Full wwPDB EM Validation Report ⓘ

Sep 11, 2026 – 02:51 am BST

PDB ID	:	9IFM / pdb_00009ifm
EMDB ID	:	EMD-52846
Title	:	STRUCTURE OF UNSTACKED C2S2-TYPE PSII-LHCII SUPERCOMPLEX FROM PISUM SATIVUM
Authors	:	Klaiman, D.; Fadeeva, M.; Kandiah, E.; Nelson, N.
Deposited on	:	2025-02-18
Resolution	:	2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

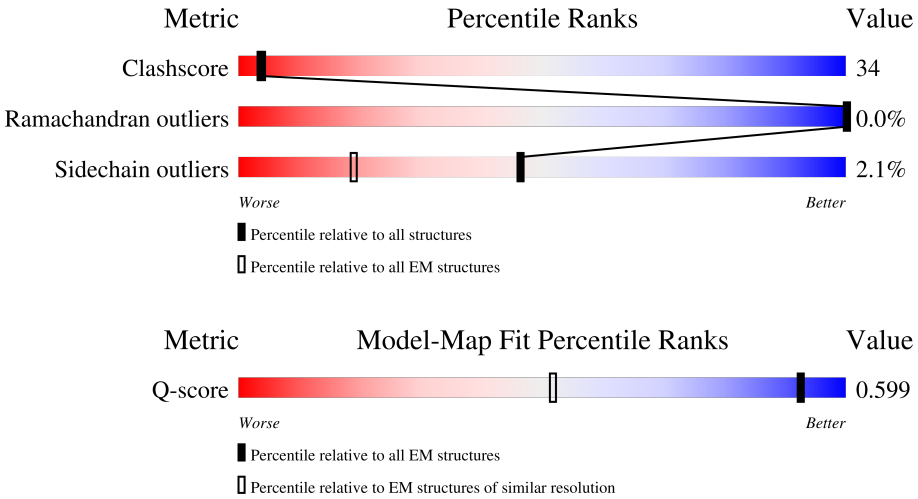
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	60% 40%
1	a	334	57% 40%
2	B	503	61% 39%
2	b	503	61% 38%

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Mol	Chain	Length	Quality of chain
3	C	450	58% 41%
3	c	450	58% 41%
4	D	352	59% 41%
4	d	352	63% 38%
5	E	75	64% 36%
5	e	75	51% 49%
6	F	30	37% 63%
6	f	30	53% 47%
7	G	216	6% 43% 56%
7	N	216	50% 48%
7	g	216	53% 46%
7	n	216	49% 49%
8	H	60	53% 45%
8	h	60	65% 35%
9	I	34	59% 41%
9	i	34	47% 53%
10	J	35	63% 34%
10	j	35	54% 40% 6%
11	K	37	35% 65%
11	k	37	32% 68%
12	L	36	50% 47%
12	l	36	64% 33%
13	M	33	12% 52% 48%
13	m	33	12% 55% 45%
14	O	248	59% 40%

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Mol	Chain	Length	Quality of chain
14	o	248	59% 40%
15	P	186	56% 41%
15	p	186	65% 33%
16	Q	148	45% 54%
16	q	148	54% 46%
17	R	224	52% 47%
17	r	224	47% 50%
18	S	218	6% 39% 59%
18	s	218	6% 39% 59%
19	T	31	71% 29%
19	t	31	52% 48%
20	W	54	6% 50% 44% 6%
20	w	54	6% 65% 35%
21	X	39	5% 59% 41%
21	x	39	8% 69% 31%
22	Y	219	52% 47%
22	y	219	55% 43%
23	Z	61	51% 46%
23	z	61	46% 49% 5%
24	U	28	54% 46%
24	u	28	7% 46% 46% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	B	603	-	-	X	-
28	CLA	C	506	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	C	507	-	-	X	-
28	CLA	G	610	-	-	X	-
28	CLA	G	613	-	-	X	-
28	CLA	N	602	-	-	X	-
28	CLA	S	303	-	-	X	-
28	CLA	S	310	-	-	X	-
28	CLA	n	603	-	-	X	-
28	CLA	n	610	-	-	X	-
28	CLA	y	304	-	-	X	-
30	BCR	B	619	-	-	X	-
30	BCR	C	514	-	X	-	-
30	BCR	C	516	-	-	X	-
30	BCR	a	410	-	-	X	-
30	BCR	t	101	-	X	-	-
35	LHG	S	317	-	-	X	-
36	DGD	C	518	-	-	X	-
38	CHL	Y	607	-	-	X	-
38	CHL	g	601	-	-	X	-
38	CHL	n	607	-	-	X	-
38	CHL	n	609	-	-	X	-
38	CHL	y	309	-	-	X	-
39	LUT	G	615	-	-	X	-
39	LUT	S	315	-	-	X	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 79416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
1	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		
2	b	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
3	c	450	Total	C	N	O	S	0	0
			3496	2300	583	603	10		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		
4	d	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 612	C 400	N 100	O 112	0	0
5	e	75	Total 612	C 400	N 100	O 112	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total 241	C 162	N 41	O 37	S 1	0	0
6	f	30	Total 241	C 162	N 41	O 37	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	26	PHE	SER	conflict	UNP P62096
f	26	PHE	SER	conflict	UNP P62096

- Molecule 7 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	216	Total 1650	C 1069	N 267	O 309	S 5	0	0
7	N	216	Total 1649	C 1068	N 267	O 309	S 5	0	0
7	g	216	Total 1650	C 1069	N 267	O 309	S 5	0	0
7	n	216	Total 1650	C 1069	N 267	O 309	S 5	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	60	Total 452	C 296	N 72	O 81	S 3	0	0
8	h	60	Total 452	C 296	N 72	O 81	S 3	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	35	Total	C	N	O	0	0
			256	174	39	43		
10	j	35	Total	C	N	O	0	0
			256	174	39	43		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			304	201	48	55		
12	l	36	Total	C	N	O	0	0
			304	201	48	55		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
13	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	248	Total 1870	C 1179	N 306	O 382	S 3	0	0

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	186	Total 1434	C 909	N 238	O 286	S 1	0	0
15	p	186	Total 1434	C 909	N 238	O 286	S 1	0	0

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total 1157	C 742	N 197	O 218	0	0
16	q	148	Total 1157	C 742	N 197	O 218	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	224	Total 1755	C 1142	N 285	O 325	S 3	0	0
17	r	224	Total 1755	C 1142	N 285	O 325	S 3	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	218	Total 1688	C 1105	N 271	O 308	S 4	0	0
18	s	218	Total 1688	C 1105	N 271	O 308	S 4	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	31	Total 252	C 176	N 35	O 40	S 1	0	0
19	t	31	Total 252	C 176	N 35	O 40	S 1	0	0

- Molecule 20 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
20	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

- Molecule 21 is a protein called Ultraviolet-B-repressible protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	39	Total	C	N	O	0	0
			276	180	46	50		
21	x	39	Total	C	N	O	0	0
			276	180	46	50		

- Molecule 22 is a protein called Chlorophyll a-b binding protein AB80, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		
22	y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		

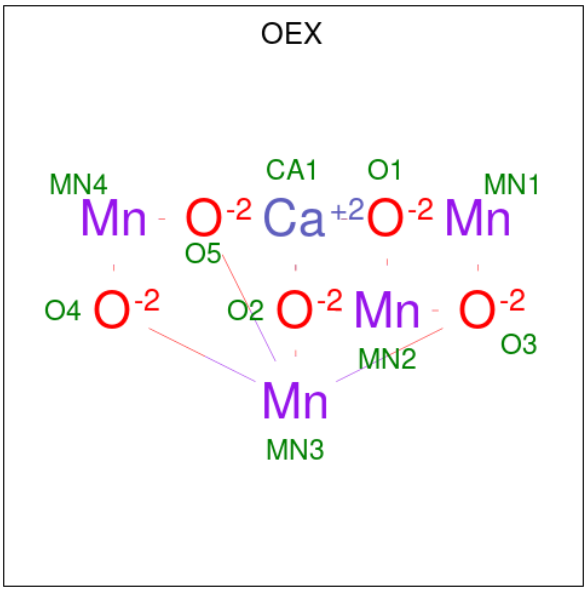
- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		
23	z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		

- Molecule 24 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	28	Total	C	N	O	S	0	0
			212	131	41	37	3		
24	u	28	Total	C	N	O	S	0	0
			212	131	41	37	3		

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
25	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

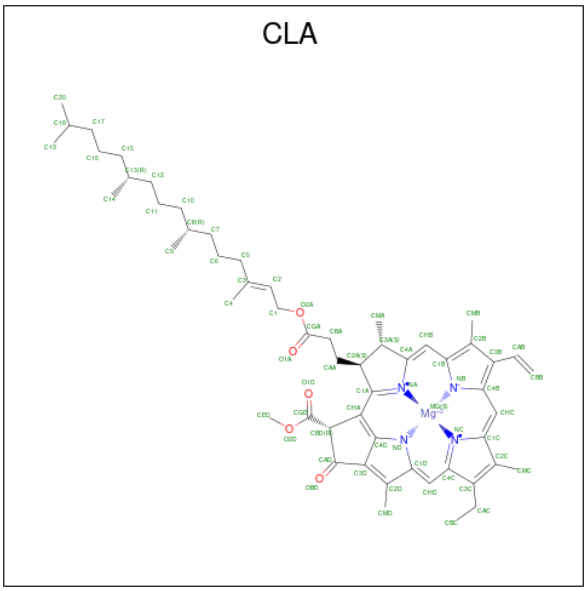
- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Fe	0
			1	1	
26	a	1	Total	Fe	0
			1	1	

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Cl	0
			2	2	
27	a	2	Total	Cl	0
			2	2	

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	g	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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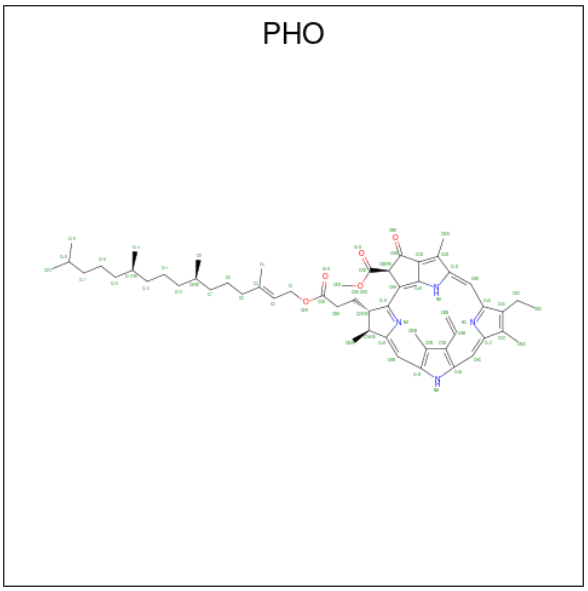
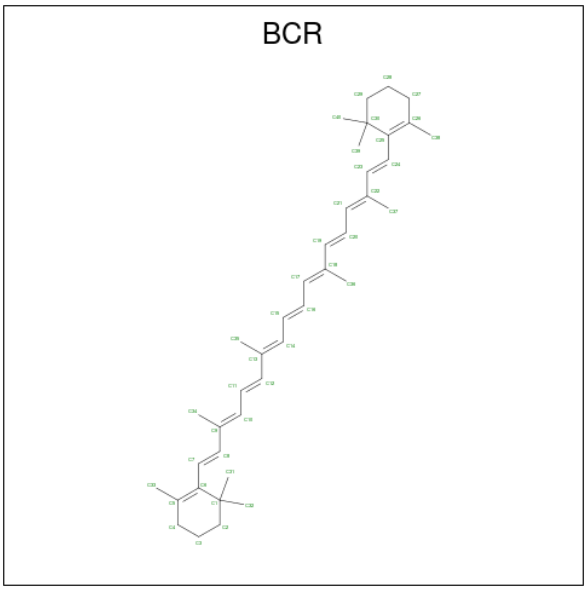
Mol	Chain	Residues	Atoms					AltConf
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 48	C 38	Mg 1	N 4	O 5	0

- Molecule 29 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



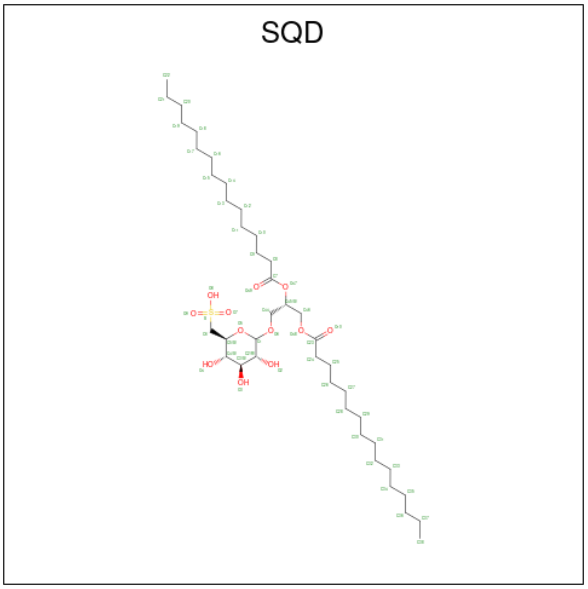
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	D	1	Total	C	N	O	0
			64	55	4	5	
29	a	1	Total	C	N	O	0
			64	55	4	5	
29	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



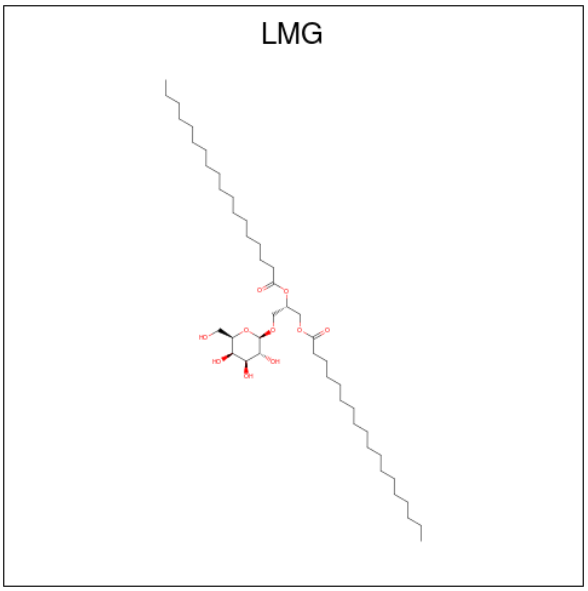
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	d	1	Total C 40 40	0
30	h	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	t	1	Total C 40 40	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



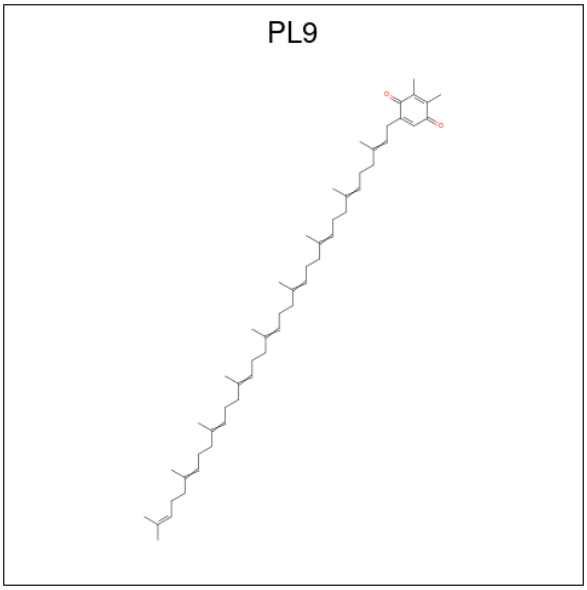
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			50	37	12	1	
31	A	1	Total	C	O	S	0
			54	41	12	1	
31	B	1	Total	C	O	S	0
			54	41	12	1	
31	L	1	Total	C	O	S	0
			42	29	12	1	
31	L	1	Total	C	O	S	0
			54	41	12	1	
31	M	1	Total	C	O	S	0
			42	29	12	1	
31	a	1	Total	C	O	S	0
			50	37	12	1	
31	a	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



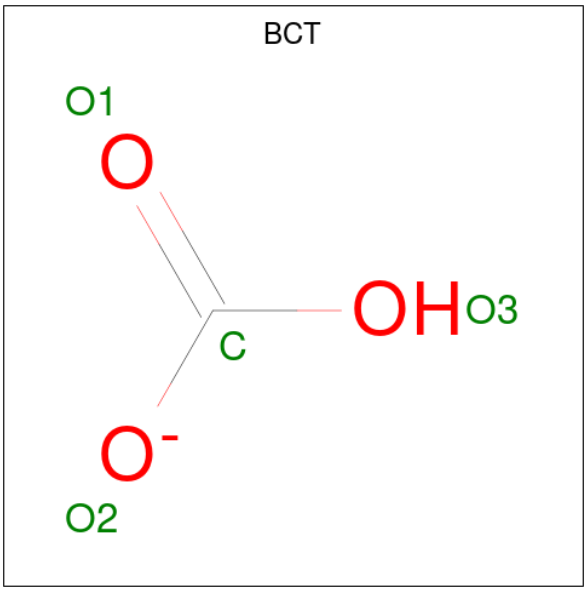
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 48 38 10	0
32	A	1	Total C O 40 30 10	0
32	B	1	Total C O 51 41 10	0
32	B	1	Total C O 31 21 10	0
32	C	1	Total C O 51 41 10	0
32	C	1	Total C O 44 34 10	0
32	D	1	Total C O 46 36 10	0
32	a	1	Total C O 40 30 10	0
32	b	1	Total C O 51 41 10	0
32	b	1	Total C O 50 40 10	0
32	c	1	Total C O 51 41 10	0
32	d	1	Total C O 46 36 10	0
32	k	1	Total C O 51 41 10	0
32	w	1	Total C O 48 38 10	0

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



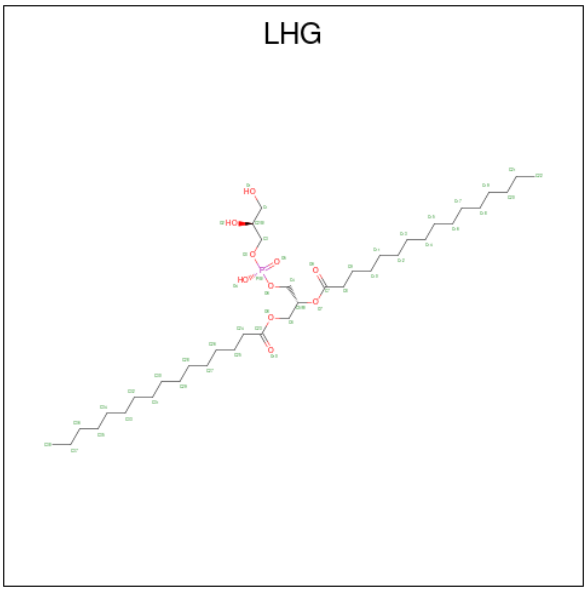
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 13 11 2	0
33	D	1	Total C O 55 53 2	0
33	a	1	Total C O 13 11 2	0
33	d	1	Total C O 55 53 2	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	d	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			30	19	10	1	
35	B	1	Total	C	O	P	0
			41	30	10	1	
35	B	1	Total	C	O	P	0
			46	35	10	1	
35	C	1	Total	C	O	P	0
			49	38	10	1	
35	D	1	Total	C	O	P	0
			49	38	10	1	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			31	20	10	1	
35	R	1	Total	C	O	P	0
			25	14	10	1	
35	S	1	Total	C	O	P	0
			34	23	10	1	
35	S	1	Total	C	O	P	0
			43	32	10	1	
35	W	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			43	32	10	1	
35	b	1	Total	C	O	P	0
			34	23	10	1	
35	b	1	Total	C	O	P	0
			41	30	10	1	
35	b	1	Total	C	O	P	0
			46	35	10	1	
35	c	1	Total	C	O	P	0
			32	21	10	1	
35	c	1	Total	C	O	P	0
			40	29	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	g	1	Total	C	O	P	0
			41	30	10	1	

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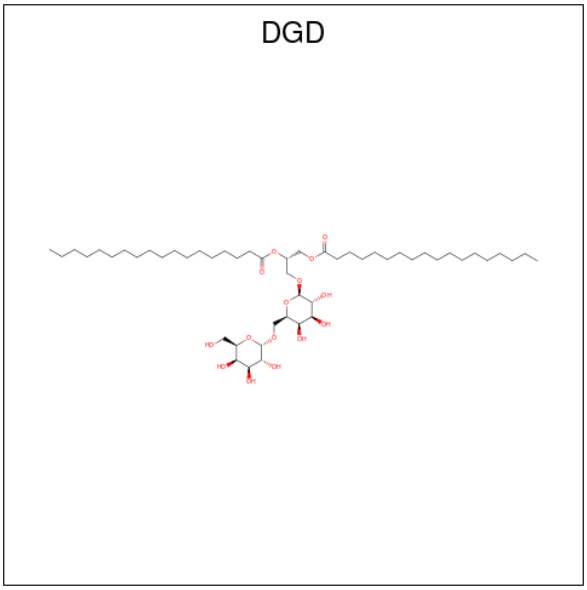
Mol	Chain	Residues	Atoms				AltConf
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			32	21	10	1	
35	r	1	Total	C	O	P	0
			30	19	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	w	1	Total	C	O	P	0
			39	28	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			59	44	15	
36	B	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			55	40	15	
36	C	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			60	45	15	

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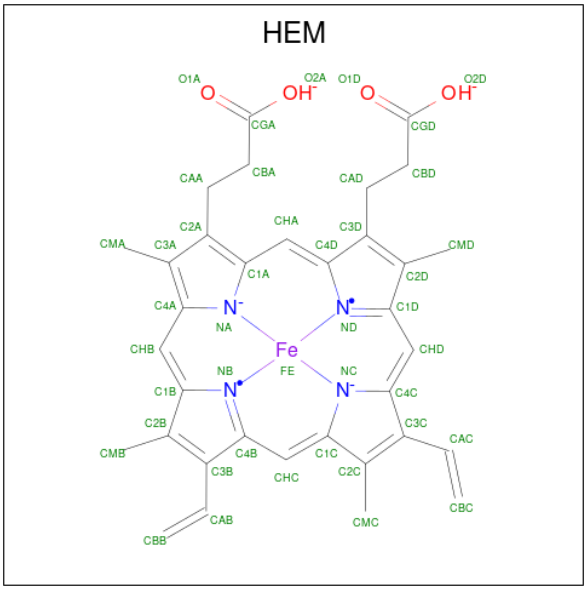
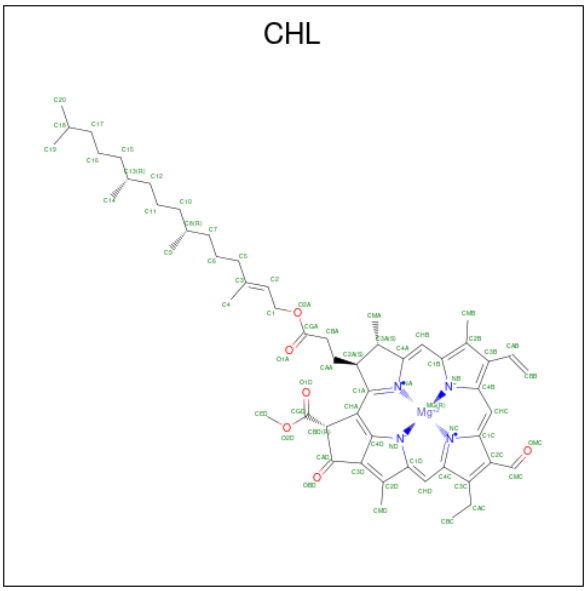
Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 59 44 15	0
36	b	1	Total C O 62 47 15	0
36	c	1	Total C O 55 40 15	0
36	c	1	Total C O 54 39 15	0
36	c	1	Total C O 59 44 15	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	AltConf
37	E	1	Total C Fe N O 43 34 1 4 4	0
37	f	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
38	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
38	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
38	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
38	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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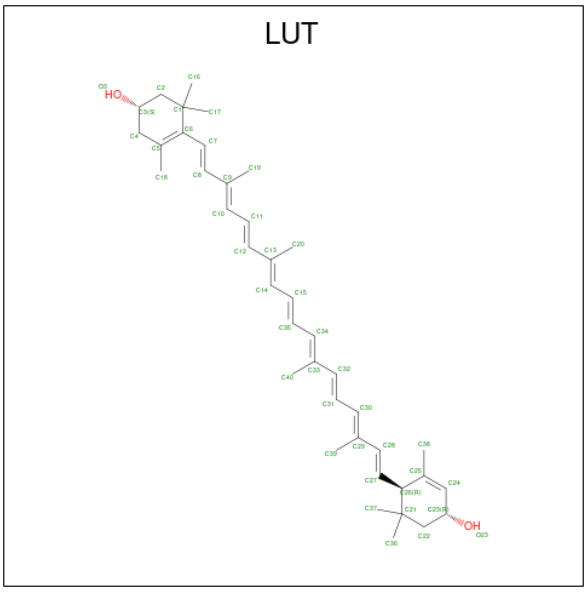
Mol	Chain	Residues	Atoms					AltConf
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	r	1	Total	C	O	0
			42	40	2	

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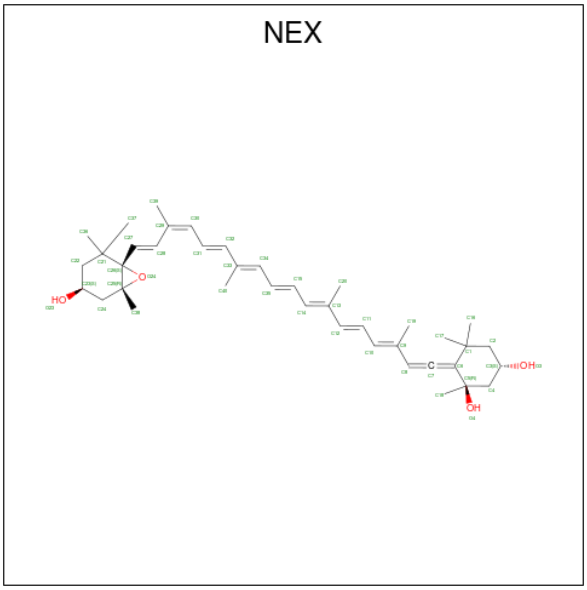
Mol	Chain	Residues	Atoms	AltConf
39	s	1	Total C O 42 40 2	0
39	s	1	Total C O 42 40 2	0
39	y	1	Total C O 42 40 2	0
39	y	1	Total C O 42 40 2	0

- Molecule 40 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
40	G	1	Total C O 44 40 4	0
40	N	1	Total C O 44 40 4	0
40	Y	1	Total C O 44 40 4	0
40	g	1	Total C O 44 40 4	0
40	n	1	Total C O 44 40 4	0
40	r	1	Total C O 44 40 4	0

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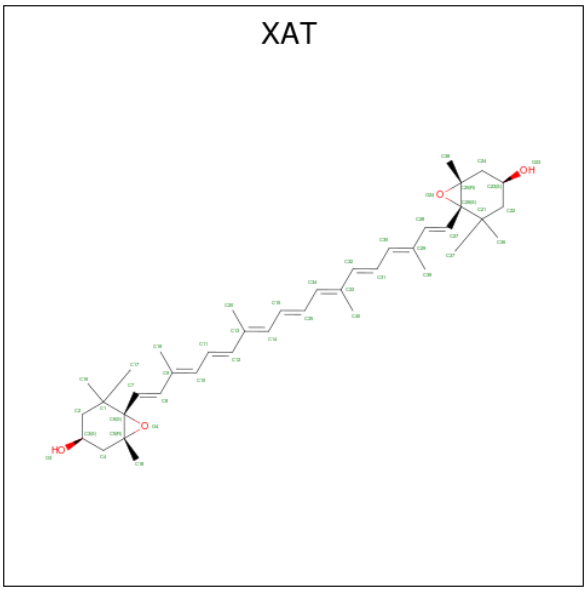
Mol	Chain	Residues	Atoms	AltConf
40	s	1	Total C O 44 40 4	0
40	y	1	Total C O 44 40 4	0
40	y	1	Total C O 44 40 4	0

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
41	R	1	Total C O 44 40 4	0
41	Y	1	Total C O 44 40 4	0
41	r	1	Total C O 44 40 4	0
41	y	1	Total C O 44 40 4	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	AltConf
42	A	92	Total O 92 92	0
42	B	151	Total O 151 151	0

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Mol	Chain	Residues	Atoms	AltConf
42	C	134	Total O 134 134	0
42	D	101	Total O 101 101	0
42	E	14	Total O 14 14	0
42	F	6	Total O 6 6	0
42	G	26	Total O 26 26	0
42	H	16	Total O 16 16	0
42	I	3	Total O 3 3	0
42	J	5	Total O 5 5	0
42	K	6	Total O 6 6	0
42	L	8	Total O 8 8	0
42	M	6	Total O 6 6	0
42	N	28	Total O 28 28	0
42	O	69	Total O 69 69	0
42	P	52	Total O 52 52	0
42	Q	28	Total O 28 28	0
42	R	40	Total O 40 40	0
42	S	24	Total O 24 24	0
42	T	7	Total O 7 7	0
42	W	11	Total O 11 11	0
42	X	10	Total O 10 10	0
42	Y	45	Total O 45 45	0

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Mol	Chain	Residues	Atoms	AltConf
42	Z	6	Total O 6 6	0
42	U	1	Total O 1 1	0
42	a	100	Total O 100 100	0
42	b	167	Total O 167 167	0
42	c	128	Total O 128 128	0
42	d	85	Total O 85 85	0
42	e	21	Total O 21 21	0
42	f	3	Total O 3 3	0
42	g	23	Total O 23 23	0
42	h	14	Total O 14 14	0
42	i	2	Total O 2 2	0
42	j	4	Total O 4 4	0
42	k	4	Total O 4 4	0
42	l	8	Total O 8 8	0
42	m	2	Total O 2 2	0
42	n	23	Total O 23 23	0
42	o	67	Total O 67 67	0
42	p	43	Total O 43 43	0
42	q	18	Total O 18 18	0
42	r	33	Total O 33 33	0
42	s	19	Total O 19 19	0

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Mol	Chain	Residues	Atoms	AltConf
42	t	3	Total O 3 3	0
42	w	11	Total O 11 11	0
42	x	7	Total O 7 7	0
42	y	31	Total O 31 31	0
42	z	2	Total O 2 2	0
42	u	4	Total O 4 4	0

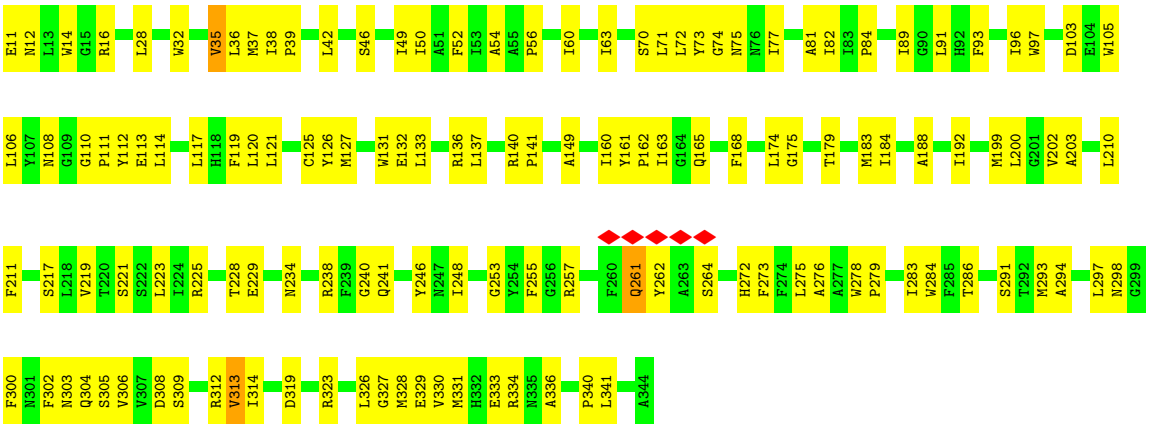
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem II protein D1

Chain A:

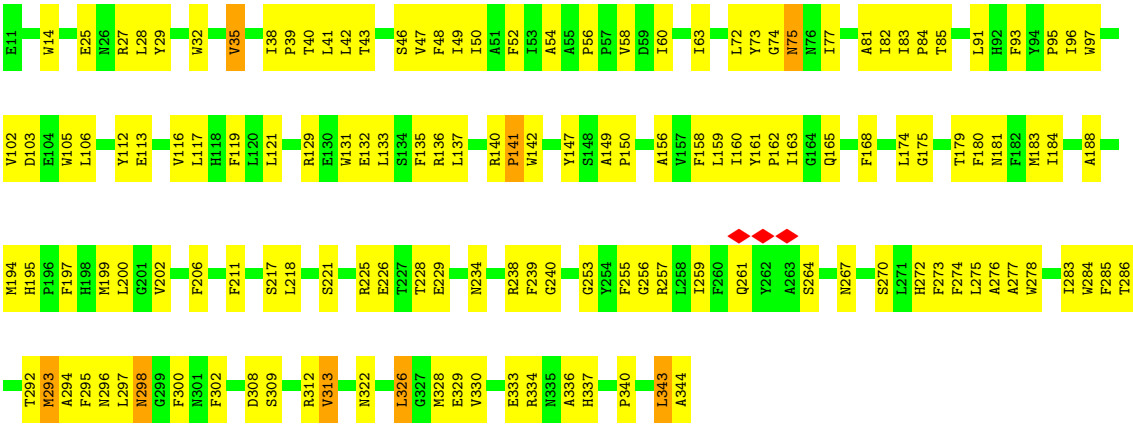




• Molecule 1: Photosystem II protein D1

Chain a:

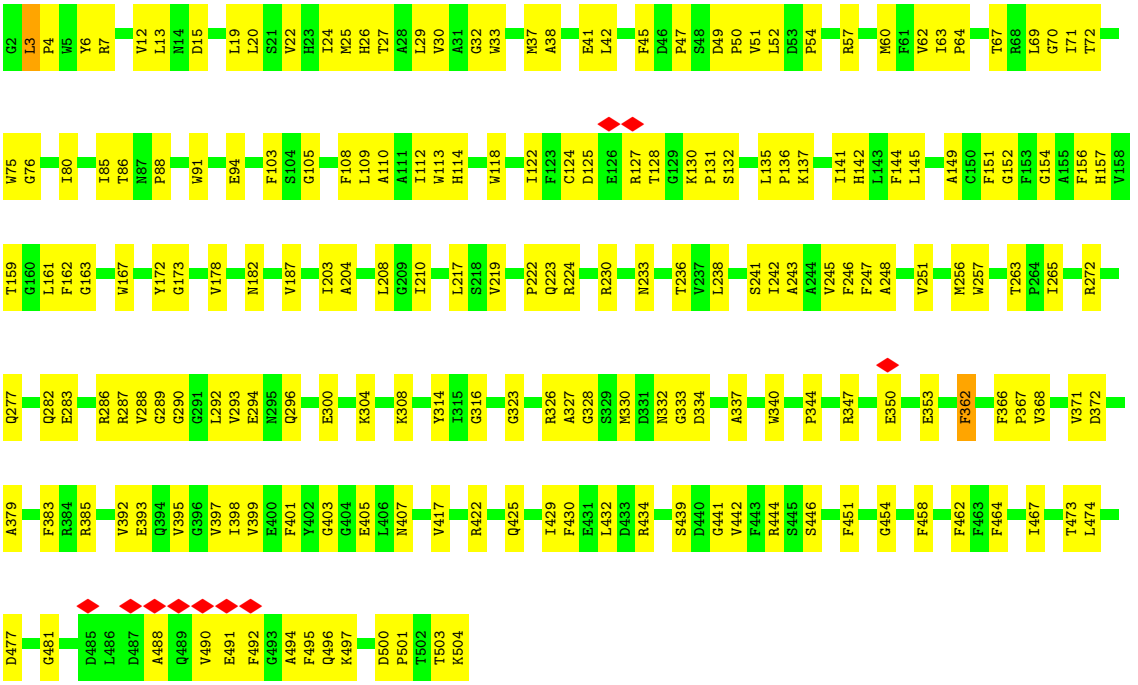




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

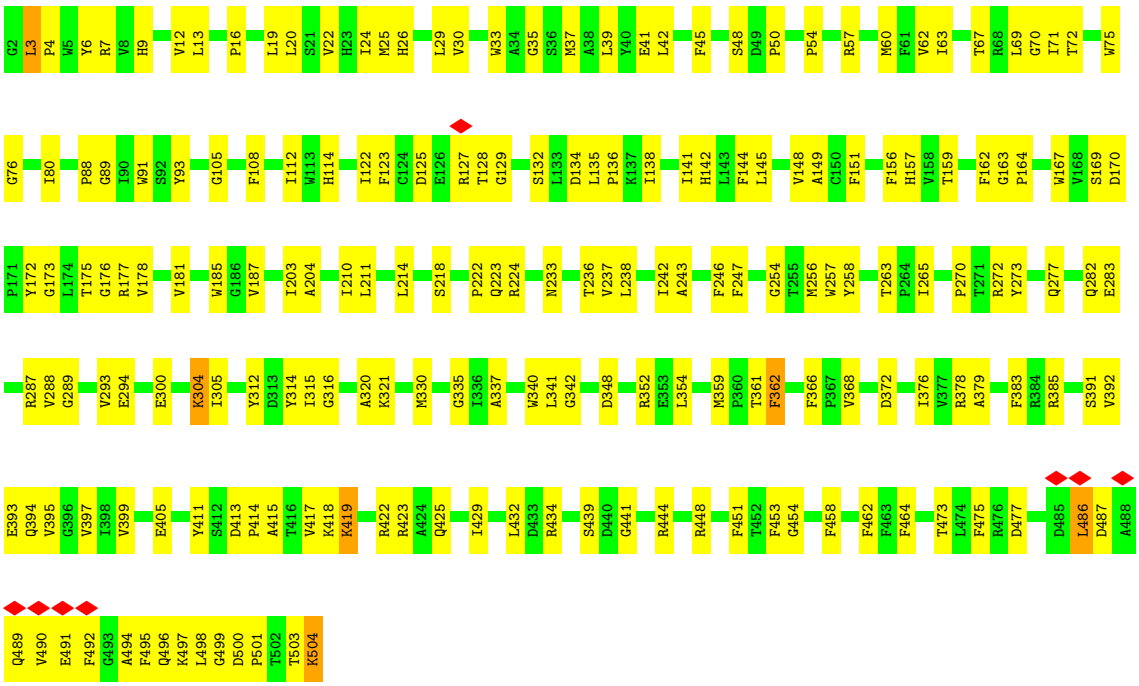




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

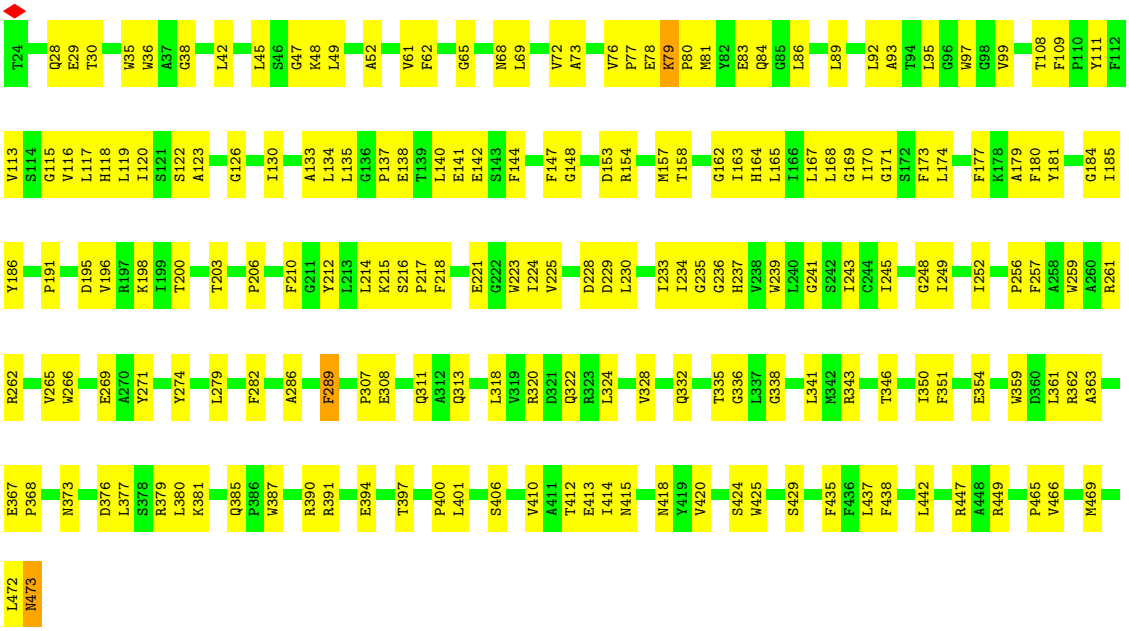




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

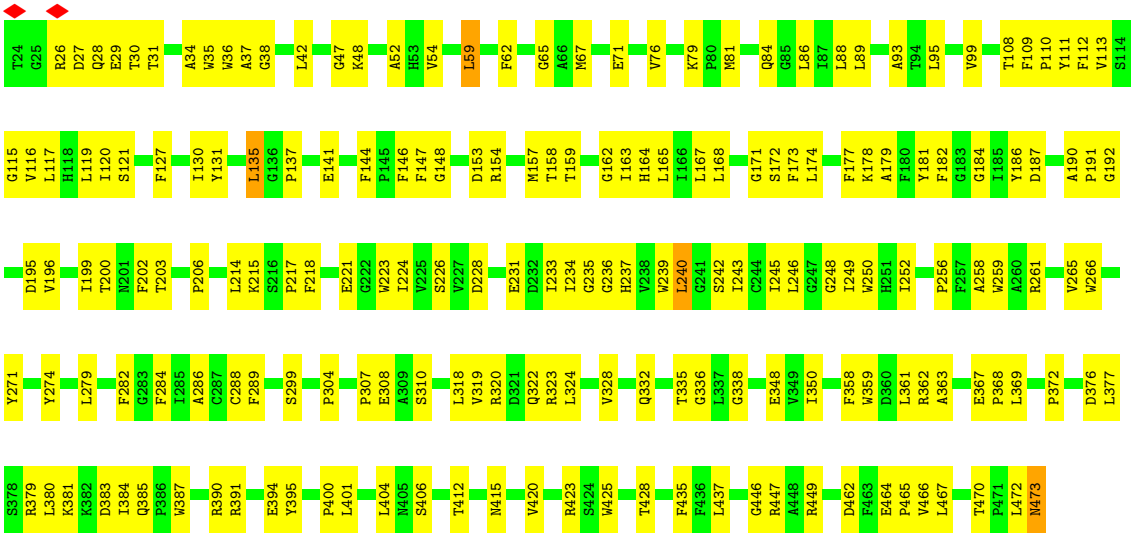




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

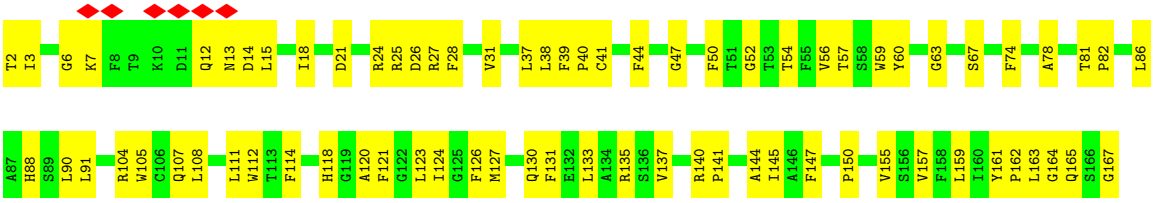




• Molecule 4: Photosystem II D2 protein

Chain D:



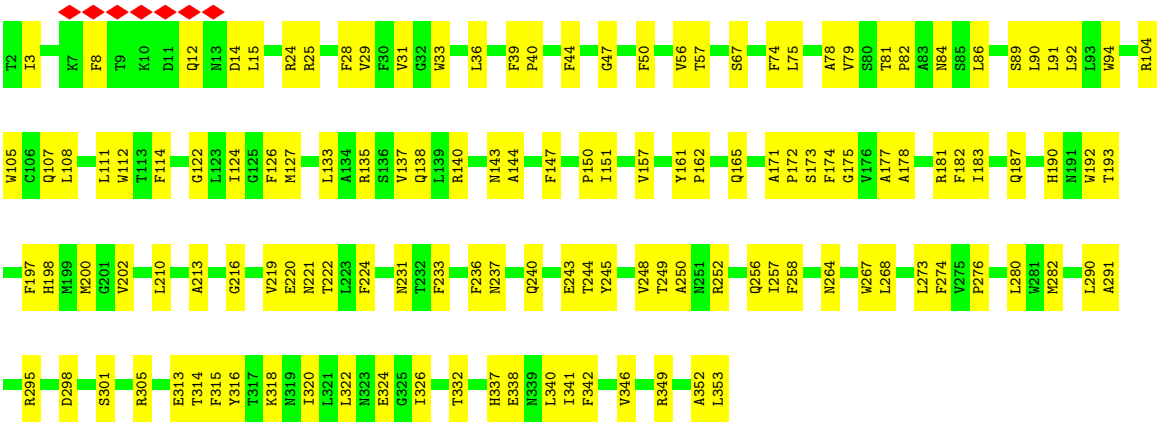




• Molecule 4: Photosystem II D2 protein

Chain d:

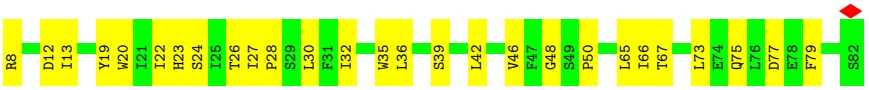




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

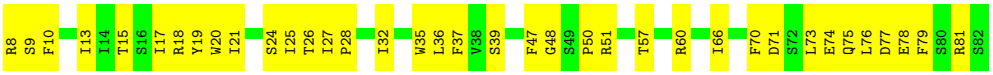




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

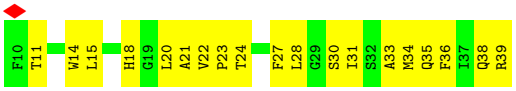




• Molecule 6: Cytochrome b559 subunit beta

Chain F:





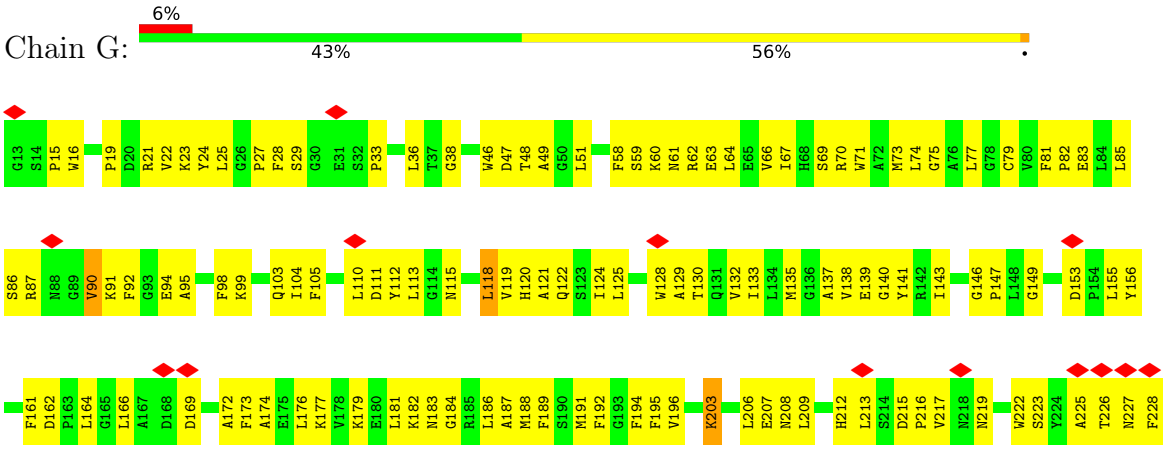
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



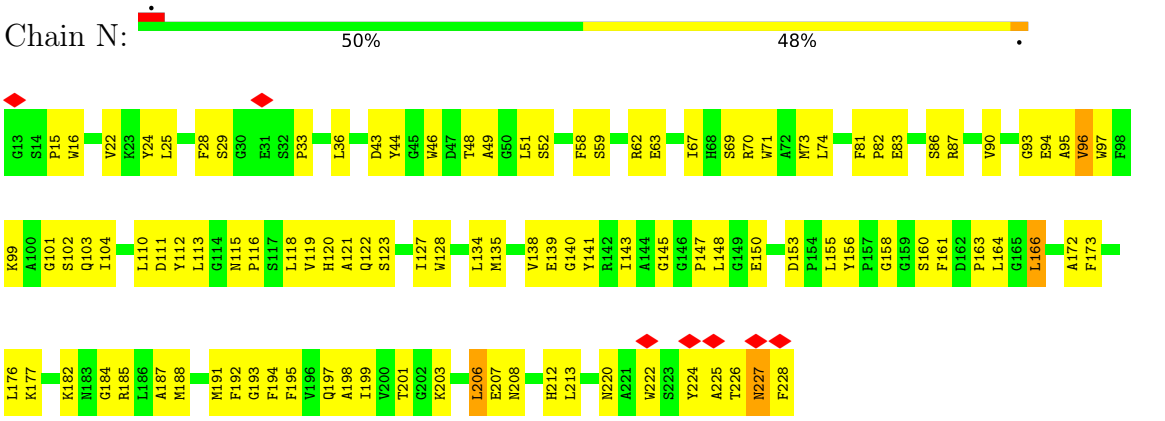
• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:



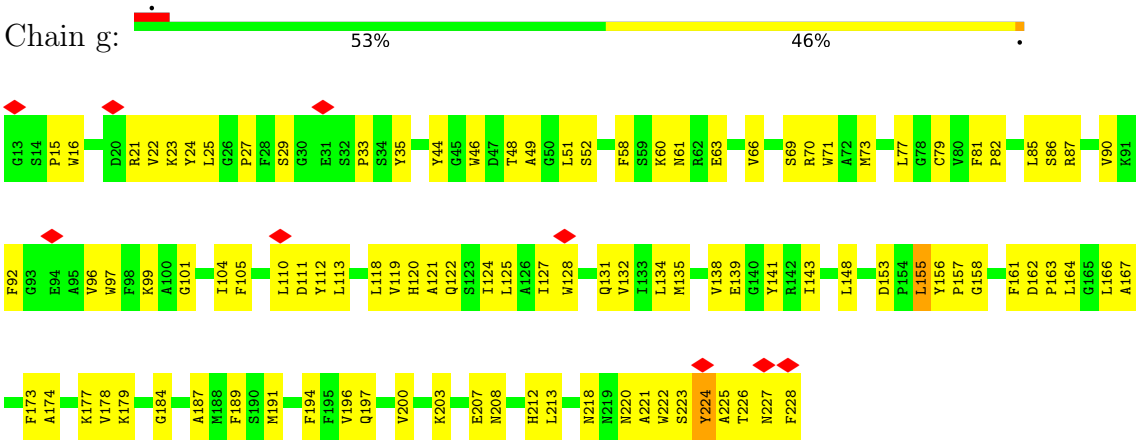
• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:



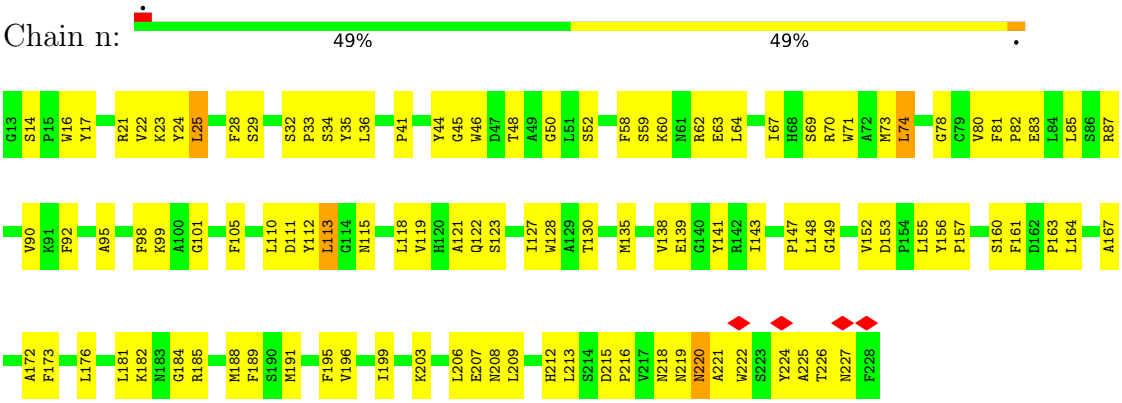
• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain g:



• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain n:



• Molecule 8: Photosystem II reaction center protein H

Chain H:



• Molecule 8: Photosystem II reaction center protein H

Chain h:



• Molecule 9: Photosystem II reaction center protein I

Chain I:



• Molecule 9: Photosystem II reaction center protein I

Chain i:



• Molecule 10: Photosystem II reaction center protein J

Chain J:



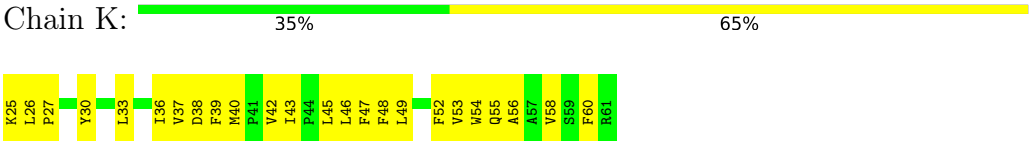
• Molecule 10: Photosystem II reaction center protein J

Chain j:



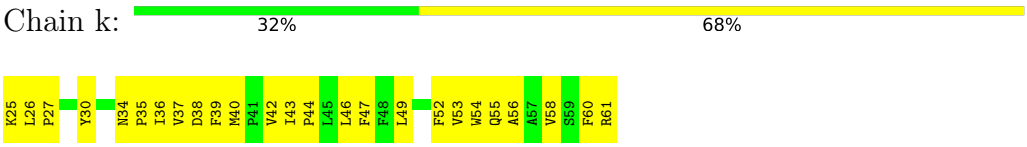
• Molecule 11: Photosystem II reaction center protein K

Chain K:



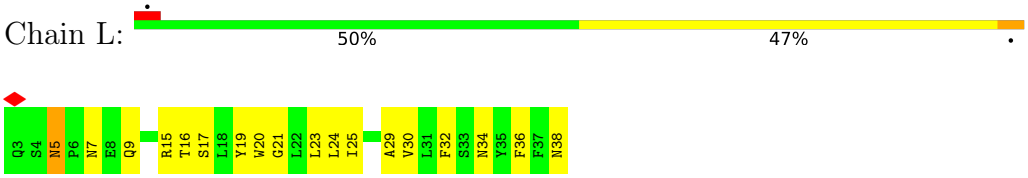
• Molecule 11: Photosystem II reaction center protein K

Chain k:



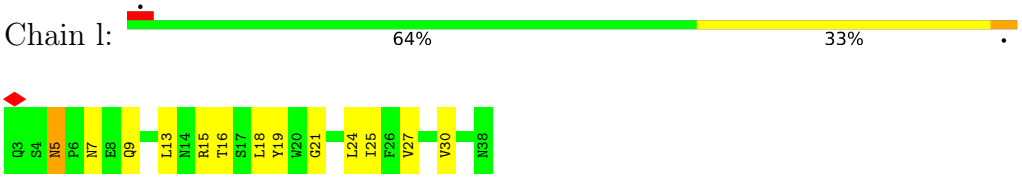
• Molecule 12: Photosystem II reaction center protein L

Chain L:



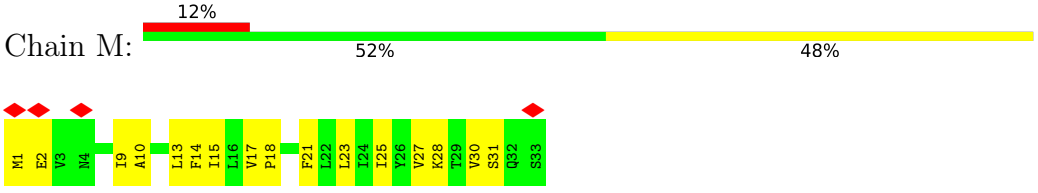
• Molecule 12: Photosystem II reaction center protein L

Chain l:



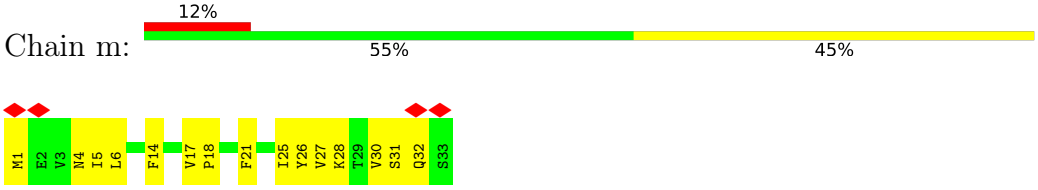
• Molecule 13: Photosystem II reaction center protein M

Chain M:



• Molecule 13: Photosystem II reaction center protein M

Chain m:



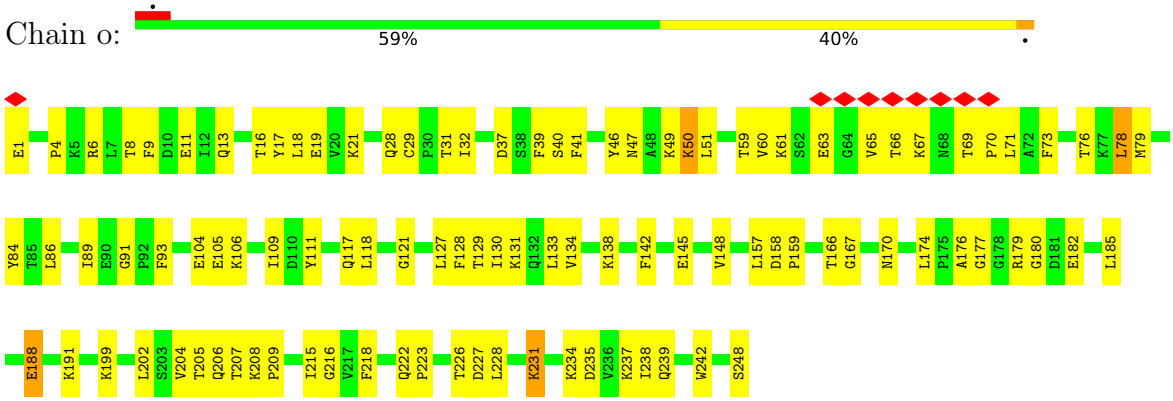
• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:



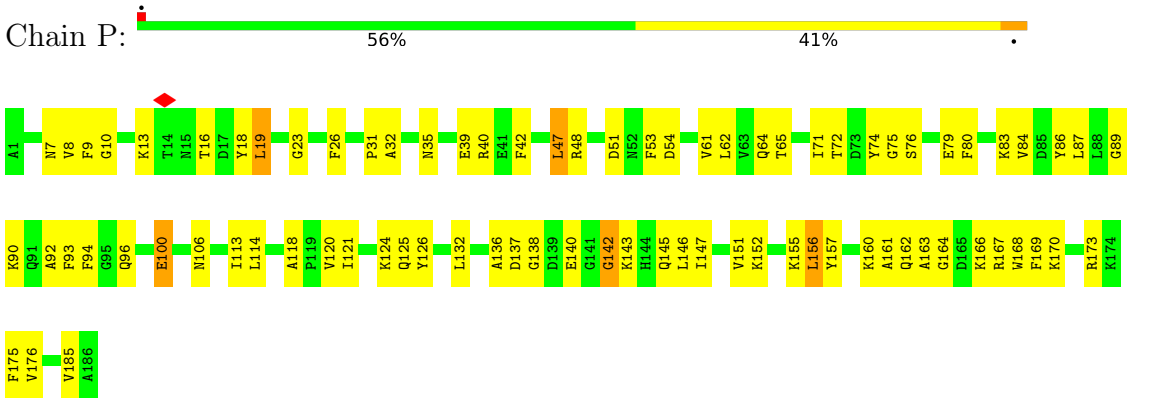
• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:



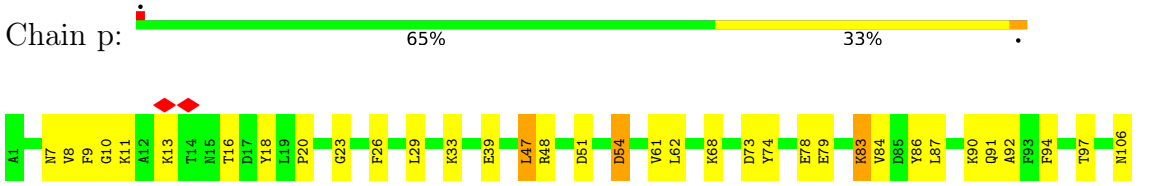
• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

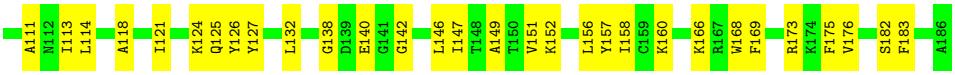
Chain P:



• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p:

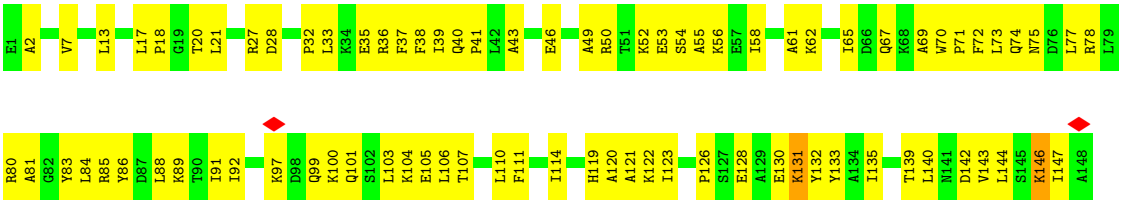




• Molecule 16: Oxygen-evolving enhancer protein 3

Chain Q:

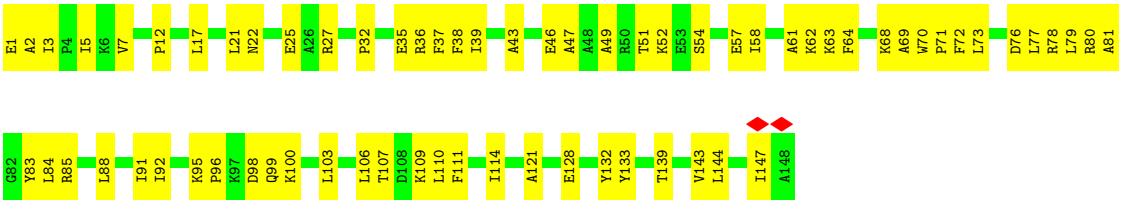




• Molecule 16: Oxygen-evolving enhancer protein 3

Chain q:

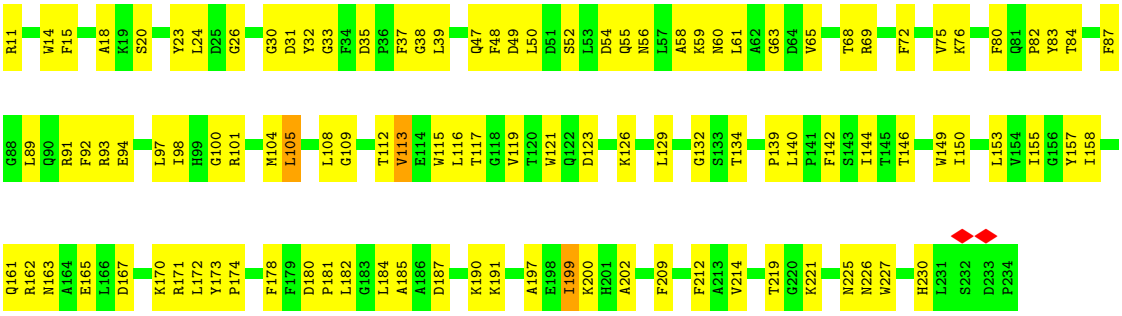




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain R:



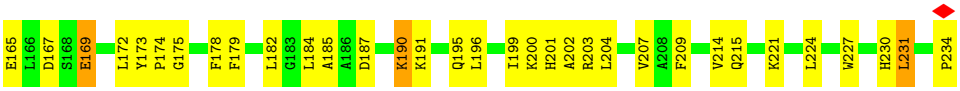


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain r:

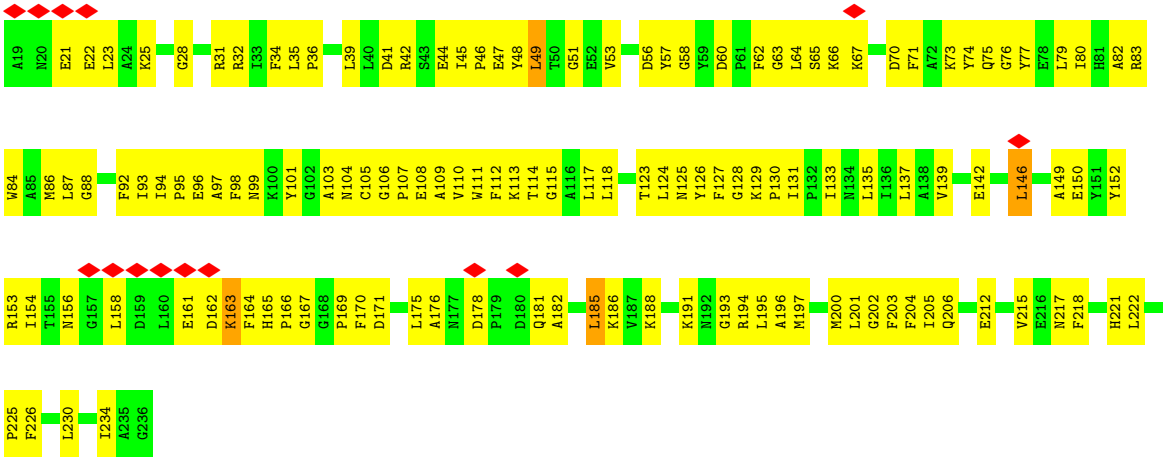






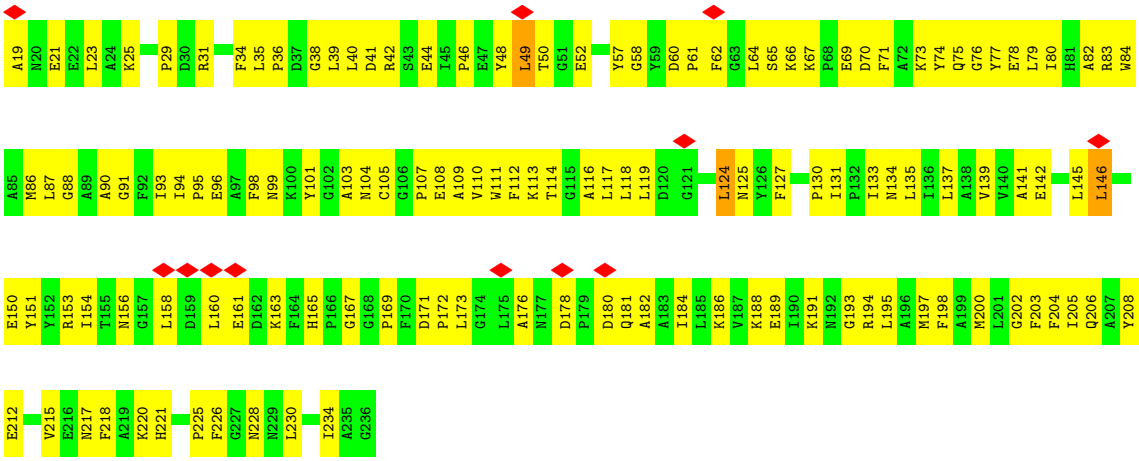
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic





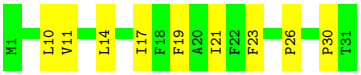
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic





• Molecule 19: Photosystem II reaction center protein T



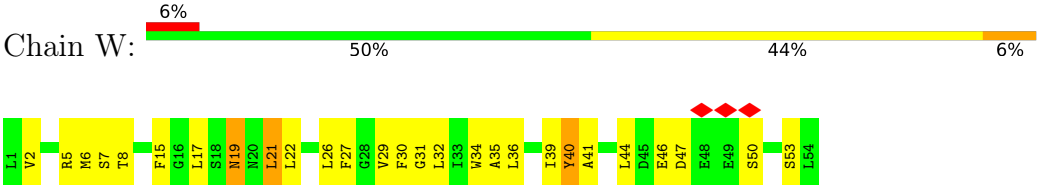


• Molecule 19: Photosystem II reaction center protein T

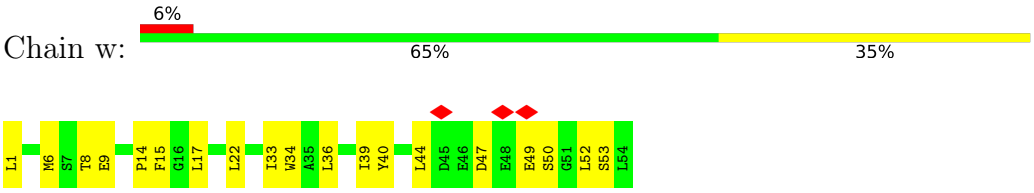




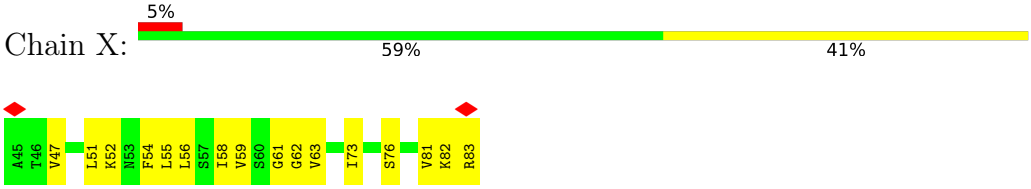
• Molecule 20: Photosystem II reaction center protein W



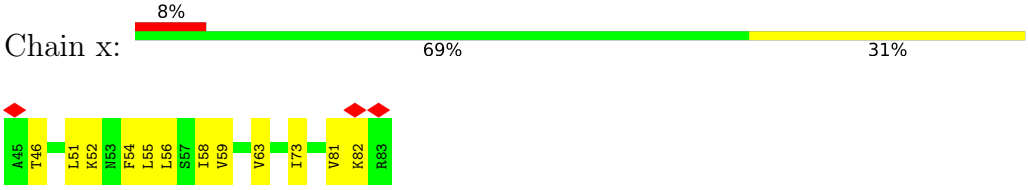
• Molecule 20: Photosystem II reaction center protein W



• Molecule 21: Ultraviolet-B-repressible protein



• Molecule 21: Ultraviolet-B-repressible protein



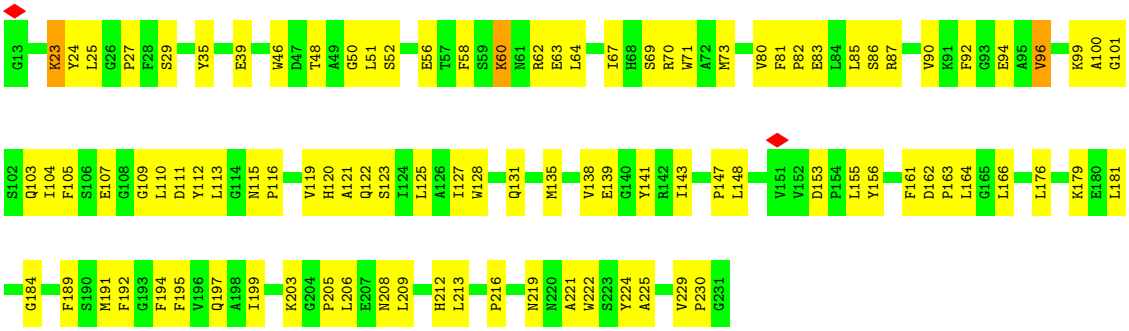
• Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic





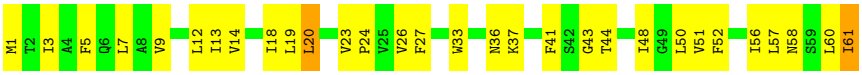
• Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic





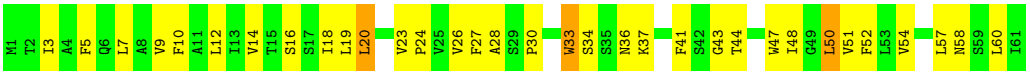
• Molecule 23: Photosystem II reaction center protein Z





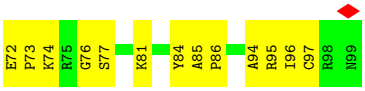
• Molecule 23: Photosystem II reaction center protein Z





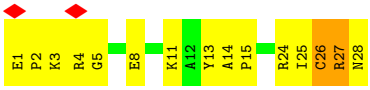
• Molecule 24: Photosystem II 5 kDa protein, chloroplastic





• Molecule 24: Photosystem II 5 kDa protein, chloroplastic





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FE2, XAT, BCT, CL, SQD, CLA, PL9, LMG, DGD, NEX, OEX, PHO, BCR, LHG, LUT, CHL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	0/2697	1.13	0/3677
1	a	0.95	0/2697	1.12	1/3677 (0.0%)
2	B	0.95	0/4071	1.13	0/5542
2	b	0.95	0/4071	1.13	2/5542 (0.0%)
3	C	0.94	1/3614 (0.0%)	1.13	0/4922
3	c	0.94	0/3613	1.12	0/4920
4	D	0.92	0/2890	1.12	0/3938
4	d	0.92	0/2890	1.12	0/3938
5	E	0.93	0/630	1.13	0/857
5	e	0.92	0/630	1.14	0/857
6	F	0.92	0/248	1.14	0/335
6	f	0.92	0/248	1.14	0/335
7	G	0.93	0/1701	1.17	0/2315
7	N	0.93	0/1700	1.16	2/2313 (0.1%)
7	g	0.93	0/1701	1.16	0/2315
7	n	0.93	0/1701	1.18	1/2315 (0.0%)
8	H	0.97	0/461	1.18	0/626
8	h	0.96	0/461	1.15	0/626
9	I	0.91	0/286	1.13	0/386
9	i	0.91	0/286	1.14	0/386
10	J	0.95	0/262	1.19	0/354
10	j	0.94	0/262	1.20	0/354
11	K	0.90	0/318	1.05	0/434
11	k	0.90	0/318	1.06	0/434
12	L	0.89	0/312	1.06	0/424
12	l	0.90	0/312	1.05	0/424
13	M	0.94	0/260	1.18	0/355
13	m	0.94	0/260	1.14	0/355
14	O	0.99	0/1906	1.09	0/2575
14	o	0.99	0/1906	1.10	0/2575
15	P	0.97	0/1464	1.08	2/1978 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	p	0.98	0/1464	1.08	1/1978 (0.1%)
16	Q	0.95	0/1179	1.17	0/1591
16	q	0.96	0/1179	1.18	0/1591
17	R	0.93	0/1804	1.14	1/2456 (0.0%)
17	r	0.92	0/1804	1.15	0/2456
18	S	0.93	0/1737	1.14	0/2361
18	s	0.91	0/1737	1.15	0/2361
19	T	0.90	0/260	1.10	0/354
19	t	0.89	0/260	1.12	0/354
20	W	0.92	0/429	1.11	0/581
20	w	0.92	0/429	1.13	0/581
21	X	0.97	0/279	1.28	0/380
21	x	0.98	0/279	1.27	0/380
22	Y	0.93	0/1719	1.17	0/2341
22	y	0.94	0/1719	1.16	0/2341
23	Z	0.97	0/467	1.23	0/640
23	z	0.96	0/467	1.22	0/640
24	U	0.94	0/216	1.21	0/291
24	u	0.94	0/216	1.17	0/291
All	All	0.94	1/61820 (0.0%)	1.14	10/84052 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	76	VAL	N-CA	5.10	1.49	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	145	GLY	CA-C-O	-6.09	118.03	122.23
15	P	89	GLY	CA-C-O	-5.92	118.05	122.37
2	b	89	GLY	CA-C-O	-5.92	118.15	122.23
17	R	132	GLY	CA-C-O	-5.89	118.17	122.23
15	p	142	GLY	CA-C-O	-5.85	118.19	122.23
15	P	142	GLY	CA-C-O	-5.61	118.09	122.52
2	b	342	GLY	CA-C-O	-5.54	118.14	122.52
7	n	152	VAL	N-CA-C	-5.47	107.30	111.62
1	a	141	PRO	N-CA-CB	-5.13	97.87	103.25
7	N	227	ASN	CB-CA-C	-5.11	110.67	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2522	138	0
1	a	2616	0	2522	178	0
2	B	3939	0	3814	208	0
2	b	3939	0	3814	180	0
3	C	3497	0	3422	198	0
3	c	3496	0	3422	208	0
4	D	2797	0	2695	152	0
4	d	2797	0	2695	134	0
5	E	612	0	595	33	0
5	e	612	0	595	38	0
6	F	241	0	246	22	0
6	f	241	0	246	18	0
7	G	1650	0	1577	168	0
7	N	1649	0	1573	135	0
7	g	1650	0	1577	137	0
7	n	1650	0	1577	136	0
8	H	452	0	473	34	0
8	h	452	0	473	31	0
9	I	278	0	291	16	0
9	i	278	0	291	17	0
10	J	256	0	269	11	0
10	j	256	0	269	15	0
11	K	306	0	313	41	0
11	k	306	0	313	32	0
12	L	304	0	292	24	0
12	l	304	0	292	12	0
13	M	256	0	284	23	0
13	m	256	0	284	22	0
14	O	1870	0	1849	86	0
14	o	1870	0	1851	92	0
15	P	1434	0	1392	80	0
15	p	1434	0	1392	51	0
16	Q	1157	0	1210	77	0
16	q	1157	0	1210	63	0
17	R	1755	0	1722	110	0
17	r	1755	0	1722	121	0
18	S	1688	0	1652	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1688	0	1652	148	0
19	T	252	0	267	13	0
19	t	252	0	267	24	0
20	W	419	0	402	34	0
20	w	419	0	402	28	0
21	X	276	0	301	23	0
21	x	276	0	301	17	0
22	Y	1667	0	1596	120	0
22	y	1667	0	1596	110	0
23	Z	457	0	488	31	0
23	z	457	0	488	40	0
24	U	212	0	220	8	0
24	u	212	0	223	16	0
25	A	10	0	0	0	0
25	a	10	0	0	0	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0
27	A	2	0	0	0	0
27	a	2	0	0	1	0
28	A	175	0	168	31	0
28	B	1040	0	1142	177	0
28	C	837	0	908	164	0
28	D	195	0	214	23	0
28	G	465	0	443	105	0
28	N	456	0	426	88	0
28	R	554	0	507	99	0
28	S	465	0	387	113	0
28	Y	463	0	440	79	0
28	a	175	0	169	32	0
28	b	1040	0	1144	176	0
28	c	808	0	837	127	0
28	d	195	0	214	34	0
28	g	440	0	402	81	0
28	n	465	0	450	97	0
28	r	563	0	524	107	0
28	s	465	0	387	84	0
28	y	473	0	463	88	0
29	A	64	0	74	9	0
29	D	64	0	74	9	0
29	a	64	0	74	12	0
29	d	64	0	74	12	0
30	A	40	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	120	0	168	51	0
30	C	120	0	168	50	0
30	D	40	0	56	11	0
30	H	40	0	56	14	0
30	K	40	0	56	13	0
30	T	40	0	56	13	0
30	a	40	0	56	22	0
30	b	120	0	168	34	0
30	c	80	0	112	30	0
30	d	40	0	56	20	0
30	h	40	0	56	19	0
30	i	40	0	56	8	0
30	k	40	0	56	16	0
30	t	40	0	56	10	0
31	A	104	0	143	23	0
31	B	54	0	77	12	0
31	L	96	0	124	21	0
31	M	42	0	47	5	0
31	a	104	0	143	30	0
32	A	88	0	116	31	0
32	B	82	0	104	23	0
32	C	95	0	130	24	0
32	D	46	0	62	15	0
32	a	40	0	50	14	0
32	b	101	0	145	22	0
32	c	51	0	72	15	0
32	d	46	0	62	20	0
32	k	51	0	72	15	0
32	w	48	0	66	13	0
33	A	13	0	7	0	0
33	D	55	0	80	8	0
33	a	13	0	7	0	0
33	d	55	0	80	6	0
34	A	4	0	0	0	0
34	d	4	0	0	0	0
35	A	43	0	56	4	0
35	B	117	0	150	30	0
35	C	49	0	74	11	0
35	D	49	0	74	13	0
35	G	49	0	74	7	0
35	L	49	0	74	6	0
35	N	31	0	32	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	25	0	20	5	0
35	S	77	0	97	26	0
35	W	49	0	74	20	0
35	Y	49	0	74	5	0
35	a	43	0	56	10	0
35	b	121	0	158	23	0
35	c	72	0	83	14	0
35	d	49	0	74	12	0
35	g	41	0	55	9	0
35	l	49	0	74	5	0
35	n	32	0	34	6	0
35	r	30	0	30	5	0
35	s	49	0	74	16	0
35	w	39	0	51	8	0
35	y	49	0	74	6	0
36	A	59	0	76	10	0
36	B	62	0	82	11	0
36	C	177	0	228	48	0
36	a	59	0	76	17	0
36	b	62	0	82	11	0
36	c	168	0	210	45	0
37	E	43	0	30	7	0
37	f	43	0	30	6	0
38	G	339	0	295	75	0
38	N	347	0	310	78	0
38	R	154	0	116	25	0
38	S	196	0	140	47	0
38	Y	362	0	345	93	0
38	g	412	0	378	99	0
38	n	350	0	317	86	0
38	r	183	0	171	37	0
38	s	196	0	140	36	0
38	y	296	0	276	67	0
39	G	84	0	112	39	0
39	N	84	0	112	27	0
39	R	42	0	56	14	0
39	S	84	0	112	43	0
39	Y	84	0	112	15	0
39	g	84	0	112	36	0
39	n	84	0	112	21	0
39	r	42	0	56	15	0
39	s	84	0	112	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	y	84	0	112	17	0
40	G	44	0	54	11	0
40	N	44	0	54	9	0
40	Y	44	0	54	9	0
40	g	44	0	55	9	0
40	n	44	0	54	8	0
40	r	44	0	54	13	0
40	s	44	0	54	7	0
40	y	88	0	108	10	0
41	R	44	0	56	13	0
41	Y	44	0	56	17	0
41	r	44	0	56	9	0
41	y	44	0	56	11	0
42	A	92	0	0	4	0
42	B	151	0	0	2	0
42	C	134	0	0	0	0
42	D	101	0	0	2	0
42	E	14	0	0	0	0
42	F	6	0	0	0	0
42	G	26	0	0	2	0
42	H	16	0	0	2	0
42	I	3	0	0	0	0
42	J	5	0	0	0	0
42	K	6	0	0	0	0
42	L	8	0	0	0	0
42	M	6	0	0	0	0
42	N	28	0	0	1	0
42	O	69	0	0	1	0
42	P	52	0	0	2	0
42	Q	28	0	0	2	0
42	R	40	0	0	3	0
42	S	24	0	0	3	0
42	T	7	0	0	2	0
42	U	1	0	0	0	0
42	W	11	0	0	0	0
42	X	10	0	0	0	0
42	Y	45	0	0	1	0
42	Z	6	0	0	0	0
42	a	100	0	0	5	0
42	b	167	0	0	1	0
42	c	128	0	0	2	0
42	d	85	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	e	21	0	0	1	0
42	f	3	0	0	0	0
42	g	23	0	0	0	0
42	h	14	0	0	0	0
42	i	2	0	0	0	0
42	j	4	0	0	0	0
42	k	4	0	0	1	0
42	l	8	0	0	0	0
42	m	2	0	0	0	0
42	n	23	0	0	2	0
42	o	67	0	0	0	0
42	p	43	0	0	1	0
42	q	18	0	0	0	0
42	r	33	0	0	1	0
42	s	19	0	0	1	0
42	t	3	0	0	0	0
42	u	4	0	0	0	0
42	w	11	0	0	0	0
42	x	7	0	0	0	0
42	y	31	0	0	1	0
42	z	2	0	0	0	0
All	All	79416	0	77862	5285	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (5285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:601:CLA:H152	30:H:101:BCR:H17C	1.34	1.09
16:Q:13:LEU:HD22	16:Q:18:PRO:HA	1.40	1.04
1:a:42:LEU:HB3	30:a:410:BCR:H353	1.38	1.04
36:a:401:DGD:HA92	32:a:413:LMG:H352	1.39	1.04
14:O:65:VAL:HA	14:O:71:LEU:HD21	1.39	1.03
28:G:610:CLA:H72	39:G:615:LUT:H371	1.40	1.03
38:g:601:CHL:H201	38:y:309:CHL:H93	1.38	1.02
28:n:610:CLA:H52	39:n:615:LUT:H28	1.42	1.01
2:B:124:CYS:HA	2:B:131:PRO:HA	1.39	1.00
30:A:409:BCR:H321	30:A:409:BCR:HC8	1.41	0.99
7:G:173:PHE:O	7:G:177:LYS:HG3	1.61	0.98
11:K:52:PHE:HB3	30:K:101:BCR:H281	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:215:ASP:HB3	7:n:218:ASN:HB3	1.45	0.97
7:G:112:TYR:HB3	7:G:118:LEU:HD12	1.45	0.97
18:s:82:ALA:HB1	18:s:193:GLY:HA3	1.47	0.97
28:s:609:CLA:H52	39:s:614:LUT:H30	1.47	0.97
32:A:413:LMG:H352	36:A:417:DGD:HA62	1.47	0.96
17:r:182:LEU:HD12	39:r:614:LUT:H222	1.48	0.96
28:C:511:CLA:H101	30:C:516:BCR:H23C	1.49	0.95
7:g:99:LYS:HA	38:g:607:CHL:HED3	1.49	0.95
28:n:612:CLA:HHC	28:n:612:CLA:HBB1	1.48	0.95
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.48	0.95
35:B:622:LHG:HC81	35:B:622:LHG:H251	1.49	0.94
7:N:24:TYR:HD2	38:N:601:CHL:HAA1	1.27	0.94
2:b:419:LYS:HD3	2:b:422:ARG:HH11	1.33	0.94
20:W:30:PHE:CZ	35:W:101:LHG:H311	2.03	0.94
3:c:86:LEU:HD13	3:c:89:LEU:HD12	1.49	0.93
28:R:609:CLA:H52	39:R:614:LUT:H30	1.48	0.93
3:c:179:ALA:HA	3:c:184:GLY:HA2	1.47	0.93
7:g:156:TYR:HB3	28:g:610:CLA:HED1	1.51	0.93
28:b:615:CLA:H102	28:b:616:CLA:H122	1.50	0.92
7:G:174:ALA:HA	7:G:177:LYS:HD3	1.49	0.92
38:G:608:CHL:H42	39:G:615:LUT:H27	1.50	0.92
28:r:609:CLA:H2	39:r:614:LUT:H28	1.52	0.92
28:B:610:CLA:HHC	28:B:610:CLA:HBB1	1.51	0.92
18:S:108:GLU:HB3	18:S:117:LEU:HD21	1.51	0.92
28:B:615:CLA:HBB1	28:B:615:CLA:HHC	1.52	0.92
28:Y:602:CLA:H62	28:Y:603:CLA:HMA3	1.49	0.92
18:s:113:LYS:HA	38:s:606:CHL:HED3	1.47	0.91
30:k:101:BCR:H332	23:z:16:SER:HB3	1.52	0.91
28:Y:603:CLA:HHC	28:Y:603:CLA:HBB1	1.51	0.91
2:B:327:ALA:HB1	32:B:621:LMG:HC91	1.50	0.91
28:S:304:CLA:HHC	28:S:304:CLA:HBB1	1.50	0.91
28:G:610:CLA:H52	39:G:615:LUT:H30	1.53	0.90
3:C:179:ALA:HA	3:C:184:GLY:HA2	1.52	0.90
28:r:601:CLA:HBB1	28:r:601:CLA:HHC	1.54	0.90
13:M:31:SER:HB3	13:m:32:GLN:HG3	1.51	0.90
11:k:42:VAL:HG21	32:k:102:LMG:H202	1.53	0.90
2:B:496:GLN:HE22	21:X:82:LYS:HB3	1.37	0.89
28:g:602:CLA:H52	39:g:616:LUT:H30	1.53	0.89
35:D:407:LHG:H322	19:T:21:ILE:HD11	1.54	0.89
28:B:616:CLA:H91	30:B:619:BCR:H14C	1.54	0.89
7:n:147:PRO:HG3	40:n:617:NEX:H181	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:608:CLA:H12	28:R:613:CLA:H12	1.54	0.89
28:r:608:CLA:HMA3	28:r:613:CLA:HAC1	1.53	0.89
18:s:171:ASP:HA	39:s:614:LUT:H24	1.55	0.89
28:b:601:CLA:HHC	28:b:601:CLA:HBB1	1.55	0.88
7:n:99:LYS:HA	38:n:607:CHL:HED3	1.55	0.88
28:s:611:CLA:HHC	28:s:611:CLA:HBB1	1.54	0.88
16:Q:49:ALA:HA	16:Q:52:LYS:HE2	1.53	0.88
18:S:82:ALA:HB1	18:S:193:GLY:HA3	1.54	0.88
28:y:312:CLA:HHC	28:y:312:CLA:HBB1	1.53	0.88
38:G:608:CHL:H42	39:G:615:LUT:C27	2.04	0.88
17:r:15:PHE:HB3	17:r:18:ALA:HB2	1.54	0.88
28:C:506:CLA:H52	30:C:515:BCR:H10C	1.54	0.88
18:S:200:MET:HE2	39:S:316:LUT:H12	1.56	0.88
38:Y:607:CHL:H43	38:Y:607:CHL:HMA2	1.53	0.87
8:H:72:MET:HE3	8:H:72:MET:HA	1.57	0.87
1:A:309:SER:HB2	15:P:13:LYS:HE3	1.56	0.87
2:B:91:TRP:HE1	35:B:623:LHG:HC61	1.38	0.87
32:D:408:LMG:H111	42:D:521:HOH:O	1.74	0.87
28:Y:603:CLA:H2	28:Y:603:CLA:H92	1.56	0.87
7:G:69:SER:HB3	7:G:184:GLY:HA3	1.55	0.87
28:S:312:CLA:HHC	28:S:312:CLA:HBB1	1.57	0.87
32:d:409:LMG:H151	32:d:409:LMG:H292	1.57	0.87
28:n:603:CLA:HHC	28:n:603:CLA:HBB1	1.57	0.87
2:b:496:GLN:HE22	21:x:82:LYS:H	1.19	0.87
28:R:611:CLA:HHC	28:R:611:CLA:HBB1	1.54	0.86
5:e:17:ILE:HA	5:e:20:TRP:HD1	1.40	0.86
28:n:612:CLA:HED2	28:n:612:CLA:H12	1.54	0.86
14:o:145:GLU:HG2	14:o:199:LYS:HG2	1.56	0.86
28:R:608:CLA:HMA3	28:R:613:CLA:HAC1	1.56	0.86
28:R:609:CLA:H2	39:R:614:LUT:H28	1.56	0.86
18:S:41:ASP:HB2	18:S:44:GLU:HG2	1.56	0.86
7:N:203:LYS:HB2	7:N:208:ASN:HD21	1.38	0.86
35:W:101:LHG:H102	28:Y:611:CLA:H51	1.57	0.86
28:b:610:CLA:HHC	28:b:610:CLA:HBB1	1.57	0.86
2:B:110:ALA:HB2	30:B:619:BCR:H17C	1.57	0.86
7:N:99:LYS:HA	38:N:607:CHL:HED3	1.57	0.86
18:S:139:VAL:HG22	38:S:307:CHL:HBC1	1.55	0.86
3:C:186:TYR:HA	3:C:196:VAL:HA	1.56	0.86
7:n:25:LEU:HD12	7:n:28:PHE:HB2	1.56	0.86
12:l:9:GLN:HE22	17:r:56:ASN:HD21	1.24	0.86
35:C:521:LHG:H223	41:Y:617:XAT:H23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:194:PHE:HZ	39:G:615:LUT:H8	1.41	0.85
22:y:161:PHE:HA	38:y:308:CHL:H51	1.57	0.85
28:b:602:CLA:H12	36:b:625:DGD:HB41	1.55	0.85
28:y:304:CLA:HHC	28:y:304:CLA:HBB1	1.57	0.85
3:C:120:ILE:HD11	30:C:516:BCR:H321	1.57	0.85
17:R:173:TYR:HB3	28:R:609:CLA:HED2	1.58	0.85
28:G:602:CLA:H142	38:Y:609:CHL:H41	1.57	0.85
38:Y:607:CHL:H42	38:Y:607:CHL:H112	1.57	0.84
7:G:216:PRO:HD2	7:G:219:ASN:HB2	1.58	0.84
30:d:406:BCR:H372	32:d:409:LMG:H301	1.59	0.84
38:n:607:CHL:H61	38:n:607:CHL:HMB1	1.59	0.84
20:W:30:PHE:HZ	35:W:101:LHG:H311	1.39	0.84
2:b:486:LEU:HD21	4:d:138:GLN:HB2	1.59	0.84
7:g:110:LEU:HD21	28:g:604:CLA:HAA2	1.60	0.84
28:n:604:CLA:H42	40:n:617:NEX:H23	1.60	0.84
2:B:497:LYS:HB3	2:B:503:THR:HG21	1.57	0.84
18:S:46:PRO:HB2	18:S:49:LEU:HD11	1.60	0.84
28:B:615:CLA:H92	28:B:615:CLA:H2	1.58	0.83
32:A:411:LMG:H372	28:C:506:CLA:H172	1.60	0.83
29:d:402:PHO:H61	28:d:404:CLA:H13	1.61	0.83
28:N:610:CLA:H52	39:N:615:LUT:H28	1.61	0.83
7:g:174:ALA:HA	7:g:177:LYS:HD3	1.61	0.83
28:c:513:CLA:NB	30:c:514:BCR:H383	1.93	0.83
7:G:194:PHE:CZ	39:G:615:LUT:H8	2.14	0.82
31:a:414:SQD:H152	30:t:101:BCR:HC41	1.60	0.82
15:p:62:LEU:HD11	15:p:87:LEU:HD21	1.60	0.82
28:B:606:CLA:HBB1	28:B:606:CLA:HHC	1.60	0.82
28:c:504:CLA:H71	36:c:518:DGD:HB72	1.61	0.82
28:r:609:CLA:H52	39:r:614:LUT:H30	1.61	0.82
28:g:610:CLA:H11	39:g:615:LUT:H26	1.61	0.82
36:C:518:DGD:HA82	36:C:518:DGD:HAW2	1.61	0.82
7:G:87:ARG:HH12	7:G:207:GLU:HA	1.45	0.82
7:n:69:SER:HB3	7:n:184:GLY:HA3	1.61	0.82
17:r:187:ASP:HB3	17:r:190:LYS:HB2	1.62	0.82
15:P:42:PHE:HB3	15:P:62:LEU:HD21	1.59	0.81
23:Z:1:MET:HG3	23:Z:61:ILE:HG22	1.62	0.81
28:g:602:CLA:H162	28:y:304:CLA:H193	1.62	0.81
30:A:409:BCR:H321	30:A:409:BCR:C8	2.10	0.81
7:N:63:GLU:HA	7:N:155:LEU:HD21	1.63	0.81
28:N:603:CLA:H2	28:N:603:CLA:H2A	1.61	0.81
7:g:222:TRP:HB3	38:g:619:CHL:H191	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:s:612:CLA:HBB1	39:s:614:LUT:H8	1.60	0.81
18:s:125:ASN:HA	18:s:130:PRO:HA	1.62	0.81
1:A:199:MET:HB2	36:C:519:DGD:HAT1	1.62	0.81
18:s:105:CYS:HA	18:s:127:PHE:HA	1.62	0.81
38:N:608:CHL:HAA2	38:N:608:CHL:H192	1.63	0.81
3:c:154:ARG:HH12	20:w:49:GLU:HG3	1.44	0.81
14:o:111:TYR:HD2	14:o:127:LEU:HD11	1.45	0.81
28:c:511:CLA:H71	30:c:515:BCR:H402	1.63	0.81
22:y:63:GLU:HA	22:y:155:LEU:HD11	1.63	0.81
28:r:604:CLA:H2	40:r:616:NEX:H241	1.61	0.81
28:S:310:CLA:H52	39:S:315:LUT:H30	1.63	0.80
28:b:616:CLA:H193	30:b:619:BCR:H343	1.61	0.80
2:b:127:ARG:HG3	2:b:128:THR:HG23	1.62	0.80
28:B:616:CLA:H192	30:B:619:BCR:HC8	1.63	0.80
18:S:113:LYS:HA	38:S:307:CHL:HED2	1.63	0.80
7:g:66:VAL:HG11	7:g:155:LEU:HD11	1.64	0.80
7:n:80:VAL:HG13	7:n:206:LEU:HD11	1.60	0.80
28:n:613:CLA:HBB1	39:n:615:LUT:H8	1.63	0.80
17:R:184:LEU:HD12	17:R:184:LEU:H	1.44	0.80
28:C:508:CLA:H202	11:K:45:LEU:HB3	1.63	0.80
12:L:9:GLN:HE22	17:R:56:ASN:HD21	1.28	0.80
22:Y:195:PHE:HB3	38:Y:607:CHL:H91	1.64	0.80
28:y:311:CLA:HHC	28:y:311:CLA:HBB1	1.62	0.80
28:R:601:CLA:HBC1	42:R:736:HOH:O	1.80	0.80
5:e:26:THR:HB	37:f:101:HEM:HAB	1.64	0.80
28:G:612:CLA:HHC	28:G:612:CLA:HBB1	1.64	0.80
32:A:411:LMG:H421	28:C:505:CLA:HBC3	1.64	0.79
7:N:69:SER:HB3	7:N:184:GLY:HA3	1.65	0.79
18:S:34:PHE:HD2	38:S:302:CHL:HAA1	1.47	0.79
28:r:611:CLA:HHC	28:r:611:CLA:HBB1	1.64	0.79
35:C:521:LHG:H201	28:Y:611:CLA:HAB	1.63	0.79
2:B:50:PRO:HD2	14:o:67:LYS:HD2	1.64	0.79
28:C:505:CLA:CMD	28:C:507:CLA:HAB	2.12	0.79
28:c:511:CLA:H51	30:c:515:BCR:H282	1.63	0.79
22:y:80:VAL:HG13	22:y:206:LEU:HD11	1.63	0.79
18:S:105:CYS:HA	18:S:127:PHE:H	1.46	0.79
38:n:601:CHL:HAC2	35:n:618:LHG:HC41	1.65	0.79
3:C:86:LEU:HD13	3:C:89:LEU:HD12	1.65	0.79
1:A:200:LEU:HD23	36:C:519:DGD:HAW2	1.65	0.78
28:B:608:CLA:H61	28:B:609:CLA:H121	1.63	0.78
2:b:491:GLU:HB2	2:b:494:ALA:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:610:CLA:H71	39:G:615:LUT:C30	2.12	0.78
7:g:48:THR:HG21	38:y:309:CHL:HAA2	1.65	0.78
28:g:610:CLA:H62	28:g:612:CLA:HMA2	1.64	0.78
14:o:128:PHE:HA	14:o:222:GLN:HE22	1.49	0.78
1:a:313:VAL:HG13	15:p:33:LYS:HD2	1.63	0.78
3:C:233:ILE:HA	30:C:515:BCR:H282	1.64	0.78
29:a:408:PHO:HBB1	29:a:408:PHO:HMB3	1.65	0.78
28:B:603:CLA:HHC	28:B:605:CLA:H171	1.65	0.78
17:R:140:LEU:HD12	17:R:142:PHE:HE2	1.49	0.78
18:s:46:PRO:HB2	18:s:49:LEU:HB2	1.65	0.78
28:C:513:CLA:HBA1	28:C:513:CLA:HBD	1.66	0.78
18:s:198:PHE:HE2	28:s:612:CLA:HAB	1.48	0.78
4:D:56:VAL:HG21	4:D:111:LEU:HD12	1.65	0.78
28:c:513:CLA:H11	30:c:514:BCR:H381	1.66	0.78
18:s:57:TYR:HB2	28:s:602:CLA:HMD1	1.63	0.78
28:G:610:CLA:H71	39:G:615:LUT:H30	1.65	0.77
4:d:193:THR:HG23	28:d:404:CLA:HBC2	1.64	0.77
7:n:81:PHE:HB3	7:n:82:PRO:HD3	1.66	0.77
1:A:63:ILE:HB	3:C:335:THR:HG21	1.64	0.77
31:B:620:SQD:H5	31:L:101:SQD:H3	1.65	0.77
2:b:497:LYS:HE3	4:d:24:ARG:HB2	1.65	0.77
33:d:407:PL9:H111	35:d:408:LHG:HC92	1.67	0.77
28:D:404:CLA:H202	21:X:63:VAL:HA	1.66	0.77
7:n:74:LEU:HD11	28:n:610:CLA:H202	1.66	0.77
14:O:94:GLU:HB2	42:O:361:HOH:O	1.83	0.77
18:s:139:VAL:HG22	38:s:606:CHL:HBC1	1.65	0.77
14:O:227:ASP:HB2	14:O:231:LYS:HE3	1.66	0.77
28:b:608:CLA:H18	28:d:405:CLA:HBA1	1.67	0.77
1:A:93:PHE:HZ	28:A:408:CLA:HAA1	1.49	0.77
3:c:178:LYS:HB2	28:c:502:CLA:H172	1.64	0.77
22:y:191:MET:HE2	39:y:316:LUT:H10	1.65	0.77
22:Y:63:GLU:HA	22:Y:155:LEU:HD11	1.67	0.77
3:c:377:LEU:HG	3:c:381:LYS:HE2	1.66	0.77
28:c:505:CLA:CMD	28:c:507:CLA:HAB	2.15	0.77
38:g:606:CHL:H3A	40:g:617:NEX:C31	2.15	0.77
36:a:401:DGD:HBT2	32:a:413:LMG:H362	1.66	0.77
7:n:130:THR:HG21	38:n:606:CHL:HED3	1.67	0.77
8:H:50:PHE:HB2	30:H:101:BCR:H12C	1.68	0.76
1:a:240:GLY:HA3	19:t:30:PRO:HG2	1.66	0.76
28:a:409:CLA:H122	32:w:101:LMG:H132	1.67	0.76
18:S:105:CYS:HA	18:S:127:PHE:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:253:GLY:HA2	2:b:492:PHE:CZ	2.20	0.76
28:g:602:CLA:H2	39:g:616:LUT:H28	1.67	0.76
38:G:601:CHL:H192	38:Y:607:CHL:H52	1.67	0.76
15:P:169:PHE:HB2	16:Q:27:ARG:HD3	1.67	0.76
3:c:154:ARG:HB3	3:c:256:PRO:HG2	1.66	0.76
2:B:434:ARG:HD2	14:O:177:GLY:HA3	1.67	0.76
38:S:302:CHL:HHD	35:S:317:LHG:HC41	1.68	0.76
38:S:308:CHL:HBC2	38:S:308:CHL:HHD	1.68	0.76
7:g:200:VAL:HG22	38:g:619:CHL:H72	1.68	0.76
28:B:616:CLA:HBB1	28:B:616:CLA:HMB1	1.68	0.76
28:N:610:CLA:H101	28:N:612:CLA:H102	1.68	0.76
7:G:73:MET:SD	28:G:610:CLA:HAB	2.26	0.76
28:R:602:CLA:HBA1	41:R:615:XAT:H382	1.67	0.76
28:c:504:CLA:H61	36:c:517:DGD:HBE2	1.68	0.76
28:c:513:CLA:HBA1	28:c:513:CLA:HBD	1.66	0.76
9:i:20:ILE:HG23	30:i:101:BCR:H332	1.67	0.76
31:A:414:SQD:H383	36:A:417:DGD:HA91	1.68	0.76
28:C:513:CLA:H193	30:C:514:BCR:H21C	1.67	0.76
7:G:189:PHE:CE1	28:G:613:CLA:HAB	2.20	0.76
38:r:605:CHL:HHC	38:r:605:CHL:HBB1	1.67	0.76
28:N:612:CLA:HMA3	28:N:612:CLA:H72	1.68	0.75
30:A:409:BCR:HC8	30:A:409:BCR:C32	2.15	0.75
35:C:521:LHG:H342	28:Y:613:CLA:H191	1.67	0.75
7:G:156:TYR:HA	28:G:610:CLA:O1D	1.86	0.75
31:B:620:SQD:H45	19:t:23:PHE:HD2	1.51	0.75
38:G:609:CHL:HAA2	7:N:48:THR:HG21	1.69	0.75
7:n:63:GLU:HA	7:n:155:LEU:HD11	1.67	0.75
14:O:157:LEU:HD21	14:O:166:THR:HG23	1.69	0.75
28:R:604:CLA:H12	40:y:301:NEX:H382	1.68	0.75
28:S:303:CLA:HMB3	28:S:303:CLA:HBB1	1.69	0.75
35:W:101:LHG:H111	28:Y:611:CLA:H72	1.69	0.75
28:b:616:CLA:HBB1	28:b:616:CLA:HMB3	1.66	0.75
7:n:164:LEU:HD12	39:n:615:LUT:H222	1.68	0.75
28:n:602:CLA:HBB1	28:n:602:CLA:HMB3	1.68	0.75
28:s:608:CLA:HBB1	28:s:608:CLA:HMB3	1.67	0.75
1:A:333:GLU:HB3	1:A:336:ALA:HB3	1.68	0.75
3:C:116:VAL:HG13	30:C:516:BCR:H313	1.68	0.75
28:Y:603:CLA:ND	38:Y:609:CHL:H8	2.02	0.75
1:A:255:PHE:HD2	1:A:264:SER:HB3	1.51	0.75
38:N:605:CHL:HHC	38:N:605:CHL:HBB1	1.69	0.75
3:c:258:ALA:H	35:c:519:LHG:HC11	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:614:CLA:HBB1	28:g:614:CLA:HMB1	1.68	0.74
4:D:3:ILE:HD13	17:R:47:GLN:HG2	1.69	0.74
28:S:312:CLA:HMB1	39:S:315:LUT:H31	1.68	0.74
28:a:407:CLA:HAA2	32:d:409:LMG:H241	1.70	0.74
18:s:105:CYS:HA	18:s:127:PHE:CA	2.17	0.74
38:G:608:CHL:H42	39:G:615:LUT:C28	2.17	0.74
3:c:186:TYR:HA	3:c:196:VAL:HA	1.69	0.74
38:G:605:CHL:HHC	38:G:605:CHL:HBB1	1.69	0.74
1:A:120:LEU:HB2	28:C:505:CLA:H202	1.69	0.74
17:R:134:THR:HG22	17:R:139:PRO:HA	1.67	0.74
3:C:154:ARG:HB3	3:C:256:PRO:HG2	1.70	0.74
38:r:605:CHL:H112	38:r:607:CHL:H93	1.68	0.74
28:B:603:CLA:H2	28:B:605:CLA:H91	1.69	0.74
18:S:126:TYR:HB2	18:S:131:ILE:HD11	1.69	0.74
28:g:604:CLA:HBB1	28:g:604:CLA:HMB1	1.70	0.74
1:A:50:ILE:HD12	30:A:409:BCR:H21C	1.69	0.74
4:d:187:GLN:HB2	28:d:404:CLA:HBC1	1.69	0.74
7:n:191:MET:HE2	39:n:616:LUT:H10	1.68	0.74
28:s:609:CLA:H62	28:s:611:CLA:HHB	1.70	0.74
38:G:608:CHL:H71	38:G:608:CHL:H2	1.68	0.74
36:a:401:DGD:HD61	30:a:410:BCR:H401	1.69	0.74
17:r:123:ASP:HA	38:r:606:CHL:HED3	1.70	0.74
3:C:117:LEU:HD12	32:C:522:LMG:H191	1.70	0.74
28:Y:612:CLA:HBB1	28:Y:612:CLA:HMB3	1.68	0.74
28:c:504:CLA:H93	36:c:518:DGD:HBE2	1.69	0.73
11:K:53:VAL:HG23	30:K:101:BCR:H21C	1.70	0.73
28:c:501:CLA:H151	28:c:507:CLA:H101	1.70	0.73
3:C:73:ALA:HB2	11:K:26:LEU:HG	1.70	0.73
7:G:83:GLU:HA	7:G:95:ALA:HB1	1.70	0.73
28:b:605:CLA:HMA2	28:b:606:CLA:HMA2	1.69	0.73
28:R:602:CLA:CAB	41:R:615:XAT:H32	2.17	0.73
1:a:277:ALA:HB3	31:a:411:SQD:H131	1.70	0.73
28:c:504:CLA:C3D	36:c:517:DGD:HB21	2.19	0.73
38:g:605:CHL:HBB1	38:g:605:CHL:HHC	1.70	0.73
7:n:189:PHE:HE2	28:n:613:CLA:HAB	1.53	0.73
17:r:97:LEU:HD23	17:r:172:LEU:HG	1.70	0.73
20:w:39:ILE:HG12	28:y:312:CLA:H41	1.70	0.73
7:G:19:PRO:HA	42:G:708:HOH:O	1.88	0.73
7:G:161:PHE:HA	38:G:608:CHL:H72	1.70	0.73
17:R:221:LYS:HB3	17:R:225:ASN:HB2	1.70	0.73
3:c:195:ASP:HB3	16:q:85:ARG:HH11	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:614:CLA:H141	30:B:617:BCR:H12C	1.70	0.73
28:y:304:CLA:H152	38:y:309:CHL:H92	1.70	0.73
7:G:51:LEU:H	7:G:51:LEU:HD12	1.51	0.73
3:c:473:ASN:HA	19:t:26:PRO:HB3	1.70	0.73
17:r:12:PRO:HB2	28:r:601:CLA:HBC3	1.71	0.73
19:t:18:PHE:HD2	30:t:101:BCR:HC7	1.52	0.73
2:B:182:ASN:OD1	32:B:624:LMG:HC62	1.89	0.73
7:N:156:TYR:HB3	28:N:610:CLA:HED3	1.71	0.73
1:a:39:PRO:HA	30:a:410:BCR:H12C	1.70	0.73
1:a:140:ARG:HB2	4:d:221:ASN:HA	1.69	0.73
38:n:601:CHL:HBB1	38:n:601:CHL:HHC	1.70	0.73
2:B:257:TRP:CD1	36:B:626:DGD:HBN1	2.23	0.73
4:D:193:THR:HG23	28:D:403:CLA:HBC2	1.71	0.73
7:G:226:THR:HG22	7:G:228:PHE:H	1.51	0.73
18:s:212:GLU:HB2	18:s:217:ASN:HD21	1.54	0.73
7:G:189:PHE:HE1	28:G:613:CLA:HAB	1.54	0.73
38:G:606:CHL:HBB1	38:G:606:CHL:HHC	1.71	0.73
28:R:610:CLA:C4A	28:R:610:CLA:H2	2.18	0.73
30:T:101:BCR:H372	42:T:206:HOH:O	1.88	0.73
28:a:407:CLA:HMB1	28:a:407:CLA:HBB1	1.70	0.73
7:N:24:TYR:CD2	38:N:601:CHL:HAA1	2.18	0.72
28:b:613:CLA:H172	30:b:618:BCR:HC22	1.70	0.72
4:d:56:VAL:HG21	4:d:111:LEU:HD12	1.70	0.72
38:g:606:CHL:HBA1	40:g:617:NEX:H31	1.69	0.72
38:g:608:CHL:HHC	38:g:608:CHL:HBB1	1.70	0.72
28:N:602:CLA:H172	39:N:616:LUT:H31	1.71	0.72
17:R:178:PHE:CD1	38:R:607:CHL:H8	2.24	0.72
1:a:50:ILE:HD12	30:a:410:BCR:H21C	1.71	0.72
28:b:602:CLA:HED3	28:b:603:CLA:HMA2	1.70	0.72
2:B:122:ILE:HA	8:H:24:LYS:HD3	1.71	0.72
28:C:502:CLA:HBB1	28:C:502:CLA:HMB3	1.71	0.72
5:E:8:ARG:HH21	5:E:13:ILE:HA	1.53	0.72
38:G:608:CHL:HBB1	38:G:608:CHL:HHC	1.70	0.72
8:H:72:MET:HA	8:H:72:MET:CE	2.18	0.72
28:c:511:CLA:H93	30:c:515:BCR:H23C	1.69	0.72
28:R:602:CLA:HAB	41:R:615:XAT:H32	1.72	0.72
38:Y:607:CHL:H43	38:Y:607:CHL:CMA	2.19	0.72
11:k:27:PRO:HB2	11:k:30:TYR:HD2	1.53	0.72
38:y:307:CHL:HHC	38:y:307:CHL:HBB1	1.70	0.72
1:A:278:TRP:HA	31:A:410:SQD:H171	1.69	0.72
12:L:25:ILE:HG22	13:M:15:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:214:VAL:HG21	28:R:612:CLA:HAC2	1.71	0.72
28:g:602:CLA:HBC1	35:g:618:LHG:H271	1.72	0.72
3:C:195:ASP:HB3	16:Q:85:ARG:HH11	1.54	0.72
7:G:227:ASN:HB2	38:Y:607:CHL:HBA1	1.70	0.72
30:K:101:BCR:H321	30:K:101:BCR:HC8	1.70	0.72
35:c:520:LHG:H112	28:s:610:CLA:HAB	1.72	0.72
28:C:512:CLA:HBB1	28:C:512:CLA:HMB1	1.69	0.72
28:R:608:CLA:H43	28:R:613:CLA:H52	1.72	0.72
18:S:195:LEU:HB2	35:S:317:LHG:H241	1.69	0.72
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.71	0.72
38:R:606:CHL:HHC	38:R:606:CHL:HBB1	1.70	0.72
3:c:259:TRP:CD1	35:w:102:LHG:HC62	2.24	0.72
7:g:191:MET:HE2	39:g:616:LUT:H10	1.72	0.72
1:A:38:ILE:HG23	31:A:414:SQD:H171	1.72	0.71
28:B:608:CLA:H18	28:D:404:CLA:HAA2	1.72	0.71
1:a:40:THR:HG21	1:a:121:LEU:HD22	1.70	0.71
38:y:308:CHL:HHC	38:y:308:CHL:HBB1	1.72	0.71
4:D:90:LEU:H	8:H:62:ASN:HD21	1.37	0.71
28:S:312:CLA:H2A	28:S:312:CLA:H12	1.72	0.71
38:Y:608:CHL:HHC	38:Y:608:CHL:HBB1	1.71	0.71
28:g:602:CLA:HAC2	35:g:618:LHG:H252	1.71	0.71
38:g:606:CHL:C3	40:g:617:NEX:H14	2.20	0.71
38:y:306:CHL:HHC	38:y:306:CHL:HBB1	1.71	0.71
1:A:302:PHE:HA	3:C:415:ASN:HD21	1.55	0.71
17:R:91:ARG:HH21	28:R:613:CLA:HBD	1.55	0.71
28:c:506:CLA:HMB3	28:c:506:CLA:HBB1	1.70	0.71
35:c:520:LHG:H181	35:s:617:LHG:H122	1.70	0.71
2:B:491:GLU:HB2	2:B:494:ALA:HB2	1.73	0.71
28:C:504:CLA:HAA2	36:C:518:DGD:HE1	1.72	0.71
28:N:610:CLA:H72	39:N:615:LUT:H30	1.71	0.71
38:g:601:CHL:HHC	38:g:601:CHL:HBB1	1.72	0.71
28:B:601:CLA:H151	28:B:601:CLA:C3B	2.21	0.71
28:B:602:CLA:H8	36:B:626:DGD:HB71	1.72	0.71
38:Y:605:CHL:HHC	38:Y:605:CHL:HBB1	1.71	0.71
4:d:192:TRP:CE3	4:d:290:LEU:HD11	2.26	0.71
18:s:62:PHE:CD1	39:s:615:LUT:H221	2.26	0.71
38:s:605:CHL:HHC	38:s:605:CHL:HBB1	1.71	0.71
31:A:414:SQD:H141	30:T:101:BCR:HC41	1.72	0.71
38:G:608:CHL:H42	39:G:615:LUT:H28	1.72	0.71
30:b:618:BCR:H323	32:b:620:LMG:H142	1.73	0.71
38:n:605:CHL:HHC	38:n:605:CHL:HBB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:HE22	4:D:231:ASN:HD22	1.39	0.70
4:D:187:GLN:HB2	28:D:403:CLA:HBC1	1.71	0.70
18:S:46:PRO:HB2	18:S:49:LEU:CD1	2.21	0.70
2:b:33:TRP:HB2	30:b:618:BCR:H353	1.73	0.70
39:n:615:LUT:H8	39:n:615:LUT:H181	1.72	0.70
16:q:106:LEU:HG	16:q:143:VAL:HG22	1.72	0.70
28:B:602:CLA:H121	36:B:626:DGD:HA71	1.73	0.70
30:B:618:BCR:H323	32:B:621:LMG:H142	1.73	0.70
38:R:607:CHL:HBB1	38:R:607:CHL:HHC	1.73	0.70
7:g:81:PHE:HB3	7:g:82:PRO:HD3	1.73	0.70
38:n:607:CHL:HBA1	22:y:229:VAL:HA	1.71	0.70
18:s:41:ASP:HB3	18:s:44:GLU:HG2	1.71	0.70
28:s:602:CLA:H2	39:s:615:LUT:H28	1.72	0.70
31:A:414:SQD:H2	31:A:414:SQD:H82	1.73	0.70
1:a:52:PHE:HB3	33:d:407:PL9:H503	1.73	0.70
28:b:606:CLA:H13	30:b:619:BCR:H10C	1.74	0.70
28:s:602:CLA:H52	39:s:615:LUT:H28	1.73	0.70
22:y:125:LEU:HA	22:y:128:TRP:CD1	2.26	0.70
28:C:513:CLA:H112	30:C:514:BCR:H24C	1.73	0.70
35:D:407:LHG:HC62	12:L:16:THR:HG23	1.74	0.70
38:G:601:CHL:HHC	38:G:601:CHL:HBB1	1.74	0.70
7:N:164:LEU:HD12	39:N:615:LUT:H222	1.71	0.70
28:S:310:CLA:H71	28:S:312:CLA:HMA3	1.74	0.70
7:g:119:VAL:HA	38:g:605:CHL:C4D	2.21	0.70
7:g:228:PHE:H	38:g:619:CHL:H162	1.57	0.70
15:p:114:LEU:HD11	15:p:132:LEU:HB2	1.74	0.70
17:r:124:ALA:HB1	28:r:604:CLA:HED1	1.74	0.70
28:s:602:CLA:H52	39:s:615:LUT:H30	1.72	0.70
15:P:94:PHE:CE1	16:Q:2:ALA:HA	2.26	0.70
15:P:168:TRP:CZ2	15:P:173:ARG:HG3	2.26	0.70
3:c:117:LEU:HD22	32:c:521:LMG:H371	1.74	0.70
4:d:237:ASN:HB3	4:d:240:GLN:HB3	1.74	0.70
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.27	0.70
28:G:603:CLA:C3D	38:G:609:CHL:H2	2.21	0.70
38:S:306:CHL:HHC	38:S:306:CHL:HBB1	1.73	0.70
22:Y:191:MET:HE2	39:Y:616:LUT:H10	1.73	0.70
38:Y:601:CHL:HHC	38:Y:601:CHL:HBB1	1.74	0.70
2:B:103:PHE:HB2	28:B:606:CLA:H71	1.73	0.70
38:N:608:CHL:HHC	38:N:608:CHL:HBB1	1.73	0.70
38:g:606:CHL:HBB1	38:g:606:CHL:HHC	1.74	0.70
28:g:612:CLA:HBB1	28:g:612:CLA:HMB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:601:CHL:HHD	35:N:618:LHG:HC41	1.73	0.70
28:Y:602:CLA:H92	28:Y:603:CLA:HMA3	1.74	0.70
28:b:603:CLA:HBB1	28:b:603:CLA:HMB1	1.72	0.70
28:B:612:CLA:H171	28:B:613:CLA:HBB2	1.74	0.70
3:C:116:VAL:HG12	30:C:514:BCR:HC8	1.74	0.70
35:C:521:LHG:HC62	28:Y:611:CLA:HBA1	1.74	0.70
23:Z:33:TRP:CE2	23:Z:37:LYS:HG2	2.27	0.70
3:c:236:GLY:HA3	30:i:101:BCR:H402	1.73	0.70
12:l:5:ASN:HD22	12:l:7:ASN:H	1.40	0.70
22:y:69:SER:HB3	22:y:184:GLY:HA3	1.74	0.70
35:C:521:LHG:H262	35:C:521:LHG:H141	1.72	0.69
38:N:601:CHL:HBB1	38:N:601:CHL:HHC	1.74	0.69
1:a:93:PHE:HZ	28:a:409:CLA:HAA1	1.56	0.69
1:a:283:ILE:HG13	29:a:408:PHO:HBC3	1.73	0.69
28:b:602:CLA:H171	36:b:625:DGD:HA92	1.73	0.69
15:p:147:ILE:HG12	15:p:160:LYS:HG3	1.73	0.69
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.26	0.69
28:c:513:CLA:C4B	30:c:514:BCR:H383	2.22	0.69
14:o:91:GLY:HA2	14:o:106:LYS:HG2	1.72	0.69
28:A:408:CLA:H142	32:A:411:LMG:H302	1.72	0.69
32:C:520:LMG:H151	11:K:39:PHE:HD1	1.57	0.69
7:G:63:GLU:HA	7:G:155:LEU:HD11	1.73	0.69
7:N:191:MET:HE2	39:N:616:LUT:H10	1.72	0.69
38:S:302:CHL:HHC	38:S:302:CHL:HBB1	1.74	0.69
22:Y:69:SER:HB3	22:Y:184:GLY:HA3	1.74	0.69
28:Y:604:CLA:H42	40:Y:618:NEX:H23	1.74	0.69
7:G:147:PRO:HG2	40:G:617:NEX:H192	1.74	0.69
7:n:119:VAL:HA	38:n:605:CHL:C4D	2.22	0.69
18:s:96:GLU:HA	18:s:109:ALA:HB1	1.75	0.69
28:B:603:CLA:HAB	28:B:605:CLA:H171	1.75	0.69
29:D:402:PHO:H152	28:D:403:CLA:H171	1.72	0.69
28:R:609:CLA:H8	39:R:614:LUT:C30	2.23	0.69
38:Y:607:CHL:H42	38:Y:607:CHL:C11	2.23	0.69
2:b:464:PHE:HD2	28:b:611:CLA:HAC2	1.56	0.69
17:r:119:VAL:HG11	17:r:127:VAL:HG21	1.73	0.69
38:y:302:CHL:HHC	38:y:302:CHL:HBB1	1.74	0.69
38:G:601:CHL:C19	38:Y:607:CHL:H52	2.23	0.69
31:M:101:SQD:H131	28:b:614:CLA:H71	1.72	0.69
38:S:308:CHL:HHC	38:S:308:CHL:HBB1	1.74	0.69
28:b:602:CLA:H93	8:h:58:LEU:HD13	1.73	0.69
30:d:406:BCR:H19C	6:f:24:THR:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:212:HIS:CG	28:g:613:CLA:HAA2	2.28	0.69
28:r:613:CLA:HBB1	28:r:613:CLA:HHC	1.73	0.69
28:y:314:CLA:HED2	41:y:317:XAT:H202	1.75	0.69
3:C:141:GLU:HA	3:C:148:GLY:HA3	1.73	0.69
38:N:607:CHL:HHC	38:N:607:CHL:HBB1	1.75	0.69
28:N:614:CLA:HBB1	28:N:614:CLA:HMB1	1.75	0.69
28:b:604:CLA:HBB1	28:b:604:CLA:HMB1	1.73	0.69
28:b:610:CLA:H151	28:b:615:CLA:HBD	1.74	0.69
38:g:619:CHL:HED3	22:y:99:LYS:HA	1.73	0.69
2:B:49:ASP:HA	14:o:67:LYS:HB2	1.74	0.69
28:N:603:CLA:ND	38:N:609:CHL:H8	2.08	0.69
16:Q:54:SER:HB3	16:Q:81:ALA:HA	1.75	0.69
28:S:303:CLA:H52	39:S:316:LUT:H28	1.75	0.69
28:S:305:CLA:HMA2	38:S:306:CHL:C3C	2.23	0.69
38:Y:606:CHL:HHC	38:Y:606:CHL:HBB1	1.75	0.69
28:b:601:CLA:C2C	30:h:101:BCR:H19C	2.23	0.69
5:e:17:ILE:HA	5:e:20:TRP:CD1	2.27	0.69
22:y:189:PHE:CE2	28:y:313:CLA:HAB	2.28	0.69
2:B:124:CYS:HA	2:B:131:PRO:CA	2.18	0.69
10:J:9:PRO:HB2	10:J:12:ILE:HG23	1.74	0.69
28:Y:604:CLA:H2	38:Y:606:CHL:HBD	1.75	0.69
3:c:26:ARG:HH11	3:c:48:LYS:HE3	1.56	0.69
13:m:17:VAL:HB	13:m:18:PRO:HD3	1.75	0.69
18:s:35:LEU:HB2	18:s:40:LEU:HB2	1.75	0.69
28:B:612:CLA:HMB1	28:B:612:CLA:HBB1	1.74	0.69
28:R:601:CLA:NC	35:R:616:LHG:HC82	2.07	0.69
38:g:608:CHL:HBA1	38:g:608:CHL:H151	1.75	0.69
38:n:608:CHL:HHC	38:n:608:CHL:HBB1	1.73	0.69
38:r:605:CHL:HBB2	38:r:606:CHL:CBB	2.23	0.69
5:e:10:PHE:CZ	6:f:13:ARG:HD2	2.28	0.68
35:W:101:LHG:H182	28:Y:612:CLA:H122	1.74	0.68
1:a:63:ILE:HB	3:c:335:THR:HG21	1.75	0.68
7:n:161:PHE:HA	38:n:608:CHL:H51	1.75	0.68
36:C:519:DGD:HA81	32:D:408:LMG:H181	1.75	0.68
28:G:610:CLA:H152	39:G:615:LUT:H393	1.75	0.68
7:N:81:PHE:HB3	7:N:82:PRO:HD3	1.75	0.68
22:Y:25:LEU:HB2	22:Y:29:SER:HA	1.75	0.68
2:b:91:TRP:HE1	35:b:622:LHG:HC61	1.57	0.68
3:c:113:VAL:HG11	32:c:521:LMG:H311	1.75	0.68
2:B:109:LEU:HB2	30:B:619:BCR:H19C	1.75	0.68
28:G:613:CLA:H13	35:G:618:LHG:H352	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:96:VAL:HG23	7:N:99:LYS:HB2	1.76	0.68
18:S:182:ALA:HB1	18:S:186:LYS:NZ	2.08	0.68
28:c:505:CLA:HMD2	28:c:507:CLA:HAB	1.74	0.68
14:o:61:LYS:HB3	14:o:235:ASP:HB2	1.75	0.68
28:s:604:CLA:O1A	40:s:616:NEX:H241	1.94	0.68
28:y:311:CLA:H92	28:y:311:CLA:H41	1.75	0.68
2:B:142:HIS:HB3	28:B:610:CLA:H102	1.75	0.68
36:C:518:DGD:HB71	32:C:520:LMG:H401	1.75	0.68
28:N:602:CLA:H102	39:N:616:LUT:H371	1.76	0.68
28:d:405:CLA:H101	21:x:58:ILE:HG23	1.75	0.68
14:o:59:THR:HB	14:o:73:PHE:HB3	1.76	0.68
17:R:197:ALA:HB2	28:R:610:CLA:HED3	1.76	0.68
28:R:601:CLA:HHC	28:R:601:CLA:HBB1	1.76	0.68
28:b:615:CLA:H172	28:b:615:CLA:H122	1.76	0.68
28:c:502:CLA:HMB1	28:c:502:CLA:HBB1	1.75	0.68
7:n:83:GLU:O	7:n:87:ARG:HG2	1.93	0.68
28:B:616:CLA:H43	28:B:616:CLA:HED3	1.76	0.68
28:C:502:CLA:H43	28:C:503:CLA:H2	1.75	0.68
28:C:508:CLA:H191	11:K:49:LEU:HD21	1.76	0.68
5:E:13:ILE:HG21	37:E:101:HEM:HAD2	1.76	0.68
14:O:111:TYR:HD2	14:O:127:LEU:HD11	1.56	0.68
28:b:604:CLA:H191	28:b:615:CLA:H101	1.76	0.68
28:b:606:CLA:HMC2	35:b:622:LHG:H321	1.76	0.68
7:g:162:ASP:HA	39:g:615:LUT:H24	1.76	0.68
38:n:608:CHL:HHB	38:n:608:CHL:H151	1.74	0.68
28:n:610:CLA:HBA1	39:n:615:LUT:H382	1.76	0.68
17:r:91:ARG:HH21	28:r:613:CLA:HBD	1.59	0.68
2:B:251:VAL:HA	36:B:626:DGD:HB61	1.74	0.68
35:B:623:LHG:H281	35:B:623:LHG:H122	1.76	0.68
28:C:508:CLA:H171	11:K:45:LEU:HD22	1.74	0.68
14:O:6:ARG:HG2	14:O:31:THR:HB	1.74	0.68
17:r:11:ARG:HH21	17:r:33:GLY:H	1.41	0.68
7:N:25:LEU:HB2	7:N:29:SER:HA	1.76	0.68
28:c:504:CLA:H91	28:c:508:CLA:H201	1.76	0.68
5:E:26:THR:HB	37:E:101:HEM:HAB	1.76	0.67
7:G:124:ILE:H	7:G:124:ILE:HD12	1.59	0.67
7:g:194:PHE:CZ	39:g:615:LUT:H8	2.29	0.67
3:C:265:VAL:HG21	3:C:449:ARG:HG2	1.76	0.67
16:Q:101:GLN:HA	16:Q:104:LYS:HE2	1.76	0.67
18:S:194:ARG:HB2	35:S:317:LHG:H252	1.74	0.67
1:a:292:THR:HG21	36:c:517:DGD:HBN1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:607:CLA:H71	32:b:620:LMG:H352	1.76	0.67
4:d:39:PHE:HB2	4:d:40:PRO:HD3	1.75	0.67
4:d:157:VAL:HG12	4:d:172:PRO:HG3	1.76	0.67
3:C:42:LEU:HD21	28:C:511:CLA:H2A	1.76	0.67
28:N:602:CLA:HAC2	35:N:618:LHG:H261	1.76	0.67
28:Y:614:CLA:HBB1	28:Y:614:CLA:HMB1	1.77	0.67
6:f:21:ALA:HB1	37:f:101:HEM:HAC	1.76	0.67
16:q:49:ALA:HA	16:q:52:LYS:HD3	1.77	0.67
36:C:518:DGD:HD3	32:C:520:LMG:HC3	1.76	0.67
16:Q:101:GLN:O	16:Q:105:GLU:HG2	1.95	0.67
18:S:162:ASP:HB3	18:S:165:HIS:O	1.94	0.67
35:S:317:LHG:H292	35:S:317:LHG:H242	1.76	0.67
38:Y:607:CHL:HHC	38:Y:607:CHL:HBB1	1.75	0.67
3:c:42:LEU:HD21	28:c:511:CLA:H2A	1.74	0.67
28:c:508:CLA:H18	32:k:102:LMG:H371	1.76	0.67
7:g:163:PRO:HD2	39:g:615:LUT:H23	1.75	0.67
11:K:37:VAL:HA	11:K:40:MET:HE2	1.75	0.67
13:M:17:VAL:HB	13:M:18:PRO:HD3	1.75	0.67
3:c:425:TRP:CD1	28:c:504:CLA:HMA2	2.29	0.67
17:r:37:PHE:HB2	17:r:39:LEU:HD13	1.76	0.67
18:S:36:PRO:HG2	18:S:39:LEU:HB2	1.77	0.67
18:S:146:LEU:HG	28:S:309:CLA:HMC2	1.77	0.67
7:G:48:THR:HG21	38:Y:609:CHL:HAA2	1.76	0.67
28:b:615:CLA:H171	28:b:616:CLA:C1C	2.25	0.67
32:b:623:LMG:HC1	32:b:623:LMG:HC92	1.75	0.67
28:c:511:CLA:H172	23:z:20:LEU:HA	1.76	0.67
15:p:169:PHE:HB2	16:q:27:ARG:HD3	1.75	0.67
38:s:607:CHL:HHC	38:s:607:CHL:HBB1	1.75	0.67
7:G:49:ALA:HB3	7:G:51:LEU:HD11	1.76	0.67
28:G:610:CLA:H2	39:G:615:LUT:H381	1.77	0.67
7:N:161:PHE:HA	38:N:608:CHL:H2	1.76	0.67
14:O:89:ILE:HD13	14:O:130:ILE:HD11	1.77	0.67
31:a:411:SQD:H5	4:d:233:PHE:HB2	1.77	0.67
2:b:12:VAL:HG23	28:b:612:CLA:HMC2	1.76	0.67
28:b:615:CLA:H142	28:b:616:CLA:H8	1.75	0.67
28:c:501:CLA:H192	28:c:507:CLA:H152	1.77	0.67
28:r:609:CLA:H92	39:r:614:LUT:H371	1.75	0.67
28:r:609:CLA:H151	39:r:614:LUT:H393	1.75	0.67
18:s:160:LEU:HG	18:s:161:GLU:HG3	1.76	0.67
7:G:51:LEU:HD11	39:G:616:LUT:H221	1.75	0.67
17:R:87:PHE:HA	17:R:92:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:212:GLU:HB2	18:S:217:ASN:HD21	1.59	0.67
38:Y:601:CHL:C4C	41:Y:617:XAT:H362	2.25	0.67
3:c:217:PRO:HB2	36:c:516:DGD:HA21	1.77	0.67
7:g:194:PHE:HZ	39:g:615:LUT:H8	1.57	0.67
38:g:609:CHL:HHC	38:g:609:CHL:HBB1	1.76	0.67
1:A:140:ARG:HH22	35:A:416:LHG:HC41	1.60	0.67
28:B:608:CLA:H121	4:D:121:PHE:CE1	2.30	0.67
22:y:156:TYR:HA	28:y:310:CLA:O1D	1.95	0.67
2:B:497:LYS:HD2	4:D:21:ASP:HA	1.75	0.66
28:C:510:CLA:H2	28:C:510:CLA:HED2	1.76	0.66
17:R:108:LEU:HD23	28:R:609:CLA:H142	1.77	0.66
18:S:188:LYS:HD3	28:S:312:CLA:HAA2	1.76	0.66
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.76	0.66
2:B:503:THR:HG22	21:X:81:VAL:HG11	1.77	0.66
30:b:618:BCR:HC42	32:b:620:LMG:H362	1.77	0.66
38:r:607:CHL:HBB1	38:r:607:CHL:HHC	1.77	0.66
18:s:208:TYR:HA	38:s:606:CHL:H62	1.77	0.66
1:A:304:GLN:HG2	1:A:313:VAL:HG21	1.78	0.66
28:A:408:CLA:H122	32:A:411:LMG:H132	1.78	0.66
32:A:413:LMG:HC2	36:A:417:DGD:HD2	1.76	0.66
20:W:19:ASN:HD22	20:W:21:LEU:H	1.42	0.66
22:Y:199:ILE:HG13	38:Y:607:CHL:H122	1.78	0.66
22:Y:225:ALA:HA	41:Y:617:XAT:H22	1.78	0.66
28:Y:604:CLA:HBB1	28:Y:604:CLA:HMB3	1.77	0.66
2:b:458:PHE:HB3	28:b:604:CLA:HBC2	1.76	0.66
3:c:147:PHE:HA	28:c:512:CLA:HMC1	1.76	0.66
4:d:338:GLU:HB3	4:d:340:LEU:HG	1.76	0.66
28:C:505:CLA:HMB1	28:C:505:CLA:HBB1	1.78	0.66
4:D:190:HIS:HA	4:D:295:ARG:HD3	1.77	0.66
28:G:611:CLA:H142	28:G:612:CLA:H141	1.78	0.66
14:O:69:THR:OG1	14:O:70:PRO:HD3	1.95	0.66
17:R:100:GLY:HA3	17:R:202:ALA:HB1	1.78	0.66
28:a:407:CLA:HAA1	36:c:518:DGD:HAF2	1.77	0.66
17:r:112:THR:HA	17:r:115:TRP:HE3	1.60	0.66
28:A:405:CLA:H41	28:D:401:CLA:HAB	1.78	0.66
36:A:417:DGD:HE4	2:b:76:GLY:HA2	1.78	0.66
28:D:403:CLA:HBB1	28:D:403:CLA:HMB1	1.76	0.66
2:B:105:GLY:HA3	30:B:618:BCR:H402	1.78	0.66
28:C:508:CLA:H2	28:C:510:CLA:H11	1.76	0.66
28:C:509:CLA:HBB1	28:C:509:CLA:HMB1	1.78	0.66
28:N:602:CLA:H172	39:N:616:LUT:C31	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:624:LHG:H151	35:l:101:LHG:H292	1.78	0.66
7:g:156:TYR:HB3	28:g:610:CLA:CED	2.23	0.66
30:k:101:BCR:H343	23:z:20:LEU:HD21	1.78	0.66
38:n:609:CHL:HAA2	22:y:48:THR:HG21	1.77	0.66
38:r:605:CHL:H91	40:r:616:NEX:H14	1.78	0.66
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.78	0.66
1:a:131:TRP:HE1	3:c:446:GLY:HA2	1.61	0.66
28:y:303:CLA:HBA1	39:y:316:LUT:H382	1.78	0.66
2:B:161:LEU:HB2	32:B:624:LMG:O2	1.95	0.66
7:g:24:TYR:CD2	38:g:601:CHL:HAA1	2.30	0.66
15:p:90:LYS:HB3	16:q:2:ALA:HB1	1.78	0.66
17:r:214:VAL:HG21	28:r:612:CLA:HAC2	1.77	0.66
28:C:508:CLA:H91	28:C:510:CLA:H72	1.78	0.66
17:R:59:LYS:HE2	17:R:61:LEU:HD21	1.78	0.66
2:b:105:GLY:HA3	30:b:618:BCR:H402	1.78	0.66
17:r:13:LEU:HD11	17:r:20:SER:HB3	1.76	0.66
18:s:125:ASN:HA	18:s:130:PRO:CA	2.26	0.66
22:y:162:ASP:HA	39:y:315:LUT:H24	1.78	0.66
28:A:406:CLA:HAA2	32:D:408:LMG:H231	1.78	0.65
2:b:187:VAL:HG12	8:h:70:ILE:HG13	1.77	0.65
4:d:301:SER:HB2	13:m:1:MET:HG3	1.78	0.65
28:r:610:CLA:HAA1	28:r:611:CLA:OBD	1.96	0.65
3:C:177:PHE:HA	3:C:181:TYR:HD2	1.61	0.65
7:G:191:MET:HE2	39:G:616:LUT:H12	1.79	0.65
38:G:608:CHL:HMA3	38:G:608:CHL:H151	1.77	0.65
28:S:310:CLA:C5	39:S:315:LUT:H30	2.27	0.65
22:Y:110:LEU:HD11	28:Y:604:CLA:HAA2	1.77	0.65
30:a:410:BCR:H321	30:a:410:BCR:HC8	1.78	0.65
2:b:385:ARG:HB3	15:p:92:ALA:HB3	1.78	0.65
28:c:509:CLA:HBB1	28:c:509:CLA:HMB1	1.78	0.65
28:n:610:CLA:H93	39:n:615:LUT:H32	1.77	0.65
17:r:15:PHE:CD1	17:r:16:PRO:HD2	2.32	0.65
28:s:609:CLA:H41	28:s:611:CLA:HMA2	1.77	0.65
22:y:164:LEU:HD12	39:y:315:LUT:H222	1.76	0.65
3:C:117:LEU:HA	30:C:514:BCR:H10C	1.78	0.65
38:G:609:CHL:HBB1	38:G:609:CHL:HHC	1.76	0.65
28:G:613:CLA:H172	28:G:614:CLA:C1D	2.25	0.65
18:S:170:PHE:O	39:S:315:LUT:H24	1.96	0.65
1:a:228:THR:HA	17:r:58:ALA:HA	1.78	0.65
29:a:408:PHO:C2B	28:d:401:CLA:H2	2.25	0.65
17:r:230:HIS:CG	28:r:612:CLA:HAA2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:83:GLU:O	22:y:87:ARG:HG2	1.96	0.65
30:B:617:BCR:HC32	13:M:10:ALA:HB2	1.79	0.65
3:C:79:LYS:HD2	3:C:84:GLN:HG2	1.78	0.65
36:C:518:DGD:CDA	36:C:519:DGD:HBT2	2.26	0.65
8:H:71:SER:O	8:H:72:MET:C	2.39	0.65
17:R:163:ASN:HD22	28:R:613:CLA:HBC3	1.61	0.65
3:c:167:LEU:HB3	28:c:512:CLA:H2	1.77	0.65
4:d:135:ARG:HA	4:d:135:ARG:HE	1.61	0.65
7:g:69:SER:HB3	7:g:184:GLY:HA3	1.77	0.65
7:g:203:LYS:HB2	7:g:208:ASN:HD21	1.60	0.65
7:n:101:GLY:HA2	38:n:606:CHL:HAC2	1.78	0.65
16:q:91:ILE:HD13	16:q:147:ILE:HG23	1.78	0.65
1:A:28:LEU:HB2	31:A:414:SQD:H101	1.79	0.65
2:B:25:MET:HG2	30:B:617:BCR:H23C	1.78	0.65
28:G:610:CLA:H2	39:G:615:LUT:C38	2.26	0.65
31:a:414:SQD:H82	31:a:414:SQD:H2	1.79	0.65
18:s:105:CYS:HA	18:s:127:PHE:N	2.11	0.65
38:y:308:CHL:H152	40:y:318:NEX:H402	1.79	0.65
28:C:504:CLA:H42	36:C:518:DGD:HB52	1.78	0.65
33:D:406:PL9:H111	35:D:407:LHG:H111	1.78	0.65
1:a:200:LEU:HD23	36:c:518:DGD:HAW2	1.79	0.65
30:d:406:BCR:H21C	32:d:409:LMG:H352	1.77	0.65
28:g:610:CLA:C1	39:g:615:LUT:H26	2.26	0.65
1:A:103:ASP:HB2	14:O:79:MET:HE1	1.78	0.65
28:S:305:CLA:HMB3	28:S:305:CLA:HBB1	1.78	0.65
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.78	0.65
7:g:87:ARG:HH12	7:g:207:GLU:HA	1.62	0.65
1:A:240:GLY:HA3	19:T:30:PRO:HG2	1.79	0.65
3:C:473:ASN:ND2	19:T:26:PRO:HG3	2.11	0.65
7:G:118:LEU:HD13	38:G:605:CHL:HED2	1.78	0.65
22:Y:92:PHE:HE2	22:Y:113:LEU:HD23	1.61	0.65
30:h:101:BCR:HC8	30:h:101:BCR:H331	1.78	0.65
1:A:131:TRP:CH2	28:C:505:CLA:HAA2	2.32	0.65
15:P:94:PHE:CZ	16:Q:2:ALA:HA	2.32	0.65
28:c:506:CLA:H43	30:i:101:BCR:HC8	1.79	0.65
38:g:619:CHL:HHC	38:g:619:CHL:HBB1	1.78	0.65
12:l:13:LEU:HD22	13:m:25:ILE:HG13	1.79	0.65
7:n:33:PRO:HG2	7:n:36:LEU:HD22	1.79	0.65
17:r:59:LYS:HE2	17:r:61:LEU:HD21	1.79	0.65
17:r:156:GLY:HA2	28:r:608:CLA:HMB1	1.79	0.65
2:B:69:LEU:HD12	28:B:605:CLA:H3A	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ALA:CB	32:B:621:LMG:HC91	2.26	0.65
28:G:613:CLA:H91	28:G:614:CLA:HBC1	1.78	0.65
31:L:103:SQD:H332	30:T:101:BCR:H16C	1.79	0.65
15:P:152:LYS:HB3	15:P:157:TYR:CE1	2.32	0.65
17:R:76:LYS:HE3	17:R:84:THR:HB	1.79	0.65
30:B:619:BCR:HC32	35:B:623:LHG:HC82	1.78	0.64
7:G:164:LEU:H	7:G:164:LEU:HD12	1.62	0.64
7:N:22:VAL:HG13	38:N:601:CHL:HBC2	1.79	0.64
28:N:602:CLA:H202	39:N:616:LUT:H31	1.78	0.64
1:a:150:PRO:HB2	28:a:406:CLA:H92	1.78	0.64
30:d:406:BCR:H363	6:f:27:PHE:HB3	1.79	0.64
28:r:604:CLA:NB	40:r:616:NEX:H242	2.12	0.64
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.79	0.64
18:S:185:LEU:HB3	28:S:310:CLA:HMA2	1.77	0.64
2:b:257:TRP:CD1	36:b:625:DGD:HBN1	2.32	0.64
28:c:508:CLA:HBB1	28:c:508:CLA:HMB3	1.79	0.64
1:A:330:VAL:HA	4:D:353:LEU:HD22	1.78	0.64
30:B:617:BCR:HC41	13:M:9:ILE:HG23	1.80	0.64
30:D:405:BCR:H372	32:D:408:LMG:H301	1.79	0.64
38:N:606:CHL:HHC	38:N:606:CHL:HBB1	1.79	0.64
28:c:508:CLA:H203	28:c:508:CLA:H151	1.78	0.64
38:g:608:CHL:H202	40:g:617:NEX:H402	1.79	0.64
28:Y:613:CLA:H8	28:Y:614:CLA:HMD3	1.79	0.64
4:d:173:SER:HB2	4:d:178:ALA:HB1	1.78	0.64
28:y:304:CLA:H101	38:y:309:CHL:H8	1.80	0.64
1:A:283:ILE:HG13	29:A:407:PHO:HBC3	1.78	0.64
8:H:42:LEU:H	8:H:42:LEU:HD22	1.62	0.64
17:R:157:TYR:O	17:R:161:GLN:HG2	1.97	0.64
2:b:156:PHE:HB3	2:b:162:PHE:HB3	1.80	0.64
2:b:247:PHE:HB2	28:b:608:CLA:HBC1	1.79	0.64
3:c:206:PRO:HG3	3:c:239:TRP:CH2	2.32	0.64
22:y:81:PHE:CE2	22:y:85:LEU:HD11	2.33	0.64
3:C:81:MET:HG3	3:C:86:LEU:HD12	1.80	0.64
7:G:119:VAL:HA	38:G:605:CHL:C4D	2.27	0.64
1:a:302:PHE:HA	3:c:415:ASN:HD21	1.62	0.64
28:b:611:CLA:H61	28:b:613:CLA:HED3	1.79	0.64
3:c:81:MET:HG3	3:c:86:LEU:HD12	1.79	0.64
38:n:607:CHL:HBB1	38:n:607:CHL:HMB3	1.79	0.64
14:o:6:ARG:HG2	14:o:31:THR:HB	1.78	0.64
28:s:604:CLA:CHB	40:s:616:NEX:H383	2.28	0.64
31:A:414:SQD:H61	30:b:619:BCR:H371	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:47:LEU:HD22	15:P:61:VAL:HG23	1.78	0.64
15:P:118:ALA:HB1	15:P:125:GLN:HE22	1.62	0.64
3:c:54:VAL:HA	28:c:512:CLA:HED1	1.79	0.64
7:g:203:LYS:HB2	7:g:208:ASN:ND2	2.13	0.64
7:G:161:PHE:HA	38:G:608:CHL:C7	2.28	0.64
38:n:609:CHL:HHC	38:n:609:CHL:HBB1	1.78	0.64
1:A:217:SER:HB3	4:D:273:LEU:HD12	1.80	0.64
28:G:602:CLA:H101	39:G:616:LUT:H371	1.79	0.64
22:Y:203:LYS:HB3	22:Y:207:GLU:HG2	1.80	0.64
28:b:601:CLA:C1C	30:h:101:BCR:H19C	2.28	0.64
28:b:601:CLA:HBB2	30:h:101:BCR:H351	1.80	0.64
3:c:286:ALA:HB2	28:c:502:CLA:HMD2	1.80	0.64
28:g:614:CLA:HAA2	22:y:128:TRP:CZ2	2.33	0.64
17:r:150:ILE:HD13	38:r:605:CHL:HED2	1.80	0.64
18:s:23:LEU:HD12	18:s:184:ILE:HD11	1.80	0.64
18:s:98:PHE:HB3	18:s:103:ALA:HB3	1.78	0.64
28:C:513:CLA:H101	30:C:514:BCR:H372	1.80	0.64
15:P:147:ILE:HG12	15:P:160:LYS:HG3	1.80	0.64
28:R:603:CLA:NC	28:R:608:CLA:H102	2.13	0.64
38:Y:607:CHL:H112	38:Y:607:CHL:C4	2.28	0.64
28:b:611:CLA:HMB1	28:b:611:CLA:HBB1	1.80	0.64
2:B:86:THR:HG22	42:B:703:HOH:O	1.97	0.63
28:G:610:CLA:H122	39:G:615:LUT:C39	2.28	0.63
16:Q:126:PRO:O	16:Q:130:GLU:HG2	1.97	0.63
38:S:307:CHL:HHC	38:S:307:CHL:HBB1	1.79	0.63
1:a:106:LEU:HD11	30:a:410:BCR:H402	1.79	0.63
28:b:603:CLA:HBC3	28:b:610:CLA:H52	1.78	0.63
36:c:517:DGD:HD3	32:k:102:LMG:HC3	1.79	0.63
4:D:276:PRO:HB2	29:D:402:PHO:HBC1	1.80	0.63
38:N:609:CHL:HAA2	22:Y:48:THR:HG21	1.80	0.63
2:b:148:VAL:HG12	35:b:622:LHG:H341	1.78	0.63
17:r:101:ARG:HA	17:r:104:MET:HE3	1.80	0.63
22:y:121:ALA:HA	38:y:306:CHL:C1C	2.28	0.63
38:y:309:CHL:HHC	38:y:309:CHL:HBB1	1.80	0.63
1:A:229:GLU:HB2	17:R:55:GLN:HA	1.79	0.63
28:C:508:CLA:H2	28:C:510:CLA:C1	2.28	0.63
38:G:606:CHL:H43	40:G:617:NEX:H35	1.81	0.63
28:b:606:CLA:HMD2	35:b:622:LHG:HC5	1.80	0.63
28:b:607:CLA:HMC2	30:b:618:BCR:HC8	1.79	0.63
28:b:612:CLA:HMB1	28:b:612:CLA:HBB1	1.79	0.63
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:13:ILE:HG21	37:f:101:HEM:HAD2	1.79	0.63
22:y:122:GLN:HB2	38:y:306:CHL:CBB	2.28	0.63
23:z:23:VAL:HB	23:z:24:PRO:HD3	1.80	0.63
38:G:608:CHL:C4	39:G:615:LUT:H27	2.27	0.63
7:N:173:PHE:CZ	7:N:177:LYS:HE3	2.33	0.63
38:S:306:CHL:HBB2	38:S:307:CHL:CBB	2.28	0.63
30:b:617:BCR:H313	32:b:620:LMG:H111	1.79	0.63
3:C:473:ASN:C	3:C:473:ASN:HD22	2.07	0.63
7:G:104:ILE:HG21	7:G:124:ILE:HG13	1.81	0.63
20:W:19:ASN:HB3	20:W:22:LEU:HD23	1.79	0.63
23:Z:5:PHE:HA	23:Z:57:LEU:HD13	1.80	0.63
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.34	0.63
28:b:614:CLA:H2	28:b:614:CLA:ND	2.14	0.63
3:c:200:THR:HA	42:c:718:HOH:O	1.97	0.63
16:q:95:LYS:HG2	16:q:103:LEU:HD11	1.79	0.63
28:R:604:CLA:C1C	40:y:301:NEX:H222	2.29	0.63
2:b:283:GLU:HG3	2:b:287:ARG:HE	1.64	0.63
28:b:608:CLA:C1D	28:b:609:CLA:H72	2.27	0.63
28:c:504:CLA:HMB1	28:c:504:CLA:HBB1	1.80	0.63
28:c:505:CLA:HMB3	28:c:505:CLA:HBB1	1.81	0.63
38:s:606:CHL:HHC	38:s:606:CHL:HBB1	1.81	0.63
22:y:64:LEU:HD13	28:y:304:CLA:HBA1	1.81	0.63
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.80	0.63
3:c:144:PHE:CE1	28:c:513:CLA:HAA1	2.33	0.63
3:c:217:PRO:HG3	36:c:516:DGD:HA72	1.81	0.63
30:c:514:BCR:H281	35:c:520:LHG:H242	1.80	0.63
28:n:602:CLA:H92	28:n:603:CLA:HMA1	1.81	0.63
15:P:169:PHE:HE1	15:P:170:LYS:HE2	1.64	0.63
11:k:56:ALA:HB2	30:k:101:BCR:H292	1.81	0.63
3:C:184:GLY:HA3	3:C:198:LYS:HA	1.80	0.62
3:C:425:TRP:CZ2	28:C:504:CLA:HBA1	2.34	0.62
16:Q:17:LEU:HD13	16:Q:21:LEU:HD22	1.81	0.62
28:b:615:CLA:H121	28:b:616:CLA:H91	1.81	0.62
17:r:87:PHE:HA	17:r:92:PHE:CZ	2.34	0.62
28:r:613:CLA:H51	28:r:613:CLA:C4B	2.29	0.62
1:A:276:ALA:HA	4:D:213:ALA:HA	1.81	0.62
28:R:609:CLA:C2	39:R:614:LUT:H28	2.28	0.62
22:Y:81:PHE:CE2	22:Y:85:LEU:HD11	2.34	0.62
2:b:451:PHE:CZ	28:b:604:CLA:HED2	2.34	0.62
7:g:218:ASN:O	7:g:223:SER:HB3	1.98	0.62
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:411:LMG:HC91	32:A:411:LMG:H121	1.81	0.62
18:S:57:TYR:HB2	28:S:303:CLA:HMD1	1.80	0.62
38:S:306:CHL:HBB1	39:S:316:LUT:H161	1.80	0.62
2:b:497:LYS:HA	4:d:25:ARG:HA	1.80	0.62
38:s:601:CHL:HHC	38:s:601:CHL:HBB1	1.81	0.62
28:s:609:CLA:O2A	39:s:614:LUT:H26	1.99	0.62
2:B:496:GLN:HB2	2:B:503:THR:HB	1.82	0.62
3:C:363:ALA:O	3:C:367:GLU:HG2	2.00	0.62
18:S:99:ASN:ND2	18:S:109:ALA:HB2	2.13	0.62
18:S:218:PHE:HB2	39:S:315:LUT:H22	1.81	0.62
3:c:391:ARG:HD2	3:c:395:TYR:CE2	2.35	0.62
28:c:510:CLA:H172	28:c:510:CLA:H121	1.82	0.62
28:g:611:CLA:H2	28:g:612:CLA:CGD	2.28	0.62
14:o:157:LEU:HD21	14:o:166:THR:HG23	1.82	0.62
28:s:604:CLA:HBA1	38:s:605:CHL:C1D	2.30	0.62
28:y:304:CLA:CAD	38:y:309:CHL:H2	2.29	0.62
23:z:26:VAL:HG12	23:z:33:TRP:HE3	1.64	0.62
28:B:609:CLA:C1B	30:H:101:BCR:HC21	2.30	0.62
3:C:123:ALA:HA	30:C:516:BCR:H16C	1.82	0.62
18:S:118:LEU:HD13	18:S:135:LEU:HA	1.80	0.62
28:g:610:CLA:H2	39:g:615:LUT:H28	1.81	0.62
32:k:102:LMG:H292	32:k:102:LMG:H152	1.81	0.62
28:y:304:CLA:H121	38:y:309:CHL:C9	2.28	0.62
28:y:313:CLA:H172	28:y:314:CLA:C4D	2.30	0.62
30:C:515:BCR:H332	9:I:20:ILE:HG23	1.82	0.62
28:N:602:CLA:H52	28:N:603:CLA:HBA1	1.81	0.62
3:c:284:PHE:HB3	36:c:516:DGD:HB82	1.81	0.62
7:g:179:LYS:HD3	28:g:612:CLA:HAA2	1.80	0.62
38:g:601:CHL:C1D	35:g:618:LHG:HC82	2.30	0.62
11:k:40:MET:HG2	30:k:101:BCR:H313	1.82	0.62
18:s:70:ASP:O	18:s:73:LYS:HG2	1.99	0.62
1:A:228:THR:HA	17:R:58:ALA:HA	1.81	0.62
2:B:383:PHE:CZ	14:O:167:GLY:HA2	2.34	0.62
28:C:508:CLA:NC	28:C:510:CLA:H51	2.14	0.62
4:D:57:THR:HG21	5:E:50:PRO:HD3	1.82	0.62
22:Y:212:HIS:CG	28:Y:613:CLA:HAA2	2.35	0.62
31:a:411:SQD:H5	4:d:233:PHE:CB	2.30	0.62
2:b:149:ALA:HA	35:b:622:LHG:H332	1.81	0.62
2:b:415:ALA:O	2:b:419:LYS:HE3	2.00	0.62
2:b:503:THR:HG22	21:x:81:VAL:HG11	1.80	0.62
7:n:156:TYR:HA	28:n:610:CLA:O1D	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:91:GLN:HE21	16:q:5:ILE:HG13	1.64	0.62
18:s:188:LYS:HD3	28:s:611:CLA:HAA2	1.81	0.62
28:A:406:CLA:CHA	28:A:406:CLA:HBA1	2.29	0.62
30:A:409:BCR:H19C	36:A:417:DGD:HB61	1.82	0.62
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.81	0.62
38:G:607:CHL:HBB1	38:G:607:CHL:HHC	1.80	0.62
8:H:24:LYS:N	8:H:25:PRO:HD2	2.13	0.62
18:S:107:PRO:HB2	18:S:117:LEU:HD11	1.82	0.62
4:d:332:THR:HG22	42:d:501:HOH:O	1.99	0.62
28:B:606:CLA:CAD	35:B:623:LHG:HC62	2.29	0.62
18:S:51:GLY:C	18:S:53:VAL:H	2.08	0.62
38:Y:609:CHL:HHC	38:Y:609:CHL:HBB1	1.81	0.62
17:r:100:GLY:HA3	17:r:202:ALA:HB1	1.81	0.62
32:A:413:LMG:HC72	9:I:1:MET:HE2	1.82	0.62
28:B:603:CLA:HMB1	28:B:603:CLA:HBB1	1.82	0.62
36:C:518:DGD:HAT1	36:C:519:DGD:CAB	2.29	0.62
28:D:404:CLA:H122	21:X:62:GLY:HA3	1.79	0.62
4:d:190:HIS:HA	4:d:295:ARG:HD2	1.80	0.62
28:g:602:CLA:C5	39:g:616:LUT:H30	2.29	0.62
3:C:362:ARG:HD2	14:O:18:LEU:HD21	1.81	0.61
4:D:56:VAL:O	4:D:67:SER:HB3	2.00	0.61
38:G:605:CHL:HBD	38:G:605:CHL:HAA2	1.82	0.61
28:G:610:CLA:HBB2	39:G:615:LUT:H34	1.81	0.61
38:R:606:CHL:HBB2	28:R:608:CLA:HBC3	1.82	0.61
28:S:303:CLA:H92	28:S:304:CLA:HHB	1.82	0.61
38:S:308:CHL:HBA2	28:S:310:CLA:HMD2	1.81	0.61
3:c:318:LEU:HG	3:c:328:VAL:HG11	1.82	0.61
28:r:603:CLA:CBC	28:r:613:CLA:H18	2.30	0.61
7:N:212:HIS:CG	28:N:613:CLA:HAA2	2.35	0.61
28:n:610:CLA:CBA	39:n:615:LUT:H382	2.30	0.61
38:r:605:CHL:H101	40:r:616:NEX:H35	1.81	0.61
28:B:604:CLA:H192	35:B:623:LHG:H332	1.82	0.61
7:N:24:TYR:N	7:N:44:TYR:HB3	2.16	0.61
28:a:406:CLA:H171	28:d:401:CLA:H151	1.82	0.61
7:n:203:LYS:HB2	7:n:208:ASN:HD21	1.66	0.61
14:o:179:ARG:HA	14:o:182:GLU:HG3	1.83	0.61
23:z:57:LEU:HD23	23:z:60:LEU:HD12	1.80	0.61
1:A:77:ILE:HD13	12:L:30:VAL:HG13	1.82	0.61
8:H:50:PHE:CB	30:H:101:BCR:H12C	2.30	0.61
28:N:602:CLA:H18	39:N:616:LUT:H402	1.81	0.61
22:Y:86:SER:HA	22:Y:90:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:411:SQD:H262	35:a:415:LHG:H112	1.82	0.61
3:C:147:PHE:HA	28:C:512:CLA:HMC1	1.81	0.61
1:a:39:PRO:HG3	30:a:410:BCR:HC8	1.83	0.61
2:b:495:PHE:HA	2:b:504:LYS:HB2	1.82	0.61
7:g:134:LEU:HD13	38:g:606:CHL:H12	1.81	0.61
10:j:8:ILE:HG23	10:j:12:ILE:HD11	1.81	0.61
2:B:159:THR:HB	32:B:624:LMG:HC2	1.82	0.61
22:Y:148:LEU:HD13	38:Y:608:CHL:H102	1.82	0.61
28:R:608:CLA:HBB1	28:R:608:CLA:HMB3	1.83	0.61
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.36	0.61
28:c:501:CLA:C1B	28:c:501:CLA:H2	2.31	0.61
7:n:220:ASN:ND2	7:n:222:TRP:HD1	1.99	0.61
15:p:68:LYS:HB3	15:p:73:ASP:HB2	1.82	0.61
2:B:161:LEU:HD11	35:B:622:LHG:HC41	1.82	0.61
7:G:81:PHE:HB3	7:G:82:PRO:HD3	1.82	0.61
15:P:168:TRP:CE2	15:P:173:ARG:HG3	2.35	0.61
28:S:311:CLA:C1C	28:S:311:CLA:H101	2.31	0.61
21:X:47:VAL:HA	21:X:51:LEU:HD23	1.82	0.61
1:a:240:GLY:HA3	19:t:30:PRO:CG	2.30	0.61
2:B:51:VAL:HG23	14:o:67:LYS:HG3	1.83	0.61
28:C:511:CLA:C10	30:C:516:BCR:H23C	2.29	0.61
36:C:519:DGD:HA32	32:D:408:LMG:H121	1.82	0.61
30:D:405:BCR:H19C	6:F:24:THR:HG23	1.82	0.61
7:G:105:PHE:CZ	7:N:225:ALA:HB3	2.36	0.61
22:Y:199:ILE:HG12	38:Y:607:CHL:H142	1.81	0.61
28:a:409:CLA:H12	32:w:101:LMG:H112	1.82	0.61
2:b:233:ASN:O	2:b:236:THR:HG22	2.01	0.61
18:s:86:MET:SD	28:s:609:CLA:HAB	2.41	0.61
28:G:611:CLA:H92	28:G:612:CLA:H111	1.83	0.61
9:I:14:PHE:CZ	9:I:18:LEU:HD11	2.36	0.61
28:N:610:CLA:H12	28:N:610:CLA:H3A	1.81	0.61
15:P:114:LEU:HD11	15:P:132:LEU:HB2	1.83	0.61
38:R:605:CHL:HBB2	38:R:606:CHL:CBB	2.29	0.61
18:S:230:LEU:HD13	28:S:313:CLA:HMD2	1.82	0.61
21:X:82:LYS:O	21:X:83:ARG:C	2.44	0.61
2:b:62:VAL:HB	28:b:605:CLA:HED3	1.82	0.61
18:s:21:GLU:O	18:s:25:LYS:HG3	2.00	0.61
18:s:150:GLU:O	18:s:154:ILE:HG13	2.00	0.61
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.82	0.60
2:B:137:LYS:HD2	8:H:26:LEU:O	2.01	0.60
2:B:333:GLY:O	2:B:439:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:501:CLA:H203	28:C:507:CLA:H152	1.83	0.60
28:C:504:CLA:HMB1	28:C:504:CLA:HBB1	1.83	0.60
28:S:312:CLA:CMB	39:S:315:LUT:H31	2.31	0.60
22:Y:116:PRO:O	22:Y:120:HIS:HB2	2.01	0.60
28:b:607:CLA:H101	32:b:620:LMG:H361	1.83	0.60
4:d:28:PHE:CD2	4:d:29:VAL:HG23	2.35	0.60
7:g:127:ILE:HG12	38:g:605:CHL:HAC1	1.83	0.60
16:q:43:ALA:HB3	16:q:46:GLU:HG2	1.82	0.60
3:C:338:GLY:HA2	14:O:111:TYR:OH	2.01	0.60
11:K:46:LEU:HB3	30:K:101:BCR:C16	2.31	0.60
28:R:609:CLA:H41	28:R:611:CLA:HMA2	1.82	0.60
18:S:49:LEU:HD21	18:S:58:GLY:HA2	1.83	0.60
28:S:303:CLA:HAC2	35:S:317:LHG:H262	1.83	0.60
28:b:603:CLA:H152	8:h:50:PHE:HE2	1.65	0.60
28:d:404:CLA:HBB1	28:d:404:CLA:HMB1	1.83	0.60
40:g:617:NEX:C28	40:g:617:NEX:H381	2.31	0.60
18:s:77:TYR:CE1	28:s:603:CLA:HBD	2.36	0.60
28:A:408:CLA:H143	32:A:411:LMG:H122	1.83	0.60
28:B:607:CLA:H2	32:B:621:LMG:H162	1.83	0.60
38:G:601:CHL:H92	22:Y:132:VAL:HG22	1.84	0.60
15:P:86:TYR:HA	15:P:90:LYS:HE3	1.82	0.60
28:S:303:CLA:HAC2	35:S:317:LHG:C26	2.31	0.60
28:S:303:CLA:H142	39:S:316:LUT:H371	1.84	0.60
28:Y:613:CLA:H172	28:Y:614:CLA:C4D	2.31	0.60
28:b:604:CLA:C4D	28:b:612:CLA:H151	2.32	0.60
4:d:162:PRO:HB3	4:d:171:ALA:HB2	1.82	0.60
14:o:40:SER:HB3	14:o:209:PRO:HG3	1.83	0.60
22:y:163:PRO:HB2	40:y:301:NEX:O3	2.01	0.60
30:B:617:BCR:HC21	32:B:621:LMG:H291	1.83	0.60
3:C:164:HIS:HA	3:C:167:LEU:HD12	1.84	0.60
23:Z:57:LEU:O	23:Z:61:ILE:HG23	2.00	0.60
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.83	0.60
36:a:401:DGD:HB81	30:a:410:BCR:H17C	1.84	0.60
32:d:409:LMG:H171	32:d:409:LMG:H312	1.82	0.60
28:n:603:CLA:H191	38:n:607:CHL:H13	1.82	0.60
17:r:129:LEU:HD22	38:r:606:CHL:HMD3	1.82	0.60
18:s:94:ILE:HB	18:s:95:PRO:HD3	1.83	0.60
24:u:27:ARG:O	24:u:28:ASN:C	2.43	0.60
2:B:347:ARG:HG2	2:B:353:GLU:HG2	1.84	0.60
2:B:462:PHE:HA	28:B:611:CLA:HMC2	1.84	0.60
28:C:501:CLA:H151	28:C:507:CLA:H101	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:601:CHL:H122	35:G:618:LHG:H211	1.82	0.60
28:N:604:CLA:HBA1	40:N:617:NEX:H241	1.82	0.60
28:R:604:CLA:HBA1	38:R:605:CHL:C1D	2.31	0.60
28:b:606:CLA:O1A	28:b:606:CLA:H3A	2.01	0.60
38:g:606:CHL:HBB2	38:g:607:CHL:CBB	2.31	0.60
30:k:101:BCR:H332	23:z:16:SER:CB	2.30	0.60
16:q:17:LEU:HD12	16:q:22:ASN:HA	1.83	0.60
28:r:612:CLA:CAB	28:r:612:CLA:H101	2.31	0.60
18:s:48:TYR:CD1	18:s:49:LEU:HD13	2.36	0.60
2:B:3:LEU:HD22	2:B:7:ARG:HB2	1.84	0.60
2:B:247:PHE:HB2	28:B:608:CLA:HBC1	1.84	0.60
35:B:625:LHG:H132	35:L:102:LHG:H281	1.82	0.60
4:D:15:LEU:HD11	21:X:73:ILE:HG23	1.82	0.60
7:g:226:THR:HB	38:g:619:CHL:HBD	1.84	0.60
18:S:49:LEU:O	18:S:49:LEU:HD22	2.02	0.60
1:a:229:GLU:HB2	17:r:55:GLN:HA	1.84	0.60
3:c:284:PHE:CZ	36:c:516:DGD:HBW2	2.37	0.60
7:g:46:TRP:O	39:g:616:LUT:H24	2.01	0.60
3:C:171:GLY:HA3	28:C:512:CLA:H41	1.82	0.60
3:C:332:GLN:HE21	3:C:336:GLY:HA2	1.66	0.60
7:G:179:LYS:HA	28:G:611:CLA:O1D	2.02	0.60
7:N:86:SER:HA	7:N:90:VAL:O	2.01	0.60
16:Q:53:GLU:HA	16:Q:56:LYS:HD3	1.84	0.60
38:S:306:CHL:CBB	39:S:316:LUT:H161	2.31	0.60
11:k:44:PRO:HA	11:k:47:PHE:HD2	1.67	0.60
28:n:612:CLA:HHC	28:n:612:CLA:CBB	2.29	0.60
17:r:126:LYS:HE2	38:r:606:CHL:HED2	1.84	0.60
17:r:157:TYR:O	17:r:161:GLN:HG2	2.02	0.60
18:s:154:ILE:HG12	28:s:608:CLA:HMA2	1.84	0.60
19:t:18:PHE:CD2	30:t:101:BCR:HC7	2.36	0.60
1:A:54:ALA:HB2	1:A:72:LEU:HD12	1.84	0.60
7:G:195:PHE:HB3	38:G:607:CHL:H91	1.82	0.60
7:N:141:TYR:HE2	40:N:617:NEX:H202	1.65	0.60
16:Q:89:LYS:O	16:Q:92:ILE:HG13	2.02	0.60
38:g:605:CHL:HHD	38:g:606:CHL:OBD	2.02	0.60
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.84	0.60
28:B:608:CLA:H13	28:B:609:CLA:H192	1.84	0.60
7:N:46:TRP:CE2	38:N:601:CHL:HBA2	2.37	0.60
7:N:116:PRO:O	7:N:120:HIS:HB2	2.02	0.60
7:g:77:LEU:HD22	28:g:612:CLA:HBB2	1.84	0.60
38:g:601:CHL:H71	38:g:601:CHL:H121	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:z:26:VAL:HG13	23:z:36:ASN:HB2	1.84	0.60
28:A:406:CLA:HMA3	32:D:408:LMG:H242	1.84	0.59
4:D:21:ASP:HB3	21:X:81:VAL:CG2	2.32	0.59
18:S:48:TYR:CD2	18:S:49:LEU:HD12	2.37	0.59
18:S:49:LEU:HD13	18:S:49:LEU:H	1.67	0.59
18:S:77:TYR:CE1	28:S:304:CLA:HBD	2.36	0.59
5:e:18:ARG:O	5:e:21:ILE:HG22	2.01	0.59
28:g:604:CLA:HMA3	38:g:606:CHL:C3C	2.31	0.59
14:o:205:THR:HG23	14:o:216:GLY:HA2	1.82	0.59
18:s:65:SER:HB2	18:s:71:PHE:HA	1.84	0.59
18:s:118:LEU:HD23	18:s:135:LEU:HA	1.84	0.59
28:C:501:CLA:CAD	28:C:503:CLA:H12	2.32	0.59
7:G:203:LYS:HG3	7:G:208:ASN:HD21	1.67	0.59
17:R:37:PHE:CD2	41:R:615:XAT:H221	2.36	0.59
18:S:70:ASP:HA	18:S:73:LYS:HG2	1.82	0.59
22:Y:163:PRO:HD2	39:Y:615:LUT:H23	1.84	0.59
1:a:81:ALA:HB2	1:a:175:GLY:HA3	1.84	0.59
2:b:495:PHE:CD2	2:b:501:PRO:HA	2.38	0.59
28:r:604:CLA:HMA3	38:r:605:CHL:C3C	2.32	0.59
1:A:52:PHE:HB3	33:D:406:PL9:H503	1.83	0.59
1:A:140:ARG:NH2	35:A:416:LHG:HC41	2.17	0.59
28:D:404:CLA:H72	21:X:58:ILE:HG23	1.83	0.59
7:G:176:LEU:HG	28:G:610:CLA:HHB	1.83	0.59
7:N:44:TYR:HB2	28:N:602:CLA:HMD1	1.84	0.59
30:d:406:BCR:H391	10:j:25:ILE:HD11	1.84	0.59
7:n:163:PRO:HD2	39:n:615:LUT:H24	1.84	0.59
16:q:61:ALA:HB1	16:q:73:LEU:HD12	1.82	0.59
18:s:110:VAL:HG11	18:s:113:LYS:HE2	1.82	0.59
28:C:508:CLA:H72	11:K:48:PHE:HZ	1.67	0.59
30:D:405:BCR:H14C	6:F:27:PHE:CE1	2.37	0.59
7:N:87:ARG:HD2	7:N:206:LEU:HD23	1.84	0.59
16:Q:69:ALA:HB1	16:Q:72:PHE:CD1	2.37	0.59
18:S:129:LYS:HD3	18:S:130:PRO:HD2	1.84	0.59
28:S:303:CLA:H2	39:S:316:LUT:H28	1.82	0.59
28:S:310:CLA:H71	28:S:312:CLA:HHB	1.82	0.59
1:a:274:PHE:HA	31:a:411:SQD:H122	1.84	0.59
28:a:409:CLA:HAC1	32:a:413:LMG:H391	1.83	0.59
9:i:14:PHE:CZ	9:i:18:LEU:HD11	2.37	0.59
28:n:603:CLA:HED1	38:n:609:CHL:H92	1.84	0.59
18:s:194:ARG:HB2	35:s:617:LHG:H252	1.84	0.59
31:A:414:SQD:H291	30:b:618:BCR:H291	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:212:HIS:CG	28:G:613:CLA:HAA2	2.37	0.59
28:S:313:CLA:H93	28:S:314:CLA:HMD3	1.84	0.59
2:b:105:GLY:CA	30:b:618:BCR:H23C	2.31	0.59
3:c:154:ARG:NH1	20:w:49:GLU:HG3	2.17	0.59
4:d:56:VAL:O	4:d:67:SER:HB3	2.02	0.59
5:e:35:TRP:HH2	6:f:36:PHE:CE2	2.18	0.59
7:g:110:LEU:HB3	7:g:121:ALA:HB3	1.83	0.59
8:h:47:MET:HG2	30:h:101:BCR:H312	1.84	0.59
16:q:85:ARG:HG2	16:q:111:PHE:CE1	2.37	0.59
17:r:140:LEU:HB3	17:r:142:PHE:CD2	2.37	0.59
17:r:174:PRO:HB3	38:r:607:CHL:HBC2	1.84	0.59
2:B:230:ARG:HD2	2:B:230:ARG:N	2.18	0.59
2:B:454:GLY:HA2	32:B:621:LMG:H212	1.84	0.59
30:C:515:BCR:H321	30:C:515:BCR:HC8	1.83	0.59
4:D:21:ASP:HB3	21:X:81:VAL:HG23	1.83	0.59
7:G:121:ALA:HA	38:G:605:CHL:C1C	2.31	0.59
3:c:372:PRO:HA	14:o:17:TYR:HA	1.83	0.59
28:g:603:CLA:H121	28:g:603:CLA:H91	1.85	0.59
38:r:606:CHL:HBB1	38:r:606:CHL:HHC	1.84	0.59
18:s:80:ILE:HG13	28:s:608:CLA:O1D	2.02	0.59
2:B:105:GLY:CA	30:B:618:BCR:H23C	2.32	0.59
2:B:233:ASN:O	2:B:236:THR:HG22	2.02	0.59
3:C:122:SER:OG	30:C:516:BCR:H14C	2.03	0.59
38:G:601:CHL:H2	38:Y:609:CHL:C1B	2.32	0.59
28:G:604:CLA:HBB1	28:G:604:CLA:HMB3	1.83	0.59
16:Q:20:THR:CG2	42:Q:226:HOH:O	2.50	0.59
28:c:504:CLA:C2D	36:c:517:DGD:HB21	2.32	0.59
28:c:509:CLA:H203	28:c:512:CLA:HAC1	1.85	0.59
4:d:114:PHE:HZ	30:d:406:BCR:H323	1.67	0.59
38:n:607:CHL:H172	38:n:609:CHL:H52	1.84	0.59
15:p:91:GLN:HB2	16:q:3:ILE:HB	1.85	0.59
23:z:12:LEU:HA	23:z:50:LEU:HD23	1.83	0.59
29:A:407:PHO:H42	35:D:407:LHG:H361	1.85	0.59
31:L:103:SQD:H331	30:T:101:BCR:H362	1.84	0.59
15:P:80:PHE:HE1	15:P:156:LEU:HD11	1.67	0.59
1:a:257:ARG:HD3	2:b:498:LEU:HD11	1.85	0.59
11:k:39:PHE:CD1	32:k:102:LMG:H162	2.37	0.59
28:r:609:CLA:H151	39:r:614:LUT:C39	2.32	0.59
28:B:609:CLA:CHC	30:H:101:BCR:HC8	2.33	0.59
28:C:508:CLA:CAB	28:C:510:CLA:HMA3	2.33	0.59
4:D:315:PHE:HA	4:D:318:LYS:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N:612:CLA:HMB2	39:N:615:LUT:C33	2.33	0.59
15:P:51:ASP:HB3	15:P:54:ASP:O	2.02	0.59
18:S:99:ASN:HA	18:S:103:ALA:O	2.02	0.59
18:S:196:ALA:HB2	39:S:315:LUT:H202	1.85	0.59
4:d:104:ARG:HH21	5:e:77:ASP:HA	1.67	0.59
7:n:24:TYR:HB3	7:n:44:TYR:HB3	1.83	0.59
17:r:178:PHE:HB3	38:r:607:CHL:H122	1.84	0.59
29:A:407:PHO:H51	31:A:414:SQD:H211	1.84	0.59
36:B:626:DGD:HB62	36:B:626:DGD:HBT1	1.84	0.59
1:a:32:TRP:O	1:a:35:VAL:HG22	2.02	0.59
1:a:333:GLU:HB3	1:a:336:ALA:HB3	1.85	0.59
2:b:300:GLU:O	2:b:304:LYS:HG2	2.02	0.59
28:b:601:CLA:H102	30:h:101:BCR:H403	1.84	0.59
3:c:338:GLY:HA2	14:o:111:TYR:OH	2.03	0.59
28:c:511:CLA:H152	23:z:20:LEU:HD13	1.83	0.59
7:g:121:ALA:HA	38:g:605:CHL:CHC	2.33	0.59
10:j:11:TRP:HB2	11:k:56:ALA:HB1	1.84	0.59
11:k:36:ILE:O	11:k:40:MET:HG3	2.02	0.59
11:k:61:ARG:HB3	42:k:201:HOH:O	2.02	0.59
17:r:15:PHE:CE1	28:r:601:CLA:H2	2.38	0.59
7:G:147:PRO:HG3	40:G:617:NEX:H183	1.85	0.58
22:Y:173:PHE:CZ	28:Y:610:CLA:HED3	2.37	0.58
28:a:406:CLA:H141	28:d:401:CLA:H143	1.85	0.58
2:b:151:PHE:CZ	32:b:623:LMG:H381	2.37	0.58
35:b:624:LHG:H141	35:l:101:LHG:H272	1.85	0.58
7:g:135:MET:HA	7:g:138:VAL:HG22	1.85	0.58
11:k:38:ASP:HB3	32:k:102:LMG:H121	1.85	0.58
7:n:73:MET:SD	28:n:610:CLA:HAB	2.43	0.58
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.38	0.58
3:C:167:LEU:HB3	28:C:512:CLA:H2	1.84	0.58
7:G:85:LEU:HB2	7:G:92:PHE:CE1	2.38	0.58
30:T:101:BCR:C37	42:T:206:HOH:O	2.49	0.58
2:b:487:ASP:O	2:b:490:VAL:HG22	2.03	0.58
3:c:135:LEU:HD21	23:z:33:TRP:CG	2.39	0.58
38:g:607:CHL:HBB1	38:g:607:CHL:HHC	1.83	0.58
38:r:607:CHL:HBA1	28:r:609:CLA:H203	1.83	0.58
18:s:200:MET:HG3	18:s:204:PHE:CE2	2.37	0.58
28:y:310:CLA:H62	28:y:312:CLA:HMA2	1.85	0.58
3:C:97:TRP:NE1	32:C:522:LMG:H141	2.19	0.58
36:C:518:DGD:HAH1	36:C:519:DGD:HBT2	1.85	0.58
8:H:32:LYS:HB2	17:R:69:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:102:SER:HB3	42:N:701:HOH:O	2.03	0.58
38:N:608:CHL:H111	38:N:608:CHL:CHB	2.32	0.58
38:N:609:CHL:HHC	38:N:609:CHL:HBB1	1.86	0.58
18:S:104:ASN:HB2	18:S:128:GLY:HA2	1.83	0.58
18:S:125:ASN:ND2	18:S:130:PRO:HA	2.17	0.58
18:S:167:GLY:CA	28:S:310:CLA:HED3	2.32	0.58
28:c:510:CLA:H102	28:c:510:CLA:HED1	1.84	0.58
4:d:108:LEU:HD23	5:e:66:ILE:HD13	1.86	0.58
30:d:406:BCR:H392	32:d:409:LMG:H141	1.85	0.58
7:n:33:PRO:HB2	7:n:36:LEU:HB2	1.85	0.58
14:o:138:LYS:HE2	14:o:138:LYS:HA	1.85	0.58
17:r:163:ASN:HD22	28:r:613:CLA:HBC3	1.68	0.58
2:B:13:LEU:HA	28:B:612:CLA:HAC2	1.86	0.58
2:B:75:TRP:CZ2	36:a:401:DGD:HG11	2.38	0.58
3:C:167:LEU:HB3	28:C:512:CLA:C2	2.34	0.58
32:C:520:LMG:H121	11:K:38:ASP:HB3	1.84	0.58
14:O:5:LYS:HD3	14:O:6:ARG:N	2.18	0.58
38:R:606:CHL:HBB2	28:R:608:CLA:CBC	2.32	0.58
18:S:46:PRO:HB3	18:S:48:TYR:CE1	2.39	0.58
3:c:308:GLU:HA	3:c:361:LEU:CD2	2.34	0.58
4:d:89:SER:HA	8:h:62:ASN:HD21	1.67	0.58
7:n:121:ALA:HA	38:n:605:CHL:C1C	2.34	0.58
18:s:61:PRO:HD2	39:s:615:LUT:H23	1.85	0.58
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.39	0.58
7:G:61:ASN:HA	7:G:64:LEU:HD12	1.85	0.58
16:Q:62:LYS:HB2	16:Q:133:TYR:CZ	2.38	0.58
38:R:605:CHL:HBC2	38:R:606:CHL:HBC3	1.84	0.58
38:R:606:CHL:HBD	38:R:606:CHL:HAA2	1.85	0.58
22:Y:81:PHE:HB3	22:Y:82:PRO:HD3	1.84	0.58
24:U:85:ALA:HB3	24:U:86:PRO:HD3	1.84	0.58
7:g:139:GLU:HG3	38:g:609:CHL:C4B	2.33	0.58
28:n:611:CLA:H62	28:n:612:CLA:C3D	2.34	0.58
18:s:34:PHE:HD2	38:s:601:CHL:HAA1	1.68	0.58
35:A:416:LHG:HC42	4:D:233:PHE:CE2	2.39	0.58
28:C:513:CLA:H71	35:S:301:LHG:H101	1.86	0.58
4:D:127:MET:HE3	4:D:144:ALA:O	2.04	0.58
7:G:138:VAL:HA	7:G:141:TYR:CD2	2.39	0.58
1:a:42:LEU:CB	30:a:410:BCR:H353	2.25	0.58
1:a:131:TRP:CH2	28:c:505:CLA:HAA2	2.38	0.58
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.86	0.58
28:g:603:CLA:NA	38:g:609:CHL:H102	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:156:ASN:ND2	18:s:160:LEU:HB2	2.19	0.58
22:y:23:LYS:HB3	22:y:29:SER:OG	2.04	0.58
22:y:110:LEU:HD21	28:y:305:CLA:HAA1	1.84	0.58
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.86	0.58
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.38	0.58
2:B:334:ASP:HA	14:O:176:ALA:HB1	1.84	0.58
28:B:611:CLA:C3B	28:B:613:CLA:HMA2	2.33	0.58
36:B:626:DGD:HBN2	4:D:164:GLY:HA2	1.85	0.58
28:N:613:CLA:H12	28:N:614:CLA:HED2	1.84	0.58
14:O:205:THR:HG23	14:O:216:GLY:HA2	1.84	0.58
28:Y:603:CLA:C3B	38:Y:609:CHL:H151	2.34	0.58
1:a:278:TRP:HA	31:a:411:SQD:H172	1.84	0.58
2:b:366:PHE:HB3	2:b:425:GLN:NE2	2.18	0.58
42:c:602:HOH:O	20:w:53:SER:HB3	2.04	0.58
35:d:408:LHG:H311	19:t:21:ILE:HD11	1.85	0.58
11:k:42:VAL:HG11	32:k:102:LMG:H172	1.84	0.58
28:s:603:CLA:HED2	28:s:603:CLA:H2A	1.86	0.58
1:A:74:GLY:HA2	13:M:1:MET:HE1	1.84	0.58
28:B:613:CLA:HAC1	30:B:618:BCR:H353	1.84	0.58
37:E:101:HEM:HAC	6:F:21:ALA:HB1	1.84	0.58
13:M:31:SER:OG	13:m:28:LYS:HB2	2.03	0.58
17:R:83:TYR:HB2	28:R:613:CLA:HED2	1.85	0.58
18:S:182:ALA:HB1	18:S:186:LYS:HZ3	1.69	0.58
22:Y:194:PHE:CE1	39:Y:615:LUT:H41	2.39	0.58
22:Y:203:LYS:HB2	22:Y:208:ASN:HD21	1.69	0.58
38:g:608:CHL:HBD	38:g:608:CHL:HAA1	1.86	0.58
7:n:87:ARG:HH12	7:n:207:GLU:HA	1.69	0.58
14:o:9:PHE:O	14:o:13:GLN:HG2	2.04	0.58
2:B:149:ALA:HB2	28:B:604:CLA:H172	1.86	0.58
28:C:506:CLA:H13	35:W:101:LHG:H382	1.85	0.58
35:D:407:LHG:H192	19:T:17:ILE:HD11	1.85	0.58
7:N:52:SER:HB3	7:N:58:PHE:CD1	2.39	0.58
16:Q:120:ALA:HB2	16:Q:132:TYR:CD2	2.39	0.58
22:Y:100:ALA:O	22:Y:103:GLN:HG2	2.04	0.58
32:a:413:LMG:H111	9:i:4:LEU:HD13	1.86	0.58
28:b:608:CLA:HMC1	36:b:625:DGD:HAF2	1.85	0.58
28:r:603:CLA:HBC3	28:r:613:CLA:H18	1.85	0.58
28:s:610:CLA:H71	28:s:610:CLA:C1C	2.34	0.58
3:C:390:ARG:HD2	16:Q:40:GLN:HE21	1.69	0.58
28:C:505:CLA:HMD1	28:C:507:CLA:HAB	1.84	0.58
28:C:506:CLA:HMC2	28:C:507:CLA:H93	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:PHE:O	7:G:85:LEU:HG	2.03	0.58
31:L:101:SQD:H282	13:M:21:PHE:HD1	1.69	0.58
31:M:101:SQD:H312	13:m:17:VAL:HG13	1.86	0.58
14:O:62:SER:O	14:O:71:LEU:HD13	2.04	0.58
14:O:93:PHE:HD1	14:O:103:PHE:HB2	1.69	0.58
4:d:15:LEU:HD11	21:x:73:ILE:HG23	1.85	0.58
7:g:25:LEU:HB2	7:g:29:SER:HA	1.86	0.58
7:g:221:ALA:HB1	38:g:619:CHL:H152	1.85	0.58
28:n:603:CLA:HHC	28:n:603:CLA:CBB	2.33	0.58
1:A:32:TRP:O	1:A:35:VAL:HG22	2.03	0.57
28:B:609:CLA:HAA1	8:H:43:MET:SD	2.44	0.57
7:G:74:LEU:HD11	28:G:610:CLA:HAC1	1.86	0.57
38:G:608:CHL:H52	38:G:608:CHL:H93	1.85	0.57
28:b:604:CLA:HBA1	28:b:612:CLA:H143	1.85	0.57
32:b:623:LMG:H302	38:r:606:CHL:H43	1.86	0.57
4:d:47:GLY:HA3	30:d:406:BCR:H341	1.86	0.57
28:g:610:CLA:C2	39:g:615:LUT:H28	2.34	0.57
28:r:604:CLA:CHC	40:r:616:NEX:H222	2.34	0.57
38:r:607:CHL:HBD	38:r:607:CHL:HAA1	1.86	0.57
22:y:189:PHE:HE2	28:y:313:CLA:HAB	1.67	0.57
2:B:497:LYS:CB	2:B:503:THR:HG21	2.33	0.57
28:B:606:CLA:C1D	35:B:623:LHG:H241	2.34	0.57
28:B:614:CLA:HBD	31:L:101:SQD:H441	1.85	0.57
31:B:620:SQD:H322	19:t:15:GLY:C	2.29	0.57
7:G:75:GLY:O	7:G:79:CYS:SG	2.61	0.57
7:G:94:GLU:HB2	7:G:103:GLN:HG3	1.85	0.57
15:P:152:LYS:HB3	15:P:157:TYR:HE1	1.68	0.57
17:R:39:LEU:HD12	41:R:615:XAT:H23	1.86	0.57
17:R:97:LEU:HD23	17:R:172:LEU:HG	1.85	0.57
28:R:604:CLA:HMA3	38:R:605:CHL:C2C	2.34	0.57
18:S:114:THR:HA	18:S:117:LEU:HD23	1.86	0.57
28:S:310:CLA:H2	39:S:315:LUT:H28	1.86	0.57
28:c:504:CLA:O1A	36:c:517:DGD:HD61	2.03	0.57
7:g:70:ARG:HA	7:g:73:MET:HE3	1.86	0.57
7:g:138:VAL:HA	7:g:141:TYR:CD2	2.39	0.57
38:g:601:CHL:H201	38:y:309:CHL:C9	2.26	0.57
28:s:611:CLA:HED2	28:s:611:CLA:H2A	1.86	0.57
1:A:140:ARG:HB2	4:D:221:ASN:HA	1.86	0.57
2:B:154:GLY:O	2:B:159:THR:HG23	2.04	0.57
28:B:614:CLA:H162	30:B:617:BCR:H12C	1.84	0.57
3:C:109:PHE:CD2	32:C:522:LMG:HC1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:613:CLA:CHB	28:G:614:CLA:HAC1	2.35	0.57
8:H:52:VAL:O	8:H:56:ILE:HG13	2.04	0.57
16:Q:101:GLN:O	16:Q:104:LYS:HG2	2.04	0.57
18:S:21:GLU:C	18:S:23:LEU:H	2.12	0.57
28:Y:603:CLA:CAB	38:Y:609:CHL:H151	2.34	0.57
1:a:276:ALA:HA	4:d:213:ALA:HA	1.86	0.57
28:b:603:CLA:H62	28:b:603:CLA:HMB2	1.86	0.57
28:b:611:CLA:C3B	28:b:613:CLA:HMA2	2.34	0.57
38:y:308:CHL:H161	40:y:318:NEX:H31	1.86	0.57
2:B:230:ARG:HH11	2:B:474:LEU:HA	1.69	0.57
3:C:308:GLU:HA	3:C:361:LEU:HD21	1.85	0.57
28:C:506:CLA:C4D	28:C:507:CLA:H202	2.35	0.57
7:G:70:ARG:HA	7:G:73:MET:HE3	1.87	0.57
7:G:182:LYS:HD3	28:G:611:CLA:CGD	2.35	0.57
28:G:612:CLA:H2	28:G:612:CLA:HMA3	1.86	0.57
14:O:49:LYS:HG2	14:O:50:LYS:HD3	1.86	0.57
16:Q:119:HIS:O	16:Q:123:ILE:HG12	2.04	0.57
18:S:22:GLU:HA	18:S:25:LYS:HD3	1.85	0.57
18:S:152:TYR:HA	18:S:156:ASN:HB2	1.86	0.57
28:S:310:CLA:H52	39:S:315:LUT:H28	1.86	0.57
28:c:503:CLA:H101	28:c:503:CLA:H52	1.87	0.57
38:n:601:CHL:HAC2	35:n:618:LHG:C4	2.32	0.57
38:n:609:CHL:NB	38:y:302:CHL:H2	2.20	0.57
14:o:51:LEU:HB3	14:o:89:ILE:HB	1.85	0.57
14:o:65:VAL:HA	14:o:71:LEU:CD2	2.34	0.57
23:z:5:PHE:HA	23:z:57:LEU:HD13	1.87	0.57
23:z:12:LEU:HD13	23:z:50:LEU:HB3	1.85	0.57
32:A:413:LMG:H122	9:I:4:LEU:HB2	1.87	0.57
3:C:279:LEU:HD22	28:C:509:CLA:HED3	1.85	0.57
12:L:20:TRP:CE3	35:L:102:LHG:H141	2.39	0.57
7:N:127:ILE:HG12	38:N:605:CHL:HBC2	1.86	0.57
28:S:311:CLA:HBA1	28:S:311:CLA:C2	2.34	0.57
22:Y:131:GLN:OE1	38:Y:607:CHL:HMC	2.05	0.57
3:C:410:VAL:O	3:C:413:GLU:HB2	2.04	0.57
28:C:506:CLA:H71	35:W:101:LHG:H312	1.86	0.57
30:D:405:BCR:H14C	6:F:27:PHE:CD1	2.40	0.57
7:G:121:ALA:HA	38:G:605:CHL:CHC	2.34	0.57
11:K:55:GLN:HA	11:K:58:VAL:HG22	1.84	0.57
38:S:302:CHL:CHD	35:S:317:LHG:HC41	2.33	0.57
28:S:304:CLA:HHC	28:S:304:CLA:CBB	2.29	0.57
22:Y:54:ASP:HB2	22:Y:57:THR:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:214:LEU:HD13	28:r:603:CLA:H111	1.85	0.57
4:d:56:VAL:HG21	4:d:111:LEU:CD1	2.34	0.57
29:d:402:PHO:HMB1	29:d:402:PHO:HBB1	1.86	0.57
28:d:405:CLA:H41	8:h:55:SER:HB3	1.87	0.57
28:g:611:CLA:H2	28:g:612:CLA:O2D	2.05	0.57
1:A:199:MET:SD	36:C:519:DGD:HA91	2.45	0.57
28:B:613:CLA:H191	32:B:621:LMG:H371	1.85	0.57
28:C:502:CLA:HBB2	28:C:510:CLA:H172	1.87	0.57
31:L:101:SQD:H91	13:m:26:TYR:HE2	1.69	0.57
7:N:33:PRO:HG2	7:N:36:LEU:HD12	1.86	0.57
14:O:117:GLN:HE21	14:O:121:GLY:HA2	1.69	0.57
2:b:368:VAL:HG21	2:b:422:ARG:HG2	1.87	0.57
3:c:377:LEU:O	3:c:381:LYS:HG3	2.04	0.57
4:d:280:LEU:HD22	29:d:402:PHO:HBC3	1.87	0.57
28:g:614:CLA:HAA2	22:y:128:TRP:CH2	2.40	0.57
11:k:60:PHE:HZ	30:k:101:BCR:H281	1.69	0.57
18:s:133:ILE:HG23	18:s:137:LEU:HB2	1.87	0.57
28:s:611:CLA:HHC	28:s:611:CLA:CBB	2.32	0.57
2:B:503:THR:HA	21:X:83:ARG:HB3	1.85	0.57
28:B:601:CLA:HBB2	30:H:101:BCR:H351	1.85	0.57
4:D:161:TYR:HA	4:D:291:ALA:HB2	1.86	0.57
28:G:613:CLA:HMB1	28:G:613:CLA:HBB1	1.87	0.57
12:L:9:GLN:HE22	17:R:56:ASN:ND2	1.98	0.57
7:N:110:LEU:HD21	28:N:604:CLA:HAA1	1.87	0.57
28:N:610:CLA:C5	39:N:615:LUT:H28	2.33	0.57
28:N:611:CLA:H62	28:N:612:CLA:C4D	2.34	0.57
17:R:230:HIS:CG	28:R:612:CLA:HAA2	2.39	0.57
2:b:48:SER:O	2:b:50:PRO:HD3	2.04	0.57
3:c:164:HIS:HA	3:c:167:LEU:HD12	1.87	0.57
7:g:24:TYR:HD2	38:g:601:CHL:HAA1	1.69	0.57
38:n:606:CHL:HMB1	38:n:606:CHL:HBB1	1.86	0.57
38:n:606:CHL:H2	40:n:617:NEX:C35	2.35	0.57
15:p:47:LEU:HD22	15:p:61:VAL:HG23	1.87	0.57
38:s:605:CHL:HBB2	38:s:606:CHL:CBB	2.35	0.57
22:y:139:GLU:O	22:y:143:ILE:HG12	2.05	0.57
18:S:80:ILE:HG13	28:S:309:CLA:O1D	2.05	0.57
28:b:616:CLA:HMA3	28:b:616:CLA:H51	1.87	0.57
28:c:510:CLA:H62	28:c:510:CLA:HMA3	1.87	0.57
15:p:124:LYS:HE2	15:p:152:LYS:HD2	1.87	0.57
38:y:307:CHL:HMB1	38:y:309:CHL:HMC	1.87	0.57
2:B:208:LEU:HD23	28:B:602:CLA:HAC2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:615:CLA:HHC	28:B:615:CLA:CBB	2.31	0.57
38:G:601:CHL:H151	38:Y:607:CHL:CHC	2.34	0.57
28:G:612:CLA:HMC2	39:G:615:LUT:C11	2.35	0.57
28:R:610:CLA:HBD	28:R:611:CLA:CAD	2.35	0.57
38:S:308:CHL:HBA2	28:S:310:CLA:CMD	2.35	0.57
22:Y:83:GLU:O	22:Y:87:ARG:HG2	2.04	0.57
1:a:28:LEU:H	31:a:414:SQD:H81	1.70	0.57
1:a:54:ALA:HB2	1:a:72:LEU:HD22	1.85	0.57
1:a:74:GLY:HA3	4:d:305:ARG:NH1	2.20	0.57
3:c:362:ARG:HD2	14:o:18:LEU:HD21	1.86	0.57
3:c:466:VAL:HG21	4:d:249:THR:HA	1.86	0.57
28:c:504:CLA:CHB	36:c:517:DGD:HB82	2.34	0.57
28:d:405:CLA:H13	21:x:58:ILE:HG22	1.87	0.57
7:g:119:VAL:HA	38:g:605:CHL:ND	2.20	0.57
7:g:155:LEU:HD12	7:g:156:TYR:CE2	2.40	0.57
28:r:609:CLA:H8	39:r:614:LUT:C30	2.35	0.57
28:B:614:CLA:HMD1	13:M:21:PHE:HE1	1.70	0.56
3:C:418:ASN:HD21	36:C:518:DGD:C4D	2.17	0.56
15:P:166:LYS:HA	15:P:169:PHE:CZ	2.40	0.56
18:S:32:ARG:HH22	35:S:301:LHG:HC31	1.70	0.56
18:S:48:TYR:OH	18:S:63:GLY:HA2	2.05	0.56
18:S:175:LEU:HB2	28:S:310:CLA:O1A	2.05	0.56
28:S:303:CLA:C2	39:S:316:LUT:H26	2.35	0.56
7:g:223:SER:C	7:g:225:ALA:H	2.13	0.56
38:g:609:CHL:HAA2	7:n:48:THR:HG21	1.87	0.56
1:A:329:GLU:HG2	4:D:353:LEU:HD21	1.87	0.56
29:A:407:PHO:C2B	28:D:401:CLA:H2	2.35	0.56
28:B:606:CLA:HMC3	35:B:623:LHG:H352	1.87	0.56
3:C:179:ALA:CA	3:C:184:GLY:HA2	2.30	0.56
3:C:308:GLU:HA	3:C:361:LEU:CD2	2.35	0.56
38:G:607:CHL:HBD	7:N:226:THR:HA	1.87	0.56
28:G:610:CLA:H122	39:G:615:LUT:H393	1.85	0.56
28:G:613:CLA:H11	28:G:613:CLA:C4D	2.34	0.56
18:S:112:PHE:CE2	18:S:113:LYS:HE3	2.40	0.56
1:a:257:ARG:HG3	2:b:492:PHE:HE1	1.68	0.56
2:b:29:LEU:HD11	30:b:617:BCR:H19C	1.88	0.56
2:b:491:GLU:HB2	2:b:494:ALA:CB	2.34	0.56
2:b:496:GLN:HB2	2:b:503:THR:HB	1.87	0.56
2:b:497:LYS:CB	2:b:503:THR:HG21	2.35	0.56
35:g:618:LHG:H181	28:y:304:CLA:H18	1.86	0.56
15:p:8:VAL:HG12	15:p:9:PHE:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:q:128:GLU:HB3	16:q:132:TYR:CE2	2.40	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.87	0.56
28:B:603:CLA:HMC3	28:B:605:CLA:H172	1.87	0.56
3:C:425:TRP:CD1	28:C:504:CLA:HMA2	2.41	0.56
5:E:67:THR:H	5:E:75:GLN:HE22	1.51	0.56
7:G:27:PRO:HD2	38:G:601:CHL:CBB	2.36	0.56
38:N:607:CHL:HMB1	38:N:607:CHL:H72	1.85	0.56
16:Q:74:GLN:HB3	16:Q:78:ARG:NH2	2.21	0.56
17:R:209:PHE:HA	17:R:212:PHE:CD2	2.39	0.56
18:S:86:MET:SD	28:S:310:CLA:HAB	2.45	0.56
1:a:46:SER:OG	36:a:401:DGD:HBH2	2.04	0.56
2:b:114:HIS:HE1	28:b:616:CLA:ND	2.03	0.56
3:c:332:GLN:HE21	3:c:336:GLY:HA2	1.70	0.56
7:g:112:TYR:CD1	7:g:113:LEU:HG	2.41	0.56
28:g:602:CLA:H52	39:g:616:LUT:H28	1.88	0.56
7:n:81:PHE:CE2	7:n:85:LEU:HD11	2.41	0.56
7:n:189:PHE:CE2	28:n:613:CLA:HAB	2.36	0.56
17:r:140:LEU:HB3	17:r:142:PHE:HD2	1.71	0.56
18:s:105:CYS:HA	18:s:127:PHE:H	1.70	0.56
38:s:601:CHL:C4D	35:s:617:LHG:H101	2.35	0.56
2:B:45:PHE:HA	2:B:60:MET:HE3	1.86	0.56
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.88	0.56
28:C:506:CLA:H203	30:C:515:BCR:H15C	1.88	0.56
36:C:518:DGD:HD1	32:C:520:LMG:O2	2.06	0.56
36:C:519:DGD:HAN2	32:D:408:LMG:H221	1.87	0.56
4:D:169:PHE:CE1	4:D:337:HIS:HE1	2.23	0.56
28:G:603:CLA:HBC1	38:G:609:CHL:HAC2	1.86	0.56
28:G:604:CLA:H43	38:G:606:CHL:HBD	1.87	0.56
31:L:101:SQD:H252	31:L:101:SQD:H131	1.87	0.56
17:R:24:LEU:HD11	17:R:35:ASP:HB2	1.87	0.56
28:R:612:CLA:HMB2	39:R:614:LUT:H8	1.87	0.56
20:W:47:ASP:H	20:W:50:SER:HB3	1.70	0.56
28:b:609:CLA:HMA3	28:b:610:CLA:C1C	2.36	0.56
28:r:608:CLA:HBA1	28:r:613:CLA:C1D	2.35	0.56
11:K:33:LEU:O	11:K:36:ILE:HG13	2.05	0.56
7:N:99:LYS:HA	38:N:607:CHL:CED	2.34	0.56
28:N:602:CLA:H141	39:N:616:LUT:H393	1.87	0.56
17:R:109:GLY:O	17:R:113:VAL:HG12	2.05	0.56
18:S:225:PRO:HG2	28:S:314:CLA:HMB2	1.88	0.56
7:n:52:SER:HB3	7:n:58:PHE:CD1	2.40	0.56
14:o:46:TYR:HA	14:o:248:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:35:LEU:CB	18:s:40:LEU:HB2	2.35	0.56
35:B:622:LHG:H282	38:R:606:CHL:C2C	2.35	0.56
28:C:501:CLA:H101	30:C:515:BCR:H17C	1.88	0.56
7:G:25:LEU:HB2	7:G:29:SER:HA	1.87	0.56
28:G:611:CLA:HAA1	28:G:612:CLA:OBD	2.04	0.56
28:N:610:CLA:H2	39:N:615:LUT:H26	1.86	0.56
18:S:49:LEU:HD13	18:S:49:LEU:N	2.21	0.56
1:a:103:ASP:HB2	14:o:79:MET:HE1	1.88	0.56
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.41	0.56
7:g:33:PRO:HB3	7:g:35:TYR:CZ	2.41	0.56
7:g:112:TYR:HB3	7:g:118:LEU:CB	2.35	0.56
17:r:173:TYR:HA	28:r:609:CLA:O1D	2.06	0.56
2:B:434:ARG:HH22	14:O:179:ARG:HD2	1.71	0.56
2:B:495:PHE:CD1	2:B:501:PRO:HA	2.40	0.56
38:R:605:CHL:HHC	38:R:605:CHL:HBB1	1.86	0.56
32:b:620:LMG:O8	32:b:620:LMG:HC1	2.06	0.56
4:d:81:THR:HG22	4:d:112:TRP:CE2	2.41	0.56
18:s:212:GLU:HB2	18:s:217:ASN:ND2	2.19	0.56
22:y:86:SER:HA	22:y:90:VAL:O	2.05	0.56
28:y:311:CLA:HHC	28:y:311:CLA:CBB	2.34	0.56
23:z:28:ALA:O	23:z:30:PRO:HD3	2.05	0.56
28:G:611:CLA:H2	28:G:612:CLA:HED3	1.87	0.56
7:N:147:PRO:HD2	38:N:608:CHL:CBB	2.36	0.56
28:S:310:CLA:HAA1	28:S:310:CLA:HED2	1.88	0.56
28:S:312:CLA:HHC	28:S:312:CLA:CBB	2.33	0.56
28:Y:604:CLA:NB	40:Y:618:NEX:H242	2.21	0.56
28:a:407:CLA:HAA1	36:c:518:DGD:CEA	2.36	0.56
6:f:21:ALA:HB1	37:f:101:HEM:CAC	2.35	0.56
6:f:22:VAL:HB	6:f:23:PRO:HD3	1.87	0.56
7:g:112:TYR:HB3	7:g:118:LEU:HB3	1.86	0.56
38:g:619:CHL:CED	22:y:99:LYS:HA	2.36	0.56
18:s:70:ASP:HA	18:s:73:LYS:HE2	1.86	0.56
2:B:6:TYR:O	28:B:611:CLA:HBD	2.05	0.56
3:C:346:THR:HG21	14:O:22:GLY:HA2	1.88	0.56
38:G:608:CHL:H71	38:G:608:CHL:C2	2.36	0.56
16:Q:104:LYS:HA	16:Q:107:THR:HG22	1.86	0.56
2:b:383:PHE:CZ	14:o:167:GLY:HA2	2.40	0.56
28:b:604:CLA:NA	28:b:612:CLA:H141	2.20	0.56
36:c:516:DGD:HA52	36:c:516:DGD:HB51	1.88	0.56
7:g:139:GLU:O	7:g:143:ILE:HG12	2.05	0.56
17:r:178:PHE:HB3	38:r:607:CHL:C12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:5:GLY:HA3	24:u:28:ASN:HA	1.87	0.56
28:C:504:CLA:H8	32:C:520:LMG:H372	1.87	0.56
28:C:505:CLA:HMD2	28:C:507:CLA:HAB	1.87	0.56
11:K:60:PHE:HZ	30:K:101:BCR:H282	1.70	0.56
28:S:304:CLA:HED2	28:S:304:CLA:H2A	1.87	0.56
20:W:31:GLY:HA3	35:W:101:LHG:H192	1.88	0.56
1:a:278:TRP:HA	31:a:411:SQD:C17	2.36	0.56
3:c:406:SER:HA	3:c:420:VAL:CG2	2.35	0.56
7:g:105:PHE:HE2	7:n:225:ALA:HB3	1.71	0.56
13:m:25:ILE:O	13:m:28:LYS:HG2	2.05	0.56
14:o:61:LYS:HD3	14:o:71:LEU:CB	2.36	0.56
16:q:96:PRO:HB2	16:q:98:ASP:OD1	2.06	0.56
3:C:223:TRP:HE3	36:C:517:DGD:HB21	1.70	0.55
38:G:606:CHL:HBC2	38:G:607:CHL:CHD	2.36	0.55
17:R:185:ALA:HB1	17:R:191:LYS:HG3	1.87	0.55
18:S:156:ASN:ND2	18:S:158:LEU:HD13	2.21	0.55
22:Y:80:VAL:HG13	22:Y:206:LEU:HD21	1.88	0.55
1:a:217:SER:HB3	4:d:273:LEU:HD12	1.87	0.55
28:b:611:CLA:H122	28:b:613:CLA:H72	1.88	0.55
8:h:32:LYS:HB2	17:r:69:ARG:NH2	2.21	0.55
14:o:32:ILE:HG12	14:o:215:ILE:HD13	1.87	0.55
18:s:83:ARG:O	18:s:87:LEU:HG	2.06	0.55
18:s:83:ARG:HA	18:s:86:MET:HE3	1.88	0.55
28:s:603:CLA:HBC1	28:s:608:CLA:HBC2	1.87	0.55
1:A:42:LEU:HD23	31:A:414:SQD:H202	1.88	0.55
2:B:290:GLY:O	2:B:294:GLU:HG3	2.06	0.55
31:B:620:SQD:H5	31:L:101:SQD:C3	2.36	0.55
36:C:518:DGD:HAH2	36:C:519:DGD:HBT2	1.87	0.55
28:G:612:CLA:HHC	28:G:612:CLA:CBB	2.35	0.55
7:N:103:GLN:HE21	7:N:110:LEU:HG	1.70	0.55
38:N:605:CHL:HBD	38:N:605:CHL:HAA1	1.87	0.55
16:Q:70:TRP:CE3	16:Q:121:ALA:HA	2.41	0.55
28:R:603:CLA:ND	28:R:608:CLA:H8	2.21	0.55
3:c:130:ILE:HD12	28:c:511:CLA:H202	1.89	0.55
3:c:261:ARG:HA	3:c:266:TRP:CZ2	2.41	0.55
22:y:138:VAL:HA	22:y:141:TYR:CD2	2.41	0.55
32:A:413:LMG:H362	36:A:417:DGD:HB82	1.88	0.55
38:G:609:CHL:C3B	38:N:601:CHL:H52	2.37	0.55
7:N:22:VAL:HG13	38:N:601:CHL:CBC	2.37	0.55
14:O:237:LYS:HD3	14:O:239:GLN:HE21	1.71	0.55
17:R:15:PHE:CD2	17:R:18:ALA:HB2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:122:ILE:HA	8:h:24:LYS:HD3	1.88	0.55
28:c:501:CLA:HMB3	28:c:501:CLA:H62	1.88	0.55
14:o:4:PRO:HG2	14:o:28:GLN:NE2	2.21	0.55
16:q:95:LYS:HG2	16:q:103:LEU:CD1	2.35	0.55
1:A:131:TRP:HZ2	3:C:449:ARG:HD2	1.71	0.55
28:N:611:CLA:H121	28:N:612:CLA:H112	1.89	0.55
16:Q:70:TRP:N	16:Q:71:PRO:HD2	2.22	0.55
16:Q:110:LEU:HD22	16:Q:143:VAL:HG21	1.88	0.55
18:S:64:LEU:HD12	28:S:303:CLA:H11	1.89	0.55
30:a:410:BCR:C17	32:a:413:LMG:H361	2.36	0.55
3:c:237:HIS:CE1	30:i:101:BCR:H272	2.40	0.55
28:c:501:CLA:H122	28:c:507:CLA:H102	1.88	0.55
30:c:515:BCR:H343	30:k:101:BCR:HC31	1.89	0.55
35:c:520:LHG:H112	28:s:610:CLA:CAB	2.36	0.55
5:e:26:THR:HB	37:f:101:HEM:CAB	2.34	0.55
22:y:25:LEU:HB2	22:y:29:SER:HA	1.87	0.55
4:D:12:GLN:O	4:D:13:ASN:C	2.48	0.55
4:D:81:THR:HG22	4:D:112:TRP:CE2	2.42	0.55
7:G:64:LEU:HD13	28:G:603:CLA:HBA1	1.89	0.55
28:R:612:CLA:H11	28:R:612:CLA:C4D	2.37	0.55
28:b:607:CLA:C10	32:b:620:LMG:H361	2.37	0.55
30:b:618:BCR:C4	32:b:620:LMG:H362	2.36	0.55
3:c:146:PHE:CZ	35:c:520:LHG:HC62	2.41	0.55
4:d:15:LEU:HD21	21:x:73:ILE:HD13	1.89	0.55
7:g:27:PRO:HD2	38:g:601:CHL:CBB	2.36	0.55
38:g:601:CHL:HAA2	38:g:601:CHL:HBD	1.89	0.55
38:g:606:CHL:HBA1	40:g:617:NEX:H403	1.88	0.55
18:s:135:LEU:O	18:s:139:VAL:HG23	2.07	0.55
28:y:304:CLA:CAB	38:y:309:CHL:H151	2.36	0.55
28:B:606:CLA:ND	35:B:623:LHG:H241	2.21	0.55
36:C:518:DGD:HAT1	36:C:519:DGD:HBT1	1.89	0.55
28:D:404:CLA:C15	21:X:59:VAL:HA	2.37	0.55
7:G:94:GLU:HB2	7:G:103:GLN:CG	2.36	0.55
28:N:612:CLA:HMB3	28:N:612:CLA:H121	1.88	0.55
17:R:121:TRP:HD1	42:R:711:HOH:O	1.89	0.55
18:S:167:GLY:HA2	28:S:310:CLA:HED3	1.87	0.55
18:S:218:PHE:HE1	28:S:314:CLA:HAC1	1.70	0.55
2:b:69:LEU:HD12	28:b:605:CLA:H3A	1.88	0.55
30:d:406:BCR:H392	32:d:409:LMG:C14	2.36	0.55
5:e:35:TRP:CH2	6:f:36:PHE:CE2	2.95	0.55
7:g:162:ASP:HA	39:g:615:LUT:C24	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:39:PHE:HA	14:o:207:THR:HG21	1.88	0.55
28:r:612:CLA:H13	28:r:612:CLA:HAB	1.88	0.55
30:B:617:BCR:HC21	32:B:621:LMG:H322	1.87	0.55
28:C:506:CLA:H41	35:W:101:LHG:H292	1.89	0.55
4:D:173:SER:HB2	4:D:178:ALA:HB1	1.89	0.55
14:O:90:GLU:HB2	14:O:107:ASP:OD1	2.06	0.55
16:Q:142:ASP:OD1	16:Q:146:LYS:HE2	2.07	0.55
18:S:218:PHE:HD1	39:S:315:LUT:H163	1.70	0.55
28:S:305:CLA:HBA1	38:S:306:CHL:C1D	2.37	0.55
31:a:411:SQD:H142	35:a:415:LHG:H162	1.87	0.55
28:b:604:CLA:H12	28:b:605:CLA:C1D	2.37	0.55
28:b:614:CLA:HMD1	13:m:21:PHE:HE1	1.71	0.55
30:d:406:BCR:H24C	32:d:409:LMG:H162	1.88	0.55
28:g:612:CLA:HMC2	39:g:615:LUT:C11	2.36	0.55
8:h:47:MET:HG3	30:h:101:BCR:H333	1.88	0.55
28:r:613:CLA:HHC	28:r:613:CLA:CBB	2.37	0.55
22:y:24:TYR:HD2	38:y:302:CHL:HAA1	1.72	0.55
28:y:305:CLA:C1C	40:y:318:NEX:H222	2.36	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.55
2:B:67:THR:HA	2:B:71:ILE:O	2.07	0.55
2:B:109:LEU:C	30:B:619:BCR:H21C	2.31	0.55
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.42	0.55
28:C:502:CLA:H2	28:C:503:CLA:C1D	2.36	0.55
4:D:161:TYR:HB3	4:D:162:PRO:HD3	1.87	0.55
38:G:606:CHL:HBB2	38:G:607:CHL:CBB	2.37	0.55
28:S:310:CLA:H12	28:S:310:CLA:H3A	1.89	0.55
22:Y:213:LEU:HD21	28:Y:614:CLA:HMC3	1.89	0.55
35:a:415:LHG:H342	28:c:508:CLA:HBC2	1.89	0.55
2:b:270:PRO:HG3	2:b:312:TYR:HD1	1.72	0.55
28:b:601:CLA:HHC	28:b:601:CLA:CBB	2.34	0.55
28:n:603:CLA:H8	38:n:609:CHL:C9	2.37	0.55
14:o:148:VAL:HG21	14:o:223:PRO:HD2	1.89	0.55
18:s:194:ARG:HA	18:s:197:MET:HE3	1.88	0.55
35:B:625:LHG:HC81	35:B:625:LHG:H371	1.89	0.55
7:G:33:PRO:HG2	7:G:36:LEU:HD12	1.88	0.55
7:G:182:LYS:HD3	28:G:611:CLA:O1D	2.07	0.55
7:N:138:VAL:HA	7:N:141:TYR:CD2	2.42	0.55
7:N:195:PHE:HD2	38:N:609:CHL:H202	1.70	0.55
18:S:185:LEU:HD21	28:S:310:CLA:H43	1.89	0.55
28:Y:604:CLA:HMA3	38:Y:606:CHL:C2C	2.36	0.55
28:n:603:CLA:HAC1	38:n:607:CHL:HBB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:611:CLA:C4C	35:n:618:LHG:HC62	2.37	0.55
17:r:209:PHE:CE2	41:r:615:XAT:H10	2.42	0.55
23:z:44:THR:O	23:z:48:ILE:HG13	2.07	0.55
3:C:142:GLU:CD	3:C:142:GLU:H	2.15	0.55
4:D:157:VAL:HG12	4:D:172:PRO:HG2	1.89	0.55
38:N:601:CHL:HBD	38:N:601:CHL:HAA2	1.88	0.55
38:N:607:CHL:H91	38:N:609:CHL:H152	1.89	0.55
18:S:112:PHE:HD2	38:S:307:CHL:H2	1.72	0.55
22:Y:66:VAL:HG22	22:Y:181:LEU:HD21	1.89	0.55
22:Y:73:MET:SD	28:Y:610:CLA:HAB	2.47	0.55
22:Y:179:LYS:HD3	28:Y:612:CLA:HAA2	1.88	0.55
1:a:195:HIS:CE1	1:a:197:PHE:HB2	2.41	0.55
35:a:415:LHG:H312	35:a:415:LHG:H171	1.88	0.55
28:n:603:CLA:H191	38:n:607:CHL:H162	1.89	0.55
38:n:605:CHL:HMA3	18:s:101:TYR:HB3	1.89	0.55
14:o:76:THR:HG22	14:o:118:LEU:HD23	1.89	0.55
21:x:51:LEU:O	21:x:55:LEU:HG	2.07	0.55
28:y:304:CLA:HHC	28:y:304:CLA:CBB	2.33	0.55
28:y:305:CLA:HMA3	38:y:307:CHL:C3C	2.37	0.55
2:B:454:GLY:CA	32:B:621:LMG:H212	2.38	0.54
28:R:612:CLA:H11	28:R:612:CLA:ND	2.22	0.54
18:S:49:LEU:HD23	18:S:56:ASP:OD1	2.07	0.54
22:Y:33:PRO:HG2	22:Y:36:LEU:HD12	1.90	0.54
1:a:298:ASN:HD22	1:a:298:ASN:N	2.04	0.54
30:a:410:BCR:C16	32:a:413:LMG:H361	2.37	0.54
28:b:608:CLA:H143	28:d:405:CLA:HHB	1.88	0.54
38:g:609:CHL:C4B	38:n:601:CHL:H52	2.37	0.54
38:r:605:CHL:C9	40:r:616:NEX:H35	2.36	0.54
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.89	0.54
1:A:106:LEU:HD11	30:A:409:BCR:H402	1.88	0.54
4:D:60:TYR:O	5:E:65:LEU:HD12	2.07	0.54
37:E:101:HEM:CAC	6:F:21:ALA:HB1	2.37	0.54
16:Q:43:ALA:HB3	16:Q:46:GLU:OE1	2.07	0.54
18:s:99:ASN:ND2	18:s:109:ALA:HB2	2.22	0.54
24:u:4:ARG:HB3	24:u:25:ILE:HA	1.88	0.54
28:B:606:CLA:HHC	28:B:606:CLA:CBB	2.35	0.54
28:C:506:CLA:C4	35:W:101:LHG:H292	2.38	0.54
4:D:108:LEU:HD23	5:E:66:ILE:HD13	1.88	0.54
4:D:211:LEU:HD21	33:D:406:PL9:H13	1.90	0.54
18:S:112:PHE:CD2	38:S:307:CHL:H2	2.42	0.54
38:S:302:CHL:ND	35:S:317:LHG:HC91	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:303:CLA:H93	28:S:303:CLA:H13	1.90	0.54
28:b:606:CLA:HBB1	28:b:606:CLA:HMB3	1.89	0.54
3:c:108:THR:HG23	3:c:111:TYR:HD2	1.70	0.54
7:n:46:TRP:HE3	28:n:602:CLA:C2D	2.21	0.54
14:o:226:THR:C	14:o:231:LYS:HG2	2.32	0.54
18:s:156:ASN:HB2	18:s:160:LEU:HD13	1.89	0.54
1:A:97:TRP:HH2	28:A:408:CLA:HBA2	1.72	0.54
36:B:626:DGD:HBE1	4:D:163:LEU:HD13	1.89	0.54
3:C:338:GLY:HA3	3:C:341:LEU:O	2.06	0.54
36:C:519:DGD:HA71	32:D:408:LMG:H161	1.89	0.54
5:E:12:ASP:HA	10:J:7:ARG:NH1	2.22	0.54
28:G:613:CLA:HHB	28:G:614:CLA:HMC1	1.89	0.54
17:R:182:LEU:HB2	17:R:184:LEU:HD11	1.88	0.54
28:R:613:CLA:HHC	28:R:613:CLA:HBB1	1.88	0.54
23:Z:3:ILE:O	23:Z:7:LEU:HG	2.07	0.54
2:b:3:LEU:HD22	2:b:7:ARG:HB2	1.88	0.54
2:b:6:TYR:O	28:b:611:CLA:HBD	2.08	0.54
28:b:603:CLA:H192	28:b:609:CLA:H91	1.88	0.54
35:b:621:LHG:H282	38:r:606:CHL:C4C	2.37	0.54
3:c:308:GLU:HA	3:c:361:LEU:HD21	1.90	0.54
7:n:24:TYR:CE2	7:n:25:LEU:HD23	2.43	0.54
18:s:34:PHE:CD2	38:s:601:CHL:HAA1	2.42	0.54
22:y:148:LEU:HD13	38:y:308:CHL:H102	1.89	0.54
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.90	0.54
28:B:602:CLA:HBA2	42:H:210:HOH:O	2.08	0.54
28:B:604:CLA:C1D	28:B:612:CLA:H172	2.37	0.54
4:D:18:ILE:HG22	21:X:76:SER:HB3	1.90	0.54
4:D:107:GLN:HE21	5:E:48:GLY:HA3	1.73	0.54
4:D:313:GLU:HB2	14:O:159:PRO:HG3	1.89	0.54
18:S:79:LEU:HD13	18:S:164:PHE:HB3	1.89	0.54
18:S:88:GLY:HA2	39:S:316:LUT:H181	1.90	0.54
1:a:77:ILE:HD13	12:l:30:VAL:HG13	1.88	0.54
32:a:413:LMG:HC1	9:i:1:MET:HE2	1.90	0.54
2:b:218:SER:HB3	17:r:86:VAL:HG11	1.90	0.54
2:b:441:GLY:C	14:o:176:ALA:HB3	2.32	0.54
4:d:298:ASP:HB2	4:d:316:TYR:OH	2.08	0.54
8:h:50:PHE:CB	30:h:101:BCR:H12C	2.37	0.54
18:s:34:PHE:HB2	38:s:601:CHL:C4D	2.38	0.54
22:y:203:LYS:HB2	22:y:208:ASN:HD21	1.73	0.54
28:C:504:CLA:H102	36:C:518:DGD:HBE2	1.89	0.54
6:F:22:VAL:HB	6:F:23:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:GLU:O	7:G:143:ILE:HG12	2.08	0.54
11:K:36:ILE:O	11:K:40:MET:HG3	2.07	0.54
13:M:28:LYS:HB2	13:m:27:VAL:HG12	1.88	0.54
18:S:34:PHE:CD2	38:S:302:CHL:HAA1	2.35	0.54
1:a:344:ALA:HB1	3:c:358:PHE:CE2	2.42	0.54
2:b:341:LEU:HD22	2:b:429:ILE:HG22	1.90	0.54
36:b:625:DGD:HAE1	4:d:124:ILE:HD11	1.88	0.54
4:d:31:VAL:HG13	4:d:39:PHE:HE2	1.72	0.54
4:d:44:PHE:HB3	4:d:114:PHE:CE1	2.43	0.54
7:g:60:LYS:HD2	7:n:48:THR:O	2.08	0.54
7:n:85:LEU:HB2	7:n:92:PHE:CE2	2.43	0.54
28:n:610:CLA:H151	39:n:615:LUT:C31	2.37	0.54
14:o:16:THR:H	14:o:19:GLU:CD	2.16	0.54
18:s:71:PHE:HE1	28:s:602:CLA:H2A	1.71	0.54
18:s:116:ALA:HA	18:s:119:LEU:HG	1.88	0.54
18:s:178:ASP:HB2	18:s:181:GLN:HB2	1.88	0.54
2:B:19:LEU:O	2:B:22:VAL:HG22	2.08	0.54
2:B:248:ALA:HB2	28:B:603:CLA:H52	1.89	0.54
28:C:506:CLA:HMB1	28:C:506:CLA:HBB1	1.88	0.54
38:G:607:CHL:H52	38:G:607:CHL:H93	1.88	0.54
7:N:195:PHE:HB2	38:N:609:CHL:H202	1.90	0.54
15:P:18:TYR:OH	15:P:175:PHE:HA	2.08	0.54
28:Y:602:CLA:H62	28:Y:603:CLA:CMA	2.30	0.54
23:Z:37:LYS:HB3	23:Z:41:PHE:CE2	2.43	0.54
1:a:56:PRO:HA	1:a:73:TYR:CE2	2.41	0.54
28:b:614:CLA:H161	30:b:617:BCR:H12C	1.88	0.54
3:c:109:PHE:CE2	32:c:521:LMG:HC1	2.42	0.54
30:h:101:BCR:H331	30:h:101:BCR:C8	2.38	0.54
2:B:30:VAL:HG12	28:B:605:CLA:HHD	1.89	0.54
2:B:75:TRP:HA	2:B:88:PRO:HG3	1.90	0.54
3:C:261:ARG:HH12	20:W:50:SER:H	1.55	0.54
28:C:501:CLA:H202	30:C:515:BCR:H353	1.89	0.54
4:D:37:LEU:HD12	28:D:404:CLA:HBB1	1.89	0.54
7:G:51:LEU:CD1	39:G:616:LUT:H221	2.38	0.54
28:N:613:CLA:H11	28:N:613:CLA:C4D	2.38	0.54
14:O:188:GLU:H	14:O:188:GLU:CD	2.13	0.54
15:P:39:GLU:O	15:P:48:ARG:HD2	2.08	0.54
16:Q:17:LEU:HB3	16:Q:21:LEU:HB3	1.90	0.54
18:S:111:TRP:HB2	39:S:316:LUT:H21	1.89	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.54
7:g:81:PHE:CD2	28:g:604:CLA:HHD	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:85:LEU:HB2	7:g:92:PHE:HE2	1.72	0.54
16:q:32:PRO:HD2	16:q:35:GLU:CD	2.33	0.54
16:q:70:TRP:N	16:q:71:PRO:HD2	2.23	0.54
22:y:139:GLU:HG3	38:y:309:CHL:C4B	2.37	0.54
36:C:518:DGD:CBB	32:C:520:LMG:H422	2.37	0.54
4:D:6:GLY:O	4:D:7:LYS:HG2	2.07	0.54
31:L:103:SQD:H211	2:b:108:PHE:HB2	1.89	0.54
16:Q:65:ILE:HG12	16:Q:73:LEU:HD22	1.89	0.54
3:c:93:ALA:HB1	3:c:99:VAL:HG11	1.89	0.54
3:c:391:ARG:HD2	3:c:395:TYR:CZ	2.42	0.54
4:d:258:PHE:HE2	35:d:408:LHG:H121	1.73	0.54
38:g:606:CHL:HAA1	40:g:617:NEX:H28	1.90	0.54
15:p:68:LYS:HE2	15:p:74:TYR:HA	1.90	0.54
18:s:83:ARG:HA	28:s:609:CLA:HMC2	1.90	0.54
22:y:125:LEU:HA	22:y:128:TRP:NE1	2.22	0.54
22:y:209:LEU:O	22:y:213:LEU:HG	2.06	0.54
23:z:19:LEU:HD21	23:z:43:GLY:HA3	1.90	0.54
2:B:167:TRP:HA	2:B:178:VAL:HA	1.90	0.54
28:B:602:CLA:H51	8:H:57:ILE:HG13	1.90	0.54
3:C:119:LEU:HG	30:C:516:BCR:H10C	1.90	0.54
4:D:211:LEU:HA	4:D:214:ILE:HG22	1.89	0.54
17:R:54:ASP:H	17:R:60:ASN:ND2	2.06	0.54
35:S:317:LHG:HC92	35:S:317:LHG:H281	1.89	0.54
38:Y:607:CHL:H143	38:Y:607:CHL:H12	1.90	0.54
1:a:93:PHE:CZ	28:a:409:CLA:HAA1	2.40	0.54
38:g:619:CHL:CBB	38:y:307:CHL:HBB2	2.37	0.54
36:A:417:DGD:HG12	36:A:417:DGD:HB21	1.90	0.53
2:B:109:LEU:O	30:B:619:BCR:H21C	2.08	0.53
3:C:42:LEU:HD23	3:C:45:LEU:HD12	1.89	0.53
7:N:224:TYR:HB3	7:N:227:ASN:OD1	2.07	0.53
14:O:39:PHE:HA	14:O:207:THR:HG21	1.90	0.53
22:Y:46:TRP:CE3	39:Y:616:LUT:H383	2.43	0.53
38:g:605:CHL:HAA2	38:g:605:CHL:HBD	1.89	0.53
28:C:501:CLA:H122	28:C:507:CLA:H102	1.90	0.53
7:G:115:ASN:HB3	7:G:118:LEU:HG	1.89	0.53
11:K:30:TYR:CZ	23:Z:5:PHE:HZ	2.26	0.53
7:N:134:LEU:HD13	38:N:606:CHL:H12	1.89	0.53
23:Z:57:LEU:HA	23:Z:60:LEU:HD12	1.90	0.53
3:c:84:GLN:HB2	3:c:86:LEU:HG	1.89	0.53
4:d:276:PRO:HB2	29:d:402:PHO:HBC1	1.90	0.53
8:h:43:MET:HG3	30:h:101:BCR:HC42	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:220:ASN:N	7:n:220:ASN:OD1	2.42	0.53
14:o:66:THR:O	14:o:67:LYS:HB3	2.08	0.53
28:r:601:CLA:HHC	28:r:601:CLA:CBB	2.32	0.53
28:s:609:CLA:H11	39:s:614:LUT:H373	1.90	0.53
1:A:221:SER:HA	4:D:140:ARG:HB2	1.88	0.53
29:D:402:PHO:HMB1	29:D:402:PHO:HBB1	1.90	0.53
7:G:186:LEU:HB3	39:G:615:LUT:H202	1.90	0.53
38:N:607:CHL:CHC	38:Y:601:CHL:H151	2.38	0.53
15:P:118:ALA:HB1	15:P:125:GLN:NE2	2.23	0.53
18:S:135:LEU:O	18:S:139:VAL:HG23	2.08	0.53
18:S:218:PHE:CD1	39:S:315:LUT:H163	2.44	0.53
1:a:270:SER:HA	31:a:411:SQD:H82	1.90	0.53
2:b:258:TYR:CE2	36:b:625:DGD:HBF2	2.43	0.53
28:b:605:CLA:CMA	28:b:606:CLA:HMA2	2.37	0.53
28:b:616:CLA:H93	30:b:619:BCR:C14	2.38	0.53
3:c:363:ALA:O	3:c:367:GLU:HG2	2.07	0.53
28:c:510:CLA:HBB1	28:c:510:CLA:HMB1	1.89	0.53
5:e:15:THR:OG1	10:j:7:ARG:HD2	2.09	0.53
28:g:602:CLA:H122	28:y:304:CLA:H143	1.90	0.53
28:n:604:CLA:H2	38:n:606:CHL:HBD	1.90	0.53
28:s:613:CLA:HBB1	28:s:613:CLA:HMB3	1.90	0.53
35:y:319:LHG:H331	35:y:319:LHG:H121	1.89	0.53
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.91	0.53
2:B:300:GLU:O	2:B:304:LYS:HG3	2.08	0.53
28:B:603:CLA:H193	28:B:609:CLA:H152	1.91	0.53
7:N:83:GLU:HA	7:N:95:ALA:HB1	1.89	0.53
7:N:87:ARG:CD	7:N:206:LEU:HD23	2.39	0.53
38:N:601:CHL:CHD	35:N:618:LHG:HC41	2.39	0.53
15:P:166:LYS:O	15:P:170:LYS:HG2	2.08	0.53
17:R:75:VAL:HG13	17:R:82:PRO:HB2	1.91	0.53
28:S:305:CLA:HBB1	28:S:305:CLA:CMB	2.38	0.53
38:S:308:CHL:HAA1	38:S:308:CHL:HBD	1.90	0.53
1:a:256:GLY:O	1:a:261:GLN:N	2.38	0.53
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.90	0.53
35:d:408:LHG:HC42	12:l:16:THR:HG21	1.89	0.53
7:g:16:TRP:HB3	7:g:178:VAL:HG21	1.89	0.53
7:n:119:VAL:HA	38:n:605:CHL:ND	2.23	0.53
14:o:111:TYR:HB3	14:o:131:LYS:HE2	1.91	0.53
2:B:12:VAL:HG23	28:B:612:CLA:HMC2	1.90	0.53
28:B:603:CLA:HAB	28:B:605:CLA:C17	2.38	0.53
3:C:92:LEU:HD21	28:C:503:CLA:HED2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.91	0.53
6:F:11:THR:O	6:F:15:LEU:HG	2.09	0.53
15:P:142:GLY:C	15:P:143:LYS:HD2	2.33	0.53
16:Q:32:PRO:HD2	16:Q:35:GLU:CD	2.34	0.53
2:b:26:HIS:CE1	28:b:612:CLA:HMA2	2.43	0.53
5:e:24:SER:O	5:e:28:PRO:HG2	2.09	0.53
28:g:603:CLA:O2D	38:g:609:CHL:H8	2.09	0.53
7:n:24:TYR:CD2	38:n:601:CHL:HAA1	2.43	0.53
14:o:104:GLU:HG2	14:o:134:VAL:HG13	1.90	0.53
22:y:121:ALA:HA	38:y:306:CHL:CHC	2.39	0.53
2:B:125:ASP:HB2	2:B:132:SER:OG	2.09	0.53
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.44	0.53
3:C:307:PRO:HB2	3:C:361:LEU:HD13	1.91	0.53
28:C:508:CLA:C1C	28:C:510:CLA:H51	2.39	0.53
3:c:223:TRP:CG	3:c:224:ILE:H	2.27	0.53
3:c:228:ASP:HB3	36:c:516:DGD:HE62	1.91	0.53
7:g:125:LEU:HD13	7:n:222:TRP:NE1	2.24	0.53
11:k:27:PRO:HB2	11:k:30:TYR:CD2	2.40	0.53
7:n:22:VAL:O	7:n:23:LYS:HB2	2.08	0.53
7:n:44:TYR:HE2	38:n:601:CHL:HBC2	1.73	0.53
28:s:603:CLA:OBD	28:s:608:CLA:HAA1	2.09	0.53
28:s:604:CLA:C1C	40:s:616:NEX:H222	2.38	0.53
22:y:81:PHE:HB3	22:y:82:PRO:HD3	1.91	0.53
1:A:199:MET:CB	36:C:519:DGD:HAT1	2.37	0.53
28:A:406:CLA:HED1	36:C:519:DGD:HA82	1.89	0.53
3:C:119:LEU:CD1	30:C:516:BCR:H12C	2.37	0.53
28:c:501:CLA:HBC1	28:c:512:CLA:H41	1.89	0.53
4:d:47:GLY:HA3	30:d:406:BCR:C34	2.38	0.53
7:g:105:PHE:CZ	7:g:124:ILE:HG21	2.44	0.53
14:o:61:LYS:HD3	14:o:71:LEU:HB3	1.90	0.53
14:o:218:PHE:HB3	14:o:242:TRP:CD1	2.44	0.53
15:p:18:TYR:OH	15:p:175:PHE:HA	2.09	0.53
19:t:8:PHE:HD1	30:t:101:BCR:H372	1.73	0.53
22:y:216:PRO:HG2	28:y:314:CLA:HMB2	1.90	0.53
2:B:495:PHE:HA	2:B:504:LYS:HB3	1.90	0.53
28:B:601:CLA:HHC	28:B:601:CLA:HBB1	1.90	0.53
14:O:86:LEU:HB3	14:O:89:ILE:HD11	1.91	0.53
28:R:603:CLA:CAC	28:R:608:CLA:HBC2	2.39	0.53
18:S:194:ARG:HA	18:S:197:MET:HE3	1.90	0.53
22:Y:24:TYR:CD2	38:Y:601:CHL:HAA1	2.44	0.53
22:Y:51:LEU:HD12	39:Y:616:LUT:H221	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:464:PHE:CZ	35:b:624:LHG:H261	2.44	0.53
28:b:610:CLA:HHC	28:b:610:CLA:CBB	2.34	0.53
3:c:385:GLN:NE2	16:q:80:ARG:HG3	2.24	0.53
3:c:472:LEU:HD11	4:d:252:ARG:HG3	1.89	0.53
7:g:191:MET:HE2	39:g:616:LUT:C10	2.38	0.53
7:g:191:MET:HG3	39:g:616:LUT:H12	1.90	0.53
11:k:53:VAL:CG2	30:k:101:BCR:H21C	2.39	0.53
28:n:603:CLA:CAD	38:n:609:CHL:H2	2.39	0.53
16:q:62:LYS:HB2	16:q:133:TYR:CZ	2.43	0.53
22:y:100:ALA:O	22:y:103:GLN:HG2	2.09	0.53
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.91	0.53
28:B:614:CLA:H43	31:B:620:SQD:H122	1.91	0.53
3:C:109:PHE:CE2	32:C:522:LMG:HC5	2.43	0.53
18:S:46:PRO:HB3	18:S:48:TYR:CZ	2.44	0.53
28:S:304:CLA:HBC1	28:S:309:CLA:HAC2	1.91	0.53
28:Y:602:CLA:H92	28:Y:603:CLA:CMA	2.39	0.53
1:a:253:GLY:HA2	2:b:492:PHE:HZ	1.69	0.53
2:b:399:VAL:HG12	2:b:417:VAL:HG22	1.91	0.53
28:b:607:CLA:HBB1	28:b:607:CLA:HMB1	1.91	0.53
28:b:610:CLA:H11	28:b:612:CLA:H191	1.91	0.53
28:c:504:CLA:H11	36:c:517:DGD:HB62	1.90	0.53
4:d:161:TYR:HA	4:d:291:ALA:HB2	1.91	0.53
28:g:613:CLA:H11	28:g:613:CLA:NA	2.24	0.53
7:n:139:GLU:O	7:n:143:ILE:HG12	2.09	0.53
1:A:82:ILE:HB	1:A:174:LEU:HB2	1.91	0.53
1:A:253:GLY:HA2	2:B:492:PHE:CE1	2.44	0.53
1:A:257:ARG:HG3	2:B:492:PHE:CE2	2.44	0.53
4:D:310:PRO:HG3	14:O:188:GLU:HB3	1.90	0.53
7:N:199:ILE:HA	22:Y:230:PRO:HB3	1.91	0.53
28:R:601:CLA:HHC	28:R:601:CLA:CBB	2.38	0.53
38:R:605:CHL:HBD	38:R:605:CHL:HAA2	1.90	0.53
28:R:611:CLA:HHC	28:R:611:CLA:CBB	2.32	0.53
41:Y:617:XAT:C29	35:Y:619:LHG:H101	2.38	0.53
23:Z:1:MET:CG	23:Z:61:ILE:HG22	2.35	0.53
1:a:218:LEU:HD11	1:a:255:PHE:HD2	1.74	0.53
2:b:75:TRP:HA	2:b:88:PRO:HG2	1.91	0.53
2:b:151:PHE:CE2	2:b:203:ILE:HG23	2.43	0.53
3:c:437:LEU:HA	28:c:508:CLA:HMC2	1.91	0.53
4:d:258:PHE:CE2	35:d:408:LHG:H301	2.44	0.53
4:d:267:TRP:CG	35:d:408:LHG:HC2	2.44	0.53
7:g:97:TRP:HB2	39:g:616:LUT:O3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:603:CLA:H2	28:g:603:CLA:HED2	1.91	0.53
38:g:606:CHL:HBC2	38:g:607:CHL:CHD	2.39	0.53
18:s:198:PHE:CE2	28:s:612:CLA:HAB	2.37	0.53
1:A:240:GLY:HA3	19:T:30:PRO:CG	2.38	0.52
2:B:488:ALA:C	2:B:490:VAL:H	2.17	0.52
28:B:603:CLA:CAD	28:B:605:CLA:H43	2.39	0.52
28:C:510:CLA:HED2	28:C:510:CLA:C2	2.39	0.52
42:D:563:HOH:O	13:M:2:GLU:HG2	2.10	0.52
7:G:66:VAL:HG21	7:G:155:LEU:HD13	1.91	0.52
28:G:603:CLA:HBC2	38:G:609:CHL:HHD	1.89	0.52
7:N:15:PRO:HG2	7:N:16:TRP:CD1	2.44	0.52
7:N:147:PRO:HD2	38:N:608:CHL:HBB2	1.89	0.52
14:O:155:SER:HA	14:O:166:THR:HG22	1.91	0.52
18:S:163:LYS:HA	38:S:308:CHL:HBC1	1.91	0.52
22:Y:96:VAL:HB	22:Y:99:LYS:HZ2	1.73	0.52
1:a:49:ILE:HG12	33:d:407:PL9:H511	1.90	0.52
28:c:506:CLA:HBB2	28:c:507:CLA:H2	1.92	0.52
28:g:602:CLA:C2	39:g:616:LUT:H28	2.37	0.52
7:n:67:ILE:HG13	38:n:609:CHL:HED2	1.91	0.52
38:n:606:CHL:CBB	38:n:609:CHL:HBC1	2.39	0.52
17:r:52:SER:HB2	17:r:60:ASN:HB3	1.92	0.52
28:r:609:CLA:HED2	28:r:609:CLA:HAA1	1.91	0.52
1:A:132:GLU:O	1:A:136:ARG:HG2	2.09	0.52
28:B:614:CLA:H8	30:B:617:BCR:H362	1.91	0.52
4:D:329:TRP:HZ2	4:D:349:ARG:HG3	1.74	0.52
6:F:24:THR:O	6:F:28:LEU:HG	2.09	0.52
28:G:613:CLA:C1B	28:G:614:CLA:HAC1	2.39	0.52
13:M:14:PHE:O	13:M:18:PRO:HG2	2.08	0.52
7:N:83:GLU:CD	7:N:206:LEU:HB2	2.35	0.52
28:N:604:CLA:HMA3	38:N:606:CHL:C2C	2.40	0.52
22:Y:103:GLN:HG3	22:Y:110:LEU:HG	1.92	0.52
38:Y:601:CHL:C3C	41:Y:617:XAT:H362	2.39	0.52
1:a:133:LEU:HD23	4:d:257:ILE:HG12	1.91	0.52
4:d:352:ALA:O	4:d:353:LEU:C	2.52	0.52
7:g:158:GLY:HA2	28:g:610:CLA:O1D	2.09	0.52
7:n:16:TRP:CE2	28:n:611:CLA:HED1	2.43	0.52
7:n:138:VAL:HA	7:n:141:TYR:CD2	2.44	0.52
20:w:47:ASP:O	20:w:50:SER:HB2	2.09	0.52
22:y:70:ARG:HA	22:y:73:MET:HE3	1.90	0.52
30:D:405:BCR:H363	6:F:27:PHE:HB3	1.91	0.52
28:G:610:CLA:HMC2	39:G:615:LUT:H31	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:103:SQD:C33	30:T:101:BCR:H16C	2.39	0.52
13:M:31:SER:HB3	13:m:32:GLN:CG	2.34	0.52
16:Q:20:THR:HG21	42:Q:226:HOH:O	2.07	0.52
17:R:191:LYS:HE2	28:R:609:CLA:HED1	1.92	0.52
28:R:604:CLA:HBB1	41:R:615:XAT:H192	1.92	0.52
22:Y:46:TRP:CD2	39:Y:616:LUT:H383	2.43	0.52
1:a:202:VAL:HG11	28:a:407:CLA:C3D	2.39	0.52
3:c:153:ASP:O	3:c:157:MET:HG2	2.09	0.52
3:c:348:GLU:OE2	14:o:21:LYS:HA	2.09	0.52
4:d:183:ILE:HG23	28:d:404:CLA:CHD	2.40	0.52
7:n:212:HIS:HB2	28:n:613:CLA:HAA2	1.91	0.52
20:w:17:LEU:HA	20:w:22:LEU:HD23	1.90	0.52
2:B:108:PHE:CD1	31:B:620:SQD:H202	2.45	0.52
3:C:29:GLU:HG3	3:C:30:THR:HG23	1.92	0.52
3:C:108:THR:HA	3:C:111:TYR:CD2	2.44	0.52
28:C:509:CLA:H143	28:C:509:CLA:CHA	2.39	0.52
4:D:114:PHE:HZ	30:D:405:BCR:H323	1.74	0.52
7:G:60:LYS:HG3	7:N:48:THR:O	2.10	0.52
7:G:99:LYS:HA	38:G:607:CHL:CED	2.40	0.52
7:G:105:PHE:HZ	7:N:225:ALA:HB3	1.75	0.52
14:O:199:LYS:HB2	14:O:199:LYS:NZ	2.24	0.52
16:Q:85:ARG:HG2	16:Q:111:PHE:CE1	2.45	0.52
28:S:313:CLA:HMB2	39:S:315:LUT:H161	1.91	0.52
2:b:475:PHE:HA	4:d:135:ARG:NH1	2.25	0.52
2:b:496:GLN:HG3	2:b:504:LYS:HG2	1.92	0.52
3:c:307:PRO:HB2	3:c:361:LEU:HD13	1.91	0.52
28:c:509:CLA:H112	28:c:512:CLA:CAD	2.40	0.52
28:r:603:CLA:H122	28:r:608:CLA:H101	1.91	0.52
22:y:192:PHE:CE2	38:y:309:CHL:H172	2.43	0.52
1:A:126:TYR:HE2	35:D:407:LHG:H382	1.73	0.52
2:B:332:ASN:ND2	32:B:621:LMG:HC61	2.24	0.52
28:C:511:CLA:C3B	30:C:516:BCR:H393	2.40	0.52
30:C:516:BCR:H281	11:K:54:TRP:CZ3	2.45	0.52
4:D:25:ARG:O	4:D:26:ASP:C	2.53	0.52
4:D:190:HIS:HA	4:D:295:ARG:CD	2.39	0.52
14:O:32:ILE:HG12	14:O:215:ILE:HD13	1.90	0.52
17:R:101:ARG:HA	17:R:104:MET:HE3	1.91	0.52
20:W:40:TYR:O	20:W:44:LEU:HD13	2.09	0.52
1:a:28:LEU:O	31:a:414:SQD:H101	2.09	0.52
2:b:434:ARG:HD2	14:o:177:GLY:HA3	1.92	0.52
36:c:517:DGD:HBT1	36:c:517:DGD:HB61	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:101:GLY:O	7:g:104:ILE:HG22	2.09	0.52
7:n:36:LEU:HD23	7:n:45:GLY:HA2	1.90	0.52
1:A:56:PRO:HB2	14:O:123:ARG:NH2	2.25	0.52
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.90	0.52
36:C:518:DGD:C7B	32:C:520:LMG:H401	2.40	0.52
9:I:21:PHE:CZ	20:W:34:TRP:HB2	2.44	0.52
28:N:602:CLA:H202	28:N:602:CLA:HMC2	1.92	0.52
38:N:607:CHL:HAA1	41:Y:617:XAT:H41	1.91	0.52
6:f:24:THR:O	6:f:28:LEU:HG	2.10	0.52
28:s:602:CLA:HMB1	28:s:602:CLA:HBB1	1.91	0.52
22:y:179:LYS:HD3	28:y:312:CLA:HAA2	1.90	0.52
28:y:313:CLA:H71	35:y:319:LHG:H161	1.92	0.52
35:A:416:LHG:HC11	28:C:508:CLA:CGD	2.40	0.52
2:B:458:PHE:CE2	32:B:621:LMG:H242	2.45	0.52
3:C:38:GLY:HA3	28:C:511:CLA:HMD2	1.91	0.52
3:C:279:LEU:HA	3:C:282:PHE:CD2	2.44	0.52
7:G:137:ALA:HB1	7:G:141:TYR:OH	2.10	0.52
7:G:215:ASP:N	7:G:216:PRO:HD3	2.25	0.52
1:a:329:GLU:HG3	42:a:588:HOH:O	2.09	0.52
7:g:128:TRP:CB	7:n:222:TRP:HH2	2.23	0.52
38:g:601:CHL:H162	38:g:619:CHL:HAB	1.91	0.52
19:t:5:VAL:O	19:t:9:LEU:HG	2.10	0.52
24:u:26:CYS:HB3	24:u:27:ARG:HH22	1.75	0.52
28:B:608:CLA:CHD	28:B:609:CLA:H102	2.40	0.52
3:C:117:LEU:CD1	32:C:522:LMG:H191	2.38	0.52
11:K:49:LEU:HB2	30:K:101:BCR:H17C	1.90	0.52
4:d:44:PHE:HB3	4:d:114:PHE:HE1	1.74	0.52
38:g:606:CHL:CBB	39:g:616:LUT:H161	2.39	0.52
38:n:607:CHL:H43	38:n:607:CHL:HMA3	1.91	0.52
19:t:19:PHE:HA	19:t:23:PHE:HD1	1.74	0.52
31:A:410:SQD:H311	28:C:508:CLA:H71	1.91	0.52
4:D:2:THR:HG1	17:R:72:PHE:HZ	1.55	0.52
14:O:47:ASN:ND2	14:O:247:GLU:HB3	2.25	0.52
1:a:102:VAL:HB	36:a:401:DGD:HD62	1.92	0.52
2:b:167:TRP:HA	2:b:178:VAL:HA	1.92	0.52
28:b:601:CLA:H101	28:b:601:CLA:C2D	2.40	0.52
3:c:27:ASP:CG	3:c:29:GLU:HG2	2.35	0.52
3:c:177:PHE:HA	3:c:181:TYR:HD2	1.75	0.52
4:d:74:PHE:CD1	32:d:409:LMG:H311	2.44	0.52
7:g:197:GLN:OE1	39:g:615:LUT:H42	2.09	0.52
28:g:603:CLA:HBC2	38:g:609:CHL:HHD	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:69:GLN:CD	8:h:69:GLN:H	2.18	0.52
7:n:110:LEU:HD21	28:n:604:CLA:HAA2	1.91	0.52
38:n:608:CHL:H152	40:n:617:NEX:H402	1.92	0.52
35:w:102:LHG:H191	28:y:312:CLA:H101	1.91	0.52
1:A:319:ASP:O	1:A:323:ARG:HG2	2.10	0.52
2:B:451:PHE:CZ	28:B:604:CLA:HED2	2.45	0.52
31:B:620:SQD:H462	19:t:23:PHE:HB3	1.92	0.52
7:G:166:LEU:HB2	28:G:610:CLA:O1A	2.10	0.52
11:K:27:PRO:HB2	11:K:30:TYR:HD2	1.74	0.52
18:S:153:ARG:HA	38:S:308:CHL:C3C	2.40	0.52
28:Y:603:CLA:HHC	28:Y:603:CLA:CBB	2.32	0.52
3:c:95:LEU:HD11	28:c:503:CLA:HAA2	1.92	0.52
36:c:517:DGD:HB22	32:k:102:LMG:H302	1.90	0.52
28:g:604:CLA:HED2	28:g:604:CLA:H2A	1.92	0.52
7:n:119:VAL:H	38:n:605:CHL:CGD	2.22	0.52
14:o:204:VAL:HG22	14:o:242:TRP:HH2	1.75	0.52
17:r:124:ALA:CB	28:r:604:CLA:HED1	2.39	0.52
18:s:49:LEU:HD23	18:s:58:GLY:HA2	1.91	0.52
22:y:96:VAL:HG22	22:y:99:LYS:HB2	1.92	0.52
23:z:37:LYS:HB3	23:z:41:PHE:CE2	2.45	0.52
2:B:33:TRP:HD1	30:t:101:BCR:H381	1.74	0.51
28:B:604:CLA:HBA1	28:B:604:CLA:CHA	2.39	0.51
28:B:606:CLA:H13	30:B:619:BCR:H12C	1.91	0.51
3:C:130:ILE:HG22	23:Z:27:PHE:HD2	1.74	0.51
28:G:613:CLA:H143	22:Y:128:TRP:CH2	2.45	0.51
14:O:117:GLN:NE2	14:O:121:GLY:HA2	2.25	0.51
16:Q:55:ALA:HB1	16:Q:140:LEU:HD21	1.91	0.51
18:S:111:TRP:CE2	18:S:112:PHE:HD1	2.28	0.51
28:S:311:CLA:HBA2	28:S:311:CLA:CHA	2.39	0.51
20:W:39:ILE:HG12	28:Y:612:CLA:H41	1.92	0.51
22:Y:141:TYR:HE2	40:Y:618:NEX:H202	1.75	0.51
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.91	0.51
2:b:142:HIS:HB3	28:b:610:CLA:H101	1.92	0.51
2:b:497:LYS:HE2	4:d:24:ARG:CZ	2.39	0.51
28:b:615:CLA:H172	28:b:615:CLA:C12	2.40	0.51
15:p:7:ASN:OD1	15:p:10:GLY:HA3	2.10	0.51
38:r:607:CHL:H12	39:r:614:LUT:H383	1.92	0.51
18:s:88:GLY:HA2	39:s:615:LUT:H181	1.93	0.51
18:s:169:PRO:O	18:s:172:PRO:HD3	2.10	0.51
18:s:221:HIS:CE1	18:s:225:PRO:HB3	2.45	0.51
22:y:116:PRO:O	22:y:120:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:y:310:CLA:H52	39:y:315:LUT:H30	1.93	0.51
28:y:312:CLA:HHC	28:y:312:CLA:CBB	2.33	0.51
28:B:616:CLA:HBA1	30:B:619:BCR:H20C	1.92	0.51
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.45	0.51
28:C:507:CLA:HBA2	28:C:509:CLA:H72	1.91	0.51
30:C:516:BCR:HC32	11:K:30:TYR:CE1	2.45	0.51
5:E:24:SER:O	5:E:28:PRO:HG2	2.09	0.51
7:G:51:LEU:HD22	28:G:602:CLA:H42	1.92	0.51
28:G:610:CLA:H2	39:G:615:LUT:C25	2.39	0.51
7:N:135:MET:O	7:N:139:GLU:HG2	2.11	0.51
28:N:602:CLA:HBA1	39:N:616:LUT:H382	1.91	0.51
18:S:104:ASN:HB2	18:S:128:GLY:CA	2.40	0.51
18:S:205:ILE:HG13	28:S:313:CLA:HAC2	1.92	0.51
28:S:310:CLA:H2	39:S:315:LUT:H26	1.92	0.51
28:a:409:CLA:H102	9:i:16:VAL:HG21	1.93	0.51
2:b:105:GLY:HA3	30:b:618:BCR:H23C	1.93	0.51
2:b:392:VAL:HG13	2:b:397:VAL:HB	1.91	0.51
2:b:496:GLN:HE22	21:x:82:LYS:N	1.98	0.51
3:c:274:TYR:HB3	28:c:507:CLA:C3B	2.41	0.51
7:n:85:LEU:HB2	7:n:92:PHE:HE2	1.75	0.51
21:x:52:LYS:O	21:x:56:LEU:HG	2.10	0.51
2:B:441:GLY:C	14:O:176:ALA:HB3	2.35	0.51
2:B:503:THR:HA	21:X:83:ARG:CB	2.40	0.51
28:C:501:CLA:C1B	28:C:501:CLA:H2	2.40	0.51
12:L:24:LEU:HA	35:L:102:LHG:H171	1.92	0.51
15:P:42:PHE:CB	15:P:62:LEU:HD21	2.37	0.51
28:S:311:CLA:C4B	28:S:311:CLA:H93	2.40	0.51
2:b:254:GLY:HA2	36:b:625:DGD:HBF1	1.92	0.51
2:b:348:ASP:HB3	2:b:354:LEU:HD11	1.91	0.51
3:c:109:PHE:CE1	32:c:521:LMG:HC3	2.44	0.51
3:c:147:PHE:HE2	30:c:514:BCR:H292	1.74	0.51
3:c:322:GLN:HE22	3:c:381:LYS:HA	1.76	0.51
28:c:506:CLA:NC	28:c:507:CLA:H151	2.25	0.51
5:e:51:ARG:HD3	42:p:241:HOH:O	2.09	0.51
7:g:157:PRO:HD2	28:g:610:CLA:OBD	2.10	0.51
7:g:196:VAL:O	7:g:200:VAL:HG23	2.10	0.51
7:n:35:TYR:CD2	7:n:36:LEU:HD13	2.45	0.51
20:w:8:THR:O	32:w:101:LMG:HC62	2.10	0.51
20:w:34:TRP:HZ2	35:w:102:LHG:HC82	1.76	0.51
2:B:488:ALA:HA	2:B:491:GLU:OE1	2.11	0.51
9:I:19:PHE:CE1	9:I:23:PHE:HE2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:M:101:SQD:C31	13:m:17:VAL:HG13	2.40	0.51
28:N:604:CLA:HMA3	38:N:606:CHL:C3C	2.40	0.51
38:N:605:CHL:HMA3	18:S:101:TYR:HB3	1.91	0.51
1:a:35:VAL:HA	30:a:410:BCR:H322	1.91	0.51
1:a:295:PHE:HD2	3:c:428:THR:HG22	1.76	0.51
28:a:406:CLA:H51	29:a:408:PHO:C3B	2.41	0.51
30:b:617:BCR:H322	32:b:620:LMG:O7	2.11	0.51
4:d:86:LEU:HD13	4:d:91:LEU:HD11	1.92	0.51
28:g:610:CLA:H8	39:g:615:LUT:C30	2.41	0.51
7:n:85:LEU:HB3	7:n:90:VAL:HG21	1.92	0.51
14:o:237:LYS:HD3	14:o:239:GLN:NE2	2.25	0.51
17:r:104:MET:SD	28:r:609:CLA:HAB	2.51	0.51
19:t:19:PHE:HA	19:t:23:PHE:CD1	2.45	0.51
22:y:212:HIS:CG	28:y:313:CLA:HAA2	2.46	0.51
1:A:272:HIS:HA	1:A:275:LEU:HD12	1.91	0.51
28:B:606:CLA:O1A	28:B:606:CLA:H3A	2.10	0.51
3:C:203:THR:O	3:C:235:GLY:HA3	2.11	0.51
3:C:466:VAL:HG21	4:D:249:THR:HA	1.92	0.51
28:C:513:CLA:HBA1	28:C:513:CLA:CBD	2.38	0.51
4:D:82:PRO:HB3	4:D:91:LEU:HD11	1.93	0.51
4:D:307:ALA:O	14:O:188:GLU:HG3	2.10	0.51
31:L:103:SQD:H291	19:T:19:PHE:CD1	2.46	0.51
7:N:73:MET:SD	28:N:610:CLA:HAB	2.50	0.51
16:Q:106:LEU:HG	16:Q:143:VAL:HG22	1.92	0.51
16:Q:143:VAL:O	16:Q:147:ILE:HG13	2.10	0.51
28:R:610:CLA:H2	28:R:610:CLA:HBA2	1.91	0.51
20:W:17:LEU:HD22	20:W:22:LEU:HB3	1.92	0.51
38:Y:606:CHL:HBD	38:Y:606:CHL:HAA2	1.91	0.51
2:b:462:PHE:HA	28:b:611:CLA:HMC2	1.90	0.51
4:d:78:ALA:HB2	4:d:175:GLY:HA3	1.91	0.51
1:A:300:PHE:HB3	1:A:302:PHE:CE2	2.45	0.51
28:B:614:CLA:H112	30:B:617:BCR:H16C	1.93	0.51
3:C:84:GLN:HB2	3:C:86:LEU:HG	1.91	0.51
3:C:191:PRO:HA	16:Q:78:ARG:CG	2.41	0.51
3:C:429:SER:HB3	36:C:518:DGD:HB92	1.91	0.51
4:D:147:PHE:C	4:D:150:PRO:HD2	2.36	0.51
19:T:21:ILE:HD12	30:T:101:BCR:HC21	1.93	0.51
38:Y:601:CHL:H8	41:Y:617:XAT:H35	1.92	0.51
38:Y:601:CHL:H111	41:Y:617:XAT:H12	1.92	0.51
1:a:344:ALA:HB3	3:c:310:SER:HB2	1.93	0.51
7:g:164:LEU:HD12	39:g:615:LUT:H222	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:161:PHE:CD1	28:n:610:CLA:HMD2	2.46	0.51
28:n:603:CLA:C3B	38:n:609:CHL:H13	2.40	0.51
1:A:74:GLY:HA3	4:D:305:ARG:NH1	2.25	0.51
31:A:414:SQD:H271	30:b:618:BCR:H271	1.93	0.51
2:B:495:PHE:HB3	2:B:503:THR:OG1	2.10	0.51
4:D:90:LEU:HG	8:H:62:ASN:ND2	2.26	0.51
4:D:200:MET:HE3	4:D:282:MET:HB3	1.93	0.51
4:D:338:GLU:HB3	4:D:340:LEU:HG	1.90	0.51
7:G:98:PHE:CE2	7:G:99:LYS:HE3	2.46	0.51
28:G:613:CLA:H143	22:Y:128:TRP:HH2	1.76	0.51
7:N:83:GLU:O	7:N:87:ARG:HG3	2.11	0.51
18:S:182:ALA:O	18:S:186:LYS:HG3	2.11	0.51
22:Y:70:ARG:HA	22:Y:73:MET:HE3	1.93	0.51
22:Y:105:PHE:CE2	38:Y:607:CHL:HMD1	2.46	0.51
23:Z:44:THR:O	23:Z:48:ILE:HG13	2.11	0.51
1:a:206:PHE:HB3	28:a:407:CLA:H11	1.92	0.51
2:b:272:ARG:NH1	4:d:165:GLN:HA	2.26	0.51
28:n:611:CLA:HBA2	28:n:612:CLA:OBD	2.11	0.51
15:p:74:TYR:HE1	15:p:151:VAL:HG21	1.76	0.51
18:s:76:GLY:O	18:s:80:ILE:HG12	2.11	0.51
28:s:604:CLA:HMA3	38:s:605:CHL:C1C	2.41	0.51
23:z:48:ILE:HG22	23:z:52:PHE:CE2	2.45	0.51
2:B:434:ARG:HH21	2:B:441:GLY:N	2.08	0.51
3:C:179:ALA:HA	3:C:184:GLY:CA	2.33	0.51
28:C:511:CLA:H193	23:Z:20:LEU:HA	1.92	0.51
7:G:147:PRO:CG	40:G:617:NEX:H192	2.41	0.51
15:P:94:PHE:HE1	16:Q:2:ALA:HA	1.74	0.51
17:R:89:LEU:HD11	28:R:602:CLA:HAA2	1.92	0.51
28:S:312:CLA:H2A	28:S:312:CLA:C1	2.41	0.51
28:c:509:CLA:C2B	28:c:510:CLA:HBA2	2.41	0.51
28:c:513:CLA:HMB3	30:c:514:BCR:H402	1.93	0.51
28:n:603:CLA:C3D	38:n:609:CHL:H62	2.41	0.51
22:y:189:PHE:CD2	28:y:313:CLA:HAB	2.46	0.51
28:y:304:CLA:H121	38:y:309:CHL:H91	1.93	0.51
32:A:411:LMG:C28	20:W:15:PHE:HA	2.41	0.51
28:C:511:CLA:H171	23:Z:20:LEU:HA	1.91	0.51
4:D:130:GLN:OE1	4:D:144:ALA:HA	2.11	0.51
7:N:73:MET:HE3	28:N:610:CLA:HMC3	1.93	0.51
14:O:56:THR:HG23	14:O:240:GLY:HA2	1.93	0.51
16:Q:110:LEU:O	16:Q:114:ILE:HG13	2.11	0.51
28:S:304:CLA:HBC2	28:S:309:CLA:HHD	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:161:TYR:HB3	1:a:162:PRO:HD3	1.92	0.51
1:a:284:TRP:CD1	3:c:435:PHE:HZ	2.29	0.51
36:a:401:DGD:HB22	30:a:410:BCR:H373	1.91	0.51
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.93	0.51
28:b:608:CLA:C1A	28:b:608:CLA:CGA	2.89	0.51
28:c:508:CLA:HBB1	28:c:508:CLA:CMB	2.41	0.51
8:h:50:PHE:HB2	30:h:101:BCR:H12C	1.93	0.51
19:t:18:PHE:CE1	19:t:23:PHE:HE1	2.29	0.51
28:y:303:CLA:H202	39:y:316:LUT:H31	1.91	0.51
1:A:49:ILE:HG23	33:D:406:PL9:H501	1.93	0.51
1:A:131:TRP:CZ2	3:C:449:ARG:HD2	2.46	0.51
3:C:170:ILE:O	3:C:174:LEU:HG	2.11	0.51
28:C:502:CLA:HBA2	28:C:502:CLA:CHA	2.40	0.51
28:C:508:CLA:C3B	28:C:510:CLA:HMA3	2.41	0.51
28:C:511:CLA:H142	11:K:47:PHE:CE1	2.46	0.51
7:G:164:LEU:HD12	7:G:164:LEU:N	2.24	0.51
3:c:121:SER:HA	30:c:514:BCR:H16C	1.92	0.51
6:f:36:PHE:CZ	10:j:27:LEU:HD21	2.45	0.51
16:q:110:LEU:O	16:q:114:ILE:HG13	2.11	0.51
2:B:103:PHE:CE1	30:B:619:BCR:H341	2.46	0.50
2:B:282:GLN:HG3	24:U:84:TYR:CE2	2.46	0.50
28:B:613:CLA:HMB1	28:B:613:CLA:HBB1	1.93	0.50
28:B:616:CLA:HED2	28:B:616:CLA:H2A	1.92	0.50
36:C:518:DGD:HAT1	36:C:519:DGD:HBT2	1.93	0.50
10:J:8:ILE:HB	10:J:13:ILE:HD11	1.93	0.50
28:N:604:CLA:CHB	40:N:617:NEX:H383	2.41	0.50
16:Q:120:ALA:HB2	16:Q:132:TYR:HD2	1.76	0.50
18:S:133:ILE:HG23	18:S:137:LEU:HB2	1.93	0.50
22:Y:189:PHE:CE1	28:Y:613:CLA:HAB	2.47	0.50
1:a:49:ILE:HG23	33:d:407:PL9:H501	1.93	0.50
3:c:62:PHE:HZ	11:k:43:ILE:HD12	1.75	0.50
3:c:165:LEU:HD21	28:c:506:CLA:CAB	2.41	0.50
5:e:28:PRO:O	5:e:32:ILE:HG12	2.11	0.50
10:j:15:THR:O	10:j:19:ILE:HG13	2.11	0.50
14:o:28:GLN:HE21	20:w:1:LEU:HD11	1.76	0.50
28:y:311:CLA:H101	28:y:312:CLA:NC	2.26	0.50
41:y:317:XAT:H361	35:y:319:LHG:HC92	1.93	0.50
23:z:3:ILE:O	23:z:7:LEU:HG	2.11	0.50
23:z:47:TRP:O	23:z:51:VAL:HG23	2.11	0.50
1:A:314:ILE:HG23	4:D:59:TRP:CZ3	2.46	0.50
2:B:330:MET:HA	2:B:444:ARG:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:611:CLA:HMB1	28:B:611:CLA:HBB1	1.93	0.50
3:C:165:LEU:HD21	28:C:506:CLA:CAB	2.41	0.50
30:C:514:BCR:H343	23:Z:51:VAL:HG12	1.93	0.50
4:D:202:VAL:HG13	28:D:403:CLA:HMB1	1.93	0.50
4:D:280:LEU:HD22	29:D:402:PHO:HBC3	1.93	0.50
35:D:407:LHG:H152	35:D:407:LHG:H291	1.92	0.50
28:N:611:CLA:C4C	35:N:618:LHG:HC62	2.40	0.50
15:P:96:GLN:HG2	15:P:106:ASN:ND2	2.26	0.50
17:R:97:LEU:HB3	17:R:172:LEU:HD11	1.93	0.50
1:a:131:TRP:NE1	3:c:446:GLY:HA2	2.25	0.50
28:b:608:CLA:H62	28:b:609:CLA:H121	1.93	0.50
32:b:623:LMG:H192	38:r:606:CHL:C4B	2.40	0.50
7:n:21:ARG:HG3	7:n:23:LYS:CD	2.41	0.50
7:n:221:ALA:N	28:n:613:CLA:O1A	2.45	0.50
38:n:607:CHL:HAA2	38:n:607:CHL:HBD	1.93	0.50
28:y:303:CLA:H61	39:y:316:LUT:H28	1.93	0.50
29:A:407:PHO:CMB	28:D:401:CLA:H2	2.42	0.50
4:D:78:ALA:HB2	4:D:175:GLY:HA3	1.93	0.50
18:S:76:GLY:HA3	18:S:164:PHE:CZ	2.47	0.50
18:S:112:PHE:HB2	38:S:307:CHL:H2	1.93	0.50
18:S:203:PHE:CZ	39:S:315:LUT:H8	2.47	0.50
1:a:85:THR:OG1	1:a:113:GLU:HG3	2.10	0.50
28:b:605:CLA:HMA2	28:b:606:CLA:CMA	2.41	0.50
28:b:609:CLA:NA	30:h:101:BCR:HC41	2.26	0.50
30:b:618:BCR:H17C	42:b:725:HOH:O	2.12	0.50
3:c:120:ILE:HD11	30:c:515:BCR:H312	1.92	0.50
3:c:195:ASP:HB3	16:q:85:ARG:NH1	2.24	0.50
7:g:124:ILE:HG13	7:n:222:TRP:CZ3	2.46	0.50
17:r:200:LYS:HD2	28:r:610:CLA:O1D	2.11	0.50
38:r:605:CHL:H111	38:r:607:CHL:HMB2	1.92	0.50
38:s:606:CHL:HAA2	38:s:606:CHL:HBD	1.93	0.50
22:y:56:GLU:O	22:y:60:LYS:HG2	2.11	0.50
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.93	0.50
28:A:408:CLA:CGA	32:A:411:LMG:H112	2.41	0.50
28:B:614:CLA:H162	30:B:617:BCR:C12	2.42	0.50
3:C:362:ARG:CD	14:O:18:LEU:HD21	2.42	0.50
3:C:385:GLN:NE2	16:Q:80:ARG:HG2	2.26	0.50
28:N:610:CLA:H3A	28:N:610:CLA:C1	2.42	0.50
15:P:8:VAL:HG12	15:P:9:PHE:CD2	2.46	0.50
17:R:49:ASP:O	17:R:63:GLY:HA3	2.12	0.50
18:S:49:LEU:HD22	18:S:49:LEU:C	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:38:ILE:HA	31:a:414:SQD:H182	1.93	0.50
1:a:221:SER:HA	4:d:140:ARG:HB2	1.94	0.50
28:b:606:CLA:H13	30:b:619:BCR:C10	2.40	0.50
28:b:614:CLA:H152	30:b:617:BCR:H353	1.93	0.50
38:n:607:CHL:HBA2	22:y:230:PRO:HD3	1.92	0.50
28:y:310:CLA:C2	39:y:315:LUT:H28	2.42	0.50
31:A:410:SQD:H332	28:C:508:CLA:H72	1.94	0.50
2:B:152:GLY:HA3	35:B:623:LHG:H371	1.93	0.50
4:D:78:ALA:CB	4:D:175:GLY:HA3	2.42	0.50
4:D:273:LEU:C	4:D:273:LEU:HD23	2.37	0.50
33:D:406:PL9:H111	35:D:407:LHG:HC92	1.94	0.50
38:G:608:CHL:C4	39:G:615:LUT:H28	2.41	0.50
28:N:611:CLA:H71	28:N:612:CLA:NA	2.26	0.50
1:a:333:GLU:HB2	1:a:337:HIS:HE1	1.76	0.50
3:c:282:PHE:HE1	28:c:501:CLA:H112	1.76	0.50
36:c:517:DGD:HBT1	36:c:517:DGD:C6B	2.41	0.50
7:g:119:VAL:H	38:g:605:CHL:CGD	2.25	0.50
28:g:604:CLA:HBB1	28:g:604:CLA:CMB	2.40	0.50
38:g:608:CHL:HAA2	38:g:608:CHL:H193	1.93	0.50
11:k:55:GLN:HA	11:k:58:VAL:HG22	1.94	0.50
35:n:618:LHG:H102	35:n:618:LHG:H272	1.92	0.50
28:r:612:CLA:H42	28:r:612:CLA:C1D	2.42	0.50
20:w:40:TYR:CE1	20:w:44:LEU:HD21	2.47	0.50
38:y:302:CHL:C3C	41:y:317:XAT:H362	2.41	0.50
1:A:36:LEU:HA	28:A:408:CLA:HBB2	1.94	0.50
1:A:179:THR:O	1:A:183:MET:HG3	2.11	0.50
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.94	0.50
28:B:601:CLA:H121	28:B:601:CLA:NB	2.26	0.50
3:C:173:PHE:HB3	3:C:177:PHE:CZ	2.47	0.50
32:C:520:LMG:H192	11:K:42:VAL:HG11	1.93	0.50
38:N:606:CHL:HAA2	38:N:606:CHL:HBD	1.92	0.50
14:O:207:THR:HG22	14:O:214:VAL:HG13	1.93	0.50
14:O:226:THR:HG22	14:O:233:PRO:HB3	1.93	0.50
17:R:184:LEU:HD11	39:R:614:LUT:H221	1.94	0.50
18:S:62:PHE:CD1	39:S:316:LUT:H222	2.46	0.50
18:S:158:LEU:HD22	38:S:308:CHL:OMC	2.12	0.50
22:Y:92:PHE:CE2	22:Y:113:LEU:HD23	2.44	0.50
22:Y:194:PHE:HE1	39:Y:615:LUT:H41	1.75	0.50
28:b:605:CLA:HBB1	28:b:605:CLA:HMB1	1.94	0.50
3:c:165:LEU:HD21	28:c:506:CLA:HAB	1.94	0.50
3:c:187:ASP:HB3	3:c:190:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:233:ILE:HA	30:i:101:BCR:H282	1.94	0.50
4:d:147:PHE:C	4:d:150:PRO:HD2	2.36	0.50
7:g:112:TYR:HE2	40:g:617:NEX:H1	1.58	0.50
7:g:200:VAL:CG2	38:g:619:CHL:H72	2.39	0.50
28:g:613:CLA:C1B	28:g:614:CLA:HMD2	2.42	0.50
12:l:24:LEU:HD13	35:l:101:LHG:H161	1.94	0.50
28:n:602:CLA:H203	28:n:602:CLA:H152	1.93	0.50
38:n:607:CHL:CBA	22:y:229:VAL:HA	2.41	0.50
17:r:24:LEU:HD21	28:r:602:CLA:HBD	1.93	0.50
28:s:609:CLA:H72	39:s:614:LUT:C30	2.42	0.50
22:y:148:LEU:HD12	38:y:308:CHL:C4B	2.42	0.50
2:B:464:PHE:HD2	28:B:611:CLA:HAC2	1.77	0.50
7:G:122:GLN:HB2	38:G:605:CHL:CBB	2.42	0.50
38:G:606:CHL:HMB1	38:G:609:CHL:HMC	1.93	0.50
14:O:63:GLU:HG2	14:O:234:LYS:HG2	1.93	0.50
15:P:96:GLN:HG2	15:P:106:ASN:HD21	1.77	0.50
17:R:39:LEU:CD1	41:R:615:XAT:H23	2.42	0.50
38:S:302:CHL:C1D	35:S:317:LHG:HC91	2.42	0.50
22:Y:153:ASP:OD2	22:Y:156:TYR:HB2	2.11	0.50
28:b:602:CLA:HED3	28:b:603:CLA:CMA	2.41	0.50
35:b:624:LHG:HC91	4:d:274:PHE:HE1	1.76	0.50
3:c:154:ARG:HH12	20:w:49:GLU:CG	2.20	0.50
3:c:203:THR:O	3:c:235:GLY:HA3	2.11	0.50
36:c:517:DGD:HD1	32:k:102:LMG:O2	2.11	0.50
4:d:12:GLN:HG2	4:d:14:ASP:HB3	1.93	0.50
4:d:273:LEU:C	4:d:273:LEU:HD23	2.36	0.50
18:s:182:ALA:O	18:s:186:LYS:HG3	2.12	0.50
1:A:284:TRP:CD1	3:C:435:PHE:HZ	2.29	0.50
28:B:603:CLA:C1C	28:B:605:CLA:H101	2.42	0.50
7:G:24:TYR:CD1	7:G:46:TRP:HB2	2.46	0.50
28:G:611:CLA:H71	28:G:612:CLA:C4D	2.42	0.50
38:N:608:CHL:C1	39:N:615:LUT:H383	2.42	0.50
22:Y:203:LYS:HB2	22:Y:208:ASN:ND2	2.26	0.50
1:a:274:PHE:CD1	31:a:411:SQD:H132	2.47	0.50
35:b:624:LHG:H162	12:l:24:LEU:HD21	1.94	0.50
36:b:625:DGD:HA31	8:h:58:LEU:HD11	1.93	0.50
3:c:76:VAL:HG23	3:c:79:LYS:HG2	1.93	0.50
3:c:131:TYR:OH	18:s:38:GLY:HA3	2.11	0.50
14:o:4:PRO:HG2	14:o:28:GLN:HE22	1.76	0.50
15:p:79:GLU:O	15:p:83:LYS:HG2	2.12	0.50
16:q:143:VAL:O	16:q:147:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:83:TYR:HB2	28:r:613:CLA:HED2	1.94	0.50
28:r:603:CLA:C3D	28:r:608:CLA:H61	2.42	0.50
18:s:99:ASN:OD1	18:s:105:CYS:HB2	2.11	0.50
18:s:205:ILE:HD12	28:s:612:CLA:HAC2	1.94	0.50
38:s:601:CHL:CAC	35:s:617:LHG:HC32	2.41	0.50
28:s:604:CLA:HBB1	39:s:615:LUT:H8	1.94	0.50
28:y:310:CLA:H42	39:y:315:LUT:H373	1.93	0.50
2:B:151:PHE:CE1	2:B:203:ILE:HG23	2.47	0.50
2:B:277:GLN:HB3	24:U:95:ARG:HD2	1.94	0.50
28:B:611:CLA:C2D	35:B:625:LHG:H372	2.42	0.50
36:C:519:DGD:HB71	36:C:519:DGD:HB22	1.93	0.50
4:D:39:PHE:HB2	4:D:40:PRO:HD3	1.94	0.50
4:D:52:GLY:HA2	4:D:56:VAL:HB	1.94	0.50
7:G:153:ASP:HB3	7:G:156:TYR:C	2.37	0.50
15:P:124:LYS:HZ3	15:P:185:VAL:HG23	1.76	0.50
16:Q:50:ARG:HA	16:Q:53:GLU:CD	2.37	0.50
18:S:31:ARG:CZ	18:S:51:GLY:H	2.24	0.50
18:S:178:ASP:HB3	18:S:181:GLN:HB2	1.93	0.50
18:S:196:ALA:O	18:S:200:MET:HG2	2.12	0.50
18:S:230:LEU:O	18:S:234:ILE:HG12	2.12	0.50
28:S:304:CLA:HBC1	28:S:309:CLA:CBC	2.41	0.50
39:S:315:LUT:H391	39:S:315:LUT:C32	2.42	0.50
28:Y:604:CLA:C1B	40:Y:618:NEX:H242	2.42	0.50
30:d:406:BCR:H363	6:f:27:PHE:CB	2.42	0.50
7:g:92:PHE:HE1	28:g:604:CLA:OBD	1.95	0.50
28:n:610:CLA:H12	28:n:610:CLA:H3A	1.93	0.50
42:n:701:HOH:O	28:s:611:CLA:H2	2.10	0.50
38:y:307:CHL:H2	40:y:318:NEX:C35	2.42	0.50
28:C:507:CLA:H2	28:C:507:CLA:HMA3	1.93	0.49
28:C:513:CLA:CAB	30:C:514:BCR:H402	2.42	0.49
7:G:49:ALA:HB3	7:G:51:LEU:CD1	2.42	0.49
7:G:203:LYS:HG3	7:G:208:ASN:ND2	2.27	0.49
18:S:83:ARG:O	18:S:87:LEU:HG	2.12	0.49
22:Y:98:PHE:HA	38:Y:607:CHL:CMA	2.42	0.49
22:Y:121:ALA:HA	38:Y:605:CHL:C1C	2.42	0.49
28:Y:611:CLA:H93	28:Y:612:CLA:CHD	2.42	0.49
2:b:489:GLN:HG2	2:b:499:GLY:HA2	1.92	0.49
3:c:65:GLY:HA2	3:c:115:GLY:HA2	1.93	0.49
28:g:602:CLA:H2	39:g:616:LUT:C28	2.40	0.49
15:p:146:LEU:HD22	15:p:176:VAL:HG12	1.94	0.49
16:q:39:ILE:HG23	16:q:83:TYR:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:r:603:CLA:O2D	28:r:608:CLA:H2	2.12	0.49
18:s:173:LEU:HD12	39:s:614:LUT:H222	1.94	0.49
28:y:304:CLA:C3B	38:y:309:CHL:H151	2.42	0.49
1:A:56:PRO:HA	1:A:73:TYR:CE2	2.47	0.49
2:B:327:ALA:HA	28:B:607:CLA:O1A	2.13	0.49
28:B:603:CLA:HAB	28:B:605:CLA:C16	2.42	0.49
7:G:92:PHE:CE2	7:G:113:LEU:HA	2.47	0.49
7:N:220:ASN:ND2	7:N:222:TRP:HD1	2.10	0.49
14:O:92:PRO:HD2	14:O:104:GLU:HB2	1.94	0.49
14:O:179:ARG:HA	14:O:182:GLU:HG3	1.94	0.49
18:S:124:LEU:HD12	18:S:131:ILE:HD12	1.94	0.49
2:b:25:MET:HG2	30:b:617:BCR:H23C	1.94	0.49
2:b:340:TRP:O	2:b:405:GLU:HG3	2.12	0.49
28:b:613:CLA:HMB1	28:b:613:CLA:HBB1	1.93	0.49
7:g:96:VAL:HG21	7:g:99:LYS:HZ3	1.77	0.49
7:g:187:ALA:O	7:g:191:MET:HG2	2.12	0.49
28:n:602:CLA:H93	28:n:603:CLA:HHB	1.95	0.49
14:o:60:VAL:HB	14:o:118:LEU:HD21	1.93	0.49
28:s:610:CLA:C4D	28:s:611:CLA:HMD3	2.42	0.49
28:y:313:CLA:H172	28:y:314:CLA:ND	2.27	0.49
2:B:114:HIS:HE1	28:B:616:CLA:ND	2.10	0.49
2:B:393:GLU:HG2	15:P:94:PHE:CE2	2.48	0.49
28:B:609:CLA:HBB1	28:B:609:CLA:HMB3	1.94	0.49
28:B:613:CLA:H172	30:B:618:BCR:H312	1.94	0.49
3:C:62:PHE:HZ	11:K:43:ILE:HD12	1.77	0.49
3:C:68:ASN:O	3:C:72:VAL:HG23	2.12	0.49
3:C:164:HIS:CD2	28:C:509:CLA:H91	2.47	0.49
28:C:511:CLA:H2	30:C:516:BCR:H272	1.93	0.49
30:C:516:BCR:H353	30:K:101:BCR:C7	2.42	0.49
4:D:126:PHE:CE2	29:D:402:PHO:HBD	2.47	0.49
7:G:81:PHE:CD2	28:G:604:CLA:HAC2	2.47	0.49
7:G:128:TRP:CE3	7:N:222:TRP:HZ2	2.31	0.49
7:G:129:ALA:O	7:G:133:ILE:HG13	2.11	0.49
28:S:310:CLA:HMC2	39:S:315:LUT:H32	1.94	0.49
3:c:179:ALA:CA	3:c:184:GLY:HA2	2.31	0.49
28:c:501:CLA:H193	28:c:506:CLA:C1B	2.42	0.49
28:d:401:CLA:H152	35:d:408:LHG:H211	1.94	0.49
35:d:408:LHG:C31	19:t:21:ILE:HD11	2.43	0.49
15:p:62:LEU:CD1	15:p:87:LEU:HD21	2.37	0.49
22:y:127:ILE:HG12	38:y:306:CHL:HAC1	1.94	0.49
38:y:302:CHL:HED3	38:y:302:CHL:H2A	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:HG23	28:B:605:CLA:HAC1	1.94	0.49
2:B:91:TRP:CD1	28:B:606:CLA:HBD	2.47	0.49
2:B:242:ILE:HA	2:B:245:VAL:HG22	1.93	0.49
10:J:15:THR:O	10:J:19:ILE:HG13	2.12	0.49
15:P:40:ARG:NH2	42:P:202:HOH:O	2.24	0.49
15:P:124:LYS:NZ	15:P:152:LYS:HD2	2.28	0.49
18:S:39:LEU:HD22	23:Z:41:PHE:HE1	1.77	0.49
22:Y:161:PHE:HA	38:Y:608:CHL:H72	1.95	0.49
1:a:273:PHE:HD2	31:a:411:SQD:H81	1.77	0.49
2:b:330:MET:HA	2:b:444:ARG:HB2	1.94	0.49
2:b:486:LEU:CD2	4:d:138:GLN:HB2	2.37	0.49
32:b:623:LMG:H111	38:r:606:CHL:HBD	1.94	0.49
28:c:501:CLA:C2D	28:c:503:CLA:H2	2.42	0.49
30:c:514:BCR:H343	23:z:51:VAL:HG12	1.94	0.49
35:c:519:LHG:HC12	35:c:519:LHG:O4	2.12	0.49
38:g:601:CHL:H52	28:y:304:CLA:HMD2	1.94	0.49
7:n:203:LYS:HB2	7:n:208:ASN:ND2	2.26	0.49
14:o:86:LEU:HB3	14:o:89:ILE:HD11	1.93	0.49
17:r:11:ARG:HH21	17:r:33:GLY:N	2.10	0.49
2:B:161:LEU:HD21	35:B:622:LHG:HC62	1.95	0.49
2:B:272:ARG:NH1	4:D:165:GLN:HA	2.27	0.49
3:C:95:LEU:HD11	28:C:503:CLA:HAA2	1.94	0.49
3:C:215:LYS:HG2	3:C:221:GLU:HB3	1.95	0.49
3:C:286:ALA:HB2	28:C:502:CLA:HMD1	1.95	0.49
4:D:126:PHE:CZ	29:D:402:PHO:HBD	2.48	0.49
28:G:610:CLA:C2	39:G:615:LUT:H26	2.42	0.49
11:K:53:VAL:CG2	30:K:101:BCR:H21C	2.38	0.49
14:O:79:MET:HE3	14:O:117:GLN:HB3	1.95	0.49
17:R:32:TYR:CD1	28:R:601:CLA:HAC2	2.48	0.49
17:R:105:LEU:HD21	28:R:609:CLA:H18	1.94	0.49
23:Z:58:ASN:HA	23:Z:61:ILE:CD1	2.42	0.49
1:a:274:PHE:HD1	31:a:411:SQD:H132	1.77	0.49
4:d:57:THR:HG21	5:e:50:PRO:HD3	1.94	0.49
28:d:401:CLA:CHA	28:d:401:CLA:HBA1	2.43	0.49
7:g:81:PHE:CE2	7:g:85:LEU:HD11	2.48	0.49
7:g:85:LEU:HB2	7:g:92:PHE:CE2	2.48	0.49
7:g:141:TYR:HB3	38:g:608:CHL:CMC	2.42	0.49
38:n:601:CHL:OBD	28:n:602:CLA:HHD	2.12	0.49
38:n:607:CHL:H192	38:y:302:CHL:H62	1.93	0.49
14:o:129:THR:OG1	14:o:131:LYS:HG3	2.12	0.49
38:r:605:CHL:HBD	38:r:605:CHL:HAA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:200:MET:HG3	18:s:204:PHE:CZ	2.48	0.49
22:y:163:PRO:HD2	39:y:315:LUT:H23	1.93	0.49
38:y:307:CHL:HAA2	38:y:307:CHL:HBD	1.95	0.49
28:y:311:CLA:C4D	28:y:312:CLA:HMD3	2.42	0.49
1:A:160:ILE:HD11	36:C:517:DGD:HBW2	1.95	0.49
28:B:606:CLA:CMC	35:B:623:LHG:H352	2.43	0.49
3:C:153:ASP:O	3:C:157:MET:HG2	2.12	0.49
3:C:274:TYR:HB3	28:C:507:CLA:C3B	2.42	0.49
28:R:603:CLA:OBD	28:R:608:CLA:HAA1	2.12	0.49
28:S:303:CLA:H2	39:S:316:LUT:H26	1.94	0.49
35:a:415:LHG:H312	35:a:415:LHG:C17	2.42	0.49
2:b:399:VAL:HG13	2:b:411:TYR:HD1	1.78	0.49
28:b:614:CLA:H161	30:b:617:BCR:C12	2.43	0.49
28:c:508:CLA:C3B	28:c:510:CLA:HMA2	2.43	0.49
28:c:512:CLA:HBB1	28:c:512:CLA:HMB3	1.94	0.49
4:d:181:ARG:C	4:d:181:ARG:HD3	2.37	0.49
7:n:157:PRO:HD2	28:n:610:CLA:OBD	2.13	0.49
15:p:51:ASP:HB3	15:p:54:ASP:O	2.12	0.49
16:q:54:SER:HB3	16:q:81:ALA:HA	1.94	0.49
28:r:609:CLA:H52	39:r:614:LUT:C30	2.38	0.49
20:w:40:TYR:CZ	20:w:44:LEU:HD11	2.48	0.49
22:y:71:TRP:CE2	38:y:308:CHL:HED2	2.47	0.49
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.95	0.49
28:C:513:CLA:H52	35:S:301:LHG:H102	1.94	0.49
35:C:521:LHG:H211	41:Y:617:XAT:H373	1.95	0.49
4:D:82:PRO:HB3	4:D:86:LEU:HD12	1.94	0.49
7:G:153:ASP:OD2	7:G:156:TYR:HB2	2.12	0.49
7:N:22:VAL:HG12	7:N:44:TYR:CE2	2.48	0.49
7:N:118:LEU:HD22	38:N:605:CHL:HED2	1.95	0.49
15:P:163:ALA:HB2	15:P:176:VAL:HG21	1.95	0.49
16:Q:88:LEU:O	16:Q:92:ILE:HG23	2.13	0.49
18:S:60:ASP:HB2	28:S:303:CLA:HBA2	1.94	0.49
18:S:64:LEU:HB2	28:S:303:CLA:O1A	2.13	0.49
30:T:101:BCR:H381	2:b:33:TRP:HD1	1.78	0.49
1:a:343:LEU:HD12	1:a:344:ALA:N	2.27	0.49
2:b:162:PHE:O	28:b:606:CLA:HMD3	2.13	0.49
3:c:171:GLY:HA2	3:c:174:LEU:HD12	1.94	0.49
6:f:36:PHE:HB2	15:p:8:VAL:HG13	1.93	0.49
7:n:59:SER:O	7:n:63:GLU:HG3	2.13	0.49
23:z:14:VAL:O	23:z:18:ILE:HG13	2.12	0.49
1:A:298:ASN:HB2	42:A:503:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:408:CLA:HMA2	32:A:411:LMG:H142	1.95	0.49
2:B:85:ILE:HG12	2:B:88:PRO:HA	1.95	0.49
2:B:112:ILE:HG22	30:B:619:BCR:H402	1.93	0.49
30:B:618:BCR:H321	30:B:618:BCR:HC8	1.95	0.49
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.95	0.49
3:C:144:PHE:CE1	28:C:513:CLA:HAA1	2.47	0.49
28:C:505:CLA:HBB1	28:C:505:CLA:CMB	2.43	0.49
6:F:20:LEU:C	6:F:23:PRO:HD2	2.38	0.49
15:P:54:ASP:OD2	15:P:167:ARG:HG3	2.12	0.49
17:R:32:TYR:CE1	28:R:601:CLA:HAC2	2.47	0.49
18:S:73:LYS:HG3	18:S:74:TYR:N	2.28	0.49
18:S:87:LEU:HD11	28:S:310:CLA:HAC1	1.95	0.49
28:S:313:CLA:CGA	28:S:313:CLA:C1A	2.91	0.49
22:Y:148:LEU:HD12	38:Y:608:CHL:C4B	2.43	0.49
28:Y:604:CLA:HMA3	38:Y:606:CHL:C3C	2.43	0.49
28:b:601:CLA:O1A	28:b:601:CLA:H143	2.13	0.49
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.93	0.49
28:g:602:CLA:C3B	28:g:602:CLA:H51	2.42	0.49
38:g:606:CHL:HMB1	38:g:609:CHL:HMC	1.95	0.49
39:g:616:LUT:H363	38:y:309:CHL:H11	1.94	0.49
20:w:34:TRP:CE3	35:w:102:LHG:H162	2.48	0.49
22:y:35:TYR:OH	22:y:50:GLY:HA2	2.12	0.49
1:A:131:TRP:CD2	28:C:505:CLA:HMA1	2.48	0.49
1:A:333:GLU:HB3	1:A:336:ALA:CB	2.42	0.49
3:C:406:SER:HA	3:C:420:VAL:CG2	2.42	0.49
28:C:511:CLA:H93	30:C:516:BCR:H383	1.95	0.49
5:E:26:THR:HB	37:E:101:HEM:CAB	2.41	0.49
7:G:77:LEU:O	7:G:81:PHE:HB2	2.13	0.49
28:G:602:CLA:H162	39:G:616:LUT:H31	1.95	0.49
9:I:9:TYR:O	9:I:13:ILE:HG22	2.13	0.49
12:L:19:TYR:CE1	31:L:103:SQD:H262	2.47	0.49
7:N:191:MET:HA	7:N:194:PHE:HD2	1.78	0.49
28:R:612:CLA:HBB1	39:R:614:LUT:H8	1.94	0.49
28:R:613:CLA:HHC	28:R:613:CLA:CBB	2.43	0.49
22:Y:22:VAL:HG22	38:Y:601:CHL:HBC3	1.95	0.49
1:a:81:ALA:CB	1:a:175:GLY:HA3	2.43	0.49
1:a:200:LEU:CD2	36:c:518:DGD:HAW2	2.43	0.49
31:a:411:SQD:H332	11:k:52:PHE:CZ	2.48	0.49
2:b:151:PHE:CE2	32:b:623:LMG:H381	2.47	0.49
2:b:453:PHE:CD2	32:b:620:LMG:H201	2.48	0.49
35:c:520:LHG:H151	28:s:610:CLA:CBB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:224:PHE:HE2	4:d:243:GLU:HG3	1.77	0.49
7:g:81:PHE:CD1	28:g:604:CLA:HAC2	2.47	0.49
38:g:606:CHL:HMC	39:g:616:LUT:H163	1.94	0.49
28:r:601:CLA:CHD	35:r:617:LHG:HC92	2.43	0.49
28:r:603:CLA:CED	28:r:608:CLA:H51	2.42	0.49
28:r:604:CLA:H2	40:r:616:NEX:C24	2.36	0.49
28:r:604:CLA:HMA3	38:r:605:CHL:C2C	2.43	0.49
18:s:46:PRO:HG2	18:s:49:LEU:HD22	1.93	0.49
18:s:87:LEU:HB3	28:s:604:CLA:HAB	1.95	0.49
22:y:221:ALA:HB3	41:y:317:XAT:H193	1.94	0.49
1:A:113:GLU:O	1:A:117:LEU:HG	2.13	0.49
2:B:29:LEU:HD11	30:B:617:BCR:H19C	1.94	0.49
28:C:509:CLA:CAD	28:C:509:CLA:H151	2.43	0.49
28:C:513:CLA:C1A	28:C:513:CLA:CGA	2.91	0.49
35:C:521:LHG:H282	28:Y:611:CLA:C2C	2.43	0.49
4:D:159:LEU:C	4:D:162:PRO:HD2	2.38	0.49
5:E:8:ARG:HE	5:E:13:ILE:HG12	1.78	0.49
7:N:141:TYR:HB3	38:N:608:CHL:CMC	2.43	0.49
7:N:203:LYS:HB3	7:N:207:GLU:CD	2.38	0.49
28:N:602:CLA:C20	39:N:616:LUT:H391	2.43	0.49
17:R:37:PHE:CE2	41:R:615:XAT:H221	2.48	0.49
17:R:52:SER:HB2	17:R:60:ASN:HB3	1.93	0.49
17:R:146:THR:O	17:R:150:ILE:HG12	2.13	0.49
1:a:43:THR:HA	30:a:410:BCR:H362	1.94	0.49
2:b:19:LEU:O	2:b:22:VAL:HG22	2.13	0.49
28:b:614:CLA:H8	30:b:617:BCR:H362	1.93	0.49
28:c:511:CLA:C7	30:c:515:BCR:H402	2.40	0.49
12:l:15:ARG:HG2	12:l:19:TYR:CE2	2.47	0.49
7:n:81:PHE:O	7:n:85:LEU:HG	2.12	0.49
15:p:84:VAL:HG23	15:p:86:TYR:CE2	2.48	0.49
17:r:94:GLU:HG2	17:r:172:LEU:HD13	1.95	0.49
28:s:609:CLA:H52	39:s:614:LUT:C30	2.30	0.49
28:s:612:CLA:CGA	28:s:612:CLA:C1A	2.91	0.49
31:B:620:SQD:H382	19:t:8:PHE:HZ	1.78	0.48
3:C:144:PHE:HD1	35:S:301:LHG:HC12	1.78	0.48
28:N:603:CLA:HMA3	28:N:603:CLA:H61	1.95	0.48
14:O:227:ASP:HB3	14:O:230:ALA:HB3	1.95	0.48
22:Y:122:GLN:HB2	38:Y:605:CHL:CBB	2.42	0.48
28:a:409:CLA:H43	32:w:101:LMG:H121	1.95	0.48
2:b:125:ASP:CG	2:b:127:ARG:HG2	2.37	0.48
35:c:520:LHG:H121	35:c:520:LHG:H152	1.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:606:CHL:HBB1	39:g:616:LUT:H161	1.95	0.48
17:r:230:HIS:CE1	17:r:234:PRO:HA	2.47	0.48
28:r:608:CLA:HBA2	28:r:608:CLA:H3A	1.44	0.48
18:s:134:ASN:H	18:s:137:LEU:HD12	1.78	0.48
18:s:221:HIS:CG	28:s:612:CLA:HAA2	2.48	0.48
28:A:408:CLA:HAA2	32:A:411:LMG:C11	2.42	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.95	0.48
3:C:163:ILE:HG21	28:C:512:CLA:C3B	2.43	0.48
3:C:257:PHE:O	3:C:261:ARG:HG3	2.13	0.48
28:C:506:CLA:H142	35:W:101:LHG:H352	1.94	0.48
4:D:74:PHE:CZ	32:D:408:LMG:H202	2.48	0.48
28:D:404:CLA:H51	21:X:61:GLY:HA3	1.96	0.48
17:R:39:LEU:HD13	28:R:602:CLA:H42	1.95	0.48
18:S:71:PHE:HE1	28:S:303:CLA:H2A	1.77	0.48
18:S:111:TRP:CH2	38:S:307:CHL:H102	2.48	0.48
28:Y:610:CLA:O1A	28:Y:610:CLA:H3A	2.13	0.48
1:a:239:PHE:O	19:t:30:PRO:HG3	2.12	0.48
1:a:330:VAL:HB	4:d:349:ARG:HG3	1.94	0.48
28:a:407:CLA:H2	29:d:402:PHO:C2B	2.43	0.48
2:b:394:GLN:HA	16:q:1:GLU:HG2	1.95	0.48
35:b:622:LHG:H102	35:b:622:LHG:H242	1.94	0.48
4:d:78:ALA:CB	4:d:175:GLY:HA3	2.42	0.48
5:e:8:ARG:NH2	5:e:13:ILE:HG23	2.28	0.48
12:l:18:LEU:HD22	13:m:26:TYR:CG	2.48	0.48
38:y:302:CHL:C4C	41:y:317:XAT:H362	2.43	0.48
1:A:291:SER:O	1:A:294:ALA:HB3	2.14	0.48
30:A:409:BCR:H401	36:A:417:DGD:HD61	1.94	0.48
31:A:414:SQD:H381	28:b:606:CLA:H112	1.94	0.48
2:B:30:VAL:HG13	28:B:613:CLA:HMC2	1.94	0.48
28:B:609:CLA:HMA3	28:B:610:CLA:C1C	2.43	0.48
5:E:28:PRO:O	5:E:32:ILE:HG12	2.14	0.48
7:G:85:LEU:HB3	7:G:90:VAL:CG1	2.43	0.48
7:N:127:ILE:HG12	38:N:605:CHL:CBC	2.42	0.48
7:N:195:PHE:CD1	38:N:607:CHL:H71	2.49	0.48
38:Y:605:CHL:HBD	38:Y:605:CHL:HAA1	1.96	0.48
3:c:28:GLN:HA	3:c:31:THR:OG1	2.13	0.48
3:c:404:LEU:HD11	36:c:518:DGD:HB71	1.95	0.48
28:d:401:CLA:H171	35:d:408:LHG:H221	1.94	0.48
28:n:603:CLA:H193	38:n:609:CHL:H51	1.95	0.48
28:n:603:CLA:H2	28:n:603:CLA:HED2	1.94	0.48
14:o:63:GLU:HA	14:o:71:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:218:PHE:HB3	14:o:242:TRP:HD1	1.78	0.48
38:r:605:CHL:H111	38:r:607:CHL:H101	1.94	0.48
22:y:67:ILE:HG13	38:y:309:CHL:HED2	1.96	0.48
3:C:113:VAL:HG13	30:C:514:BCR:H313	1.95	0.48
3:C:168:LEU:HA	28:C:512:CLA:H42	1.95	0.48
28:C:512:CLA:C3B	30:C:514:BCR:H291	2.44	0.48
30:C:516:BCR:H19C	11:K:47:PHE:CE1	2.49	0.48
4:D:181:ARG:C	4:D:181:ARG:HD3	2.38	0.48
6:F:14:TRP:CE2	6:F:18:HIS:CE1	3.02	0.48
7:N:150:GLU:O	38:N:608:CHL:HBC1	2.13	0.48
38:N:606:CHL:C4	40:N:617:NEX:H14	2.43	0.48
14:O:76:THR:HB	14:O:116:VAL:HB	1.95	0.48
28:S:304:CLA:OBD	28:S:309:CLA:HAA1	2.13	0.48
22:Y:139:GLU:O	22:Y:143:ILE:HG12	2.14	0.48
28:Y:602:CLA:H202	39:Y:616:LUT:H391	1.95	0.48
28:Y:603:CLA:H91	38:Y:609:CHL:C9	2.43	0.48
1:a:43:THR:HG23	30:a:410:BCR:C36	2.43	0.48
28:b:604:CLA:C2D	28:b:612:CLA:H171	2.43	0.48
28:b:606:CLA:CAD	35:b:622:LHG:HC62	2.44	0.48
28:b:616:CLA:HMA1	28:b:616:CLA:H92	1.95	0.48
28:c:513:CLA:CGA	28:c:513:CLA:C1A	2.91	0.48
35:c:520:LHG:O9	35:c:520:LHG:HC12	2.13	0.48
4:d:216:GLY:O	4:d:220:GLU:HG2	2.14	0.48
8:h:52:VAL:O	8:h:56:ILE:HG13	2.13	0.48
7:n:85:LEU:HD12	7:n:92:PHE:HZ	1.77	0.48
28:n:602:CLA:H141	39:n:616:LUT:H393	1.95	0.48
28:r:603:CLA:HBB1	28:r:603:CLA:HMB3	1.95	0.48
28:r:611:CLA:HHC	28:r:611:CLA:CBB	2.39	0.48
22:y:109:GLY:HA3	22:y:122:GLN:HG2	1.94	0.48
1:A:93:PHE:CZ	28:A:408:CLA:HAA1	2.40	0.48
1:A:273:PHE:CE2	31:A:410:SQD:H121	2.48	0.48
3:C:373:ASN:ND2	14:O:26:ALA:HA	2.28	0.48
28:G:610:CLA:H2	39:G:615:LUT:H26	1.95	0.48
8:H:69:GLN:H	8:H:69:GLN:CD	2.22	0.48
38:N:606:CHL:HBB1	39:N:616:LUT:H161	1.96	0.48
14:O:194:ALA:HA	15:P:96:GLN:OE1	2.13	0.48
17:R:167:ASP:OD2	17:R:170:LYS:HG2	2.13	0.48
18:S:83:ARG:HA	18:S:86:MET:HE3	1.96	0.48
1:a:131:TRP:CZ2	3:c:449:ARG:HG3	2.49	0.48
28:c:506:CLA:CHA	28:c:507:CLA:H192	2.44	0.48
28:c:506:CLA:HMC2	28:c:507:CLA:H93	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:513:CLA:HBA1	28:c:513:CLA:CBD	2.38	0.48
4:d:74:PHE:HB2	32:d:409:LMG:H291	1.96	0.48
4:d:114:PHE:CZ	30:d:406:BCR:H323	2.47	0.48
28:d:401:CLA:HBB1	28:d:401:CLA:HMB3	1.96	0.48
30:d:406:BCR:H383	32:d:409:LMG:H182	1.95	0.48
5:e:37:PHE:CZ	5:e:47:PHE:HE1	2.31	0.48
7:g:77:LEU:HD22	28:g:612:CLA:CBB	2.44	0.48
38:g:601:CHL:H13	38:g:601:CHL:H203	1.94	0.48
14:o:185:LEU:HA	14:o:188:GLU:OE2	2.14	0.48
17:r:23:TYR:OH	17:r:38:GLY:HA2	2.14	0.48
17:r:196:LEU:O	17:r:199:ILE:HG22	2.13	0.48
18:s:80:ILE:HG22	18:s:84:TRP:HD1	1.79	0.48
18:s:114:THR:HG23	18:s:117:LEU:HD12	1.95	0.48
28:y:310:CLA:HBA1	39:y:315:LUT:H382	1.96	0.48
28:y:311:CLA:H62	28:y:312:CLA:C4D	2.43	0.48
1:A:70:SER:HB3	1:A:73:TYR:CD1	2.49	0.48
1:A:211:PHE:HE2	1:A:278:TRP:CG	2.31	0.48
32:A:411:LMG:HC62	20:W:8:THR:O	2.13	0.48
42:A:504:HOH:O	3:C:424:SER:HB3	2.12	0.48
2:B:51:VAL:CG2	14:o:67:LYS:HG3	2.43	0.48
28:B:601:CLA:H151	28:B:601:CLA:C4B	2.43	0.48
28:B:615:CLA:H143	28:B:616:CLA:HED1	1.94	0.48
3:C:165:LEU:HD21	28:C:506:CLA:HAB	1.94	0.48
3:C:180:PHE:CE2	3:C:200:THR:HA	2.48	0.48
3:C:225:VAL:CG2	36:C:517:DGD:HB22	2.43	0.48
3:C:261:ARG:NH1	20:W:50:SER:H	2.11	0.48
3:C:437:LEU:HA	28:C:508:CLA:HMC2	1.94	0.48
7:N:160:SER:O	7:N:163:PRO:HD3	2.14	0.48
18:S:124:LEU:C	18:S:125:ASN:HD22	2.22	0.48
18:S:221:HIS:CG	28:S:313:CLA:HAA2	2.48	0.48
21:X:81:VAL:HB	21:X:83:ARG:NH2	2.29	0.48
22:Y:135:MET:HB2	38:Y:609:CHL:CBB	2.43	0.48
2:b:70:GLY:HA2	2:b:178:VAL:CG2	2.41	0.48
2:b:224:ARG:HG3	8:h:37:TRP:CD2	2.49	0.48
28:b:607:CLA:C1C	32:b:620:LMG:H141	2.43	0.48
30:c:514:BCR:H352	32:c:521:LMG:H402	1.94	0.48
4:d:352:ALA:HA	15:p:138:GLY:O	2.13	0.48
5:e:74:GLU:O	5:e:78:GLU:HG3	2.14	0.48
7:g:44:TYR:HE2	38:g:601:CHL:HBC2	1.79	0.48
7:g:227:ASN:HB2	38:g:619:CHL:C1D	2.44	0.48
38:g:608:CHL:H42	39:g:615:LUT:H27	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:26:LEU:HG	11:k:27:PRO:HD2	1.94	0.48
14:o:39:PHE:CE2	14:o:41:PHE:HB2	2.48	0.48
18:s:116:ALA:HB2	38:s:606:CHL:HED2	1.96	0.48
22:y:209:LEU:HD11	28:y:314:CLA:HMC1	1.96	0.48
1:A:42:LEU:CD2	31:A:414:SQD:H202	2.43	0.48
1:A:49:ILE:HG12	33:D:406:PL9:H511	1.96	0.48
1:A:334:ARG:HD2	14:O:157:LEU:HB2	1.96	0.48
30:A:409:BCR:H363	32:A:413:LMG:H342	1.94	0.48
28:B:603:CLA:H171	8:H:50:PHE:CE2	2.49	0.48
3:C:180:PHE:O	3:C:198:LYS:HD3	2.14	0.48
7:G:189:PHE:CD1	28:G:613:CLA:HAB	2.49	0.48
7:G:209:LEU:O	7:G:213:LEU:N	2.47	0.48
8:H:30:TYR:CE1	17:R:50:LEU:HG	2.49	0.48
31:L:101:SQD:H272	31:L:101:SQD:H152	1.96	0.48
7:N:58:PHE:CE2	7:N:62:ARG:HD2	2.49	0.48
7:N:139:GLU:O	7:N:143:ILE:HG12	2.13	0.48
15:P:47:LEU:HD23	15:P:47:LEU:C	2.39	0.48
15:P:146:LEU:HD22	15:P:176:VAL:HG12	1.94	0.48
17:R:23:TYR:OH	17:R:38:GLY:HA2	2.13	0.48
17:R:174:PRO:HB3	38:R:607:CHL:HBC2	1.96	0.48
28:R:602:CLA:H112	28:R:602:CLA:H93	1.58	0.48
22:Y:81:PHE:CD2	28:Y:604:CLA:HHD	2.49	0.48
1:a:52:PHE:CD1	33:d:407:PL9:H48	2.48	0.48
3:c:42:LEU:HD22	3:c:48:LYS:HB3	1.95	0.48
3:c:271:TYR:HA	3:c:274:TYR:CD2	2.49	0.48
28:c:501:CLA:H171	28:c:507:CLA:H122	1.95	0.48
4:d:313:GLU:HB2	14:o:159:PRO:HG3	1.94	0.48
7:n:141:TYR:HB3	38:n:608:CHL:CMC	2.43	0.48
14:o:199:LYS:NZ	14:o:199:LYS:HB3	2.28	0.48
38:r:605:CHL:H93	40:r:616:NEX:H35	1.96	0.48
20:w:40:TYR:CE2	20:w:44:LEU:HD11	2.49	0.48
22:y:225:ALA:O	41:y:317:XAT:H42	2.14	0.48
1:A:46:SER:CB	30:A:409:BCR:H17C	2.44	0.48
2:B:379:ALA:HB2	2:B:395:VAL:HG11	1.96	0.48
2:B:434:ARG:NH2	14:O:179:ARG:HD2	2.29	0.48
5:E:22:ILE:O	5:E:26:THR:HG23	2.14	0.48
28:N:614:CLA:H11	28:N:614:CLA:CHA	2.44	0.48
14:O:104:GLU:HB2	14:O:106:LYS:HE2	1.95	0.48
17:R:149:TRP:O	17:R:153:LEU:HG	2.14	0.48
18:S:124:LEU:CD1	18:S:131:ILE:HD12	2.42	0.48
18:S:149:ALA:HA	18:S:152:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:139:GLU:HG3	38:Y:609:CHL:C4B	2.44	0.48
28:Y:604:CLA:H12	40:Y:618:NEX:H241	1.96	0.48
1:a:131:TRP:HZ2	3:c:449:ARG:HG3	1.78	0.48
1:a:147:TYR:CE1	28:a:406:CLA:H91	2.49	0.48
4:d:222:THR:HG21	4:d:250:ALA:HB2	1.96	0.48
29:d:402:PHO:HBB1	29:d:402:PHO:CMB	2.43	0.48
7:g:155:LEU:HD12	7:g:156:TYR:CZ	2.48	0.48
9:i:6:LEU:HD23	20:w:22:LEU:HD13	1.96	0.48
9:i:16:VAL:HG13	32:w:101:LMG:C21	2.44	0.48
3:C:52:ALA:HB2	28:C:511:CLA:HMA1	1.96	0.48
28:C:503:CLA:HBA2	28:C:503:CLA:CHA	2.43	0.48
4:D:44:PHE:HB3	4:D:114:PHE:CZ	2.49	0.48
5:E:75:GLN:HG2	5:E:79:PHE:CE2	2.49	0.48
7:G:119:VAL:HG13	38:G:605:CHL:CHD	2.42	0.48
28:G:610:CLA:CBB	39:G:615:LUT:H34	2.43	0.48
7:N:63:GLU:HA	7:N:155:LEU:HD11	1.96	0.48
7:N:101:GLY:HA2	38:N:606:CHL:HAC2	1.96	0.48
14:O:4:PRO:HG2	14:O:28:GLN:NE2	2.29	0.48
18:S:65:SER:HB2	42:S:403:HOH:O	2.14	0.48
1:a:82:ILE:HB	1:a:174:LEU:HB2	1.95	0.48
28:b:601:CLA:H192	30:h:101:BCR:C17	2.43	0.48
7:g:166:LEU:HD12	28:g:610:CLA:H12	1.96	0.48
7:n:176:LEU:HB3	28:n:610:CLA:HMA2	1.96	0.48
28:n:604:CLA:NB	40:n:617:NEX:H242	2.29	0.48
16:q:69:ALA:HB1	16:q:72:PHE:HD2	1.78	0.48
2:B:347:ARG:HB2	2:B:398:ILE:HD11	1.96	0.48
3:C:135:LEU:HD21	23:Z:33:TRP:CE2	2.49	0.48
7:G:147:PRO:HD2	38:G:608:CHL:CBB	2.44	0.48
28:N:602:CLA:H72	39:N:616:LUT:H30	1.96	0.48
15:P:19:LEU:HD13	15:P:32:ALA:HB2	1.95	0.48
15:P:84:VAL:HA	15:P:86:TYR:CE1	2.49	0.48
17:R:182:LEU:N	17:R:182:LEU:HD12	2.29	0.48
18:S:230:LEU:HD13	28:S:313:CLA:CMD	2.43	0.48
19:T:10:LEU:O	19:T:14:LEU:HG	2.14	0.48
22:Y:138:VAL:HA	22:Y:141:TYR:HD2	1.79	0.48
1:a:308:ASP:OD1	1:a:312:ARG:N	2.46	0.48
36:a:401:DGD:HAE2	32:a:413:LMG:H371	1.96	0.48
28:b:609:CLA:HAA1	8:h:43:MET:SD	2.54	0.48
28:c:501:CLA:C3	28:c:503:CLA:H92	2.43	0.48
6:f:30:SER:O	6:f:34:MET:HG3	2.14	0.48
7:g:81:PHE:CG	28:g:604:CLA:HAC2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:603:CLA:C4B	38:n:609:CHL:H122	2.44	0.48
15:p:78:GLU:HG3	15:p:113:ILE:HD12	1.95	0.48
16:q:73:LEU:O	16:q:77:LEU:HD13	2.13	0.48
38:r:605:CHL:H101	40:r:616:NEX:C35	2.44	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
30:B:617:BCR:H383	31:B:620:SQD:H102	1.96	0.47
7:G:128:TRP:HH2	28:N:614:CLA:CGA	2.26	0.47
7:G:146:GLY:H	38:G:608:CHL:CMC	2.27	0.47
7:G:153:ASP:HB3	7:G:156:TYR:O	2.14	0.47
7:G:187:ALA:O	7:G:191:MET:HG2	2.14	0.47
28:G:604:CLA:C4A	40:G:617:NEX:H242	2.44	0.47
8:H:63:SER:OG	8:H:72:MET:HE2	2.14	0.47
18:S:176:ALA:HB3	28:S:310:CLA:HED1	1.96	0.47
41:Y:617:XAT:H31	41:Y:617:XAT:H391	1.60	0.47
28:b:615:CLA:H192	28:b:616:CLA:HMC2	1.96	0.47
3:c:202:PHE:HA	3:c:231:GLU:HB3	1.96	0.47
7:g:63:GLU:O	7:g:66:VAL:HG22	2.14	0.47
28:g:603:CLA:H152	28:n:602:CLA:H122	1.95	0.47
13:m:4:ASN:HD22	13:m:5:ILE:N	2.11	0.47
38:n:607:CHL:H142	38:n:609:CHL:H121	1.95	0.47
14:o:216:GLY:HA3	14:o:242:TRP:CZ2	2.49	0.47
28:r:612:CLA:H13	28:r:612:CLA:H91	1.95	0.47
38:s:605:CHL:HAA2	38:s:605:CHL:HBD	1.94	0.47
22:y:27:PRO:HD2	38:y:302:CHL:CBB	2.44	0.47
22:y:94:GLU:HG2	22:y:99:LYS:C	2.39	0.47
38:y:307:CHL:H2	40:y:318:NEX:H401	1.96	0.47
1:A:121:LEU:HB2	28:C:505:CLA:H18	1.95	0.47
2:B:467:ILE:HG21	4:D:127:MET:CE	2.43	0.47
28:B:601:CLA:HHC	28:B:601:CLA:CBB	2.45	0.47
28:B:603:CLA:HMD3	28:B:606:CLA:HAB	1.95	0.47
28:B:613:CLA:H192	30:B:618:BCR:HC42	1.95	0.47
28:C:506:CLA:H52	30:C:515:BCR:C10	2.37	0.47
4:D:224:PHE:HE2	4:D:243:GLU:HG3	1.77	0.47
28:G:603:CLA:CAD	38:G:609:CHL:H2	2.43	0.47
10:J:20:VAL:O	10:J:24:LEU:HG	2.14	0.47
13:M:28:LYS:HG3	13:m:31:SER:HB2	1.96	0.47
7:N:158:GLY:N	28:N:610:CLA:HED2	2.29	0.47
22:Y:153:ASP:HB3	22:Y:156:TYR:O	2.14	0.47
38:Y:601:CHL:HED3	35:Y:619:LHG:H131	1.95	0.47
28:Y:613:CLA:H13	28:Y:613:CLA:H101	1.53	0.47
1:a:131:TRP:CD2	28:c:505:CLA:HMA1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:408:PHO:C3B	28:d:401:CLA:H2	2.43	0.47
28:c:510:CLA:H3A	28:c:510:CLA:HBA1	1.39	0.47
32:c:521:LMG:H161	18:s:226:PHE:CE2	2.49	0.47
4:d:240:GLN:HE22	4:d:244:THR:HB	1.78	0.47
5:e:76:LEU:HA	5:e:79:PHE:CD2	2.49	0.47
7:g:81:PHE:O	7:g:85:LEU:HG	2.14	0.47
7:g:189:PHE:CE1	28:g:613:CLA:HAB	2.49	0.47
16:q:47:ALA:O	16:q:51:THR:HG23	2.14	0.47
28:r:610:CLA:HHC	28:r:610:CLA:HBB1	1.95	0.47
28:B:608:CLA:C1A	28:B:608:CLA:CGA	2.92	0.47
3:C:177:PHE:HA	3:C:181:TYR:CD2	2.45	0.47
36:C:518:DGD:HB22	32:C:520:LMG:H302	1.97	0.47
4:D:3:ILE:CD1	17:R:47:GLN:HG2	2.42	0.47
14:O:79:MET:HE3	14:O:117:GLN:CB	2.44	0.47
15:P:157:TYR:CG	15:P:185:VAL:HG11	2.50	0.47
38:R:605:CHL:HMB2	28:R:608:CLA:HMC2	1.94	0.47
28:R:609:CLA:O2A	39:R:614:LUT:H26	2.14	0.47
18:S:96:GLU:HA	18:S:109:ALA:HB1	1.97	0.47
28:S:311:CLA:HHB	35:S:317:LHG:HC11	1.96	0.47
22:Y:35:TYR:OH	22:Y:50:GLY:HA2	2.14	0.47
28:Y:610:CLA:H3A	28:Y:610:CLA:CGA	2.44	0.47
1:a:285:PHE:CE1	36:c:518:DGD:HBW1	2.49	0.47
1:a:300:PHE:HB3	1:a:302:PHE:CE2	2.49	0.47
28:a:406:CLA:H93	29:a:408:PHO:NA	2.29	0.47
2:b:236:THR:HB	2:b:473:THR:HG21	1.96	0.47
28:c:506:CLA:HBB1	28:c:506:CLA:CMB	2.43	0.47
4:d:12:GLN:CD	4:d:14:ASP:HB3	2.39	0.47
4:d:79:VAL:HB	4:d:174:PHE:HB2	1.95	0.47
4:d:192:TRP:CE2	4:d:198:HIS:HB2	2.48	0.47
29:d:402:PHO:H152	28:d:404:CLA:H202	1.96	0.47
7:g:124:ILE:HG13	7:n:222:TRP:HZ3	1.79	0.47
38:g:601:CHL:H122	28:y:304:CLA:H202	1.96	0.47
38:n:606:CHL:HAB	39:n:616:LUT:H161	1.96	0.47
17:r:57:LEU:HB2	17:r:60:ASN:OD1	2.14	0.47
28:r:609:CLA:C2	39:r:614:LUT:H28	2.33	0.47
18:s:108:GLU:H	18:s:117:LEU:HD11	1.78	0.47
18:s:163:LYS:HA	38:s:607:CHL:CBC	2.44	0.47
2:B:152:GLY:C	28:B:606:CLA:HMC2	2.40	0.47
28:B:614:CLA:H2	28:B:614:CLA:ND	2.29	0.47
35:B:623:LHG:H292	35:B:623:LHG:H131	1.95	0.47
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:PRO:HG2	7:G:16:TRP:CD1	2.48	0.47
7:N:112:TYR:CD1	7:N:113:LEU:HG	2.50	0.47
28:N:604:CLA:NA	40:N:617:NEX:H242	2.29	0.47
16:Q:81:ALA:HB1	16:Q:84:LEU:HD12	1.95	0.47
17:R:30:GLY:HA3	17:R:199:ILE:HG21	1.95	0.47
38:R:605:CHL:HMA1	38:R:605:CHL:O1A	2.14	0.47
28:S:313:CLA:H42	28:S:313:CLA:C1D	2.44	0.47
38:Y:606:CHL:HBB2	38:Y:607:CHL:CBB	2.44	0.47
1:a:161:TYR:HA	1:a:294:ALA:HB2	1.95	0.47
28:a:407:CLA:O2D	36:c:518:DGD:HAF1	2.15	0.47
3:c:141:GLU:HA	3:c:148:GLY:HA3	1.96	0.47
30:c:514:BCR:H352	32:c:521:LMG:H382	1.96	0.47
9:i:2:LEU:O	9:i:6:LEU:HG	2.15	0.47
28:n:610:CLA:H61	28:n:610:CLA:H41	1.62	0.47
14:o:170:ASN:HB2	14:o:180:GLY:O	2.14	0.47
15:p:74:TYR:HE1	15:p:151:VAL:CG2	2.27	0.47
15:p:157:TYR:HB3	15:p:183:PHE:HZ	1.80	0.47
18:s:134:ASN:OD1	18:s:137:LEU:HG	2.14	0.47
1:A:246:TYR:CE2	1:A:248:ILE:HG12	2.49	0.47
1:A:323:ARG:HA	1:A:326:LEU:HD12	1.96	0.47
2:B:464:PHE:CZ	35:B:625:LHG:H261	2.50	0.47
28:B:601:CLA:H102	30:H:101:BCR:H21C	1.95	0.47
36:C:518:DGD:HG12	36:C:518:DGD:O6D	2.14	0.47
4:D:240:GLN:HE22	4:D:244:THR:HB	1.79	0.47
7:N:173:PHE:CE2	7:N:177:LYS:HE3	2.48	0.47
28:N:613:CLA:H2	28:N:613:CLA:H61	1.59	0.47
22:Y:21:ARG:HD3	22:Y:38:GLY:HA3	1.95	0.47
22:Y:145:GLY:HA2	38:Y:608:CHL:HAC1	1.96	0.47
28:b:611:CLA:HBC2	35:b:624:LHG:H341	1.95	0.47
30:b:618:BCR:HC8	30:b:618:BCR:H321	1.95	0.47
30:c:514:BCR:H332	23:z:54:VAL:HG12	1.95	0.47
28:n:613:CLA:H2	28:n:613:CLA:H61	1.57	0.47
39:s:615:LUT:H35	39:s:615:LUT:H401	1.77	0.47
22:y:101:GLY:O	22:y:104:ILE:HG22	2.14	0.47
22:y:138:VAL:HA	22:y:141:TYR:HD2	1.80	0.47
28:y:310:CLA:H61	28:y:310:CLA:H92	1.63	0.47
1:A:341:LEU:H	3:C:313:GLN:HE22	1.63	0.47
28:B:602:CLA:H92	8:H:58:LEU:HD13	1.96	0.47
35:B:623:LHG:H102	35:B:623:LHG:H242	1.96	0.47
3:C:49:LEU:HD11	28:C:509:CLA:C1C	2.44	0.47
30:C:514:BCR:H321	32:C:522:LMG:H352	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:GLY:O	38:G:608:CHL:HMC	2.15	0.47
12:L:24:LEU:HB2	35:L:102:LHG:H151	1.95	0.47
13:M:31:SER:HA	31:M:101:SQD:O9	2.14	0.47
28:N:603:CLA:HBC2	38:N:609:CHL:HHD	1.96	0.47
14:O:61:LYS:HA	14:O:73:PHE:HA	1.96	0.47
28:R:603:CLA:HAC2	28:R:608:CLA:HBC2	1.97	0.47
28:R:604:CLA:H3A	28:R:604:CLA:HBA2	1.55	0.47
18:S:41:ASP:HB2	18:S:44:GLU:CG	2.38	0.47
18:S:200:MET:HA	18:S:203:PHE:CD2	2.49	0.47
23:Z:57:LEU:HD23	23:Z:60:LEU:HD12	1.97	0.47
1:a:135:PHE:CE2	9:i:31:ASN:HB3	2.49	0.47
28:b:606:CLA:C13	30:b:619:BCR:H10C	2.42	0.47
28:b:611:CLA:H112	28:b:611:CLA:H72	1.47	0.47
28:c:510:CLA:HED2	28:c:510:CLA:H61	1.97	0.47
32:c:521:LMG:H372	28:s:613:CLA:HAA2	1.96	0.47
14:o:63:GLU:OE1	14:o:234:LYS:HG2	2.15	0.47
17:r:37:PHE:CD2	41:r:615:XAT:H221	2.49	0.47
17:r:184:LEU:HB2	28:r:609:CLA:O1A	2.14	0.47
18:s:80:ILE:HG22	18:s:84:TRP:CD1	2.49	0.47
30:A:409:BCR:C19	36:A:417:DGD:HB61	2.43	0.47
2:B:103:PHE:CD1	30:B:619:BCR:H353	2.50	0.47
2:B:230:ARG:NH1	2:B:474:LEU:HA	2.29	0.47
28:C:512:CLA:H93	28:C:512:CLA:H111	1.70	0.47
36:C:518:DGD:HA22	36:C:518:DGD:HA52	1.77	0.47
4:D:200:MET:HG2	33:D:406:PL9:H321	1.96	0.47
6:F:31:ILE:O	6:F:35:GLN:HG2	2.15	0.47
7:G:99:LYS:HA	38:G:607:CHL:HED3	1.97	0.47
7:G:192:PHE:CE1	28:G:613:CLA:HAC1	2.49	0.47
8:H:53:PHE:HB2	30:H:101:BCR:H363	1.96	0.47
12:L:5:ASN:HD22	12:L:7:ASN:H	1.61	0.47
28:N:604:CLA:NB	40:N:617:NEX:H222	2.29	0.47
18:S:94:ILE:HG23	18:S:98:PHE:CE2	2.50	0.47
18:S:206:GLN:HG2	28:S:313:CLA:C1D	2.45	0.47
28:S:311:CLA:C2B	35:S:317:LHG:HC2	2.45	0.47
19:T:19:PHE:HA	19:T:23:PHE:HD1	1.80	0.47
30:T:101:BCR:H381	2:b:33:TRP:CD1	2.49	0.47
22:Y:80:VAL:HG13	22:Y:206:LEU:HD11	1.95	0.47
38:Y:608:CHL:HAA1	38:Y:608:CHL:HBD	1.97	0.47
23:Z:23:VAL:N	23:Z:24:PRO:HD2	2.30	0.47
1:a:42:LEU:HB3	30:a:410:BCR:C35	2.28	0.47
28:a:409:CLA:H101	32:w:101:LMG:H161	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:141:ILE:O	2:b:145:LEU:HG	2.14	0.47
2:b:144:PHE:CE2	2:b:210:ILE:HG23	2.49	0.47
3:c:109:PHE:CZ	32:c:521:LMG:HC3	2.50	0.47
3:c:191:PRO:HG3	16:q:78:ARG:NH2	2.30	0.47
3:c:385:GLN:HE21	16:q:79:LEU:HG	1.80	0.47
28:c:506:CLA:C3C	28:c:507:CLA:H143	2.45	0.47
5:e:25:ILE:C	5:e:28:PRO:HD2	2.40	0.47
7:g:92:PHE:CZ	7:g:113:LEU:HD23	2.50	0.47
28:g:603:CLA:HED2	28:g:603:CLA:C2	2.44	0.47
38:g:609:CHL:H11	39:n:616:LUT:C36	2.45	0.47
16:q:88:LEU:HD12	16:q:111:PHE:CZ	2.49	0.47
18:s:19:ALA:O	18:s:23:LEU:HD22	2.14	0.47
18:s:112:PHE:HA	38:s:606:CHL:HMA2	1.97	0.47
18:s:139:VAL:CG2	38:s:606:CHL:HBC1	2.41	0.47
18:s:156:ASN:CG	18:s:160:LEU:HB2	2.40	0.47
18:s:205:ILE:HD12	28:s:612:CLA:CAC	2.44	0.47
22:y:51:LEU:HD13	28:y:303:CLA:H42	1.95	0.47
22:y:191:MET:HA	22:y:194:PHE:HD2	1.80	0.47
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.95	0.47
3:C:257:PHE:CD1	35:C:521:LHG:HC41	2.50	0.47
28:C:502:CLA:ND	28:C:503:CLA:H172	2.30	0.47
36:C:518:DGD:HE5	36:C:518:DGD:HD4	1.97	0.47
4:D:352:ALA:N	15:P:137:ASP:O	2.48	0.47
29:D:402:PHO:HBB1	29:D:402:PHO:CMB	2.45	0.47
6:F:38:GLN:HG3	15:P:10:GLY:O	2.14	0.47
28:G:613:CLA:H91	35:G:618:LHG:H341	1.96	0.47
16:Q:104:LYS:O	16:Q:107:THR:HG22	2.14	0.47
17:R:91:ARG:O	17:R:94:GLU:HG2	2.15	0.47
22:Y:33:PRO:HB3	22:Y:35:TYR:CZ	2.50	0.47
22:Y:195:PHE:HB2	38:Y:609:CHL:H201	1.95	0.47
32:b:620:LMG:H292	13:m:6:LEU:HB2	1.96	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.47
28:c:504:CLA:H43	36:c:517:DGD:O1A	2.15	0.47
7:g:157:PRO:CG	38:g:608:CHL:HMD2	2.44	0.47
28:g:613:CLA:H42	28:g:613:CLA:C1D	2.44	0.47
17:r:182:LEU:CD1	39:r:614:LUT:H222	2.33	0.47
17:r:185:ALA:HB2	28:r:609:CLA:HAA2	1.96	0.47
24:u:14:ALA:HB3	24:u:15:PRO:HD3	1.96	0.47
2:B:103:PHE:CE1	30:B:619:BCR:H353	2.50	0.47
2:B:141:ILE:HG13	2:B:217:LEU:HD21	1.97	0.47
3:C:322:GLN:NE2	3:C:381:LYS:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:401:CLA:HBA1	28:D:401:CLA:CHA	2.42	0.47
7:G:203:LYS:HD3	7:G:207:GLU:OE1	2.14	0.47
7:G:209:LEU:HD13	7:G:209:LEU:C	2.40	0.47
31:L:103:SQD:H101	30:b:617:BCR:H24C	1.97	0.47
28:R:612:CLA:CGA	28:R:612:CLA:C1A	2.93	0.47
28:Y:602:CLA:H3A	28:Y:602:CLA:CGA	2.45	0.47
1:a:132:GLU:O	1:a:136:ARG:HG2	2.15	0.47
1:a:255:PHE:O	1:a:259:ILE:HG12	2.14	0.47
28:c:501:CLA:HBC1	28:c:512:CLA:C4	2.45	0.47
7:n:209:LEU:HA	28:n:613:CLA:HMA1	1.97	0.47
14:o:109:ILE:H	14:o:109:ILE:HD12	1.80	0.47
17:r:105:LEU:HD23	39:r:614:LUT:H402	1.97	0.47
17:r:130:VAL:HG13	17:r:131:GLU:HG2	1.97	0.47
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.15	0.47
3:C:137:PRO:HG2	3:C:140:LEU:HD23	1.96	0.47
28:C:509:CLA:HBB1	28:C:509:CLA:CMB	2.45	0.47
28:C:510:CLA:H122	28:C:510:CLA:H91	1.97	0.47
28:C:512:CLA:H2	28:C:512:CLA:H72	1.97	0.47
28:C:512:CLA:H92	28:C:512:CLA:H62	1.66	0.47
6:F:36:PHE:HB2	15:P:8:VAL:HG13	1.96	0.47
11:K:55:GLN:HB3	11:K:60:PHE:CD2	2.50	0.47
7:N:197:GLN:O	7:N:201:THR:N	2.42	0.47
28:N:603:CLA:H2A	28:N:603:CLA:C2	2.36	0.47
28:N:612:CLA:HBB1	28:N:612:CLA:HMB1	1.96	0.47
14:O:142:PHE:HE1	14:O:204:VAL:HG23	1.79	0.47
17:R:226:ASN:HB3	28:R:612:CLA:O1D	2.14	0.47
28:R:610:CLA:HAA1	28:R:611:CLA:OBD	2.15	0.47
18:S:153:ARG:HG3	38:S:308:CHL:CHD	2.45	0.47
18:S:202:GLY:O	18:S:206:GLN:HG3	2.15	0.47
22:Y:98:PHE:HA	38:Y:607:CHL:HMA3	1.97	0.47
22:Y:138:VAL:HA	22:Y:141:TYR:CD2	2.50	0.47
28:Y:611:CLA:C4D	28:Y:612:CLA:HMD3	2.45	0.47
2:b:30:VAL:HG12	28:b:605:CLA:HHD	1.97	0.47
2:b:352:ARG:HE	2:b:372:ASP:HB2	1.79	0.47
28:b:613:CLA:H92	28:b:613:CLA:H62	1.69	0.47
28:c:509:CLA:HBB1	28:c:509:CLA:CMB	2.42	0.47
4:d:50:PHE:CZ	32:d:409:LMG:H341	2.50	0.47
28:g:602:CLA:H91	28:y:304:CLA:H92	1.97	0.47
9:i:9:TYR:O	9:i:13:ILE:HG22	2.14	0.47
7:n:163:PRO:HD2	39:n:615:LUT:C24	2.45	0.47
14:o:8:THR:HA	14:o:31:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:165:GLU:OE2	17:r:167:ASP:HB3	2.14	0.47
22:y:52:SER:HB3	22:y:58:PHE:CD1	2.50	0.47
22:y:82:PRO:HB3	28:y:305:CLA:HED3	1.97	0.47
23:z:30:PRO:HA	23:z:33:TRP:HB3	1.96	0.47
23:z:33:TRP:CZ2	23:z:37:LYS:HG2	2.50	0.47
1:A:323:ARG:NH1	15:P:53:PHE:HA	2.30	0.46
2:B:156:PHE:HE1	35:B:622:LHG:HC61	1.80	0.46
28:B:612:CLA:HBB1	28:B:612:CLA:CMB	2.44	0.46
36:C:518:DGD:HB22	32:C:520:LMG:C30	2.45	0.46
7:G:98:PHE:HB2	38:G:607:CHL:H43	1.97	0.46
7:G:103:GLN:CD	7:G:110:LEU:HG	2.39	0.46
7:G:174:ALA:HA	7:G:177:LYS:CD	2.33	0.46
28:G:611:CLA:H71	28:G:612:CLA:ND	2.30	0.46
7:N:43:ASP:HA	28:N:602:CLA:O1D	2.14	0.46
7:N:188:MET:HE3	28:N:602:CLA:HMC3	1.97	0.46
28:R:601:CLA:C1C	35:R:616:LHG:HC82	2.45	0.46
28:R:604:CLA:HMB2	41:R:615:XAT:H7	1.96	0.46
28:R:608:CLA:H62	28:R:608:CLA:H2	1.60	0.46
28:S:305:CLA:C4A	28:S:305:CLA:HBA2	2.37	0.46
28:S:309:CLA:HBC3	28:S:309:CLA:HMC3	1.97	0.46
28:S:310:CLA:CMC	39:S:315:LUT:H32	2.45	0.46
39:S:315:LUT:H391	39:S:315:LUT:H32	1.96	0.46
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.97	0.46
1:a:194:MET:HE1	4:d:177:ALA:HB2	1.97	0.46
3:c:223:TRP:HE3	36:c:516:DGD:HB21	1.80	0.46
5:e:77:ASP:O	5:e:81:ARG:HG3	2.15	0.46
7:g:138:VAL:HA	7:g:141:TYR:HD2	1.78	0.46
28:g:611:CLA:H111	28:g:611:CLA:H93	1.54	0.46
30:h:101:BCR:H281	21:x:46:THR:O	2.15	0.46
7:n:121:ALA:HA	38:n:605:CHL:CHC	2.44	0.46
14:o:128:PHE:HA	14:o:222:GLN:NE2	2.25	0.46
16:q:57:GLU:OE2	16:q:79:LEU:HB3	2.15	0.46
16:q:139:THR:O	16:q:143:VAL:HG23	2.15	0.46
20:w:40:TYR:O	20:w:44:LEU:HG	2.15	0.46
22:y:164:LEU:CD1	39:y:315:LUT:H222	2.44	0.46
28:B:611:CLA:HMD1	35:B:625:LHG:H351	1.97	0.46
28:B:616:CLA:H92	28:B:616:CLA:H62	1.53	0.46
3:C:245:ILE:O	3:C:249:ILE:HG13	2.16	0.46
3:C:400:PRO:C	3:C:401:LEU:HD12	2.39	0.46
7:G:128:TRP:CE3	7:N:222:TRP:CZ2	3.04	0.46
28:G:611:CLA:H8	28:G:611:CLA:H122	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:128:TRP:HE1	41:Y:617:XAT:C14	2.27	0.46
22:Y:163:PRO:HD2	39:Y:615:LUT:C23	2.44	0.46
24:U:84:TYR:CD1	24:U:96:ILE:HG12	2.51	0.46
1:a:140:ARG:NH2	35:a:415:LHG:HC41	2.30	0.46
3:c:119:LEU:HD22	11:k:40:MET:HE1	1.96	0.46
28:c:503:CLA:CHA	28:c:503:CLA:HBA2	2.43	0.46
30:d:406:BCR:C24	32:d:409:LMG:H162	2.45	0.46
30:d:406:BCR:C21	32:d:409:LMG:H352	2.44	0.46
28:n:604:CLA:CHB	40:n:617:NEX:H383	2.45	0.46
14:o:174:LEU:HB3	14:o:179:ARG:HB3	1.97	0.46
15:p:23:GLY:HA3	15:p:26:PHE:CZ	2.50	0.46
17:r:98:ILE:HG13	28:r:608:CLA:O1D	2.16	0.46
17:r:154:VAL:HG13	40:r:616:NEX:H15	1.97	0.46
17:r:230:HIS:CE1	28:r:612:CLA:HBA1	2.50	0.46
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.44	0.46
1:A:163:ILE:HD11	36:C:517:DGD:HA31	1.97	0.46
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.97	0.46
28:C:501:CLA:HHC	28:C:501:CLA:HBB1	1.96	0.46
28:C:507:CLA:CAD	28:C:509:CLA:H152	2.46	0.46
4:D:120:ALA:O	4:D:124:ILE:HG13	2.14	0.46
5:E:36:LEU:HA	5:E:39:SER:OG	2.16	0.46
7:G:135:MET:HB2	38:G:609:CHL:CBB	2.46	0.46
7:N:97:TRP:HA	39:N:616:LUT:O3	2.14	0.46
28:N:602:CLA:CAC	35:N:618:LHG:H261	2.45	0.46
14:O:32:ILE:HD12	14:O:35:GLY:HA3	1.98	0.46
18:S:86:MET:HB3	39:S:315:LUT:C35	2.45	0.46
23:Z:19:LEU:HD21	23:Z:43:GLY:HA3	1.96	0.46
23:Z:33:TRP:O	23:Z:37:LYS:HG3	2.15	0.46
1:a:147:TYR:HE1	28:a:406:CLA:H91	1.80	0.46
28:a:409:CLA:H3A	32:w:101:LMG:H142	1.97	0.46
28:b:612:CLA:H111	28:b:613:CLA:CAB	2.45	0.46
28:b:616:CLA:C5	30:b:619:BCR:H362	2.46	0.46
28:b:616:CLA:HMA2	30:b:619:BCR:C18	2.45	0.46
5:e:70:PHE:HB2	24:u:28:ASN:ND2	2.30	0.46
10:j:21:VAL:O	10:j:25:ILE:HD13	2.16	0.46
7:n:212:HIS:CG	28:n:613:CLA:HAA2	2.51	0.46
28:n:610:CLA:H93	28:n:610:CLA:H111	1.62	0.46
14:o:105:GLU:HB3	14:o:133:LEU:H	1.80	0.46
17:r:94:GLU:O	17:r:98:ILE:HG12	2.15	0.46
28:r:603:CLA:C1C	28:r:608:CLA:H111	2.45	0.46
18:s:200:MET:HA	18:s:203:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:y:304:CLA:C1B	38:y:309:CHL:H122	2.45	0.46
1:A:119:PHE:CD1	29:A:407:PHO:H8	2.50	0.46
17:R:26:GLY:HA2	17:R:31:ASP:HB3	1.97	0.46
21:X:52:LYS:O	21:X:56:LEU:HG	2.16	0.46
1:a:25:GLU:OE2	3:c:470:THR:HG22	2.14	0.46
1:a:27:ARG:HB3	31:a:414:SQD:C7	2.45	0.46
1:a:344:ALA:HB1	3:c:358:PHE:HE2	1.79	0.46
2:b:67:THR:HA	2:b:71:ILE:O	2.15	0.46
28:b:615:CLA:H172	28:b:615:CLA:H91	1.97	0.46
35:b:622:LHG:C14	35:b:622:LHG:H322	2.45	0.46
35:c:519:LHG:HC12	35:c:519:LHG:P	2.55	0.46
4:d:82:PRO:HB3	4:d:91:LEU:HD11	1.96	0.46
38:g:619:CHL:H161	38:g:619:CHL:H122	1.72	0.46
14:o:89:ILE:HD13	14:o:130:ILE:HD11	1.96	0.46
17:r:19:LYS:HB3	17:r:19:LYS:NZ	2.31	0.46
17:r:227:TRP:O	17:r:231:LEU:HB2	2.16	0.46
28:r:611:CLA:H3A	28:r:611:CLA:HBA1	1.68	0.46
18:s:71:PHE:CE1	28:s:602:CLA:H2A	2.50	0.46
21:x:54:PHE:O	21:x:58:ILE:HG12	2.16	0.46
22:y:153:ASP:HB3	22:y:156:TYR:O	2.15	0.46
28:y:304:CLA:C4B	38:y:309:CHL:H122	2.45	0.46
2:B:26:HIS:CE1	28:B:612:CLA:HMA2	2.50	0.46
2:B:118:TRP:CZ2	12:L:5:ASN:HA	2.49	0.46
2:B:323:GLY:N	2:B:326:ARG:HD2	2.30	0.46
2:B:467:ILE:HG21	4:D:127:MET:HE2	1.98	0.46
35:B:622:LHG:O5	17:R:144:ILE:HG21	2.16	0.46
3:C:158:THR:HG21	3:C:256:PRO:HD3	1.98	0.46
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.46
36:C:518:DGD:HA81	32:C:520:LMG:H342	1.98	0.46
4:D:147:PHE:O	4:D:150:PRO:HD2	2.15	0.46
4:D:299:PHE:HA	12:L:38:ASN:OD1	2.16	0.46
8:H:22:LEU:HB3	17:R:80:PHE:CE2	2.50	0.46
7:N:44:TYR:CE2	38:N:601:CHL:HMD1	2.51	0.46
15:P:35:ASN:OD1	42:P:201:HOH:O	2.20	0.46
15:P:75:GLY:HA3	15:P:79:GLU:OE2	2.15	0.46
15:P:140:GLU:HA	15:P:166:LYS:HD2	1.97	0.46
16:Q:61:ALA:HB1	16:Q:73:LEU:HD12	1.97	0.46
22:Y:21:ARG:HD3	22:Y:38:GLY:CA	2.45	0.46
22:Y:135:MET:HA	22:Y:138:VAL:HG22	1.98	0.46
22:Y:200:VAL:HG13	22:Y:228:PHE:HZ	1.80	0.46
41:Y:617:XAT:H363	35:Y:619:LHG:C7	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:60:ILE:HB	1:a:83:ILE:HG22	1.97	0.46
1:a:159:LEU:O	1:a:163:ILE:HG13	2.16	0.46
28:b:612:CLA:HBB1	28:b:612:CLA:CMB	2.45	0.46
3:c:466:VAL:HG13	4:d:252:ARG:HD2	1.98	0.46
28:c:505:CLA:H61	28:c:505:CLA:H92	1.67	0.46
36:c:517:DGD:HB92	32:k:102:LMG:C42	2.46	0.46
4:d:135:ARG:HA	4:d:135:ARG:NE	2.29	0.46
35:g:618:LHG:H202	28:y:304:CLA:H201	1.96	0.46
14:o:37:ASP:HA	14:o:206:GLN:HA	1.98	0.46
14:o:91:GLY:HA2	14:o:106:LYS:CG	2.42	0.46
1:A:210:LEU:HD13	28:A:406:CLA:C5	2.46	0.46
2:B:224:ARG:HG3	8:H:37:TRP:CD2	2.51	0.46
28:B:612:CLA:H111	28:B:613:CLA:CAB	2.46	0.46
28:B:613:CLA:H203	30:B:618:BCR:HC7	1.97	0.46
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.98	0.46
7:G:212:HIS:CB	28:G:613:CLA:HAA2	2.45	0.46
38:G:606:CHL:HBA1	40:G:617:NEX:H403	1.97	0.46
14:O:213:GLU:HG2	14:O:245:GLN:HG2	1.97	0.46
1:a:50:ILE:CD1	30:a:410:BCR:H21C	2.43	0.46
2:b:45:PHE:HA	2:b:60:MET:HE3	1.97	0.46
2:b:135:LEU:HB2	2:b:136:PRO:HD3	1.98	0.46
28:c:504:CLA:C7	36:c:518:DGD:HB72	2.41	0.46
36:c:518:DGD:HA22	32:d:409:LMG:H111	1.96	0.46
4:d:320:ILE:O	4:d:324:GLU:HG3	2.15	0.46
7:g:24:TYR:N	7:g:44:TYR:HB3	2.31	0.46
10:j:10:LEU:O	10:j:13:ILE:HG12	2.16	0.46
7:n:199:ILE:HA	22:y:230:PRO:HB3	1.96	0.46
17:r:12:PRO:HB2	28:r:601:CLA:CBC	2.43	0.46
28:r:610:CLA:HHC	28:r:610:CLA:CBB	2.46	0.46
30:t:101:BCR:H321	30:t:101:BCR:HC8	1.97	0.46
20:w:34:TRP:CD2	35:w:102:LHG:H162	2.51	0.46
23:z:33:TRP:O	23:z:37:LYS:N	2.49	0.46
28:B:606:CLA:H102	30:B:619:BCR:HC7	1.98	0.46
28:B:613:CLA:H122	30:B:618:BCR:H312	1.98	0.46
28:B:614:CLA:HBC2	31:L:101:SQD:H281	1.98	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.46
4:D:265:LYS:HD2	4:D:269:HIS:HE1	1.79	0.46
28:D:403:CLA:HBA2	28:D:403:CLA:H3A	1.41	0.46
5:E:32:ILE:O	5:E:36:LEU:HG	2.15	0.46
7:N:118:LEU:O	7:N:120:HIS:N	2.48	0.46
17:R:39:LEU:HD11	41:R:615:XAT:H373	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:94:GLU:O	17:R:98:ILE:HG12	2.16	0.46
17:R:126:LYS:HB2	38:R:606:CHL:O2D	2.16	0.46
18:S:86:MET:HB3	39:S:315:LUT:C34	2.46	0.46
28:Y:612:CLA:HMB2	28:Y:612:CLA:H141	1.97	0.46
24:U:94:ALA:HB3	24:U:97:CYS:SG	2.56	0.46
2:b:282:GLN:NE2	24:u:25:ILE:HD12	2.31	0.46
2:b:419:LYS:O	2:b:423:ARG:HG3	2.16	0.46
28:b:614:CLA:C9	28:b:614:CLA:HBC3	2.46	0.46
3:c:154:ARG:NH2	20:w:49:GLU:HA	2.30	0.46
28:c:501:CLA:C10	30:i:101:BCR:H17C	2.45	0.46
39:n:615:LUT:H181	39:n:615:LUT:C8	2.43	0.46
15:p:97:THR:HG22	15:p:106:ASN:HA	1.98	0.46
17:r:124:ALA:HA	17:r:127:VAL:HG22	1.98	0.46
28:r:609:CLA:H61	39:r:614:LUT:H371	1.97	0.46
28:s:609:CLA:H2	39:s:614:LUT:H28	1.97	0.46
19:t:15:GLY:HA2	30:t:101:BCR:H12C	1.97	0.46
22:y:24:TYR:CD1	22:y:46:TRP:HB2	2.51	0.46
22:y:166:LEU:HB2	28:y:310:CLA:O1A	2.16	0.46
3:C:237:HIS:CE1	30:C:515:BCR:H272	2.51	0.46
3:C:390:ARG:HD3	16:Q:38:PHE:O	2.15	0.46
3:C:465:PRO:HB2	3:C:469:MET:HE3	1.98	0.46
4:D:86:LEU:HD13	4:D:91:LEU:HD11	1.98	0.46
4:D:325:GLY:O	4:D:329:TRP:HD1	1.99	0.46
5:E:20:TRP:CD1	10:J:8:ILE:HG13	2.51	0.46
7:G:59:SER:HA	7:G:62:ARG:CZ	2.45	0.46
7:G:85:LEU:HB3	7:G:90:VAL:HG11	1.98	0.46
28:G:612:CLA:CHB	28:G:612:CLA:H121	2.46	0.46
39:G:616:LUT:H35	39:G:616:LUT:H401	1.85	0.46
15:P:31:PRO:HG3	15:P:175:PHE:HB3	1.98	0.46
28:Y:603:CLA:H2	28:Y:603:CLA:H61	1.76	0.46
38:Y:607:CHL:H42	38:Y:607:CHL:H151	1.97	0.46
2:b:162:PHE:HB2	35:b:621:LHG:HC61	1.97	0.46
4:d:84:ASN:HD22	4:d:337:HIS:CD2	2.33	0.46
5:e:32:ILE:O	5:e:36:LEU:HG	2.15	0.46
7:g:131:GLN:OE1	38:g:607:CHL:HMC	2.15	0.46
11:k:46:LEU:HB2	30:k:101:BCR:H352	1.98	0.46
7:n:157:PRO:HB3	38:n:608:CHL:HBC2	1.98	0.46
7:n:182:LYS:HB3	28:n:611:CLA:HMD1	1.98	0.46
18:s:191:LYS:HE3	35:s:617:LHG:C23	2.46	0.46
18:s:197:MET:HE3	28:s:602:CLA:HMC2	1.97	0.46
28:s:602:CLA:H2	39:s:615:LUT:C28	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:24:TYR:CD2	38:y:302:CHL:HAA1	2.50	0.46
24:u:3:LYS:HE2	24:u:3:LYS:HA	1.97	0.46
30:A:409:BCR:H11C	30:A:409:BCR:H341	1.85	0.46
2:B:105:GLY:HA2	30:B:618:BCR:H23C	1.97	0.46
28:B:602:CLA:H202	36:B:626:DGD:HAT1	1.98	0.46
3:C:367:GLU:N	3:C:368:PRO:CD	2.78	0.46
7:G:21:ARG:HD3	7:G:38:GLY:HA3	1.96	0.46
13:M:27:VAL:HG12	13:m:28:LYS:HB3	1.98	0.46
16:Q:32:PRO:O	16:Q:36:ARG:HG2	2.16	0.46
18:S:36:PRO:HD3	38:S:302:CHL:C3B	2.46	0.46
18:S:212:GLU:HB2	18:S:217:ASN:ND2	2.27	0.46
35:S:317:LHG:H271	35:S:317:LHG:C23	2.46	0.46
22:Y:44:TYR:HE2	38:Y:601:CHL:HBC2	1.79	0.46
1:a:179:THR:O	1:a:183:MET:HG3	2.16	0.46
2:b:169:SER:HA	2:b:176:GLY:HA2	1.97	0.46
2:b:283:GLU:CG	2:b:287:ARG:HE	2.27	0.46
2:b:497:LYS:HB3	2:b:503:THR:HG21	1.98	0.46
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.96	0.46
28:d:401:CLA:HMB1	28:d:401:CLA:H122	1.98	0.46
30:d:406:BCR:C19	6:f:24:THR:HG23	2.44	0.46
32:d:409:LMG:H131	10:j:28:PHE:HD2	1.81	0.46
7:n:83:GLU:HA	7:n:95:ALA:HB1	1.97	0.46
28:n:612:CLA:H91	28:n:612:CLA:H111	1.65	0.46
14:o:59:THR:OG1	14:o:237:LYS:HB3	2.16	0.46
15:p:118:ALA:HB1	15:p:125:GLN:NE2	2.31	0.46
18:s:78:GLU:HB2	28:s:602:CLA:C2B	2.45	0.46
1:A:297:LEU:HB2	42:A:504:HOH:O	2.15	0.46
1:A:323:ARG:HH12	15:P:53:PHE:HA	1.80	0.46
2:B:328:GLY:HA3	2:B:332:ASN:HD22	1.81	0.46
28:B:602:CLA:HED3	28:B:603:CLA:HMA2	1.97	0.46
28:B:603:CLA:H12	28:B:603:CLA:CHB	2.46	0.46
7:G:24:TYR:HD2	38:G:601:CHL:HAA1	1.81	0.46
7:G:91:LYS:HD2	7:G:92:PHE:N	2.30	0.46
28:G:613:CLA:H2	28:G:613:CLA:H8	1.96	0.46
16:Q:37:PHE:CE2	16:Q:39:ILE:HB	2.51	0.46
28:R:601:CLA:HMC1	35:R:616:LHG:O5	2.15	0.46
18:S:48:TYR:CE2	18:S:49:LEU:HD12	2.51	0.46
28:S:303:CLA:H62	28:S:304:CLA:HMA3	1.98	0.46
28:S:311:CLA:C1D	28:S:312:CLA:HMD3	2.46	0.46
28:S:314:CLA:CGA	28:S:314:CLA:C1A	2.93	0.46
1:a:272:HIS:HA	1:a:275:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:134:ASP:O	2:b:138:ILE:HG13	2.16	0.46
2:b:170:ASP:CG	2:b:175:THR:H	2.23	0.46
3:c:62:PHE:CZ	30:k:101:BCR:H311	2.51	0.46
28:g:613:CLA:HMD2	38:g:619:CHL:H143	1.98	0.46
9:i:14:PHE:O	9:i:18:LEU:HG	2.16	0.46
14:o:65:VAL:HA	14:o:71:LEU:HD21	1.98	0.46
18:s:158:LEU:O	38:s:607:CHL:HBC3	2.16	0.46
28:y:313:CLA:H121	41:y:317:XAT:H34	1.98	0.46
2:B:242:ILE:O	2:B:245:VAL:HG22	2.17	0.45
3:C:257:PHE:HB2	3:C:259:TRP:CD1	2.51	0.45
30:C:514:BCR:H341	30:C:514:BCR:H11C	1.55	0.45
5:E:36:LEU:HA	5:E:39:SER:HG	1.80	0.45
7:G:46:TRP:HE3	28:G:602:CLA:C2D	2.29	0.45
7:G:176:LEU:HB3	28:G:610:CLA:HMA2	1.98	0.45
28:G:610:CLA:H41	28:G:612:CLA:HMA2	1.98	0.45
8:H:42:LEU:HD22	8:H:42:LEU:N	2.31	0.45
7:N:25:LEU:HB2	7:N:29:SER:CA	2.45	0.45
14:O:93:PHE:CD1	14:O:103:PHE:HB2	2.50	0.45
16:Q:97:LYS:HE2	16:Q:100:LYS:NZ	2.31	0.45
18:S:71:PHE:O	18:S:75:GLN:HG3	2.16	0.45
18:S:150:GLU:HG3	28:S:309:CLA:C4B	2.46	0.45
38:S:302:CHL:CMD	35:S:317:LHG:H272	2.46	0.45
2:b:42:LEU:HD21	2:b:93:TYR:HB3	1.98	0.45
2:b:223:GLN:HE22	4:d:8:PHE:HZ	1.61	0.45
28:b:611:CLA:HBB1	28:b:611:CLA:CMB	2.45	0.45
28:c:505:CLA:H3A	28:c:505:CLA:HBA2	1.69	0.45
4:d:147:PHE:O	4:d:151:ILE:HG12	2.16	0.45
11:k:43:ILE:HG22	11:k:47:PHE:CE2	2.50	0.45
28:n:611:CLA:H112	28:n:612:CLA:C1C	2.45	0.45
14:o:142:PHE:CE2	14:o:202:LEU:HB2	2.50	0.45
16:q:21:LEU:O	16:q:25:GLU:HG3	2.16	0.45
17:r:207:VAL:HG11	28:r:612:CLA:H111	1.97	0.45
18:s:200:MET:HG2	39:s:615:LUT:H14	1.98	0.45
18:s:221:HIS:ND1	28:s:612:CLA:HAA2	2.32	0.45
22:y:135:MET:HB2	38:y:309:CHL:CBB	2.46	0.45
1:A:126:TYR:CE2	35:D:407:LHG:H382	2.50	0.45
2:B:223:GLN:NE2	17:R:65:VAL:HG21	2.30	0.45
28:B:610:CLA:HHC	28:B:610:CLA:CBB	2.32	0.45
3:C:116:VAL:HG13	30:C:516:BCR:H322	1.98	0.45
3:C:266:TRP:HB2	20:W:53:SER:HB3	1.98	0.45
7:N:212:HIS:ND1	28:N:613:CLA:HAA2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:606:CHL:HBB2	38:N:607:CHL:CBB	2.47	0.45
28:N:612:CLA:H11	28:N:612:CLA:HMA2	1.98	0.45
28:R:613:CLA:H91	28:R:613:CLA:H111	1.79	0.45
22:Y:24:TYR:HD2	38:Y:601:CHL:HAA1	1.81	0.45
28:Y:613:CLA:H152	28:Y:614:CLA:CAD	2.47	0.45
41:Y:617:XAT:H15	41:Y:617:XAT:H201	1.70	0.45
1:a:343:LEU:CD1	3:c:310:SER:HA	2.46	0.45
2:b:16:PRO:HG2	2:b:123:PHE:HB3	1.99	0.45
28:c:501:CLA:C3B	28:c:501:CLA:H51	2.46	0.45
4:d:126:PHE:CZ	29:d:402:PHO:HBD	2.50	0.45
4:d:340:LEU:HB3	4:d:342:PHE:CE2	2.52	0.45
7:g:24:TYR:CD1	7:g:46:TRP:HB2	2.51	0.45
7:n:98:PHE:HB2	38:n:607:CHL:HMA1	1.98	0.45
7:n:135:MET:HA	7:n:138:VAL:HG22	1.98	0.45
38:n:606:CHL:HBB2	38:n:607:CHL:HAB	1.97	0.45
28:n:610:CLA:C1B	28:n:610:CLA:H51	2.46	0.45
14:o:109:ILE:HD12	14:o:109:ILE:N	2.30	0.45
16:q:54:SER:O	16:q:58:ILE:HG13	2.16	0.45
17:r:54:ASP:H	17:r:60:ASN:ND2	2.14	0.45
17:r:97:LEU:HB3	17:r:172:LEU:HD11	1.97	0.45
28:r:608:CLA:C1	28:r:613:CLA:H61	2.46	0.45
18:s:176:ALA:HB2	28:s:609:CLA:HAA2	1.97	0.45
38:s:601:CHL:CHA	35:s:617:LHG:H101	2.47	0.45
23:z:5:PHE:O	23:z:9:VAL:HG23	2.17	0.45
1:A:91:LEU:HA	1:A:168:PHE:CE2	2.51	0.45
28:B:611:CLA:C3D	35:B:625:LHG:H372	2.47	0.45
3:C:214:LEU:HD22	20:W:15:PHE:CE2	2.51	0.45
4:D:162:PRO:HG3	4:D:171:ALA:HB2	1.97	0.45
7:G:130:THR:HB	38:G:606:CHL:HED3	1.97	0.45
38:G:601:CHL:H143	38:Y:607:CHL:C2C	2.46	0.45
9:I:14:PHE:O	9:I:18:LEU:HG	2.16	0.45
10:J:18:GLY:O	10:J:22:ILE:HG13	2.17	0.45
14:O:128:PHE:HA	14:O:222:GLN:HE22	1.81	0.45
14:O:208:LYS:NZ	14:O:210:GLU:HB2	2.31	0.45
15:P:161:ALA:CB	15:P:176:VAL:HG13	2.46	0.45
18:S:200:MET:HE3	18:S:204:PHE:CZ	2.52	0.45
20:W:35:ALA:O	20:W:39:ILE:HG13	2.16	0.45
22:Y:97:TRP:CE2	22:Y:98:PHE:HD2	2.35	0.45
38:Y:605:CHL:HHC	38:Y:605:CHL:CBB	2.45	0.45
28:b:608:CLA:H62	28:b:608:CLA:H92	1.68	0.45
3:c:35:TRP:C	3:c:37:ALA:H	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:508:CLA:C18	32:k:102:LMG:H371	2.45	0.45
30:c:514:BCR:H15C	30:c:514:BCR:H351	1.80	0.45
4:d:200:MET:HE3	4:d:282:MET:HB3	1.97	0.45
7:g:52:SER:HB3	7:g:58:PHE:CD1	2.51	0.45
11:k:55:GLN:HB3	11:k:60:PHE:CD2	2.52	0.45
7:n:80:VAL:O	7:n:81:PHE:C	2.59	0.45
28:n:611:CLA:H102	28:n:611:CLA:H13	1.69	0.45
28:r:604:CLA:C1B	40:r:616:NEX:H242	2.46	0.45
22:y:112:TYR:CD1	22:y:113:LEU:HG	2.51	0.45
24:u:8:GLU:HA	24:u:11:LYS:HG2	1.97	0.45
3:C:77:PRO:HG2	3:C:78:GLU:OE2	2.15	0.45
28:C:511:CLA:H142	11:K:47:PHE:HE1	1.82	0.45
7:G:85:LEU:HB2	7:G:92:PHE:HE1	1.80	0.45
12:L:21:GLY:O	12:L:25:ILE:HG12	2.16	0.45
7:N:59:SER:O	7:N:63:GLU:HG3	2.16	0.45
28:N:611:CLA:HHC	28:N:611:CLA:CBB	2.47	0.45
40:N:617:NEX:H8	28:S:312:CLA:C4	2.46	0.45
14:O:204:VAL:HG22	14:O:242:TRP:HH2	1.81	0.45
15:P:71:ILE:HG22	15:P:125:GLN:HG3	1.99	0.45
16:Q:139:THR:O	16:Q:143:VAL:HG23	2.16	0.45
22:Y:81:PHE:O	22:Y:85:LEU:HG	2.16	0.45
22:Y:162:ASP:HA	39:Y:615:LUT:H24	1.97	0.45
23:Z:58:ASN:HA	23:Z:61:ILE:HD13	1.98	0.45
1:a:106:LEU:CD1	36:a:401:DGD:HE1	2.46	0.45
2:b:211:LEU:HD22	28:r:603:CLA:H121	1.97	0.45
2:b:272:ARG:HG3	2:b:273:TYR:N	2.32	0.45
28:b:608:CLA:HAB	36:b:625:DGD:HAN2	1.98	0.45
28:b:609:CLA:C3D	8:h:43:MET:HB2	2.46	0.45
3:c:154:ARG:HH22	20:w:49:GLU:HA	1.81	0.45
3:c:217:PRO:HD3	32:w:101:LMG:H332	1.97	0.45
3:c:261:ARG:HD2	20:w:49:GLU:HA	1.98	0.45
3:c:319:VAL:HG22	3:c:384:ILE:HD13	1.97	0.45
36:c:518:DGD:HAE1	36:c:518:DGD:HAN1	1.98	0.45
4:d:107:GLN:HE21	5:e:48:GLY:HA3	1.81	0.45
7:g:162:ASP:HB2	28:g:610:CLA:O1D	2.17	0.45
38:g:601:CHL:H52	28:y:304:CLA:CMD	2.46	0.45
10:j:9:PRO:O	10:j:12:ILE:HG12	2.17	0.45
7:n:46:TRP:HB3	28:n:602:CLA:CAD	2.47	0.45
28:n:611:CLA:HHC	28:n:611:CLA:CBB	2.46	0.45
16:q:144:LEU:HA	16:q:147:ILE:HD12	1.98	0.45
18:s:195:LEU:HB2	35:s:617:LHG:H261	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TRP:HA	2:B:91:TRP:CE3	2.51	0.45
28:B:603:CLA:CHC	28:B:605:CLA:H101	2.46	0.45
28:C:510:CLA:HBB1	28:C:510:CLA:HMB1	1.99	0.45
4:D:258:PHE:CE2	35:D:407:LHG:H312	2.52	0.45
7:G:86:SER:HA	7:G:90:VAL:O	2.16	0.45
7:G:135:MET:O	7:G:139:GLU:HG2	2.17	0.45
38:G:609:CHL:HBD	38:G:609:CHL:HAA1	1.98	0.45
7:N:58:PHE:CZ	7:N:62:ARG:HD2	2.51	0.45
7:N:135:MET:HA	7:N:138:VAL:HG22	1.97	0.45
7:N:139:GLU:HG3	38:N:609:CHL:C4B	2.47	0.45
38:N:601:CHL:HAC2	35:N:618:LHG:HC41	1.98	0.45
28:N:604:CLA:C4B	40:N:617:NEX:H222	2.46	0.45
14:O:185:LEU:HA	14:O:188:GLU:OE2	2.17	0.45
38:R:606:CHL:HHC	38:R:606:CHL:CBB	2.45	0.45
28:R:610:CLA:C2C	35:R:616:LHG:HC62	2.47	0.45
18:S:65:SER:O	18:S:66:LYS:C	2.59	0.45
28:S:311:CLA:HHC	28:S:311:CLA:HBB1	1.99	0.45
23:Z:12:LEU:HA	23:Z:50:LEU:HD13	1.98	0.45
24:U:74:LYS:HB2	24:U:77:SER:HB3	1.99	0.45
1:a:103:ASP:HB3	14:o:117:GLN:HE22	1.82	0.45
2:b:256:MET:HG3	2:b:448:ARG:HG3	1.97	0.45
2:b:379:ALA:HB2	2:b:395:VAL:HG11	1.98	0.45
2:b:393:GLU:O	16:q:1:GLU:HG3	2.16	0.45
30:d:406:BCR:H341	30:d:406:BCR:H11C	1.84	0.45
7:g:46:TRP:HE3	28:g:602:CLA:C2D	2.29	0.45
12:l:13:LEU:HD23	13:m:26:TYR:HB2	1.98	0.45
12:l:21:GLY:O	12:l:25:ILE:HG12	2.16	0.45
13:m:4:ASN:HD22	13:m:4:ASN:C	2.24	0.45
7:n:167:ALA:HB1	7:n:173:PHE:CG	2.51	0.45
39:n:615:LUT:H11	39:n:615:LUT:H191	1.81	0.45
16:q:32:PRO:O	16:q:36:ARG:HG2	2.16	0.45
16:q:63:LYS:HG3	16:q:64:PHE:N	2.31	0.45
17:r:23:TYR:CD2	17:r:24:LEU:HD13	2.52	0.45
17:r:126:LYS:O	17:r:130:VAL:HG12	2.17	0.45
17:r:175:GLY:CA	28:r:609:CLA:HED3	2.47	0.45
22:y:141:TYR:HB3	38:y:308:CHL:CMC	2.46	0.45
41:y:317:XAT:H15	41:y:317:XAT:H201	1.72	0.45
1:A:121:LEU:HD13	28:C:505:CLA:H162	1.98	0.45
1:A:303:ASN:HB2	3:C:414:ILE:HA	1.97	0.45
2:B:113:TRP:CZ2	8:H:15:ARG:NH2	2.84	0.45
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:511:CLA:H71	30:C:516:BCR:H402	1.99	0.45
28:C:512:CLA:H101	28:C:513:CLA:H203	1.98	0.45
4:D:114:PHE:CE1	30:D:405:BCR:HC21	2.52	0.45
7:G:217:VAL:O	7:G:223:SER:HB3	2.16	0.45
7:N:172:ALA:O	7:N:176:LEU:HG	2.17	0.45
28:R:604:CLA:HBA1	38:R:605:CHL:CHD	2.47	0.45
18:S:106:GLY:O	18:S:107:PRO:C	2.60	0.45
38:Y:605:CHL:H12	17:r:136:LEU:HB2	1.99	0.45
1:a:74:GLY:HA3	4:d:305:ARG:HH12	1.81	0.45
1:a:113:GLU:O	1:a:117:LEU:HD13	2.17	0.45
1:a:322:ASN:OD1	3:c:412:THR:HA	2.17	0.45
28:b:608:CLA:CMC	28:b:609:CLA:H143	2.45	0.45
28:b:612:CLA:H3A	28:b:612:CLA:HBA2	1.56	0.45
3:c:223:TRP:CG	3:c:224:ILE:N	2.84	0.45
28:c:511:CLA:C4A	30:c:515:BCR:H271	2.47	0.45
40:n:617:NEX:H3	40:n:617:NEX:H173	1.43	0.45
28:r:604:CLA:CHA	28:r:604:CLA:HBA1	2.40	0.45
28:r:613:CLA:H62	28:r:613:CLA:H101	1.50	0.45
28:s:602:CLA:H93	28:s:602:CLA:H111	1.62	0.45
38:s:607:CHL:HAA1	38:s:607:CHL:HBD	1.98	0.45
28:y:313:CLA:H111	28:y:313:CLA:H152	1.70	0.45
2:B:141:ILE:O	2:B:145:LEU:HG	2.16	0.45
2:B:467:ILE:HG23	4:D:131:PHE:HZ	1.82	0.45
28:B:601:CLA:HHD	30:H:101:BCR:H383	1.98	0.45
28:B:611:CLA:H122	28:B:613:CLA:H102	1.97	0.45
4:D:192:TRP:CE2	4:D:198:HIS:HB2	2.52	0.45
4:D:340:LEU:HB3	4:D:342:PHE:CZ	2.52	0.45
28:G:604:CLA:NB	40:G:617:NEX:H222	2.32	0.45
38:G:608:CHL:O1A	38:G:608:CHL:H43	2.17	0.45
28:N:612:CLA:H11	28:N:612:CLA:CMA	2.47	0.45
17:R:184:LEU:HD11	39:R:614:LUT:C22	2.47	0.45
18:S:142:GLU:HA	38:S:306:CHL:HMA1	1.98	0.45
28:S:311:CLA:CHD	35:S:317:LHG:HC62	2.47	0.45
38:Y:607:CHL:HBB2	38:Y:609:CHL:CBC	2.47	0.45
23:Z:52:PHE:O	23:Z:56:ILE:HG13	2.17	0.45
1:a:309:SER:HB3	15:p:13:LYS:HE3	1.99	0.45
30:a:410:BCR:H17C	32:a:413:LMG:H361	1.99	0.45
3:c:79:LYS:CD	3:c:84:GLN:HG2	2.47	0.45
28:c:509:CLA:H93	28:c:509:CLA:H62	1.77	0.45
7:g:86:SER:HA	7:g:90:VAL:O	2.17	0.45
7:g:173:PHE:HE1	28:g:610:CLA:H2A	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:16:VAL:HG13	32:w:101:LMG:H212	1.99	0.45
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.99	0.45
1:A:308:ASP:OD1	1:A:312:ARG:N	2.50	0.45
2:B:51:VAL:HA	2:B:308:LYS:NZ	2.31	0.45
28:B:615:CLA:H2	28:B:615:CLA:H61	1.68	0.45
3:C:266:TRP:CZ3	28:C:507:CLA:HMC1	2.52	0.45
3:C:271:TYR:CE1	28:C:507:CLA:HAC2	2.52	0.45
28:C:504:CLA:HBC1	11:K:42:VAL:HA	1.99	0.45
28:C:506:CLA:HBB1	28:C:506:CLA:CMB	2.47	0.45
5:E:19:TYR:HE2	37:E:101:HEM:C3D	2.35	0.45
7:G:81:PHE:CE1	7:G:85:LEU:HD11	2.52	0.45
7:N:148:LEU:HD12	38:N:608:CHL:C4B	2.47	0.45
38:N:607:CHL:C4A	38:Y:601:CHL:H203	2.46	0.45
16:Q:128:GLU:HB3	16:Q:132:TYR:CE2	2.52	0.45
17:R:20:SER:HA	17:R:33:GLY:HA3	1.99	0.45
28:S:305:CLA:HBA2	28:S:305:CLA:H11	1.73	0.45
20:W:17:LEU:HD21	20:W:26:LEU:HD11	1.97	0.45
22:Y:27:PRO:HD2	38:Y:601:CHL:CBB	2.46	0.45
22:Y:71:TRP:CD1	38:Y:609:CHL:HMD3	2.52	0.45
22:Y:135:MET:HG3	38:Y:609:CHL:OMC	2.17	0.45
1:a:293:MET:HG3	42:a:502:HOH:O	2.16	0.45
28:b:602:CLA:H18	28:b:602:CLA:H151	1.73	0.45
36:c:518:DGD:C7A	4:d:75:LEU:HD21	2.46	0.45
8:h:41:PRO:O	8:h:45:ILE:HG13	2.17	0.45
7:n:71:TRP:CD1	38:n:609:CHL:HMD3	2.52	0.45
7:n:122:GLN:HB2	38:n:605:CHL:CBB	2.47	0.45
7:n:224:TYR:HB3	7:n:227:ASN:OD1	2.17	0.45
15:p:47:LEU:HD23	15:p:47:LEU:C	2.42	0.45
17:r:41:LYS:HG2	17:r:42:PRO:HD2	1.99	0.45
17:r:47:GLN:NE2	17:r:69:ARG:HH21	2.15	0.45
18:s:200:MET:HA	18:s:203:PHE:CD2	2.51	0.45
2:B:29:LEU:CD1	30:B:617:BCR:H19C	2.47	0.45
28:C:501:CLA:H151	28:C:507:CLA:C10	2.46	0.45
36:C:518:DGD:HBE1	32:C:520:LMG:H422	1.99	0.45
5:E:26:THR:O	5:E:30:LEU:HG	2.17	0.45
7:G:63:GLU:HA	7:G:155:LEU:HD21	1.99	0.45
38:G:607:CHL:HBD	38:G:607:CHL:HAA2	1.98	0.45
35:G:618:LHG:H223	35:G:618:LHG:H191	1.64	0.45
12:L:23:LEU:HG	35:L:102:LHG:H181	1.99	0.45
28:N:602:CLA:H202	39:N:616:LUT:H391	1.98	0.45
28:N:603:CLA:HMD2	38:N:609:CHL:H52	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:219:THR:HG21	28:R:612:CLA:O1D	2.17	0.45
18:S:104:ASN:O	18:S:105:CYS:C	2.59	0.45
22:Y:182:LYS:HD3	28:Y:611:CLA:O1D	2.17	0.45
38:Y:605:CHL:H11	17:r:135:TYR:HD2	1.81	0.45
1:a:180:PHE:O	1:a:184:ILE:HG13	2.17	0.45
36:a:401:DGD:HBT2	32:a:413:LMG:C36	2.42	0.45
3:c:116:VAL:O	3:c:120:ILE:HG12	2.17	0.45
28:c:504:CLA:H42	36:c:517:DGD:HB62	1.99	0.45
39:g:616:LUT:H35	39:g:616:LUT:H401	1.80	0.45
8:h:45:ILE:O	8:h:49:LEU:HG	2.17	0.45
7:n:160:SER:O	7:n:163:PRO:HD3	2.16	0.45
28:n:610:CLA:C9	28:n:612:CLA:HHB	2.47	0.45
14:o:128:PHE:CA	14:o:222:GLN:HE22	2.26	0.45
16:q:96:PRO:HD2	16:q:99:GLN:OE1	2.17	0.45
17:r:23:TYR:CE2	17:r:24:LEU:HD13	2.52	0.45
17:r:93:ARG:NH2	17:r:199:ILE:HG12	2.31	0.45
28:r:603:CLA:H92	28:r:603:CLA:H61	1.53	0.45
39:s:614:LUT:H35	39:s:614:LUT:H401	1.79	0.45
22:y:73:MET:SD	28:y:310:CLA:HAB	2.56	0.45
22:y:191:MET:HA	22:y:194:PHE:CD2	2.52	0.45
2:B:366:PHE:HD2	2:B:425:GLN:NE2	2.15	0.45
28:B:609:CLA:C3B	30:H:101:BCR:H323	2.46	0.45
30:B:618:BCR:H323	32:B:621:LMG:C14	2.45	0.45
3:C:259:TRP:CD1	35:W:101:LHG:HC62	2.51	0.45
28:C:507:CLA:HMA3	28:C:507:CLA:C2	2.47	0.45
36:C:517:DGD:HA22	36:C:517:DGD:C5B	2.47	0.45
4:D:44:PHE:HB3	4:D:114:PHE:CE2	2.53	0.45
4:D:260:VAL:HG23	19:T:21:ILE:HG12	1.98	0.45
28:G:603:CLA:C1A	38:G:609:CHL:H92	2.46	0.45
31:L:101:SQD:H282	13:M:21:PHE:CD1	2.52	0.45
7:N:46:TRP:HE3	28:N:602:CLA:C2D	2.29	0.45
14:O:8:THR:OG1	14:O:11:GLU:HG3	2.17	0.45
15:P:65:THR:HA	15:P:155:LYS:HA	1.98	0.45
18:S:74:TYR:HD2	42:S:403:HOH:O	1.98	0.45
18:S:92:PHE:HE1	39:S:316:LUT:C6	2.30	0.45
18:S:115:GLY:HA3	38:S:307:CHL:C4D	2.47	0.45
18:S:150:GLU:HG3	28:S:309:CLA:C3B	2.47	0.45
18:S:201:LEU:O	18:S:205:ILE:HG12	2.17	0.45
1:a:75:ASN:HD22	1:a:75:ASN:N	2.15	0.45
1:a:161:TYR:O	1:a:165:GLN:HG2	2.16	0.45
28:b:603:CLA:HMC3	28:b:605:CLA:H202	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:265:VAL:HG22	20:w:52:LEU:HD23	1.99	0.45
36:c:516:DGD:HB41	36:c:516:DGD:HA22	1.99	0.45
4:d:322:LEU:O	4:d:326:ILE:HG13	2.17	0.45
29:d:402:PHO:H143	28:d:404:CLA:H171	1.99	0.45
35:d:408:LHG:H292	35:d:408:LHG:H122	1.99	0.45
7:g:24:TYR:CE2	38:g:601:CHL:HAA1	2.52	0.45
28:g:610:CLA:HBB1	28:g:612:CLA:HBA1	1.99	0.45
28:n:611:CLA:HHC	28:n:611:CLA:HBB1	1.99	0.45
28:n:613:CLA:HBB1	39:n:615:LUT:H181	1.99	0.45
22:y:81:PHE:O	22:y:85:LEU:HG	2.16	0.45
1:A:261:GLN:O	1:A:262:TYR:C	2.60	0.44
1:A:336:ALA:O	3:C:354:GLU:HG3	2.17	0.44
32:A:411:LMG:HC91	32:A:411:LMG:C12	2.47	0.44
28:B:601:CLA:H102	28:B:601:CLA:NC	2.32	0.44
3:C:206:PRO:O	3:C:210:PHE:HD1	2.01	0.44
3:C:376:ASP:O	3:C:380:LEU:HD13	2.17	0.44
3:C:472:LEU:HD11	4:D:252:ARG:HG3	1.98	0.44
28:C:501:CLA:C3B	28:C:501:CLA:H51	2.46	0.44
28:C:512:CLA:C4B	30:C:514:BCR:H291	2.47	0.44
4:D:155:VAL:O	4:D:159:LEU:HB2	2.18	0.44
7:G:28:PHE:CD1	22:Y:140:GLY:HA3	2.52	0.44
28:G:611:CLA:H62	28:G:612:CLA:C3D	2.47	0.44
14:O:129:THR:OG1	14:O:131:LYS:HG3	2.17	0.44
18:S:200:MET:HE2	39:S:316:LUT:C12	2.38	0.44
21:X:51:LEU:O	21:X:55:LEU:HD13	2.17	0.44
22:Y:92:PHE:CE2	22:Y:113:LEU:HA	2.52	0.44
38:Y:607:CHL:H42	38:Y:607:CHL:C12	2.47	0.44
1:a:93:PHE:HB2	3:c:218:PHE:CG	2.52	0.44
1:a:142:TRP:HZ2	3:c:447:ARG:HD2	1.82	0.44
31:a:411:SQD:H161	35:a:415:LHG:H162	1.99	0.44
2:b:454:GLY:HA2	32:b:620:LMG:C22	2.47	0.44
28:b:614:CLA:H52	28:b:614:CLA:NC	2.31	0.44
28:b:615:CLA:H121	28:b:616:CLA:C9	2.46	0.44
35:b:622:LHG:H342	35:b:622:LHG:H371	1.44	0.44
3:c:52:ALA:HB2	28:c:511:CLA:HMA1	1.99	0.44
7:g:135:MET:HB2	38:g:609:CHL:CBB	2.48	0.44
38:g:608:CHL:HHC	38:g:608:CHL:CBB	2.45	0.44
17:r:106:ALA:HA	41:r:615:XAT:C18	2.48	0.44
17:r:203:ARG:O	17:r:207:VAL:HG23	2.17	0.44
18:s:50:THR:HG23	18:s:52:GLU:H	1.83	0.44
18:s:90:ALA:HB1	18:s:94:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:408:CLA:HBC1	32:A:413:LMG:H341	1.99	0.44
32:A:411:LMG:H312	3:C:215:LYS:O	2.17	0.44
2:B:33:TRP:CD1	30:B:618:BCR:H12C	2.52	0.44
2:B:385:ARG:NH1	14:O:167:GLY:O	2.46	0.44
28:B:602:CLA:H152	28:B:602:CLA:H18	1.73	0.44
35:B:625:LHG:H321	35:B:625:LHG:H291	1.69	0.44
3:C:269:GLU:OE2	3:C:447:ARG:HB3	2.18	0.44
4:D:57:THR:HG21	5:E:50:PRO:CD	2.45	0.44
8:H:56:ILE:HG12	21:X:54:PHE:CE2	2.52	0.44
7:N:49:ALA:HB3	7:N:51:LEU:HG	1.97	0.44
14:O:5:LYS:HD3	14:O:6:ARG:O	2.18	0.44
14:O:58:PHE:CD2	20:W:2:VAL:HG21	2.52	0.44
17:R:23:TYR:HH	17:R:38:GLY:HA2	1.82	0.44
18:S:126:TYR:HA	28:S:305:CLA:OBD	2.16	0.44
38:S:307:CHL:HAA2	38:S:307:CHL:HBD	1.99	0.44
28:S:314:CLA:H11	28:S:314:CLA:ND	2.32	0.44
28:Y:602:CLA:HBB1	28:Y:602:CLA:HMB1	2.00	0.44
1:a:97:TRP:HZ3	9:i:8:VAL:HG21	1.81	0.44
1:a:195:HIS:ND1	1:a:197:PHE:HB2	2.32	0.44
1:a:218:LEU:HD11	1:a:255:PHE:CD2	2.50	0.44
1:a:273:PHE:CD2	31:a:411:SQD:H81	2.52	0.44
2:b:162:PHE:CG	35:b:621:LHG:H101	2.52	0.44
36:c:516:DGD:HA81	32:w:101:LMG:H371	1.99	0.44
4:d:200:MET:HG2	33:d:407:PL9:H321	1.99	0.44
28:d:404:CLA:HBB1	28:d:404:CLA:CMB	2.47	0.44
7:g:148:LEU:HD13	38:g:608:CHL:CBB	2.47	0.44
28:g:602:CLA:HED2	28:g:602:CLA:H2A	2.00	0.44
8:h:30:TYR:CE1	17:r:50:LEU:HD13	2.52	0.44
8:h:33:VAL:HG21	17:r:48:PHE:CE2	2.53	0.44
7:n:216:PRO:HB2	28:n:614:CLA:HMB2	1.99	0.44
18:s:153:ARG:HG2	18:s:163:LYS:HE3	1.99	0.44
28:s:602:CLA:C2	39:s:615:LUT:H28	2.43	0.44
38:s:605:CHL:HBC2	38:s:606:CHL:CHD	2.46	0.44
28:A:408:CLA:H111	32:A:411:LMG:H161	2.00	0.44
2:B:50:PRO:HD2	14:o:67:LYS:CD	2.42	0.44
3:C:69:LEU:HD12	11:K:40:MET:HE1	1.98	0.44
28:C:502:CLA:H92	28:C:502:CLA:H62	1.62	0.44
35:C:521:LHG:H351	28:Y:614:CLA:C2C	2.46	0.44
4:D:268:LEU:HD23	4:D:268:LEU:C	2.42	0.44
7:G:25:LEU:HB2	7:G:29:SER:CA	2.48	0.44
7:G:63:GLU:O	7:G:67:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:605:CHL:HHC	38:G:605:CHL:CBB	2.43	0.44
8:H:56:ILE:HD13	30:H:101:BCR:H373	1.98	0.44
12:L:15:ARG:HG2	12:L:19:TYR:CE2	2.53	0.44
7:N:185:ARG:HB2	35:N:618:LHG:H252	1.99	0.44
28:N:602:CLA:H101	39:N:616:LUT:C30	2.47	0.44
28:N:604:CLA:C4A	40:N:617:NEX:H242	2.47	0.44
28:N:613:CLA:C1A	28:N:613:CLA:CGA	2.94	0.44
17:R:117:THR:HG22	17:R:119:VAL:H	1.83	0.44
38:Y:608:CHL:H2	39:Y:615:LUT:H383	1.99	0.44
28:b:608:CLA:H112	28:b:609:CLA:H202	1.98	0.44
3:c:173:PHE:HB3	3:c:177:PHE:CZ	2.52	0.44
3:c:261:ARG:HA	3:c:266:TRP:HZ2	1.79	0.44
28:g:603:CLA:C3D	38:g:609:CHL:H62	2.47	0.44
15:p:168:TRP:CZ2	15:p:173:ARG:HG3	2.53	0.44
17:r:73:GLU:CG	17:r:90:GLN:HB3	2.47	0.44
18:s:93:ILE:HG23	18:s:215:VAL:HG22	1.98	0.44
28:s:610:CLA:H93	28:s:610:CLA:CMC	2.48	0.44
22:y:166:LEU:HD12	28:y:310:CLA:H11	1.98	0.44
28:y:313:CLA:CGA	28:y:313:CLA:C1A	2.96	0.44
1:A:340:PRO:HB2	15:P:166:LYS:HB3	1.98	0.44
2:B:69:LEU:HD21	28:B:603:CLA:OBD	2.18	0.44
36:B:626:DGD:HBN2	4:D:164:GLY:CA	2.48	0.44
3:C:387:TRP:HD1	16:Q:83:TYR:CZ	2.35	0.44
28:C:511:CLA:H92	28:C:511:CLA:H62	1.67	0.44
7:G:225:ALA:HB3	22:Y:105:PHE:CZ	2.53	0.44
7:N:191:MET:HA	7:N:194:PHE:CD2	2.53	0.44
28:S:303:CLA:H91	28:S:303:CLA:H112	1.75	0.44
20:W:5:ARG:HG3	20:W:7:SER:OG	2.17	0.44
22:Y:52:SER:HB3	22:Y:58:PHE:CD1	2.52	0.44
31:a:411:SQD:H252	3:c:36:TRP:CG	2.53	0.44
2:b:376:ILE:HD12	2:b:378:ARG:HH11	1.82	0.44
2:b:454:GLY:HA2	32:b:620:LMG:H222	1.99	0.44
35:c:519:LHG:H272	28:y:311:CLA:C1C	2.47	0.44
5:e:36:LEU:O	5:e:37:PHE:C	2.61	0.44
28:g:613:CLA:H11	28:g:613:CLA:ND	2.32	0.44
7:n:87:ARG:HH22	7:n:207:GLU:N	2.15	0.44
17:r:95:CYS:SG	28:r:608:CLA:HED3	2.57	0.44
28:r:610:CLA:HBC3	35:r:617:LHG:H252	2.00	0.44
18:s:46:PRO:HB3	18:s:48:TYR:CZ	2.53	0.44
19:t:20:ALA:O	19:t:24:ARG:HB3	2.17	0.44
22:y:119:VAL:HA	38:y:306:CHL:C4D	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:13:TYR:CG	24:u:25:ILE:HD13	2.52	0.44
2:B:283:GLU:O	2:B:287:ARG:HG3	2.17	0.44
4:D:258:PHE:HA	35:D:407:LHG:H383	2.00	0.44
6:F:30:SER:O	6:F:34:MET:HG3	2.17	0.44
7:G:104:ILE:CG2	7:G:124:ILE:HG13	2.47	0.44
28:G:610:CLA:H192	40:G:617:NEX:H372	1.99	0.44
38:N:605:CHL:HHC	38:N:605:CHL:CBB	2.44	0.44
15:P:76:SER:OG	15:P:79:GLU:HG3	2.17	0.44
16:Q:41:PRO:HG3	16:Q:86:TYR:OH	2.17	0.44
17:R:227:TRP:HE3	28:R:612:CLA:HMA2	1.82	0.44
28:R:609:CLA:H2A	28:R:609:CLA:HED3	2.00	0.44
28:R:612:CLA:H42	28:R:612:CLA:C1D	2.47	0.44
18:S:218:PHE:O	18:S:222:LEU:HD23	2.18	0.44
28:Y:604:CLA:H2	38:Y:606:CHL:CBD	2.46	0.44
28:Y:612:CLA:HED2	28:Y:612:CLA:H2A	1.99	0.44
28:b:603:CLA:HAB	28:b:605:CLA:H18	2.00	0.44
3:c:59:LEU:HD13	30:c:515:BCR:H372	2.00	0.44
3:c:242:SER:O	3:c:246:LEU:HG	2.17	0.44
28:c:508:CLA:C19	32:k:102:LMG:H371	2.47	0.44
28:c:513:CLA:C1	30:c:514:BCR:H381	2.44	0.44
6:f:39:ARG:HH12	15:p:16:THR:HG21	1.83	0.44
7:g:122:GLN:HB2	38:g:605:CHL:CBB	2.48	0.44
28:g:604:CLA:HED2	28:g:604:CLA:C2A	2.47	0.44
28:g:604:CLA:H2	38:g:606:CHL:HBD	2.00	0.44
7:n:176:LEU:HB3	28:n:610:CLA:CMA	2.47	0.44
28:n:603:CLA:H143	28:y:303:CLA:H122	1.99	0.44
38:n:609:CHL:C1B	38:y:302:CHL:H2	2.47	0.44
14:o:1:GLU:HB2	20:w:6:MET:HG3	1.99	0.44
15:p:121:ILE:N	15:p:124:LYS:O	2.49	0.44
16:q:69:ALA:HB1	16:q:72:PHE:CD2	2.53	0.44
28:B:615:CLA:H111	28:B:615:CLA:H93	1.61	0.44
28:C:508:CLA:HMB1	28:C:508:CLA:HBB1	2.00	0.44
7:G:111:ASP:OD1	7:G:120:HIS:HA	2.18	0.44
10:J:11:TRP:HB2	11:K:56:ALA:HB1	2.00	0.44
28:N:611:CLA:HHC	28:N:611:CLA:HBB1	1.98	0.44
14:O:29:CYS:SG	14:O:54:GLU:HB2	2.58	0.44
16:Q:37:PHE:HD2	16:Q:39:ILE:O	2.00	0.44
16:Q:58:ILE:HD11	16:Q:84:LEU:HD11	1.99	0.44
17:R:162:ARG:HH12	28:R:608:CLA:HED2	1.83	0.44
39:R:614:LUT:H11	39:R:614:LUT:H191	1.87	0.44
20:W:19:ASN:ND2	20:W:21:LEU:H	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:225:ALA:O	41:Y:617:XAT:H42	2.16	0.44
28:Y:611:CLA:HBA2	28:Y:612:CLA:OBD	2.18	0.44
23:Z:14:VAL:O	23:Z:18:ILE:HD13	2.18	0.44
1:a:29:TYR:HB2	4:d:256:GLN:HE21	1.81	0.44
1:a:255:PHE:CD1	1:a:264:SER:HA	2.53	0.44
28:a:406:CLA:H171	28:d:401:CLA:H111	1.99	0.44
28:a:406:CLA:H151	28:d:401:CLA:H151	2.00	0.44
2:b:72:THR:HB	2:b:80:ILE:HG22	2.00	0.44
28:c:504:CLA:C4	32:k:102:LMG:H362	2.48	0.44
28:c:504:CLA:HAA1	36:c:517:DGD:HE1	1.99	0.44
28:c:512:CLA:H2	28:c:512:CLA:H61	1.68	0.44
38:g:601:CHL:H161	38:g:601:CHL:H141	1.78	0.44
11:k:53:VAL:HA	30:k:101:BCR:H402	1.99	0.44
14:o:50:LYS:HA	14:o:50:LYS:HE3	1.99	0.44
14:o:191:LYS:HB3	14:o:228:LEU:HD13	2.00	0.44
28:r:602:CLA:C2	41:r:615:XAT:O24	2.66	0.44
28:r:602:CLA:HBB1	28:r:602:CLA:HMB1	1.99	0.44
38:r:605:CHL:H161	38:r:605:CHL:H141	1.76	0.44
28:r:609:CLA:H92	28:r:609:CLA:H61	1.68	0.44
18:s:125:ASN:HA	18:s:130:PRO:N	2.33	0.44
18:s:220:LYS:HB3	18:s:228:ASN:HD22	1.83	0.44
35:s:617:LHG:H262	35:s:617:LHG:HC62	1.99	0.44
35:s:617:LHG:HC81	35:s:617:LHG:H111	1.57	0.44
22:y:111:ASP:HB3	22:y:115:ASN:C	2.42	0.44
22:y:203:LYS:HB2	22:y:208:ASN:ND2	2.32	0.44
1:A:234:ASN:HB3	4:D:264:ASN:ND2	2.33	0.44
2:B:233:ASN:ND2	2:B:473:THR:HG23	2.33	0.44
28:B:601:CLA:H61	30:H:101:BCR:H403	1.99	0.44
28:B:614:CLA:H62	31:L:101:SQD:H152	1.99	0.44
3:C:126:GLY:O	3:C:130:ILE:HG13	2.18	0.44
28:C:506:CLA:H102	28:C:506:CLA:H61	1.27	0.44
4:D:41:CYS:HB3	4:D:118:HIS:O	2.18	0.44
28:D:404:CLA:H122	21:X:62:GLY:CA	2.46	0.44
5:E:19:TYR:HE2	37:E:101:HEM:C4D	2.36	0.44
7:G:98:PHE:HA	38:G:607:CHL:HMA3	1.99	0.44
7:G:169:ASP:HB3	7:G:172:ALA:HB3	1.99	0.44
11:K:39:PHE:HZ	11:K:46:LEU:HD11	1.82	0.44
14:O:237:LYS:HD3	14:O:239:GLN:NE2	2.32	0.44
18:S:34:PHE:CD2	18:S:35:LEU:HG	2.52	0.44
18:S:86:MET:HE3	28:S:310:CLA:HMC3	2.00	0.44
20:W:34:TRP:CZ2	35:W:101:LHG:H112	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:613:CLA:H11	28:Y:613:CLA:C4D	2.48	0.44
1:a:238:ARG:HH22	19:t:30:PRO:HB3	1.82	0.44
2:b:91:TRP:HD1	35:b:622:LHG:O3	2.01	0.44
2:b:434:ARG:HB3	2:b:439:SER:HB2	1.99	0.44
3:c:367:GLU:N	3:c:368:PRO:CD	2.81	0.44
4:d:127:MET:HE3	4:d:144:ALA:O	2.17	0.44
7:g:128:TRP:O	7:g:132:VAL:HG23	2.17	0.44
39:g:615:LUT:H31	39:g:615:LUT:H391	1.90	0.44
28:n:603:CLA:HAC1	38:n:607:CHL:CBB	2.48	0.44
18:s:39:LEU:HD22	23:z:41:PHE:CE1	2.53	0.44
18:s:117:LEU:HD13	18:s:124:LEU:HD21	2.00	0.44
28:s:609:CLA:H41	28:s:609:CLA:H61	1.72	0.44
28:s:613:CLA:HBB1	28:s:613:CLA:CMB	2.48	0.44
22:y:206:LEU:N	22:y:206:LEU:HD12	2.32	0.44
38:y:309:CHL:HAA1	38:y:309:CHL:HBD	2.00	0.44
23:z:34:SER:HA	23:z:37:LYS:HG3	2.00	0.44
1:A:136:ARG:O	9:I:32:PRO:HD3	2.18	0.44
1:A:188:ALA:CB	1:A:328:MET:HB2	2.46	0.44
1:A:331:MET:HB2	4:D:322:LEU:HD13	1.99	0.44
28:B:607:CLA:H143	12:L:36:PHE:HZ	1.83	0.44
30:B:619:BCR:H341	30:B:619:BCR:H11C	1.88	0.44
3:C:119:LEU:HG	30:C:516:BCR:C10	2.47	0.44
5:E:35:TRP:CD2	6:F:33:ALA:HB2	2.53	0.44
7:N:112:TYR:HB3	7:N:118:LEU:HB3	2.00	0.44
7:N:164:LEU:HB2	7:N:166:LEU:HD13	1.99	0.44
7:N:192:PHE:CD2	38:N:609:CHL:H203	2.53	0.44
17:R:184:LEU:H	17:R:184:LEU:CD1	2.22	0.44
28:R:604:CLA:C3B	41:R:615:XAT:H183	2.47	0.44
18:S:34:PHE:CE2	18:S:35:LEU:HG	2.53	0.44
1:a:297:LEU:HB2	42:a:501:HOH:O	2.18	0.44
2:b:224:ARG:HG3	8:h:37:TRP:CE2	2.53	0.44
28:b:603:CLA:HBB1	28:b:603:CLA:CMB	2.44	0.44
28:b:610:CLA:H13	28:b:612:CLA:H2	2.00	0.44
3:c:221:GLU:O	3:c:226:SER:HB3	2.18	0.44
30:d:406:BCR:C39	10:j:25:ILE:HD11	2.46	0.44
14:o:158:ASP:HB2	14:o:159:PRO:HD2	2.00	0.44
17:r:114:GLU:OE2	17:r:224:LEU:HD13	2.18	0.44
28:r:601:CLA:HAC1	35:r:617:LHG:O3	2.18	0.44
18:s:107:PRO:HD2	18:s:117:LEU:HD13	2.00	0.44
38:y:306:CHL:HAA1	38:y:306:CHL:HBD	1.99	0.44
38:y:308:CHL:H101	38:y:308:CHL:H62	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:y:317:XAT:C36	35:y:319:LHG:HC81	2.48	0.44
1:A:161:TYR:O	1:A:165:GLN:HG2	2.17	0.44
31:A:410:SQD:H112	31:A:410:SQD:H141	1.85	0.44
2:B:72:THR:HB	2:B:80:ILE:HG22	1.98	0.44
28:B:614:CLA:H2	28:B:614:CLA:NC	2.33	0.44
30:B:617:BCR:H24C	31:B:620:SQD:H121	2.00	0.44
3:C:379:ARG:NH2	16:Q:75:ASN:HD22	2.15	0.44
28:C:509:CLA:O1A	28:C:509:CLA:HBD	2.18	0.44
28:C:512:CLA:CHB	30:C:514:BCR:H401	2.47	0.44
32:C:520:LMG:H162	11:K:42:VAL:HG21	2.00	0.44
4:D:265:LYS:HB2	4:D:265:LYS:NZ	2.32	0.44
7:G:132:VAL:HA	38:G:609:CHL:HBB2	1.99	0.44
7:N:93:GLY:O	7:N:94:GLU:HG3	2.18	0.44
14:O:68:ASN:HB3	14:O:70:PRO:HD2	2.00	0.44
15:P:7:ASN:OD1	15:P:10:GLY:HA3	2.17	0.44
15:P:62:LEU:HD23	15:P:64:GLN:HE21	1.82	0.44
15:P:169:PHE:CE1	15:P:170:LYS:HE2	2.48	0.44
17:R:184:LEU:HB2	28:R:609:CLA:O1A	2.18	0.44
18:S:51:GLY:O	18:S:53:VAL:N	2.51	0.44
22:Y:141:TYR:HB3	38:Y:608:CHL:CMC	2.47	0.44
28:Y:602:CLA:H92	28:Y:603:CLA:HHB	2.00	0.44
28:Y:613:CLA:H61	28:Y:613:CLA:H2	1.63	0.44
23:Z:33:TRP:O	23:Z:37:LYS:N	2.51	0.44
1:a:131:TRP:CE2	28:c:505:CLA:HMA1	2.52	0.44
1:a:156:ALA:HA	1:a:160:ILE:HB	1.99	0.44
2:b:237:VAL:HG22	28:b:610:CLA:HBC2	2.00	0.44
28:b:601:CLA:C1D	28:b:601:CLA:H122	2.47	0.44
32:b:623:LMG:H132	32:b:623:LMG:H161	1.83	0.44
28:g:604:CLA:H3A	28:g:604:CLA:HBA2	1.53	0.44
28:g:612:CLA:HBA1	28:g:612:CLA:H3A	1.70	0.44
12:l:27:VAL:HG11	35:l:101:LHG:H201	2.00	0.44
28:n:602:CLA:H2	39:n:616:LUT:H26	1.99	0.44
28:n:603:CLA:HMD1	38:n:609:CHL:C1D	2.48	0.44
28:n:611:CLA:H43	28:n:612:CLA:HMD2	2.00	0.44
16:q:70:TRP:CE3	16:q:121:ALA:HA	2.53	0.44
17:r:76:LYS:HB2	17:r:76:LYS:NZ	2.33	0.44
17:r:182:LEU:HB2	17:r:184:LEU:HG	1.99	0.44
18:s:29:PRO:C	18:s:31:ARG:N	2.76	0.44
21:x:59:VAL:O	21:x:63:VAL:HG23	2.18	0.44
22:y:110:LEU:HD23	22:y:110:LEU:C	2.43	0.44
22:y:112:TYR:HD2	28:y:305:CLA:HBA2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:y:315:LUT:H35	39:y:315:LUT:H401	1.87	0.44
1:A:184:ILE:HA	28:A:405:CLA:HBC1	1.99	0.43
2:B:3:LEU:HD12	12:L:9:GLN:HB2	1.99	0.43
2:B:124:CYS:CA	2:B:131:PRO:HA	2.29	0.43
28:B:604:CLA:H71	28:B:604:CLA:H111	1.75	0.43
28:B:611:CLA:H61	28:B:611:CLA:H2	1.65	0.43
3:C:311:GLN:HE22	3:C:351:PHE:HB2	1.83	0.43
28:C:507:CLA:CBA	28:C:509:CLA:H72	2.48	0.43
7:G:115:ASN:O	7:G:118:LEU:HB2	2.17	0.43
8:H:29:GLU:HA	17:R:69:ARG:HH12	1.83	0.43
7:N:70:ARG:HA	7:N:73:MET:HE3	2.00	0.43
7:N:140:GLY:CA	22:Y:28:PHE:HB3	2.47	0.43
7:N:203:LYS:HB2	7:N:208:ASN:ND2	2.19	0.43
15:P:124:LYS:HZ3	15:P:152:LYS:HD2	1.82	0.43
17:R:14:TRP:HD1	17:R:32:TYR:O	2.01	0.43
17:R:155:ILE:O	17:R:158:ILE:HG12	2.17	0.43
22:Y:209:LEU:O	22:Y:213:LEU:HG	2.17	0.43
1:a:277:ALA:CB	31:a:411:SQD:H131	2.45	0.43
2:b:13:LEU:HA	28:b:612:CLA:HAC2	2.00	0.43
2:b:246:PHE:CE1	28:b:608:CLA:HBC2	2.52	0.43
4:d:92:LEU:HD13	4:d:94:TRP:CZ2	2.53	0.43
4:d:192:TRP:CZ2	4:d:198:HIS:HB2	2.53	0.43
15:p:20:PRO:HA	15:p:29:LEU:HD23	1.99	0.43
18:s:91:GLY:HA3	39:s:615:LUT:H182	1.98	0.43
18:s:154:ILE:HG12	28:s:608:CLA:CMA	2.48	0.43
18:s:230:LEU:O	18:s:234:ILE:HG12	2.18	0.43
28:s:603:CLA:HBC1	28:s:608:CLA:CBC	2.48	0.43
35:w:102:LHG:HC81	28:y:311:CLA:C2	2.48	0.43
28:A:408:CLA:H61	20:W:15:PHE:HD1	1.83	0.43
2:B:127:ARG:NH2	4:D:3:ILE:HD11	2.33	0.43
28:B:602:CLA:H171	36:B:626:DGD:HAT1	1.98	0.43
28:B:603:CLA:C1D	28:B:605:CLA:H62	2.47	0.43
28:B:606:CLA:H102	30:B:619:BCR:C10	2.48	0.43
28:B:606:CLA:H161	30:B:619:BCR:H12C	2.00	0.43
28:B:611:CLA:HBB1	28:B:611:CLA:CMB	2.48	0.43
28:B:616:CLA:HBB1	28:B:616:CLA:CMB	2.45	0.43
3:C:185:ILE:HG13	3:C:230:LEU:HD13	1.99	0.43
28:C:506:CLA:C2C	28:C:507:CLA:H143	2.48	0.43
28:C:513:CLA:CHC	30:C:514:BCR:H23C	2.48	0.43
30:C:514:BCR:H343	23:Z:51:VAL:CG1	2.48	0.43
4:D:25:ARG:CD	21:X:81:VAL:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:TRP:HB3	28:G:602:CLA:CAD	2.48	0.43
28:G:612:CLA:HMA3	28:G:612:CLA:C2	2.47	0.43
12:L:17:SER:OG	35:L:102:LHG:HC62	2.18	0.43
7:N:24:TYR:H	7:N:44:TYR:HB3	1.82	0.43
14:O:164:ALA:HB1	15:P:93:PHE:HE1	1.83	0.43
28:R:601:CLA:CMC	35:R:616:LHG:HC42	2.49	0.43
18:S:42:ARG:O	18:S:45:ILE:HG12	2.18	0.43
28:Y:611:CLA:H93	28:Y:612:CLA:C1D	2.48	0.43
28:Y:613:CLA:C1A	28:Y:613:CLA:CGA	2.95	0.43
36:a:401:DGD:HA92	32:a:413:LMG:C35	2.29	0.43
28:a:406:CLA:H71	29:a:408:PHO:C1B	2.49	0.43
28:b:605:CLA:CBB	28:b:606:CLA:H52	2.47	0.43
28:b:611:CLA:CHD	35:b:624:LHG:H352	2.48	0.43
3:c:117:LEU:CD2	32:c:521:LMG:H371	2.45	0.43
28:c:510:CLA:HBB1	28:c:510:CLA:CMB	2.48	0.43
4:d:268:LEU:HD23	4:d:268:LEU:C	2.43	0.43
7:g:128:TRP:CE3	7:n:222:TRP:HZ2	2.36	0.43
7:g:227:ASN:HB2	38:g:619:CHL:C2D	2.48	0.43
28:g:604:CLA:HMA3	38:g:606:CHL:C2C	2.48	0.43
28:g:614:CLA:HAA2	22:y:128:TRP:HZ2	1.81	0.43
8:h:33:VAL:HG21	17:r:48:PHE:HE2	1.83	0.43
11:k:37:VAL:HA	11:k:40:MET:SD	2.58	0.43
7:n:78:GLY:HA3	39:n:616:LUT:H183	2.00	0.43
7:n:139:GLU:HG3	38:n:609:CHL:C4B	2.48	0.43
28:n:610:CLA:HMB2	28:n:612:CLA:HBA2	1.99	0.43
16:q:38:PHE:CE2	16:q:39:ILE:HG13	2.53	0.43
16:q:88:LEU:HD13	16:q:107:THR:HG23	2.00	0.43
28:r:602:CLA:H111	28:r:602:CLA:H71	1.41	0.43
28:r:602:CLA:H2	41:r:615:XAT:O24	2.18	0.43
28:r:608:CLA:H11	28:r:613:CLA:H61	1.99	0.43
18:s:19:ALA:N	18:s:180:ASP:HB3	2.32	0.43
18:s:77:TYR:CE2	28:s:603:CLA:HBA1	2.53	0.43
21:x:52:LYS:HZ3	21:x:56:LEU:HD11	1.82	0.43
22:y:222:TRP:C	22:y:224:TYR:H	2.27	0.43
28:y:304:CLA:H121	38:y:309:CHL:H92	1.98	0.43
2:B:76:GLY:HA2	36:a:401:DGD:HE4	1.99	0.43
2:B:151:PHE:CZ	32:B:624:LMG:H161	2.53	0.43
28:B:616:CLA:HBA2	30:B:619:BCR:H372	1.99	0.43
3:C:418:ASN:HD21	36:C:518:DGD:HD4	1.83	0.43
28:C:506:CLA:CHA	28:C:507:CLA:H202	2.49	0.43
28:C:506:CLA:H112	35:W:101:LHG:H361	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:510:CLA:H102	28:C:510:CLA:H62	1.47	0.43
4:D:133:LEU:O	4:D:137:VAL:HG23	2.18	0.43
5:E:35:TRP:HZ2	15:P:9:PHE:CE2	2.35	0.43
7:G:47:ASP:OD1	7:G:51:LEU:HD12	2.17	0.43
7:G:64:LEU:HD13	28:G:603:CLA:CBA	2.47	0.43
9:I:13:ILE:HG23	20:W:29:VAL:HG11	2.01	0.43
11:K:26:LEU:HD11	11:K:37:VAL:HG21	2.00	0.43
31:L:103:SQD:H45	31:L:103:SQD:H81	1.76	0.43
7:N:182:LYS:HB3	28:N:611:CLA:HMD1	1.99	0.43
38:N:607:CHL:C2C	38:Y:601:CHL:H143	2.47	0.43
14:O:219:GLU:HG3	14:O:239:GLN:HG2	2.01	0.43
16:Q:131:LYS:O	16:Q:135:ILE:HG13	2.17	0.43
16:Q:144:LEU:HA	16:Q:147:ILE:HD12	2.01	0.43
28:S:304:CLA:HBC1	28:S:309:CLA:CAC	2.48	0.43
1:a:102:VAL:O	1:a:106:LEU:HG	2.18	0.43
1:a:119:PHE:CD1	29:a:408:PHO:H121	2.54	0.43
3:c:135:LEU:HD23	23:z:27:PHE:HA	1.99	0.43
3:c:158:THR:HG21	3:c:256:PRO:HD3	2.00	0.43
3:c:223:TRP:CE2	3:c:224:ILE:HG23	2.53	0.43
3:c:369:LEU:HA	3:c:379:ARG:HD2	2.00	0.43
5:e:71:ASP:O	5:e:75:GLN:HG3	2.18	0.43
7:g:220:ASN:HB2	7:g:222:TRP:CZ3	2.53	0.43
28:g:611:CLA:CHD	35:g:618:LHG:HC62	2.48	0.43
38:r:607:CHL:O2A	28:r:609:CLA:HMD1	2.17	0.43
18:s:77:TYR:CD1	28:s:603:CLA:HBD	2.52	0.43
24:u:2:PRO:HG3	24:u:8:GLU:HG2	2.00	0.43
1:A:202:VAL:HG11	28:A:406:CLA:C3D	2.48	0.43
1:A:306:VAL:HG12	1:A:314:ILE:HB	2.01	0.43
32:A:411:LMG:O10	20:W:15:PHE:HA	2.18	0.43
31:A:414:SQD:C38	36:A:417:DGD:HA91	2.44	0.43
28:B:615:CLA:H122	28:B:616:CLA:C1B	2.48	0.43
3:C:438:PHE:CE2	3:C:442:LEU:HD11	2.52	0.43
3:C:473:ASN:HA	19:T:26:PRO:HB3	1.98	0.43
4:D:172:PRO:HG3	4:D:182:PHE:CZ	2.53	0.43
28:G:602:CLA:C2	39:G:616:LUT:H26	2.48	0.43
17:R:115:TRP:CE3	17:R:116:LEU:HD21	2.54	0.43
18:S:56:ASP:HA	28:S:303:CLA:O1D	2.19	0.43
18:S:67:LYS:HB2	18:S:70:ASP:CG	2.43	0.43
18:S:88:GLY:HA2	39:S:316:LUT:C18	2.47	0.43
18:S:96:GLU:CD	18:S:215:VAL:HB	2.43	0.43
18:S:109:ALA:HA	28:S:305:CLA:HED1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:150:GLU:O	18:S:154:ILE:HG22	2.18	0.43
38:Y:608:CHL:C2	39:Y:615:LUT:H383	2.48	0.43
38:Y:609:CHL:HAA1	38:Y:609:CHL:HBD	2.00	0.43
1:a:103:ASP:HB3	14:o:117:GLN:NE2	2.33	0.43
1:a:116:VAL:HG13	1:a:158:PHE:HB3	1.99	0.43
1:a:326:LEU:HD13	1:a:326:LEU:HA	1.87	0.43
36:a:401:DGD:C8B	30:a:410:BCR:H17C	2.47	0.43
2:b:6:TYR:OH	35:b:624:LHG:HC2	2.18	0.43
2:b:35:GLY:O	2:b:39:LEU:HG	2.18	0.43
2:b:451:PHE:HZ	28:b:604:CLA:HED2	1.83	0.43
2:b:491:GLU:H	2:b:491:GLU:CD	2.26	0.43
28:b:610:CLA:H13	28:b:612:CLA:C2	2.48	0.43
28:b:615:CLA:H191	28:b:615:CLA:CHB	2.49	0.43
3:c:34:ALA:HB2	4:d:231:ASN:HD22	1.84	0.43
3:c:284:PHE:CG	36:c:516:DGD:HBT2	2.53	0.43
3:c:320:ARG:O	3:c:324:LEU:HD23	2.19	0.43
28:c:511:CLA:H122	23:z:24:PRO:HG3	2.00	0.43
36:c:517:DGD:HB72	32:k:102:LMG:H422	1.99	0.43
32:c:521:LMG:H291	18:s:226:PHE:O	2.18	0.43
38:g:609:CHL:H51	38:g:609:CHL:H92	2.01	0.43
7:n:44:TYR:CE2	38:n:601:CHL:HBC2	2.52	0.43
14:o:16:THR:O	14:o:19:GLU:HG2	2.18	0.43
17:r:209:PHE:CZ	41:r:615:XAT:H8	2.54	0.43
18:s:79:LEU:HD21	18:s:165:HIS:NE2	2.33	0.43
28:s:602:CLA:HBB1	28:s:602:CLA:CMB	2.48	0.43
28:s:612:CLA:HMB2	39:s:614:LUT:H161	2.01	0.43
1:A:273:PHE:CD2	31:A:410:SQD:H121	2.53	0.43
28:A:405:CLA:H18	28:D:401:CLA:H72	2.01	0.43
29:A:407:PHO:H101	28:D:401:CLA:H203	2.00	0.43
2:B:288:VAL:O	2:B:292:LEU:HG	2.18	0.43
28:B:612:CLA:H111	28:B:613:CLA:HHC	2.00	0.43
32:B:621:LMG:C43	13:M:13:LEU:HB3	2.48	0.43
3:C:335:THR:HG22	14:O:156:PHE:HE1	1.84	0.43
32:C:520:LMG:H182	11:K:42:VAL:HG21	2.00	0.43
4:D:81:THR:HG22	4:D:112:TRP:NE1	2.33	0.43
4:D:114:PHE:CZ	30:D:405:BCR:HC21	2.54	0.43
28:D:403:CLA:HBB1	28:D:403:CLA:CMB	2.46	0.43
7:G:212:HIS:C	7:G:215:ASP:H	2.26	0.43
39:G:615:LUT:H35	39:G:615:LUT:H401	1.62	0.43
8:H:33:VAL:HG21	17:R:48:PHE:CE2	2.53	0.43
15:P:169:PHE:CB	16:Q:27:ARG:HD3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:28:ASP:O	16:Q:36:ARG:HD3	2.18	0.43
28:S:310:CLA:HHC	39:S:315:LUT:C32	2.49	0.43
22:Y:112:TYR:CD1	22:Y:113:LEU:HG	2.53	0.43
22:Y:118:LEU:O	22:Y:120:HIS:N	2.51	0.43
35:Y:619:LHG:H291	35:Y:619:LHG:H262	1.61	0.43
28:a:406:CLA:H72	28:a:406:CLA:H111	1.28	0.43
2:b:33:TRP:HD1	30:b:618:BCR:H12C	1.83	0.43
2:b:362:PHE:HE1	4:d:190:HIS:CE1	2.37	0.43
28:b:603:CLA:C1D	28:b:605:CLA:H51	2.48	0.43
3:c:259:TRP:CG	35:w:102:LHG:HC62	2.54	0.43
3:c:304:PRO:HB3	3:c:395:TYR:CG	2.54	0.43
3:c:391:ARG:O	3:c:394:GLU:HG3	2.19	0.43
7:n:123:SER:O	7:n:127:ILE:HG13	2.18	0.43
17:r:135:TYR:CD2	17:r:136:LEU:HD23	2.54	0.43
41:r:615:XAT:H35	41:r:615:XAT:H401	1.92	0.43
18:s:104:ASN:O	18:s:105:CYS:C	2.61	0.43
28:B:611:CLA:H71	28:B:611:CLA:H112	1.78	0.43
28:B:613:CLA:HBB1	28:B:613:CLA:CMB	2.49	0.43
3:C:236:GLY:HA3	30:C:515:BCR:H402	2.01	0.43
28:C:511:CLA:H51	30:C:516:BCR:H282	1.99	0.43
30:D:405:BCR:C39	10:J:25:ILE:HD11	2.49	0.43
7:G:51:LEU:CD2	28:Y:603:CLA:H43	2.49	0.43
7:G:71:TRP:CD1	38:G:609:CHL:HMD3	2.53	0.43
28:G:613:CLA:H172	28:G:614:CLA:CHD	2.49	0.43
15:P:145:GLN:HG2	15:P:162:GLN:HG3	2.00	0.43
15:P:161:ALA:HB1	15:P:176:VAL:HG13	2.00	0.43
28:R:609:CLA:H112	39:R:614:LUT:C31	2.49	0.43
18:S:185:LEU:HD22	28:S:310:CLA:HHB	2.00	0.43
38:S:306:CHL:HBB2	38:S:307:CHL:HBB1	2.00	0.43
36:a:401:DGD:C9A	32:a:413:LMG:H352	2.29	0.43
29:a:408:PHO:HMA1	28:d:401:CLA:H72	1.99	0.43
2:b:277:GLN:HB3	24:u:24:ARG:HB3	2.00	0.43
5:e:35:TRP:CD2	6:f:33:ALA:HB2	2.53	0.43
6:f:31:ILE:O	6:f:35:GLN:HG2	2.18	0.43
7:g:61:ASN:HB2	28:g:602:CLA:HMA2	2.01	0.43
7:g:164:LEU:CD1	39:g:615:LUT:H222	2.48	0.43
39:g:616:LUT:H15	39:g:616:LUT:H201	1.92	0.43
30:k:101:BCR:H11C	30:k:101:BCR:H341	1.83	0.43
7:n:148:LEU:HD12	38:n:608:CHL:C4B	2.49	0.43
15:p:39:GLU:HB2	15:p:48:ARG:HD3	2.00	0.43
15:p:140:GLU:HG2	15:p:166:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:110:ALA:HA	17:r:121:TRP:HB3	2.00	0.43
17:r:227:TRP:HB2	39:r:614:LUT:H21	1.99	0.43
39:r:614:LUT:H31	39:r:614:LUT:H391	1.76	0.43
28:s:610:CLA:HBC3	28:s:610:CLA:H101	2.01	0.43
32:w:101:LMG:H332	32:w:101:LMG:H301	1.55	0.43
1:A:114:LEU:HD23	1:A:114:LEU:C	2.44	0.43
28:B:609:CLA:HBA2	28:B:609:CLA:H3A	1.34	0.43
30:B:619:BCR:HC31	35:B:623:LHG:H251	2.01	0.43
35:B:622:LHG:H251	35:B:622:LHG:C8	2.35	0.43
28:C:501:CLA:HHC	28:C:501:CLA:CBB	2.48	0.43
28:C:506:CLA:HBA2	28:C:507:CLA:H203	2.01	0.43
4:D:14:ASP:C	4:D:14:ASP:OD1	2.62	0.43
7:G:73:MET:HB3	39:G:615:LUT:C40	2.48	0.43
7:N:63:GLU:O	7:N:67:ILE:HG12	2.19	0.43
7:N:139:GLU:HG3	38:N:609:CHL:C3B	2.48	0.43
7:N:163:PRO:HD2	39:N:615:LUT:H24	2.01	0.43
38:N:606:CHL:HAC2	38:N:606:CHL:OMC	2.18	0.43
17:R:93:ARG:NH2	28:R:602:CLA:HED3	2.34	0.43
28:R:603:CLA:HMD2	28:R:613:CLA:H121	2.01	0.43
28:R:608:CLA:H93	28:R:608:CLA:H111	1.80	0.43
1:a:35:VAL:HA	30:a:410:BCR:C32	2.48	0.43
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.99	0.43
2:b:497:LYS:HB2	2:b:503:THR:HG21	2.01	0.43
28:b:610:CLA:H151	28:b:615:CLA:CBD	2.45	0.43
3:c:108:THR:HA	3:c:111:TYR:CD2	2.53	0.43
28:c:507:CLA:H111	30:i:101:BCR:C16	2.49	0.43
7:g:21:ARG:CZ	7:g:23:LYS:HE2	2.49	0.43
7:n:35:TYR:OH	7:n:50:GLY:HA2	2.18	0.43
7:n:161:PHE:HZ	38:n:608:CHL:NB	2.16	0.43
15:p:11:LYS:NZ	15:p:11:LYS:HB3	2.34	0.43
17:r:49:ASP:HB2	17:r:66:ILE:CG2	2.49	0.43
18:s:133:ILE:HG12	38:s:605:CHL:HED3	1.99	0.43
28:y:312:CLA:C2	28:y:312:CLA:H71	2.49	0.43
1:A:12:ASN:O	1:A:16:ARG:HG3	2.19	0.43
28:A:405:CLA:H112	28:A:405:CLA:H71	1.65	0.43
28:A:408:CLA:HAC1	32:A:413:LMG:H391	2.01	0.43
2:B:32:GLY:HA3	30:B:618:BCR:C17	2.48	0.43
2:B:63:ILE:HB	2:B:64:PRO:HD3	2.00	0.43
2:B:500:ASP:CG	2:B:503:THR:HG23	2.43	0.43
3:C:162:GLY:HA3	3:C:252:ILE:HG13	1.99	0.43
3:C:262:ARG:O	9:I:26:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:C:518:DGD:HA62	36:C:518:DGD:HA91	1.76	0.43
4:D:14:ASP:O	4:D:18:ILE:HG13	2.18	0.43
8:H:43:MET:O	8:H:47:MET:HG3	2.19	0.43
11:K:39:PHE:CZ	11:K:46:LEU:HD11	2.53	0.43
28:N:602:CLA:H102	39:N:616:LUT:C37	2.47	0.43
38:N:608:CHL:HBA2	38:N:608:CHL:CHA	2.48	0.43
15:P:121:ILE:HB	15:P:126:TYR:CE1	2.53	0.43
17:R:31:ASP:HB2	28:R:602:CLA:HED2	2.01	0.43
17:R:89:LEU:CD1	28:R:602:CLA:HAA2	2.48	0.43
28:S:311:CLA:HHC	28:S:311:CLA:CBB	2.48	0.43
28:S:311:CLA:C4A	28:S:311:CLA:H62	2.48	0.43
22:Y:199:ILE:HG12	38:Y:607:CHL:H111	2.01	0.43
28:Y:604:CLA:HBB1	28:Y:604:CLA:CMB	2.45	0.43
28:Y:604:CLA:O1A	40:Y:618:NEX:H241	2.18	0.43
1:a:32:TRP:HB2	9:i:23:PHE:CE2	2.54	0.43
1:a:149:ALA:N	1:a:150:PRO:HD2	2.33	0.43
2:b:159:THR:HA	2:b:181:VAL:O	2.19	0.43
28:b:601:CLA:H141	28:b:601:CLA:H162	1.77	0.43
3:c:179:ALA:HA	3:c:184:GLY:CA	2.34	0.43
3:c:245:ILE:O	3:c:249:ILE:HG13	2.18	0.43
3:c:299:SER:HA	3:c:423:ARG:HH21	1.84	0.43
28:c:509:CLA:H141	28:c:509:CLA:H161	1.80	0.43
4:d:314:THR:O	4:d:318:LYS:HG3	2.19	0.43
28:d:405:CLA:H13	21:x:58:ILE:CG2	2.49	0.43
28:g:602:CLA:H93	28:g:602:CLA:H111	1.63	0.43
38:g:619:CHL:HMC	22:y:131:GLN:OE1	2.19	0.43
35:l:101:LHG:H112	35:l:101:LHG:H142	1.89	0.43
28:n:603:CLA:H71	28:n:603:CLA:H112	1.40	0.43
38:n:608:CHL:H61	38:n:608:CHL:H101	1.68	0.43
14:o:238:ILE:N	14:o:238:ILE:HD12	2.34	0.43
15:p:78:GLU:HG3	15:p:113:ILE:CD1	2.49	0.43
16:q:88:LEU:O	16:q:92:ILE:HG13	2.18	0.43
28:r:610:CLA:HBC1	28:r:612:CLA:H143	2.00	0.43
28:s:604:CLA:HMA3	38:s:605:CHL:C2C	2.48	0.43
28:s:604:CLA:HBA2	28:s:604:CLA:H3A	1.31	0.43
40:s:616:NEX:H11	40:s:616:NEX:H191	1.89	0.43
28:y:304:CLA:HED1	28:y:304:CLA:C9	2.49	0.43
38:y:308:CHL:HAA2	38:y:308:CHL:H172	2.00	0.43
1:A:203:ALA:HB2	36:C:519:DGD:HAH1	2.01	0.43
28:A:408:CLA:HAA2	32:A:411:LMG:H111	2.01	0.43
28:A:408:CLA:H12	9:I:9:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:413:LMG:H341	32:A:413:LMG:H372	1.66	0.43
2:B:94:GLU:H	2:B:94:GLU:CD	2.27	0.43
2:B:236:THR:HB	2:B:473:THR:HG21	2.00	0.43
2:B:393:GLU:HG2	15:P:94:PHE:HE2	1.83	0.43
35:B:623:LHG:H242	35:B:623:LHG:C10	2.49	0.43
4:D:210:LEU:HD23	4:D:210:LEU:C	2.44	0.43
7:G:59:SER:O	7:G:63:GLU:HG3	2.19	0.43
7:G:156:TYR:HA	28:G:610:CLA:CGD	2.49	0.43
38:G:601:CHL:C1D	35:G:618:LHG:HC82	2.49	0.43
28:G:604:CLA:HBB1	28:G:604:CLA:CMB	2.46	0.43
10:J:9:PRO:O	10:J:13:ILE:HG13	2.18	0.43
7:N:121:ALA:HA	38:N:605:CHL:CHC	2.48	0.43
7:N:187:ALA:O	7:N:191:MET:HG2	2.18	0.43
38:N:606:CHL:HAB	38:N:609:CHL:HBC1	2.00	0.43
28:R:601:CLA:HMC1	28:R:601:CLA:HBC2	2.01	0.43
30:T:101:BCR:H15C	30:b:618:BCR:H373	2.00	0.43
1:a:200:LEU:HD23	36:c:518:DGD:CCA	2.48	0.43
2:b:9:HIS:HE1	28:b:613:CLA:HED1	1.84	0.43
2:b:164:PRO:HB3	28:b:606:CLA:O1D	2.19	0.43
2:b:218:SER:HB2	28:r:603:CLA:H52	2.01	0.43
2:b:414:PRO:O	2:b:418:LYS:HG3	2.19	0.43
2:b:504:LYS:HB3	2:b:504:LYS:NZ	2.34	0.43
28:b:608:CLA:H143	28:d:405:CLA:CHB	2.48	0.43
3:c:369:LEU:HD22	3:c:379:ARG:HB3	2.00	0.43
4:d:267:TRP:CD1	35:d:408:LHG:HC2	2.54	0.43
7:g:161:PHE:HE1	38:g:608:CHL:HBA2	1.84	0.43
7:g:179:LYS:HG2	28:g:611:CLA:HED2	2.00	0.43
38:g:601:CHL:H162	38:g:619:CHL:CAB	2.49	0.43
10:j:9:PRO:HG2	10:j:12:ILE:HD13	2.00	0.43
11:k:30:TYR:CZ	23:z:5:PHE:HZ	2.37	0.43
15:p:111:ALA:O	16:q:7:VAL:HA	2.19	0.43
16:q:85:ARG:HG2	16:q:111:PHE:CZ	2.53	0.43
38:r:605:CHL:H151	40:r:616:NEX:C11	2.48	0.43
18:s:71:PHE:O	18:s:75:GLN:HG3	2.19	0.43
18:s:111:TRP:CZ3	18:s:112:PHE:HB3	2.54	0.43
19:t:12:SER:O	19:t:16:ILE:HG13	2.19	0.43
28:y:312:CLA:H121	28:y:312:CLA:H91	2.01	0.43
32:A:411:LMG:H142	32:A:411:LMG:H111	1.89	0.43
2:B:326:ARG:HD3	2:B:442:VAL:HG12	2.01	0.43
2:B:495:PHE:HA	2:B:504:LYS:CB	2.49	0.43
28:B:603:CLA:CMC	28:B:605:CLA:H172	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:603:CLA:C3D	28:B:605:CLA:H43	2.49	0.43
3:C:163:ILE:HD13	28:C:512:CLA:HAB	2.01	0.43
6:F:27:PHE:O	6:F:31:ILE:HG13	2.19	0.43
6:F:31:ILE:HG22	6:F:35:GLN:HE21	1.84	0.43
38:N:601:CHL:HHD	35:N:618:LHG:C4	2.47	0.43
28:N:602:CLA:H52	28:N:603:CLA:CBA	2.49	0.43
28:N:603:CLA:C4D	38:N:609:CHL:H8	2.48	0.43
15:P:92:ALA:HA	15:P:94:PHE:CZ	2.54	0.43
16:Q:92:ILE:HG22	16:Q:103:LEU:HG	2.01	0.43
28:R:603:CLA:CHC	28:R:608:CLA:H122	2.49	0.43
28:R:608:CLA:HBA2	28:R:613:CLA:H101	2.01	0.43
28:R:608:CLA:H52	28:R:613:CLA:H18	2.01	0.43
18:S:60:ASP:HA	39:S:316:LUT:H24	1.99	0.43
20:W:34:TRP:CH2	28:Y:612:CLA:H61	2.54	0.43
1:a:267:ASN:HA	4:d:236:PHE:CE2	2.54	0.43
31:a:411:SQD:H252	3:c:36:TRP:CD1	2.54	0.43
2:b:41:GLU:OE1	2:b:63:ILE:HG13	2.19	0.43
2:b:256:MET:HA	2:b:263:THR:HG21	2.00	0.43
2:b:289:GLY:O	2:b:293:VAL:HG23	2.19	0.43
2:b:352:ARG:HE	2:b:372:ASP:CB	2.32	0.43
3:c:177:PHE:HB3	3:c:182:PHE:HE2	1.83	0.43
29:d:402:PHO:H152	28:d:404:CLA:H171	2.00	0.43
7:g:73:MET:HB3	39:g:615:LUT:C35	2.48	0.43
7:g:224:TYR:HA	22:y:105:PHE:CD1	2.53	0.43
35:g:618:LHG:H223	28:y:304:CLA:H201	2.01	0.43
30:h:101:BCR:HC8	30:h:101:BCR:C33	2.48	0.43
9:i:24:LEU:HG	30:i:101:BCR:HC41	2.00	0.43
7:n:23:LYS:HB3	7:n:29:SER:OG	2.18	0.43
7:n:24:TYR:HD2	38:n:601:CHL:HAA1	1.84	0.43
7:n:203:LYS:HB3	7:n:207:GLU:OE1	2.19	0.43
28:n:612:CLA:H3A	28:n:612:CLA:HBA1	1.81	0.43
15:p:125:GLN:HE21	15:p:127:TYR:HD1	1.66	0.43
16:q:39:ILE:HG23	16:q:83:TYR:CD1	2.52	0.43
28:r:604:CLA:C4B	40:r:616:NEX:H222	2.49	0.43
18:s:60:ASP:HA	39:s:615:LUT:H24	2.01	0.43
18:s:189:GLU:HG3	28:s:609:CLA:C4B	2.49	0.43
28:s:604:CLA:CGA	40:s:616:NEX:H382	2.48	0.43
22:y:46:TRP:HE3	28:y:303:CLA:C2D	2.32	0.43
1:A:327:GLY:O	1:A:331:MET:HG2	2.19	0.42
2:B:371:VAL:HG12	2:B:372:ASP:O	2.19	0.42
3:C:257:PHE:HB2	3:C:259:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.00	0.42
3:C:391:ARG:O	3:C:394:GLU:HG2	2.19	0.42
28:C:502:CLA:H171	28:C:502:CLA:H13	1.71	0.42
28:C:508:CLA:H8	28:C:510:CLA:HED3	2.00	0.42
28:C:510:CLA:HED1	28:C:510:CLA:H93	2.00	0.42
35:C:521:LHG:H241	35:C:521:LHG:H121	2.01	0.42
4:D:203:ALA:HB2	33:D:406:PL9:H353	2.00	0.42
7:G:79:CYS:HA	39:G:616:LUT:H41	2.00	0.42
7:G:140:GLY:HA3	7:N:28:PHE:CD1	2.54	0.42
7:G:162:ASP:CG	28:G:610:CLA:HBA2	2.44	0.42
28:G:612:CLA:H121	28:G:612:CLA:C1B	2.49	0.42
31:L:103:SQD:H441	19:T:23:PHE:HD2	1.84	0.42
28:N:611:CLA:HBA2	28:N:612:CLA:OBD	2.19	0.42
17:R:14:TRP:HA	28:R:601:CLA:NC	2.34	0.42
18:S:21:GLU:O	18:S:23:LEU:N	2.48	0.42
28:Y:602:CLA:H51	28:Y:603:CLA:HBA1	2.01	0.42
32:a:413:LMG:H322	32:a:413:LMG:H291	1.66	0.42
2:b:288:VAL:HG23	2:b:305:ILE:HD11	2.01	0.42
28:b:601:CLA:H101	28:b:601:CLA:HMD2	2.00	0.42
28:b:602:CLA:H122	28:b:602:CLA:H8	1.78	0.42
3:c:308:GLU:HA	3:c:361:LEU:HD22	2.01	0.42
3:c:350:ILE:CG2	3:c:359:TRP:HB2	2.47	0.42
4:d:81:THR:HG22	4:d:112:TRP:NE1	2.34	0.42
4:d:181:ARG:HD3	4:d:182:PHE:N	2.34	0.42
28:g:614:CLA:HBB1	28:g:614:CLA:CMB	2.44	0.42
7:n:153:ASP:HB3	7:n:156:TYR:O	2.19	0.42
28:n:602:CLA:H13	28:n:602:CLA:H102	1.46	0.42
14:o:8:THR:OG1	14:o:11:GLU:HG3	2.19	0.42
14:o:47:ASN:O	14:o:49:LYS:HG2	2.19	0.42
16:q:37:PHE:CE2	16:q:39:ILE:HB	2.54	0.42
28:r:603:CLA:C15	28:r:603:CLA:H91	2.49	0.42
18:s:65:SER:HB2	18:s:71:PHE:CA	2.48	0.42
39:s:615:LUT:H15	39:s:615:LUT:H201	1.88	0.42
19:t:18:PHE:HE1	19:t:23:PHE:HE1	1.65	0.42
22:y:147:PRO:HD2	38:y:308:CHL:CBB	2.48	0.42
29:A:407:PHO:H71	28:D:401:CLA:H191	1.99	0.42
2:B:296:GLN:NE2	2:B:304:LYS:HE3	2.35	0.42
2:B:340:TRP:HB2	2:B:430:PHE:CE2	2.54	0.42
28:C:513:CLA:NB	30:C:514:BCR:H383	2.34	0.42
4:D:54:THR:HG22	6:F:34:MET:HE1	2.01	0.42
7:G:179:LYS:HD3	28:G:612:CLA:CBA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:119:VAL:HA	38:N:605:CHL:C4D	2.49	0.42
7:N:224:TYR:HE2	28:N:613:CLA:HED2	1.84	0.42
14:O:89:ILE:HA	14:O:108:GLY:HA3	2.01	0.42
18:S:74:TYR:HB3	28:S:303:CLA:HHB	2.01	0.42
18:S:206:GLN:OE1	39:S:315:LUT:H42	2.19	0.42
35:S:301:LHG:H112	28:S:311:CLA:CAB	2.49	0.42
38:S:302:CHL:HAA2	38:S:302:CHL:HBD	2.01	0.42
28:Y:603:CLA:H92	28:Y:603:CLA:H61	1.58	0.42
38:Y:606:CHL:CBB	39:Y:616:LUT:H161	2.50	0.42
28:Y:613:CLA:H121	41:Y:617:XAT:H34	2.01	0.42
1:a:161:TYR:HA	1:a:294:ALA:CB	2.49	0.42
2:b:237:VAL:CG2	28:b:610:CLA:HBC2	2.50	0.42
2:b:320:ALA:HB3	2:b:361:THR:HG21	1.99	0.42
3:c:28:GLN:C	3:c:30:THR:N	2.75	0.42
3:c:159:THR:O	3:c:163:ILE:HG13	2.18	0.42
4:d:133:LEU:O	4:d:137:VAL:HG23	2.20	0.42
28:d:401:CLA:H93	28:d:401:CLA:H62	1.88	0.42
5:e:9:SER:O	5:e:13:ILE:HG13	2.19	0.42
9:i:17:SER:HB2	20:w:33:ILE:HG13	2.01	0.42
13:m:21:PHE:O	13:m:25:ILE:HG12	2.19	0.42
7:n:147:PRO:HD2	38:n:608:CHL:CBB	2.49	0.42
38:n:601:CHL:HHC	38:n:601:CHL:CBB	2.46	0.42
15:p:156:LEU:HD21	15:p:158:ILE:HD11	2.01	0.42
17:r:146:THR:O	17:r:150:ILE:HG13	2.19	0.42
17:r:201:HIS:CE1	28:r:610:CLA:OBD	2.72	0.42
17:r:215:GLN:HG2	28:r:612:CLA:C4D	2.48	0.42
18:s:171:ASP:OD1	28:s:609:CLA:HBA2	2.20	0.42
22:y:205:PRO:HG2	22:y:206:LEU:HD12	2.00	0.42
28:y:311:CLA:H102	28:y:312:CLA:H141	2.00	0.42
23:z:26:VAL:CG1	23:z:33:TRP:HE3	2.30	0.42
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.01	0.42
1:A:279:PRO:O	1:A:283:ILE:HG12	2.19	0.42
2:B:41:GLU:O	2:B:45:PHE:N	2.51	0.42
28:B:616:CLA:HMA3	28:B:616:CLA:C6	2.49	0.42
32:B:621:LMG:H392	13:M:14:PHE:N	2.34	0.42
3:C:228:ASP:HB3	36:C:517:DGD:HE62	2.02	0.42
3:C:271:TYR:HA	3:C:274:TYR:CD2	2.54	0.42
3:C:397:THR:OG1	16:Q:27:ARG:HG2	2.20	0.42
4:D:104:ARG:HG3	5:E:73:LEU:CD1	2.49	0.42
7:G:73:MET:HG3	7:G:184:GLY:HA2	2.00	0.42
7:G:125:LEU:HD11	28:N:614:CLA:HAA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:176:LEU:CD1	28:G:612:CLA:HBA2	2.48	0.42
35:G:618:LHG:H312	35:G:618:LHG:H282	1.84	0.42
8:H:29:GLU:HG3	42:H:203:HOH:O	2.20	0.42
30:H:101:BCR:H351	30:H:101:BCR:H15C	1.88	0.42
7:N:119:VAL:HG12	7:N:121:ALA:H	1.84	0.42
7:N:123:SER:O	7:N:127:ILE:HG13	2.19	0.42
7:N:156:TYR:HA	28:N:610:CLA:O1D	2.20	0.42
7:N:182:LYS:HD3	28:N:611:CLA:C3D	2.48	0.42
16:Q:49:ALA:O	16:Q:53:GLU:HG3	2.20	0.42
28:R:610:CLA:H2	28:R:610:CLA:CHB	2.49	0.42
18:S:98:PHE:CD1	18:S:127:PHE:HE1	2.36	0.42
28:Y:602:CLA:HBB1	28:Y:602:CLA:CMB	2.50	0.42
28:Y:611:CLA:C4C	35:Y:619:LHG:HC62	2.49	0.42
1:a:28:LEU:HB2	31:a:414:SQD:C11	2.49	0.42
31:a:411:SQD:H271	35:a:415:LHG:H131	2.01	0.42
2:b:413:ASP:N	2:b:413:ASP:OD1	2.51	0.42
28:b:604:CLA:ND	28:b:612:CLA:H151	2.34	0.42
28:b:607:CLA:HBB1	28:b:607:CLA:CMB	2.49	0.42
3:c:154:ARG:HE	3:c:266:TRP:CD1	2.37	0.42
3:c:259:TRP:CZ2	28:c:506:CLA:HBD	2.54	0.42
3:c:376:ASP:O	3:c:380:LEU:HD13	2.20	0.42
3:c:390:ARG:HD2	16:q:22:ASN:HD21	1.84	0.42
28:c:502:CLA:H93	28:c:502:CLA:H62	1.82	0.42
7:g:22:VAL:HG23	7:g:44:TYR:CE2	2.54	0.42
7:g:49:ALA:HB3	7:g:51:LEU:HG	2.01	0.42
11:k:60:PHE:O	11:k:61:ARG:C	2.62	0.42
13:m:27:VAL:O	13:m:30:VAL:HG22	2.19	0.42
7:n:216:PRO:HB3	28:n:614:CLA:C2B	2.49	0.42
38:n:607:CHL:H61	38:n:607:CHL:H101	1.74	0.42
38:n:607:CHL:HBC2	22:y:222:TRP:CH2	2.53	0.42
38:n:607:CHL:HBC2	22:y:222:TRP:HH2	1.83	0.42
28:n:610:CLA:H91	28:n:612:CLA:HMB1	2.00	0.42
15:p:166:LYS:HA	15:p:169:PHE:CZ	2.55	0.42
28:r:603:CLA:H122	28:r:608:CLA:H93	2.00	0.42
18:s:36:PRO:HG3	38:s:601:CHL:CBB	2.49	0.42
1:A:32:TRP:HB2	9:I:23:PHE:CE2	2.55	0.42
30:A:409:BCR:H352	32:A:413:LMG:H392	2.01	0.42
28:B:605:CLA:HBA1	28:B:605:CLA:H12	1.75	0.42
28:B:614:CLA:CGA	28:B:614:CLA:C1A	2.98	0.42
3:C:186:TYR:HB2	3:C:196:VAL:HG22	2.00	0.42
28:C:509:CLA:H93	28:C:512:CLA:CGA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:C:522:LMG:H162	18:S:226:PHE:CE2	2.54	0.42
4:D:59:TRP:O	4:D:63:GLY:HA2	2.19	0.42
4:D:141:PRO:O	4:D:145:ILE:HG13	2.19	0.42
4:D:316:TYR:O	4:D:320:ILE:HG12	2.20	0.42
4:D:344:GLU:HA	4:D:347:LEU:HD12	2.00	0.42
5:E:20:TRP:CE3	5:E:20:TRP:HA	2.54	0.42
7:N:24:TYR:CG	7:N:46:TRP:HB2	2.54	0.42
14:O:76:THR:HG22	14:O:118:LEU:HD23	2.00	0.42
15:P:23:GLY:HA3	15:P:26:PHE:CZ	2.54	0.42
15:P:62:LEU:HD23	15:P:64:GLN:NE2	2.34	0.42
15:P:113:ILE:HG13	16:Q:7:VAL:HG12	2.01	0.42
18:S:76:GLY:O	18:S:80:ILE:HG12	2.18	0.42
18:S:84:TRP:CD1	28:S:309:CLA:HMD2	2.54	0.42
18:S:94:ILE:HB	18:S:95:PRO:HD3	2.02	0.42
18:S:111:TRP:HH2	38:S:307:CHL:H102	1.85	0.42
18:S:142:GLU:HA	38:S:306:CHL:CMA	2.49	0.42
19:T:11:VAL:HG12	30:T:101:BCR:H363	2.02	0.42
20:W:41:ALA:O	20:W:44:LEU:HB2	2.19	0.42
2:b:238:LEU:O	2:b:242:ILE:HG13	2.20	0.42
28:b:601:CLA:H52	28:b:601:CLA:H12	1.66	0.42
28:b:607:CLA:H143	28:b:607:CLA:H111	1.79	0.42
28:b:608:CLA:HBB1	28:b:608:CLA:HMB3	2.01	0.42
28:c:513:CLA:H91	28:c:513:CLA:H112	1.70	0.42
30:c:514:BCR:H17C	35:s:617:LHG:H201	2.01	0.42
28:d:401:CLA:HBB1	28:d:401:CLA:CMB	2.50	0.42
5:e:36:LEU:HA	5:e:39:SER:OG	2.18	0.42
7:g:15:PRO:HB2	7:g:22:VAL:HG13	2.01	0.42
35:g:618:LHG:H182	35:g:618:LHG:H211	1.86	0.42
8:h:56:ILE:HG12	21:x:54:PHE:CE2	2.54	0.42
10:j:38:SER:O	10:j:40:LEU:HD13	2.20	0.42
7:n:115:ASN:ND2	7:n:118:LEU:HG	2.35	0.42
15:p:94:PHE:CE1	16:q:3:ILE:HG12	2.55	0.42
28:r:608:CLA:C4B	28:r:613:CLA:H13	2.50	0.42
38:y:307:CHL:OMC	38:y:307:CHL:HAC2	2.19	0.42
2:B:15:ASP:HB2	12:L:7:ASN:HD22	1.85	0.42
28:B:602:CLA:H8	36:B:626:DGD:C7B	2.44	0.42
28:B:607:CLA:C1D	32:B:621:LMG:H122	2.50	0.42
28:B:615:CLA:H51	28:B:616:CLA:H203	2.01	0.42
32:B:621:LMG:C43	32:B:621:LMG:H391	2.50	0.42
4:D:31:VAL:HA	4:D:39:PHE:CE2	2.55	0.42
4:D:105:TRP:CH2	4:D:114:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:ARG:HD3	4:D:182:PHE:N	2.33	0.42
38:G:606:CHL:HHC	38:G:606:CHL:CBB	2.46	0.42
10:J:9:PRO:O	10:J:12:ILE:HG13	2.20	0.42
7:N:121:ALA:HA	38:N:605:CHL:C1C	2.49	0.42
7:N:161:PHE:HA	38:N:608:CHL:H61	2.01	0.42
14:O:216:GLY:HA3	14:O:242:TRP:CZ2	2.54	0.42
17:R:165:GLU:OE2	17:R:167:ASP:HB3	2.20	0.42
17:R:180:ASP:N	17:R:181:PRO:HD3	2.34	0.42
17:R:182:LEU:HB2	17:R:184:LEU:CD1	2.50	0.42
28:R:603:CLA:HMD1	28:R:613:CLA:H142	2.02	0.42
28:R:604:CLA:CHC	40:y:301:NEX:H222	2.48	0.42
18:S:70:ASP:HB3	18:S:74:TYR:CE2	2.53	0.42
18:S:87:LEU:HD23	39:S:315:LUT:H402	2.01	0.42
38:S:307:CHL:CMA	38:S:307:CHL:H71	2.49	0.42
35:W:101:LHG:H221	28:Y:612:CLA:H93	2.01	0.42
22:Y:128:TRP:O	22:Y:132:VAL:HG23	2.19	0.42
22:Y:222:TRP:CD2	41:Y:617:XAT:H192	2.54	0.42
1:a:234:ASN:HB3	4:d:264:ASN:ND2	2.35	0.42
2:b:337:ALA:HA	2:b:432:LEU:HD23	2.02	0.42
2:b:391:SER:O	2:b:394:GLN:HG2	2.20	0.42
28:b:601:CLA:CBB	30:h:101:BCR:H15C	2.50	0.42
3:c:214:LEU:HD22	20:w:15:PHE:CE2	2.54	0.42
30:d:406:BCR:H15C	30:d:406:BCR:H351	1.87	0.42
38:g:605:CHL:HHC	38:g:605:CHL:CBB	2.44	0.42
38:n:609:CHL:HAA1	38:n:609:CHL:HBD	2.01	0.42
28:n:610:CLA:H91	28:n:612:CLA:HHB	1.99	0.42
14:o:188:GLU:H	14:o:188:GLU:CD	2.26	0.42
15:p:149:ALA:HA	15:p:157:TYR:O	2.20	0.42
17:r:47:GLN:HE22	17:r:69:ARG:HH21	1.68	0.42
22:y:219:ASN:HB3	42:y:429:HOH:O	2.19	0.42
39:y:316:LUT:H35	39:y:316:LUT:H401	1.86	0.42
35:y:319:LHG:H262	35:y:319:LHG:H291	1.37	0.42
1:A:71:LEU:HA	1:A:75:ASN:O	2.20	0.42
1:A:119:PHE:CD1	29:A:407:PHO:H121	2.54	0.42
1:A:133:LEU:O	1:A:137:LEU:HG	2.19	0.42
2:B:340:TRP:O	2:B:405:GLU:HG3	2.20	0.42
2:B:403:GLY:H	2:B:407:ASN:CG	2.28	0.42
28:B:615:CLA:H203	28:B:616:CLA:C4C	2.50	0.42
3:C:472:LEU:O	3:C:473:ASN:HB3	2.19	0.42
3:C:473:ASN:ND2	3:C:473:ASN:C	2.75	0.42
28:C:502:CLA:HBB1	28:C:502:CLA:CMB	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:LEU:HD23	29:D:402:PHO:H42	2.01	0.42
5:E:23:HIS:HA	5:E:26:THR:OG1	2.20	0.42
7:G:192:PHE:CG	28:G:602:CLA:H18	2.54	0.42
28:G:603:CLA:HBA2	28:G:603:CLA:HBD	2.01	0.42
13:M:21:PHE:O	13:M:25:ILE:HG12	2.19	0.42
7:N:140:GLY:HA2	22:Y:28:PHE:HB3	2.01	0.42
7:N:197:GLN:O	7:N:198:ALA:C	2.62	0.42
38:N:608:CHL:H202	28:N:610:CLA:H202	2.01	0.42
17:R:184:LEU:CD1	39:R:614:LUT:H221	2.50	0.42
28:R:613:CLA:H62	28:R:613:CLA:CHC	2.49	0.42
38:S:302:CHL:HMD2	35:S:317:LHG:H272	2.01	0.42
28:S:310:CLA:HBB1	28:S:310:CLA:HMB1	2.01	0.42
28:Y:610:CLA:H52	39:Y:615:LUT:H30	2.00	0.42
24:U:76:GLY:O	24:U:81:LYS:HE2	2.20	0.42
1:a:211:PHE:HE2	1:a:278:TRP:CG	2.38	0.42
1:a:225:ARG:C	1:a:226:GLU:HG3	2.43	0.42
1:a:234:ASN:HD21	35:b:624:LHG:HC11	1.83	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.54	0.42
2:b:489:GLN:CG	2:b:499:GLY:HA2	2.50	0.42
28:b:603:CLA:H121	28:b:603:CLA:H91	2.00	0.42
28:b:610:CLA:H61	28:b:610:CLA:H92	1.70	0.42
28:b:615:CLA:H71	28:b:616:CLA:H152	2.00	0.42
3:c:223:TRP:CE3	3:c:224:ILE:HG12	2.54	0.42
3:c:348:GLU:OE1	3:c:348:GLU:N	2.50	0.42
28:c:511:CLA:C9	30:c:515:BCR:H23C	2.44	0.42
28:c:512:CLA:HBB1	28:c:512:CLA:CMB	2.49	0.42
7:g:227:ASN:O	7:g:228:PHE:C	2.63	0.42
8:h:24:LYS:HB3	8:h:25:PRO:HD3	2.02	0.42
7:n:110:LEU:HD13	38:n:606:CHL:HHD	2.01	0.42
7:n:172:ALA:O	7:n:176:LEU:HG	2.20	0.42
14:o:142:PHE:HE1	14:o:204:VAL:HG23	1.84	0.42
17:r:14:TRP:HA	28:r:601:CLA:CHD	2.50	0.42
17:r:21:PRO:HD2	17:r:33:GLY:HA2	2.02	0.42
38:r:605:CHL:OMC	38:r:605:CHL:HAC2	2.19	0.42
28:r:608:CLA:HED2	28:r:608:CLA:HBD	1.82	0.42
38:s:601:CHL:HAC1	35:s:617:LHG:HC32	2.01	0.42
38:s:601:CHL:C2B	35:s:617:LHG:H141	2.49	0.42
30:t:101:BCR:H11C	30:t:101:BCR:H341	1.92	0.42
28:y:304:CLA:HBD	28:y:304:CLA:HBA2	2.01	0.42
1:A:238:ARG:CZ	1:A:241:GLN:HA	2.50	0.42
2:B:20:LEU:O	2:B:24:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B:622:LHG:HC42	17:R:129:LEU:HD11	2.01	0.42
3:C:163:ILE:HD13	28:C:512:CLA:CAB	2.50	0.42
4:D:343:PRO:O	4:D:346:VAL:HG22	2.19	0.42
7:G:183:ASN:N	28:G:611:CLA:HMD1	2.35	0.42
7:G:225:ALA:HB3	22:Y:105:PHE:HZ	1.85	0.42
28:G:614:CLA:HHC	28:G:614:CLA:CBB	2.50	0.42
39:G:616:LUT:H15	39:G:616:LUT:H201	1.85	0.42
7:N:24:TYR:CE2	7:N:25:LEU:HG	2.54	0.42
7:N:71:TRP:CD1	38:N:609:CHL:HMD3	2.55	0.42
38:N:608:CHL:H11	39:N:615:LUT:H383	2.02	0.42
28:N:611:CLA:H93	28:N:611:CLA:H111	1.60	0.42
14:O:61:LYS:HE2	14:O:71:LEU:O	2.20	0.42
16:Q:119:HIS:HA	16:Q:122:LYS:HE2	2.01	0.42
38:R:605:CHL:HAC2	38:R:605:CHL:OMC	2.19	0.42
39:S:316:LUT:H31	39:S:316:LUT:H391	1.83	0.42
22:Y:58:PHE:O	22:Y:62:ARG:HG3	2.18	0.42
22:Y:224:TYR:HD2	22:Y:227:ASN:ND2	2.18	0.42
28:Y:611:CLA:H2	28:Y:611:CLA:H62	1.59	0.42
1:a:41:LEU:HB3	31:a:414:SQD:H211	2.02	0.42
1:a:142:TRP:HB3	35:a:415:LHG:H251	2.00	0.42
1:a:283:ILE:CG1	29:a:408:PHO:HBC3	2.45	0.42
2:b:185:TRP:HZ3	2:b:204:ALA:HB2	1.84	0.42
28:b:608:CLA:H162	28:b:608:CLA:H141	1.79	0.42
3:c:109:PHE:HB3	3:c:110:PRO:HD3	2.01	0.42
3:c:112:PHE:HE2	30:c:514:BCR:HC32	1.85	0.42
3:c:400:PRO:C	3:c:401:LEU:HD12	2.45	0.42
28:c:501:CLA:C1D	28:c:503:CLA:H51	2.50	0.42
35:c:520:LHG:H223	35:s:617:LHG:H331	2.02	0.42
4:d:50:PHE:CZ	32:d:409:LMG:H372	2.55	0.42
5:e:35:TRP:CH2	6:f:36:PHE:CD2	3.08	0.42
5:e:70:PHE:HB2	24:u:28:ASN:HD21	1.84	0.42
13:m:14:PHE:O	13:m:18:PRO:HG2	2.19	0.42
7:n:149:GLY:O	38:n:608:CHL:HMC	2.19	0.42
7:n:176:LEU:CB	28:n:610:CLA:HMA2	2.50	0.42
14:o:32:ILE:HD12	14:o:208:LYS:HB2	2.01	0.42
17:r:14:TRP:HD1	17:r:32:TYR:O	2.03	0.42
17:r:169:GLU:OE1	17:r:173:TYR:HB2	2.19	0.42
17:r:196:LEU:HD11	17:r:200:LYS:HE3	2.00	0.42
28:s:612:CLA:H2	28:s:612:CLA:H61	1.66	0.42
24:u:1:GLU:N	24:u:2:PRO:HD2	2.35	0.42
28:A:405:CLA:H3A	28:A:405:CLA:HBA1	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:PRO:HD2	2:B:7:ARG:HD2	2.01	0.42
2:B:398:ILE:C	2:B:398:ILE:HD12	2.45	0.42
4:D:281:TRP:O	4:D:285:LEU:HD13	2.20	0.42
28:G:611:CLA:CBB	28:G:611:CLA:HHC	2.50	0.42
28:G:613:CLA:C9	35:G:618:LHG:H341	2.49	0.42
7:N:161:PHE:CZ	38:N:608:CHL:NC	2.87	0.42
14:O:59:THR:HB	14:O:73:PHE:HB3	2.02	0.42
16:Q:140:LEU:O	16:Q:144:LEU:HD13	2.19	0.42
17:R:221:LYS:HB3	17:R:225:ASN:CB	2.45	0.42
18:S:162:ASP:HB3	18:S:165:HIS:C	2.45	0.42
18:S:195:LEU:HD21	28:S:312:CLA:HAC1	2.02	0.42
22:Y:18:GLY:HA3	42:Y:702:HOH:O	2.19	0.42
22:Y:160:SER:O	38:Y:608:CHL:H61	2.19	0.42
22:Y:193:GLY:O	22:Y:197:GLN:HG3	2.20	0.42
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.00	0.42
2:b:41:GLU:CD	2:b:62:VAL:HG22	2.44	0.42
2:b:497:LYS:HE2	4:d:24:ARG:NH1	2.35	0.42
28:c:513:CLA:HAB	30:c:514:BCR:H24C	2.01	0.42
5:e:57:THR:HG1	5:e:60:ARG:H	1.68	0.42
15:p:124:LYS:HB2	15:p:126:TYR:HE1	1.83	0.42
28:r:601:CLA:C4C	35:r:617:LHG:HC92	2.50	0.42
18:s:48:TYR:CE1	18:s:49:LEU:HD13	2.54	0.42
18:s:225:PRO:HG2	28:s:613:CLA:C2B	2.50	0.42
28:s:609:CLA:C4D	39:s:614:LUT:H382	2.49	0.42
23:z:16:SER:O	23:z:20:LEU:HB2	2.20	0.42
2:B:37:MET:SD	30:t:101:BCR:H282	2.60	0.42
2:B:128:THR:O	2:B:130:LYS:HG3	2.19	0.42
2:B:204:ALA:CB	28:B:602:CLA:HAB	2.50	0.42
2:B:241:SER:O	2:B:245:VAL:HG13	2.19	0.42
28:B:608:CLA:H112	28:D:404:CLA:HMB1	2.02	0.42
28:B:615:CLA:H72	30:B:619:BCR:C11	2.50	0.42
36:C:518:DGD:HA91	36:C:519:DGD:HB81	2.00	0.42
4:D:31:VAL:HG13	4:D:39:PHE:HE2	1.84	0.42
7:G:222:TRP:CZ2	28:G:614:CLA:CGD	3.02	0.42
28:G:604:CLA:NA	40:G:617:NEX:H242	2.34	0.42
11:K:43:ILE:HG23	30:K:101:BCR:H11C	2.00	0.42
7:N:36:LEU:HB3	7:N:43:ASP:OD1	2.20	0.42
28:N:612:CLA:H72	28:N:612:CLA:CMA	2.45	0.42
15:P:120:VAL:HG22	15:P:125:GLN:OE1	2.20	0.42
16:Q:69:ALA:HB1	16:Q:72:PHE:HD1	1.81	0.42
17:R:75:VAL:HG21	17:R:171:ARG:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:180:ASP:HA	39:R:614:LUT:H24	2.01	0.42
28:S:311:CLA:C4C	35:S:317:LHG:HC62	2.50	0.42
20:W:46:GLU:HB3	20:W:50:SER:OG	2.19	0.42
22:Y:195:PHE:HB3	38:Y:607:CHL:H102	2.01	0.42
1:a:131:TRP:HH2	3:c:449:ARG:NH2	2.17	0.42
28:b:602:CLA:H91	36:b:625:DGD:HB81	2.02	0.42
28:b:603:CLA:CHC	28:b:605:CLA:H101	2.50	0.42
28:b:613:CLA:HBB1	28:b:613:CLA:CMB	2.50	0.42
3:c:38:GLY:HA3	28:c:511:CLA:HMD2	2.02	0.42
3:c:62:PHE:CE2	30:k:101:BCR:H311	2.55	0.42
3:c:109:PHE:HE2	32:c:521:LMG:HC8	1.84	0.42
3:c:266:TRP:HZ3	28:c:507:CLA:HBC2	1.85	0.42
28:c:511:CLA:C3B	30:c:515:BCR:H393	2.50	0.42
28:c:513:CLA:H51	35:s:617:LHG:H151	2.02	0.42
4:d:316:TYR:O	4:d:320:ILE:HG12	2.19	0.42
7:g:111:ASP:OD1	7:g:120:HIS:HA	2.20	0.42
8:h:50:PHE:CA	30:h:101:BCR:H12C	2.49	0.42
7:n:17:TYR:OH	7:n:41:PRO:HB3	2.20	0.42
7:n:113:LEU:CD2	28:n:604:CLA:HMD3	2.49	0.42
7:n:119:VAL:N	38:n:605:CHL:O2D	2.53	0.42
38:n:606:CHL:O2A	40:n:617:NEX:H403	2.20	0.42
28:r:608:CLA:H11	28:r:613:CLA:H12	2.00	0.42
18:s:124:LEU:HD22	28:s:604:CLA:O1D	2.20	0.42
18:s:202:GLY:O	18:s:206:GLN:HG3	2.20	0.42
22:y:58:PHE:O	22:y:62:ARG:HG3	2.20	0.42
22:y:63:GLU:O	22:y:67:ILE:HG12	2.19	0.42
38:y:302:CHL:H91	38:y:302:CHL:H111	1.76	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
28:B:601:CLA:O1A	28:B:601:CLA:H112	2.20	0.42
28:B:607:CLA:H202	28:B:607:CLA:H162	1.85	0.42
28:B:608:CLA:H93	28:B:608:CLA:H62	1.70	0.42
28:B:609:CLA:HBB1	28:B:609:CLA:CMB	2.49	0.42
30:B:617:BCR:C21	31:B:620:SQD:H171	2.49	0.42
3:C:133:ALA:C	3:C:134:LEU:HD12	2.45	0.42
28:C:501:CLA:CHA	28:C:501:CLA:HBA1	2.50	0.42
28:C:505:CLA:H3A	28:C:505:CLA:HBA2	1.67	0.42
4:D:38:LEU:HD22	4:D:126:PHE:HA	2.01	0.42
4:D:352:ALA:HA	15:P:138:GLY:O	2.20	0.42
38:G:606:CHL:CBB	39:G:616:LUT:H171	2.50	0.42
28:G:610:CLA:H93	28:G:612:CLA:HMB1	2.02	0.42
7:N:111:ASP:HB3	7:N:115:ASN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N:612:CLA:HBB1	28:N:612:CLA:CMB	2.50	0.42
17:R:221:LYS:HG2	42:R:733:HOH:O	2.20	0.42
28:R:610:CLA:HBA2	28:R:610:CLA:C2	2.48	0.42
18:S:149:ALA:HA	18:S:152:TYR:CD2	2.55	0.42
28:S:303:CLA:HAC2	35:S:317:LHG:H261	2.01	0.42
28:S:311:CLA:CHB	35:S:317:LHG:HC11	2.49	0.42
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.42
28:b:608:CLA:C6	28:b:609:CLA:H121	2.49	0.42
28:b:615:CLA:H143	28:b:616:CLA:C4A	2.50	0.42
3:c:113:VAL:HB	32:c:521:LMG:H142	2.02	0.42
4:d:126:PHE:CE2	29:d:402:PHO:HBD	2.54	0.42
7:g:71:TRP:CD1	38:g:609:CHL:HMD3	2.54	0.42
7:g:223:SER:C	7:g:225:ALA:N	2.77	0.42
28:g:613:CLA:H2	28:g:613:CLA:H62	1.76	0.42
28:g:614:CLA:HMA1	22:y:125:LEU:HD11	2.01	0.42
11:k:30:TYR:CE1	23:z:5:PHE:HZ	2.38	0.42
7:n:182:LYS:HB3	28:n:611:CLA:CMD	2.49	0.42
7:n:182:LYS:HE3	35:n:618:LHG:HC61	2.02	0.42
38:n:605:CHL:HHC	38:n:605:CHL:CBB	2.46	0.42
28:n:611:CLA:H111	28:n:611:CLA:H93	1.52	0.42
14:o:46:TYR:N	14:o:93:PHE:O	2.53	0.42
16:q:96:PRO:O	16:q:100:LYS:HG3	2.20	0.42
17:r:124:ALA:O	17:r:127:VAL:HG22	2.20	0.42
18:s:131:ILE:HG22	18:s:133:ILE:H	1.84	0.42
18:s:141:ALA:CB	38:s:605:CHL:HED2	2.50	0.42
28:s:609:CLA:C2	39:s:614:LUT:H28	2.50	0.42
40:s:616:NEX:H15	40:s:616:NEX:H201	1.92	0.42
21:x:52:LYS:NZ	21:x:56:LEU:HD11	2.35	0.42
38:y:307:CHL:HBB1	39:y:316:LUT:H161	2.00	0.42
1:A:77:ILE:HB	12:L:34:ASN:HD21	1.85	0.41
1:A:149:ALA:HA	1:A:284:TRP:CD1	2.55	0.41
1:A:223:LEU:HD23	1:A:246:TYR:HB3	2.01	0.41
28:A:406:CLA:HMB2	29:D:402:PHO:H161	2.02	0.41
2:B:362:PHE:HE1	4:D:190:HIS:CE1	2.37	0.41
2:B:462:PHE:HA	28:B:611:CLA:CMC	2.48	0.41
28:B:610:CLA:H93	28:B:610:CLA:H111	1.95	0.41
3:C:225:VAL:HG23	36:C:517:DGD:HB22	2.02	0.41
28:C:506:CLA:C11	35:W:101:LHG:H361	2.50	0.41
28:C:509:CLA:H93	28:C:509:CLA:H62	1.79	0.41
28:C:511:CLA:C4A	30:C:516:BCR:H271	2.50	0.41
36:C:519:DGD:HA52	32:D:408:LMG:H141	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:HIS:CE1	4:D:295:ARG:HH11	2.38	0.41
4:D:298:ASP:HB2	4:D:316:TYR:OH	2.19	0.41
4:D:320:ILE:O	4:D:324:GLU:HG3	2.20	0.41
7:G:22:VAL:O	7:G:23:LYS:HD2	2.20	0.41
18:S:111:TRP:CZ3	18:S:112:PHE:HB3	2.55	0.41
18:S:162:ASP:HB2	18:S:166:PRO:HA	2.02	0.41
28:S:309:CLA:HBC1	39:S:316:LUT:H193	2.01	0.41
28:Y:610:CLA:H92	28:Y:610:CLA:H61	1.74	0.41
28:Y:612:CLA:H2	28:Y:612:CLA:H62	1.72	0.41
1:a:199:MET:C	36:c:518:DGD:HAH1	2.45	0.41
2:b:125:ASP:HB2	2:b:132:SER:OG	2.19	0.41
28:b:601:CLA:H102	30:h:101:BCR:C40	2.46	0.41
28:b:606:CLA:H172	28:b:606:CLA:H122	2.01	0.41
28:b:606:CLA:H61	30:b:619:BCR:H311	2.01	0.41
28:b:611:CLA:H2	28:b:611:CLA:H62	1.79	0.41
28:b:614:CLA:H192	28:b:614:CLA:H162	1.83	0.41
3:c:28:GLN:C	3:c:30:THR:H	2.28	0.41
3:c:248:GLY:O	3:c:252:ILE:HG13	2.20	0.41
3:c:288:CYS:SG	36:c:516:DGD:HB61	2.60	0.41
28:c:510:CLA:H203	28:c:510:CLA:C3D	2.49	0.41
4:d:50:PHE:HZ	32:d:409:LMG:H341	1.83	0.41
4:d:104:ARG:HG3	5:e:73:LEU:CD1	2.50	0.41
7:g:148:LEU:HD22	38:g:608:CHL:C3B	2.50	0.41
38:g:601:CHL:HHC	38:g:601:CHL:CBB	2.47	0.41
28:n:611:CLA:H112	28:n:612:CLA:NC	2.35	0.41
28:r:603:CLA:HBB1	28:r:603:CLA:CMB	2.50	0.41
28:r:603:CLA:C2D	28:r:608:CLA:H61	2.50	0.41
18:s:34:PHE:HA	38:s:601:CHL:C1D	2.50	0.41
18:s:99:ASN:HA	18:s:103:ALA:O	2.19	0.41
28:s:602:CLA:C4A	28:s:602:CLA:H12	2.49	0.41
2:B:38:ALA:O	2:B:42:LEU:HG	2.19	0.41
2:B:41:GLU:CD	2:B:62:VAL:HG22	2.45	0.41
2:B:52:LEU:HB3	2:B:337:ALA:HB3	2.02	0.41
28:B:608:CLA:C4C	28:B:609:CLA:H102	2.50	0.41
3:C:65:GLY:HA2	3:C:115:GLY:HA2	2.03	0.41
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.41
3:C:230:LEU:O	3:C:234:ILE:HG12	2.19	0.41
3:C:239:TRP:O	3:C:243:ILE:HG13	2.20	0.41
4:D:88:HIS:CD2	4:D:167:GLY:HA2	2.55	0.41
4:D:192:TRP:CZ2	4:D:198:HIS:HB2	2.55	0.41
4:D:278:THR:O	4:D:282:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:405:BCR:H363	6:F:27:PHE:CB	2.50	0.41
7:G:74:LEU:HD11	28:G:610:CLA:CAC	2.49	0.41
7:G:164:LEU:H	7:G:164:LEU:CD1	2.30	0.41
28:G:610:CLA:HBB1	28:G:610:CLA:H51	2.01	0.41
31:M:101:SQD:H122	28:b:614:CLA:H42	2.02	0.41
7:N:101:GLY:O	7:N:104:ILE:HG22	2.20	0.41
28:N:612:CLA:HMA1	28:N:612:CLA:H101	2.03	0.41
39:N:616:LUT:H15	39:N:616:LUT:H201	1.93	0.41
14:O:142:PHE:CE2	14:O:202:LEU:HB2	2.55	0.41
15:P:72:THR:C	15:P:74:TYR:N	2.76	0.41
18:S:47:GLU:CD	18:S:47:GLU:H	2.26	0.41
30:T:101:BCR:H24C	30:T:101:BCR:H371	1.90	0.41
40:Y:618:NEX:H15	40:Y:618:NEX:H201	1.92	0.41
2:b:4:PRO:HD2	2:b:7:ARG:HD2	2.02	0.41
2:b:210:ILE:O	2:b:214:LEU:HG	2.19	0.41
2:b:335:GLY:HA2	2:b:439:SER:OG	2.19	0.41
28:b:613:CLA:H71	28:b:613:CLA:H111	1.90	0.41
32:b:623:LMG:H302	38:r:606:CHL:C4	2.50	0.41
3:c:322:GLN:NE2	3:c:381:LYS:HA	2.35	0.41
4:d:197:PHE:HA	4:d:200:MET:HE2	2.02	0.41
28:g:603:CLA:H162	28:g:603:CLA:H202	1.79	0.41
8:h:40:THR:HB	8:h:41:PRO:HD3	2.02	0.41
7:n:32:SER:HA	42:n:708:HOH:O	2.19	0.41
28:n:602:CLA:H92	28:n:603:CLA:CMA	2.50	0.41
16:q:37:PHE:HD2	16:q:39:ILE:O	2.02	0.41
16:q:84:LEU:O	16:q:88:LEU:HG	2.20	0.41
18:s:67:LYS:HB2	18:s:70:ASP:CG	2.45	0.41
18:s:218:PHE:HE1	28:s:613:CLA:HAC1	1.84	0.41
22:y:194:PHE:CZ	39:y:315:LUT:H8	2.55	0.41
22:y:195:PHE:O	22:y:199:ILE:HG13	2.19	0.41
22:y:197:GLN:OE1	39:y:315:LUT:H42	2.20	0.41
28:y:304:CLA:C15	38:y:309:CHL:H62	2.51	0.41
2:B:109:LEU:CB	30:B:619:BCR:H19C	2.48	0.41
2:B:219:VAL:HG22	17:R:87:PHE:HZ	1.85	0.41
2:B:337:ALA:HA	2:B:432:LEU:HD23	2.02	0.41
2:B:477:ASP:O	17:R:59:LYS:HG3	2.20	0.41
28:C:504:CLA:C1D	36:C:518:DGD:HB21	2.50	0.41
4:D:135:ARG:HA	4:D:135:ARG:HE	1.84	0.41
7:G:112:TYR:CD1	7:G:113:LEU:HG	2.55	0.41
38:G:606:CHL:HBD	38:G:606:CHL:HAA2	2.01	0.41
12:L:29:ALA:CB	13:M:15:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:195:PHE:CD2	38:N:609:CHL:H202	2.52	0.41
15:P:140:GLU:OE1	15:P:164:GLY:HA3	2.20	0.41
15:P:168:TRP:HZ3	15:P:176:VAL:HG11	1.85	0.41
17:R:187:ASP:OD1	17:R:190:LYS:HB2	2.20	0.41
18:S:25:LYS:HE3	18:S:32:ARG:HH11	1.85	0.41
20:W:27:PHE:CZ	35:W:101:LHG:H162	2.55	0.41
20:W:32:LEU:O	20:W:36:LEU:HD13	2.20	0.41
35:W:101:LHG:H332	35:W:101:LHG:H362	1.68	0.41
1:a:28:LEU:HB2	31:a:414:SQD:H111	2.02	0.41
1:a:91:LEU:HA	1:a:168:PHE:CE2	2.55	0.41
1:a:333:GLU:HB2	1:a:337:HIS:CE1	2.56	0.41
30:a:410:BCR:H373	32:a:413:LMG:H302	2.02	0.41
7:g:227:ASN:CG	38:g:619:CHL:H18	2.45	0.41
38:g:601:CHL:OBD	28:g:602:CLA:HHD	2.21	0.41
38:g:601:CHL:H41	38:y:309:CHL:C4B	2.50	0.41
38:g:609:CHL:H11	39:n:616:LUT:H363	2.03	0.41
35:g:618:LHG:H191	35:g:618:LHG:H162	1.62	0.41
11:k:34:ASN:HB2	11:k:35:PRO:HD3	2.02	0.41
7:n:70:ARG:HA	7:n:73:MET:HE3	2.02	0.41
7:n:118:LEU:HD22	38:n:605:CHL:HED2	2.02	0.41
7:n:161:PHE:O	39:n:615:LUT:H383	2.19	0.41
14:o:6:ARG:HD2	14:o:29:CYS:O	2.21	0.41
16:q:62:LYS:HE2	16:q:133:TYR:CE2	2.56	0.41
17:r:109:GLY:O	17:r:113:VAL:HG12	2.19	0.41
17:r:113:VAL:O	17:r:117:THR:N	2.52	0.41
18:s:64:LEU:O	18:s:74:TYR:HE2	2.04	0.41
18:s:96:GLU:HA	18:s:109:ALA:CB	2.48	0.41
18:s:142:GLU:O	18:s:146:LEU:HB2	2.21	0.41
22:y:176:LEU:HB3	28:y:310:CLA:CMA	2.50	0.41
1:A:219:VAL:HG13	1:A:246:TYR:CD1	2.55	0.41
28:B:605:CLA:CHA	28:B:605:CLA:HBA2	2.47	0.41
28:B:611:CLA:H72	28:B:613:CLA:HED3	2.01	0.41
28:B:611:CLA:H121	28:B:613:CLA:O1D	2.20	0.41
31:B:620:SQD:H352	19:t:12:SER:HB3	2.01	0.41
28:G:603:CLA:ND	38:G:609:CHL:H72	2.35	0.41
15:P:74:TYR:HE1	15:P:151:VAL:HG21	1.85	0.41
16:Q:120:ALA:HB2	16:Q:132:TYR:CE2	2.56	0.41
17:R:165:GLU:HG3	17:R:171:ARG:HG3	2.02	0.41
28:S:311:CLA:HMA1	35:S:317:LHG:HC11	2.03	0.41
20:W:19:ASN:HB3	20:W:22:LEU:CD2	2.46	0.41
22:Y:173:PHE:O	22:Y:177:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:608:CHL:HHC	38:Y:608:CHL:CBB	2.46	0.41
1:a:239:PHE:CZ	4:d:248:VAL:HA	2.55	0.41
2:b:214:LEU:CD1	28:r:603:CLA:H111	2.50	0.41
3:c:323:ARG:NH2	16:q:12:PRO:O	2.53	0.41
4:d:90:LEU:H	8:h:62:ASN:HD21	1.68	0.41
28:g:604:CLA:CHC	40:g:617:NEX:H362	2.49	0.41
7:n:185:ARG:HD2	28:n:602:CLA:C4C	2.50	0.41
17:r:21:PRO:HG2	17:r:24:LEU:HD22	2.02	0.41
17:r:149:TRP:O	17:r:153:LEU:HG	2.19	0.41
17:r:155:ILE:O	17:r:158:ILE:HG12	2.20	0.41
17:r:175:GLY:O	17:r:179:PHE:HB2	2.20	0.41
18:s:93:ILE:O	18:s:94:ILE:C	2.64	0.41
18:s:145:LEU:O	40:s:616:NEX:H15	2.20	0.41
18:s:150:GLU:HG3	28:s:608:CLA:C3B	2.51	0.41
22:y:222:TRP:CD2	41:y:317:XAT:H192	2.55	0.41
31:A:410:SQD:H101	31:A:410:SQD:H261	2.02	0.41
2:B:13:LEU:C	2:B:13:LEU:HD23	2.45	0.41
2:B:187:VAL:HG23	28:B:601:CLA:HMD2	2.02	0.41
2:B:289:GLY:O	2:B:293:VAL:HG23	2.19	0.41
28:B:603:CLA:HMB1	28:B:603:CLA:CBB	2.49	0.41
28:B:607:CLA:HMC3	30:B:618:BCR:C10	2.51	0.41
3:C:225:VAL:HG22	3:C:289:PHE:CD2	2.56	0.41
4:D:262:PHE:CE2	35:D:407:LHG:HC81	2.55	0.41
13:M:23:LEU:O	13:M:27:VAL:HG23	2.20	0.41
7:N:96:VAL:HG21	7:N:99:LYS:HZ3	1.85	0.41
7:N:128:TRP:HE1	41:Y:617:XAT:C15	2.33	0.41
38:N:607:CHL:HBB2	38:N:609:CHL:HBC2	2.03	0.41
14:O:47:ASN:N	14:O:247:GLU:O	2.48	0.41
16:Q:17:LEU:HA	16:Q:18:PRO:HD3	1.92	0.41
16:Q:73:LEU:O	16:Q:77:LEU:HD13	2.20	0.41
28:R:608:CLA:H2A	28:R:608:CLA:HED3	2.01	0.41
41:R:615:XAT:H35	41:R:615:XAT:H401	1.92	0.41
18:S:124:LEU:HD12	18:S:124:LEU:C	2.45	0.41
18:S:166:PRO:HB2	18:S:170:PHE:CD1	2.56	0.41
22:Y:105:PHE:HE2	38:Y:607:CHL:OBD	2.03	0.41
22:Y:195:PHE:O	22:Y:199:ILE:HG13	2.20	0.41
28:Y:614:CLA:HMB1	28:Y:614:CLA:CBB	2.49	0.41
28:b:611:CLA:H143	28:b:613:CLA:O1D	2.20	0.41
3:c:172:SER:OG	3:c:240:LEU:HD23	2.21	0.41
30:c:514:BCR:H11C	30:c:514:BCR:H341	1.87	0.41
7:g:44:TYR:CE2	38:g:601:CHL:HBC2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:601:CHL:H172	28:y:304:CLA:HMC2	2.02	0.41
32:k:102:LMG:H161	32:k:102:LMG:H132	1.84	0.41
7:n:105:PHE:CE2	38:n:607:CHL:HMD1	2.55	0.41
7:n:215:ASP:HB2	7:n:219:ASN:CG	2.46	0.41
38:n:605:CHL:HAA1	38:n:605:CHL:HBD	2.02	0.41
19:t:22:PHE:HZ	30:t:101:BCR:HC42	1.84	0.41
1:A:37:MET:HB2	1:A:125:CYS:HB2	2.02	0.41
28:B:605:CLA:H152	28:B:605:CLA:H112	1.91	0.41
28:B:605:CLA:H92	28:B:605:CLA:H61	1.58	0.41
28:C:508:CLA:H92	28:C:508:CLA:H61	1.65	0.41
4:D:121:PHE:HA	4:D:124:ILE:HD12	2.01	0.41
35:D:407:LHG:H242	12:L:20:TRP:CE2	2.55	0.41
7:G:91:LYS:HD2	7:G:92:PHE:O	2.20	0.41
7:G:196:VAL:HG11	28:G:613:CLA:HAC2	2.02	0.41
28:G:602:CLA:H101	39:G:616:LUT:C37	2.48	0.41
28:G:613:CLA:H11	28:G:613:CLA:ND	2.35	0.41
28:N:610:CLA:H92	28:N:610:CLA:H61	1.59	0.41
16:Q:91:ILE:HD13	16:Q:147:ILE:HG23	2.02	0.41
39:R:614:LUT:H23	39:R:614:LUT:H362	1.81	0.41
18:S:108:GLU:CB	18:S:117:LEU:HD21	2.36	0.41
18:S:221:HIS:CE1	18:S:225:PRO:HB3	2.55	0.41
35:W:101:LHG:H252	35:W:101:LHG:H282	1.71	0.41
22:Y:22:VAL:CG2	38:Y:601:CHL:HBC3	2.50	0.41
28:Y:604:CLA:H3A	28:Y:604:CLA:HBA2	1.37	0.41
38:Y:606:CHL:OMC	38:Y:606:CHL:HAC2	2.20	0.41
1:a:129:ARG:NH2	4:d:256:GLN:O	2.54	0.41
1:a:296:ASN:HB2	3:c:400:PRO:O	2.20	0.41
2:b:315:ILE:HG12	2:b:321:LYS:HG3	2.03	0.41
28:b:604:CLA:H162	28:b:604:CLA:H141	1.80	0.41
3:c:135:LEU:HD21	23:z:33:TRP:CD1	2.56	0.41
7:g:71:TRP:CE2	38:g:608:CHL:HED3	2.55	0.41
7:n:21:ARG:HG3	7:n:23:LYS:HD2	2.02	0.41
7:n:64:LEU:HD13	28:n:603:CLA:HBA2	2.02	0.41
7:n:148:LEU:HD13	38:n:608:CHL:H102	2.02	0.41
28:n:610:CLA:HBA1	28:n:610:CLA:CHA	2.47	0.41
15:p:84:VAL:HG22	15:p:87:LEU:HG	2.02	0.41
17:r:204:LEU:HA	35:r:617:LHG:H251	2.03	0.41
28:r:613:CLA:H51	28:r:613:CLA:NB	2.34	0.41
28:r:613:CLA:H172	28:r:613:CLA:H143	2.03	0.41
18:s:42:ARG:HD2	42:s:715:HOH:O	2.20	0.41
38:s:601:CHL:C1B	35:s:617:LHG:H141	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:s:602:CLA:H52	39:s:615:LUT:C28	2.48	0.41
28:y:312:CLA:H2A	28:y:312:CLA:HED2	2.03	0.41
24:u:26:CYS:HB3	24:u:27:ARG:NH2	2.35	0.41
1:A:261:GLN:HB2	4:D:28:PHE:O	2.19	0.41
3:C:257:PHE:HB3	35:C:521:LHG:O5	2.20	0.41
7:G:77:LEU:HD11	7:G:81:PHE:HD2	1.86	0.41
38:G:608:CHL:H202	40:G:617:NEX:H371	2.02	0.41
7:N:71:TRP:CE2	38:N:608:CHL:HED2	2.56	0.41
28:N:611:CLA:H43	28:N:612:CLA:C2D	2.51	0.41
15:P:100:GLU:HG3	15:P:136:ALA:HB1	2.03	0.41
17:R:161:GLN:HB3	38:R:607:CHL:OMC	2.21	0.41
17:R:200:LYS:HD2	28:R:610:CLA:O1D	2.21	0.41
18:S:79:LEU:C	18:S:79:LEU:HD23	2.45	0.41
18:S:169:PRO:C	18:S:171:ASP:H	2.28	0.41
28:S:303:CLA:CHA	28:S:303:CLA:HBA1	2.42	0.41
28:S:303:CLA:HAA2	42:S:403:HOH:O	2.20	0.41
22:Y:118:LEU:HA	38:Y:605:CHL:O1D	2.20	0.41
22:Y:119:VAL:HA	38:Y:605:CHL:ND	2.35	0.41
22:Y:121:ALA:HA	38:Y:605:CHL:CHC	2.51	0.41
22:Y:161:PHE:CE1	38:Y:608:CHL:H101	2.56	0.41
22:Y:189:PHE:HE1	28:Y:613:CLA:HAB	1.84	0.41
1:a:343:LEU:HD13	3:c:310:SER:HA	2.02	0.41
28:b:609:CLA:H18	28:b:609:CLA:H152	1.88	0.41
28:b:615:CLA:HBB2	28:r:613:CLA:CAB	2.51	0.41
3:c:217:PRO:HG3	32:w:101:LMG:H341	2.03	0.41
3:c:379:ARG:HA	3:c:383:ASP:HB2	2.02	0.41
36:c:517:DGD:O2G	36:c:517:DGD:C1A	2.69	0.41
4:d:258:PHE:CZ	35:d:408:LHG:H322	2.56	0.41
5:e:8:ARG:NH1	42:e:101:HOH:O	2.53	0.41
7:g:112:TYR:HB3	7:g:118:LEU:HB2	2.02	0.41
38:g:619:CHL:HBB2	38:y:309:CHL:CBC	2.51	0.41
11:k:49:LEU:C	30:k:101:BCR:H19C	2.45	0.41
7:n:25:LEU:HB3	7:n:29:SER:HA	2.02	0.41
7:n:203:LYS:HB3	7:n:207:GLU:CD	2.45	0.41
28:n:603:CLA:H143	28:y:303:CLA:H111	2.02	0.41
14:o:227:ASP:HB2	14:o:231:LYS:HD2	2.02	0.41
28:r:613:CLA:H192	28:r:613:CLA:H162	1.88	0.41
18:s:194:ARG:HA	18:s:197:MET:CE	2.51	0.41
23:z:26:VAL:CG1	23:z:36:ASN:HB2	2.50	0.41
2:B:238:LEU:O	2:B:242:ILE:HG13	2.20	0.41
2:B:330:MET:HE3	2:B:446:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:ILE:HG13	42:B:702:HOH:O	2.19	0.41
2:B:454:GLY:HA2	32:B:621:LMG:H241	2.02	0.41
28:B:612:CLA:H122	28:B:612:CLA:H8	1.56	0.41
28:B:614:CLA:H92	28:B:614:CLA:H61	1.73	0.41
4:D:50:PHE:HE1	32:D:408:LMG:H312	1.86	0.41
7:G:58:PHE:O	7:G:62:ARG:HG3	2.21	0.41
11:K:40:MET:HG2	30:K:101:BCR:H332	2.02	0.41
13:M:27:VAL:HA	13:M:30:VAL:HG22	2.02	0.41
7:N:158:GLY:CA	28:N:610:CLA:HED2	2.51	0.41
28:N:611:CLA:C15	28:N:612:CLA:H13	2.50	0.41
15:P:42:PHE:CE1	15:P:87:LEU:HA	2.55	0.41
15:P:90:LYS:HB3	16:Q:2:ALA:HB1	2.03	0.41
18:S:28:GLY:H	18:S:51:GLY:HA3	1.85	0.41
18:S:49:LEU:CD1	18:S:49:LEU:N	2.82	0.41
18:S:57:TYR:CE2	38:S:302:CHL:HMD1	2.56	0.41
18:S:84:TRP:CZ3	28:S:309:CLA:HAC1	2.56	0.41
22:Y:124:ILE:HD13	38:Y:607:CHL:HMD3	2.03	0.41
40:Y:618:NEX:H35	40:Y:618:NEX:H401	1.89	0.41
24:U:72:GLU:N	24:U:73:PRO:HD2	2.36	0.41
1:a:328:MET:HG2	4:d:326:ILE:HG12	2.02	0.41
31:a:411:SQD:H5	4:d:233:PHE:HB3	2.02	0.41
2:b:222:PRO:HB3	8:h:37:TRP:C	2.45	0.41
2:b:498:LEU:HD23	2:b:499:GLY:N	2.36	0.41
30:b:619:BCR:H371	30:b:619:BCR:H24C	1.93	0.41
28:c:503:CLA:H93	28:c:503:CLA:H111	1.68	0.41
28:c:505:CLA:H62	28:c:505:CLA:H2	1.62	0.41
7:g:66:VAL:HG21	7:g:155:LEU:CD1	2.50	0.41
14:o:69:THR:N	14:o:70:PRO:HD2	2.36	0.41
16:q:57:GLU:HG2	16:q:76:ASP:HB3	2.02	0.41
17:r:24:LEU:HD11	28:r:602:CLA:HAA1	2.02	0.41
17:r:49:ASP:HB2	17:r:66:ILE:HG23	2.02	0.41
28:r:610:CLA:H12	28:r:611:CLA:HMD2	2.03	0.41
28:y:311:CLA:H93	28:y:312:CLA:CHD	2.51	0.41
28:y:311:CLA:HAC1	35:y:319:LHG:H302	2.03	0.41
28:A:406:CLA:HMA1	32:D:408:LMG:H212	2.03	0.41
32:A:411:LMG:H352	3:C:223:TRP:CD2	2.56	0.41
32:A:413:LMG:H291	32:A:413:LMG:H322	1.80	0.41
2:B:246:PHE:CD1	2:B:246:PHE:C	2.99	0.41
2:B:344:PRO:HB3	2:B:401:PHE:CZ	2.56	0.41
2:B:488:ALA:C	2:B:490:VAL:N	2.79	0.41
28:B:601:CLA:C1C	30:H:101:BCR:H19C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:607:CLA:H102	28:B:607:CLA:H62	1.22	0.41
28:B:614:CLA:HMD3	31:L:101:SQD:H242	2.02	0.41
28:B:615:CLA:H122	28:B:616:CLA:CHB	2.51	0.41
3:C:79:LYS:C	16:Q:33:LEU:HD12	2.45	0.41
3:C:191:PRO:HA	16:Q:78:ARG:HG3	2.02	0.41
3:C:216:SER:OG	3:C:218:PHE:HD1	2.03	0.41
28:C:501:CLA:HMB2	28:C:501:CLA:H62	2.03	0.41
4:D:47:GLY:HA3	30:D:405:BCR:C34	2.51	0.41
5:E:75:GLN:HG2	5:E:79:PHE:CZ	2.56	0.41
7:G:74:LEU:HD11	28:G:610:CLA:CBC	2.51	0.41
28:G:603:CLA:CBC	38:G:609:CHL:HHD	2.50	0.41
9:I:34:ARG:HD2	9:I:34:ARG:HA	1.89	0.41
11:K:46:LEU:HB3	30:K:101:BCR:C15	2.51	0.41
7:N:191:MET:HE2	39:N:616:LUT:C10	2.48	0.41
28:N:611:CLA:C4D	28:N:612:CLA:HMD3	2.50	0.41
16:Q:67:GLN:HE21	16:Q:67:GLN:HB2	1.57	0.41
16:Q:73:LEU:HD23	16:Q:121:ALA:HB2	2.03	0.41
17:R:11:ARG:HH21	17:R:33:GLY:H	1.68	0.41
17:R:155:ILE:HD11	38:R:605:CHL:HMA3	2.03	0.41
28:R:603:CLA:C3D	28:R:608:CLA:H2	2.50	0.41
18:S:93:ILE:O	18:S:94:ILE:C	2.64	0.41
18:S:97:ALA:O	18:S:101:TYR:HD1	2.04	0.41
18:S:123:THR:HB	18:S:131:ILE:O	2.21	0.41
18:S:191:LYS:HD3	28:S:311:CLA:O1D	2.21	0.41
30:T:101:BCR:H282	2:b:37:MET:SD	2.61	0.41
35:W:101:LHG:H182	35:W:101:LHG:H212	1.90	0.41
22:Y:111:ASP:HB3	22:Y:115:ASN:C	2.46	0.41
23:Z:5:PHE:O	23:Z:9:VAL:HG23	2.21	0.41
1:a:48:PHE:CD2	28:d:401:CLA:H202	2.55	0.41
1:a:58:VAL:HB	1:a:83:ILE:HB	2.03	0.41
1:a:181:ASN:HD22	4:d:315:PHE:HD1	1.69	0.41
1:a:298:ASN:ND2	42:a:502:HOH:O	2.54	0.41
1:a:334:ARG:HB2	14:o:157:LEU:HD12	2.02	0.41
36:a:401:DGD:HBN2	31:a:414:SQD:H301	2.03	0.41
28:a:406:CLA:H51	29:a:408:PHO:C2B	2.50	0.41
2:b:359:MET:HE3	2:b:425:GLN:HE21	1.85	0.41
28:b:601:CLA:H172	30:h:101:BCR:H17C	2.02	0.41
28:b:614:CLA:H93	28:b:614:CLA:H61	1.79	0.41
3:c:109:PHE:CE2	32:c:521:LMG:HC8	2.56	0.41
3:c:113:VAL:O	3:c:117:LEU:HG	2.20	0.41
3:c:162:GLY:HA3	3:c:252:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:214:LEU:O	20:w:14:PRO:HA	2.21	0.41
3:c:215:LYS:HG2	3:c:221:GLU:HB3	2.03	0.41
3:c:284:PHE:CD1	36:c:516:DGD:HBT2	2.56	0.41
3:c:332:GLN:NE2	3:c:336:GLY:HA2	2.35	0.41
3:c:387:TRP:HD1	16:q:83:TYR:CZ	2.38	0.41
28:c:502:CLA:H72	28:c:503:CLA:C4B	2.50	0.41
4:d:210:LEU:HD23	4:d:210:LEU:C	2.46	0.41
28:d:405:CLA:H151	21:x:58:ILE:O	2.21	0.41
5:e:8:ARG:HH21	5:e:13:ILE:HG23	1.84	0.41
7:g:49:ALA:HA	22:y:64:LEU:HD11	2.02	0.41
7:g:79:CYS:SG	39:g:616:LUT:H8	2.61	0.41
8:h:50:PHE:O	8:h:54:LEU:HG	2.21	0.41
10:j:12:ILE:HG13	10:j:13:ILE:N	2.36	0.41
7:n:33:PRO:O	7:n:34:SER:C	2.64	0.41
7:n:58:PHE:O	7:n:62:ARG:HG3	2.21	0.41
7:n:73:MET:HG3	7:n:184:GLY:HA2	2.03	0.41
7:n:128:TRP:CZ3	28:y:314:CLA:HAA2	2.56	0.41
17:r:37:PHE:CE2	41:r:615:XAT:H372	2.55	0.41
17:r:156:GLY:O	17:r:160:PHE:HD1	2.03	0.41
17:r:221:LYS:HG3	42:r:727:HOH:O	2.21	0.41
28:r:602:CLA:H72	41:r:615:XAT:H28	2.02	0.41
20:w:34:TRP:HZ3	28:y:312:CLA:H62	1.85	0.41
38:y:302:CHL:HHC	38:y:302:CHL:CBB	2.48	0.41
28:y:304:CLA:H61	28:y:304:CLA:H2	1.59	0.41
38:y:308:CHL:HHC	38:y:308:CHL:CBB	2.47	0.41
23:z:10:PHE:O	23:z:14:VAL:HG23	2.20	0.41
1:A:127:MET:HE3	28:C:505:CLA:HMB1	2.03	0.41
1:A:210:LEU:C	1:A:210:LEU:HD23	2.46	0.41
28:A:406:CLA:CMA	32:D:408:LMG:H242	2.51	0.41
32:A:411:LMG:H211	9:I:16:VAL:HG13	2.03	0.41
2:B:272:ARG:HH12	4:D:165:GLN:HA	1.86	0.41
2:B:283:GLU:CD	2:B:286:ARG:HH21	2.29	0.41
28:B:608:CLA:H152	4:D:121:PHE:CZ	2.56	0.41
3:C:212:TYR:HA	3:C:215:LYS:HE2	2.04	0.41
28:C:504:CLA:H8	32:C:520:LMG:H392	2.02	0.41
28:C:506:CLA:H141	28:C:506:CLA:H162	1.93	0.41
30:C:516:BCR:H343	30:K:101:BCR:HC22	2.03	0.41
36:C:519:DGD:C8A	32:D:408:LMG:H181	2.47	0.41
4:D:329:TRP:CZ2	4:D:349:ARG:HG3	2.54	0.41
7:G:24:TYR:CD2	38:G:601:CHL:HAA1	2.55	0.41
7:G:110:LEU:N	42:G:701:HOH:O	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:VAL:HG13	38:G:605:CHL:C1D	2.51	0.41
7:G:147:PRO:CG	40:G:617:NEX:H183	2.51	0.41
28:G:614:CLA:C3	22:Y:128:TRP:HZ3	2.33	0.41
7:N:185:ARG:HA	7:N:188:MET:HE3	2.02	0.41
28:N:603:CLA:NB	38:N:609:CHL:H111	2.36	0.41
28:N:614:CLA:HMB1	28:N:614:CLA:CBB	2.48	0.41
18:S:98:PHE:C	18:S:103:ALA:HB3	2.45	0.41
18:S:181:GLN:O	18:S:185:LEU:HB2	2.21	0.41
38:S:302:CHL:HAC2	35:S:317:LHG:O6	2.21	0.41
28:S:303:CLA:H52	39:S:316:LUT:H30	2.02	0.41
38:S:306:CHL:HHC	38:S:306:CHL:CBB	2.48	0.41
28:S:314:CLA:HBB1	28:S:314:CLA:HMB3	2.02	0.41
39:S:315:LUT:H11	39:S:315:LUT:H191	1.96	0.41
22:Y:181:LEU:HD23	22:Y:181:LEU:HA	1.95	0.41
38:Y:606:CHL:H43	40:Y:618:NEX:C35	2.51	0.41
38:Y:607:CHL:H112	38:Y:607:CHL:C3	2.51	0.41
23:Z:26:VAL:HG13	23:Z:36:ASN:HB2	2.03	0.41
35:a:415:LHG:H181	35:a:415:LHG:H152	1.86	0.41
28:b:604:CLA:H162	28:b:604:CLA:H192	1.79	0.41
28:b:604:CLA:H2A	28:b:604:CLA:O1D	2.21	0.41
3:c:127:PHE:HA	28:c:511:CLA:H201	2.01	0.41
3:c:141:GLU:CD	3:c:141:GLU:H	2.28	0.41
3:c:168:LEU:HD11	28:c:507:CLA:HED2	2.03	0.41
3:c:199:ILE:HG13	3:c:234:ILE:HG13	2.02	0.41
28:c:508:CLA:CHB	28:c:510:CLA:H11	2.51	0.41
28:c:511:CLA:O1A	28:c:511:CLA:HBD	2.21	0.41
30:c:514:BCR:HC31	23:z:58:ASN:ND2	2.36	0.41
30:c:514:BCR:C35	32:c:521:LMG:H402	2.51	0.41
4:d:33:TRP:HA	4:d:36:LEU:HD13	2.03	0.41
7:g:119:VAL:N	38:g:605:CHL:O2D	2.54	0.41
7:g:220:ASN:HB2	7:g:222:TRP:CH2	2.55	0.41
9:i:27:ASP:N	9:i:28:PRO:CD	2.84	0.41
7:n:14:SER:OG	7:n:17:TYR:HB2	2.21	0.41
38:n:606:CHL:HAC2	38:n:606:CHL:OMC	2.21	0.41
38:n:606:CHL:HBD	38:n:606:CHL:HAA2	2.01	0.41
38:n:609:CHL:C4B	38:y:302:CHL:H2	2.51	0.41
17:r:126:LYS:N	38:r:606:CHL:O1D	2.47	0.41
28:r:609:CLA:HED2	28:r:609:CLA:HBD	1.90	0.41
18:s:48:TYR:CD2	18:s:66:LYS:HA	2.56	0.41
18:s:195:LEU:HD11	39:s:614:LUT:H192	2.02	0.41
1:A:28:LEU:HD12	31:A:414:SQD:H111	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:ND2	42:A:503:HOH:O	2.53	0.40
1:A:341:LEU:N	3:C:313:GLN:HE22	2.20	0.40
2:B:6:TYR:CE1	35:B:625:LHG:HC41	2.56	0.40
2:B:497:LYS:HE2	4:D:24:ARG:NH1	2.36	0.40
32:B:624:LMG:H122	38:R:606:CHL:HAA1	2.02	0.40
3:C:318:LEU:HD23	3:C:318:LEU:C	2.46	0.40
28:C:502:CLA:H2	28:C:503:CLA:ND	2.35	0.40
28:C:503:CLA:H102	28:C:503:CLA:H13	1.76	0.40
28:C:505:CLA:H161	28:C:505:CLA:H122	1.77	0.40
4:D:25:ARG:O	4:D:27:ARG:HG2	2.21	0.40
4:D:338:GLU:CB	4:D:340:LEU:HG	2.51	0.40
7:G:22:VAL:C	7:G:23:LYS:HD2	2.46	0.40
7:G:147:PRO:HB2	38:G:608:CHL:HBB2	2.02	0.40
8:H:24:LYS:N	8:H:25:PRO:CD	2.84	0.40
9:I:19:PHE:CZ	9:I:23:PHE:HE2	2.38	0.40
7:N:193:GLY:O	7:N:197:GLN:HG3	2.20	0.40
28:N:604:CLA:CHA	28:N:604:CLA:HBA2	2.51	0.40
38:N:607:CHL:H72	38:N:607:CHL:CMB	2.50	0.40
22:Y:127:ILE:HG12	38:Y:605:CHL:HAC1	2.03	0.40
22:Y:198:ALA:HB3	38:Y:607:CHL:C12	2.51	0.40
23:Z:9:VAL:O	23:Z:13:ILE:HG13	2.21	0.40
2:b:108:PHE:O	2:b:112:ILE:HG13	2.22	0.40
2:b:477:ASP:O	17:r:59:LYS:HG3	2.21	0.40
28:b:608:CLA:HBB1	28:b:608:CLA:CMB	2.51	0.40
3:c:47:GLY:HA3	3:c:137:PRO:O	2.21	0.40
4:d:161:TYR:N	4:d:162:PRO:HD2	2.36	0.40
4:d:219:VAL:HG13	4:d:245:TYR:CD1	2.56	0.40
7:g:189:PHE:CD2	28:g:602:CLA:H201	2.56	0.40
7:g:221:ALA:O	38:g:619:CHL:H141	2.22	0.40
11:k:52:PHE:HB3	30:k:101:BCR:H282	2.03	0.40
7:n:111:ASP:HB3	7:n:115:ASN:O	2.20	0.40
7:n:195:PHE:O	7:n:199:ILE:HG13	2.21	0.40
38:n:601:CHL:C1D	35:n:618:LHG:HC82	2.51	0.40
28:n:602:CLA:HED2	28:n:602:CLA:H2A	2.03	0.40
28:n:603:CLA:H193	38:n:609:CHL:H72	2.04	0.40
28:n:613:CLA:H2	28:n:614:CLA:HMD2	2.03	0.40
28:n:613:CLA:C1A	28:n:613:CLA:CGA	2.99	0.40
16:q:98:ASP:OD1	16:q:99:GLN:N	2.54	0.40
16:q:107:THR:HG22	16:q:111:PHE:CE2	2.56	0.40
17:r:73:GLU:HG2	17:r:90:GLN:HB3	2.02	0.40
17:r:102:TRP:CE2	38:r:607:CHL:HED3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:161:GLN:HB3	38:r:607:CHL:OMC	2.21	0.40
28:r:612:CLA:H101	28:r:612:CLA:CBB	2.51	0.40
38:s:601:CHL:HAC1	38:s:601:CHL:OMC	2.22	0.40
28:s:602:CLA:C5	39:s:615:LUT:H28	2.47	0.40
28:s:609:CLA:C10	39:s:614:LUT:H371	2.51	0.40
39:s:614:LUT:H15	39:s:614:LUT:H201	1.83	0.40
22:y:112:TYR:CE2	28:y:305:CLA:H42	2.57	0.40
28:y:304:CLA:H61	28:y:304:CLA:H93	1.85	0.40
38:y:307:CHL:HHC	38:y:307:CHL:CBB	2.45	0.40
1:A:278:TRP:CE2	31:A:410:SQD:H223	2.57	0.40
28:A:405:CLA:H93	28:A:405:CLA:H62	1.72	0.40
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.56	0.40
28:B:607:CLA:H172	12:L:32:PHE:CE1	2.57	0.40
3:C:61:VAL:HG12	3:C:118:HIS:O	2.20	0.40
3:C:223:TRP:CE2	3:C:224:ILE:HG23	2.57	0.40
28:C:507:CLA:HHC	28:C:507:CLA:CBB	2.52	0.40
28:C:510:CLA:H3A	28:C:510:CLA:HBA1	1.83	0.40
30:C:516:BCR:H353	30:K:101:BCR:HC7	2.02	0.40
4:D:104:ARG:HH21	5:E:77:ASP:HA	1.87	0.40
32:D:408:LMG:H342	32:D:408:LMG:H311	1.85	0.40
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.40
6:F:14:TRP:HE3	6:F:15:LEU:HD23	1.86	0.40
6:F:39:ARG:HH12	15:P:16:THR:HG21	1.86	0.40
7:G:111:ASP:HB3	7:G:115:ASN:O	2.20	0.40
7:G:206:LEU:HD22	7:G:206:LEU:HA	1.92	0.40
12:L:19:TYR:HE1	31:L:103:SQD:H262	1.84	0.40
38:N:609:CHL:H161	38:N:609:CHL:H141	1.84	0.40
15:P:80:PHE:CE1	15:P:156:LEU:HD11	2.52	0.40
16:Q:62:LYS:HD2	16:Q:65:ILE:HD12	2.03	0.40
17:R:83:TYR:CB	28:R:613:CLA:HED2	2.48	0.40
17:R:209:PHE:CZ	41:R:615:XAT:H8	2.56	0.40
28:Y:602:CLA:H202	39:Y:616:LUT:H31	2.04	0.40
38:Y:607:CHL:C4	38:Y:607:CHL:H151	2.51	0.40
23:Z:33:TRP:CZ2	23:Z:37:LYS:HG2	2.55	0.40
1:a:217:SER:HB2	4:d:143:ASN:HA	2.03	0.40
1:a:340:PRO:HB2	15:p:166:LYS:HB3	2.02	0.40
27:a:404:CL:CL	42:a:594:HOH:O	2.59	0.40
28:a:409:CLA:CHA	28:a:409:CLA:HBA2	2.51	0.40
28:a:409:CLA:H72	28:a:409:CLA:H121	2.03	0.40
2:b:20:LEU:O	2:b:24:ILE:HG13	2.21	0.40
2:b:500:ASP:CG	2:b:503:THR:HG23	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:624:LHG:HC91	4:d:274:PHE:CE1	2.56	0.40
3:c:35:TRP:C	3:c:37:ALA:N	2.79	0.40
3:c:154:ARG:NH1	20:w:49:GLU:HA	2.36	0.40
3:c:465:PRO:HD2	42:d:552:HOH:O	2.21	0.40
4:d:28:PHE:HD2	4:d:29:VAL:HG23	1.82	0.40
32:d:409:LMG:H292	32:d:409:LMG:C15	2.42	0.40
7:g:110:LEU:HD13	38:g:606:CHL:HMD3	2.02	0.40
7:g:153:ASP:HB3	7:g:156:TYR:O	2.21	0.40
7:n:161:PHE:HD1	28:n:610:CLA:HMD2	1.86	0.40
7:n:188:MET:HE3	28:n:602:CLA:HMC3	2.02	0.40
14:o:117:GLN:OE1	14:o:121:GLY:HA2	2.21	0.40
15:p:78:GLU:H	15:p:78:GLU:CD	2.27	0.40
17:r:191:LYS:HE2	17:r:195:GLN:NE2	2.37	0.40
18:s:60:ASP:N	18:s:61:PRO:HD3	2.37	0.40
18:s:64:LEU:HD11	39:s:615:LUT:H373	2.03	0.40
38:y:306:CHL:HHC	38:y:306:CHL:CBB	2.45	0.40
23:z:34:SER:O	23:z:37:LYS:HB2	2.22	0.40
1:A:110:GLY:N	1:A:111:PRO:CD	2.84	0.40
1:A:284:TRP:CG	3:C:435:PHE:HZ	2.40	0.40
2:B:51:VAL:HA	2:B:308:LYS:HZ3	1.87	0.40
3:C:45:LEU:HD22	3:C:138:GLU:HG2	2.03	0.40
3:C:72:VAL:HG12	11:K:26:LEU:HD23	2.04	0.40
3:C:229:ASP:N	3:C:229:ASP:OD1	2.52	0.40
3:C:343:ARG:NH1	14:O:27:ASN:HA	2.36	0.40
3:C:376:ASP:OD2	3:C:379:ARG:HG3	2.21	0.40
30:C:514:BCR:H11C	30:C:514:BCR:H353	1.98	0.40
32:C:520:LMG:C19	11:K:42:VAL:HG11	2.51	0.40
7:G:66:VAL:HG22	7:G:181:LEU:HD21	2.03	0.40
7:G:105:PHE:HZ	7:N:225:ALA:CB	2.34	0.40
28:G:610:CLA:H112	28:G:612:CLA:HMB1	2.03	0.40
14:O:37:ASP:HA	14:O:206:GLN:HG2	2.03	0.40
17:R:123:ASP:HA	38:R:606:CHL:HED2	2.03	0.40
38:R:606:CHL:OMC	38:R:606:CHL:HAC2	2.21	0.40
28:R:609:CLA:H61	28:R:609:CLA:H92	1.62	0.40
18:S:64:LEU:CD1	39:S:316:LUT:H221	2.52	0.40
18:S:110:VAL:HG13	18:S:112:PHE:CE1	2.57	0.40
28:Y:613:CLA:H71	28:Y:613:CLA:H112	1.67	0.40
1:a:47:VAL:HG23	30:a:410:BCR:H361	2.04	0.40
28:b:609:CLA:H3A	28:b:609:CLA:HBA2	1.40	0.40
3:c:67:MET:HB3	3:c:88:LEU:HD11	2.02	0.40
3:c:192:GLY:HA2	16:q:81:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:502:CLA:HBB1	28:c:502:CLA:CMB	2.45	0.40
28:c:505:CLA:HMB3	28:c:505:CLA:CBB	2.50	0.40
28:c:511:CLA:C4D	11:k:54:TRP:HH2	2.35	0.40
30:c:515:BCR:H11C	30:c:515:BCR:H341	1.84	0.40
4:d:12:GLN:CG	4:d:14:ASP:HB3	2.50	0.40
7:g:128:TRP:HB3	7:n:222:TRP:CH2	2.57	0.40
10:j:25:ILE:HG23	10:j:29:PHE:CE2	2.56	0.40
28:r:603:CLA:C4D	28:r:608:CLA:H61	2.51	0.40
18:s:167:GLY:HA2	18:s:171:ASP:HB2	2.03	0.40
22:y:92:PHE:CE2	22:y:113:LEU:HA	2.57	0.40
22:y:123:SER:O	22:y:127:ILE:HG13	2.22	0.40
24:u:1:GLU:HB2	24:u:2:PRO:HD3	2.03	0.40
1:A:14:TRP:HD1	20:W:40:TYR:CG	2.39	0.40
1:A:305:SER:OG	3:C:415:ASN:ND2	2.54	0.40
1:A:326:LEU:CD2	3:C:412:THR:HB	2.52	0.40
2:B:222:PRO:HB3	8:H:37:TRP:C	2.47	0.40
3:C:35:TRP:CD2	11:K:60:PHE:HD2	2.38	0.40
3:C:47:GLY:HA3	3:C:137:PRO:O	2.22	0.40
3:C:212:TYR:HB3	3:C:224:ILE:HA	2.03	0.40
3:C:274:TYR:CD1	28:C:505:CLA:HMD2	2.56	0.40
4:D:7:LYS:HE3	17:R:68:THR:HB	2.04	0.40
7:G:135:MET:O	7:G:138:VAL:HG22	2.22	0.40
7:G:188:MET:HE3	28:G:602:CLA:HMC3	2.03	0.40
39:G:615:LUT:H27	39:G:615:LUT:H362	1.83	0.40
8:H:45:ILE:O	8:H:49:LEU:HG	2.22	0.40
7:N:115:ASN:ND2	7:N:118:LEU:HG	2.36	0.40
39:N:615:LUT:H15	39:N:615:LUT:H201	1.92	0.40
14:O:58:PHE:CE2	20:W:2:VAL:HG21	2.56	0.40
17:R:112:THR:HG21	28:R:604:CLA:HHD	2.03	0.40
18:S:118:LEU:HD12	38:S:306:CHL:HBC3	2.03	0.40
18:S:200:MET:HA	18:S:203:PHE:HD2	1.86	0.40
38:S:302:CHL:OMC	38:S:302:CHL:HAC1	2.22	0.40
21:X:59:VAL:O	21:X:63:VAL:HG23	2.21	0.40
1:a:74:GLY:C	1:a:75:ASN:HD22	2.29	0.40
1:a:195:HIS:HD1	1:a:197:PHE:HB2	1.86	0.40
1:a:328:MET:H	1:a:328:MET:HG3	1.70	0.40
2:b:462:PHE:HA	28:b:611:CLA:CMC	2.51	0.40
28:b:603:CLA:H2	28:b:605:CLA:H91	2.04	0.40
28:b:604:CLA:H193	28:b:615:CLA:H93	2.03	0.40
28:b:608:CLA:H122	28:d:405:CLA:HMB1	2.04	0.40
28:b:611:CLA:H18	28:b:613:CLA:NA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:239:TRP:O	3:c:243:ILE:HG13	2.21	0.40
3:c:464:GLU:HB3	3:c:467:LEU:HD22	2.02	0.40
28:c:503:CLA:H102	28:c:503:CLA:H13	1.88	0.40
4:d:105:TRP:HH2	4:d:114:PHE:CD2	2.40	0.40
32:d:409:LMG:H341	32:d:409:LMG:H372	1.90	0.40
7:g:52:SER:HB3	7:g:58:PHE:CG	2.56	0.40
38:g:608:CHL:H151	38:g:608:CHL:C10	2.51	0.40
11:k:25:LYS:NZ	11:k:25:LYS:HB2	2.36	0.40
30:k:101:BCR:H21C	30:k:101:BCR:H24C	1.86	0.40
7:n:148:LEU:CD1	38:n:608:CHL:H102	2.51	0.40
7:n:196:VAL:HG21	28:n:613:CLA:HAC2	2.03	0.40
28:n:610:CLA:H8	28:n:612:CLA:H101	2.04	0.40
14:o:78:LEU:HD11	14:o:84:TYR:CE1	2.56	0.40
16:q:64:PHE:O	16:q:68:LYS:N	2.54	0.40
38:s:601:CHL:C1D	35:s:617:LHG:HC82	2.51	0.40
35:w:102:LHG:HC81	28:y:311:CLA:C3	2.51	0.40
22:y:107:GLU:H	22:y:107:GLU:CD	2.30	0.40
22:y:206:LEU:HD12	22:y:206:LEU:H	1.87	0.40
40:y:318:NEX:H192	40:y:318:NEX:H183	2.03	0.40
31:A:410:SQD:H241	3:C:36:TRP:CD2	2.56	0.40
32:A:411:LMG:H332	3:C:217:PRO:HD3	2.03	0.40
28:B:604:CLA:H92	28:B:604:CLA:H61	1.66	0.40
28:B:615:CLA:H92	28:B:615:CLA:H61	1.62	0.40
30:B:617:BCR:H322	32:B:621:LMG:H111	2.04	0.40
3:C:320:ARG:O	3:C:324:LEU:HG	2.21	0.40
28:C:506:CLA:H192	28:C:506:CLA:H161	1.81	0.40
30:C:514:BCR:H15C	30:C:514:BCR:H351	1.63	0.40
4:D:25:ARG:NE	21:X:81:VAL:HG22	2.36	0.40
5:E:19:TYR:CE2	5:E:23:HIS:CE1	3.09	0.40
7:G:66:VAL:HB	7:G:155:LEU:HD22	2.04	0.40
28:G:613:CLA:HMB1	28:G:613:CLA:CBB	2.51	0.40
7:N:24:TYR:H	7:N:24:TYR:HD1	1.69	0.40
7:N:70:ARG:O	7:N:74:LEU:HG	2.21	0.40
7:N:153:ASP:OD2	7:N:156:TYR:HB2	2.21	0.40
38:N:609:CHL:C3B	38:Y:601:CHL:H52	2.52	0.40
14:O:147:LEU:HD11	14:O:195:SER:HB2	2.04	0.40
14:O:208:LYS:NZ	14:O:211:THR:HG23	2.37	0.40
17:R:32:TYR:CZ	28:R:601:CLA:HAC2	2.56	0.40
17:R:230:HIS:HB2	28:R:612:CLA:HAA2	2.02	0.40
18:S:57:TYR:HE2	38:S:302:CHL:HBC2	1.86	0.40
18:S:112:PHE:HE2	18:S:113:LYS:HE3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:S:307:CHL:H71	38:S:307:CHL:HMA3	2.04	0.40
28:S:310:CLA:HBB1	28:S:310:CLA:CMB	2.51	0.40
20:W:6:MET:HG2	20:W:8:THR:OG1	2.21	0.40
22:Y:199:ILE:CG1	38:Y:607:CHL:H122	2.49	0.40
1:a:14:TRP:HB2	20:w:36:LEU:HB3	2.03	0.40
1:a:106:LEU:HD12	36:a:401:DGD:HE1	2.03	0.40
1:a:133:LEU:O	1:a:137:LEU:HG	2.22	0.40
28:a:406:CLA:H152	29:a:408:PHO:H43	2.03	0.40
2:b:125:ASP:O	2:b:129:GLY:N	2.50	0.40
2:b:258:TYR:CZ	36:b:625:DGD:HBF2	2.57	0.40
3:c:279:LEU:HB3	3:c:437:LEU:HD23	2.04	0.40
3:c:332:GLN:HA	14:o:111:TYR:OH	2.22	0.40
35:c:519:LHG:H262	28:y:312:CLA:CMD	2.52	0.40
4:d:122:GLY:C	29:d:402:PHO:H41	2.46	0.40
4:d:202:VAL:HG11	28:d:401:CLA:C3D	2.51	0.40
5:e:19:TYR:HE2	37:f:101:HEM:C3D	2.40	0.40
7:g:167:ALA:HB2	28:g:610:CLA:CAA	2.52	0.40
39:g:615:LUT:H35	39:g:615:LUT:H401	1.77	0.40
7:n:112:TYR:HB3	7:n:118:LEU:HB3	2.03	0.40
7:n:215:ASP:O	7:n:219:ASN:N	2.53	0.40
15:p:29:LEU:H	15:p:182:SER:CB	2.34	0.40
38:s:607:CHL:HBA2	28:s:609:CLA:HMD2	2.04	0.40
32:w:101:LMG:H142	32:w:101:LMG:H111	1.85	0.40
38:y:308:CHL:H91	38:y:308:CHL:H112	1.82	0.40
41:y:317:XAT:H31	41:y:317:XAT:H391	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	332/334 (99%)	317 (96%)	14 (4%)	1 (0%)	36	42
2	B	501/503 (100%)	489 (98%)	12 (2%)	0	100	100
2	b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
3	C	448/450 (100%)	432 (96%)	16 (4%)	0	100	100
3	c	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
4	D	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
4	d	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
5	e	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
6	F	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
6	f	28/30 (93%)	28 (100%)	0	0	100	100
7	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
7	N	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	g	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	n	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
8	H	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
8	h	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
10	J	33/35 (94%)	33 (100%)	0	0	100	100
10	j	33/35 (94%)	33 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/36 (94%)	34 (100%)	0	0	100	100
12	l	34/36 (94%)	34 (100%)	0	0	100	100
13	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
13	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	234 (95%)	12 (5%)	0	100	100
15	P	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
15	p	184/186 (99%)	180 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
16	q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
17	R	222/224 (99%)	215 (97%)	7 (3%)	0	100	100
17	r	222/224 (99%)	216 (97%)	6 (3%)	0	100	100
18	S	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	24	27
18	s	216/218 (99%)	202 (94%)	14 (6%)	0	100	100
19	T	29/31 (94%)	29 (100%)	0	0	100	100
19	t	29/31 (94%)	29 (100%)	0	0	100	100
20	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
20	w	52/54 (96%)	52 (100%)	0	0	100	100
21	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
21	x	37/39 (95%)	37 (100%)	0	0	100	100
22	Y	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
22	y	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
23	Z	59/61 (97%)	59 (100%)	0	0	100	100
23	z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
24	U	26/28 (93%)	26 (100%)	0	0	100	100
24	u	26/28 (93%)	26 (100%)	0	0	100	100
All	All	7634/7734 (99%)	7353 (96%)	278 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	161	GLU
1	a	141	PRO
1	A	141	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/270 (100%)	265 (98%)	5 (2%)	50 66
1	a	270/270 (100%)	262 (97%)	8 (3%)	36 49
2	B	399/399 (100%)	396 (99%)	3 (1%)	73 85
2	b	399/399 (100%)	391 (98%)	8 (2%)	48 64
3	C	352/352 (100%)	348 (99%)	4 (1%)	65 79
3	c	352/352 (100%)	345 (98%)	7 (2%)	48 64
4	D	284/284 (100%)	281 (99%)	3 (1%)	65 79
4	d	284/284 (100%)	281 (99%)	3 (1%)	65 79
5	E	67/67 (100%)	67 (100%)	0	100 100
5	e	67/67 (100%)	67 (100%)	0	100 100
6	F	25/25 (100%)	25 (100%)	0	100 100
6	f	25/25 (100%)	25 (100%)	0	100 100
7	G	169/169 (100%)	166 (98%)	3 (2%)	51 68
7	N	168/169 (99%)	162 (96%)	6 (4%)	31 42
7	g	169/169 (100%)	166 (98%)	3 (2%)	51 68
7	n	169/169 (100%)	161 (95%)	8 (5%)	23 31
8	H	49/49 (100%)	46 (94%)	3 (6%)	17 20
8	h	49/49 (100%)	49 (100%)	0	100 100
9	I	31/31 (100%)	31 (100%)	0	100 100
9	i	31/31 (100%)	30 (97%)	1 (3%)	34 47
10	J	26/26 (100%)	25 (96%)	1 (4%)	29 40
10	j	26/26 (100%)	24 (92%)	2 (8%)	12 13
11	K	32/32 (100%)	31 (97%)	1 (3%)	35 48
11	k	32/32 (100%)	32 (100%)	0	100 100
12	L	34/34 (100%)	33 (97%)	1 (3%)	37 51
12	l	34/34 (100%)	33 (97%)	1 (3%)	37 51
13	M	29/29 (100%)	29 (100%)	0	100 100
13	m	29/29 (100%)	29 (100%)	0	100 100
14	O	204/204 (100%)	201 (98%)	3 (2%)	57 73
14	o	204/204 (100%)	200 (98%)	4 (2%)	48 64
15	P	150/150 (100%)	145 (97%)	5 (3%)	33 45
15	p	150/150 (100%)	147 (98%)	3 (2%)	48 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	Q	125/125 (100%)	122 (98%)	3 (2%)	43 58
16	q	125/125 (100%)	124 (99%)	1 (1%)	73 85
17	R	181/181 (100%)	178 (98%)	3 (2%)	53 69
17	r	181/181 (100%)	174 (96%)	7 (4%)	28 39
18	S	169/169 (100%)	165 (98%)	4 (2%)	43 58
18	s	169/169 (100%)	164 (97%)	5 (3%)	36 49
19	T	28/28 (100%)	28 (100%)	0	100 100
19	t	28/28 (100%)	28 (100%)	0	100 100
20	W	44/44 (100%)	41 (93%)	3 (7%)	14 17
20	w	44/44 (100%)	43 (98%)	1 (2%)	44 59
21	X	32/32 (100%)	32 (100%)	0	100 100
21	x	32/32 (100%)	32 (100%)	0	100 100
22	Y	170/170 (100%)	166 (98%)	4 (2%)	43 58
22	y	170/170 (100%)	165 (97%)	5 (3%)	37 51
23	Z	53/53 (100%)	51 (96%)	2 (4%)	29 40
23	z	53/53 (100%)	50 (94%)	3 (6%)	18 23
24	U	23/23 (100%)	23 (100%)	0	100 100
24	u	23/23 (100%)	21 (91%)	2 (9%)	9 10
All	All	6229/6230 (100%)	6100 (98%)	129 (2%)	46 63

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	35	VAL
1	A	261	GLN
1	A	286	THR
1	A	313	VAL
2	B	3	LEU
2	B	350	GLU
2	B	362	PHE
3	C	79	LYS
3	C	289	PHE
3	C	377	LEU
3	C	473	ASN
4	D	247	MET

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Mol	Chain	Res	Type
4	D	265	LYS
4	D	353	LEU
7	G	90	VAL
7	G	118	LEU
7	G	203	LYS
8	H	64	SER
8	H	70	ILE
8	H	72	MET
10	J	12	ILE
11	K	25	LYS
12	L	5	ASN
7	N	96	VAL
7	N	122	GLN
7	N	166	LEU
7	N	206	LEU
7	N	213	LEU
7	N	228	PHE
14	O	13	GLN
14	O	188	GLU
14	O	199	LYS
15	P	19	LEU
15	P	47	LEU
15	P	83	LYS
15	P	100	GLU
15	P	156	LEU
16	Q	99	GLN
16	Q	131	LYS
16	Q	146	LYS
17	R	105	LEU
17	R	113	VAL
17	R	199	ILE
18	S	49	LEU
18	S	146	LEU
18	S	163	LYS
18	S	185	LEU
20	W	19	ASN
20	W	21	LEU
20	W	40	TYR
22	Y	60	LYS
22	Y	87	ARG
22	Y	125	LEU
22	Y	228	PHE

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Mol	Chain	Res	Type
23	Z	20	LEU
23	Z	61	ILE
1	a	35	VAL
1	a	75	ASN
1	a	286	THR
1	a	293	MET
1	a	298	ASN
1	a	313	VAL
1	a	326	LEU
1	a	343	LEU
2	b	3	LEU
2	b	177	ARG
2	b	294	GLU
2	b	304	LYS
2	b	362	PHE
2	b	419	LYS
2	b	486	LEU
2	b	504	LYS
3	c	59	LEU
3	c	135	LEU
3	c	240	LEU
3	c	250	TRP
3	c	289	PHE
3	c	462	ASP
3	c	473	ASN
4	d	3	ILE
4	d	341	ILE
4	d	346	VAL
7	g	155	LEU
7	g	213	LEU
7	g	224	TYR
9	i	34	ARG
10	j	13	ILE
10	j	27	LEU
12	l	5	ASN
7	n	25	LEU
7	n	60	LYS
7	n	74	LEU
7	n	113	LEU
7	n	181	LEU
7	n	213	LEU
7	n	220	ASN

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Mol	Chain	Res	Type
7	n	226	THR
14	o	50	LYS
14	o	78	LEU
14	o	188	GLU
14	o	231	LYS
15	p	47	LEU
15	p	54	ASP
15	p	83	LYS
16	q	109	LYS
17	r	24	LEU
17	r	39	LEU
17	r	76	LYS
17	r	94	GLU
17	r	169	GLU
17	r	190	LYS
17	r	231	LEU
18	s	49	LEU
18	s	69	GLU
18	s	124	LEU
18	s	146	LEU
18	s	151	TYR
20	w	9	GLU
22	y	23	LYS
22	y	39	GLU
22	y	60	LYS
22	y	96	VAL
22	y	181	LEU
23	z	20	LEU
23	z	33	TRP
23	z	50	LEU
24	u	26	CYS
24	u	27	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	261	GLN
1	A	266	ASN
1	A	304	GLN
1	A	310	GLN
2	B	9	HIS

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Mol	Chain	Res	Type
2	B	26	HIS
2	B	79	ASN
2	B	100	HIS
2	B	216	HIS
2	B	332	ASN
2	B	343	HIS
2	B	425	GLN
2	B	455	HIS
3	C	28	GLN
3	C	68	ASN
3	C	201	ASN
3	C	311	GLN
3	C	313	GLN
3	C	322	GLN
3	C	332	GLN
3	C	385	GLN
3	C	415	ASN
3	C	418	ASN
3	C	473	ASN
4	D	138	GLN
4	D	191	ASN
4	D	198	HIS
4	D	256	GLN
4	D	337	HIS
4	D	339	ASN
4	D	351	ASN
6	F	38	GLN
7	G	61	ASN
7	G	88	ASN
7	G	122	GLN
7	G	197	GLN
7	G	208	ASN
7	G	218	ASN
7	G	227	ASN
8	H	62	ASN
11	K	34	ASN
12	L	5	ASN
7	N	88	ASN
7	N	120	HIS
7	N	197	GLN
7	N	208	ASN
7	N	218	ASN

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Mol	Chain	Res	Type
7	N	220	ASN
14	O	28	GLN
14	O	47	ASN
14	O	75	ASN
14	O	117	GLN
14	O	190	ASN
14	O	222	GLN
14	O	239	GLN
15	P	64	GLN
15	P	162	GLN
16	Q	40	GLN
16	Q	67	GLN
16	Q	74	GLN
16	Q	99	GLN
16	Q	141	ASN
17	R	56	ASN
17	R	161	GLN
18	S	75	GLN
18	S	125	ASN
18	S	181	GLN
18	S	217	ASN
18	S	228	ASN
20	W	19	ASN
21	X	77	ASN
22	Y	88	ASN
22	Y	120	HIS
22	Y	197	GLN
22	Y	208	ASN
23	Z	6	GLN
23	Z	36	ASN
1	a	75	ASN
1	a	108	ASN
1	a	165	GLN
1	a	261	GLN
1	a	266	ASN
1	a	298	ASN
1	a	304	GLN
2	b	9	HIS
2	b	73	ASN
2	b	157	HIS
2	b	182	ASN
2	b	216	HIS

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Mol	Chain	Res	Type
2	b	425	GLN
2	b	489	GLN
2	b	496	GLN
3	c	68	ASN
3	c	132	HIS
3	c	201	ASN
3	c	311	GLN
3	c	313	GLN
3	c	322	GLN
3	c	332	GLN
3	c	385	GLN
3	c	415	ASN
3	c	473	ASN
4	d	12	GLN
4	d	13	ASN
4	d	84	ASN
4	d	99	GLN
4	d	198	HIS
4	d	256	GLN
6	f	38	GLN
7	g	220	ASN
8	h	62	ASN
12	l	5	ASN
12	l	10	ASN
13	m	4	ASN
13	m	32	GLN
7	n	88	ASN
7	n	120	HIS
7	n	197	GLN
7	n	208	ASN
14	o	28	GLN
14	o	75	ASN
14	o	190	ASN
14	o	222	GLN
14	o	239	GLN
15	p	35	ASN
15	p	91	GLN
15	p	112	ASN
15	p	125	GLN
16	q	22	ASN
16	q	112	GLN
17	r	47	GLN

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Mol	Chain	Res	Type
17	r	55	GLN
17	r	56	ASN
17	r	60	ASN
17	r	81	GLN
17	r	90	GLN
17	r	195	GLN
18	s	75	GLN
18	s	104	ASN
18	s	156	ASN
18	s	206	GLN
18	s	217	ASN
22	y	88	ASN
22	y	197	GLN
22	y	208	ASN
22	y	218	ASN
22	y	227	ASN
23	z	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 339 ligands modelled in this entry, 6 are monoatomic - leaving 333 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	r	612	17	64,68,73	1.40	7 (10%)	77,107,113	2.02	18 (23%)
30	BCR	K	101	-	41,41,41	4.77	27 (65%)	56,56,56	2.41	21 (37%)
38	CHL	R	607	42	65,69,74	0.80	2 (3%)	74,108,114	1.33	14 (18%)
32	LMG	A	413	-	40,40,55	0.92	3 (7%)	48,48,63	1.11	3 (6%)
38	CHL	N	609	7	68,72,74	0.80	2 (2%)	77,111,114	1.30	11 (14%)
36	DGD	B	626	-	63,63,67	1.13	6 (9%)	77,77,81	0.94	2 (2%)
35	LHG	l	101	-	48,48,48	0.42	0	51,54,54	1.09	2 (3%)
30	BCR	a	410	-	41,41,41	4.79	27 (65%)	56,56,56	2.31	21 (37%)
30	BCR	A	409	-	41,41,41	4.79	27 (65%)	56,56,56	2.23	18 (32%)
28	CLA	Y	602	22	69,73,73	1.43	7 (10%)	83,113,113	1.90	22 (26%)
28	CLA	s	603	18	49,53,73	1.60	7 (14%)	59,89,113	2.07	16 (27%)
28	CLA	G	610	7	68,72,73	1.36	6 (8%)	81,111,113	1.98	19 (23%)
33	PL9	a	412	-	13,13,55	1.47	1 (7%)	17,17,69	1.04	0
38	CHL	g	608	42	70,74,74	0.80	2 (2%)	80,114,114	1.35	14 (17%)
30	BCR	k	101	-	41,41,41	4.80	27 (65%)	56,56,56	2.31	19 (33%)
35	LHG	Y	619	28	48,48,48	0.47	1 (2%)	51,54,54	1.07	2 (3%)
28	CLA	d	405	4	69,73,73	1.36	6 (8%)	83,113,113	1.96	18 (21%)
28	CLA	C	513	3	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
28	CLA	s	604	42	54,58,73	1.52	6 (11%)	65,95,113	2.15	17 (26%)
28	CLA	B	606	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
28	CLA	S	311	35	60,64,73	1.44	6 (10%)	72,102,113	2.09	20 (27%)
28	CLA	g	610	7	62,66,73	1.43	6 (9%)	74,104,113	2.26	22 (29%)
28	CLA	n	611	35	64,68,73	1.43	6 (9%)	77,107,113	2.03	22 (28%)
33	PL9	A	412	-	13,13,55	1.49	1 (7%)	17,17,69	1.02	0
38	CHL	r	605	42	70,74,74	0.81	2 (2%)	80,114,114	1.31	12 (15%)
28	CLA	b	616	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
36	DGD	a	401	-	60,60,67	1.06	6 (10%)	74,74,81	0.92	2 (2%)
28	CLA	r	604	42,40	52,56,73	1.55	7 (13%)	62,92,113	2.12	17 (27%)
28	CLA	r	602	17	64,68,73	1.40	6 (9%)	77,107,113	1.98	20 (25%)
38	CHL	N	607	42	70,74,74	0.78	2 (2%)	80,114,114	1.26	13 (16%)
38	CHL	y	308	42	70,74,74	0.79	2 (2%)	80,114,114	1.30	14 (17%)
28	CLA	N	612	7	64,68,73	1.41	7 (10%)	77,107,113	1.97	19 (24%)
31	SQD	A	410	-	49,50,54	0.81	0	58,61,65	0.94	2 (3%)
28	CLA	G	614	7	52,56,73	1.55	6 (11%)	62,92,113	2.08	18 (29%)
28	CLA	b	603	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	d	401	42	69,73,73	1.36	6 (8%)	83,113,113	1.89	19 (22%)
38	CHL	n	601	7	58,62,74	0.86	2 (3%)	65,99,114	1.47	14 (21%)
28	CLA	s	602	18	65,69,73	1.39	7 (10%)	78,108,113	2.00	19 (24%)
28	CLA	G	604	40	54,58,73	1.53	7 (12%)	65,95,113	2.14	18 (27%)
37	HEM	E	101	5,6	50,50,50	1.56	8 (16%)	66,82,82	1.77	13 (19%)
41	XAT	y	317	-	39,47,47	0.67	0	54,74,74	1.87	12 (22%)
32	LMG	A	411	-	48,48,55	0.99	5 (10%)	56,56,63	1.16	4 (7%)
39	LUT	S	315	-	42,43,43	6.07	27 (64%)	51,60,60	1.87	13 (25%)
36	DGD	A	417	-	60,60,67	1.07	6 (10%)	74,74,81	1.03	5 (6%)
35	LHG	a	415	-	42,42,48	0.40	0	45,48,54	1.09	3 (6%)
35	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
38	CHL	G	607	42	60,64,74	0.83	1 (1%)	68,102,114	1.35	14 (20%)
38	CHL	r	606	42	60,64,74	0.87	2 (3%)	68,102,114	1.39	13 (19%)
35	LHG	R	616	28	24,24,48	0.51	0	27,30,54	1.21	2 (7%)
38	CHL	N	605	7	52,56,74	0.90	2 (3%)	58,92,114	1.42	13 (22%)
35	LHG	G	618	28	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
30	BCR	B	617	-	41,41,41	4.80	27 (65%)	56,56,56	2.20	19 (33%)
31	SQD	L	103	-	53,54,54	0.79	0	62,65,65	0.92	3 (4%)
28	CLA	C	505	3	69,73,73	1.36	7 (10%)	83,113,113	1.90	18 (21%)
28	CLA	G	602	7	69,73,73	1.36	6 (8%)	83,113,113	1.96	21 (25%)
28	CLA	R	610	35	53,57,73	1.53	6 (11%)	62,93,113	2.17	16 (25%)
28	CLA	Y	611	35	64,68,73	1.40	6 (9%)	77,107,113	2.00	18 (23%)
28	CLA	B	608	2	69,73,73	1.35	7 (10%)	83,113,113	1.89	18 (21%)
38	CHL	s	606	42	62,66,74	0.82	1 (1%)	70,104,114	1.40	14 (20%)
28	CLA	G	611	35	64,68,73	1.40	6 (9%)	77,107,113	1.96	17 (22%)
28	CLA	G	613	-	69,73,73	1.35	7 (10%)	83,113,113	1.99	18 (21%)
28	CLA	b	608	2	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
31	SQD	B	620	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
36	DGD	C	517	-	56,56,67	1.00	4 (7%)	70,70,81	1.00	3 (4%)
32	LMG	C	522	-	44,44,55	0.86	3 (6%)	52,52,63	1.10	2 (3%)
28	CLA	g	602	7	69,73,73	1.34	6 (8%)	83,113,113	1.94	20 (24%)
28	CLA	c	513	3	61,65,73	1.44	6 (9%)	73,103,113	2.05	19 (26%)
38	CHL	Y	608	42	70,74,74	0.79	2 (2%)	80,114,114	1.29	13 (16%)
39	LUT	g	616	-	42,43,43	6.04	28 (66%)	51,60,60	2.02	14 (27%)
28	CLA	y	304	22	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	a	406	1	69,73,73	1.35	6 (8%)	83,113,113	1.89	18 (21%)
28	CLA	Y	604	42,40	54,58,73	1.53	7 (12%)	65,95,113	2.14	17 (26%)
32	LMG	k	102	-	51,51,55	1.07	5 (9%)	59,59,63	1.08	3 (5%)
30	BCR	b	617	-	41,41,41	4.80	27 (65%)	56,56,56	2.25	19 (33%)
35	LHG	b	621	-	33,33,48	0.45	0	36,39,54	1.13	3 (8%)
38	CHL	Y	605	22	52,56,74	0.90	1 (1%)	58,92,114	1.42	13 (22%)
35	LHG	D	407	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
38	CHL	G	605	7	50,54,74	0.91	2 (4%)	56,90,114	1.46	13 (23%)
35	LHG	g	618	28	40,40,48	0.41	0	43,46,54	1.14	3 (6%)
38	CHL	g	607	42	61,65,74	0.84	1 (1%)	69,103,114	1.35	14 (20%)
39	LUT	s	615	-	42,43,43	6.04	27 (64%)	51,60,60	2.18	15 (29%)
31	SQD	L	101	-	41,42,54	0.88	0	50,53,65	0.98	2 (4%)
28	CLA	B	610	42	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
32	LMG	C	520	-	51,51,55	1.07	6 (11%)	59,59,63	1.11	3 (5%)
32	LMG	c	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.04	3 (5%)
40	NEX	N	617	28	38,46,46	3.37	11 (28%)	50,70,70	1.54	10 (20%)
28	CLA	r	603	17	64,68,73	1.41	7 (10%)	77,107,113	1.97	18 (23%)
28	CLA	b	610	42	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
38	CHL	r	607	42	65,69,74	0.80	2 (3%)	74,108,114	1.30	13 (17%)
32	LMG	D	408	-	46,46,55	0.93	4 (8%)	54,54,63	1.02	2 (3%)
28	CLA	B	615	2	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
31	SQD	a	411	-	49,50,54	0.81	0	58,61,65	0.96	2 (3%)
30	BCR	C	514	-	41,41,41	4.78	27 (65%)	56,56,56	3.63	27 (48%)
28	CLA	Y	603	22	59,63,73	1.45	7 (11%)	71,101,113	2.11	20 (28%)
28	CLA	c	501	3	69,73,73	1.36	6 (8%)	83,113,113	1.90	19 (22%)
28	CLA	G	603	7	57,61,73	1.49	7 (12%)	68,98,113	2.11	19 (27%)
35	LHG	b	624	-	45,45,48	0.40	0	48,51,54	1.12	4 (8%)
35	LHG	A	416	-	42,42,48	0.41	0	45,48,54	1.09	3 (6%)
38	CHL	G	608	42	70,74,74	0.80	2 (2%)	80,114,114	1.31	14 (17%)
28	CLA	r	613	17	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
30	BCR	b	619	-	41,41,41	4.72	26 (63%)	56,56,56	2.42	24 (42%)
28	CLA	B	614	2	69,73,73	1.35	7 (10%)	83,113,113	1.93	19 (22%)
28	CLA	C	507	42	69,73,73	1.36	6 (8%)	83,113,113	1.95	20 (24%)
28	CLA	s	612	18	59,63,73	1.45	6 (10%)	71,101,113	2.00	18 (25%)
40	NEX	G	617	28	38,46,46	3.50	11 (28%)	50,70,70	1.99	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	a	409	1	64,68,73	1.40	6 (9%)	77,107,113	2.03	18 (23%)
28	CLA	b	605	2	69,73,73	1.40	6 (8%)	83,113,113	2.01	18 (21%)
28	CLA	b	614	2	69,73,73	1.35	7 (10%)	83,113,113	1.96	18 (21%)
28	CLA	R	609	17	69,73,73	1.35	7 (10%)	83,113,113	1.92	18 (21%)
28	CLA	n	604	42,40	54,58,73	1.54	7 (12%)	65,95,113	2.18	18 (27%)
28	CLA	y	312	22	64,68,73	1.40	7 (10%)	77,107,113	2.00	17 (22%)
40	NEX	s	616	-	38,46,46	3.38	11 (28%)	50,70,70	1.58	9 (18%)
28	CLA	N	614	7	52,56,73	1.55	6 (11%)	62,92,113	2.09	18 (29%)
39	LUT	Y	615	-	42,43,43	5.92	29 (69%)	51,60,60	2.13	21 (41%)
28	CLA	s	611	-	53,57,73	1.54	7 (13%)	62,93,113	2.11	17 (27%)
39	LUT	G	615	-	42,43,43	6.09	27 (64%)	51,60,60	2.68	16 (31%)
35	LHG	N	618	28	30,30,48	0.48	0	33,36,54	1.38	4 (12%)
38	CHL	n	607	42	70,74,74	0.77	2 (2%)	80,114,114	1.20	14 (17%)
34	BCT	A	415	26	2,3,3	0.98	0	2,3,3	1.65	1 (50%)
28	CLA	C	504	42	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
35	LHG	S	317	28	42,42,48	0.41	0	45,48,54	1.09	3 (6%)
28	CLA	c	512	3	61,65,73	1.44	6 (9%)	73,103,113	2.08	19 (26%)
28	CLA	N	602	7	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
30	BCR	d	406	-	41,41,41	4.77	27 (65%)	56,56,56	2.52	20 (35%)
38	CHL	s	607	-	50,54,74	0.92	1 (2%)	56,90,114	1.48	11 (19%)
28	CLA	c	510	3	69,73,73	1.35	7 (10%)	83,113,113	1.95	17 (20%)
30	BCR	h	101	-	41,41,41	4.83	27 (65%)	56,56,56	2.25	19 (33%)
28	CLA	C	511	3	69,73,73	1.35	6 (8%)	83,113,113	1.99	21 (25%)
28	CLA	r	601	17	53,57,73	1.54	7 (13%)	62,93,113	2.13	17 (27%)
28	CLA	B	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.96	17 (20%)
38	CHL	n	609	7	70,74,74	0.78	1 (1%)	80,114,114	1.31	14 (17%)
28	CLA	y	303	22	69,73,73	1.36	6 (8%)	83,113,113	1.95	22 (26%)
28	CLA	b	606	2	69,73,73	1.35	7 (10%)	83,113,113	1.89	20 (24%)
40	NEX	y	301	-	38,46,46	3.46	11 (28%)	50,70,70	1.48	8 (16%)
28	CLA	b	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.92	18 (21%)
28	CLA	C	502	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
28	CLA	B	613	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	17 (20%)
38	CHL	S	308	-	50,54,74	0.92	2 (4%)	56,90,114	1.52	12 (21%)
28	CLA	R	613	17	69,73,73	1.34	6 (8%)	83,113,113	1.91	19 (22%)
38	CHL	g	601	7	70,74,74	0.76	2 (2%)	80,114,114	1.33	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	NEX	g	617	-	38,46,46	3.42	11 (28%)	50,70,70	1.57	8 (16%)
35	LHG	B	622	-	29,29,48	0.48	0	32,35,54	1.20	3 (9%)
28	CLA	D	403	4	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
35	LHG	y	319	28	48,48,48	0.48	1 (2%)	51,54,54	1.12	3 (5%)
35	LHG	b	622	-	40,40,48	0.41	0	43,46,54	1.11	3 (6%)
28	CLA	c	511	3	69,73,73	1.35	6 (8%)	83,113,113	1.95	20 (24%)
28	CLA	r	610	35	53,57,73	1.54	6 (11%)	62,93,113	2.16	17 (27%)
37	HEM	f	101	5,6	50,50,50	1.56	8 (16%)	66,82,82	1.71	12 (18%)
28	CLA	a	407	42	54,58,73	1.52	6 (11%)	65,95,113	2.13	18 (27%)
36	DGD	c	516	-	56,56,67	0.99	4 (7%)	70,70,81	0.97	3 (4%)
28	CLA	y	305	42	54,58,73	1.53	7 (12%)	65,95,113	2.13	17 (26%)
28	CLA	B	607	42	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
30	BCR	B	619	-	41,41,41	4.80	27 (65%)	56,56,56	2.43	19 (33%)
35	LHG	S	301	-	33,33,48	0.46	0	36,39,54	1.13	3 (8%)
38	CHL	N	601	7	56,60,74	0.86	2 (3%)	63,97,114	1.49	14 (22%)
28	CLA	b	607	42	69,73,73	1.36	7 (10%)	83,113,113	1.94	20 (24%)
38	CHL	y	306	22	52,56,74	0.89	2 (3%)	58,92,114	1.39	12 (20%)
30	BCR	D	405	-	41,41,41	4.76	27 (65%)	56,56,56	2.51	20 (35%)
38	CHL	Y	607	42	70,74,74	0.80	3 (4%)	80,114,114	1.22	12 (15%)
28	CLA	Y	612	22	64,68,73	1.40	7 (10%)	77,107,113	1.98	18 (23%)
38	CHL	S	306	42	50,54,74	0.94	1 (2%)	56,90,114	1.47	12 (21%)
28	CLA	N	613	7	57,61,73	1.49	7 (12%)	68,98,113	2.07	18 (26%)
25	OEX	A	401	42,1,3	0,14,14	-	-	-		
38	CHL	g	606	42	54,58,74	0.95	1 (1%)	59,94,114	1.40	9 (15%)
38	CHL	y	307	42	54,58,74	0.90	1 (1%)	59,94,114	1.43	11 (18%)
28	CLA	S	303	18	65,69,73	1.39	7 (10%)	78,108,113	2.00	18 (23%)
28	CLA	G	612	-	64,68,73	1.40	6 (9%)	77,107,113	2.04	19 (24%)
38	CHL	R	605	42	51,55,74	0.94	1 (1%)	57,91,114	1.43	11 (19%)
28	CLA	c	504	42	63,67,73	1.42	6 (9%)	75,105,113	1.96	20 (26%)
39	LUT	g	615	-	42,43,43	6.08	28 (66%)	51,60,60	1.94	12 (23%)
32	LMG	b	620	-	51,51,55	1.07	6 (11%)	59,59,63	1.04	3 (5%)
25	OEX	a	402	42,1,3	0,14,14	-	-	-		
28	CLA	C	512	3	61,65,73	1.43	6 (9%)	73,103,113	2.02	20 (27%)
28	CLA	N	604	42,40	54,58,73	1.52	5 (9%)	65,95,113	2.18	18 (27%)
30	BCR	c	515	-	41,41,41	4.81	27 (65%)	56,56,56	2.26	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PHO	A	407	-	58,69,69	0.79	2 (3%)	56,99,99	0.95	3 (5%)
38	CHL	S	302	18	50,54,74	0.95	2 (4%)	56,90,114	1.46	12 (21%)
28	CLA	g	614	7	49,53,73	1.60	7 (14%)	59,89,113	2.12	16 (27%)
35	LHG	C	521	-	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
28	CLA	A	405	1	69,73,73	1.35	6 (8%)	83,113,113	1.88	18 (21%)
39	LUT	N	615	-	42,43,43	6.06	28 (66%)	51,60,60	1.92	15 (29%)
39	LUT	y	315	-	42,43,43	6.09	28 (66%)	51,60,60	1.79	15 (29%)
36	DGD	C	518	-	63,63,67	1.12	7 (11%)	77,77,81	0.91	3 (3%)
38	CHL	y	309	22	70,74,74	0.80	2 (2%)	80,114,114	1.33	13 (16%)
39	LUT	G	616	-	42,43,43	6.01	27 (64%)	51,60,60	2.15	13 (25%)
28	CLA	r	608	17	62,66,73	1.42	6 (9%)	74,104,113	2.05	17 (22%)
41	XAT	R	615	-	39,47,47	0.65	0	54,74,74	1.89	15 (27%)
28	CLA	Y	610	22	64,68,73	1.44	6 (9%)	77,107,113	1.97	20 (25%)
39	LUT	r	614	-	42,43,43	6.08	28 (66%)	51,60,60	3.37	21 (41%)
30	BCR	t	101	-	41,41,41	4.78	27 (65%)	56,56,56	2.56	23 (41%)
28	CLA	B	604	2	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
35	LHG	r	617	28	29,29,48	0.48	0	32,35,54	1.35	4 (12%)
28	CLA	n	612	7	64,68,73	1.42	6 (9%)	77,107,113	1.99	18 (23%)
30	BCR	C	515	-	41,41,41	4.81	27 (65%)	56,56,56	2.30	20 (35%)
30	BCR	i	101	-	41,41,41	4.81	27 (65%)	56,56,56	2.43	22 (39%)
32	LMG	a	413	-	40,40,55	0.91	3 (7%)	48,48,63	1.09	4 (8%)
31	SQD	A	414	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
29	PHO	d	402	-	58,69,69	0.78	2 (3%)	56,99,99	0.97	3 (5%)
28	CLA	g	613	7	56,60,73	1.49	5 (8%)	67,97,113	2.20	19 (28%)
38	CHL	G	609	7	59,63,74	0.86	2 (3%)	66,100,114	1.47	13 (19%)
38	CHL	g	619	42	70,74,74	0.79	2 (2%)	80,114,114	1.28	14 (17%)
33	PL9	d	407	-	55,55,55	0.69	1 (1%)	68,69,69	0.61	1 (1%)
36	DGD	C	519	-	61,61,67	1.08	6 (9%)	75,75,81	0.93	3 (4%)
40	NEX	Y	618	28	38,46,46	3.33	11 (28%)	50,70,70	1.53	9 (18%)
35	LHG	B	625	-	45,45,48	0.41	0	48,51,54	1.01	3 (6%)
38	CHL	R	606	42	50,54,74	0.93	1 (2%)	56,90,114	1.49	11 (19%)
28	CLA	A	406	42	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
28	CLA	s	608	-	49,53,73	1.60	6 (12%)	59,89,113	2.07	16 (27%)
38	CHL	n	608	42	70,74,74	0.78	2 (2%)	80,114,114	1.33	14 (17%)
39	LUT	R	614	-	42,43,43	6.05	28 (66%)	51,60,60	2.26	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	C	503	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
35	LHG	s	617	28	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
28	CLA	n	610	7	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
28	CLA	s	613	18	53,57,73	1.54	6 (11%)	62,93,113	2.15	18 (29%)
32	LMG	b	623	-	50,50,55	1.03	5 (10%)	58,58,63	0.96	2 (3%)
28	CLA	N	610	7	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
28	CLA	S	312	18	53,57,73	1.54	7 (13%)	62,93,113	2.14	16 (25%)
28	CLA	Y	614	22	52,56,73	1.55	5 (9%)	62,92,113	2.10	17 (27%)
35	LHG	L	102	-	48,48,48	0.38	0	51,54,54	0.98	2 (3%)
38	CHL	Y	606	42	54,58,74	0.91	1 (1%)	59,94,114	1.43	12 (20%)
28	CLA	R	603	17	64,68,73	1.44	6 (9%)	77,107,113	1.98	19 (24%)
35	LHG	n	618	28	31,31,48	0.50	0	34,37,54	1.18	2 (5%)
39	LUT	S	316	-	42,43,43	6.11	28 (66%)	51,60,60	2.07	13 (25%)
38	CHL	N	608	42	70,74,74	0.79	2 (2%)	80,114,114	1.31	14 (17%)
28	CLA	R	612	17	59,63,73	1.47	7 (11%)	71,101,113	2.09	19 (26%)
28	CLA	S	310	18	59,63,73	1.47	7 (11%)	71,101,113	2.09	21 (29%)
38	CHL	g	609	-	65,69,74	0.82	2 (3%)	74,108,114	1.41	14 (18%)
28	CLA	r	611	17	53,57,73	1.61	5 (9%)	62,93,113	2.27	18 (29%)
28	CLA	N	611	35	64,68,73	1.40	7 (10%)	77,107,113	1.95	18 (23%)
28	CLA	y	314	22	52,56,73	1.55	7 (13%)	62,92,113	2.08	17 (27%)
38	CHL	g	605	7	50,54,74	0.91	2 (4%)	56,90,114	1.44	12 (21%)
28	CLA	d	404	4	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
28	CLA	R	611	17	53,57,73	1.54	6 (11%)	62,93,113	2.19	18 (29%)
28	CLA	R	601	17	49,53,73	1.61	6 (12%)	59,89,113	2.12	15 (25%)
28	CLA	S	304	18	49,53,73	1.59	6 (12%)	59,89,113	2.11	17 (28%)
28	CLA	C	501	3	69,73,73	1.36	6 (8%)	83,113,113	1.89	19 (22%)
39	LUT	y	316	-	42,43,43	6.09	28 (66%)	51,60,60	1.94	14 (27%)
28	CLA	b	615	2	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
28	CLA	B	603	2	69,73,73	1.35	6 (8%)	83,113,113	1.89	18 (21%)
29	PHO	D	402	-	58,69,69	0.78	3 (5%)	56,99,99	0.96	3 (5%)
29	PHO	a	408	-	58,69,69	0.79	2 (3%)	56,99,99	0.96	3 (5%)
28	CLA	B	612	2	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)
28	CLA	B	616	2	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
38	CHL	s	605	42	50,54,74	0.93	1 (2%)	56,90,114	1.49	12 (21%)
35	LHG	c	519	-	30,30,48	0.47	0	32,35,54	1.26	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	Y	613	22	69,73,73	1.35	7 (10%)	83,113,113	1.89	19 (22%)
34	BCT	d	403	26	2,3,3	0.98	0	2,3,3	1.67	1 (50%)
28	CLA	g	603	7	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
38	CHL	s	601	18	50,54,74	0.93	2 (4%)	56,90,114	1.44	12 (21%)
28	CLA	S	314	18	53,57,73	1.54	7 (13%)	62,93,113	2.15	17 (27%)
30	BCR	C	516	-	41,41,41	4.80	27 (65%)	56,56,56	2.44	19 (33%)
28	CLA	B	611	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
32	LMG	w	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.17	3 (5%)
35	LHG	w	102	-	38,38,48	0.43	0	41,44,54	1.04	3 (7%)
35	LHG	W	101	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
28	CLA	b	611	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	20 (24%)
30	BCR	c	514	-	41,41,41	4.77	27 (65%)	56,56,56	2.54	21 (37%)
28	CLA	c	503	3	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
41	XAT	Y	617	-	39,47,47	0.66	0	54,74,74	1.99	13 (24%)
41	XAT	r	615	-	39,47,47	0.64	0	54,74,74	1.90	15 (27%)
28	CLA	S	309	18	49,53,73	1.60	5 (10%)	59,89,113	2.11	16 (27%)
33	PL9	D	406	-	55,55,55	0.69	1 (1%)	68,69,69	0.60	1 (1%)
28	CLA	c	508	3	69,73,73	1.37	6 (8%)	83,113,113	1.94	19 (22%)
28	CLA	N	603	7	59,63,73	1.45	7 (11%)	71,101,113	2.07	17 (23%)
28	CLA	S	313	18	59,63,73	1.46	6 (10%)	71,101,113	2.01	18 (25%)
28	CLA	n	603	7	69,73,73	1.35	7 (10%)	83,113,113	2.01	19 (22%)
28	CLA	c	509	3	69,73,73	1.38	6 (8%)	83,113,113	1.99	18 (21%)
38	CHL	G	606	42	54,58,74	0.93	2 (3%)	59,94,114	1.42	10 (16%)
28	CLA	B	605	2	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
28	CLA	b	612	2	69,73,73	1.34	6 (8%)	83,113,113	1.98	18 (21%)
28	CLA	R	604	42	52,56,73	1.60	9 (17%)	62,92,113	2.16	18 (29%)
28	CLA	R	602	17	64,68,73	1.45	6 (9%)	77,107,113	1.98	20 (25%)
28	CLA	b	609	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	17 (20%)
31	SQD	M	101	-	41,42,54	0.86	0	50,53,65	0.97	2 (4%)
28	CLA	B	601	42	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
30	BCR	T	101	-	41,41,41	4.76	26 (63%)	56,56,56	2.58	20 (35%)
39	LUT	Y	616	-	42,43,43	6.09	28 (66%)	51,60,60	1.82	12 (23%)
40	NEX	n	617	28	38,46,46	3.44	11 (28%)	50,70,70	1.74	9 (18%)
28	CLA	D	404	4	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
28	CLA	y	313	22	69,73,73	1.35	7 (10%)	83,113,113	1.95	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	b	613	2	69,73,73	1.36	6 (8%)	83,113,113	1.90	18 (21%)
28	CLA	n	613	7	59,63,73	1.48	6 (10%)	71,101,113	2.14	17 (23%)
28	CLA	r	609	17	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
38	CHL	Y	601	22	70,74,74	0.79	2 (2%)	80,114,114	1.34	13 (16%)
28	CLA	y	310	22	64,68,73	1.40	6 (9%)	77,107,113	2.01	20 (25%)
28	CLA	y	311	35	64,68,73	1.40	6 (9%)	77,107,113	1.98	18 (23%)
28	CLA	S	305	42	54,58,73	1.56	6 (11%)	65,95,113	2.17	21 (32%)
39	LUT	n	615	-	42,43,43	6.08	28 (66%)	51,60,60	2.00	17 (33%)
28	CLA	c	505	3	61,65,73	1.44	7 (11%)	73,103,113	2.00	18 (24%)
28	CLA	b	604	2	69,73,73	1.36	7 (10%)	83,113,113	2.00	19 (22%)
38	CHL	G	601	7	70,74,74	0.76	2 (2%)	80,114,114	1.28	15 (18%)
32	LMG	d	409	-	46,46,55	0.92	3 (6%)	54,54,63	1.03	3 (5%)
31	SQD	a	414	-	53,54,54	0.78	0	62,65,65	0.91	2 (3%)
28	CLA	B	609	2	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
35	LHG	c	520	-	39,39,48	0.42	0	42,45,54	1.19	3 (7%)
30	BCR	b	618	-	41,41,41	4.81	27 (65%)	56,56,56	2.22	19 (33%)
28	CLA	b	601	42	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
28	CLA	g	604	42	54,58,73	1.58	7 (12%)	65,95,113	2.20	18 (27%)
28	CLA	g	612	7	49,53,73	1.60	7 (14%)	59,89,113	2.08	17 (28%)
38	CHL	Y	609	22	70,74,74	0.80	2 (2%)	80,114,114	1.35	14 (17%)
28	CLA	c	502	3	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
36	DGD	c	518	-	60,60,67	4.56	7 (11%)	74,74,81	1.17	4 (5%)
32	LMG	B	621	-	51,51,55	1.07	6 (11%)	59,59,63	1.23	4 (6%)
28	CLA	g	611	35	64,68,73	1.43	6 (9%)	77,107,113	2.00	17 (22%)
32	LMG	B	624	-	31,31,55	0.53	0	39,39,63	1.29	3 (7%)
39	LUT	N	616	-	42,43,43	6.01	29 (69%)	51,60,60	2.12	17 (33%)
38	CHL	n	606	42	54,58,74	0.90	2 (3%)	59,94,114	1.43	13 (22%)
28	CLA	c	506	3	60,64,73	1.45	7 (11%)	72,102,113	2.03	19 (26%)
28	CLA	C	506	3	69,73,73	1.36	6 (8%)	83,113,113	1.93	18 (21%)
39	LUT	s	614	-	42,43,43	6.07	27 (64%)	51,60,60	2.08	15 (29%)
38	CHL	y	302	22	70,74,74	0.78	2 (2%)	80,114,114	1.30	14 (17%)
28	CLA	A	408	1	64,68,73	1.40	6 (9%)	77,107,113	1.97	16 (20%)
38	CHL	N	606	42	54,58,74	0.92	2 (3%)	59,94,114	1.46	11 (18%)
30	BCR	H	101	-	41,41,41	4.80	27 (65%)	56,56,56	2.42	21 (37%)
40	NEX	y	318	-	38,46,46	3.29	11 (28%)	50,70,70	1.73	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	c	507	42	69,73,73	1.35	6 (8%)	83,113,113	1.98	18 (21%)
28	CLA	C	508	3	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
38	CHL	n	605	7	52,56,74	0.89	2 (3%)	58,92,114	1.42	13 (22%)
28	CLA	n	602	7	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
28	CLA	D	401	42	69,73,73	1.35	6 (8%)	83,113,113	1.89	20 (24%)
28	CLA	C	509	3	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
28	CLA	s	609	18	59,63,73	1.47	6 (10%)	71,101,113	2.04	18 (25%)
30	BCR	B	618	-	41,41,41	4.81	27 (65%)	56,56,56	2.25	21 (37%)
40	NEX	r	616	28	38,46,46	3.35	11 (28%)	50,70,70	1.58	9 (18%)
28	CLA	C	510	3	69,73,73	1.34	6 (8%)	83,113,113	1.91	18 (21%)
28	CLA	s	610	35	60,64,73	1.45	6 (10%)	72,102,113	2.03	18 (25%)
39	LUT	n	616	-	42,43,43	5.99	28 (66%)	51,60,60	2.12	17 (33%)
36	DGD	b	625	-	63,63,67	1.12	6 (9%)	77,77,81	0.96	2 (2%)
36	DGD	c	517	-	55,55,67	1.00	3 (5%)	69,69,81	1.00	4 (5%)
28	CLA	n	614	7	49,53,73	1.60	6 (12%)	59,89,113	2.05	16 (27%)
28	CLA	R	608	17	62,66,73	1.42	5 (8%)	74,104,113	2.04	18 (24%)
35	LHG	B	623	-	40,40,48	0.42	0	43,46,54	1.09	3 (6%)
38	CHL	S	307	42	62,66,74	0.82	2 (3%)	70,104,114	1.35	14 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	r	612	17	-	19/33/109/115	-
30	BCR	K	101	-	-	14/29/63/63	0/2/2/2
38	CHL	R	607	42	-	11/35/111/117	-
32	LMG	A	413	-	-	7/35/55/70	0/1/1/1
38	CHL	N	609	7	-	14/35/111/117	-
36	DGD	B	626	-	-	9/51/91/95	0/2/2/2
35	LHG	l	101	-	-	25/53/53/53	-
30	BCR	a	410	-	-	15/29/63/63	0/2/2/2
30	BCR	A	409	-	-	14/29/63/63	0/2/2/2
28	CLA	Y	602	22	-	12/39/115/115	-
28	CLA	s	603	18	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	G	610	7	-	13/38/114/115	-
33	PL9	a	412	-	-	0/5/18/73	0/1/1/1
38	CHL	g	608	42	-	14/41/117/117	-
30	BCR	k	101	-	-	13/29/63/63	0/2/2/2
35	LHG	Y	619	28	-	33/53/53/53	-
28	CLA	d	405	4	-	16/39/115/115	-
28	CLA	C	513	3	-	11/39/115/115	-
28	CLA	s	604	42	-	8/21/97/115	-
28	CLA	B	606	2	-	13/39/115/115	-
28	CLA	S	311	35	-	15/29/105/115	-
28	CLA	g	610	7	-	11/31/107/115	-
28	CLA	n	611	35	-	16/33/109/115	-
33	PL9	A	412	-	-	0/5/18/73	0/1/1/1
38	CHL	r	605	42	-	7/41/117/117	-
28	CLA	b	616	2	-	17/39/115/115	-
36	DGD	a	401	-	-	10/48/88/95	0/2/2/2
28	CLA	r	604	42,40	-	10/19/95/115	-
28	CLA	r	602	17	-	12/33/109/115	-
38	CHL	N	607	42	-	10/41/117/117	-
38	CHL	y	308	42	-	14/41/117/117	-
28	CLA	N	612	7	-	13/33/109/115	-
31	SQD	A	410	-	-	9/45/65/69	0/1/1/1
28	CLA	G	614	7	-	7/19/95/115	-
28	CLA	b	603	-	-	14/39/115/115	-
28	CLA	d	401	42	-	15/39/115/115	-
38	CHL	n	601	7	-	4/27/103/117	-
28	CLA	s	602	18	-	15/35/111/115	-
28	CLA	G	604	40	-	11/21/97/115	-
37	HEM	E	101	5,6	-	7/14/54/54	-
41	XAT	y	317	-	-	2/31/93/93	0/4/4/4
32	LMG	A	411	-	-	6/43/63/70	0/1/1/1
39	LUT	S	315	-	-	7/29/67/67	0/2/2/2
36	DGD	A	417	-	-	14/48/88/95	0/2/2/2
35	LHG	a	415	-	-	30/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	d	408	-	-	30/53/53/53	-
38	CHL	G	607	42	-	8/29/105/117	-
38	CHL	r	606	42	-	7/29/105/117	-
35	LHG	R	616	28	-	18/29/29/53	-
38	CHL	N	605	7	-	6/20/96/117	-
35	LHG	G	618	28	-	31/53/53/53	-
30	BCR	B	617	-	-	14/29/63/63	0/2/2/2
31	SQD	L	103	-	-	8/49/69/69	0/1/1/1
28	CLA	C	505	3	-	11/39/115/115	-
28	CLA	G	602	7	-	16/39/115/115	-
28	CLA	R	610	35	-	12/20/96/115	-
28	CLA	Y	611	35	-	12/33/109/115	-
28	CLA	B	608	2	-	13/39/115/115	-
38	CHL	s	606	42	-	6/32/108/117	-
28	CLA	G	611	35	-	15/33/109/115	-
28	CLA	G	613	-	-	20/39/115/115	-
28	CLA	b	608	2	-	9/39/115/115	-
31	SQD	B	620	-	-	8/49/69/69	0/1/1/1
36	DGD	C	517	-	-	4/44/84/95	0/2/2/2
32	LMG	C	522	-	-	14/39/59/70	0/1/1/1
28	CLA	g	602	7	-	18/39/115/115	-
28	CLA	c	513	3	-	8/30/106/115	-
38	CHL	Y	608	42	-	12/41/117/117	-
39	LUT	g	616	-	-	7/29/67/67	0/2/2/2
28	CLA	y	304	22	-	11/39/115/115	-
28	CLA	a	406	1	-	13/39/115/115	-
28	CLA	Y	604	42,40	-	8/21/97/115	-
32	LMG	k	102	-	-	9/46/66/70	0/1/1/1
30	BCR	b	617	-	-	14/29/63/63	0/2/2/2
35	LHG	b	621	-	-	23/38/38/53	-
38	CHL	Y	605	22	-	2/20/96/117	-
35	LHG	D	407	-	-	37/53/53/53	-
38	CHL	G	605	7	-	8/17/93/117	-
35	LHG	g	618	28	-	29/45/45/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	g	607	42	-	10/31/107/117	-
39	LUT	s	615	-	-	6/29/67/67	0/2/2/2
31	SQD	L	101	-	-	5/37/57/69	0/1/1/1
28	CLA	B	610	42	-	18/39/115/115	-
32	LMG	C	520	-	-	13/46/66/70	0/1/1/1
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1
40	NEX	N	617	28	-	5/27/83/83	0/3/3/3
28	CLA	r	603	17	-	18/33/109/115	-
28	CLA	b	610	42	-	4/39/115/115	-
38	CHL	r	607	42	-	14/35/111/117	-
32	LMG	D	408	-	-	8/41/61/70	0/1/1/1
28	CLA	B	615	2	-	17/39/115/115	-
31	SQD	a	411	-	-	12/45/65/69	0/1/1/1
30	BCR	C	514	-	-	14/29/63/63	0/2/2/2
28	CLA	Y	603	22	-	12/27/103/115	-
28	CLA	c	501	3	-	12/39/115/115	-
28	CLA	G	603	7	-	10/25/101/115	-
35	LHG	b	624	-	-	31/50/50/53	-
35	LHG	A	416	-	-	31/47/47/53	-
38	CHL	G	608	42	-	7/41/117/117	-
28	CLA	r	613	17	-	14/39/115/115	-
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
28	CLA	B	614	2	-	16/39/115/115	-
28	CLA	C	507	42	-	15/39/115/115	-
28	CLA	s	612	18	-	10/27/103/115	-
40	NEX	G	617	28	-	8/27/83/83	0/3/3/3
28	CLA	a	409	1	-	13/33/109/115	-
28	CLA	b	605	2	-	10/39/115/115	-
28	CLA	b	614	2	-	13/39/115/115	-
28	CLA	R	609	17	-	12/39/115/115	-
28	CLA	n	604	42,40	-	11/21/97/115	-
28	CLA	y	312	22	-	14/33/109/115	-
40	NEX	s	616	-	-	8/27/83/83	0/3/3/3
28	CLA	N	614	7	-	10/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	Y	615	-	-	3/29/67/67	0/2/2/2
28	CLA	s	611	-	-	7/20/96/115	-
39	LUT	G	615	-	-	10/29/67/67	0/2/2/2
35	LHG	N	618	28	-	23/35/35/53	-
38	CHL	n	607	42	-	11/41/117/117	-
28	CLA	C	504	42	-	16/39/115/115	-
35	LHG	S	317	28	-	29/47/47/53	-
28	CLA	c	512	3	-	19/30/106/115	-
28	CLA	N	602	7	-	16/39/115/115	-
30	BCR	d	406	-	-	10/29/63/63	0/2/2/2
38	CHL	s	607	-	-	4/17/93/117	-
28	CLA	c	510	3	-	16/39/115/115	-
30	BCR	h	101	-	-	13/29/63/63	0/2/2/2
28	CLA	C	511	3	-	15/39/115/115	-
28	CLA	r	601	17	-	8/20/96/115	-
28	CLA	B	602	2	-	16/39/115/115	-
38	CHL	n	609	7	-	10/41/117/117	-
28	CLA	y	303	22	-	13/39/115/115	-
28	CLA	b	606	2	-	15/39/115/115	-
40	NEX	y	301	-	-	13/27/83/83	0/3/3/3
28	CLA	b	602	2	-	20/39/115/115	-
28	CLA	C	502	-	-	18/39/115/115	-
28	CLA	B	613	2	-	13/39/115/115	-
38	CHL	S	308	-	-	5/17/93/117	-
28	CLA	R	613	17	-	13/39/115/115	-
38	CHL	g	601	7	-	10/41/117/117	-
40	NEX	g	617	-	-	18/27/83/83	0/3/3/3
35	LHG	B	622	-	-	28/34/34/53	-
28	CLA	D	403	4	-	13/39/115/115	-
35	LHG	y	319	28	-	34/53/53/53	-
35	LHG	b	622	-	-	28/45/45/53	-
28	CLA	c	511	3	-	16/39/115/115	-
28	CLA	r	610	35	-	13/20/96/115	-
37	HEM	f	101	5,6	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	a	407	42	-	5/21/97/115	-
36	DGD	c	516	-	-	6/44/84/95	0/2/2/2
28	CLA	y	305	42	-	10/21/97/115	-
28	CLA	B	607	42	-	20/39/115/115	-
30	BCR	B	619	-	-	14/29/63/63	0/2/2/2
35	LHG	S	301	-	-	27/38/38/53	-
38	CHL	N	601	7	-	4/25/101/117	-
28	CLA	b	607	42	-	20/39/115/115	-
38	CHL	y	306	22	-	2/20/96/117	-
30	BCR	D	405	-	-	15/29/63/63	0/2/2/2
38	CHL	Y	607	42	-	17/41/117/117	-
28	CLA	Y	612	22	-	11/33/109/115	-
38	CHL	S	306	42	-	3/17/93/117	-
28	CLA	N	613	7	-	8/25/101/115	-
38	CHL	g	606	42	-	7/22/98/117	-
38	CHL	y	307	42	-	3/22/98/117	-
28	CLA	S	303	18	-	16/35/111/115	-
28	CLA	G	612	-	-	12/33/109/115	-
38	CHL	R	605	42	-	2/19/95/117	-
28	CLA	c	504	42	-	15/29/105/115	-
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
32	LMG	b	620	-	-	12/46/66/70	0/1/1/1
28	CLA	C	512	3	-	19/30/106/115	-
28	CLA	N	604	42,40	-	9/21/97/115	-
30	BCR	c	515	-	-	13/29/63/63	0/2/2/2
29	PHO	A	407	-	-	6/37/103/103	0/5/6/6
38	CHL	S	302	18	-	2/17/93/117	-
28	CLA	g	614	7	-	6/15/91/115	-
35	LHG	C	521	-	-	35/53/53/53	-
28	CLA	A	405	1	-	13/39/115/115	-
39	LUT	N	615	-	-	5/29/67/67	0/2/2/2
39	LUT	y	315	-	-	5/29/67/67	0/2/2/2
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
38	CHL	y	309	22	-	7/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	G	616	-	-	5/29/67/67	0/2/2/2
28	CLA	r	608	17	-	14/31/107/115	-
41	XAT	R	615	-	-	7/31/93/93	0/4/4/4
28	CLA	Y	610	22	-	13/33/109/115	-
39	LUT	r	614	-	-	8/29/67/67	0/2/2/2
30	BCR	t	101	-	-	15/29/63/63	0/2/2/2
28	CLA	B	604	2	-	17/39/115/115	-
35	LHG	r	617	28	-	23/34/34/53	-
28	CLA	n	612	7	-	12/33/109/115	-
30	BCR	C	515	-	-	14/29/63/63	0/2/2/2
30	BCR	i	101	-	-	14/29/63/63	0/2/2/2
32	LMG	a	413	-	-	5/35/55/70	0/1/1/1
31	SQD	A	414	-	-	12/49/69/69	0/1/1/1
29	PHO	d	402	-	-	2/37/103/103	0/5/6/6
28	CLA	g	613	7	-	10/24/100/115	-
38	CHL	G	609	7	-	5/28/104/117	-
38	CHL	g	619	42	-	16/41/117/117	-
33	PL9	d	407	-	-	7/53/73/73	0/1/1/1
36	DGD	C	519	-	-	11/49/89/95	0/2/2/2
40	NEX	Y	618	28	-	4/27/83/83	0/3/3/3
35	LHG	B	625	-	-	33/50/50/53	-
38	CHL	R	606	42	-	4/17/93/117	-
28	CLA	A	406	42	-	11/21/97/115	-
28	CLA	s	608	-	-	6/15/91/115	-
38	CHL	n	608	42	-	15/41/117/117	-
39	LUT	R	614	-	-	5/29/67/67	0/2/2/2
28	CLA	C	503	-	-	18/39/115/115	-
35	LHG	s	617	28	-	35/53/53/53	-
28	CLA	n	610	7	-	22/39/115/115	-
28	CLA	s	613	18	-	8/20/96/115	-
32	LMG	b	623	-	-	13/45/65/70	0/1/1/1
28	CLA	N	610	7	-	20/39/115/115	-
28	CLA	S	312	18	-	9/20/96/115	-
28	CLA	Y	614	22	-	8/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	L	102	-	-	30/53/53/53	-
38	CHL	Y	606	42	-	2/22/98/117	-
28	CLA	R	603	17	-	14/33/109/115	-
35	LHG	n	618	28	-	22/36/36/53	-
39	LUT	S	316	-	-	6/29/67/67	0/2/2/2
38	CHL	N	608	42	-	11/41/117/117	-
28	CLA	R	612	17	-	10/27/103/115	-
28	CLA	S	310	18	-	12/27/103/115	-
38	CHL	g	609	-	-	15/35/111/117	-
28	CLA	r	611	17	-	9/20/96/115	-
28	CLA	N	611	35	-	17/33/109/115	-
28	CLA	y	314	22	-	9/19/95/115	-
38	CHL	g	605	7	-	6/17/93/117	-
28	CLA	d	404	4	-	12/39/115/115	-
28	CLA	R	611	17	-	8/20/96/115	-
28	CLA	R	601	17	-	8/15/91/115	-
28	CLA	S	304	18	-	8/15/91/115	-
28	CLA	C	501	3	-	10/39/115/115	-
39	LUT	y	316	-	-	7/29/67/67	0/2/2/2
28	CLA	b	615	2	-	11/39/115/115	-
28	CLA	B	603	2	-	13/39/115/115	-
29	PHO	D	402	-	-	4/37/103/103	0/5/6/6
29	PHO	a	408	-	-	5/37/103/103	0/5/6/6
28	CLA	B	612	2	-	15/39/115/115	-
28	CLA	B	616	2	-	14/39/115/115	-
38	CHL	s	605	42	-	7/17/93/117	-
35	LHG	c	519	-	-	24/34/34/53	-
28	CLA	Y	613	22	-	11/39/115/115	-
28	CLA	g	603	7	-	11/39/115/115	-
38	CHL	s	601	18	-	5/17/93/117	-
28	CLA	S	314	18	-	4/20/96/115	-
30	BCR	C	516	-	-	16/29/63/63	0/2/2/2
28	CLA	B	611	2	-	16/39/115/115	-
32	LMG	w	101	-	-	7/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	w	102	-	-	28/43/43/53	-
35	LHG	W	101	-	-	35/53/53/53	-
28	CLA	b	611	2	-	17/39/115/115	-
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
28	CLA	c	503	3	-	18/39/115/115	-
41	XAT	Y	617	-	-	4/31/93/93	0/4/4/4
41	XAT	r	615	-	-	7/31/93/93	0/4/4/4
28	CLA	S	309	18	-	8/15/91/115	-
33	PL9	D	406	-	-	8/53/73/73	0/1/1/1
28	CLA	c	508	3	-	16/39/115/115	-
28	CLA	N	603	7	-	11/27/103/115	-
28	CLA	S	313	18	-	9/27/103/115	-
28	CLA	n	603	7	-	18/39/115/115	-
28	CLA	c	509	3	-	11/39/115/115	-
38	CHL	G	606	42	-	5/22/98/117	-
28	CLA	B	605	2	-	17/39/115/115	-
28	CLA	b	612	2	-	20/39/115/115	-
28	CLA	R	604	42	-	8/19/95/115	-
28	CLA	R	602	17	-	11/33/109/115	-
28	CLA	b	609	-	-	14/39/115/115	-
31	SQD	M	101	-	-	12/37/57/69	0/1/1/1
28	CLA	B	601	42	-	12/39/115/115	-
30	BCR	T	101	-	-	9/29/63/63	0/2/2/2
39	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
40	NEX	n	617	28	-	12/27/83/83	0/3/3/3
28	CLA	D	404	4	-	12/39/115/115	-
28	CLA	y	313	22	-	11/39/115/115	-
28	CLA	b	613	2	-	9/39/115/115	-
28	CLA	n	613	7	-	5/27/103/115	-
28	CLA	r	609	17	-	15/39/115/115	-
38	CHL	Y	601	22	-	11/41/117/117	-
28	CLA	y	310	22	-	14/33/109/115	-
28	CLA	y	311	35	-	12/33/109/115	-
28	CLA	S	305	42	-	11/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	n	615	-	-	7/29/67/67	0/2/2/2
28	CLA	c	505	3	-	14/30/106/115	-
28	CLA	b	604	2	-	14/39/115/115	-
38	CHL	G	601	7	-	11/41/117/117	-
32	LMG	d	409	-	-	4/41/61/70	0/1/1/1
31	SQD	a	414	-	-	10/49/69/69	0/1/1/1
28	CLA	B	609	2	-	17/39/115/115	-
35	LHG	c	520	-	-	27/44/44/53	-
30	BCR	b	618	-	-	15/29/63/63	0/2/2/2
28	CLA	b	601	42	-	14/39/115/115	-
28	CLA	g	604	42	-	6/21/97/115	-
28	CLA	g	612	7	-	6/15/91/115	-
38	CHL	Y	609	22	-	7/41/117/117	-
28	CLA	c	502	3	-	18/39/115/115	-
36	DGD	c	518	-	-	13/48/88/95	0/2/2/2
32	LMG	B	621	-	-	10/46/66/70	0/1/1/1
28	CLA	g	611	35	-	16/33/109/115	-
32	LMG	B	624	-	-	14/26/46/70	0/1/1/1
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
38	CHL	n	606	42	-	6/22/98/117	-
28	CLA	c	506	3	-	11/29/105/115	-
28	CLA	C	506	3	-	16/39/115/115	-
39	LUT	s	614	-	-	9/29/67/67	0/2/2/2
38	CHL	y	302	22	-	17/41/117/117	-
28	CLA	A	408	1	-	18/33/109/115	-
38	CHL	N	606	42	-	2/22/98/117	-
30	BCR	H	101	-	-	13/29/63/63	0/2/2/2
40	NEX	y	318	-	-	8/27/83/83	0/3/3/3
28	CLA	c	507	42	-	10/39/115/115	-
28	CLA	C	508	3	-	12/39/115/115	-
38	CHL	n	605	7	-	8/20/96/117	-
28	CLA	n	602	7	-	20/39/115/115	-
28	CLA	D	401	42	-	16/39/115/115	-
28	CLA	C	509	3	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	s	609	18	-	11/27/103/115	-
30	BCR	B	618	-	-	14/29/63/63	0/2/2/2
40	NEX	r	616	28	-	6/27/83/83	0/3/3/3
28	CLA	C	510	3	-	17/39/115/115	-
28	CLA	s	610	35	-	11/29/105/115	-
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
36	DGD	b	625	-	-	6/51/91/95	0/2/2/2
36	DGD	c	517	-	-	13/43/83/95	0/2/2/2
28	CLA	n	614	7	-	5/15/91/115	-
28	CLA	R	608	17	-	13/31/107/115	-
35	LHG	B	623	-	-	25/45/45/53	-
38	CHL	S	307	42	-	13/32/108/117	-

All (2412) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518	DGD	C6B-C5B	34.31	3.44	1.51
39	S	316	LUT	C24-C25	23.38	1.62	1.33
39	n	615	LUT	C24-C25	23.19	1.62	1.33
39	y	315	LUT	C24-C25	23.19	1.62	1.33
39	g	615	LUT	C24-C25	23.18	1.62	1.33
39	s	614	LUT	C24-C25	23.17	1.62	1.33
39	N	615	LUT	C24-C25	23.16	1.62	1.33
39	y	316	LUT	C24-C25	23.14	1.62	1.33
39	G	615	LUT	C24-C25	23.11	1.61	1.33
39	S	315	LUT	C24-C25	23.10	1.61	1.33
39	r	614	LUT	C24-C25	23.08	1.61	1.33
39	Y	616	LUT	C24-C25	23.01	1.61	1.33
39	g	616	LUT	C24-C25	22.97	1.61	1.33
39	R	614	LUT	C24-C25	22.90	1.61	1.33
39	s	615	LUT	C24-C25	22.86	1.61	1.33
39	N	616	LUT	C24-C25	22.83	1.61	1.33
39	n	616	LUT	C24-C25	22.72	1.61	1.33
39	G	616	LUT	C24-C25	22.38	1.61	1.33
39	Y	615	LUT	C24-C25	22.24	1.60	1.33
30	B	618	BCR	C26-C25	15.61	1.61	1.34
30	b	618	BCR	C26-C25	15.55	1.61	1.34
30	c	515	BCR	C26-C25	15.53	1.61	1.34
39	Y	616	LUT	C5-C6	15.53	1.61	1.34
30	k	101	BCR	C26-C25	15.53	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	101	BCR	C26-C25	15.51	1.61	1.34
39	y	316	LUT	C5-C6	15.50	1.61	1.34
30	a	410	BCR	C26-C25	15.44	1.61	1.34
30	A	409	BCR	C26-C25	15.43	1.61	1.34
30	h	101	BCR	C26-C25	15.43	1.61	1.34
30	H	101	BCR	C26-C25	15.41	1.61	1.34
30	b	617	BCR	C26-C25	15.36	1.61	1.34
30	C	516	BCR	C26-C25	15.36	1.61	1.34
30	B	617	BCR	C26-C25	15.36	1.61	1.34
39	S	316	LUT	C5-C6	15.35	1.61	1.34
30	B	619	BCR	C26-C25	15.33	1.61	1.34
39	y	315	LUT	C5-C6	15.32	1.61	1.34
39	G	615	LUT	C5-C6	15.30	1.60	1.34
30	C	515	BCR	C26-C25	15.26	1.60	1.34
39	S	315	LUT	C5-C6	15.25	1.60	1.34
39	g	616	LUT	C5-C6	15.24	1.60	1.34
39	g	615	LUT	C5-C6	15.16	1.60	1.34
30	t	101	BCR	C26-C25	15.16	1.60	1.34
30	K	101	BCR	C26-C25	15.15	1.60	1.34
30	C	514	BCR	C26-C25	15.15	1.60	1.34
30	d	406	BCR	C26-C25	15.13	1.60	1.34
39	s	615	LUT	C5-C6	15.11	1.60	1.34
39	n	615	LUT	C5-C6	15.11	1.60	1.34
30	b	619	BCR	C26-C25	15.08	1.60	1.34
30	D	405	BCR	C26-C25	15.07	1.60	1.34
30	c	514	BCR	C26-C25	15.05	1.60	1.34
39	s	614	LUT	C5-C6	15.05	1.60	1.34
39	r	614	LUT	C5-C6	14.97	1.60	1.34
30	T	101	BCR	C26-C25	14.95	1.60	1.34
39	Y	615	LUT	C5-C6	14.75	1.60	1.34
39	N	616	LUT	C5-C6	14.72	1.59	1.34
39	N	615	LUT	C5-C6	14.69	1.59	1.34
39	n	616	LUT	C5-C6	14.68	1.59	1.34
39	R	614	LUT	C5-C6	14.67	1.59	1.34
39	G	616	LUT	C5-C6	14.66	1.59	1.34
30	h	101	BCR	C5-C6	14.37	1.59	1.34
30	C	515	BCR	C5-C6	14.09	1.58	1.34
30	T	101	BCR	C5-C6	14.08	1.58	1.34
30	B	617	BCR	C5-C6	14.07	1.58	1.34
30	b	617	BCR	C5-C6	14.06	1.58	1.34
30	i	101	BCR	C5-C6	14.05	1.58	1.34
30	B	619	BCR	C5-C6	14.04	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	101	BCR	C5-C6	14.02	1.58	1.34
30	c	514	BCR	C5-C6	14.01	1.58	1.34
30	A	409	BCR	C5-C6	14.01	1.58	1.34
30	b	618	BCR	C5-C6	14.00	1.58	1.34
30	C	516	BCR	C5-C6	13.99	1.58	1.34
30	k	101	BCR	C5-C6	13.99	1.58	1.34
30	a	410	BCR	C5-C6	13.98	1.58	1.34
30	B	618	BCR	C5-C6	13.97	1.58	1.34
30	c	515	BCR	C5-C6	13.97	1.58	1.34
30	H	101	BCR	C5-C6	13.93	1.58	1.34
30	C	514	BCR	C5-C6	13.90	1.58	1.34
30	b	619	BCR	C5-C6	13.82	1.58	1.34
30	d	406	BCR	C5-C6	13.77	1.58	1.34
30	D	405	BCR	C5-C6	13.71	1.58	1.34
30	t	101	BCR	C5-C6	13.71	1.58	1.34
39	G	616	LUT	C22-C21	-13.62	1.37	1.54
39	r	614	LUT	C22-C21	-13.53	1.37	1.54
39	N	615	LUT	C22-C21	-13.51	1.37	1.54
39	Y	616	LUT	C22-C21	-13.50	1.37	1.54
39	R	614	LUT	C22-C21	-13.50	1.37	1.54
39	n	616	LUT	C22-C21	-13.39	1.37	1.54
39	N	616	LUT	C22-C21	-13.34	1.38	1.54
39	n	615	LUT	C22-C21	-13.19	1.38	1.54
39	g	615	LUT	C22-C21	-13.07	1.38	1.54
39	y	315	LUT	C22-C21	-13.05	1.38	1.54
39	S	316	LUT	C22-C21	-13.01	1.38	1.54
39	Y	615	LUT	C22-C21	-12.80	1.38	1.54
39	S	315	LUT	C22-C21	-12.77	1.38	1.54
39	s	614	LUT	C22-C21	-12.70	1.38	1.54
39	y	316	LUT	C22-C21	-12.70	1.38	1.54
39	G	615	LUT	C22-C21	-12.61	1.38	1.54
39	s	615	LUT	C22-C21	-12.46	1.39	1.54
39	g	616	LUT	C22-C21	-12.37	1.39	1.54
39	Y	616	LUT	C2-C3	-11.97	1.35	1.52
39	N	615	LUT	C2-C3	-11.55	1.35	1.52
39	Y	615	LUT	C2-C3	-11.47	1.35	1.52
39	N	616	LUT	C2-C3	-11.37	1.36	1.52
39	G	616	LUT	C2-C3	-11.25	1.36	1.52
39	n	616	LUT	C2-C3	-11.24	1.36	1.52
39	y	315	LUT	C2-C3	-11.22	1.36	1.52
39	n	615	LUT	C2-C3	-11.21	1.36	1.52
39	y	316	LUT	C2-C3	-11.17	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	615	LUT	C2-C3	-11.17	1.36	1.52
39	G	615	LUT	C2-C3	-11.12	1.36	1.52
39	S	316	LUT	C2-C3	-11.05	1.36	1.52
39	r	614	LUT	C2-C3	-11.01	1.36	1.52
39	S	315	LUT	C2-C3	-10.93	1.36	1.52
39	s	615	LUT	C2-C3	-10.89	1.36	1.52
39	s	614	LUT	C2-C3	-10.89	1.36	1.52
39	g	616	LUT	C2-C3	-10.89	1.36	1.52
39	R	614	LUT	C2-C3	-10.73	1.36	1.52
40	G	617	NEX	C30-C29	-8.35	1.24	1.35
39	y	316	LUT	C22-C23	8.26	1.66	1.53
39	g	616	LUT	C22-C23	8.15	1.66	1.53
39	S	315	LUT	C22-C23	8.13	1.66	1.53
39	n	615	LUT	C22-C23	8.11	1.66	1.53
39	s	615	LUT	C22-C23	8.08	1.66	1.53
40	y	301	NEX	C34-C33	-8.08	1.25	1.35
39	s	614	LUT	C4-C3	8.07	1.66	1.52
39	s	615	LUT	C4-C3	8.04	1.66	1.52
39	S	316	LUT	C22-C23	8.03	1.66	1.53
39	s	614	LUT	C22-C23	8.03	1.66	1.53
39	g	615	LUT	C22-C23	8.00	1.66	1.53
39	y	315	LUT	C22-C23	7.99	1.66	1.53
39	S	315	LUT	C4-C3	7.98	1.66	1.52
39	R	614	LUT	C22-C23	7.94	1.66	1.53
40	n	617	NEX	C34-C33	-7.92	1.25	1.35
39	Y	616	LUT	C22-C23	7.91	1.66	1.53
39	G	616	LUT	C4-C3	7.90	1.66	1.52
39	g	616	LUT	C4-C3	7.89	1.66	1.52
39	R	614	LUT	C4-C3	7.89	1.66	1.52
39	g	615	LUT	C4-C3	7.86	1.65	1.52
39	G	615	LUT	C22-C23	7.86	1.66	1.53
39	S	316	LUT	C4-C3	7.84	1.65	1.52
39	G	615	LUT	C4-C3	7.84	1.65	1.52
40	G	617	NEX	C34-C33	-7.82	1.25	1.35
40	y	301	NEX	C14-C13	-7.81	1.25	1.35
39	y	315	LUT	C4-C3	7.81	1.65	1.52
40	n	617	NEX	C14-C13	-7.80	1.25	1.35
40	G	617	NEX	C14-C13	-7.79	1.25	1.35
40	y	301	NEX	C30-C29	-7.78	1.25	1.35
39	y	316	LUT	C4-C3	7.75	1.65	1.52
40	n	617	NEX	C30-C29	-7.74	1.25	1.35
39	n	616	LUT	C22-C23	7.73	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	615	LUT	C22-C23	7.73	1.65	1.53
40	g	617	NEX	C30-C29	-7.73	1.25	1.35
39	n	616	LUT	C4-C3	7.73	1.65	1.52
39	N	616	LUT	C22-C23	7.69	1.65	1.53
40	g	617	NEX	C34-C33	-7.69	1.25	1.35
30	b	619	BCR	C30-C25	-7.67	1.43	1.53
40	g	617	NEX	C10-C9	-7.67	1.25	1.35
39	G	615	LUT	C32-C33	7.67	1.62	1.45
39	Y	615	LUT	C4-C3	7.63	1.65	1.52
39	r	614	LUT	C4-C3	7.62	1.65	1.52
39	r	614	LUT	C22-C23	7.60	1.65	1.53
40	s	616	NEX	C14-C13	-7.59	1.25	1.35
40	s	616	NEX	C30-C29	-7.59	1.25	1.35
40	s	616	NEX	C10-C9	-7.56	1.25	1.35
40	y	318	NEX	C30-C29	-7.55	1.25	1.35
40	s	616	NEX	C34-C33	-7.55	1.25	1.35
40	n	617	NEX	C10-C9	-7.55	1.25	1.35
39	N	615	LUT	C4-C3	7.55	1.65	1.52
40	r	616	NEX	C30-C29	-7.55	1.25	1.35
40	N	617	NEX	C30-C29	-7.55	1.25	1.35
39	s	614	LUT	C32-C33	7.54	1.62	1.45
39	G	616	LUT	C32-C33	7.51	1.62	1.45
40	g	617	NEX	C14-C13	-7.51	1.25	1.35
39	n	615	LUT	C4-C3	7.50	1.65	1.52
40	r	616	NEX	C34-C33	-7.50	1.25	1.35
40	N	617	NEX	C14-C13	-7.50	1.25	1.35
40	y	301	NEX	C10-C9	-7.50	1.25	1.35
40	r	616	NEX	C14-C13	-7.48	1.25	1.35
39	s	615	LUT	C32-C33	7.48	1.62	1.45
39	S	316	LUT	C32-C33	7.47	1.62	1.45
40	N	617	NEX	C34-C33	-7.47	1.25	1.35
39	g	616	LUT	C32-C33	7.46	1.62	1.45
39	G	616	LUT	C22-C23	7.45	1.65	1.53
39	R	614	LUT	C1-C6	-7.44	1.43	1.53
40	Y	618	NEX	C14-C13	-7.44	1.25	1.35
40	N	617	NEX	C10-C9	-7.44	1.25	1.35
40	Y	618	NEX	C30-C29	-7.42	1.25	1.35
39	y	316	LUT	C32-C33	7.42	1.61	1.45
40	Y	618	NEX	C34-C33	-7.41	1.26	1.35
40	r	616	NEX	C10-C9	-7.40	1.26	1.35
30	T	101	BCR	C30-C25	-7.40	1.43	1.53
39	g	615	LUT	C32-C33	7.40	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	616	LUT	C4-C3	7.37	1.65	1.52
39	S	315	LUT	C32-C33	7.36	1.61	1.45
39	N	616	LUT	C4-C3	7.34	1.65	1.52
39	Y	615	LUT	C22-C23	7.31	1.65	1.53
40	Y	618	NEX	C10-C9	-7.31	1.26	1.35
39	N	615	LUT	C1-C6	-7.30	1.43	1.53
39	y	315	LUT	C32-C33	7.30	1.61	1.45
39	N	616	LUT	C32-C33	7.29	1.61	1.45
39	n	615	LUT	C32-C33	7.27	1.61	1.45
39	G	616	LUT	C1-C6	-7.24	1.43	1.53
39	R	614	LUT	C32-C33	7.22	1.61	1.45
40	G	617	NEX	C10-C9	-7.20	1.26	1.35
30	K	101	BCR	C30-C25	-7.12	1.44	1.53
30	D	405	BCR	C30-C25	-7.12	1.44	1.53
40	y	301	NEX	C35-C15	-7.09	1.17	1.36
39	r	614	LUT	C32-C33	7.09	1.61	1.45
40	y	318	NEX	C34-C33	-7.07	1.26	1.35
40	n	617	NEX	C35-C15	-7.06	1.17	1.36
30	c	514	BCR	C30-C25	-7.04	1.44	1.53
30	C	515	BCR	C30-C25	-7.02	1.44	1.53
40	y	318	NEX	C14-C13	-7.02	1.26	1.35
40	G	617	NEX	C35-C15	-7.01	1.17	1.36
40	y	318	NEX	C10-C9	-7.01	1.26	1.35
39	N	615	LUT	C32-C33	7.00	1.61	1.45
30	d	406	BCR	C30-C25	-6.99	1.44	1.53
39	Y	615	LUT	C32-C33	6.97	1.60	1.45
39	n	616	LUT	C32-C33	6.97	1.60	1.45
30	T	101	BCR	C1-C6	-6.96	1.44	1.53
30	C	514	BCR	C30-C25	-6.96	1.44	1.53
30	H	101	BCR	C30-C25	-6.94	1.44	1.53
30	t	101	BCR	C30-C25	-6.90	1.44	1.53
39	Y	616	LUT	C32-C33	6.90	1.60	1.45
40	s	616	NEX	C35-C15	-6.81	1.18	1.36
30	c	515	BCR	C30-C25	-6.80	1.44	1.53
30	C	516	BCR	C30-C25	-6.80	1.44	1.53
40	r	616	NEX	C35-C15	-6.78	1.18	1.36
30	h	101	BCR	C30-C25	-6.78	1.44	1.53
40	N	617	NEX	C35-C15	-6.78	1.18	1.36
30	B	619	BCR	C30-C25	-6.76	1.44	1.53
30	b	617	BCR	C30-C25	-6.75	1.44	1.53
40	Y	618	NEX	C35-C15	-6.73	1.18	1.36
30	T	101	BCR	C2-C3	-6.72	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	410	BCR	C30-C25	-6.72	1.44	1.53
40	g	617	NEX	C35-C15	-6.72	1.18	1.36
30	h	101	BCR	C2-C3	-6.72	1.36	1.52
30	B	617	BCR	C30-C25	-6.71	1.44	1.53
30	D	405	BCR	C1-C6	-6.71	1.44	1.53
30	b	619	BCR	C2-C3	-6.70	1.36	1.52
30	d	406	BCR	C1-C6	-6.70	1.44	1.53
30	t	101	BCR	C1-C6	-6.69	1.44	1.53
30	b	617	BCR	C1-C6	-6.69	1.44	1.53
39	n	616	LUT	C1-C6	-6.68	1.44	1.53
30	K	101	BCR	C2-C3	-6.67	1.36	1.52
30	i	101	BCR	C2-C3	-6.67	1.36	1.52
30	C	516	BCR	C1-C6	-6.66	1.44	1.53
39	n	615	LUT	C1-C6	-6.65	1.44	1.53
30	C	515	BCR	C2-C3	-6.65	1.36	1.52
30	C	514	BCR	C1-C6	-6.65	1.44	1.53
30	b	618	BCR	C30-C25	-6.64	1.44	1.53
30	B	619	BCR	C2-C3	-6.63	1.36	1.52
30	a	410	BCR	C2-C3	-6.63	1.36	1.52
30	c	514	BCR	C1-C6	-6.62	1.44	1.53
30	B	617	BCR	C2-C3	-6.62	1.36	1.52
30	h	101	BCR	C1-C6	-6.62	1.44	1.53
30	k	101	BCR	C30-C25	-6.62	1.44	1.53
39	N	616	LUT	C1-C6	-6.61	1.44	1.53
30	A	409	BCR	C30-C25	-6.61	1.44	1.53
30	H	101	BCR	C1-C6	-6.61	1.44	1.53
30	b	619	BCR	C1-C6	-6.60	1.44	1.53
30	C	516	BCR	C2-C3	-6.59	1.36	1.52
40	n	617	NEX	C11-C12	-6.59	1.17	1.34
30	i	101	BCR	C30-C25	-6.58	1.44	1.53
30	A	409	BCR	C2-C3	-6.58	1.36	1.52
30	B	618	BCR	C30-C25	-6.57	1.44	1.53
40	G	617	NEX	C31-C32	-6.57	1.17	1.34
30	b	617	BCR	C2-C3	-6.56	1.36	1.52
30	B	618	BCR	C2-C3	-6.55	1.36	1.52
30	c	515	BCR	C2-C3	-6.55	1.36	1.52
30	B	619	BCR	C1-C6	-6.55	1.44	1.53
30	k	101	BCR	C1-C6	-6.55	1.44	1.53
28	R	603	CLA	MG-NA	6.55	2.21	2.06
30	H	101	BCR	C2-C3	-6.54	1.36	1.52
40	g	617	NEX	C11-C12	-6.54	1.17	1.34
30	c	514	BCR	C2-C3	-6.54	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	604	CLA	MG-NA	6.53	2.21	2.06
30	b	618	BCR	C2-C3	-6.53	1.36	1.52
30	k	101	BCR	C2-C3	-6.53	1.36	1.52
30	B	617	BCR	C1-C6	-6.53	1.44	1.53
40	y	301	NEX	C31-C32	-6.52	1.17	1.34
40	y	318	NEX	C35-C15	-6.51	1.19	1.36
30	T	101	BCR	C29-C28	-6.48	1.36	1.52
30	C	514	BCR	C2-C3	-6.48	1.36	1.52
30	D	405	BCR	C2-C3	-6.46	1.36	1.52
30	i	101	BCR	C1-C6	-6.45	1.44	1.53
40	n	617	NEX	C31-C32	-6.45	1.18	1.34
30	t	101	BCR	C2-C3	-6.44	1.36	1.52
30	b	618	BCR	C1-C6	-6.44	1.44	1.53
30	c	515	BCR	C1-C6	-6.44	1.44	1.53
30	C	515	BCR	C1-C6	-6.43	1.44	1.53
30	B	618	BCR	C1-C6	-6.43	1.44	1.53
28	Y	602	CLA	MG-NA	6.42	2.21	2.06
30	d	406	BCR	C2-C3	-6.42	1.36	1.52
30	A	409	BCR	C1-C6	-6.40	1.45	1.53
30	k	101	BCR	C29-C28	-6.39	1.36	1.52
40	g	617	NEX	C31-C32	-6.37	1.18	1.34
28	R	601	CLA	MG-NA	6.37	2.21	2.06
28	B	604	CLA	MG-NA	6.36	2.21	2.06
40	G	617	NEX	C11-C12	-6.36	1.18	1.34
40	s	616	NEX	C11-C12	-6.35	1.18	1.34
39	r	614	LUT	C1-C6	-6.35	1.45	1.53
40	y	301	NEX	C11-C12	-6.35	1.18	1.34
39	s	614	LUT	C1-C6	-6.34	1.45	1.53
30	b	619	BCR	C29-C28	-6.34	1.36	1.52
30	B	618	BCR	C29-C28	-6.34	1.36	1.52
40	s	616	NEX	C31-C32	-6.34	1.18	1.34
30	h	101	BCR	C29-C28	-6.34	1.36	1.52
30	b	618	BCR	C29-C28	-6.34	1.36	1.52
30	a	410	BCR	C29-C28	-6.33	1.36	1.52
28	d	401	CLA	MG-NA	6.32	2.21	2.06
30	A	409	BCR	C29-C28	-6.32	1.37	1.52
30	i	101	BCR	C29-C28	-6.32	1.37	1.52
28	c	511	CLA	MG-NA	6.31	2.21	2.06
28	s	612	CLA	MG-NA	6.31	2.21	2.06
30	c	515	BCR	C29-C28	-6.31	1.37	1.52
28	B	615	CLA	MG-NA	6.31	2.21	2.06
28	b	604	CLA	MG-NA	6.30	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	313	CLA	MG-NA	6.30	2.21	2.06
28	r	603	CLA	MG-NA	6.30	2.21	2.06
28	S	312	CLA	MG-NA	6.30	2.21	2.06
30	a	410	BCR	C1-C6	-6.30	1.45	1.53
28	D	401	CLA	MG-NA	6.29	2.21	2.06
28	b	613	CLA	MG-NA	6.29	2.21	2.06
28	R	613	CLA	MG-NA	6.29	2.21	2.06
28	C	511	CLA	MG-NA	6.29	2.21	2.06
28	N	613	CLA	MG-NA	6.29	2.21	2.06
28	R	611	CLA	MG-NA	6.29	2.21	2.06
28	c	503	CLA	MG-NA	6.29	2.21	2.06
28	r	601	CLA	MG-NA	6.29	2.21	2.06
28	C	513	CLA	MG-NA	6.29	2.21	2.06
28	B	610	CLA	MG-NA	6.29	2.21	2.06
39	s	615	LUT	C1-C6	-6.29	1.45	1.53
28	s	608	CLA	MG-NA	6.28	2.21	2.06
28	c	502	CLA	MG-NA	6.28	2.21	2.06
28	y	303	CLA	MG-NA	6.28	2.21	2.06
28	C	501	CLA	MG-NA	6.28	2.21	2.06
28	Y	613	CLA	MG-NA	6.28	2.21	2.06
28	s	604	CLA	MG-NA	6.28	2.21	2.06
28	G	602	CLA	MG-NA	6.28	2.21	2.06
28	c	513	CLA	MG-NA	6.28	2.21	2.06
28	B	601	CLA	MG-NA	6.28	2.21	2.06
28	r	613	CLA	MG-NA	6.28	2.21	2.06
28	d	405	CLA	MG-NA	6.28	2.21	2.06
28	n	614	CLA	MG-NA	6.28	2.21	2.06
28	b	615	CLA	MG-NA	6.27	2.21	2.06
40	N	617	NEX	C11-C12	-6.27	1.18	1.34
28	S	304	CLA	MG-NA	6.27	2.21	2.06
40	N	617	NEX	C31-C32	-6.27	1.18	1.34
28	C	509	CLA	MG-NA	6.27	2.21	2.06
28	b	607	CLA	MG-NA	6.27	2.21	2.06
28	y	311	CLA	MG-NA	6.27	2.21	2.06
30	B	619	BCR	C29-C28	-6.27	1.37	1.52
28	y	313	CLA	MG-NA	6.27	2.21	2.06
28	A	406	CLA	MG-NA	6.27	2.21	2.06
40	r	616	NEX	C31-C32	-6.27	1.18	1.34
28	n	602	CLA	MG-NA	6.27	2.21	2.06
28	b	601	CLA	MG-NA	6.27	2.21	2.06
28	b	611	CLA	MG-NA	6.27	2.21	2.06
28	B	606	CLA	MG-NA	6.26	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	y	304	CLA	MG-NA	6.26	2.21	2.06
28	n	604	CLA	MG-NA	6.26	2.21	2.06
28	s	611	CLA	MG-NA	6.26	2.21	2.06
28	C	506	CLA	MG-NA	6.26	2.21	2.06
40	Y	618	NEX	C31-C32	-6.26	1.18	1.34
28	C	503	CLA	MG-NA	6.26	2.21	2.06
28	C	507	CLA	MG-NA	6.26	2.21	2.06
28	a	409	CLA	MG-NA	6.26	2.21	2.06
28	s	613	CLA	MG-NA	6.26	2.21	2.06
30	C	516	BCR	C29-C28	-6.26	1.37	1.52
30	H	101	BCR	C29-C28	-6.26	1.37	1.52
28	b	610	CLA	MG-NA	6.25	2.21	2.06
28	R	612	CLA	MG-NA	6.25	2.21	2.06
30	B	617	BCR	C29-C28	-6.25	1.37	1.52
28	C	512	CLA	MG-NA	6.25	2.21	2.06
28	c	507	CLA	MG-NA	6.25	2.21	2.06
28	r	602	CLA	MG-NA	6.25	2.21	2.06
28	G	603	CLA	MG-NA	6.25	2.21	2.06
28	d	404	CLA	MG-NA	6.25	2.21	2.06
28	D	404	CLA	MG-NA	6.25	2.21	2.06
28	a	407	CLA	MG-NA	6.25	2.21	2.06
28	g	612	CLA	MG-NA	6.24	2.21	2.06
28	B	608	CLA	MG-NA	6.24	2.21	2.06
28	B	607	CLA	MG-NA	6.24	2.21	2.06
28	C	502	CLA	MG-NA	6.24	2.21	2.06
28	s	609	CLA	MG-NA	6.24	2.21	2.06
28	S	311	CLA	MG-NA	6.24	2.21	2.06
28	b	603	CLA	MG-NA	6.24	2.21	2.06
28	G	611	CLA	MG-NA	6.24	2.21	2.06
28	c	506	CLA	MG-NA	6.24	2.21	2.06
28	s	610	CLA	MG-NA	6.24	2.21	2.06
28	r	612	CLA	MG-NA	6.24	2.21	2.06
28	A	405	CLA	MG-NA	6.24	2.21	2.06
28	C	508	CLA	MG-NA	6.24	2.21	2.06
28	g	604	CLA	MG-NA	6.24	2.21	2.06
28	S	314	CLA	MG-NA	6.24	2.21	2.06
28	S	309	CLA	MG-NA	6.24	2.21	2.06
28	g	613	CLA	MG-NA	6.24	2.21	2.06
28	n	610	CLA	MG-NA	6.24	2.21	2.06
40	r	616	NEX	C11-C12	-6.23	1.18	1.34
28	Y	611	CLA	MG-NA	6.23	2.21	2.06
28	a	406	CLA	MG-NA	6.23	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	y	318	NEX	C11-C12	-6.23	1.18	1.34
28	B	611	CLA	MG-NA	6.23	2.21	2.06
28	B	613	CLA	MG-NA	6.23	2.21	2.06
28	Y	614	CLA	MG-NA	6.23	2.21	2.06
28	Y	603	CLA	MG-NA	6.22	2.21	2.06
28	c	501	CLA	MG-NA	6.22	2.21	2.06
28	b	614	CLA	MG-NA	6.22	2.21	2.06
28	N	611	CLA	MG-NA	6.22	2.21	2.06
28	R	609	CLA	MG-NA	6.22	2.21	2.06
28	D	403	CLA	MG-NA	6.22	2.21	2.06
39	Y	616	LUT	C1-C6	-6.22	1.45	1.53
28	G	614	CLA	MG-NA	6.22	2.21	2.06
28	B	603	CLA	MG-NA	6.22	2.21	2.06
28	y	312	CLA	MG-NA	6.22	2.21	2.06
28	n	603	CLA	MG-NA	6.21	2.21	2.06
28	r	608	CLA	MG-NA	6.21	2.21	2.06
40	y	318	NEX	C31-C32	-6.21	1.18	1.34
28	N	610	CLA	MG-NA	6.21	2.21	2.06
28	S	303	CLA	MG-NA	6.21	2.21	2.06
28	g	602	CLA	MG-NA	6.21	2.21	2.06
28	g	614	CLA	MG-NA	6.20	2.21	2.06
28	N	612	CLA	MG-NA	6.20	2.21	2.06
28	y	314	CLA	MG-NA	6.20	2.21	2.06
30	b	617	BCR	C29-C28	-6.20	1.37	1.52
30	t	101	BCR	C29-C28	-6.20	1.37	1.52
28	G	613	CLA	MG-NA	6.20	2.21	2.06
28	c	512	CLA	MG-NA	6.20	2.21	2.06
28	R	610	CLA	MG-NA	6.20	2.21	2.06
30	d	406	BCR	C29-C28	-6.19	1.37	1.52
28	N	602	CLA	MG-NA	6.19	2.21	2.06
28	r	610	CLA	MG-NA	6.19	2.21	2.06
28	B	614	CLA	MG-NA	6.19	2.21	2.06
28	S	310	CLA	MG-NA	6.19	2.21	2.06
40	Y	618	NEX	C11-C12	-6.19	1.18	1.34
28	R	608	CLA	MG-NA	6.19	2.21	2.06
28	B	605	CLA	MG-NA	6.19	2.21	2.06
28	s	603	CLA	MG-NA	6.19	2.21	2.06
28	r	604	CLA	MG-NA	6.19	2.21	2.06
28	C	510	CLA	MG-NA	6.18	2.21	2.06
28	B	616	CLA	MG-NA	6.18	2.21	2.06
28	Y	612	CLA	MG-NA	6.18	2.20	2.06
28	b	602	CLA	MG-NA	6.18	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	608	CLA	MG-NA	6.18	2.20	2.06
28	y	305	CLA	MG-NA	6.18	2.20	2.06
28	C	505	CLA	MG-NA	6.17	2.20	2.06
28	N	614	CLA	MG-NA	6.17	2.20	2.06
28	c	505	CLA	MG-NA	6.17	2.20	2.06
28	B	612	CLA	MG-NA	6.17	2.20	2.06
39	Y	615	LUT	C1-C6	-6.17	1.45	1.53
28	s	602	CLA	MG-NA	6.17	2.20	2.06
28	C	504	CLA	MG-NA	6.17	2.20	2.06
28	c	510	CLA	MG-NA	6.17	2.20	2.06
28	G	604	CLA	MG-NA	6.17	2.20	2.06
39	S	316	LUT	C1-C6	-6.17	1.45	1.53
30	C	514	BCR	C29-C28	-6.17	1.37	1.52
28	N	603	CLA	MG-NA	6.16	2.20	2.06
28	y	310	CLA	MG-NA	6.16	2.20	2.06
28	G	612	CLA	MG-NA	6.15	2.20	2.06
28	Y	604	CLA	MG-NA	6.15	2.20	2.06
28	G	610	CLA	MG-NA	6.15	2.20	2.06
28	c	504	CLA	MG-NA	6.15	2.20	2.06
28	b	616	CLA	MG-NA	6.15	2.20	2.06
28	N	604	CLA	MG-NA	6.15	2.20	2.06
28	b	606	CLA	MG-NA	6.14	2.20	2.06
28	g	610	CLA	MG-NA	6.14	2.20	2.06
28	b	612	CLA	MG-NA	6.14	2.20	2.06
28	r	609	CLA	MG-NA	6.14	2.20	2.06
30	D	405	BCR	C29-C28	-6.13	1.37	1.52
28	B	602	CLA	MG-NA	6.13	2.20	2.06
30	C	515	BCR	C29-C28	-6.13	1.37	1.52
28	A	408	CLA	MG-NA	6.13	2.20	2.06
40	G	617	NEX	C28-C29	-6.13	1.32	1.45
28	b	609	CLA	MG-NA	6.12	2.20	2.06
28	n	611	CLA	MG-NA	6.12	2.20	2.06
30	K	101	BCR	C1-C6	-6.12	1.45	1.53
28	B	609	CLA	MG-NA	6.12	2.20	2.06
28	Y	610	CLA	MG-NA	6.11	2.20	2.06
30	K	101	BCR	C29-C28	-6.10	1.37	1.52
28	c	508	CLA	MG-NA	6.10	2.20	2.06
39	y	316	LUT	C1-C6	-6.10	1.45	1.53
39	G	615	LUT	C1-C6	-6.09	1.45	1.53
39	g	616	LUT	C1-C6	-6.08	1.45	1.53
30	c	514	BCR	C29-C28	-6.06	1.37	1.52
39	y	315	LUT	C1-C6	-6.05	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	613	CLA	MG-NA	6.05	2.20	2.06
39	S	315	LUT	C1-C6	-6.02	1.45	1.53
28	n	612	CLA	MG-NA	6.02	2.20	2.06
28	R	602	CLA	MG-NA	6.02	2.20	2.06
28	c	509	CLA	MG-NA	6.01	2.20	2.06
39	g	615	LUT	C1-C6	-6.00	1.45	1.53
28	b	605	CLA	MG-NA	5.95	2.20	2.06
28	g	611	CLA	MG-NA	5.92	2.20	2.06
28	r	611	CLA	MG-NA	5.91	2.20	2.06
28	g	603	CLA	MG-NA	5.88	2.20	2.06
28	S	305	CLA	MG-NA	5.82	2.20	2.06
30	i	101	BCR	C12-C13	5.78	1.58	1.45
30	C	515	BCR	C12-C13	5.77	1.58	1.45
30	B	617	BCR	C12-C13	5.77	1.58	1.45
30	C	516	BCR	C12-C13	5.76	1.58	1.45
30	C	514	BCR	C12-C13	5.76	1.58	1.45
30	d	406	BCR	C12-C13	5.75	1.58	1.45
30	t	101	BCR	C12-C13	5.75	1.58	1.45
30	k	101	BCR	C12-C13	5.74	1.58	1.45
30	B	619	BCR	C12-C13	5.73	1.58	1.45
30	b	617	BCR	C12-C13	5.73	1.58	1.45
30	K	101	BCR	C12-C13	5.73	1.58	1.45
30	a	410	BCR	C12-C13	5.73	1.58	1.45
30	D	405	BCR	C12-C13	5.72	1.58	1.45
30	c	515	BCR	C12-C13	5.72	1.58	1.45
30	B	618	BCR	C12-C13	5.69	1.58	1.45
30	h	101	BCR	C12-C13	5.68	1.58	1.45
30	H	101	BCR	C12-C13	5.67	1.58	1.45
30	c	514	BCR	C12-C13	5.65	1.58	1.45
30	b	618	BCR	C12-C13	5.64	1.58	1.45
30	A	409	BCR	C12-C13	5.63	1.58	1.45
30	B	617	BCR	C8-C9	5.55	1.57	1.45
40	N	617	NEX	C28-C29	-5.52	1.34	1.45
40	y	301	NEX	C28-C29	-5.52	1.34	1.45
30	C	514	BCR	C8-C9	5.51	1.57	1.45
30	b	617	BCR	C8-C9	5.48	1.57	1.45
40	G	617	NEX	C7-C8	5.47	1.41	1.32
30	k	101	BCR	C8-C9	5.47	1.57	1.45
30	b	618	BCR	C8-C9	5.47	1.57	1.45
30	B	618	BCR	C8-C9	5.47	1.57	1.45
30	t	101	BCR	C8-C9	5.47	1.57	1.45
30	c	515	BCR	C8-C9	5.46	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	617	NEX	C28-C29	-5.46	1.34	1.45
40	s	616	NEX	C28-C29	-5.45	1.34	1.45
30	d	406	BCR	C8-C9	5.44	1.57	1.45
40	r	616	NEX	C28-C29	-5.42	1.34	1.45
30	C	516	BCR	C8-C9	5.42	1.57	1.45
30	K	101	BCR	C8-C9	5.42	1.57	1.45
30	D	405	BCR	C8-C9	5.42	1.57	1.45
30	C	515	BCR	C8-C9	5.41	1.57	1.45
30	A	409	BCR	C8-C9	5.41	1.57	1.45
30	h	101	BCR	C8-C9	5.41	1.57	1.45
40	y	318	NEX	C7-C8	5.41	1.41	1.32
40	Y	618	NEX	C28-C29	-5.41	1.34	1.45
30	B	619	BCR	C8-C9	5.39	1.57	1.45
39	Y	615	LUT	C4-C5	-5.39	1.42	1.51
40	Y	618	NEX	C7-C8	5.38	1.40	1.32
30	i	101	BCR	C8-C9	5.38	1.57	1.45
30	H	101	BCR	C8-C9	5.38	1.57	1.45
30	a	410	BCR	C8-C9	5.37	1.57	1.45
30	c	514	BCR	C8-C9	5.37	1.57	1.45
40	n	617	NEX	C28-C29	-5.36	1.34	1.45
30	C	515	BCR	C29-C30	5.33	1.66	1.54
30	b	619	BCR	C12-C13	5.32	1.57	1.45
30	K	101	BCR	C29-C30	5.32	1.66	1.54
30	t	101	BCR	C23-C22	5.32	1.57	1.45
30	h	101	BCR	C23-C22	5.31	1.57	1.45
40	y	318	NEX	C28-C29	-5.29	1.34	1.45
30	C	515	BCR	C23-C22	5.28	1.57	1.45
30	B	619	BCR	C23-C22	5.28	1.57	1.45
40	N	617	NEX	C7-C8	5.28	1.40	1.32
30	A	409	BCR	C23-C22	5.27	1.57	1.45
30	i	101	BCR	C29-C30	5.27	1.66	1.54
30	B	618	BCR	C23-C22	5.27	1.57	1.45
40	r	616	NEX	C7-C8	5.27	1.40	1.32
30	H	101	BCR	C23-C22	5.27	1.57	1.45
30	b	618	BCR	C23-C22	5.26	1.57	1.45
37	f	101	HEM	FE-NB	5.26	2.11	1.94
30	i	101	BCR	C23-C22	5.26	1.57	1.45
30	C	516	BCR	C23-C22	5.26	1.57	1.45
30	t	101	BCR	C29-C30	5.26	1.66	1.54
30	c	515	BCR	C23-C22	5.26	1.57	1.45
30	T	101	BCR	C12-C13	5.25	1.57	1.45
30	k	101	BCR	C23-C22	5.24	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	101	HEM	FE-NB	5.24	2.11	1.94
28	r	611	CLA	C1C-NC	-5.24	1.30	1.37
30	D	405	BCR	C29-C30	5.24	1.66	1.54
30	c	514	BCR	C29-C30	5.24	1.66	1.54
30	A	409	BCR	C29-C30	5.23	1.66	1.54
30	B	618	BCR	C29-C30	5.23	1.66	1.54
30	B	619	BCR	C29-C30	5.23	1.66	1.54
30	B	617	BCR	C23-C22	5.23	1.57	1.45
30	a	410	BCR	C23-C22	5.22	1.57	1.45
30	c	514	BCR	C23-C22	5.20	1.57	1.45
30	a	410	BCR	C29-C30	5.20	1.66	1.54
30	B	617	BCR	C29-C30	5.20	1.66	1.54
30	k	101	BCR	C29-C30	5.20	1.66	1.54
30	C	514	BCR	C29-C30	5.20	1.66	1.54
30	b	617	BCR	C23-C22	5.20	1.57	1.45
30	C	514	BCR	C23-C22	5.19	1.57	1.45
30	d	406	BCR	C23-C22	5.19	1.57	1.45
30	b	618	BCR	C29-C30	5.19	1.66	1.54
30	b	617	BCR	C29-C30	5.18	1.66	1.54
30	H	101	BCR	C29-C30	5.18	1.66	1.54
30	D	405	BCR	C23-C22	5.18	1.57	1.45
30	d	406	BCR	C29-C30	5.17	1.66	1.54
30	C	516	BCR	C29-C30	5.17	1.66	1.54
30	b	619	BCR	C8-C9	5.16	1.57	1.45
30	T	101	BCR	C23-C22	5.16	1.57	1.45
30	c	515	BCR	C29-C30	5.16	1.66	1.54
30	h	101	BCR	C29-C30	5.14	1.66	1.54
30	K	101	BCR	C23-C22	5.11	1.56	1.45
39	N	616	LUT	C4-C5	-5.11	1.43	1.51
40	g	617	NEX	C7-C8	5.10	1.40	1.32
40	s	616	NEX	C7-C8	5.08	1.40	1.32
39	G	615	LUT	C8-C9	5.05	1.56	1.45
39	s	614	LUT	C8-C9	5.01	1.56	1.45
39	S	315	LUT	C8-C9	5.00	1.56	1.45
39	n	616	LUT	C4-C5	-5.00	1.43	1.51
39	s	615	LUT	C8-C9	4.99	1.56	1.45
39	g	616	LUT	C8-C9	4.99	1.56	1.45
39	S	316	LUT	C8-C9	4.98	1.56	1.45
30	T	101	BCR	C8-C9	4.98	1.56	1.45
39	Y	616	LUT	C4-C5	-4.95	1.43	1.51
39	g	615	LUT	C8-C9	4.95	1.56	1.45
39	y	316	LUT	C8-C9	4.90	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	614	LUT	C8-C9	4.88	1.56	1.45
39	y	315	LUT	C8-C9	4.85	1.56	1.45
39	G	615	LUT	C12-C13	4.83	1.56	1.45
30	i	101	BCR	C15-C14	4.81	1.58	1.43
40	y	301	NEX	C7-C8	4.81	1.40	1.32
30	c	515	BCR	C15-C14	4.80	1.58	1.43
30	C	515	BCR	C15-C14	4.80	1.58	1.43
30	k	101	BCR	C15-C14	4.78	1.58	1.43
30	t	101	BCR	C15-C14	4.78	1.58	1.43
39	n	615	LUT	C8-C9	4.78	1.56	1.45
30	B	617	BCR	C15-C14	4.77	1.58	1.43
30	T	101	BCR	C29-C30	4.77	1.65	1.54
30	a	410	BCR	C15-C14	4.76	1.58	1.43
30	C	514	BCR	C15-C14	4.76	1.58	1.43
30	B	618	BCR	C15-C14	4.76	1.58	1.43
30	b	619	BCR	C29-C30	4.76	1.65	1.54
30	C	516	BCR	C15-C14	4.75	1.58	1.43
30	b	617	BCR	C15-C14	4.74	1.58	1.43
30	K	101	BCR	C15-C14	4.74	1.58	1.43
30	d	406	BCR	C15-C14	4.73	1.58	1.43
30	B	619	BCR	C15-C14	4.73	1.58	1.43
30	b	619	BCR	C2-C1	4.73	1.65	1.54
30	b	618	BCR	C15-C14	4.73	1.58	1.43
30	i	101	BCR	C19-C18	4.73	1.56	1.45
30	A	409	BCR	C15-C14	4.73	1.58	1.43
40	n	617	NEX	C7-C8	4.73	1.39	1.32
30	h	101	BCR	C15-C14	4.72	1.58	1.43
39	r	614	LUT	C4-C5	-4.72	1.43	1.51
30	D	405	BCR	C15-C14	4.71	1.58	1.43
39	s	614	LUT	C12-C13	4.71	1.56	1.45
33	A	412	PL9	C3-C4	-4.70	1.42	1.49
30	C	514	BCR	C2-C1	4.69	1.64	1.54
30	c	515	BCR	C19-C18	4.69	1.56	1.45
39	n	615	LUT	C4-C5	-4.68	1.43	1.51
39	G	616	LUT	C8-C9	4.68	1.56	1.45
30	b	617	BCR	C2-C1	4.67	1.64	1.54
30	C	515	BCR	C19-C18	4.67	1.56	1.45
30	H	101	BCR	C15-C14	4.67	1.57	1.43
30	t	101	BCR	C19-C18	4.66	1.56	1.45
30	b	618	BCR	C19-C18	4.66	1.56	1.45
30	t	101	BCR	C2-C1	4.66	1.64	1.54
30	B	618	BCR	C19-C18	4.65	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	514	BCR	C15-C14	4.65	1.57	1.43
39	S	315	LUT	C12-C13	4.65	1.55	1.45
30	d	406	BCR	C2-C1	4.64	1.64	1.54
30	D	405	BCR	C2-C1	4.64	1.64	1.54
30	b	619	BCR	C23-C22	4.64	1.55	1.45
33	a	412	PL9	C3-C4	-4.64	1.42	1.49
39	s	615	LUT	C12-C13	4.62	1.55	1.45
30	C	516	BCR	C19-C18	4.62	1.55	1.45
39	r	614	LUT	C12-C13	4.62	1.55	1.45
39	S	316	LUT	C12-C13	4.61	1.55	1.45
30	B	619	BCR	C19-C18	4.61	1.55	1.45
30	c	514	BCR	C19-C18	4.61	1.55	1.45
30	h	101	BCR	C19-C18	4.60	1.55	1.45
30	K	101	BCR	C2-C1	4.60	1.64	1.54
30	B	617	BCR	C19-C18	4.60	1.55	1.45
30	C	514	BCR	C19-C18	4.60	1.55	1.45
30	A	409	BCR	C2-C1	4.59	1.64	1.54
30	B	619	BCR	C2-C1	4.59	1.64	1.54
30	B	617	BCR	C2-C1	4.59	1.64	1.54
30	c	514	BCR	C2-C1	4.58	1.64	1.54
30	H	101	BCR	C19-C18	4.58	1.55	1.45
30	b	617	BCR	C19-C18	4.58	1.55	1.45
39	R	614	LUT	C8-C9	4.58	1.55	1.45
30	T	101	BCR	C15-C14	4.58	1.57	1.43
30	H	101	BCR	C2-C1	4.57	1.64	1.54
39	N	615	LUT	C8-C9	4.57	1.55	1.45
30	b	618	BCR	C2-C1	4.57	1.64	1.54
39	G	616	LUT	C12-C13	4.56	1.55	1.45
39	g	616	LUT	C12-C13	4.56	1.55	1.45
30	B	618	BCR	C2-C1	4.55	1.64	1.54
30	c	515	BCR	C2-C1	4.55	1.64	1.54
30	k	101	BCR	C2-C1	4.55	1.64	1.54
30	A	409	BCR	C19-C18	4.55	1.55	1.45
30	k	101	BCR	C19-C18	4.54	1.55	1.45
39	g	615	LUT	C4-C5	-4.54	1.44	1.51
39	Y	616	LUT	C8-C9	4.54	1.55	1.45
30	d	406	BCR	C19-C18	4.53	1.55	1.45
30	a	410	BCR	C19-C18	4.53	1.55	1.45
39	y	316	LUT	C12-C13	4.52	1.55	1.45
39	g	615	LUT	C12-C13	4.52	1.55	1.45
30	D	405	BCR	C19-C18	4.51	1.55	1.45
30	i	101	BCR	C2-C1	4.51	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	406	PL9	C3-C4	-4.50	1.42	1.49
30	a	410	BCR	C2-C1	4.50	1.64	1.54
30	T	101	BCR	C2-C1	4.50	1.64	1.54
39	G	616	LUT	C4-C5	-4.50	1.44	1.51
30	C	515	BCR	C2-C1	4.50	1.64	1.54
33	d	407	PL9	C3-C4	-4.49	1.42	1.49
30	C	516	BCR	C2-C1	4.47	1.64	1.54
30	h	101	BCR	C2-C1	4.46	1.64	1.54
30	K	101	BCR	C19-C18	4.46	1.55	1.45
39	n	616	LUT	C8-C9	4.46	1.55	1.45
39	N	616	LUT	C8-C9	4.46	1.55	1.45
39	n	615	LUT	C12-C13	4.45	1.55	1.45
39	g	616	LUT	C4-C5	-4.44	1.44	1.51
39	G	615	LUT	C15-C14	4.44	1.57	1.43
39	G	615	LUT	C31-C30	4.43	1.57	1.43
39	y	315	LUT	C12-C13	4.43	1.55	1.45
39	R	614	LUT	C4-C5	-4.41	1.44	1.51
39	y	315	LUT	C4-C5	-4.40	1.44	1.51
39	S	315	LUT	C31-C30	4.40	1.57	1.43
39	S	315	LUT	C4-C5	-4.39	1.44	1.51
39	s	614	LUT	C15-C14	4.39	1.57	1.43
39	G	615	LUT	C35-C34	4.39	1.57	1.43
39	R	614	LUT	C12-C13	4.39	1.55	1.45
39	s	614	LUT	C31-C30	4.38	1.57	1.43
39	s	615	LUT	C15-C14	4.38	1.57	1.43
30	b	619	BCR	C15-C14	4.37	1.57	1.43
39	s	614	LUT	C4-C5	-4.36	1.44	1.51
30	T	101	BCR	C19-C18	4.35	1.55	1.45
39	g	616	LUT	C15-C14	4.35	1.56	1.43
39	S	316	LUT	C15-C14	4.35	1.56	1.43
39	G	616	LUT	C15-C14	4.34	1.56	1.43
30	C	516	BCR	C20-C21	4.33	1.56	1.43
39	S	316	LUT	C31-C30	4.32	1.56	1.43
30	i	101	BCR	C20-C21	4.32	1.56	1.43
28	s	603	CLA	CBB-CAB	4.32	1.51	1.30
28	n	612	CLA	CBB-CAB	4.32	1.51	1.30
30	c	515	BCR	C20-C21	4.32	1.56	1.43
39	s	615	LUT	C31-C30	4.31	1.56	1.43
30	c	514	BCR	C28-C27	4.31	1.66	1.52
39	S	315	LUT	C15-C14	4.31	1.56	1.43
39	N	616	LUT	C12-C13	4.31	1.55	1.45
38	g	605	CHL	CBB-CAB	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	316	LUT	C4-C5	-4.31	1.44	1.51
30	C	515	BCR	C20-C21	4.30	1.56	1.43
36	C	517	DGD	O1G-C1A	4.30	1.45	1.33
39	r	614	LUT	C15-C14	4.30	1.56	1.43
39	s	614	LUT	C35-C34	4.30	1.56	1.43
30	t	101	BCR	C20-C21	4.30	1.56	1.43
28	c	507	CLA	CBB-CAB	4.30	1.51	1.30
38	g	608	CHL	CBB-CAB	4.29	1.51	1.30
28	d	405	CLA	CBB-CAB	4.29	1.51	1.30
28	G	602	CLA	CBB-CAB	4.29	1.51	1.30
28	n	602	CLA	CBB-CAB	4.29	1.51	1.30
30	B	619	BCR	C20-C21	4.29	1.56	1.43
28	Y	603	CLA	CBB-CAB	4.29	1.51	1.30
39	S	316	LUT	C4-C5	-4.29	1.44	1.51
28	G	603	CLA	CBB-CAB	4.29	1.51	1.30
30	D	405	BCR	C28-C27	4.29	1.66	1.52
30	h	101	BCR	C20-C21	4.29	1.56	1.43
38	n	607	CHL	CBB-CAB	4.29	1.51	1.30
39	Y	615	LUT	C8-C9	4.29	1.55	1.45
30	b	618	BCR	C20-C21	4.29	1.56	1.43
39	y	316	LUT	C15-C14	4.29	1.56	1.43
39	y	316	LUT	C31-C30	4.29	1.56	1.43
28	B	611	CLA	CBB-CAB	4.29	1.51	1.30
28	C	508	CLA	CBB-CAB	4.29	1.51	1.30
28	r	602	CLA	CBB-CAB	4.29	1.51	1.30
28	c	502	CLA	CBB-CAB	4.29	1.51	1.30
28	G	614	CLA	CBB-CAB	4.29	1.51	1.30
28	s	602	CLA	CBB-CAB	4.28	1.51	1.30
30	d	406	BCR	C28-C27	4.28	1.65	1.52
28	N	613	CLA	CBB-CAB	4.28	1.51	1.30
28	y	303	CLA	CBB-CAB	4.28	1.51	1.30
28	c	510	CLA	CBB-CAB	4.28	1.51	1.30
39	g	615	LUT	C15-C14	4.28	1.56	1.43
28	Y	612	CLA	CBB-CAB	4.28	1.51	1.30
28	c	504	CLA	CBB-CAB	4.28	1.51	1.30
28	S	303	CLA	CBB-CAB	4.28	1.51	1.30
28	r	612	CLA	CBB-CAB	4.28	1.51	1.30
28	S	312	CLA	CBB-CAB	4.28	1.51	1.30
28	a	406	CLA	CBB-CAB	4.28	1.51	1.30
28	B	607	CLA	CBB-CAB	4.28	1.51	1.30
28	C	511	CLA	CBB-CAB	4.28	1.51	1.30
28	d	401	CLA	CBB-CAB	4.28	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	602	CLA	CBB-CAB	4.28	1.51	1.30
28	C	509	CLA	CBB-CAB	4.28	1.51	1.30
28	b	608	CLA	CBB-CAB	4.28	1.51	1.30
28	R	610	CLA	CBB-CAB	4.28	1.51	1.30
28	b	602	CLA	CBB-CAB	4.28	1.51	1.30
28	c	511	CLA	CBB-CAB	4.28	1.51	1.30
38	n	605	CHL	CBB-CAB	4.28	1.51	1.30
28	b	610	CLA	CBB-CAB	4.28	1.51	1.30
28	A	405	CLA	CBB-CAB	4.28	1.51	1.30
28	A	406	CLA	CBB-CAB	4.28	1.51	1.30
28	s	613	CLA	CBB-CAB	4.28	1.51	1.30
28	b	614	CLA	CBB-CAB	4.28	1.51	1.30
28	Y	613	CLA	CBB-CAB	4.28	1.51	1.30
28	n	614	CLA	CBB-CAB	4.28	1.51	1.30
28	R	609	CLA	CBB-CAB	4.28	1.51	1.30
28	C	505	CLA	CBB-CAB	4.28	1.51	1.30
28	b	606	CLA	CBB-CAB	4.28	1.51	1.30
28	S	304	CLA	CBB-CAB	4.28	1.51	1.30
36	c	517	DGD	O1G-C1A	4.28	1.45	1.33
28	B	605	CLA	CBB-CAB	4.28	1.51	1.30
28	R	612	CLA	CBB-CAB	4.28	1.51	1.30
28	g	602	CLA	CBB-CAB	4.28	1.51	1.30
28	C	504	CLA	CBB-CAB	4.28	1.51	1.30
28	b	616	CLA	CBB-CAB	4.28	1.51	1.30
28	r	603	CLA	CBB-CAB	4.28	1.51	1.30
28	s	608	CLA	CBB-CAB	4.28	1.51	1.30
38	G	605	CHL	CBB-CAB	4.28	1.51	1.30
28	R	613	CLA	CBB-CAB	4.28	1.51	1.30
28	b	607	CLA	CBB-CAB	4.28	1.51	1.30
28	r	608	CLA	CBB-CAB	4.28	1.51	1.30
30	C	515	BCR	C28-C27	4.28	1.65	1.52
28	R	608	CLA	CBB-CAB	4.28	1.51	1.30
28	R	601	CLA	CBB-CAB	4.28	1.51	1.30
28	B	602	CLA	CBB-CAB	4.28	1.51	1.30
28	r	610	CLA	CBB-CAB	4.28	1.51	1.30
30	B	617	BCR	C20-C21	4.27	1.56	1.43
28	r	613	CLA	CBB-CAB	4.27	1.51	1.30
38	Y	605	CHL	CBB-CAB	4.27	1.51	1.30
28	D	401	CLA	CBB-CAB	4.27	1.51	1.30
28	S	313	CLA	CBB-CAB	4.27	1.51	1.30
28	c	506	CLA	CBB-CAB	4.27	1.51	1.30
28	G	613	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	s	604	CLA	CBB-CAB	4.27	1.51	1.30
39	s	615	LUT	C4-C5	-4.27	1.44	1.51
28	b	612	CLA	CBB-CAB	4.27	1.51	1.30
28	r	601	CLA	CBB-CAB	4.27	1.51	1.30
28	C	507	CLA	CBB-CAB	4.27	1.51	1.30
28	b	613	CLA	CBB-CAB	4.27	1.51	1.30
28	c	512	CLA	CBB-CAB	4.27	1.51	1.30
28	C	506	CLA	CBB-CAB	4.27	1.51	1.30
28	b	603	CLA	CBB-CAB	4.27	1.51	1.30
28	r	609	CLA	CBB-CAB	4.27	1.51	1.30
28	g	613	CLA	CBB-CAB	4.27	1.51	1.30
28	B	616	CLA	CBB-CAB	4.27	1.51	1.30
28	N	611	CLA	CBB-CAB	4.27	1.51	1.30
28	y	313	CLA	CBB-CAB	4.27	1.51	1.30
28	y	314	CLA	CBB-CAB	4.27	1.51	1.30
28	n	603	CLA	CBB-CAB	4.27	1.51	1.30
28	B	609	CLA	CBB-CAB	4.27	1.51	1.30
28	c	503	CLA	CBB-CAB	4.27	1.51	1.30
28	B	612	CLA	CBB-CAB	4.27	1.51	1.30
38	Y	608	CHL	CBB-CAB	4.27	1.51	1.30
28	d	404	CLA	CBB-CAB	4.27	1.51	1.30
38	N	605	CHL	CBB-CAB	4.27	1.51	1.30
28	B	614	CLA	CBB-CAB	4.27	1.51	1.30
28	B	606	CLA	CBB-CAB	4.27	1.51	1.30
28	G	611	CLA	CBB-CAB	4.27	1.51	1.30
28	S	309	CLA	CBB-CAB	4.27	1.51	1.30
28	b	611	CLA	CBB-CAB	4.27	1.51	1.30
28	R	611	CLA	CBB-CAB	4.27	1.51	1.30
28	g	604	CLA	CBB-CAB	4.27	1.51	1.30
38	y	306	CHL	CBB-CAB	4.27	1.51	1.30
28	S	311	CLA	CBB-CAB	4.27	1.51	1.30
28	a	409	CLA	CBB-CAB	4.27	1.51	1.30
28	N	612	CLA	CBB-CAB	4.27	1.51	1.30
30	K	101	BCR	C28-C27	4.27	1.65	1.52
39	G	615	LUT	C21-C26	4.27	1.68	1.56
28	y	311	CLA	CBB-CAB	4.27	1.51	1.30
28	B	608	CLA	CBB-CAB	4.27	1.51	1.30
28	b	604	CLA	CBB-CAB	4.27	1.51	1.30
28	b	609	CLA	CBB-CAB	4.27	1.51	1.30
39	g	615	LUT	C31-C30	4.27	1.56	1.43
28	G	604	CLA	CBB-CAB	4.27	1.51	1.30
28	C	510	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	513	CLA	CBB-CAB	4.26	1.51	1.30
28	Y	604	CLA	CBB-CAB	4.26	1.51	1.30
28	Y	611	CLA	CBB-CAB	4.26	1.51	1.30
28	s	610	CLA	CBB-CAB	4.26	1.51	1.30
28	B	604	CLA	CBB-CAB	4.26	1.51	1.30
30	B	618	BCR	C20-C21	4.26	1.56	1.43
28	y	312	CLA	CBB-CAB	4.26	1.51	1.30
28	A	408	CLA	CBB-CAB	4.26	1.51	1.30
28	C	503	CLA	CBB-CAB	4.26	1.51	1.30
30	T	101	BCR	C20-C21	4.26	1.56	1.43
39	s	615	LUT	C35-C34	4.26	1.56	1.43
28	a	407	CLA	CBB-CAB	4.26	1.51	1.30
38	R	607	CHL	CBB-CAB	4.26	1.51	1.30
28	y	304	CLA	CBB-CAB	4.26	1.51	1.30
28	G	610	CLA	CBB-CAB	4.26	1.51	1.30
28	c	501	CLA	CBB-CAB	4.26	1.51	1.30
28	y	310	CLA	CBB-CAB	4.26	1.51	1.30
28	C	502	CLA	CBB-CAB	4.26	1.51	1.30
28	C	501	CLA	CBB-CAB	4.26	1.51	1.30
28	G	612	CLA	CBB-CAB	4.26	1.51	1.30
28	D	403	CLA	CBB-CAB	4.26	1.51	1.30
28	N	614	CLA	CBB-CAB	4.26	1.51	1.30
28	N	604	CLA	CBB-CAB	4.26	1.51	1.30
28	S	314	CLA	CBB-CAB	4.26	1.51	1.30
28	b	615	CLA	CBB-CAB	4.26	1.51	1.30
28	C	513	CLA	CBB-CAB	4.26	1.51	1.30
28	s	611	CLA	CBB-CAB	4.26	1.51	1.30
38	r	607	CHL	CBB-CAB	4.26	1.51	1.30
28	r	604	CLA	CBB-CAB	4.26	1.51	1.30
28	B	603	CLA	CBB-CAB	4.26	1.51	1.30
28	B	610	CLA	CBB-CAB	4.26	1.51	1.30
28	N	610	CLA	CBB-CAB	4.26	1.51	1.30
28	g	614	CLA	CBB-CAB	4.26	1.51	1.30
39	g	616	LUT	C31-C30	4.26	1.56	1.43
28	D	404	CLA	CBB-CAB	4.26	1.51	1.30
28	n	604	CLA	CBB-CAB	4.26	1.51	1.30
28	Y	614	CLA	CBB-CAB	4.26	1.51	1.30
36	B	626	DGD	O1G-C1A	4.26	1.45	1.33
30	C	514	BCR	C28-C27	4.26	1.65	1.52
28	s	612	CLA	CBB-CAB	4.26	1.51	1.30
28	r	611	CLA	CBB-CAB	4.26	1.51	1.30
30	H	101	BCR	C20-C21	4.26	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	505	CLA	CBB-CAB	4.26	1.51	1.30
39	N	615	LUT	C4-C5	-4.25	1.44	1.51
30	t	101	BCR	C28-C27	4.25	1.65	1.52
28	y	305	CLA	CBB-CAB	4.25	1.51	1.30
38	S	308	CHL	CBB-CAB	4.25	1.51	1.30
28	n	610	CLA	CBB-CAB	4.25	1.51	1.30
36	A	417	DGD	O1G-C1A	4.25	1.45	1.33
28	s	609	CLA	CBB-CAB	4.25	1.51	1.30
30	k	101	BCR	C20-C21	4.25	1.56	1.43
28	B	615	CLA	CBB-CAB	4.25	1.51	1.30
28	B	613	CLA	CBB-CAB	4.25	1.51	1.30
28	B	601	CLA	CBB-CAB	4.25	1.51	1.30
28	N	603	CLA	CBB-CAB	4.25	1.51	1.30
30	c	514	BCR	C20-C21	4.25	1.56	1.43
38	g	609	CHL	CBB-CAB	4.24	1.51	1.30
28	n	611	CLA	CBB-CAB	4.24	1.51	1.30
28	C	512	CLA	CBB-CAB	4.24	1.51	1.30
38	s	607	CHL	CBB-CAB	4.24	1.51	1.30
28	g	612	CLA	CBB-CAB	4.24	1.51	1.30
36	c	518	DGD	O1G-C1A	4.24	1.45	1.33
28	b	601	CLA	CBB-CAB	4.24	1.51	1.30
38	Y	601	CHL	CBB-CAB	4.24	1.51	1.30
28	g	610	CLA	CBB-CAB	4.24	1.51	1.30
38	r	606	CHL	CBB-CAB	4.24	1.51	1.30
30	C	514	BCR	C20-C21	4.24	1.56	1.43
38	G	609	CHL	CBB-CAB	4.24	1.51	1.30
38	Y	609	CHL	CBB-CAB	4.23	1.51	1.30
38	S	302	CHL	CBB-CAB	4.23	1.51	1.30
38	s	606	CHL	CBB-CAB	4.23	1.51	1.30
39	S	316	LUT	C35-C34	4.23	1.56	1.43
30	b	617	BCR	C20-C21	4.23	1.56	1.43
38	n	601	CHL	CBB-CAB	4.23	1.51	1.30
28	n	613	CLA	CBB-CAB	4.23	1.51	1.30
39	G	615	LUT	C28-C29	4.23	1.55	1.45
28	S	310	CLA	CBB-CAB	4.23	1.51	1.30
38	g	601	CHL	CBB-CAB	4.23	1.51	1.30
38	n	608	CHL	CBB-CAB	4.23	1.51	1.30
39	R	614	LUT	C15-C14	4.22	1.56	1.43
28	S	305	CLA	CBB-CAB	4.22	1.51	1.30
38	g	619	CHL	CBB-CAB	4.22	1.51	1.30
36	b	625	DGD	O1G-C1A	4.22	1.45	1.33
39	y	315	LUT	C31-C30	4.22	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	516	DGD	O1G-C1A	4.22	1.45	1.33
38	N	601	CHL	CBB-CAB	4.22	1.51	1.30
30	H	101	BCR	C28-C27	4.22	1.65	1.52
38	G	607	CHL	CBB-CAB	4.22	1.51	1.30
30	A	409	BCR	C20-C21	4.22	1.56	1.43
38	y	309	CHL	CBB-CAB	4.22	1.51	1.30
36	C	519	DGD	O1G-C1A	4.22	1.45	1.33
30	D	405	BCR	C20-C21	4.21	1.56	1.43
39	y	315	LUT	C15-C14	4.21	1.56	1.43
38	n	609	CHL	CBB-CAB	4.21	1.51	1.30
39	G	615	LUT	C4-C5	-4.21	1.44	1.51
30	b	617	BCR	C28-C27	4.21	1.65	1.52
30	B	619	BCR	C28-C27	4.21	1.65	1.52
38	N	609	CHL	CBB-CAB	4.20	1.51	1.30
38	y	308	CHL	CBB-CAB	4.20	1.51	1.30
30	C	516	BCR	C28-C27	4.20	1.65	1.52
38	S	307	CHL	CBB-CAB	4.20	1.51	1.30
30	d	406	BCR	C20-C21	4.20	1.56	1.43
39	N	615	LUT	C12-C13	4.20	1.55	1.45
38	g	607	CHL	CBB-CAB	4.20	1.51	1.30
30	a	410	BCR	C20-C21	4.20	1.56	1.43
38	S	306	CHL	CBB-CAB	4.20	1.51	1.30
39	G	616	LUT	C35-C34	4.20	1.56	1.43
39	n	615	LUT	C31-C30	4.20	1.56	1.43
38	G	601	CHL	CBB-CAB	4.20	1.51	1.30
38	N	606	CHL	CBB-CAB	4.19	1.51	1.30
38	y	307	CHL	CBB-CAB	4.19	1.51	1.30
28	c	508	CLA	CBB-CAB	4.19	1.51	1.30
39	Y	616	LUT	C12-C13	4.19	1.54	1.45
38	G	606	CHL	CBB-CAB	4.19	1.51	1.30
39	g	615	LUT	C35-C34	4.19	1.56	1.43
30	h	101	BCR	C28-C27	4.19	1.65	1.52
38	R	605	CHL	CBB-CAB	4.19	1.51	1.30
30	K	101	BCR	C20-C21	4.19	1.56	1.43
28	R	603	CLA	CBB-CAB	4.19	1.51	1.30
39	g	616	LUT	C35-C34	4.19	1.56	1.43
38	N	608	CHL	CBB-CAB	4.19	1.51	1.30
38	R	606	CHL	CBB-CAB	4.18	1.51	1.30
38	y	302	CHL	CBB-CAB	4.18	1.51	1.30
30	c	515	BCR	C28-C27	4.18	1.65	1.52
36	C	518	DGD	O1G-C1A	4.18	1.45	1.33
39	S	315	LUT	C28-C29	4.18	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	617	BCR	C28-C27	4.17	1.65	1.52
30	T	101	BCR	C28-C27	4.17	1.65	1.52
38	Y	606	CHL	CBB-CAB	4.17	1.51	1.30
28	R	604	CLA	CBB-CAB	4.17	1.51	1.30
39	G	616	LUT	C31-C30	4.17	1.56	1.43
28	g	603	CLA	CBB-CAB	4.17	1.51	1.30
38	N	607	CHL	CBB-CAB	4.17	1.50	1.30
39	y	316	LUT	C35-C34	4.17	1.56	1.43
38	s	605	CHL	CBB-CAB	4.16	1.50	1.30
28	Y	602	CLA	CBB-CAB	4.16	1.50	1.30
38	G	608	CHL	CBB-CAB	4.16	1.50	1.30
30	a	410	BCR	C28-C27	4.16	1.65	1.52
38	Y	607	CHL	CBB-CAB	4.16	1.50	1.30
39	R	614	LUT	C35-C34	4.16	1.56	1.43
39	r	614	LUT	C31-C30	4.15	1.56	1.43
39	S	315	LUT	C35-C34	4.15	1.56	1.43
39	r	614	LUT	C35-C34	4.15	1.56	1.43
38	g	606	CHL	CBB-CAB	4.14	1.50	1.30
28	g	611	CLA	CBB-CAB	4.14	1.50	1.30
38	s	601	CHL	CBB-CAB	4.14	1.50	1.30
30	A	409	BCR	C28-C27	4.14	1.65	1.52
28	Y	610	CLA	CBB-CAB	4.14	1.50	1.30
39	N	616	LUT	C31-C30	4.14	1.56	1.43
30	b	618	BCR	C28-C27	4.13	1.65	1.52
39	n	615	LUT	C35-C34	4.13	1.56	1.43
28	R	602	CLA	CBB-CAB	4.13	1.50	1.30
30	B	618	BCR	C28-C27	4.13	1.65	1.52
38	n	606	CHL	CBB-CAB	4.13	1.50	1.30
30	i	101	BCR	C28-C27	4.13	1.65	1.52
39	N	615	LUT	C15-C14	4.12	1.56	1.43
37	E	101	HEM	FE-NC	4.12	2.09	1.95
28	c	509	CLA	CBB-CAB	4.12	1.50	1.30
39	G	615	LUT	C7-C6	4.11	1.59	1.45
39	y	315	LUT	C35-C34	4.11	1.56	1.43
39	n	615	LUT	C15-C14	4.11	1.56	1.43
30	b	619	BCR	C28-C27	4.11	1.65	1.52
39	n	616	LUT	C12-C13	4.10	1.54	1.45
36	a	401	DGD	O1G-C1A	4.10	1.45	1.33
39	N	615	LUT	C31-C30	4.10	1.56	1.43
39	s	614	LUT	C28-C29	4.10	1.54	1.45
39	Y	616	LUT	C15-C14	4.10	1.56	1.43
30	k	101	BCR	C28-C27	4.10	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	FE-NC	4.10	2.09	1.95
38	r	605	CHL	CBB-CAB	4.09	1.50	1.30
39	s	615	LUT	C28-C29	4.06	1.54	1.45
39	g	616	LUT	C28-C29	4.06	1.54	1.45
39	n	615	LUT	C7-C6	4.05	1.59	1.45
39	g	616	LUT	C7-C6	4.04	1.59	1.45
39	N	616	LUT	C15-C14	4.04	1.56	1.43
39	S	316	LUT	C28-C29	4.04	1.54	1.45
39	n	616	LUT	C31-C30	4.04	1.56	1.43
39	S	315	LUT	C7-C6	4.04	1.59	1.45
39	S	316	LUT	C7-C6	4.03	1.59	1.45
28	b	605	CLA	CBB-CAB	4.03	1.50	1.30
39	s	615	LUT	C7-C6	4.02	1.59	1.45
39	s	614	LUT	C7-C6	4.01	1.59	1.45
39	N	615	LUT	C35-C34	4.01	1.55	1.43
39	y	316	LUT	C28-C29	4.01	1.54	1.45
28	Y	602	CLA	MG-ND	-4.00	1.97	2.05
39	g	616	LUT	C21-C26	4.00	1.67	1.56
39	N	616	LUT	C35-C34	4.00	1.55	1.43
39	g	615	LUT	C7-C6	4.00	1.59	1.45
39	s	615	LUT	C21-C26	4.00	1.67	1.56
39	y	316	LUT	C7-C6	3.99	1.59	1.45
39	Y	616	LUT	C35-C34	3.99	1.55	1.43
30	t	101	BCR	C3-C4	3.99	1.65	1.52
39	Y	615	LUT	C31-C30	3.99	1.55	1.43
30	b	619	BCR	C19-C18	3.98	1.54	1.45
28	S	305	CLA	MG-ND	-3.98	1.97	2.05
39	s	614	LUT	C21-C26	3.97	1.67	1.56
39	g	615	LUT	C28-C29	3.95	1.54	1.45
30	D	405	BCR	C3-C4	3.95	1.64	1.52
39	y	315	LUT	C7-C6	3.95	1.59	1.45
28	r	611	CLA	MG-ND	-3.95	1.98	2.05
30	b	619	BCR	C20-C21	3.94	1.55	1.43
39	n	616	LUT	C15-C14	3.93	1.55	1.43
30	C	516	BCR	C3-C4	3.93	1.64	1.52
30	H	101	BCR	C3-C4	3.93	1.64	1.52
28	R	602	CLA	C4B-NB	-3.93	1.33	1.37
28	n	611	CLA	MG-ND	-3.92	1.98	2.05
30	b	618	BCR	C3-C4	3.92	1.64	1.52
39	Y	615	LUT	C12-C13	3.92	1.54	1.45
30	d	406	BCR	C3-C4	3.91	1.64	1.52
30	B	618	BCR	C3-C4	3.91	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	514	BCR	C3-C4	3.91	1.64	1.52
39	G	615	LUT	C11-C10	3.90	1.55	1.43
39	S	315	LUT	C21-C26	3.90	1.67	1.56
39	n	616	LUT	C35-C34	3.89	1.55	1.43
39	R	614	LUT	C21-C26	3.89	1.67	1.56
39	R	614	LUT	C31-C30	3.89	1.55	1.43
30	k	101	BCR	C3-C4	3.89	1.64	1.52
39	Y	615	LUT	C15-C14	3.89	1.55	1.43
39	y	315	LUT	C28-C29	3.89	1.54	1.45
30	B	619	BCR	C3-C4	3.88	1.64	1.52
30	c	514	BCR	C3-C4	3.88	1.64	1.52
39	N	616	LUT	C28-C29	3.87	1.54	1.45
39	y	316	LUT	C21-C26	3.87	1.67	1.56
30	C	515	BCR	C3-C4	3.87	1.64	1.52
30	a	410	BCR	C3-C4	3.87	1.64	1.52
39	n	615	LUT	C28-C29	3.86	1.54	1.45
30	b	617	BCR	C3-C4	3.86	1.64	1.52
30	c	515	BCR	C3-C4	3.86	1.64	1.52
30	h	101	BCR	C3-C4	3.86	1.64	1.52
30	i	101	BCR	C3-C4	3.86	1.64	1.52
28	b	605	CLA	C4B-NB	-3.85	1.33	1.37
39	S	316	LUT	C21-C26	3.84	1.67	1.56
39	r	614	LUT	C21-C26	3.84	1.67	1.56
30	A	409	BCR	C3-C4	3.84	1.64	1.52
39	Y	616	LUT	C31-C30	3.84	1.55	1.43
28	R	602	CLA	MG-ND	-3.84	1.98	2.05
39	Y	615	LUT	C21-C26	3.84	1.67	1.56
30	B	617	BCR	C3-C4	3.83	1.64	1.52
39	R	614	LUT	C28-C29	3.83	1.54	1.45
28	n	612	CLA	MG-ND	-3.83	1.98	2.05
28	g	603	CLA	MG-ND	-3.83	1.98	2.05
39	Y	616	LUT	C7-C6	3.82	1.58	1.45
39	r	614	LUT	C7-C6	3.82	1.58	1.45
30	K	101	BCR	C3-C4	3.81	1.64	1.52
30	i	101	BCR	C16-C17	3.81	1.55	1.43
39	y	315	LUT	C21-C26	3.80	1.67	1.56
30	c	515	BCR	C16-C17	3.80	1.55	1.43
30	T	101	BCR	C3-C4	3.79	1.64	1.52
39	Y	615	LUT	C35-C34	3.79	1.55	1.43
30	B	617	BCR	C16-C17	3.79	1.55	1.43
39	G	616	LUT	C7-C6	3.78	1.58	1.45
39	r	614	LUT	C28-C29	3.78	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	516	BCR	C16-C17	3.77	1.55	1.43
30	C	514	BCR	C16-C17	3.77	1.55	1.43
30	C	515	BCR	C16-C17	3.77	1.55	1.43
30	h	101	BCR	C16-C17	3.76	1.55	1.43
39	s	614	LUT	C11-C10	3.76	1.55	1.43
30	t	101	BCR	C16-C17	3.76	1.55	1.43
39	R	614	LUT	C23-C24	-3.76	1.44	1.50
39	g	615	LUT	C21-C26	3.76	1.66	1.56
30	k	101	BCR	C16-C17	3.76	1.55	1.43
39	S	316	LUT	C11-C10	3.76	1.55	1.43
39	n	616	LUT	C7-C6	3.75	1.58	1.45
28	R	602	CLA	C1C-NC	-3.75	1.32	1.37
39	N	615	LUT	C7-C6	3.74	1.58	1.45
28	c	509	CLA	MG-ND	-3.74	1.98	2.05
28	Y	610	CLA	MG-ND	-3.73	1.98	2.05
30	B	618	BCR	C16-C17	3.73	1.55	1.43
39	r	614	LUT	C19-C9	3.73	1.58	1.50
30	d	406	BCR	C16-C17	3.73	1.55	1.43
30	H	101	BCR	C16-C17	3.73	1.55	1.43
30	C	516	BCR	C11-C10	3.73	1.55	1.43
30	b	617	BCR	C16-C17	3.72	1.55	1.43
30	b	618	BCR	C16-C17	3.72	1.55	1.43
30	B	619	BCR	C16-C17	3.72	1.55	1.43
39	s	615	LUT	C11-C10	3.72	1.55	1.43
39	Y	616	LUT	C21-C26	3.72	1.66	1.56
39	N	615	LUT	C28-C29	3.72	1.53	1.45
39	S	315	LUT	C11-C10	3.72	1.55	1.43
30	h	101	BCR	C11-C10	3.72	1.55	1.43
30	H	101	BCR	C11-C10	3.72	1.55	1.43
28	b	605	CLA	C1C-NC	-3.72	1.32	1.37
39	Y	615	LUT	C7-C6	3.71	1.58	1.45
30	B	617	BCR	C11-C10	3.71	1.55	1.43
30	d	406	BCR	C11-C10	3.71	1.55	1.43
30	K	101	BCR	C16-C17	3.71	1.54	1.43
30	a	410	BCR	C16-C17	3.71	1.54	1.43
28	g	610	CLA	MG-ND	-3.71	1.98	2.05
30	D	405	BCR	C11-C10	3.71	1.54	1.43
30	i	101	BCR	C11-C10	3.70	1.54	1.43
39	R	614	LUT	C7-C6	3.70	1.58	1.45
30	k	101	BCR	C11-C10	3.70	1.54	1.43
39	r	614	LUT	C11-C10	3.70	1.54	1.43
39	G	616	LUT	C11-C10	3.70	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	613	CLA	MG-ND	-3.70	1.98	2.05
30	D	405	BCR	C16-C17	3.70	1.54	1.43
30	A	409	BCR	C16-C17	3.69	1.54	1.43
28	c	509	CLA	C1C-NC	-3.69	1.32	1.37
30	K	101	BCR	C11-C10	3.69	1.54	1.43
30	C	515	BCR	C11-C10	3.69	1.54	1.43
39	g	616	LUT	C11-C10	3.69	1.54	1.43
30	a	410	BCR	C11-C10	3.69	1.54	1.43
30	C	514	BCR	C11-C10	3.69	1.54	1.43
30	b	617	BCR	C11-C10	3.68	1.54	1.43
39	g	615	LUT	C11-C10	3.68	1.54	1.43
39	R	614	LUT	C11-C10	3.68	1.54	1.43
30	c	514	BCR	C16-C17	3.67	1.54	1.43
39	Y	615	LUT	C28-C29	3.67	1.53	1.45
28	s	611	CLA	MG-ND	-3.67	1.98	2.05
28	g	611	CLA	C1C-NC	-3.67	1.32	1.37
30	c	515	BCR	C11-C10	3.67	1.54	1.43
39	y	316	LUT	C11-C10	3.67	1.54	1.43
30	A	409	BCR	C11-C10	3.67	1.54	1.43
39	G	615	LUT	C19-C9	3.66	1.58	1.50
39	n	615	LUT	C11-C10	3.66	1.54	1.43
30	t	101	BCR	C11-C10	3.66	1.54	1.43
28	Y	610	CLA	C1C-NC	-3.66	1.32	1.37
28	g	611	CLA	MG-ND	-3.66	1.98	2.05
28	c	505	CLA	MG-ND	-3.66	1.98	2.05
30	B	619	BCR	C11-C10	3.66	1.54	1.43
30	b	619	BCR	C4-C5	-3.66	1.43	1.51
28	C	505	CLA	MG-ND	-3.65	1.98	2.05
39	G	616	LUT	C23-C24	-3.65	1.45	1.50
28	S	305	CLA	C1C-NC	-3.65	1.32	1.37
28	R	612	CLA	MG-ND	-3.65	1.98	2.05
39	N	616	LUT	C21-C26	3.65	1.66	1.56
28	Y	610	CLA	C4B-NB	-3.65	1.33	1.37
28	g	604	CLA	MG-ND	-3.65	1.98	2.05
28	g	612	CLA	MG-ND	-3.65	1.98	2.05
30	B	618	BCR	C11-C10	3.64	1.54	1.43
28	y	313	CLA	MG-ND	-3.64	1.98	2.05
28	b	608	CLA	MG-ND	-3.64	1.98	2.05
39	N	616	LUT	C7-C6	3.64	1.58	1.45
28	G	612	CLA	MG-ND	-3.63	1.98	2.05
39	N	615	LUT	C21-C26	3.63	1.66	1.56
39	n	616	LUT	C28-C29	3.63	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	s	615	LUT	C19-C9	3.63	1.58	1.50
39	G	616	LUT	C19-C9	3.63	1.58	1.50
39	Y	615	LUT	C23-C24	-3.63	1.45	1.50
30	c	514	BCR	C11-C10	3.63	1.54	1.43
28	N	612	CLA	MG-ND	-3.63	1.98	2.05
30	b	618	BCR	C11-C10	3.63	1.54	1.43
28	s	610	CLA	MG-ND	-3.63	1.98	2.05
30	T	101	BCR	C27-C26	-3.62	1.43	1.51
28	c	512	CLA	MG-ND	-3.62	1.98	2.05
39	y	316	LUT	C38-C25	3.62	1.57	1.50
30	T	101	BCR	C16-C17	3.62	1.54	1.43
28	N	611	CLA	MG-ND	-3.62	1.98	2.05
28	n	610	CLA	MG-ND	-3.62	1.98	2.05
28	Y	613	CLA	MG-ND	-3.61	1.98	2.05
39	N	616	LUT	C11-C10	3.61	1.54	1.43
28	G	603	CLA	MG-ND	-3.61	1.98	2.05
28	c	513	CLA	MG-ND	-3.61	1.98	2.05
28	N	604	CLA	MG-ND	-3.61	1.98	2.05
28	r	604	CLA	MG-ND	-3.61	1.98	2.05
39	S	315	LUT	C38-C25	3.61	1.57	1.50
30	B	618	BCR	C24-C25	3.61	1.57	1.45
28	C	507	CLA	MG-ND	-3.61	1.98	2.05
28	c	509	CLA	C4B-NB	-3.61	1.33	1.37
28	b	613	CLA	MG-ND	-3.61	1.98	2.05
39	g	615	LUT	C19-C9	3.60	1.58	1.50
30	c	515	BCR	C24-C25	3.60	1.57	1.45
28	S	310	CLA	MG-ND	-3.60	1.98	2.05
28	c	506	CLA	MG-ND	-3.60	1.98	2.05
39	g	616	LUT	C19-C9	3.60	1.58	1.50
39	g	616	LUT	C38-C25	3.60	1.57	1.50
28	C	512	CLA	MG-ND	-3.60	1.98	2.05
28	B	601	CLA	MG-ND	-3.60	1.98	2.05
28	g	603	CLA	C1C-NC	-3.60	1.32	1.37
28	N	613	CLA	MG-ND	-3.60	1.98	2.05
28	n	613	CLA	C4B-NB	-3.60	1.33	1.37
28	Y	611	CLA	MG-ND	-3.60	1.98	2.05
28	C	513	CLA	MG-ND	-3.60	1.98	2.05
28	Y	612	CLA	MG-ND	-3.60	1.98	2.05
30	b	618	BCR	C24-C25	3.60	1.57	1.45
28	B	609	CLA	MG-ND	-3.60	1.98	2.05
28	C	506	CLA	MG-ND	-3.60	1.98	2.05
28	n	613	CLA	C1C-NC	-3.59	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	s	614	LUT	C38-C25	3.59	1.57	1.50
28	S	314	CLA	MG-ND	-3.59	1.98	2.05
28	B	608	CLA	MG-ND	-3.59	1.98	2.05
39	n	616	LUT	C23-C24	-3.59	1.45	1.50
28	c	508	CLA	MG-ND	-3.59	1.98	2.05
30	b	619	BCR	C3-C4	3.59	1.63	1.52
28	b	604	CLA	MG-ND	-3.58	1.98	2.05
28	s	609	CLA	MG-ND	-3.58	1.98	2.05
39	y	315	LUT	C11-C10	3.58	1.54	1.43
28	G	611	CLA	MG-ND	-3.58	1.98	2.05
28	A	406	CLA	MG-ND	-3.58	1.98	2.05
28	A	408	CLA	MG-ND	-3.58	1.98	2.05
28	b	612	CLA	MG-ND	-3.58	1.98	2.05
28	d	404	CLA	MG-ND	-3.58	1.98	2.05
28	n	604	CLA	MG-ND	-3.58	1.98	2.05
28	B	604	CLA	MG-ND	-3.58	1.98	2.05
39	s	615	LUT	C38-C25	3.58	1.57	1.50
28	g	613	CLA	MG-ND	-3.58	1.98	2.05
39	S	316	LUT	C38-C25	3.58	1.57	1.50
39	y	315	LUT	C19-C9	3.58	1.58	1.50
28	b	615	CLA	MG-ND	-3.57	1.98	2.05
28	r	610	CLA	MG-ND	-3.57	1.98	2.05
28	s	613	CLA	MG-ND	-3.57	1.98	2.05
28	B	603	CLA	MG-ND	-3.57	1.98	2.05
28	G	613	CLA	MG-ND	-3.57	1.98	2.05
28	N	610	CLA	MG-ND	-3.57	1.98	2.05
28	b	616	CLA	MG-ND	-3.57	1.98	2.05
28	y	305	CLA	MG-ND	-3.57	1.98	2.05
28	S	312	CLA	MG-ND	-3.57	1.98	2.05
28	D	404	CLA	MG-ND	-3.57	1.98	2.05
30	i	101	BCR	C24-C25	3.57	1.57	1.45
39	S	316	LUT	C19-C9	3.57	1.58	1.50
39	y	316	LUT	C19-C9	3.57	1.58	1.50
28	S	313	CLA	MG-ND	-3.57	1.98	2.05
28	y	311	CLA	MG-ND	-3.57	1.98	2.05
28	s	603	CLA	MG-ND	-3.57	1.98	2.05
30	h	101	BCR	C24-C25	3.56	1.57	1.45
30	b	617	BCR	C24-C25	3.56	1.57	1.45
28	a	407	CLA	MG-ND	-3.56	1.98	2.05
28	C	501	CLA	MG-ND	-3.56	1.98	2.05
28	B	615	CLA	MG-ND	-3.56	1.98	2.05
30	B	619	BCR	C24-C25	3.56	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	406	BCR	C24-C25	3.56	1.57	1.45
28	R	610	CLA	MG-ND	-3.56	1.98	2.05
28	c	502	CLA	MG-ND	-3.56	1.98	2.05
28	C	503	CLA	MG-ND	-3.56	1.98	2.05
39	G	616	LUT	C28-C29	3.56	1.53	1.45
28	n	614	CLA	MG-ND	-3.56	1.98	2.05
30	C	515	BCR	C24-C25	3.56	1.57	1.45
28	b	607	CLA	MG-ND	-3.56	1.98	2.05
28	s	604	CLA	MG-ND	-3.56	1.98	2.05
28	y	314	CLA	MG-ND	-3.56	1.98	2.05
39	S	315	LUT	C19-C9	3.55	1.58	1.50
28	Y	604	CLA	MG-ND	-3.55	1.98	2.05
28	c	501	CLA	MG-ND	-3.55	1.98	2.05
28	D	403	CLA	MG-ND	-3.55	1.98	2.05
28	r	602	CLA	MG-ND	-3.55	1.98	2.05
28	n	603	CLA	MG-ND	-3.55	1.98	2.05
30	B	617	BCR	C24-C25	3.55	1.57	1.45
28	G	614	CLA	MG-ND	-3.55	1.98	2.05
28	C	502	CLA	MG-ND	-3.55	1.98	2.05
28	S	311	CLA	MG-ND	-3.55	1.98	2.05
28	Y	614	CLA	MG-ND	-3.55	1.98	2.05
28	y	303	CLA	MG-ND	-3.55	1.98	2.05
28	g	614	CLA	MG-ND	-3.55	1.98	2.05
28	b	605	CLA	MG-ND	-3.55	1.98	2.05
28	B	612	CLA	MG-ND	-3.55	1.98	2.05
30	H	101	BCR	C24-C25	3.55	1.57	1.45
28	B	614	CLA	MG-ND	-3.55	1.98	2.05
30	A	409	BCR	C24-C25	3.55	1.57	1.45
30	C	516	BCR	C24-C25	3.55	1.57	1.45
28	a	409	CLA	MG-ND	-3.55	1.98	2.05
30	k	101	BCR	C24-C25	3.55	1.57	1.45
39	n	616	LUT	C21-C26	3.55	1.66	1.56
28	R	611	CLA	MG-ND	-3.54	1.98	2.05
28	A	405	CLA	MG-ND	-3.54	1.98	2.05
39	y	315	LUT	C38-C25	3.54	1.57	1.50
28	R	609	CLA	MG-ND	-3.54	1.98	2.05
28	y	310	CLA	MG-ND	-3.54	1.98	2.05
28	c	507	CLA	MG-ND	-3.54	1.98	2.05
28	G	602	CLA	MG-ND	-3.54	1.98	2.05
28	C	508	CLA	MG-ND	-3.54	1.98	2.05
28	C	510	CLA	MG-ND	-3.54	1.98	2.05
28	N	603	CLA	MG-ND	-3.54	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	603	CLA	C1C-NC	-3.54	1.32	1.37
28	y	312	CLA	MG-ND	-3.54	1.98	2.05
30	T	101	BCR	C24-C25	3.54	1.57	1.45
28	G	604	CLA	MG-ND	-3.54	1.98	2.05
39	G	616	LUT	C21-C26	3.54	1.66	1.56
28	B	610	CLA	MG-ND	-3.54	1.98	2.05
28	N	602	CLA	MG-ND	-3.54	1.98	2.05
28	d	401	CLA	MG-ND	-3.54	1.98	2.05
28	n	612	CLA	C1C-NC	-3.53	1.32	1.37
28	y	304	CLA	MG-ND	-3.53	1.98	2.05
30	t	101	BCR	C24-C25	3.53	1.57	1.45
28	s	612	CLA	MG-ND	-3.53	1.98	2.05
28	c	511	CLA	MG-ND	-3.53	1.98	2.05
28	b	603	CLA	MG-ND	-3.53	1.98	2.05
28	c	503	CLA	MG-ND	-3.53	1.98	2.05
28	B	616	CLA	MG-ND	-3.53	1.98	2.05
28	d	405	CLA	MG-ND	-3.53	1.98	2.05
28	B	613	CLA	MG-ND	-3.53	1.98	2.05
28	c	510	CLA	MG-ND	-3.53	1.98	2.05
28	R	601	CLA	MG-ND	-3.53	1.98	2.05
28	b	602	CLA	MG-ND	-3.53	1.98	2.05
30	a	410	BCR	C24-C25	3.53	1.57	1.45
28	C	504	CLA	MG-ND	-3.53	1.98	2.05
28	b	601	CLA	MG-ND	-3.53	1.98	2.05
28	b	609	CLA	MG-ND	-3.53	1.98	2.05
28	r	612	CLA	MG-ND	-3.53	1.98	2.05
28	B	607	CLA	MG-ND	-3.53	1.98	2.05
28	R	608	CLA	MG-ND	-3.53	1.98	2.05
28	r	608	CLA	MG-ND	-3.53	1.98	2.05
28	r	613	CLA	MG-ND	-3.53	1.98	2.05
28	N	614	CLA	MG-ND	-3.52	1.98	2.05
28	s	608	CLA	MG-ND	-3.52	1.98	2.05
28	r	609	CLA	MG-ND	-3.52	1.98	2.05
30	D	405	BCR	C24-C25	3.52	1.57	1.45
28	r	603	CLA	MG-ND	-3.52	1.98	2.05
39	R	614	LUT	C30-C29	-3.52	1.31	1.35
28	b	614	CLA	MG-ND	-3.52	1.98	2.05
28	a	406	CLA	MG-ND	-3.52	1.98	2.05
28	D	401	CLA	MG-ND	-3.51	1.98	2.05
39	g	615	LUT	C38-C25	3.51	1.57	1.50
28	b	606	CLA	MG-ND	-3.51	1.98	2.05
39	N	615	LUT	C19-C9	3.51	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	611	CLA	C4B-NB	-3.51	1.33	1.37
28	B	602	CLA	MG-ND	-3.50	1.98	2.05
28	n	611	CLA	C1C-NC	-3.50	1.32	1.37
28	s	602	CLA	MG-ND	-3.50	1.98	2.05
28	b	611	CLA	MG-ND	-3.50	1.98	2.05
28	G	610	CLA	MG-ND	-3.50	1.98	2.05
28	g	602	CLA	MG-ND	-3.50	1.98	2.05
28	C	511	CLA	MG-ND	-3.50	1.98	2.05
28	S	304	CLA	MG-ND	-3.49	1.98	2.05
39	N	615	LUT	C11-C10	3.49	1.54	1.43
28	b	610	CLA	MG-ND	-3.49	1.98	2.05
39	s	614	LUT	C19-C9	3.49	1.58	1.50
28	n	602	CLA	MG-ND	-3.49	1.98	2.05
30	c	514	BCR	C24-C25	3.49	1.57	1.45
28	C	509	CLA	MG-ND	-3.49	1.98	2.05
28	B	611	CLA	MG-ND	-3.49	1.98	2.05
28	g	603	CLA	C4B-NB	-3.48	1.33	1.37
30	C	514	BCR	C24-C25	3.48	1.57	1.45
28	g	604	CLA	C1C-NC	-3.47	1.32	1.37
28	B	605	CLA	MG-ND	-3.47	1.98	2.05
28	Y	602	CLA	C1C-NC	-3.47	1.32	1.37
30	K	101	BCR	C24-C25	3.47	1.57	1.45
28	S	303	CLA	MG-ND	-3.47	1.98	2.05
30	b	619	BCR	C27-C26	-3.46	1.44	1.51
28	R	613	CLA	MG-ND	-3.46	1.98	2.05
28	S	309	CLA	MG-ND	-3.46	1.98	2.05
39	n	615	LUT	C21-C26	3.45	1.66	1.56
39	g	616	LUT	C2-C1	3.45	1.65	1.54
28	Y	603	CLA	MG-ND	-3.45	1.98	2.05
28	S	305	CLA	C4B-NB	-3.45	1.33	1.37
28	r	601	CLA	MG-ND	-3.45	1.99	2.05
39	r	614	LUT	C38-C25	3.45	1.57	1.50
28	c	504	CLA	MG-ND	-3.45	1.99	2.05
39	Y	616	LUT	C19-C9	3.45	1.58	1.50
39	n	615	LUT	C38-C25	3.44	1.57	1.50
39	G	615	LUT	C23-C24	-3.44	1.45	1.50
30	b	619	BCR	C16-C17	3.44	1.54	1.43
28	c	508	CLA	C1C-NC	-3.43	1.32	1.37
39	r	614	LUT	C23-C24	-3.43	1.45	1.50
37	E	101	HEM	C1B-NB	-3.43	1.34	1.40
39	Y	615	LUT	C19-C9	3.43	1.58	1.50
39	Y	616	LUT	C28-C29	3.42	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	606	CLA	MG-ND	-3.42	1.99	2.05
30	d	406	BCR	C4-C5	-3.40	1.44	1.51
30	t	101	BCR	C4-C5	-3.40	1.44	1.51
39	y	315	LUT	C2-C1	3.40	1.65	1.54
30	K	101	BCR	C27-C26	-3.39	1.44	1.51
39	R	614	LUT	C38-C25	3.39	1.56	1.50
39	Y	615	LUT	C11-C10	3.39	1.53	1.43
39	g	615	LUT	C2-C1	3.39	1.65	1.54
39	G	615	LUT	C40-C33	3.39	1.57	1.50
39	r	614	LUT	C2-C1	3.38	1.65	1.54
39	n	615	LUT	C19-C9	3.38	1.57	1.50
30	D	405	BCR	C4-C5	-3.38	1.44	1.51
39	g	615	LUT	C40-C33	3.38	1.57	1.50
39	G	615	LUT	C2-C1	3.37	1.65	1.54
39	s	615	LUT	C2-C1	3.37	1.65	1.54
39	S	315	LUT	C40-C33	3.36	1.57	1.50
28	g	610	CLA	C1C-NC	-3.36	1.32	1.37
28	c	508	CLA	C4B-NB	-3.36	1.33	1.37
39	g	616	LUT	C40-C33	3.36	1.57	1.50
39	s	614	LUT	C2-C1	3.36	1.65	1.54
39	s	614	LUT	C40-C33	3.36	1.57	1.50
39	S	316	LUT	C40-C33	3.36	1.57	1.50
39	S	315	LUT	C2-C1	3.35	1.65	1.54
39	y	315	LUT	C40-C33	3.35	1.57	1.50
30	b	618	BCR	C27-C26	-3.35	1.44	1.51
28	Y	602	CLA	C4B-NB	-3.35	1.33	1.37
39	n	616	LUT	C11-C10	3.35	1.53	1.43
28	g	610	CLA	C4B-NB	-3.34	1.33	1.37
39	y	316	LUT	C2-C1	3.34	1.65	1.54
30	C	514	BCR	C4-C5	-3.34	1.44	1.51
30	T	101	BCR	C4-C5	-3.34	1.44	1.51
39	s	615	LUT	C23-C24	-3.33	1.45	1.50
39	S	316	LUT	C2-C1	3.33	1.65	1.54
39	n	616	LUT	C19-C9	3.33	1.57	1.50
37	f	101	HEM	C1B-NB	-3.33	1.34	1.40
30	i	101	BCR	C4-C5	-3.32	1.44	1.51
39	s	615	LUT	C40-C33	3.32	1.57	1.50
30	H	101	BCR	C4-C5	-3.32	1.44	1.51
39	Y	616	LUT	C38-C25	3.31	1.56	1.50
28	R	604	CLA	C1C-NC	-3.31	1.32	1.37
28	G	612	CLA	C1C-NC	-3.31	1.32	1.37
30	c	515	BCR	C4-C5	-3.31	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	618	BCR	C27-C26	-3.31	1.44	1.51
37	f	101	HEM	C4D-ND	-3.31	1.34	1.40
30	B	617	BCR	C4-C5	-3.31	1.44	1.51
30	K	101	BCR	C4-C5	-3.31	1.44	1.51
30	C	514	BCR	C27-C26	-3.31	1.44	1.51
30	B	619	BCR	C27-C26	-3.31	1.44	1.51
28	R	601	CLA	C1C-NC	-3.31	1.32	1.37
30	A	409	BCR	C27-C26	-3.31	1.44	1.51
30	D	405	BCR	C27-C26	-3.31	1.44	1.51
30	b	617	BCR	C4-C5	-3.31	1.44	1.51
30	b	619	BCR	C11-C10	3.30	1.53	1.43
36	C	519	DGD	CAB-C9B	-3.30	1.33	1.51
39	N	616	LUT	C23-C24	-3.30	1.45	1.50
39	n	615	LUT	C2-C1	3.29	1.65	1.54
28	B	616	CLA	C1C-NC	-3.29	1.32	1.37
28	g	604	CLA	C4B-NB	-3.29	1.33	1.37
39	Y	615	LUT	C38-C25	3.29	1.56	1.50
30	C	515	BCR	C27-C26	-3.29	1.44	1.51
30	k	101	BCR	C4-C5	-3.29	1.44	1.51
32	C	522	LMG	C22-C21	-3.29	1.33	1.51
39	G	615	LUT	C38-C25	3.29	1.56	1.50
30	a	410	BCR	C27-C26	-3.28	1.44	1.51
30	i	101	BCR	C27-C26	-3.28	1.44	1.51
36	B	626	DGD	CDB-CCB	-3.28	1.33	1.51
32	C	522	LMG	C19-C18	-3.28	1.33	1.51
39	Y	616	LUT	C11-C10	3.28	1.53	1.43
32	A	413	LMG	C40-C39	-3.28	1.33	1.51
39	y	316	LUT	C40-C33	3.28	1.57	1.50
32	A	413	LMG	C37-C36	-3.27	1.33	1.51
30	c	514	BCR	C4-C5	-3.27	1.44	1.51
30	b	618	BCR	C4-C5	-3.27	1.44	1.51
32	B	621	LMG	C19-C18	-3.27	1.33	1.51
28	R	604	CLA	C4B-NB	-3.27	1.33	1.37
32	w	101	LMG	C37-C36	-3.27	1.33	1.51
32	a	413	LMG	C40-C39	-3.26	1.33	1.51
32	a	413	LMG	C37-C36	-3.26	1.33	1.51
36	C	518	DGD	CDA-CCA	-3.26	1.33	1.51
30	a	410	BCR	C4-C5	-3.26	1.44	1.51
39	g	616	LUT	C23-C24	-3.26	1.45	1.50
30	t	101	BCR	C27-C26	-3.26	1.44	1.51
32	k	102	LMG	C40-C39	-3.26	1.33	1.51
30	C	515	BCR	C4-C5	-3.26	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518	DGD	C9B-C8B	-3.26	1.33	1.51
32	k	102	LMG	C19-C18	-3.26	1.33	1.51
28	R	604	CLA	MG-ND	-3.26	1.99	2.05
36	B	626	DGD	CAB-C9B	-3.26	1.33	1.51
32	c	521	LMG	C40-C39	-3.26	1.33	1.51
32	b	620	LMG	C37-C36	-3.26	1.33	1.51
30	c	514	BCR	C27-C26	-3.26	1.44	1.51
28	G	614	CLA	C1C-NC	-3.26	1.32	1.37
32	C	520	LMG	C22-C21	-3.25	1.33	1.51
28	S	312	CLA	C1C-NC	-3.25	1.32	1.37
36	C	519	DGD	CAA-C9A	-3.25	1.33	1.51
30	B	618	BCR	C4-C5	-3.25	1.44	1.51
36	b	625	DGD	CDA-CCA	-3.25	1.33	1.51
32	d	409	LMG	C19-C18	-3.25	1.33	1.51
36	C	519	DGD	CDA-CCA	-3.25	1.33	1.51
32	b	620	LMG	C40-C39	-3.25	1.33	1.51
36	c	517	DGD	CAB-C9B	-3.25	1.33	1.51
39	N	616	LUT	C38-C25	3.25	1.56	1.50
36	C	517	DGD	CDB-CCB	-3.25	1.33	1.51
30	C	516	BCR	C4-C5	-3.25	1.44	1.51
39	n	616	LUT	C2-C1	3.25	1.65	1.54
36	b	625	DGD	CAA-C9A	-3.25	1.33	1.51
32	c	521	LMG	C37-C36	-3.25	1.33	1.51
36	a	401	DGD	CAA-C9A	-3.25	1.33	1.51
36	c	518	DGD	CAA-C9A	-3.25	1.33	1.51
28	c	501	CLA	C1C-NC	-3.25	1.33	1.37
28	c	504	CLA	C1C-NC	-3.25	1.33	1.37
28	s	609	CLA	C1C-NC	-3.25	1.33	1.37
36	b	625	DGD	CDB-CCB	-3.25	1.33	1.51
32	b	623	LMG	C19-C18	-3.25	1.33	1.51
36	B	626	DGD	CDA-CCA	-3.25	1.33	1.51
28	R	608	CLA	C1C-NC	-3.25	1.33	1.37
28	c	507	CLA	C1C-NC	-3.25	1.33	1.37
28	r	601	CLA	C1C-NC	-3.25	1.33	1.37
36	B	626	DGD	CAA-C9A	-3.24	1.33	1.51
30	C	516	BCR	C27-C26	-3.24	1.44	1.51
36	a	401	DGD	CAB-C9B	-3.24	1.33	1.51
30	A	409	BCR	C4-C5	-3.24	1.44	1.51
30	B	619	BCR	C4-C5	-3.24	1.44	1.51
36	A	417	DGD	CAB-C9B	-3.24	1.33	1.51
39	N	616	LUT	C19-C9	3.24	1.57	1.50
36	b	625	DGD	CAB-C9B	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	517	DGD	CDB-CCB	-3.24	1.33	1.51
32	C	520	LMG	C19-C18	-3.24	1.33	1.51
28	b	616	CLA	C1C-NC	-3.24	1.33	1.37
36	A	417	DGD	CAA-C9A	-3.24	1.33	1.51
32	D	408	LMG	C22-C21	-3.24	1.33	1.51
32	B	621	LMG	C22-C21	-3.24	1.33	1.51
32	b	620	LMG	C19-C18	-3.24	1.33	1.51
30	k	101	BCR	C27-C26	-3.24	1.44	1.51
28	C	507	CLA	C1C-NC	-3.24	1.33	1.37
28	s	611	CLA	C1C-NC	-3.24	1.33	1.37
32	D	408	LMG	C19-C18	-3.24	1.33	1.51
30	b	617	BCR	C27-C26	-3.24	1.44	1.51
36	c	516	DGD	CDB-CCB	-3.24	1.33	1.51
32	k	102	LMG	C22-C21	-3.24	1.33	1.51
32	c	521	LMG	C22-C21	-3.24	1.33	1.51
32	b	620	LMG	C22-C21	-3.24	1.33	1.51
36	c	516	DGD	CAB-C9B	-3.23	1.33	1.51
32	k	102	LMG	C37-C36	-3.23	1.33	1.51
36	c	518	DGD	CDA-CCA	-3.23	1.33	1.51
28	s	602	CLA	C1C-NC	-3.23	1.33	1.37
32	w	101	LMG	C40-C39	-3.23	1.33	1.51
36	C	517	DGD	CAB-C9B	-3.23	1.33	1.51
36	a	401	DGD	CDB-CCB	-3.23	1.33	1.51
30	h	101	BCR	C4-C5	-3.23	1.44	1.51
32	c	521	LMG	C19-C18	-3.23	1.33	1.51
32	A	411	LMG	C37-C36	-3.23	1.33	1.51
39	N	615	LUT	C23-C24	-3.23	1.45	1.50
36	C	518	DGD	CAB-C9B	-3.23	1.33	1.51
32	C	520	LMG	C40-C39	-3.23	1.33	1.51
30	B	617	BCR	C27-C26	-3.23	1.44	1.51
32	A	411	LMG	C19-C18	-3.23	1.33	1.51
39	R	614	LUT	C19-C9	3.22	1.57	1.50
36	A	417	DGD	CDB-CCB	-3.22	1.33	1.51
32	w	101	LMG	C19-C18	-3.22	1.33	1.51
32	d	409	LMG	C22-C21	-3.22	1.33	1.51
32	B	621	LMG	C37-C36	-3.22	1.33	1.51
32	B	621	LMG	C40-C39	-3.22	1.33	1.51
28	r	603	CLA	C1C-NC	-3.22	1.33	1.37
28	r	613	CLA	C1C-NC	-3.22	1.33	1.37
37	E	101	HEM	C4D-ND	-3.22	1.34	1.40
32	A	411	LMG	C40-C39	-3.22	1.33	1.51
39	N	615	LUT	C38-C25	3.22	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	623	LMG	C43-C42	-3.22	1.33	1.51
32	b	623	LMG	C37-C36	-3.22	1.33	1.51
28	y	312	CLA	C1C-NC	-3.22	1.33	1.37
39	n	615	LUT	C40-C33	3.22	1.57	1.50
32	C	520	LMG	C37-C36	-3.22	1.33	1.51
28	n	612	CLA	C4B-NB	-3.22	1.33	1.37
30	H	101	BCR	C27-C26	-3.21	1.44	1.51
32	b	623	LMG	C40-C39	-3.21	1.33	1.51
28	S	304	CLA	C1C-NC	-3.21	1.33	1.37
36	C	518	DGD	CDB-CCB	-3.21	1.33	1.51
28	y	311	CLA	C1C-NC	-3.21	1.33	1.37
28	R	603	CLA	MG-ND	-3.21	1.99	2.05
28	S	314	CLA	C1C-NC	-3.21	1.33	1.37
28	S	310	CLA	C1C-NC	-3.21	1.33	1.37
28	B	611	CLA	C1C-NC	-3.21	1.33	1.37
28	Y	604	CLA	C1C-NC	-3.21	1.33	1.37
28	b	601	CLA	C1C-NC	-3.21	1.33	1.37
30	d	406	BCR	C27-C26	-3.20	1.44	1.51
28	r	610	CLA	C1C-NC	-3.20	1.33	1.37
39	Y	615	LUT	C40-C33	3.20	1.57	1.50
28	B	615	CLA	C1C-NC	-3.20	1.33	1.37
28	s	603	CLA	C1C-NC	-3.20	1.33	1.37
36	C	518	DGD	CAA-C9A	-3.20	1.33	1.51
39	Y	615	LUT	C2-C1	3.20	1.64	1.54
28	N	612	CLA	C1C-NC	-3.20	1.33	1.37
28	R	611	CLA	C1C-NC	-3.20	1.33	1.37
39	R	614	LUT	C2-C1	3.20	1.64	1.54
28	R	613	CLA	C1C-NC	-3.19	1.33	1.37
28	n	603	CLA	C1C-NC	-3.19	1.33	1.37
28	B	610	CLA	C1C-NC	-3.19	1.33	1.37
28	N	603	CLA	C1C-NC	-3.19	1.33	1.37
28	r	609	CLA	C1C-NC	-3.19	1.33	1.37
28	B	602	CLA	C1C-NC	-3.19	1.33	1.37
39	G	616	LUT	O23-C23	-3.19	1.37	1.43
28	Y	603	CLA	C1C-NC	-3.19	1.33	1.37
28	G	610	CLA	C1C-NC	-3.18	1.33	1.37
28	y	305	CLA	C1C-NC	-3.18	1.33	1.37
28	N	604	CLA	C1C-NC	-3.18	1.33	1.37
28	B	601	CLA	C1C-NC	-3.18	1.33	1.37
28	g	612	CLA	C1C-NC	-3.18	1.33	1.37
28	B	609	CLA	C1C-NC	-3.18	1.33	1.37
28	b	609	CLA	C1C-NC	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	603	CLA	C1C-NC	-3.17	1.33	1.37
28	N	610	CLA	C1C-NC	-3.17	1.33	1.37
28	b	604	CLA	C1C-NC	-3.17	1.33	1.37
28	c	503	CLA	C1C-NC	-3.17	1.33	1.37
30	T	101	BCR	C11-C10	3.17	1.53	1.43
28	S	309	CLA	C1C-NC	-3.17	1.33	1.37
28	G	611	CLA	C1C-NC	-3.17	1.33	1.37
28	R	612	CLA	C1C-NC	-3.17	1.33	1.37
28	C	513	CLA	C1C-NC	-3.17	1.33	1.37
39	r	614	LUT	C30-C29	-3.17	1.31	1.35
30	b	619	BCR	C24-C25	3.17	1.56	1.45
28	y	304	CLA	C1C-NC	-3.16	1.33	1.37
28	N	611	CLA	C1C-NC	-3.16	1.33	1.37
30	h	101	BCR	C27-C26	-3.16	1.44	1.51
28	D	403	CLA	C1C-NC	-3.16	1.33	1.37
28	d	401	CLA	C1C-NC	-3.16	1.33	1.37
28	C	501	CLA	C1C-NC	-3.16	1.33	1.37
28	C	504	CLA	C1C-NC	-3.16	1.33	1.37
28	R	610	CLA	C1C-NC	-3.16	1.33	1.37
28	b	615	CLA	C1C-NC	-3.16	1.33	1.37
28	A	408	CLA	C1C-NC	-3.16	1.33	1.37
28	B	612	CLA	C1C-NC	-3.16	1.33	1.37
28	c	506	CLA	C1C-NC	-3.16	1.33	1.37
28	G	602	CLA	C1C-NC	-3.16	1.33	1.37
39	N	616	LUT	C2-C1	3.16	1.64	1.54
28	A	405	CLA	C1C-NC	-3.15	1.33	1.37
39	n	616	LUT	C38-C25	3.15	1.56	1.50
28	B	604	CLA	C1C-NC	-3.15	1.33	1.37
28	s	613	CLA	C1C-NC	-3.15	1.33	1.37
28	r	608	CLA	C1C-NC	-3.15	1.33	1.37
28	B	605	CLA	C1C-NC	-3.15	1.33	1.37
28	G	613	CLA	C1C-NC	-3.15	1.33	1.37
28	n	611	CLA	C4B-NB	-3.15	1.33	1.37
39	Y	616	LUT	C40-C33	3.14	1.57	1.50
28	B	606	CLA	C1C-NC	-3.14	1.33	1.37
28	C	506	CLA	C1C-NC	-3.14	1.33	1.37
28	s	610	CLA	C1C-NC	-3.14	1.33	1.37
28	B	608	CLA	C1C-NC	-3.14	1.33	1.37
28	D	404	CLA	C1C-NC	-3.14	1.33	1.37
28	r	612	CLA	C1C-NC	-3.14	1.33	1.37
39	R	614	LUT	C40-C33	3.14	1.57	1.50
28	c	505	CLA	C1C-NC	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	609	CLA	C1C-NC	-3.14	1.33	1.37
28	b	613	CLA	C1C-NC	-3.14	1.33	1.37
39	Y	616	LUT	C23-C24	-3.14	1.45	1.50
39	N	615	LUT	C2-C1	3.14	1.64	1.54
28	Y	611	CLA	C1C-NC	-3.14	1.33	1.37
28	r	604	CLA	C1C-NC	-3.14	1.33	1.37
28	n	610	CLA	C1C-NC	-3.14	1.33	1.37
28	N	602	CLA	C1C-NC	-3.14	1.33	1.37
39	y	315	LUT	C23-C24	-3.14	1.45	1.50
28	S	311	CLA	C1C-NC	-3.14	1.33	1.37
28	Y	612	CLA	C1C-NC	-3.13	1.33	1.37
28	C	503	CLA	C1C-NC	-3.13	1.33	1.37
28	N	613	CLA	C1C-NC	-3.13	1.33	1.37
28	b	610	CLA	C1C-NC	-3.13	1.33	1.37
28	b	611	CLA	C1C-NC	-3.13	1.33	1.37
28	S	313	CLA	C1C-NC	-3.13	1.33	1.37
28	d	405	CLA	C1C-NC	-3.13	1.33	1.37
28	s	604	CLA	C1C-NC	-3.13	1.33	1.37
28	y	303	CLA	C1C-NC	-3.13	1.33	1.37
28	y	313	CLA	C1C-NC	-3.13	1.33	1.37
28	B	613	CLA	C1C-NC	-3.12	1.33	1.37
28	G	604	CLA	C1C-NC	-3.12	1.33	1.37
28	N	614	CLA	C1C-NC	-3.12	1.33	1.37
28	a	407	CLA	C1C-NC	-3.12	1.33	1.37
28	B	614	CLA	C1C-NC	-3.12	1.33	1.37
28	C	502	CLA	C1C-NC	-3.12	1.33	1.37
28	B	609	CLA	C4B-NB	-3.12	1.33	1.37
28	a	406	CLA	C1C-NC	-3.12	1.33	1.37
28	c	512	CLA	C1C-NC	-3.12	1.33	1.37
28	d	404	CLA	C1C-NC	-3.12	1.33	1.37
39	n	616	LUT	C40-C33	3.12	1.57	1.50
28	b	603	CLA	C1C-NC	-3.12	1.33	1.37
28	g	613	CLA	C1C-NC	-3.12	1.33	1.37
28	y	310	CLA	C1C-NC	-3.12	1.33	1.37
39	N	615	LUT	C40-C33	3.12	1.57	1.50
28	b	607	CLA	C1C-NC	-3.12	1.33	1.37
28	n	604	CLA	C1C-NC	-3.11	1.33	1.37
28	n	602	CLA	C1C-NC	-3.11	1.33	1.37
28	A	406	CLA	C1C-NC	-3.11	1.33	1.37
28	C	505	CLA	C1C-NC	-3.11	1.33	1.37
28	Y	614	CLA	C1C-NC	-3.11	1.33	1.37
28	C	508	CLA	C1C-NC	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	515	BCR	C27-C26	-3.11	1.44	1.51
39	N	616	LUT	C40-C33	3.11	1.57	1.50
28	Y	613	CLA	C1C-NC	-3.11	1.33	1.37
28	g	614	CLA	C1C-NC	-3.10	1.33	1.37
39	G	616	LUT	C2-C1	3.10	1.64	1.54
39	Y	616	LUT	C2-C1	3.10	1.64	1.54
28	b	606	CLA	C1C-NC	-3.10	1.33	1.37
28	g	602	CLA	C1C-NC	-3.10	1.33	1.37
28	y	314	CLA	C1C-NC	-3.10	1.33	1.37
28	D	401	CLA	C1C-NC	-3.10	1.33	1.37
28	C	511	CLA	C1C-NC	-3.10	1.33	1.37
28	b	602	CLA	C1C-NC	-3.10	1.33	1.37
28	c	511	CLA	C1C-NC	-3.09	1.33	1.37
28	n	614	CLA	C1C-NC	-3.09	1.33	1.37
28	s	613	CLA	C4B-NB	-3.09	1.34	1.37
28	c	513	CLA	C1C-NC	-3.09	1.33	1.37
28	C	510	CLA	C1C-NC	-3.09	1.33	1.37
28	b	608	CLA	C1C-NC	-3.09	1.33	1.37
28	B	603	CLA	C1C-NC	-3.09	1.33	1.37
28	c	502	CLA	C1C-NC	-3.08	1.33	1.37
39	n	615	LUT	C23-C24	-3.08	1.45	1.50
28	a	409	CLA	C1C-NC	-3.08	1.33	1.37
28	C	509	CLA	C1C-NC	-3.08	1.33	1.37
39	G	616	LUT	C38-C25	3.08	1.56	1.50
28	r	602	CLA	C1C-NC	-3.08	1.33	1.37
28	B	607	CLA	C1C-NC	-3.07	1.33	1.37
28	s	608	CLA	C1C-NC	-3.07	1.33	1.37
28	B	602	CLA	C4B-NB	-3.07	1.34	1.37
28	c	505	CLA	C4B-NB	-3.07	1.34	1.37
28	s	612	CLA	C1C-NC	-3.07	1.33	1.37
28	R	608	CLA	C4B-NB	-3.07	1.34	1.37
28	b	612	CLA	C1C-NC	-3.07	1.33	1.37
28	c	510	CLA	C1C-NC	-3.07	1.33	1.37
28	b	614	CLA	C1C-NC	-3.07	1.33	1.37
39	s	614	LUT	C23-C24	-3.07	1.45	1.50
28	S	303	CLA	C1C-NC	-3.07	1.33	1.37
28	D	403	CLA	C4B-NB	-3.07	1.34	1.37
28	B	616	CLA	C4B-NB	-3.07	1.34	1.37
28	S	310	CLA	C4B-NB	-3.06	1.34	1.37
28	S	314	CLA	C4B-NB	-3.06	1.34	1.37
28	N	604	CLA	C4B-NB	-3.06	1.34	1.37
28	G	604	CLA	C4B-NB	-3.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	610	CLA	C4B-NB	-3.05	1.34	1.37
28	N	602	CLA	C4B-NB	-3.05	1.34	1.37
28	N	603	CLA	C4B-NB	-3.05	1.34	1.37
28	N	614	CLA	C4B-NB	-3.05	1.34	1.37
28	b	616	CLA	C4B-NB	-3.05	1.34	1.37
28	y	305	CLA	C4B-NB	-3.05	1.34	1.37
28	C	512	CLA	C1C-NC	-3.05	1.33	1.37
28	y	310	CLA	C4B-NB	-3.05	1.34	1.37
28	G	610	CLA	C4B-NB	-3.04	1.34	1.37
28	S	303	CLA	C4B-NB	-3.04	1.34	1.37
28	s	602	CLA	C4B-NB	-3.04	1.34	1.37
28	s	609	CLA	C4B-NB	-3.04	1.34	1.37
28	C	506	CLA	C4B-NB	-3.03	1.34	1.37
28	S	309	CLA	C4B-NB	-3.03	1.34	1.37
28	c	507	CLA	C4B-NB	-3.03	1.34	1.37
28	C	505	CLA	C4B-NB	-3.03	1.34	1.37
28	n	604	CLA	C4B-NB	-3.03	1.34	1.37
39	G	616	LUT	C40-C33	3.03	1.57	1.50
39	S	316	LUT	C23-C24	-3.03	1.45	1.50
29	A	407	PHO	C4D-CHA	3.02	1.44	1.39
28	B	611	CLA	C4B-NB	-3.02	1.34	1.37
28	Y	604	CLA	C4B-NB	-3.02	1.34	1.37
39	r	614	LUT	C40-C33	3.02	1.57	1.50
28	b	611	CLA	C4B-NB	-3.02	1.34	1.37
28	C	507	CLA	C4B-NB	-3.01	1.34	1.37
28	b	607	CLA	C4B-NB	-3.01	1.34	1.37
28	c	504	CLA	C4B-NB	-3.01	1.34	1.37
28	r	603	CLA	C4B-NB	-3.01	1.34	1.37
28	s	603	CLA	C4B-NB	-3.01	1.34	1.37
28	Y	612	CLA	C4B-NB	-3.01	1.34	1.37
28	G	603	CLA	C4B-NB	-3.01	1.34	1.37
28	c	513	CLA	C4B-NB	-3.01	1.34	1.37
39	S	315	LUT	C23-C24	-3.00	1.45	1.50
28	n	602	CLA	C4B-NB	-3.00	1.34	1.37
28	r	602	CLA	C4B-NB	-3.00	1.34	1.37
28	s	608	CLA	C4B-NB	-3.00	1.34	1.37
28	R	603	CLA	C4B-NB	-3.00	1.34	1.37
28	B	608	CLA	C4B-NB	-3.00	1.34	1.37
28	G	602	CLA	C4B-NB	-3.00	1.34	1.37
28	b	609	CLA	C4B-NB	-3.00	1.34	1.37
28	d	405	CLA	C4B-NB	-3.00	1.34	1.37
28	b	606	CLA	C4B-NB	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	614	CLA	C4B-NB	-2.99	1.34	1.37
28	a	409	CLA	C4B-NB	-2.99	1.34	1.37
28	y	313	CLA	C4B-NB	-2.99	1.34	1.37
28	A	408	CLA	C4B-NB	-2.99	1.34	1.37
28	C	502	CLA	C4B-NB	-2.99	1.34	1.37
28	C	513	CLA	C4B-NB	-2.99	1.34	1.37
28	n	614	CLA	C4B-NB	-2.99	1.34	1.37
28	R	609	CLA	C4B-NB	-2.99	1.34	1.37
28	B	612	CLA	C4B-NB	-2.98	1.34	1.37
28	g	614	CLA	C4B-NB	-2.98	1.34	1.37
28	n	610	CLA	C4B-NB	-2.98	1.34	1.37
28	C	504	CLA	C4B-NB	-2.98	1.34	1.37
28	B	613	CLA	C4B-NB	-2.97	1.34	1.37
28	C	509	CLA	C4B-NB	-2.97	1.34	1.37
28	r	609	CLA	C4B-NB	-2.97	1.34	1.37
28	B	605	CLA	C4B-NB	-2.97	1.34	1.37
28	A	406	CLA	C4B-NB	-2.97	1.34	1.37
39	Y	615	LUT	C30-C29	-2.97	1.31	1.35
28	y	314	CLA	C4B-NB	-2.97	1.34	1.37
28	b	608	CLA	C4B-NB	-2.97	1.34	1.37
28	Y	613	CLA	C4B-NB	-2.96	1.34	1.37
28	c	512	CLA	C4B-NB	-2.96	1.34	1.37
28	c	503	CLA	C4B-NB	-2.96	1.34	1.37
28	c	510	CLA	C4B-NB	-2.96	1.34	1.37
29	a	408	PHO	C4D-CHA	2.96	1.44	1.39
28	a	407	CLA	C4B-NB	-2.96	1.34	1.37
28	s	604	CLA	C4B-NB	-2.96	1.34	1.37
28	g	612	CLA	C4B-NB	-2.96	1.34	1.37
28	c	502	CLA	C4B-NB	-2.95	1.34	1.37
28	C	508	CLA	C4B-NB	-2.95	1.34	1.37
28	D	404	CLA	C4B-NB	-2.95	1.34	1.37
28	b	602	CLA	C4B-NB	-2.95	1.34	1.37
28	g	602	CLA	C4B-NB	-2.95	1.34	1.37
28	r	608	CLA	C4B-NB	-2.95	1.34	1.37
28	B	604	CLA	C4B-NB	-2.94	1.34	1.37
28	b	604	CLA	C4B-NB	-2.94	1.34	1.37
28	c	506	CLA	C4B-NB	-2.94	1.34	1.37
28	Y	611	CLA	C4B-NB	-2.94	1.34	1.37
28	R	612	CLA	C4B-NB	-2.93	1.34	1.37
28	C	503	CLA	C4B-NB	-2.93	1.34	1.37
28	C	510	CLA	C4B-NB	-2.93	1.34	1.37
28	a	406	CLA	C4B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	y	303	CLA	C4B-NB	-2.93	1.34	1.37
28	b	603	CLA	C4B-NB	-2.92	1.34	1.37
28	N	612	CLA	C4B-NB	-2.92	1.34	1.37
28	D	401	CLA	C4B-NB	-2.92	1.34	1.37
28	s	612	CLA	C4B-NB	-2.92	1.34	1.37
28	C	511	CLA	C4B-NB	-2.92	1.34	1.37
39	g	615	LUT	C23-C24	-2.92	1.46	1.50
28	d	404	CLA	C4B-NB	-2.92	1.34	1.37
28	b	613	CLA	C4B-NB	-2.92	1.34	1.37
28	r	604	CLA	C4B-NB	-2.92	1.34	1.37
28	A	405	CLA	C4B-NB	-2.91	1.34	1.37
28	N	613	CLA	C4B-NB	-2.91	1.34	1.37
28	g	613	CLA	C4B-NB	-2.91	1.34	1.37
28	N	611	CLA	C4B-NB	-2.91	1.34	1.37
28	d	401	CLA	C4B-NB	-2.91	1.34	1.37
28	B	614	CLA	C4B-NB	-2.91	1.34	1.37
28	G	613	CLA	C4B-NB	-2.91	1.34	1.37
28	r	612	CLA	C4B-NB	-2.91	1.34	1.37
39	R	614	LUT	O23-C23	-2.90	1.38	1.43
28	C	512	CLA	C4B-NB	-2.90	1.34	1.37
28	b	615	CLA	C4B-NB	-2.90	1.34	1.37
28	r	610	CLA	C4B-NB	-2.90	1.34	1.37
28	b	614	CLA	C4B-NB	-2.90	1.34	1.37
28	B	607	CLA	C4B-NB	-2.90	1.34	1.37
28	b	612	CLA	C4B-NB	-2.89	1.34	1.37
28	B	603	CLA	C4B-NB	-2.89	1.34	1.37
39	Y	616	LUT	C30-C29	-2.89	1.32	1.35
39	r	614	LUT	O23-C23	-2.88	1.38	1.43
28	c	511	CLA	C4B-NB	-2.88	1.34	1.37
30	B	618	BCR	C34-C9	2.86	1.56	1.50
28	G	611	CLA	C4B-NB	-2.85	1.34	1.37
28	S	313	CLA	C4B-NB	-2.85	1.34	1.37
28	c	501	CLA	C4B-NB	-2.85	1.34	1.37
28	s	610	CLA	C4B-NB	-2.85	1.34	1.37
30	B	617	BCR	C34-C9	2.85	1.56	1.50
28	R	610	CLA	C4B-NB	-2.85	1.34	1.37
30	H	101	BCR	C34-C9	2.85	1.56	1.50
30	b	617	BCR	C34-C9	2.85	1.56	1.50
30	c	514	BCR	C34-C9	2.85	1.56	1.50
28	S	311	CLA	C4B-NB	-2.84	1.34	1.37
30	D	405	BCR	C34-C9	2.84	1.56	1.50
29	D	402	PHO	C4D-CHA	2.84	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	618	BCR	C34-C9	2.84	1.56	1.50
28	r	601	CLA	C4B-NB	-2.83	1.34	1.37
30	h	101	BCR	C34-C9	2.83	1.56	1.50
39	y	316	LUT	C23-C24	-2.83	1.46	1.50
28	C	501	CLA	C4B-NB	-2.83	1.34	1.37
30	t	101	BCR	C34-C9	2.83	1.56	1.50
39	N	616	LUT	O23-C23	-2.83	1.38	1.43
30	C	515	BCR	C34-C9	2.83	1.56	1.50
28	G	614	CLA	C4B-NB	-2.82	1.34	1.37
29	d	402	PHO	C4D-CHA	2.82	1.44	1.39
28	R	601	CLA	C4B-NB	-2.82	1.34	1.37
30	i	101	BCR	C34-C9	2.81	1.56	1.50
30	d	406	BCR	C34-C9	2.81	1.56	1.50
30	A	409	BCR	C34-C9	2.81	1.56	1.50
30	a	410	BCR	C34-C9	2.80	1.56	1.50
28	r	613	CLA	C4B-NB	-2.80	1.34	1.37
28	G	612	CLA	C4B-NB	-2.80	1.34	1.37
30	C	514	BCR	C34-C9	2.80	1.56	1.50
30	b	619	BCR	C34-C9	2.79	1.56	1.50
28	R	613	CLA	C4B-NB	-2.78	1.34	1.37
30	K	101	BCR	C34-C9	2.78	1.56	1.50
30	c	515	BCR	C34-C9	2.78	1.56	1.50
39	Y	615	LUT	C34-C33	-2.77	1.32	1.35
28	S	304	CLA	C4B-NB	-2.77	1.34	1.37
39	n	616	LUT	O23-C23	-2.77	1.38	1.43
28	B	610	CLA	C4B-NB	-2.75	1.34	1.37
30	K	101	BCR	C7-C6	2.75	1.54	1.45
30	k	101	BCR	C34-C9	2.74	1.56	1.50
39	N	615	LUT	O23-C23	-2.74	1.38	1.43
28	y	311	CLA	C4B-NB	-2.74	1.34	1.37
30	h	101	BCR	C7-C6	2.74	1.54	1.45
40	n	617	NEX	C1-C6	-2.74	1.50	1.54
28	S	312	CLA	C4B-NB	-2.73	1.34	1.37
28	B	601	CLA	C4B-NB	-2.72	1.34	1.37
28	s	611	CLA	C4B-NB	-2.72	1.34	1.37
28	y	304	CLA	C4B-NB	-2.72	1.34	1.37
39	y	315	LUT	C18-C5	2.72	1.55	1.50
30	C	515	BCR	C7-C6	2.71	1.54	1.45
39	S	315	LUT	C18-C5	2.71	1.55	1.50
39	n	616	LUT	C30-C29	-2.71	1.32	1.35
30	B	619	BCR	C34-C9	2.71	1.56	1.50
28	R	611	CLA	C4B-NB	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	618	BCR	C7-C6	2.70	1.54	1.45
30	C	516	BCR	C7-C6	2.70	1.54	1.45
30	k	101	BCR	C7-C6	2.70	1.54	1.45
30	a	410	BCR	C7-C6	2.69	1.54	1.45
30	B	618	BCR	C7-C6	2.69	1.54	1.45
39	r	614	LUT	C18-C5	2.69	1.55	1.50
30	C	516	BCR	C34-C9	2.69	1.56	1.50
30	c	515	BCR	C7-C6	2.68	1.54	1.45
28	b	610	CLA	C4B-NB	-2.68	1.34	1.37
30	t	101	BCR	C7-C6	2.67	1.54	1.45
28	B	615	CLA	C4B-NB	-2.67	1.34	1.37
28	b	601	CLA	C4B-NB	-2.66	1.34	1.37
30	C	514	BCR	C7-C6	2.66	1.54	1.45
30	b	617	BCR	C7-C6	2.66	1.54	1.45
30	B	619	BCR	C7-C6	2.66	1.54	1.45
39	Y	616	LUT	O23-C23	-2.66	1.38	1.43
30	B	617	BCR	C7-C6	2.66	1.54	1.45
30	A	409	BCR	C7-C6	2.66	1.54	1.45
30	i	101	BCR	C7-C6	2.65	1.54	1.45
30	H	101	BCR	C7-C6	2.65	1.54	1.45
28	n	603	CLA	C4B-NB	-2.65	1.34	1.37
30	D	405	BCR	C7-C6	2.65	1.54	1.45
28	Y	603	CLA	C4B-NB	-2.65	1.34	1.37
30	c	514	BCR	C7-C6	2.65	1.54	1.45
39	g	615	LUT	C18-C5	2.64	1.55	1.50
28	y	312	CLA	C4B-NB	-2.64	1.34	1.37
30	d	406	BCR	C7-C6	2.63	1.54	1.45
39	y	316	LUT	C18-C5	2.63	1.55	1.50
30	T	101	BCR	C34-C9	2.63	1.56	1.50
39	g	616	LUT	C18-C5	2.62	1.55	1.50
28	B	606	CLA	C4B-NB	-2.62	1.34	1.37
28	b	605	CLA	C3D-C4D	-2.61	1.38	1.44
39	g	615	LUT	O23-C23	-2.59	1.38	1.43
28	r	611	CLA	C4B-NB	-2.58	1.34	1.37
39	R	614	LUT	C18-C5	2.58	1.55	1.50
36	c	518	DGD	CCB-CBB	-2.58	1.33	1.51
39	y	315	LUT	O23-C23	-2.58	1.38	1.43
39	Y	615	LUT	O23-C23	-2.56	1.39	1.43
39	s	615	LUT	C18-C5	2.56	1.55	1.50
39	G	615	LUT	O23-C23	-2.56	1.39	1.43
32	D	408	LMG	C37-C36	-2.56	1.33	1.51
32	d	409	LMG	C37-C36	-2.56	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	619	BCR	C7-C6	2.56	1.54	1.45
39	Y	616	LUT	C34-C33	-2.55	1.32	1.35
29	D	402	PHO	C1B-C2B	2.55	1.42	1.39
39	S	316	LUT	C18-C5	2.54	1.55	1.50
36	C	519	DGD	CDB-CCB	-2.54	1.33	1.51
39	y	316	LUT	O23-C23	-2.53	1.39	1.43
37	E	101	HEM	C1C-C2C	-2.53	1.40	1.45
28	g	603	CLA	C3D-C4D	-2.52	1.38	1.44
39	G	615	LUT	C18-C5	2.52	1.55	1.50
39	s	615	LUT	O23-C23	-2.52	1.39	1.43
40	y	301	NEX	C1-C6	-2.51	1.50	1.54
39	s	614	LUT	C18-C5	2.51	1.55	1.50
40	y	318	NEX	O24-C25	-2.50	1.42	1.46
29	d	402	PHO	C1B-C2B	2.49	1.42	1.39
39	S	316	LUT	O23-C23	-2.49	1.39	1.43
39	s	614	LUT	O23-C23	-2.48	1.39	1.43
39	Y	615	LUT	C18-C5	2.48	1.55	1.50
39	N	615	LUT	C30-C29	-2.47	1.32	1.35
39	S	315	LUT	O23-C23	-2.46	1.39	1.43
30	C	516	BCR	C36-C18	2.46	1.56	1.50
39	n	616	LUT	C34-C33	-2.46	1.32	1.35
29	A	407	PHO	C1B-C2B	2.46	1.42	1.39
28	c	509	CLA	C3D-C4D	-2.45	1.38	1.44
39	g	616	LUT	O23-C23	-2.45	1.39	1.43
39	N	615	LUT	C18-C5	2.45	1.54	1.50
30	C	514	BCR	C36-C18	2.44	1.55	1.50
30	t	101	BCR	C36-C18	2.44	1.55	1.50
39	n	615	LUT	O23-C23	-2.44	1.39	1.43
28	R	604	CLA	C3D-C4D	-2.43	1.38	1.44
28	n	612	CLA	C3D-C4D	-2.42	1.38	1.44
29	a	408	PHO	C1B-C2B	2.41	1.42	1.39
39	Y	616	LUT	C18-C5	2.41	1.54	1.50
30	b	617	BCR	C36-C18	2.41	1.55	1.50
39	n	615	LUT	C30-C29	-2.41	1.32	1.35
39	y	315	LUT	C30-C29	-2.41	1.32	1.35
30	T	101	BCR	C39-C30	-2.40	1.49	1.53
30	c	514	BCR	C36-C18	2.40	1.55	1.50
30	c	515	BCR	C36-C18	2.39	1.55	1.50
37	f	101	HEM	FE-ND	-2.39	1.87	1.94
30	B	617	BCR	C36-C18	2.39	1.55	1.50
37	E	101	HEM	FE-ND	-2.38	1.87	1.94
28	Y	602	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	T	101	BCR	C7-C6	2.38	1.53	1.45
30	C	515	BCR	C36-C18	2.38	1.55	1.50
40	g	617	NEX	C1-C6	-2.38	1.50	1.54
39	n	615	LUT	C18-C5	2.37	1.54	1.50
30	b	618	BCR	C36-C18	2.37	1.55	1.50
28	s	603	CLA	C1C-C2C	2.37	1.49	1.44
30	h	101	BCR	C36-C18	2.37	1.55	1.50
39	N	615	LUT	C34-C33	-2.37	1.32	1.35
38	y	302	CHL	C1B-NB	-2.36	1.34	1.37
30	D	405	BCR	C36-C18	2.36	1.55	1.50
39	G	616	LUT	C18-C5	2.36	1.54	1.50
28	c	508	CLA	C3D-C4D	-2.36	1.38	1.44
39	S	315	LUT	C26-C27	2.36	1.53	1.50
30	B	619	BCR	C36-C18	2.36	1.55	1.50
30	K	101	BCR	C36-C18	2.36	1.55	1.50
40	y	301	NEX	O24-C25	-2.36	1.42	1.46
30	k	101	BCR	C36-C18	2.35	1.55	1.50
30	B	618	BCR	C36-C18	2.35	1.55	1.50
30	H	101	BCR	C36-C18	2.35	1.55	1.50
37	f	101	HEM	C1C-C2C	-2.34	1.40	1.45
39	n	616	LUT	C18-C5	2.34	1.54	1.50
30	i	101	BCR	C36-C18	2.34	1.55	1.50
38	n	601	CHL	C1B-NB	-2.33	1.34	1.37
39	N	616	LUT	C34-C33	-2.33	1.32	1.35
30	d	406	BCR	C36-C18	2.33	1.55	1.50
28	n	613	CLA	C3D-C4D	-2.33	1.38	1.44
39	r	614	LUT	C34-C33	-2.33	1.32	1.35
40	n	617	NEX	O24-C25	-2.32	1.42	1.46
28	Y	610	CLA	C3D-C4D	-2.32	1.38	1.44
30	a	410	BCR	C36-C18	2.32	1.55	1.50
30	A	409	BCR	C36-C18	2.32	1.55	1.50
39	N	616	LUT	C30-C29	-2.31	1.32	1.35
28	R	602	CLA	C3D-C4D	-2.31	1.39	1.44
40	N	617	NEX	O24-C25	-2.31	1.42	1.46
30	d	406	BCR	C39-C30	-2.31	1.49	1.53
28	g	604	CLA	C3D-C4D	-2.30	1.39	1.44
39	G	616	LUT	C34-C33	-2.30	1.32	1.35
39	G	615	LUT	C28-C27	2.30	1.37	1.32
28	B	612	CLA	C1C-C2C	2.29	1.49	1.44
39	g	616	LUT	C26-C27	2.29	1.53	1.50
30	B	619	BCR	C39-C30	-2.28	1.49	1.53
38	r	605	CHL	C3A-C2A	-2.28	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	y	318	NEX	C1-C6	-2.28	1.50	1.54
28	R	603	CLA	C3D-C4D	-2.28	1.39	1.44
39	s	615	LUT	C26-C27	2.27	1.53	1.50
39	R	614	LUT	C34-C33	-2.27	1.32	1.35
28	B	603	CLA	C1C-C2C	2.27	1.49	1.44
39	g	615	LUT	C30-C29	-2.27	1.32	1.35
39	G	616	LUT	C30-C29	-2.25	1.32	1.35
28	Y	602	CLA	C1C-C2C	2.25	1.48	1.44
30	b	619	BCR	C39-C30	-2.25	1.49	1.53
38	N	601	CHL	C1B-NB	-2.25	1.35	1.37
39	y	316	LUT	C30-C29	-2.24	1.32	1.35
39	N	616	LUT	C18-C5	2.23	1.54	1.50
35	y	319	LHG	O7-C5	-2.23	1.41	1.46
30	B	618	BCR	C39-C30	-2.23	1.49	1.53
40	s	616	NEX	C1-C6	-2.23	1.50	1.54
39	G	615	LUT	C30-C29	-2.23	1.32	1.35
28	S	305	CLA	C3D-C4D	-2.23	1.39	1.44
28	n	611	CLA	C3D-C4D	-2.23	1.39	1.44
28	b	612	CLA	C1C-C2C	2.23	1.48	1.44
39	g	616	LUT	C30-C29	-2.22	1.32	1.35
39	Y	615	LUT	C14-C13	-2.22	1.32	1.35
39	y	316	LUT	C26-C27	2.22	1.53	1.50
28	b	610	CLA	C1C-C2C	2.22	1.48	1.44
39	n	615	LUT	C34-C33	-2.22	1.32	1.35
38	y	309	CHL	C3A-C2A	-2.21	1.48	1.54
39	N	616	LUT	C26-C27	2.21	1.53	1.50
39	n	615	LUT	C26-C27	2.21	1.53	1.50
39	S	316	LUT	C26-C27	2.21	1.53	1.50
30	D	405	BCR	C39-C30	-2.20	1.49	1.53
39	y	315	LUT	C34-C33	-2.20	1.32	1.35
39	s	614	LUT	C26-C27	2.19	1.53	1.50
30	i	101	BCR	C39-C30	-2.19	1.49	1.53
28	b	601	CLA	C1C-C2C	2.19	1.48	1.44
28	C	501	CLA	C1C-C2C	2.19	1.48	1.44
28	n	602	CLA	C1C-C2C	2.19	1.48	1.44
28	C	509	CLA	C1C-C2C	2.19	1.48	1.44
28	r	602	CLA	C1C-C2C	2.19	1.48	1.44
30	H	101	BCR	C39-C30	-2.19	1.49	1.53
38	Y	609	CHL	C3A-C2A	-2.19	1.48	1.54
30	b	617	BCR	C39-C30	-2.19	1.49	1.53
30	T	101	BCR	C37-C22	2.19	1.55	1.50
30	T	101	BCR	C36-C18	2.18	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	N	607	CHL	C1B-NB	-2.18	1.35	1.37
28	B	608	CLA	C1C-C2C	2.18	1.48	1.44
28	c	501	CLA	C1C-C2C	2.18	1.48	1.44
30	h	101	BCR	C39-C30	-2.18	1.49	1.53
40	G	617	NEX	O24-C25	-2.18	1.43	1.46
28	B	610	CLA	C1C-C2C	2.18	1.48	1.44
28	s	602	CLA	C1C-C2C	2.18	1.48	1.44
30	C	514	BCR	C39-C30	-2.18	1.49	1.53
39	y	316	LUT	C34-C33	-2.17	1.32	1.35
28	B	606	CLA	C1C-C2C	2.17	1.48	1.44
30	b	618	BCR	C39-C30	-2.17	1.49	1.53
30	t	101	BCR	C39-C30	-2.17	1.49	1.53
30	k	101	BCR	C39-C30	-2.17	1.49	1.53
28	G	602	CLA	C1C-C2C	2.17	1.48	1.44
30	b	618	BCR	C38-C26	2.17	1.54	1.50
28	y	303	CLA	C1C-C2C	2.17	1.48	1.44
28	D	401	CLA	C1C-C2C	2.16	1.48	1.44
28	c	503	CLA	C1C-C2C	2.16	1.48	1.44
39	s	614	LUT	C30-C29	-2.16	1.32	1.35
30	C	515	BCR	C39-C30	-2.16	1.49	1.53
38	G	609	CHL	C3A-C2A	-2.16	1.48	1.54
30	c	515	BCR	C39-C30	-2.16	1.49	1.53
30	C	516	BCR	C38-C26	2.16	1.54	1.50
30	a	410	BCR	C39-C30	-2.16	1.49	1.53
28	R	601	CLA	C1C-C2C	2.15	1.48	1.44
28	B	611	CLA	C1C-C2C	2.15	1.48	1.44
28	g	602	CLA	C1C-C2C	2.15	1.48	1.44
40	g	617	NEX	O24-C25	-2.15	1.43	1.46
28	c	511	CLA	C1C-C2C	2.15	1.48	1.44
30	B	617	BCR	C38-C26	2.15	1.54	1.50
38	Y	608	CHL	C1B-NB	-2.15	1.35	1.37
28	y	310	CLA	C1C-C2C	2.15	1.48	1.44
28	y	313	CLA	C1C-C2C	2.15	1.48	1.44
28	N	602	CLA	C1C-C2C	2.15	1.48	1.44
30	b	617	BCR	C38-C26	2.15	1.54	1.50
39	g	615	LUT	C34-C33	-2.15	1.32	1.35
30	C	516	BCR	C39-C30	-2.15	1.49	1.53
28	n	614	CLA	C1C-C2C	2.15	1.48	1.44
30	B	617	BCR	C39-C30	-2.15	1.49	1.53
30	c	515	BCR	C38-C26	2.15	1.54	1.50
28	R	604	CLA	C1C-C2C	2.15	1.48	1.44
28	d	404	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	s	601	CHL	C1B-NB	-2.14	1.35	1.37
28	g	611	CLA	C3D-C4D	-2.14	1.39	1.44
28	b	608	CLA	C1C-C2C	2.14	1.48	1.44
28	C	512	CLA	C1C-C2C	2.14	1.48	1.44
28	G	610	CLA	C1C-C2C	2.14	1.48	1.44
28	S	303	CLA	C1C-C2C	2.14	1.48	1.44
28	c	513	CLA	C1C-C2C	2.14	1.48	1.44
30	b	619	BCR	C10-C9	-2.14	1.32	1.35
35	Y	619	LHG	O7-C5	-2.14	1.41	1.46
28	N	610	CLA	C1C-C2C	2.14	1.48	1.44
28	n	603	CLA	C1C-C2C	2.13	1.48	1.44
30	A	409	BCR	C38-C26	2.13	1.54	1.50
28	C	506	CLA	C1C-C2C	2.13	1.48	1.44
28	R	612	CLA	C1C-C2C	2.13	1.48	1.44
28	c	510	CLA	C1C-C2C	2.13	1.48	1.44
28	B	614	CLA	C1C-C2C	2.13	1.48	1.44
28	G	611	CLA	C1C-C2C	2.13	1.48	1.44
37	f	101	HEM	C3C-C4C	-2.13	1.42	1.46
38	G	605	CHL	C1B-NB	-2.13	1.35	1.37
28	G	614	CLA	C1C-C2C	2.13	1.48	1.44
30	t	101	BCR	C37-C22	2.13	1.55	1.50
30	k	101	BCR	C38-C26	2.13	1.54	1.50
28	g	604	CLA	C1C-C2C	2.13	1.48	1.44
30	d	406	BCR	C38-C26	2.13	1.54	1.50
39	S	316	LUT	C30-C29	-2.13	1.33	1.35
30	K	101	BCR	C39-C30	-2.12	1.49	1.53
38	g	605	CHL	C1B-NB	-2.12	1.35	1.37
38	r	607	CHL	C1B-NB	-2.12	1.35	1.37
30	D	405	BCR	C38-C26	2.12	1.54	1.50
38	N	608	CHL	C1B-NB	-2.12	1.35	1.37
28	y	305	CLA	C1C-C2C	2.12	1.48	1.44
28	C	513	CLA	C1C-C2C	2.12	1.48	1.44
30	K	101	BCR	C37-C22	2.12	1.55	1.50
28	G	613	CLA	C1C-C2C	2.12	1.48	1.44
30	C	515	BCR	C38-C26	2.12	1.54	1.50
30	A	409	BCR	C39-C30	-2.12	1.49	1.53
30	i	101	BCR	C38-C26	2.12	1.54	1.50
28	C	503	CLA	C1C-C2C	2.12	1.48	1.44
28	A	406	CLA	C1C-C2C	2.12	1.48	1.44
28	g	614	CLA	C1C-C2C	2.12	1.48	1.44
38	Y	607	CHL	C1B-NB	-2.12	1.35	1.37
38	n	605	CHL	C1B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	607	CLA	C1C-C2C	2.12	1.48	1.44
28	B	602	CLA	C1C-C2C	2.11	1.48	1.44
28	C	511	CLA	C1C-C2C	2.11	1.48	1.44
28	R	611	CLA	C1C-C2C	2.11	1.48	1.44
28	b	603	CLA	C1C-C2C	2.11	1.48	1.44
28	D	403	CLA	C1C-C2C	2.11	1.48	1.44
30	B	618	BCR	C38-C26	2.11	1.54	1.50
28	c	512	CLA	C1C-C2C	2.11	1.48	1.44
28	r	610	CLA	C1C-C2C	2.11	1.48	1.44
28	S	311	CLA	C1C-C2C	2.11	1.48	1.44
28	B	601	CLA	C1C-C2C	2.11	1.48	1.44
39	S	315	LUT	C34-C33	-2.11	1.33	1.35
28	N	614	CLA	C1C-C2C	2.11	1.48	1.44
28	c	506	CLA	C1C-C2C	2.11	1.48	1.44
38	G	601	CHL	C1B-NB	-2.11	1.35	1.37
28	d	401	CLA	C1C-C2C	2.11	1.48	1.44
40	N	617	NEX	C1-C6	-2.10	1.51	1.54
28	b	614	CLA	C1C-C2C	2.10	1.48	1.44
28	B	605	CLA	C1C-C2C	2.10	1.48	1.44
28	s	611	CLA	C1C-C2C	2.10	1.48	1.44
30	k	101	BCR	C37-C22	2.10	1.55	1.50
28	s	609	CLA	C1C-C2C	2.10	1.48	1.44
28	C	502	CLA	C1C-C2C	2.10	1.48	1.44
28	n	610	CLA	C1C-C2C	2.10	1.48	1.44
30	K	101	BCR	C38-C26	2.10	1.54	1.50
38	R	607	CHL	C1B-NB	-2.10	1.35	1.37
38	n	608	CHL	C1B-NB	-2.10	1.35	1.37
30	c	514	BCR	C37-C22	2.10	1.55	1.50
28	b	602	CLA	C1C-C2C	2.10	1.48	1.44
28	Y	612	CLA	C1C-C2C	2.10	1.48	1.44
28	n	604	CLA	C1C-C2C	2.10	1.48	1.44
28	s	610	CLA	C1C-C2C	2.10	1.48	1.44
30	b	618	BCR	C37-C22	2.10	1.55	1.50
38	S	308	CHL	C1B-NB	-2.10	1.35	1.37
30	h	101	BCR	C38-C26	2.10	1.54	1.50
28	B	613	CLA	C1C-C2C	2.10	1.48	1.44
28	b	611	CLA	C1C-C2C	2.10	1.48	1.44
40	r	616	NEX	O24-C25	-2.10	1.43	1.46
28	Y	604	CLA	C1C-C2C	2.09	1.48	1.44
38	n	606	CHL	C1B-NB	-2.09	1.35	1.37
28	Y	613	CLA	C1C-C2C	2.09	1.48	1.44
28	B	615	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	404	CLA	C1C-C2C	2.09	1.48	1.44
28	c	502	CLA	C1C-C2C	2.09	1.48	1.44
28	r	609	CLA	C1C-C2C	2.09	1.48	1.44
28	B	604	CLA	C1C-C2C	2.09	1.48	1.44
28	S	313	CLA	C1C-C2C	2.09	1.48	1.44
28	C	504	CLA	C1C-C2C	2.09	1.48	1.44
28	R	610	CLA	C1C-C2C	2.09	1.48	1.44
28	b	613	CLA	C1C-C2C	2.09	1.48	1.44
30	B	619	BCR	C37-C22	2.09	1.55	1.50
39	N	616	LUT	C14-C13	-2.09	1.33	1.35
40	Y	618	NEX	O24-C25	-2.09	1.43	1.46
40	s	616	NEX	O24-C25	-2.09	1.43	1.46
38	S	302	CHL	C1B-NB	-2.09	1.35	1.37
28	N	612	CLA	C1C-C2C	2.09	1.48	1.44
30	H	101	BCR	C38-C26	2.09	1.54	1.50
30	c	514	BCR	C38-C26	2.09	1.54	1.50
28	a	406	CLA	C1C-C2C	2.09	1.48	1.44
30	t	101	BCR	C38-C26	2.08	1.54	1.50
28	r	608	CLA	C1C-C2C	2.08	1.48	1.44
30	c	514	BCR	C39-C30	-2.08	1.49	1.53
30	D	405	BCR	C37-C22	2.08	1.55	1.50
28	r	604	CLA	C1C-C2C	2.08	1.48	1.44
30	C	514	BCR	C37-C22	2.08	1.55	1.50
30	b	617	BCR	C37-C22	2.08	1.55	1.50
28	b	615	CLA	C1C-C2C	2.08	1.48	1.44
38	y	308	CHL	C1B-NB	-2.08	1.35	1.37
28	C	507	CLA	C1C-C2C	2.08	1.48	1.44
28	s	613	CLA	C1C-C2C	2.08	1.48	1.44
28	r	601	CLA	C1C-C2C	2.08	1.48	1.44
28	c	504	CLA	C1C-C2C	2.08	1.48	1.44
28	C	510	CLA	C1C-C2C	2.08	1.48	1.44
30	A	409	BCR	C37-C22	2.08	1.55	1.50
38	G	608	CHL	C1B-NB	-2.08	1.35	1.37
28	y	312	CLA	C1C-C2C	2.08	1.48	1.44
28	b	604	CLA	C1A-CHA	2.07	1.51	1.43
28	g	612	CLA	C1C-C2C	2.07	1.48	1.44
37	f	101	HEM	C1D-ND	-2.07	1.34	1.38
30	a	410	BCR	C38-C26	2.07	1.54	1.50
28	y	304	CLA	C1C-C2C	2.07	1.48	1.44
28	y	314	CLA	C1C-C2C	2.07	1.48	1.44
39	R	614	LUT	C26-C27	2.07	1.53	1.50
28	d	405	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	410	BCR	C37-C22	2.07	1.55	1.50
30	i	101	BCR	C37-C22	2.07	1.55	1.50
37	E	101	HEM	C3C-C4C	-2.07	1.42	1.46
28	s	608	CLA	C1C-C2C	2.07	1.48	1.44
28	b	607	CLA	C1C-C2C	2.07	1.48	1.44
30	B	619	BCR	C38-C26	2.07	1.54	1.50
28	b	606	CLA	C3D-C4D	-2.07	1.39	1.44
28	C	505	CLA	C1C-C2C	2.07	1.48	1.44
30	C	514	BCR	C38-C26	2.06	1.54	1.50
39	Y	616	LUT	C14-C13	-2.06	1.33	1.35
28	s	611	CLA	C3D-C4D	-2.06	1.39	1.44
28	C	508	CLA	C1C-C2C	2.06	1.48	1.44
28	N	613	CLA	C1C-C2C	2.06	1.48	1.44
30	B	618	BCR	C37-C22	2.06	1.55	1.50
28	A	405	CLA	C1C-C2C	2.06	1.48	1.44
28	N	603	CLA	C1C-C2C	2.06	1.48	1.44
28	N	611	CLA	C1C-C2C	2.06	1.48	1.44
30	c	515	BCR	C37-C22	2.06	1.55	1.50
28	Y	603	CLA	C1C-C2C	2.06	1.48	1.44
28	s	612	CLA	C1C-C2C	2.06	1.48	1.44
30	C	515	BCR	C37-C22	2.06	1.55	1.50
39	y	315	LUT	C26-C27	2.06	1.53	1.50
28	B	616	CLA	C1C-C2C	2.06	1.48	1.44
28	G	604	CLA	C1C-C2C	2.06	1.48	1.44
28	S	310	CLA	C1C-C2C	2.06	1.48	1.44
28	a	409	CLA	C1C-C2C	2.06	1.48	1.44
28	g	610	CLA	C3D-C4D	-2.06	1.39	1.44
40	r	616	NEX	C1-C6	-2.06	1.51	1.54
28	r	613	CLA	C1C-C2C	2.06	1.48	1.44
28	c	505	CLA	C3D-C4D	-2.05	1.39	1.44
28	b	606	CLA	C1C-C2C	2.05	1.48	1.44
30	h	101	BCR	C37-C22	2.05	1.55	1.50
39	s	615	LUT	C30-C29	-2.05	1.33	1.35
28	c	505	CLA	C1C-C2C	2.05	1.48	1.44
40	Y	618	NEX	C1-C6	-2.05	1.51	1.54
28	s	603	CLA	C3D-C4D	-2.05	1.39	1.44
28	y	305	CLA	C3D-C4D	-2.05	1.39	1.44
30	B	617	BCR	C37-C22	2.05	1.55	1.50
38	g	619	CHL	C1B-NB	-2.05	1.35	1.37
28	y	311	CLA	C1C-C2C	2.05	1.48	1.44
28	C	505	CLA	C3D-C4D	-2.05	1.39	1.44
28	b	608	CLA	C3D-C4D	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	s	602	CLA	C3D-C4D	-2.05	1.39	1.44
28	a	407	CLA	C1C-C2C	2.05	1.48	1.44
28	n	603	CLA	C3D-C4D	-2.05	1.39	1.44
38	G	606	CHL	C3A-C2A	-2.05	1.48	1.54
28	r	609	CLA	C3D-C4D	-2.05	1.39	1.44
28	A	408	CLA	C1C-C2C	2.04	1.48	1.44
28	Y	611	CLA	C1C-C2C	2.04	1.48	1.44
38	N	609	CHL	C1B-NB	-2.04	1.35	1.37
32	C	522	LMG	C25-C24	-2.04	1.33	1.49
28	R	612	CLA	C3D-C4D	-2.04	1.39	1.44
28	c	507	CLA	C1C-C2C	2.04	1.48	1.44
39	g	616	LUT	C34-C33	-2.04	1.33	1.35
28	r	603	CLA	C3D-C4D	-2.04	1.39	1.44
30	b	619	BCR	C36-C18	2.04	1.55	1.50
28	B	614	CLA	C3D-C4D	-2.04	1.39	1.44
28	S	310	CLA	C3D-C4D	-2.04	1.39	1.44
28	R	609	CLA	C1C-C2C	2.04	1.48	1.44
28	S	314	CLA	C1C-C2C	2.04	1.48	1.44
28	G	604	CLA	C3D-C4D	-2.04	1.39	1.44
28	S	312	CLA	C1C-C2C	2.04	1.48	1.44
28	Y	612	CLA	C3D-C4D	-2.04	1.39	1.44
29	D	402	PHO	C1D-C2D	2.04	1.41	1.39
38	y	306	CHL	C1B-NB	-2.04	1.35	1.37
28	B	616	CLA	C3D-C4D	-2.04	1.39	1.44
28	N	611	CLA	C3D-C4D	-2.04	1.39	1.44
28	c	510	CLA	C3D-C4D	-2.04	1.39	1.44
28	G	612	CLA	C1A-CHA	2.04	1.51	1.43
28	b	607	CLA	C1A-CHA	2.04	1.51	1.43
38	n	607	CHL	C1B-NB	-2.04	1.35	1.37
39	S	316	LUT	C34-C33	-2.03	1.33	1.35
38	g	609	CHL	C3A-C2A	-2.03	1.48	1.54
28	S	312	CLA	C3D-C4D	-2.03	1.39	1.44
28	g	614	CLA	C3D-C4D	-2.03	1.39	1.44
28	g	612	CLA	C3D-C4D	-2.03	1.39	1.44
28	N	613	CLA	C3D-C4D	-2.03	1.39	1.44
28	r	612	CLA	C3D-C4D	-2.03	1.39	1.44
38	Y	601	CHL	C1B-NB	-2.03	1.35	1.37
28	n	604	CLA	C3D-C4D	-2.03	1.39	1.44
30	H	101	BCR	C37-C22	2.03	1.55	1.50
28	N	603	CLA	C3D-C4D	-2.03	1.39	1.44
30	d	406	BCR	C37-C22	2.03	1.55	1.50
28	r	601	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	y	312	CLA	C3D-C4D	-2.03	1.39	1.44
36	B	626	DGD	CGB-CFB	-2.03	1.33	1.49
28	B	609	CLA	C1C-C2C	2.03	1.48	1.44
28	N	612	CLA	C3D-C4D	-2.03	1.39	1.44
28	S	314	CLA	C3D-C4D	-2.03	1.39	1.44
28	b	604	CLA	C1C-C2C	2.02	1.48	1.44
39	Y	615	LUT	C35-C15	-2.02	1.30	1.36
38	g	601	CHL	C1B-NB	-2.02	1.35	1.37
39	N	615	LUT	C26-C27	2.02	1.53	1.50
28	B	604	CLA	C1A-CHA	2.02	1.51	1.43
28	R	609	CLA	C3D-C4D	-2.02	1.39	1.44
28	c	506	CLA	C3D-C4D	-2.02	1.39	1.44
28	s	604	CLA	C1C-C2C	2.02	1.48	1.44
36	a	401	DGD	CDA-CCA	-2.02	1.33	1.49
28	N	602	CLA	C3D-C4D	-2.02	1.39	1.44
38	Y	607	CHL	C1A-CHA	-2.02	1.34	1.43
28	r	604	CLA	C1A-CHA	2.02	1.51	1.43
28	Y	604	CLA	C3D-C4D	-2.02	1.39	1.44
32	B	621	LMG	C43-C42	-2.02	1.33	1.49
38	S	307	CHL	C1B-NB	-2.02	1.35	1.37
32	k	102	LMG	C43-C42	-2.02	1.33	1.49
28	B	602	CLA	C3D-C4D	-2.02	1.39	1.44
28	R	604	CLA	MG-NC	2.02	2.11	2.06
40	G	617	NEX	C1-C6	-2.02	1.51	1.54
32	a	413	LMG	C43-C42	-2.02	1.33	1.49
32	w	101	LMG	C22-C21	-2.01	1.33	1.49
32	b	623	LMG	C22-C21	-2.01	1.33	1.49
28	b	614	CLA	C3D-C4D	-2.01	1.39	1.44
28	r	612	CLA	C1C-C2C	2.01	1.48	1.44
36	C	519	DGD	CGA-CFA	-2.01	1.33	1.49
38	N	605	CHL	C1B-NB	-2.01	1.35	1.37
36	A	417	DGD	CGB-CFB	-2.01	1.33	1.49
28	y	314	CLA	C3D-C4D	-2.01	1.39	1.44
28	b	602	CLA	C3D-C4D	-2.01	1.39	1.44
37	E	101	HEM	C1D-ND	-2.01	1.34	1.38
28	G	603	CLA	C1C-C2C	2.01	1.48	1.44
28	R	604	CLA	C1A-CHA	2.01	1.51	1.43
28	r	603	CLA	C1C-C2C	2.01	1.48	1.44
32	B	621	LMG	C25-C24	-2.01	1.33	1.49
28	b	615	CLA	C3D-C4D	-2.01	1.39	1.44
36	c	518	DGD	CGA-CFA	-2.01	1.33	1.49
28	b	609	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	608	CHL	C1B-NB	-2.01	1.35	1.37
32	w	101	LMG	C43-C42	-2.01	1.33	1.49
36	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
36	A	417	DGD	CDA-CCA	-2.01	1.33	1.49
28	B	608	CLA	C3D-C4D	-2.01	1.39	1.44
28	C	502	CLA	C1A-CHA	2.01	1.51	1.43
32	c	521	LMG	C25-C24	-2.01	1.33	1.49
36	b	625	DGD	CGB-CFB	-2.01	1.33	1.49
32	c	521	LMG	C43-C42	-2.01	1.33	1.49
28	G	603	CLA	C3D-C4D	-2.01	1.39	1.44
28	b	616	CLA	C3D-C4D	-2.01	1.39	1.44
30	C	516	BCR	C37-C22	2.01	1.55	1.50
28	Y	603	CLA	C3D-C4D	-2.01	1.39	1.44
36	C	517	DGD	CGB-CFB	-2.01	1.33	1.49
36	C	518	DGD	CGA-CFA	-2.01	1.33	1.49
28	R	613	CLA	C1C-C2C	2.01	1.48	1.44
32	A	411	LMG	C43-C42	-2.01	1.33	1.49
32	C	520	LMG	C43-C42	-2.00	1.33	1.49
28	S	304	CLA	C1C-C2C	2.00	1.48	1.44
38	r	606	CHL	C1B-NB	-2.00	1.35	1.37
32	A	413	LMG	C43-C42	-2.00	1.33	1.49
32	C	520	LMG	C25-C24	-2.00	1.33	1.49
32	b	620	LMG	C43-C42	-2.00	1.33	1.49
39	g	615	LUT	C26-C27	2.00	1.53	1.50
39	r	614	LUT	C26-C27	2.00	1.53	1.50
32	D	408	LMG	C25-C24	-2.00	1.33	1.49
28	G	613	CLA	C3D-C4D	-2.00	1.39	1.44
32	A	411	LMG	C22-C21	-2.00	1.33	1.49
32	b	620	LMG	C25-C24	-2.00	1.33	1.49
28	y	313	CLA	C3D-C4D	-2.00	1.39	1.44
39	n	616	LUT	C14-C13	-2.00	1.33	1.35
36	c	516	DGD	CGB-CFB	-2.00	1.33	1.49
28	S	303	CLA	C3D-C4D	-2.00	1.39	1.44
28	Y	613	CLA	C3D-C4D	-2.00	1.39	1.44
36	a	401	DGD	CGB-CFB	-2.00	1.33	1.49
38	N	606	CHL	C3A-C2A	-2.00	1.48	1.54

All (4591) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	r	614	LUT	C15-C14-C13	-13.17	108.51	127.31
28	r	611	CLA	C4A-NA-C1A	10.37	111.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	514	BCR	C16-C17-C18	-9.95	113.12	127.31
30	C	514	BCR	C15-C14-C13	-9.81	113.30	127.31
39	G	615	LUT	C31-C30-C29	-9.61	113.59	127.31
28	b	605	CLA	C4A-NA-C1A	9.58	111.02	106.71
28	R	601	CLA	C4A-NA-C1A	9.40	110.93	106.71
28	n	613	CLA	C4A-NA-C1A	9.35	110.91	106.71
28	b	609	CLA	C4A-NA-C1A	9.14	110.81	106.71
28	b	612	CLA	C4A-NA-C1A	9.14	110.81	106.71
28	g	610	CLA	C4A-NA-C1A	9.07	110.78	106.71
28	Y	610	CLA	C4A-NA-C1A	9.06	110.78	106.71
28	B	604	CLA	C4A-NA-C1A	9.05	110.78	106.71
28	B	612	CLA	C4A-NA-C1A	9.05	110.77	106.71
28	b	604	CLA	C4A-NA-C1A	9.00	110.75	106.71
28	b	616	CLA	C4A-NA-C1A	8.99	110.75	106.71
30	C	514	BCR	C20-C21-C22	-8.99	114.48	127.31
28	G	603	CLA	C4A-NA-C1A	8.98	110.74	106.71
28	r	604	CLA	C4A-NA-C1A	8.97	110.74	106.71
28	C	513	CLA	C4A-NA-C1A	8.96	110.73	106.71
28	C	506	CLA	C4A-NA-C1A	8.96	110.73	106.71
28	n	611	CLA	C4A-NA-C1A	8.96	110.73	106.71
28	C	502	CLA	C4A-NA-C1A	8.96	110.73	106.71
28	R	604	CLA	C4A-NA-C1A	8.95	110.73	106.71
39	r	614	LUT	C7-C8-C9	-8.94	112.72	126.23
28	G	612	CLA	C4A-NA-C1A	8.94	110.73	106.71
28	c	512	CLA	C4A-NA-C1A	8.94	110.72	106.71
28	N	604	CLA	C4A-NA-C1A	8.93	110.72	106.71
28	c	507	CLA	C4A-NA-C1A	8.93	110.72	106.71
28	n	604	CLA	C4A-NA-C1A	8.93	110.72	106.71
28	B	609	CLA	C4A-NA-C1A	8.92	110.72	106.71
28	y	304	CLA	C4A-NA-C1A	8.92	110.72	106.71
28	s	604	CLA	C4A-NA-C1A	8.91	110.71	106.71
28	Y	604	CLA	C4A-NA-C1A	8.90	110.71	106.71
28	c	506	CLA	C4A-NA-C1A	8.90	110.71	106.71
28	b	607	CLA	C4A-NA-C1A	8.89	110.70	106.71
28	R	608	CLA	C4A-NA-C1A	8.89	110.70	106.71
28	b	611	CLA	C4A-NA-C1A	8.87	110.69	106.71
28	s	612	CLA	C4A-NA-C1A	8.87	110.69	106.71
28	b	614	CLA	C4A-NA-C1A	8.87	110.69	106.71
28	B	616	CLA	C4A-NA-C1A	8.86	110.69	106.71
28	B	607	CLA	C4A-NA-C1A	8.86	110.69	106.71
28	C	504	CLA	C4A-NA-C1A	8.85	110.69	106.71
28	N	603	CLA	C4A-NA-C1A	8.85	110.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	507	CLA	C4A-NA-C1A	8.84	110.68	106.71
28	c	505	CLA	C4A-NA-C1A	8.84	110.68	106.71
28	C	509	CLA	C4A-NA-C1A	8.84	110.68	106.71
28	A	406	CLA	C4A-NA-C1A	8.83	110.68	106.71
28	R	610	CLA	C4A-NA-C1A	8.79	110.66	106.71
28	a	407	CLA	C4A-NA-C1A	8.79	110.66	106.71
28	d	401	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	g	614	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	G	613	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	y	305	CLA	C4A-NA-C1A	8.77	110.65	106.71
28	c	513	CLA	C4A-NA-C1A	8.77	110.65	106.71
28	c	502	CLA	C4A-NA-C1A	8.76	110.64	106.71
28	R	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
28	S	311	CLA	C4A-NA-C1A	8.75	110.64	106.71
28	B	602	CLA	C4A-NA-C1A	8.74	110.64	106.71
28	C	505	CLA	C4A-NA-C1A	8.74	110.63	106.71
28	C	503	CLA	C4A-NA-C1A	8.72	110.63	106.71
28	R	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
28	g	613	CLA	C4A-NA-C1A	8.72	110.63	106.71
28	S	304	CLA	C4A-NA-C1A	8.72	110.63	106.71
28	S	312	CLA	C4A-NA-C1A	8.71	110.62	106.71
28	c	503	CLA	C4A-NA-C1A	8.70	110.62	106.71
28	B	611	CLA	C4A-NA-C1A	8.70	110.62	106.71
28	n	602	CLA	C4A-NA-C1A	8.70	110.62	106.71
28	C	512	CLA	C4A-NA-C1A	8.69	110.61	106.71
28	s	613	CLA	C4A-NA-C1A	8.69	110.61	106.71
28	r	610	CLA	C4A-NA-C1A	8.69	110.61	106.71
28	d	405	CLA	C4A-NA-C1A	8.68	110.61	106.71
28	r	612	CLA	C4A-NA-C1A	8.68	110.61	106.71
28	d	404	CLA	C4A-NA-C1A	8.67	110.61	106.71
28	Y	603	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	B	608	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	N	612	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	y	314	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	n	603	CLA	C4A-NA-C1A	8.66	110.60	106.71
28	a	409	CLA	C4A-NA-C1A	8.65	110.60	106.71
28	B	601	CLA	C4A-NA-C1A	8.65	110.60	106.71
28	B	614	CLA	C4A-NA-C1A	8.65	110.59	106.71
28	r	608	CLA	C4A-NA-C1A	8.65	110.59	106.71
28	B	605	CLA	C4A-NA-C1A	8.64	110.59	106.71
28	Y	614	CLA	C4A-NA-C1A	8.64	110.59	106.71
28	G	604	CLA	C4A-NA-C1A	8.63	110.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	611	CLA	C4A-NA-C1A	8.63	110.59	106.71
28	s	603	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	S	305	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	S	309	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	s	610	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	S	314	CLA	C4A-NA-C1A	8.61	110.58	106.71
28	b	608	CLA	C4A-NA-C1A	8.61	110.58	106.71
28	y	303	CLA	C4A-NA-C1A	8.61	110.58	106.71
28	R	612	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	C	511	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	g	611	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	b	601	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	n	614	CLA	C4A-NA-C1A	8.59	110.57	106.71
28	D	403	CLA	C4A-NA-C1A	8.58	110.56	106.71
28	g	612	CLA	C4A-NA-C1A	8.58	110.56	106.71
28	S	303	CLA	C4A-NA-C1A	8.58	110.56	106.71
28	c	509	CLA	C4A-NA-C1A	8.58	110.56	106.71
28	S	313	CLA	C4A-NA-C1A	8.57	110.56	106.71
28	D	401	CLA	C4A-NA-C1A	8.56	110.55	106.71
28	G	611	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	r	613	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	g	602	CLA	C4A-NA-C1A	8.54	110.55	106.71
28	b	603	CLA	C4A-NA-C1A	8.54	110.54	106.71
28	G	602	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	Y	612	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	s	609	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	n	612	CLA	C4A-NA-C1A	8.51	110.53	106.71
28	c	511	CLA	C4A-NA-C1A	8.51	110.53	106.71
28	s	602	CLA	C4A-NA-C1A	8.51	110.53	106.71
28	D	404	CLA	C4A-NA-C1A	8.50	110.53	106.71
28	a	406	CLA	C4A-NA-C1A	8.50	110.53	106.71
28	Y	611	CLA	C4A-NA-C1A	8.49	110.52	106.71
28	N	613	CLA	C4A-NA-C1A	8.48	110.52	106.71
28	r	602	CLA	C4A-NA-C1A	8.47	110.51	106.71
28	N	602	CLA	C4A-NA-C1A	8.47	110.51	106.71
28	n	610	CLA	C4A-NA-C1A	8.47	110.51	106.71
28	A	408	CLA	C4A-NA-C1A	8.46	110.51	106.71
28	y	311	CLA	C4A-NA-C1A	8.46	110.51	106.71
28	A	405	CLA	C4A-NA-C1A	8.45	110.50	106.71
28	b	602	CLA	C4A-NA-C1A	8.44	110.50	106.71
28	N	610	CLA	C4A-NA-C1A	8.43	110.50	106.71
28	N	611	CLA	C4A-NA-C1A	8.42	110.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	504	CLA	C4A-NA-C1A	8.41	110.49	106.71
28	G	610	CLA	C4A-NA-C1A	8.41	110.48	106.71
28	y	313	CLA	C4A-NA-C1A	8.41	110.48	106.71
28	y	310	CLA	C4A-NA-C1A	8.40	110.48	106.71
28	B	603	CLA	C4A-NA-C1A	8.38	110.47	106.71
28	R	609	CLA	C4A-NA-C1A	8.38	110.47	106.71
28	Y	613	CLA	C4A-NA-C1A	8.37	110.47	106.71
28	c	508	CLA	C4A-NA-C1A	8.37	110.47	106.71
28	S	310	CLA	C4A-NA-C1A	8.36	110.46	106.71
28	G	614	CLA	C4A-NA-C1A	8.34	110.46	106.71
28	B	613	CLA	C4A-NA-C1A	8.34	110.46	106.71
28	N	614	CLA	C4A-NA-C1A	8.34	110.46	106.71
28	s	608	CLA	C4A-NA-C1A	8.34	110.46	106.71
28	r	603	CLA	C4A-NA-C1A	8.33	110.45	106.71
28	C	510	CLA	C4A-NA-C1A	8.32	110.45	106.71
28	b	613	CLA	C4A-NA-C1A	8.31	110.44	106.71
28	r	609	CLA	C4A-NA-C1A	8.29	110.43	106.71
28	C	508	CLA	C4A-NA-C1A	8.27	110.43	106.71
28	y	312	CLA	C4A-NA-C1A	8.27	110.42	106.71
28	C	501	CLA	C4A-NA-C1A	8.27	110.42	106.71
28	c	510	CLA	C4A-NA-C1A	8.25	110.42	106.71
28	b	610	CLA	C4A-NA-C1A	8.23	110.41	106.71
28	R	603	CLA	C4A-NA-C1A	8.23	110.41	106.71
30	C	514	BCR	C11-C10-C9	-8.23	115.57	127.31
28	c	501	CLA	C4A-NA-C1A	8.22	110.40	106.71
28	s	611	CLA	C4A-NA-C1A	8.15	110.37	106.71
28	b	615	CLA	C4A-NA-C1A	8.15	110.37	106.71
28	r	601	CLA	C4A-NA-C1A	8.14	110.36	106.71
28	B	610	CLA	C4A-NA-C1A	8.08	110.34	106.71
28	B	606	CLA	C4A-NA-C1A	8.04	110.32	106.71
28	b	606	CLA	C4A-NA-C1A	8.04	110.32	106.71
28	B	615	CLA	C4A-NA-C1A	7.98	110.30	106.71
28	g	603	CLA	C4A-NA-C1A	7.88	110.25	106.71
39	G	615	LUT	C35-C34-C33	-7.24	116.97	127.31
28	g	604	CLA	C4A-NA-C1A	7.06	109.88	106.71
28	g	610	CLA	O2D-CGD-CBD	7.02	123.74	111.27
28	Y	602	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	c	514	BCR	C15-C14-C13	-6.55	117.96	127.31
30	C	516	BCR	C15-C14-C13	-6.45	118.11	127.31
39	s	614	LUT	C11-C10-C9	-6.42	118.14	127.31
41	Y	617	XAT	C31-C30-C29	-6.41	118.17	127.31
30	b	618	BCR	C15-C14-C13	-6.39	118.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	n	615	LUT	C11-C10-C9	-6.34	118.26	127.31
30	K	101	BCR	C16-C17-C18	-6.32	118.29	127.31
30	T	101	BCR	C7-C8-C9	-6.32	116.69	126.23
30	C	516	BCR	C11-C10-C9	-6.26	118.38	127.31
30	C	514	BCR	C24-C23-C22	-6.25	116.79	126.23
39	N	616	LUT	C7-C8-C9	-6.19	116.88	126.23
30	c	514	BCR	C16-C17-C18	-6.18	118.49	127.31
30	B	619	BCR	C16-C17-C18	-6.18	118.50	127.31
39	r	614	LUT	C18-C5-C6	-6.13	117.64	124.53
39	G	616	LUT	C11-C10-C9	-6.12	118.58	127.31
30	D	405	BCR	C15-C14-C13	-6.12	118.58	127.31
39	n	616	LUT	C18-C5-C6	-6.06	117.72	124.53
28	n	612	CLA	CMD-C2D-C1D	6.03	135.34	124.71
30	K	101	BCR	C24-C23-C22	-6.01	117.15	126.23
30	T	101	BCR	C38-C26-C25	-6.00	117.79	124.53
39	R	614	LUT	C7-C8-C9	-5.94	117.25	126.23
28	g	614	CLA	CMD-C2D-C1D	5.93	135.16	124.71
30	B	619	BCR	C15-C14-C13	-5.91	118.88	127.31
30	T	101	BCR	C30-C25-C26	-5.89	114.31	122.61
39	R	614	LUT	C11-C10-C9	-5.89	118.91	127.31
39	r	614	LUT	C12-C13-C14	5.82	127.88	118.94
28	R	609	CLA	CMD-C2D-C1D	5.82	134.97	124.71
30	i	101	BCR	C15-C14-C13	-5.82	119.00	127.31
28	n	611	CLA	O2D-CGD-CBD	5.81	121.60	111.27
28	c	509	CLA	O2D-CGD-CBD	5.81	121.59	111.27
30	H	101	BCR	C15-C14-C13	-5.81	119.02	127.31
40	G	617	NEX	C27-C28-C29	-5.81	116.52	125.53
28	Y	614	CLA	CMD-C2D-C1D	5.80	134.94	124.71
28	b	606	CLA	CMD-C2D-C1D	5.77	134.88	124.71
30	B	618	BCR	C15-C14-C13	-5.77	119.08	127.31
28	S	303	CLA	CMD-C2D-C1D	5.76	134.87	124.71
28	G	604	CLA	CMD-C2D-C1D	5.73	134.81	124.71
28	R	604	CLA	O2D-CGD-CBD	5.70	121.40	111.27
28	r	602	CLA	CMD-C2D-C1D	5.70	134.75	124.71
28	G	613	CLA	O2A-C1-C2	5.69	123.59	108.64
28	n	603	CLA	CMD-C2D-C1D	5.69	134.74	124.71
30	t	101	BCR	C11-C10-C9	-5.69	119.19	127.31
30	d	406	BCR	C24-C23-C22	-5.68	117.64	126.23
39	g	616	LUT	C35-C34-C33	-5.68	119.21	127.31
28	n	614	CLA	CMD-C2D-C1D	5.67	134.71	124.71
30	k	101	BCR	C24-C23-C22	-5.67	117.67	126.23
28	r	603	CLA	CMD-C2D-C1D	5.67	134.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	309	CLA	CMD-C2D-C1D	5.67	134.70	124.71
28	b	614	CLA	CMD-C2D-C1D	5.66	134.69	124.71
28	g	602	CLA	CMD-C2D-C1D	5.65	134.68	124.71
28	y	314	CLA	CMD-C2D-C1D	5.65	134.67	124.71
30	a	410	BCR	C16-C17-C18	-5.65	119.25	127.31
30	h	101	BCR	C20-C21-C22	-5.65	119.25	127.31
28	Y	604	CLA	CMD-C2D-C1D	5.65	134.67	124.71
28	g	613	CLA	O2A-C1-C2	5.64	123.46	108.64
28	B	602	CLA	CMD-C2D-C1D	5.64	134.65	124.71
28	n	613	CLA	CMD-C2D-C1D	5.64	134.65	124.71
39	r	614	LUT	C20-C13-C14	-5.64	115.02	122.92
28	b	602	CLA	CMD-C2D-C1D	5.63	134.64	124.71
28	n	603	CLA	O2D-CGD-CBD	5.63	121.28	111.27
28	s	602	CLA	CMD-C2D-C1D	5.63	134.64	124.71
30	T	101	BCR	C27-C26-C25	-5.63	114.56	122.73
28	B	611	CLA	CMD-C2D-C1D	5.63	134.63	124.71
28	g	612	CLA	CMD-C2D-C1D	5.62	134.63	124.71
28	Y	603	CLA	CMD-C2D-C1D	5.62	134.62	124.71
28	c	510	CLA	CMD-C2D-C1D	5.62	134.62	124.71
28	y	304	CLA	CMD-C2D-C1D	5.62	134.62	124.71
28	S	310	CLA	CMD-C2D-C1D	5.62	134.61	124.71
28	N	614	CLA	CMD-C2D-C1D	5.62	134.61	124.71
28	r	609	CLA	O2D-CGD-CBD	5.62	121.25	111.27
28	d	405	CLA	CMD-C2D-C1D	5.62	134.61	124.71
28	y	303	CLA	CMD-C2D-C1D	5.61	134.60	124.71
28	n	604	CLA	CMD-C2D-C1D	5.61	134.59	124.71
39	G	615	LUT	C28-C29-C30	5.60	127.54	118.94
28	r	609	CLA	CMD-C2D-C1D	5.60	134.59	124.71
28	n	610	CLA	CMD-C2D-C1D	5.58	134.56	124.71
28	N	602	CLA	CMD-C2D-C1D	5.58	134.55	124.71
39	R	614	LUT	C18-C5-C6	-5.58	118.26	124.53
28	S	314	CLA	CMD-C2D-C1D	5.58	134.54	124.71
28	b	611	CLA	CMD-C2D-C1D	5.58	134.54	124.71
28	b	603	CLA	CMD-C2D-C1D	5.58	134.54	124.71
28	b	605	CLA	CMD-C2D-C1D	5.58	134.54	124.71
28	c	504	CLA	CMD-C2D-C1D	5.58	134.54	124.71
28	C	512	CLA	CMD-C2D-C1D	5.57	134.54	124.71
28	N	603	CLA	CMD-C2D-C1D	5.57	134.53	124.71
40	g	617	NEX	C27-C28-C29	-5.57	116.88	125.53
28	N	610	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	c	501	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	b	605	CLA	O2D-CGD-CBD	5.56	121.15	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	503	CLA	CMD-C2D-C1D	5.56	134.52	124.71
28	C	510	CLA	CMD-C2D-C1D	5.56	134.51	124.71
28	D	404	CLA	CMD-C2D-C1D	5.56	134.51	124.71
28	R	603	CLA	CMD-C2D-C1D	5.56	134.51	124.71
39	g	615	LUT	C35-C34-C33	-5.56	119.37	127.31
28	A	408	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	B	609	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	c	511	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	b	609	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	S	304	CLA	CMD-C2D-C1D	5.55	134.49	124.71
28	N	604	CLA	CMD-C2D-C1D	5.55	134.49	124.71
28	G	610	CLA	CMD-C2D-C1D	5.54	134.48	124.71
28	C	504	CLA	CMD-C2D-C1D	5.54	134.48	124.71
28	B	605	CLA	CMD-C2D-C1D	5.54	134.47	124.71
28	y	310	CLA	CMD-C2D-C1D	5.54	134.47	124.71
28	g	604	CLA	CMD-C2D-C1D	5.54	134.47	124.71
28	r	601	CLA	CMD-C2D-C1D	5.53	134.47	124.71
39	s	615	LUT	C11-C10-C9	-5.53	119.41	127.31
28	B	601	CLA	CMD-C2D-C1D	5.53	134.45	124.71
28	R	612	CLA	CMD-C2D-C1D	5.52	134.45	124.71
28	B	614	CLA	CMD-C2D-C1D	5.52	134.45	124.71
30	C	514	BCR	C38-C26-C25	-5.52	118.33	124.53
28	n	602	CLA	CMD-C2D-C1D	5.52	134.44	124.71
28	a	409	CLA	CMD-C2D-C1D	5.52	134.44	124.71
30	C	514	BCR	C27-C26-C25	-5.52	114.72	122.73
28	C	509	CLA	CMD-C2D-C1D	5.52	134.43	124.71
39	Y	616	LUT	C7-C8-C9	-5.51	117.90	126.23
28	C	503	CLA	CMD-C2D-C1D	5.51	134.43	124.71
28	r	604	CLA	O2D-CGD-CBD	5.51	121.06	111.27
28	C	511	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	G	602	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	c	513	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	g	604	CLA	O2A-C1-C2	5.50	123.10	108.64
28	b	608	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	R	604	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	Y	613	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	r	612	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	b	615	CLA	CMD-C2D-C1D	5.50	134.40	124.71
28	d	404	CLA	CMD-C2D-C1D	5.50	134.40	124.71
28	C	501	CLA	CMD-C2D-C1D	5.49	134.40	124.71
28	c	506	CLA	CMD-C2D-C1D	5.49	134.39	124.71
28	B	610	CLA	CMD-C2D-C1D	5.49	134.39	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	607	CLA	CMD-C2D-C1D	5.49	134.39	124.71
28	C	508	CLA	CMD-C2D-C1D	5.49	134.39	124.71
28	B	616	CLA	CMD-C2D-C1D	5.49	134.39	124.71
28	a	406	CLA	CMD-C2D-C1D	5.49	134.39	124.71
28	y	312	CLA	CMD-C2D-C1D	5.49	134.38	124.71
30	i	101	BCR	C20-C21-C22	-5.49	119.48	127.31
28	R	611	CLA	CMD-C2D-C1D	5.49	134.38	124.71
28	b	601	CLA	CMD-C2D-C1D	5.49	134.38	124.71
28	R	613	CLA	CMD-C2D-C1D	5.48	134.38	124.71
28	b	607	CLA	CMD-C2D-C1D	5.48	134.38	124.71
28	y	305	CLA	CMD-C2D-C1D	5.48	134.38	124.71
28	b	604	CLA	CMD-C2D-C1D	5.48	134.38	124.71
28	D	401	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	C	507	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	Y	612	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	S	305	CLA	O2D-CGD-CBD	5.48	121.00	111.27
28	B	603	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	c	507	CLA	CMD-C2D-C1D	5.48	134.37	124.71
30	C	515	BCR	C20-C21-C22	-5.48	119.50	127.31
41	r	615	XAT	C31-C30-C29	-5.47	119.50	127.31
28	N	613	CLA	CMD-C2D-C1D	5.47	134.36	124.71
28	B	615	CLA	CMD-C2D-C1D	5.47	134.36	124.71
28	y	313	CLA	CMD-C2D-C1D	5.47	134.35	124.71
28	G	610	CLA	O2D-CGD-CBD	5.47	120.99	111.27
28	R	608	CLA	CMD-C2D-C1D	5.47	134.35	124.71
28	B	604	CLA	CMD-C2D-C1D	5.46	134.33	124.71
28	a	407	CLA	CMD-C2D-C1D	5.46	134.33	124.71
28	C	513	CLA	CMD-C2D-C1D	5.45	134.32	124.71
41	R	615	XAT	C31-C30-C29	-5.45	119.53	127.31
28	R	610	CLA	O2A-C1-C2	5.45	121.71	108.97
28	b	610	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	A	405	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	b	613	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	d	401	CLA	CMD-C2D-C1D	5.44	134.31	124.71
28	s	604	CLA	CMD-C2D-C1D	5.44	134.31	124.71
28	G	612	CLA	CMD-C2D-C1D	5.44	134.30	124.71
28	D	403	CLA	CMD-C2D-C1D	5.43	134.28	124.71
28	N	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
28	G	613	CLA	CMD-C2D-C1D	5.42	134.27	124.71
28	c	505	CLA	CMD-C2D-C1D	5.42	134.27	124.71
40	s	616	NEX	C38-C25-C24	5.42	120.38	114.28
28	B	606	CLA	CMD-C2D-C1D	5.42	134.27	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	603	CLA	CMD-C2D-C1D	5.42	134.26	124.71
28	G	611	CLA	O2D-CGD-CBD	5.42	120.89	111.27
28	c	502	CLA	CMD-C2D-C1D	5.41	134.25	124.71
28	r	613	CLA	CMD-C2D-C1D	5.41	134.24	124.71
30	i	101	BCR	C33-C5-C6	-5.41	118.46	124.53
28	A	406	CLA	CMD-C2D-C1D	5.41	134.24	124.71
28	C	502	CLA	CMD-C2D-C1D	5.40	134.24	124.71
30	t	101	BCR	C4-C5-C6	-5.40	114.89	122.73
28	B	613	CLA	CMD-C2D-C1D	5.40	134.23	124.71
28	g	613	CLA	CMD-C2D-C1D	5.39	134.22	124.71
28	g	612	CLA	O2D-CGD-CBD	5.39	120.85	111.27
39	N	616	LUT	C35-C34-C33	-5.39	119.62	127.31
28	b	616	CLA	CMD-C2D-C1D	5.39	134.21	124.71
41	r	615	XAT	C38-C25-C24	5.38	120.33	114.28
28	G	603	CLA	CMD-C2D-C1D	5.38	134.20	124.71
28	s	613	CLA	CMD-C2D-C1D	5.38	134.20	124.71
28	C	506	CLA	CMD-C2D-C1D	5.38	134.19	124.71
28	s	608	CLA	CMD-C2D-C1D	5.38	134.19	124.71
28	C	505	CLA	CMD-C2D-C1D	5.37	134.18	124.71
28	B	608	CLA	CMD-C2D-C1D	5.37	134.18	124.71
37	E	101	HEM	CHC-C4B-NB	5.37	130.26	124.42
28	s	611	CLA	CMD-C2D-C1D	5.37	134.18	124.71
28	g	611	CLA	O2D-CGD-CBD	5.37	120.81	111.27
28	s	603	CLA	CMD-C2D-C1D	5.37	134.17	124.71
41	R	615	XAT	C38-C25-C24	5.37	120.32	114.28
41	Y	617	XAT	C15-C14-C13	-5.36	119.66	127.31
30	i	101	BCR	C16-C17-C18	-5.35	119.67	127.31
28	g	610	CLA	O2A-C1-C2	5.35	122.70	108.64
30	c	515	BCR	C11-C10-C9	-5.35	119.67	127.31
28	r	604	CLA	CMD-C2D-C1D	5.35	134.14	124.71
28	S	312	CLA	CMD-C2D-C1D	5.34	134.13	124.71
39	s	615	LUT	C35-C34-C33	-5.34	119.69	127.31
28	c	509	CLA	CMD-C2D-C1D	5.34	134.12	124.71
28	c	512	CLA	CMD-C2D-C1D	5.34	134.12	124.71
28	r	603	CLA	O2A-C1-C2	5.33	122.65	108.64
28	c	510	CLA	O2A-C1-C2	5.33	122.65	108.64
30	t	101	BCR	C38-C26-C25	-5.33	118.54	124.53
28	y	310	CLA	O2D-CGD-CBD	5.33	120.73	111.27
28	g	611	CLA	CMD-C2D-C1D	5.33	134.10	124.71
28	Y	603	CLA	O2A-C1-C2	5.32	122.62	108.64
37	f	101	HEM	CHC-C4B-NB	5.32	130.20	124.42
28	r	603	CLA	O2D-CGD-CBD	5.32	120.71	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	611	CLA	CMD-C2D-C1D	5.31	134.08	124.71
30	k	101	BCR	C16-C17-C18	-5.31	119.73	127.31
28	S	311	CLA	CMD-C2D-C1D	5.31	134.07	124.71
28	r	608	CLA	CMD-C2D-C1D	5.31	134.07	124.71
30	c	514	BCR	C38-C26-C25	-5.30	118.57	124.53
28	B	605	CLA	O2A-C1-C2	5.30	122.56	108.64
39	N	615	LUT	C18-C5-C6	-5.29	118.58	124.53
28	r	610	CLA	O2A-C1-C2	5.29	121.34	108.97
39	S	315	LUT	C35-C34-C33	-5.29	119.76	127.31
28	y	311	CLA	CMD-C2D-C1D	5.28	134.03	124.71
28	N	602	CLA	O2A-C1-C2	5.28	122.52	108.64
28	D	404	CLA	O2D-CGD-CBD	5.28	120.65	111.27
28	N	611	CLA	CMD-C2D-C1D	5.28	134.02	124.71
28	G	614	CLA	CMD-C2D-C1D	5.28	134.01	124.71
30	c	514	BCR	C20-C21-C22	-5.27	119.78	127.31
28	s	609	CLA	CMD-C2D-C1D	5.27	134.00	124.71
28	S	305	CLA	CMD-C2D-C1D	5.27	134.00	124.71
28	g	614	CLA	O2D-CGD-CBD	5.27	120.62	111.27
28	g	610	CLA	CMD-C2D-C1D	5.26	133.99	124.71
30	b	617	BCR	C15-C14-C13	-5.26	119.80	127.31
30	d	406	BCR	C11-C10-C9	-5.26	119.80	127.31
28	S	311	CLA	O2A-C1-C2	5.26	122.45	108.64
28	s	610	CLA	CMD-C2D-C1D	5.25	133.97	124.71
30	C	514	BCR	C30-C25-C26	-5.25	115.22	122.61
40	r	616	NEX	C38-C25-C24	5.25	120.19	114.28
28	R	611	CLA	O2A-C1-C2	5.24	121.23	108.97
28	R	602	CLA	CMD-C2D-C1D	5.24	133.95	124.71
41	Y	617	XAT	C38-C25-C24	5.24	120.17	114.28
28	C	504	CLA	O2D-CGD-CBD	5.24	120.57	111.27
28	s	608	CLA	O2D-CGD-CBD	5.24	120.57	111.27
28	S	310	CLA	O2D-CGD-CBD	5.23	120.57	111.27
28	B	602	CLA	O2A-C1-C2	5.23	122.39	108.64
28	S	313	CLA	CMD-C2D-C1D	5.23	133.93	124.71
28	r	610	CLA	CMD-C2D-C1D	5.22	133.92	124.71
28	b	604	CLA	O2A-C1-C2	5.22	122.36	108.64
40	G	617	NEX	C38-C25-C24	5.22	120.15	114.28
28	S	314	CLA	O2A-C1-C2	5.22	121.17	108.97
39	G	615	LUT	C18-C5-C6	-5.21	118.67	124.53
28	s	612	CLA	CMD-C2D-C1D	5.21	133.90	124.71
28	C	511	CLA	O2A-C1-C2	5.21	122.33	108.64
28	R	601	CLA	CMD-C2D-C1D	5.21	133.90	124.71
28	B	612	CLA	CMD-C2D-C1D	5.21	133.89	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	615	CLA	O2D-CGD-CBD	5.21	120.52	111.27
30	K	101	BCR	C27-C26-C25	-5.20	115.18	122.73
28	d	405	CLA	O2D-CGD-CBD	5.20	120.51	111.27
28	y	304	CLA	O2D-CGD-CBD	5.20	120.51	111.27
28	S	314	CLA	O2D-CGD-CBD	5.20	120.50	111.27
28	b	606	CLA	O2D-CGD-CBD	5.20	120.50	111.27
30	d	406	BCR	C7-C8-C9	-5.19	118.40	126.23
28	b	612	CLA	CMD-C2D-C1D	5.18	133.85	124.71
40	y	318	NEX	C27-C28-C29	-5.18	117.49	125.53
28	C	502	CLA	O2D-CGD-CBD	5.18	120.47	111.27
28	c	508	CLA	CMD-C2D-C1D	5.18	133.84	124.71
28	y	313	CLA	O2A-C1-C2	5.17	122.23	108.64
28	r	601	CLA	O2A-C1-C2	5.17	121.07	108.97
28	c	502	CLA	O2D-CGD-CBD	5.17	120.46	111.27
30	d	406	BCR	C1-C6-C5	-5.17	115.33	122.61
28	B	604	CLA	O2A-C1-C2	5.17	122.21	108.64
28	b	615	CLA	O2D-CGD-CBD	5.17	120.45	111.27
28	R	611	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	R	612	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	Y	603	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	n	604	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	S	309	CLA	O2D-CGD-CBD	5.15	120.43	111.27
28	d	404	CLA	O2A-C1-C2	5.15	122.18	108.64
30	B	618	BCR	C11-C10-C9	-5.15	119.96	127.31
39	S	316	LUT	C11-C10-C9	-5.15	119.96	127.31
28	b	612	CLA	O2D-CGD-CBD	5.15	120.42	111.27
30	B	617	BCR	C15-C14-C13	-5.15	119.96	127.31
28	C	510	CLA	O2A-C1-C2	5.15	122.16	108.64
28	S	312	CLA	O2A-C1-C2	5.14	121.00	108.97
28	G	603	CLA	O2D-CGD-CBD	5.14	120.41	111.27
28	g	603	CLA	O2D-CGD-CBD	5.14	120.41	111.27
28	s	613	CLA	O2A-C1-C2	5.14	121.00	108.97
28	b	616	CLA	O2D-CGD-CBD	5.14	120.40	111.27
28	b	602	CLA	O2A-C1-C2	5.13	122.13	108.64
28	C	512	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	g	604	CLA	C1-C2-C3	-5.13	118.45	126.75
28	A	408	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	s	613	CLA	O2D-CGD-CBD	5.13	120.39	111.27
41	y	317	XAT	C38-C25-C24	5.13	120.05	114.28
28	S	305	CLA	O2A-C1-C2	5.13	122.12	108.64
28	s	604	CLA	O2D-CGD-CBD	5.13	120.38	111.27
28	R	610	CLA	CMD-C2D-C1D	5.13	133.75	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	101	BCR	C16-C17-C18	-5.13	120.00	127.31
28	y	312	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	n	610	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	r	608	CLA	O2A-C1-C2	5.12	122.09	108.64
28	G	602	CLA	O2D-CGD-CBD	5.12	120.36	111.27
28	a	409	CLA	O2D-CGD-CBD	5.12	120.36	111.27
28	y	311	CLA	O2D-CGD-CBD	5.12	120.36	111.27
40	G	617	NEX	C38-C25-C26	-5.11	113.69	122.26
28	Y	611	CLA	O2D-CGD-CBD	5.11	120.35	111.27
28	c	508	CLA	O2A-C1-C2	5.11	122.07	108.64
28	c	504	CLA	O2D-CGD-CBD	5.11	120.35	111.27
30	a	410	BCR	C11-C10-C9	-5.11	120.02	127.31
28	n	603	CLA	O2A-C1-C2	5.11	122.06	108.64
28	a	409	CLA	O2A-C1-C2	5.11	122.06	108.64
30	T	101	BCR	C11-C10-C9	-5.10	120.03	127.31
30	t	101	BCR	C20-C21-C22	-5.10	120.03	127.31
28	b	603	CLA	O2A-C1-C2	5.10	122.04	108.64
28	B	612	CLA	O2D-CGD-CBD	5.10	120.33	111.27
28	B	610	CLA	O2D-CGD-CBD	5.10	120.32	111.27
28	b	609	CLA	O2D-CGD-CBD	5.09	120.30	111.27
28	b	609	CLA	O2A-C1-C2	5.08	121.99	108.64
28	R	603	CLA	O2A-C1-C2	5.08	121.98	108.64
28	n	613	CLA	O2D-CGD-CBD	5.07	120.28	111.27
28	S	304	CLA	O2D-CGD-CBD	5.07	120.28	111.27
28	R	612	CLA	O2A-C1-C2	5.07	121.96	108.64
28	b	603	CLA	O2D-CGD-CBD	5.07	120.27	111.27
28	Y	612	CLA	O2D-CGD-CBD	5.06	120.27	111.27
28	Y	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
28	g	604	CLA	O2D-CGD-CBD	5.06	120.25	111.27
28	g	602	CLA	O2D-CGD-CBD	5.05	120.25	111.27
28	Y	604	CLA	O2D-CGD-CBD	5.05	120.24	111.27
28	R	608	CLA	O2A-C1-C2	5.05	121.90	108.64
28	n	602	CLA	O2D-CGD-CBD	5.05	120.23	111.27
28	D	403	CLA	O2A-C1-C2	5.05	121.90	108.64
30	C	515	BCR	C33-C5-C6	-5.05	118.86	124.53
28	R	603	CLA	O2D-CGD-CBD	5.04	120.23	111.27
39	r	614	LUT	C15-C35-C34	-5.04	113.14	123.47
28	B	607	CLA	O2D-CGD-CBD	5.04	120.22	111.27
39	Y	615	LUT	C18-C5-C6	-5.04	118.87	124.53
28	B	606	CLA	O2A-C1-C2	5.04	121.88	108.64
28	c	512	CLA	O2D-CGD-CBD	5.04	120.22	111.27
28	y	312	CLA	O2A-C1-C2	5.03	121.86	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	101	BCR	C11-C10-C9	-5.03	120.13	127.31
28	N	610	CLA	O2D-CGD-CBD	5.03	120.21	111.27
30	h	101	BCR	C38-C26-C25	-5.03	118.88	124.53
28	R	609	CLA	O2D-CGD-CBD	5.02	120.19	111.27
28	c	510	CLA	O2D-CGD-CBD	5.02	120.19	111.27
30	H	101	BCR	C33-C5-C6	-5.02	118.89	124.53
28	c	503	CLA	O2D-CGD-CBD	5.02	120.19	111.27
28	b	601	CLA	O2D-CGD-CBD	5.02	120.19	111.27
30	C	514	BCR	C20-C19-C18	-5.02	112.32	126.42
28	G	604	CLA	O2D-CGD-CBD	5.02	120.18	111.27
28	D	404	CLA	O2A-C1-C2	5.00	121.79	108.64
28	B	603	CLA	O2D-CGD-CBD	5.00	120.16	111.27
28	B	605	CLA	O2D-CGD-CBD	5.00	120.15	111.27
39	r	614	LUT	C8-C9-C10	5.00	126.61	118.94
28	c	509	CLA	O2A-C1-C2	5.00	121.77	108.64
28	B	609	CLA	O2D-CGD-CBD	5.00	120.15	111.27
28	C	508	CLA	O2D-CGD-CBD	5.00	120.15	111.27
28	B	609	CLA	O2A-C1-C2	5.00	121.77	108.64
28	B	611	CLA	O2D-CGD-CBD	4.99	120.14	111.27
30	c	514	BCR	C27-C26-C25	-4.99	115.48	122.73
28	y	303	CLA	O2D-CGD-CBD	4.99	120.13	111.27
28	s	611	CLA	O2D-CGD-CBD	4.99	120.13	111.27
30	H	101	BCR	C11-C10-C9	-4.98	120.20	127.31
28	B	608	CLA	O2D-CGD-CBD	4.98	120.12	111.27
28	N	604	CLA	O2A-C1-C2	4.98	121.72	108.64
28	c	513	CLA	O2D-CGD-CBD	4.98	120.12	111.27
28	A	408	CLA	O2A-C1-C2	4.98	121.72	108.64
28	g	610	CLA	C1-C2-C3	-4.98	117.44	126.04
28	R	601	CLA	O2D-CGD-CBD	4.97	120.11	111.27
28	r	601	CLA	O2D-CGD-CBD	4.97	120.11	111.27
28	c	506	CLA	O2A-C1-C2	4.97	121.70	108.64
28	s	611	CLA	O2A-C1-C2	4.97	120.60	108.97
28	r	611	CLA	O2A-C1-C2	4.97	120.58	108.97
30	H	101	BCR	C20-C21-C22	-4.97	120.22	127.31
28	r	608	CLA	O2D-CGD-CBD	4.96	120.09	111.27
39	r	614	LUT	C19-C9-C10	-4.96	115.97	122.92
28	N	604	CLA	O2D-CGD-CBD	4.96	120.08	111.27
41	y	317	XAT	C15-C14-C13	-4.96	120.23	127.31
28	Y	610	CLA	CMD-C2D-C1D	4.96	133.45	124.71
28	N	602	CLA	O2D-CGD-CBD	4.96	120.08	111.27
28	N	612	CLA	O2D-CGD-CBD	4.96	120.08	111.27
28	c	512	CLA	O2A-C1-C2	4.96	121.66	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	505	CLA	O2D-CGD-CBD	4.96	120.08	111.27
28	r	611	CLA	O2D-CGD-CBD	4.96	120.08	111.27
39	S	316	LUT	C15-C14-C13	-4.96	120.24	127.31
28	B	606	CLA	O2D-CGD-CBD	4.95	120.07	111.27
28	r	612	CLA	O2A-C1-C2	4.95	121.64	108.64
30	D	405	BCR	C11-C10-C9	-4.95	120.25	127.31
39	s	614	LUT	C35-C34-C33	-4.95	120.25	127.31
28	c	501	CLA	O2D-CGD-CBD	4.95	120.06	111.27
28	B	613	CLA	O2D-CGD-CBD	4.94	120.06	111.27
28	g	613	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	614	CLA	O2A-C1-C2	4.94	121.63	108.64
28	C	503	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	N	603	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	611	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	608	CLA	O2D-CGD-CBD	4.94	120.04	111.27
28	N	603	CLA	O2A-C1-C2	4.94	121.61	108.64
28	b	607	CLA	O2D-CGD-CBD	4.93	120.03	111.27
28	G	602	CLA	O2A-C1-C2	4.93	121.60	108.64
28	b	615	CLA	O2A-C1-C2	4.93	121.60	108.64
39	y	316	LUT	C35-C34-C33	-4.93	120.28	127.31
28	y	305	CLA	O2D-CGD-CBD	4.93	120.02	111.27
28	s	609	CLA	O2D-CGD-CBD	4.92	120.02	111.27
28	B	611	CLA	O2A-C1-C2	4.92	121.57	108.64
28	B	602	CLA	O2D-CGD-CBD	4.92	120.01	111.27
39	G	616	LUT	C1-C6-C5	-4.92	115.69	122.61
28	d	404	CLA	O2D-CGD-CBD	4.92	120.01	111.27
28	b	604	CLA	O2D-CGD-CBD	4.92	120.00	111.27
30	k	101	BCR	C1-C6-C5	-4.92	115.69	122.61
28	b	602	CLA	O2D-CGD-CBD	4.91	120.00	111.27
40	s	616	NEX	C27-C28-C29	-4.91	117.91	125.53
40	Y	618	NEX	C27-C28-C29	-4.91	117.91	125.53
28	y	313	CLA	O2D-CGD-CBD	4.91	119.99	111.27
28	c	507	CLA	O2A-C1-C2	4.91	121.53	108.64
28	a	406	CLA	O2D-CGD-CBD	4.91	119.99	111.27
28	C	501	CLA	O2A-C1-C2	4.91	121.53	108.64
28	B	604	CLA	O2D-CGD-CBD	4.90	119.98	111.27
28	C	507	CLA	O2D-CGD-CBD	4.90	119.98	111.27
28	r	612	CLA	O2D-CGD-CBD	4.90	119.98	111.27
28	s	603	CLA	O2D-CGD-CBD	4.90	119.98	111.27
28	C	503	CLA	O2A-C1-C2	4.90	121.52	108.64
28	D	403	CLA	O2D-CGD-CBD	4.90	119.97	111.27
28	b	611	CLA	O2A-C1-C2	4.90	121.50	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	611	CLA	CMD-C2D-C1D	4.89	133.33	124.71
28	G	612	CLA	O2D-CGD-CBD	4.89	119.96	111.27
28	C	501	CLA	O2D-CGD-CBD	4.88	119.95	111.27
28	A	405	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	C	505	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	C	506	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	N	613	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	B	601	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	B	616	CLA	O2A-C1-C2	4.88	121.45	108.64
28	r	602	CLA	O2D-CGD-CBD	4.87	119.93	111.27
28	s	610	CLA	O2D-CGD-CBD	4.87	119.93	111.27
28	C	509	CLA	O2D-CGD-CBD	4.87	119.93	111.27
28	S	313	CLA	O2D-CGD-CBD	4.87	119.92	111.27
28	Y	613	CLA	O2D-CGD-CBD	4.87	119.92	111.27
28	N	612	CLA	O2A-C1-C2	4.87	121.43	108.64
28	C	513	CLA	O2D-CGD-CBD	4.86	119.91	111.27
28	G	613	CLA	O2D-CGD-CBD	4.86	119.91	111.27
28	S	311	CLA	O2D-CGD-CBD	4.86	119.91	111.27
28	s	612	CLA	O2D-CGD-CBD	4.86	119.90	111.27
28	G	614	CLA	O2D-CGD-CBD	4.86	119.90	111.27
28	g	603	CLA	O2A-C1-C2	4.86	121.40	108.64
30	t	101	BCR	C27-C26-C25	-4.86	115.68	122.73
28	a	407	CLA	O2D-CGD-CBD	4.86	119.90	111.27
28	c	511	CLA	O2D-CGD-CBD	4.85	119.89	111.27
28	B	610	CLA	O2A-C1-C2	4.85	121.39	108.64
28	B	614	CLA	O2D-CGD-CBD	4.85	119.89	111.27
30	a	410	BCR	C15-C14-C13	-4.84	120.40	127.31
28	R	602	CLA	O2D-CGD-CBD	4.84	119.87	111.27
30	b	619	BCR	C16-C17-C18	-4.84	120.41	127.31
30	t	101	BCR	C16-C17-C18	-4.83	120.41	127.31
28	A	406	CLA	O2D-CGD-CBD	4.83	119.85	111.27
28	b	613	CLA	O2D-CGD-CBD	4.83	119.85	111.27
40	n	617	NEX	C1-C2-C3	-4.83	102.74	113.64
30	C	515	BCR	C16-C17-C18	-4.83	120.42	127.31
39	G	615	LUT	C21-C26-C27	-4.82	106.60	112.70
30	c	515	BCR	C7-C8-C9	-4.82	118.95	126.23
28	c	507	CLA	O2D-CGD-CBD	4.82	119.84	111.27
30	t	101	BCR	C1-C6-C5	-4.82	115.83	122.61
28	B	613	CLA	O2A-C1-C2	4.81	121.29	108.64
39	S	316	LUT	C35-C34-C33	-4.81	120.44	127.31
28	S	303	CLA	O2D-CGD-CBD	4.81	119.82	111.27
38	N	609	CHL	CHD-C1D-ND	-4.81	120.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	602	CLA	O2D-CGD-CBD	4.81	119.81	111.27
28	b	610	CLA	O2D-CGD-CBD	4.80	119.80	111.27
28	y	304	CLA	O2A-C1-C2	4.80	121.26	108.64
28	Y	614	CLA	O2D-CGD-CBD	4.80	119.80	111.27
30	d	406	BCR	C30-C25-C26	-4.80	115.85	122.61
28	y	314	CLA	O2D-CGD-CBD	4.80	119.80	111.27
28	b	607	CLA	O2A-C1-C2	4.79	121.24	108.64
39	S	315	LUT	C18-C5-C6	-4.79	119.14	124.53
30	B	619	BCR	C7-C8-C9	-4.79	118.99	126.23
30	A	409	BCR	C11-C10-C9	-4.79	120.47	127.31
28	D	401	CLA	O2D-CGD-CBD	4.79	119.78	111.27
39	r	614	LUT	C10-C11-C12	-4.79	108.28	123.22
30	H	101	BCR	C16-C17-C18	-4.79	120.48	127.31
28	C	511	CLA	O2D-CGD-CBD	4.79	119.77	111.27
28	c	511	CLA	O2A-C1-C2	4.78	121.19	108.64
28	r	610	CLA	O2D-CGD-CBD	4.78	119.76	111.27
28	c	501	CLA	O2A-C1-C2	4.78	121.19	108.64
28	r	611	CLA	CMD-C2D-C1D	4.78	133.13	124.71
28	Y	612	CLA	O2A-C1-C2	4.78	121.19	108.64
28	d	401	CLA	O2D-CGD-CBD	4.78	119.75	111.27
28	R	608	CLA	O2D-CGD-CBD	4.77	119.75	111.27
28	N	611	CLA	O2D-CGD-CBD	4.77	119.75	111.27
30	a	410	BCR	C33-C5-C6	-4.77	119.17	124.53
28	Y	604	CLA	O2A-C1-C2	4.77	121.16	108.64
28	b	601	CLA	O2A-C1-C2	4.77	121.16	108.64
30	D	405	BCR	C33-C5-C6	-4.77	119.18	124.53
28	C	513	CLA	O2A-C1-C2	4.76	121.16	108.64
30	b	619	BCR	C24-C23-C22	-4.76	119.04	126.23
39	S	316	LUT	C7-C8-C9	-4.76	119.05	126.23
28	B	616	CLA	O2D-CGD-CBD	4.76	119.72	111.27
28	N	604	CLA	C1-C2-C3	-4.75	119.06	126.75
28	Y	602	CLA	CMD-C2D-C1D	4.75	133.08	124.71
30	c	515	BCR	C15-C14-C13	-4.74	120.54	127.31
28	b	610	CLA	O2A-C1-C2	4.74	121.10	108.64
28	y	310	CLA	O2A-C1-C2	4.74	121.09	108.64
28	n	602	CLA	O2A-C1-C2	4.74	121.09	108.64
28	r	609	CLA	O2A-C1-C2	4.74	121.09	108.64
30	t	101	BCR	C24-C23-C22	-4.74	119.07	126.23
38	g	606	CHL	CHD-C1D-ND	-4.73	120.10	124.45
30	D	405	BCR	C1-C6-C5	-4.73	115.95	122.61
28	Y	610	CLA	O2A-C1-C2	4.73	121.08	108.64
28	G	610	CLA	O2A-C1-C2	4.73	121.07	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	y	316	LUT	C7-C8-C9	-4.73	119.09	126.23
30	C	514	BCR	C1-C6-C5	-4.73	115.96	122.61
28	G	613	CLA	C1-C2-C3	-4.72	117.88	126.04
30	D	405	BCR	C24-C23-C22	-4.72	119.11	126.23
28	b	613	CLA	O2A-C1-C2	4.72	121.03	108.64
28	S	312	CLA	O2D-CGD-CBD	4.71	119.64	111.27
30	K	101	BCR	C30-C25-C26	-4.71	115.98	122.61
28	b	612	CLA	O2A-C1-C2	4.70	120.99	108.64
30	b	619	BCR	C2-C1-C6	4.70	117.72	110.48
28	Y	611	CLA	O2A-C1-C2	4.70	120.98	108.64
28	B	615	CLA	O2A-C1-C2	4.69	120.97	108.64
30	K	101	BCR	C33-C5-C6	-4.69	119.26	124.53
28	b	606	CLA	O2A-C1-C2	4.69	120.96	108.64
30	k	101	BCR	C38-C26-C25	-4.69	119.26	124.53
28	S	310	CLA	O2A-C1-C2	4.69	120.96	108.64
30	T	101	BCR	C16-C17-C18	-4.69	120.62	127.31
28	d	405	CLA	O2A-C1-C2	4.68	120.94	108.64
39	n	616	LUT	C11-C10-C9	-4.68	120.63	127.31
30	B	619	BCR	C11-C10-C9	-4.68	120.63	127.31
41	y	317	XAT	C31-C30-C29	-4.68	120.64	127.31
39	s	615	LUT	C7-C8-C9	-4.67	119.17	126.23
28	B	612	CLA	O2A-C1-C2	4.67	120.91	108.64
39	N	616	LUT	C11-C10-C9	-4.67	120.64	127.31
30	C	516	BCR	C16-C17-C18	-4.67	120.65	127.31
30	d	406	BCR	C38-C26-C25	-4.67	119.29	124.53
30	k	101	BCR	C11-C10-C9	-4.67	120.65	127.31
28	R	610	CLA	O2D-CGD-CBD	4.67	119.56	111.27
28	C	510	CLA	O2D-CGD-CBD	4.66	119.55	111.27
28	n	612	CLA	O2D-CGD-CBD	4.66	119.55	111.27
28	g	602	CLA	O2A-C1-C2	4.66	120.88	108.64
28	c	513	CLA	O2A-C1-C2	4.66	120.88	108.64
30	b	619	BCR	C33-C5-C6	-4.66	119.30	124.53
30	b	618	BCR	C11-C10-C9	-4.65	120.67	127.31
30	c	514	BCR	C11-C10-C9	-4.65	120.67	127.31
39	G	616	LUT	C15-C14-C13	-4.65	120.67	127.31
28	s	609	CLA	O2A-C1-C2	4.65	120.85	108.64
28	b	614	CLA	O2D-CGD-CBD	4.64	119.52	111.27
30	B	618	BCR	C16-C17-C18	-4.64	120.69	127.31
30	b	619	BCR	C7-C8-C9	-4.62	119.25	126.23
28	r	602	CLA	O2A-C1-C2	4.62	120.77	108.64
28	a	406	CLA	O2A-C1-C2	4.62	120.77	108.64
37	E	101	HEM	CHD-C1D-ND	4.62	129.43	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N	614	CLA	O2D-CGD-CBD	4.61	119.47	111.27
28	b	608	CLA	O2A-C1-C2	4.61	120.75	108.64
28	S	303	CLA	O2A-C1-C2	4.61	120.74	108.64
28	Y	602	CLA	O2A-C1-C2	4.60	120.74	108.64
38	g	609	CHL	CHD-C1D-ND	-4.60	120.22	124.45
39	r	614	LUT	C31-C30-C29	-4.60	120.74	127.31
28	s	602	CLA	O2A-C1-C2	4.59	120.69	108.64
32	B	624	LMG	O7-C10-C11	4.59	121.38	111.50
28	n	613	CLA	O2A-C1-C2	4.58	120.67	108.64
39	s	615	LUT	C31-C30-C29	-4.58	120.78	127.31
39	S	316	LUT	C18-C5-C6	-4.57	119.39	124.53
28	r	613	CLA	O2A-C1-C2	4.57	120.65	108.64
28	A	406	CLA	O2A-C1-C2	4.57	120.64	108.64
28	r	613	CLA	O2D-CGD-CBD	4.56	119.37	111.27
40	Y	618	NEX	C38-C25-C24	4.56	119.41	114.28
38	S	306	CHL	CHD-C1D-ND	-4.56	120.27	124.45
28	C	504	CLA	O2A-C1-C2	4.56	120.61	108.64
28	y	303	CLA	O2A-C1-C2	4.55	120.60	108.64
28	c	506	CLA	O2D-CGD-CBD	4.55	119.35	111.27
39	s	614	LUT	C15-C14-C13	-4.54	120.82	127.31
40	N	617	NEX	C38-C25-C24	4.54	119.39	114.28
28	a	407	CLA	O2A-C1-C2	4.54	120.56	108.64
28	n	614	CLA	O2D-CGD-CBD	4.54	119.33	111.27
30	C	514	BCR	C11-C12-C13	-4.54	113.67	126.42
28	C	507	CLA	O2A-C1-C2	4.53	120.55	108.64
28	n	611	CLA	O2A-C1-C2	4.53	120.55	108.64
38	s	607	CHL	CHD-C1D-ND	-4.53	120.29	124.45
28	A	406	CLA	C1-C2-C3	-4.52	119.43	126.75
28	n	610	CLA	O2A-C1-C2	4.52	120.52	108.64
28	G	604	CLA	O2A-C1-C2	4.52	120.51	108.64
30	K	101	BCR	C38-C26-C25	-4.52	119.45	124.53
30	b	617	BCR	C38-C26-C25	-4.52	119.46	124.53
38	R	606	CHL	CHD-C1D-ND	-4.51	120.31	124.45
38	S	302	CHL	CHD-C1D-ND	-4.51	120.31	124.45
30	T	101	BCR	C20-C21-C22	-4.51	120.88	127.31
28	R	613	CLA	O2D-CGD-CBD	4.51	119.28	111.27
30	b	619	BCR	C4-C5-C6	-4.51	116.19	122.73
28	c	508	CLA	O2D-CGD-CBD	4.51	119.28	111.27
28	G	611	CLA	O2A-C1-C2	4.50	120.47	108.64
28	B	614	CLA	O2A-C1-C2	4.50	120.46	108.64
35	N	618	LHG	O7-C7-C8	4.50	121.19	111.50
28	c	503	CLA	O2A-C1-C2	4.49	120.44	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	603	CLA	O2A-C1-C2	4.49	120.44	108.64
28	g	613	CLA	C1-C2-C3	-4.49	118.27	126.04
30	d	406	BCR	C27-C26-C25	-4.49	116.21	122.73
28	n	604	CLA	O2A-C1-C2	4.49	120.43	108.64
28	C	506	CLA	O2A-C1-C2	4.49	120.43	108.64
30	b	619	BCR	C15-C14-C13	-4.49	120.91	127.31
28	N	613	CLA	O2A-C1-C2	4.48	120.42	108.64
28	b	616	CLA	O2A-C1-C2	4.48	120.42	108.64
39	s	615	LUT	C15-C14-C13	-4.48	120.91	127.31
30	t	101	BCR	C33-C5-C6	-4.48	119.50	124.53
28	C	508	CLA	O2A-C1-C2	4.48	120.41	108.64
38	g	608	CHL	CHD-C1D-ND	-4.48	120.34	124.45
28	c	502	CLA	O2A-C1-C2	4.48	120.41	108.64
28	s	604	CLA	O2A-C1-C2	4.48	120.40	108.64
39	g	615	LUT	C18-C5-C6	-4.47	119.50	124.53
28	R	609	CLA	O2A-C1-C2	4.47	120.39	108.64
30	C	515	BCR	C27-C26-C25	-4.47	116.24	122.73
28	C	505	CLA	O2A-C1-C2	4.47	120.38	108.64
30	h	101	BCR	C15-C14-C13	-4.47	120.94	127.31
30	b	618	BCR	C1-C6-C5	-4.47	116.32	122.61
28	g	611	CLA	O2A-C1-C2	4.46	120.35	108.64
30	D	405	BCR	C7-C8-C9	-4.46	119.50	126.23
28	B	607	CLA	O2A-C1-C2	4.45	120.33	108.64
30	B	617	BCR	C38-C26-C25	-4.45	119.53	124.53
38	Y	609	CHL	CHD-C1D-ND	-4.44	120.37	124.45
28	B	603	CLA	O2A-C1-C2	4.44	120.30	108.64
30	D	405	BCR	C27-C26-C25	-4.43	116.30	122.73
37	f	101	HEM	CHD-C1D-ND	4.43	129.23	124.42
38	r	605	CHL	CHD-C1D-ND	-4.43	120.39	124.45
39	y	315	LUT	C35-C34-C33	-4.42	121.01	127.31
38	R	605	CHL	CHD-C1D-ND	-4.42	120.40	124.45
28	y	305	CLA	O2A-C1-C2	4.41	120.23	108.64
40	G	617	NEX	C2-C1-C6	4.41	113.50	109.21
28	n	611	CLA	CMD-C2D-C1D	4.41	132.48	124.71
28	G	612	CLA	O2A-C1-C2	4.41	120.22	108.64
28	C	511	CLA	C1-C2-C3	-4.41	118.42	126.04
32	w	101	LMG	O7-C10-C11	4.41	121.00	111.50
32	A	411	LMG	O7-C10-C11	4.40	120.98	111.50
36	c	518	DGD	C7B-C6B-C5B	4.40	136.75	114.42
30	C	515	BCR	C30-C25-C26	-4.39	116.42	122.61
39	y	315	LUT	C18-C5-C6	-4.39	119.59	124.53
38	s	605	CHL	CHD-C1D-ND	-4.39	120.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	502	CLA	O2A-C1-C2	4.39	120.18	108.64
30	H	101	BCR	C38-C26-C25	-4.39	119.60	124.53
36	A	417	DGD	O2G-C1B-C2B	4.39	120.96	111.50
30	H	101	BCR	C7-C8-C9	-4.39	119.61	126.23
28	N	602	CLA	C1-C2-C3	-4.38	118.47	126.04
30	D	405	BCR	C30-C25-C26	-4.38	116.45	122.61
30	C	516	BCR	C33-C5-C6	-4.38	119.61	124.53
28	y	311	CLA	O2A-C1-C2	4.37	120.13	108.64
41	y	317	XAT	C18-C5-C4	4.37	119.20	114.28
30	C	514	BCR	C7-C8-C9	-4.37	119.63	126.23
30	i	101	BCR	C7-C8-C9	-4.37	119.64	126.23
28	B	608	CLA	O2A-C1-C2	4.37	120.11	108.64
36	c	518	DGD	O2G-C1B-C2B	4.36	120.91	111.50
38	y	308	CHL	CHD-C1D-ND	-4.36	120.45	124.45
30	c	515	BCR	C33-C5-C6	-4.36	119.64	124.53
28	B	601	CLA	O2A-C1-C2	4.35	120.08	108.64
28	N	611	CLA	O2A-C1-C2	4.35	120.08	108.64
30	H	101	BCR	C4-C5-C6	-4.35	116.42	122.73
30	A	409	BCR	C20-C21-C22	-4.35	121.11	127.31
30	B	618	BCR	C1-C6-C5	-4.34	116.50	122.61
30	D	405	BCR	C4-C5-C6	-4.34	116.43	122.73
39	G	615	LUT	C39-C29-C30	-4.34	116.85	122.92
38	G	609	CHL	CHD-C1D-ND	-4.33	120.47	124.45
30	T	101	BCR	C24-C23-C22	-4.33	119.69	126.23
28	A	405	CLA	O2A-C1-C2	4.33	120.01	108.64
28	Y	610	CLA	O2D-CGD-CBD	4.33	118.96	111.27
39	S	316	LUT	C31-C30-C29	-4.33	121.14	127.31
32	B	621	LMG	O7-C10-C11	4.32	120.81	111.50
30	B	619	BCR	C33-C5-C6	-4.32	119.68	124.53
30	a	410	BCR	C38-C26-C25	-4.32	119.68	124.53
30	d	406	BCR	C4-C5-C6	-4.31	116.47	122.73
28	b	614	CLA	C1-C2-C3	-4.30	118.61	126.04
30	A	409	BCR	C15-C14-C13	-4.29	121.18	127.31
38	g	605	CHL	CHD-C1D-ND	-4.29	120.51	124.45
39	G	616	LUT	C7-C8-C9	-4.29	119.75	126.23
38	n	608	CHL	CHD-C1D-ND	-4.29	120.51	124.45
35	c	520	LHG	O7-C7-C8	4.27	120.71	111.50
40	r	616	NEX	C27-C28-C29	-4.27	118.90	125.53
38	y	309	CHL	CHD-C1D-ND	-4.27	120.53	124.45
30	C	514	BCR	C4-C5-C6	-4.27	116.53	122.73
38	s	601	CHL	CHD-C1D-ND	-4.27	120.53	124.45
40	y	318	NEX	C38-C25-C24	4.27	119.08	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Y	617	XAT	C18-C5-C4	4.26	119.08	114.28
28	S	313	CLA	O2A-C1-C2	4.26	119.83	108.64
38	N	606	CHL	CHD-C1D-ND	-4.26	120.54	124.45
40	n	617	NEX	C27-C28-C29	-4.26	118.92	125.53
30	C	514	BCR	C33-C5-C6	-4.26	119.75	124.53
38	G	607	CHL	CHD-C1D-ND	-4.26	120.54	124.45
28	R	602	CLA	O2A-C1-C2	4.26	119.82	108.64
28	C	509	CLA	O2A-C1-C2	4.25	119.82	108.64
39	g	615	LUT	C11-C10-C9	-4.25	121.25	127.31
28	a	409	CLA	C1-C2-C3	-4.25	118.70	126.04
38	Y	601	CHL	C1-C2-C3	-4.24	118.70	126.04
40	n	617	NEX	C5-C6-C1	4.24	123.91	119.70
28	C	512	CLA	O2A-C1-C2	4.24	119.78	108.64
38	G	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
30	c	515	BCR	C38-C26-C25	-4.23	119.78	124.53
30	h	101	BCR	C24-C23-C22	-4.23	119.85	126.23
30	b	618	BCR	C33-C5-C6	-4.23	119.78	124.53
28	R	613	CLA	O2A-C1-C2	4.22	119.72	108.64
30	C	516	BCR	C7-C8-C9	-4.22	119.86	126.23
30	d	406	BCR	C16-C17-C18	-4.22	121.29	127.31
28	s	604	CLA	C1-C2-C3	-4.21	119.94	126.75
40	y	301	NEX	C27-C28-C29	-4.21	119.00	125.53
30	C	516	BCR	C20-C21-C22	-4.21	121.31	127.31
41	r	615	XAT	C15-C14-C13	-4.21	121.31	127.31
35	b	624	LHG	O7-C7-C8	4.20	120.55	111.50
30	H	101	BCR	C24-C23-C22	-4.20	119.89	126.23
35	G	618	LHG	O7-C7-C8	4.20	120.55	111.50
38	y	307	CHL	CHD-C1D-ND	-4.20	120.59	124.45
28	n	604	CLA	C1-C2-C3	-4.20	119.96	126.75
38	Y	606	CHL	CHD-C1D-ND	-4.20	120.60	124.45
39	n	615	LUT	C1-C6-C5	-4.19	116.71	122.61
28	C	503	CLA	C1-C2-C3	-4.19	118.79	126.04
41	R	615	XAT	C15-C14-C13	-4.19	121.33	127.31
30	B	619	BCR	C24-C23-C22	-4.18	119.91	126.23
28	y	305	CLA	C1-C2-C3	-4.18	119.98	126.75
30	D	405	BCR	C38-C26-C25	-4.18	119.83	124.53
38	g	601	CHL	CHD-C1D-ND	-4.18	120.62	124.45
38	n	609	CHL	CHD-C1D-ND	-4.18	120.62	124.45
38	S	308	CHL	CHD-C1D-ND	-4.17	120.62	124.45
30	C	516	BCR	C1-C6-C5	-4.17	116.73	122.61
38	s	606	CHL	C1-O2A-CGA	4.16	127.37	116.44
30	t	101	BCR	C30-C25-C26	-4.16	116.75	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	617	BCR	C11-C10-C9	-4.16	121.38	127.31
38	G	608	CHL	CHD-C1D-ND	-4.16	120.63	124.45
29	d	402	PHO	C4D-CHA-CBD	-4.15	106.64	108.52
38	Y	601	CHL	CHD-C1D-ND	-4.15	120.64	124.45
28	c	510	CLA	C1-C2-C3	-4.15	118.87	126.04
28	Y	613	CLA	O2A-C1-C2	4.14	119.53	108.64
38	G	605	CHL	CHD-C1D-ND	-4.14	120.65	124.45
38	r	607	CHL	CHD-C1D-ND	-4.14	120.65	124.45
38	Y	607	CHL	CHD-C1D-ND	-4.14	120.65	124.45
30	d	406	BCR	C15-C14-C13	-4.14	121.40	127.31
28	b	604	CLA	C1-C2-C3	-4.14	118.89	126.04
41	r	615	XAT	C18-C5-C4	4.14	118.93	114.28
28	c	505	CLA	O2A-C1-C2	4.13	119.50	108.64
28	D	404	CLA	C1-C2-C3	-4.13	118.90	126.04
41	R	615	XAT	C18-C5-C4	4.13	118.92	114.28
38	N	608	CHL	CHD-C1D-ND	-4.12	120.67	124.45
29	A	407	PHO	C4D-CHA-CBD	-4.12	106.65	108.52
29	D	402	PHO	C4D-CHA-CBD	-4.12	106.66	108.52
39	g	616	LUT	C15-C14-C13	-4.11	121.44	127.31
28	N	610	CLA	O2A-C1-C2	4.11	119.44	108.64
28	D	401	CLA	O2A-C1-C2	4.11	119.43	108.64
30	b	619	BCR	C38-C26-C25	-4.10	119.92	124.53
38	N	605	CHL	CHD-C1D-ND	-4.10	120.68	124.45
35	g	618	LHG	O7-C7-C8	4.10	120.34	111.50
30	A	409	BCR	C38-C26-C25	-4.10	119.92	124.53
32	C	522	LMG	O7-C10-C11	4.10	120.33	111.50
28	y	312	CLA	C1-C2-C3	-4.09	118.96	126.04
30	b	617	BCR	C33-C5-C6	-4.09	119.94	124.53
38	r	606	CHL	CHD-C1D-ND	-4.09	120.70	124.45
30	B	619	BCR	C38-C26-C25	-4.09	119.94	124.53
28	d	401	CLA	O2A-C1-C2	4.09	119.38	108.64
35	c	519	LHG	O7-C7-C8	4.09	120.31	111.50
35	A	416	LHG	O7-C7-C8	4.08	120.30	111.50
39	Y	615	LUT	C35-C34-C33	-4.08	121.49	127.31
30	B	617	BCR	C24-C23-C22	-4.08	120.07	126.23
35	d	408	LHG	O7-C7-C8	4.08	120.29	111.50
30	k	101	BCR	C4-C5-C6	-4.08	116.81	122.73
38	g	619	CHL	CHD-C1D-ND	-4.08	120.71	124.45
30	d	406	BCR	C33-C5-C6	-4.08	119.95	124.53
40	g	617	NEX	C38-C25-C24	4.07	118.86	114.28
40	y	301	NEX	C38-C25-C24	4.07	118.86	114.28
30	i	101	BCR	C24-C23-C22	-4.07	120.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	616	LUT	C35-C34-C33	-4.06	121.51	127.31
36	c	517	DGD	O2G-C1B-C2B	4.06	120.26	111.50
30	D	405	BCR	C16-C17-C18	-4.06	121.52	127.31
39	G	615	LUT	C15-C14-C13	-4.06	121.52	127.31
37	f	101	HEM	C1B-NB-C4B	4.06	109.26	105.07
30	B	619	BCR	C1-C6-C5	-4.05	116.90	122.61
38	R	607	CHL	CHD-C1D-ND	-4.05	120.73	124.45
39	s	615	LUT	C18-C5-C6	-4.05	119.98	124.53
28	s	610	CLA	O2A-C1-C2	4.05	119.28	108.64
38	S	307	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	b	617	BCR	C16-C17-C18	-4.05	121.53	127.31
30	T	101	BCR	C11-C12-C13	-4.05	115.04	126.42
30	A	409	BCR	C16-C17-C18	-4.05	121.53	127.31
38	s	606	CHL	CHD-C1D-ND	-4.05	120.74	124.45
30	C	515	BCR	C15-C14-C13	-4.05	121.54	127.31
38	Y	605	CHL	CHD-C1D-ND	-4.04	120.74	124.45
38	G	601	CHL	CHD-C1D-ND	-4.04	120.74	124.45
30	C	516	BCR	C30-C25-C26	-4.04	116.92	122.61
39	n	616	LUT	C15-C14-C13	-4.03	121.56	127.31
39	N	615	LUT	C35-C34-C33	-4.03	121.56	127.31
39	g	616	LUT	C18-C5-C6	-4.02	120.01	124.53
38	y	302	CHL	CHD-C1D-ND	-4.02	120.76	124.45
38	Y	608	CHL	CHD-C1D-ND	-4.02	120.76	124.45
38	N	601	CHL	CHD-C1D-ND	-4.02	120.76	124.45
28	b	601	CLA	C1-C2-C3	-4.01	119.11	126.04
30	b	617	BCR	C24-C23-C22	-4.01	120.18	126.23
28	G	602	CLA	C1-C2-C3	-4.00	119.12	126.04
35	a	415	LHG	O7-C7-C8	4.00	120.12	111.50
29	a	408	PHO	C4D-CHA-CBD	-4.00	106.71	108.52
38	n	601	CHL	CHD-C1D-ND	-3.99	120.79	124.45
28	B	613	CLA	C1-C2-C3	-3.99	119.14	126.04
41	r	615	XAT	C38-C25-C26	-3.99	115.58	122.26
35	S	317	LHG	O7-C7-C8	3.98	120.09	111.50
36	C	517	DGD	O2G-C1B-C2B	3.98	120.09	111.50
38	n	606	CHL	CHD-C1D-ND	-3.98	120.79	124.45
30	b	617	BCR	C11-C10-C9	-3.98	121.63	127.31
35	n	618	LHG	O7-C7-C8	3.98	120.08	111.50
30	k	101	BCR	C33-C5-C6	-3.98	120.06	124.53
39	g	615	LUT	C15-C14-C13	-3.98	121.63	127.31
39	g	616	LUT	C7-C8-C9	-3.97	120.23	126.23
35	b	622	LHG	O7-C7-C8	3.97	120.06	111.50
38	y	306	CHL	CHD-C1D-ND	-3.97	120.81	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	101	LHG	O7-C7-C8	3.97	120.05	111.50
41	R	615	XAT	C38-C25-C26	-3.96	115.62	122.26
38	R	606	CHL	C4D-CHA-C1A	3.96	126.06	121.25
38	n	605	CHL	CHD-C1D-ND	-3.95	120.82	124.45
28	y	313	CLA	C1-C2-C3	-3.95	119.20	126.04
28	r	612	CLA	C1-C2-C3	-3.95	119.21	126.04
32	a	413	LMG	O7-C10-C11	3.95	120.01	111.50
35	B	622	LHG	O7-C7-C8	3.94	119.99	111.50
30	C	515	BCR	C24-C23-C22	-3.94	120.29	126.23
35	r	617	LHG	O7-C7-C8	3.93	119.97	111.50
28	Y	611	CLA	C1-C2-C3	-3.93	119.25	126.04
30	B	618	BCR	C33-C5-C6	-3.92	120.13	124.53
32	C	520	LMG	O7-C10-C11	3.91	119.94	111.50
30	h	101	BCR	C11-C10-C9	-3.91	121.73	127.31
30	A	409	BCR	C33-C5-C6	-3.91	120.14	124.53
28	r	613	CLA	C1-C2-C3	-3.91	119.29	126.04
30	c	515	BCR	C24-C23-C22	-3.90	120.33	126.23
30	c	515	BCR	C4-C5-C6	-3.90	117.06	122.73
28	G	604	CLA	C1-C2-C3	-3.90	120.44	126.75
30	a	410	BCR	C20-C21-C22	-3.90	121.75	127.31
28	c	512	CLA	C1-C2-C3	-3.90	119.31	126.04
36	b	625	DGD	O2G-C1B-C2B	3.90	119.90	111.50
30	c	515	BCR	C20-C21-C22	-3.89	121.76	127.31
28	r	608	CLA	C1-C2-C3	-3.88	119.32	126.04
36	C	519	DGD	O2G-C1B-C2B	3.88	119.87	111.50
39	y	316	LUT	C15-C14-C13	-3.88	121.77	127.31
28	n	613	CLA	C1-C2-C3	-3.88	119.33	126.04
32	d	409	LMG	O7-C10-C11	3.88	119.86	111.50
40	G	617	NEX	C16-C1-C6	-3.87	107.00	110.47
39	s	614	LUT	C1-C6-C5	-3.87	117.16	122.61
39	G	616	LUT	C18-C5-C6	-3.87	120.18	124.53
28	a	407	CLA	C1-C2-C3	-3.87	120.49	126.75
30	C	515	BCR	C38-C26-C25	-3.86	120.19	124.53
30	h	101	BCR	C33-C5-C6	-3.86	120.20	124.53
35	C	521	LHG	O7-C7-C8	3.86	119.81	111.50
39	g	616	LUT	C31-C30-C29	-3.85	121.81	127.31
30	b	618	BCR	C38-C26-C25	-3.85	120.21	124.53
30	b	619	BCR	C20-C21-C22	-3.85	121.82	127.31
28	B	601	CLA	C1-C2-C3	-3.84	119.40	126.04
39	n	616	LUT	C7-C8-C9	-3.84	120.43	126.23
30	B	617	BCR	C33-C5-C6	-3.84	120.21	124.53
30	A	409	BCR	C1-C6-C5	-3.84	117.20	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	409	BCR	C24-C23-C22	-3.84	120.44	126.23
30	c	514	BCR	C4-C5-C6	-3.83	117.17	122.73
33	d	407	PL9	C7-C3-C4	3.83	119.99	116.88
32	A	413	LMG	O7-C10-C11	3.83	119.75	111.50
39	R	614	LUT	C35-C34-C33	-3.83	121.85	127.31
32	k	102	LMG	O7-C10-C11	3.83	119.75	111.50
28	s	612	CLA	O2A-C1-C2	3.82	118.67	108.64
38	N	607	CHL	CHD-C1D-ND	-3.82	120.95	124.45
28	c	511	CLA	C1-C2-C3	-3.82	119.44	126.04
30	b	617	BCR	C4-C5-C6	-3.82	117.19	122.73
28	c	507	CLA	C1-C2-C3	-3.82	119.44	126.04
30	C	515	BCR	C11-C10-C9	-3.82	121.86	127.31
28	B	606	CLA	C1-C2-C3	-3.81	119.44	126.04
35	l	101	LHG	O7-C7-C8	3.81	119.72	111.50
28	c	508	CLA	CHD-C1D-ND	-3.81	120.95	124.45
28	G	612	CLA	C1-C2-C3	-3.81	119.45	126.04
35	b	621	LHG	O7-C7-C8	3.81	119.71	111.50
35	s	617	LHG	O7-C7-C8	3.81	119.71	111.50
38	n	601	CHL	C1-C2-C3	-3.81	119.46	126.04
30	C	516	BCR	C4-C5-C6	-3.80	117.21	122.73
39	s	615	LUT	C1-C6-C5	-3.80	117.26	122.61
30	B	619	BCR	C27-C26-C25	-3.80	117.21	122.73
30	T	101	BCR	C33-C5-C6	-3.80	120.26	124.53
30	t	101	BCR	C15-C14-C13	-3.80	121.89	127.31
30	B	617	BCR	C16-C17-C18	-3.80	121.89	127.31
28	R	612	CLA	C1-C2-C3	-3.79	119.48	126.04
28	S	311	CLA	C1-C2-C3	-3.79	119.48	126.04
30	h	101	BCR	C7-C8-C9	-3.79	120.50	126.23
39	Y	615	LUT	C21-C26-C27	-3.79	107.91	112.70
35	B	623	LHG	O7-C7-C8	3.79	119.67	111.50
30	b	617	BCR	C27-C26-C25	-3.79	117.23	122.73
38	g	607	CHL	CHD-C1D-ND	-3.79	120.97	124.45
28	c	509	CLA	C1-C2-C3	-3.79	119.50	126.04
28	b	608	CLA	C1-C2-C3	-3.78	119.50	126.04
28	B	614	CLA	C1-C2-C3	-3.78	119.51	126.04
28	b	605	CLA	C2D-C1D-ND	3.78	112.89	110.10
28	B	615	CLA	C1-C2-C3	-3.78	119.51	126.04
28	n	612	CLA	O2A-C1-C2	3.77	118.55	108.64
30	d	406	BCR	C20-C21-C22	-3.77	121.93	127.31
28	c	504	CLA	O2A-C1-C2	3.76	118.51	108.64
28	n	603	CLA	C1-C2-C3	-3.75	119.56	126.04
30	c	514	BCR	C7-C8-C9	-3.75	120.57	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	303	CLA	C1-C2-C3	-3.75	119.56	126.04
38	S	308	CHL	C3C-C4C-NC	-3.75	106.37	110.57
35	B	625	LHG	O7-C7-C8	3.74	119.56	111.50
40	N	617	NEX	C27-C28-C29	-3.74	119.72	125.53
30	H	101	BCR	C1-C6-C5	-3.74	117.34	122.61
37	E	101	HEM	C1B-NB-C4B	3.74	108.93	105.07
32	c	521	LMG	O7-C10-C11	3.73	119.55	111.50
39	n	615	LUT	C7-C8-C9	-3.73	120.60	126.23
39	Y	615	LUT	C15-C14-C13	-3.73	121.99	127.31
28	b	605	CLA	C1D-ND-C4D	-3.73	103.69	106.33
28	N	614	CLA	O2A-C1-C2	3.72	122.07	109.49
30	C	515	BCR	C1-C6-C5	-3.72	117.38	122.61
28	s	602	CLA	C1-C2-C3	-3.71	119.62	126.04
30	c	515	BCR	C1-C6-C5	-3.71	117.39	122.61
37	E	101	HEM	CHA-C4D-ND	3.71	128.95	124.37
31	a	411	SQD	O7-S-C6	-3.71	102.53	106.94
39	R	614	LUT	C1-C6-C5	-3.71	117.39	122.61
36	B	626	DGD	O2G-C1B-C2B	3.71	119.49	111.50
33	D	406	PL9	C7-C3-C4	3.71	119.89	116.88
30	c	514	BCR	C33-C5-C6	-3.70	120.38	124.53
30	B	619	BCR	C4-C5-C6	-3.70	117.36	122.73
32	b	623	LMG	O7-C10-C11	3.69	119.46	111.50
38	n	607	CHL	CHD-C1D-ND	-3.69	121.06	124.45
35	D	407	LHG	O7-C7-C8	3.69	119.46	111.50
30	i	101	BCR	C38-C26-C25	-3.69	120.38	124.53
32	D	408	LMG	O7-C10-C11	3.69	119.45	111.50
28	N	612	CLA	C1-C2-C3	-3.68	119.67	126.04
28	n	613	CLA	C2C-C1C-NC	3.68	113.42	109.97
39	g	615	LUT	C31-C30-C29	-3.67	122.07	127.31
28	R	604	CLA	CHD-C1D-ND	-3.67	121.08	124.45
28	r	611	CLA	C2D-C1D-ND	3.66	112.80	110.10
28	n	610	CLA	C1-C2-C3	-3.66	119.71	126.04
28	c	508	CLA	C2D-C1D-ND	3.65	112.79	110.10
30	c	515	BCR	C16-C17-C18	-3.64	122.11	127.31
38	G	609	CHL	C1-O2A-CGA	3.64	125.99	116.44
35	L	102	LHG	O7-C7-C8	3.63	119.33	111.50
30	B	617	BCR	C27-C26-C25	-3.62	117.47	122.73
28	g	610	CLA	C2D-C1D-ND	3.62	112.77	110.10
35	y	319	LHG	O7-C7-C8	3.62	119.31	111.50
30	B	618	BCR	C20-C21-C22	-3.62	122.14	127.31
39	N	616	LUT	C15-C14-C13	-3.62	122.15	127.31
38	N	601	CHL	C3C-C4C-NC	-3.62	106.52	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	604	CLA	C1-C2-C3	-3.61	120.90	126.75
28	b	612	CLA	C1-C2-C3	-3.61	119.79	126.04
30	b	618	BCR	C4-C5-C6	-3.61	117.49	122.73
36	c	516	DGD	O2G-C1B-C2B	3.61	119.28	111.50
28	C	513	CLA	C1-C2-C3	-3.60	119.81	126.04
35	w	102	LHG	O7-C7-C8	3.60	119.26	111.50
39	Y	616	LUT	C11-C10-C9	-3.60	122.17	127.31
30	t	101	BCR	C7-C8-C9	-3.60	120.80	126.23
31	L	103	SQD	O7-S-C6	-3.59	102.67	106.94
30	B	617	BCR	C4-C5-C6	-3.59	117.52	122.73
30	C	514	BCR	C19-C18-C17	3.59	124.44	118.94
28	S	310	CLA	C1-C2-C3	-3.58	119.84	126.04
38	g	607	CHL	C1-C2-C3	-3.58	119.85	126.04
30	B	618	BCR	C38-C26-C25	-3.58	120.51	124.53
31	B	620	SQD	O7-S-C6	-3.58	102.68	106.94
30	C	514	BCR	C36-C18-C17	-3.58	117.91	122.92
28	R	602	CLA	C1-C2-C3	-3.57	119.86	126.04
28	Y	610	CLA	CHD-C1D-ND	-3.57	121.17	124.45
38	r	605	CHL	CMA-C3A-C4A	3.57	121.36	111.77
32	b	620	LMG	O7-C10-C11	3.57	119.19	111.50
39	n	616	LUT	C21-C26-C27	-3.56	108.20	112.70
31	A	414	SQD	O7-S-C6	-3.56	102.70	106.94
28	Y	612	CLA	C1-C2-C3	-3.56	119.88	126.04
39	S	315	LUT	C11-C10-C9	-3.56	122.23	127.31
36	a	401	DGD	O2G-C1B-C2B	3.56	119.17	111.50
39	y	316	LUT	C18-C5-C6	-3.55	120.54	124.53
36	C	518	DGD	O2G-C1B-C2B	3.55	119.15	111.50
30	b	618	BCR	C20-C21-C22	-3.55	122.25	127.31
38	y	302	CHL	C4D-CHA-C1A	3.55	125.56	121.25
28	g	604	CLA	CHD-C1D-ND	-3.55	121.19	124.45
30	i	101	BCR	C27-C26-C25	-3.55	117.58	122.73
30	B	617	BCR	C30-C25-C26	-3.54	117.63	122.61
30	C	516	BCR	C38-C26-C27	3.54	120.42	113.62
39	y	316	LUT	C21-C26-C27	-3.54	108.22	112.70
28	b	611	CLA	C1-C2-C3	-3.54	119.92	126.04
30	B	619	BCR	C30-C25-C26	-3.54	117.63	122.61
30	D	405	BCR	C38-C26-C27	3.54	120.41	113.62
39	s	614	LUT	C18-C5-C6	-3.53	120.56	124.53
30	C	516	BCR	C38-C26-C25	-3.53	120.56	124.53
38	g	609	CHL	C3C-C4C-NC	-3.53	106.61	110.57
30	b	619	BCR	C11-C10-C9	-3.53	122.28	127.31
38	g	606	CHL	C3B-C4B-NB	-3.53	107.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	301	LHG	O7-C7-C8	3.52	119.10	111.50
30	c	514	BCR	C30-C25-C26	-3.51	117.66	122.61
31	A	410	SQD	O7-S-C6	-3.51	102.76	106.94
28	g	603	CLA	C1-C2-C3	-3.51	119.97	126.04
28	g	604	CLA	C3B-C4B-NB	-3.51	107.26	110.52
38	Y	609	CHL	C1-C2-C3	-3.51	119.98	126.04
38	Y	607	CHL	C3C-C4C-NC	-3.51	106.64	110.57
38	g	601	CHL	C4D-CHA-C1A	3.50	125.51	121.25
28	B	611	CLA	C1-C2-C3	-3.50	119.98	126.04
40	G	617	NEX	C26-C27-C28	-3.50	118.58	125.99
30	B	618	BCR	C4-C5-C6	-3.50	117.65	122.73
31	a	414	SQD	O7-S-C6	-3.50	102.78	106.94
30	T	101	BCR	C4-C5-C6	-3.50	117.65	122.73
28	b	610	CLA	C1-C2-C3	-3.49	120.00	126.04
38	N	609	CHL	C3C-C4C-NC	-3.49	106.65	110.57
28	B	604	CLA	C1-C2-C3	-3.49	120.01	126.04
38	n	609	CHL	C3C-C4C-NC	-3.48	106.66	110.57
28	N	613	CLA	C1-C2-C3	-3.48	120.03	126.04
28	g	604	CLA	C1D-ND-C4D	-3.48	103.86	106.33
28	y	310	CLA	C1-C2-C3	-3.47	120.03	126.04
30	a	410	BCR	C24-C23-C22	-3.47	120.99	126.23
40	n	617	NEX	C2-C1-C6	-3.47	105.84	109.21
38	Y	609	CHL	C3C-C4C-NC	-3.47	106.68	110.57
39	g	616	LUT	C21-C26-C27	-3.47	108.32	112.70
28	B	609	CLA	C1-C2-C3	-3.47	120.05	126.04
28	C	505	CLA	C1-C2-C3	-3.46	120.05	126.04
39	g	615	LUT	C7-C8-C9	-3.46	121.00	126.23
30	B	618	BCR	C33-C5-C4	3.46	120.27	113.62
30	C	514	BCR	C35-C13-C14	-3.46	118.07	122.92
28	g	602	CLA	C1-C2-C3	-3.46	120.06	126.04
40	r	616	NEX	C38-C25-C26	-3.46	116.47	122.26
30	b	617	BCR	C30-C25-C26	-3.46	117.74	122.61
38	Y	609	CHL	CMA-C3A-C4A	3.46	121.06	111.77
28	y	310	CLA	CHD-C1D-ND	-3.46	121.28	124.45
39	g	616	LUT	C1-C6-C5	-3.46	117.75	122.61
30	H	101	BCR	C27-C26-C25	-3.45	117.72	122.73
38	y	309	CHL	C3C-C4C-NC	-3.45	106.70	110.57
37	E	101	HEM	CHB-C1B-NB	3.45	128.63	124.37
29	A	407	PHO	C2B-C1B-NB	-3.45	107.14	109.53
38	y	309	CHL	CMA-C3A-C4A	3.45	121.05	111.77
39	G	615	LUT	C11-C12-C13	-3.45	116.72	126.42
30	h	101	BCR	C1-C6-C5	-3.45	117.75	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	315	LUT	C15-C14-C13	-3.45	122.39	127.31
30	A	409	BCR	C33-C5-C4	3.45	120.24	113.62
28	R	604	CLA	O2A-C1-C2	3.45	121.14	109.49
38	r	605	CHL	C4D-CHA-C1A	3.44	125.44	121.25
39	Y	615	LUT	C8-C7-C6	-3.44	117.53	127.20
28	c	508	CLA	C3B-C4B-NB	-3.44	107.32	110.52
28	s	609	CLA	C1-C2-C3	-3.44	120.09	126.04
39	r	614	LUT	C7-C6-C5	-3.44	113.13	121.46
30	K	101	BCR	C7-C8-C9	-3.44	121.04	126.23
39	s	614	LUT	C7-C8-C9	-3.44	121.04	126.23
38	G	609	CHL	C3C-C4C-NC	-3.44	106.72	110.57
38	N	606	CHL	CMA-C3A-C4A	3.44	121.01	111.77
39	G	616	LUT	C18-C5-C4	3.44	120.72	114.36
38	n	601	CHL	C3C-C4C-NC	-3.44	106.72	110.57
38	g	606	CHL	C4D-CHA-C1A	3.44	125.43	121.25
39	n	615	LUT	C21-C26-C27	-3.43	108.36	112.70
28	b	615	CLA	C1-C2-C3	-3.43	120.11	126.04
28	G	610	CLA	CHD-C1D-ND	-3.43	121.30	124.45
28	Y	602	CLA	C3B-C4B-NB	-3.43	107.33	110.52
38	n	608	CHL	C3C-C4C-NC	-3.43	106.72	110.57
28	n	611	CLA	C2D-C1D-ND	3.43	112.63	110.10
28	y	311	CLA	C1-C2-C3	-3.43	120.12	126.04
30	K	101	BCR	C4-C5-C6	-3.42	117.77	122.73
28	B	612	CLA	C2D-C1D-ND	3.42	112.62	110.10
39	n	615	LUT	C18-C5-C6	-3.42	120.69	124.53
37	f	101	HEM	CHA-C4D-ND	3.41	128.58	124.37
28	g	604	CLA	O2A-CGA-CBA	3.41	122.62	111.91
28	b	603	CLA	C1-C2-C3	-3.41	120.14	126.04
28	r	609	CLA	C1-C2-C3	-3.41	120.14	126.04
39	N	615	LUT	C35-C15-C14	-3.41	116.49	123.47
39	y	316	LUT	C22-C23-C24	3.41	115.62	111.74
28	g	611	CLA	CHD-C1D-ND	-3.41	121.32	124.45
28	d	405	CLA	C1-C2-C3	-3.41	120.15	126.04
38	s	605	CHL	C4D-CHA-C1A	3.40	125.39	121.25
38	g	609	CHL	CMA-C3A-C4A	3.40	120.91	111.77
38	N	608	CHL	C1-O2A-CGA	3.40	125.36	116.44
28	g	604	CLA	C2D-C1D-ND	3.40	112.61	110.10
38	N	608	CHL	C3C-C4C-NC	-3.40	106.76	110.57
39	Y	616	LUT	C31-C30-C29	-3.39	122.47	127.31
38	S	308	CHL	C2C-C3C-C4C	3.39	108.91	106.49
38	n	606	CHL	CMA-C3A-C4A	3.39	120.89	111.77
28	d	404	CLA	C1-C2-C3	-3.39	120.18	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	s	607	CHL	C3C-C4C-NC	-3.39	106.77	110.57
30	C	514	BCR	C12-C13-C14	3.38	124.13	118.94
38	G	609	CHL	CMA-C3A-C4A	3.38	120.86	111.77
28	S	303	CLA	CHD-C1D-ND	-3.38	121.35	124.45
38	G	605	CHL	C4D-CHA-C1A	3.38	125.36	121.25
32	B	621	LMG	C8-O7-C10	-3.38	109.48	117.79
28	S	309	CLA	CHD-C1D-ND	-3.38	121.35	124.45
28	r	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45
39	Y	615	LUT	C2-C3-C4	3.37	114.92	110.30
28	b	607	CLA	C1-C2-C3	-3.37	120.21	126.04
38	G	606	CHL	CMA-C3A-C4A	3.37	120.84	111.77
38	g	608	CHL	C3C-C4C-NC	-3.37	106.79	110.57
30	k	101	BCR	C15-C14-C13	-3.37	122.50	127.31
28	b	612	CLA	C2D-C1D-ND	3.37	112.59	110.10
28	C	502	CLA	C1-C2-C3	-3.37	120.22	126.04
30	d	406	BCR	C33-C5-C4	3.36	120.08	113.62
35	Y	619	LHG	O7-C7-C8	3.36	118.75	111.50
30	d	406	BCR	C20-C19-C18	-3.36	116.97	126.42
30	T	101	BCR	C1-C6-C5	-3.36	117.88	122.61
38	n	609	CHL	C2C-C3C-C4C	3.36	108.89	106.49
38	r	606	CHL	CMA-C3A-C4A	3.36	120.81	111.77
39	N	616	LUT	C18-C5-C6	-3.36	120.75	124.53
29	a	408	PHO	C2B-C1B-NB	-3.36	107.20	109.53
28	g	610	CLA	CHD-C1D-ND	-3.36	121.37	124.45
38	Y	601	CHL	C3C-C4C-NC	-3.36	106.80	110.57
38	y	308	CHL	C3C-C4C-NC	-3.36	106.81	110.57
28	n	602	CLA	CHD-C1D-ND	-3.36	121.37	124.45
38	y	307	CHL	C4D-CHA-C1A	3.35	125.33	121.25
29	D	402	PHO	C2B-C1B-NB	-3.35	107.21	109.53
28	S	309	CLA	C2C-C1C-NC	3.35	113.11	109.97
28	g	602	CLA	CHD-C1D-ND	-3.35	121.37	124.45
39	y	315	LUT	C7-C8-C9	-3.35	121.17	126.23
28	y	303	CLA	CHD-C1D-ND	-3.35	121.38	124.45
39	N	615	LUT	C8-C7-C6	-3.35	117.80	127.20
28	r	604	CLA	O2A-C1-C2	3.34	120.79	109.49
38	N	601	CHL	C1-C2-C3	-3.34	120.27	126.04
30	a	410	BCR	C7-C8-C9	-3.34	121.19	126.23
38	G	608	CHL	C3C-C4C-NC	-3.34	106.83	110.57
38	y	309	CHL	C1-O2A-CGA	3.33	125.19	116.44
28	R	603	CLA	CHD-C1D-ND	-3.33	121.40	124.45
39	S	315	LUT	C7-C8-C9	-3.32	121.21	126.23
28	R	613	CLA	C2D-C1D-ND	3.32	112.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	602	CLA	C1-C2-C3	-3.32	120.30	126.04
39	g	616	LUT	C11-C10-C9	-3.32	122.57	127.31
30	a	410	BCR	C4-C5-C6	-3.32	117.92	122.73
40	g	617	NEX	C39-C29-C30	-3.32	118.28	122.92
28	R	609	CLA	CHD-C1D-ND	-3.31	121.41	124.45
30	i	101	BCR	C4-C5-C6	-3.31	117.92	122.73
38	s	607	CHL	C2C-C3C-C4C	3.31	108.85	106.49
28	b	613	CLA	C1-C2-C3	-3.31	120.31	126.04
28	G	612	CLA	C2D-C1D-ND	3.31	112.54	110.10
41	y	317	XAT	C7-C8-C9	-3.31	120.39	125.53
28	c	508	CLA	C1-C2-C3	-3.31	120.32	126.04
38	Y	608	CHL	C3C-C4C-NC	-3.31	106.86	110.57
28	c	507	CLA	C2C-C1C-NC	3.30	113.07	109.97
38	g	619	CHL	C3C-C4C-NC	-3.30	106.86	110.57
28	C	502	CLA	C2D-C1D-ND	3.30	112.54	110.10
28	Y	603	CLA	C1-C2-C3	-3.30	120.33	126.04
28	b	605	CLA	O2A-C1-C2	3.30	117.31	108.64
28	C	507	CLA	C2C-C1C-NC	3.30	113.06	109.97
38	y	306	CHL	C4D-CHA-C1A	3.30	125.27	121.25
41	y	317	XAT	C6-C7-C8	-3.30	119.01	125.99
28	g	611	CLA	C2C-C1C-NC	3.30	113.06	109.97
28	b	609	CLA	C1-C2-C3	-3.30	120.34	126.04
28	R	608	CLA	C1-C2-C3	-3.30	120.34	126.04
28	Y	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
30	D	405	BCR	C16-C15-C14	-3.29	116.73	123.47
31	M	101	SQD	O7-S-C6	-3.29	103.03	106.94
39	s	615	LUT	C21-C26-C27	-3.29	108.55	112.70
39	r	614	LUT	C11-C10-C9	3.29	132.00	127.31
28	G	612	CLA	C2C-C1C-NC	3.29	113.05	109.97
28	n	612	CLA	C2C-C1C-NC	3.29	113.05	109.97
28	B	607	CLA	C1-C2-C3	-3.29	120.36	126.04
39	S	315	LUT	C21-C26-C27	-3.29	108.55	112.70
38	S	306	CHL	C4D-CHA-C1A	3.29	125.25	121.25
28	g	610	CLA	O1D-CGD-CBD	-3.28	117.76	124.48
39	G	615	LUT	C1-C6-C5	-3.28	117.99	122.61
31	L	101	SQD	O7-S-C6	-3.28	103.04	106.94
38	n	609	CHL	CMA-C3A-C4A	3.28	120.59	111.77
40	N	617	NEX	C26-C27-C28	-3.28	119.06	125.99
28	c	502	CLA	C1-C2-C3	-3.28	120.37	126.04
38	s	606	CHL	C3C-C4C-NC	-3.28	106.89	110.57
28	c	510	CLA	CHD-C1D-ND	-3.28	121.44	124.45
28	R	613	CLA	CHD-C1D-ND	-3.28	121.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	514	BCR	C24-C23-C22	-3.28	121.28	126.23
29	d	402	PHO	C2B-C1B-NB	-3.27	107.27	109.53
28	n	610	CLA	CHD-C1D-ND	-3.27	121.44	124.45
30	b	617	BCR	C20-C21-C22	-3.27	122.64	127.31
38	g	606	CHL	C4B-CHC-C1C	3.27	134.10	126.34
38	R	607	CHL	C3C-C4C-NC	-3.27	106.90	110.57
28	b	605	CLA	CHD-C1D-ND	-3.27	121.45	124.45
30	C	516	BCR	C24-C23-C22	-3.27	121.30	126.23
28	G	614	CLA	C2D-C1D-ND	3.27	112.51	110.10
30	B	619	BCR	C38-C26-C27	3.27	119.89	113.62
30	C	515	BCR	C4-C5-C6	-3.27	117.99	122.73
28	s	602	CLA	CHD-C1D-ND	-3.27	121.45	124.45
28	Y	614	CLA	O2A-C1-C2	3.27	120.53	109.49
28	C	508	CLA	C1-C2-C3	-3.26	120.40	126.04
28	g	610	CLA	C1D-ND-C4D	-3.26	104.02	106.33
35	R	616	LHG	O7-C7-C8	3.26	119.90	110.80
28	C	510	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	G	603	CLA	C1-C2-C3	-3.26	120.40	126.04
39	R	614	LUT	C39-C29-C28	3.26	123.22	118.08
38	G	606	CHL	C4D-CHA-C1A	3.26	125.22	121.25
40	y	318	NEX	C31-C30-C29	3.26	131.96	127.31
39	G	615	LUT	C40-C33-C34	-3.26	118.36	122.92
30	a	410	BCR	C38-C26-C27	3.25	119.87	113.62
38	r	605	CHL	C3B-C4B-NB	-3.25	107.50	110.52
28	N	610	CLA	C1-C2-C3	-3.25	120.42	126.04
28	s	604	CLA	CHD-C1D-ND	-3.25	121.46	124.45
39	y	315	LUT	C15-C14-C13	-3.25	122.67	127.31
28	b	604	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	c	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
28	R	601	CLA	C2D-C1D-ND	3.25	112.50	110.10
28	N	613	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	S	304	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	c	513	CLA	C1-C2-C3	-3.25	120.43	126.04
28	B	612	CLA	C1-C2-C3	-3.25	120.43	126.04
30	d	406	BCR	C38-C26-C27	3.25	119.85	113.62
37	f	101	HEM	CHB-C1B-NB	3.25	128.38	124.37
30	A	409	BCR	C38-C26-C27	3.24	119.85	113.62
30	a	410	BCR	C30-C25-C26	-3.24	118.05	122.61
28	c	506	CLA	CHD-C1D-ND	-3.24	121.47	124.45
28	B	602	CLA	CHD-C1D-ND	-3.24	121.48	124.45
28	Y	611	CLA	C2C-C1C-NC	3.23	113.00	109.97
28	b	602	CLA	CHD-C1D-ND	-3.23	121.48	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	602	CLA	C2C-C1C-NC	3.23	113.00	109.97
38	n	605	CHL	C2C-C3C-C4C	3.23	108.79	106.49
28	y	314	CLA	O2A-C1-C2	3.23	120.42	109.49
28	n	602	CLA	C1-C2-C3	-3.23	120.45	126.04
30	B	619	BCR	C20-C21-C22	-3.23	122.70	127.31
28	C	512	CLA	C2D-C1D-ND	3.23	112.48	110.10
40	y	318	NEX	C39-C29-C30	-3.23	118.40	122.92
28	B	604	CLA	C2C-C1C-NC	3.23	113.00	109.97
28	d	404	CLA	C2D-C1D-ND	3.23	112.48	110.10
38	N	606	CHL	C4D-CHA-C1A	3.23	125.17	121.25
40	N	617	NEX	C38-C25-C26	-3.22	116.86	122.26
28	c	506	CLA	C2D-C1D-ND	3.22	112.48	110.10
28	R	610	CLA	C2D-C1D-ND	3.22	112.48	110.10
28	G	604	CLA	CHD-C1D-ND	-3.22	121.50	124.45
30	c	514	BCR	C33-C5-C4	3.22	119.80	113.62
28	S	311	CLA	C2D-C1D-ND	3.22	112.47	110.10
28	R	612	CLA	CHD-C1D-ND	-3.22	121.50	124.45
28	B	610	CLA	C2D-C1D-ND	3.21	112.47	110.10
38	s	605	CHL	CMA-C3A-C4A	3.21	120.41	111.77
30	c	514	BCR	C1-C6-C5	-3.21	118.09	122.61
38	g	609	CHL	C2C-C3C-C4C	3.21	108.78	106.49
30	b	619	BCR	C38-C26-C27	3.21	119.78	113.62
30	c	515	BCR	C33-C5-C4	3.21	119.78	113.62
28	G	610	CLA	C2D-C1D-ND	3.21	112.47	110.10
28	R	601	CLA	C2C-C1C-NC	3.20	112.97	109.97
39	N	615	LUT	C30-C31-C32	-3.20	113.22	123.22
28	y	304	CLA	C1-C2-C3	-3.20	120.50	126.04
28	b	609	CLA	C2D-C1D-ND	3.20	112.46	110.10
28	g	603	CLA	C2C-C1C-NC	3.20	112.97	109.97
41	Y	617	XAT	C7-C8-C9	-3.20	120.56	125.53
28	Y	602	CLA	CMA-C3A-C4A	3.20	120.37	111.77
28	y	303	CLA	C2D-C1D-ND	3.20	112.46	110.10
28	C	509	CLA	C1-C2-C3	-3.20	120.51	126.04
38	n	606	CHL	C4D-CHA-C1A	3.20	125.14	121.25
28	Y	602	CLA	C1-C2-C3	-3.19	120.52	126.04
28	S	312	CLA	C2C-C1C-NC	3.19	112.96	109.97
28	n	604	CLA	CHD-C1D-ND	-3.19	121.52	124.45
28	b	601	CLA	C2D-C1D-ND	3.19	112.46	110.10
28	s	608	CLA	CHD-C1D-ND	-3.19	121.52	124.45
38	Y	609	CHL	C2C-C3C-C4C	3.19	108.76	106.49
28	G	614	CLA	O2A-C1-C2	3.19	120.28	109.49
28	d	404	CLA	CHD-C1D-ND	-3.19	121.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	y	307	CHL	CMA-C3A-C4A	3.19	120.35	111.77
28	N	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45
39	n	616	LUT	C35-C15-C14	-3.19	116.94	123.47
28	c	502	CLA	C2D-C1D-ND	3.19	112.45	110.10
38	G	601	CHL	C4D-CHA-C1A	3.19	125.13	121.25
28	R	611	CLA	C2D-C1D-ND	3.18	112.45	110.10
28	b	613	CLA	C2C-C1C-NC	3.18	112.95	109.97
28	c	509	CLA	CHD-C1D-ND	-3.18	121.53	124.45
38	R	606	CHL	C4B-CHC-C1C	3.18	133.89	126.34
38	r	605	CHL	C4B-CHC-C1C	3.18	133.89	126.34
30	b	618	BCR	C38-C26-C27	3.18	119.73	113.62
30	C	514	BCR	C37-C22-C21	-3.18	118.47	122.92
38	n	605	CHL	C3C-C4C-NC	-3.18	107.00	110.57
38	g	608	CHL	C1-O2A-CGA	3.18	124.79	116.44
28	B	611	CLA	C2D-C1D-ND	3.18	112.45	110.10
38	N	609	CHL	C2C-C3C-C4C	3.18	108.76	106.49
38	G	601	CHL	C3C-C4C-NC	-3.18	107.00	110.57
41	Y	617	XAT	C6-C7-C8	-3.18	119.27	125.99
28	n	612	CLA	CHD-C1D-ND	-3.18	121.53	124.45
30	B	618	BCR	C38-C26-C27	3.18	119.72	113.62
28	Y	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
28	G	602	CLA	CHD-C1D-ND	-3.18	121.53	124.45
38	g	601	CHL	C3C-C4C-NC	-3.18	107.01	110.57
28	G	603	CLA	C2C-C1C-NC	3.17	112.95	109.97
28	n	611	CLA	C3B-C4B-NB	-3.17	107.57	110.52
38	g	607	CHL	C3C-C4C-NC	-3.17	107.01	110.57
28	B	615	CLA	C2C-C1C-NC	3.17	112.94	109.97
30	k	101	BCR	C29-C30-C25	3.17	115.36	110.48
28	Y	613	CLA	C2C-C1C-NC	3.17	112.94	109.97
28	r	612	CLA	CHD-C1D-ND	-3.17	121.54	124.45
28	g	613	CLA	C2C-C1C-NC	3.17	112.94	109.97
28	C	502	CLA	C2C-C1C-NC	3.17	112.94	109.97
28	r	611	CLA	C2C-C1C-NC	3.17	112.94	109.97
40	G	617	NEX	C19-C9-C10	-3.17	118.49	122.92
38	n	607	CHL	C3C-C4C-NC	-3.17	107.02	110.57
28	d	405	CLA	CHD-C1D-ND	-3.17	121.55	124.45
28	r	602	CLA	CHD-C1D-ND	-3.17	121.55	124.45
38	S	306	CHL	CMA-C3A-C4A	3.16	120.27	111.77
38	N	607	CHL	C3C-C4C-NC	-3.16	107.03	110.57
30	b	618	BCR	C33-C5-C4	3.16	119.69	113.62
28	B	616	CLA	C1-C2-C3	-3.16	120.58	126.04
28	c	512	CLA	C2D-C1D-ND	3.16	112.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Y	606	CHL	CMA-C3A-C4A	3.16	120.27	111.77
39	y	316	LUT	C11-C10-C9	-3.16	122.80	127.31
28	R	602	CLA	CHD-C1D-ND	-3.16	121.55	124.45
28	S	310	CLA	CHD-C1D-ND	-3.16	121.55	124.45
28	N	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	b	619	BCR	C23-C24-C25	-3.16	118.33	127.20
28	y	305	CLA	C2C-C1C-NC	3.16	112.93	109.97
30	b	617	BCR	C7-C8-C9	-3.16	121.46	126.23
38	S	307	CHL	C3C-C4C-NC	-3.16	107.03	110.57
38	s	601	CHL	C3C-C4C-NC	-3.16	107.03	110.57
38	y	302	CHL	C3C-C4C-NC	-3.16	107.03	110.57
28	r	603	CLA	C2C-C1C-NC	3.16	112.93	109.97
28	N	604	CLA	C2C-C1C-NC	3.16	112.93	109.97
30	a	410	BCR	C27-C26-C25	-3.16	118.15	122.73
38	N	606	CHL	C3B-C4B-NB	-3.16	107.59	110.52
28	b	611	CLA	C2D-C1D-ND	3.15	112.43	110.10
30	B	617	BCR	C33-C5-C4	3.15	119.67	113.62
28	A	408	CLA	CHD-C1D-ND	-3.15	121.56	124.45
30	C	516	BCR	C27-C26-C25	-3.15	118.16	122.73
28	D	403	CLA	C2D-C1D-ND	3.15	112.42	110.10
28	b	615	CLA	C2C-C1C-NC	3.15	112.92	109.97
30	b	617	BCR	C38-C26-C27	3.15	119.67	113.62
28	r	604	CLA	C2C-C1C-NC	3.15	112.92	109.97
30	B	617	BCR	C38-C26-C27	3.15	119.66	113.62
39	R	614	LUT	C21-C26-C27	-3.15	108.72	112.70
28	y	311	CLA	C2C-C1C-NC	3.15	112.92	109.97
38	N	601	CHL	C2C-C3C-C4C	3.15	108.73	106.49
28	g	612	CLA	C2C-C1C-NC	3.14	112.92	109.97
39	N	616	LUT	C20-C13-C12	3.14	123.03	118.08
30	B	617	BCR	C20-C21-C22	-3.14	122.82	127.31
39	Y	615	LUT	C11-C10-C9	-3.14	122.82	127.31
39	Y	615	LUT	C7-C8-C9	-3.14	121.49	126.23
28	C	513	CLA	C2C-C1C-NC	3.14	112.92	109.97
30	b	619	BCR	C1-C6-C5	-3.14	118.19	122.61
28	r	613	CLA	C2D-C1D-ND	3.14	112.42	110.10
38	G	609	CHL	C2C-C3C-C4C	3.14	108.73	106.49
30	h	101	BCR	C27-C26-C25	-3.14	118.17	122.73
28	r	604	CLA	C2D-C1D-ND	3.14	112.42	110.10
28	D	403	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	c	502	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	r	608	CLA	CHD-C1D-ND	-3.14	121.57	124.45
38	Y	601	CHL	C2C-C3C-C4C	3.14	108.72	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	G	606	CHL	C3B-C4B-NB	-3.14	107.61	110.52
28	G	614	CLA	CMA-C3A-C4A	3.14	120.20	111.77
28	y	303	CLA	C1-C2-C3	-3.13	120.62	126.04
38	N	609	CHL	CMA-C3A-C4A	3.13	120.20	111.77
28	B	612	CLA	C1D-ND-C4D	-3.13	104.11	106.33
28	C	506	CLA	C2C-C1C-NC	3.13	112.91	109.97
28	a	407	CLA	CHD-C1D-ND	-3.13	121.58	124.45
28	b	611	CLA	CHD-C1D-ND	-3.13	121.58	124.45
28	y	304	CLA	CHD-C1D-ND	-3.13	121.58	124.45
28	B	603	CLA	C2D-C1D-ND	3.13	112.41	110.10
28	N	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
38	g	609	CHL	C4D-CHA-C1A	3.13	125.06	121.25
28	B	610	CLA	C1-C2-C3	-3.13	120.63	126.04
39	N	615	LUT	C15-C14-C13	-3.13	122.85	127.31
28	B	609	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	C	514	BCR	C34-C9-C10	-3.13	118.54	122.92
28	Y	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
28	S	310	CLA	C2C-C1C-NC	3.13	112.90	109.97
30	K	101	BCR	C11-C10-C9	-3.13	122.85	127.31
38	r	606	CHL	C3C-C4C-NC	-3.12	107.07	110.57
28	r	612	CLA	C2C-C1C-NC	3.12	112.90	109.97
30	b	617	BCR	C1-C6-C5	-3.12	118.21	122.61
28	C	512	CLA	CHD-C1D-ND	-3.12	121.58	124.45
28	g	603	CLA	CHD-C1D-ND	-3.12	121.58	124.45
28	N	603	CLA	C1-C2-C3	-3.12	120.64	126.04
28	n	604	CLA	C2C-C1C-NC	3.12	112.90	109.97
28	C	503	CLA	CHD-C1D-ND	-3.12	121.58	124.45
28	B	606	CLA	C2D-C1D-ND	3.12	112.41	110.10
28	n	603	CLA	C2D-C1D-ND	3.12	112.40	110.10
28	c	504	CLA	CHD-C1D-ND	-3.12	121.59	124.45
38	r	607	CHL	C3C-C4C-NC	-3.12	107.07	110.57
28	s	612	CLA	C2C-C1C-NC	3.12	112.89	109.97
28	c	501	CLA	CHD-C1D-ND	-3.12	121.59	124.45
28	n	602	CLA	C2D-C1D-ND	3.12	112.40	110.10
28	D	404	CLA	C2C-C1C-NC	3.12	112.89	109.97
28	Y	614	CLA	C2C-C1C-NC	3.12	112.89	109.97
28	b	613	CLA	CHD-C1D-ND	-3.12	121.59	124.45
28	y	310	CLA	C2D-C1D-ND	3.12	112.40	110.10
30	A	409	BCR	C30-C25-C26	-3.11	118.23	122.61
28	a	409	CLA	C2C-C1C-NC	3.11	112.89	109.97
30	K	101	BCR	C1-C6-C5	-3.11	118.23	122.61
39	n	615	LUT	C35-C34-C33	-3.11	122.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	613	CLA	C2C-C1C-NC	3.11	112.89	109.97
38	S	302	CHL	C3C-C4C-NC	-3.11	107.08	110.57
38	N	607	CHL	C4D-CHA-C1A	3.11	125.03	121.25
39	S	315	LUT	C1-C6-C5	-3.11	118.23	122.61
28	s	610	CLA	C2C-C1C-NC	3.11	112.89	109.97
28	S	313	CLA	C1-C2-C3	-3.11	120.66	126.04
30	A	409	BCR	C8-C7-C6	-3.11	118.47	127.20
28	B	607	CLA	C2D-C1D-ND	3.11	112.39	110.10
28	B	601	CLA	C2C-C1C-NC	3.11	112.88	109.97
30	A	409	BCR	C27-C26-C25	-3.11	118.22	122.73
28	r	609	CLA	C2D-C1D-ND	3.11	112.39	110.10
28	S	314	CLA	CHD-C1D-ND	-3.11	121.60	124.45
28	R	608	CLA	C2C-C1C-NC	3.11	112.88	109.97
28	S	313	CLA	C2C-C1C-NC	3.11	112.88	109.97
28	B	605	CLA	C2D-C1D-ND	3.11	112.39	110.10
28	r	611	CLA	C1D-ND-C4D	-3.11	104.13	106.33
28	b	607	CLA	C2C-C1C-NC	3.11	112.88	109.97
38	y	309	CHL	C2C-C3C-C4C	3.10	108.70	106.49
28	N	611	CLA	C2C-C1C-NC	3.10	112.88	109.97
28	a	409	CLA	CHD-C1D-ND	-3.10	121.60	124.45
28	r	610	CLA	C2D-C1D-ND	3.10	112.39	110.10
28	C	508	CLA	CHD-C1D-ND	-3.10	121.60	124.45
28	g	613	CLA	CHD-C1D-ND	-3.10	121.60	124.45
28	d	401	CLA	C2C-C1C-NC	3.10	112.88	109.97
40	N	617	NEX	C17-C1-C6	-3.10	107.70	110.47
28	D	401	CLA	CHD-C1D-ND	-3.10	121.61	124.45
28	N	602	CLA	C2D-C1D-ND	3.10	112.39	110.10
28	C	510	CLA	C1-C2-C3	-3.10	120.68	126.04
30	b	617	BCR	C33-C5-C4	3.10	119.57	113.62
30	b	618	BCR	C23-C24-C25	-3.10	118.50	127.20
28	n	603	CLA	CHD-C1D-ND	-3.10	121.61	124.45
38	Y	606	CHL	C3B-C4B-NB	-3.10	107.64	110.52
40	n	617	NEX	O24-C25-C38	-3.10	111.34	115.06
38	G	608	CHL	C4D-CHA-C1A	3.10	125.02	121.25
28	G	604	CLA	C2C-C1C-NC	3.10	112.87	109.97
28	b	601	CLA	C2C-C1C-NC	3.10	112.87	109.97
28	c	513	CLA	C2D-C1D-ND	3.10	112.39	110.10
28	C	504	CLA	C1-C2-C3	-3.10	120.69	126.04
30	h	101	BCR	C4-C5-C6	-3.10	118.24	122.73
38	n	601	CHL	C4D-CHA-C1A	3.10	125.02	121.25
30	D	405	BCR	C33-C5-C4	3.10	119.56	113.62
30	a	410	BCR	C1-C6-C5	-3.10	118.25	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Y	616	LUT	C35-C15-C14	-3.09	117.14	123.47
28	s	613	CLA	C2D-C1D-ND	3.09	112.38	110.10
35	d	408	LHG	C5-O7-C7	-3.09	110.18	117.79
28	B	601	CLA	CHD-C1D-ND	-3.09	121.61	124.45
28	D	403	CLA	CHD-C1D-ND	-3.09	121.61	124.45
28	C	509	CLA	C2D-C1D-ND	3.09	112.38	110.10
38	n	601	CHL	C2C-C3C-C4C	3.09	108.69	106.49
28	C	509	CLA	C2C-C1C-NC	3.09	112.87	109.97
28	r	610	CLA	C2C-C1C-NC	3.09	112.87	109.97
38	g	608	CHL	CMA-C3A-C4A	3.09	120.08	111.77
28	g	602	CLA	C2D-C1D-ND	3.09	112.38	110.10
38	N	608	CHL	CMA-C3A-C4A	3.09	120.07	111.77
28	C	501	CLA	C2D-C1D-ND	3.09	112.38	110.10
28	b	604	CLA	CMA-C3A-C4A	3.09	120.07	111.77
28	d	405	CLA	C2D-C1D-ND	3.09	112.38	110.10
40	r	616	NEX	C17-C1-C6	-3.09	107.71	110.47
38	g	608	CHL	C2C-C3C-C4C	3.08	108.69	106.49
28	C	504	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	s	608	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	C	509	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	b	610	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	B	613	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	C	512	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	b	609	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	C	503	CLA	C2D-C1D-ND	3.08	112.38	110.10
28	C	511	CLA	C2D-C1D-ND	3.08	112.38	110.10
28	Y	612	CLA	C2D-C1D-ND	3.08	112.38	110.10
38	R	606	CHL	C3C-C4C-NC	-3.08	107.11	110.57
28	A	408	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	B	611	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	C	506	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	c	511	CLA	C2D-C1D-ND	3.08	112.37	110.10
28	B	610	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	B	613	CLA	CHD-C1D-ND	-3.08	121.62	124.45
38	y	308	CHL	C2C-C3C-C4C	3.08	108.68	106.49
28	y	304	CLA	C2D-C1D-ND	3.08	112.37	110.10
28	C	504	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	y	312	CLA	C2D-C1D-ND	3.08	112.37	110.10
39	n	616	LUT	C35-C34-C33	-3.08	122.92	127.31
28	C	513	CLA	C2D-C1D-ND	3.08	112.37	110.10
38	y	307	CHL	C4B-CHC-C1C	3.08	133.63	126.34
30	b	619	BCR	C27-C26-C25	-3.08	118.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	407	CLA	C2D-C1D-ND	3.07	112.37	110.10
38	G	607	CHL	C3C-C4C-NC	-3.07	107.12	110.57
28	b	605	CLA	C3B-C4B-NB	-3.07	107.66	110.52
28	D	404	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	G	614	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	G	610	CLA	CMA-C3A-C4A	3.07	120.03	111.77
28	G	611	CLA	C1-C2-C3	-3.07	120.73	126.04
28	C	502	CLA	CHD-C1D-ND	-3.07	121.63	124.45
37	f	101	HEM	C4C-NC-C1C	3.07	108.36	105.35
38	Y	607	CHL	C3B-C4B-NB	-3.07	107.67	110.52
28	r	609	CLA	C1D-ND-C4D	-3.07	104.16	106.33
28	S	304	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	N	610	CLA	CHD-C1D-ND	-3.07	121.64	124.45
28	s	612	CLA	C2D-C1D-ND	3.07	112.36	110.10
28	b	615	CLA	CHD-C1D-ND	-3.07	121.64	124.45
28	r	613	CLA	C2C-C1C-NC	3.07	112.84	109.97
28	C	511	CLA	CMA-C3A-C4A	3.07	120.01	111.77
28	Y	604	CLA	C2C-C1C-NC	3.06	112.84	109.97
32	A	411	LMG	C8-O7-C10	-3.06	110.25	117.79
28	c	511	CLA	CMA-C3A-C4A	3.06	120.01	111.77
28	C	508	CLA	C2D-C1D-ND	3.06	112.36	110.10
28	n	612	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
28	D	403	CLA	C1-C2-C3	-3.06	120.75	126.04
28	N	614	CLA	C2D-C1D-ND	3.06	112.36	110.10
28	r	613	CLA	CHD-C1D-ND	-3.06	121.64	124.45
28	a	407	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	A	405	CLA	CHD-C1D-ND	-3.06	121.64	124.45
41	Y	617	XAT	C38-C25-C26	-3.06	117.13	122.26
28	R	612	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	s	609	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	b	603	CLA	CHD-C1D-ND	-3.06	121.64	124.45
38	G	606	CHL	C4B-CHC-C1C	3.06	133.59	126.34
28	b	610	CLA	C2D-C1D-ND	3.06	112.36	110.10
28	c	509	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	b	606	CLA	CHD-C1D-ND	-3.06	121.64	124.45
38	r	606	CHL	C1-C2-C3	-3.06	120.76	126.04
28	B	615	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	y	314	CLA	CHD-C1D-ND	-3.06	121.65	124.45
39	n	616	LUT	C8-C7-C6	-3.05	118.62	127.20
28	s	608	CLA	CMA-C3A-C4A	3.05	119.98	111.77
28	y	303	CLA	C2C-C1C-NC	3.05	112.83	109.97
36	c	518	DGD	C6B-C5B-C4B	3.05	129.92	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	s	606	CHL	C2C-C3C-C4C	3.05	108.67	106.49
28	d	405	CLA	C2C-C1C-NC	3.05	112.83	109.97
28	C	511	CLA	CHD-C1D-ND	-3.05	121.65	124.45
28	r	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
28	N	612	CLA	C2D-C1D-ND	3.05	112.35	110.10
40	n	617	NEX	C40-C33-C34	-3.05	118.65	122.92
41	r	615	XAT	C7-C8-C9	-3.05	120.80	125.53
38	S	308	CHL	CHD-C4C-C3C	3.05	129.32	124.84
30	K	101	BCR	C16-C15-C14	-3.05	117.23	123.47
28	c	504	CLA	C2D-C1D-ND	3.05	112.35	110.10
28	Y	602	CLA	C11-C10-C8	-3.05	106.07	115.92
28	G	614	CLA	C3B-C4B-NB	-3.05	107.69	110.52
38	s	605	CHL	C4B-CHC-C1C	3.05	133.56	126.34
38	Y	605	CHL	C4D-CHA-C1A	3.05	124.96	121.25
28	A	405	CLA	C2D-C1D-ND	3.05	112.35	110.10
28	B	602	CLA	C2D-C1D-ND	3.05	112.35	110.10
28	B	616	CLA	CHD-C1D-ND	-3.05	121.66	124.45
35	b	624	LHG	C5-O7-C7	-3.05	110.29	117.79
28	G	611	CLA	C2C-C1C-NC	3.05	112.83	109.97
38	G	608	CHL	CMA-C3A-C4A	3.04	119.95	111.77
28	c	503	CLA	C2D-C1D-ND	3.04	112.35	110.10
28	c	502	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	b	616	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	g	614	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	s	613	CLA	CHD-C1D-ND	-3.04	121.66	124.45
39	Y	616	LUT	C35-C34-C33	-3.04	122.97	127.31
28	a	409	CLA	C2D-C1D-ND	3.04	112.35	110.10
28	C	511	CLA	C2C-C1C-NC	3.04	112.82	109.97
30	i	101	BCR	C38-C26-C27	3.04	119.46	113.62
28	y	305	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	y	304	CLA	C2C-C1C-NC	3.04	112.82	109.97
37	E	101	HEM	C4C-NC-C1C	3.04	108.33	105.35
28	G	602	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	G	613	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	D	404	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	r	608	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	b	608	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	G	611	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	b	607	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	S	312	CLA	CMA-C3A-C4A	3.04	119.94	111.77
39	N	616	LUT	C21-C26-C27	-3.04	108.86	112.70
28	c	505	CLA	C2C-C1C-NC	3.04	112.82	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	506	CLA	C1D-ND-C4D	-3.04	104.18	106.33
30	K	101	BCR	C15-C14-C13	-3.04	122.98	127.31
30	C	516	BCR	C15-C16-C17	-3.04	117.25	123.47
28	B	609	CLA	C2D-C1D-ND	3.04	112.34	110.10
28	C	506	CLA	C1-C2-C3	-3.04	120.79	126.04
41	R	615	XAT	C7-C8-C9	-3.04	120.82	125.53
28	g	612	CLA	C2D-C1D-ND	3.03	112.34	110.10
38	G	605	CHL	C4B-CHC-C1C	3.03	133.53	126.34
28	Y	613	CLA	CMA-C3A-C4A	3.03	119.92	111.77
28	G	610	CLA	C1D-ND-C4D	-3.03	104.18	106.33
28	b	614	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	y	313	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	B	613	CLA	C2D-C1D-ND	3.03	112.34	110.10
38	S	307	CHL	C4D-CHA-C1A	3.03	124.94	121.25
38	G	605	CHL	C3C-C4C-NC	-3.03	107.17	110.57
28	c	507	CLA	CHD-C1D-ND	-3.03	121.67	124.45
38	N	609	CHL	C4D-CHA-C1A	3.03	124.94	121.25
28	c	512	CLA	C2C-C1C-NC	3.03	112.81	109.97
38	y	307	CHL	C3B-C4B-NB	-3.03	107.70	110.52
28	r	602	CLA	C2D-C1D-ND	3.03	112.34	110.10
28	d	401	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	B	607	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	s	611	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	r	612	CLA	CMA-C3A-C4A	3.03	119.91	111.77
39	Y	616	LUT	C21-C26-C27	-3.03	108.87	112.70
30	C	515	BCR	C38-C26-C27	3.03	119.43	113.62
39	s	614	LUT	C18-C5-C4	3.03	119.96	114.36
28	D	401	CLA	C2D-C1D-ND	3.03	112.33	110.10
28	N	610	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	N	612	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	b	614	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	c	506	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	Y	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
41	y	317	XAT	C38-C25-C26	-3.03	117.19	122.26
28	C	504	CLA	C2D-C1D-ND	3.03	112.33	110.10
28	n	610	CLA	C2D-C1D-ND	3.03	112.33	110.10
28	c	509	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	B	618	BCR	C23-C24-C25	-3.03	118.70	127.20
28	g	613	CLA	C6-C5-C3	-3.03	109.67	114.62
28	G	602	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	c	514	BCR	C23-C24-C25	-3.03	118.71	127.20
28	Y	602	CLA	C1C-C2C-C3C	-3.03	103.78	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	409	BCR	C7-C8-C9	-3.02	121.67	126.23
28	B	605	CLA	CHD-C1D-ND	-3.02	121.67	124.45
28	R	608	CLA	CHD-C1D-ND	-3.02	121.67	124.45
28	c	511	CLA	C2C-C1C-NC	3.02	112.80	109.97
38	s	601	CHL	C3B-C4B-NB	-3.02	107.71	110.52
39	Y	615	LUT	C30-C31-C32	-3.02	113.79	123.22
28	B	616	CLA	C2D-C1D-ND	3.02	112.33	110.10
28	y	314	CLA	C2D-C1D-ND	3.02	112.33	110.10
28	b	605	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
38	Y	608	CHL	C4B-CHC-C1C	3.02	133.50	126.34
28	a	406	CLA	C2D-C1D-ND	3.02	112.33	110.10
28	d	401	CLA	C2D-C1D-ND	3.02	112.33	110.10
28	C	503	CLA	CMA-C3A-C4A	3.02	119.89	111.77
30	T	101	BCR	C33-C5-C4	3.02	119.42	113.62
30	T	101	BCR	C15-C14-C13	-3.02	123.00	127.31
28	C	506	CLA	C2D-C1D-ND	3.02	112.33	110.10
28	A	406	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	n	614	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	g	612	CLA	CHD-C1D-ND	-3.02	121.68	124.45
28	D	401	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	N	614	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	B	614	CLA	CHD-C1D-ND	-3.02	121.68	124.45
38	s	601	CHL	C4D-CHA-C1A	3.02	124.92	121.25
28	s	613	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	s	611	CLA	C2D-C1D-ND	3.02	112.33	110.10
30	i	101	BCR	C1-C6-C5	-3.01	118.37	122.61
38	N	605	CHL	C3C-C4C-NC	-3.01	107.19	110.57
28	n	610	CLA	C2C-C1C-NC	3.01	112.80	109.97
40	s	616	NEX	C38-C25-C26	-3.01	117.21	122.26
28	c	501	CLA	C2D-C1D-ND	3.01	112.33	110.10
30	c	514	BCR	C38-C26-C27	3.01	119.41	113.62
28	N	613	CLA	CMA-C3A-C4A	3.01	119.87	111.77
28	b	602	CLA	C1-C2-C3	-3.01	120.83	126.04
28	Y	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	D	404	CLA	CMA-C3A-C4A	3.01	119.87	111.77
28	b	609	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	y	313	CLA	C2C-C1C-NC	3.01	112.79	109.97
35	l	101	LHG	O8-C23-C24	3.01	121.35	111.91
28	R	611	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	c	511	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	R	610	CLA	C2C-C1C-NC	3.01	112.79	109.97
38	G	608	CHL	C4B-CHC-C1C	3.01	133.47	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	601	CLA	CHD-C1D-ND	-3.01	121.69	124.45
38	g	608	CHL	C4B-CHC-C1C	3.01	133.47	126.34
28	S	314	CLA	C2C-C1C-NC	3.01	112.79	109.97
38	Y	606	CHL	C4D-CHA-C1A	3.01	124.91	121.25
38	G	608	CHL	C3B-C4B-NB	-3.00	107.73	110.52
38	n	601	CHL	C4B-CHC-C1C	3.00	133.46	126.34
28	B	606	CLA	C1D-ND-C4D	-3.00	104.20	106.33
38	n	608	CHL	C2C-C3C-C4C	3.00	108.63	106.49
38	n	606	CHL	C4B-CHC-C1C	3.00	133.46	126.34
28	n	603	CLA	C2C-C1C-NC	3.00	112.78	109.97
28	a	406	CLA	CHD-C1D-ND	-3.00	121.69	124.45
28	N	603	CLA	C2C-C1C-NC	3.00	112.78	109.97
28	b	603	CLA	C2D-C1D-ND	3.00	112.32	110.10
30	K	101	BCR	C38-C26-C27	3.00	119.38	113.62
38	y	302	CHL	C4B-CHC-C1C	3.00	133.46	126.34
28	c	507	CLA	C2D-C1D-ND	3.00	112.31	110.10
28	B	614	CLA	C2C-C1C-NC	3.00	112.78	109.97
38	n	608	CHL	C1-O2A-CGA	3.00	124.31	116.44
28	R	611	CLA	CHD-C1D-ND	-3.00	121.70	124.45
28	R	612	CLA	CMA-C3A-C4A	3.00	119.83	111.77
38	g	601	CHL	C4B-CHC-C1C	3.00	133.45	126.34
28	b	602	CLA	C2D-C1D-ND	3.00	112.31	110.10
28	g	614	CLA	C2D-C1D-ND	3.00	112.31	110.10
28	B	610	CLA	C3B-C4B-NB	-3.00	107.73	110.52
28	G	610	CLA	C1-C2-C3	-3.00	120.86	126.04
28	n	604	CLA	C2D-C1D-ND	3.00	112.31	110.10
38	S	306	CHL	C3B-C4B-NB	-3.00	107.74	110.52
30	H	101	BCR	C30-C25-C26	-2.99	118.39	122.61
28	Y	612	CLA	CHD-C1D-ND	-2.99	121.70	124.45
28	y	304	CLA	CMA-C3A-C4A	2.99	119.82	111.77
28	N	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
28	c	510	CLA	C2D-C1D-ND	2.99	112.31	110.10
28	d	404	CLA	C2C-C1C-NC	2.99	112.78	109.97
39	G	616	LUT	C8-C7-C6	-2.99	118.80	127.20
30	k	101	BCR	C33-C5-C4	2.99	119.36	113.62
38	N	607	CHL	C4B-CHC-C1C	2.99	133.44	126.34
28	y	303	CLA	CMA-C3A-C4A	2.99	119.81	111.77
38	g	605	CHL	C3C-C4C-NC	-2.99	107.22	110.57
30	k	101	BCR	C38-C26-C27	2.99	119.36	113.62
28	c	513	CLA	C2C-C1C-NC	2.99	112.77	109.97
28	s	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
30	k	101	BCR	C8-C7-C6	-2.99	118.80	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	602	CLA	C2C-C1C-NC	2.99	112.77	109.97
35	c	520	LHG	C5-O7-C7	-2.99	110.43	117.79
28	R	612	CLA	C2D-C1D-ND	2.99	112.31	110.10
28	n	614	CLA	C2D-C1D-ND	2.99	112.31	110.10
30	C	516	BCR	C33-C5-C4	2.99	119.36	113.62
35	C	521	LHG	O8-C23-C24	2.99	121.29	111.91
30	b	619	BCR	C34-C9-C8	2.99	122.78	118.08
28	d	401	CLA	CMA-C3A-C4A	2.99	119.80	111.77
38	g	608	CHL	C4D-CHA-C1A	2.99	124.88	121.25
40	n	617	NEX	C38-C25-C24	2.99	117.64	114.28
28	G	603	CLA	CMA-C3A-C4A	2.99	119.80	111.77
32	B	621	LMG	O8-C28-C29	2.99	121.28	111.91
28	y	312	CLA	CHD-C1D-ND	-2.98	121.71	124.45
30	C	514	BCR	C33-C5-C4	2.98	119.35	113.62
28	b	612	CLA	C1D-ND-C4D	-2.98	104.22	106.33
28	R	609	CLA	CMA-C3A-C4A	2.98	119.79	111.77
28	s	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
38	S	302	CHL	CMA-C3A-C4A	2.98	119.79	111.77
38	S	306	CHL	C3C-C4C-NC	-2.98	107.23	110.57
30	H	101	BCR	C38-C26-C27	2.98	119.34	113.62
28	B	602	CLA	CMA-C3A-C4A	2.98	119.78	111.77
28	G	611	CLA	C3B-C4B-NB	-2.98	107.75	110.52
28	r	601	CLA	C2C-C1C-NC	2.98	112.76	109.97
28	b	613	CLA	C2D-C1D-ND	2.98	112.30	110.10
28	n	612	CLA	CMA-C3A-C4A	2.98	119.78	111.77
28	B	606	CLA	CHD-C1D-ND	-2.98	121.72	124.45
28	R	611	CLA	CMA-C3A-C4A	2.98	119.78	111.77
38	S	308	CHL	C4B-CHC-C1C	2.98	133.40	126.34
28	B	601	CLA	C2D-C1D-ND	2.98	112.30	110.10
38	N	606	CHL	C4B-CHC-C1C	2.98	133.40	126.34
39	R	614	LUT	C15-C14-C13	-2.98	123.06	127.31
28	n	612	CLA	O2A-CGA-CBA	2.98	121.25	111.91
28	S	303	CLA	CMA-C3A-C4A	2.98	119.78	111.77
28	C	507	CLA	C2D-C1D-ND	2.98	112.30	110.10
28	R	608	CLA	C2D-C1D-ND	2.98	112.30	110.10
28	S	303	CLA	C2D-C1D-ND	2.98	112.30	110.10
39	G	615	LUT	C32-C33-C34	2.98	123.51	118.94
28	y	310	CLA	C1D-ND-C4D	-2.98	104.22	106.33
28	C	508	CLA	CMA-C3A-C4A	2.98	119.77	111.77
38	Y	608	CHL	C4D-CHA-C1A	2.98	124.87	121.25
30	c	515	BCR	C30-C25-C26	-2.98	118.42	122.61
28	s	612	CLA	CMA-C3A-C4A	2.98	119.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N	602	CLA	C2C-C1C-NC	2.97	112.76	109.97
28	y	313	CLA	CMA-C3A-C4A	2.97	119.77	111.77
28	A	406	CLA	C2D-C1D-ND	2.97	112.30	110.10
38	R	605	CHL	C3C-C4C-NC	-2.97	107.24	110.57
28	S	311	CLA	C2C-C1C-NC	2.97	112.76	109.97
28	g	602	CLA	C2C-C1C-NC	2.97	112.76	109.97
38	S	307	CHL	C2C-C3C-C4C	2.97	108.61	106.49
28	c	506	CLA	C1-C2-C3	-2.97	120.90	126.04
28	A	406	CLA	CHD-C1D-ND	-2.97	121.72	124.45
28	b	601	CLA	CHD-C1D-ND	-2.97	121.72	124.45
30	K	101	BCR	C33-C5-C4	2.97	119.32	113.62
28	r	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
28	a	406	CLA	C1-C2-C3	-2.97	120.91	126.04
30	t	101	BCR	C11-C12-C13	-2.97	118.08	126.42
28	b	601	CLA	CMA-C3A-C4A	2.97	119.75	111.77
38	r	607	CHL	C4D-CHA-C1A	2.97	124.86	121.25
28	n	611	CLA	C2C-C1C-NC	2.97	112.75	109.97
30	B	617	BCR	C1-C6-C5	-2.97	118.43	122.61
38	g	601	CHL	C2C-C3C-C4C	2.97	108.60	106.49
38	R	605	CHL	C3B-C4B-NB	-2.97	107.76	110.52
28	Y	612	CLA	C2C-C1C-NC	2.97	112.75	109.97
28	B	615	CLA	C2D-C1D-ND	2.97	112.29	110.10
28	y	311	CLA	C2D-C1D-ND	2.97	112.29	110.10
28	d	405	CLA	CMA-C3A-C4A	2.97	119.75	111.77
28	G	614	CLA	C1D-ND-C4D	-2.97	104.23	106.33
28	y	312	CLA	C1D-ND-C4D	-2.97	104.23	106.33
28	C	510	CLA	C2C-C1C-NC	2.97	112.75	109.97
28	r	609	CLA	CMA-C3A-C4A	2.97	119.74	111.77
38	n	608	CHL	CMA-C3A-C4A	2.97	119.74	111.77
28	b	602	CLA	C2C-C1C-NC	2.96	112.75	109.97
38	n	607	CHL	C2C-C3C-C4C	2.96	108.60	106.49
28	Y	604	CLA	C2D-C1D-ND	2.96	112.29	110.10
28	g	602	CLA	CMA-C3A-C4A	2.96	119.74	111.77
28	b	604	CLA	C2D-C1D-ND	2.96	112.29	110.10
38	G	609	CHL	C4D-CHA-C1A	2.96	124.85	121.25
28	r	613	CLA	CMA-C3A-C4A	2.96	119.73	111.77
28	C	508	CLA	C2C-C1C-NC	2.96	112.75	109.97
28	B	609	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	c	503	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	n	614	CLA	CHD-C1D-ND	-2.96	121.74	124.45
28	S	303	CLA	C1D-ND-C4D	-2.96	104.23	106.33
28	c	509	CLA	C2D-C1D-ND	2.96	112.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	603	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	C	505	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	S	304	CLA	C2D-C1D-ND	2.96	112.28	110.10
28	S	313	CLA	C2D-C1D-ND	2.96	112.28	110.10
28	G	603	CLA	CHD-C1D-ND	-2.96	121.74	124.45
28	S	310	CLA	CMA-C3A-C4A	2.96	119.72	111.77
28	y	303	CLA	C1D-ND-C4D	-2.95	104.24	106.33
28	N	604	CLA	CHD-C1D-ND	-2.95	121.74	124.45
30	k	101	BCR	C16-C15-C14	-2.95	117.42	123.47
28	n	613	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
28	y	312	CLA	C3B-C4B-NB	-2.95	107.78	110.52
28	r	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
38	y	306	CHL	C4B-CHC-C1C	2.95	133.34	126.34
28	B	610	CLA	C2C-C1C-NC	2.95	112.74	109.97
28	y	313	CLA	C2D-C1D-ND	2.95	112.28	110.10
28	c	512	CLA	CMA-C3A-C4A	2.95	119.70	111.77
28	D	401	CLA	CMA-C3A-C4A	2.95	119.70	111.77
28	c	501	CLA	C2C-C1C-NC	2.95	112.74	109.97
28	y	314	CLA	C2C-C1C-NC	2.95	112.74	109.97
39	G	616	LUT	C21-C26-C27	-2.95	108.97	112.70
28	G	610	CLA	C2C-C1C-NC	2.95	112.73	109.97
28	Y	612	CLA	CMA-C3A-C4A	2.95	119.70	111.77
38	y	308	CHL	CMA-C3A-C4A	2.95	119.69	111.77
28	S	305	CLA	CMA-C3A-C4A	2.95	119.69	111.77
38	r	606	CHL	C4D-CHA-C1A	2.95	124.83	121.25
28	s	603	CLA	CMA-C3A-C4A	2.94	119.69	111.77
28	Y	610	CLA	C1-C2-C3	-2.94	120.95	126.04
30	t	101	BCR	C38-C26-C27	2.94	119.27	113.62
28	C	507	CLA	C1-C2-C3	-2.94	120.95	126.04
28	s	602	CLA	C2C-C1C-NC	2.94	112.73	109.97
39	n	616	LUT	C10-C11-C12	-2.94	114.03	123.22
38	g	607	CHL	C3B-C4B-NB	-2.94	107.78	110.52
28	B	608	CLA	CMA-C3A-C4A	2.94	119.68	111.77
30	B	617	BCR	C8-C7-C6	-2.94	118.94	127.20
38	g	619	CHL	C2C-C3C-C4C	2.94	108.58	106.49
39	s	614	LUT	C31-C30-C29	-2.94	123.11	127.31
28	B	604	CLA	CMA-C3A-C4A	2.94	119.67	111.77
28	B	602	CLA	C2C-C1C-NC	2.94	112.73	109.97
28	b	608	CLA	CMA-C3A-C4A	2.94	119.67	111.77
38	Y	606	CHL	C4B-CHC-C1C	2.94	133.31	126.34
39	r	614	LUT	C35-C15-C14	2.94	129.50	123.47
28	s	609	CLA	C2D-C1D-ND	2.94	112.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	G	607	CHL	C2C-C3C-C4C	2.94	108.58	106.49
28	s	604	CLA	C2C-C1C-NC	2.94	112.72	109.97
38	S	308	CHL	C4D-CHA-C1A	2.94	124.83	121.25
30	C	515	BCR	C7-C8-C9	-2.94	121.80	126.23
30	a	410	BCR	C33-C5-C4	2.94	119.26	113.62
28	G	612	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	Y	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	N	602	CLA	C1D-ND-C4D	-2.94	104.25	106.33
28	C	507	CLA	C3B-C4B-NB	-2.94	107.79	110.52
28	B	607	CLA	CMA-C3A-C4A	2.94	119.66	111.77
28	C	501	CLA	CMA-C3A-C4A	2.94	119.66	111.77
39	R	614	LUT	C30-C31-C32	-2.94	114.06	123.22
38	R	606	CHL	CMA-C3A-C4A	2.93	119.66	111.77
28	N	613	CLA	CHD-C1D-ND	-2.93	121.76	124.45
38	N	605	CHL	C3B-C4B-NB	-2.93	107.79	110.52
28	Y	603	CLA	C2D-C1D-ND	2.93	112.27	110.10
28	C	501	CLA	CHD-C1D-ND	-2.93	121.76	124.45
38	N	605	CHL	C4B-CHC-C1C	2.93	133.30	126.34
38	Y	606	CHL	C3C-C4C-NC	-2.93	107.28	110.57
28	R	603	CLA	C2D-C1D-ND	2.93	112.27	110.10
28	b	603	CLA	C2C-C1C-NC	2.93	112.72	109.97
28	C	509	CLA	CMA-C3A-C4A	2.93	119.65	111.77
28	c	505	CLA	C1-C2-C3	-2.93	120.97	126.04
28	c	510	CLA	C2C-C1C-NC	2.93	112.72	109.97
28	b	609	CLA	C1D-ND-C4D	-2.93	104.25	106.33
28	y	310	CLA	C2C-C1C-NC	2.93	112.72	109.97
38	Y	607	CHL	C4B-CHC-C1C	2.93	133.28	126.34
28	R	613	CLA	C2C-C1C-NC	2.93	112.72	109.97
38	g	609	CHL	C4B-CHC-C1C	2.93	133.28	126.34
28	C	503	CLA	C2C-C1C-NC	2.93	112.71	109.97
28	B	606	CLA	C3B-C4B-NB	-2.93	107.80	110.52
28	C	501	CLA	C3B-C4B-NB	-2.93	107.80	110.52
38	G	601	CHL	C3B-C4B-NB	-2.93	107.80	110.52
28	S	303	CLA	C2C-C1C-NC	2.93	112.71	109.97
28	R	609	CLA	C1D-ND-C4D	-2.93	104.26	106.33
28	d	404	CLA	C1D-ND-C4D	-2.93	104.26	106.33
38	N	605	CHL	C4D-CHA-C1A	2.92	124.81	121.25
28	s	611	CLA	C3B-C4B-NB	-2.92	107.80	110.52
28	R	610	CLA	CMA-C3A-C4A	2.92	119.63	111.77
38	R	607	CHL	C2C-C3C-C4C	2.92	108.57	106.49
38	r	606	CHL	C4B-CHC-C1C	2.92	133.27	126.34
28	Y	611	CLA	C2D-C1D-ND	2.92	112.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	603	CLA	C1D-ND-C4D	-2.92	104.26	106.33
28	s	610	CLA	C3B-C4B-NB	-2.92	107.80	110.52
28	B	608	CLA	CHD-C1D-ND	-2.92	121.77	124.45
28	N	603	CLA	C2D-C1D-ND	2.92	112.26	110.10
28	B	603	CLA	C3B-C4B-NB	-2.92	107.81	110.52
28	N	611	CLA	CMA-C3A-C4A	2.92	119.62	111.77
28	c	502	CLA	CMA-C3A-C4A	2.92	119.62	111.77
28	R	609	CLA	C2D-C1D-ND	2.92	112.26	110.10
28	b	608	CLA	C2D-C1D-ND	2.92	112.26	110.10
28	c	512	CLA	CHD-C1D-ND	-2.92	121.77	124.45
28	R	601	CLA	C3B-C4B-NB	-2.92	107.81	110.52
28	B	604	CLA	C2D-C1D-ND	2.92	112.25	110.10
28	S	312	CLA	C2D-C1D-ND	2.92	112.25	110.10
28	R	609	CLA	C2C-C1C-NC	2.92	112.71	109.97
39	Y	615	LUT	C39-C29-C28	2.92	122.67	118.08
28	n	612	CLA	C1D-ND-C4D	-2.92	104.26	106.33
38	Y	608	CHL	CMA-C3A-C4A	2.92	119.61	111.77
28	s	609	CLA	CHD-C1D-ND	-2.92	121.77	124.45
38	g	619	CHL	C1-C2-C3	-2.92	121.00	126.04
30	B	618	BCR	C29-C30-C25	2.92	114.97	110.48
28	s	612	CLA	CHD-C1D-ND	-2.92	121.77	124.45
38	y	302	CHL	C3B-C4B-NB	-2.92	107.81	110.52
38	S	302	CHL	C4D-CHA-C1A	2.92	124.80	121.25
28	G	602	CLA	CMA-C3A-C4A	2.92	119.61	111.77
28	Y	610	CLA	C2D-C1D-ND	2.91	112.25	110.10
38	Y	608	CHL	C1-C2-C3	-2.91	121.00	126.04
28	g	614	CLA	C2C-C1C-NC	2.91	112.70	109.97
30	h	101	BCR	C30-C25-C26	-2.91	118.51	122.61
28	N	612	CLA	CHD-C1D-ND	-2.91	121.78	124.45
39	s	614	LUT	C19-C9-C10	-2.91	118.84	122.92
28	R	610	CLA	C3B-C4B-NB	-2.91	107.81	110.52
38	Y	605	CHL	C3C-C4C-NC	-2.91	107.31	110.57
38	R	605	CHL	C4D-CHA-C1A	2.91	124.79	121.25
28	s	609	CLA	CMA-C3A-C4A	2.91	119.60	111.77
28	S	305	CLA	C2C-C1C-NC	2.91	112.70	109.97
28	b	615	CLA	C2D-C1D-ND	2.91	112.25	110.10
28	B	607	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	B	602	CLA	C1D-ND-C4D	-2.91	104.27	106.33
28	g	614	CLA	C1D-ND-C4D	-2.91	104.27	106.33
28	B	608	CLA	C1-C2-C3	-2.91	121.01	126.04
28	R	613	CLA	CMA-C3A-C4A	2.91	119.59	111.77
28	r	604	CLA	CHD-C1D-ND	-2.91	121.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	N	601	CHL	C4D-CHA-C1A	2.91	124.79	121.25
28	b	616	CLA	C2D-C1D-ND	2.91	112.25	110.10
28	B	603	CLA	CMA-C3A-C4A	2.91	119.59	111.77
32	w	101	LMG	O8-C28-C29	2.91	121.03	111.91
28	B	602	CLA	C1-C2-C3	-2.91	121.02	126.04
28	S	311	CLA	C1D-ND-C4D	-2.91	104.27	106.33
35	N	618	LHG	O8-C23-C24	2.91	121.03	111.91
32	k	102	LMG	O8-C28-C29	2.91	121.03	111.91
28	S	313	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	c	501	CLA	CMA-C3A-C4A	2.91	119.58	111.77
28	c	507	CLA	CMA-C3A-C4A	2.91	119.58	111.77
38	N	606	CHL	C3C-C4C-NC	-2.91	107.31	110.57
38	r	605	CHL	C3C-C4C-NC	-2.91	107.31	110.57
28	A	408	CLA	CMA-C3A-C4A	2.90	119.58	111.77
28	S	304	CLA	CMA-C3A-C4A	2.90	119.58	111.77
28	B	603	CLA	CHD-C1D-ND	-2.90	121.78	124.45
28	S	313	CLA	CMA-C3A-C4A	2.90	119.58	111.77
28	c	510	CLA	C1D-ND-C4D	-2.90	104.27	106.33
28	C	504	CLA	CMA-C3A-C4A	2.90	119.57	111.77
28	B	601	CLA	CMA-C3A-C4A	2.90	119.57	111.77
28	c	506	CLA	CMA-C3A-C4A	2.90	119.57	111.77
28	G	614	CLA	C2C-C1C-NC	2.90	112.69	109.97
28	c	513	CLA	CHD-C1D-ND	-2.90	121.79	124.45
28	c	503	CLA	CMA-C3A-C4A	2.90	119.57	111.77
28	B	612	CLA	CHD-C1D-ND	-2.90	121.79	124.45
28	r	610	CLA	CMA-C3A-C4A	2.90	119.56	111.77
38	G	601	CHL	C2C-C3C-C4C	2.90	108.56	106.49
38	S	306	CHL	C4B-CHC-C1C	2.90	133.21	126.34
28	r	613	CLA	C3B-C4B-NB	-2.90	107.83	110.52
28	b	614	CLA	C2D-C1D-ND	2.90	112.24	110.10
38	G	601	CHL	C4B-CHC-C1C	2.90	133.21	126.34
28	Y	602	CLA	C2C-C1C-NC	2.90	112.69	109.97
28	b	602	CLA	C1D-ND-C4D	-2.90	104.28	106.33
28	d	405	CLA	C1D-ND-C4D	-2.90	104.28	106.33
28	b	610	CLA	C3B-C4B-NB	-2.90	107.83	110.52
28	r	602	CLA	C2C-C1C-NC	2.89	112.68	109.97
28	B	611	CLA	C1D-ND-C4D	-2.89	104.28	106.33
38	g	601	CHL	C3B-C4B-NB	-2.89	107.83	110.52
28	G	604	CLA	C2D-C1D-ND	2.89	112.24	110.10
28	g	603	CLA	CMA-C3A-C4A	2.89	119.55	111.77
38	n	608	CHL	C4D-CHA-C1A	2.89	124.77	121.25
28	n	604	CLA	C1D-ND-C4D	-2.89	104.28	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	N	608	CHL	C3B-C4B-NB	-2.89	107.83	110.52
38	S	302	CHL	C3B-C4B-NB	-2.89	107.83	110.52
28	b	607	CLA	CMA-C3A-C4A	2.89	119.54	111.77
28	n	603	CLA	C3B-C4B-NB	-2.89	107.83	110.52
38	r	607	CHL	C3B-C4B-NB	-2.89	107.83	110.52
28	y	311	CLA	CMA-C3A-C4A	2.89	119.54	111.77
28	r	610	CLA	CHD-C1D-ND	-2.89	121.80	124.45
28	s	602	CLA	C2D-C1D-ND	2.89	112.23	110.10
28	Y	610	CLA	C3B-C4B-NB	-2.89	107.83	110.52
28	s	602	CLA	C1D-ND-C4D	-2.89	104.28	106.33
28	G	613	CLA	CMA-C3A-C4A	2.89	119.53	111.77
28	R	601	CLA	CMA-C3A-C4A	2.89	119.53	111.77
28	b	616	CLA	C2C-C1C-NC	2.89	112.68	109.97
28	r	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
28	G	613	CLA	C2D-C1D-ND	2.89	112.23	110.10
30	b	618	BCR	C8-C7-C6	-2.89	119.10	127.20
28	B	608	CLA	C2C-C1C-NC	2.89	112.67	109.97
38	n	609	CHL	C1-C2-C3	-2.89	121.05	126.04
30	t	101	BCR	C33-C5-C4	2.88	119.16	113.62
28	B	605	CLA	C1D-ND-C4D	-2.88	104.29	106.33
38	N	608	CHL	C2C-C3C-C4C	2.88	108.55	106.49
38	g	619	CHL	CMA-C3A-C4A	2.88	119.53	111.77
38	G	609	CHL	C4B-CHC-C1C	2.88	133.18	126.34
28	n	613	CLA	CHD-C1D-ND	-2.88	121.81	124.45
28	B	616	CLA	CMA-C3A-C4A	2.88	119.52	111.77
28	s	611	CLA	C1D-ND-C4D	-2.88	104.29	106.33
30	k	101	BCR	C7-C8-C9	-2.88	121.88	126.23
38	S	307	CHL	C3B-C4B-NB	-2.88	107.84	110.52
38	n	608	CHL	C4B-CHC-C1C	2.88	133.17	126.34
28	A	408	CLA	C2D-C1D-ND	2.88	112.23	110.10
28	C	513	CLA	CHD-C1D-ND	-2.88	121.81	124.45
28	R	613	CLA	C1D-ND-C4D	-2.88	104.29	106.33
38	Y	609	CHL	C3B-C4B-NB	-2.88	107.84	110.52
28	S	311	CLA	CMA-C3A-C4A	2.88	119.51	111.77
38	N	608	CHL	C4B-CHC-C1C	2.88	133.17	126.34
38	n	606	CHL	C3C-C4C-NC	-2.88	107.34	110.57
28	s	613	CLA	CMA-C3A-C4A	2.88	119.51	111.77
28	G	610	CLA	O1D-CGD-CBD	-2.88	118.59	124.48
28	A	405	CLA	C2C-C1C-NC	2.88	112.67	109.97
28	c	504	CLA	C2C-C1C-NC	2.88	112.67	109.97
36	c	517	DGD	O1G-C1A-C2A	2.88	120.94	111.91
28	A	405	CLA	C1D-ND-C4D	-2.88	104.29	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	409	CLA	CMA-C3A-C4A	2.88	119.51	111.77
28	b	610	CLA	CMA-C3A-C4A	2.88	119.51	111.77
28	g	603	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
28	s	603	CLA	C2D-C1D-ND	2.88	112.22	110.10
28	Y	602	CLA	C4B-CHC-C1C	2.87	133.16	126.34
38	Y	609	CHL	C4D-CHA-C1A	2.87	124.75	121.25
38	y	308	CHL	C4D-CHA-C1A	2.87	124.75	121.25
28	s	610	CLA	CHD-C1D-ND	-2.87	121.81	124.45
38	N	607	CHL	C3B-C4B-NB	-2.87	107.85	110.52
28	R	604	CLA	C2C-C1C-NC	2.87	112.66	109.97
28	C	502	CLA	CMA-C3A-C4A	2.87	119.49	111.77
28	C	507	CLA	CHD-C1D-ND	-2.87	121.81	124.45
28	N	604	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	S	314	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	C	505	CLA	CHD-C1D-ND	-2.87	121.82	124.45
28	B	608	CLA	C2D-C1D-ND	2.87	112.22	110.10
30	B	617	BCR	C7-C8-C9	-2.87	121.90	126.23
38	g	619	CHL	C3B-C4B-NB	-2.87	107.85	110.52
38	Y	605	CHL	C4B-CHC-C1C	2.87	133.14	126.34
28	Y	614	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	c	505	CLA	CHD-C1D-ND	-2.87	121.82	124.45
38	r	606	CHL	C3B-C4B-NB	-2.87	107.85	110.52
38	y	308	CHL	C3B-C4B-NB	-2.87	107.85	110.52
28	r	609	CLA	C2C-C1C-NC	2.87	112.66	109.97
30	b	618	BCR	C27-C26-C25	-2.87	118.57	122.73
28	B	609	CLA	C1D-ND-C4D	-2.87	104.30	106.33
28	b	611	CLA	C1D-ND-C4D	-2.87	104.30	106.33
28	R	610	CLA	CHD-C1D-ND	-2.87	121.82	124.45
28	B	605	CLA	C2C-C1C-NC	2.87	112.66	109.97
38	Y	605	CHL	CMA-C3A-C4A	2.87	119.48	111.77
39	N	615	LUT	C7-C8-C9	-2.87	121.90	126.23
28	B	610	CLA	C1D-ND-C4D	-2.87	104.30	106.33
28	B	605	CLA	CMA-C3A-C4A	2.87	119.48	111.77
28	Y	613	CLA	C2D-C1D-ND	2.87	112.22	110.10
38	s	605	CHL	C3C-C4C-NC	-2.87	107.36	110.57
28	C	509	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	c	508	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	n	611	CLA	C1-C2-C3	-2.86	121.09	126.04
28	y	312	CLA	C2C-C1C-NC	2.86	112.66	109.97
28	Y	610	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
28	r	612	CLA	C2D-C1D-ND	2.86	112.21	110.10
28	g	604	CLA	CMA-C3A-C4A	2.86	119.47	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	611	CLA	C3B-C4B-NB	-2.86	107.86	110.52
28	R	609	CLA	C1-C2-C3	-2.86	121.09	126.04
28	c	501	CLA	C3B-C4B-NB	-2.86	107.86	110.52
38	r	607	CHL	C2C-C3C-C4C	2.86	108.53	106.49
28	R	603	CLA	C2C-C1C-NC	2.86	112.65	109.97
28	b	610	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	g	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
28	n	612	CLA	C3B-C4B-NB	-2.86	107.86	110.52
30	b	618	BCR	C16-C17-C18	-2.86	123.23	127.31
28	s	608	CLA	C2D-C1D-ND	2.86	112.21	110.10
28	Y	604	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	Y	612	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	a	407	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	g	602	CLA	C1D-ND-C4D	-2.86	104.30	106.33
30	b	619	BCR	C16-C15-C14	-2.86	117.62	123.47
28	r	601	CLA	CMA-C3A-C4A	2.86	119.45	111.77
28	D	403	CLA	C1D-ND-C4D	-2.86	104.31	106.33
28	R	610	CLA	C1D-ND-C4D	-2.86	104.31	106.33
28	r	608	CLA	C1D-ND-C4D	-2.86	104.31	106.33
28	b	607	CLA	CHD-C1D-ND	-2.86	121.83	124.45
28	G	611	CLA	CMA-C3A-C4A	2.86	119.45	111.77
28	y	305	CLA	C2D-C1D-ND	2.86	112.21	110.10
35	c	519	LHG	C5-O7-C7	-2.86	110.76	117.79
38	y	306	CHL	C3C-C4C-NC	-2.86	107.37	110.57
35	b	624	LHG	O8-C23-C24	2.86	120.87	111.91
28	N	611	CLA	C3B-C4B-NB	-2.86	107.87	110.52
28	a	406	CLA	C2C-C1C-NC	2.86	112.65	109.97
28	s	611	CLA	CHD-C1D-ND	-2.86	121.83	124.45
28	C	510	CLA	C2D-C1D-ND	2.86	112.21	110.10
28	b	611	CLA	C2C-C1C-NC	2.85	112.65	109.97
38	N	601	CHL	C4B-CHC-C1C	2.85	133.11	126.34
28	Y	614	CLA	CMA-C3A-C4A	2.85	119.44	111.77
38	s	607	CHL	CMA-C3A-C4A	2.85	119.44	111.77
28	n	603	CLA	CMA-C3A-C4A	2.85	119.44	111.77
28	R	611	CLA	C1D-ND-C4D	-2.85	104.31	106.33
28	b	608	CLA	C2C-C1C-NC	2.85	112.64	109.97
28	r	601	CLA	C3B-C4B-NB	-2.85	107.87	110.52
28	n	611	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
38	R	606	CHL	C3B-C4B-NB	-2.85	107.87	110.52
38	n	608	CHL	C3B-C4B-NB	-2.85	107.87	110.52
38	s	607	CHL	C3B-C4B-NB	-2.85	107.87	110.52
28	g	613	CLA	CMA-C3A-C4A	2.85	119.44	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	601	CLA	C3B-C4B-NB	-2.85	107.87	110.52
28	r	610	CLA	C3B-C4B-NB	-2.85	107.87	110.52
38	N	607	CHL	C2C-C3C-C4C	2.85	108.52	106.49
28	B	611	CLA	CMA-C3A-C4A	2.85	119.43	111.77
28	R	603	CLA	CMA-C3A-C4A	2.85	119.43	111.77
28	c	507	CLA	C3B-C4B-NB	-2.85	107.87	110.52
38	g	607	CHL	C2C-C3C-C4C	2.85	108.52	106.49
28	b	603	CLA	CMA-C3A-C4A	2.85	119.43	111.77
28	C	513	CLA	CMA-C3A-C4A	2.85	119.43	111.77
38	Y	605	CHL	C3B-C4B-NB	-2.85	107.87	110.52
30	D	405	BCR	C20-C21-C22	-2.85	123.25	127.31
38	s	605	CHL	C3B-C4B-NB	-2.85	107.88	110.52
38	R	607	CHL	C4B-CHC-C1C	2.85	133.09	126.34
28	R	602	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
38	N	608	CHL	C4D-CHA-C1A	2.84	124.71	121.25
28	B	613	CLA	C1D-ND-C4D	-2.84	104.31	106.33
38	r	607	CHL	C4B-CHC-C1C	2.84	133.08	126.34
28	s	609	CLA	C1D-ND-C4D	-2.84	104.32	106.33
28	b	610	CLA	C2C-C1C-NC	2.84	112.63	109.97
28	B	614	CLA	C2D-C1D-ND	2.84	112.20	110.10
38	y	307	CHL	C3C-C4C-NC	-2.84	107.39	110.57
28	S	310	CLA	C2D-C1D-ND	2.84	112.20	110.10
28	y	311	CLA	C3B-C4B-NB	-2.84	107.88	110.52
28	S	304	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
28	B	603	CLA	C1D-ND-C4D	-2.84	104.32	106.33
28	N	612	CLA	CMA-C3A-C4A	2.84	119.39	111.77
28	n	602	CLA	CMA-C3A-C4A	2.84	119.39	111.77
28	S	309	CLA	CMA-C3A-C4A	2.84	119.39	111.77
28	y	314	CLA	C1D-ND-C4D	-2.84	104.32	106.33
38	s	607	CHL	C4D-CHA-C1A	2.83	124.70	121.25
28	B	612	CLA	CMA-C3A-C4A	2.83	119.39	111.77
28	N	611	CLA	C2D-C1D-ND	2.83	112.19	110.10
28	N	614	CLA	CMA-C3A-C4A	2.83	119.39	111.77
38	G	607	CHL	C3B-C4B-NB	-2.83	107.89	110.52
36	C	517	DGD	O1G-C1A-C2A	2.83	120.80	111.91
38	Y	601	CHL	C4D-CHA-C1A	2.83	124.70	121.25
39	N	616	LUT	C18-C5-C4	2.83	119.60	114.36
38	g	619	CHL	C4B-CHC-C1C	2.83	133.05	126.34
28	R	604	CLA	C1D-ND-C4D	-2.83	104.33	106.33
38	G	608	CHL	C1-C2-C3	-2.83	121.15	126.04
28	b	611	CLA	CMA-C3A-C4A	2.83	119.37	111.77
28	c	504	CLA	CMA-C3A-C4A	2.83	119.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	601	CLA	C1C-C2C-C3C	-2.83	103.99	106.96
39	y	315	LUT	C8-C7-C6	-2.82	119.27	127.20
38	R	607	CHL	C4D-CHA-C1A	2.82	124.69	121.25
38	Y	601	CHL	C3B-C4B-NB	-2.82	107.89	110.52
28	c	503	CLA	CHD-C1D-ND	-2.82	121.86	124.45
28	G	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
35	r	617	LHG	C5-O7-C7	-2.82	110.84	117.79
28	S	305	CLA	C3B-C4B-NB	-2.82	107.90	110.52
28	C	503	CLA	C1D-ND-C4D	-2.82	104.33	106.33
28	r	610	CLA	C1D-ND-C4D	-2.82	104.33	106.33
38	g	601	CHL	CMA-C3A-C4A	2.82	119.35	111.77
38	y	308	CHL	C4B-CHC-C1C	2.82	133.03	126.34
28	a	406	CLA	C1D-ND-C4D	-2.82	104.33	106.33
28	s	613	CLA	C1D-ND-C4D	-2.82	104.33	106.33
28	g	611	CLA	C3B-C4B-NB	-2.82	107.90	110.52
28	y	311	CLA	CHD-C1D-ND	-2.82	121.86	124.45
38	Y	609	CHL	C4B-CHC-C1C	2.82	133.02	126.34
28	N	613	CLA	C2D-C1D-ND	2.82	112.18	110.10
28	B	616	CLA	C2C-C1C-NC	2.82	112.61	109.97
38	S	302	CHL	C4B-CHC-C1C	2.82	133.02	126.34
28	R	612	CLA	C1D-ND-C4D	-2.82	104.33	106.33
28	C	507	CLA	CMA-C3A-C4A	2.82	119.34	111.77
28	N	611	CLA	CHD-C1D-ND	-2.82	121.87	124.45
28	s	610	CLA	CMA-C3A-C4A	2.82	119.34	111.77
38	Y	601	CHL	CMA-C3A-C4A	2.82	119.34	111.77
30	B	618	BCR	C7-C8-C9	-2.81	121.98	126.23
39	N	616	LUT	C8-C7-C6	-2.81	119.30	127.20
28	b	612	CLA	CHD-C1D-ND	-2.81	121.87	124.45
28	s	608	CLA	C1D-ND-C4D	-2.81	104.34	106.33
28	G	613	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
28	R	613	CLA	C3B-C4B-NB	-2.81	107.91	110.52
30	C	514	BCR	C23-C22-C21	2.81	123.26	118.94
37	f	101	HEM	CHD-C4C-NC	2.81	127.48	124.44
28	N	614	CLA	C1D-ND-C4D	-2.81	104.34	106.33
38	G	607	CHL	C4D-CHA-C1A	2.81	124.67	121.25
28	C	508	CLA	C1D-ND-C4D	-2.81	104.34	106.33
28	b	606	CLA	C1D-ND-C4D	-2.81	104.34	106.33
28	C	501	CLA	C2C-C1C-NC	2.81	112.61	109.97
28	b	606	CLA	C2D-C1D-ND	2.81	112.17	110.10
28	S	305	CLA	C1-C2-C3	-2.81	122.20	126.75
28	B	615	CLA	C1D-ND-C4D	-2.81	104.34	106.33
28	n	610	CLA	C1D-ND-C4D	-2.81	104.34	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	601	CLA	C3B-C4B-NB	-2.81	107.91	110.52
28	s	602	CLA	C6-C5-C3	-2.81	106.09	113.45
28	N	610	CLA	C1D-ND-C4D	-2.81	104.34	106.33
30	B	618	BCR	C8-C7-C6	-2.81	119.31	127.20
38	R	605	CHL	CMA-C3A-C4A	2.81	119.32	111.77
28	y	310	CLA	CMA-C3A-C4A	2.81	119.32	111.77
28	N	602	CLA	CMA-C3A-C4A	2.81	119.32	111.77
28	c	505	CLA	C2D-C1D-ND	2.81	112.17	110.10
38	Y	608	CHL	C2C-C3C-C4C	2.81	108.49	106.49
32	w	101	LMG	C8-O7-C10	-2.81	110.89	117.79
36	c	516	DGD	O1G-C1A-C2A	2.80	120.71	111.91
39	Y	615	LUT	C35-C15-C14	-2.80	117.73	123.47
28	y	304	CLA	C1D-ND-C4D	-2.80	104.34	106.33
30	b	617	BCR	C8-C7-C6	-2.80	119.33	127.20
28	G	603	CLA	C2D-C1D-ND	2.80	112.17	110.10
28	g	613	CLA	C2D-C1D-ND	2.80	112.17	110.10
28	B	615	CLA	C3B-C4B-NB	-2.80	107.92	110.52
38	Y	607	CHL	C2C-C3C-C4C	2.80	108.49	106.49
30	B	619	BCR	C35-C13-C14	-2.80	119.00	122.92
39	y	315	LUT	C11-C10-C9	-2.80	123.31	127.31
28	R	603	CLA	C3B-C4B-NB	-2.80	107.92	110.52
28	R	604	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
28	y	314	CLA	CMA-C3A-C4A	2.80	119.29	111.77
38	g	601	CHL	C1-O2A-CGA	2.80	123.78	116.44
28	R	601	CLA	C1D-ND-C4D	-2.80	104.35	106.33
28	r	603	CLA	CMA-C3A-C4A	2.80	119.29	111.77
28	b	602	CLA	CMA-C3A-C4A	2.80	119.29	111.77
28	n	602	CLA	C1D-ND-C4D	-2.80	104.35	106.33
28	R	604	CLA	C2D-C1D-ND	2.80	112.16	110.10
28	C	506	CLA	CMA-C3A-C4A	2.79	119.28	111.77
28	N	613	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
28	r	608	CLA	CMA-C3A-C4A	2.79	119.28	111.77
28	S	311	CLA	C3B-C4B-NB	-2.79	107.92	110.52
28	C	512	CLA	C1D-ND-C4D	-2.79	104.35	106.33
28	b	608	CLA	C1D-ND-C4D	-2.79	104.35	106.33
28	n	603	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
39	r	614	LUT	C1-C6-C5	-2.79	118.68	122.61
38	s	607	CHL	C4B-CHC-C1C	2.79	132.96	126.34
39	Y	616	LUT	C30-C31-C32	-2.79	114.51	123.22
30	k	101	BCR	C20-C21-C22	-2.79	123.33	127.31
28	C	512	CLA	CMA-C3A-C4A	2.79	119.27	111.77
30	A	409	BCR	C4-C5-C6	-2.79	118.68	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	513	CLA	C1D-ND-C4D	-2.79	104.35	106.33
28	Y	611	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
28	A	408	CLA	C1D-ND-C4D	-2.79	104.36	106.33
28	B	616	CLA	C1D-ND-C4D	-2.79	104.36	106.33
28	C	501	CLA	C1D-ND-C4D	-2.79	104.36	106.33
38	g	605	CHL	C2C-C3C-C4C	2.79	108.47	106.49
28	G	604	CLA	C1D-ND-C4D	-2.79	104.36	106.33
38	g	619	CHL	C4D-CHA-C1A	2.79	124.64	121.25
39	Y	615	LUT	C31-C30-C29	-2.79	123.33	127.31
38	G	608	CHL	C2C-C3C-C4C	2.78	108.47	106.49
28	S	310	CLA	C1D-ND-C4D	-2.78	104.36	106.33
37	E	101	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
35	y	319	LHG	O8-C23-C24	2.78	120.64	111.91
28	c	513	CLA	CMA-C3A-C4A	2.78	119.25	111.77
28	y	312	CLA	CMA-C3A-C4A	2.78	119.25	111.77
39	g	615	LUT	C8-C7-C6	-2.78	119.39	127.20
35	b	622	LHG	O8-C23-C24	2.78	120.64	111.91
37	f	101	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
38	S	307	CHL	C4B-CHC-C1C	2.78	132.93	126.34
28	B	606	CLA	CMA-C3A-C4A	2.78	119.25	111.77
28	n	610	CLA	CMA-C3A-C4A	2.78	119.25	111.77
28	S	312	CLA	C3B-C4B-NB	-2.78	107.94	110.52
28	B	615	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	c	502	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	S	312	CLA	CHD-C1D-ND	-2.78	121.90	124.45
28	C	505	CLA	C2D-C1D-ND	2.78	112.15	110.10
38	s	606	CHL	C4D-CHA-C1A	2.78	124.63	121.25
28	g	613	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
28	s	604	CLA	C1D-ND-C4D	-2.78	104.36	106.33
38	S	307	CHL	C1-O2A-CGA	2.78	123.73	116.44
30	a	410	BCR	C23-C24-C25	-2.78	119.40	127.20
28	r	613	CLA	C1D-ND-C4D	-2.78	104.36	106.33
28	S	311	CLA	CHD-C1D-ND	-2.78	121.90	124.45
28	C	507	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
28	C	502	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
28	S	305	CLA	CHD-C1D-ND	-2.77	121.90	124.45
28	G	611	CLA	C1D-ND-C4D	-2.77	104.36	106.33
28	s	612	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
28	c	509	CLA	C3B-C4B-NB	-2.77	107.94	110.52
38	N	601	CHL	C3B-C4B-NB	-2.77	107.94	110.52
28	S	314	CLA	CMA-C3A-C4A	2.77	119.23	111.77
38	s	606	CHL	C3B-C4B-NB	-2.77	107.94	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	612	CLA	CMA-C3A-C4A	2.77	119.22	111.77
28	G	610	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
28	D	401	CLA	C1D-ND-C4D	-2.77	104.37	106.33
28	n	614	CLA	CMA-C3A-C4A	2.77	119.22	111.77
28	d	401	CLA	C1D-ND-C4D	-2.77	104.37	106.33
28	r	609	CLA	O1D-CGD-CBD	-2.77	118.82	124.48
28	G	603	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
39	s	615	LUT	C18-C5-C4	2.77	119.48	114.36
28	R	602	CLA	C6-C5-C3	-2.77	106.20	113.45
30	c	515	BCR	C38-C26-C27	2.77	118.93	113.62
28	B	608	CLA	C1D-ND-C4D	-2.77	104.37	106.33
28	Y	614	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
38	s	601	CHL	C4B-CHC-C1C	2.76	132.90	126.34
28	D	404	CLA	C1D-ND-C4D	-2.76	104.37	106.33
32	b	620	LMG	O8-C28-C29	2.76	120.58	111.91
28	s	611	CLA	CMA-C3A-C4A	2.76	119.20	111.77
28	R	601	CLA	CHD-C1D-ND	-2.76	121.91	124.45
28	b	606	CLA	C2C-C1C-NC	2.76	112.56	109.97
39	R	614	LUT	C2-C3-C4	2.76	114.09	110.30
28	G	612	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
28	N	610	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
28	S	310	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
32	A	411	LMG	O8-C28-C29	2.76	120.58	111.91
28	G	612	CLA	C1D-ND-C4D	-2.76	104.37	106.33
28	B	615	CLA	CMA-C3A-C4A	2.76	119.20	111.77
28	R	612	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
38	n	609	CHL	C3B-C4B-NB	-2.76	107.95	110.52
38	y	309	CHL	C4D-CHA-C1A	2.76	124.61	121.25
28	g	611	CLA	C1-O2A-CGA	2.76	123.69	116.44
38	g	608	CHL	C1-C2-C3	-2.76	121.27	126.04
28	n	604	CLA	CMA-C3A-C4A	2.76	119.19	111.77
38	s	605	CHL	C2B-C1B-NB	-2.76	108.38	110.23
28	r	612	CLA	C1D-ND-C4D	-2.76	104.38	106.33
38	G	605	CHL	C2C-C3C-C4C	2.76	108.45	106.49
28	n	613	CLA	CMA-C3A-C4A	2.76	119.19	111.77
28	a	407	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
39	n	616	LUT	C2-C3-C4	2.76	114.08	110.30
28	Y	614	CLA	C1D-ND-C4D	-2.76	104.38	106.33
38	n	601	CHL	C3B-C4B-NB	-2.76	107.96	110.52
28	A	405	CLA	CMA-C3A-C4A	2.76	119.18	111.77
28	B	612	CLA	C2C-C1C-NC	2.76	112.55	109.97
28	B	602	CLA	C1C-C2C-C3C	-2.76	104.06	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	k	101	BCR	C27-C26-C25	-2.76	118.73	122.73
39	y	316	LUT	C31-C30-C29	-2.75	123.38	127.31
28	s	602	CLA	CMA-C3A-C4A	2.75	119.18	111.77
28	Y	613	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
35	a	415	LHG	O8-C23-C24	2.75	120.55	111.91
38	y	302	CHL	C2C-C3C-C4C	2.75	108.45	106.49
30	C	516	BCR	C35-C13-C14	-2.75	119.07	122.92
28	b	615	CLA	C1D-ND-C4D	-2.75	104.38	106.33
28	r	612	CLA	C3B-C4B-NB	-2.75	107.96	110.52
28	y	311	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
38	R	607	CHL	C1-C2-C3	-2.75	121.28	126.04
30	b	618	BCR	C7-C8-C9	-2.75	122.08	126.23
30	C	516	BCR	C23-C24-C25	-2.75	119.47	127.20
38	S	308	CHL	CMA-C3A-C4A	2.75	119.17	111.77
38	g	605	CHL	C2B-C1B-NB	-2.75	108.39	110.23
28	c	507	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
28	r	604	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
28	b	613	CLA	C1D-ND-C4D	-2.75	104.38	106.33
38	g	608	CHL	C3B-C4B-NB	-2.75	107.96	110.52
28	g	614	CLA	CMA-C3A-C4A	2.75	119.17	111.77
28	N	610	CLA	CMA-C3A-C4A	2.75	119.17	111.77
38	g	606	CHL	C3C-C4C-NC	-2.75	107.49	110.57
30	i	101	BCR	C30-C25-C26	-2.75	118.74	122.61
28	b	613	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
38	G	605	CHL	C3B-C4B-NB	-2.75	107.97	110.52
28	A	406	CLA	C1D-ND-C4D	-2.75	104.38	106.33
28	c	501	CLA	C1D-ND-C4D	-2.75	104.38	106.33
38	N	609	CHL	C4B-CHC-C1C	2.75	132.85	126.34
28	b	606	CLA	C3B-C4B-NB	-2.75	107.97	110.52
38	g	609	CHL	C3B-C4B-NB	-2.75	107.97	110.52
38	y	309	CHL	C3B-C4B-NB	-2.75	107.97	110.52
28	B	611	CLA	C2C-C1C-NC	2.75	112.55	109.97
28	C	510	CLA	C1D-ND-C4D	-2.75	104.38	106.33
30	B	619	BCR	C33-C5-C4	2.75	118.89	113.62
28	g	603	CLA	O2A-CGA-CBA	2.75	120.52	111.91
39	s	614	LUT	C11-C12-C13	-2.75	118.70	126.42
38	y	309	CHL	C4B-CHC-C1C	2.75	132.85	126.34
28	c	504	CLA	C1D-ND-C4D	-2.74	104.39	106.33
40	s	616	NEX	O24-C25-C24	2.74	115.44	113.38
28	a	406	CLA	CMA-C3A-C4A	2.74	119.14	111.77
38	s	606	CHL	C4B-CHC-C1C	2.74	132.84	126.34
30	h	101	BCR	C38-C26-C27	2.74	118.88	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	612	CLA	C2D-C1D-ND	2.74	112.12	110.10
28	Y	603	CLA	C3B-C4B-NB	-2.74	107.97	110.52
38	Y	608	CHL	C3B-C4B-NB	-2.74	107.97	110.52
28	g	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
40	y	318	NEX	O24-C25-C24	-2.74	111.33	113.38
28	B	607	CLA	C1D-ND-C4D	-2.74	104.39	106.33
28	G	602	CLA	C1D-ND-C4D	-2.74	104.39	106.33
28	s	612	CLA	C1D-ND-C4D	-2.74	104.39	106.33
28	C	502	CLA	C1D-ND-C4D	-2.74	104.39	106.33
28	C	511	CLA	C1D-ND-C4D	-2.74	104.39	106.33
28	c	503	CLA	C3B-C4B-NB	-2.73	107.98	110.52
28	y	303	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	Y	610	CLA	C2C-C1C-NC	2.73	112.53	109.97
28	g	610	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	T	101	BCR	C8-C7-C6	-2.73	119.53	127.20
28	b	601	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	y	310	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
38	g	609	CHL	C1-C2-C3	-2.73	121.32	126.04
38	R	607	CHL	C3B-C4B-NB	-2.73	107.98	110.52
39	N	615	LUT	C18-C5-C4	2.73	119.42	114.36
30	c	514	BCR	C8-C7-C6	-2.73	119.53	127.20
28	a	407	CLA	CMA-C3A-C4A	2.73	119.11	111.77
38	G	608	CHL	C1-O2A-CGA	2.73	123.61	116.44
28	C	506	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
39	Y	615	LUT	C10-C11-C12	-2.73	114.70	123.22
28	R	603	CLA	C1D-ND-C4D	-2.73	104.40	106.33
28	Y	611	CLA	CMA-C3A-C4A	2.73	119.10	111.77
28	D	401	CLA	C1-C2-C3	-2.73	121.33	126.04
28	c	511	CLA	C1D-ND-C4D	-2.73	104.40	106.33
28	C	504	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
28	S	309	CLA	C2D-C1D-ND	2.73	112.11	110.10
28	d	401	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
28	S	312	CLA	C1D-ND-C4D	-2.73	104.40	106.33
28	b	612	CLA	C2C-C1C-NC	2.73	112.53	109.97
28	b	604	CLA	CHD-C1D-ND	-2.72	121.95	124.45
28	C	512	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
28	y	305	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
28	B	613	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
28	c	507	CLA	C1D-ND-C4D	-2.72	104.40	106.33
28	b	615	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
37	E	101	HEM	CHD-C4C-NC	2.72	127.38	124.44
38	n	605	CHL	C4D-CHA-C1A	2.72	124.56	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	510	CLA	CMA-C3A-C4A	2.72	119.09	111.77
28	y	305	CLA	C1D-ND-C4D	-2.72	104.40	106.33
38	S	308	CHL	C3B-C4B-NB	-2.72	107.99	110.52
28	B	606	CLA	C4B-CHC-C1C	2.72	132.79	126.34
28	c	502	CLA	C1D-ND-C4D	-2.72	104.40	106.33
38	G	607	CHL	C4B-CHC-C1C	2.72	132.79	126.34
38	n	605	CHL	C4B-CHC-C1C	2.72	132.79	126.34
39	S	315	LUT	C8-C7-C6	-2.72	119.56	127.20
28	d	404	CLA	CMA-C3A-C4A	2.72	119.08	111.77
38	g	605	CHL	CMA-C3A-C4A	2.72	119.08	111.77
28	D	401	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	a	409	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	b	614	CLA	C1D-ND-C4D	-2.72	104.41	106.33
28	S	309	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	s	610	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
41	r	615	XAT	C6-C7-C8	-2.72	120.25	125.99
28	D	403	CLA	CMA-C3A-C4A	2.71	119.07	111.77
28	D	403	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
28	S	313	CLA	C3B-C4B-NB	-2.71	108.00	110.52
28	n	604	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
28	b	616	CLA	CMA-C3A-C4A	2.71	119.07	111.77
28	d	401	CLA	C1-C2-C3	-2.71	121.35	126.04
32	A	413	LMG	C8-O7-C10	-2.71	111.11	117.79
28	s	602	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
28	R	608	CLA	C1D-ND-C4D	-2.71	104.41	106.33
28	S	305	CLA	O2A-CGA-CBA	2.71	120.42	111.91
28	C	513	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
28	S	313	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
28	C	504	CLA	C1D-ND-C4D	-2.71	104.41	106.33
28	r	612	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
28	Y	602	CLA	C6-C5-C3	-2.71	106.35	113.45
28	g	610	CLA	CHA-C1A-NA	-2.71	120.19	126.40
28	r	603	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
28	b	614	CLA	CMA-C3A-C4A	2.71	119.06	111.77
38	y	308	CHL	C1-C2-C3	-2.71	121.36	126.04
41	Y	617	XAT	C26-C27-C28	-2.71	120.27	125.99
28	b	606	CLA	C1-C2-C3	-2.71	121.36	126.04
28	G	613	CLA	C1D-ND-C4D	-2.71	104.41	106.33
28	R	602	CLA	C3B-C4B-NB	-2.71	108.00	110.52
28	y	304	CLA	C3B-C4B-NB	-2.71	108.00	110.52
28	Y	604	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
28	g	611	CLA	C1C-C2C-C3C	-2.71	104.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	612	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
35	N	618	LHG	C5-O7-C7	-2.71	111.13	117.79
28	c	501	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
38	N	609	CHL	C3B-C4B-NB	-2.70	108.01	110.52
41	R	615	XAT	C6-C7-C8	-2.70	120.28	125.99
28	C	505	CLA	C1D-ND-C4D	-2.70	104.41	106.33
28	B	604	CLA	CHD-C1D-ND	-2.70	121.97	124.45
38	G	609	CHL	C3B-C4B-NB	-2.70	108.01	110.52
38	g	605	CHL	C4B-CHC-C1C	2.70	132.75	126.34
35	c	519	LHG	O8-C23-C24	2.70	120.38	111.91
28	A	406	CLA	CMA-C3A-C4A	2.70	119.03	111.77
28	Y	603	CLA	C1D-ND-C4D	-2.70	104.42	106.33
28	c	508	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
28	C	503	CLA	C3B-C4B-NB	-2.70	108.01	110.52
38	g	605	CHL	C3B-C4B-NB	-2.70	108.01	110.52
28	B	601	CLA	C1D-ND-C4D	-2.69	104.42	106.33
28	G	604	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
28	b	605	CLA	C1-O2A-CGA	2.69	123.51	116.44
38	s	601	CHL	CMA-C3A-C4A	2.69	119.01	111.77
28	y	304	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
28	B	603	CLA	C2C-C1C-NC	2.69	112.49	109.97
28	R	604	CLA	CMA-C3A-C4A	2.69	119.01	111.77
28	s	610	CLA	C1D-ND-C4D	-2.69	104.42	106.33
28	B	610	CLA	C4B-CHC-C1C	2.69	132.72	126.34
28	r	603	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
38	R	605	CHL	C4B-CHC-C1C	2.69	132.72	126.34
28	c	512	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	S	313	CLA	C1D-ND-C4D	-2.69	104.42	106.33
39	R	614	LUT	C11-C12-C13	-2.69	118.86	126.42
28	B	601	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	D	404	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
39	G	615	LUT	C8-C7-C6	-2.69	119.66	127.20
28	b	602	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	d	405	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	c	502	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
38	y	306	CHL	C3B-C4B-NB	-2.69	108.02	110.52
41	y	317	XAT	C18-C5-C6	-2.68	117.76	122.26
28	g	603	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
28	r	610	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
28	Y	602	CLA	O2A-CGA-CBA	2.68	120.33	111.91
28	b	603	CLA	C1D-ND-C4D	-2.68	104.43	106.33
32	b	623	LMG	O8-C28-C29	2.68	120.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	N	605	CHL	C2C-C3C-C4C	2.68	108.40	106.49
28	N	614	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	c	515	BCR	C27-C26-C25	-2.68	118.83	122.73
30	C	515	BCR	C8-C7-C6	-2.68	119.67	127.20
28	B	614	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	C	510	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	s	611	CLA	C4B-CHC-C1C	2.68	132.70	126.34
40	G	617	NEX	C17-C1-C6	-2.68	108.07	110.47
28	a	409	CLA	C1D-ND-C4D	-2.68	104.43	106.33
28	n	614	CLA	C1D-ND-C4D	-2.68	104.43	106.33
32	B	624	LMG	O8-C28-C29	2.68	120.32	111.91
28	G	604	CLA	CMA-C3A-C4A	2.68	118.98	111.77
28	s	609	CLA	C3B-C4B-NB	-2.68	108.03	110.52
28	N	603	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	A	408	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	c	510	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	C	509	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	n	613	CLA	O2A-CGA-CBA	2.68	120.31	111.91
28	b	604	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	g	602	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
28	R	611	CLA	C4B-CHC-C1C	2.68	132.69	126.34
28	S	314	CLA	C1D-ND-C4D	-2.68	104.43	106.33
28	y	313	CLA	C3B-C4B-NB	-2.68	108.03	110.52
28	B	615	CLA	C4B-CHC-C1C	2.68	132.69	126.34
28	B	609	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
38	r	605	CHL	C1-C2-C3	-2.68	121.42	126.04
28	c	509	CLA	O2A-CGA-CBA	2.67	120.30	111.91
30	i	101	BCR	C33-C5-C4	2.67	118.75	113.62
28	b	609	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
28	N	612	CLA	C1D-ND-C4D	-2.67	104.44	106.33
28	b	601	CLA	C1D-ND-C4D	-2.67	104.44	106.33
28	s	609	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	N	611	CLA	C1D-ND-C4D	-2.67	104.44	106.33
30	T	101	BCR	C15-C16-C17	-2.67	118.00	123.47
28	r	609	CLA	C3B-C4B-NB	-2.67	108.04	110.52
39	S	316	LUT	C1-C6-C5	-2.67	118.85	122.61
38	Y	601	CHL	C4B-CHC-C1C	2.67	132.67	126.34
28	S	314	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	G	612	CLA	C3B-C4B-NB	-2.67	108.04	110.52
28	C	510	CLA	CMA-C3A-C4A	2.67	118.95	111.77
35	B	623	LHG	O8-C23-C24	2.67	120.28	111.91
39	n	616	LUT	C4-C5-C6	-2.67	114.90	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	G	617	NEX	C5-C4-C3	-2.67	108.59	111.75
28	S	303	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	B	613	CLA	CMA-C3A-C4A	2.67	118.94	111.77
28	r	604	CLA	C1D-ND-C4D	-2.67	104.44	106.33
28	b	607	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	B	606	CLA	C2C-C1C-NC	2.67	112.47	109.97
28	b	606	CLA	CMA-C3A-C4A	2.67	118.94	111.77
40	Y	618	NEX	C39-C29-C30	-2.66	119.19	122.92
38	n	605	CHL	C3B-C4B-NB	-2.66	108.04	110.52
28	y	313	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
38	y	308	CHL	C1-O2A-CGA	2.66	123.43	116.44
38	y	302	CHL	CMA-C3A-C4A	2.66	118.93	111.77
28	c	512	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
35	b	621	LHG	O8-C23-C24	2.66	120.27	111.91
28	y	313	CLA	C1D-ND-C4D	-2.66	104.44	106.33
38	n	609	CHL	C4B-CHC-C1C	2.66	132.65	126.34
28	Y	610	CLA	O2A-CGA-CBA	2.66	120.26	111.91
28	C	502	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
28	S	312	CLA	O2A-CGA-CBA	2.66	120.25	111.91
41	Y	617	XAT	C39-C29-C30	-2.66	119.20	122.92
28	N	612	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
28	c	504	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
38	n	609	CHL	C4D-CHA-C1A	2.66	124.48	121.25
28	S	312	CLA	C4B-CHC-C1C	2.66	132.64	126.34
28	Y	603	CLA	C4B-CHC-C1C	2.66	132.64	126.34
28	d	404	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
40	y	301	NEX	C38-C25-C26	-2.66	117.81	122.26
28	r	608	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
28	r	601	CLA	C4B-CHC-C1C	2.65	132.63	126.34
28	R	611	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	c	513	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	b	601	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
28	c	505	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	s	613	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	b	608	CLA	C3B-C4B-NB	-2.65	108.06	110.52
39	N	616	LUT	C38-C25-C24	-2.65	117.89	123.56
38	G	606	CHL	C3C-C4C-NC	-2.65	107.60	110.57
28	c	512	CLA	C1D-ND-C4D	-2.65	104.45	106.33
28	A	406	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	b	610	CLA	C4B-CHC-C1C	2.65	132.62	126.34
39	n	616	LUT	C31-C30-C29	-2.65	123.53	127.31
28	n	614	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	g	618	LHG	C5-O7-C7	-2.65	111.27	117.79
28	y	312	CLA	C4B-CHC-C1C	2.65	132.62	126.34
28	S	311	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
41	Y	617	XAT	C18-C5-C6	-2.65	117.82	122.26
28	n	611	CLA	CMA-C3A-C4A	2.65	118.89	111.77
30	b	618	BCR	C30-C25-C26	-2.65	118.89	122.61
28	b	612	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
28	b	615	CLA	CMA-C3A-C4A	2.65	118.89	111.77
28	G	602	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
32	C	520	LMG	O8-C28-C29	2.64	120.21	111.91
35	r	617	LHG	O8-C23-C24	2.64	120.20	111.91
28	c	513	CLA	C1D-ND-C4D	-2.64	104.46	106.33
38	S	307	CHL	C1-C2-C3	-2.64	121.47	126.04
28	R	601	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	Y	612	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	B	610	CLA	CMA-C3A-C4A	2.64	118.87	111.77
28	B	607	CLA	C3B-C4B-NB	-2.64	108.06	110.52
28	b	614	CLA	C3B-C4B-NB	-2.64	108.06	110.52
28	G	610	CLA	C3B-C4B-NB	-2.64	108.06	110.52
28	s	604	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
40	s	616	NEX	C39-C29-C30	-2.64	119.22	122.92
28	c	505	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
28	s	602	CLA	C4B-CHC-C1C	2.64	132.60	126.34
36	c	518	DGD	O1G-C1A-C2A	2.64	120.19	111.91
39	g	615	LUT	C1-C6-C5	-2.64	118.90	122.61
28	y	304	CLA	C4B-CHC-C1C	2.64	132.59	126.34
40	s	616	NEX	O24-C25-C38	-2.64	111.90	115.06
28	N	602	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
28	R	601	CLA	C4B-CHC-C1C	2.64	132.59	126.34
28	y	305	CLA	CMA-C3A-C4A	2.64	118.86	111.77
38	G	607	CHL	C1-O2A-CGA	2.64	123.36	116.44
28	g	612	CLA	C1D-ND-C4D	-2.64	104.46	106.33
39	Y	616	LUT	C15-C14-C13	-2.63	123.55	127.31
40	r	616	NEX	C26-C27-C28	-2.63	120.42	125.99
35	W	101	LHG	C5-O7-C7	-2.63	111.31	117.79
28	Y	603	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	S	304	CLA	C4B-CHC-C1C	2.63	132.58	126.34
28	b	605	CLA	C2C-C1C-NC	2.63	112.44	109.97
38	n	606	CHL	C3B-C4B-NB	-2.63	108.07	110.52
28	r	609	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
30	b	617	BCR	C23-C24-C25	-2.63	119.81	127.20
28	C	506	CLA	C1D-ND-C4D	-2.63	104.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	y	310	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
28	C	511	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	N	603	CLA	CMA-C3A-C4A	2.63	118.85	111.77
28	b	613	CLA	CMA-C3A-C4A	2.63	118.85	111.77
41	y	317	XAT	C26-C27-C28	-2.63	120.43	125.99
28	c	511	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	N	603	CLA	C1D-ND-C4D	-2.63	104.47	106.33
35	g	618	LHG	O8-C23-C24	2.63	120.16	111.91
28	R	604	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
28	s	608	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	y	311	CLA	C1D-ND-C4D	-2.63	104.47	106.33
28	y	314	CLA	C3B-C4B-NB	-2.63	108.08	110.52
38	Y	605	CHL	C2C-C3C-C4C	2.63	108.36	106.49
30	D	405	BCR	C20-C19-C18	-2.63	119.04	126.42
28	Y	613	CLA	C1D-ND-C4D	-2.63	104.47	106.33
39	r	614	LUT	C31-C32-C33	-2.63	119.04	126.42
38	g	605	CHL	C4D-CHA-C1A	2.63	124.44	121.25
28	n	602	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
28	n	603	CLA	C4B-CHC-C1C	2.63	132.56	126.34
28	G	612	CLA	C4B-CHC-C1C	2.62	132.56	126.34
30	t	101	BCR	C15-C16-C17	-2.62	118.10	123.47
28	B	602	CLA	C3B-C4B-NB	-2.62	108.08	110.52
28	B	614	CLA	C3B-C4B-NB	-2.62	108.08	110.52
28	S	304	CLA	C3B-C4B-NB	-2.62	108.08	110.52
28	c	501	CLA	C4B-CHC-C1C	2.62	132.56	126.34
28	r	604	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
28	B	607	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	G	614	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	N	604	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	r	608	CLA	C3B-C4B-NB	-2.62	108.08	110.52
28	Y	603	CLA	CMA-C3A-C4A	2.62	118.82	111.77
28	b	616	CLA	C1-C2-C3	-2.62	121.51	126.04
28	r	610	CLA	C4B-CHC-C1C	2.62	132.56	126.34
28	S	312	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	r	602	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
40	y	301	NEX	C16-C1-C6	-2.62	108.13	110.47
30	b	619	BCR	C21-C20-C19	-2.62	115.04	123.22
28	B	614	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
40	Y	618	NEX	C38-C25-C26	-2.62	117.87	122.26
38	G	601	CHL	CMA-C3A-C4A	2.62	118.81	111.77
30	b	619	BCR	C31-C1-C6	-2.62	106.05	110.30
40	y	301	NEX	C39-C29-C30	-2.62	119.25	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	613	CLA	C4B-CHC-C1C	2.62	132.55	126.34
28	S	305	CLA	C2D-C1D-ND	2.62	112.03	110.10
28	N	611	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	G	611	CLA	CHD-C1D-ND	-2.62	122.05	124.45
28	Y	602	CLA	CMC-C2C-C1C	2.62	129.02	125.04
28	R	612	CLA	C3B-C4B-NB	-2.62	108.09	110.52
28	r	613	CLA	C4B-CHC-C1C	2.61	132.54	126.34
28	C	501	CLA	C4B-CHC-C1C	2.61	132.54	126.34
28	Y	613	CLA	C3B-C4B-NB	-2.61	108.09	110.52
28	s	603	CLA	CHD-C1D-ND	-2.61	122.05	124.45
30	a	410	BCR	C8-C7-C6	-2.61	119.86	127.20
38	s	601	CHL	C2C-C3C-C4C	2.61	108.35	106.49
28	C	501	CLA	C1-C2-C3	-2.61	121.53	126.04
35	c	520	LHG	O8-C23-C24	2.61	120.10	111.91
38	N	607	CHL	C1-O2A-CGA	2.61	123.29	116.44
38	r	606	CHL	C2C-C3C-C4C	2.61	108.35	106.49
28	c	508	CLA	CMA-C3A-C4A	2.61	118.79	111.77
41	R	615	XAT	C26-C27-C28	-2.61	120.48	125.99
28	N	611	CLA	C1-C2-C3	-2.61	121.53	126.04
28	B	614	CLA	C1D-ND-C4D	-2.61	104.48	106.33
28	S	309	CLA	C1D-ND-C4D	-2.61	104.48	106.33
28	n	610	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
38	g	607	CHL	C4B-CHC-C1C	2.60	132.51	126.34
36	b	625	DGD	O1G-C1A-C2A	2.60	120.08	111.91
28	y	312	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
28	N	613	CLA	C1D-ND-C4D	-2.60	104.49	106.33
28	c	503	CLA	C1D-ND-C4D	-2.60	104.49	106.33
28	c	504	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
28	r	601	CLA	C2D-C1D-ND	2.60	112.02	110.10
28	c	506	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
28	s	611	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
35	B	622	LHG	O8-C23-C24	2.60	120.07	111.91
28	d	405	CLA	C3B-C4B-NB	-2.60	108.10	110.52
38	R	607	CHL	CMA-C3A-C4A	2.60	118.76	111.77
28	y	311	CLA	C4B-CHC-C1C	2.60	132.50	126.34
28	n	612	CLA	C4B-CHC-C1C	2.60	132.50	126.34
40	n	617	NEX	C39-C29-C30	-2.60	119.28	122.92
28	B	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
28	B	608	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
39	S	315	LUT	C35-C15-C14	-2.60	118.15	123.47
28	b	609	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
28	b	604	CLA	O2D-CGD-O1D	-2.60	118.76	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	515	BCR	C23-C24-C25	-2.60	119.91	127.20
28	b	603	CLA	O2A-CGA-CBA	2.60	120.06	111.91
35	s	617	LHG	O8-C23-C24	2.60	120.06	111.91
28	B	610	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
28	C	507	CLA	C1D-ND-C4D	-2.60	104.49	106.33
28	R	602	CLA	C4B-CHC-C1C	2.60	132.49	126.34
28	N	604	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
39	n	616	LUT	C15-C35-C34	-2.60	118.16	123.47
28	b	601	CLA	C4B-CHC-C1C	2.60	132.49	126.34
30	H	101	BCR	C23-C24-C25	-2.59	119.91	127.20
28	C	505	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
28	n	614	CLA	C3B-C4B-NB	-2.59	108.11	110.52
28	R	604	CLA	C4B-CHC-C1C	2.59	132.49	126.34
28	c	503	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
28	B	614	CLA	CMA-C3A-C4A	2.59	118.75	111.77
28	G	610	CLA	C4B-CHC-C1C	2.59	132.49	126.34
28	G	614	CLA	C4B-CHC-C1C	2.59	132.49	126.34
28	r	609	CLA	C4B-CHC-C1C	2.59	132.49	126.34
28	N	604	CLA	C1D-ND-C4D	-2.59	104.49	106.33
28	B	612	CLA	C3B-C4B-NB	-2.59	108.11	110.52
28	R	608	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
28	g	613	CLA	O2A-CGA-CBA	2.59	120.04	111.91
39	s	615	LUT	C11-C12-C13	-2.59	119.14	126.42
28	G	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
28	b	612	CLA	C3B-C4B-NB	-2.59	108.11	110.52
30	a	410	BCR	C15-C16-C17	-2.59	118.17	123.47
28	C	508	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
28	S	305	CLA	CHA-C4D-ND	2.59	137.91	132.50
30	C	515	BCR	C33-C5-C4	2.59	118.59	113.62
28	R	610	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
38	n	607	CHL	C4B-CHC-C1C	2.59	132.48	126.34
41	r	615	XAT	C26-C27-C28	-2.59	120.52	125.99
28	b	614	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
28	C	504	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
28	s	603	CLA	CHA-C4D-ND	2.59	137.91	132.50
28	c	513	CLA	C3B-C4B-NB	-2.58	108.12	110.52
28	n	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	D	404	CLA	C3B-C4B-NB	-2.58	108.12	110.52
38	n	607	CHL	C4D-CHA-C1A	2.58	124.39	121.25
39	n	615	LUT	C19-C9-C10	-2.58	119.31	122.92
28	c	510	CLA	C3B-C4B-NB	-2.58	108.12	110.52
39	y	315	LUT	C30-C31-C32	-2.58	115.16	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	609	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	G	614	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	N	614	CLA	C3B-C4B-NB	-2.58	108.12	110.52
28	n	612	CLA	CMD-C2D-C3D	-2.58	121.68	127.61
28	B	608	CLA	C3B-C4B-NB	-2.58	108.12	110.52
28	R	603	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
28	g	611	CLA	CMA-C3A-C4A	2.58	118.70	111.77
28	n	604	CLA	C3B-C4B-NB	-2.58	108.12	110.52
30	B	618	BCR	C24-C23-C22	-2.58	122.34	126.23
30	C	514	BCR	C16-C15-C14	2.58	128.75	123.47
28	r	613	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
30	C	514	BCR	C15-C16-C17	2.58	128.75	123.47
28	c	503	CLA	C1-C2-C3	-2.58	121.59	126.04
28	b	612	CLA	C6-C5-C3	-2.58	106.70	113.45
28	C	503	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
38	y	306	CHL	C2C-C3C-C4C	2.57	108.32	106.49
28	C	501	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
28	B	605	CLA	C3B-C4B-NB	-2.57	108.13	110.52
28	S	305	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
38	y	302	CHL	C4A-NA-C1A	2.57	107.86	106.71
28	c	505	CLA	C1D-ND-C4D	-2.57	104.51	106.33
28	b	612	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
28	N	611	CLA	C4B-CHC-C1C	2.57	132.44	126.34
30	D	405	BCR	C8-C7-C6	-2.57	119.98	127.20
35	W	101	LHG	O8-C23-C24	2.57	119.98	111.91
28	A	406	CLA	C3B-C4B-NB	-2.57	108.13	110.52
28	y	305	CLA	C3B-C4B-NB	-2.57	108.13	110.52
39	n	615	LUT	C15-C14-C13	-2.57	123.64	127.31
28	G	611	CLA	C4B-CHC-C1C	2.57	132.44	126.34
28	s	610	CLA	C1-C2-C3	-2.57	121.60	126.04
28	G	613	CLA	O2A-CGA-CBA	2.57	119.97	111.91
28	g	603	CLA	C6-C5-C3	-2.57	106.72	113.45
28	Y	604	CLA	CMA-C3A-C4A	2.57	118.68	111.77
28	g	614	CLA	CHA-C4D-ND	2.57	137.87	132.50
28	S	311	CLA	C4B-CHC-C1C	2.57	132.43	126.34
38	Y	601	CHL	C2B-C1B-NB	-2.57	108.51	110.23
28	b	608	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
28	C	505	CLA	C3B-C4B-NB	-2.57	108.13	110.52
28	b	607	CLA	C1D-ND-C4D	-2.57	104.51	106.33
28	y	314	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
28	Y	610	CLA	C4B-CHC-C1C	2.57	132.42	126.34
28	y	310	CLA	C4B-CHC-C1C	2.57	132.42	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	R	606	CHL	CHC-C1C-NC	2.57	128.09	124.20
28	C	507	CLA	C4B-CHC-C1C	2.57	132.42	126.34
28	g	614	CLA	CMD-C2D-C3D	-2.56	121.72	127.61
28	R	609	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
28	C	512	CLA	C3B-C4B-NB	-2.56	108.14	110.52
39	N	615	LUT	C21-C26-C27	-2.56	109.46	112.70
30	T	101	BCR	C20-C19-C18	-2.56	119.22	126.42
28	R	603	CLA	C4B-CHC-C1C	2.56	132.41	126.34
28	g	614	CLA	C3B-C4B-NB	-2.56	108.14	110.52
28	B	612	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
28	C	513	CLA	C3B-C4B-NB	-2.56	108.14	110.52
38	S	308	CHL	CHC-C1C-NC	2.56	128.08	124.20
30	C	514	BCR	C38-C26-C27	2.56	118.53	113.62
40	y	318	NEX	O24-C25-C38	-2.56	111.99	115.06
28	y	303	CLA	C3B-C4B-NB	-2.56	108.14	110.52
28	b	606	CLA	CHA-C4D-ND	2.55	137.84	132.50
39	Y	615	LUT	C15-C35-C34	-2.55	118.24	123.47
28	s	610	CLA	C4B-CHC-C1C	2.55	132.40	126.34
30	D	405	BCR	C23-C24-C25	-2.55	120.03	127.20
28	g	612	CLA	CHA-C4D-ND	2.55	137.84	132.50
30	C	516	BCR	C34-C9-C10	-2.55	119.35	122.92
35	d	408	LHG	O8-C23-C24	2.55	119.92	111.91
28	C	511	CLA	C3B-C4B-NB	-2.55	108.15	110.52
38	S	302	CHL	C2C-C3C-C4C	2.55	108.31	106.49
28	b	605	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
38	y	302	CHL	C2B-C1B-NB	-2.55	108.52	110.23
35	Y	619	LHG	O8-C23-C24	2.55	119.91	111.91
28	G	613	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	y	310	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	b	603	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
28	N	602	CLA	C4B-CHC-C1C	2.55	132.39	126.34
28	N	611	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
28	s	609	CLA	C4B-CHC-C1C	2.55	132.38	126.34
28	S	304	CLA	C1D-ND-C4D	-2.55	104.52	106.33
28	b	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	R	604	CLA	O2A-CGA-CBA	2.55	119.91	111.91
28	c	513	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
28	b	611	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
28	r	602	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	N	613	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	b	602	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	N	615	LUT	C1-C6-C5	-2.55	119.03	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	615	LUT	C31-C32-C33	-2.55	119.26	126.42
38	R	605	CHL	C2C-C3C-C4C	2.55	108.30	106.49
30	B	618	BCR	C16-C15-C14	-2.55	118.26	123.47
28	S	305	CLA	C1-O2A-CGA	2.55	123.12	116.44
28	G	602	CLA	C4B-CHC-C1C	2.55	132.38	126.34
28	b	604	CLA	C1D-ND-C4D	-2.55	104.53	106.33
28	C	508	CLA	C3B-C4B-NB	-2.54	108.15	110.52
28	g	610	CLA	C6-C5-C3	-2.54	106.78	113.45
28	y	305	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
28	n	603	CLA	O2A-CGA-CBA	2.54	119.89	111.91
28	C	505	CLA	CHA-C4D-ND	2.54	137.82	132.50
28	R	608	CLA	CMA-C3A-C4A	2.54	118.61	111.77
28	r	603	CLA	CHA-C4D-ND	2.54	137.82	132.50
28	n	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
28	R	602	CLA	O2A-CGA-CBA	2.54	119.88	111.91
28	g	611	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	R	603	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
28	g	614	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
28	C	504	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	Y	615	LUT	C4-C5-C6	-2.54	115.19	120.85
28	B	604	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
28	R	610	CLA	C4B-CHC-C1C	2.54	132.36	126.34
39	r	614	LUT	C39-C29-C30	-2.54	119.37	122.92
28	S	303	CLA	C4B-CHC-C1C	2.54	132.36	126.34
30	A	409	BCR	C23-C24-C25	-2.54	120.07	127.20
40	g	617	NEX	O24-C25-C24	-2.54	111.48	113.38
28	n	603	CLA	CHA-C4D-ND	2.54	137.81	132.50
28	b	610	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
28	c	505	CLA	CHA-C4D-ND	2.54	137.80	132.50
38	g	601	CHL	C2B-C1B-NB	-2.54	108.53	110.23
32	C	520	LMG	C8-O7-C10	-2.54	111.55	117.79
38	g	607	CHL	CHB-C4A-NA	2.54	128.02	124.51
35	G	618	LHG	O8-C23-C24	2.53	119.86	111.91
38	n	601	CHL	C1-O2A-CGA	2.53	123.09	116.44
35	D	407	LHG	O8-C23-C24	2.53	119.86	111.91
38	g	605	CHL	C4A-NA-C1A	2.53	107.84	106.71
28	C	512	CLA	C1-C2-C3	-2.53	121.66	126.04
28	B	607	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
28	y	311	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
28	B	604	CLA	C1D-ND-C4D	-2.53	104.54	106.33
28	b	607	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	C	510	CLA	C3B-C4B-NB	-2.53	108.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	g	601	CHL	C1-C2-C3	-2.53	121.67	126.04
28	g	612	CLA	CMA-C3A-C4A	2.53	118.57	111.77
28	s	612	CLA	C3B-C4B-NB	-2.53	108.17	110.52
28	B	603	CLA	C4B-CHC-C1C	2.53	132.33	126.34
28	b	616	CLA	C1D-ND-C4D	-2.53	104.54	106.33
28	b	604	CLA	CHA-C4D-ND	2.53	137.78	132.50
28	n	610	CLA	C4B-CHC-C1C	2.53	132.33	126.34
28	B	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
28	s	604	CLA	C3B-C4B-NB	-2.53	108.17	110.52
38	n	607	CHL	C3B-C4B-NB	-2.52	108.17	110.52
28	Y	610	CLA	CMA-C3A-C4A	2.52	118.56	111.77
28	R	603	CLA	C1-C2-C3	-2.52	121.68	126.04
28	b	614	CLA	CHA-C4D-ND	2.52	137.78	132.50
28	n	613	CLA	C4B-CHC-C1C	2.52	132.32	126.34
30	B	617	BCR	C16-C15-C14	-2.52	118.31	123.47
28	g	613	CLA	C1D-ND-C4D	-2.52	104.54	106.33
28	B	611	CLA	C3B-C4B-NB	-2.52	108.17	110.52
28	g	612	CLA	C3B-C4B-NB	-2.52	108.17	110.52
40	g	617	NEX	C40-C33-C34	-2.52	119.39	122.92
40	y	318	NEX	C16-C1-C6	-2.52	108.22	110.47
28	c	509	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
38	s	606	CHL	CHB-C4A-NA	2.52	128.00	124.51
39	n	615	LUT	C38-C25-C24	-2.52	118.17	123.56
28	s	603	CLA	C1D-ND-C4D	-2.52	104.55	106.33
28	C	509	CLA	C4B-CHC-C1C	2.52	132.31	126.34
28	C	505	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
28	g	613	CLA	C3B-C4B-NB	-2.52	108.18	110.52
28	B	604	CLA	CHA-C4D-ND	2.52	137.77	132.50
28	R	609	CLA	C3B-C4B-NB	-2.52	108.18	110.52
28	G	603	CLA	C1D-ND-C4D	-2.52	104.55	106.33
38	n	608	CHL	C1-C2-C3	-2.52	121.69	126.04
38	y	302	CHL	C1-O2A-CGA	2.52	123.05	116.44
28	B	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
36	B	626	DGD	O1G-C1A-C2A	2.52	119.80	111.91
35	L	102	LHG	O8-C23-C24	2.52	119.80	111.91
28	r	604	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	A	405	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
38	y	306	CHL	CMA-C3A-C4A	2.51	118.53	111.77
28	r	610	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
38	Y	608	CHL	CHD-C4C-C3C	2.51	128.53	124.84
28	c	507	CLA	C4B-CHC-C1C	2.51	132.30	126.34
28	R	609	CLA	CMD-C2D-C3D	-2.51	121.83	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	S	306	CHL	C2B-C1B-NB	-2.51	108.55	110.23
28	s	603	CLA	C4B-CHC-C1C	2.51	132.29	126.34
41	R	615	XAT	C18-C5-C6	-2.51	118.05	122.26
28	S	311	CLA	O2A-CGA-CBA	2.51	119.79	111.91
28	R	613	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
38	G	605	CHL	CMA-C3A-C4A	2.51	118.52	111.77
28	B	615	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
35	B	622	LHG	C5-O7-C7	-2.51	111.61	117.79
28	G	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
28	Y	614	CLA	C3B-C4B-NB	-2.51	108.19	110.52
28	s	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
28	c	501	CLA	C1-C2-C3	-2.51	121.70	126.04
28	B	603	CLA	C1-C2-C3	-2.51	121.71	126.04
28	Y	602	CLA	CHD-C1D-ND	-2.51	122.15	124.45
30	b	619	BCR	C33-C5-C4	2.51	118.43	113.62
28	r	612	CLA	C4B-CHC-C1C	2.51	132.28	126.34
35	S	317	LHG	O8-C23-C24	2.51	119.77	111.91
35	w	102	LHG	O8-C23-C24	2.51	119.77	111.91
28	N	610	CLA	C4B-CHC-C1C	2.51	132.28	126.34
28	Y	614	CLA	CMD-C2D-C3D	-2.51	121.85	127.61
28	b	601	CLA	CHA-C4D-ND	2.51	137.74	132.50
41	r	615	XAT	C18-C5-C6	-2.51	118.06	122.26
28	B	610	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	N	604	CLA	CHA-C4D-ND	2.50	137.74	132.50
38	N	605	CHL	CMA-C3A-C4A	2.50	118.50	111.77
28	n	613	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
38	n	601	CHL	CHB-C4A-NA	2.50	127.97	124.51
28	B	605	CLA	C4B-CHC-C1C	2.50	132.28	126.34
28	c	511	CLA	C3B-C4B-NB	-2.50	108.19	110.52
39	g	615	LUT	C18-C5-C4	2.50	118.99	114.36
40	N	617	NEX	C39-C29-C30	-2.50	119.42	122.92
38	y	302	CHL	C1-C2-C3	-2.50	121.72	126.04
28	c	503	CLA	CHA-C4D-ND	2.50	137.73	132.50
28	b	605	CLA	C2B-C1B-NB	-2.50	108.56	110.23
40	y	318	NEX	C40-C33-C34	-2.50	119.42	122.92
28	C	508	CLA	C4B-CHC-C1C	2.50	132.27	126.34
28	B	601	CLA	C4B-CHC-C1C	2.50	132.26	126.34
38	Y	607	CHL	C4D-CHA-C1A	2.50	124.29	121.25
28	b	615	CLA	C3B-C4B-NB	-2.50	108.20	110.52
28	s	613	CLA	C3B-C4B-NB	-2.50	108.20	110.52
28	B	607	CLA	CHA-C4D-ND	2.50	137.72	132.50
38	n	605	CHL	C2B-C1B-NB	-2.50	108.56	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	n	607	CHL	CHB-C4A-NA	2.50	127.96	124.51
28	Y	611	CLA	C3B-C4B-NB	-2.50	108.20	110.52
28	n	602	CLA	C4B-CHC-C1C	2.50	132.26	126.34
28	b	613	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
28	B	614	CLA	CHA-C4D-ND	2.49	137.72	132.50
28	b	606	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
28	Y	611	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
28	r	603	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
32	D	408	LMG	O8-C28-C29	2.49	119.73	111.91
28	s	604	CLA	CMA-C3A-C4A	2.49	118.47	111.77
28	R	609	CLA	C4B-CHC-C1C	2.49	132.25	126.34
39	s	614	LUT	C8-C7-C6	-2.49	120.20	127.20
28	c	512	CLA	C3B-C4B-NB	-2.49	108.20	110.52
30	c	515	BCR	C23-C24-C25	-2.49	120.21	127.20
28	N	612	CLA	CHA-C4D-ND	2.49	137.71	132.50
28	s	603	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
35	B	625	LHG	O8-C23-C24	2.49	119.72	111.91
30	B	617	BCR	C23-C24-C25	-2.49	120.21	127.20
28	s	612	CLA	C1-C2-C3	-2.49	121.74	126.04
28	r	601	CLA	CHA-C4D-ND	2.49	137.71	132.50
38	Y	607	CHL	CHD-C4C-C3C	2.49	128.50	124.84
30	b	618	BCR	C29-C30-C25	2.49	114.31	110.48
28	Y	613	CLA	C1-C2-C3	-2.49	121.74	126.04
28	B	606	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
28	c	513	CLA	CHA-C4D-ND	2.49	137.70	132.50
28	N	602	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	c	506	CLA	C3B-C4B-NB	-2.49	108.21	110.52
39	R	614	LUT	C35-C15-C14	-2.49	118.38	123.47
28	B	603	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
28	S	305	CLA	CAC-C3C-C4C	2.49	128.04	124.81
28	B	616	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	B	601	CLA	CHA-C4D-ND	2.49	137.70	132.50
28	b	611	CLA	C4B-CHC-C1C	2.49	132.23	126.34
39	y	315	LUT	C31-C30-C29	-2.49	123.76	127.31
28	R	608	CLA	C4B-CHC-C1C	2.48	132.23	126.34
28	G	610	CLA	O2A-CGA-CBA	2.48	119.70	111.91
28	b	615	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
28	N	610	CLA	C3B-C4B-NB	-2.48	108.21	110.52
28	S	312	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	b	609	CLA	C4B-CHC-C1C	2.48	132.23	126.34
28	y	303	CLA	C4B-CHC-C1C	2.48	132.23	126.34
37	E	101	HEM	C4D-ND-C1D	2.48	107.64	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	N	615	LUT	C11-C10-C9	-2.48	123.77	127.31
28	N	611	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	c	511	CLA	C4B-CHC-C1C	2.48	132.23	126.34
28	A	405	CLA	C1-C2-C3	-2.48	121.75	126.04
28	B	602	CLA	C4B-CHC-C1C	2.48	132.22	126.34
28	b	605	CLA	CMA-C3A-C4A	2.48	118.44	111.77
28	c	511	CLA	O2A-CGA-CBA	2.48	119.69	111.91
38	Y	605	CHL	C2B-C1B-NB	-2.48	108.57	110.23
38	R	605	CHL	CMA-C3A-C2A	2.48	123.83	113.83
38	N	601	CHL	CHD-C4C-C3C	2.48	128.49	124.84
38	n	608	CHL	CHD-C4C-C3C	2.48	128.49	124.84
28	g	602	CLA	C4B-CHC-C1C	2.48	132.22	126.34
28	D	401	CLA	C3B-C4B-NB	-2.48	108.21	110.52
28	d	404	CLA	C3B-C4B-NB	-2.48	108.21	110.52
28	g	604	CLA	CHA-C4D-ND	2.48	137.69	132.50
30	h	101	BCR	C23-C24-C25	-2.48	120.24	127.20
28	b	609	CLA	C3B-C4B-NB	-2.48	108.22	110.52
28	n	602	CLA	C3B-C4B-NB	-2.48	108.22	110.52
28	D	404	CLA	O2A-CGA-CBA	2.48	119.69	111.91
38	n	601	CHL	CHD-C4C-C3C	2.48	128.48	124.84
28	b	611	CLA	C3B-C4B-NB	-2.48	108.22	110.52
28	b	605	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	c	504	CLA	C4B-CHC-C1C	2.48	132.21	126.34
28	Y	604	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	r	609	CLA	O2A-CGA-CBA	2.48	119.68	111.91
28	Y	603	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	n	614	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	y	304	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	r	602	CLA	C4B-CHC-C1C	2.47	132.21	126.34
28	s	608	CLA	C4B-CHC-C1C	2.47	132.21	126.34
28	b	607	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
28	Y	612	CLA	C4B-CHC-C1C	2.47	132.21	126.34
28	s	604	CLA	CHA-C4D-ND	2.47	137.68	132.50
28	b	606	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
28	A	405	CLA	C3B-C4B-NB	-2.47	108.22	110.52
28	S	310	CLA	C4B-CHC-C1C	2.47	132.21	126.34
39	r	614	LUT	C2-C3-C4	2.47	113.69	110.30
28	B	609	CLA	CMA-C3A-C4A	2.47	118.42	111.77
28	S	314	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
28	N	611	CLA	O2A-CGA-CBA	2.47	119.67	111.91
38	G	601	CHL	C1-O2A-CGA	2.47	122.93	116.44
35	D	407	LHG	C5-O7-C7	-2.47	111.70	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	406	CLA	C4B-CHC-C1C	2.47	132.20	126.34
28	s	613	CLA	C4B-CHC-C1C	2.47	132.20	126.34
28	Y	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52
28	s	603	CLA	C3B-C4B-NB	-2.47	108.22	110.52
30	b	617	BCR	C2-C1-C6	2.47	114.29	110.48
36	c	517	DGD	C2G-O2G-C1B	-2.47	111.71	117.79
28	b	606	CLA	C4B-CHC-C1C	2.47	132.20	126.34
28	c	509	CLA	CHA-C4D-ND	2.47	137.67	132.50
28	S	313	CLA	C4B-CHC-C1C	2.47	132.20	126.34
28	b	603	CLA	CHA-C4D-ND	2.47	137.67	132.50
28	B	608	CLA	C4B-CHC-C1C	2.47	132.20	126.34
28	G	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
28	A	405	CLA	C4B-CHC-C1C	2.47	132.19	126.34
28	y	305	CLA	CHA-C4D-ND	2.47	137.66	132.50
28	a	406	CLA	C4B-CHC-C1C	2.47	132.19	126.34
28	C	506	CLA	CHA-C4D-ND	2.47	137.66	132.50
39	n	616	LUT	C18-C5-C4	2.47	118.93	114.36
28	r	608	CLA	C4B-CHC-C1C	2.47	132.19	126.34
28	Y	611	CLA	CHA-C4D-ND	2.47	137.66	132.50
28	b	616	CLA	CHA-C4D-ND	2.47	137.66	132.50
38	N	601	CHL	CHB-C4A-NA	2.47	127.92	124.51
28	y	314	CLA	CHA-C4D-ND	2.47	137.66	132.50
38	g	607	CHL	C1-O2A-CGA	2.47	122.91	116.44
28	S	314	CLA	C3B-C4B-NB	-2.47	108.23	110.52
28	Y	611	CLA	C1D-ND-C4D	-2.46	104.58	106.33
28	D	401	CLA	C4B-CHC-C1C	2.46	132.18	126.34
28	r	611	CLA	CMA-C3A-C4A	2.46	118.40	111.77
28	b	616	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
28	B	609	CLA	C4B-CHC-C1C	2.46	132.18	126.34
28	N	603	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	a	406	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
28	n	611	CLA	CHA-C4D-ND	2.46	137.65	132.50
28	a	406	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	g	602	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	B	611	CLA	C4B-CHC-C1C	2.46	132.18	126.34
28	c	506	CLA	C4B-CHC-C1C	2.46	132.18	126.34
38	G	607	CHL	C2B-C1B-NB	-2.46	108.58	110.23
28	C	510	CLA	C4B-CHC-C1C	2.46	132.18	126.34
28	B	616	CLA	C4B-CHC-C1C	2.46	132.17	126.34
28	N	612	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	y	314	CLA	C4B-CHC-C1C	2.46	132.17	126.34
28	C	503	CLA	CHA-C4D-ND	2.46	137.64	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	614	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	c	505	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	B	605	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
28	s	611	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	r	611	CLA	CHC-C1C-C2C	-2.46	119.90	126.73
28	b	603	CLA	C4B-CHC-C1C	2.46	132.17	126.34
38	g	607	CHL	C4D-CHA-C1A	2.46	124.24	121.25
28	y	312	CLA	CHA-C4D-ND	2.46	137.64	132.50
38	Y	601	CHL	CHB-C4A-NA	2.46	127.91	124.51
28	G	603	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	G	604	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	N	603	CLA	CHA-C4D-ND	2.46	137.64	132.50
38	R	607	CHL	C2B-C1B-NB	-2.46	108.58	110.23
28	Y	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	b	602	CLA	C4B-CHC-C1C	2.46	132.16	126.34
28	n	611	CLA	CHA-C1A-NA	-2.46	120.77	126.40
28	S	304	CLA	CHA-C4D-ND	2.46	137.64	132.50
38	N	607	CHL	CMA-C3A-C4A	2.46	118.37	111.77
28	s	603	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
28	N	612	CLA	C4B-CHC-C1C	2.46	132.16	126.34
28	D	404	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
35	R	616	LHG	O8-C23-C24	2.45	119.61	111.91
28	c	502	CLA	C4B-CHC-C1C	2.45	132.16	126.34
28	R	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
28	y	313	CLA	C4B-CHC-C1C	2.45	132.16	126.34
28	C	513	CLA	CHA-C4D-ND	2.45	137.63	132.50
28	a	409	CLA	CHA-C4D-ND	2.45	137.63	132.50
38	g	609	CHL	CMA-C3A-C2A	2.45	123.73	113.83
28	a	407	CLA	C3B-C4B-NB	-2.45	108.24	110.52
28	g	614	CLA	C4B-CHC-C1C	2.45	132.16	126.34
28	N	614	CLA	CHA-C4D-ND	2.45	137.63	132.50
30	c	515	BCR	C1-C6-C7	2.45	122.72	115.78
38	g	619	CHL	C2B-C1B-NB	-2.45	108.59	110.23
28	g	610	CLA	C2C-C1C-NC	2.45	112.27	109.97
28	r	612	CLA	O2A-CGA-CBA	2.45	119.60	111.91
28	C	507	CLA	CHA-C4D-ND	2.45	137.63	132.50
28	c	511	CLA	CHA-C4D-ND	2.45	137.63	132.50
28	b	612	CLA	C4B-CHC-C1C	2.45	132.15	126.34
28	Y	613	CLA	C4B-CHC-C1C	2.45	132.15	126.34
28	r	604	CLA	C3B-C4B-NB	-2.45	108.24	110.52
39	r	614	LUT	C18-C5-C4	2.45	118.90	114.36
38	N	606	CHL	C2B-C1B-NB	-2.45	108.59	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	R	605	CHL	CHC-C1C-NC	2.45	127.92	124.20
30	b	617	BCR	C16-C15-C14	-2.45	118.45	123.47
28	C	513	CLA	C4B-CHC-C1C	2.45	132.15	126.34
28	S	303	CLA	C3B-C4B-NB	-2.45	108.24	110.52
38	G	607	CHL	CMA-C3A-C4A	2.45	118.36	111.77
38	g	607	CHL	CMA-C3A-C4A	2.45	118.36	111.77
28	R	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	n	610	CLA	O2A-CGA-CBA	2.45	119.59	111.91
28	C	503	CLA	C4B-CHC-C1C	2.45	132.15	126.34
28	S	314	CLA	C4B-CHC-C1C	2.45	132.15	126.34
32	A	413	LMG	O8-C28-C29	2.45	119.59	111.91
28	c	503	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	G	604	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
28	y	313	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	b	614	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	R	612	CLA	C4B-CHC-C1C	2.45	132.14	126.34
28	a	407	CLA	C4B-CHC-C1C	2.45	132.14	126.34
28	S	303	CLA	CMD-C2D-C3D	-2.45	121.99	127.61
28	B	608	CLA	CHA-C4D-ND	2.44	137.61	132.50
30	A	409	BCR	C29-C30-C25	2.44	114.24	110.48
39	N	616	LUT	C40-C33-C34	-2.44	119.50	122.92
28	B	601	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
28	s	613	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
28	C	512	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	c	510	CLA	C4B-CHC-C1C	2.44	132.13	126.34
28	B	605	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
28	g	610	CLA	C4B-CHC-C1C	2.44	132.13	126.34
28	Y	612	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	y	311	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	Y	613	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	c	513	CLA	C4B-CHC-C1C	2.44	132.13	126.34
28	S	305	CLA	CAA-C2A-C1A	-2.44	103.97	111.97
28	B	609	CLA	CHA-C4D-ND	2.44	137.60	132.50
39	s	615	LUT	C19-C9-C10	-2.44	119.50	122.92
40	y	301	NEX	C40-C33-C34	-2.44	119.50	122.92
35	S	317	LHG	C5-O7-C7	-2.44	111.78	117.79
28	b	614	CLA	C4B-CHC-C1C	2.44	132.13	126.34
30	i	101	BCR	C35-C13-C14	-2.44	119.50	122.92
28	C	507	CLA	O2A-CGA-CBA	2.44	119.56	111.91
28	c	504	CLA	C3B-C4B-NB	-2.44	108.25	110.52
38	R	606	CHL	CHD-C4C-C3C	2.44	128.43	124.84
28	s	604	CLA	O1D-CGD-CBD	-2.44	119.49	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	314	CLA	CHA-C4D-ND	2.44	137.60	132.50
28	b	605	CLA	C4B-CHC-C1C	2.44	132.12	126.34
28	C	511	CLA	C4B-CHC-C1C	2.44	132.12	126.34
28	C	512	CLA	C4B-CHC-C1C	2.44	132.12	126.34
28	D	403	CLA	C4B-CHC-C1C	2.44	132.12	126.34
28	D	404	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	b	608	CLA	CHA-C4D-ND	2.44	137.59	132.50
38	G	609	CHL	CHD-C4C-C3C	2.43	128.42	124.84
28	b	615	CLA	C4B-CHC-C1C	2.43	132.11	126.34
30	B	619	BCR	C36-C18-C17	-2.43	119.51	122.92
40	Y	618	NEX	C31-C30-C29	2.43	130.78	127.31
28	b	609	CLA	CHA-C4D-ND	2.43	137.59	132.50
30	i	101	BCR	C23-C24-C25	-2.43	120.37	127.20
28	S	309	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
28	N	602	CLA	O2A-CGA-CBA	2.43	119.55	111.91
28	B	613	CLA	C3B-C4B-NB	-2.43	108.26	110.52
28	c	512	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	r	603	CLA	C4B-CHC-C1C	2.43	132.11	126.34
39	G	615	LUT	C38-C25-C24	-2.43	118.36	123.56
28	d	405	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
28	g	611	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	C	504	CLA	C4B-CHC-C1C	2.43	132.10	126.34
28	d	404	CLA	O2A-CGA-CBA	2.43	119.54	111.91
28	S	311	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	n	604	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	B	605	CLA	O2A-CGA-CBA	2.43	119.53	111.91
28	R	611	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
38	y	309	CHL	CMA-C3A-C2A	2.43	123.62	113.83
32	C	522	LMG	O8-C28-C29	2.43	119.53	111.91
28	Y	614	CLA	C4B-CHC-C1C	2.43	132.10	126.34
28	C	501	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	B	605	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	d	404	CLA	CHA-C4D-ND	2.43	137.58	132.50
40	y	301	NEX	C20-C13-C14	-2.43	119.52	122.92
28	d	404	CLA	C4B-CHC-C1C	2.43	132.09	126.34
28	n	612	CLA	CHA-C4D-ND	2.43	137.58	132.50
38	s	607	CHL	C2B-C1B-NB	-2.43	108.61	110.23
28	B	613	CLA	C4B-CHC-C1C	2.43	132.09	126.34
28	R	604	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	N	614	CLA	C4B-CHC-C1C	2.43	132.09	126.34
30	B	618	BCR	C27-C26-C25	-2.43	119.21	122.73
28	s	602	CLA	O2A-CGA-CBA	2.43	119.52	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	603	CLA	CHA-C4D-ND	2.43	137.57	132.50
38	Y	609	CHL	CMA-C3A-C2A	2.43	123.61	113.83
28	B	612	CLA	C4B-CHC-C1C	2.43	132.09	126.34
28	c	510	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	d	401	CLA	C4B-CHC-C1C	2.42	132.09	126.34
28	C	510	CLA	CHA-C4D-ND	2.42	137.57	132.50
28	c	503	CLA	C4B-CHC-C1C	2.42	132.09	126.34
28	C	512	CLA	O2A-CGA-CBA	2.42	119.51	111.91
28	C	505	CLA	C4B-CHC-C1C	2.42	132.08	126.34
28	B	609	CLA	C3B-C4B-NB	-2.42	108.27	110.52
28	S	310	CLA	C3B-C4B-NB	-2.42	108.27	110.52
28	Y	602	CLA	C16-C15-C13	-2.42	108.09	115.92
28	N	613	CLA	C4B-CHC-C1C	2.42	132.08	126.34
28	r	602	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
28	C	509	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	D	401	CLA	O2A-CGA-CBA	2.42	119.51	111.91
28	d	405	CLA	C4B-CHC-C1C	2.42	132.08	126.34
28	r	603	CLA	C3B-C4B-NB	-2.42	108.27	110.52
28	G	602	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	N	613	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	g	603	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	c	504	CLA	CHA-C4D-ND	2.42	137.56	132.50
38	s	605	CHL	CHC-C1C-NC	2.42	127.87	124.20
28	d	405	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	R	604	CLA	C3B-C4B-NB	-2.42	108.27	110.52
38	n	601	CHL	CHC-C1C-NC	2.42	127.87	124.20
30	C	516	BCR	C8-C7-C6	-2.42	120.41	127.20
28	c	507	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	i	101	BCR	C8-C7-C6	-2.42	120.41	127.20
35	A	416	LHG	C5-O7-C7	-2.42	111.84	117.79
28	B	604	CLA	C4B-CHC-C1C	2.42	132.07	126.34
28	b	607	CLA	C4B-CHC-C1C	2.42	132.07	126.34
38	S	302	CHL	C2B-C1B-NB	-2.42	108.61	110.23
28	b	602	CLA	CHA-C4D-ND	2.42	137.55	132.50
28	g	613	CLA	CHA-C4D-ND	2.42	137.55	132.50
28	B	611	CLA	CHA-C4D-ND	2.42	137.55	132.50
28	d	401	CLA	CHA-C4D-ND	2.42	137.55	132.50
28	d	401	CLA	C3B-C4B-NB	-2.42	108.27	110.52
28	Y	602	CLA	C11-C12-C13	-2.42	108.11	115.92
35	A	416	LHG	O8-C23-C24	2.42	119.49	111.91
28	g	604	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
28	b	612	CLA	CMA-C3A-C4A	2.42	118.26	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	t	101	BCR	C8-C7-C6	-2.41	120.42	127.20
28	b	611	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	S	310	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	r	603	CLA	C2D-C1D-ND	2.41	111.88	110.10
28	N	602	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	D	404	CLA	C4B-CHC-C1C	2.41	132.06	126.34
28	Y	603	CLA	O2A-CGA-CBA	2.41	119.48	111.91
30	T	101	BCR	C38-C26-C27	2.41	118.25	113.62
28	A	408	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	r	611	CLA	CAC-C3C-C4C	2.41	127.94	124.81
30	B	619	BCR	C23-C24-C25	-2.41	120.42	127.20
28	N	603	CLA	C4B-CHC-C1C	2.41	132.06	126.34
28	y	305	CLA	C4B-CHC-C1C	2.41	132.06	126.34
28	c	508	CLA	C2C-C1C-NC	2.41	112.23	109.97
28	C	504	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	s	610	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	a	409	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
38	n	601	CHL	CMA-C3A-C4A	2.41	118.26	111.77
30	H	101	BCR	C15-C16-C17	-2.41	118.53	123.47
39	S	316	LUT	C21-C26-C27	-2.41	109.65	112.70
38	r	605	CHL	CMA-C3A-C2A	2.41	123.56	113.83
28	S	311	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
38	N	606	CHL	CMA-C3A-C2A	2.41	123.56	113.83
40	y	301	NEX	C17-C1-C6	-2.41	108.31	110.47
28	C	502	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	r	602	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	r	613	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	c	501	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	B	610	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	C	501	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	B	606	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	b	612	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	s	610	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	c	506	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	b	616	CLA	C4B-CHC-C1C	2.41	132.05	126.34
28	a	409	CLA	C3B-C4B-NB	-2.41	108.28	110.52
28	R	610	CLA	O2A-CGA-CBA	2.41	119.46	111.91
38	n	608	CHL	CHC-C1C-NC	2.41	127.86	124.20
28	c	512	CLA	C4B-CHC-C1C	2.41	132.05	126.34
28	s	604	CLA	C4B-CHC-C1C	2.41	132.05	126.34
28	B	607	CLA	C4B-CHC-C1C	2.41	132.05	126.34
35	B	625	LHG	C5-O7-C7	-2.41	111.87	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	406	CLA	CHA-C4D-ND	2.41	137.53	132.50
28	n	613	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
38	n	609	CHL	CHB-C4A-NA	2.41	127.84	124.51
38	Y	608	CHL	CHC-C1C-NC	2.41	127.85	124.20
28	D	403	CLA	CHA-C4D-ND	2.41	137.53	132.50
28	b	613	CLA	CHA-C4D-ND	2.41	137.53	132.50
38	G	605	CHL	C2B-C1B-NB	-2.40	108.62	110.23
28	r	608	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
28	y	303	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	g	602	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	C	513	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
28	G	613	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	r	610	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	s	610	CLA	O2A-CGA-CBA	2.40	119.45	111.91
28	b	616	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	D	401	CLA	CHA-C4D-ND	2.40	137.53	132.50
38	R	607	CHL	CHB-C4A-NA	2.40	127.83	124.51
28	n	602	CLA	CHA-C4D-ND	2.40	137.52	132.50
28	C	506	CLA	C4B-CHC-C1C	2.40	132.03	126.34
28	b	614	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
28	C	509	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	n	610	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
28	s	609	CLA	CHA-C4D-ND	2.40	137.52	132.50
38	n	606	CHL	CMA-C3A-C2A	2.40	123.51	113.83
28	g	613	CLA	C4B-CHC-C1C	2.40	132.03	126.34
30	b	618	BCR	C24-C23-C22	-2.40	122.61	126.23
30	C	514	BCR	C8-C7-C6	-2.40	120.46	127.20
28	A	408	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	S	309	CLA	C4B-CHC-C1C	2.40	132.03	126.34
28	G	611	CLA	CHA-C4D-ND	2.40	137.52	132.50
28	R	603	CLA	O2A-CGA-CBA	2.40	119.44	111.91
28	c	503	CLA	O2A-CGA-CBA	2.40	119.44	111.91
28	n	613	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	b	613	CLA	C4B-CHC-C1C	2.40	132.03	126.34
28	Y	611	CLA	C11-C10-C8	-2.40	108.16	115.92
28	R	609	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
39	G	615	LUT	C20-C13-C14	-2.40	119.56	122.92
28	a	409	CLA	C4B-CHC-C1C	2.40	132.03	126.34
28	G	604	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	A	408	CLA	C4B-CHC-C1C	2.40	132.02	126.34
40	Y	618	NEX	C20-C13-C14	-2.40	119.56	122.92
28	B	605	CLA	C1-C2-C3	-2.40	121.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	N	601	CHL	C1-O2A-CGA	2.40	122.73	116.44
28	R	613	CLA	C1-C2-C3	-2.40	121.90	126.04
28	A	406	CLA	CHA-C4D-ND	2.40	137.51	132.50
28	b	615	CLA	CHA-C4D-ND	2.40	137.51	132.50
28	g	611	CLA	C1D-ND-C4D	-2.40	104.63	106.33
28	B	615	CLA	CHA-C4D-ND	2.40	137.51	132.50
28	R	608	CLA	C3B-C4B-NB	-2.40	108.29	110.52
28	S	303	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	n	610	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	g	612	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	b	610	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	C	504	CLA	O2A-CGA-CBA	2.39	119.42	111.91
28	Y	604	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
38	g	606	CHL	C2B-C1B-NB	-2.39	108.63	110.23
28	R	601	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	c	502	CLA	CHA-C4D-ND	2.39	137.51	132.50
38	y	302	CHL	CHC-C1C-NC	2.39	127.83	124.20
38	Y	606	CHL	CMA-C3A-C2A	2.39	123.48	113.83
28	n	614	CLA	C4B-CHC-C1C	2.39	132.02	126.34
39	n	615	LUT	C11-C12-C13	-2.39	119.69	126.42
28	G	613	CLA	C4B-CHC-C1C	2.39	132.01	126.34
28	B	606	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	C	511	CLA	CHA-C4D-ND	2.39	137.50	132.50
28	D	403	CLA	C3B-C4B-NB	-2.39	108.30	110.52
28	c	502	CLA	C3B-C4B-NB	-2.39	108.30	110.52
38	r	606	CHL	C2B-C1B-NB	-2.39	108.63	110.23
28	r	611	CLA	C4B-CHC-C1C	2.39	132.01	126.34
38	g	609	CHL	CHD-C4C-C3C	2.39	128.36	124.84
40	y	318	NEX	C28-C29-C30	2.39	122.61	118.94
28	R	609	CLA	CHA-C4D-ND	2.39	137.50	132.50
28	c	513	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
30	c	514	BCR	C35-C13-C14	-2.39	119.58	122.92
28	B	603	CLA	O2A-CGA-CBA	2.39	119.41	111.91
28	c	505	CLA	C4B-CHC-C1C	2.39	132.00	126.34
28	B	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
38	g	605	CHL	CHB-C4A-NA	2.39	127.81	124.51
39	N	616	LUT	C15-C35-C34	-2.39	118.58	123.47
28	C	502	CLA	C4B-CHC-C1C	2.39	132.00	126.34
38	N	608	CHL	C1-C2-C3	-2.39	121.91	126.04
28	Y	604	CLA	C4B-CHC-C1C	2.39	132.00	126.34
38	G	605	CHL	CHD-C4C-C3C	2.39	128.35	124.84
28	a	407	CLA	CHA-C4D-ND	2.39	137.49	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	612	CLA	C4B-CHC-C1C	2.39	132.00	126.34
28	b	604	CLA	C4B-CHC-C1C	2.39	132.00	126.34
38	N	601	CHL	CHC-C1C-NC	2.39	127.82	124.20
28	N	610	CLA	CHA-C4D-ND	2.39	137.49	132.50
28	B	614	CLA	C4B-CHC-C1C	2.39	132.00	126.34
28	N	604	CLA	C4B-CHC-C1C	2.38	131.99	126.34
28	C	509	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	C	508	CLA	CHA-C4D-ND	2.38	137.49	132.50
28	s	608	CLA	C3B-C4B-NB	-2.38	108.30	110.52
28	r	604	CLA	CMA-C3A-C4A	2.38	118.18	111.77
38	y	309	CHL	CHB-C4A-NA	2.38	127.81	124.51
39	y	316	LUT	C30-C31-C32	-2.38	115.78	123.22
28	A	405	CLA	CHA-C4D-ND	2.38	137.48	132.50
28	R	610	CLA	CHA-C4D-ND	2.38	137.48	132.50
28	y	312	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	C	508	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	R	608	CLA	CHA-C4D-ND	2.38	137.48	132.50
28	B	611	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	G	604	CLA	C4B-CHC-C1C	2.38	131.99	126.34
28	b	608	CLA	C4B-CHC-C1C	2.38	131.99	126.34
38	g	601	CHL	CHC-C1C-NC	2.38	127.81	124.20
28	y	310	CLA	O2A-CGA-CBA	2.38	119.38	111.91
36	C	518	DGD	O1G-C1A-C2A	2.38	119.38	111.91
38	n	607	CHL	CMA-C3A-C4A	2.38	118.17	111.77
30	a	410	BCR	C29-C30-C25	2.38	114.14	110.48
38	s	606	CHL	C4A-NA-C1A	2.38	107.78	106.71
35	N	618	LHG	O7-C7-O9	-2.38	117.95	123.70
28	b	612	CLA	O2A-CGA-CBA	2.38	119.38	111.91
28	C	502	CLA	O2A-CGA-CBA	2.38	119.37	111.91
28	S	310	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
39	y	315	LUT	C35-C15-C14	-2.38	118.61	123.47
28	B	612	CLA	CHA-C4D-ND	2.38	137.47	132.50
38	N	607	CHL	CHD-C4C-C3C	2.38	128.33	124.84
28	s	613	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	c	509	CLA	C4B-CHC-C1C	2.38	131.97	126.34
28	S	313	CLA	CHA-C4D-ND	2.37	137.47	132.50
28	D	403	CLA	O2A-CGA-CBA	2.37	119.36	111.91
38	n	605	CHL	CHB-C4A-NA	2.37	127.79	124.51
28	b	607	CLA	C3B-C4B-NB	-2.37	108.31	110.52
28	N	604	CLA	CMA-C3A-C4A	2.37	118.15	111.77
38	G	607	CHL	C1-C2-C3	-2.37	121.94	126.04
28	A	408	CLA	O2D-CGD-O1D	-2.37	119.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	616	CLA	CHA-C4D-ND	2.37	137.46	132.50
28	G	603	CLA	C4B-CHC-C1C	2.37	131.96	126.34
39	Y	616	LUT	C20-C13-C12	2.37	121.81	118.08
28	c	510	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
30	C	514	BCR	C8-C9-C10	2.37	122.58	118.94
28	b	605	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
28	r	612	CLA	CHA-C4D-ND	2.37	137.45	132.50
38	N	601	CHL	CMA-C3A-C4A	2.37	118.14	111.77
28	n	604	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
28	b	609	CLA	CMA-C3A-C4A	2.37	118.14	111.77
28	r	602	CLA	O2A-CGA-CBA	2.37	119.34	111.91
28	D	401	CLA	C6-C5-C3	-2.37	107.25	113.45
38	g	607	CHL	CMA-C3A-C2A	2.37	123.38	113.83
28	c	501	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
30	b	619	BCR	C10-C11-C12	-2.37	115.83	123.22
28	y	303	CLA	O2A-CGA-CBA	2.37	119.33	111.91
28	y	314	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
28	s	602	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
38	s	601	CHL	CHB-C4A-NA	2.36	127.78	124.51
36	A	417	DGD	O1G-C1A-C2A	2.36	119.33	111.91
30	c	514	BCR	C36-C18-C17	-2.36	119.61	122.92
28	Y	612	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	f	101	HEM	C4A-NA-C1A	2.36	107.66	105.35
38	y	306	CHL	C2B-C1B-NB	-2.36	108.65	110.23
28	n	604	CLA	C4B-CHC-C1C	2.36	131.94	126.34
30	t	101	BCR	C20-C19-C18	-2.36	119.78	126.42
30	i	101	BCR	C29-C30-C25	2.36	114.12	110.48
28	n	613	CLA	CHA-C4D-ND	2.36	137.44	132.50
38	n	605	CHL	CMA-C3A-C4A	2.36	118.12	111.77
28	B	604	CLA	C3B-C4B-NB	-2.36	108.32	110.52
28	n	603	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
28	r	611	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
30	H	101	BCR	C8-C7-C6	-2.36	120.58	127.20
28	Y	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
28	b	613	CLA	C3B-C4B-NB	-2.36	108.33	110.52
28	c	508	CLA	O2A-CGA-CBA	2.36	119.31	111.91
38	G	601	CHL	C2B-C1B-NB	-2.36	108.65	110.23
38	n	608	CHL	C2B-C1B-NB	-2.36	108.65	110.23
36	A	417	DGD	C2G-O2G-C1B	-2.36	111.98	117.79
28	c	508	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
38	G	609	CHL	CMA-C3A-C2A	2.36	123.34	113.83
28	N	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	602	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
28	R	609	CLA	O2A-CGA-CBA	2.36	119.30	111.91
28	s	602	CLA	CHA-C4D-ND	2.36	137.43	132.50
39	Y	615	LUT	C20-C13-C12	2.36	121.79	118.08
28	C	506	CLA	C3B-C4B-NB	-2.36	108.33	110.52
28	b	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
39	Y	615	LUT	C18-C5-C4	2.35	118.72	114.36
28	Y	603	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
28	c	501	CLA	O2A-CGA-CBA	2.35	119.30	111.91
30	i	101	BCR	C11-C12-C13	-2.35	119.80	126.42
31	M	101	SQD	O3-C3-C2	-2.35	104.91	110.35
28	b	603	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
39	n	615	LUT	C35-C15-C14	-2.35	118.65	123.47
38	S	306	CHL	CHC-C1C-NC	2.35	127.77	124.20
28	n	604	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
28	Y	611	CLA	C4B-CHC-C1C	2.35	131.92	126.34
28	n	611	CLA	C4B-CHC-C1C	2.35	131.92	126.34
38	n	609	CHL	CMA-C3A-C2A	2.35	123.31	113.83
28	b	616	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
28	n	614	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
28	G	603	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
38	s	601	CHL	CHC-C1C-NC	2.35	127.77	124.20
28	N	603	CLA	O2A-CGA-CBA	2.35	119.28	111.91
28	R	612	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	B	614	CLA	O2A-CGA-CBA	2.35	119.28	111.91
28	r	611	CLA	O2A-CGA-CBA	2.35	119.28	111.91
28	G	613	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
28	G	614	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	B	601	CLA	O2A-CGA-CBA	2.35	119.28	111.91
28	s	612	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	r	604	CLA	C4B-CHC-C1C	2.35	131.91	126.34
38	G	608	CHL	CHD-C4C-C3C	2.35	128.29	124.84
28	B	616	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
28	g	604	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
28	S	309	CLA	CHA-C4D-ND	2.35	137.41	132.50
30	b	617	BCR	C30-C25-C24	2.35	122.41	115.78
39	N	616	LUT	C1-C6-C5	-2.34	119.31	122.61
38	Y	607	CHL	CHC-C1C-NC	2.34	127.76	124.20
28	Y	603	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
28	r	611	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
28	B	602	CLA	CHA-C4D-ND	2.34	137.40	132.50
41	r	615	XAT	C40-C33-C34	-2.34	119.64	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	603	CLA	C3B-C4B-NB	-2.34	108.34	110.52
35	a	415	LHG	C5-O7-C7	-2.34	112.02	117.79
38	n	607	CHL	C4A-NA-C1A	2.34	107.76	106.71
38	S	308	CHL	C2B-C1B-NB	-2.34	108.66	110.23
39	n	616	LUT	C30-C31-C32	-2.34	115.91	123.22
38	N	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
38	N	609	CHL	CHC-C1C-NC	2.34	127.75	124.20
28	A	405	CLA	O2A-CGA-CBA	2.34	119.25	111.91
40	G	617	NEX	O24-C25-C24	2.34	115.14	113.38
28	B	602	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
28	A	405	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
38	G	606	CHL	CMA-C3A-C2A	2.34	123.26	113.83
38	R	607	CHL	C1-O2A-CGA	2.34	122.58	116.44
32	k	102	LMG	C8-O7-C10	-2.34	112.04	117.79
35	S	301	LHG	O8-C23-C24	2.34	119.24	111.91
30	i	101	BCR	C36-C18-C17	-2.34	119.65	122.92
28	G	612	CLA	O2A-CGA-CBA	2.34	119.24	111.91
28	y	304	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
28	r	603	CLA	O2A-CGA-CBA	2.33	119.22	111.91
28	n	602	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
28	C	502	CLA	C3B-C4B-NB	-2.33	108.35	110.52
39	R	614	LUT	C19-C9-C10	-2.33	119.66	122.92
28	d	405	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
28	c	508	CLA	C4B-CHC-C1C	2.33	131.86	126.34
28	C	508	CLA	O2A-CGA-CBA	2.33	119.22	111.91
28	B	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
28	s	612	CLA	C4B-CHC-C1C	2.33	131.86	126.34
38	N	607	CHL	CHB-C4A-NA	2.33	127.73	124.51
39	N	615	LUT	C20-C13-C12	2.33	121.74	118.08
28	C	510	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
28	r	608	CLA	CHA-C4D-ND	2.33	137.37	132.50
32	c	521	LMG	O8-C28-C29	2.33	119.21	111.91
28	Y	610	CLA	CHA-C1A-NA	-2.33	121.07	126.40
28	S	314	CLA	CMD-C2D-C3D	-2.33	122.27	127.61
28	c	510	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
28	A	408	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
38	r	607	CHL	C2B-C1B-NB	-2.32	108.67	110.23
30	h	101	BCR	C37-C22-C21	-2.32	119.67	122.92
28	B	612	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
41	R	615	XAT	C40-C33-C34	-2.32	119.67	122.92
28	y	313	CLA	O2A-CGA-CBA	2.32	119.19	111.91
28	s	602	CLA	O2D-CGD-O1D	-2.32	119.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	610	CLA	O2A-CGA-CBA	2.32	119.19	111.91
28	g	604	CLA	C4B-CHC-C1C	2.32	131.84	126.34
28	N	604	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
28	g	602	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
39	N	616	LUT	C30-C31-C32	-2.32	115.97	123.22
28	Y	604	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
28	S	303	CLA	O2A-CGA-CBA	2.32	119.19	111.91
28	C	510	CLA	O2A-CGA-CBA	2.32	119.19	111.91
39	G	615	LUT	C7-C8-C9	-2.32	122.73	126.23
28	n	602	CLA	O2A-CGA-CBA	2.32	119.19	111.91
28	b	611	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	a	414	SQD	O3-C3-C2	-2.32	104.99	110.35
39	r	614	LUT	C38-C25-C24	-2.32	118.60	123.56
28	r	601	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
39	n	615	LUT	C20-C13-C12	2.32	121.73	118.08
38	G	606	CHL	C2B-C1B-NB	-2.32	108.68	110.23
28	s	611	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
28	S	305	CLA	C4B-CHC-C1C	2.32	131.84	126.34
28	B	606	CLA	O2A-CGA-CBA	2.32	119.18	111.91
28	C	511	CLA	O2A-CGA-CBA	2.32	119.18	111.91
38	N	605	CHL	C2B-C1B-NB	-2.32	108.68	110.23
28	R	613	CLA	CHA-C4D-ND	2.32	137.34	132.50
28	r	609	CLA	CHA-C4D-ND	2.31	137.34	132.50
28	R	612	CLA	O2A-CGA-CBA	2.31	119.17	111.91
38	n	606	CHL	C1-O2A-CGA	2.31	122.51	116.44
38	Y	607	CHL	CHB-C4A-NA	2.31	127.71	124.51
28	B	610	CLA	O2A-CGA-CBA	2.31	119.16	111.91
28	S	310	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
28	C	501	CLA	O2A-CGA-CBA	2.31	119.16	111.91
28	s	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
28	R	602	CLA	CHA-C4D-ND	2.31	137.33	132.50
28	N	614	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
28	r	601	CLA	C1D-ND-C4D	-2.31	104.69	106.33
38	g	609	CHL	CHC-C1C-NC	2.31	127.70	124.20
28	N	610	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
28	B	615	CLA	C16-C15-C13	-2.31	108.46	115.92
38	y	308	CHL	C2B-C1B-NB	-2.31	108.69	110.23
38	R	605	CHL	CHB-C4A-NA	2.31	127.70	124.51
28	R	610	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
28	Y	614	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
28	n	611	CLA	C1D-ND-C4D	-2.31	104.70	106.33
28	B	609	CLA	CMD-C2D-C3D	-2.31	122.31	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	y	304	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
28	G	603	CLA	C3B-C4B-NB	-2.31	108.38	110.52
38	g	609	CHL	C1-O2A-CGA	2.31	122.49	116.44
38	G	609	CHL	CHB-C4A-NA	2.30	127.70	124.51
30	d	406	BCR	C8-C7-C6	-2.30	120.73	127.20
28	B	608	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
28	r	611	CLA	CHA-C4D-ND	2.30	137.32	132.50
28	B	612	CLA	O2A-CGA-CBA	2.30	119.13	111.91
28	b	608	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
28	Y	610	CLA	C1D-ND-C4D	-2.30	104.70	106.33
39	S	315	LUT	C18-C5-C4	2.30	118.62	114.36
28	c	513	CLA	CHA-C1A-NA	-2.30	121.13	126.40
28	C	512	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
40	s	616	NEX	C26-C27-C28	-2.30	121.13	125.99
38	N	607	CHL	C2B-C1B-NB	-2.30	108.69	110.23
39	S	316	LUT	C11-C12-C13	-2.30	119.96	126.42
38	G	601	CHL	CHC-C1C-NC	2.30	127.69	124.20
28	b	610	CLA	O2A-CGA-CBA	2.30	119.12	111.91
28	b	608	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
38	N	606	CHL	CHC-C1C-NC	2.30	127.69	124.20
28	b	603	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
38	Y	606	CHL	CHC-C1C-NC	2.30	127.69	124.20
28	N	603	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
36	C	519	DGD	O1G-C1A-C2A	2.30	119.11	111.91
28	N	612	CLA	O2A-CGA-CBA	2.30	119.11	111.91
39	y	315	LUT	C18-C5-C4	2.30	118.61	114.36
40	g	617	NEX	C26-C27-C28	-2.29	121.14	125.99
38	N	609	CHL	CHB-C4A-NA	2.29	127.69	124.51
28	g	613	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
38	Y	608	CHL	C2B-C1B-NB	-2.29	108.69	110.23
38	g	608	CHL	CHD-C4C-C3C	2.29	128.21	124.84
38	Y	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
28	G	602	CLA	O2A-CGA-CBA	2.29	119.10	111.91
28	C	506	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	S	312	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	y	313	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	s	608	CLA	CHA-C4D-ND	2.29	137.29	132.50
28	y	310	CLA	CHA-C4D-ND	2.29	137.29	132.50
28	n	610	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
28	r	609	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
38	r	606	CHL	CMA-C3A-C2A	2.29	123.06	113.83
28	g	602	CLA	O2D-CGD-O1D	-2.29	119.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	623	LHG	C5-O7-C7	-2.29	112.16	117.79
28	N	610	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
28	B	602	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	B	611	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
38	y	309	CHL	CHC-C1C-NC	2.29	127.67	124.20
38	G	609	CHL	CHC-C1C-NC	2.29	127.67	124.20
38	S	302	CHL	CHC-C1C-NC	2.29	127.67	124.20
28	a	406	CLA	O2A-CGA-CBA	2.29	119.08	111.91
28	a	406	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
28	Y	602	CLA	CHA-C1A-NA	-2.29	121.16	126.40
28	c	508	CLA	CHA-C4D-ND	2.29	137.28	132.50
28	g	603	CLA	C4B-CHC-C1C	2.28	131.76	126.34
28	b	615	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
28	r	611	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
28	r	612	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
39	y	316	LUT	C18-C5-C4	2.28	118.59	114.36
28	R	602	CLA	CMA-C3A-C4A	2.28	117.91	111.77
28	B	614	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
28	C	505	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
31	L	101	SQD	O3-C3-C2	-2.28	105.07	110.35
28	C	511	CLA	C11-C12-C13	-2.28	108.54	115.92
38	n	605	CHL	CHD-C4C-C3C	2.28	128.19	124.84
28	N	602	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
38	N	605	CHL	CHB-C4A-NA	2.28	127.67	124.51
38	r	607	CHL	C1-O2A-CGA	2.28	122.43	116.44
28	c	505	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
31	A	414	SQD	O3-C3-C2	-2.28	105.08	110.35
39	S	316	LUT	C19-C9-C10	-2.28	119.73	122.92
38	g	608	CHL	C2B-C1B-NB	-2.28	108.70	110.23
28	b	609	CLA	O2A-CGA-CBA	2.28	119.06	111.91
28	S	304	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
38	Y	609	CHL	CHC-C1C-NC	2.28	127.66	124.20
28	S	310	CLA	C6-C5-C3	-2.28	107.48	113.45
28	s	613	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	B	620	SQD	O3-C3-C2	-2.28	105.08	110.35
40	n	617	NEX	C5-C4-C3	2.28	114.44	111.75
28	D	404	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
28	Y	610	CLA	CHA-C4D-ND	2.28	137.26	132.50
38	G	608	CHL	CHC-C1C-NC	2.28	127.66	124.20
38	s	606	CHL	CMA-C3A-C4A	2.28	117.89	111.77
28	b	602	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
38	S	302	CHL	CHB-C4A-NA	2.27	127.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	515	BCR	C11-C12-C13	-2.27	120.03	126.42
39	g	616	LUT	C18-C5-C4	2.27	118.57	114.36
38	g	619	CHL	C1-O2A-CGA	2.27	122.41	116.44
28	c	504	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
28	C	513	CLA	CHA-C1A-NA	-2.27	121.19	126.40
28	N	603	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
28	g	611	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
28	Y	613	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
28	d	404	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
28	r	601	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
28	r	601	CLA	O2A-CGA-CBA	2.27	119.03	111.91
28	y	303	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
38	R	606	CHL	C2C-C3C-C4C	2.27	108.11	106.49
28	C	503	CLA	O2A-CGA-CBA	2.27	119.03	111.91
30	c	514	BCR	C15-C16-C17	-2.27	118.83	123.47
28	R	602	CLA	C2D-C1D-ND	2.27	111.78	110.10
38	G	601	CHL	CHB-C4A-NA	2.27	127.65	124.51
28	b	609	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
28	r	610	CLA	O2A-CGA-CBA	2.27	119.02	111.91
28	a	409	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
28	y	305	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
35	s	617	LHG	C5-O7-C7	-2.27	112.21	117.79
28	b	613	CLA	O2A-CGA-CBA	2.27	119.02	111.91
28	c	501	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
28	y	312	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
38	s	606	CHL	CMA-C3A-C2A	2.26	122.96	113.83
38	y	307	CHL	CMA-C3A-C2A	2.26	122.96	113.83
28	g	610	CLA	CMA-C3A-C4A	2.26	117.86	111.77
39	Y	616	LUT	C19-C9-C8	2.26	121.64	118.08
39	s	615	LUT	C40-C33-C34	-2.26	119.75	122.92
28	D	403	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
28	C	505	CLA	CMA-C3A-C4A	2.26	117.86	111.77
28	N	614	CLA	O2A-CGA-CBA	2.26	119.01	111.91
28	g	612	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	t	101	BCR	C23-C24-C25	-2.26	120.84	127.20
28	C	507	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
28	C	513	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
28	s	609	CLA	O2A-CGA-CBA	2.26	119.01	111.91
28	b	616	CLA	O2A-CGA-CBA	2.26	119.01	111.91
28	c	503	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
38	R	606	CHL	C2B-C1B-NB	-2.26	108.72	110.23
28	Y	613	CLA	CMD-C2D-C3D	-2.26	122.41	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	101	BCR	C33-C5-C4	2.26	117.96	113.62
28	B	615	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
28	S	314	CLA	O2A-CGA-CBA	2.26	119.00	111.91
38	g	619	CHL	CMA-C3A-C2A	2.26	122.95	113.83
28	R	612	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	S	309	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
38	S	306	CHL	CMA-C3A-C2A	2.26	122.94	113.83
28	R	611	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	a	411	SQD	O3-C3-C2	-2.26	105.13	110.35
28	R	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	n	611	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
28	n	614	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
28	G	604	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
38	r	605	CHL	CHC-C1C-NC	2.26	127.63	124.20
28	b	611	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
38	r	607	CHL	CMA-C3A-C4A	2.26	117.84	111.77
28	B	601	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	c	511	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	N	610	CLA	O2A-CGA-CBA	2.26	118.99	111.91
28	b	601	CLA	O2A-CGA-CBA	2.26	118.99	111.91
31	A	410	SQD	O3-C3-C2	-2.26	105.13	110.35
39	R	614	LUT	C4-C5-C6	-2.26	115.82	120.85
28	S	304	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
38	G	605	CHL	CHC-C1C-NC	2.26	127.62	124.20
38	r	607	CHL	C4A-NA-C1A	2.26	107.72	106.71
28	C	509	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
38	n	608	CHL	CHB-C4A-NA	2.25	127.63	124.51
28	N	614	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
38	g	601	CHL	CHD-C4C-C3C	2.25	128.15	124.84
28	b	606	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
28	s	609	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
38	Y	605	CHL	C1-O2A-CGA	2.25	123.27	116.73
41	R	615	XAT	C24-C23-C22	-2.25	106.42	110.77
38	g	607	CHL	C2B-C1B-NB	-2.25	108.72	110.23
28	R	602	CLA	C1D-ND-C4D	-2.25	104.73	106.33
28	r	603	CLA	C1D-ND-C4D	-2.25	104.73	106.33
28	G	602	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
30	b	618	BCR	C16-C15-C14	-2.25	118.86	123.47
38	r	606	CHL	CHC-C1C-NC	2.25	127.62	124.20
38	y	309	CHL	CHD-C4C-C3C	2.25	128.15	124.84
28	s	612	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
28	g	602	CLA	O2A-CGA-CBA	2.25	118.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	r	617	LHG	O8-C23-O10	-2.25	117.91	123.59
28	G	610	CLA	CHA-C4D-ND	2.25	137.21	132.50
28	r	601	CLA	CHA-C1A-NA	-2.25	121.25	126.40
28	B	608	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	g	604	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
38	y	307	CHL	CHC-C1C-NC	2.25	127.61	124.20
28	c	511	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
28	n	611	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	C	509	CLA	O2A-CGA-CBA	2.25	118.96	111.91
28	C	504	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
38	N	608	CHL	CHD-C4C-C3C	2.25	128.14	124.84
28	r	613	CLA	O2A-CGA-CBA	2.25	118.96	111.91
28	y	310	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
38	N	607	CHL	CHC-C1C-NC	2.24	127.61	124.20
38	Y	606	CHL	C2B-C1B-NB	-2.24	108.73	110.23
28	S	309	CLA	C3B-C4B-NB	-2.24	108.43	110.52
28	c	509	CLA	CHA-C1A-NA	-2.24	121.26	126.40
28	B	605	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
28	g	614	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
38	n	606	CHL	CHD-C4C-C3C	2.24	128.14	124.84
38	Y	607	CHL	C4A-NA-C1A	2.24	107.71	106.71
28	a	406	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
38	Y	606	CHL	C2C-C3C-C4C	2.24	108.09	106.49
38	G	601	CHL	C1-C2-C3	-2.24	122.17	126.04
38	s	605	CHL	CMA-C3A-C2A	2.24	122.87	113.83
30	K	101	BCR	C23-C24-C25	-2.24	120.91	127.20
38	y	308	CHL	CHB-C4A-NA	2.24	127.61	124.51
36	C	517	DGD	O6D-C5D-C6D	2.24	111.19	106.67
38	y	308	CHL	CHD-C4C-C3C	2.24	128.13	124.84
38	G	609	CHL	C2B-C1B-NB	-2.24	108.73	110.23
38	N	608	CHL	CHC-C1C-NC	2.24	127.60	124.20
38	S	307	CHL	CMA-C3A-C4A	2.24	117.79	111.77
28	Y	614	CLA	O2A-CGA-CBA	2.24	118.94	111.91
30	B	619	BCR	C8-C7-C6	-2.24	120.91	127.20
40	r	616	NEX	C20-C13-C14	-2.24	119.79	122.92
30	K	101	BCR	C20-C19-C18	-2.24	120.12	126.42
38	G	608	CHL	C2B-C1B-NB	-2.24	108.73	110.23
28	Y	602	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
37	E	101	HEM	C4A-NA-C1A	2.24	107.54	105.35
28	d	401	CLA	O2A-CGA-CBA	2.24	118.93	111.91
28	N	613	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
28	s	608	CLA	CMD-C2D-C3D	-2.24	122.47	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	602	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
41	r	615	XAT	C24-C23-C22	-2.24	106.45	110.77
28	y	314	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
28	G	610	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
30	K	101	BCR	C20-C21-C22	-2.23	124.12	127.31
30	b	618	BCR	C35-C13-C14	-2.23	119.79	122.92
28	G	613	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
30	B	617	BCR	C10-C11-C12	-2.23	116.25	123.22
38	S	306	CHL	C2C-C3C-C4C	2.23	108.08	106.49
39	N	615	LUT	C10-C11-C12	-2.23	116.25	123.22
28	g	603	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
28	R	608	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
32	d	409	LMG	O8-C28-C29	2.23	118.91	111.91
30	i	101	BCR	C37-C22-C21	-2.23	119.80	122.92
28	y	303	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
38	n	606	CHL	CHC-C1C-NC	2.23	127.59	124.20
36	C	519	DGD	C2G-O2G-C1B	-2.23	112.30	117.79
41	Y	617	XAT	C40-C33-C34	-2.23	119.80	122.92
30	d	406	BCR	C11-C12-C13	-2.23	120.15	126.42
30	c	515	BCR	C20-C19-C18	-2.23	120.15	126.42
28	R	601	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
28	R	608	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
28	g	614	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
28	g	603	CLA	C2D-C1D-ND	2.23	111.75	110.10
28	N	602	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
39	G	616	LUT	C31-C30-C29	-2.23	124.13	127.31
38	S	307	CHL	CHB-C4A-NA	2.23	127.59	124.51
38	s	601	CHL	C2B-C1B-NB	-2.23	108.74	110.23
28	B	615	CLA	O2A-CGA-CBA	2.23	118.90	111.91
28	c	509	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
28	C	503	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
28	b	613	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
28	b	608	CLA	O2A-CGA-CBA	2.23	118.89	111.91
28	b	601	CLA	C16-C15-C13	-2.23	108.73	115.92
28	Y	611	CLA	CHA-C1A-NA	-2.22	121.30	126.40
28	B	613	CLA	O2A-CGA-CBA	2.22	118.89	111.91
28	n	603	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
38	r	607	CHL	CHC-C1C-NC	2.22	127.58	124.20
28	B	616	CLA	O2A-CGA-CBA	2.22	118.88	111.91
28	B	607	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	C	512	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	C	513	CLA	CMD-C2D-C3D	-2.22	122.50	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	n	609	CHL	CHC-C1C-NC	2.22	127.58	124.20
28	C	510	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
28	C	508	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	C	511	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
39	g	616	LUT	C40-C33-C34	-2.22	119.81	122.92
28	G	612	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
38	y	302	CHL	CHD-C4C-C3C	2.22	128.10	124.84
38	N	607	CHL	CMA-C3A-C2A	2.22	122.78	113.83
38	g	606	CHL	CHC-C1C-NC	2.22	127.57	124.20
28	R	604	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
28	d	404	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
29	D	402	PHO	C1C-C2C-C3C	-2.22	106.77	108.61
28	B	603	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
39	y	316	LUT	C1-C6-C5	-2.22	119.49	122.61
39	y	315	LUT	C10-C11-C12	-2.22	116.30	123.22
38	R	607	CHL	CHC-C1C-NC	2.22	127.56	124.20
39	G	616	LUT	C11-C12-C13	-2.22	120.19	126.42
28	N	612	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
29	a	408	PHO	C1C-C2C-C3C	-2.22	106.77	108.61
38	n	609	CHL	C2B-C1B-NB	-2.22	108.75	110.23
38	G	608	CHL	CHB-C4A-NA	2.22	127.58	124.51
39	s	614	LUT	C21-C26-C27	-2.21	109.90	112.70
30	K	101	BCR	C1-C6-C7	2.21	122.04	115.78
28	b	604	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
28	c	513	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
38	n	606	CHL	C2C-C3C-C4C	2.21	108.07	106.49
38	g	609	CHL	C2B-C1B-NB	-2.21	108.75	110.23
28	N	613	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
28	R	602	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
39	N	615	LUT	C19-C9-C8	2.21	121.56	118.08
31	L	103	SQD	O3-C3-C2	-2.21	105.23	110.35
28	c	505	CLA	CMA-C3A-C4A	2.21	117.72	111.77
28	n	611	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
38	y	307	CHL	C2C-C3C-C4C	2.21	108.07	106.49
28	c	507	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
28	n	602	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
28	b	607	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
32	a	413	LMG	O8-C28-C29	2.21	118.85	111.91
28	C	501	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
40	r	616	NEX	C19-C9-C10	-2.21	119.83	122.92
28	g	610	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
28	C	503	CLA	CMD-C2D-C3D	-2.21	122.53	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	401	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
35	n	618	LHG	O8-C23-C24	2.21	118.84	111.91
28	B	604	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
38	g	619	CHL	CHB-C4A-NA	2.21	127.57	124.51
28	Y	604	CLA	O2A-CGA-CBA	2.21	118.84	111.91
28	c	506	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
37	f	101	HEM	C4D-ND-C1D	2.21	107.35	105.07
28	R	612	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
38	Y	609	CHL	CHD-C4C-C3C	2.21	128.08	124.84
28	n	610	CLA	CHA-C1A-NA	-2.21	121.34	126.40
34	d	403	BCT	O2-C-O1	2.21	125.27	119.55
28	B	616	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
38	y	306	CHL	CHC-C1C-NC	2.21	127.55	124.20
28	n	612	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
28	y	313	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
28	R	602	CLA	C6-C7-C8	-2.21	108.79	115.92
28	G	602	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
28	R	603	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
28	d	401	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
38	Y	607	CHL	C1-O2A-CGA	2.20	122.23	116.44
28	C	511	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
28	g	610	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
39	y	315	LUT	C38-C25-C24	-2.20	118.85	123.56
28	a	409	CLA	O2A-CGA-CBA	2.20	118.82	111.91
28	a	407	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
28	B	604	CLA	CHA-C1A-NA	-2.20	121.36	126.40
38	s	606	CHL	C2B-C1B-NB	-2.20	108.76	110.23
28	n	613	CLA	C6-C5-C3	-2.20	107.69	113.45
38	g	608	CHL	CMA-C3A-C2A	2.20	122.70	113.83
38	n	601	CHL	C2B-C1B-NB	-2.20	108.76	110.23
28	g	604	CLA	C2C-C1C-NC	2.20	112.03	109.97
28	C	507	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
28	A	405	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
28	G	603	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
40	s	616	NEX	C19-C9-C10	-2.20	119.84	122.92
28	C	507	CLA	CHA-C1A-NA	-2.20	121.37	126.40
38	N	601	CHL	C2B-C1B-NB	-2.20	108.76	110.23
38	s	606	CHL	CHC-C1C-NC	2.20	127.53	124.20
28	B	609	CLA	O2A-CGA-CBA	2.19	118.79	111.91
28	g	612	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
38	n	605	CHL	C1-O2A-CGA	2.19	123.10	116.73
41	y	317	XAT	O4-C5-C4	-2.19	111.73	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	507	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
28	D	401	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
40	N	617	NEX	C20-C13-C14	-2.19	119.85	122.92
41	R	615	XAT	C39-C29-C30	-2.19	119.85	122.92
39	Y	615	LUT	C40-C33-C32	2.19	121.53	118.08
39	g	616	LUT	C38-C25-C24	-2.19	118.87	123.56
28	R	611	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
28	b	610	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
41	Y	617	XAT	C20-C13-C14	-2.19	119.86	122.92
34	A	415	BCT	O2-C-O1	2.19	125.22	119.55
38	r	605	CHL	CHD-C4C-C3C	2.19	128.06	124.84
28	b	606	CLA	O2A-CGA-CBA	2.19	118.78	111.91
30	h	101	BCR	C36-C18-C17	-2.19	119.86	122.92
38	Y	605	CHL	CHD-C4C-C3C	2.19	128.06	124.84
30	B	619	BCR	C16-C15-C14	-2.19	118.99	123.47
40	g	617	NEX	C32-C33-C34	2.19	122.30	118.94
30	b	619	BCR	C3-C4-C5	-2.19	110.17	114.08
28	b	604	CLA	CHA-C1A-NA	-2.19	121.39	126.40
28	B	616	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
35	b	622	LHG	C5-O7-C7	-2.19	112.41	117.79
41	r	615	XAT	O4-C5-C18	-2.19	112.44	115.06
28	A	406	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
28	B	604	CLA	C6-C5-C3	-2.19	107.72	113.45
28	b	610	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
28	b	602	CLA	O2A-CGA-CBA	2.19	118.77	111.91
36	A	417	DGD	O2G-C1B-O1B	-2.18	118.42	123.70
28	c	509	CLA	CMA-C3A-C4A	2.18	117.64	111.77
28	B	613	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
28	s	604	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
38	r	605	CHL	C2C-C3C-C4C	2.18	108.05	106.49
28	S	305	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
28	B	610	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
39	G	616	LUT	C19-C9-C10	-2.18	119.87	122.92
38	n	609	CHL	C1-O2A-CGA	2.18	122.17	116.44
28	B	606	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
39	N	616	LUT	C40-C33-C32	2.18	121.51	118.08
28	C	506	CLA	O2A-CGA-CBA	2.18	118.75	111.91
38	Y	606	CHL	CHB-C4A-NA	2.18	127.53	124.51
28	g	613	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
38	g	608	CHL	CHC-C1C-NC	2.18	127.51	124.20
36	c	517	DGD	O2G-C1B-O1B	-2.18	118.44	123.70
28	r	603	CLA	C1-C2-C3	-2.18	122.28	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	N	606	CHL	C2C-C3C-C4C	2.18	108.04	106.49
28	D	403	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
28	Y	612	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
40	r	616	NEX	C39-C29-C30	-2.17	119.88	122.92
41	r	615	XAT	C39-C29-C30	-2.17	119.88	122.92
28	s	611	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
30	h	101	BCR	C11-C12-C13	-2.17	120.31	126.42
38	R	607	CHL	CHD-C4C-C3C	2.17	128.03	124.84
38	Y	607	CHL	C2B-C1B-NB	-2.17	108.78	110.23
38	y	307	CHL	C2B-C1B-NB	-2.17	108.78	110.23
28	s	604	CLA	O2A-CGA-CBA	2.17	118.73	111.91
30	t	101	BCR	C34-C9-C10	-2.17	119.88	122.92
38	N	608	CHL	CMA-C3A-C2A	2.17	122.59	113.83
35	C	521	LHG	C5-O7-C7	-2.17	112.44	117.79
38	Y	609	CHL	C2B-C1B-NB	-2.17	108.78	110.23
38	S	307	CHL	CHC-C1C-NC	2.17	127.50	124.20
28	b	604	CLA	O2A-CGA-CBA	2.17	118.72	111.91
30	a	410	BCR	C36-C18-C17	-2.17	119.88	122.92
28	R	612	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
38	r	605	CHL	C2B-C1B-NB	-2.17	108.78	110.23
30	A	409	BCR	C2-C1-C6	2.17	113.82	110.48
28	b	607	CLA	O2A-CGA-CBA	2.17	118.71	111.91
39	Y	615	LUT	C12-C13-C14	-2.17	115.61	118.94
38	g	609	CHL	CHB-C4A-NA	2.17	127.51	124.51
28	S	313	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
41	R	615	XAT	O4-C5-C18	-2.17	112.46	115.06
39	R	614	LUT	C3-C4-C5	2.17	116.17	111.85
38	S	308	CHL	CHB-C4A-NA	2.16	127.50	124.51
28	G	611	CLA	O2A-CGA-CBA	2.16	118.70	111.91
28	C	511	CLA	C6-C5-C3	-2.16	107.78	113.45
28	C	505	CLA	O2A-CGA-CBA	2.16	118.70	111.91
28	y	311	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
28	S	310	CLA	O2A-CGA-CBA	2.16	118.69	111.91
28	c	510	CLA	O2A-CGA-CBA	2.16	118.69	111.91
35	S	301	LHG	C6-C5-C4	-2.16	106.67	111.79
32	B	624	LMG	O6-C5-C6	2.16	111.81	106.44
30	C	515	BCR	C20-C19-C18	-2.16	120.34	126.42
28	S	312	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	y	312	CLA	O2A-CGA-CBA	2.16	118.69	111.91
28	b	606	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
38	Y	605	CHL	CMA-C3A-C2A	2.16	122.54	113.83
30	K	101	BCR	C37-C22-C23	2.16	121.48	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	601	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
39	Y	615	LUT	O3-C3-C2	-2.16	105.51	109.80
38	y	308	CHL	CHC-C1C-NC	2.16	127.48	124.20
28	N	610	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	N	613	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	R	613	CLA	O2A-CGA-CBA	2.16	118.68	111.91
32	c	521	LMG	C8-O7-C10	-2.16	112.48	117.79
28	S	311	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	b	604	CLA	C16-C15-C13	-2.16	108.95	115.92
28	y	314	CLA	O2A-CGA-CBA	2.16	118.67	111.91
28	B	616	CLA	C6-C7-C8	-2.16	108.95	115.92
28	Y	603	CLA	C1-O2A-CGA	2.16	122.10	116.44
28	S	303	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
28	C	506	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	r	602	CLA	C6-C5-C3	-2.16	107.80	113.45
28	r	613	CLA	CHA-C1A-NA	-2.15	121.46	126.40
29	A	407	PHO	C1C-C2C-C3C	-2.15	106.82	108.61
38	y	306	CHL	CHD-C4C-C3C	2.15	128.01	124.84
39	s	614	LUT	C40-C33-C34	-2.15	119.91	122.92
38	N	601	CHL	CMA-C3A-C2A	2.15	122.52	113.83
37	E	101	HEM	C1A-CHA-C4D	-2.15	121.23	126.34
39	n	616	LUT	C38-C25-C24	-2.15	118.95	123.56
39	N	616	LUT	C10-C11-C12	-2.15	116.50	123.22
28	G	614	CLA	O2A-CGA-CBA	2.15	118.66	111.91
39	y	315	LUT	C20-C13-C12	2.15	121.47	118.08
40	N	617	NEX	C2-C1-C6	2.15	111.30	109.21
28	A	406	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
28	s	609	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
38	N	608	CHL	C2B-C1B-NB	-2.15	108.79	110.23
28	d	405	CLA	O2A-CGA-CBA	2.15	118.65	111.91
40	Y	618	NEX	C26-C27-C28	-2.15	121.45	125.99
38	N	605	CHL	CMA-C3A-C2A	2.15	122.49	113.83
38	N	609	CHL	CHD-C4C-C3C	2.15	128.00	124.84
28	C	508	CLA	CHA-C1A-NA	-2.15	121.48	126.40
28	c	511	CLA	CHA-C1A-NA	-2.15	121.48	126.40
38	S	307	CHL	C2B-C1B-NB	-2.15	108.79	110.23
39	N	615	LUT	C38-C25-C24	-2.15	118.97	123.56
28	Y	613	CLA	C6-C5-C3	-2.15	107.83	113.45
28	c	508	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
28	b	616	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
28	D	404	CLA	CHA-C1A-NA	-2.15	121.48	126.40
41	r	615	XAT	C19-C9-C10	-2.14	119.92	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	611	CLA	O2A-CGA-CBA	2.14	118.64	111.91
38	G	608	CHL	CMA-C3A-C2A	2.14	122.48	113.83
30	D	405	BCR	C35-C13-C14	-2.14	119.92	122.92
28	d	401	CLA	C6-C5-C3	-2.14	107.83	113.45
28	s	612	CLA	C1-O2A-CGA	2.14	122.07	116.44
40	Y	618	NEX	C19-C9-C10	-2.14	119.92	122.92
28	G	602	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	s	608	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
41	R	615	XAT	C19-C9-C10	-2.14	119.92	122.92
38	G	601	CHL	CHD-C4C-C3C	2.14	127.99	124.84
28	C	506	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
28	r	613	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
28	B	611	CLA	CHA-C1A-NA	-2.14	121.50	126.40
38	g	619	CHL	CHC-C1C-NC	2.14	127.45	124.20
28	b	612	CLA	C16-C15-C13	-2.14	109.00	115.92
28	C	502	CLA	CHA-C1A-NA	-2.14	121.50	126.40
28	G	612	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
28	c	509	CLA	C1D-ND-C4D	-2.14	104.81	106.33
38	G	605	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	c	514	BCR	C21-C20-C19	-2.14	116.54	123.22
38	g	606	CHL	CAA-C2A-C1A	-2.14	104.97	111.97
28	C	509	CLA	CHA-C1A-NA	-2.14	121.51	126.40
28	R	613	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
38	R	606	CHL	CMA-C3A-C2A	2.14	122.44	113.83
28	b	615	CLA	O2A-CGA-CBA	2.14	118.61	111.91
28	R	613	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
28	s	603	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
39	r	614	LUT	C35-C34-C33	-2.13	124.26	127.31
38	s	607	CHL	CHB-C4A-NA	2.13	127.46	124.51
28	a	407	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
38	Y	608	CHL	CHB-C4A-NA	2.13	127.46	124.51
41	Y	617	XAT	O4-C5-C18	-2.13	112.50	115.06
28	N	611	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
39	S	315	LUT	C31-C32-C33	-2.13	120.42	126.42
28	S	310	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
28	C	508	CLA	C11-C10-C8	-2.13	109.03	115.92
28	N	612	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
38	Y	609	CHL	C1-O2A-CGA	2.13	122.03	116.44
38	n	606	CHL	C2B-C1B-NB	-2.13	108.80	110.23
38	y	309	CHL	C2B-C1B-NB	-2.13	108.80	110.23
40	y	318	NEX	C11-C10-C9	2.13	130.35	127.31
28	s	613	CLA	CMD-C2D-C3D	-2.13	122.71	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	607	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	d	401	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
28	r	604	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
28	b	616	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	K	101	BCR	C8-C7-C6	-2.13	121.22	127.20
28	N	604	CLA	O2A-CGA-CBA	2.13	118.59	111.91
28	R	608	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	R	613	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	y	311	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	C	502	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
36	A	417	DGD	O3G-C3G-C2G	-2.13	105.77	110.90
28	r	611	CLA	CHA-C1A-NA	-2.13	121.53	126.40
28	n	611	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
28	c	508	CLA	CHA-C1A-NA	-2.13	121.53	126.40
38	n	606	CHL	CHB-C4A-NA	2.13	127.45	124.51
28	r	608	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
28	r	602	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
28	r	612	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
28	Y	613	CLA	CHA-C1A-NA	-2.12	121.53	126.40
28	b	606	CLA	CHA-C1A-NA	-2.12	121.53	126.40
41	y	317	XAT	C40-C33-C34	-2.12	119.95	122.92
28	y	303	CLA	C6-C7-C8	-2.12	109.06	115.92
38	g	608	CHL	CHB-C4A-NA	2.12	127.45	124.51
38	r	607	CHL	CHB-C4A-NA	2.12	127.45	124.51
28	y	311	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
28	c	502	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
38	g	605	CHL	CHD-C4C-C3C	2.12	127.96	124.84
28	d	401	CLA	CHA-C1A-NA	-2.12	121.54	126.40
39	g	616	LUT	C11-C12-C13	-2.12	120.46	126.42
30	H	101	BCR	C35-C13-C14	-2.12	119.95	122.92
30	b	619	BCR	C15-C16-C17	-2.12	119.13	123.47
28	Y	610	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
28	B	610	CLA	CHA-C1A-NA	-2.12	121.54	126.40
28	S	309	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
30	B	618	BCR	C34-C9-C10	-2.12	119.96	122.92
38	G	606	CHL	CHC-C1C-NC	2.12	127.42	124.20
38	s	606	CHL	CHD-C4C-C3C	2.12	127.95	124.84
28	B	604	CLA	O2A-CGA-CBA	2.12	118.55	111.91
28	A	406	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	d	402	PHO	C1C-C2C-C3C	-2.12	106.85	108.61
28	S	311	CLA	C1-O2A-CGA	2.12	122.00	116.44
28	R	603	CLA	C3D-C2D-C1D	-2.12	102.94	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	316	LUT	C20-C13-C14	-2.12	119.96	122.92
41	y	317	XAT	C39-C29-C30	-2.12	119.96	122.92
28	C	501	CLA	CHA-C1A-NA	-2.12	121.55	126.40
28	Y	612	CLA	O2A-CGA-CBA	2.11	118.54	111.91
38	Y	601	CHL	CHC-C1C-NC	2.11	127.41	124.20
37	f	101	HEM	C1A-CHA-C4D	-2.11	121.33	126.34
28	Y	611	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
28	n	611	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
30	C	515	BCR	C36-C18-C17	-2.11	119.96	122.92
38	G	607	CHL	CHB-C4A-NA	2.11	127.43	124.51
39	g	616	LUT	C8-C7-C6	-2.11	121.27	127.20
28	y	303	CLA	C6-C5-C3	-2.11	107.92	113.45
28	b	611	CLA	CHA-C1A-NA	-2.11	121.56	126.40
30	B	618	BCR	C30-C25-C26	-2.11	119.64	122.61
28	B	608	CLA	O2A-CGA-CBA	2.11	118.53	111.91
30	k	101	BCR	C30-C25-C26	-2.11	119.64	122.61
28	a	407	CLA	O2A-CGA-CBA	2.11	118.53	111.91
36	a	401	DGD	O1G-C1A-C2A	2.11	118.52	111.91
38	s	601	CHL	CMA-C3A-C2A	2.11	122.33	113.83
30	C	515	BCR	C37-C22-C21	-2.11	119.97	122.92
30	K	101	BCR	C36-C18-C17	-2.11	119.97	122.92
30	H	101	BCR	C2-C1-C6	2.11	113.72	110.48
38	s	605	CHL	CHD-C4C-C3C	2.11	127.94	124.84
38	g	601	CHL	CMA-C3A-C2A	2.11	122.32	113.83
30	c	515	BCR	C15-C16-C17	-2.11	119.16	123.47
30	B	618	BCR	C35-C13-C14	-2.11	119.97	122.92
38	G	605	CHL	CHB-C4A-NA	2.11	127.42	124.51
28	a	409	CLA	CHA-C1A-NA	-2.10	121.58	126.40
38	S	302	CHL	CMA-C3A-C2A	2.10	122.32	113.83
28	R	601	CLA	CHA-C1A-NA	-2.10	121.58	126.40
32	A	411	LMG	O7-C10-O9	-2.10	118.62	123.70
28	Y	613	CLA	O2A-CGA-CBA	2.10	118.51	111.91
28	C	512	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
28	n	614	CLA	CHA-C1A-NA	-2.10	121.59	126.40
37	E	101	HEM	CHA-C4D-C3D	-2.10	121.38	125.33
28	B	607	CLA	O2A-CGA-CBA	2.10	118.50	111.91
30	c	515	BCR	C34-C9-C10	-2.10	119.98	122.92
37	f	101	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
28	g	612	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
30	T	101	BCR	C23-C24-C25	-2.10	121.31	127.20
38	g	605	CHL	CMA-C3A-C2A	2.10	122.29	113.83
38	Y	605	CHL	CHB-C4A-NA	2.10	127.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
28	S	305	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
28	G	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
39	y	315	LUT	C15-C35-C34	-2.10	119.18	123.47
39	g	615	LUT	C40-C33-C34	-2.10	119.99	122.92
28	c	506	CLA	O2A-CGA-CBA	2.10	118.48	111.91
28	a	407	CLA	CHA-C1A-NA	-2.10	121.60	126.40
38	n	607	CHL	C1-C2-C3	-2.10	122.42	126.04
28	G	612	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
28	g	610	CLA	CHA-C4D-ND	2.09	136.88	132.50
28	b	601	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
28	G	603	CLA	CHA-C1A-NA	-2.09	121.60	126.40
38	g	619	CHL	CHD-C4C-C3C	2.09	127.92	124.84
28	B	611	CLA	O2A-CGA-CBA	2.09	118.48	111.91
28	A	406	CLA	O2A-CGA-CBA	2.09	118.48	111.91
28	r	608	CLA	CHA-C1A-NA	-2.09	121.60	126.40
38	G	601	CHL	C4A-NA-C1A	2.09	107.65	106.71
39	n	615	LUT	C39-C29-C28	2.09	121.37	118.08
28	B	601	CLA	CHA-C1A-NA	-2.09	121.61	126.40
39	y	316	LUT	C40-C33-C34	-2.09	119.99	122.92
28	G	602	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
30	t	101	BCR	C1-C6-C7	2.09	121.70	115.78
28	B	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
28	C	511	CLA	CHA-C1A-NA	-2.09	121.61	126.40
38	n	609	CHL	CHD-C4C-C3C	2.09	127.91	124.84
28	G	614	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
28	n	611	CLA	CED-O2D-CGD	-2.09	111.21	115.94
28	n	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
28	c	505	CLA	O2A-CGA-CBA	2.09	118.47	111.91
38	n	607	CHL	CHD-C4C-C3C	2.09	127.91	124.84
38	N	606	CHL	CHB-C4A-NA	2.09	127.40	124.51
30	k	101	BCR	C34-C9-C10	-2.09	120.00	122.92
38	n	607	CHL	CHC-C1C-NC	2.09	127.37	124.20
38	s	605	CHL	CHB-C4A-NA	2.09	127.40	124.51
38	N	609	CHL	C2B-C1B-NB	-2.09	108.83	110.23
28	R	608	CLA	O2A-CGA-CBA	2.09	118.46	111.91
28	S	314	CLA	CHA-C1A-NA	-2.09	121.62	126.40
28	c	511	CLA	C6-C5-C3	-2.09	107.98	113.45
39	G	616	LUT	C2-C3-C4	2.09	113.16	110.30
28	S	313	CLA	CHA-C1A-NA	-2.09	121.62	126.40
28	y	310	CLA	CHA-C1A-NA	-2.09	121.62	126.40
39	g	615	LUT	C35-C15-C14	-2.09	119.20	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	613	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
28	c	504	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
30	a	410	BCR	C35-C13-C14	-2.09	120.00	122.92
38	r	607	CHL	CHD-C4C-C3C	2.09	127.91	124.84
28	y	304	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
38	Y	601	CHL	CMA-C3A-C2A	2.09	122.24	113.83
28	b	603	CLA	CHA-C1A-NA	-2.08	121.62	126.40
28	c	503	CLA	CHA-C1A-NA	-2.08	121.62	126.40
28	g	611	CLA	C4B-CHC-C1C	2.08	131.28	126.34
30	B	617	BCR	C30-C25-C24	2.08	121.67	115.78
28	s	603	CLA	CHA-C1A-NA	-2.08	121.63	126.40
39	s	614	LUT	C8-C9-C10	2.08	122.14	118.94
28	s	612	CLA	CHA-C1A-NA	-2.08	121.63	126.40
35	y	319	LHG	O8-C23-O10	-2.08	118.33	123.59
28	B	606	CLA	CHA-C1A-NA	-2.08	121.63	126.40
28	R	603	CLA	CHA-C1A-NA	-2.08	121.63	126.40
28	S	313	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
28	s	608	CLA	CHA-C1A-NA	-2.08	121.63	126.40
38	s	607	CHL	CMA-C3A-C2A	2.08	122.22	113.83
28	Y	602	CLA	C2D-C1D-ND	2.08	111.64	110.10
28	R	602	CLA	CHA-C1A-NA	-2.08	121.63	126.40
28	r	604	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
28	S	309	CLA	CHA-C1A-NA	-2.08	121.64	126.40
38	Y	606	CHL	CHD-C4C-C3C	2.08	127.90	124.84
28	c	512	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
30	d	406	BCR	C16-C15-C14	-2.08	119.22	123.47
30	H	101	BCR	C37-C22-C21	-2.08	120.01	122.92
28	s	611	CLA	O2A-CGA-CBA	2.08	118.43	111.91
30	c	514	BCR	C11-C12-C13	-2.08	120.58	126.42
39	R	614	LUT	C28-C29-C30	-2.08	115.75	118.94
28	C	503	CLA	CHA-C1A-NA	-2.08	121.64	126.40
28	N	604	CLA	CHA-C1A-NA	-2.08	121.64	126.40
40	y	318	NEX	C38-C25-C26	-2.08	118.78	122.26
39	y	316	LUT	C40-C33-C32	2.08	121.35	118.08
28	C	502	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
28	s	610	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
28	G	614	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	d	406	BCR	C23-C24-C25	-2.08	121.37	127.20
38	g	606	CHL	C3A-C2A-C1A	2.08	104.45	101.34
28	n	611	CLA	O2A-CGA-CBA	2.07	118.42	111.91
40	Y	618	NEX	C40-C33-C34	-2.07	120.02	122.92
28	c	501	CLA	CHA-C1A-NA	-2.07	121.65	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	g	601	CHL	CHB-C4A-NA	2.07	127.38	124.51
40	N	617	NEX	C40-C33-C34	-2.07	120.02	122.92
28	C	513	CLA	C1-O2A-CGA	2.07	121.89	116.44
28	y	304	CLA	O2A-CGA-CBA	2.07	118.42	111.91
39	S	315	LUT	C10-C11-C12	-2.07	116.75	123.22
39	S	315	LUT	C20-C13-C12	2.07	121.34	118.08
39	s	615	LUT	C31-C32-C33	-2.07	120.59	126.42
39	s	615	LUT	C8-C7-C6	-2.07	121.38	127.20
30	C	515	BCR	C15-C16-C17	-2.07	119.23	123.47
39	y	315	LUT	C21-C26-C27	-2.07	110.08	112.70
28	b	613	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	c	512	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	y	304	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	R	601	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
28	D	403	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	i	101	BCR	C20-C19-C18	-2.07	120.60	126.42
38	Y	608	CHL	CMA-C3A-C2A	2.07	122.18	113.83
28	b	610	CLA	CHA-C1A-NA	-2.07	121.66	126.40
38	s	607	CHL	CHC-C1C-NC	2.07	127.34	124.20
28	S	311	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
32	d	409	LMG	C8-O7-C10	-2.07	112.70	117.79
28	y	303	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
28	g	613	CLA	CHA-C1A-NA	-2.07	121.66	126.40
28	c	504	CLA	O2A-CGA-CBA	2.07	118.39	111.91
28	N	612	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
39	n	615	LUT	C4-C5-C6	-2.07	116.24	120.85
28	R	609	CLA	CHA-C1A-NA	-2.07	121.67	126.40
28	n	602	CLA	CHA-C1A-NA	-2.07	121.67	126.40
28	b	605	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
28	N	611	CLA	CHA-C1A-NA	-2.07	121.67	126.40
28	R	612	CLA	CHA-C1A-NA	-2.07	121.67	126.40
38	y	302	CHL	CHB-C4A-NA	2.07	127.37	124.51
38	G	607	CHL	CMA-C3A-C2A	2.06	122.16	113.83
28	B	610	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
28	c	502	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
28	Y	603	CLA	CHA-C1A-NA	-2.06	121.67	126.40
28	y	313	CLA	CHA-C1A-NA	-2.06	121.67	126.40
38	S	306	CHL	CHD-C4C-C3C	2.06	127.88	124.84
36	C	518	DGD	O1G-C1A-O1A	-2.06	118.38	123.59
28	g	602	CLA	CHA-C1A-NA	-2.06	121.67	126.40
28	r	604	CLA	CHA-C1A-NA	-2.06	121.67	126.40
28	g	610	CLA	C4D-CHA-C1A	2.06	123.76	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	610	CLA	CHA-C1A-NA	-2.06	121.67	126.40
38	r	606	CHL	C1-O2A-CGA	2.06	121.86	116.44
40	s	616	NEX	C40-C33-C34	-2.06	120.03	122.92
28	R	611	CLA	CHA-C1A-NA	-2.06	121.67	126.40
28	S	304	CLA	CHA-C1A-NA	-2.06	121.67	126.40
40	N	617	NEX	C16-C1-C6	-2.06	108.63	110.47
28	S	305	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
28	B	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
30	b	619	BCR	C11-C12-C13	-2.06	120.62	126.42
28	c	506	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
28	c	505	CLA	CHA-C1A-NA	-2.06	121.68	126.40
30	H	101	BCR	C36-C18-C17	-2.06	120.04	122.92
28	Y	612	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	d	404	CLA	CHA-C1A-NA	-2.06	121.68	126.40
39	n	615	LUT	C8-C7-C6	-2.06	121.42	127.20
28	C	512	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
28	g	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40
28	G	602	CLA	C6-C5-C3	-2.06	108.05	113.45
38	Y	601	CHL	C4A-NA-C1A	2.06	107.63	106.71
28	c	502	CLA	CHA-C1A-NA	-2.06	121.68	126.40
28	N	613	CLA	O2A-CGA-CBA	2.06	118.37	111.91
28	S	310	CLA	CHA-C1A-NA	-2.06	121.68	126.40
28	c	507	CLA	O2A-CGA-CBA	2.06	118.37	111.91
38	N	605	CHL	CHD-C4C-C3C	2.06	127.87	124.84
30	d	406	BCR	C30-C25-C24	2.06	121.60	115.78
28	s	613	CLA	CHA-C1A-NA	-2.06	121.69	126.40
39	g	615	LUT	C11-C12-C13	-2.06	120.64	126.42
39	N	616	LUT	C31-C30-C29	-2.06	124.38	127.31
28	y	305	CLA	CHA-C1A-NA	-2.06	121.69	126.40
28	C	512	CLA	CHA-C1A-NA	-2.05	121.69	126.40
38	N	605	CHL	C1-O2A-CGA	2.05	122.70	116.73
28	G	611	CLA	CHA-C1A-NA	-2.05	121.69	126.40
28	B	616	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
28	G	603	CLA	O2A-CGA-CBA	2.05	118.35	111.91
38	n	605	CHL	CHC-C1C-NC	2.05	127.32	124.20
28	b	606	CLA	CAA-C2A-C3A	-2.05	107.15	112.78
28	D	401	CLA	CHA-C1A-NA	-2.05	121.69	126.40
39	s	614	LUT	C20-C13-C14	-2.05	120.05	122.92
28	A	405	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	b	620	LMG	O8-C28-O10	-2.05	118.41	123.59
28	n	612	CLA	C1-C2-C3	-2.05	122.49	126.04
28	r	610	CLA	CMD-C2D-C3D	-2.05	122.89	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	610	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	t	101	BCR	C37-C22-C21	-2.05	120.05	122.92
28	c	504	CLA	C1-O2A-CGA	2.05	121.82	116.44
28	s	603	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
35	w	102	LHG	C5-O7-C7	-2.05	112.74	117.79
28	Y	602	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
28	n	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
32	a	413	LMG	O7-C10-O9	-2.05	118.75	123.70
28	c	504	CLA	C1-C2-C3	-2.05	122.50	126.04
28	d	405	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	G	612	CLA	CHA-C1A-NA	-2.05	121.71	126.40
38	G	606	CHL	CHB-C4A-NA	2.05	127.34	124.51
32	a	413	LMG	C8-O7-C10	-2.05	112.75	117.79
28	b	611	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
38	s	601	CHL	CHD-C4C-C3C	2.05	127.85	124.84
28	Y	610	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
28	s	609	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	G	602	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
38	S	302	CHL	CHD-C4C-C3C	2.05	127.85	124.84
28	n	611	CLA	C11-C10-C8	-2.05	109.31	115.92
28	g	611	CLA	CBB-CAB-C3B	-2.05	117.44	127.62
28	C	503	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
28	G	604	CLA	O2A-CGA-CBA	2.04	118.33	111.91
38	G	605	CHL	C4A-NA-C1A	2.04	107.62	106.71
28	B	614	CLA	C6-C5-C3	-2.04	108.09	113.45
38	r	606	CHL	CHD-C4C-C3C	2.04	127.84	124.84
35	G	618	LHG	O7-C7-O9	-2.04	118.76	123.70
28	g	610	CLA	C2A-C1A-CHA	2.04	127.43	123.86
28	b	608	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	r	610	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	Y	614	CLA	CHA-C1A-NA	-2.04	121.72	126.40
30	B	618	BCR	C20-C19-C18	-2.04	120.68	126.42
28	R	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	D	404	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
28	y	310	CLA	C11-C10-C8	-2.04	109.32	115.92
39	Y	616	LUT	C18-C5-C6	-2.04	122.24	124.53
35	b	621	LHG	C5-O7-C7	-2.04	112.77	117.79
28	N	602	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	Y	603	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
28	b	614	CLA	O2A-CGA-CBA	2.04	118.31	111.91
39	g	616	LUT	C21-C26-C25	2.04	115.07	111.42
38	G	601	CHL	CMA-C3A-C2A	2.04	122.05	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	612	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
28	G	610	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	g	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
38	y	307	CHL	CHD-C4C-C3C	2.04	127.83	124.84
28	c	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
37	E	101	HEM	CAA-CBA-CGA	-2.04	109.22	113.60
28	N	612	CLA	CHA-C1A-NA	-2.04	121.73	126.40
28	N	614	CLA	CHA-C1A-NA	-2.04	121.73	126.40
28	S	313	CLA	O2A-CGA-CBA	2.04	118.30	111.91
39	Y	616	LUT	C11-C12-C13	-2.04	120.70	126.42
28	C	507	CLA	C16-C15-C13	-2.04	109.34	115.92
38	S	307	CHL	C4A-NA-C1A	2.04	107.62	106.71
28	a	406	CLA	CHA-C1A-NA	-2.04	121.74	126.40
38	n	608	CHL	CMA-C3A-C2A	2.03	122.04	113.83
39	n	615	LUT	C40-C33-C32	2.03	121.28	118.08
28	S	310	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
28	B	614	CLA	CHA-C1A-NA	-2.03	121.74	126.40
28	y	303	CLA	CHA-C1A-NA	-2.03	121.74	126.40
39	n	615	LUT	C31-C30-C29	-2.03	124.41	127.31
28	n	613	CLA	CAC-C3C-C4C	2.03	127.45	124.81
28	B	615	CLA	CHA-C1A-NA	-2.03	121.74	126.40
28	s	602	CLA	CHA-C1A-NA	-2.03	121.74	126.40
38	y	306	CHL	CHB-C4A-NA	2.03	127.32	124.51
39	y	316	LUT	C15-C35-C34	-2.03	119.31	123.47
28	B	609	CLA	CHA-C1A-NA	-2.03	121.74	126.40
28	Y	610	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
38	g	607	CHL	CHD-C4C-C3C	2.03	127.83	124.84
28	y	314	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	A	408	CLA	C1-C2-C3	-2.03	122.53	126.04
30	k	101	BCR	C23-C24-C25	-2.03	121.50	127.20
28	r	612	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
36	c	516	DGD	O6D-C5D-C6D	2.03	110.76	106.67
38	y	306	CHL	C1-O2A-CGA	2.03	122.63	116.73
28	n	604	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	r	613	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
28	G	613	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	g	614	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	c	513	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	S	304	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
41	r	615	XAT	C20-C13-C14	-2.03	120.08	122.92
39	S	316	LUT	C38-C25-C24	-2.03	119.22	123.56
38	n	607	CHL	CMA-C3A-C2A	2.03	122.00	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	n	616	LUT	C21-C26-C25	2.03	115.05	111.42
41	R	615	XAT	C20-C13-C14	-2.03	120.08	122.92
28	c	506	CLA	CHA-C1A-NA	-2.03	121.76	126.40
28	B	608	CLA	CHA-C1A-NA	-2.02	121.76	126.40
28	r	609	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	r	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
39	Y	615	LUT	C19-C9-C8	2.02	121.27	118.08
28	C	505	CLA	CHA-C1A-NA	-2.02	121.76	126.40
38	R	605	CHL	CHD-C4C-C3C	2.02	127.81	124.84
30	D	405	BCR	C2-C1-C6	2.02	113.60	110.48
30	T	101	BCR	C29-C30-C25	2.02	113.60	110.48
38	y	308	CHL	CMA-C3A-C2A	2.02	121.99	113.83
39	R	614	LUT	C18-C5-C4	2.02	118.10	114.36
28	c	506	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	n	603	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	y	304	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	R	610	CLA	CHA-C1A-NA	-2.02	121.77	126.40
28	C	507	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	c	501	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
35	b	624	LHG	O7-C7-O9	-2.02	118.82	123.70
28	b	611	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
28	G	603	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
28	C	511	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	c	503	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
38	G	607	CHL	C4A-NA-C1A	2.02	107.61	106.71
28	r	611	CLA	C1D-CHD-C4C	-2.02	121.70	126.06
28	g	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
28	S	311	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
28	c	504	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
32	B	621	LMG	O8-C28-O10	-2.02	118.50	123.59
28	B	605	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
28	C	501	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
38	S	308	CHL	CMA-C3A-C2A	2.02	121.97	113.83
28	C	510	CLA	CHA-C1A-NA	-2.02	121.78	126.40
38	N	605	CHL	CHC-C1C-NC	2.02	127.26	124.20
28	C	504	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
28	b	615	CLA	CHA-C1A-NA	-2.02	121.78	126.40
38	G	607	CHL	CHC-C1C-NC	2.02	127.26	124.20
38	g	607	CHL	CHC-C1C-NC	2.02	127.26	124.20
39	r	614	LUT	C11-C12-C13	2.02	132.08	126.42
28	c	511	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
28	b	607	CLA	CAA-C2A-C3A	-2.02	107.26	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	614	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
28	b	601	CLA	CHA-C1A-NA	-2.01	121.78	126.40
28	y	310	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
30	h	101	BCR	C8-C7-C6	-2.01	121.55	127.20
28	B	612	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
28	N	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
30	h	101	BCR	C16-C15-C14	-2.01	119.35	123.47
38	S	307	CHL	CMA-C3A-C2A	2.01	121.94	113.83
38	s	605	CHL	C2C-C3C-C4C	2.01	107.92	106.49
28	b	614	CLA	CHA-C1A-NA	-2.01	121.79	126.40
28	S	304	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	b	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
38	n	607	CHL	C2B-C1B-NB	-2.01	108.88	110.23
28	N	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	B	612	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
28	d	404	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	g	604	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	s	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
40	r	616	NEX	C40-C33-C34	-2.01	120.11	122.92
38	n	601	CHL	CMA-C3A-C2A	2.01	121.93	113.83
28	r	609	CLA	CHA-C1A-NA	-2.01	121.80	126.40
38	S	306	CHL	CHB-C4A-NA	2.01	127.29	124.51
39	R	614	LUT	C8-C7-C6	-2.01	121.56	127.20
28	c	507	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	s	611	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	r	609	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
28	B	602	CLA	O2A-CGA-CBA	2.01	118.20	111.91
38	Y	605	CHL	CHC-C1C-NC	2.01	127.25	124.20
38	R	607	CHL	C4A-NA-C1A	2.01	107.61	106.71
39	R	614	LUT	C17-C1-C6	-2.01	107.05	110.30
28	r	602	CLA	CHA-C1A-NA	-2.01	121.81	126.40
39	s	615	LUT	C20-C13-C14	-2.01	120.11	122.92
28	n	604	CLA	O2A-CGA-CBA	2.00	118.20	111.91
39	S	316	LUT	C15-C35-C34	-2.00	119.37	123.47
28	b	607	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
38	n	605	CHL	CMA-C3A-C2A	2.00	121.91	113.83
28	C	502	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
30	a	410	BCR	C34-C9-C10	-2.00	120.12	122.92
28	R	604	CLA	CHA-C1A-NA	-2.00	121.81	126.40
28	D	401	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
28	b	610	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
30	b	619	BCR	C34-C9-C10	-2.00	120.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	t	101	BCR	C36-C18-C17	-2.00	120.12	122.92
40	g	617	NEX	C20-C13-C14	-2.00	120.12	122.92
28	g	602	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	r	602	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	G	614	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
31	L	103	SQD	O8-S-C6	-2.00	102.55	105.74
28	c	512	CLA	O2A-CGA-CBA	2.00	118.19	111.91
28	G	604	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	y	303	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	S	305	CLA	C1D-ND-C4D	-2.00	104.91	106.33
28	S	303	CLA	CHA-C1A-NA	-2.00	121.82	126.40

There are no chirality outliers.

All (4063) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	405	CLA	C6-C7-C8-C9
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	408	CLA	O2A-C1-C2-C3
28	B	601	CLA	O1A-CGA-O2A-C1
28	B	601	CLA	CAD-CBD-CGD-O1D
28	B	601	CLA	CAD-CBD-CGD-O2D
28	B	603	CLA	CBD-CGD-O2D-CED
28	B	604	CLA	C1A-C2A-CAA-CBA
28	B	604	CLA	CAD-CBD-CGD-O1D
28	B	604	CLA	CAD-CBD-CGD-O2D
28	B	605	CLA	CBA-CGA-O2A-C1
28	B	605	CLA	O1A-CGA-O2A-C1
28	B	605	CLA	CHA-CBD-CGD-O1D
28	B	605	CLA	CAD-CBD-CGD-O1D
28	B	605	CLA	O2A-C1-C2-C3
28	B	605	CLA	C6-C7-C8-C9
28	B	607	CLA	C1A-C2A-CAA-CBA
28	B	607	CLA	C3A-C2A-CAA-CBA
28	B	607	CLA	CHA-CBD-CGD-O1D
28	B	607	CLA	CAD-CBD-CGD-O1D
28	B	607	CLA	CAD-CBD-CGD-O2D
28	B	608	CLA	C6-C7-C8-C9
28	B	609	CLA	C3A-C2A-CAA-CBA
28	B	609	CLA	CAD-CBD-CGD-O1D
28	B	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	B	610	CLA	CBD-CGD-O2D-CED
28	B	611	CLA	C1A-C2A-CAA-CBA
28	B	612	CLA	C1A-C2A-CAA-CBA
28	B	612	CLA	C3A-C2A-CAA-CBA
28	B	612	CLA	C2-C1-O2A-CGA
28	B	613	CLA	CBD-CGD-O2D-CED
28	B	614	CLA	CAD-CBD-CGD-O1D
28	B	614	CLA	CAD-CBD-CGD-O2D
28	C	502	CLA	C1A-C2A-CAA-CBA
28	C	502	CLA	CAD-CBD-CGD-O1D
28	C	502	CLA	CAD-CBD-CGD-O2D
28	C	502	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	C1A-C2A-CAA-CBA
28	C	504	CLA	C1A-C2A-CAA-CBA
28	C	504	CLA	C3A-C2A-CAA-CBA
28	C	504	CLA	CHA-CBD-CGD-O1D
28	C	504	CLA	CHA-CBD-CGD-O2D
28	C	504	CLA	CAD-CBD-CGD-O1D
28	C	504	CLA	CAD-CBD-CGD-O2D
28	C	505	CLA	CAD-CBD-CGD-O1D
28	C	507	CLA	C1A-C2A-CAA-CBA
28	C	507	CLA	C3A-C2A-CAA-CBA
28	C	507	CLA	CHA-CBD-CGD-O2D
28	C	507	CLA	C11-C12-C13-C14
28	C	509	CLA	C1A-C2A-CAA-CBA
28	C	509	CLA	C6-C7-C8-C9
28	C	512	CLA	C1A-C2A-CAA-CBA
28	C	512	CLA	C3A-C2A-CAA-CBA
28	C	512	CLA	C6-C7-C8-C9
28	C	513	CLA	C1A-C2A-CAA-CBA
28	D	401	CLA	C1A-C2A-CAA-CBA
28	D	403	CLA	C1A-C2A-CAA-CBA
28	D	403	CLA	C3A-C2A-CAA-CBA
28	D	403	CLA	C6-C7-C8-C9
28	D	404	CLA	CBD-CGD-O2D-CED
28	G	603	CLA	C1A-C2A-CAA-CBA
28	G	603	CLA	C3A-C2A-CAA-CBA
28	G	603	CLA	CHA-CBD-CGD-O2D
28	G	604	CLA	C3A-C2A-CAA-CBA
28	G	610	CLA	CBD-CGD-O2D-CED
28	G	611	CLA	C3A-C2A-CAA-CBA
28	G	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	G	612	CLA	CHA-CBD-CGD-O2D
28	G	613	CLA	CHA-CBD-CGD-O1D
28	G	613	CLA	CHA-CBD-CGD-O2D
28	G	614	CLA	CHA-CBD-CGD-O1D
28	G	614	CLA	CHA-CBD-CGD-O2D
28	N	603	CLA	C2-C1-O2A-CGA
28	N	604	CLA	CAD-CBD-CGD-O1D
28	N	604	CLA	CAD-CBD-CGD-O2D
28	N	610	CLA	C2-C1-O2A-CGA
28	N	612	CLA	CHA-CBD-CGD-O1D
28	N	612	CLA	CHA-CBD-CGD-O2D
28	N	614	CLA	CBA-CGA-O2A-C1
28	R	601	CLA	C3A-C2A-CAA-CBA
28	R	601	CLA	CBD-CGD-O2D-CED
28	R	604	CLA	C1A-C2A-CAA-CBA
28	R	604	CLA	CHA-CBD-CGD-O1D
28	R	604	CLA	CHA-CBD-CGD-O2D
28	R	608	CLA	C1A-C2A-CAA-CBA
28	R	608	CLA	C3A-C2A-CAA-CBA
28	R	610	CLA	C1A-C2A-CAA-CBA
28	R	610	CLA	C3A-C2A-CAA-CBA
28	R	610	CLA	CHA-CBD-CGD-O1D
28	R	610	CLA	CBD-CGD-O2D-CED
28	R	611	CLA	CBA-CGA-O2A-C1
28	R	611	CLA	O1A-CGA-O2A-C1
28	R	612	CLA	CBD-CGD-O2D-CED
28	R	613	CLA	C1A-C2A-CAA-CBA
28	R	613	CLA	C3A-C2A-CAA-CBA
28	R	613	CLA	CHA-CBD-CGD-O1D
28	R	613	CLA	CHA-CBD-CGD-O2D
28	S	303	CLA	C11-C10-C8-C9
28	S	304	CLA	C1A-C2A-CAA-CBA
28	S	304	CLA	C3A-C2A-CAA-CBA
28	S	305	CLA	C1A-C2A-CAA-CBA
28	S	305	CLA	C3A-C2A-CAA-CBA
28	S	305	CLA	CBA-CGA-O2A-C1
28	S	305	CLA	O1A-CGA-O2A-C1
28	S	305	CLA	CHA-CBD-CGD-O1D
28	S	305	CLA	CHA-CBD-CGD-O2D
28	S	305	CLA	CAD-CBD-CGD-O1D
28	S	309	CLA	C3A-C2A-CAA-CBA
28	S	310	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	S	310	CLA	CHA-CBD-CGD-O2D
28	S	310	CLA	CBD-CGD-O2D-CED
28	S	311	CLA	C1A-C2A-CAA-CBA
28	S	311	CLA	CBA-CGA-O2A-C1
28	S	311	CLA	O1A-CGA-O2A-C1
28	S	312	CLA	C2-C1-O2A-CGA
28	Y	603	CLA	C2-C1-O2A-CGA
28	Y	604	CLA	C1A-C2A-CAA-CBA
28	Y	604	CLA	C3A-C2A-CAA-CBA
28	Y	611	CLA	CBA-CGA-O2A-C1
28	Y	613	CLA	CBD-CGD-O2D-CED
28	Y	614	CLA	C2-C1-O2A-CGA
28	Y	614	CLA	CBD-CGD-O2D-CED
28	a	406	CLA	C11-C10-C8-C7
28	a	407	CLA	C1A-C2A-CAA-CBA
28	a	407	CLA	C2A-CAA-CBA-CGA
28	b	601	CLA	C2A-CAA-CBA-CGA
28	b	601	CLA	CAD-CBD-CGD-O1D
28	b	601	CLA	CAD-CBD-CGD-O2D
28	b	602	CLA	C6-C7-C8-C9
28	b	604	CLA	C1A-C2A-CAA-CBA
28	b	604	CLA	CAD-CBD-CGD-O1D
28	b	606	CLA	CHA-CBD-CGD-O1D
28	b	607	CLA	CAD-CBD-CGD-O1D
28	b	607	CLA	CAD-CBD-CGD-O2D
28	b	608	CLA	CBD-CGD-O2D-CED
28	b	609	CLA	C1A-C2A-CAA-CBA
28	b	609	CLA	C3A-C2A-CAA-CBA
28	b	609	CLA	CHA-CBD-CGD-O1D
28	b	609	CLA	CAD-CBD-CGD-O1D
28	b	609	CLA	CAD-CBD-CGD-O2D
28	b	611	CLA	C1A-C2A-CAA-CBA
28	b	612	CLA	C1A-C2A-CAA-CBA
28	b	612	CLA	C3A-C2A-CAA-CBA
28	b	612	CLA	CHA-CBD-CGD-O1D
28	b	612	CLA	CHA-CBD-CGD-O2D
28	b	612	CLA	CAD-CBD-CGD-O1D
28	b	612	CLA	CAD-CBD-CGD-O2D
28	b	614	CLA	C1A-C2A-CAA-CBA
28	b	614	CLA	C3A-C2A-CAA-CBA
28	b	614	CLA	CAD-CBD-CGD-O1D
28	b	614	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	b	616	CLA	CBA-CGA-O2A-C1
28	b	616	CLA	O1A-CGA-O2A-C1
28	c	501	CLA	C14-C13-C15-C16
28	c	502	CLA	CAD-CBD-CGD-O1D
28	c	502	CLA	CAD-CBD-CGD-O2D
28	c	502	CLA	CBD-CGD-O2D-CED
28	c	502	CLA	C6-C7-C8-C9
28	c	503	CLA	CHA-CBD-CGD-O1D
28	c	503	CLA	CHA-CBD-CGD-O2D
28	c	503	CLA	CAD-CBD-CGD-O1D
28	c	504	CLA	CAD-CBD-CGD-O1D
28	c	504	CLA	CAD-CBD-CGD-O2D
28	c	505	CLA	CAD-CBD-CGD-O1D
28	c	505	CLA	CAD-CBD-CGD-O2D
28	c	506	CLA	C1A-C2A-CAA-CBA
28	c	506	CLA	C3A-C2A-CAA-CBA
28	c	506	CLA	O2A-C1-C2-C3
28	c	507	CLA	CHA-CBD-CGD-O2D
28	c	510	CLA	C1A-C2A-CAA-CBA
28	c	510	CLA	C3A-C2A-CAA-CBA
28	c	512	CLA	CAD-CBD-CGD-O1D
28	c	512	CLA	CAD-CBD-CGD-O2D
28	c	513	CLA	C1A-C2A-CAA-CBA
28	c	513	CLA	C11-C10-C8-C9
28	d	401	CLA	C1A-C2A-CAA-CBA
28	d	404	CLA	C1A-C2A-CAA-CBA
28	d	404	CLA	C3A-C2A-CAA-CBA
28	d	405	CLA	C1A-C2A-CAA-CBA
28	d	405	CLA	C3A-C2A-CAA-CBA
28	d	405	CLA	CBD-CGD-O2D-CED
28	g	604	CLA	C1A-C2A-CAA-CBA
28	g	604	CLA	C3A-C2A-CAA-CBA
28	g	612	CLA	CHA-CBD-CGD-O1D
28	g	612	CLA	CHA-CBD-CGD-O2D
28	g	614	CLA	C3A-C2A-CAA-CBA
28	g	614	CLA	CHA-CBD-CGD-O1D
28	g	614	CLA	CHA-CBD-CGD-O2D
28	g	614	CLA	CBD-CGD-O2D-CED
28	n	603	CLA	C1A-C2A-CAA-CBA
28	n	603	CLA	CHA-CBD-CGD-O1D
28	n	603	CLA	CHA-CBD-CGD-O2D
28	n	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	n	604	CLA	CHA-CBD-CGD-O1D
28	n	604	CLA	CHA-CBD-CGD-O2D
28	n	610	CLA	C1A-C2A-CAA-CBA
28	n	610	CLA	C2-C1-O2A-CGA
28	n	610	CLA	CBD-CGD-O2D-CED
28	n	612	CLA	C2-C1-O2A-CGA
28	n	613	CLA	CBD-CGD-O2D-CED
28	n	614	CLA	CBD-CGD-O2D-CED
28	r	601	CLA	CBD-CGD-O2D-CED
28	r	603	CLA	CHA-CBD-CGD-O1D
28	r	603	CLA	CHA-CBD-CGD-O2D
28	r	603	CLA	CAD-CBD-CGD-O1D
28	r	603	CLA	O2A-C1-C2-C3
28	r	604	CLA	C1A-C2A-CAA-CBA
28	r	604	CLA	C2-C1-O2A-CGA
28	r	604	CLA	CHA-CBD-CGD-O1D
28	r	604	CLA	CHA-CBD-CGD-O2D
28	r	608	CLA	C1A-C2A-CAA-CBA
28	r	608	CLA	C3A-C2A-CAA-CBA
28	r	608	CLA	CBD-CGD-O2D-CED
28	r	609	CLA	CBD-CGD-O2D-CED
28	r	610	CLA	C1A-C2A-CAA-CBA
28	r	610	CLA	C3A-C2A-CAA-CBA
28	r	610	CLA	CBA-CGA-O2A-C1
28	r	610	CLA	O1A-CGA-O2A-C1
28	r	610	CLA	CHA-CBD-CGD-O1D
28	r	610	CLA	CHA-CBD-CGD-O2D
28	r	610	CLA	CBD-CGD-O2D-CED
28	r	611	CLA	CBD-CGD-O2D-CED
28	r	612	CLA	C1A-C2A-CAA-CBA
28	r	612	CLA	C3A-C2A-CAA-CBA
28	r	613	CLA	C1A-C2A-CAA-CBA
28	r	613	CLA	C3A-C2A-CAA-CBA
28	s	604	CLA	C1A-C2A-CAA-CBA
28	s	604	CLA	C3A-C2A-CAA-CBA
28	s	608	CLA	C3A-C2A-CAA-CBA
28	s	609	CLA	CHA-CBD-CGD-O1D
28	s	609	CLA	CHA-CBD-CGD-O2D
28	s	609	CLA	CBD-CGD-O2D-CED
28	s	610	CLA	CBA-CGA-O2A-C1
28	s	612	CLA	CBD-CGD-O2D-CED
28	y	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	y	304	CLA	C6-C7-C8-C9
28	y	305	CLA	C1A-C2A-CAA-CBA
28	y	310	CLA	CBD-CGD-O2D-CED
28	y	310	CLA	C2-C3-C5-C6
28	y	310	CLA	C4-C3-C5-C6
28	y	313	CLA	CBD-CGD-O2D-CED
28	y	314	CLA	C3A-C2A-CAA-CBA
29	A	407	PHO	CBA-CGA-O2A-C1
29	A	407	PHO	O1A-CGA-O2A-C1
29	a	408	PHO	CBA-CGA-O2A-C1
29	a	408	PHO	O1A-CGA-O2A-C1
30	A	409	BCR	C1-C6-C7-C8
30	A	409	BCR	C17-C18-C19-C20
30	A	409	BCR	C36-C18-C19-C20
30	A	409	BCR	C19-C20-C21-C22
30	A	409	BCR	C21-C22-C23-C24
30	A	409	BCR	C37-C22-C23-C24
30	A	409	BCR	C23-C24-C25-C26
30	B	617	BCR	C21-C22-C23-C24
30	B	617	BCR	C37-C22-C23-C24
30	B	618	BCR	C1-C6-C7-C8
30	B	618	BCR	C9-C10-C11-C12
30	B	618	BCR	C11-C12-C13-C14
30	B	618	BCR	C17-C18-C19-C20
30	B	618	BCR	C36-C18-C19-C20
30	B	619	BCR	C1-C6-C7-C8
30	B	619	BCR	C21-C22-C23-C24
30	B	619	BCR	C37-C22-C23-C24
30	C	514	BCR	C7-C8-C9-C10
30	C	514	BCR	C7-C8-C9-C34
30	C	514	BCR	C11-C12-C13-C14
30	C	514	BCR	C11-C12-C13-C35
30	C	514	BCR	C36-C18-C19-C20
30	C	514	BCR	C23-C24-C25-C26
30	C	515	BCR	C1-C6-C7-C8
30	C	515	BCR	C7-C8-C9-C10
30	C	515	BCR	C7-C8-C9-C34
30	C	515	BCR	C11-C12-C13-C14
30	C	515	BCR	C11-C12-C13-C35
30	C	515	BCR	C13-C14-C15-C16
30	C	515	BCR	C19-C20-C21-C22
30	C	516	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	516	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C34
30	C	516	BCR	C9-C10-C11-C12
30	C	516	BCR	C17-C18-C19-C20
30	C	516	BCR	C36-C18-C19-C20
30	C	516	BCR	C19-C20-C21-C22
30	D	405	BCR	C7-C8-C9-C10
30	D	405	BCR	C7-C8-C9-C34
30	D	405	BCR	C15-C16-C17-C18
30	D	405	BCR	C19-C20-C21-C22
30	D	405	BCR	C23-C24-C25-C26
30	D	405	BCR	C23-C24-C25-C30
30	H	101	BCR	C7-C8-C9-C10
30	H	101	BCR	C7-C8-C9-C34
30	H	101	BCR	C9-C10-C11-C12
30	H	101	BCR	C11-C12-C13-C14
30	H	101	BCR	C11-C12-C13-C35
30	K	101	BCR	C5-C6-C7-C8
30	K	101	BCR	C7-C8-C9-C10
30	K	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C11-C12-C13-C35
30	K	101	BCR	C17-C18-C19-C20
30	K	101	BCR	C36-C18-C19-C20
30	a	410	BCR	C1-C6-C7-C8
30	a	410	BCR	C7-C8-C9-C10
30	a	410	BCR	C7-C8-C9-C34
30	a	410	BCR	C21-C22-C23-C24
30	a	410	BCR	C37-C22-C23-C24
30	a	410	BCR	C23-C24-C25-C26
30	b	617	BCR	C7-C8-C9-C34
30	b	617	BCR	C37-C22-C23-C24
30	b	617	BCR	C23-C24-C25-C30
30	b	618	BCR	C1-C6-C7-C8
30	b	618	BCR	C21-C22-C23-C24
30	b	618	BCR	C37-C22-C23-C24
30	b	619	BCR	C7-C8-C9-C34
30	c	514	BCR	C7-C8-C9-C34
30	c	514	BCR	C21-C22-C23-C24
30	c	514	BCR	C37-C22-C23-C24
30	c	515	BCR	C1-C6-C7-C8
30	c	515	BCR	C5-C6-C7-C8
30	c	515	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
30	c	515	BCR	C21-C22-C23-C24
30	c	515	BCR	C37-C22-C23-C24
30	h	101	BCR	C1-C6-C7-C8
30	h	101	BCR	C5-C6-C7-C8
30	h	101	BCR	C7-C8-C9-C10
30	h	101	BCR	C7-C8-C9-C34
30	h	101	BCR	C9-C10-C11-C12
30	h	101	BCR	C11-C12-C13-C14
30	h	101	BCR	C11-C12-C13-C35
30	h	101	BCR	C21-C22-C23-C24
30	h	101	BCR	C37-C22-C23-C24
30	k	101	BCR	C11-C12-C13-C14
30	k	101	BCR	C11-C12-C13-C35
30	k	101	BCR	C15-C16-C17-C18
30	k	101	BCR	C23-C24-C25-C26
30	t	101	BCR	C1-C6-C7-C8
30	t	101	BCR	C7-C8-C9-C10
30	t	101	BCR	C7-C8-C9-C34
30	t	101	BCR	C11-C12-C13-C14
30	t	101	BCR	C11-C12-C13-C35
31	A	410	SQD	O5-C5-C6-S
31	A	414	SQD	O5-C1-O6-C44
31	A	414	SQD	O5-C5-C6-S
31	B	620	SQD	O49-C7-O47-C45
31	B	620	SQD	C8-C7-O47-C45
31	L	101	SQD	O49-C7-O47-C45
31	L	101	SQD	C8-C7-O47-C45
31	L	101	SQD	O5-C5-C6-S
31	L	103	SQD	O49-C7-O47-C45
31	M	101	SQD	O5-C1-O6-C44
31	M	101	SQD	O49-C7-O47-C45
31	M	101	SQD	O5-C5-C6-S
31	a	411	SQD	O49-C7-O47-C45
31	a	411	SQD	C8-C7-O47-C45
31	a	411	SQD	O5-C5-C6-S
31	a	414	SQD	O5-C1-O6-C44
31	a	414	SQD	O5-C5-C6-S
32	A	413	LMG	C11-C10-O7-C8
32	B	621	LMG	O9-C10-O7-C8
32	B	621	LMG	C11-C10-O7-C8
32	B	624	LMG	C11-C10-O7-C8
32	C	520	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	C	522	LMG	O6-C1-O1-C7
32	C	522	LMG	C11-C10-O7-C8
32	b	620	LMG	O9-C10-O7-C8
32	b	620	LMG	C11-C10-O7-C8
32	c	521	LMG	C11-C10-O7-C8
35	A	416	LHG	O1-C1-C2-C3
35	A	416	LHG	C4-O6-P-O5
35	A	416	LHG	O6-C4-C5-O7
35	B	622	LHG	O1-C1-C2-C3
35	B	622	LHG	C3-O3-P-O5
35	B	622	LHG	C4-O6-P-O3
35	B	622	LHG	C4-O6-P-O4
35	B	622	LHG	C4-O6-P-O5
35	B	622	LHG	O6-C4-C5-O7
35	B	623	LHG	O1-C1-C2-C3
35	B	623	LHG	O2-C2-C3-O3
35	B	623	LHG	C4-O6-P-O3
35	B	625	LHG	O1-C1-C2-C3
35	B	625	LHG	C1-C2-C3-O3
35	B	625	LHG	C4-O6-P-O5
35	C	521	LHG	O1-C1-C2-C3
35	C	521	LHG	C1-C2-C3-O3
35	C	521	LHG	C4-O6-P-O3
35	D	407	LHG	O1-C1-C2-C3
35	D	407	LHG	C1-C2-C3-O3
35	D	407	LHG	C4-O6-P-O3
35	D	407	LHG	C4-O6-P-O4
35	D	407	LHG	C4-O6-P-O5
35	G	618	LHG	O1-C1-C2-O2
35	G	618	LHG	O1-C1-C2-C3
35	G	618	LHG	C1-C2-C3-O3
35	G	618	LHG	C3-O3-P-O5
35	G	618	LHG	C4-O6-P-O3
35	G	618	LHG	C4-O6-P-O4
35	G	618	LHG	C4-O6-P-O5
35	L	102	LHG	C4-O6-P-O3
35	L	102	LHG	C4-O6-P-O4
35	L	102	LHG	C4-O6-P-O5
35	L	102	LHG	C5-C6-O8-C23
35	N	618	LHG	C3-O3-P-O4
35	N	618	LHG	C4-O6-P-O4
35	R	616	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
35	R	616	LHG	C4-O6-P-O4
35	R	616	LHG	O7-C5-C6-O8
35	R	616	LHG	O9-C7-O7-C5
35	R	616	LHG	C8-C7-O7-C5
35	S	301	LHG	O1-C1-C2-C3
35	S	301	LHG	C3-O3-P-O4
35	S	301	LHG	C4-O6-P-O3
35	S	301	LHG	C4-O6-P-O4
35	S	301	LHG	C4-O6-P-O5
35	S	317	LHG	O1-C1-C2-C3
35	S	317	LHG	C1-C2-C3-O3
35	S	317	LHG	C3-O3-P-O4
35	S	317	LHG	C3-O3-P-O5
35	S	317	LHG	C3-O3-P-O6
35	W	101	LHG	O1-C1-C2-C3
35	W	101	LHG	C1-C2-C3-O3
35	W	101	LHG	C2-C3-O3-P
35	W	101	LHG	C3-O3-P-O4
35	W	101	LHG	C4-O6-P-O4
35	W	101	LHG	C4-O6-P-O5
35	Y	619	LHG	O1-C1-C2-O2
35	Y	619	LHG	O1-C1-C2-C3
35	Y	619	LHG	O2-C2-C3-O3
35	Y	619	LHG	C3-O3-P-O4
35	Y	619	LHG	C3-O3-P-O5
35	Y	619	LHG	C3-O3-P-O6
35	Y	619	LHG	C4-O6-P-O4
35	a	415	LHG	O1-C1-C2-O2
35	a	415	LHG	C1-C2-C3-O3
35	a	415	LHG	O6-C4-C5-O7
35	b	621	LHG	C4-O6-P-O3
35	b	621	LHG	C8-C7-O7-C5
35	b	622	LHG	O1-C1-C2-O2
35	b	622	LHG	C1-C2-C3-O3
35	b	622	LHG	C2-C3-O3-P
35	b	624	LHG	C1-C2-C3-O3
35	b	624	LHG	C3-O3-P-O4
35	b	624	LHG	C3-O3-P-O5
35	b	624	LHG	C3-O3-P-O6
35	c	519	LHG	O1-C1-C2-O2
35	c	519	LHG	C3-O3-P-O4
35	c	520	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
35	c	520	LHG	C3-O3-P-O4
35	c	520	LHG	C4-O6-P-O3
35	c	520	LHG	C4-O6-P-O4
35	c	520	LHG	C4-O6-P-O5
35	d	408	LHG	O1-C1-C2-C3
35	g	618	LHG	C1-C2-C3-O3
35	g	618	LHG	C4-O6-P-O3
35	g	618	LHG	C4-O6-P-O4
35	g	618	LHG	C4-O6-P-O5
35	n	618	LHG	C3-O3-P-O4
35	n	618	LHG	C4-O6-P-O4
35	r	617	LHG	O2-C2-C3-O3
35	r	617	LHG	C4-O6-P-O3
35	r	617	LHG	C4-O6-P-O4
35	r	617	LHG	C4-O6-P-O5
35	r	617	LHG	O7-C5-C6-O8
35	s	617	LHG	O1-C1-C2-C3
35	s	617	LHG	C3-O3-P-O5
35	s	617	LHG	O10-C23-O8-C6
35	s	617	LHG	C24-C23-O8-C6
35	w	102	LHG	C1-C2-C3-O3
35	y	319	LHG	C3-O3-P-O4
36	A	417	DGD	C2A-C1A-O1G-C1G
36	A	417	DGD	O1A-C1A-O1G-C1G
36	A	417	DGD	C2B-C1B-O2G-C2G
36	A	417	DGD	C2D-C1D-O3G-C3G
36	A	417	DGD	O6D-C1D-O3G-C3G
36	a	401	DGD	C2A-C1A-O1G-C1G
36	a	401	DGD	O1A-C1A-O1G-C1G
37	E	101	HEM	C2C-C3C-CAC-CBC
37	f	101	HEM	C2C-C3C-CAC-CBC
38	G	601	CHL	C1A-C2A-CAA-CBA
38	G	601	CHL	C3A-C2A-CAA-CBA
38	G	601	CHL	CHA-CBD-CGD-O1D
38	G	601	CHL	CHA-CBD-CGD-O2D
38	G	606	CHL	CHA-CBD-CGD-O1D
38	G	606	CHL	CHA-CBD-CGD-O2D
38	G	607	CHL	C1A-C2A-CAA-CBA
38	N	601	CHL	CHA-CBD-CGD-O1D
38	N	601	CHL	CHA-CBD-CGD-O2D
38	R	607	CHL	C1A-C2A-CAA-CBA
38	S	302	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
38	S	302	CHL	CHA-CBD-CGD-O2D
38	S	306	CHL	C3A-C2A-CAA-CBA
38	Y	601	CHL	CHA-CBD-CGD-O1D
38	Y	601	CHL	CHA-CBD-CGD-O2D
38	Y	607	CHL	C1A-C2A-CAA-CBA
38	g	607	CHL	C1A-C2A-CAA-CBA
38	g	609	CHL	C1A-C2A-CAA-CBA
38	g	609	CHL	C3A-C2A-CAA-CBA
38	g	609	CHL	CBD-CGD-O2D-CED
38	g	619	CHL	C1A-C2A-CAA-CBA
38	g	619	CHL	C3A-C2A-CAA-CBA
38	n	601	CHL	C1A-C2A-CAA-CBA
38	n	601	CHL	C3A-C2A-CAA-CBA
38	n	601	CHL	CHA-CBD-CGD-O1D
38	n	601	CHL	CHA-CBD-CGD-O2D
38	n	606	CHL	CHA-CBD-CGD-O1D
38	n	606	CHL	CHA-CBD-CGD-O2D
38	n	609	CHL	C11-C12-C13-C14
38	r	606	CHL	CHA-CBD-CGD-O1D
38	r	606	CHL	CHA-CBD-CGD-O2D
38	r	607	CHL	C2-C1-O2A-CGA
38	y	302	CHL	C1A-C2A-CAA-CBA
38	y	302	CHL	C3A-C2A-CAA-CBA
39	G	615	LUT	C31-C32-C33-C34
39	G	615	LUT	C31-C32-C33-C40
39	G	616	LUT	C11-C12-C13-C14
39	G	616	LUT	C11-C12-C13-C20
39	N	615	LUT	C31-C32-C33-C34
39	N	615	LUT	C31-C32-C33-C40
39	N	616	LUT	C31-C32-C33-C34
39	N	616	LUT	C31-C32-C33-C40
39	R	614	LUT	C11-C12-C13-C14
39	R	614	LUT	C11-C12-C13-C20
39	S	316	LUT	C11-C12-C13-C14
39	S	316	LUT	C11-C12-C13-C20
39	S	316	LUT	C31-C32-C33-C34
39	S	316	LUT	C31-C32-C33-C40
39	g	615	LUT	C11-C12-C13-C14
39	g	615	LUT	C11-C12-C13-C20
39	g	615	LUT	C31-C32-C33-C40
39	g	616	LUT	C11-C12-C13-C14
39	g	616	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
39	g	616	LUT	C31-C32-C33-C34
39	g	616	LUT	C31-C32-C33-C40
39	n	615	LUT	C11-C12-C13-C14
39	n	615	LUT	C11-C12-C13-C20
39	n	615	LUT	C31-C32-C33-C34
39	n	615	LUT	C31-C32-C33-C40
39	n	616	LUT	C31-C32-C33-C34
39	n	616	LUT	C31-C32-C33-C40
39	r	614	LUT	C5-C6-C7-C8
39	r	614	LUT	C11-C12-C13-C14
39	r	614	LUT	C11-C12-C13-C20
39	s	614	LUT	C11-C12-C13-C14
39	s	614	LUT	C11-C12-C13-C20
39	s	614	LUT	C27-C28-C29-C30
39	s	614	LUT	C27-C28-C29-C39
39	s	614	LUT	C31-C32-C33-C40
39	s	615	LUT	C11-C12-C13-C14
39	s	615	LUT	C11-C12-C13-C20
39	s	615	LUT	C31-C32-C33-C34
39	s	615	LUT	C31-C32-C33-C40
39	y	315	LUT	C11-C12-C13-C14
39	y	315	LUT	C11-C12-C13-C20
39	y	315	LUT	C31-C32-C33-C34
39	y	315	LUT	C31-C32-C33-C40
39	y	316	LUT	C7-C8-C9-C10
39	y	316	LUT	C7-C8-C9-C19
39	y	316	LUT	C31-C32-C33-C34
39	y	316	LUT	C31-C32-C33-C40
40	G	617	NEX	C11-C12-C13-C14
40	G	617	NEX	C11-C12-C13-C20
40	G	617	NEX	O24-C26-C27-C28
40	G	617	NEX	C29-C30-C31-C32
40	N	617	NEX	O24-C26-C27-C28
40	N	617	NEX	C26-C27-C28-C29
40	N	617	NEX	C28-C29-C30-C31
40	g	617	NEX	C11-C10-C9-C8
40	g	617	NEX	C11-C10-C9-C19
40	g	617	NEX	C10-C11-C12-C13
40	g	617	NEX	C25-C26-C27-C28
40	g	617	NEX	C26-C27-C28-C29
40	g	617	NEX	C27-C28-C29-C30
40	g	617	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	n	617	NEX	O24-C26-C27-C28
40	n	617	NEX	C26-C27-C28-C29
40	r	616	NEX	O24-C26-C27-C28
40	r	616	NEX	C26-C27-C28-C29
40	s	616	NEX	C11-C12-C13-C14
40	s	616	NEX	C11-C12-C13-C20
40	s	616	NEX	C39-C29-C30-C31
40	s	616	NEX	C30-C31-C32-C33
40	s	616	NEX	C32-C33-C34-C35
40	s	616	NEX	C40-C33-C34-C35
40	y	301	NEX	C11-C10-C9-C8
40	y	301	NEX	C11-C10-C9-C19
40	y	301	NEX	C28-C29-C30-C31
40	y	318	NEX	C11-C10-C9-C19
40	y	318	NEX	C28-C29-C30-C31
40	y	318	NEX	C39-C29-C30-C31
41	R	615	XAT	O24-C26-C27-C28
41	r	615	XAT	O24-C26-C27-C28
28	A	405	CLA	O1D-CGD-O2D-CED
28	G	610	CLA	O1D-CGD-O2D-CED
28	R	610	CLA	O1D-CGD-O2D-CED
28	Y	614	CLA	O1D-CGD-O2D-CED
28	b	613	CLA	O1D-CGD-O2D-CED
28	g	604	CLA	O1D-CGD-O2D-CED
28	g	613	CLA	O1D-CGD-O2D-CED
28	n	610	CLA	O1D-CGD-O2D-CED
28	n	614	CLA	O1D-CGD-O2D-CED
28	y	310	CLA	O1D-CGD-O2D-CED
28	C	501	CLA	O1D-CGD-O2D-CED
28	G	613	CLA	O1D-CGD-O2D-CED
28	N	613	CLA	O1D-CGD-O2D-CED
28	S	310	CLA	O1D-CGD-O2D-CED
28	a	406	CLA	O1D-CGD-O2D-CED
28	r	601	CLA	O1D-CGD-O2D-CED
28	r	610	CLA	O1D-CGD-O2D-CED
28	r	611	CLA	O1D-CGD-O2D-CED
28	y	313	CLA	O1D-CGD-O2D-CED
28	A	408	CLA	CBD-CGD-O2D-CED
28	B	605	CLA	CBD-CGD-O2D-CED
28	B	608	CLA	CBD-CGD-O2D-CED
28	B	609	CLA	CBD-CGD-O2D-CED
28	B	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	B	616	CLA	CBD-CGD-O2D-CED
28	C	501	CLA	CBD-CGD-O2D-CED
28	C	504	CLA	CBD-CGD-O2D-CED
28	C	506	CLA	CBD-CGD-O2D-CED
28	C	508	CLA	CBD-CGD-O2D-CED
28	C	509	CLA	CBD-CGD-O2D-CED
28	C	511	CLA	CBD-CGD-O2D-CED
28	C	513	CLA	CBD-CGD-O2D-CED
28	G	602	CLA	CBD-CGD-O2D-CED
28	G	604	CLA	CBD-CGD-O2D-CED
28	G	611	CLA	CBD-CGD-O2D-CED
28	G	613	CLA	CBD-CGD-O2D-CED
28	N	604	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	CBD-CGD-O2D-CED
28	N	613	CLA	CBD-CGD-O2D-CED
28	N	614	CLA	CBD-CGD-O2D-CED
28	R	608	CLA	CBD-CGD-O2D-CED
28	R	611	CLA	CBD-CGD-O2D-CED
28	S	304	CLA	CBD-CGD-O2D-CED
28	S	305	CLA	CBD-CGD-O2D-CED
28	S	309	CLA	CBD-CGD-O2D-CED
28	S	311	CLA	CBD-CGD-O2D-CED
28	S	312	CLA	CBD-CGD-O2D-CED
28	Y	612	CLA	CBD-CGD-O2D-CED
28	a	406	CLA	CBD-CGD-O2D-CED
28	a	409	CLA	CBD-CGD-O2D-CED
28	b	603	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	CBD-CGD-O2D-CED
28	b	607	CLA	CBD-CGD-O2D-CED
28	b	609	CLA	CBD-CGD-O2D-CED
28	b	612	CLA	CBD-CGD-O2D-CED
28	b	613	CLA	CBD-CGD-O2D-CED
28	c	503	CLA	CBD-CGD-O2D-CED
28	c	508	CLA	CBD-CGD-O2D-CED
28	c	511	CLA	CBD-CGD-O2D-CED
28	c	512	CLA	CBD-CGD-O2D-CED
28	d	404	CLA	CBD-CGD-O2D-CED
28	g	602	CLA	CBD-CGD-O2D-CED
28	g	604	CLA	CBD-CGD-O2D-CED
28	g	613	CLA	CBD-CGD-O2D-CED
28	n	602	CLA	CBD-CGD-O2D-CED
28	n	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	r	612	CLA	CBD-CGD-O2D-CED
28	s	602	CLA	CBD-CGD-O2D-CED
28	s	603	CLA	CBD-CGD-O2D-CED
28	y	303	CLA	CBD-CGD-O2D-CED
28	y	305	CLA	CBD-CGD-O2D-CED
28	y	314	CLA	CBD-CGD-O2D-CED
38	G	605	CHL	CBD-CGD-O2D-CED
38	G	608	CHL	CBD-CGD-O2D-CED
38	N	605	CHL	CBD-CGD-O2D-CED
38	S	307	CHL	CBD-CGD-O2D-CED
38	g	605	CHL	CBD-CGD-O2D-CED
38	g	608	CHL	CBD-CGD-O2D-CED
38	n	605	CHL	CBD-CGD-O2D-CED
38	y	302	CHL	CBD-CGD-O2D-CED
28	G	611	CLA	O1A-CGA-O2A-C1
28	G	614	CLA	O1A-CGA-O2A-C1
28	N	604	CLA	O1A-CGA-O2A-C1
28	N	611	CLA	O1A-CGA-O2A-C1
28	N	614	CLA	O1A-CGA-O2A-C1
28	R	610	CLA	O1A-CGA-O2A-C1
28	S	310	CLA	O1A-CGA-O2A-C1
28	Y	611	CLA	O1A-CGA-O2A-C1
28	n	611	CLA	O1A-CGA-O2A-C1
28	s	610	CLA	O1A-CGA-O2A-C1
28	y	311	CLA	O1A-CGA-O2A-C1
32	C	522	LMG	O10-C28-O8-C9
32	b	620	LMG	O10-C28-O8-C9
32	c	521	LMG	O10-C28-O8-C9
35	B	622	LHG	O10-C23-O8-C6
28	B	605	CLA	O1D-CGD-O2D-CED
28	B	616	CLA	O1D-CGD-O2D-CED
28	C	508	CLA	O1D-CGD-O2D-CED
28	R	611	CLA	O1D-CGD-O2D-CED
28	S	312	CLA	O1D-CGD-O2D-CED
28	Y	613	CLA	O1D-CGD-O2D-CED
28	c	503	CLA	O1D-CGD-O2D-CED
28	y	314	CLA	O1D-CGD-O2D-CED
28	B	607	CLA	C8-C10-C11-C12
28	b	615	CLA	C8-C10-C11-C12
28	B	603	CLA	O1D-CGD-O2D-CED
28	B	613	CLA	O1D-CGD-O2D-CED
28	G	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	R	601	CLA	O1D-CGD-O2D-CED
28	c	508	CLA	O1D-CGD-O2D-CED
28	d	405	CLA	O1D-CGD-O2D-CED
28	g	614	CLA	O1D-CGD-O2D-CED
28	n	613	CLA	O1D-CGD-O2D-CED
28	r	608	CLA	O1D-CGD-O2D-CED
28	r	609	CLA	O1D-CGD-O2D-CED
28	s	609	CLA	O1D-CGD-O2D-CED
28	s	612	CLA	O1D-CGD-O2D-CED
28	N	612	CLA	C3-C5-C6-C7
28	B	601	CLA	CBA-CGA-O2A-C1
28	G	614	CLA	CBA-CGA-O2A-C1
28	R	610	CLA	CBA-CGA-O2A-C1
28	S	310	CLA	CBA-CGA-O2A-C1
28	n	611	CLA	CBA-CGA-O2A-C1
28	y	311	CLA	CBA-CGA-O2A-C1
32	C	522	LMG	C29-C28-O8-C9
32	b	620	LMG	C29-C28-O8-C9
32	c	521	LMG	C29-C28-O8-C9
28	B	607	CLA	CBD-CGD-O2D-CED
28	B	611	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	CBD-CGD-O2D-CED
28	D	403	CLA	CBD-CGD-O2D-CED
28	G	614	CLA	CBD-CGD-O2D-CED
28	N	602	CLA	CBD-CGD-O2D-CED
28	R	609	CLA	CBD-CGD-O2D-CED
28	S	303	CLA	CBD-CGD-O2D-CED
28	S	313	CLA	CBD-CGD-O2D-CED
28	S	314	CLA	CBD-CGD-O2D-CED
28	Y	611	CLA	CBD-CGD-O2D-CED
28	b	615	CLA	CBD-CGD-O2D-CED
28	b	616	CLA	CBD-CGD-O2D-CED
28	c	501	CLA	CBD-CGD-O2D-CED
28	c	513	CLA	CBD-CGD-O2D-CED
28	g	611	CLA	CBD-CGD-O2D-CED
28	g	612	CLA	CBD-CGD-O2D-CED
28	r	604	CLA	CBD-CGD-O2D-CED
28	s	610	CLA	CBD-CGD-O2D-CED
28	s	611	CLA	CBD-CGD-O2D-CED
28	y	311	CLA	CBD-CGD-O2D-CED
28	y	312	CLA	CBD-CGD-O2D-CED
38	N	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	N	609	CHL	CBD-CGD-O2D-CED
38	R	606	CHL	CBD-CGD-O2D-CED
38	S	308	CHL	CBD-CGD-O2D-CED
38	n	606	CHL	CBD-CGD-O2D-CED
38	s	605	CHL	CBD-CGD-O2D-CED
38	y	308	CHL	CBD-CGD-O2D-CED
28	A	405	CLA	O1A-CGA-O2A-C1
28	C	502	CLA	O1A-CGA-O2A-C1
28	D	404	CLA	O1A-CGA-O2A-C1
28	N	612	CLA	O1A-CGA-O2A-C1
28	a	409	CLA	O1A-CGA-O2A-C1
28	y	305	CLA	O1A-CGA-O2A-C1
28	y	314	CLA	O1A-CGA-O2A-C1
31	M	101	SQD	O10-C23-O48-C46
32	B	621	LMG	O10-C28-O8-C9
38	g	619	CHL	O1A-CGA-O2A-C1
28	B	610	CLA	O1D-CGD-O2D-CED
28	C	502	CLA	O1D-CGD-O2D-CED
28	R	612	CLA	O1D-CGD-O2D-CED
28	n	602	CLA	C10-C11-C12-C13
38	S	308	CHL	C2C-C3C-CAC-CBC
28	D	404	CLA	O1D-CGD-O2D-CED
28	b	608	CLA	O1D-CGD-O2D-CED
28	r	612	CLA	O1D-CGD-O2D-CED
28	B	602	CLA	CBD-CGD-O2D-CED
28	Y	604	CLA	CBD-CGD-O2D-CED
28	c	504	CLA	CBD-CGD-O2D-CED
38	r	606	CHL	CBD-CGD-O2D-CED
28	b	603	CLA	O1D-CGD-O2D-CED
28	c	502	CLA	O1D-CGD-O2D-CED
38	g	608	CHL	O1D-CGD-O2D-CED
38	g	609	CHL	O1D-CGD-O2D-CED
32	A	413	LMG	O9-C10-O7-C8
32	B	624	LMG	O9-C10-O7-C8
32	C	522	LMG	O9-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
35	b	621	LHG	O9-C7-O7-C5
35	y	319	LHG	O9-C7-O7-C5
36	A	417	DGD	O1B-C1B-O2G-C2G
28	b	607	CLA	O1A-CGA-O2A-C1
38	S	308	CHL	C4C-C3C-CAC-CBC
28	A	405	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	B	608	CLA	C3-C5-C6-C7
28	B	614	CLA	C3-C5-C6-C7
28	B	615	CLA	C3-C5-C6-C7
28	C	501	CLA	C3-C5-C6-C7
28	C	510	CLA	C3-C5-C6-C7
28	D	403	CLA	C3-C5-C6-C7
28	D	404	CLA	C3-C5-C6-C7
28	G	602	CLA	C3-C5-C6-C7
28	G	613	CLA	C3-C5-C6-C7
28	R	608	CLA	C3-C5-C6-C7
28	b	602	CLA	C3-C5-C6-C7
28	b	614	CLA	C3-C5-C6-C7
28	c	502	CLA	C3-C5-C6-C7
28	c	503	CLA	C3-C5-C6-C7
28	g	610	CLA	C3-C5-C6-C7
28	n	603	CLA	C3-C5-C6-C7
28	n	612	CLA	C3-C5-C6-C7
38	y	309	CHL	C3-C5-C6-C7
28	A	405	CLA	CBA-CGA-O2A-C1
28	B	604	CLA	CBA-CGA-O2A-C1
28	C	506	CLA	CBA-CGA-O2A-C1
28	C	512	CLA	CBA-CGA-O2A-C1
28	D	404	CLA	CBA-CGA-O2A-C1
28	G	611	CLA	CBA-CGA-O2A-C1
28	N	604	CLA	CBA-CGA-O2A-C1
28	N	611	CLA	CBA-CGA-O2A-C1
28	N	612	CLA	CBA-CGA-O2A-C1
28	Y	614	CLA	CBA-CGA-O2A-C1
28	b	612	CLA	CBA-CGA-O2A-C1
28	c	510	CLA	CBA-CGA-O2A-C1
28	n	610	CLA	CBA-CGA-O2A-C1
28	r	613	CLA	CBA-CGA-O2A-C1
31	M	101	SQD	C24-C23-O48-C46
32	B	621	LMG	C29-C28-O8-C9
35	B	622	LHG	C24-C23-O8-C6
31	L	103	SQD	C8-C7-O47-C45
31	M	101	SQD	C8-C7-O47-C45
32	A	411	LMG	C11-C10-O7-C8
35	y	319	LHG	C8-C7-O7-C5
28	N	610	CLA	O1D-CGD-O2D-CED
28	a	409	CLA	O1D-CGD-O2D-CED
28	b	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	s	604	CLA	CBD-CGD-O2D-CED
28	s	613	CLA	CBD-CGD-O2D-CED
38	Y	608	CHL	CBD-CGD-O2D-CED
28	D	404	CLA	C4-C3-C5-C6
28	b	602	CLA	C4-C3-C5-C6
28	g	611	CLA	C4-C3-C5-C6
28	b	611	CLA	CBD-CGD-O2D-CED
28	r	603	CLA	CBD-CGD-O2D-CED
28	C	504	CLA	C2A-CAA-CBA-CGA
28	c	510	CLA	C2A-CAA-CBA-CGA
28	n	610	CLA	C2A-CAA-CBA-CGA
28	y	305	CLA	C2A-CAA-CBA-CGA
38	R	605	CHL	C2A-CAA-CBA-CGA
38	g	606	CHL	C2A-CAA-CBA-CGA
28	B	612	CLA	O1A-CGA-O2A-C1
32	B	621	LMG	C35-C36-C37-C38
32	C	520	LMG	C17-C18-C19-C20
32	C	520	LMG	C35-C36-C37-C38
32	D	408	LMG	C17-C18-C19-C20
32	b	620	LMG	C35-C36-C37-C38
32	b	623	LMG	C35-C36-C37-C38
32	d	409	LMG	C17-C18-C19-C20
32	k	102	LMG	C17-C18-C19-C20
32	k	102	LMG	C35-C36-C37-C38
36	A	417	DGD	C8B-C9B-CAB-CBB
36	B	626	DGD	CBA-CCA-CDA-CEA
36	C	518	DGD	C8A-C9A-CAA-CBA
36	C	518	DGD	CBB-CCB-CDB-CEB
36	C	519	DGD	C8A-C9A-CAA-CBA
36	C	519	DGD	CBA-CCA-CDA-CEA
36	a	401	DGD	C8B-C9B-CAB-CBB
36	b	625	DGD	CBA-CCA-CDA-CEA
36	c	517	DGD	CBB-CCB-CDB-CEB
36	c	518	DGD	C8A-C9A-CAA-CBA
36	c	518	DGD	CBA-CCA-CDA-CEA
28	B	611	CLA	C3-C5-C6-C7
28	B	613	CLA	C3-C5-C6-C7
28	D	401	CLA	C3-C5-C6-C7
28	S	303	CLA	C3-C5-C6-C7
28	c	511	CLA	C3-C5-C6-C7
28	s	610	CLA	C3-C5-C6-C7
28	y	304	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
38	r	605	CHL	C3-C5-C6-C7
28	B	610	CLA	CBA-CGA-O2A-C1
28	B	612	CLA	CBA-CGA-O2A-C1
28	C	502	CLA	CBA-CGA-O2A-C1
28	C	511	CLA	CBA-CGA-O2A-C1
28	N	610	CLA	CBA-CGA-O2A-C1
28	S	312	CLA	CBA-CGA-O2A-C1
28	a	409	CLA	CBA-CGA-O2A-C1
28	b	607	CLA	CBA-CGA-O2A-C1
28	c	502	CLA	CBA-CGA-O2A-C1
28	c	504	CLA	CBA-CGA-O2A-C1
28	r	604	CLA	CBA-CGA-O2A-C1
28	y	305	CLA	CBA-CGA-O2A-C1
28	y	314	CLA	CBA-CGA-O2A-C1
38	g	619	CHL	CBA-CGA-O2A-C1
28	B	609	CLA	O1D-CGD-O2D-CED
28	C	511	CLA	O1D-CGD-O2D-CED
28	s	603	CLA	O1D-CGD-O2D-CED
28	y	305	CLA	O1D-CGD-O2D-CED
28	c	510	CLA	CBD-CGD-O2D-CED
28	A	408	CLA	O1D-CGD-O2D-CED
28	B	608	CLA	O1D-CGD-O2D-CED
28	C	504	CLA	O1D-CGD-O2D-CED
28	C	506	CLA	O1D-CGD-O2D-CED
28	C	509	CLA	O1D-CGD-O2D-CED
28	G	604	CLA	O1D-CGD-O2D-CED
28	S	304	CLA	O1D-CGD-O2D-CED
28	b	609	CLA	O1D-CGD-O2D-CED
28	c	511	CLA	O1D-CGD-O2D-CED
28	c	512	CLA	O1D-CGD-O2D-CED
28	n	602	CLA	O1D-CGD-O2D-CED
38	G	605	CHL	O1D-CGD-O2D-CED
32	A	411	LMG	O9-C10-O7-C8
32	a	413	LMG	O9-C10-O7-C8
35	S	317	LHG	O9-C7-O7-C5
28	B	604	CLA	O1A-CGA-O2A-C1
28	B	616	CLA	O1A-CGA-O2A-C1
28	C	506	CLA	O1A-CGA-O2A-C1
28	C	509	CLA	O1A-CGA-O2A-C1
28	C	511	CLA	O1A-CGA-O2A-C1
28	C	512	CLA	O1A-CGA-O2A-C1
28	S	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	Y	614	CLA	O1A-CGA-O2A-C1
28	a	406	CLA	O1A-CGA-O2A-C1
28	b	601	CLA	O1A-CGA-O2A-C1
28	b	612	CLA	O1A-CGA-O2A-C1
28	c	510	CLA	O1A-CGA-O2A-C1
28	r	601	CLA	O1A-CGA-O2A-C1
28	r	613	CLA	O1A-CGA-O2A-C1
35	W	101	LHG	O10-C23-O8-C6
35	G	618	LHG	C28-C29-C30-C31
28	S	311	CLA	O1D-CGD-O2D-CED
28	b	606	CLA	O1D-CGD-O2D-CED
28	s	602	CLA	O1D-CGD-O2D-CED
28	y	303	CLA	O1D-CGD-O2D-CED
30	B	617	BCR	C15-C16-C17-C18
30	C	515	BCR	C15-C16-C17-C18
30	C	516	BCR	C13-C14-C15-C16
30	D	405	BCR	C13-C14-C15-C16
30	H	101	BCR	C15-C16-C17-C18
30	H	101	BCR	C19-C20-C21-C22
30	K	101	BCR	C15-C16-C17-C18
30	a	410	BCR	C9-C10-C11-C12
30	b	617	BCR	C9-C10-C11-C12
30	c	514	BCR	C19-C20-C21-C22
30	d	406	BCR	C19-C20-C21-C22
30	h	101	BCR	C19-C20-C21-C22
30	t	101	BCR	C15-C16-C17-C18
39	G	615	LUT	C9-C10-C11-C12
28	C	511	CLA	C8-C10-C11-C12
28	N	611	CLA	CBD-CGD-O2D-CED
28	N	612	CLA	CBD-CGD-O2D-CED
28	r	602	CLA	CBD-CGD-O2D-CED
38	G	609	CHL	CBD-CGD-O2D-CED
38	Y	605	CHL	CBD-CGD-O2D-CED
28	B	615	CLA	O1D-CGD-O2D-CED
28	C	513	CLA	O1D-CGD-O2D-CED
28	N	614	CLA	O1D-CGD-O2D-CED
35	A	416	LHG	O2-C2-C3-O3
35	C	521	LHG	O2-C2-C3-O3
35	R	616	LHG	O2-C2-C3-O3
35	s	617	LHG	O2-C2-C3-O3
35	w	102	LHG	O2-C2-C3-O3
35	y	319	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	A	408	CLA	C3-C5-C6-C7
28	B	609	CLA	C3-C5-C6-C7
28	B	616	CLA	C3-C5-C6-C7
28	G	611	CLA	C3-C5-C6-C7
28	N	613	CLA	C3-C5-C6-C7
28	S	313	CLA	C3-C5-C6-C7
28	Y	602	CLA	C3-C5-C6-C7
28	b	606	CLA	C3-C5-C6-C7
28	c	501	CLA	C3-C5-C6-C7
28	A	406	CLA	CBA-CGA-O2A-C1
28	A	408	CLA	CBA-CGA-O2A-C1
28	B	616	CLA	CBA-CGA-O2A-C1
28	Y	603	CLA	CBA-CGA-O2A-C1
28	a	406	CLA	CBA-CGA-O2A-C1
28	b	601	CLA	CBA-CGA-O2A-C1
28	c	511	CLA	CBA-CGA-O2A-C1
28	n	612	CLA	CBA-CGA-O2A-C1
35	S	301	LHG	C24-C23-O8-C6
35	W	101	LHG	C24-C23-O8-C6
35	b	621	LHG	C24-C23-O8-C6
35	B	625	LHG	C11-C12-C13-C14
35	b	624	LHG	C11-C12-C13-C14
35	b	624	LHG	C13-C14-C15-C16
35	l	101	LHG	C11-C12-C13-C14
28	B	610	CLA	O1A-CGA-O2A-C1
28	c	511	CLA	O1A-CGA-O2A-C1
28	n	610	CLA	O1A-CGA-O2A-C1
28	b	607	CLA	O1D-CGD-O2D-CED
28	g	602	CLA	O1D-CGD-O2D-CED
38	S	307	CHL	O1D-CGD-O2D-CED
38	g	605	CHL	O1D-CGD-O2D-CED
32	a	413	LMG	C11-C10-O7-C8
32	w	101	LMG	C11-C10-O7-C8
35	C	521	LHG	C8-C7-O7-C5
35	S	317	LHG	C8-C7-O7-C5
35	b	624	LHG	C8-C7-O7-C5
35	A	416	LHG	C13-C14-C15-C16
35	y	319	LHG	C28-C29-C30-C31
28	N	604	CLA	O1D-CGD-O2D-CED
28	S	309	CLA	O1D-CGD-O2D-CED
28	C	510	CLA	CBD-CGD-O2D-CED
28	g	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	W	101	LHG	C33-C34-C35-C36
35	b	622	LHG	C34-C35-C36-C37
28	d	404	CLA	O1D-CGD-O2D-CED
28	A	406	CLA	O1A-CGA-O2A-C1
35	a	415	LHG	C11-C12-C13-C14
35	y	319	LHG	C26-C27-C28-C29
28	Y	612	CLA	O1D-CGD-O2D-CED
38	G	608	CHL	O1D-CGD-O2D-CED
28	r	603	CLA	C2C-C3C-CAC-CBC
35	Y	619	LHG	C33-C34-C35-C36
28	b	602	CLA	C8-C10-C11-C12
28	B	607	CLA	C3-C5-C6-C7
28	s	612	CLA	C3-C5-C6-C7
38	y	302	CHL	C3-C5-C6-C7
28	C	509	CLA	CBA-CGA-O2A-C1
28	r	601	CLA	CBA-CGA-O2A-C1
28	s	611	CLA	CBA-CGA-O2A-C1
28	n	604	CLA	O1D-CGD-O2D-CED
38	N	605	CHL	O1D-CGD-O2D-CED
35	s	617	LHG	C11-C10-C9-C8
35	C	521	LHG	C2-C3-O3-P
28	N	610	CLA	O1A-CGA-O2A-C1
28	Y	603	CLA	O1A-CGA-O2A-C1
28	r	604	CLA	O1A-CGA-O2A-C1
35	S	317	LHG	C26-C27-C28-C29
28	B	608	CLA	C8-C10-C11-C12
28	n	611	CLA	C10-C11-C12-C13
28	N	610	CLA	C2A-CAA-CBA-CGA
28	G	602	CLA	O1D-CGD-O2D-CED
28	S	305	CLA	O1D-CGD-O2D-CED
38	n	605	CHL	O1D-CGD-O2D-CED
38	y	302	CHL	O1D-CGD-O2D-CED
28	A	408	CLA	O1A-CGA-O2A-C1
28	c	502	CLA	O1A-CGA-O2A-C1
28	c	504	CLA	O1A-CGA-O2A-C1
28	n	612	CLA	O1A-CGA-O2A-C1
28	d	404	CLA	C3-C5-C6-C7
38	g	608	CHL	C3-C5-C6-C7
28	S	303	CLA	CBA-CGA-O2A-C1
28	Y	604	CLA	CBA-CGA-O2A-C1
38	R	607	CHL	CBA-CGA-O2A-C1
28	R	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	615	CLA	O1D-CGD-O2D-CED
28	s	611	CLA	O1D-CGD-O2D-CED
28	s	611	CLA	O1A-CGA-O2A-C1
35	S	301	LHG	O10-C23-O8-C6
35	g	618	LHG	C8-C7-O7-C5
35	b	621	LHG	C26-C27-C28-C29
28	D	403	CLA	O1D-CGD-O2D-CED
28	G	614	CLA	O1D-CGD-O2D-CED
28	c	513	CLA	O1D-CGD-O2D-CED
28	s	610	CLA	O1D-CGD-O2D-CED
38	n	606	CHL	O1D-CGD-O2D-CED
28	B	607	CLA	O1D-CGD-O2D-CED
28	Y	611	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	C1-C2-C3-O3
35	N	618	LHG	C1-C2-C3-O3
35	S	301	LHG	C1-C2-C3-O3
35	Y	619	LHG	C1-C2-C3-O3
35	b	621	LHG	C1-C2-C3-O3
35	c	519	LHG	C1-C2-C3-O3
35	d	408	LHG	C1-C2-C3-O3
35	r	617	LHG	C1-C2-C3-O3
32	w	101	LMG	O9-C10-O7-C8
35	b	621	LHG	O10-C23-O8-C6
28	g	602	CLA	C3-C5-C6-C7
28	r	613	CLA	C3-C5-C6-C7
28	C	503	CLA	O1D-CGD-O2D-CED
38	y	308	CHL	O1D-CGD-O2D-CED
28	B	602	CLA	CBA-CGA-O2A-C1
28	C	510	CLA	CBA-CGA-O2A-C1
28	N	603	CLA	CBA-CGA-O2A-C1
28	R	604	CLA	CBA-CGA-O2A-C1
28	b	611	CLA	CBA-CGA-O2A-C1
28	c	503	CLA	CBA-CGA-O2A-C1
28	c	509	CLA	CBA-CGA-O2A-C1
28	n	604	CLA	CBA-CGA-O2A-C1
28	s	602	CLA	CBA-CGA-O2A-C1
35	A	416	LHG	C24-C23-O8-C6
35	a	415	LHG	C24-C23-O8-C6
35	b	622	LHG	C24-C23-O8-C6
36	c	516	DGD	C2A-C1A-O1G-C1G
38	r	607	CHL	CBA-CGA-O2A-C1
28	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	y	312	CLA	O1D-CGD-O2D-CED
30	B	618	BCR	C13-C14-C15-C16
30	C	516	BCR	C15-C16-C17-C18
30	K	101	BCR	C13-C14-C15-C16
30	b	617	BCR	C15-C16-C17-C18
30	b	618	BCR	C15-C16-C17-C18
35	W	101	LHG	C25-C26-C27-C28
35	d	408	LHG	C34-C35-C36-C37
35	w	102	LHG	C9-C10-C11-C12
28	B	609	CLA	C8-C10-C11-C12
28	B	612	CLA	C8-C10-C11-C12
28	Y	603	CLA	C5-C6-C7-C8
38	g	607	CHL	C5-C6-C7-C8
35	B	625	LHG	O2-C2-C3-O3
35	D	407	LHG	O2-C2-C3-O3
35	b	624	LHG	O2-C2-C3-O3
35	C	521	LHG	C23-C24-C25-C26
28	g	613	CLA	C3-C5-C6-C7
32	C	520	LMG	C2-C1-O1-C7
35	c	520	LHG	C12-C13-C14-C15
28	C	510	CLA	O1A-CGA-O2A-C1
28	c	503	CLA	O1A-CGA-O2A-C1
28	s	602	CLA	O1A-CGA-O2A-C1
28	D	404	CLA	C2-C3-C5-C6
28	b	602	CLA	C2-C3-C5-C6
28	g	611	CLA	C2-C3-C5-C6
28	A	408	CLA	C11-C10-C8-C9
28	B	601	CLA	C6-C7-C8-C9
28	B	601	CLA	C11-C10-C8-C9
28	B	602	CLA	C6-C7-C8-C9
28	B	604	CLA	C6-C7-C8-C9
28	B	611	CLA	C6-C7-C8-C9
28	B	613	CLA	C6-C7-C8-C9
28	B	614	CLA	C6-C7-C8-C9
28	B	615	CLA	C6-C7-C8-C9
28	B	616	CLA	C6-C7-C8-C9
28	C	501	CLA	C6-C7-C8-C9
28	C	502	CLA	C11-C12-C13-C14
28	C	503	CLA	C11-C10-C8-C9
28	C	504	CLA	C11-C12-C13-C14
28	C	507	CLA	C11-C10-C8-C9
28	C	511	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	513	CLA	C11-C10-C8-C9
28	D	401	CLA	C6-C7-C8-C9
28	D	404	CLA	C6-C7-C8-C9
28	G	602	CLA	C11-C10-C8-C9
28	G	610	CLA	C6-C7-C8-C9
28	G	610	CLA	C11-C10-C8-C9
28	N	611	CLA	C6-C7-C8-C9
28	N	611	CLA	C11-C10-C8-C9
28	N	612	CLA	C11-C10-C8-C9
28	R	602	CLA	C11-C10-C8-C9
28	R	603	CLA	C11-C10-C8-C9
28	R	609	CLA	C11-C12-C13-C14
28	S	311	CLA	C6-C7-C8-C9
28	Y	611	CLA	C6-C7-C8-C9
28	Y	613	CLA	C6-C7-C8-C9
28	b	601	CLA	C6-C7-C8-C9
28	b	604	CLA	C6-C7-C8-C9
28	b	605	CLA	C14-C13-C15-C16
28	b	607	CLA	C6-C7-C8-C9
28	b	609	CLA	C6-C7-C8-C9
28	b	615	CLA	C6-C7-C8-C9
28	b	616	CLA	C11-C10-C8-C9
28	c	501	CLA	C6-C7-C8-C9
28	c	506	CLA	C6-C7-C8-C9
28	c	507	CLA	C11-C10-C8-C9
28	c	508	CLA	C6-C7-C8-C9
28	c	509	CLA	C6-C7-C8-C9
28	c	510	CLA	C11-C12-C13-C14
28	c	511	CLA	C11-C10-C8-C9
28	c	512	CLA	C6-C7-C8-C9
28	d	401	CLA	C6-C7-C8-C9
28	d	405	CLA	C6-C7-C8-C9
28	g	610	CLA	C6-C7-C8-C9
28	g	611	CLA	C6-C7-C8-C9
28	n	602	CLA	C6-C7-C8-C9
28	n	603	CLA	C6-C7-C8-C9
28	n	610	CLA	C6-C7-C8-C9
28	n	610	CLA	C11-C10-C8-C9
28	n	611	CLA	C6-C7-C8-C9
28	n	611	CLA	C11-C10-C8-C9
28	n	612	CLA	C6-C7-C8-C9
28	n	612	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	r	602	CLA	C6-C7-C8-C9
28	r	603	CLA	C6-C7-C8-C9
28	r	608	CLA	C6-C7-C8-C9
28	r	609	CLA	C11-C12-C13-C14
28	r	612	CLA	C6-C7-C8-C9
28	r	613	CLA	C11-C10-C8-C9
28	s	602	CLA	C6-C7-C8-C9
28	s	602	CLA	C11-C10-C8-C9
28	y	303	CLA	C11-C10-C8-C9
28	y	311	CLA	C6-C7-C8-C9
38	G	601	CHL	C11-C10-C8-C9
38	G	608	CHL	C6-C7-C8-C9
38	N	607	CHL	C11-C10-C8-C9
38	N	608	CHL	C11-C10-C8-C9
38	N	609	CHL	C11-C10-C8-C9
38	Y	601	CHL	C11-C10-C8-C9
38	Y	608	CHL	C11-C10-C8-C9
38	Y	608	CHL	C14-C13-C15-C16
38	Y	609	CHL	C11-C10-C8-C9
38	g	608	CHL	C11-C10-C8-C9
38	g	608	CHL	C14-C13-C15-C16
38	g	609	CHL	C11-C10-C8-C9
38	n	608	CHL	C11-C10-C8-C9
38	n	608	CHL	C14-C13-C15-C16
38	n	609	CHL	C11-C10-C8-C9
38	r	605	CHL	C14-C13-C15-C16
38	y	302	CHL	C6-C7-C8-C9
38	y	302	CHL	C11-C10-C8-C9
38	y	308	CHL	C11-C10-C8-C9
38	y	308	CHL	C14-C13-C15-C16
38	y	309	CHL	C14-C13-C15-C16
28	R	609	CLA	O1D-CGD-O2D-CED
28	c	501	CLA	O1D-CGD-O2D-CED
38	R	606	CHL	O1D-CGD-O2D-CED
38	S	308	CHL	O1D-CGD-O2D-CED
28	n	603	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	C2A-CAA-CBA-CGA
38	N	601	CHL	C2A-CAA-CBA-CGA
30	A	409	BCR	C7-C8-C9-C34
30	B	617	BCR	C7-C8-C9-C34
30	B	617	BCR	C11-C12-C13-C35
30	B	617	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	B	618	BCR	C7-C8-C9-C34
30	B	618	BCR	C11-C12-C13-C35
30	B	618	BCR	C37-C22-C23-C24
30	B	619	BCR	C7-C8-C9-C34
30	B	619	BCR	C11-C12-C13-C35
30	B	619	BCR	C36-C18-C19-C20
30	C	514	BCR	C37-C22-C23-C24
30	C	516	BCR	C37-C22-C23-C24
30	D	405	BCR	C11-C12-C13-C35
30	D	405	BCR	C36-C18-C19-C20
30	H	101	BCR	C36-C18-C19-C20
30	H	101	BCR	C37-C22-C23-C24
30	T	101	BCR	C11-C12-C13-C35
30	T	101	BCR	C36-C18-C19-C20
30	a	410	BCR	C11-C12-C13-C35
30	a	410	BCR	C36-C18-C19-C20
30	b	617	BCR	C11-C12-C13-C35
30	b	618	BCR	C11-C12-C13-C35
30	b	618	BCR	C36-C18-C19-C20
30	c	514	BCR	C11-C12-C13-C35
30	d	406	BCR	C36-C18-C19-C20
30	d	406	BCR	C37-C22-C23-C24
30	h	101	BCR	C36-C18-C19-C20
30	k	101	BCR	C7-C8-C9-C34
30	k	101	BCR	C36-C18-C19-C20
30	k	101	BCR	C37-C22-C23-C24
30	t	101	BCR	C36-C18-C19-C20
30	t	101	BCR	C37-C22-C23-C24
39	G	615	LUT	C27-C28-C29-C39
39	N	616	LUT	C7-C8-C9-C19
39	R	614	LUT	C7-C8-C9-C19
39	S	315	LUT	C27-C28-C29-C39
39	Y	615	LUT	C11-C12-C13-C20
39	Y	616	LUT	C7-C8-C9-C19
39	r	614	LUT	C27-C28-C29-C39
39	s	614	LUT	C7-C8-C9-C19
39	y	316	LUT	C11-C12-C13-C20
40	g	617	NEX	C11-C12-C13-C20
41	R	615	XAT	C27-C28-C29-C39
41	r	615	XAT	C27-C28-C29-C39
30	A	409	BCR	C7-C8-C9-C10
30	B	617	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	B	617	BCR	C17-C18-C19-C20
30	B	618	BCR	C7-C8-C9-C10
30	B	619	BCR	C11-C12-C13-C14
30	B	619	BCR	C17-C18-C19-C20
30	C	514	BCR	C17-C18-C19-C20
30	C	516	BCR	C21-C22-C23-C24
30	D	405	BCR	C11-C12-C13-C14
30	D	405	BCR	C21-C22-C23-C24
30	T	101	BCR	C17-C18-C19-C20
30	a	410	BCR	C11-C12-C13-C14
30	a	410	BCR	C17-C18-C19-C20
30	b	617	BCR	C7-C8-C9-C10
30	b	617	BCR	C11-C12-C13-C14
30	b	617	BCR	C21-C22-C23-C24
30	b	618	BCR	C11-C12-C13-C14
30	b	618	BCR	C17-C18-C19-C20
30	b	619	BCR	C7-C8-C9-C10
30	c	514	BCR	C7-C8-C9-C10
30	c	515	BCR	C11-C12-C13-C14
30	d	406	BCR	C21-C22-C23-C24
30	h	101	BCR	C17-C18-C19-C20
30	i	101	BCR	C17-C18-C19-C20
30	k	101	BCR	C7-C8-C9-C10
30	k	101	BCR	C17-C18-C19-C20
30	k	101	BCR	C21-C22-C23-C24
30	t	101	BCR	C21-C22-C23-C24
39	G	615	LUT	C27-C28-C29-C30
39	N	616	LUT	C7-C8-C9-C10
39	R	614	LUT	C7-C8-C9-C10
39	Y	616	LUT	C7-C8-C9-C10
39	s	614	LUT	C7-C8-C9-C10
40	g	617	NEX	C11-C12-C13-C14
35	S	301	LHG	C23-C24-C25-C26
35	a	415	LHG	C7-C8-C9-C10
35	a	415	LHG	C23-C24-C25-C26
35	c	519	LHG	C23-C24-C25-C26
35	l	101	LHG	C23-C24-C25-C26
28	B	602	CLA	O1A-CGA-O2A-C1
28	N	603	CLA	O1A-CGA-O2A-C1
28	R	604	CLA	O1A-CGA-O2A-C1
28	b	611	CLA	O1A-CGA-O2A-C1
28	c	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	c	516	DGD	O1A-C1A-O1G-C1G
28	A	405	CLA	C8-C10-C11-C12
28	b	616	CLA	O1D-CGD-O2D-CED
28	g	612	CLA	O1D-CGD-O2D-CED
28	r	604	CLA	O1D-CGD-O2D-CED
38	N	608	CHL	O1D-CGD-O2D-CED
28	N	611	CLA	C3-C5-C6-C7
28	d	401	CLA	C3-C5-C6-C7
28	b	602	CLA	CBA-CGA-O2A-C1
28	n	603	CLA	CBA-CGA-O2A-C1
35	B	623	LHG	C24-C23-O8-C6
36	C	519	DGD	C2A-C1A-O1G-C1G
28	B	615	CLA	C5-C6-C7-C8
28	r	612	CLA	C8-C10-C11-C12
38	y	302	CHL	C8-C10-C11-C12
35	Y	619	LHG	C7-C8-C9-C10
35	b	621	LHG	C7-C8-C9-C10
35	b	622	LHG	C23-C24-C25-C26
35	b	624	LHG	C7-C8-C9-C10
35	r	617	LHG	C23-C24-C25-C26
28	B	611	CLA	O1D-CGD-O2D-CED
36	C	518	DGD	C4A-C5A-C6A-C7A
28	N	611	CLA	C8-C10-C11-C12
28	R	602	CLA	C8-C10-C11-C12
28	R	613	CLA	C8-C10-C11-C12
28	Y	610	CLA	C5-C6-C7-C8
28	b	612	CLA	C8-C10-C11-C12
28	n	610	CLA	C8-C10-C11-C12
28	n	611	CLA	C8-C10-C11-C12
38	N	607	CHL	C5-C6-C7-C8
35	A	416	LHG	C9-C10-C11-C12
28	S	303	CLA	O1D-CGD-O2D-CED
28	y	311	CLA	O1D-CGD-O2D-CED
35	N	618	LHG	O1-C1-C2-O2
35	b	621	LHG	O1-C1-C2-O2
35	c	520	LHG	O1-C1-C2-O2
35	B	622	LHG	C7-C8-C9-C10
35	B	623	LHG	C23-C24-C25-C26
35	B	625	LHG	C23-C24-C25-C26
35	C	521	LHG	C7-C8-C9-C10
35	L	102	LHG	C23-C24-C25-C26
35	S	317	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	W	101	LHG	C7-C8-C9-C10
35	b	624	LHG	C23-C24-C25-C26
35	c	519	LHG	C7-C8-C9-C10
35	c	520	LHG	C23-C24-C25-C26
35	w	102	LHG	C7-C8-C9-C10
35	y	319	LHG	C7-C8-C9-C10
35	y	319	LHG	C23-C24-C25-C26
36	C	519	DGD	C1B-C2B-C3B-C4B
28	N	602	CLA	O1D-CGD-O2D-CED
28	S	313	CLA	O1D-CGD-O2D-CED
28	S	314	CLA	O1D-CGD-O2D-CED
28	C	502	CLA	C5-C6-C7-C8
38	g	608	CHL	C8-C10-C11-C12
28	C	503	CLA	CBA-CGA-O2A-C1
28	y	303	CLA	CBA-CGA-O2A-C1
38	g	601	CHL	CBA-CGA-O2A-C1
28	B	602	CLA	O1D-CGD-O2D-CED
28	g	611	CLA	O1D-CGD-O2D-CED
38	N	609	CHL	O1D-CGD-O2D-CED
38	r	606	CHL	O1D-CGD-O2D-CED
38	s	605	CHL	O1D-CGD-O2D-CED
35	C	521	LHG	O9-C7-O7-C5
35	b	624	LHG	O9-C7-O7-C5
28	C	510	CLA	C2-C1-O2A-CGA
28	C	512	CLA	C2-C1-O2A-CGA
28	N	614	CLA	C2-C1-O2A-CGA
28	S	311	CLA	C2-C1-O2A-CGA
28	b	613	CLA	C2-C1-O2A-CGA
28	c	502	CLA	C2-C1-O2A-CGA
28	c	509	CLA	C2-C1-O2A-CGA
28	r	611	CLA	C2-C1-O2A-CGA
28	c	508	CLA	C8-C10-C11-C12
35	B	622	LHG	C23-C24-C25-C26
35	n	618	LHG	C23-C24-C25-C26
35	r	617	LHG	C7-C8-C9-C10
35	s	617	LHG	C23-C24-C25-C26
28	n	611	CLA	CBD-CGD-O2D-CED
32	b	623	LMG	C11-C10-O7-C8
28	B	614	CLA	C5-C6-C7-C8
28	C	504	CLA	C8-C10-C11-C12
28	S	303	CLA	C8-C10-C11-C12
28	A	408	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	B	606	CLA	C6-C7-C8-C10
28	B	607	CLA	C6-C7-C8-C10
28	C	506	CLA	C6-C7-C8-C10
28	C	510	CLA	C6-C7-C8-C10
28	G	611	CLA	C6-C7-C8-C10
28	R	602	CLA	C11-C10-C8-C7
28	b	612	CLA	C6-C7-C8-C10
28	b	616	CLA	C11-C10-C8-C7
28	n	603	CLA	C11-C10-C8-C7
28	n	610	CLA	C11-C12-C13-C15
28	r	602	CLA	C11-C10-C8-C7
28	r	613	CLA	C6-C7-C8-C10
28	y	312	CLA	C6-C7-C8-C10
38	Y	607	CHL	C11-C10-C8-C7
38	g	608	CHL	C11-C12-C13-C15
38	y	302	CHL	C11-C12-C13-C15
28	C	509	CLA	C3-C5-C6-C7
28	b	607	CLA	C3-C5-C6-C7
28	s	609	CLA	C3-C5-C6-C7
35	b	622	LHG	O10-C23-O8-C6
36	C	519	DGD	O1A-C1A-O1G-C1G
38	r	607	CHL	O1A-CGA-O2A-C1
35	b	621	LHG	C9-C10-C11-C12
30	B	617	BCR	C9-C10-C11-C12
30	B	617	BCR	C13-C14-C15-C16
30	B	618	BCR	C15-C16-C17-C18
30	B	618	BCR	C19-C20-C21-C22
30	C	515	BCR	C9-C10-C11-C12
30	T	101	BCR	C13-C14-C15-C16
30	T	101	BCR	C15-C16-C17-C18
30	a	410	BCR	C15-C16-C17-C18
30	b	617	BCR	C13-C14-C15-C16
30	b	618	BCR	C9-C10-C11-C12
30	b	618	BCR	C19-C20-C21-C22
30	i	101	BCR	C13-C14-C15-C16
30	i	101	BCR	C19-C20-C21-C22
28	C	507	CLA	C2A-CAA-CBA-CGA
28	S	305	CLA	C2A-CAA-CBA-CGA
28	c	504	CLA	O1D-CGD-O2D-CED
28	y	313	CLA	C5-C6-C7-C8
28	n	604	CLA	O1A-CGA-O2A-C1
35	A	416	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
28	R	613	CLA	CBD-CGD-O2D-CED
38	G	606	CHL	CBD-CGD-O2D-CED
35	A	416	LHG	C7-C8-C9-C10
35	d	408	LHG	C23-C24-C25-C26
40	g	617	NEX	C30-C31-C32-C33
40	n	617	NEX	C10-C11-C12-C13
40	s	616	NEX	C10-C11-C12-C13
40	y	301	NEX	C10-C11-C12-C13
40	y	318	NEX	C30-C31-C32-C33
41	Y	617	XAT	C10-C11-C12-C13
41	y	317	XAT	C10-C11-C12-C13
41	y	317	XAT	C30-C31-C32-C33
36	c	518	DGD	CAB-CBB-CCB-CDB
28	s	604	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	O2-C2-C3-O3
35	G	618	LHG	O2-C2-C3-O3
35	L	102	LHG	O2-C2-C3-O3
35	N	618	LHG	O2-C2-C3-O3
35	S	301	LHG	O2-C2-C3-O3
35	S	317	LHG	O2-C2-C3-O3
35	W	101	LHG	O2-C2-C3-O3
35	a	415	LHG	O2-C2-C3-O3
35	b	621	LHG	O2-C2-C3-O3
35	b	622	LHG	O2-C2-C3-O3
35	c	519	LHG	O2-C2-C3-O3
35	d	408	LHG	O2-C2-C3-O3
35	g	618	LHG	O2-C2-C3-O3
35	n	618	LHG	O2-C2-C3-O3
35	g	618	LHG	O9-C7-O7-C5
28	Y	611	CLA	C3-C5-C6-C7
28	d	405	CLA	C3-C5-C6-C7
28	c	513	CLA	C8-C10-C11-C12
28	B	606	CLA	C8-C10-C11-C12
28	B	614	CLA	C8-C10-C11-C12
28	n	603	CLA	C13-C15-C16-C17
28	r	603	CLA	C5-C6-C7-C8
38	N	609	CHL	C13-C15-C16-C17
38	S	307	CHL	C5-C6-C7-C8
28	R	602	CLA	CBA-CGA-O2A-C1
35	c	519	LHG	C24-C23-O8-C6
35	B	623	LHG	C29-C30-C31-C32
28	Y	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	S	303	CLA	O1A-CGA-O2A-C1
28	Y	604	CLA	O1A-CGA-O2A-C1
28	b	602	CLA	O1A-CGA-O2A-C1
28	y	303	CLA	O1A-CGA-O2A-C1
35	a	415	LHG	O10-C23-O8-C6
38	R	607	CHL	O1A-CGA-O2A-C1
35	D	407	LHG	C23-C24-C25-C26
35	G	618	LHG	C23-C24-C25-C26
35	W	101	LHG	C23-C24-C25-C26
36	C	519	DGD	CBB-CCB-CDB-CEB
28	b	601	CLA	C5-C6-C7-C8
28	c	508	CLA	C13-C15-C16-C17
28	c	510	CLA	C13-C15-C16-C17
28	d	405	CLA	C8-C10-C11-C12
28	g	610	CLA	C5-C6-C7-C8
28	r	609	CLA	C8-C10-C11-C12
28	s	609	CLA	C5-C6-C7-C8
38	N	607	CHL	C8-C10-C11-C12
38	Y	609	CHL	C5-C6-C7-C8
35	G	618	LHG	C33-C34-C35-C36
28	s	613	CLA	O1D-CGD-O2D-CED
28	b	614	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	O1A-CGA-O2A-C1
28	n	603	CLA	O1A-CGA-O2A-C1
35	A	416	LHG	C25-C26-C27-C28
28	B	605	CLA	C5-C6-C7-C8
28	Y	612	CLA	C8-C10-C11-C12
28	b	602	CLA	C5-C6-C7-C8
28	b	603	CLA	C5-C6-C7-C8
28	b	611	CLA	C8-C10-C11-C12
28	b	614	CLA	C5-C6-C7-C8
28	y	310	CLA	C5-C6-C7-C8
38	y	308	CHL	C8-C10-C11-C12
35	G	618	LHG	C3-O3-P-O6
35	N	618	LHG	C3-O3-P-O6
35	N	618	LHG	C4-O6-P-O3
35	R	616	LHG	C4-O6-P-O3
35	S	301	LHG	C3-O3-P-O6
35	W	101	LHG	C4-O6-P-O3
35	Y	619	LHG	C4-O6-P-O3
35	a	415	LHG	C4-O6-P-O3
35	b	622	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
35	b	624	LHG	C4-O6-P-O3
35	c	519	LHG	C3-O3-P-O6
35	c	520	LHG	C3-O3-P-O6
35	d	408	LHG	C3-O3-P-O6
35	l	101	LHG	C4-O6-P-O3
35	n	618	LHG	C3-O3-P-O6
35	n	618	LHG	C4-O6-P-O3
35	s	617	LHG	C3-O3-P-O6
35	s	617	LHG	C4-O6-P-O3
35	y	319	LHG	C3-O3-P-O6
28	Y	612	CLA	C3-C5-C6-C7
28	a	406	CLA	C3-C5-C6-C7
28	g	611	CLA	C3-C5-C6-C7
28	d	401	CLA	CBA-CGA-O2A-C1
28	g	603	CLA	CBA-CGA-O2A-C1
35	L	102	LHG	C24-C23-O8-C6
35	w	102	LHG	C24-C23-O8-C6
36	C	517	DGD	C2A-C1A-O1G-C1G
28	B	604	CLA	C5-C6-C7-C8
28	C	502	CLA	C8-C10-C11-C12
28	c	507	CLA	C8-C10-C11-C12
38	g	601	CHL	C13-C15-C16-C17
38	Y	608	CHL	O1D-CGD-O2D-CED
35	B	623	LHG	C1-C2-C3-O3
35	L	102	LHG	C1-C2-C3-O3
35	R	616	LHG	C1-C2-C3-O3
35	c	520	LHG	C1-C2-C3-O3
35	n	618	LHG	C1-C2-C3-O3
35	s	617	LHG	C1-C2-C3-O3
35	y	319	LHG	C1-C2-C3-O3
32	b	623	LMG	O9-C10-O7-C8
35	D	407	LHG	O9-C7-O7-C5
35	c	520	LHG	C16-C17-C18-C19
28	b	607	CLA	C5-C6-C7-C8
38	y	309	CHL	C8-C10-C11-C12
36	C	517	DGD	O1A-C1A-O1G-C1G
28	B	606	CLA	C2A-CAA-CBA-CGA
28	G	603	CLA	C2A-CAA-CBA-CGA
28	R	604	CLA	C2A-CAA-CBA-CGA
28	g	604	CLA	C2A-CAA-CBA-CGA
28	s	604	CLA	C2A-CAA-CBA-CGA
38	G	605	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
38	G	607	CHL	C2A-CAA-CBA-CGA
38	N	607	CHL	C2A-CAA-CBA-CGA
38	S	307	CHL	C2A-CAA-CBA-CGA
38	Y	607	CHL	C2A-CAA-CBA-CGA
38	g	605	CHL	C2A-CAA-CBA-CGA
38	g	607	CHL	C2A-CAA-CBA-CGA
38	n	607	CHL	C2A-CAA-CBA-CGA
38	s	601	CHL	C2A-CAA-CBA-CGA
38	N	609	CHL	C16-C17-C18-C20
28	C	508	CLA	CBA-CGA-O2A-C1
28	N	602	CLA	CBA-CGA-O2A-C1
28	d	405	CLA	CBA-CGA-O2A-C1
28	r	611	CLA	CBA-CGA-O2A-C1
35	B	625	LHG	C24-C23-O8-C6
35	D	407	LHG	C24-C23-O8-C6
38	y	307	CHL	CBA-CGA-O2A-C1
30	b	618	BCR	C13-C14-C15-C16
30	h	101	BCR	C15-C16-C17-C18
30	t	101	BCR	C13-C14-C15-C16
35	b	621	LHG	C23-C24-C25-C26
28	r	603	CLA	C4C-C3C-CAC-CBC
35	Y	619	LHG	C26-C27-C28-C29
28	s	608	CLA	CBD-CGD-O2D-CED
35	B	622	LHG	C8-C7-O7-C5
35	D	407	LHG	C8-C7-O7-C5
35	c	520	LHG	C8-C7-O7-C5
35	n	618	LHG	C8-C7-O7-C5
35	s	617	LHG	C8-C7-O7-C5
28	c	510	CLA	C8-C10-C11-C12
40	N	617	NEX	C39-C29-C30-C31
40	g	617	NEX	C39-C29-C30-C31
40	g	617	NEX	C40-C33-C34-C35
40	n	617	NEX	C11-C10-C9-C19
40	n	617	NEX	C20-C13-C14-C15
40	r	616	NEX	C39-C29-C30-C31
40	y	301	NEX	C40-C33-C34-C35
41	R	615	XAT	C20-C13-C14-C15
41	r	615	XAT	C20-C13-C14-C15
28	Y	603	CLA	C3-C5-C6-C7
28	n	611	CLA	C3-C5-C6-C7
35	D	407	LHG	C28-C29-C30-C31
35	W	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	w	102	LHG	C11-C12-C13-C14
35	w	102	LHG	C13-C14-C15-C16
35	y	319	LHG	C11-C12-C13-C14
28	b	611	CLA	O1D-CGD-O2D-CED
28	S	313	CLA	C6-C7-C8-C10
28	Y	602	CLA	C16-C17-C18-C20
36	c	518	DGD	C2A-C1A-O1G-C1G
32	b	620	LMG	C11-C12-C13-C14
35	L	102	LHG	C11-C12-C13-C14
35	S	317	LHG	C11-C12-C13-C14
35	a	415	LHG	C13-C14-C15-C16
35	b	621	LHG	C11-C12-C13-C14
35	g	618	LHG	C11-C12-C13-C14
35	l	101	LHG	C13-C14-C15-C16
35	s	617	LHG	C28-C29-C30-C31
36	c	518	DGD	C4B-C5B-C6B-C7B
28	c	510	CLA	O1D-CGD-O2D-CED
32	D	408	LMG	O9-C10-O7-C8
35	B	622	LHG	O9-C7-O7-C5
35	c	520	LHG	O9-C7-O7-C5
35	n	618	LHG	O9-C7-O7-C5
35	s	617	LHG	O9-C7-O7-C5
28	b	605	CLA	C15-C16-C17-C18
28	R	603	CLA	CBD-CGD-O2D-CED
35	D	407	LHG	C11-C12-C13-C14
35	G	618	LHG	C25-C26-C27-C28
35	S	317	LHG	C25-C26-C27-C28
36	B	626	DGD	C2B-C3B-C4B-C5B
28	r	603	CLA	O1D-CGD-O2D-CED
35	Y	619	LHG	C11-C12-C13-C14
37	E	101	HEM	C2A-CAA-CBA-CGA
35	C	521	LHG	C13-C14-C15-C16
35	d	408	LHG	C11-C12-C13-C14
28	b	611	CLA	C3-C5-C6-C7
28	c	506	CLA	C3-C5-C6-C7
28	c	508	CLA	C3-C5-C6-C7
32	b	623	LMG	C10-C11-C12-C13
35	g	618	LHG	C23-C24-C25-C26
28	N	611	CLA	O1D-CGD-O2D-CED
28	r	602	CLA	O1D-CGD-O2D-CED
31	M	101	SQD	C2-C1-O6-C44
40	G	617	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	g	617	NEX	C32-C33-C34-C35
40	n	617	NEX	C11-C10-C9-C8
40	n	617	NEX	C12-C13-C14-C15
40	r	616	NEX	C28-C29-C30-C31
40	s	616	NEX	C28-C29-C30-C31
40	y	301	NEX	C32-C33-C34-C35
40	y	318	NEX	C11-C10-C9-C8
31	M	101	SQD	O47-C45-C46-O48
35	s	617	LHG	C13-C14-C15-C16
28	d	405	CLA	O1A-CGA-O2A-C1
35	B	623	LHG	O10-C23-O8-C6
28	Y	610	CLA	C11-C12-C13-C14
28	n	611	CLA	C11-C12-C13-C15
28	n	613	CLA	C6-C7-C8-C10
38	R	607	CHL	C11-C12-C13-C15
28	S	313	CLA	C4-C3-C5-C6
35	B	625	LHG	C13-C14-C15-C16
35	a	415	LHG	C28-C29-C30-C31
35	y	319	LHG	C13-C14-C15-C16
36	c	518	DGD	C5B-C6B-C7B-C8B
28	B	606	CLA	C2-C3-C5-C6
28	B	612	CLA	C6-C7-C8-C9
28	C	502	CLA	C6-C7-C8-C9
28	C	512	CLA	C11-C10-C8-C9
28	C	513	CLA	C6-C7-C8-C9
28	N	612	CLA	C6-C7-C8-C9
28	R	608	CLA	C11-C10-C8-C9
28	a	406	CLA	C11-C10-C8-C9
38	g	608	CHL	C11-C12-C13-C14
38	G	609	CHL	O1D-CGD-O2D-CED
35	N	618	LHG	C23-C24-C25-C26
28	c	507	CLA	C2A-CAA-CBA-CGA
28	R	602	CLA	O1A-CGA-O2A-C1
28	r	611	CLA	O1A-CGA-O2A-C1
35	c	519	LHG	O10-C23-O8-C6
35	w	102	LHG	O10-C23-O8-C6
38	g	601	CHL	O1A-CGA-O2A-C1
30	C	515	BCR	C36-C18-C19-C20
30	C	515	BCR	C37-C22-C23-C24
30	C	516	BCR	C11-C12-C13-C35
30	D	405	BCR	C37-C22-C23-C24
30	K	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
30	b	617	BCR	C36-C18-C19-C20
30	b	618	BCR	C7-C8-C9-C34
30	c	514	BCR	C36-C18-C19-C20
30	c	515	BCR	C36-C18-C19-C20
30	i	101	BCR	C7-C8-C9-C34
30	i	101	BCR	C11-C12-C13-C35
30	i	101	BCR	C36-C18-C19-C20
39	G	616	LUT	C7-C8-C9-C19
39	g	616	LUT	C7-C8-C9-C19
40	y	301	NEX	C11-C12-C13-C20
40	y	301	NEX	C31-C32-C33-C40
35	d	408	LHG	C28-C29-C30-C31
35	L	102	LHG	O1-C1-C2-C3
35	N	618	LHG	O1-C1-C2-C3
35	R	616	LHG	O1-C1-C2-C3
35	a	415	LHG	O1-C1-C2-C3
35	b	621	LHG	O1-C1-C2-C3
35	b	622	LHG	O1-C1-C2-C3
35	b	624	LHG	O1-C1-C2-C3
35	c	519	LHG	O1-C1-C2-C3
35	c	520	LHG	O1-C1-C2-C3
35	g	618	LHG	O1-C1-C2-C3
35	n	618	LHG	O1-C1-C2-C3
35	r	617	LHG	O1-C1-C2-C3
35	w	102	LHG	O1-C1-C2-C3
35	y	319	LHG	O1-C1-C2-C3
30	B	617	BCR	C7-C8-C9-C10
30	B	619	BCR	C7-C8-C9-C10
30	C	514	BCR	C21-C22-C23-C24
30	C	515	BCR	C17-C18-C19-C20
30	C	515	BCR	C21-C22-C23-C24
30	C	516	BCR	C11-C12-C13-C14
30	D	405	BCR	C17-C18-C19-C20
30	H	101	BCR	C17-C18-C19-C20
30	K	101	BCR	C11-C12-C13-C14
30	K	101	BCR	C21-C22-C23-C24
30	T	101	BCR	C11-C12-C13-C14
30	b	617	BCR	C17-C18-C19-C20
30	b	618	BCR	C7-C8-C9-C10
30	c	514	BCR	C17-C18-C19-C20
30	c	515	BCR	C17-C18-C19-C20
30	d	406	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	i	101	BCR	C7-C8-C9-C10
30	i	101	BCR	C11-C12-C13-C14
30	t	101	BCR	C17-C18-C19-C20
39	G	616	LUT	C7-C8-C9-C10
39	g	615	LUT	C31-C32-C33-C34
39	g	616	LUT	C7-C8-C9-C10
39	s	614	LUT	C31-C32-C33-C34
39	s	615	LUT	C7-C8-C9-C10
28	n	610	CLA	C3-C5-C6-C7
28	r	602	CLA	C3-C5-C6-C7
32	C	520	LMG	O9-C10-O7-C8
35	S	301	LHG	O9-C7-O7-C5
28	y	311	CLA	C5-C6-C7-C8
32	C	520	LMG	C11-C10-O7-C8
32	D	408	LMG	C11-C10-O7-C8
35	S	301	LHG	C8-C7-O7-C5
35	S	317	LHG	C9-C10-C11-C12
35	b	624	LHG	C30-C31-C32-C33
35	s	617	LHG	C11-C12-C13-C14
35	N	618	LHG	C7-C8-C9-C10
35	S	317	LHG	C23-C24-C25-C26
35	n	618	LHG	C7-C8-C9-C10
35	A	416	LHG	C11-C12-C13-C14
35	G	618	LHG	C13-C14-C15-C16
35	W	101	LHG	C28-C29-C30-C31
35	l	101	LHG	C33-C34-C35-C36
35	n	618	LHG	C25-C26-C27-C28
35	y	319	LHG	C29-C30-C31-C32
28	g	611	CLA	C4B-C3B-CAB-CBB
28	s	609	CLA	C6-C7-C8-C9
28	s	612	CLA	C6-C7-C8-C9
38	g	609	CHL	C11-C12-C13-C15
38	r	607	CHL	C11-C12-C13-C14
38	r	607	CHL	C11-C12-C13-C15
28	B	616	CLA	C8-C10-C11-C12
28	b	607	CLA	C8-C10-C11-C12
32	a	413	LMG	C34-C35-C36-C37
35	C	521	LHG	C11-C12-C13-C14
35	b	622	LHG	C26-C27-C28-C29
35	d	408	LHG	C26-C27-C28-C29
38	Y	609	CHL	CBD-CGD-O2D-CED
28	N	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	Y	605	CHL	O1D-CGD-O2D-CED
35	A	416	LHG	C28-C29-C30-C31
35	D	407	LHG	C13-C14-C15-C16
35	N	618	LHG	C26-C27-C28-C29
35	l	101	LHG	C25-C26-C27-C28
28	R	609	CLA	C8-C10-C11-C12
28	N	602	CLA	O1A-CGA-O2A-C1
28	d	401	CLA	O1A-CGA-O2A-C1
28	g	603	CLA	O1A-CGA-O2A-C1
32	a	413	LMG	C30-C31-C32-C33
35	b	624	LHG	C28-C29-C30-C31
35	y	319	LHG	C25-C26-C27-C28
28	S	311	CLA	C3-C5-C6-C7
28	n	602	CLA	CBA-CGA-O2A-C1
28	A	406	CLA	C3A-C2A-CAA-CBA
28	B	604	CLA	C3A-C2A-CAA-CBA
28	C	509	CLA	C3A-C2A-CAA-CBA
28	C	513	CLA	C3A-C2A-CAA-CBA
28	R	604	CLA	C3A-C2A-CAA-CBA
28	a	407	CLA	C3A-C2A-CAA-CBA
28	b	604	CLA	C3A-C2A-CAA-CBA
28	c	512	CLA	C3A-C2A-CAA-CBA
28	c	513	CLA	C3A-C2A-CAA-CBA
28	n	603	CLA	C3A-C2A-CAA-CBA
28	s	603	CLA	C3A-C2A-CAA-CBA
38	G	607	CHL	C3A-C2A-CAA-CBA
38	R	607	CHL	C3A-C2A-CAA-CBA
38	Y	601	CHL	C3A-C2A-CAA-CBA
38	Y	607	CHL	C3A-C2A-CAA-CBA
38	g	607	CHL	C3A-C2A-CAA-CBA
28	B	611	CLA	C15-C16-C17-C18
28	N	610	CLA	C5-C6-C7-C8
28	R	609	CLA	C5-C6-C7-C8
32	B	624	LMG	C8-C9-O8-C28
35	C	521	LHG	C33-C34-C35-C36
35	N	618	LHG	C25-C26-C27-C28
35	c	520	LHG	C13-C14-C15-C16
28	g	603	CLA	O1D-CGD-O2D-CED
38	y	307	CHL	O1A-CGA-O2A-C1
28	s	609	CLA	C6-C7-C8-C10
38	N	609	CHL	C16-C17-C18-C19
38	R	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	g	609	CHL	C11-C12-C13-C14
35	B	623	LHG	C28-C29-C30-C31
35	Y	619	LHG	C34-C35-C36-C37
35	d	408	LHG	C13-C14-C15-C16
35	S	301	LHG	C11-C12-C13-C14
35	s	617	LHG	C9-C10-C11-C12
35	y	319	LHG	C15-C16-C17-C18
40	G	617	NEX	C14-C15-C35-C34
40	Y	618	NEX	C14-C15-C35-C34
28	B	602	CLA	C3-C5-C6-C7
35	B	623	LHG	C7-C8-C9-C10
36	C	519	DGD	C2B-C3B-C4B-C5B
35	D	407	LHG	O10-C23-O8-C6
28	r	609	CLA	C5-C6-C7-C8
28	G	613	CLA	C4-C3-C5-C6
28	y	312	CLA	C4-C3-C5-C6
28	y	312	CLA	C2-C3-C5-C6
35	A	416	LHG	C8-C7-O7-C5
35	c	519	LHG	C8-C7-O7-C5
35	d	408	LHG	C8-C7-O7-C5
35	r	617	LHG	C8-C7-O7-C5
35	Y	619	LHG	C13-C14-C15-C16
28	b	612	CLA	C2A-CAA-CBA-CGA
35	A	416	LHG	O1-C1-C2-O2
35	B	622	LHG	O1-C1-C2-O2
35	B	623	LHG	O1-C1-C2-O2
35	D	407	LHG	O1-C1-C2-O2
35	L	102	LHG	O1-C1-C2-O2
35	S	301	LHG	O1-C1-C2-O2
35	S	317	LHG	O1-C1-C2-O2
35	b	624	LHG	O1-C1-C2-O2
35	d	408	LHG	O1-C1-C2-O2
35	g	618	LHG	O1-C1-C2-O2
35	s	617	LHG	O1-C1-C2-O2
35	w	102	LHG	O1-C1-C2-O2
35	L	102	LHG	C13-C14-C15-C16
35	c	520	LHG	C11-C12-C13-C14
35	n	618	LHG	C26-C27-C28-C29
35	B	625	LHG	O10-C23-O8-C6
36	c	518	DGD	O1A-C1A-O1G-C1G
35	G	618	LHG	C7-C8-C9-C10
28	n	611	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	w	102	LHG	C11-C10-C9-C8
28	g	611	CLA	C2B-C3B-CAB-CBB
28	Y	610	CLA	C8-C10-C11-C12
28	c	513	CLA	C5-C6-C7-C8
35	B	625	LHG	C30-C31-C32-C33
28	r	603	CLA	C3-C5-C6-C7
28	G	610	CLA	CBA-CGA-O2A-C1
35	g	618	LHG	C13-C14-C15-C16
28	C	508	CLA	O1A-CGA-O2A-C1
35	L	102	LHG	O10-C23-O8-C6
35	B	625	LHG	C7-C8-C9-C10
35	w	102	LHG	C23-C24-C25-C26
35	A	416	LHG	C1-C2-C3-O3
35	S	317	LHG	C28-C29-C30-C31
35	W	101	LHG	C26-C27-C28-C29
35	A	416	LHG	O9-C7-O7-C5
35	d	408	LHG	O9-C7-O7-C5
35	r	617	LHG	O9-C7-O7-C5
28	B	610	CLA	C2-C1-O2A-CGA
28	B	616	CLA	C2-C1-O2A-CGA
28	C	509	CLA	C2-C1-O2A-CGA
28	b	612	CLA	C2-C1-O2A-CGA
28	c	512	CLA	C2-C1-O2A-CGA
28	d	405	CLA	C2-C1-O2A-CGA
28	s	604	CLA	C2-C1-O2A-CGA
28	y	304	CLA	C2-C1-O2A-CGA
28	y	305	CLA	C2-C1-O2A-CGA
35	y	319	LHG	C14-C15-C16-C17
28	D	401	CLA	C8-C10-C11-C12
28	Y	611	CLA	C8-C10-C11-C12
28	b	606	CLA	C13-C15-C16-C17
35	B	625	LHG	C26-C27-C28-C29
35	L	102	LHG	C29-C30-C31-C32
35	Y	619	LHG	C28-C29-C30-C31
28	Y	602	CLA	C16-C17-C18-C19
28	N	602	CLA	C3-C5-C6-C7
28	c	512	CLA	C3-C5-C6-C7
30	A	409	BCR	C5-C6-C7-C8
30	B	617	BCR	C23-C24-C25-C26
30	B	617	BCR	C23-C24-C25-C30
30	B	618	BCR	C5-C6-C7-C8
30	B	619	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	B	619	BCR	C23-C24-C25-C30
30	C	515	BCR	C5-C6-C7-C8
30	C	516	BCR	C5-C6-C7-C8
30	C	516	BCR	C23-C24-C25-C30
30	D	405	BCR	C5-C6-C7-C8
30	K	101	BCR	C1-C6-C7-C8
30	K	101	BCR	C23-C24-C25-C26
30	a	410	BCR	C5-C6-C7-C8
30	b	617	BCR	C23-C24-C25-C26
30	b	619	BCR	C5-C6-C7-C8
30	b	619	BCR	C23-C24-C25-C30
30	d	406	BCR	C5-C6-C7-C8
30	d	406	BCR	C23-C24-C25-C30
30	i	101	BCR	C1-C6-C7-C8
30	k	101	BCR	C5-C6-C7-C8
30	k	101	BCR	C23-C24-C25-C30
30	t	101	BCR	C5-C6-C7-C8
30	t	101	BCR	C23-C24-C25-C26
39	G	615	LUT	C5-C6-C7-C8
28	c	505	CLA	C8-C10-C11-C12
35	G	618	LHG	C34-C35-C36-C37
35	W	101	LHG	C13-C14-C15-C16
35	a	415	LHG	C9-C10-C11-C12
35	b	624	LHG	C10-C11-C12-C13
36	C	517	DGD	C2B-C3B-C4B-C5B
28	B	611	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	C2A-C1A-O1G-C1G
38	Y	601	CHL	C5-C6-C7-C8
35	d	408	LHG	C31-C32-C33-C34
35	g	618	LHG	C16-C17-C18-C19
35	w	102	LHG	C24-C25-C26-C27
35	g	618	LHG	C7-C8-C9-C10
35	B	622	LHG	C26-C27-C28-C29
35	B	623	LHG	C26-C27-C28-C29
35	C	521	LHG	C26-C27-C28-C29
35	d	408	LHG	C32-C33-C34-C35
35	g	618	LHG	C11-C10-C9-C8
28	A	408	CLA	C8-C10-C11-C12
28	r	608	CLA	C8-C10-C11-C12
28	C	510	CLA	O1D-CGD-O2D-CED
28	N	610	CLA	C4-C3-C5-C6
28	n	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
38	G	601	CHL	C4-C3-C5-C6
38	N	607	CHL	C4-C3-C5-C6
38	N	608	CHL	C4-C3-C5-C6
38	g	607	CHL	C4-C3-C5-C6
38	n	607	CHL	C4-C3-C5-C6
38	n	609	CHL	C4-C3-C5-C6
38	r	607	CHL	C4-C3-C5-C6
28	B	609	CLA	C11-C12-C13-C15
28	B	612	CLA	C6-C7-C8-C10
28	C	502	CLA	C11-C12-C13-C15
28	C	503	CLA	C11-C10-C8-C7
28	C	504	CLA	C6-C7-C8-C10
28	C	504	CLA	C11-C12-C13-C15
28	C	505	CLA	C11-C10-C8-C7
28	C	507	CLA	C11-C12-C13-C15
28	C	513	CLA	C11-C10-C8-C7
28	G	602	CLA	C11-C10-C8-C7
28	G	612	CLA	C6-C7-C8-C10
28	N	610	CLA	C11-C12-C13-C15
28	R	602	CLA	C6-C7-C8-C10
28	R	608	CLA	C6-C7-C8-C10
28	R	609	CLA	C11-C12-C13-C15
28	R	613	CLA	C6-C7-C8-C10
28	S	313	CLA	C2-C3-C5-C6
28	Y	612	CLA	C6-C7-C8-C10
28	Y	613	CLA	C11-C10-C8-C7
28	b	602	CLA	C11-C12-C13-C15
28	b	610	CLA	C11-C10-C8-C7
28	b	611	CLA	C11-C10-C8-C7
28	b	613	CLA	C11-C10-C8-C7
28	b	616	CLA	C6-C7-C8-C10
28	c	501	CLA	C12-C13-C15-C16
28	c	504	CLA	C6-C7-C8-C10
28	c	507	CLA	C11-C10-C8-C7
28	c	511	CLA	C6-C7-C8-C10
28	d	401	CLA	C11-C12-C13-C15
28	n	610	CLA	C11-C10-C8-C7
28	r	609	CLA	C11-C12-C13-C15
28	r	613	CLA	C11-C10-C8-C7
28	s	602	CLA	C11-C10-C8-C7
28	y	303	CLA	C11-C10-C8-C7
38	G	608	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
38	N	608	CHL	C2-C3-C5-C6
38	S	307	CHL	C2-C3-C5-C6
38	Y	607	CHL	C11-C12-C13-C15
38	g	607	CHL	C2-C3-C5-C6
38	g	609	CHL	C2-C3-C5-C6
38	n	607	CHL	C2-C3-C5-C6
38	n	609	CHL	C2-C3-C5-C6
38	s	606	CHL	C2-C3-C5-C6
28	r	608	CLA	C3-C5-C6-C7
28	G	610	CLA	O1A-CGA-O2A-C1
28	n	602	CLA	O1A-CGA-O2A-C1
36	C	518	DGD	O1A-C1A-O1G-C1G
35	b	621	LHG	C11-C10-C9-C8
35	b	624	LHG	C26-C27-C28-C29
35	b	624	LHG	C29-C30-C31-C32
35	y	319	LHG	C35-C36-C37-C38
28	D	401	CLA	C5-C6-C7-C8
30	D	405	BCR	C9-C10-C11-C12
30	a	410	BCR	C13-C14-C15-C16
30	i	101	BCR	C15-C16-C17-C18
40	n	617	NEX	C13-C14-C15-C35
28	N	603	CLA	C6-C7-C8-C10
28	N	611	CLA	C11-C12-C13-C15
35	d	408	LHG	C7-C8-C9-C10
28	b	613	CLA	CBA-CGA-O2A-C1
28	g	602	CLA	CBA-CGA-O2A-C1
28	r	602	CLA	CBA-CGA-O2A-C1
36	b	625	DGD	C2A-C1A-O1G-C1G
28	G	603	CLA	C5-C6-C7-C8
35	B	623	LHG	C30-C31-C32-C33
35	C	521	LHG	C34-C35-C36-C37
28	Y	604	CLA	C2A-CAA-CBA-CGA
28	c	506	CLA	C2A-CAA-CBA-CGA
28	r	604	CLA	C2A-CAA-CBA-CGA
28	B	611	CLA	C10-C11-C12-C13
28	C	511	CLA	C5-C6-C7-C8
35	S	301	LHG	C11-C10-C9-C8
35	w	102	LHG	C25-C26-C27-C28
38	G	609	CHL	C6-C7-C8-C9
31	A	414	SQD	C29-C30-C31-C32
28	G	611	CLA	C8-C10-C11-C12
28	Y	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	a	409	CLA	C8-C10-C11-C12
35	G	618	LHG	C30-C31-C32-C33
35	L	102	LHG	C26-C27-C28-C29
35	W	101	LHG	C11-C10-C9-C8
35	W	101	LHG	C30-C31-C32-C33
35	b	624	LHG	C9-C10-C11-C12
35	c	519	LHG	C25-C26-C27-C28
28	R	612	CLA	C3-C5-C6-C7
28	Y	612	CLA	C11-C12-C13-C15
28	C	506	CLA	C5-C6-C7-C8
28	y	310	CLA	C8-C10-C11-C12
35	B	625	LHG	C29-C30-C31-C32
35	Y	619	LHG	C23-C24-C25-C26
32	k	102	LMG	C11-C10-O7-C8
35	N	618	LHG	C8-C7-O7-C5
36	c	517	DGD	C2B-C1B-O2G-C2G
35	L	102	LHG	C11-C10-C9-C8
35	b	624	LHG	C25-C26-C27-C28
37	E	101	HEM	C4C-C3C-CAC-CBC
37	f	101	HEM	C4C-C3C-CAC-CBC
28	B	612	CLA	C5-C6-C7-C8
38	y	302	CHL	C10-C11-C12-C13
28	b	601	CLA	CBD-CGD-O2D-CED
35	c	519	LHG	O9-C7-O7-C5
36	c	517	DGD	O1B-C1B-O2G-C2G
28	B	606	CLA	C3-C5-C6-C7
28	R	603	CLA	C3-C5-C6-C7
35	b	622	LHG	C28-C29-C30-C31
38	s	606	CHL	C5-C6-C7-C8
35	B	623	LHG	O7-C5-C6-O8
35	D	407	LHG	O7-C5-C6-O8
35	N	618	LHG	O7-C5-C6-O8
35	S	301	LHG	O7-C5-C6-O8
35	W	101	LHG	O7-C5-C6-O8
35	Y	619	LHG	O7-C5-C6-O8
35	c	520	LHG	O7-C5-C6-O8
35	g	618	LHG	O7-C5-C6-O8
36	c	517	DGD	C2A-C1A-O1G-C1G
35	B	622	LHG	C9-C10-C11-C12
35	d	408	LHG	C25-C26-C27-C28
28	A	408	CLA	C5-C6-C7-C8
28	Y	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	b	605	CLA	C8-C10-C11-C12
28	r	603	CLA	C8-C10-C11-C12
28	B	603	CLA	C4-C3-C5-C6
28	B	606	CLA	C4-C3-C5-C6
38	g	609	CHL	C4-C3-C5-C6
35	D	407	LHG	C7-C8-C9-C10
35	b	622	LHG	C7-C8-C9-C10
38	N	607	CHL	C2-C3-C5-C6
38	r	607	CHL	C2-C3-C5-C6
35	y	319	LHG	C9-C10-C11-C12
28	B	603	CLA	C6-C7-C8-C9
28	B	606	CLA	C6-C7-C8-C9
28	C	504	CLA	C6-C7-C8-C9
28	C	507	CLA	C6-C7-C8-C9
28	G	612	CLA	C6-C7-C8-C9
28	N	602	CLA	C11-C10-C8-C9
28	R	602	CLA	C6-C7-C8-C9
28	R	608	CLA	C6-C7-C8-C9
28	Y	612	CLA	C6-C7-C8-C9
28	b	616	CLA	C6-C7-C8-C9
28	c	504	CLA	C6-C7-C8-C9
28	c	511	CLA	C6-C7-C8-C9
28	d	401	CLA	C14-C13-C15-C16
28	g	611	CLA	C11-C10-C8-C9
28	n	602	CLA	C11-C12-C13-C14
28	n	603	CLA	C11-C10-C8-C9
28	n	610	CLA	C11-C12-C13-C14
28	r	613	CLA	C6-C7-C8-C9
38	N	609	CHL	C11-C12-C13-C14
28	B	604	CLA	C3-C5-C6-C7
28	G	610	CLA	C3-C5-C6-C7
28	b	604	CLA	C3-C5-C6-C7
28	c	509	CLA	C3-C5-C6-C7
32	B	624	LMG	O6-C5-C6-O5
28	G	613	CLA	CBA-CGA-O2A-C1
39	G	615	LUT	C11-C12-C13-C20
39	s	615	LUT	C7-C8-C9-C19
28	c	503	CLA	C15-C16-C17-C18
28	c	507	CLA	C5-C6-C7-C8
39	G	615	LUT	C11-C12-C13-C14
39	y	316	LUT	C11-C12-C13-C14
28	B	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	g	602	CLA	O1A-CGA-O2A-C1
28	A	408	CLA	C1A-C2A-CAA-CBA
28	B	605	CLA	C1A-C2A-CAA-CBA
28	B	606	CLA	C1A-C2A-CAA-CBA
28	B	609	CLA	C1A-C2A-CAA-CBA
28	C	501	CLA	C1A-C2A-CAA-CBA
28	C	505	CLA	C1A-C2A-CAA-CBA
28	C	506	CLA	C1A-C2A-CAA-CBA
28	C	511	CLA	C1A-C2A-CAA-CBA
28	D	404	CLA	C1A-C2A-CAA-CBA
28	G	602	CLA	C1A-C2A-CAA-CBA
28	G	604	CLA	C1A-C2A-CAA-CBA
28	G	610	CLA	C1A-C2A-CAA-CBA
28	G	611	CLA	C1A-C2A-CAA-CBA
28	N	602	CLA	C1A-C2A-CAA-CBA
28	N	604	CLA	C1A-C2A-CAA-CBA
28	N	610	CLA	C1A-C2A-CAA-CBA
28	N	614	CLA	C1A-C2A-CAA-CBA
28	R	601	CLA	C1A-C2A-CAA-CBA
28	R	609	CLA	C1A-C2A-CAA-CBA
28	S	303	CLA	C1A-C2A-CAA-CBA
28	S	309	CLA	C1A-C2A-CAA-CBA
28	S	310	CLA	C1A-C2A-CAA-CBA
28	Y	610	CLA	C1A-C2A-CAA-CBA
28	Y	611	CLA	C1A-C2A-CAA-CBA
28	Y	614	CLA	C1A-C2A-CAA-CBA
28	a	409	CLA	C1A-C2A-CAA-CBA
28	b	607	CLA	C1A-C2A-CAA-CBA
28	c	501	CLA	C1A-C2A-CAA-CBA
28	c	503	CLA	C1A-C2A-CAA-CBA
28	c	504	CLA	C1A-C2A-CAA-CBA
28	c	511	CLA	C1A-C2A-CAA-CBA
28	c	512	CLA	C1A-C2A-CAA-CBA
28	g	602	CLA	C1A-C2A-CAA-CBA
28	g	610	CLA	C1A-C2A-CAA-CBA
28	g	614	CLA	C1A-C2A-CAA-CBA
28	n	602	CLA	C1A-C2A-CAA-CBA
28	n	604	CLA	C1A-C2A-CAA-CBA
28	n	611	CLA	C1A-C2A-CAA-CBA
28	n	614	CLA	C1A-C2A-CAA-CBA
28	r	602	CLA	C1A-C2A-CAA-CBA
28	r	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	s	602	CLA	C1A-C2A-CAA-CBA
28	s	603	CLA	C1A-C2A-CAA-CBA
28	s	608	CLA	C1A-C2A-CAA-CBA
28	s	609	CLA	C1A-C2A-CAA-CBA
28	y	303	CLA	C1A-C2A-CAA-CBA
28	y	304	CLA	C1A-C2A-CAA-CBA
28	y	310	CLA	C1A-C2A-CAA-CBA
28	y	311	CLA	C1A-C2A-CAA-CBA
28	y	314	CLA	C1A-C2A-CAA-CBA
38	N	608	CHL	C1A-C2A-CAA-CBA
38	S	306	CHL	C1A-C2A-CAA-CBA
38	Y	601	CHL	C1A-C2A-CAA-CBA
28	s	612	CLA	C6-C7-C8-C10
32	k	102	LMG	O9-C10-O7-C8
35	N	618	LHG	O9-C7-O7-C5
35	s	617	LHG	C25-C26-C27-C28
30	B	619	BCR	C13-C14-C15-C16
30	c	515	BCR	C19-C20-C21-C22
30	k	101	BCR	C13-C14-C15-C16
40	g	617	NEX	C13-C14-C15-C35
40	g	617	NEX	C33-C34-C35-C15
40	n	617	NEX	C29-C30-C31-C32
28	s	602	CLA	C8-C10-C11-C12
38	R	607	CHL	C10-C11-C12-C13
35	B	625	LHG	C4-O6-P-O3
35	R	616	LHG	C3-O3-P-O6
35	W	101	LHG	C3-O3-P-O6
32	C	522	LMG	C32-C33-C34-C35
31	A	410	SQD	C23-C24-C25-C26
28	B	610	CLA	C3-C5-C6-C7
35	s	617	LHG	C2-C3-O3-P
28	B	601	CLA	C5-C6-C7-C8
28	C	505	CLA	C5-C6-C7-C8
28	G	611	CLA	C5-C6-C7-C8
28	c	512	CLA	CBA-CGA-O2A-C1
35	A	416	LHG	O6-C4-C5-C6
35	L	102	LHG	O6-C4-C5-C6
35	W	101	LHG	O6-C4-C5-C6
35	a	415	LHG	O6-C4-C5-C6
35	g	618	LHG	O6-C4-C5-C6
35	r	617	LHG	O6-C4-C5-C6
35	s	617	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	G	602	CLA	C13-C15-C16-C17
28	B	614	CLA	O1D-CGD-O2D-CED
28	n	603	CLA	O1D-CGD-O2D-CED
32	d	409	LMG	O6-C5-C6-O5
35	y	319	LHG	C11-C10-C9-C8
28	C	504	CLA	C3-C5-C6-C7
28	n	613	CLA	C3-C5-C6-C7
28	B	604	CLA	C8-C10-C11-C12
28	g	602	CLA	C4-C3-C5-C6
38	S	307	CHL	C4-C3-C5-C6
38	r	606	CHL	C4-C3-C5-C6
38	s	606	CHL	C4-C3-C5-C6
35	G	618	LHG	C18-C19-C20-C21
28	B	616	CLA	C5-C6-C7-C8
28	c	502	CLA	C13-C15-C16-C17
28	b	613	CLA	O1A-CGA-O2A-C1
36	b	625	DGD	O1A-C1A-O1G-C1G
28	S	303	CLA	C2A-CAA-CBA-CGA
38	R	607	CHL	C2A-CAA-CBA-CGA
31	A	414	SQD	O6-C44-C45-C46
31	L	103	SQD	C44-C45-C46-O48
31	a	414	SQD	C44-C45-C46-O48
32	c	521	LMG	O1-C7-C8-C9
35	A	416	LHG	C4-C5-C6-O8
35	B	623	LHG	C4-C5-C6-O8
35	D	407	LHG	C4-C5-C6-O8
35	R	616	LHG	C4-C5-C6-O8
35	S	317	LHG	C4-C5-C6-O8
35	a	415	LHG	C4-C5-C6-O8
35	b	621	LHG	C4-C5-C6-O8
35	b	624	LHG	C4-C5-C6-O8
35	c	519	LHG	C4-C5-C6-O8
35	c	520	LHG	C4-C5-C6-O8
35	g	618	LHG	C4-C5-C6-O8
35	s	617	LHG	C29-C30-C31-C32
35	w	102	LHG	C4-C5-C6-O8
36	a	401	DGD	O6E-C5E-C6E-O5E
36	b	625	DGD	O6E-C5E-C6E-O5E
31	a	411	SQD	C17-C18-C19-C20
35	G	618	LHG	C31-C32-C33-C34
35	Y	619	LHG	C29-C30-C31-C32
32	c	521	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	C2G-C3G-O3G-C1D
36	c	517	DGD	C5D-C6D-O5D-C1E
32	b	620	LMG	C8-C9-O8-C28
31	A	410	SQD	C11-C10-C9-C8
35	b	622	LHG	C25-C26-C27-C28
28	c	512	CLA	C8-C10-C11-C12
28	B	615	CLA	C8-C10-C11-C12
28	y	304	CLA	C5-C6-C7-C8
32	a	413	LMG	C29-C30-C31-C32
35	B	623	LHG	C11-C12-C13-C14
35	G	618	LHG	C19-C20-C21-C22
35	S	317	LHG	C13-C14-C15-C16
28	R	613	CLA	O1D-CGD-O2D-CED
36	B	626	DGD	O6E-C5E-C6E-O5E
32	B	621	LMG	C10-C11-C12-C13
28	r	602	CLA	O1A-CGA-O2A-C1
35	r	617	LHG	C10-C11-C12-C13
32	D	408	LMG	O6-C5-C6-O5
35	B	625	LHG	O1-C1-C2-O2
35	C	521	LHG	O1-C1-C2-O2
35	W	101	LHG	O1-C1-C2-O2
35	b	622	LHG	C30-C31-C32-C33
28	s	610	CLA	C5-C6-C7-C8
35	N	618	LHG	C28-C29-C30-C31
28	G	610	CLA	C16-C17-C18-C19
35	D	407	LHG	C25-C26-C27-C28
28	n	611	CLA	C5-C6-C7-C8
36	A	417	DGD	O6E-C5E-C6E-O5E
36	C	517	DGD	O6E-C5E-C6E-O5E
36	c	516	DGD	O6E-C5E-C6E-O5E
40	Y	618	NEX	C39-C29-C30-C31
40	y	301	NEX	C39-C29-C30-C31
40	y	318	NEX	C40-C33-C34-C35
35	B	625	LHG	C28-C29-C30-C31
35	B	625	LHG	C34-C35-C36-C37
35	C	521	LHG	C28-C29-C30-C31
35	L	102	LHG	C33-C34-C35-C36
28	R	612	CLA	C6-C7-C8-C10
28	G	602	CLA	CBA-CGA-O2A-C1
35	l	101	LHG	C34-C35-C36-C37
28	b	604	CLA	C5-C6-C7-C8
28	b	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
38	g	609	CHL	C8-C10-C11-C12
35	b	622	LHG	C35-C36-C37-C38
35	g	618	LHG	C26-C27-C28-C29
31	M	101	SQD	C44-C45-O47-C7
28	C	506	CLA	C8-C10-C11-C12
28	G	613	CLA	C5-C6-C7-C8
28	n	603	CLA	C5-C6-C7-C8
28	r	601	CLA	C2-C1-O2A-CGA
28	C	512	CLA	CBD-CGD-O2D-CED
35	Y	619	LHG	C24-C25-C26-C27
28	s	608	CLA	O1D-CGD-O2D-CED
28	y	312	CLA	C8-C10-C11-C12
28	g	613	CLA	CBA-CGA-O2A-C1
36	B	626	DGD	C2A-C1A-O1G-C1G
38	n	608	CHL	CBA-CGA-O2A-C1
35	d	408	LHG	O6-C4-C5-O7
35	y	319	LHG	O6-C4-C5-O7
31	B	620	SQD	C10-C11-C12-C13
28	C	509	CLA	C8-C10-C11-C12
28	N	603	CLA	C5-C6-C7-C8
28	R	612	CLA	C5-C6-C7-C8
28	c	506	CLA	C5-C6-C7-C8
38	n	607	CHL	C5-C6-C7-C8
38	G	606	CHL	O1D-CGD-O2D-CED
28	c	512	CLA	O1A-CGA-O2A-C1
36	c	517	DGD	O1A-C1A-O1G-C1G
35	G	618	LHG	C8-C7-O7-C5
28	B	605	CLA	C8-C10-C11-C12
38	R	607	CHL	C5-C6-C7-C8
41	R	615	XAT	C12-C13-C14-C15
41	r	615	XAT	C12-C13-C14-C15
35	b	622	LHG	C11-C12-C13-C14
35	c	520	LHG	C9-C10-C11-C12
28	C	510	CLA	CAA-CBA-CGA-O2A
35	S	301	LHG	O7-C7-C8-C9
32	B	624	LMG	O1-C7-C8-O7
35	A	416	LHG	O7-C5-C6-O8
35	a	415	LHG	O7-C5-C6-O8
35	y	319	LHG	O7-C5-C6-O8
35	c	520	LHG	C24-C25-C26-C27
35	l	101	LHG	C17-C18-C19-C20
28	g	611	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	G	613	CLA	O1A-CGA-O2A-C1
32	B	624	LMG	C14-C15-C16-C17
28	g	602	CLA	C5-C6-C7-C8
28	A	405	CLA	C6-C7-C8-C10
28	A	405	CLA	C11-C10-C8-C7
28	A	408	CLA	C11-C10-C8-C7
28	B	601	CLA	C11-C10-C8-C7
28	B	603	CLA	C6-C7-C8-C10
28	B	608	CLA	C6-C7-C8-C10
28	B	610	CLA	C6-C7-C8-C10
28	B	614	CLA	C6-C7-C8-C10
28	C	501	CLA	C11-C10-C8-C7
28	C	507	CLA	C6-C7-C8-C10
28	C	507	CLA	C11-C10-C8-C7
28	C	513	CLA	C6-C7-C8-C10
28	D	404	CLA	C11-C10-C8-C7
28	G	610	CLA	C11-C10-C8-C7
28	N	602	CLA	C6-C7-C8-C10
28	N	602	CLA	C11-C12-C13-C15
28	N	611	CLA	C11-C10-C8-C7
28	N	612	CLA	C11-C10-C8-C7
28	R	603	CLA	C11-C10-C8-C7
28	R	613	CLA	C11-C12-C13-C15
28	b	601	CLA	C11-C10-C8-C7
28	b	603	CLA	C6-C7-C8-C10
28	b	605	CLA	C11-C10-C8-C7
28	b	612	CLA	C11-C12-C13-C15
28	b	615	CLA	C6-C7-C8-C10
28	b	615	CLA	C11-C12-C13-C15
28	c	501	CLA	C11-C10-C8-C7
28	c	502	CLA	C12-C13-C15-C16
28	c	507	CLA	C6-C7-C8-C10
28	c	510	CLA	C11-C12-C13-C15
28	c	511	CLA	C11-C10-C8-C7
28	c	512	CLA	C11-C10-C8-C7
28	c	513	CLA	C11-C10-C8-C7
28	n	602	CLA	C11-C12-C13-C15
28	n	611	CLA	C6-C7-C8-C10
28	n	611	CLA	C11-C10-C8-C7
28	r	612	CLA	C11-C10-C8-C7
38	N	608	CHL	C11-C10-C8-C7
38	S	307	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
38	Y	601	CHL	C6-C7-C8-C10
38	Y	608	CHL	C11-C10-C8-C7
38	Y	608	CHL	C12-C13-C15-C16
38	g	608	CHL	C12-C13-C15-C16
38	g	619	CHL	C6-C7-C8-C10
38	g	619	CHL	C12-C13-C15-C16
38	n	607	CHL	C11-C12-C13-C15
38	n	608	CHL	C6-C7-C8-C10
38	n	608	CHL	C12-C13-C15-C16
38	r	605	CHL	C11-C10-C8-C7
38	r	607	CHL	C11-C10-C8-C7
38	y	302	CHL	C11-C10-C8-C7
38	y	308	CHL	C12-C13-C15-C16
38	y	309	CHL	C12-C13-C15-C16
28	N	603	CLA	C3-C5-C6-C7
28	y	310	CLA	C3-C5-C6-C7
28	B	609	CLA	C6-C7-C8-C9
28	B	610	CLA	C6-C7-C8-C9
28	C	510	CLA	C6-C7-C8-C9
28	G	602	CLA	C6-C7-C8-C9
28	G	611	CLA	C6-C7-C8-C9
28	N	602	CLA	C6-C7-C8-C9
28	R	613	CLA	C6-C7-C8-C9
28	S	303	CLA	C6-C7-C8-C9
28	a	409	CLA	C11-C10-C8-C9
28	b	603	CLA	C6-C7-C8-C9
28	b	612	CLA	C6-C7-C8-C9
28	b	615	CLA	C11-C12-C13-C14
28	c	507	CLA	C6-C7-C8-C9
38	S	307	CHL	C11-C10-C8-C9
38	Y	607	CHL	C11-C10-C8-C9
38	r	605	CHL	C11-C10-C8-C9
38	r	607	CHL	C11-C10-C8-C9
38	y	302	CHL	C14-C13-C15-C16
30	B	619	BCR	C19-C20-C21-C22
35	C	521	LHG	C25-C26-C27-C28
35	Y	619	LHG	C11-C10-C9-C8
28	A	405	CLA	C5-C6-C7-C8
28	r	608	CLA	C2A-CAA-CBA-CGA
35	D	407	LHG	C33-C34-C35-C36
30	c	515	BCR	C7-C8-C9-C34
30	d	406	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
39	N	615	LUT	C11-C12-C13-C20
39	S	315	LUT	C31-C32-C33-C40
39	n	615	LUT	C7-C8-C9-C19
28	S	310	CLA	C6-C7-C8-C9
39	S	315	LUT	C27-C28-C29-C30
39	S	315	LUT	C31-C32-C33-C34
39	S	316	LUT	C7-C8-C9-C10
39	Y	615	LUT	C11-C12-C13-C14
39	n	615	LUT	C7-C8-C9-C10
35	G	618	LHG	C12-C13-C14-C15
28	D	401	CLA	CBA-CGA-O2A-C1
38	Y	607	CHL	CBA-CGA-O2A-C1
32	k	102	LMG	C32-C33-C34-C35
35	Y	619	LHG	C35-C36-C37-C38
28	N	612	CLA	C5-C6-C7-C8
28	b	616	CLA	C8-C10-C11-C12
35	Y	619	LHG	C30-C31-C32-C33
36	C	519	DGD	O6D-C5D-C6D-O5D
28	n	613	CLA	C6-C7-C8-C9
28	Y	602	CLA	C8-C10-C11-C12
28	r	613	CLA	C13-C15-C16-C17
35	D	407	LHG	O6-C4-C5-C6
35	c	519	LHG	O6-C4-C5-C6
35	c	520	LHG	O6-C4-C5-C6
35	y	319	LHG	O6-C4-C5-C6
32	c	521	LMG	C10-C11-C12-C13
35	a	415	LHG	C11-C10-C9-C8
36	b	625	DGD	C3B-C4B-C5B-C6B
28	G	612	CLA	CBA-CGA-O2A-C1
28	r	612	CLA	CBA-CGA-O2A-C1
28	G	612	CLA	C8-C10-C11-C12
28	c	505	CLA	C5-C6-C7-C8
28	g	611	CLA	C5-C6-C7-C8
28	G	613	CLA	C2-C3-C5-C6
38	y	302	CHL	C16-C17-C18-C20
35	B	623	LHG	C33-C34-C35-C36
35	l	101	LHG	C31-C32-C33-C34
36	B	626	DGD	C3B-C4B-C5B-C6B
28	b	606	CLA	CBA-CGA-O2A-C1
32	b	623	LMG	O7-C10-C11-C12
35	L	102	LHG	C7-C8-C9-C10
35	B	625	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
28	b	614	CLA	O1D-CGD-O2D-CED
28	C	505	CLA	C3A-C2A-CAA-CBA
28	G	613	CLA	C3A-C2A-CAA-CBA
28	N	603	CLA	C3A-C2A-CAA-CBA
28	Y	603	CLA	C3A-C2A-CAA-CBA
28	b	616	CLA	C3A-C2A-CAA-CBA
28	c	505	CLA	C3A-C2A-CAA-CBA
28	n	610	CLA	C3A-C2A-CAA-CBA
38	s	601	CHL	C3A-C2A-CAA-CBA
28	G	602	CLA	C8-C10-C11-C12
35	L	102	LHG	C30-C31-C32-C33
30	C	514	BCR	C19-C20-C21-C22
30	K	101	BCR	C9-C10-C11-C12
30	b	617	BCR	C19-C20-C21-C22
30	c	515	BCR	C13-C14-C15-C16
28	G	603	CLA	C3-C5-C6-C7
28	B	610	CLA	C5-C6-C7-C8
28	C	510	CLA	C8-C10-C11-C12
28	b	601	CLA	C8-C10-C11-C12
28	n	603	CLA	C8-C10-C11-C12
35	S	301	LHG	C12-C13-C14-C15
36	c	518	DGD	O6D-C5D-C6D-O5D
38	N	609	CHL	C4-C3-C5-C6
29	D	402	PHO	CBA-CGA-O2A-C1
28	b	611	CLA	C13-C15-C16-C17
31	A	414	SQD	C44-C45-C46-O48
31	B	620	SQD	C44-C45-C46-O48
31	M	101	SQD	O6-C44-C45-C46
31	M	101	SQD	C44-C45-C46-O48
35	B	622	LHG	C4-C5-C6-O8
35	B	625	LHG	C4-C5-C6-O8
35	N	618	LHG	C4-C5-C6-O8
35	S	301	LHG	C4-C5-C6-O8
35	W	101	LHG	C4-C5-C6-O8
35	Y	619	LHG	C4-C5-C6-O8
35	y	319	LHG	C4-C5-C6-O8
35	B	625	LHG	C11-C10-C9-C8
28	R	603	CLA	O2A-C1-C2-C3
28	n	602	CLA	C5-C6-C7-C8
35	G	618	LHG	C9-C10-C11-C12
28	S	310	CLA	C3-C5-C6-C7
28	c	505	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	n	611	CLA	O1D-CGD-O2D-CED
35	G	618	LHG	C27-C28-C29-C30
35	b	624	LHG	C33-C34-C35-C36
38	Y	609	CHL	O1D-CGD-O2D-CED
35	A	416	LHG	C4-O6-P-O3
35	l	101	LHG	C3-O3-P-O6
28	G	602	CLA	O1A-CGA-O2A-C1
28	g	613	CLA	O1A-CGA-O2A-C1
36	B	626	DGD	O1A-C1A-O1G-C1G
28	c	511	CLA	C2A-CAA-CBA-CGA
28	s	602	CLA	C2A-CAA-CBA-CGA
35	y	319	LHG	O1-C1-C2-O2
28	B	602	CLA	C8-C10-C11-C12
35	C	521	LHG	C30-C31-C32-C33
35	l	101	LHG	C12-C13-C14-C15
35	D	407	LHG	O6-C4-C5-O7
35	W	101	LHG	O6-C4-C5-O7
35	c	520	LHG	O6-C4-C5-O7
35	r	617	LHG	O6-C4-C5-O7
35	R	616	LHG	C23-C24-C25-C26
28	N	611	CLA	C11-C12-C13-C14
28	Y	612	CLA	C11-C12-C13-C14
38	y	302	CHL	C16-C17-C18-C19
35	C	521	LHG	C15-C16-C17-C18
35	N	618	LHG	C11-C10-C9-C8
28	B	611	CLA	C8-C10-C11-C12
38	n	608	CHL	O1A-CGA-O2A-C1
35	b	622	LHG	C29-C30-C31-C32
31	M	101	SQD	O6-C44-C45-O47
31	a	414	SQD	O47-C45-C46-O48
35	B	622	LHG	O7-C5-C6-O8
35	B	625	LHG	O7-C5-C6-O8
35	S	317	LHG	O7-C5-C6-O8
35	w	102	LHG	O7-C5-C6-O8
38	S	307	CHL	CBA-CGA-O2A-C1
28	g	603	CLA	C8-C10-C11-C12
32	A	413	LMG	C34-C35-C36-C37
35	C	521	LHG	C35-C36-C37-C38
35	L	102	LHG	C31-C32-C33-C34
35	L	102	LHG	C8-C7-O7-C5
35	a	415	LHG	C8-C7-O7-C5
28	R	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	A	413	LMG	C29-C30-C31-C32
32	b	620	LMG	O6-C1-O1-C7
28	c	503	CLA	C5-C6-C7-C8
35	G	618	LHG	O9-C7-O7-C5
28	B	615	CLA	C2-C1-O2A-CGA
28	C	501	CLA	C2-C1-O2A-CGA
28	b	606	CLA	C2-C1-O2A-CGA
28	b	607	CLA	C2-C1-O2A-CGA
28	c	503	CLA	C2-C1-O2A-CGA
35	a	415	LHG	C31-C32-C33-C34
28	A	408	CLA	C6-C7-C8-C9
28	B	613	CLA	C14-C13-C15-C16
28	B	615	CLA	C11-C10-C8-C9
28	b	607	CLA	C11-C12-C13-C14
28	b	611	CLA	C6-C7-C8-C9
28	c	505	CLA	C6-C7-C8-C9
28	g	602	CLA	C11-C10-C8-C9
28	s	610	CLA	C6-C7-C8-C9
28	y	310	CLA	C6-C7-C8-C9
28	y	312	CLA	C6-C7-C8-C9
38	G	601	CHL	C11-C12-C13-C14
38	G	608	CHL	C11-C12-C13-C14
38	Y	601	CHL	C11-C12-C13-C14
38	Y	607	CHL	C11-C12-C13-C14
35	G	618	LHG	C17-C18-C19-C20
35	C	521	LHG	C11-C10-C9-C8
28	C	508	CLA	C5-C6-C7-C8
38	N	608	CHL	C8-C10-C11-C12
38	N	609	CHL	C5-C6-C7-C8
35	A	416	LHG	C2-C3-O3-P
35	B	622	LHG	C5-C4-O6-P
35	D	407	LHG	C5-C4-O6-P
35	G	618	LHG	C5-C4-O6-P
35	c	519	LHG	C2-C3-O3-P
28	B	604	CLA	C2A-CAA-CBA-CGA
28	B	607	CLA	C2A-CAA-CBA-CGA
38	n	605	CHL	C2A-CAA-CBA-CGA
28	N	603	CLA	C6-C7-C8-C9
28	S	310	CLA	C6-C7-C8-C10
28	Y	603	CLA	C6-C7-C8-C9
28	Y	610	CLA	C11-C12-C13-C15
28	R	611	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	g	606	CHL	O2A-C1-C2-C3
38	n	606	CHL	O2A-C1-C2-C3
28	b	612	CLA	C3-C5-C6-C7
30	A	409	BCR	C23-C24-C25-C30
30	C	514	BCR	C5-C6-C7-C8
30	C	516	BCR	C23-C24-C25-C26
30	a	410	BCR	C23-C24-C25-C30
30	b	618	BCR	C5-C6-C7-C8
30	d	406	BCR	C23-C24-C25-C26
30	i	101	BCR	C5-C6-C7-C8
39	Y	615	LUT	C1-C6-C7-C8
39	g	615	LUT	C5-C6-C7-C8
35	D	407	LHG	C11-C10-C9-C8
36	B	626	DGD	C5B-C6B-C7B-C8B
39	S	316	LUT	C7-C8-C9-C19
35	G	618	LHG	C24-C25-C26-C27
30	H	101	BCR	C21-C22-C23-C24
30	c	514	BCR	C11-C12-C13-C14
30	c	515	BCR	C7-C8-C9-C10
39	N	615	LUT	C11-C12-C13-C14
40	y	301	NEX	C11-C12-C13-C14
40	y	301	NEX	C27-C28-C29-C30
41	R	615	XAT	C27-C28-C29-C30
41	r	615	XAT	C27-C28-C29-C30
28	B	607	CLA	C5-C6-C7-C8
28	b	616	CLA	C5-C6-C7-C8
28	N	613	CLA	C5-C6-C7-C8
35	L	102	LHG	O9-C7-O7-C5
35	B	622	LHG	C11-C10-C9-C8
35	L	102	LHG	C34-C35-C36-C37
35	B	623	LHG	C11-C10-C9-C8
35	B	623	LHG	C35-C36-C37-C38
35	d	408	LHG	C16-C17-C18-C19
28	S	313	CLA	C6-C7-C8-C9
35	s	617	LHG	C34-C35-C36-C37
28	b	601	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	O6-C4-C5-C6
35	C	521	LHG	O6-C4-C5-C6
35	S	301	LHG	O6-C4-C5-C6
35	S	317	LHG	O6-C4-C5-C6
35	d	408	LHG	O6-C4-C5-C6
35	l	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
35	w	102	LHG	O6-C4-C5-C6
28	B	602	CLA	C6-C7-C8-C10
28	B	602	CLA	C11-C10-C8-C7
28	B	607	CLA	C11-C10-C8-C7
28	B	609	CLA	C6-C7-C8-C10
28	B	611	CLA	C11-C10-C8-C7
28	B	613	CLA	C6-C7-C8-C10
28	B	615	CLA	C11-C12-C13-C15
28	C	501	CLA	C6-C7-C8-C10
28	C	506	CLA	C11-C10-C8-C7
28	C	509	CLA	C6-C7-C8-C10
28	C	509	CLA	C11-C10-C8-C7
28	D	401	CLA	C11-C12-C13-C15
28	D	403	CLA	C6-C7-C8-C10
28	D	404	CLA	C6-C7-C8-C10
28	G	602	CLA	C6-C7-C8-C10
28	G	602	CLA	C12-C13-C15-C16
28	G	610	CLA	C6-C7-C8-C10
28	G	612	CLA	C11-C10-C8-C7
28	G	613	CLA	C6-C7-C8-C10
28	N	610	CLA	C11-C10-C8-C7
28	S	303	CLA	C6-C7-C8-C10
28	S	303	CLA	C11-C10-C8-C7
28	S	303	CLA	C11-C12-C13-C15
28	Y	611	CLA	C6-C7-C8-C10
28	Y	613	CLA	C11-C12-C13-C15
28	a	406	CLA	C6-C7-C8-C10
28	b	602	CLA	C6-C7-C8-C10
28	b	606	CLA	C6-C7-C8-C10
28	b	611	CLA	C6-C7-C8-C10
28	b	614	CLA	C6-C7-C8-C10
28	c	502	CLA	C6-C7-C8-C10
28	c	505	CLA	C11-C10-C8-C7
28	c	508	CLA	C11-C12-C13-C15
28	c	509	CLA	C6-C7-C8-C10
28	c	512	CLA	C6-C7-C8-C10
28	d	401	CLA	C6-C7-C8-C10
28	d	405	CLA	C11-C10-C8-C7
28	g	602	CLA	C6-C7-C8-C10
28	g	602	CLA	C11-C12-C13-C15
28	n	602	CLA	C6-C7-C8-C10
28	n	612	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
28	r	602	CLA	C6-C7-C8-C10
28	s	602	CLA	C6-C7-C8-C10
28	s	610	CLA	C6-C7-C8-C10
28	y	304	CLA	C6-C7-C8-C10
28	y	311	CLA	C6-C7-C8-C10
38	G	601	CHL	C12-C13-C15-C16
38	Y	607	CHL	C6-C7-C8-C10
38	Y	608	CHL	C11-C12-C13-C15
38	Y	609	CHL	C11-C12-C13-C15
38	g	601	CHL	C11-C12-C13-C15
38	g	609	CHL	C6-C7-C8-C10
38	g	619	CHL	C11-C12-C13-C15
38	n	609	CHL	C11-C12-C13-C15
38	y	308	CHL	C11-C12-C13-C15
30	B	617	BCR	C19-C20-C21-C22
30	C	514	BCR	C13-C14-C15-C16
30	c	514	BCR	C15-C16-C17-C18
30	t	101	BCR	C9-C10-C11-C12
39	S	315	LUT	C29-C30-C31-C32
39	g	616	LUT	C9-C10-C11-C12
40	G	617	NEX	C9-C10-C11-C12
41	R	615	XAT	C29-C30-C31-C32
41	r	615	XAT	C29-C30-C31-C32
28	A	408	CLA	C11-C12-C13-C15
35	b	622	LHG	C31-C32-C33-C34
35	a	415	LHG	O9-C7-O7-C5
28	g	610	CLA	C8-C10-C11-C12
38	Y	607	CHL	O1A-CGA-O2A-C1
38	g	619	CHL	C2A-CAA-CBA-CGA
38	s	606	CHL	C2A-CAA-CBA-CGA
38	g	601	CHL	C5-C6-C7-C8
28	B	603	CLA	C3-C5-C6-C7
36	c	516	DGD	C2G-C1G-O1G-C1A
35	L	102	LHG	C16-C17-C18-C19
35	a	415	LHG	C26-C27-C28-C29
28	C	502	CLA	C13-C15-C16-C17
28	g	603	CLA	C5-C6-C7-C8
28	R	609	CLA	CBA-CGA-O2A-C1
38	n	609	CHL	CBA-CGA-O2A-C1
38	s	606	CHL	CBA-CGA-O2A-C1
28	c	506	CLA	C11-C10-C8-C7
28	R	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	R	601	CLA	C2C-C3C-CAC-CBC
28	C	505	CLA	CAD-CBD-CGD-O2D
28	b	614	CLA	CAD-CBD-CGD-O2D
28	c	503	CLA	CAD-CBD-CGD-O2D
28	c	509	CLA	CAD-CBD-CGD-O2D
28	r	603	CLA	CAD-CBD-CGD-O2D
35	r	617	LHG	C4-C5-O7-C7
37	E	101	HEM	C2B-C3B-CAB-CBB
37	f	101	HEM	C2B-C3B-CAB-CBB
38	R	606	CHL	CAD-CBD-CGD-O2D
35	L	102	LHG	C35-C36-C37-C38
35	g	618	LHG	C25-C26-C27-C28
28	R	613	CLA	C5-C6-C7-C8
38	N	608	CHL	C13-C15-C16-C17
29	D	402	PHO	O1A-CGA-O2A-C1
31	a	411	SQD	C24-C23-O48-C46
35	g	618	LHG	C24-C23-O8-C6
28	C	512	CLA	O1D-CGD-O2D-CED
38	g	619	CHL	C4-C3-C5-C6
28	S	311	CLA	C5-C6-C7-C8
28	b	603	CLA	C8-C10-C11-C12
28	b	610	CLA	C5-C6-C7-C8
38	Y	608	CHL	C8-C10-C11-C12
31	L	103	SQD	O6-C44-C45-C46
32	B	624	LMG	O1-C7-C8-C9
32	B	624	LMG	C7-C8-C9-O8
32	C	522	LMG	O1-C7-C8-C9
35	Y	619	LHG	C5-C4-O6-P
35	b	622	LHG	C4-C5-C6-O8
35	d	408	LHG	C4-C5-C6-O8
35	r	617	LHG	C4-C5-C6-O8
35	s	617	LHG	C4-C5-C6-O8
28	r	612	CLA	O1A-CGA-O2A-C1
35	B	625	LHG	O6-C4-C5-O7
35	R	616	LHG	O6-C4-C5-O7
35	S	301	LHG	O6-C4-C5-O7
35	S	317	LHG	O6-C4-C5-O7
35	l	101	LHG	O6-C4-C5-O7
28	B	601	CLA	C13-C15-C16-C17
28	C	507	CLA	C8-C10-C11-C12
38	N	608	CHL	C15-C16-C17-C18
28	S	314	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	R	606	CHL	C2A-CAA-CBA-CGA
28	C	503	CLA	C5-C6-C7-C8
35	a	415	LHG	C30-C31-C32-C33
28	R	609	CLA	O1A-CGA-O2A-C1
28	R	602	CLA	C11-C12-C13-C15
28	R	603	CLA	O1D-CGD-O2D-CED
35	l	101	LHG	C1-C2-C3-O3
35	l	101	LHG	O2-C2-C3-O3
28	B	605	CLA	CHA-CBD-CGD-O2D
28	B	607	CLA	CHA-CBD-CGD-O2D
28	B	610	CLA	CHA-CBD-CGD-O1D
28	B	610	CLA	CHA-CBD-CGD-O2D
28	B	612	CLA	CHA-CBD-CGD-O1D
28	B	612	CLA	CHA-CBD-CGD-O2D
28	C	502	CLA	CHA-CBD-CGD-O1D
28	C	502	CLA	CHA-CBD-CGD-O2D
28	C	507	CLA	CHA-CBD-CGD-O1D
28	C	508	CLA	CHA-CBD-CGD-O1D
28	C	512	CLA	CHA-CBD-CGD-O1D
28	C	512	CLA	CHA-CBD-CGD-O2D
28	D	401	CLA	CHA-CBD-CGD-O1D
28	G	602	CLA	CHA-CBD-CGD-O1D
28	G	602	CLA	CHA-CBD-CGD-O2D
28	G	603	CLA	CHA-CBD-CGD-O1D
28	G	604	CLA	CHA-CBD-CGD-O1D
28	G	604	CLA	CHA-CBD-CGD-O2D
28	G	610	CLA	CHA-CBD-CGD-O2D
28	N	602	CLA	CHA-CBD-CGD-O1D
28	N	602	CLA	CHA-CBD-CGD-O2D
28	N	603	CLA	CHA-CBD-CGD-O1D
28	N	603	CLA	CHA-CBD-CGD-O2D
28	R	603	CLA	CHA-CBD-CGD-O1D
28	R	603	CLA	CHA-CBD-CGD-O2D
28	R	610	CLA	CHA-CBD-CGD-O2D
28	S	304	CLA	CHA-CBD-CGD-O1D
28	S	304	CLA	CHA-CBD-CGD-O2D
28	Y	603	CLA	CHA-CBD-CGD-O1D
28	Y	603	CLA	CHA-CBD-CGD-O2D
28	Y	612	CLA	CHA-CBD-CGD-O1D
28	Y	612	CLA	CHA-CBD-CGD-O2D
28	b	606	CLA	CHA-CBD-CGD-O2D
28	b	609	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	b	616	CLA	CHA-CBD-CGD-O1D
28	b	616	CLA	CHA-CBD-CGD-O2D
28	c	504	CLA	CHA-CBD-CGD-O1D
28	c	507	CLA	CHA-CBD-CGD-O1D
28	c	510	CLA	CHA-CBD-CGD-O1D
28	c	510	CLA	CHA-CBD-CGD-O2D
28	g	603	CLA	CHA-CBD-CGD-O1D
28	g	603	CLA	CHA-CBD-CGD-O2D
28	g	613	CLA	CHA-CBD-CGD-O1D
28	g	613	CLA	CHA-CBD-CGD-O2D
28	n	602	CLA	CHA-CBD-CGD-O1D
28	n	602	CLA	CHA-CBD-CGD-O2D
28	n	612	CLA	CHA-CBD-CGD-O1D
28	n	612	CLA	CHA-CBD-CGD-O2D
28	r	613	CLA	CHA-CBD-CGD-O1D
28	r	613	CLA	CHA-CBD-CGD-O2D
28	s	603	CLA	CHA-CBD-CGD-O1D
28	s	603	CLA	CHA-CBD-CGD-O2D
28	s	611	CLA	CHA-CBD-CGD-O1D
28	s	611	CLA	CHA-CBD-CGD-O2D
28	y	303	CLA	CHA-CBD-CGD-O1D
28	y	303	CLA	CHA-CBD-CGD-O2D
28	y	304	CLA	CHA-CBD-CGD-O1D
28	y	304	CLA	CHA-CBD-CGD-O2D
28	y	305	CLA	CHA-CBD-CGD-O1D
28	y	305	CLA	CHA-CBD-CGD-O2D
28	y	312	CLA	CHA-CBD-CGD-O1D
28	y	312	CLA	CHA-CBD-CGD-O2D
38	G	605	CHL	CHA-CBD-CGD-O1D
38	N	605	CHL	CHA-CBD-CGD-O1D
38	g	605	CHL	CHA-CBD-CGD-O1D
38	n	605	CHL	CHA-CBD-CGD-O1D
38	n	605	CHL	CHA-CBD-CGD-O2D
38	s	605	CHL	CHA-CBD-CGD-O1D
28	B	605	CLA	C3-C5-C6-C7
28	Y	613	CLA	C3-C5-C6-C7
28	D	401	CLA	O1A-CGA-O2A-C1
28	G	612	CLA	O1A-CGA-O2A-C1
28	b	606	CLA	O1A-CGA-O2A-C1
40	y	318	NEX	C32-C33-C34-C35
31	A	414	SQD	O6-C44-C45-O47
31	A	414	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
31	L	103	SQD	O47-C45-C46-O48
32	A	411	LMG	O7-C8-C9-O8
32	c	521	LMG	O1-C7-C8-O7
35	C	521	LHG	O7-C5-C6-O8
35	b	622	LHG	O7-C5-C6-O8
35	d	408	LHG	O7-C5-C6-O8
35	s	617	LHG	O7-C5-C6-O8
35	D	407	LHG	C10-C11-C12-C13
38	S	307	CHL	O1A-CGA-O2A-C1
35	l	101	LHG	O1-C1-C2-O2
35	A	416	LHG	C11-C10-C9-C8
35	y	319	LHG	C24-C25-C26-C27
28	y	303	CLA	C3-C5-C6-C7
28	y	311	CLA	C3-C5-C6-C7
35	B	623	LHG	C31-C32-C33-C34
28	B	607	CLA	C6-C7-C8-C9
28	C	506	CLA	C6-C7-C8-C9
28	G	602	CLA	C14-C13-C15-C16
28	S	303	CLA	C11-C12-C13-C14
28	a	406	CLA	C6-C7-C8-C9
28	c	508	CLA	C11-C12-C13-C14
28	g	602	CLA	C6-C7-C8-C9
28	g	603	CLA	C6-C7-C8-C9
38	Y	608	CHL	C11-C12-C13-C14
38	Y	609	CHL	C11-C12-C13-C14
38	y	308	CHL	C11-C12-C13-C14
35	b	624	LHG	C11-C10-C9-C8
36	c	518	DGD	C3B-C4B-C5B-C6B
38	s	606	CHL	O1A-CGA-O2A-C1
32	B	624	LMG	C13-C14-C15-C16
35	D	407	LHG	C32-C33-C34-C35
35	S	317	LHG	C11-C10-C9-C8
31	a	411	SQD	C4-C5-C6-S
38	y	306	CHL	C2A-CAA-CBA-CGA
28	b	601	CLA	CAA-CBA-CGA-O2A
28	C	512	CLA	C5-C6-C7-C8
28	B	603	CLA	CBA-CGA-O2A-C1
30	A	409	BCR	C11-C12-C13-C35
30	T	101	BCR	C7-C8-C9-C34
30	i	101	BCR	C37-C22-C23-C24
40	g	617	NEX	C31-C32-C33-C40
28	N	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	A	409	BCR	C11-C12-C13-C14
30	B	618	BCR	C21-C22-C23-C24
30	T	101	BCR	C7-C8-C9-C10
30	d	406	BCR	C7-C8-C9-C10
30	i	101	BCR	C21-C22-C23-C24
40	y	301	NEX	C31-C32-C33-C34
28	y	313	CLA	C3-C5-C6-C7
28	B	603	CLA	C1A-C2A-CAA-CBA
28	G	613	CLA	C1A-C2A-CAA-CBA
28	N	603	CLA	C1A-C2A-CAA-CBA
28	Y	602	CLA	C1A-C2A-CAA-CBA
38	s	601	CHL	C1A-C2A-CAA-CBA
28	a	409	CLA	C11-C12-C13-C15
28	c	511	CLA	C2-C1-O2A-CGA
28	G	603	CLA	CBA-CGA-O2A-C1
38	y	308	CHL	CBA-CGA-O2A-C1
30	C	514	BCR	C15-C16-C17-C18
30	T	101	BCR	C9-C10-C11-C12
40	y	318	NEX	C13-C14-C15-C35
35	B	625	LHG	C3-O3-P-O6
35	S	317	LHG	C4-O6-P-O3
35	b	622	LHG	C3-O3-P-O6
35	g	618	LHG	C3-O3-P-O6
35	y	319	LHG	C4-O6-P-O3
35	N	618	LHG	C24-C25-C26-C27
35	d	408	LHG	C30-C31-C32-C33
35	b	624	LHG	C34-C35-C36-C37
33	d	407	PL9	C15-C14-C16-C17
35	B	622	LHG	C2-C3-O3-P
35	B	625	LHG	C5-C4-O6-P
35	c	519	LHG	C5-C4-O6-P
35	w	102	LHG	C2-C3-O3-P
35	y	319	LHG	C5-C4-O6-P
28	B	603	CLA	C2-C3-C5-C6
28	n	610	CLA	C2-C3-C5-C6
38	n	609	CHL	O1A-CGA-O2A-C1
35	A	416	LHG	C3-O3-P-O5
35	B	623	LHG	C4-O6-P-O5
35	B	625	LHG	C4-O6-P-O4
35	C	521	LHG	C4-O6-P-O5
35	G	618	LHG	C3-O3-P-O4
35	R	616	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
35	W	101	LHG	C3-O3-P-O5
35	a	415	LHG	C4-O6-P-O5
35	b	621	LHG	C4-O6-P-O4
35	b	622	LHG	C4-O6-P-O4
35	b	624	LHG	C4-O6-P-O4
35	b	624	LHG	C4-O6-P-O5
35	d	408	LHG	C3-O3-P-O5
35	l	101	LHG	C4-O6-P-O5
35	s	617	LHG	C3-O3-P-O4
35	s	617	LHG	C4-O6-P-O4
35	w	102	LHG	C4-O6-P-O4
36	A	417	DGD	C7A-C8A-C9A-CAA
28	R	608	CLA	CBA-CGA-O2A-C1
35	B	623	LHG	O6-C4-C5-C6
35	B	625	LHG	O6-C4-C5-C6
35	R	616	LHG	O6-C4-C5-C6
35	b	621	LHG	O6-C4-C5-C6
35	c	520	LHG	C25-C26-C27-C28
28	b	603	CLA	C3-C5-C6-C7
38	n	607	CHL	C3-C5-C6-C7
28	Y	603	CLA	C6-C7-C8-C10
32	A	413	LMG	C33-C34-C35-C36
28	B	610	CLA	CAD-CBD-CGD-O1D
28	C	508	CLA	CAD-CBD-CGD-O1D
28	c	508	CLA	CAD-CBD-CGD-O1D
31	B	620	SQD	O5-C5-C6-S
31	L	103	SQD	O5-C5-C6-S
38	G	605	CHL	CAD-CBD-CGD-O1D
38	N	605	CHL	CAD-CBD-CGD-O1D
38	g	605	CHL	CAD-CBD-CGD-O1D
38	n	605	CHL	CAD-CBD-CGD-O1D
38	s	605	CHL	CAD-CBD-CGD-O1D
38	y	302	CHL	C5-C6-C7-C8
35	C	521	LHG	C12-C13-C14-C15
28	C	506	CLA	C3-C5-C6-C7
28	g	602	CLA	C8-C10-C11-C12
35	G	618	LHG	C26-C27-C28-C29
38	g	601	CHL	O1D-CGD-O2D-CED
35	D	407	LHG	C34-C35-C36-C37
28	b	607	CLA	C16-C17-C18-C20
28	n	612	CLA	C11-C12-C13-C15
38	g	619	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	C	512	CLA	C4-C3-C5-C6
28	s	609	CLA	C4-C3-C5-C6
28	A	405	CLA	C11-C12-C13-C15
28	B	603	CLA	C11-C10-C8-C7
28	B	604	CLA	C6-C7-C8-C10
28	B	607	CLA	C11-C12-C13-C15
28	B	611	CLA	C6-C7-C8-C10
28	B	613	CLA	C11-C10-C8-C7
28	B	613	CLA	C11-C12-C13-C15
28	B	614	CLA	C11-C10-C8-C7
28	B	614	CLA	C11-C12-C13-C15
28	B	615	CLA	C6-C7-C8-C10
28	B	615	CLA	C12-C13-C15-C16
28	B	616	CLA	C11-C12-C13-C15
28	C	510	CLA	C11-C12-C13-C15
28	C	511	CLA	C6-C7-C8-C10
28	C	513	CLA	C11-C12-C13-C15
28	D	401	CLA	C6-C7-C8-C10
28	D	403	CLA	C11-C10-C8-C7
28	G	611	CLA	C11-C10-C8-C7
28	N	610	CLA	C2-C3-C5-C6
28	N	611	CLA	C6-C7-C8-C10
28	R	609	CLA	C11-C10-C8-C7
28	S	311	CLA	C6-C7-C8-C10
28	Y	602	CLA	C11-C12-C13-C15
28	Y	613	CLA	C6-C7-C8-C10
28	b	602	CLA	C11-C10-C8-C7
28	b	603	CLA	C11-C10-C8-C7
28	b	604	CLA	C6-C7-C8-C10
28	b	604	CLA	C11-C10-C8-C7
28	b	604	CLA	C11-C12-C13-C15
28	b	606	CLA	C11-C10-C8-C7
28	b	607	CLA	C6-C7-C8-C10
28	b	616	CLA	C11-C12-C13-C15
28	c	501	CLA	C6-C7-C8-C10
28	c	506	CLA	C6-C7-C8-C10
28	c	508	CLA	C6-C7-C8-C10
28	c	509	CLA	C11-C10-C8-C7
28	d	401	CLA	C11-C10-C8-C7
28	d	404	CLA	C6-C7-C8-C10
28	d	405	CLA	C6-C7-C8-C10
28	g	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	g	610	CLA	C6-C7-C8-C10
28	g	611	CLA	C6-C7-C8-C10
28	n	603	CLA	C6-C7-C8-C10
28	r	603	CLA	C11-C10-C8-C7
28	r	609	CLA	C11-C10-C8-C7
28	r	612	CLA	C6-C7-C8-C10
28	y	303	CLA	C11-C12-C13-C15
35	C	521	LHG	O6-C4-C5-O7
35	L	102	LHG	O6-C4-C5-O7
35	b	621	LHG	O6-C4-C5-O7
35	c	519	LHG	O6-C4-C5-O7
35	w	102	LHG	O6-C4-C5-O7
38	N	607	CHL	C11-C10-C8-C7
38	Y	601	CHL	C11-C10-C8-C7
38	Y	601	CHL	C12-C13-C15-C16
38	Y	609	CHL	C11-C10-C8-C7
38	g	608	CHL	C11-C10-C8-C7
38	g	609	CHL	C11-C10-C8-C7
38	n	608	CHL	C11-C10-C8-C7
38	n	609	CHL	C11-C10-C8-C7
38	n	609	CHL	C12-C13-C15-C16
38	r	605	CHL	C12-C13-C15-C16
38	y	302	CHL	C6-C7-C8-C10
38	y	308	CHL	C11-C10-C8-C7
32	b	620	LMG	C34-C35-C36-C37
35	c	519	LHG	C24-C25-C26-C27
36	a	401	DGD	C6A-C7A-C8A-C9A
28	c	509	CLA	C13-C15-C16-C17
35	A	416	LHG	C26-C27-C28-C29
35	W	101	LHG	C19-C20-C21-C22
35	c	519	LHG	C11-C10-C9-C8
28	C	512	CLA	C8-C10-C11-C12
35	s	617	LHG	C27-C28-C29-C30
35	w	102	LHG	C16-C17-C18-C19
28	c	511	CLA	C5-C6-C7-C8
28	s	610	CLA	C2A-CAA-CBA-CGA
28	y	304	CLA	C2A-CAA-CBA-CGA
38	S	308	CHL	C2A-CAA-CBA-CGA
38	s	607	CHL	C2A-CAA-CBA-CGA
28	B	615	CLA	C16-C17-C18-C20
28	N	612	CLA	C11-C12-C13-C15
28	r	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
35	D	407	LHG	C35-C36-C37-C38
35	W	101	LHG	C34-C35-C36-C37
31	A	410	SQD	C44-C45-C46-O48
28	B	603	CLA	O1A-CGA-O2A-C1
31	L	103	SQD	O6-C44-C45-O47
32	B	624	LMG	O7-C8-C9-O8
32	b	623	LMG	O1-C7-C8-O7
35	b	621	LHG	O7-C5-C6-O8
35	b	624	LHG	O7-C5-C6-O8
31	A	414	SQD	C11-C10-C9-C8
35	B	625	LHG	C25-C26-C27-C28
28	b	602	CLA	O2A-C1-C2-C3
28	R	608	CLA	O1A-CGA-O2A-C1
31	A	410	SQD	C45-C44-O6-C1
31	B	620	SQD	C45-C44-O6-C1
32	C	522	LMG	C8-C7-O1-C1
32	D	408	LMG	C8-C7-O1-C1
32	b	623	LMG	C8-C7-O1-C1
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C2G-C3G-O3G-C1D
28	n	612	CLA	CAA-CBA-CGA-O2A
35	b	621	LHG	C2-C3-O3-P
35	W	101	LHG	C31-C32-C33-C34
35	c	519	LHG	C26-C27-C28-C29
35	g	618	LHG	O10-C23-O8-C6
38	y	308	CHL	O1A-CGA-O2A-C1
35	B	625	LHG	C9-C10-C11-C12
35	C	521	LHG	C29-C30-C31-C32
35	w	102	LHG	C12-C13-C14-C15
28	c	512	CLA	CAA-CBA-CGA-O2A
35	r	617	LHG	O8-C23-C24-C25
32	C	522	LMG	C12-C13-C14-C15
28	B	602	CLA	C11-C10-C8-C9
28	B	607	CLA	C11-C10-C8-C9
28	B	607	CLA	C11-C12-C13-C14
28	B	615	CLA	C11-C12-C13-C14
28	C	506	CLA	C11-C10-C8-C9
28	C	508	CLA	C6-C7-C8-C9
28	C	509	CLA	C11-C10-C8-C9
28	D	401	CLA	C11-C12-C13-C14
28	G	612	CLA	C11-C10-C8-C9
28	G	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	N	602	CLA	C11-C12-C13-C14
28	N	610	CLA	C11-C10-C8-C9
28	b	606	CLA	C6-C7-C8-C9
28	c	502	CLA	C14-C13-C15-C16
28	c	512	CLA	C11-C10-C8-C9
28	d	405	CLA	C11-C10-C8-C9
28	g	602	CLA	C11-C12-C13-C14
28	r	609	CLA	C11-C10-C8-C9
28	y	303	CLA	C11-C12-C13-C14
38	N	607	CHL	C11-C12-C13-C14
38	Y	607	CHL	C6-C7-C8-C9
38	g	601	CHL	C11-C12-C13-C14
38	g	619	CHL	C6-C7-C8-C9
38	g	619	CHL	C11-C12-C13-C14
38	n	607	CHL	C11-C12-C13-C14
38	n	608	CHL	C11-C12-C13-C14
32	C	522	LMG	C30-C31-C32-C33
28	b	613	CLA	C3-C5-C6-C7
28	C	507	CLA	C5-C6-C7-C8
28	G	613	CLA	C10-C11-C12-C13
35	B	625	LHG	C33-C34-C35-C36
31	a	411	SQD	O10-C23-O48-C46
35	n	618	LHG	O1-C1-C2-O2
35	W	101	LHG	C35-C36-C37-C38
38	G	609	CHL	C5-C6-C7-C8
28	b	615	CLA	C13-C15-C16-C17
28	G	603	CLA	O1A-CGA-O2A-C1
32	b	620	LMG	C12-C13-C14-C15
35	l	101	LHG	C30-C31-C32-C33
41	Y	617	XAT	C40-C33-C34-C35
33	D	406	PL9	C15-C14-C16-C17
38	r	606	CHL	C2-C3-C5-C6
36	C	518	DGD	C7B-C8B-C9B-CAB
35	b	624	LHG	C35-C36-C37-C38
28	B	602	CLA	C13-C15-C16-C17
28	R	610	CLA	C1-C2-C3-C4
28	R	611	CLA	C1-C2-C3-C4
28	S	312	CLA	C1-C2-C3-C4
28	r	601	CLA	C1-C2-C3-C4
28	r	610	CLA	C1-C2-C3-C4
28	r	611	CLA	C1-C2-C3-C4
28	s	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
38	G	606	CHL	C1-C2-C3-C4
38	N	606	CHL	C1-C2-C3-C4
38	Y	606	CHL	C1-C2-C3-C4
38	g	606	CHL	C1-C2-C3-C4
38	n	606	CHL	C1-C2-C3-C4
38	y	307	CHL	C1-C2-C3-C4
28	Y	610	CLA	C3-C5-C6-C7
28	b	610	CLA	C3-C5-C6-C7
28	n	610	CLA	CAA-CBA-CGA-O2A
35	C	521	LHG	C31-C32-C33-C34
35	G	618	LHG	C35-C36-C37-C38
35	d	408	LHG	C33-C34-C35-C36
32	b	623	LMG	C9-C8-O7-C10
35	D	407	LHG	C4-C5-O7-C7
35	Y	619	LHG	O6-C4-C5-C6
35	b	622	LHG	O6-C4-C5-C6
35	b	624	LHG	O6-C4-C5-C6
38	g	601	CHL	CBD-CGD-O2D-CED
28	C	511	CLA	C2A-CAA-CBA-CGA
28	N	602	CLA	C2A-CAA-CBA-CGA
28	B	613	CLA	C2-C1-O2A-CGA
28	C	507	CLA	C2-C1-O2A-CGA
28	D	401	CLA	C2-C1-O2A-CGA
28	D	403	CLA	C2-C1-O2A-CGA
28	r	603	CLA	C2-C1-O2A-CGA
38	y	302	CHL	C2-C1-O2A-CGA
35	d	408	LHG	C35-C36-C37-C38
35	N	618	LHG	C5-C4-O6-P
35	c	520	LHG	C5-C4-O6-P
35	g	618	LHG	C5-C4-O6-P
35	w	102	LHG	C5-C4-O6-P
28	c	508	CLA	CBA-CGA-O2A-C1
35	B	623	LHG	O6-C4-C5-O7
35	b	622	LHG	O6-C4-C5-O7
35	b	624	LHG	O6-C4-C5-O7
35	g	618	LHG	O6-C4-C5-O7
35	s	617	LHG	O6-C4-C5-O7
28	n	602	CLA	C16-C17-C18-C19
28	n	603	CLA	C16-C17-C18-C20
33	D	406	PL9	C45-C44-C46-C47
31	A	410	SQD	C27-C28-C29-C30
31	A	414	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	B	624	LMG	C12-C13-C14-C15
28	n	602	CLA	C3-C5-C6-C7
30	H	101	BCR	C1-C6-C7-C8
30	c	514	BCR	C23-C24-C25-C30
28	g	602	CLA	C2-C3-C5-C6
38	G	601	CHL	C2-C3-C5-C6
28	b	604	CLA	O1D-CGD-O2D-CED
28	R	603	CLA	C11-C12-C13-C15
28	S	310	CLA	C2A-CAA-CBA-CGA
38	Y	608	CHL	C2A-CAA-CBA-CGA
28	R	604	CLA	O2A-C1-C2-C3
31	a	414	SQD	C2-C1-O6-C44
31	B	620	SQD	O47-C45-C46-O48
35	c	519	LHG	O7-C5-C6-O8
35	l	101	LHG	C28-C29-C30-C31
35	c	520	LHG	C24-C23-O8-C6
35	A	416	LHG	C3-O3-P-O6
35	B	622	LHG	C3-O3-P-O6
35	D	407	LHG	C3-O3-P-O6
35	b	621	LHG	C3-O3-P-O6
35	r	617	LHG	C3-O3-P-O6
28	y	312	CLA	C11-C12-C13-C14
36	c	517	DGD	C2G-C1G-O1G-C1A
28	N	611	CLA	C5-C6-C7-C8
35	S	317	LHG	C24-C25-C26-C27
28	B	606	CLA	O1D-CGD-O2D-CED
28	g	611	CLA	CBA-CGA-O2A-C1
31	a	414	SQD	O6-C44-C45-C46
32	b	623	LMG	O1-C7-C8-C9
36	c	518	DGD	O1G-C1G-C2G-C3G
29	A	407	PHO	C4-C3-C5-C6
35	W	101	LHG	C16-C17-C18-C19
28	B	604	CLA	C11-C10-C8-C7
28	B	604	CLA	C11-C12-C13-C15
28	C	508	CLA	C11-C10-C8-C7
28	C	512	CLA	C2-C3-C5-C6
28	R	603	CLA	C6-C7-C8-C10
28	R	608	CLA	C11-C10-C8-C7
28	b	615	CLA	C11-C10-C8-C7
28	y	313	CLA	C11-C12-C13-C15
28	D	403	CLA	CAA-CBA-CGA-O2A
28	S	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C11-C12-C13-C14
28	B	613	CLA	C11-C12-C13-C14
28	C	513	CLA	C11-C12-C13-C14
28	G	611	CLA	C11-C10-C8-C9
28	R	613	CLA	C11-C12-C13-C14
28	Y	602	CLA	C11-C12-C13-C14
28	b	602	CLA	C11-C10-C8-C9
28	b	605	CLA	C11-C10-C8-C9
28	b	612	CLA	C11-C12-C13-C14
28	b	616	CLA	C11-C12-C13-C14
28	c	505	CLA	C11-C10-C8-C9
28	d	401	CLA	C11-C10-C8-C9
28	d	404	CLA	C6-C7-C8-C9
28	r	612	CLA	C11-C10-C8-C9
38	g	609	CHL	C6-C7-C8-C9
30	H	101	BCR	C13-C14-C15-C16
39	G	615	LUT	C29-C30-C31-C32
40	n	617	NEX	C33-C34-C35-C15
28	y	311	CLA	C11-C12-C13-C14
32	c	521	LMG	C33-C34-C35-C36
35	W	101	LHG	C12-C13-C14-C15
36	a	401	DGD	C6B-C7B-C8B-C9B
35	b	622	LHG	C9-C10-C11-C12
28	R	602	CLA	C2A-CAA-CBA-CGA
35	s	617	LHG	C33-C34-C35-C36
28	G	604	CLA	CBA-CGA-O2A-C1
35	S	317	LHG	C5-C4-O6-P
35	n	618	LHG	C2-C3-O3-P
36	a	401	DGD	C9B-CAB-CBB-CCB
40	g	617	NEX	C31-C32-C33-C34
38	r	607	CHL	CBD-CGD-O2D-CED
28	S	311	CLA	C11-C10-C8-C7
29	d	402	PHO	C4-C3-C5-C6
33	d	407	PL9	C45-C44-C46-C47
35	r	617	LHG	O1-C1-C2-O2
35	B	623	LHG	C32-C33-C34-C35
35	y	319	LHG	C30-C31-C32-C33
28	d	404	CLA	CAA-CBA-CGA-O2A
28	C	506	CLA	C15-C16-C17-C18
28	G	604	CLA	O1A-CGA-O2A-C1
36	c	517	DGD	O6E-C1E-O5D-C6D
30	B	619	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	c	515	BCR	C15-C16-C17-C18
39	G	616	LUT	C9-C10-C11-C12
39	R	614	LUT	C9-C10-C11-C12
35	C	521	LHG	C9-C10-C11-C12
28	c	504	CLA	C3-C5-C6-C7
35	c	520	LHG	O10-C23-O8-C6
28	d	401	CLA	C5-C6-C7-C8
28	y	311	CLA	C8-C10-C11-C12
28	B	606	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	CAA-CBA-CGA-O2A
28	C	512	CLA	C3-C5-C6-C7
32	B	621	LMG	C12-C13-C14-C15
28	b	605	CLA	C4-C3-C5-C6
28	b	611	CLA	C15-C16-C17-C18
28	n	602	CLA	C8-C10-C11-C12
28	n	610	CLA	C5-C6-C7-C8
35	D	407	LHG	C31-C32-C33-C34
28	g	611	CLA	O1A-CGA-O2A-C1
38	n	608	CHL	C5-C6-C7-C8
36	a	401	DGD	C7B-C8B-C9B-CAB
28	B	606	CLA	C2-C1-O2A-CGA
28	a	406	CLA	C2-C1-O2A-CGA
35	Y	619	LHG	O10-C23-O8-C6
35	L	102	LHG	C17-C18-C19-C20
36	c	517	DGD	C2E-C1E-O5D-C6D
28	c	508	CLA	O1A-CGA-O2A-C1
37	E	101	HEM	CAD-CBD-CGD-O1D
28	r	613	CLA	C2A-CAA-CBA-CGA
28	y	303	CLA	C2A-CAA-CBA-CGA
35	n	618	LHG	O7-C5-C6-O8
28	R	601	CLA	C4C-C3C-CAC-CBC
35	A	416	LHG	C31-C32-C33-C34
28	B	608	CLA	C3A-C2A-CAA-CBA
28	B	610	CLA	C3A-C2A-CAA-CBA
28	g	613	CLA	C3A-C2A-CAA-CBA
28	s	613	CLA	C3A-C2A-CAA-CBA
29	D	402	PHO	C3A-C2A-CAA-CBA
28	A	408	CLA	C11-C12-C13-C14
32	b	623	LMG	C11-C12-C13-C14
38	G	605	CHL	CAA-CBA-CGA-O2A
38	s	605	CHL	CAA-CBA-CGA-O2A
33	D	406	PL9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
33	d	407	PL9	C13-C14-C16-C17
28	B	612	CLA	C11-C12-C13-C14
28	B	614	CLA	C11-C12-C13-C14
28	B	615	CLA	C14-C13-C15-C16
28	C	501	CLA	C14-C13-C15-C16
28	N	610	CLA	C6-C7-C8-C9
28	R	603	CLA	C6-C7-C8-C9
28	R	609	CLA	C6-C7-C8-C9
28	R	609	CLA	C11-C10-C8-C9
28	Y	610	CLA	C6-C7-C8-C9
28	b	608	CLA	C6-C7-C8-C9
28	b	613	CLA	C6-C7-C8-C9
28	c	503	CLA	C11-C10-C8-C9
28	c	509	CLA	C11-C10-C8-C9
29	A	407	PHO	C14-C13-C15-C16
29	a	408	PHO	C14-C13-C15-C16
28	r	609	CLA	C16-C17-C18-C19
35	C	521	LHG	C10-C11-C12-C13
28	S	309	CLA	CAA-CBA-CGA-O2A
28	n	614	CLA	CAA-CBA-CGA-O2A
37	f	101	HEM	CAA-CBA-CGA-O2A
38	s	607	CHL	CAA-CBA-CGA-O2A
35	S	317	LHG	C16-C17-C18-C19
38	r	607	CHL	O1D-CGD-O2D-CED
35	A	416	LHG	C30-C31-C32-C33
35	C	521	LHG	C4-C5-C6-O8
35	n	618	LHG	C4-C5-C6-O8
39	r	614	LUT	C11-C10-C9-C19
40	G	617	NEX	C39-C29-C30-C31
40	n	617	NEX	C39-C29-C30-C31
35	C	521	LHG	C16-C17-C18-C19
38	G	605	CHL	CAA-CBA-CGA-O1A
28	A	408	CLA	C2A-CAA-CBA-CGA
28	R	610	CLA	C2A-CAA-CBA-CGA
28	n	602	CLA	C2A-CAA-CBA-CGA
35	S	301	LHG	O9-C7-C8-C9
28	C	503	CLA	C16-C17-C18-C19
28	A	406	CLA	O2A-C1-C2-C3
28	B	602	CLA	O2A-C1-C2-C3
28	B	604	CLA	O2A-C1-C2-C3
28	s	613	CLA	CBA-CGA-O2A-C1
38	g	607	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	O6E-C1E-O5D-C6D
35	b	622	LHG	C11-C10-C9-C8
35	y	319	LHG	C34-C35-C36-C37
38	s	607	CHL	CAA-CBA-CGA-O1A
39	S	315	LUT	C11-C12-C13-C20
40	g	617	NEX	C27-C28-C29-C39
28	a	409	CLA	C3-C5-C6-C7
38	Y	607	CHL	C3-C5-C6-C7
32	c	521	LMG	C7-C8-O7-C10
32	c	521	LMG	C9-C8-O7-C10
28	Y	610	CLA	C4-C3-C5-C6
29	a	408	PHO	C4-C3-C5-C6
28	B	610	CLA	C1A-C2A-CAA-CBA
28	G	614	CLA	C1A-C2A-CAA-CBA
28	N	611	CLA	C1A-C2A-CAA-CBA
28	Y	603	CLA	C1A-C2A-CAA-CBA
28	b	616	CLA	C1A-C2A-CAA-CBA
28	c	505	CLA	C1A-C2A-CAA-CBA
36	A	417	DGD	C2B-C3B-C4B-C5B
28	R	603	CLA	C11-C12-C13-C14
28	c	508	CLA	C16-C17-C18-C19
28	B	605	CLA	C11-C10-C8-C7
28	C	503	CLA	C11-C12-C13-C15
28	C	512	CLA	C11-C10-C8-C7
28	N	602	CLA	C11-C10-C8-C7
28	Y	602	CLA	C6-C7-C8-C10
28	Y	610	CLA	C11-C10-C8-C7
28	b	601	CLA	C6-C7-C8-C10
28	b	605	CLA	C12-C13-C15-C16
28	b	609	CLA	C11-C12-C13-C15
28	b	611	CLA	C11-C12-C13-C15
28	c	502	CLA	C11-C10-C8-C7
28	d	404	CLA	C11-C10-C8-C7
28	g	611	CLA	C11-C10-C8-C7
28	n	610	CLA	C6-C7-C8-C10
28	r	603	CLA	C6-C7-C8-C10
28	r	608	CLA	C6-C7-C8-C10
28	y	312	CLA	C11-C10-C8-C7
38	G	601	CHL	C11-C10-C8-C7
31	a	411	SQD	C16-C17-C18-C19
32	C	520	LMG	C36-C37-C38-C39
28	s	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	n	614	CLA	CAA-CBA-CGA-O1A
37	E	101	HEM	CAD-CBD-CGD-O2D
38	s	601	CHL	CAA-CBA-CGA-O1A
38	s	601	CHL	CAA-CBA-CGA-O2A
38	s	605	CHL	CAA-CBA-CGA-O1A
28	b	602	CLA	O1D-CGD-O2D-CED
35	D	407	LHG	C30-C31-C32-C33
39	y	316	LUT	C13-C14-C15-C35
35	L	102	LHG	C19-C20-C21-C22
28	n	603	CLA	CAA-CBA-CGA-O2A
28	S	309	CLA	CAA-CBA-CGA-O1A
36	C	518	DGD	C6A-C7A-C8A-C9A
36	C	518	DGD	CAB-CBB-CCB-CDB
28	b	604	CLA	CBD-CGD-O2D-CED
35	Y	619	LHG	C31-C32-C33-C34
28	Y	611	CLA	C5-C6-C7-C8
37	f	101	HEM	CAA-CBA-CGA-O1A
28	d	405	CLA	C5-C6-C7-C8
32	k	102	LMG	C13-C14-C15-C16
35	d	408	LHG	C29-C30-C31-C32
28	c	506	CLA	C11-C10-C8-C9
36	C	518	DGD	C2G-C1G-O1G-C1A
28	r	603	CLA	C11-C12-C13-C15
28	C	502	CLA	C4-C3-C5-C6
28	b	609	CLA	C8-C10-C11-C12
28	y	313	CLA	C8-C10-C11-C12
29	A	407	PHO	C2-C3-C5-C6
33	D	406	PL9	C12-C11-C9-C8
35	S	317	LHG	C17-C18-C19-C20
39	r	614	LUT	C11-C10-C9-C8
40	Y	618	NEX	C28-C29-C30-C31
35	L	102	LHG	C28-C29-C30-C31
28	b	603	CLA	CBA-CGA-O2A-C1
35	N	618	LHG	C24-C23-O8-C6
32	b	623	LMG	O9-C10-C11-C12
30	c	514	BCR	C13-C14-C15-C16
30	i	101	BCR	C9-C10-C11-C12
39	n	615	LUT	C9-C10-C11-C12
40	r	616	NEX	C33-C34-C35-C15
41	Y	617	XAT	C33-C34-C35-C15
28	C	507	CLA	C3-C5-C6-C7
28	n	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
35	B	625	LHG	C35-C36-C37-C38
35	l	101	LHG	C9-C10-C11-C12
28	G	612	CLA	C5-C6-C7-C8
38	n	608	CHL	C4-C3-C5-C6
38	y	309	CHL	C4-C3-C5-C6
35	w	102	LHG	C10-C11-C12-C13
28	A	406	CLA	C2-C1-O2A-CGA
28	A	408	CLA	C2-C1-O2A-CGA
28	g	610	CLA	C2-C1-O2A-CGA
28	g	611	CLA	C2-C1-O2A-CGA
28	y	312	CLA	C2-C1-O2A-CGA
29	d	402	PHO	C2-C3-C5-C6
33	d	407	PL9	C43-C44-C46-C47
28	C	503	CLA	C6-C7-C8-C9
28	a	409	CLA	C6-C7-C8-C9
28	c	510	CLA	C6-C7-C8-C9
28	r	602	CLA	C11-C10-C8-C9
28	y	313	CLA	C6-C7-C8-C9
32	w	101	LMG	C31-C32-C33-C34
28	D	401	CLA	CBD-CGD-O2D-CED
38	N	609	CHL	C2C-C3C-CAC-CBC
28	C	513	CLA	C3-C5-C6-C7
35	S	317	LHG	C29-C30-C31-C32
35	n	618	LHG	C24-C25-C26-C27
28	G	613	CLA	C13-C15-C16-C17
28	B	612	CLA	C2A-CAA-CBA-CGA
28	Y	611	CLA	C11-C12-C13-C15
35	Y	619	LHG	C24-C23-O8-C6
28	s	608	CLA	CAA-CBA-CGA-O2A
28	b	603	CLA	O1A-CGA-O2A-C1
35	d	408	LHG	O10-C23-O8-C6
30	C	514	BCR	C23-C24-C25-C30
30	b	618	BCR	C23-C24-C25-C30
30	t	101	BCR	C23-C24-C25-C30
39	G	615	LUT	C1-C6-C7-C8
39	N	615	LUT	C5-C6-C7-C8
39	n	616	LUT	C1-C6-C7-C8
39	r	614	LUT	C1-C6-C7-C8
39	s	614	LUT	C5-C6-C7-C8
35	B	622	LHG	C25-C26-C27-C28
36	b	625	DGD	C2B-C3B-C4B-C5B
28	B	601	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	C	522	LMG	C7-C8-C9-O8
32	C	522	LMG	C10-C11-C12-C13
28	s	608	CLA	CAA-CBA-CGA-O1A
38	g	607	CHL	CBD-CGD-O2D-CED
35	l	101	LHG	O1-C1-C2-C3
38	g	607	CHL	O1A-CGA-O2A-C1
30	A	409	BCR	C13-C14-C15-C16
40	N	617	NEX	C13-C14-C15-C35
38	G	607	CHL	C4-C3-C5-C6
38	Y	607	CHL	C4-C3-C5-C6
28	c	503	CLA	C8-C10-C11-C12
28	B	609	CLA	C2-C3-C5-C6
33	D	406	PL9	C13-C14-C16-C17
33	D	406	PL9	C43-C44-C46-C47
28	C	508	CLA	C8-C10-C11-C12
36	c	516	DGD	C5D-C6D-O5D-C1E
28	b	614	CLA	CAA-CBA-CGA-O2A
28	C	506	CLA	C16-C17-C18-C19
38	G	607	CHL	C6-C7-C8-C10
28	c	504	CLA	C11-C10-C8-C9
32	A	413	LMG	C39-C40-C41-C42
35	a	415	LHG	C25-C26-C27-C28
28	n	604	CLA	C2A-CAA-CBA-CGA
28	r	609	CLA	CBA-CGA-O2A-C1
28	C	503	CLA	C15-C16-C17-C18
35	S	301	LHG	C26-C27-C28-C29
28	r	612	CLA	C3-C5-C6-C7
28	y	310	CLA	C11-C12-C13-C15
36	A	417	DGD	C6B-C7B-C8B-C9B
28	b	602	CLA	CBD-CGD-O2D-CED
28	c	505	CLA	O1D-CGD-O2D-CED
35	n	618	LHG	C9-C10-C11-C12
38	G	609	CHL	C4-C3-C5-C6
28	B	616	CLA	C6-C7-C8-C10
28	a	409	CLA	C6-C7-C8-C10
28	a	409	CLA	C11-C10-C8-C7
28	b	607	CLA	C12-C13-C15-C16
28	s	612	CLA	C2-C3-C5-C6
29	a	408	PHO	C2-C3-C5-C6
38	Y	607	CHL	C2-C3-C5-C6
38	g	607	CHL	CBA-CGA-O2A-C1
31	L	103	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	s	617	LHG	C16-C17-C18-C19
38	N	609	CHL	C4C-C3C-CAC-CBC
35	R	616	LHG	O1-C1-C2-O2
29	A	407	PHO	C1-C2-C3-C4
28	r	608	CLA	C5-C6-C7-C8
30	b	619	BCR	C9-C10-C11-C12
31	A	414	SQD	C2-C1-O6-C44
35	S	301	LHG	C5-C4-O6-P
35	s	617	LHG	C30-C31-C32-C33
31	A	410	SQD	O47-C45-C46-O48
32	C	522	LMG	O7-C8-C9-O8
28	r	609	CLA	O1A-CGA-O2A-C1
35	N	618	LHG	O10-C23-O8-C6
28	S	309	CLA	C2C-C3C-CAC-CBC
35	g	618	LHG	C9-C10-C11-C12
35	a	415	LHG	C16-C17-C18-C19
28	B	608	CLA	C13-C15-C16-C17
28	C	503	CLA	C3-C5-C6-C7
28	r	608	CLA	CAA-CBA-CGA-O2A
35	W	101	LHG	C29-C30-C31-C32
28	Y	610	CLA	O1A-CGA-O2A-C1
28	B	610	CLA	C8-C10-C11-C12
35	C	521	LHG	C24-C23-O8-C6
28	G	612	CLA	C11-C12-C13-C15
38	g	619	CHL	C16-C17-C18-C19
28	S	309	CLA	C4C-C3C-CAC-CBC
35	b	622	LHG	C33-C34-C35-C36
28	c	504	CLA	C11-C10-C8-C7
28	B	603	CLA	C11-C10-C8-C9
28	B	605	CLA	C11-C10-C8-C9
28	B	613	CLA	C11-C10-C8-C9
28	B	614	CLA	C11-C10-C8-C9
28	B	616	CLA	C11-C12-C13-C14
28	C	503	CLA	C11-C12-C13-C14
28	C	510	CLA	C11-C12-C13-C14
28	D	403	CLA	C11-C10-C8-C9
28	Y	602	CLA	C6-C7-C8-C9
28	Y	610	CLA	C11-C10-C8-C9
28	Y	613	CLA	C11-C12-C13-C14
28	b	603	CLA	C11-C10-C8-C9
28	b	604	CLA	C11-C10-C8-C9
28	b	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	606	CLA	C11-C10-C8-C9
28	b	615	CLA	C11-C10-C8-C9
28	c	502	CLA	C11-C10-C8-C9
28	r	603	CLA	C11-C10-C8-C9
28	y	312	CLA	C11-C10-C8-C9
36	C	518	DGD	CAA-CBA-CCA-CDA
28	C	502	CLA	C3A-C2A-CAA-CBA
28	S	311	CLA	C3A-C2A-CAA-CBA
28	d	401	CLA	C3A-C2A-CAA-CBA
28	g	612	CLA	C3A-C2A-CAA-CBA
38	N	609	CHL	C3A-C2A-CAA-CBA
38	S	307	CHL	C3A-C2A-CAA-CBA
35	r	617	LHG	C24-C25-C26-C27
28	B	616	CLA	CAD-CBD-CGD-O2D
28	N	614	CLA	CAD-CBD-CGD-O2D
28	S	305	CLA	CAD-CBD-CGD-O2D
28	S	312	CLA	CAD-CBD-CGD-O2D
28	b	604	CLA	CAD-CBD-CGD-O2D
28	c	506	CLA	CAD-CBD-CGD-O2D
28	n	611	CLA	CAD-CBD-CGD-O2D
38	N	608	CHL	CAD-CBD-CGD-O2D
38	R	605	CHL	CAD-CBD-CGD-O2D
38	S	306	CHL	CAD-CBD-CGD-O2D
38	S	307	CHL	CAD-CBD-CGD-O2D
38	Y	606	CHL	CAD-CBD-CGD-O2D
38	g	606	CHL	CAD-CBD-CGD-O2D
38	n	609	CHL	CAD-CBD-CGD-O2D
38	r	605	CHL	CAD-CBD-CGD-O2D
38	s	607	CHL	CAD-CBD-CGD-O2D
38	y	306	CHL	CAD-CBD-CGD-O2D
38	y	308	CHL	CAD-CBD-CGD-O2D
38	y	309	CHL	CAD-CBD-CGD-O2D
28	Y	610	CLA	CBA-CGA-O2A-C1
28	C	510	CLA	CAA-CBA-CGA-O1A
35	B	625	LHG	C16-C17-C18-C19
35	D	407	LHG	C26-C27-C28-C29
35	c	520	LHG	C26-C27-C28-C29
28	N	612	CLA	C8-C10-C11-C12
35	B	623	LHG	O9-C7-O7-C5
35	Y	619	LHG	C15-C16-C17-C18
28	G	604	CLA	C2-C1-O2A-CGA
35	y	319	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
36	c	518	DGD	O2G-C1B-C2B-C3B
35	d	408	LHG	C24-C23-O8-C6
28	B	609	CLA	C4-C3-C5-C6
28	s	612	CLA	C4-C3-C5-C6
38	R	607	CHL	C4-C3-C5-C6
28	C	502	CLA	C2-C3-C5-C6
32	b	623	LMG	O8-C28-C29-C30
39	S	315	LUT	C11-C12-C13-C14
39	r	614	LUT	C27-C28-C29-C30
32	A	411	LMG	C30-C31-C32-C33
32	A	411	LMG	C7-C8-C9-O8
32	C	520	LMG	C7-C8-C9-O8
32	w	101	LMG	C7-C8-C9-O8
40	y	301	NEX	O24-C26-C27-C28
41	Y	617	XAT	O24-C26-C27-C28
32	B	624	LMG	O10-C28-O8-C9
31	A	410	SQD	C12-C13-C14-C15
31	B	620	SQD	C12-C13-C14-C15
35	a	415	LHG	C24-C25-C26-C27
35	Y	619	LHG	O6-C4-C5-O7
28	B	602	CLA	CAA-CBA-CGA-O2A
28	B	610	CLA	CAA-CBA-CGA-O2A
28	R	608	CLA	CAA-CBA-CGA-O2A
28	R	610	CLA	CAA-CBA-CGA-O2A
28	Y	603	CLA	CAA-CBA-CGA-O2A
35	S	301	LHG	O8-C23-C24-C25
38	N	607	CHL	O2A-C1-C2-C3
38	Y	607	CHL	O2A-C1-C2-C3
38	n	607	CHL	O2A-C1-C2-C3
38	r	605	CHL	O2A-C1-C2-C3
37	E	101	HEM	C4B-C3B-CAB-CBB
37	f	101	HEM	C4B-C3B-CAB-CBB
35	r	617	LHG	C24-C23-O8-C6
28	B	609	CLA	C2A-CAA-CBA-CGA
28	G	613	CLA	C2A-CAA-CBA-CGA
28	r	612	CLA	CAA-CBA-CGA-O2A
36	c	517	DGD	C3A-C4A-C5A-C6A
28	B	601	CLA	C8-C10-C11-C12
31	a	411	SQD	C28-C29-C30-C31
36	C	519	DGD	C6A-C7A-C8A-C9A
28	A	406	CLA	CHA-CBD-CGD-O1D
28	A	406	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	B	602	CLA	CHA-CBD-CGD-O1D
28	B	602	CLA	CHA-CBD-CGD-O2D
28	B	606	CLA	CHA-CBD-CGD-O1D
28	B	606	CLA	CHA-CBD-CGD-O2D
28	B	608	CLA	CHA-CBD-CGD-O1D
28	B	608	CLA	CHA-CBD-CGD-O2D
28	B	609	CLA	CHA-CBD-CGD-O1D
28	B	609	CLA	CHA-CBD-CGD-O2D
28	B	611	CLA	CHA-CBD-CGD-O2D
28	B	616	CLA	CHA-CBD-CGD-O2D
28	C	503	CLA	CHA-CBD-CGD-O1D
28	C	503	CLA	CHA-CBD-CGD-O2D
28	C	506	CLA	CHA-CBD-CGD-O1D
28	C	506	CLA	CHA-CBD-CGD-O2D
28	C	508	CLA	CHA-CBD-CGD-O2D
28	C	509	CLA	CHA-CBD-CGD-O1D
28	C	509	CLA	CHA-CBD-CGD-O2D
28	C	510	CLA	CHA-CBD-CGD-O1D
28	C	510	CLA	CHA-CBD-CGD-O2D
28	C	511	CLA	CHA-CBD-CGD-O1D
28	C	511	CLA	CHA-CBD-CGD-O2D
28	D	401	CLA	CHA-CBD-CGD-O2D
28	D	403	CLA	CHA-CBD-CGD-O1D
28	D	403	CLA	CHA-CBD-CGD-O2D
28	G	610	CLA	CHA-CBD-CGD-O1D
28	N	604	CLA	CHA-CBD-CGD-O1D
28	N	604	CLA	CHA-CBD-CGD-O2D
28	N	610	CLA	CHA-CBD-CGD-O1D
28	N	610	CLA	CHA-CBD-CGD-O2D
28	N	611	CLA	CHA-CBD-CGD-O1D
28	N	611	CLA	CHA-CBD-CGD-O2D
28	N	613	CLA	CHA-CBD-CGD-O2D
28	R	601	CLA	CHA-CBD-CGD-O1D
28	R	601	CLA	CHA-CBD-CGD-O2D
28	R	602	CLA	CHA-CBD-CGD-O1D
28	R	602	CLA	CHA-CBD-CGD-O2D
28	R	611	CLA	CHA-CBD-CGD-O1D
28	R	611	CLA	CHA-CBD-CGD-O2D
28	R	612	CLA	CHA-CBD-CGD-O2D
28	S	303	CLA	CHA-CBD-CGD-O1D
28	S	303	CLA	CHA-CBD-CGD-O2D
28	S	311	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	S	311	CLA	CHA-CBD-CGD-O2D
28	Y	602	CLA	CHA-CBD-CGD-O1D
28	Y	602	CLA	CHA-CBD-CGD-O2D
28	Y	604	CLA	CHA-CBD-CGD-O2D
28	Y	613	CLA	CHA-CBD-CGD-O2D
28	Y	614	CLA	CHA-CBD-CGD-O2D
28	a	406	CLA	CHA-CBD-CGD-O2D
28	a	407	CLA	CHA-CBD-CGD-O1D
28	a	407	CLA	CHA-CBD-CGD-O2D
28	b	602	CLA	CHA-CBD-CGD-O1D
28	b	602	CLA	CHA-CBD-CGD-O2D
28	b	607	CLA	CHA-CBD-CGD-O1D
28	b	607	CLA	CHA-CBD-CGD-O2D
28	b	608	CLA	CHA-CBD-CGD-O1D
28	b	608	CLA	CHA-CBD-CGD-O2D
28	c	501	CLA	CHA-CBD-CGD-O1D
28	c	501	CLA	CHA-CBD-CGD-O2D
28	c	502	CLA	CHA-CBD-CGD-O1D
28	c	502	CLA	CHA-CBD-CGD-O2D
28	c	504	CLA	CHA-CBD-CGD-O2D
28	c	508	CLA	CHA-CBD-CGD-O1D
28	c	511	CLA	CHA-CBD-CGD-O2D
28	c	512	CLA	CHA-CBD-CGD-O1D
28	c	512	CLA	CHA-CBD-CGD-O2D
28	d	401	CLA	CHA-CBD-CGD-O1D
28	d	401	CLA	CHA-CBD-CGD-O2D
28	d	404	CLA	CHA-CBD-CGD-O1D
28	d	404	CLA	CHA-CBD-CGD-O2D
28	g	602	CLA	CHA-CBD-CGD-O1D
28	g	602	CLA	CHA-CBD-CGD-O2D
28	g	604	CLA	CHA-CBD-CGD-O1D
28	g	610	CLA	CHA-CBD-CGD-O2D
28	n	610	CLA	CHA-CBD-CGD-O1D
28	n	610	CLA	CHA-CBD-CGD-O2D
28	r	601	CLA	CHA-CBD-CGD-O1D
28	r	601	CLA	CHA-CBD-CGD-O2D
28	r	602	CLA	CHA-CBD-CGD-O1D
28	r	602	CLA	CHA-CBD-CGD-O2D
28	r	608	CLA	CHA-CBD-CGD-O1D
28	r	608	CLA	CHA-CBD-CGD-O2D
28	r	609	CLA	CHA-CBD-CGD-O1D
28	r	609	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	r	611	CLA	CHA-CBD-CGD-O1D
28	r	611	CLA	CHA-CBD-CGD-O2D
28	r	612	CLA	CHA-CBD-CGD-O1D
28	r	612	CLA	CHA-CBD-CGD-O2D
28	s	602	CLA	CHA-CBD-CGD-O1D
28	s	602	CLA	CHA-CBD-CGD-O2D
28	s	604	CLA	CHA-CBD-CGD-O1D
28	s	604	CLA	CHA-CBD-CGD-O2D
28	s	612	CLA	CHA-CBD-CGD-O1D
28	s	612	CLA	CHA-CBD-CGD-O2D
28	y	310	CLA	CHA-CBD-CGD-O1D
28	y	310	CLA	CHA-CBD-CGD-O2D
28	y	313	CLA	CHA-CBD-CGD-O1D
28	y	313	CLA	CHA-CBD-CGD-O2D
28	y	314	CLA	CHA-CBD-CGD-O1D
28	y	314	CLA	CHA-CBD-CGD-O2D
38	G	605	CHL	CHA-CBD-CGD-O2D
38	N	605	CHL	CHA-CBD-CGD-O2D
38	g	605	CHL	CHA-CBD-CGD-O2D
38	s	605	CHL	CHA-CBD-CGD-O2D
28	S	304	CLA	CAA-CBA-CGA-O2A
28	b	602	CLA	CAA-CBA-CGA-O2A
36	A	417	DGD	O1G-C1A-C2A-C3A
36	C	519	DGD	O1G-C1A-C2A-C3A
38	n	608	CHL	C2-C3-C5-C6
32	B	621	LMG	C21-C22-C23-C24
36	c	517	DGD	C5B-C6B-C7B-C8B
35	A	416	LHG	C32-C33-C34-C35
35	N	618	LHG	O6-C4-C5-C6
35	n	618	LHG	O6-C4-C5-C6
40	n	617	NEX	C28-C29-C30-C31
28	y	312	CLA	C11-C12-C13-C15
28	N	614	CLA	CAA-CBA-CGA-O2A
28	r	610	CLA	CAA-CBA-CGA-O2A
32	b	620	LMG	O7-C10-C11-C12
35	w	102	LHG	O8-C23-C24-C25
32	c	521	LMG	C15-C16-C17-C18
31	a	414	SQD	O6-C44-C45-O47
32	C	520	LMG	O7-C8-C9-O8
32	w	101	LMG	O7-C8-C9-O8
36	B	626	DGD	O1G-C1G-C2G-O2G
36	c	517	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
28	B	605	CLA	C10-C11-C12-C13
28	b	602	CLA	C15-C16-C17-C18
28	r	612	CLA	C10-C11-C12-C13
28	r	613	CLA	C8-C10-C11-C12
36	c	518	DGD	C6B-C7B-C8B-C9B
28	D	404	CLA	C8-C10-C11-C12
28	B	607	CLA	CAA-CBA-CGA-O2A
28	G	613	CLA	CAA-CBA-CGA-O2A
28	d	405	CLA	CAA-CBA-CGA-O2A
32	D	408	LMG	O7-C10-C11-C12
35	Y	619	LHG	O8-C23-C24-C25
36	a	401	DGD	O1G-C1A-C2A-C3A
38	n	608	CHL	CAA-CBA-CGA-O2A
28	r	610	CLA	C2A-CAA-CBA-CGA
28	Y	602	CLA	C10-C11-C12-C13
28	b	611	CLA	C5-C6-C7-C8
28	D	401	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	O8-C23-C24-C25
35	D	407	LHG	O8-C23-C24-C25
38	y	308	CHL	CAA-CBA-CGA-O2A
32	w	101	LMG	C8-C9-O8-C28
28	B	605	CLA	C6-C7-C8-C10
28	B	612	CLA	C11-C10-C8-C7
28	B	613	CLA	C12-C13-C15-C16
28	C	510	CLA	C11-C10-C8-C7
28	C	511	CLA	C11-C12-C13-C15
28	b	608	CLA	C11-C10-C8-C7
28	b	612	CLA	C11-C10-C8-C7
28	c	510	CLA	C6-C7-C8-C10
28	g	602	CLA	C11-C10-C8-C7
28	g	610	CLA	C11-C10-C8-C7
28	n	602	CLA	C11-C10-C8-C7
28	n	612	CLA	C6-C7-C8-C10
28	s	609	CLA	C2-C3-C5-C6
28	y	310	CLA	C11-C10-C8-C7
38	N	609	CHL	C11-C10-C8-C7
28	N	602	CLA	C13-C15-C16-C17
28	c	510	CLA	CAA-CBA-CGA-O2A
28	B	612	CLA	C11-C10-C8-C9
28	C	508	CLA	C11-C10-C8-C9
28	C	511	CLA	C11-C12-C13-C14
28	N	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	610	CLA	C11-C10-C8-C9
28	b	611	CLA	C11-C12-C13-C14
28	b	612	CLA	C11-C10-C8-C9
28	b	613	CLA	C11-C10-C8-C9
28	c	503	CLA	C6-C7-C8-C9
28	d	404	CLA	C11-C10-C8-C9
28	g	610	CLA	C11-C10-C8-C9
28	b	603	CLA	C2B-C3B-CAB-CBB
38	n	607	CHL	C2B-C3B-CAB-CBB
32	C	520	LMG	C39-C40-C41-C42
31	a	411	SQD	O47-C7-C8-C9
32	B	621	LMG	O8-C28-C29-C30
35	l	101	LHG	O7-C7-C8-C9
31	A	414	SQD	C4-C5-C6-S
31	L	101	SQD	C4-C5-C6-S
31	a	414	SQD	C4-C5-C6-S
28	C	503	CLA	C16-C17-C18-C20
35	A	416	LHG	C29-C30-C31-C32
38	Y	607	CHL	C5-C6-C7-C8
28	D	401	CLA	C2A-CAA-CBA-CGA
33	d	407	PL9	C11-C12-C13-C14
33	d	407	PL9	C46-C47-C48-C49
35	y	319	LHG	C33-C34-C35-C36
28	c	508	CLA	C16-C17-C18-C20
35	C	521	LHG	O10-C23-O8-C6
35	r	617	LHG	O10-C23-O8-C6
28	r	612	CLA	C2-C3-C5-C6
28	B	602	CLA	CAA-CBA-CGA-O1A
28	r	608	CLA	CAA-CBA-CGA-O1A
28	A	405	CLA	C1A-C2A-CAA-CBA
28	B	608	CLA	C1A-C2A-CAA-CBA
28	a	406	CLA	C1A-C2A-CAA-CBA
28	b	603	CLA	C1A-C2A-CAA-CBA
28	g	612	CLA	C1A-C2A-CAA-CBA
28	g	613	CLA	C1A-C2A-CAA-CBA
28	r	611	CLA	C1A-C2A-CAA-CBA
28	s	610	CLA	C1A-C2A-CAA-CBA
28	s	613	CLA	C1A-C2A-CAA-CBA
38	N	605	CHL	C1A-C2A-CAA-CBA
38	N	609	CHL	C1A-C2A-CAA-CBA
38	S	307	CHL	C1A-C2A-CAA-CBA
38	g	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
38	r	606	CHL	C1A-C2A-CAA-CBA
38	r	607	CHL	C1A-C2A-CAA-CBA
28	y	311	CLA	C11-C12-C13-C15
38	G	607	CHL	CAA-CBA-CGA-O2A
32	k	102	LMG	C34-C35-C36-C37
33	D	406	PL9	C46-C47-C48-C49
28	c	505	CLA	O1A-CGA-O2A-C1
28	a	409	CLA	C2-C1-O2A-CGA
28	c	501	CLA	C2-C1-O2A-CGA
28	g	603	CLA	C2-C1-O2A-CGA
28	c	505	CLA	CBA-CGA-O2A-C1
32	B	624	LMG	C29-C28-O8-C9
32	b	623	LMG	O10-C28-C29-C30
35	y	319	LHG	O10-C23-C24-C25
36	A	417	DGD	O1A-C1A-C2A-C3A
36	c	518	DGD	O1B-C1B-C2B-C3B
35	g	618	LHG	O8-C23-C24-C25
38	G	608	CHL	CAA-CBA-CGA-O2A
38	n	605	CHL	CAA-CBA-CGA-O2A
35	s	617	LHG	C19-C20-C21-C22
28	G	612	CLA	C11-C12-C13-C14
28	Y	611	CLA	C11-C12-C13-C14
35	S	301	LHG	O10-C23-C24-C25
38	n	608	CHL	C13-C15-C16-C17
28	r	612	CLA	C4-C3-C5-C6
35	s	617	LHG	O8-C23-C24-C25
38	r	607	CHL	CAA-CBA-CGA-O2A
35	w	102	LHG	O9-C7-O7-C5
28	b	601	CLA	C3-C5-C6-C7
28	b	602	CLA	CAA-CBA-CGA-O1A
28	r	610	CLA	CAA-CBA-CGA-O1A
35	D	407	LHG	O10-C23-C24-C25
35	l	101	LHG	O9-C7-C8-C9
38	G	607	CHL	C2-C3-C5-C6
28	B	615	CLA	O1A-CGA-O2A-C1
28	d	401	CLA	C13-C15-C16-C17
28	B	610	CLA	C4B-C3B-CAB-CBB
28	c	507	CLA	C4B-C3B-CAB-CBB
35	D	407	LHG	C3-O3-P-O5
35	a	415	LHG	C3-O3-P-O5
35	b	621	LHG	C3-O3-P-O5
35	l	101	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
35	w	102	LHG	C4-O6-P-O5
38	g	601	CHL	C4B-C3B-CAB-CBB
38	g	608	CHL	C4B-C3B-CAB-CBB
33	d	407	PL9	C31-C32-C33-C34
31	L	101	SQD	C27-C28-C29-C30
32	C	520	LMG	C19-C20-C21-C22
35	B	622	LHG	C24-C25-C26-C27
35	C	521	LHG	C19-C20-C21-C22
28	B	607	CLA	CAA-CBA-CGA-O1A
28	N	614	CLA	CAA-CBA-CGA-O1A
28	R	608	CLA	CAA-CBA-CGA-O1A
28	R	610	CLA	CAA-CBA-CGA-O1A
28	r	612	CLA	CAA-CBA-CGA-O1A
36	C	519	DGD	O1A-C1A-C2A-C3A
28	S	312	CLA	O2A-C1-C2-C3
28	r	610	CLA	O2A-C1-C2-C3
28	s	612	CLA	CAA-CBA-CGA-O2A
35	A	416	LHG	O7-C7-C8-C9
38	g	601	CHL	C8-C10-C11-C12
38	y	309	CHL	C5-C6-C7-C8
40	r	616	NEX	C40-C33-C34-C35
35	a	415	LHG	C27-C28-C29-C30
41	R	615	XAT	C26-C27-C28-C29
41	r	615	XAT	C26-C27-C28-C29
35	w	102	LHG	O10-C23-C24-C25
32	A	413	LMG	C36-C37-C38-C39
28	A	408	CLA	CAA-CBA-CGA-O2A
32	d	409	LMG	O7-C10-C11-C12
35	R	616	LHG	O8-C23-C24-C25
28	A	406	CLA	C2A-CAA-CBA-CGA
28	B	610	CLA	CAA-CBA-CGA-O1A
28	C	505	CLA	O1A-CGA-O2A-C1
28	b	603	CLA	C13-C15-C16-C17
31	A	410	SQD	C13-C14-C15-C16
35	d	408	LHG	C10-C11-C12-C13
28	C	511	CLA	CAA-CBA-CGA-O2A
28	b	616	CLA	CAA-CBA-CGA-O2A
28	c	505	CLA	CAA-CBA-CGA-O2A
36	a	401	DGD	O1A-C1A-C2A-C3A
28	B	614	CLA	C4-C3-C5-C6
28	C	504	CLA	C2C-C3C-CAC-CBC
28	B	611	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	B	613	CLA	CAD-CBD-CGD-O1D
28	C	501	CLA	CAD-CBD-CGD-O1D
28	N	613	CLA	CAD-CBD-CGD-O1D
28	R	612	CLA	CAD-CBD-CGD-O1D
28	Y	614	CLA	CAD-CBD-CGD-O1D
28	a	406	CLA	CAD-CBD-CGD-O1D
28	b	605	CLA	CAD-CBD-CGD-O1D
28	c	511	CLA	CAD-CBD-CGD-O1D
28	s	613	CLA	CAD-CBD-CGD-O1D
35	g	618	LHG	C4-C5-O7-C7
31	a	414	SQD	C7-C8-C9-C10
28	G	613	CLA	CAA-CBA-CGA-O1A
35	Y	619	LHG	O10-C23-C24-C25
38	y	308	CHL	CAA-CBA-CGA-O1A
28	y	305	CLA	CAA-CBA-CGA-O2A
28	y	314	CLA	CAA-CBA-CGA-O2A
31	A	414	SQD	O47-C7-C8-C9
32	A	411	LMG	O7-C10-C11-C12
38	g	608	CHL	CAA-CBA-CGA-O2A
28	B	611	CLA	C5-C6-C7-C8
28	c	512	CLA	C5-C6-C7-C8
38	g	619	CHL	C8-C10-C11-C12
28	C	510	CLA	C11-C10-C8-C9
28	b	605	CLA	C6-C7-C8-C9
28	b	607	CLA	C14-C13-C15-C16
28	b	608	CLA	C11-C10-C8-C9
28	c	509	CLA	C11-C12-C13-C14
28	s	602	CLA	C11-C12-C13-C14
28	y	310	CLA	C11-C10-C8-C9
29	D	402	PHO	C6-C7-C8-C9
38	R	607	CHL	C6-C7-C8-C9
38	Y	601	CHL	C14-C13-C15-C16
38	n	608	CHL	C6-C7-C8-C9
32	D	408	LMG	C32-C33-C34-C35
35	n	618	LHG	C10-C11-C12-C13
32	c	521	LMG	C29-C30-C31-C32
28	S	304	CLA	CAA-CBA-CGA-O1A
28	S	311	CLA	C11-C10-C8-C9
28	R	603	CLA	C5-C6-C7-C8
38	N	607	CHL	C10-C11-C12-C13
28	g	610	CLA	O1A-CGA-O2A-C1
28	A	406	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	B	608	CLA	CAA-CBA-CGA-O2A
28	B	614	CLA	CAA-CBA-CGA-O2A
28	G	604	CLA	CAA-CBA-CGA-O2A
28	s	610	CLA	CAA-CBA-CGA-O2A
31	a	414	SQD	O47-C7-C8-C9
32	B	624	LMG	O8-C28-C29-C30
35	W	101	LHG	O8-C23-C24-C25
38	N	606	CHL	CAA-CBA-CGA-O2A
38	Y	608	CHL	CAA-CBA-CGA-O2A
38	g	609	CHL	CAA-CBA-CGA-O2A
38	n	607	CHL	CAA-CBA-CGA-O2A
28	d	405	CLA	CAA-CBA-CGA-O1A
35	r	617	LHG	C25-C26-C27-C28
35	y	319	LHG	C19-C20-C21-C22
28	B	604	CLA	CAA-CBA-CGA-O2A
28	C	505	CLA	CAA-CBA-CGA-O2A
28	G	611	CLA	CAA-CBA-CGA-O2A
28	N	613	CLA	CAA-CBA-CGA-O2A
28	b	608	CLA	CAA-CBA-CGA-O2A
28	b	609	CLA	CAA-CBA-CGA-O2A
28	c	511	CLA	CAA-CBA-CGA-O2A
28	s	613	CLA	CAA-CBA-CGA-O2A
35	B	625	LHG	O8-C23-C24-C25
35	S	317	LHG	O8-C23-C24-C25
35	a	415	LHG	O7-C7-C8-C9
35	n	618	LHG	O8-C23-C24-C25
28	c	508	CLA	C15-C16-C17-C18
28	n	602	CLA	C15-C16-C17-C18
35	l	101	LHG	C35-C36-C37-C38
32	b	620	LMG	O9-C10-C11-C12
38	n	608	CHL	CAA-CBA-CGA-O1A
38	r	607	CHL	CAA-CBA-CGA-O1A
32	w	101	LMG	C30-C31-C32-C33
28	b	614	CLA	C8-C10-C11-C12
28	b	609	CLA	O1A-CGA-O2A-C1
28	B	601	CLA	C6-C7-C8-C10
28	B	603	CLA	C11-C12-C13-C15
28	B	611	CLA	C3A-C2A-CAA-CBA
28	B	615	CLA	C11-C10-C8-C7
28	C	503	CLA	C6-C7-C8-C10
28	C	505	CLA	C2-C3-C5-C6
28	C	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	G	613	CLA	C11-C10-C8-C7
28	b	605	CLA	C2-C3-C5-C6
28	b	607	CLA	C11-C12-C13-C15
28	b	611	CLA	C3A-C2A-CAA-CBA
28	b	614	CLA	C11-C10-C8-C7
28	c	503	CLA	C6-C7-C8-C10
28	c	503	CLA	C11-C12-C13-C15
28	r	604	CLA	C3A-C2A-CAA-CBA
28	s	602	CLA	C11-C12-C13-C15
28	y	313	CLA	C11-C10-C8-C7
38	g	619	CHL	C2-C3-C5-C6
28	G	604	CLA	CAA-CBA-CGA-O1A
32	D	408	LMG	O9-C10-C11-C12
35	g	618	LHG	O10-C23-C24-C25
38	G	607	CHL	CAA-CBA-CGA-O1A
38	Y	608	CHL	CAA-CBA-CGA-O1A
38	g	606	CHL	CAA-CBA-CGA-O1A
28	s	603	CLA	CAA-CBA-CGA-O2A
28	B	609	CLA	CAA-CBA-CGA-O2A
28	R	612	CLA	CAA-CBA-CGA-O2A
28	S	313	CLA	CAA-CBA-CGA-O2A
28	S	314	CLA	CAA-CBA-CGA-O2A
28	Y	613	CLA	CAA-CBA-CGA-O2A
28	g	613	CLA	CAA-CBA-CGA-O2A
32	C	520	LMG	O7-C10-C11-C12
35	c	519	LHG	O8-C23-C24-C25
38	N	601	CHL	CAA-CBA-CGA-O2A
38	g	606	CHL	CAA-CBA-CGA-O2A
35	s	617	LHG	C35-C36-C37-C38
36	B	626	DGD	C6B-C7B-C8B-C9B
31	a	411	SQD	C7-C8-C9-C10
39	y	315	LUT	C7-C8-C9-C10
40	Y	618	NEX	C11-C12-C13-C14
32	C	520	LMG	O9-C10-C11-C12
32	k	102	LMG	O9-C10-C11-C12
35	s	617	LHG	O10-C23-C24-C25
38	g	608	CHL	CAA-CBA-CGA-O1A
39	n	616	LUT	C9-C10-C11-C12
36	A	417	DGD	C2A-C3A-C4A-C5A
28	G	603	CLA	CAA-CBA-CGA-O2A
28	N	611	CLA	CAA-CBA-CGA-O2A
28	c	502	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	n	604	CLA	CAA-CBA-CGA-O2A
35	D	407	LHG	O7-C7-C8-C9
38	Y	607	CHL	CAA-CBA-CGA-O2A
36	c	516	DGD	C2A-C3A-C4A-C5A
28	b	611	CLA	C10-C11-C12-C13
38	G	601	CHL	C10-C11-C12-C13
38	g	619	CHL	C10-C11-C12-C13
28	B	604	CLA	CAA-CBA-CGA-O1A
28	C	505	CLA	CAA-CBA-CGA-O1A
28	G	611	CLA	CAA-CBA-CGA-O1A
28	N	613	CLA	CAA-CBA-CGA-O1A
28	R	612	CLA	CAA-CBA-CGA-O1A
28	n	604	CLA	CAA-CBA-CGA-O1A
35	B	622	LHG	O10-C23-C24-C25
35	B	625	LHG	O10-C23-C24-C25
35	R	616	LHG	O10-C23-C24-C25
35	c	519	LHG	O10-C23-C24-C25
38	G	608	CHL	CAA-CBA-CGA-O1A
38	n	607	CHL	CAA-CBA-CGA-O1A
32	C	522	LMG	C4-C5-C6-O5
38	g	608	CHL	C10-C11-C12-C13
33	D	406	PL9	C31-C32-C33-C34
28	C	512	CLA	CAA-CBA-CGA-O2A
28	y	304	CLA	CAA-CBA-CGA-O2A
28	y	313	CLA	CAA-CBA-CGA-O2A
32	k	102	LMG	O7-C10-C11-C12
28	N	610	CLA	C13-C15-C16-C17
28	b	608	CLA	C5-C6-C7-C8
31	a	411	SQD	O49-C7-C8-C9
32	B	621	LMG	O10-C28-C29-C30
35	A	416	LHG	O9-C7-C8-C9
38	g	609	CHL	CAA-CBA-CGA-O1A
38	n	605	CHL	CAA-CBA-CGA-O1A
28	N	614	CLA	C2A-CAA-CBA-CGA
28	b	609	CLA	C2A-CAA-CBA-CGA
28	Y	612	CLA	C5-C6-C7-C8
28	b	606	CLA	C10-C11-C12-C13
28	c	504	CLA	C5-C6-C7-C8
28	B	615	CLA	CBA-CGA-O2A-C1
28	C	505	CLA	CBA-CGA-O2A-C1
32	d	409	LMG	C30-C31-C32-C33
28	A	406	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	B	608	CLA	CAA-CBA-CGA-O1A
28	B	614	CLA	CAA-CBA-CGA-O1A
28	S	313	CLA	CAA-CBA-CGA-O1A
28	R	613	CLA	CAA-CBA-CGA-O2A
28	S	310	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

327 monomers are involved in 3043 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	r	612	CLA	11	0
30	K	101	BCR	13	0
38	R	607	CHL	4	0
32	A	413	LMG	11	0
38	N	609	CHL	19	0
36	B	626	DGD	11	0
35	l	101	LHG	5	0
30	a	410	BCR	22	0
30	A	409	BCR	12	0
28	Y	602	CLA	11	0
28	s	603	CLA	7	0
28	G	610	CLA	30	0
38	g	608	CHL	14	0
30	k	101	BCR	16	0
35	Y	619	LHG	5	0
28	d	405	CLA	9	0
28	C	513	CLA	13	0
28	s	604	CLA	11	0
28	B	606	CLA	16	0
28	S	311	CLA	16	0
28	g	610	CLA	15	0
28	n	611	CLA	13	0
38	r	605	CHL	17	0
28	b	616	CLA	16	0
36	a	401	DGD	17	0
28	r	604	CLA	11	0
28	r	602	CLA	7	0
38	N	607	CHL	13	0
38	y	308	CHL	13	0
28	N	612	CLA	17	0
31	A	410	SQD	9	0
28	G	614	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	603	CLA	14	0
28	d	401	CLA	16	0
38	n	601	CHL	11	0
28	s	602	CLA	16	0
28	G	604	CLA	7	0
37	E	101	HEM	7	0
41	y	317	XAT	11	0
32	A	411	LMG	20	0
39	S	315	LUT	24	0
36	A	417	DGD	10	0
35	a	415	LHG	10	0
35	d	408	LHG	12	0
38	G	607	CHL	11	0
38	r	606	CHL	11	0
35	R	616	LHG	5	0
38	N	605	CHL	10	0
35	G	618	LHG	7	0
30	B	617	BCR	16	0
31	L	103	SQD	10	0
28	C	505	CLA	15	0
28	G	602	CLA	10	0
28	R	610	CLA	9	0
28	Y	611	CLA	12	0
28	B	608	CLA	11	0
38	s	606	CHL	10	0
28	G	611	CLA	13	0
28	G	613	CLA	23	0
28	b	608	CLA	18	0
31	B	620	SQD	12	0
36	C	517	DGD	7	0
32	C	522	LMG	7	0
28	g	602	CLA	18	0
28	c	513	CLA	12	0
38	Y	608	CHL	12	0
39	g	616	LUT	18	0
28	y	304	CLA	28	0
28	a	406	CLA	13	0
28	Y	604	CLA	14	0
32	k	102	LMG	15	0
30	b	617	BCR	9	0
35	b	621	LHG	3	0
38	Y	605	CHL	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	407	LHG	13	0
38	G	605	CHL	10	0
35	g	618	LHG	9	0
38	g	607	CHL	5	0
39	s	615	LUT	17	0
31	L	101	SQD	11	0
28	B	610	CLA	5	0
32	C	520	LMG	17	0
32	c	521	LMG	15	0
40	N	617	NEX	9	0
28	r	603	CLA	18	0
28	b	610	CLA	13	0
38	r	607	CHL	13	0
32	D	408	LMG	15	0
28	B	615	CLA	12	0
31	a	411	SQD	20	0
30	C	514	BCR	18	0
28	Y	603	CLA	16	0
28	c	501	CLA	15	0
28	G	603	CLA	10	0
35	b	624	LHG	10	0
35	A	416	LHG	4	0
38	G	608	CHL	19	0
28	r	613	CLA	19	0
30	b	619	BCR	10	0
28	B	614	CLA	15	0
28	C	507	CLA	21	0
28	s	612	CLA	10	0
40	G	617	NEX	11	0
28	a	409	CLA	11	0
28	b	605	CLA	14	0
28	b	614	CLA	12	0
28	R	609	CLA	14	0
28	n	604	CLA	6	0
28	y	312	CLA	16	0
40	s	616	NEX	7	0
28	N	614	CLA	6	0
39	Y	615	LUT	8	0
28	s	611	CLA	8	0
39	G	615	LUT	28	0
35	N	618	LHG	8	0
38	n	607	CHL	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	504	CLA	10	0
35	S	317	LHG	21	0
28	c	512	CLA	10	0
28	N	602	CLA	21	0
30	d	406	BCR	20	0
38	s	607	CHL	5	0
28	c	510	CLA	11	0
30	h	101	BCR	19	0
28	C	511	CLA	16	0
28	r	601	CLA	9	0
28	B	602	CLA	12	0
38	n	609	CHL	21	0
28	y	303	CLA	7	0
28	b	606	CLA	17	0
40	y	301	NEX	4	0
28	b	602	CLA	8	0
28	C	502	CLA	11	0
28	B	613	CLA	16	0
38	S	308	CHL	9	0
28	R	613	CLA	15	0
38	g	601	CHL	23	0
40	g	617	NEX	9	0
35	B	622	LHG	8	0
28	D	403	CLA	7	0
35	y	319	LHG	6	0
35	b	622	LHG	10	0
28	c	511	CLA	17	0
28	r	610	CLA	8	0
37	f	101	HEM	6	0
28	a	407	CLA	8	0
36	c	516	DGD	12	0
28	y	305	CLA	6	0
28	B	607	CLA	8	0
30	B	619	BCR	21	0
35	S	301	LHG	5	0
38	N	601	CHL	13	0
28	b	607	CLA	8	0
38	y	306	CHL	8	0
30	D	405	BCR	11	0
38	Y	607	CHL	31	0
28	Y	612	CLA	13	0
38	S	306	CHL	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	N	613	CLA	7	0
38	g	606	CHL	18	0
38	y	307	CHL	10	0
28	S	303	CLA	23	0
28	G	612	CLA	19	0
38	R	605	CHL	11	0
28	c	504	CLA	16	0
39	g	615	LUT	18	0
32	b	620	LMG	14	0
28	C	512	CLA	17	0
28	N	604	CLA	10	0
30	c	515	BCR	11	0
29	A	407	PHO	9	0
38	S	302	CHL	15	0
28	g	614	CLA	7	0
35	C	521	LHG	11	0
28	A	405	CLA	6	0
39	N	615	LUT	10	0
39	y	315	LUT	11	0
36	C	518	DGD	28	0
38	y	309	CHL	24	0
39	G	616	LUT	11	0
28	r	608	CLA	19	0
41	R	615	XAT	13	0
28	Y	610	CLA	6	0
39	r	614	LUT	15	0
30	t	101	BCR	10	0
28	B	604	CLA	7	0
35	r	617	LHG	5	0
28	n	612	CLA	15	0
30	C	515	BCR	10	0
30	i	101	BCR	8	0
32	a	413	LMG	14	0
31	A	414	SQD	14	0
29	d	402	PHO	12	0
28	g	613	CLA	8	0
38	G	609	CHL	15	0
38	g	619	CHL	20	0
33	d	407	PL9	6	0
36	C	519	DGD	20	0
40	Y	618	NEX	9	0
35	B	625	LHG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	R	606	CHL	12	0
28	A	406	CLA	9	0
28	s	608	CLA	8	0
38	n	608	CHL	13	0
39	R	614	LUT	14	0
28	C	503	CLA	9	0
35	s	617	LHG	16	0
28	n	610	CLA	24	0
28	s	613	CLA	5	0
32	b	623	LMG	8	0
28	N	610	CLA	15	0
28	S	312	CLA	12	0
28	Y	614	CLA	7	0
35	L	102	LHG	6	0
38	Y	606	CHL	10	0
28	R	603	CLA	9	0
35	n	618	LHG	6	0
39	S	316	LUT	19	0
38	N	608	CHL	16	0
28	R	612	CLA	12	0
28	S	310	CLA	26	0
38	g	609	CHL	14	0
28	r	611	CLA	5	0
28	N	611	CLA	13	0
28	y	314	CLA	6	0
38	g	605	CHL	11	0
28	d	404	CLA	9	0
28	R	611	CLA	5	0
28	R	601	CLA	12	0
28	S	304	CLA	11	0
28	C	501	CLA	13	0
39	y	316	LUT	6	0
28	b	615	CLA	17	0
28	B	603	CLA	21	0
29	D	402	PHO	9	0
29	a	408	PHO	12	0
28	B	612	CLA	10	0
28	B	616	CLA	16	0
38	s	605	CHL	9	0
35	c	519	LHG	5	0
28	Y	613	CLA	13	0
28	g	603	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	s	601	CHL	14	0
28	S	314	CLA	6	0
30	C	516	BCR	22	0
28	B	611	CLA	15	0
32	w	101	LMG	13	0
35	w	102	LHG	8	0
35	W	101	LHG	20	0
28	b	611	CLA	15	0
30	c	514	BCR	19	0
28	c	503	CLA	9	0
41	Y	617	XAT	17	0
41	r	615	XAT	9	0
28	S	309	CLA	13	0
33	D	406	PL9	8	0
28	c	508	CLA	11	0
28	N	603	CLA	10	0
28	S	313	CLA	9	0
28	n	603	CLA	23	0
28	c	509	CLA	7	0
38	G	606	CHL	11	0
28	B	605	CLA	19	0
28	b	612	CLA	15	0
28	R	604	CLA	11	0
28	R	602	CLA	9	0
28	b	609	CLA	12	0
31	M	101	SQD	5	0
28	B	601	CLA	14	0
30	T	101	BCR	13	0
39	Y	616	LUT	7	0
40	n	617	NEX	8	0
28	D	404	CLA	9	0
28	y	313	CLA	10	0
28	b	613	CLA	12	0
28	n	613	CLA	12	0
28	r	609	CLA	19	0
38	Y	601	CHL	16	0
28	y	310	CLA	11	0
28	y	311	CLA	12	0
28	S	305	CLA	8	0
39	n	615	LUT	14	0
28	c	505	CLA	10	0
28	b	604	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	G	601	CHL	12	0
32	d	409	LMG	20	0
31	a	414	SQD	10	0
28	B	609	CLA	13	0
35	c	520	LHG	9	0
30	b	618	BCR	15	0
28	b	601	CLA	16	0
28	g	604	CLA	14	0
28	g	612	CLA	10	0
38	Y	609	CHL	15	0
28	c	502	CLA	6	0
36	c	518	DGD	15	0
32	B	621	LMG	18	0
28	g	611	CLA	5	0
32	B	624	LMG	5	0
39	N	616	LUT	17	0
38	n	606	CHL	12	0
28	c	506	CLA	12	0
28	C	506	CLA	23	0
39	s	614	LUT	16	0
38	y	302	CHL	13	0
28	A	408	CLA	16	0
38	N	606	CHL	11	0
30	H	101	BCR	14	0
40	y	318	NEX	6	0
28	c	507	CLA	15	0
28	C	508	CLA	18	0
38	n	605	CHL	12	0
28	n	602	CLA	15	0
28	D	401	CLA	7	0
28	C	509	CLA	13	0
28	s	609	CLA	18	0
30	B	618	BCR	14	0
40	r	616	NEX	13	0
28	C	510	CLA	16	0
28	s	610	CLA	7	0
39	n	616	LUT	7	0
36	b	625	DGD	11	0
36	c	517	DGD	18	0
28	n	614	CLA	3	0
28	R	608	CLA	20	0
35	B	623	LHG	14	0

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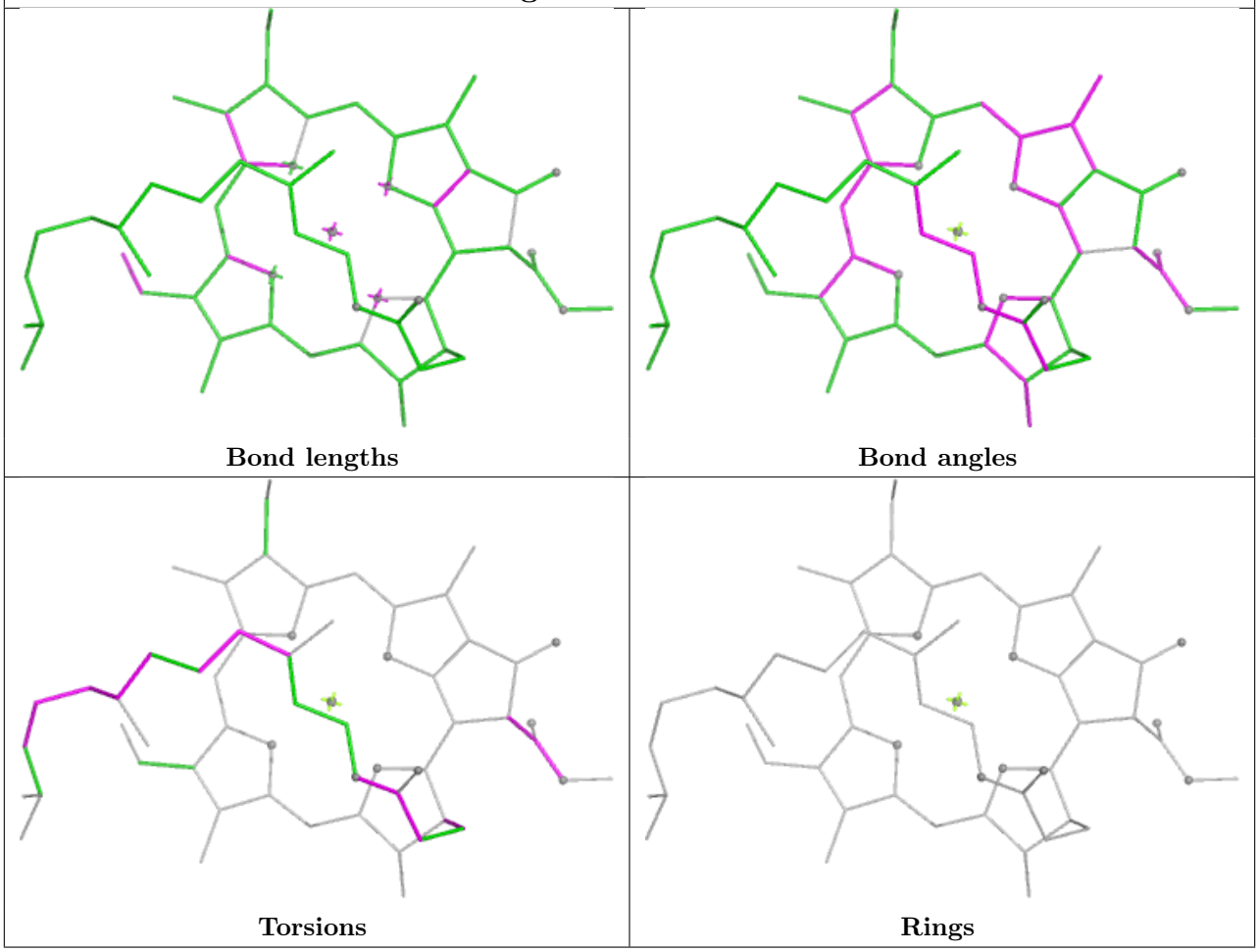
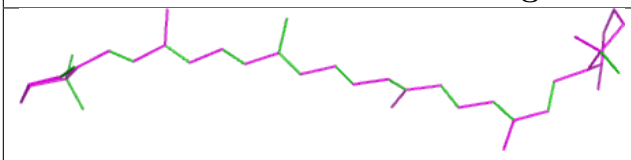
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	S	307	CHL	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA r 612



Ligand BCR K 101



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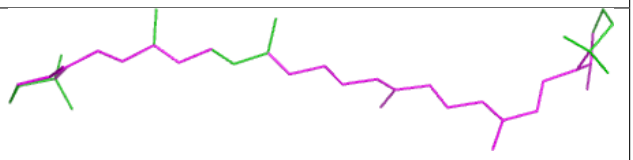

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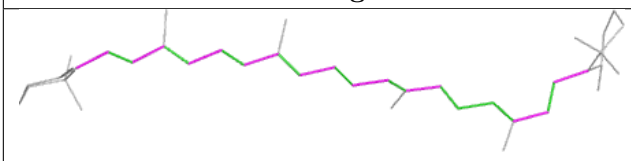
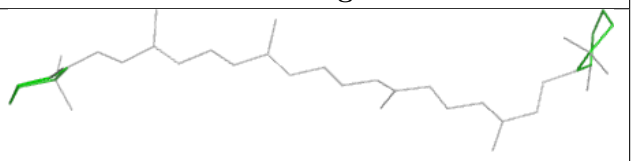
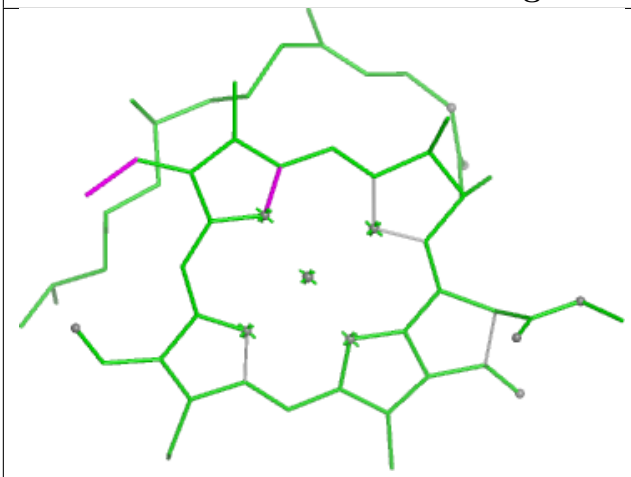


Torsions



Rings

Ligand CHL R 607



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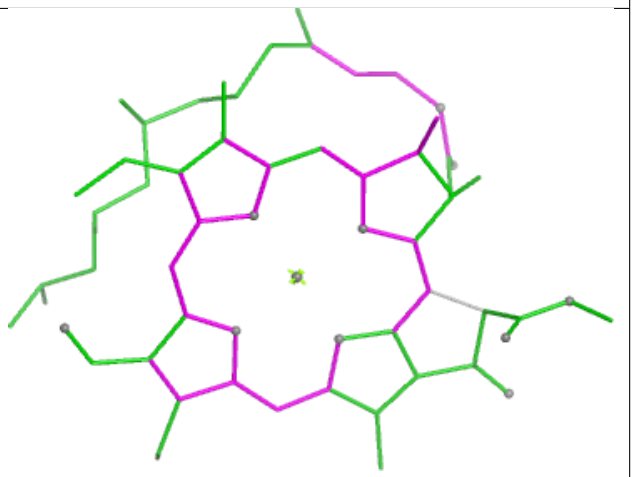
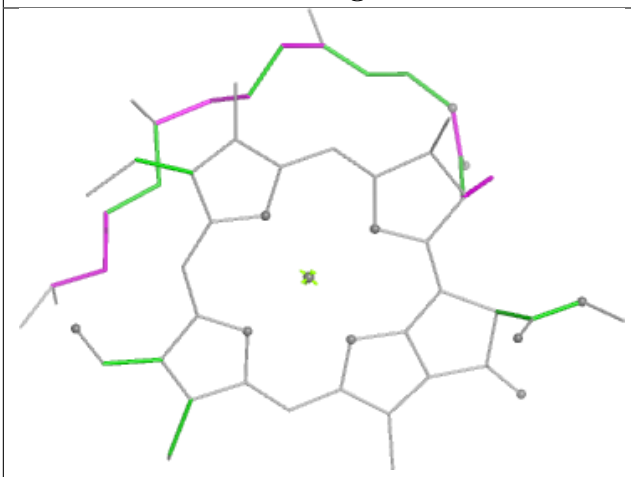
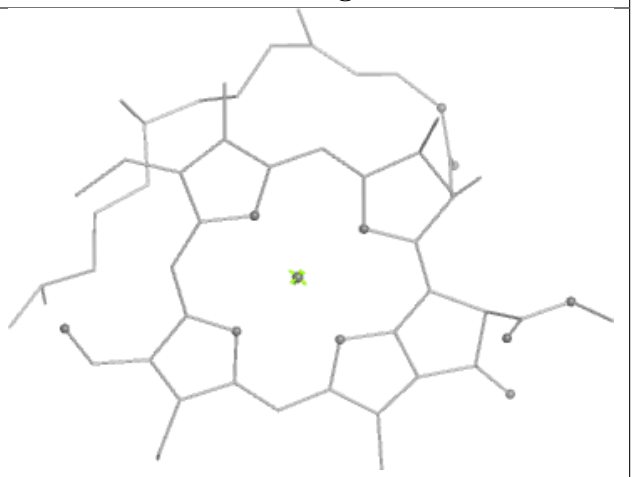


Bond angles

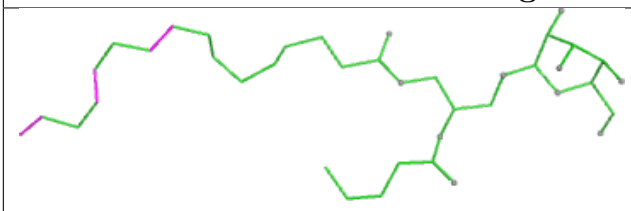


Torsions



Rings

Ligand LMG A 413



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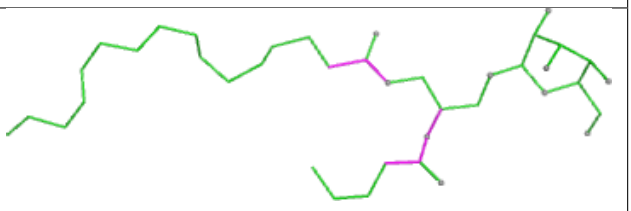

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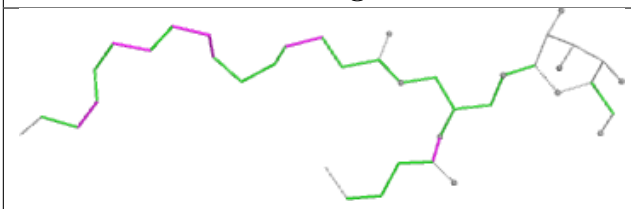

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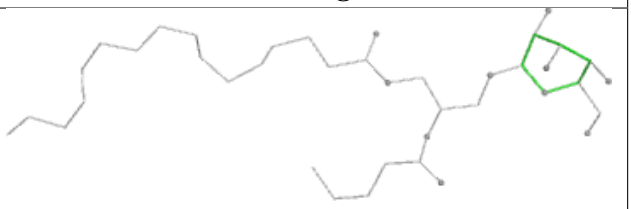
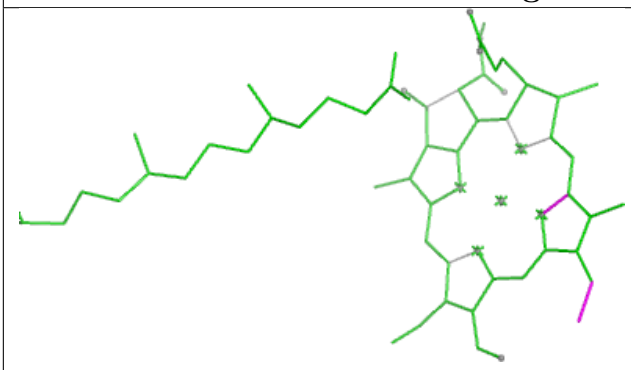


Rings

Ligand CHL N 609



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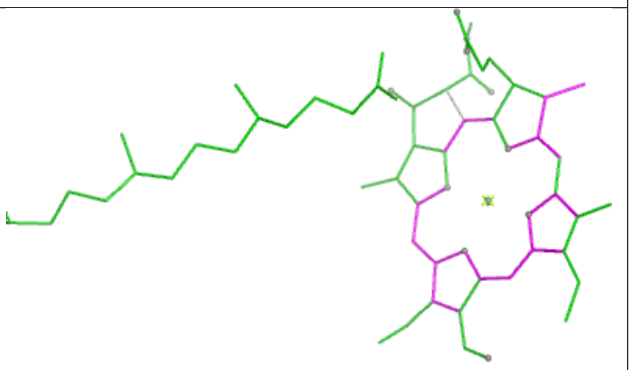

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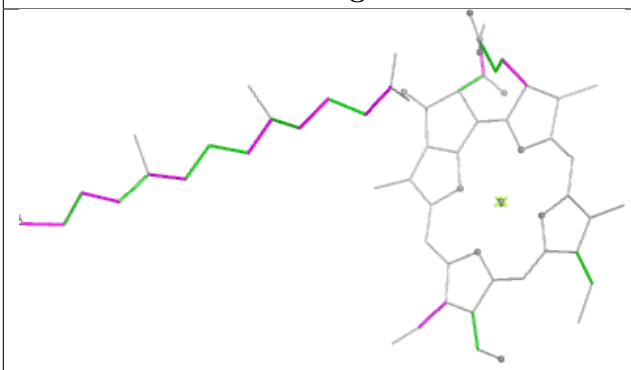

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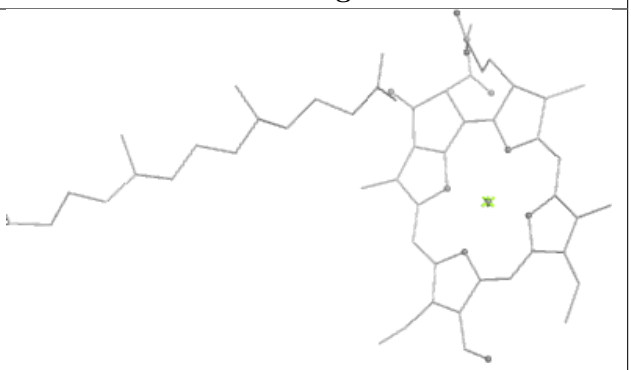
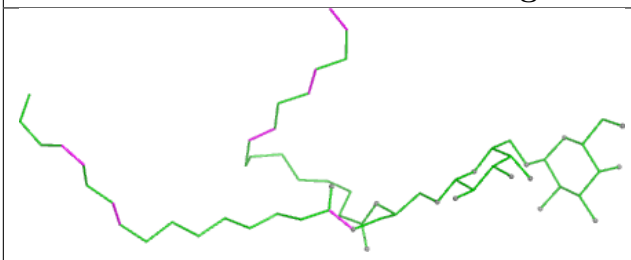


Rings

Ligand DGD B 626



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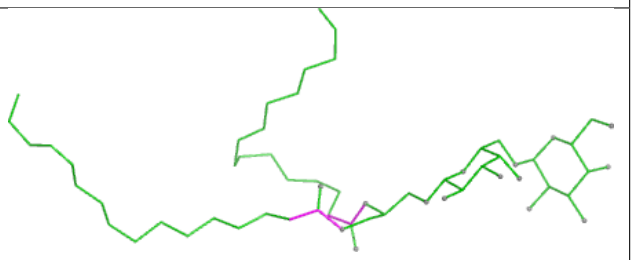

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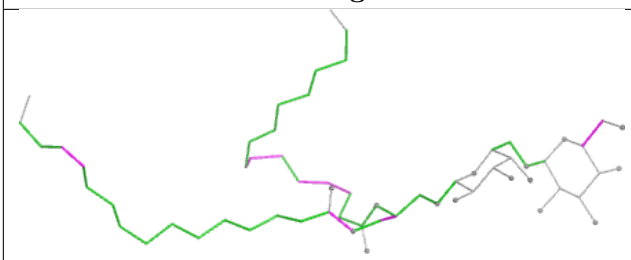

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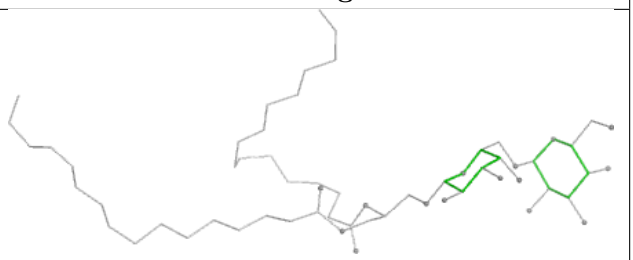


Rings

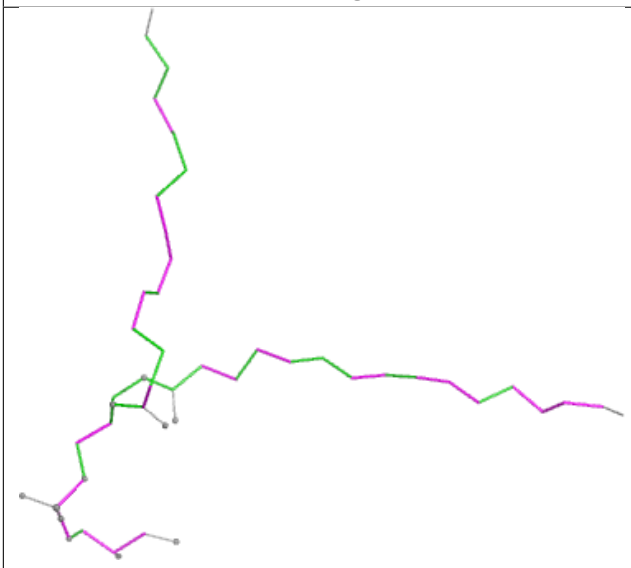
Ligand LHG l 101



Bond lengths



Bond angles

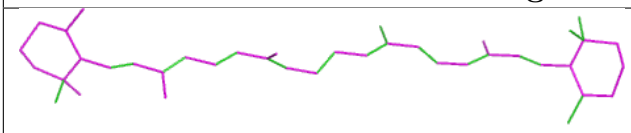


Torsions



Rings

Ligand BCR a 410



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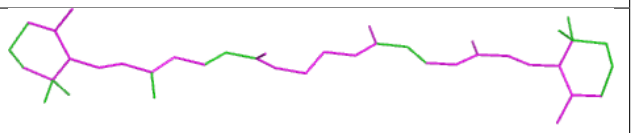

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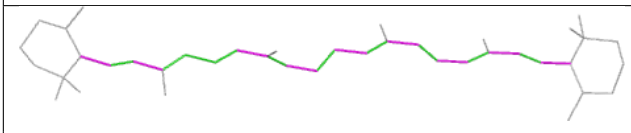

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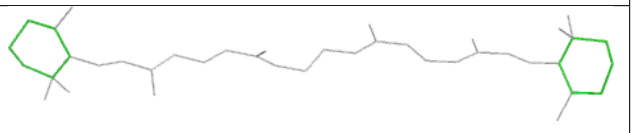

Rings

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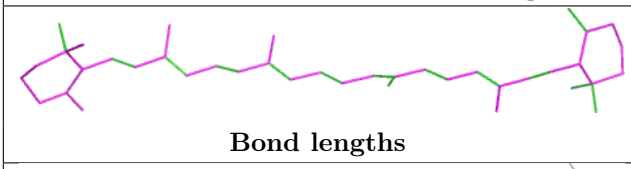

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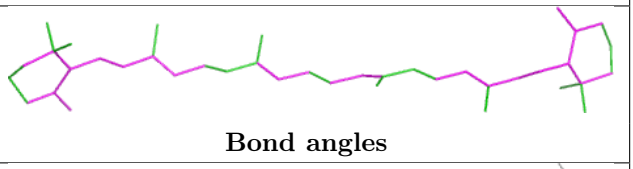

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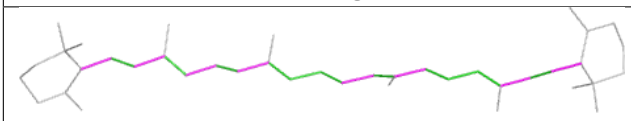

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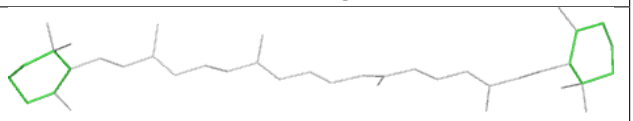
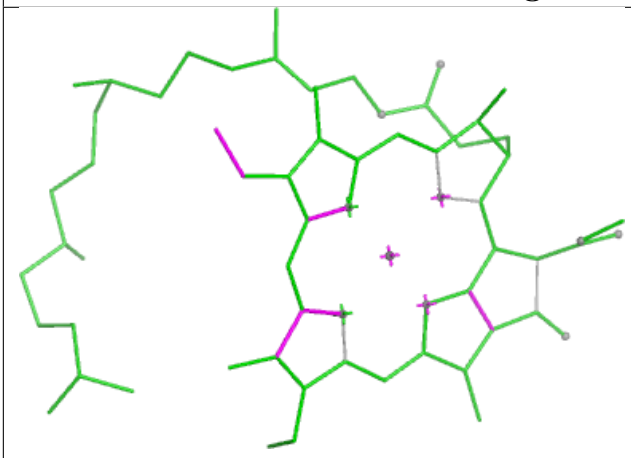


Rings

Ligand CLA Y 602



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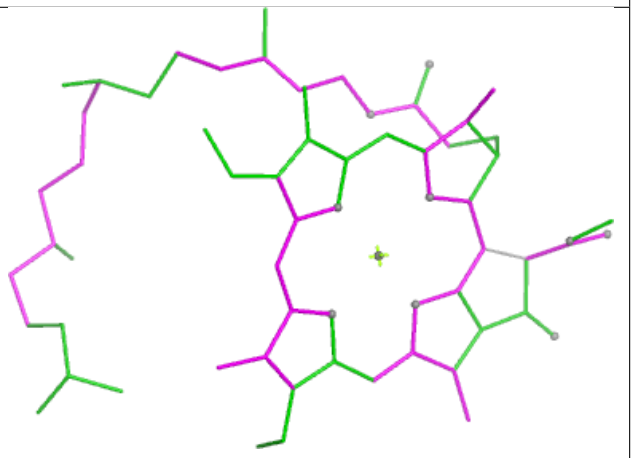

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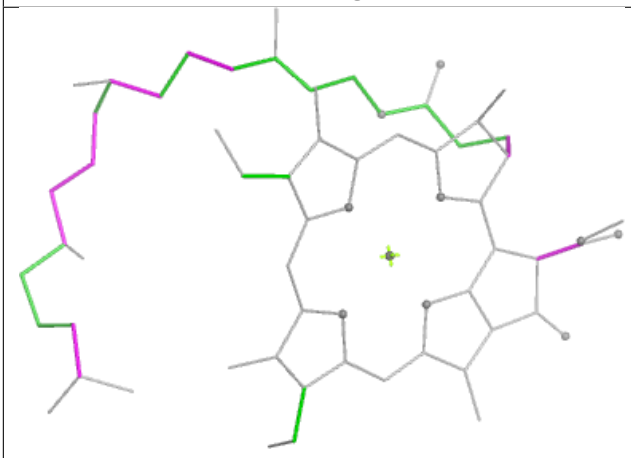

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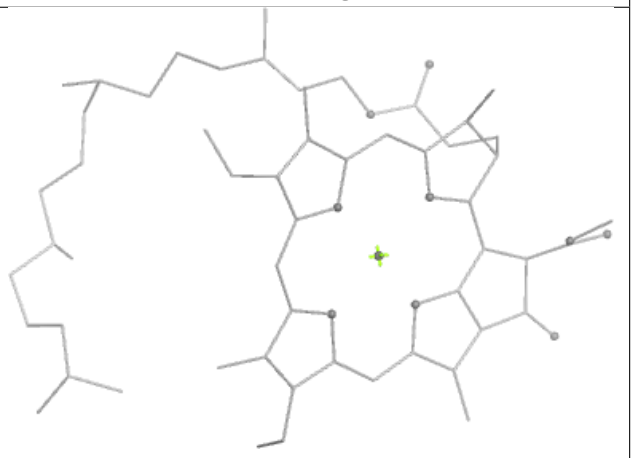
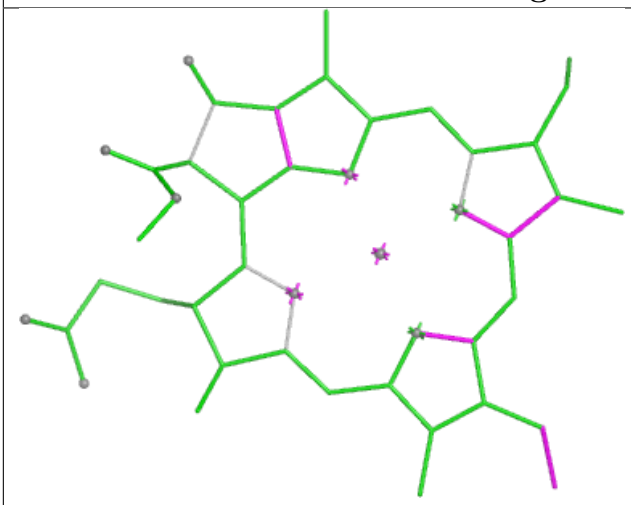


Rings

Ligand CLA s 603



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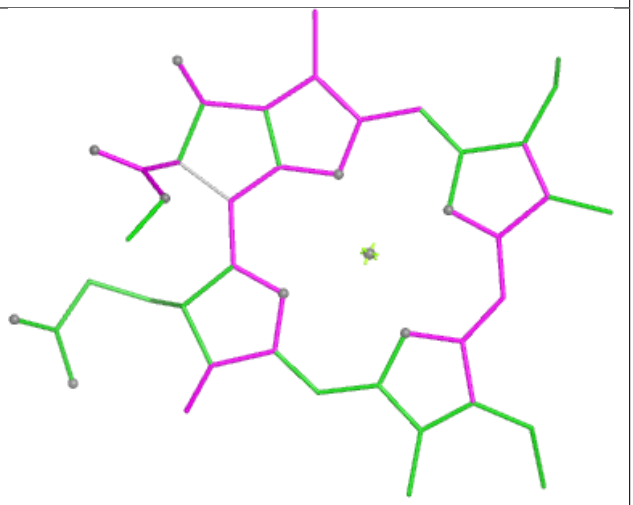

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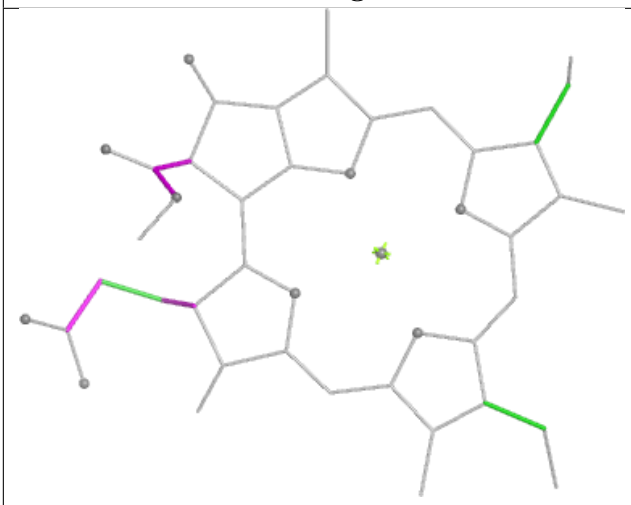

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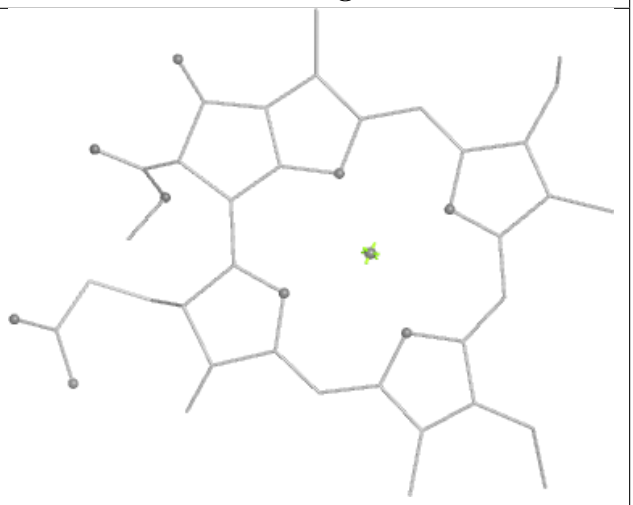

Rings

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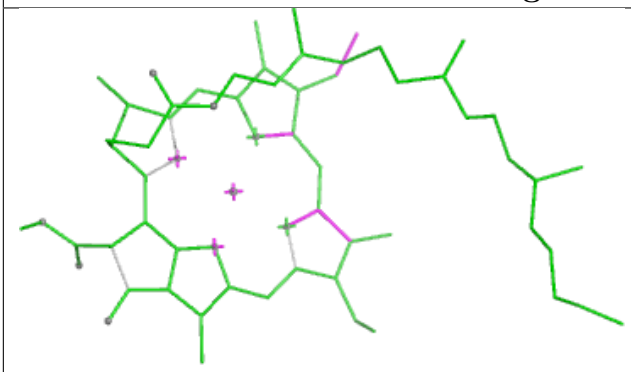

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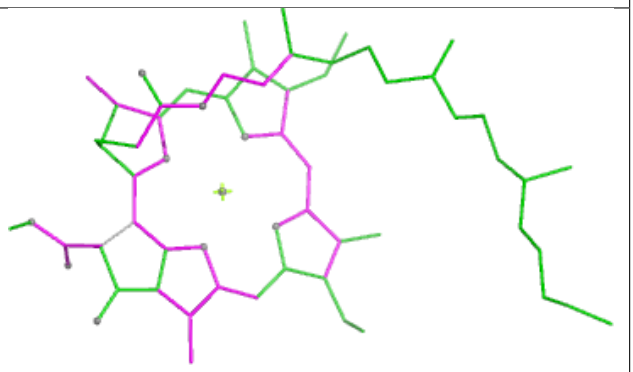

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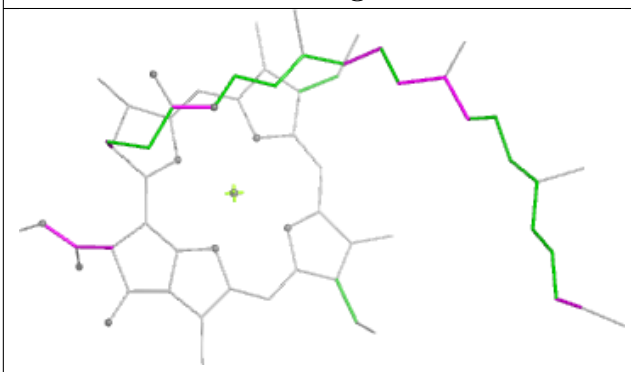

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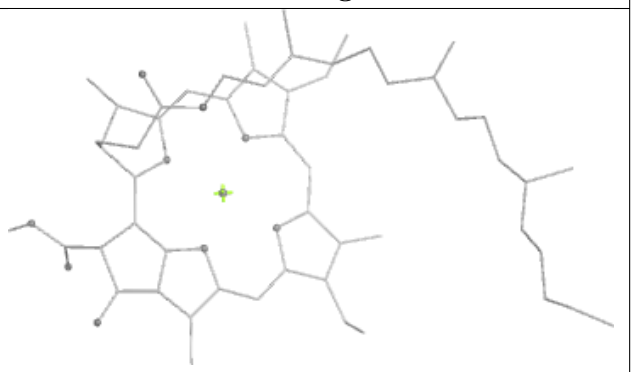
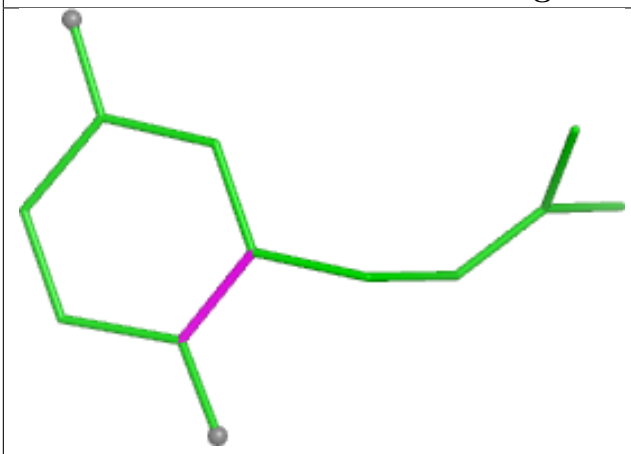


Rings

Ligand PL9 a 412



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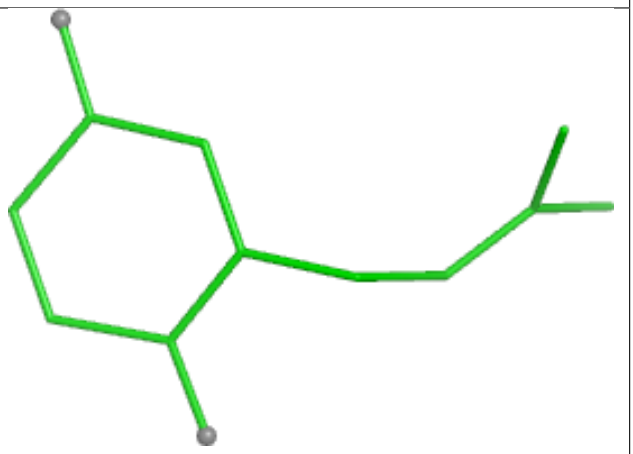

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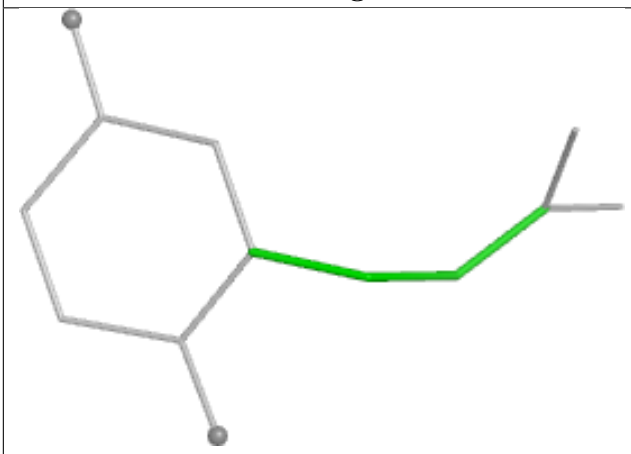

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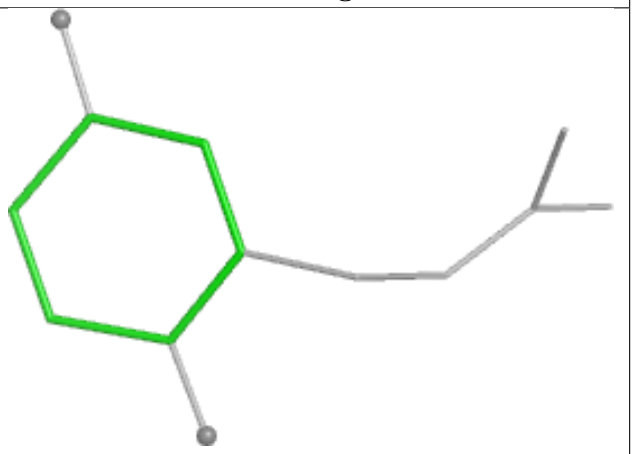
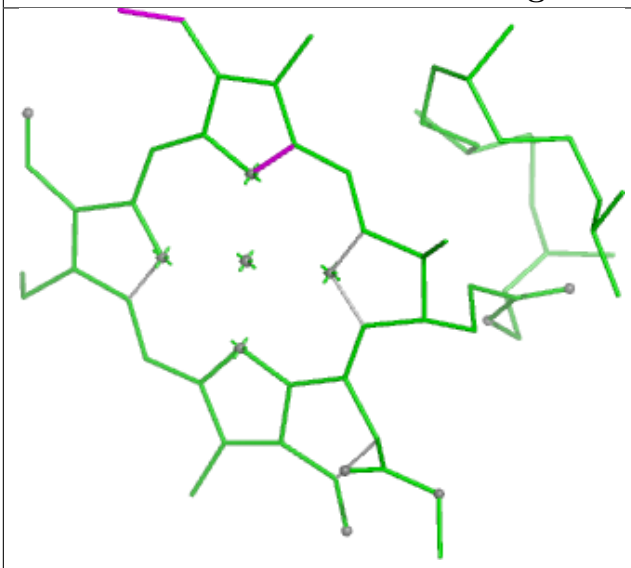


Rings

Ligand CHL g 608



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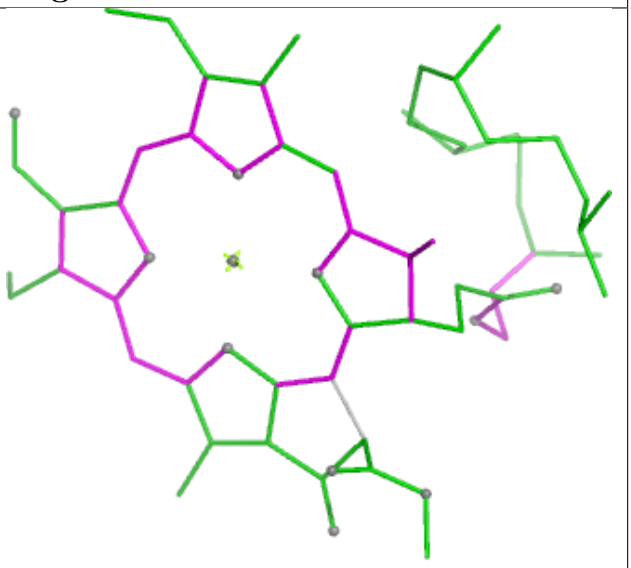
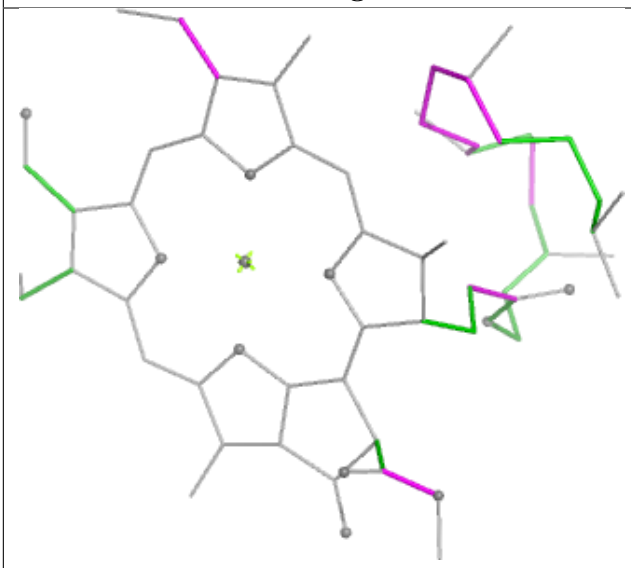


Bond angles



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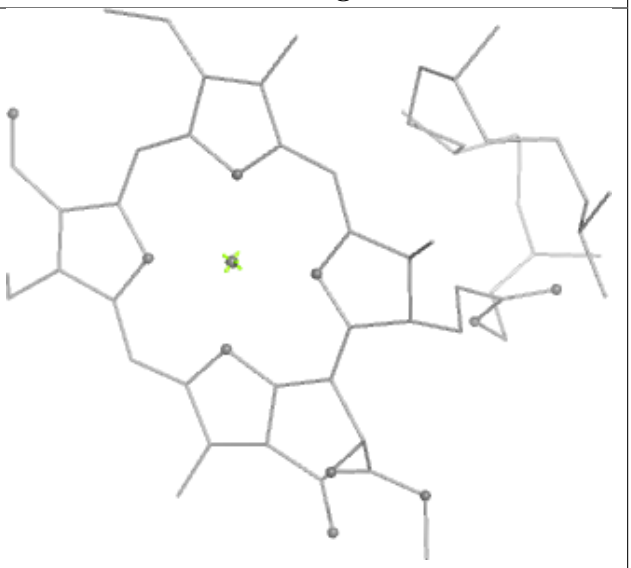
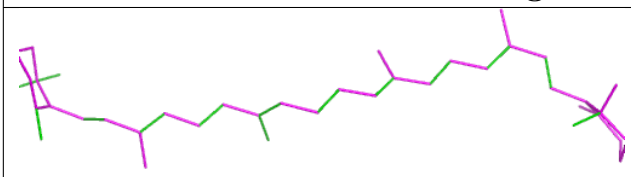
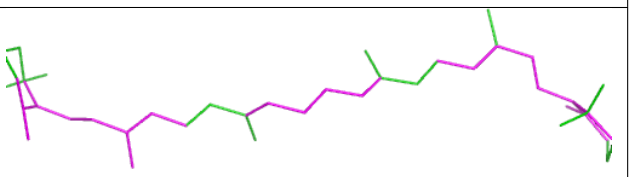


Rings

Ligand BCR k 101



Bond lengths



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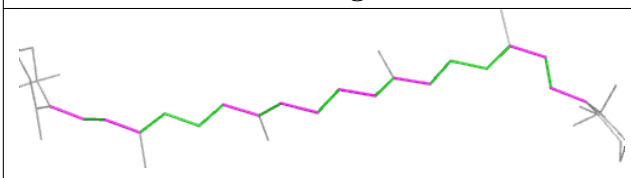
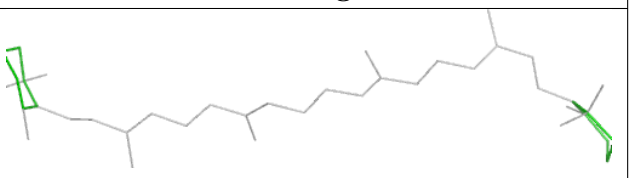


Torsions



Rings

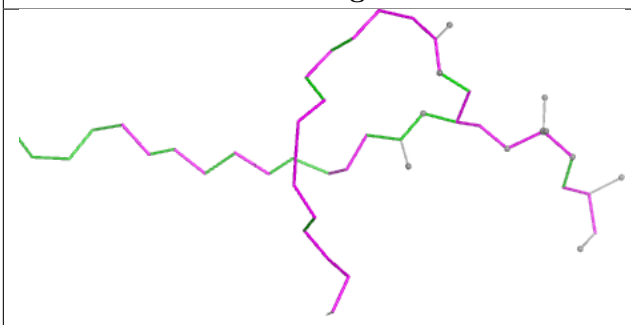
Ligand LHG Y 619



Bond lengths



Bond angles

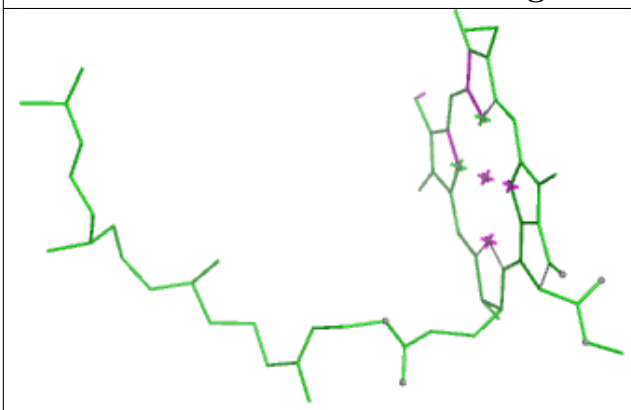


Torsions



Rings

Ligand CLA d 405



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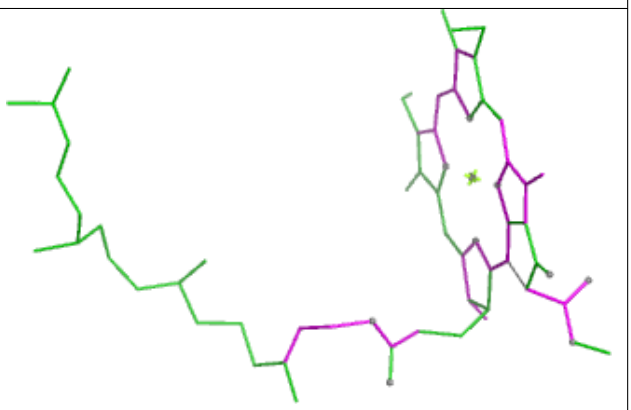

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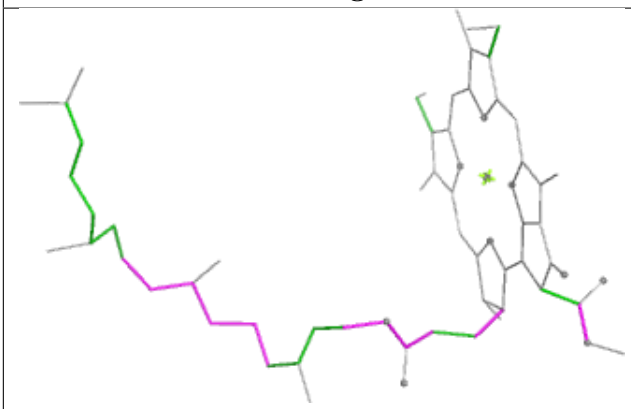

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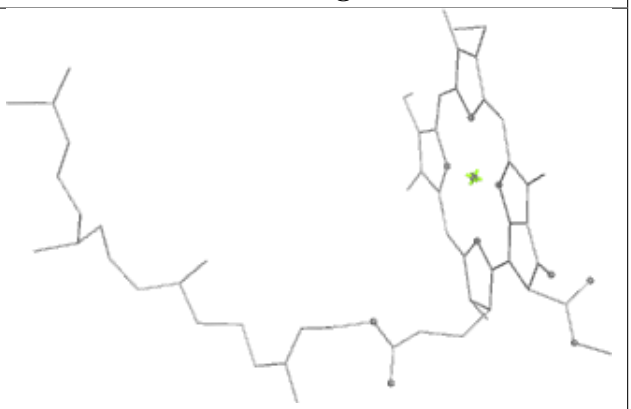
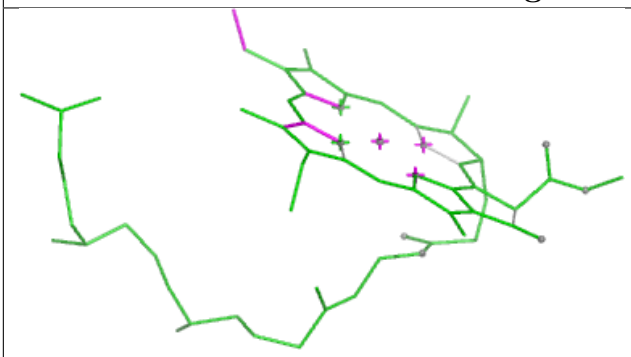


Rings

Ligand CLA C 513



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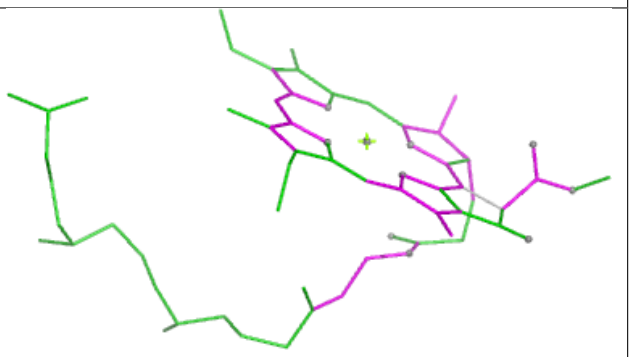
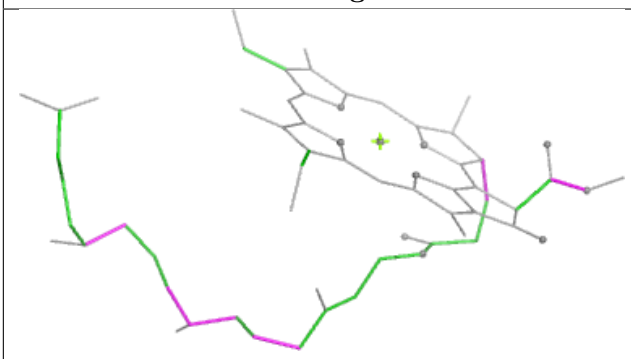


Bond angles



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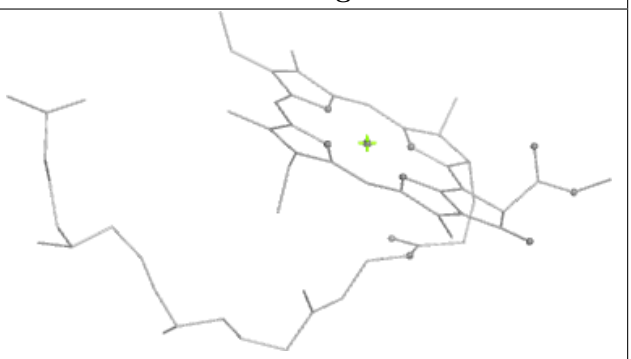

Rings

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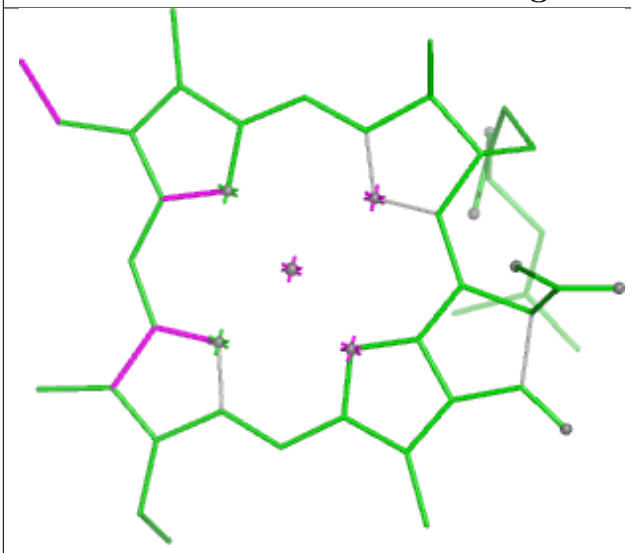

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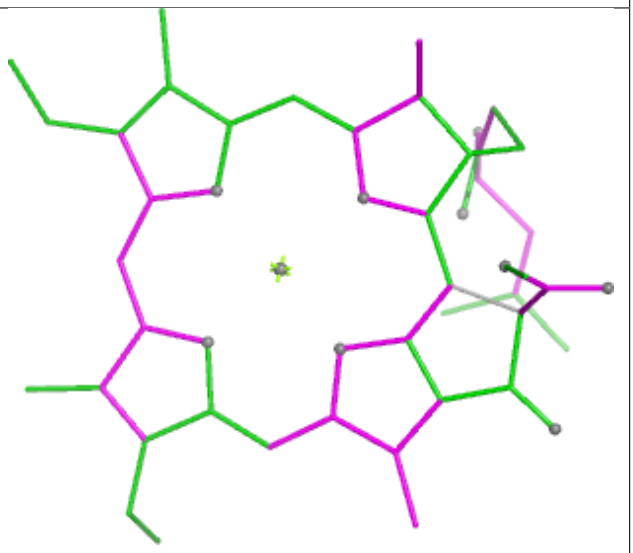

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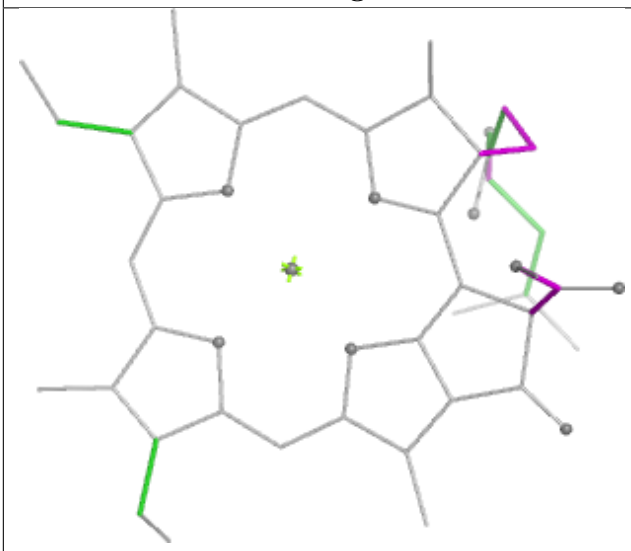

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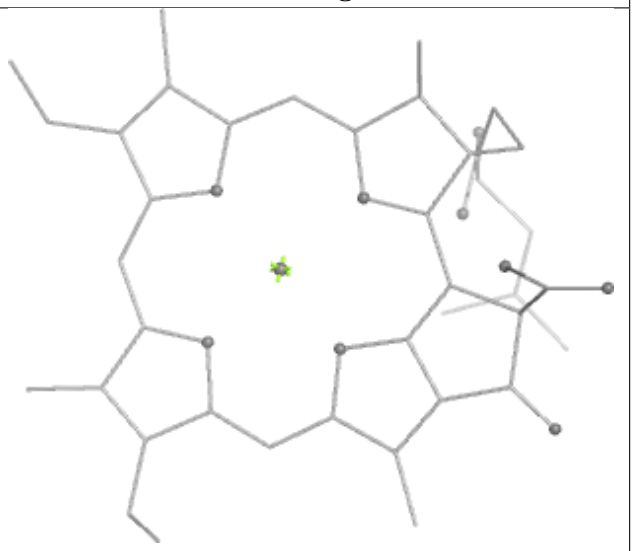
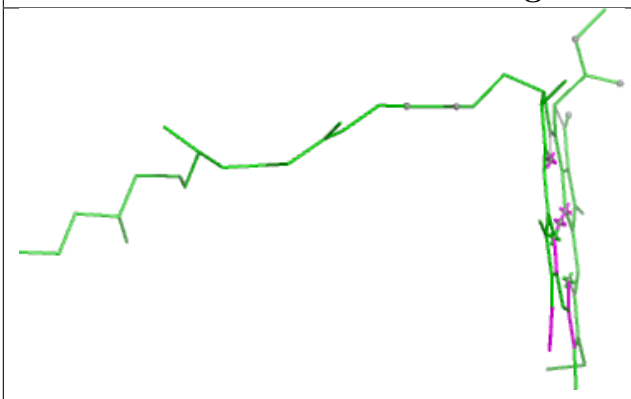


Rings

Ligand CLA B 606



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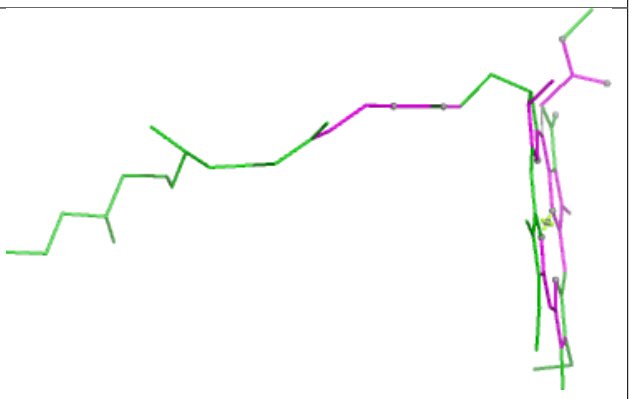

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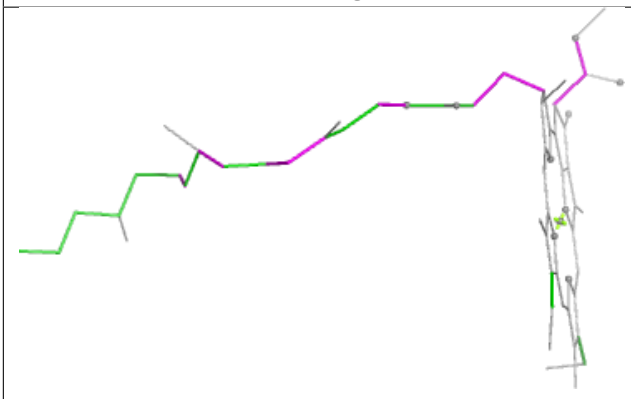

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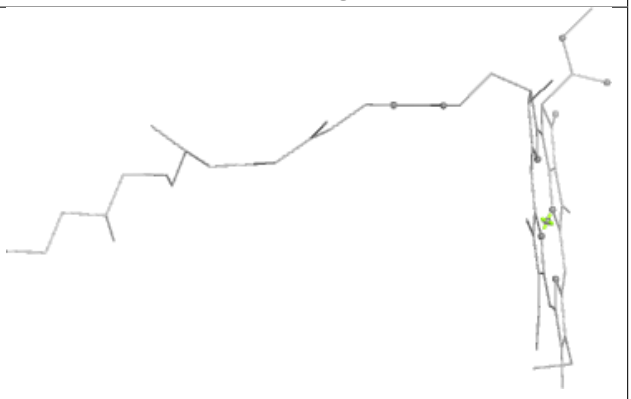
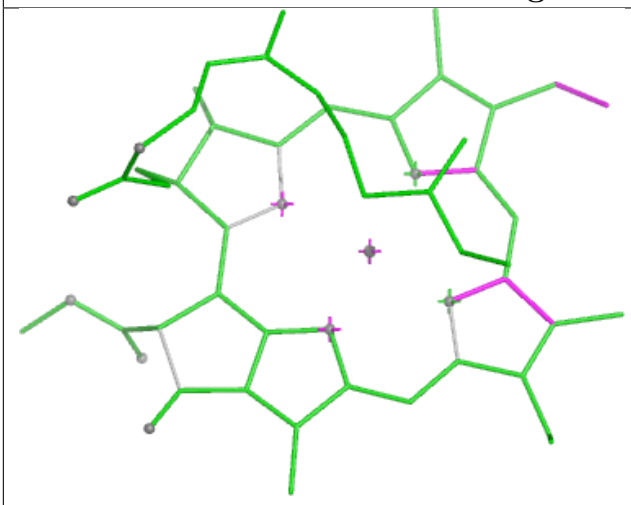


Rings

Ligand CLA S 311



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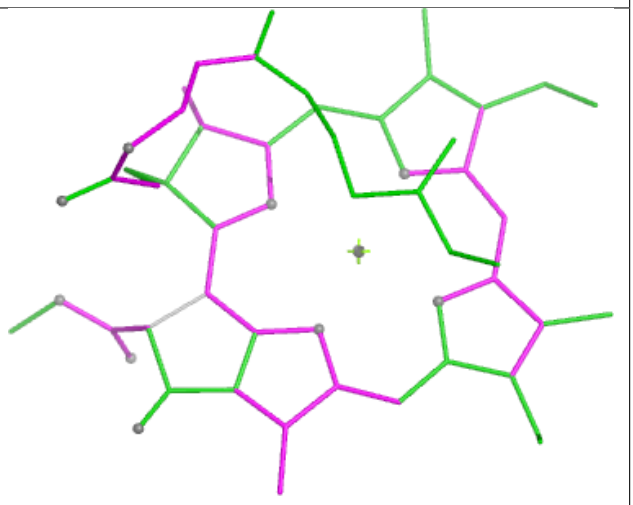

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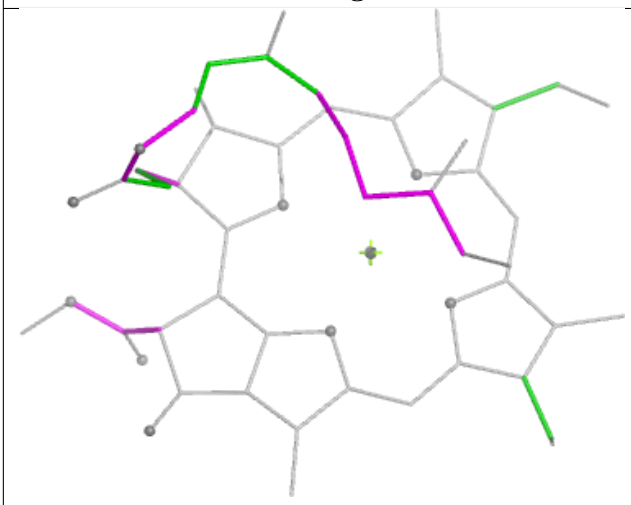

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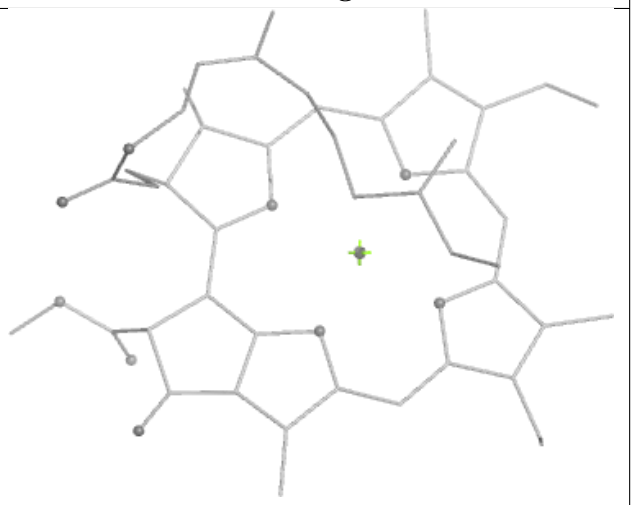
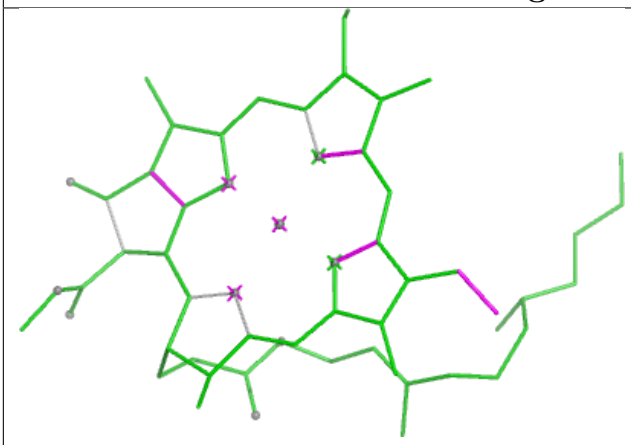


Rings

Ligand CLA g 610



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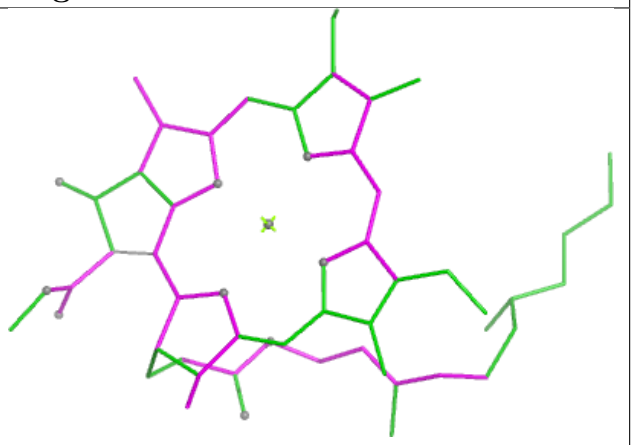

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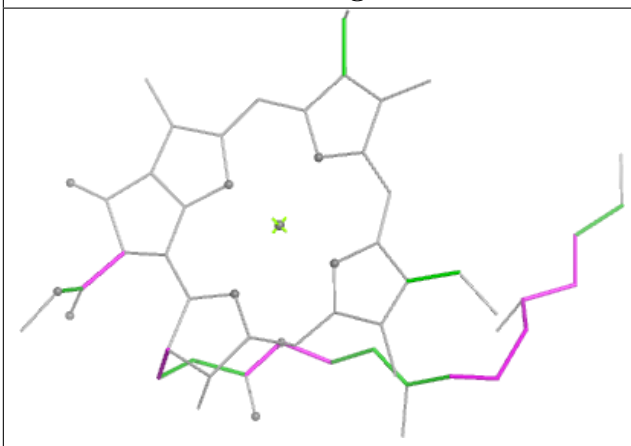

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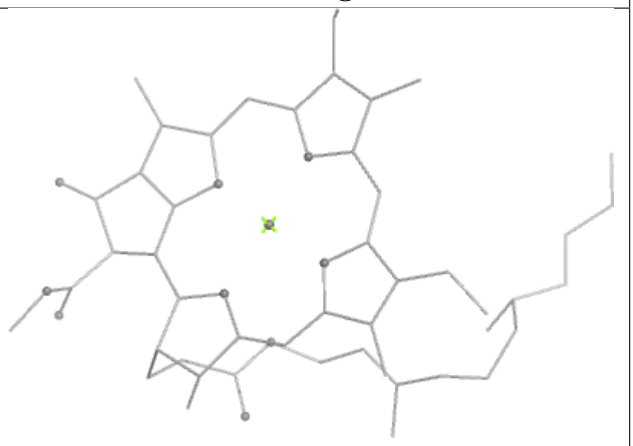
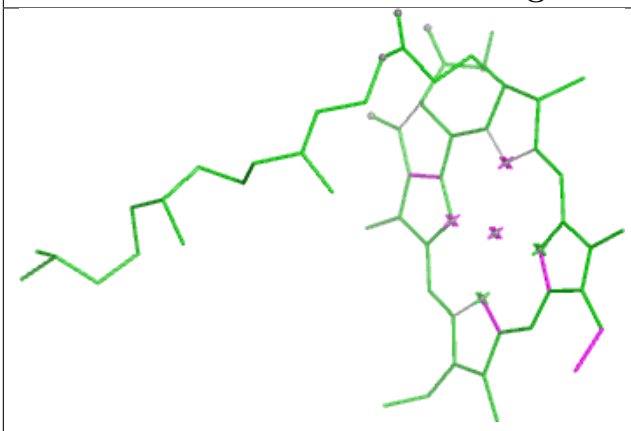


Rings

Ligand CLA n 611



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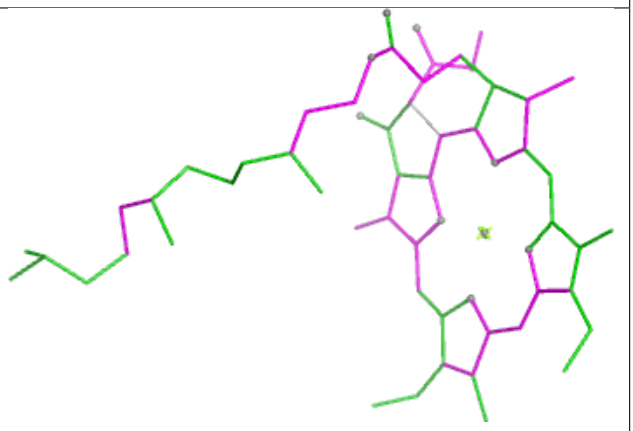

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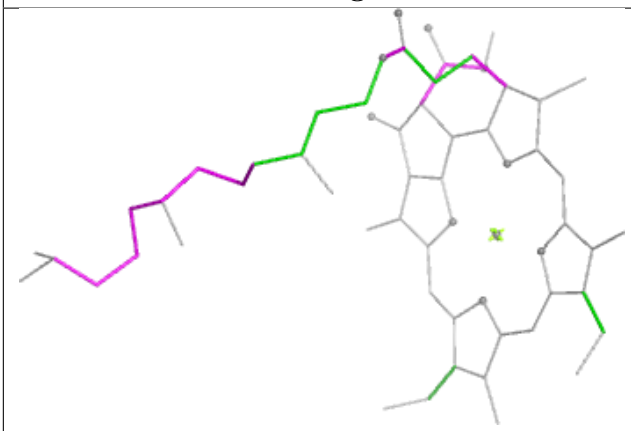
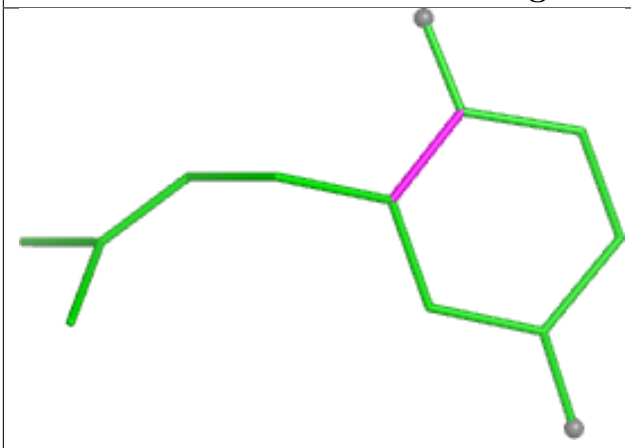


Torsions



Rings

Ligand PL9 A 412



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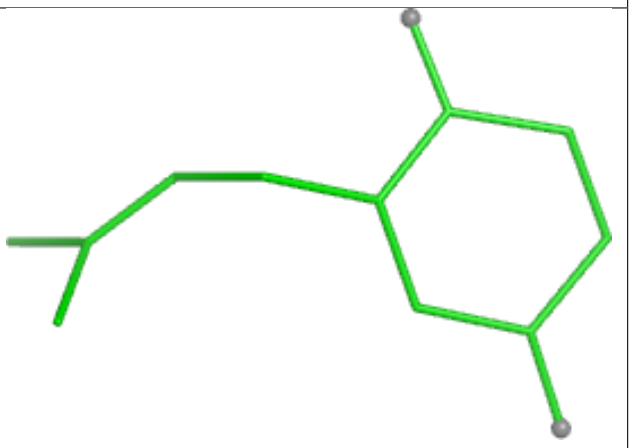

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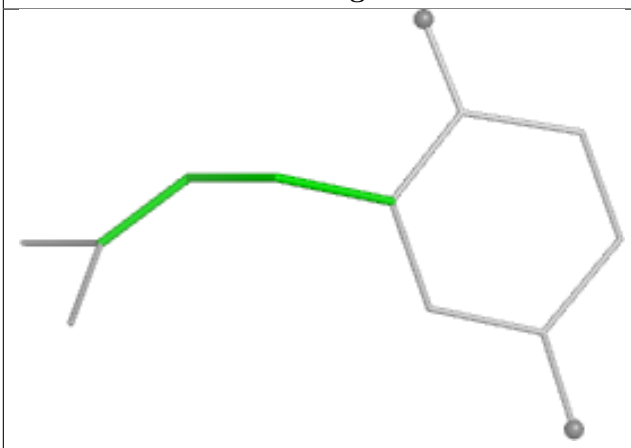

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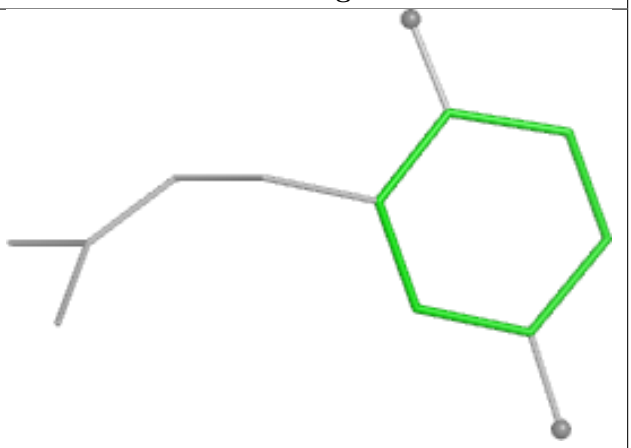
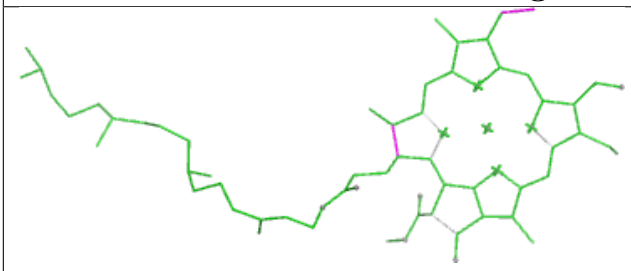


Rings

Ligand CHL r 605



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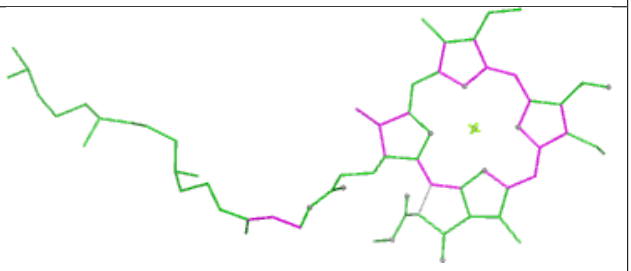

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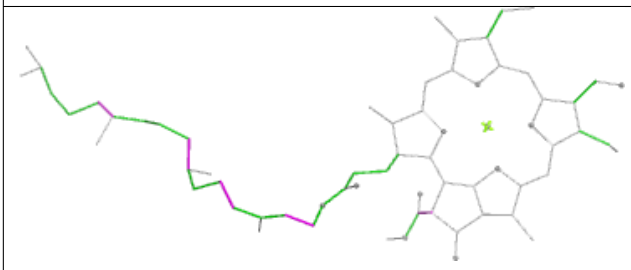

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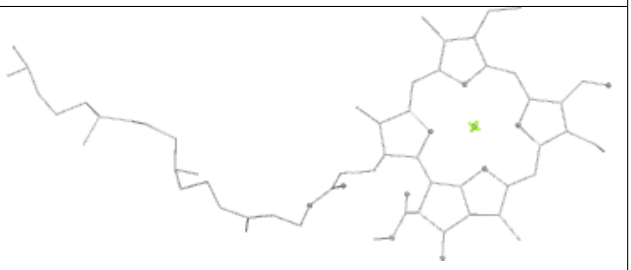
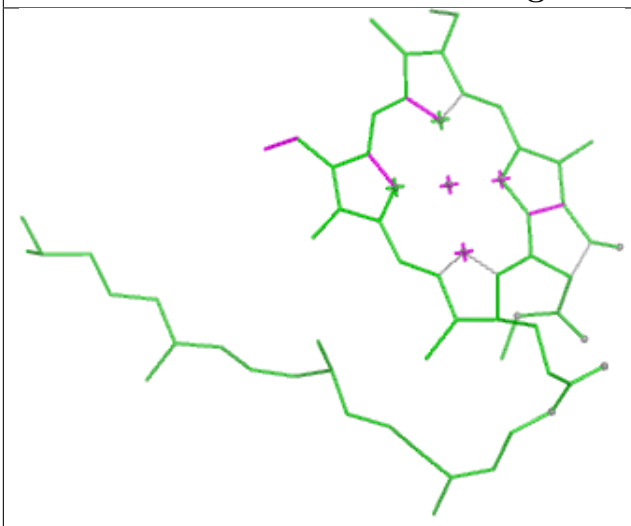


Rings

Ligand CLA b 616



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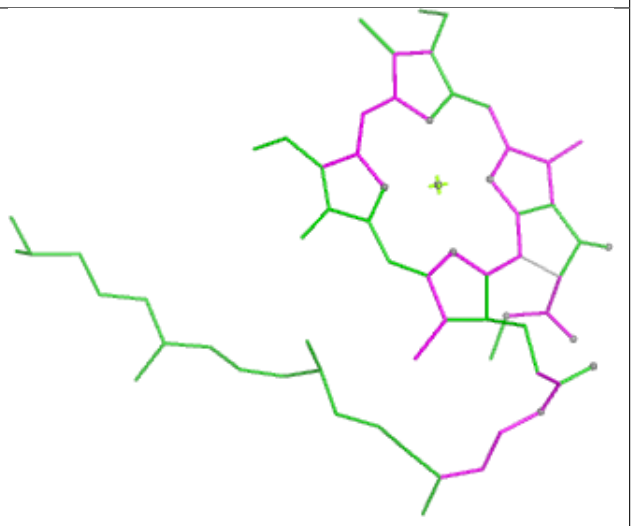

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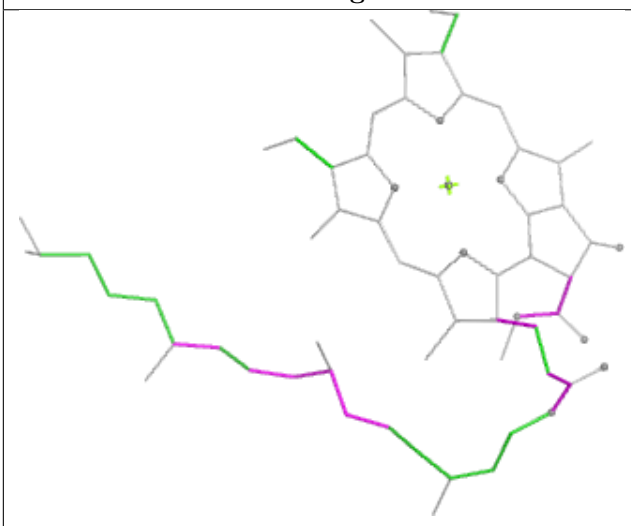

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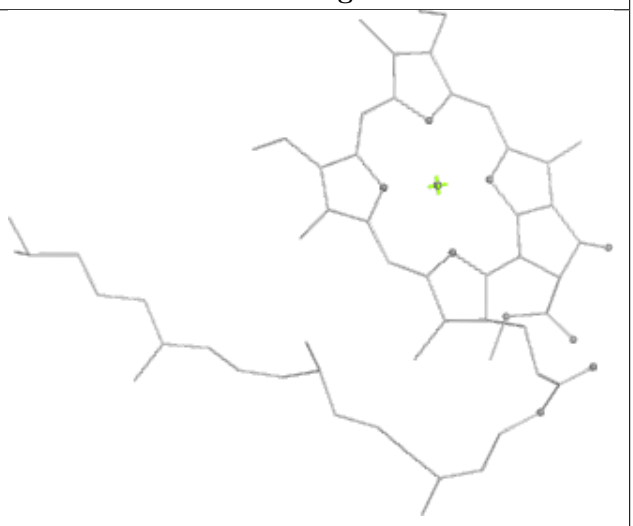
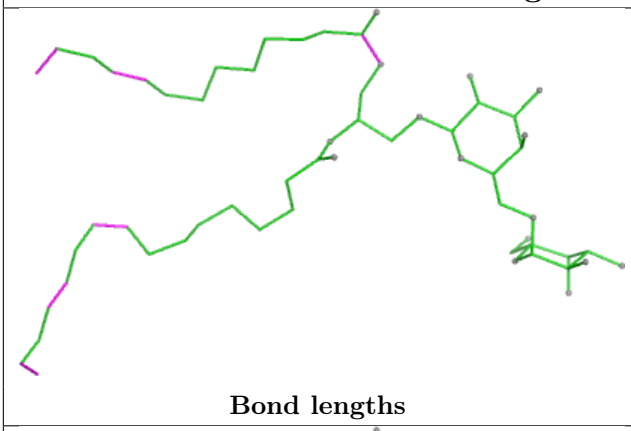


Rings

Ligand DGD a 401



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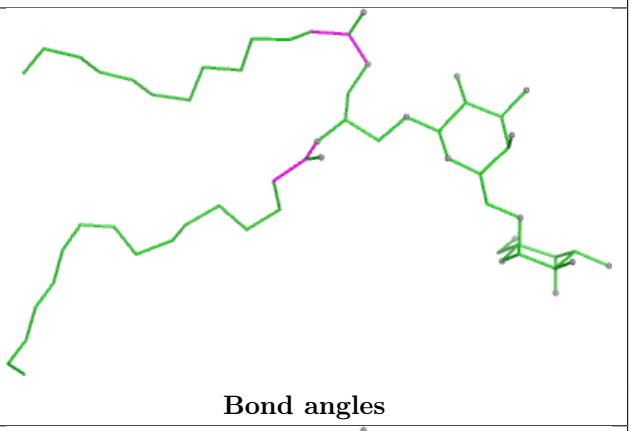

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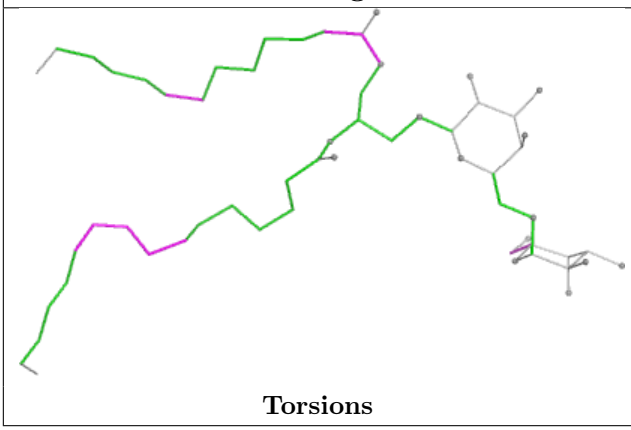

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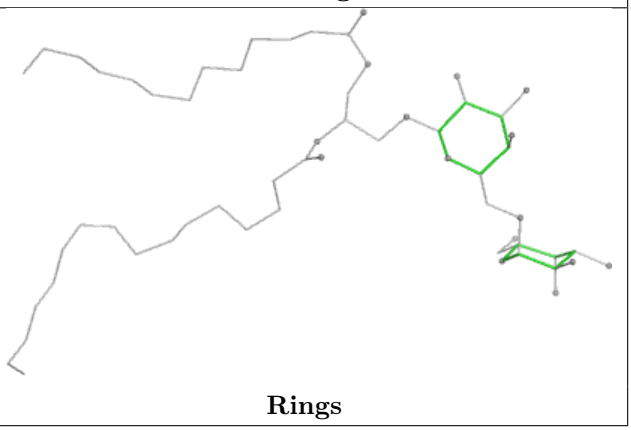
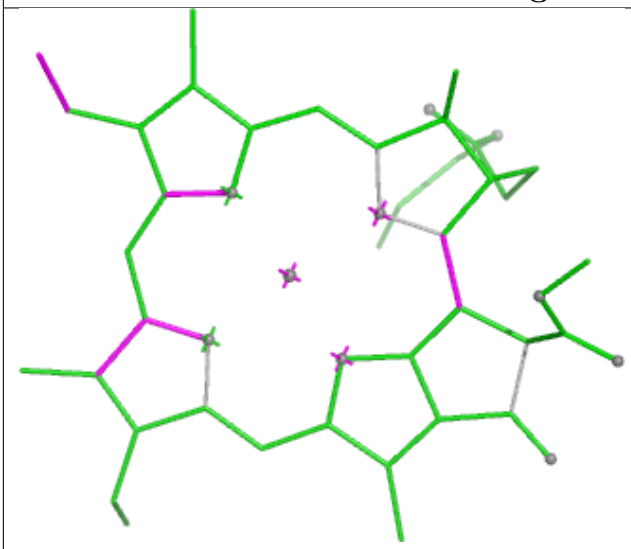


Rings

Ligand CLA r 604



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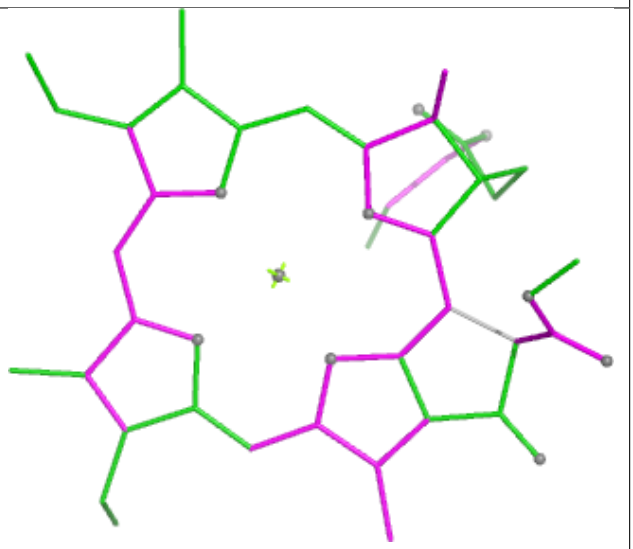
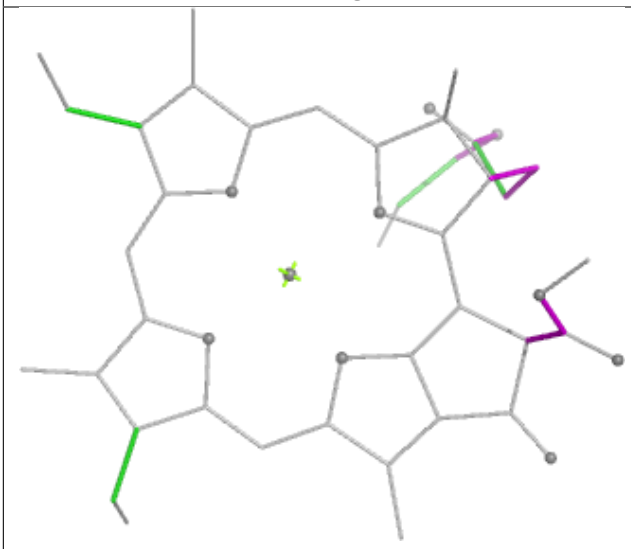


Bond angles



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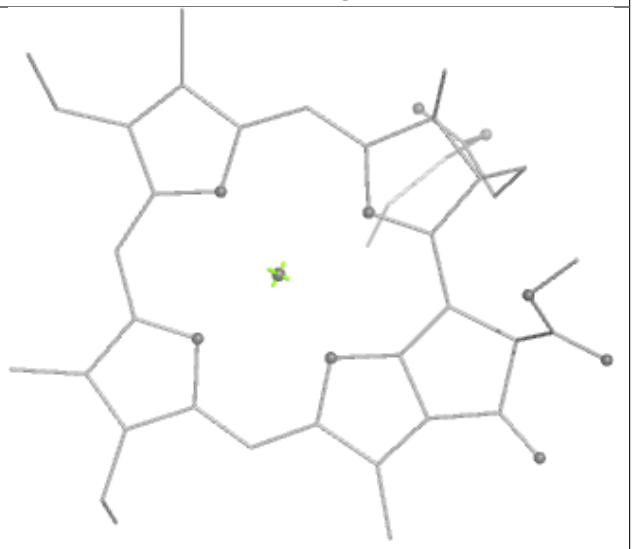

Rings

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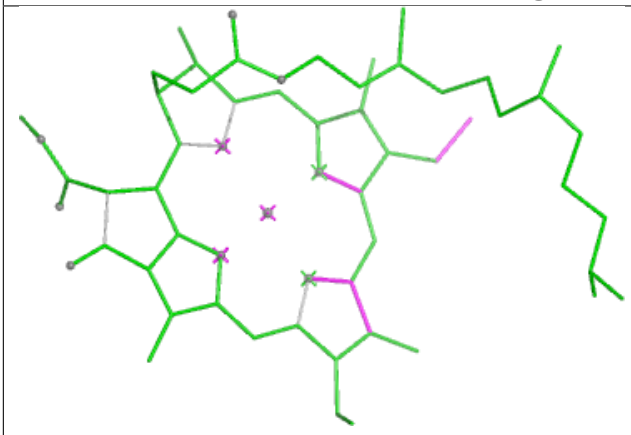

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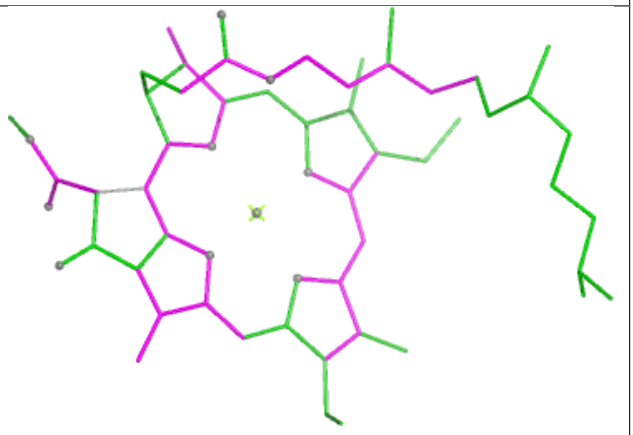
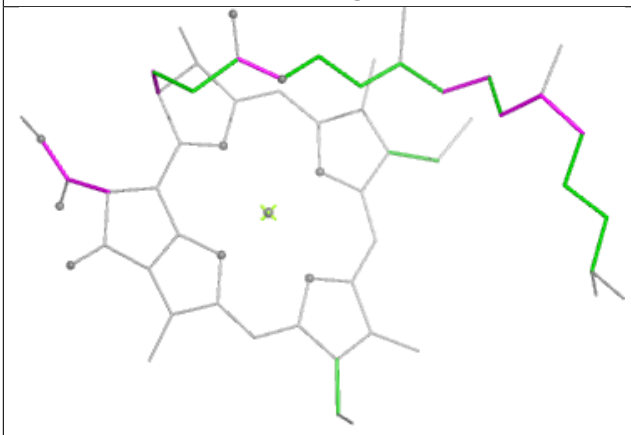


Bond angles



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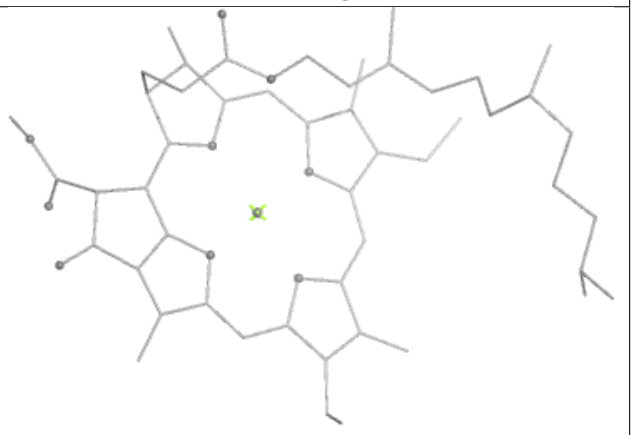
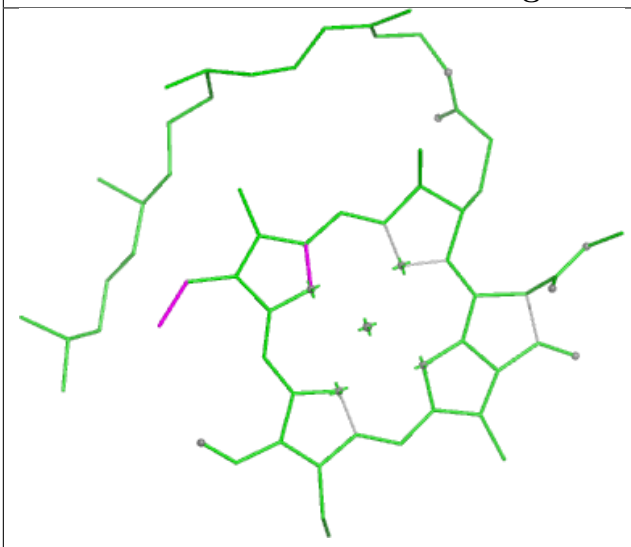


Rings

Ligand CHL N 607



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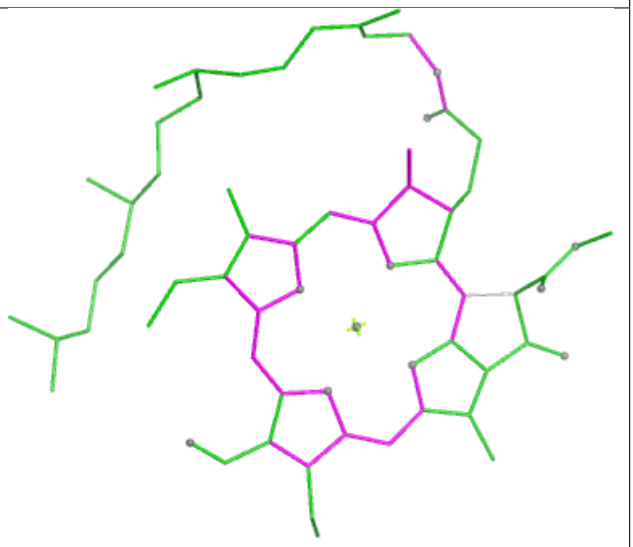
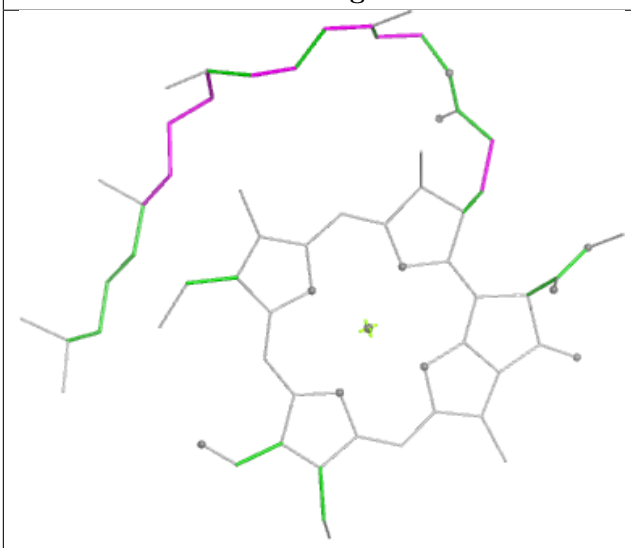
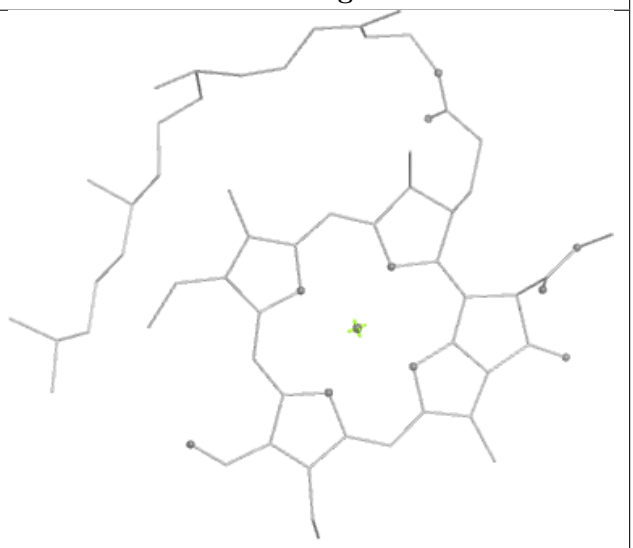


Bond angles

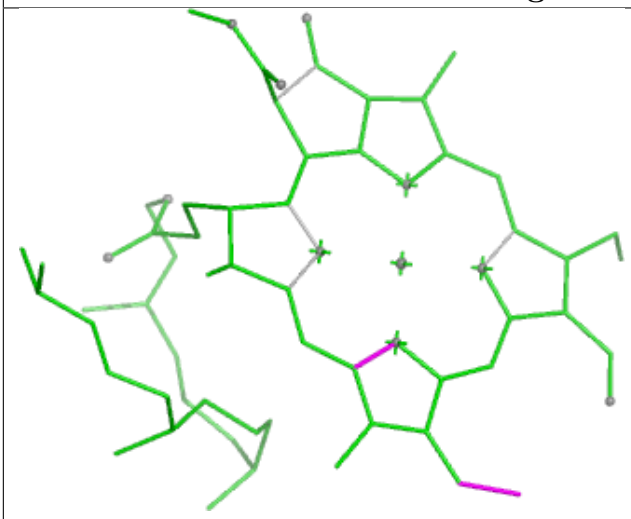


Torsions

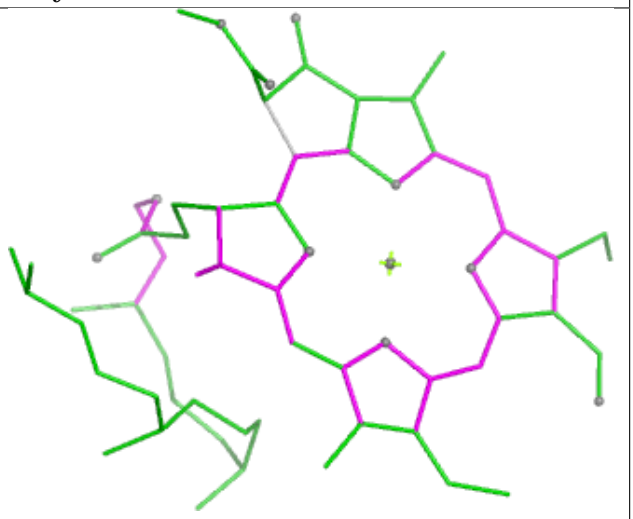


Rings

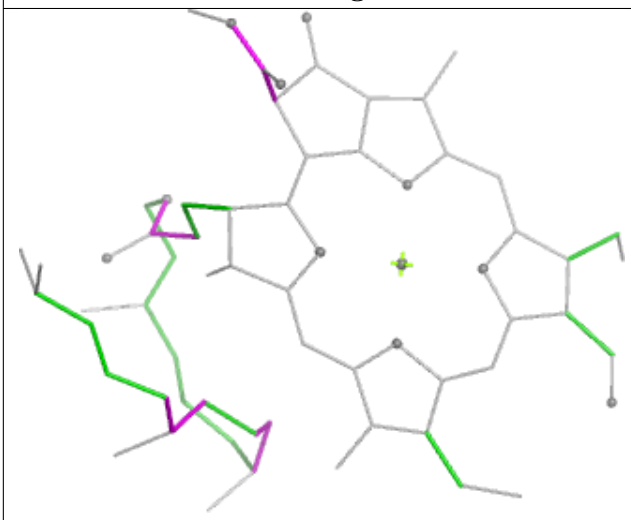
Ligand CHL y 308



Bond lengths



Bond angles



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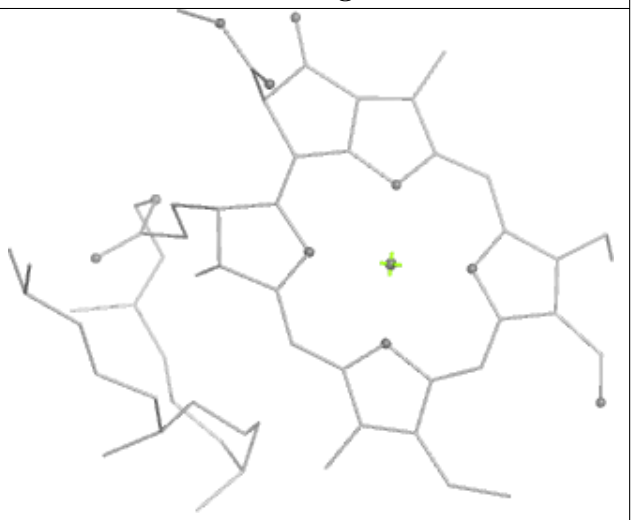
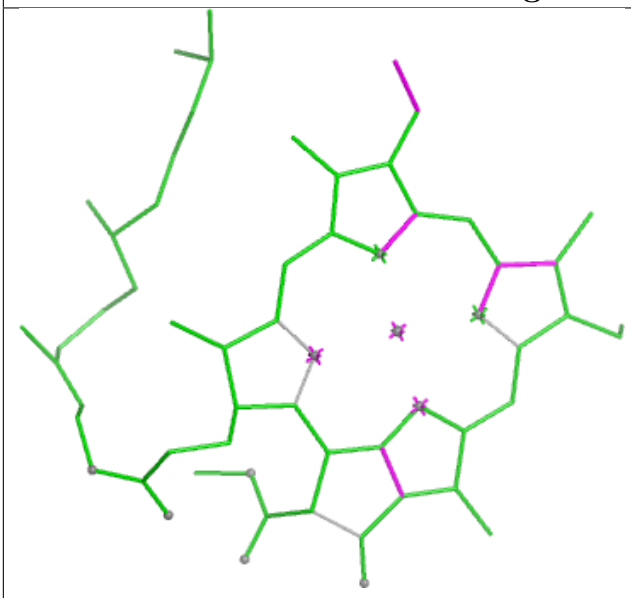


Rings

Ligand CLA N 612



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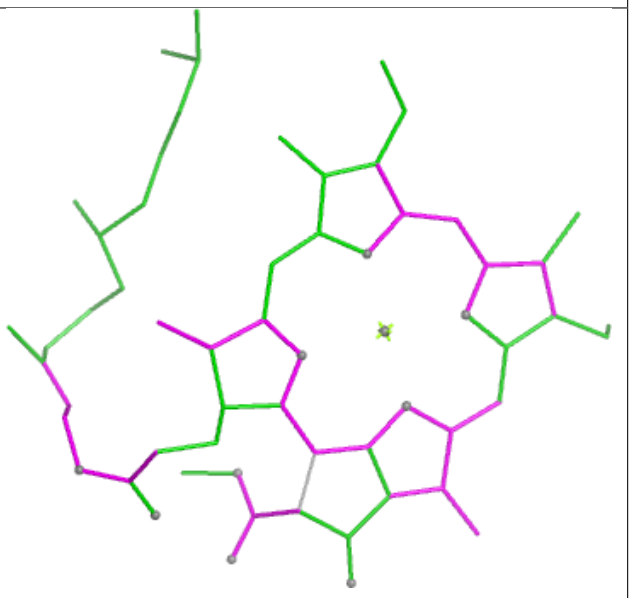
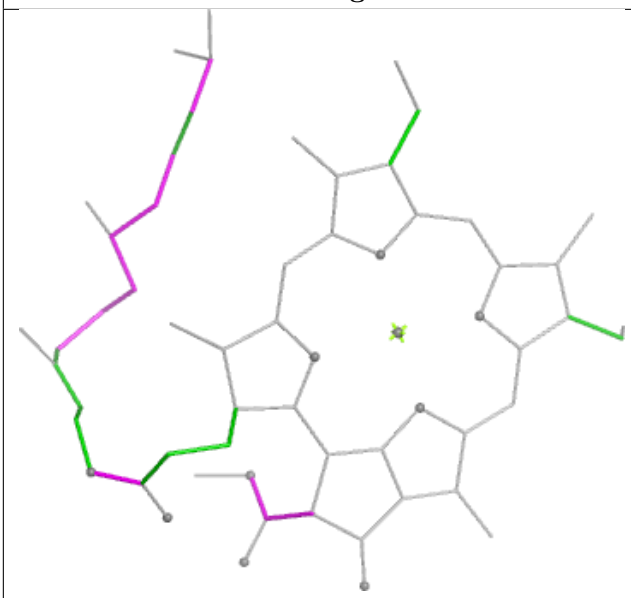


Bond angles



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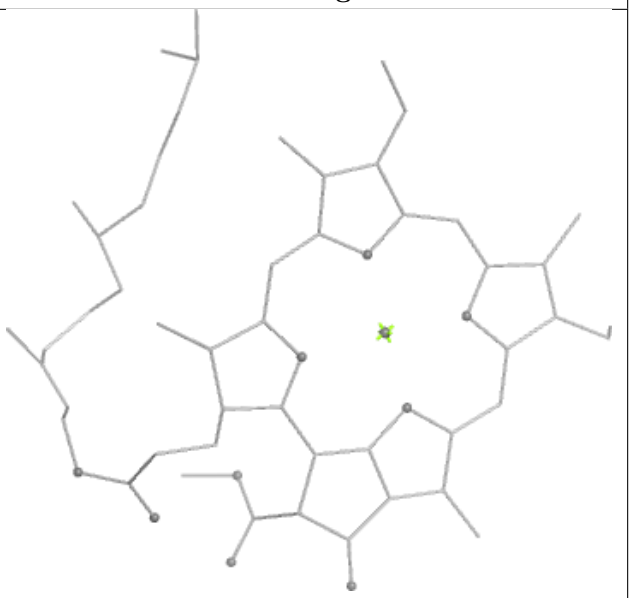
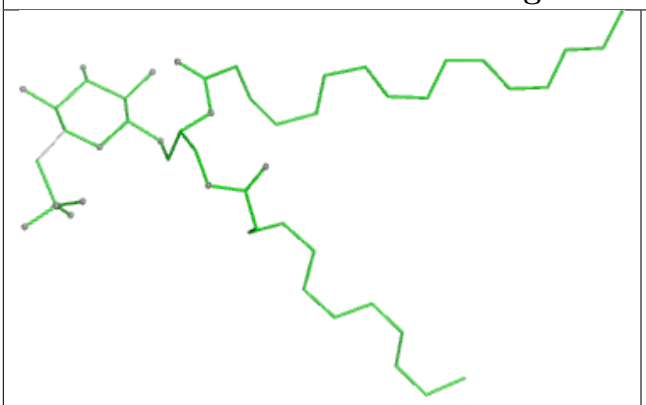


Rings

Ligand SQD A 410



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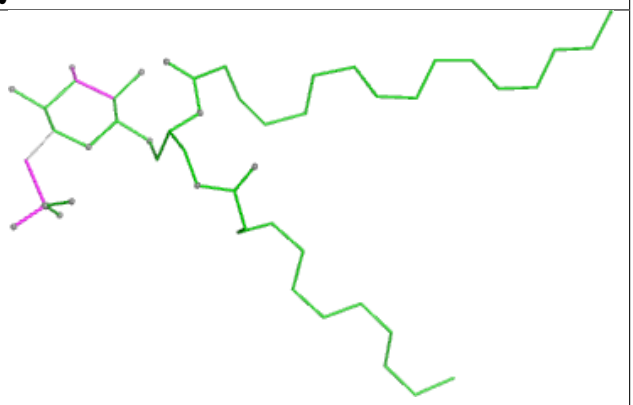
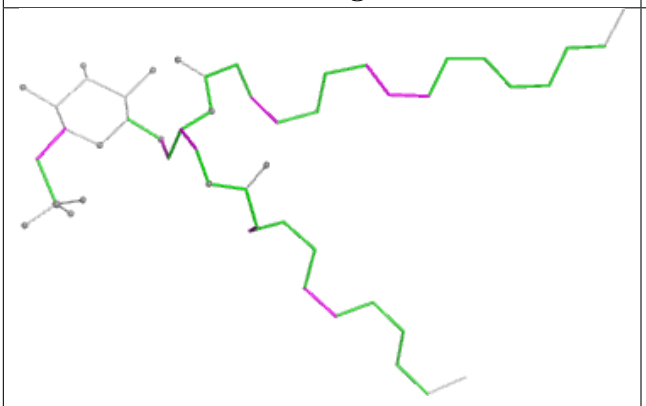


Bond angles



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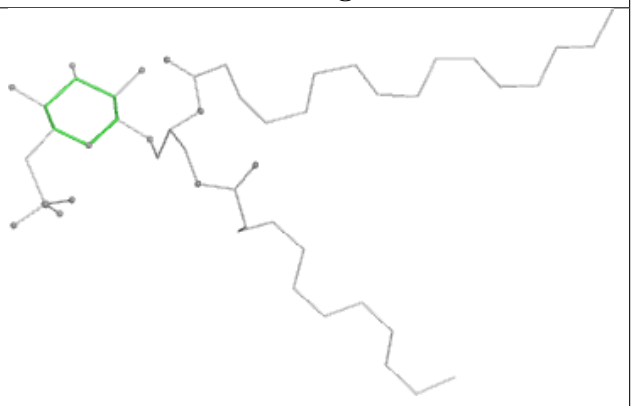
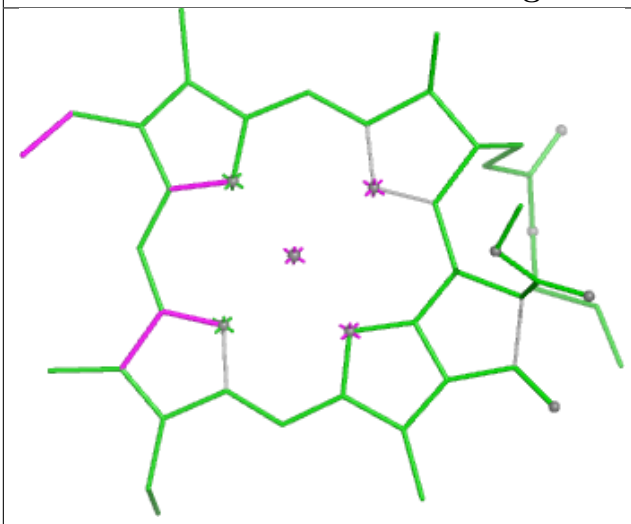


Rings

Ligand CLA G 614



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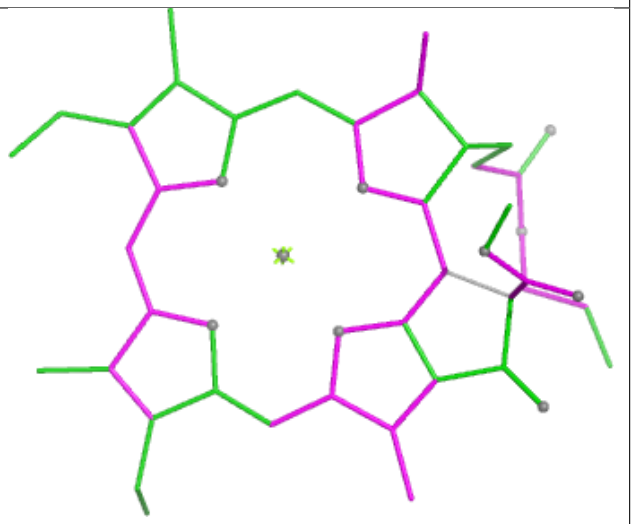
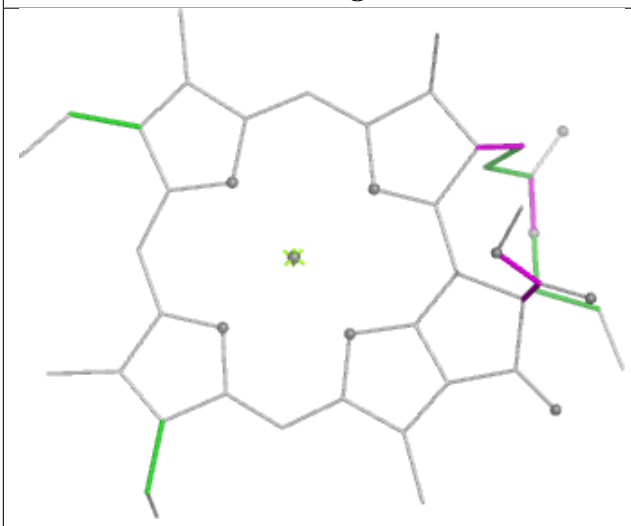


Bond angles



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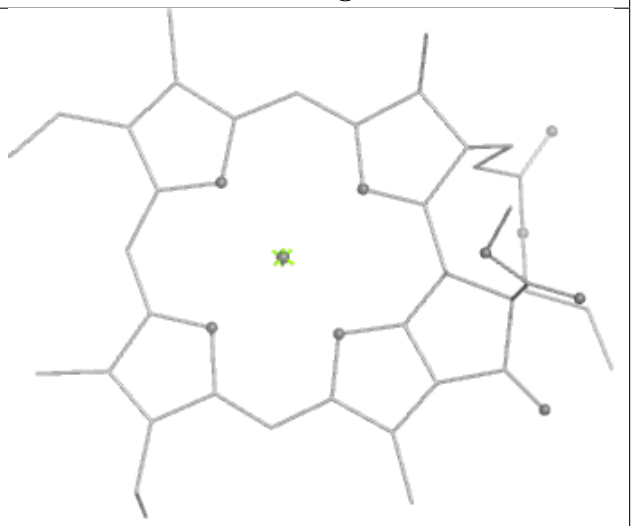
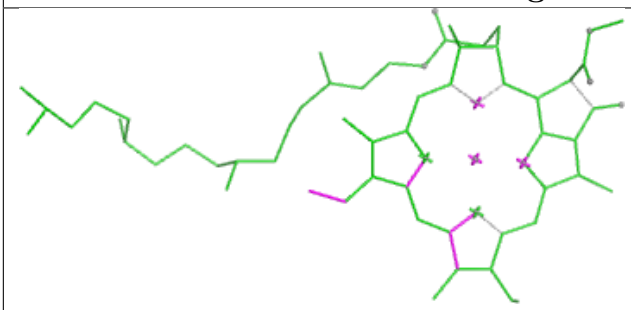


Rings

Ligand CLA b 603



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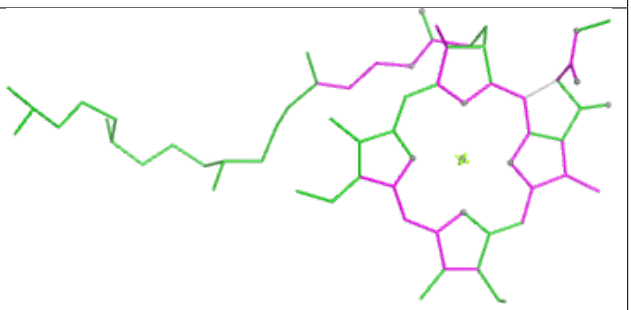

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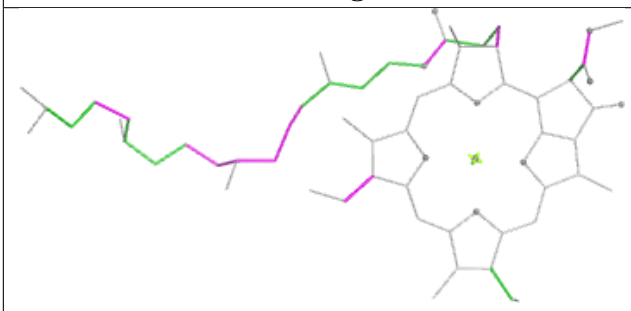
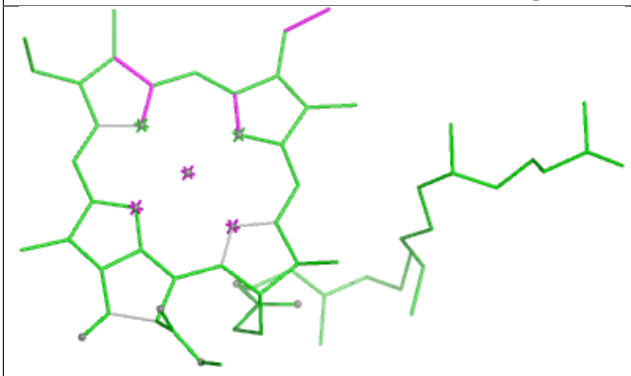


Torsions



Rings

Ligand CLA d 401



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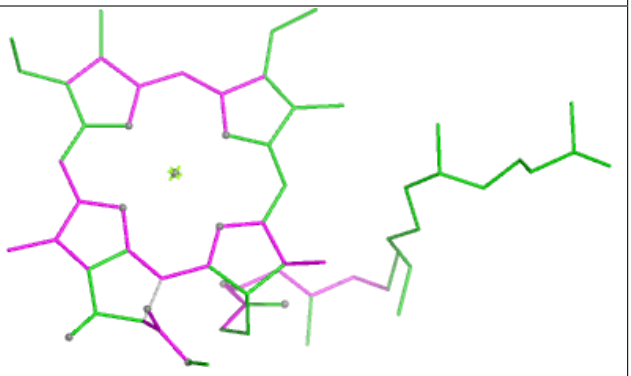
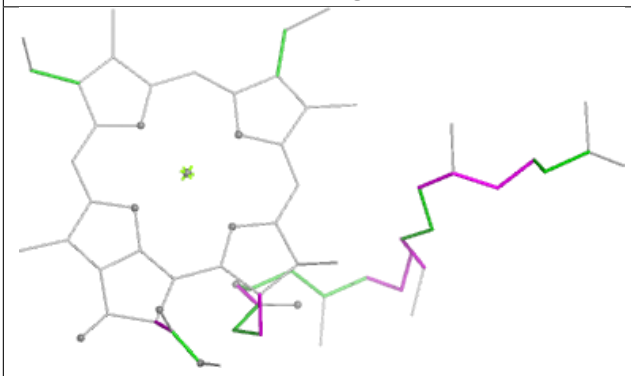


Bond angles



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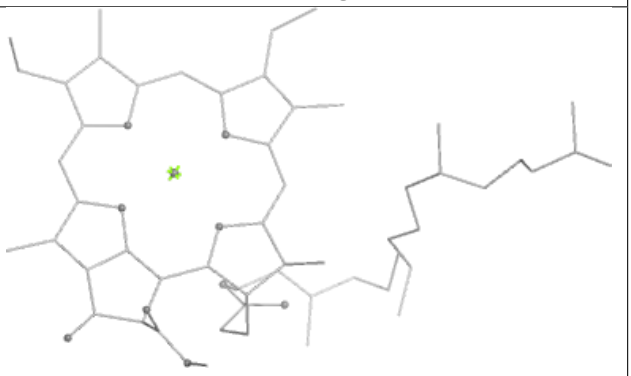
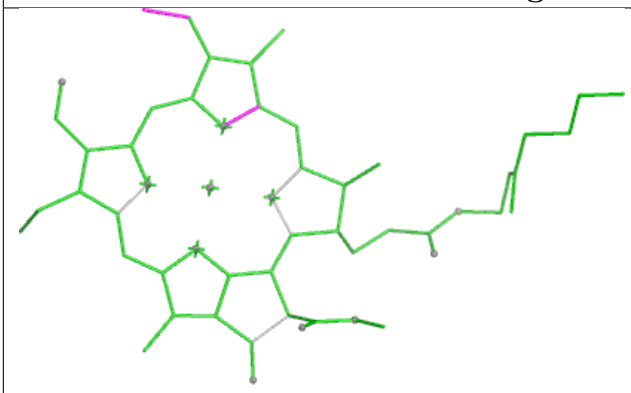


Rings

Ligand CHL n 601



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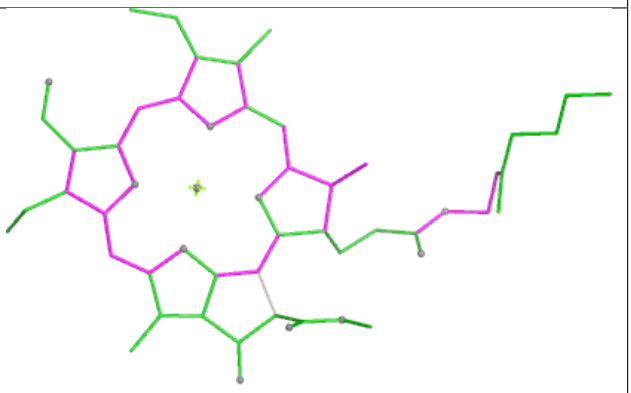
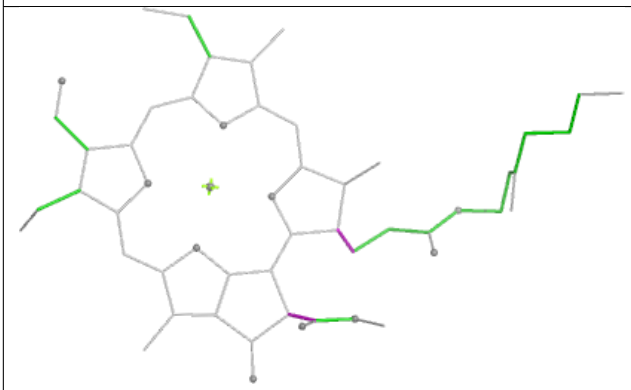


Bond angles



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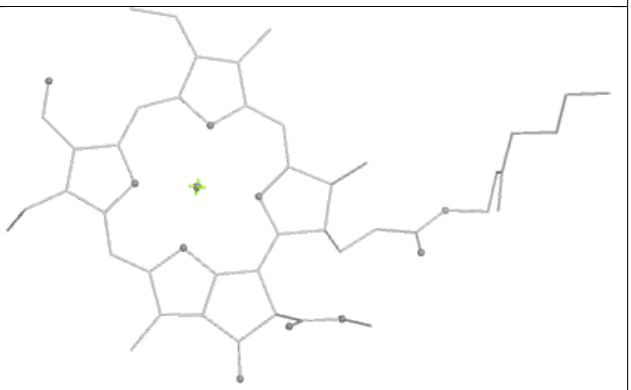
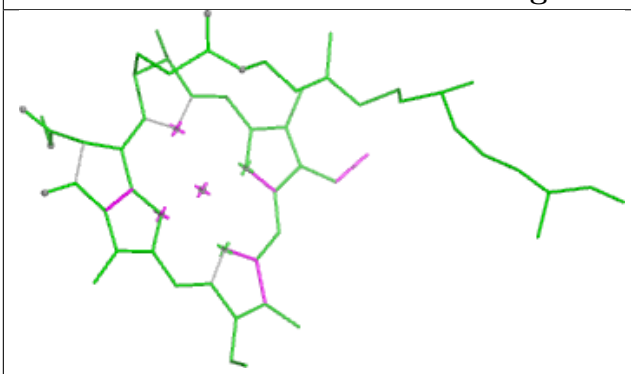


Rings

Ligand CLA s 602



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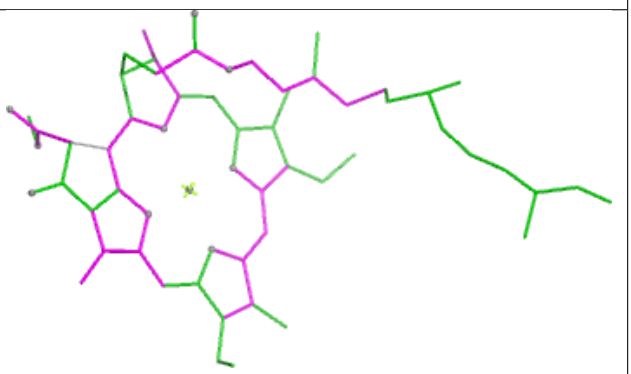
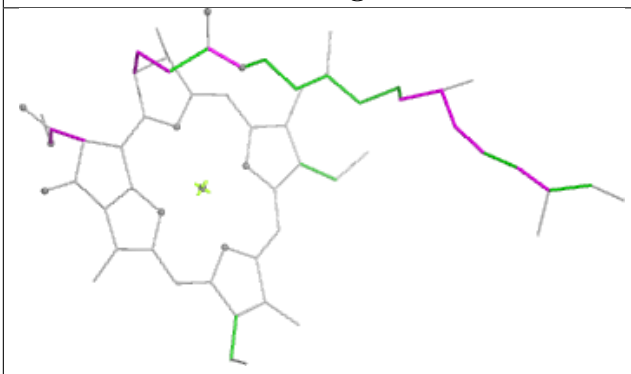


Bond angles

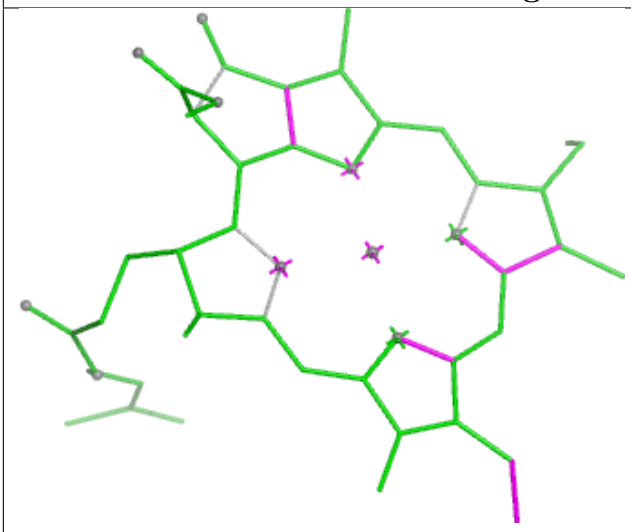


Torsions



Rings

Ligand CLA G 604



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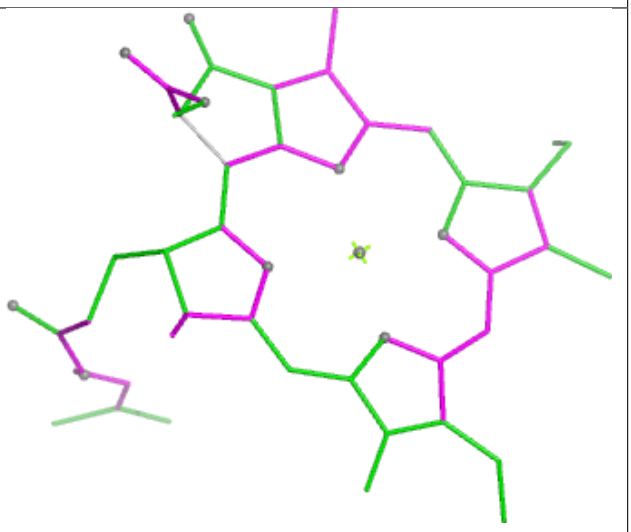
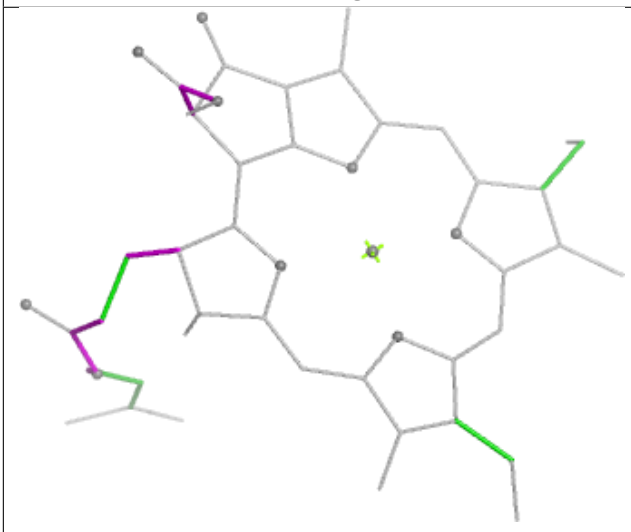


Bond angles



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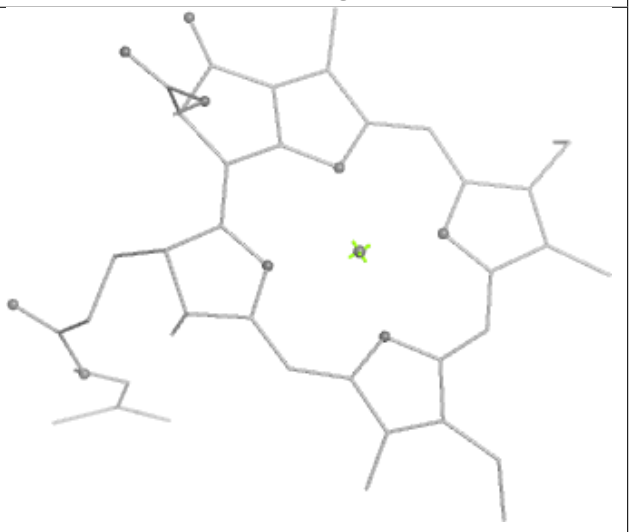
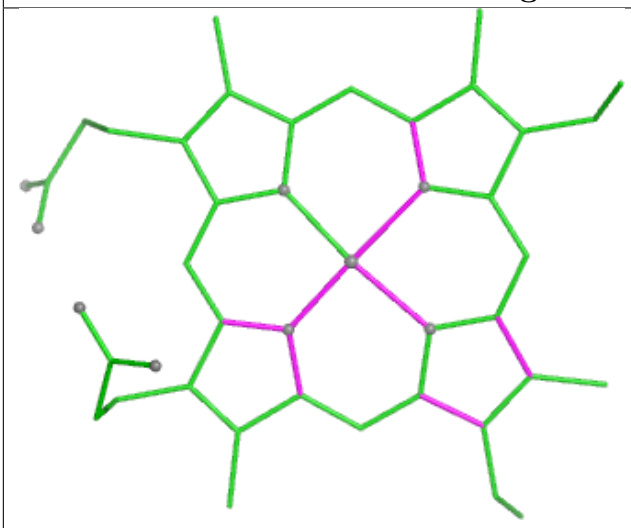


Rings

Ligand HEM E 101



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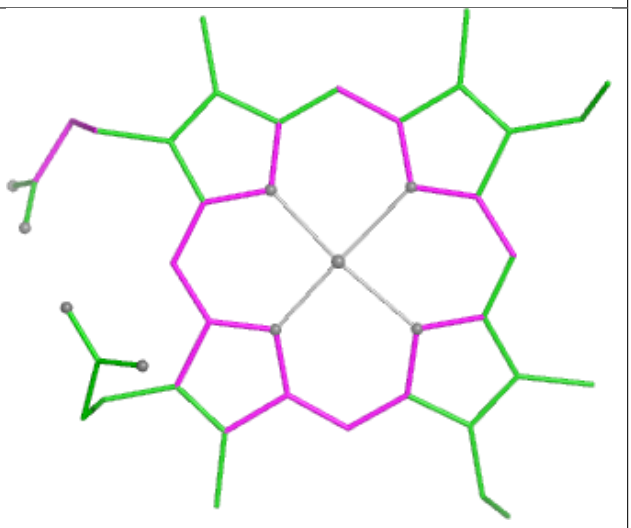
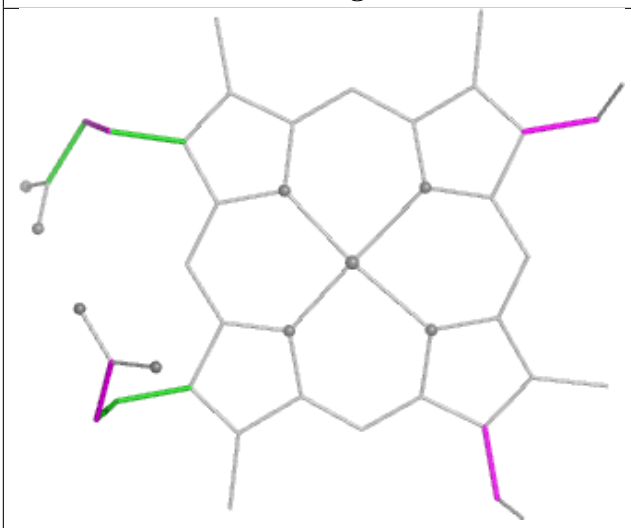


Bond angles



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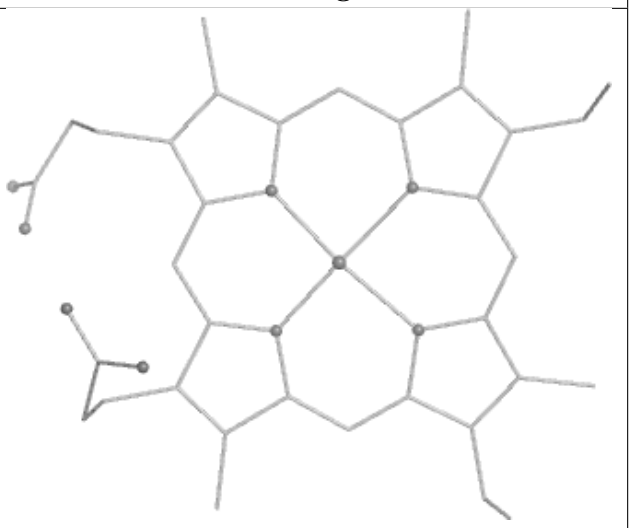
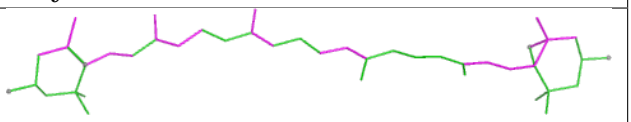


Rings

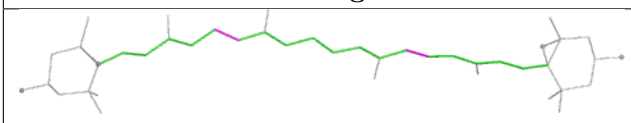
Ligand XAT y 317



Bond lengths



Bond angles



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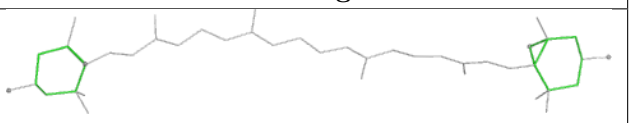
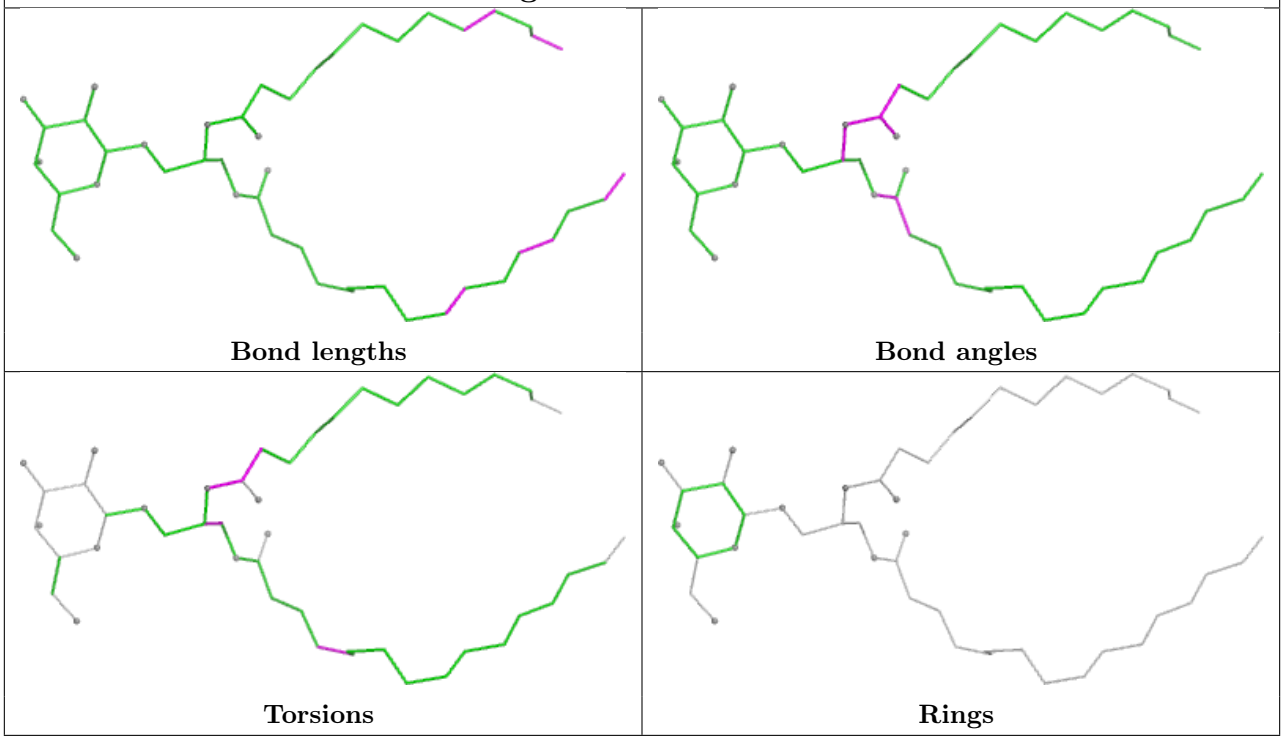


Rings

Ligand LMG A 411



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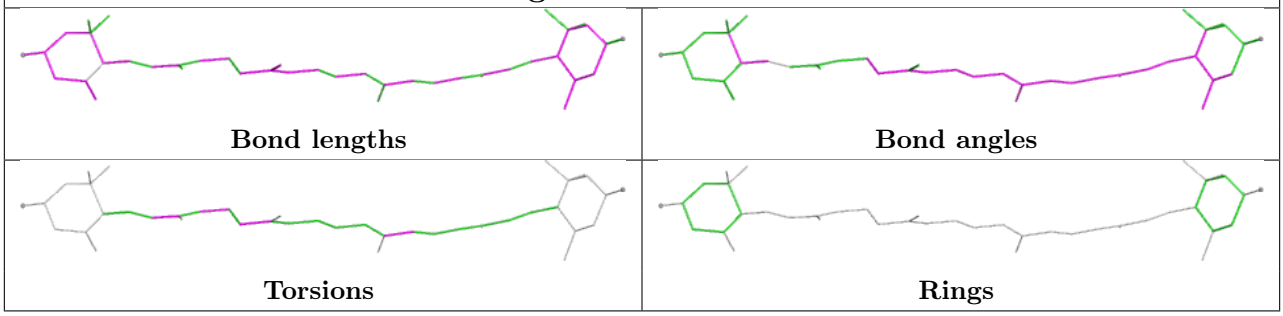

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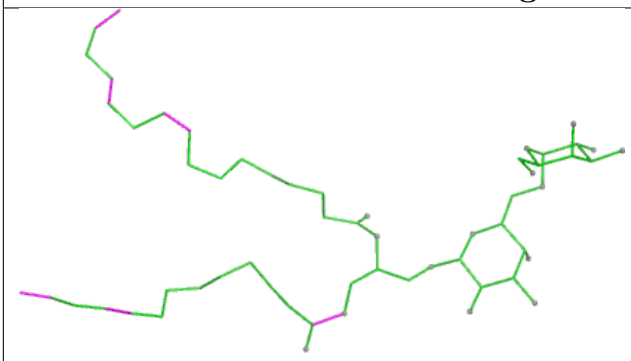

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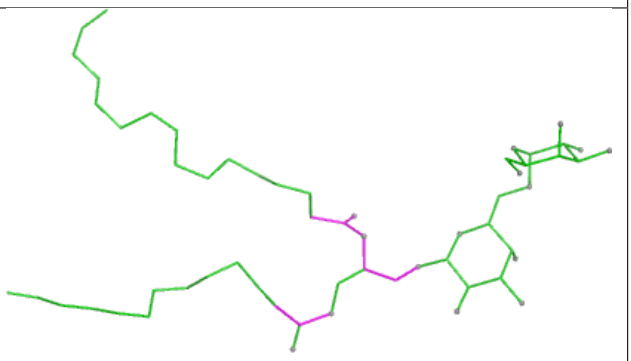
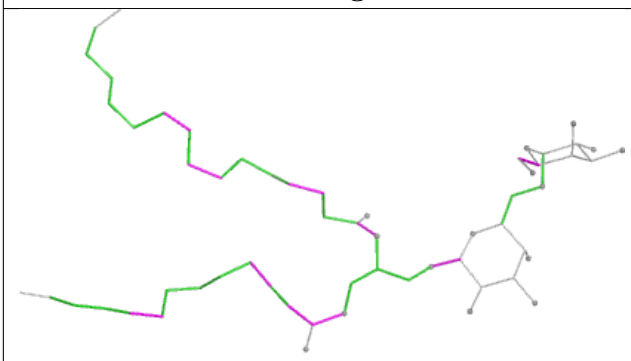


Bond angles



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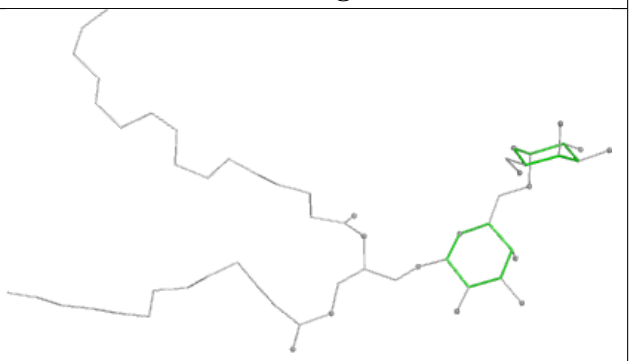
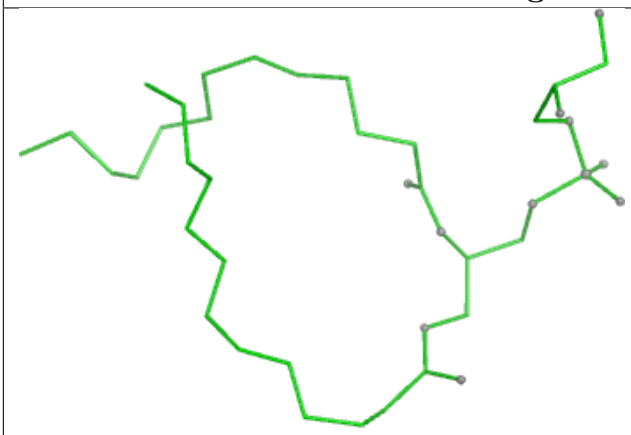


Rings

Ligand LHG a 415



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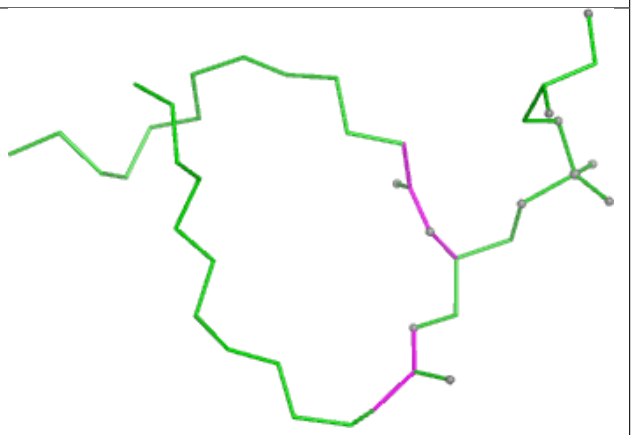
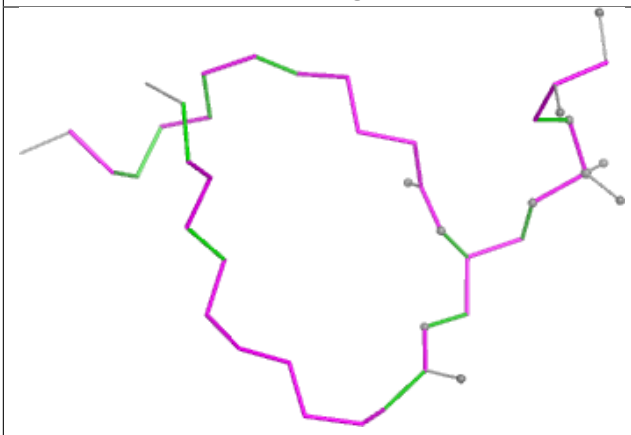


Bond angles



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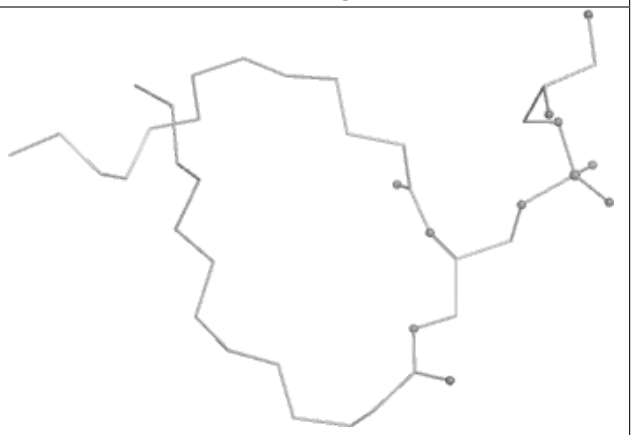
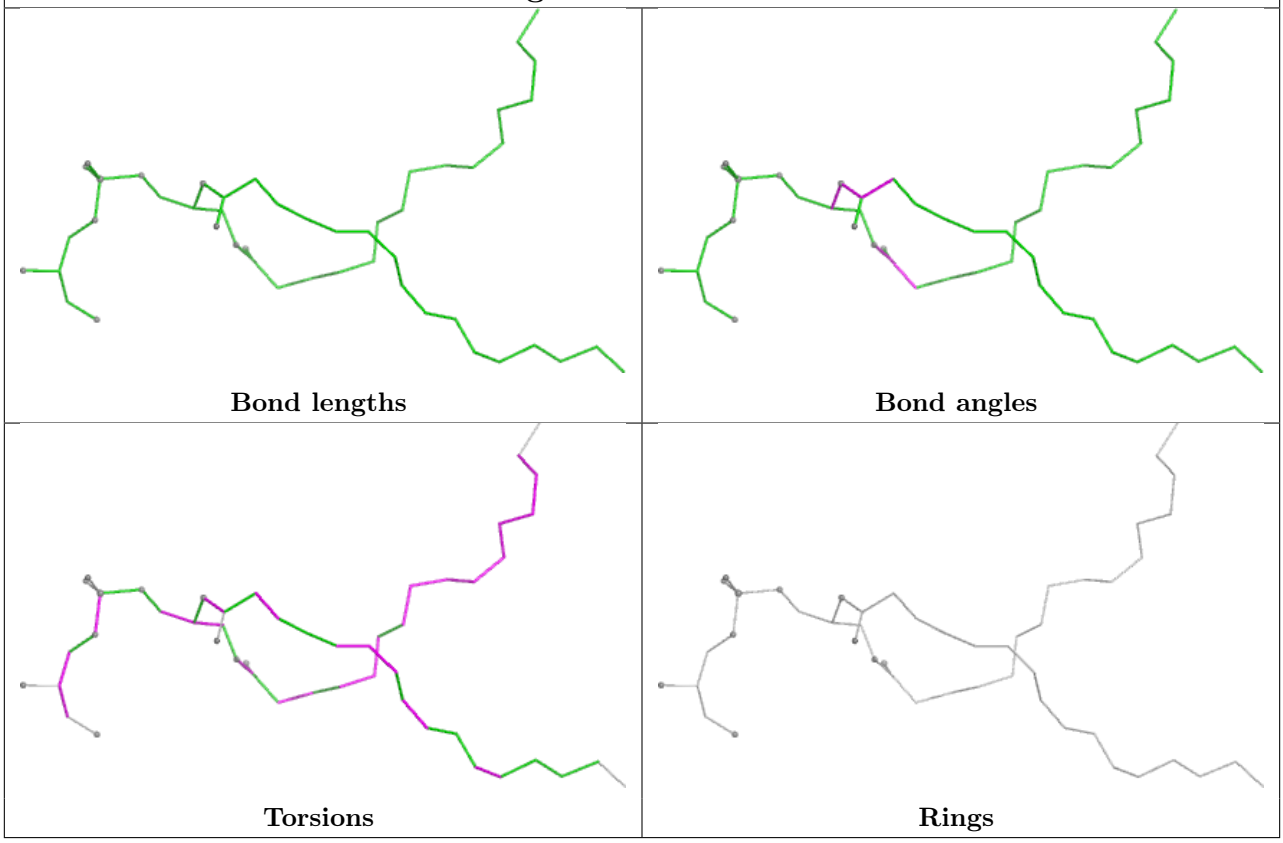
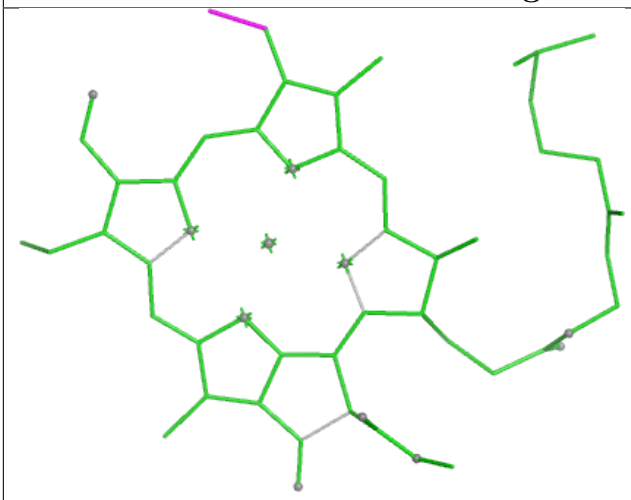


Rings

Ligand LHG d 408



Ligand CHL G 607



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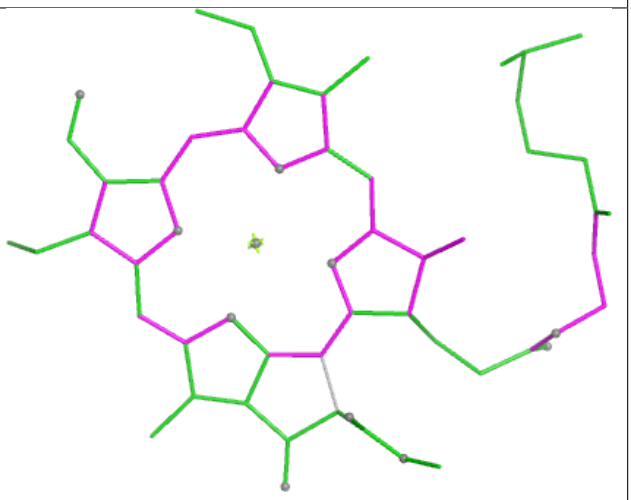
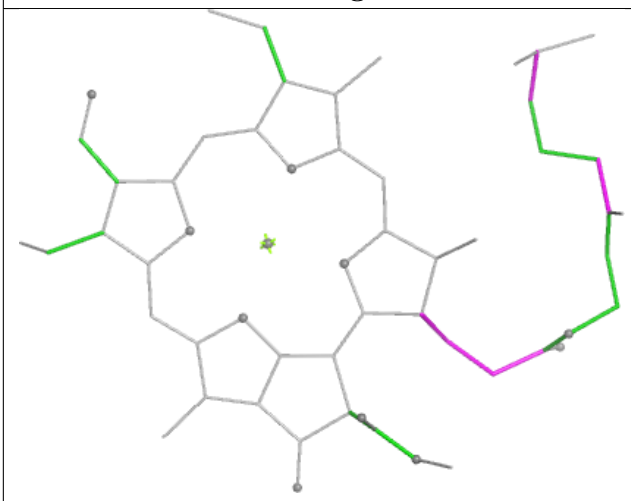


Bond angles



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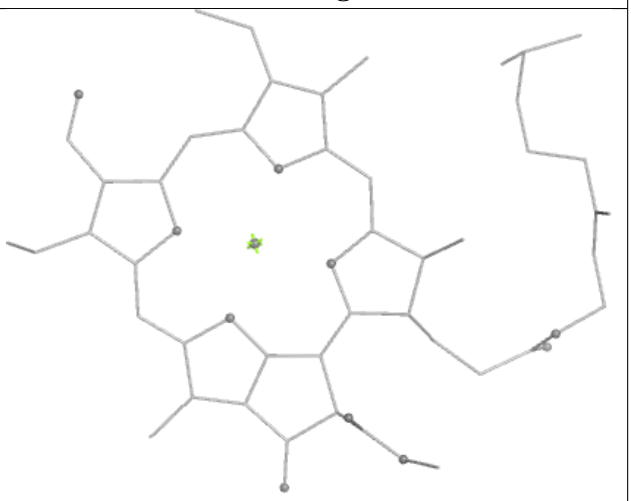
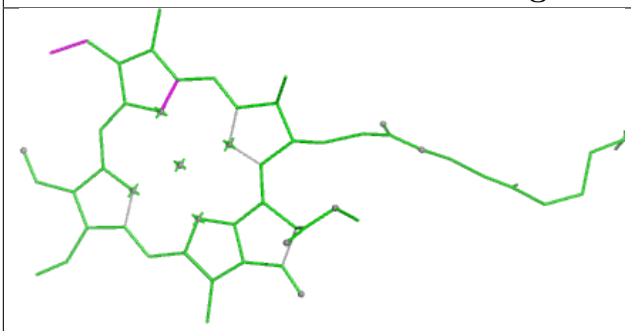
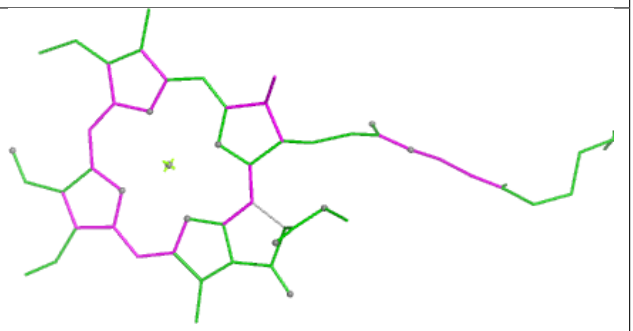


Rings

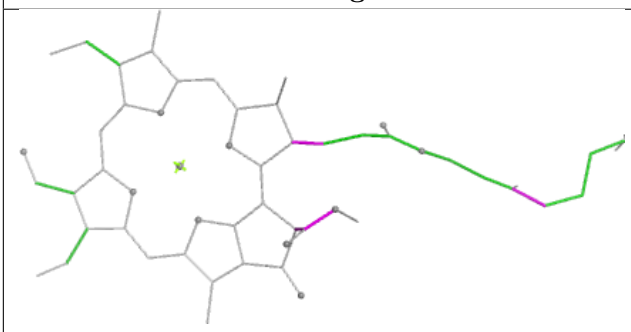
Ligand CHL r 606



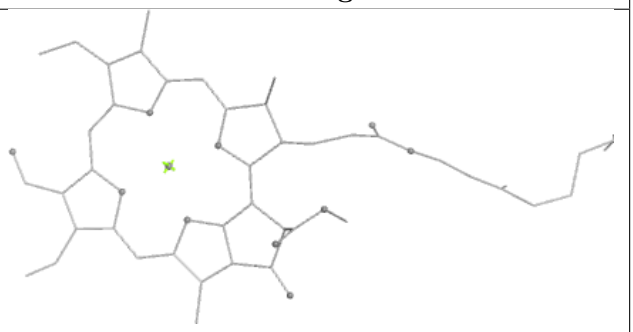
Bond lengths



Bond angles

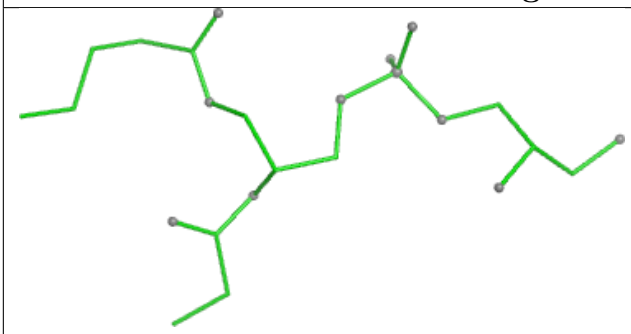


Torsions



Rings

Ligand LHG R 616



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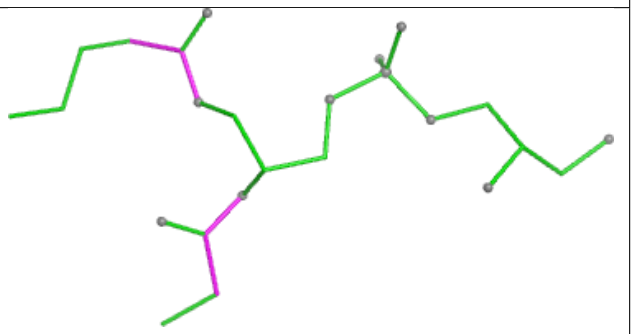
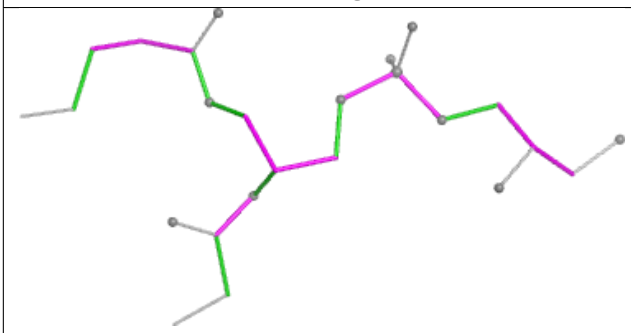


Bond angles



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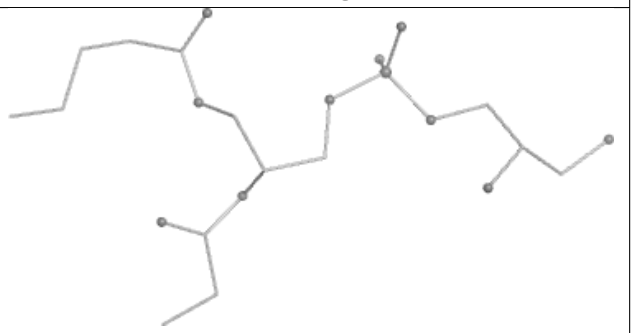
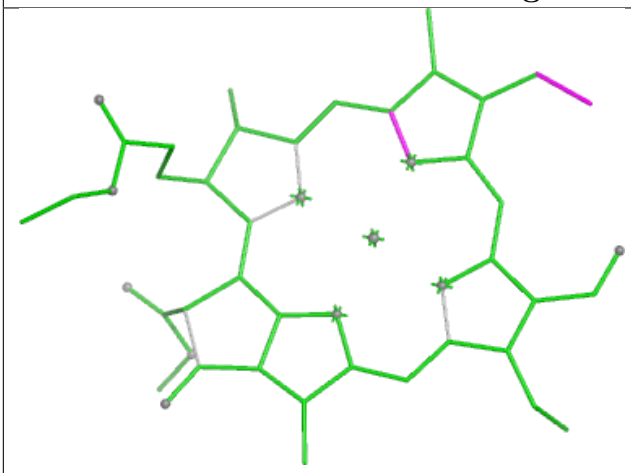
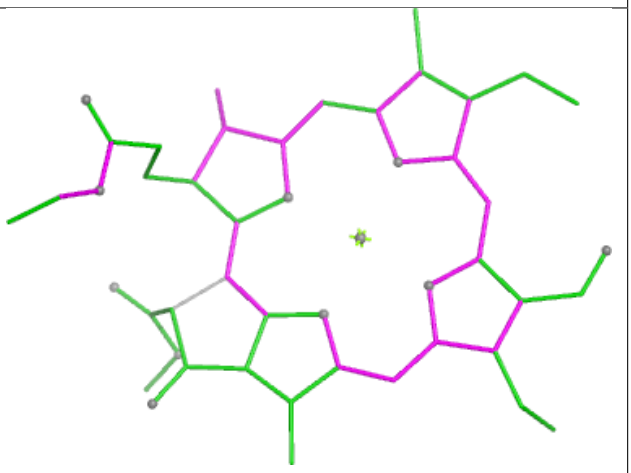


Rings

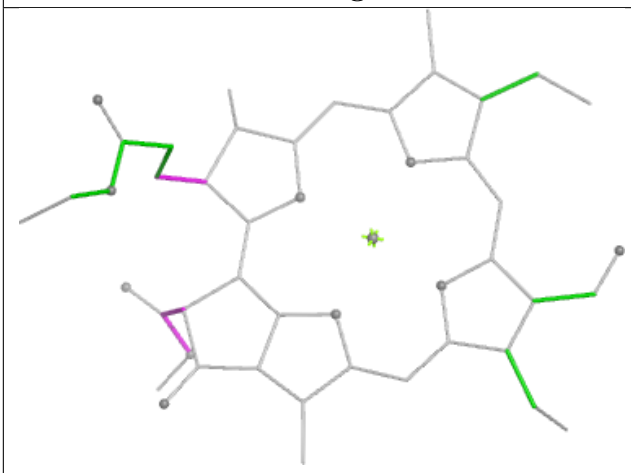
Ligand CHL N 605



Bond lengths



Bond angles



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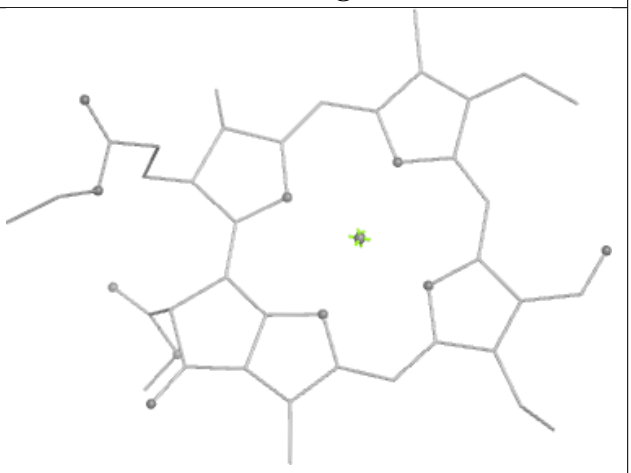
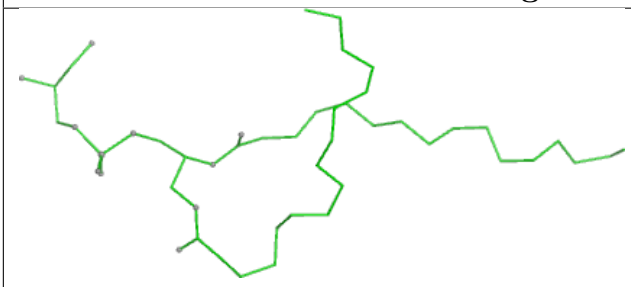


Rings

Ligand LHG G 618



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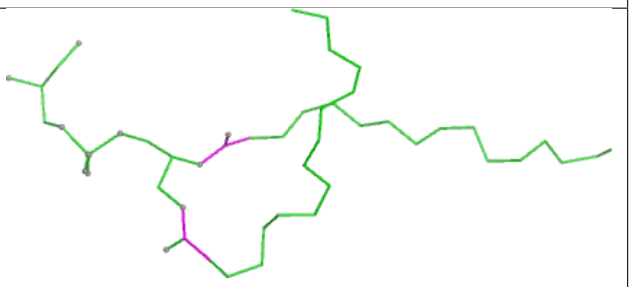
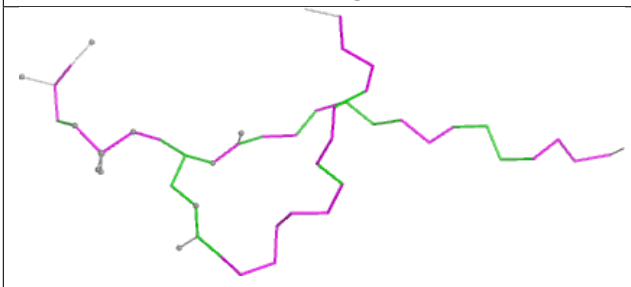


Bond angles

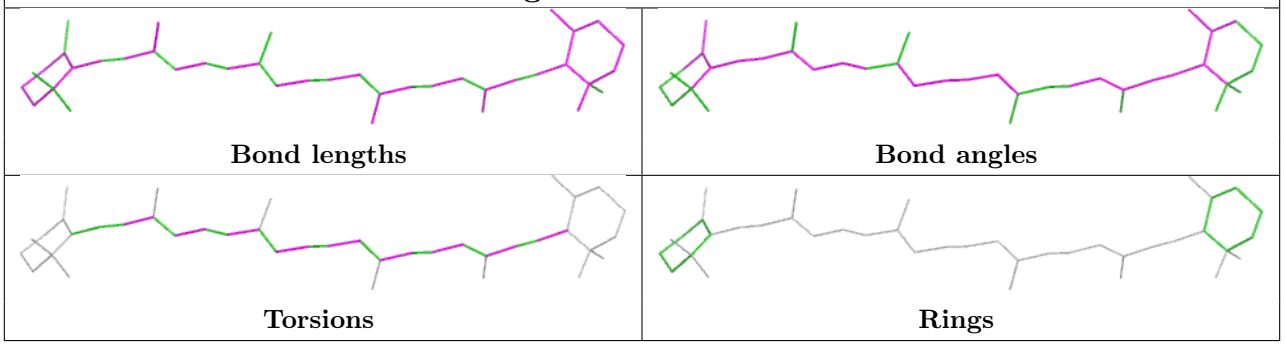


Torsions

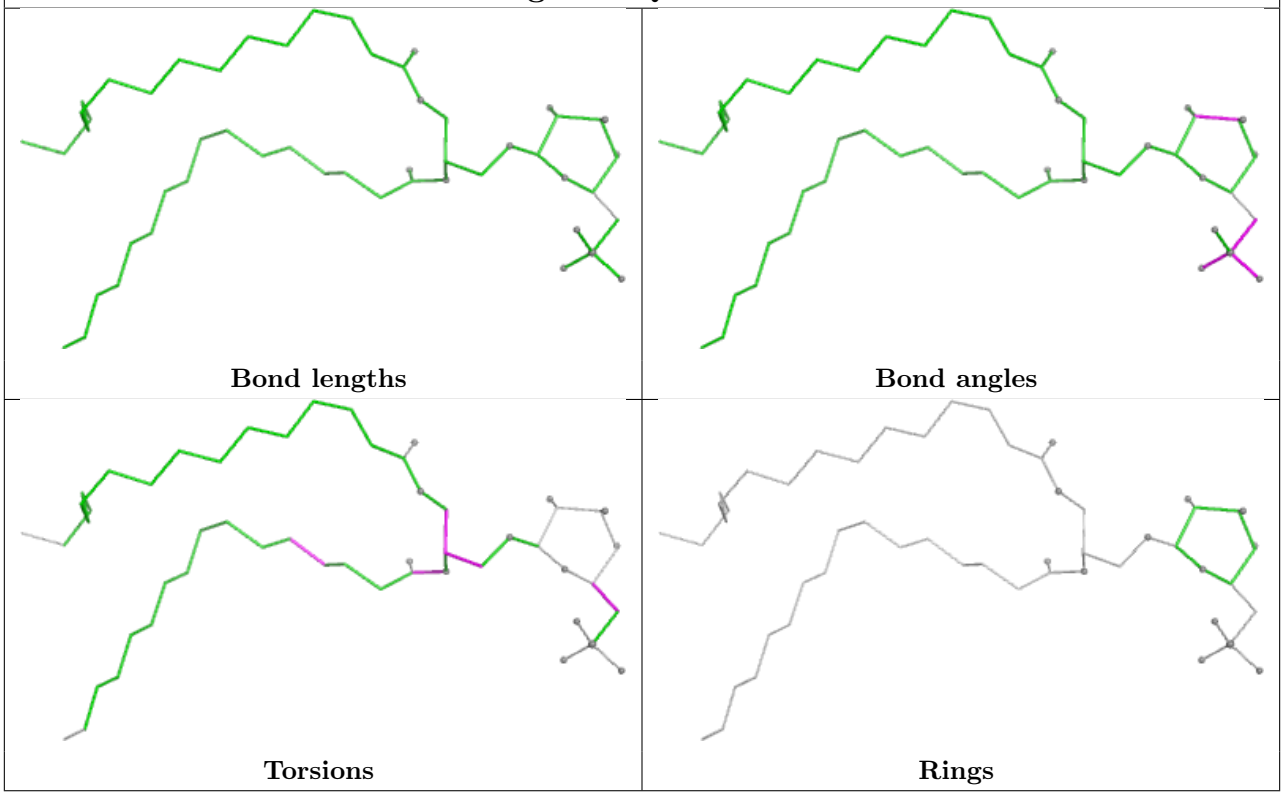


Rings

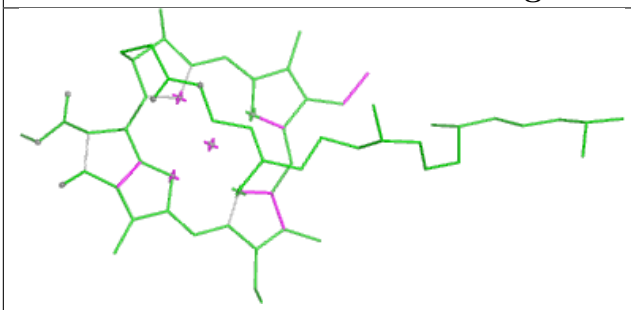
Ligand BCR B 617



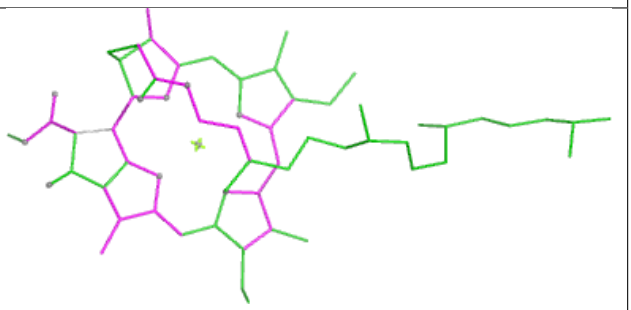
Ligand SQD L 103



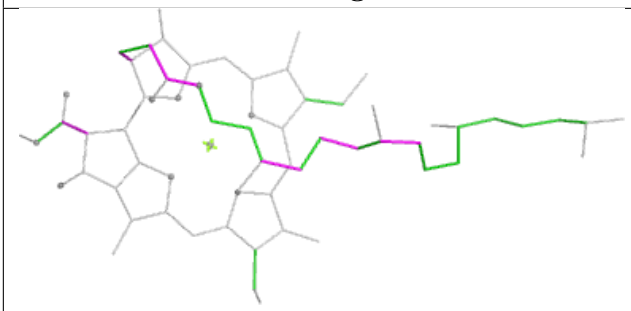
Ligand CLA C 505



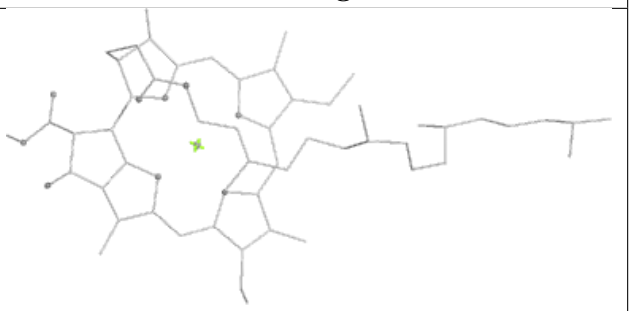
Bond lengths



Bond angles

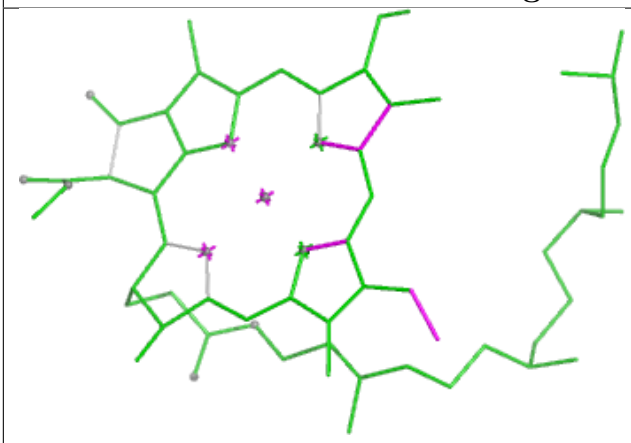


Torsions



Rings

Ligand CLA G 602



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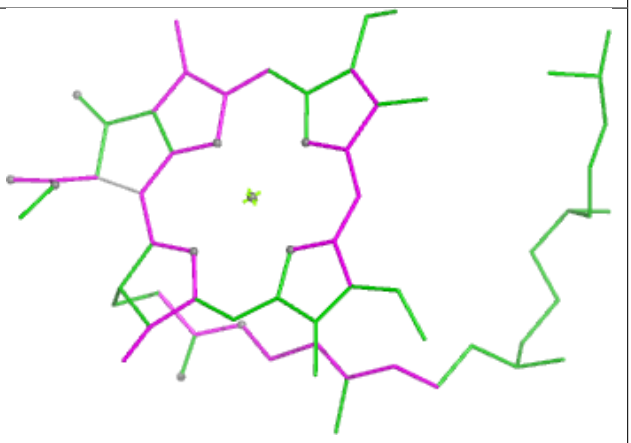
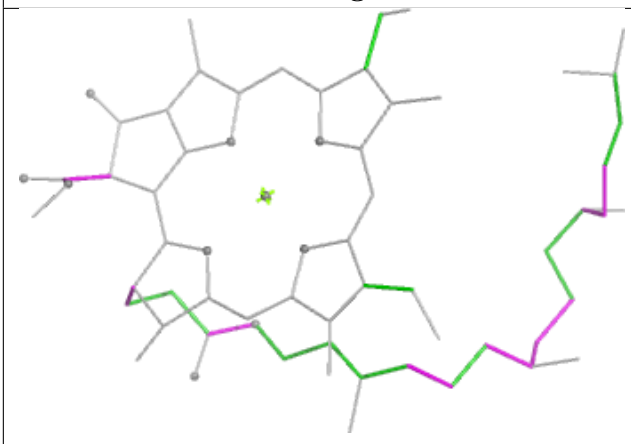


Bond angles



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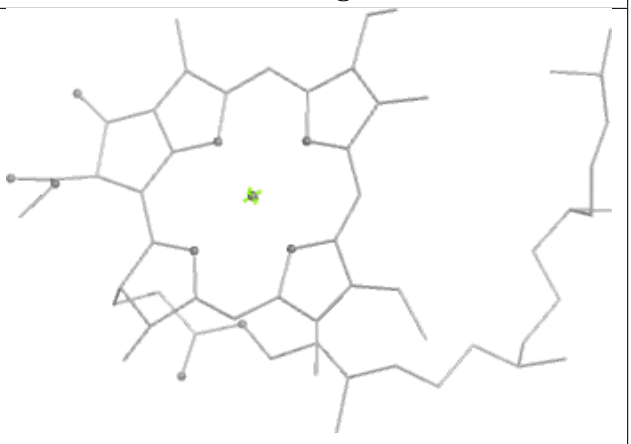
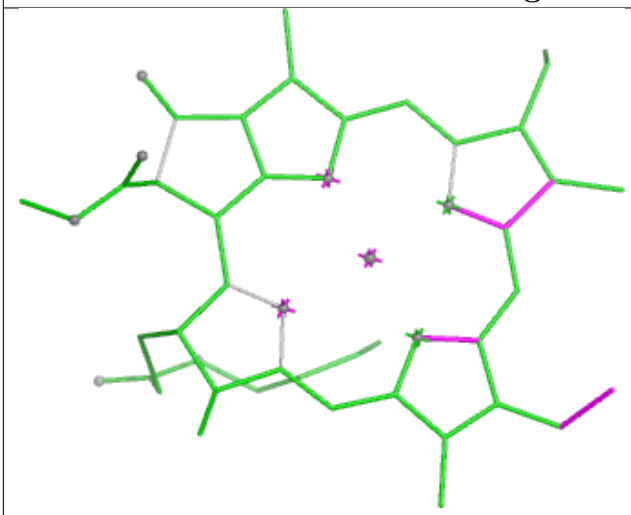


Rings

Ligand CLA R 610



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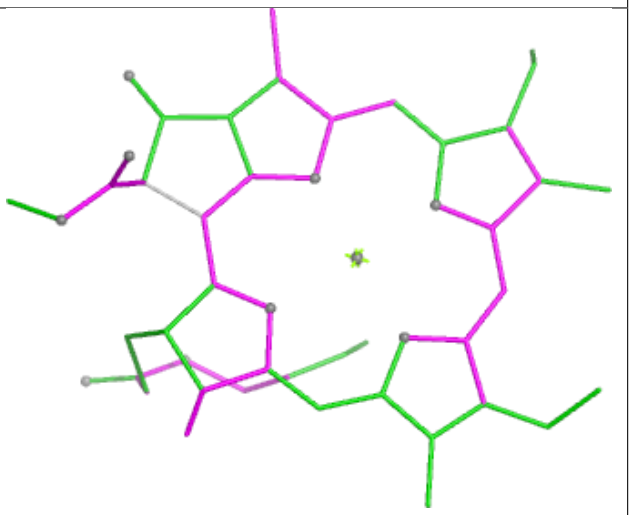
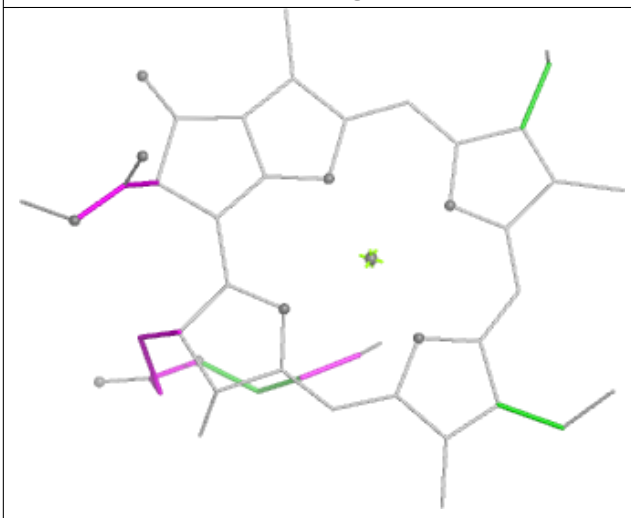


Bond angles



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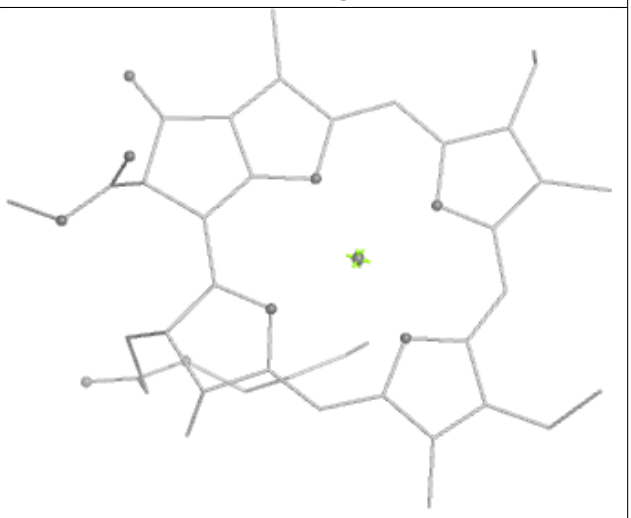
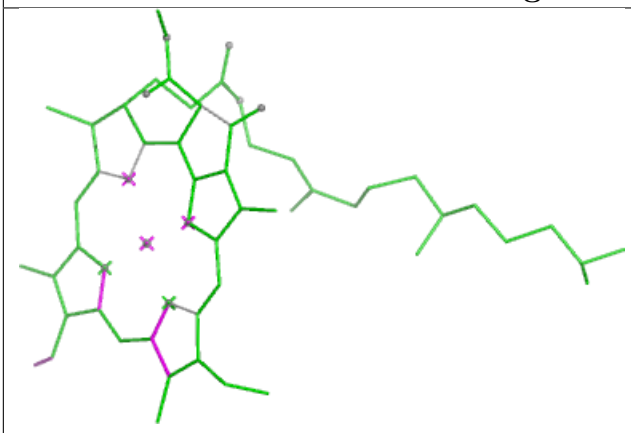


Rings

Ligand CLA Y 611



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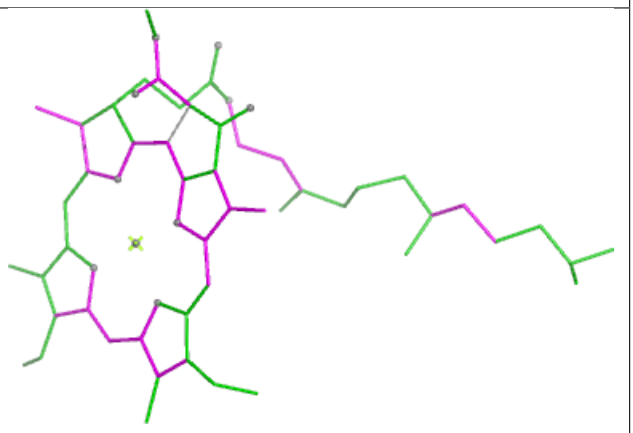
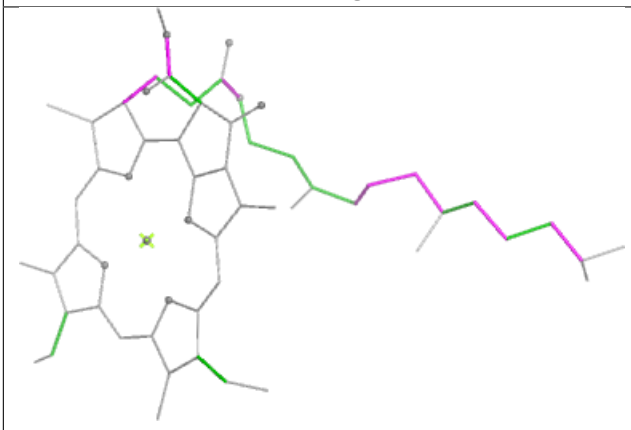


Bond angles



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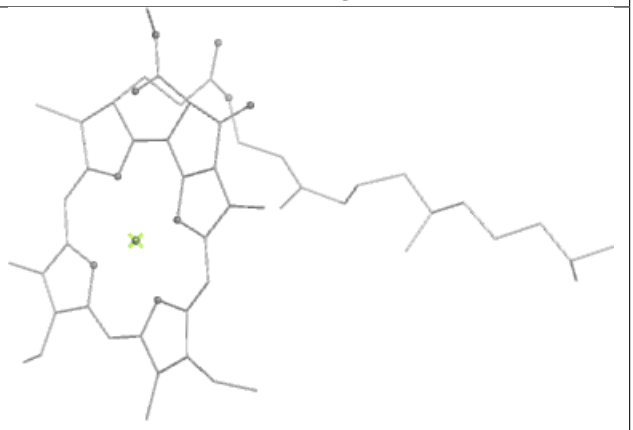
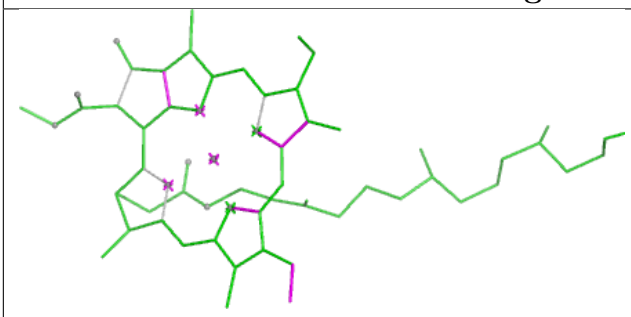


Rings

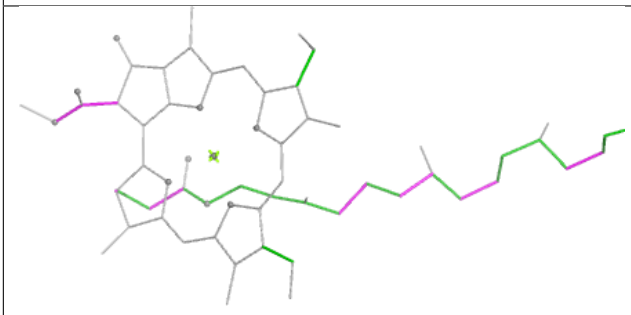
Ligand CLA B 608



Bond lengths



Bond angles



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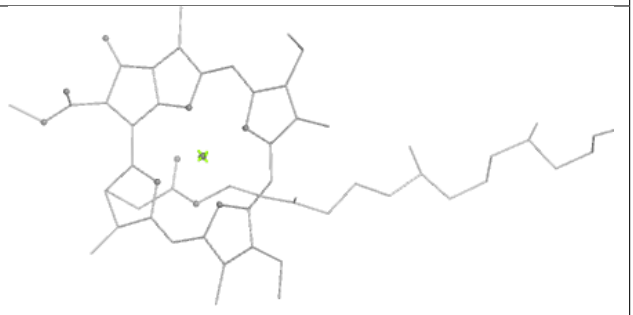
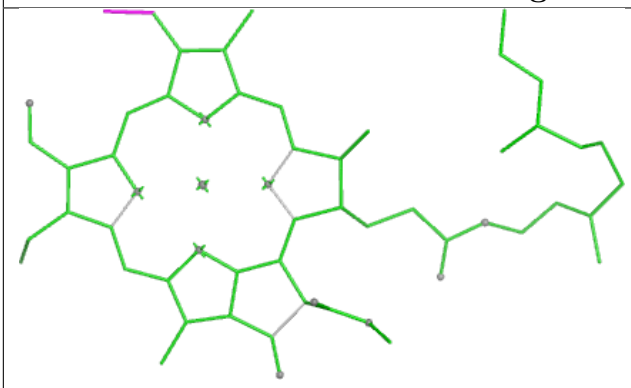


Rings

Ligand CHL s 606



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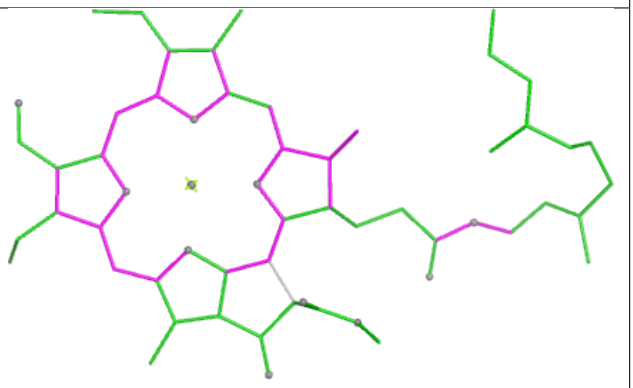
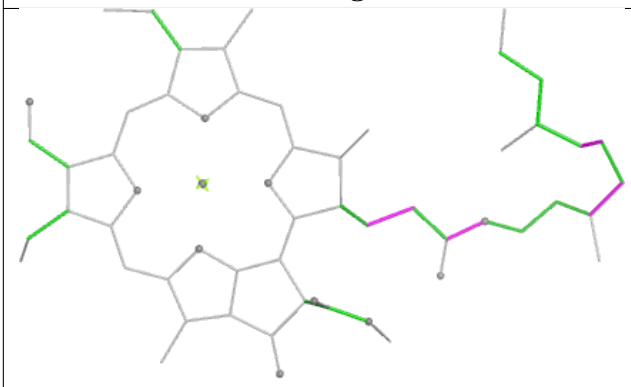


Bond angles

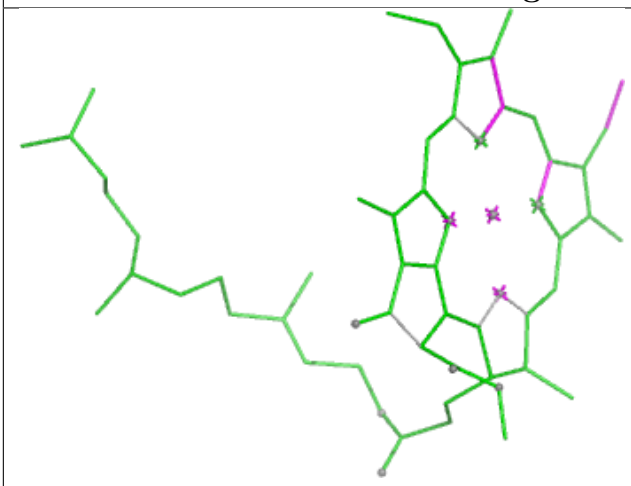


Torsions



Rings

Ligand CLA G 611



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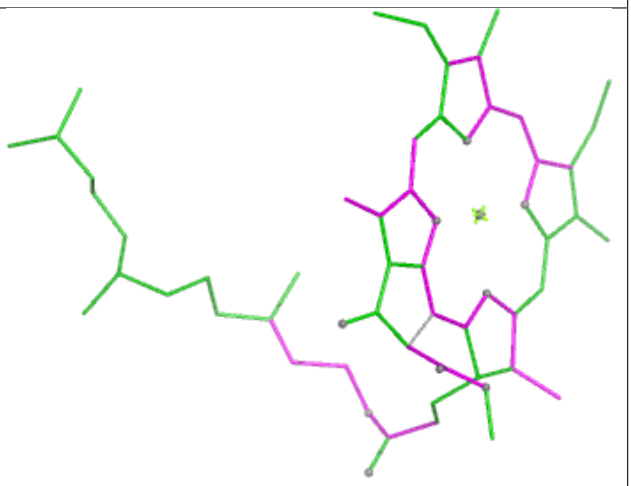
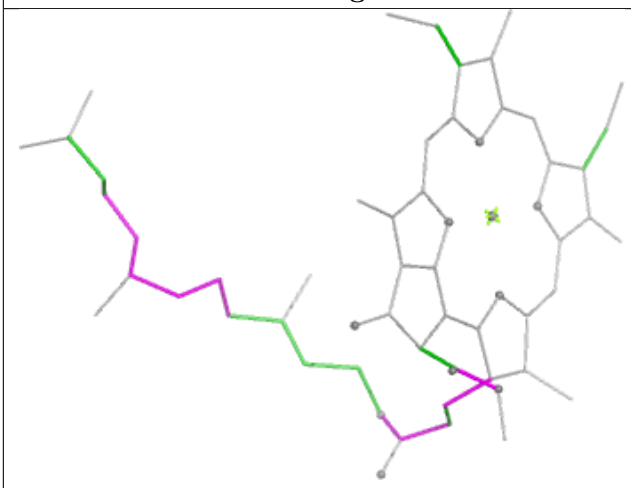


Bond angles



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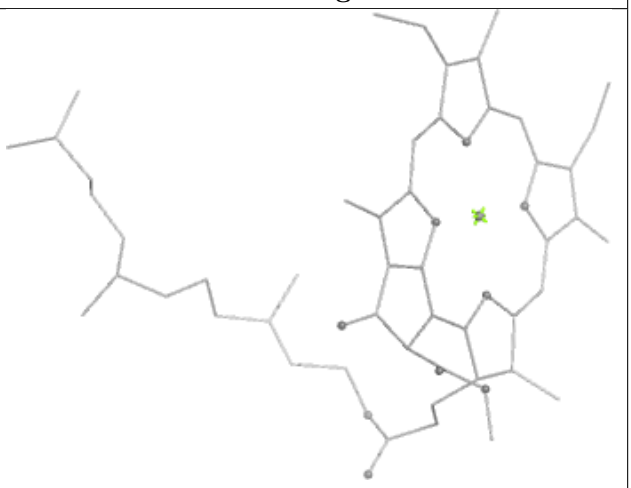
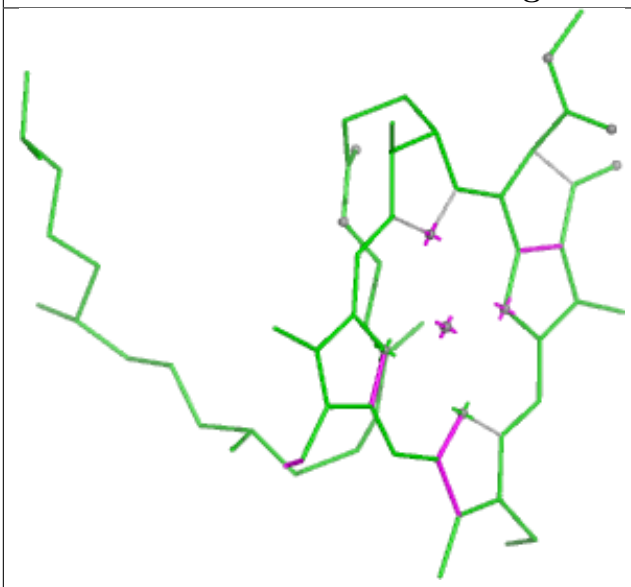


Rings

Ligand CLA G 613



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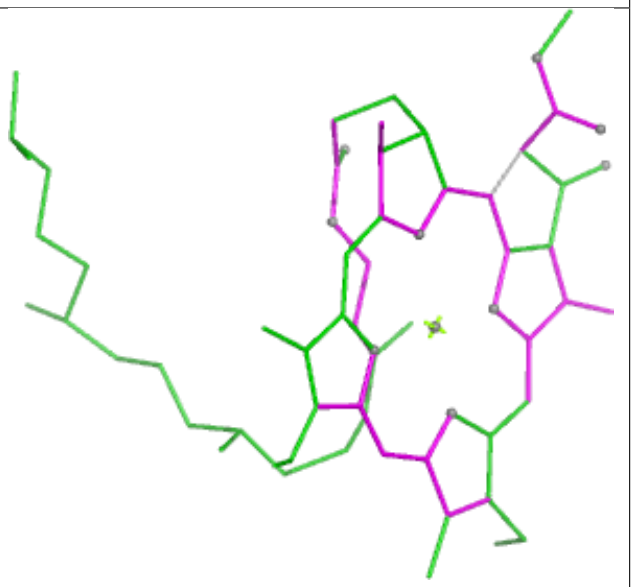
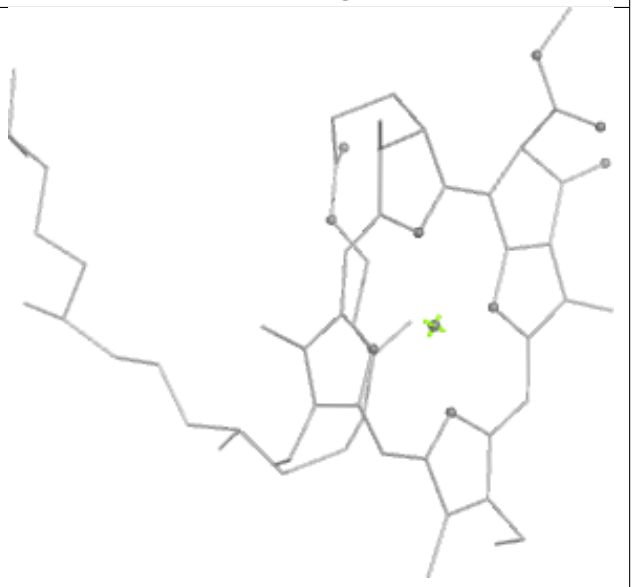


Bond angles

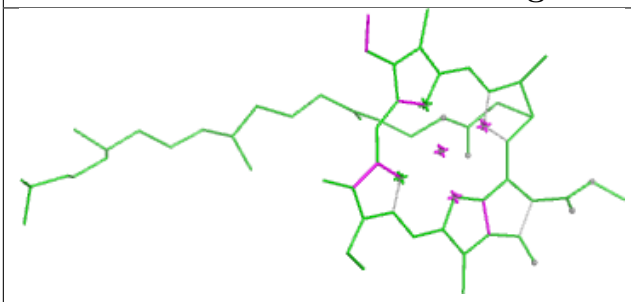


Torsions



Rings

Ligand CLA b 608



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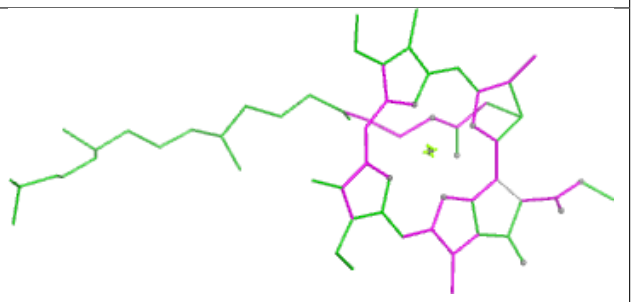
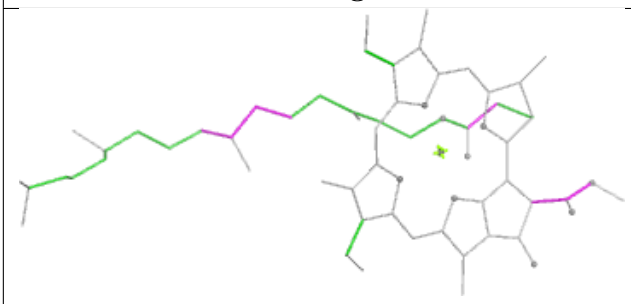


Bond angles

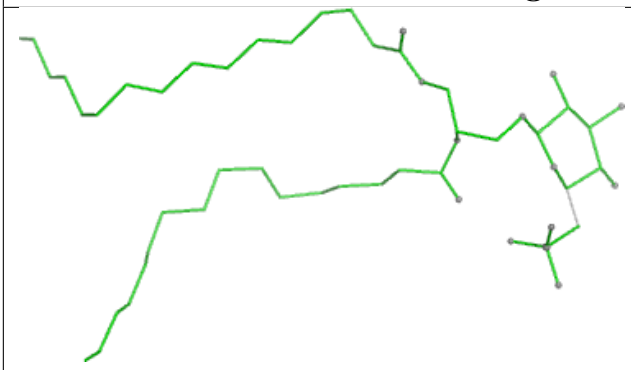


Torsions



Rings

Ligand SQD B 620



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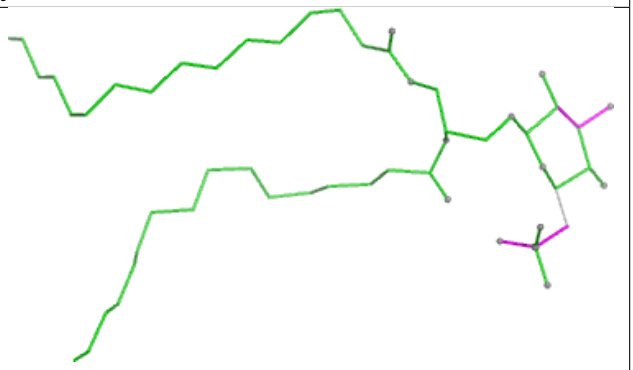
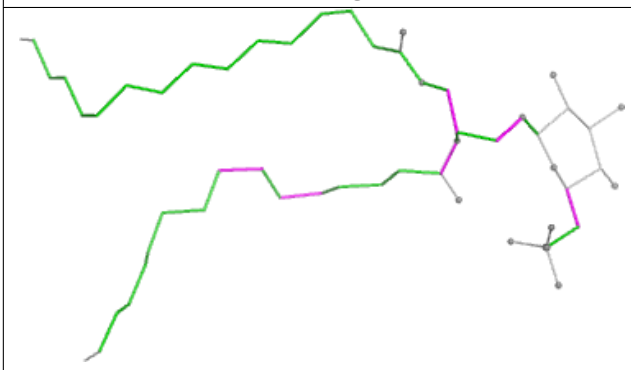


Bond angles

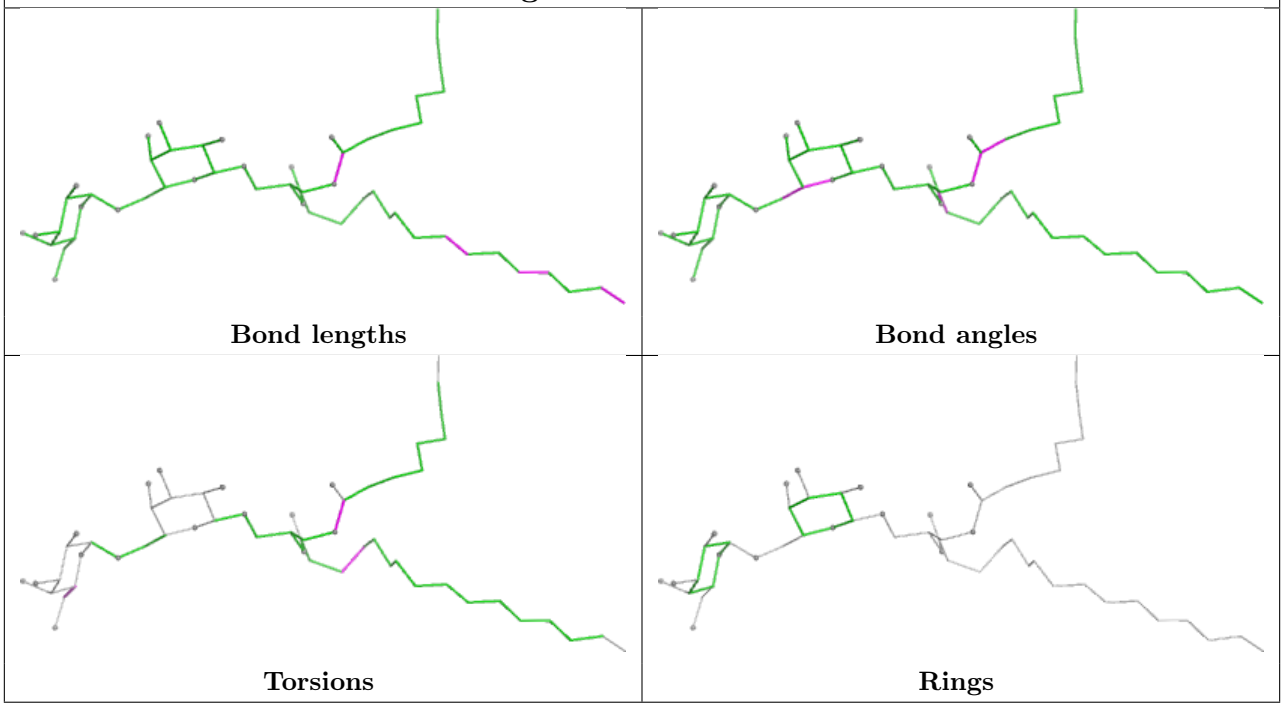


Torsions

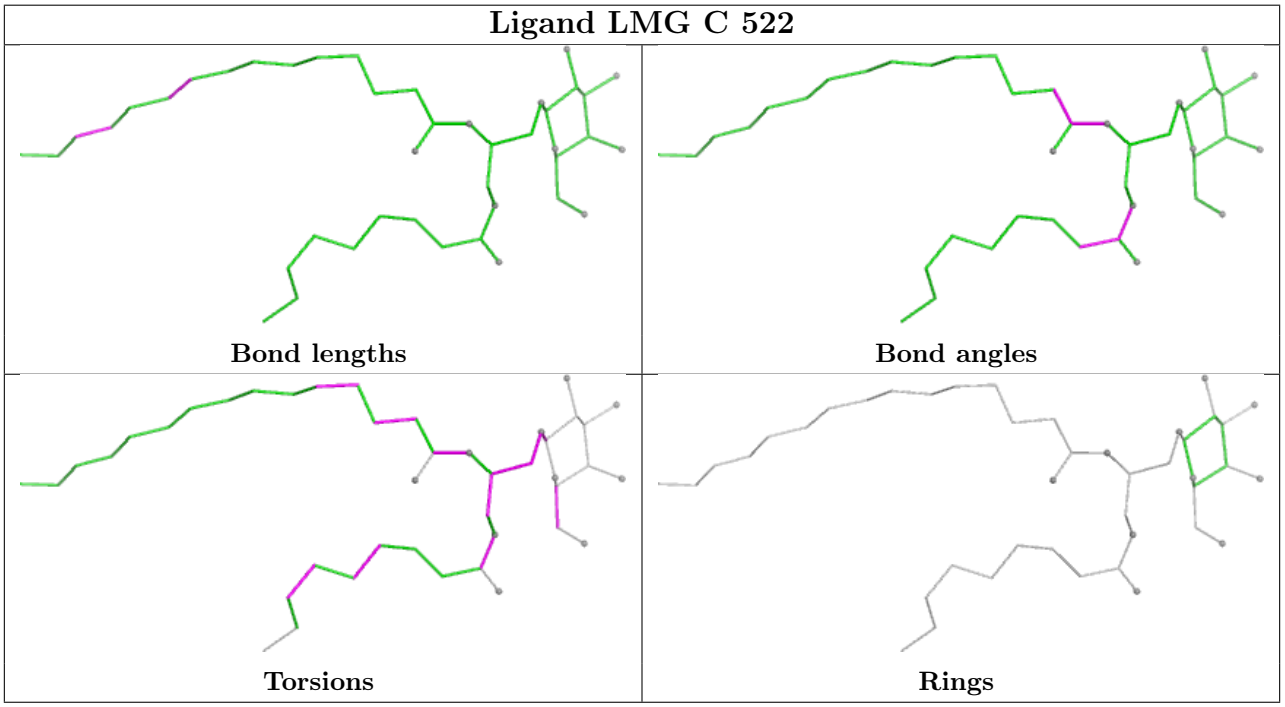


Rings

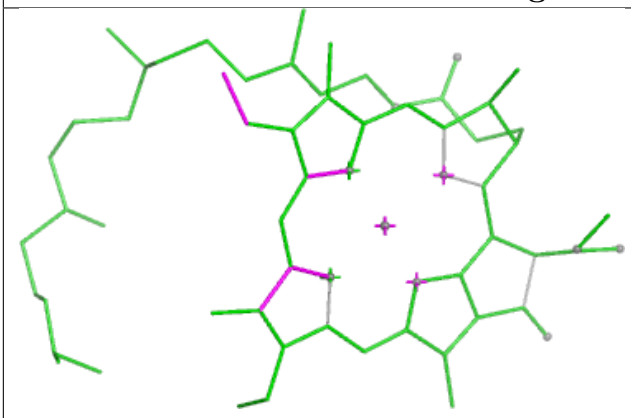
Ligand DGD C 517



Ligand LMG C 522



Ligand CLA g 602



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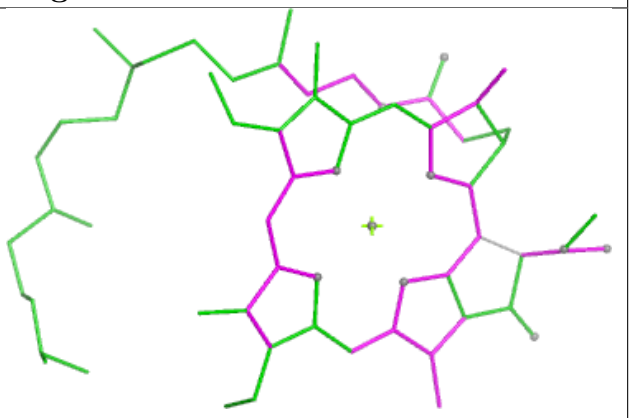
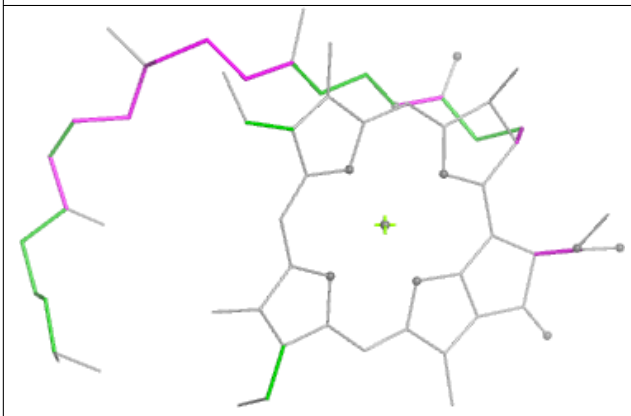
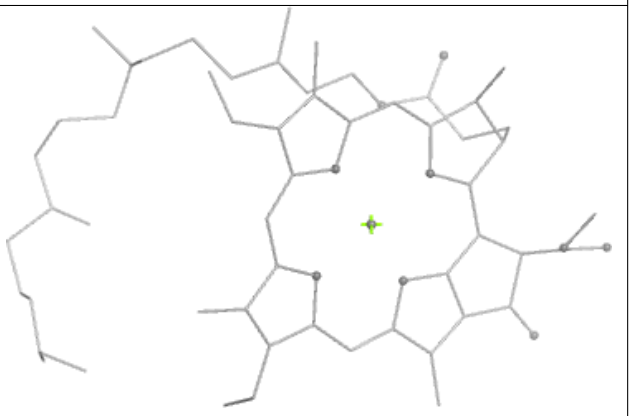


Bond angles



Torsions



Rings

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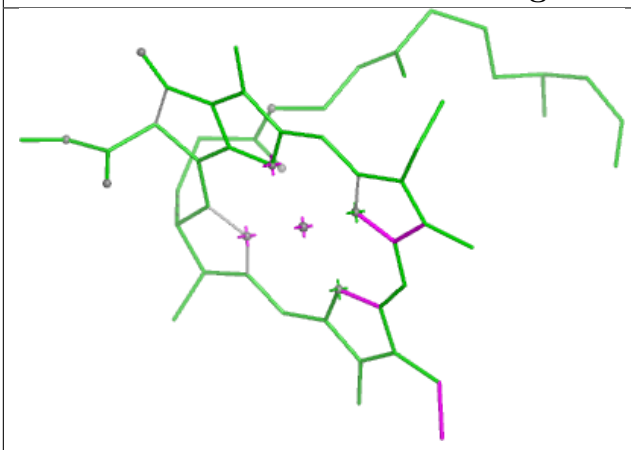
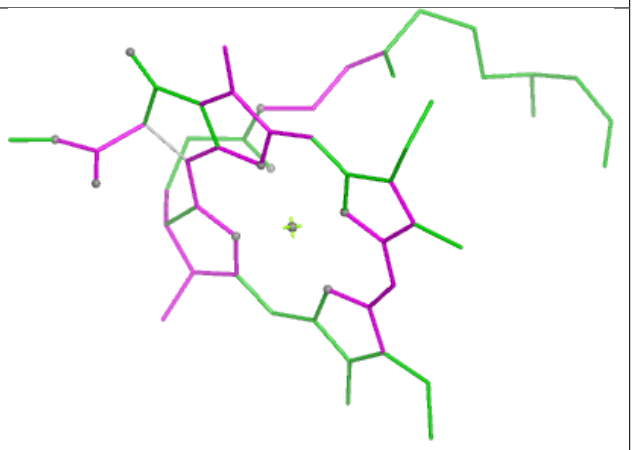
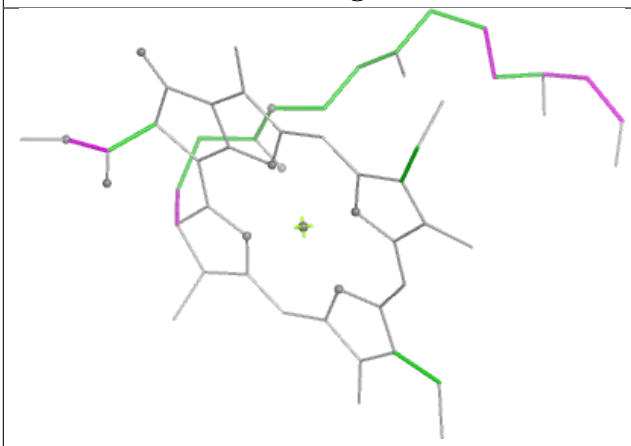


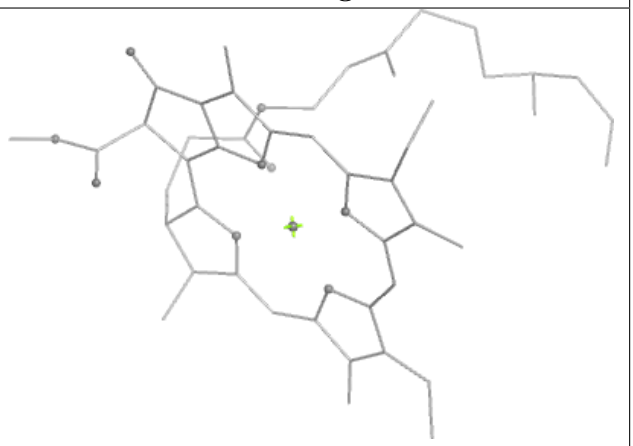
Bond lengths



Bond angles

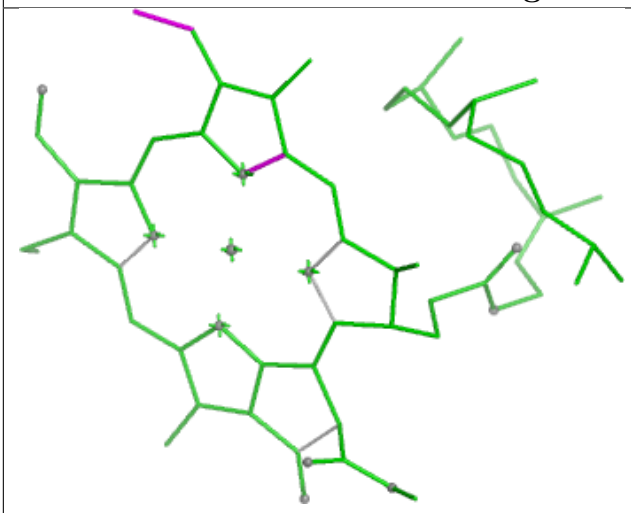


Torsions



Rings

Ligand CHL Y 608



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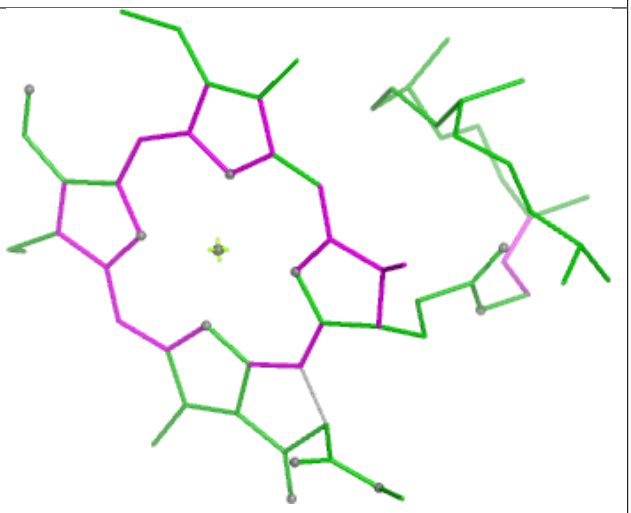

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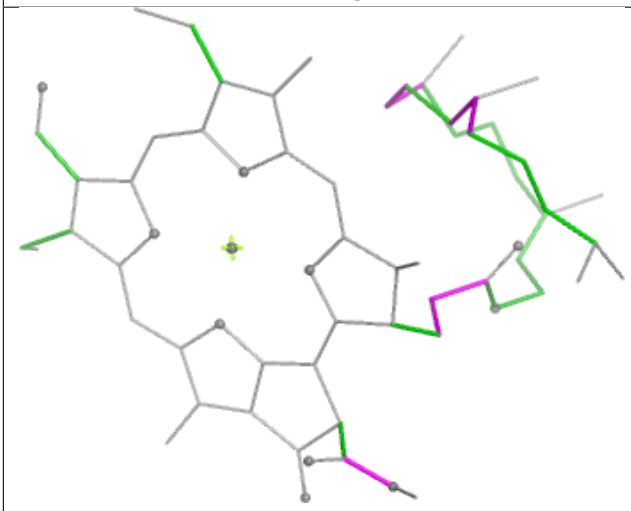

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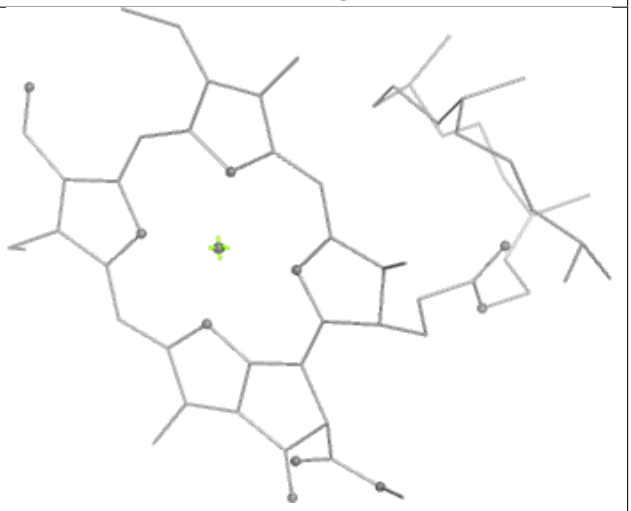
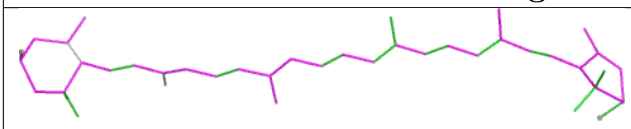


Rings

Ligand LUT g 616



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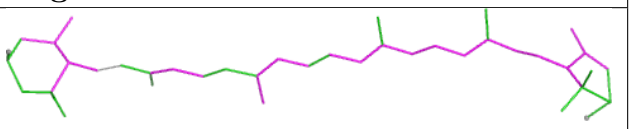

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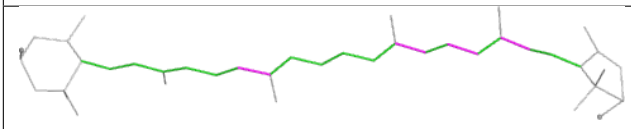

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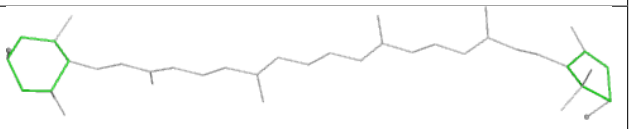
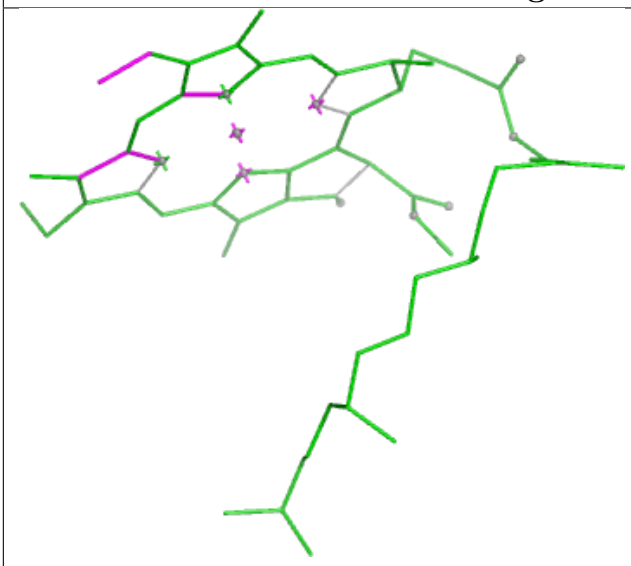


Rings

Ligand CLA y 304



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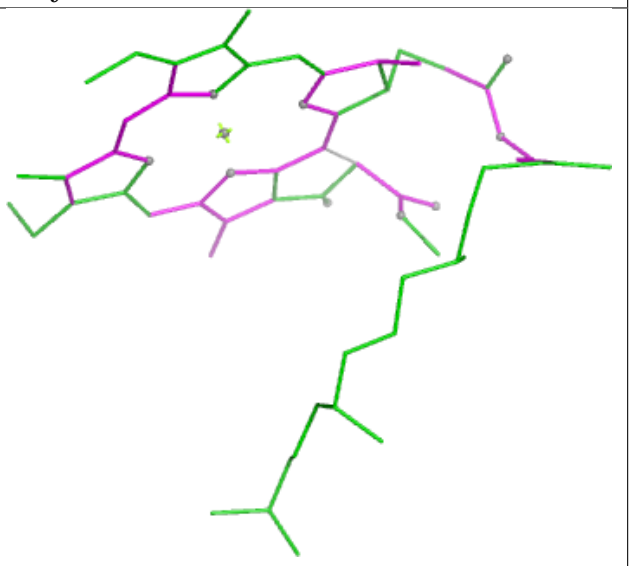

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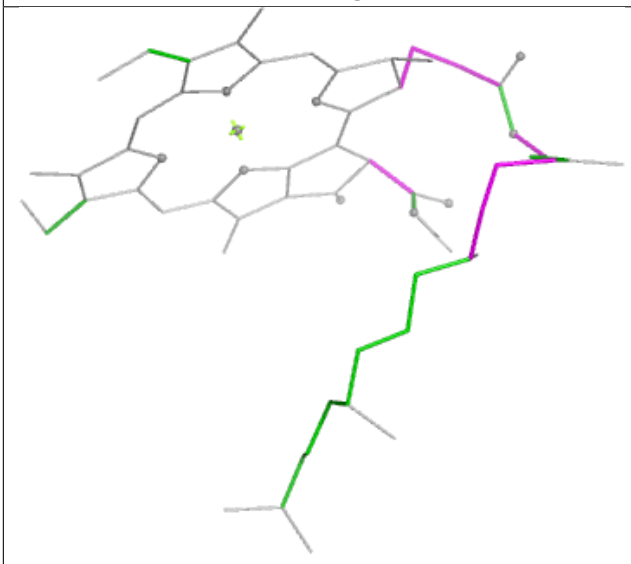

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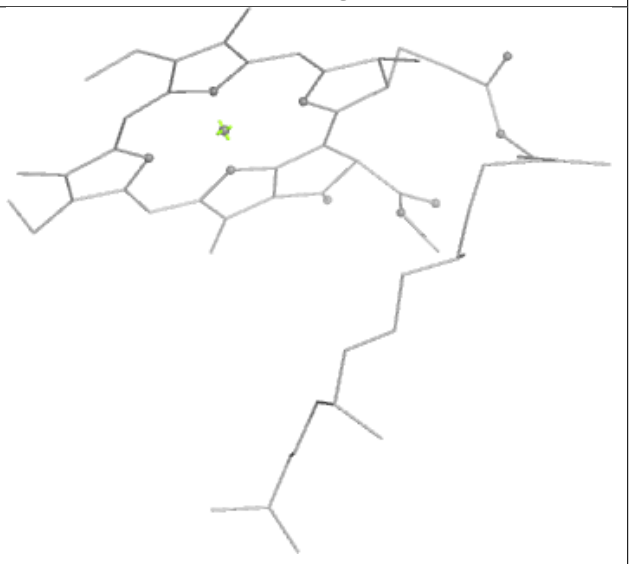
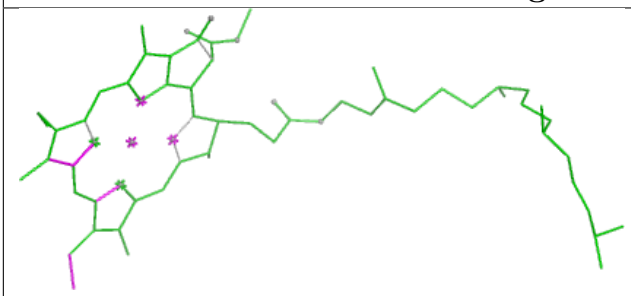


Rings

Ligand CLA a 406



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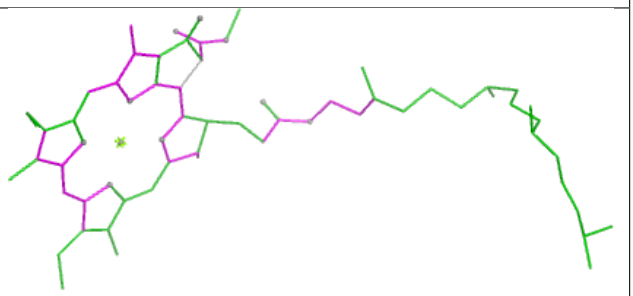
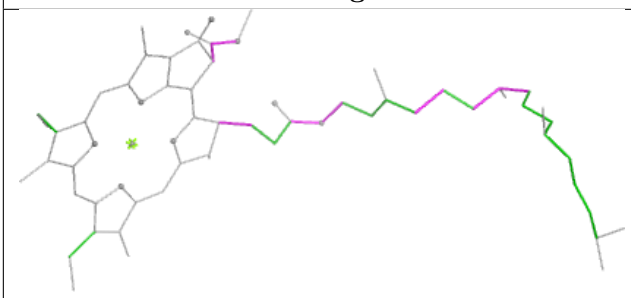


Bond angles



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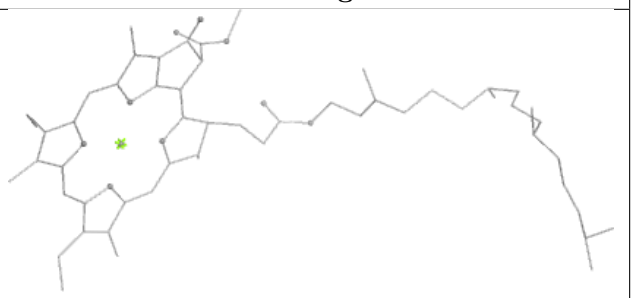
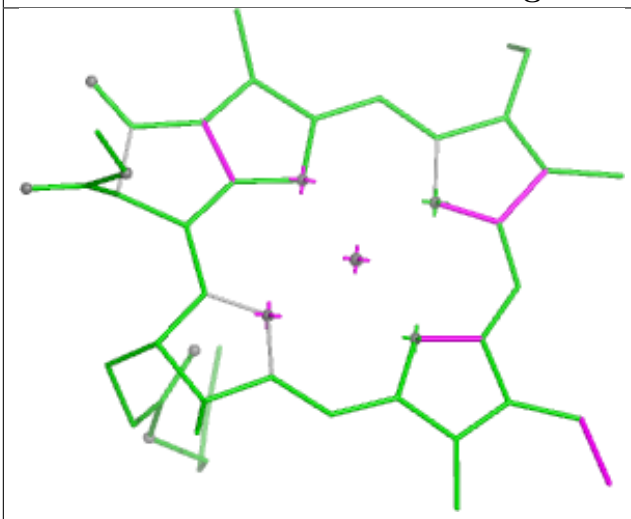


Rings

Ligand CLA Y 604



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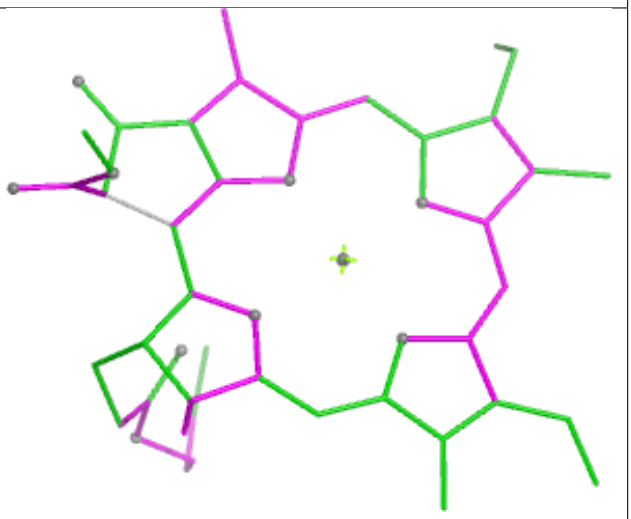

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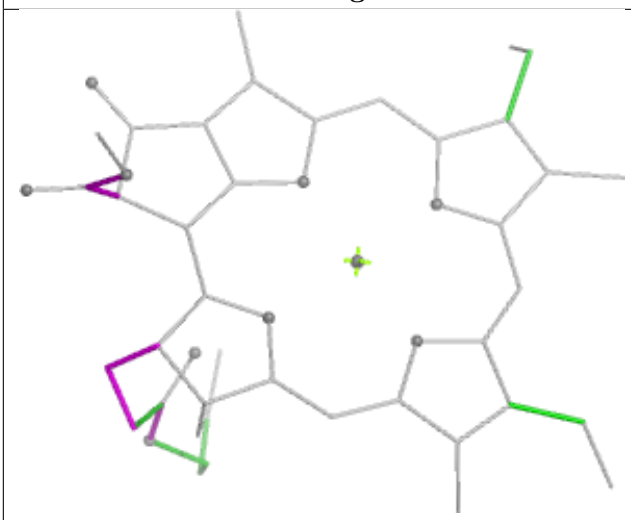

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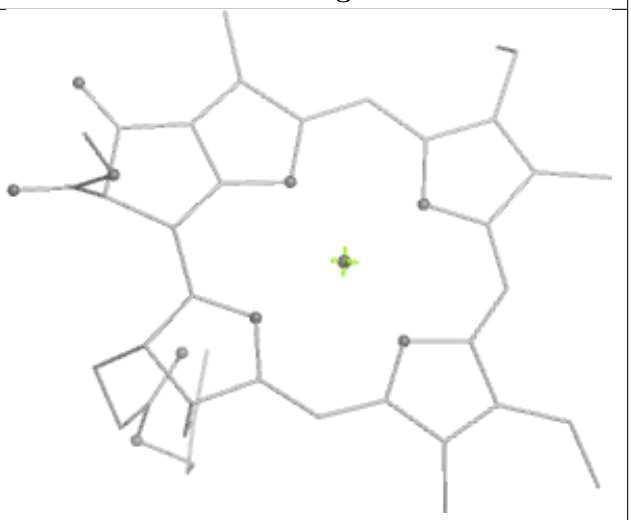
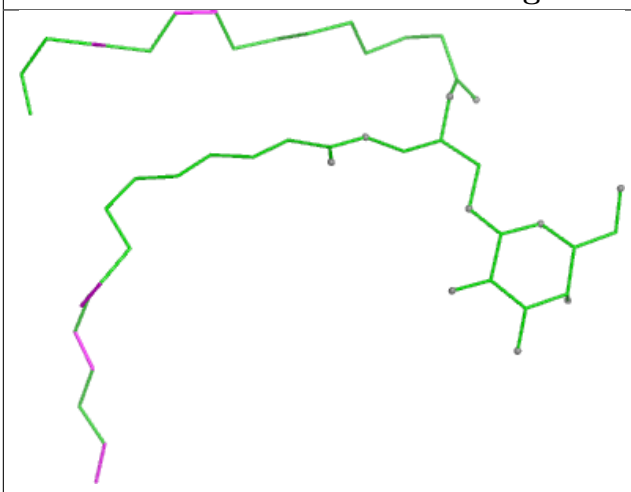


Rings

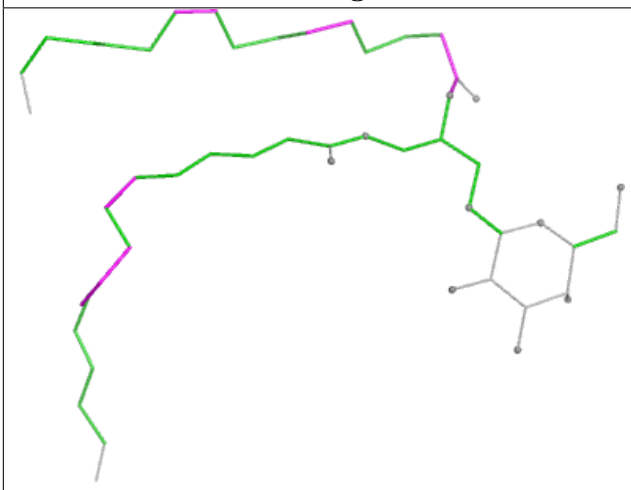
Ligand LMG k 102



Bond lengths



Bond angles



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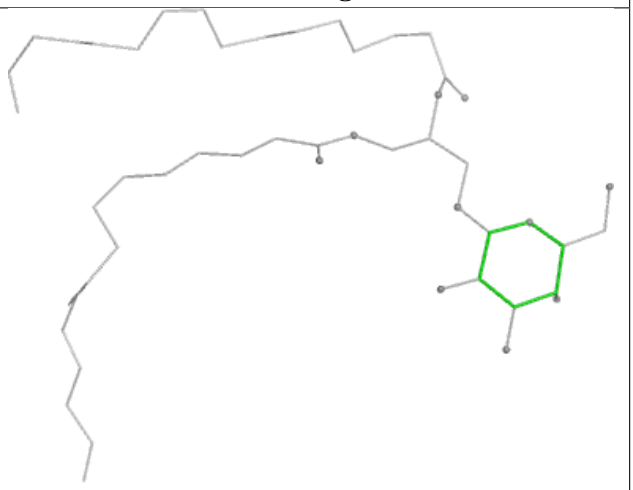
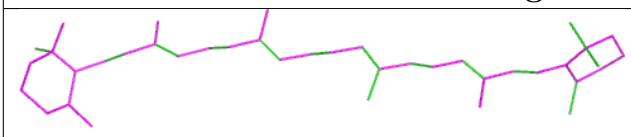


Rings

Ligand BCR b 617



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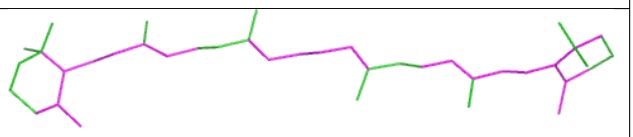
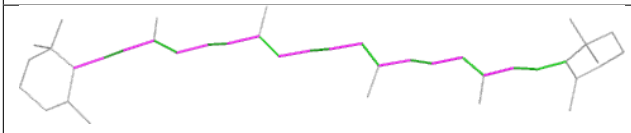


Bond angles



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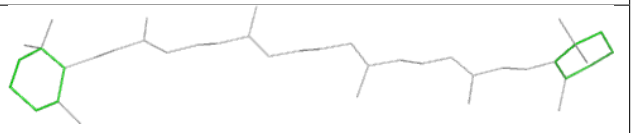
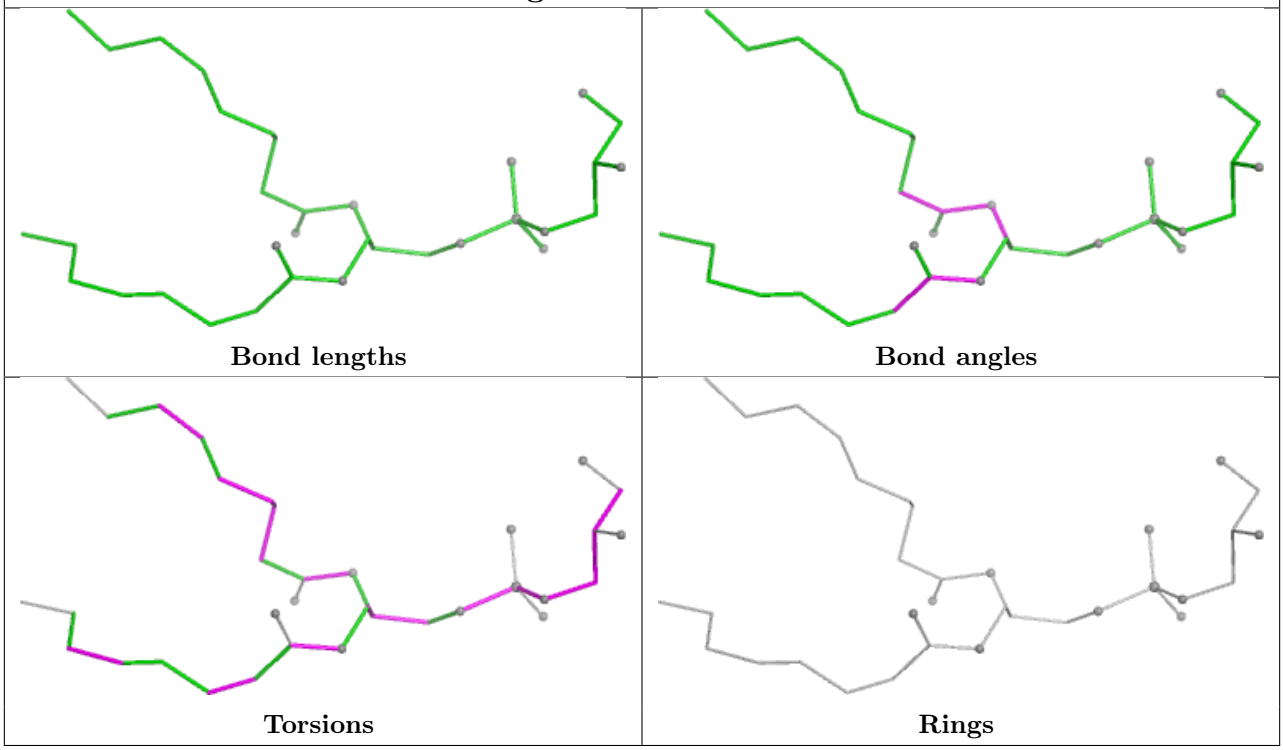
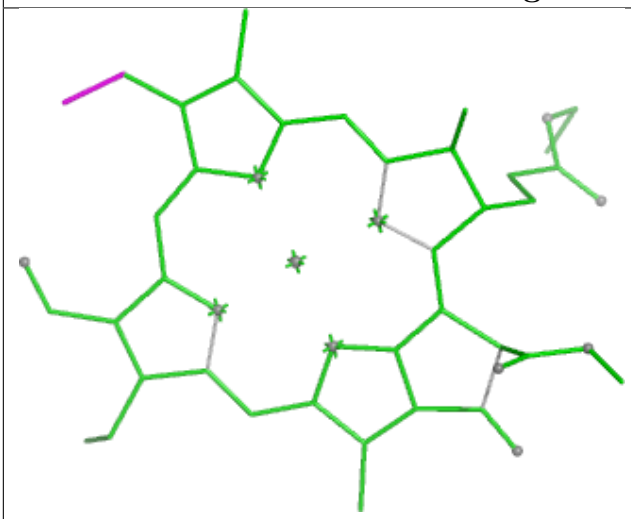


Rings

Ligand LHG b 621



Ligand CHL Y 605



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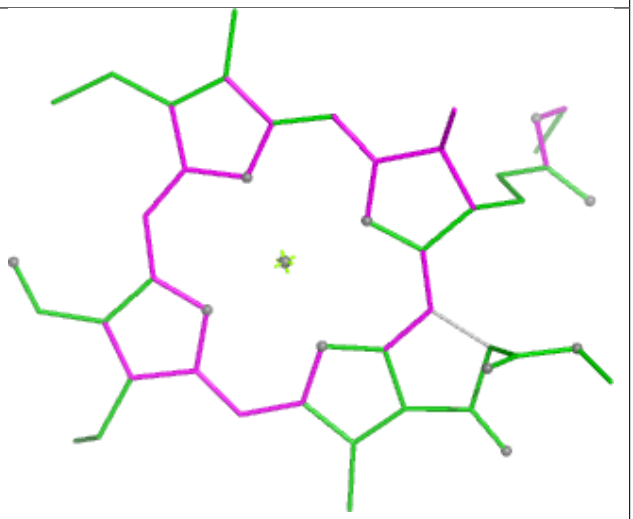
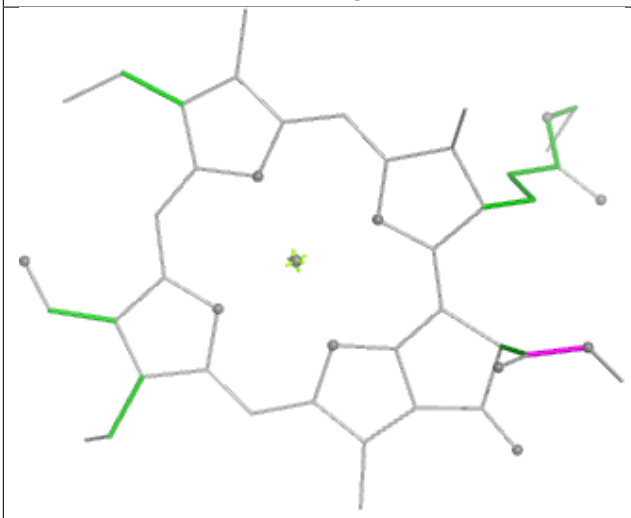


Bond angles



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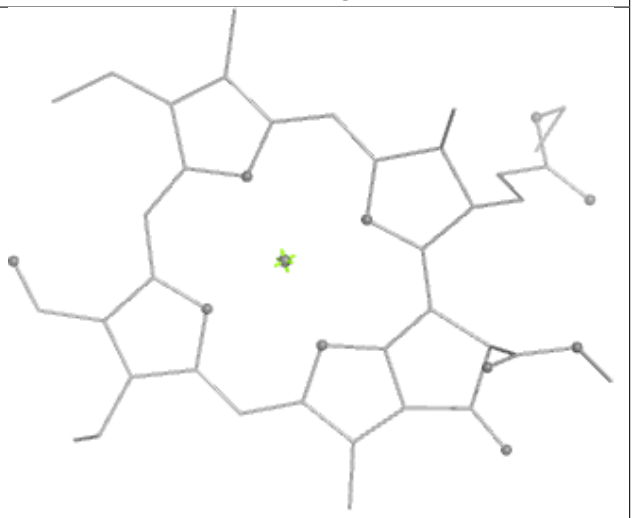
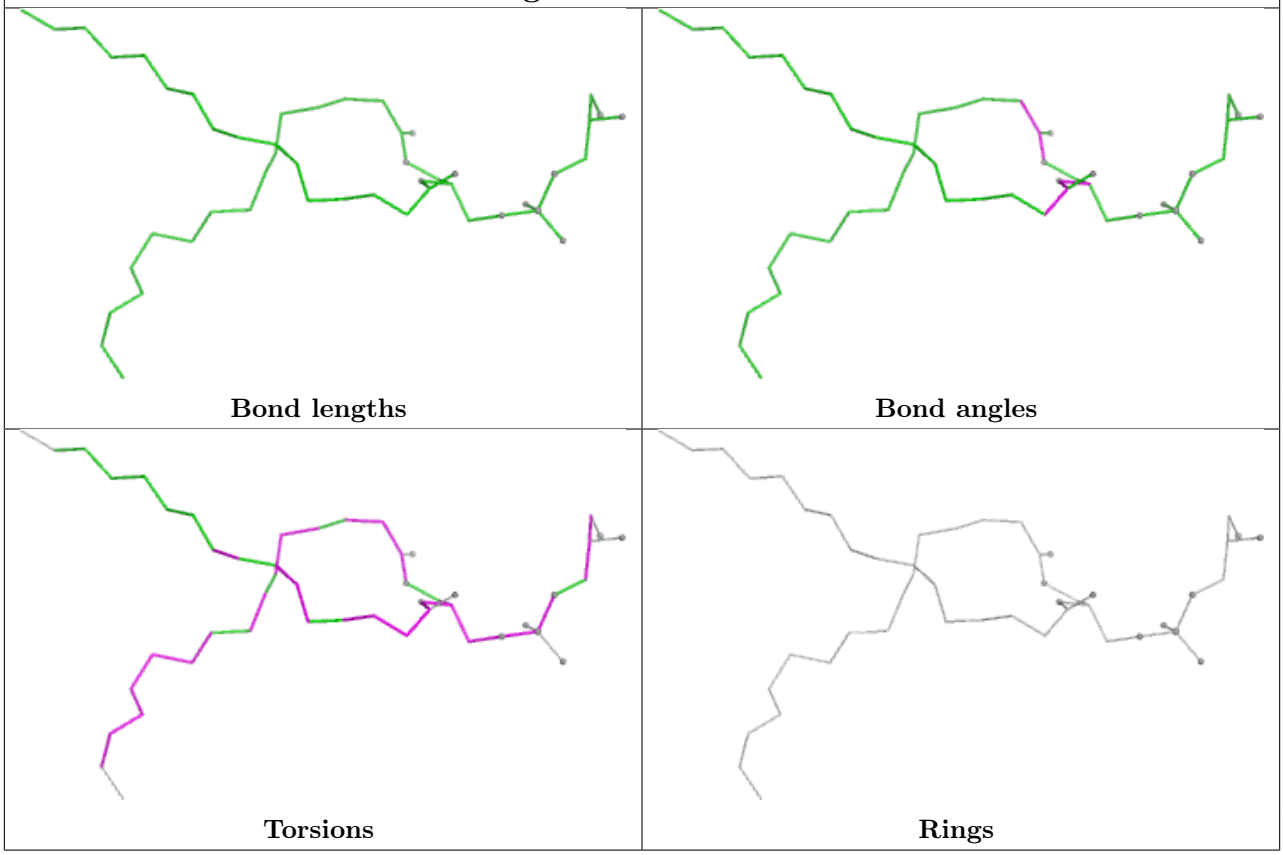
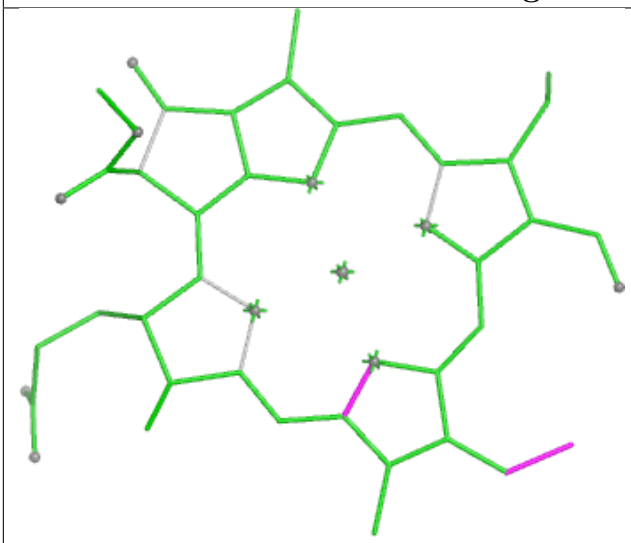


Rings

Ligand LHG D 407



Ligand CHL G 605



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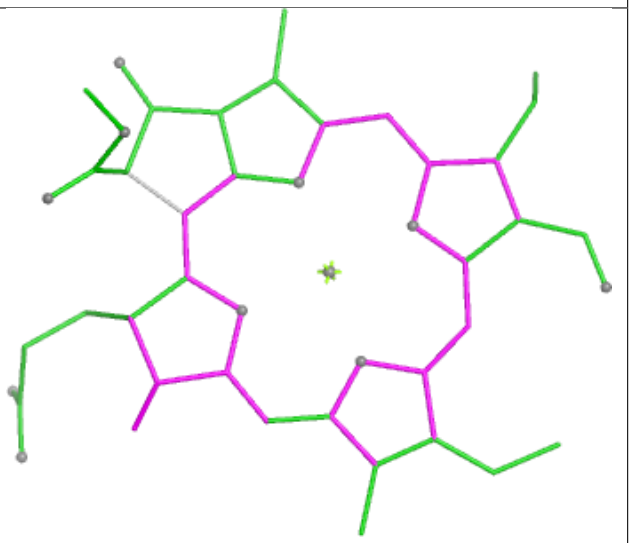
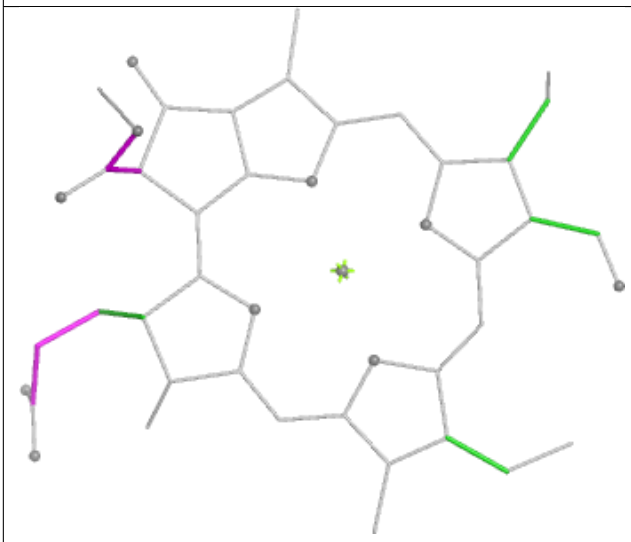


Bond angles



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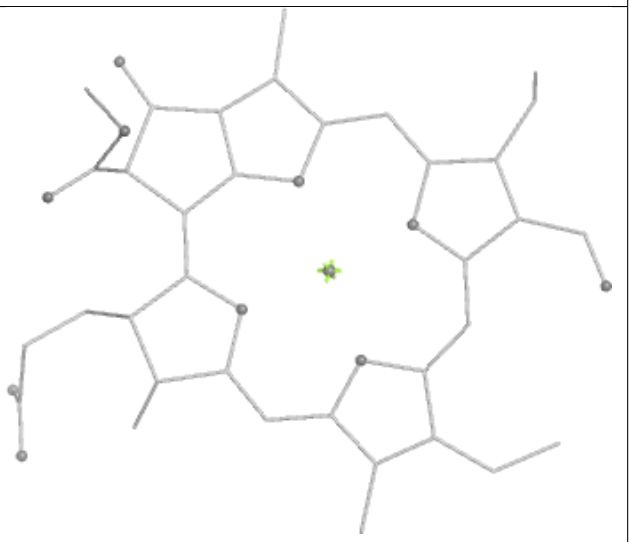
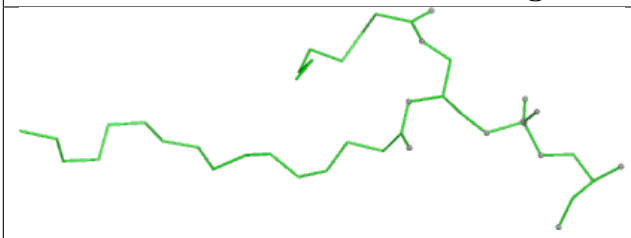


Rings

Ligand LHG g 618



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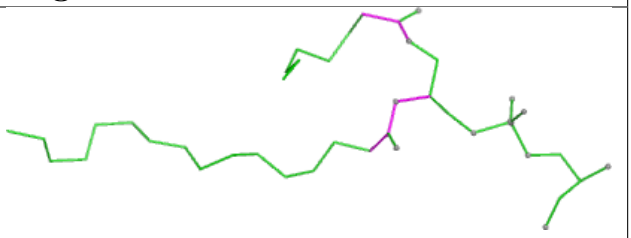
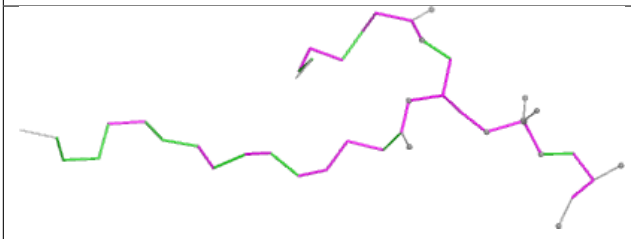


Bond angles



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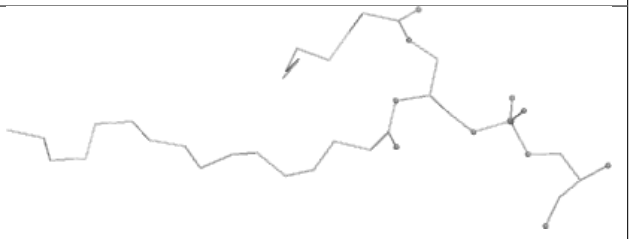
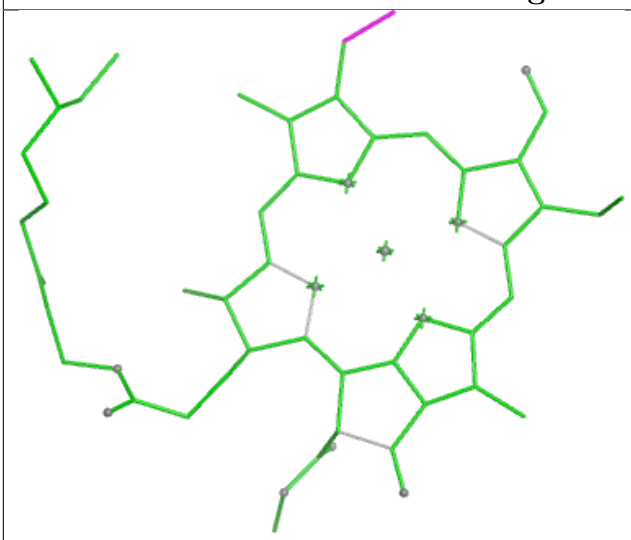


Rings

Ligand CHL g 607



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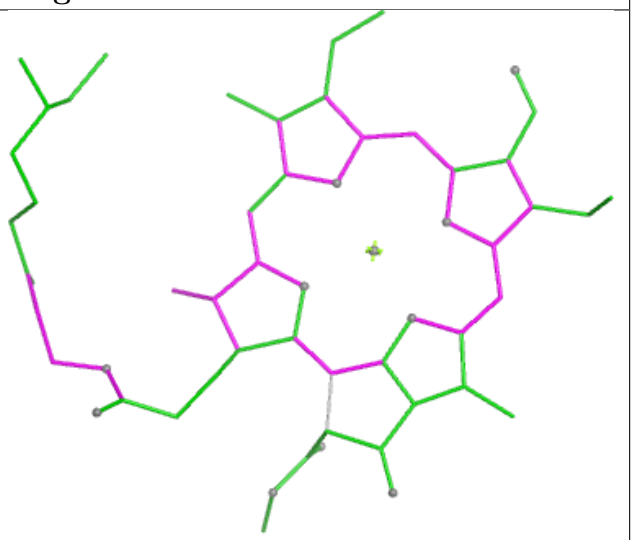
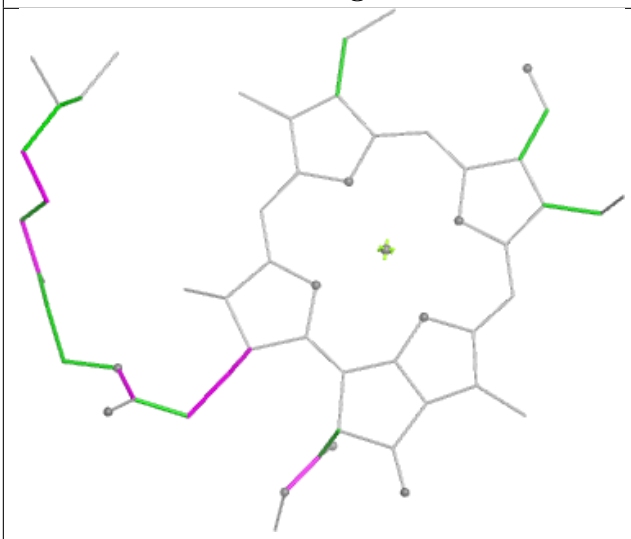


Bond angles

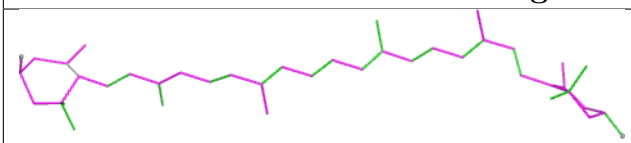


Torsions



Rings

Ligand LUT s 615



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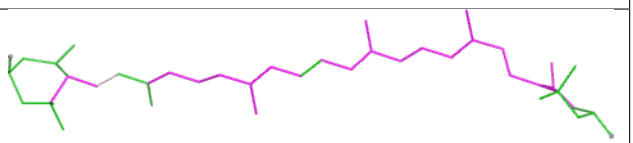
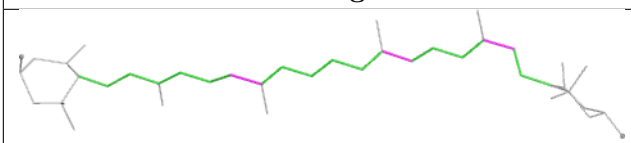


Bond angles



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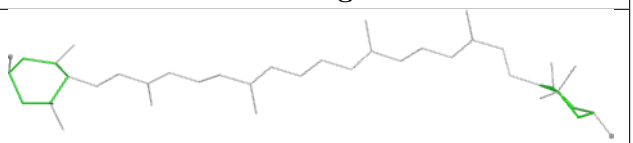
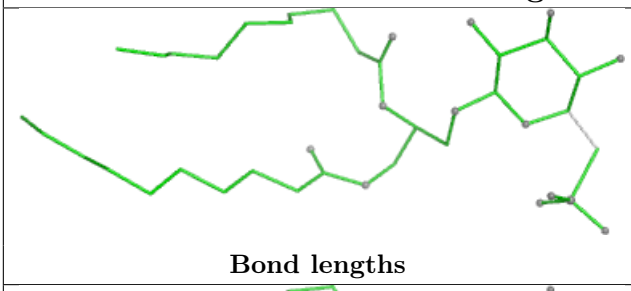


Rings

Ligand SQD L 101



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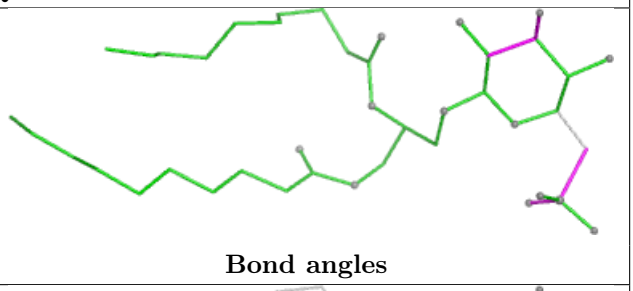
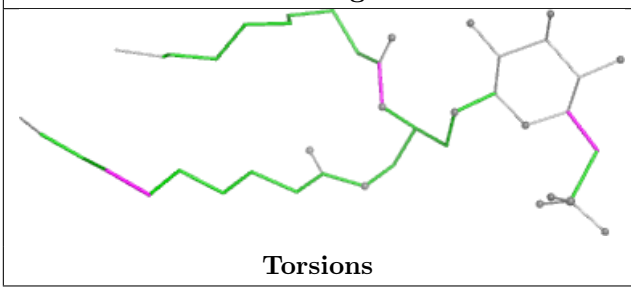


Bond angles



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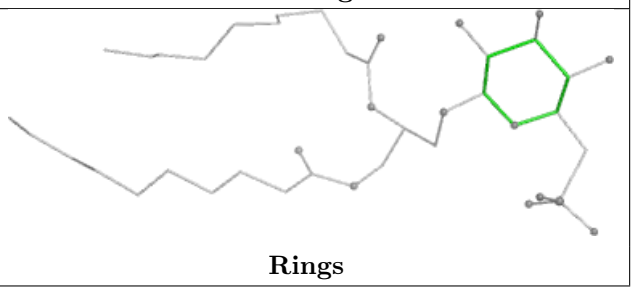
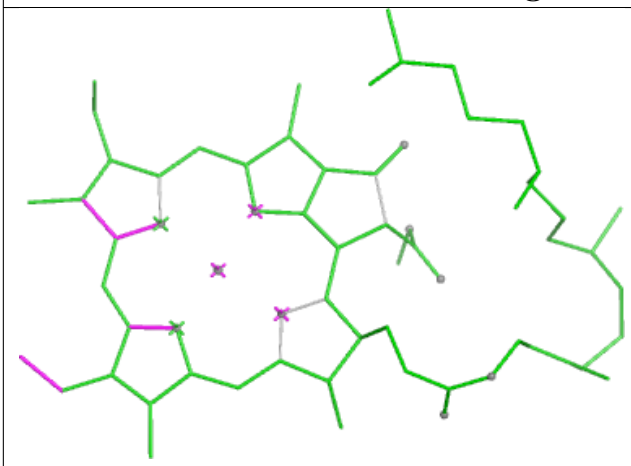


Rings

Ligand CLA B 610



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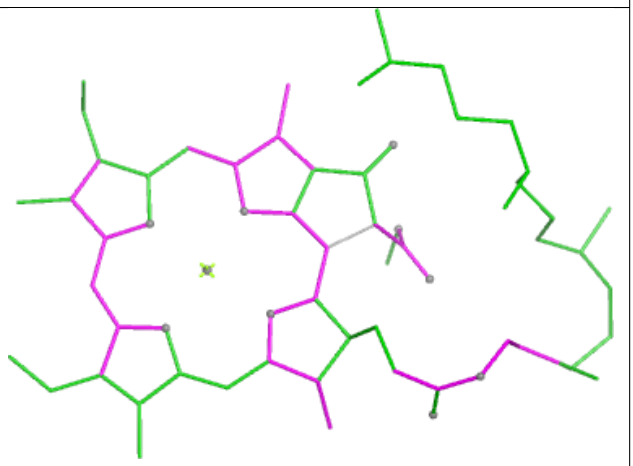
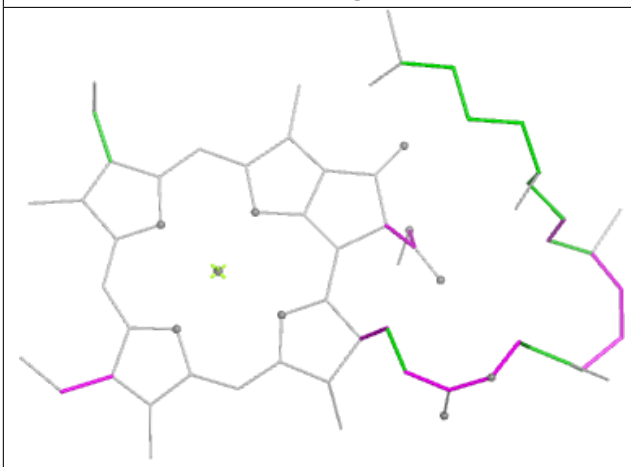


Bond angles



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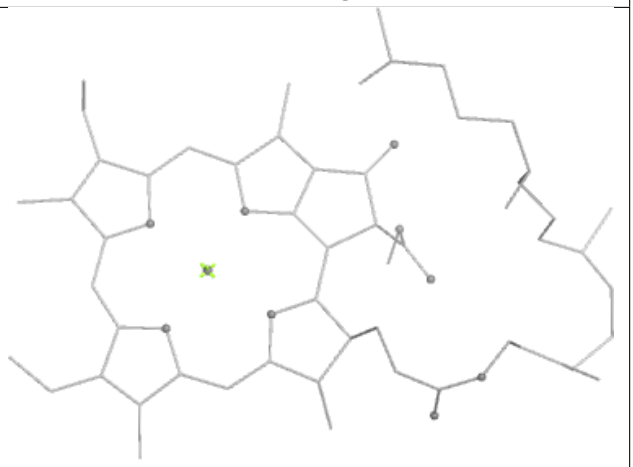
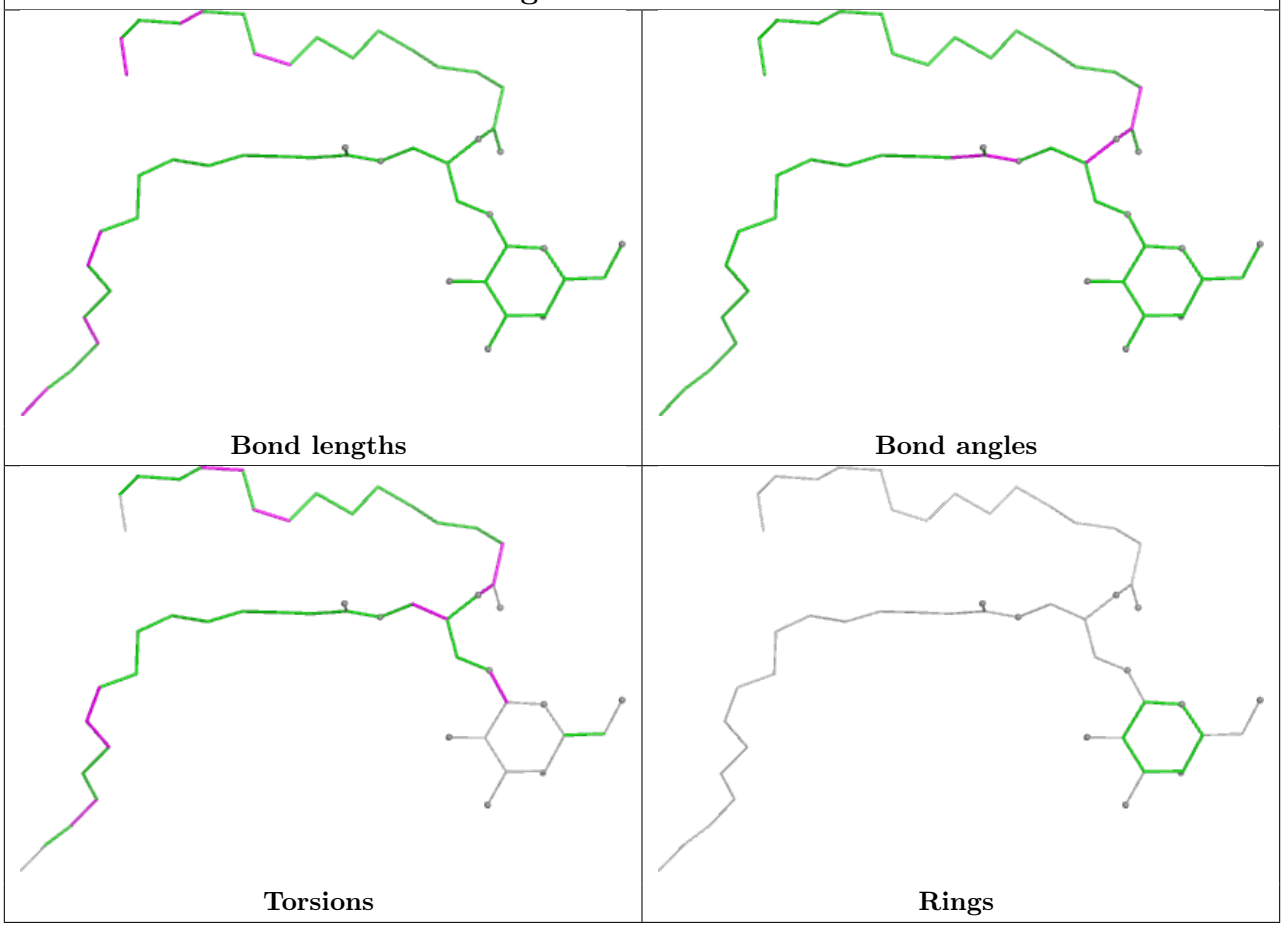


Rings

Ligand LMG C 520



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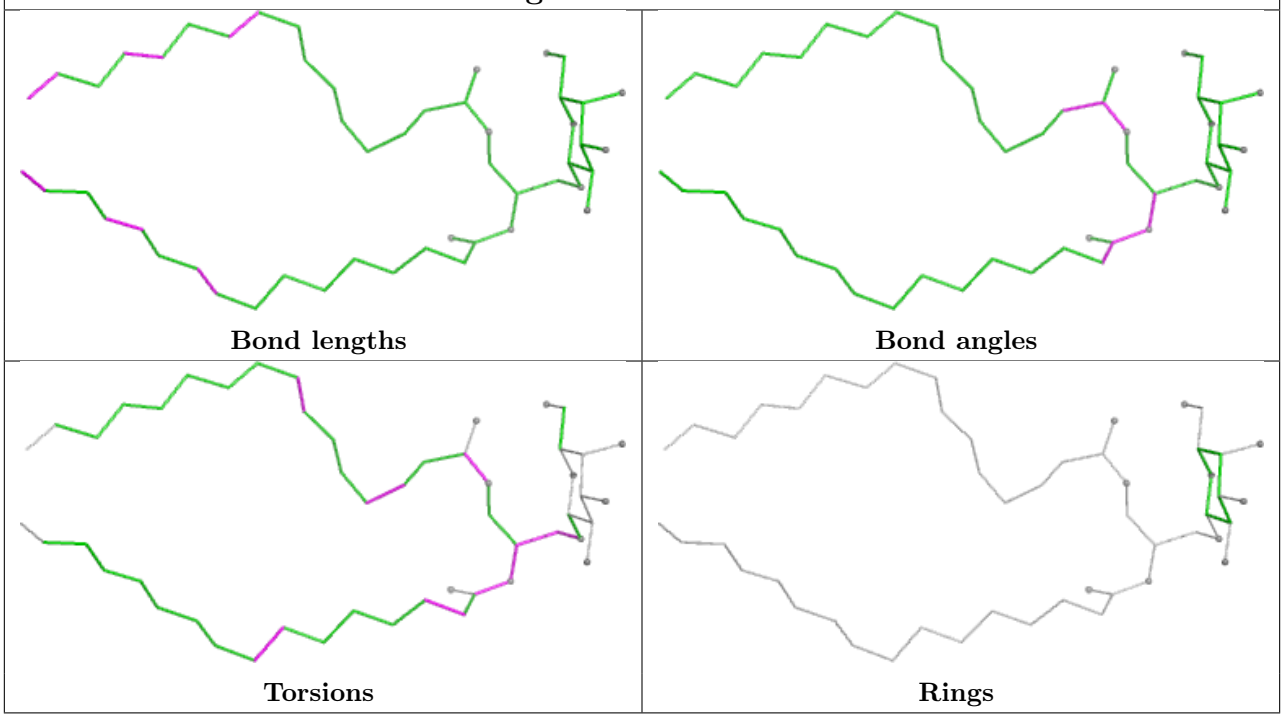
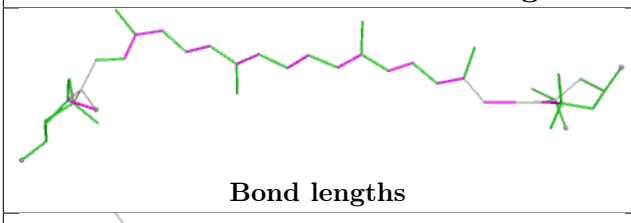
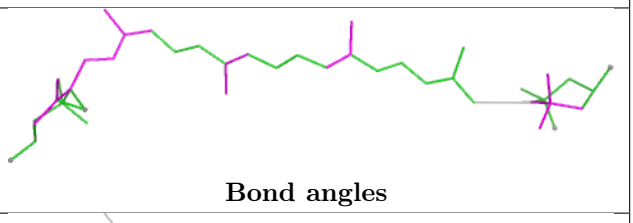


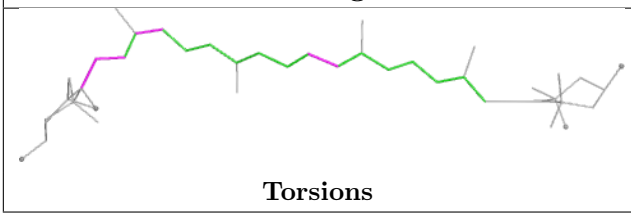
Ligand NEX N 617



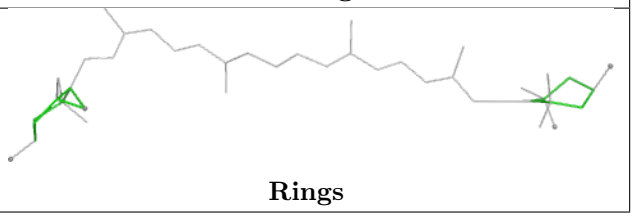
Bond lengths



Bond angles

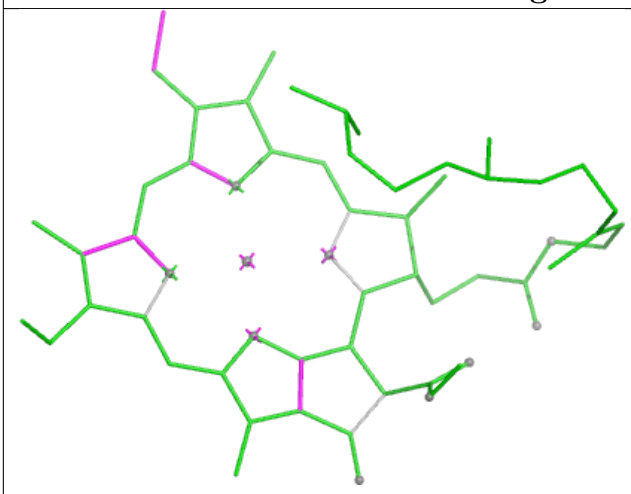


Torsions



Rings

Ligand CLA r 603



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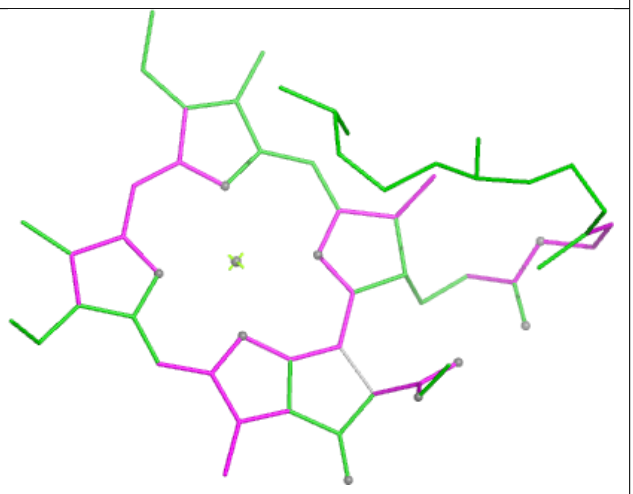
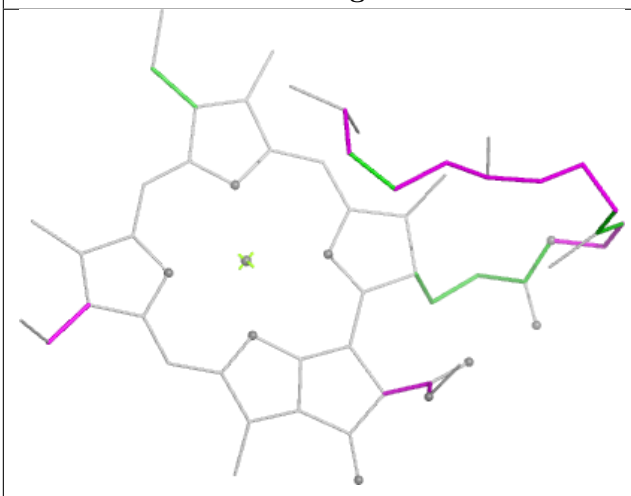


Bond angles



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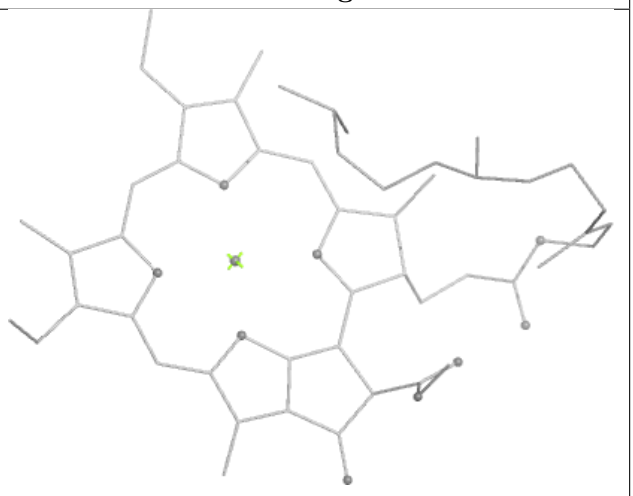
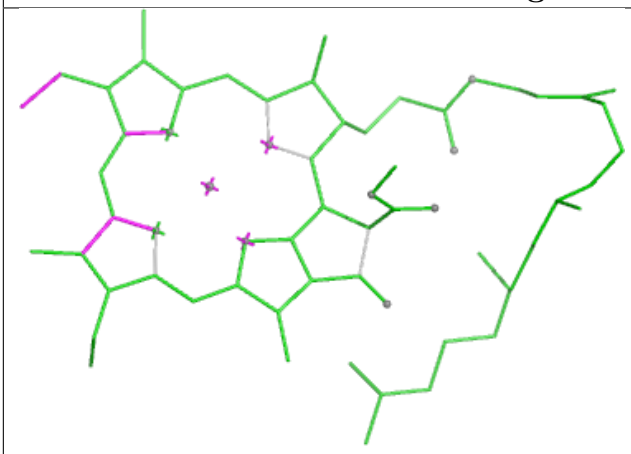


Rings

Ligand CLA b 610



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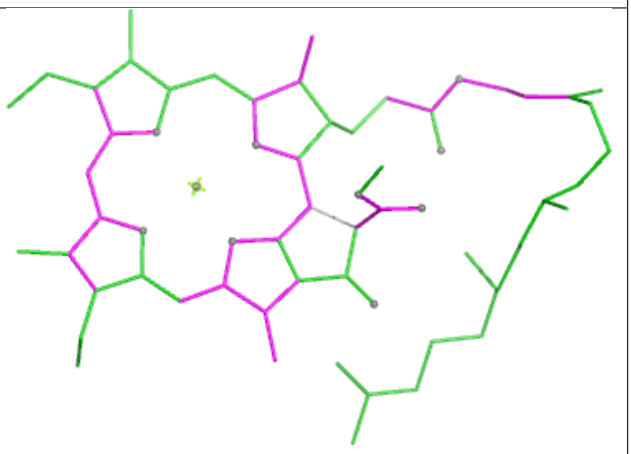
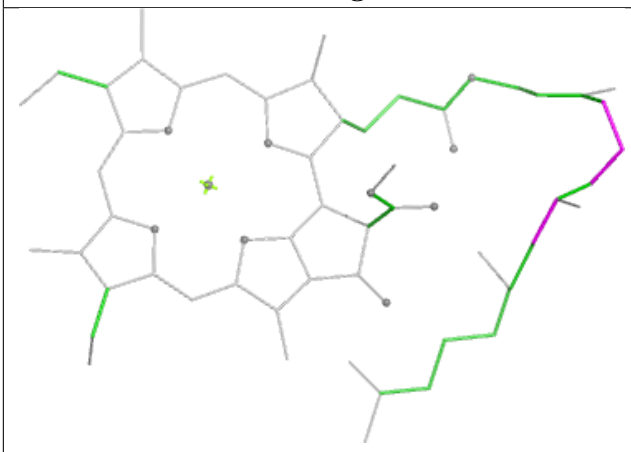


Bond angles



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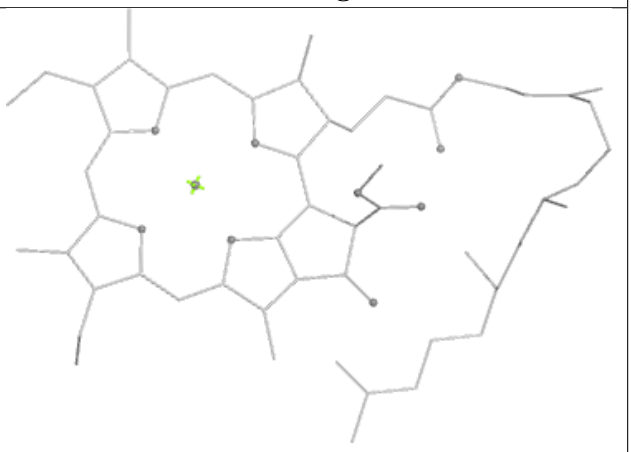
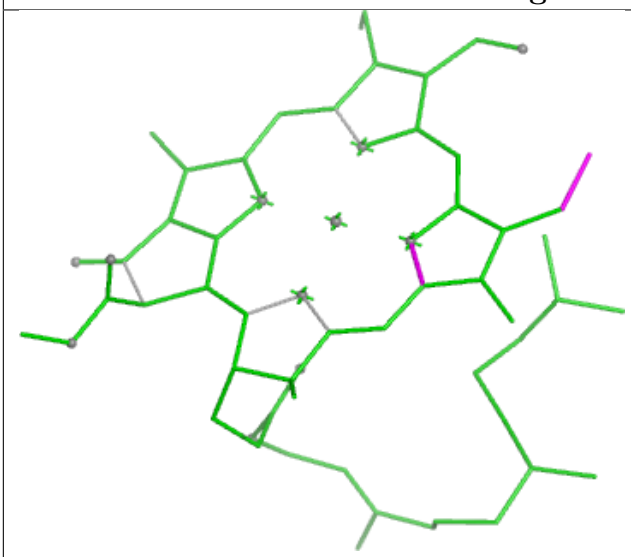


Rings

Ligand CHL r 607



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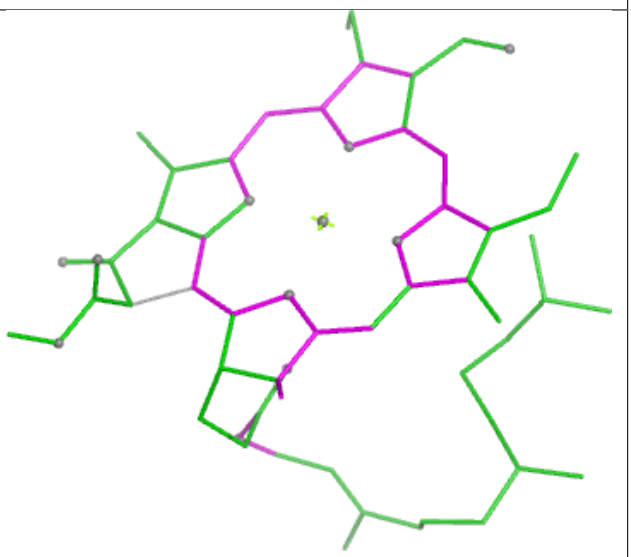
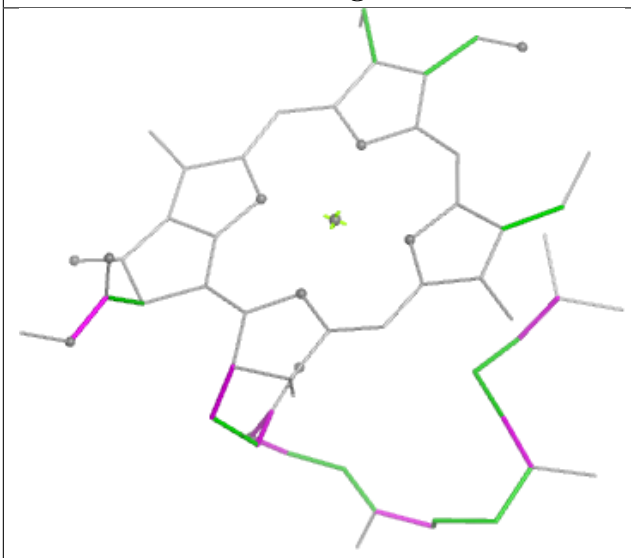


Bond angles



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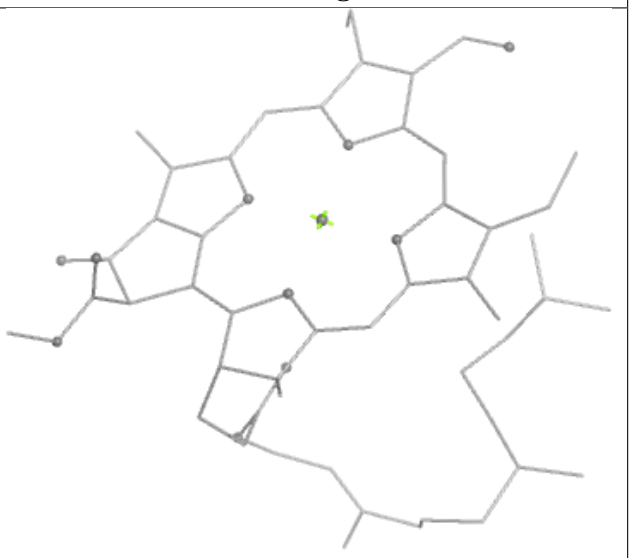
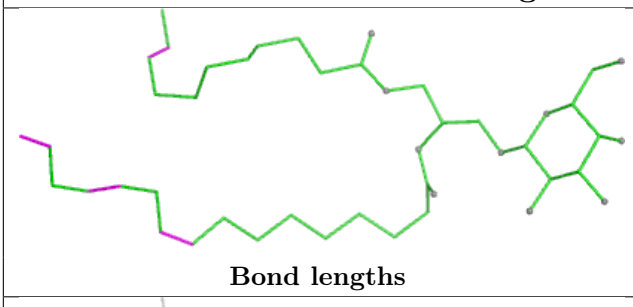


Rings

Ligand LMG D 408



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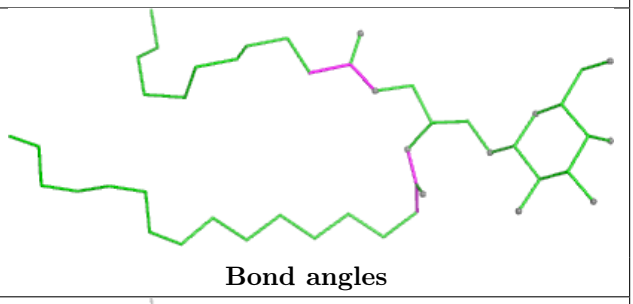
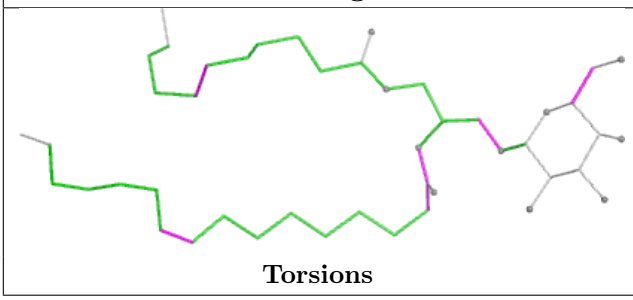


Bond angles



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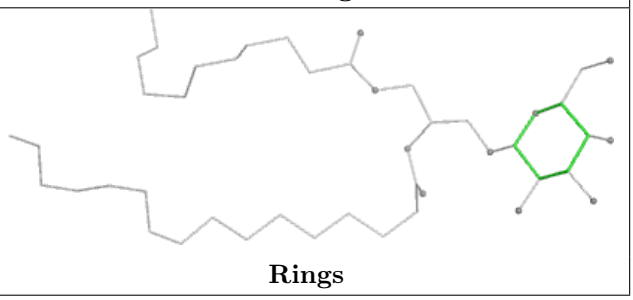
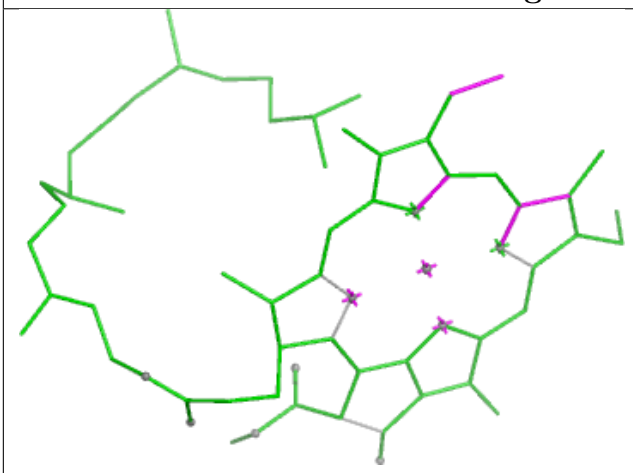


Rings

Ligand CLA B 615



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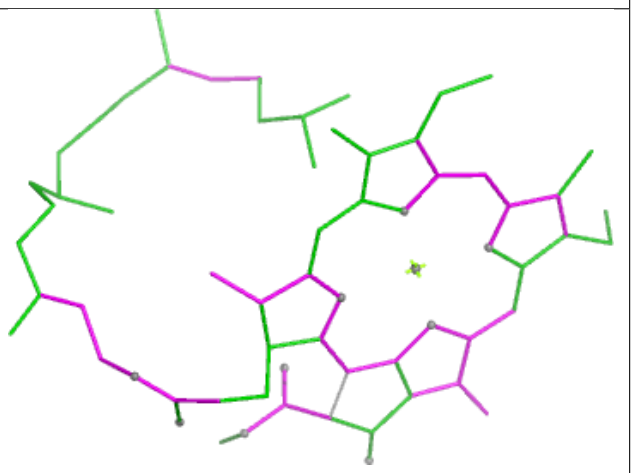
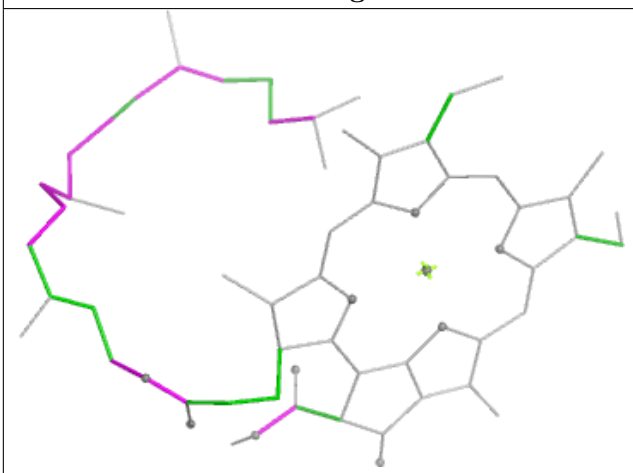


Bond angles



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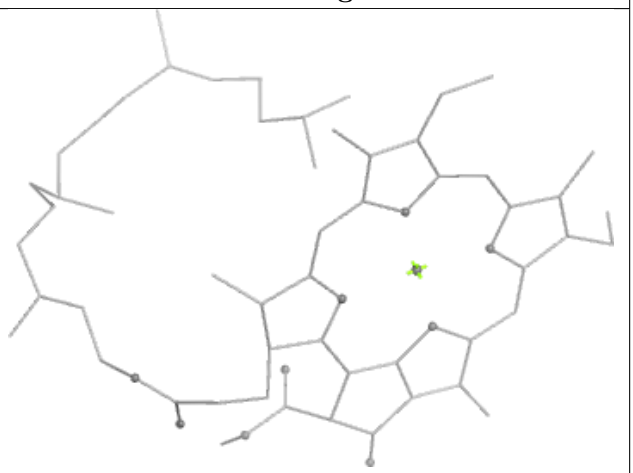
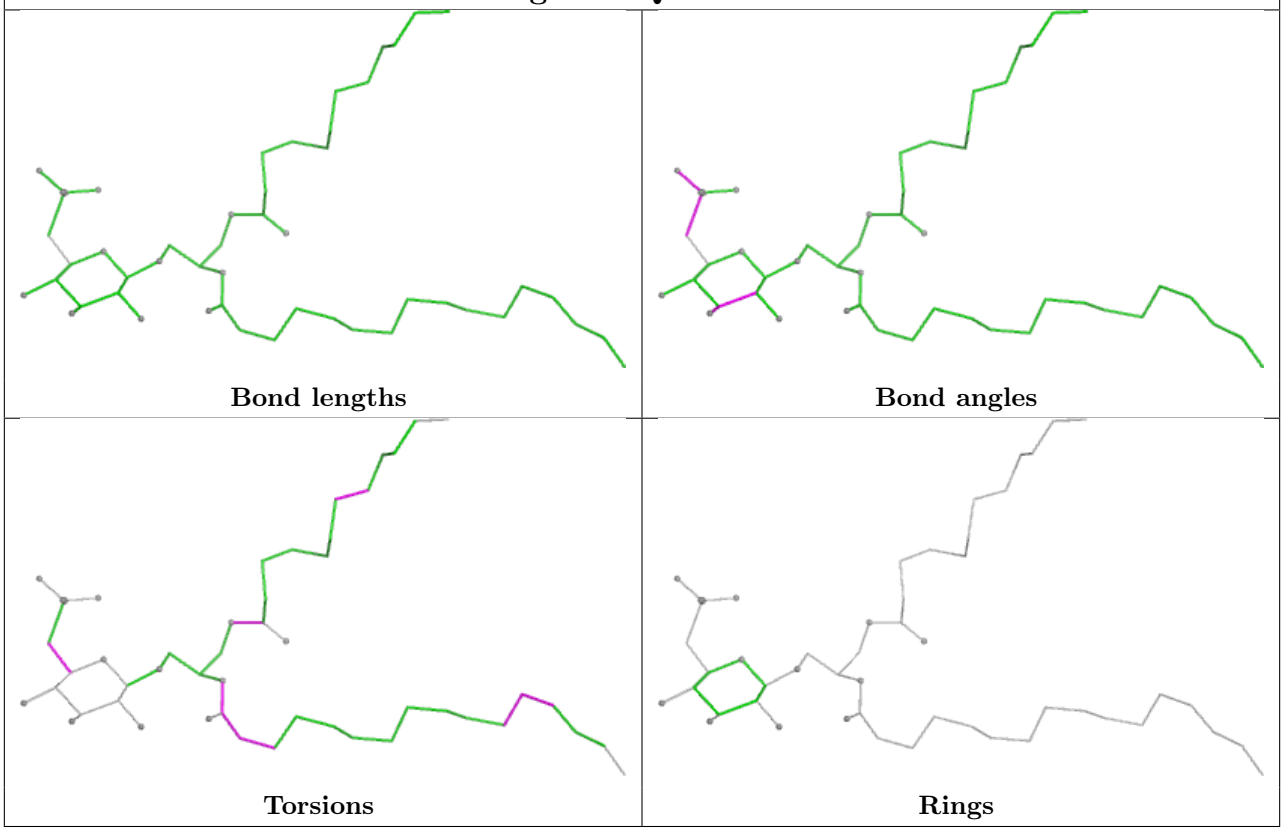
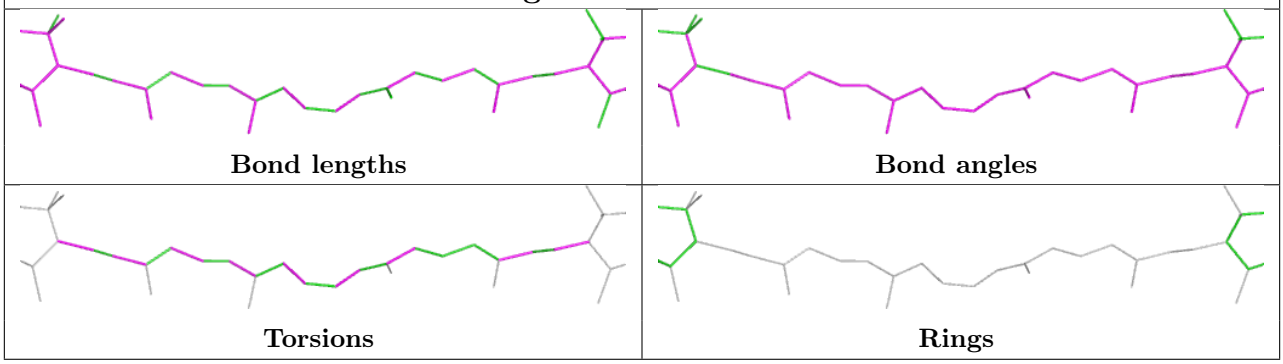


Rings

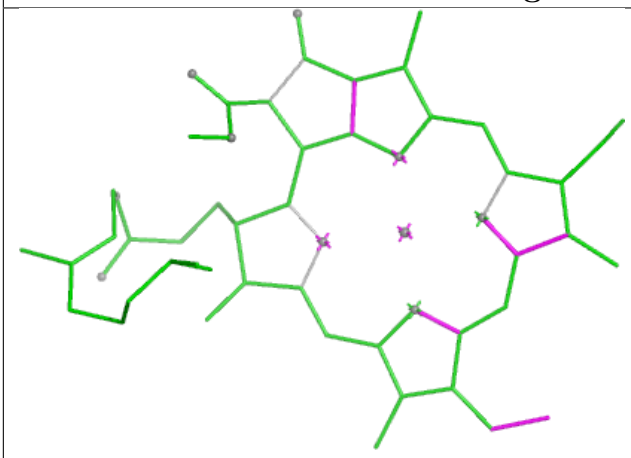
Ligand SQD a 411



Ligand BCR C 514



Ligand CLA Y 603



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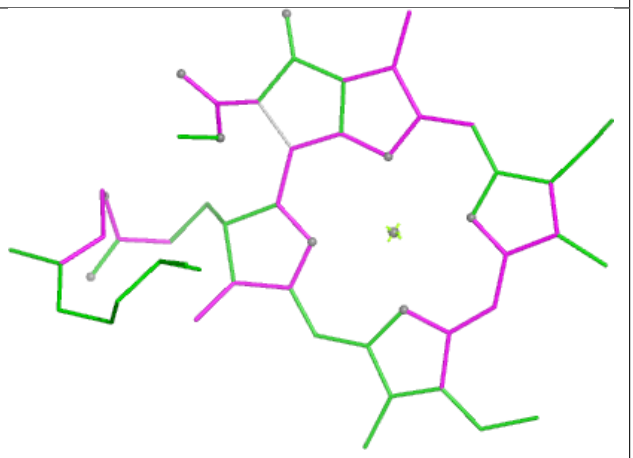
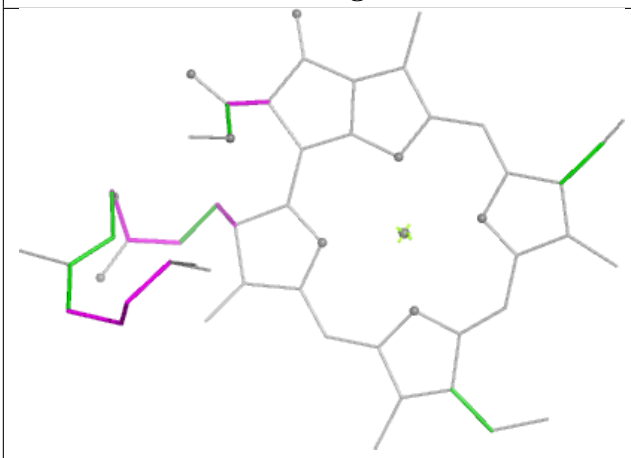


Bond angles



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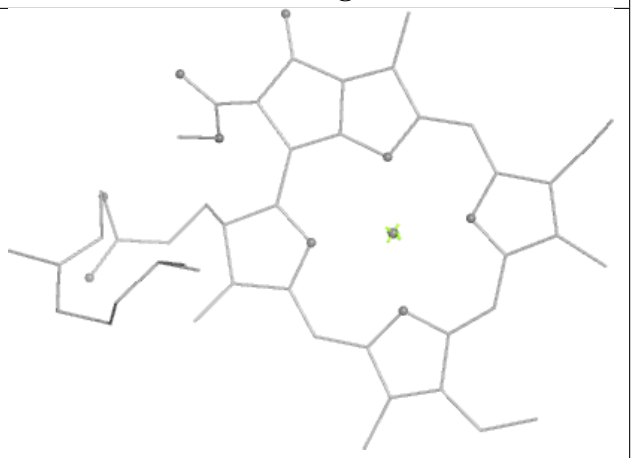
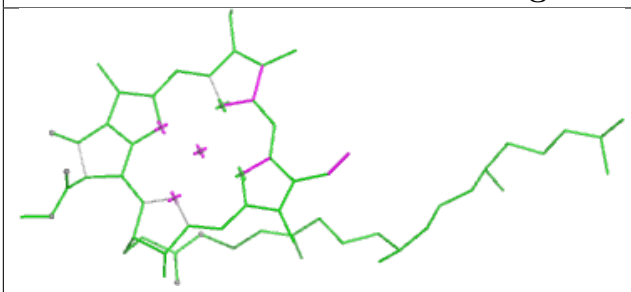


Rings

Ligand CLA c 501



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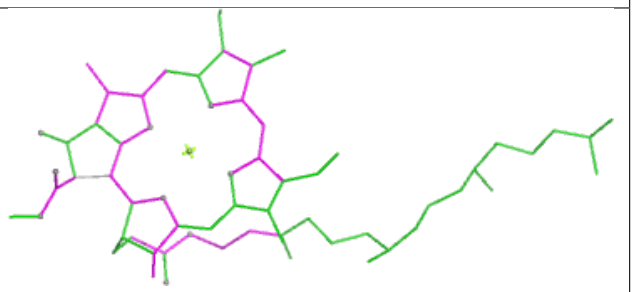
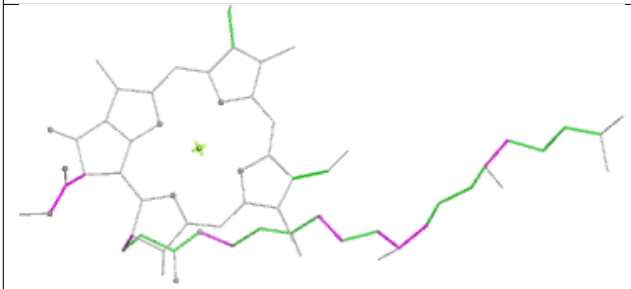


Bond angles

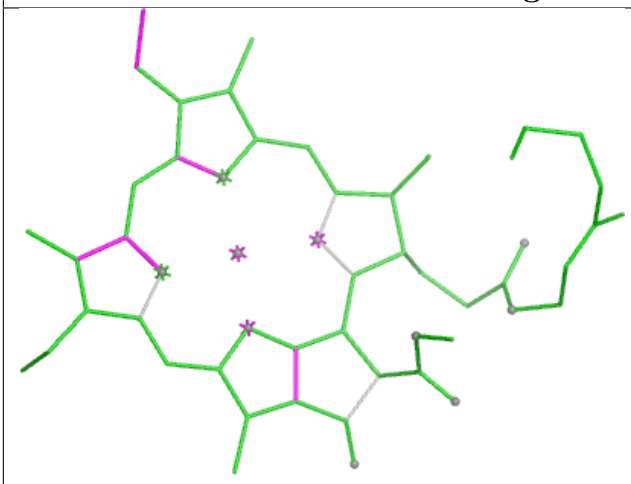


Torsions



Rings

Ligand CLA G 603



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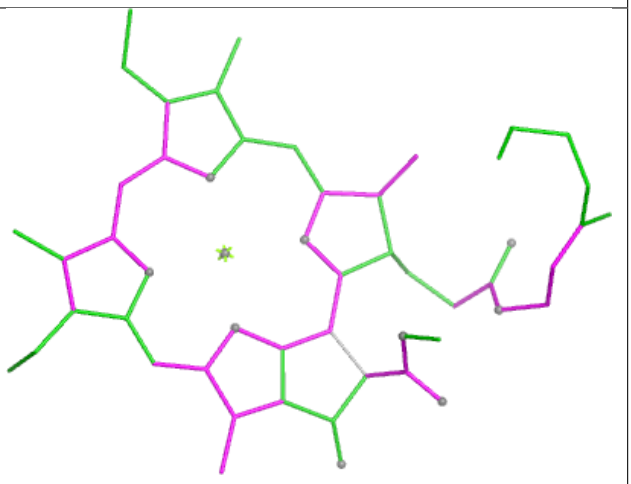
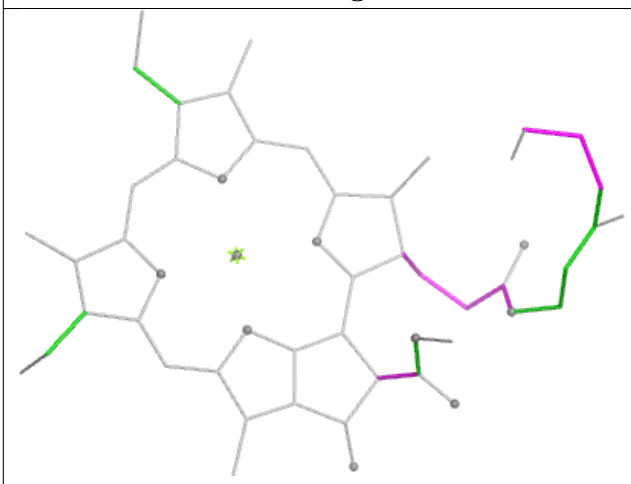


Bond angles



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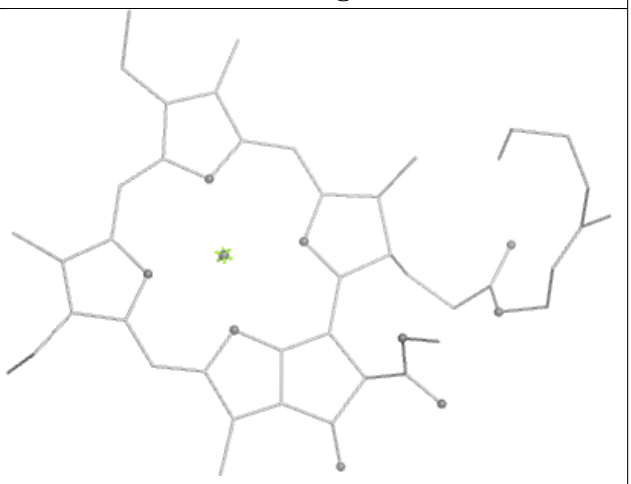
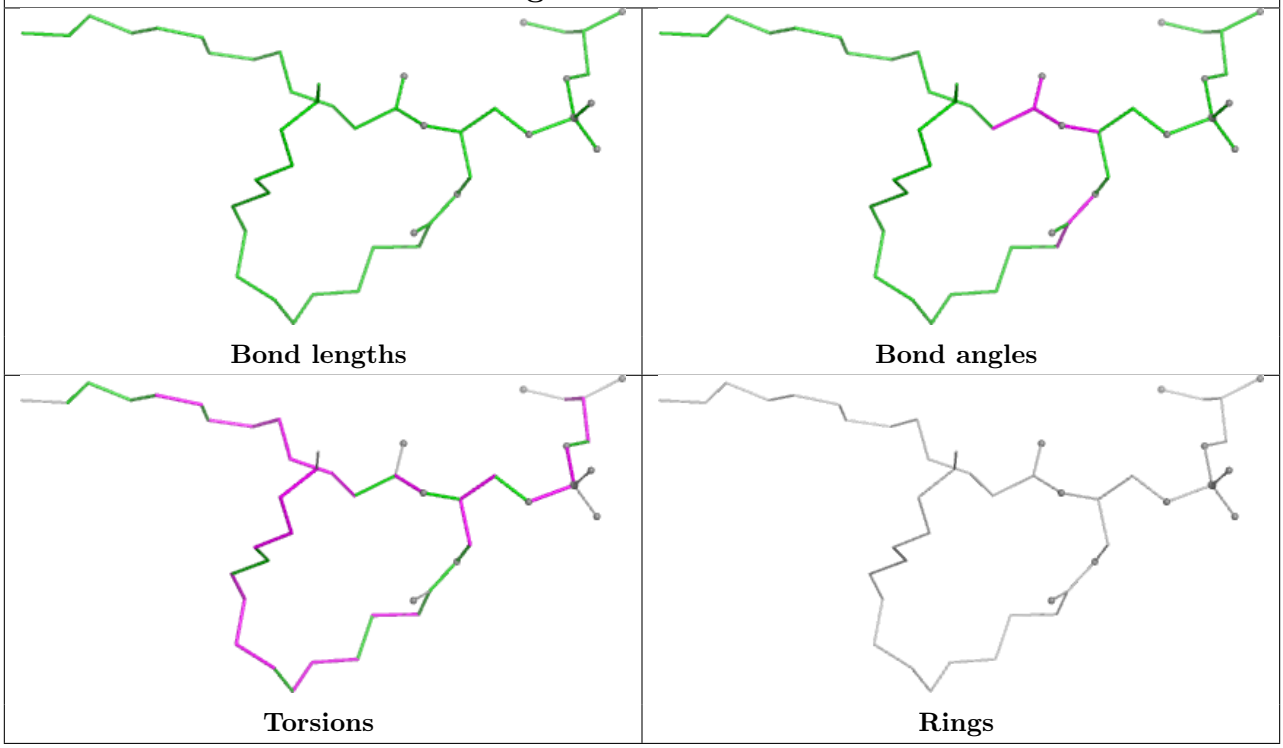


Rings

Ligand LHG b 624



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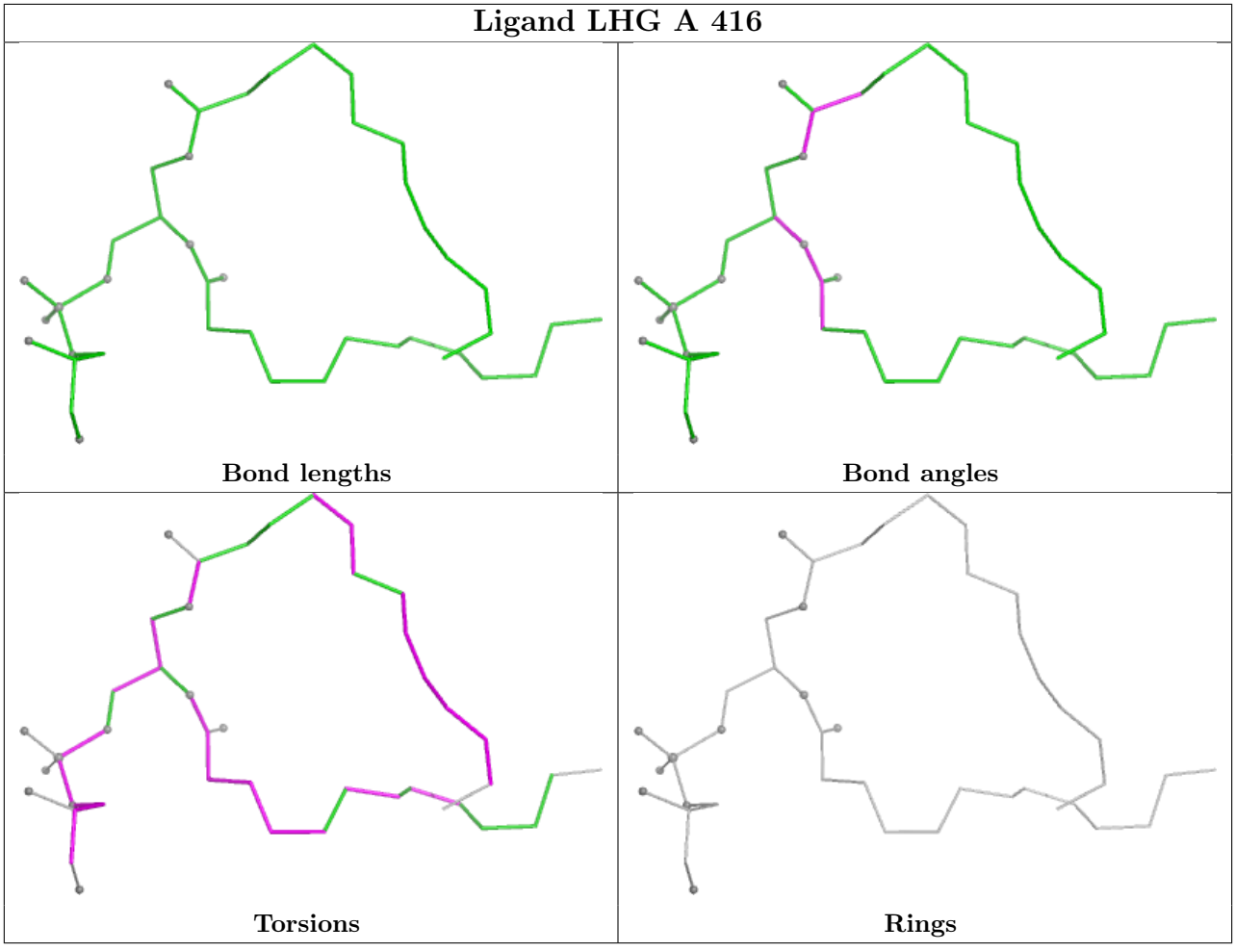
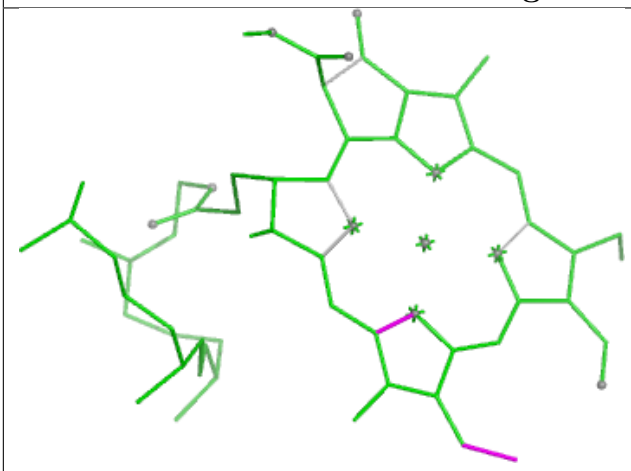


Ligand CHL G 608



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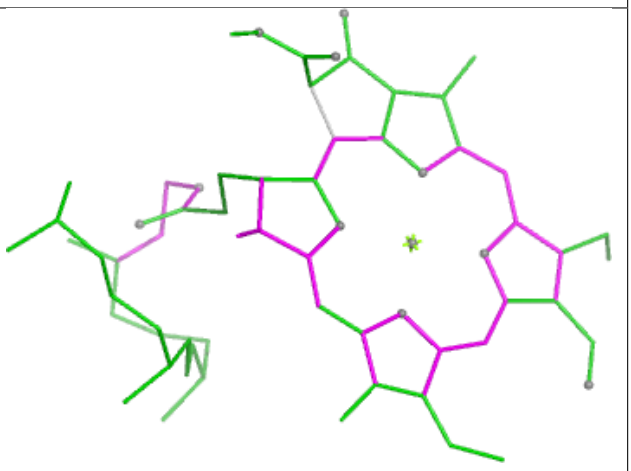
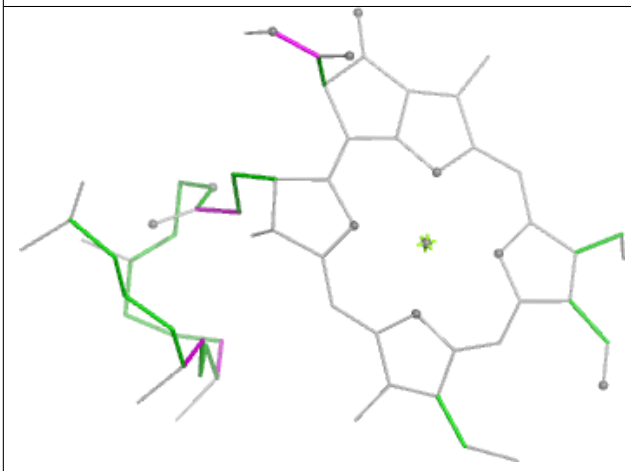


Bond angles



Torsions

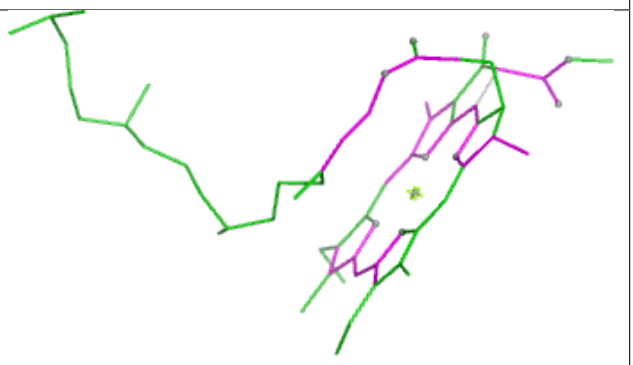


Rings

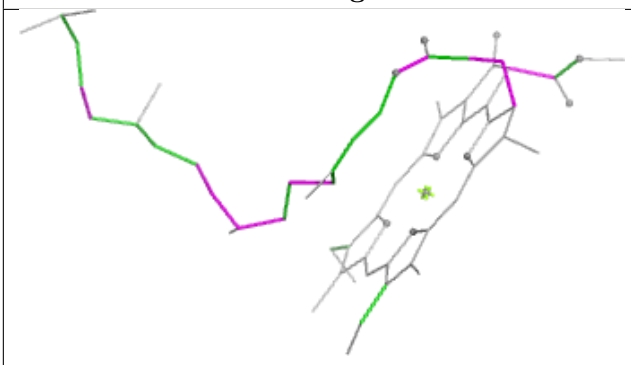
Ligand CLA r 613



Bond lengths



Bond angles

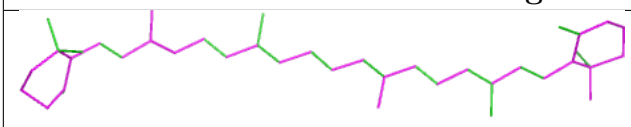


Torsions



Rings

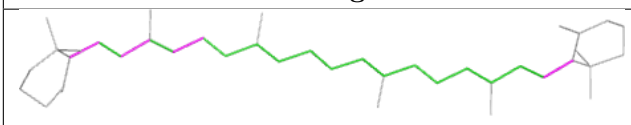
Ligand BCR b 619



Bond lengths



Bond angles



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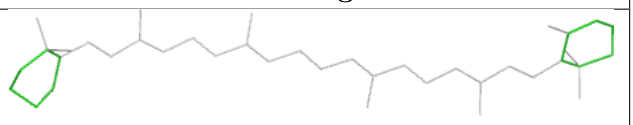
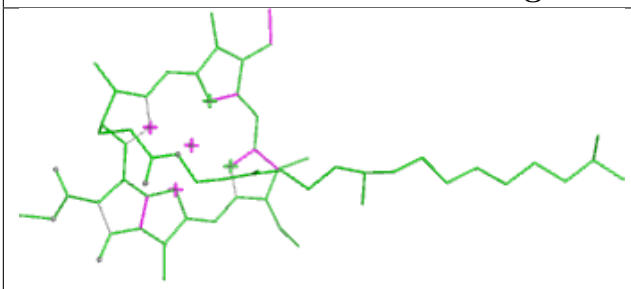
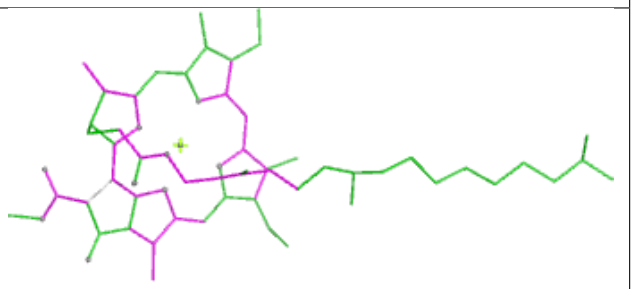


Rings

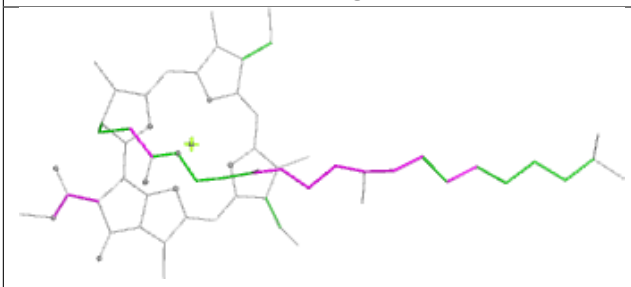
Ligand CLA B 614



Bond lengths



Bond angles



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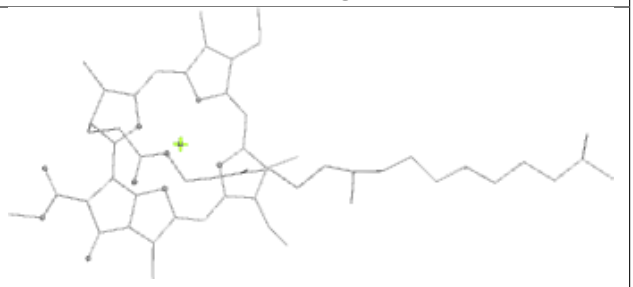
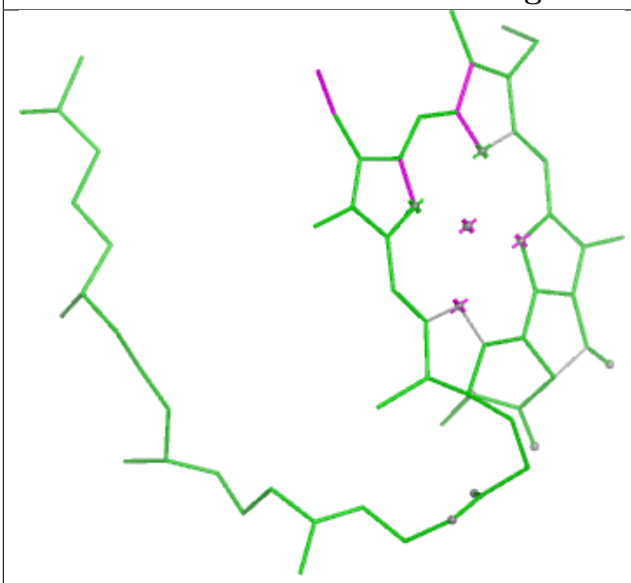
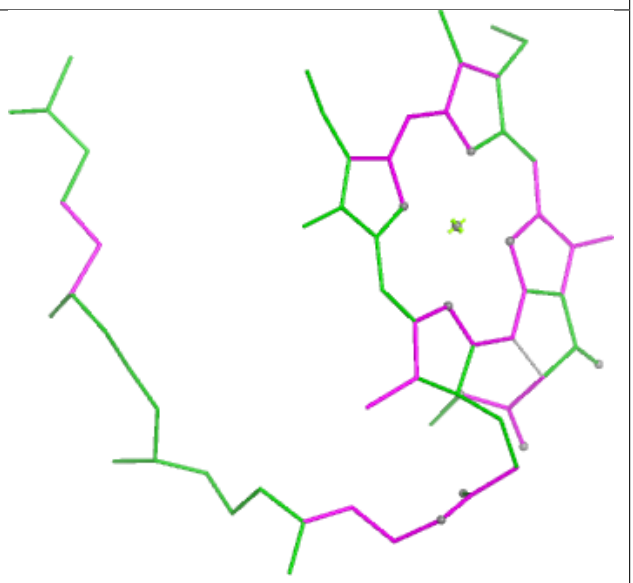


Rings

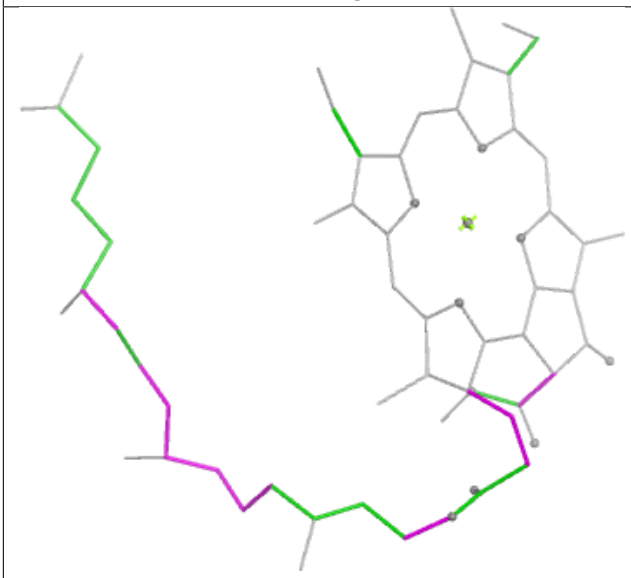
Ligand CLA C 507



Bond lengths



Bond angles



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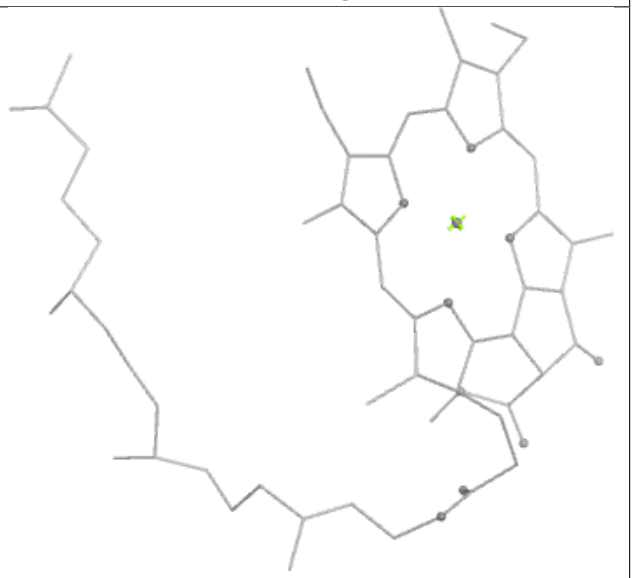
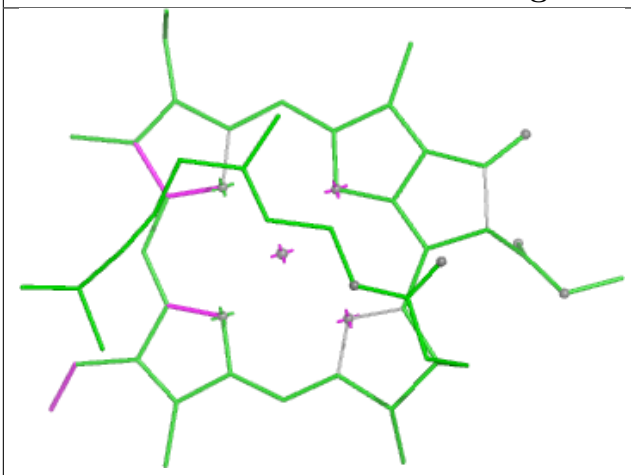
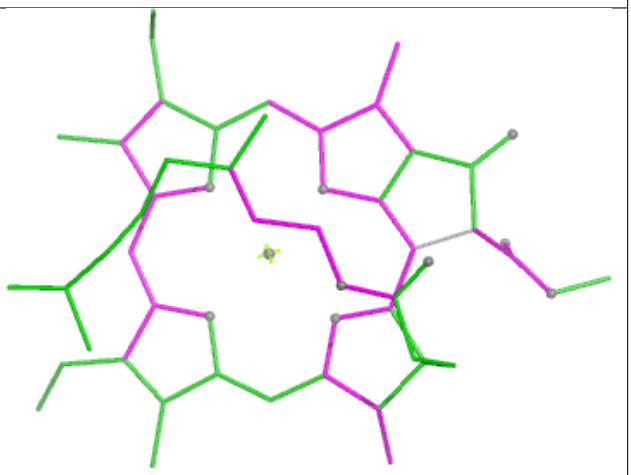


Rings

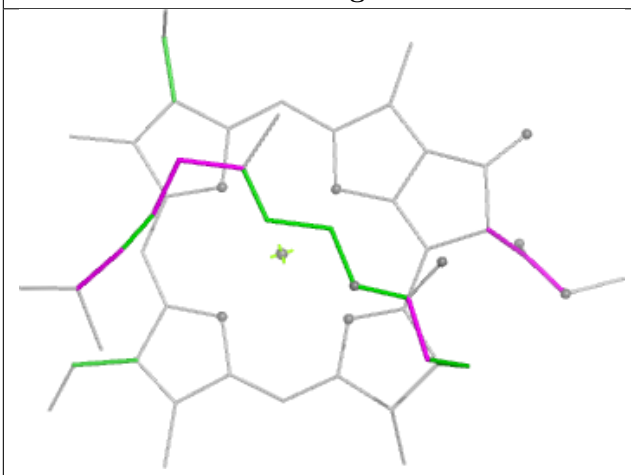
Ligand CLA s 612



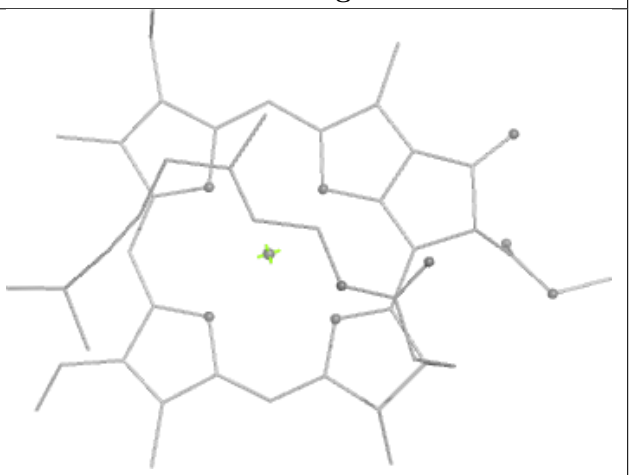
Bond lengths



Bond angles

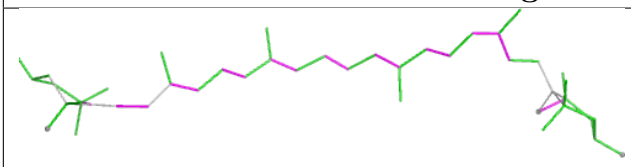


Torsions



Rings

Ligand NEX G 617



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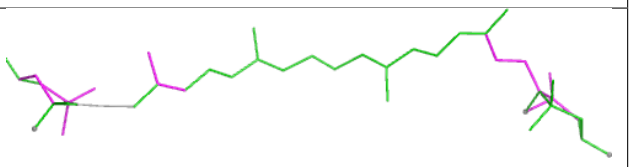
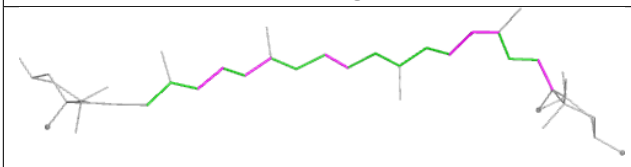
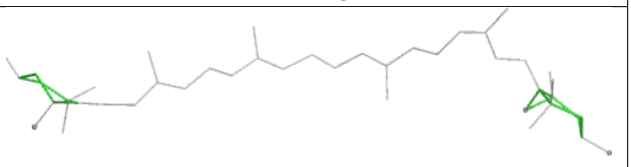


Bond angles

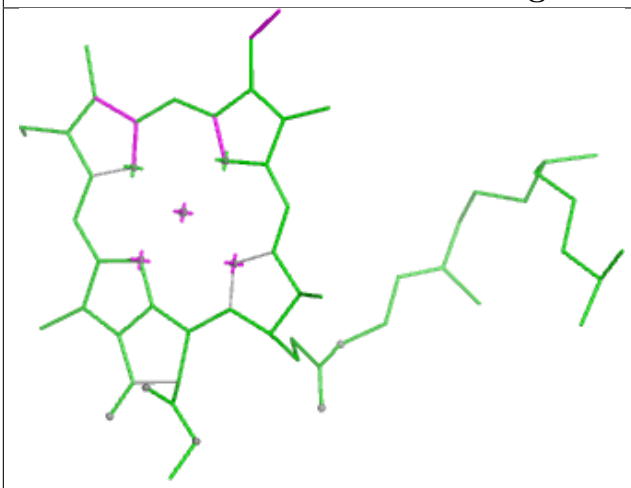


Torsions



Rings

Ligand CLA a 409



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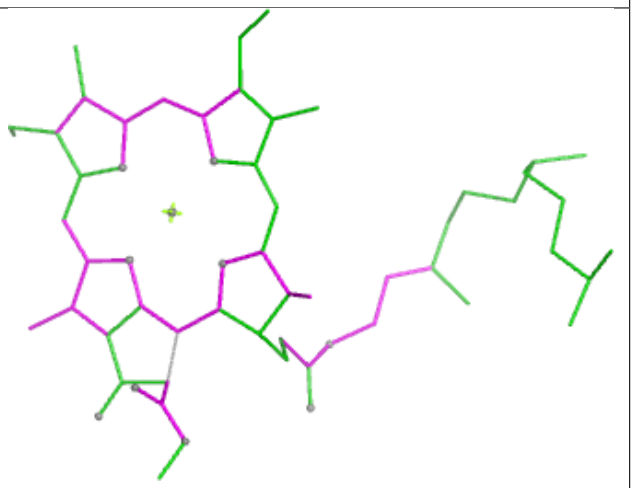
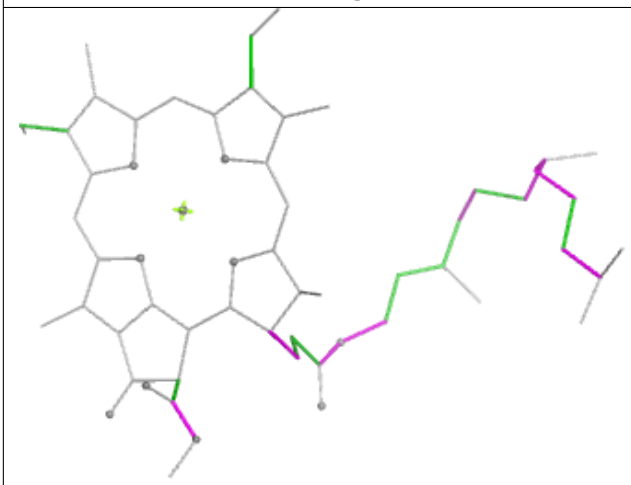


Bond angles



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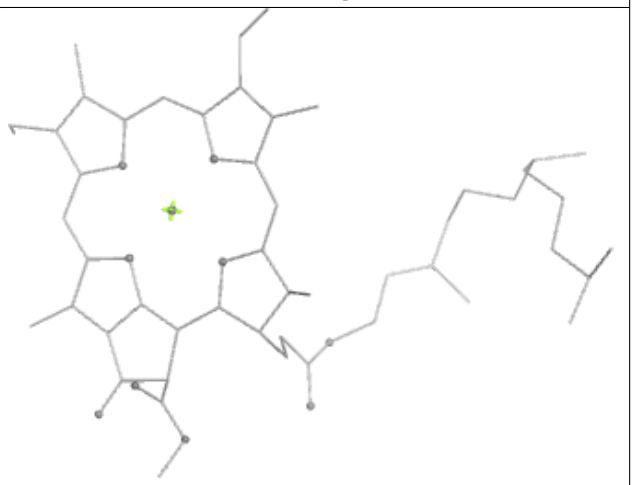
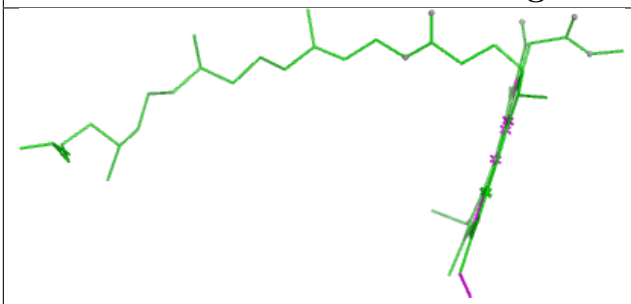


Rings

Ligand CLA b 605



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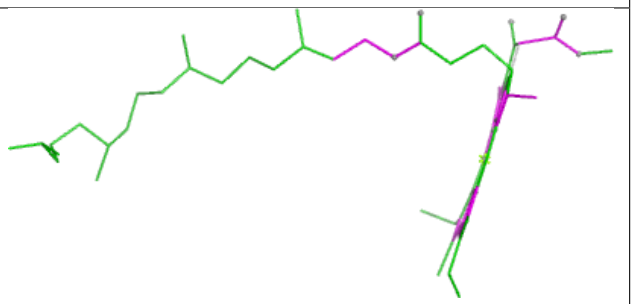
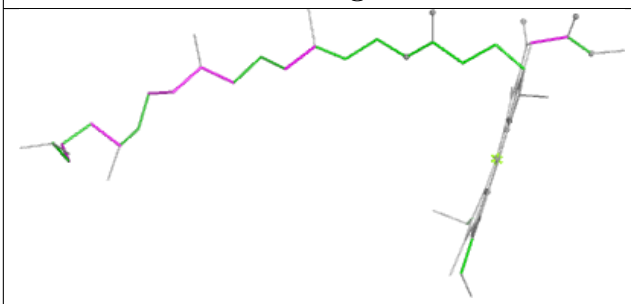
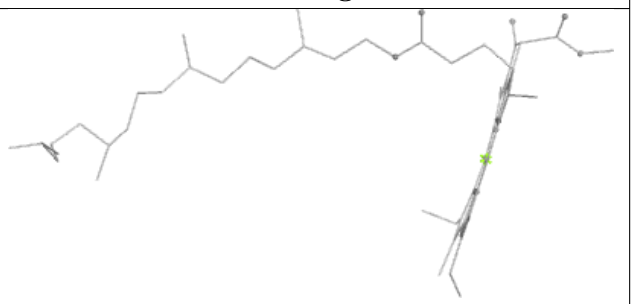


Bond angles

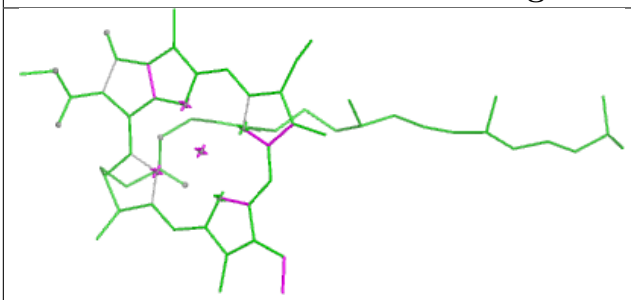


Torsions



Rings

Ligand CLA b 614



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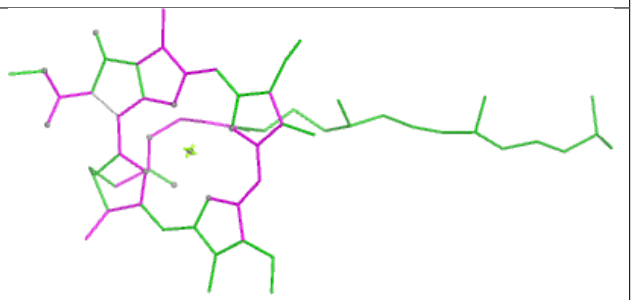
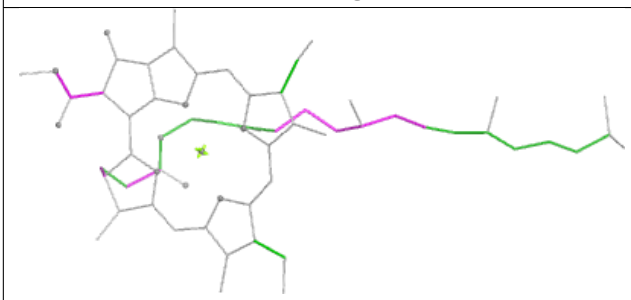


Bond angles

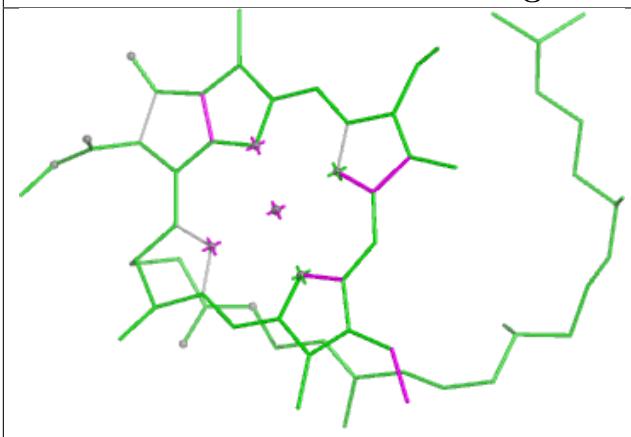


Torsions



Rings

Ligand CLA R 609



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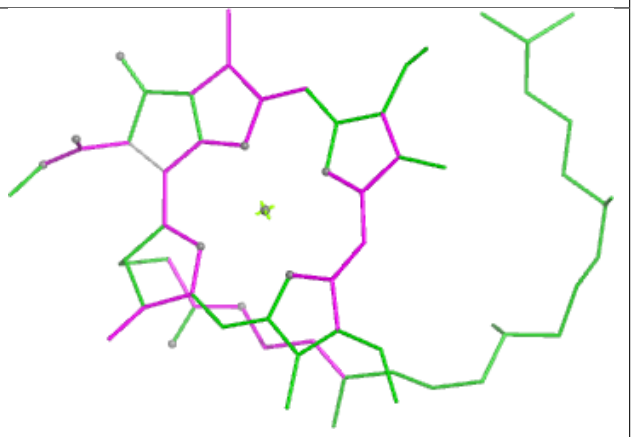
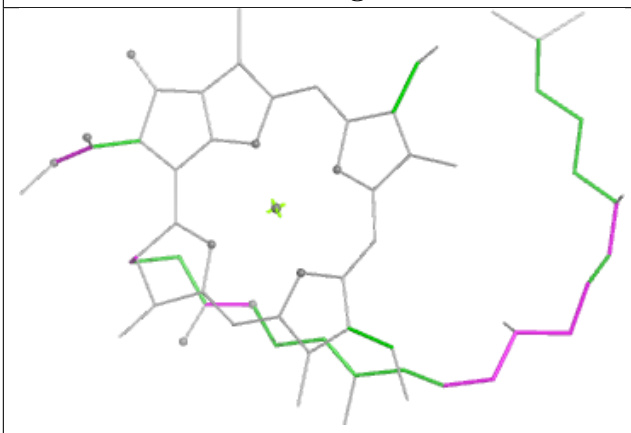


Bond angles



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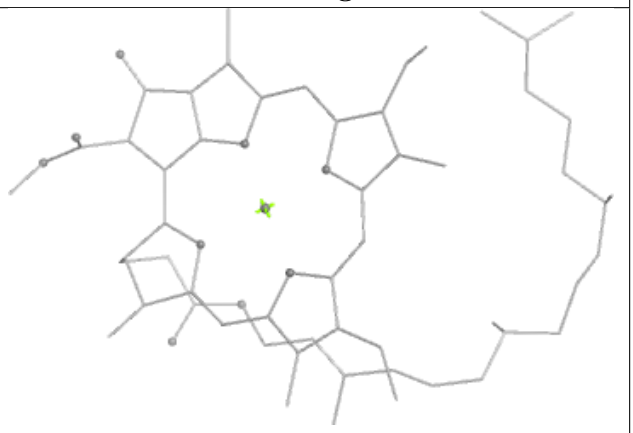
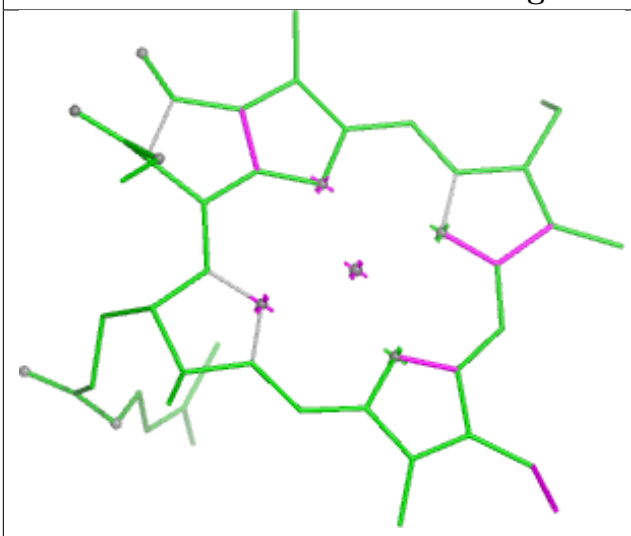


Rings

Ligand CLA n 604



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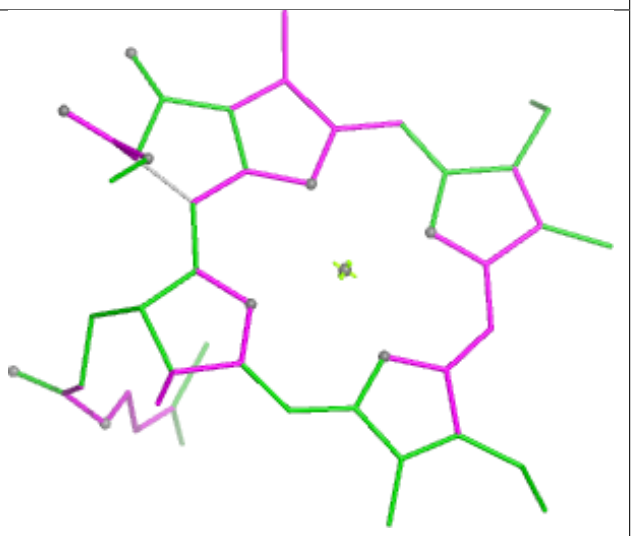
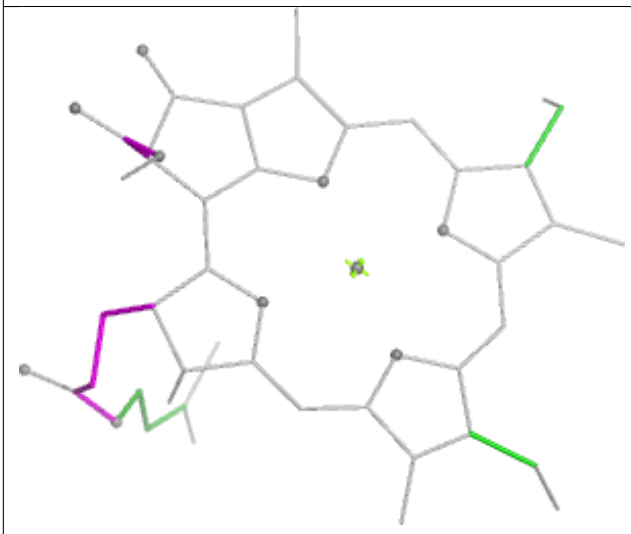


Bond angles



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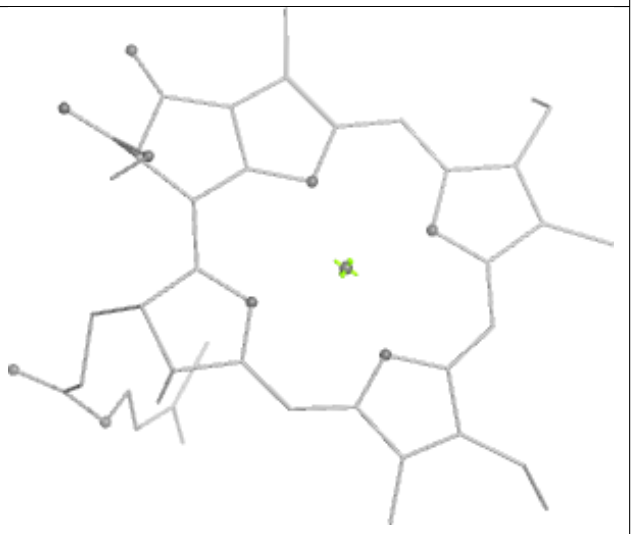
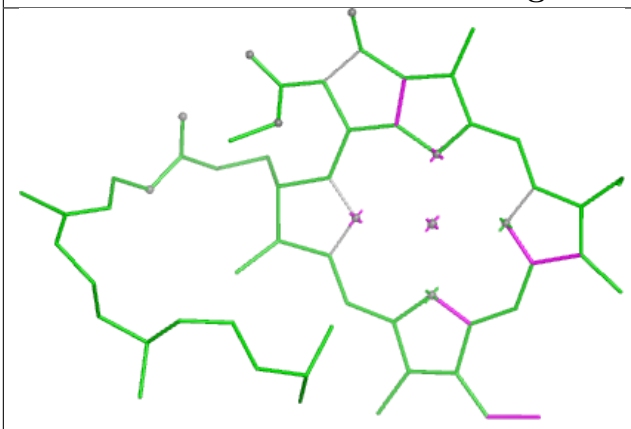


Rings

Ligand CLA y 312



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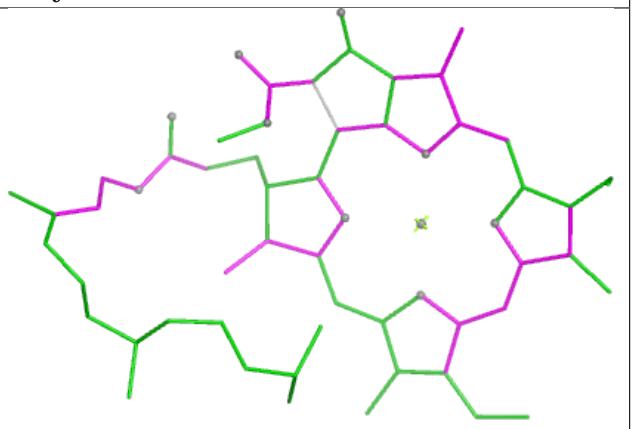
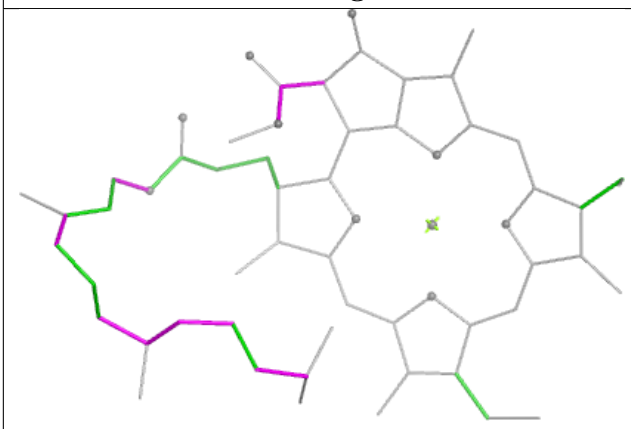


Bond angles



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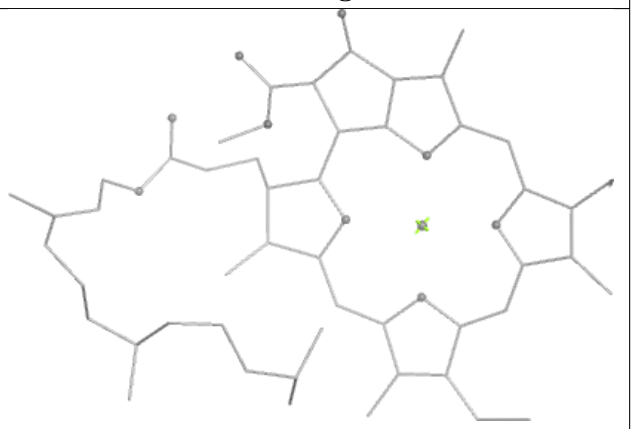
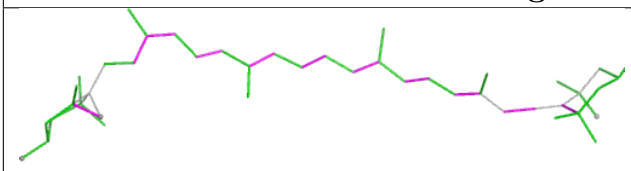


Rings

Ligand NEX s 616



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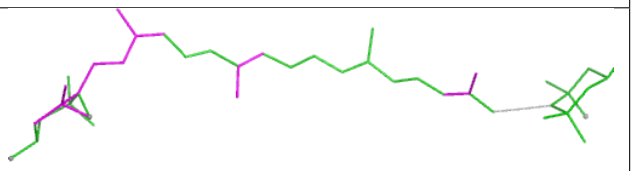
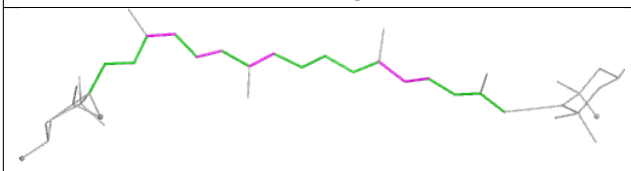


Bond angles



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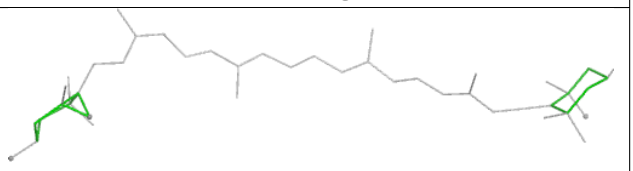
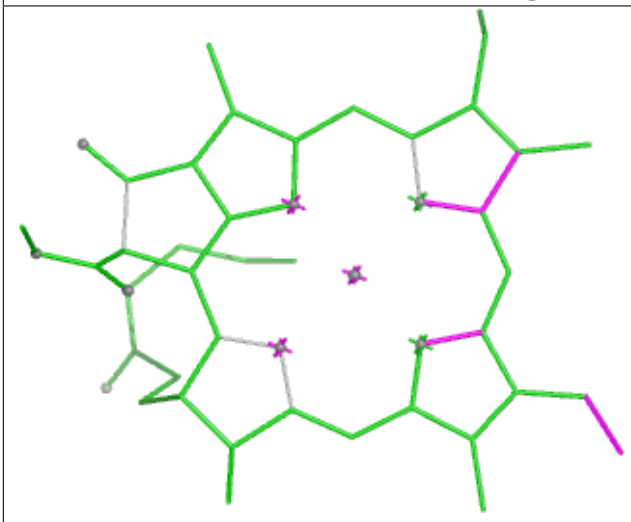


Rings

Ligand CLA N 614



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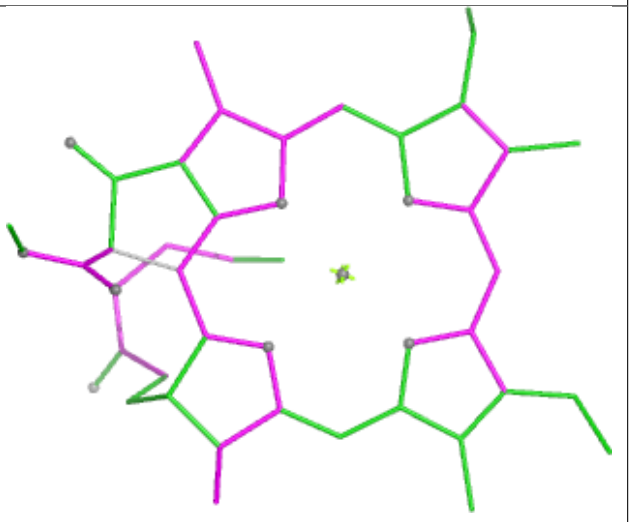
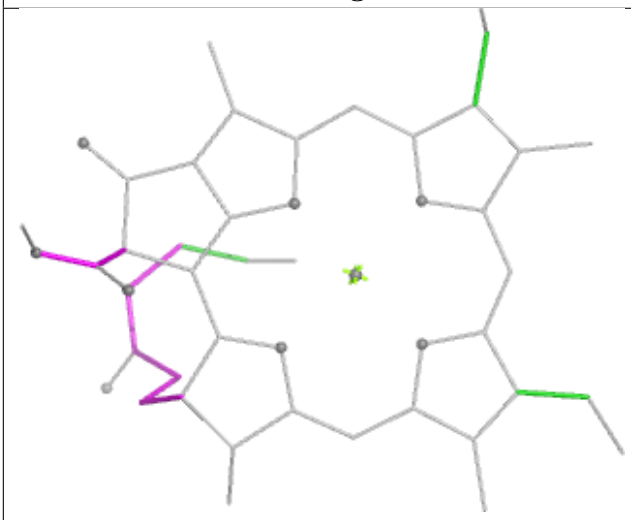


Bond angles



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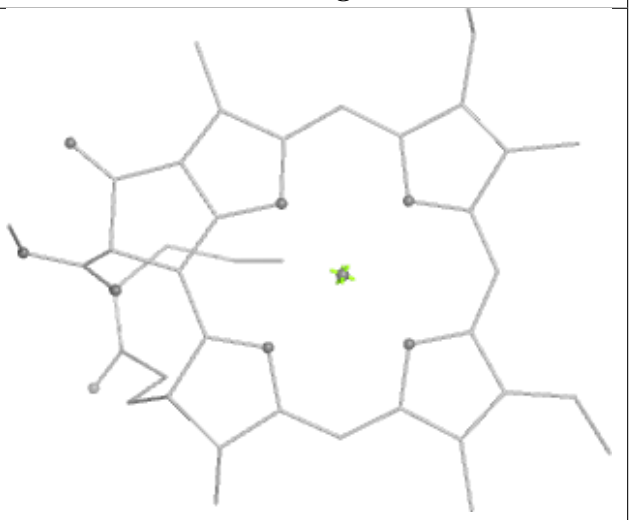
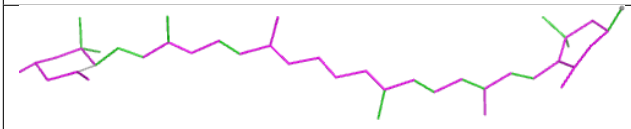


Rings

Ligand LUT Y 615



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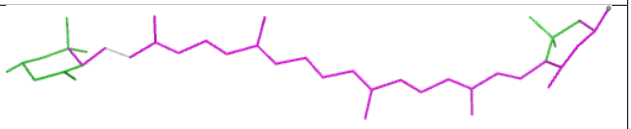
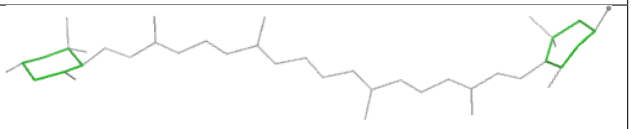


Bond angles

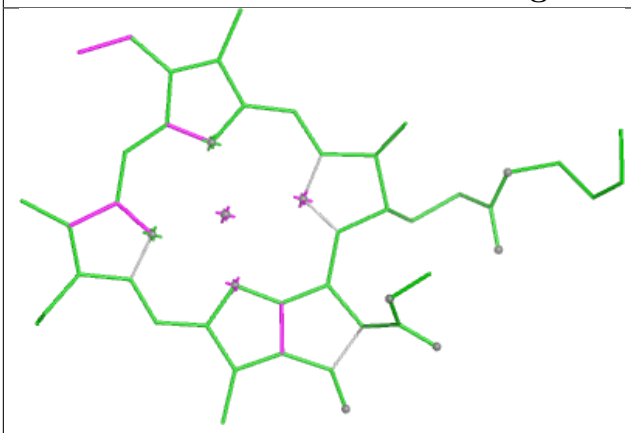


Torsions



Rings

Ligand CLA s 611



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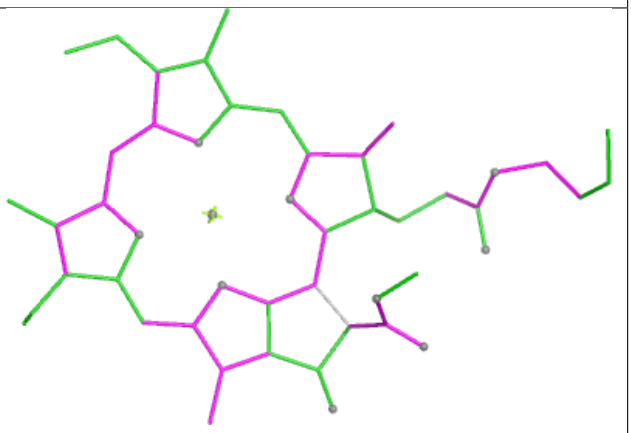
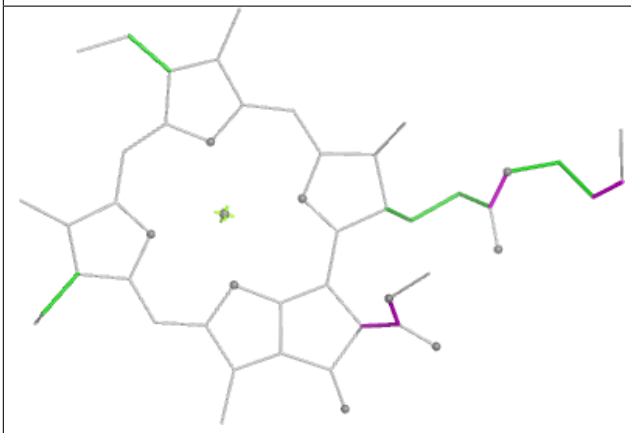


Bond angles

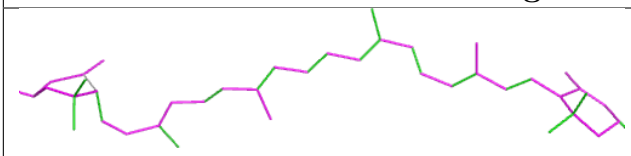


Torsions



Rings

Ligand LUT G 615



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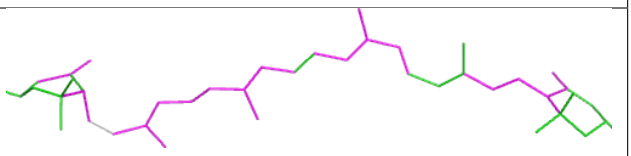
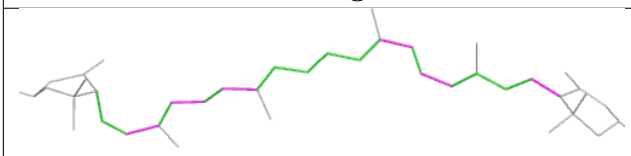


Bond angles



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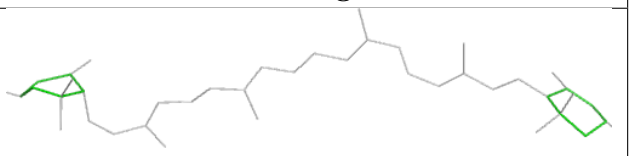
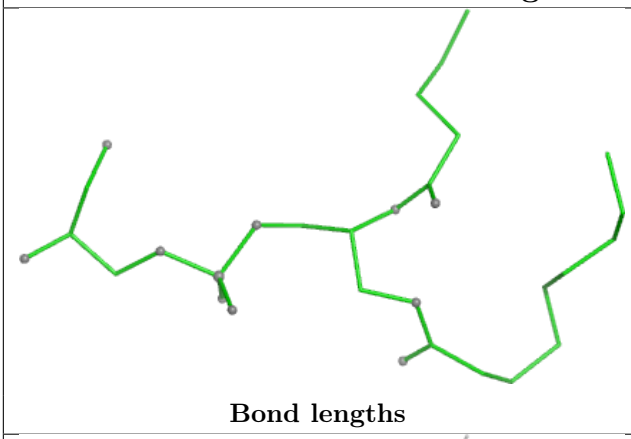


Rings

Ligand LHG N 618



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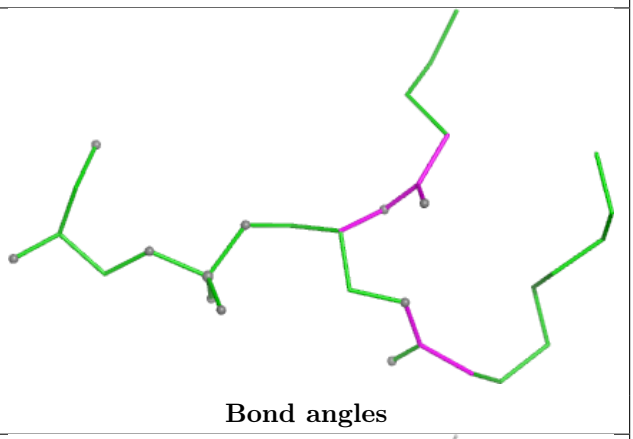
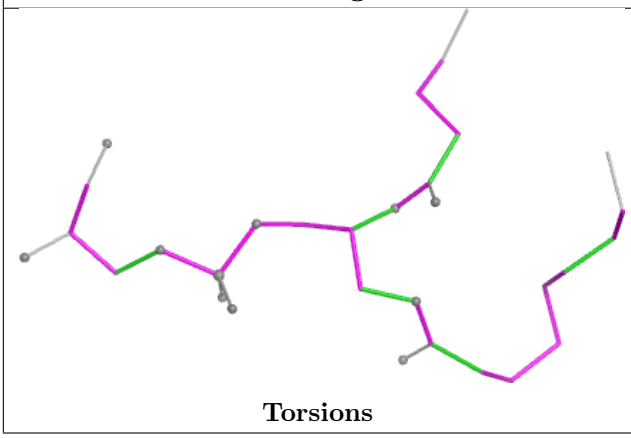


Bond angles



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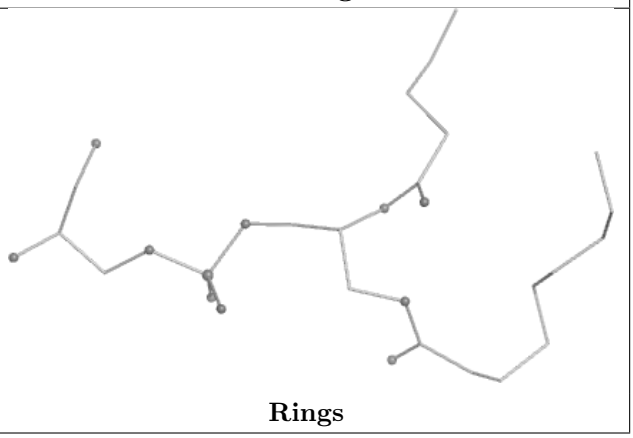
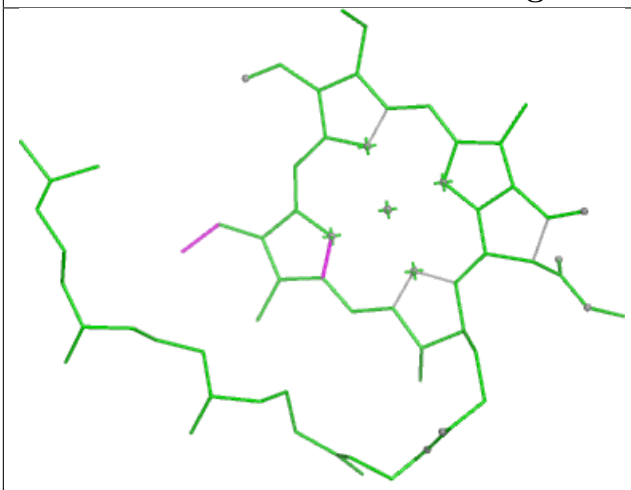


Rings

Ligand CHL n 607



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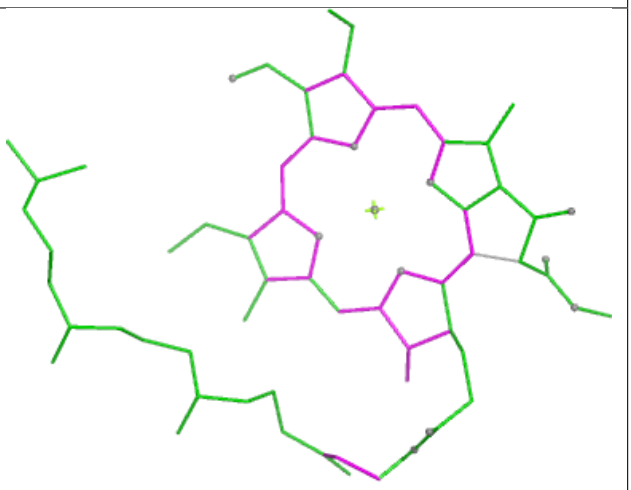
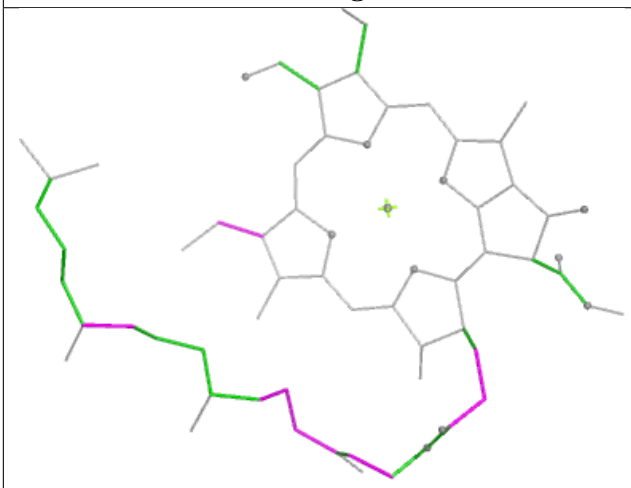


Bond angles



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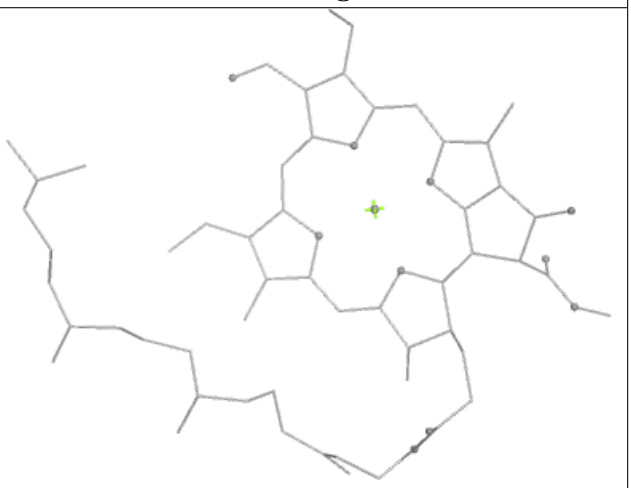
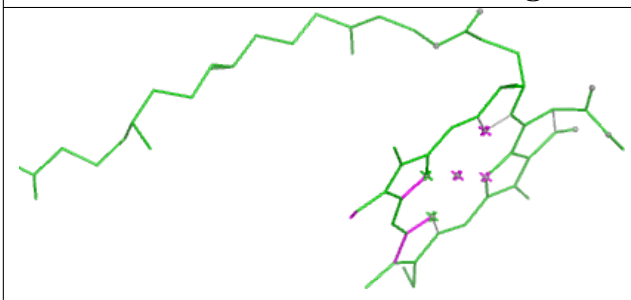
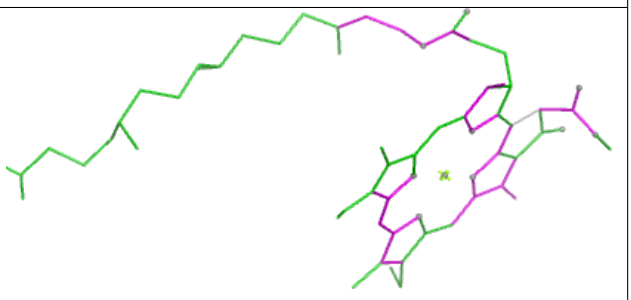


Rings

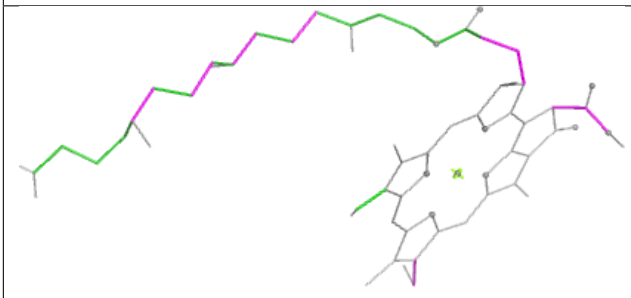
Ligand CLA C 504



Bond lengths



Bond angles

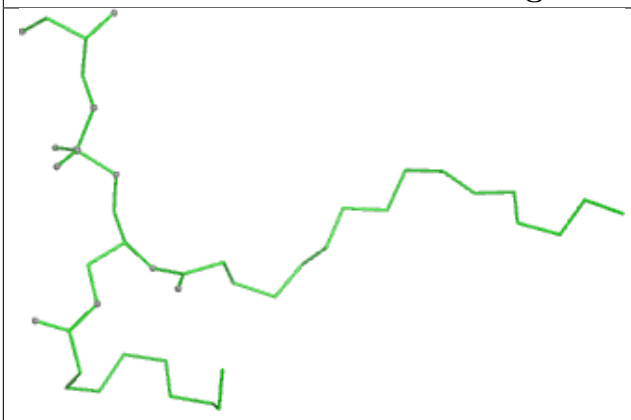


Torsions



Rings

Ligand LHG S 317



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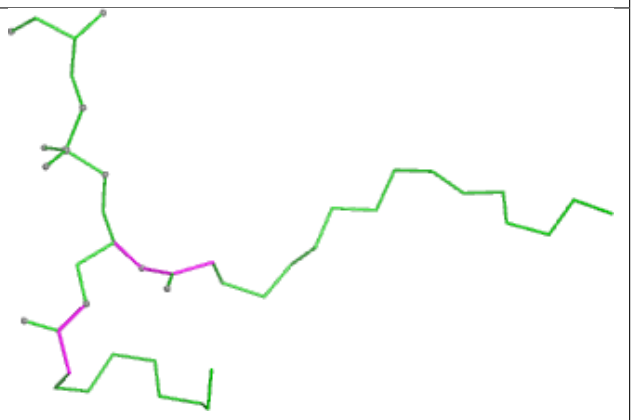
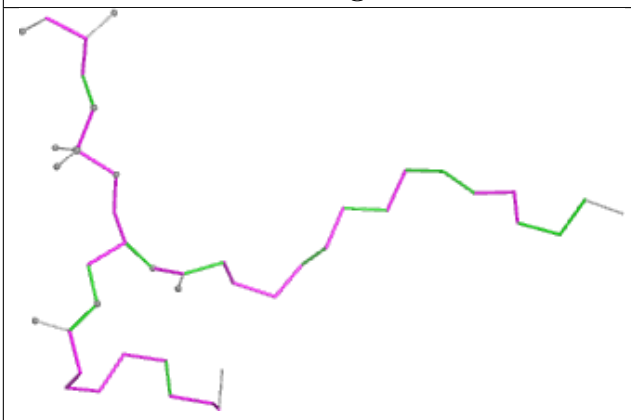


Bond angles

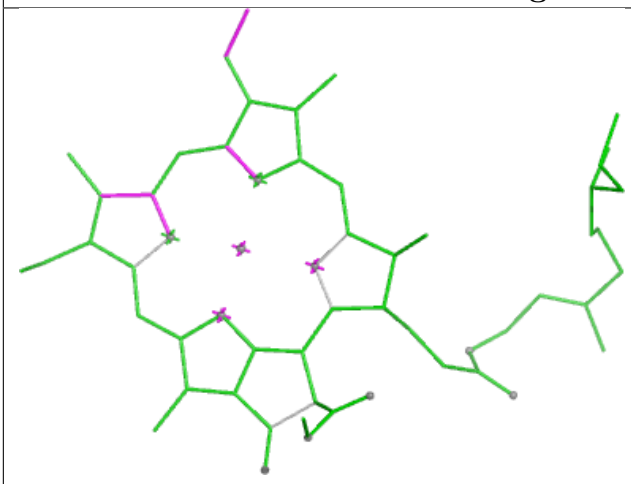


Torsions



Rings

Ligand CLA c 512



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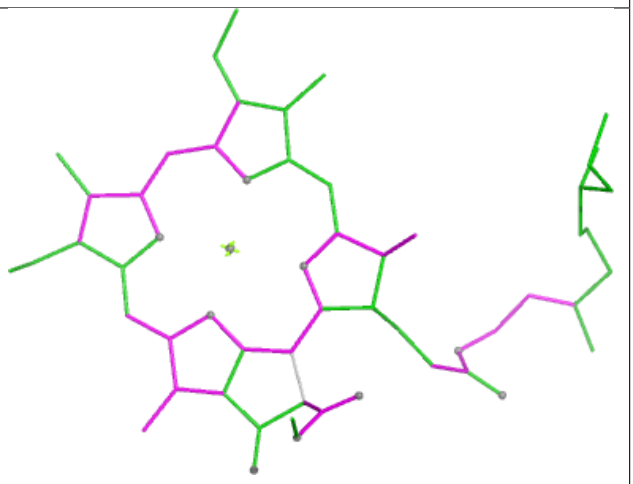
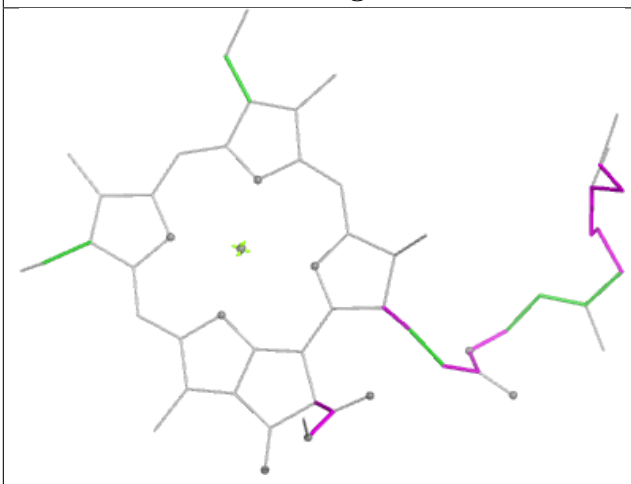


Bond angles



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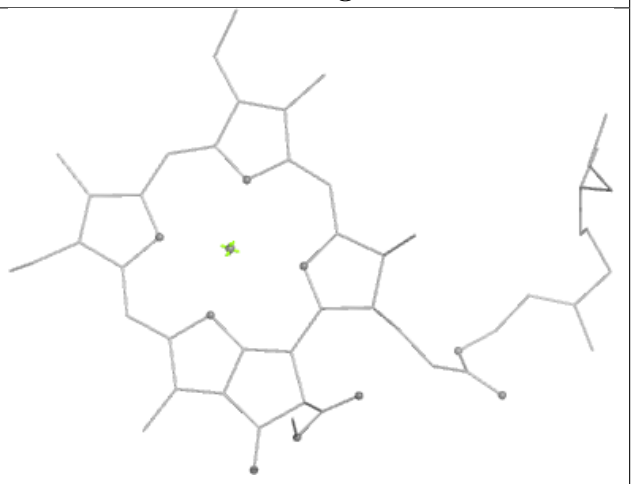
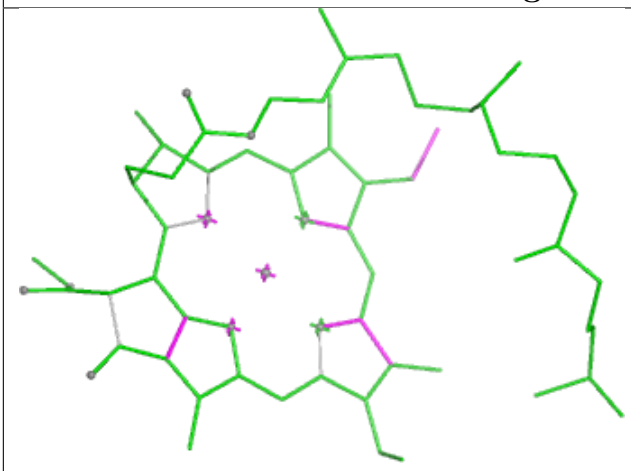


Rings

Ligand CLA N 602



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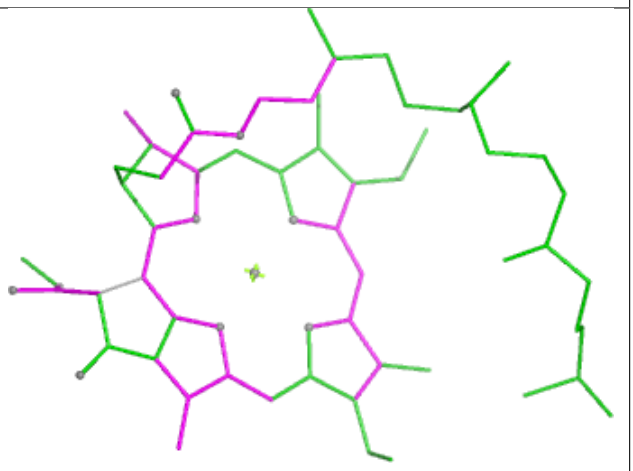
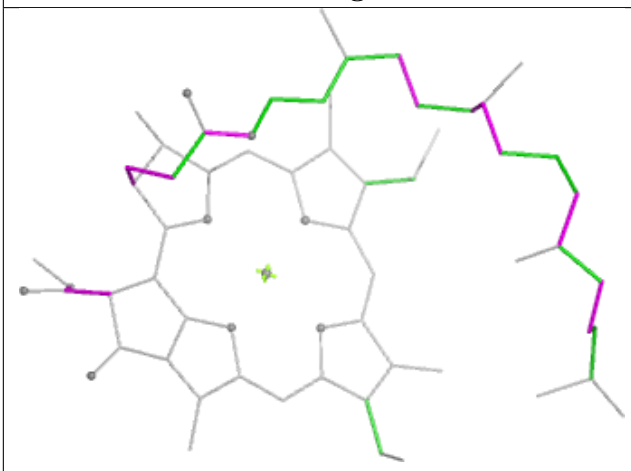


Bond angles



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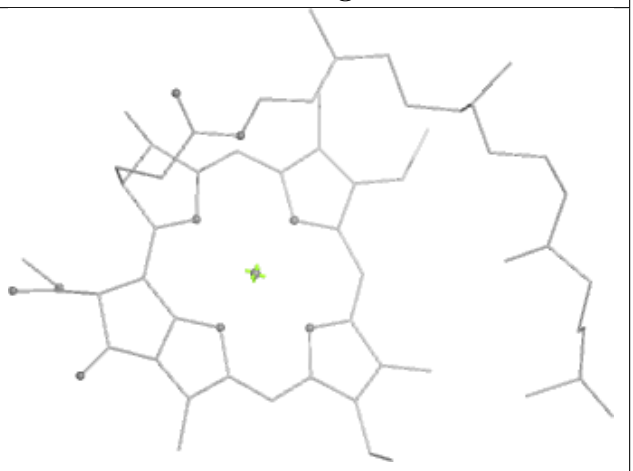


Rings

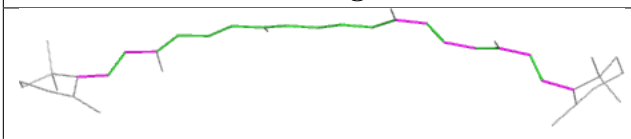
Ligand BCR d 406



Bond lengths



Bond angles

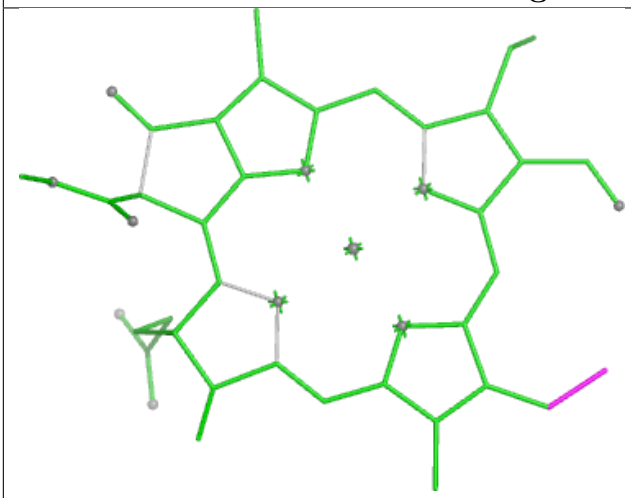


Torsions



Rings

Ligand CHL s 607



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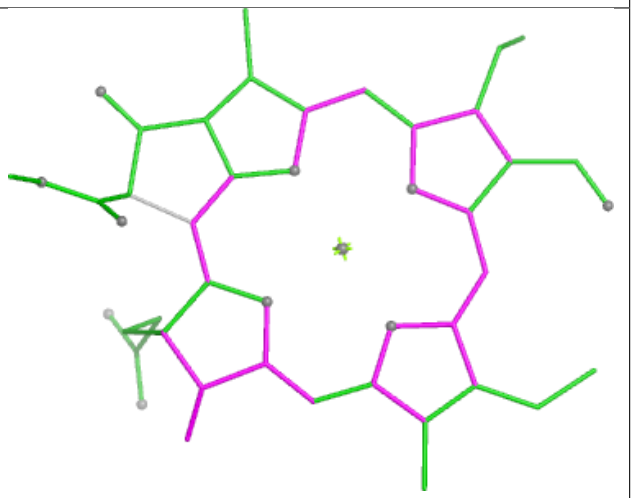
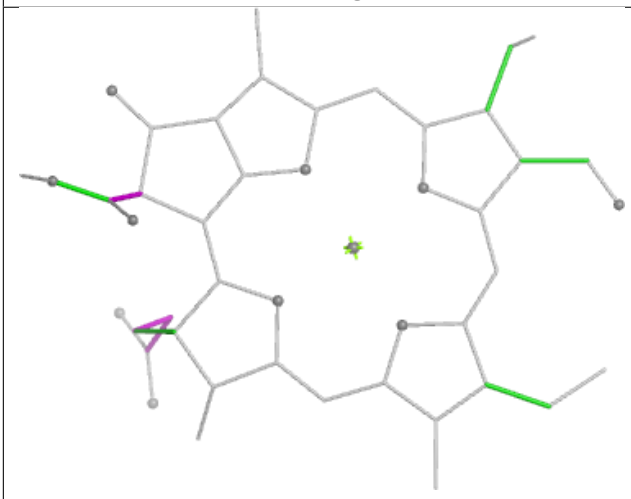


Bond angles



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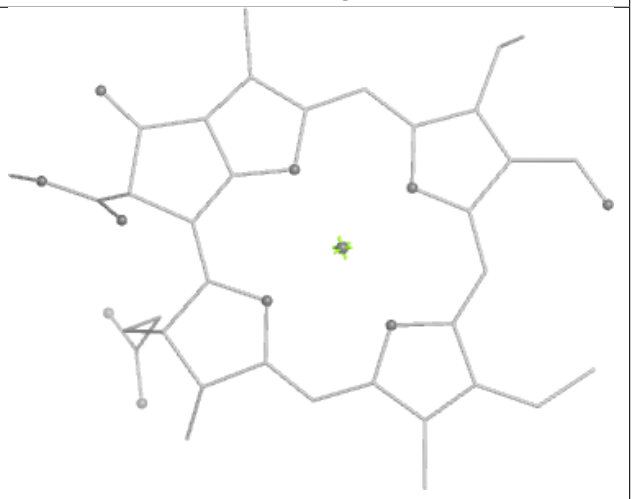
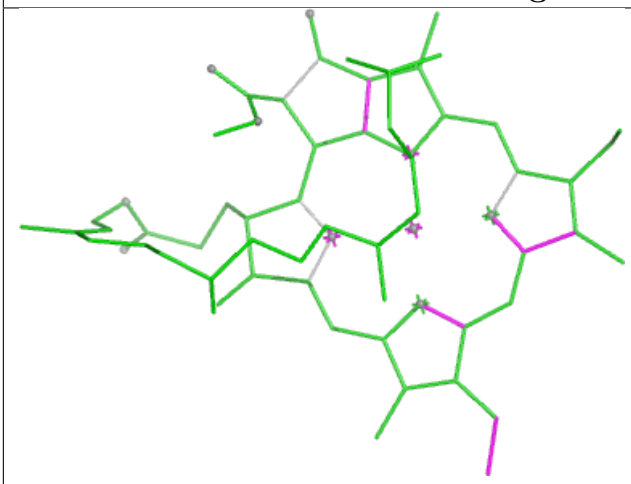


Rings

Ligand CLA c 510



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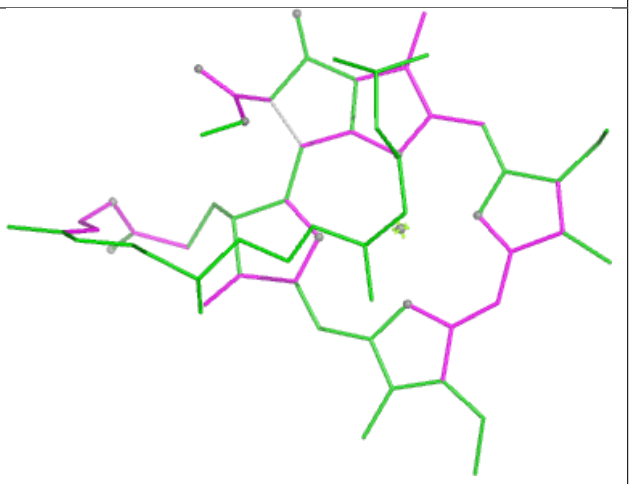
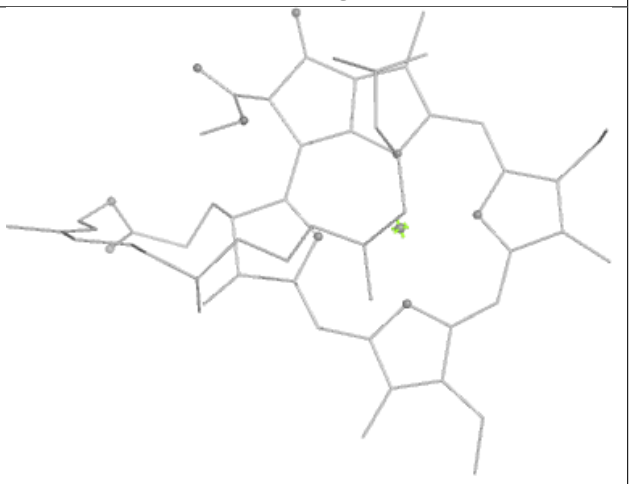


Bond angles

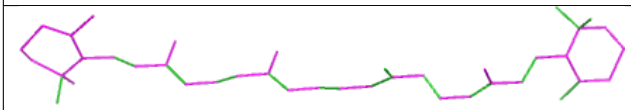


Torsions



Rings

Ligand BCR h 101



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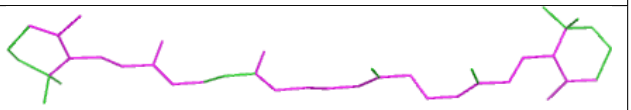
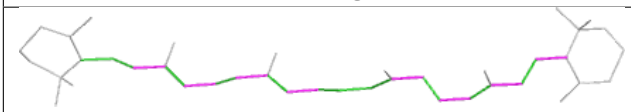


Bond angles



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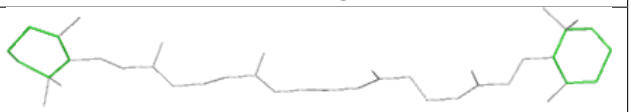
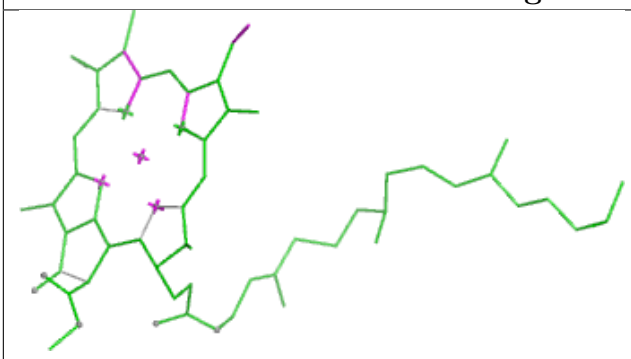


Rings

Ligand CLA C 511



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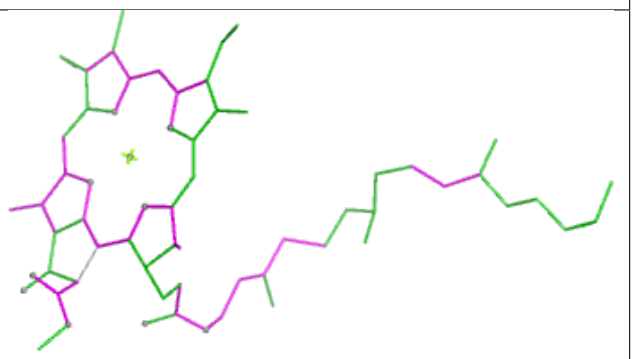
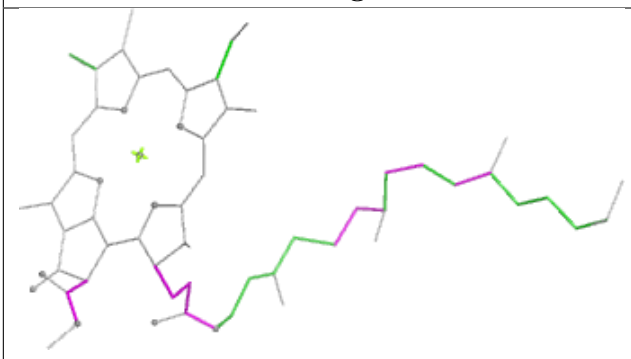


Bond angles



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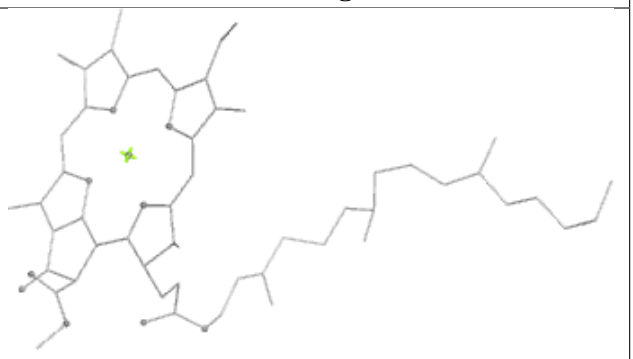
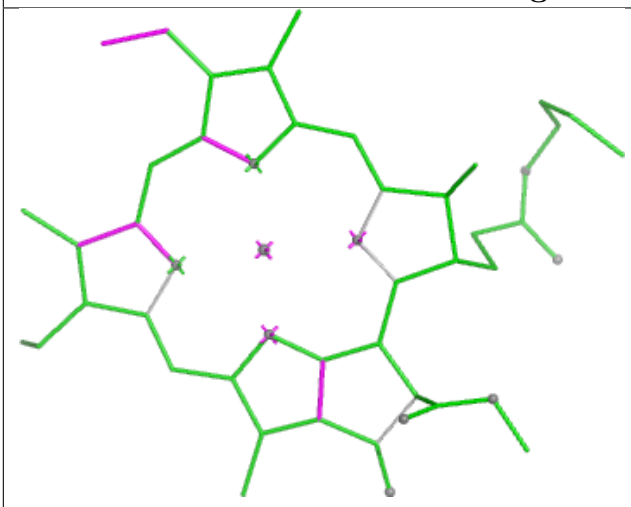


Rings

Ligand CLA r 601



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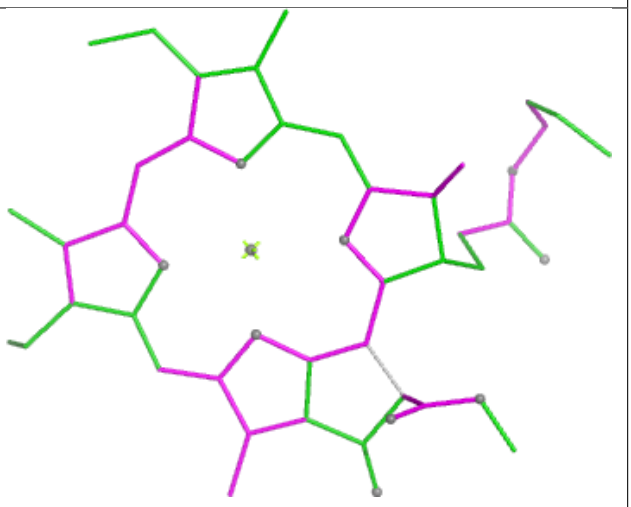
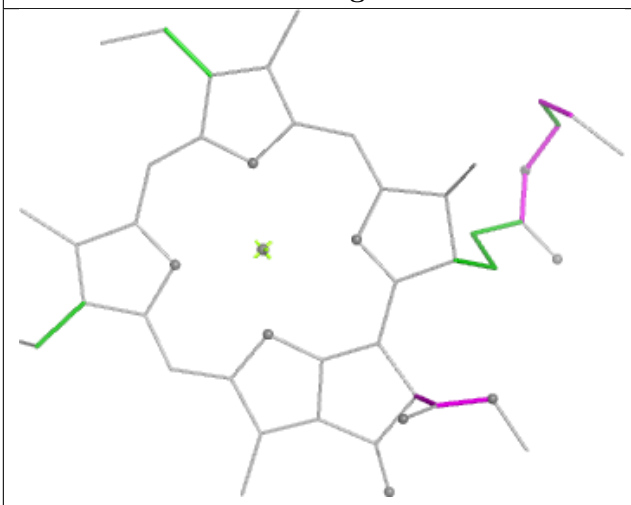


Bond angles



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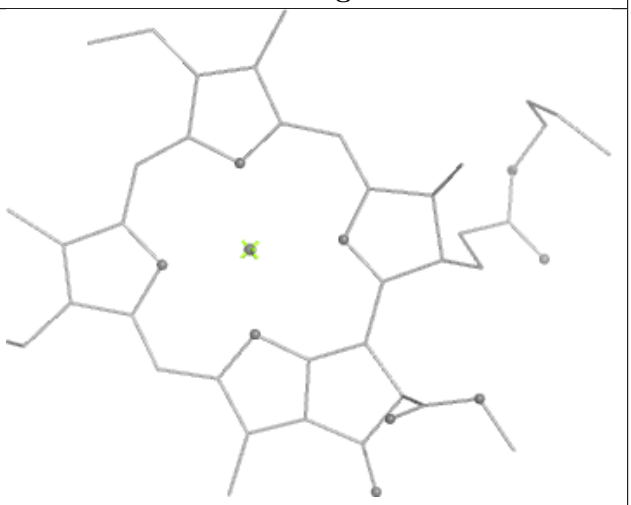
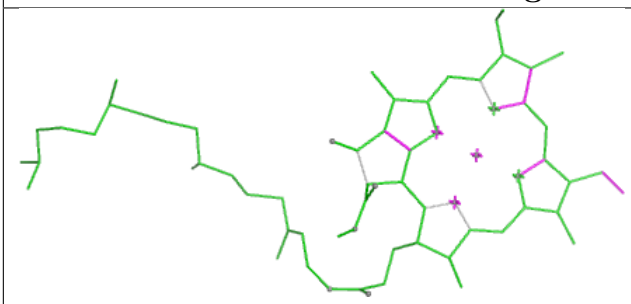


Rings

Ligand CLA B 602



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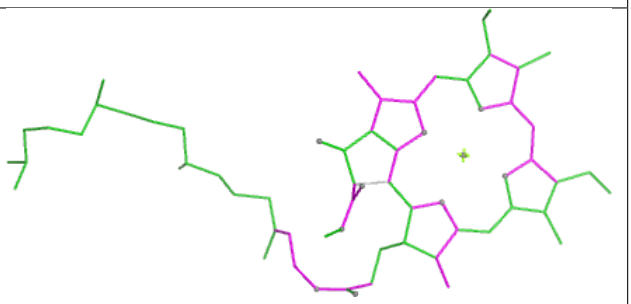
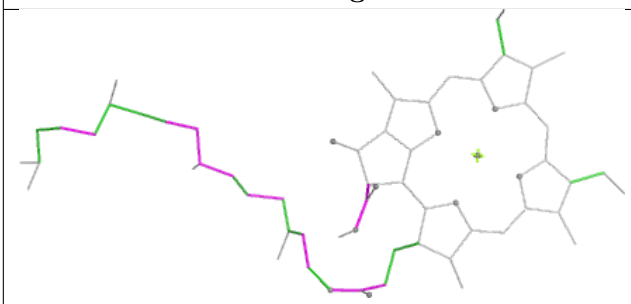


Bond angles



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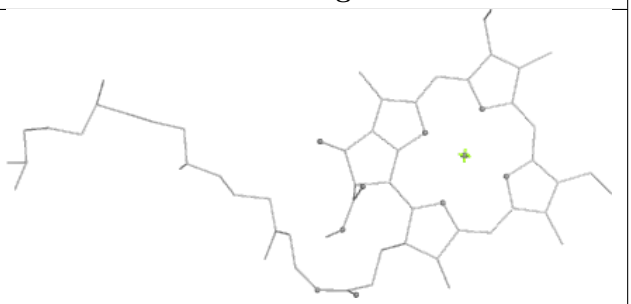
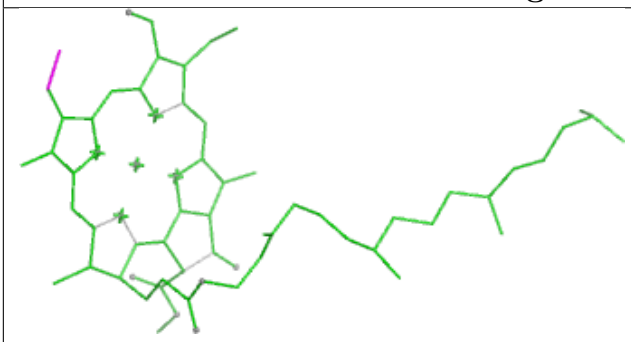


Rings

Ligand CHL n 609



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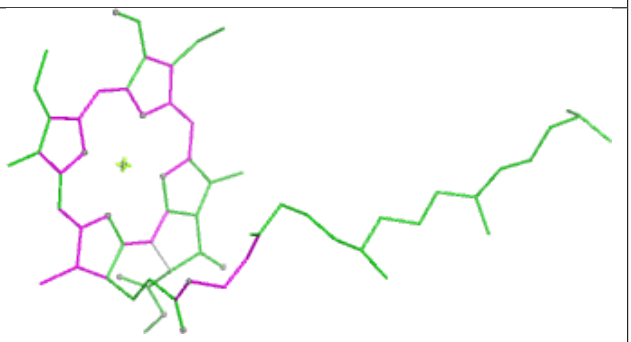
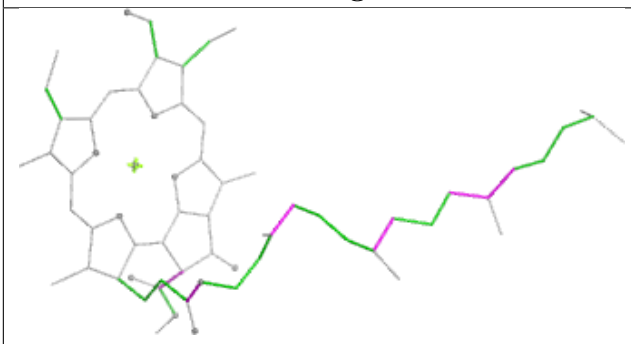


Bond angles



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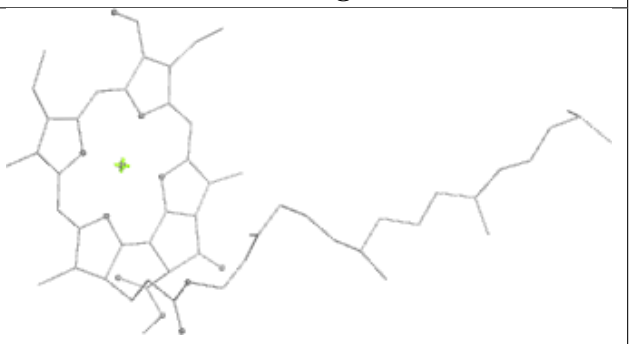
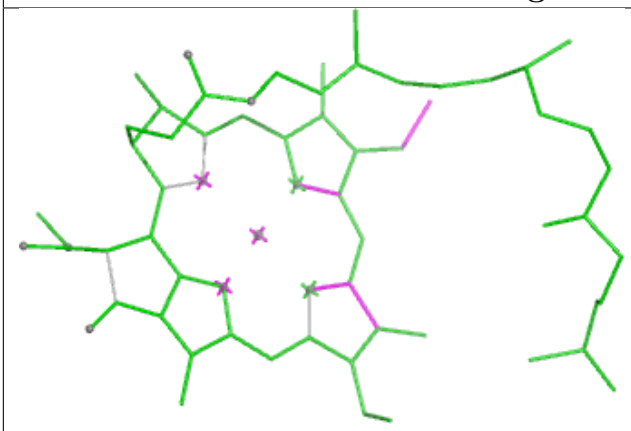


Rings

Ligand CLA y 303



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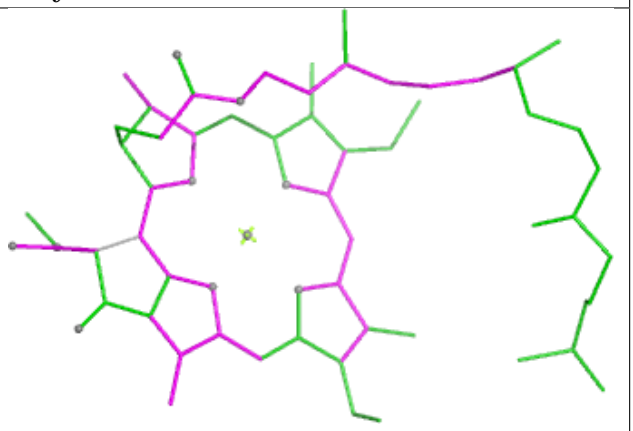
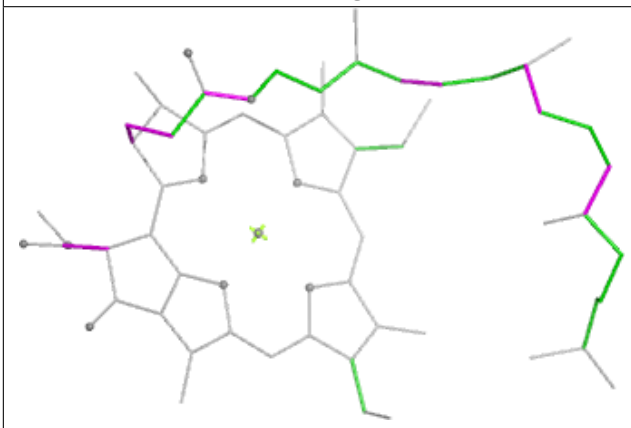


Bond angles



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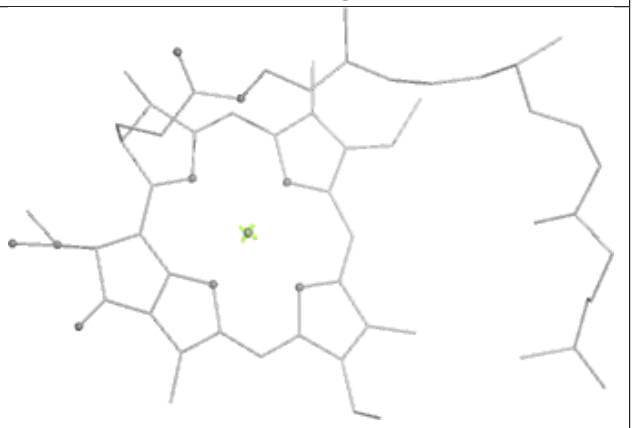
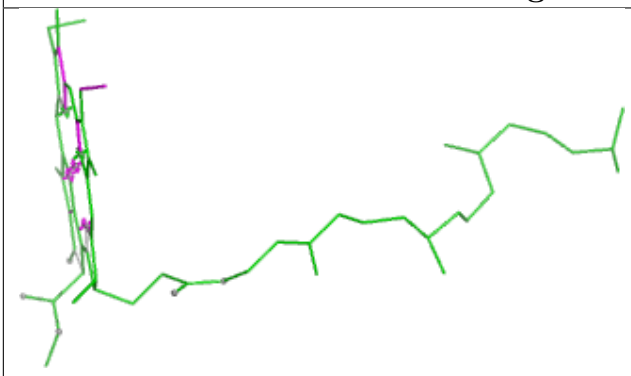


Rings

Ligand CLA b 606



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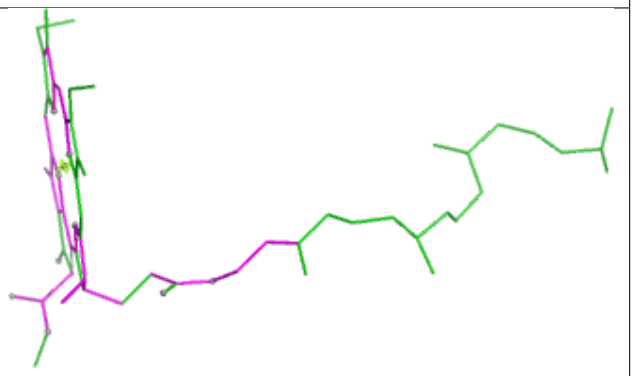
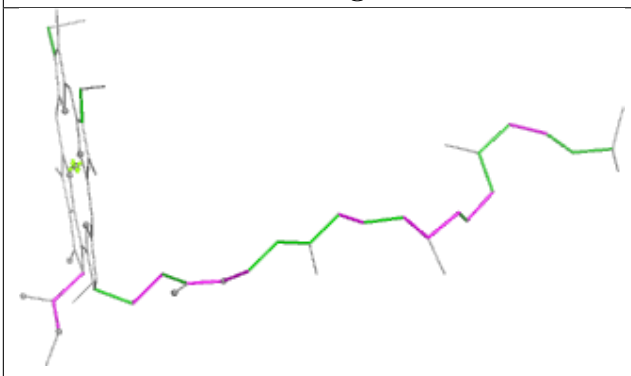


Bond angles



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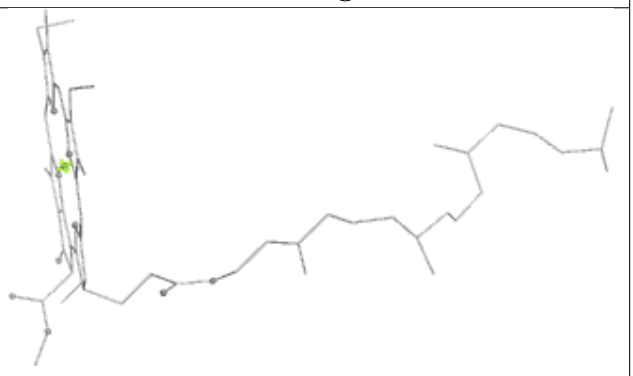
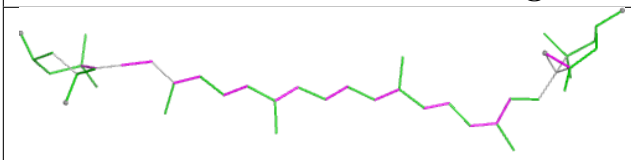
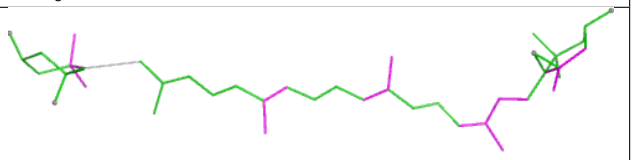


Rings

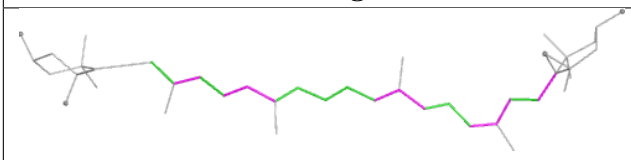
Ligand NEX y 301



Bond lengths



Bond angles



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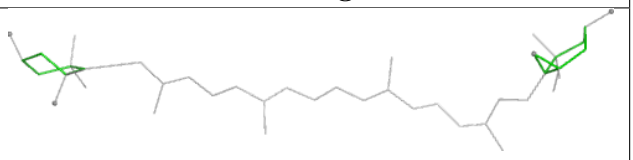
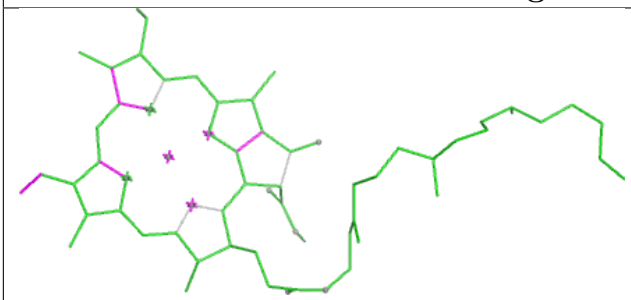


Rings

Ligand CLA b 602



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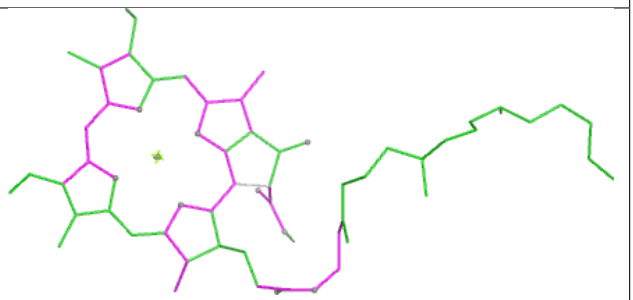
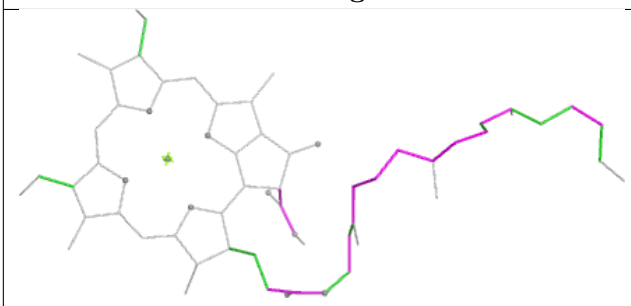
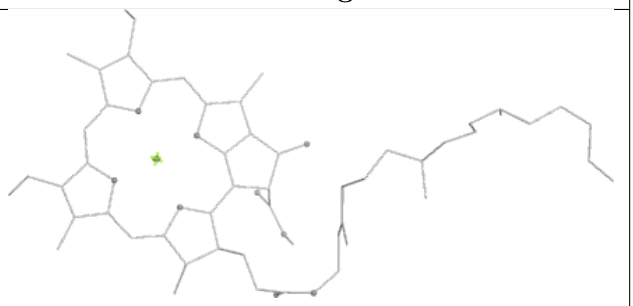


Bond angles

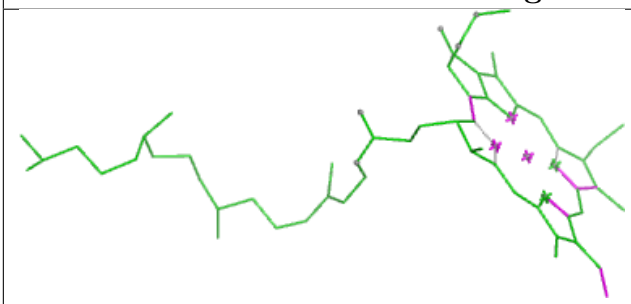


Torsions

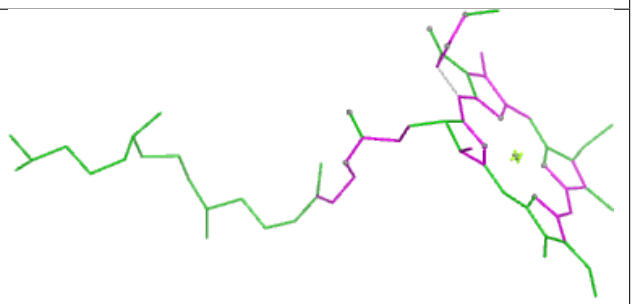


Rings

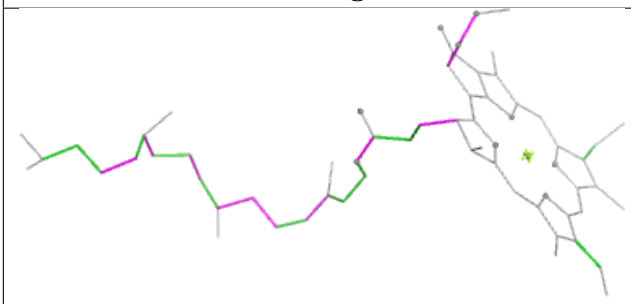
Ligand CLA C 502



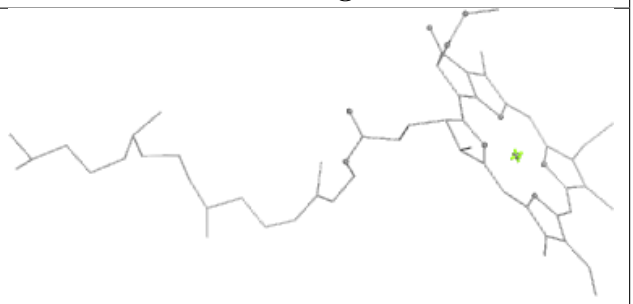
Bond lengths



Bond angles

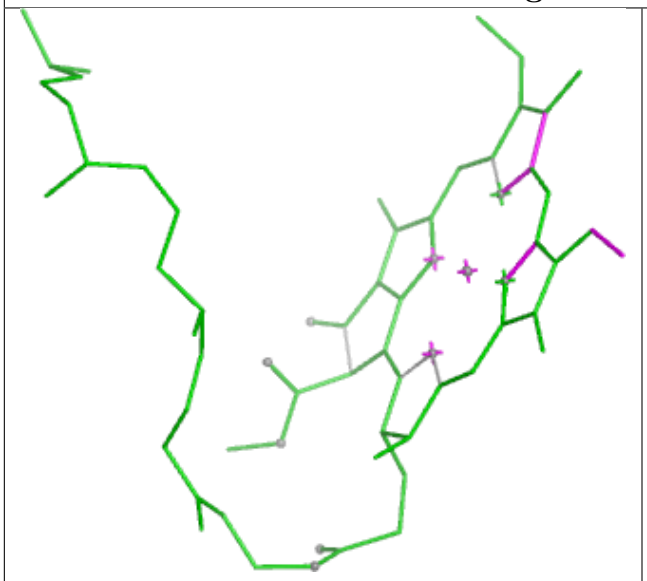


Torsions

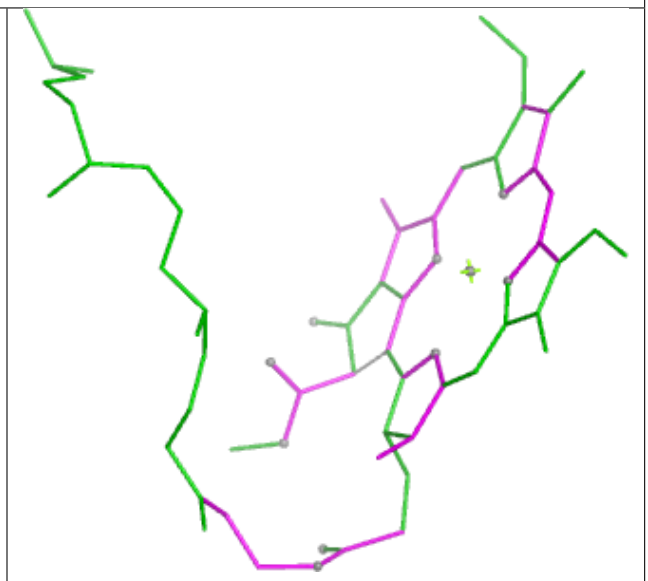


Rings

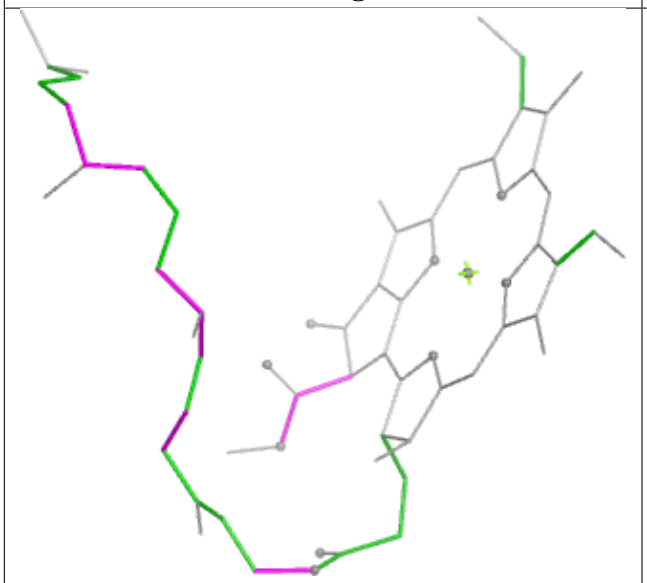
Ligand CLA B 613



Bond lengths



Bond angles

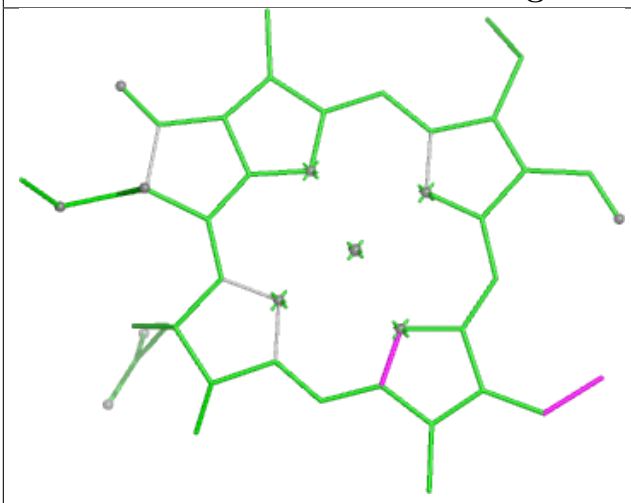


Torsions



Rings

Ligand CHL S 308



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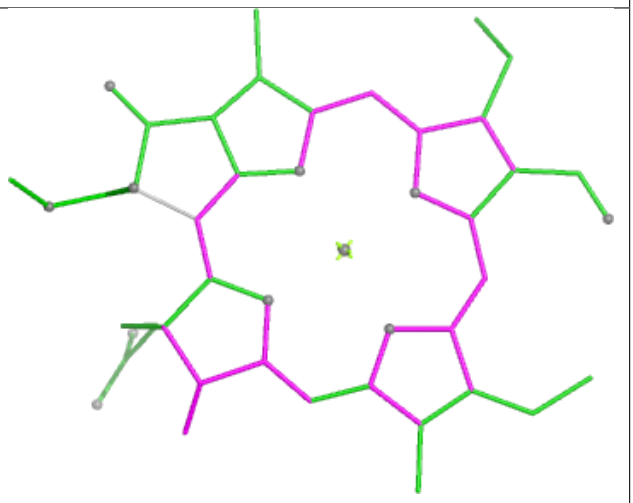
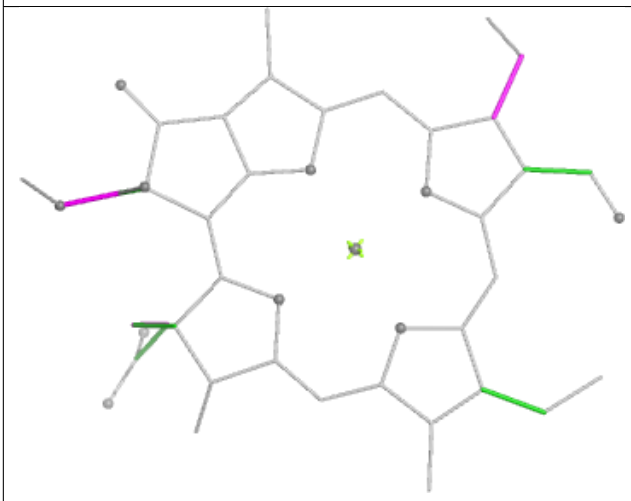


Bond angles



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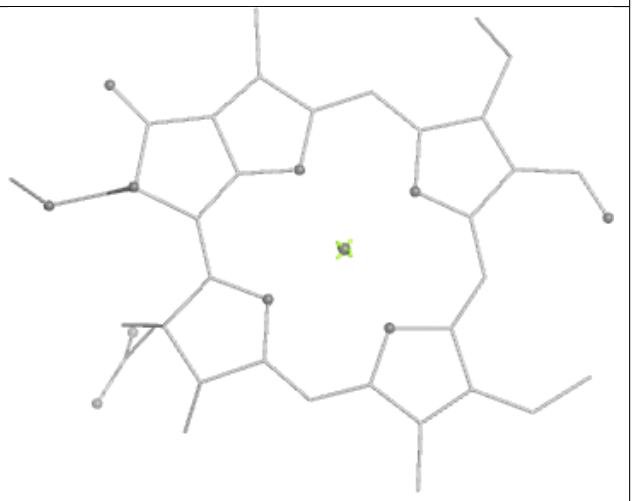
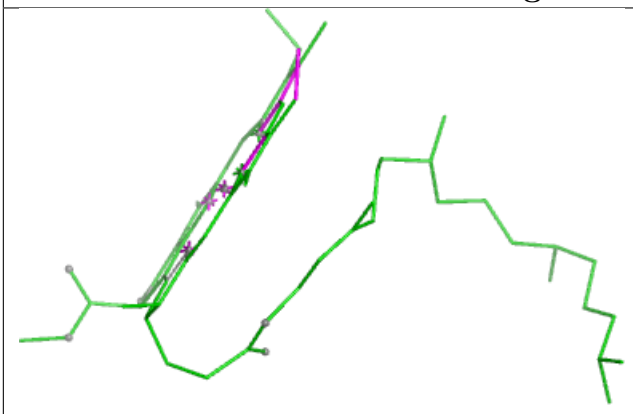


Rings

Ligand CLA R 613



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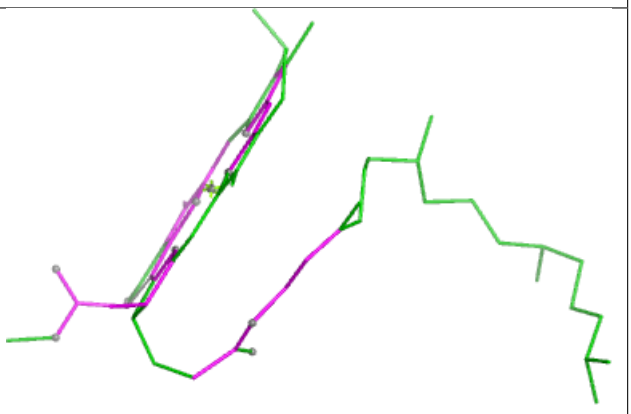
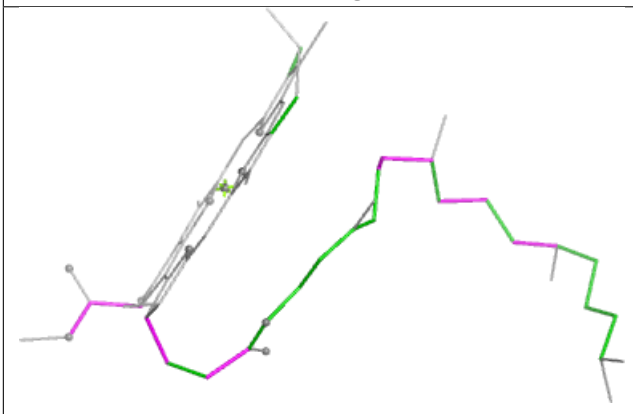


Bond angles

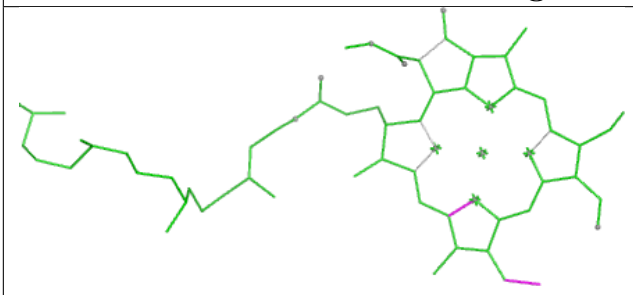


Torsions



Rings

Ligand CHL g 601



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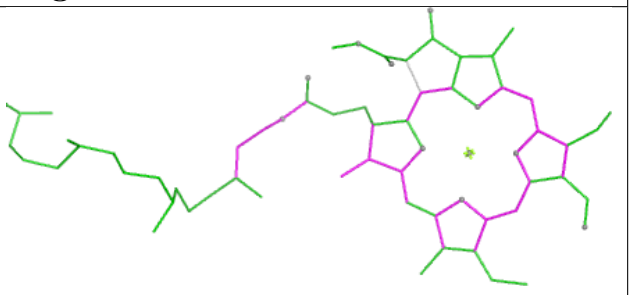
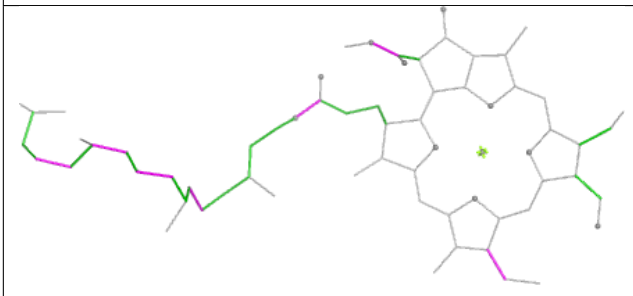


Bond angles



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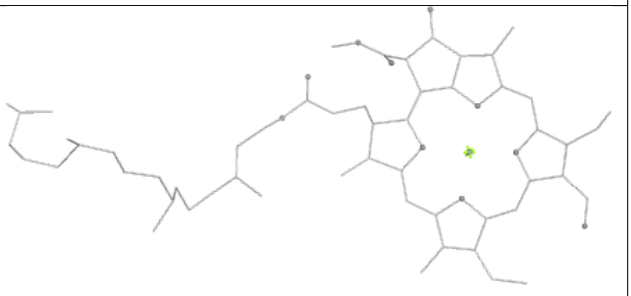
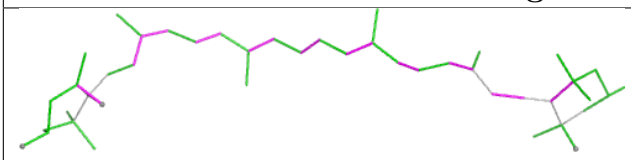


Rings

Ligand NEX g 617



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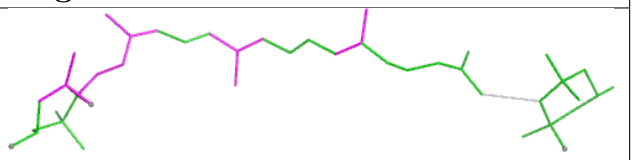
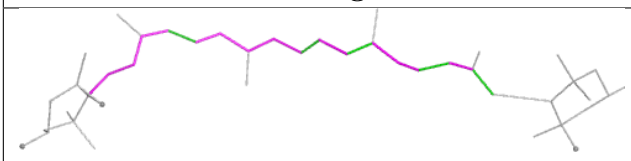


Bond angles



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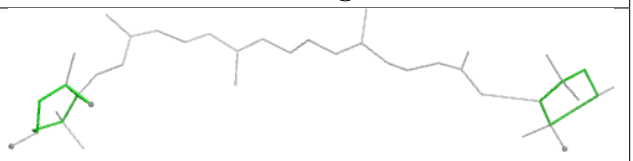
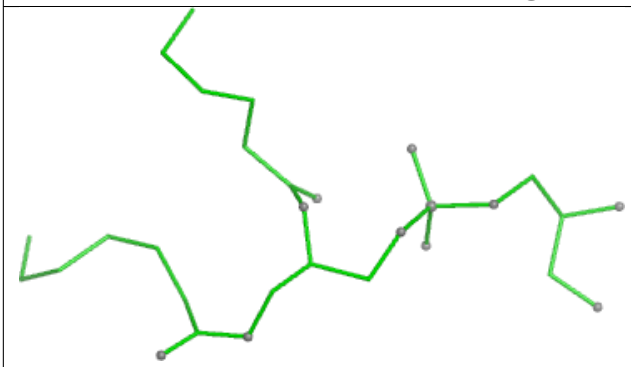


Rings

Ligand LHG B 622



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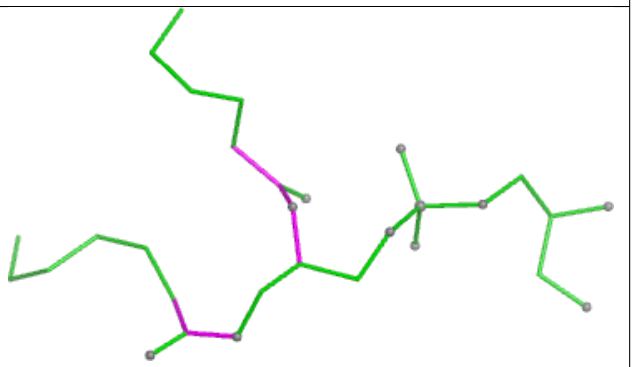

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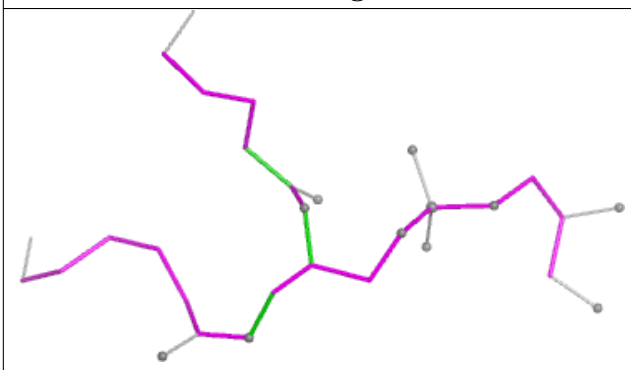

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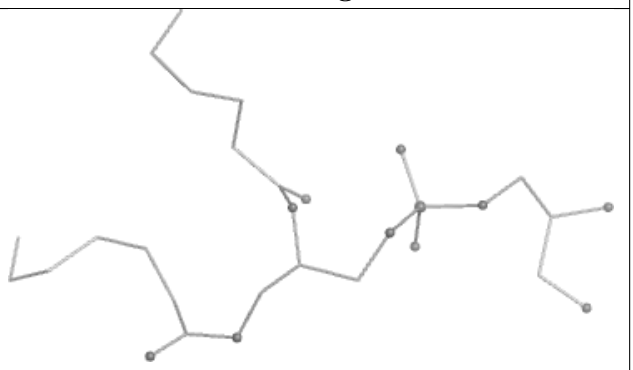
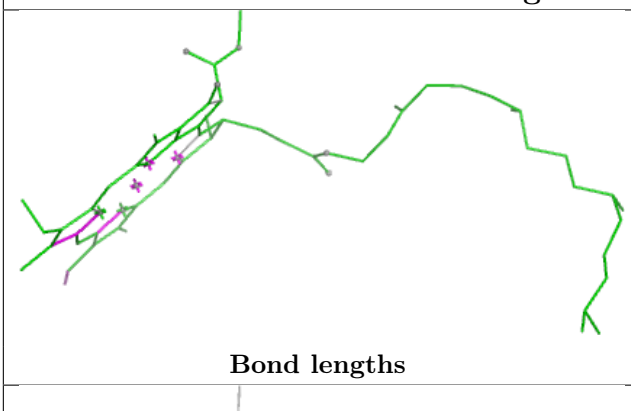


Rings

Ligand CLA D 403



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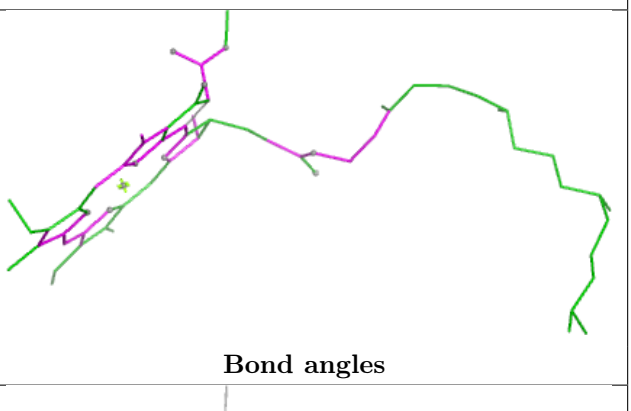
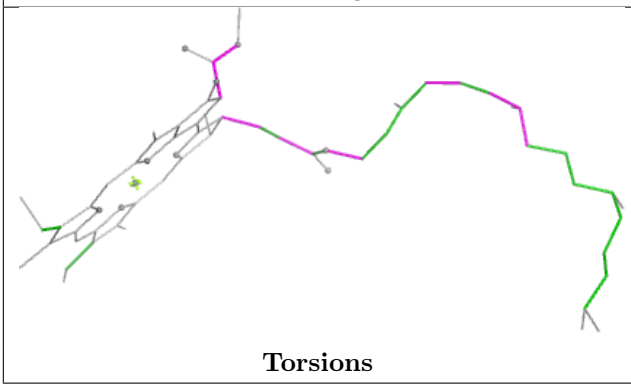


Bond angles



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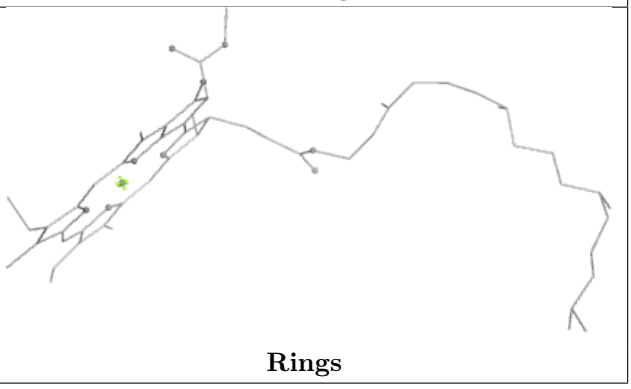
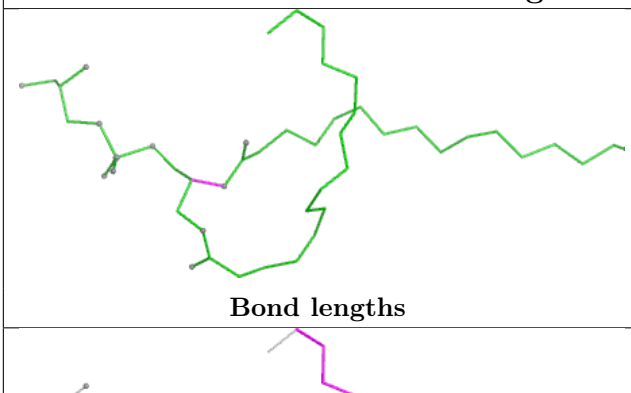


Rings

Ligand LHG y 319



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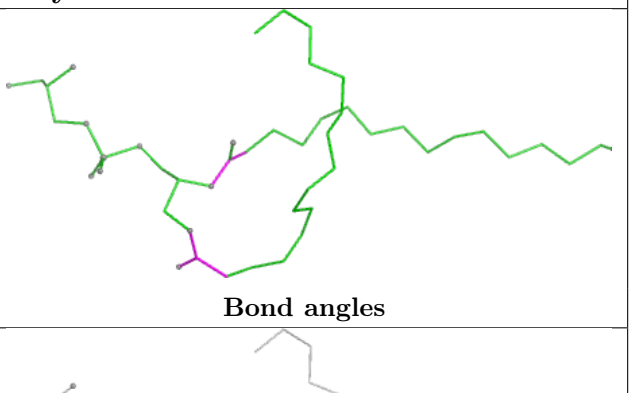
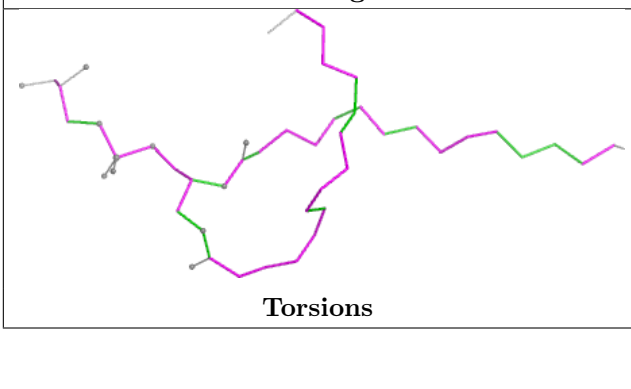


Bond angles



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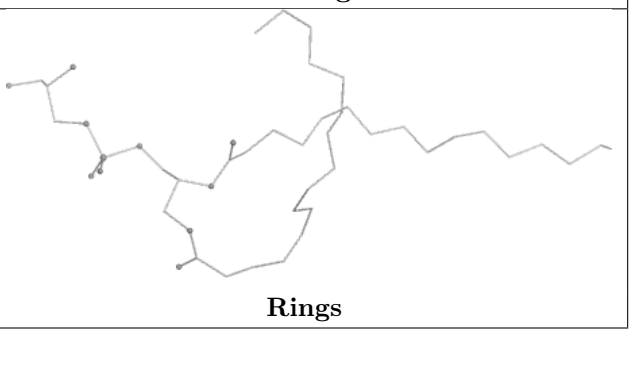
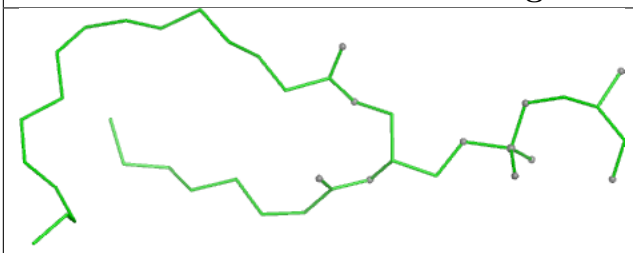


Rings

Ligand LHG b 622



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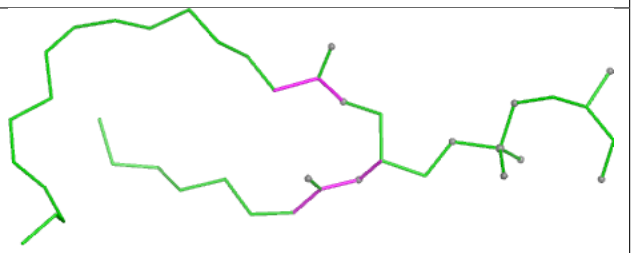
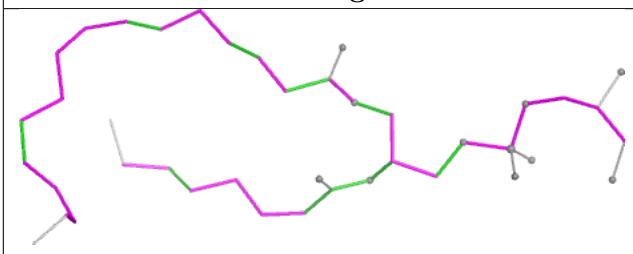


Bond angles



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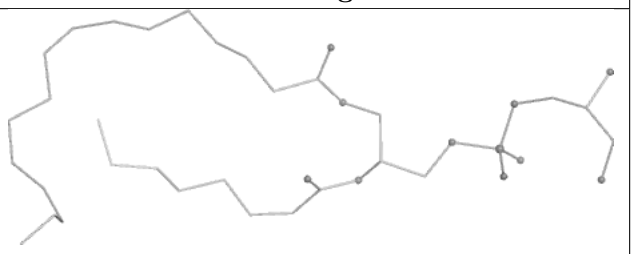
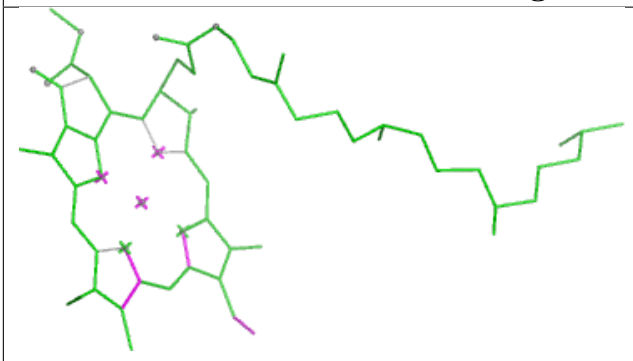


Rings

Ligand CLA c 511



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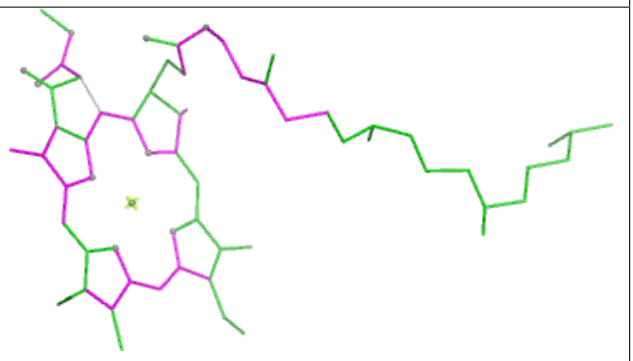
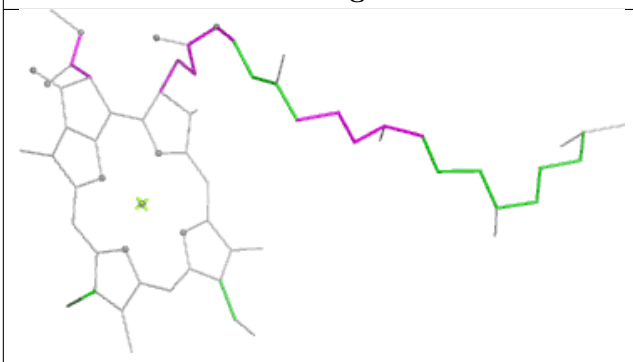


Bond angles



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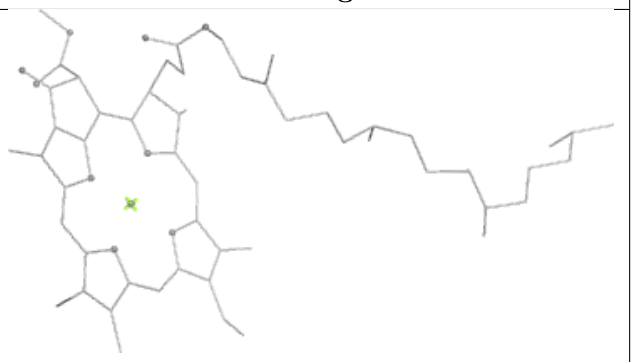
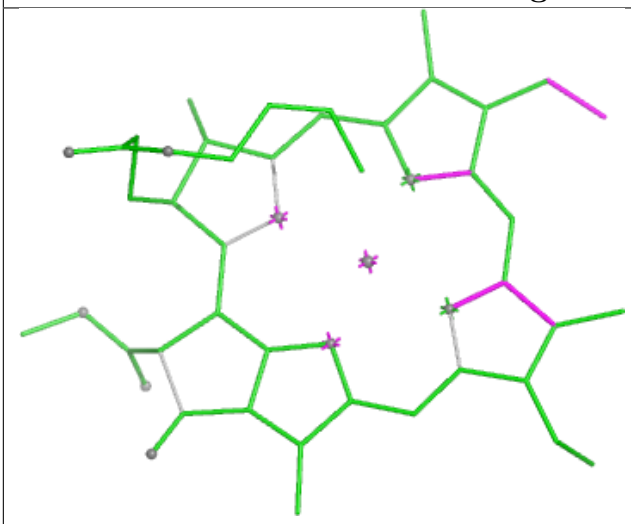


Rings

Ligand CLA r 610



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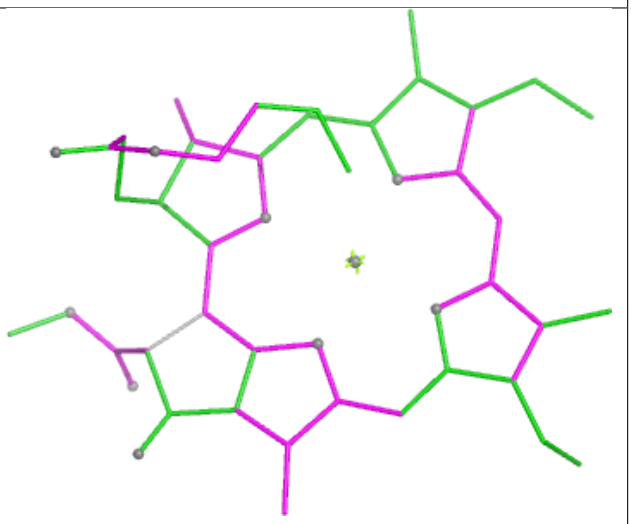
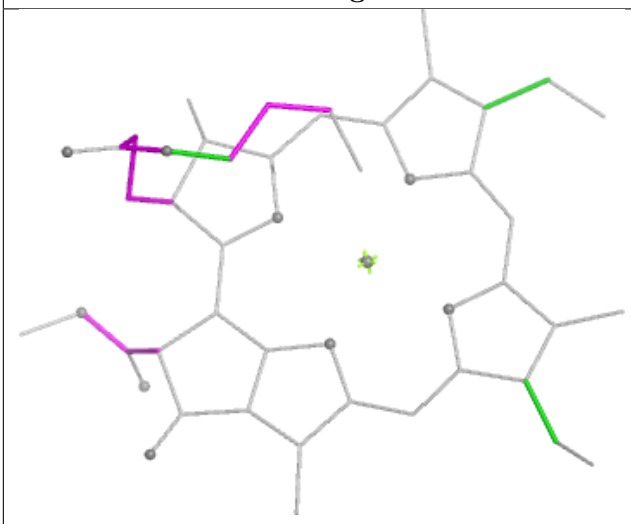


Bond angles



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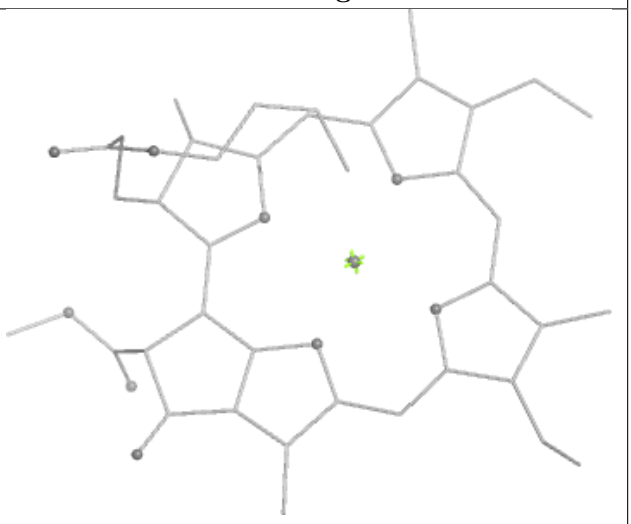
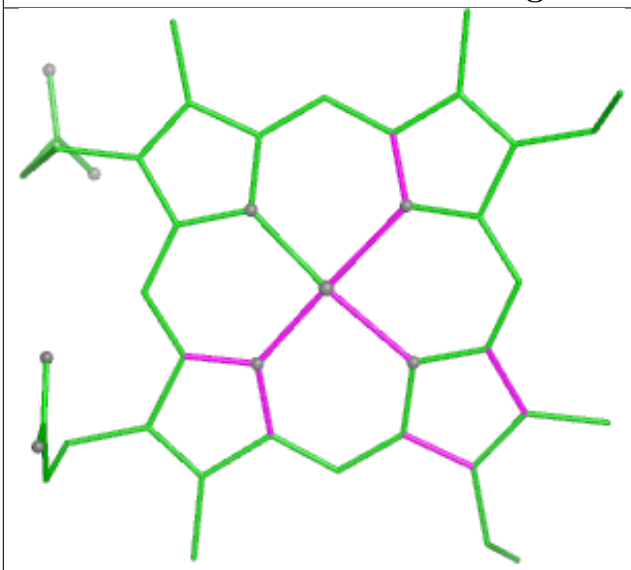


Rings

Ligand HEM f 101



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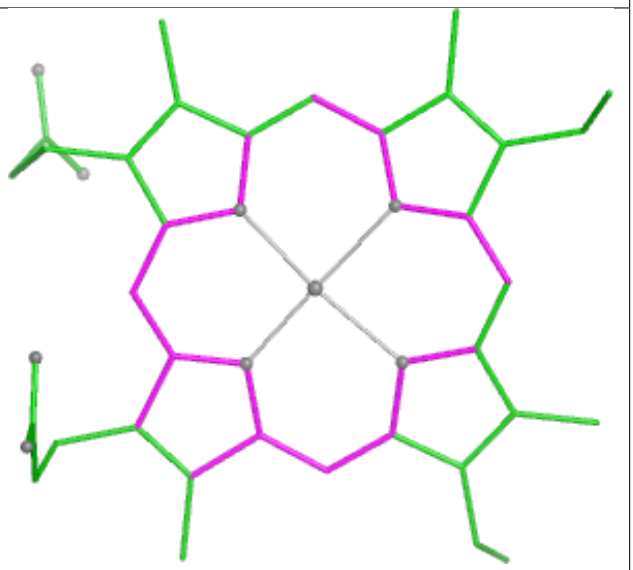
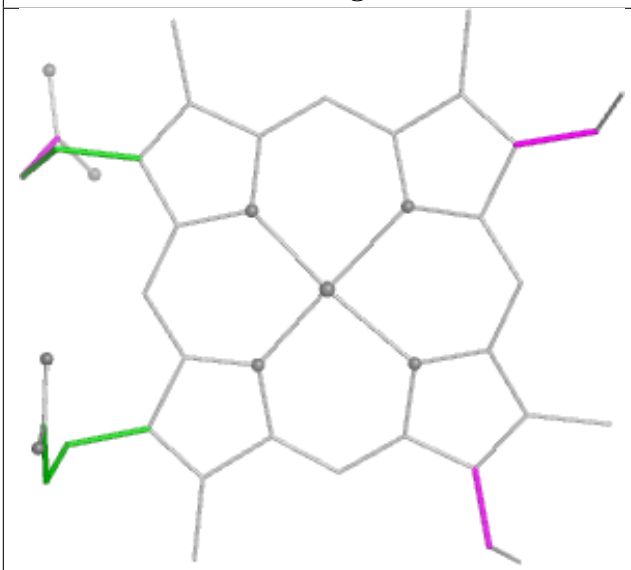


Bond angles



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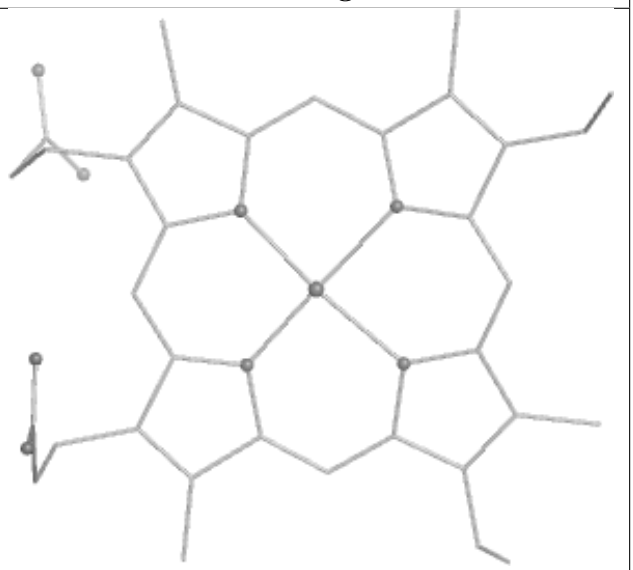
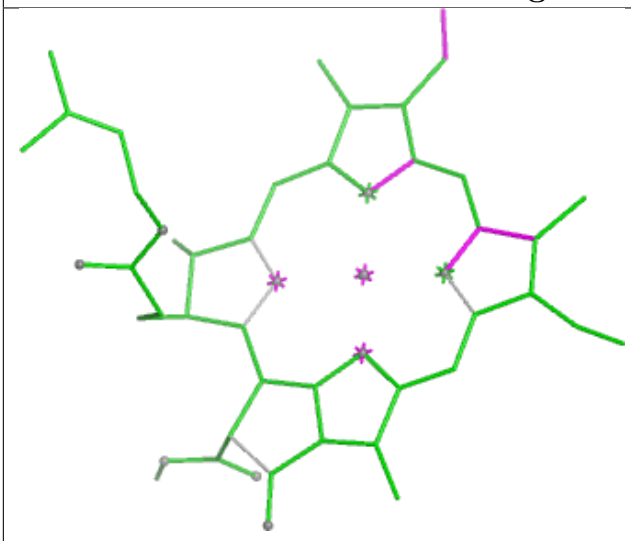
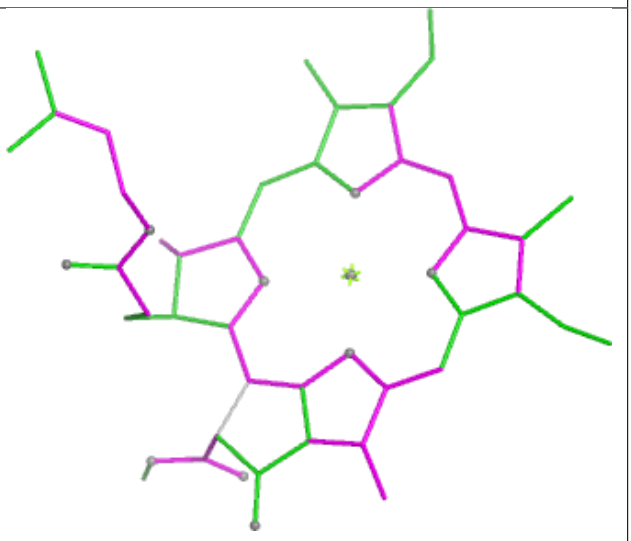


Rings

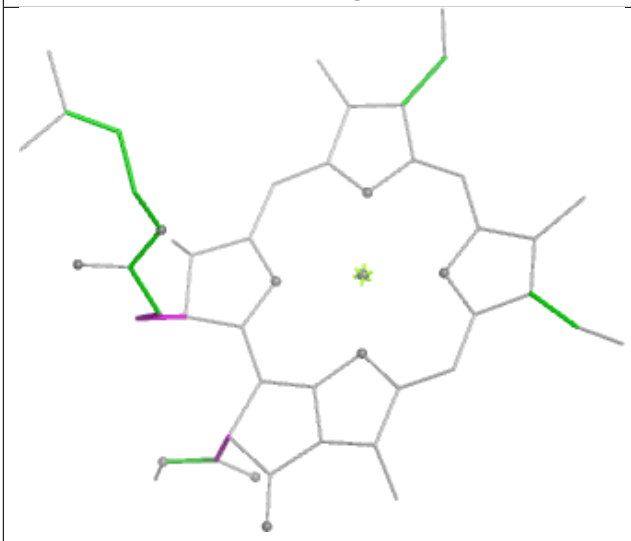
Ligand CLA a 407



Bond lengths



Bond angles



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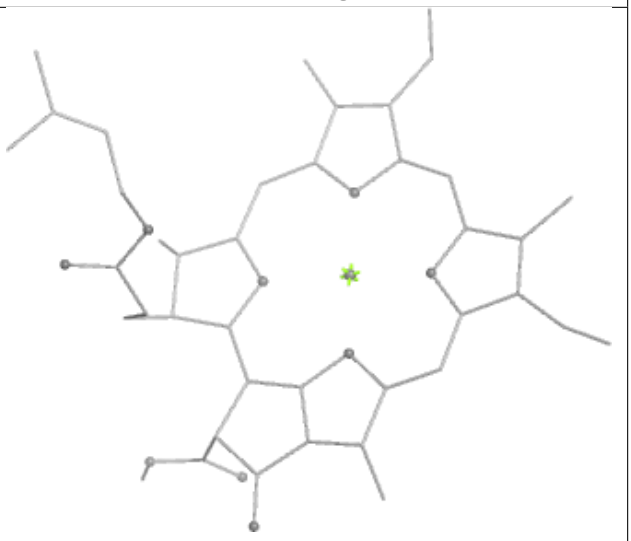
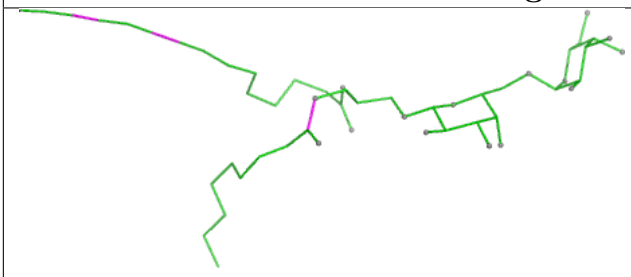
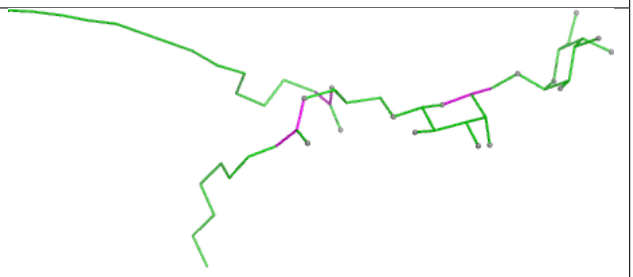


Rings

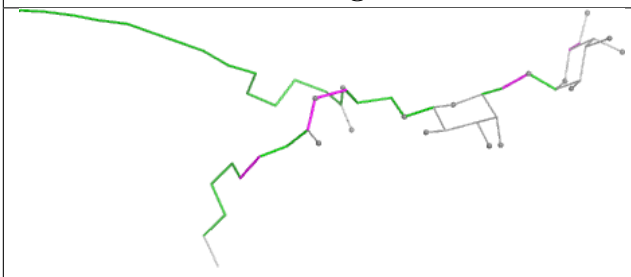
Ligand DGD c 516



Bond lengths



Bond angles



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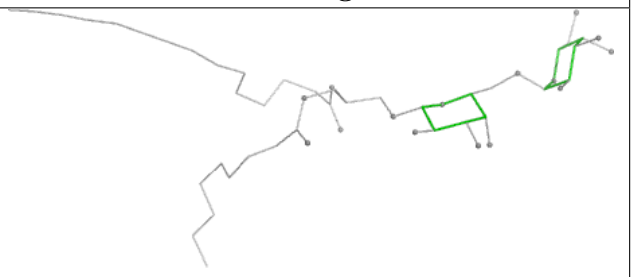
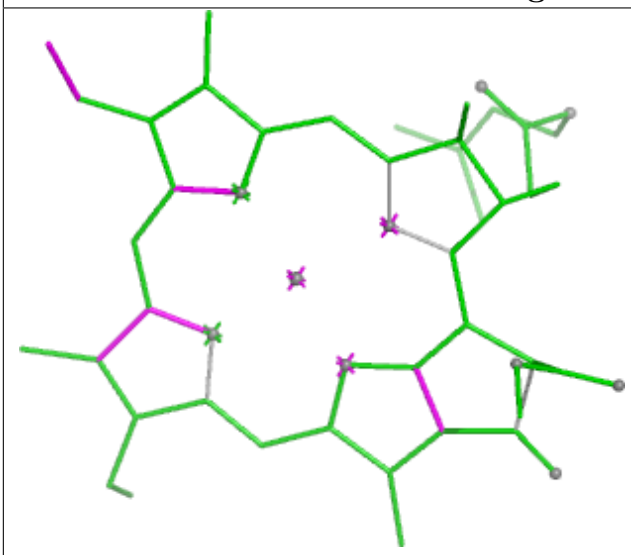
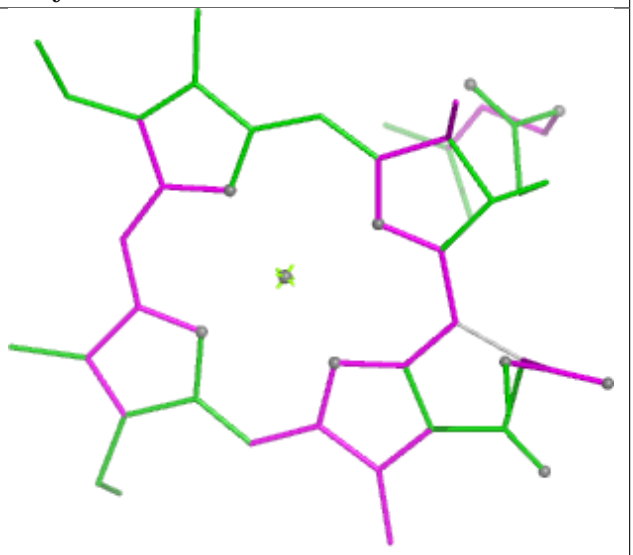


Rings

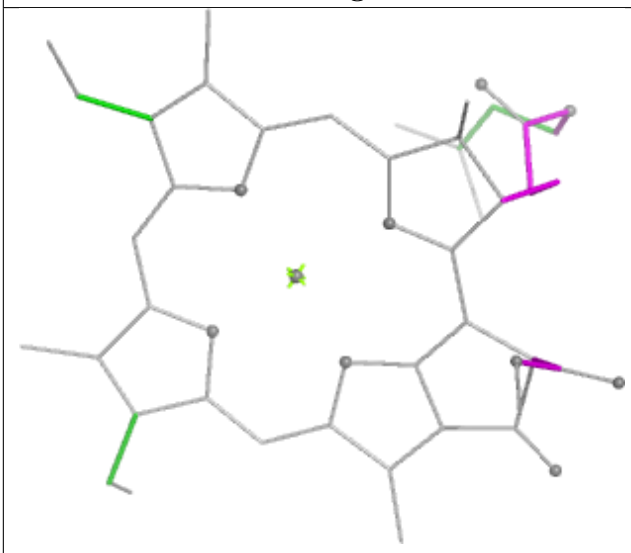
Ligand CLA y 305



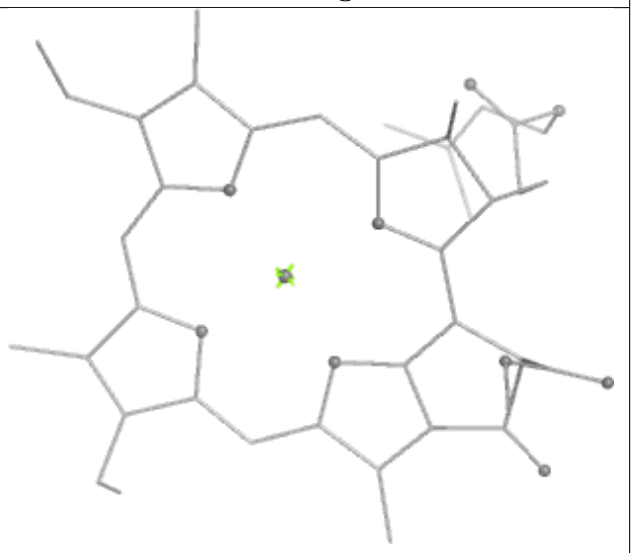
Bond lengths



Bond angles

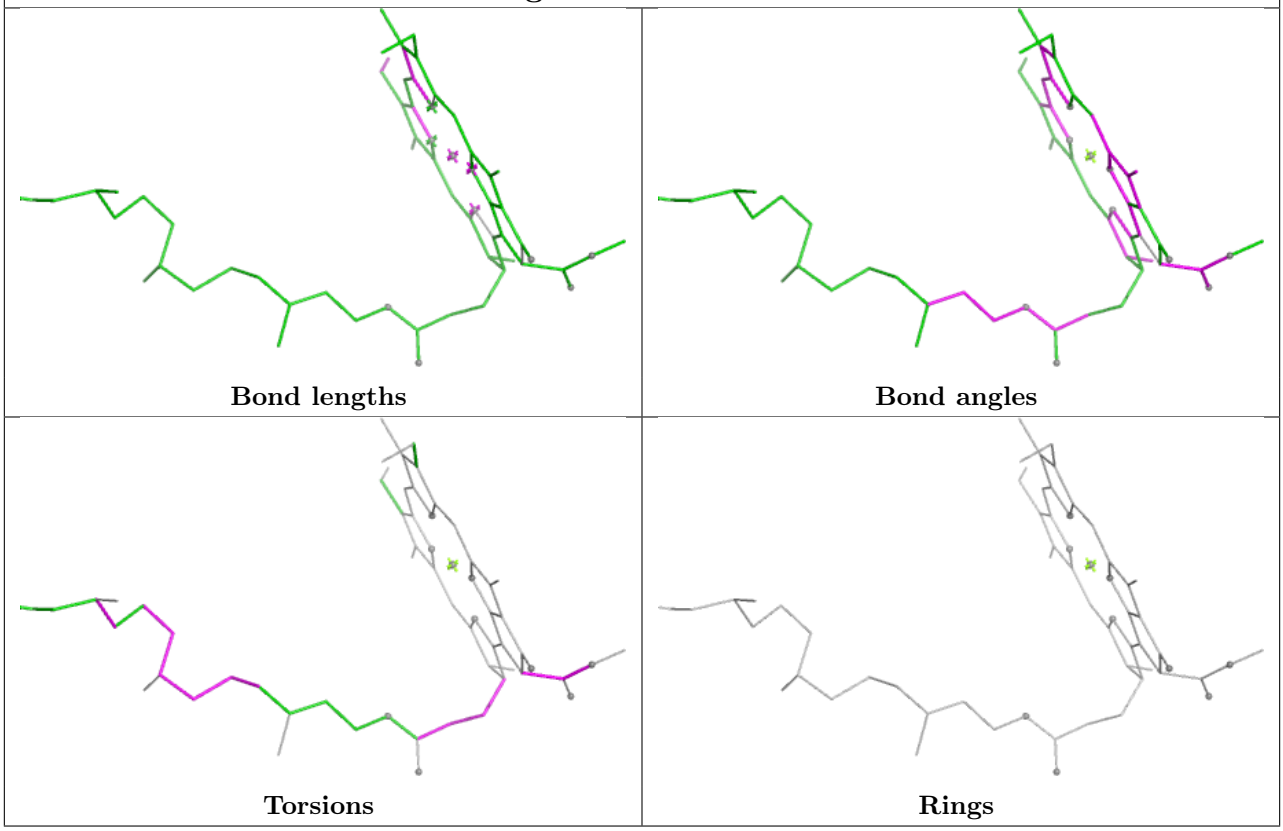


Torsions



Rings

Ligand CLA B 607



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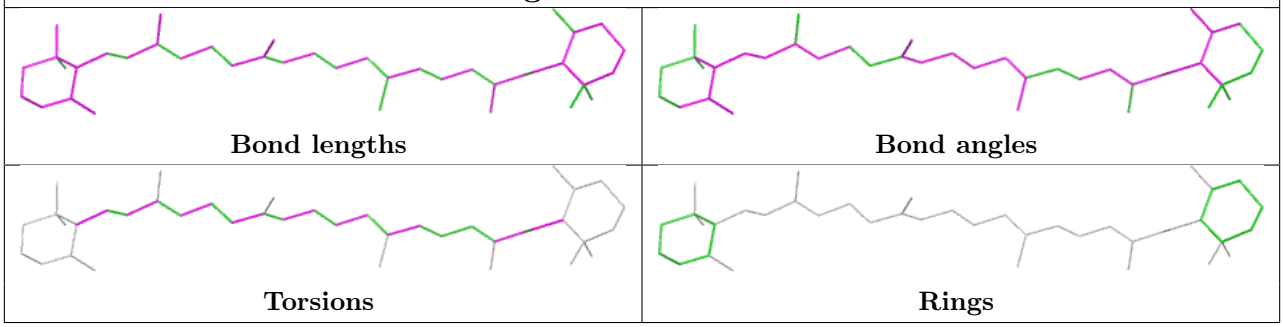
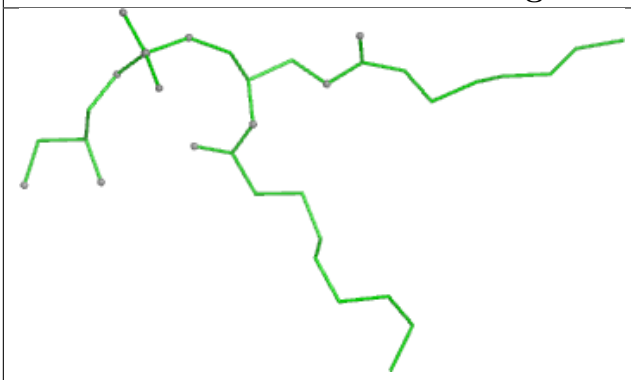
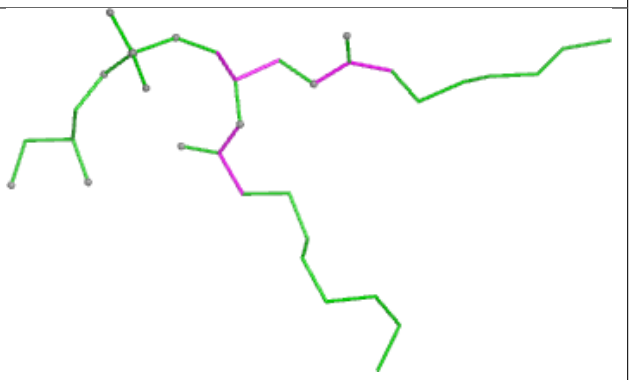


Ligand LHG S 301



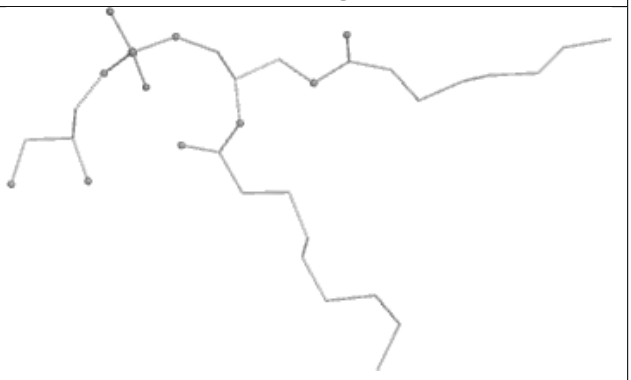
Bond lengths



Bond angles

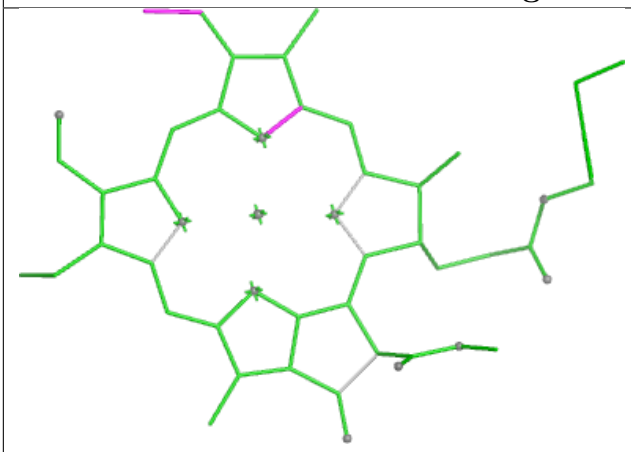


Torsions



Rings

Ligand CHL N 601



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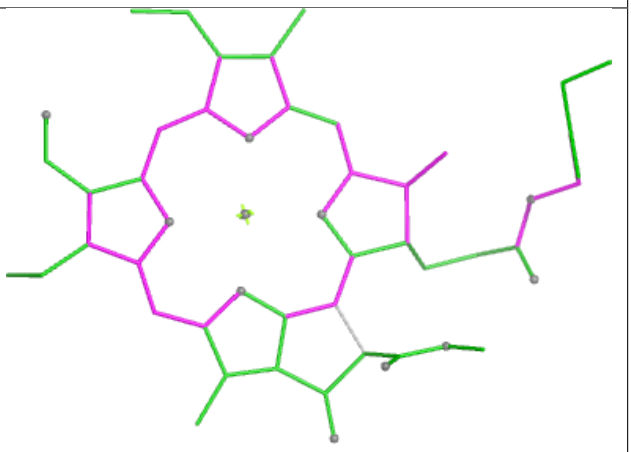
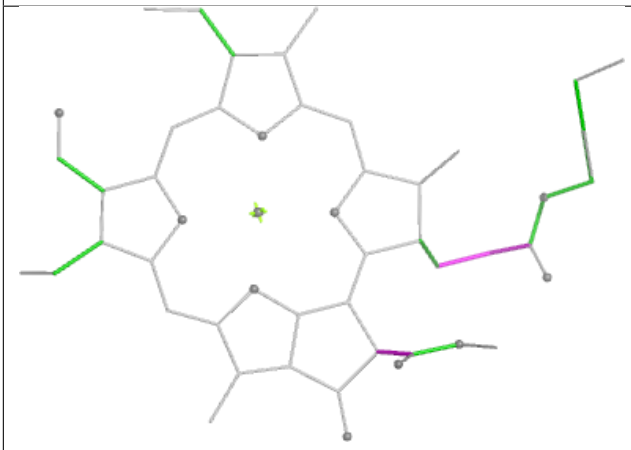


Bond angles



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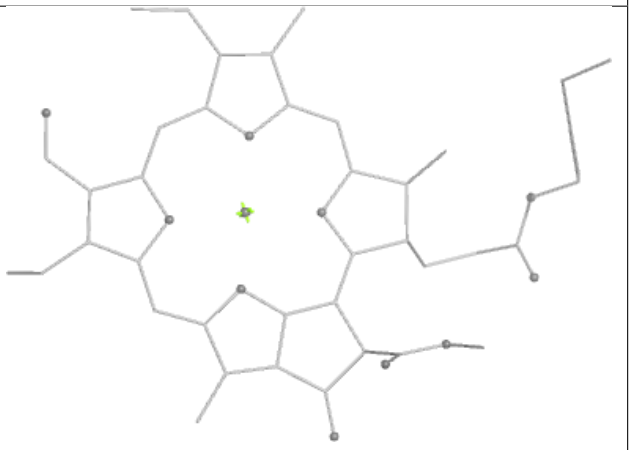
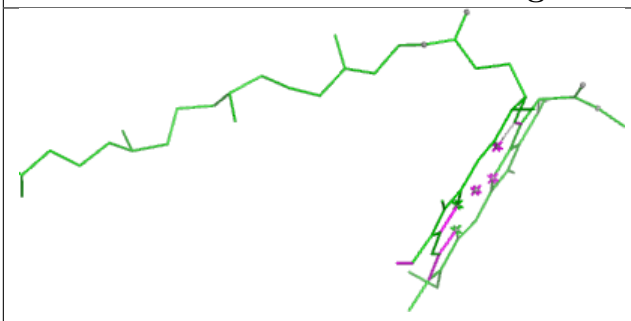


Rings

Ligand CLA b 607



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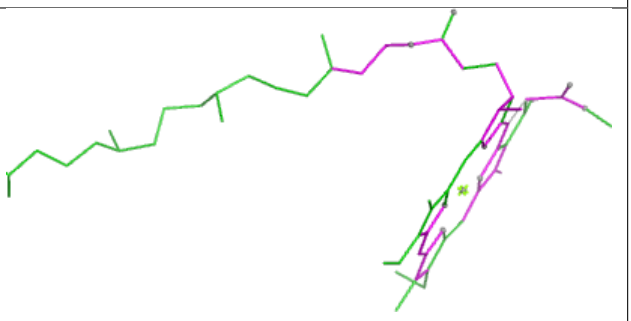
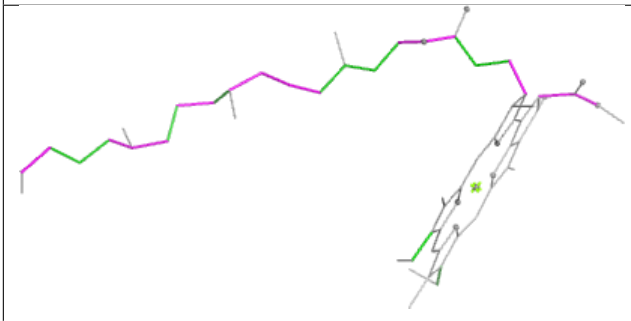


Bond angles

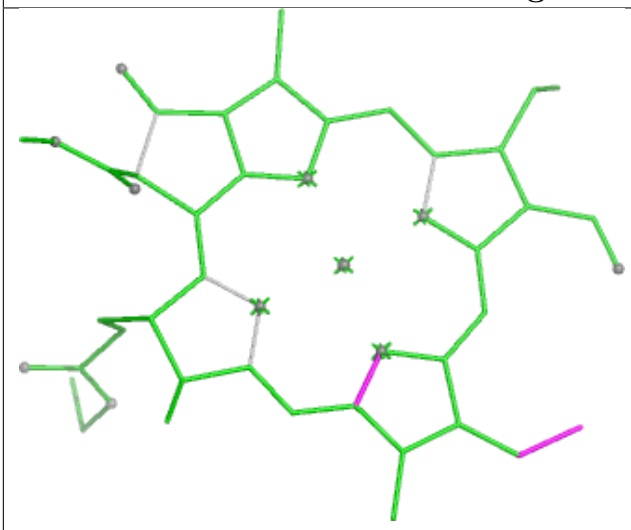


Torsions



Rings

Ligand CHL y 306



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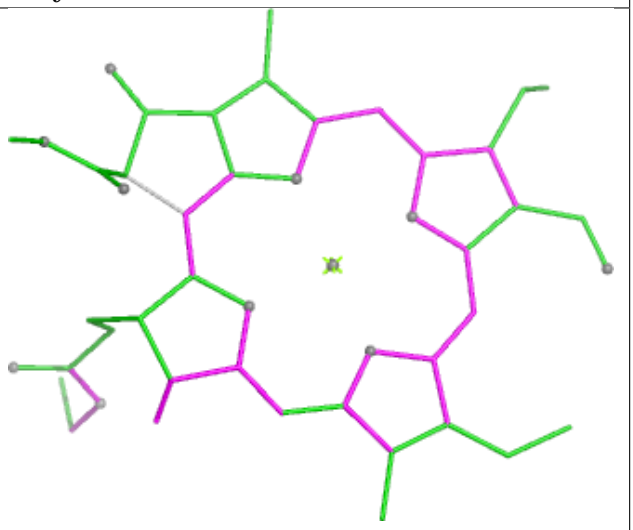
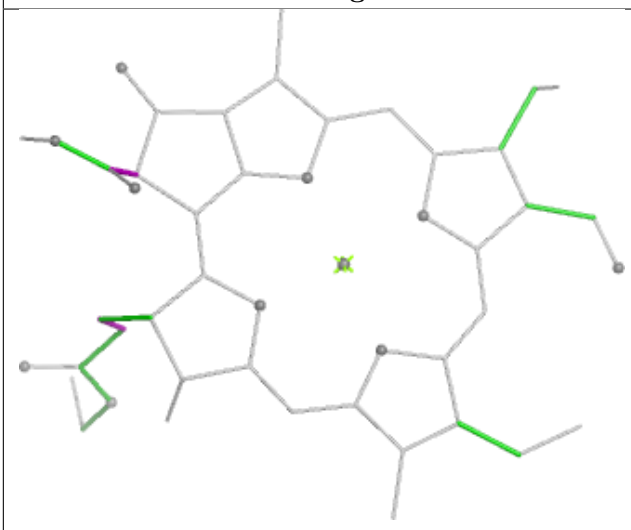


Bond angles



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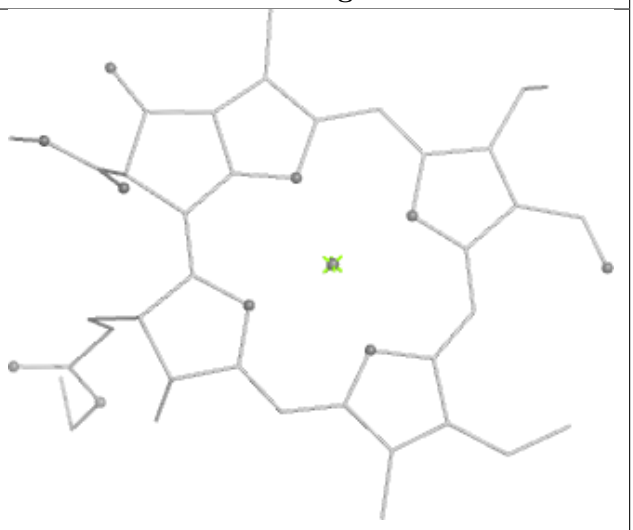
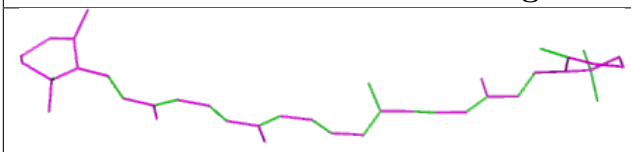


Rings

Ligand BCR D 405



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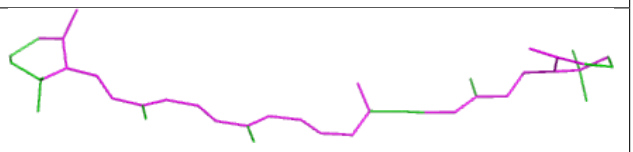
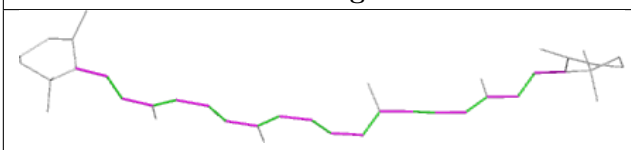


Bond angles



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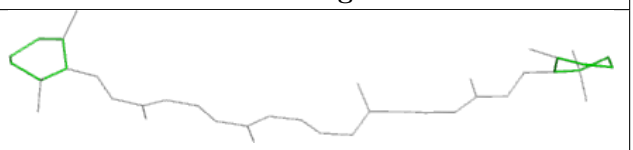
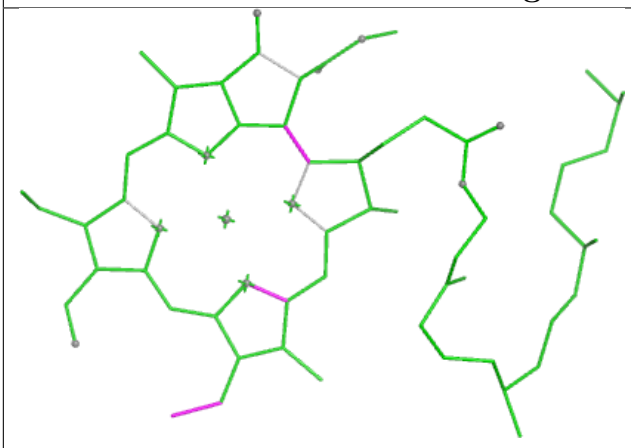


Rings

Ligand CHL Y 607



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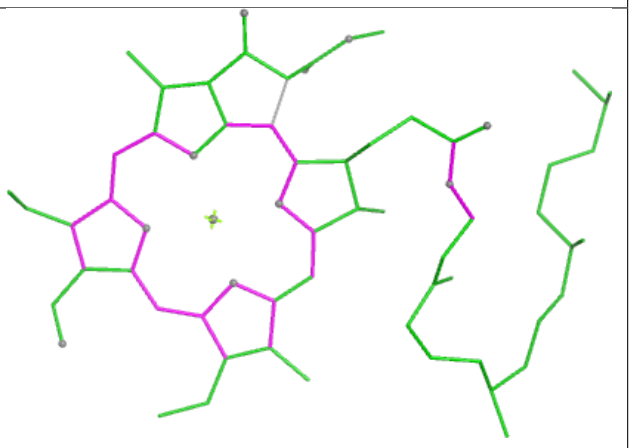
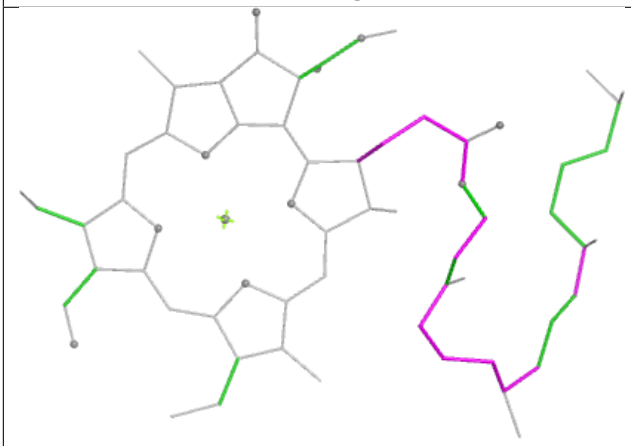


Bond angles



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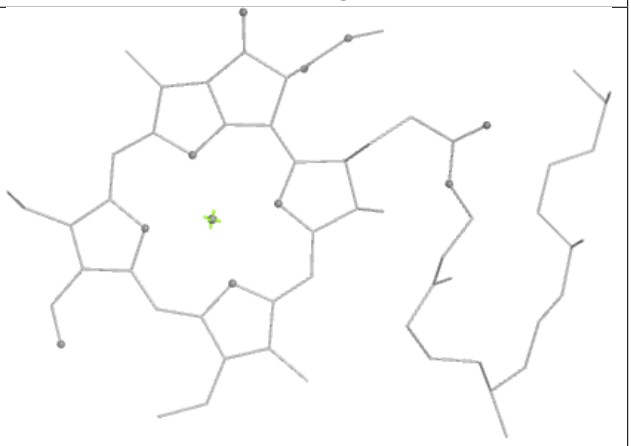
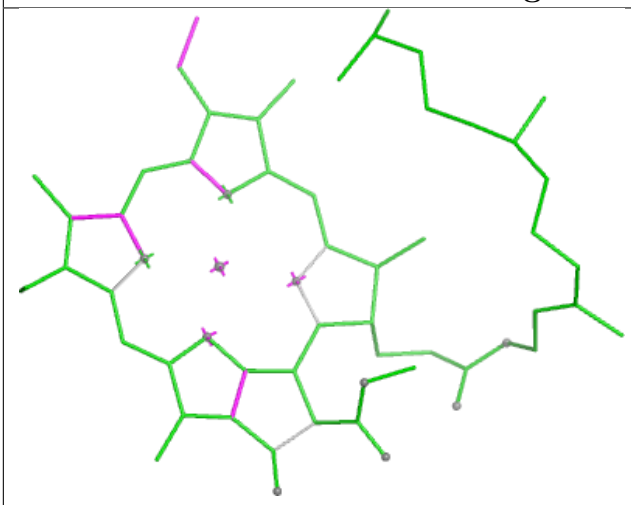


Rings

Ligand CLA Y 612



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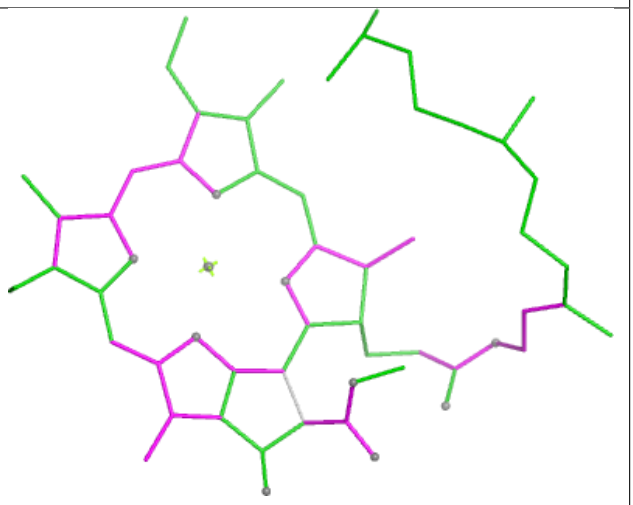
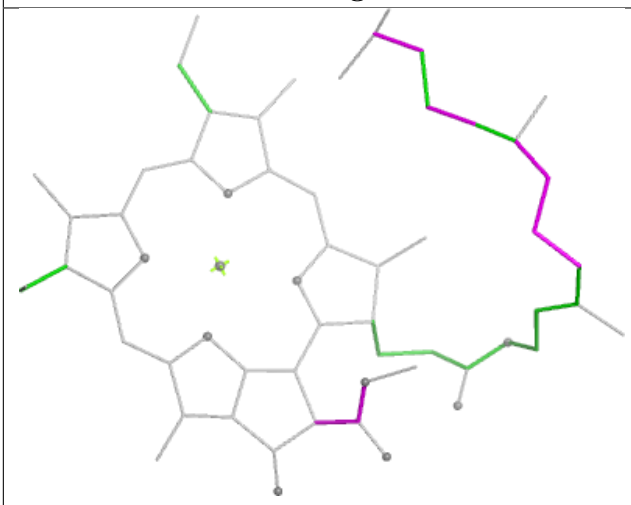


Bond angles



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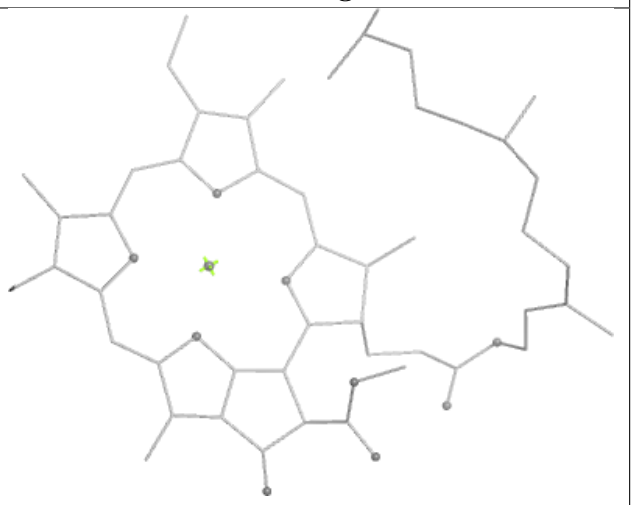
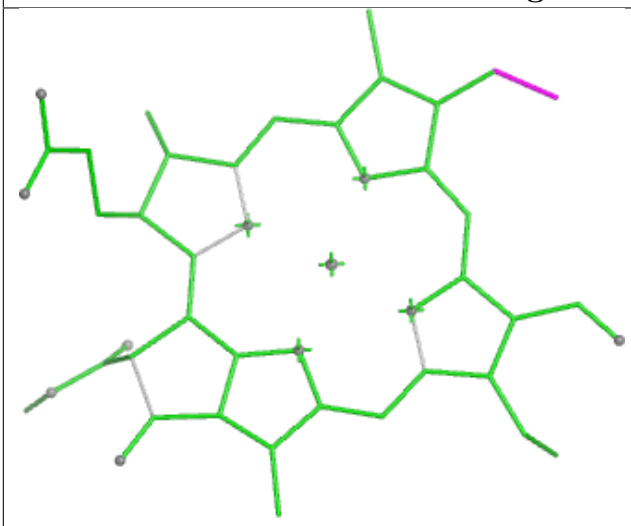


Rings

Ligand CHL S 306



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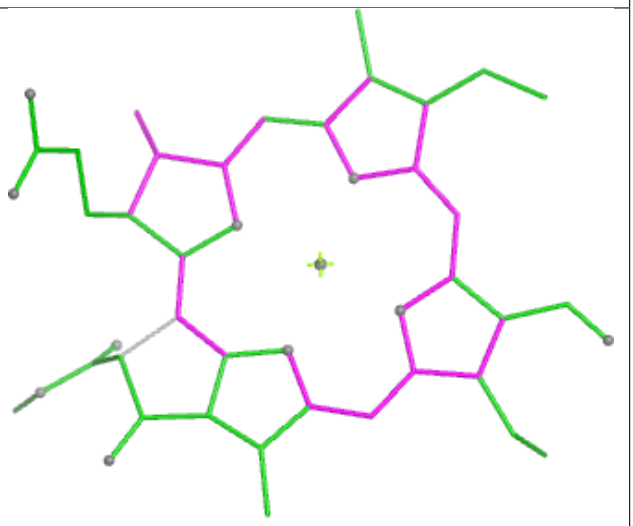
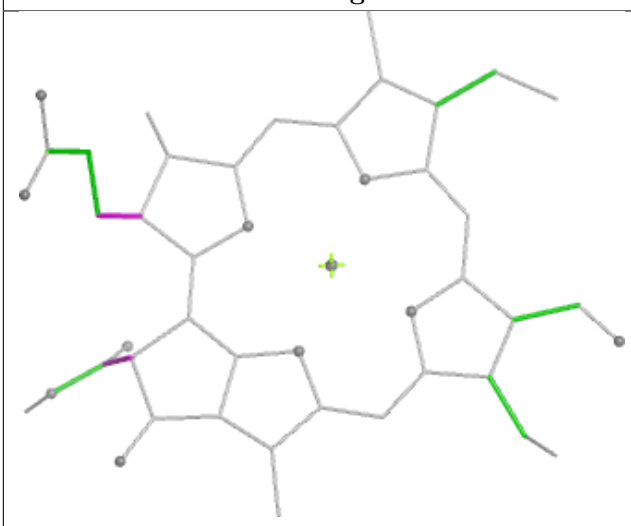


Bond angles



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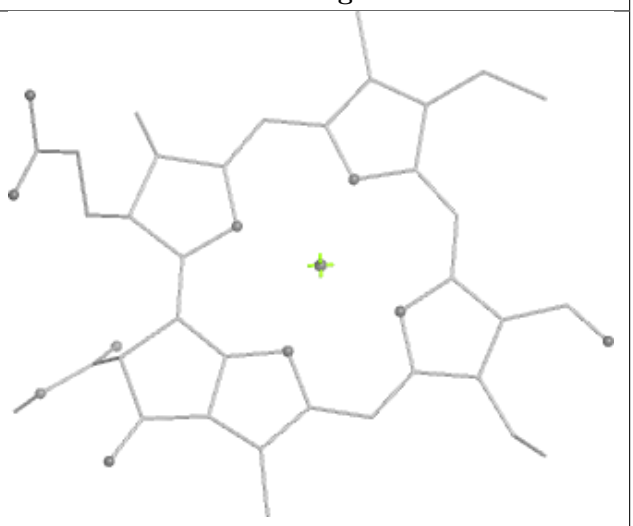
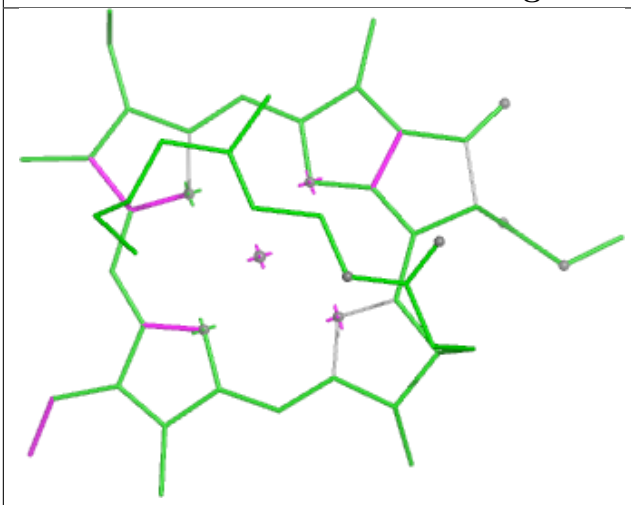


Rings

Ligand CLA N 613



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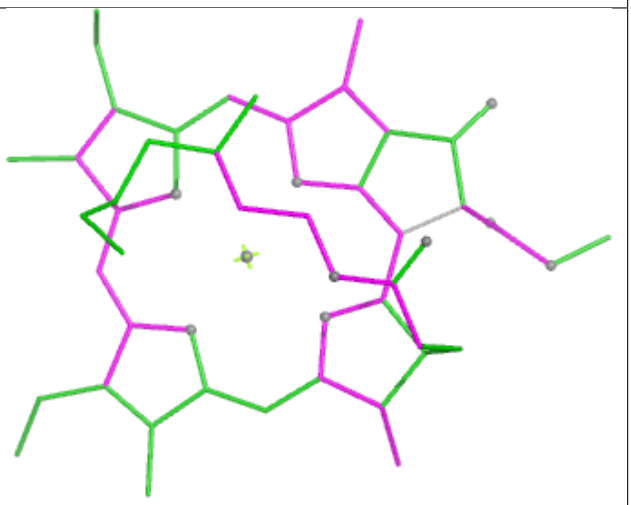
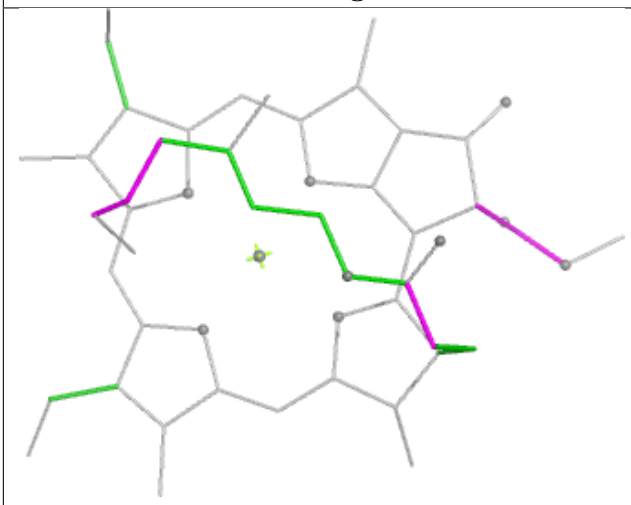


Bond angles



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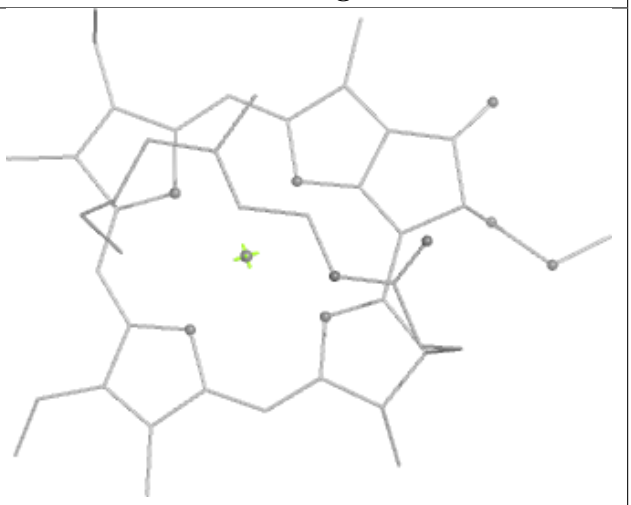
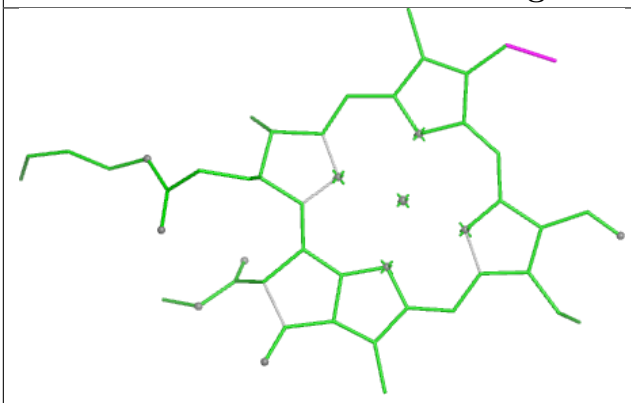


Rings

Ligand CHL g 606



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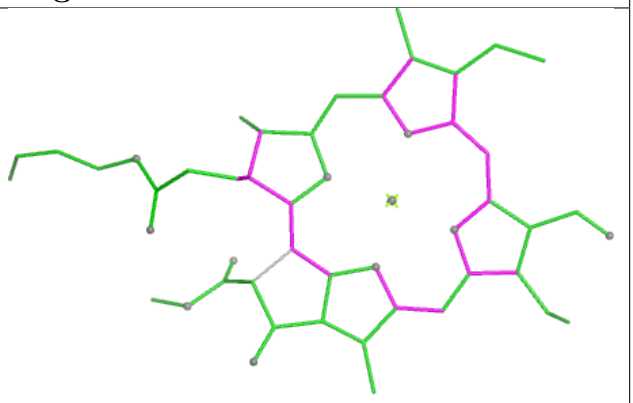
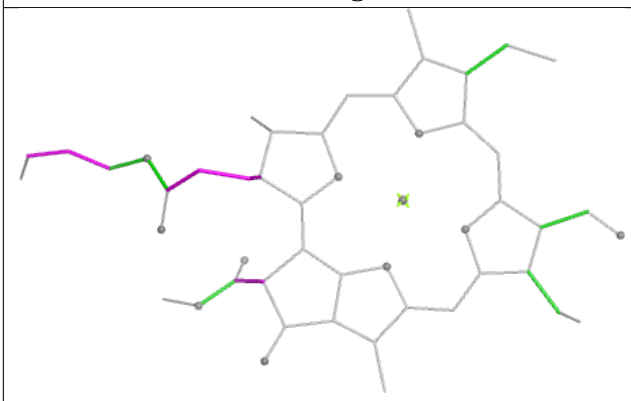


Bond angles



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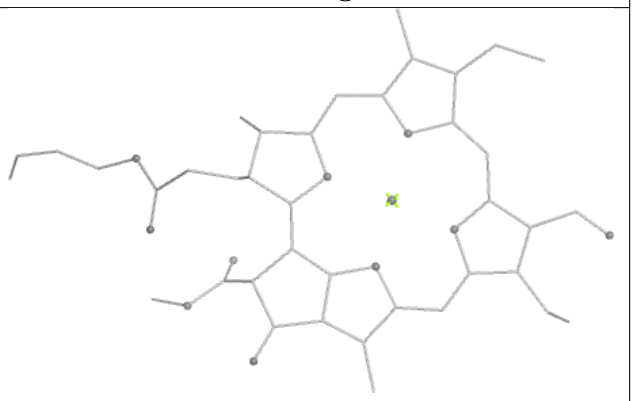
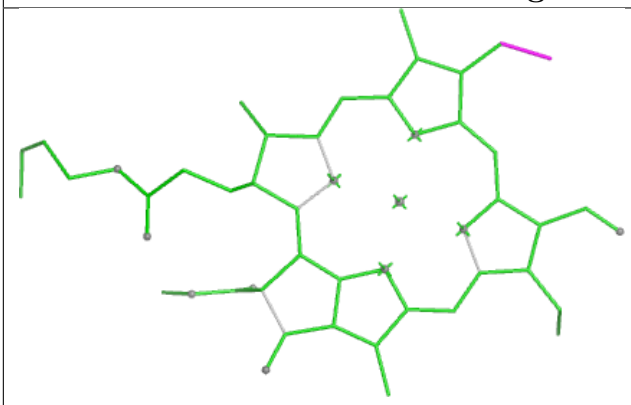


Rings

Ligand CHL y 307



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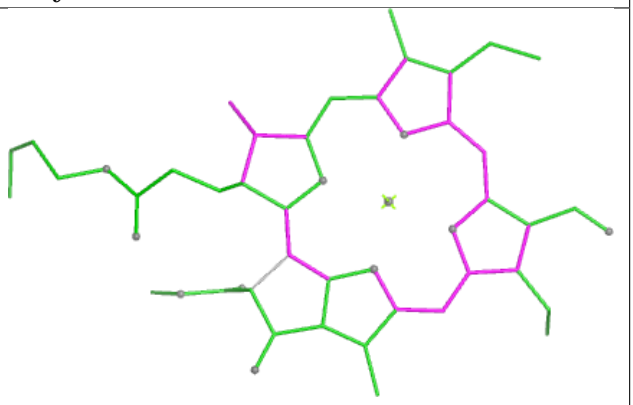
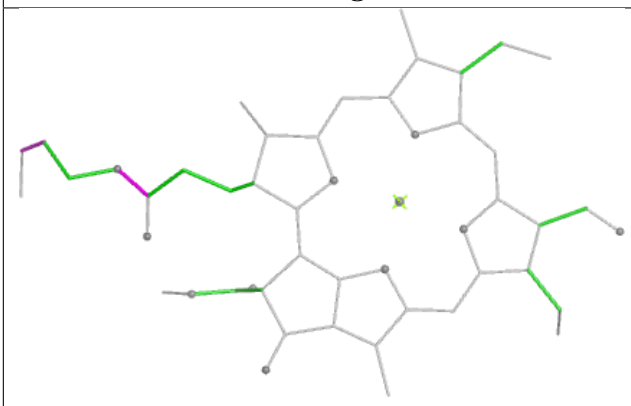


Bond angles



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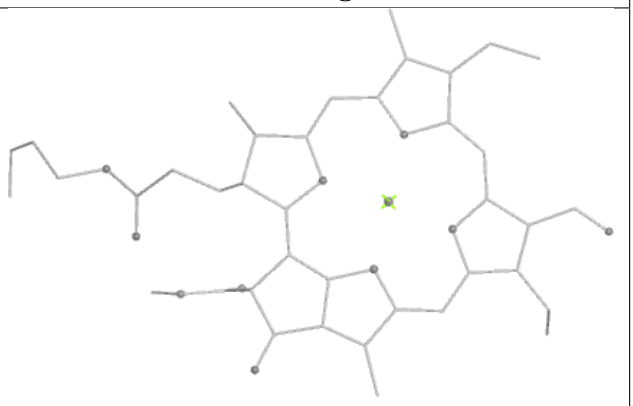
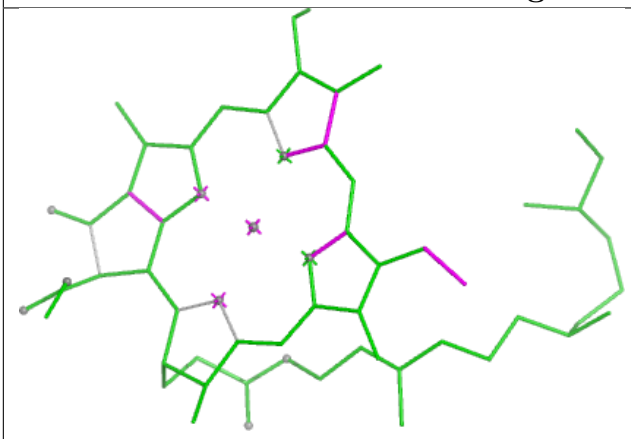


Rings

Ligand CLA S 303



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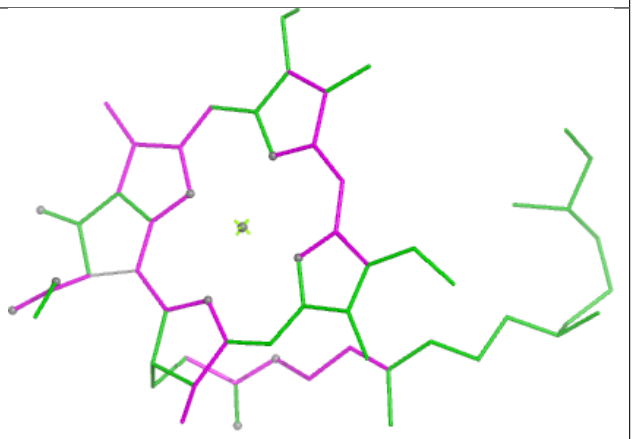

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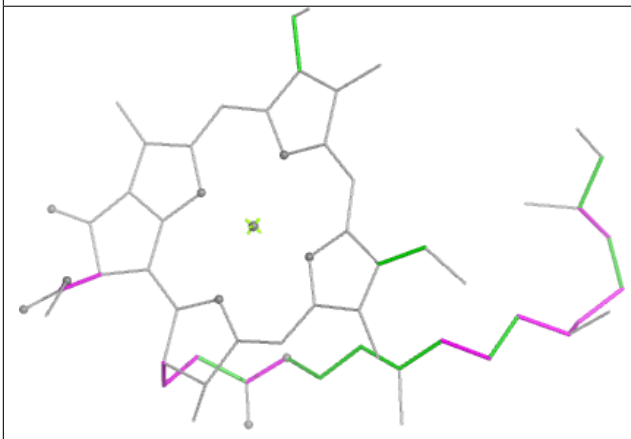
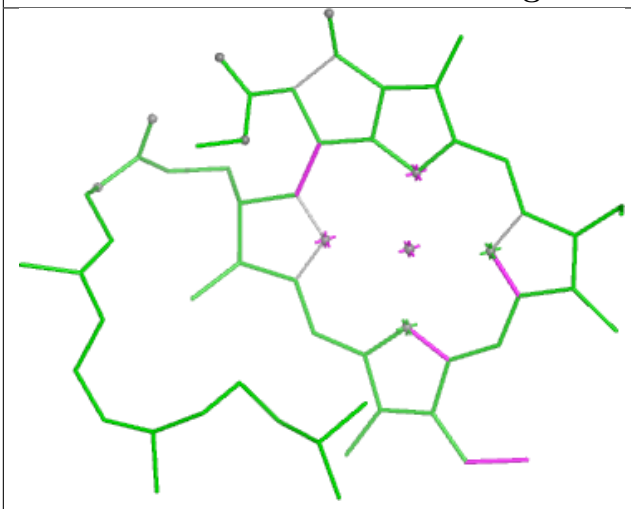


Torsions



Rings

Ligand CLA G 612



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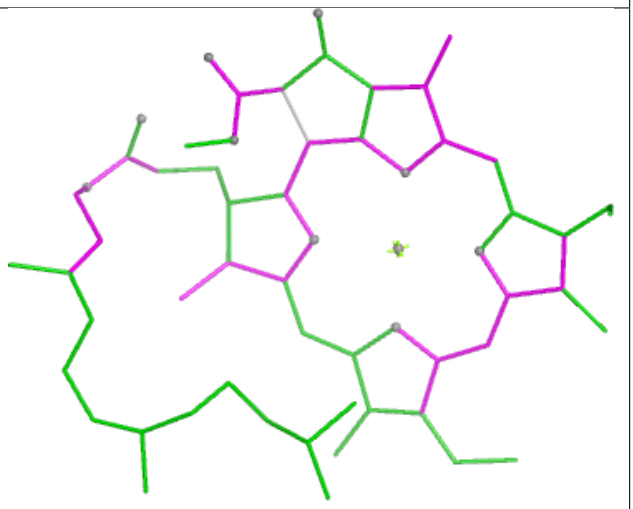
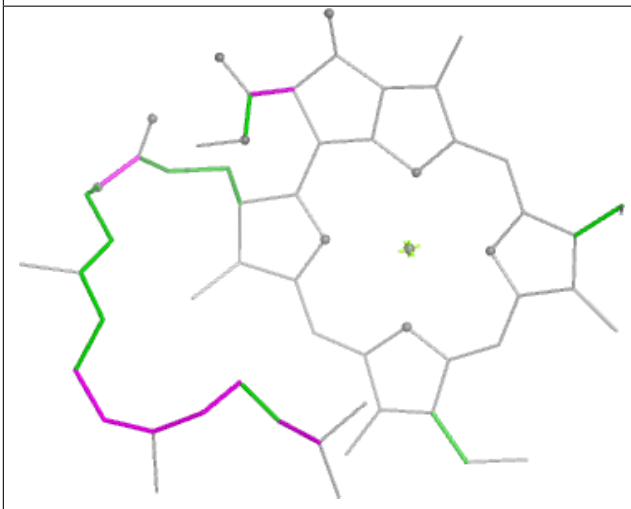


Bond angles



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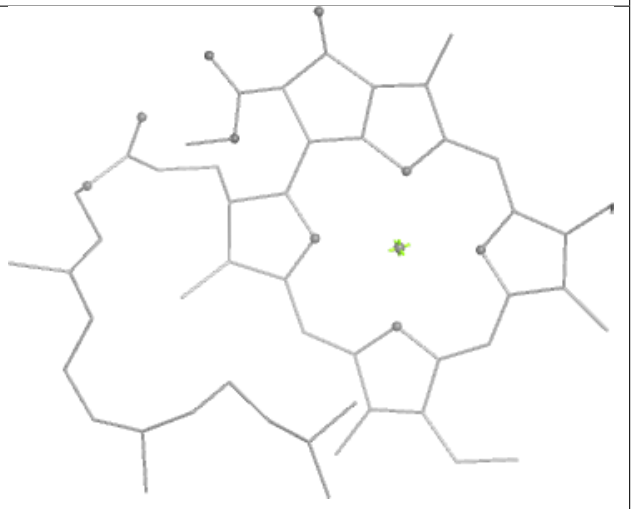
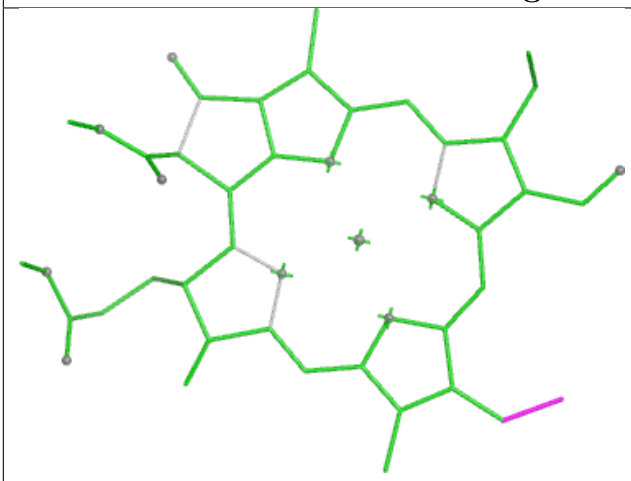


Rings

Ligand CHL R 605



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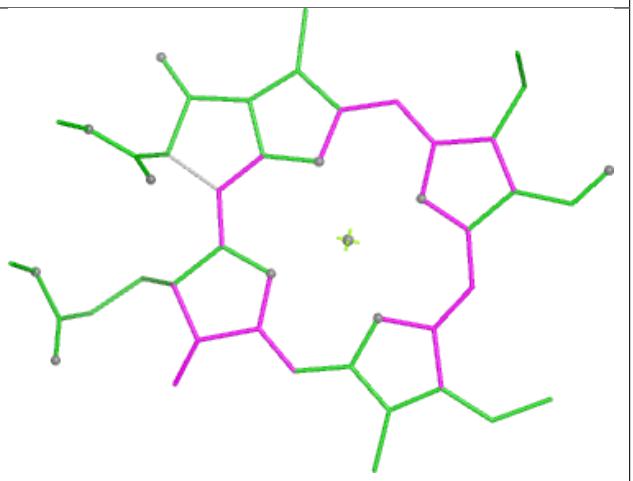
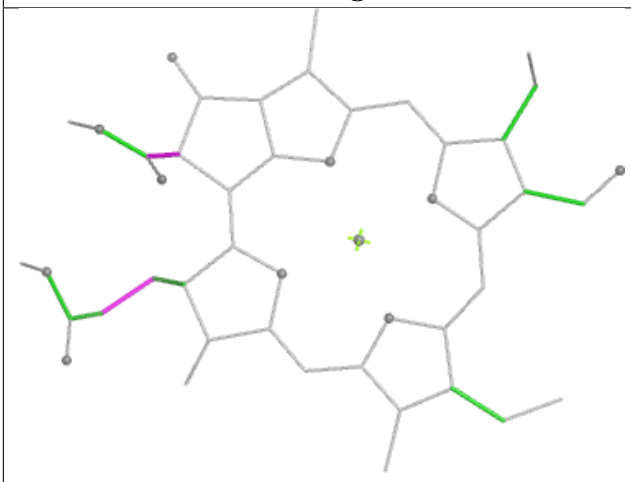


Bond angles



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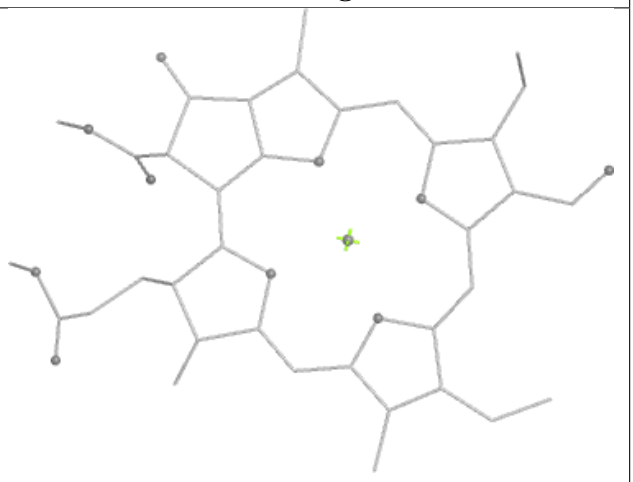
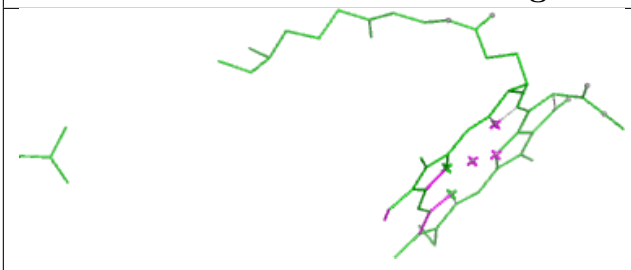
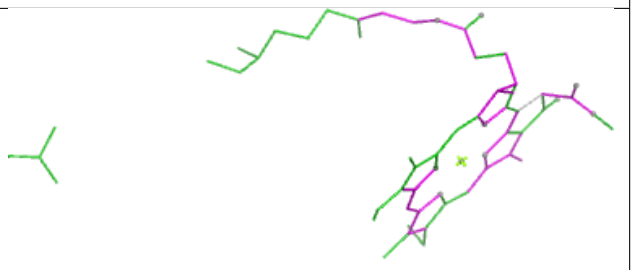


Rings

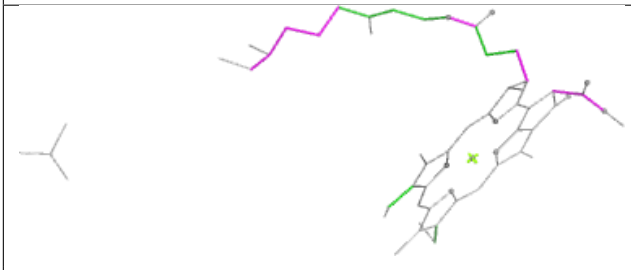
Ligand CLA c 504



Bond lengths



Bond angles

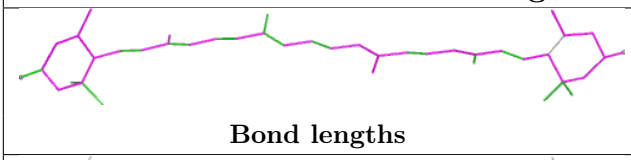


Torsions



Rings

Ligand LUT g 615



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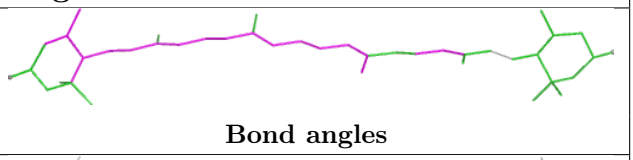
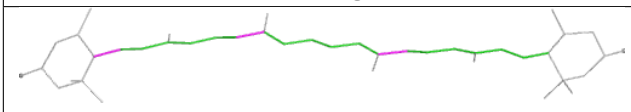


Bond angles



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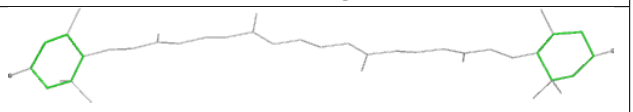
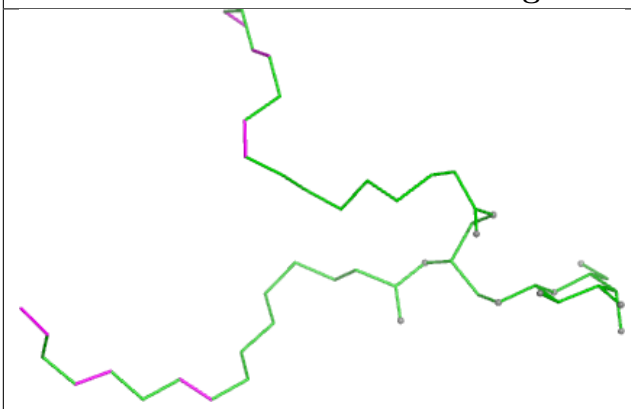


Rings

Ligand LMG b 620



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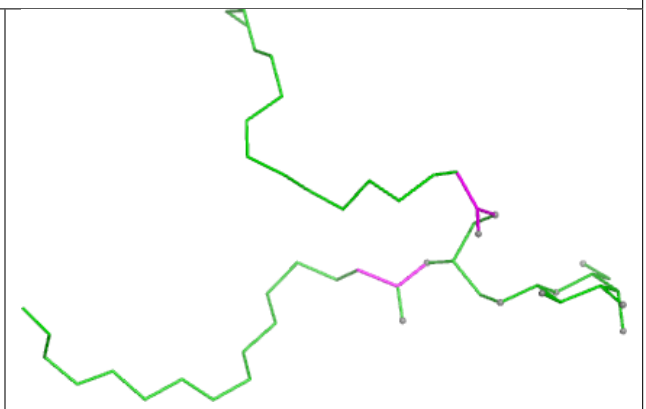
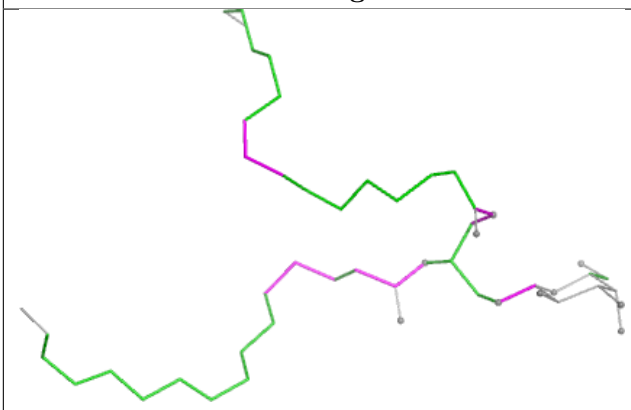


Bond angles



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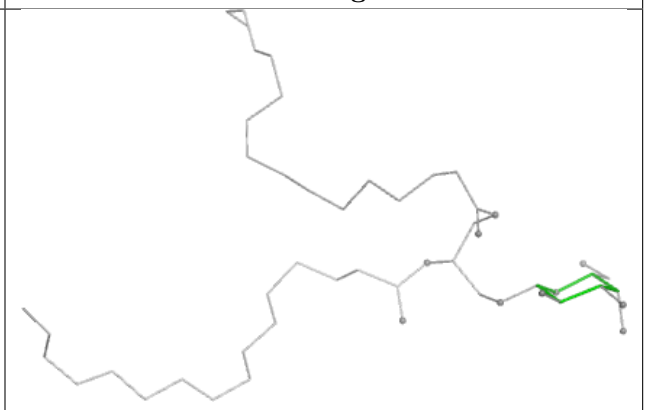
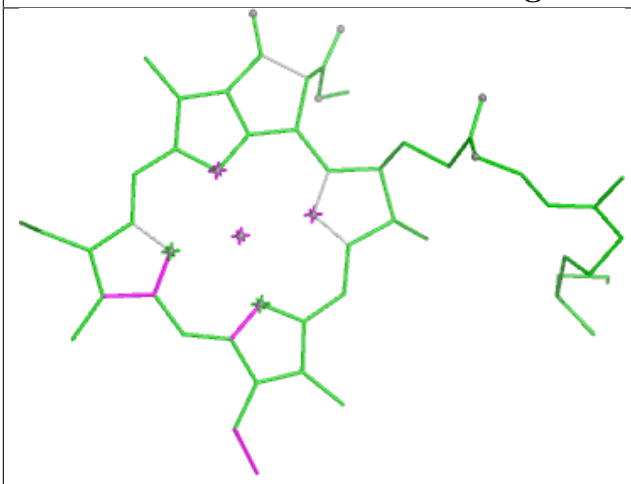


Rings

Ligand CLA C 512



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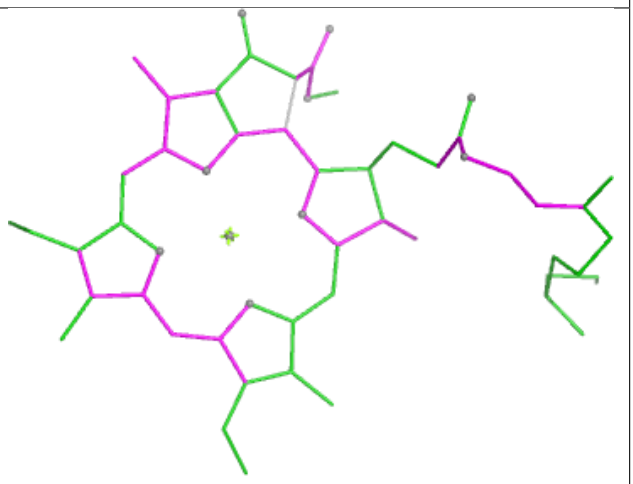
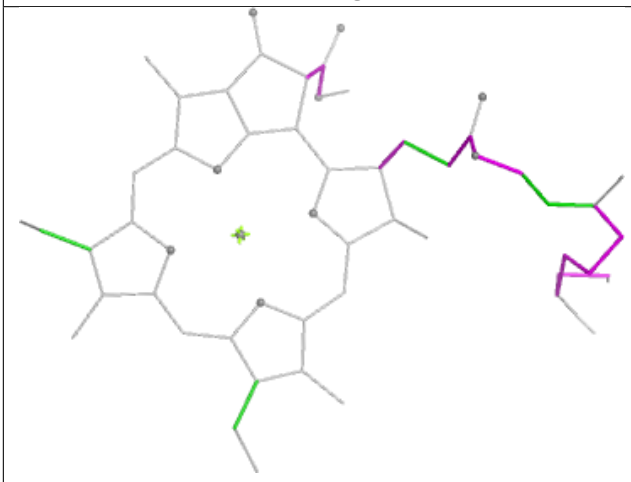


Bond angles



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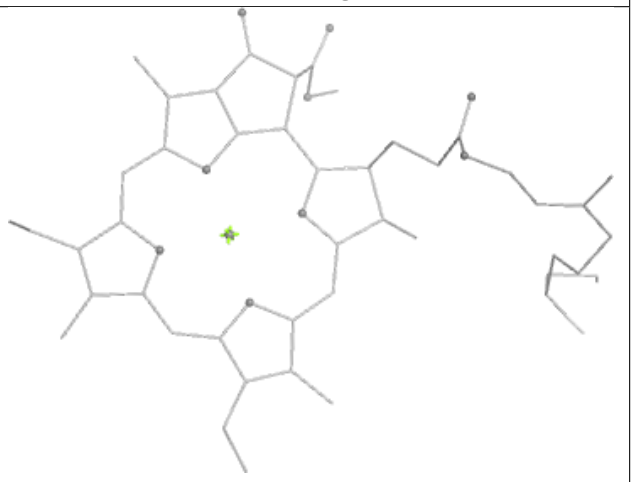
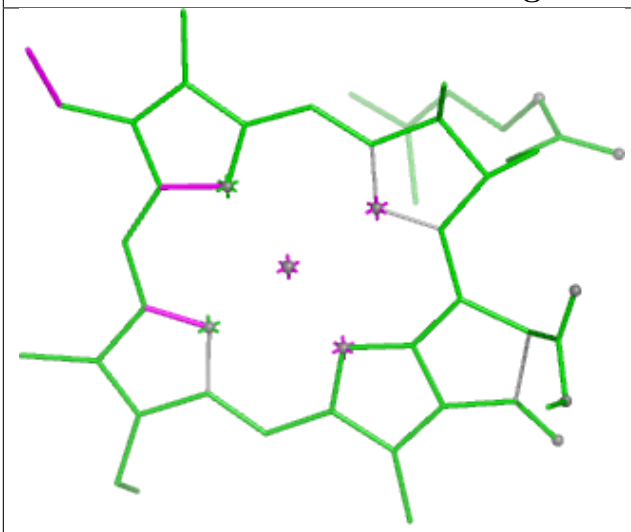


Rings

Ligand CLA N 604



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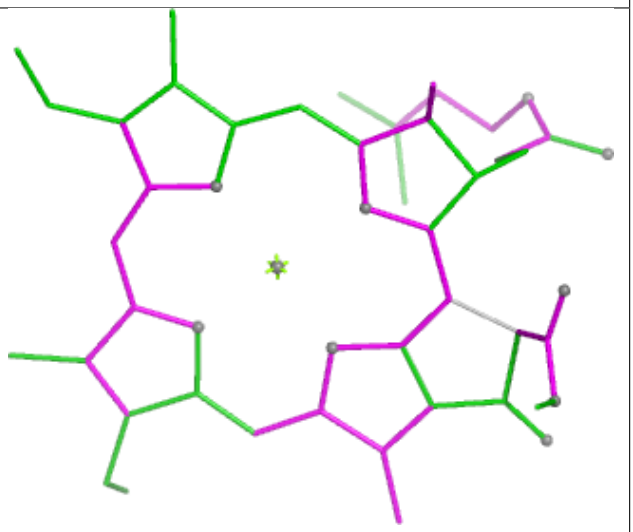
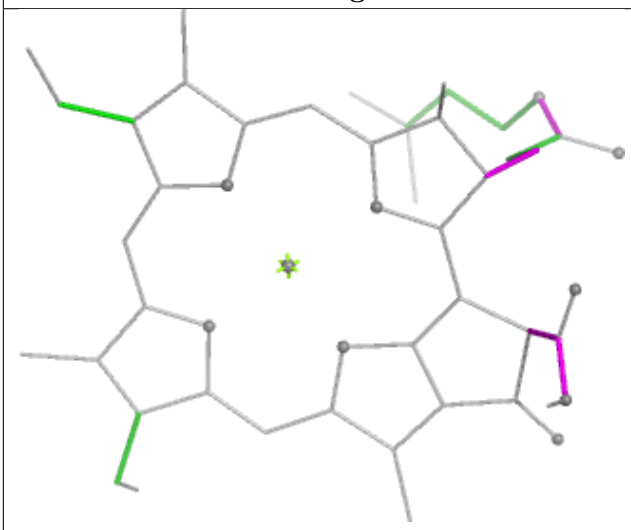


Bond angles



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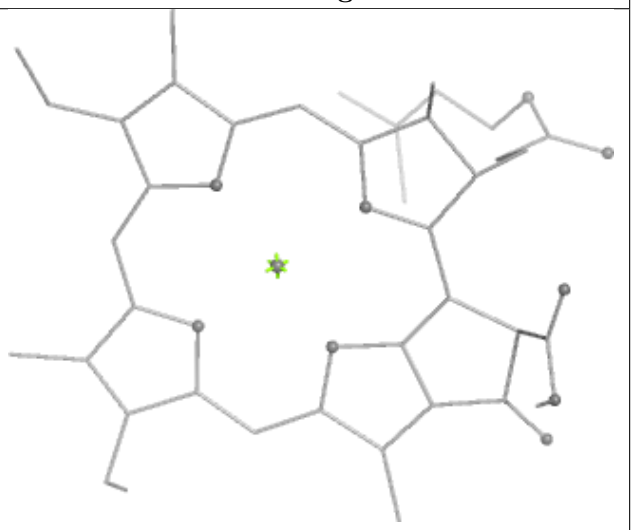
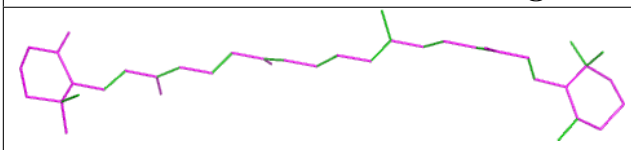


Rings

Ligand BCR c 515



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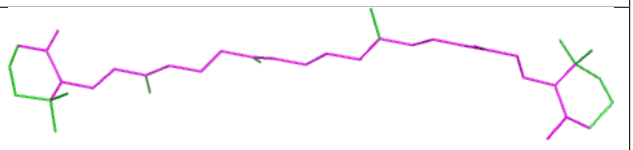

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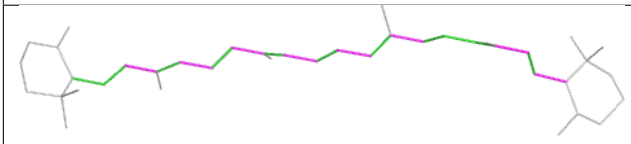
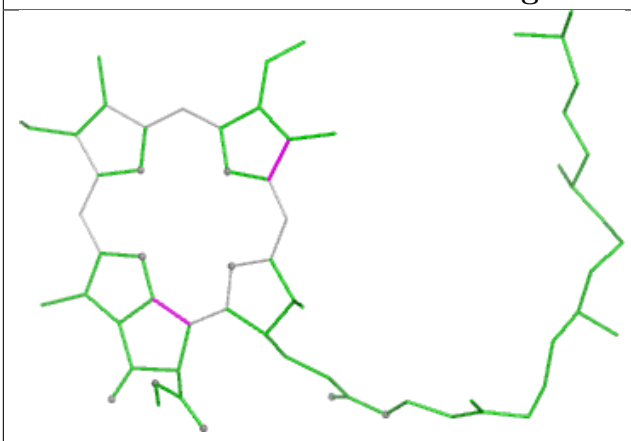


Torsions



Rings

Ligand PHO A 407



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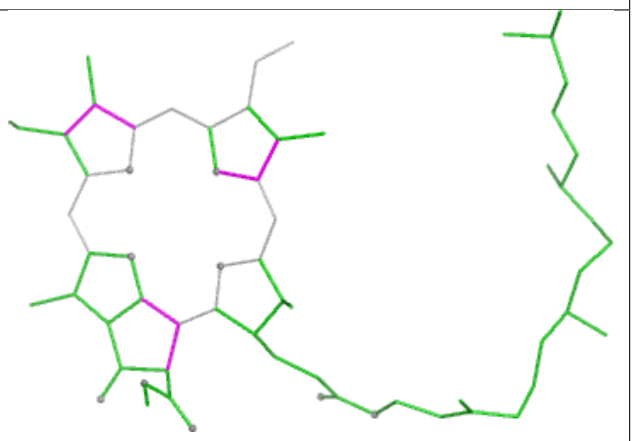
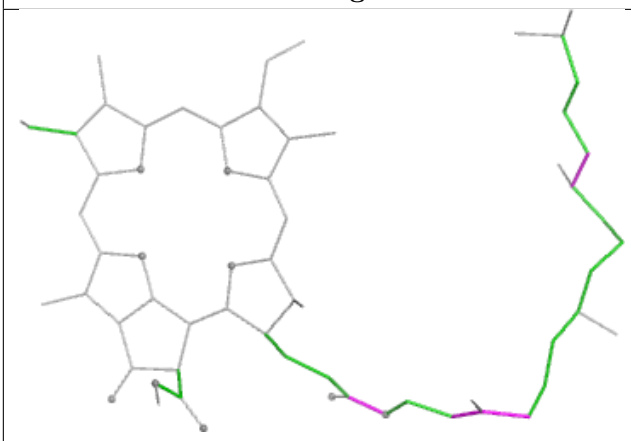


Bond angles



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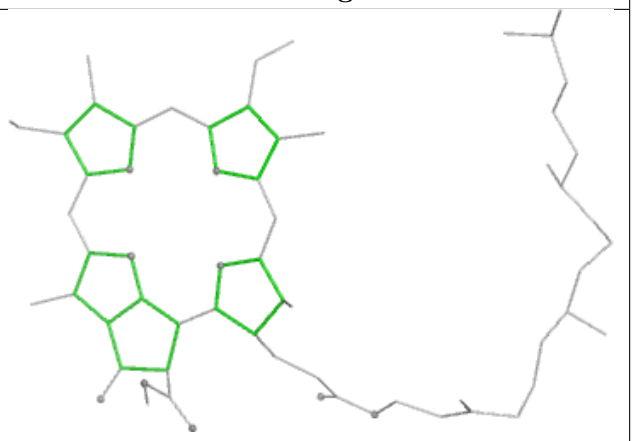
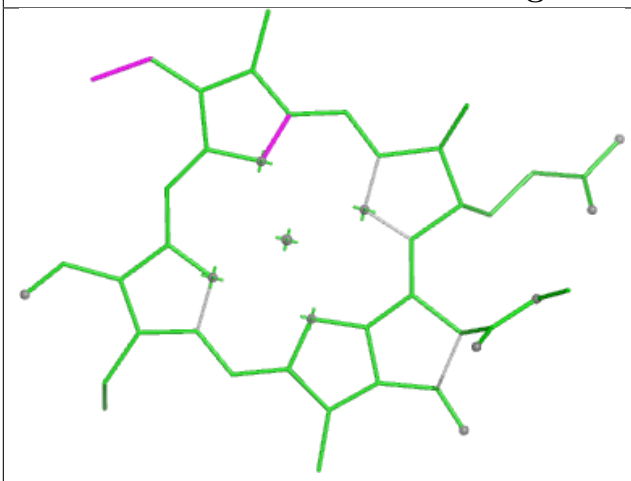


Rings

Ligand CHL S 302



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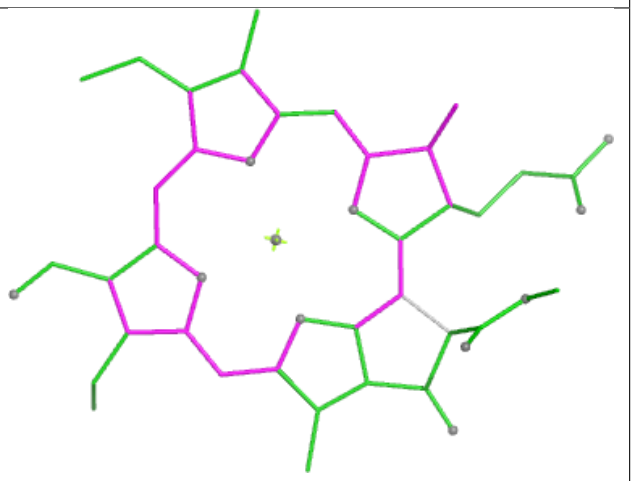
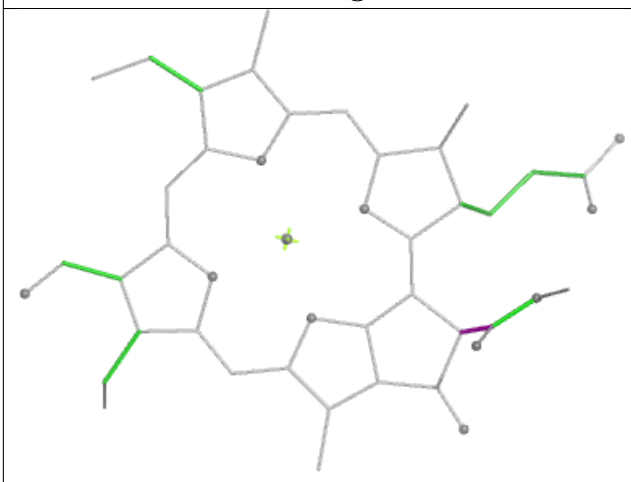


Bond angles



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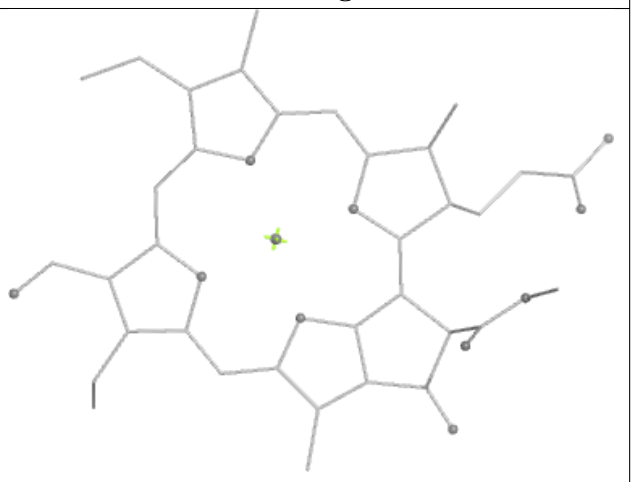
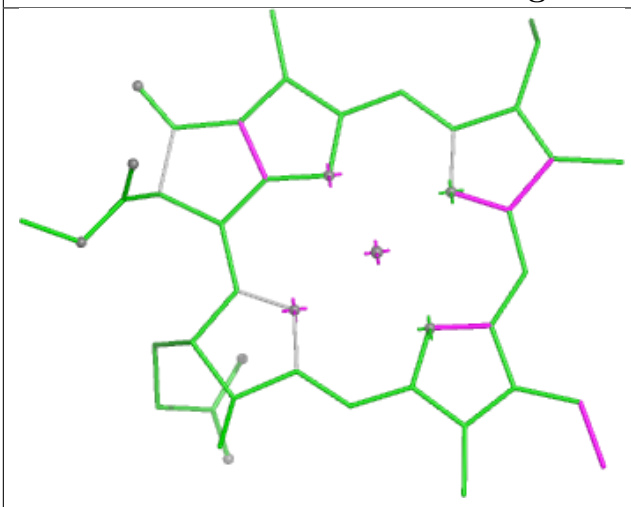


Rings

Ligand CLA g 614



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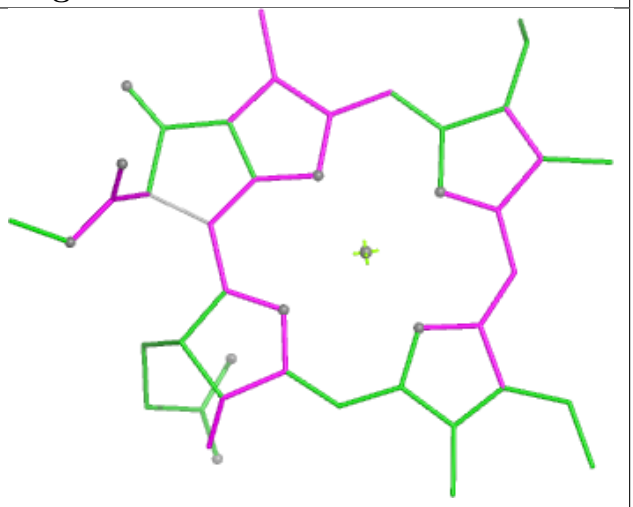
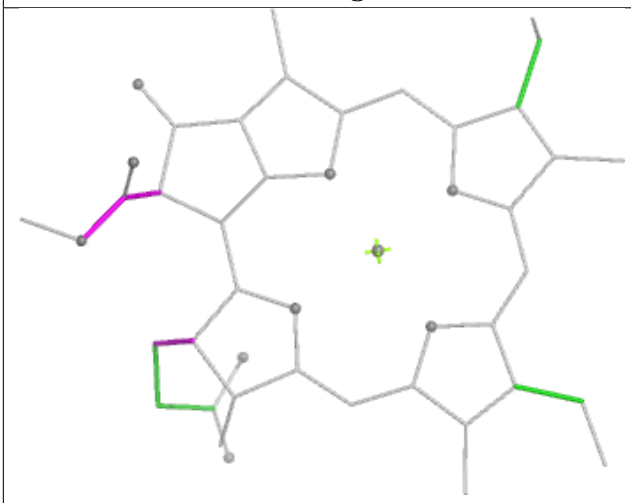


Bond angles



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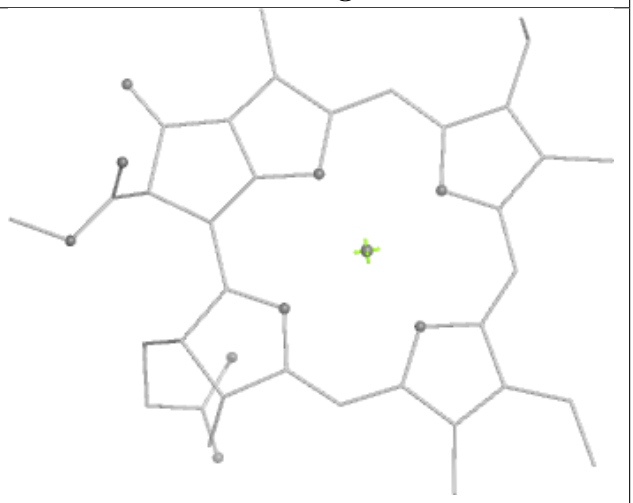
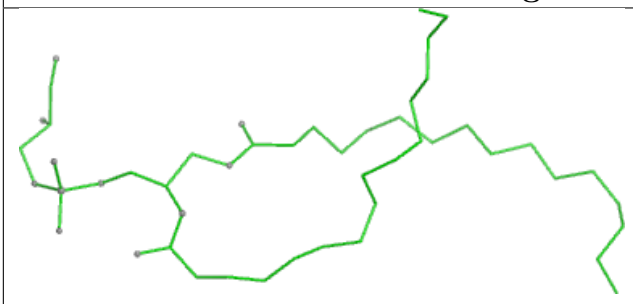


Rings

Ligand LHG C 521



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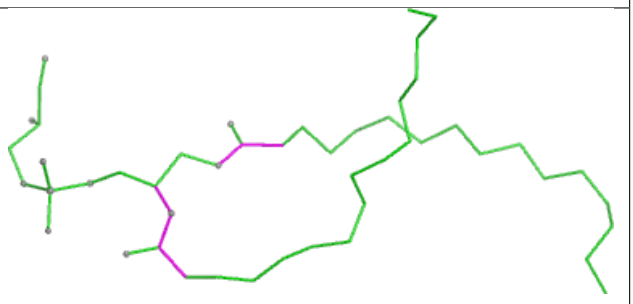
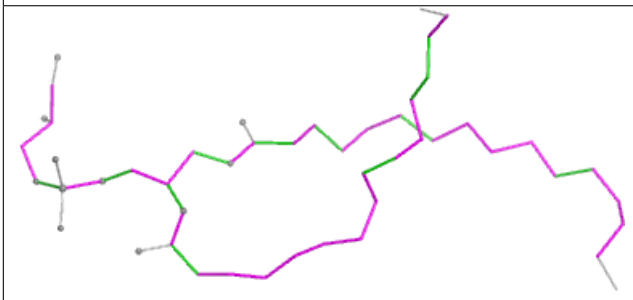


Bond angles



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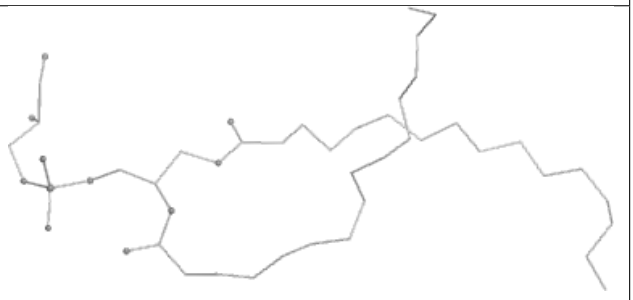
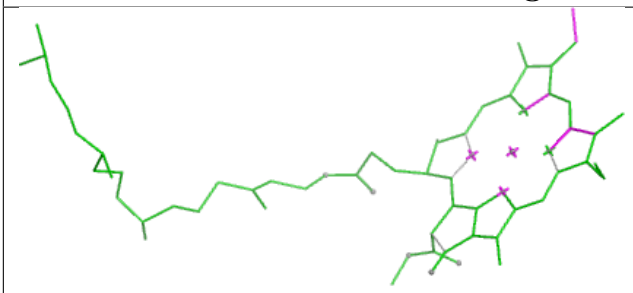


Rings

Ligand CLA A 405



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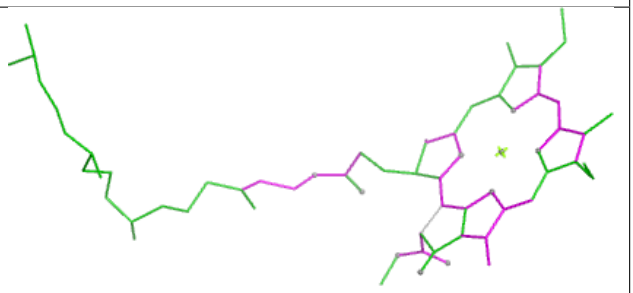
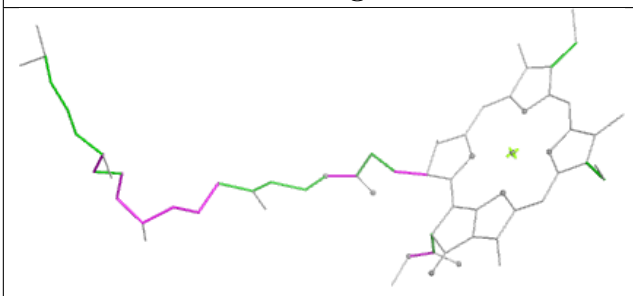


Bond angles



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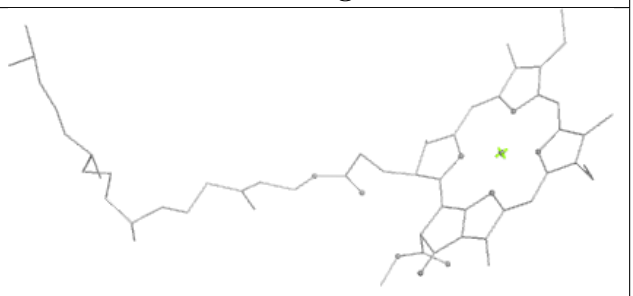
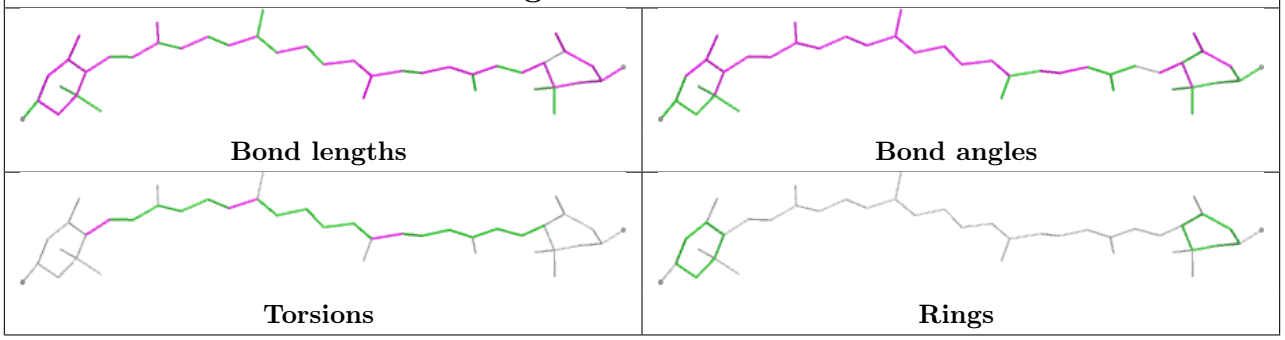
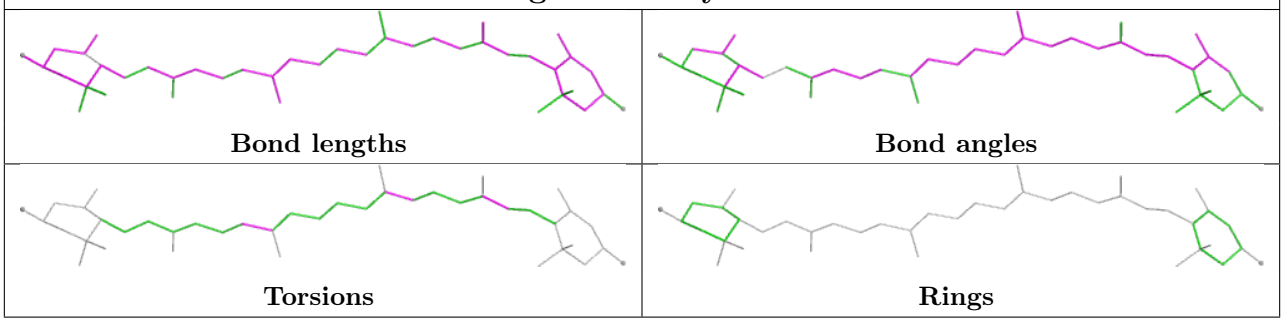


Rings

Ligand LUT N 615



Ligand LUT y 315



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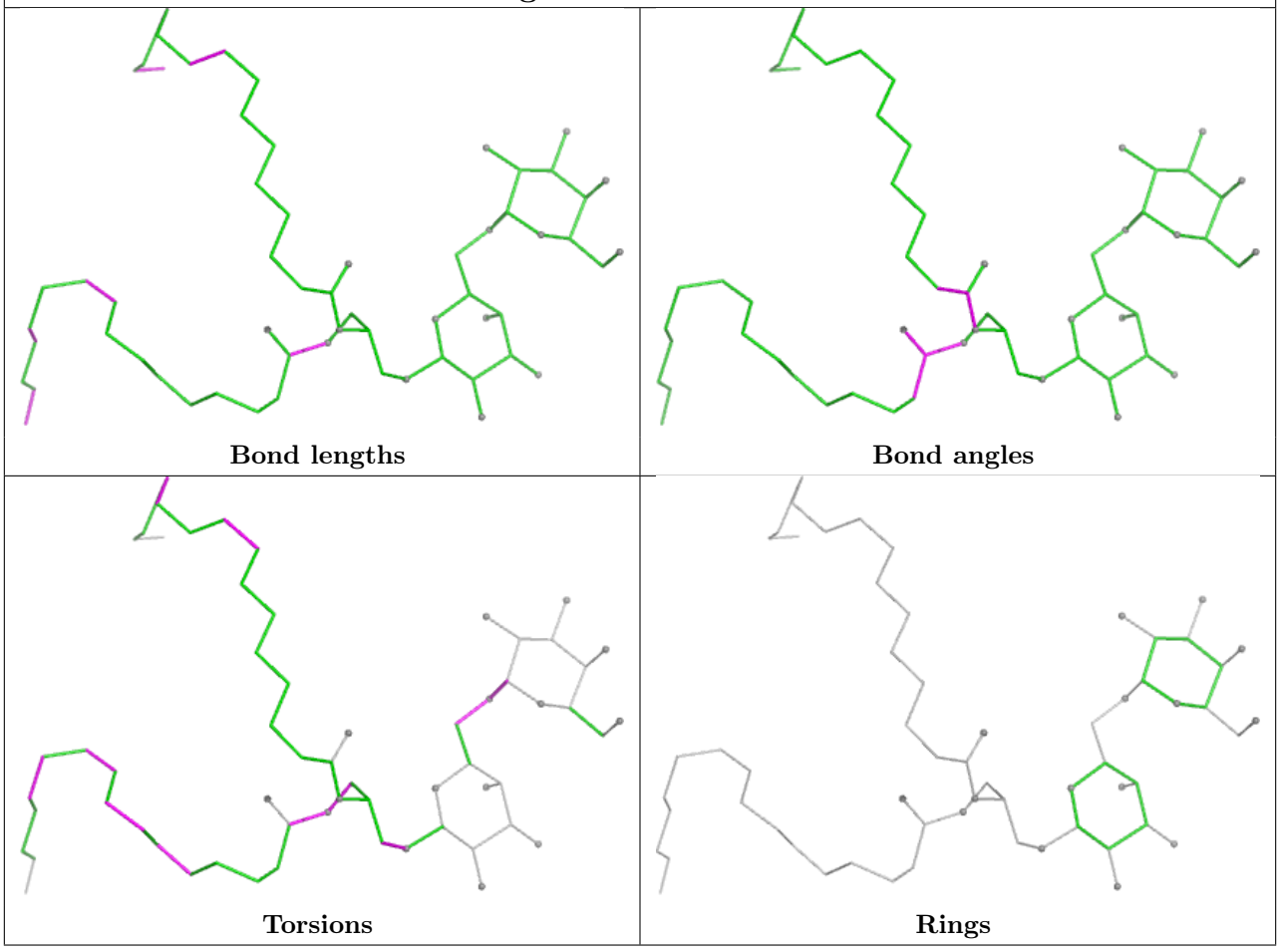

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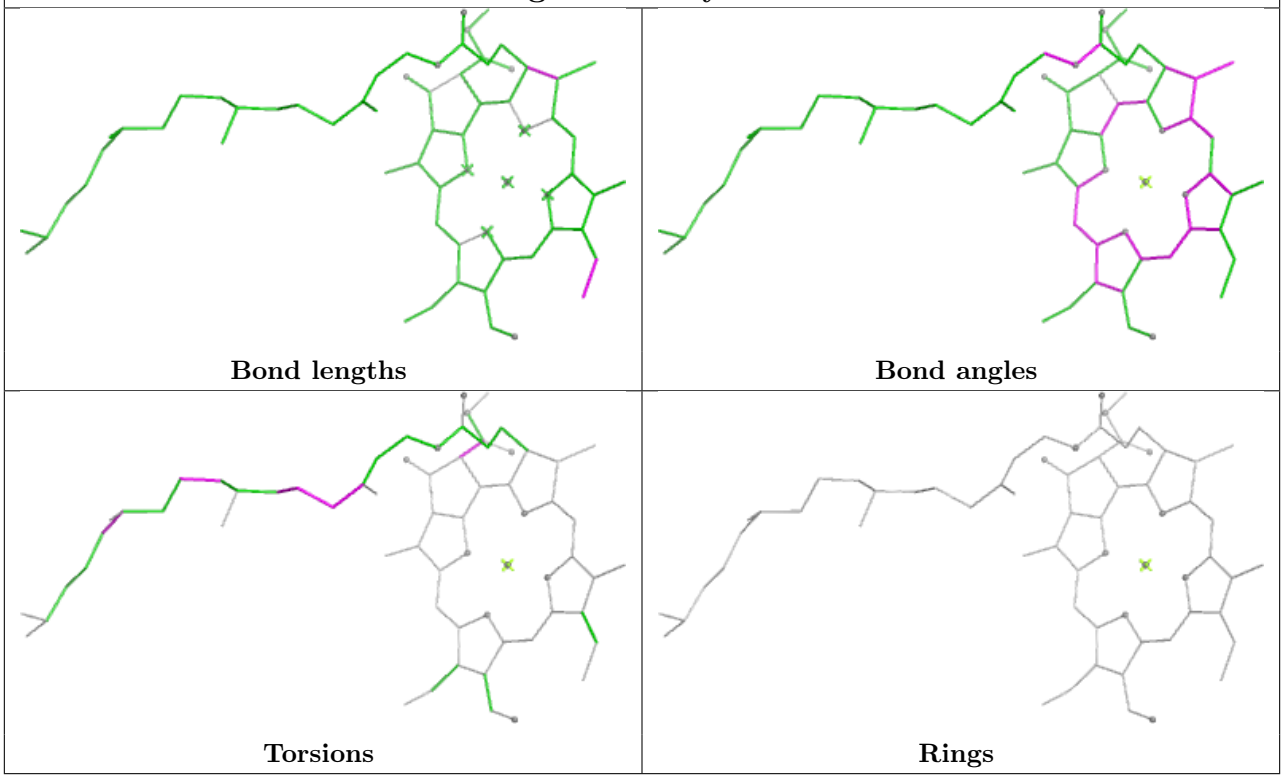

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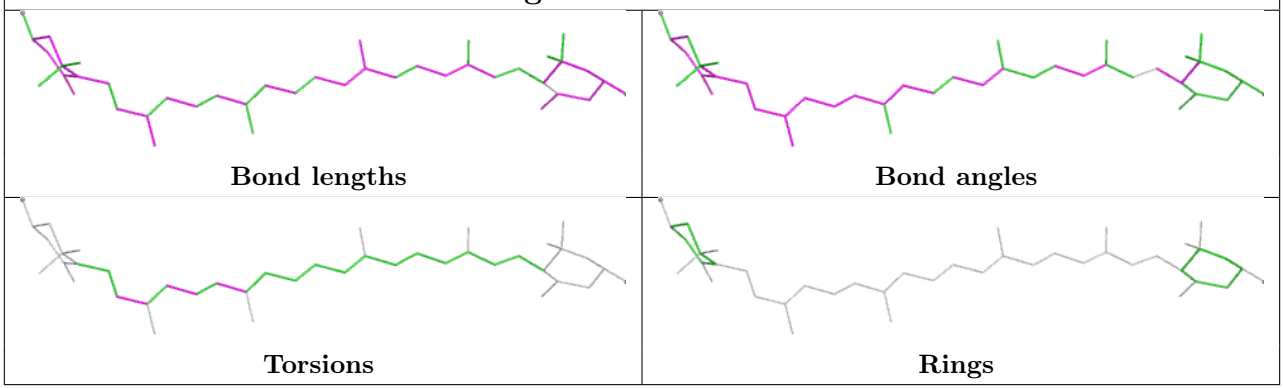
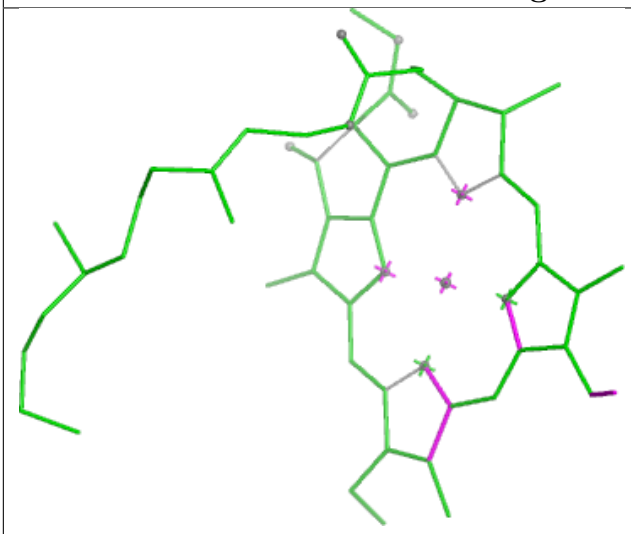
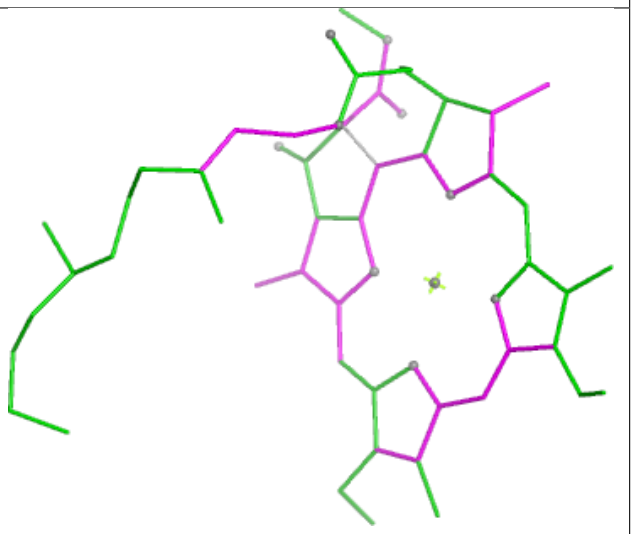


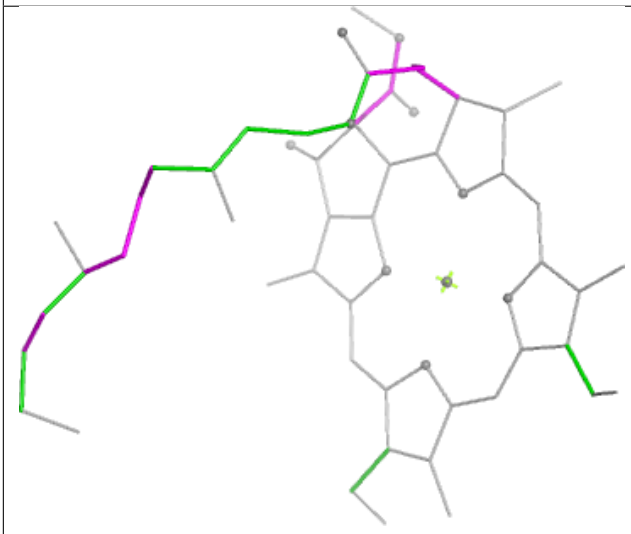
Ligand CLA r 608



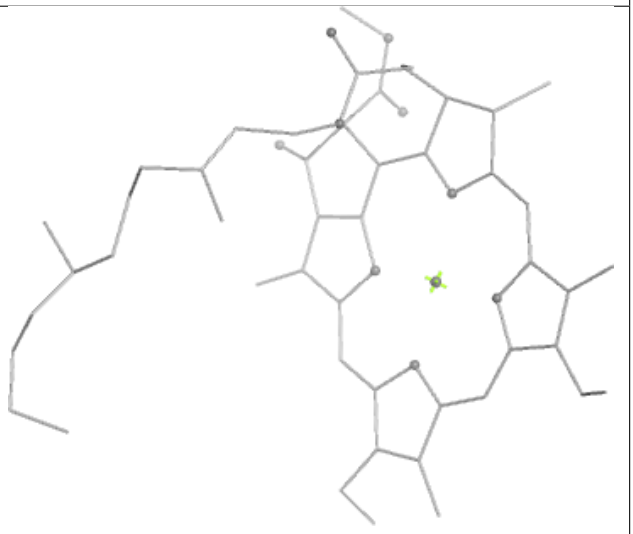
Bond lengths



Bond angles

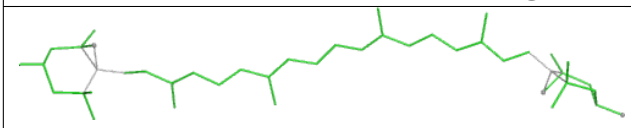


Torsions



Rings

Ligand XAT R 615



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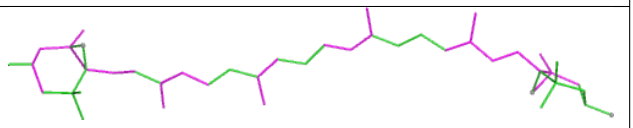
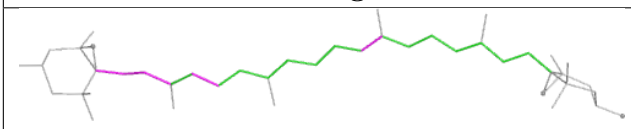


Bond angles



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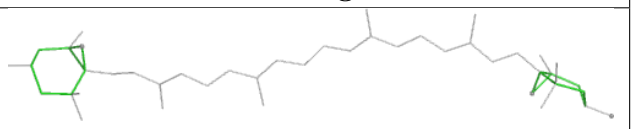
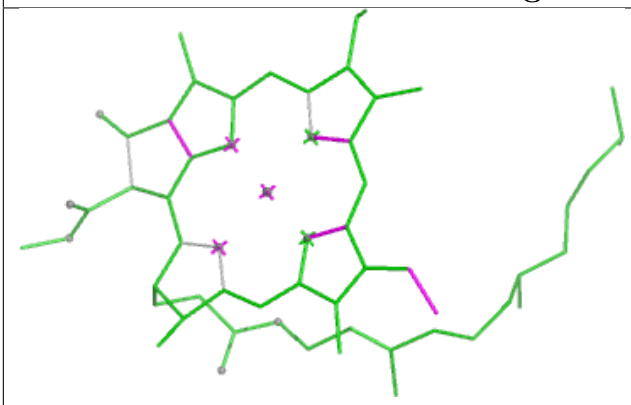
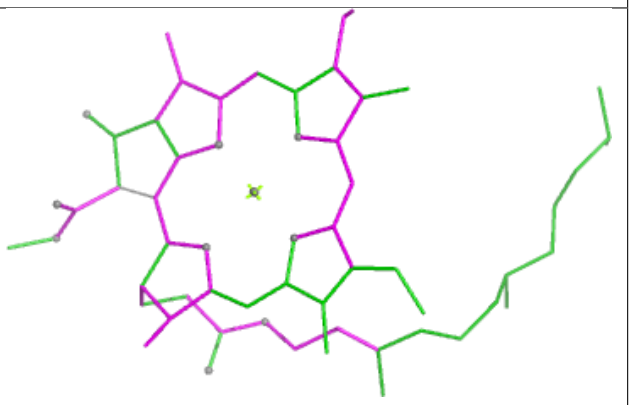


Rings

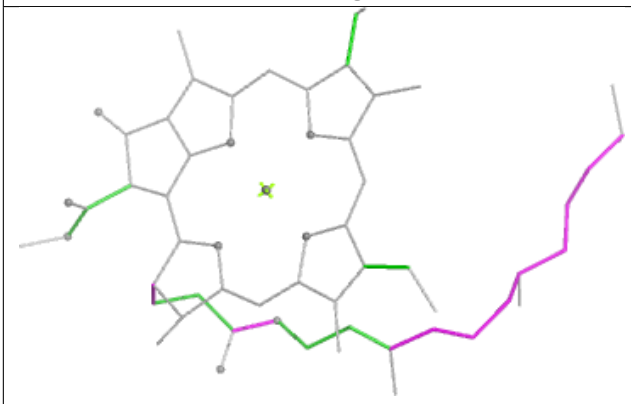
Ligand CLA Y 610



Bond lengths



Bond angles



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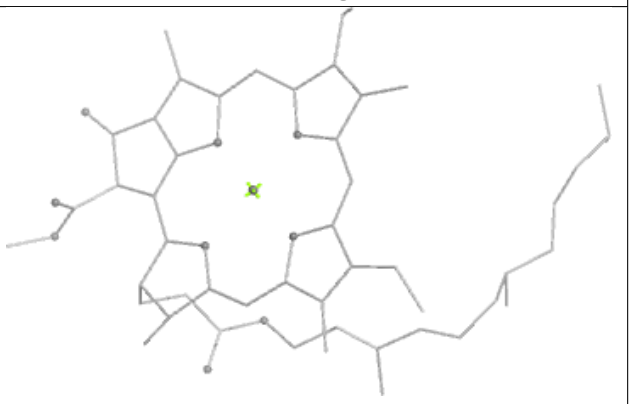
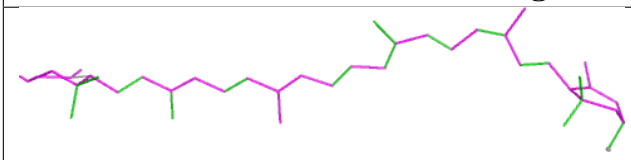


Rings

Ligand LUT r 614



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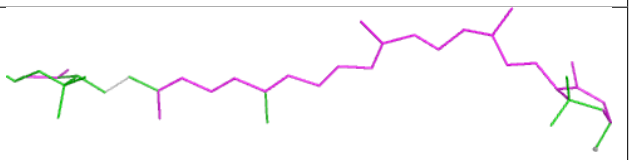

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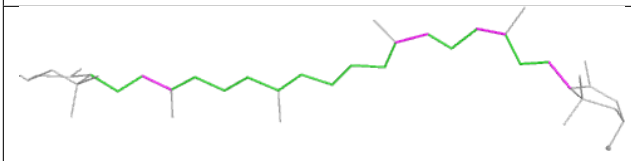
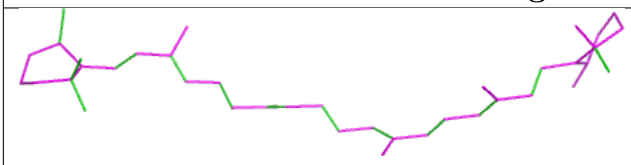


Torsions



Rings

Ligand BCR t 101



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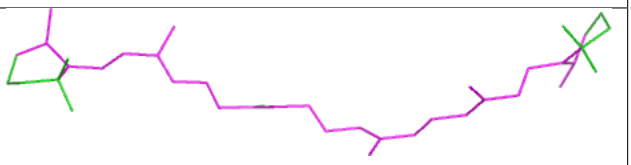

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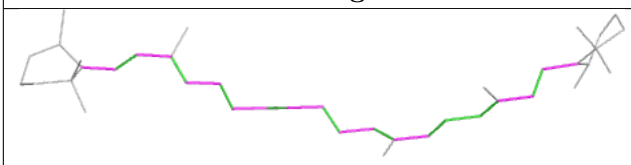

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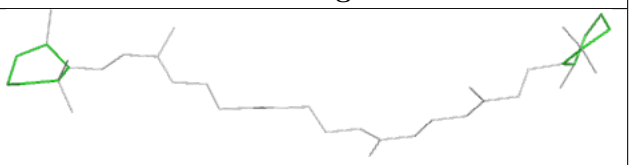
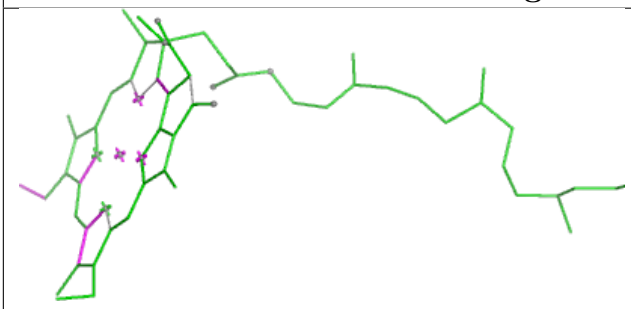


Rings

Ligand CLA B 604



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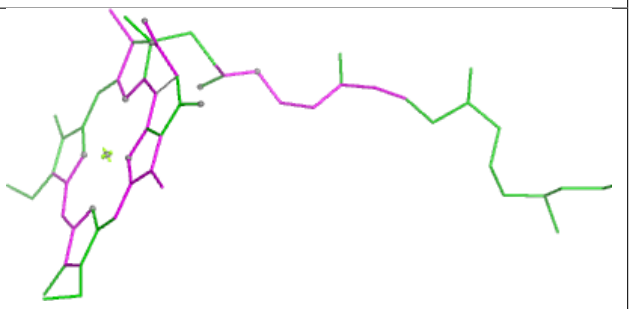

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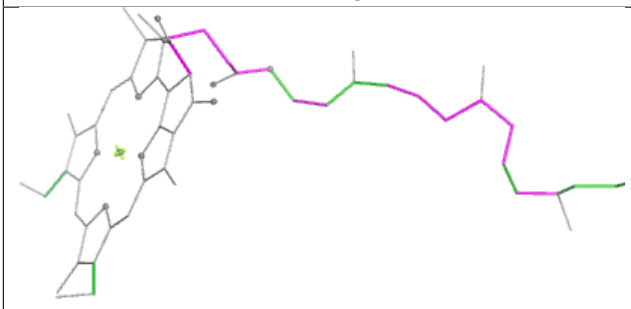

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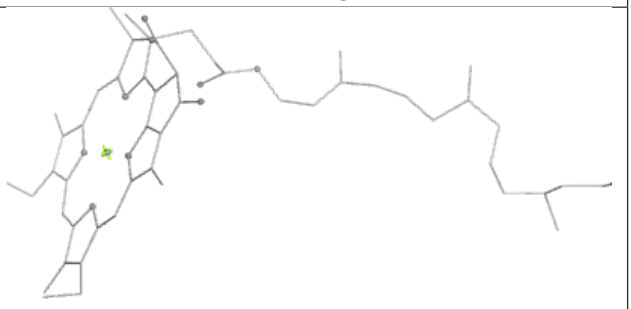
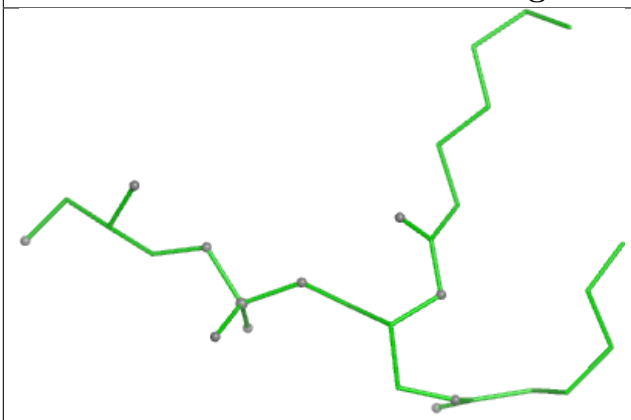


Rings

Ligand LHG r 617



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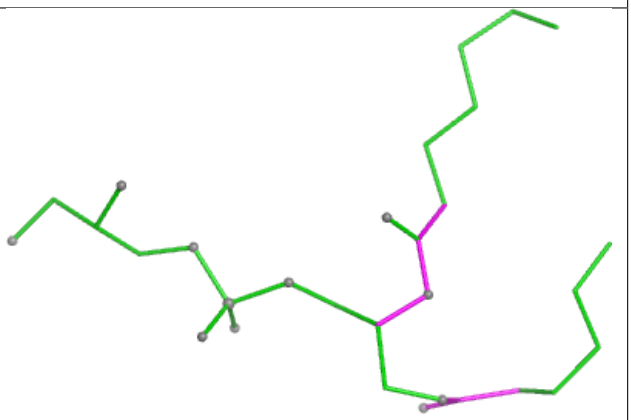

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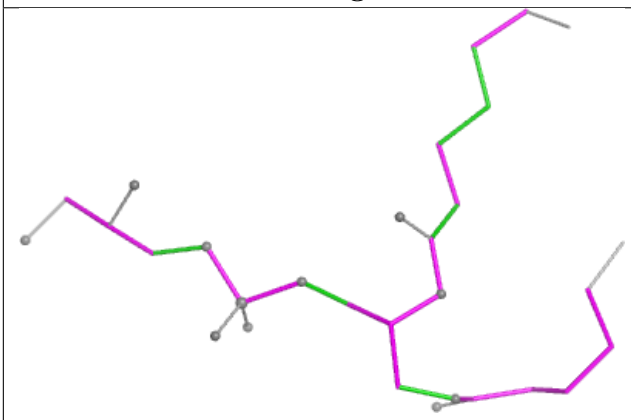

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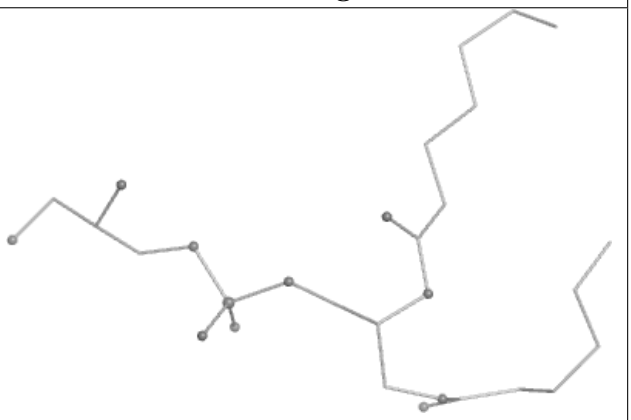
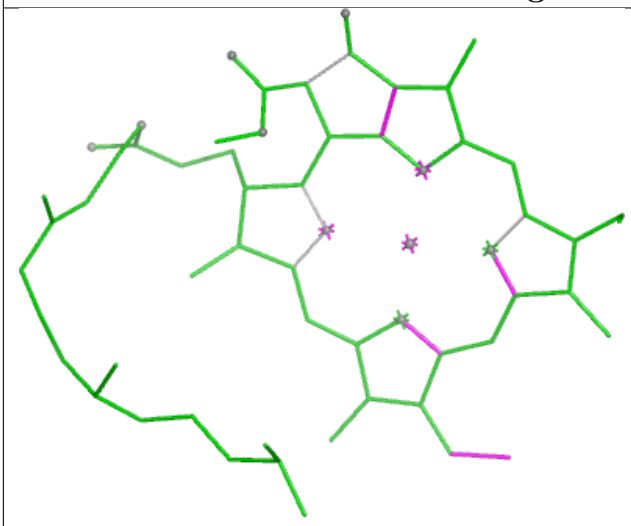


Rings

Ligand CLA n 612



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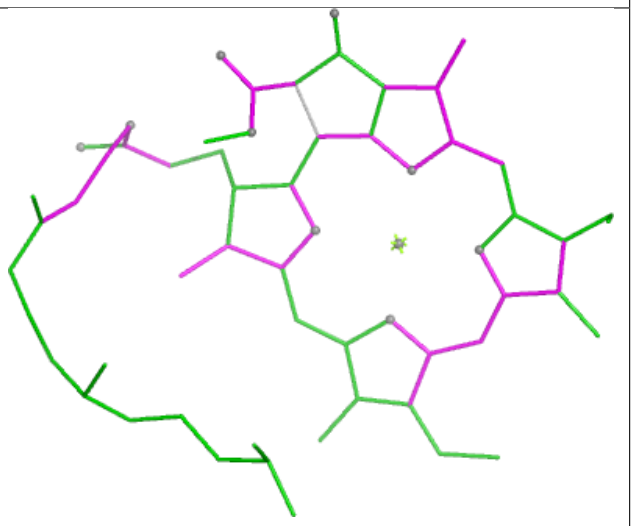
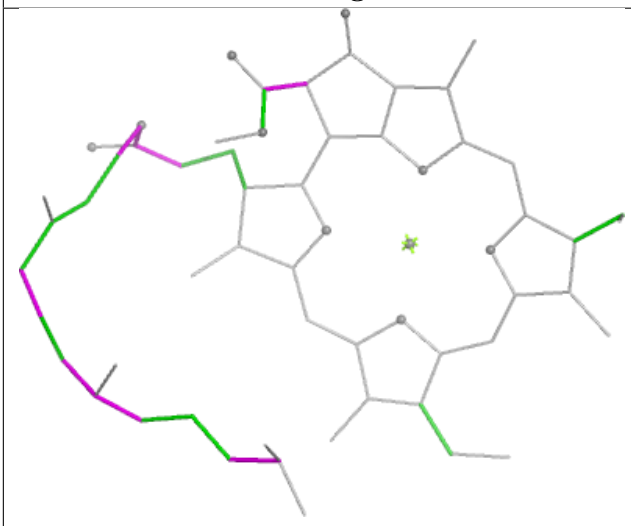


Bond angles



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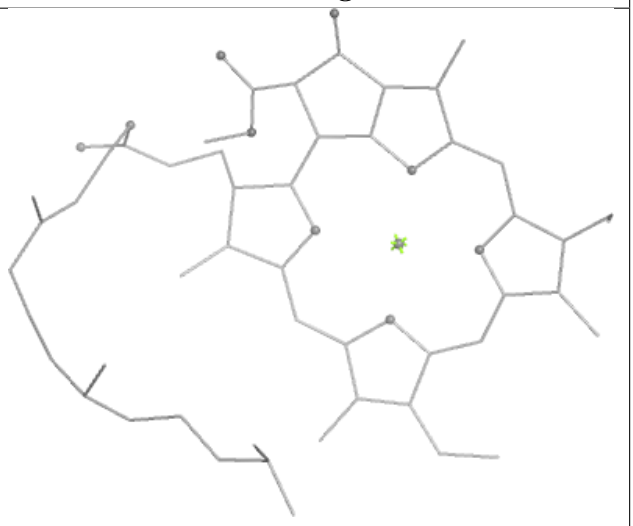
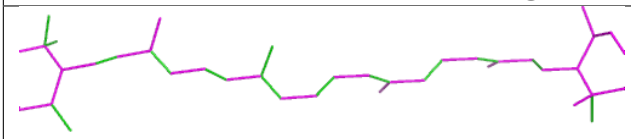


Rings

Ligand BCR C 515



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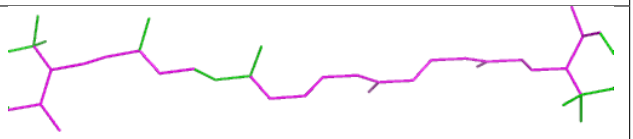

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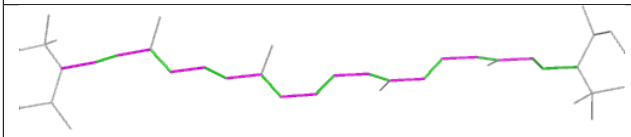

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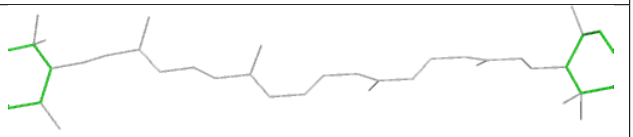
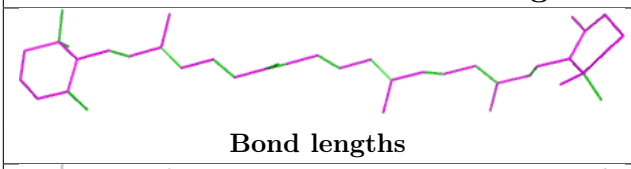


Rings

Ligand BCR i 101



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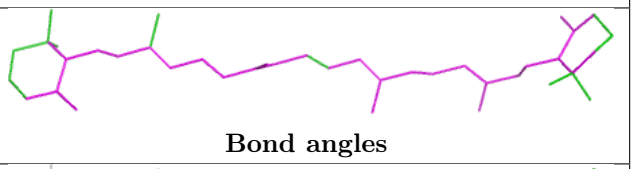

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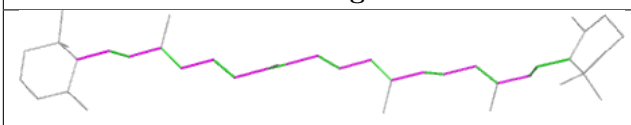

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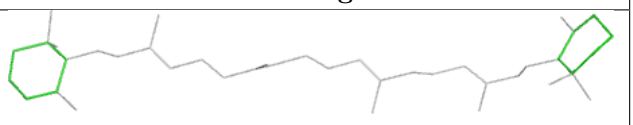
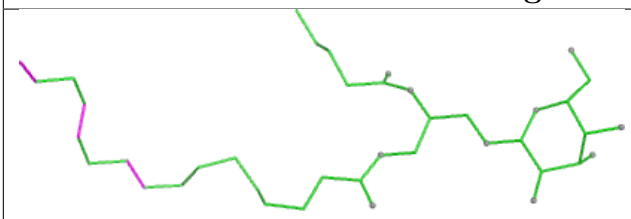


Rings

Ligand LMG a 413



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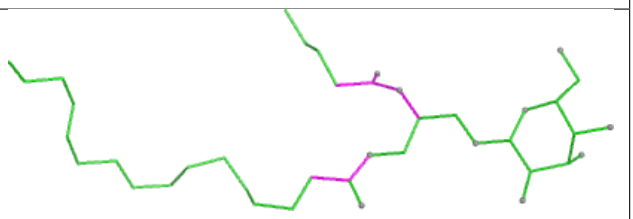

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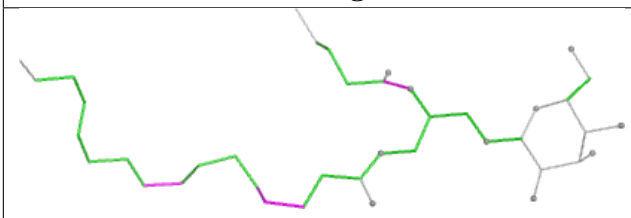

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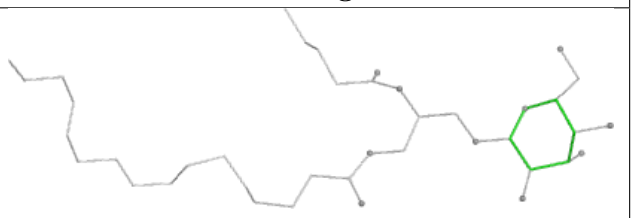
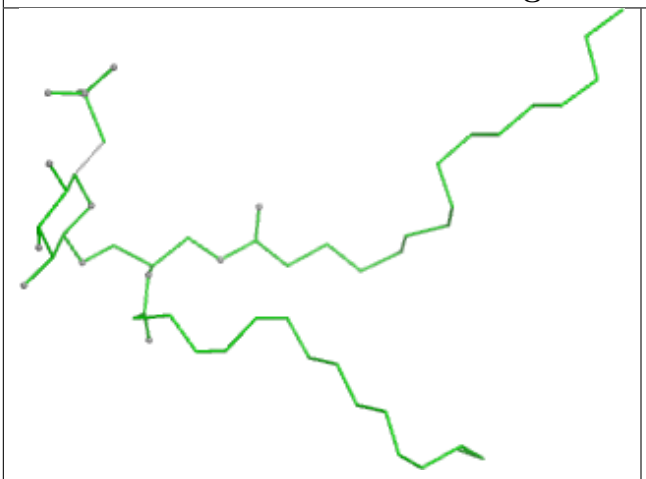


Rings

Ligand SQD A 414



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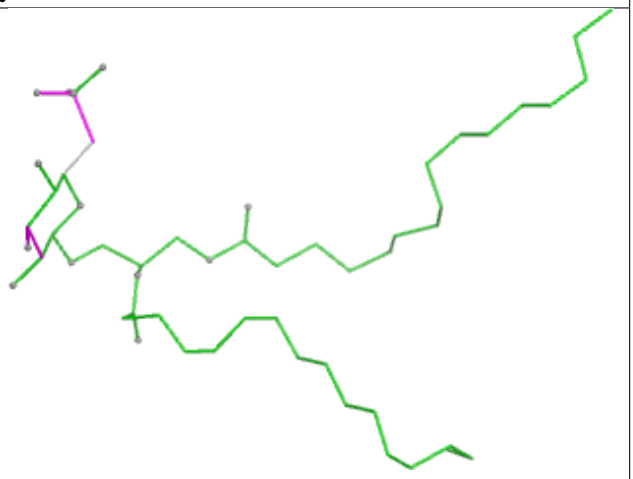

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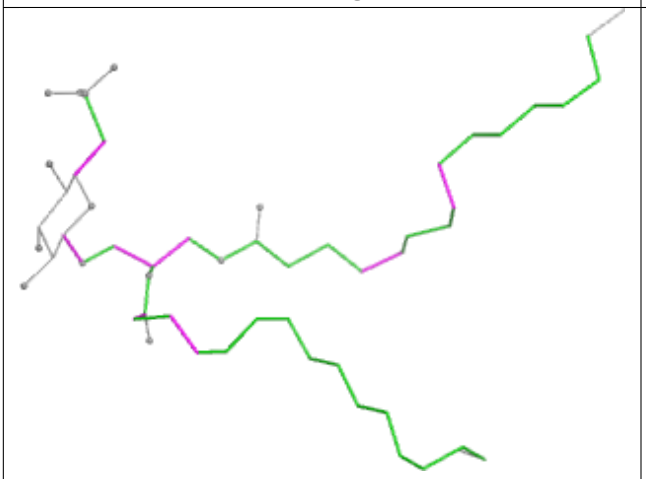

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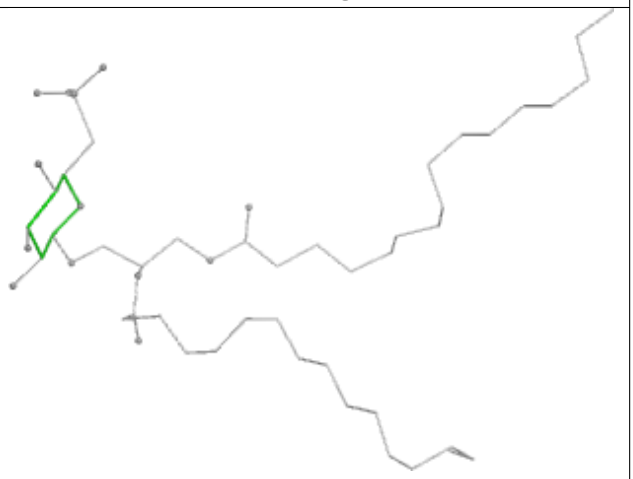
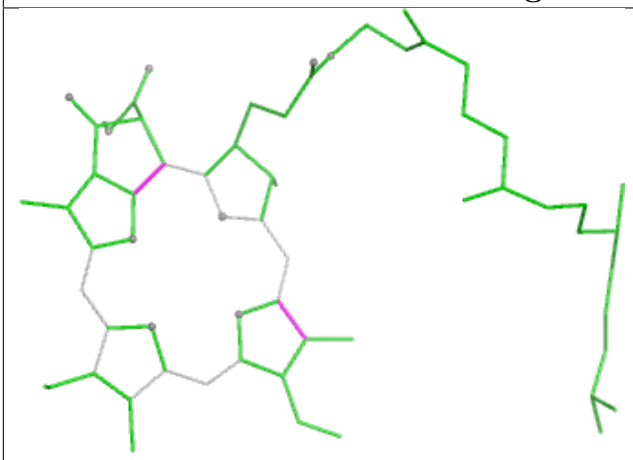


Rings

Ligand PHO d 402



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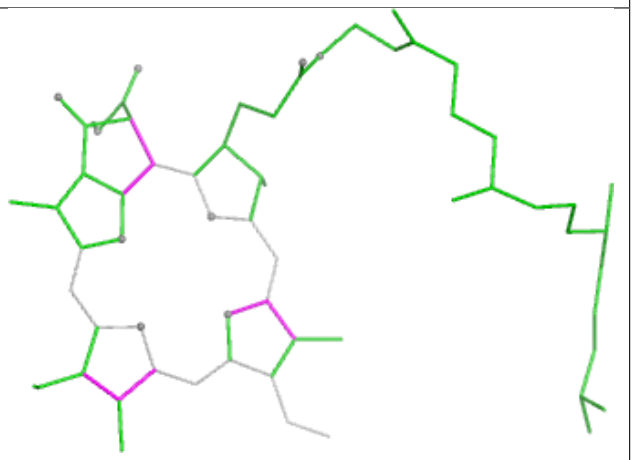

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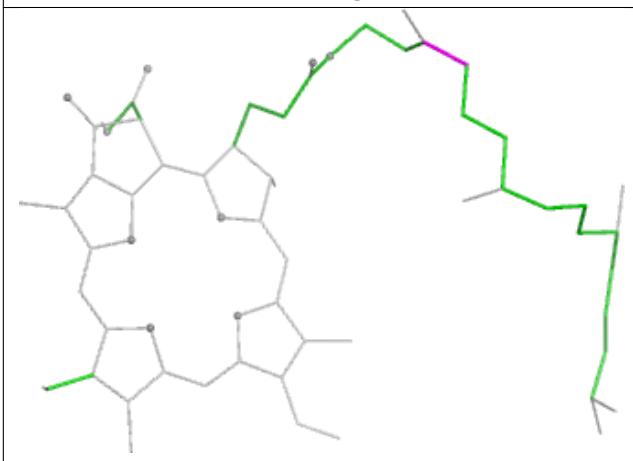

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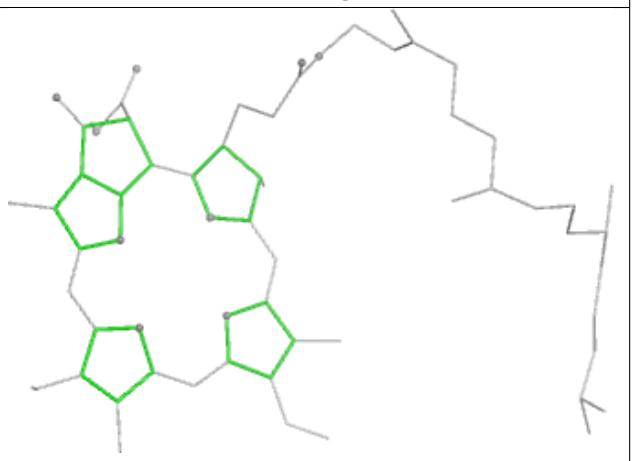
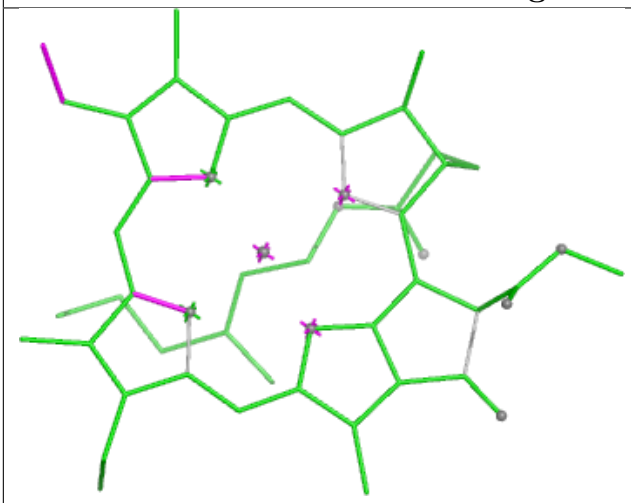


Rings

Ligand CLA g 613



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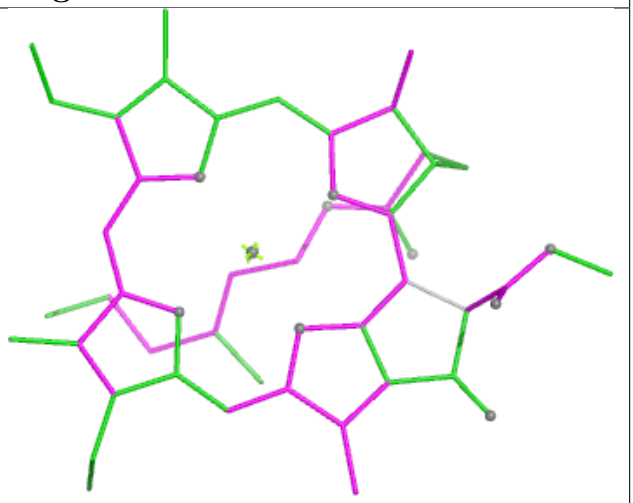

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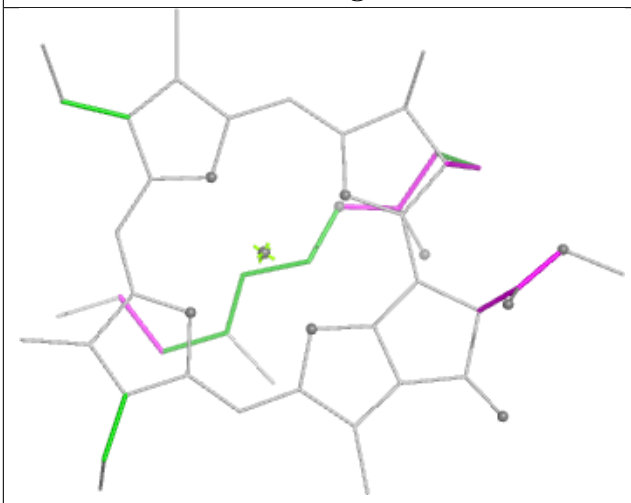

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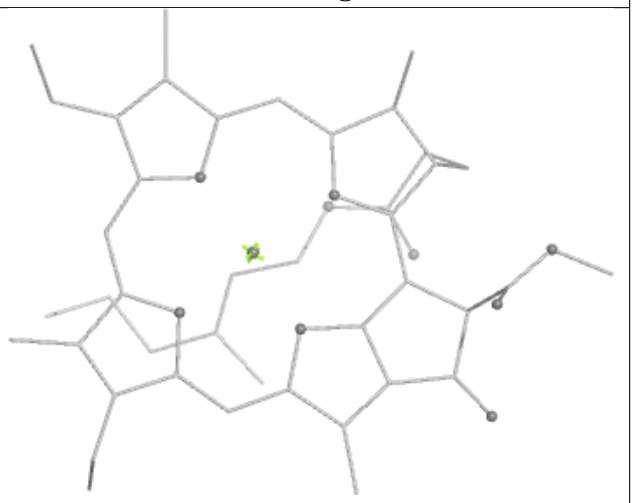
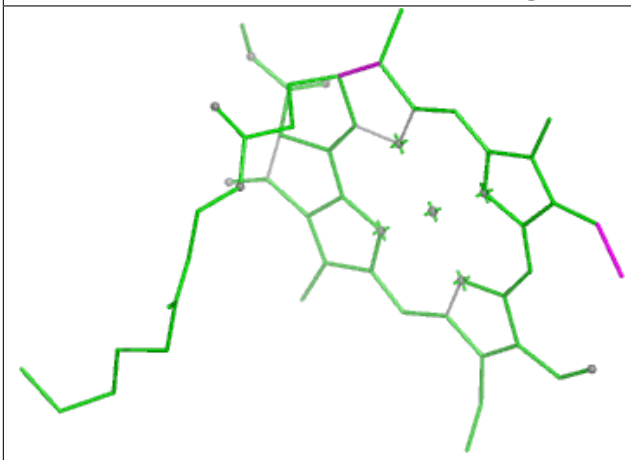


Rings

Ligand CHL G 609



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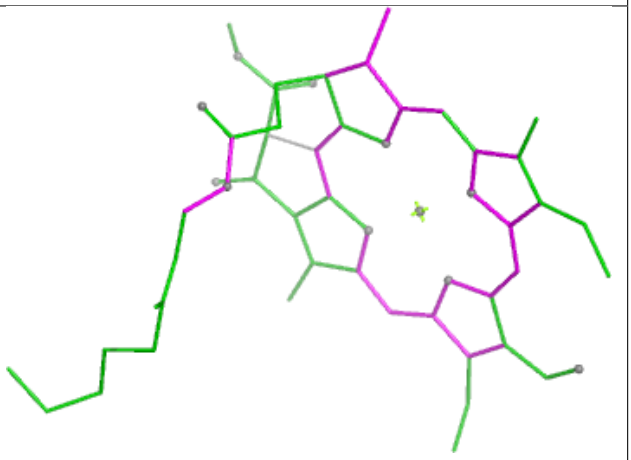
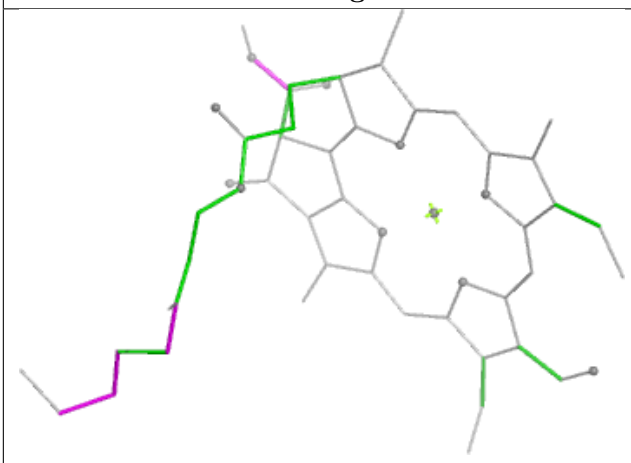


Bond angles



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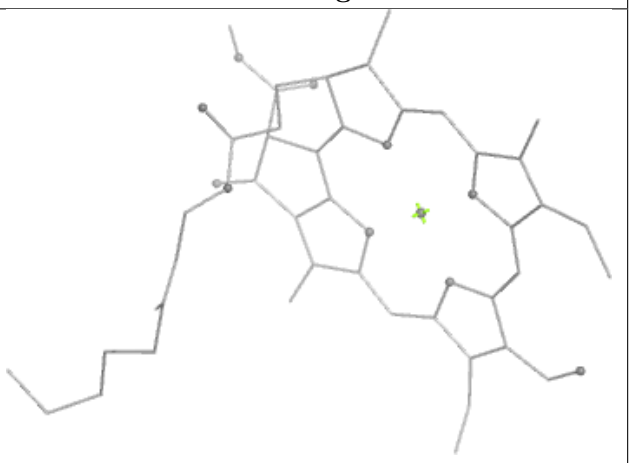
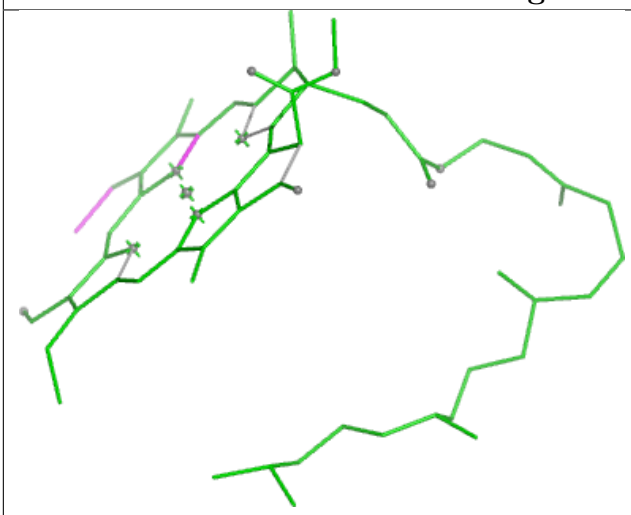


Rings

Ligand CHL g 619



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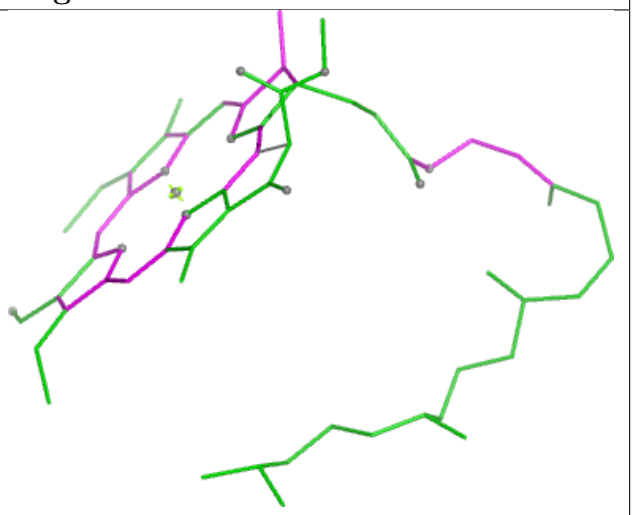
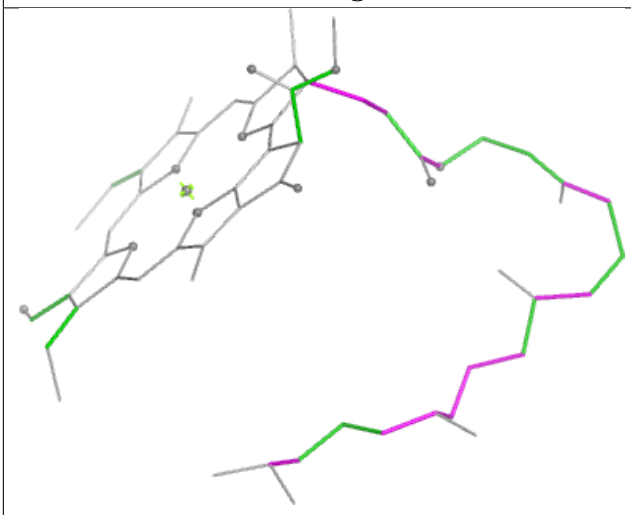


Bond angles



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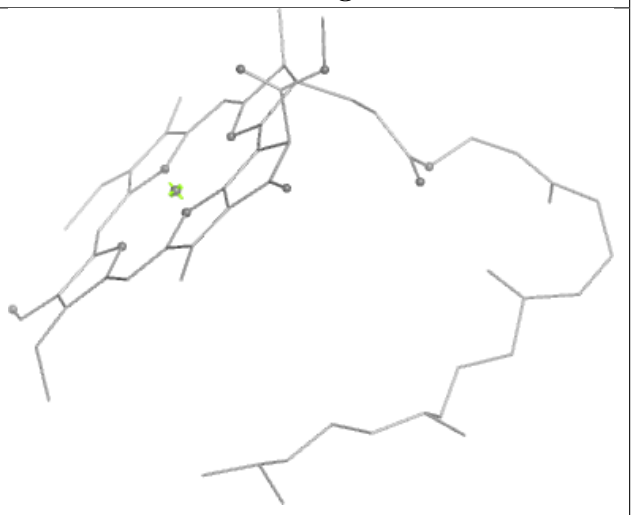
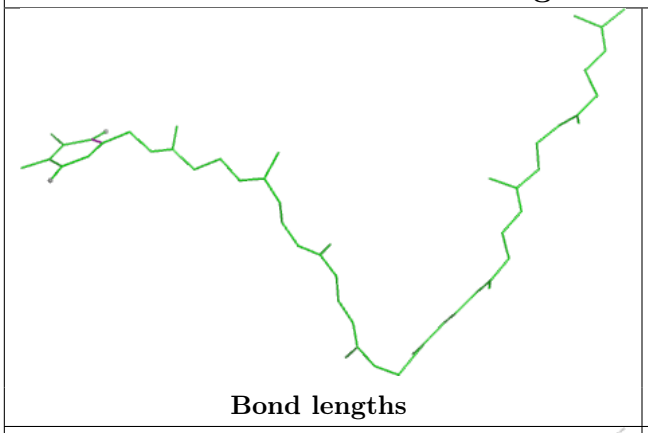


Rings

Ligand PL9 d 407



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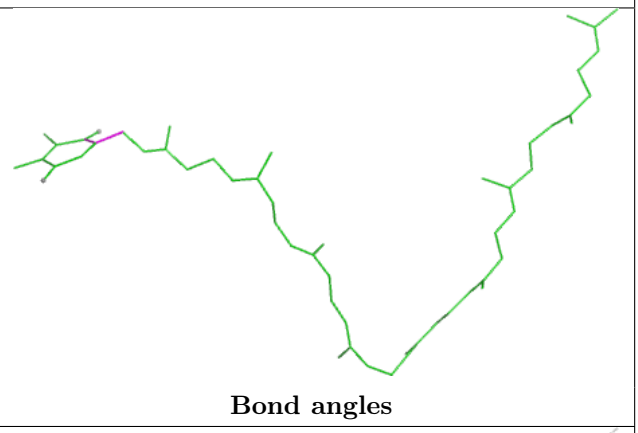
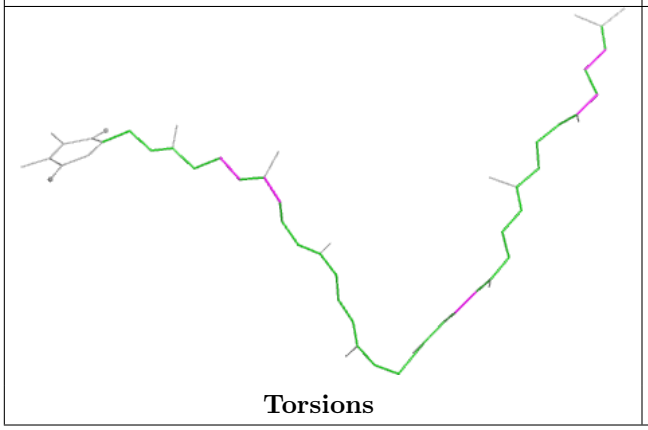


Bond angles



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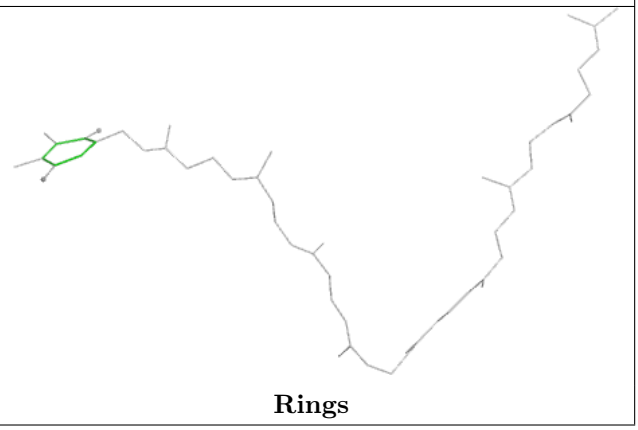
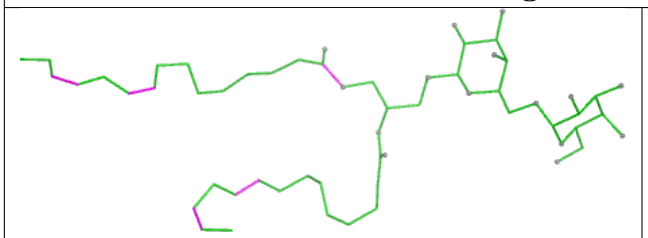


Rings

Ligand DGD C 519



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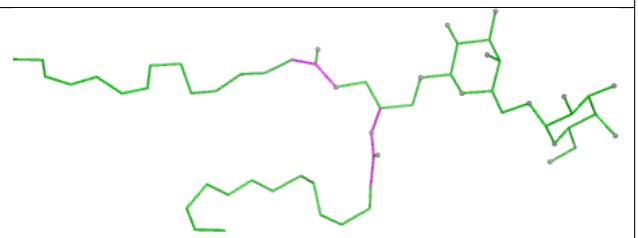
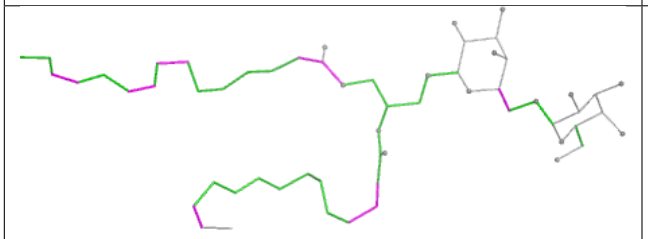


Bond angles



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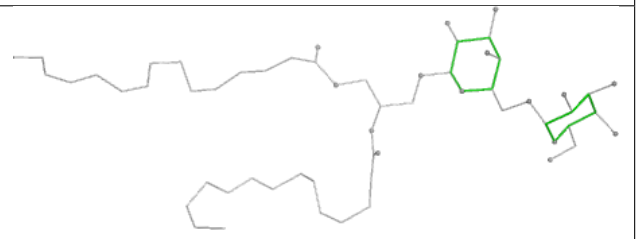
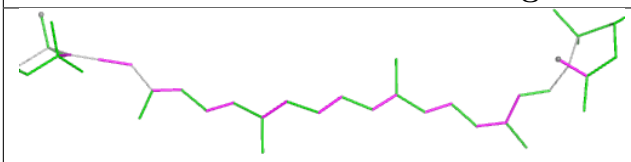
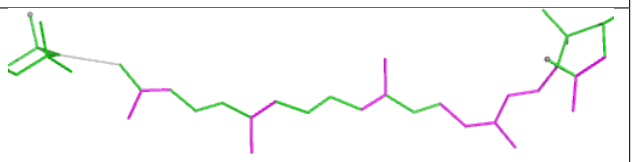


Rings

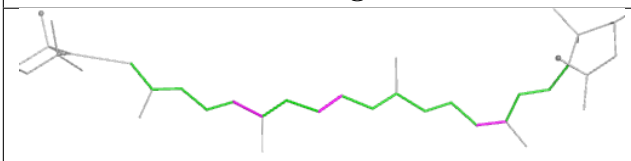
Ligand NEX Y 618



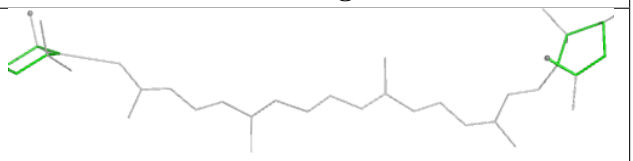
Bond lengths



Bond angles

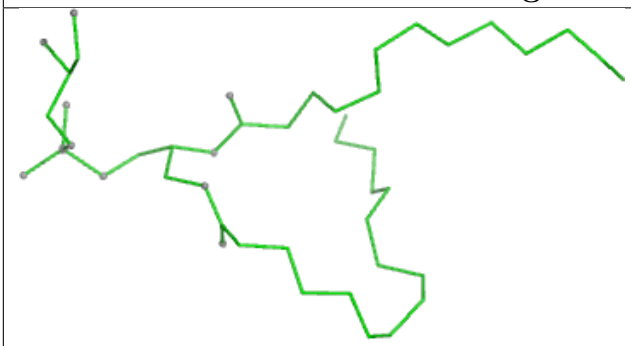


Torsions



Rings

Ligand LHG B 625



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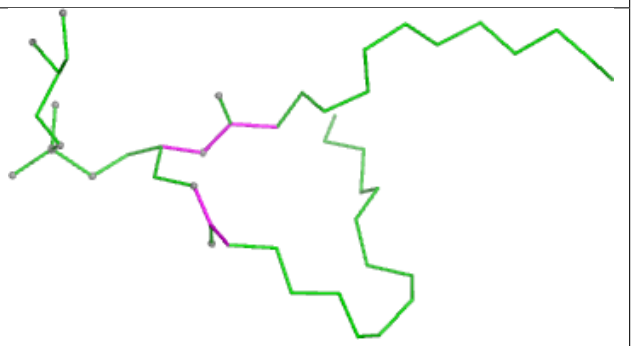

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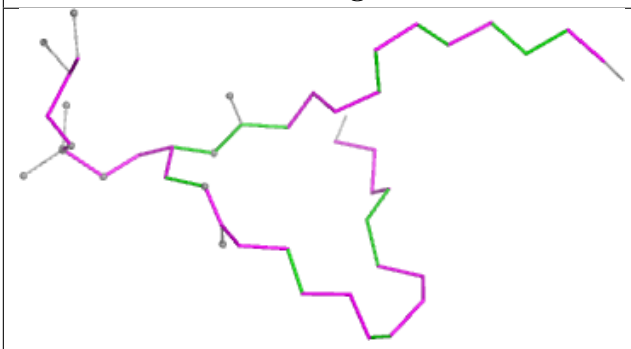

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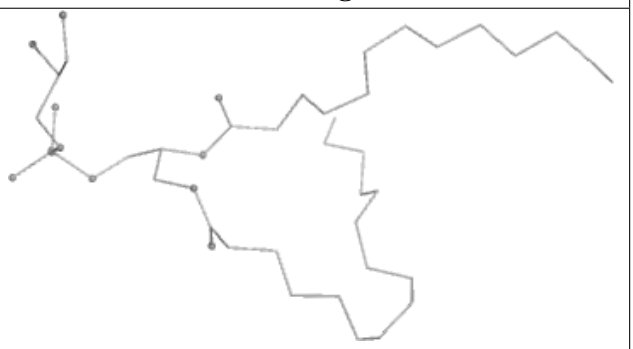
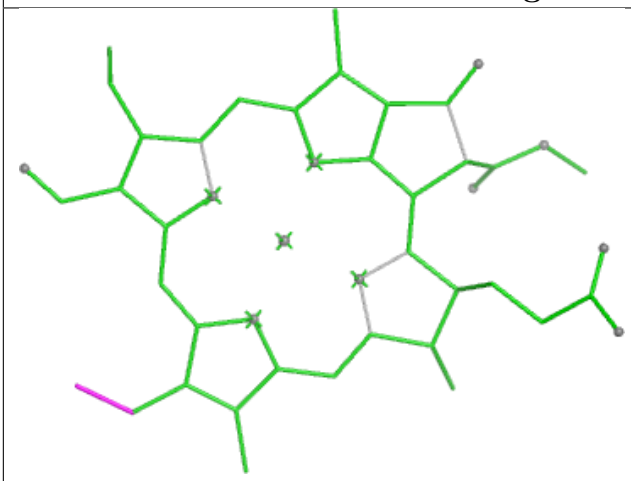


Rings

Ligand CHL R 606



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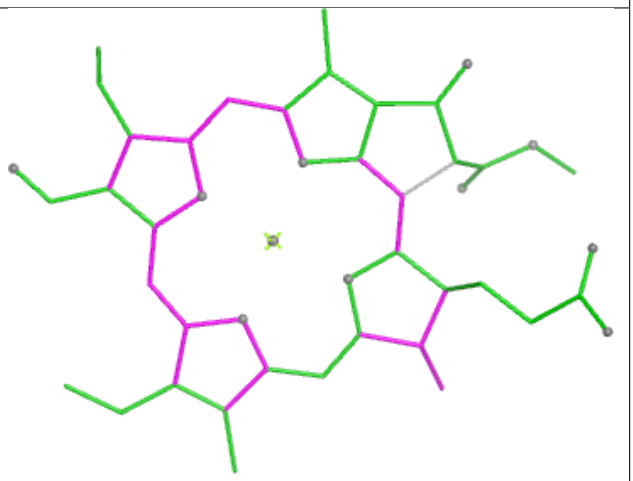
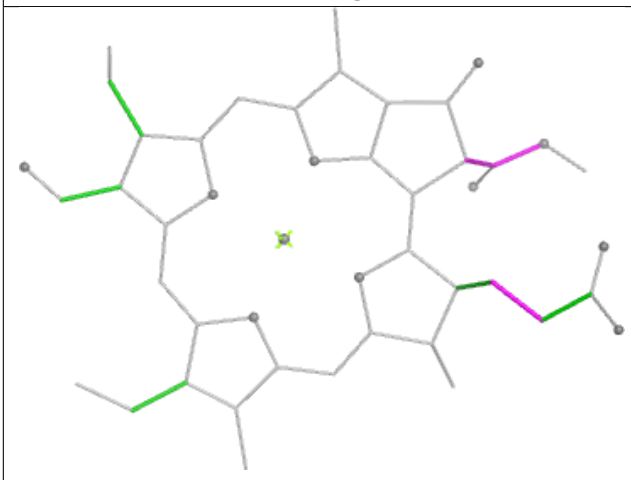


Bond angles



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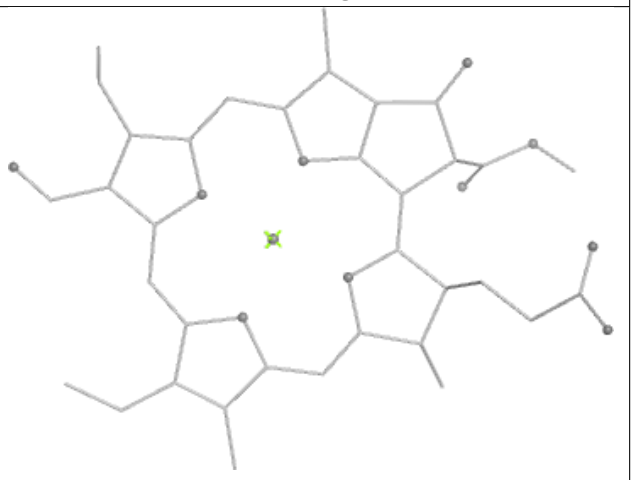
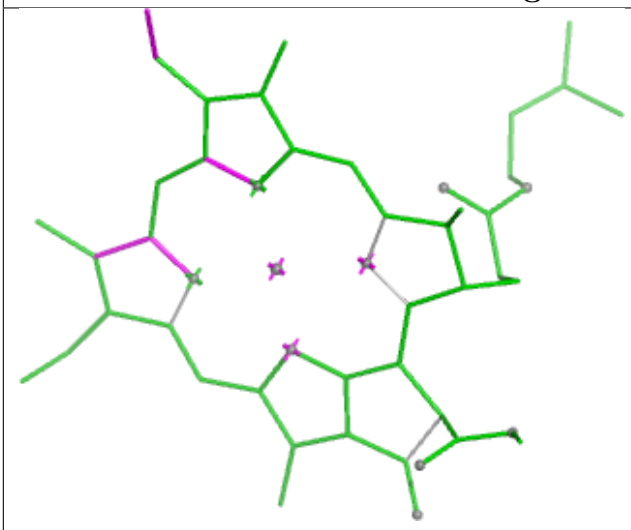


Rings

Ligand CLA A 406



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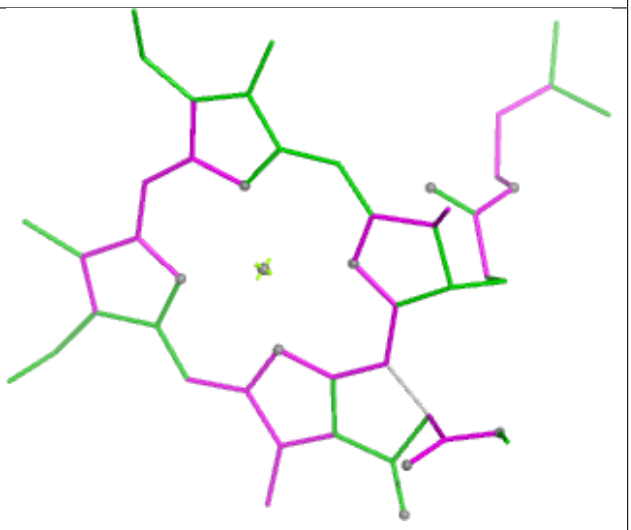

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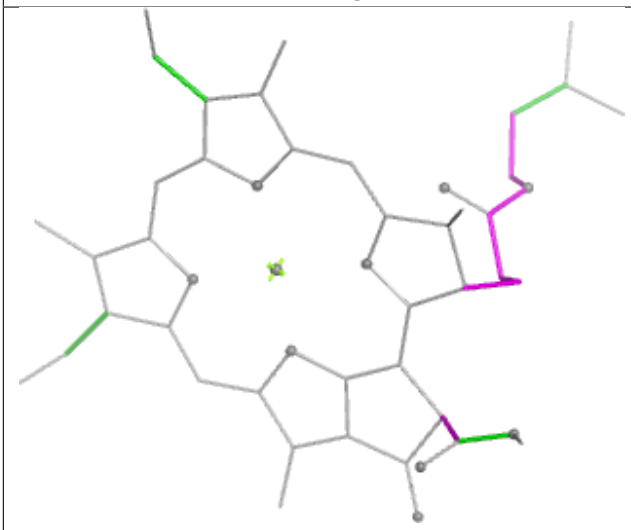

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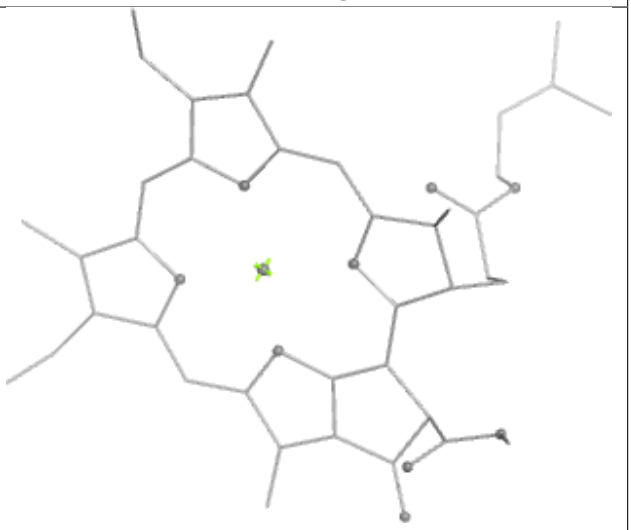
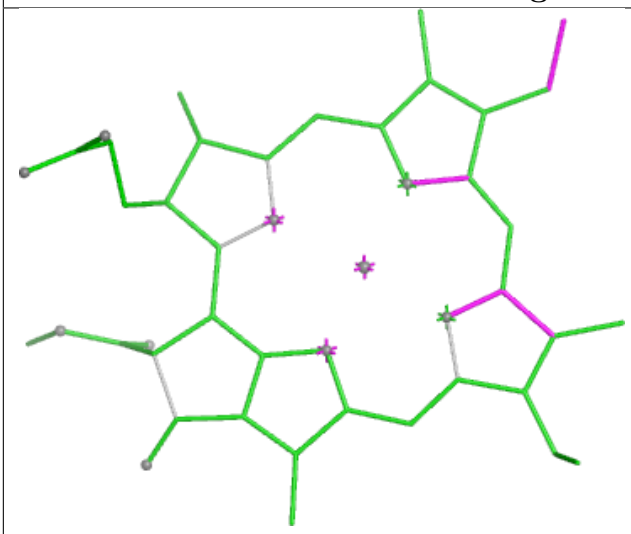


Rings

Ligand CLA s 608



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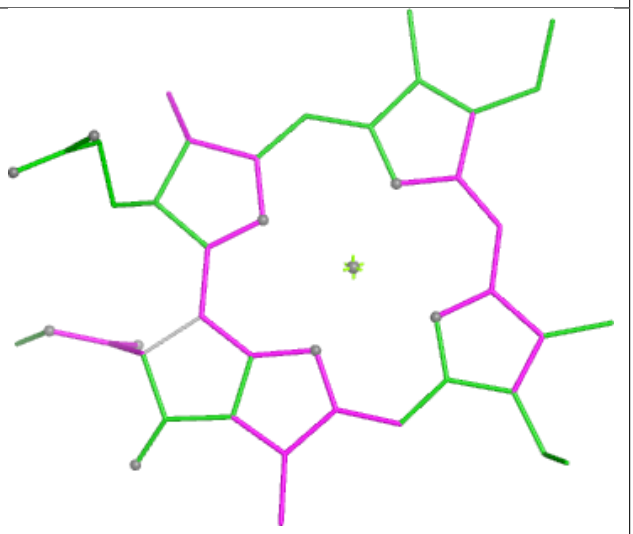

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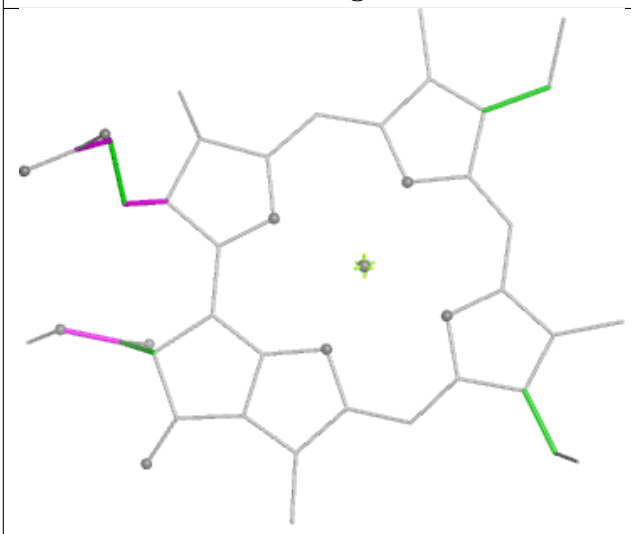
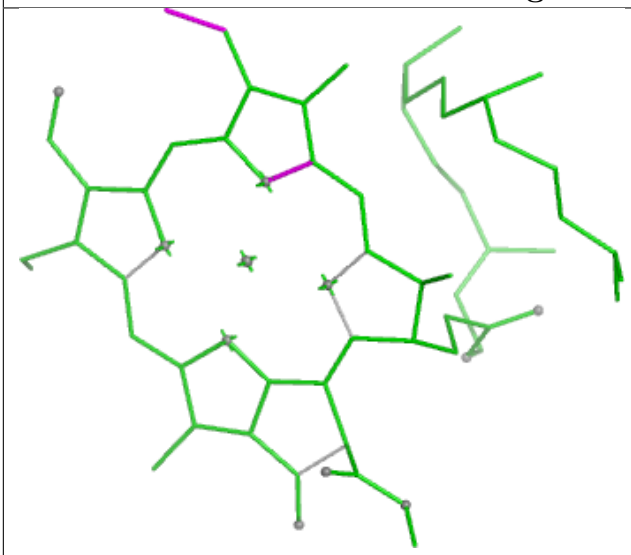


Torsions



Rings

Ligand CHL n 608



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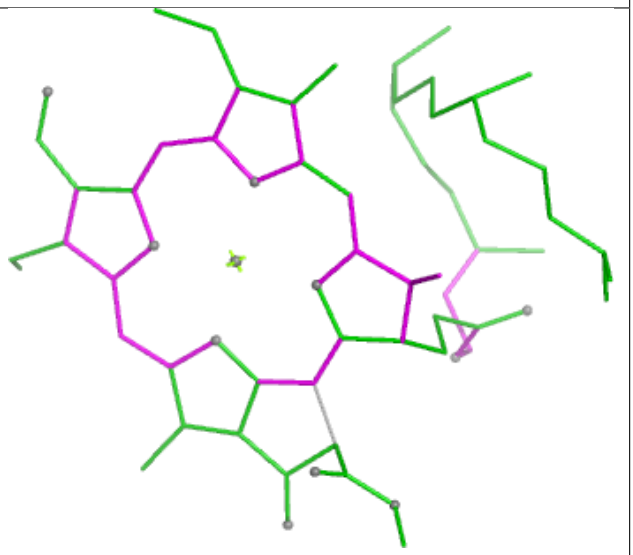

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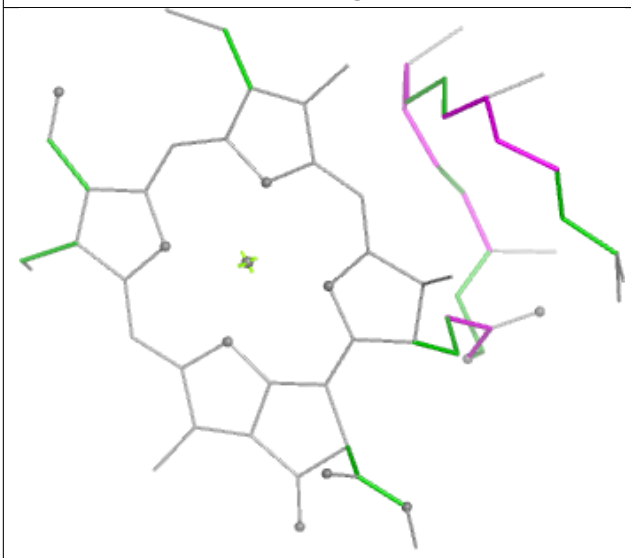

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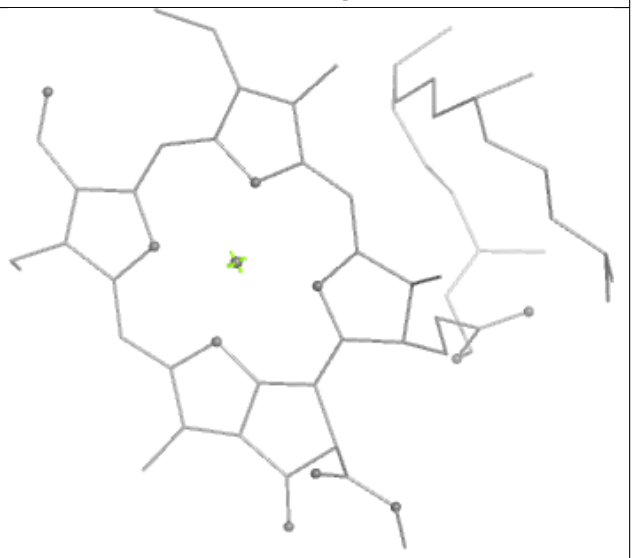
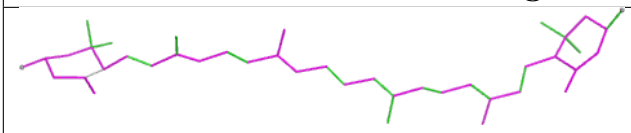


Rings

Ligand LUT R 614



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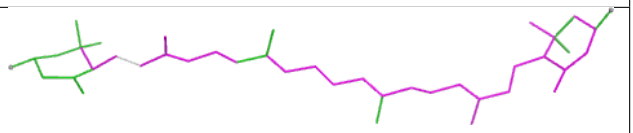
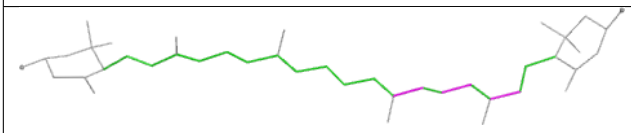


Bond angles



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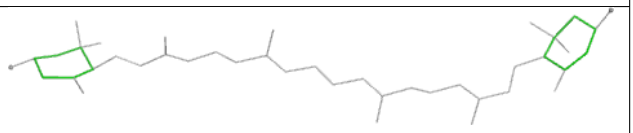
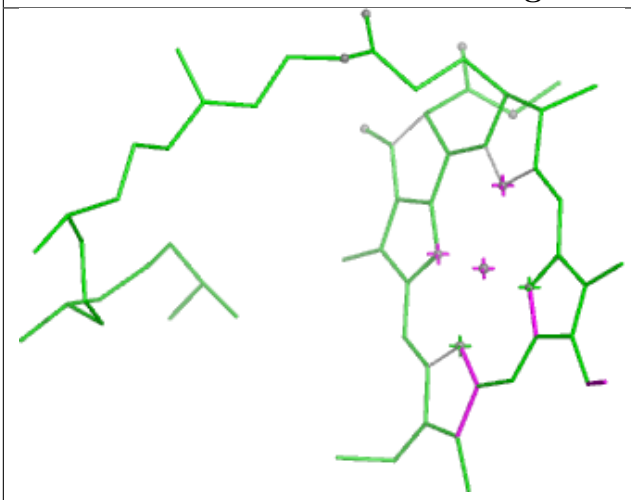


Rings

Ligand CLA C 503



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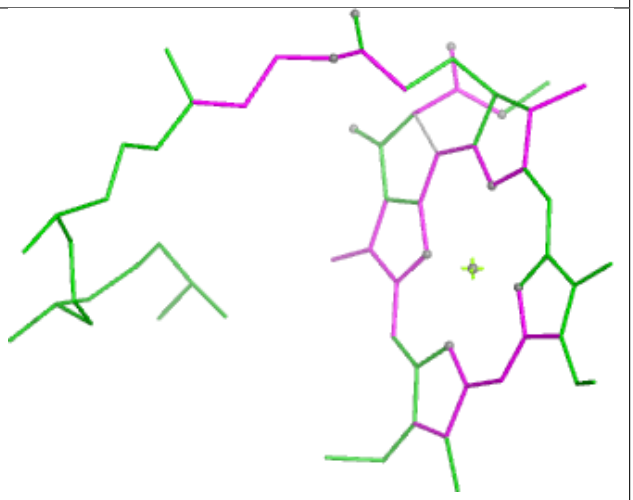
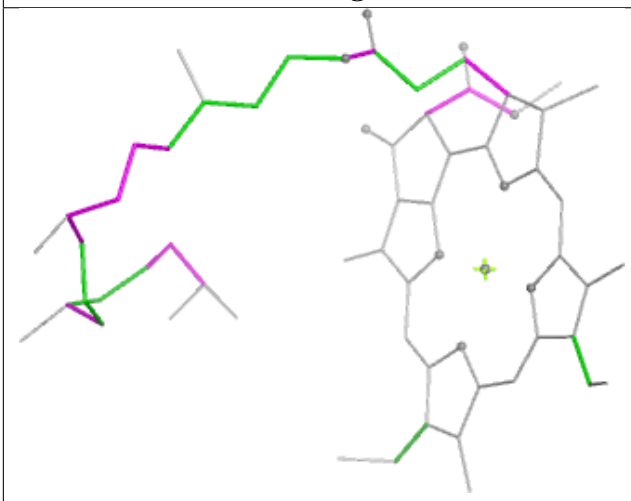


Bond angles



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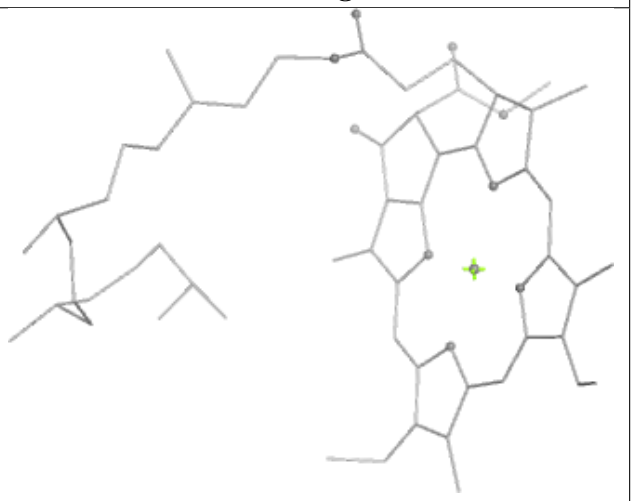
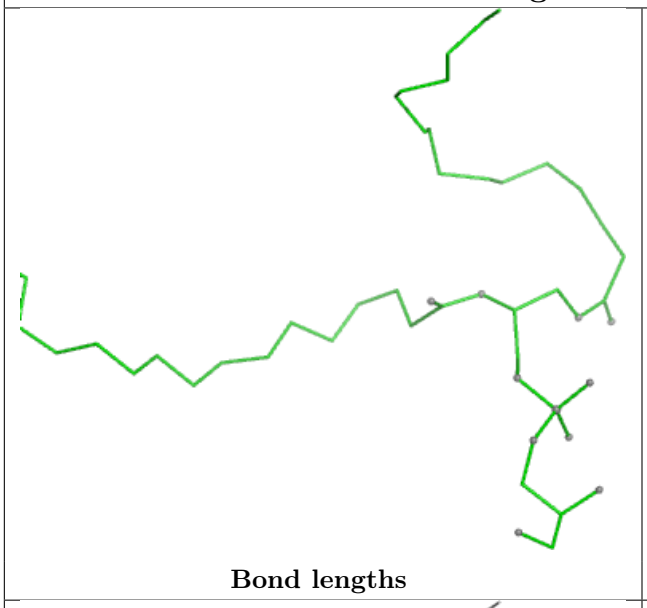


Rings

Ligand LHG s 617



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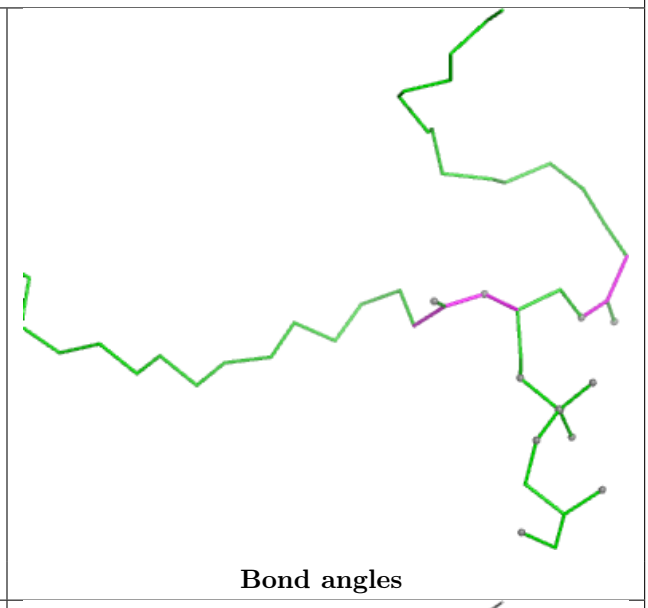
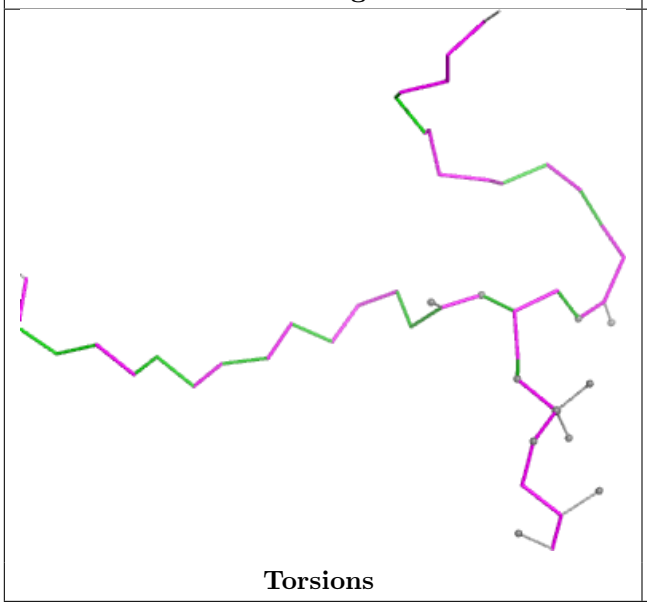


Bond angles



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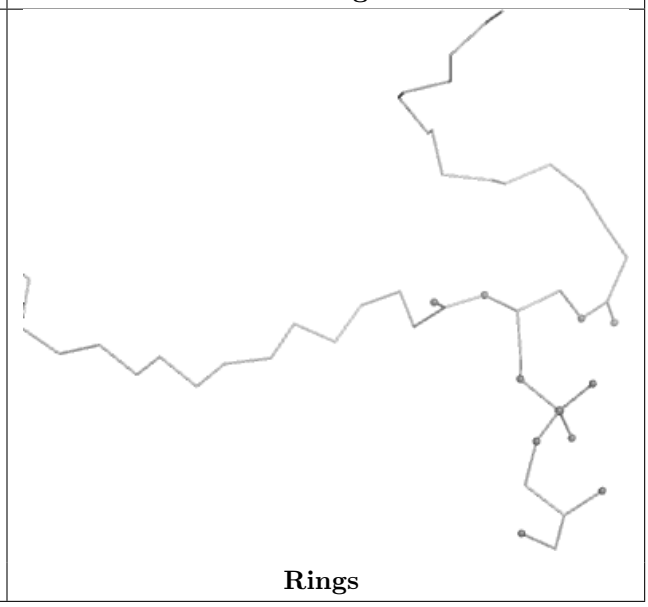
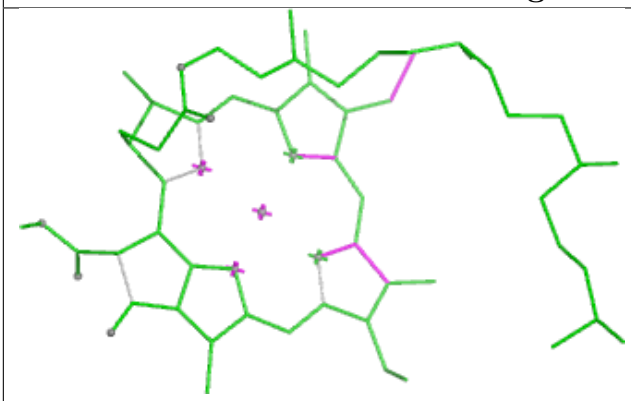


Rings

Ligand CLA n 610



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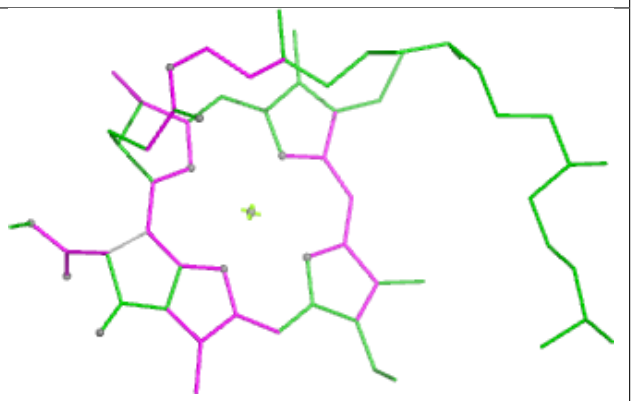
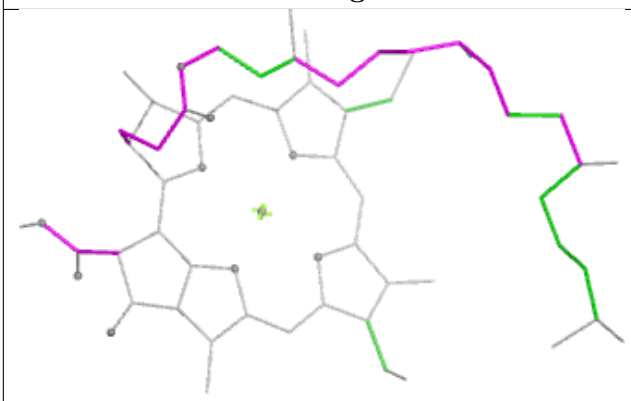


Bond angles

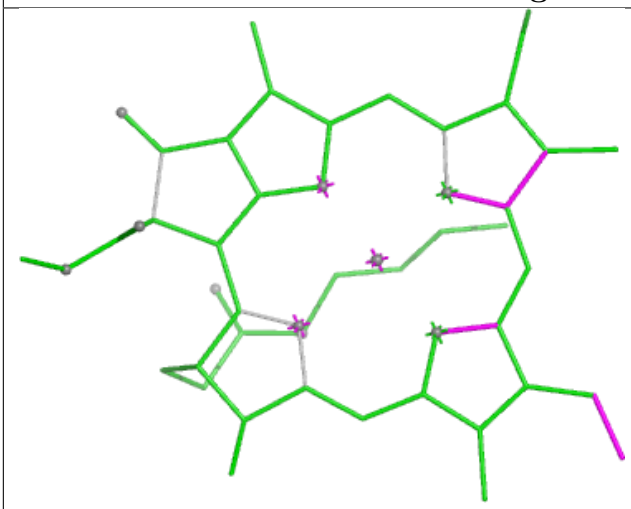


Torsions



Rings

Ligand CLA s 613



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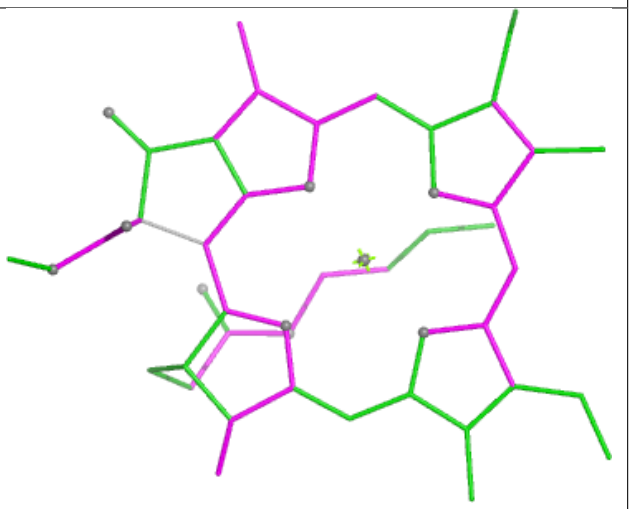
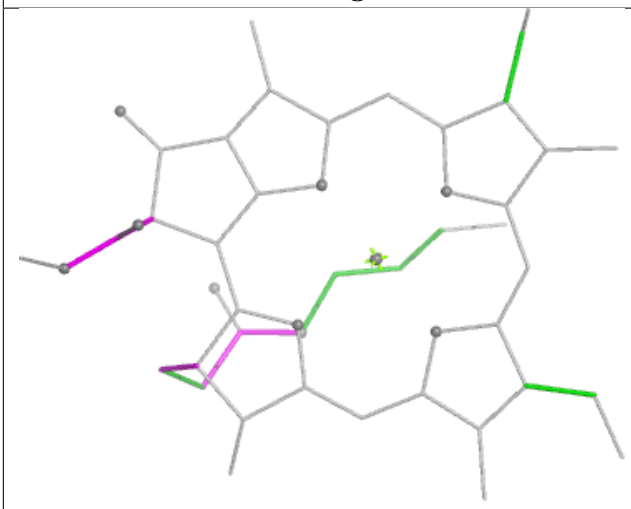


Bond angles



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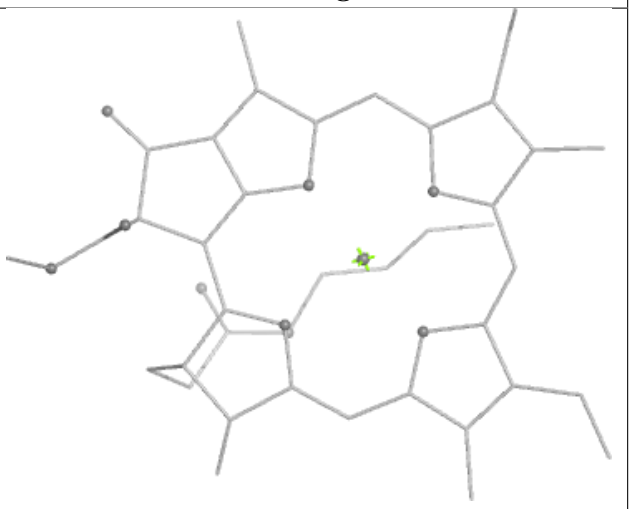
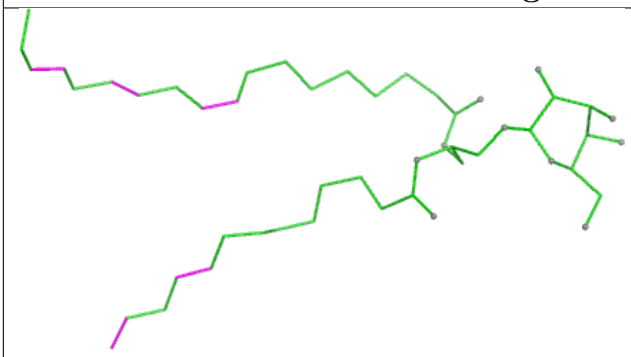


Rings

Ligand LMG b 623



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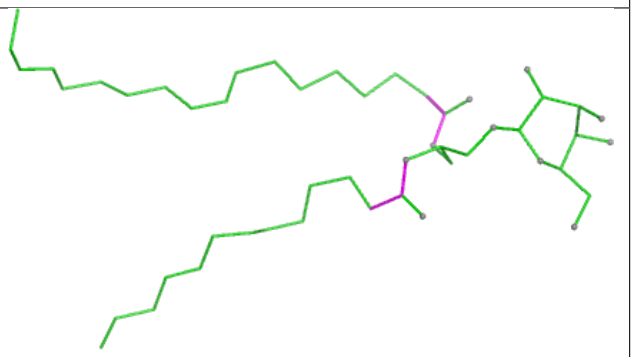
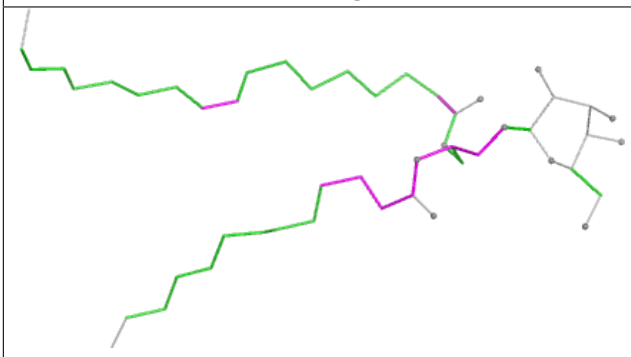


Bond angles



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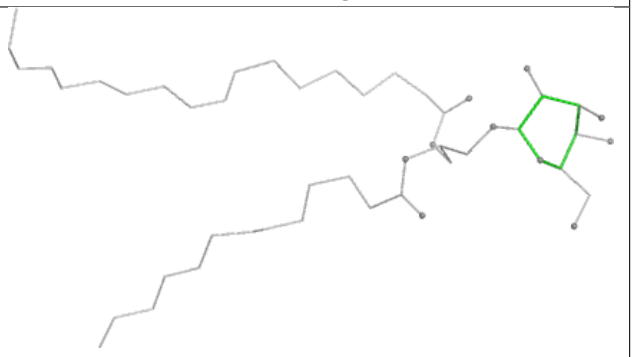
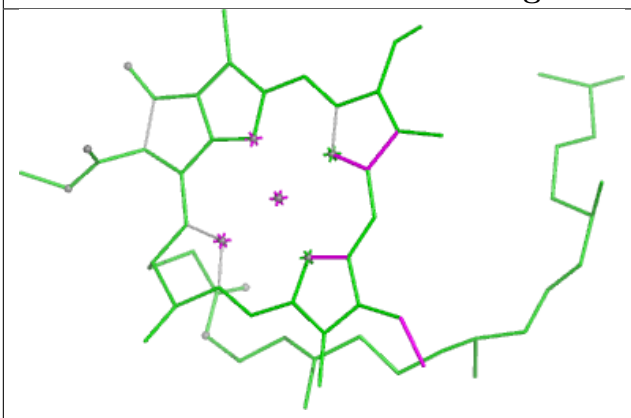


Rings

Ligand CLA N 610



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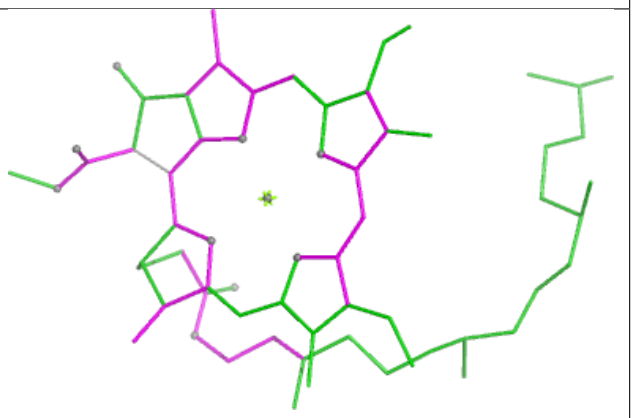
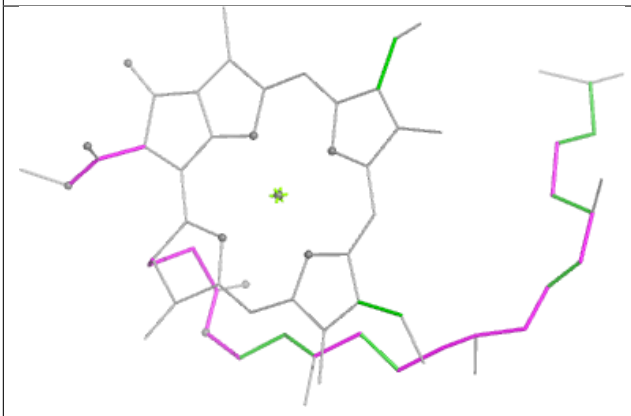


Bond angles



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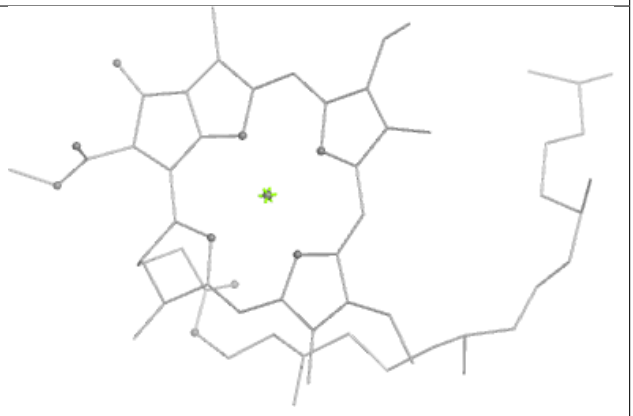
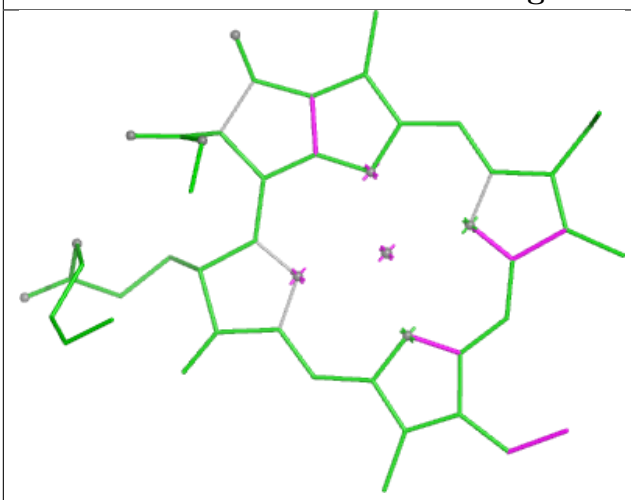


Rings

Ligand CLA S 312



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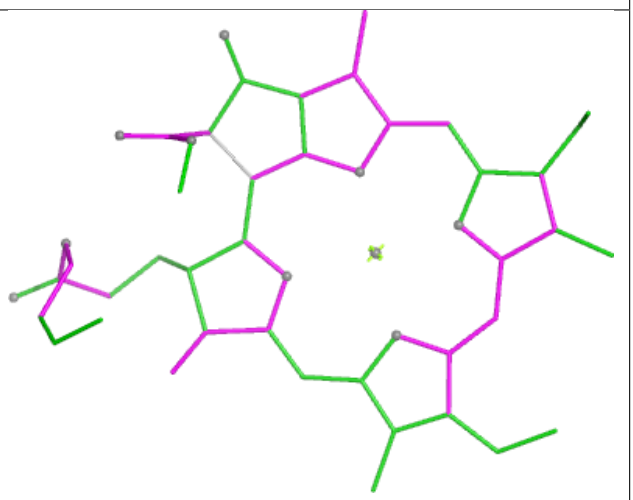
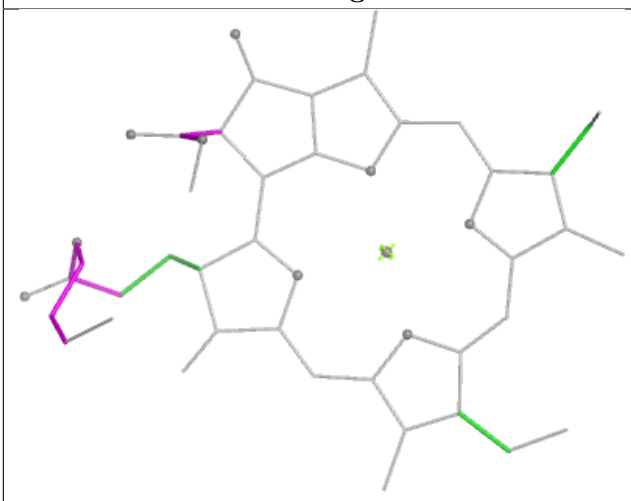


Bond angles



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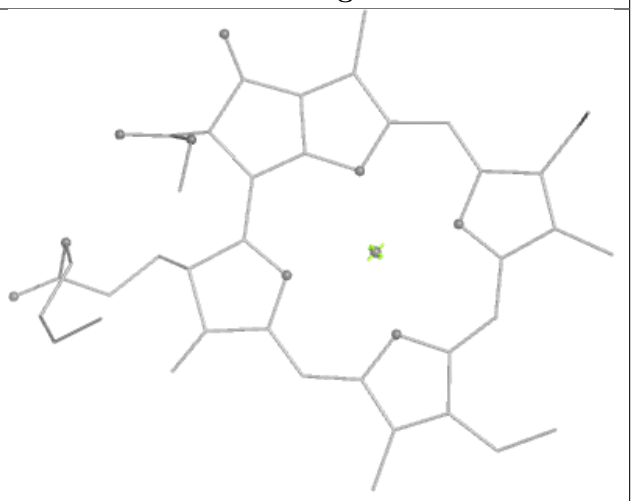
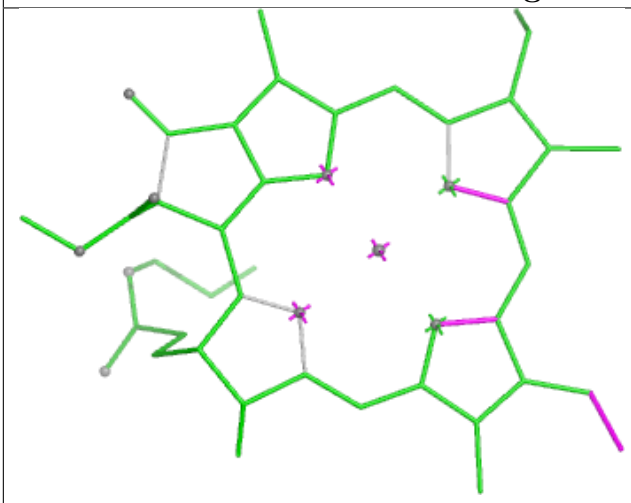


Rings

Ligand CLA Y 614



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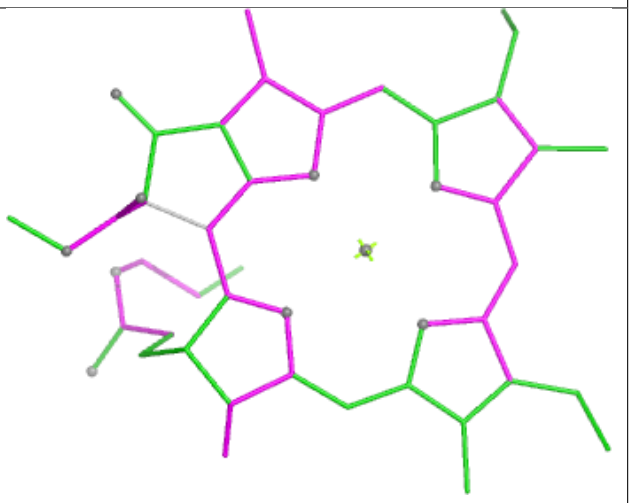
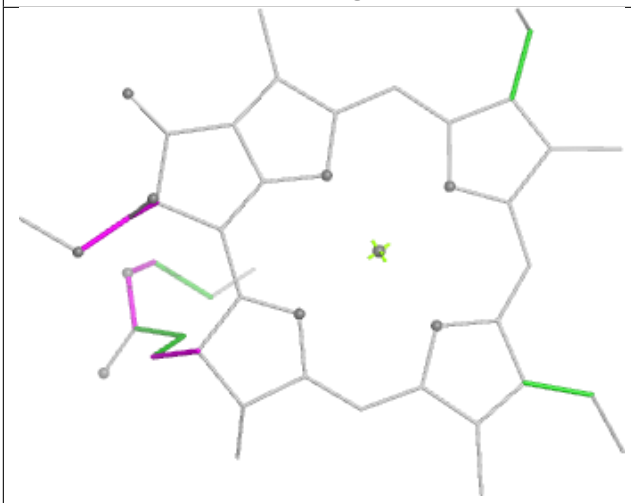


Bond angles



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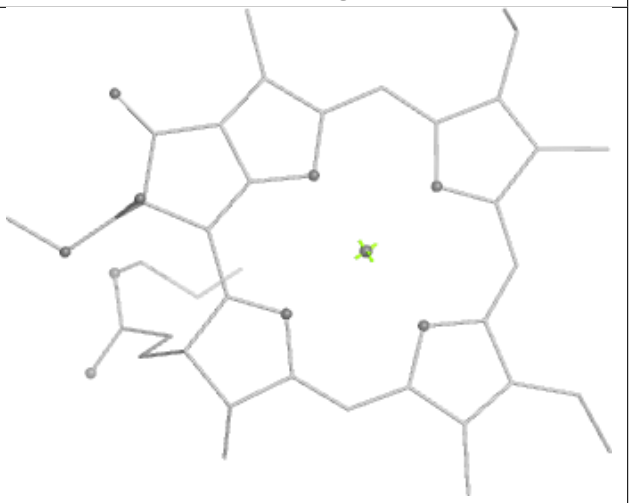
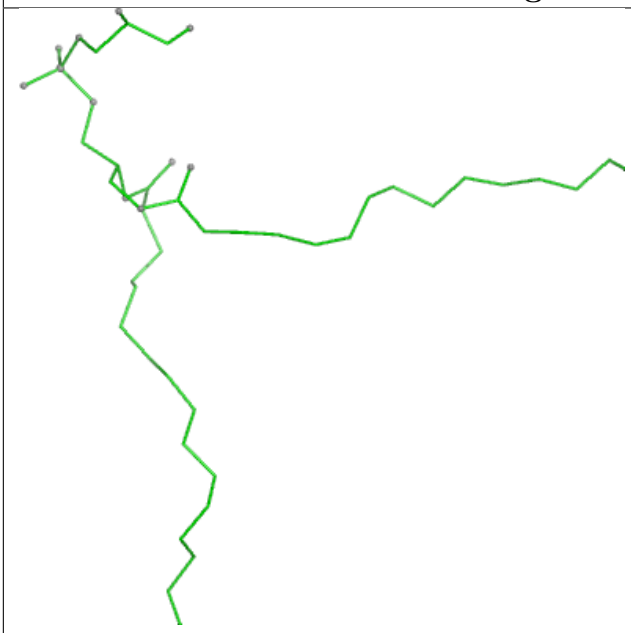


Rings

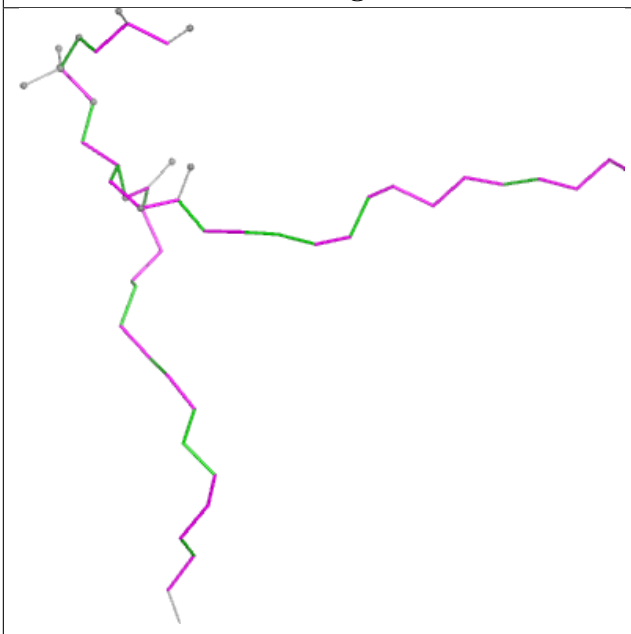
Ligand LHG L 102



Bond lengths



Bond angles

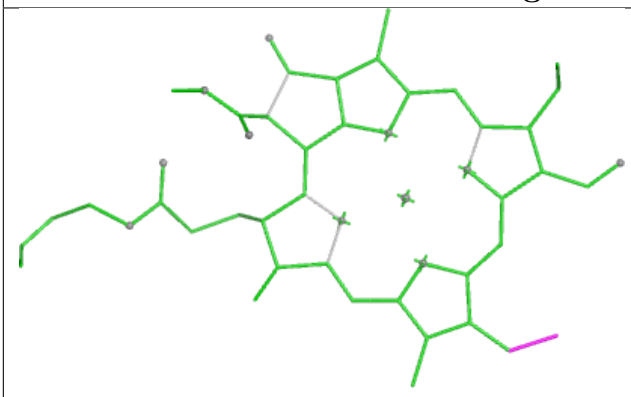


Torsions

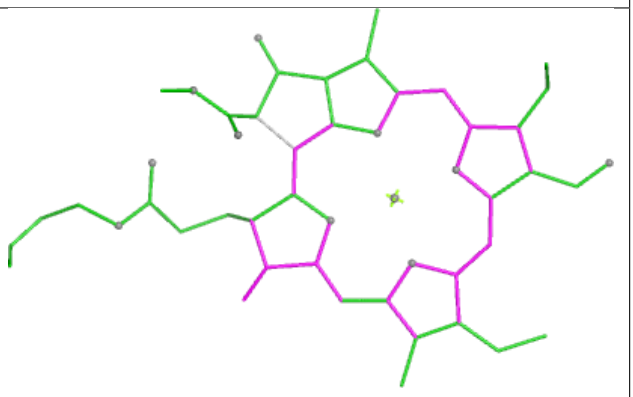


Rings

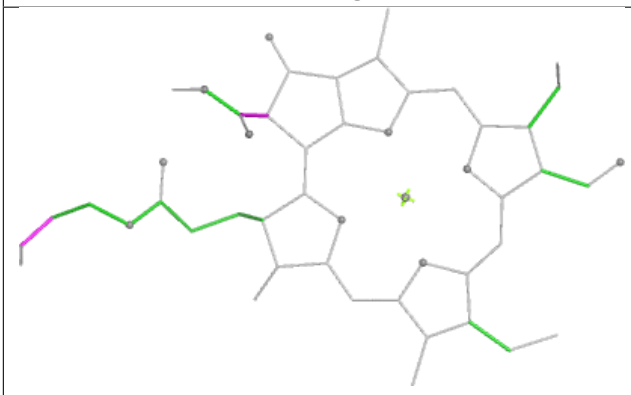
Ligand CHL Y 606



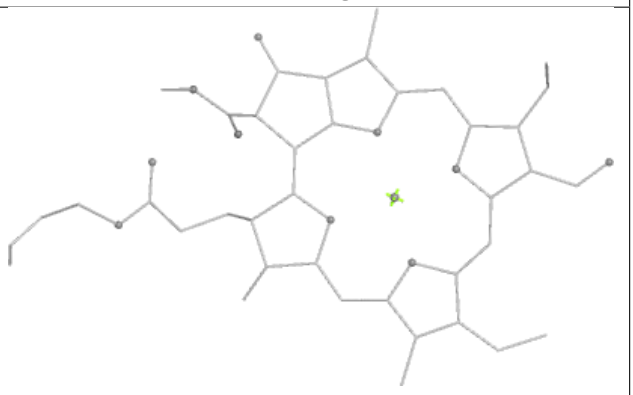
Bond lengths



Bond angles

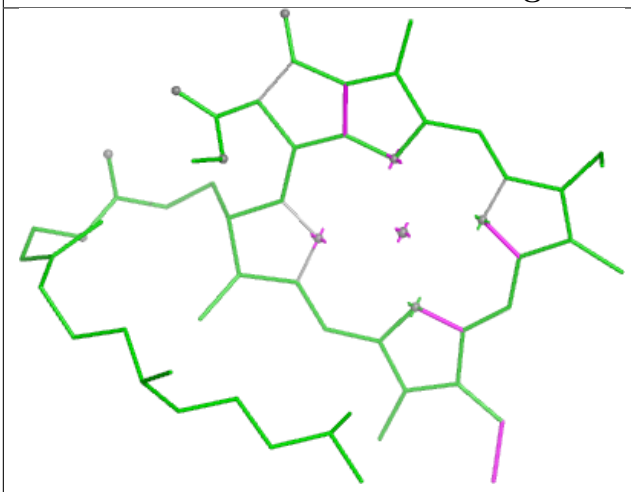


Torsions



Rings

Ligand CLA R 603



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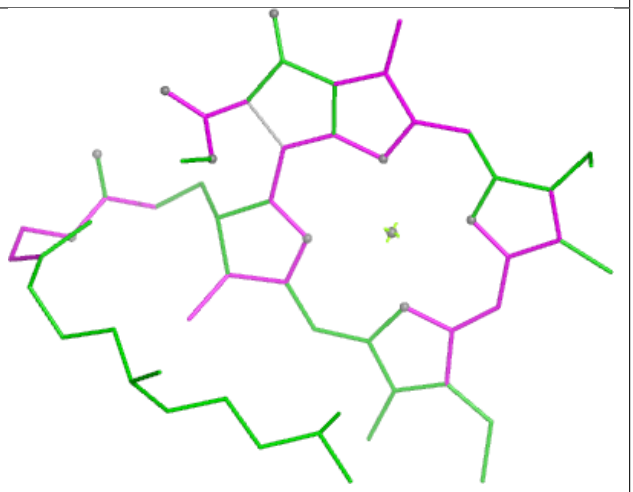

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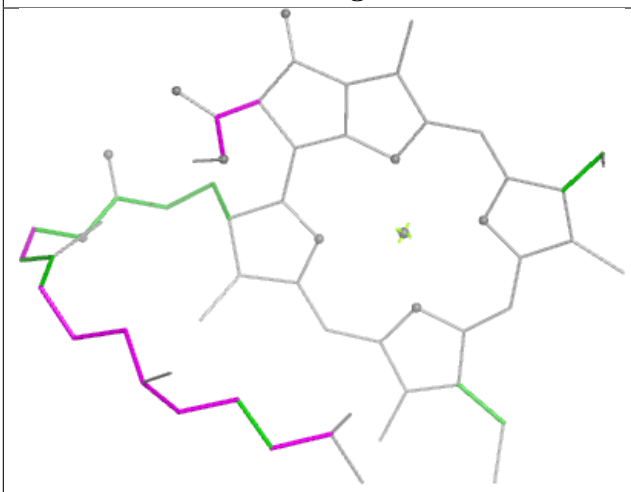

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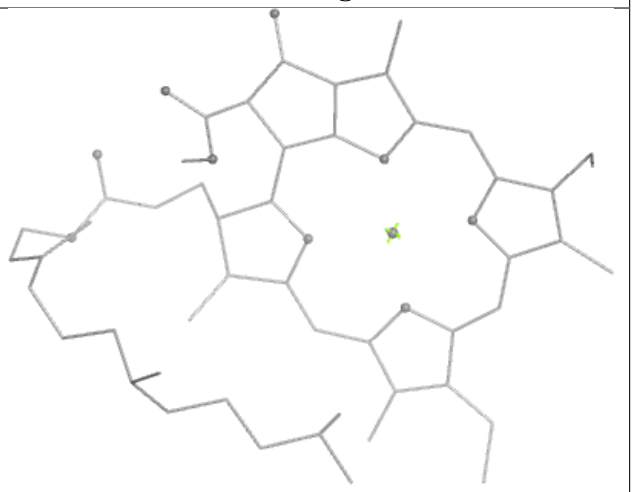
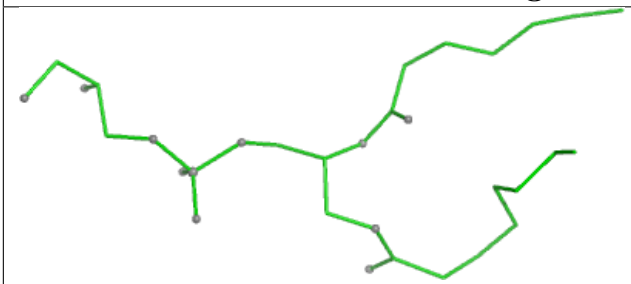


Rings

Ligand LHG n 618



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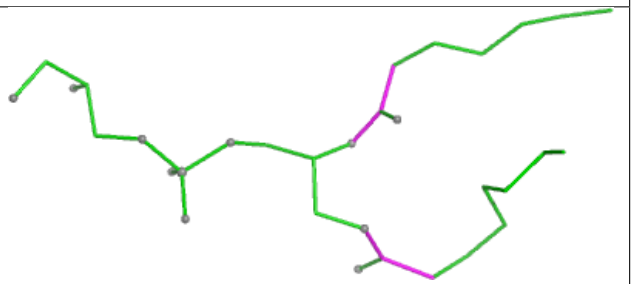

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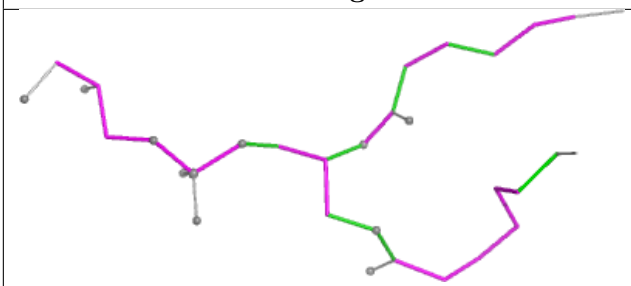

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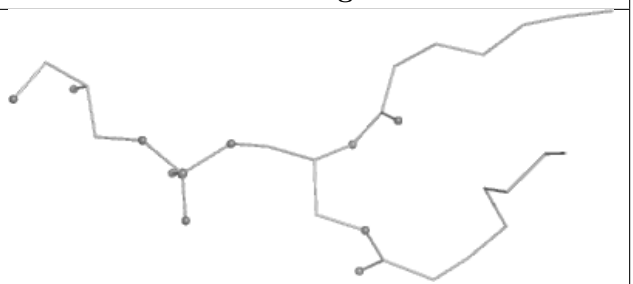
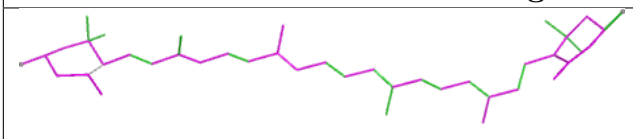


Rings

Ligand LUT S 316



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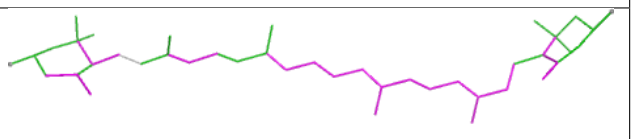

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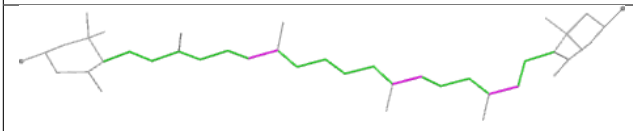

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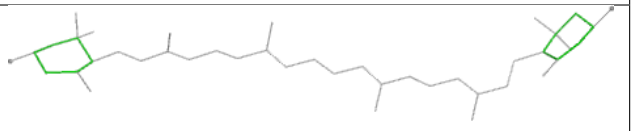
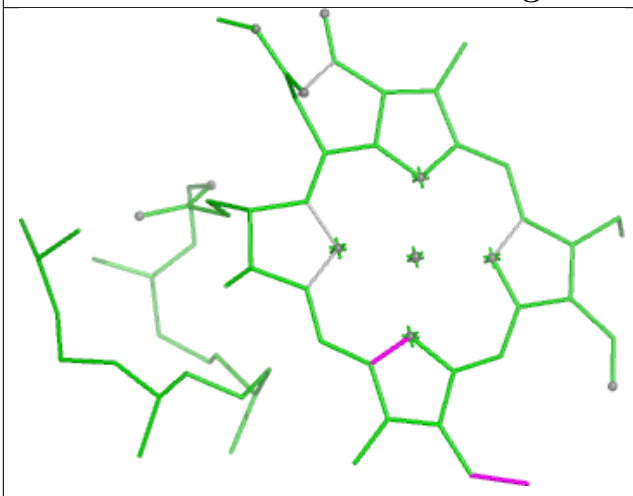


Rings

Ligand CHL N 608



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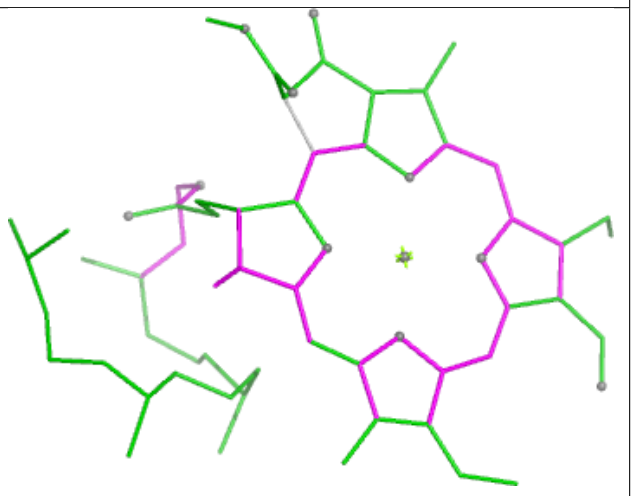

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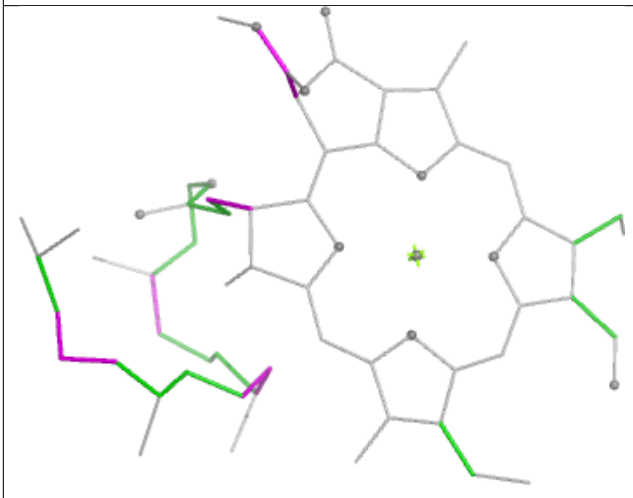

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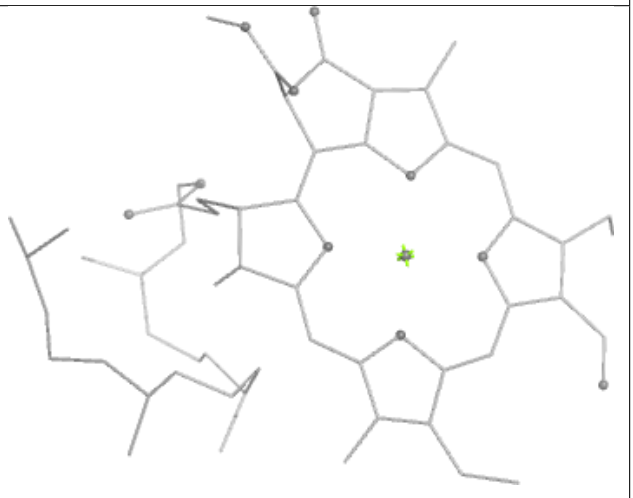
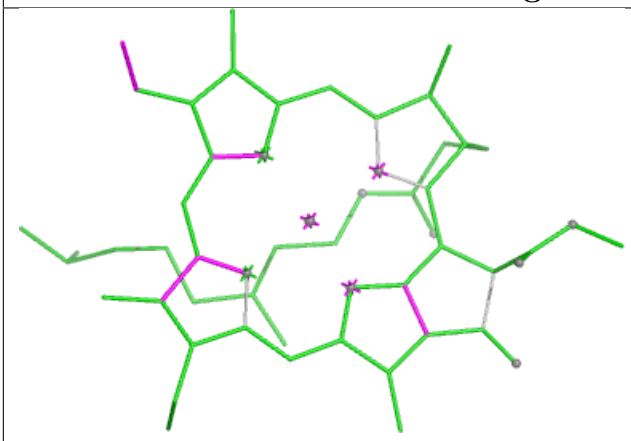


Rings

Ligand CLA R 612



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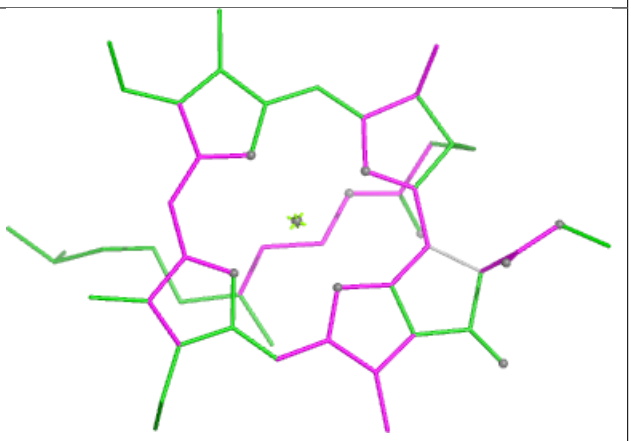

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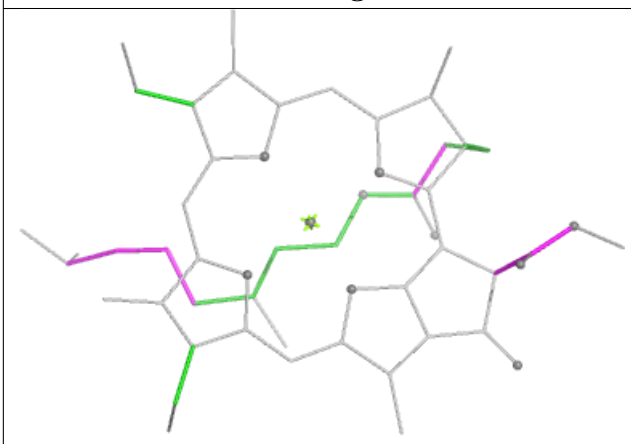

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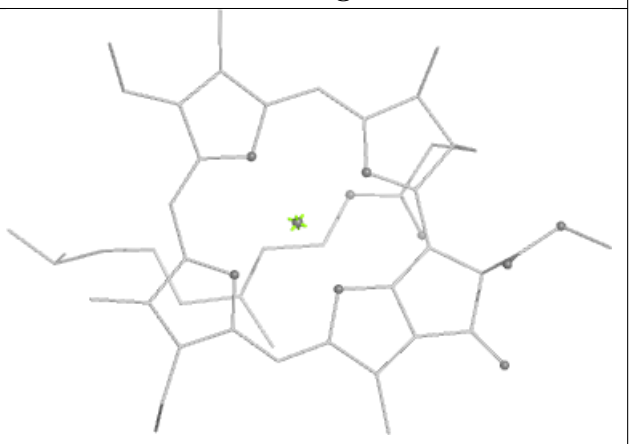
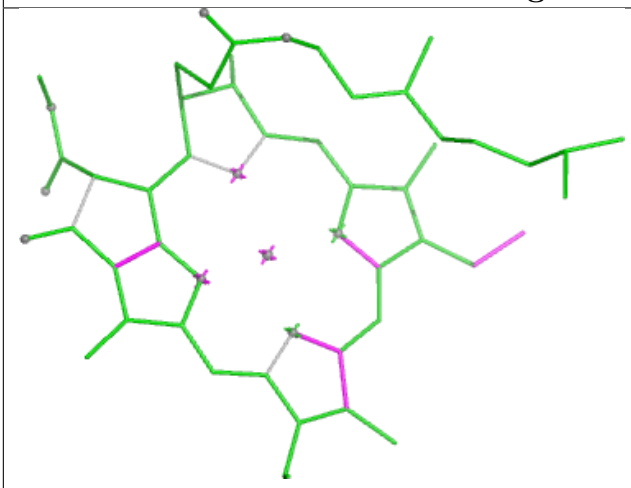


Rings

Ligand CLA S 310



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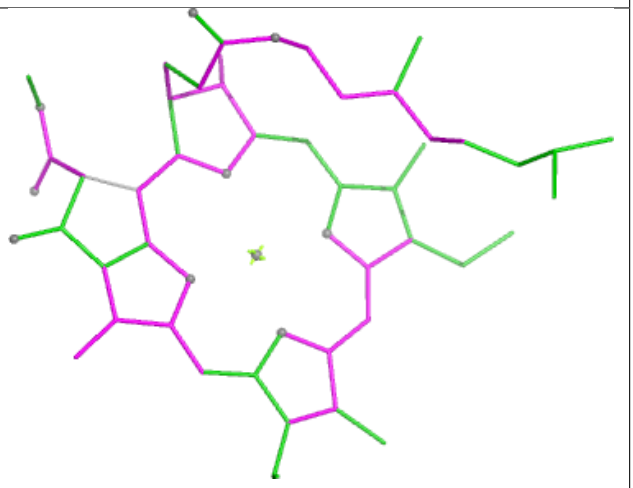

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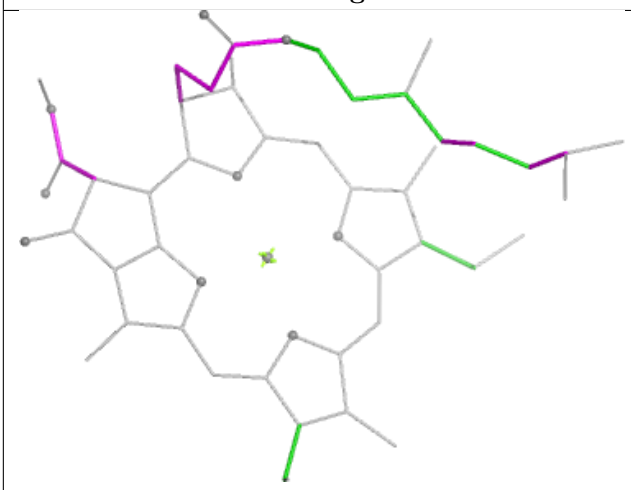

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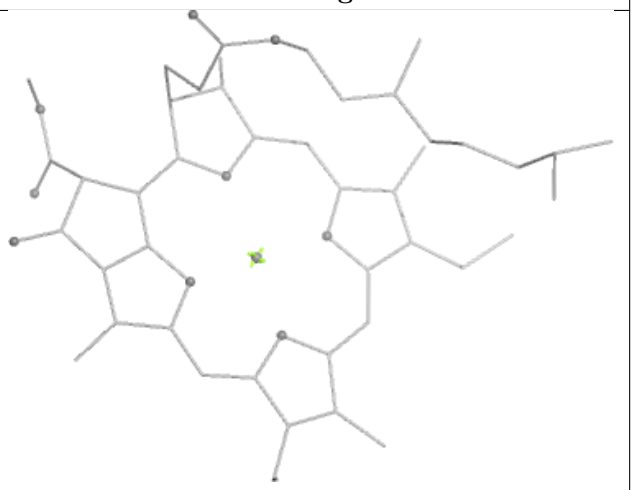
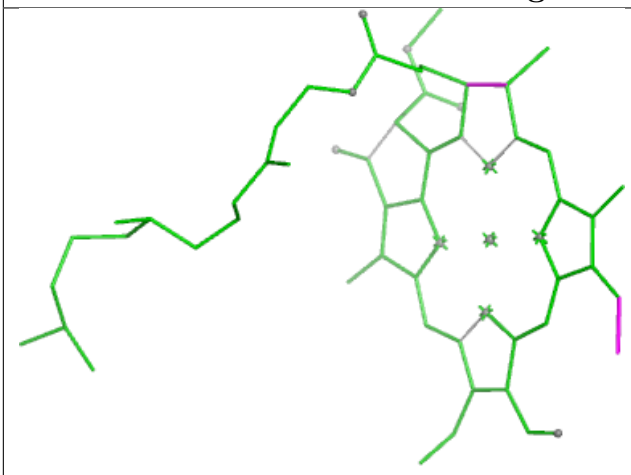


Rings

Ligand CHL g 609



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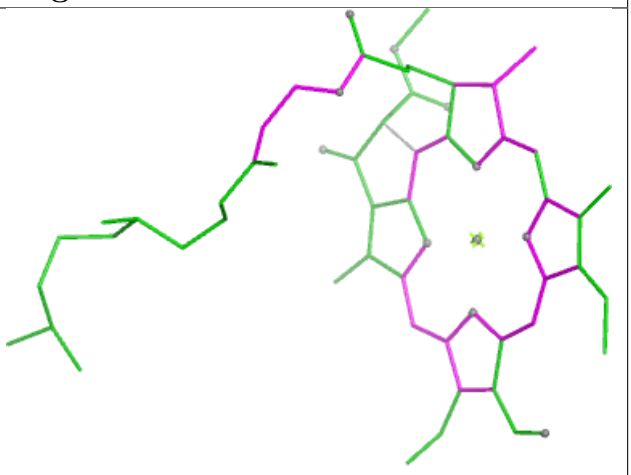

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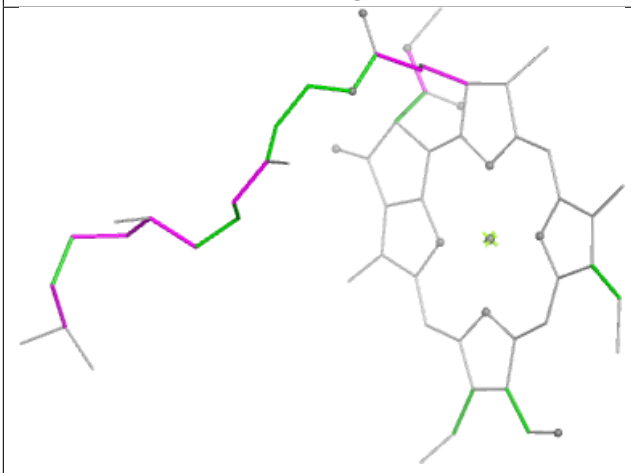
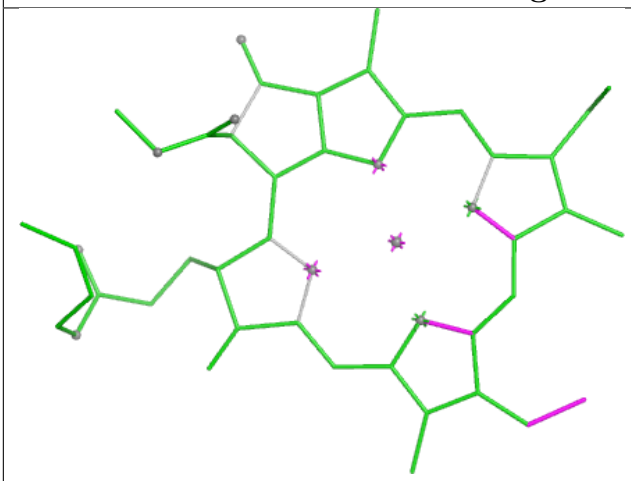


Torsions



Rings

Ligand CLA r 611



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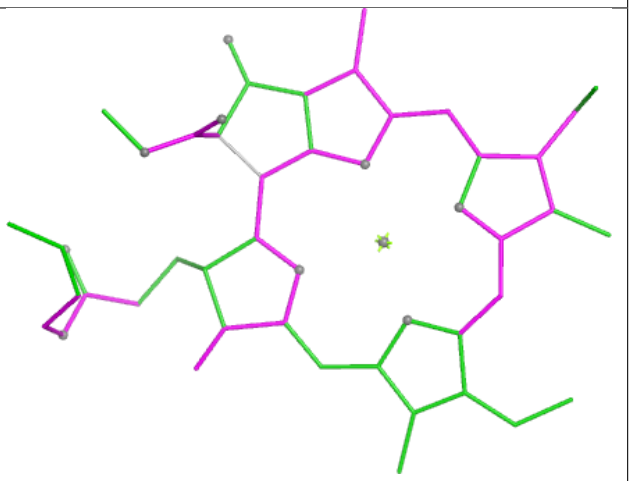

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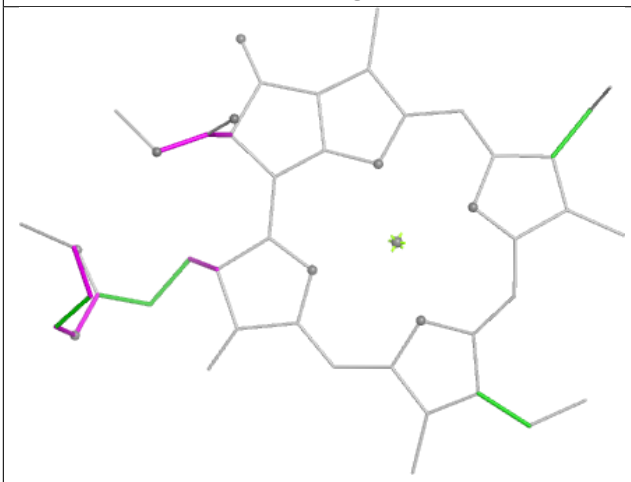
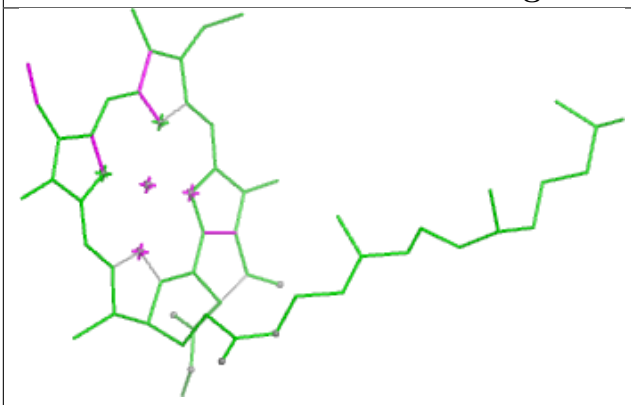


Torsions



Rings

Ligand CLA N 611



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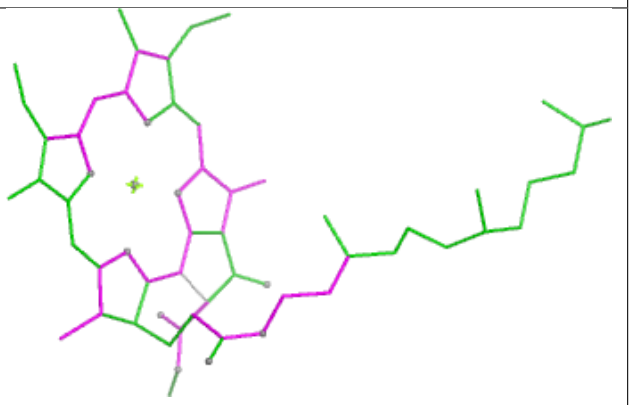

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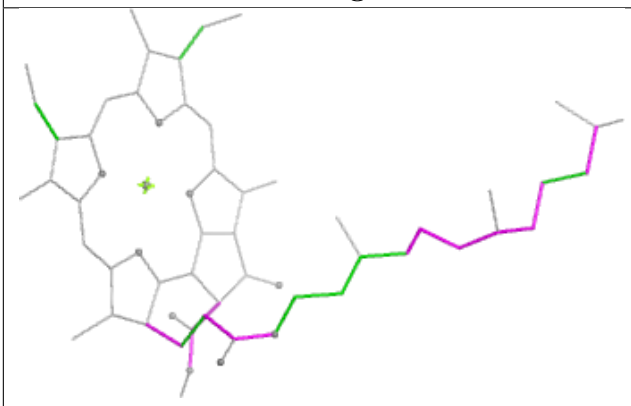

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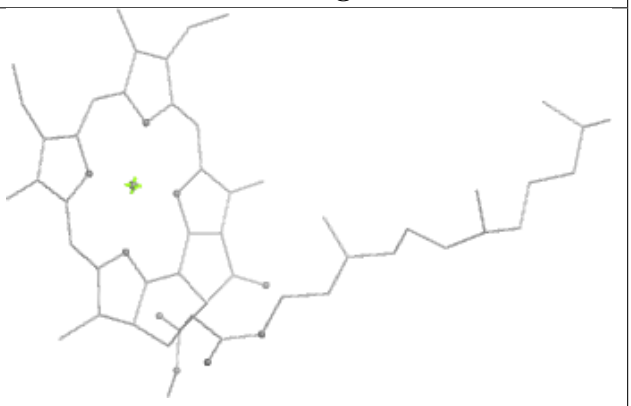
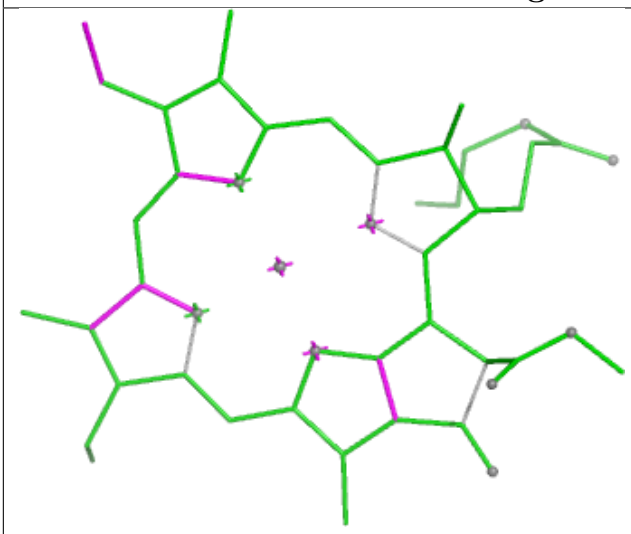


Rings

Ligand CLA y 314



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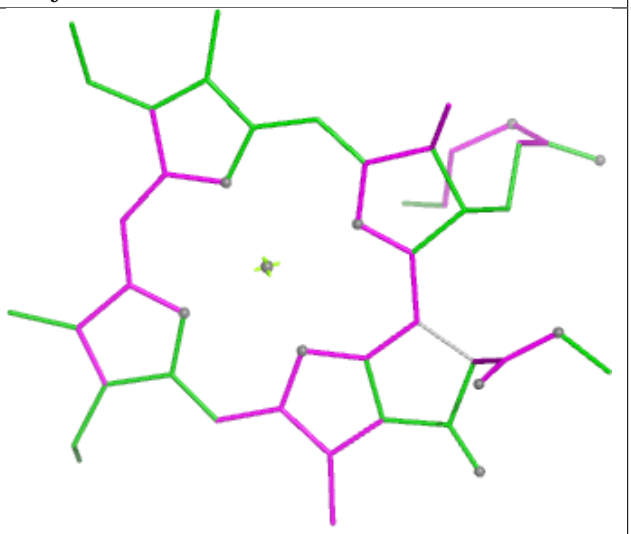
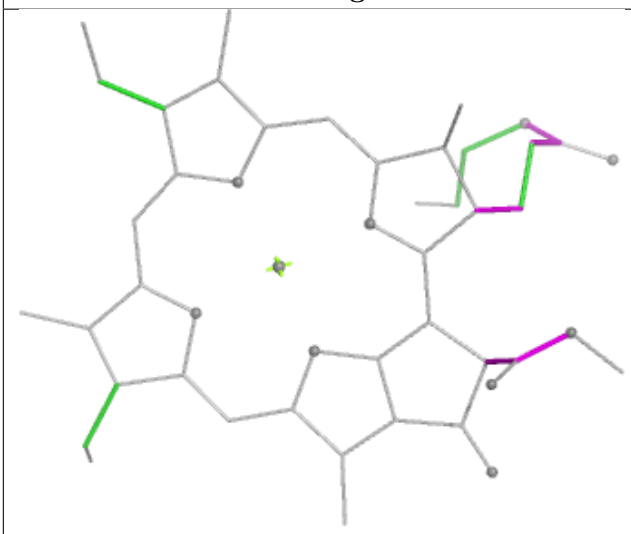


Bond angles



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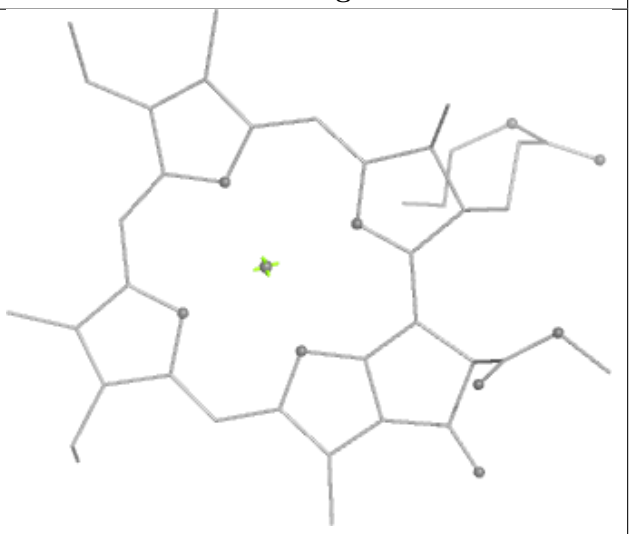
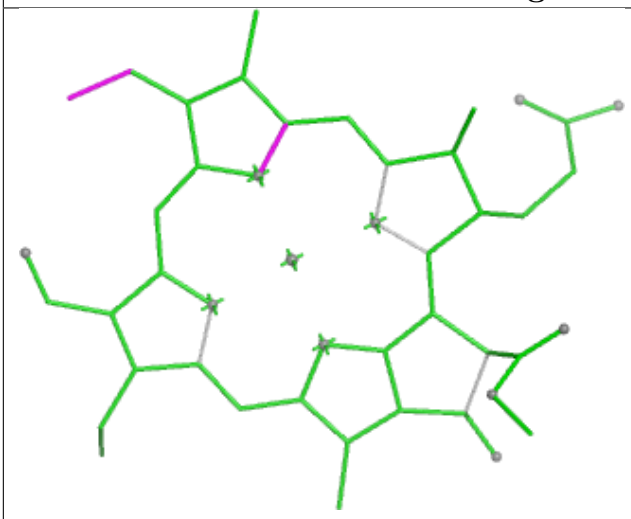


Rings

Ligand CHL g 605



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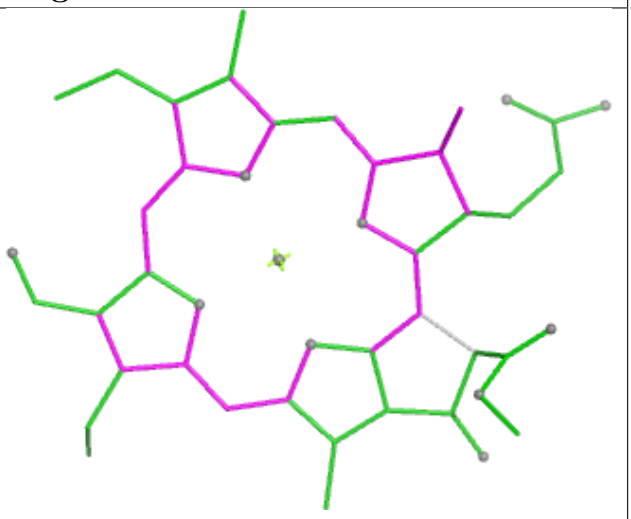
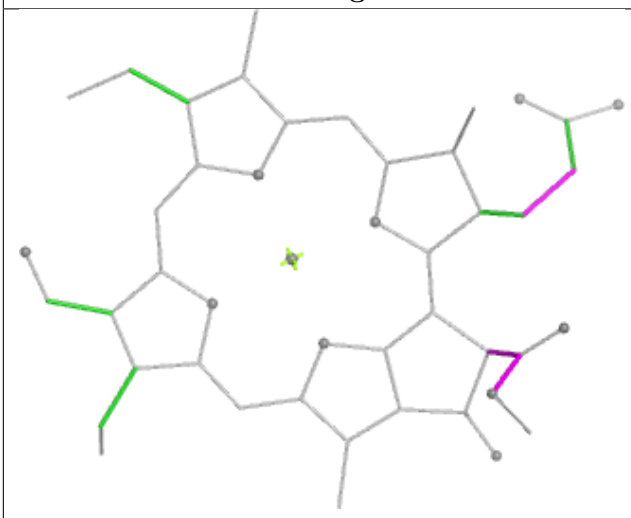


Bond angles



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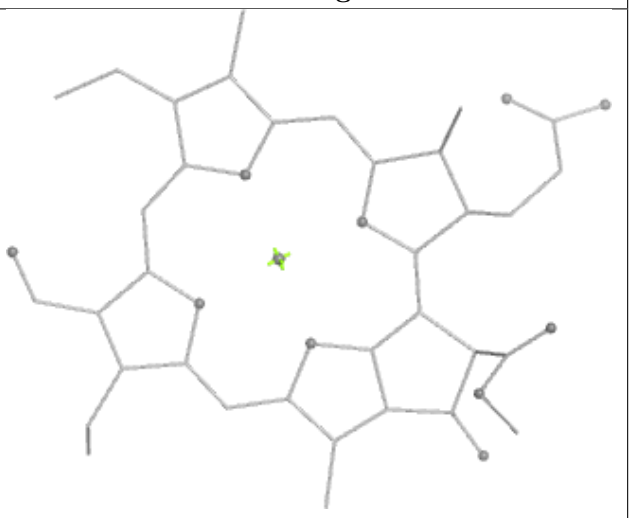
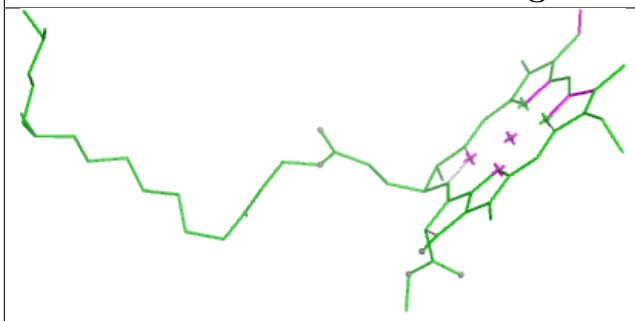


Rings

Ligand CLA d 404



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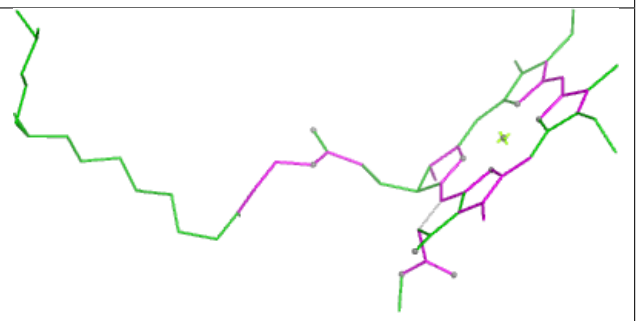
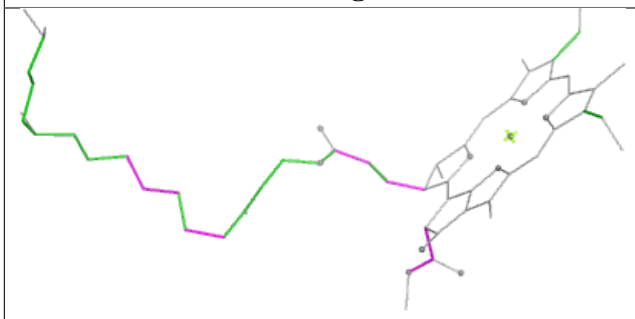


Bond angles



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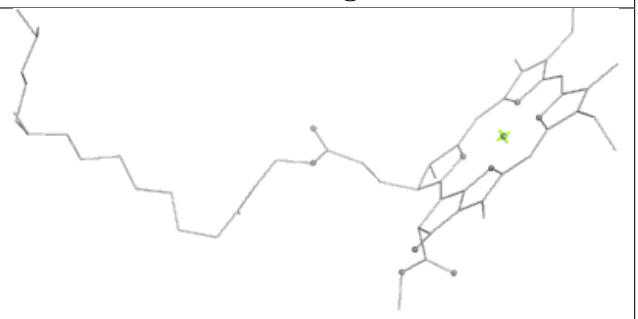
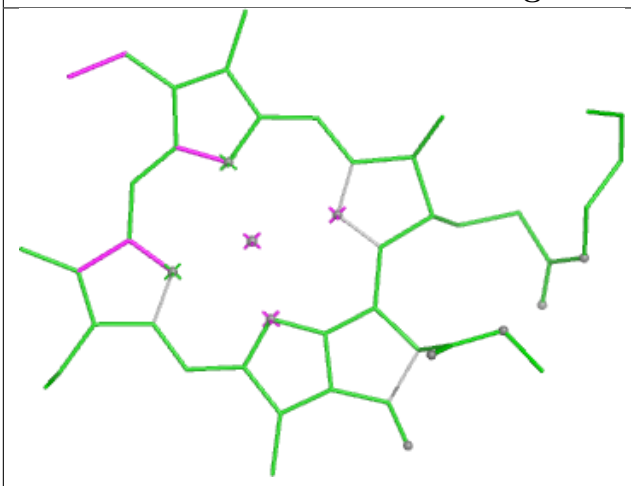


Rings

Ligand CLA R 611



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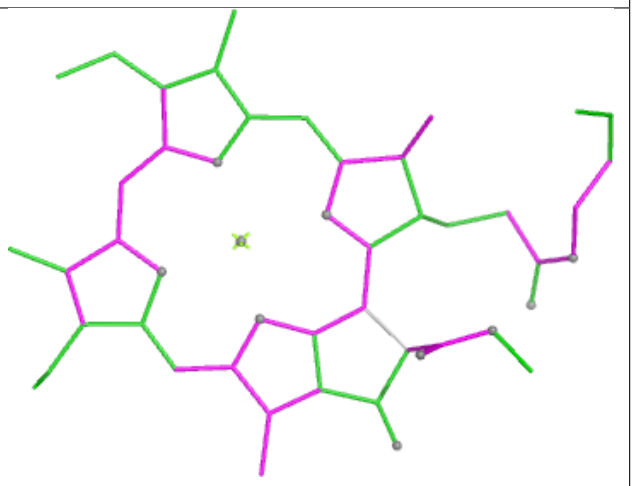
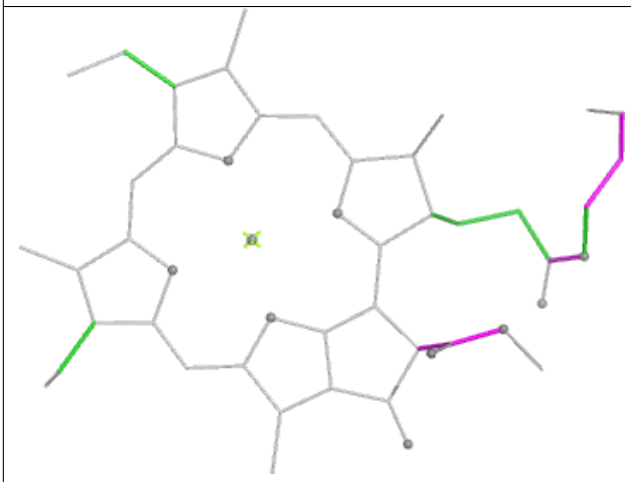


Bond angles



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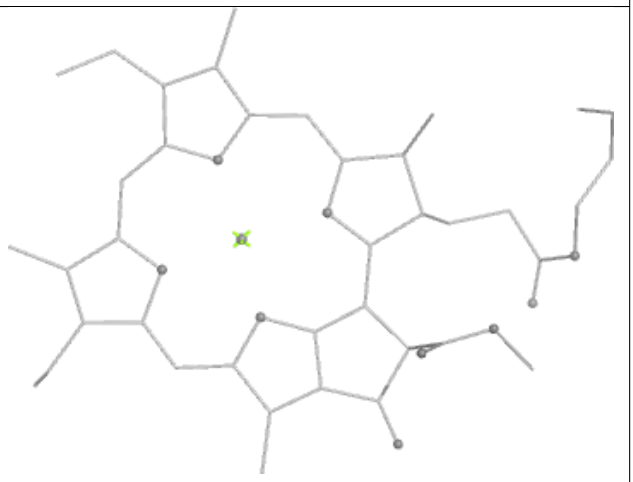
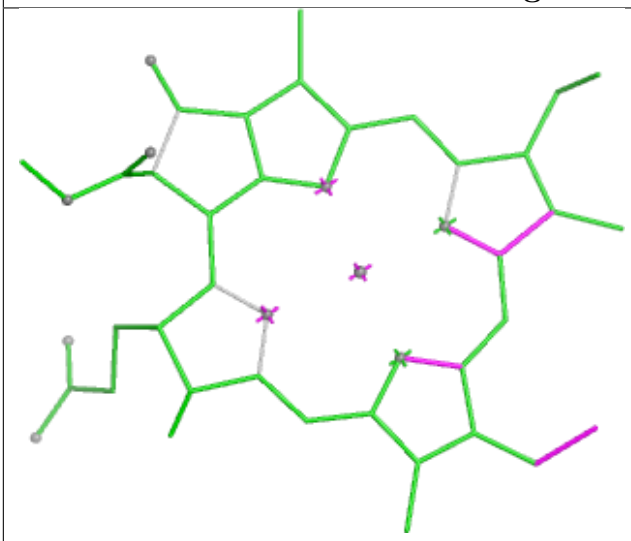


Rings

Ligand CLA R 601



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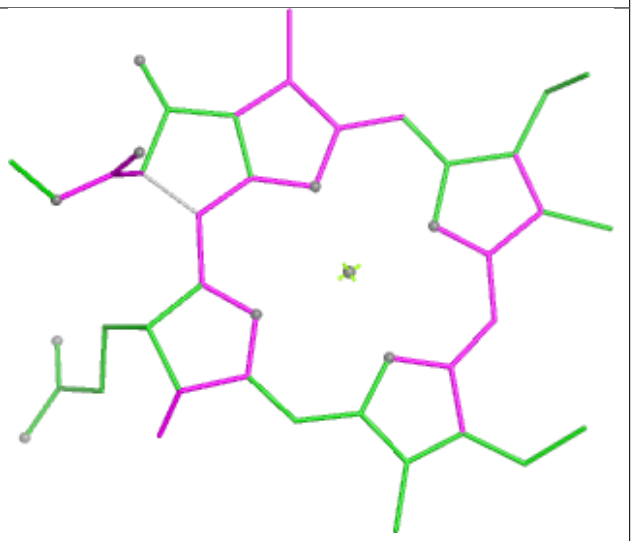
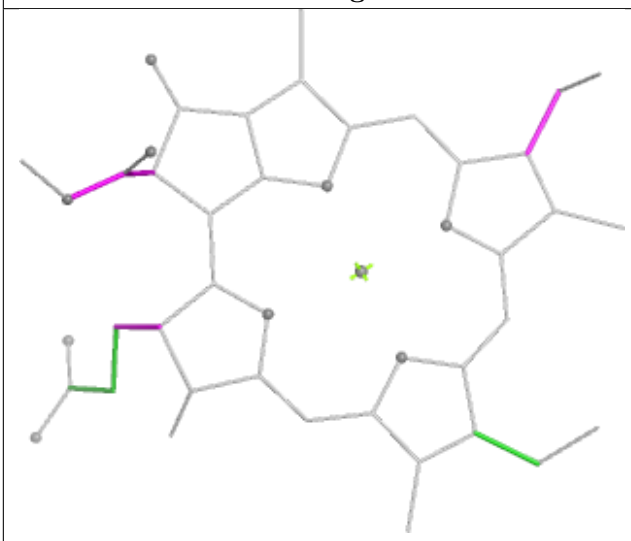


Bond angles



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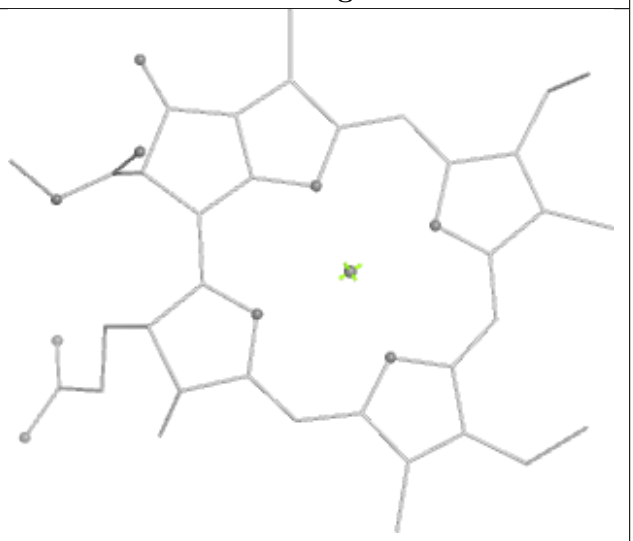
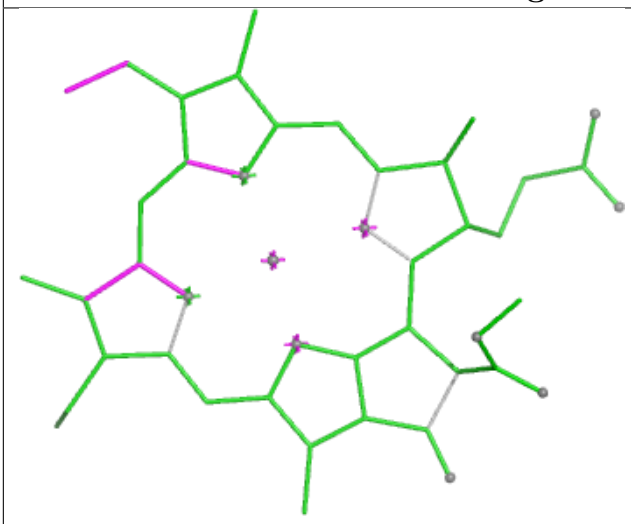
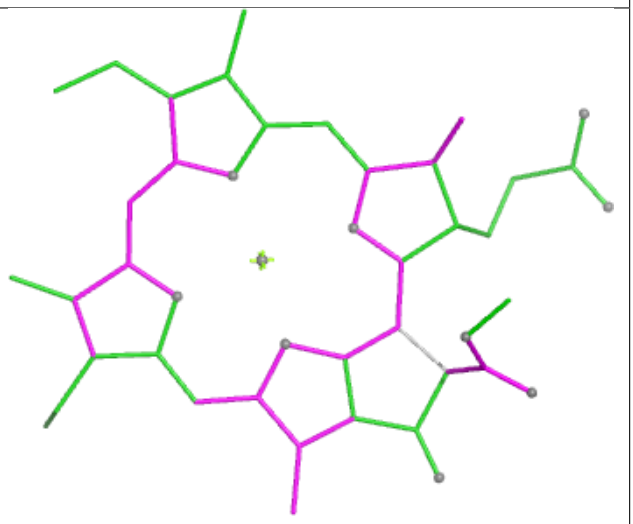


Rings

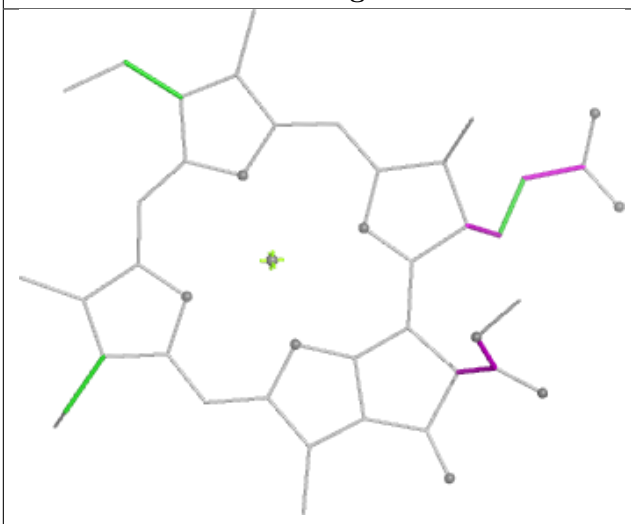
Ligand CLA S 304



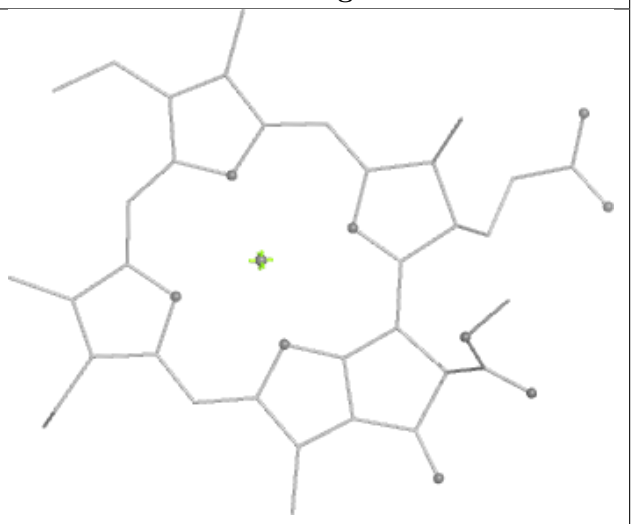
Bond lengths



Bond angles

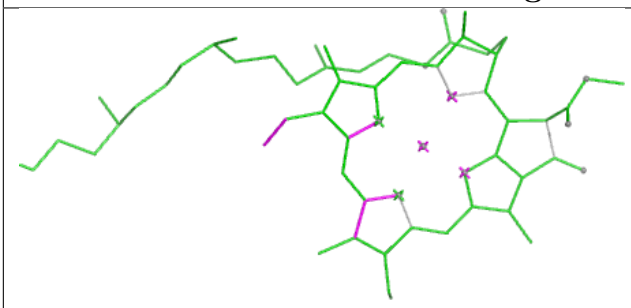


Torsions



Rings

Ligand CLA C 501



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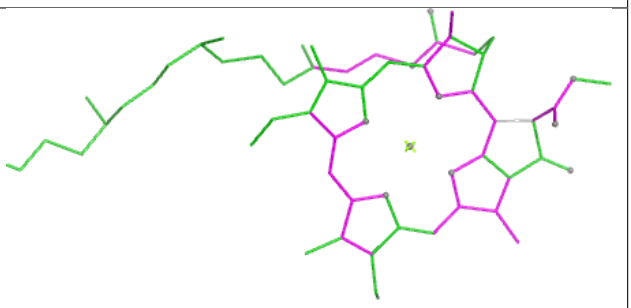

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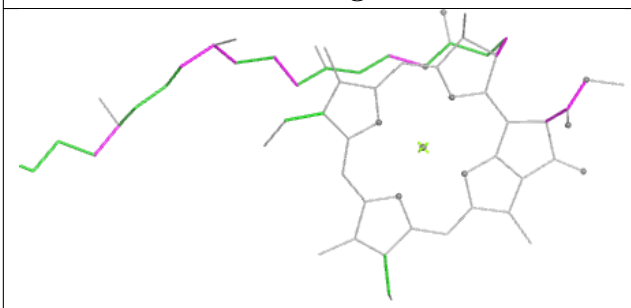

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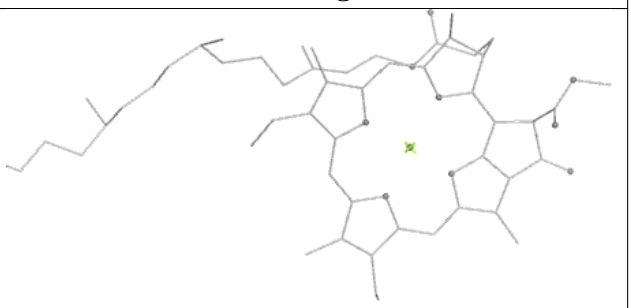
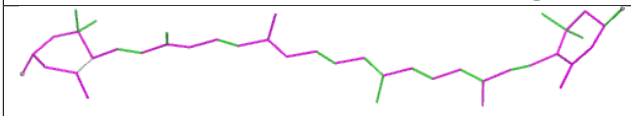


Rings

Ligand LUT y 316



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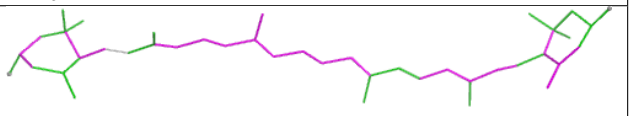
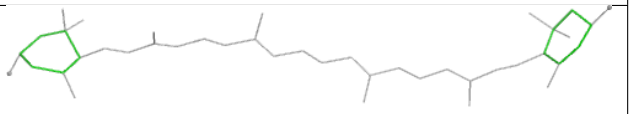


Bond angles

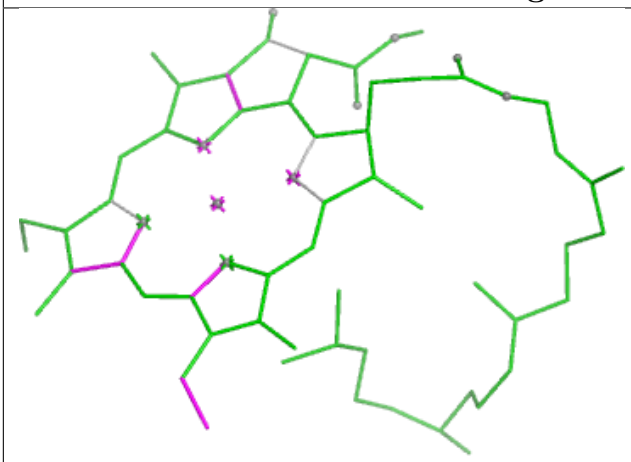


Torsions



Rings

Ligand CLA b 615



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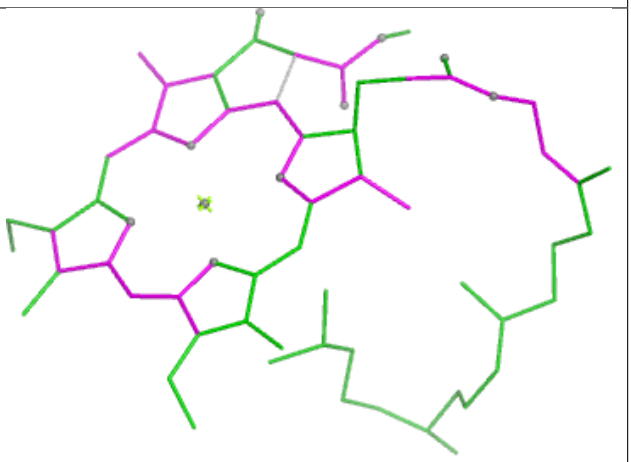

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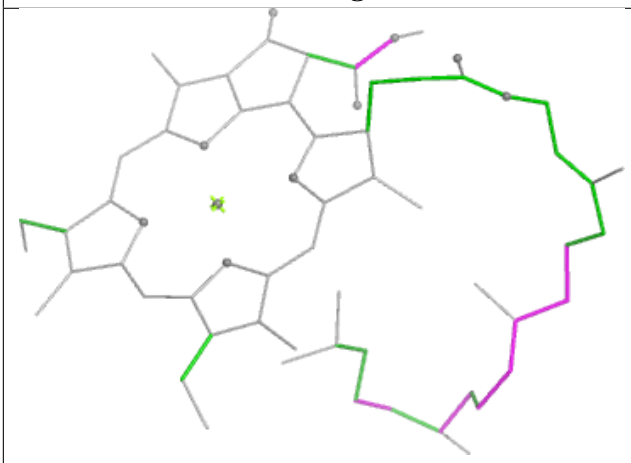

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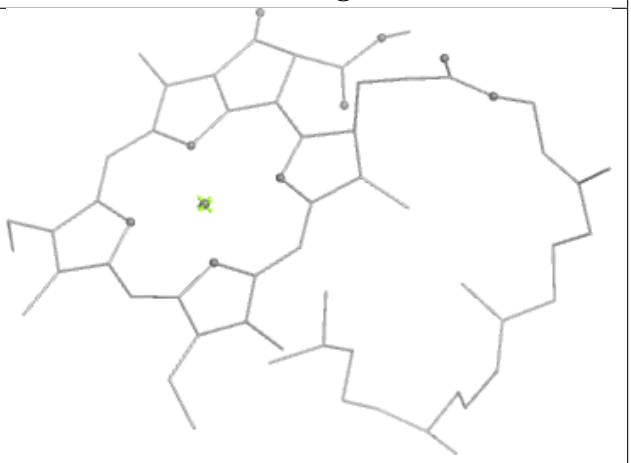
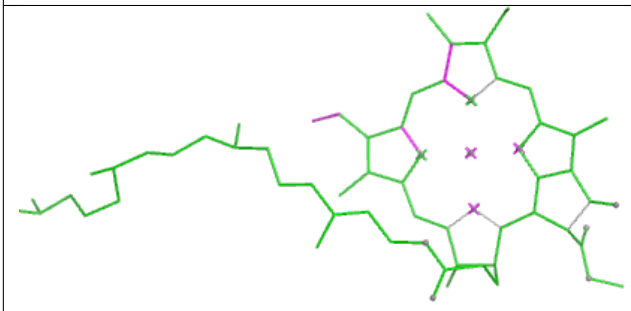


Rings

Ligand CLA B 603



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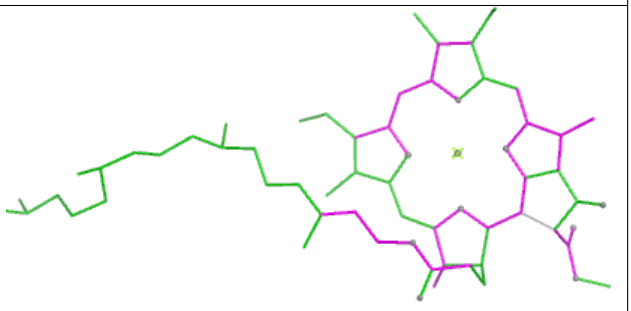
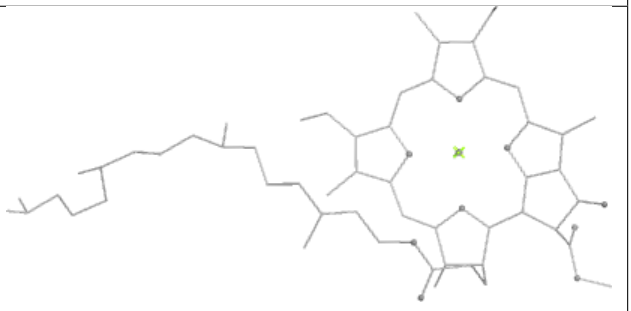


Bond angles

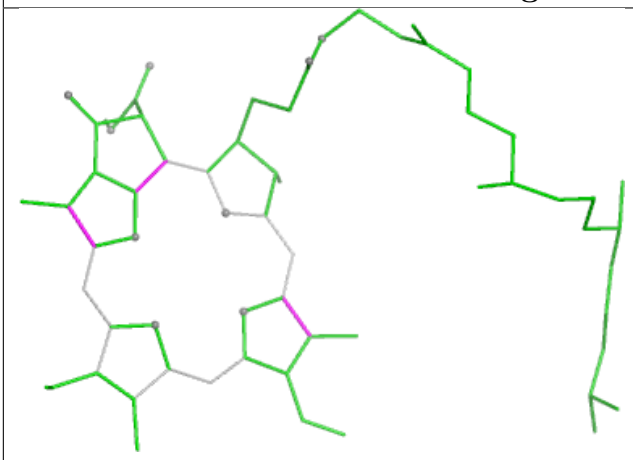


Torsions



Rings

Ligand PHO D 402



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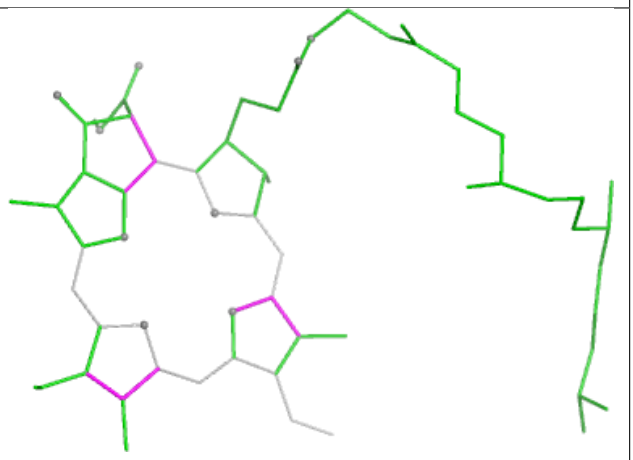
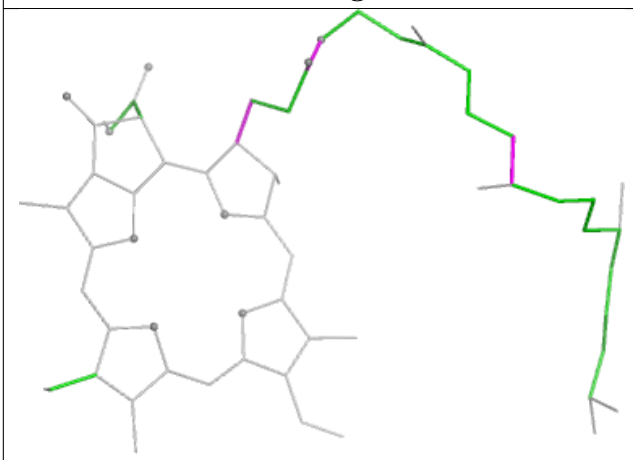


Bond angles



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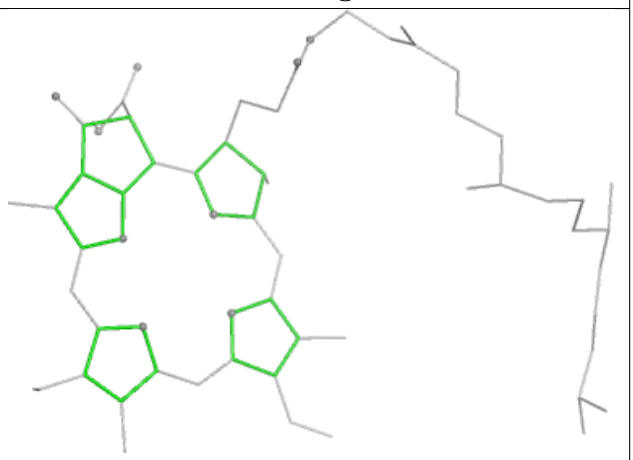
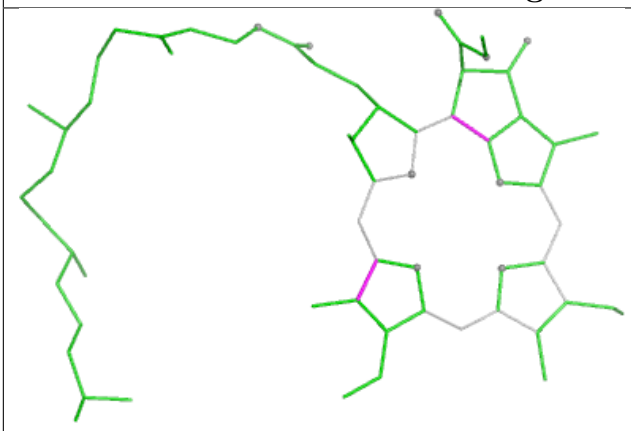


Rings

Ligand PHO a 408



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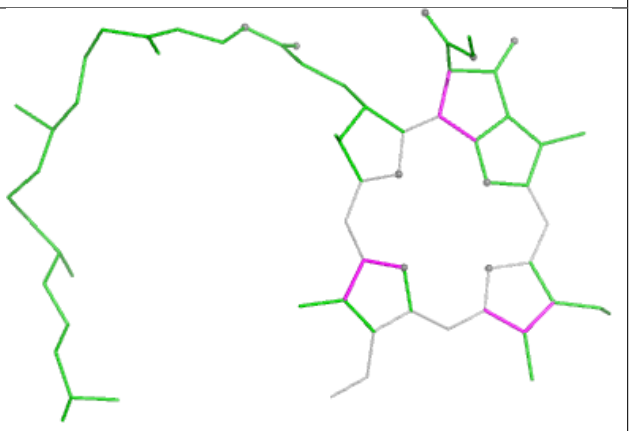
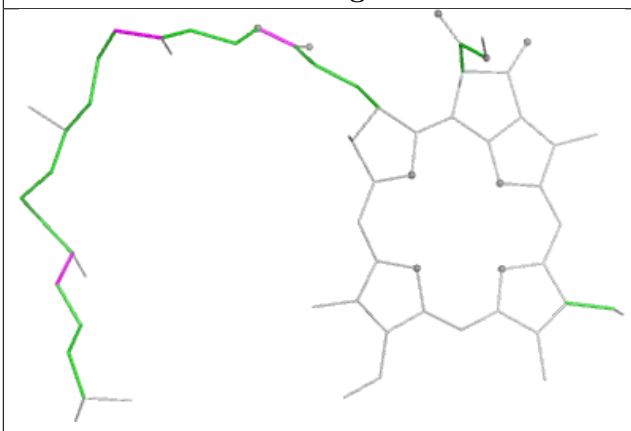


Bond angles



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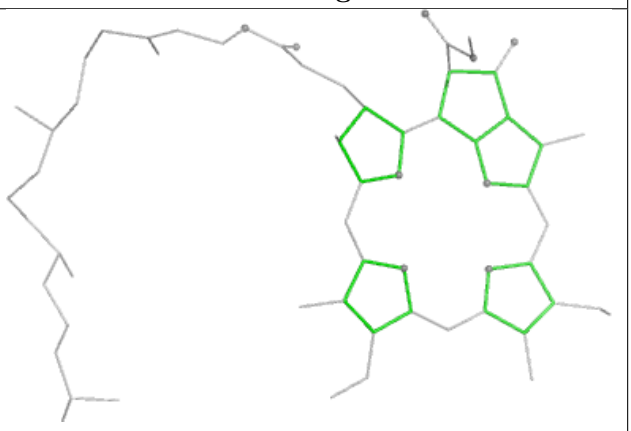
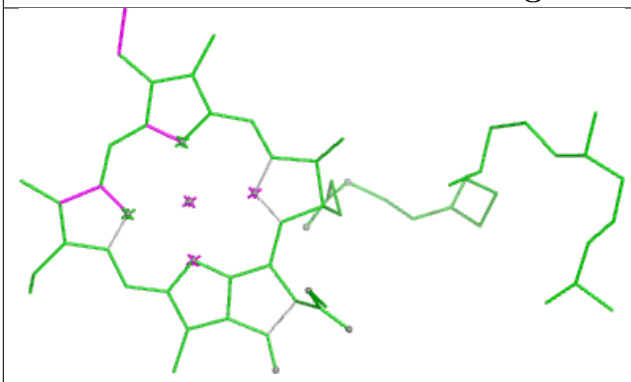


Rings

Ligand CLA B 612



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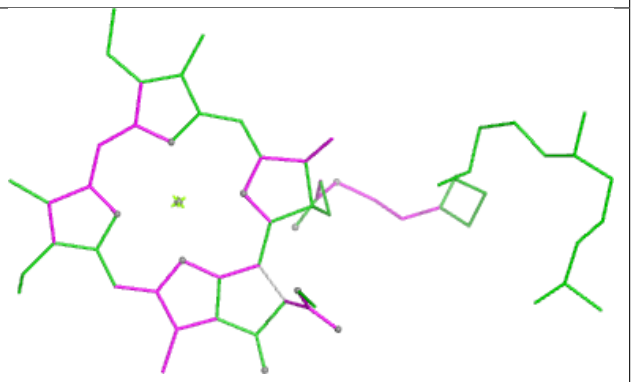
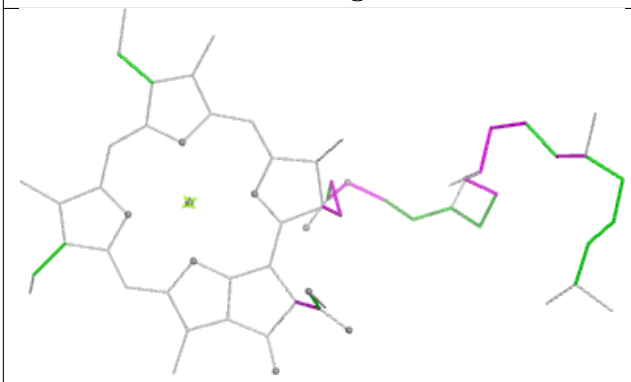


Bond angles



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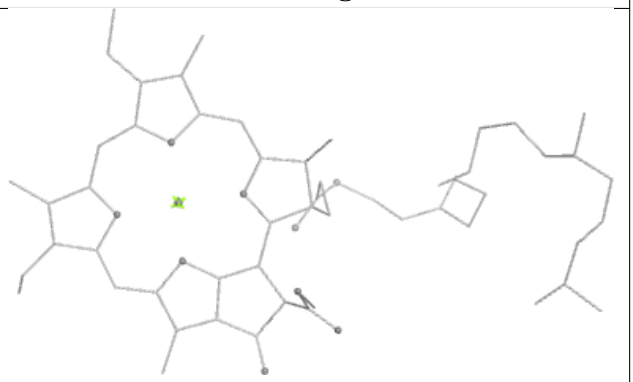
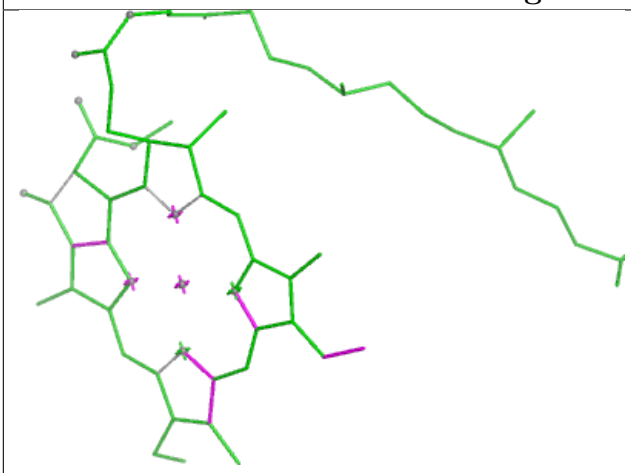


Rings

Ligand CLA B 616



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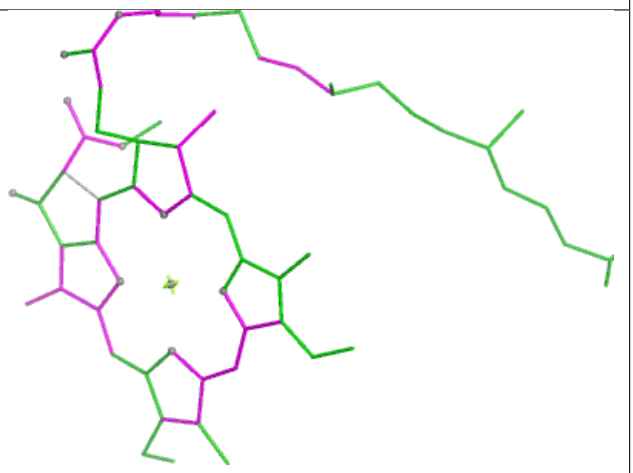
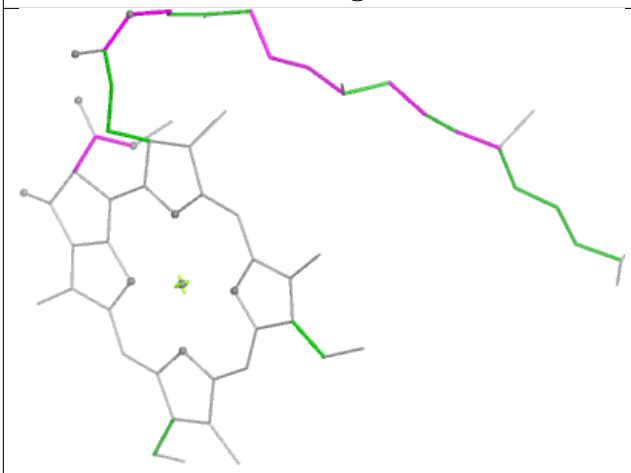


Bond angles



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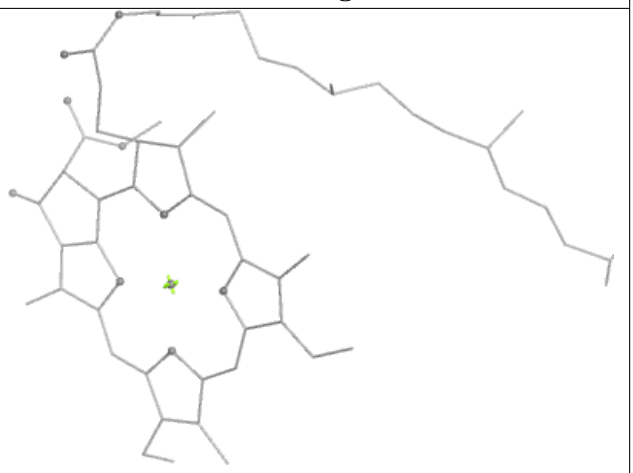
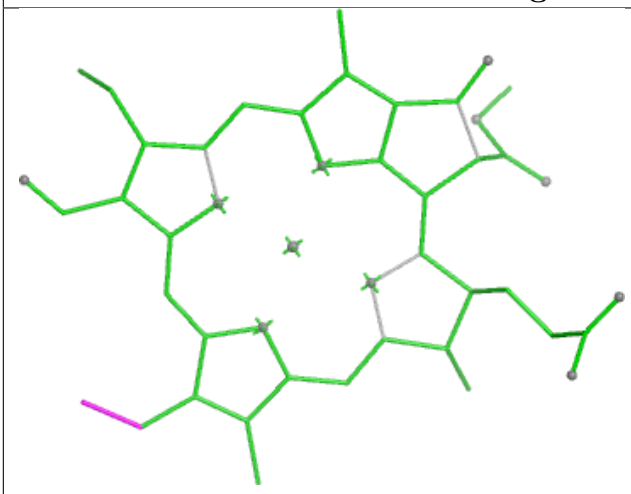


Rings

Ligand CHL s 605



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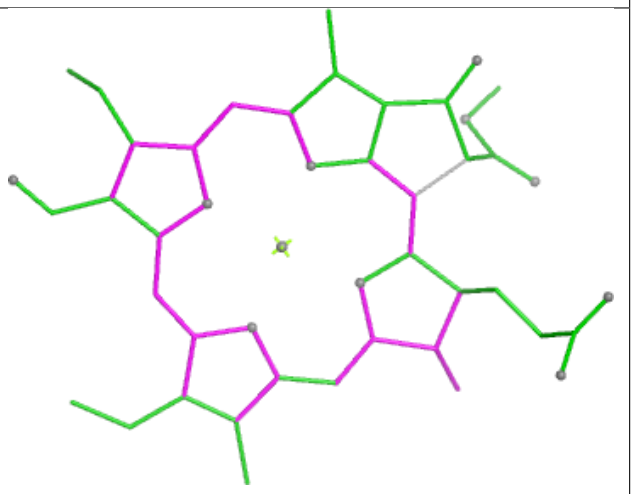
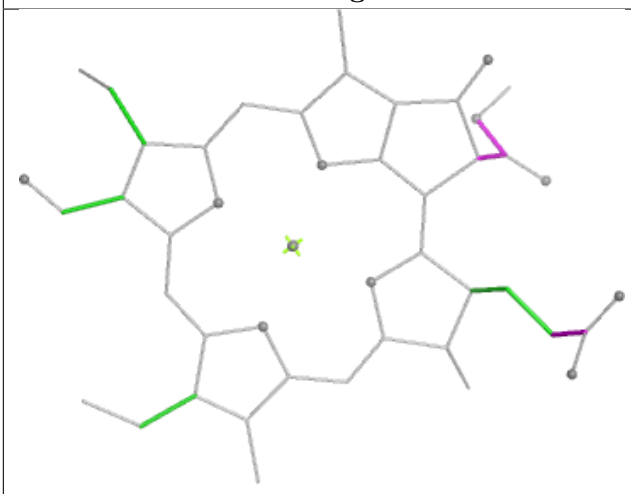


Bond angles



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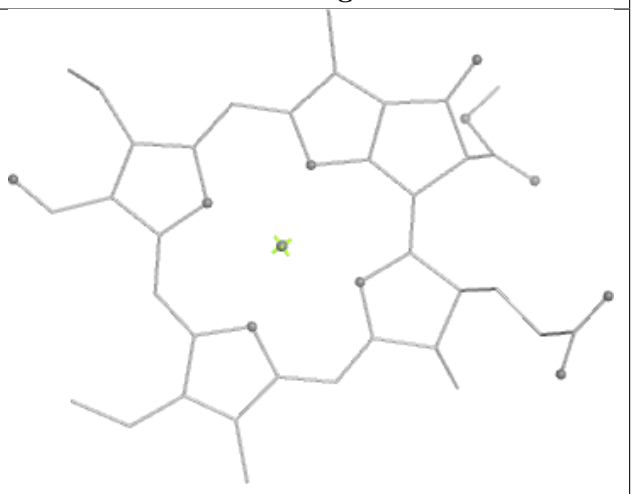
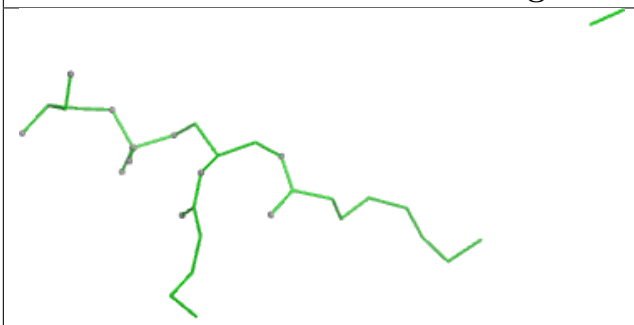


Rings

Ligand LHG c 519



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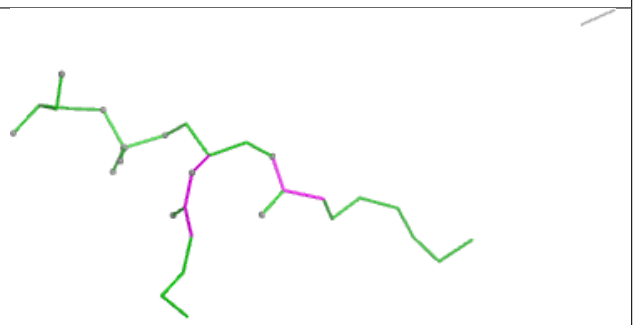

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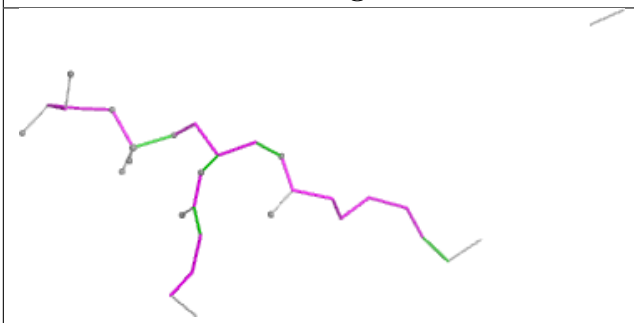

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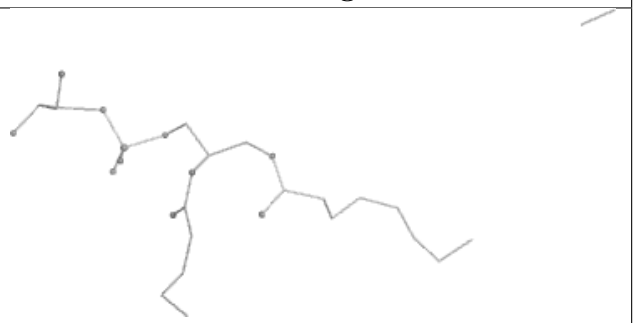
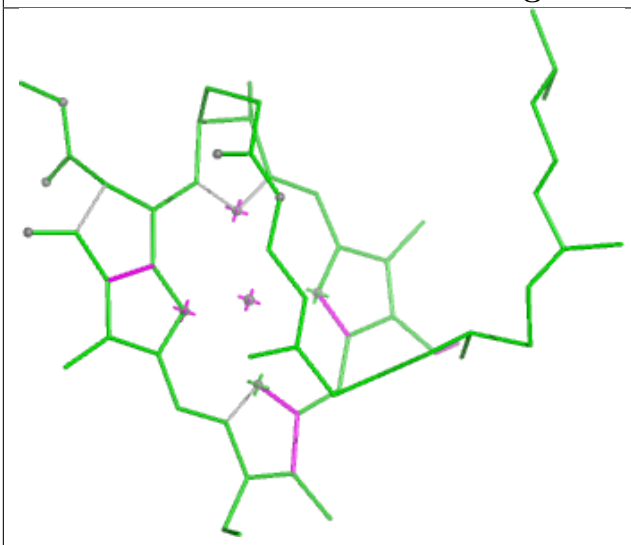


Rings

Ligand CLA Y 613



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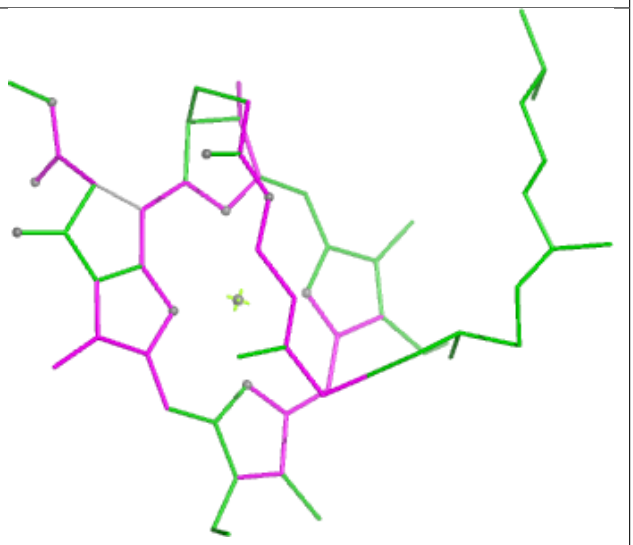

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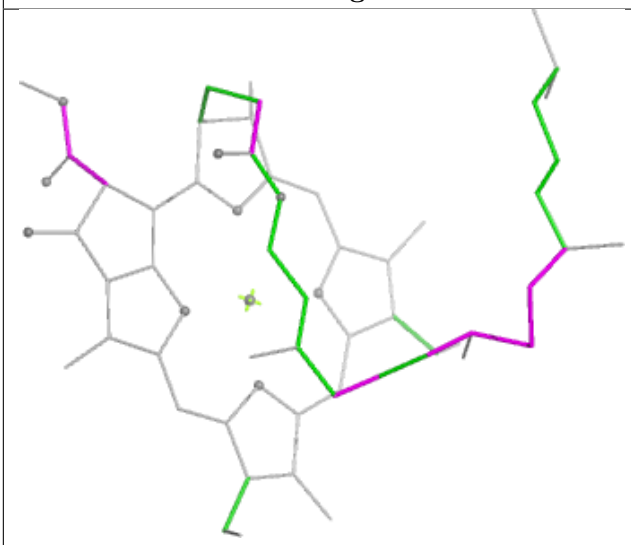

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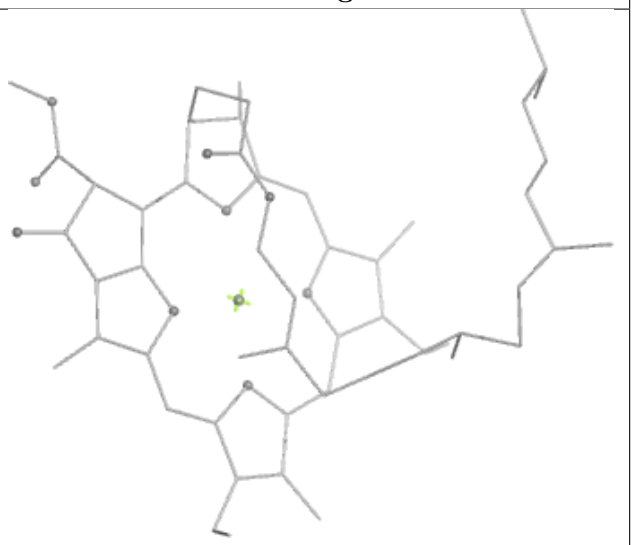
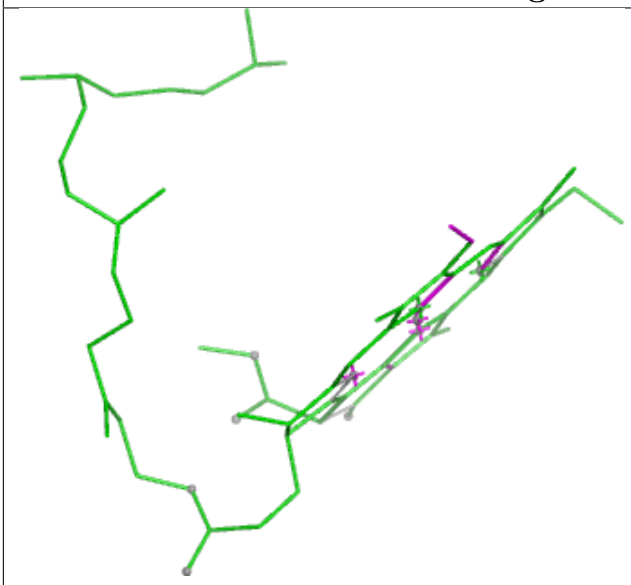


Rings

Ligand CLA g 603



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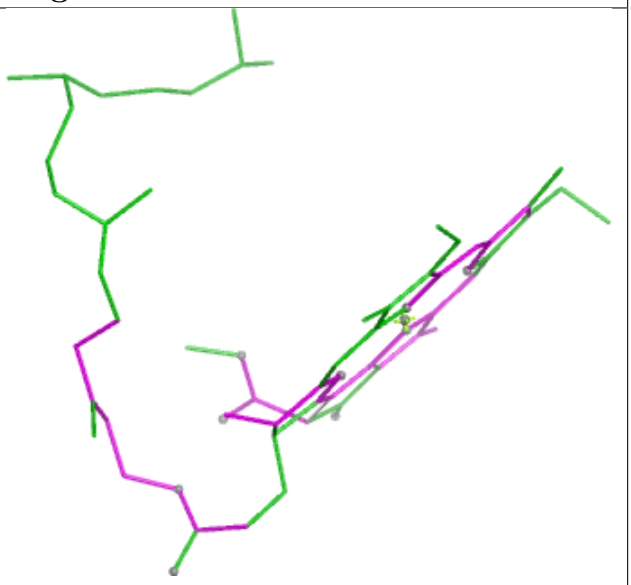
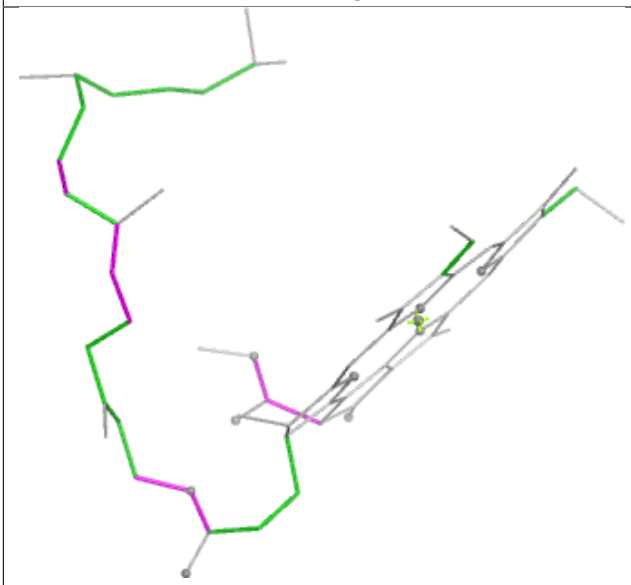


Bond angles

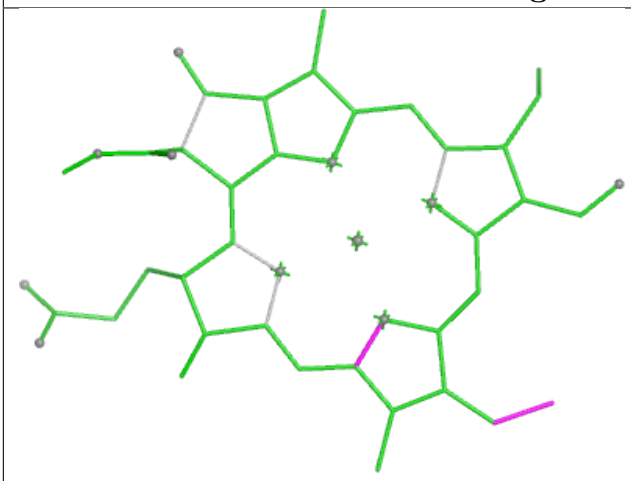


Torsions



Rings

Ligand CHL s 601



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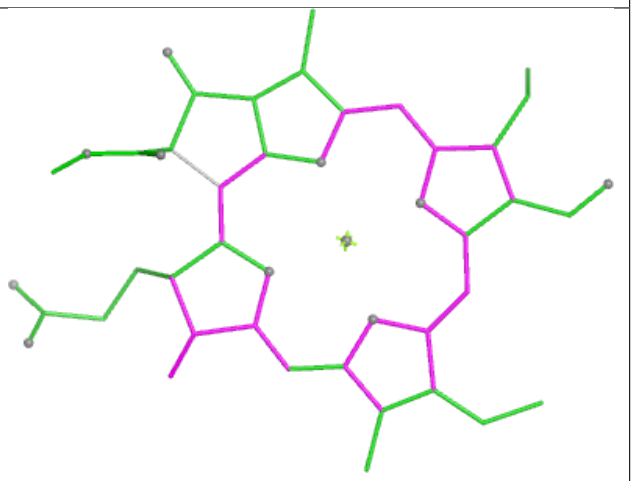
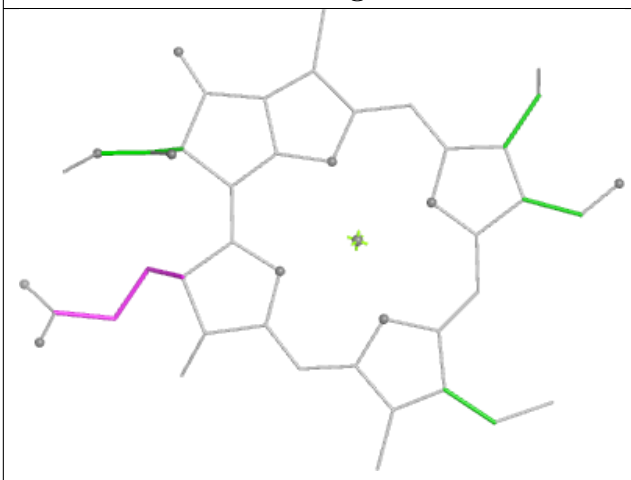


Bond angles



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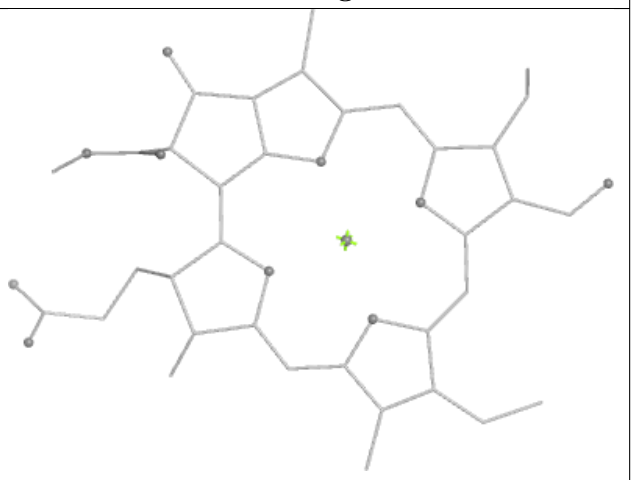
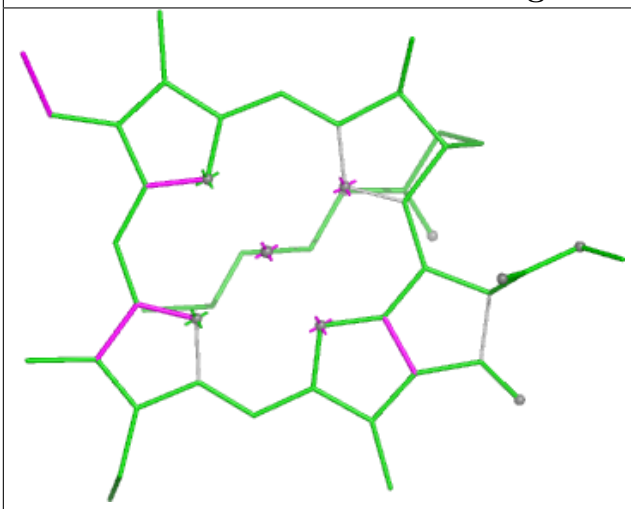


Rings

Ligand CLA S 314



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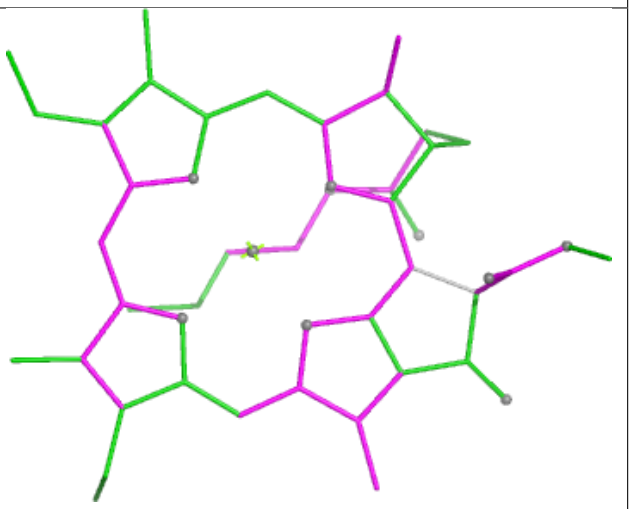
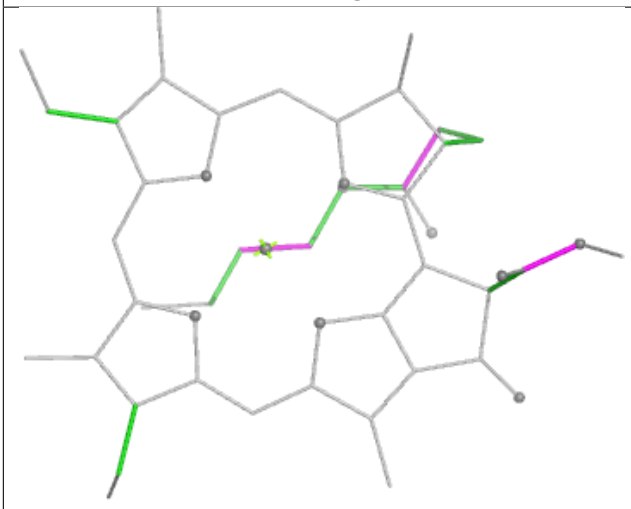


Bond angles



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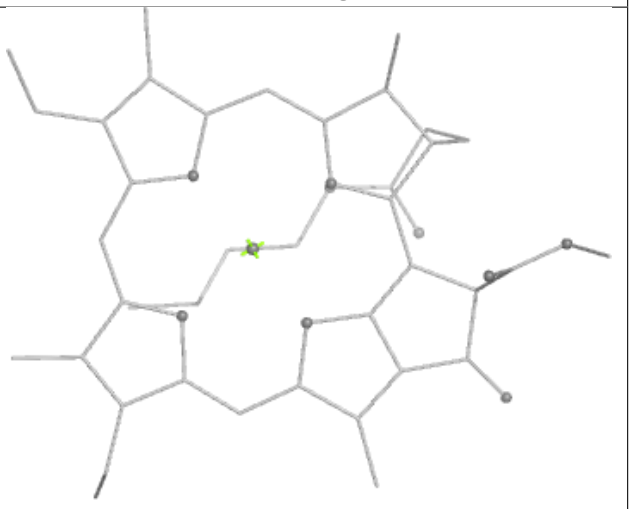
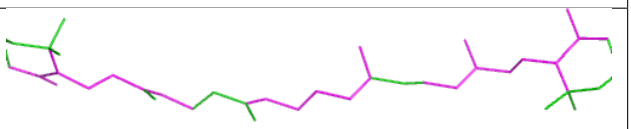


Rings

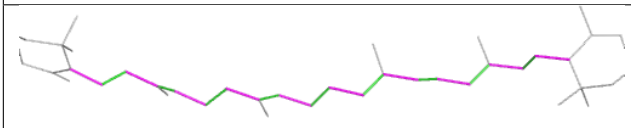
Ligand BCR C 516



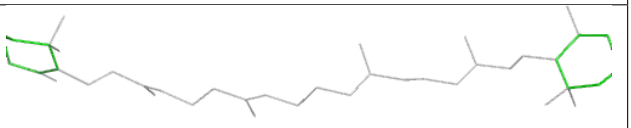
Bond lengths



Bond angles

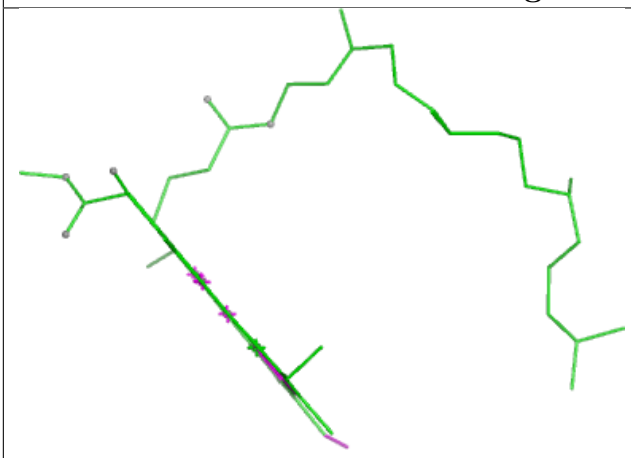


Torsions



Rings

Ligand CLA B 611



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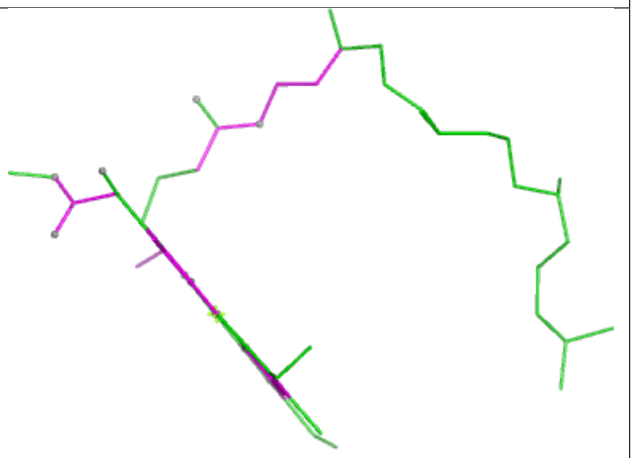


Bond angles

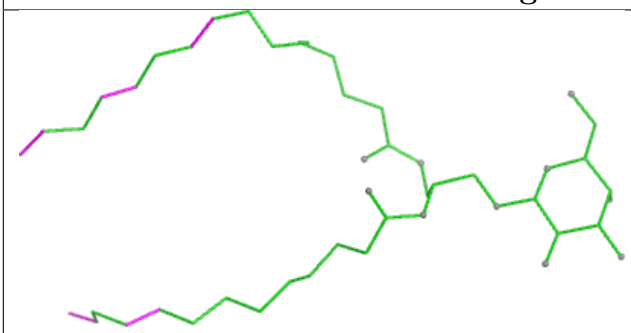


Torsions



Rings

Ligand LMG w 101



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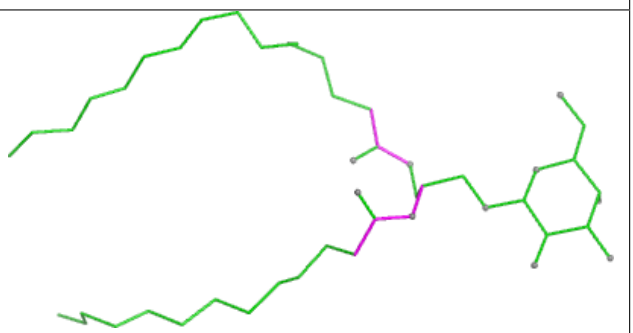
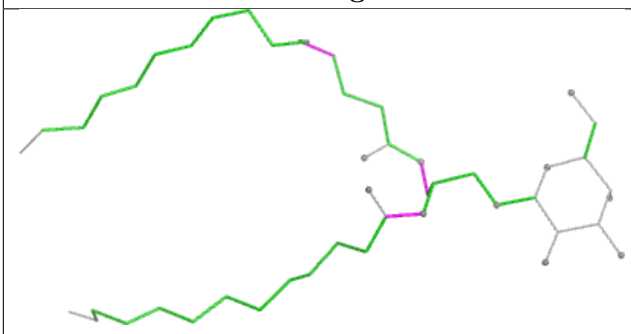


Bond angles



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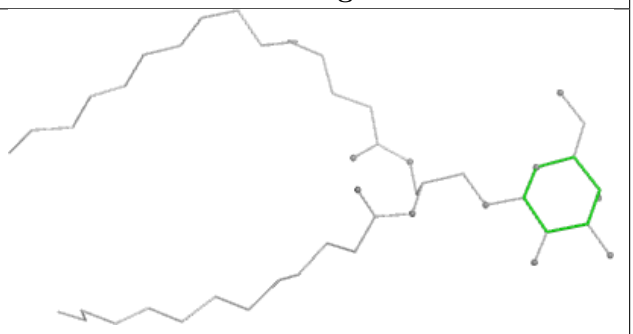
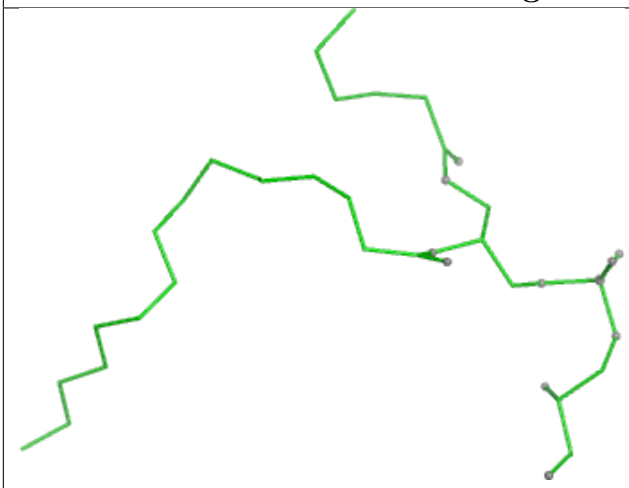


Rings

Ligand LHG w 102



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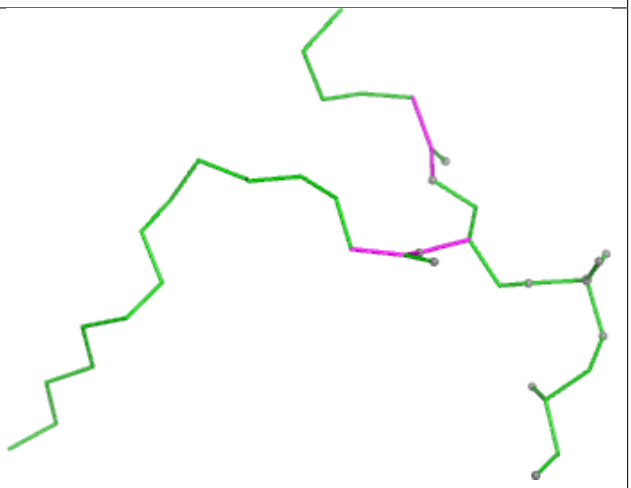
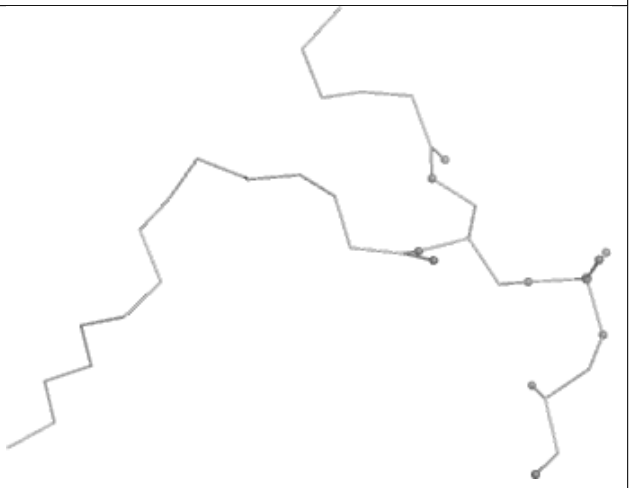


Bond angles

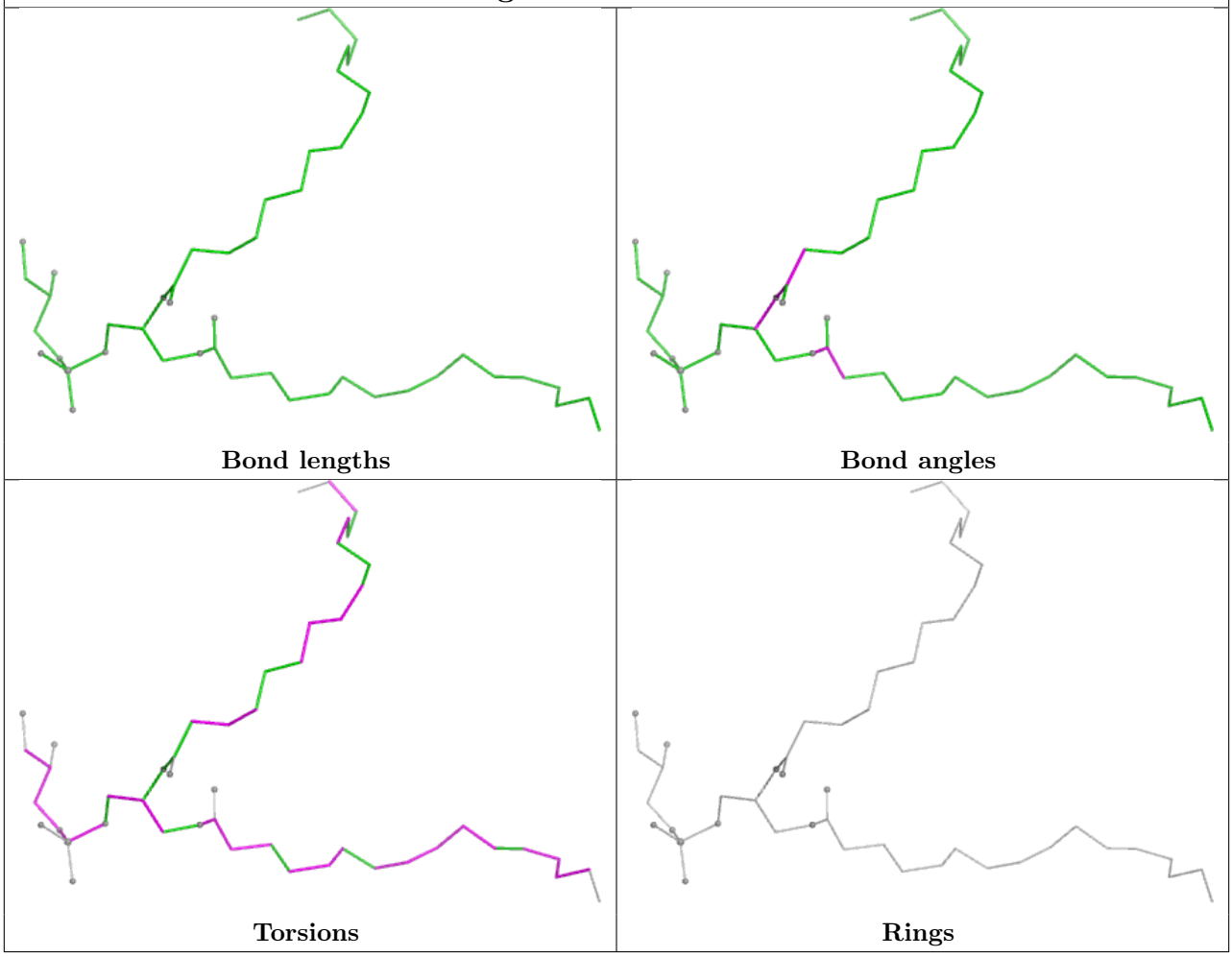


Torsions

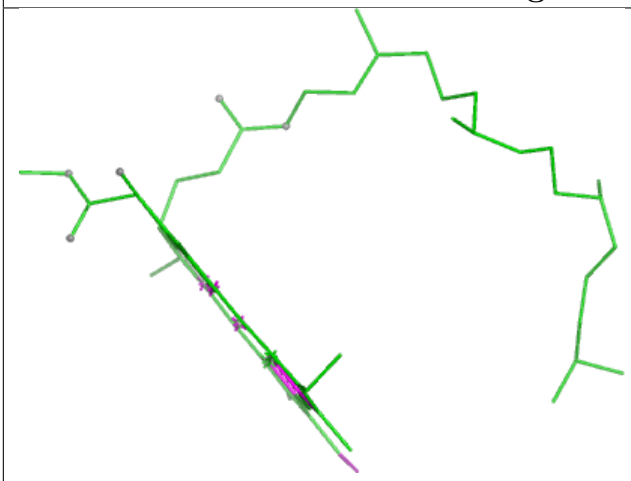


Rings

Ligand LHG W 101



Ligand CLA b 611



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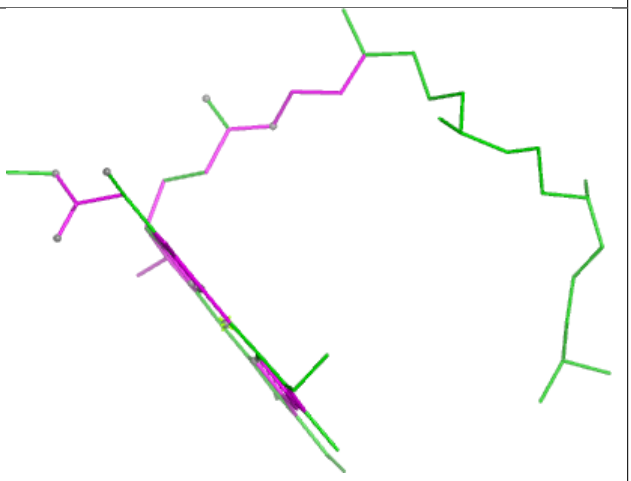
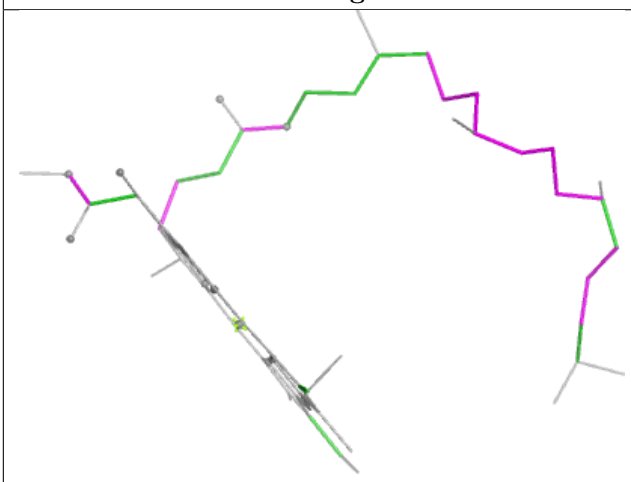


Bond angles



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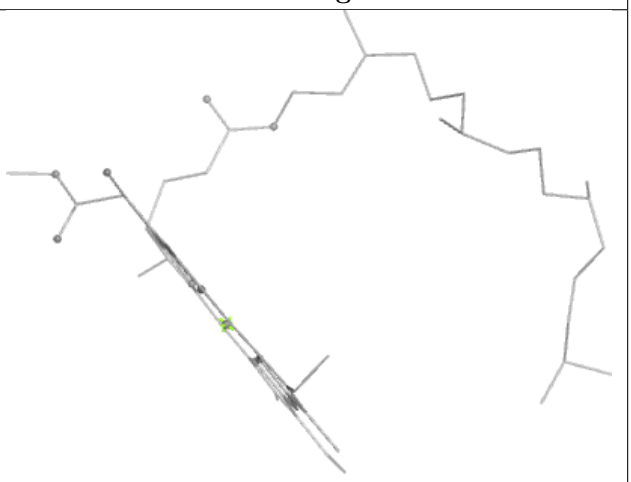
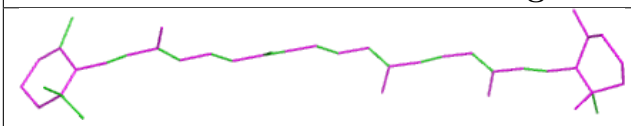


Rings

Ligand BCR c 514



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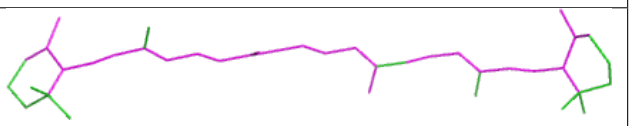
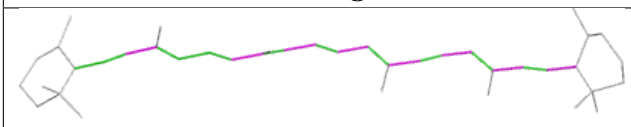


Bond angles



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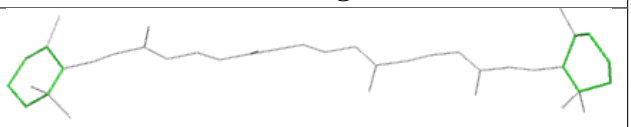
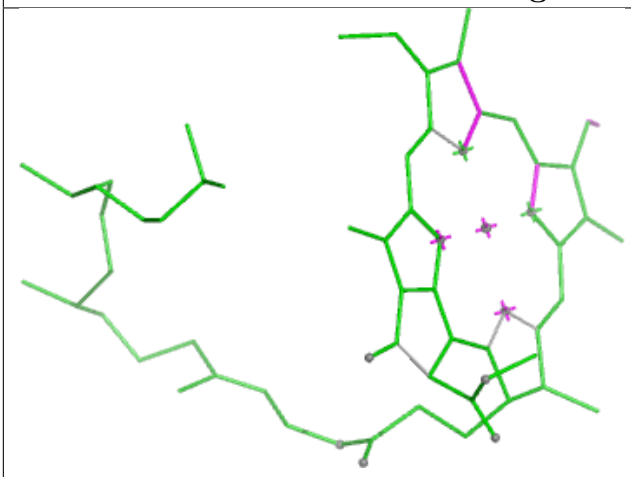


Rings

Ligand CLA c 503



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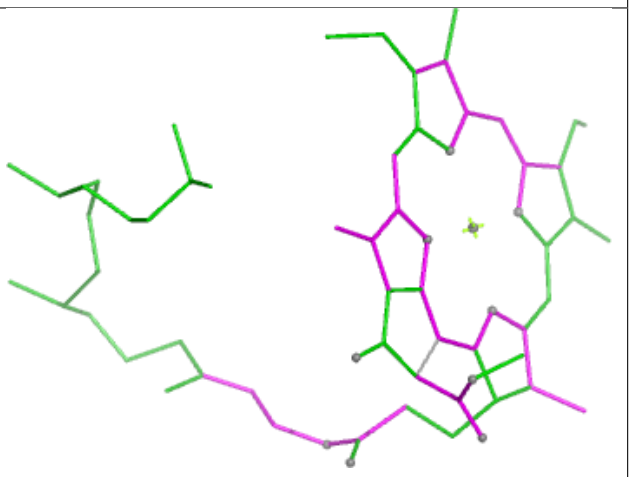

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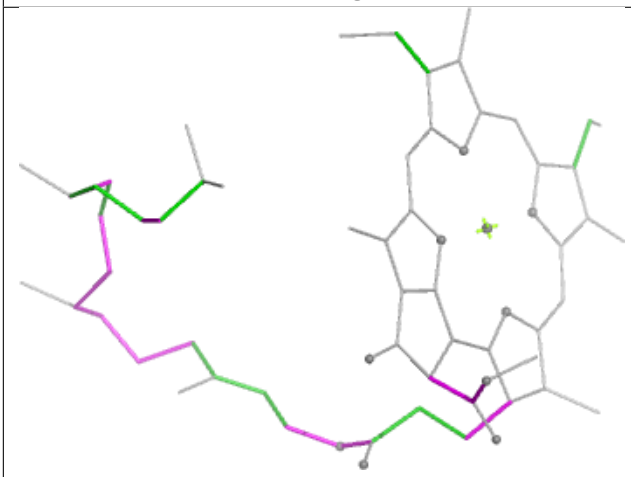

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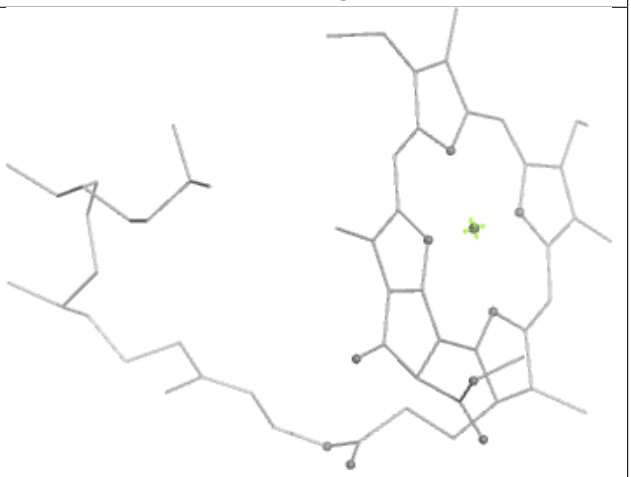
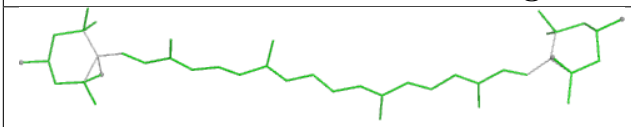


Rings

Ligand XAT Y 617



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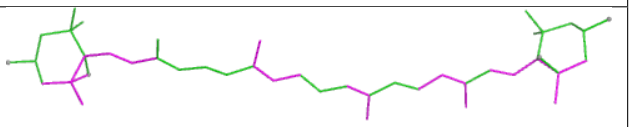
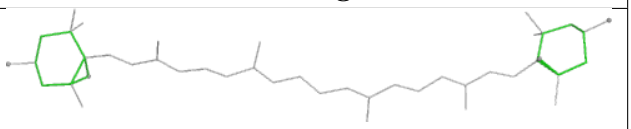


Bond angles

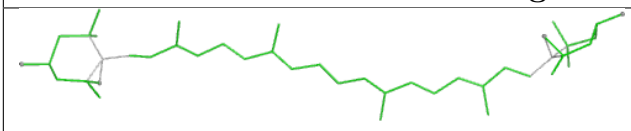


Torsions



Rings

Ligand XAT r 615



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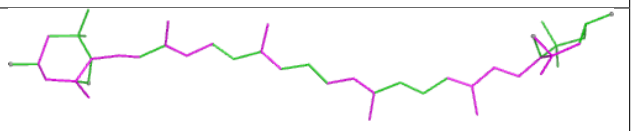
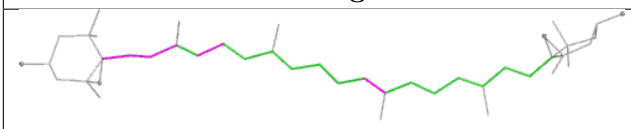


Bond angles



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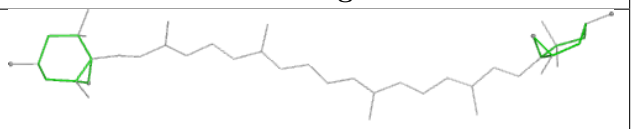
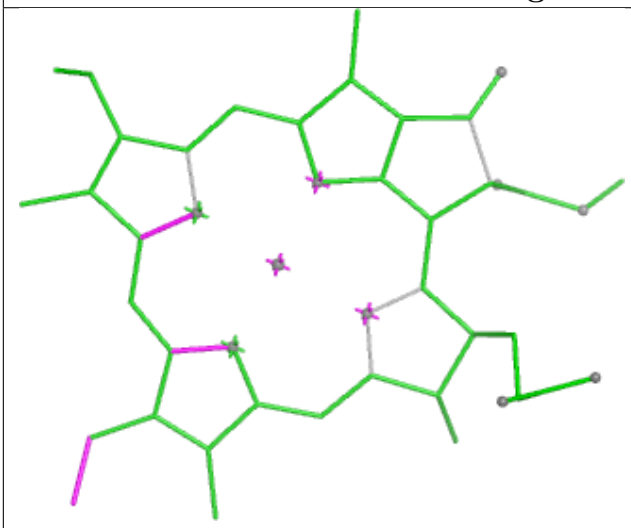


Rings

Ligand CLA S 309



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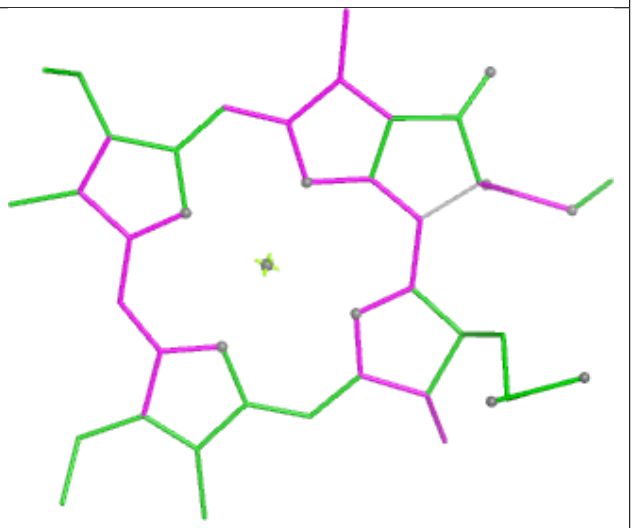
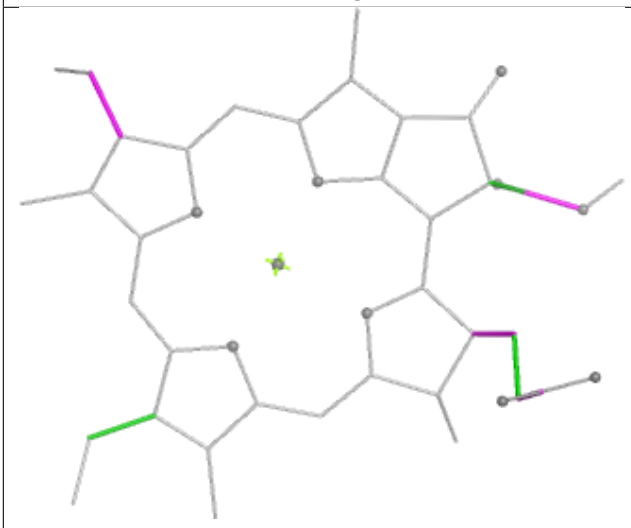


Bond angles



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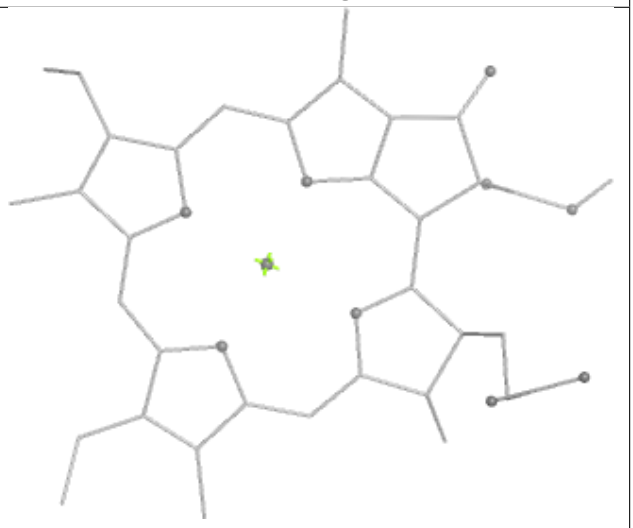
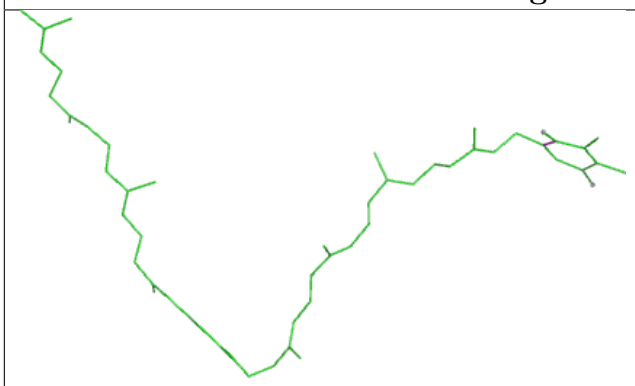


Rings

Ligand PL9 D 406



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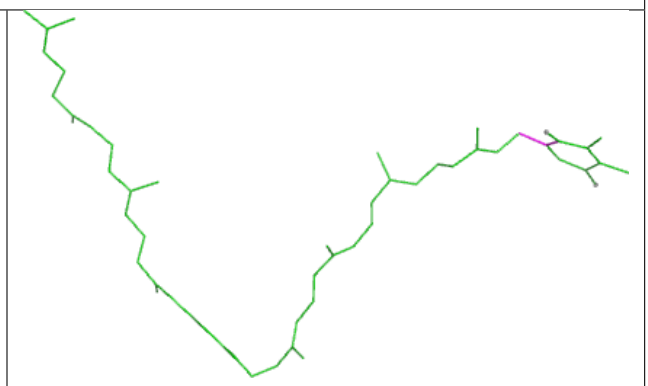
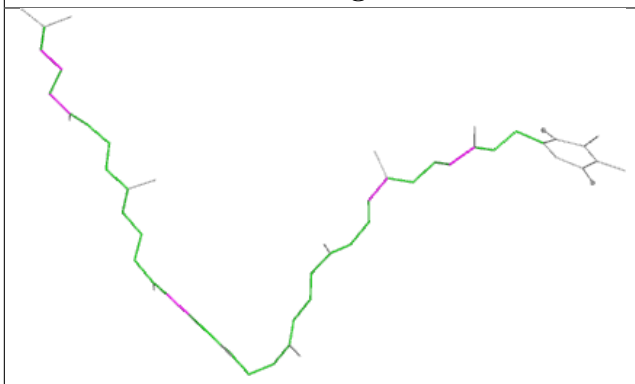


Bond angles



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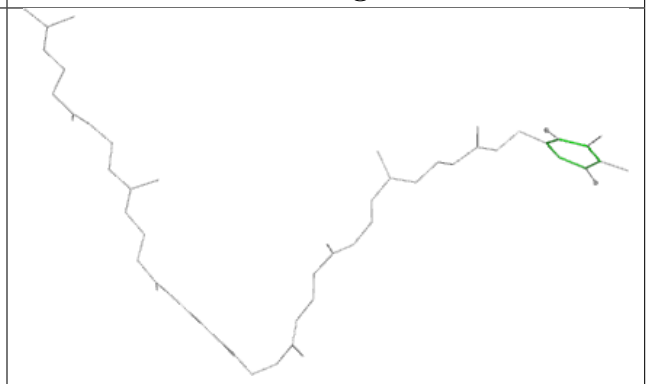
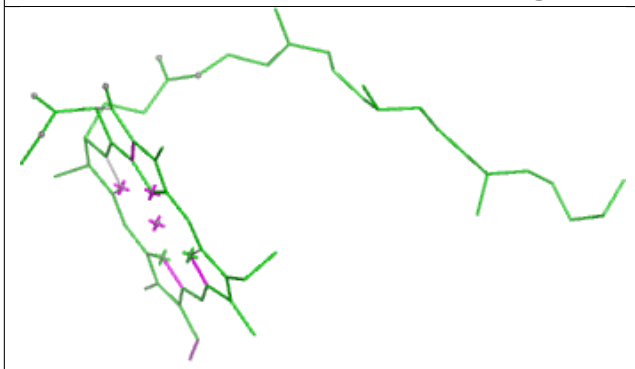


Rings

Ligand CLA c 508



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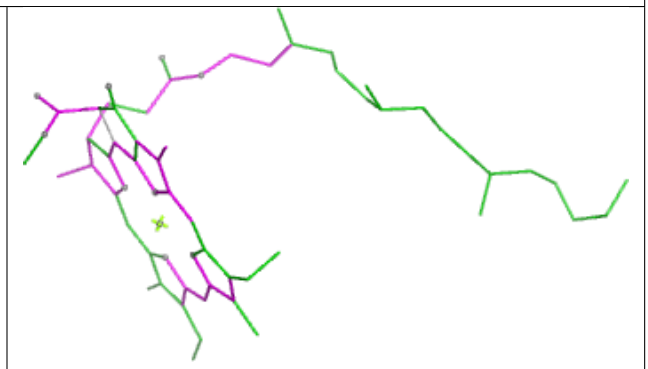
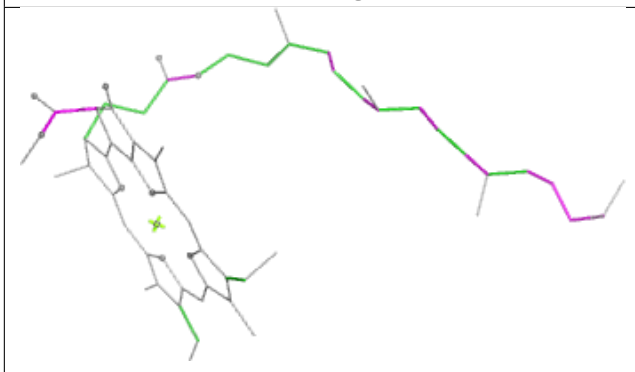


Bond angles



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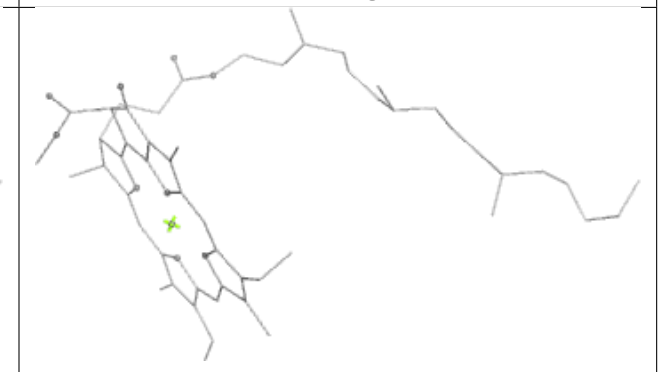
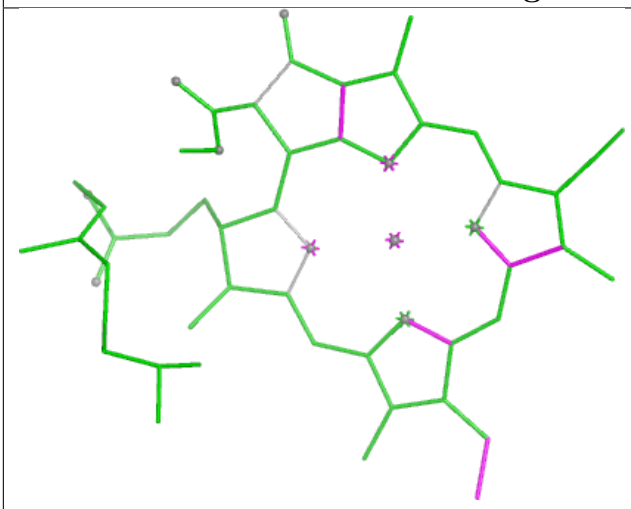


Rings

Ligand CLA N 603



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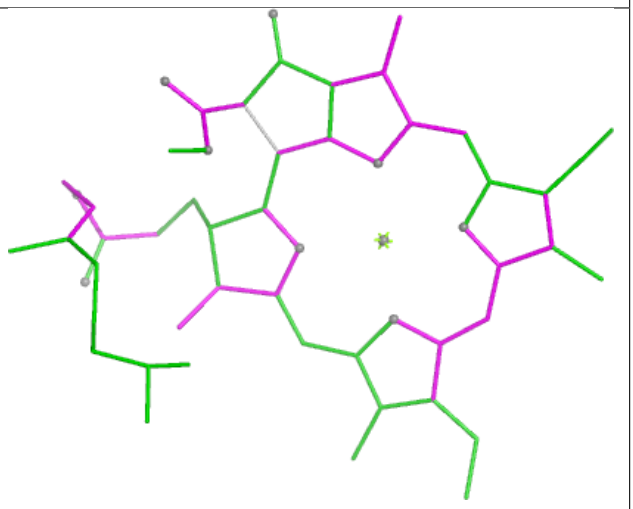
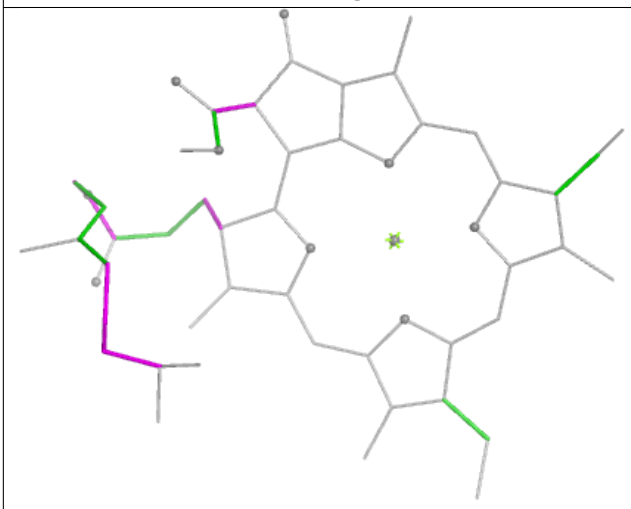


Bond angles



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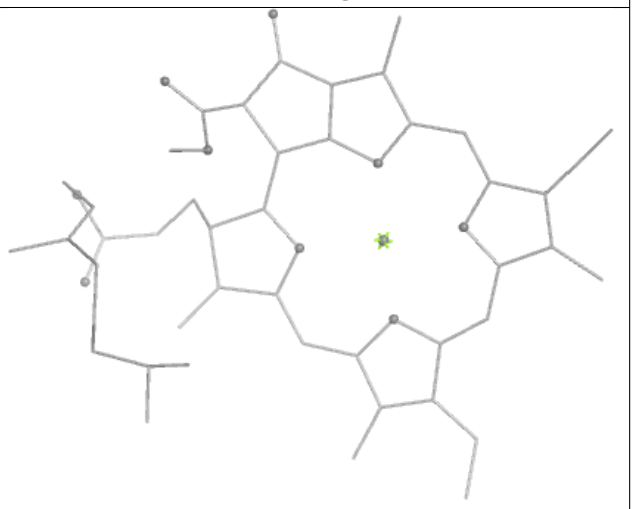
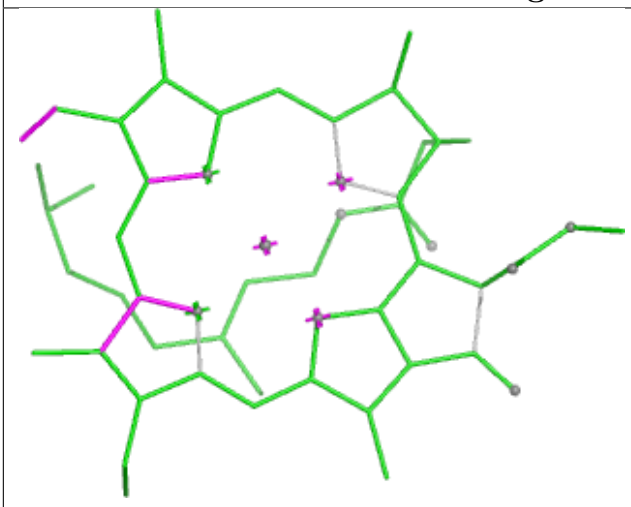


Rings

Ligand CLA S 313



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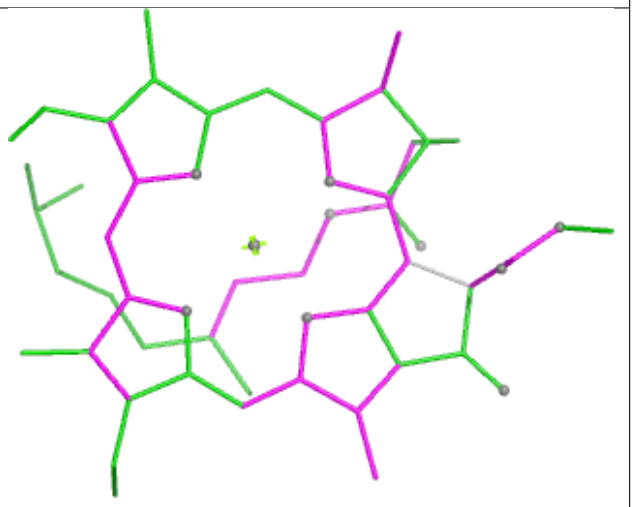
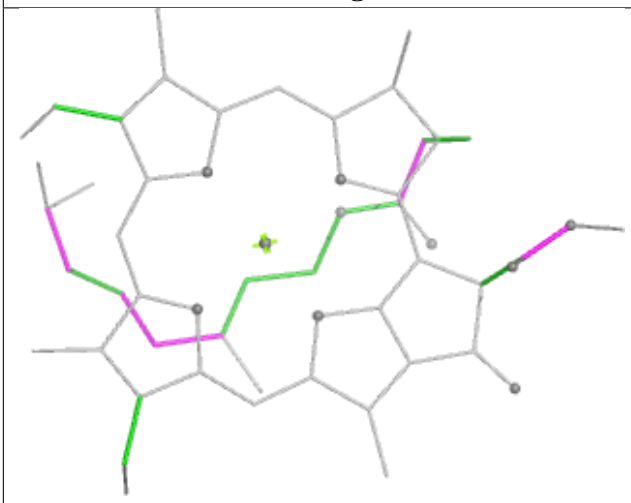


Bond angles



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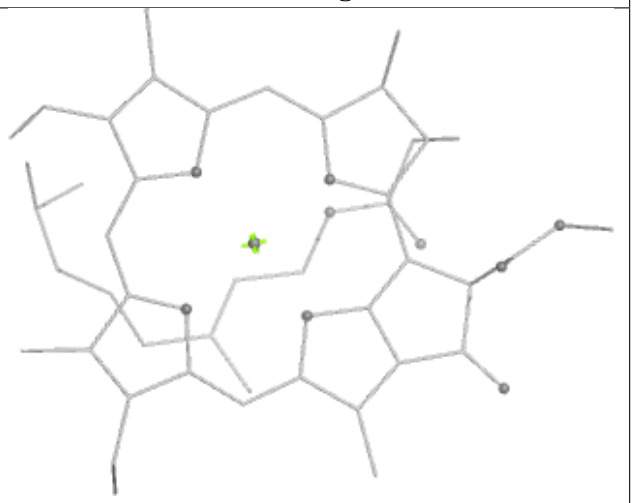
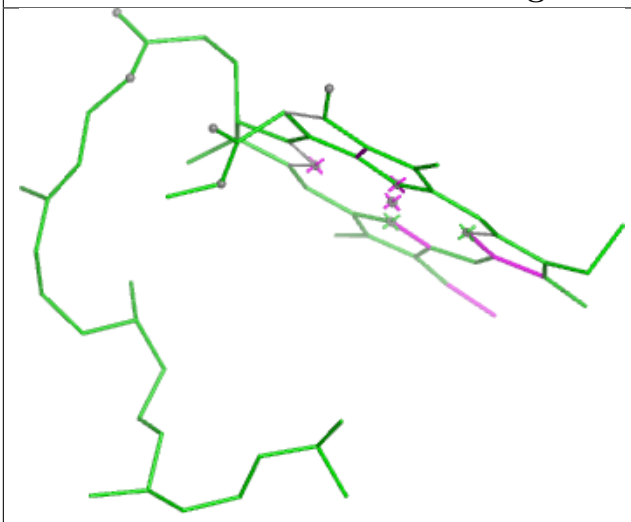


Rings

Ligand CLA n 603



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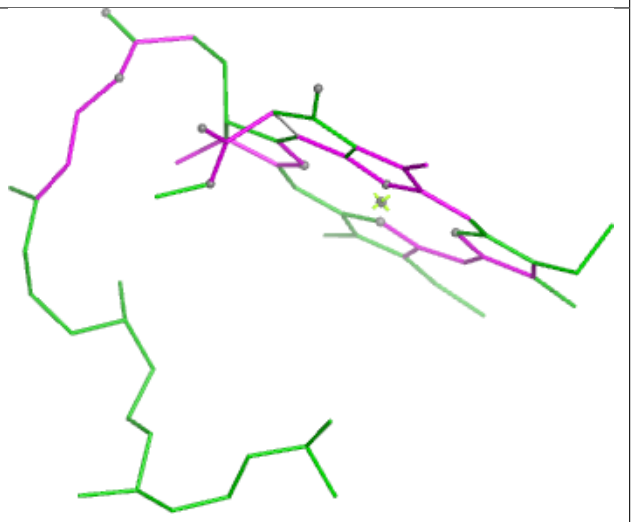
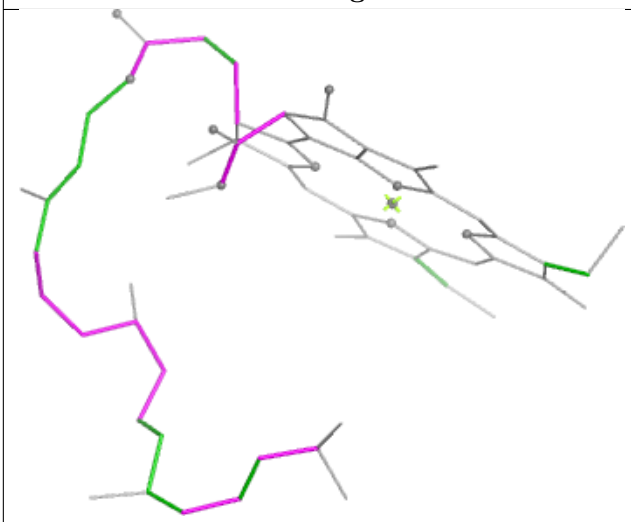


Bond angles



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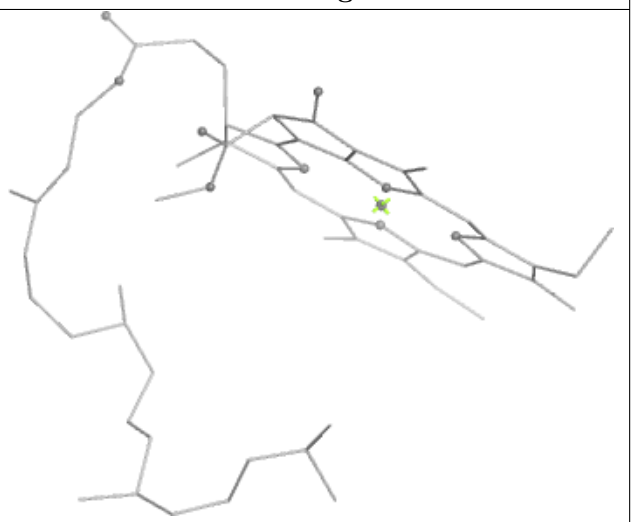
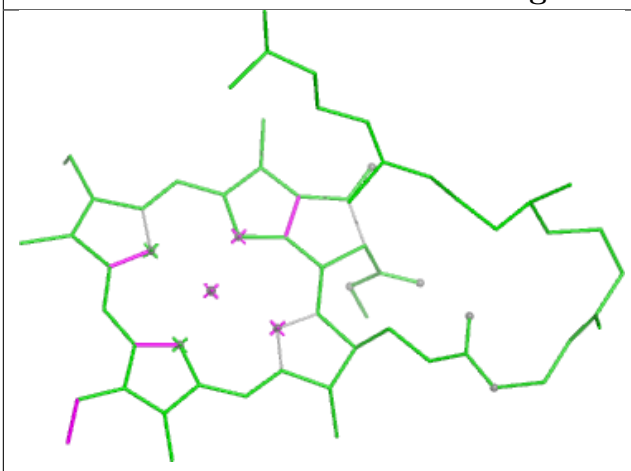


Rings

Ligand CLA c 509



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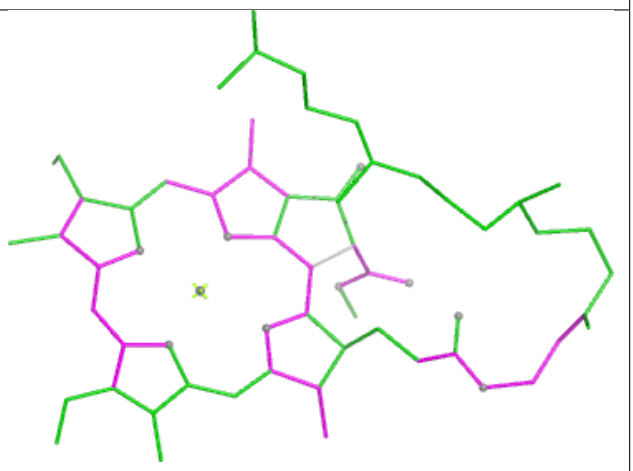
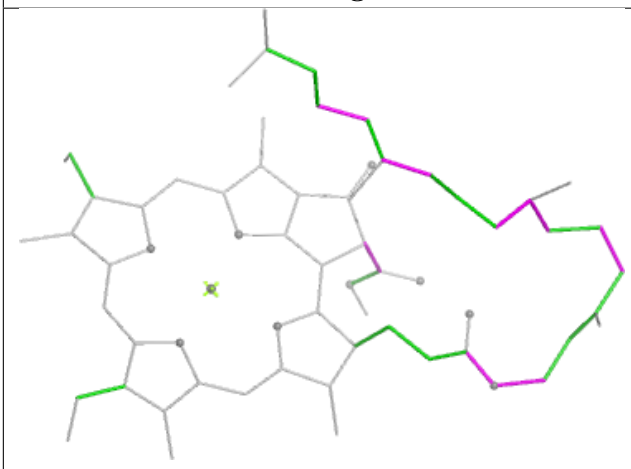


Bond angles



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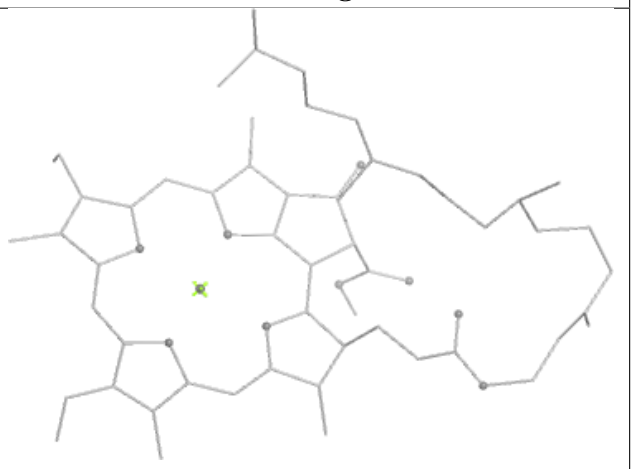
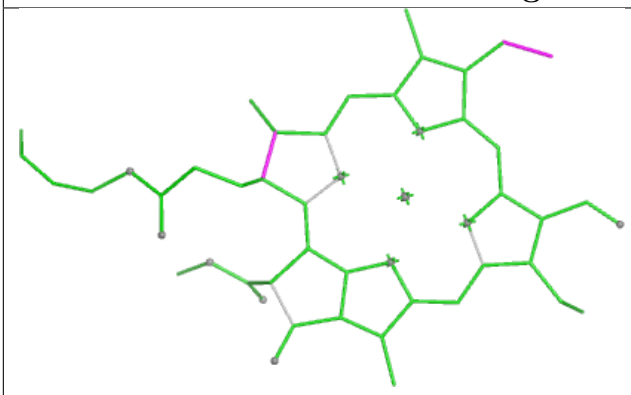
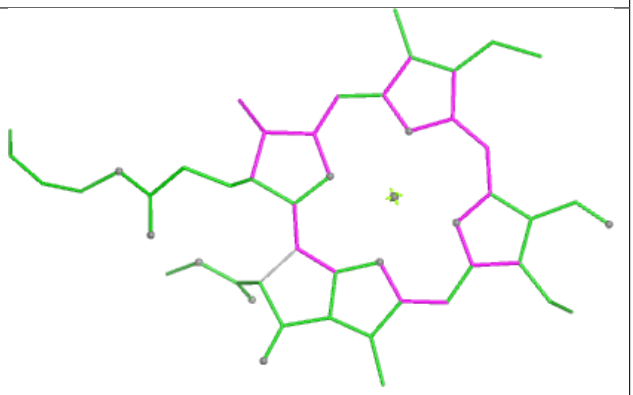


Rings

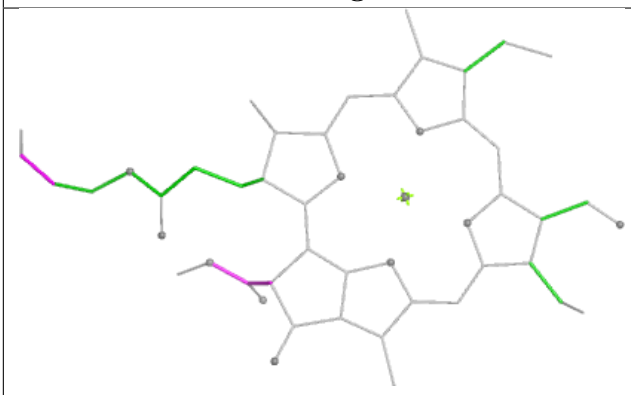
Ligand CHL G 606



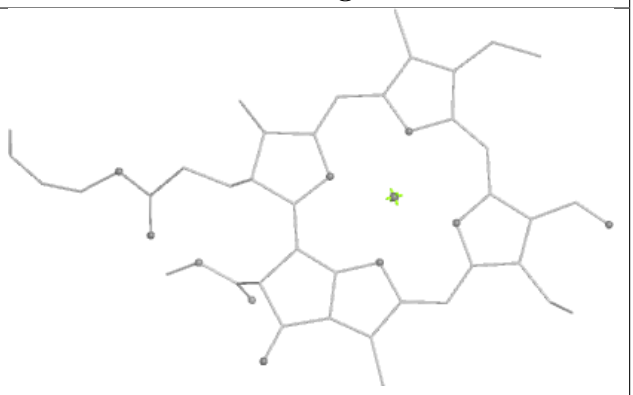
Bond lengths



Bond angles

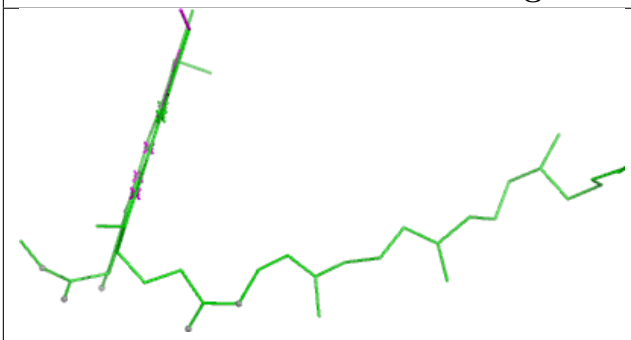


Torsions



Rings

Ligand CLA B 605



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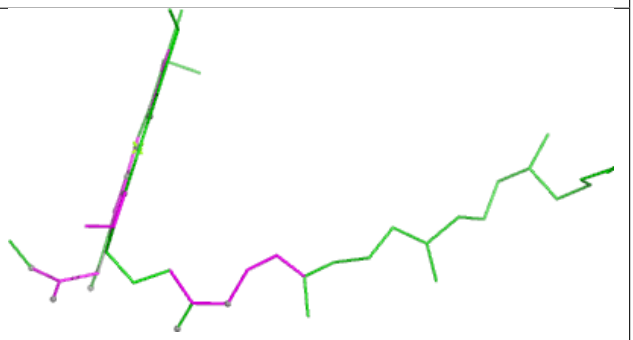

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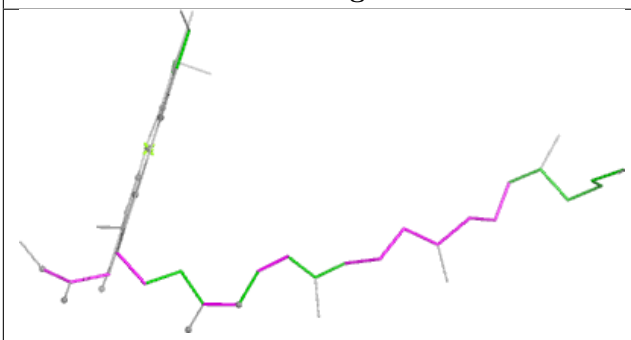

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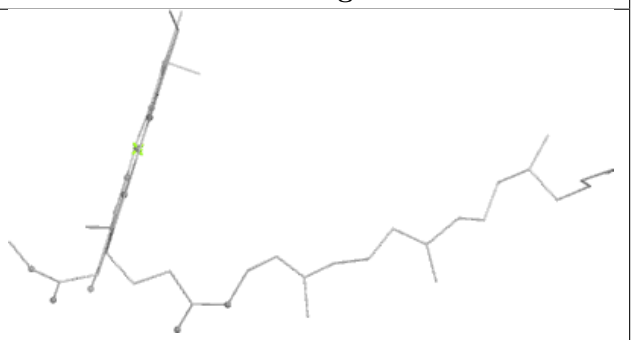
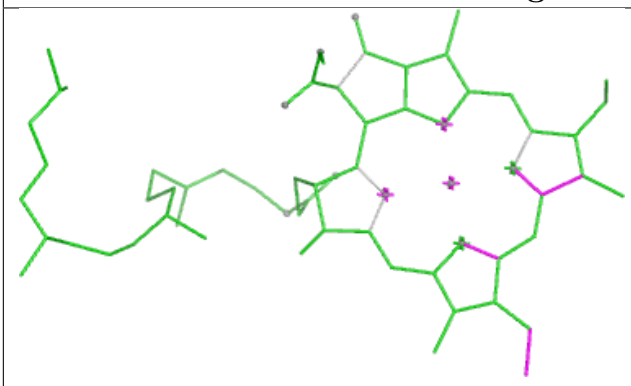


Rings

Ligand CLA b 612



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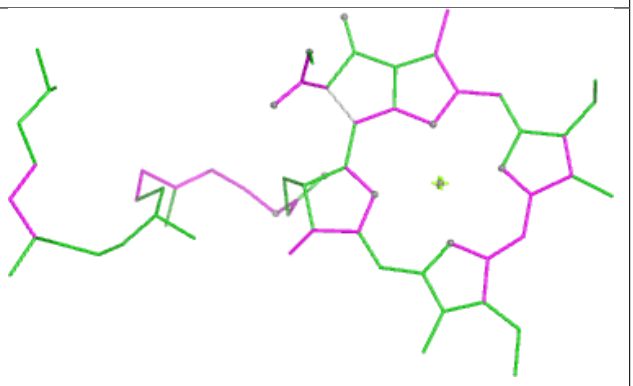

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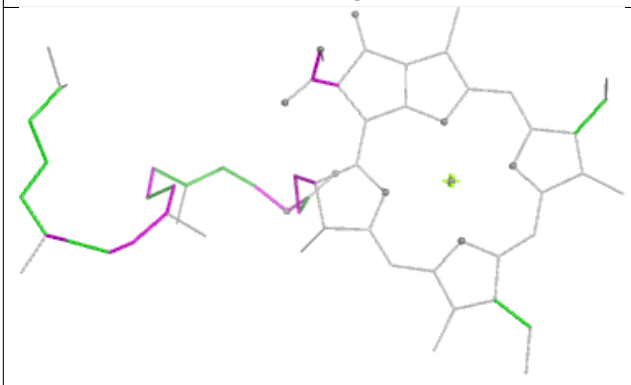

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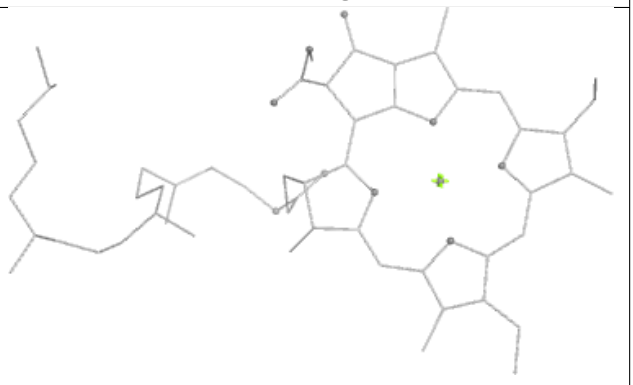
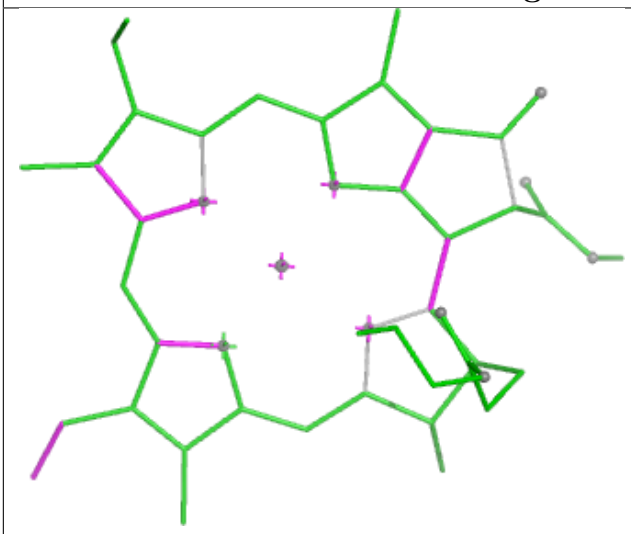


Rings

Ligand CLA R 604



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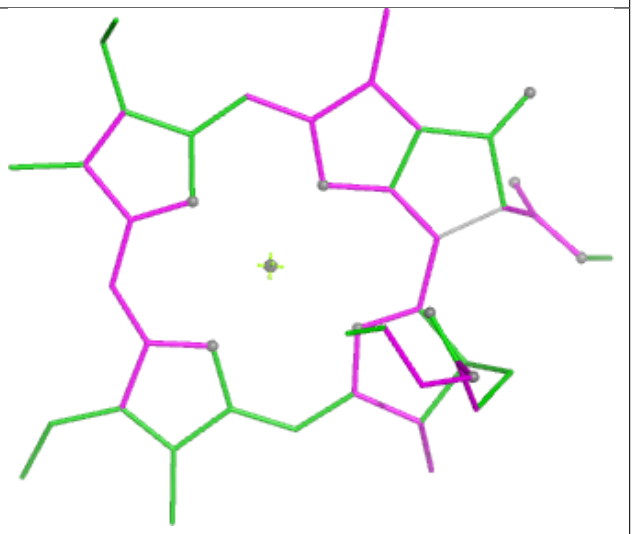

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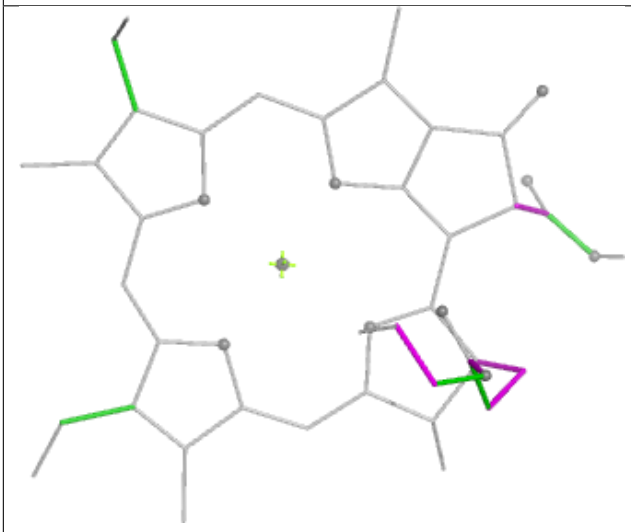

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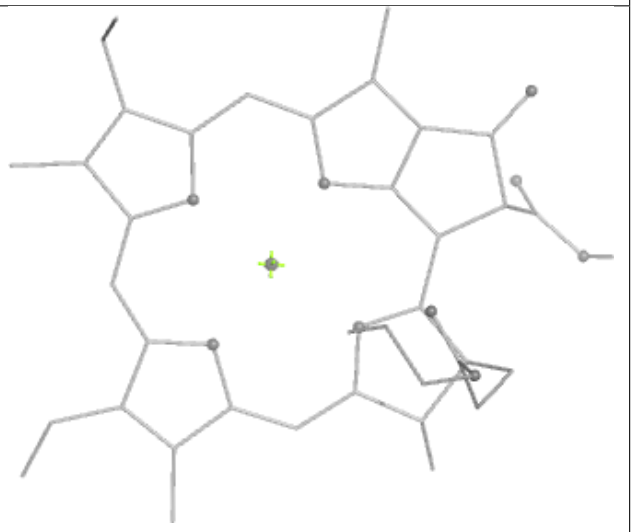

Rings

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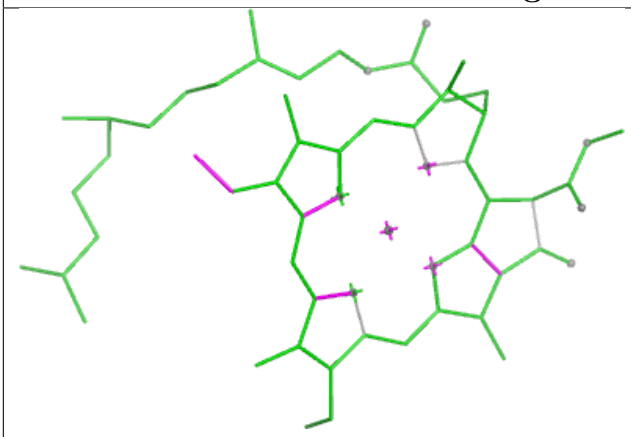

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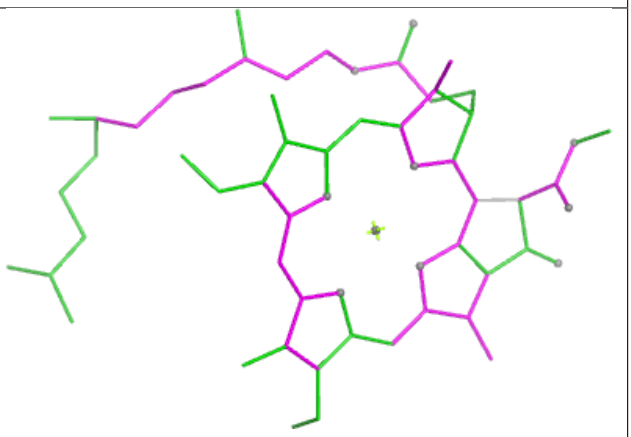

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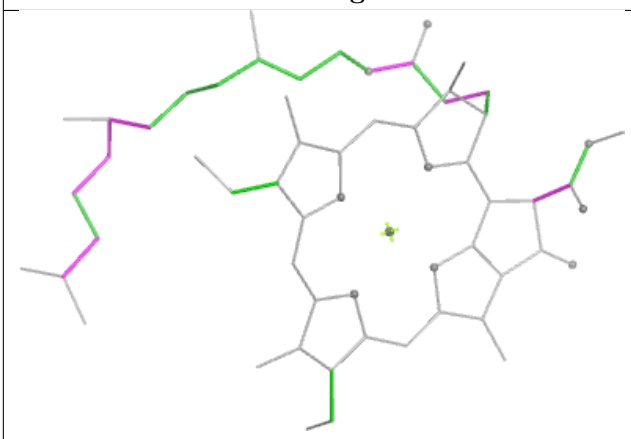

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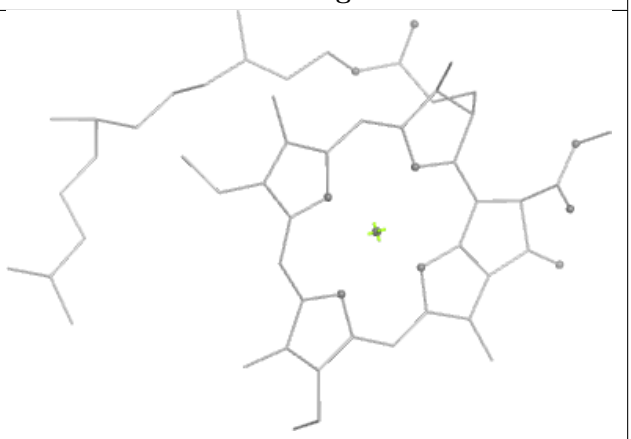
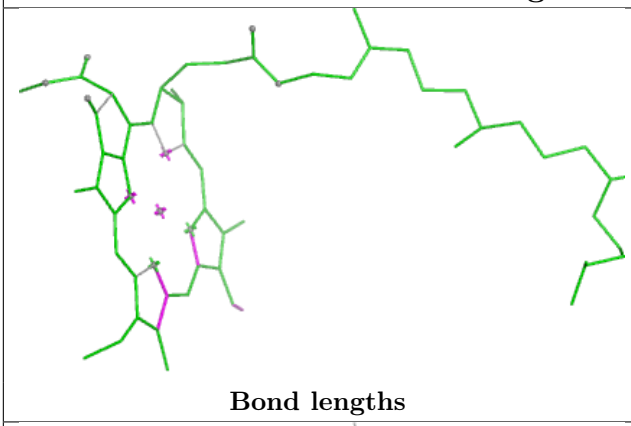


Rings

Ligand CLA b 609



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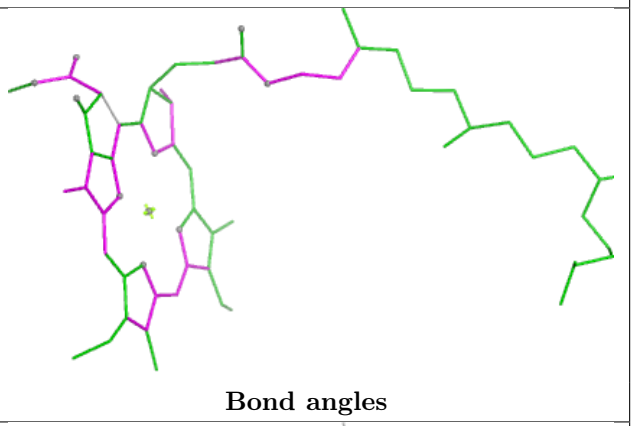

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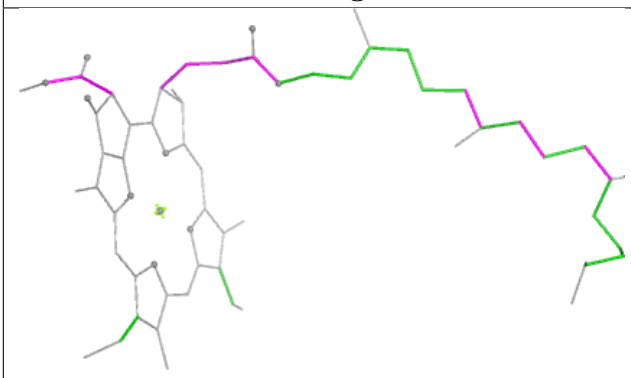
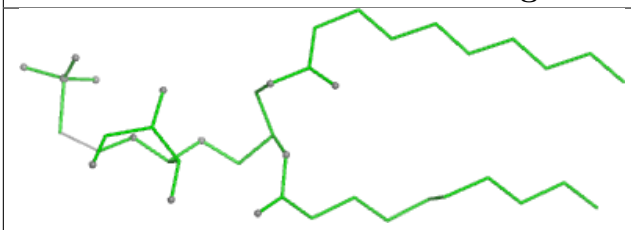


Torsions



Rings

Ligand SQD M 101



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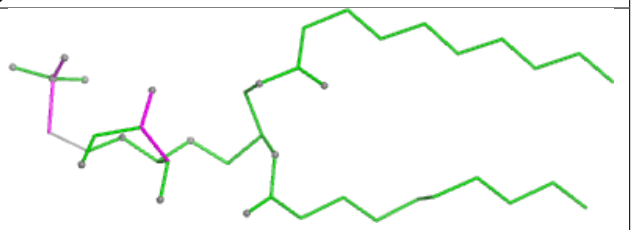

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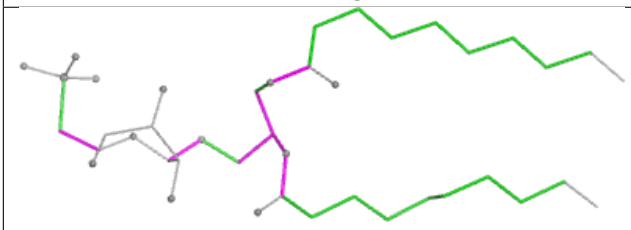

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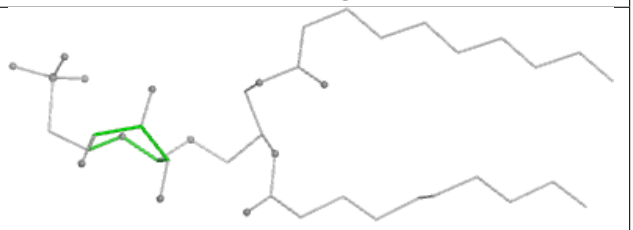
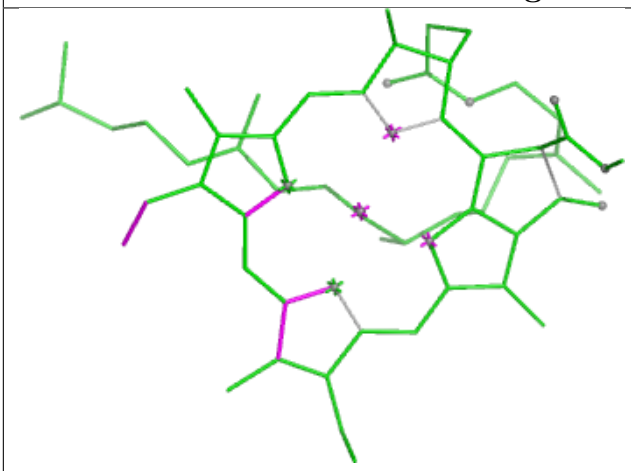


Rings

Ligand CLA B 601



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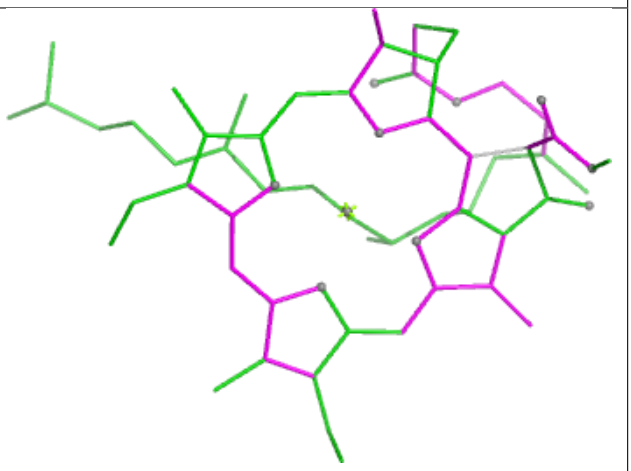

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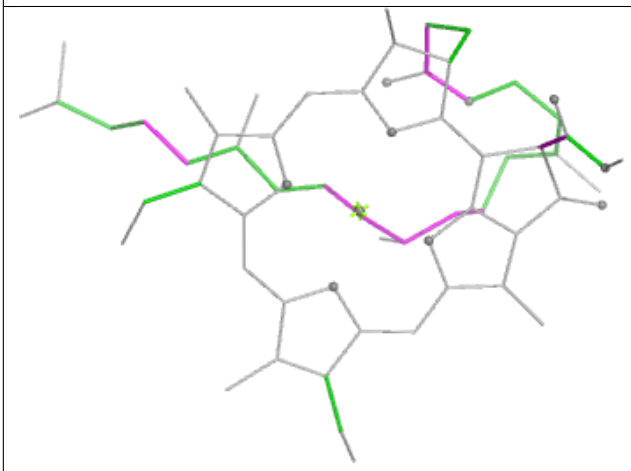

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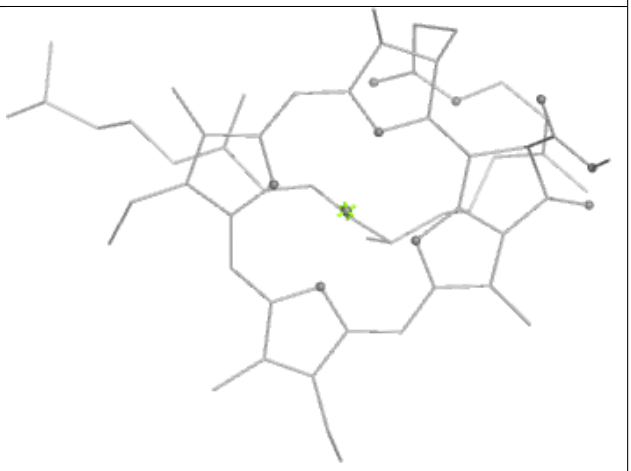
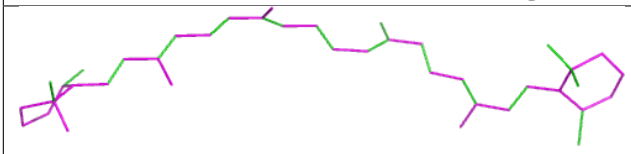


Rings

Ligand BCR T 101



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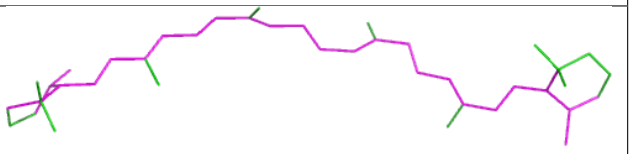

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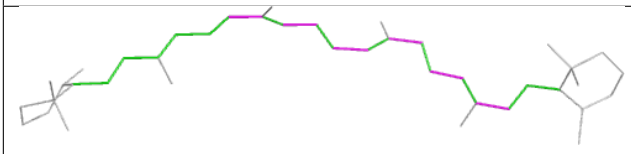

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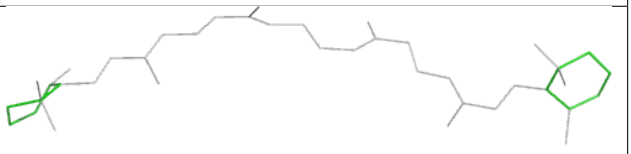
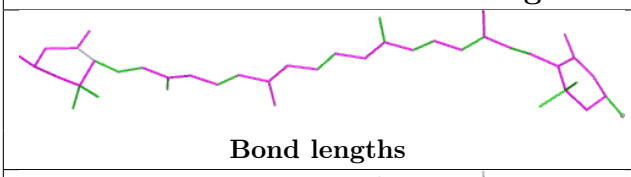


Rings

Ligand LUT Y 616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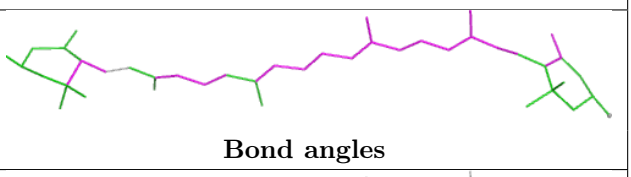
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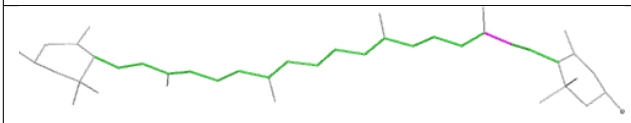
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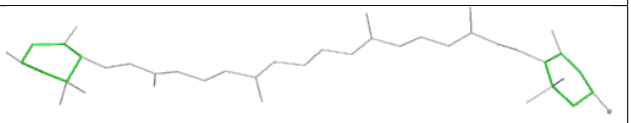
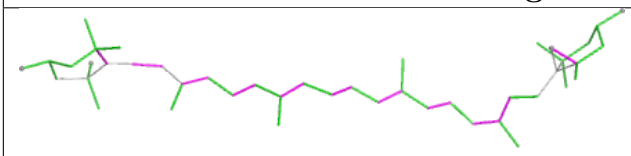

Rings

Ligand NEX n 617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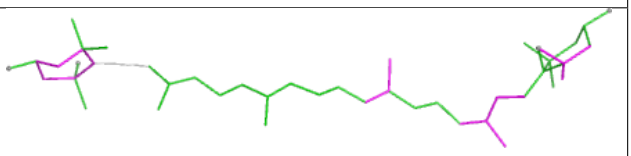
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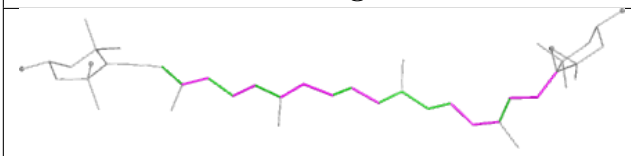
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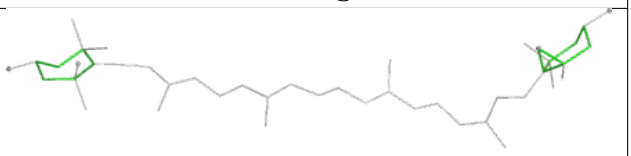
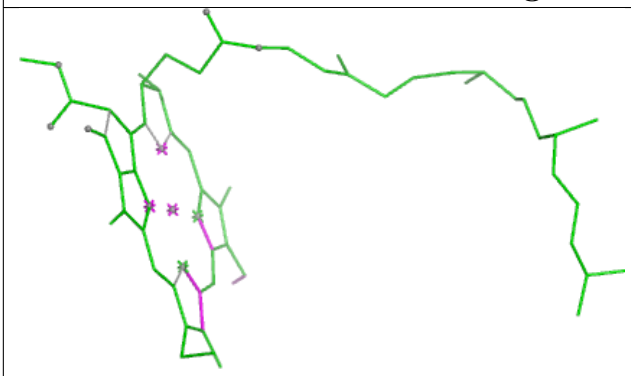

Rings

Ligand CLA D 404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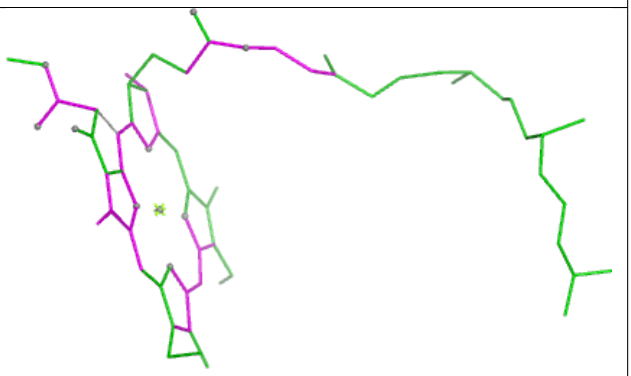
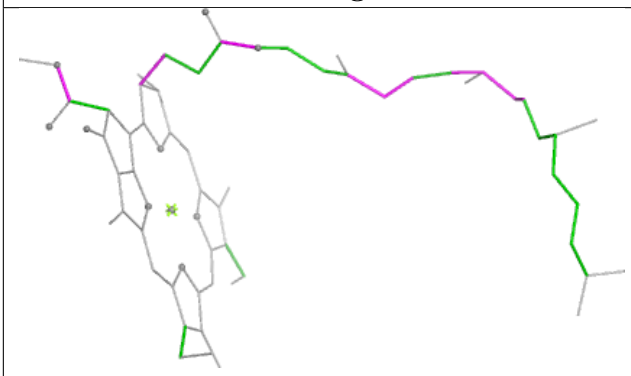
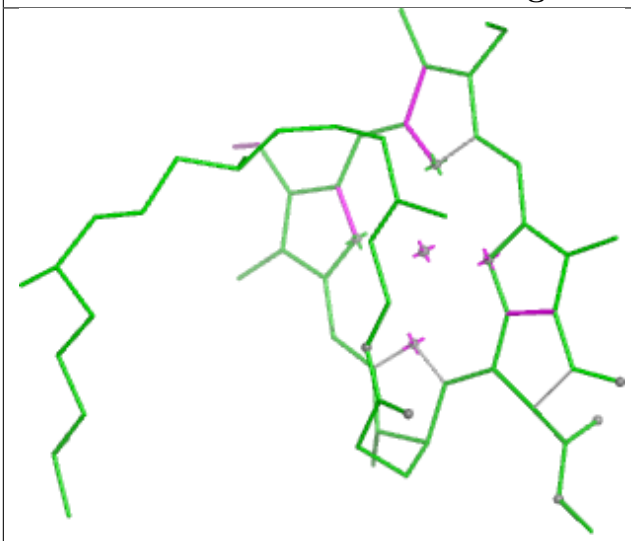

Bond angles


Torsions


Rings

Ligand CLA y 313



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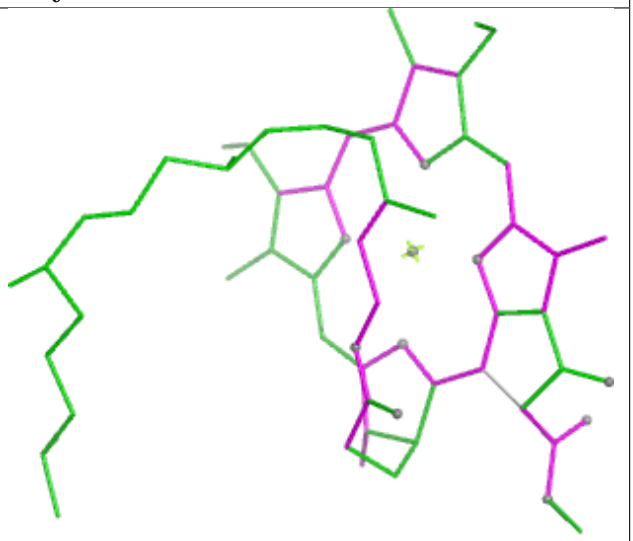
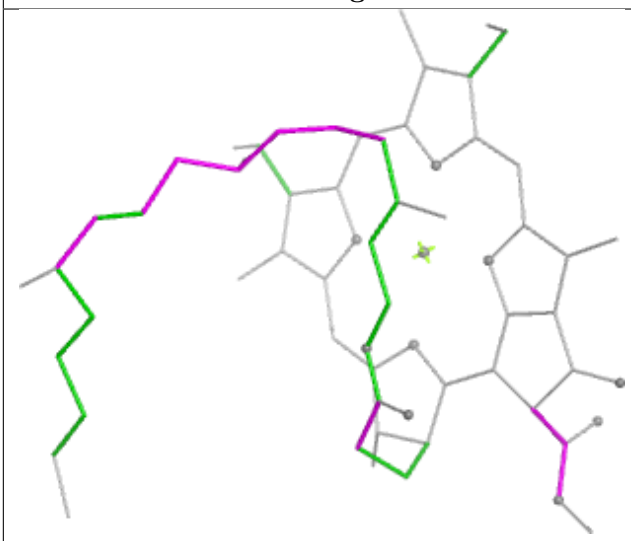


Bond angles



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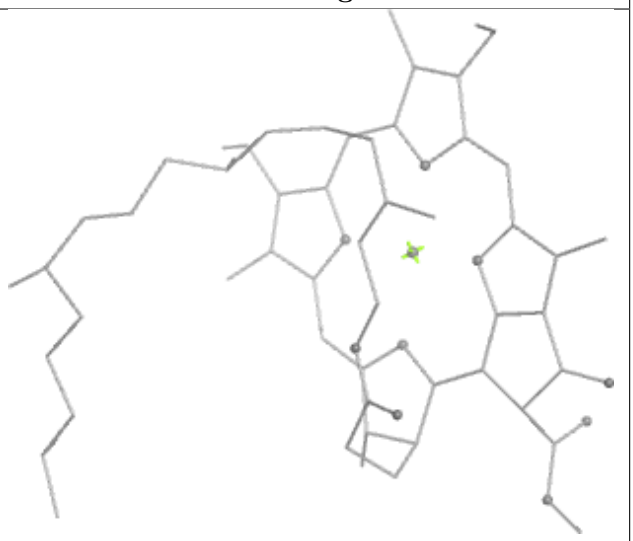
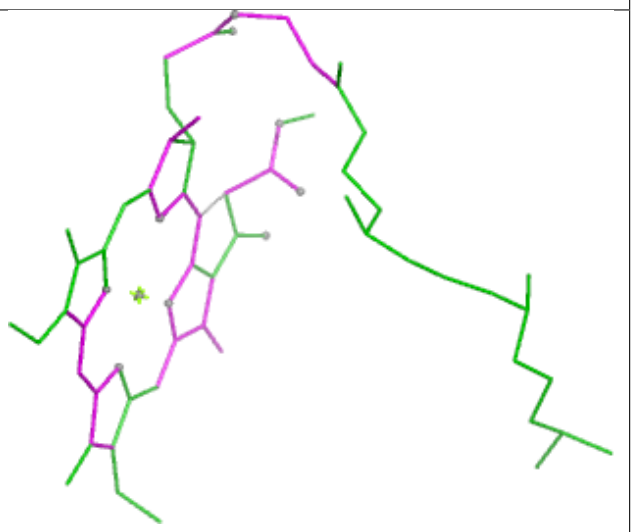


Rings

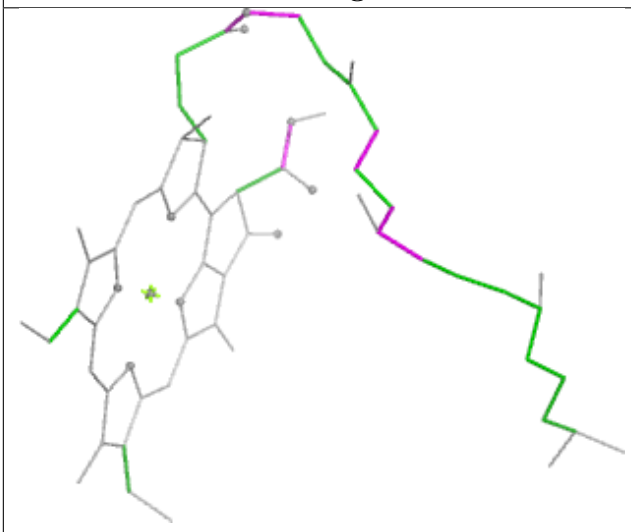
Ligand CLA b 613



Bond lengths



Bond angles



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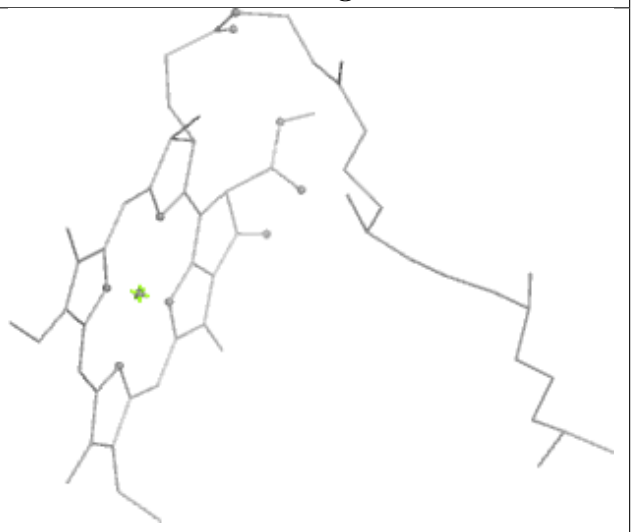
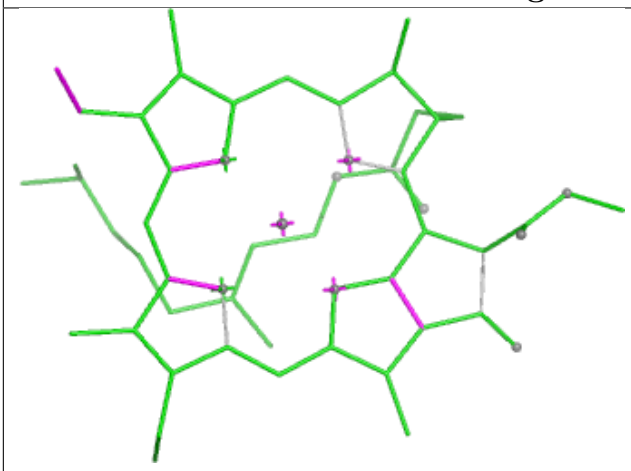


Rings

Ligand CLA n 613



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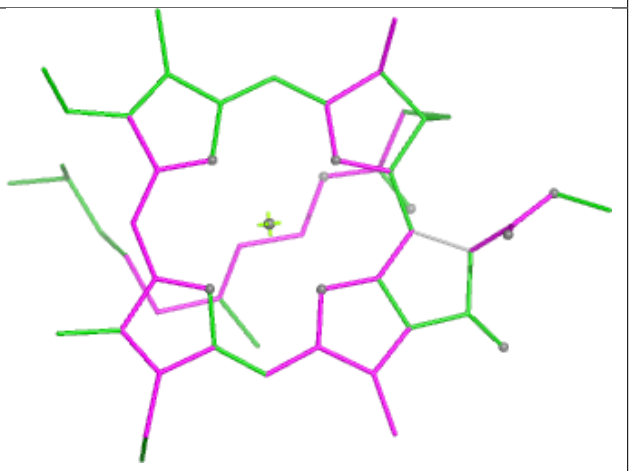
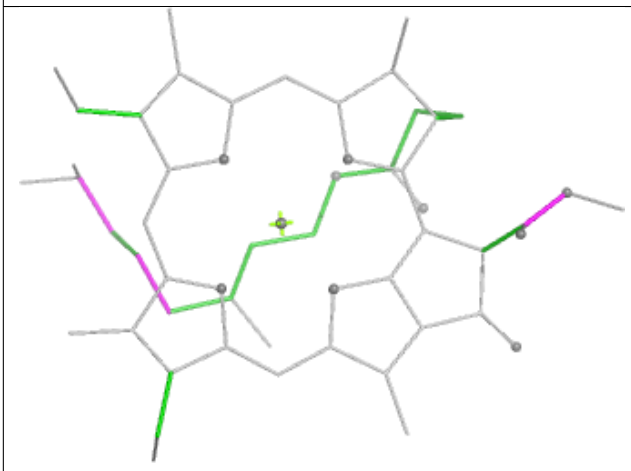


Bond angles



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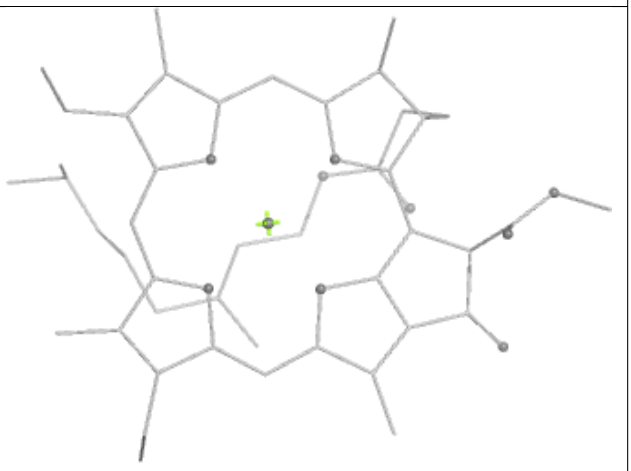
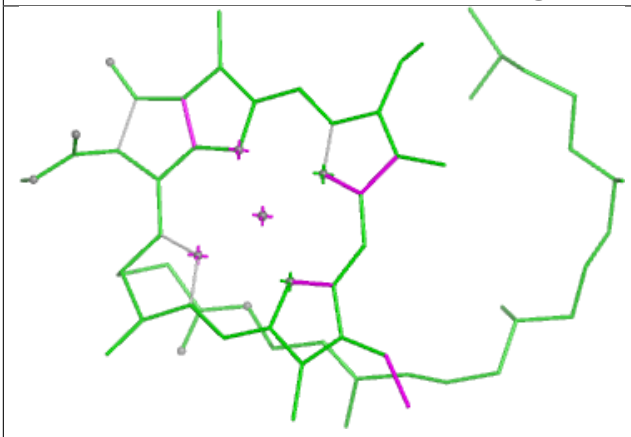


Rings

Ligand CLA r 609



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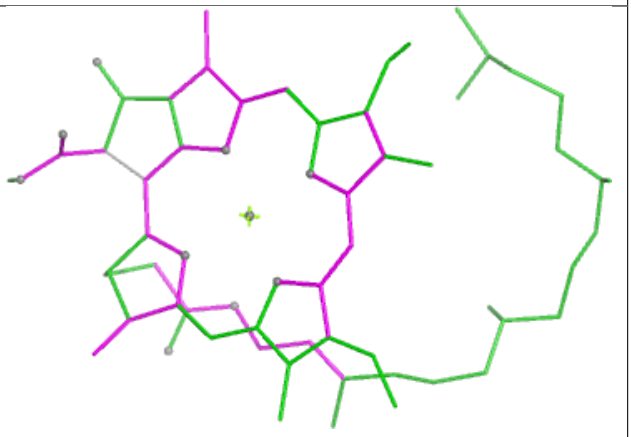
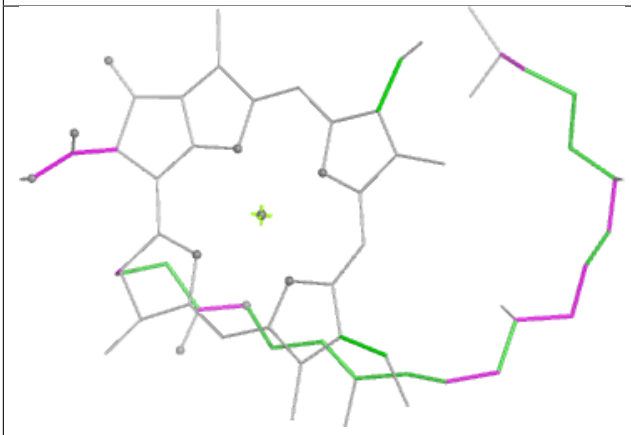
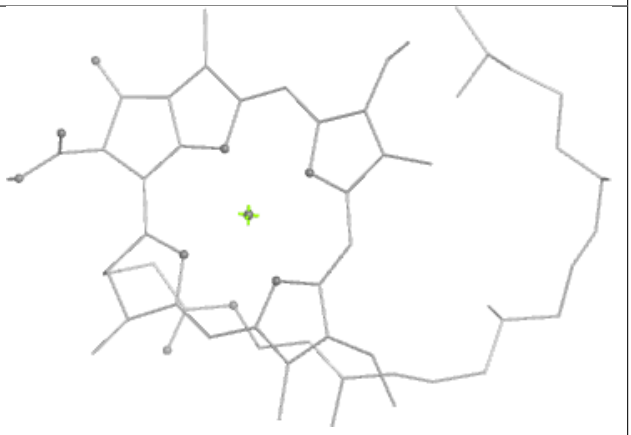


Bond angles

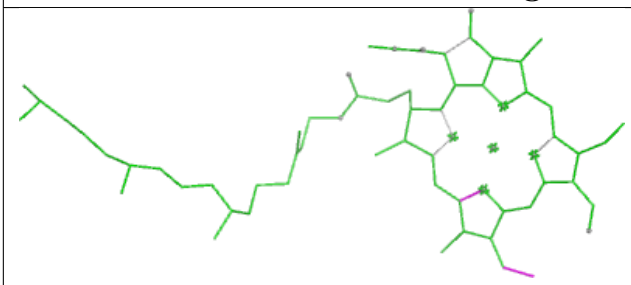


Torsions



Rings

Ligand CHL Y 601



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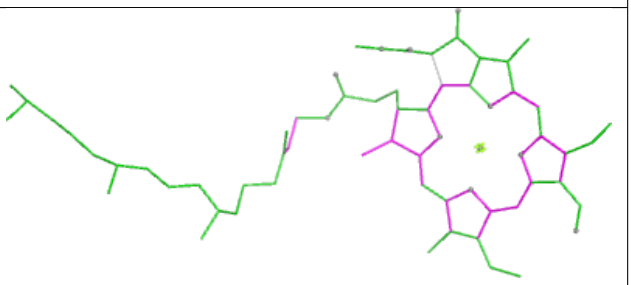
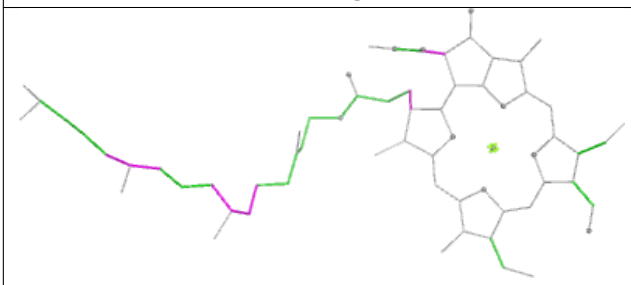


Bond angles



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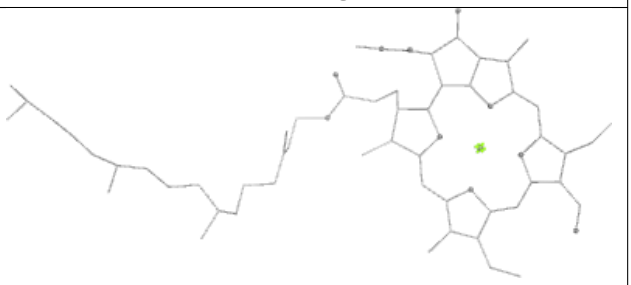
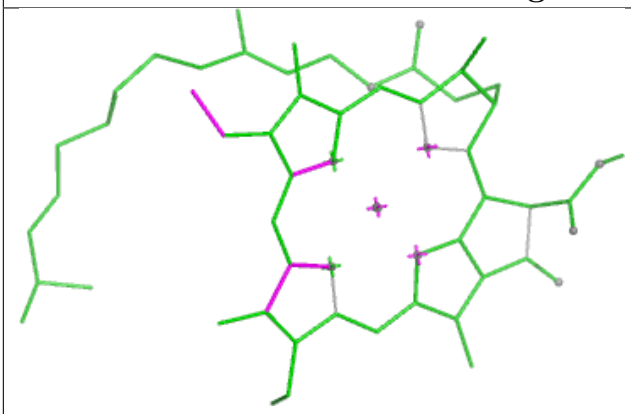


Rings

Ligand CLA y 310



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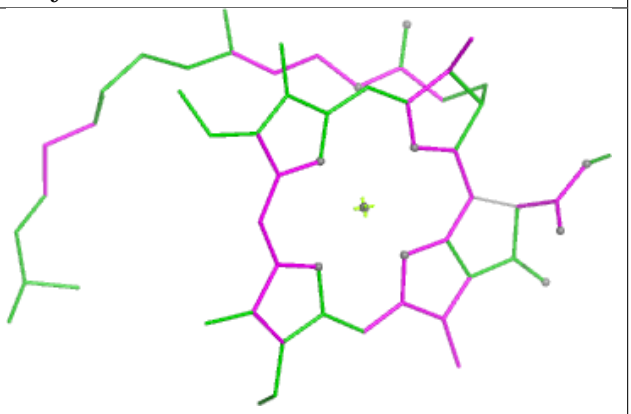
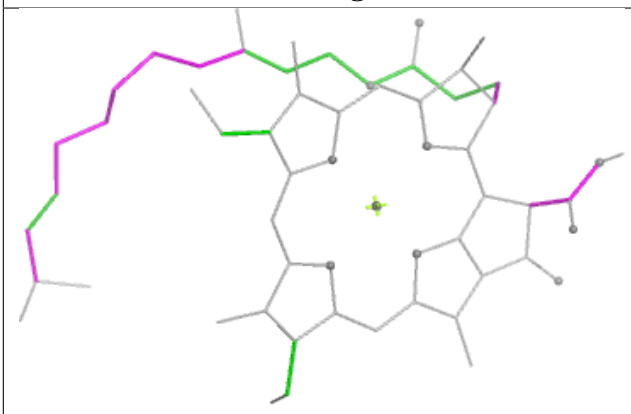


Bond angles



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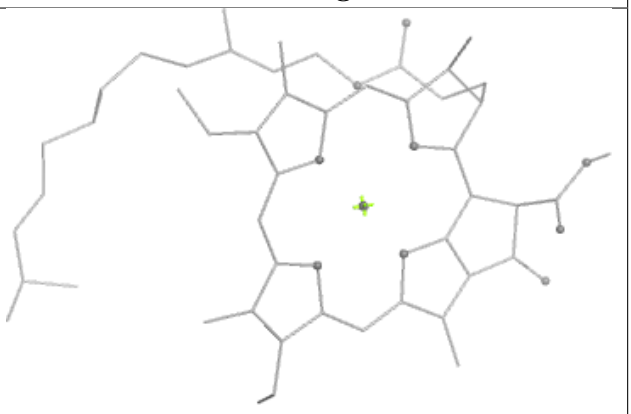
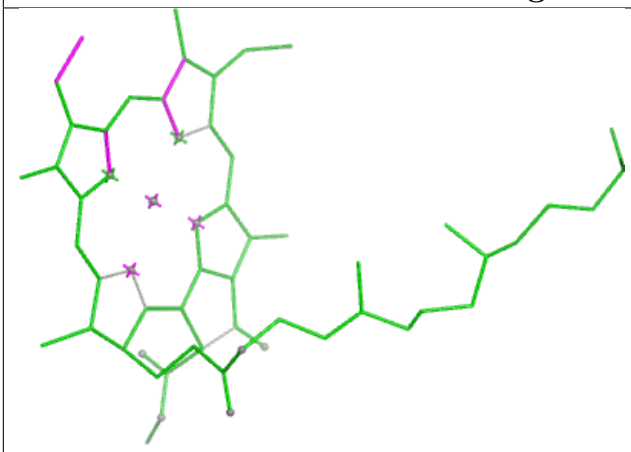


Rings

Ligand CLA y 311



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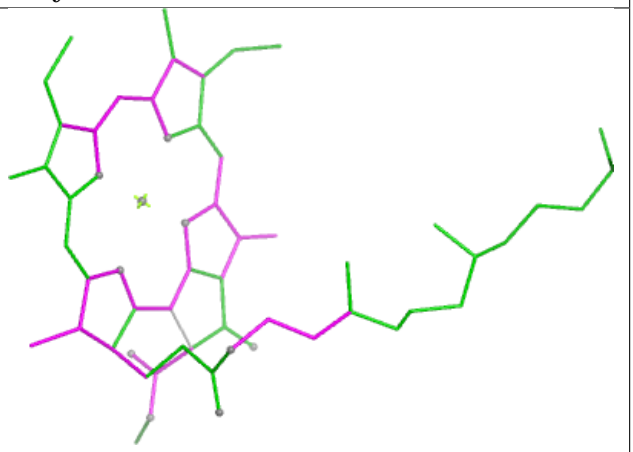

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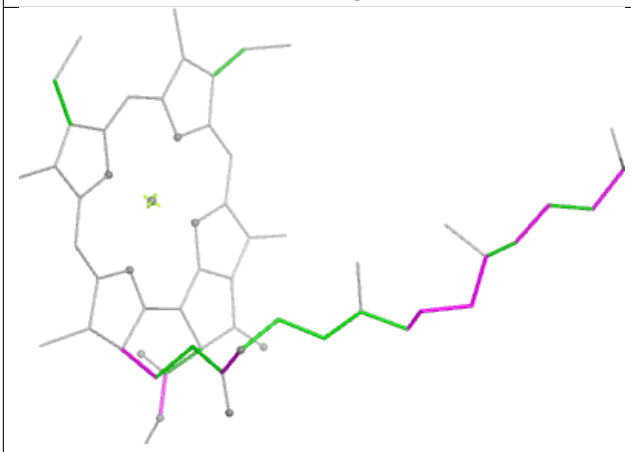

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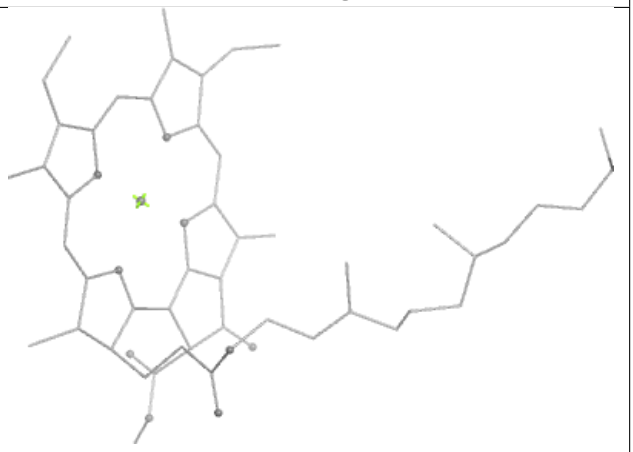
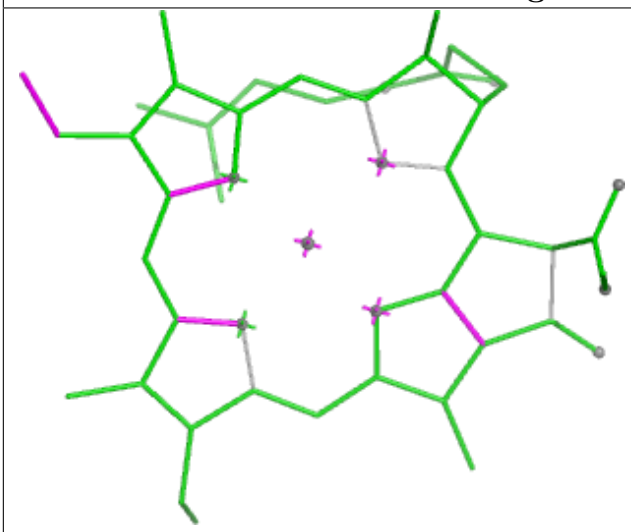


Rings

Ligand CLA S 305



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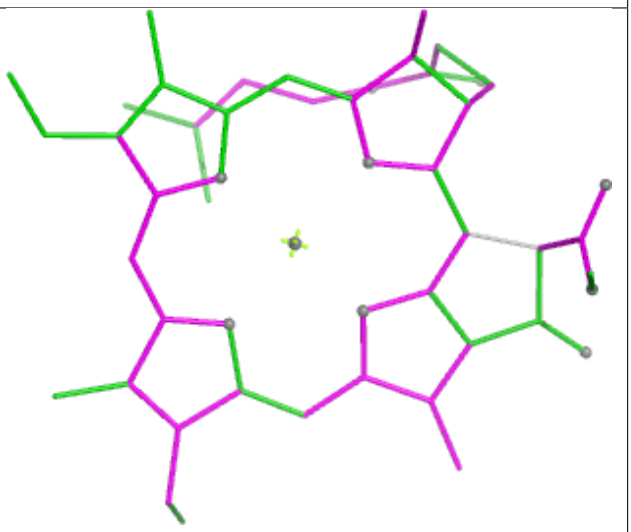
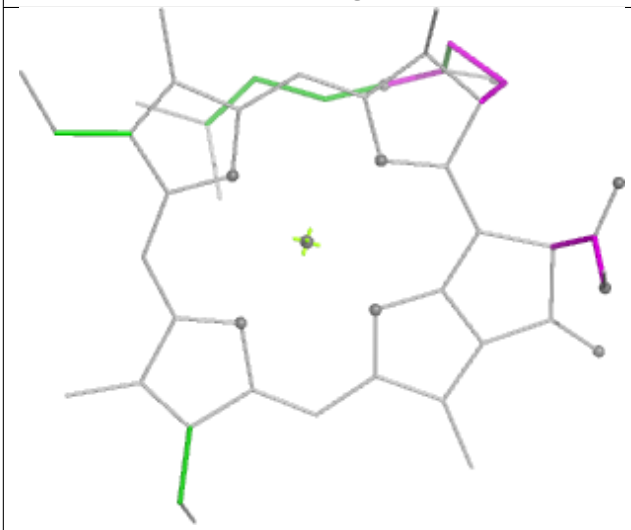


Bond angles



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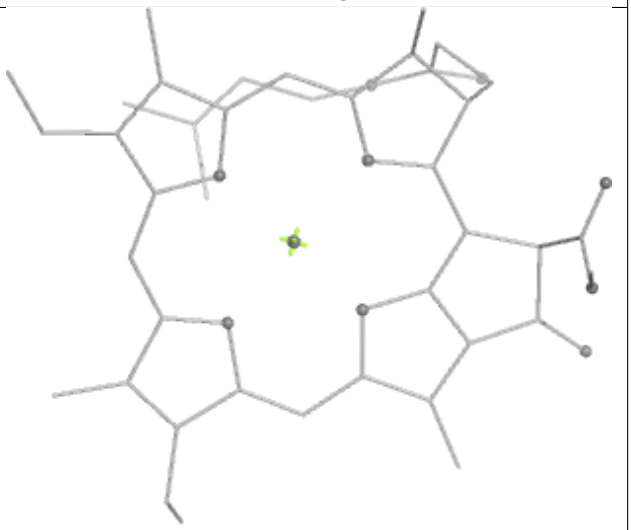
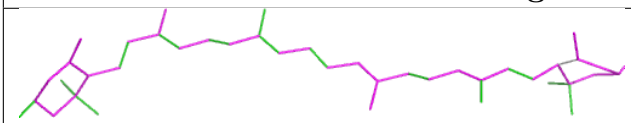


Rings

Ligand LUT n 615



Bond lengths



Bond angles

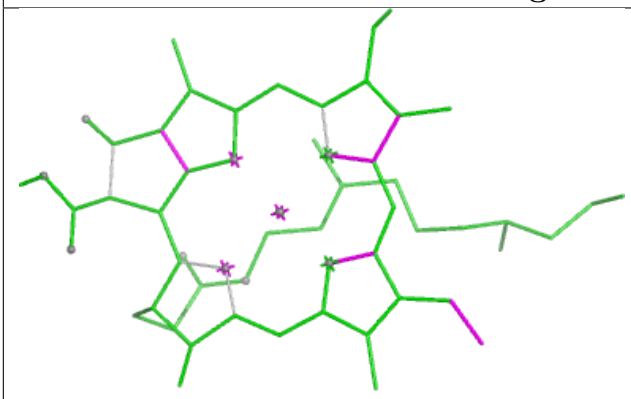


Torsions



Rings

Ligand CLA c 505



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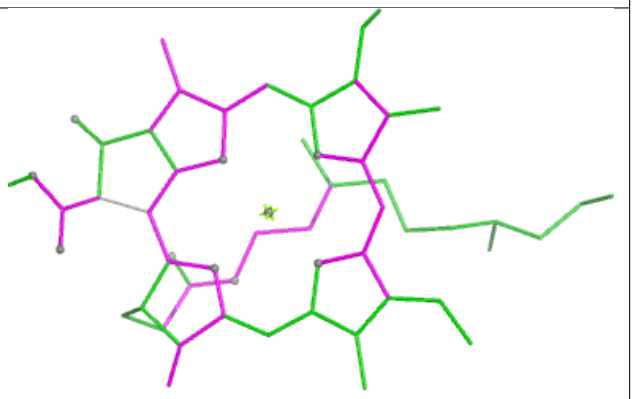
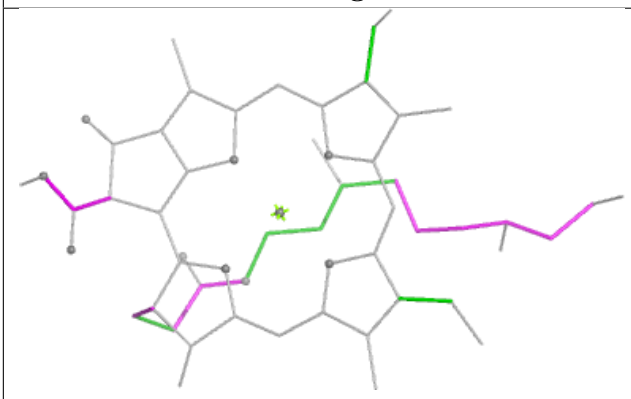


Bond angles



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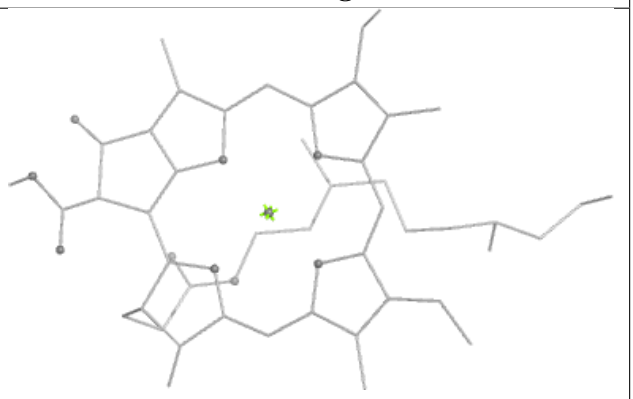
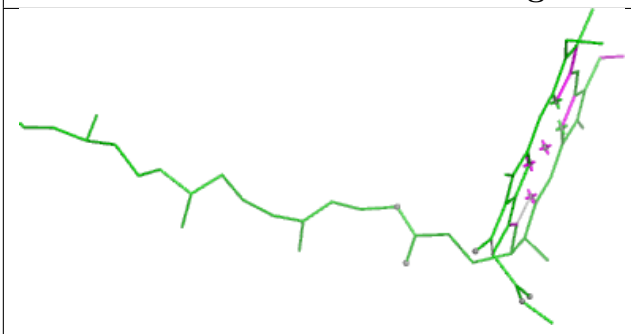


Rings

Ligand CLA b 604



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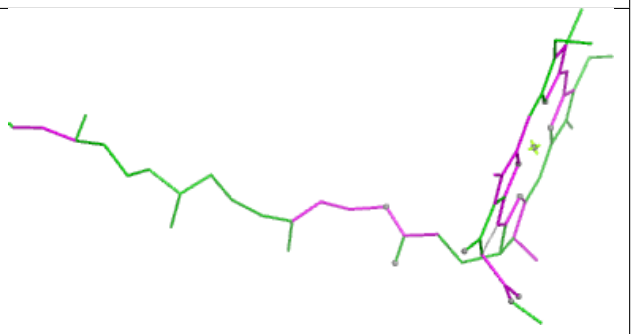
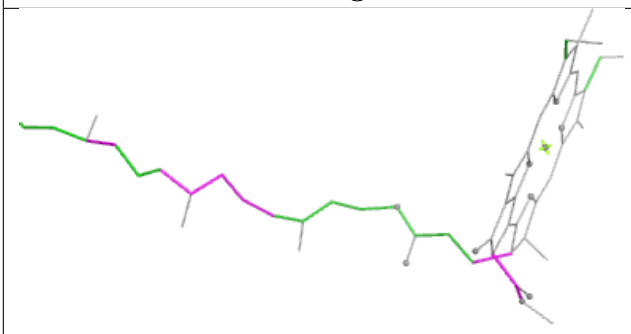


Bond angles



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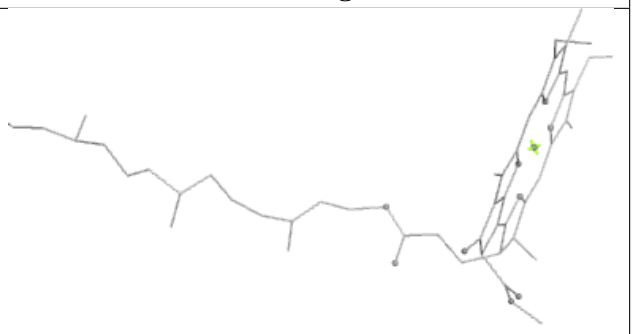
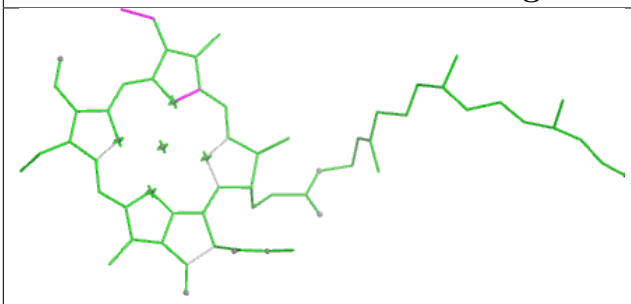


Rings

Ligand CHL G 601



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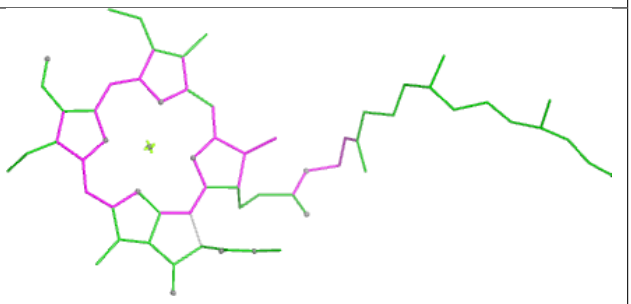

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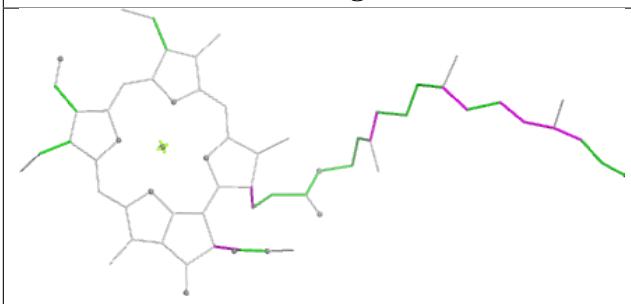

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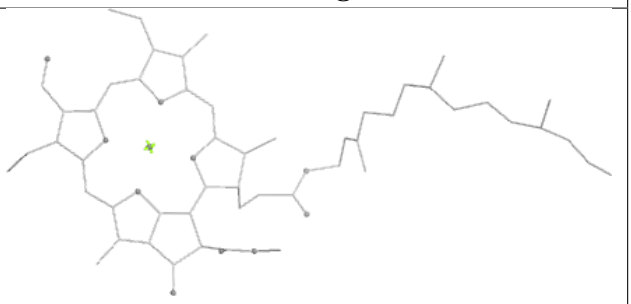
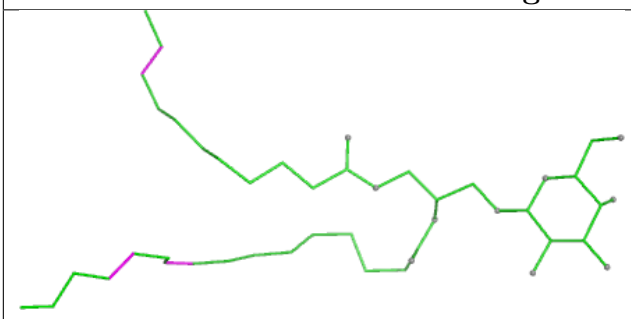


Rings

Ligand LMG d 409



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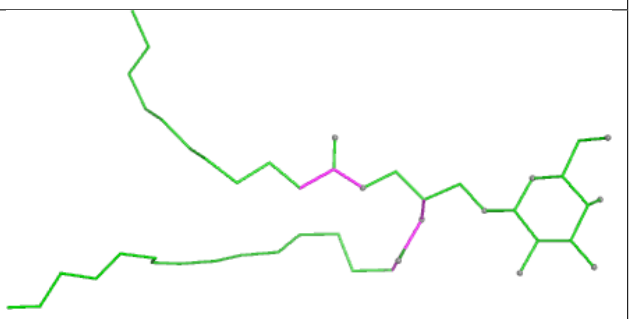
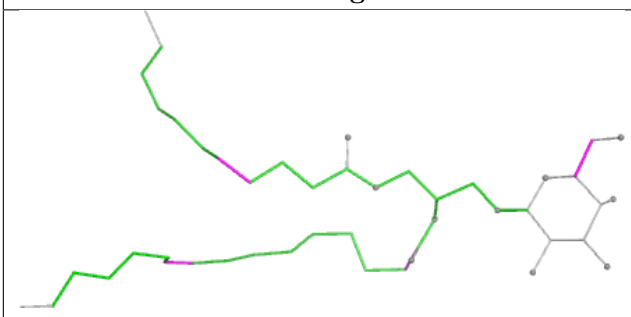


Bond angles



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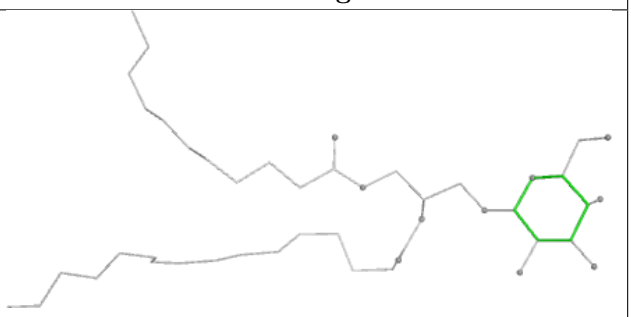
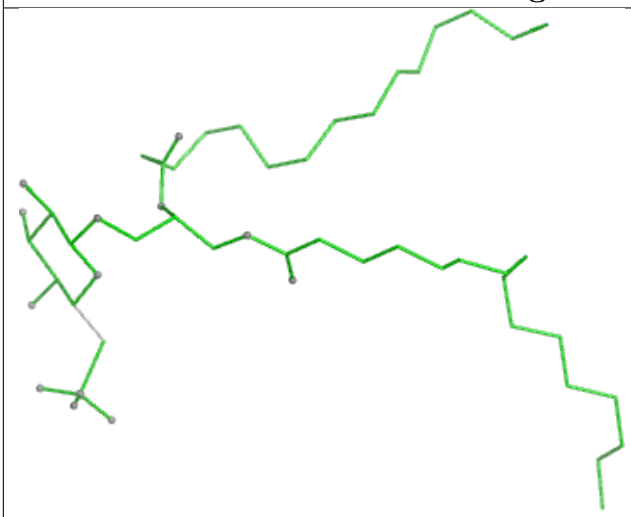


Rings

Ligand SQD a 414



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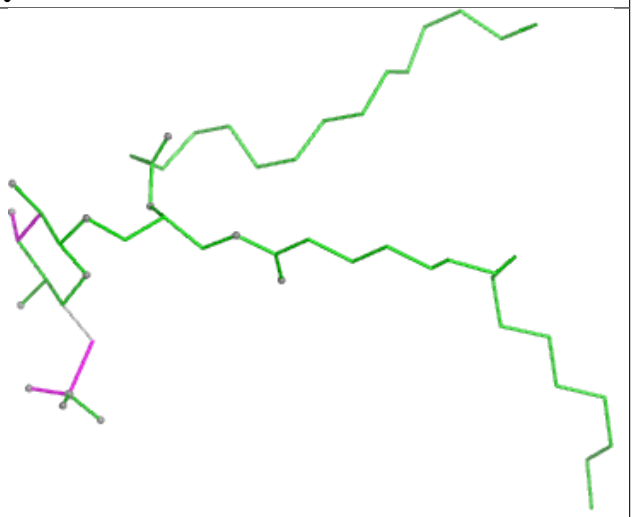
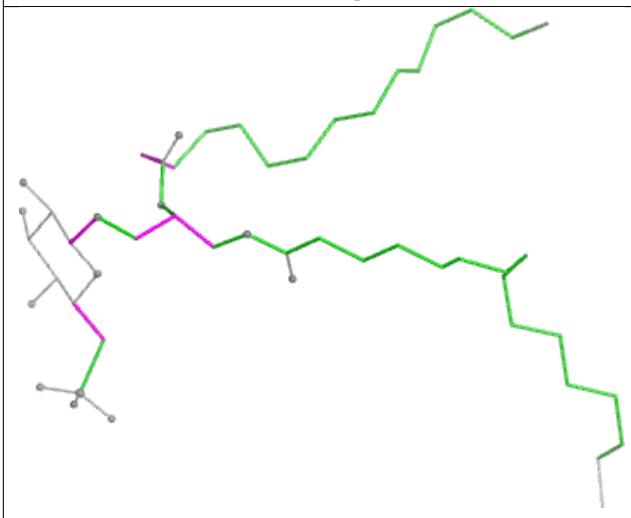


Bond angles



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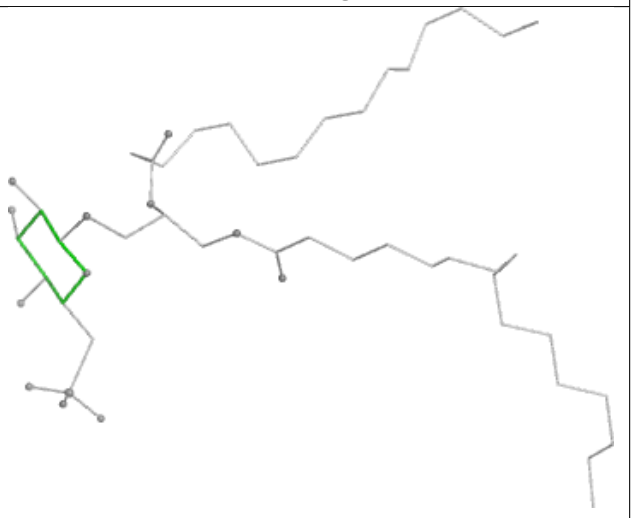
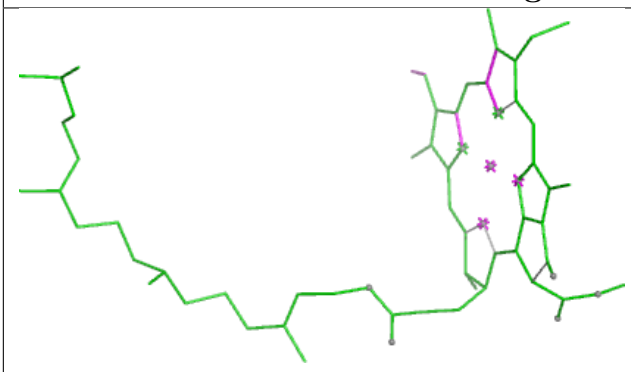


Rings

Ligand CLA B 609



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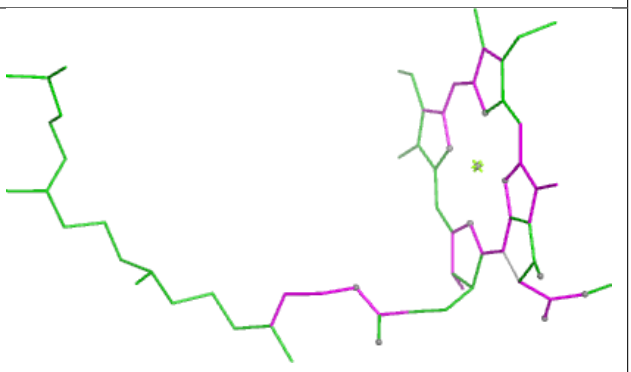
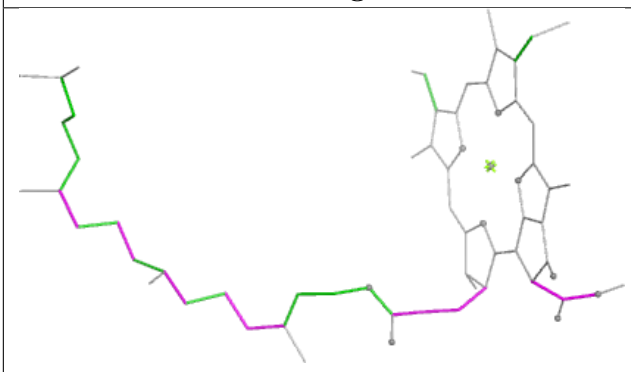


Bond angles

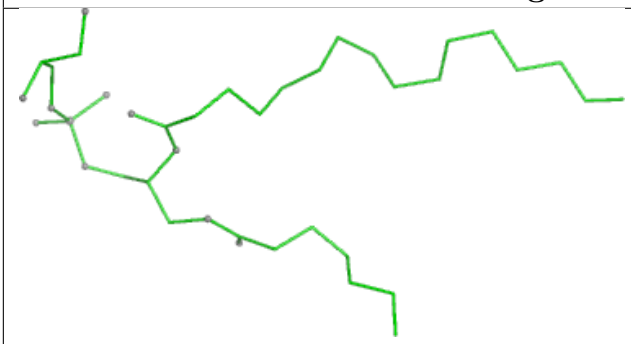


Torsions



Rings

Ligand LHG c 520



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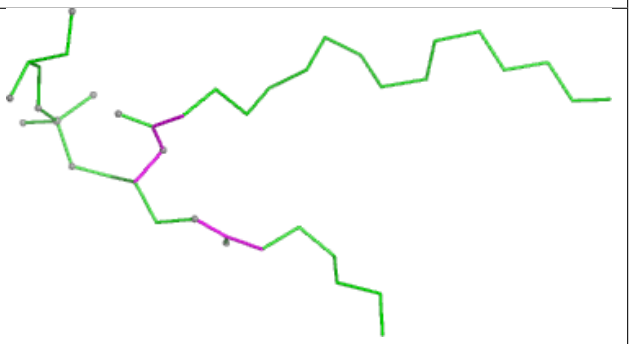
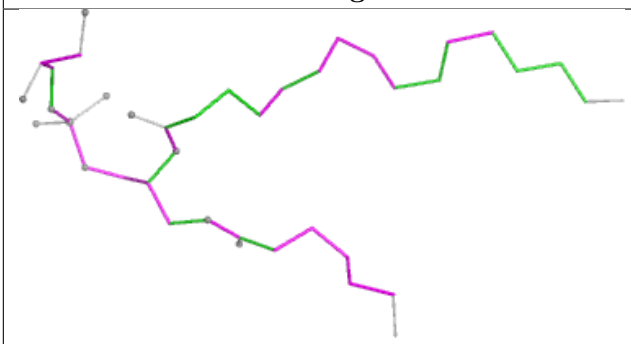


Bond angles



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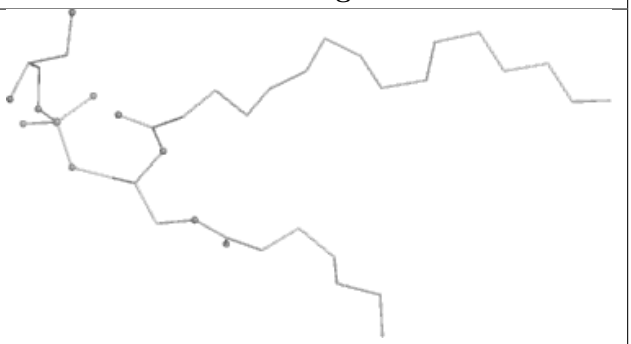
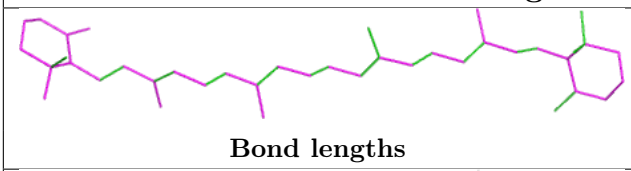


Rings

Ligand BCR b 618



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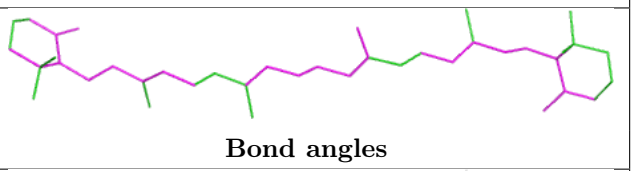
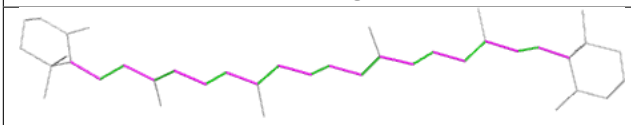


Bond angles



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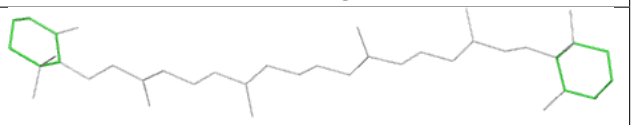
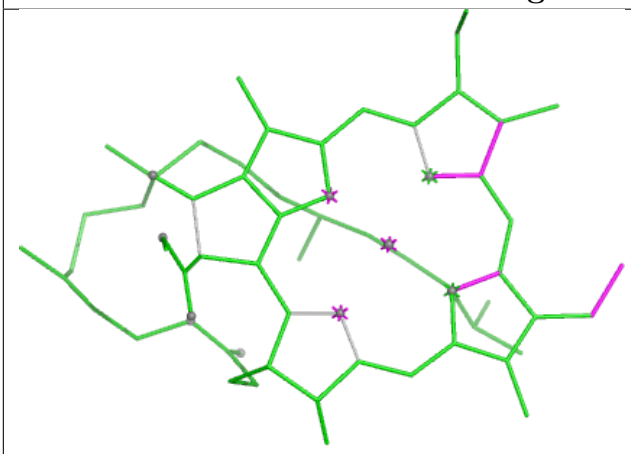


Rings

Ligand CLA b 601



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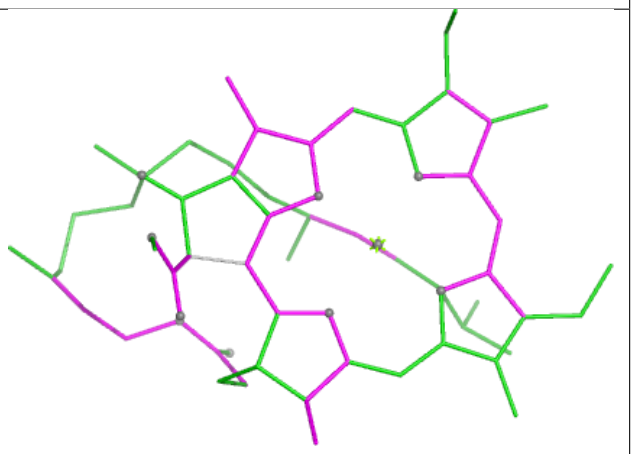
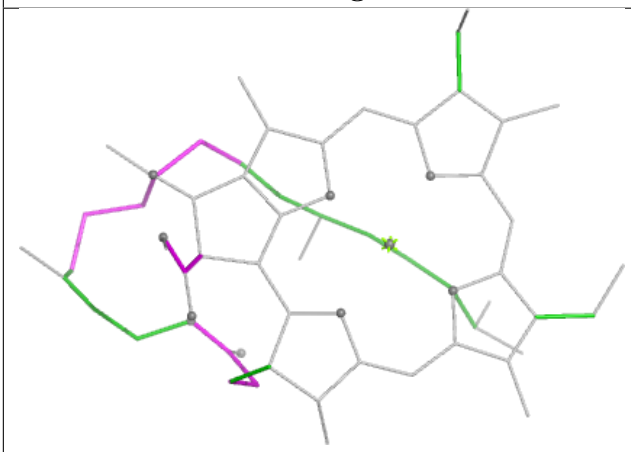


Bond angles



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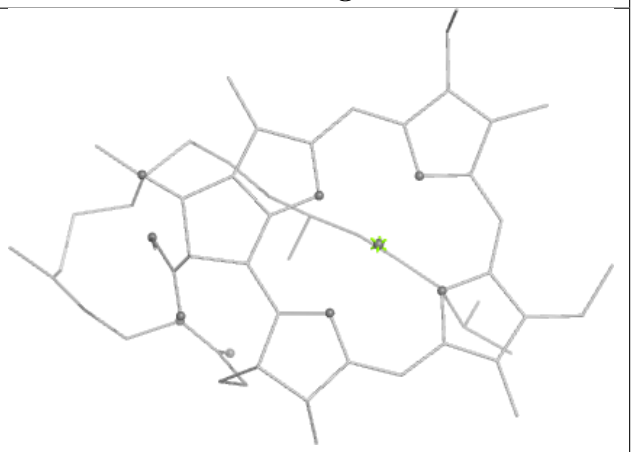
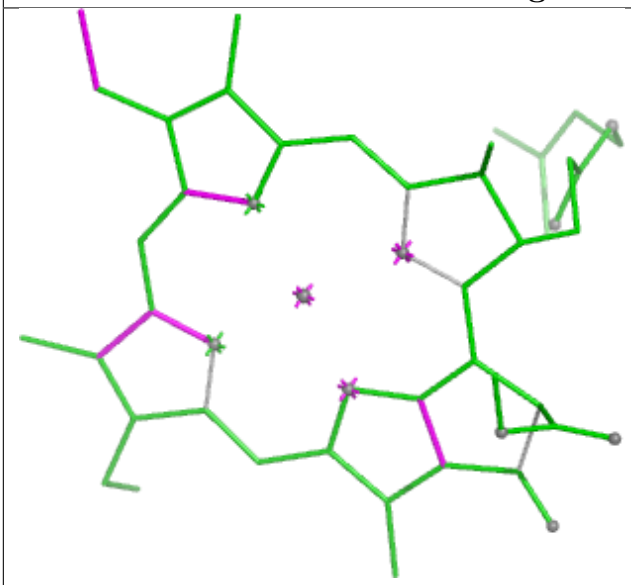


Rings

Ligand CLA g 604



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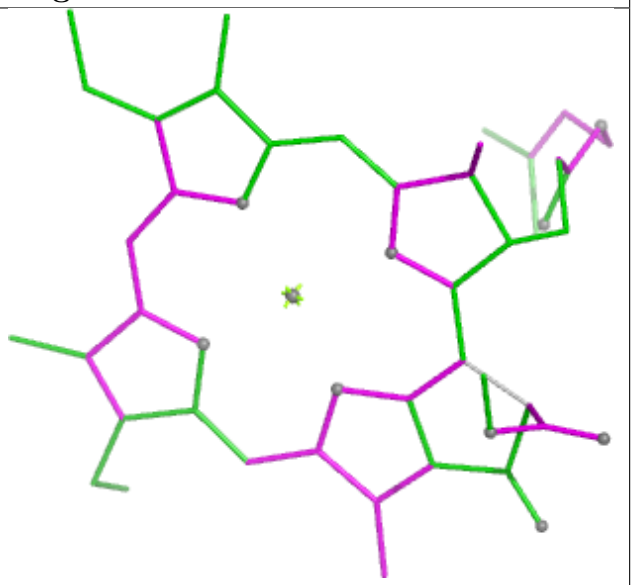
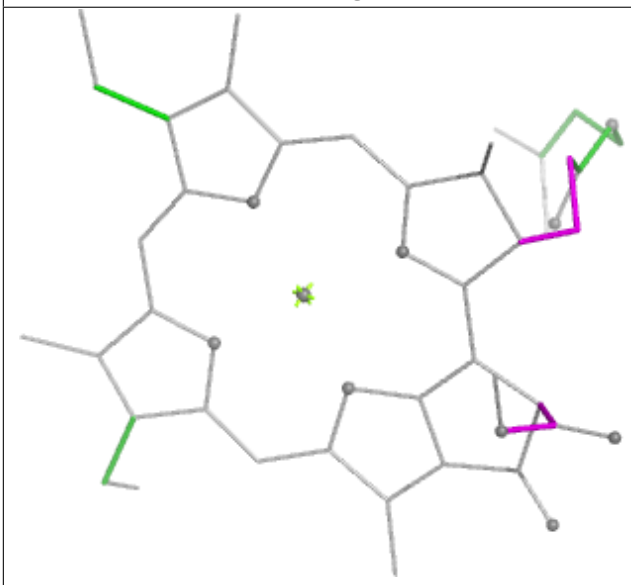


Bond angles



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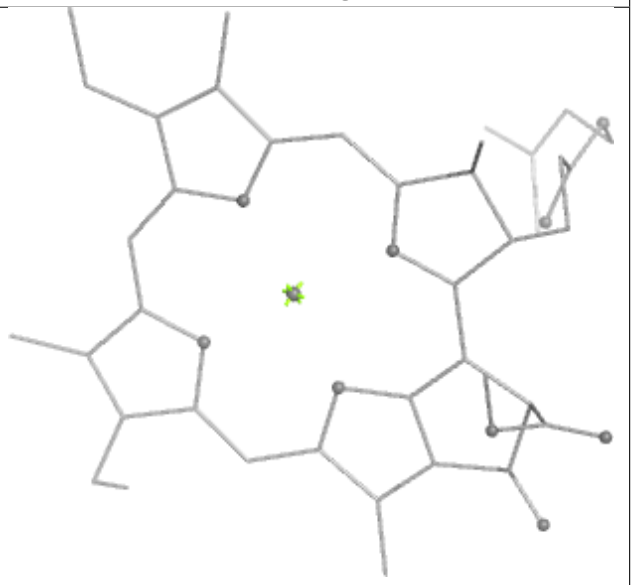
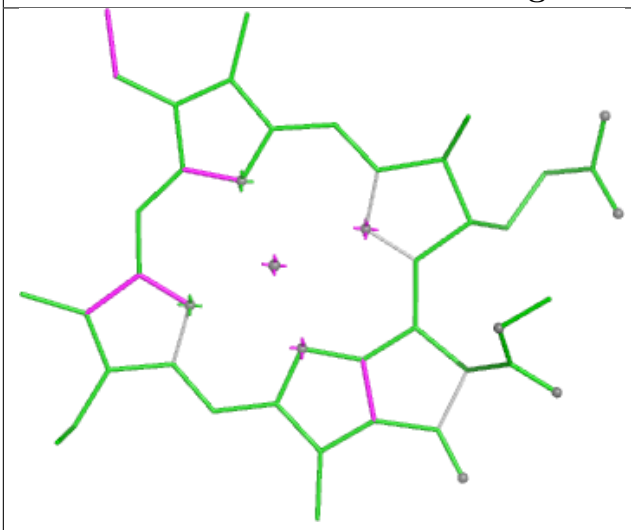
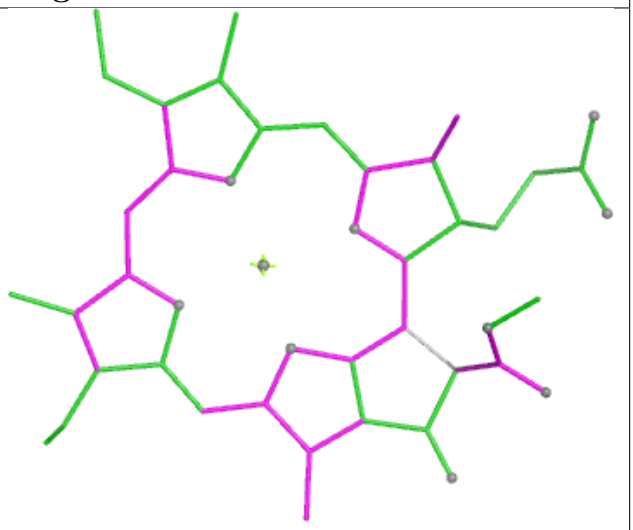


Rings

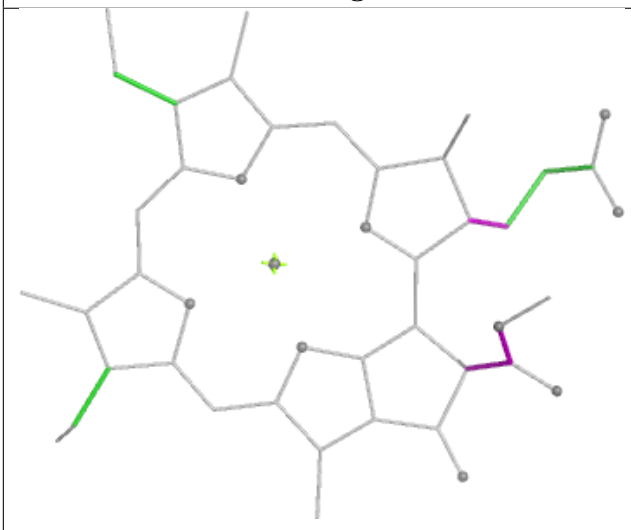
Ligand CLA g 612



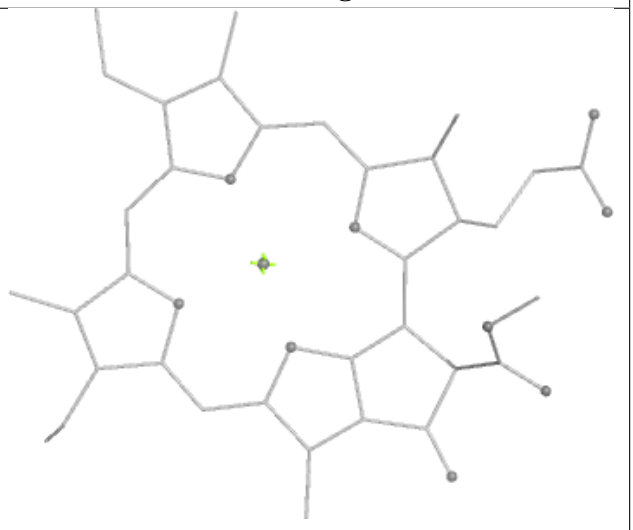
Bond lengths



Bond angles

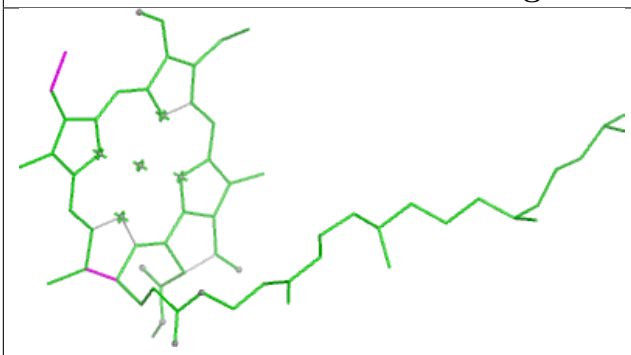


Torsions



Rings

Ligand CHL Y 609



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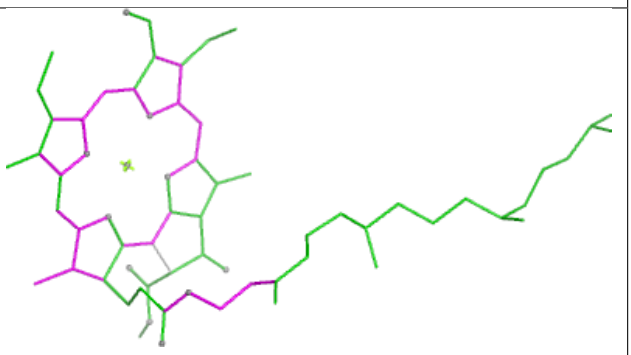

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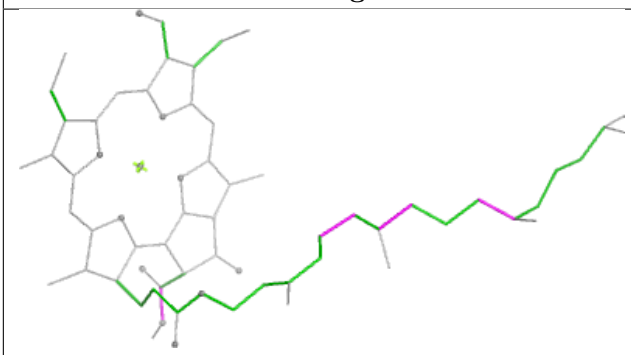

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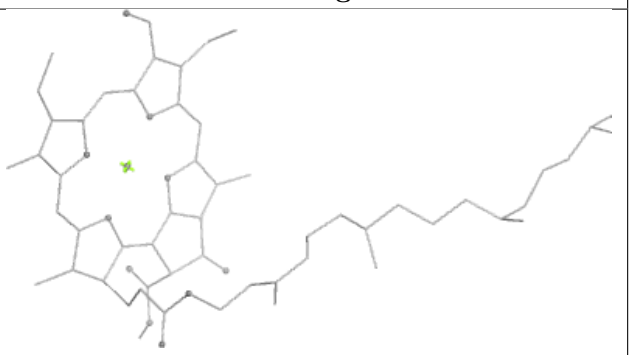
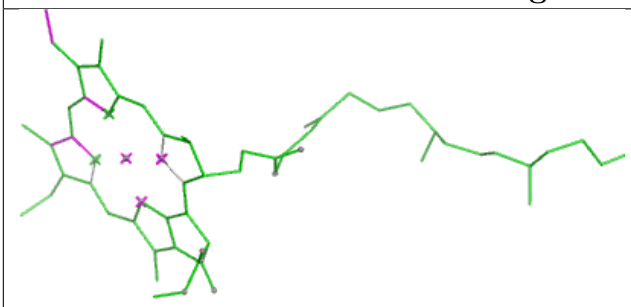


Rings

Ligand CLA c 502



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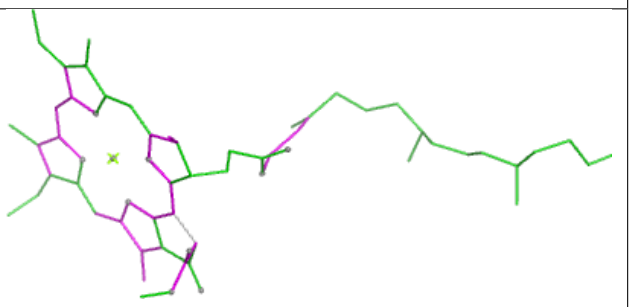

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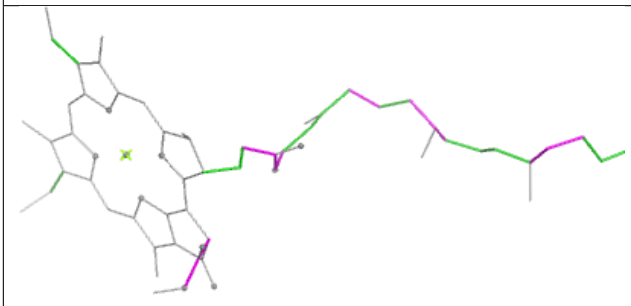

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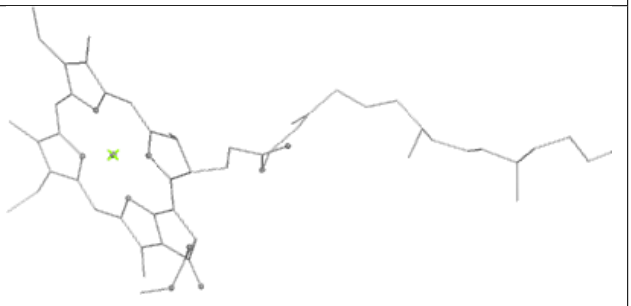
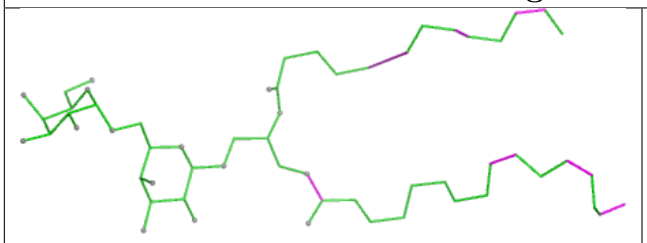


Rings

Ligand DGD c 518



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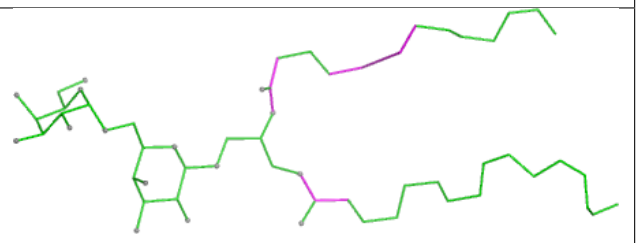
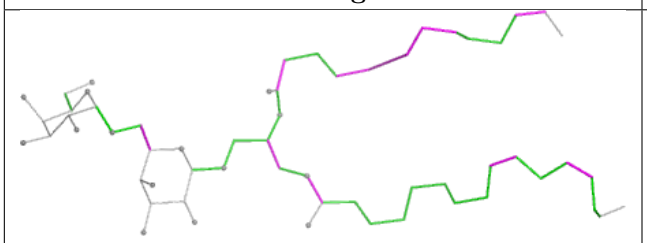


Bond angles



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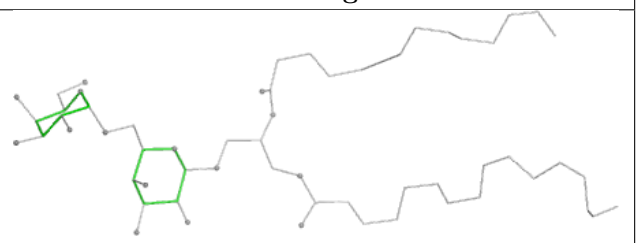
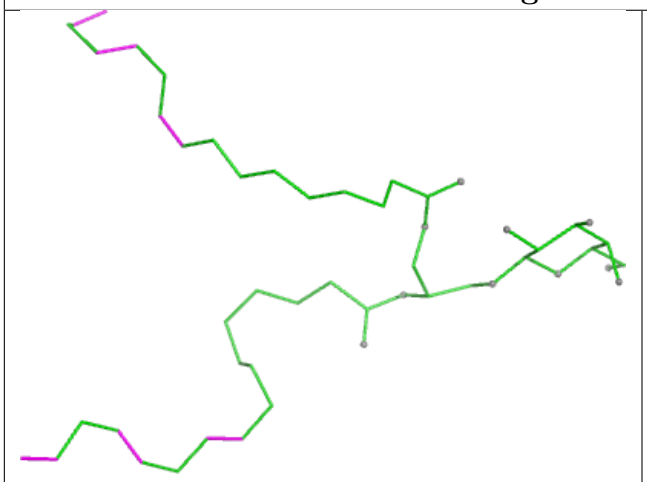


Rings

Ligand LMG B 621



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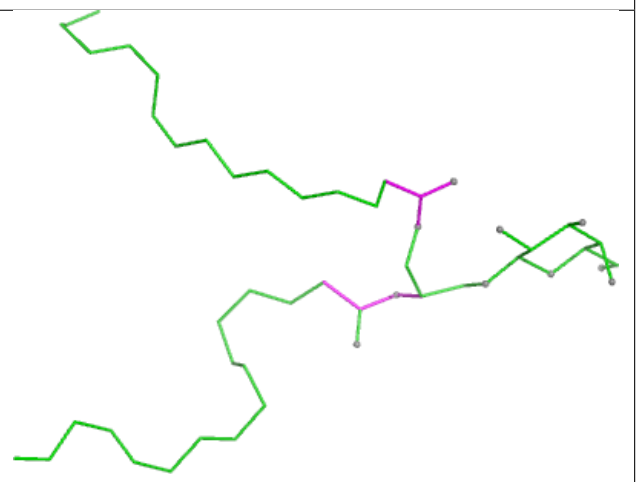

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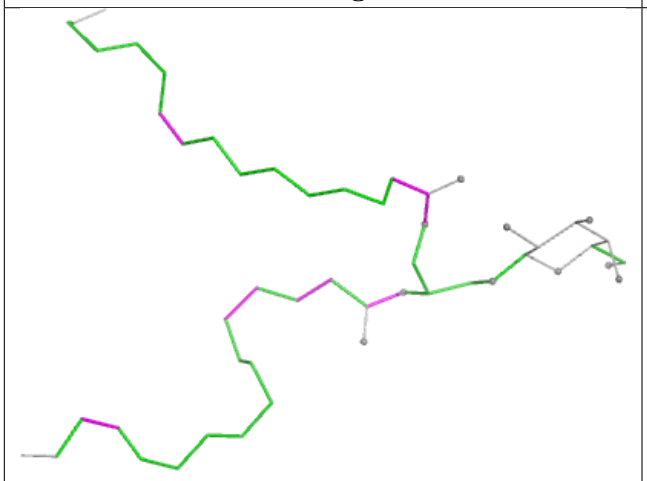

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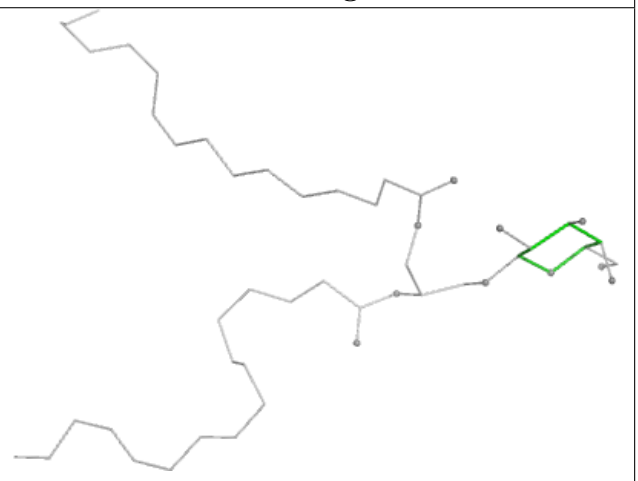
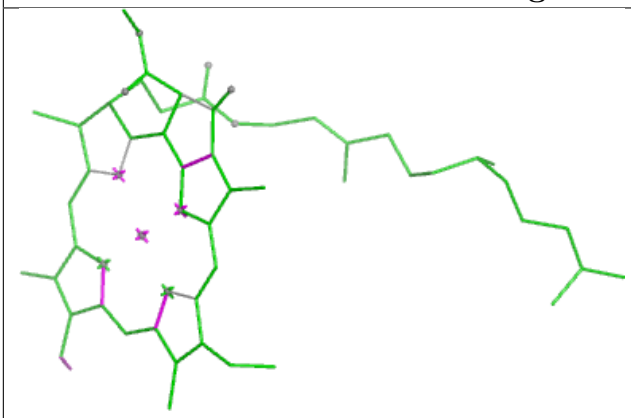


Rings

Ligand CLA g 611



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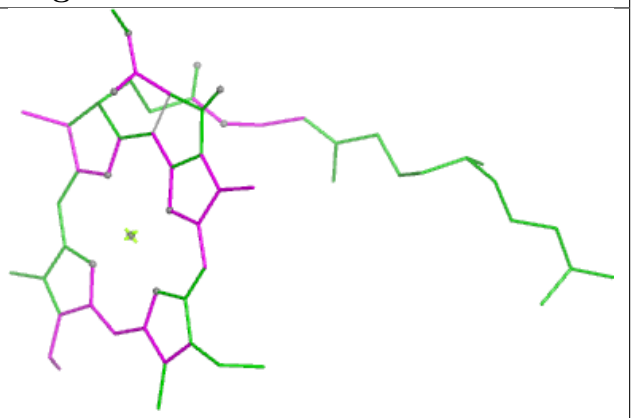
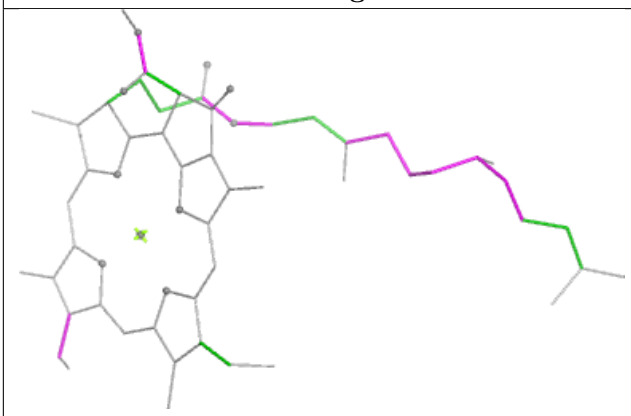


Bond angles



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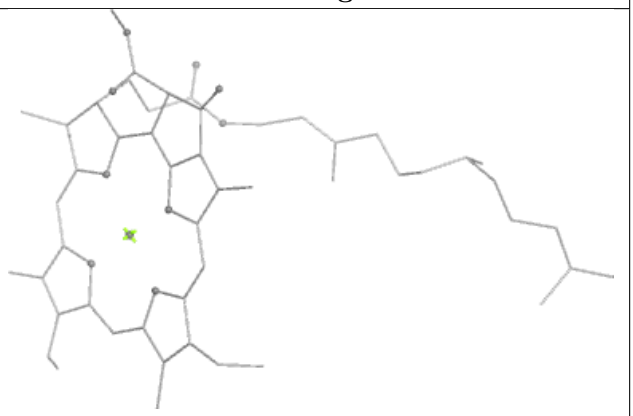
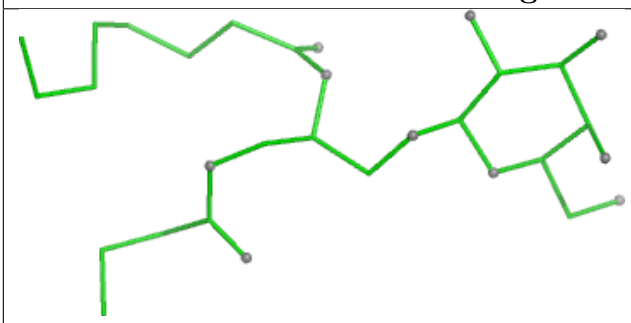


Rings

Ligand LMG B 624



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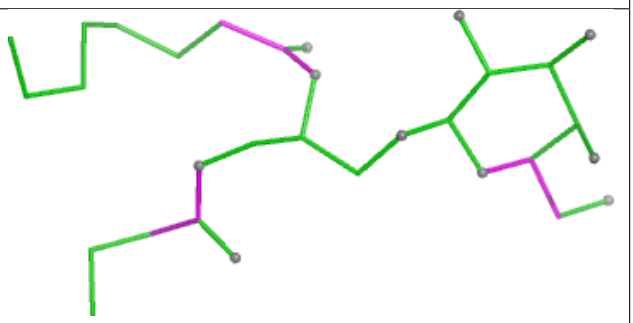
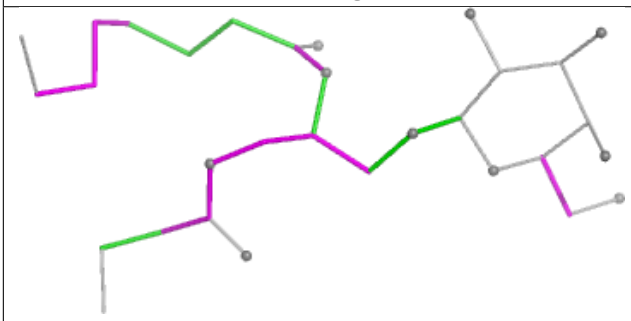


Bond angles



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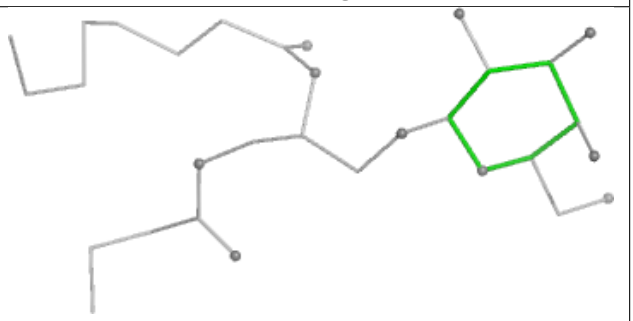
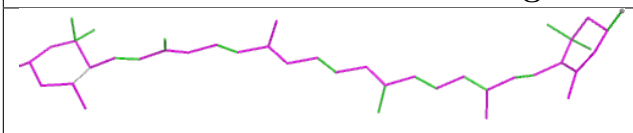


Rings

Ligand LUT N 616



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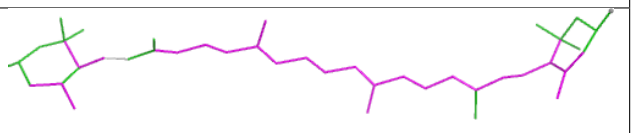
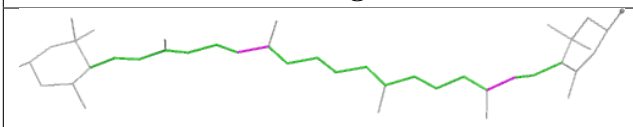


Bond angles



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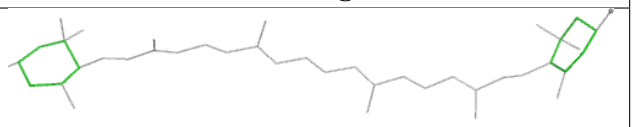
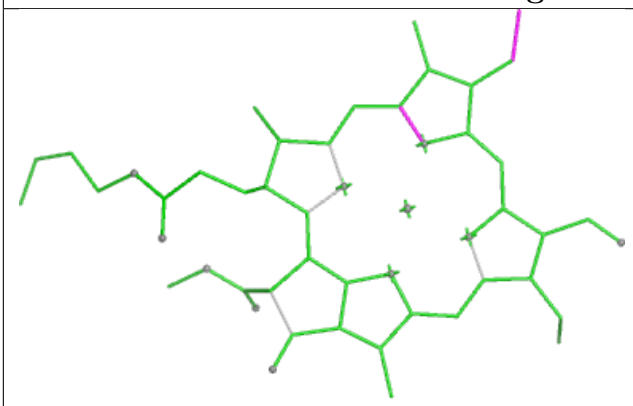
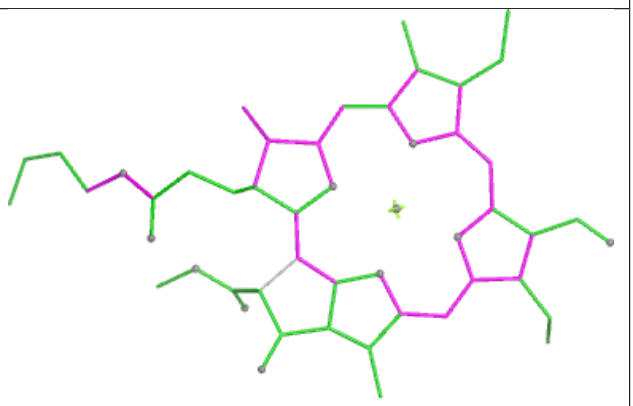


Rings

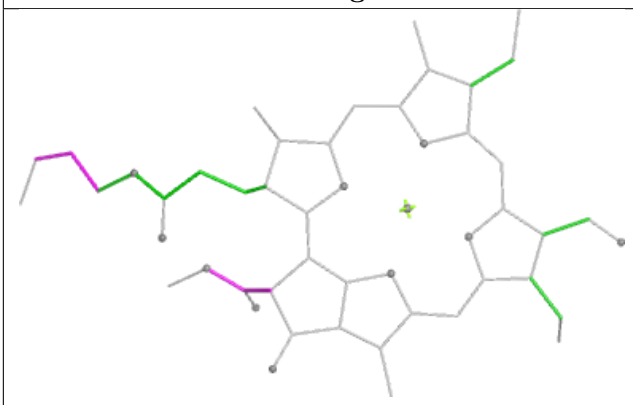
Ligand CHL n 606



Bond lengths



Bond angles



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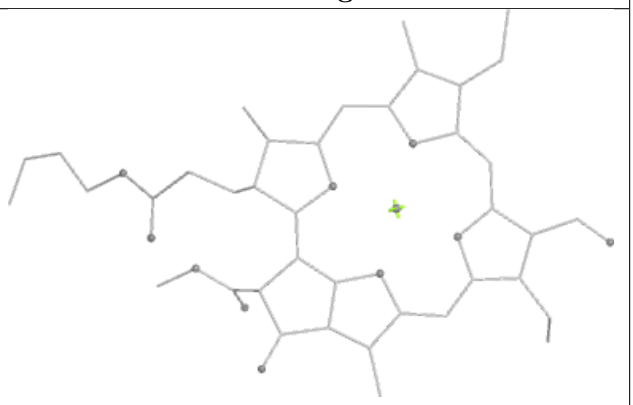
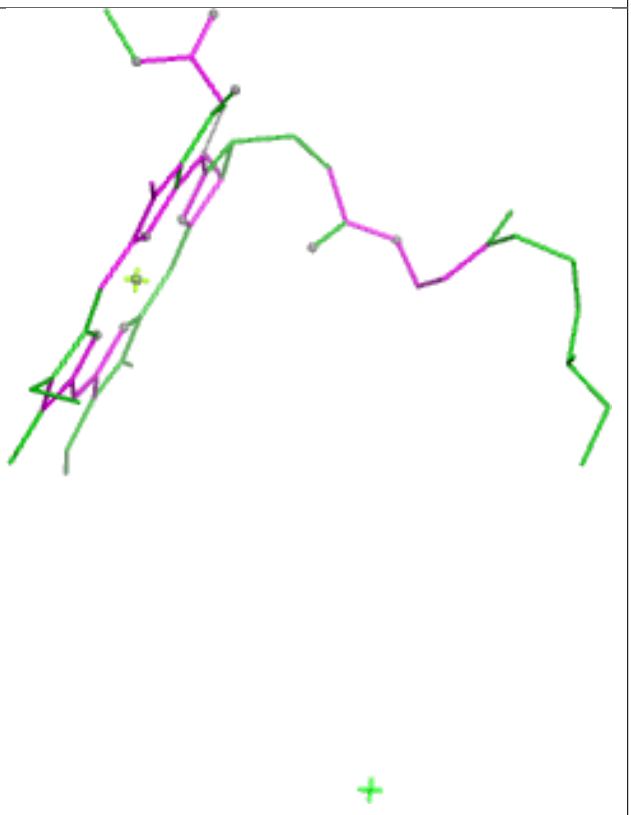


Rings

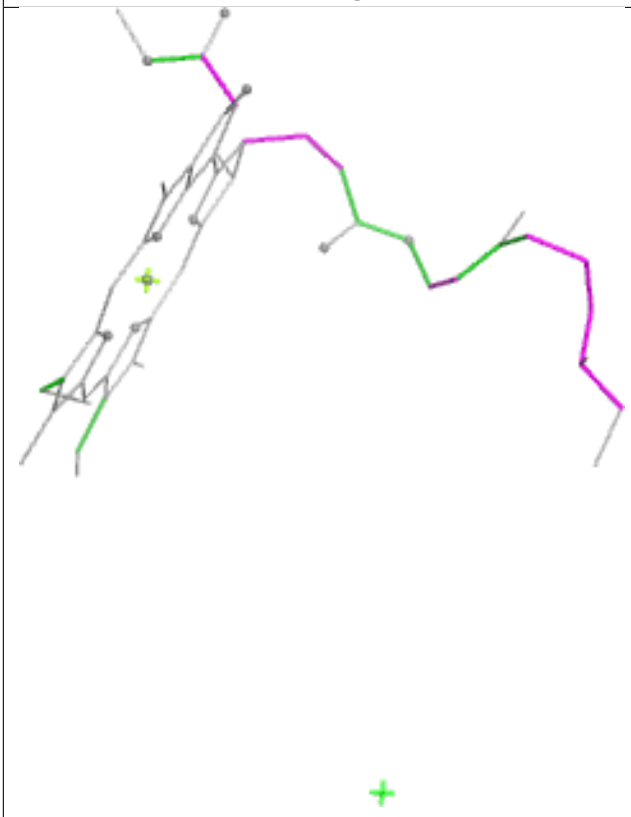
Ligand CLA c 506



Bond lengths



Bond angles

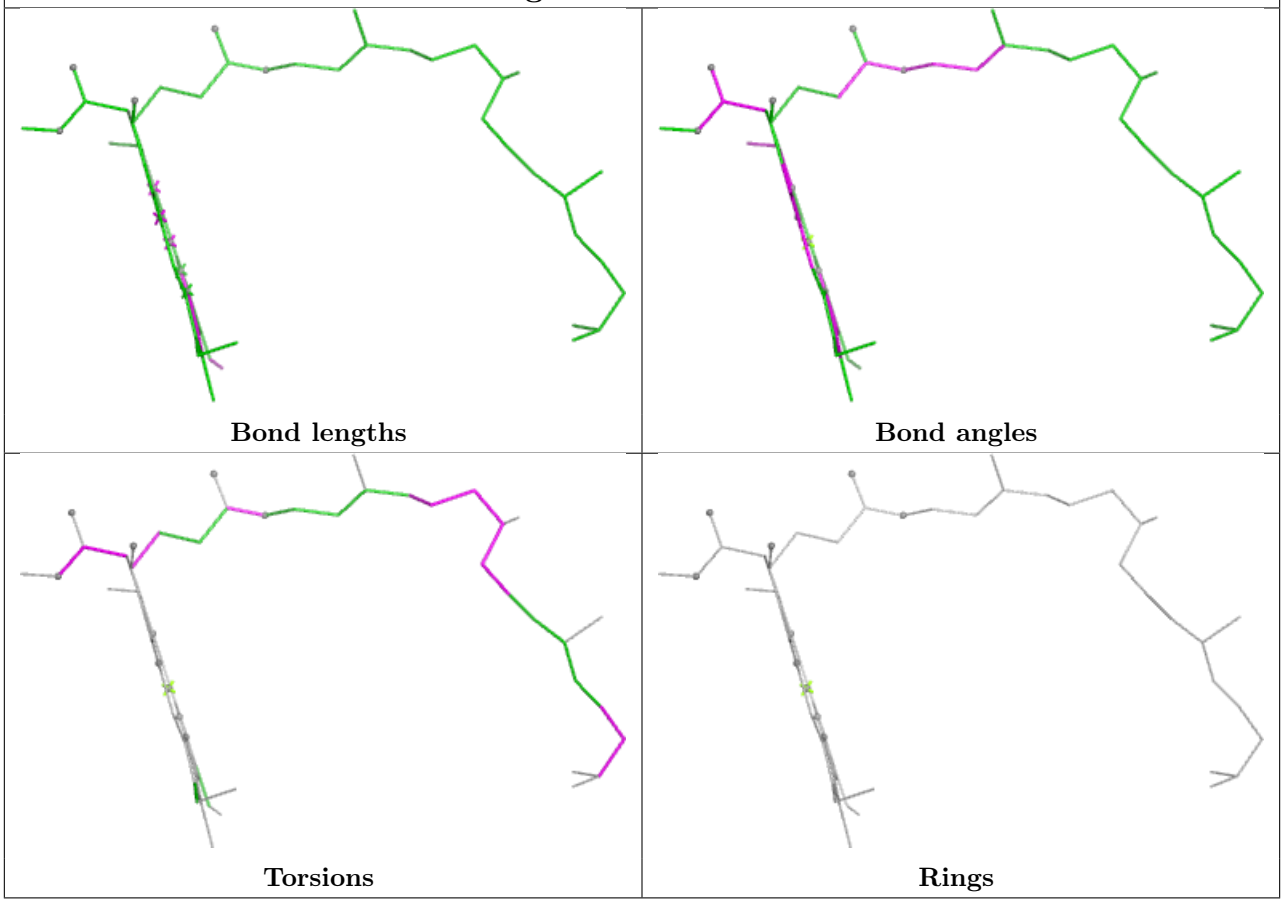


Torsions

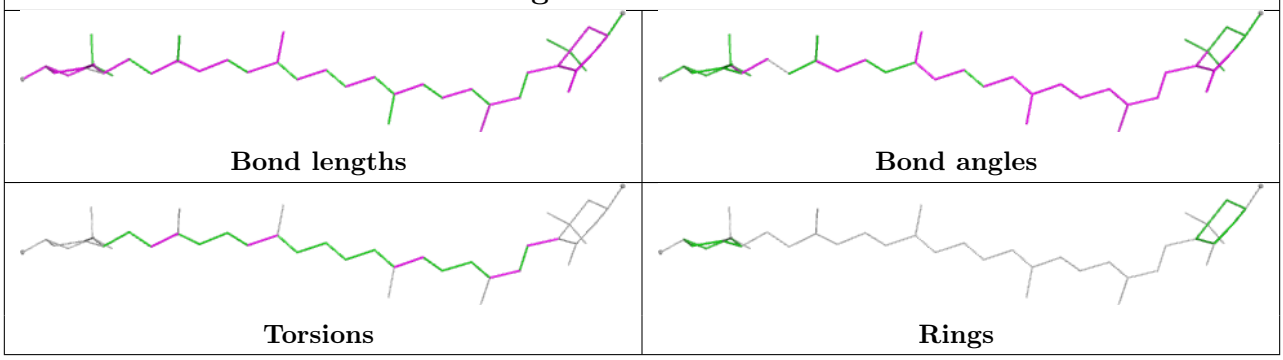


Rings

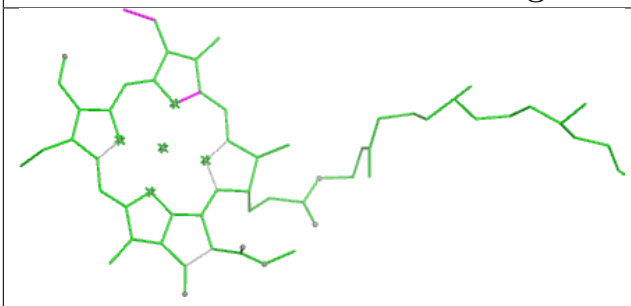
Ligand CLA C 506



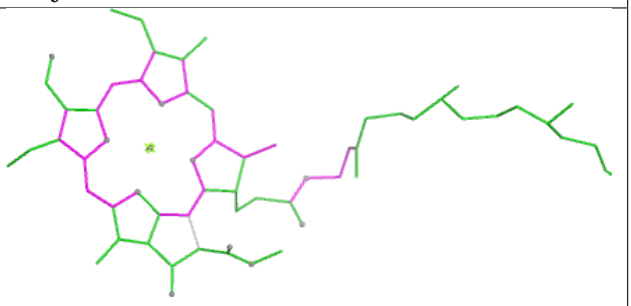
Ligand LUT s 614



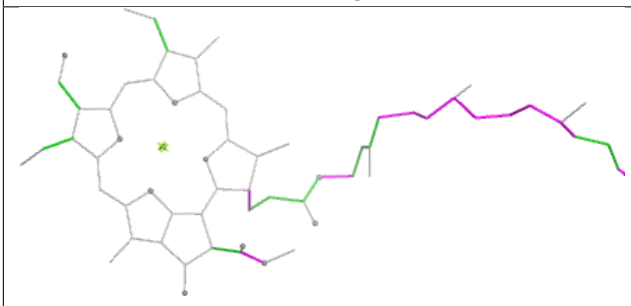
Ligand CHL y 302



Bond lengths



Bond angles



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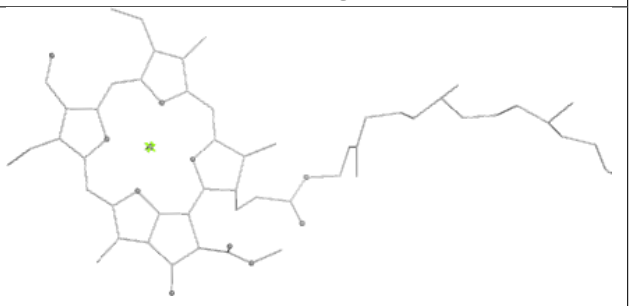
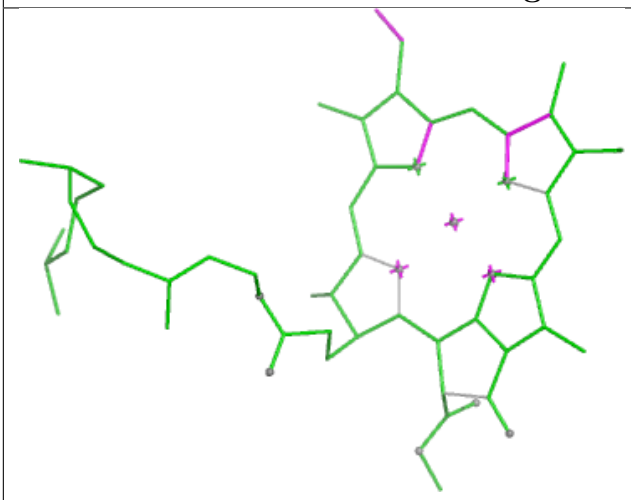


Rings

Ligand CLA A 408



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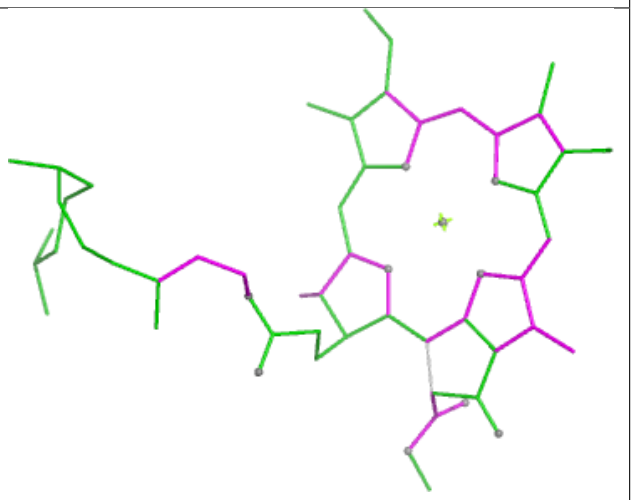

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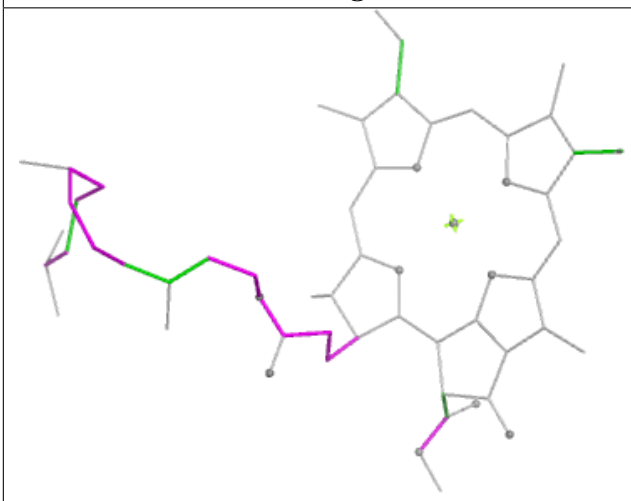

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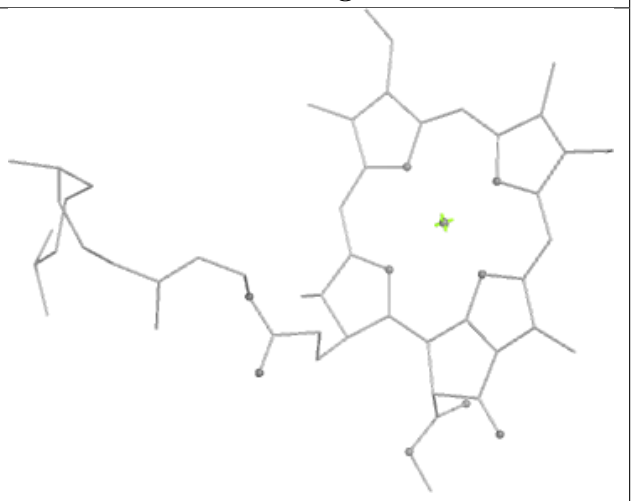
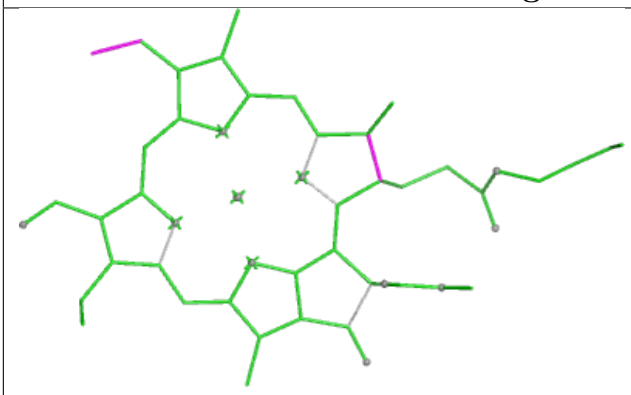


Rings

Ligand CHL N 606



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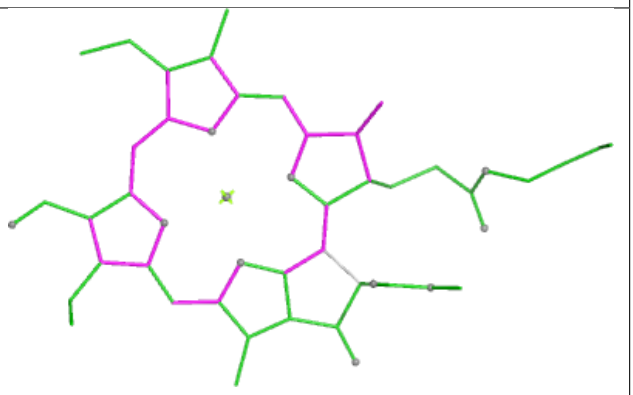
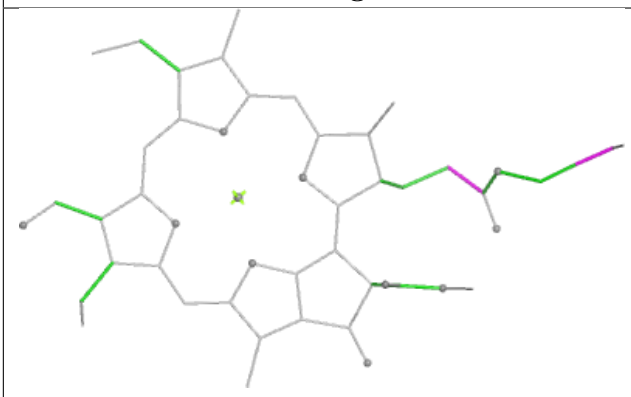


Bond angles



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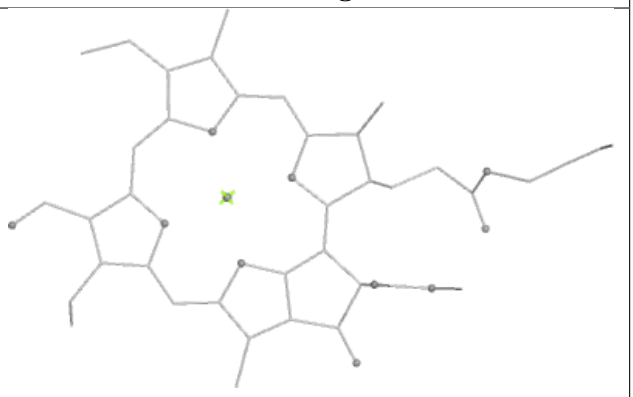
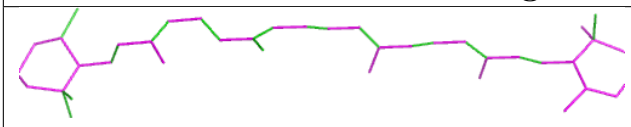
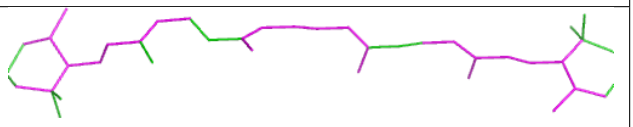


Rings

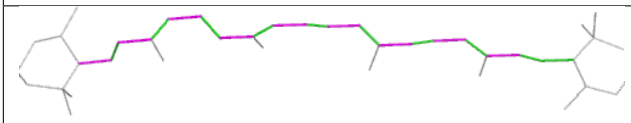
Ligand BCR H 101



Bond lengths



Bond angles



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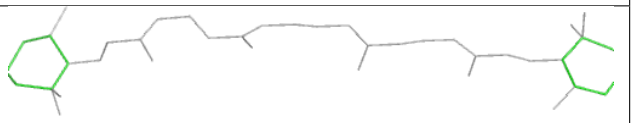
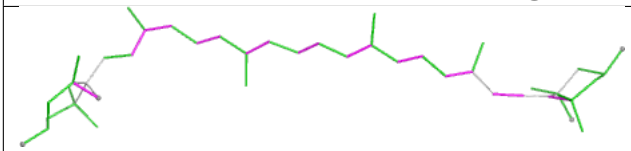


Rings

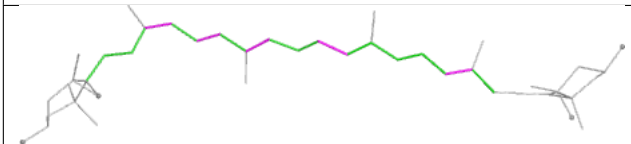
Ligand NEX y 318



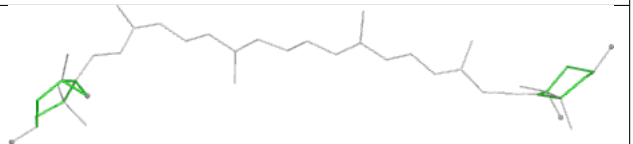
Bond lengths



Bond angles

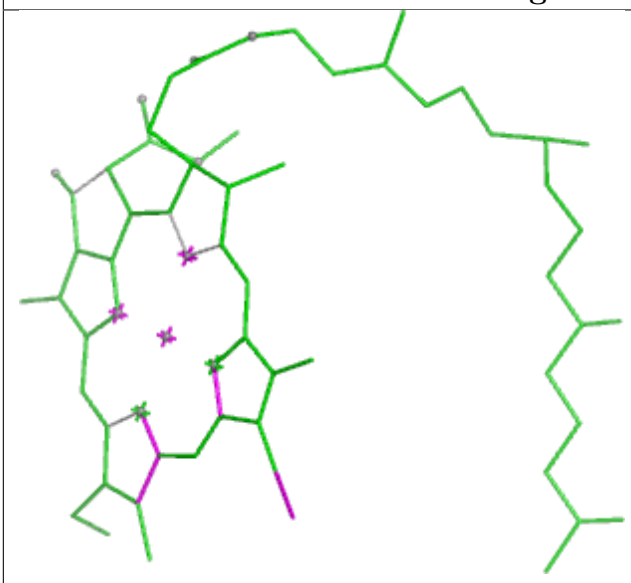


Torsions

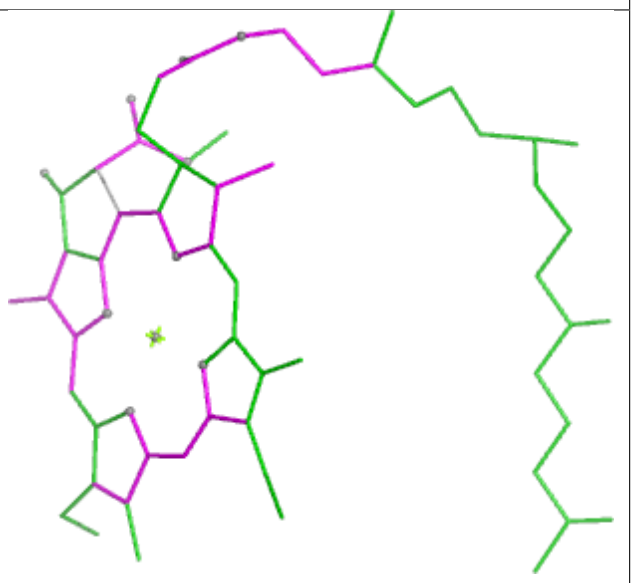


Rings

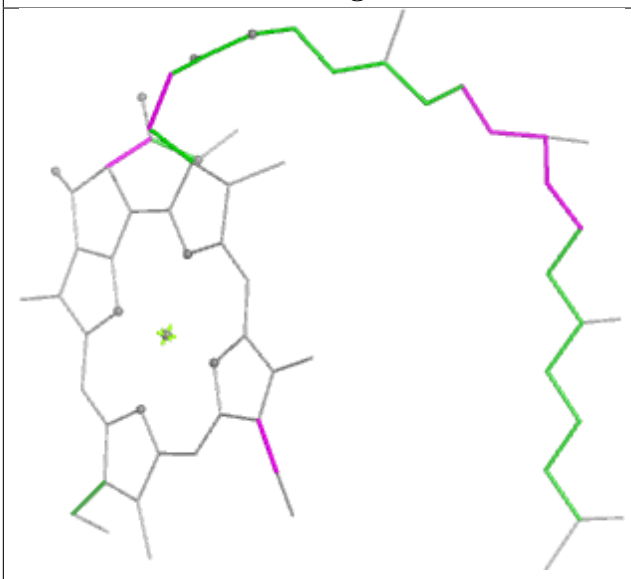
Ligand CLA c 507



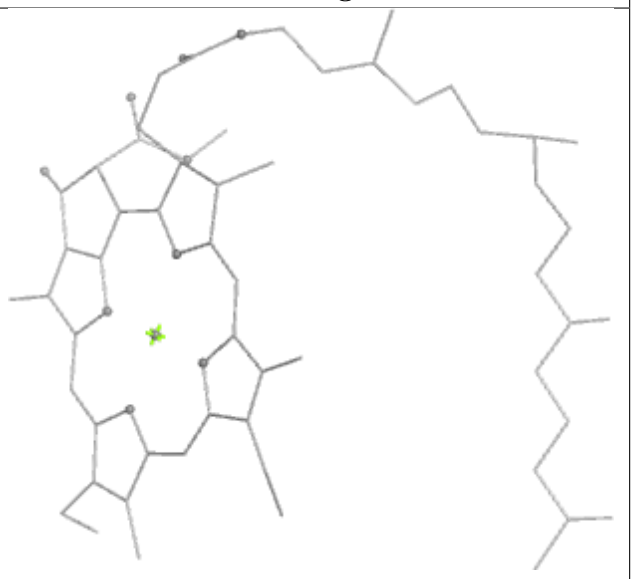
Bond lengths



Bond angles

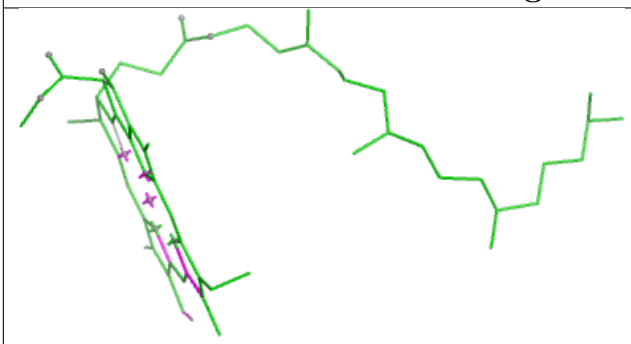


Torsions



Rings

Ligand CLA C 508



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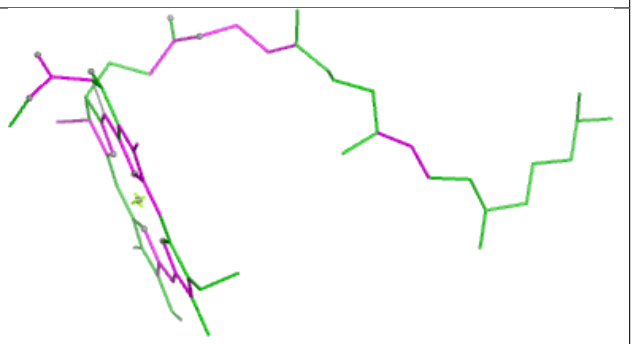

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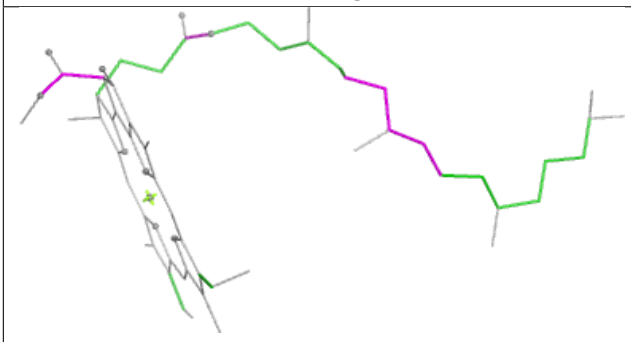
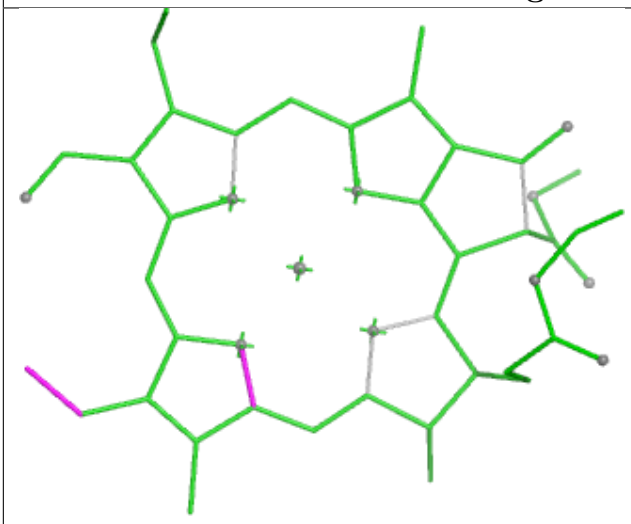


Torsions



Rings

Ligand CHL n 605



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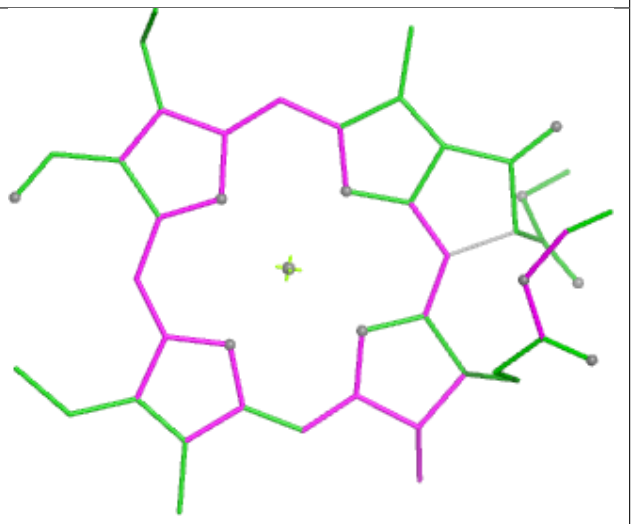
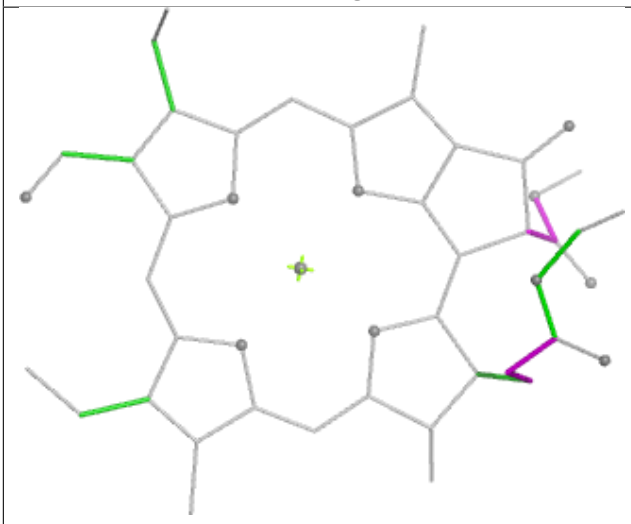


Bond angles



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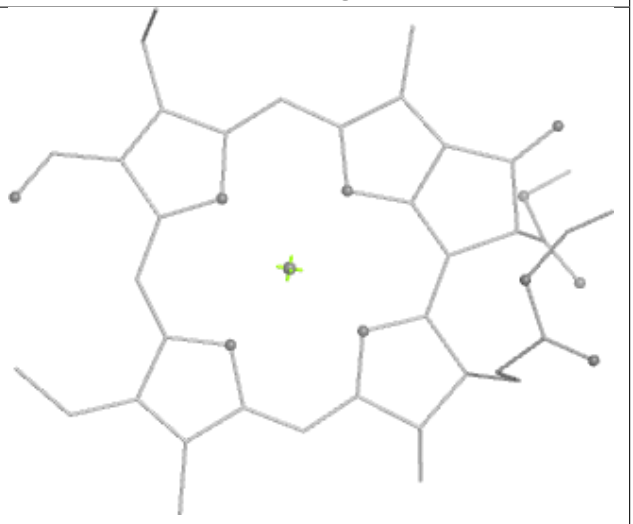
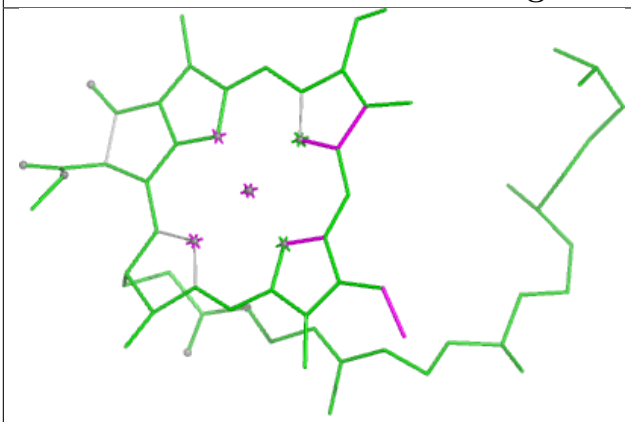


Rings

Ligand CLA n 602



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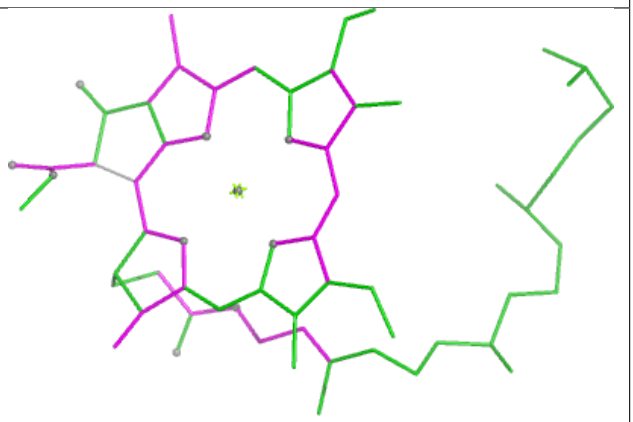

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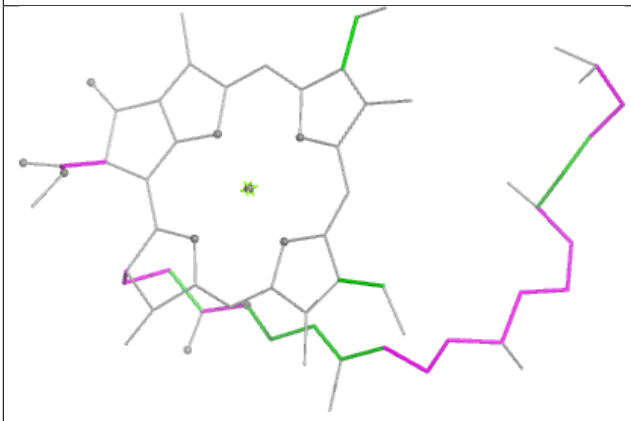

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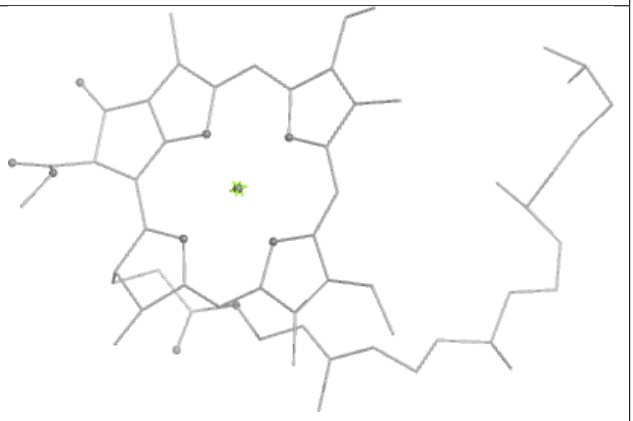
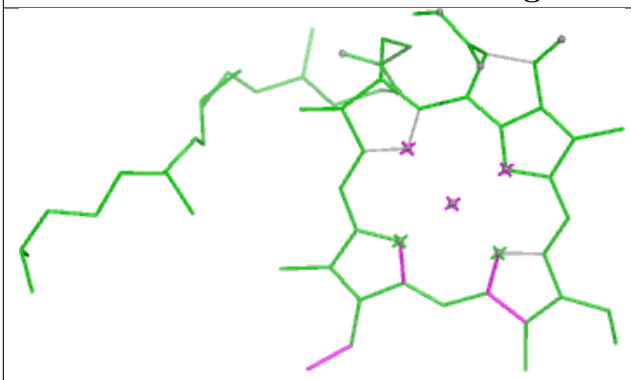


Rings

Ligand CLA D 401



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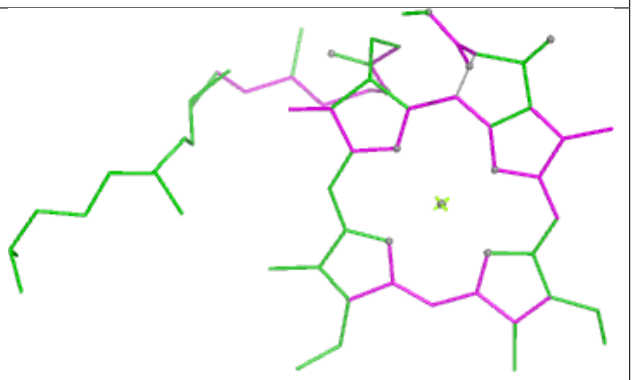

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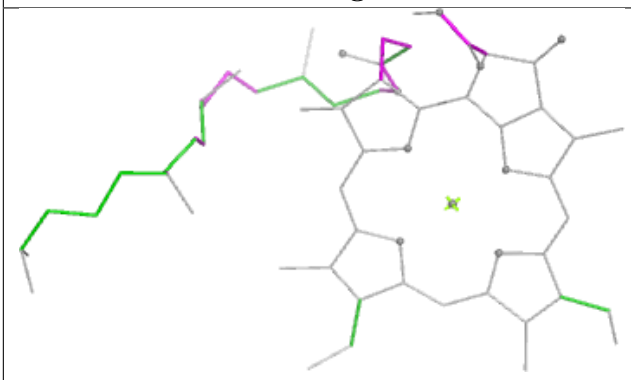
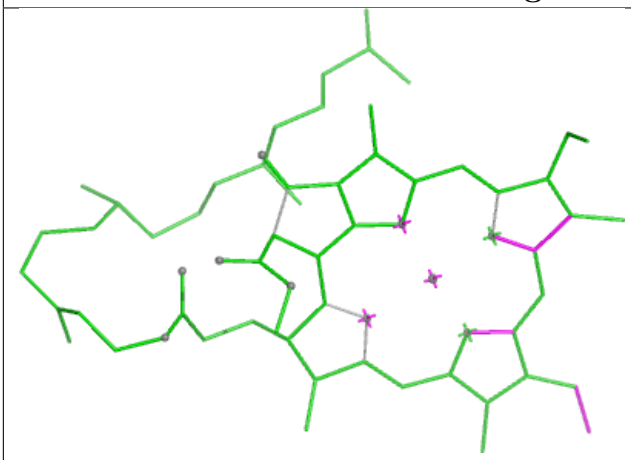


Torsions



Rings

Ligand CLA C 509



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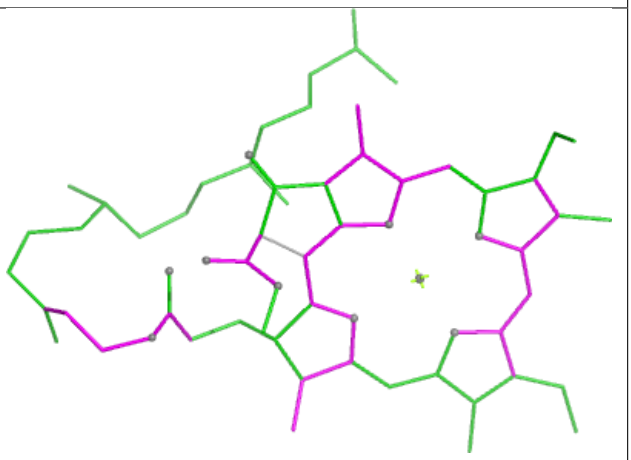

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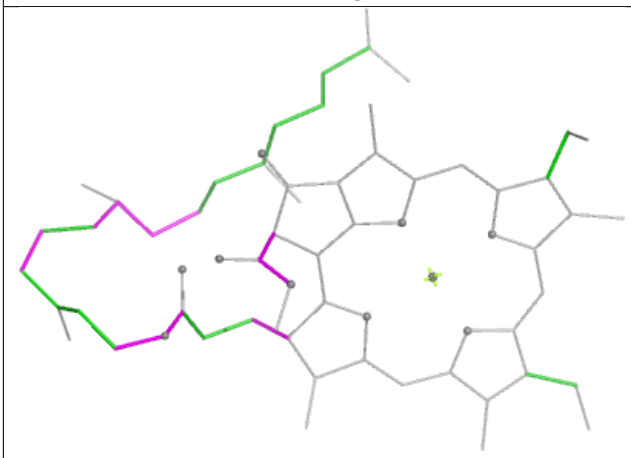

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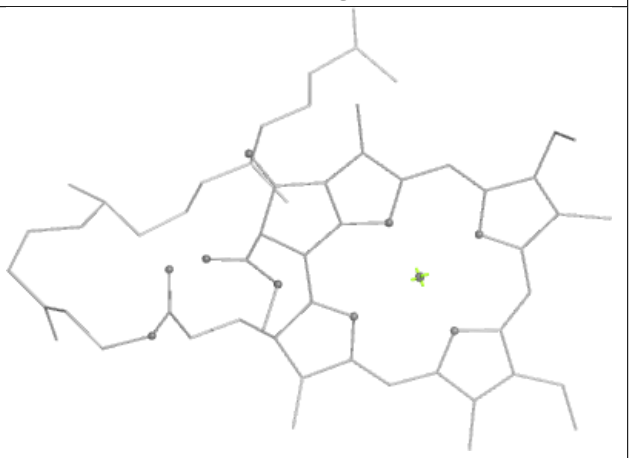
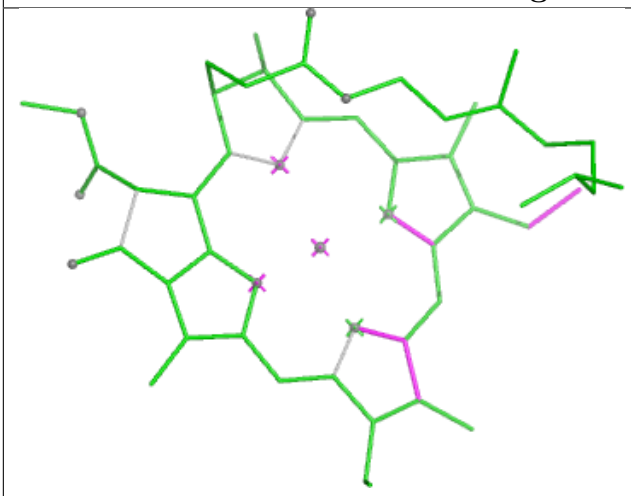


Rings

Ligand CLA s 609



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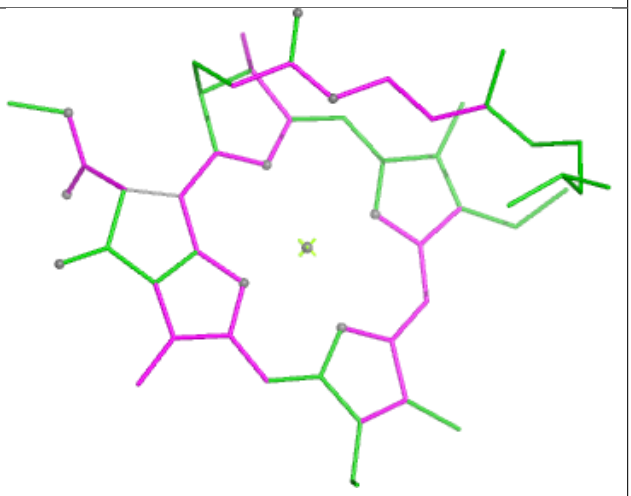
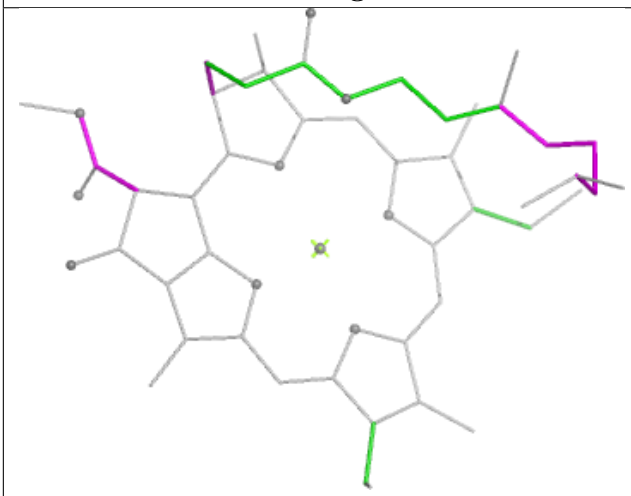


Bond angles



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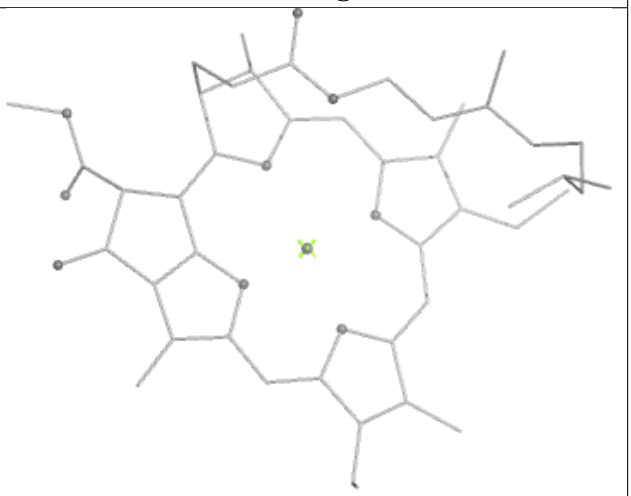
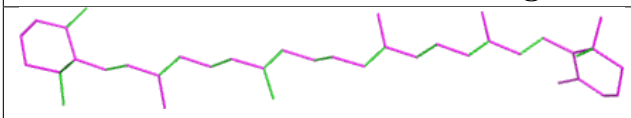


Rings

Ligand BCR B 618



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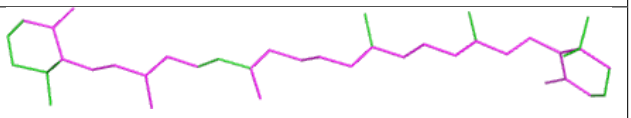
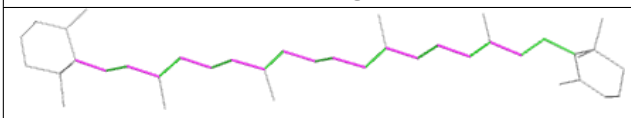


Bond angles



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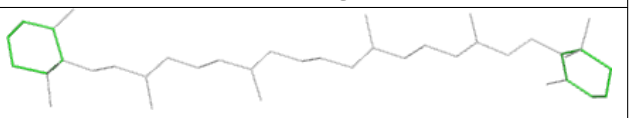
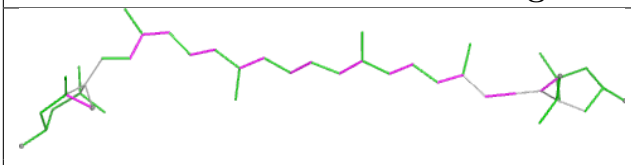


Rings

Ligand NEX r 616



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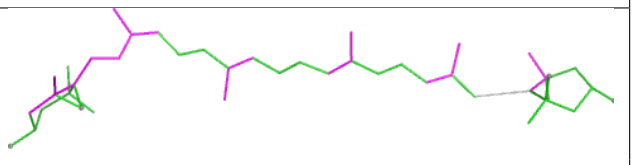
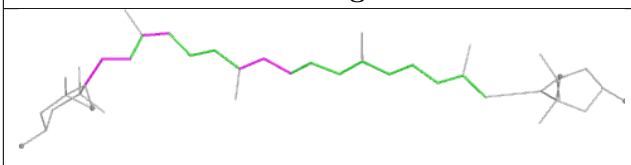


Bond angles



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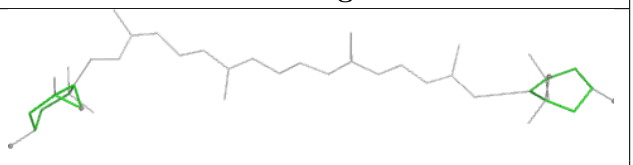
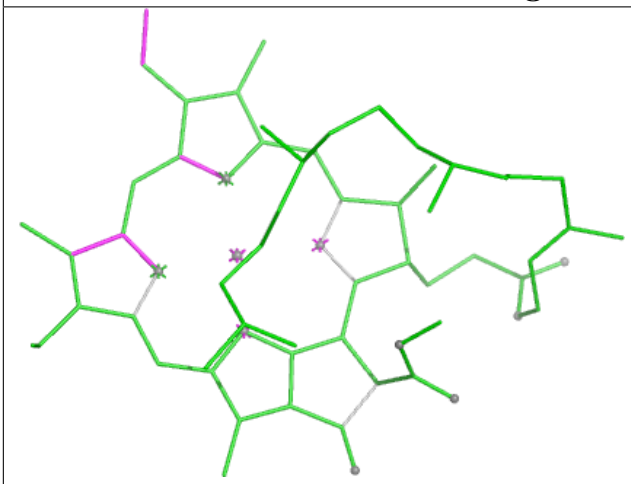


Rings

Ligand CLA C 510



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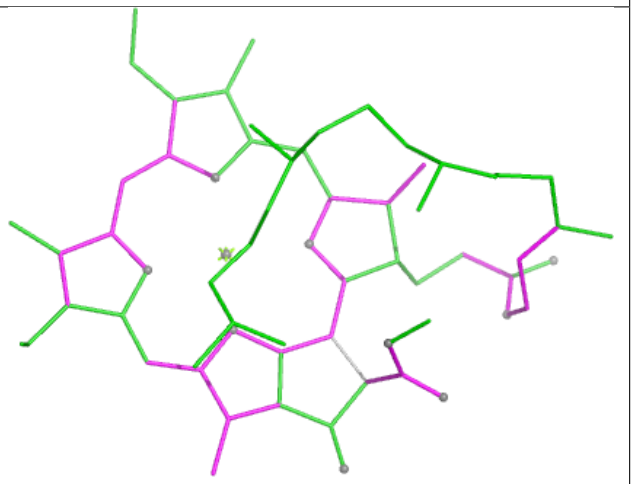
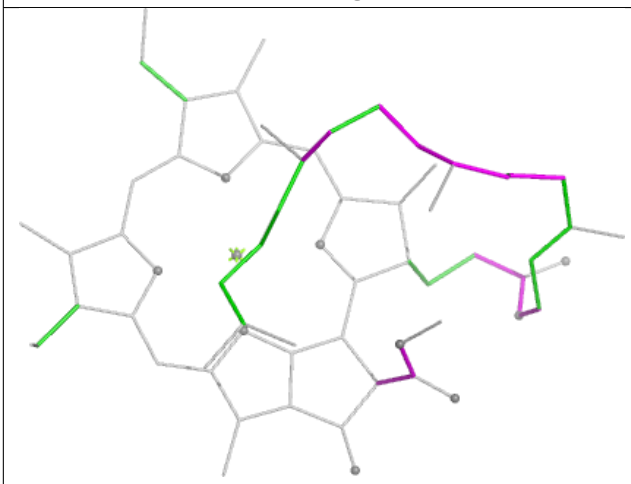


Bond angles



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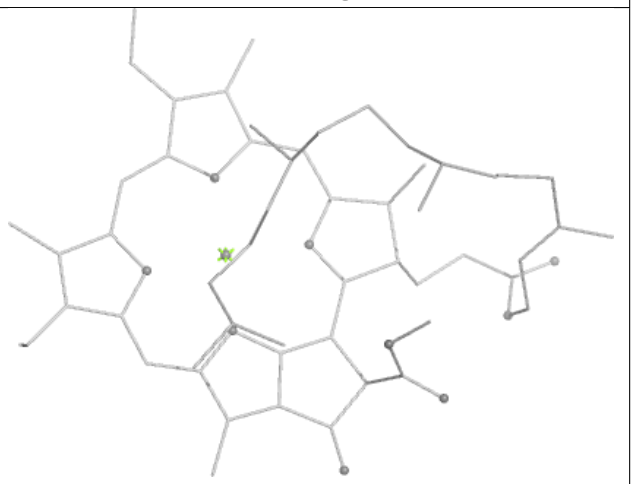

Rings

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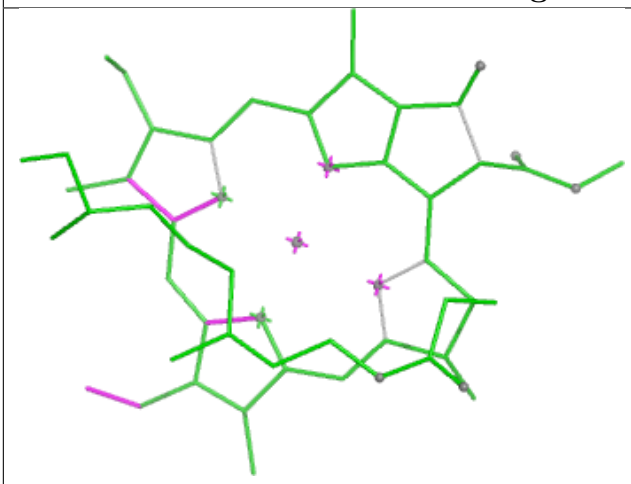

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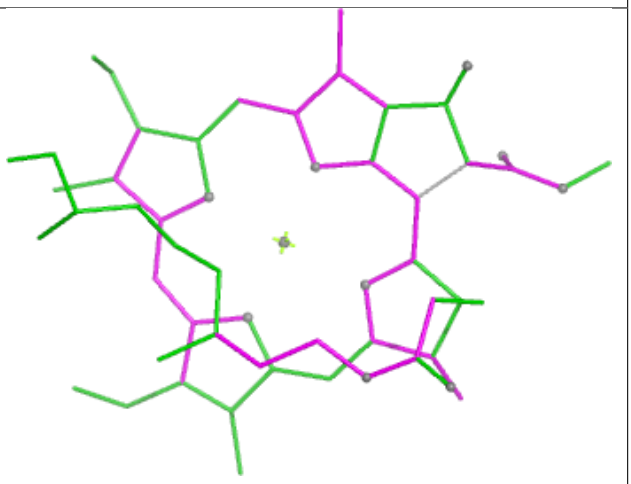

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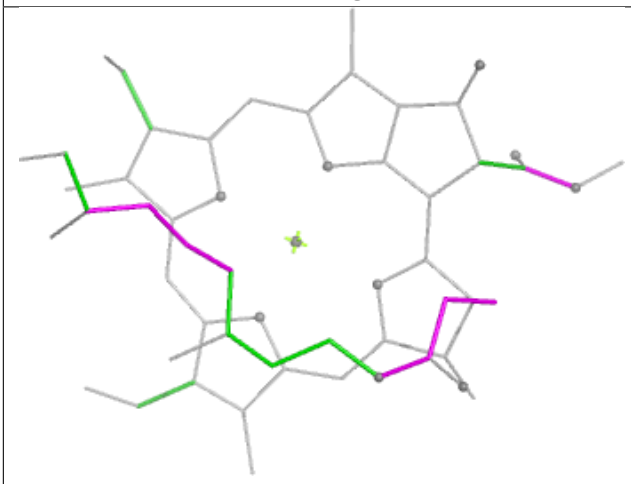

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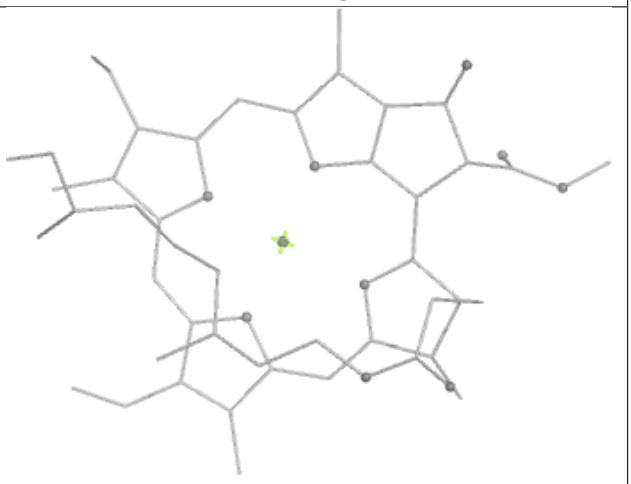
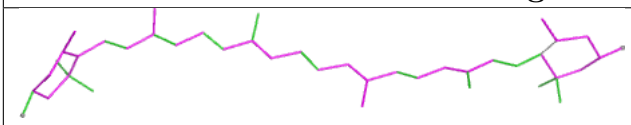


Rings

Ligand LUT n 616



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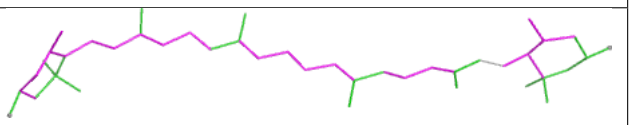


Bond angles

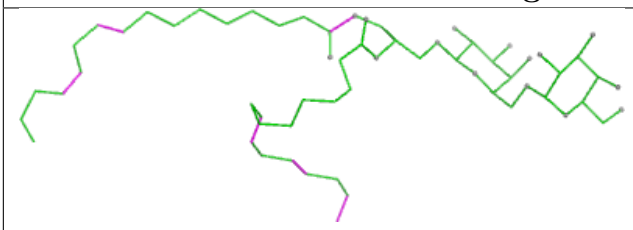


Torsions



Rings

Ligand DGD b 625



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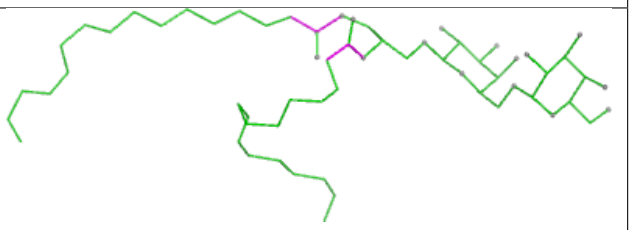
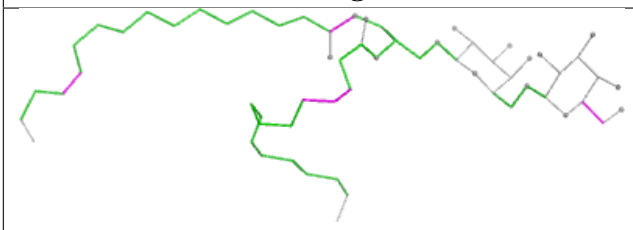


Bond angles



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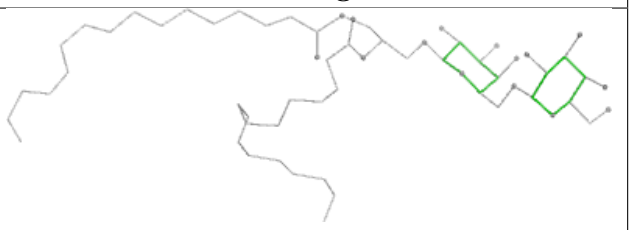

Rings

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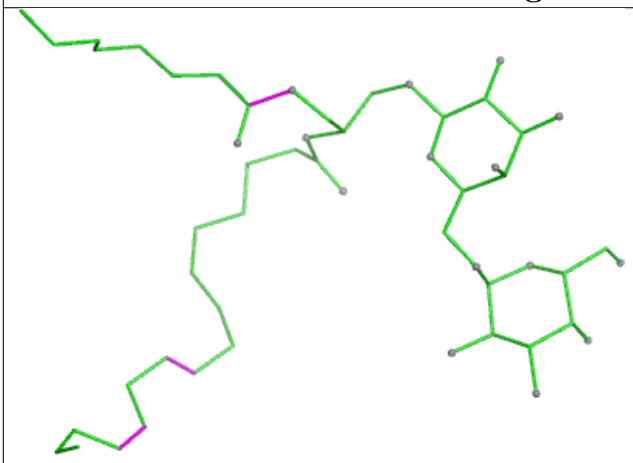

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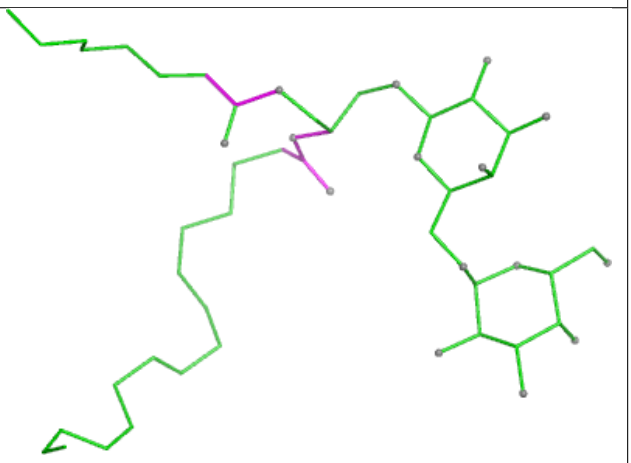
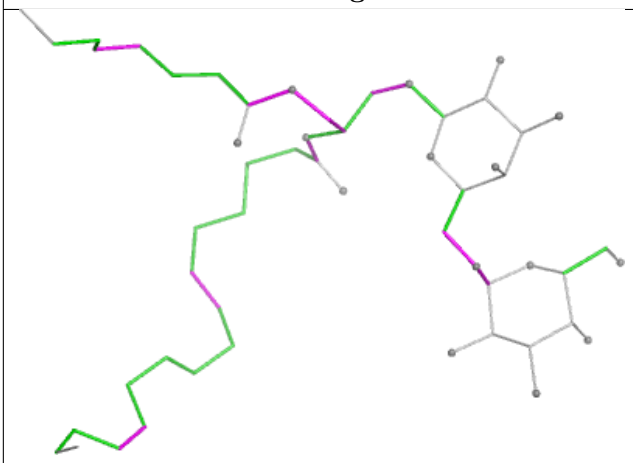


Bond angles



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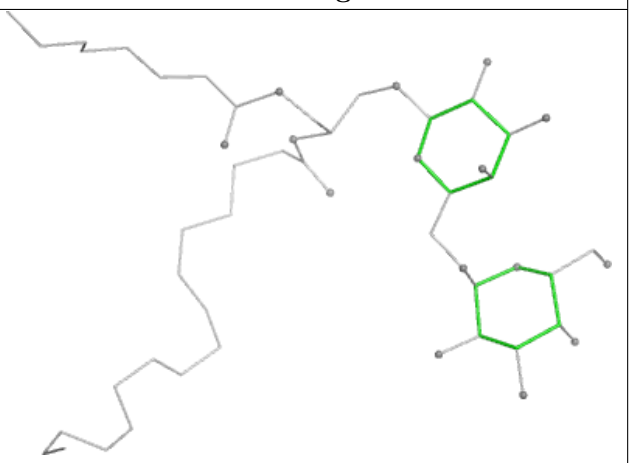
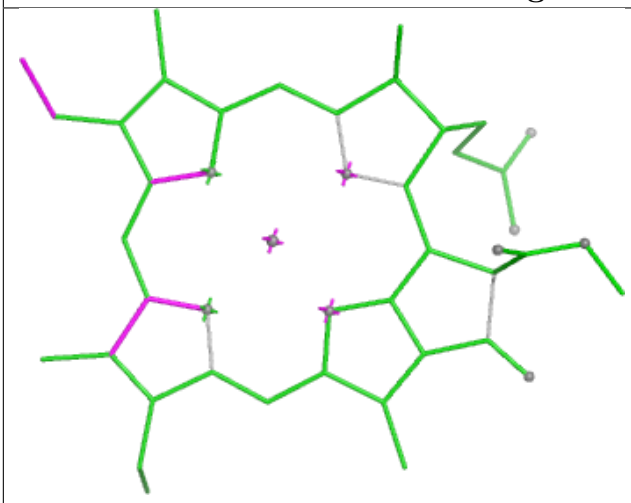


Rings

Ligand CLA n 614



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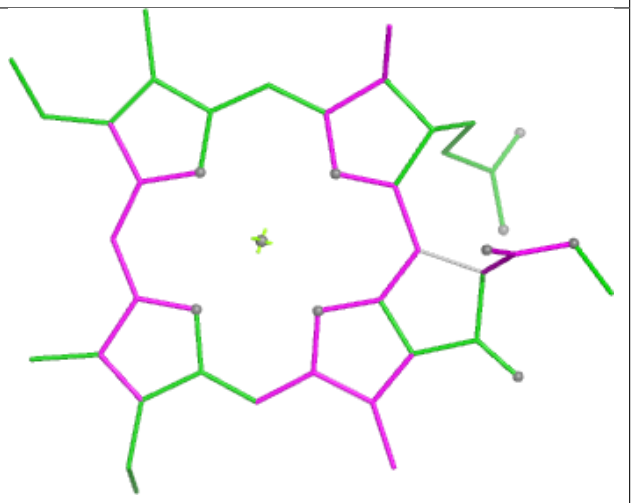
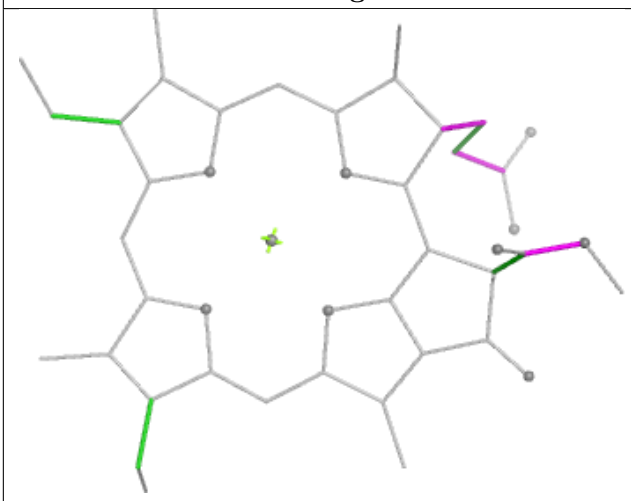


Bond angles



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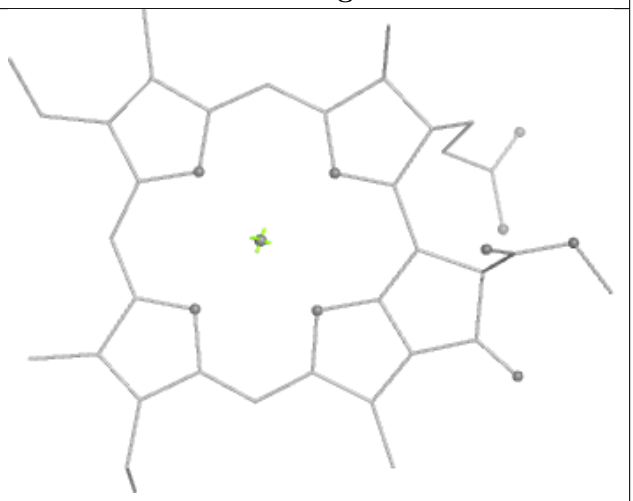
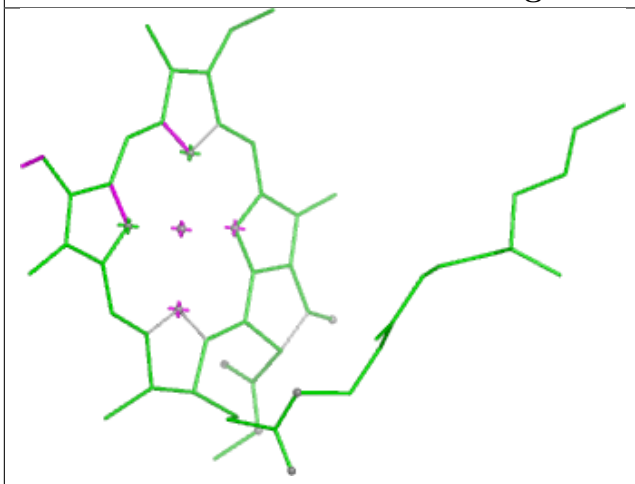
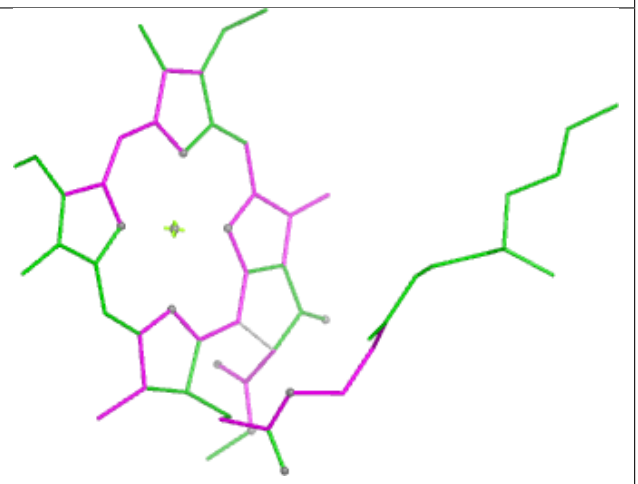


Rings

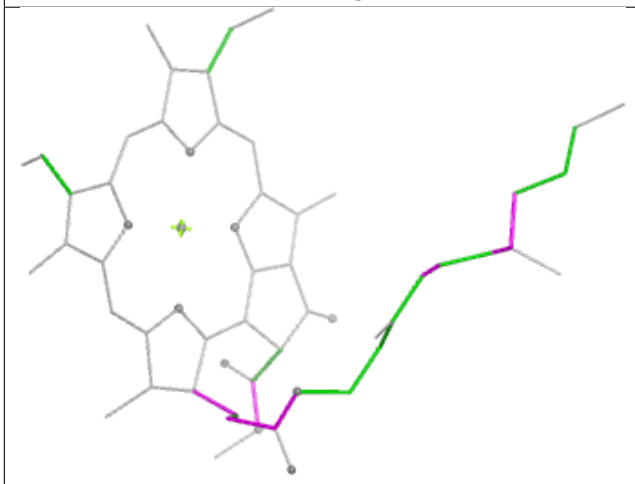
Ligand CLA R 608



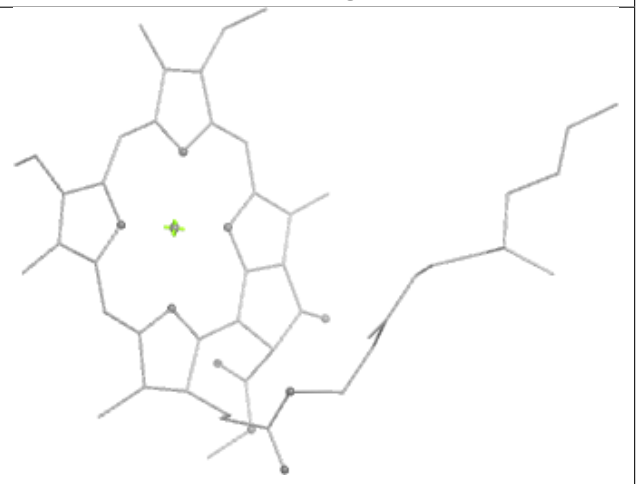
Bond lengths



Bond angles

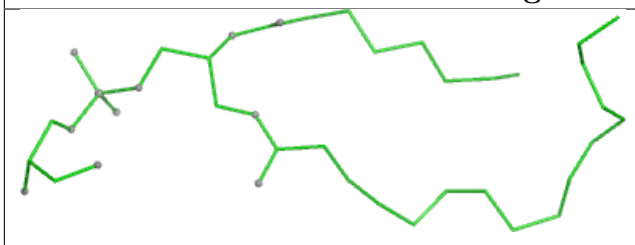


Torsions

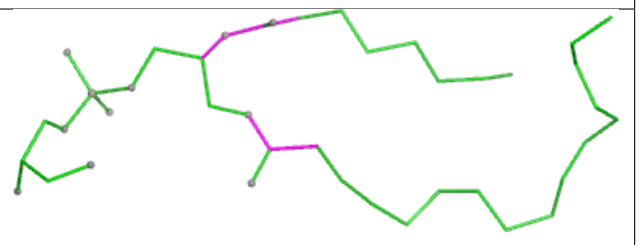


Rings

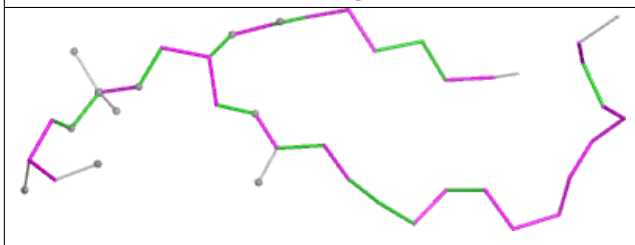
Ligand LHG B 623



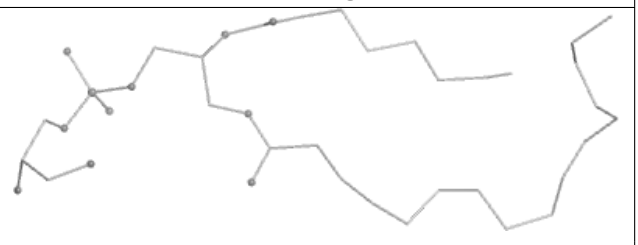
Bond lengths



Bond angles

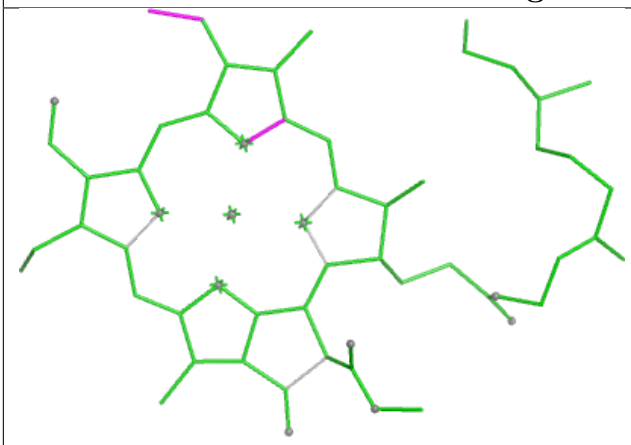


Torsions

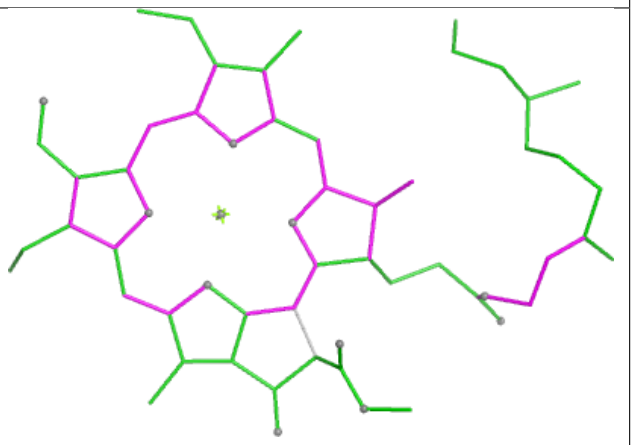


Rings

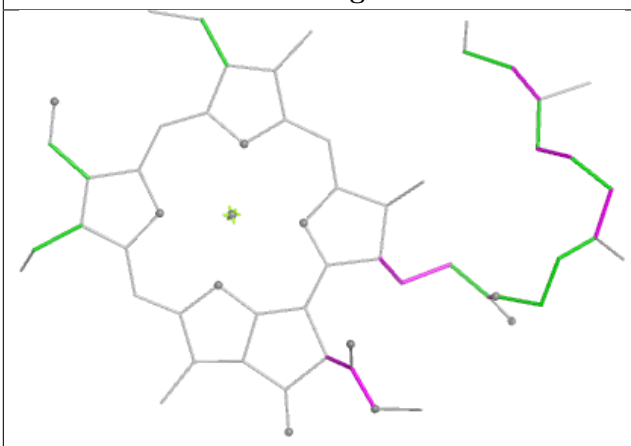
Ligand CHL S 307



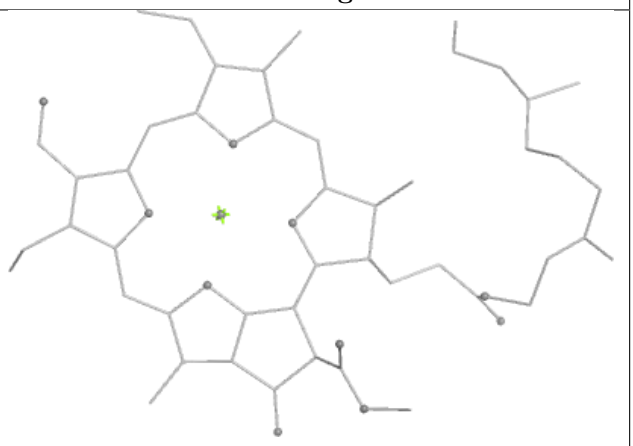
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

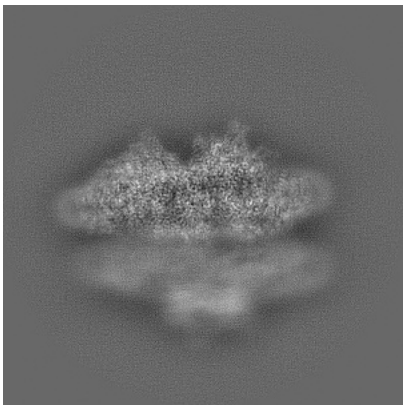
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52846. These allow visual inspection of the internal detail of the map and identification of artifacts.

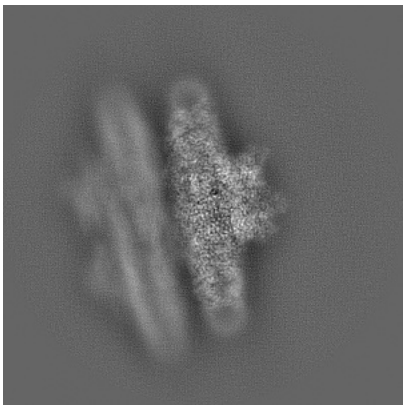
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

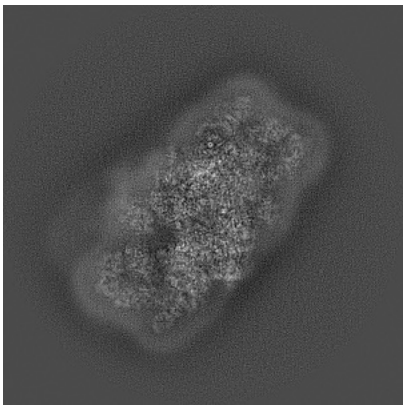
6.1.1 Primary map



X

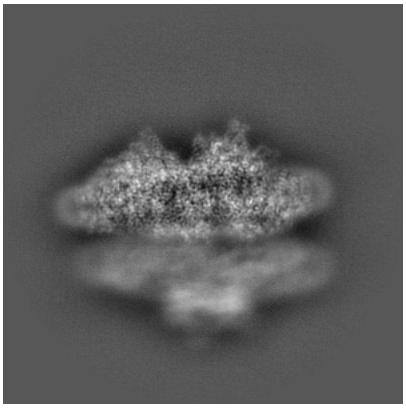


Y

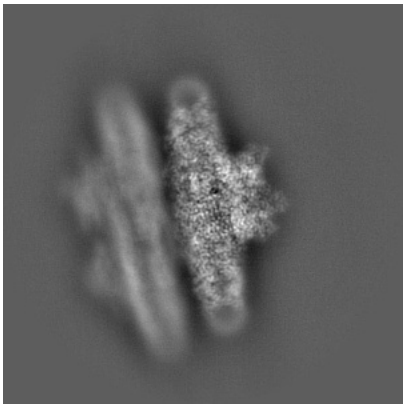


Z

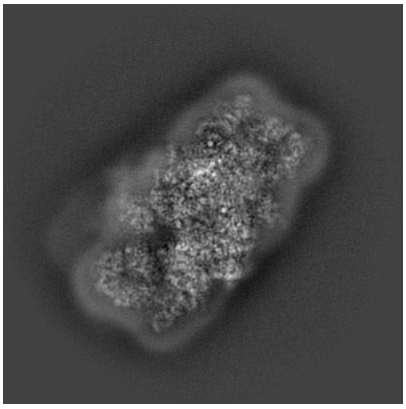
6.1.2 Raw map



X



Y

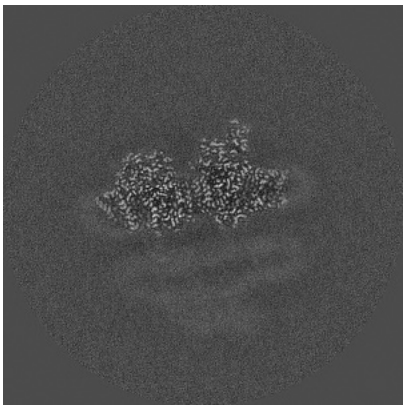


Z

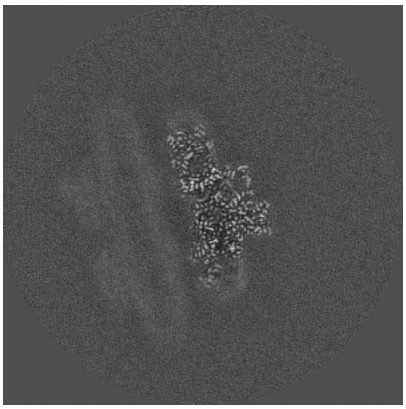
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

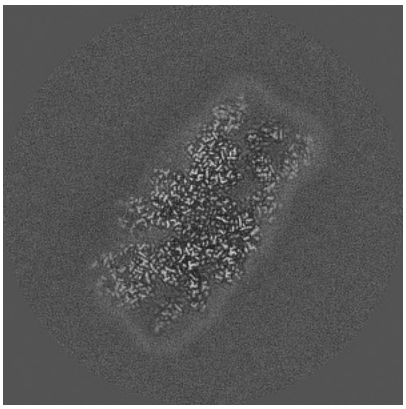
6.2.1 Primary map



X Index: 250

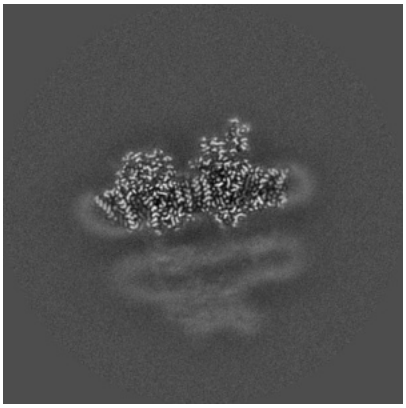


Y Index: 250

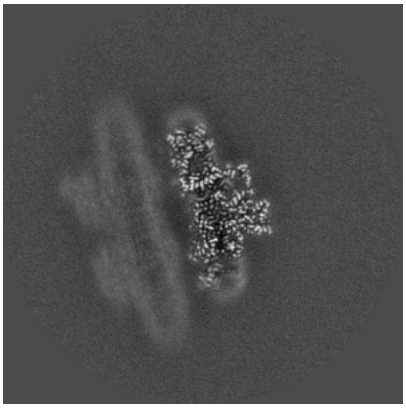


Z Index: 250

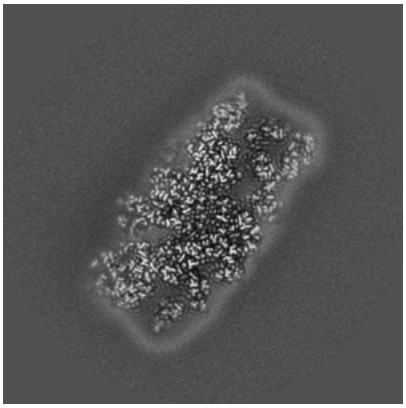
6.2.2 Raw map



X Index: 250



Y Index: 250

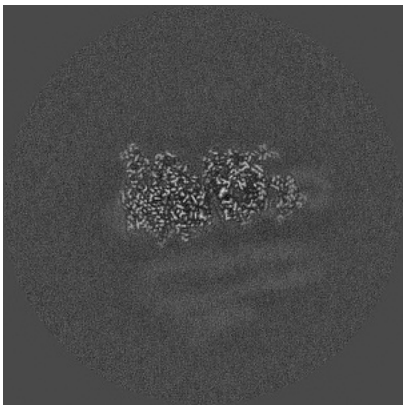


Z Index: 250

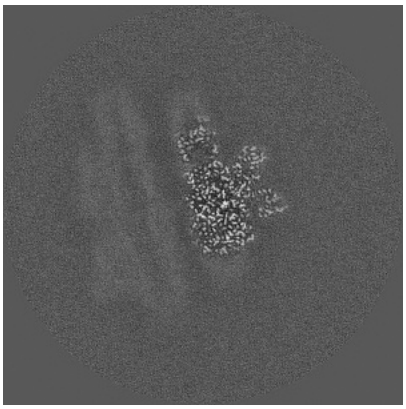
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

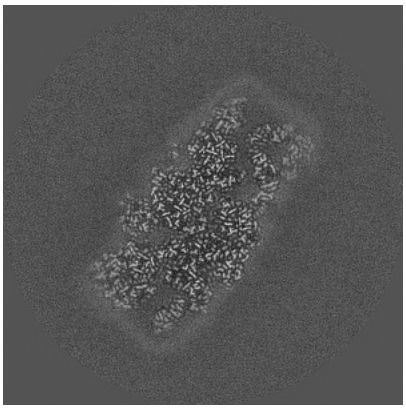
6.3.1 Primary map



X Index: 283

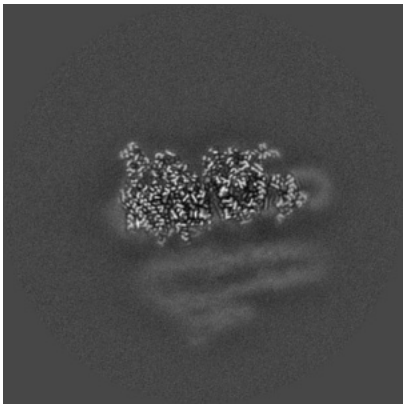


Y Index: 282

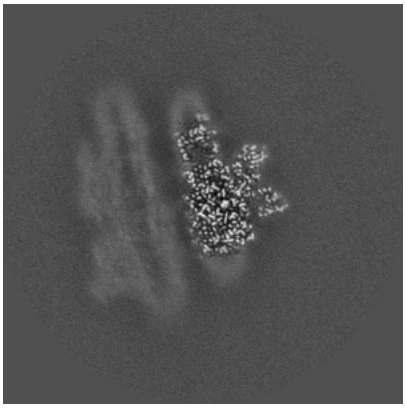


Z Index: 254

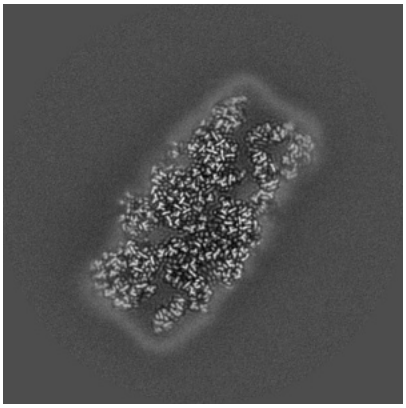
6.3.2 Raw map



X Index: 283



Y Index: 282

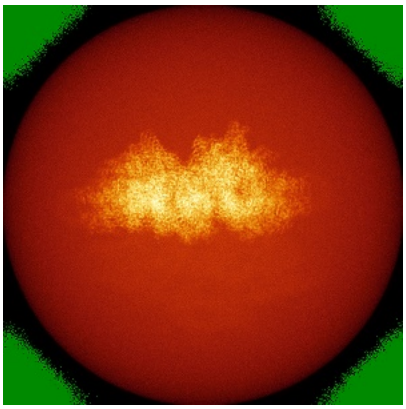


Z Index: 254

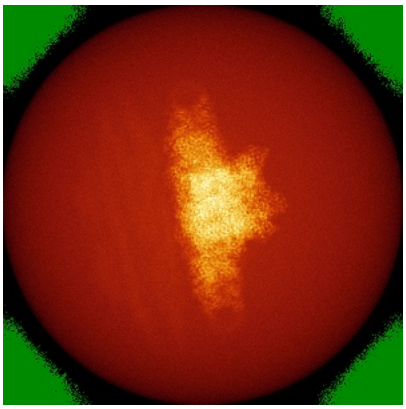
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

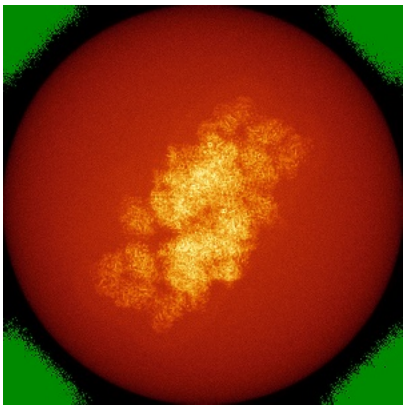
6.4.1 Primary map



X

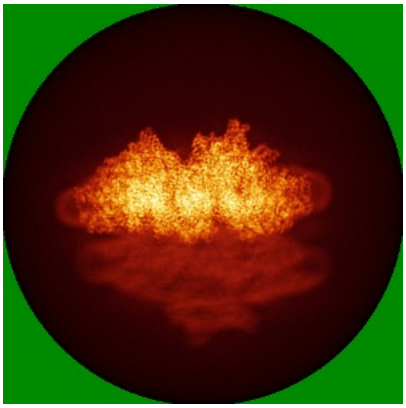


Y

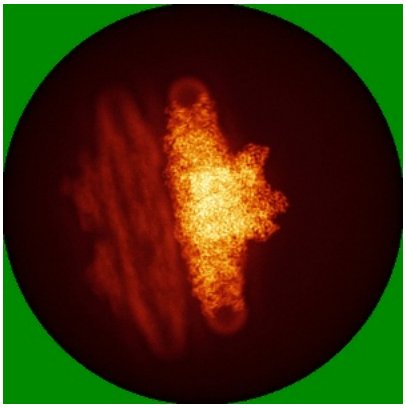


Z

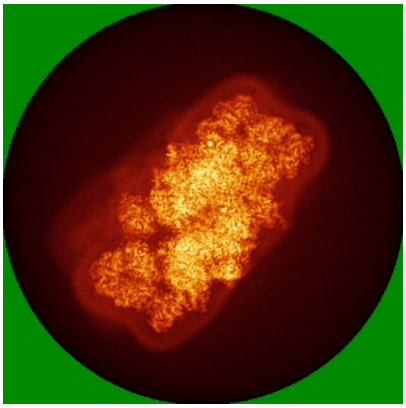
6.4.2 Raw map



X



Y

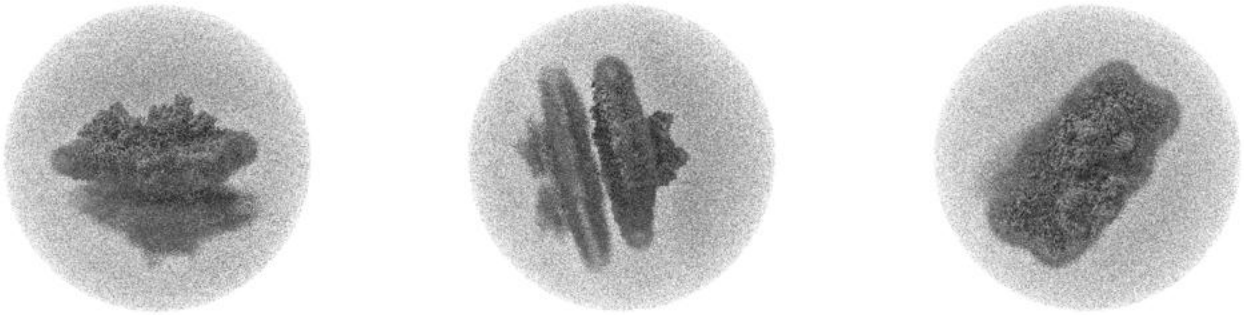


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

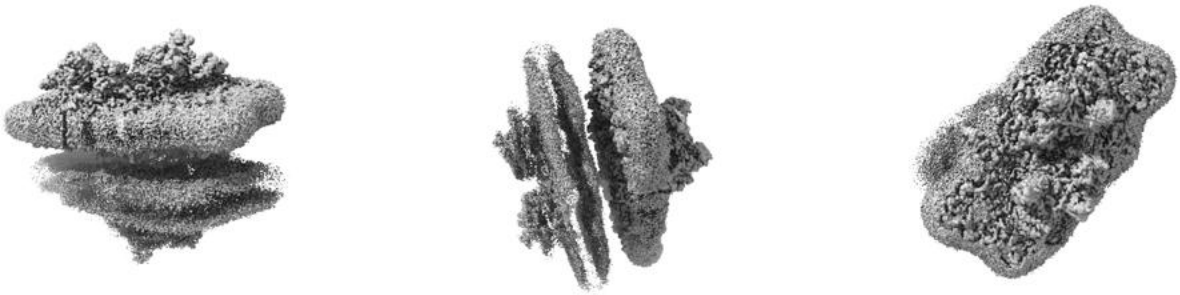
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

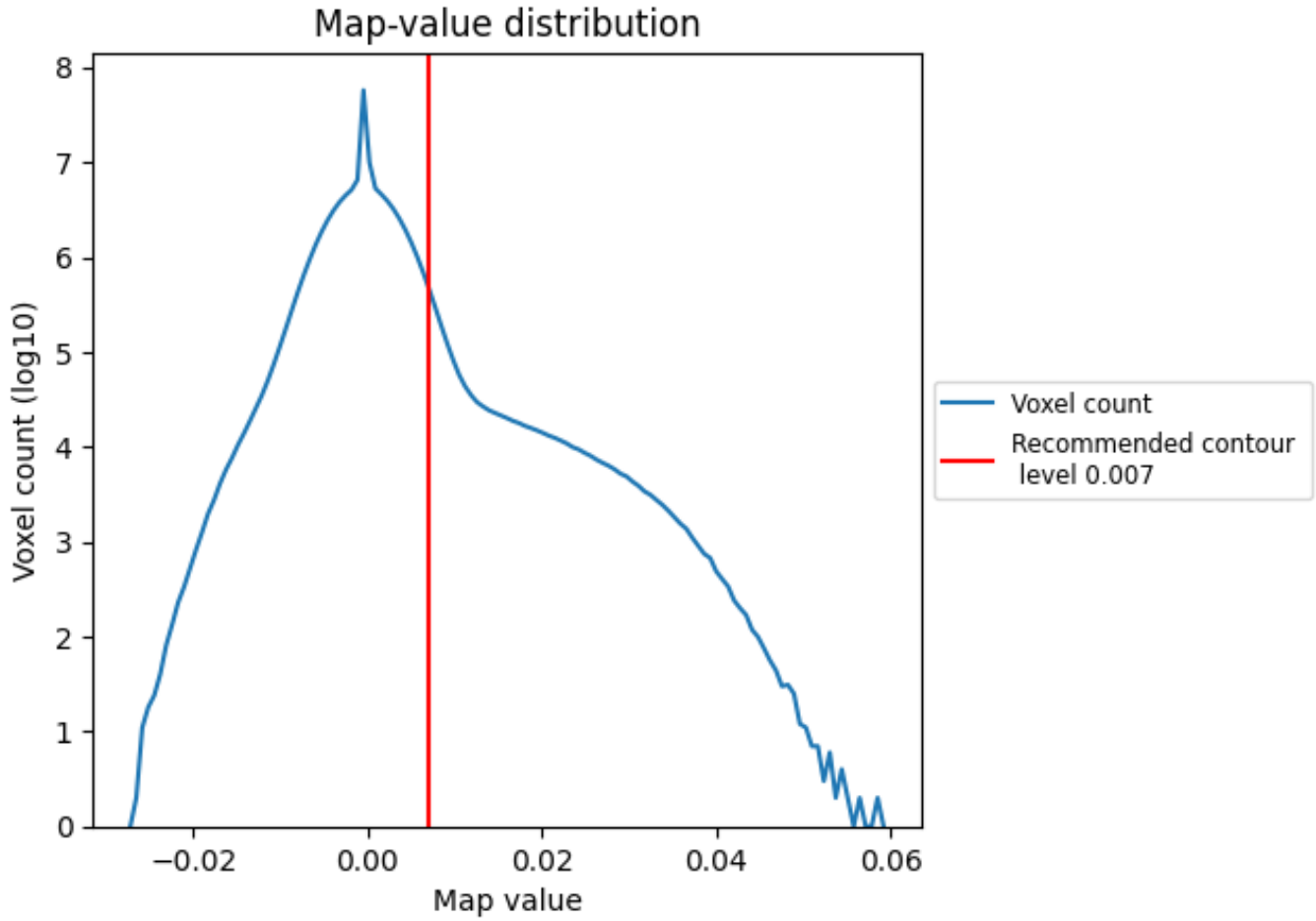
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

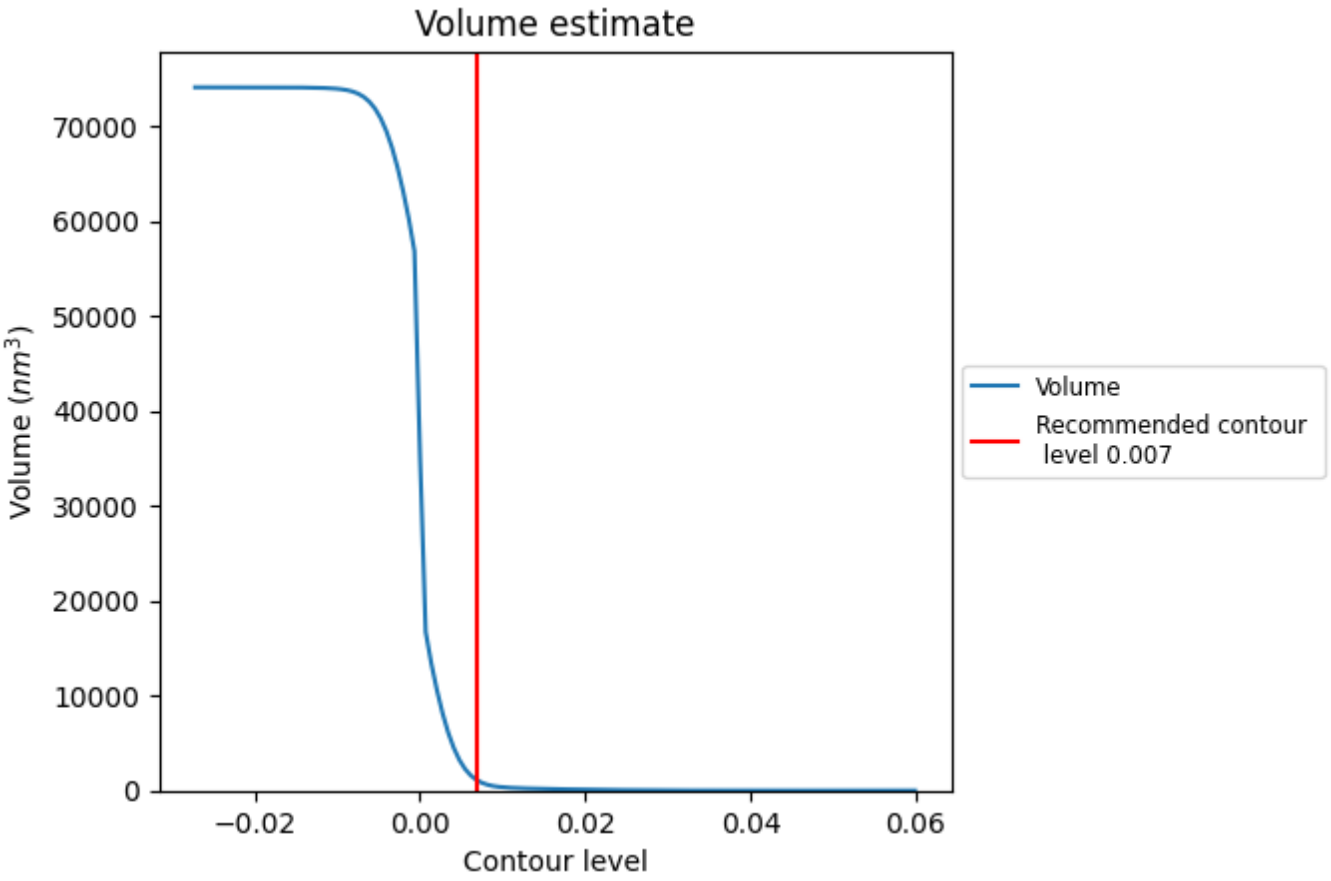
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

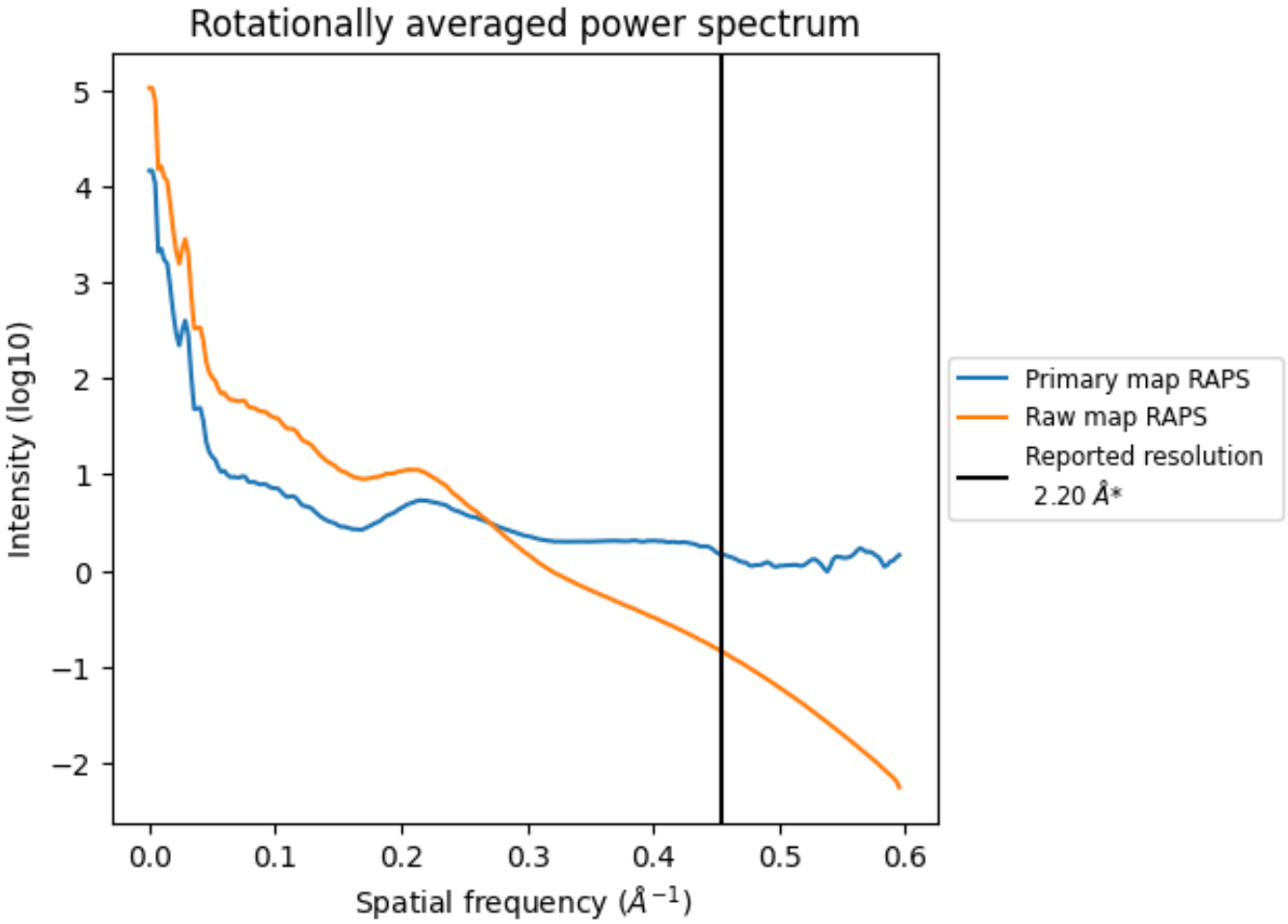
7.2 Volume estimate



The volume at the recommended contour level is 1052 nm^3; this corresponds to an approximate mass of 950 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

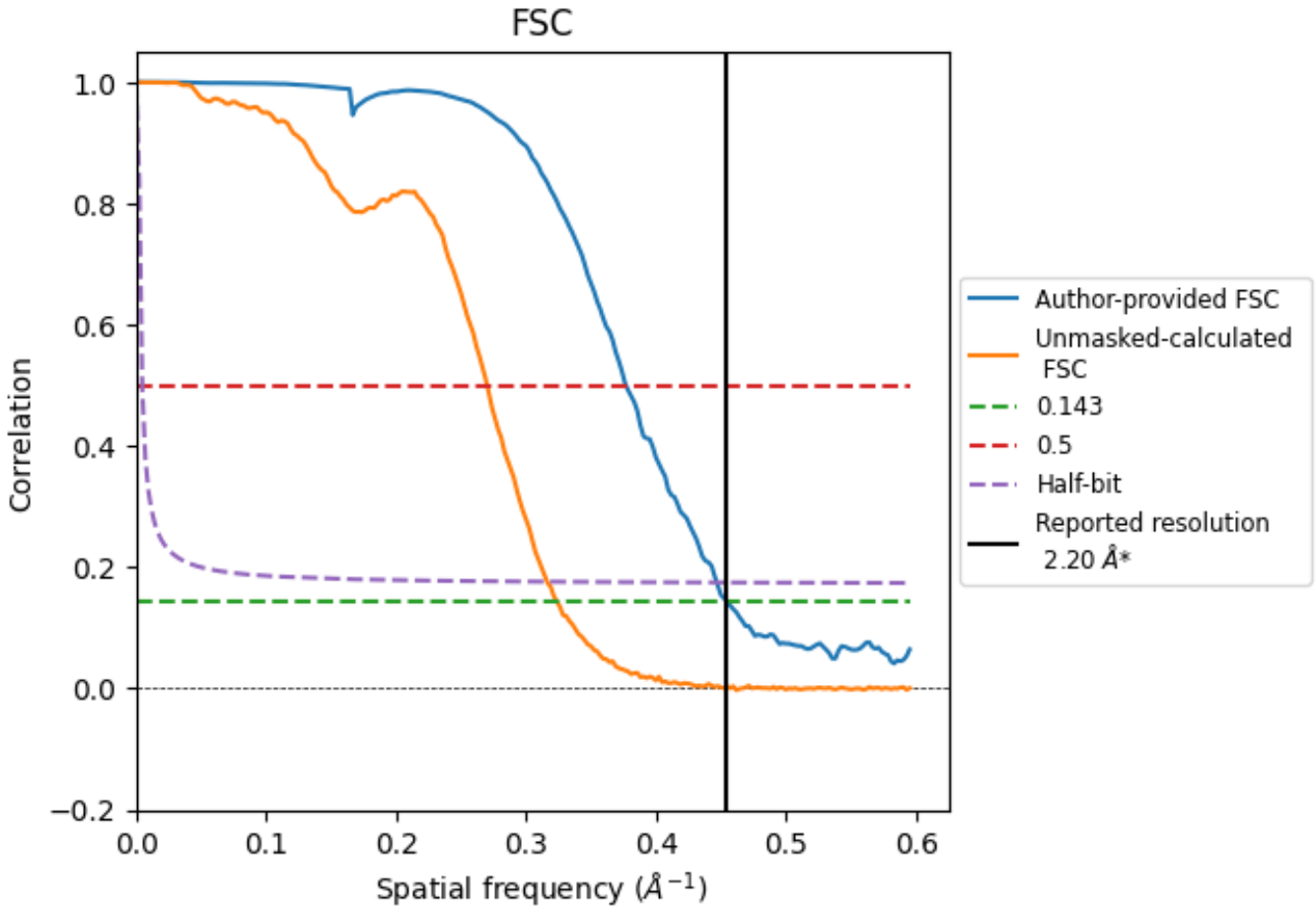


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8.2 Resolution estimates (i)

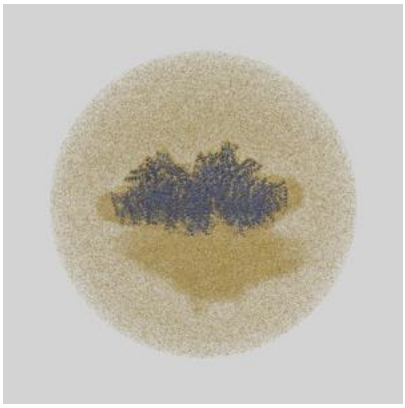
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.65	2.24
Unmasked-calculated*	3.09	3.70	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.2 by more than 10 %

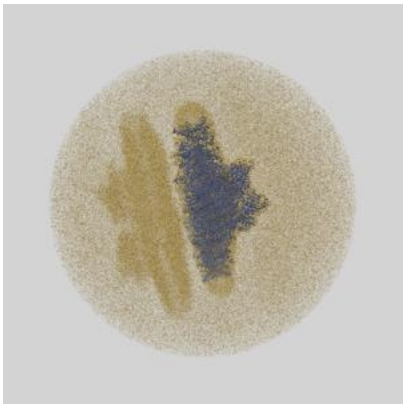
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52846 and PDB model 9IFM. Per-residue inclusion information can be found in section 3 on page 38.

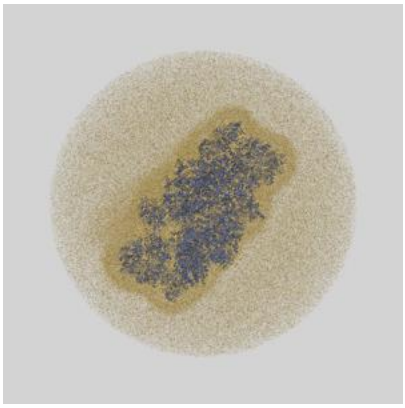
9.1 Map-model overlay



X



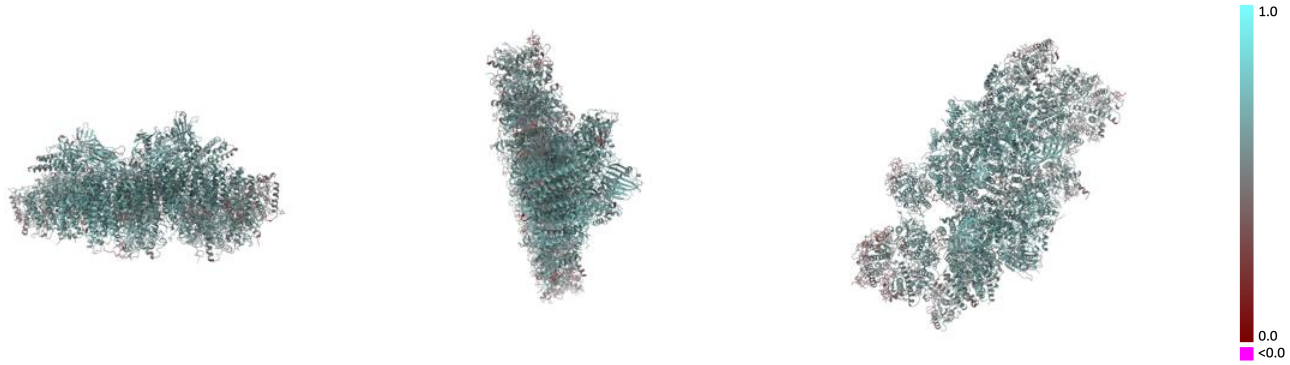
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

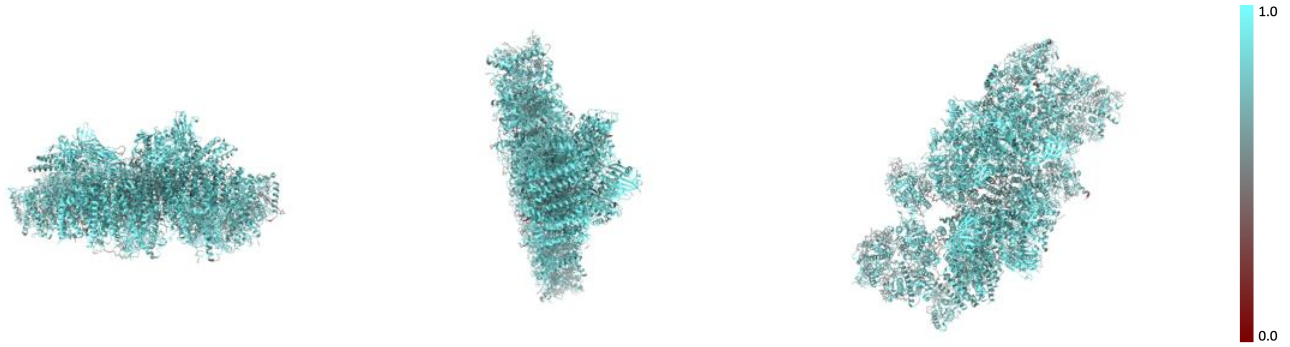
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

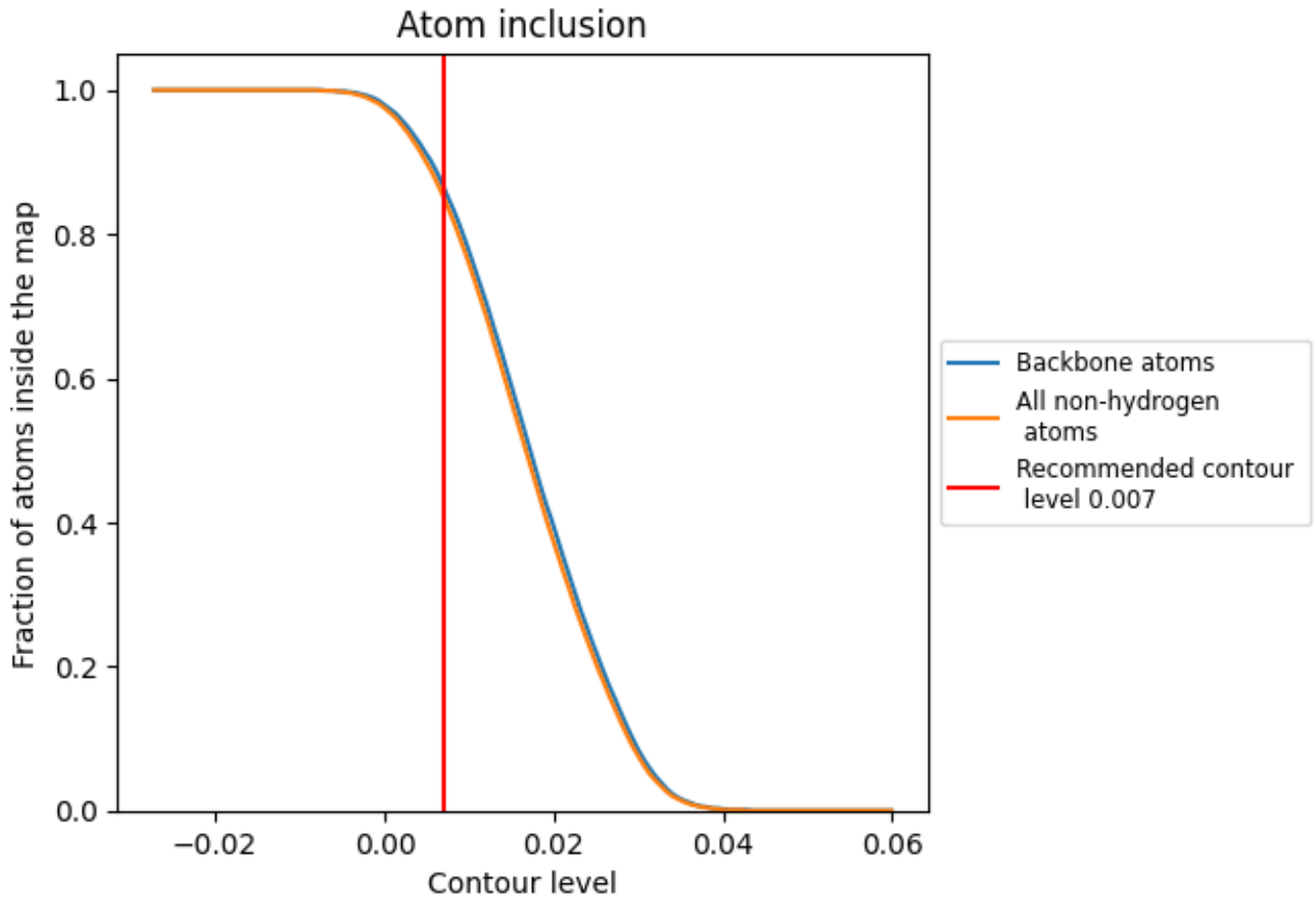
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.5990
A	0.9000	0.6540
B	0.8850	0.6340
C	0.8900	0.6310
D	0.9200	0.6580
E	0.8960	0.6110
F	0.9150	0.6340
G	0.7160	0.4780
H	0.9220	0.6500
I	0.9340	0.6660
J	0.8370	0.6090
K	0.8300	0.6090
L	0.7790	0.6010
M	0.7140	0.5630
N	0.7700	0.5190
O	0.8690	0.6070
P	0.8720	0.6040
Q	0.8090	0.5690
R	0.8240	0.5660
S	0.7490	0.4950
T	0.8480	0.6410
U	0.7800	0.5290
W	0.7900	0.5670
X	0.8390	0.5890
Y	0.8580	0.5970
Z	0.7800	0.5590
a	0.9030	0.6500
b	0.9000	0.6400
c	0.9070	0.6470
d	0.9200	0.6610
e	0.9090	0.6080
f	0.8980	0.6340
g	0.7540	0.5090
h	0.9260	0.6400
i	0.9390	0.6610



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	0.8490	0.6150
k	0.7760	0.5710
l	0.9170	0.6630
m	0.7800	0.6070
n	0.7870	0.5420
o	0.8690	0.6110
p	0.8870	0.6100
q	0.8160	0.5660
r	0.8070	0.5620
s	0.7410	0.4970
t	0.8300	0.6340
u	0.7710	0.5200
w	0.8060	0.5830
x	0.8290	0.5910
y	0.8670	0.6060
z	0.7520	0.5530