Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 08:49 am BST

PDB ID	:	9GNW / pdb_00009gnw
EMDB ID	:	EMD-51482
Title	:	Universal PSII assembly intermediate
Authors	:	Fadeeva, M.; Klaiman, D.; Nelson, N.
Deposited on	:	2024-09-04
Resolution	:	2.93 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:

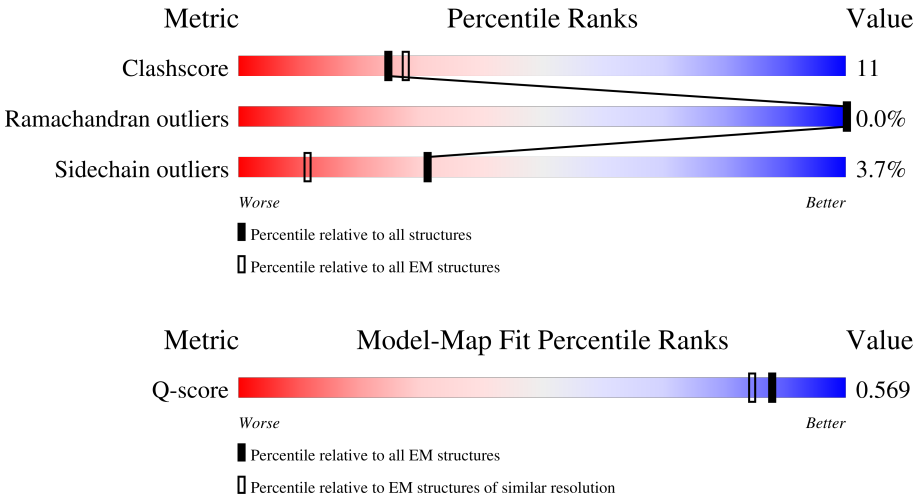
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.93 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	13037 (2.43 - 3.43)

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	336	9% 74% 26%
2	B	484	79% 20%
3	V	33	82% 18%
4	C	449	79% 20%

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Mol	Chain	Length	Quality of chain
5	D	348	79% 20%
6	E	76	80% 16%
7	F	31	74% 26%
8	H	67	81% 18%
9	I	33	88% 12%
10	J	36	6% 92% 6%
11	K	37	81% 16%
12	L	36	94% 6%
13	M	31	6% 87% 13%
14	O	238	7% 76% 23%
15	P	187	18% 78% 20%
16	T	30	7% 83% 17%
17	W	45	29% 93% 7%
18	X	33	6% 76% 24%
19	Z	61	82% 16%
20	U	28	11% 75% 18% 7%

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 24204 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
			Total	C	N	O	S		
1	A	336	2635	1719	432	468	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	484	3785	2480	630	665	10	0	0

- Molecule 3 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	V	33	235	157	38	39	1	0	0

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	449	3483	2282	581	607	13	0	0

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	348	2766	1824	454	477	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	76	621	404	102	115	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			265	182	39	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			265	181	40	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- 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	0	0
			297	207	43	47		

- 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
			300	201	49	50		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			235	161	33	41		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1819	1148	295	370	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	101	ASP	ASN	conflict	UNP A0A7S3QTM3
O	103	LYS	ARG	conflict	UNP A0A7S3QTM3
O	150	ASN	GLY	conflict	UNP A0A7S3QTM3
O	151	ASN	GLY	conflict	UNP A0A7S3QTM3
O	156	GLU	GLN	conflict	UNP A0A7S3QTM3
O	160	ASP	GLU	conflict	UNP A0A7S3QTM3
O	219	ALA	SER	conflict	UNP A0A7S3QTM3
O	220	THR	SER	conflict	UNP A0A7S3QTM3
O	226	ILE	VAL	conflict	UNP A0A7S3QTM3
O	240	LEU	VAL	conflict	UNP A0A7S3QTM3
O	244	SER	THR	conflict	UNP A0A7S3QTM3
O	248	GLY	SER	conflict	UNP A0A7S3QTM3
O	261	THR	ALA	conflict	UNP A0A7S3QTM3
O	272	SER	THR	conflict	UNP A0A7S3QTM3
O	285	ALA	SER	conflict	UNP A0A7S3QTM3

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1453	923	243	286	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	96	GLN	GLU	conflict	UNP A0A9J4RF14
P	100	GLU	ASP	conflict	UNP A0A9J4RF14
P	107	GLU	ALA	conflict	UNP A0A9J4RF14
P	116	LEU	VAL	conflict	UNP A0A9J4RF14
P	119	VAL	ILE	conflict	UNP A0A9J4RF14
P	120	GLU	ALA	conflict	UNP A0A9J4RF14

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Chain	Residue	Modelled	Actual	Comment	Reference
P	121	ASP	GLN	conflict	UNP A0A9J4RF14
P	122	LYS	ASP	conflict	UNP A0A9J4RF14
P	123	SER	THR	conflict	UNP A0A9J4RF14
P	129	GLU	GLN	conflict	UNP A0A9J4RF14
P	130	ALA	ASP	conflict	UNP A0A9J4RF14
P	133	THR	SER	conflict	UNP A0A9J4RF14
P	147	LYS	ARG	conflict	UNP A0A9J4RF14
P	164	ARG	LYS	conflict	UNP A0A9J4RF14
P	167	ASN	SER	conflict	UNP A0A9J4RF14
P	191	THR	SER	conflict	UNP A0A9J4RF14

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	45	Total	C	N	O	S	0	0
			335	217	54	63	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	104	GLY	-	expression tag	UNP A0A9J4RF15

- Molecule 18 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	33	Total	C	N	O	0	0
			225	148	36	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3

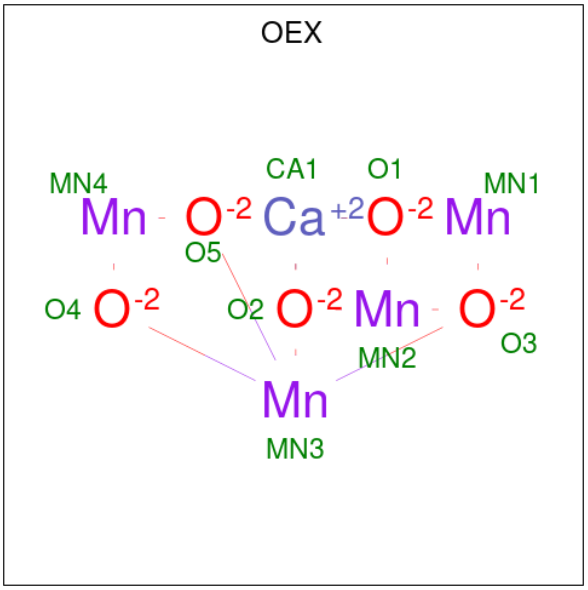
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Photosystem II reaction center protein U, PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			235	141	46	47	1		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

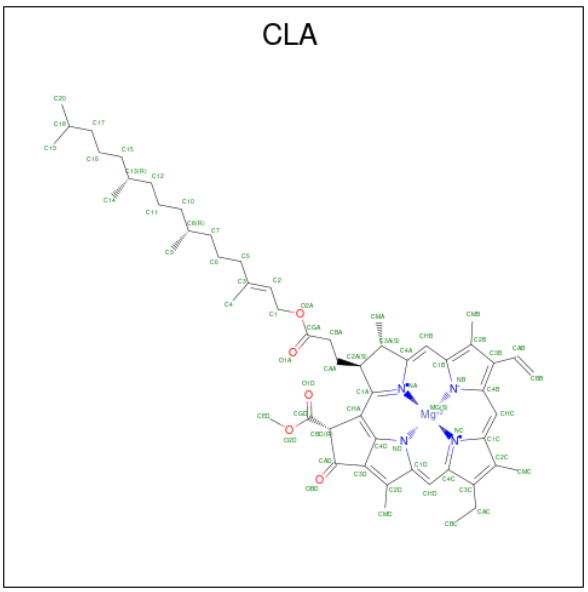
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Cl	0
			2	2	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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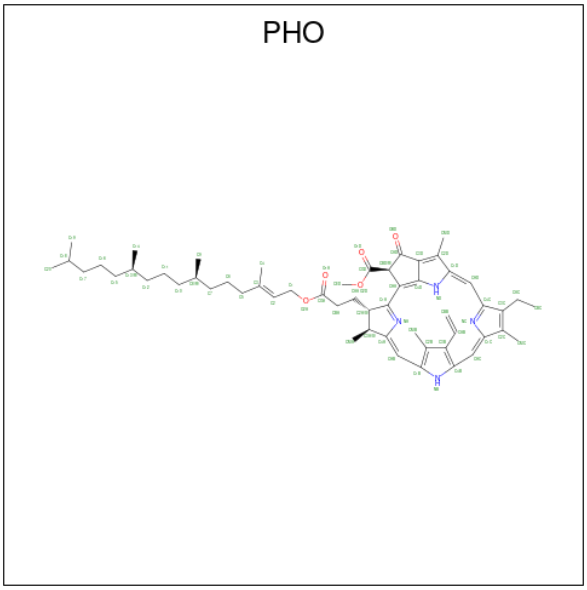
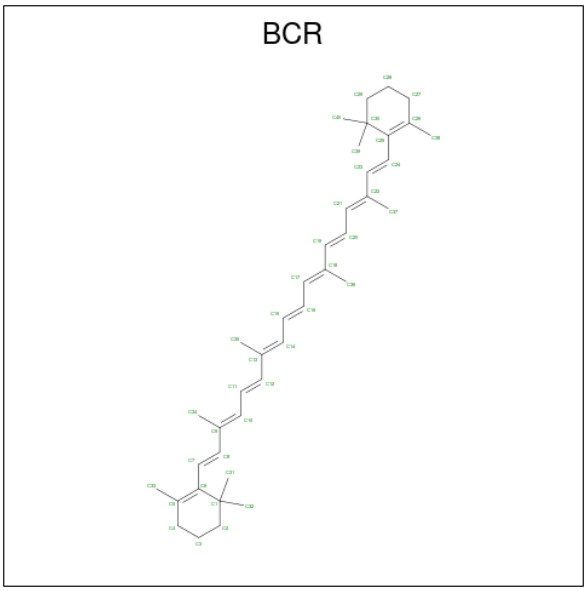
Mol	Chain	Residues	Atoms					AltConf
24	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



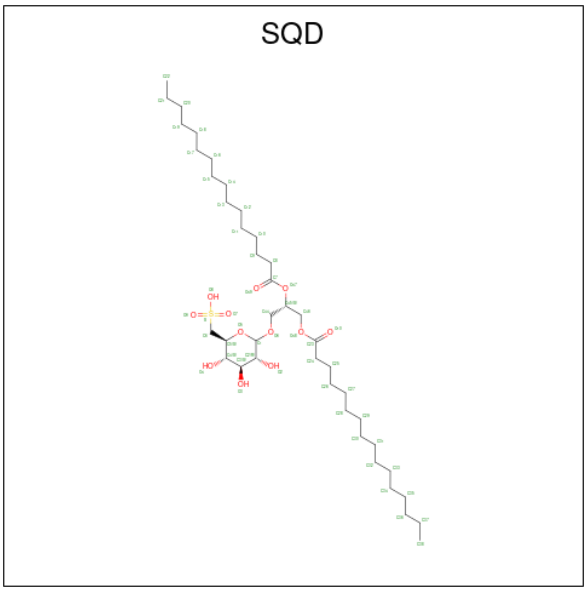
Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	N	O		0
			64	55	4	5		
25	D	1	Total	C	N	O		0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



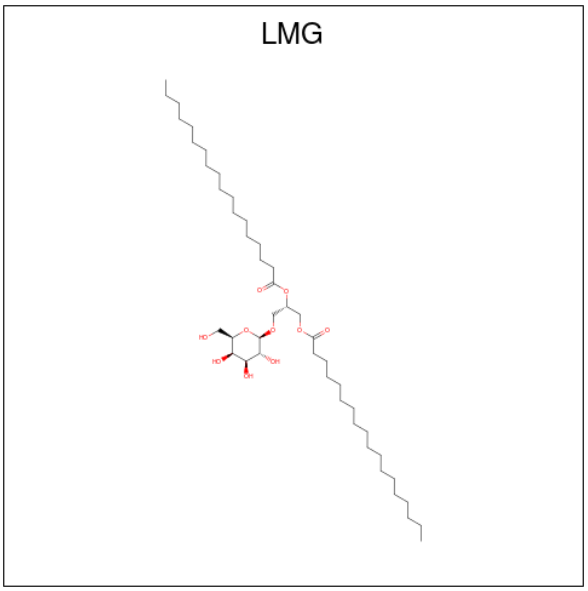
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	J	1	Total C 40 40	0

- Molecule 27 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
27	A	1	Total	C	O	S	0
			42	29	12	1	
27	M	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			34	24	10	

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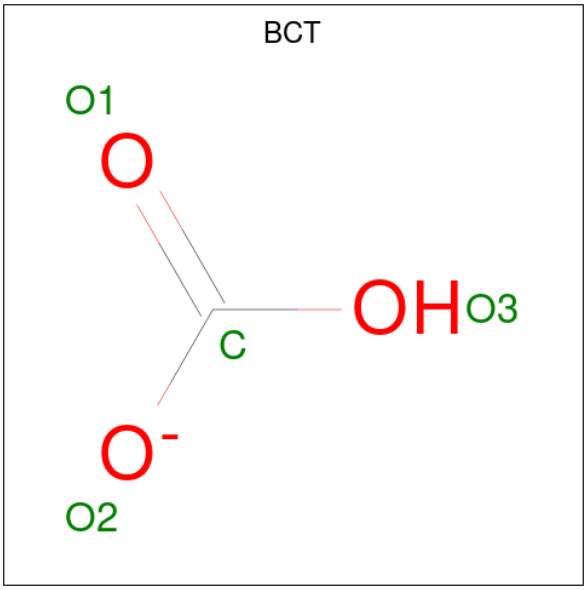
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C O 37 27 10	0
28	B	1	Total C O 44 34 10	0
28	C	1	Total C O 40 30 10	0
28	C	1	Total C O 47 37 10	0
28	C	1	Total C O 33 24 9	0
28	D	1	Total C O 42 32 10	0
28	H	1	Total C O 48 38 10	0

- Molecule 29 is SODIUM ION (CCD ID: NA) (formula: Na).

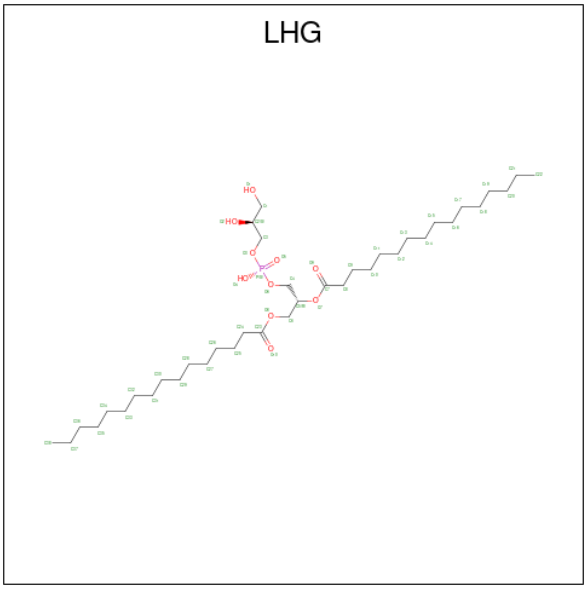
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Na 1 1	0

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



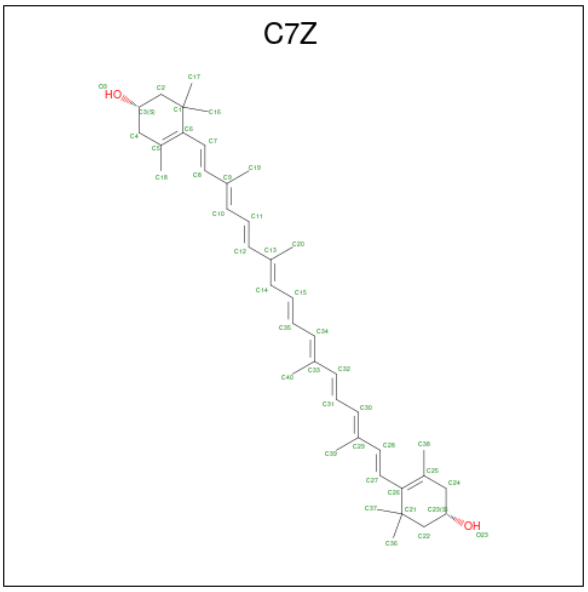
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C O 4 1 3	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



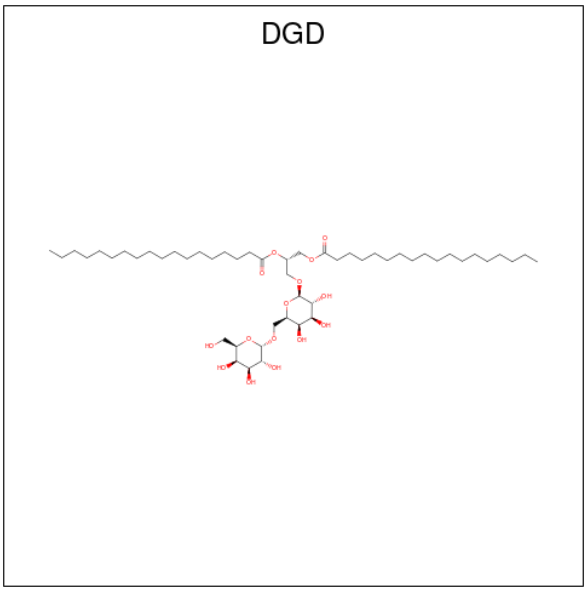
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			39	28	10	1	
31	D	1	Total	C	O	P	0
			44	33	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			39	28	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			42	40	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			43	28	15	
33	C	1	Total	C	O	0
			44	29	15	

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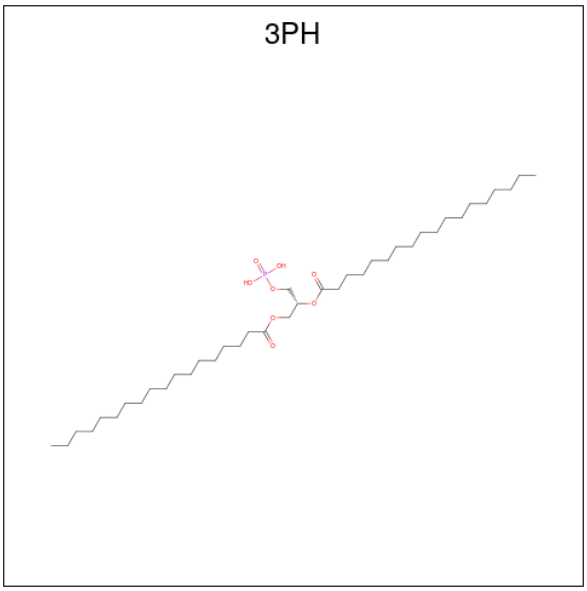
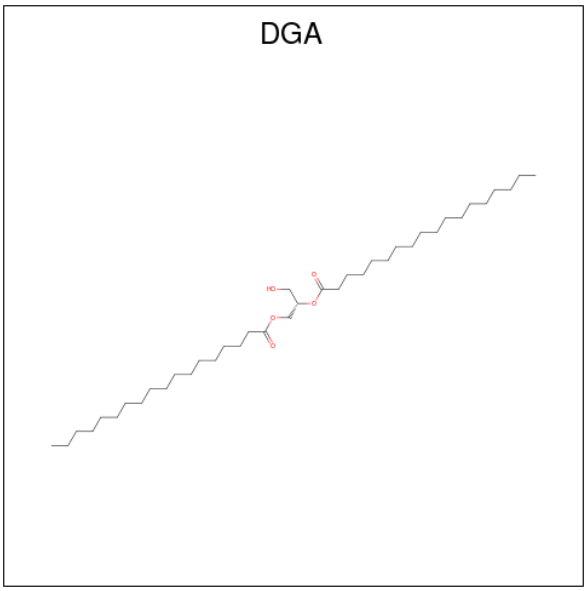
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C O 53 38 15	0
33	C	1	Total C O 53 38 15	0

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



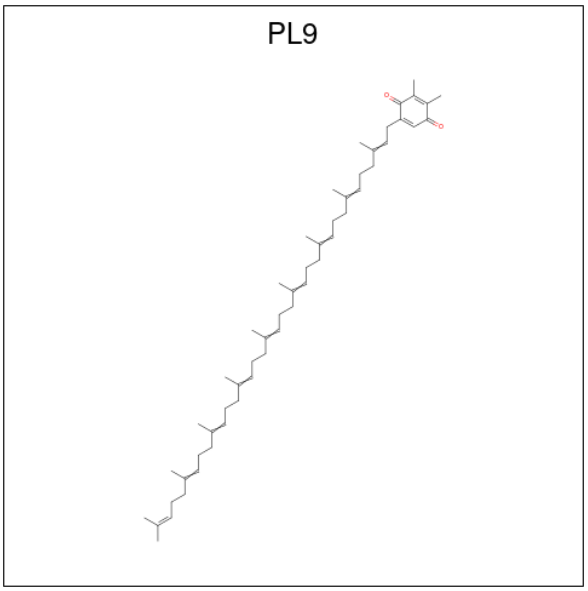
Mol	Chain	Residues	Atoms	AltConf
34	B	1	Total C O P 48 39 8 1	0

- Molecule 35 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	B	1	37	32	5	0

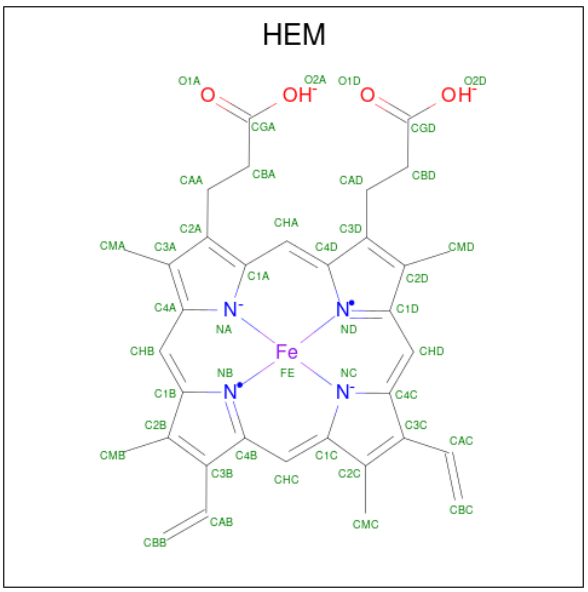
- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	D	1	55	53	2	0

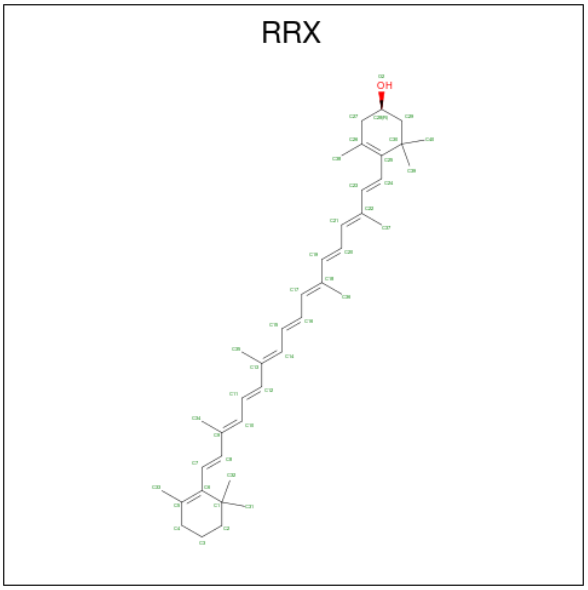
- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



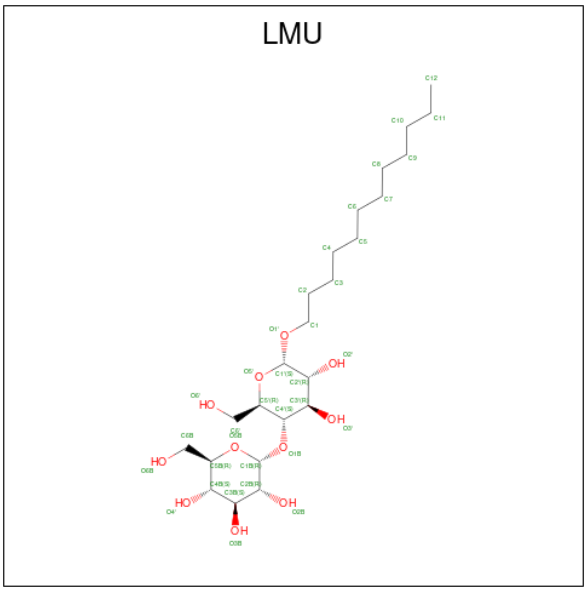
Mol	Chain	Residues	Atoms					AltConf
37	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			41	40	1	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
39	J	1	Total C O 35 24 11	0

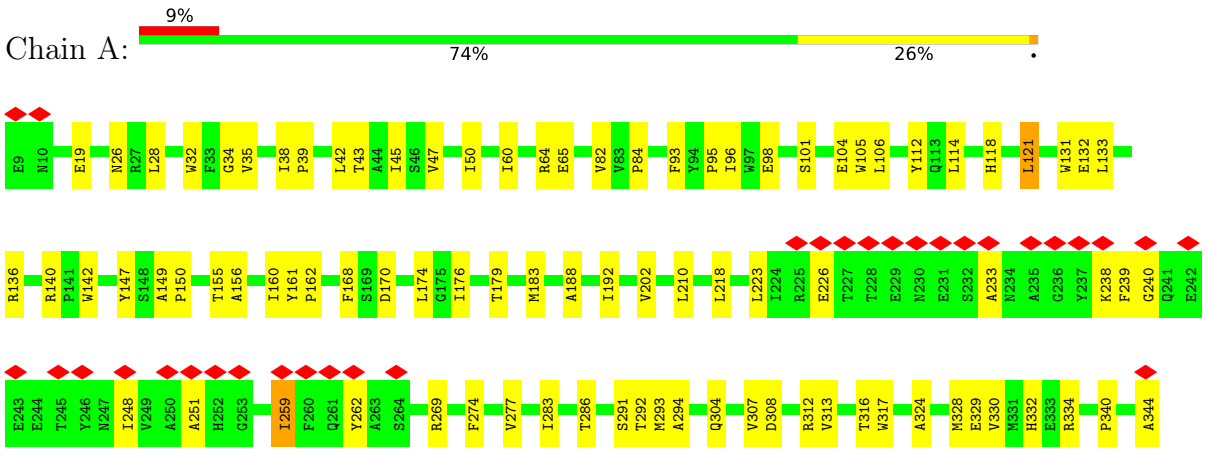
- Molecule 40 is water.

Mol	Chain	Residues	Atoms	AltConf
40	A	6	Total O 6 6	0
40	B	3	Total O 3 3	0
40	C	1	Total O 1 1	0
40	D	1	Total O 1 1	0

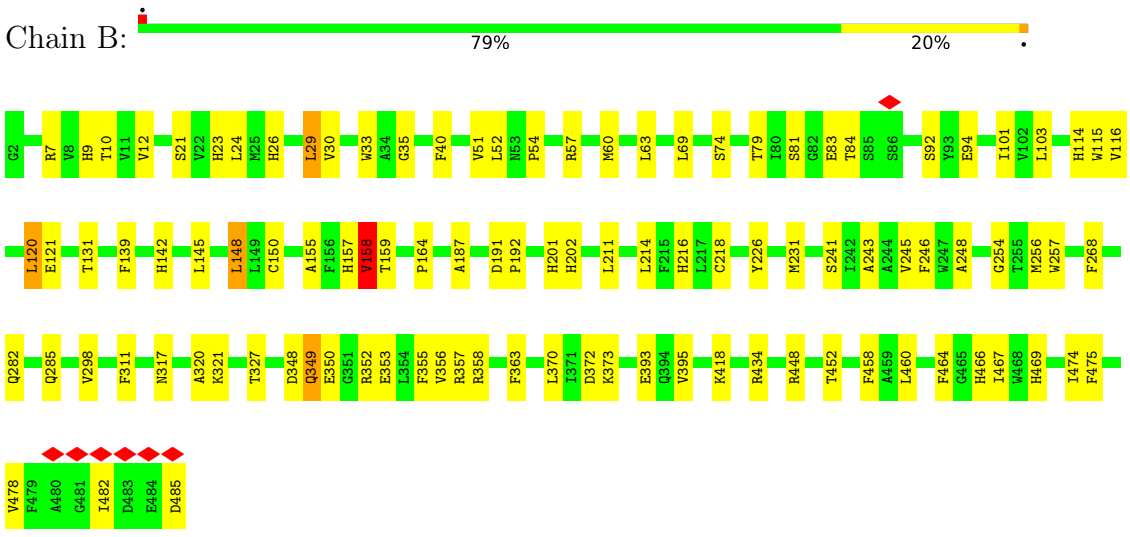
3 Residue-property plots (i)

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.

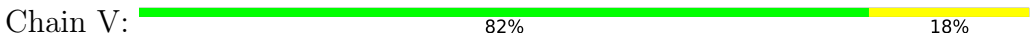
• Molecule 1: Photosystem II protein D1

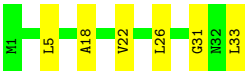


• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II reaction center protein Psb30

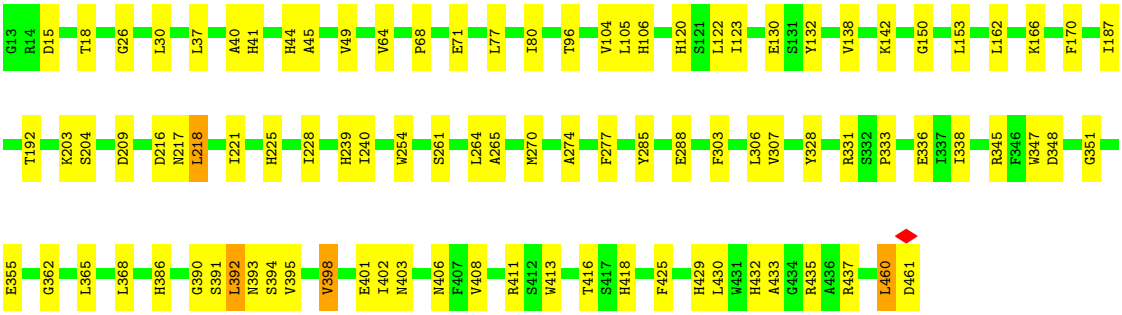




• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:

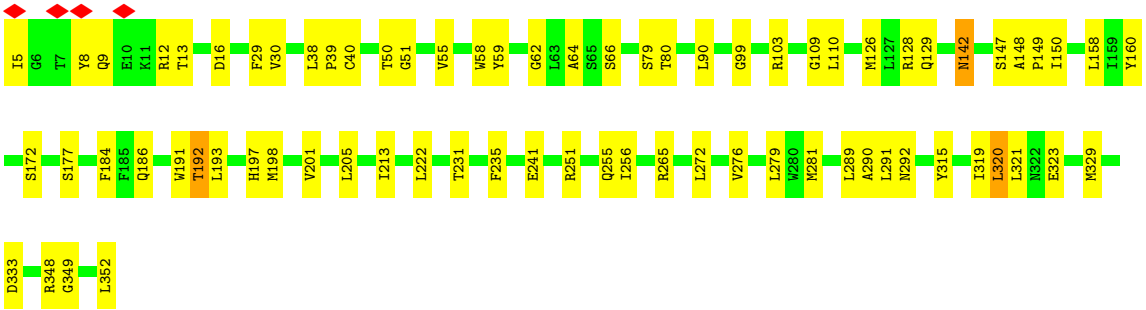




• Molecule 5: Photosystem II D2 protein

Chain D:

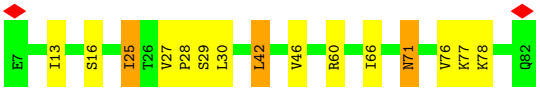




• Molecule 6: Cytochrome b559 subunit alpha

Chain E:

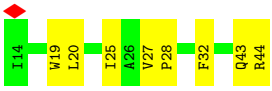




• Molecule 7: Cytochrome b559 subunit beta

Chain F:

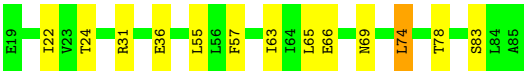




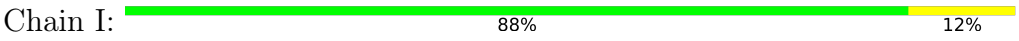
• Molecule 8: Photosystem II reaction center protein H

Chain H:



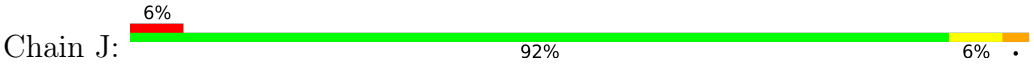


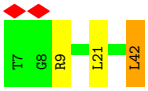
• Molecule 9: Photosystem II reaction center protein I



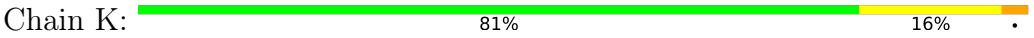


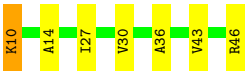
• Molecule 10: Photosystem II reaction center protein J



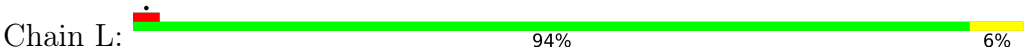


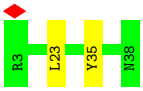
• Molecule 11: Photosystem II reaction center protein K



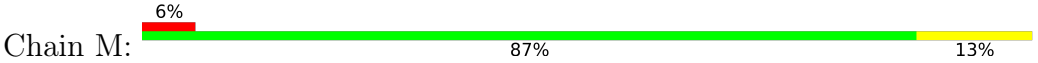


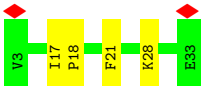
• Molecule 12: Photosystem II reaction center protein L



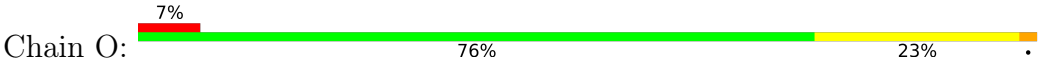


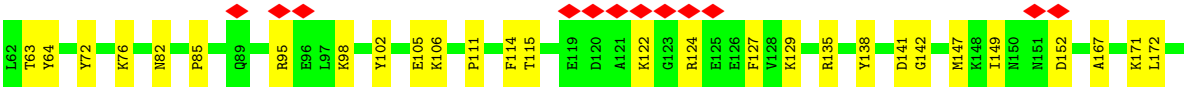
• Molecule 13: Photosystem II reaction center protein M

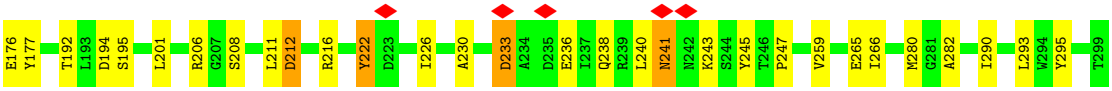




• Molecule 14: PsbO

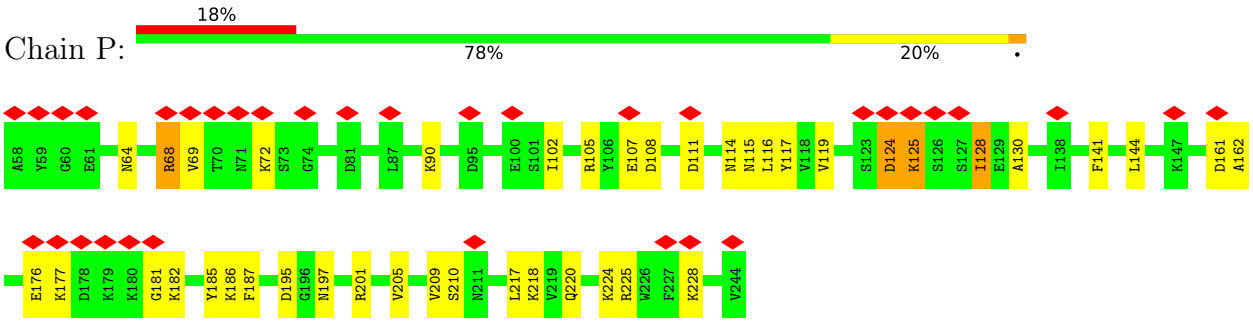






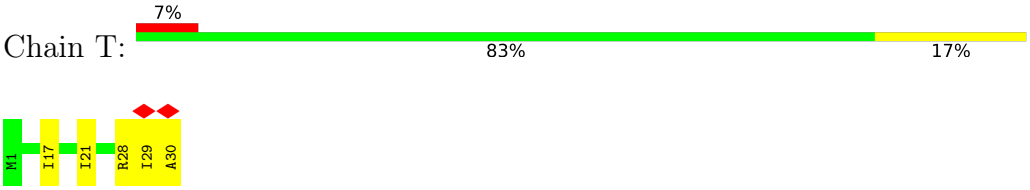
• Molecule 15: PsbP

Chain P:



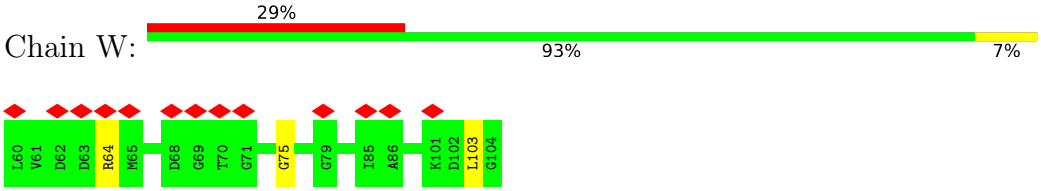
• Molecule 16: Photosystem II reaction center protein T

Chain T:



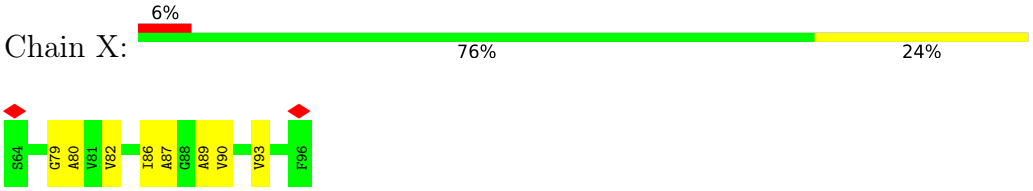
• Molecule 17: PSII 6.1 kDa protein

Chain W:



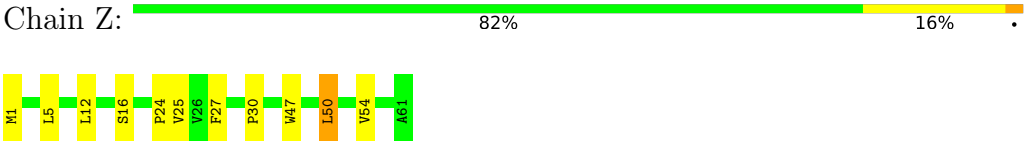
• Molecule 18: Photosystem II PsbX

Chain X:



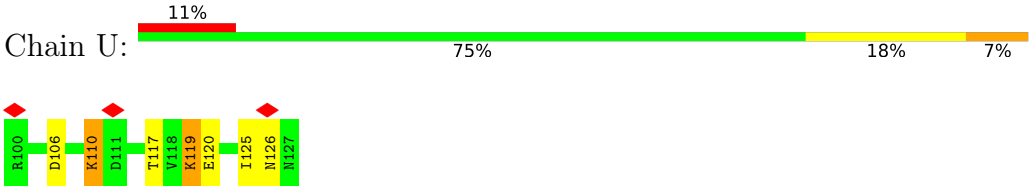
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein U, PsbU

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0047	Depositor
Map size (Å)	193.5, 193.5, 193.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.645, 0.645, 0.645	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CL, C7Z, FE2, LHG, CSD, CLA, PHO, OEX, NA, DGA, SQD, PL9, HEM, DGD, LMU, RRX, BCT, 3PH, BCR

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	0.26	0/2717	0.34	0/3707
2	B	0.22	0/3906	0.31	0/5319
3	V	0.16	0/236	0.24	0/321
4	C	0.30	0/3602	0.37	0/4913
5	D	0.31	0/2860	0.37	0/3899
6	E	0.18	0/639	0.31	0/870
7	F	0.19	0/259	0.29	0/351
8	H	0.19	0/513	0.24	0/703
9	I	0.21	0/273	0.29	0/370
10	J	0.25	0/271	0.29	0/368
11	K	0.23	0/308	0.36	0/423
12	L	0.21	0/308	0.26	0/418
13	M	0.17	0/238	0.24	0/324
14	O	0.21	0/1854	0.31	0/2503
15	P	0.13	0/1482	0.26	0/1999
16	T	0.18	0/254	0.23	0/342
17	W	0.14	0/342	0.26	0/465
18	X	0.18	0/227	0.27	0/311
19	Z	0.15	0/469	0.25	0/641
20	U	0.15	0/235	0.25	0/311
All	All	0.24	0/20993	0.32	0/28558

There are no bond length outliers.

There are no bond angle outliers.

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	2635	0	2536	84	0
2	B	3785	0	3662	85	0
3	V	235	0	273	8	0
4	C	3483	0	3376	76	0
5	D	2766	0	2655	58	0
6	E	621	0	605	8	0
7	F	252	0	265	6	0
8	H	503	0	532	11	0
9	I	265	0	272	2	0
10	J	265	0	282	4	0
11	K	297	0	312	6	0
12	L	300	0	308	2	0
13	M	235	0	262	3	0
14	O	1819	0	1772	39	0
15	P	1453	0	1416	27	0
16	T	247	0	260	7	0
17	W	335	0	326	3	0
18	X	225	0	244	5	0
19	Z	457	0	478	10	0
20	U	235	0	244	6	0
21	A	10	0	0	0	0
22	A	1	0	0	0	0
23	A	2	0	0	0	0
24	A	190	0	203	16	0
24	B	1017	0	1095	82	0
24	C	794	0	824	53	0
24	D	190	0	203	20	0
25	A	64	0	74	5	0
25	D	64	0	74	5	0
26	A	40	0	56	5	0
26	B	80	0	112	6	0
26	C	120	0	168	9	0
26	D	40	0	56	1	0
26	J	40	0	56	2	0
27	A	42	0	47	0	0
27	M	42	0	47	4	0
28	A	71	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	44	0	58	2	0
28	C	120	0	156	7	0
28	D	42	0	54	1	0
28	H	48	0	66	5	0
29	A	1	0	0	0	0
30	A	4	0	1	0	0
31	A	39	0	48	3	0
31	D	132	0	185	11	0
31	L	49	0	74	1	0
32	B	42	0	0	3	0
33	B	43	0	44	2	0
33	C	150	0	174	7	0
34	B	48	0	75	4	0
35	B	37	0	56	3	0
36	D	55	0	80	1	0
37	E	43	0	30	2	0
38	H	41	0	56	6	0
39	J	35	0	46	4	0
40	A	6	0	0	0	0
40	B	3	0	0	0	0
40	C	1	0	0	0	0
40	D	1	0	0	0	0
All	All	24204	0	24380	513	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 11.

All (513) 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)
2:B:24:LEU:HD21	24:B:516:CLA:HAB	1.56	0.88
5:D:192:THR:HG23	24:D:403:CLA:HBC2	1.67	0.77
24:B:514:CLA:H18	26:B:517:BCR:H11C	1.68	0.75
4:C:187:ILE:HD11	4:C:218:LEU:HD23	1.68	0.74
1:A:26:ASN:HA	28:A:415:LMG:HC71	1.68	0.73
2:B:142:HIS:HE1	24:B:515:CLA:ND	1.87	0.73
2:B:469:HIS:HE1	24:B:511:CLA:NA	1.89	0.70
1:A:42:LEU:HB3	26:A:409:BCR:H353	1.74	0.70
14:O:240:LEU:O	14:O:241:ASN:ND2	2.26	0.69
1:A:106:LEU:HD11	26:A:409:BCR:H402	1.74	0.69
24:B:502:CLA:H2	24:B:502:CLA:HBD	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HH12	5:D:222:LEU:HD12	1.56	0.69
5:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.74	0.69
4:C:392:LEU:HD12	33:C:520:DGD:HB51	1.74	0.68
5:D:55:VAL:O	5:D:66:SER:HB3	1.94	0.68
5:D:129:GLN:NE2	25:D:402:PHO:OBD	2.27	0.68
20:U:106:ASP:OD1	20:U:110:LYS:NZ	2.26	0.68
5:D:5:ILE:N	5:D:8:TYR:O	2.27	0.67
3:V:26:LEU:HB3	3:V:33:LEU:HD21	1.75	0.67
31:D:408:LHG:H272	12:L:23:LEU:HD22	1.78	0.66
15:P:182:LYS:HZ1	15:P:210:SER:HB3	1.60	0.66
24:B:501:CLA:H122	38:H:101:RRX:H50	1.78	0.65
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.78	0.65
1:A:26:ASN:HB3	28:A:415:LMG:HC91	1.78	0.65
5:D:279:LEU:HD22	25:D:402:PHO:HBC3	1.78	0.65
4:C:104:VAL:HG11	26:C:515:BCR:HC42	1.78	0.65
24:B:501:CLA:H143	24:B:501:CLA:H12	1.79	0.64
14:O:172:LEU:HB2	14:O:176:GLU:HB2	1.79	0.64
14:O:233:ASP:OD1	14:O:233:ASP:N	2.21	0.64
1:A:233:ALA:O	5:D:265:ARG:NH1	2.31	0.64
2:B:202:HIS:HE1	24:B:503:CLA:NA	1.94	0.63
8:H:69:ASN:ND2	28:H:102:LMG:O10	2.29	0.63
2:B:30:VAL:HG12	24:B:505:CLA:HHD	1.80	0.63
1:A:334:ARG:HB3	14:O:211:LEU:HD12	1.80	0.63
1:A:64:ARG:NH1	14:O:167:ALA:O	2.32	0.63
1:A:28:LEU:HD12	28:A:415:LMG:H312	1.80	0.62
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.32	0.62
24:C:507:CLA:HBB2	24:C:508:CLA:H52	1.82	0.62
4:C:71:GLU:OE2	4:C:386:HIS:NE2	2.32	0.62
31:D:408:LHG:H281	31:D:408:LHG:H131	1.82	0.62
10:J:21:LEU:HD21	26:J:101:BCR:H361	1.81	0.62
26:B:518:BCR:H14C	34:B:522:3PH:H2E1	1.82	0.62
24:D:404:CLA:NB	31:D:410:LHG:H202	2.15	0.61
15:P:107:GLU:HG3	15:P:115:ASN:HB3	1.81	0.61
4:C:461:ASP:O	5:D:251:ARG:NH2	2.34	0.61
15:P:128:ILE:HG12	15:P:209:VAL:HG23	1.81	0.61
24:A:405:CLA:H143	25:A:407:PHO:H72	1.81	0.60
1:A:43:THR:HA	26:A:409:BCR:H15C	1.83	0.60
26:C:516:BCR:H332	9:I:20:ILE:HG23	1.83	0.60
10:J:42:LEU:OXT	15:P:72:LYS:NZ	2.34	0.60
28:C:521:LMG:H172	39:J:102:LMU:H51	1.82	0.60
7:F:44:ARG:NH2	10:J:42:LEU:OXT	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:348:ARG:NH1	5:D:352:LEU:OXT	2.33	0.60
2:B:285:GLN:HG3	20:U:110:LYS:HE2	1.83	0.60
24:D:404:CLA:C1B	31:D:410:LHG:H202	2.32	0.59
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.84	0.59
13:M:28:LYS:HE3	27:M:101:SQD:H462	1.85	0.59
24:A:405:CLA:H112	24:D:401:CLA:HBB1	1.84	0.59
2:B:74:SER:HA	2:B:92:SER:HB2	1.83	0.59
24:B:508:CLA:H162	24:D:404:CLA:HBA1	1.83	0.59
4:C:285:TYR:O	4:C:411:ARG:NH2	2.36	0.59
2:B:157:HIS:O	2:B:159:THR:N	2.32	0.59
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.59
14:O:95:ARG:NH1	14:O:194:ASP:OD1	2.35	0.59
1:A:93:PHE:HZ	24:A:408:CLA:HAA1	1.66	0.58
2:B:474:ILE:HD11	24:B:508:CLA:HAA2	1.85	0.58
4:C:432:HIS:HE1	24:C:509:CLA:NA	2.01	0.58
28:C:501:LMG:HC2	17:W:75:GLY:HA3	1.83	0.58
1:A:133:LEU:HD23	5:D:256:ILE:HG12	1.85	0.58
4:C:221:ILE:HA	26:C:516:BCR:H282	1.85	0.58
4:C:390:GLY:HA3	4:C:408:VAL:HG22	1.85	0.58
15:P:141:PHE:HB3	15:P:144:LEU:HD13	1.86	0.58
2:B:350:GLU:OE1	2:B:352:ARG:NH2	2.37	0.58
2:B:434:ARG:NH1	14:O:230:ALA:O	2.36	0.58
5:D:79:SER:HA	5:D:172:SER:HB3	1.86	0.58
7:F:43:GLN:O	15:P:64:ASN:ND2	2.32	0.58
24:D:404:CLA:H43	18:X:79:GLY:HA3	1.86	0.57
14:O:243:LYS:HD2	14:O:280:MET:HE2	1.86	0.57
2:B:79:THR:HG22	2:B:81:SER:H	1.69	0.57
14:O:259:VAL:HG22	14:O:266:ILE:HG22	1.87	0.57
37:E:101:HEM:HBC2	37:E:101:HEM:HMC2	1.85	0.57
4:C:68:PRO:HD2	4:C:71:GLU:HG3	1.85	0.57
4:C:430:LEU:HD21	24:C:506:CLA:HMB2	1.86	0.57
14:O:147:MET:HE2	14:O:149:ILE:HD11	1.86	0.57
1:A:47:VAL:HG21	1:A:114:LEU:HD22	1.87	0.57
24:A:408:CLA:HBB1	24:A:408:CLA:HMB3	1.86	0.57
4:C:331:ARG:NH2	14:O:82:ASN:HA	2.19	0.57
14:O:212:ASP:OD1	14:O:216:ARG:N	2.36	0.57
2:B:321:LYS:NZ	2:B:363:PHE:O	2.38	0.56
24:B:503:CLA:HMB2	24:B:503:CLA:H51	1.86	0.56
4:C:239:HIS:HE1	24:C:507:CLA:C1A	2.19	0.56
5:D:126:MET:HE1	5:D:147:SER:HA	1.88	0.56
1:A:118:HIS:HE1	24:A:408:CLA:C4D	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HB2	24:A:408:CLA:HAB	1.88	0.56
3:V:22:VAL:HG23	19:Z:25:VAL:HG23	1.87	0.56
4:C:398:VAL:O	4:C:401:GLU:HG2	2.05	0.56
24:C:512:CLA:H202	26:C:517:BCR:H17C	1.88	0.56
13:M:17:ILE:HB	13:M:18:PRO:HD3	1.86	0.56
14:O:122:LYS:H	14:O:122:LYS:HD3	1.71	0.56
4:C:395:VAL:CG1	4:C:403:ASN:HA	2.36	0.55
24:B:511:CLA:H52	24:B:513:CLA:HED3	1.89	0.55
4:C:30:LEU:HD21	24:C:512:CLA:H2A	1.89	0.55
14:O:122:LYS:HE2	14:O:124:ARG:HB2	1.89	0.55
24:B:513:CLA:OBD	24:B:514:CLA:HAB	2.06	0.55
2:B:355:PHE:HZ	2:B:373:LYS:HZ3	1.54	0.55
4:C:391:SER:OG	4:C:393:ASN:OD1	2.20	0.55
4:C:45:ALA:O	4:C:49:VAL:HG23	2.06	0.55
32:B:519:C7Z:C4	33:B:521:DGD:HA31	2.37	0.54
24:C:511:CLA:H191	11:K:30:VAL:HG12	1.87	0.54
15:P:225:ARG:HH11	15:P:228:LYS:HZ1	1.56	0.54
2:B:121:GLU:OE1	8:H:31:ARG:NH2	2.41	0.54
2:B:327:THR:HG22	24:B:507:CLA:H11	1.88	0.54
15:P:125:LYS:HB3	15:P:130:ALA:HB3	1.89	0.54
1:A:45:ILE:HD11	25:A:407:PHO:H51	1.88	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.43	0.53
24:B:502:CLA:H42	28:H:102:LMG:H131	1.91	0.53
3:V:26:LEU:HD21	19:Z:25:VAL:HA	1.91	0.53
2:B:35:GLY:HA3	2:B:101:ILE:HG12	1.89	0.53
5:D:193:LEU:O	12:L:35:TYR:OH	2.24	0.53
1:A:240:GLY:H	16:T:30:ALA:H	1.57	0.53
26:D:405:BCR:H20C	28:D:409:LMG:H321	1.91	0.53
1:A:93:PHE:CE2	1:A:95:PRO:HG3	2.44	0.53
1:A:283:ILE:HA	1:A:286:THR:HG22	1.89	0.53
3:V:5:LEU:HD22	39:J:102:LMU:H6'1	1.91	0.53
5:D:201:VAL:HG22	24:D:403:CLA:C2B	2.39	0.53
24:B:510:CLA:H112	24:B:515:CLA:HAA1	1.90	0.53
5:D:172:SER:HB2	5:D:177:SER:HB2	1.90	0.53
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.53
2:B:202:HIS:HE1	24:B:503:CLA:C1A	2.22	0.53
2:B:357:ARG:NH1	2:B:358:ARG:O	2.42	0.52
2:B:458:PHE:HB3	24:B:504:CLA:HBC2	1.89	0.52
1:A:223:LEU:HD11	5:D:265:ARG:NH1	2.25	0.52
2:B:282:GLN:HA	20:U:110:LYS:HD3	1.92	0.52
33:C:519:DGD:HO2D	39:J:102:LMU:H2O2	1.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:21:PHE:HD1	27:M:101:SQD:H271	1.73	0.52
15:P:68:ARG:HD3	15:P:69:VAL:N	2.25	0.52
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.52
24:C:507:CLA:H43	26:C:516:BCR:H10C	1.90	0.52
7:F:19:TRP:HE3	7:F:20:LEU:HD22	1.74	0.52
2:B:372:ASP:OD1	2:B:373:LYS:N	2.41	0.52
3:V:33:LEU:OXT	11:K:46:ARG:NH2	2.39	0.52
14:O:115:THR:HB	14:O:127:PHE:HB3	1.90	0.52
24:B:510:CLA:H101	24:B:515:CLA:HBA2	1.90	0.52
1:A:179:THR:O	1:A:183:MET:HG3	2.10	0.52
5:D:99:GLY:HA2	31:D:410:LHG:HC62	1.91	0.52
24:D:404:CLA:H102	18:X:80:ALA:HB2	1.91	0.52
2:B:7:ARG:O	2:B:10:THR:OG1	2.20	0.52
2:B:393:GLU:OE2	2:B:418:LYS:NZ	2.39	0.52
2:B:348:ASP:OD1	2:B:352:ARG:N	2.43	0.52
2:B:216:HIS:HE1	24:B:509:CLA:NC	2.07	0.51
24:B:505:CLA:HMA3	24:B:506:CLA:H3A	1.92	0.51
4:C:331:ARG:HH21	14:O:82:ASN:HA	1.74	0.51
4:C:432:HIS:HE1	24:C:509:CLA:C1A	2.23	0.51
24:D:404:CLA:H8	8:H:55:LEU:HD11	1.92	0.51
1:A:101:SER:HA	28:A:411:LMG:HC61	1.91	0.51
5:D:103:ARG:HD2	6:E:76:VAL:HG13	1.93	0.51
37:E:101:HEM:HBB2	37:E:101:HEM:HMB2	1.92	0.51
15:P:177:LYS:NZ	15:P:181:GLY:O	2.41	0.51
4:C:225:HIS:HE1	24:C:502:CLA:NA	2.09	0.51
5:D:5:ILE:O	5:D:9:GLN:NE2	2.43	0.51
24:B:514:CLA:H71	26:B:517:BCR:H20C	1.94	0.50
5:D:201:VAL:HG13	24:D:403:CLA:HMB2	1.92	0.50
1:A:308:ASP:OD1	1:A:312:ARG:N	2.44	0.50
2:B:12:VAL:HG23	24:B:512:CLA:HMC2	1.93	0.50
4:C:26:GLY:HA3	24:C:512:CLA:HMD2	1.93	0.50
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.92	0.50
5:D:142:ASN:HD22	5:D:142:ASN:H	1.60	0.50
24:B:507:CLA:H202	28:B:520:LMG:H351	1.92	0.50
2:B:201:HIS:HE1	24:B:502:CLA:C1D	2.16	0.50
34:B:522:3PH:H3H1	34:B:522:3PH:H2I3	1.93	0.50
1:A:269:ARG:HD2	5:D:235:PHE:HB2	1.92	0.50
33:C:519:DGD:O2D	39:J:102:LMU:O2'	2.26	0.50
31:D:408:LHG:H191	16:T:17:ILE:HD11	1.94	0.50
8:H:65:LEU:HD11	28:H:102:LMG:H302	1.94	0.50
11:K:14:ALA:HB1	19:Z:5:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:HIS:HE1	24:B:516:CLA:C1D	2.25	0.49
24:B:508:CLA:HBB1	24:B:508:CLA:HMB1	1.93	0.49
5:D:58:TRP:O	5:D:62:GLY:HA2	2.12	0.49
2:B:452:THR:HB	5:D:291:LEU:HD11	1.94	0.49
26:B:517:BCR:H383	27:M:101:SQD:H162	1.94	0.49
4:C:239:HIS:HE1	24:C:507:CLA:NA	2.05	0.49
4:C:40:ALA:HB2	24:C:512:CLA:HMA2	1.95	0.49
26:C:517:BCR:H391	11:K:36:ALA:HB2	1.93	0.49
1:A:223:LEU:HD21	5:D:265:ARG:NE	2.27	0.49
24:B:508:CLA:H92	35:B:523:DGA:HBH1	1.93	0.49
15:P:205:VAL:HG22	15:P:218:LYS:HG3	1.94	0.49
1:A:64:ARG:O	14:O:206:ARG:NH2	2.44	0.49
1:A:176:ILE:HD13	24:D:401:CLA:HED3	1.94	0.49
31:A:414:LHG:O1	4:C:435:ARG:NE	2.29	0.49
26:C:515:BCR:H332	19:Z:54:VAL:HG12	1.94	0.49
5:D:148:ALA:HB2	5:D:276:VAL:HG13	1.94	0.49
1:A:160:ILE:HD11	33:C:518:DGD:HB82	1.94	0.49
1:A:340:PRO:HB2	15:P:224:LYS:HB2	1.94	0.49
24:B:509:CLA:H42	35:B:523:DGA:HB71	1.94	0.49
14:O:238:GLN:NE2	14:O:282:ALA:O	2.46	0.49
4:C:288:GLU:OE1	4:C:288:GLU:N	2.41	0.48
15:P:161:ASP:OD1	15:P:162:ALA:N	2.42	0.48
2:B:29:LEU:HD21	26:B:517:BCR:H19C	1.95	0.48
2:B:464:PHE:HD2	24:B:511:CLA:HAC2	1.76	0.48
4:C:122:LEU:HD21	24:C:512:CLA:H2	1.95	0.48
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.40	0.48
24:C:502:CLA:H121	24:C:508:CLA:H92	1.95	0.48
10:J:9:ARG:H	10:J:9:ARG:HD2	1.78	0.48
2:B:349:GLN:NE2	2:B:395:VAL:O	2.47	0.48
3:V:22:VAL:HG21	19:Z:24:PRO:HB2	1.94	0.48
15:P:114:ASN:HA	15:P:220:GLN:O	2.14	0.48
2:B:214:LEU:O	2:B:218:CSD:OD2	2.29	0.48
4:C:418:HIS:CD2	24:C:503:CLA:ND	2.80	0.48
4:C:41:HIS:CD2	24:C:510:CLA:NA	2.82	0.48
4:C:80:ILE:HD11	24:C:504:CLA:HED3	1.95	0.48
14:O:236:GLU:HB3	14:O:240:LEU:HD13	1.95	0.48
24:B:504:CLA:CMB	24:B:507:CLA:HAB	2.44	0.48
1:A:93:PHE:CZ	24:A:408:CLA:HAA1	2.47	0.48
4:C:394:SER:HA	4:C:408:VAL:HG23	1.96	0.48
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.96	0.48
4:C:264:LEU:HD21	24:C:509:CLA:CAB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG12	2:B:52:LEU:HG	1.94	0.47
2:B:142:HIS:HA	2:B:145:LEU:HD12	1.95	0.47
4:C:274:ALA:HB2	24:C:503:CLA:HMD2	1.96	0.47
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.96	0.47
4:C:153:LEU:HD11	24:C:507:CLA:HAB	1.95	0.47
8:H:78:THR:OG1	8:H:83:SER:OG	2.31	0.47
24:A:405:CLA:HBA1	24:A:405:CLA:H3A	1.64	0.47
2:B:21:SER:OG	2:B:115:TRP:HB2	2.13	0.47
24:B:504:CLA:HBB1	24:B:504:CLA:HMB1	1.97	0.47
4:C:425:PHE:HA	24:C:509:CLA:HMC2	1.97	0.47
5:D:29:PHE:O	5:D:128:ARG:NH1	2.41	0.47
1:A:239:PHE:HB3	16:T:29:ILE:HA	1.96	0.47
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.96	0.47
1:A:155:THR:HG22	1:A:160:ILE:HG12	1.97	0.47
4:C:132:TYR:CE1	24:C:514:CLA:HAA2	2.50	0.47
15:P:185:TYR:HB3	15:P:187:PHE:CZ	2.50	0.47
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.97	0.47
25:A:407:PHO:HAB	5:D:205:LEU:HD13	1.97	0.47
4:C:265:ALA:HB2	4:C:429:HIS:CG	2.49	0.47
31:D:408:LHG:H322	16:T:21:ILE:HD11	1.96	0.47
14:O:85:PRO:HG2	14:O:295:TYR:CD2	2.49	0.47
2:B:157:HIS:CD2	2:B:164:PRO:HD2	2.49	0.47
2:B:191:ASP:OD2	8:H:83:SER:OG	2.32	0.47
2:B:348:ASP:OD2	2:B:352:ARG:NH1	2.48	0.47
5:D:50:THR:HG22	7:F:32:PHE:HZ	1.79	0.47
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.97	0.47
1:A:26:ASN:O	5:D:255:GLN:NE2	2.45	0.47
2:B:23:HIS:CD2	24:B:512:CLA:NB	2.82	0.47
24:C:502:CLA:H93	24:C:502:CLA:H112	1.73	0.47
2:B:60:MET:HB3	2:B:63:LEU:HB2	1.96	0.46
5:D:90:LEU:HD13	5:D:109:GLY:HA2	1.98	0.46
1:A:50:ILE:HG22	26:A:409:BCR:H271	1.97	0.46
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.50	0.46
2:B:268:PHE:HB3	2:B:448:ARG:HB3	1.98	0.46
4:C:261:SER:HB2	4:C:433:ALA:HB2	1.98	0.46
4:C:333:PRO:HB3	14:O:135:ARG:HD3	1.96	0.46
6:E:71:ASN:OD1	6:E:71:ASN:N	2.46	0.46
1:A:334:ARG:HD3	5:D:320:LEU:HD23	1.97	0.46
24:B:502:CLA:H61	24:B:502:CLA:H41	1.37	0.46
24:B:512:CLA:H102	24:B:512:CLA:H61	1.68	0.46
1:A:316:THR:HG23	5:D:64:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:HA	5:D:321:LEU:HD21	1.97	0.46
2:B:24:LEU:HD21	24:B:516:CLA:CAB	2.36	0.46
2:B:201:HIS:HB2	24:B:502:CLA:C1B	2.45	0.46
24:B:508:CLA:H3A	24:B:508:CLA:HBA2	1.60	0.46
24:B:508:CLA:H61	24:B:508:CLA:H41	1.60	0.46
8:H:63:ILE:HD13	38:H:101:RRX:H45	1.96	0.46
14:O:63:THR:OG1	14:O:64:TYR:N	2.49	0.46
4:C:406:ASN:HD21	33:C:519:DGD:HD4	1.79	0.46
4:C:413:TRP:CD1	24:C:505:CLA:HMA2	2.50	0.46
31:D:407:LHG:H111	31:D:407:LHG:H141	1.70	0.46
2:B:245:VAL:HG12	24:B:504:CLA:HAC1	1.98	0.46
24:C:510:CLA:H91	24:C:510:CLA:H111	1.73	0.46
24:C:513:CLA:H51	24:C:513:CLA:H11	1.75	0.46
5:D:198:MET:SD	24:D:401:CLA:HED2	2.56	0.46
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.80	0.46
2:B:120:LEU:HD12	8:H:22:ILE:HB	1.98	0.46
2:B:349:GLN:OE1	2:B:350:GLU:N	2.48	0.46
24:B:507:CLA:C2B	28:B:520:LMG:H162	2.45	0.46
19:Z:16:SER:OG	19:Z:47:TRP:NE1	2.37	0.46
4:C:153:LEU:CD1	24:C:507:CLA:HAB	2.47	0.45
24:C:504:CLA:H61	24:C:504:CLA:H41	1.83	0.45
1:A:28:LEU:HB2	28:A:415:LMG:H301	1.98	0.45
24:D:404:CLA:H41	24:D:404:CLA:H62	1.41	0.45
6:E:25:ILE:O	6:E:29:SER:OG	2.29	0.45
24:A:408:CLA:H2	9:I:12:VAL:HG11	1.99	0.45
4:C:306:LEU:HD12	4:C:328:TYR:HB3	1.96	0.45
15:P:182:LYS:NZ	15:P:210:SER:HB3	2.30	0.45
1:A:269:ARG:NH1	5:D:231:THR:O	2.50	0.45
2:B:83:GLU:HG2	2:B:84:THR:H	1.82	0.45
24:B:516:CLA:H52	24:B:516:CLA:H11	1.69	0.45
25:D:402:PHO:HBA1	25:D:402:PHO:H3A	1.36	0.45
24:B:511:CLA:H193	24:B:511:CLA:H162	1.74	0.45
3:V:31:GLY:HA2	19:Z:30:PRO:HD3	1.99	0.45
1:A:307:VAL:HG23	7:F:44:ARG:HD3	1.98	0.45
2:B:116:VAL:HG21	32:B:519:C7Z:O23	2.15	0.45
6:E:27:VAL:HB	6:E:28:PRO:HD3	1.98	0.45
1:A:202:VAL:HG11	24:A:406:CLA:C3D	2.47	0.45
24:B:501:CLA:HBB2	38:H:101:RRX:H28	1.99	0.45
4:C:120:HIS:HE1	24:C:514:CLA:NA	2.09	0.45
1:A:43:THR:HG23	26:A:409:BCR:H362	1.99	0.45
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.98	0.45
2:B:69:LEU:HA	2:B:69:LEU:HD12	1.75	0.45
2:B:192:PRO:HB3	24:B:502:CLA:O1A	2.17	0.45
2:B:469:HIS:HE1	24:B:511:CLA:C1A	2.29	0.45
4:C:395:VAL:HG11	4:C:403:ASN:HA	1.99	0.45
14:O:201:LEU:HD11	14:O:247:PRO:HB2	1.99	0.45
2:B:9:HIS:CG	24:B:512:CLA:HBB2	2.52	0.45
4:C:270:MET:HE1	24:C:508:CLA:H11	1.98	0.45
6:E:13:ILE:O	6:E:16:SER:OG	2.29	0.45
2:B:40:PHE:HD1	34:B:522:3PH:H3B2	1.82	0.44
24:D:403:CLA:H41	24:D:403:CLA:H62	1.74	0.44
1:A:210:LEU:HD13	24:A:406:CLA:H43	1.98	0.44
24:B:514:CLA:H141	24:B:514:CLA:H161	1.66	0.44
5:D:323:GLU:OE2	14:O:222:TYR:OH	2.29	0.44
1:A:240:GLY:HA3	16:T:29:ILE:HG13	1.99	0.44
24:B:503:CLA:H152	8:H:57:PHE:HE2	1.82	0.44
24:B:510:CLA:H141	24:B:510:CLA:H162	1.70	0.44
5:D:12:ARG:HG3	5:D:16:ASP:HB2	1.99	0.44
5:D:320:LEU:HD12	5:D:320:LEU:HA	1.81	0.44
14:O:98:LYS:O	14:O:102:TYR:OH	2.22	0.44
15:P:68:ARG:HD3	15:P:69:VAL:H	1.83	0.44
2:B:320:ALA:HB1	5:D:292:ASN:HD22	1.82	0.44
26:B:517:BCR:H15C	26:B:517:BCR:H351	1.72	0.44
4:C:150:GLY:HA3	4:C:240:ILE:HG13	1.99	0.44
5:D:40:CYS:SG	24:D:404:CLA:HBB1	2.57	0.44
15:P:197:ASN:HD22	15:P:201:ARG:HH21	1.65	0.44
15:P:197:ASN:ND2	15:P:201:ARG:HH21	2.15	0.44
24:B:505:CLA:H102	24:B:510:CLA:H42	1.98	0.44
1:A:174:LEU:HD22	25:A:407:PHO:H143	2.00	0.44
24:B:502:CLA:H201	5:D:158:LEU:HD23	2.00	0.44
24:B:503:CLA:H141	24:B:503:CLA:H161	1.79	0.44
14:O:105:GLU:HG3	14:O:106:LYS:HG2	2.00	0.44
20:U:110:LYS:N	20:U:110:LYS:HE3	2.33	0.44
1:A:344:ALA:O	4:C:345:ARG:NH1	2.51	0.44
2:B:157:HIS:O	2:B:158:VAL:HG22	2.17	0.44
24:C:508:CLA:H62	24:C:508:CLA:H41	1.63	0.44
15:P:68:ARG:HH11	15:P:69:VAL:H	1.64	0.44
20:U:117:THR:HG22	20:U:119:LYS:H	1.82	0.44
31:A:414:LHG:H342	24:C:509:CLA:HBC2	1.99	0.44
2:B:478:VAL:HB	2:B:482:ILE:HG22	2.00	0.44
24:C:502:CLA:H41	24:C:502:CLA:H61	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:510:CLA:H62	24:C:510:CLA:H101	1.64	0.44
5:D:38:LEU:HB2	5:D:39:PRO:HD3	1.99	0.44
14:O:265:GLU:OE1	14:O:295:TYR:OH	2.32	0.44
24:B:504:CLA:HAB	24:B:511:CLA:H191	1.99	0.44
25:D:402:PHO:H112	25:D:402:PHO:H72	1.80	0.44
16:T:28:ARG:CZ	16:T:28:ARG:HA	2.48	0.44
25:A:407:PHO:H8	25:A:407:PHO:H121	1.78	0.43
24:B:508:CLA:HMC2	24:B:509:CLA:H142	2.00	0.43
24:B:515:CLA:H93	24:B:515:CLA:H62	1.69	0.43
24:C:510:CLA:H142	24:C:510:CLA:H112	1.75	0.43
5:D:329:MET:HG2	5:D:333:ASP:HB2	1.99	0.43
38:H:101:RRX:H40	38:H:101:RRX:H36	1.83	0.43
31:L:101:LHG:HC81	31:L:101:LHG:H112	1.52	0.43
1:A:149:ALA:HB3	1:A:150:PRO:HD3	2.00	0.43
14:O:135:ARG:HA	17:W:64:ARG:NH2	2.33	0.43
14:O:208:SER:HA	14:O:245:TYR:CZ	2.53	0.43
4:C:395:VAL:HG13	4:C:403:ASN:HA	2.00	0.43
5:D:51:GLY:HA2	5:D:55:VAL:HB	2.00	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.18	0.43
1:A:316:THR:HG22	1:A:317:TRP:H	1.84	0.43
1:A:324:ALA:O	1:A:328:MET:HG3	2.19	0.43
2:B:248:ALA:HA	24:B:503:CLA:H42	2.00	0.43
24:B:510:CLA:H161	24:B:510:CLA:H192	1.72	0.43
4:C:216:ASP:OD1	4:C:216:ASP:N	2.48	0.43
4:C:351:GLY:O	4:C:355:GLU:HG2	2.19	0.43
24:C:507:CLA:HBA1	24:C:507:CLA:H3A	1.88	0.43
1:A:140:ARG:HH21	1:A:142:TRP:HZ3	1.66	0.43
2:B:30:VAL:HG22	24:B:513:CLA:C3C	2.49	0.43
2:B:466:HIS:CE1	24:B:508:CLA:C4D	3.02	0.43
24:B:503:CLA:H193	24:B:503:CLA:H162	1.68	0.43
24:B:504:CLA:H92	24:B:504:CLA:H41	2.00	0.43
24:B:505:CLA:H41	24:B:505:CLA:H62	1.55	0.43
1:A:32:TRP:O	1:A:35:VAL:HG22	2.18	0.43
2:B:150:CYS:HB2	24:B:503:CLA:CMC	2.49	0.43
24:B:504:CLA:H92	24:B:504:CLA:H61	1.83	0.43
4:C:26:GLY:HA3	24:C:512:CLA:C2D	2.49	0.43
18:X:87:ALA:O	18:X:90:VAL:HG12	2.19	0.43
2:B:475:PHE:HB3	2:B:478:VAL:HG22	2.00	0.43
4:C:105:LEU:HB2	28:C:522:LMG:H171	2.01	0.43
24:C:508:CLA:H193	24:C:508:CLA:H162	1.76	0.43
14:O:141:ASP:OD1	14:O:141:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:O	2:B:30:VAL:HG23	2.19	0.42
24:B:504:CLA:H41	24:B:504:CLA:H61	1.71	0.42
24:D:401:CLA:H62	24:D:401:CLA:H92	1.81	0.42
4:C:204:SER:HB2	28:C:501:LMG:HC71	2.00	0.42
24:C:504:CLA:H61	24:C:504:CLA:H101	1.88	0.42
4:C:365:LEU:HD12	14:O:142:GLY:HA3	2.01	0.42
5:D:59:TYR:O	6:E:66:ILE:HG12	2.20	0.42
19:Z:12:LEU:HA	19:Z:50:LEU:HD23	2.01	0.42
2:B:74:SER:HG	2:B:94:GLU:CD	2.27	0.42
24:B:514:CLA:H3A	24:B:514:CLA:HBA2	1.50	0.42
5:D:160:TYR:HA	5:D:290:ALA:HB2	2.01	0.42
1:A:104:GLU:CD	17:W:64:ARG:HH12	2.28	0.42
4:C:15:ASP:OD1	4:C:18:THR:OG1	2.35	0.42
5:D:55:VAL:HG21	5:D:110:LEU:HD22	2.02	0.42
2:B:460:LEU:HD23	2:B:460:LEU:HA	1.88	0.42
24:B:513:CLA:H92	24:B:513:CLA:H61	1.82	0.42
24:B:513:CLA:CAD	24:B:514:CLA:HAB	2.48	0.42
15:P:124:ASP:OD1	15:P:124:ASP:N	2.51	0.42
20:U:110:LYS:HG2	20:U:117:THR:HG21	2.01	0.42
1:A:329:GLU:O	1:A:332:HIS:ND1	2.52	0.42
31:A:414:LHG:H331	31:A:414:LHG:H361	1.68	0.42
24:B:503:CLA:H91	24:B:503:CLA:H111	1.83	0.42
24:B:504:CLA:HBD	24:B:505:CLA:H42	2.02	0.42
24:B:513:CLA:HBB1	24:B:513:CLA:HMB1	2.02	0.42
35:B:523:DGA:HBE2	35:B:523:DGA:HB81	1.38	0.42
5:D:148:ALA:HB3	5:D:149:PRO:HD3	2.01	0.42
15:P:105:ARG:HG3	15:P:117:TYR:HB3	2.01	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.02	0.42
24:A:406:CLA:HBB1	25:D:402:PHO:H122	2.01	0.42
2:B:485:ASP:OD1	2:B:485:ASP:N	2.51	0.42
24:B:511:CLA:H142	24:B:511:CLA:H111	1.82	0.42
24:B:512:CLA:H3A	24:B:512:CLA:HBA2	1.62	0.42
34:B:522:3PH:H361	34:B:522:3PH:H331	1.71	0.42
4:C:106:HIS:CE1	28:C:522:LMG:H202	2.55	0.42
4:C:142:LYS:HZ2	4:C:254:TRP:CG	2.37	0.42
4:C:203:LYS:HG2	4:C:209:ASP:HB3	2.02	0.42
5:D:191:TRP:CE2	5:D:197:HIS:HB2	2.55	0.42
11:K:10:LYS:NZ	11:K:10:LYS:HB3	2.34	0.42
18:X:89:ALA:O	18:X:93:VAL:HG23	2.20	0.42
3:V:18:ALA:HB3	26:J:101:BCR:H12C	2.01	0.42
4:C:460:LEU:HD22	4:C:460:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:77:LYS:HE3	6:E:77:LYS:HB2	1.91	0.42
14:O:72:TYR:CE2	14:O:76:LYS:HD2	2.54	0.42
14:O:152:ASP:OD1	14:O:152:ASP:N	2.51	0.42
14:O:192:THR:HG23	14:O:195:SER:H	1.85	0.42
14:O:226:ILE:H	14:O:226:ILE:HG13	1.66	0.42
15:P:176:GLU:OE2	15:P:186:LYS:HD3	2.20	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.42
4:C:44:HIS:HE1	24:C:511:CLA:C4B	2.33	0.42
24:C:504:CLA:H203	24:C:511:CLA:HAB	2.01	0.42
8:H:63:ILE:CD1	38:H:101:RRX:H45	2.50	0.42
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.41
1:A:274:PHE:HA	1:A:277:VAL:HG12	2.00	0.41
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.41
24:B:501:CLA:HBB1	38:H:101:RRX:H34	2.01	0.41
4:C:49:VAL:HG12	4:C:106:HIS:O	2.20	0.41
24:D:401:CLA:HBA2	24:D:401:CLA:H3A	1.54	0.41
14:O:171:LYS:HD2	14:O:177:TYR:HE1	1.85	0.41
1:A:259:ILE:HG22	24:A:406:CLA:H201	2.01	0.41
1:A:291:SER:O	1:A:294:ALA:HB3	2.19	0.41
5:D:191:TRP:CE3	5:D:289:LEU:HD11	2.55	0.41
31:D:407:LHG:H102	31:D:407:LHG:H362	2.02	0.41
15:P:102:ILE:HG12	15:P:119:VAL:HG22	2.01	0.41
19:Z:1:MET:SD	19:Z:1:MET:N	2.89	0.41
1:A:147:TYR:O	1:A:150:PRO:HD2	2.21	0.41
1:A:161:TYR:HA	1:A:294:ALA:HB1	2.02	0.41
1:A:218:LEU:HD12	1:A:251:ALA:HB1	2.02	0.41
15:P:108:ASP:HB3	15:P:111:ASP:O	2.20	0.41
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	2.01	0.41
2:B:103:LEU:HB2	24:B:506:CLA:H71	2.02	0.41
24:B:505:CLA:HBB2	32:B:519:C7Z:C19	2.51	0.41
4:C:264:LEU:HD21	24:C:509:CLA:HAB	2.01	0.41
24:A:405:CLA:H141	24:A:405:CLA:H162	1.72	0.41
2:B:74:SER:OG	2:B:94:GLU:OE2	2.34	0.41
24:B:502:CLA:H92	24:B:502:CLA:H62	1.79	0.41
4:C:44:HIS:HE1	24:C:511:CLA:NB	2.14	0.41
4:C:303:PHE:O	4:C:307:VAL:HG13	2.20	0.41
28:C:501:LMG:H322	28:C:501:LMG:H291	1.76	0.41
24:C:507:CLA:H8	26:C:516:BCR:H14C	2.03	0.41
4:C:406:ASN:HB2	33:C:520:DGD:O3E	2.20	0.41
6:E:42:LEU:O	6:E:46:VAL:HG22	2.21	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:HE1	24:A:408:CLA:ND	2.16	0.41
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.91	0.41
4:C:362:GLY:HA2	14:O:72:TYR:CE1	2.56	0.41
24:C:511:CLA:H111	24:C:511:CLA:H152	1.69	0.41
5:D:201:VAL:HG22	24:D:403:CLA:C1B	2.50	0.41
1:A:34:GLY:O	1:A:38:ILE:HG12	2.21	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.91	0.41
1:A:238:LYS:HB3	16:T:30:ALA:HA	2.01	0.41
1:A:238:LYS:HE2	1:A:238:LYS:HB2	1.83	0.41
1:A:330:VAL:O	5:D:349:GLY:N	2.47	0.41
24:C:502:CLA:H191	24:C:508:CLA:HBB1	2.03	0.41
24:C:510:CLA:H161	24:C:510:CLA:H141	1.84	0.41
5:D:160:TYR:HA	5:D:290:ALA:CB	2.51	0.41
11:K:27:ILE:O	11:K:30:VAL:HG22	2.21	0.41
14:O:111:PRO:HD2	14:O:138:TYR:HD1	1.86	0.41
14:O:114:PHE:HD1	14:O:290:ILE:HG12	1.85	0.41
15:P:195:ASP:OD1	15:P:195:ASP:N	2.53	0.41
2:B:254:GLY:HA2	28:H:102:LMG:H212	2.02	0.41
4:C:433:ALA:HB1	24:C:506:CLA:HED2	2.03	0.41
5:D:315:TYR:O	5:D:319:ILE:HG12	2.21	0.41
18:X:82:VAL:O	18:X:86:ILE:HG12	2.21	0.41
1:A:131:TRP:CH2	24:C:506:CLA:HAA2	2.56	0.40
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.91	0.40
2:B:187:ALA:HB1	8:H:74:LEU:HD23	2.03	0.40
2:B:466:HIS:HE1	24:B:508:CLA:C4D	2.33	0.40
24:B:511:CLA:H112	24:B:511:CLA:H72	1.68	0.40
33:B:521:DGD:HG31	33:B:521:DGD:HD2	1.68	0.40
4:C:15:ASP:OD1	4:C:15:ASP:N	2.54	0.40
4:C:336:GLU:OE1	4:C:336:GLU:N	2.54	0.40
5:D:184:PHE:HA	5:D:329:MET:HE1	2.03	0.40
31:D:410:LHG:H112	31:D:410:LHG:H142	1.49	0.40
27:M:101:SQD:H81	27:M:101:SQD:H112	1.86	0.40
2:B:241:SER:O	2:B:245:VAL:HG23	2.22	0.40
2:B:467:ILE:HD13	2:B:467:ILE:HA	1.83	0.40
4:C:166:LYS:HA	4:C:170:PHE:HB2	2.03	0.40
33:C:519:DGD:HB61	33:C:519:DGD:HB32	1.84	0.40
24:D:401:CLA:HMA2	36:D:406:PL9:H411	2.02	0.40
31:D:410:LHG:H131	31:D:410:LHG:H161	1.81	0.40
1:A:226:GLU:HB2	5:D:265:ARG:HH22	1.87	0.40
1:A:292:THR:HA	4:C:416:THR:HG22	2.04	0.40
4:C:37:LEU:HD12	4:C:37:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:123:ILE:HD11	19:Z:27:PHE:O	2.21	0.40
7:F:27:VAL:HB	7:F:28:PRO:HD3	2.04	0.40
28:H:102:LMG:O4	28:H:102:LMG:O5	2.36	0.40
15:P:177:LYS:HA	15:P:177:LYS:HE2	2.03	0.40
2:B:33:TRP:HE1	24:B:507:CLA:C3C	2.35	0.40
2:B:148:LEU:HD22	2:B:148:LEU:HA	1.96	0.40
24:A:408:CLA:O1A	28:C:501:LMG:H131	2.21	0.40
2:B:139:PHE:HE2	2:B:216:HIS:CD2	2.39	0.40
2:B:311:PHE:O	2:B:317:ASN:ND2	2.54	0.40
24:C:512:CLA:H141	24:C:512:CLA:H162	1.90	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	334/336 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	481/484 (99%)	466 (97%)	14 (3%)	1 (0%)	43	65
3	V	31/33 (94%)	31 (100%)	0	0	100	100
4	C	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
5	D	346/348 (99%)	336 (97%)	10 (3%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
9	I	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	34/36 (94%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
15	P	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
17	W	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
18	X	31/33 (94%)	31 (100%)	0	0	100	100
19	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
20	U	26/28 (93%)	26 (100%)	0	0	100	100
All	All	2578/2619 (98%)	2498 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	VAL

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	275/275 (100%)	270 (98%)	5 (2%)	51	72
2	B	387/387 (100%)	378 (98%)	9 (2%)	44	68
3	V	26/26 (100%)	26 (100%)	0	100	100
4	C	350/350 (100%)	332 (95%)	18 (5%)	21	45
5	D	279/279 (100%)	268 (96%)	11 (4%)	28	53
6	E	68/68 (100%)	62 (91%)	6 (9%)	9	23
7	F	25/25 (100%)	24 (96%)	1 (4%)	28	53
8	H	56/56 (100%)	52 (93%)	4 (7%)	13	31
9	I	30/30 (100%)	28 (93%)	2 (7%)	15	34
10	J	27/27 (100%)	26 (96%)	1 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	33/33 (100%)	31 (94%)	2 (6%)	17 38
12	L	34/34 (100%)	34 (100%)	0	100 100
13	M	26/26 (100%)	26 (100%)	0	100 100
14	O	195/195 (100%)	189 (97%)	6 (3%)	35 60
15	P	152/152 (100%)	145 (95%)	7 (5%)	24 49
16	T	26/26 (100%)	26 (100%)	0	100 100
17	W	34/34 (100%)	33 (97%)	1 (3%)	37 62
18	X	24/24 (100%)	24 (100%)	0	100 100
19	Z	50/50 (100%)	49 (98%)	1 (2%)	48 70
20	U	27/27 (100%)	22 (82%)	5 (18%)	1 3
All	All	2124/2124 (100%)	2045 (96%)	79 (4%)	31 55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	121	LEU
1	A	248	ILE
1	A	259	ILE
1	A	262	TYR
2	B	29	LEU
2	B	120	LEU
2	B	131	THR
2	B	148	LEU
2	B	158	VAL
2	B	211	LEU
2	B	298	VAL
2	B	349	GLN
2	B	353	GLU
4	C	64	VAL
4	C	77	LEU
4	C	96	THR
4	C	130	GLU
4	C	138	VAL
4	C	162	LEU
4	C	192	THR
4	C	217	ASN
4	C	218	LEU

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Mol	Chain	Res	Type
4	C	228	ILE
4	C	277	PHE
4	C	348	ASP
4	C	368	LEU
4	C	392	LEU
4	C	398	VAL
4	C	402	ILE
4	C	437	ARG
4	C	460	LEU
5	D	13	THR
5	D	30	VAL
5	D	80	THR
5	D	142	ASN
5	D	150	ILE
5	D	192	THR
5	D	213	ILE
5	D	241	GLU
5	D	272	LEU
5	D	281	MET
5	D	320	LEU
6	E	25	ILE
6	E	30	LEU
6	E	42	LEU
6	E	60	ARG
6	E	71	ASN
6	E	78	LYS
7	F	25	ILE
8	H	24	THR
8	H	36	GLU
8	H	66	GLU
8	H	74	LEU
9	I	6	ILE
9	I	23	PHE
10	J	42	LEU
11	K	10	LYS
11	K	43	VAL
14	O	129	LYS
14	O	212	ASP
14	O	222	TYR
14	O	233	ASP
14	O	241	ASN
14	O	293	LEU

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Mol	Chain	Res	Type
15	P	68	ARG
15	P	90	LYS
15	P	116	LEU
15	P	124	ASP
15	P	125	LYS
15	P	128	ILE
15	P	217	LEU
17	W	103	LEU
19	Z	50	LEU
20	U	110	LYS
20	U	119	LYS
20	U	120	GLU
20	U	125	ILE
20	U	126	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	317	ASN
2	B	394	GLN
4	C	403	ASN
4	C	406	ASN
5	D	83	ASN
5	D	142	ASN
5	D	336	HIS
8	H	79	ASN
9	I	31	ASN
14	O	242	ASN
15	P	71	ASN
15	P	115	ASN
15	P	197	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
2	CSD	B	218	2	3,7,8	0.87	0	1,8,10	0.10	0

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
2	CSD	B	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	218	CSD	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 4 are monoatomic - leaving 73 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	$\#\|Z\| > 2$
24	CLA	A	408	1	64,68,73	1.41	7 (10%)	77,107,113	2.13	20 (25%)
24	CLA	B	501	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)
24	CLA	B	508	2	69,73,73	1.37	6 (8%)	83,113,113	1.88	17 (20%)
24	CLA	C	503	4	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
24	CLA	C	509	4	69,73,73	1.38	6 (8%)	83,113,113	1.92	18 (21%)
36	PL9	D	406	-	55,55,55	1.39	5 (9%)	68,69,69	1.52	13 (19%)
24	CLA	C	506	4	58,62,73	1.50	7 (12%)	69,99,113	2.08	17 (24%)
24	CLA	B	503	2	69,73,73	1.38	7 (10%)	83,113,113	1.88	17 (20%)
28	LMG	H	102	-	48,48,55	0.99	5 (10%)	56,56,63	1.13	2 (3%)
24	CLA	B	509	2	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
31	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
24	CLA	C	505	-	59,63,73	1.46	7 (11%)	71,101,113	2.11	17 (23%)
28	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.09	3 (5%)
24	CLA	C	513	4	59,63,73	1.47	7 (11%)	71,101,113	2.01	17 (23%)
25	PHO	D	402	-	58,69,69	1.98	10 (17%)	56,99,99	1.52	8 (14%)
30	BCT	A	413	22	2,3,3	1.28	0	2,3,3	4.11	1 (50%)
26	BCR	B	518	-	41,41,41	4.76	26 (63%)	56,56,56	2.24	19 (33%)
26	BCR	B	517	-	41,41,41	4.74	25 (60%)	56,56,56	2.47	20 (35%)
28	LMG	A	411	-	34,34,55	0.46	0	42,42,63	1.27	5 (11%)
24	CLA	B	515	2	69,73,73	1.34	7 (10%)	83,113,113	1.93	18 (21%)
37	HEM	E	101	7,6	50,50,50	1.36	6 (12%)	66,82,82	1.07	5 (7%)
24	CLA	C	511	4	69,73,73	1.35	6 (8%)	83,113,113	1.99	17 (20%)
24	CLA	D	404	-	64,68,73	1.42	7 (10%)	77,107,113	2.06	16 (20%)
24	CLA	C	512	4	69,73,73	1.37	6 (8%)	83,113,113	1.98	20 (24%)
24	CLA	A	406	40	69,73,73	1.37	7 (10%)	83,113,113	1.94	21 (25%)
28	LMG	B	520	-	44,44,55	0.87	3 (6%)	52,52,63	1.14	2 (3%)
28	LMG	C	522	-	33,33,55	0.93	2 (6%)	40,40,63	1.10	2 (5%)
24	CLA	B	512	2	69,73,73	1.36	6 (8%)	83,113,113	1.93	16 (19%)
21	OEX	A	401	4,1	0,14,14	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	504	4	69,73,73	1.37	7 (10%)	83,113,113	1.92	19 (22%)
28	LMG	C	501	-	40,40,55	0.76	2 (5%)	48,48,63	1.24	4 (8%)
33	DGD	C	520	-	54,54,67	0.94	4 (7%)	68,68,81	1.16	5 (7%)
26	BCR	J	101	-	41,41,41	4.79	26 (63%)	56,56,56	2.39	20 (35%)
28	LMG	D	409	-	42,42,55	0.77	2 (4%)	50,50,63	1.08	3 (6%)
24	CLA	B	511	2	69,73,73	1.37	6 (8%)	83,113,113	1.90	17 (20%)
24	CLA	D	403	5	69,73,73	1.36	7 (10%)	83,113,113	1.87	16 (19%)
24	CLA	B	506	-	61,65,73	1.45	6 (9%)	73,103,113	1.99	18 (24%)
24	CLA	B	510	40	69,73,73	1.36	6 (8%)	83,113,113	1.93	17 (20%)
26	BCR	D	405	-	41,41,41	4.77	26 (63%)	56,56,56	2.20	19 (33%)
31	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.12	4 (7%)
32	C7Z	B	519	-	43,43,43	5.30	27 (62%)	58,60,60	2.33	18 (31%)
33	DGD	C	519	-	54,54,67	1.01	4 (7%)	68,68,81	1.21	5 (7%)
39	LMU	J	102	-	36,36,36	0.39	0	47,47,47	0.77	2 (4%)
31	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.20	4 (9%)
24	CLA	B	516	2	59,63,73	1.47	6 (10%)	71,101,113	2.00	17 (23%)
25	PHO	A	407	-	58,69,69	1.97	10 (17%)	56,99,99	1.52	7 (12%)
27	SQD	M	101	-	41,42,54	0.87	0	50,53,65	0.93	2 (4%)
33	DGD	C	518	-	45,45,67	0.80	1 (2%)	59,59,81	1.11	4 (6%)
31	LHG	A	414	-	38,38,48	0.43	0	41,44,54	1.19	3 (7%)
24	CLA	B	505	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	18 (21%)
26	BCR	C	516	-	41,41,41	4.73	25 (60%)	56,56,56	2.40	22 (39%)
24	CLA	D	401	40	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
26	BCR	C	517	-	41,41,41	4.78	26 (63%)	56,56,56	2.38	19 (33%)
34	3PH	B	522	-	47,47,47	0.85	4 (8%)	51,52,52	1.15	2 (3%)
24	CLA	A	405	1	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
35	DGA	B	523	-	36,36,43	1.17	3 (8%)	38,38,45	1.38	3 (7%)
24	CLA	C	514	4	49,53,73	1.61	6 (12%)	59,89,113	2.09	14 (23%)
24	CLA	B	513	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	15 (18%)
38	RRX	H	101	-	42,42,42	5.02	26 (61%)	57,58,58	2.57	23 (40%)
24	CLA	B	504	2	64,68,73	1.44	7 (10%)	77,107,113	2.02	16 (20%)
24	CLA	B	514	2	69,73,73	1.37	6 (8%)	83,113,113	1.95	18 (21%)
33	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	0.93	2 (3%)
24	CLA	B	507	40	69,73,73	1.36	7 (10%)	83,113,113	1.94	18 (21%)
24	CLA	C	502	4	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LMG	A	415	-	37,37,55	0.59	1 (2%)	45,45,63	1.07	3 (6%)
24	CLA	C	508	40	69,73,73	1.36	6 (8%)	83,113,113	1.96	16 (19%)
26	BCR	C	515	-	41,41,41	4.77	26 (63%)	56,56,56	2.23	20 (35%)
24	CLA	C	507	4	69,73,73	1.37	6 (8%)	83,113,113	1.92	19 (22%)
27	SQD	A	410	-	41,42,54	0.87	0	50,53,65	1.01	2 (4%)
31	LHG	D	407	-	43,43,48	0.42	0	46,49,54	1.05	3 (6%)
24	CLA	B	502	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
24	CLA	C	510	4	69,73,73	1.37	6 (8%)	83,113,113	1.92	17 (20%)
26	BCR	A	409	-	41,41,41	4.79	26 (63%)	56,56,56	3.00	25 (44%)

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
24	CLA	A	408	1	-	15/33/109/115	-
24	CLA	B	501	-	-	16/39/115/115	-
24	CLA	B	508	2	-	15/39/115/115	-
24	CLA	C	503	4	-	15/39/115/115	-
24	CLA	C	509	4	-	15/39/115/115	-
36	PL9	D	406	-	-	8/53/73/73	0/1/1/1
24	CLA	C	506	4	-	13/26/102/115	-
24	CLA	B	503	2	-	21/39/115/115	-
28	LMG	H	102	-	-	13/43/63/70	0/1/1/1
24	CLA	B	509	2	-	15/39/115/115	-
31	LHG	D	408	-	-	26/53/53/53	-
24	CLA	C	505	-	-	9/27/103/115	-
28	LMG	C	521	-	-	9/42/62/70	0/1/1/1
24	CLA	C	513	4	-	11/27/103/115	-
25	PHO	D	402	-	-	7/37/103/103	0/5/6/6
26	BCR	B	518	-	-	13/29/63/63	0/2/2/2
26	BCR	B	517	-	-	10/29/63/63	0/2/2/2
28	LMG	A	411	-	-	8/29/49/70	0/1/1/1
24	CLA	B	515	2	-	20/39/115/115	-
37	HEM	E	101	7,6	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	511	4	-	16/39/115/115	-
24	CLA	D	404	-	-	16/33/109/115	-
24	CLA	C	512	4	-	13/39/115/115	-
24	CLA	A	406	40	-	13/39/115/115	-
28	LMG	B	520	-	-	9/39/59/70	0/1/1/1
28	LMG	C	522	-	-	8/27/47/70	0/1/1/1
24	CLA	B	512	2	-	15/39/115/115	-
24	CLA	C	504	4	-	15/39/115/115	-
28	LMG	C	501	-	-	8/35/55/70	0/1/1/1
33	DGD	C	520	-	-	9/42/82/95	0/2/2/2
26	BCR	J	101	-	-	11/29/63/63	0/2/2/2
28	LMG	D	409	-	-	9/37/57/70	0/1/1/1
24	CLA	B	511	2	-	16/39/115/115	-
24	CLA	D	403	5	-	14/39/115/115	-
24	CLA	B	506	-	-	7/30/106/115	-
24	CLA	B	510	40	-	19/39/115/115	-
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
31	LHG	L	101	-	-	30/53/53/53	-
32	C7Z	B	519	-	-	12/29/67/67	0/2/2/2
33	DGD	C	519	-	-	16/42/82/95	0/2/2/2
39	LMU	J	102	-	-	6/21/61/61	0/2/2/2
31	LHG	D	410	-	-	25/43/43/53	-
24	CLA	B	516	2	-	15/27/103/115	-
25	PHO	A	407	-	-	13/37/103/103	0/5/6/6
27	SQD	M	101	-	-	14/37/57/69	0/1/1/1
33	DGD	C	518	-	-	6/33/73/95	0/2/2/2
31	LHG	A	414	-	-	26/43/43/53	-
24	CLA	B	505	2	-	15/39/115/115	-
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	CLA	D	401	40	-	21/39/115/115	-
26	BCR	C	517	-	-	10/29/63/63	0/2/2/2
34	3PH	B	522	-	-	25/49/49/49	-
24	CLA	A	405	1	-	14/39/115/115	-
35	DGA	B	523	-	-	24/38/38/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	514	4	-	7/15/91/115	-
24	CLA	B	513	2	-	18/39/115/115	-
38	RRX	H	101	-	-	6/29/65/65	0/2/2/2
24	CLA	B	504	2	-	18/33/109/115	-
24	CLA	B	514	2	-	17/39/115/115	-
33	DGD	B	521	-	-	14/32/72/95	0/2/2/2
24	CLA	B	507	40	-	24/39/115/115	-
24	CLA	C	502	4	-	18/39/115/115	-
28	LMG	A	415	-	-	4/32/52/70	0/1/1/1
24	CLA	C	508	40	-	14/39/115/115	-
26	BCR	C	515	-	-	13/29/63/63	0/2/2/2
24	CLA	C	507	4	-	19/39/115/115	-
27	SQD	A	410	-	-	8/37/57/69	0/1/1/1
31	LHG	D	407	-	-	23/48/48/53	-
24	CLA	B	502	2	-	14/39/115/115	-
24	CLA	C	510	4	-	9/39/115/115	-
26	BCR	A	409	-	-	13/29/63/63	0/2/2/2

All (549) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C25-C26	15.87	1.61	1.34
26	A	409	BCR	C26-C25	15.47	1.61	1.34
26	D	405	BCR	C26-C25	15.44	1.61	1.34
26	J	101	BCR	C26-C25	15.43	1.61	1.34
26	B	518	BCR	C26-C25	15.41	1.61	1.34
26	C	517	BCR	C26-C25	15.39	1.61	1.34
26	C	516	BCR	C26-C25	15.34	1.61	1.34
38	H	101	RRX	C26-C25	15.12	1.60	1.34
26	B	517	BCR	C26-C25	15.06	1.60	1.34
26	C	515	BCR	C26-C25	15.06	1.60	1.34
32	B	519	C7Z	C5-C6	14.79	1.60	1.34
38	H	101	RRX	C5-C6	14.11	1.58	1.34
26	J	101	BCR	C5-C6	14.06	1.58	1.34
26	A	409	BCR	C5-C6	14.04	1.58	1.34
26	C	515	BCR	C5-C6	14.00	1.58	1.34
26	C	517	BCR	C5-C6	13.99	1.58	1.34
26	B	518	BCR	C5-C6	13.90	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	BCR	C5-C6	13.81	1.58	1.34
26	B	517	BCR	C5-C6	13.66	1.58	1.34
26	C	516	BCR	C5-C6	13.58	1.58	1.34
32	B	519	C7Z	C24-C23	11.36	1.72	1.52
32	B	519	C7Z	C22-C23	-11.25	1.36	1.52
38	H	101	RRX	C29-C28	-10.70	1.36	1.52
32	B	519	C7Z	C2-C3	-10.06	1.37	1.52
25	D	402	PHO	C1B-C2B	8.97	1.49	1.39
25	A	407	PHO	C1B-C2B	8.90	1.49	1.39
32	B	519	C7Z	C4-C3	8.26	1.66	1.52
38	H	101	RRX	C27-C28	7.94	1.66	1.52
38	H	101	RRX	C30-C25	-7.34	1.43	1.53
26	B	517	BCR	C30-C25	-7.33	1.43	1.53
25	D	402	PHO	C3B-C4B	7.30	1.49	1.41
25	A	407	PHO	C3B-C4B	7.19	1.49	1.41
26	C	517	BCR	C30-C25	-7.17	1.43	1.53
26	C	515	BCR	C30-C25	-7.15	1.43	1.53
26	B	517	BCR	C1-C6	-7.11	1.44	1.53
26	D	405	BCR	C30-C25	-7.08	1.44	1.53
26	C	516	BCR	C1-C6	-7.04	1.44	1.53
26	C	516	BCR	C30-C25	-6.99	1.44	1.53
26	J	101	BCR	C1-C6	-6.98	1.44	1.53
26	B	518	BCR	C30-C25	-6.87	1.44	1.53
26	J	101	BCR	C30-C25	-6.81	1.44	1.53
38	H	101	RRX	C1-C6	-6.79	1.44	1.53
26	J	101	BCR	C2-C3	-6.78	1.35	1.52
26	A	409	BCR	C2-C3	-6.78	1.35	1.52
26	D	405	BCR	C1-C6	-6.77	1.44	1.53
26	A	409	BCR	C30-C25	-6.76	1.44	1.53
26	C	515	BCR	C1-C6	-6.74	1.44	1.53
26	C	517	BCR	C2-C3	-6.73	1.36	1.52
26	B	517	BCR	C2-C3	-6.71	1.36	1.52
38	H	101	RRX	C2-C3	-6.71	1.36	1.52
26	D	405	BCR	C2-C3	-6.71	1.36	1.52
26	B	518	BCR	C2-C3	-6.66	1.36	1.52
26	C	517	BCR	C1-C6	-6.63	1.44	1.53
26	C	515	BCR	C2-C3	-6.63	1.36	1.52
26	C	516	BCR	C2-C3	-6.55	1.36	1.52
26	A	409	BCR	C1-C6	-6.52	1.44	1.53
26	A	409	BCR	C29-C28	-6.50	1.36	1.52
26	B	518	BCR	C1-C6	-6.47	1.44	1.53
26	B	518	BCR	C29-C28	-6.47	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	517	BCR	C29-C28	-6.46	1.36	1.52
26	C	516	BCR	C29-C28	-6.44	1.36	1.52
26	J	101	BCR	C29-C28	-6.43	1.36	1.52
26	B	517	BCR	C29-C28	-6.42	1.36	1.52
26	C	515	BCR	C29-C28	-6.27	1.37	1.52
24	C	504	CLA	MG-NA	6.26	2.21	2.06
26	D	405	BCR	C29-C28	-6.26	1.37	1.52
24	C	508	CLA	MG-NA	6.26	2.21	2.06
24	B	516	CLA	MG-NA	6.24	2.21	2.06
24	B	504	CLA	MG-NA	6.24	2.21	2.06
24	C	506	CLA	MG-NA	6.23	2.21	2.06
24	B	510	CLA	MG-NA	6.21	2.21	2.06
24	C	512	CLA	MG-NA	6.21	2.21	2.06
24	C	507	CLA	MG-NA	6.20	2.21	2.06
24	B	501	CLA	MG-NA	6.16	2.20	2.06
24	C	509	CLA	MG-NA	6.15	2.20	2.06
24	C	514	CLA	MG-NA	6.15	2.20	2.06
24	C	513	CLA	MG-NA	6.15	2.20	2.06
24	D	404	CLA	MG-NA	6.15	2.20	2.06
24	C	503	CLA	MG-NA	6.13	2.20	2.06
24	B	514	CLA	MG-NA	6.13	2.20	2.06
24	A	406	CLA	MG-NA	6.12	2.20	2.06
24	B	503	CLA	MG-NA	6.12	2.20	2.06
24	C	502	CLA	MG-NA	6.11	2.20	2.06
24	B	508	CLA	MG-NA	6.11	2.20	2.06
24	B	507	CLA	MG-NA	6.11	2.20	2.06
24	B	502	CLA	MG-NA	6.08	2.20	2.06
24	B	511	CLA	MG-NA	6.07	2.20	2.06
24	A	408	CLA	MG-NA	6.05	2.20	2.06
24	D	403	CLA	MG-NA	6.05	2.20	2.06
24	B	515	CLA	MG-NA	6.04	2.20	2.06
24	B	513	CLA	MG-NA	6.03	2.20	2.06
24	C	510	CLA	MG-NA	6.03	2.20	2.06
24	C	511	CLA	MG-NA	6.02	2.20	2.06
24	C	505	CLA	MG-NA	6.02	2.20	2.06
24	B	505	CLA	MG-NA	6.00	2.20	2.06
24	B	509	CLA	MG-NA	6.00	2.20	2.06
24	B	506	CLA	MG-NA	5.98	2.20	2.06
24	B	512	CLA	MG-NA	5.96	2.20	2.06
24	D	401	CLA	MG-NA	5.96	2.20	2.06
24	A	405	CLA	MG-NA	5.93	2.20	2.06
32	B	519	C7Z	C12-C13	5.82	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	H	101	RRX	C19-C18	5.68	1.58	1.45
26	C	517	BCR	C12-C13	5.66	1.58	1.45
26	A	409	BCR	C12-C13	5.65	1.58	1.45
26	C	515	BCR	C12-C13	5.60	1.58	1.45
26	J	101	BCR	C12-C13	5.55	1.57	1.45
26	B	517	BCR	C12-C13	5.54	1.57	1.45
26	D	405	BCR	C12-C13	5.47	1.57	1.45
26	B	518	BCR	C12-C13	5.43	1.57	1.45
32	B	519	C7Z	C1-C6	-5.41	1.46	1.53
26	C	516	BCR	C12-C13	5.39	1.57	1.45
26	C	515	BCR	C8-C9	5.30	1.57	1.45
26	A	409	BCR	C8-C9	5.26	1.57	1.45
26	D	405	BCR	C8-C9	5.24	1.57	1.45
26	J	101	BCR	C8-C9	5.21	1.57	1.45
26	C	515	BCR	C29-C30	5.20	1.66	1.54
26	C	517	BCR	C8-C9	5.19	1.57	1.45
26	B	518	BCR	C8-C9	5.17	1.57	1.45
26	B	517	BCR	C8-C9	5.17	1.57	1.45
26	D	405	BCR	C29-C30	5.15	1.66	1.54
26	C	516	BCR	C8-C9	5.13	1.57	1.45
26	J	101	BCR	C29-C30	5.12	1.65	1.54
26	A	409	BCR	C23-C22	5.11	1.56	1.45
26	B	518	BCR	C23-C22	5.07	1.56	1.45
26	J	101	BCR	C23-C22	5.06	1.56	1.45
26	C	515	BCR	C23-C22	5.05	1.56	1.45
26	D	405	BCR	C23-C22	5.04	1.56	1.45
32	B	519	C7Z	C24-C25	-5.04	1.43	1.51
26	B	518	BCR	C29-C30	5.03	1.65	1.54
26	B	517	BCR	C29-C30	5.02	1.65	1.54
26	A	409	BCR	C29-C30	4.99	1.65	1.54
26	C	516	BCR	C29-C30	4.95	1.65	1.54
26	C	517	BCR	C23-C22	4.93	1.56	1.45
26	C	517	BCR	C29-C30	4.91	1.65	1.54
26	B	517	BCR	C23-C22	4.90	1.56	1.45
26	C	516	BCR	C23-C22	4.84	1.56	1.45
26	A	409	BCR	C15-C14	4.83	1.58	1.43
38	H	101	RRX	C8-C9	4.78	1.56	1.45
26	C	517	BCR	C15-C14	4.73	1.58	1.43
38	H	101	RRX	C12-C13	4.71	1.56	1.45
26	C	515	BCR	C15-C14	4.70	1.58	1.43
26	B	518	BCR	C15-C14	4.64	1.57	1.43
26	J	101	BCR	C15-C14	4.59	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	517	BCR	C15-C14	4.58	1.57	1.43
26	D	405	BCR	C15-C14	4.58	1.57	1.43
38	H	101	RRX	C2-C1	4.56	1.64	1.54
26	C	516	BCR	C15-C14	4.53	1.57	1.43
26	C	515	BCR	C19-C18	4.52	1.55	1.45
32	B	519	C7Z	C28-C29	4.47	1.55	1.45
26	C	517	BCR	C2-C1	4.45	1.64	1.54
36	D	406	PL9	C7-C3	-4.44	1.46	1.51
26	D	405	BCR	C2-C1	4.44	1.64	1.54
26	B	518	BCR	C19-C18	4.42	1.55	1.45
26	C	517	BCR	C19-C18	4.41	1.55	1.45
38	H	101	RRX	C27-C26	-4.40	1.44	1.51
38	H	101	RRX	C23-C22	4.38	1.55	1.45
26	C	516	BCR	C2-C1	4.38	1.64	1.54
26	D	405	BCR	C19-C18	4.37	1.55	1.45
26	J	101	BCR	C19-C18	4.36	1.55	1.45
26	B	517	BCR	C2-C1	4.36	1.64	1.54
26	B	518	BCR	C2-C1	4.34	1.64	1.54
32	B	519	C7Z	C31-C30	4.33	1.56	1.43
26	C	515	BCR	C2-C1	4.32	1.64	1.54
38	H	101	RRX	C24-C25	4.31	1.60	1.45
26	A	409	BCR	C19-C18	4.30	1.55	1.45
26	J	101	BCR	C2-C1	4.29	1.64	1.54
26	B	517	BCR	C19-C18	4.29	1.55	1.45
38	H	101	RRX	C3-C4	4.28	1.65	1.52
24	C	506	CLA	CBB-CAB	4.27	1.51	1.30
24	B	507	CLA	CBB-CAB	4.27	1.51	1.30
24	D	404	CLA	CBB-CAB	4.27	1.51	1.30
24	B	509	CLA	CBB-CAB	4.26	1.51	1.30
24	C	504	CLA	CBB-CAB	4.26	1.51	1.30
26	C	515	BCR	C20-C21	4.26	1.56	1.43
24	B	514	CLA	CBB-CAB	4.25	1.51	1.30
24	B	505	CLA	CBB-CAB	4.25	1.51	1.30
24	C	505	CLA	CBB-CAB	4.25	1.51	1.30
24	B	513	CLA	CBB-CAB	4.25	1.51	1.30
24	B	504	CLA	CBB-CAB	4.25	1.51	1.30
33	C	518	DGD	O1G-C1A	4.25	1.45	1.33
24	B	502	CLA	CBB-CAB	4.25	1.51	1.30
24	B	503	CLA	CBB-CAB	4.25	1.51	1.30
24	B	515	CLA	CBB-CAB	4.25	1.51	1.30
26	D	405	BCR	C28-C27	4.25	1.65	1.52
24	B	510	CLA	CBB-CAB	4.25	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	508	CLA	CBB-CAB	4.24	1.51	1.30
26	B	518	BCR	C20-C21	4.24	1.56	1.43
24	C	503	CLA	CBB-CAB	4.24	1.51	1.30
24	C	507	CLA	CBB-CAB	4.24	1.51	1.30
24	C	511	CLA	CBB-CAB	4.24	1.51	1.30
24	C	512	CLA	CBB-CAB	4.24	1.51	1.30
24	A	405	CLA	CBB-CAB	4.24	1.51	1.30
24	C	514	CLA	CBB-CAB	4.23	1.51	1.30
24	C	509	CLA	CBB-CAB	4.23	1.51	1.30
33	B	521	DGD	O1G-C1A	4.23	1.45	1.33
26	A	409	BCR	C2-C1	4.23	1.63	1.54
24	C	508	CLA	CBB-CAB	4.23	1.51	1.30
24	B	506	CLA	CBB-CAB	4.22	1.51	1.30
24	C	513	CLA	CBB-CAB	4.22	1.51	1.30
38	H	101	RRX	C11-C10	4.22	1.56	1.43
24	C	502	CLA	CBB-CAB	4.22	1.51	1.30
26	C	516	BCR	C19-C18	4.20	1.55	1.45
24	A	406	CLA	CBB-CAB	4.20	1.51	1.30
24	B	511	CLA	CBB-CAB	4.20	1.51	1.30
24	B	516	CLA	CBB-CAB	4.19	1.51	1.30
26	C	517	BCR	C20-C21	4.19	1.56	1.43
24	D	401	CLA	CBB-CAB	4.19	1.51	1.30
24	B	501	CLA	CBB-CAB	4.19	1.51	1.30
26	J	101	BCR	C20-C21	4.18	1.56	1.43
24	A	408	CLA	CBB-CAB	4.18	1.51	1.30
24	B	512	CLA	CBB-CAB	4.18	1.51	1.30
24	C	510	CLA	CBB-CAB	4.18	1.51	1.30
26	A	409	BCR	C20-C21	4.15	1.56	1.43
26	C	515	BCR	C28-C27	4.14	1.65	1.52
33	C	519	DGD	O1G-C1A	4.14	1.45	1.33
24	D	403	CLA	CBB-CAB	4.14	1.50	1.30
24	B	513	CLA	MG-ND	-4.13	1.97	2.05
26	D	405	BCR	C20-C21	4.13	1.56	1.43
26	B	517	BCR	C20-C21	4.12	1.56	1.43
26	B	517	BCR	C28-C27	4.11	1.65	1.52
26	C	517	BCR	C28-C27	4.10	1.65	1.52
24	B	508	CLA	MG-ND	-4.10	1.97	2.05
24	C	513	CLA	MG-ND	-4.09	1.97	2.05
26	C	516	BCR	C28-C27	4.09	1.65	1.52
26	A	409	BCR	C28-C27	4.08	1.65	1.52
26	B	518	BCR	C28-C27	4.08	1.65	1.52
26	J	101	BCR	C28-C27	4.08	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	512	CLA	MG-ND	-4.07	1.97	2.05
32	B	519	C7Z	C32-C33	4.05	1.54	1.45
24	C	510	CLA	MG-ND	-4.05	1.97	2.05
24	B	504	CLA	MG-ND	-4.04	1.97	2.05
24	B	503	CLA	MG-ND	-4.04	1.97	2.05
24	C	509	CLA	MG-ND	-4.03	1.97	2.05
33	C	520	DGD	O1G-C1A	4.02	1.45	1.33
24	D	403	CLA	MG-ND	-4.02	1.97	2.05
24	C	503	CLA	MG-ND	-4.01	1.97	2.05
26	C	516	BCR	C20-C21	4.01	1.55	1.43
36	D	406	PL9	C3-C4	-4.00	1.42	1.49
24	C	508	CLA	MG-ND	-3.99	1.97	2.05
32	B	519	C7Z	C4-C5	-3.98	1.44	1.51
24	B	516	CLA	MG-ND	-3.98	1.97	2.05
24	B	506	CLA	MG-ND	-3.98	1.97	2.05
24	C	507	CLA	MG-ND	-3.96	1.97	2.05
24	D	401	CLA	MG-ND	-3.96	1.97	2.05
24	A	406	CLA	MG-ND	-3.96	1.97	2.05
24	C	511	CLA	MG-ND	-3.96	1.97	2.05
24	B	507	CLA	MG-ND	-3.95	1.98	2.05
24	C	512	CLA	MG-ND	-3.95	1.98	2.05
24	B	515	CLA	MG-ND	-3.94	1.98	2.05
24	B	501	CLA	MG-ND	-3.94	1.98	2.05
24	B	514	CLA	MG-ND	-3.93	1.98	2.05
24	A	405	CLA	MG-ND	-3.93	1.98	2.05
24	D	404	CLA	MG-ND	-3.92	1.98	2.05
24	B	505	CLA	MG-ND	-3.92	1.98	2.05
24	B	510	CLA	MG-ND	-3.91	1.98	2.05
24	C	506	CLA	MG-ND	-3.91	1.98	2.05
26	C	516	BCR	C3-C4	3.91	1.64	1.52
38	H	101	RRX	C29-C30	3.90	1.67	1.54
24	C	514	CLA	MG-ND	-3.89	1.98	2.05
24	B	509	CLA	MG-ND	-3.88	1.98	2.05
38	H	101	RRX	C15-C14	3.87	1.55	1.43
26	B	518	BCR	C3-C4	3.86	1.64	1.52
26	C	515	BCR	C3-C4	3.85	1.64	1.52
26	B	517	BCR	C3-C4	3.84	1.64	1.52
24	B	511	CLA	MG-ND	-3.82	1.98	2.05
24	C	505	CLA	MG-ND	-3.81	1.98	2.05
24	C	504	CLA	MG-ND	-3.79	1.98	2.05
26	D	405	BCR	C3-C4	3.77	1.64	1.52
32	B	519	C7Z	C22-C21	3.77	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	BCR	C16-C17	3.76	1.55	1.43
26	J	101	BCR	C3-C4	3.76	1.64	1.52
24	C	502	CLA	MG-ND	-3.76	1.98	2.05
32	B	519	C7Z	C11-C10	3.76	1.55	1.43
24	D	401	CLA	C1C-NC	-3.75	1.32	1.37
26	C	517	BCR	C3-C4	3.73	1.64	1.52
26	A	409	BCR	C3-C4	3.73	1.64	1.52
38	H	101	RRX	C16-C17	3.72	1.55	1.43
32	B	519	C7Z	C15-C14	3.72	1.55	1.43
24	A	408	CLA	MG-ND	-3.72	1.98	2.05
26	A	409	BCR	C11-C10	3.71	1.55	1.43
24	B	502	CLA	MG-ND	-3.68	1.98	2.05
26	B	518	BCR	C16-C17	3.67	1.54	1.43
26	C	517	BCR	C11-C10	3.67	1.54	1.43
24	B	505	CLA	C1C-NC	-3.67	1.32	1.37
24	B	511	CLA	C1C-NC	-3.66	1.32	1.37
24	A	405	CLA	C1C-NC	-3.66	1.32	1.37
26	C	515	BCR	C16-C17	3.66	1.54	1.43
26	C	517	BCR	C16-C17	3.65	1.54	1.43
26	C	515	BCR	C11-C10	3.64	1.54	1.43
38	H	101	RRX	C20-C21	3.63	1.54	1.43
26	B	517	BCR	C11-C10	3.63	1.54	1.43
32	B	519	C7Z	C27-C26	3.62	1.58	1.45
24	C	509	CLA	C1C-NC	-3.60	1.32	1.37
26	D	405	BCR	C16-C17	3.60	1.54	1.43
26	J	101	BCR	C16-C17	3.60	1.54	1.43
24	C	505	CLA	C1C-NC	-3.59	1.32	1.37
26	J	101	BCR	C11-C10	3.58	1.54	1.43
24	A	406	CLA	C1C-NC	-3.58	1.32	1.37
24	C	503	CLA	C1C-NC	-3.58	1.32	1.37
26	B	517	BCR	C16-C17	3.58	1.54	1.43
24	B	506	CLA	C1C-NC	-3.57	1.32	1.37
24	B	512	CLA	C1C-NC	-3.57	1.32	1.37
24	B	510	CLA	C1C-NC	-3.57	1.32	1.37
24	B	504	CLA	C1C-NC	-3.56	1.32	1.37
26	D	405	BCR	C11-C10	3.56	1.54	1.43
25	D	402	PHO	C1D-C2D	3.55	1.43	1.39
26	A	409	BCR	C27-C26	-3.54	1.44	1.51
26	D	405	BCR	C24-C25	3.54	1.57	1.45
26	A	409	BCR	C24-C25	3.54	1.57	1.45
24	B	502	CLA	C1C-NC	-3.52	1.32	1.37
26	D	405	BCR	C4-C5	-3.52	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	518	BCR	C24-C25	3.52	1.57	1.45
24	C	510	CLA	C1C-NC	-3.52	1.32	1.37
24	C	507	CLA	C1C-NC	-3.51	1.32	1.37
24	B	507	CLA	C1C-NC	-3.50	1.32	1.37
26	B	518	BCR	C11-C10	3.50	1.54	1.43
24	C	512	CLA	C1C-NC	-3.50	1.32	1.37
24	C	514	CLA	C1C-NC	-3.50	1.32	1.37
35	B	523	DGA	OG2-CB1	3.50	1.44	1.34
24	D	404	CLA	C1C-NC	-3.50	1.32	1.37
24	B	501	CLA	C1C-NC	-3.50	1.32	1.37
32	B	519	C7Z	C2-C1	3.50	1.65	1.54
24	B	514	CLA	C1C-NC	-3.50	1.32	1.37
24	B	509	CLA	C1C-NC	-3.49	1.32	1.37
24	C	506	CLA	C1C-NC	-3.49	1.32	1.37
26	J	101	BCR	C24-C25	3.49	1.57	1.45
32	B	519	C7Z	C35-C34	3.49	1.54	1.43
26	C	516	BCR	C16-C17	3.48	1.54	1.43
24	B	503	CLA	C1C-NC	-3.48	1.32	1.37
26	A	409	BCR	C4-C5	-3.48	1.44	1.51
26	C	515	BCR	C27-C26	-3.47	1.44	1.51
24	A	408	CLA	C1C-NC	-3.47	1.32	1.37
26	C	517	BCR	C4-C5	-3.46	1.44	1.51
24	C	502	CLA	C1C-NC	-3.46	1.32	1.37
26	C	517	BCR	C24-C25	3.45	1.57	1.45
24	C	511	CLA	C1C-NC	-3.45	1.32	1.37
26	C	516	BCR	C4-C5	-3.45	1.44	1.51
26	C	516	BCR	C11-C10	3.45	1.54	1.43
26	C	516	BCR	C24-C25	3.45	1.57	1.45
26	B	517	BCR	C27-C26	-3.43	1.44	1.51
25	A	407	PHO	C1D-C2D	3.43	1.43	1.39
26	C	516	BCR	C27-C26	-3.42	1.44	1.51
26	B	517	BCR	C24-C25	3.41	1.57	1.45
24	B	508	CLA	C1C-NC	-3.41	1.32	1.37
26	C	515	BCR	C24-C25	3.41	1.57	1.45
24	C	504	CLA	C1C-NC	-3.41	1.32	1.37
24	D	401	CLA	C4B-NB	-3.40	1.33	1.37
26	J	101	BCR	C4-C5	-3.40	1.44	1.51
26	C	517	BCR	C27-C26	-3.39	1.44	1.51
24	B	516	CLA	C1C-NC	-3.39	1.32	1.37
24	C	508	CLA	C1C-NC	-3.38	1.32	1.37
24	B	513	CLA	C1C-NC	-3.36	1.32	1.37
26	C	515	BCR	C4-C5	-3.36	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	518	BCR	C4-C5	-3.36	1.44	1.51
26	B	518	BCR	C27-C26	-3.35	1.44	1.51
24	A	408	CLA	C4B-NB	-3.35	1.33	1.37
26	B	517	BCR	C4-C5	-3.35	1.44	1.51
32	B	519	C7Z	C18-C5	3.34	1.56	1.50
26	J	101	BCR	C27-C26	-3.33	1.44	1.51
24	C	513	CLA	C1C-NC	-3.33	1.32	1.37
24	D	403	CLA	C1C-NC	-3.33	1.32	1.37
24	C	510	CLA	C4B-NB	-3.32	1.33	1.37
35	B	523	DGA	OG1-CA1	3.32	1.43	1.33
38	H	101	RRX	C7-C6	3.31	1.56	1.45
38	H	101	RRX	C17-C18	-3.29	1.31	1.35
28	B	520	LMG	C22-C21	-3.29	1.33	1.51
33	C	519	DGD	CAB-C9B	-3.29	1.33	1.51
24	B	515	CLA	C1C-NC	-3.29	1.32	1.37
25	D	402	PHO	C4D-CHA	3.29	1.44	1.39
24	B	511	CLA	C4B-NB	-3.29	1.33	1.37
24	B	504	CLA	C4B-NB	-3.28	1.33	1.37
28	C	522	LMG	C19-C18	-3.28	1.33	1.51
28	C	521	LMG	C19-C18	-3.28	1.33	1.51
33	C	519	DGD	CDB-CCB	-3.27	1.33	1.51
28	C	522	LMG	C22-C21	-3.27	1.33	1.51
33	C	520	DGD	CAA-C9A	-3.27	1.33	1.51
24	A	405	CLA	C4B-NB	-3.26	1.33	1.37
28	B	520	LMG	C19-C18	-3.26	1.33	1.51
28	H	102	LMG	C19-C18	-3.25	1.33	1.51
28	C	521	LMG	C40-C39	-3.25	1.33	1.51
24	B	502	CLA	C4B-NB	-3.24	1.33	1.37
28	C	521	LMG	C37-C36	-3.24	1.33	1.51
38	H	101	RRX	C4-C5	-3.23	1.44	1.51
24	C	509	CLA	C4B-NB	-3.23	1.33	1.37
28	D	409	LMG	C19-C18	-3.22	1.33	1.51
28	H	102	LMG	C40-C39	-3.22	1.33	1.51
24	A	406	CLA	C4B-NB	-3.22	1.33	1.37
24	B	512	CLA	C4B-NB	-3.21	1.33	1.37
26	D	405	BCR	C27-C26	-3.21	1.44	1.51
28	C	501	LMG	C19-C18	-3.20	1.33	1.51
24	B	514	CLA	C4B-NB	-3.20	1.33	1.37
28	H	102	LMG	C37-C36	-3.19	1.33	1.51
24	C	506	CLA	C4B-NB	-3.18	1.33	1.37
32	B	519	C7Z	C7-C6	3.18	1.56	1.45
24	B	506	CLA	C4B-NB	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C21-C26	-3.17	1.49	1.53
36	D	406	PL9	C6-C1	-3.16	1.42	1.48
24	C	503	CLA	C4B-NB	-3.15	1.33	1.37
32	B	519	C7Z	C8-C9	3.13	1.52	1.45
24	C	512	CLA	C4B-NB	-3.12	1.33	1.37
25	A	407	PHO	C4D-CHA	3.11	1.44	1.39
24	C	505	CLA	C4B-NB	-3.11	1.34	1.37
24	C	508	CLA	C4B-NB	-3.11	1.34	1.37
24	C	504	CLA	C4B-NB	-3.09	1.34	1.37
24	B	509	CLA	C4B-NB	-3.09	1.34	1.37
24	C	514	CLA	C4B-NB	-3.08	1.34	1.37
24	D	404	CLA	C4B-NB	-3.07	1.34	1.37
24	B	515	CLA	C4B-NB	-3.06	1.34	1.37
24	C	507	CLA	C4B-NB	-3.06	1.34	1.37
37	E	101	HEM	FE-NA	3.03	2.05	1.95
24	B	503	CLA	C4B-NB	-3.03	1.34	1.37
24	B	507	CLA	C4B-NB	-3.01	1.34	1.37
24	C	511	CLA	C4B-NB	-3.01	1.34	1.37
24	B	508	CLA	C4B-NB	-3.00	1.34	1.37
24	B	513	CLA	C4B-NB	-2.99	1.34	1.37
37	E	101	HEM	FE-ND	2.95	2.04	1.94
37	E	101	HEM	CAB-C3B	2.94	1.55	1.47
24	B	516	CLA	C4B-NB	-2.93	1.34	1.37
24	B	505	CLA	C4B-NB	-2.92	1.34	1.37
24	C	513	CLA	C4B-NB	-2.89	1.34	1.37
37	E	101	HEM	CAC-C3C	2.84	1.55	1.47
26	A	409	BCR	C34-C9	2.80	1.56	1.50
24	B	510	CLA	C4B-NB	-2.77	1.34	1.37
25	A	407	PHO	CMC-C2C	-2.77	1.46	1.50
26	B	517	BCR	C34-C9	2.76	1.56	1.50
24	C	502	CLA	C4B-NB	-2.74	1.34	1.37
25	D	402	PHO	CMC-C2C	-2.73	1.46	1.50
24	D	403	CLA	C4B-NB	-2.72	1.34	1.37
26	C	515	BCR	C34-C9	2.72	1.56	1.50
37	E	101	HEM	FE-NC	2.68	2.04	1.95
26	C	515	BCR	C7-C6	2.66	1.54	1.45
26	B	518	BCR	C34-C9	2.65	1.56	1.50
26	J	101	BCR	C34-C9	2.63	1.56	1.50
24	B	501	CLA	C4B-NB	-2.62	1.34	1.37
26	C	516	BCR	C34-C9	2.61	1.56	1.50
26	D	405	BCR	C34-C9	2.60	1.56	1.50
26	J	101	BCR	C7-C6	2.59	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	BCR	C7-C6	2.59	1.54	1.45
37	E	101	HEM	FE-NB	2.58	2.02	1.94
26	A	409	BCR	C7-C6	2.58	1.54	1.45
26	B	518	BCR	C7-C6	2.58	1.54	1.45
25	D	402	PHO	CMD-C2D	-2.56	1.46	1.51
25	A	407	PHO	CMD-C2D	-2.55	1.46	1.51
28	D	409	LMG	C37-C36	-2.55	1.33	1.51
26	C	517	BCR	C7-C6	2.55	1.54	1.45
25	A	407	PHO	C4D-ND	-2.55	1.35	1.38
26	B	517	BCR	C7-C6	2.52	1.54	1.45
26	C	516	BCR	C7-C6	2.52	1.54	1.45
26	C	517	BCR	C34-C9	2.52	1.56	1.50
36	D	406	PL9	C53-C6	-2.48	1.45	1.50
26	C	516	BCR	C39-C30	-2.48	1.48	1.53
25	A	407	PHO	CMB-C2B	-2.46	1.46	1.51
25	D	402	PHO	CMB-C2B	-2.46	1.46	1.51
34	B	522	3PH	O31-C31	2.42	1.40	1.33
26	C	517	BCR	C39-C30	-2.41	1.49	1.53
25	D	402	PHO	CAC-C3C	-2.41	1.47	1.51
32	B	519	C7Z	C38-C25	2.40	1.54	1.50
25	A	407	PHO	CAC-C3C	-2.39	1.47	1.51
32	B	519	C7Z	C20-C13	2.38	1.55	1.50
26	J	101	BCR	C39-C30	-2.37	1.49	1.53
36	D	406	PL9	C52-C5	-2.37	1.45	1.50
26	C	515	BCR	C39-C30	-2.35	1.49	1.53
25	D	402	PHO	C4D-ND	-2.32	1.35	1.38
38	H	101	RRX	C14-C13	-2.31	1.32	1.35
24	D	403	CLA	C3D-C4D	-2.30	1.39	1.44
26	C	516	BCR	C36-C18	2.30	1.55	1.50
24	B	503	CLA	C3D-C4D	-2.29	1.39	1.44
24	A	406	CLA	C3D-C4D	-2.29	1.39	1.44
26	A	409	BCR	C39-C30	-2.29	1.49	1.53
26	B	518	BCR	C39-C30	-2.28	1.49	1.53
38	H	101	RRX	C34-C9	2.28	1.55	1.50
26	B	517	BCR	C39-C30	-2.28	1.49	1.53
26	D	405	BCR	C39-C30	-2.27	1.49	1.53
26	C	515	BCR	C36-C18	2.27	1.55	1.50
26	J	101	BCR	C36-C18	2.25	1.55	1.50
24	C	502	CLA	C3D-C4D	-2.25	1.39	1.44
24	C	510	CLA	C3D-C4D	-2.24	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.23	1.39	1.44
32	B	519	C7Z	C40-C33	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	517	BCR	C36-C18	2.22	1.55	1.50
24	A	408	CLA	C3D-C4D	-2.22	1.39	1.44
26	B	518	BCR	C36-C18	2.22	1.55	1.50
34	B	522	3PH	O21-C2	-2.22	1.41	1.46
26	D	405	BCR	C36-C18	2.21	1.55	1.50
24	D	401	CLA	C3D-C4D	-2.21	1.39	1.44
24	B	504	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	405	CLA	C3D-C4D	-2.21	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.20	1.39	1.44
26	C	517	BCR	C36-C18	2.20	1.55	1.50
34	B	522	3PH	O21-C21	2.19	1.40	1.34
24	B	508	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	504	CLA	C3D-C4D	-2.18	1.39	1.44
24	B	505	CLA	C3D-C4D	-2.17	1.39	1.44
24	C	512	CLA	C3D-C4D	-2.17	1.39	1.44
34	B	522	3PH	O31-C3	-2.17	1.40	1.45
26	D	405	BCR	C38-C26	2.17	1.54	1.50
24	B	506	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	514	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	512	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	514	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	506	CLA	C3D-C4D	-2.15	1.39	1.44
32	B	519	C7Z	C19-C9	2.15	1.55	1.50
24	B	511	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	516	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	501	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	502	CLA	C3D-C4D	-2.13	1.39	1.44
24	C	508	CLA	C3D-C4D	-2.12	1.39	1.44
24	C	507	CLA	C3D-C4D	-2.12	1.39	1.44
24	D	404	CLA	C3D-C4D	-2.12	1.39	1.44
24	C	505	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	507	CLA	C1A-CHA	2.11	1.51	1.43
26	A	409	BCR	C36-C18	2.11	1.55	1.50
24	B	513	CLA	C3D-C4D	-2.10	1.39	1.44
24	B	507	CLA	C3D-C4D	-2.10	1.39	1.44
24	B	510	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	503	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	509	CLA	C3D-C4D	-2.08	1.39	1.44
38	H	101	RRX	C33-C5	2.08	1.54	1.50
24	B	515	CLA	C3D-C4D	-2.08	1.39	1.44
24	A	408	CLA	C1A-CHA	2.07	1.51	1.43
26	A	409	BCR	C37-C22	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C3D-C4D	-2.06	1.39	1.44
24	C	504	CLA	C1C-C2C	2.05	1.48	1.44
24	C	505	CLA	C1A-CHA	2.04	1.51	1.43
33	C	520	DGD	CDA-CCA	-2.04	1.33	1.49
24	B	504	CLA	C1A-CHA	2.04	1.51	1.43
28	H	102	LMG	C22-C21	-2.04	1.33	1.49
24	B	503	CLA	C1A-CHA	2.04	1.51	1.43
26	B	518	BCR	C38-C26	2.04	1.54	1.50
33	C	520	DGD	CAB-C9B	-2.04	1.33	1.49
24	A	406	CLA	C1A-CHA	2.03	1.51	1.43
25	A	407	PHO	C3B-C2B	-2.03	1.37	1.40
33	C	519	DGD	CGB-CFB	-2.03	1.33	1.49
26	J	101	BCR	C38-C26	2.03	1.54	1.50
26	C	515	BCR	C38-C26	2.02	1.54	1.50
28	A	415	LMG	C37-C36	-2.02	1.33	1.49
25	D	402	PHO	C3D-C4D	2.02	1.44	1.41
28	B	520	LMG	C25-C24	-2.02	1.33	1.49
28	C	501	LMG	C22-C21	-2.02	1.33	1.49
28	C	521	LMG	C43-C42	-2.02	1.33	1.49
24	D	404	CLA	C1A-CHA	2.02	1.51	1.43
35	B	523	DGA	OG2-CG2	-2.02	1.41	1.46
26	C	517	BCR	C38-C26	2.01	1.54	1.50
24	B	515	CLA	C1A-CHA	2.01	1.51	1.43
24	C	513	CLA	C1C-C2C	2.01	1.48	1.44
28	H	102	LMG	C43-C42	-2.01	1.33	1.49
24	C	506	CLA	C1A-CHA	2.01	1.51	1.43
24	B	509	CLA	C1A-CHA	2.00	1.51	1.43
24	D	403	CLA	C1C-C2C	2.00	1.48	1.44

All (926) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	408	CLA	C4A-NA-C1A	9.70	111.06	106.71
26	A	409	BCR	C7-C8-C9	-9.68	111.60	126.23
24	B	512	CLA	C4A-NA-C1A	9.65	111.05	106.71
24	D	404	CLA	C4A-NA-C1A	9.55	111.00	106.71
24	B	509	CLA	C4A-NA-C1A	9.44	110.95	106.71
24	B	513	CLA	C4A-NA-C1A	9.36	110.91	106.71
24	B	507	CLA	C4A-NA-C1A	9.30	110.89	106.71
24	C	505	CLA	C4A-NA-C1A	9.28	110.88	106.71
24	B	506	CLA	C4A-NA-C1A	9.20	110.84	106.71
24	A	405	CLA	C4A-NA-C1A	9.17	110.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	515	CLA	C4A-NA-C1A	9.14	110.81	106.71
24	C	503	CLA	C4A-NA-C1A	9.12	110.81	106.71
24	C	512	CLA	C4A-NA-C1A	9.11	110.80	106.71
24	C	508	CLA	C4A-NA-C1A	9.01	110.76	106.71
24	C	511	CLA	C4A-NA-C1A	9.01	110.76	106.71
24	C	514	CLA	C4A-NA-C1A	8.93	110.72	106.71
24	C	510	CLA	C4A-NA-C1A	8.91	110.71	106.71
24	B	510	CLA	C4A-NA-C1A	8.89	110.70	106.71
24	B	514	CLA	C4A-NA-C1A	8.89	110.70	106.71
24	C	513	CLA	C4A-NA-C1A	8.81	110.67	106.71
24	D	401	CLA	C4A-NA-C1A	8.78	110.65	106.71
24	B	501	CLA	C4A-NA-C1A	8.76	110.64	106.71
24	C	506	CLA	C4A-NA-C1A	8.75	110.64	106.71
24	B	502	CLA	C4A-NA-C1A	8.72	110.63	106.71
24	C	507	CLA	C4A-NA-C1A	8.69	110.61	106.71
24	B	508	CLA	C4A-NA-C1A	8.64	110.59	106.71
24	A	406	CLA	C4A-NA-C1A	8.63	110.59	106.71
24	B	511	CLA	C4A-NA-C1A	8.58	110.56	106.71
24	B	504	CLA	C4A-NA-C1A	8.58	110.56	106.71
24	B	503	CLA	C4A-NA-C1A	8.54	110.54	106.71
24	C	502	CLA	C4A-NA-C1A	8.44	110.50	106.71
26	A	409	BCR	C15-C14-C13	-8.39	115.34	127.31
24	B	505	CLA	C4A-NA-C1A	8.35	110.46	106.71
24	B	516	CLA	C4A-NA-C1A	8.33	110.45	106.71
24	C	504	CLA	C4A-NA-C1A	8.29	110.44	106.71
24	C	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
38	H	101	RRX	C11-C10-C9	-7.90	116.03	127.31
24	D	403	CLA	C4A-NA-C1A	7.90	110.26	106.71
26	C	517	BCR	C7-C8-C9	-7.18	115.38	126.23
26	A	409	BCR	C20-C21-C22	-6.75	117.68	127.31
26	B	517	BCR	C33-C5-C6	-6.61	117.11	124.53
25	A	407	PHO	C4D-CHA-CBD	-6.51	105.57	108.52
38	H	101	RRX	C20-C21-C22	-6.36	118.24	127.31
25	D	402	PHO	C4D-CHA-CBD	-6.30	105.67	108.52
26	B	517	BCR	C15-C14-C13	-6.27	118.37	127.31
24	A	408	CLA	O2D-CGD-CBD	6.25	122.37	111.27
24	B	501	CLA	O2D-CGD-CBD	6.05	122.02	111.27
38	H	101	RRX	C15-C14-C13	-6.03	118.70	127.31
26	A	409	BCR	C33-C5-C6	-5.92	117.88	124.53
32	B	519	C7Z	C11-C10-C9	-5.91	118.88	127.31
24	C	510	CLA	O2D-CGD-CBD	5.91	121.76	111.27
24	C	502	CLA	CMD-C2D-C1D	5.89	135.09	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	517	BCR	C11-C10-C9	-5.77	119.08	127.31
24	A	405	CLA	O2A-C1-C2	5.71	123.65	108.64
24	C	511	CLA	CMD-C2D-C1D	5.63	134.64	124.71
26	C	515	BCR	C16-C17-C18	-5.63	119.27	127.31
24	C	512	CLA	CMD-C2D-C1D	5.63	134.63	124.71
24	B	507	CLA	CMD-C2D-C1D	5.61	134.61	124.71
24	D	401	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	D	404	CLA	O2D-CGD-CBD	5.59	121.20	111.27
24	C	509	CLA	O2A-C1-C2	5.59	123.32	108.64
24	B	506	CLA	CMD-C2D-C1D	5.58	134.55	124.71
24	B	512	CLA	O2D-CGD-CBD	5.56	121.15	111.27
24	C	509	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	B	514	CLA	O2A-C1-C2	5.54	123.20	108.64
24	C	503	CLA	O2A-C1-C2	5.53	123.17	108.64
24	B	505	CLA	CMD-C2D-C1D	5.52	134.45	124.71
24	C	502	CLA	O2D-CGD-CBD	5.52	121.07	111.27
24	C	513	CLA	O2D-CGD-CBD	5.50	121.04	111.27
26	A	409	BCR	C8-C9-C10	5.50	127.38	118.94
24	B	503	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	C	504	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	B	501	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	B	510	CLA	O2D-CGD-CBD	5.48	121.01	111.27
30	A	413	BCT	O2-C-O1	5.48	133.76	119.55
24	B	504	CLA	CMD-C2D-C1D	5.47	134.36	124.71
24	C	514	CLA	O2D-CGD-CBD	5.47	120.99	111.27
24	B	505	CLA	O2D-CGD-CBD	5.46	120.96	111.27
24	C	503	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	B	504	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	C	510	CLA	CMD-C2D-C1D	5.44	134.31	124.71
24	A	406	CLA	O2A-C1-C2	5.43	122.90	108.64
24	C	508	CLA	O2D-CGD-CBD	5.43	120.91	111.27
24	B	509	CLA	O2D-CGD-CBD	5.42	120.90	111.27
24	B	514	CLA	CMD-C2D-C1D	5.42	134.26	124.71
24	A	406	CLA	CMD-C2D-C1D	5.41	134.25	124.71
24	A	408	CLA	O2A-C1-C2	5.41	122.86	108.64
26	C	516	BCR	C15-C14-C13	-5.40	119.61	127.31
24	B	502	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	C	505	CLA	O2D-CGD-CBD	5.39	120.84	111.27
24	C	514	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	C	508	CLA	CMD-C2D-C1D	5.37	134.18	124.71
24	C	505	CLA	O2A-C1-C2	5.36	122.71	108.64
24	B	506	CLA	O2D-CGD-CBD	5.35	120.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	A	408	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	C	507	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	C	505	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	D	403	CLA	CMD-C2D-C1D	5.34	134.12	124.71
24	D	404	CLA	O2A-C1-C2	5.33	122.66	108.64
24	B	508	CLA	O2A-C1-C2	5.33	122.65	108.64
26	C	517	BCR	C20-C21-C22	-5.32	119.71	127.31
26	C	517	BCR	C11-C10-C9	-5.32	119.72	127.31
24	B	515	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	C	506	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	C	511	CLA	O2D-CGD-CBD	5.29	120.66	111.27
32	B	519	C7Z	C15-C14-C13	-5.28	119.77	127.31
24	D	401	CLA	O2A-C1-C2	5.28	122.52	108.64
24	C	506	CLA	CMD-C2D-C1D	5.28	134.02	124.71
24	B	513	CLA	CMD-C2D-C1D	5.27	134.00	124.71
24	B	505	CLA	O2A-C1-C2	5.24	122.40	108.64
24	B	507	CLA	O2A-C1-C2	5.23	122.38	108.64
24	C	511	CLA	O2A-C1-C2	5.23	122.37	108.64
24	D	404	CLA	CMD-C2D-C1D	5.22	133.92	124.71
24	B	509	CLA	CMD-C2D-C1D	5.20	133.87	124.71
26	J	101	BCR	C24-C23-C22	-5.19	118.39	126.23
24	C	504	CLA	O2A-C1-C2	5.18	122.24	108.64
24	C	507	CLA	O2A-C1-C2	5.18	122.24	108.64
26	J	101	BCR	C11-C10-C9	-5.16	119.95	127.31
24	B	516	CLA	CMD-C2D-C1D	5.16	133.80	124.71
24	C	512	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	B	511	CLA	CMD-C2D-C1D	5.15	133.80	124.71
24	B	515	CLA	CMD-C2D-C1D	5.15	133.78	124.71
24	B	501	CLA	O2A-C1-C2	5.14	122.15	108.64
24	A	406	CLA	O2D-CGD-CBD	5.13	120.38	111.27
24	B	511	CLA	O2D-CGD-CBD	5.13	120.38	111.27
26	J	101	BCR	C16-C17-C18	-5.12	120.00	127.31
24	C	509	CLA	CMD-C2D-C1D	5.12	133.74	124.71
24	C	508	CLA	O2A-C1-C2	5.12	122.08	108.64
26	C	516	BCR	C38-C26-C25	-5.11	118.79	124.53
24	B	502	CLA	O2D-CGD-CBD	5.07	120.28	111.27
24	B	513	CLA	O2A-C1-C2	5.07	121.96	108.64
24	B	510	CLA	CMD-C2D-C1D	5.07	133.64	124.71
26	A	409	BCR	C34-C9-C10	-5.06	115.83	122.92
24	C	504	CLA	O2D-CGD-CBD	5.06	120.26	111.27
24	D	403	CLA	O2A-C1-C2	5.05	121.92	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	508	CLA	O2D-CGD-CBD	5.05	120.25	111.27
24	B	503	CLA	O2D-CGD-CBD	5.04	120.23	111.27
24	C	512	CLA	O2A-C1-C2	5.04	121.87	108.64
26	C	516	BCR	C11-C10-C9	-5.03	120.14	127.31
24	B	504	CLA	O2A-C1-C2	5.03	121.85	108.64
26	A	409	BCR	C10-C11-C12	-5.02	107.54	123.22
26	J	101	BCR	C33-C5-C6	-5.02	118.89	124.53
24	B	516	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	C	507	CLA	O2D-CGD-CBD	5.00	120.15	111.27
24	C	503	CLA	CMD-C2D-C1D	4.99	133.50	124.71
24	B	511	CLA	O2A-C1-C2	4.99	121.74	108.64
26	C	515	BCR	C24-C23-C22	-4.99	118.70	126.23
24	C	506	CLA	O2A-C1-C2	4.99	121.74	108.64
24	D	403	CLA	O2D-CGD-CBD	4.98	120.13	111.27
24	B	516	CLA	O2A-C1-C2	4.98	121.74	108.64
24	B	507	CLA	O2D-CGD-CBD	4.97	120.10	111.27
24	B	509	CLA	O2A-C1-C2	4.93	121.60	108.64
26	C	516	BCR	C1-C6-C5	-4.93	115.67	122.61
24	B	513	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	B	512	CLA	CMD-C2D-C1D	4.93	133.39	124.71
24	C	513	CLA	CMD-C2D-C1D	4.91	133.36	124.71
26	D	405	BCR	C16-C17-C18	-4.90	120.32	127.31
26	B	517	BCR	C38-C26-C25	-4.90	119.03	124.53
24	B	514	CLA	O2D-CGD-CBD	4.89	119.96	111.27
32	B	519	C7Z	C35-C34-C33	-4.88	120.34	127.31
24	D	401	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	B	503	CLA	O2A-C1-C2	4.84	121.35	108.64
24	B	510	CLA	O2A-C1-C2	4.83	121.32	108.64
24	B	515	CLA	O2A-C1-C2	4.81	121.29	108.64
26	B	518	BCR	C38-C26-C25	-4.80	119.14	124.53
26	C	517	BCR	C16-C17-C18	-4.79	120.47	127.31
36	D	406	PL9	C7-C3-C4	4.78	120.76	116.88
24	B	508	CLA	CMD-C2D-C1D	4.77	133.13	124.71
26	B	518	BCR	C33-C5-C6	-4.77	119.18	124.53
26	J	101	BCR	C7-C8-C9	-4.75	119.06	126.23
26	B	518	BCR	C20-C21-C22	-4.74	120.54	127.31
26	J	101	BCR	C38-C26-C25	-4.74	119.20	124.53
26	C	517	BCR	C38-C26-C25	-4.73	119.21	124.53
28	B	520	LMG	O7-C10-C11	4.72	121.67	111.50
26	C	516	BCR	C16-C17-C18	-4.71	120.59	127.31
32	B	519	C7Z	C1-C6-C5	-4.68	116.02	122.61
24	C	502	CLA	O2A-C1-C2	4.67	120.91	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	518	BCR	C15-C14-C13	-4.67	120.65	127.31
24	C	510	CLA	O2A-C1-C2	4.66	120.88	108.64
24	A	405	CLA	O2D-CGD-CBD	4.65	119.53	111.27
26	C	516	BCR	C4-C5-C6	-4.63	116.01	122.73
26	J	101	BCR	C15-C14-C13	-4.56	120.80	127.31
32	B	519	C7Z	C18-C5-C6	-4.55	119.42	124.53
32	B	519	C7Z	C31-C30-C29	-4.53	120.84	127.31
28	C	501	LMG	O7-C10-C11	4.51	121.21	111.50
26	B	517	BCR	C7-C8-C9	-4.46	119.50	126.23
32	B	519	C7Z	C27-C28-C29	-4.45	119.51	126.23
26	B	518	BCR	C16-C17-C18	-4.43	120.99	127.31
26	C	515	BCR	C20-C21-C22	-4.43	120.99	127.31
31	D	410	LHG	O7-C7-C8	4.42	121.02	111.50
26	D	405	BCR	C20-C21-C22	-4.41	121.01	127.31
26	C	516	BCR	C33-C5-C6	-4.41	119.58	124.53
38	H	101	RRX	C24-C23-C22	-4.41	119.58	126.23
32	B	519	C7Z	C38-C25-C26	-4.40	119.59	124.53
38	H	101	RRX	C1-C6-C5	-4.37	116.45	122.61
32	B	519	C7Z	C7-C8-C9	-4.33	119.70	126.23
31	A	414	LHG	O7-C7-C8	4.31	120.80	111.50
33	C	518	DGD	O2G-C1B-C2B	4.30	120.78	111.50
24	B	512	CLA	O2A-C1-C2	4.30	119.95	108.64
28	A	411	LMG	O7-C10-C11	4.29	120.74	111.50
38	H	101	RRX	C16-C17-C18	-4.28	121.21	127.31
31	L	101	LHG	O7-C7-C8	4.27	120.71	111.50
28	C	522	LMG	O7-C10-C11	4.24	120.65	111.50
38	H	101	RRX	C4-C5-C6	-4.21	116.62	122.73
34	B	522	3PH	O21-C21-C22	4.21	120.57	111.50
35	B	523	DGA	OG2-CB1-CB2	4.18	120.51	111.50
38	H	101	RRX	C33-C5-C6	-4.18	119.84	124.53
26	J	101	BCR	C20-C21-C22	-4.17	121.36	127.31
28	H	102	LMG	O7-C10-C11	4.15	120.44	111.50
24	C	511	CLA	C1-C2-C3	-4.13	118.90	126.04
24	B	504	CLA	C1-C2-C3	-4.13	118.91	126.04
24	C	513	CLA	O2A-C1-C2	4.11	119.44	108.64
26	B	518	BCR	C24-C23-C22	-4.08	120.07	126.23
26	B	517	BCR	C4-C5-C6	-4.07	116.82	122.73
26	C	515	BCR	C27-C26-C25	-4.07	116.82	122.73
26	C	517	BCR	C24-C23-C22	-4.06	120.10	126.23
28	A	415	LMG	O7-C10-C11	4.06	120.24	111.50
26	D	405	BCR	C30-C25-C26	-4.05	116.91	122.61
33	C	519	DGD	O2G-C1B-C2B	4.04	120.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	401	CLA	C1-C2-C3	-4.00	119.13	126.04
31	D	408	LHG	O7-C7-C8	3.99	120.10	111.50
26	A	409	BCR	C11-C10-C9	3.99	133.00	127.31
28	C	521	LMG	O7-C10-C11	3.98	120.07	111.50
33	C	520	DGD	O2G-C1B-C2B	3.97	120.06	111.50
28	D	409	LMG	O7-C10-C11	3.96	120.03	111.50
24	B	502	CLA	O2A-C1-C2	3.96	119.03	108.64
33	B	521	DGD	O2G-C1B-C2B	3.91	119.93	111.50
31	D	407	LHG	O7-C7-C8	3.89	119.89	111.50
24	B	506	CLA	O2A-C1-C2	3.88	118.83	108.64
26	D	405	BCR	C33-C5-C6	-3.88	120.18	124.53
26	C	515	BCR	C7-C8-C9	-3.86	120.39	126.23
24	D	404	CLA	C1-C2-C3	-3.86	119.36	126.04
26	B	517	BCR	C16-C17-C18	-3.86	121.80	127.31
24	C	503	CLA	C1-C2-C3	-3.85	119.39	126.04
26	D	405	BCR	C27-C26-C25	-3.83	117.17	122.73
26	B	518	BCR	C4-C5-C6	-3.83	117.17	122.73
26	D	405	BCR	C15-C14-C13	-3.83	121.85	127.31
24	B	514	CLA	C1-C2-C3	-3.79	119.48	126.04
26	J	101	BCR	C1-C6-C5	-3.79	117.27	122.61
26	A	409	BCR	C12-C13-C14	3.78	124.75	118.94
35	B	523	DGA	CDB-CCB-CBB	-3.78	80.21	115.30
24	A	406	CLA	C1-C2-C3	-3.77	119.52	126.04
26	B	518	BCR	C11-C10-C9	-3.75	121.95	127.31
26	C	516	BCR	C7-C8-C9	-3.73	120.59	126.23
24	C	509	CLA	C1-C2-C3	-3.72	119.62	126.04
26	B	518	BCR	C1-C6-C5	-3.69	117.42	122.61
25	A	407	PHO	C2B-C1B-NB	-3.68	106.99	109.53
26	B	517	BCR	C30-C25-C26	-3.68	117.44	122.61
25	D	402	PHO	C2B-C1B-NB	-3.68	106.99	109.53
24	B	508	CLA	C1-C2-C3	-3.67	119.70	126.04
26	D	405	BCR	C38-C26-C25	-3.67	120.41	124.53
26	C	515	BCR	C1-C6-C5	-3.67	117.45	122.61
26	C	515	BCR	C15-C14-C13	-3.66	122.09	127.31
26	C	515	BCR	C38-C26-C25	-3.65	120.43	124.53
38	H	101	RRX	C38-C26-C25	-3.64	120.44	124.53
26	B	517	BCR	C27-C26-C25	-3.61	117.49	122.73
38	H	101	RRX	C30-C25-C26	-3.60	117.54	122.61
26	D	405	BCR	C1-C6-C5	-3.60	117.55	122.61
24	C	505	CLA	C1-C2-C3	-3.59	119.84	126.04
24	B	513	CLA	C1-C2-C3	-3.58	119.85	126.04
27	A	410	SQD	O7-S-C6	-3.58	102.69	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C4-C5-C6	-3.57	117.55	122.73
26	C	517	BCR	C27-C26-C25	-3.57	117.56	122.73
26	B	517	BCR	C23-C24-C25	-3.56	117.20	127.20
26	A	409	BCR	C27-C26-C25	-3.55	117.58	122.73
26	C	516	BCR	C23-C24-C25	-3.53	117.29	127.20
26	C	515	BCR	C38-C26-C27	3.49	120.33	113.62
24	C	504	CLA	C1-C2-C3	-3.49	120.01	126.04
24	B	505	CLA	C1-C2-C3	-3.48	120.03	126.04
24	C	511	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	C	502	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	B	511	CLA	C1-C2-C3	-3.45	120.08	126.04
24	C	505	CLA	CHD-C1D-ND	-3.44	121.29	124.45
24	D	401	CLA	CHD-C1D-ND	-3.44	121.29	124.45
26	C	516	BCR	C27-C26-C25	-3.43	117.75	122.73
24	B	515	CLA	C1-C2-C3	-3.43	120.11	126.04
24	B	515	CLA	C2C-C1C-NC	3.40	113.16	109.97
24	B	502	CLA	CHD-C1D-ND	-3.40	121.33	124.45
24	B	516	CLA	C1-C2-C3	-3.36	120.24	126.04
24	C	512	CLA	C1-C2-C3	-3.36	120.24	126.04
24	C	512	CLA	CMA-C3A-C4A	3.35	120.77	111.77
24	B	513	CLA	CHD-C1D-ND	-3.34	121.38	124.45
24	C	510	CLA	CHD-C1D-ND	-3.34	121.39	124.45
26	C	515	BCR	C11-C10-C9	-3.33	122.55	127.31
24	B	506	CLA	CHD-C1D-ND	-3.33	121.40	124.45
24	B	516	CLA	C2C-C1C-NC	3.32	113.08	109.97
26	C	517	BCR	C4-C5-C6	-3.31	117.92	122.73
26	D	405	BCR	C4-C5-C6	-3.31	117.92	122.73
25	D	402	PHO	CMB-C2B-C3B	3.30	130.86	124.68
24	D	404	CLA	CHD-C1D-ND	-3.30	121.42	124.45
38	H	101	RRX	C29-C28-C27	3.30	114.81	110.30
24	D	403	CLA	C1-C2-C3	-3.30	120.34	126.04
26	C	515	BCR	C33-C5-C6	-3.29	120.83	124.53
24	D	403	CLA	C3B-C4B-NB	-3.29	107.46	110.52
24	B	516	CLA	CHD-C1D-ND	-3.29	121.43	124.45
26	D	405	BCR	C11-C10-C9	-3.28	122.62	127.31
24	C	506	CLA	C1-C2-C3	-3.28	120.37	126.04
24	C	510	CLA	C2C-C1C-NC	3.28	113.04	109.97
24	A	406	CLA	CHD-C1D-ND	-3.27	121.45	124.45
27	M	101	SQD	O7-S-C6	-3.27	103.06	106.94
24	C	508	CLA	C2C-C1C-NC	3.26	113.03	109.97
26	C	516	BCR	C20-C21-C22	-3.26	122.66	127.31
26	B	518	BCR	C8-C7-C6	-3.25	118.06	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C2C-C1C-NC	3.25	113.02	109.97
26	C	516	BCR	C33-C5-C4	3.24	119.85	113.62
24	B	504	CLA	C2C-C1C-NC	3.24	113.01	109.97
24	A	408	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	C	502	CLA	C1-C2-C3	-3.24	120.44	126.04
26	C	517	BCR	C1-C6-C5	-3.24	118.05	122.61
36	D	406	PL9	C7-C3-C2	-3.23	119.05	123.30
24	A	408	CLA	C2C-C1C-NC	3.23	113.00	109.97
38	H	101	RRX	C8-C7-C6	-3.21	118.18	127.20
26	A	409	BCR	C4-C5-C6	-3.21	118.07	122.73
24	C	508	CLA	C1-C2-C3	-3.20	120.51	126.04
24	B	513	CLA	C2C-C1C-NC	3.20	112.97	109.97
24	B	501	CLA	C1-C2-C3	-3.19	120.53	126.04
24	C	513	CLA	C2C-C1C-NC	3.19	112.96	109.97
24	C	512	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	B	505	CLA	CHD-C1D-ND	-3.18	121.53	124.45
26	A	409	BCR	C23-C24-C25	-3.17	118.29	127.20
24	B	507	CLA	CHD-C1D-ND	-3.17	121.54	124.45
26	C	517	BCR	C15-C14-C13	-3.17	122.79	127.31
26	C	517	BCR	C30-C25-C26	-3.16	118.16	122.61
26	B	517	BCR	C38-C26-C27	3.16	119.69	113.62
24	B	514	CLA	CHD-C1D-ND	-3.15	121.56	124.45
24	C	514	CLA	CHD-C1D-ND	-3.15	121.56	124.45
26	D	405	BCR	C24-C23-C22	-3.15	121.47	126.23
26	D	405	BCR	C8-C7-C6	-3.15	118.36	127.20
26	D	405	BCR	C7-C8-C9	-3.15	121.48	126.23
26	C	517	BCR	C15-C16-C17	-3.12	117.08	123.47
24	B	511	CLA	CHD-C1D-ND	-3.12	121.59	124.45
24	D	403	CLA	CHD-C1D-ND	-3.11	121.59	124.45
24	B	510	CLA	C2C-C1C-NC	3.11	112.89	109.97
24	B	504	CLA	CMA-C3A-C4A	3.11	120.13	111.77
26	D	405	BCR	C33-C5-C4	3.10	119.58	113.62
24	C	504	CLA	CHD-C1D-ND	-3.10	121.60	124.45
26	A	409	BCR	C35-C13-C14	-3.09	118.60	122.92
24	C	512	CLA	C2C-C1C-NC	3.09	112.86	109.97
24	C	508	CLA	CHD-C1D-ND	-3.08	121.62	124.45
26	A	409	BCR	C16-C15-C14	-3.08	117.17	123.47
26	B	517	BCR	C15-C16-C17	-3.08	117.17	123.47
24	B	515	CLA	CHD-C1D-ND	-3.07	121.63	124.45
24	C	513	CLA	CHD-C1D-ND	-3.07	121.63	124.45
26	D	405	BCR	C23-C24-C25	-3.06	118.61	127.20
24	C	503	CLA	C2C-C1C-NC	3.05	112.83	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	406	PL9	C7-C8-C9	-3.05	121.71	126.79
24	B	510	CLA	CHD-C1D-ND	-3.04	121.66	124.45
24	B	509	CLA	C2D-C1D-ND	3.03	112.34	110.10
32	B	519	C7Z	C18-C5-C4	3.03	119.97	114.36
25	D	402	PHO	O1D-CGD-CBD	3.03	129.78	124.74
24	B	512	CLA	C2C-C1C-NC	3.03	112.81	109.97
24	D	401	CLA	C2C-C1C-NC	3.02	112.81	109.97
24	C	504	CLA	CMA-C3A-C4A	3.02	119.90	111.77
24	C	507	CLA	CHD-C1D-ND	-3.02	121.68	124.45
26	A	409	BCR	C1-C6-C5	-3.02	118.37	122.61
26	C	516	BCR	C8-C7-C6	-3.01	118.74	127.20
26	J	101	BCR	C38-C26-C27	3.00	119.39	113.62
24	C	511	CLA	C2C-C1C-NC	3.00	112.78	109.97
24	B	512	CLA	C1-C2-C3	-3.00	120.85	126.04
24	B	502	CLA	C2D-C1D-ND	2.99	112.31	110.10
24	B	510	CLA	C2D-C1D-ND	2.99	112.31	110.10
26	B	517	BCR	C1-C6-C5	-2.99	118.41	122.61
24	B	511	CLA	C2C-C1C-NC	2.99	112.77	109.97
33	C	519	DGD	C1D-O6D-C5D	2.98	119.54	113.69
28	A	411	LMG	C8-O7-C10	-2.98	110.45	117.79
24	B	514	CLA	C2C-C1C-NC	2.98	112.77	109.97
26	A	409	BCR	C38-C26-C25	-2.98	121.18	124.53
26	B	517	BCR	C21-C20-C19	-2.98	113.92	123.22
24	C	507	CLA	C1-C2-C3	-2.98	120.90	126.04
24	A	405	CLA	CHD-C1D-ND	-2.97	121.72	124.45
24	C	506	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	C	516	BCR	C21-C20-C19	-2.97	113.96	123.22
25	D	402	PHO	O2D-CGD-O1D	-2.97	118.04	123.84
24	B	509	CLA	C2C-C1C-NC	2.97	112.75	109.97
38	H	101	RRX	C23-C24-C25	-2.97	118.87	127.20
24	B	509	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	D	404	CLA	C2C-C1C-NC	2.96	112.75	109.97
24	B	510	CLA	C1-C2-C3	-2.96	120.93	126.04
24	C	503	CLA	C2D-C1D-ND	2.95	112.28	110.10
24	B	509	CLA	C1-C2-C3	-2.95	120.94	126.04
24	B	508	CLA	C2C-C1C-NC	2.95	112.73	109.97
24	B	507	CLA	C2C-C1C-NC	2.94	112.73	109.97
33	C	519	DGD	O1G-C1A-C2A	2.94	121.14	111.91
33	C	518	DGD	O1G-C1A-C2A	2.94	121.14	111.91
24	C	505	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	B	502	CLA	C2C-C1C-NC	2.94	112.72	109.97
24	B	507	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C2C-C1C-NC	2.93	112.72	109.97
24	A	406	CLA	C2C-C1C-NC	2.93	112.72	109.97
24	D	403	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	D	410	LHG	O8-C23-C24	2.92	121.08	111.91
24	A	405	CLA	C2D-C1D-ND	2.92	112.26	110.10
24	B	510	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	C	517	BCR	C2-C1-C6	2.92	114.97	110.48
32	B	519	C7Z	C38-C25-C24	2.91	119.75	114.36
24	C	509	CLA	CHD-C1D-ND	-2.91	121.78	124.45
26	J	101	BCR	C29-C30-C25	2.91	114.96	110.48
24	C	514	CLA	C2C-C1C-NC	2.91	112.70	109.97
24	B	505	CLA	C2C-C1C-NC	2.91	112.70	109.97
24	B	505	CLA	C2D-C1D-ND	2.90	112.24	110.10
24	B	501	CLA	C2C-C1C-NC	2.90	112.69	109.97
24	C	504	CLA	C2D-C1D-ND	2.90	112.24	110.10
24	C	503	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	C	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	C	508	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
24	B	513	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	L	101	LHG	O8-C23-C24	2.90	121.00	111.91
24	B	506	CLA	C2C-C1C-NC	2.89	112.68	109.97
24	A	405	CLA	C1-C2-C3	-2.88	121.06	126.04
26	C	517	BCR	C33-C5-C4	2.88	119.15	113.62
32	B	519	C7Z	C8-C7-C6	-2.88	119.11	127.20
31	D	407	LHG	O8-C23-C24	2.88	120.95	111.91
24	B	512	CLA	CHD-C1D-ND	-2.88	121.81	124.45
25	A	407	PHO	CMB-C2B-C3B	2.88	130.06	124.68
24	B	512	CLA	C2D-C1D-ND	2.88	112.22	110.10
26	C	515	BCR	C30-C25-C26	-2.88	118.56	122.61
28	H	102	LMG	O8-C28-C29	2.88	120.93	111.91
24	B	502	CLA	O2A-CGA-CBA	2.87	120.91	111.91
24	B	511	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	D	408	LHG	O8-C23-C24	2.87	120.91	111.91
24	C	511	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
24	B	501	CLA	CMA-C3A-C4A	2.86	119.46	111.77
25	A	407	PHO	O2D-CGD-O1D	-2.86	118.25	123.84
24	D	401	CLA	O2A-CGA-CBA	2.86	120.88	111.91
26	D	405	BCR	C38-C26-C27	2.86	119.10	113.62
24	B	503	CLA	C1-C2-C3	-2.85	121.11	126.04
24	B	512	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
33	C	519	DGD	O6D-C5D-C6D	2.84	112.40	106.67
24	C	503	CLA	O2D-CGD-O1D	-2.84	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	520	DGD	O1G-C1A-C2A	2.83	120.80	111.91
24	A	408	CLA	C2D-C1D-ND	2.83	112.19	110.10
24	B	513	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
24	C	502	CLA	C3B-C4B-NB	-2.83	107.89	110.52
38	H	101	RRX	C11-C12-C13	-2.82	118.48	126.42
24	B	501	CLA	C2D-C1D-ND	2.82	112.19	110.10
26	J	101	BCR	C30-C25-C26	-2.82	118.64	122.61
24	B	501	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	B	508	CLA	C2D-C1D-ND	2.82	112.18	110.10
26	A	409	BCR	C38-C26-C27	2.82	119.03	113.62
28	B	520	LMG	O8-C28-C29	2.81	120.74	111.91
24	A	408	CLA	CHD-C1D-ND	-2.81	121.87	124.45
24	C	513	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
24	C	506	CLA	C2D-C1D-ND	2.81	112.17	110.10
24	B	501	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	C	513	CLA	C2D-C1D-ND	2.81	112.17	110.10
24	D	404	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
26	C	517	BCR	C33-C5-C6	-2.80	121.38	124.53
24	B	508	CLA	CHD-C1D-ND	-2.80	121.88	124.45
24	C	506	CLA	C3B-C4B-NB	-2.80	107.92	110.52
26	C	515	BCR	C33-C5-C4	2.80	118.99	113.62
24	B	503	CLA	C2C-C1C-NC	2.80	112.59	109.97
24	B	502	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
24	C	511	CLA	C2D-C1D-ND	2.79	112.16	110.10
24	B	503	CLA	CHD-C1D-ND	-2.79	121.89	124.45
24	D	404	CLA	C2D-C1D-ND	2.79	112.16	110.10
24	C	505	CLA	C2D-C1D-ND	2.78	112.15	110.10
24	C	505	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	A	408	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
24	B	515	CLA	C2D-C1D-ND	2.78	112.15	110.10
26	C	516	BCR	C15-C16-C17	-2.78	117.78	123.47
31	L	101	LHG	C5-O7-C7	-2.78	110.96	117.79
24	C	506	CLA	CHD-C1D-ND	-2.77	121.90	124.45
38	H	101	RRX	C35-C13-C14	-2.77	119.04	122.92
24	C	512	CLA	C2D-C1D-ND	2.77	112.15	110.10
24	C	506	CLA	C2C-C1C-NC	2.77	112.57	109.97
26	B	518	BCR	C33-C5-C4	2.77	118.93	113.62
24	B	505	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
24	C	514	CLA	C2D-C1D-ND	2.76	112.14	110.10
24	B	505	CLA	C3B-C4B-NB	-2.76	107.95	110.52
24	C	504	CLA	C2C-C1C-NC	2.76	112.56	109.97
38	H	101	RRX	C34-C9-C10	-2.76	119.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	517	BCR	C23-C24-C25	-2.76	119.46	127.20
24	B	514	CLA	C2D-C1D-ND	2.76	112.14	110.10
24	B	504	CLA	O2A-CGA-CBA	2.74	120.52	111.91
26	B	517	BCR	C20-C21-C22	-2.74	123.40	127.31
24	C	502	CLA	CMA-C3A-C4A	2.74	119.13	111.77
24	D	401	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
38	H	101	RRX	C7-C8-C9	-2.74	122.10	126.23
24	C	502	CLA	C2D-C1D-ND	2.73	112.12	110.10
31	A	414	LHG	C5-O7-C7	-2.73	111.08	117.79
26	B	518	BCR	C38-C26-C27	2.73	118.85	113.62
25	A	407	PHO	O1D-CGD-CBD	2.72	129.28	124.74
24	B	504	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	B	510	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
26	C	515	BCR	C16-C15-C14	-2.72	117.90	123.47
24	C	510	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
26	B	517	BCR	C8-C7-C6	-2.71	119.58	127.20
28	C	521	LMG	O8-C28-C29	2.71	120.41	111.91
24	B	501	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
36	D	406	PL9	C22-C23-C24	-2.71	121.14	127.66
24	D	403	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	508	CLA	CMA-C3A-C4A	2.70	119.03	111.77
24	B	504	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
24	D	403	CLA	C1D-ND-C4D	-2.70	104.42	106.33
24	B	501	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	C	507	CLA	C2D-C1D-ND	2.70	112.09	110.10
26	B	518	BCR	C23-C24-C25	-2.70	119.63	127.20
24	C	505	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	A	414	LHG	O8-C23-C24	2.69	120.35	111.91
24	A	406	CLA	C2D-C1D-ND	2.69	112.08	110.10
24	C	508	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	A	406	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	C	511	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
24	B	510	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	B	514	CLA	CMA-C3A-C4A	2.68	118.98	111.77
24	C	513	CLA	C1-C2-C3	-2.68	121.40	126.04
24	C	514	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	C	514	CLA	CMA-C3A-C4A	2.67	118.96	111.77
24	B	516	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
24	B	503	CLA	O2A-CGA-CBA	2.66	120.27	111.91
24	C	513	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	B	508	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
24	B	515	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	518	BCR	C27-C26-C25	-2.65	118.88	122.73
24	A	405	CLA	C2C-C1C-NC	2.65	112.46	109.97
24	A	408	CLA	CMA-C3A-C4A	2.65	118.91	111.77
24	B	507	CLA	C2D-C1D-ND	2.65	112.06	110.10
24	C	509	CLA	C2D-C1D-ND	2.65	112.06	110.10
24	B	508	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
24	A	406	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	C	507	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	D	404	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
33	C	520	DGD	O3G-C3G-C2G	-2.65	104.51	110.90
24	B	504	CLA	CHD-C1D-ND	-2.65	122.02	124.45
28	C	501	LMG	C7-O1-C1	-2.65	108.57	113.74
24	C	508	CLA	C2D-C1D-ND	2.64	112.05	110.10
24	C	502	CLA	C2C-C1C-NC	2.64	112.44	109.97
24	B	510	CLA	C4B-CHC-C1C	2.64	132.59	126.34
24	A	408	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
24	A	408	CLA	C1-C2-C3	-2.64	121.48	126.04
24	B	510	CLA	C3B-C4B-NB	-2.63	108.07	110.52
26	J	101	BCR	C27-C26-C25	-2.63	118.91	122.73
24	C	512	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
24	B	514	CLA	C1-O2A-CGA	2.63	123.33	116.44
24	B	509	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	C	517	BCR	C21-C20-C19	-2.62	115.03	123.22
24	B	501	CLA	O2A-CGA-CBA	2.62	120.12	111.91
28	D	409	LMG	O8-C28-C29	2.62	120.12	111.91
24	B	512	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
26	B	518	BCR	C7-C8-C9	-2.61	122.29	126.23
24	B	516	CLA	C3B-C4B-NB	-2.61	108.09	110.52
24	C	513	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
32	B	519	C7Z	C28-C27-C26	-2.61	119.88	127.20
24	B	514	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
24	B	506	CLA	C2D-C1D-ND	2.60	112.02	110.10
24	B	505	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	B	517	BCR	C24-C23-C22	-2.60	122.31	126.23
26	A	409	BCR	C30-C25-C26	-2.59	118.96	122.61
24	B	504	CLA	CHA-C4D-ND	2.59	137.92	132.50
24	C	502	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
26	B	518	BCR	C15-C16-C17	-2.59	118.17	123.47
24	B	511	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
26	B	518	BCR	C29-C30-C25	2.59	114.46	110.48
24	B	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77
24	C	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	513	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
35	B	523	DGA	OG1-CA1-CA2	2.58	120.00	111.91
24	B	506	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
34	B	522	3PH	O31-C31-C32	2.58	120.00	111.91
24	B	502	CLA	CMA-C3A-C4A	2.58	118.69	111.77
24	B	502	CLA	C1D-ND-C4D	-2.57	104.51	106.33
24	C	509	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	B	505	CLA	C4B-CHC-C1C	2.57	132.43	126.34
24	B	507	CLA	CHA-C4D-ND	2.57	137.87	132.50
24	C	503	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
24	B	507	CLA	C1-C2-C3	-2.56	121.61	126.04
26	D	405	BCR	C10-C11-C12	-2.56	115.22	123.22
24	C	514	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
24	B	503	CLA	CHA-C4D-ND	2.56	137.84	132.50
26	J	101	BCR	C4-C5-C6	-2.55	119.03	122.73
24	C	502	CLA	C1D-ND-C4D	-2.55	104.52	106.33
24	B	509	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
26	D	405	BCR	C16-C15-C14	-2.55	118.25	123.47
33	B	521	DGD	O1G-C1A-C2A	2.54	119.89	111.91
24	C	509	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
24	B	515	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	D	404	CLA	CMA-C3A-C4A	2.53	118.59	111.77
24	C	502	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
24	B	506	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
26	C	515	BCR	C8-C7-C6	-2.53	120.10	127.20
24	C	508	CLA	CMA-C3A-C4A	2.53	118.56	111.77
24	C	504	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
24	B	505	CLA	C1D-ND-C4D	-2.52	104.55	106.33
24	C	502	CLA	CMD-C2D-C3D	-2.52	121.83	127.61
38	H	101	RRX	C38-C26-C27	2.52	119.02	114.36
24	C	502	CLA	C4B-CHC-C1C	2.51	132.30	126.34
24	A	406	CLA	C3B-C4B-NB	-2.51	108.19	110.52
24	B	501	CLA	C4B-CHC-C1C	2.51	132.29	126.34
24	B	507	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	B	514	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
24	B	501	CLA	CHA-C4D-ND	2.50	137.73	132.50
32	B	519	C7Z	C15-C35-C34	-2.50	118.36	123.47
24	B	506	CLA	CHA-C4D-ND	2.49	137.72	132.50
24	D	403	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
24	C	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
26	A	409	BCR	C29-C30-C25	2.49	114.31	110.48
24	B	507	CLA	C1C-C2C-C3C	-2.49	104.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J	101	BCR	C8-C7-C6	-2.49	120.22	127.20
32	B	519	C7Z	C4-C5-C6	-2.49	115.31	120.85
24	C	506	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
26	A	409	BCR	C37-C22-C21	-2.48	119.44	122.92
36	D	406	PL9	C27-C28-C29	-2.48	121.69	127.66
24	D	401	CLA	C2D-C1D-ND	2.48	111.93	110.10
24	C	507	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
24	D	403	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
24	C	509	CLA	CHA-C4D-ND	2.48	137.68	132.50
24	A	408	CLA	C1D-ND-C4D	-2.48	104.58	106.33
24	C	512	CLA	CHA-C4D-ND	2.47	137.67	132.50
24	B	511	CLA	O2A-CGA-CBA	2.47	119.67	111.91
28	C	501	LMG	C8-O7-C10	-2.47	111.71	117.79
24	B	503	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	B	516	CLA	C2D-C1D-ND	2.46	111.92	110.10
24	C	511	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	C	511	CLA	CHA-C4D-ND	2.46	137.65	132.50
24	C	509	CLA	CMA-C3A-C4A	2.46	118.39	111.77
24	C	506	CLA	O2A-CGA-CBA	2.46	119.63	111.91
24	B	516	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	508	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	510	CLA	C2D-C1D-ND	2.46	111.92	110.10
24	D	403	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	504	CLA	C4B-CHC-C1C	2.45	132.16	126.34
24	C	502	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	B	505	CLA	CHA-C4D-ND	2.45	137.63	132.50
24	B	502	CLA	C4B-CHC-C1C	2.45	132.15	126.34
24	C	504	CLA	CHA-C4D-ND	2.45	137.62	132.50
24	C	502	CLA	CHA-C4D-ND	2.45	137.61	132.50
24	C	505	CLA	CMA-C3A-C4A	2.44	118.34	111.77
24	C	506	CLA	CMA-C3A-C4A	2.44	118.33	111.77
28	A	411	LMG	O8-C28-C29	2.43	119.54	111.91
24	B	516	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
24	B	503	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
24	B	506	CLA	CMA-C3A-C4A	2.43	118.30	111.77
24	B	514	CLA	CHA-C4D-ND	2.43	137.57	132.50
24	C	507	CLA	CHA-C4D-ND	2.43	137.57	132.50
26	B	518	BCR	C30-C25-C26	-2.42	119.20	122.61
24	C	510	CLA	C4B-CHC-C1C	2.42	132.08	126.34
24	C	504	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	D	403	CLA	C2C-C1C-NC	2.41	112.23	109.97
24	C	507	CLA	C3B-C4B-NB	-2.41	108.28	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C23-C24-C25	-2.41	120.44	127.20
24	B	513	CLA	CHA-C4D-ND	2.41	137.53	132.50
39	J	102	LMU	C1B-O1B-C4'	-2.40	112.02	117.96
31	D	408	LHG	C5-O7-C7	-2.40	111.88	117.79
25	A	407	PHO	C1C-C2C-C3C	-2.40	106.61	108.61
24	C	507	CLA	O2A-CGA-CBA	2.40	119.44	111.91
24	C	514	CLA	CHA-C4D-ND	2.40	137.52	132.50
24	D	401	CLA	C4B-CHC-C1C	2.40	132.03	126.34
24	B	503	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
24	D	403	CLA	C4B-CHC-C1C	2.40	132.02	126.34
36	D	406	PL9	C20-C19-C21	2.39	119.29	115.27
24	B	504	CLA	C4B-CHC-C1C	2.39	132.00	126.34
24	A	405	CLA	CHA-C4D-ND	2.39	137.49	132.50
24	B	511	CLA	CMA-C3A-C4A	2.38	118.17	111.77
24	A	405	CLA	C1D-ND-C4D	-2.38	104.64	106.33
24	B	511	CLA	C1D-ND-C4D	-2.38	104.64	106.33
24	C	504	CLA	O2A-CGA-CBA	2.38	119.37	111.91
24	C	504	CLA	C1D-ND-C4D	-2.38	104.65	106.33
38	H	101	RRX	C20-C19-C18	-2.37	119.75	126.42
24	B	501	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
28	A	415	LMG	O8-C28-C29	2.37	119.35	111.91
24	C	503	CLA	C4B-CHC-C1C	2.37	131.96	126.34
24	C	504	CLA	C3B-C4B-NB	-2.37	108.31	110.52
24	D	404	CLA	CHA-C4D-ND	2.37	137.46	132.50
24	B	504	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
26	C	516	BCR	C30-C25-C26	-2.37	119.28	122.61
24	A	406	CLA	CHA-C4D-ND	2.37	137.46	132.50
24	C	509	CLA	C4B-CHC-C1C	2.37	131.96	126.34
24	D	401	CLA	CHA-C4D-ND	2.37	137.45	132.50
33	C	520	DGD	C2G-O2G-C1B	-2.37	111.97	117.79
24	B	510	CLA	CHA-C4D-ND	2.36	137.45	132.50
24	B	505	CLA	O2A-CGA-CBA	2.36	119.33	111.91
24	D	401	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
24	C	505	CLA	CHA-C4D-ND	2.36	137.44	132.50
24	C	509	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
24	A	405	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
24	C	503	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	D	410	LHG	C5-O7-C7	-2.36	111.98	117.79
24	A	406	CLA	C4B-CHC-C1C	2.36	131.93	126.34
24	C	513	CLA	CHA-C4D-ND	2.36	137.43	132.50
26	J	101	BCR	C11-C12-C13	-2.36	119.80	126.42
24	B	502	CLA	O2D-CGD-O1D	-2.35	119.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	C4B-CHC-C1C	2.35	131.92	126.34
24	B	516	CLA	C4B-CHC-C1C	2.35	131.92	126.34
24	B	515	CLA	CHA-C4D-ND	2.35	137.42	132.50
24	D	404	CLA	C3B-C4B-NB	-2.35	108.33	110.52
24	C	510	CLA	CHA-C4D-ND	2.35	137.41	132.50
24	A	406	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	D	402	PHO	C1-C2-C3	-2.35	121.99	126.04
24	B	502	CLA	C3B-C4B-NB	-2.34	108.34	110.52
24	B	509	CLA	C4B-CHC-C1C	2.34	131.88	126.34
24	B	512	CLA	CHA-C4D-ND	2.34	137.39	132.50
24	C	507	CLA	CMA-C3A-C4A	2.33	118.05	111.77
24	C	506	CLA	C4B-CHC-C1C	2.33	131.87	126.34
24	A	408	CLA	C4B-CHC-C1C	2.33	131.86	126.34
38	H	101	RRX	C15-C16-C17	-2.33	118.71	123.47
24	C	511	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
24	C	507	CLA	C4B-CHC-C1C	2.33	131.85	126.34
24	B	509	CLA	O2A-CGA-CBA	2.32	119.20	111.91
25	D	402	PHO	C1C-C2C-C3C	-2.32	106.68	108.61
27	M	101	SQD	O3-C3-C2	-2.32	104.99	110.35
24	C	508	CLA	C3B-C4B-NB	-2.32	108.37	110.52
24	B	509	CLA	CHA-C4D-ND	2.32	137.34	132.50
24	A	405	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
24	B	506	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
24	B	503	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
24	B	507	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
28	C	501	LMG	O8-C28-C29	2.31	119.16	111.91
24	B	503	CLA	C3B-C4B-NB	-2.31	108.37	110.52
24	B	503	CLA	C4B-CHC-C1C	2.31	131.81	126.34
24	C	514	CLA	C4B-CHC-C1C	2.31	131.81	126.34
24	B	511	CLA	CHA-C4D-ND	2.31	137.32	132.50
24	B	510	CLA	C1D-ND-C4D	-2.31	104.70	106.33
24	B	502	CLA	CHA-C4D-ND	2.30	137.32	132.50
24	B	511	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
24	C	512	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
24	D	401	CLA	CMA-C3A-C4A	2.30	117.95	111.77
24	C	512	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	B	505	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
24	B	511	CLA	C4B-CHC-C1C	2.29	131.78	126.34
24	C	512	CLA	C4B-CHC-C1C	2.29	131.77	126.34
27	A	410	SQD	O3-C3-C2	-2.29	105.06	110.35
24	B	512	CLA	C4B-CHC-C1C	2.29	131.77	126.34
37	E	101	HEM	C4D-ND-C1D	2.29	107.44	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	508	CLA	CHA-C4D-ND	2.28	137.28	132.50
26	C	517	BCR	C38-C26-C27	2.28	118.00	113.62
32	B	519	C7Z	C21-C26-C25	-2.28	119.40	122.61
24	B	508	CLA	C1D-ND-C4D	-2.28	104.72	106.33
24	D	404	CLA	C4B-CHC-C1C	2.27	131.73	126.34
24	A	408	CLA	O2A-CGA-CBA	2.27	119.04	111.91
24	C	508	CLA	C4B-CHC-C1C	2.27	131.72	126.34
24	A	406	CLA	C1D-ND-C4D	-2.27	104.72	106.33
28	C	521	LMG	C8-O7-C10	-2.27	112.21	117.79
24	B	516	CLA	O2A-CGA-CBA	2.27	119.02	111.91
24	C	513	CLA	C4B-CHC-C1C	2.27	131.71	126.34
24	C	509	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	B	507	CLA	O2A-CGA-CBA	2.26	119.00	111.91
24	B	514	CLA	C4B-CHC-C1C	2.26	131.70	126.34
26	J	101	BCR	C23-C24-C25	-2.26	120.86	127.20
24	D	403	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
24	C	510	CLA	O2A-CGA-CBA	2.25	118.98	111.91
24	B	507	CLA	C4B-CHC-C1C	2.25	131.67	126.34
24	B	513	CLA	O2A-CGA-CBA	2.24	118.94	111.91
26	A	409	BCR	C1-C6-C7	2.24	122.12	115.78
24	B	512	CLA	O2A-CGA-CBA	2.24	118.93	111.91
36	D	406	PL9	O1-C4-C3	-2.24	118.26	120.72
24	C	505	CLA	C4B-CHC-C1C	2.23	131.64	126.34
26	A	409	BCR	C21-C20-C19	-2.23	116.25	123.22
24	C	514	CLA	C1D-ND-C4D	-2.23	104.75	106.33
24	D	401	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
37	E	101	HEM	C4A-NA-C1A	2.23	107.53	105.35
24	A	408	CLA	CHA-C4D-ND	2.23	137.16	132.50
24	B	515	CLA	CMA-C3A-C4A	2.22	117.75	111.77
26	J	101	BCR	C33-C5-C4	2.22	117.89	113.62
24	B	512	CLA	CMA-C3A-C4A	2.22	117.74	111.77
37	E	101	HEM	C1B-NB-C4B	2.22	107.36	105.07
26	B	517	BCR	C35-C13-C14	-2.22	119.82	122.92
24	B	508	CLA	C3B-C4B-NB	-2.22	108.46	110.52
24	C	513	CLA	O2A-CGA-CBA	2.21	118.86	111.91
24	B	515	CLA	C3B-C4B-NB	-2.21	108.46	110.52
24	B	502	CLA	C1-C2-C3	-2.21	122.21	126.04
26	J	101	BCR	C16-C15-C14	-2.21	118.94	123.47
24	C	511	CLA	C3B-C4B-NB	-2.21	108.47	110.52
26	A	409	BCR	C24-C23-C22	-2.21	122.90	126.23
24	C	512	CLA	O2A-CGA-CBA	2.21	118.83	111.91
24	D	401	CLA	C1D-ND-C4D	-2.20	104.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C1-O2A-CGA	2.20	122.22	116.44
24	B	503	CLA	C2D-C1D-ND	2.20	111.72	110.10
24	B	506	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	C	509	CLA	CHA-C1A-NA	-2.20	121.36	126.40
24	C	510	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
24	D	401	CLA	C1-O2A-CGA	2.20	122.21	116.44
26	C	515	BCR	C20-C19-C18	-2.20	120.24	126.42
36	D	406	PL9	C37-C38-C39	-2.20	122.37	127.66
24	C	511	CLA	C4B-CHC-C1C	2.20	131.55	126.34
24	A	405	CLA	CMA-C3A-C4A	2.19	117.67	111.77
24	A	405	CLA	O2A-CGA-CBA	2.19	118.78	111.91
24	B	509	CLA	C1D-ND-C4D	-2.19	104.78	106.33
24	B	501	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
24	A	406	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	B	516	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	C	506	CLA	C1D-ND-C4D	-2.18	104.78	106.33
24	B	514	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
24	C	511	CLA	C1D-ND-C4D	-2.18	104.79	106.33
24	B	515	CLA	C4B-CHC-C1C	2.18	131.51	126.34
28	A	415	LMG	C8-O7-C10	-2.18	112.42	117.79
24	B	508	CLA	C4B-CHC-C1C	2.18	131.51	126.34
24	C	504	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
24	B	513	CLA	C4B-CHC-C1C	2.18	131.50	126.34
24	C	507	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	B	514	CLA	C1D-ND-C4D	-2.18	104.79	106.33
26	A	409	BCR	C33-C5-C4	2.18	117.80	113.62
24	B	509	CLA	C3B-C4B-NB	-2.18	108.50	110.52
24	B	504	CLA	CHA-C1A-NA	-2.17	121.42	126.40
26	C	516	BCR	C11-C12-C13	-2.17	120.31	126.42
24	C	509	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
36	D	406	PL9	C12-C13-C14	-2.17	122.44	127.66
38	H	101	RRX	C33-C5-C4	2.17	117.78	113.62
24	C	510	CLA	CMA-C3A-C4A	2.17	117.59	111.77
24	B	512	CLA	C3B-C4B-NB	-2.16	108.51	110.52
24	C	510	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
32	B	519	C7Z	C11-C12-C13	-2.16	120.34	126.42
24	B	516	CLA	CMA-C3A-C4A	2.16	117.58	111.77
38	H	101	RRX	C8-C9-C10	2.16	122.26	118.94
24	C	514	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
24	B	506	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
24	B	515	CLA	CHA-C1A-NA	-2.16	121.45	126.40
25	D	402	PHO	O2A-CGA-O1A	-2.16	118.15	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
26	C	516	BCR	C37-C22-C23	2.15	121.47	118.08
24	D	401	CLA	C6-C5-C3	-2.15	107.81	113.45
24	B	506	CLA	C4B-CHC-C1C	2.15	131.44	126.34
24	B	507	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	C	516	BCR	C1-C6-C7	2.14	121.84	115.78
26	B	517	BCR	C37-C22-C23	2.14	121.45	118.08
24	B	509	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	C	513	CLA	CMA-C3A-C4A	2.14	117.52	111.77
26	C	515	BCR	C36-C18-C17	-2.14	119.93	122.92
24	C	510	CLA	C1-C2-C3	-2.14	122.35	126.04
24	C	513	CLA	CHA-C1A-NA	-2.13	121.51	126.40
26	C	516	BCR	C24-C23-C22	-2.13	123.01	126.23
24	A	408	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	C	508	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
32	B	519	C7Z	C19-C9-C10	-2.13	119.94	122.92
24	C	505	CLA	O2A-CGA-CBA	2.12	118.57	111.91
24	C	503	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	B	502	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
26	B	518	BCR	C11-C12-C13	-2.12	120.47	126.42
24	C	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	C	502	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
26	D	405	BCR	C20-C19-C18	-2.12	120.47	126.42
24	A	408	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
24	C	514	CLA	C3B-C4B-NB	-2.11	108.56	110.52
24	C	507	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
24	C	503	CLA	C1D-ND-C4D	-2.11	104.84	106.33
24	B	506	CLA	C3B-C4B-NB	-2.11	108.56	110.52
38	H	101	RRX	C27-C26-C25	-2.11	116.16	120.85
28	C	522	LMG	C8-O7-C10	-2.10	112.61	117.79
24	B	508	CLA	C1-O2A-CGA	2.10	121.97	116.44
26	C	516	BCR	C16-C15-C14	-2.10	119.17	123.47
24	B	504	CLA	C2D-C1D-ND	2.10	111.65	110.10
24	C	512	CLA	C1D-ND-C4D	-2.10	104.84	106.33
24	A	405	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
24	C	503	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	C	509	CLA	C3B-C4B-NB	-2.10	108.57	110.52
24	C	505	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
31	D	407	LHG	C5-O7-C7	-2.10	112.63	117.79
24	B	513	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
24	C	506	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
24	A	406	CLA	CHA-C1A-NA	-2.09	121.61	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C10-C11-C12	-2.09	116.69	123.22
31	D	410	LHG	O7-C7-O9	-2.09	118.65	123.70
24	B	501	CLA	C1D-ND-C4D	-2.09	104.85	106.33
26	B	517	BCR	C33-C5-C4	2.09	117.63	113.62
24	C	507	CLA	C1D-ND-C4D	-2.09	104.85	106.33
24	B	506	CLA	C1-O2A-CGA	2.09	121.92	116.44
24	C	513	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	B	511	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	B	514	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	A	406	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
24	C	512	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	C	503	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	B	507	CLA	C1-O2A-CGA	2.08	121.90	116.44
33	C	518	DGD	C2G-O2G-C1B	-2.08	112.68	117.79
24	D	404	CLA	O2A-CGA-CBA	2.07	118.42	111.91
28	A	411	LMG	O7-C10-O9	-2.07	118.70	123.70
24	C	505	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	A	405	CLA	C3B-C4B-NB	-2.07	108.60	110.52
24	B	512	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	C	504	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
31	L	101	LHG	O8-C23-O10	-2.06	118.39	123.59
26	A	409	BCR	C7-C6-C5	-2.06	116.47	121.46
24	B	510	CLA	O2A-CGA-CBA	2.06	118.37	111.91
36	D	406	PL9	C31-C32-C33	-2.06	105.11	111.88
24	B	509	CLA	CMA-C3A-C4A	2.06	117.30	111.77
24	B	505	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
24	C	512	CLA	C3B-C4B-NB	-2.06	108.61	110.52
36	D	406	PL9	O2-C1-C6	2.05	124.15	120.59
24	B	511	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
36	D	406	PL9	C40-C39-C41	2.05	118.72	115.27
25	A	407	PHO	C1-C2-C3	-2.05	122.50	126.04
37	E	101	HEM	CAD-CBD-CGD	-2.04	109.20	113.60
24	C	503	CLA	C6-C5-C3	-2.04	108.09	113.45
24	B	509	CLA	CHA-C1A-NA	-2.04	121.72	126.40
24	D	401	CLA	C3B-C4B-NB	-2.04	108.62	110.52
24	B	501	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	C	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	A	408	CLA	C3B-C4B-NB	-2.04	108.62	110.52
24	B	502	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	B	515	CLA	O2A-CGA-CBA	2.04	118.30	111.91
24	B	506	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
24	C	512	CLA	CHA-C1A-NA	-2.04	121.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	409	LMG	C8-O7-C10	-2.03	112.79	117.79
24	C	510	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	C	520	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
24	B	508	CLA	O2A-CGA-CBA	2.03	118.27	111.91
24	D	404	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
26	C	516	BCR	C38-C26-C27	2.03	117.51	113.62
37	E	101	HEM	C4C-NC-C1C	2.03	107.33	105.35
39	J	102	LMU	C1-O1'-C1'	-2.02	110.48	113.84
24	C	504	CLA	CHA-C1A-NA	-2.02	121.76	126.40
24	B	515	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	B	515	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	C	505	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	B	501	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	B	514	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	J	101	BCR	C37-C22-C21	-2.02	120.09	122.92
26	C	517	BCR	C37-C22-C21	-2.02	120.10	122.92
24	B	516	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	B	510	CLA	CHA-C1A-NA	-2.01	121.79	126.40
36	D	406	PL9	O2-C1-C2	-2.01	117.17	121.78
24	B	513	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	A	406	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
24	C	502	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	B	505	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
33	C	519	DGD	C3G-O3G-C1D	-2.01	109.81	113.74
24	A	408	CLA	C1-O2A-CGA	2.01	121.71	116.44
24	C	511	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	A	406	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	C	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
33	C	518	DGD	C3G-C2G-C1G	-2.00	107.05	111.79
24	A	405	CLA	CAC-C3C-C4C	2.00	127.41	124.81
24	B	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	B	509	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	A	411	LMG	C9-C8-C7	-2.00	107.06	111.79

There are no chirality outliers.

All (987) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C1A-C2A-CAA-CBA
24	A	405	CLA	C3A-C2A-CAA-CBA
24	A	406	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	A	408	CLA	C1A-C2A-CAA-CBA
24	A	408	CLA	CHA-CBD-CGD-O1D
24	A	408	CLA	CHA-CBD-CGD-O2D
24	A	408	CLA	C2-C3-C5-C6
24	A	408	CLA	C4-C3-C5-C6
24	B	501	CLA	C2-C1-O2A-CGA
24	B	501	CLA	CHA-CBD-CGD-O2D
24	B	502	CLA	CHA-CBD-CGD-O1D
24	B	502	CLA	CHA-CBD-CGD-O2D
24	B	503	CLA	CBD-CGD-O2D-CED
24	B	504	CLA	CHA-CBD-CGD-O1D
24	B	504	CLA	CHA-CBD-CGD-O2D
24	B	504	CLA	CAD-CBD-CGD-O1D
24	B	504	CLA	C6-C7-C8-C9
24	B	505	CLA	C4-C3-C5-C6
24	B	506	CLA	CHA-CBD-CGD-O1D
24	B	506	CLA	CHA-CBD-CGD-O2D
24	B	506	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	C1A-C2A-CAA-CBA
24	B	507	CLA	C3A-C2A-CAA-CBA
24	B	507	CLA	CAD-CBD-CGD-O1D
24	B	507	CLA	CAD-CBD-CGD-O2D
24	B	508	CLA	C1A-C2A-CAA-CBA
24	B	508	CLA	C3A-C2A-CAA-CBA
24	B	508	CLA	CBD-CGD-O2D-CED
24	B	508	CLA	C2-C3-C5-C6
24	B	508	CLA	C4-C3-C5-C6
24	B	509	CLA	C1A-C2A-CAA-CBA
24	B	509	CLA	C3A-C2A-CAA-CBA
24	B	509	CLA	CHA-CBD-CGD-O1D
24	B	509	CLA	CBD-CGD-O2D-CED
24	B	509	CLA	C4-C3-C5-C6
24	B	510	CLA	CHA-CBD-CGD-O1D
24	B	510	CLA	CHA-CBD-CGD-O2D
24	B	511	CLA	CHA-CBD-CGD-O1D
24	B	511	CLA	CHA-CBD-CGD-O2D
24	B	511	CLA	CBD-CGD-O2D-CED
24	B	512	CLA	C1A-C2A-CAA-CBA
24	B	512	CLA	C3A-C2A-CAA-CBA
24	B	512	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	514	CLA	C1A-C2A-CAA-CBA
24	B	514	CLA	C3A-C2A-CAA-CBA
24	B	514	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	C2-C3-C5-C6
24	C	502	CLA	C4-C3-C5-C6
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	CHA-CBD-CGD-O1D
24	C	506	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	C2-C1-O2A-CGA
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CHA-CBD-CGD-O1D
24	C	512	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C3A-C2A-CAA-CBA
24	C	514	CLA	C2A-CAA-CBA-CGA
24	C	514	CLA	CBD-CGD-O2D-CED
24	D	401	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C3A-C2A-CAA-CBA
24	D	401	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	D	404	CLA	C1A-C2A-CAA-CBA
24	D	404	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	D	402	PHO	C3A-C2A-CAA-CBA
26	A	409	BCR	C5-C6-C7-C8
26	A	409	BCR	C11-C12-C13-C14
26	A	409	BCR	C11-C12-C13-C35
26	A	409	BCR	C17-C18-C19-C20
26	A	409	BCR	C36-C18-C19-C20
26	B	517	BCR	C11-C12-C13-C14
26	B	517	BCR	C11-C12-C13-C35
26	B	517	BCR	C17-C18-C19-C20
26	B	517	BCR	C36-C18-C19-C20
26	B	517	BCR	C21-C22-C23-C24
26	B	517	BCR	C37-C22-C23-C24
26	B	518	BCR	C7-C8-C9-C10
26	B	518	BCR	C7-C8-C9-C34
26	B	518	BCR	C9-C10-C11-C12
26	B	518	BCR	C17-C18-C19-C20
26	B	518	BCR	C36-C18-C19-C20
26	B	518	BCR	C19-C20-C21-C22
26	C	515	BCR	C7-C8-C9-C10
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C11-C12-C13-C14
26	C	515	BCR	C11-C12-C13-C35
26	C	515	BCR	C17-C18-C19-C20
26	C	516	BCR	C17-C18-C19-C20
26	C	516	BCR	C36-C18-C19-C20
26	C	516	BCR	C19-C20-C21-C22
26	C	517	BCR	C7-C8-C9-C10
26	C	517	BCR	C7-C8-C9-C34
26	D	405	BCR	C19-C20-C21-C22
26	D	405	BCR	C23-C24-C25-C30
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
27	A	410	SQD	O5-C5-C6-S
27	M	101	SQD	O5-C1-O6-C44
28	A	411	LMG	C11-C10-O7-C8
28	B	520	LMG	O9-C10-O7-C8
28	B	520	LMG	C11-C10-O7-C8
28	C	521	LMG	O7-C8-C9-O8
31	A	414	LHG	O1-C1-C2-C3
31	A	414	LHG	C4-O6-P-O3
31	A	414	LHG	C4-O6-P-O4
31	A	414	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
31	D	407	LHG	C1-C2-C3-O3
31	D	408	LHG	O1-C1-C2-O2
31	D	408	LHG	O1-C1-C2-C3
31	D	408	LHG	C1-C2-C3-O3
31	D	408	LHG	C4-O6-P-O5
31	D	410	LHG	C2-C3-O3-P
31	D	410	LHG	C3-O3-P-O4
31	L	101	LHG	O1-C1-C2-C3
31	L	101	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
32	B	519	C7Z	C21-C26-C27-C28
32	B	519	C7Z	C7-C8-C9-C19
32	B	519	C7Z	C7-C8-C9-C10
32	B	519	C7Z	C11-C12-C13-C20
32	B	519	C7Z	C11-C12-C13-C14
32	B	519	C7Z	C31-C32-C33-C34
32	B	519	C7Z	C31-C32-C33-C40
33	B	521	DGD	O6E-C1E-O5D-C6D
33	C	520	DGD	O6D-C1D-O3G-C3G
34	B	522	3PH	C1-O11-P-O14
34	B	522	3PH	C2-C1-O11-P
34	B	522	3PH	C22-C21-O21-C2
35	B	523	DGA	CB2-CB1-OG2-CG2
35	B	523	DGA	OB1-CB1-OG2-CG2
36	D	406	PL9	C37-C38-C39-C41
38	H	101	RRX	C37-C22-C23-C24
38	H	101	RRX	C21-C22-C23-C24
24	A	405	CLA	O1D-CGD-O2D-CED
24	A	405	CLA	CBD-CGD-O2D-CED
24	A	408	CLA	CBD-CGD-O2D-CED
24	B	502	CLA	CBD-CGD-O2D-CED
24	B	505	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	CBD-CGD-O2D-CED
24	B	513	CLA	CBD-CGD-O2D-CED
24	B	515	CLA	CBD-CGD-O2D-CED
24	B	516	CLA	CBD-CGD-O2D-CED
24	C	503	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	D	403	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	O1A-CGA-O2A-C1
24	D	401	CLA	O1A-CGA-O2A-C1
28	A	411	LMG	O10-C28-O8-C9
24	B	505	CLA	O1D-CGD-O2D-CED
24	B	506	CLA	O1D-CGD-O2D-CED
24	B	513	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	O1D-CGD-O2D-CED
24	B	508	CLA	O1D-CGD-O2D-CED
24	B	511	CLA	O1D-CGD-O2D-CED
24	C	504	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
24	C	512	CLA	O1D-CGD-O2D-CED
24	B	501	CLA	CBA-CGA-O2A-C1
24	B	510	CLA	CBA-CGA-O2A-C1
24	D	401	CLA	CBA-CGA-O2A-C1
28	A	411	LMG	C29-C28-O8-C9
24	B	501	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	CBD-CGD-O2D-CED
24	B	512	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CBD-CGD-O2D-CED
24	D	404	CLA	CBD-CGD-O2D-CED
24	B	501	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	O1A-CGA-O2A-C1
28	C	521	LMG	O10-C28-O8-C9
24	B	514	CLA	O1D-CGD-O2D-CED
24	C	507	CLA	O1D-CGD-O2D-CED
24	B	509	CLA	O1D-CGD-O2D-CED
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	O1D-CGD-O2D-CED
24	C	514	CLA	O1D-CGD-O2D-CED
28	A	411	LMG	O9-C10-O7-C8
28	C	521	LMG	O9-C10-O7-C8
31	D	410	LHG	O9-C7-O7-C5
34	B	522	3PH	O22-C21-O21-C2
24	A	408	CLA	C3-C5-C6-C7
24	B	502	CLA	C3-C5-C6-C7
24	B	504	CLA	C3-C5-C6-C7
24	C	505	CLA	C3-C5-C6-C7
24	C	513	CLA	C3-C5-C6-C7
25	D	402	PHO	C3-C5-C6-C7
24	B	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	C	518	DGD	C2A-C1A-O1G-C1G
34	B	522	3PH	C32-C31-O31-C3
31	D	410	LHG	C8-C7-O7-C5
24	B	502	CLA	O1D-CGD-O2D-CED
24	B	507	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	C4-C3-C5-C6
24	B	503	CLA	C2-C3-C5-C6
24	B	505	CLA	C2-C3-C5-C6
24	B	509	CLA	C2-C3-C5-C6
24	C	513	CLA	CBD-CGD-O2D-CED
24	B	506	CLA	C2A-CAA-CBA-CGA
24	C	506	CLA	C2A-CAA-CBA-CGA
28	B	520	LMG	C17-C18-C19-C20
28	C	501	LMG	C17-C18-C19-C20
28	C	521	LMG	C35-C36-C37-C38
28	C	522	LMG	C17-C18-C19-C20
28	D	409	LMG	C17-C18-C19-C20
28	H	102	LMG	C35-C36-C37-C38
28	H	102	LMG	C38-C39-C40-C41
33	C	519	DGD	CBB-CCB-CDB-CEB
24	B	515	CLA	C3-C5-C6-C7
24	B	512	CLA	CBA-CGA-O2A-C1
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1
28	B	520	LMG	C29-C28-O8-C9
28	C	521	LMG	C29-C28-O8-C9
31	D	410	LHG	C13-C14-C15-C16
24	B	515	CLA	O1D-CGD-O2D-CED
24	C	511	CLA	O1D-CGD-O2D-CED
24	D	403	CLA	O1D-CGD-O2D-CED
24	B	502	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	O1A-C1A-O1G-C1G
31	D	407	LHG	C11-C12-C13-C14
24	C	503	CLA	O1D-CGD-O2D-CED
26	A	409	BCR	C19-C20-C21-C22
26	C	515	BCR	C13-C14-C15-C16
26	C	517	BCR	C13-C14-C15-C16
24	A	406	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CBD-CGD-O2D-CED
31	A	414	LHG	O2-C2-C3-O3
24	C	510	CLA	CBA-CGA-O2A-C1
33	B	521	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
28	B	520	LMG	O10-C28-O8-C9
34	B	522	3PH	O32-C31-O31-C3
28	C	521	LMG	C11-C10-O7-C8
31	D	407	LHG	C28-C29-C30-C31
31	D	410	LHG	C11-C12-C13-C14
24	B	516	CLA	O1D-CGD-O2D-CED
24	C	513	CLA	O1A-CGA-O2A-C1
33	B	521	DGD	O1A-C1A-O1G-C1G
24	B	502	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	D	404	CLA	C4-C3-C5-C6
24	B	502	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	D	404	CLA	C2-C3-C5-C6
24	A	406	CLA	C2A-CAA-CBA-CGA
24	A	408	CLA	C2A-CAA-CBA-CGA
24	B	512	CLA	O1A-CGA-O2A-C1
36	D	406	PL9	C39-C41-C42-C43
24	C	507	CLA	CBA-CGA-O2A-C1
24	A	408	CLA	O1D-CGD-O2D-CED
27	M	101	SQD	C8-C7-O47-C45
24	B	512	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	O1D-CGD-O2D-CED
24	B	510	CLA	O1D-CGD-O2D-CED
31	D	410	LHG	C1-C2-C3-O3
31	L	101	LHG	C1-C2-C3-O3
24	C	507	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
24	A	406	CLA	CBA-CGA-O2A-C1
24	B	507	CLA	CBA-CGA-O2A-C1
24	B	510	CLA	C13-C15-C16-C17
26	B	517	BCR	C9-C10-C11-C12
24	B	515	CLA	C5-C6-C7-C8
24	B	503	CLA	C15-C16-C17-C18
24	B	513	CLA	C5-C6-C7-C8
31	D	407	LHG	O2-C2-C3-O3
31	D	408	LHG	O2-C2-C3-O3
28	C	522	LMG	C2-C1-O1-C7
33	B	521	DGD	C2E-C1E-O5D-C6D
24	A	406	CLA	C11-C12-C13-C14
24	B	503	CLA	C14-C13-C15-C16
24	B	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	511	CLA	C11-C12-C13-C14
24	B	515	CLA	C6-C7-C8-C9
24	C	502	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
25	A	407	PHO	C6-C7-C8-C9
24	B	501	CLA	O1D-CGD-O2D-CED
35	B	523	DGA	CBB-CAB-CB9-CB8
24	B	501	CLA	C8-C10-C11-C12
26	A	409	BCR	C37-C22-C23-C24
26	C	515	BCR	C36-C18-C19-C20
26	C	516	BCR	C7-C8-C9-C34
26	C	517	BCR	C36-C18-C19-C20
26	C	517	BCR	C37-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	J	101	BCR	C37-C22-C23-C24
32	B	519	C7Z	C27-C28-C29-C39
38	H	101	RRX	C7-C8-C9-C34
26	A	409	BCR	C21-C22-C23-C24
26	C	516	BCR	C7-C8-C9-C10
26	C	517	BCR	C17-C18-C19-C20
26	D	405	BCR	C21-C22-C23-C24
26	J	101	BCR	C21-C22-C23-C24
32	B	519	C7Z	C27-C28-C29-C30
38	H	101	RRX	C7-C8-C9-C10
39	J	102	LMU	O5B-C5B-C6B-O6B
28	A	415	LMG	C11-C10-O7-C8
31	A	414	LHG	C23-C24-C25-C26
24	B	507	CLA	C15-C16-C17-C18
24	B	512	CLA	C15-C16-C17-C18
24	C	507	CLA	C15-C16-C17-C18
24	B	505	CLA	C15-C16-C17-C18
24	B	508	CLA	C15-C16-C17-C18
24	B	515	CLA	C15-C16-C17-C18
24	C	502	CLA	C10-C11-C12-C13
24	D	401	CLA	C15-C16-C17-C18
28	C	522	LMG	C10-C11-C12-C13
24	B	501	CLA	C10-C11-C12-C13
24	B	502	CLA	C13-C15-C16-C17
24	B	504	CLA	C8-C10-C11-C12
24	B	508	CLA	C13-C15-C16-C17
24	B	511	CLA	C13-C15-C16-C17
24	B	514	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
31	D	407	LHG	O1-C1-C2-O2
28	B	520	LMG	C10-C11-C12-C13
31	D	410	LHG	C7-C8-C9-C10
31	L	101	LHG	C7-C8-C9-C10
35	B	523	DGA	CA1-CA2-CA3-CA4
39	J	102	LMU	C4B-C5B-C6B-O6B
24	A	405	CLA	C15-C16-C17-C18
24	B	503	CLA	C5-C6-C7-C8
24	B	510	CLA	C15-C16-C17-C18
24	B	512	CLA	C13-C15-C16-C17
24	B	513	CLA	C10-C11-C12-C13
31	L	101	LHG	C11-C10-C9-C8
27	M	101	SQD	O49-C7-O47-C45
24	B	509	CLA	C2-C1-O2A-CGA
24	B	515	CLA	C2-C1-O2A-CGA
24	B	516	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	A	408	CLA	C8-C10-C11-C12
24	B	507	CLA	C5-C6-C7-C8
31	D	410	LHG	C23-C24-C25-C26
37	E	101	HEM	C3D-CAD-CBD-CGD
24	A	408	CLA	C11-C10-C8-C7
26	A	409	BCR	C13-C14-C15-C16
26	C	515	BCR	C15-C16-C17-C18
26	C	515	BCR	C19-C20-C21-C22
26	C	517	BCR	C15-C16-C17-C18
26	C	517	BCR	C19-C20-C21-C22
24	A	405	CLA	C2A-CAA-CBA-CGA
24	C	502	CLA	C2A-CAA-CBA-CGA
24	C	508	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	C10-C11-C12-C13
24	B	511	CLA	C15-C16-C17-C18
24	A	406	CLA	O1A-CGA-O2A-C1
24	B	507	CLA	O1A-CGA-O2A-C1
24	B	508	CLA	C5-C6-C7-C8
28	D	409	LMG	C35-C36-C37-C38
31	D	410	LHG	O2-C2-C3-O3
31	L	101	LHG	O2-C2-C3-O3
28	A	415	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	D	404	CLA	C8-C10-C11-C12
24	B	510	CLA	C5-C6-C7-C8
24	B	510	CLA	C10-C11-C12-C13
24	B	511	CLA	C8-C10-C11-C12
24	C	502	CLA	C15-C16-C17-C18
24	C	511	CLA	C15-C16-C17-C18
31	D	407	LHG	C3-O3-P-O6
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	D	410	LHG	C3-O3-P-O6
31	D	410	LHG	C4-O6-P-O3
31	L	101	LHG	C23-C24-C25-C26
24	C	511	CLA	CBA-CGA-O2A-C1
36	D	406	PL9	C37-C38-C39-C40
27	M	101	SQD	C7-C8-C9-C10
24	C	513	CLA	O1D-CGD-O2D-CED
31	A	414	LHG	C1-C2-C3-O3
33	C	519	DGD	C9B-CAB-CBB-CCB
24	B	509	CLA	C5-C6-C7-C8
24	C	502	CLA	C16-C17-C18-C20
33	C	519	DGD	C2A-C1A-O1G-C1G
24	C	509	CLA	C5-C6-C7-C8
24	C	511	CLA	C13-C15-C16-C17
26	A	409	BCR	C15-C16-C17-C18
28	B	520	LMG	C28-C29-C30-C31
31	L	101	LHG	C13-C14-C15-C16
24	D	404	CLA	C3-C5-C6-C7
31	L	101	LHG	C26-C27-C28-C29
33	C	520	DGD	C2A-C3A-C4A-C5A
24	B	513	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	CBA-CGA-O2A-C1
34	B	522	3PH	C3-C2-O21-C21
35	B	523	DGA	CB1-CB2-CB3-CB4
35	B	523	DGA	CA6-CA7-CA8-CA9
39	J	102	LMU	C6-C7-C8-C9
31	A	414	LHG	O7-C5-C6-O8
34	B	522	3PH	C29-C2A-C2B-C2C
24	C	508	CLA	C8-C10-C11-C12
24	C	506	CLA	O1D-CGD-O2D-CED
31	A	414	LHG	C28-C29-C30-C31
24	B	505	CLA	C11-C12-C13-C14
24	C	512	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	506	CLA	C5-C6-C7-C8
28	D	409	LMG	C13-C14-C15-C16
31	A	414	LHG	C25-C26-C27-C28
31	D	407	LHG	C13-C14-C15-C16
33	C	519	DGD	O1A-C1A-O1G-C1G
26	B	518	BCR	C11-C12-C13-C35
26	D	405	BCR	C36-C18-C19-C20
34	B	522	3PH	C39-C3A-C3B-C3C
31	D	407	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
26	B	518	BCR	C11-C12-C13-C14
26	D	405	BCR	C17-C18-C19-C20
24	B	507	CLA	C8-C10-C11-C12
31	D	408	LHG	C7-C8-C9-C10
31	D	410	LHG	C10-C11-C12-C13
35	B	523	DGA	CB3-CB4-CB5-CB6
35	B	523	DGA	CB5-CB6-CB7-CB8
24	B	516	CLA	C6-C7-C8-C9
24	B	516	CLA	C6-C7-C8-C10
33	C	518	DGD	C2G-C1G-O1G-C1A
27	M	101	SQD	C24-C25-C26-C27
31	L	101	LHG	C11-C12-C13-C14
24	B	516	CLA	C5-C6-C7-C8
24	C	511	CLA	O1A-CGA-O2A-C1
24	C	504	CLA	CBA-CGA-O2A-C1
33	C	520	DGD	C2A-C1A-O1G-C1G
28	H	102	LMG	C16-C17-C18-C19
31	A	414	LHG	C11-C10-C9-C8
24	A	406	CLA	O1D-CGD-O2D-CED
24	B	510	CLA	C3A-C2A-CAA-CBA
34	B	522	3PH	C2B-C2C-C2D-C2E
27	A	410	SQD	C11-C10-C9-C8
31	L	101	LHG	C34-C35-C36-C37
31	A	414	LHG	C31-C32-C33-C34
25	A	407	PHO	C2-C3-C5-C6
31	D	410	LHG	C14-C15-C16-C17
31	A	414	LHG	O1-C1-C2-O2
31	L	101	LHG	O1-C1-C2-O2
31	A	414	LHG	C26-C27-C28-C29
31	D	408	LHG	C13-C14-C15-C16
35	B	523	DGA	CB9-CAB-CBB-CCB
24	B	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	D	404	CLA	O1A-CGA-O2A-C1
33	C	520	DGD	O1A-C1A-O1G-C1G
28	C	501	LMG	O9-C10-O7-C8
24	A	405	CLA	C2-C1-O2A-CGA
24	A	408	CLA	C2-C1-O2A-CGA
24	B	507	CLA	C2-C1-O2A-CGA
24	B	513	CLA	C2-C1-O2A-CGA
24	B	514	CLA	C2-C1-O2A-CGA
24	C	503	CLA	C2-C1-O2A-CGA
24	C	508	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	D	401	CLA	C2-C1-O2A-CGA
28	B	520	LMG	C11-C12-C13-C14
24	C	512	CLA	C10-C11-C12-C13
34	B	522	3PH	C3A-C3B-C3C-C3D
31	D	408	LHG	C23-C24-C25-C26
24	B	516	CLA	C3-C5-C6-C7
26	A	409	BCR	C1-C6-C7-C8
26	B	517	BCR	C23-C24-C25-C26
26	B	518	BCR	C1-C6-C7-C8
26	B	518	BCR	C23-C24-C25-C26
26	C	516	BCR	C1-C6-C7-C8
26	J	101	BCR	C5-C6-C7-C8
26	J	101	BCR	C23-C24-C25-C26
32	B	519	C7Z	C1-C6-C7-C8
32	B	519	C7Z	C25-C26-C27-C28
28	D	409	LMG	C12-C13-C14-C15
24	B	505	CLA	CBA-CGA-O2A-C1
24	A	405	CLA	C13-C15-C16-C17
24	B	513	CLA	C13-C15-C16-C17
24	C	509	CLA	C13-C15-C16-C17
28	C	501	LMG	C11-C10-O7-C8
31	A	414	LHG	C24-C25-C26-C27
31	D	408	LHG	C28-C29-C30-C31
31	D	408	LHG	C33-C34-C35-C36
24	C	504	CLA	O1A-CGA-O2A-C1
31	L	101	LHG	C33-C34-C35-C36
24	B	503	CLA	C8-C10-C11-C12
24	B	510	CLA	C8-C10-C11-C12
24	B	504	CLA	C4-C3-C5-C6
25	A	407	PHO	C4-C3-C5-C6
24	A	405	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	B	503	CLA	C6-C7-C8-C10
24	B	505	CLA	C11-C12-C13-C15
24	B	515	CLA	C6-C7-C8-C10
24	C	502	CLA	C11-C10-C8-C7
24	C	512	CLA	C6-C7-C8-C10
25	A	407	PHO	C11-C10-C8-C7
24	C	508	CLA	C13-C15-C16-C17
24	D	401	CLA	C8-C10-C11-C12
34	B	522	3PH	C31-C32-C33-C34
24	B	516	CLA	CBA-CGA-O2A-C1
24	B	512	CLA	C10-C11-C12-C13
24	C	508	CLA	C15-C16-C17-C18
33	B	521	DGD	C3A-C4A-C5A-C6A
31	D	408	LHG	C9-C10-C11-C12
31	D	408	LHG	C34-C35-C36-C37
33	C	519	DGD	CCB-CDB-CEB-CFB
24	B	509	CLA	C8-C10-C11-C12
24	C	503	CLA	C8-C10-C11-C12
31	D	408	LHG	C11-C12-C13-C14
24	C	508	CLA	C5-C6-C7-C8
28	H	102	LMG	C33-C34-C35-C36
24	B	501	CLA	C13-C15-C16-C17
27	M	101	SQD	C2-C1-O6-C44
24	B	505	CLA	C8-C10-C11-C12
27	A	410	SQD	C28-C29-C30-C31
24	A	405	CLA	C11-C12-C13-C14
24	A	408	CLA	C11-C10-C8-C9
24	B	503	CLA	C6-C7-C8-C9
24	B	513	CLA	C11-C12-C13-C14
24	C	502	CLA	C6-C7-C8-C9
24	C	509	CLA	C11-C12-C13-C14
24	C	511	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C10-C8-C9
24	D	401	CLA	C14-C13-C15-C16
25	A	407	PHO	C11-C10-C8-C9
33	B	521	DGD	C2A-C3A-C4A-C5A
24	C	507	CLA	C3-C5-C6-C7
24	B	502	CLA	C2A-CAA-CBA-CGA
24	D	404	CLA	C2A-CAA-CBA-CGA
24	B	505	CLA	O1A-CGA-O2A-C1
24	B	504	CLA	C1A-C2A-CAA-CBA
24	B	510	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C16-C17-C18-C19
31	D	407	LHG	C27-C28-C29-C30
24	B	503	CLA	C13-C15-C16-C17
33	C	519	DGD	C3A-C4A-C5A-C6A
24	B	504	CLA	C10-C11-C12-C13
31	D	407	LHG	C7-C8-C9-C10
31	L	101	LHG	C31-C32-C33-C34
34	B	522	3PH	C27-C28-C29-C2A
35	B	523	DGA	CAB-CBB-CCB-CDB
31	A	414	LHG	C33-C34-C35-C36
35	B	523	DGA	CA2-CA3-CA4-CA5
24	C	504	CLA	C8-C10-C11-C12
24	C	509	CLA	C8-C10-C11-C12
31	D	407	LHG	C4-C5-C6-O8
33	C	520	DGD	O6E-C5E-C6E-O5E
24	D	401	CLA	C13-C15-C16-C17
28	A	415	LMG	C8-C7-O1-C1
33	C	519	DGD	C5D-C6D-O5D-C1E
31	D	408	LHG	C11-C10-C9-C8
24	B	516	CLA	O1A-CGA-O2A-C1
28	C	522	LMG	O6-C1-O1-C7
27	A	410	SQD	C24-C25-C26-C27
28	D	409	LMG	O6-C5-C6-O5
33	C	519	DGD	O6D-C5D-C6D-O5D
36	D	406	PL9	C40-C39-C41-C42
24	C	505	CLA	CBA-CGA-O2A-C1
24	C	512	CLA	CBA-CGA-O2A-C1
24	B	502	CLA	C15-C16-C17-C18
24	B	507	CLA	C13-C15-C16-C17
31	D	410	LHG	C17-C18-C19-C20
27	M	101	SQD	C46-C45-O47-C7
33	C	518	DGD	O6E-C5E-C6E-O5E
24	B	503	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	C2A-CAA-CBA-CGA
24	B	514	CLA	C15-C16-C17-C18
31	A	414	LHG	C34-C35-C36-C37
24	C	502	CLA	CBA-CGA-O2A-C1
24	A	405	CLA	C16-C17-C18-C19
24	C	502	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	B	501	CLA	C5-C6-C7-C8
33	B	521	DGD	C2D-C1D-O3G-C3G
33	C	520	DGD	C2D-C1D-O3G-C3G
31	D	410	LHG	C18-C19-C20-C21
33	C	519	DGD	O1G-C1G-C2G-O2G
24	A	406	CLA	C11-C10-C8-C7
24	B	503	CLA	C11-C12-C13-C15
24	B	504	CLA	C2-C3-C5-C6
24	B	504	CLA	C6-C7-C8-C10
24	B	504	CLA	C11-C10-C8-C7
24	B	513	CLA	C11-C10-C8-C7
24	B	513	CLA	C11-C12-C13-C15
24	C	502	CLA	C6-C7-C8-C10
24	C	509	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	C	511	CLA	C11-C10-C8-C7
24	C	511	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	D	401	CLA	C12-C13-C15-C16
24	D	403	CLA	C11-C12-C13-C15
25	A	407	PHO	C3-C5-C6-C7
24	B	507	CLA	C14-C13-C15-C16
24	B	513	CLA	C11-C10-C8-C9
24	B	514	CLA	C6-C7-C8-C9
24	C	511	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C12-C13-C14
31	D	407	LHG	C23-C24-C25-C26
24	B	515	CLA	C8-C10-C11-C12
26	B	517	BCR	C7-C8-C9-C34
26	B	518	BCR	C37-C22-C23-C24
26	B	517	BCR	C7-C8-C9-C10
26	B	518	BCR	C21-C22-C23-C24
26	C	517	BCR	C21-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C10
31	A	414	LHG	C30-C31-C32-C33
34	B	522	3PH	C25-C26-C27-C28
24	C	508	CLA	C4B-C3B-CAB-CBB
24	B	507	CLA	C16-C17-C18-C20
24	C	512	CLA	C3-C5-C6-C7
24	B	515	CLA	C13-C15-C16-C17
24	C	510	CLA	C13-C15-C16-C17
24	C	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	503	CLA	CBA-CGA-O2A-C1
24	B	514	CLA	CAA-CBA-CGA-O2A
24	C	507	CLA	C3A-C2A-CAA-CBA
26	C	516	BCR	C9-C10-C11-C12
24	B	511	CLA	C5-C6-C7-C8
31	A	414	LHG	C24-C23-O8-C6
28	A	411	LMG	O1-C7-C8-C9
28	C	521	LMG	C7-C8-C9-O8
28	H	102	LMG	C7-C8-C9-O8
31	A	414	LHG	C4-C5-C6-O8
31	D	408	LHG	C4-C5-C6-O8
33	B	521	DGD	C1G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-CG3
24	C	512	CLA	O1A-CGA-O2A-C1
33	C	520	DGD	O6D-C5D-C6D-O5D
24	B	504	CLA	C5-C6-C7-C8
31	D	410	LHG	O6-C4-C5-O7
24	B	511	CLA	CBA-CGA-O2A-C1
24	B	515	CLA	CBA-CGA-O2A-C1
35	B	523	DGA	CBB-CCB-CDB-CEB
28	A	411	LMG	O1-C7-C8-O7
28	H	102	LMG	O7-C8-C9-O8
31	D	407	LHG	C35-C36-C37-C38
34	B	522	3PH	C24-C25-C26-C27
35	B	523	DGA	CG1-CG2-CG3-OXT
24	B	503	CLA	C2-C1-O2A-CGA
25	A	407	PHO	C13-C15-C16-C17
24	B	515	CLA	C11-C12-C13-C14
24	C	503	CLA	C14-C13-C15-C16
28	C	522	LMG	C15-C16-C17-C18
31	D	408	LHG	C19-C20-C21-C22
25	D	402	PHO	C2A-CAA-CBA-CGA
24	B	514	CLA	C3-C5-C6-C7
26	C	515	BCR	C23-C24-C25-C30
26	C	516	BCR	C5-C6-C7-C8
26	D	405	BCR	C5-C6-C7-C8
25	A	407	PHO	C10-C11-C12-C13
31	D	408	LHG	C25-C26-C27-C28
33	C	519	DGD	C6B-C7B-C8B-C9B
35	B	523	DGA	CB7-CB8-CB9-CAB
24	A	405	CLA	C8-C10-C11-C12
39	J	102	LMU	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C16-C17-C18-C20
24	C	504	CLA	C16-C17-C18-C19
31	A	414	LHG	O6-C4-C5-C6
31	D	407	LHG	O6-C4-C5-C6
24	B	507	CLA	C12-C13-C15-C16
24	B	508	CLA	C6-C7-C8-C10
24	B	508	CLA	C11-C12-C13-C15
24	B	514	CLA	C6-C7-C8-C10
24	B	515	CLA	C11-C12-C13-C15
24	C	503	CLA	C12-C13-C15-C16
35	B	523	DGA	OG2-CG2-CG3-OXT
32	B	519	C7Z	C9-C10-C11-C12
34	B	522	3PH	C1-O11-P-O13
24	B	513	CLA	C3-C5-C6-C7
24	B	507	CLA	C16-C17-C18-C19
28	H	102	LMG	C36-C37-C38-C39
33	C	518	DGD	C1B-C2B-C3B-C4B
24	B	514	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
35	B	523	DGA	CG1-CG2-OG2-CB1
24	C	508	CLA	C16-C17-C18-C19
28	H	102	LMG	C32-C33-C34-C35
31	D	407	LHG	C31-C32-C33-C34
28	A	415	LMG	O6-C1-O1-C7
31	D	407	LHG	C34-C35-C36-C37
31	A	414	LHG	O6-C4-C5-O7
31	D	407	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
34	B	522	3PH	C32-C33-C34-C35
24	B	501	CLA	CHA-CBD-CGD-O1D
24	B	505	CLA	CHA-CBD-CGD-O1D
24	B	509	CLA	CHA-CBD-CGD-O2D
24	B	512	CLA	CHA-CBD-CGD-O1D
24	B	512	CLA	CHA-CBD-CGD-O2D
24	B	513	CLA	CHA-CBD-CGD-O1D
34	B	522	3PH	C2A-C2B-C2C-C2D
24	B	503	CLA	O1A-CGA-O2A-C1
31	D	407	LHG	O7-C5-C6-O8
31	L	101	LHG	O7-C5-C6-O8
24	B	515	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C10-C11-C12-C13
24	C	503	CLA	C3-C5-C6-C7
24	B	511	CLA	O1A-CGA-O2A-C1
31	A	414	LHG	O10-C23-O8-C6
33	B	521	DGD	O1B-C1B-O2G-C2G
33	C	520	DGD	O1B-C1B-O2G-C2G
24	B	501	CLA	C11-C12-C13-C14
24	B	508	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C12-C13-C14
24	D	401	CLA	C2A-CAA-CBA-CGA
26	C	515	BCR	C37-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C34
26	C	515	BCR	C21-C22-C23-C24
24	C	507	CLA	C1A-C2A-CAA-CBA
24	B	503	CLA	C16-C17-C18-C19
24	C	512	CLA	C2-C1-O2A-CGA
26	D	405	BCR	C9-C10-C11-C12
31	D	407	LHG	C4-O6-P-O3
31	A	414	LHG	C2-C3-O3-P
24	B	516	CLA	C4B-C3B-CAB-CBB
24	C	513	CLA	C4B-C3B-CAB-CBB
31	D	407	LHG	C3-O3-P-O5
31	D	408	LHG	C3-O3-P-O5
31	D	408	LHG	C4-O6-P-O4
31	D	410	LHG	C4-O6-P-O5
24	C	510	CLA	C8-C10-C11-C12
24	B	509	CLA	CBA-CGA-O2A-C1
31	D	410	LHG	O6-C4-C5-C6
31	L	101	LHG	O6-C4-C5-C6
24	B	505	CLA	CAD-CBD-CGD-O1D
24	B	509	CLA	CAD-CBD-CGD-O1D
24	B	512	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
27	M	101	SQD	C5-C6-S-O9
24	B	502	CLA	CAA-CBA-CGA-O2A
28	H	102	LMG	O7-C10-C11-C12
24	D	401	CLA	C3-C5-C6-C7
24	C	504	CLA	C16-C17-C18-C20
24	B	503	CLA	C12-C13-C15-C16
24	B	507	CLA	C6-C7-C8-C10
24	B	510	CLA	C12-C13-C15-C16
24	B	515	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	D	401	CLA	C11-C12-C13-C15
33	B	521	DGD	C1A-C2A-C3A-C4A
33	B	521	DGD	C2B-C1B-O2G-C2G
31	L	101	LHG	O8-C23-C24-C25
35	B	523	DGA	CB2-CB3-CB4-CB5
31	D	408	LHG	O7-C5-C6-O8
33	B	521	DGD	O2G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-OG2
33	B	521	DGD	C2G-C3G-O3G-C1D
24	B	509	CLA	O1A-CGA-O2A-C1
28	C	501	LMG	C29-C28-O8-C9
24	A	406	CLA	C11-C10-C8-C9
24	B	504	CLA	C11-C10-C8-C9
24	B	508	CLA	C6-C7-C8-C9
24	B	514	CLA	C14-C13-C15-C16
24	D	403	CLA	C14-C13-C15-C16
28	C	501	LMG	O10-C28-O8-C9
24	B	510	CLA	C16-C17-C18-C19
35	B	523	DGA	CB6-CB7-CB8-CB9
28	A	411	LMG	C28-C29-C30-C31
24	B	516	CLA	CAA-CBA-CGA-O2A
24	C	509	CLA	C3-C5-C6-C7
24	C	507	CLA	C16-C17-C18-C20
31	L	101	LHG	C28-C29-C30-C31
24	B	516	CLA	C2B-C3B-CAB-CBB
24	C	508	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	D	404	CLA	C2B-C3B-CAB-CBB
24	B	505	CLA	C16-C17-C18-C20
28	D	409	LMG	C31-C32-C33-C34
24	B	514	CLA	C10-C11-C12-C13
28	B	520	LMG	C9-C8-O7-C10
24	B	510	CLA	C2-C1-O2A-CGA
24	B	511	CLA	C2-C1-O2A-CGA
27	M	101	SQD	C23-C24-C25-C26
24	A	405	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	C10-C11-C12-C13
34	B	522	3PH	C1-O11-P-O12
24	C	509	CLA	CBA-CGA-O2A-C1
31	D	410	LHG	C9-C10-C11-C12
31	D	407	LHG	C26-C27-C28-C29
24	C	503	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
33	C	519	DGD	C2D-C1D-O3G-C3G
39	J	102	LMU	C1-C2-C3-C4
24	B	511	CLA	C10-C11-C12-C13
31	D	407	LHG	C9-C10-C11-C12
31	A	414	LHG	C3-O3-P-O6
25	D	402	PHO	CHA-CBD-CGD-O2D
33	C	519	DGD	O1G-C1G-C2G-C3G
33	C	519	DGD	C4D-C5D-C6D-O5D
24	B	501	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	B	503	CLA	C11-C12-C13-C14
24	D	401	CLA	C11-C12-C13-C14
33	C	520	DGD	C2B-C1B-O2G-C2G
24	A	406	CLA	C10-C11-C12-C13
24	B	503	CLA	C3-C5-C6-C7
31	D	410	LHG	C25-C26-C27-C28
34	B	522	3PH	C28-C29-C2A-C2B
31	D	410	LHG	O1-C1-C2-O2
35	B	523	DGA	CA5-CA6-CA7-CA8
39	J	102	LMU	C5-C6-C7-C8
24	C	509	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	C4B-C3B-CAB-CBB
26	J	101	BCR	C9-C10-C11-C12
26	J	101	BCR	C15-C16-C17-C18
38	H	101	RRX	C15-C16-C17-C18
27	M	101	SQD	C25-C26-C27-C28
24	D	401	CLA	C16-C17-C18-C19
24	B	513	CLA	C4-C3-C5-C6
36	D	406	PL9	C30-C29-C31-C32
36	D	406	PL9	C13-C14-C16-C17
28	C	522	LMG	O9-C10-O7-C8
31	L	101	LHG	C9-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
35	B	523	DGA	CA9-CAA-CBA-CCA
24	B	507	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	B	510	CLA	C16-C17-C18-C20
26	A	409	BCR	C11-C10-C9-C34
31	L	101	LHG	C4-C5-C6-O8
24	B	511	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C24-C25-C26-C27
24	B	503	CLA	C1A-C2A-CAA-CBA
24	B	506	CLA	C6-C7-C8-C10
25	A	407	PHO	C6-C7-C8-C10
25	D	402	PHO	C6-C7-C8-C10
24	B	504	CLA	O1A-CGA-O2A-C1
27	M	101	SQD	O47-C7-C8-C9
24	C	503	CLA	C13-C15-C16-C17
24	D	401	CLA	C5-C6-C7-C8
24	B	515	CLA	C2B-C3B-CAB-CBB
34	B	522	3PH	C2C-C2D-C2E-C2F
24	B	514	CLA	C16-C17-C18-C20
26	A	409	BCR	C11-C10-C9-C8
28	H	102	LMG	C30-C31-C32-C33
24	C	503	CLA	C16-C17-C18-C19
28	D	409	LMG	C11-C12-C13-C14
36	D	406	PL9	C38-C39-C41-C42
31	L	101	LHG	C35-C36-C37-C38
24	C	502	CLA	C11-C12-C13-C14
24	B	501	CLA	C3-C5-C6-C7
31	L	101	LHG	C2-C3-O3-P
24	D	403	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	C30-C31-C32-C33
26	C	517	BCR	C23-C24-C25-C30
26	J	101	BCR	C13-C14-C15-C16
24	C	511	CLA	C2-C3-C5-C6
24	B	504	CLA	CBA-CGA-O2A-C1
24	B	515	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
31	D	407	LHG	C12-C13-C14-C15
26	C	515	BCR	C9-C10-C11-C12
24	B	514	CLA	CAA-CBA-CGA-O1A
24	D	403	CLA	C15-C16-C17-C18
24	A	408	CLA	C11-C12-C13-C15
24	C	514	CLA	CAA-CBA-CGA-O2A
24	C	503	CLA	C4-C3-C5-C6
28	C	501	LMG	C31-C32-C33-C34
34	B	522	3PH	O21-C21-C22-C23
24	B	501	CLA	C14-C13-C15-C16
24	B	502	CLA	C14-C13-C15-C16
24	B	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	506	CLA	C6-C7-C8-C9
24	B	515	CLA	C11-C10-C8-C9
25	D	402	PHO	C6-C7-C8-C9
24	A	406	CLA	C3A-C2A-CAA-CBA
24	B	504	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	509	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
38	H	101	RRX	C19-C20-C21-C22
24	C	504	CLA	C2-C1-O2A-CGA
31	D	408	LHG	C30-C31-C32-C33
24	B	511	CLA	C4-C3-C5-C6
24	B	513	CLA	C16-C17-C18-C20
28	C	521	LMG	O7-C10-C11-C12
27	A	410	SQD	C10-C11-C12-C13
24	C	514	CLA	CAA-CBA-CGA-O1A
25	A	407	PHO	O2A-C1-C2-C3
24	B	512	CLA	C8-C10-C11-C12
24	B	507	CLA	CAA-CBA-CGA-O2A
33	C	519	DGD	O2G-C1B-C2B-C3B
24	D	401	CLA	C16-C17-C18-C20
24	B	505	CLA	CHA-CBD-CGD-O2D
24	B	507	CLA	CHA-CBD-CGD-O1D
24	B	507	CLA	CHA-CBD-CGD-O2D
24	B	513	CLA	CHA-CBD-CGD-O2D
24	B	515	CLA	CHA-CBD-CGD-O1D
24	B	515	CLA	CHA-CBD-CGD-O2D
24	B	516	CLA	CHA-CBD-CGD-O1D
24	B	516	CLA	CHA-CBD-CGD-O2D
24	D	403	CLA	CHA-CBD-CGD-O2D
26	B	518	BCR	C15-C16-C17-C18
24	C	511	CLA	C4-C3-C5-C6
28	A	411	LMG	C31-C32-C33-C34
31	D	408	LHG	C32-C33-C34-C35
27	A	410	SQD	C25-C26-C27-C28
24	C	506	CLA	CAA-CBA-CGA-O2A
25	A	407	PHO	CHA-CBD-CGD-O1D
25	D	402	PHO	CHA-CBD-CGD-O1D
31	D	410	LHG	C24-C23-O8-C6
28	C	501	LMG	O7-C10-C11-C12
35	B	523	DGA	CA7-CA8-CA9-CAA

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C2-C3-O3-P
33	C	519	DGD	O1B-C1B-C2B-C3B
27	M	101	SQD	C4-C5-C6-S
27	M	101	SQD	C5-C6-S-O8
24	C	509	CLA	CAA-CBA-CGA-O2A
24	C	513	CLA	CAA-CBA-CGA-O2A
34	B	522	3PH	O22-C21-C22-C23
28	H	102	LMG	C12-C13-C14-C15
24	C	511	CLA	C16-C17-C18-C20
28	C	521	LMG	O9-C10-C11-C12
28	C	501	LMG	C16-C17-C18-C19
24	B	514	CLA	C2A-CAA-CBA-CGA
36	D	406	PL9	C15-C14-C16-C17
34	B	522	3PH	O31-C31-C32-C33
28	H	102	LMG	C40-C41-C42-C43
24	D	403	CLA	C4B-C3B-CAB-CBB
31	A	414	LHG	C3-O3-P-O5
28	C	522	LMG	C11-C10-O7-C8
28	C	522	LMG	O7-C10-C11-C12
26	C	516	BCR	C23-C24-C25-C30
35	B	523	DGA	CA4-CA5-CA6-CA7
24	B	504	CLA	CAA-CBA-CGA-O2A
24	B	509	CLA	CAA-CBA-CGA-O2A
24	B	516	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	CAA-CBA-CGA-O1A
24	D	403	CLA	CAD-CBD-CGD-O1D
27	M	101	SQD	O5-C5-C6-S
24	C	506	CLA	CAA-CBA-CGA-O1A
24	C	509	CLA	CAA-CBA-CGA-O1A
24	C	504	CLA	CAA-CBA-CGA-O2A
24	B	510	CLA	C11-C12-C13-C14
24	C	509	CLA	C14-C13-C15-C16
24	D	401	CLA	C11-C10-C8-C9
24	D	403	CLA	C6-C7-C8-C9
24	D	403	CLA	C11-C10-C8-C9
31	D	408	LHG	C15-C16-C17-C18
37	E	101	HEM	CAA-CBA-CGA-O2A
28	H	102	LMG	C14-C15-C16-C17
24	B	508	CLA	CAA-CBA-CGA-O2A
24	D	404	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O7-C10-C11-C12
24	C	513	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	B	501	CLA	C11-C12-C13-C15
24	B	511	CLA	C11-C12-C13-C15
24	B	513	CLA	C2-C3-C5-C6
24	C	510	CLA	C6-C7-C8-C10
24	D	401	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
27	A	410	SQD	O47-C7-C8-C9
33	B	521	DGD	O2G-C1B-C2B-C3B
33	C	518	DGD	O2G-C1B-C2B-C3B
27	A	410	SQD	O49-C7-C8-C9
34	B	522	3PH	O32-C31-C32-C33
33	C	519	DGD	O6D-C1D-O3G-C3G
25	A	407	PHO	C15-C16-C17-C18
24	C	504	CLA	CAA-CBA-CGA-O1A
24	B	508	CLA	CAA-CBA-CGA-O1A
24	B	512	CLA	C2A-CAA-CBA-CGA
24	D	403	CLA	C4-C3-C5-C6
24	C	505	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

70 monomers are involved in 245 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	408	CLA	8	0
24	B	501	CLA	4	0
24	B	508	CLA	9	0
24	C	503	CLA	2	0
24	C	509	CLA	7	0
36	D	406	PL9	1	0
24	C	506	CLA	3	0
24	B	503	CLA	9	0
28	H	102	LMG	5	0
24	B	509	CLA	3	0
31	D	408	LHG	4	0
24	C	505	CLA	1	0
28	C	521	LMG	1	0
24	C	513	CLA	1	0
25	D	402	PHO	5	0
26	B	518	BCR	1	0
26	B	517	BCR	5	0
28	A	411	LMG	1	0
24	B	515	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	101	HEM	2	0
24	C	511	CLA	5	0
24	D	404	CLA	8	0
24	C	512	CLA	7	0
24	A	406	CLA	4	0
28	B	520	LMG	2	0
28	C	522	LMG	2	0
24	B	512	CLA	5	0
24	C	504	CLA	4	0
28	C	501	LMG	4	0
33	C	520	DGD	2	0
26	J	101	BCR	2	0
28	D	409	LMG	1	0
24	B	511	CLA	8	0
24	D	403	CLA	6	0
24	B	506	CLA	2	0
24	B	510	CLA	5	0
26	D	405	BCR	1	0
31	L	101	LHG	1	0
32	B	519	C7Z	3	0
33	C	519	DGD	4	0
39	J	102	LMU	4	0
31	D	410	LHG	5	0
24	B	516	CLA	4	0
25	A	407	PHO	5	0
27	M	101	SQD	4	0
33	C	518	DGD	1	0
31	A	414	LHG	3	0
24	B	505	CLA	6	0
26	C	516	BCR	5	0
24	D	401	CLA	6	0
26	C	517	BCR	2	0
34	B	522	3PH	4	0
24	A	405	CLA	4	0
35	B	523	DGA	3	0
24	C	514	CLA	2	0
24	B	513	CLA	6	0
38	H	101	RRX	6	0
24	B	504	CLA	9	0
24	B	514	CLA	6	0
33	B	521	DGD	2	0
24	B	507	CLA	5	0

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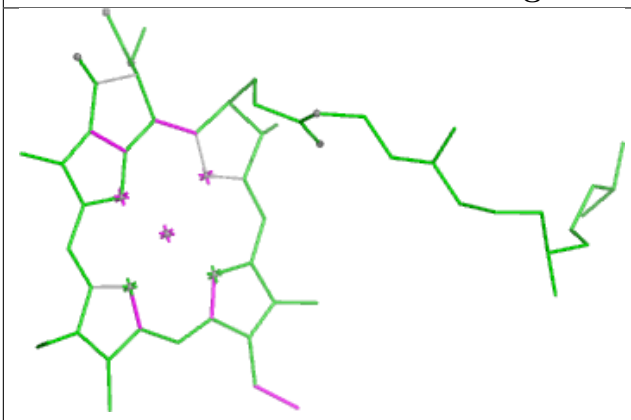
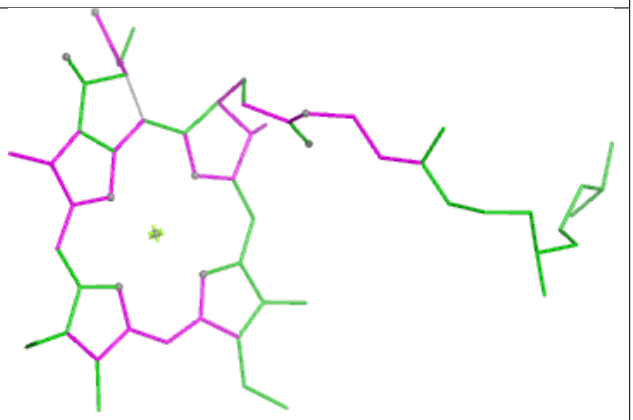
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	502	CLA	5	0
28	A	415	LMG	4	0
24	C	508	CLA	6	0
26	C	515	BCR	2	0
24	C	507	CLA	8	0
31	D	407	LHG	2	0
24	B	502	CLA	8	0
24	C	510	CLA	6	0
26	A	409	BCR	5	0

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.

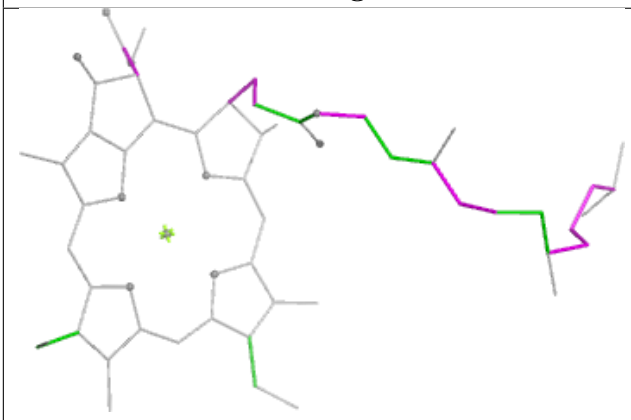
Ligand CLA A 408



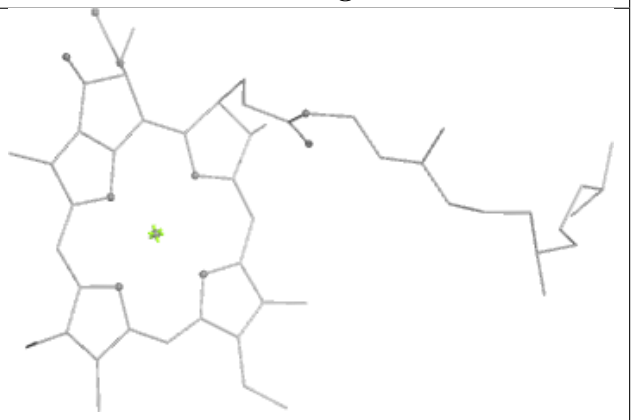
Bond lengths



Bond angles

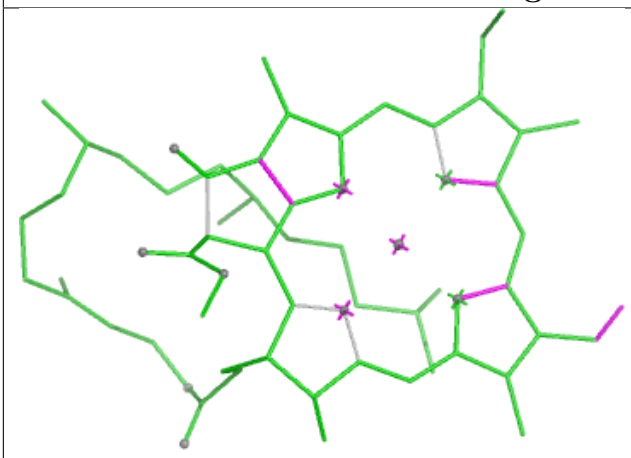


Torsions

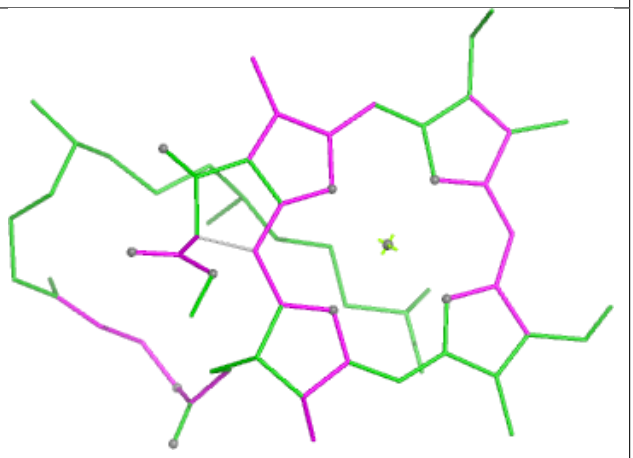


Rings

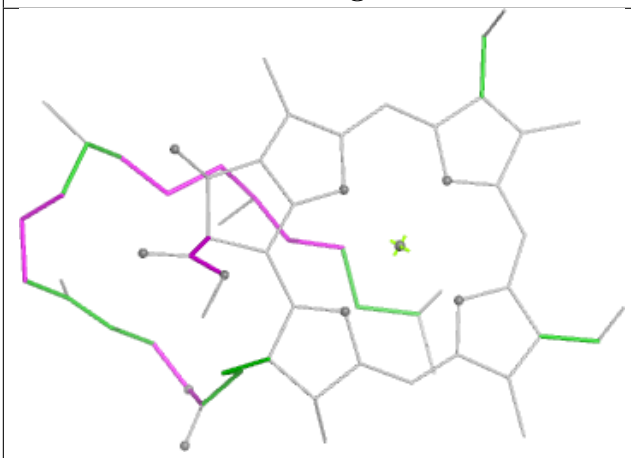
Ligand CLA B 501



Bond lengths



Bond angles



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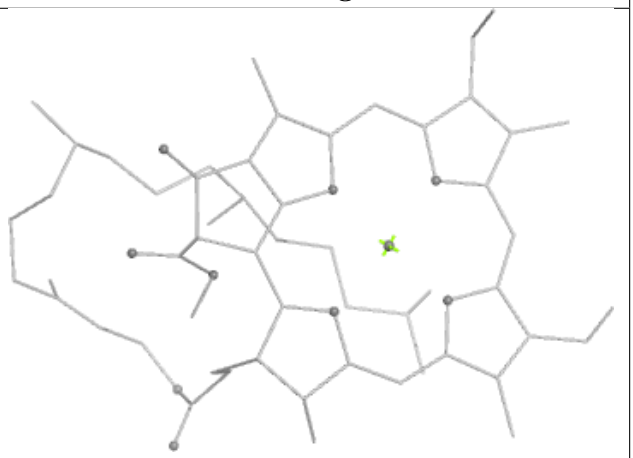
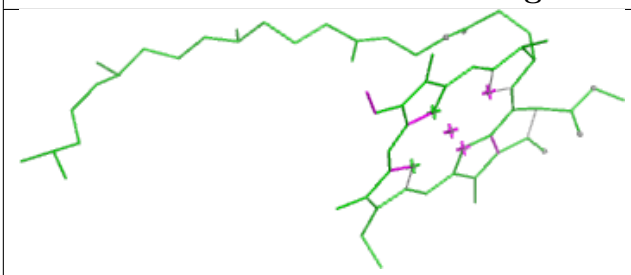


Rings

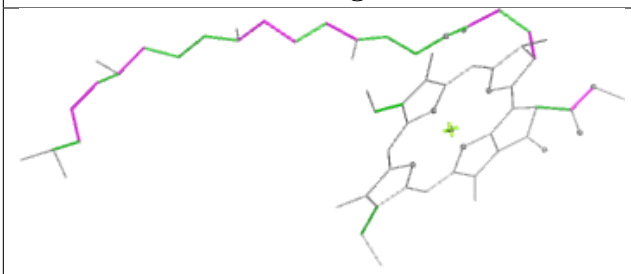
Ligand CLA B 508



Bond lengths



Bond angles

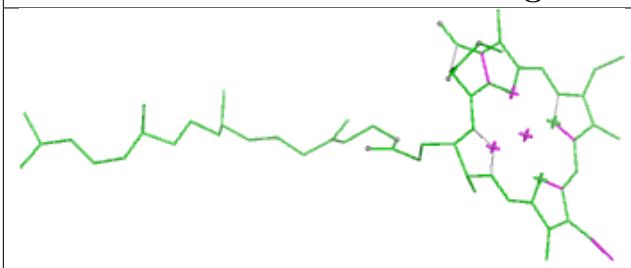


Torsions

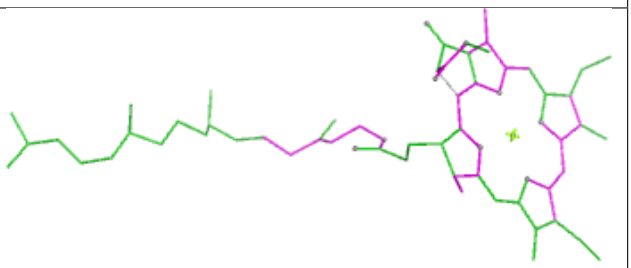


Rings

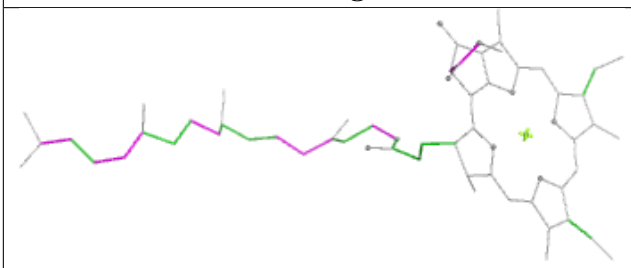
Ligand CLA C 503



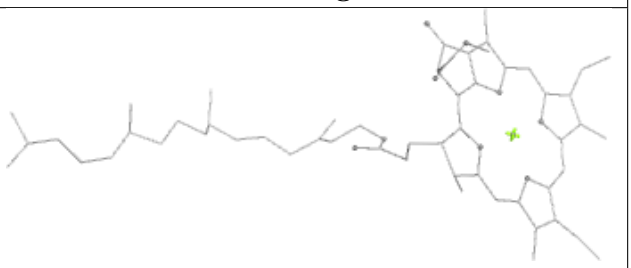
Bond lengths



Bond angles

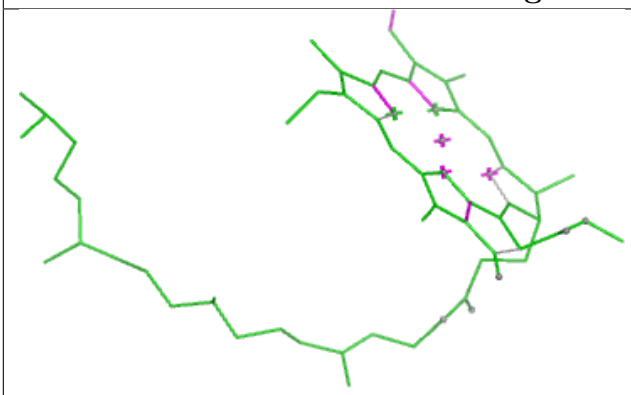


Torsions

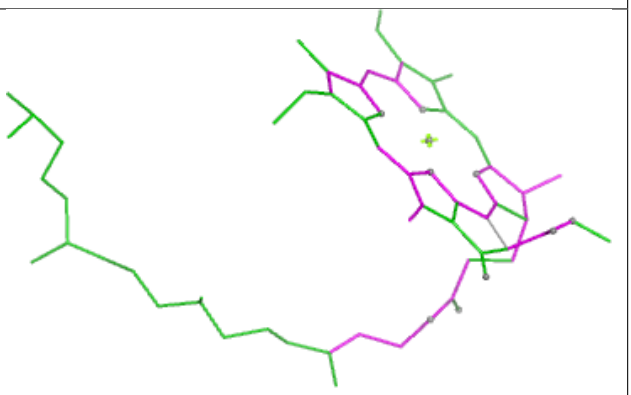


Rings

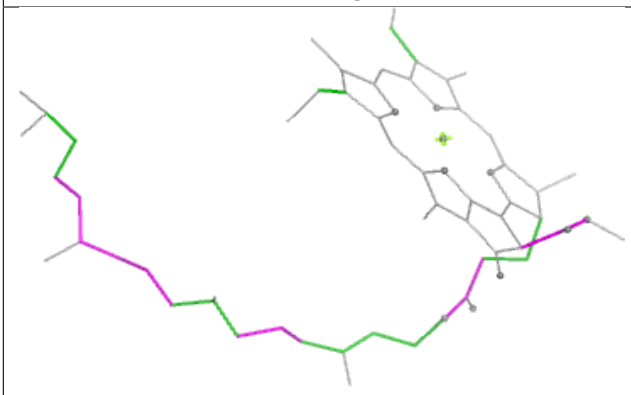
Ligand CLA C 509



Bond lengths



Bond angles

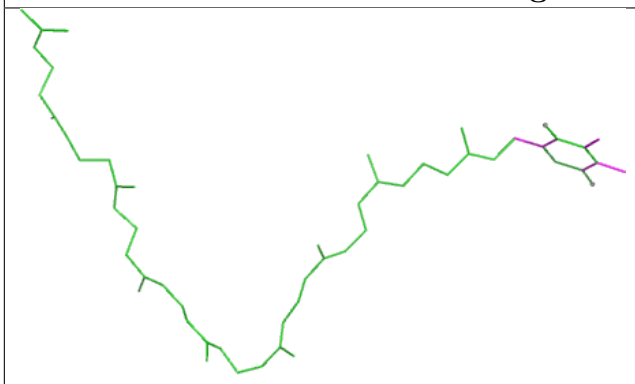


Torsions

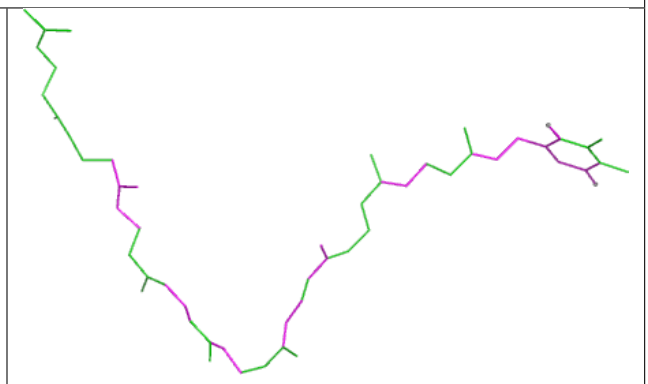


Rings

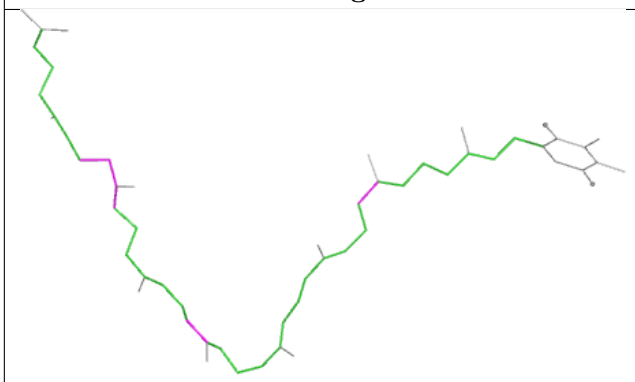
Ligand PL9 D 406



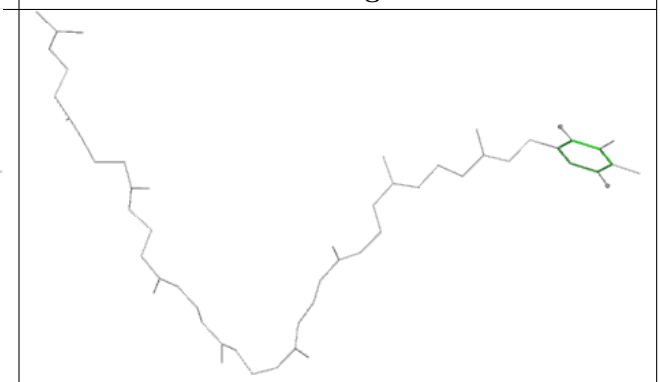
Bond lengths



Bond angles

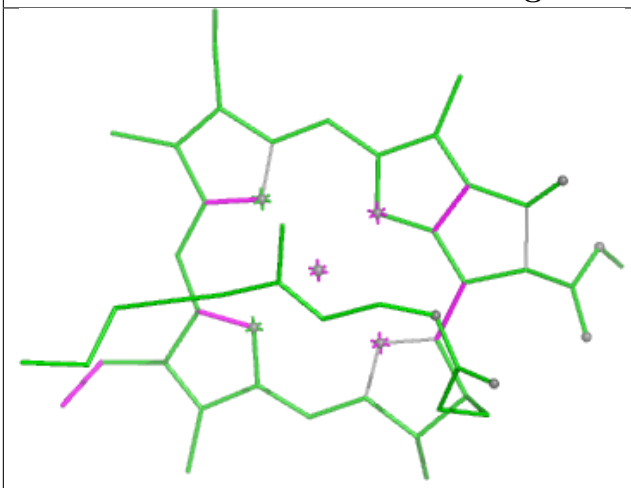


Torsions

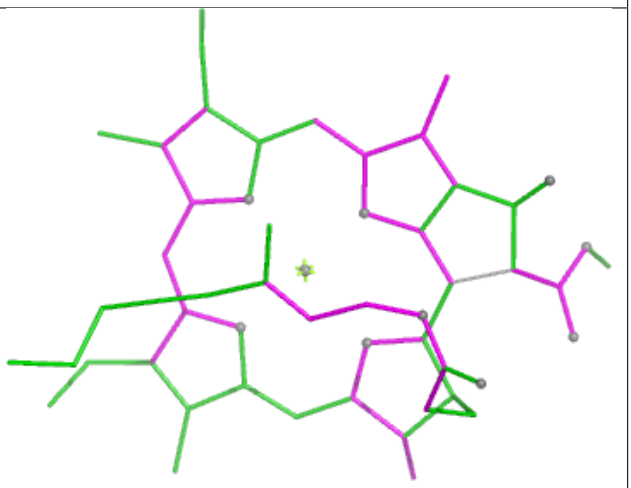


Rings

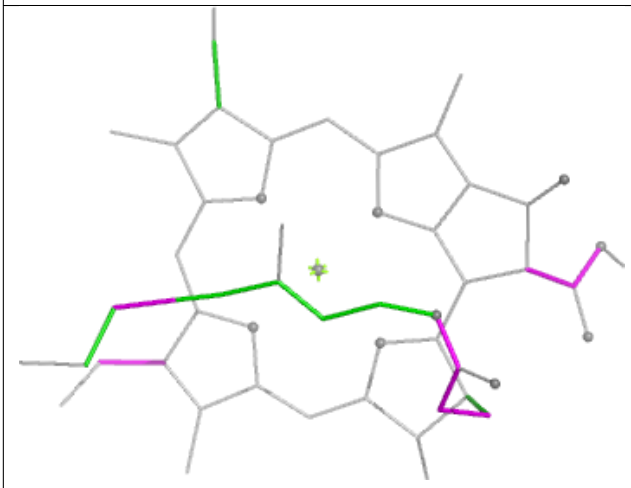
Ligand CLA C 506



Bond lengths



Bond angles



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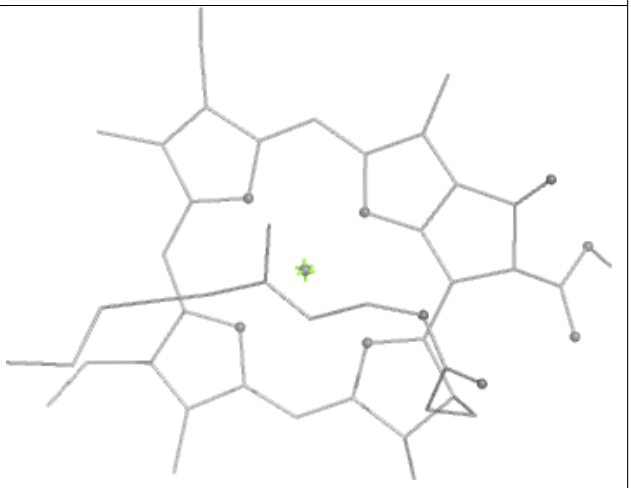
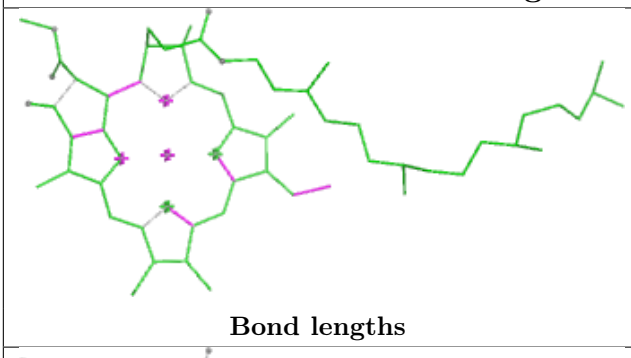


Rings

Ligand CLA B 503



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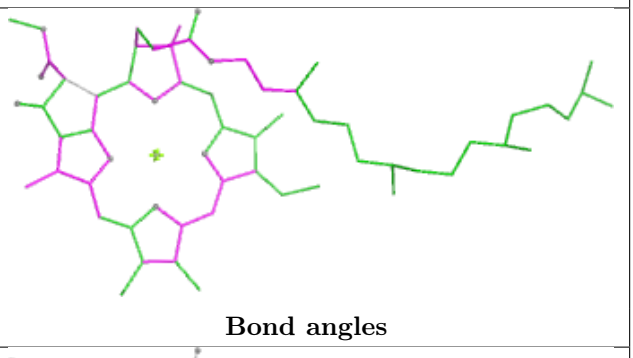
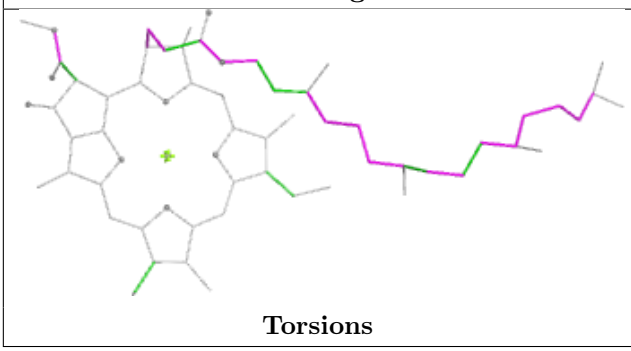


Bond angles



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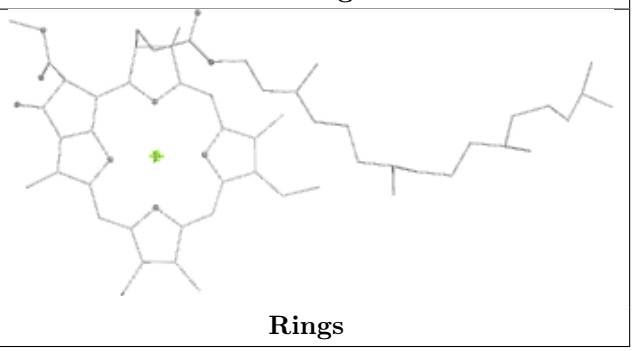
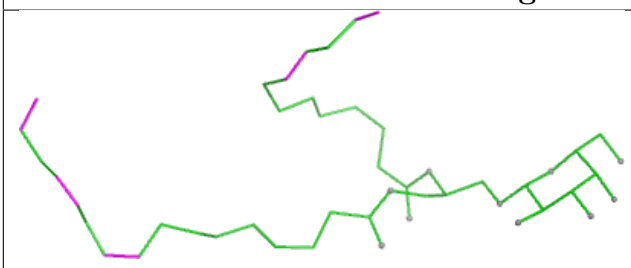


Rings

Ligand LMG H 102



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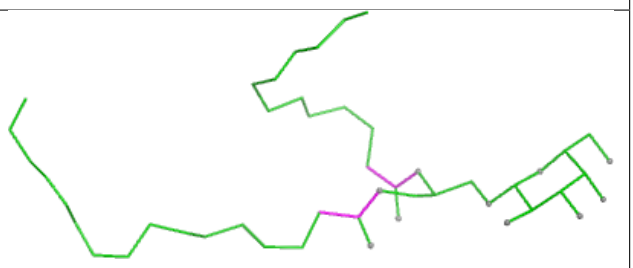
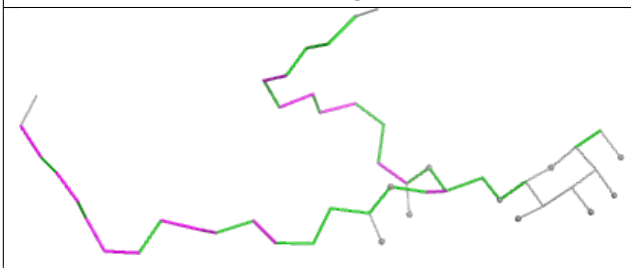


Bond angles



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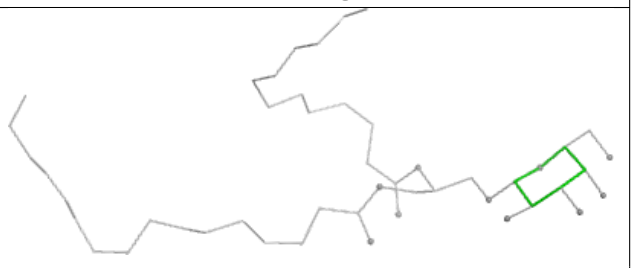
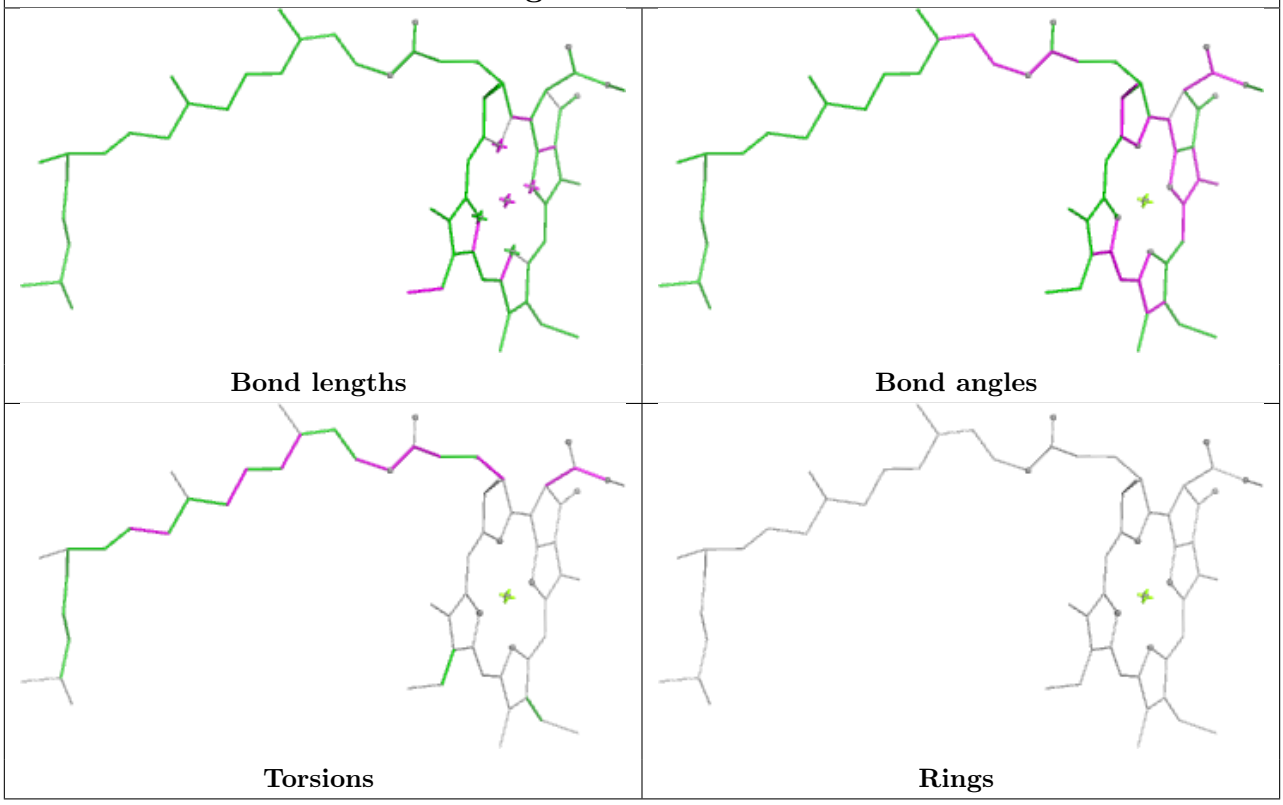
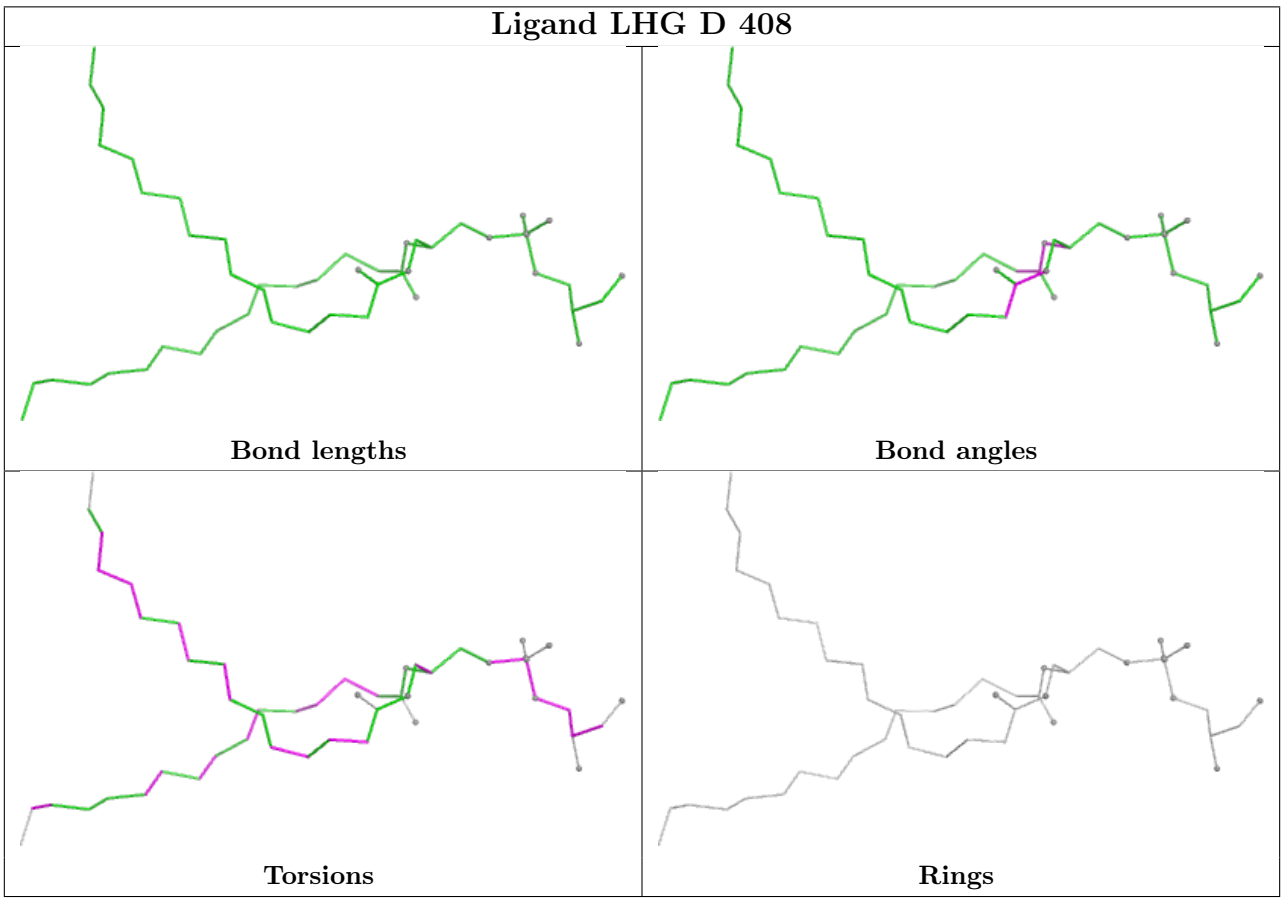


Rings

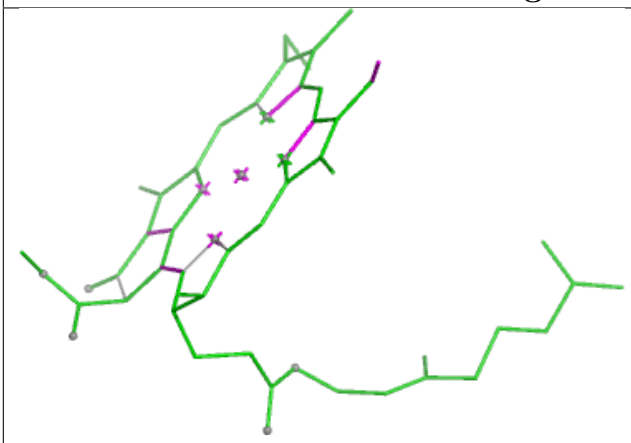
Ligand CLA B 509



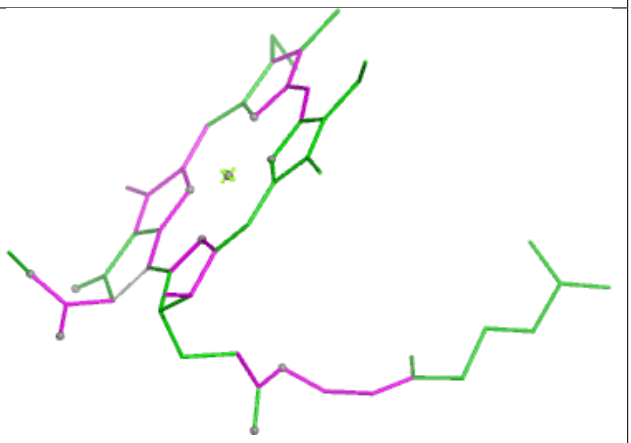
Ligand LHG D 408



Ligand CLA C 505



Bond lengths



Bond angles

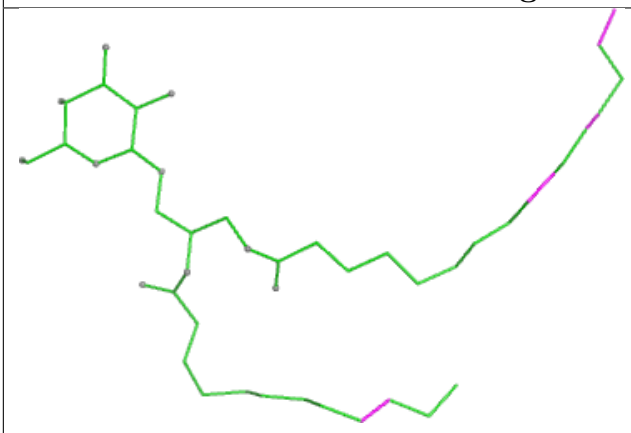


Torsions



Rings

Ligand LMG C 521



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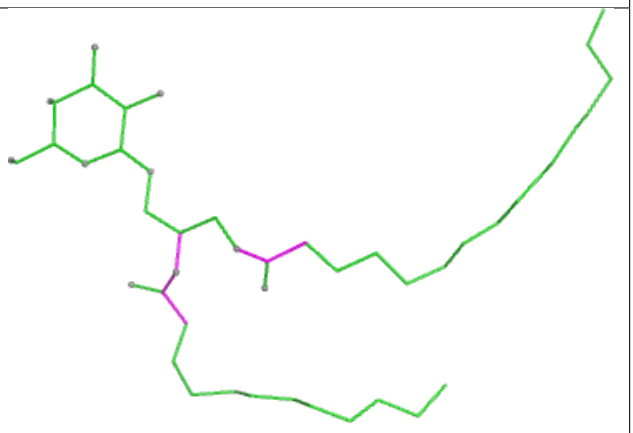
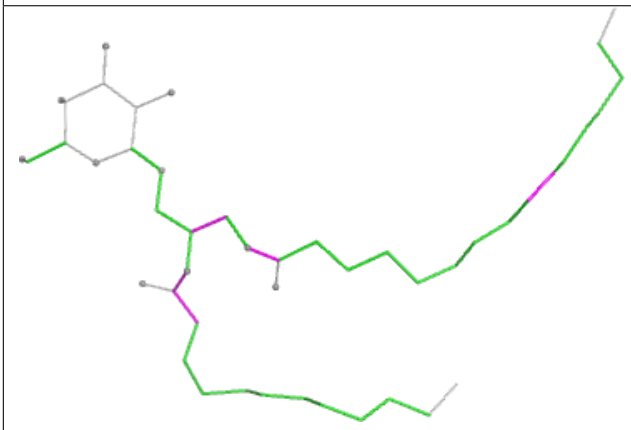


Bond angles



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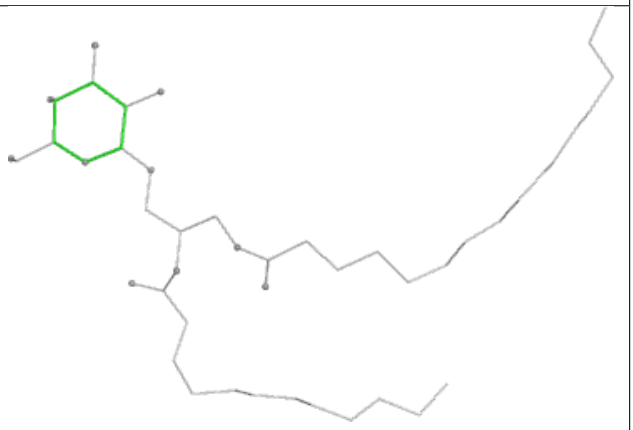
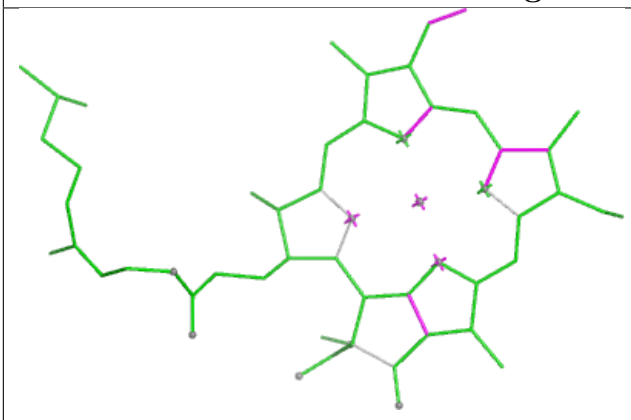


Rings

Ligand CLA C 513



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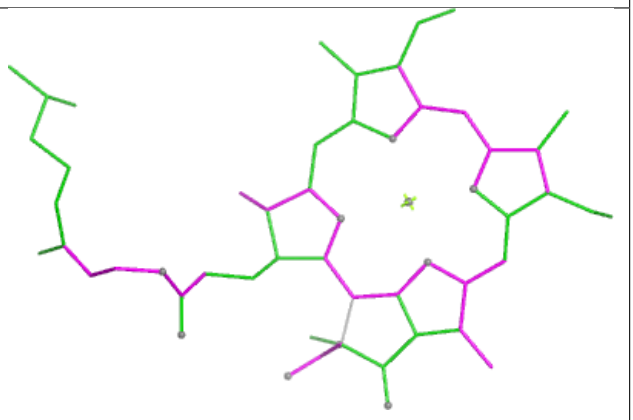
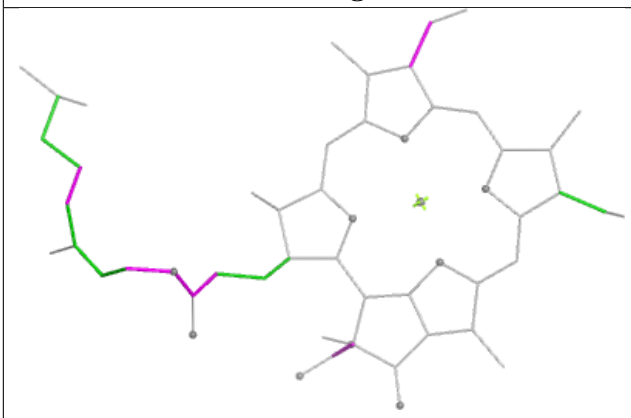


Bond angles



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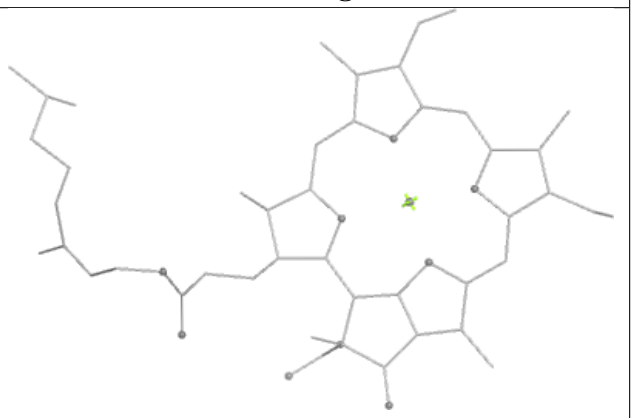
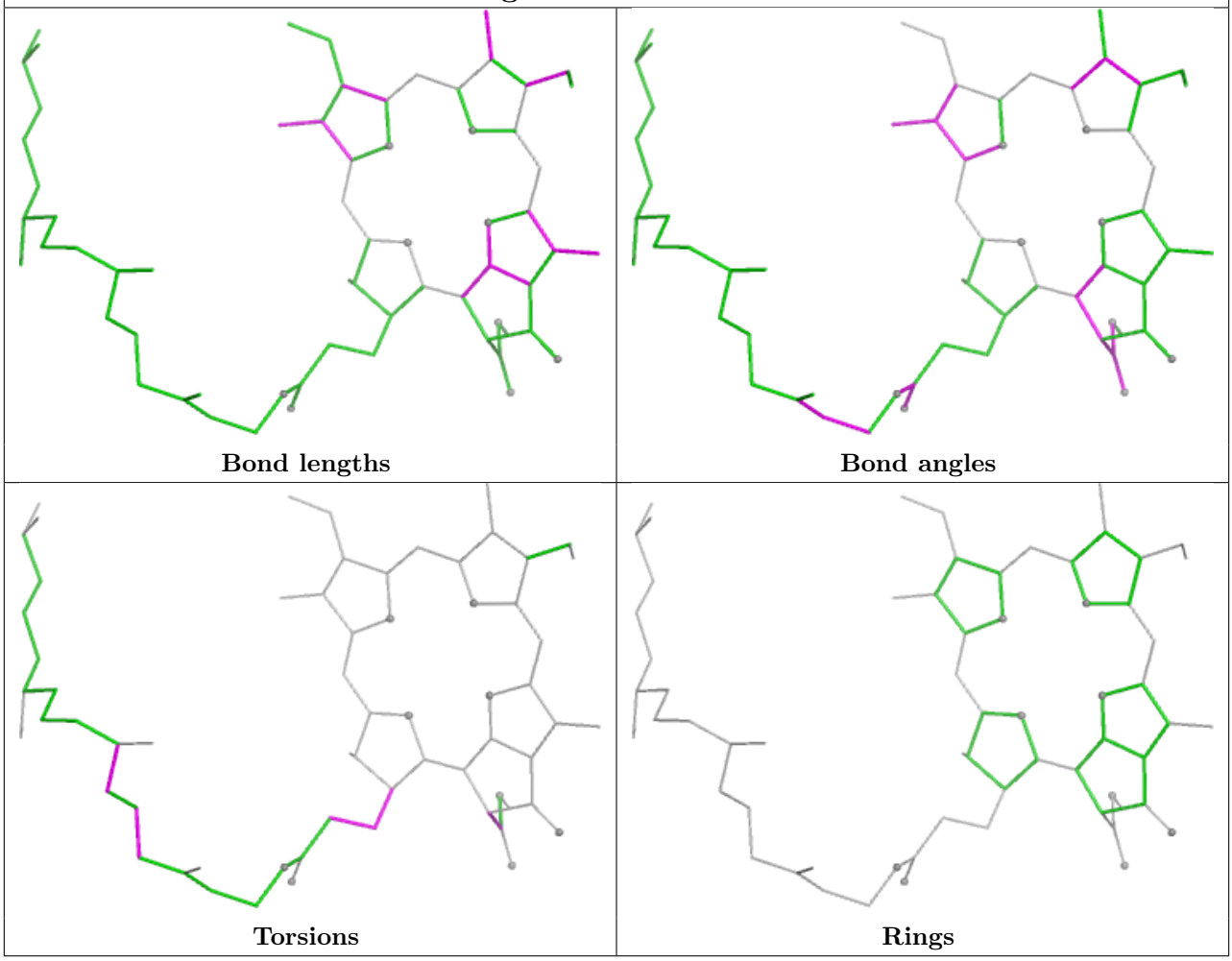
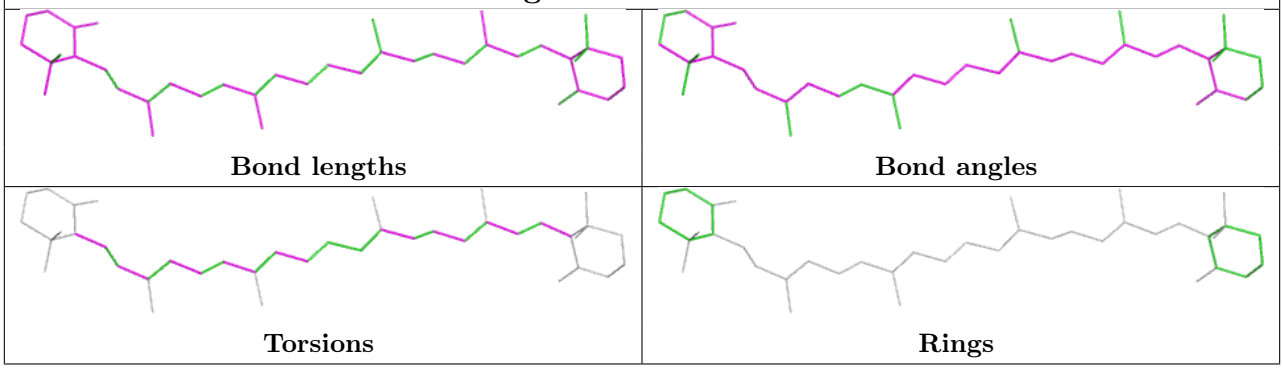


Rings

Ligand PHO D 402



Ligand BCR B 518



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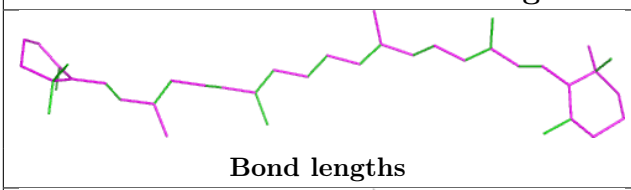

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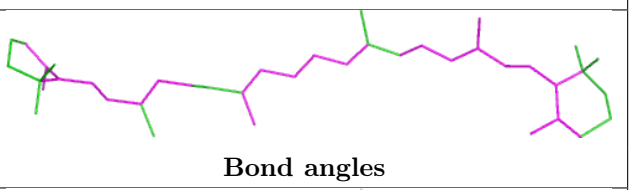
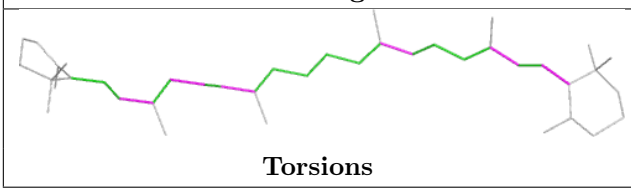


Bond angles



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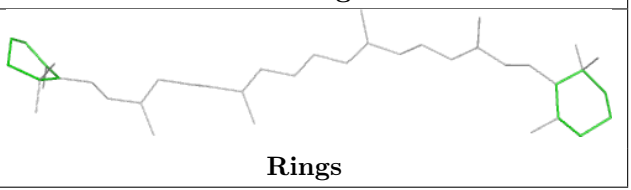
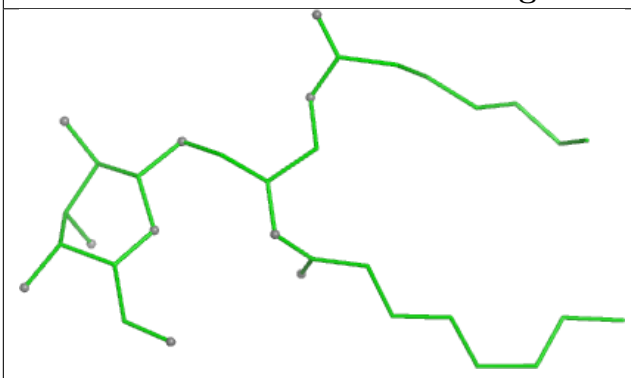


Rings

Ligand LMG A 411



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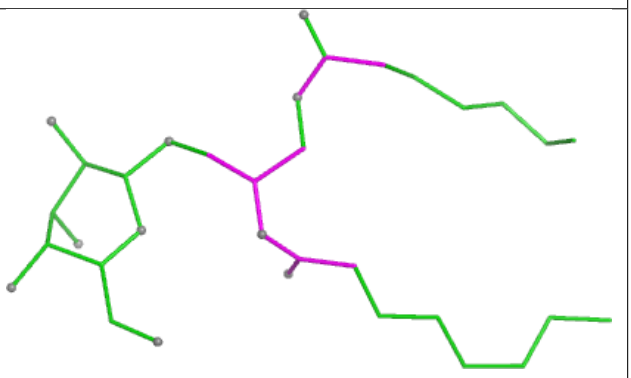
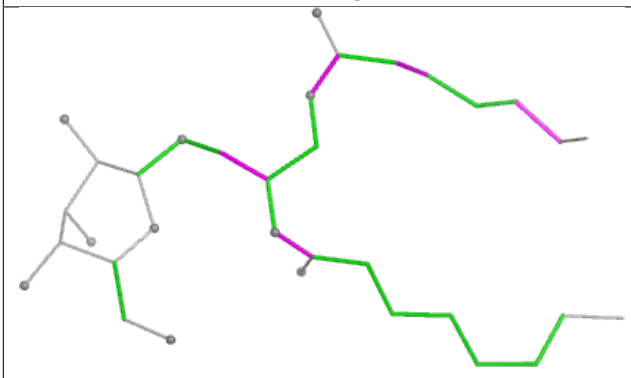


Bond angles



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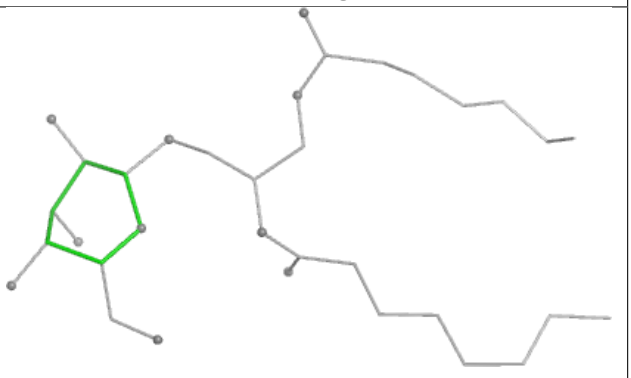
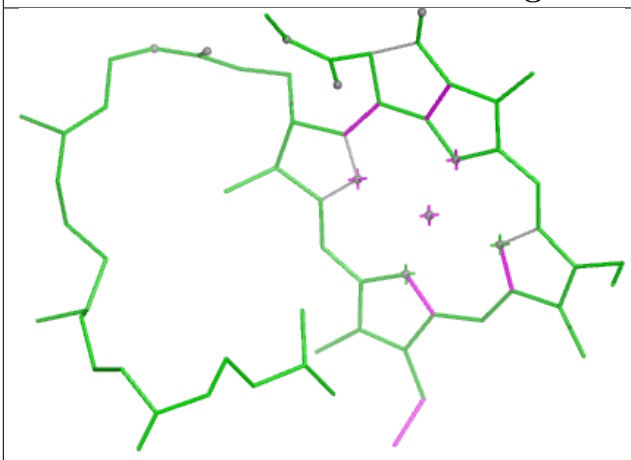


Rings

Ligand CLA B 515



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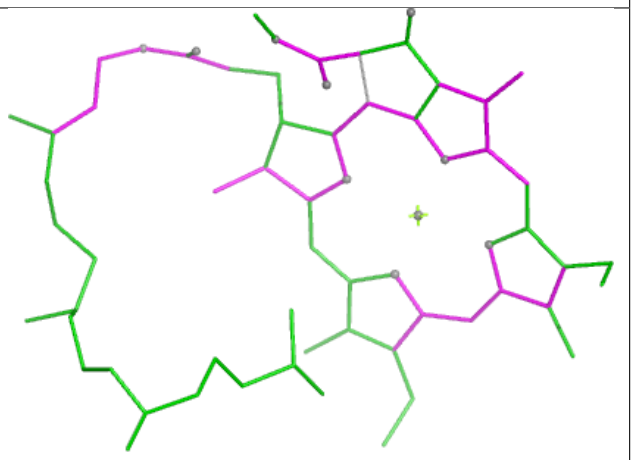
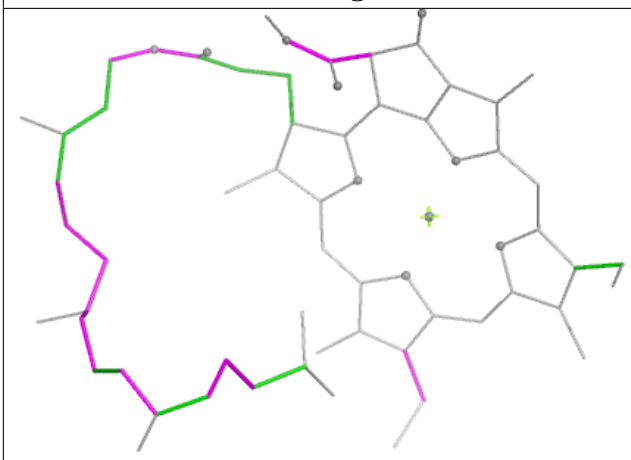


Bond angles



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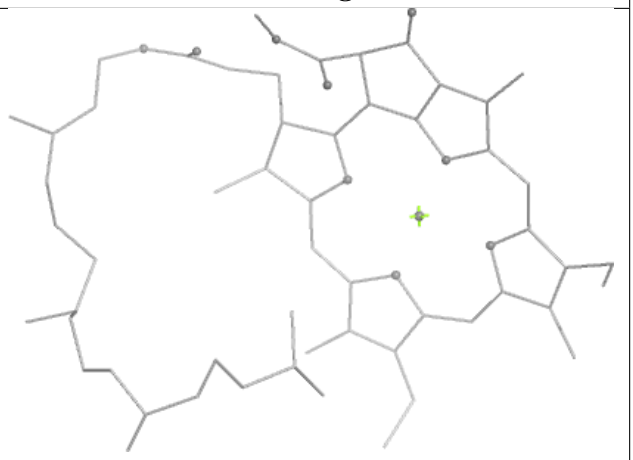
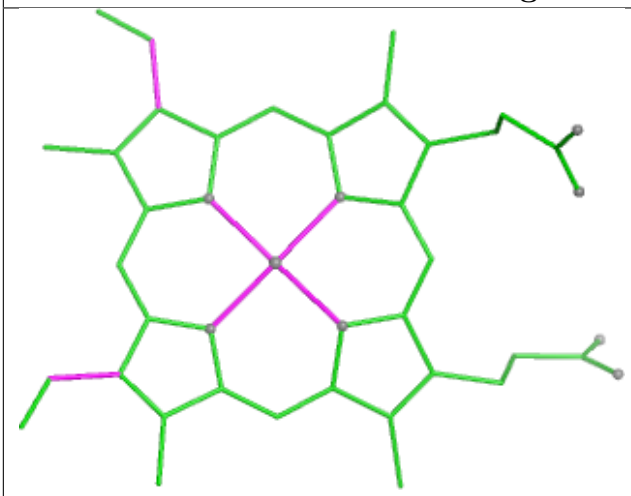


Rings

Ligand HEM E 101



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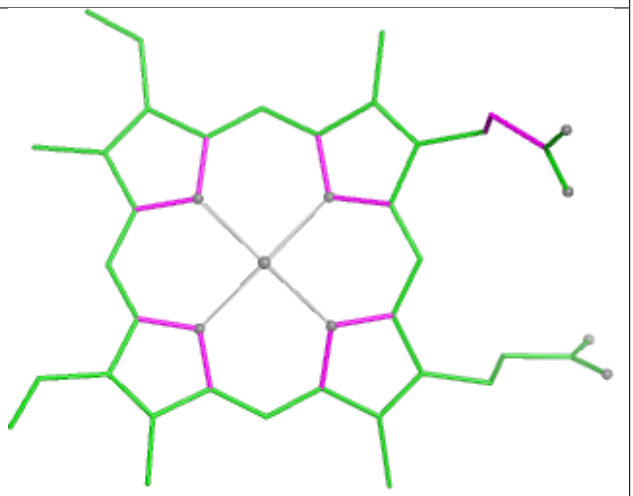
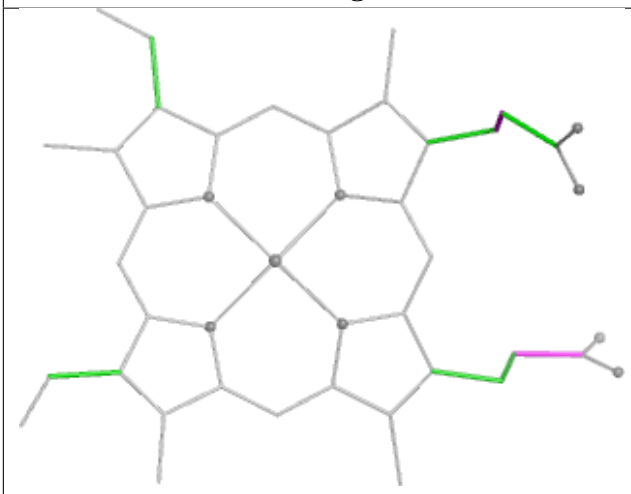


Bond angles



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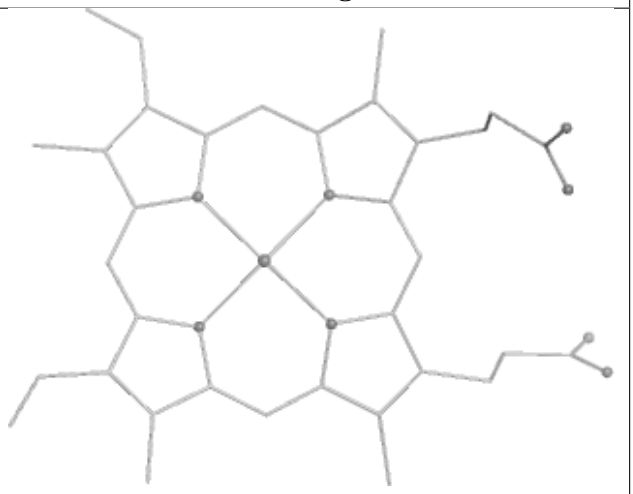
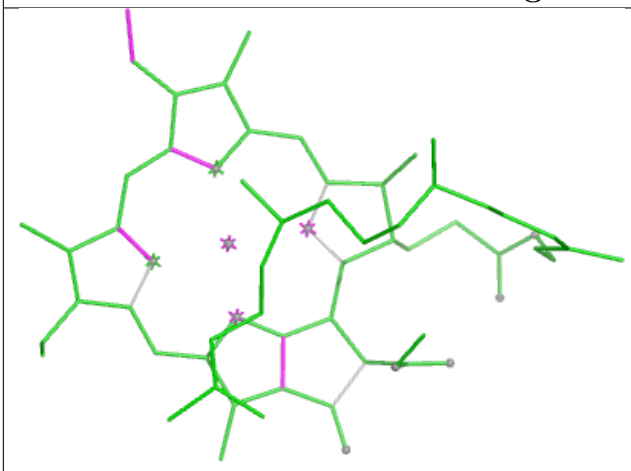


Rings

Ligand CLA C 511



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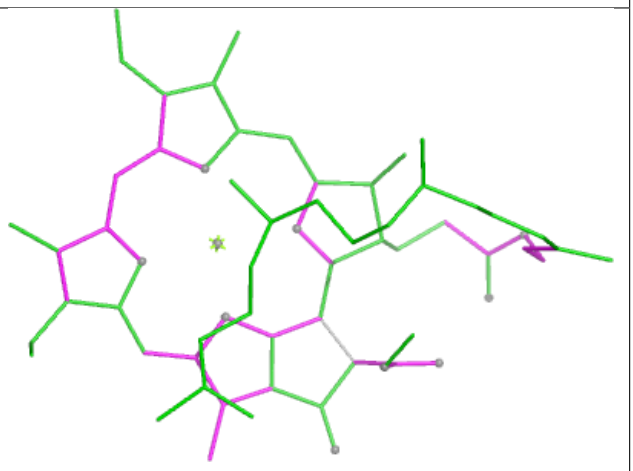
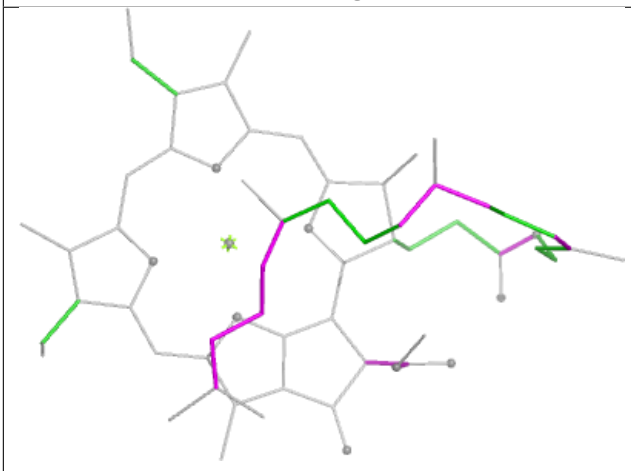


Bond angles



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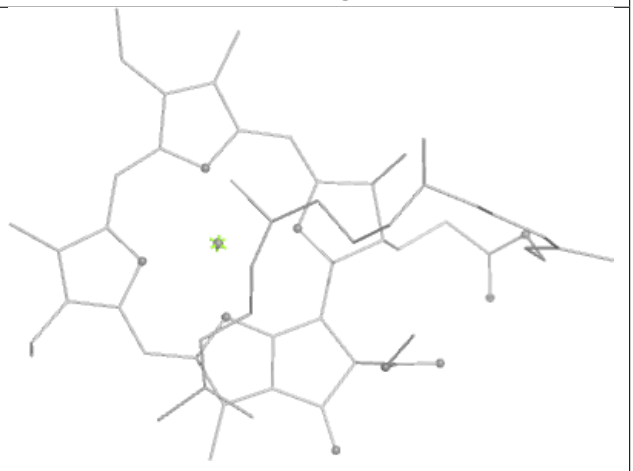
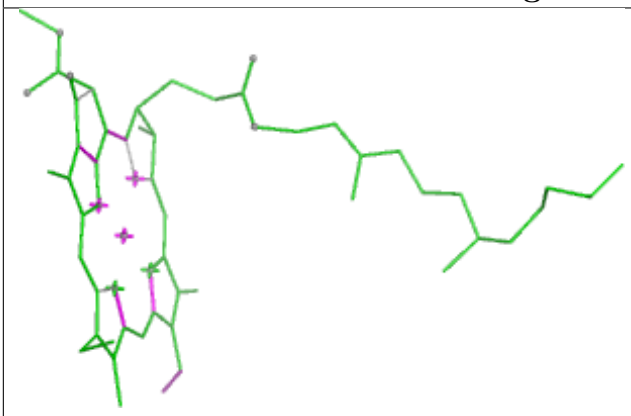


Rings

Ligand CLA D 404



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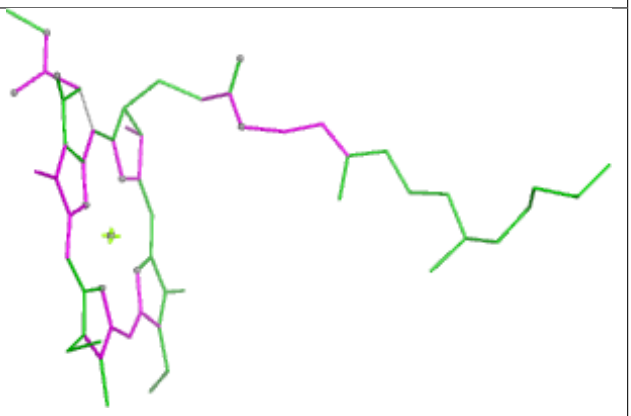
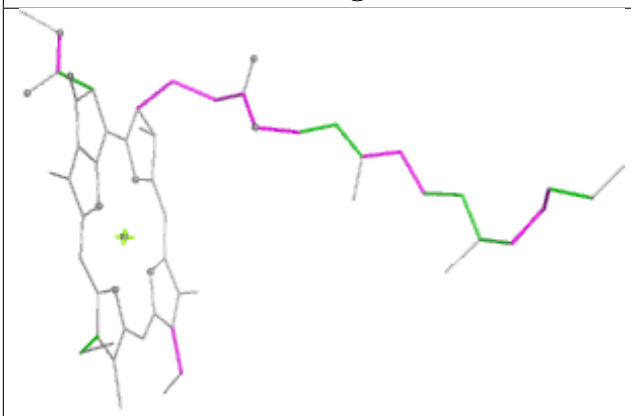


Bond angles



Torsions



Rings

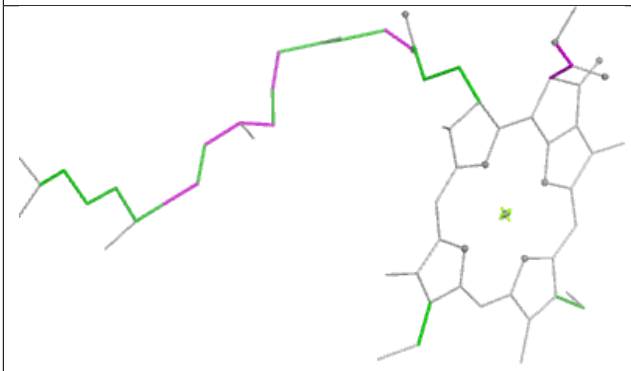
Ligand CLA C 512



Bond lengths



Bond angles

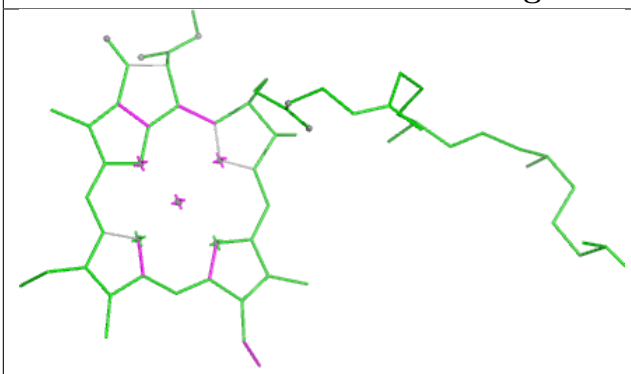


Torsions

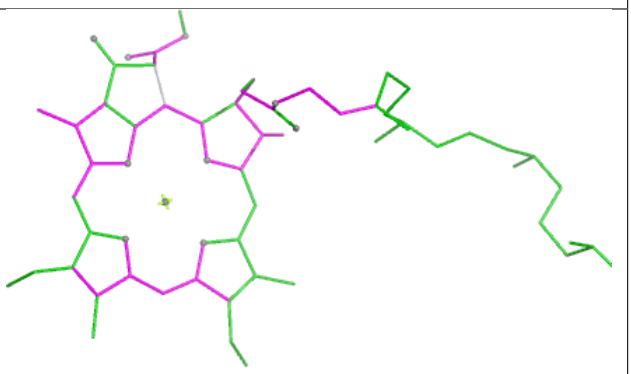


Rings

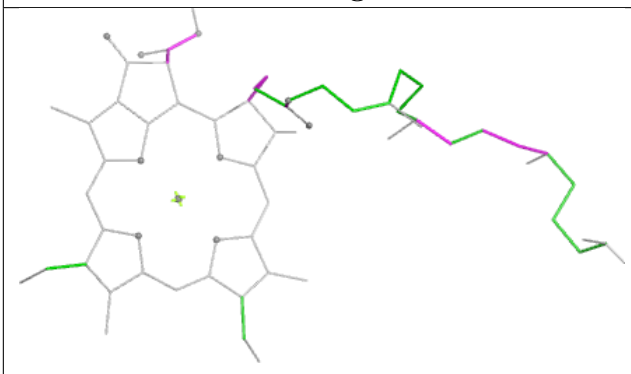
Ligand CLA A 406



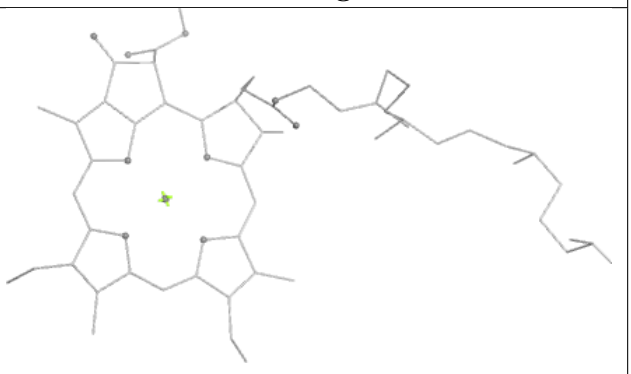
Bond lengths



Bond angles

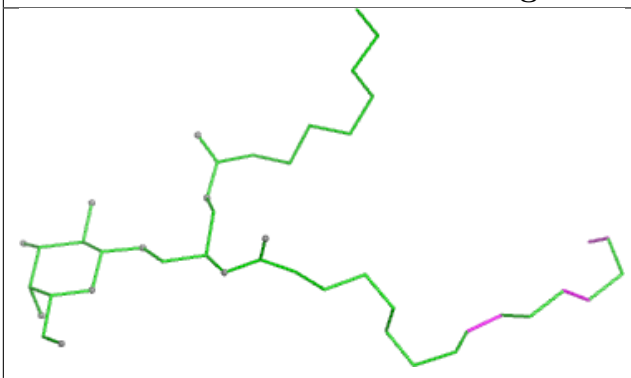


Torsions

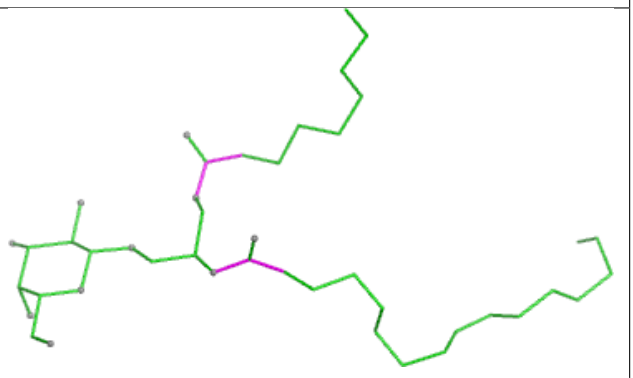


Rings

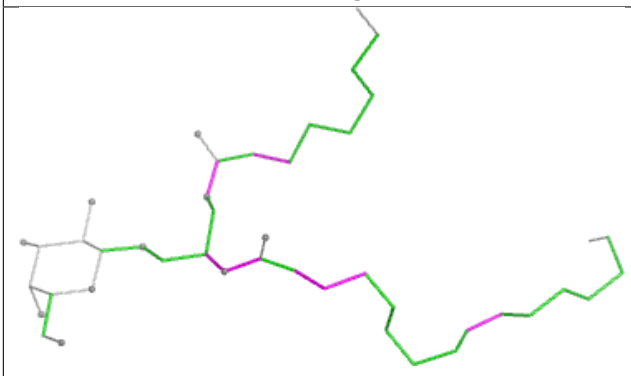
Ligand LMG B 520



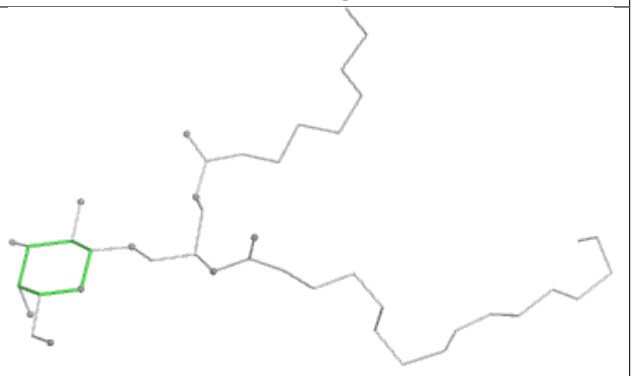
Bond lengths



Bond angles

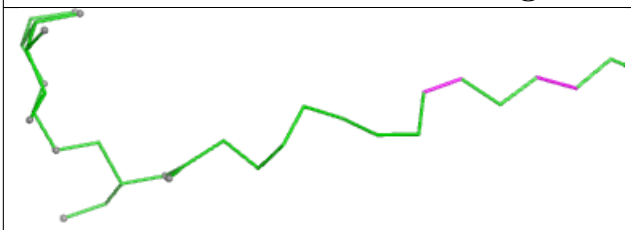


Torsions

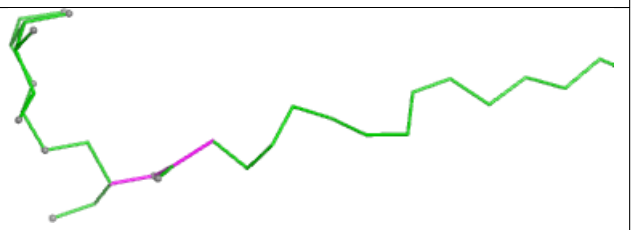


Rings

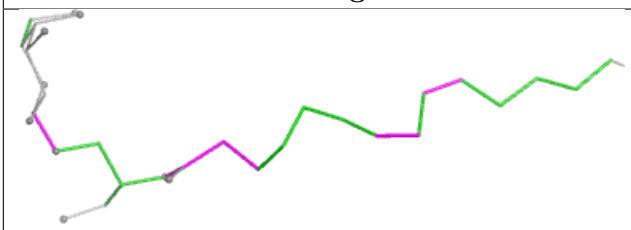
Ligand LMG C 522



Bond lengths



Bond angles



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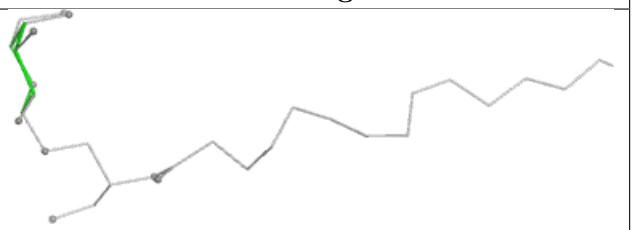
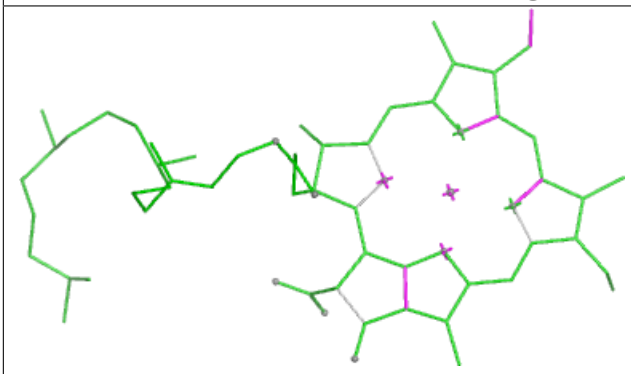
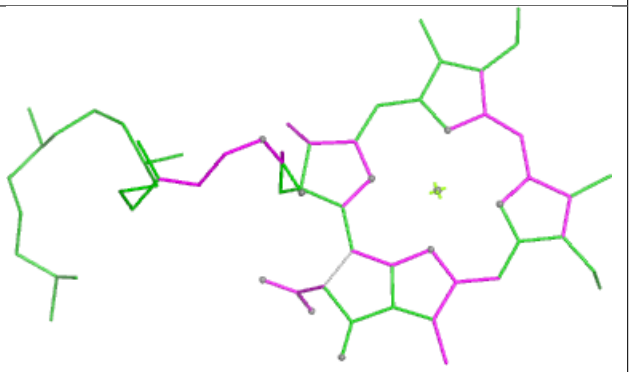
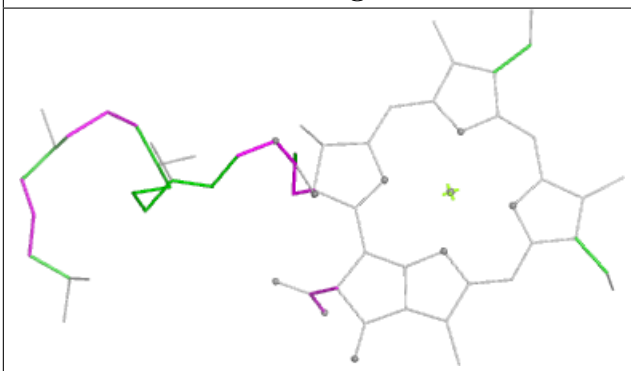
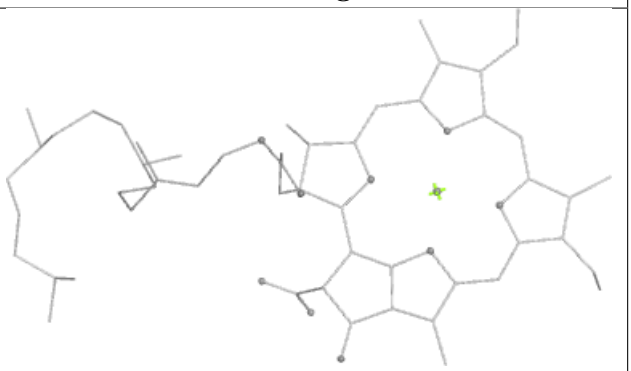
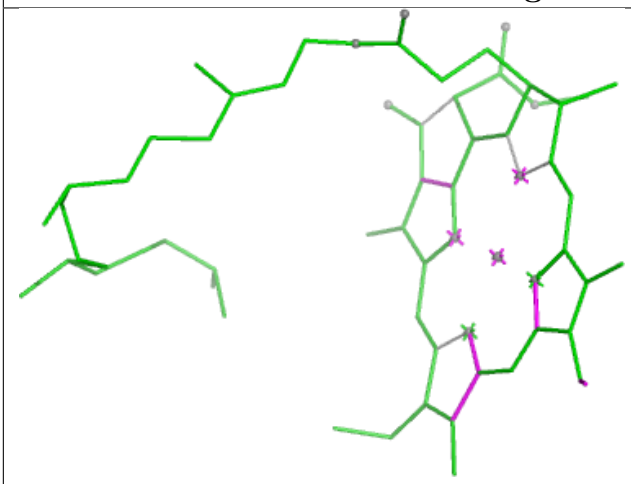


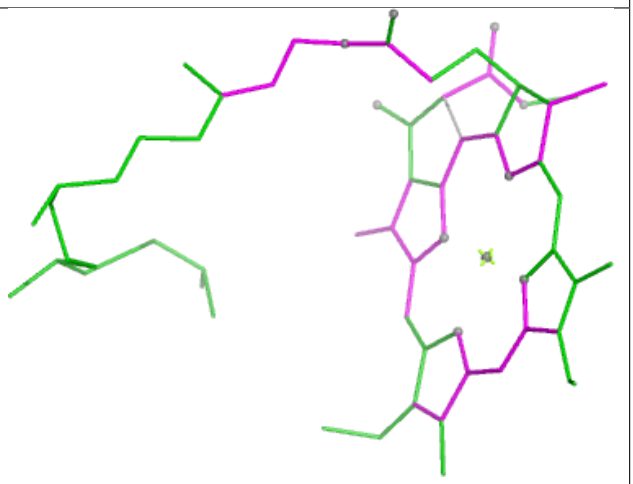
Rings

Ligand CLA B 512	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

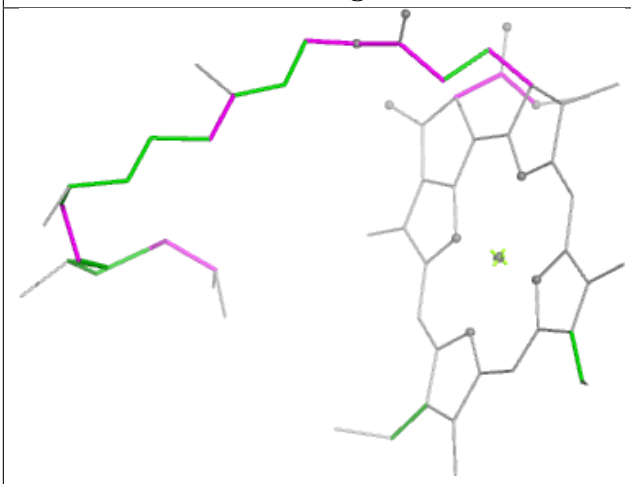
Ligand CLA C 504



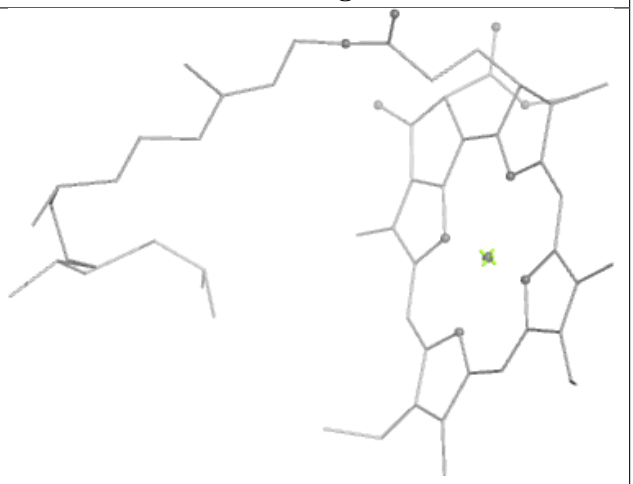
Bond lengths



Bond angles

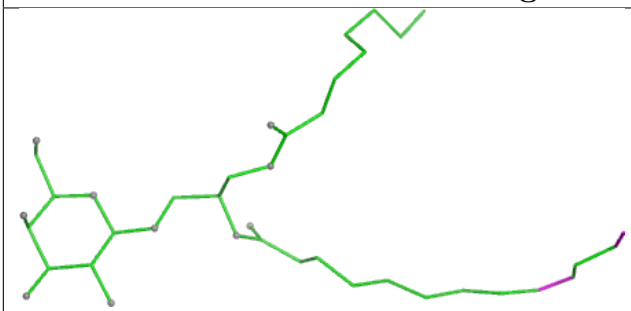


Torsions



Rings

Ligand LMG C 501



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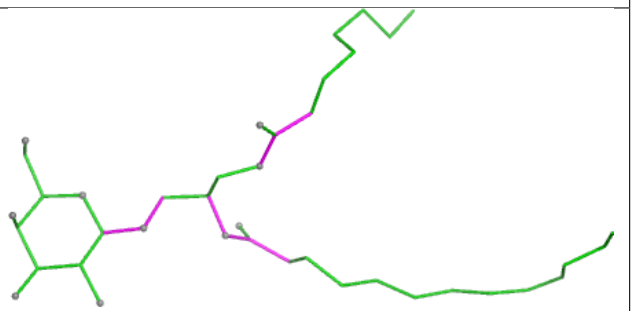
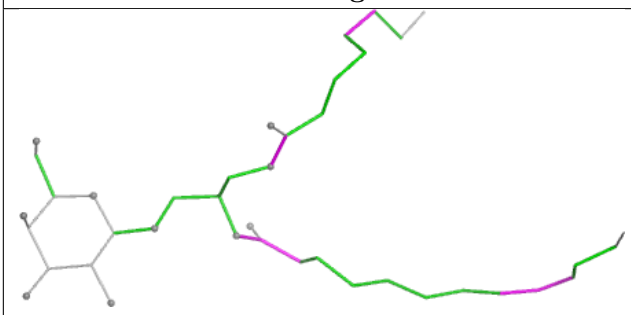


Bond angles



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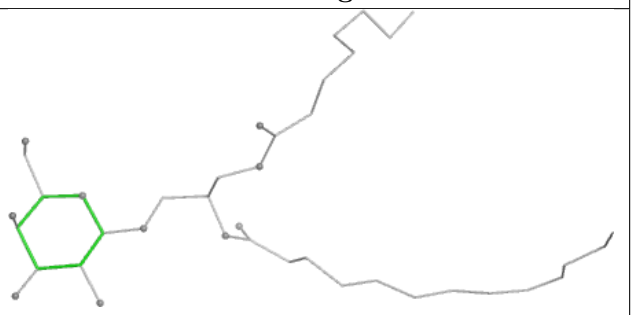
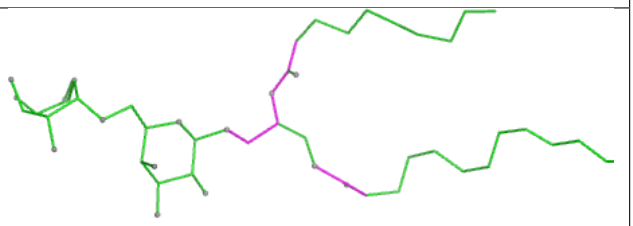


Rings

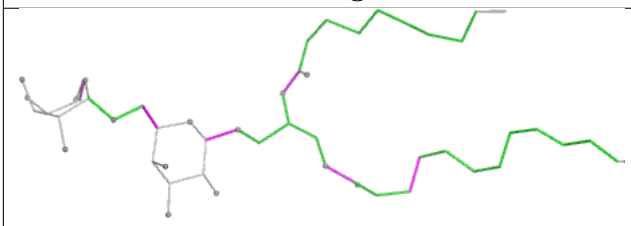
Ligand DGD C 520



Bond lengths



Bond angles



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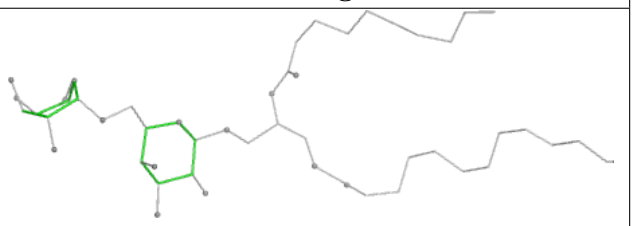
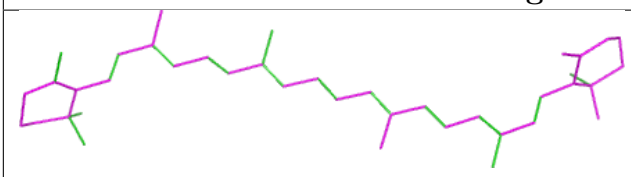


Rings

Ligand BCR J 101



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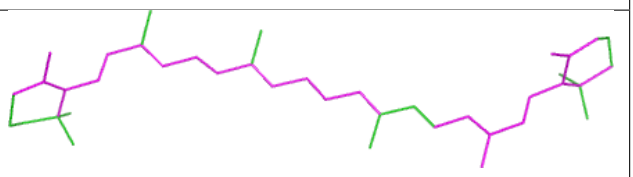
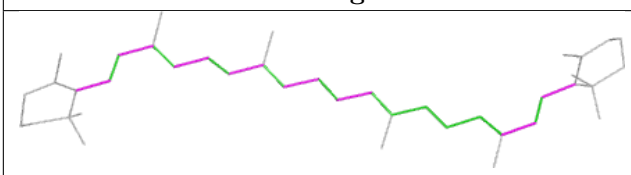


Bond angles



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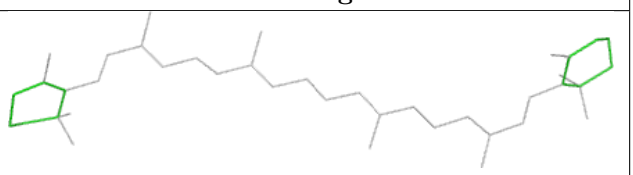
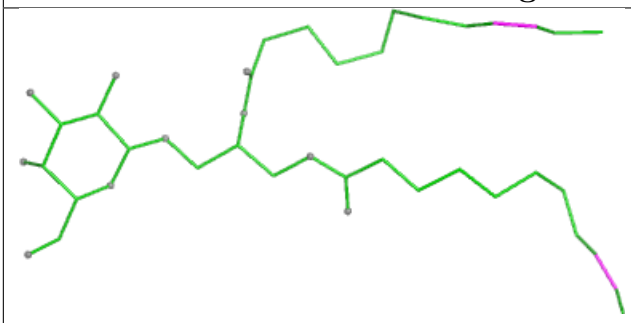


Rings

Ligand LMG D 409



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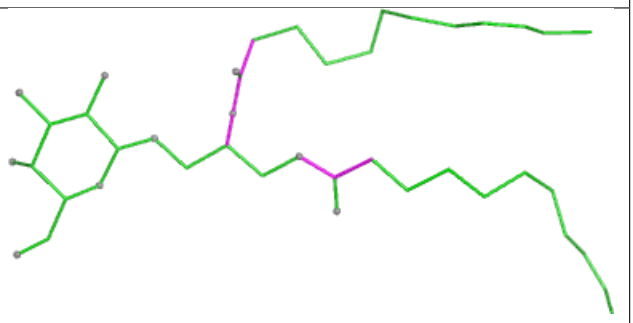
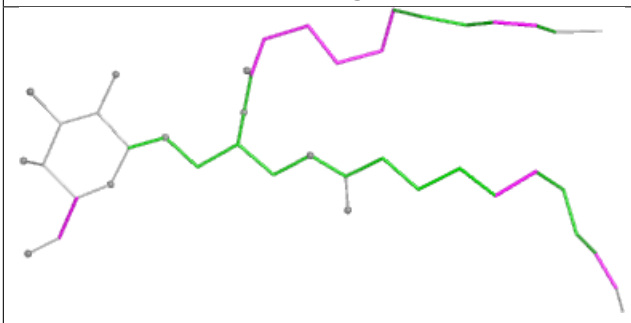


Bond angles



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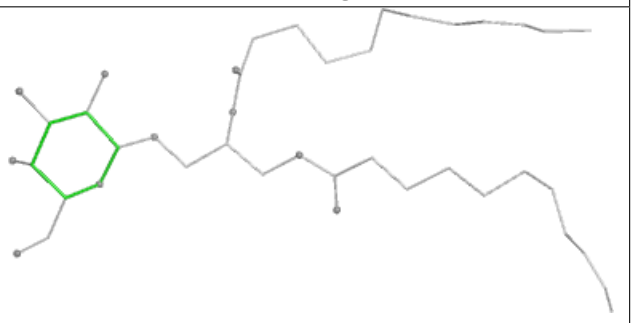
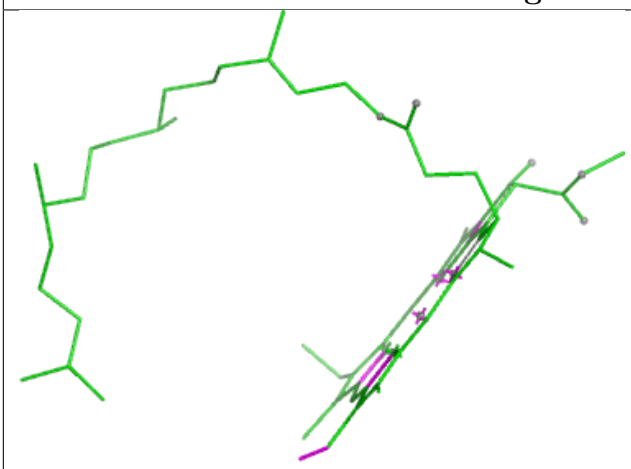


Rings

Ligand CLA B 511



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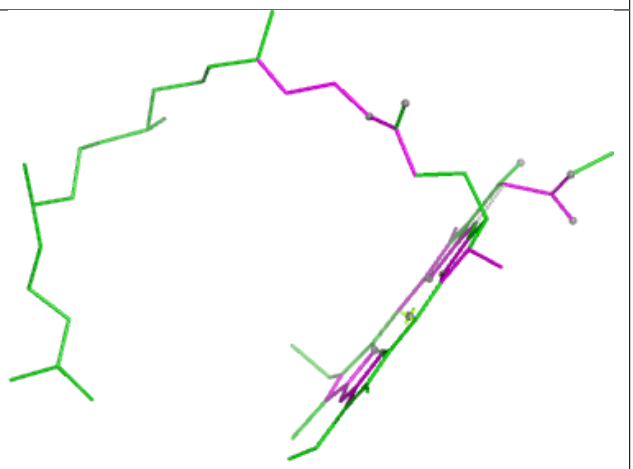
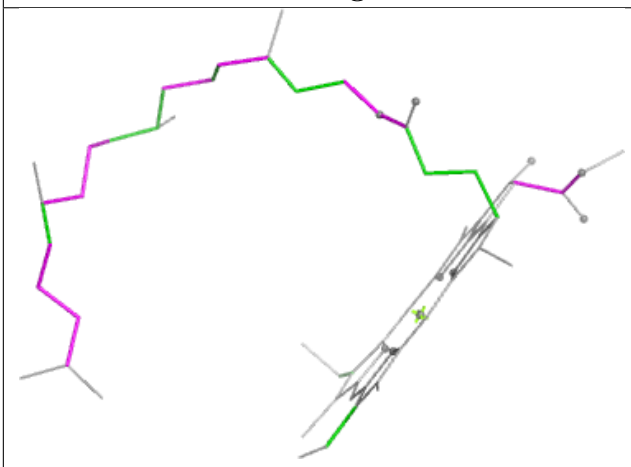


Bond angles

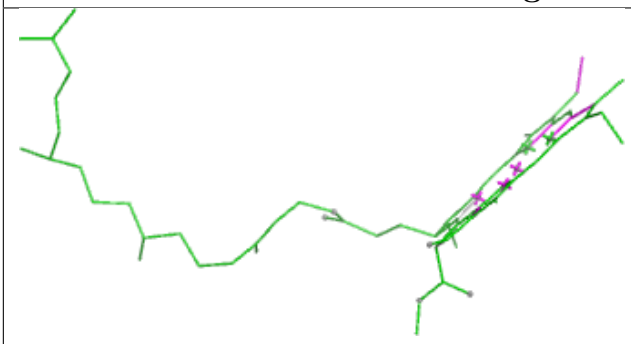


Torsions



Rings

Ligand CLA D 403



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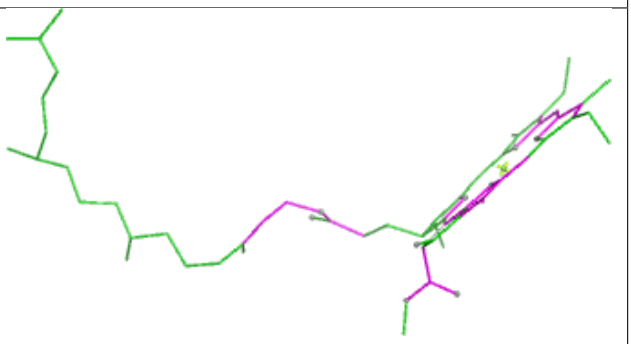
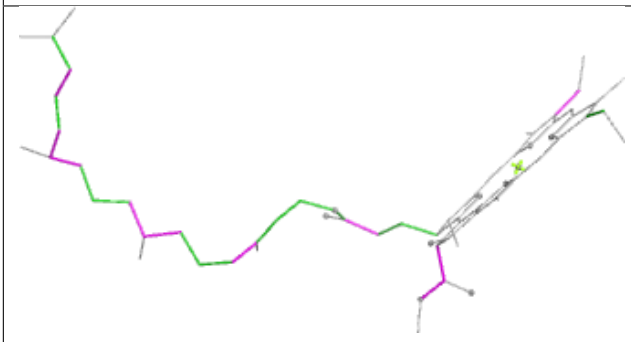


Bond angles



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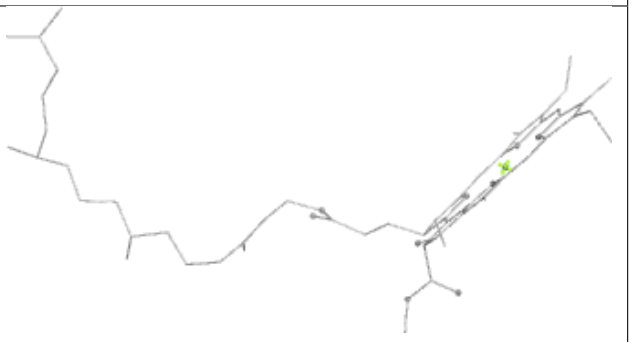
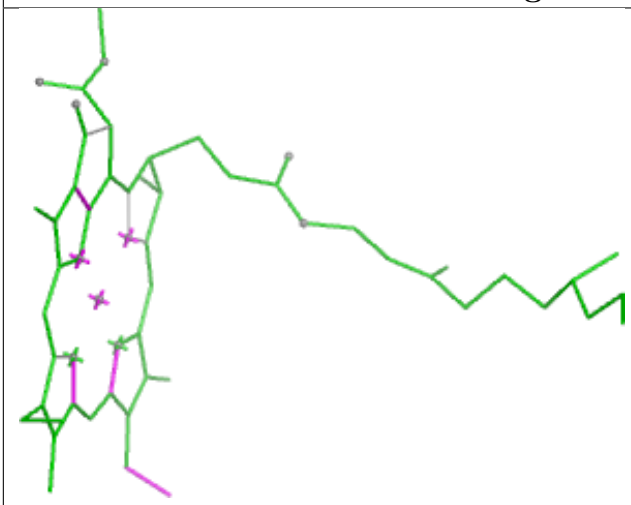


Rings

Ligand CLA B 506



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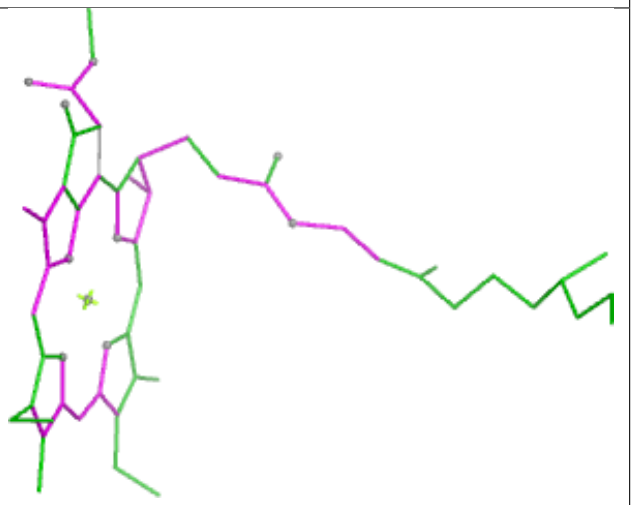

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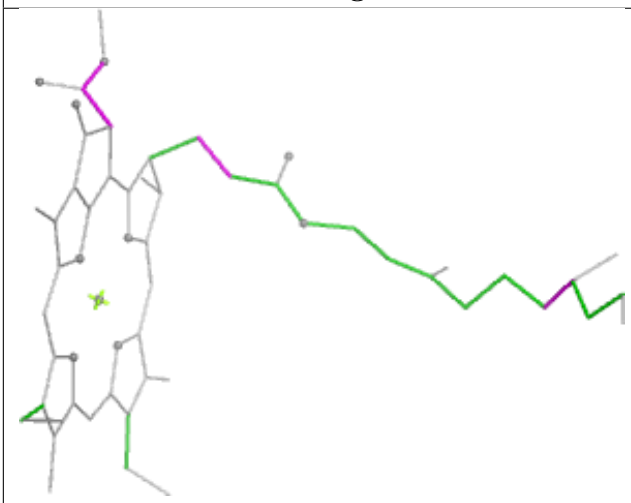
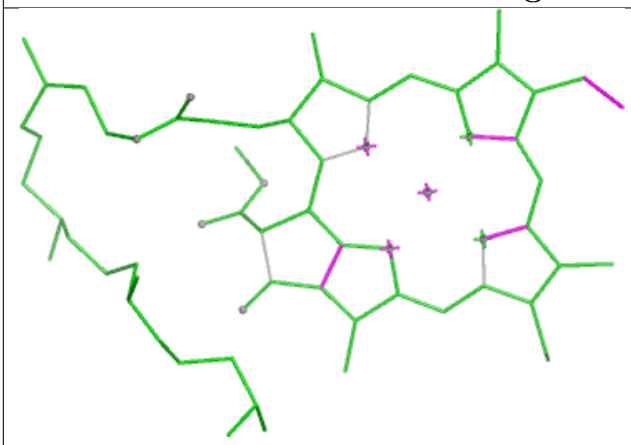


Torsions



Rings

Ligand CLA B 510



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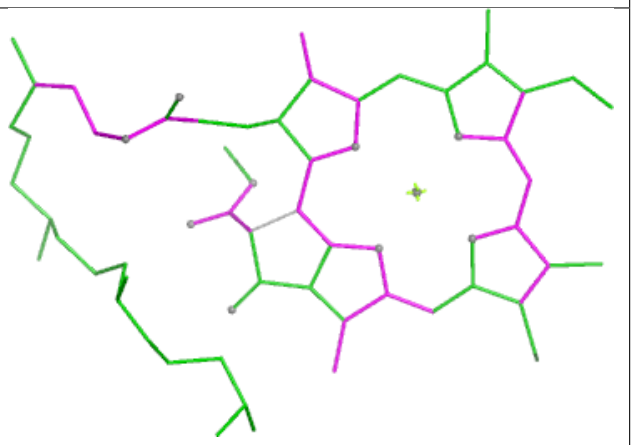
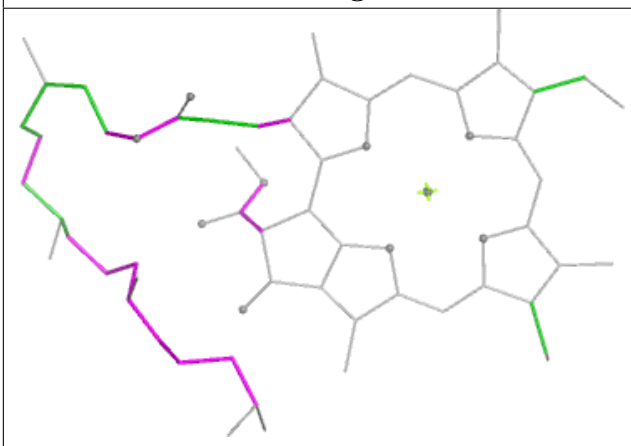


Bond angles



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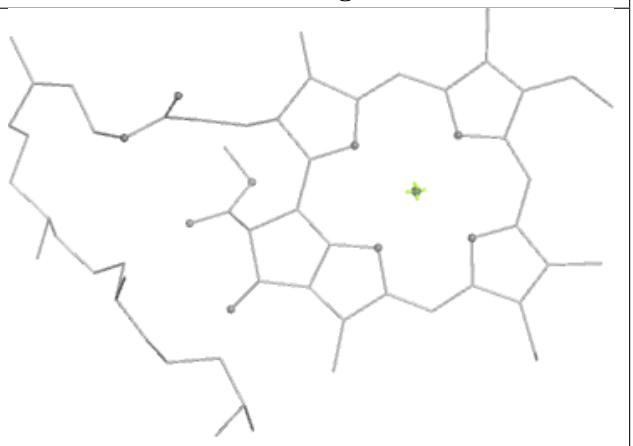
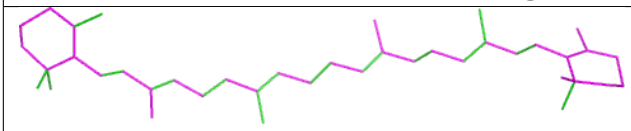


Rings

Ligand BCR D 405



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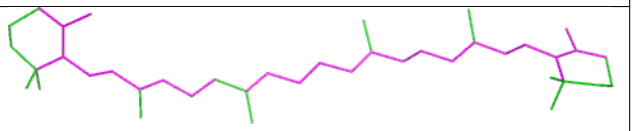
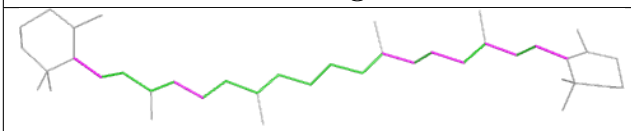


Bond angles



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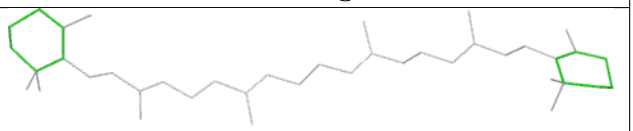
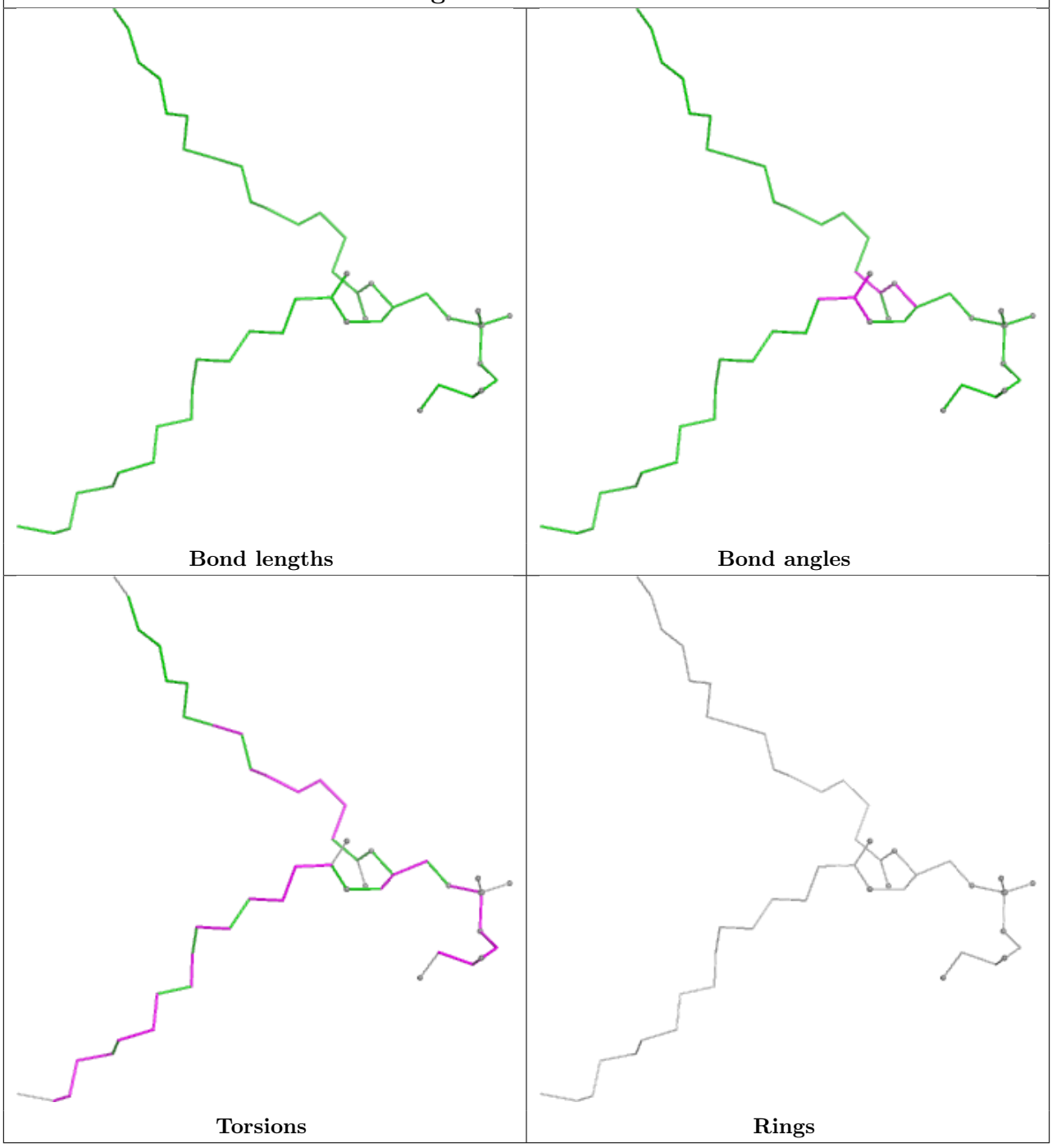
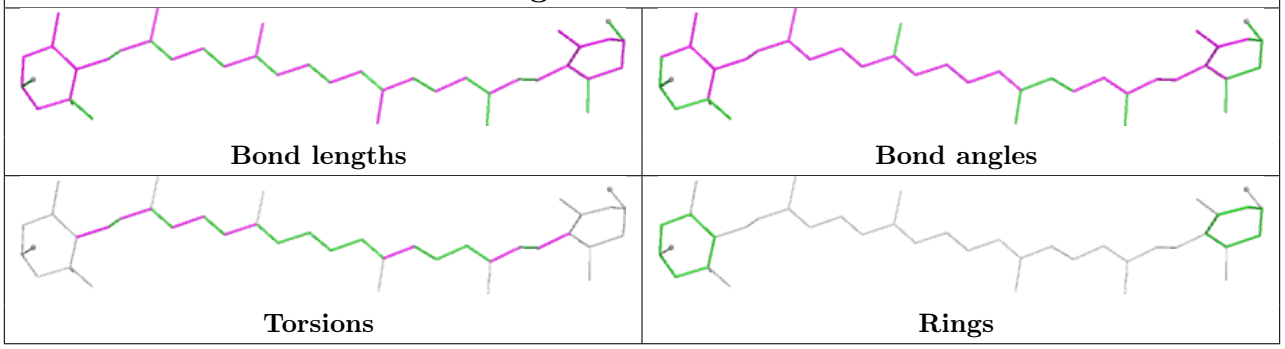


Rings

Ligand LHG L 101



Ligand C7Z B 519



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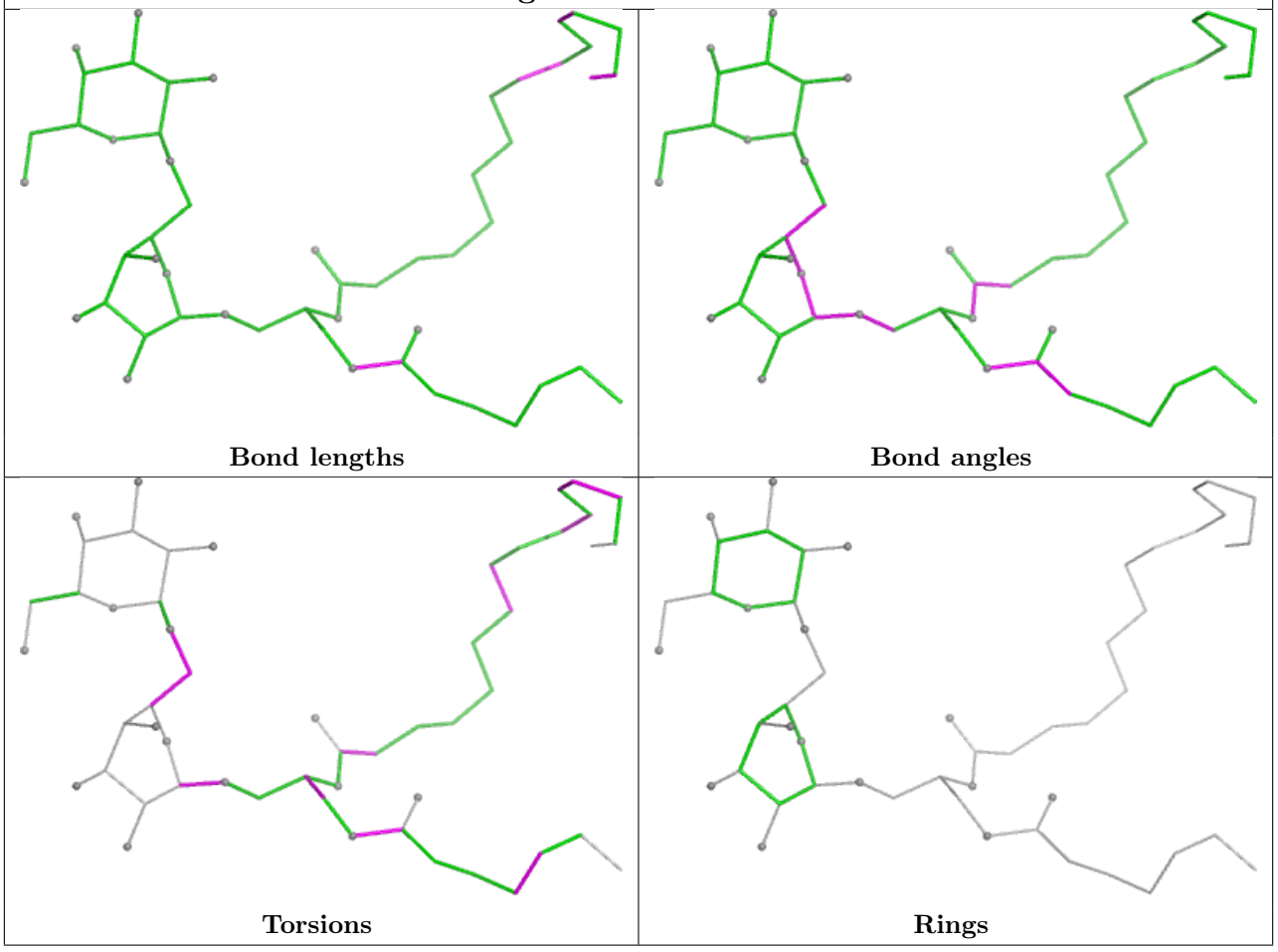
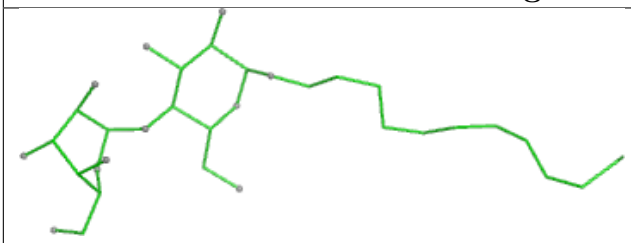
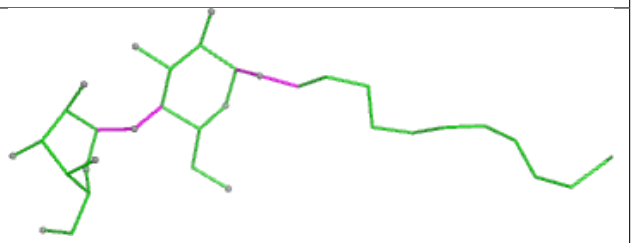


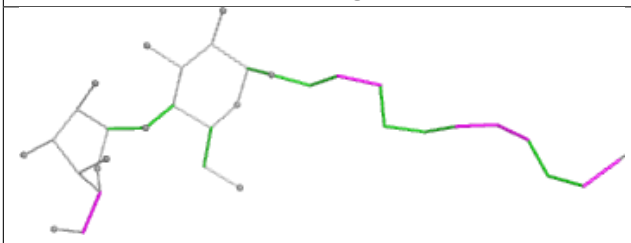
Ligand LMU J 102



Bond lengths



Bond angles



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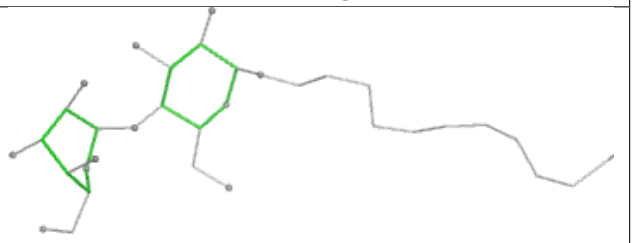
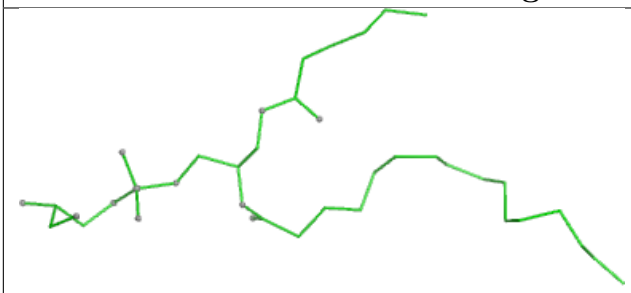


Rings

Ligand LHG D 410



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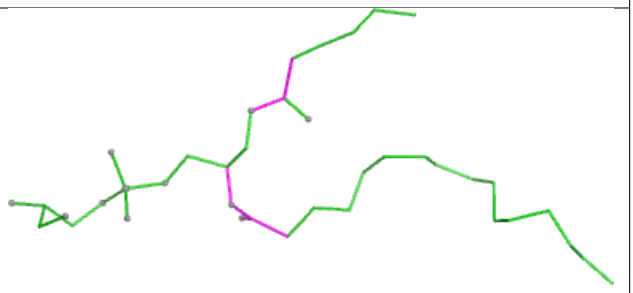
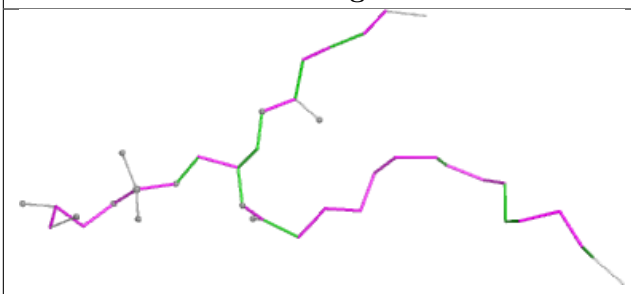
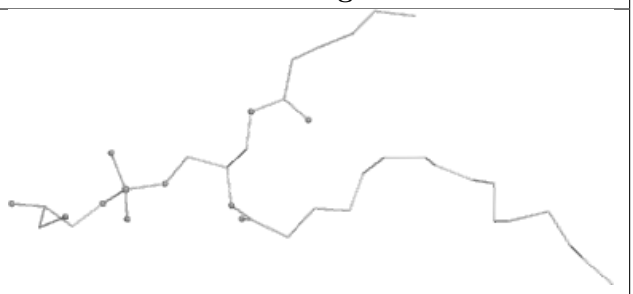


Bond angles

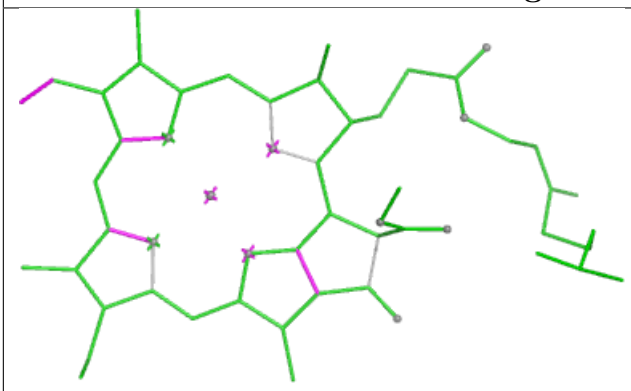


Torsions

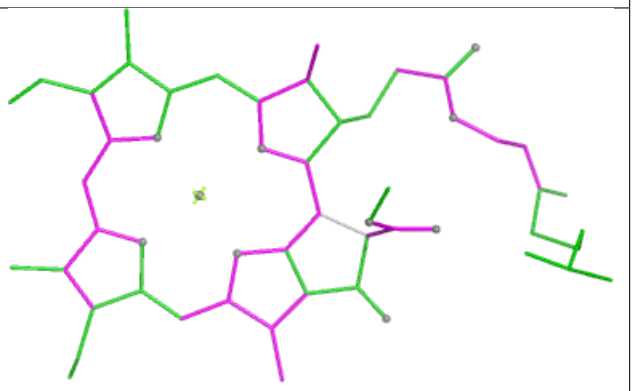


Rings

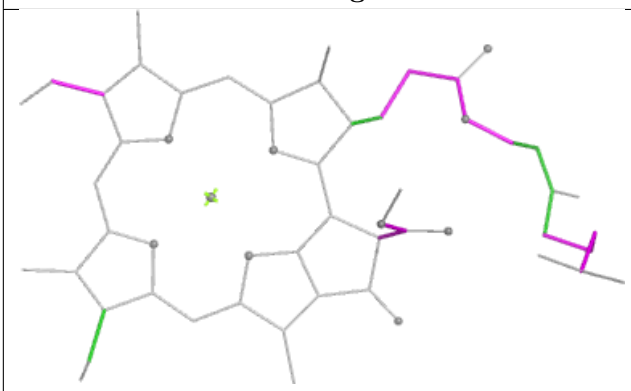
Ligand CLA B 516



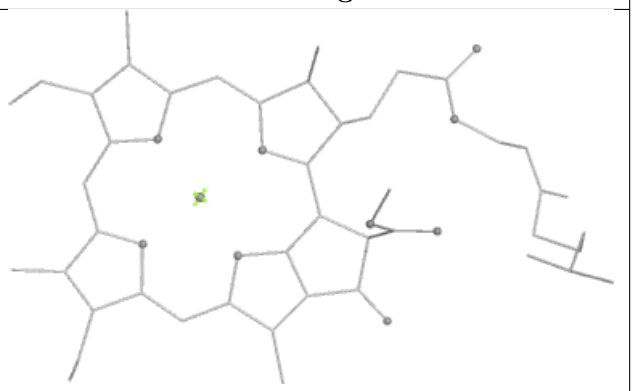
Bond lengths



Bond angles

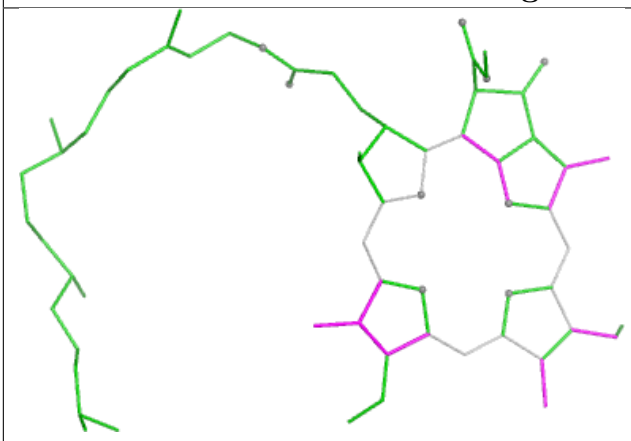


Torsions



Rings

Ligand PHO A 407



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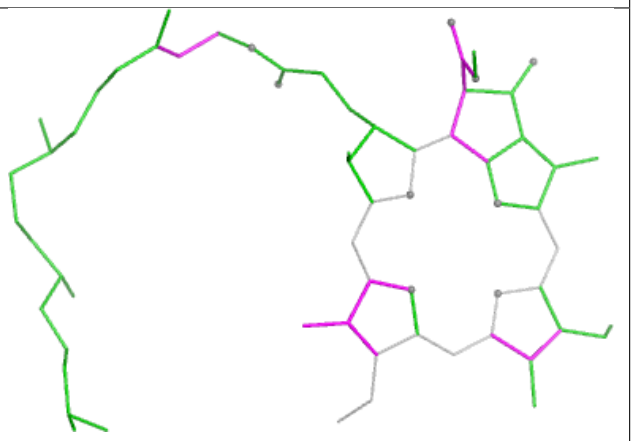
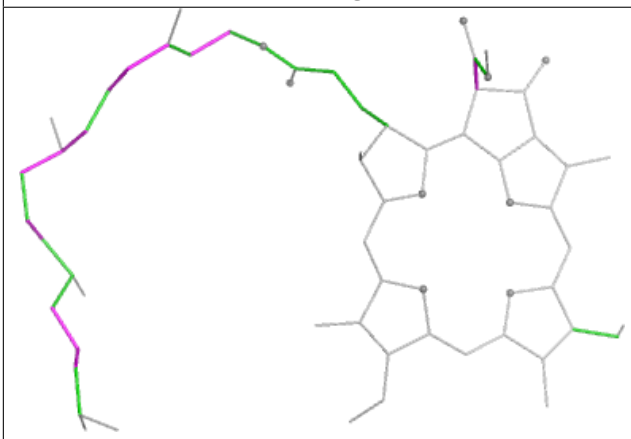


Bond angles



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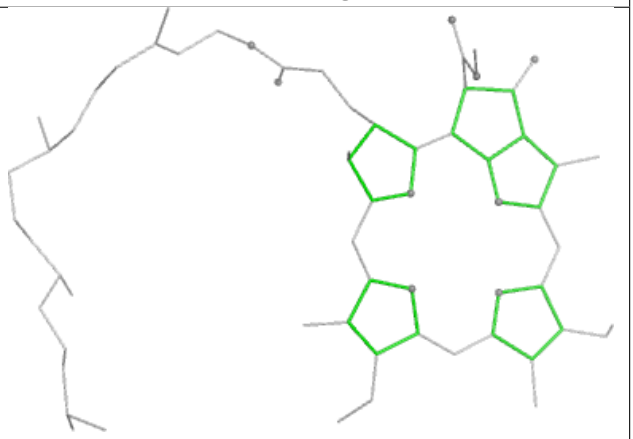


Rings

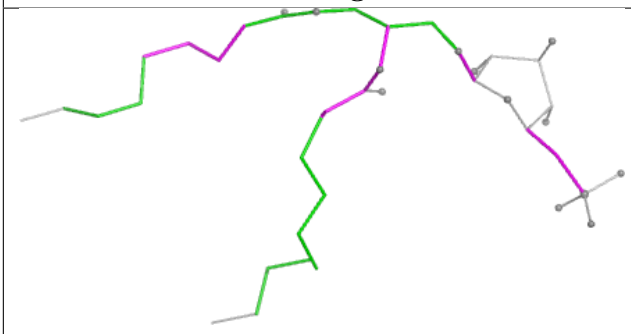
Ligand SQD M 101



Bond lengths



Bond angles

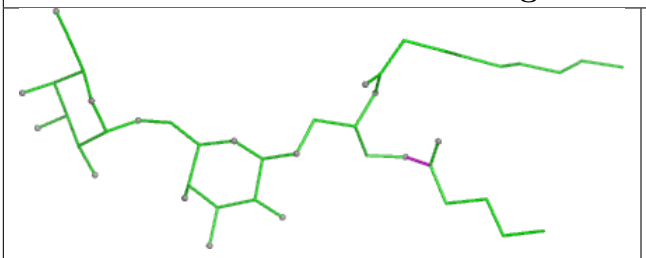


Torsions

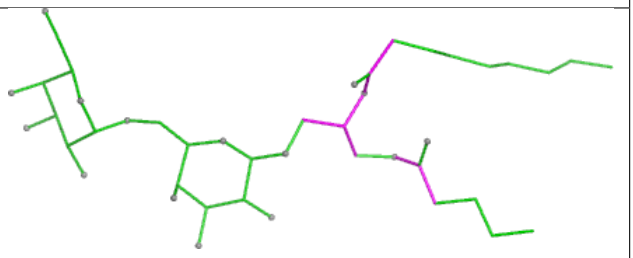


Rings

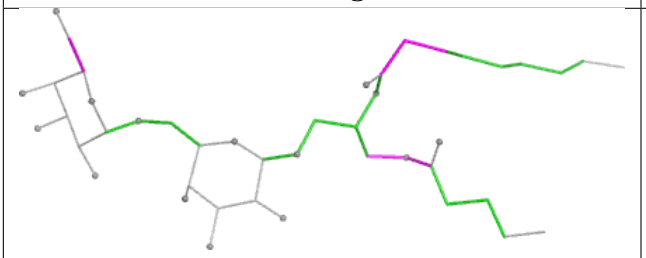
Ligand DGD C 518



Bond lengths



Bond angles



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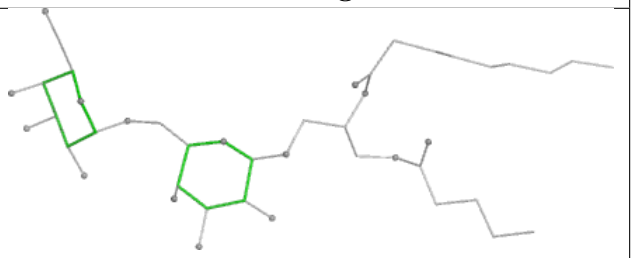
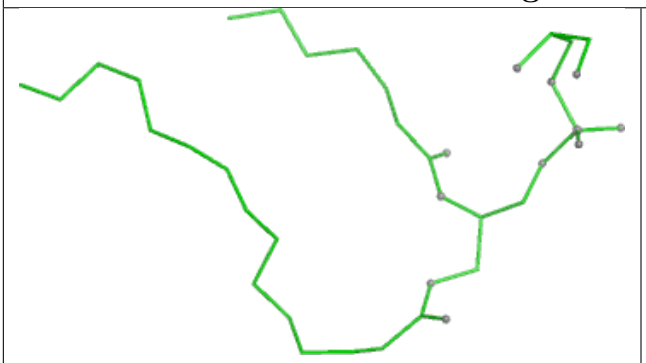


Rings

Ligand LHG A 414



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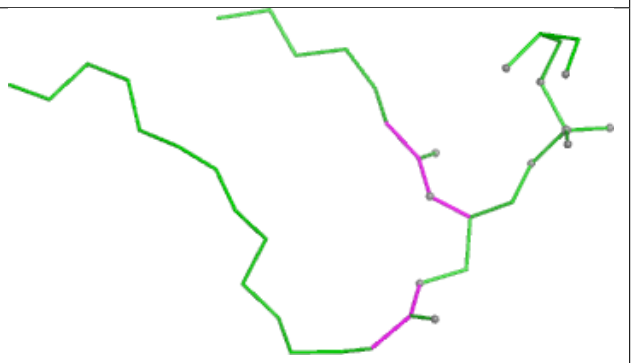
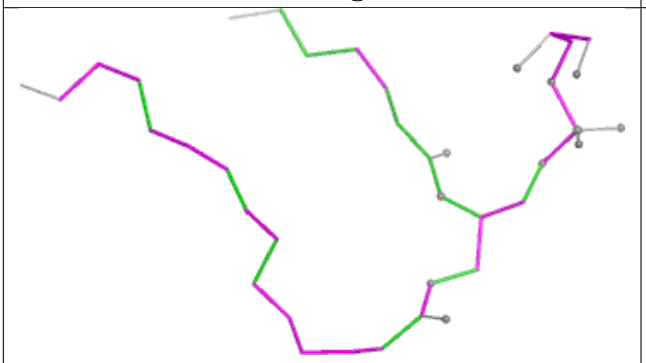


Bond angles



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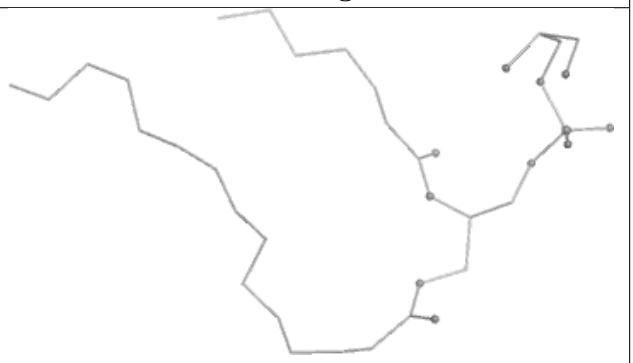
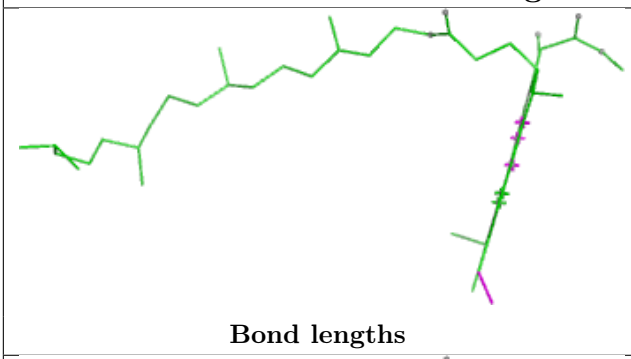


Rings

Ligand CLA B 505



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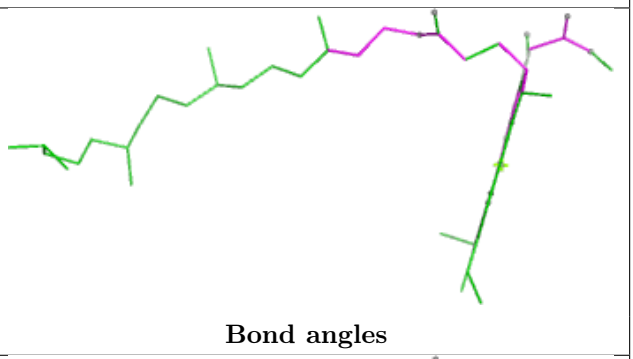
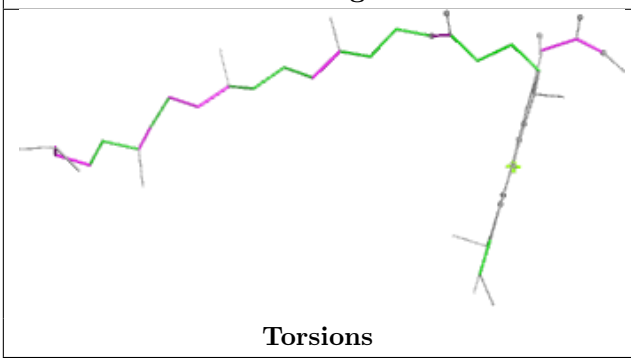


Bond angles



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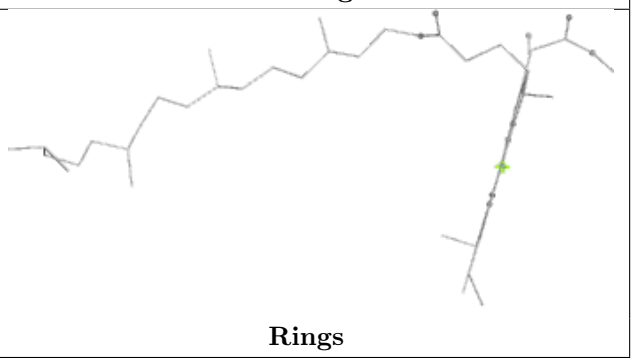
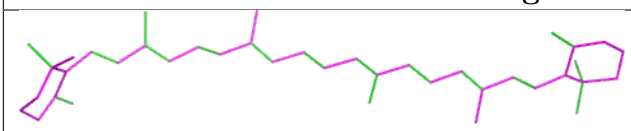


Rings

Ligand BCR C 516



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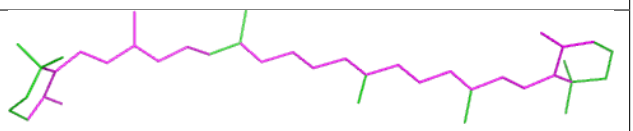
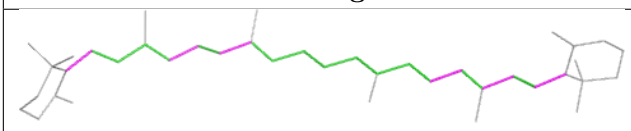


Bond angles



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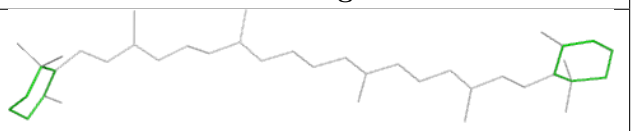
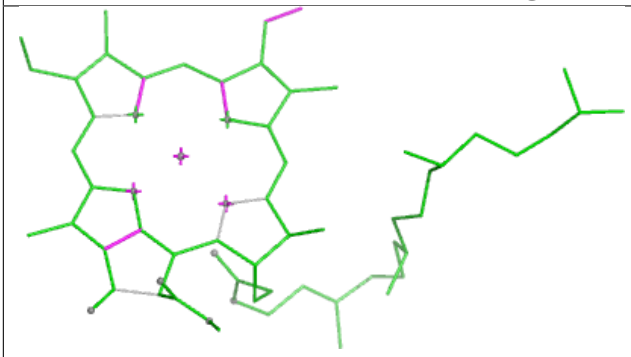


Rings

Ligand CLA D 401



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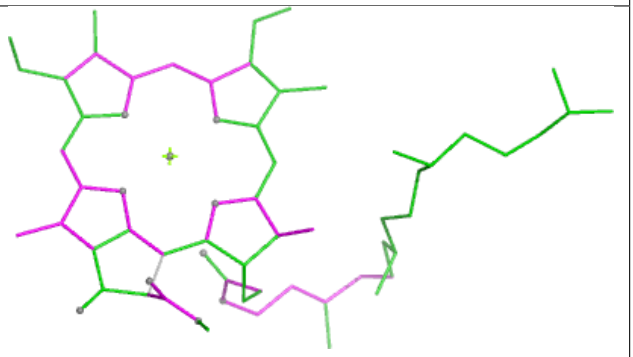
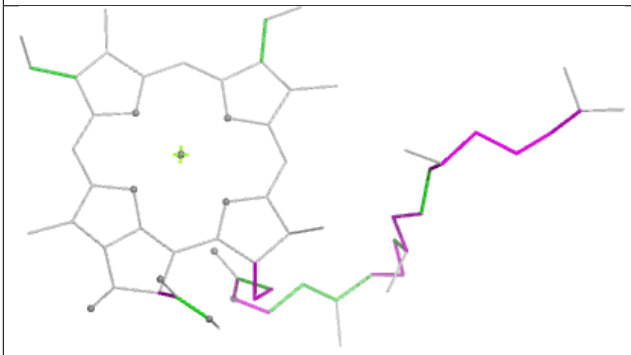


Bond angles



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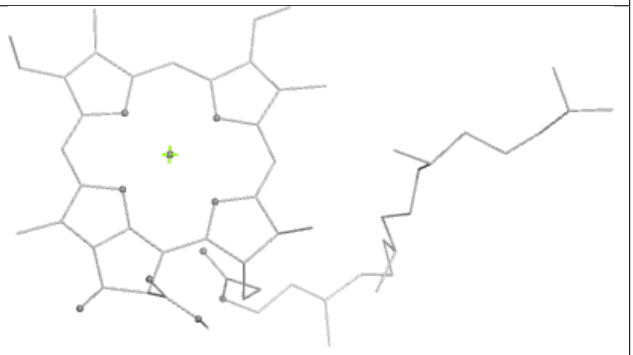
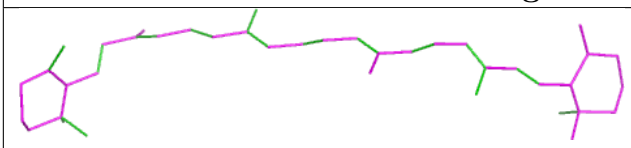


Rings

Ligand BCR C 517



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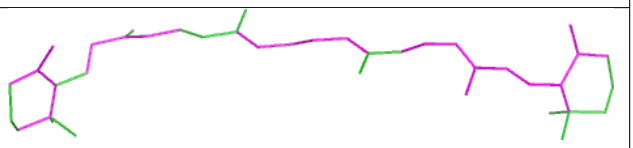
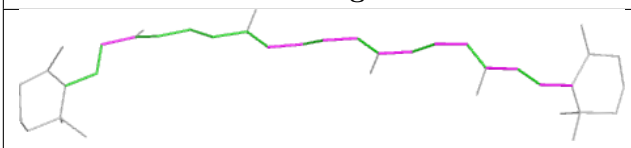


Bond angles



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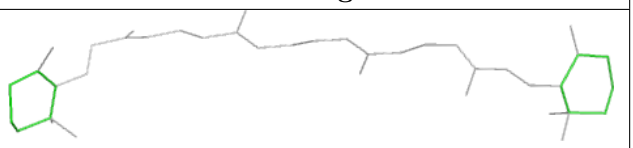
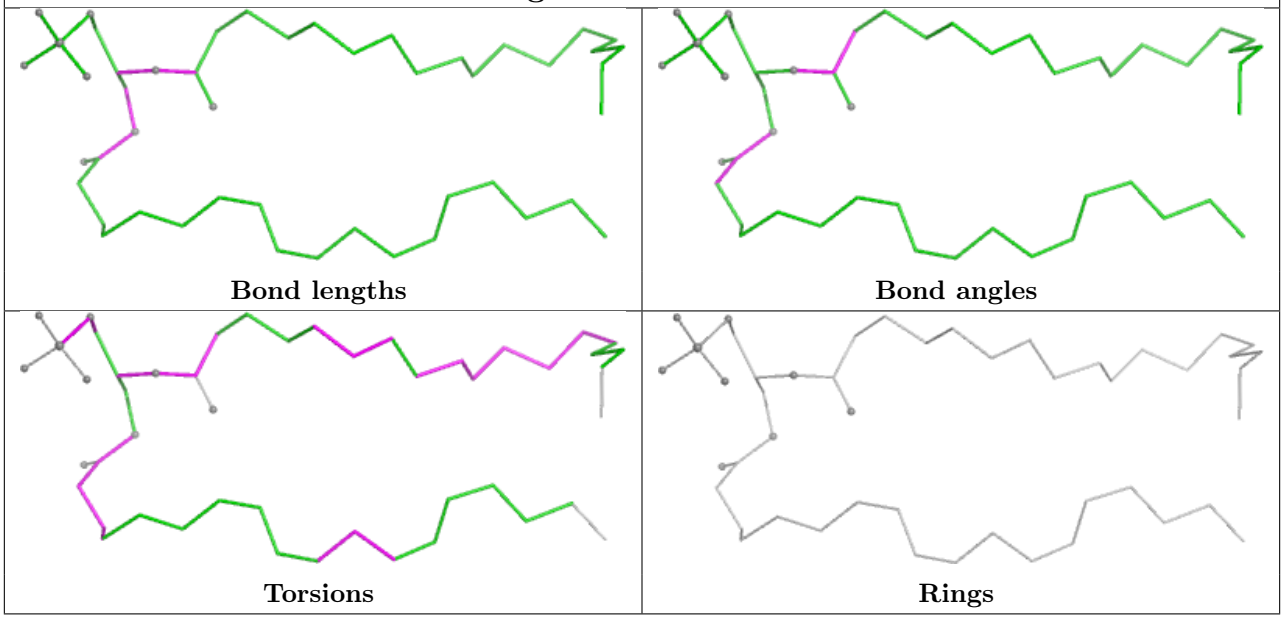
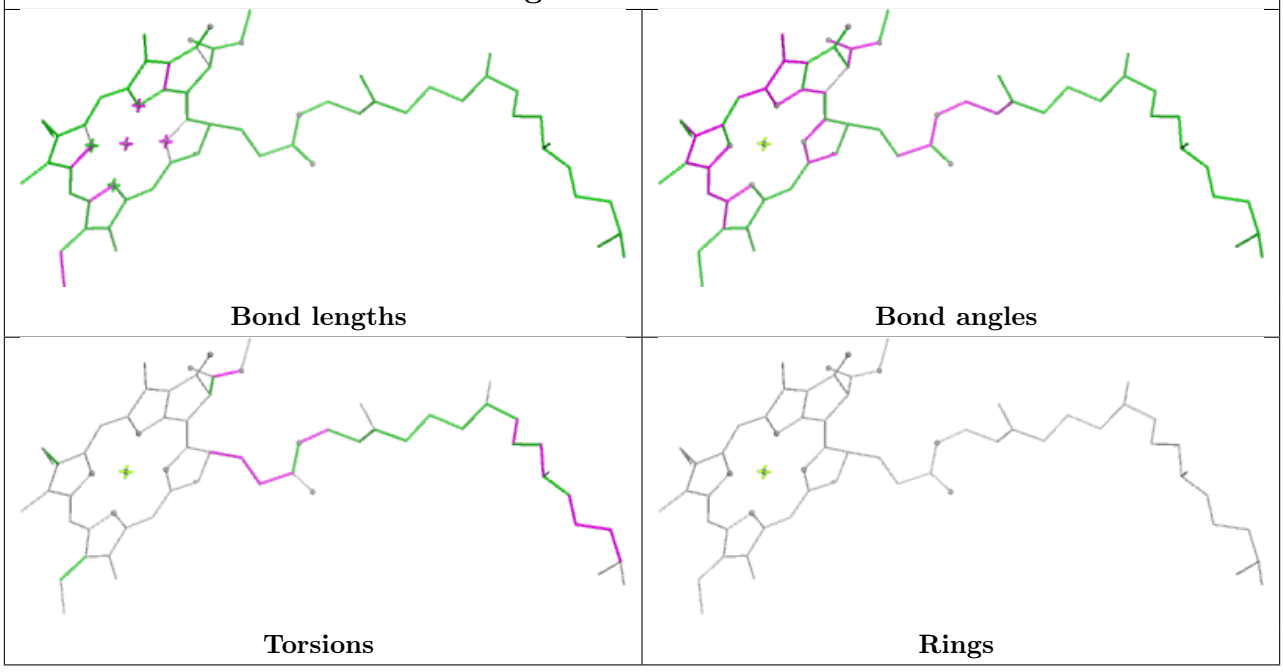


Rings

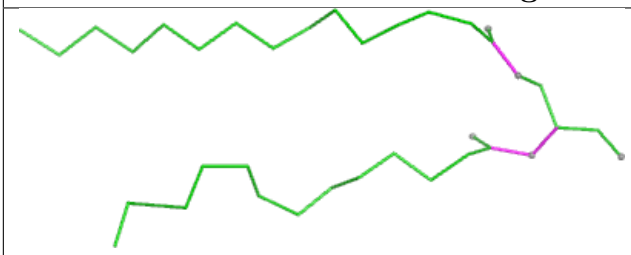
Ligand 3PH B 522



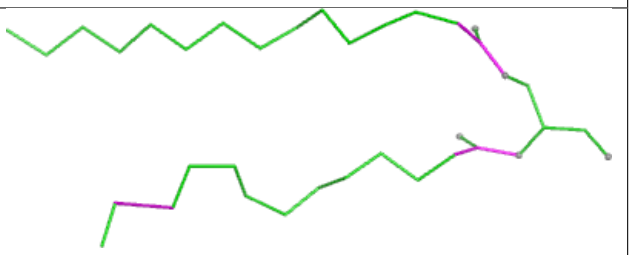
Ligand CLA A 405



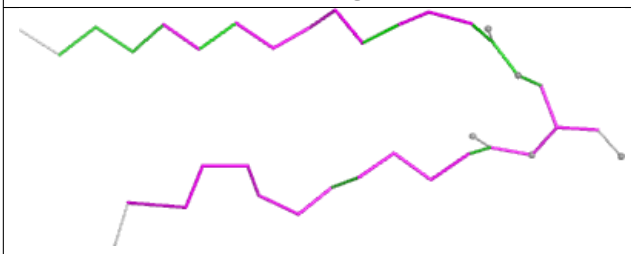
Ligand DGA B 523



Bond lengths



Bond angles



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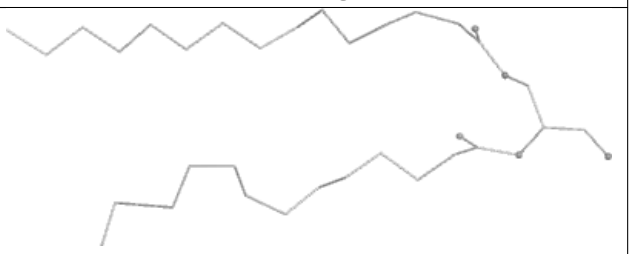
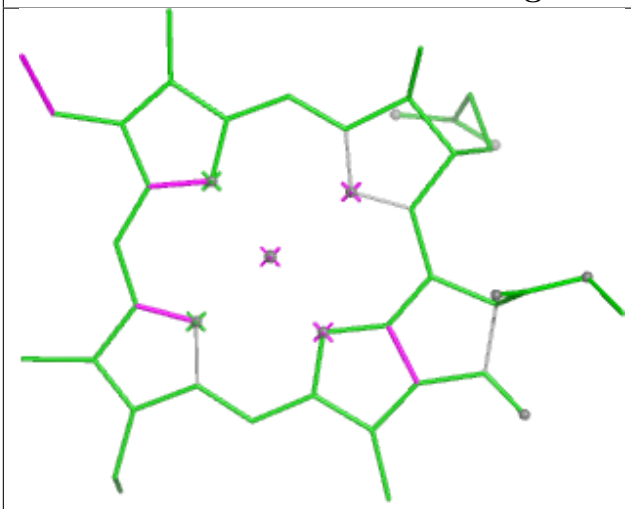


Rings

Ligand CLA C 514



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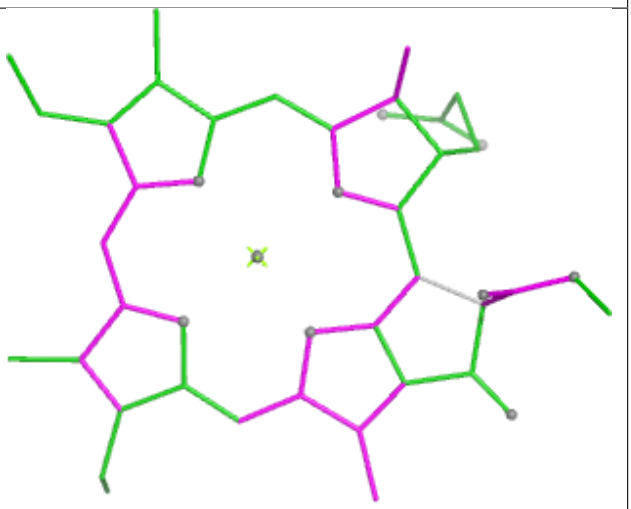
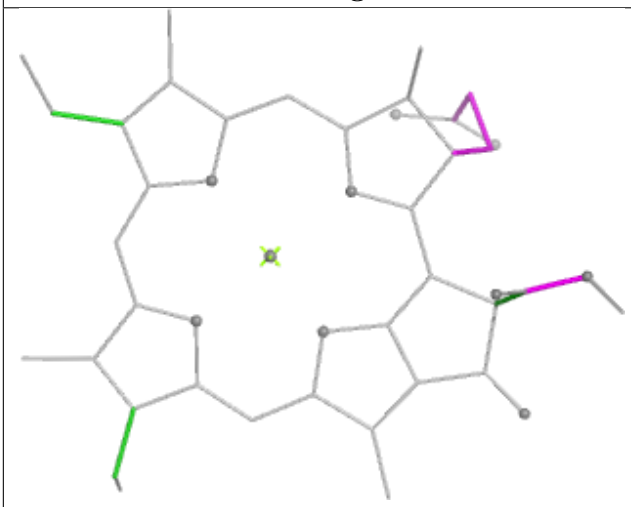


Bond angles



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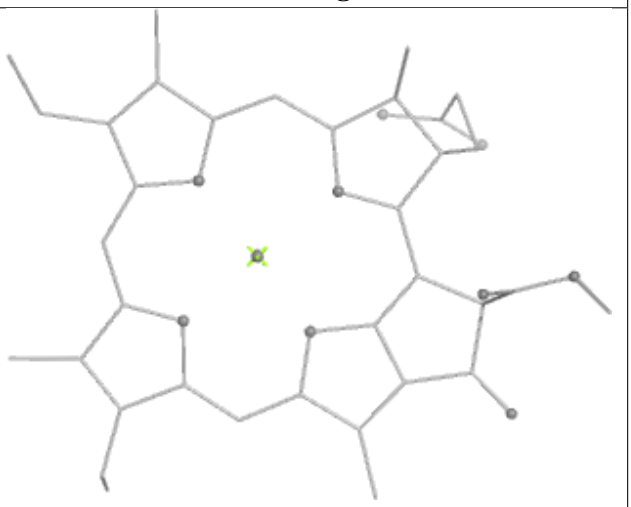
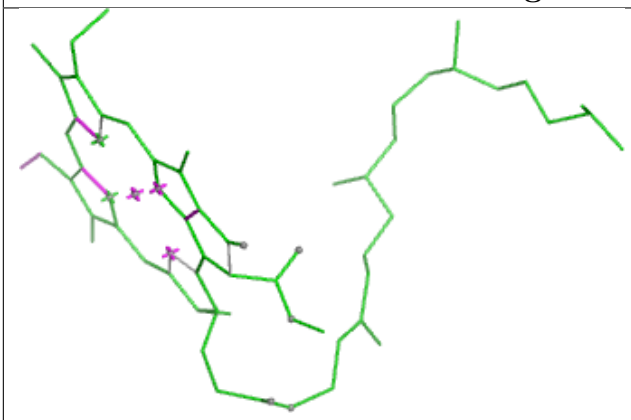
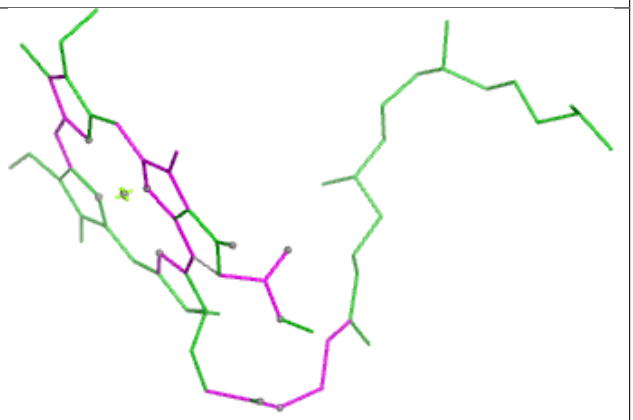


Rings

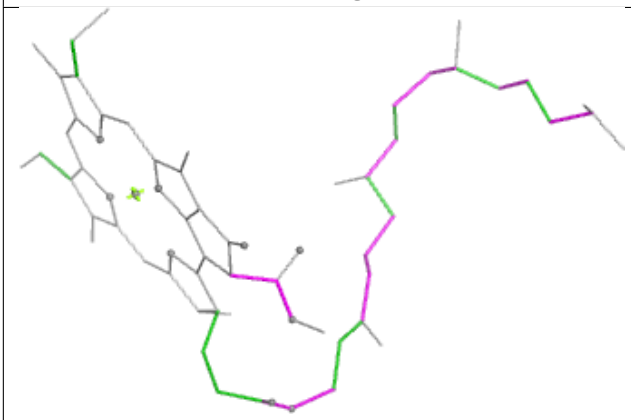
Ligand CLA B 513



Bond lengths



Bond angles

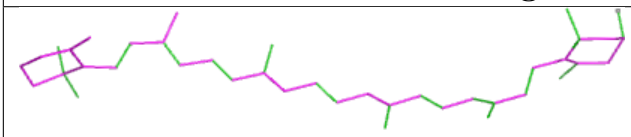


Torsions



Rings

Ligand RRX H 101



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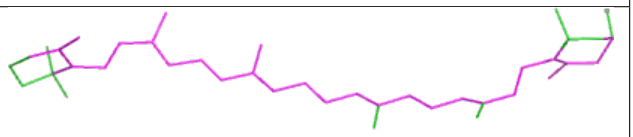
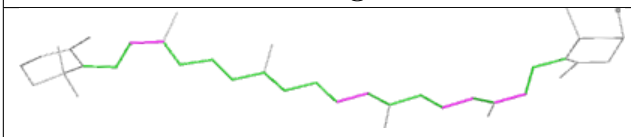
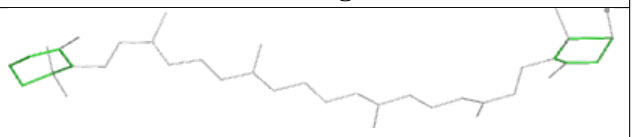


Bond angles

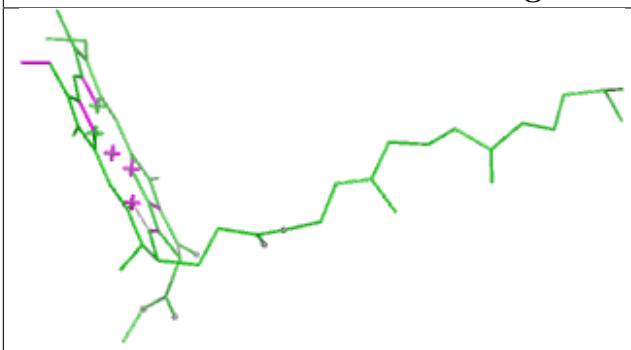


Torsions



Rings

Ligand CLA B 504



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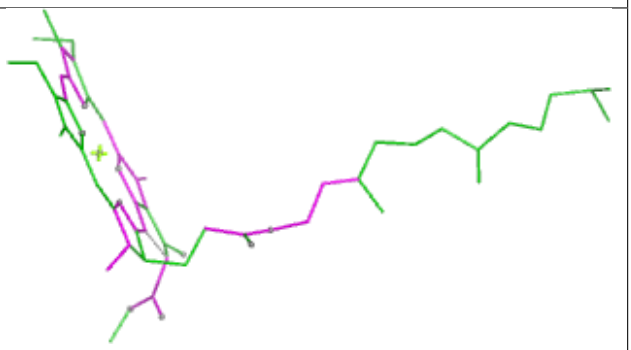
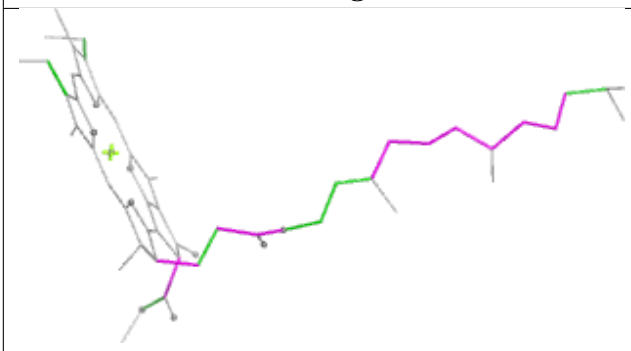
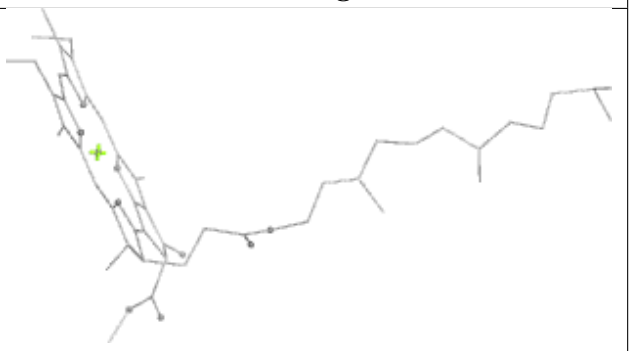


Bond angles

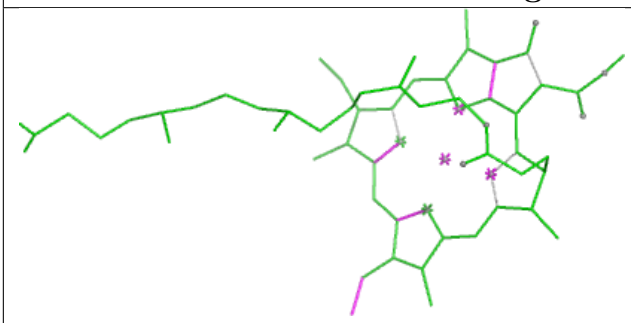


Torsions

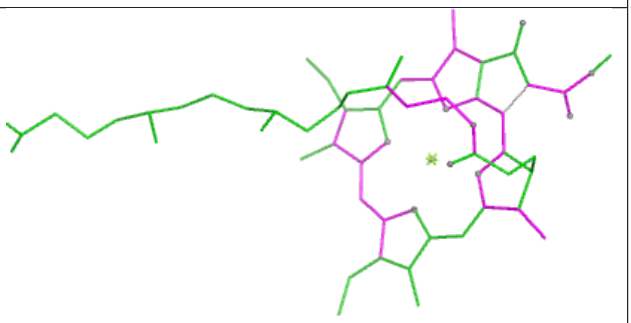


Rings

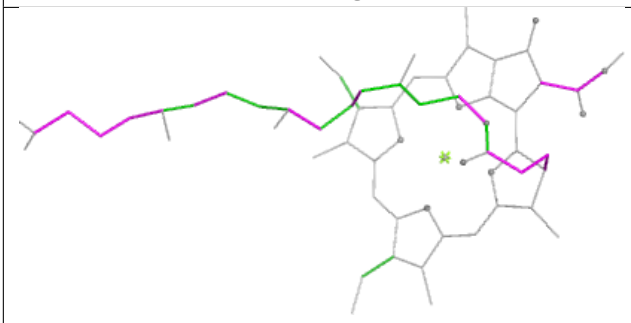
Ligand CLA B 514



Bond lengths



Bond angles

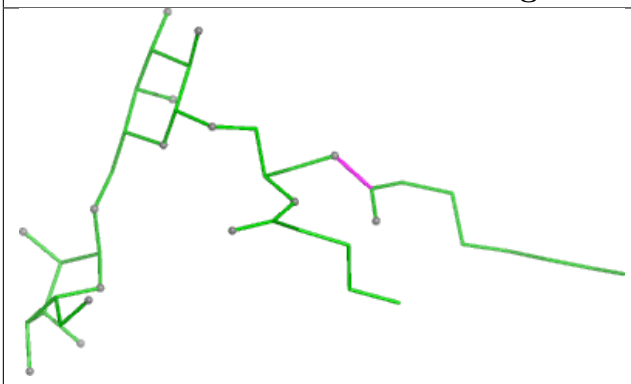


Torsions

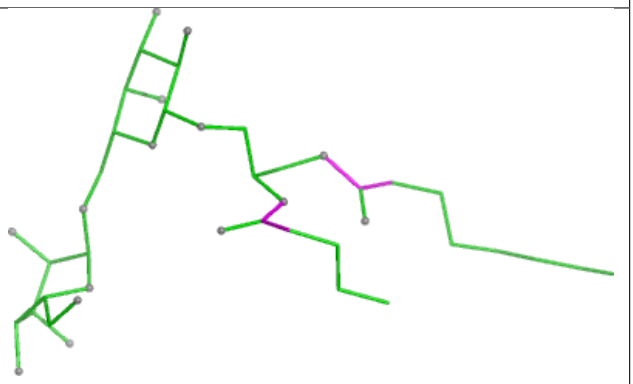


Rings

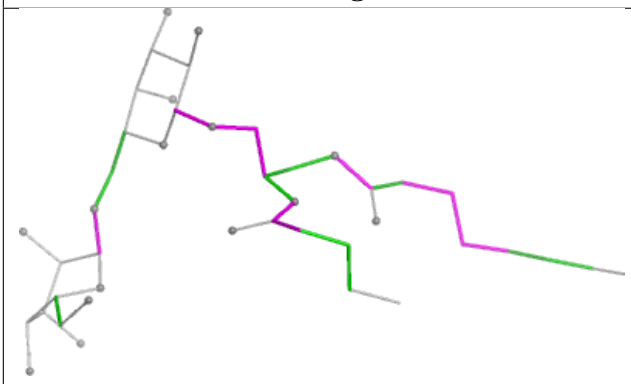
Ligand DGD B 521



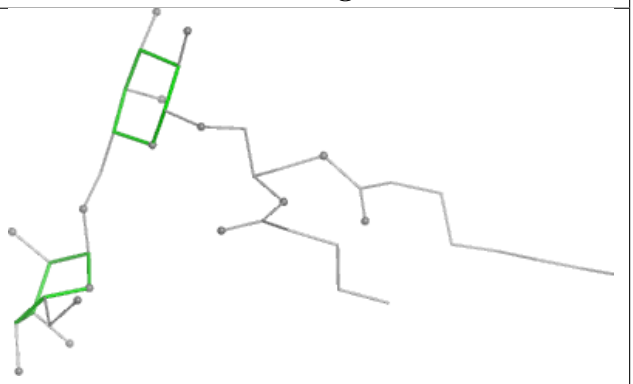
Bond lengths



Bond angles

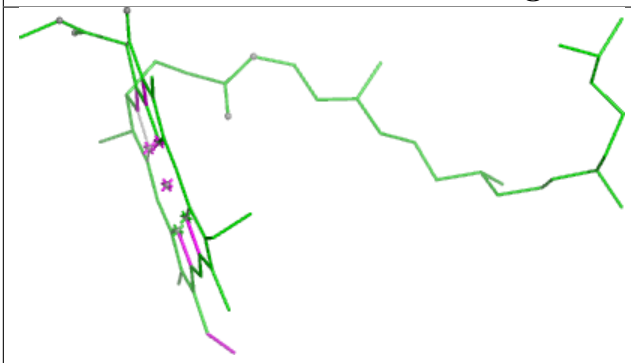


Torsions

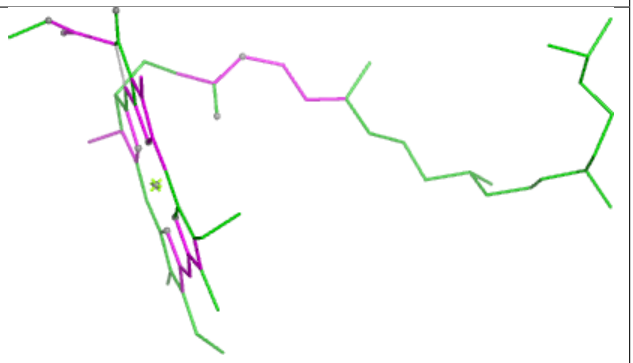


Rings

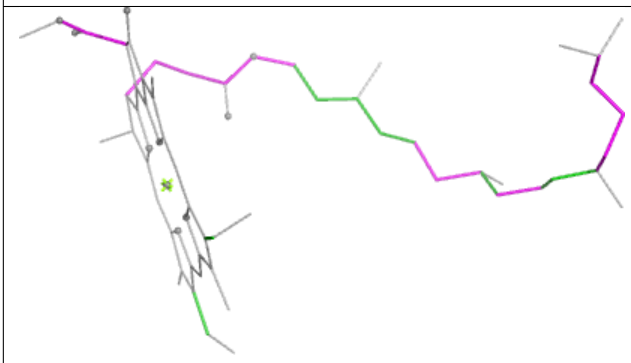
Ligand CLA B 507



Bond lengths



Bond angles

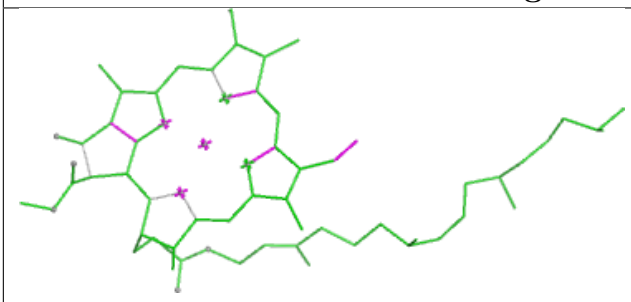


Torsions

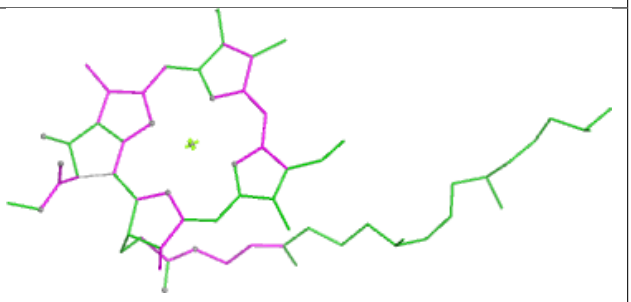


Rings

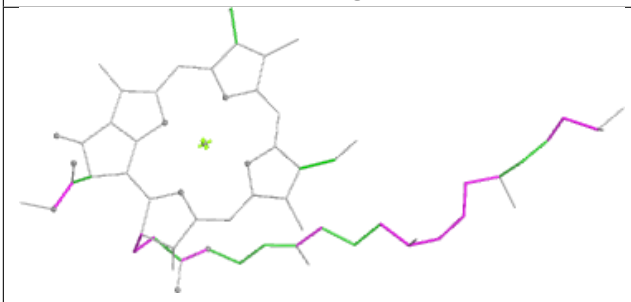
Ligand CLA C 502



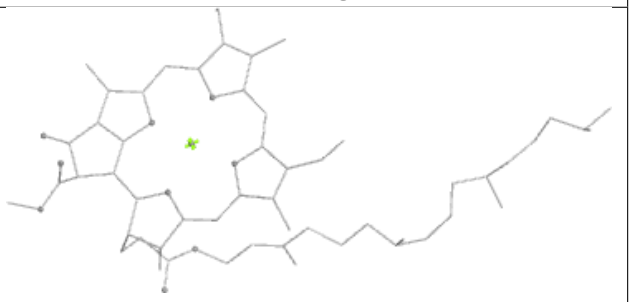
Bond lengths



Bond angles

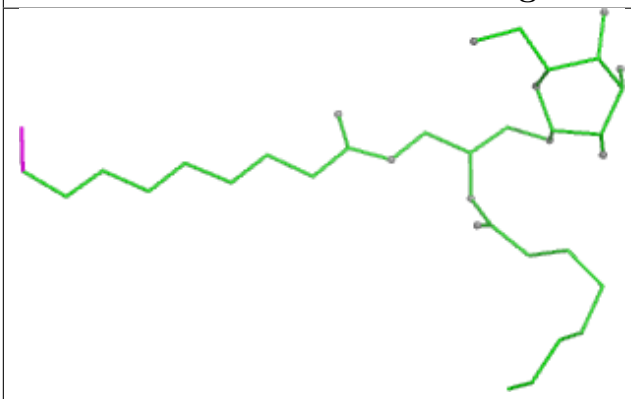


Torsions

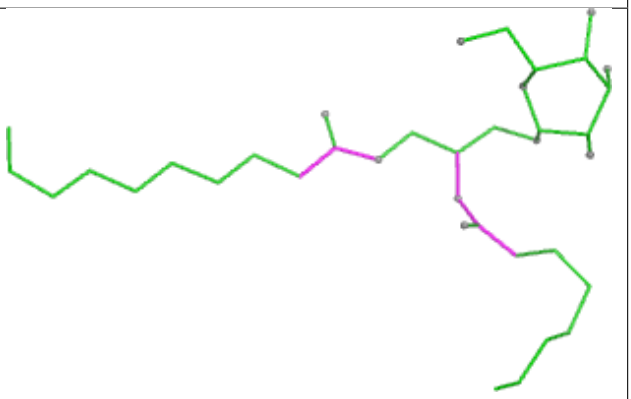


Rings

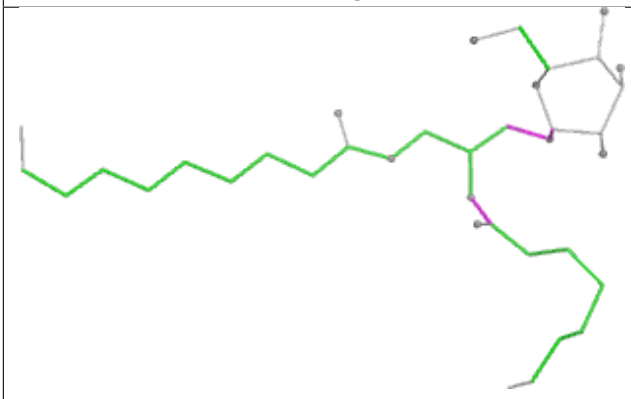
Ligand LMG A 415



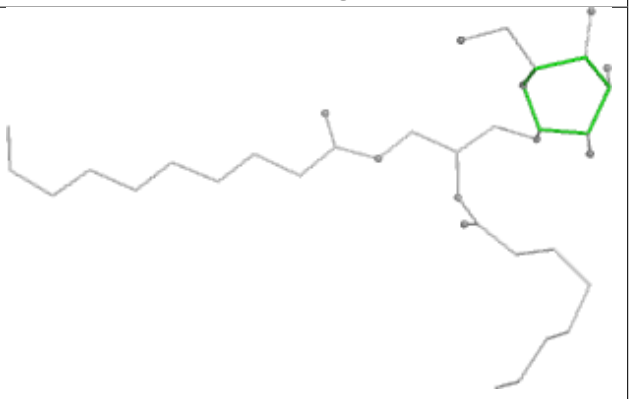
Bond lengths



Bond angles

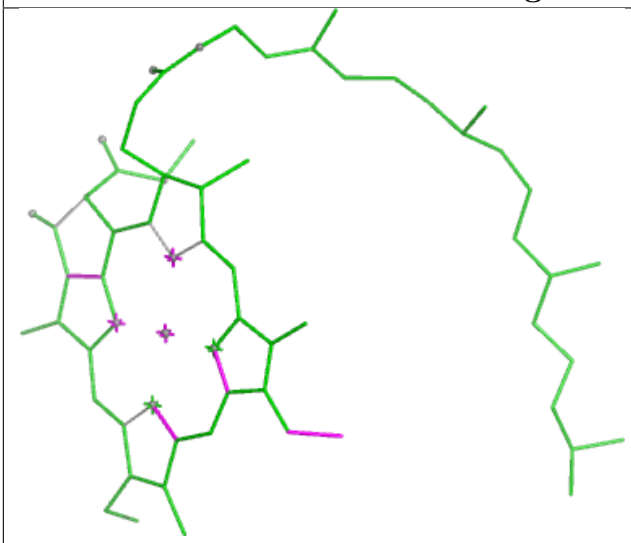


Torsions

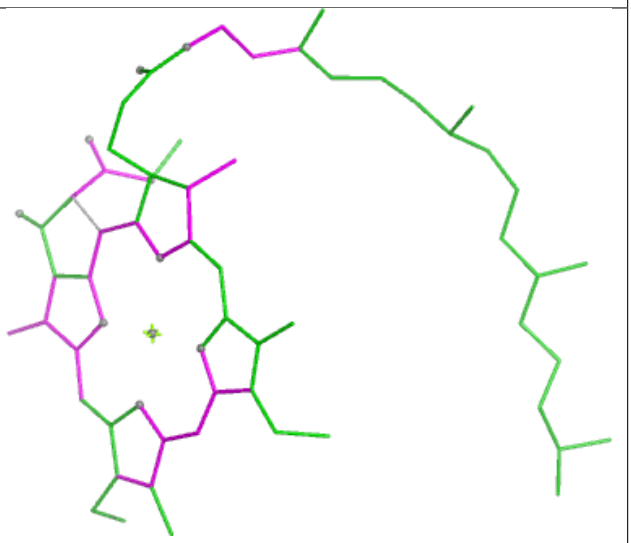


Rings

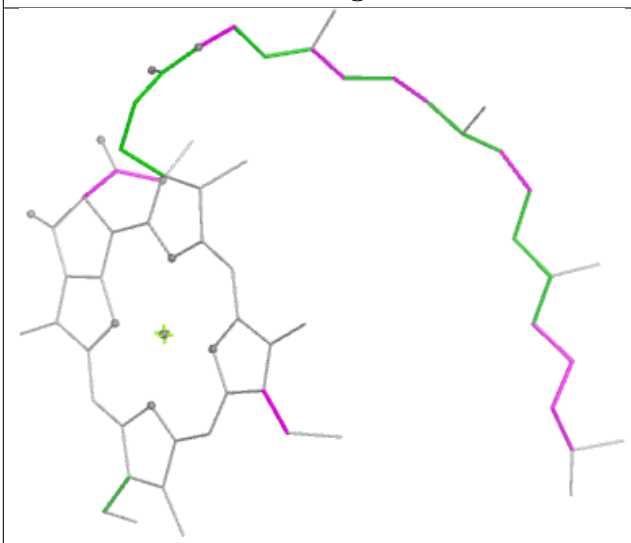
Ligand CLA C 508



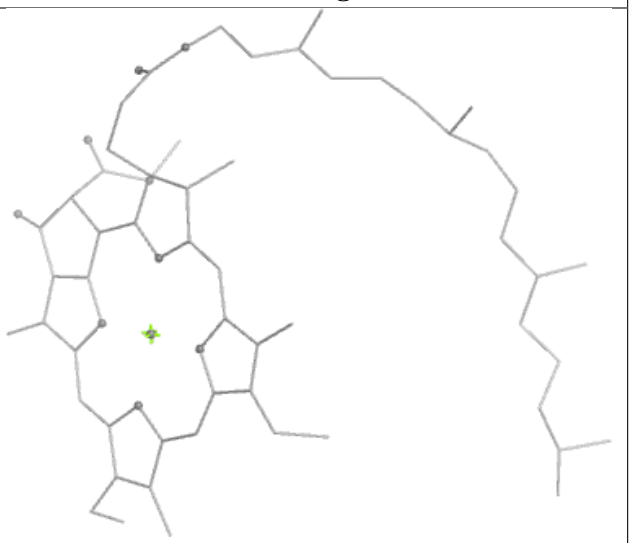
Bond lengths



Bond angles

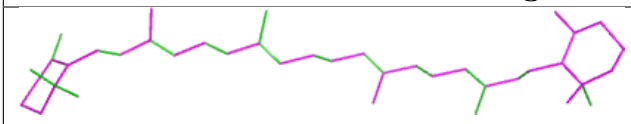


Torsions

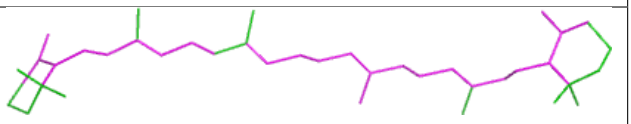


Rings

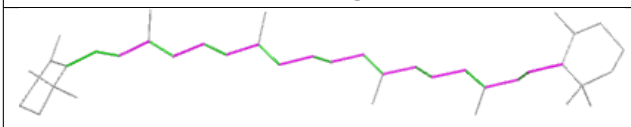
Ligand BCR C 515



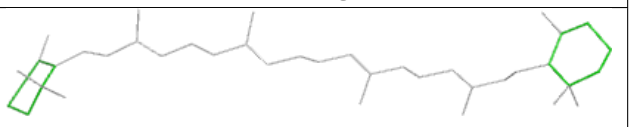
Bond lengths



Bond angles

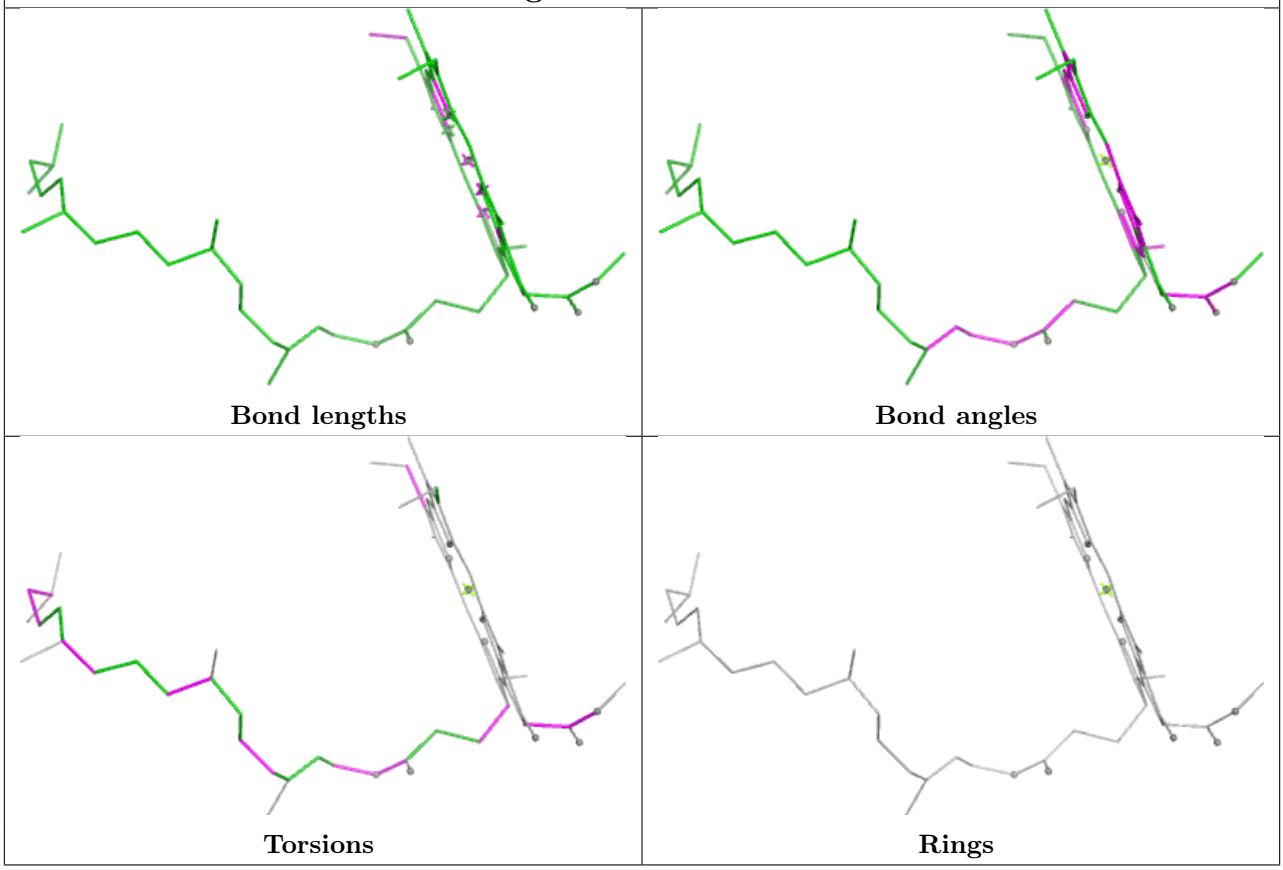


Torsions

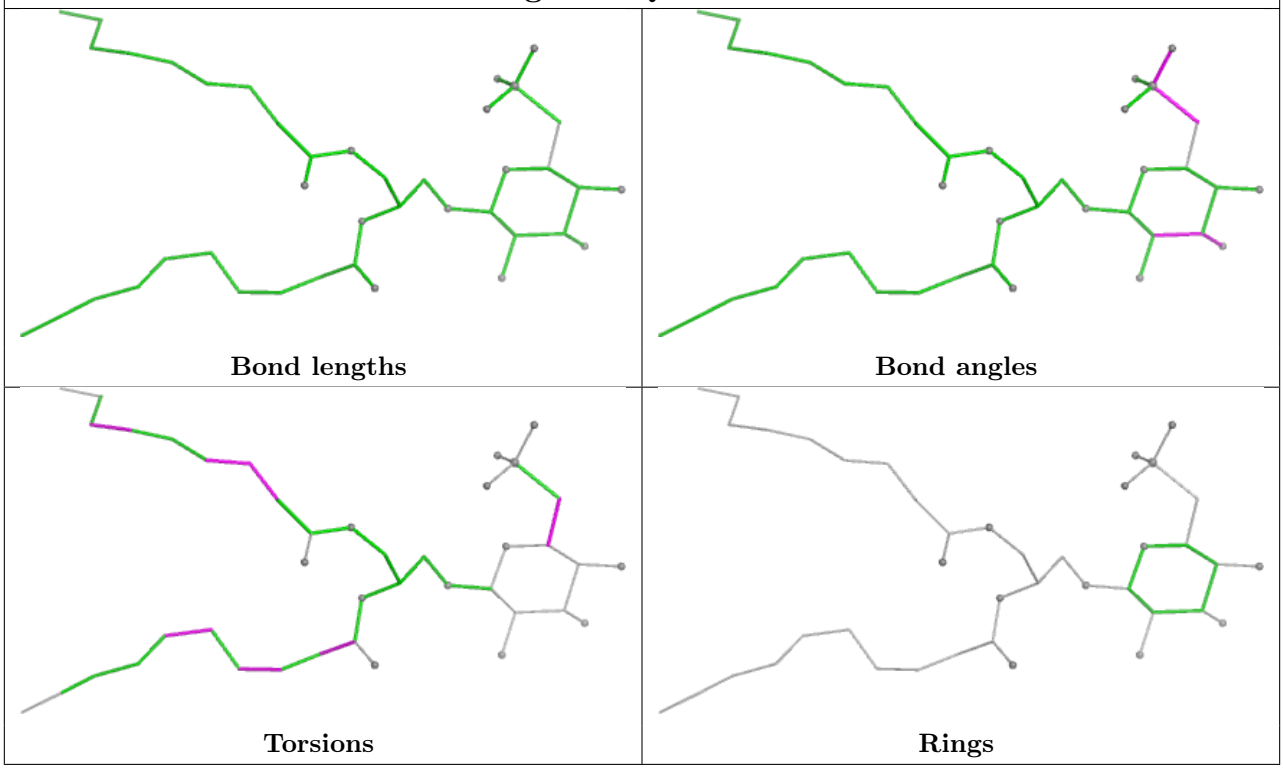


Rings

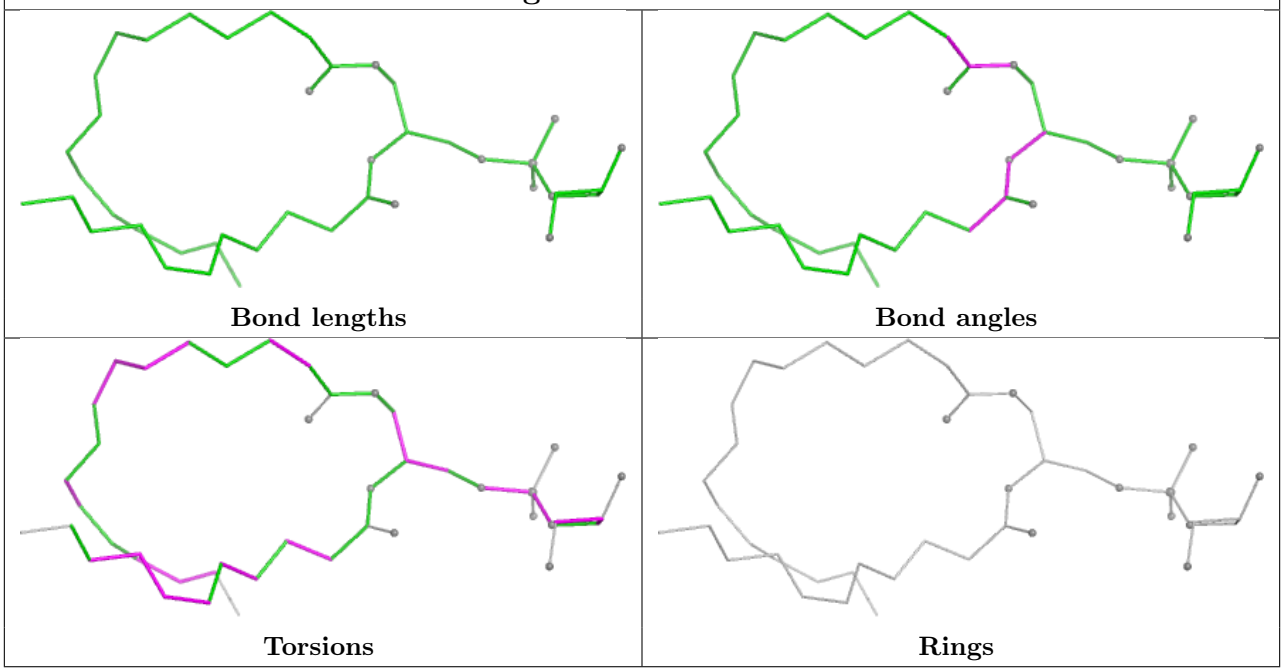
Ligand CLA C 507



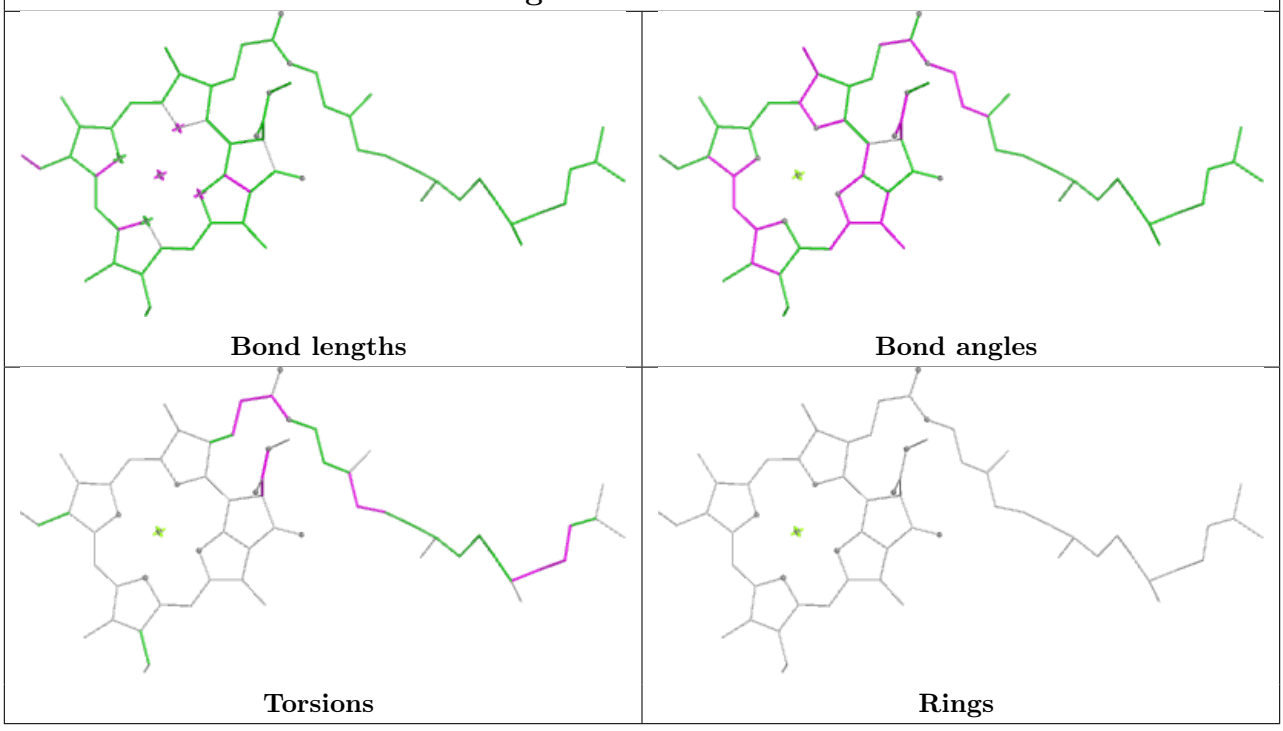
Ligand SQD A 410



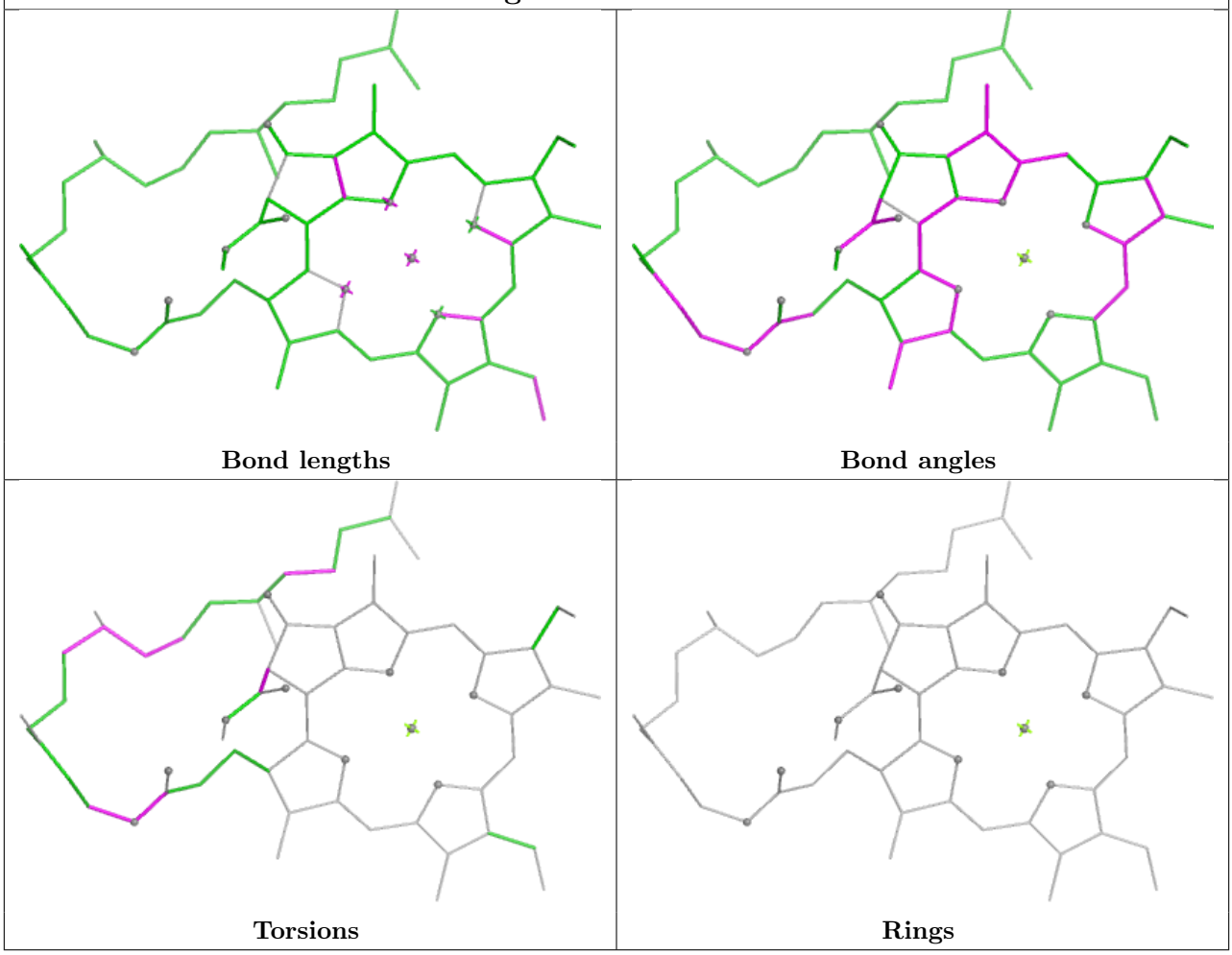
Ligand LHG D 407



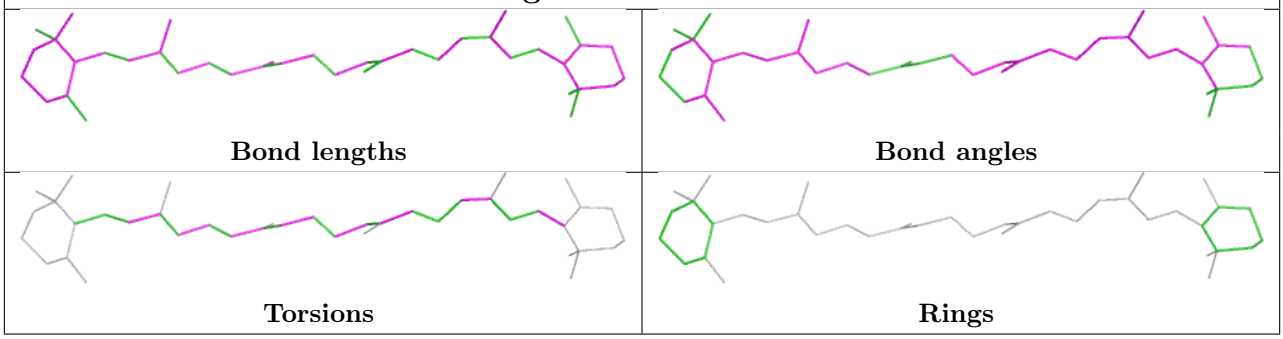
Ligand CLA B 502



Ligand CLA C 510



Ligand BCR A 409



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

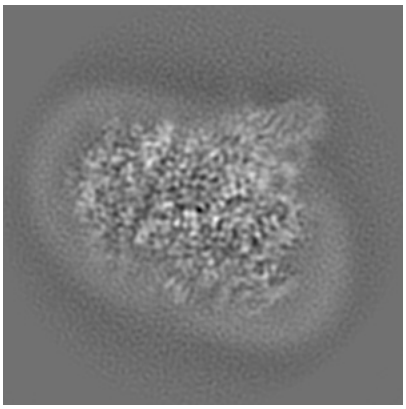
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51482. These allow visual inspection of the internal detail of the map and identification of artifacts.

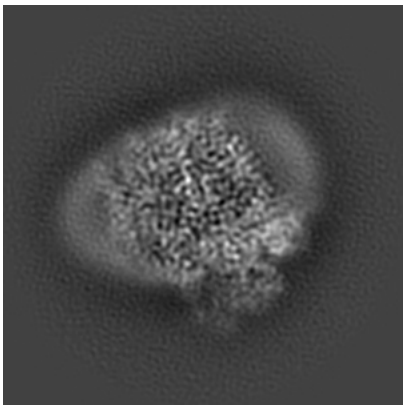
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

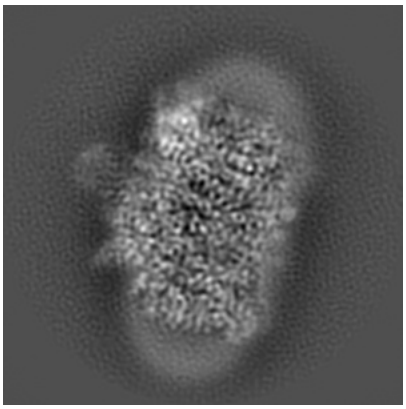
6.1.1 Primary map



X

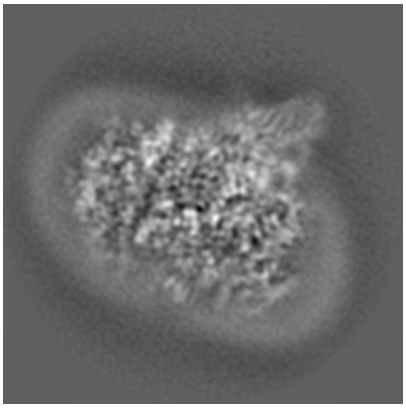


Y

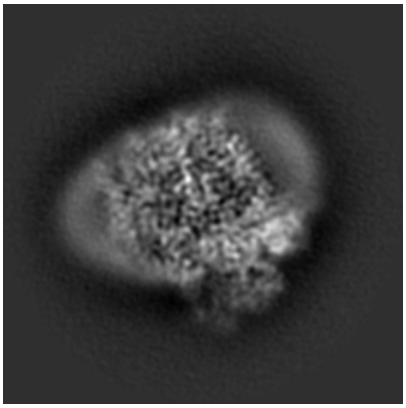


Z

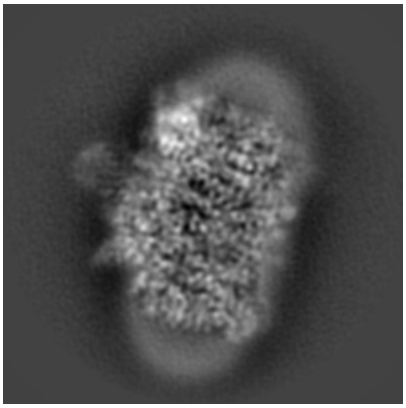
6.1.2 Raw map



X



Y

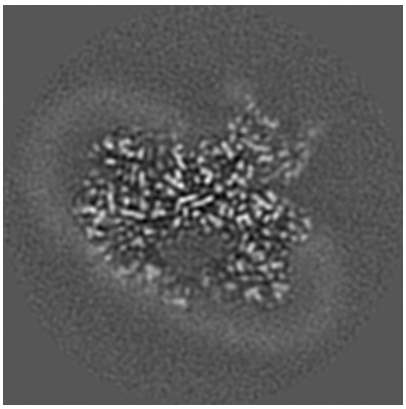


Z

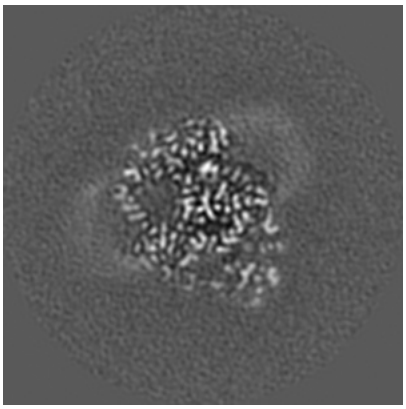
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

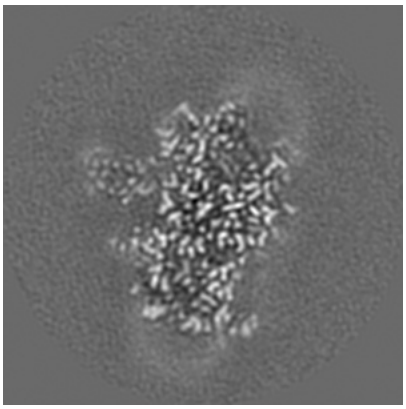
6.2.1 Primary map



X Index: 150

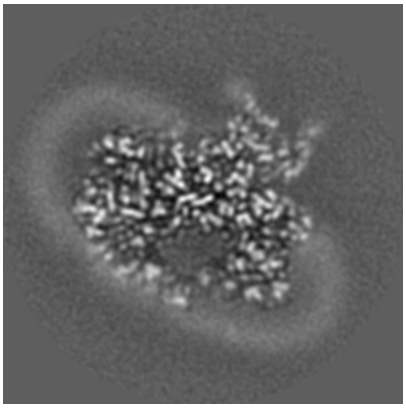


Y Index: 150

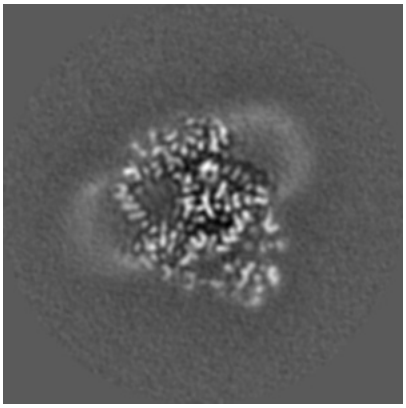


Z Index: 150

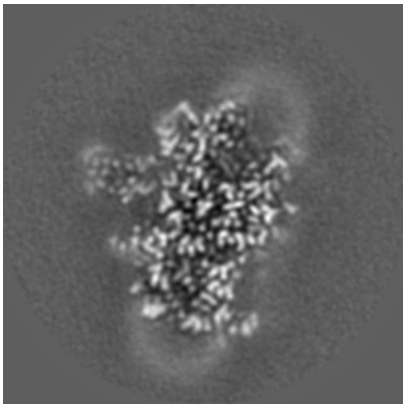
6.2.2 Raw map



X Index: 150



Y Index: 150

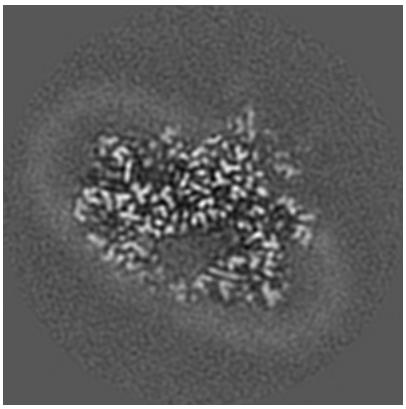


Z Index: 150

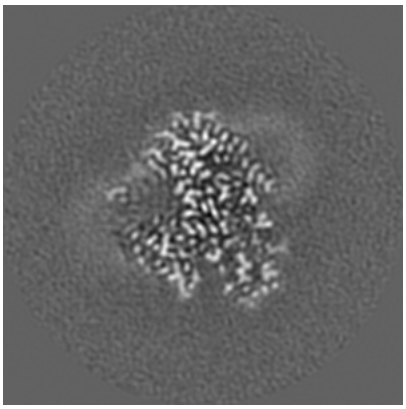
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

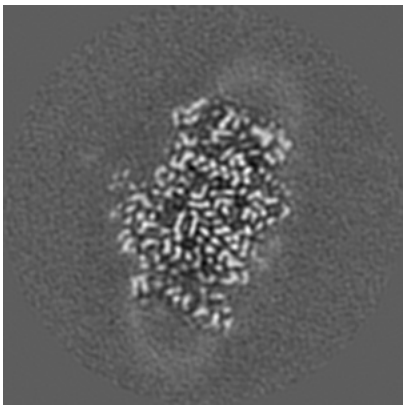
6.3.1 Primary map



X Index: 154

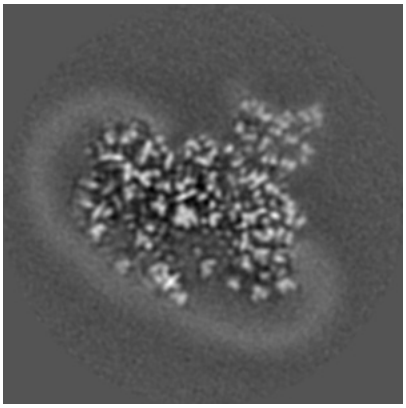


Y Index: 143

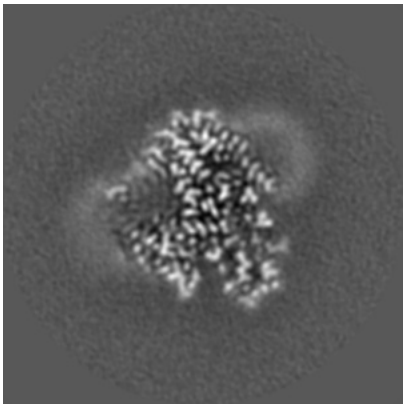


Z Index: 137

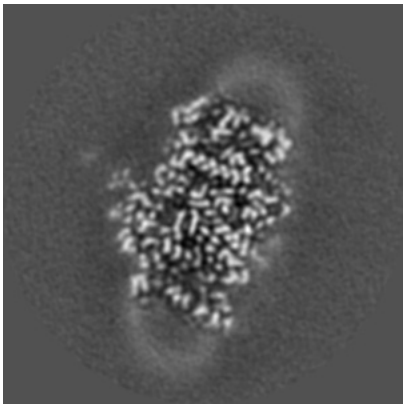
6.3.2 Raw map



X Index: 142



Y Index: 143

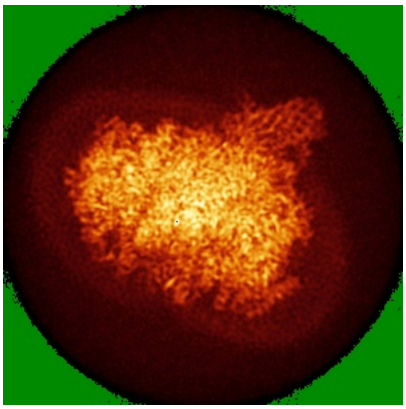


Z Index: 137

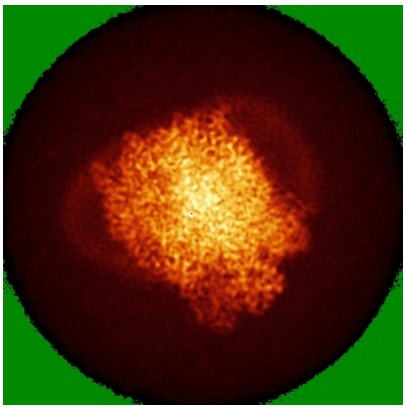
The images above show the largest variance slices of the map in three orthogonal directions.

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

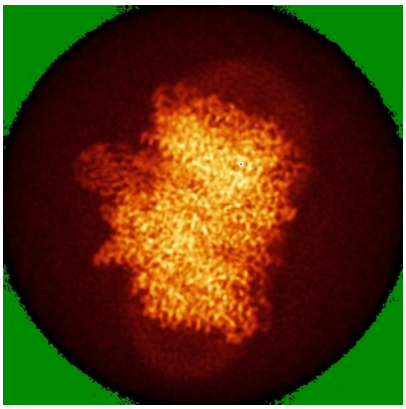
6.4.1 Primary map



X

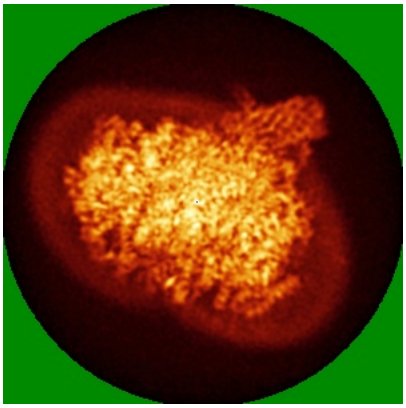


Y

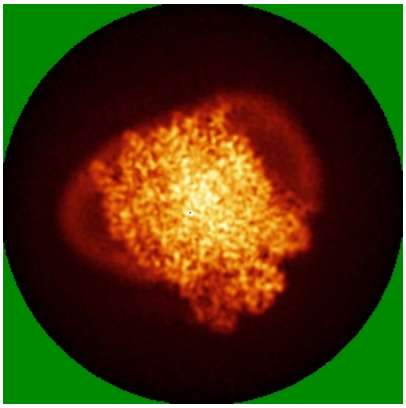


Z

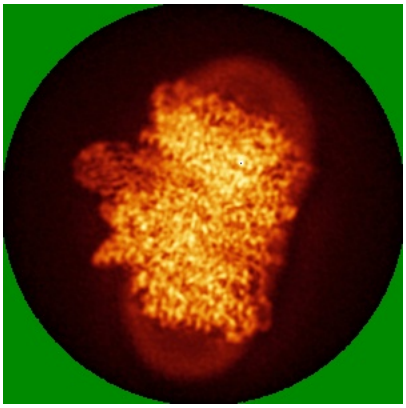
6.4.2 Raw map



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 0.0047. 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.

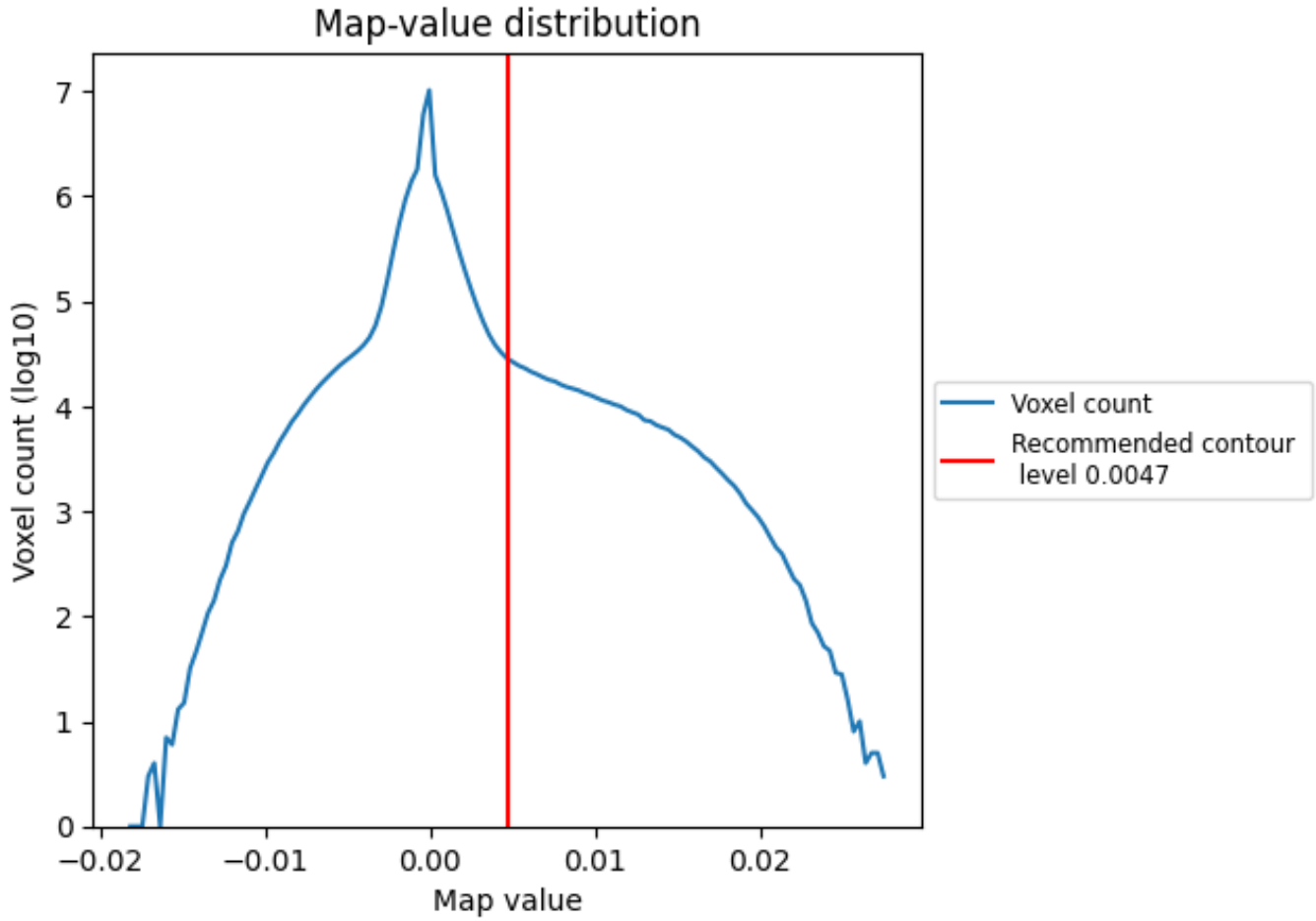
6.6 Mask visualisation (i)

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

7 Map analysis

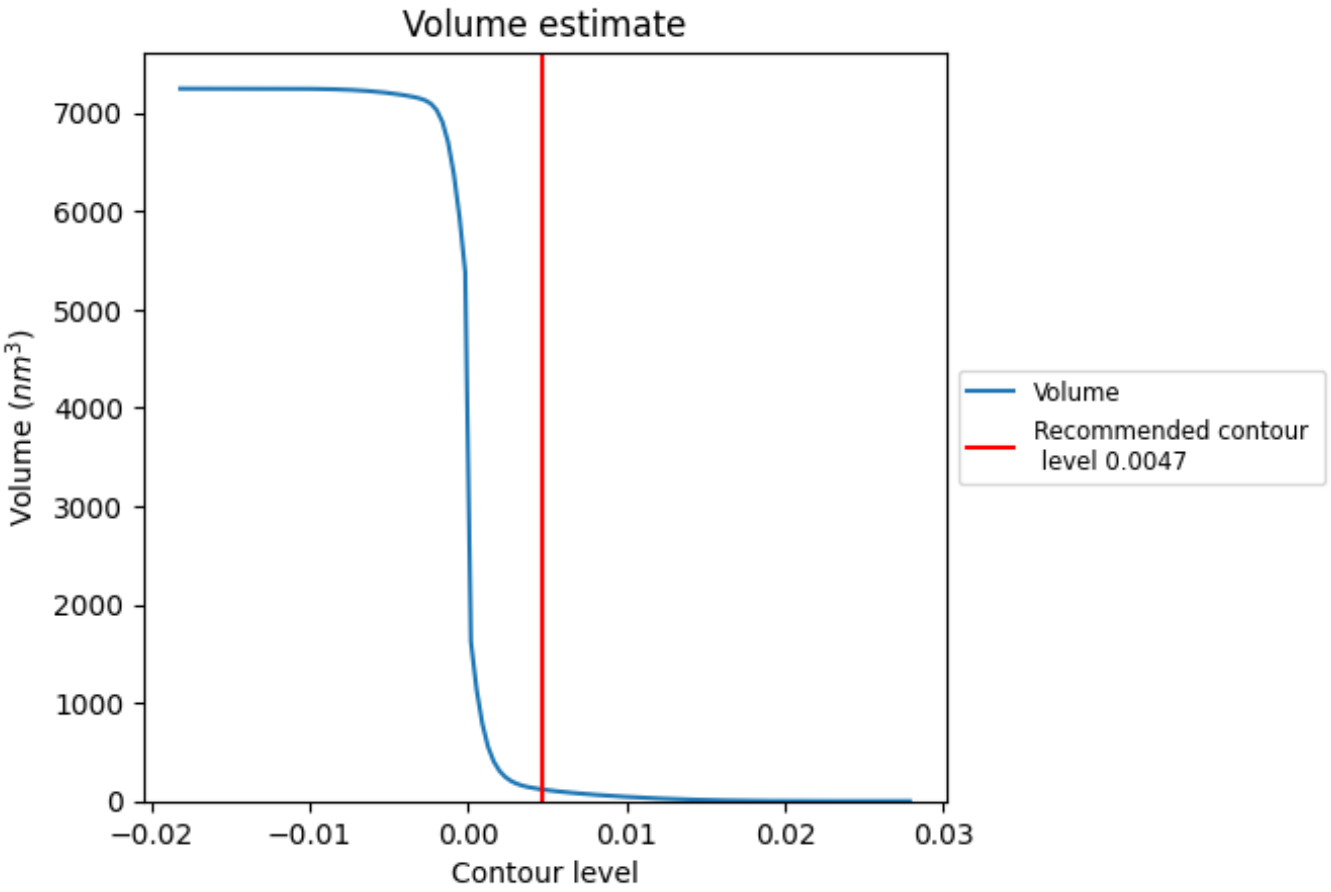
This section contains the results of statistical analysis of the map.

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.

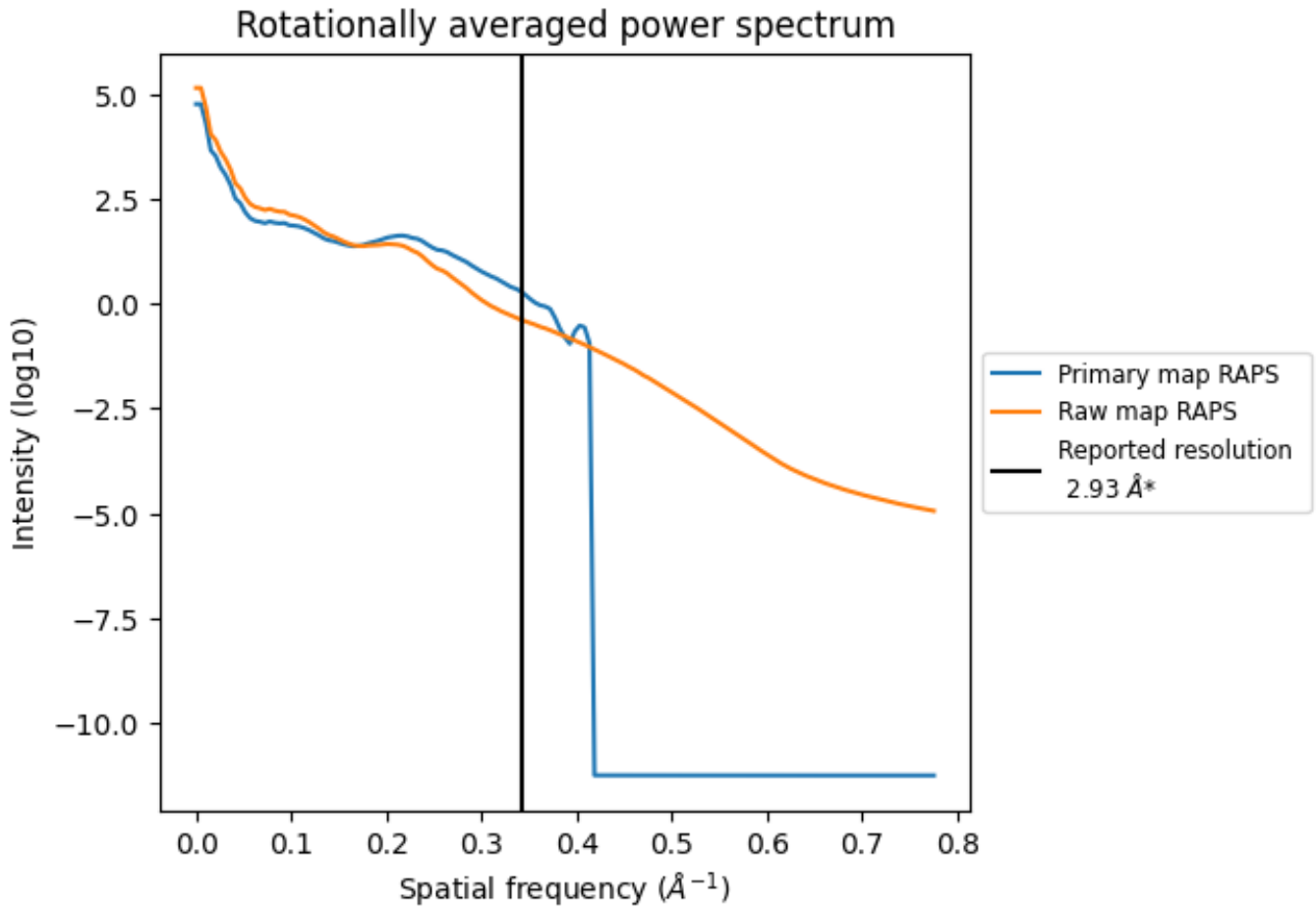
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 107 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)

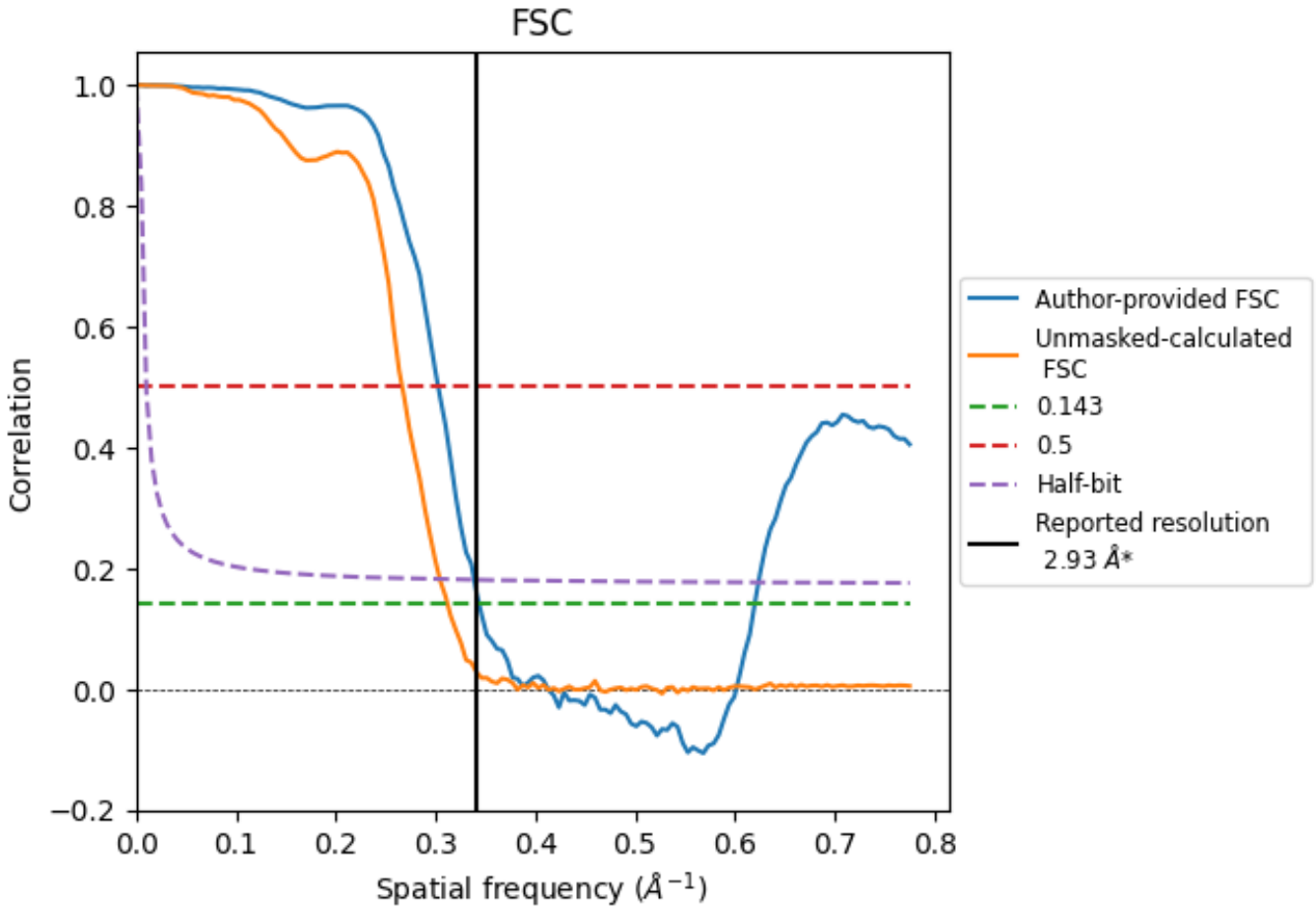


*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

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 0.341 Å^{-1}

8.2 Resolution estimates (i)

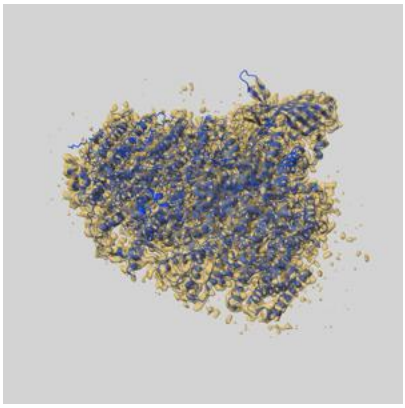
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.91	3.30	2.95
Unmasked-calculated*	3.21	3.75	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

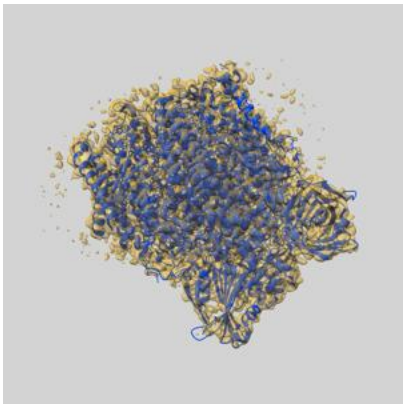
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51482 and PDB model 9GNW. Per-residue inclusion information can be found in section 3 on page 21.

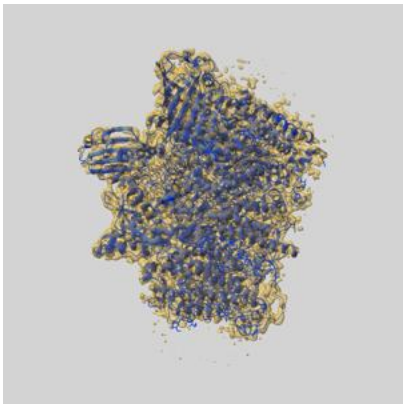
9.1 Map-model overlay



X



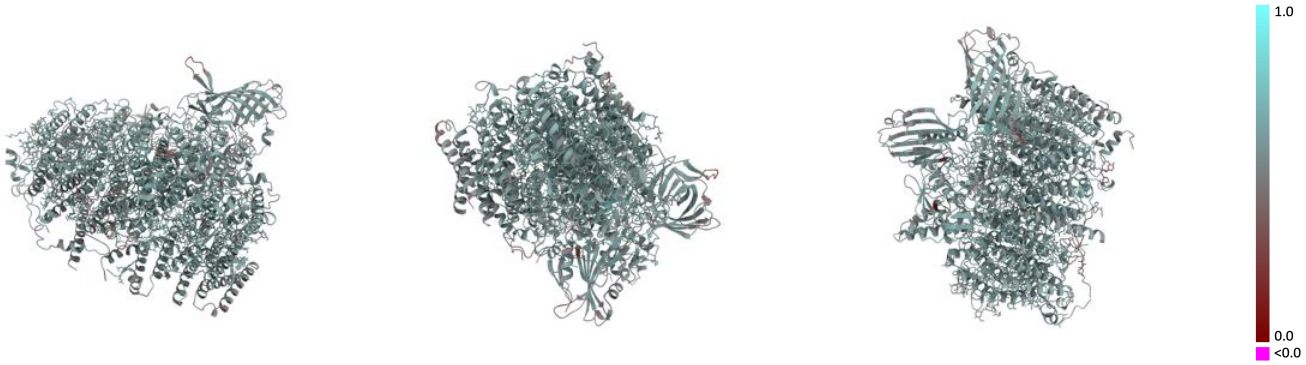
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0047 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.

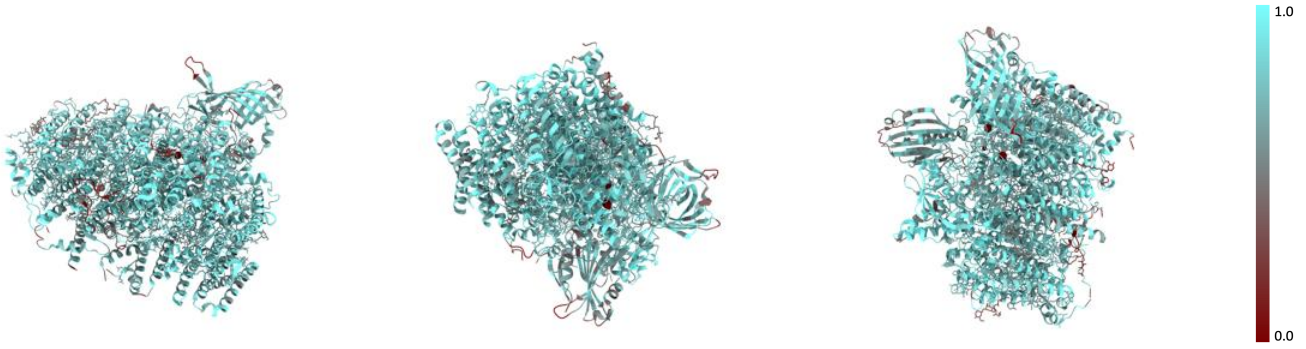
9.2 Q-score mapped to coordinate model (i)



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.

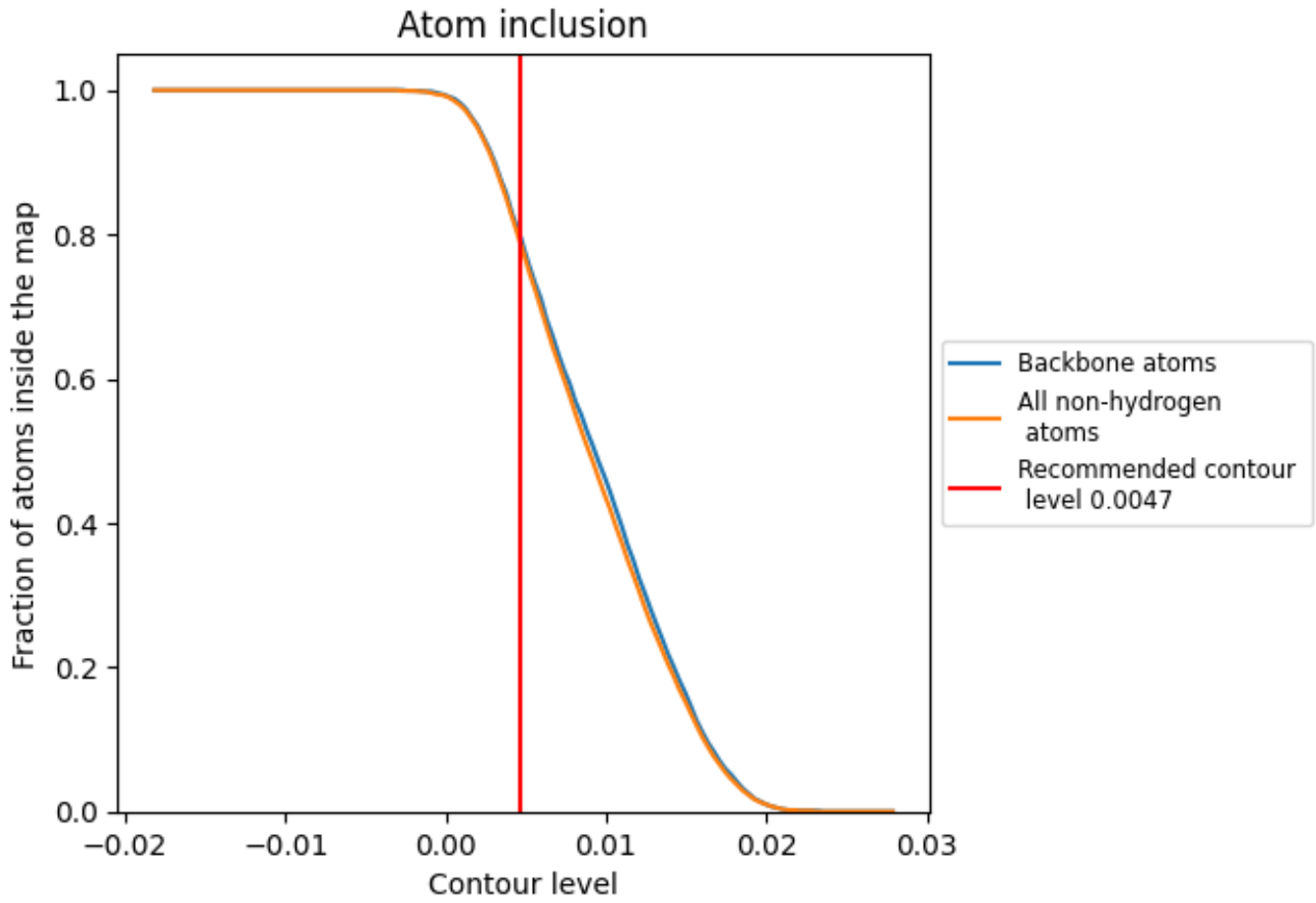
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0047).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.5690
A	0.7720	0.5710
B	0.8280	0.5800
C	0.8450	0.5850
D	0.8440	0.5940
E	0.8120	0.5530
F	0.7850	0.5490
H	0.8020	0.5590
I	0.8740	0.5830
J	0.7080	0.5580
K	0.8120	0.5530
L	0.8280	0.5780
M	0.6450	0.5220
O	0.7270	0.5420
P	0.5960	0.5350
T	0.7560	0.5580
U	0.6040	0.4710
V	0.7470	0.5420
W	0.5480	0.5110
X	0.7200	0.5210
Z	0.7280	0.5050

