Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 03:02 am BST

PDB ID	:	9QEF / pdb_00009qef
EMDB ID	:	EMD-53065
Title	:	Respiratory supercomplex from Mycobacterium smegmatis with decylubiquinone
Authors	:	Kovalova, T.; Krol, S.; Brzezinski, P.; Hogbom, M.
Deposited on	:	2025-03-09
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

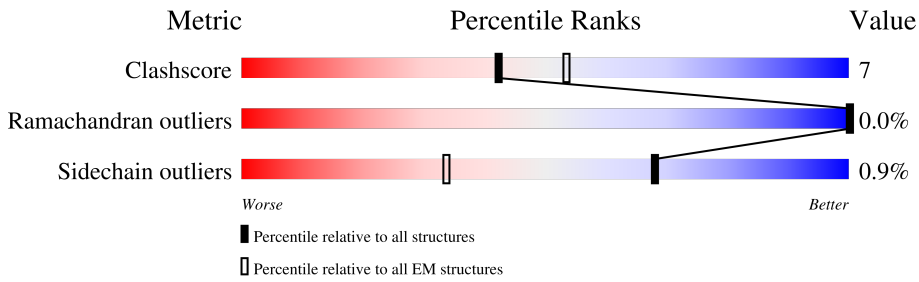
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

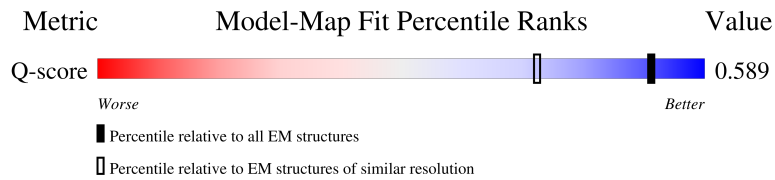
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	C	278	68% 10% • 20%
1	O	278	66% 13% • 20%
2	G	408	84% 9% 7%
2	M	408	84% 10% 7%

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Mol	Chain	Length	Quality of chain
3	H	556	84% 12% •
3	N	556	84% 11% •
4	I	100	66% 7% 27%
4	P	100	64% 9% 27%
5	J	203	• 76% 16% 8%
5	S	203	79% 12% 8%
6	K	139	• 89% 11%
6	T	139	86% 14%
7	L	575	74% 22% •
7	R	575	75% 20% •
8	Q	341	• 73% 11% 16%
8	X	341	• 74% 11% • 14%
9	U	79	• 80% • 16%
9	Z	79	• 77% 8% 15%
10	V	157	78% 13% • 9%
10	a	157	• 76% 15% 9%
11	W	186	23% 69% 10% 20%
11	b	186	38% 72% 8% 20%
12	Y	236	10% 89%
12	c	236	10% • 89%
13	A	123	22% 63% • 33%
13	E	123	15% 67% • 29%
14	B	65	9% 74% 11% 15%
14	F	65	6% 66% 15% • 15%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEC	C	301	X	-	-	-
15	HEC	C	302	X	-	-	-
15	HEC	O	301	X	-	-	-
15	HEC	O	302	X	-	-	-
28	HEA	R	603	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 49157 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 Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	O	223	1623	1008	289	314	12	0	0
1	C	223	1623	1008	289	314	12	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	MET	-	initiating methionine	UNP A0R050
O	18	HIS	-	expression tag	UNP A0R050
O	19	HIS	-	expression tag	UNP A0R050
O	20	HIS	-	expression tag	UNP A0R050
O	21	HIS	-	expression tag	UNP A0R050
O	22	HIS	-	expression tag	UNP A0R050
O	23	HIS	-	expression tag	UNP A0R050
O	24	MET	-	expression tag	UNP A0R050
O	25	GLY	-	expression tag	UNP A0R050
O	26	SER	-	expression tag	UNP A0R050
C	17	MET	-	initiating methionine	UNP A0R050
C	18	HIS	-	expression tag	UNP A0R050
C	19	HIS	-	expression tag	UNP A0R050
C	20	HIS	-	expression tag	UNP A0R050
C	21	HIS	-	expression tag	UNP A0R050
C	22	HIS	-	expression tag	UNP A0R050
C	23	HIS	-	expression tag	UNP A0R050
C	24	MET	-	expression tag	UNP A0R050
C	25	GLY	-	expression tag	UNP A0R050
C	26	SER	-	expression tag	UNP A0R050

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	380	2967	1919	502	535	11	0	0
2	G	380	2967	1919	502	535	11	0	0

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	533	4167	2743	707	699	18	0	0
3	H	533	4167	2743	707	699	18	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	547	LYS	-	expression tag	UNP A0R052
N	548	LEU	-	expression tag	UNP A0R052
N	549	ASP	-	expression tag	UNP A0R052
N	550	TYR	-	expression tag	UNP A0R052
N	551	LYS	-	expression tag	UNP A0R052
N	552	ASP	-	expression tag	UNP A0R052
N	553	ASP	-	expression tag	UNP A0R052
N	554	ASP	-	expression tag	UNP A0R052
N	555	ASP	-	expression tag	UNP A0R052
N	556	LYS	-	expression tag	UNP A0R052
H	547	LYS	-	expression tag	UNP A0R052
H	548	LEU	-	expression tag	UNP A0R052
H	549	ASP	-	expression tag	UNP A0R052
H	550	TYR	-	expression tag	UNP A0R052
H	551	LYS	-	expression tag	UNP A0R052
H	552	ASP	-	expression tag	UNP A0R052
H	553	ASP	-	expression tag	UNP A0R052
H	554	ASP	-	expression tag	UNP A0R052
H	555	ASP	-	expression tag	UNP A0R052
H	556	LYS	-	expression tag	UNP A0R052

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	73	586	385	107	90	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	73	586	385	107	90	4	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4
I	1	MET	-	initiating methionine	UNP A0QVH4
I	2	SER	-	expression tag	UNP A0QVH4
I	3	SER	-	expression tag	UNP A0QVH4
I	4	THR	-	expression tag	UNP A0QVH4
I	5	GLN	-	expression tag	UNP A0QVH4
I	6	ASP	-	expression tag	UNP A0QVH4
I	7	ARG	-	expression tag	UNP A0QVH4
I	8	SER	-	expression tag	UNP A0QVH4
I	9	GLN	-	expression tag	UNP A0QVH4
I	10	LEU	-	expression tag	UNP A0QVH4
I	11	ASP	-	expression tag	UNP A0QVH4
I	12	PRO	-	expression tag	UNP A0QVH4
I	13	GLU	-	expression tag	UNP A0QVH4
I	14	GLU	-	expression tag	UNP A0QVH4
I	15	GLN	-	expression tag	UNP A0QVH4
I	16	PRO	-	expression tag	UNP A0QVH4
I	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	187	1465	982	234	242	7	0	0
5	J	187	1465	982	234	242	7	0	0

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	139	1077	719	167	188	3	0	0
6	K	139	1077	719	167	188	3	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	551	4369	2936	694	713	26	0	0
7	L	551	4369	2936	694	713	26	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2U9PNL2
R	2	VAL	-	expression tag	UNP A0A2U9PNL2
R	3	ALA	-	expression tag	UNP A0A2U9PNL2
R	4	GLU	-	expression tag	UNP A0A2U9PNL2
R	5	ALA	-	expression tag	UNP A0A2U9PNL2
R	6	PRO	-	expression tag	UNP A0A2U9PNL2
R	7	PRO	-	expression tag	UNP A0A2U9PNL2
R	8	ILE	-	expression tag	UNP A0A2U9PNL2
R	9	GLY	-	expression tag	UNP A0A2U9PNL2
R	10	GLU	-	expression tag	UNP A0A2U9PNL2
R	11	LEU	-	expression tag	UNP A0A2U9PNL2
R	12	GLU	-	expression tag	UNP A0A2U9PNL2
R	13	ALA	-	expression tag	UNP A0A2U9PNL2
R	14	ARG	-	expression tag	UNP A0A2U9PNL2
R	15	ARG	-	expression tag	UNP A0A2U9PNL2
R	16	PRO	-	expression tag	UNP A0A2U9PNL2
R	17	PHE	-	expression tag	UNP A0A2U9PNL2
R	18	PRO	-	expression tag	UNP A0A2U9PNL2
R	19	GLU	-	expression tag	UNP A0A2U9PNL2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	20	ARG	-	expression tag	UNP A0A2U9PNL2
L	1	MET	-	initiating methionine	UNP A0A2U9PNL2
L	2	VAL	-	expression tag	UNP A0A2U9PNL2
L	3	ALA	-	expression tag	UNP A0A2U9PNL2
L	4	GLU	-	expression tag	UNP A0A2U9PNL2
L	5	ALA	-	expression tag	UNP A0A2U9PNL2
L	6	PRO	-	expression tag	UNP A0A2U9PNL2
L	7	PRO	-	expression tag	UNP A0A2U9PNL2
L	8	ILE	-	expression tag	UNP A0A2U9PNL2
L	9	GLY	-	expression tag	UNP A0A2U9PNL2
L	10	GLU	-	expression tag	UNP A0A2U9PNL2
L	11	LEU	-	expression tag	UNP A0A2U9PNL2
L	12	GLU	-	expression tag	UNP A0A2U9PNL2
L	13	ALA	-	expression tag	UNP A0A2U9PNL2
L	14	ARG	-	expression tag	UNP A0A2U9PNL2
L	15	ARG	-	expression tag	UNP A0A2U9PNL2
L	16	PRO	-	expression tag	UNP A0A2U9PNL2
L	17	PHE	-	expression tag	UNP A0A2U9PNL2
L	18	PRO	-	expression tag	UNP A0A2U9PNL2
L	19	GLU	-	expression tag	UNP A0A2U9PNL2
L	20	ARG	-	expression tag	UNP A0A2U9PNL2

- Molecule 8 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Q	287	2293	1487	378	419	9	0	0
8	X	292	2328	1508	383	427	10	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	U	66	499	329	84	85	1	0	0
9	Z	67	507	334	85	86	2	0	0

- Molecule 10 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	V	143	1024	647	174	201	2	0	0
10	a	143	1024	647	174	201	2	0	0

- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	148	1075	664	180	230	1	0	0
11	b	149	1083	670	181	231	1	0	0

- Molecule 12 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Y	25	168	103	26	38	1	0	0
12	c	25	168	103	26	38	1	0	0

- Molecule 13 is a protein called Co-purified transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	87	660	427	121	110	2	0	0
13	A	83	620	404	109	106	1	0	0

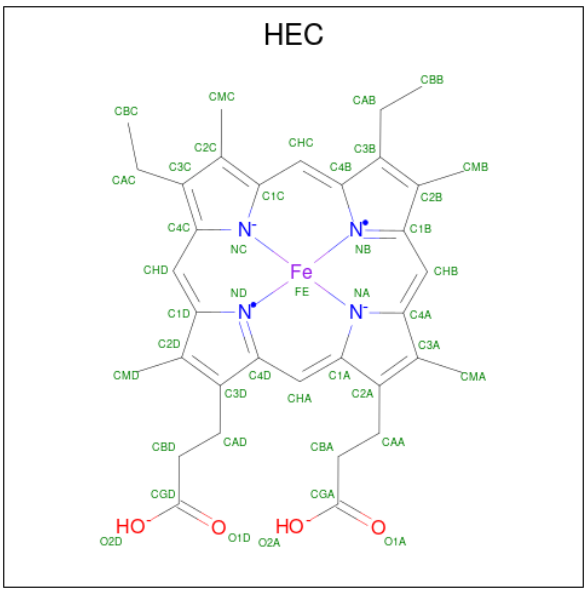
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	126	ALA	VAL	conflict	UNP A0A653FDI6
A	126	ALA	VAL	conflict	UNP A0A653FDI6

- Molecule 14 is a protein called Co-purified peptide.

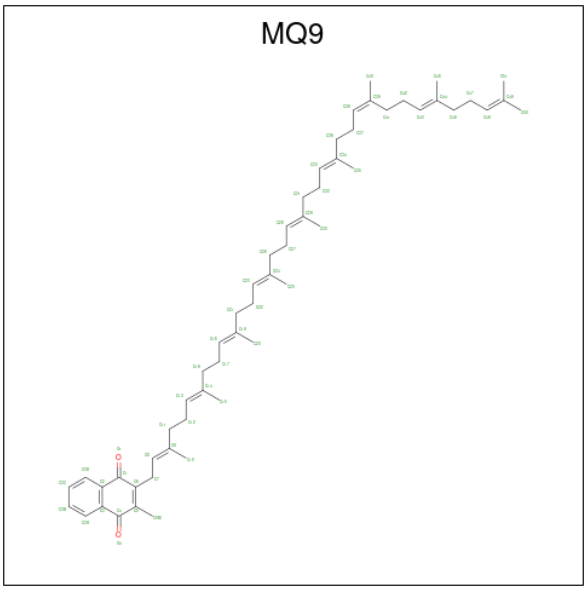
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	F	55	417	266	68	83	0	0
14	B	55	417	266	68	83	0	0

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



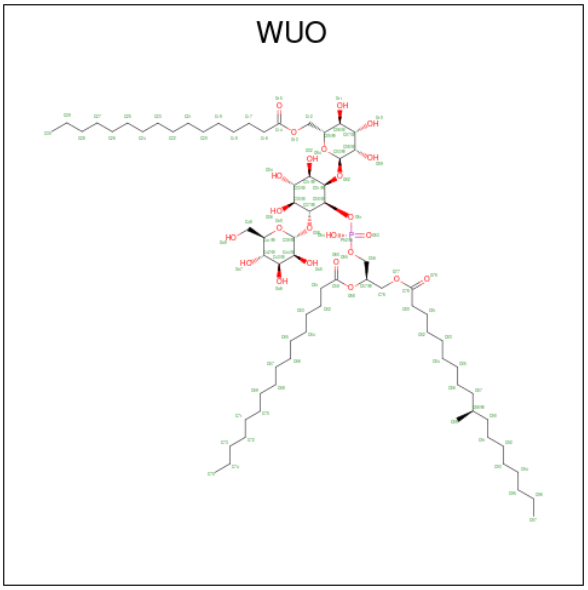
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



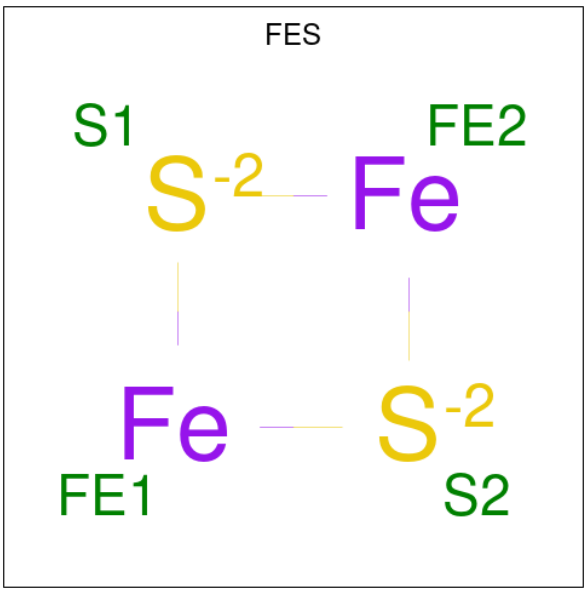
Mol	Chain	Residues	Atoms				AltConf
16	O	1	Total	C	O		0
			58	56	2		
16	N	1	Total	C	O		0
			58	56	2		
16	N	1	Total	C	O		0
			58	56	2		
16	T	1	Total	C	O		0
			58	56	2		
16	C	1	Total	C	O		0
			58	56	2		
16	C	1	Total	C	O		0
			58	56	2		
16	H	1	Total	C	O		0
			58	56	2		

- Molecule 17 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: $C_{72}H_{135}O_{24}P$).



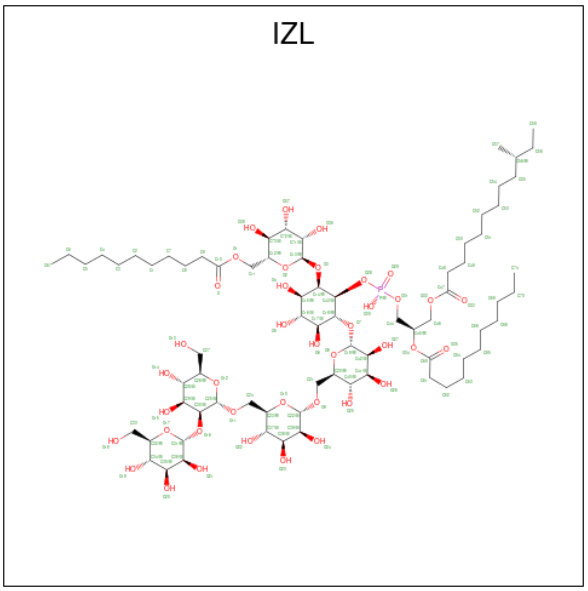
Mol	Chain	Residues	Atoms				AltConf
17	O	1	Total	C	O	P	0
			97	72	24	1	
17	P	1	Total	C	O	P	0
			97	72	24	1	
17	C	1	Total	C	O	P	0
			97	72	24	1	
17	I	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



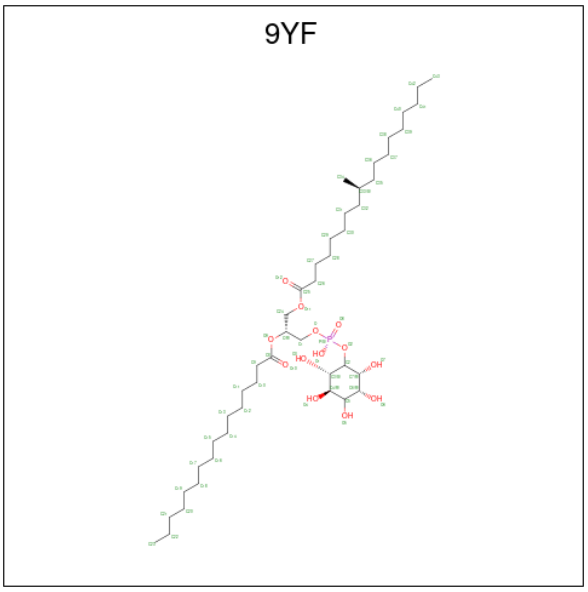
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	M	1	4	2	2	0
18	G	1	4	2	2	0

- Molecule 19 is [(2 {R})-3-[[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: $C_{74}H_{133}O_{39}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	M	1	114	74	39	1	0
			Total	C	O	P	
19	G	1	114	74	39	1	0

- Molecule 20 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	58	44	13	1	0

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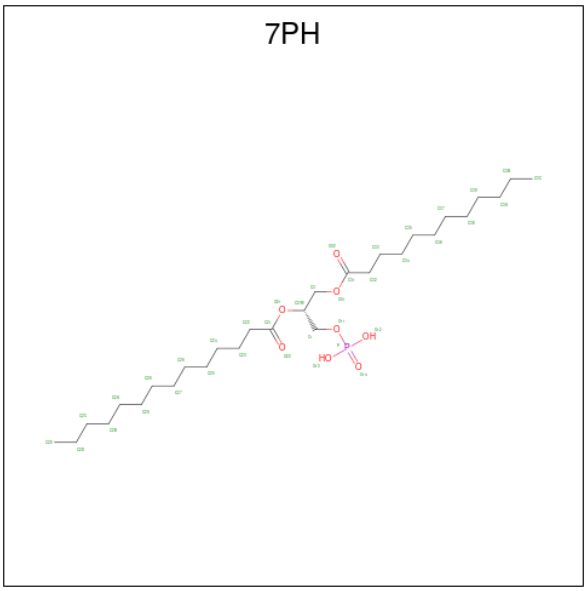
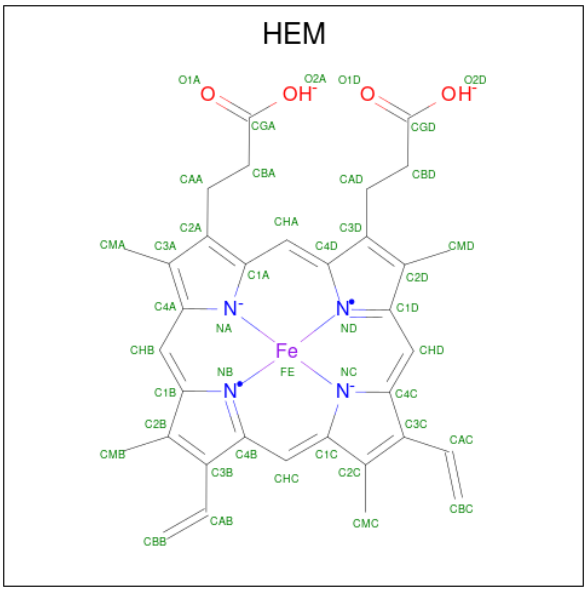
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	W	1	58	44	13	1	0
20	G	1	58	44	13	1	0
20	b	1	58	44	13	1	0

- Molecule 21 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



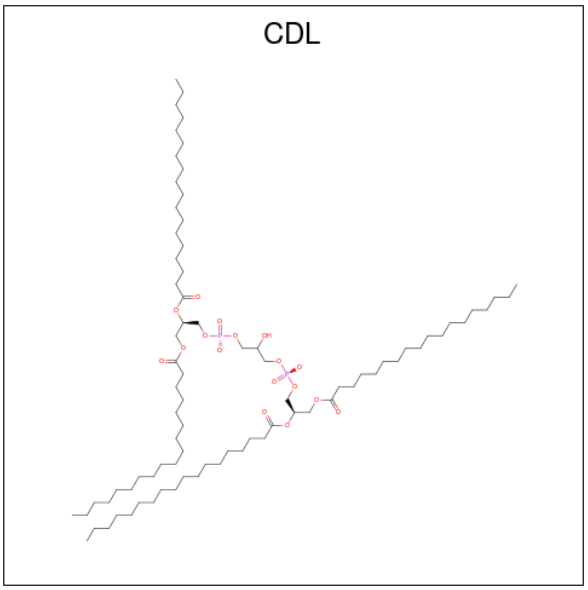
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	M	1	38	29	8	1	0
21	S	1	38	29	8	1	0
21	G	1	38	29	8	1	0
21	G	1	38	29	8	1	0
21	H	1	38	29	8	1	0

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



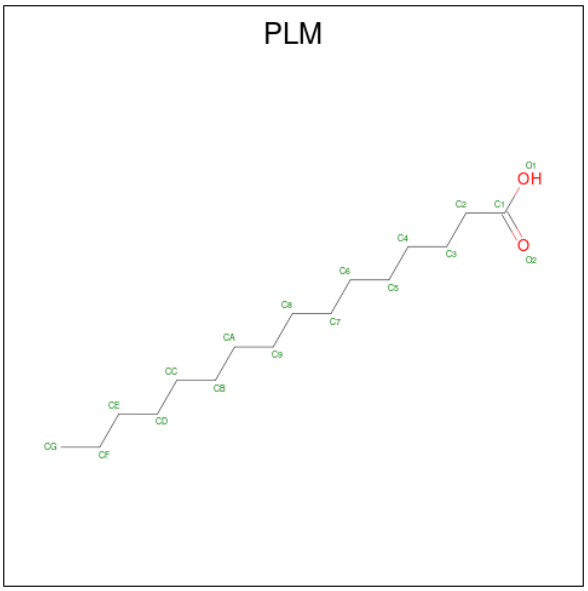
Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 23 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



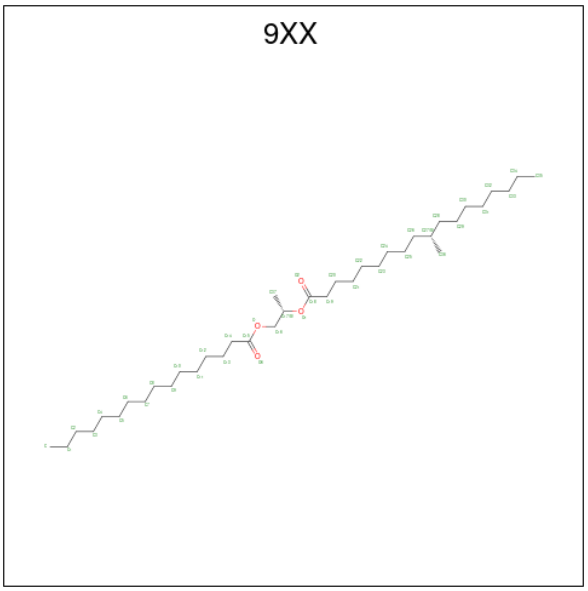
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	N	1	74	55	17	2	0
23	N	1	77	58	17	2	0
23	N	1	79	60	17	2	0
23	P	1	77	58	17	2	0
23	P	1	77	58	17	2	0
23	T	1	79	60	17	2	0
23	R	1	77	58	17	2	0
23	R	1	77	58	17	2	0
23	G	1	79	60	17	2	0
23	H	1	74	55	17	2	0
23	H	1	77	58	17	2	0
23	H	1	79	60	17	2	0
23	I	1	77	58	17	2	0
23	I	1	77	58	17	2	0
23	K	1	79	60	17	2	0
23	L	1	79	60	17	2	0
23	L	1	77	58	17	2	0

- Molecule 24 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



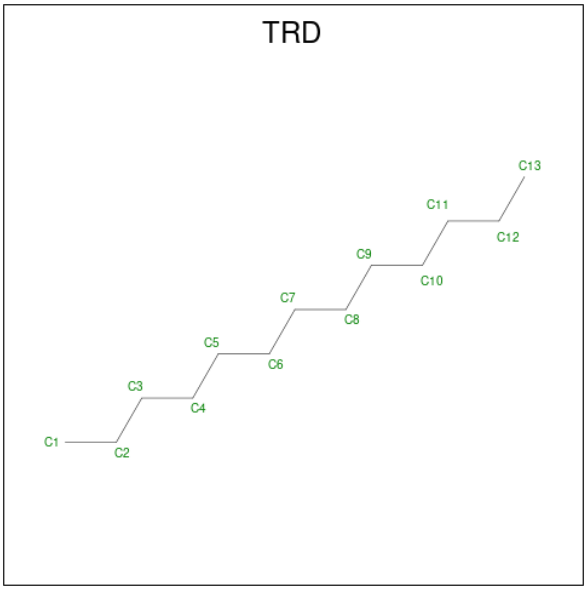
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	N	1	11	10	1	0
			Total	C	O	
24	W	1	11	10	1	0
			Total	C	O	
24	L	1	11	10	1	0
			Total	C	O	
24	c	1	11	10	1	0

- Molecule 25 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	N	1	32	28	4	0
25	W	1	42	38	4	0
25	b	1	32	28	4	0
25	c	1	32	28	4	0

- Molecule 26 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	S	1	13	13	0
26	T	1	13	13	0
26	R	1	13	13	0
26	R	1	13	13	0
26	Q	1	13	13	0
26	J	1	13	13	0
26	K	1	13	13	0
26	L	1	13	13	0

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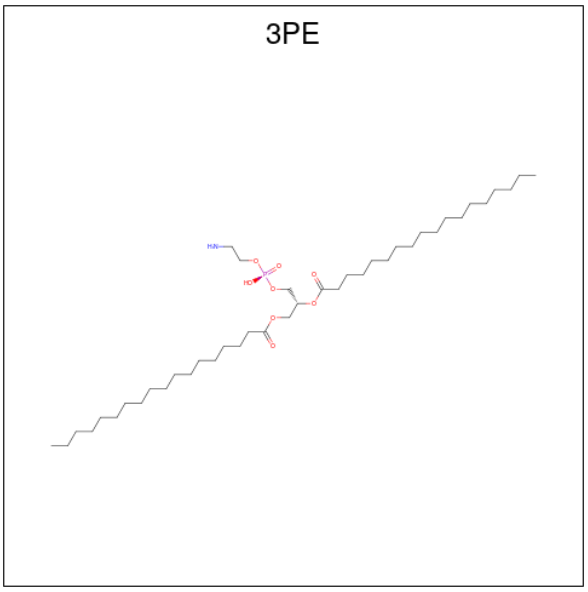
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	L	1	13	13	0
			Total	C	
26	X	1	13	13	0

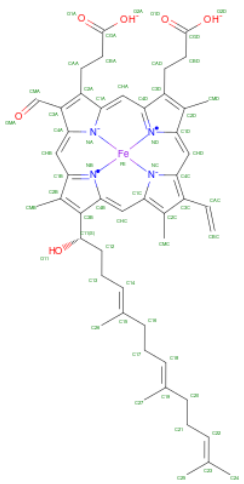
- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	S	1	32	22	1	8	1	0
			Total	C	N	O	P	
27	J	1	32	22	1	8	1	0

- Molecule 28 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

HEA



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
28	R	1	60	49	1	4	6	0
28	R	1	60	49	1	4	6	0
28	L	1	60	49	1	4	6	0
28	L	1	60	49	1	4	6	0

- Molecule 29 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
29	R	1	1	1	0
29	Q	2	2	2	0
29	L	1	1	1	0
29	X	2	2	2	0

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
30	R	1	1	1	0

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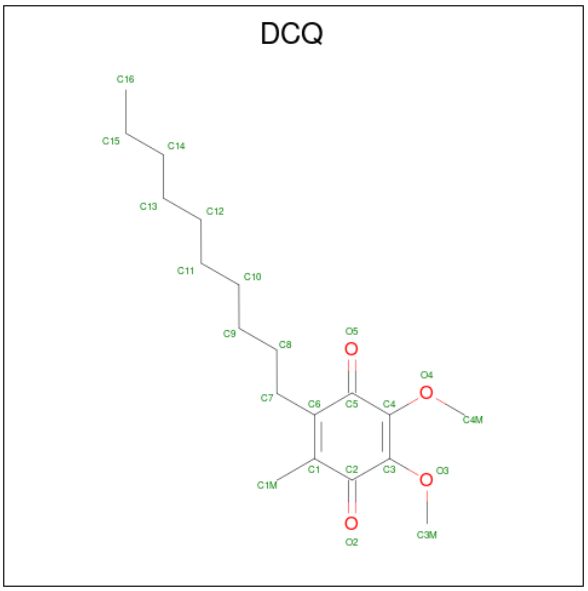
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
30	L	1	1	1	0

- Molecule 31 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
31	R	1	1	1	0
			Total	Ca	
31	L	1	1	1	0

- Molecule 32 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	H	1	23	19	4	0

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
33	O	46	46	46	0
			Total	O	
33	M	54	54	54	0

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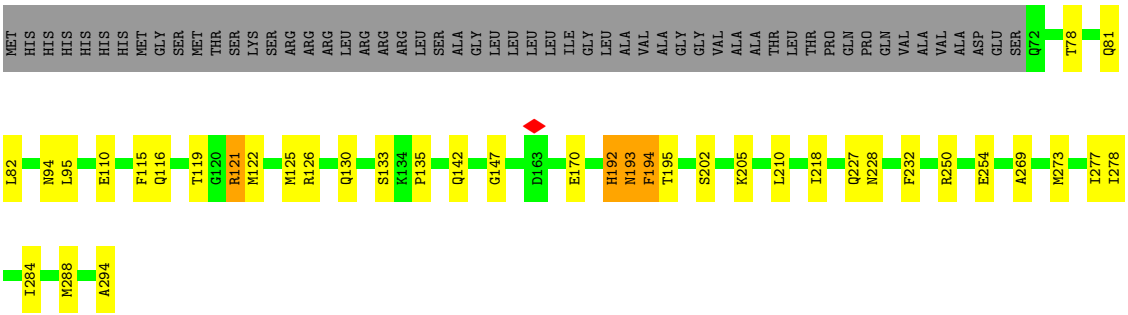
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
33	N	75	75	75	0
			Total	O	
33	P	6	6	6	0
			Total	O	
33	S	3	3	3	0
			Total	O	
33	T	10	10	10	0
			Total	O	
33	R	51	51	51	0
			Total	O	
33	Q	23	23	23	0
			Total	O	
33	W	6	6	6	0
			Total	O	
33	C	54	54	54	0
			Total	O	
33	G	61	61	61	0
			Total	O	
33	H	90	90	90	0
			Total	O	
33	I	6	6	6	0
			Total	O	
33	J	4	4	4	0
			Total	O	
33	K	9	9	9	0
			Total	O	
33	L	52	52	52	0
			Total	O	
33	X	29	29	29	0
			Total	O	
33	Z	2	2	2	0
			Total	O	
33	a	2	2	2	0
			Total	O	
33	b	10	10	10	0
			Total	O	
33	c	1	1	1	0
			Total	O	
33	F	6	6	6	0
			Total	O	
33	B	6	6	6	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.

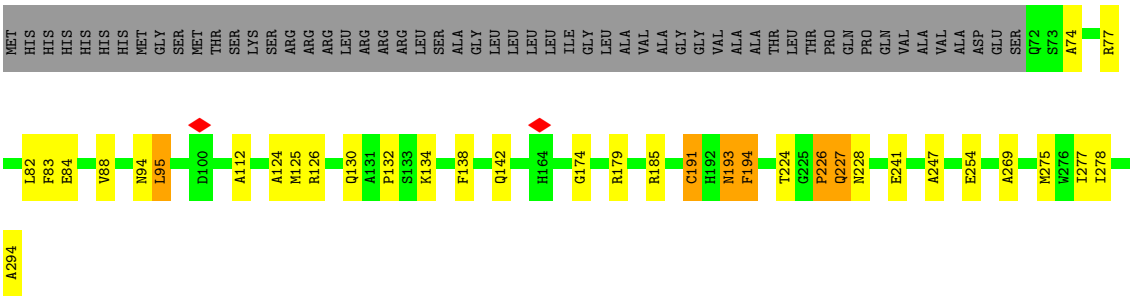
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain O:



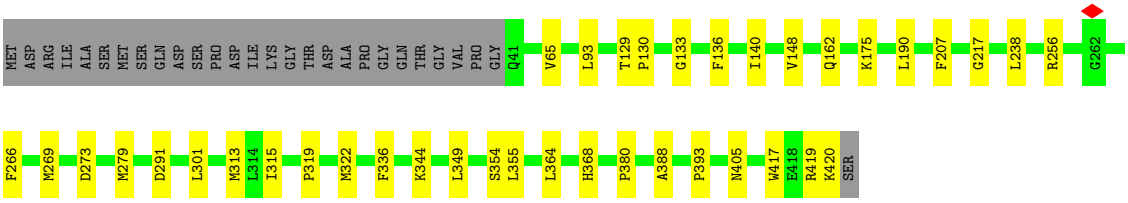
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain C:



• Molecule 2: Cytochrome bc1 complex cytochrome c subunit

Chain M:



• Molecule 2: Cytochrome bc1 complex cytochrome c subunit

Chain G: 84% 9% 7%

MET ASP ARG ILE ALA SER MET SER GLN ASP SER PRO ASP ILE LYS GLY THR ASP ALA PRO GLY GLN THR GLY VAL PRO GLY Q41 E46 M50 V65 A90 M94 F107 F117 G133 L134 I140 V148 L149 K152 Q162 S199 L204 L238

L254 R260 P261 G262 F266 P271 M279 D291 L301 M313 L314 I315 R316 I317 K318 P319 M322 L339 K344 S354 L355 L364 Q369 P393 L402 N405 W417 K420 SER

• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

Chain N: 84% 11%

MET SER PRO D4 L8 A9 A10 A11 Q12 L30 L41 L42 G43 E44 L55 P66 Q78 R87 F104 V122 F156 Y159 S160 D164 S167 T179 V184 T187 W188 M189 L203 Y208 A209 L210 H211 I212 L213 L214 L229 Q233

P239 V253 M254 P255 V256 F257 A263 M267 L272 G277 Y290 S296 M305 M306 W315 W318 Q329 G338 L339 P371 I402 S403 T407 F424 Y427 S432 S436 V440 P464 H473 P474 E478 P483 T499

H511 T527 E531 I536 HIS GLY ASN GLY GLU THR ASN GLY HIS HIS LYS LEU ASP TYR LYS ASP ASP ASP ASP LYS

• Molecule 3: Cytochrome bc1 complex cytochrome b subunit

Chain H: 84% 12%

MET SER PRO D4 A10 L42 T56 P66 S67 Y77 R87 W111 L114 I120 M121 V122 H123 L124 L147 L165 A174 I178 T179 V184 M189 G195 I202 P205 Y208 A209 L210 H211 I212 L213 L214 L229 V230 W231 F232 Q233

V253 F257 A258 V259 A266 M275 G276 G277 W285 G288 F303 M306 D309 I312 R313 L314 V333 L344 M379 L386 M392 S403 L404 T407 R412 M415 V416 P419 Y423 R428 S432 L441 E446 Y458

H462 L477 E478 P483 K490 L526 I536 HIS GLY ASN GLY GLU THR ASN GLY HIS HIS LYS LEU ASP TYR LYS ASP ASP ASP ASP LYS

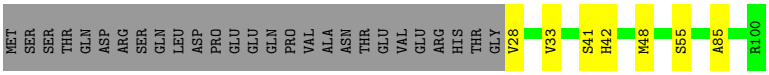
• Molecule 4: Transmembrane protein

Chain P: 64% 9% 27%

MET SER SER THR GLN ASP ARG SER GLN LEU ASP PRO GLU GLU GLN PRO VAL ALA ASN THR GLU VAL GLU ARG HIS THR GLY V28 H42 V47 G52 M62 E72 L76 R89 W92 R100

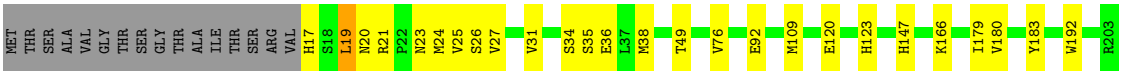
• Molecule 4: Transmembrane protein

Chain I: 66% 7% 27%



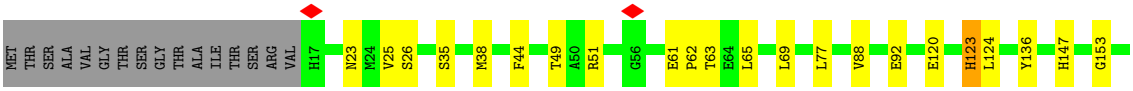
• Molecule 5: Probable cytochrome c oxidase subunit 3

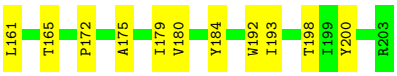
Chain S:



• Molecule 5: Probable cytochrome c oxidase subunit 3

Chain J:





• Molecule 6: Cytochrome c oxidase polypeptide 4

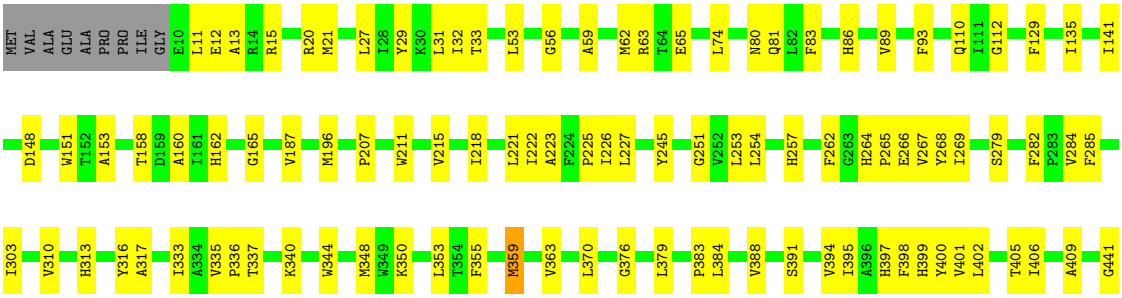
Chain T:

• Molecule 6: Cytochrome c oxidase polypeptide 4

Chain K:

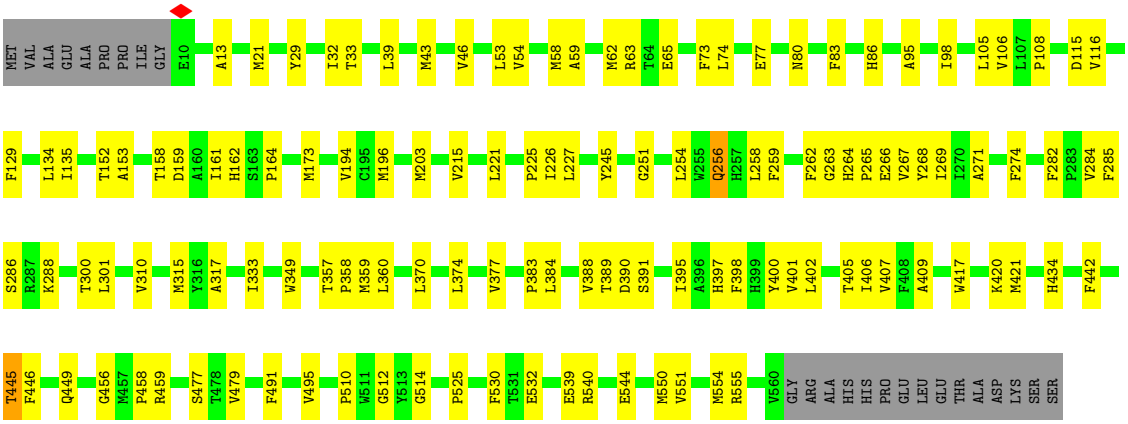
• Molecule 7: Cytochrome c oxidase subunit 1

Chain R:



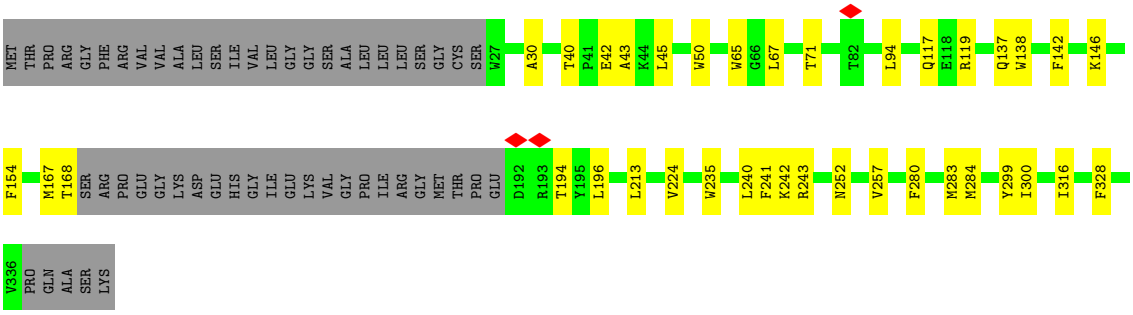
• Molecule 7: Cytochrome c oxidase subunit 1

Chain L:



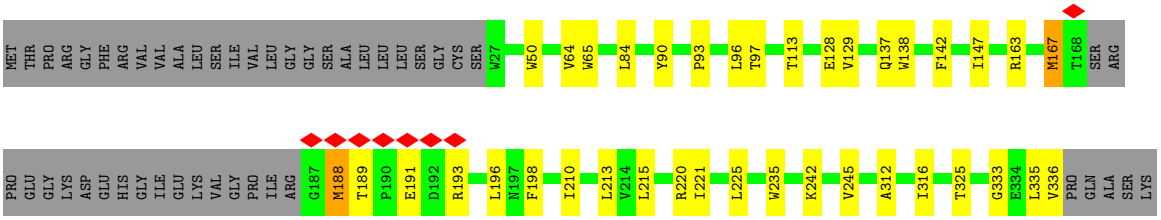
• Molecule 8: cytochrome-c oxidase

Chain Q:



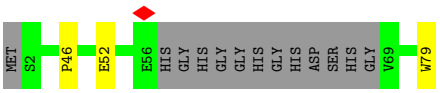
• Molecule 8: cytochrome-c oxidase

Chain X:



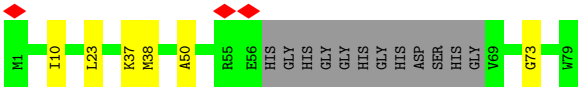
• Molecule 9: Cytochrome c oxidase subunit

Chain U:



• Molecule 9: Cytochrome c oxidase subunit

Chain Z:

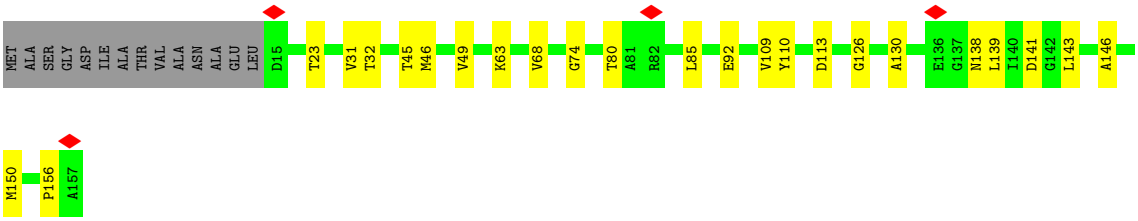


• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:

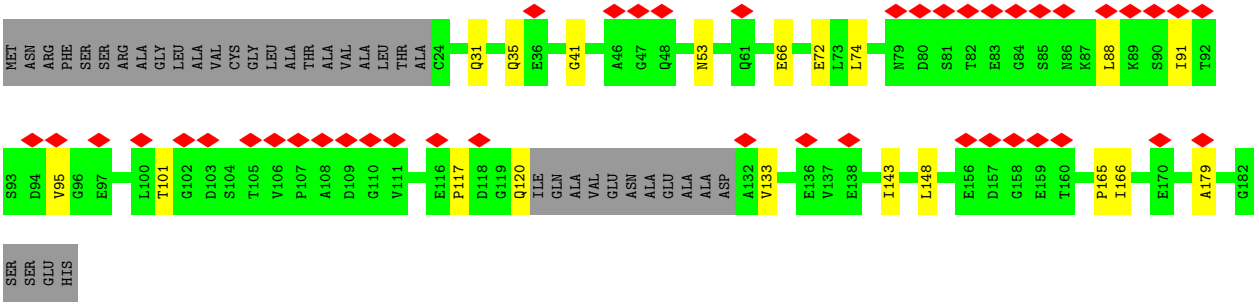
• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain a:



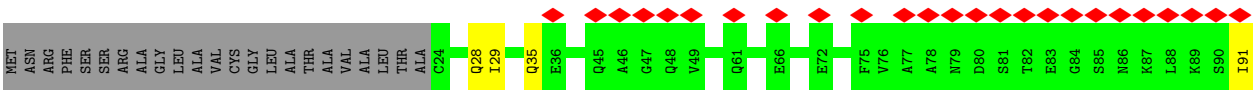
• Molecule 11: LpqE protein

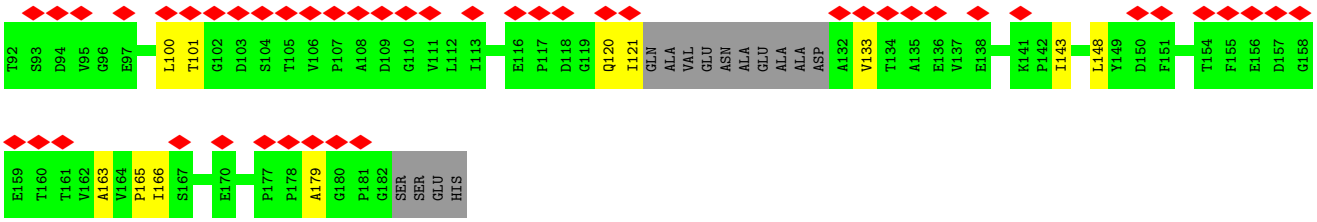
Chain W:



• Molecule 11: LpqE protein

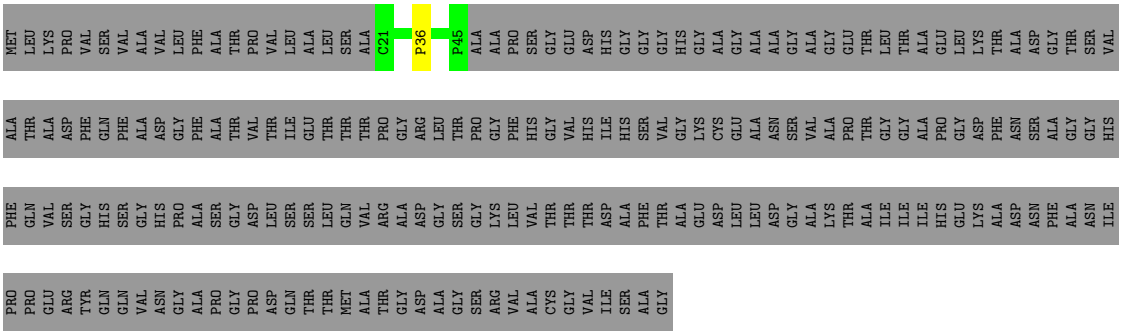
Chain b:





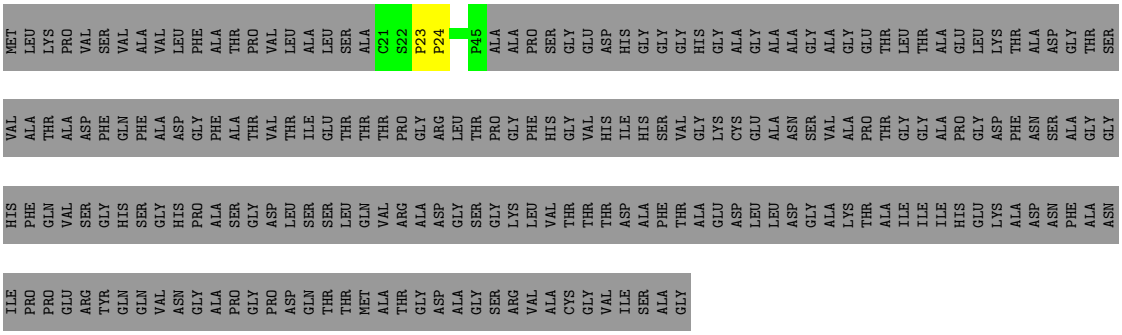
• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain Y:



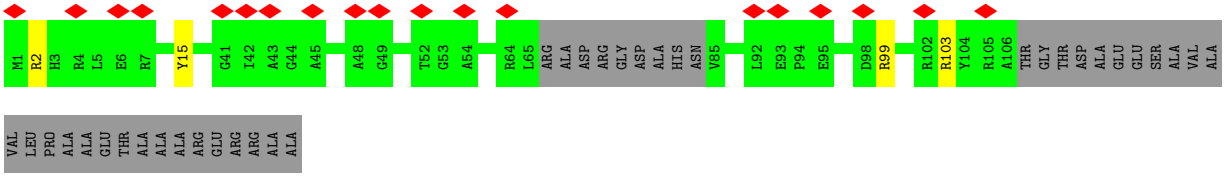
• Molecule 12: Superoxide dismutase [Cu-Zn]

Chain c:



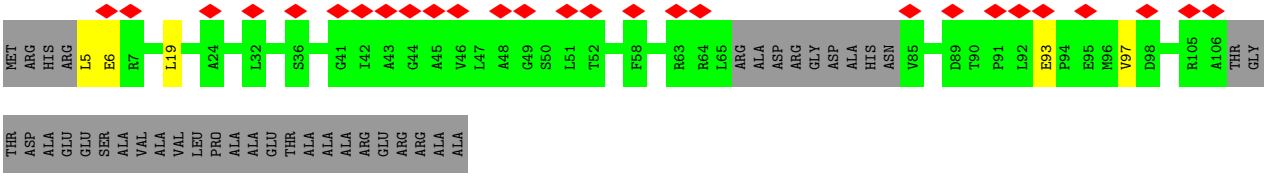
• Molecule 13: Co-purified transmembrane protein

Chain E:



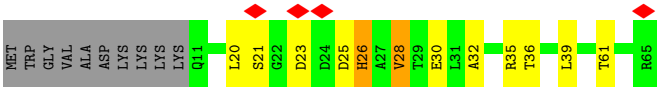
• Molecule 13: Co-purified transmembrane protein

Chain A:



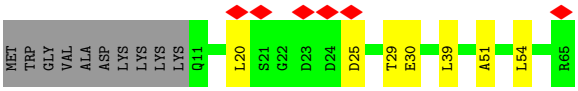
• Molecule 14: Co-purified peptide

Chain F:



• Molecule 14: Co-purified peptide

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.831	Depositor
Minimum map value	-0.397	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	445.5, 445.5, 445.5	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: 7PH, HEC, 3PE, FES, WUO, PLM, CA, 9YF, CU, TRD, MG, DCQ, IZL, CDL, 9XX, HEA, MQ9, HEM

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	C	0.34	2/1660 (0.1%)	0.49	3/2250 (0.1%)
1	O	0.44	3/1660 (0.2%)	0.62	5/2250 (0.2%)
2	G	0.19	0/3046	0.32	0/4129
2	M	0.14	0/3046	0.27	0/4129
3	H	0.24	0/4299	0.32	0/5862
3	N	0.20	0/4299	0.32	2/5862 (0.0%)
4	I	0.13	0/606	0.25	0/825
4	P	0.12	0/606	0.21	0/825
5	J	0.19	0/1513	0.29	0/2066
5	S	0.20	0/1513	0.33	0/2066
6	K	0.15	0/1112	0.28	0/1524
6	T	0.18	0/1112	0.31	0/1524
7	L	0.21	0/4529	0.38	0/6187
7	R	0.21	0/4529	0.36	0/6187
8	Q	0.14	0/2356	0.27	0/3207
8	X	0.15	0/2392	0.33	0/3256
9	U	0.11	0/515	0.20	0/704
9	Z	0.11	0/523	0.25	0/714
10	V	0.23	0/1042	0.34	0/1423
10	a	0.14	0/1042	0.28	0/1423
11	W	0.14	0/1092	0.31	0/1497
11	b	0.12	0/1100	0.32	0/1508
12	Y	0.12	0/175	0.26	0/244
12	c	0.14	0/175	0.35	0/244
13	A	0.10	0/632	0.33	0/859
13	E	0.13	0/673	0.34	0/912
14	B	0.14	0/429	0.34	0/592
14	F	0.33	0/429	0.57	0/592
All	All	0.21	5/46105 (0.0%)	0.35	10/62861 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	194	PHE	C-N	6.10	1.41	1.33
1	C	95	LEU	C-N	-5.98	1.24	1.33
1	O	228	ASN	C-N	-5.16	1.23	1.33
1	C	228	ASN	C-N	-5.14	1.23	1.33
1	O	192	HIS	CE1-NE2	-5.07	1.27	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	192	HIS	CA-C-O	-7.91	109.70	119.28
1	C	228	ASN	N-CA-C	7.24	121.71	113.02
3	N	187	THR	CA-C-N	-6.72	110.75	120.29
3	N	187	THR	C-N-CA	-6.72	110.75	120.29
1	C	227	GLN	N-CA-C	-6.08	98.53	108.67
1	O	194	PHE	O-C-N	-5.82	114.84	122.59
1	O	192	HIS	CA-CB-CG	-5.64	108.16	113.80
1	O	232	PHE	O-C-N	-5.38	116.01	123.01
1	O	193	ASN	CA-CB-CG	5.36	117.96	112.60
1	C	226	PRO	N-CA-C	5.04	118.42	110.50

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	C	1623	0	1561	31	0
1	O	1623	0	1560	32	0
2	G	2967	0	2976	27	0
2	M	2967	0	2976	30	0
3	H	4167	0	4192	53	0
3	N	4167	0	4192	44	0
4	I	586	0	578	5	0
4	P	586	0	578	6	0
5	J	1465	0	1462	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1465	0	1462	31	0
6	K	1077	0	1058	14	0
6	T	1077	0	1058	15	0
7	L	4369	0	4346	107	0
7	R	4369	0	4346	111	0
8	Q	2293	0	2242	26	0
8	X	2328	0	2274	29	0
9	U	499	0	504	3	0
9	Z	507	0	516	5	0
10	V	1024	0	1035	14	0
10	a	1024	0	1035	16	0
11	W	1075	0	1044	14	0
11	b	1083	0	1055	12	0
12	Y	168	0	151	1	0
12	c	168	0	151	1	0
13	A	620	0	640	3	0
13	E	660	0	685	7	0
14	B	417	0	393	4	0
14	F	417	0	393	17	0
15	C	86	0	61	6	0
15	O	86	0	60	4	0
16	C	116	0	160	4	0
16	H	58	0	80	10	0
16	N	116	0	160	8	0
16	O	58	0	80	3	0
16	T	58	0	80	7	0
17	C	97	0	0	0	0
17	I	97	0	0	0	0
17	O	97	0	0	0	0
17	P	97	0	0	0	0
18	G	4	0	0	0	0
18	M	4	0	0	0	0
19	G	114	0	0	0	0
19	M	114	0	0	0	0
20	G	58	0	0	0	0
20	M	58	0	0	0	0
20	W	58	0	0	0	0
20	b	58	0	0	0	0
21	G	76	0	110	3	0
21	H	38	0	55	1	0
21	M	38	0	55	3	0
21	S	38	0	55	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	86	0	60	6	0
22	N	86	0	60	5	0
23	G	79	0	105	1	0
23	H	230	0	295	6	0
23	I	154	0	196	7	0
23	K	79	0	105	2	0
23	L	156	0	203	6	0
23	N	230	0	295	9	0
23	P	154	0	196	13	0
23	R	154	0	196	6	0
23	T	79	0	105	5	0
24	L	11	0	16	0	0
24	N	11	0	16	1	0
24	W	11	0	16	0	0
24	c	11	0	16	0	0
25	N	32	0	0	0	0
25	W	42	0	0	0	0
25	b	32	0	0	0	0
25	c	32	0	0	0	0
26	J	13	0	28	1	0
26	K	13	0	28	0	0
26	L	26	0	56	0	0
26	Q	13	0	28	1	0
26	R	26	0	56	0	0
26	S	13	0	28	0	0
26	T	13	0	28	0	0
26	X	13	0	28	0	0
27	J	32	0	38	0	0
27	S	32	0	38	0	0
28	L	120	0	108	12	0
28	R	120	0	108	38	0
29	L	1	0	0	0	0
29	Q	2	0	0	0	0
29	R	1	0	0	0	0
29	X	2	0	0	0	0
30	L	1	0	0	0	0
30	R	1	0	0	0	0
31	L	1	0	0	0	0
31	R	1	0	0	0	0
32	H	23	0	30	0	0
33	B	6	0	0	0	0
33	C	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	F	6	0	0	0	0
33	G	61	0	0	0	0
33	H	90	0	0	0	0
33	I	6	0	0	0	0
33	J	4	0	0	0	0
33	K	9	0	0	0	0
33	L	52	0	0	0	0
33	M	54	0	0	0	0
33	N	75	0	0	0	0
33	O	46	0	0	0	0
33	P	6	0	0	0	0
33	Q	23	0	0	0	0
33	R	51	0	0	0	0
33	S	3	0	0	0	0
33	T	10	0	0	0	0
33	W	6	0	0	0	0
33	X	29	0	0	0	0
33	Z	2	0	0	0	0
33	a	2	0	0	0	0
33	b	10	0	0	0	0
33	c	1	0	0	0	0
All	All	49157	0	47901	645	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 7.

All (645) 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)
7:R:264:HIS:CE1	7:R:268:TYR:HE2	1.42	1.35
7:L:264:HIS:NE2	7:L:268:TYR:HE2	1.31	1.28
7:L:264:HIS:CE1	7:L:268:TYR:HE2	1.54	1.25
7:R:264:HIS:NE2	7:R:268:TYR:HE2	1.39	1.19
7:R:264:HIS:CE1	7:R:268:TYR:CE2	2.31	1.19
7:L:264:HIS:CE1	7:L:268:TYR:CE2	2.38	1.11
7:L:264:HIS:NE2	7:L:268:TYR:CE2	2.18	1.09
7:R:264:HIS:NE2	7:R:268:TYR:CE2	2.21	1.07
3:H:120:ILE:HG12	22:H:1007:HEM:HAB	1.38	1.01
28:R:603:HEA:HHD	28:R:603:HEA:HBC1	1.43	1.01
28:R:603:HEA:H18	28:R:603:HEA:H261	1.43	0.98
7:R:406:ILE:HD11	28:R:603:HEA:HAC	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:CYS:SG	15:C:302:HEC:HAC	2.05	0.96
7:L:401:VAL:HG22	28:L:602:HEA:HBC1	1.53	0.88
28:R:603:HEA:H261	28:R:603:HEA:C18	2.03	0.84
7:L:285:PHE:HB2	7:L:359:MET:HE3	1.60	0.83
7:R:395:ILE:HD13	28:R:603:HEA:CAA	2.07	0.82
7:R:401:VAL:HG12	28:R:602:HEA:HBC1	1.62	0.81
3:H:412:ARG:HA	3:H:415:MET:HE3	1.61	0.80
7:R:53:LEU:HD22	28:R:603:HEA:H272	1.62	0.80
14:F:20:LEU:HD12	14:F:20:LEU:O	1.83	0.79
3:N:464:PRO:HB3	3:N:474:PRO:HB3	1.64	0.79
8:X:333:GLY:O	8:X:336:VAL:HG22	1.82	0.78
7:R:395:ILE:HD13	28:R:603:HEA:HAA2	1.67	0.76
1:O:121:ARG:HG3	1:O:121:ARG:HH11	1.51	0.76
1:C:269:ALA:HB1	3:H:392:MET:HE3	1.67	0.75
7:R:56:GLY:HA3	28:R:603:HEA:H262	1.66	0.75
2:M:344:LYS:HE3	2:M:354:SER:HB3	1.68	0.75
2:G:254:LEU:HD12	2:G:402:LEU:HB3	1.69	0.75
7:R:56:GLY:HA3	28:R:603:HEA:C26	2.18	0.74
14:F:20:LEU:HD13	14:F:25:ASP:O	1.86	0.74
28:L:602:HEA:HBA2	28:L:602:HEA:HHA	1.69	0.73
7:R:266:GLU:HA	7:R:269:ILE:HD12	1.70	0.73
22:H:1002:HEM:HBC2	22:H:1002:HEM:HHD	1.68	0.73
7:L:271:ALA:HA	7:L:405:THR:HG21	1.70	0.71
2:M:133:GLY:HA3	3:N:277:GLY:HA3	1.71	0.71
2:G:90:ALA:O	2:G:94:MET:HG3	1.92	0.70
2:M:279:MET:HG2	2:M:315:ILE:HG22	1.72	0.70
28:R:603:HEA:HBC1	28:R:603:HEA:CHD	2.21	0.69
9:Z:38:MET:HE1	10:a:139:LEU:HD13	1.72	0.69
7:R:56:GLY:HA3	28:R:603:HEA:C15	2.23	0.68
5:S:20:ASN:HB3	13:E:103:ARG:HH11	1.59	0.68
6:K:95:ILE:HG12	6:K:124:SER:HB3	1.75	0.68
2:G:133:GLY:HA3	3:H:277:GLY:HA3	1.75	0.68
2:G:319:PRO:HG3	11:b:165:PRO:HG3	1.76	0.68
5:S:23:ASN:HB3	5:S:26:SER:HB2	1.75	0.68
6:T:70:TYR:HB3	6:T:73:ALA:HB2	1.75	0.67
28:R:603:HEA:CMB	28:R:603:HEA:H121	2.24	0.67
2:G:317:ILE:HD11	2:G:322:MET:HE2	1.77	0.67
1:C:275:MET:HE1	3:H:275:MET:HE1	1.78	0.66
10:a:74:GLY:H	10:a:80:THR:HG21	1.60	0.66
7:L:266:GLU:HA	7:L:269:ILE:HD12	1.76	0.66
2:G:344:LYS:HE3	2:G:354:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:603:HEA:HBD2	28:R:603:HEA:HHA	1.77	0.65
10:a:130:ALA:HB2	10:a:146:ALA:HB2	1.79	0.65
1:O:82:LEU:HD11	1:O:142:GLN:HG2	1.78	0.65
7:L:398:PHE:HA	7:L:401:VAL:HG12	1.79	0.65
7:R:395:ILE:HD13	28:R:603:HEA:HAA1	1.76	0.64
7:R:303:ILE:HG13	7:R:336:PRO:HB2	1.79	0.64
1:O:227:GLN:HG3	15:O:302:HEC:O1D	1.98	0.64
28:R:603:HEA:O11	28:R:603:HEA:HHC	1.98	0.64
1:C:227:GLN:HG3	15:C:302:HEC:O1D	1.98	0.64
22:N:606:HEM:HMC2	22:N:606:HEM:HBC2	1.80	0.63
3:N:527:THR:O	3:N:531:GLU:HG2	1.97	0.63
1:O:130:GLN:HG3	1:O:227:GLN:NE2	2.14	0.63
23:N:603:CDL:H521	23:N:603:CDL:H722	1.80	0.63
8:Q:299:TYR:HB2	8:Q:316:ILE:HD13	1.80	0.63
22:N:601:HEM:HBC1	3:H:213:LEU:HD21	1.81	0.63
8:X:163:ARG:HH21	8:X:198:PHE:HB3	1.64	0.62
23:N:603:CDL:H152	23:N:603:CDL:H352	1.81	0.62
7:R:348:MET:HB3	8:Q:71:THR:HG21	1.80	0.62
5:J:25:VAL:HG12	5:J:180:VAL:HG11	1.81	0.62
1:O:119:THR:HB	1:O:121:ARG:HD2	1.82	0.62
1:O:202:SER:HB3	1:O:205:LYS:HZ1	1.64	0.62
8:X:210:ILE:HD13	8:X:325:THR:HG23	1.81	0.62
2:M:355:LEU:HB2	2:M:364:LEU:O	2.01	0.61
7:R:395:ILE:CD1	28:R:603:HEA:HAA1	2.29	0.61
8:Q:45:LEU:HD22	8:Q:119:ARG:HD3	1.82	0.61
7:L:73:PHE:HA	8:X:335:LEU:HD11	1.81	0.61
7:L:108:PRO:HG3	7:L:116:VAL:HG13	1.82	0.61
16:H:1006:MQ9:H3B	22:H:1007:HEM:HAA2	1.83	0.61
10:V:73:LEU:O	10:V:77:THR:HA	2.01	0.60
7:L:267:VAL:CG1	28:L:602:HEA:HAC	2.31	0.60
8:X:336:VAL:HG13	11:b:28:GLN:HB3	1.83	0.60
4:P:89:ARG:HB2	23:P:303:CDL:H122	1.83	0.60
11:W:95:VAL:HG12	11:W:95:VAL:O	2.01	0.60
2:G:279:MET:HG2	2:G:315:ILE:HG22	1.83	0.60
5:J:38:MET:HB2	7:L:225:PRO:HB2	1.82	0.60
7:R:395:ILE:CD1	28:R:603:HEA:CAA	2.79	0.60
1:O:273:MET:HE3	16:T:1301:MQ9:H112	1.84	0.60
7:R:264:HIS:CD2	7:R:310:VAL:HG23	2.37	0.60
11:b:143:ILE:HD12	11:b:166:ILE:HD11	1.84	0.60
7:L:495:VAL:HG11	23:L:609:CDL:H391	1.83	0.60
8:X:336:VAL:HG12	11:b:29:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:601:HEM:HBB2	22:N:601:HEM:HMB2	1.84	0.59
7:R:264:HIS:O	7:R:267:VAL:HG22	2.02	0.59
3:N:253:VAL:HA	3:N:257:PHE:HB3	1.83	0.59
1:C:130:GLN:HG3	1:C:227:GLN:NE2	2.16	0.59
5:J:49:THR:HG21	7:L:254:LEU:HB2	1.85	0.59
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.85	0.59
6:T:95:ILE:HG12	6:T:124:SER:HB3	1.84	0.59
3:N:318:TRP:CD1	24:N:608:PLM:H21	2.37	0.59
5:J:147:HIS:NE2	5:J:192:TRP:HB2	2.17	0.59
3:H:266:ALA:HB2	16:H:1006:MQ9:H321	1.82	0.59
3:N:41:LEU:HA	3:N:44:GLU:HG3	1.85	0.59
8:X:235:TRP:CD1	8:X:242:LYS:HB3	2.38	0.59
14:F:20:LEU:HD22	14:F:25:ASP:O	2.03	0.59
1:O:121:ARG:HH11	1:O:121:ARG:CG	2.14	0.59
7:L:105:LEU:HD22	7:L:421:MET:HG3	1.83	0.59
11:W:101:THR:O	11:W:133:VAL:HA	2.02	0.58
1:O:284:ILE:O	1:O:288:MET:HG3	2.04	0.58
7:L:65:GLU:HB2	7:L:74:LEU:HD12	1.86	0.58
7:R:32:ILE:HG13	7:R:33:THR:HG23	1.86	0.58
4:I:28:VAL:HG13	4:I:42:HIS:HB2	1.85	0.58
7:R:11:LEU:HD21	9:U:46:PRO:HB2	1.85	0.57
7:R:395:ILE:HA	7:R:398:PHE:CE2	2.39	0.57
4:P:28:VAL:HG13	4:P:42:HIS:HB2	1.85	0.57
5:S:38:MET:HB2	7:R:225:PRO:HB2	1.85	0.57
5:S:17:HIS:CE1	5:S:19:LEU:HD23	2.40	0.57
7:L:264:HIS:CD2	7:L:310:VAL:HG23	2.40	0.57
2:M:130:PRO:HA	3:N:277:GLY:O	2.05	0.57
7:R:379:LEU:HD21	7:R:394:VAL:HG22	1.87	0.57
7:R:211:TRP:O	7:R:215:VAL:HG23	2.04	0.56
3:H:253:VAL:HA	3:H:257:PHE:HB3	1.87	0.56
7:L:80:ASN:HA	7:L:83:PHE:CE2	2.40	0.56
5:S:147:HIS:CE1	5:S:192:TRP:HB2	2.40	0.56
7:R:56:GLY:C	28:R:603:HEA:H172	2.30	0.56
1:C:126:ARG:HB2	7:L:77:GLU:HG2	1.87	0.56
1:C:226:PRO:HB2	15:C:302:HEC:HBD1	1.86	0.56
7:L:264:HIS:CD2	7:L:310:VAL:CG2	2.89	0.56
7:L:256:GLN:HG2	7:L:315:MET:HG2	1.88	0.56
3:H:379:MET:HG3	3:H:419:PRO:HB3	1.87	0.56
23:H:1004:CDL:HA4	23:H:1005:CDL:H511	1.87	0.56
7:R:267:VAL:HB	28:R:602:HEA:HAC	1.86	0.56
6:K:90:TRP:HB3	7:L:33:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:301:CDL:H202	23:R:605:CDL:H362	1.88	0.56
2:G:393:PRO:HB2	2:G:405:ASN:HB3	1.88	0.56
3:H:174:ALA:HA	3:H:178:ILE:HD12	1.87	0.56
7:R:284:VAL:HG22	7:R:514:GLY:HA2	1.88	0.56
5:J:147:HIS:CE1	5:J:192:TRP:HB2	2.40	0.56
7:L:282:PHE:HA	7:L:359:MET:HE1	1.88	0.55
7:L:370:LEU:HD23	8:X:65:TRP:CD1	2.41	0.55
3:H:124:LEU:HD11	3:H:344:LEU:HD11	1.88	0.55
7:R:406:ILE:CD1	28:R:603:HEA:HAC	2.30	0.55
6:T:90:TRP:HB3	7:R:33:THR:HG22	1.89	0.55
3:N:55:LEU:HD13	16:N:605:MQ9:H451	1.88	0.55
10:V:130:ALA:HB2	10:V:146:ALA:HB2	1.89	0.55
5:S:147:HIS:NE2	5:S:192:TRP:HB2	2.22	0.55
7:L:406:ILE:HD12	7:L:407:VAL:HG23	1.89	0.55
7:R:59:ALA:HA	7:R:62:MET:HE2	1.87	0.55
7:R:406:ILE:HD11	28:R:603:HEA:CAC	2.31	0.55
10:V:76:ASP:O	10:V:77:THR:HG22	2.06	0.55
5:J:23:ASN:HB3	5:J:26:SER:HB2	1.88	0.55
7:L:550:MET:HE1	8:X:84:LEU:HB2	1.88	0.55
7:L:264:HIS:HB3	7:L:265:PRO:HD3	1.89	0.54
14:F:20:LEU:HD12	14:F:20:LEU:C	2.32	0.54
10:V:74:GLY:HA3	10:V:80:THR:HG21	1.90	0.54
6:K:4:GLU:HG3	7:L:203:MET:HE2	1.88	0.54
2:M:291:ASP:HB3	11:W:179:ALA:HB3	1.90	0.54
11:W:41:GLY:HA3	11:W:53:ASN:HA	1.90	0.54
7:L:13:ALA:HB1	9:Z:50:ALA:HB3	1.89	0.54
3:H:416:VAL:HG13	4:I:55:SER:HB2	1.90	0.54
7:R:65:GLU:HB2	7:R:74:LEU:HD12	1.90	0.54
3:N:315:TRP:HB3	3:N:329:GLN:HE21	1.72	0.54
7:R:370:LEU:HD23	8:Q:65:TRP:CE2	2.43	0.54
3:H:446:GLU:HG2	3:H:462:HIS:NE2	2.21	0.54
8:X:128:GLU:HG3	8:X:220:ARG:HB3	1.90	0.54
3:H:147:LEU:HD13	22:H:1007:HEM:HBB2	1.89	0.54
5:J:123:HIS:CE1	5:J:124:LEU:HG	2.43	0.54
5:S:49:THR:HG21	7:R:254:LEU:HB2	1.90	0.54
7:R:15:ARG:HD2	9:U:52:GLU:HG3	1.90	0.54
1:C:185:ARG:NH1	3:H:288:GLY:HA3	2.23	0.53
3:N:473:HIS:ND1	3:N:474:PRO:HD2	2.23	0.53
7:R:512:GLY:HA2	10:V:31:VAL:HB	1.90	0.53
9:U:79:TRP:C	10:V:104:ARG:HH21	2.16	0.53
2:G:355:LEU:HB2	2:G:364:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:112:TRP:CH2	16:T:1301:MQ9:H8	2.43	0.53
2:M:65:VAL:HG22	2:M:162:GLN:HB2	1.90	0.53
2:M:148:VAL:HG21	3:N:267:MET:HE2	1.90	0.53
5:S:21:ARG:HD2	14:F:36:THR:HA	1.90	0.53
8:X:189:THR:C	8:X:191:GLU:H	2.16	0.53
7:R:355:PHE:HE1	7:R:363:VAL:HG21	1.74	0.53
2:G:65:VAL:HG22	2:G:162:GLN:HB2	1.91	0.53
2:M:256:ARG:HH22	2:M:273:ASP:HB3	1.73	0.53
1:O:78:THR:HA	1:O:81:GLN:CD	2.34	0.53
1:O:192:HIS:CE1	1:O:210:LEU:HD21	2.43	0.53
1:C:191:CYS:HG	15:C:302:HEC:HAC	1.74	0.53
7:L:539:GLU:HG2	7:L:540:ARG:HG3	1.90	0.53
7:L:32:ILE:HG13	7:L:33:THR:HG23	1.90	0.53
7:L:395:ILE:HD12	28:L:603:HEA:HAA2	1.90	0.53
3:N:402:ILE:HD11	16:T:1301:MQ9:H38	1.91	0.52
8:X:312:ALA:O	8:X:316:ILE:HG12	2.09	0.52
1:O:78:THR:O	1:O:81:GLN:HG2	2.09	0.52
7:R:400:TYR:HA	7:R:442:PHE:HZ	1.75	0.52
5:S:19:LEU:HB3	14:F:32:ALA:HB1	1.91	0.52
7:L:59:ALA:HA	7:L:62:MET:HE2	1.92	0.52
8:Q:241:PHE:HZ	8:Q:243:ARG:HH21	1.56	0.52
3:H:259:VAL:HG22	16:H:1006:MQ9:H251	1.92	0.52
4:I:85:ALA:HA	23:I:302:CDL:H362	1.92	0.52
7:R:441:GLY:O	7:R:445:THR:HG22	2.09	0.52
2:G:279:MET:SD	2:G:313:MET:HG2	2.50	0.52
22:H:1002:HEM:HMB1	22:H:1002:HEM:HBB2	1.91	0.52
7:L:456:GLY:HA2	8:X:235:TRP:CH2	2.45	0.52
8:X:225:LEU:HB3	8:X:245:VAL:HG13	1.91	0.52
7:R:63:ARG:HD3	7:R:478:THR:HA	1.92	0.51
2:M:319:PRO:HG3	11:W:165:PRO:HG3	1.92	0.51
6:T:100:SER:HB3	7:R:135:ILE:HD11	1.91	0.51
28:R:603:HEA:O11	28:R:603:HEA:H14	2.10	0.51
3:H:42:LEU:HD13	3:H:122:VAL:HG12	1.92	0.51
1:O:273:MET:HE2	16:O:303:MQ9:H3D	1.92	0.51
7:R:279:SER:HB3	7:R:344:TRP:HE1	1.74	0.51
1:O:277:ILE:HG23	1:O:278:ILE:HG13	1.91	0.51
7:L:263:GLY:O	7:L:267:VAL:HG23	2.11	0.51
7:R:110:GLN:HG2	7:R:518:GLU:OE1	2.11	0.51
3:N:229:LEU:O	3:N:233:GLN:HB2	2.10	0.51
3:N:424:PHE:HB2	23:P:301:CDL:H512	1.93	0.51
11:W:88:LEU:HD21	11:W:91:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:39:LEU:O	7:L:43:MET:HG3	2.10	0.51
7:L:434:HIS:CD2	7:L:491:PHE:HB2	2.46	0.51
23:P:301:CDL:HA61	23:R:605:CDL:H312	1.92	0.51
7:R:384:LEU:O	7:R:388:VAL:HG22	2.11	0.51
4:I:48:MET:HG2	23:I:301:CDL:HB61	1.93	0.51
10:a:138:ASN:HB3	10:a:141:ASP:HB2	1.93	0.51
7:R:110:GLN:HB3	7:R:207:PRO:HG2	1.92	0.51
22:N:606:HEM:HMB1	22:N:606:HEM:HBB2	1.93	0.50
2:G:369:GLN:HG2	3:H:404:LEU:HD11	1.92	0.50
1:O:130:GLN:HG3	1:O:227:GLN:HE22	1.76	0.50
5:S:34:SER:HB2	6:T:48:LEU:HG	1.93	0.50
3:H:312:ILE:HG12	3:H:333:VAL:HG21	1.93	0.50
1:O:110:GLU:O	1:O:110:GLU:HG2	2.11	0.50
3:N:42:LEU:HD13	3:N:122:VAL:HG12	1.92	0.50
23:L:601:CDL:H721	23:L:601:CDL:H542	1.93	0.50
14:B:20:LEU:HD22	14:B:25:ASP:HB3	1.92	0.50
7:R:245:TYR:HA	7:R:251:GLY:HA3	1.94	0.50
7:R:395:ILE:HG23	7:R:399:HIS:CE1	2.47	0.50
3:N:156:PHE:HA	3:N:159:TYR:CE2	2.47	0.50
7:L:383:PRO:HD2	8:X:113:THR:HG23	1.94	0.50
16:T:1301:MQ9:H362	7:R:141:ILE:HD11	1.94	0.50
7:R:485:GLY:HA2	28:R:603:HEA:H161	1.94	0.50
5:J:35:SER:HB2	7:L:221:LEU:HB3	1.93	0.50
7:R:353:LEU:HD11	8:Q:71:THR:HG22	1.94	0.49
7:R:398:PHE:O	7:R:402:LEU:HB2	2.12	0.49
3:H:231:TRP:CE3	16:H:1006:MQ9:H3D	2.47	0.49
3:H:490:LYS:NZ	23:K:201:CDL:HA22	2.27	0.49
5:S:31:VAL:HG12	7:R:187:VAL:HG22	1.94	0.49
8:X:90:TYR:O	8:X:90:TYR:CD1	2.65	0.49
7:L:445:THR:HG23	7:L:446:PHE:CE1	2.47	0.49
2:M:393:PRO:HB2	2:M:405:ASN:HB3	1.92	0.49
10:V:85:LEU:HD22	10:V:109:VAL:HG12	1.94	0.49
23:N:604:CDL:H312	23:N:604:CDL:HB4	1.95	0.49
7:R:384:LEU:HD13	8:Q:50:TRP:HE3	1.78	0.49
1:C:124:ALA:O	1:C:125:MET:HE2	2.12	0.49
1:C:294:ALA:HA	3:H:483:PRO:HG2	1.95	0.49
3:H:428:ARG:HH22	23:I:301:CDL:HB21	1.76	0.49
2:M:279:MET:SD	2:M:313:MET:HG2	2.52	0.49
4:P:92:TRP:HE1	23:P:303:CDL:HB32	1.77	0.49
23:P:303:CDL:H171	23:P:303:CDL:H781	1.95	0.49
5:S:31:VAL:HG13	7:R:221:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:231:TRP:HE3	16:H:1006:MQ9:H3D	1.77	0.49
1:O:135:PRO:HD2	7:R:160:ALA:O	2.13	0.49
7:R:215:VAL:HA	7:R:218:ILE:HD12	1.94	0.49
2:M:148:VAL:HG23	3:N:263:ALA:HB1	1.93	0.48
10:a:45:THR:HG22	10:a:46:MET:HE2	1.95	0.48
2:M:419:ARG:HD3	2:M:420:LYS:HZ3	1.77	0.48
1:C:130:GLN:HG3	1:C:227:GLN:HE22	1.77	0.48
5:J:153:GLY:HA3	23:L:601:CDL:H592	1.95	0.48
1:O:194:PHE:CZ	3:N:296:SER:HB3	2.48	0.48
7:R:80:ASN:HA	7:R:83:PHE:CE2	2.48	0.48
7:R:395:ILE:CD1	28:R:603:HEA:HAA2	2.41	0.48
16:H:1006:MQ9:H322	16:H:1006:MQ9:H303	1.62	0.48
6:K:100:SER:HB3	7:L:135:ILE:HD11	1.95	0.48
7:R:456:GLY:HA2	8:Q:235:TRP:CH2	2.48	0.48
7:L:532:GLU:HG3	10:a:23:THR:HB	1.94	0.48
3:N:66:PRO:HG3	3:N:208:TYR:CD2	2.48	0.48
10:V:77:THR:HG23	10:V:107:GLU:CD	2.39	0.48
14:F:20:LEU:CD1	14:F:25:ASP:O	2.61	0.48
1:O:121:ARG:CG	1:O:121:ARG:NH1	2.74	0.48
5:S:17:HIS:O	5:S:19:LEU:HD22	2.14	0.48
8:Q:40:THR:HG22	8:Q:42:GLU:H	1.78	0.48
7:L:115:ASP:O	7:L:196:MET:HE2	2.14	0.48
23:P:303:CDL:H132	23:P:303:CDL:HA62	1.95	0.48
5:J:69:LEU:HD22	5:J:120:GLU:HB2	1.95	0.48
16:N:605:MQ9:H453	16:N:605:MQ9:H472	1.57	0.48
7:R:282:PHE:HA	7:R:359:MET:HE1	1.95	0.48
28:R:603:HEA:C27	28:R:603:HEA:C22	2.86	0.48
3:H:67:SER:HB3	3:H:87:ARG:HB2	1.95	0.48
7:L:53:LEU:HB3	28:L:603:HEA:H22	1.96	0.48
7:L:445:THR:HG23	7:L:446:PHE:CD1	2.49	0.48
11:W:143:ILE:HB	11:W:166:ILE:HD11	1.96	0.47
1:C:112:ALA:HA	1:C:224:THR:HG21	1.96	0.47
7:L:215:VAL:HG21	7:L:300:THR:HG22	1.95	0.47
23:R:601:CDL:H521	23:R:601:CDL:H761	1.96	0.47
3:H:77:TYR:CE2	3:H:285:TRP:HB2	2.49	0.47
21:M:504:7PH:H22	21:M:504:7PH:H25	1.57	0.47
8:Q:224:VAL:HG22	8:Q:257:VAL:HG22	1.97	0.47
8:X:189:THR:C	8:X:191:GLU:N	2.71	0.47
1:O:116:GLN:HE21	1:O:122:MET:HG2	1.79	0.47
23:H:1005:CDL:HB4	23:H:1005:CDL:H311	1.95	0.47
5:J:184:TYR:CZ	23:L:601:CDL:H572	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:374:LEU:O	7:L:377:VAL:HG12	2.14	0.47
11:b:101:THR:O	11:b:133:VAL:HA	2.15	0.47
11:b:148:LEU:HB3	11:b:163:ALA:HB1	1.95	0.47
15:C:301:HEC:HBD2	11:b:35:GLN:NE2	2.29	0.47
10:a:85:LEU:HD22	10:a:109:VAL:HG12	1.95	0.47
14:F:26:HIS:H	14:F:26:HIS:CD2	2.31	0.47
3:N:239:PRO:HB3	14:F:61:THR:HG21	1.96	0.47
23:P:303:CDL:H731	23:P:303:CDL:H111	1.97	0.47
7:R:264:HIS:O	7:R:265:PRO:C	2.54	0.47
2:G:46:GLU:O	2:G:50:MET:HG3	2.15	0.47
5:J:77:LEU:HD23	5:J:192:TRP:CD1	2.49	0.47
5:J:175:ALA:O	5:J:179:ILE:HD12	2.14	0.47
8:X:188:MET:O	8:X:189:THR:C	2.57	0.47
8:X:193:ARG:HB3	8:X:196:LEU:HD12	1.95	0.47
2:M:129:THR:HG23	3:N:104:PHE:HB2	1.97	0.47
7:R:445:THR:HA	7:R:477:SER:HA	1.96	0.47
23:R:605:CDL:H352	23:R:605:CDL:H382	1.71	0.47
3:N:432:SER:HB3	7:R:29:TYR:HB2	1.96	0.47
3:N:499:THR:HG23	3:N:511:HIS:ND1	2.30	0.47
28:R:603:HEA:H132	28:R:603:HEA:H162	1.58	0.47
7:L:398:PHE:HD1	7:L:402:LEU:HD12	1.79	0.47
6:T:1:MET:HG2	6:T:59:VAL:HG12	1.97	0.46
7:R:532:GLU:HG3	10:V:23:THR:HB	1.97	0.46
1:C:194:PHE:HE1	3:H:165:LEU:HD23	1.80	0.46
2:M:190:LEU:HD22	21:H:1001:7PH:H3BA	1.96	0.46
2:M:417:TRP:CG	3:N:184:VAL:H	2.33	0.46
23:T:1302:CDL:H311	23:T:1302:CDL:H341	1.65	0.46
7:R:383:PRO:HG3	8:Q:117:GLN:HB3	1.96	0.46
2:G:149:LEU:HD21	23:G:506:CDL:HB31	1.97	0.46
7:L:402:LEU:O	7:L:406:ILE:HG13	2.15	0.46
8:Q:137:GLN:HA	8:Q:138:TRP:HA	1.60	0.46
3:H:423:TYR:CD1	23:I:301:CDL:H512	2.50	0.46
6:K:7:LEU:CD1	7:L:301:LEU:HD21	2.46	0.46
16:O:303:MQ9:H301	16:O:303:MQ9:H512	1.98	0.46
2:M:380:PRO:HD3	2:M:388:ALA:HA	1.97	0.46
5:S:120:GLU:OE1	5:S:123:HIS:HD2	1.99	0.46
16:T:1301:MQ9:H472	16:T:1301:MQ9:H453	1.57	0.46
7:R:264:HIS:CD2	7:R:310:VAL:CG2	2.99	0.46
11:W:95:VAL:O	11:W:95:VAL:CG1	2.63	0.46
3:H:478:GLU:HA	3:H:478:GLU:OE1	2.15	0.46
13:A:5:LEU:HG	13:A:6:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:92:TRP:CD1	23:P:303:CDL:H511	2.51	0.46
1:C:138:PHE:HB3	1:C:142:GLN:HB2	1.97	0.46
1:C:227:GLN:HA	11:b:35:GLN:HE22	1.80	0.46
7:L:288:LYS:HE2	7:L:349:TRP:O	2.15	0.46
23:T:1302:CDL:H562	23:T:1302:CDL:H531	1.68	0.46
7:L:550:MET:CE	8:X:84:LEU:HB2	2.46	0.46
1:O:218:ILE:HG23	15:O:302:HEC:HMA3	1.96	0.46
16:N:607:MQ9:H203	16:N:607:MQ9:H221	1.75	0.46
16:C:305:MQ9:H153	16:C:305:MQ9:H412	1.98	0.46
21:G:504:7PH:H25	21:G:504:7PH:H22	1.51	0.46
10:a:63:LYS:HG2	10:a:156:PRO:HB3	1.98	0.46
7:R:223:ALA:O	7:R:226:ILE:HG22	2.16	0.46
1:C:179:ARG:NH2	1:C:241:GLU:HG3	2.31	0.46
7:L:284:VAL:HG22	7:L:514:GLY:HA2	1.98	0.46
7:L:359:MET:HE2	7:L:359:MET:HA	1.98	0.46
7:R:384:LEU:HD22	8:Q:50:TRP:HB2	1.97	0.45
23:H:1005:CDL:H141	23:H:1005:CDL:H112	1.67	0.45
23:N:604:CDL:H222	23:N:604:CDL:H191	1.54	0.45
16:N:607:MQ9:H33	16:N:607:MQ9:H303	1.98	0.45
7:L:397:HIS:NE2	28:L:602:HEA:NA	2.64	0.45
8:X:167:MET:HB3	8:X:167:MET:HE3	1.63	0.45
7:R:391:SER:HA	7:R:458:PRO:HA	1.98	0.45
11:W:66:GLU:OE1	11:W:66:GLU:HA	2.16	0.45
1:C:125:MET:HG3	7:L:162:HIS:HA	1.99	0.45
2:G:417:TRP:CG	3:H:184:VAL:H	2.34	0.45
1:O:269:ALA:HA	3:N:306:MET:HE1	1.98	0.45
23:N:603:CDL:H772	23:N:603:CDL:H742	1.82	0.45
23:N:604:CDL:H331	23:N:604:CDL:H141	1.99	0.45
3:H:66:PRO:HG3	3:H:208:TYR:CD2	2.49	0.45
23:L:609:CDL:H351	23:L:609:CDL:H382	1.70	0.45
8:X:129:VAL:HG22	8:X:147:ILE:HG23	1.97	0.45
5:S:92:GLU:OE2	14:F:30:GLU:HB2	2.16	0.45
7:L:384:LEU:O	7:L:388:VAL:HG22	2.17	0.45
16:N:605:MQ9:H203	16:N:605:MQ9:H222	1.48	0.45
5:S:35:SER:HB2	7:R:221:LEU:HD22	1.99	0.45
21:S:501:7PH:H28	21:S:501:7PH:H2BA	1.68	0.45
7:R:81:GLN:HG3	7:R:148:ASP:HB3	1.99	0.45
28:R:602:HEA:H202	28:R:602:HEA:H172	1.63	0.45
1:C:277:ILE:HG23	1:C:278:ILE:HG13	1.99	0.45
23:R:605:CDL:H731	23:R:605:CDL:H762	1.60	0.45
7:L:274:PHE:CE2	7:L:406:ILE:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:179:THR:HG23	3:N:189:MET:HE2	1.99	0.45
7:R:550:MET:HE3	7:R:550:MET:HB3	1.85	0.45
6:K:1:MET:HE1	7:L:194:VAL:HG13	1.99	0.45
7:L:282:PHE:O	7:L:286:SER:HB2	2.16	0.45
1:O:121:ARG:NH1	1:O:133:SER:HB3	2.32	0.45
2:M:322:MET:HG3	11:W:148:LEU:HD11	1.99	0.45
21:M:504:7PH:H23A	3:H:10:ALA:HA	1.99	0.45
7:L:46:VAL:HG21	23:L:609:CDL:H131	1.98	0.45
7:L:317:ALA:HB2	7:L:389:THR:HG21	1.99	0.45
2:M:266:PHE:HD2	2:M:301:LEU:HD22	1.82	0.45
5:S:92:GLU:HG2	14:F:28:VAL:O	2.17	0.45
23:T:1302:CDL:H521	23:T:1302:CDL:H141	1.98	0.45
7:L:400:TYR:HA	7:L:442:PHE:HZ	1.82	0.45
7:L:446:PHE:HA	7:L:449:GLN:HG3	1.99	0.45
10:a:68:VAL:HG11	10:a:143:LEU:HD13	1.99	0.45
1:O:110:GLU:HG3	1:O:147:GLY:HA3	1.99	0.44
3:H:195:GLY:HA3	3:H:202:ILE:HD11	1.99	0.44
7:L:384:LEU:HD13	8:X:50:TRP:HE3	1.82	0.44
5:S:17:HIS:CD2	5:S:19:LEU:HB2	2.52	0.44
7:R:253:LEU:HD12	8:Q:252:ASN:O	2.17	0.44
22:H:1007:HEM:HBC2	22:H:1007:HEM:HMC2	2.00	0.44
3:N:160:SER:HA	3:N:167:SER:HB2	2.00	0.44
23:N:603:CDL:HB62	23:N:604:CDL:H322	2.00	0.44
3:H:179:THR:HG23	3:H:189:MET:HE2	1.98	0.44
3:H:210:LEU:HA	3:H:214:LEU:HB2	1.99	0.44
3:H:229:LEU:O	3:H:233:GLN:HB2	2.18	0.44
7:L:267:VAL:HG11	28:L:602:HEA:CHD	2.48	0.44
1:O:115:PHE:HZ	15:O:302:HEC:HAA2	1.82	0.44
2:M:419:ARG:HH11	2:M:420:LYS:HG3	1.82	0.44
8:Q:235:TRP:CD1	8:Q:242:LYS:HB3	2.52	0.44
7:L:159:ASP:OD1	7:L:161:ILE:HG22	2.17	0.44
9:Z:73:GLY:HA3	10:a:110:TYR:CE1	2.52	0.44
10:a:92:GLU:HB2	10:a:113:ASP:OD2	2.16	0.44
3:H:314:LEU:HB3	3:H:415:MET:HE1	1.98	0.44
28:L:602:HEA:O11	28:L:602:HEA:HHC	2.18	0.44
9:Z:37:LYS:HE3	9:Z:37:LYS:HB2	1.70	0.44
5:S:179:ILE:HD13	14:F:30:GLU:HA	1.99	0.44
1:C:174:GLY:H	1:C:247:ALA:HB2	1.82	0.44
3:H:403:SER:O	3:H:407:THR:HG23	2.18	0.44
3:H:432:SER:HB3	7:L:29:TYR:HB2	1.99	0.44
5:J:65:LEU:HD23	5:J:65:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:226:ILE:HD11	7:L:258:LEU:HD22	1.98	0.44
8:X:215:LEU:HD13	8:X:221:ILE:HG21	1.99	0.44
10:a:45:THR:O	10:a:49:VAL:HG23	2.18	0.44
23:P:303:CDL:H321	23:P:303:CDL:H352	1.61	0.44
16:T:1301:MQ9:H203	16:T:1301:MQ9:H221	1.79	0.44
7:R:376:GLY:O	28:R:602:HEA:HHB	2.17	0.44
7:R:397:HIS:NE2	28:R:602:HEA:NA	2.66	0.44
1:C:227:GLN:HE21	15:C:302:HEC:CGD	2.30	0.44
3:N:407:THR:HB	16:T:1301:MQ9:H502	1.99	0.44
4:P:52:GLY:HA2	23:P:301:CDL:H752	2.00	0.44
7:R:398:PHE:CE1	7:R:399:HIS:CE1	3.05	0.44
5:J:61:GLU:OE2	5:J:62:PRO:HA	2.18	0.44
7:L:54:VAL:HG12	7:L:58:MET:HE3	2.00	0.44
7:L:420:LYS:HG3	7:L:421:MET:HE2	2.00	0.44
7:L:420:LYS:O	7:L:525:PRO:HD3	2.18	0.44
1:O:227:GLN:HE21	15:O:302:HEC:CGD	2.30	0.44
21:S:501:7PH:H35	23:T:1302:CDL:H161	2.00	0.44
7:R:504:PRO:HB2	10:V:39:VAL:HG21	2.00	0.44
1:C:193:ASN:O	1:C:194:PHE:C	2.61	0.43
6:K:17:LEU:HD22	13:A:19:LEU:HB3	2.00	0.43
7:L:445:THR:HA	7:L:477:SER:HA	2.00	0.43
7:L:510:PRO:HA	10:a:32:THR:HG22	1.99	0.43
7:R:21:MET:HG3	7:R:500:ARG:HG2	1.99	0.43
10:V:126:GLY:HA3	10:V:150:MET:HG3	2.01	0.43
16:H:1006:MQ9:H203	16:H:1006:MQ9:H221	1.58	0.43
1:O:250:ARG:O	1:O:254:GLU:HG2	2.18	0.43
23:N:604:CDL:H532	23:N:604:CDL:H712	2.00	0.43
6:T:2:HIS:HB2	13:E:2:ARG:HH12	1.82	0.43
7:R:112:GLY:HA2	7:R:530:PHE:CE2	2.53	0.43
7:R:313:HIS:ND1	28:R:602:HEA:CMA	2.81	0.43
16:C:303:MQ9:H153	16:C:303:MQ9:H172	1.72	0.43
6:K:91:TRP:O	6:K:95:ILE:HG13	2.19	0.43
7:L:227:LEU:HB2	7:L:262:PHE:CG	2.54	0.43
7:L:267:VAL:CG1	28:L:602:HEA:CAC	2.96	0.43
3:N:315:TRP:HB3	3:N:329:GLN:NE2	2.33	0.43
5:S:27:VAL:HG12	6:T:55:PHE:HE2	1.82	0.43
10:V:138:ASN:HB3	10:V:141:ASP:HB2	2.01	0.43
16:H:1006:MQ9:H422	16:H:1006:MQ9:H403	1.79	0.43
7:L:59:ALA:HB2	7:L:86:HIS:CE1	2.54	0.43
7:L:512:GLY:HA2	10:a:31:VAL:HB	2.00	0.43
7:R:53:LEU:HD22	28:R:603:HEA:C27	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:196:MET:HE3	7:R:196:MET:HB3	1.75	0.43
7:R:402:LEU:HD13	28:R:603:HEA:CBC	2.48	0.43
8:Q:283:MET:HG2	8:Q:328:PHE:CG	2.53	0.43
2:G:238:LEU:HD23	2:G:238:LEU:HA	1.89	0.43
7:L:479:VAL:HG22	9:Z:10:ILE:HA	2.00	0.43
14:F:35:ARG:HA	14:F:35:ARG:HD3	1.82	0.43
4:P:72:GLU:O	4:P:76:LEU:HG	2.19	0.43
6:T:10:ILE:HG23	13:E:15:TYR:CZ	2.54	0.43
5:J:63:THR:HG21	5:J:136:TYR:HE2	1.83	0.43
7:L:384:LEU:HD22	8:X:50:TRP:HB2	1.99	0.43
7:L:554:MET:HE2	7:L:554:MET:HB2	1.81	0.43
11:b:91:ILE:HD12	11:b:100:LEU:HD21	2.00	0.43
5:S:20:ASN:CB	13:E:103:ARG:HH11	2.30	0.43
7:R:80:ASN:HA	7:R:83:PHE:CD2	2.53	0.43
5:J:38:MET:HE3	5:J:38:MET:HB3	1.91	0.43
8:X:137:GLN:HA	8:X:138:TRP:HA	1.58	0.43
11:b:120:GLN:HG2	11:b:121:ILE:HG23	2.00	0.43
3:H:441:LEU:HD22	3:H:477:LEU:HB2	2.01	0.43
10:a:126:GLY:HA3	10:a:150:MET:HG3	2.01	0.43
2:G:204:LEU:HD23	2:G:204:LEU:HA	1.81	0.43
7:L:245:TYR:HA	7:L:251:GLY:HA3	2.01	0.43
7:L:544:GLU:HG2	7:L:551:VAL:HG22	2.01	0.43
7:L:555:ARG:HG2	7:L:555:ARG:HH11	1.83	0.43
2:M:207:PHE:CE1	2:G:140:ILE:HB	2.54	0.43
21:M:504:7PH:H29A	21:M:504:7PH:H2CA	1.79	0.43
7:R:56:GLY:HA3	28:R:603:HEA:H172	2.00	0.43
2:G:291:ASP:HB3	11:b:179:ALA:HB3	2.01	0.43
2:M:279:MET:HE3	2:M:279:MET:HB3	1.91	0.42
2:M:349:LEU:HD12	2:M:368:HIS:CE1	2.53	0.42
8:Q:194:THR:HG22	8:Q:196:LEU:H	1.84	0.42
1:C:275:MET:HG2	3:H:114:LEU:HB3	2.01	0.42
16:C:305:MQ9:H253	16:C:305:MQ9:H271	1.76	0.42
23:I:302:CDL:H772	23:I:302:CDL:H741	1.85	0.42
7:L:196:MET:HB3	7:L:196:MET:HE3	1.77	0.42
2:M:175:LYS:HE3	2:M:175:LYS:HB3	1.87	0.42
3:N:305:MET:HE1	16:N:607:MQ9:H3B	2.00	0.42
7:R:59:ALA:HB2	7:R:86:HIS:CE1	2.54	0.42
23:R:601:CDL:HB62	23:R:601:CDL:HA32	2.01	0.42
10:V:135:LYS:HZ2	10:V:135:LYS:HG2	1.77	0.42
3:H:309:ASP:HA	3:H:312:ILE:HD12	2.01	0.42
16:H:1006:MQ9:H103	16:H:1006:MQ9:H122	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:142:PHE:HB3	8:X:213:LEU:HD13	2.00	0.42
8:Q:43:ALA:HB1	8:Q:240:LEU:HD12	2.02	0.42
11:W:72:GLU:HG2	11:W:74:LEU:CD1	2.48	0.42
2:G:266:PHE:HD2	2:G:301:LEU:HD22	1.84	0.42
1:O:126:ARG:HH21	7:R:165:GLY:H	1.66	0.42
1:O:294:ALA:HA	3:N:483:PRO:HG2	2.02	0.42
2:M:217:GLY:HA3	2:G:107:PHE:HE2	1.84	0.42
7:R:317:ALA:O	8:Q:243:ARG:HD3	2.19	0.42
2:G:148:VAL:O	2:G:152:LYS:HG2	2.19	0.42
3:N:436:SER:O	3:N:440:VAL:HG23	2.19	0.42
7:R:227:LEU:HB2	7:R:262:PHE:CG	2.54	0.42
7:R:405:THR:O	7:R:409:ALA:HB3	2.19	0.42
2:G:279:MET:HE3	2:G:279:MET:HB3	1.83	0.42
7:L:398:PHE:HB2	28:L:602:HEA:C2D	2.49	0.42
14:F:21:SER:C	14:F:23:ASP:H	2.25	0.42
2:M:238:LEU:HD23	2:M:238:LEU:HA	1.92	0.42
5:S:38:MET:HG3	7:R:222:ILE:HA	2.02	0.42
7:R:397:HIS:O	7:R:401:VAL:HG23	2.19	0.42
8:Q:142:PHE:HB3	8:Q:213:LEU:HD13	2.01	0.42
11:W:117:PRO:HD2	11:W:120:GLN:OE1	2.19	0.42
6:K:17:LEU:O	6:K:21:VAL:HG23	2.20	0.42
5:S:36:GLU:O	5:S:36:GLU:HG3	2.17	0.42
3:H:111:TRP:HD1	3:H:276:GLY:HA2	1.85	0.42
3:H:458:TYR:HD2	7:L:530:PHE:HB2	1.85	0.42
3:H:526:LEU:HD23	3:H:526:LEU:HA	1.83	0.42
5:J:44:PHE:HE1	5:J:198:THR:HG21	1.84	0.42
7:L:405:THR:O	7:L:409:ALA:HB3	2.20	0.42
8:Q:138:TRP:O	8:Q:284:MET:HB3	2.20	0.42
7:L:63:ARG:NH2	7:L:477:SER:HB3	2.35	0.42
14:B:29:THR:O	14:B:30:GLU:HB3	2.20	0.42
2:M:136:PHE:O	2:M:140:ILE:HG22	2.19	0.42
3:N:30:LEU:HD22	3:N:254:MET:HB2	2.01	0.42
5:S:76:VAL:HG13	5:S:109:MET:HB3	2.01	0.42
7:R:89:VAL:HA	7:R:93:PHE:CD2	2.55	0.42
5:J:63:THR:HG21	5:J:136:TYR:CE2	2.54	0.42
7:L:357:THR:OG1	7:L:358:PRO:HD3	2.20	0.42
13:E:99:ARG:HB2	13:E:99:ARG:NH1	2.34	0.42
3:N:212:ILE:HD11	3:H:212:ILE:HD11	2.01	0.42
3:N:272:LEU:HD23	3:N:272:LEU:HA	1.91	0.42
3:N:338:GLY:HA2	16:N:607:MQ9:H161	2.01	0.42
23:P:301:CDL:H391	7:R:492:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:17:HIS:C	5:S:19:LEU:H	2.27	0.42
6:T:26:THR:HG21	6:T:35:GLU:H	1.85	0.42
7:R:313:HIS:HB2	7:R:316:TYR:CZ	2.55	0.42
2:G:322:MET:HG3	11:b:148:LEU:HD11	2.01	0.42
13:A:93:GLU:O	13:A:97:VAL:HG23	2.19	0.42
8:Q:146:LYS:HB3	8:Q:146:LYS:HE3	1.90	0.41
1:C:82:LEU:O	1:C:83:PHE:C	2.62	0.41
5:J:172:PRO:HB2	14:B:39:LEU:HD13	2.02	0.41
7:R:285:PHE:HB2	7:R:359:MET:HE2	2.01	0.41
4:I:33:VAL:HG11	4:I:41:SER:HB2	2.02	0.41
7:L:391:SER:HA	7:L:458:PRO:HA	2.02	0.41
5:S:20:ASN:HB3	13:E:103:ARG:NH1	2.30	0.41
7:R:151:TRP:HD1	28:R:603:HEA:O2D	2.02	0.41
7:L:153:ALA:HB1	7:L:158:THR:HG21	2.02	0.41
2:M:93:LEU:HB2	2:G:199:SER:HB3	2.02	0.41
3:N:10:ALA:HA	21:G:504:7PH:H23A	2.01	0.41
6:T:6:ARG:HD3	6:T:6:ARG:HA	1.97	0.41
7:R:336:PRO:O	7:R:340:LYS:HG3	2.20	0.41
23:H:1003:CDL:H152	23:H:1003:CDL:H182	1.82	0.41
7:L:360:LEU:HD12	7:L:360:LEU:HA	1.94	0.41
7:L:370:LEU:HD21	8:X:64:VAL:HB	2.03	0.41
3:N:371:PRO:HB2	3:N:427:TYR:CD1	2.55	0.41
22:N:601:HEM:CBC	3:H:213:LEU:HD21	2.49	0.41
16:N:607:MQ9:H372	16:N:607:MQ9:H353	1.64	0.41
7:R:153:ALA:HB1	7:R:158:THR:HG21	2.03	0.41
7:R:335:VAL:HB	7:R:336:PRO:HD3	2.02	0.41
7:R:484:LEU:HD13	28:R:603:HEA:H11	2.01	0.41
28:R:603:HEA:H171	28:R:603:HEA:H202	1.73	0.41
1:C:132:PRO:HG2	7:L:164:PRO:HB2	2.03	0.41
1:C:254:GLU:HB2	2:G:117:PHE:CE1	2.55	0.41
21:G:504:7PH:H36A	21:G:504:7PH:H39	1.77	0.41
5:J:88:VAL:O	5:J:92:GLU:HG2	2.20	0.41
3:N:210:LEU:HA	3:N:214:LEU:HB2	2.03	0.41
7:R:337:THR:HG22	28:R:602:HEA:H171	2.03	0.41
8:Q:154:PHE:HZ	8:Q:300:ILE:HG21	1.84	0.41
3:H:423:TYR:HD1	23:I:301:CDL:H512	1.85	0.41
7:L:95:ALA:O	7:L:98:ILE:HG22	2.20	0.41
1:O:94:ASN:O	1:O:95:LEU:HB2	2.20	0.41
7:R:282:PHE:HD1	7:R:359:MET:HE1	1.85	0.41
1:C:94:ASN:O	1:C:95:LEU:HB2	2.19	0.41
2:G:271:PRO:HB3	2:G:339:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:21:MET:HE2	7:L:21:MET:HB2	1.86	0.41
7:L:267:VAL:HG13	28:L:602:HEA:HAC	2.01	0.41
12:c:23:PRO:HA	12:c:24:PRO:HD3	1.96	0.41
3:N:8:LEU:O	3:N:12:GLN:HG2	2.21	0.41
3:N:87:ARG:HA	3:N:87:ARG:HD2	1.88	0.41
23:P:301:CDL:H742	23:P:301:CDL:H541	2.03	0.41
5:S:24:MET:HE2	5:S:24:MET:HB3	1.80	0.41
8:Q:67:LEU:HD23	8:Q:67:LEU:HA	1.91	0.41
1:C:269:ALA:HA	3:H:306:MET:HE1	2.02	0.41
6:K:11:LEU:HD23	6:K:11:LEU:HA	1.92	0.41
7:L:390:ASP:HA	7:L:459:ARG:HD3	2.02	0.41
1:O:125:MET:HE3	7:R:162:HIS:CD2	2.56	0.41
16:O:303:MQ9:H161	23:N:603:CDL:H571	2.02	0.41
3:N:403:SER:O	3:N:407:THR:HG23	2.21	0.41
5:S:120:GLU:OE1	5:S:120:GLU:HA	2.21	0.41
6:T:123:THR:HG23	23:T:1302:CDL:H132	2.03	0.41
7:R:27:LEU:HG	7:R:31:LEU:HG	2.03	0.41
1:C:134:LYS:HD3	7:L:164:PRO:HG3	2.02	0.41
16:C:305:MQ9:H422	16:C:305:MQ9:H38	1.66	0.41
3:H:56:THR:HG23	16:H:1006:MQ9:H453	2.03	0.41
3:H:458:TYR:HE1	6:K:82:LEU:HD11	1.86	0.41
5:J:51:ARG:HH12	26:J:601:TRD:H41	1.86	0.41
7:L:83:PHE:CD1	7:L:83:PHE:C	2.98	0.41
7:L:152:THR:HA	7:L:259:PHE:CZ	2.56	0.41
28:L:602:HEA:H18	28:L:602:HEA:H212	1.72	0.41
1:O:125:MET:HE3	7:R:162:HIS:HA	2.01	0.41
11:W:72:GLU:HG2	11:W:74:LEU:HD11	2.02	0.41
1:C:74:ALA:HA	1:C:77:ARG:HG2	2.02	0.41
3:H:66:PRO:O	3:H:205:PRO:HG3	2.21	0.41
23:H:1005:CDL:H192	6:K:94:LEU:HD13	2.03	0.41
10:a:63:LYS:HE3	10:a:63:LYS:HA	2.03	0.41
14:F:35:ARG:HB2	14:F:39:LEU:HD23	2.03	0.41
2:M:336:PHE:HD1	12:Y:36:PRO:HG2	1.85	0.40
6:T:35:GLU:OE2	7:R:257:HIS:NE2	2.54	0.40
11:W:31:GLN:O	11:W:35:GLN:HG3	2.22	0.40
7:L:134:LEU:HD23	7:L:134:LEU:HA	1.87	0.40
7:L:395:ILE:HA	7:L:398:PHE:CE2	2.56	0.40
8:X:93:PRO:O	8:X:97:THR:HG22	2.21	0.40
5:S:183:TYR:OH	14:F:30:GLU:HG2	2.21	0.40
8:Q:138:TRP:CG	8:Q:280:PHE:HB2	2.56	0.40
1:C:84:GLU:HA	1:C:88:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:301:CDL:H511	23:I:301:CDL:H542	1.97	0.40
5:J:161:LEU:O	5:J:165:THR:HG23	2.22	0.40
7:L:106:VAL:HG11	7:L:417:TRP:CE2	2.56	0.40
3:H:303:PHE:HA	3:H:306:MET:HG3	2.03	0.40
23:H:1005:CDL:H111	23:K:201:CDL:HA4	2.03	0.40
6:K:103:ALA:O	7:L:173:MET:HG3	2.21	0.40
6:K:112:TRP:CD1	6:K:112:TRP:H	2.38	0.40
14:B:51:ALA:HA	14:B:54:LEU:HB2	2.02	0.40
3:N:164:ASP:O	3:N:290:TYR:HB2	2.20	0.40
5:S:19:LEU:HB3	14:F:32:ALA:CB	2.51	0.40
6:T:2:HIS:HB2	13:E:2:ARG:NH1	2.36	0.40
7:R:12:GLU:HG2	7:R:13:ALA:N	2.36	0.40
10:V:76:ASP:O	10:V:78:ALA:N	2.49	0.40
5:J:65:LEU:HD13	5:J:200:TYR:HA	2.04	0.40
5:J:193:ILE:HD13	5:J:193:ILE:HA	1.90	0.40
3:N:254:MET:HA	3:N:255:PRO:HA	1.85	0.40
7:R:350:LYS:HD3	7:R:350:LYS:HA	1.85	0.40
8:Q:30:ALA:HA	26:Q:403:TRD:H12	2.03	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	C	221/278 (80%)	214 (97%)	6 (3%)	1 (0%)	24 43
1	O	221/278 (80%)	210 (95%)	11 (5%)	0	100 100
2	G	378/408 (93%)	366 (97%)	12 (3%)	0	100 100
2	M	378/408 (93%)	368 (97%)	10 (3%)	0	100 100
3	H	531/556 (96%)	519 (98%)	12 (2%)	0	100 100
3	N	531/556 (96%)	521 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	J	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
5	S	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
6	K	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	L	549/575 (96%)	534 (97%)	15 (3%)	0	100	100
7	R	549/575 (96%)	535 (97%)	14 (3%)	0	100	100
8	Q	283/341 (83%)	274 (97%)	9 (3%)	0	100	100
8	X	288/341 (84%)	277 (96%)	11 (4%)	0	100	100
9	U	62/79 (78%)	61 (98%)	1 (2%)	0	100	100
9	Z	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	a	141/157 (90%)	139 (99%)	2 (1%)	0	100	100
11	W	144/186 (77%)	138 (96%)	6 (4%)	0	100	100
11	b	145/186 (78%)	143 (99%)	2 (1%)	0	100	100
12	Y	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
12	c	23/236 (10%)	22 (96%)	1 (4%)	0	100	100
13	A	79/123 (64%)	76 (96%)	3 (4%)	0	100	100
13	E	83/123 (68%)	78 (94%)	5 (6%)	0	100	100
14	B	53/65 (82%)	50 (94%)	3 (6%)	0	100	100
14	F	53/65 (82%)	48 (91%)	5 (9%)	0	100	100
All	All	5725/6892 (83%)	5569 (97%)	155 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	194	PHE

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	C	163/206 (79%)	161 (99%)	2 (1%)	63	83
1	O	163/206 (79%)	159 (98%)	4 (2%)	42	69
2	G	311/333 (93%)	310 (100%)	1 (0%)	86	94
2	M	311/333 (93%)	310 (100%)	1 (0%)	86	94
3	H	428/448 (96%)	427 (100%)	1 (0%)	87	95
3	N	428/448 (96%)	422 (99%)	6 (1%)	59	81
4	I	58/83 (70%)	58 (100%)	0	100	100
4	P	58/83 (70%)	56 (97%)	2 (3%)	32	60
5	J	149/161 (92%)	148 (99%)	1 (1%)	76	89
5	S	149/161 (92%)	147 (99%)	2 (1%)	61	82
6	K	106/106 (100%)	106 (100%)	0	100	100
6	T	106/106 (100%)	104 (98%)	2 (2%)	50	76
7	L	453/471 (96%)	449 (99%)	4 (1%)	70	87
7	R	453/471 (96%)	449 (99%)	4 (1%)	70	87
8	Q	245/288 (85%)	242 (99%)	3 (1%)	63	83
8	X	249/288 (86%)	246 (99%)	3 (1%)	63	83
9	U	51/59 (86%)	51 (100%)	0	100	100
9	Z	52/59 (88%)	51 (98%)	1 (2%)	50	76
10	V	105/114 (92%)	103 (98%)	2 (2%)	50	76
10	a	105/114 (92%)	105 (100%)	0	100	100
11	W	120/146 (82%)	120 (100%)	0	100	100
11	b	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100
12	c	20/167 (12%)	20 (100%)	0	100	100
13	A	60/86 (70%)	60 (100%)	0	100	100
13	E	64/86 (74%)	64 (100%)	0	100	100
14	B	46/54 (85%)	46 (100%)	0	100	100
14	F	46/54 (85%)	44 (96%)	2 (4%)	26	51
All	All	4640/5444 (85%)	4599 (99%)	41 (1%)	68	87

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	121	ARG
1	O	170	GLU
1	O	193	ASN
1	O	195	THR
2	M	269	MET
3	N	8	LEU
3	N	78	GLN
3	N	203	LEU
3	N	339	LEU
3	N	402	ILE
3	N	478	GLU
4	P	47	VAL
4	P	62	MET
5	S	19	LEU
5	S	166	LYS
6	T	9	GLU
6	T	29	PHE
7	R	20	ARG
7	R	129	PHE
7	R	333	ILE
7	R	359	MET
8	Q	94	LEU
8	Q	167	MET
8	Q	168	THR
10	V	53	ASP
10	V	77	THR
1	C	191	CYS
1	C	193	ASN
2	G	134	LEU
3	H	386	LEU
5	J	123	HIS
7	L	129	PHE
7	L	256	GLN
7	L	333	ILE
7	L	445	THR
8	X	96	LEU
8	X	167	MET
8	X	188	MET
9	Z	23	LEU
14	F	26	HIS
14	F	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	116	GLN
1	O	227	GLN
2	M	222	ASN
2	M	368	HIS
3	N	78	GLN
3	N	110	HIS
3	N	233	GLN
5	S	17	HIS
5	S	23	ASN
5	S	53	GLN
5	S	123	HIS
7	R	264	HIS
7	R	343	ASN
7	R	559	HIS
8	Q	226	ASN
8	Q	285	ASN
1	C	227	GLN
1	C	228	ASN
2	G	368	HIS
5	J	23	ASN
7	L	26	ASN
7	L	264	HIS
8	X	137	GLN
8	X	226	ASN
8	X	232	HIS
9	Z	7	HIS
10	a	138	ASN
11	b	35	GLN
11	b	61	GLN
14	F	26	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 84 ligands modelled in this entry, 10 are monoatomic - leaving 74 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	$\#\|Z\| > 2$
19	IZL	G	502	-	119,119,119	1.74	22 (18%)	161,163,163	1.27	16 (9%)
16	MQ9	O	303	-	59,59,59	1.54	5 (8%)	72,75,75	1.66	20 (27%)
15	HEC	O	302	1	50,50,50	1.44	6 (12%)	68,82,82	1.42	12 (17%)
23	CDL	G	506	-	78,78,99	1.35	10 (12%)	84,90,111	1.10	4 (4%)
23	CDL	H	1003	-	73,73,99	1.38	10 (13%)	79,85,111	1.18	4 (5%)
18	FES	M	501	2	0,4,4	-	-	-		
15	HEC	C	302	1	50,50,50	1.44	6 (12%)	68,82,82	1.42	12 (17%)
23	CDL	I	302	-	76,76,99	1.37	11 (14%)	82,88,111	1.11	4 (4%)
28	HEA	L	602	7	66,67,67	2.46	27 (40%)	78,103,103	2.63	35 (44%)
23	CDL	N	602	-	73,73,99	1.38	10 (13%)	79,85,111	1.18	4 (5%)
21	7PH	H	1001	-	37,37,37	0.95	4 (10%)	41,42,42	1.11	2 (4%)
26	TRD	L	607	-	12,12,12	0.29	0	11,11,11	0.83	0
23	CDL	H	1005	-	78,78,99	1.33	10 (12%)	84,90,111	1.17	4 (4%)
23	CDL	L	601	-	78,78,99	1.35	10 (12%)	84,90,111	1.15	4 (4%)
21	7PH	S	501	-	37,37,37	0.96	4 (10%)	41,42,42	1.13	2 (4%)
19	IZL	M	502	-	119,119,119	1.75	22 (18%)	161,163,163	1.18	13 (8%)
22	HEM	N	601	3	50,50,50	1.42	6 (12%)	66,82,82	1.14	6 (9%)
26	TRD	T	1303	-	12,12,12	0.29	0	11,11,11	0.85	0
24	PLM	N	608	-	10,10,17	0.44	0	9,9,17	0.54	0
26	TRD	Q	403	-	12,12,12	0.28	0	11,11,11	0.86	0
27	3PE	J	602	-	31,31,50	1.07	4 (12%)	34,36,55	1.19	2 (5%)
16	MQ9	C	305	-	59,59,59	1.54	5 (8%)	72,75,75	1.70	21 (29%)
23	CDL	L	609	-	76,76,99	1.38	11 (14%)	82,88,111	1.13	4 (4%)
26	TRD	L	608	-	12,12,12	0.28	0	11,11,11	0.83	0
23	CDL	I	301	-	76,76,99	1.37	11 (14%)	82,88,111	1.13	4 (4%)
25	9XX	b	202	-	31,31,41	1.08	4 (12%)	34,34,44	1.29	3 (8%)
26	TRD	R	608	-	12,12,12	0.28	0	11,11,11	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	9XX	c	302	-	31,31,41	1.09	4 (12%)	34,34,44	1.37	3 (8%)
23	CDL	T	1302	-	78,78,99	1.34	10 (12%)	84,90,111	1.17	5 (5%)
17	WUO	I	303	-	99,99,99	1.53	8 (8%)	123,125,125	1.30	15 (12%)
23	CDL	P	303	-	76,76,99	1.37	10 (13%)	82,88,111	1.12	4 (4%)
17	WUO	C	304	-	99,99,99	1.53	8 (8%)	123,125,125	1.27	12 (9%)
16	MQ9	N	605	-	59,59,59	1.60	5 (8%)	72,75,75	1.62	17 (23%)
16	MQ9	C	303	-	59,59,59	1.19	2 (3%)	72,75,75	1.73	20 (27%)
25	9XX	N	609	-	31,31,41	1.10	4 (12%)	34,34,44	1.38	4 (11%)
16	MQ9	T	1301	-	59,59,59	1.54	5 (8%)	72,75,75	1.70	19 (26%)
22	HEM	N	606	3	50,50,50	1.40	6 (12%)	66,82,82	1.12	5 (7%)
15	HEC	C	301	1	50,50,50	1.38	6 (12%)	68,82,82	1.17	6 (8%)
20	9YF	G	503	-	58,58,58	1.34	5 (8%)	69,71,71	1.16	4 (5%)
23	CDL	P	301	-	76,76,99	1.38	11 (14%)	82,88,111	1.16	4 (4%)
21	7PH	M	504	-	37,37,37	0.95	4 (10%)	41,42,42	1.12	2 (4%)
28	HEA	L	603	7	66,67,67	2.46	26 (39%)	78,103,103	2.47	35 (44%)
22	HEM	H	1002	3	50,50,50	1.39	7 (14%)	66,82,82	1.27	8 (12%)
23	CDL	H	1004	-	76,76,99	1.35	10 (13%)	82,88,111	1.17	5 (6%)
15	HEC	O	301	1	50,50,50	1.38	6 (12%)	68,82,82	1.18	6 (8%)
25	9XX	W	202	-	41,41,41	0.97	4 (9%)	44,44,44	1.26	4 (9%)
23	CDL	R	605	-	76,76,99	1.38	11 (14%)	82,88,111	1.13	4 (4%)
24	PLM	c	301	-	10,10,17	0.45	0	9,9,17	0.55	0
22	HEM	H	1007	3	50,50,50	1.65	10 (20%)	66,82,82	1.67	15 (22%)
26	TRD	X	403	-	12,12,12	0.28	0	11,11,11	0.85	0
28	HEA	R	602	7	66,67,67	2.45	26 (39%)	78,103,103	2.54	33 (42%)
24	PLM	L	610	-	10,10,17	0.40	0	9,9,17	0.80	0
18	FES	G	501	2	0,4,4	-	-	-		
26	TRD	S	502	-	12,12,12	0.29	0	11,11,11	0.84	0
17	WUO	P	302	-	99,99,99	1.56	8 (8%)	123,125,125	1.31	15 (12%)
16	MQ9	N	607	-	59,59,59	1.65	5 (8%)	72,75,75	1.56	19 (26%)
20	9YF	b	201	-	58,58,58	1.33	4 (6%)	69,71,71	1.11	3 (4%)
20	9YF	M	503	-	58,58,58	1.33	6 (10%)	69,71,71	1.22	4 (5%)
21	7PH	G	504	-	37,37,37	0.94	4 (10%)	41,42,42	1.14	2 (4%)
21	7PH	G	505	-	37,37,37	0.96	4 (10%)	41,42,42	1.09	2 (4%)
23	CDL	N	604	-	78,78,99	1.32	10 (12%)	84,90,111	1.18	4 (4%)
23	CDL	K	201	-	78,78,99	1.35	11 (14%)	84,90,111	1.15	4 (4%)
26	TRD	K	202	-	12,12,12	0.29	0	11,11,11	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	3PE	S	503	-	31,31,50	1.08	4 (12%)	34,36,55	1.13	2 (5%)
20	9YF	W	201	-	58,58,58	1.36	5 (8%)	69,71,71	1.13	3 (4%)
28	HEA	R	603	7	66,67,67	2.15	23 (34%)	78,103,103	2.57	32 (41%)
32	DCQ	H	1008	-	23,23,23	0.59	0	26,29,29	0.45	0
23	CDL	R	601	-	76,76,99	1.36	10 (13%)	82,88,111	1.15	4 (4%)
24	PLM	W	203	-	10,10,17	0.46	0	9,9,17	0.53	0
23	CDL	N	603	-	76,76,99	1.36	10 (13%)	82,88,111	1.15	4 (4%)
26	TRD	J	601	-	12,12,12	0.29	0	11,11,11	0.85	0
26	TRD	R	609	-	12,12,12	0.28	0	11,11,11	0.85	0
17	WUO	O	304	-	99,99,99	1.54	8 (8%)	123,125,125	1.30	14 (11%)
16	MQ9	H	1006	-	59,59,59	1.55	5 (8%)	72,75,75	1.69	19 (26%)

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
19	IZL	G	502	-	-	29/84/208/208	0/6/6/6
16	MQ9	O	303	-	-	10/53/73/73	0/2/2/2
15	HEC	O	302	1	1/1/3/7	4/14/54/54	-
23	CDL	G	506	-	-	56/89/89/110	-
23	CDL	H	1003	-	-	40/84/84/110	-
18	FES	M	501	2	-	-	0/1/1/1
15	HEC	C	302	1	1/1/3/7	4/14/54/54	-
23	CDL	I	302	-	-	54/87/87/110	-
28	HEA	L	602	7	-	14/36/76/76	-
23	CDL	N	602	-	-	52/84/84/110	-
21	7PH	H	1001	-	-	13/39/39/39	-
26	TRD	L	607	-	-	1/10/10/10	-
23	CDL	H	1005	-	-	48/89/89/110	-
23	CDL	L	601	-	-	45/89/89/110	-
21	7PH	S	501	-	-	15/39/39/39	-
19	IZL	M	502	-	-	40/84/208/208	0/6/6/6
22	HEM	N	601	3	-	1/14/54/54	-
26	TRD	T	1303	-	-	2/10/10/10	-
24	PLM	N	608	-	-	0/7/8/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	TRD	Q	403	-	-	0/10/10/10	-
27	3PE	J	602	-	-	14/35/35/54	-
16	MQ9	C	305	-	-	15/53/73/73	0/2/2/2
23	CDL	L	609	-	-	51/87/87/110	-
26	TRD	L	608	-	-	0/10/10/10	-
23	CDL	I	301	-	-	49/87/87/110	-
25	9XX	b	202	-	-	12/33/33/43	-
26	TRD	R	608	-	-	0/10/10/10	-
25	9XX	c	302	-	-	9/33/33/43	-
23	CDL	T	1302	-	-	57/89/89/110	-
17	WUO	I	303	-	-	36/84/148/148	0/3/3/3
23	CDL	P	303	-	-	59/87/87/110	-
17	WUO	C	304	-	-	46/84/148/148	0/3/3/3
16	MQ9	N	605	-	-	20/53/73/73	0/2/2/2
16	MQ9	C	303	-	-	6/53/73/73	0/2/2/2
25	9XX	N	609	-	-	12/33/33/43	-
16	MQ9	T	1301	-	-	10/53/73/73	0/2/2/2
22	HEM	N	606	3	-	4/14/54/54	-
15	HEC	C	301	1	1/1/3/7	5/14/54/54	-
20	9YF	G	503	-	-	39/54/78/78	0/1/1/1
23	CDL	P	301	-	-	53/87/87/110	-
21	7PH	M	504	-	-	15/39/39/39	-
28	HEA	L	603	7	-	10/36/76/76	-
22	HEM	H	1002	3	-	3/14/54/54	-
23	CDL	H	1004	-	-	45/87/87/110	-
15	HEC	O	301	1	1/1/3/7	5/14/54/54	-
25	9XX	W	202	-	-	21/43/43/43	-
23	CDL	R	605	-	-	58/87/87/110	-
24	PLM	c	301	-	-	0/7/8/15	-
22	HEM	H	1007	3	-	5/14/54/54	-
26	TRD	X	403	-	-	1/10/10/10	-
28	HEA	R	602	7	-	15/36/76/76	-
24	PLM	L	610	-	-	5/7/8/15	-
18	FES	G	501	2	-	-	0/1/1/1
26	TRD	S	502	-	-	1/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	WUO	P	302	-	-	43/84/148/148	0/3/3/3
16	MQ9	N	607	-	-	21/53/73/73	0/2/2/2
20	9YF	b	201	-	-	33/54/78/78	0/1/1/1
20	9YF	M	503	-	-	33/54/78/78	0/1/1/1
21	7PH	G	504	-	-	15/39/39/39	-
21	7PH	G	505	-	-	12/39/39/39	-
23	CDL	N	604	-	-	52/89/89/110	-
23	CDL	K	201	-	-	54/89/89/110	-
26	TRD	K	202	-	-	0/10/10/10	-
27	3PE	S	503	-	-	18/35/35/54	-
20	9YF	W	201	-	-	25/54/78/78	0/1/1/1
28	HEA	R	603	7	-	14/36/76/76	-
32	DCQ	H	1008	-	-	4/14/38/38	0/1/1/1
23	CDL	R	601	-	-	45/87/87/110	-
24	PLM	W	203	-	-	2/7/8/15	-
23	CDL	N	603	-	-	50/87/87/110	-
26	TRD	J	601	-	-	1/10/10/10	-
26	TRD	R	609	-	-	1/10/10/10	-
17	WUO	O	304	-	-	35/84/148/148	0/3/3/3
16	MQ9	H	1006	-	-	19/53/73/73	0/2/2/2

All (503) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	607	MQ9	C6-C5	8.01	1.49	1.35
16	N	605	MQ9	C6-C5	7.72	1.49	1.35
16	H	1006	MQ9	C6-C5	7.35	1.48	1.35
16	O	303	MQ9	C6-C5	7.34	1.48	1.35
16	T	1301	MQ9	C6-C5	7.34	1.48	1.35
16	C	303	MQ9	C6-C5	7.33	1.48	1.35
16	C	305	MQ9	C6-C5	7.29	1.48	1.35
19	G	502	IZL	P-O28	7.08	1.79	1.60
19	M	502	IZL	P-O28	6.59	1.77	1.60
17	C	304	WUO	P52-O51	6.25	1.76	1.60
17	O	304	WUO	P52-O51	6.24	1.76	1.60
17	P	302	WUO	P52-O51	6.23	1.76	1.60
17	I	303	WUO	P52-O51	6.22	1.76	1.60
28	L	603	HEA	C3B-C2B	5.58	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	W	201	9YF	P-O2	5.56	1.75	1.60
28	L	602	HEA	FE-NB	5.41	2.11	1.94
20	b	201	9YF	P-O2	5.40	1.74	1.60
17	O	304	WUO	C50-C01	5.39	1.63	1.52
28	L	602	HEA	C3B-C2B	5.37	1.46	1.34
28	R	602	HEA	FE-NB	5.32	2.11	1.94
17	P	302	WUO	C50-C01	5.30	1.63	1.52
28	R	602	HEA	C3B-C2B	5.29	1.46	1.34
28	L	602	HEA	C3A-C2A	5.27	1.48	1.36
20	G	503	9YF	P-O2	5.23	1.74	1.60
28	L	603	HEA	C3A-C2A	5.23	1.47	1.36
28	R	602	HEA	C3A-C2A	5.20	1.47	1.36
28	R	602	HEA	FE-ND	5.16	2.10	1.94
17	P	302	WUO	P52-O55	5.15	1.80	1.59
17	C	304	WUO	P52-O55	5.12	1.80	1.59
28	L	602	HEA	FE-ND	5.10	2.10	1.94
28	L	603	HEA	FE-ND	5.08	2.10	1.94
28	R	602	HEA	C3D-C2D	5.07	1.47	1.36
28	L	603	HEA	C3D-C2D	5.05	1.47	1.36
28	L	602	HEA	C3D-C2D	5.02	1.47	1.36
20	M	503	9YF	P-O2	5.01	1.73	1.60
17	I	303	WUO	P52-O55	4.99	1.79	1.59
17	O	304	WUO	P52-O55	4.96	1.79	1.59
17	C	304	WUO	C50-C01	4.96	1.62	1.52
17	I	303	WUO	C50-C01	4.94	1.62	1.52
28	R	603	HEA	FE-ND	4.93	2.10	1.94
22	H	1007	HEM	FE-NB	4.92	2.10	1.94
28	L	602	HEA	FE-NC	4.88	2.11	1.95
28	L	603	HEA	FE-NB	4.87	2.09	1.94
16	C	305	MQ9	C2-C1	4.80	1.57	1.48
16	T	1301	MQ9	C2-C1	4.79	1.57	1.48
16	O	303	MQ9	C3-C4	4.77	1.57	1.48
16	N	605	MQ9	C2-C1	4.77	1.57	1.48
16	N	607	MQ9	C2-C1	4.76	1.57	1.48
16	N	607	MQ9	C3-C4	4.75	1.57	1.48
16	H	1006	MQ9	C2-C1	4.71	1.57	1.48
17	C	304	WUO	C56-C57	4.70	1.65	1.50
16	N	605	MQ9	C3-C4	4.70	1.57	1.48
17	P	302	WUO	C56-C57	4.69	1.65	1.50
16	C	303	MQ9	C2-C3	4.69	1.48	1.40
28	L	603	HEA	CHD-C1D	4.68	1.48	1.38
16	H	1006	MQ9	C3-C4	4.68	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	1301	MQ9	C3-C4	4.65	1.57	1.48
19	G	502	IZL	C44-C45	4.65	1.64	1.50
28	R	602	HEA	FE-NC	4.64	2.10	1.95
16	O	303	MQ9	C2-C1	4.63	1.57	1.48
28	L	602	HEA	CHD-C1D	4.59	1.47	1.38
19	M	502	IZL	C44-C45	4.59	1.64	1.50
16	C	305	MQ9	C3-C4	4.58	1.56	1.48
28	R	603	HEA	C3B-C2B	4.52	1.44	1.34
19	G	502	IZL	C43-C14	4.48	1.61	1.52
17	I	303	WUO	C56-C57	4.48	1.64	1.50
28	L	603	HEA	CHB-C4A	4.48	1.47	1.38
28	L	603	HEA	CHC-C4B	4.45	1.47	1.38
28	R	602	HEA	CHD-C1D	4.45	1.47	1.38
28	L	602	HEA	CHA-C1A	4.45	1.47	1.38
28	R	602	HEA	CHA-C1A	4.38	1.46	1.38
28	R	603	HEA	C4B-NB	-4.38	1.32	1.40
28	L	603	HEA	CHA-C1A	4.34	1.46	1.38
17	O	304	WUO	C56-C57	4.32	1.63	1.50
28	R	603	HEA	FE-NC	4.31	2.09	1.95
28	L	602	HEA	C1A-NA	4.30	1.48	1.39
28	R	603	HEA	FE-NB	4.29	2.08	1.94
28	R	602	HEA	CHC-C4B	4.29	1.47	1.38
19	M	502	IZL	P-O31	4.24	1.76	1.59
28	R	602	HEA	C1A-NA	4.24	1.48	1.39
19	M	502	IZL	C43-C14	4.24	1.61	1.52
28	L	603	HEA	FE-NC	4.22	2.09	1.95
20	W	201	9YF	P-O	4.19	1.76	1.59
19	G	502	IZL	P-O31	4.19	1.76	1.59
28	R	602	HEA	CHB-C4A	4.18	1.46	1.38
28	R	603	HEA	C3A-C2A	4.17	1.45	1.36
22	H	1007	HEM	FE-NC	4.06	2.08	1.95
20	M	503	9YF	P-O	4.05	1.75	1.59
20	G	503	9YF	P-O	4.04	1.75	1.59
28	L	602	HEA	CHB-C4A	4.01	1.46	1.38
28	L	602	HEA	CHC-C4B	3.92	1.46	1.38
20	b	201	9YF	P-O	3.90	1.75	1.59
28	R	602	HEA	C4A-NA	3.89	1.47	1.39
25	W	202	9XX	O1-C17	-3.89	1.40	1.47
28	L	603	HEA	C1A-NA	3.89	1.47	1.39
25	N	609	9XX	O1-C17	-3.88	1.40	1.47
23	P	301	CDL	OA8-CA7	3.87	1.44	1.33
25	c	302	9XX	O1-C17	-3.84	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	602	HEA	C4A-NA	3.84	1.47	1.39
23	R	605	CDL	OA8-CA7	3.83	1.44	1.33
28	R	603	HEA	CHD-C1D	3.83	1.46	1.38
17	P	302	WUO	C50-C37	3.82	1.60	1.52
23	I	301	CDL	OA8-CA7	3.82	1.44	1.33
17	I	303	WUO	C50-C37	3.81	1.60	1.52
23	I	302	CDL	OA8-CA7	3.80	1.44	1.33
23	L	601	CDL	OA8-CA7	3.79	1.44	1.33
28	L	603	HEA	C4A-NA	3.79	1.47	1.39
22	H	1007	HEM	C1B-NB	-3.76	1.33	1.40
23	L	609	CDL	OA8-CA7	3.75	1.44	1.33
23	G	506	CDL	OA8-CA7	3.74	1.44	1.33
23	H	1003	CDL	OA8-CA7	3.74	1.44	1.33
23	N	602	CDL	OA8-CA7	3.73	1.44	1.33
23	K	201	CDL	OA8-CA7	3.73	1.44	1.33
28	R	603	HEA	C1D-ND	-3.72	1.33	1.40
22	N	606	HEM	FE-ND	3.72	2.06	1.94
23	T	1302	CDL	OA8-CA7	3.72	1.44	1.33
22	N	601	HEM	FE-ND	3.72	2.06	1.94
23	P	303	CDL	OA8-CA7	3.71	1.44	1.33
28	L	603	HEA	CHD-C4C	3.70	1.47	1.39
23	R	601	CDL	OA8-CA7	3.68	1.44	1.33
23	N	604	CDL	OA8-CA7	3.67	1.44	1.33
28	R	603	HEA	C3D-C2D	3.67	1.44	1.36
17	O	304	WUO	C50-C37	3.66	1.59	1.52
23	L	609	CDL	OB8-CB7	3.64	1.44	1.33
22	H	1007	HEM	C4D-ND	-3.63	1.34	1.40
23	N	603	CDL	OB8-CB7	3.61	1.43	1.33
23	H	1004	CDL	OA8-CA7	3.59	1.43	1.33
28	L	603	HEA	CHC-C1C	3.59	1.47	1.39
23	R	601	CDL	OB8-CB7	3.58	1.43	1.33
23	N	603	CDL	OA8-CA7	3.58	1.43	1.33
23	H	1005	CDL	OA8-CA7	3.58	1.43	1.33
25	b	202	9XX	O1-C17	-3.57	1.41	1.47
23	G	506	CDL	OB8-CB7	3.56	1.43	1.33
15	O	302	HEC	CBC-CAC	-3.56	1.35	1.51
15	C	302	HEC	CBC-CAC	-3.56	1.35	1.51
23	R	605	CDL	OB8-CB7	3.55	1.43	1.33
23	P	301	CDL	OB8-CB7	3.55	1.43	1.33
28	R	602	HEA	CHD-C4C	3.55	1.47	1.39
23	H	1004	CDL	OB8-CB7	3.55	1.43	1.33
23	I	302	CDL	OB8-CB7	3.54	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	1005	CDL	OB8-CB7	3.54	1.43	1.33
23	P	303	CDL	OB8-CB7	3.53	1.43	1.33
23	N	604	CDL	OB8-CB7	3.52	1.43	1.33
28	R	603	HEA	CHB-C4A	3.52	1.45	1.38
28	L	602	HEA	CHD-C4C	3.51	1.47	1.39
23	T	1302	CDL	OB8-CB7	3.50	1.43	1.33
23	K	201	CDL	OB8-CB7	3.49	1.43	1.33
23	I	301	CDL	OB8-CB7	3.48	1.43	1.33
28	L	602	HEA	CHA-C4D	3.47	1.47	1.39
23	L	601	CDL	OB8-CB7	3.47	1.43	1.33
28	R	602	HEA	CHA-C4D	3.47	1.47	1.39
23	H	1003	CDL	OB8-CB7	3.47	1.43	1.33
23	N	602	CDL	OB8-CB7	3.46	1.43	1.33
28	L	603	HEA	CHB-C1B	3.42	1.47	1.39
28	L	603	HEA	CHA-C4D	3.39	1.47	1.39
23	G	506	CDL	OA6-CA5	3.36	1.43	1.34
28	R	603	HEA	CHA-C1A	3.34	1.44	1.38
15	O	302	HEC	CAC-C3C	3.34	1.59	1.51
28	R	603	HEA	CHC-C4B	3.33	1.45	1.38
28	R	603	HEA	C1C-NC	-3.33	1.33	1.39
15	O	301	HEC	CBC-CAC	-3.33	1.36	1.51
15	C	302	HEC	CAC-C3C	3.32	1.59	1.51
23	L	601	CDL	OA6-CA5	3.31	1.43	1.34
15	C	301	HEC	CBC-CAC	-3.31	1.36	1.51
23	P	301	CDL	OA6-CA5	3.31	1.43	1.34
28	R	602	HEA	CHB-C1B	3.31	1.46	1.39
17	C	304	WUO	C50-C37	3.30	1.59	1.52
15	O	301	HEC	CAC-C3C	3.29	1.59	1.51
15	C	301	HEC	CAC-C3C	3.28	1.59	1.51
23	N	604	CDL	OA6-CA5	3.28	1.43	1.34
23	N	602	CDL	OA6-CA5	3.28	1.43	1.34
23	R	605	CDL	OA6-CA5	3.28	1.43	1.34
23	H	1005	CDL	OA6-CA5	3.27	1.43	1.34
23	I	301	CDL	OA6-CA5	3.27	1.43	1.34
23	K	201	CDL	OA6-CA5	3.26	1.43	1.34
23	H	1003	CDL	OA6-CA5	3.26	1.43	1.34
23	P	303	CDL	OA6-CA5	3.26	1.43	1.34
28	R	602	HEA	CHC-C1C	3.25	1.46	1.39
23	I	302	CDL	OA6-CA5	3.24	1.43	1.34
23	L	609	CDL	OA6-CA5	3.24	1.43	1.34
17	P	302	WUO	C76-C57	3.23	1.60	1.50
23	R	601	CDL	OA6-CA5	3.22	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	603	HEA	C4B-NB	-3.22	1.34	1.40
22	N	601	HEM	FE-NB	3.22	2.04	1.94
23	H	1004	CDL	OA6-CA5	3.22	1.43	1.34
23	T	1302	CDL	OA6-CA5	3.21	1.43	1.34
23	N	603	CDL	OA6-CA5	3.21	1.43	1.34
19	M	502	IZL	C43-C18	3.20	1.58	1.52
19	G	502	IZL	C43-C18	3.18	1.58	1.52
28	L	603	HEA	C1D-ND	-3.16	1.34	1.40
17	C	304	WUO	C76-C57	3.15	1.60	1.50
22	N	601	HEM	FE-NA	3.14	2.05	1.95
28	L	602	HEA	C4B-NB	-3.10	1.35	1.40
22	H	1002	HEM	FE-ND	3.10	2.04	1.94
28	R	603	HEA	C4A-NA	3.07	1.45	1.39
22	H	1002	HEM	FE-NB	3.06	2.04	1.94
22	H	1002	HEM	FE-NA	3.06	2.05	1.95
28	L	602	HEA	CHC-C1C	3.06	1.46	1.39
17	O	304	WUO	C76-C57	3.05	1.60	1.50
28	R	603	HEA	C4C-NC	-3.05	1.33	1.39
22	N	606	HEM	FE-NA	3.02	2.05	1.95
28	R	603	HEA	CHD-C4C	3.00	1.46	1.39
22	N	601	HEM	FE-NC	2.99	2.05	1.95
19	G	502	IZL	C11-C12	2.98	1.60	1.51
28	L	602	HEA	CHB-C1B	2.98	1.46	1.39
17	I	303	WUO	C76-C57	2.95	1.59	1.50
19	G	502	IZL	O1-C10	2.95	1.42	1.33
22	N	606	HEM	CAB-C3B	2.95	1.55	1.47
28	R	603	HEA	CHC-C1C	2.94	1.46	1.39
28	R	603	HEA	C1A-NA	2.94	1.45	1.39
22	H	1002	HEM	FE-NC	2.94	2.05	1.95
22	H	1002	HEM	CAB-C3B	2.93	1.55	1.47
23	N	604	CDL	OB6-CB4	-2.91	1.39	1.46
22	N	601	HEM	CAB-C3B	2.90	1.55	1.47
23	K	201	CDL	OB6-CB4	-2.89	1.39	1.46
23	H	1004	CDL	OB6-CB4	-2.89	1.39	1.46
19	M	502	IZL	C25-C30	2.88	1.59	1.52
23	T	1302	CDL	OB6-CB4	-2.87	1.39	1.46
28	R	602	HEA	C4B-NB	-2.87	1.35	1.40
23	R	605	CDL	OB6-CB5	2.87	1.42	1.34
22	N	606	HEM	FE-NC	2.86	2.04	1.95
23	G	506	CDL	OB6-CB5	2.86	1.42	1.34
22	N	606	HEM	CAC-C3C	2.85	1.55	1.47
23	H	1005	CDL	OB6-CB4	-2.85	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	602	HEA	C1D-ND	-2.85	1.35	1.40
23	I	302	CDL	OB6-CB5	2.85	1.42	1.34
23	H	1003	CDL	OB6-CB5	2.84	1.42	1.34
23	R	601	CDL	OB6-CB4	-2.84	1.39	1.46
23	N	603	CDL	OB6-CB4	-2.83	1.39	1.46
23	L	601	CDL	OB6-CB4	-2.82	1.39	1.46
23	P	303	CDL	OB6-CB5	2.82	1.42	1.34
23	P	301	CDL	OB6-CB5	2.82	1.42	1.34
23	L	609	CDL	OB6-CB4	-2.80	1.39	1.46
23	N	603	CDL	OB6-CB5	2.80	1.42	1.34
28	L	602	HEA	C1A-C2A	2.80	1.50	1.45
23	N	602	CDL	OB6-CB4	-2.79	1.39	1.46
23	I	301	CDL	OB6-CB5	2.79	1.42	1.34
23	H	1003	CDL	OB6-CB4	-2.78	1.39	1.46
23	N	602	CDL	OB6-CB5	2.78	1.42	1.34
19	M	502	IZL	O1-C10	2.78	1.41	1.33
23	G	506	CDL	OB6-CB4	-2.78	1.39	1.46
23	I	301	CDL	OB6-CB4	-2.78	1.39	1.46
23	K	201	CDL	OB6-CB5	2.77	1.42	1.34
23	L	601	CDL	OB6-CB5	2.76	1.42	1.34
23	L	609	CDL	OB6-CB5	2.76	1.42	1.34
28	L	602	HEA	C3C-C4C	2.76	1.49	1.42
19	M	502	IZL	C11-C12	2.76	1.60	1.51
22	N	601	HEM	CAC-C3C	2.75	1.54	1.47
23	R	605	CDL	OB6-CB4	-2.74	1.39	1.46
23	P	301	CDL	OB6-CB4	-2.74	1.39	1.46
19	M	502	IZL	C24-C23	2.74	1.60	1.51
22	H	1007	HEM	C1C-C2C	-2.73	1.39	1.45
22	N	606	HEM	FE-NB	2.71	2.03	1.94
23	H	1005	CDL	OB6-CB5	2.70	1.41	1.34
28	L	602	HEA	C1D-ND	-2.70	1.35	1.40
22	H	1002	HEM	CAC-C3C	2.70	1.54	1.47
23	T	1302	CDL	OB6-CB5	2.69	1.41	1.34
23	P	303	CDL	OB6-CB4	-2.69	1.39	1.46
23	R	601	CDL	OB6-CB5	2.68	1.41	1.34
28	L	603	HEA	C4C-NC	-2.66	1.34	1.39
23	N	604	CDL	OB6-CB5	2.66	1.41	1.34
23	H	1004	CDL	OB6-CB5	2.65	1.41	1.34
28	R	602	HEA	C4B-C3B	2.56	1.48	1.44
28	R	603	HEA	CHA-C4D	2.54	1.45	1.39
22	H	1007	HEM	FE-ND	-2.54	1.86	1.94
28	R	603	HEA	CHB-C1B	2.53	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	502	IZL	C24-C23	2.52	1.59	1.51
21	G	505	7PH	O21-C2	-2.51	1.40	1.46
21	S	501	7PH	O21-C2	-2.51	1.40	1.46
19	M	502	IZL	C48-C47	2.51	1.58	1.50
23	I	302	CDL	OB6-CB4	-2.50	1.40	1.46
28	R	603	HEA	C1B-NB	-2.49	1.33	1.38
19	G	502	IZL	C48-C47	2.48	1.58	1.50
19	M	502	IZL	O34-C60	2.47	1.41	1.34
28	R	603	HEA	C4D-ND	-2.45	1.33	1.38
19	M	502	IZL	C61-C60	2.45	1.57	1.50
28	L	603	HEA	C4B-C3B	2.44	1.48	1.44
19	G	502	IZL	C31-C36	2.42	1.59	1.52
15	C	301	HEC	CBB-CAB	-2.42	1.40	1.51
25	c	302	9XX	O-C15	2.42	1.40	1.33
15	O	301	HEC	CBB-CAB	-2.42	1.40	1.51
21	G	505	7PH	O31-C31	2.41	1.40	1.33
28	L	603	HEA	C3C-C4C	2.41	1.48	1.42
23	P	301	CDL	C11-CA5	2.40	1.57	1.50
25	b	202	9XX	O-C15	2.40	1.40	1.33
19	M	502	IZL	C46-C45	2.40	1.58	1.50
23	G	506	CDL	C11-CA5	2.40	1.57	1.50
23	N	602	CDL	OA6-CA4	-2.39	1.40	1.46
15	O	302	HEC	CBB-CAB	-2.39	1.40	1.51
20	G	503	9YF	C1-C	2.39	1.58	1.50
25	N	609	9XX	O-C15	2.39	1.40	1.33
21	S	501	7PH	O31-C31	2.39	1.40	1.33
15	C	302	HEC	CBB-CAB	-2.39	1.40	1.51
19	G	502	IZL	O32-C47	2.38	1.40	1.33
23	P	303	CDL	C11-CA5	2.37	1.57	1.50
19	G	502	IZL	C46-C45	2.37	1.58	1.50
21	H	1001	7PH	O31-C31	2.36	1.40	1.33
19	G	502	IZL	C61-C60	2.36	1.57	1.50
22	H	1007	HEM	C1D-ND	-2.36	1.33	1.38
20	W	201	9YF	C1-C	2.36	1.57	1.50
23	R	601	CDL	OA6-CA4	-2.36	1.40	1.46
23	L	601	CDL	C11-CA5	2.36	1.57	1.50
23	I	302	CDL	C11-CA5	2.35	1.57	1.50
23	L	609	CDL	C11-CA5	2.35	1.57	1.50
20	M	503	9YF	C1-C	2.34	1.57	1.50
28	R	602	HEA	C3C-C4C	2.34	1.48	1.42
27	J	602	3PE	O31-C31	2.34	1.40	1.33
23	I	301	CDL	C11-CA5	2.34	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	605	CDL	C11-CA5	2.34	1.57	1.50
28	L	602	HEA	C4B-C3B	2.34	1.48	1.44
15	O	301	HEC	CMD-C2D	2.34	1.55	1.50
27	S	503	3PE	O31-C31	2.34	1.40	1.33
15	C	301	HEC	CMD-C2D	2.33	1.55	1.50
28	L	603	HEA	C1C-NC	-2.33	1.35	1.39
21	M	504	7PH	O31-C31	2.33	1.40	1.33
23	P	303	CDL	OA6-CA4	-2.33	1.40	1.46
22	H	1007	HEM	C4B-NB	-2.33	1.34	1.38
25	W	202	9XX	O-C15	2.33	1.40	1.33
23	H	1004	CDL	OA6-CA4	-2.32	1.40	1.46
23	I	302	CDL	OA6-CA4	-2.32	1.40	1.46
23	H	1003	CDL	OA6-CA4	-2.32	1.40	1.46
25	W	202	9XX	O1-C18	2.32	1.40	1.34
28	R	602	HEA	C1C-C2C	2.32	1.48	1.43
25	b	202	9XX	O1-C18	2.31	1.40	1.34
23	T	1302	CDL	C11-CA5	2.31	1.57	1.50
23	L	609	CDL	OA6-CA4	-2.31	1.40	1.46
23	H	1003	CDL	C11-CA5	2.30	1.57	1.50
15	O	301	HEC	CAB-C3B	2.30	1.57	1.51
21	G	504	7PH	O31-C31	2.30	1.40	1.33
21	H	1001	7PH	O21-C21	2.30	1.40	1.34
15	C	301	HEC	CAB-C3B	2.30	1.57	1.51
27	S	503	3PE	O21-C21	2.30	1.40	1.34
20	b	201	9YF	C1-C	2.30	1.57	1.50
23	K	201	CDL	C11-CA5	2.30	1.57	1.50
19	M	502	IZL	O32-C47	2.29	1.40	1.33
23	R	601	CDL	C11-CA5	2.29	1.57	1.50
23	N	603	CDL	OA6-CA4	-2.29	1.40	1.46
27	S	503	3PE	O21-C2	-2.29	1.40	1.46
23	K	201	CDL	OA6-CA4	-2.29	1.40	1.46
23	H	1005	CDL	OA6-CA4	-2.29	1.40	1.46
23	T	1302	CDL	OA6-CA4	-2.29	1.40	1.46
19	G	502	IZL	O34-C60	2.29	1.40	1.34
15	C	302	HEC	CAB-C3B	2.28	1.57	1.51
21	M	504	7PH	O21-C2	-2.28	1.40	1.46
21	G	504	7PH	O21-C2	-2.28	1.40	1.46
23	H	1005	CDL	C11-CA5	2.28	1.57	1.50
21	M	504	7PH	O21-C21	2.28	1.40	1.34
15	O	302	HEC	CAB-C3B	2.28	1.56	1.51
23	N	602	CDL	C11-CA5	2.28	1.57	1.50
23	L	609	CDL	PB2-OB5	2.28	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	303	CDL	PB2-OB5	2.27	1.68	1.59
28	L	602	HEA	C1D-C2D	2.27	1.49	1.44
28	R	602	HEA	C4C-NC	-2.27	1.35	1.39
23	K	201	CDL	PB2-OB5	2.27	1.68	1.59
28	L	602	HEA	C1C-C2C	2.27	1.48	1.43
28	L	603	HEA	C1C-C2C	2.27	1.48	1.43
23	N	603	CDL	C11-CA5	2.27	1.57	1.50
23	G	506	CDL	PB2-OB5	2.26	1.68	1.59
23	L	601	CDL	OA6-CA4	-2.26	1.40	1.46
17	P	302	WUO	O77-C78	2.26	1.39	1.33
27	J	602	3PE	O21-C21	2.26	1.40	1.34
19	G	502	IZL	C13-C71	2.26	1.59	1.52
23	H	1004	CDL	C11-CA5	2.26	1.57	1.50
23	N	604	CDL	C11-CA5	2.25	1.57	1.50
23	I	301	CDL	OA6-CA4	-2.25	1.41	1.46
23	H	1003	CDL	PB2-OB5	2.25	1.68	1.59
28	R	602	HEA	C1A-C2A	2.25	1.49	1.45
17	C	304	WUO	O77-C78	2.25	1.39	1.33
23	H	1005	CDL	PB2-OB5	2.25	1.68	1.59
16	O	303	MQ9	O4-C4	-2.24	1.18	1.23
23	R	605	CDL	PA1-OA5	2.24	1.68	1.59
27	J	602	3PE	O31-C3	-2.24	1.40	1.45
23	P	301	CDL	OA6-CA4	-2.24	1.41	1.46
23	R	605	CDL	OA6-CA4	-2.24	1.41	1.46
20	b	201	9YF	O9-C	-2.24	1.41	1.46
17	I	303	WUO	O51-C50	-2.23	1.36	1.44
23	P	303	CDL	PA1-OA5	2.23	1.68	1.59
23	L	609	CDL	PA1-OA5	2.23	1.68	1.59
23	I	301	CDL	PB2-OB2	2.23	1.68	1.59
23	I	302	CDL	PB2-OB5	2.23	1.68	1.59
23	G	506	CDL	PA1-OA5	2.23	1.68	1.59
23	N	603	CDL	PB2-OB5	2.23	1.68	1.59
23	I	301	CDL	PA1-OA5	2.22	1.68	1.59
23	P	301	CDL	PA1-OA5	2.22	1.68	1.59
23	R	605	CDL	PB2-OB5	2.22	1.68	1.59
16	H	1006	MQ9	O4-C4	-2.22	1.18	1.23
16	N	605	MQ9	O4-C4	-2.22	1.18	1.23
21	G	504	7PH	O21-C21	2.22	1.40	1.34
16	C	305	MQ9	O4-C4	-2.21	1.18	1.23
23	T	1302	CDL	PA1-OA5	2.21	1.68	1.59
19	M	502	IZL	O28-C43	-2.21	1.36	1.44
23	I	301	CDL	PB2-OB5	2.21	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	601	CDL	PA1-OA5	2.20	1.68	1.59
17	O	304	WUO	O51-C50	-2.20	1.36	1.44
27	S	503	3PE	O31-C3	-2.20	1.40	1.45
16	N	607	MQ9	O4-C4	-2.20	1.18	1.23
21	H	1001	7PH	O21-C2	-2.20	1.41	1.46
28	L	603	HEA	C1D-C2D	2.20	1.48	1.44
28	R	603	HEA	O2D-CGD	-2.20	1.23	1.30
23	L	601	CDL	PB2-OB5	2.20	1.68	1.59
17	C	304	WUO	O51-C50	-2.19	1.36	1.44
23	G	506	CDL	PB2-OB2	2.19	1.68	1.59
23	N	604	CDL	PA1-OA5	2.19	1.68	1.59
23	P	303	CDL	PB2-OB2	2.19	1.68	1.59
17	O	304	WUO	O77-C78	2.19	1.39	1.33
28	L	602	HEA	C4C-NC	-2.19	1.35	1.39
25	W	202	9XX	O-C16	-2.19	1.40	1.45
19	M	502	IZL	C29-C28	2.19	1.57	1.52
28	R	602	HEA	C1C-NC	-2.19	1.35	1.39
23	P	301	CDL	PB2-OB2	2.19	1.68	1.59
23	N	604	CDL	PB2-OB5	2.19	1.68	1.59
23	H	1005	CDL	PA1-OA5	2.19	1.68	1.59
23	H	1003	CDL	PA1-OA5	2.18	1.68	1.59
23	P	301	CDL	PB2-OB5	2.18	1.68	1.59
28	R	602	HEA	C1D-C2D	2.18	1.48	1.44
16	T	1301	MQ9	O4-C4	-2.18	1.18	1.23
23	N	602	CDL	PB2-OB2	2.18	1.68	1.59
25	N	609	9XX	O1-C18	2.18	1.40	1.34
17	P	302	WUO	O51-C50	-2.18	1.36	1.44
23	T	1302	CDL	PB2-OB2	2.18	1.68	1.59
23	I	302	CDL	PB2-OB2	2.17	1.68	1.59
16	N	607	MQ9	O1-C1	-2.17	1.18	1.23
16	O	303	MQ9	O1-C1	-2.17	1.18	1.23
16	T	1301	MQ9	O1-C1	-2.17	1.18	1.23
23	I	302	CDL	PA1-OA5	2.17	1.68	1.59
20	M	503	9YF	O7-C7	-2.17	1.37	1.43
23	K	201	CDL	PA1-OA5	2.17	1.68	1.59
23	K	201	CDL	PB2-OB2	2.16	1.68	1.59
19	M	502	IZL	C13-C71	2.16	1.58	1.52
23	R	601	CDL	PB2-OB5	2.16	1.68	1.59
23	N	603	CDL	PB2-OB2	2.16	1.68	1.59
21	G	504	7PH	O31-C3	-2.16	1.40	1.45
27	J	602	3PE	O21-C2	-2.16	1.41	1.46
23	N	602	CDL	PA1-OA5	2.16	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	T	1302	CDL	PB2-OB5	2.16	1.68	1.59
23	H	1004	CDL	PB2-OB5	2.16	1.68	1.59
19	M	502	IZL	O38-C73	-2.16	1.37	1.43
21	S	501	7PH	O31-C3	-2.15	1.40	1.45
19	G	502	IZL	O38-C73	-2.15	1.37	1.43
23	H	1004	CDL	PB2-OB2	2.15	1.68	1.59
25	c	302	9XX	O-C16	-2.15	1.40	1.45
23	R	605	CDL	PB2-OB2	2.14	1.68	1.59
21	M	504	7PH	O31-C3	-2.14	1.40	1.45
23	L	601	CDL	PB2-OB2	2.14	1.68	1.59
21	G	505	7PH	O21-C21	2.14	1.40	1.34
19	M	502	IZL	C31-C36	2.14	1.58	1.52
25	c	302	9XX	O1-C18	2.14	1.40	1.34
23	N	602	CDL	PB2-OB5	2.14	1.67	1.59
20	G	503	9YF	C24-C	2.13	1.57	1.50
23	H	1005	CDL	PB2-OB2	2.13	1.67	1.59
23	N	603	CDL	PA1-OA5	2.13	1.67	1.59
21	H	1001	7PH	O31-C3	-2.13	1.40	1.45
28	L	602	HEA	C1C-NC	-2.13	1.35	1.39
25	b	202	9XX	O-C16	-2.13	1.40	1.45
28	L	603	HEA	C4D-C3D	2.13	1.48	1.45
23	R	601	CDL	PA1-OA5	2.13	1.67	1.59
16	C	305	MQ9	O1-C1	-2.12	1.18	1.23
21	S	501	7PH	O21-C21	2.11	1.40	1.34
15	O	301	HEC	FE-ND	2.11	2.01	1.94
23	R	601	CDL	PB2-OB2	2.11	1.67	1.59
20	W	201	9YF	O9-C	-2.10	1.41	1.46
23	H	1003	CDL	PB2-OB2	2.10	1.67	1.59
28	R	602	HEA	C1B-C2B	2.10	1.48	1.44
20	M	503	9YF	O9-C	-2.10	1.41	1.46
19	G	502	IZL	C9-C10	2.10	1.56	1.50
22	H	1007	HEM	C3C-C4C	-2.10	1.42	1.46
17	I	303	WUO	O77-C78	2.09	1.39	1.33
22	H	1002	HEM	C3C-C2C	-2.09	1.33	1.37
15	C	301	HEC	FE-ND	2.09	2.01	1.94
28	L	602	HEA	C4D-C3D	2.09	1.48	1.45
20	G	503	9YF	O7-C7	-2.08	1.38	1.43
23	H	1004	CDL	PA1-OA5	2.08	1.67	1.59
25	N	609	9XX	O-C16	-2.08	1.40	1.45
23	L	609	CDL	PB2-OB2	2.08	1.67	1.59
16	N	605	MQ9	O1-C1	-2.08	1.18	1.23
23	N	604	CDL	PB2-OB2	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1006	MQ9	O1-C1	-2.07	1.18	1.23
21	G	505	7PH	O31-C3	-2.06	1.40	1.45
23	R	605	CDL	C31-CA7	2.06	1.56	1.50
23	P	301	CDL	C31-CA7	2.06	1.56	1.50
23	N	604	CDL	OA6-CA4	-2.06	1.41	1.46
15	C	302	HEC	C4B-NB	-2.05	1.36	1.40
15	C	302	HEC	C3D-C2D	-2.05	1.32	1.36
15	O	302	HEC	C4B-NB	-2.05	1.36	1.40
22	H	1007	HEM	C1C-NC	-2.04	1.35	1.39
19	G	502	IZL	C25-C30	2.04	1.57	1.52
23	I	301	CDL	C31-CA7	2.04	1.56	1.50
20	W	201	9YF	C24-C	2.04	1.56	1.50
23	G	506	CDL	OA6-CA4	-2.03	1.41	1.46
19	G	502	IZL	C21-C20	2.03	1.57	1.51
19	G	502	IZL	C17-C18	2.03	1.57	1.52
23	L	609	CDL	C31-CA7	2.03	1.56	1.50
28	L	603	HEA	C1B-NB	-2.02	1.34	1.38
15	O	302	HEC	C3D-C2D	-2.02	1.32	1.36
19	M	502	IZL	C35-C34	2.02	1.57	1.52
20	M	503	9YF	O2-C2	-2.02	1.36	1.44
19	M	502	IZL	C34-C32	2.01	1.57	1.53
19	G	502	IZL	C17-C16	2.01	1.57	1.52
19	G	502	IZL	P-O30	-2.01	1.45	1.55
19	M	502	IZL	C21-C20	2.01	1.57	1.51
23	K	201	CDL	C31-CA7	2.01	1.56	1.50
28	L	602	HEA	C1B-C2B	2.00	1.48	1.44
23	I	302	CDL	C31-CA7	2.00	1.56	1.50

All (537) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	602	HEA	C3C-C4C-NC	6.54	114.27	110.25
28	R	603	HEA	C3D-C4D-ND	6.34	116.50	110.36
28	R	602	HEA	C3C-C4C-NC	5.98	113.93	110.25
28	R	603	HEA	C3C-C4C-NC	5.75	113.79	110.25
28	L	602	HEA	C2B-C1B-NB	5.72	116.74	109.88
28	L	602	HEA	C3D-C4D-ND	5.71	115.89	110.36
28	L	602	HEA	C3B-C4B-NB	5.70	116.60	109.84
28	R	602	HEA	C3D-C4D-ND	5.69	115.87	110.36
28	L	602	HEA	C3C-C2C-C1C	-5.52	100.50	107.16
28	L	603	HEA	C3D-C4D-ND	5.47	115.66	110.36
28	R	602	HEA	C3C-C2C-C1C	-5.47	100.56	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	603	HEA	CHA-C4D-ND	-5.38	118.57	124.42
28	L	603	HEA	C3C-C2C-C1C	-5.28	100.79	107.16
28	R	603	HEA	C2B-C1B-NB	5.25	116.17	109.88
28	R	603	HEA	C3C-C2C-C1C	-5.16	100.94	107.16
28	R	602	HEA	C3B-C4B-NB	5.09	115.87	109.84
28	R	602	HEA	C2B-C1B-NB	5.05	115.93	109.88
28	R	602	HEA	C2D-C1D-ND	5.01	115.78	109.84
28	L	602	HEA	C2C-C1C-NC	4.93	117.59	110.08
22	H	1007	HEM	CHC-C4B-NB	4.90	129.74	124.42
28	L	602	HEA	C4A-NA-C1A	-4.86	100.59	105.35
28	L	602	HEA	C2D-C1D-ND	4.73	115.45	109.84
28	R	602	HEA	C4A-NA-C1A	-4.68	100.76	105.35
28	L	602	HEA	C2A-C1A-NA	4.67	114.87	110.32
28	R	602	HEA	C2A-C1A-NA	4.66	114.86	110.32
28	R	603	HEA	C3B-C4B-NB	4.64	115.33	109.84
20	M	503	9YF	C7-C2-C3	-4.60	104.21	110.85
25	W	202	9XX	O1-C18-C19	4.59	121.40	111.50
19	M	502	IZL	O10-C23-C24	4.56	115.88	106.67
28	R	603	HEA	C2C-C1C-NC	4.54	117.00	110.08
28	R	603	HEA	C13-C14-C15	-4.54	116.72	127.66
28	L	603	HEA	C2B-C1B-NB	4.54	115.31	109.88
28	L	603	HEA	C2A-C1A-NA	4.51	114.71	110.32
20	W	201	9YF	C7-C2-C3	-4.50	104.36	110.85
28	R	603	HEA	CAD-CBD-CGD	-4.48	103.96	113.60
28	L	602	HEA	CHA-C1A-NA	-4.45	119.62	124.44
19	G	502	IZL	O10-C23-C24	4.44	115.64	106.67
20	b	201	9YF	C7-C2-C3	-4.44	104.44	110.85
28	R	602	HEA	C1D-C2D-C3D	-4.43	102.30	106.96
28	L	603	HEA	CHA-C1A-NA	-4.43	119.65	124.44
28	R	602	HEA	C2C-C1C-NC	4.41	116.80	110.08
23	L	601	CDL	OA6-CA5-C11	4.39	120.96	111.50
28	L	603	HEA	C3B-C4B-NB	4.37	115.02	109.84
28	L	603	HEA	C3C-C4C-NC	4.33	112.91	110.25
28	R	603	HEA	C1B-C2B-C3B	-4.32	101.63	106.80
23	T	1302	CDL	OA6-CA5-C11	4.32	120.80	111.50
23	H	1003	CDL	OA6-CA5-C11	4.30	120.77	111.50
23	N	603	CDL	OA6-CA5-C11	4.27	120.70	111.50
16	N	605	MQ9	C7-C8-C9	-4.23	119.75	126.79
23	H	1005	CDL	OA6-CA5-C11	4.22	120.59	111.50
28	L	602	HEA	C3A-C2A-C1A	-4.21	103.05	107.08
27	J	602	3PE	O21-C21-C22	4.19	120.54	111.50
16	C	305	MQ9	C7-C8-C9	-4.19	119.81	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	603	HEA	C2D-C1D-ND	4.19	114.80	109.84
23	N	602	CDL	OB6-CB5-C51	4.17	120.49	111.50
23	P	301	CDL	OA6-CA5-C11	4.16	120.48	111.50
23	T	1302	CDL	OB6-CB5-C51	4.16	120.47	111.50
23	P	301	CDL	OB6-CB5-C51	4.16	120.47	111.50
23	H	1004	CDL	OB6-CB5-C51	4.15	120.45	111.50
23	P	303	CDL	OB6-CB5-C51	4.15	120.44	111.50
23	K	201	CDL	OB6-CB5-C51	4.14	120.43	111.50
28	R	603	HEA	C4A-NA-C1A	-4.14	101.29	105.35
28	L	602	HEA	C1D-C2D-C3D	-4.14	102.61	106.96
23	H	1004	CDL	OA6-CA5-C11	4.14	120.42	111.50
28	L	603	HEA	C2D-C1D-ND	4.12	114.72	109.84
23	H	1005	CDL	OB6-CB5-C51	4.11	120.37	111.50
28	R	603	HEA	C2A-C1A-NA	4.11	114.32	110.32
23	N	604	CDL	OB6-CB5-C51	4.09	120.31	111.50
17	O	304	WUO	O04-C05-C12	4.08	114.90	106.67
21	S	501	7PH	O21-C21-C22	4.07	120.27	111.50
25	c	302	9XX	O1-C18-C19	4.05	120.24	111.50
20	b	201	9YF	O1-P-O8	4.05	132.24	112.24
17	P	302	WUO	C03-O04-C05	4.04	121.63	113.69
22	H	1007	HEM	CHD-C1D-ND	4.04	128.81	124.42
23	H	1003	CDL	OB6-CB5-C51	4.04	120.21	111.50
23	P	303	CDL	OA6-CA5-C11	4.03	120.20	111.50
23	R	605	CDL	OA6-CA5-C11	4.03	120.18	111.50
23	I	302	CDL	OA6-CA5-C11	4.03	120.18	111.50
23	N	604	CDL	OA6-CA5-C11	4.02	120.17	111.50
20	W	201	9YF	O1-P-O8	4.01	132.08	112.24
23	N	602	CDL	OA6-CA5-C11	4.01	120.14	111.50
23	L	609	CDL	OB6-CB5-C51	4.01	120.14	111.50
28	L	603	HEA	C1A-CHA-C4D	-4.00	117.43	126.06
25	N	609	9XX	O1-C18-C19	3.99	120.10	111.50
23	N	603	CDL	OB6-CB5-C51	3.98	120.07	111.50
23	R	601	CDL	OA6-CA5-C11	3.98	120.07	111.50
17	P	302	WUO	O58-C59-C61	3.97	120.06	111.50
23	G	506	CDL	OB6-CB5-C51	3.97	120.06	111.50
17	I	303	WUO	C03-O04-C05	3.97	121.47	113.69
23	R	605	CDL	OB6-CB5-C51	3.96	120.05	111.50
28	L	603	HEA	C4A-NA-C1A	-3.95	101.48	105.35
27	S	503	3PE	O21-C21-C22	3.94	120.00	111.50
23	I	301	CDL	OA6-CA5-C11	3.94	119.99	111.50
23	K	201	CDL	OA6-CA5-C11	3.92	119.95	111.50
20	M	503	9YF	O1-P-O8	3.92	131.62	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	304	WUO	O58-C59-C61	3.92	119.94	111.50
23	L	601	CDL	OB6-CB5-C51	3.91	119.94	111.50
23	L	609	CDL	OA6-CA5-C11	3.91	119.92	111.50
22	H	1007	HEM	C1B-NB-C4B	3.90	109.10	105.07
20	G	503	9YF	O1-P-O8	3.86	131.32	112.24
22	H	1007	HEM	C4C-NC-C1C	3.86	109.13	105.35
23	R	601	CDL	OB6-CB5-C51	3.86	119.81	111.50
23	I	301	CDL	OB6-CB5-C51	3.86	119.81	111.50
28	R	602	HEA	CHB-C1B-NB	-3.85	120.23	124.42
28	R	602	HEA	C3A-C2A-C1A	-3.85	103.40	107.08
21	H	1001	7PH	O21-C21-C22	3.84	119.77	111.50
28	L	602	HEA	C1B-C2B-C3B	-3.83	102.22	106.80
17	C	304	WUO	O58-C59-C61	3.82	119.74	111.50
17	I	303	WUO	O58-C59-C61	3.80	119.70	111.50
23	G	506	CDL	OA6-CA5-C11	3.78	119.65	111.50
23	I	302	CDL	OB6-CB5-C51	3.75	119.59	111.50
28	L	603	HEA	C2C-C1C-NC	3.75	115.79	110.08
16	C	303	MQ9	C7-C8-C9	-3.74	120.57	126.79
17	C	304	WUO	O04-C05-C12	3.72	114.17	106.67
21	G	505	7PH	O21-C21-C22	3.70	119.47	111.50
28	L	602	HEA	CHB-C1B-NB	-3.68	120.42	124.42
20	G	503	9YF	C7-C2-C3	-3.68	105.55	110.85
16	T	1301	MQ9	C7-C8-C9	-3.67	120.68	126.79
28	L	603	HEA	C3A-C2A-C1A	-3.66	103.58	107.08
17	I	303	WUO	O04-C05-C12	3.64	114.02	106.67
25	b	202	9XX	O1-C18-C19	3.61	119.28	111.50
17	P	302	WUO	O04-C05-C12	3.58	113.90	106.67
19	G	502	IZL	C24-O11-C25	3.56	120.69	113.74
21	G	504	7PH	O21-C21-C22	3.51	119.07	111.50
28	R	603	HEA	CMB-C2B-C1B	3.51	130.38	125.04
28	L	603	HEA	C1D-C2D-C3D	-3.49	103.28	106.96
28	R	603	HEA	CBA-CAA-C2A	-3.48	102.97	112.63
28	R	602	HEA	CAD-CBD-CGD	-3.44	106.20	113.60
16	C	303	MQ9	C37-C38-C39	-3.43	119.39	127.66
21	M	504	7PH	O21-C21-C22	3.42	118.86	111.50
28	R	603	HEA	CMD-C2D-C1D	3.40	130.22	125.04
19	G	502	IZL	O34-C60-C61	3.40	118.82	111.50
28	R	602	HEA	C1B-C2B-C3B	-3.39	102.74	106.80
16	C	305	MQ9	C27-C28-C29	-3.39	119.50	127.66
28	L	603	HEA	C1B-C2B-C3B	-3.39	102.75	106.80
16	C	305	MQ9	C32-C33-C34	-3.35	119.59	127.66
19	M	502	IZL	C24-O11-C25	3.35	120.28	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	607	MQ9	C12-C13-C14	-3.34	119.61	127.66
17	C	304	WUO	C03-O04-C05	3.34	120.24	113.69
19	G	502	IZL	O28-C43-C14	3.33	116.55	108.69
19	M	502	IZL	O34-C60-C61	3.33	118.67	111.50
28	R	603	HEA	C1D-C2D-C3D	-3.32	103.46	106.96
16	H	1006	MQ9	C27-C28-C29	-3.31	119.68	127.66
28	L	603	HEA	C4D-C3D-C2D	-3.31	102.08	106.90
17	O	304	WUO	O55-P52-O53	-3.28	96.25	109.07
17	I	303	WUO	O55-P52-O53	-3.27	96.28	109.07
17	P	302	WUO	O55-P52-O53	-3.26	96.34	109.07
15	O	302	HEC	C1D-ND-C4D	3.26	108.44	105.07
22	H	1007	HEM	CHA-C4D-ND	3.26	128.39	124.37
17	C	304	WUO	O55-P52-O53	-3.26	96.34	109.07
15	C	302	HEC	C1D-ND-C4D	3.25	108.44	105.07
22	H	1007	HEM	CHB-C1B-NB	3.25	128.38	124.37
16	H	1006	MQ9	C17-C18-C19	-3.25	119.84	127.66
28	R	603	HEA	CMC-C2C-C1C	3.25	130.31	125.37
16	T	1301	MQ9	C10-C9-C11	3.24	120.72	115.27
16	C	303	MQ9	C32-C33-C34	-3.23	119.88	127.66
19	M	502	IZL	O11-C24-C23	3.23	115.03	109.05
17	I	303	WUO	O54-P52-O53	3.23	128.21	112.24
16	O	303	MQ9	C7-C8-C9	-3.22	121.43	126.79
28	R	603	HEA	C4D-C3D-C2D	-3.22	102.21	106.90
16	C	303	MQ9	C27-C28-C29	-3.21	119.92	127.66
16	C	305	MQ9	C22-C23-C24	-3.21	119.92	127.66
16	N	607	MQ9	C10-C9-C11	3.21	120.67	115.27
15	C	302	HEC	O1D-CGD-CBD	-3.20	112.79	123.08
28	R	602	HEA	CHA-C1A-NA	-3.20	120.97	124.44
15	O	302	HEC	O1D-CGD-CBD	-3.20	112.80	123.08
17	P	302	WUO	O54-P52-O53	3.20	128.04	112.24
16	H	1006	MQ9	C42-C43-C44	-3.20	119.97	127.66
16	T	1301	MQ9	C15-C14-C16	3.19	120.64	115.27
16	N	605	MQ9	C42-C43-C44	-3.18	120.01	127.66
17	O	304	WUO	O54-P52-O53	3.16	127.88	112.24
15	O	302	HEC	CBC-CAC-C3C	3.16	121.13	112.43
28	R	603	HEA	C17-C18-C19	-3.15	120.07	127.66
28	L	602	HEA	C13-C14-C15	-3.15	120.07	127.66
28	R	602	HEA	CMB-C2B-C1B	3.15	129.84	125.04
28	L	603	HEA	CAD-C3D-C4D	3.15	130.16	124.66
15	C	302	HEC	CBC-CAC-C3C	3.14	121.09	112.43
16	T	1301	MQ9	C22-C23-C24	-3.13	120.13	127.66
16	H	1006	MQ9	C7-C8-C9	-3.13	121.58	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	603	HEA	C13-C12-C11	-3.12	109.66	114.35
16	O	303	MQ9	C32-C33-C34	-3.12	120.14	127.66
16	N	605	MQ9	C32-C33-C34	-3.12	120.16	127.66
28	L	603	HEA	C17-C18-C19	-3.10	120.19	127.66
17	C	304	WUO	O54-P52-O53	3.10	127.57	112.24
16	T	1301	MQ9	C20-C19-C21	3.09	120.47	115.27
16	O	303	MQ9	C27-C28-C29	-3.09	120.22	127.66
16	N	607	MQ9	C30-C29-C31	3.09	120.46	115.27
16	H	1006	MQ9	C12-C13-C14	-3.08	120.24	127.66
16	O	303	MQ9	C17-C18-C19	-3.08	120.25	127.66
28	R	602	HEA	C17-C18-C19	-3.08	120.25	127.66
19	G	502	IZL	O1-C11-C12	3.07	114.93	108.43
17	P	302	WUO	C08-C07-C06	-3.06	105.49	110.82
16	H	1006	MQ9	C37-C38-C39	-3.05	120.31	127.66
28	R	602	HEA	CHB-C4A-NA	-3.05	121.14	124.44
16	C	303	MQ9	C17-C18-C19	-3.04	120.34	127.66
17	O	304	WUO	C03-O04-C05	3.04	119.65	113.69
28	L	602	HEA	CAA-C2A-C1A	3.03	130.62	124.89
15	O	301	HEC	C1D-ND-C4D	3.02	108.19	105.07
17	C	304	WUO	C08-C07-C06	-3.01	105.57	110.82
28	L	602	HEA	C4B-C3B-C2B	-3.01	102.28	107.41
19	G	502	IZL	C15-C14-C43	-3.01	104.80	111.66
16	H	1006	MQ9	C22-C23-C24	-3.00	120.44	127.66
16	O	303	MQ9	C25-C24-C26	2.99	120.31	115.27
16	N	605	MQ9	C12-C13-C14	-2.99	120.46	127.66
16	C	303	MQ9	C20-C19-C21	2.99	120.30	115.27
15	C	301	HEC	C1D-ND-C4D	2.99	108.16	105.07
16	O	303	MQ9	C37-C38-C39	-2.98	120.48	127.66
16	C	303	MQ9	C22-C23-C24	-2.98	120.48	127.66
16	T	1301	MQ9	C25-C24-C26	2.98	120.28	115.27
16	H	1006	MQ9	C32-C33-C34	-2.98	120.49	127.66
17	I	303	WUO	C08-C07-C06	-2.97	105.63	110.82
28	R	602	HEA	C13-C14-C15	-2.97	120.51	127.66
21	G	504	7PH	O31-C31-C32	2.97	121.22	111.91
16	O	303	MQ9	C42-C43-C44	-2.97	120.52	127.66
16	C	303	MQ9	C35-C34-C36	2.96	120.25	115.27
16	T	1301	MQ9	C12-C13-C14	-2.96	120.54	127.66
28	L	603	HEA	CBA-CAA-C2A	-2.96	104.42	112.63
16	N	605	MQ9	C45-C44-C46	2.96	120.24	115.27
16	T	1301	MQ9	C32-C33-C34	-2.95	120.55	127.66
16	N	607	MQ9	C25-C24-C26	2.95	120.24	115.27
28	L	602	HEA	C4D-C3D-C2D	-2.95	102.60	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	1301	MQ9	C27-C28-C29	-2.95	120.56	127.66
28	R	603	HEA	CAA-CBA-CGA	-2.95	107.26	113.60
16	T	1301	MQ9	C45-C44-C46	2.94	120.22	115.27
16	O	303	MQ9	C22-C23-C24	-2.94	120.58	127.66
15	C	302	HEC	CAD-CBD-CGD	2.93	119.91	113.60
15	O	302	HEC	CAD-CBD-CGD	2.93	119.90	113.60
21	M	504	7PH	O31-C31-C32	2.92	121.08	111.91
19	G	502	IZL	C21-O9-C22	2.92	119.44	113.74
16	O	303	MQ9	C10-C9-C11	2.92	120.18	115.27
25	c	302	9XX	C17-O1-C18	-2.91	114.14	117.88
16	C	305	MQ9	C30-C29-C31	2.90	120.16	115.27
28	R	602	HEA	C4B-C3B-C2B	-2.90	102.45	107.41
23	R	605	CDL	OA8-CA7-C31	2.90	121.02	111.91
16	N	605	MQ9	C27-C28-C29	-2.90	120.67	127.66
16	N	605	MQ9	C10-C9-C11	2.90	120.14	115.27
28	L	603	HEA	C13-C14-C15	-2.90	120.69	127.66
16	H	1006	MQ9	C10-C9-C11	2.89	120.14	115.27
16	H	1006	MQ9	C30-C29-C31	2.88	120.12	115.27
16	C	305	MQ9	C10-C9-C11	2.88	120.12	115.27
28	R	603	HEA	C21-C20-C19	-2.88	103.50	112.98
16	C	305	MQ9	C37-C38-C39	-2.88	120.73	127.66
20	M	503	9YF	O6-C6-C7	-2.88	103.70	110.35
16	N	607	MQ9	C45-C44-C46	2.88	120.11	115.27
16	N	607	MQ9	C17-C18-C19	-2.87	120.75	127.66
16	T	1301	MQ9	C5M-C5-C6	-2.87	119.72	124.40
28	L	603	HEA	OMA-CMA-C3A	-2.86	119.22	125.69
16	N	605	MQ9	C22-C23-C24	-2.86	120.77	127.66
16	O	303	MQ9	C30-C29-C31	2.86	120.08	115.27
28	R	602	HEA	C4D-C3D-C2D	-2.86	102.73	106.90
16	N	605	MQ9	C20-C19-C21	2.85	120.07	115.27
16	N	607	MQ9	C15-C14-C16	2.85	120.07	115.27
22	N	606	HEM	C4D-ND-C1D	2.85	108.02	105.07
16	T	1301	MQ9	C42-C43-C44	-2.85	120.81	127.66
16	C	303	MQ9	C45-C44-C46	2.85	120.06	115.27
28	L	603	HEA	CMC-C2C-C1C	2.84	129.70	125.37
16	C	303	MQ9	C5M-C5-C6	-2.84	119.76	124.40
23	R	601	CDL	OB8-CB7-C71	2.84	120.82	111.91
16	H	1006	MQ9	C20-C19-C21	2.84	120.05	115.27
23	N	602	CDL	OB8-CB7-C71	2.83	120.80	111.91
16	O	303	MQ9	C40-C39-C41	2.83	120.04	115.27
16	C	305	MQ9	C12-C13-C14	-2.83	120.84	127.66
28	L	602	HEA	C4B-NB-C1B	-2.83	102.15	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	502	IZL	C21-O9-C22	2.82	119.25	113.74
16	C	305	MQ9	C17-C18-C19	-2.82	120.88	127.66
16	C	303	MQ9	C42-C43-C44	-2.82	120.88	127.66
19	G	502	IZL	P-O28-C43	2.82	129.65	119.41
16	N	605	MQ9	C30-C29-C31	2.81	120.00	115.27
16	N	607	MQ9	C20-C19-C21	2.81	120.00	115.27
28	L	602	HEA	C17-C18-C19	-2.80	120.91	127.66
19	M	502	IZL	O2-C12-C11	2.80	112.32	106.67
25	N	609	9XX	C17-O1-C18	-2.80	114.28	117.88
16	C	305	MQ9	C15-C14-C16	2.80	119.97	115.27
28	L	603	HEA	CHC-C4B-NB	-2.80	120.93	124.37
17	P	302	WUO	C33-C31-C01	2.80	116.06	109.68
16	H	1006	MQ9	C15-C14-C16	2.79	119.97	115.27
27	S	503	3PE	O31-C31-C32	2.79	120.66	111.91
16	N	605	MQ9	C35-C34-C36	2.79	119.96	115.27
16	H	1006	MQ9	C35-C34-C36	2.78	119.95	115.27
23	N	602	CDL	OA8-CA7-C31	2.78	120.63	111.91
28	L	602	HEA	C26-C15-C16	2.78	119.94	115.27
28	L	603	HEA	C4B-C3B-C2B	-2.78	102.67	107.41
16	C	305	MQ9	C35-C34-C36	2.77	119.94	115.27
28	R	603	HEA	C25-C23-C24	2.77	120.72	114.60
19	G	502	IZL	O11-C24-C23	2.76	114.16	109.05
16	C	303	MQ9	C15-C14-C16	2.75	119.90	115.27
16	O	303	MQ9	C15-C14-C16	2.74	119.89	115.27
16	T	1301	MQ9	C30-C29-C31	2.74	119.89	115.27
15	C	302	HEC	C4B-NB-C1B	2.74	107.91	105.07
16	C	305	MQ9	C5M-C5-C6	-2.74	119.93	124.40
16	O	303	MQ9	C45-C44-C46	2.74	119.88	115.27
17	O	304	WUO	P52-O51-C50	2.74	129.37	119.41
23	N	603	CDL	OB8-CB7-C71	2.73	120.49	111.91
15	O	302	HEC	C4B-NB-C1B	2.73	107.90	105.07
16	T	1301	MQ9	C17-C18-C19	-2.73	121.08	127.66
23	P	301	CDL	OA8-CA7-C31	2.73	120.47	111.91
20	G	503	9YF	O7-C7-C6	-2.73	104.04	110.35
23	H	1003	CDL	OB8-CB7-C71	2.73	120.46	111.91
16	H	1006	MQ9	C45-C44-C46	2.72	119.85	115.27
27	J	602	3PE	O31-C31-C32	2.72	120.45	111.91
16	H	1006	MQ9	C40-C39-C41	2.72	119.85	115.27
28	L	602	HEA	C4C-NC-C1C	-2.72	102.68	105.35
17	I	303	WUO	O10-C07-C08	-2.72	104.07	110.35
16	C	303	MQ9	C51-C49-C50	2.72	120.60	114.60
17	I	303	WUO	C33-C31-C01	2.71	115.88	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	H	1005	CDL	OB8-CB7-C71	2.71	120.42	111.91
16	N	605	MQ9	C40-C39-C41	2.71	119.83	115.27
15	O	302	HEC	CBA-CAA-C2A	-2.71	105.09	112.63
20	M	503	9YF	O7-C7-C6	-2.71	104.09	110.35
16	O	303	MQ9	C5M-C5-C6	-2.71	119.98	124.40
28	R	602	HEA	OMA-CMA-C3A	-2.71	119.57	125.69
16	C	303	MQ9	C10-C9-C11	2.70	119.82	115.27
15	C	302	HEC	CBA-CAA-C2A	-2.70	105.12	112.63
28	R	603	HEA	CAD-C3D-C4D	2.70	129.38	124.66
25	N	609	9XX	O-C15-C14	2.70	120.38	111.91
16	C	305	MQ9	C42-C43-C44	-2.69	121.18	127.66
28	L	603	HEA	CAD-CBD-CGD	-2.69	107.81	113.60
23	K	201	CDL	OA8-CA7-C31	2.69	120.34	111.91
28	L	602	HEA	CMB-C2B-C1B	2.68	129.12	125.04
20	G	503	9YF	O6-C6-C7	-2.68	104.16	110.35
28	R	603	HEA	C3A-C2A-C1A	-2.68	104.52	107.08
17	P	302	WUO	P52-O51-C50	2.67	129.12	119.41
28	L	603	HEA	CHB-C1B-NB	-2.67	121.52	124.42
23	L	601	CDL	OA8-CA7-C31	2.66	120.26	111.91
23	L	609	CDL	OA8-CA7-C31	2.66	120.25	111.91
23	N	604	CDL	OB8-CB7-C71	2.66	120.25	111.91
28	R	602	HEA	C27-C19-C20	2.66	119.74	115.27
16	C	303	MQ9	C40-C39-C41	2.66	119.74	115.27
23	T	1302	CDL	OA8-CA7-C31	2.65	120.22	111.91
17	O	304	WUO	O10-C07-C08	-2.65	104.23	110.35
16	O	303	MQ9	C20-C19-C21	2.64	119.72	115.27
28	L	602	HEA	CHA-C4D-ND	-2.64	121.55	124.42
23	P	301	CDL	OB8-CB7-C71	2.64	120.19	111.91
17	P	302	WUO	O10-C07-C08	-2.64	104.25	110.35
23	H	1003	CDL	OA8-CA7-C31	2.64	120.18	111.91
23	T	1302	CDL	OB8-CB7-C71	2.63	120.17	111.91
23	L	609	CDL	OB8-CB7-C71	2.63	120.16	111.91
22	H	1002	HEM	C4C-NC-C1C	2.63	107.92	105.35
22	H	1002	HEM	C4D-ND-C1D	2.62	107.78	105.07
16	C	305	MQ9	C20-C19-C21	2.62	119.68	115.27
22	H	1002	HEM	C4A-NA-C1A	2.62	107.91	105.35
23	I	301	CDL	OB8-CB7-C71	2.62	120.13	111.91
16	C	303	MQ9	C25-C24-C26	2.62	119.67	115.27
28	L	602	HEA	CAD-CBD-CGD	-2.61	107.98	113.60
16	H	1006	MQ9	C5M-C5-C6	-2.61	120.14	124.40
23	G	506	CDL	OA8-CA7-C31	2.61	120.09	111.91
23	I	301	CDL	OA8-CA7-C31	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	304	WUO	C33-C31-C01	2.60	115.62	109.68
17	P	302	WUO	O02-C01-C50	2.60	114.09	107.48
23	R	605	CDL	OB8-CB7-C71	2.60	120.07	111.91
17	O	304	WUO	O02-C01-C50	2.60	114.08	107.48
22	H	1007	HEM	C4D-ND-C1D	2.60	107.76	105.07
17	O	304	WUO	C08-C07-C06	-2.60	106.29	110.82
28	L	603	HEA	C27-C19-C20	2.60	119.64	115.27
16	T	1301	MQ9	C40-C39-C41	2.60	119.64	115.27
28	R	603	HEA	CHA-C4D-C3D	-2.60	121.03	124.84
23	H	1004	CDL	OB8-CB7-C71	2.59	120.05	111.91
22	N	601	HEM	C4A-NA-C1A	2.59	107.89	105.35
16	C	303	MQ9	C30-C29-C31	2.59	119.63	115.27
28	L	602	HEA	CMC-C2C-C1C	2.59	129.31	125.37
23	G	506	CDL	OB8-CB7-C71	2.58	120.02	111.91
16	N	605	MQ9	C37-C38-C39	-2.58	121.44	127.66
23	I	302	CDL	OA8-CA7-C31	2.58	120.02	111.91
17	C	304	WUO	O10-C07-C08	-2.58	104.38	110.35
23	H	1005	CDL	OA8-CA7-C31	2.58	120.01	111.91
16	C	303	MQ9	C47-C48-C49	-2.57	118.98	127.75
16	N	607	MQ9	C22-C23-C24	-2.56	121.49	127.66
17	C	304	WUO	P52-O51-C50	2.56	128.74	119.41
19	G	502	IZL	O32-C47-C48	2.55	119.92	111.91
28	L	603	HEA	C26-C15-C16	2.55	119.56	115.27
28	L	603	HEA	C25-C23-C24	2.55	120.24	114.60
23	P	303	CDL	OA8-CA7-C31	2.55	119.90	111.91
16	O	303	MQ9	C35-C34-C36	2.55	119.55	115.27
16	N	607	MQ9	C35-C34-C36	2.55	119.55	115.27
23	H	1004	CDL	OA8-CA7-C31	2.54	119.89	111.91
16	O	303	MQ9	C12-C13-C14	-2.54	121.54	127.66
16	N	607	MQ9	C42-C43-C44	-2.54	121.55	127.66
23	P	303	CDL	OB8-CB7-C71	2.54	119.87	111.91
16	T	1301	MQ9	C37-C38-C39	-2.53	121.56	127.66
21	H	1001	7PH	O31-C31-C32	2.53	119.85	111.91
25	b	202	9XX	O-C15-C14	2.53	119.85	111.91
16	C	305	MQ9	C7-C6-C1	2.53	121.21	118.50
25	c	302	9XX	O-C15-C14	2.53	119.84	111.91
23	N	604	CDL	OA8-CA7-C31	2.52	119.83	111.91
16	C	303	MQ9	C12-C13-C14	-2.52	121.59	127.66
23	I	302	CDL	OB8-CB7-C71	2.52	119.81	111.91
22	N	606	HEM	C1B-NB-C4B	2.52	107.67	105.07
16	C	305	MQ9	C40-C39-C41	2.52	119.51	115.27
16	N	607	MQ9	C37-C38-C39	-2.51	121.61	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	301	HEC	C3D-C4D-ND	-2.51	107.92	110.36
28	R	603	HEA	CHC-C1C-C2C	-2.51	120.16	127.24
21	G	505	7PH	O31-C31-C32	2.50	119.76	111.91
17	O	304	WUO	C33-C31-C01	2.50	115.39	109.68
28	R	603	HEA	OMA-CMA-C3A	-2.50	120.04	125.69
17	I	303	WUO	P52-O51-C50	2.50	128.49	119.41
23	K	201	CDL	OB8-CB7-C71	2.50	119.74	111.91
16	N	605	MQ9	C25-C24-C26	2.49	119.46	115.27
22	N	606	HEM	C4A-NA-C1A	2.49	107.78	105.35
28	L	602	HEA	CHC-C1C-C2C	-2.49	120.22	127.24
22	H	1002	HEM	CAD-CBD-CGD	-2.48	108.26	113.60
15	C	302	HEC	O1A-CGA-CBA	-2.48	115.10	123.08
16	C	305	MQ9	C45-C44-C46	2.48	119.44	115.27
15	O	302	HEC	O1A-CGA-CBA	-2.48	115.12	123.08
28	R	603	HEA	CHB-C1B-C2B	-2.48	121.11	124.98
17	I	303	WUO	O02-C01-C50	2.47	113.76	107.48
15	C	301	HEC	C3D-C4D-ND	-2.47	107.96	110.36
16	O	303	MQ9	C51-C49-C50	2.47	120.06	114.60
19	M	502	IZL	O32-C47-C48	2.46	119.63	111.91
19	M	502	IZL	O1-C11-C12	2.46	113.64	108.43
22	N	601	HEM	C1B-NB-C4B	2.46	107.61	105.07
22	H	1007	HEM	CHD-C1D-C2D	-2.46	121.14	124.98
22	N	601	HEM	C4D-ND-C1D	2.45	107.61	105.07
28	R	602	HEA	CMC-C2C-C1C	2.45	129.10	125.37
19	M	502	IZL	O1-C10-C9	2.45	119.60	111.91
19	G	502	IZL	O1-C10-C9	2.45	119.59	111.91
28	R	602	HEA	C4A-CHB-C1B	-2.45	120.78	126.06
16	N	605	MQ9	C15-C14-C16	2.44	119.38	115.27
16	N	607	MQ9	C40-C39-C41	2.44	119.38	115.27
23	R	601	CDL	OA8-CA7-C31	2.44	119.57	111.91
15	C	302	HEC	C2D-C1D-ND	-2.44	106.95	109.84
16	H	1006	MQ9	C25-C24-C26	2.43	119.37	115.27
16	C	303	MQ9	C5M-C5-C4	2.43	120.30	116.27
15	C	301	HEC	O1D-CGD-CBD	-2.43	115.27	123.08
15	O	301	HEC	O1D-CGD-CBD	-2.43	115.27	123.08
25	b	202	9XX	O1-C17-C16	2.43	111.75	106.13
28	L	602	HEA	C27-C19-C20	2.42	119.35	115.27
15	O	302	HEC	C2D-C1D-ND	-2.42	106.97	109.84
16	O	303	MQ9	C5M-C5-C4	2.42	120.28	116.27
19	G	502	IZL	O2-C12-C11	2.42	111.55	106.67
28	R	602	HEA	C25-C23-C24	2.42	119.94	114.60
28	L	603	HEA	CMD-C2D-C1D	2.41	128.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	602	HEA	C25-C23-C24	2.40	119.91	114.60
16	T	1301	MQ9	C51-C49-C50	2.40	119.90	114.60
23	L	601	CDL	OB8-CB7-C71	2.40	119.43	111.91
23	N	603	CDL	OA8-CA7-C31	2.40	119.43	111.91
17	I	303	WUO	C31-C01-C50	-2.37	106.24	111.66
16	H	1006	MQ9	C51-C49-C50	2.37	119.84	114.60
28	L	602	HEA	CMD-C2D-C1D	2.37	128.64	125.04
19	M	502	IZL	O1-C10-O	-2.36	117.63	123.59
16	N	605	MQ9	C51-C49-C50	2.35	119.80	114.60
15	C	302	HEC	C3B-C4B-NB	-2.35	107.55	110.17
16	N	605	MQ9	C17-C18-C19	-2.35	122.00	127.66
16	O	303	MQ9	C47-C48-C49	-2.35	119.72	127.75
16	C	305	MQ9	C51-C49-C50	2.35	119.79	114.60
28	R	602	HEA	C21-C22-C23	-2.34	119.75	127.75
22	N	606	HEM	C4C-NC-C1C	2.34	107.64	105.35
15	C	302	HEC	CAA-CBA-CGA	2.34	118.63	113.60
25	W	202	9XX	O-C15-C14	2.33	119.23	111.91
28	R	603	HEA	C26-C15-C16	2.33	119.19	115.27
15	O	302	HEC	C3B-C4B-NB	-2.33	107.57	110.17
28	L	602	HEA	OMA-CMA-C3A	-2.33	120.42	125.69
28	R	602	HEA	C26-C15-C16	2.33	119.18	115.27
15	O	302	HEC	CAA-CBA-CGA	2.32	118.61	113.60
15	C	301	HEC	CBD-CAD-C3D	2.32	119.08	112.63
16	T	1301	MQ9	C35-C34-C36	2.32	119.18	115.27
28	L	602	HEA	CHB-C4A-NA	-2.32	121.93	124.44
15	O	301	HEC	CBD-CAD-C3D	2.32	119.07	112.63
19	G	502	IZL	O1-C10-O	-2.31	117.77	123.59
19	M	502	IZL	O30-P-O29	2.30	123.63	112.24
17	C	304	WUO	O02-C01-C50	2.30	113.31	107.48
16	H	1006	MQ9	C5M-C5-C4	2.30	120.07	116.27
28	R	602	HEA	CHA-C4D-ND	-2.29	121.93	124.42
22	H	1002	HEM	C1B-NB-C4B	2.29	107.44	105.07
17	O	304	WUO	O58-C59-O60	-2.28	118.20	123.70
21	S	501	7PH	O31-C31-C32	2.27	119.05	111.91
16	C	305	MQ9	C47-C48-C49	-2.26	120.01	127.75
17	I	303	WUO	O04-C05-C06	2.26	113.79	109.69
16	N	607	MQ9	C47-C48-C49	-2.25	120.05	127.75
15	C	301	HEC	CBC-CAC-C3C	2.25	118.63	112.43
16	N	607	MQ9	C27-C28-C29	-2.25	122.24	127.66
15	O	301	HEC	CBC-CAC-C3C	2.25	118.62	112.43
23	T	1302	CDL	CB4-OB6-CB5	-2.24	112.28	117.79
28	L	602	HEA	C13-C12-C11	-2.23	110.99	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	502	IZL	O28-P-O29	-2.23	101.08	109.47
17	P	302	WUO	O40-C39-C44	2.23	115.07	110.35
16	N	607	MQ9	C51-C49-C50	2.23	119.53	114.60
28	R	603	HEA	C4B-C3B-C2B	-2.23	103.61	107.41
17	I	303	WUO	O40-C39-C44	2.23	115.06	110.35
17	I	303	WUO	C33-C35-C37	2.22	114.75	109.68
17	C	304	WUO	O58-C59-O60	-2.20	118.38	123.70
22	H	1007	HEM	C4C-CHD-C1D	-2.20	121.31	126.06
22	H	1007	HEM	CHD-C4C-NC	2.20	126.82	124.44
22	N	601	HEM	C4C-NC-C1C	2.20	107.50	105.35
15	C	302	HEC	CHC-C4B-NB	2.20	127.08	124.37
19	M	502	IZL	O11-C25-C30	2.19	112.45	108.22
28	L	603	HEA	C21-C22-C23	-2.19	120.26	127.75
28	L	603	HEA	CMB-C2B-C1B	2.19	128.37	125.04
22	H	1007	HEM	C4A-NA-C1A	2.18	107.49	105.35
28	L	603	HEA	CHD-C1D-ND	-2.17	121.69	124.37
22	N	606	HEM	C3D-C4D-ND	-2.17	107.75	110.17
15	O	302	HEC	CHC-C4B-NB	2.17	127.05	124.37
17	P	302	WUO	O58-C59-O60	-2.17	118.46	123.70
22	H	1002	HEM	C3D-C4D-ND	-2.17	107.75	110.17
17	O	304	WUO	C31-C01-C50	-2.17	106.71	111.66
15	C	301	HEC	O1A-CGA-CBA	-2.16	116.13	123.08
28	L	602	HEA	CAD-C3D-C4D	2.15	128.42	124.66
16	C	305	MQ9	C5M-C5-C4	2.15	119.84	116.27
25	W	202	9XX	C25-C26-C27	-2.15	108.96	115.92
16	C	305	MQ9	C25-C24-C26	2.15	118.89	115.27
15	O	301	HEC	O1A-CGA-CBA	-2.15	116.17	123.08
17	C	304	WUO	C31-C01-C50	-2.15	106.75	111.66
22	H	1007	HEM	C1A-CHA-C4D	-2.14	121.26	126.34
17	P	302	WUO	O04-C05-C06	2.14	113.58	109.69
22	H	1007	HEM	C4A-CHB-C1B	-2.13	121.28	126.34
28	R	602	HEA	CMD-C2D-C1D	2.12	128.27	125.04
28	R	602	HEA	CHC-C1C-C2C	-2.12	121.24	127.24
20	W	201	9YF	O11-C25-C26	2.12	118.57	111.91
28	L	602	HEA	C4A-CHB-C1B	-2.12	121.48	126.06
22	H	1007	HEM	CAD-CBD-CGD	-2.12	109.04	113.60
16	N	607	MQ9	C10-C9-C8	-2.12	118.24	123.68
15	C	302	HEC	C3D-C4D-ND	-2.12	108.30	110.36
19	G	502	IZL	O28-C43-C18	2.12	113.68	108.69
15	O	302	HEC	C3D-C4D-ND	-2.12	108.31	110.36
17	P	302	WUO	C31-C01-C50	-2.11	106.85	111.66
16	T	1301	MQ9	C5M-C5-C4	2.10	119.76	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	603	HEA	CHB-C4A-NA	-2.10	122.17	124.44
28	R	603	HEA	C21-C22-C23	-2.10	120.57	127.75
17	I	303	WUO	O58-C59-O60	-2.09	118.64	123.70
19	G	502	IZL	O8-C20-C21	2.09	110.88	106.67
22	N	601	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
28	R	603	HEA	C4C-NC-C1C	-2.08	103.31	105.35
19	G	502	IZL	O30-P-O29	2.08	122.52	112.24
17	O	304	WUO	O77-C76-C57	2.08	114.48	108.43
23	H	1004	CDL	CB4-OB6-CB5	-2.08	112.68	117.79
16	N	607	MQ9	C32-C33-C34	-2.07	122.68	127.66
22	H	1002	HEM	C2A-C1A-NA	-2.06	107.85	110.15
28	R	602	HEA	CHC-C4B-NB	-2.05	121.85	124.37
17	P	302	WUO	C33-C35-C37	2.04	114.35	109.68
22	N	601	HEM	C2A-C1A-NA	-2.04	107.86	110.15
17	O	304	WUO	O40-C39-C44	2.04	114.67	110.35
22	H	1002	HEM	CHC-C1C-NC	2.03	126.64	124.44
16	N	607	MQ9	C30-C29-C28	-2.03	118.47	123.68
28	R	602	HEA	C4B-NB-C1B	-2.03	102.98	105.07
25	W	202	9XX	O1-C18-O2	-2.02	118.81	123.70
25	N	609	9XX	C25-C26-C27	-2.02	109.40	115.92
22	H	1007	HEM	CHB-C1B-C2B	-2.01	121.14	126.73
20	b	201	9YF	O6-C6-C7	-2.00	105.72	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	O	301	HEC	NA
15	O	302	HEC	NA
15	C	301	HEC	NA
15	C	302	HEC	NA

All (1586) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	N	605	MQ9	C14-C16-C17-C18
16	N	605	MQ9	C38-C39-C41-C42
16	N	605	MQ9	C40-C39-C41-C42
16	N	605	MQ9	C39-C41-C42-C43
16	N	605	MQ9	C43-C44-C46-C47
16	N	605	MQ9	C45-C44-C46-C47
16	N	607	MQ9	C12-C11-C9-C10
16	N	607	MQ9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
16	N	607	MQ9	C14-C16-C17-C18
16	N	607	MQ9	C24-C26-C27-C28
16	N	607	MQ9	C35-C34-C36-C37
16	N	607	MQ9	C43-C44-C46-C47
16	N	607	MQ9	C45-C44-C46-C47
16	T	1301	MQ9	C45-C44-C46-C47
16	C	305	MQ9	C39-C41-C42-C43
16	C	305	MQ9	C44-C46-C47-C48
16	H	1006	MQ9	C12-C11-C9-C8
16	H	1006	MQ9	C12-C11-C9-C10
16	H	1006	MQ9	C18-C19-C21-C22
16	H	1006	MQ9	C20-C19-C21-C22
16	H	1006	MQ9	C28-C29-C31-C32
16	H	1006	MQ9	C30-C29-C31-C32
16	H	1006	MQ9	C34-C36-C37-C38
17	P	302	WUO	C80-C78-O77-C76
17	P	302	WUO	O79-C78-O77-C76
17	C	304	WUO	C61-C59-O58-C57
17	C	304	WUO	C86-C87-C88-C89
19	M	502	IZL	C48-C47-O32-C46
19	M	502	IZL	O33-C47-O32-C46
19	M	502	IZL	C44-O31-P-O30
19	G	502	IZL	C14-C43-O28-P
19	G	502	IZL	C18-C43-O28-P
19	G	502	IZL	C48-C47-O32-C46
19	G	502	IZL	O33-C47-O32-C46
20	M	503	9YF	C2-O2-P-O1
20	M	503	9YF	C1-O-P-O2
20	M	503	9YF	C1-O-P-O8
20	W	201	9YF	C2-O2-P-O1
20	W	201	9YF	O9-C-C1-O
20	W	201	9YF	O10-C8-O9-C
20	G	503	9YF	C2-O2-P-O1
20	b	201	9YF	C2-O2-P-O1
20	b	201	9YF	C1-O-P-O8
20	b	201	9YF	C31-C32-C33-C34
20	b	201	9YF	C9-C8-O9-C
20	b	201	9YF	O10-C8-O9-C
21	M	504	7PH	C1-O11-P-O12
21	M	504	7PH	C1-O11-P-O13
21	M	504	7PH	C1-O11-P-O14
21	S	501	7PH	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
21	S	501	7PH	C1-O11-P-O14
21	G	504	7PH	C1-O11-P-O12
21	G	504	7PH	C1-O11-P-O13
21	G	504	7PH	C1-O11-P-O14
21	G	505	7PH	C1-O11-P-O12
21	G	505	7PH	C1-O11-P-O13
21	G	505	7PH	C1-O11-P-O14
21	H	1001	7PH	C1-O11-P-O12
21	H	1001	7PH	C1-O11-P-O13
21	H	1001	7PH	C1-O11-P-O14
22	N	601	HEM	C3D-CAD-CBD-CGD
22	H	1007	HEM	C2B-C3B-CAB-CBB
22	H	1007	HEM	C4B-C3B-CAB-CBB
23	N	602	CDL	CA2-C1-CB2-OB2
23	N	602	CDL	CA2-OA2-PA1-OA3
23	N	602	CDL	CA2-OA2-PA1-OA4
23	N	602	CDL	CA2-OA2-PA1-OA5
23	N	602	CDL	CA3-OA5-PA1-OA4
23	N	602	CDL	C11-CA5-OA6-CA4
23	N	602	CDL	CB2-OB2-PB2-OB3
23	N	602	CDL	CB2-OB2-PB2-OB4
23	N	602	CDL	CB2-OB2-PB2-OB5
23	N	603	CDL	CB2-C1-CA2-OA2
23	N	603	CDL	CA2-OA2-PA1-OA3
23	N	603	CDL	CA2-OA2-PA1-OA4
23	N	603	CDL	CA2-OA2-PA1-OA5
23	N	603	CDL	CA3-OA5-PA1-OA3
23	N	603	CDL	CB2-OB2-PB2-OB3
23	N	603	CDL	CB2-OB2-PB2-OB4
23	N	603	CDL	CB3-OB5-PB2-OB3
23	N	603	CDL	CB3-OB5-PB2-OB4
23	N	604	CDL	CB2-C1-CA2-OA2
23	N	604	CDL	CA2-OA2-PA1-OA3
23	N	604	CDL	CA2-OA2-PA1-OA4
23	N	604	CDL	CA2-OA2-PA1-OA5
23	N	604	CDL	CA3-OA5-PA1-OA2
23	N	604	CDL	CA3-OA5-PA1-OA3
23	N	604	CDL	CA3-OA5-PA1-OA4
23	N	604	CDL	OA9-CA7-OA8-CA6
23	N	604	CDL	C31-CA7-OA8-CA6
23	N	604	CDL	CB2-OB2-PB2-OB3
23	N	604	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
23	N	604	CDL	CB3-OB5-PB2-OB2
23	N	604	CDL	CB3-OB5-PB2-OB3
23	N	604	CDL	CB3-OB5-PB2-OB4
23	P	301	CDL	CA3-OA5-PA1-OA2
23	P	301	CDL	CA3-OA5-PA1-OA3
23	P	301	CDL	CA3-OA5-PA1-OA4
23	P	301	CDL	C11-CA5-OA6-CA4
23	P	301	CDL	OB6-CB4-CB6-OB8
23	P	303	CDL	CA2-C1-CB2-OB2
23	P	303	CDL	CA3-OA5-PA1-OA2
23	P	303	CDL	CA3-OA5-PA1-OA3
23	P	303	CDL	CA3-OA5-PA1-OA4
23	P	303	CDL	C11-CA5-OA6-CA4
23	P	303	CDL	CB2-OB2-PB2-OB3
23	P	303	CDL	CB2-OB2-PB2-OB4
23	P	303	CDL	CB2-OB2-PB2-OB5
23	P	303	CDL	CB3-OB5-PB2-OB3
23	P	303	CDL	C51-CB5-OB6-CB4
23	T	1302	CDL	CA2-OA2-PA1-OA4
23	T	1302	CDL	OA5-CA3-CA4-OA6
23	T	1302	CDL	C11-CA5-OA6-CA4
23	T	1302	CDL	CB2-OB2-PB2-OB3
23	R	601	CDL	CA2-OA2-PA1-OA4
23	R	601	CDL	CA2-OA2-PA1-OA5
23	R	601	CDL	CB2-OB2-PB2-OB3
23	R	601	CDL	CB2-OB2-PB2-OB4
23	R	601	CDL	CB2-OB2-PB2-OB5
23	R	601	CDL	CB3-OB5-PB2-OB4
23	R	605	CDL	CA2-OA2-PA1-OA3
23	R	605	CDL	CA2-OA2-PA1-OA4
23	R	605	CDL	CA2-OA2-PA1-OA5
23	R	605	CDL	CA3-OA5-PA1-OA3
23	R	605	CDL	CB2-OB2-PB2-OB3
23	R	605	CDL	CB2-OB2-PB2-OB4
23	R	605	CDL	CB3-OB5-PB2-OB2
23	R	605	CDL	CB3-OB5-PB2-OB3
23	R	605	CDL	CB3-OB5-PB2-OB4
23	R	605	CDL	OB9-CB7-OB8-CB6
23	G	506	CDL	C1-CA2-OA2-PA1
23	G	506	CDL	CA2-OA2-PA1-OA3
23	G	506	CDL	CA2-OA2-PA1-OA4
23	G	506	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
23	G	506	CDL	C11-CA5-OA6-CA4
23	G	506	CDL	CB2-OB2-PB2-OB3
23	G	506	CDL	CB2-OB2-PB2-OB4
23	G	506	CDL	CB2-OB2-PB2-OB5
23	H	1003	CDL	CA2-C1-CB2-OB2
23	H	1003	CDL	CA2-OA2-PA1-OA3
23	H	1003	CDL	CA2-OA2-PA1-OA4
23	H	1003	CDL	CA2-OA2-PA1-OA5
23	H	1003	CDL	CA3-OA5-PA1-OA4
23	H	1003	CDL	CB2-OB2-PB2-OB4
23	H	1003	CDL	CB2-OB2-PB2-OB5
23	H	1003	CDL	OB5-CB3-CB4-OB6
23	H	1004	CDL	CA2-C1-CB2-OB2
23	H	1004	CDL	CA3-OA5-PA1-OA3
23	H	1004	CDL	CB2-OB2-PB2-OB3
23	H	1004	CDL	CB2-OB2-PB2-OB4
23	H	1005	CDL	CA2-OA2-PA1-OA3
23	H	1005	CDL	CA2-OA2-PA1-OA4
23	H	1005	CDL	CB2-OB2-PB2-OB3
23	H	1005	CDL	CB2-OB2-PB2-OB4
23	H	1005	CDL	OB7-CB5-OB6-CB4
23	H	1005	CDL	C51-CB5-OB6-CB4
23	I	301	CDL	CA2-OA2-PA1-OA4
23	I	301	CDL	C11-CA5-OA6-CA4
23	I	301	CDL	CB2-OB2-PB2-OB3
23	I	301	CDL	CB3-OB5-PB2-OB3
23	I	302	CDL	CA2-C1-CB2-OB2
23	I	302	CDL	CA2-OA2-PA1-OA3
23	I	302	CDL	CA2-OA2-PA1-OA4
23	I	302	CDL	CA3-OA5-PA1-OA4
23	I	302	CDL	CB2-OB2-PB2-OB3
23	I	302	CDL	CB2-OB2-PB2-OB4
23	I	302	CDL	CB2-OB2-PB2-OB5
23	I	302	CDL	CB3-OB5-PB2-OB2
23	I	302	CDL	CB3-OB5-PB2-OB3
23	I	302	CDL	CB3-OB5-PB2-OB4
23	K	201	CDL	CA2-OA2-PA1-OA3
23	K	201	CDL	CA2-OA2-PA1-OA4
23	K	201	CDL	CA3-OA5-PA1-OA4
23	K	201	CDL	CB2-OB2-PB2-OB3
23	K	201	CDL	CB2-OB2-PB2-OB4
23	K	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
23	K	201	CDL	CB3-OB5-PB2-OB2
23	L	601	CDL	O1-C1-CA2-OA2
23	L	601	CDL	CB2-C1-CA2-OA2
23	L	601	CDL	CA2-C1-CB2-OB2
23	L	601	CDL	CA2-OA2-PA1-OA3
23	L	601	CDL	CA2-OA2-PA1-OA4
23	L	601	CDL	CA3-OA5-PA1-OA3
23	L	601	CDL	OA7-CA5-OA6-CA4
23	L	601	CDL	C11-CA5-OA6-CA4
23	L	601	CDL	CB2-OB2-PB2-OB4
23	L	609	CDL	CA2-OA2-PA1-OA4
24	W	203	PLM	C1-C2-C3-C4
25	N	609	9XX	O-C16-C17-C37
25	N	609	9XX	O-C16-C17-O1
25	N	609	9XX	C19-C18-O1-C17
25	N	609	9XX	O2-C18-O1-C17
25	W	202	9XX	C19-C18-O1-C17
25	W	202	9XX	O2-C18-O1-C17
25	b	202	9XX	O-C16-C17-C37
25	b	202	9XX	O-C16-C17-O1
25	b	202	9XX	C16-C17-O1-C18
27	S	503	3PE	C1-O11-P-O12
27	S	503	3PE	C1-O11-P-O13
27	S	503	3PE	C1-O11-P-O14
27	S	503	3PE	C22-C21-O21-C2
27	J	602	3PE	C1-O11-P-O14
27	J	602	3PE	C22-C21-O21-C2
28	R	602	HEA	C2A-C3A-CMA-OMA
28	R	602	HEA	C4A-C3A-CMA-OMA
28	R	602	HEA	C3B-C11-C12-C13
28	R	602	HEA	O11-C11-C12-C13
28	R	603	HEA	C2A-C3A-CMA-OMA
28	R	603	HEA	C12-C11-C3B-C2B
28	L	602	HEA	C3B-C11-C12-C13
28	L	602	HEA	O11-C11-C12-C13
28	L	603	HEA	C2A-C3A-CMA-OMA
28	L	603	HEA	C4A-C3A-CMA-OMA
28	L	603	HEA	C4C-C3C-CAC-CBC
28	L	603	HEA	C14-C15-C16-C17
28	L	603	HEA	C26-C15-C16-C17
17	P	302	WUO	O15-C14-O13-C12
17	I	303	WUO	O15-C14-O13-C12

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Mol	Chain	Res	Type	Atoms
19	G	502	IZL	O-C10-O1-C11
23	P	303	CDL	OA9-CA7-OA8-CA6
23	I	301	CDL	OA9-CA7-OA8-CA6
17	P	302	WUO	C16-C14-O13-C12
17	I	303	WUO	C16-C14-O13-C12
19	G	502	IZL	C9-C10-O1-C11
23	P	303	CDL	C31-CA7-OA8-CA6
23	I	302	CDL	C71-CB7-OB8-CB6
23	P	303	CDL	OB9-CB7-OB8-CB6
23	G	506	CDL	OA9-CA7-OA8-CA6
23	G	506	CDL	OB9-CB7-OB8-CB6
23	I	301	CDL	OB9-CB7-OB8-CB6
23	I	302	CDL	OA9-CA7-OA8-CA6
23	I	302	CDL	OB9-CB7-OB8-CB6
27	S	503	3PE	O32-C31-O31-C3
27	J	602	3PE	O32-C31-O31-C3
19	M	502	IZL	O10-C23-C24-O11
17	C	304	WUO	O60-C59-O58-C57
23	N	602	CDL	OA7-CA5-OA6-CA4
23	N	604	CDL	OA7-CA5-OA6-CA4
23	P	301	CDL	OA7-CA5-OA6-CA4
23	P	303	CDL	OA7-CA5-OA6-CA4
23	P	303	CDL	OB7-CB5-OB6-CB4
23	T	1302	CDL	OA7-CA5-OA6-CA4
23	I	301	CDL	OA7-CA5-OA6-CA4
27	S	503	3PE	O22-C21-O21-C2
27	J	602	3PE	O22-C21-O21-C2
25	c	302	9XX	O6-C15-O-C16
23	R	605	CDL	C71-CB7-OB8-CB6
23	I	301	CDL	C31-CA7-OA8-CA6
23	L	601	CDL	C31-CA7-OA8-CA6
23	L	609	CDL	C71-CB7-OB8-CB6
27	J	602	3PE	C32-C31-O31-C3
20	W	201	9YF	C9-C8-O9-C
23	N	604	CDL	C11-CA5-OA6-CA4
17	P	302	WUO	O40-C41-C48-O49
16	N	607	MQ9	C20-C19-C21-C22
16	T	1301	MQ9	C20-C19-C21-C22
28	R	603	HEA	C26-C15-C16-C17
16	N	607	MQ9	C12-C11-C9-C8
16	N	607	MQ9	C13-C14-C16-C17
16	N	607	MQ9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
16	T	1301	MQ9	C43-C44-C46-C47
25	b	202	9XX	O6-C15-O-C16
20	M	503	9YF	C26-C25-O11-C24
23	P	303	CDL	C71-CB7-OB8-CB6
23	G	506	CDL	C31-CA7-OA8-CA6
23	G	506	CDL	C71-CB7-OB8-CB6
23	H	1004	CDL	C71-CB7-OB8-CB6
23	I	301	CDL	C71-CB7-OB8-CB6
23	I	302	CDL	C31-CA7-OA8-CA6
23	L	609	CDL	C31-CA7-OA8-CA6
25	c	302	9XX	C14-C15-O-C16
27	S	503	3PE	C32-C31-O31-C3
17	O	304	WUO	O40-C41-C48-O49
20	G	503	9YF	C39-C40-C41-C42
28	L	602	HEA	C1A-C2A-CAA-CBA
23	H	1003	CDL	OA7-CA5-OA6-CA4
19	M	502	IZL	O-C10-O1-C11
23	H	1004	CDL	OB9-CB7-OB8-CB6
23	L	609	CDL	OB9-CB7-OB8-CB6
23	N	602	CDL	O1-C1-CB2-OB2
23	N	603	CDL	O1-C1-CA2-OA2
23	N	604	CDL	O1-C1-CA2-OA2
23	P	303	CDL	O1-C1-CB2-OB2
23	T	1302	CDL	O1-C1-CB2-OB2
23	R	601	CDL	O1-C1-CB2-OB2
23	H	1003	CDL	O1-C1-CA2-OA2
23	H	1003	CDL	O1-C1-CB2-OB2
23	I	302	CDL	O1-C1-CB2-OB2
19	M	502	IZL	C9-C10-O1-C11
20	G	503	9YF	C26-C25-O11-C24
25	b	202	9XX	C14-C15-O-C16
23	L	601	CDL	OA9-CA7-OA8-CA6
19	M	502	IZL	O17-C32-C33-O18
17	P	302	WUO	C61-C59-O58-C57
23	N	604	CDL	C51-CB5-OB6-CB4
23	H	1003	CDL	C11-CA5-OA6-CA4
23	H	1004	CDL	C51-CB5-OB6-CB4
23	H	1005	CDL	C11-CA5-OA6-CA4
23	I	302	CDL	C51-CB5-OB6-CB4
23	K	201	CDL	C51-CB5-OB6-CB4
20	b	201	9YF	C29-C30-C31-C32
17	P	302	WUO	C59-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
19	M	502	IZL	O12-C26-C27-O13
17	O	304	WUO	C42-C41-C48-O49
17	O	304	WUO	C65-C66-C67-C68
17	P	302	WUO	C24-C25-C26-C27
20	M	503	9YF	C13-C14-C15-C16
20	W	201	9YF	C38-C39-C40-C41
17	C	304	WUO	C64-C65-C66-C67
17	I	303	WUO	C90-C91-C92-C93
20	G	503	9YF	C9-C10-C11-C12
20	b	201	9YF	C38-C39-C40-C41
23	T	1302	CDL	C76-C77-C78-C79
23	H	1003	CDL	C15-C16-C17-C18
28	L	602	HEA	C3A-C2A-CAA-CBA
17	I	303	WUO	O40-C41-C48-O49
23	H	1005	CDL	OA7-CA5-OA6-CA4
20	G	503	9YF	C16-C17-C18-C19
20	M	503	9YF	O12-C25-O11-C24
16	O	303	MQ9	C25-C24-C26-C27
16	N	605	MQ9	C20-C19-C21-C22
16	N	605	MQ9	C35-C34-C36-C37
16	N	607	MQ9	C25-C24-C26-C27
16	C	305	MQ9	C12-C11-C9-C10
16	O	303	MQ9	C23-C24-C26-C27
16	N	605	MQ9	C18-C19-C21-C22
16	N	607	MQ9	C23-C24-C26-C27
16	C	305	MQ9	C12-C11-C9-C8
23	T	1302	CDL	C31-C32-C33-C34
20	G	503	9YF	O12-C25-O11-C24
23	L	609	CDL	OA9-CA7-OA8-CA6
19	M	502	IZL	O12-C25-O11-C24
16	N	605	MQ9	C19-C21-C22-C23
16	N	605	MQ9	C29-C31-C32-C33
16	N	607	MQ9	C19-C21-C22-C23
16	T	1301	MQ9	C14-C16-C17-C18
16	C	305	MQ9	C14-C16-C17-C18
16	C	305	MQ9	C29-C31-C32-C33
16	H	1006	MQ9	C19-C21-C22-C23
17	I	303	WUO	C42-C41-C48-O49
23	R	605	CDL	C51-CB5-OB6-CB4
23	P	301	CDL	CA2-C1-CB2-OB2
23	T	1302	CDL	CA2-C1-CB2-OB2
23	R	601	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
23	R	605	CDL	CA2-C1-CB2-OB2
23	H	1003	CDL	CB2-C1-CA2-OA2
23	I	301	CDL	CB2-C1-CA2-OA2
17	P	302	WUO	O60-C59-O58-C57
23	H	1004	CDL	OB7-CB5-OB6-CB4
23	I	302	CDL	OB7-CB5-OB6-CB4
23	H	1005	CDL	C71-CB7-OB8-CB6
23	K	201	CDL	CB5-C51-C52-C53
17	I	303	WUO	C67-C68-C69-C70
19	G	502	IZL	O31-C44-C45-O34
21	M	504	7PH	O11-C1-C2-O21
21	G	504	7PH	O11-C1-C2-O21
17	P	302	WUO	C42-C41-C48-O49
20	W	201	9YF	C33-C35-C36-C37
23	N	604	CDL	O1-C1-CB2-OB2
23	I	301	CDL	O1-C1-CA2-OA2
17	O	304	WUO	C14-C16-C17-C18
20	G	503	9YF	C25-C26-C27-C28
23	I	302	CDL	OA6-CA4-CA6-OA8
16	O	303	MQ9	C20-C19-C21-C22
16	T	1301	MQ9	C18-C19-C21-C22
17	O	304	WUO	C86-C87-C88-C89
17	O	304	WUO	C89-C88-C90-C91
17	P	302	WUO	C86-C87-C88-C89
17	I	303	WUO	C86-C87-C88-C89
19	M	502	IZL	C54-C55-C56-C57
19	G	502	IZL	C54-C55-C56-C57
20	G	503	9YF	C31-C32-C33-C34
23	K	201	CDL	OB7-CB5-OB6-CB4
19	M	502	IZL	C61-C60-O34-C45
21	G	504	7PH	C22-C21-O21-C2
23	L	609	CDL	C51-CB5-OB6-CB4
19	M	502	IZL	C65-C66-C68-C69
23	R	605	CDL	C73-C74-C75-C76
23	P	303	CDL	CB5-C51-C52-C53
23	K	201	CDL	CA7-C31-C32-C33
20	b	201	9YF	C33-C35-C36-C37
17	P	302	WUO	C17-C18-C19-C20
17	C	304	WUO	C62-C63-C64-C65
23	N	604	CDL	CA7-C31-C32-C33
23	N	604	CDL	CB5-C51-C52-C53
23	R	601	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
23	I	301	CDL	CA7-C31-C32-C33
23	L	609	CDL	CA5-C11-C12-C13
20	b	201	9YF	C30-C31-C32-C33
17	I	303	WUO	C14-C16-C17-C18
20	M	503	9YF	C25-C26-C27-C28
21	G	505	7PH	C21-C22-C23-C24
23	N	602	CDL	CB5-C51-C52-C53
23	N	603	CDL	CB5-C51-C52-C53
23	N	603	CDL	CB7-C71-C72-C73
23	P	301	CDL	CA7-C31-C32-C33
23	K	201	CDL	CA5-C11-C12-C13
23	L	601	CDL	CB5-C51-C52-C53
23	L	609	CDL	CA7-C31-C32-C33
27	S	503	3PE	C21-C22-C23-C24
23	G	506	CDL	C11-C12-C13-C14
19	M	502	IZL	C28-C26-C27-O13
23	N	603	CDL	C74-C75-C76-C77
21	H	1001	7PH	C24-C25-C26-C27
23	R	605	CDL	CB7-C71-C72-C73
23	G	506	CDL	CB5-C51-C52-C53
27	J	602	3PE	C21-C22-C23-C24
21	G	504	7PH	C22-C23-C24-C25
23	T	1302	CDL	C51-CB5-OB6-CB4
20	G	503	9YF	C30-C31-C32-C33
20	M	503	9YF	C31-C32-C33-C35
20	G	503	9YF	C31-C32-C33-C35
23	H	1005	CDL	OB9-CB7-OB8-CB6
21	M	504	7PH	C22-C23-C24-C25
20	G	503	9YF	C33-C35-C36-C37
17	P	302	WUO	C85-C86-C87-C88
16	T	1301	MQ9	C29-C31-C32-C33
16	T	1301	MQ9	C44-C46-C47-C48
16	C	303	MQ9	C14-C16-C17-C18
16	C	305	MQ9	C19-C21-C22-C23
28	R	602	HEA	C15-C16-C17-C18
21	G	504	7PH	C24-C25-C26-C27
23	N	602	CDL	O1-C1-CA2-OA2
23	P	301	CDL	O1-C1-CB2-OB2
23	P	303	CDL	O1-C1-CA2-OA2
23	R	605	CDL	O1-C1-CB2-OB2
23	H	1004	CDL	O1-C1-CB2-OB2
23	I	301	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
23	L	601	CDL	O1-C1-CB2-OB2
21	G	504	7PH	O22-C21-O21-C2
23	N	604	CDL	OB7-CB5-OB6-CB4
23	R	605	CDL	OB7-CB5-OB6-CB4
17	C	304	WUO	C88-C90-C91-C92
23	T	1302	CDL	C71-CB7-OB8-CB6
23	P	303	CDL	C71-C72-C73-C74
19	M	502	IZL	C2-C3-C4-C5
21	M	504	7PH	C24-C25-C26-C27
19	M	502	IZL	C37-C23-C24-O11
21	M	504	7PH	C22-C21-O21-C2
25	b	202	9XX	C19-C18-O1-C17
19	M	502	IZL	C53-C54-C55-C56
19	M	502	IZL	C44-O31-P-O28
19	G	502	IZL	C44-O31-P-O28
20	G	503	9YF	C1-O-P-O2
20	b	201	9YF	C1-O-P-O2
23	N	602	CDL	CA3-OA5-PA1-OA2
23	N	602	CDL	CB3-OB5-PB2-OB2
23	N	603	CDL	CB2-OB2-PB2-OB5
23	N	603	CDL	CB3-OB5-PB2-OB2
23	N	604	CDL	CB2-OB2-PB2-OB5
23	P	301	CDL	CB2-OB2-PB2-OB5
23	P	301	CDL	CB3-OB5-PB2-OB2
23	P	303	CDL	CB3-OB5-PB2-OB2
23	T	1302	CDL	CA3-OA5-PA1-OA2
23	T	1302	CDL	CB2-OB2-PB2-OB5
23	T	1302	CDL	CB3-OB5-PB2-OB2
23	R	601	CDL	CA3-OA5-PA1-OA2
23	R	601	CDL	CB3-OB5-PB2-OB2
23	R	605	CDL	CB2-OB2-PB2-OB5
23	G	506	CDL	CA2-OA2-PA1-OA5
23	G	506	CDL	CA3-OA5-PA1-OA2
23	H	1003	CDL	CA3-OA5-PA1-OA2
23	H	1004	CDL	CA3-OA5-PA1-OA2
23	H	1005	CDL	CA2-OA2-PA1-OA5
23	H	1005	CDL	CA3-OA5-PA1-OA2
23	H	1005	CDL	CB2-OB2-PB2-OB5
23	I	301	CDL	CB3-OB5-PB2-OB2
23	I	302	CDL	CA2-OA2-PA1-OA5
23	I	302	CDL	CA3-OA5-PA1-OA2
23	K	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
23	L	601	CDL	CA2-OA2-PA1-OA5
23	L	601	CDL	CA3-OA5-PA1-OA2
23	L	601	CDL	CB2-OB2-PB2-OB5
23	L	609	CDL	CA3-OA5-PA1-OA2
27	J	602	3PE	C1-O11-P-O13
17	O	304	WUO	C70-C71-C72-C73
17	I	303	WUO	C85-C86-C87-C88
23	R	601	CDL	CB5-C51-C52-C53
23	N	602	CDL	CB2-C1-CA2-OA2
23	N	604	CDL	CA2-C1-CB2-OB2
23	P	303	CDL	CB2-C1-CA2-OA2
23	I	301	CDL	CA2-C1-CB2-OB2
19	M	502	IZL	O35-C60-O34-C45
21	M	504	7PH	O22-C21-O21-C2
23	T	1302	CDL	OB7-CB5-OB6-CB4
23	L	609	CDL	OB7-CB5-OB6-CB4
25	b	202	9XX	O2-C18-O1-C17
23	H	1004	CDL	C71-C72-C73-C74
23	N	604	CDL	C19-C20-C21-C22
23	L	601	CDL	CA7-C31-C32-C33
17	P	302	WUO	C25-C26-C27-C28
23	P	301	CDL	C35-C36-C37-C38
23	T	1302	CDL	C12-C13-C14-C15
23	R	605	CDL	C57-C58-C59-C60
23	G	506	CDL	C76-C77-C78-C79
21	H	1001	7PH	C22-C21-O21-C2
23	N	603	CDL	C11-CA5-OA6-CA4
23	P	301	CDL	C51-CB5-OB6-CB4
17	C	304	WUO	C25-C26-C27-C28
17	I	303	WUO	C64-C65-C66-C67
23	N	602	CDL	C54-C55-C56-C57
23	P	303	CDL	C51-C52-C53-C54
23	T	1302	CDL	C15-C16-C17-C18
23	T	1302	CDL	C78-C79-C80-C81
23	G	506	CDL	C57-C58-C59-C60
23	G	506	CDL	C71-C72-C73-C74
23	H	1003	CDL	C57-C58-C59-C60
23	H	1004	CDL	C53-C54-C55-C56
23	H	1005	CDL	C16-C17-C18-C19
23	H	1005	CDL	C73-C74-C75-C76
23	I	301	CDL	C57-C58-C59-C60
23	K	201	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
23	P	301	CDL	C31-CA7-OA8-CA6
17	O	304	WUO	C83-C84-C85-C86
17	P	302	WUO	C90-C91-C92-C93
20	G	503	9YF	C11-C12-C13-C14
20	G	503	9YF	C17-C18-C19-C20
23	P	301	CDL	C57-C58-C59-C60
23	R	605	CDL	C59-C60-C61-C62
23	H	1005	CDL	C13-C14-C15-C16
23	L	609	CDL	C16-C17-C18-C19
27	J	602	3PE	C3-C2-O21-C21
21	H	1001	7PH	O22-C21-O21-C2
23	N	603	CDL	OA7-CA5-OA6-CA4
23	P	301	CDL	OB7-CB5-OB6-CB4
17	I	303	WUO	C24-C25-C26-C27
17	I	303	WUO	C84-C85-C86-C87
17	I	303	WUO	C91-C92-C93-C94
20	M	503	9YF	C18-C19-C20-C21
20	W	201	9YF	C29-C30-C31-C32
20	W	201	9YF	C39-C40-C41-C42
20	G	503	9YF	C13-C14-C15-C16
20	G	503	9YF	C38-C39-C40-C41
20	b	201	9YF	C13-C14-C15-C16
23	N	602	CDL	C57-C58-C59-C60
23	H	1003	CDL	C76-C77-C78-C79
23	H	1005	CDL	C21-C22-C23-C24
20	b	201	9YF	O9-C-C1-O
17	O	304	WUO	C61-C62-C63-C64
17	O	304	WUO	C91-C92-C93-C94
17	C	304	WUO	C22-C23-C24-C25
20	M	503	9YF	C16-C17-C18-C19
23	N	602	CDL	C11-C12-C13-C14
23	N	602	CDL	C51-C52-C53-C54
23	T	1302	CDL	C74-C75-C76-C77
23	R	605	CDL	C33-C34-C35-C36
23	H	1005	CDL	C18-C19-C20-C21
23	I	301	CDL	C55-C56-C57-C58
20	W	201	9YF	C30-C31-C32-C33
23	N	604	CDL	C76-C77-C78-C79
23	R	601	CDL	C32-C33-C34-C35
23	R	605	CDL	C32-C33-C34-C35
23	G	506	CDL	C15-C16-C17-C18
23	K	201	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
23	L	601	CDL	CA5-C11-C12-C13
17	C	304	WUO	C65-C66-C67-C68
20	M	503	9YF	C39-C40-C41-C42
23	N	603	CDL	C57-C58-C59-C60
23	N	604	CDL	C16-C17-C18-C19
23	P	303	CDL	C37-C38-C39-C40
23	G	506	CDL	C16-C17-C18-C19
23	H	1004	CDL	C57-C58-C59-C60
23	I	301	CDL	C16-C17-C18-C19
23	I	301	CDL	C71-C72-C73-C74
23	K	201	CDL	C81-C82-C83-C84
23	L	601	CDL	C53-C54-C55-C56
23	L	609	CDL	C32-C33-C34-C35
25	W	202	9XX	C4-C5-C6-C7
20	G	503	9YF	C3-C2-O2-P
20	W	201	9YF	C13-C14-C15-C16
20	G	503	9YF	C15-C16-C17-C18
23	N	604	CDL	C51-C52-C53-C54
23	N	604	CDL	C75-C76-C77-C78
23	P	303	CDL	C72-C73-C74-C75
23	H	1003	CDL	C74-C75-C76-C77
23	K	201	CDL	C74-C75-C76-C77
26	X	403	TRD	C11-C10-C9-C8
20	M	503	9YF	C31-C32-C33-C34
25	N	609	9XX	C25-C26-C27-C36
23	P	303	CDL	CA5-C11-C12-C13
23	I	302	CDL	CB5-C51-C52-C53
23	L	609	CDL	CB5-C51-C52-C53
17	I	303	WUO	C21-C22-C23-C24
17	I	303	WUO	C61-C62-C63-C64
20	W	201	9YF	C10-C11-C12-C13
23	P	301	CDL	C51-C52-C53-C54
23	P	303	CDL	C16-C17-C18-C19
23	P	303	CDL	C57-C58-C59-C60
23	R	605	CDL	C16-C17-C18-C19
23	G	506	CDL	C78-C79-C80-C81
23	H	1003	CDL	C16-C17-C18-C19
23	K	201	CDL	C16-C17-C18-C19
23	L	601	CDL	C81-C82-C83-C84
23	L	609	CDL	C57-C58-C59-C60
25	W	202	9XX	C10-C11-C12-C13
23	T	1302	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
17	O	304	WUO	C90-C91-C92-C93
20	b	201	9YF	C27-C28-C29-C30
23	N	602	CDL	C13-C14-C15-C16
23	P	301	CDL	C59-C60-C61-C62
23	I	302	CDL	C16-C17-C18-C19
19	G	502	IZL	O12-C26-C27-O13
20	G	503	9YF	O10-C8-O9-C
20	G	503	9YF	C9-C8-O9-C
23	I	301	CDL	C51-CB5-OB6-CB4
17	P	302	WUO	C71-C72-C73-C74
17	P	302	WUO	C83-C84-C85-C86
20	M	503	9YF	C19-C20-C21-C22
20	W	201	9YF	C16-C17-C18-C19
23	T	1302	CDL	C71-C72-C73-C74
23	R	605	CDL	C13-C14-C15-C16
23	R	605	CDL	C15-C16-C17-C18
23	H	1004	CDL	C16-C17-C18-C19
23	I	302	CDL	C35-C36-C37-C38
23	I	302	CDL	C51-C52-C53-C54
23	I	302	CDL	C57-C58-C59-C60
23	K	201	CDL	C12-C13-C14-C15
23	I	301	CDL	CA5-C11-C12-C13
23	I	302	CDL	CA7-C31-C32-C33
17	O	304	WUO	C64-C65-C66-C67
17	C	304	WUO	C82-C83-C84-C85
20	M	503	9YF	C38-C39-C40-C41
21	S	501	7PH	C26-C27-C28-C29
23	N	603	CDL	C32-C33-C34-C35
23	R	601	CDL	C53-C54-C55-C56
23	H	1005	CDL	C22-C23-C24-C25
23	I	302	CDL	C55-C56-C57-C58
25	W	202	9XX	C6-C7-C8-C9
25	c	302	9XX	C19-C20-C21-C22
19	M	502	IZL	C34-C32-C33-O18
17	I	303	WUO	C88-C90-C91-C92
20	M	503	9YF	C12-C13-C14-C15
21	G	504	7PH	C23-C24-C25-C26
23	R	605	CDL	C51-C52-C53-C54
23	H	1003	CDL	C11-C12-C13-C14
23	H	1005	CDL	C57-C58-C59-C60
23	K	201	CDL	C73-C74-C75-C76
23	L	601	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
23	L	609	CDL	C59-C60-C61-C62
32	H	1008	DCQ	C9-C10-C11-C12
27	S	503	3PE	O13-C11-C12-N
23	N	604	CDL	C55-C56-C57-C58
23	K	201	CDL	C53-C54-C55-C56
17	P	302	WUO	C14-C16-C17-C18
23	T	1302	CDL	CB5-C51-C52-C53
17	P	302	WUO	C84-C85-C86-C87
17	C	304	WUO	C83-C84-C85-C86
17	I	303	WUO	C65-C66-C67-C68
20	W	201	9YF	C27-C28-C29-C30
23	N	602	CDL	C16-C17-C18-C19
23	N	604	CDL	C18-C19-C20-C21
23	R	601	CDL	C59-C60-C61-C62
17	O	304	WUO	C71-C72-C73-C74
17	P	302	WUO	C65-C66-C67-C68
17	C	304	WUO	C61-C62-C63-C64
17	I	303	WUO	C83-C84-C85-C86
23	P	301	CDL	C12-C13-C14-C15
23	G	506	CDL	C81-C82-C83-C84
23	H	1004	CDL	C51-C52-C53-C54
17	O	304	WUO	C88-C90-C91-C92
19	M	502	IZL	C51-C52-C53-C54
20	M	503	9YF	C14-C15-C16-C17
20	M	503	9YF	C29-C30-C31-C32
21	G	505	7PH	C24-C25-C26-C27
23	N	603	CDL	C51-C52-C53-C54
23	N	604	CDL	C31-C32-C33-C34
23	R	601	CDL	C74-C75-C76-C77
23	H	1005	CDL	C12-C13-C14-C15
23	H	1005	CDL	C76-C77-C78-C79
23	K	201	CDL	C79-C80-C81-C82
23	L	609	CDL	C74-C75-C76-C77
20	G	503	9YF	C29-C30-C31-C32
23	H	1005	CDL	C19-C20-C21-C22
17	P	302	WUO	C82-C83-C84-C85
20	b	201	9YF	C18-C19-C20-C21
23	N	603	CDL	C54-C55-C56-C57
23	P	301	CDL	C11-C12-C13-C14
23	H	1003	CDL	C78-C79-C80-C81
23	H	1004	CDL	C74-C75-C76-C77
23	I	301	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
23	I	302	CDL	C33-C34-C35-C36
21	S	501	7PH	C21-C22-C23-C24
23	G	506	CDL	CA5-C11-C12-C13
23	T	1302	CDL	C16-C17-C18-C19
16	N	605	MQ9	C33-C34-C36-C37
16	N	607	MQ9	C18-C19-C21-C22
17	P	302	WUO	C21-C22-C23-C24
23	N	603	CDL	C55-C56-C57-C58
23	R	605	CDL	C34-C35-C36-C37
20	b	201	9YF	C10-C11-C12-C13
21	M	504	7PH	C28-C29-C2A-C2B
23	K	201	CDL	C51-C52-C53-C54
23	L	601	CDL	C76-C77-C78-C79
20	M	503	9YF	C10-C11-C12-C13
28	L	603	HEA	C2C-C3C-CAC-CBC
23	L	601	CDL	C15-C16-C17-C18
17	O	304	WUO	C21-C22-C23-C24
20	W	201	9YF	C15-C16-C17-C18
20	G	503	9YF	C18-C19-C20-C21
21	M	504	7PH	C23-C24-C25-C26
23	N	603	CDL	C37-C38-C39-C40
23	N	604	CDL	C74-C75-C76-C77
23	N	602	CDL	C18-C19-C20-C21
23	N	602	CDL	C76-C77-C78-C79
23	P	301	CDL	C15-C16-C17-C18
23	I	302	CDL	C14-C15-C16-C17
23	I	301	CDL	OB7-CB5-OB6-CB4
23	T	1302	CDL	C32-C33-C34-C35
23	I	301	CDL	C15-C16-C17-C18
23	L	601	CDL	C51-C52-C53-C54
23	P	301	CDL	OA9-CA7-OA8-CA6
17	O	304	WUO	C69-C70-C71-C72
23	P	301	CDL	C33-C34-C35-C36
25	W	202	9XX	C1-C2-C3-C4
19	M	502	IZL	C3-C4-C5-C6
23	H	1003	CDL	C73-C74-C75-C76
17	C	304	WUO	C85-C86-C87-C88
25	W	202	9XX	C24-C25-C26-C27
17	P	302	WUO	C61-C62-C63-C64
17	I	303	WUO	C20-C21-C22-C23
23	P	301	CDL	C16-C17-C18-C19
23	G	506	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	I	302	CDL	C32-C33-C34-C35
23	H	1004	CDL	CB5-C51-C52-C53
23	L	601	CDL	C52-C53-C54-C55
16	C	303	MQ9	C15-C14-C16-C17
16	H	1006	MQ9	C35-C34-C36-C37
28	R	603	HEA	C27-C19-C20-C21
16	O	303	MQ9	C18-C19-C21-C22
16	H	1006	MQ9	C33-C34-C36-C37
25	N	609	9XX	C25-C26-C27-C28
28	R	603	HEA	C14-C15-C16-C17
17	P	302	WUO	C64-C65-C66-C67
21	S	501	7PH	O22-C21-O21-C2
23	R	601	CDL	OB7-CB5-OB6-CB4
23	R	605	CDL	OA7-CA5-OA6-CA4
23	N	603	CDL	CA5-C11-C12-C13
23	K	201	CDL	C71-CB7-OB8-CB6
23	R	601	CDL	C73-C74-C75-C76
23	R	605	CDL	C74-C75-C76-C77
19	M	502	IZL	O1-C11-C12-C73
21	S	501	7PH	C34-C35-C36-C37
21	S	501	7PH	C29-C2A-C2B-C2C
23	T	1302	CDL	C11-C12-C13-C14
23	K	201	CDL	C14-C15-C16-C17
23	N	604	CDL	C12-C13-C14-C15
23	N	604	CDL	C56-C57-C58-C59
23	N	604	CDL	C57-C58-C59-C60
23	T	1302	CDL	C13-C14-C15-C16
23	H	1004	CDL	C35-C36-C37-C38
17	I	303	WUO	C93-C94-C95-C96
21	G	504	7PH	C28-C29-C2A-C2B
23	R	605	CDL	C31-C32-C33-C34
23	H	1003	CDL	C79-C80-C81-C82
17	O	304	WUO	C85-C86-C87-C88
16	N	607	MQ9	C9-C11-C12-C13
23	P	303	CDL	C59-C60-C61-C62
23	G	506	CDL	C74-C75-C76-C77
23	G	506	CDL	CB7-C71-C72-C73
20	M	503	9YF	C9-C8-O9-C
21	S	501	7PH	C22-C21-O21-C2
23	R	601	CDL	C51-CB5-OB6-CB4
23	R	605	CDL	C11-CA5-OA6-CA4
21	H	1001	7PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
23	G	506	CDL	C34-C35-C36-C37
23	H	1004	CDL	C33-C34-C35-C36
23	K	201	CDL	C78-C79-C80-C81
23	L	601	CDL	C34-C35-C36-C37
24	L	610	PLM	C6-C7-C8-C9
23	H	1004	CDL	O1-C1-CA2-OA2
20	M	503	9YF	O10-C8-O9-C
25	N	609	9XX	C12-C13-C14-C15
17	C	304	WUO	C84-C85-C86-C87
17	I	303	WUO	C82-C83-C84-C85
23	N	602	CDL	C15-C16-C17-C18
23	N	603	CDL	C73-C74-C75-C76
17	C	304	WUO	O58-C57-C76-O77
23	R	605	CDL	OA6-CA4-CA6-OA8
23	N	603	CDL	C71-C72-C73-C74
23	N	604	CDL	C11-C12-C13-C14
23	G	506	CDL	C12-C13-C14-C15
23	K	201	CDL	C34-C35-C36-C37
16	H	1006	MQ9	C25-C24-C26-C27
23	N	602	CDL	C55-C56-C57-C58
23	P	303	CDL	C74-C75-C76-C77
23	G	506	CDL	C13-C14-C15-C16
23	H	1003	CDL	C54-C55-C56-C57
23	H	1005	CDL	C32-C33-C34-C35
25	b	202	9XX	C25-C26-C27-C36
20	M	503	9YF	C37-C38-C39-C40
20	b	201	9YF	C39-C40-C41-C42
23	H	1003	CDL	C13-C14-C15-C16
28	R	602	HEA	C4D-C3D-CAD-CBD
28	R	603	HEA	C4D-C3D-CAD-CBD
23	T	1302	CDL	C55-C56-C57-C58
23	R	601	CDL	C51-C52-C53-C54
23	H	1005	CDL	C74-C75-C76-C77
23	G	506	CDL	OB7-CB5-OB6-CB4
19	G	502	IZL	C61-C60-O34-C45
23	G	506	CDL	C51-CB5-OB6-CB4
23	P	303	CDL	C53-C54-C55-C56
23	T	1302	CDL	C57-C58-C59-C60
17	C	304	WUO	C56-O55-P52-O51
23	R	605	CDL	CA3-OA5-PA1-OA2
23	H	1004	CDL	CB2-OB2-PB2-OB5
23	H	1005	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
23	K	201	CDL	CA3-OA5-PA1-OA2
17	C	304	WUO	C24-C25-C26-C27
20	b	201	9YF	C26-C27-C28-C29
23	H	1005	CDL	CB5-C51-C52-C53
23	H	1003	CDL	C53-C54-C55-C56
23	K	201	CDL	C80-C81-C82-C83
20	W	201	9YF	C24-C-C1-O
21	M	504	7PH	O11-C1-C2-C3
23	P	301	CDL	OB5-CB3-CB4-CB6
23	R	601	CDL	OB5-CB3-CB4-CB6
27	S	503	3PE	O11-C1-C2-C3
24	L	610	PLM	C5-C6-C7-C8
23	N	602	CDL	C53-C54-C55-C56
23	L	609	CDL	C15-C16-C17-C18
20	b	201	9YF	C11-C12-C13-C14
23	H	1004	CDL	C34-C35-C36-C37
19	M	502	IZL	C47-C48-C49-C50
17	O	304	WUO	C80-C81-C82-C83
19	G	502	IZL	O35-C60-O34-C45
19	M	502	IZL	C49-C50-C51-C52
20	M	503	9YF	C36-C37-C38-C39
20	W	201	9YF	C37-C38-C39-C40
23	N	603	CDL	C33-C34-C35-C36
23	P	303	CDL	C11-C12-C13-C14
23	H	1005	CDL	C11-C12-C13-C14
23	I	302	CDL	C59-C60-C61-C62
25	c	302	9XX	C18-C19-C20-C21
23	K	201	CDL	O1-C1-CA2-OA2
23	T	1302	CDL	C72-C73-C74-C75
20	W	201	9YF	C1-C-C24-O11
20	b	201	9YF	C1-C-C24-O11
23	N	602	CDL	CB3-CB4-CB6-OB8
23	N	603	CDL	CB3-CB4-CB6-OB8
23	P	301	CDL	CB3-CB4-CB6-OB8
23	P	303	CDL	CB3-CB4-CB6-OB8
23	T	1302	CDL	CA3-CA4-CA6-OA8
23	T	1302	CDL	CB3-CB4-CB6-OB8
23	G	506	CDL	CA3-CA4-CA6-OA8
23	H	1003	CDL	CB3-CB4-CB6-OB8
23	H	1004	CDL	CA3-CA4-CA6-OA8
23	I	302	CDL	CA3-CA4-CA6-OA8
23	I	302	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
23	K	201	CDL	CB3-CB4-CB6-OB8
26	L	607	TRD	C9-C10-C11-C12
27	S	503	3PE	C1-C2-C3-O31
23	T	1302	CDL	C81-C82-C83-C84
23	H	1004	CDL	C76-C77-C78-C79
24	L	610	PLM	C2-C3-C4-C5
23	K	201	CDL	OB9-CB7-OB8-CB6
19	M	502	IZL	C7-C1-C2-C3
23	R	605	CDL	C71-C72-C73-C74
23	H	1005	CDL	C79-C80-C81-C82
23	I	301	CDL	C18-C19-C20-C21
23	I	302	CDL	C11-C12-C13-C14
23	I	302	CDL	C15-C16-C17-C18
23	L	609	CDL	C60-C61-C62-C63
17	I	303	WUO	C27-C28-C29-C30
23	P	303	CDL	C18-C19-C20-C21
23	H	1003	CDL	C59-C60-C61-C62
23	I	302	CDL	C76-C77-C78-C79
23	R	605	CDL	C52-C51-CB5-OB6
23	P	303	CDL	CB7-C71-C72-C73
23	R	605	CDL	CB5-C51-C52-C53
20	G	503	9YF	C37-C38-C39-C40
23	H	1005	CDL	C34-C35-C36-C37
16	T	1301	MQ9	C34-C36-C37-C38
19	M	502	IZL	O1-C11-C12-O2
17	P	302	WUO	C94-C95-C96-C97
23	P	303	CDL	C60-C61-C62-C63
17	C	304	WUO	C80-C78-O77-C76
20	M	503	9YF	C2-O2-P-O
25	N	609	9XX	C19-C20-C21-C22
16	N	605	MQ9	C15-C14-C16-C17
17	P	302	WUO	C27-C28-C29-C30
23	N	602	CDL	C78-C79-C80-C81
23	R	605	CDL	C18-C19-C20-C21
23	H	1005	CDL	C51-C52-C53-C54
16	N	607	MQ9	C1-C6-C7-C8
19	G	502	IZL	C2-C3-C4-C5
23	I	302	CDL	C13-C14-C15-C16
17	P	302	WUO	C56-C57-O58-C59
17	C	304	WUO	C56-C57-O58-C59
23	N	604	CDL	CA6-CA4-OA6-CA5
23	G	506	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
23	I	302	CDL	CB6-CB4-OB6-CB5
27	S	503	3PE	C3-C2-O21-C21
28	R	602	HEA	C11-C12-C13-C14
17	I	303	WUO	C81-C82-C83-C84
23	P	301	CDL	C76-C77-C78-C79
23	H	1003	CDL	C18-C19-C20-C21
23	L	601	CDL	C36-C37-C38-C39
19	M	502	IZL	O31-C44-C45-O34
23	K	201	CDL	OB5-CB3-CB4-OB6
23	R	605	CDL	C32-C31-CA7-OA8
19	G	502	IZL	C47-C48-C49-C50
23	H	1004	CDL	CA5-C11-C12-C13
17	I	303	WUO	C71-C72-C73-C74
25	c	302	9XX	C9-C10-C11-C12
17	O	304	WUO	C27-C28-C29-C30
23	I	301	CDL	C38-C39-C40-C41
15	O	301	HEC	C3D-CAD-CBD-CGD
15	C	301	HEC	C3D-CAD-CBD-CGD
23	G	506	CDL	C51-C52-C53-C54
23	H	1005	CDL	C75-C76-C77-C78
23	L	609	CDL	C71-C72-C73-C74
17	I	303	WUO	C69-C70-C71-C72
17	I	303	WUO	C94-C95-C96-C97
23	N	603	CDL	C76-C77-C78-C79
23	P	303	CDL	OB6-CB4-CB6-OB8
23	I	301	CDL	OA6-CA4-CA6-OA8
23	I	301	CDL	C73-C74-C75-C76
23	I	302	CDL	C18-C19-C20-C21
23	L	609	CDL	C18-C19-C20-C21
16	C	305	MQ9	C30-C29-C31-C32
16	N	605	MQ9	C13-C14-C16-C17
16	C	305	MQ9	C28-C29-C31-C32
20	b	201	9YF	C31-C32-C33-C35
25	W	202	9XX	C25-C26-C27-C28
25	b	202	9XX	C25-C26-C27-C28
28	R	602	HEA	C2D-C3D-CAD-CBD
23	P	301	CDL	C52-C51-CB5-OB6
17	C	304	WUO	O79-C78-O77-C76
17	C	304	WUO	C27-C28-C29-C30
23	P	303	CDL	C35-C36-C37-C38
23	H	1004	CDL	C55-C56-C57-C58
23	P	301	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	R	605	CDL	C76-C77-C78-C79
17	O	304	WUO	C94-C95-C96-C97
23	P	303	CDL	C76-C77-C78-C79
17	P	302	WUO	C62-C63-C64-C65
23	N	602	CDL	C59-C60-C61-C62
23	L	601	CDL	C17-C18-C19-C20
23	P	301	CDL	CB5-C51-C52-C53
28	R	602	HEA	C4C-C3C-CAC-CBC
19	G	502	IZL	O31-C44-C45-C46
21	G	504	7PH	O11-C1-C2-C3
21	H	1001	7PH	O11-C1-C2-C3
23	N	602	CDL	OB5-CB3-CB4-CB6
23	P	301	CDL	OA5-CA3-CA4-CA6
23	T	1302	CDL	OA5-CA3-CA4-CA6
23	H	1003	CDL	OA5-CA3-CA4-CA6
23	H	1003	CDL	OB5-CB3-CB4-CB6
23	H	1004	CDL	OB5-CB3-CB4-CB6
23	I	301	CDL	OB5-CB3-CB4-CB6
23	K	201	CDL	OB5-CB3-CB4-CB6
27	J	602	3PE	O11-C1-C2-C3
16	C	305	MQ9	C34-C36-C37-C38
16	H	1006	MQ9	C9-C11-C12-C13
17	C	304	WUO	C91-C92-C93-C94
23	P	303	CDL	C34-C35-C36-C37
23	H	1004	CDL	C15-C16-C17-C18
17	I	303	WUO	C92-C93-C94-C95
20	M	503	9YF	C11-C12-C13-C14
23	I	301	CDL	C60-C61-C62-C63
20	W	201	9YF	C26-C25-O11-C24
28	R	603	HEA	C2D-C3D-CAD-CBD
20	M	503	9YF	C20-C21-C22-C23
23	P	301	CDL	C60-C61-C62-C63
23	L	609	CDL	O1-C1-CA2-OA2
23	R	601	CDL	C60-C61-C62-C63
23	G	506	CDL	C80-C81-C82-C83
25	N	609	9XX	C10-C11-C12-C13
25	N	609	9XX	C11-C10-C9-C8
20	M	503	9YF	C30-C31-C32-C33
23	L	609	CDL	C11-CA5-OA6-CA4
23	P	303	CDL	CA7-C31-C32-C33
23	H	1005	CDL	C1-CB2-OB2-PB2
23	K	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
23	N	603	CDL	C60-C61-C62-C63
20	b	201	9YF	C16-C17-C18-C19
17	C	304	WUO	C56-C57-C76-O77
20	G	503	9YF	C1-C-C24-O11
21	S	501	7PH	C1-C2-C3-O31
23	R	605	CDL	CA3-CA4-CA6-OA8
27	J	602	3PE	C1-C2-C3-O31
17	C	304	WUO	C21-C22-C23-C24
23	L	601	CDL	C31-C32-C33-C34
23	T	1302	CDL	C32-C31-CA7-OA8
20	M	503	9YF	C2-O2-P-O8
16	C	303	MQ9	C13-C14-C16-C17
17	C	304	WUO	C94-C95-C96-C97
23	N	603	CDL	C16-C17-C18-C19
23	T	1302	CDL	C53-C54-C55-C56
23	T	1302	CDL	CA2-OA2-PA1-OA5
23	I	301	CDL	CB2-OB2-PB2-OB5
23	L	609	CDL	CA2-OA2-PA1-OA5
23	R	605	CDL	C60-C61-C62-C63
23	R	605	CDL	C37-C38-C39-C40
23	L	609	CDL	C13-C14-C15-C16
23	P	301	CDL	OA5-CA3-CA4-OA6
23	R	601	CDL	OB5-CB3-CB4-OB6
23	H	1004	CDL	OB5-CB3-CB4-OB6
23	I	301	CDL	OB5-CB3-CB4-OB6
27	J	602	3PE	O11-C1-C2-O21
23	H	1005	CDL	C52-C53-C54-C55
23	I	302	CDL	C12-C13-C14-C15
25	b	202	9XX	C11-C12-C13-C14
23	N	604	CDL	C79-C80-C81-C82
23	N	603	CDL	C18-C19-C20-C21
23	P	301	CDL	C18-C19-C20-C21
23	R	601	CDL	C33-C34-C35-C36
23	G	506	CDL	C55-C56-C57-C58
20	W	201	9YF	O9-C-C24-O11
20	G	503	9YF	O9-C-C24-O11
21	S	501	7PH	O21-C2-C3-O31
23	N	602	CDL	OB6-CB4-CB6-OB8
23	N	603	CDL	OB6-CB4-CB6-OB8
23	T	1302	CDL	OA6-CA4-CA6-OA8
23	G	506	CDL	OB6-CB4-CB6-OB8
27	S	503	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
27	J	602	3PE	O21-C2-C3-O31
23	K	201	CDL	CA2-C1-CB2-OB2
28	R	602	HEA	C19-C20-C21-C22
23	P	303	CDL	C56-C57-C58-C59
20	W	201	9YF	C11-C12-C13-C14
23	N	604	CDL	C1-CA2-OA2-PA1
23	I	302	CDL	C1-CA2-OA2-PA1
23	K	201	CDL	CB4-CB3-OB5-PB2
23	H	1004	CDL	C37-C38-C39-C40
23	I	301	CDL	C32-C33-C34-C35
25	c	302	9XX	C11-C12-C13-C14
23	I	302	CDL	C34-C35-C36-C37
17	P	302	WUO	C88-C90-C91-C92
17	O	304	WUO	C61-C59-O58-C57
23	H	1003	CDL	C12-C13-C14-C15
23	H	1005	CDL	C15-C16-C17-C18
23	K	201	CDL	C75-C76-C77-C78
17	O	304	WUO	C93-C94-C95-C96
17	C	304	WUO	O55-C56-C57-C76
20	b	201	9YF	C24-C-C1-O
21	G	504	7PH	O31-C31-C32-C33
20	M	503	9YF	C35-C36-C37-C38
23	H	1005	CDL	C53-C54-C55-C56
19	G	502	IZL	C54-C55-C56-C58
17	P	302	WUO	C91-C92-C93-C94
25	W	202	9XX	C19-C20-C21-C22
23	N	603	CDL	C59-C60-C61-C62
23	P	301	CDL	C31-C32-C33-C34
19	M	502	IZL	C48-C49-C50-C51
23	P	301	CDL	C53-C54-C55-C56
23	H	1005	CDL	C72-C73-C74-C75
20	G	503	9YF	C10-C11-C12-C13
21	S	501	7PH	C1-O11-P-O13
32	H	1008	DCQ	C10-C11-C12-C13
17	C	304	WUO	C80-C81-C82-C83
17	C	304	WUO	C93-C94-C95-C96
21	S	501	7PH	C32-C31-O31-C3
23	N	602	CDL	C31-CA7-OA8-CA6
17	P	302	WUO	C67-C68-C69-C70
23	N	603	CDL	C14-C15-C16-C17
17	O	304	WUO	C59-C61-C62-C63
20	M	503	9YF	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	K	201	CDL	C77-C78-C79-C80
25	W	202	9XX	C22-C23-C24-C25
23	K	201	CDL	C72-C73-C74-C75
21	M	504	7PH	C3-C2-O21-C21
21	G	504	7PH	C3-C2-O21-C21
23	L	609	CDL	OA7-CA5-OA6-CA4
23	P	301	CDL	C73-C74-C75-C76
23	L	609	CDL	C36-C37-C38-C39
23	H	1005	CDL	C71-C72-C73-C74
17	C	304	WUO	C92-C93-C94-C95
21	H	1001	7PH	C1-C2-C3-O31
23	N	604	CDL	C1-CB2-OB2-PB2
23	H	1003	CDL	C1-CA2-OA2-PA1
23	N	602	CDL	C73-C74-C75-C76
23	N	602	CDL	OA5-CA3-CA4-OA6
23	H	1003	CDL	OA5-CA3-CA4-OA6
27	S	503	3PE	O11-C1-C2-O21
22	H	1002	HEM	C4C-C3C-CAC-CBC
21	S	501	7PH	C33-C34-C35-C36
23	I	301	CDL	C34-C35-C36-C37
23	G	506	CDL	CA2-C1-CB2-OB2
17	O	304	WUO	O60-C59-O58-C57
20	W	201	9YF	O12-C25-O11-C24
23	N	602	CDL	C79-C80-C81-C82
23	L	601	CDL	C11-C12-C13-C14
17	P	302	WUO	O58-C57-C76-O77
23	L	601	CDL	OA6-CA4-CA6-OA8
21	G	505	7PH	C34-C35-C36-C37
23	T	1302	CDL	C34-C35-C36-C37
23	H	1004	CDL	C36-C37-C38-C39
20	G	503	9YF	C27-C28-C29-C30
23	N	603	CDL	C35-C36-C37-C38
23	H	1004	CDL	C18-C19-C20-C21
21	S	501	7PH	O32-C31-O31-C3
23	N	602	CDL	OA9-CA7-OA8-CA6
19	M	502	IZL	C62-C63-C64-C65
23	G	506	CDL	C31-C32-C33-C34
23	P	301	CDL	CA5-C11-C12-C13
23	R	601	CDL	C11-CA5-OA6-CA4
23	P	301	CDL	C58-C59-C60-C61
23	N	603	CDL	CA3-OA5-PA1-OA2
23	P	303	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
23	G	506	CDL	CB3-OB5-PB2-OB2
23	I	301	CDL	CA2-OA2-PA1-OA5
23	P	303	CDL	C15-C16-C17-C18
23	N	602	CDL	C1-CB2-OB2-PB2
23	R	601	CDL	CB4-CB3-OB5-PB2
16	H	1006	MQ9	C23-C24-C26-C27
23	R	605	CDL	C55-C56-C57-C58
16	N	607	MQ9	C6-C7-C8-C9
17	C	304	WUO	C56-O55-P52-O53
17	C	304	WUO	C56-O55-P52-O54
19	M	502	IZL	C44-O31-P-O29
19	G	502	IZL	C44-O31-P-O29
19	G	502	IZL	C44-O31-P-O30
20	G	503	9YF	C1-O-P-O8
20	b	201	9YF	C1-O-P-O1
23	N	602	CDL	CA3-OA5-PA1-OA3
23	N	602	CDL	CB3-OB5-PB2-OB3
23	N	602	CDL	CB3-OB5-PB2-OB4
23	N	603	CDL	CA3-OA5-PA1-OA4
23	P	301	CDL	CA2-OA2-PA1-OA4
23	P	301	CDL	CB2-OB2-PB2-OB3
23	P	301	CDL	CB2-OB2-PB2-OB4
23	P	301	CDL	CB3-OB5-PB2-OB3
23	P	303	CDL	CA2-OA2-PA1-OA3
23	P	303	CDL	CB3-OB5-PB2-OB4
23	T	1302	CDL	CA2-OA2-PA1-OA3
23	T	1302	CDL	CA3-OA5-PA1-OA3
23	T	1302	CDL	CA3-OA5-PA1-OA4
23	T	1302	CDL	CB2-OB2-PB2-OB4
23	T	1302	CDL	CB3-OB5-PB2-OB3
23	T	1302	CDL	CB3-OB5-PB2-OB4
23	R	601	CDL	CA2-OA2-PA1-OA3
23	R	601	CDL	CA3-OA5-PA1-OA4
23	R	601	CDL	CB3-OB5-PB2-OB3
23	R	605	CDL	CA3-OA5-PA1-OA4
23	G	506	CDL	CA3-OA5-PA1-OA3
23	G	506	CDL	CA3-OA5-PA1-OA4
23	G	506	CDL	CB3-OB5-PB2-OB3
23	G	506	CDL	CB3-OB5-PB2-OB4
23	H	1003	CDL	CA3-OA5-PA1-OA3
23	H	1003	CDL	CB2-OB2-PB2-OB3
23	H	1004	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
23	H	1004	CDL	CA3-OA5-PA1-OA4
23	H	1005	CDL	CA3-OA5-PA1-OA3
23	H	1005	CDL	CB3-OB5-PB2-OB4
23	I	301	CDL	CA2-OA2-PA1-OA3
23	I	301	CDL	CB2-OB2-PB2-OB4
23	I	302	CDL	CA3-OA5-PA1-OA3
23	K	201	CDL	CA3-OA5-PA1-OA3
23	K	201	CDL	CB3-OB5-PB2-OB4
23	L	601	CDL	CA3-OA5-PA1-OA4
23	L	601	CDL	CB2-OB2-PB2-OB3
23	L	609	CDL	CA2-OA2-PA1-OA3
23	L	609	CDL	CA3-OA5-PA1-OA3
23	L	609	CDL	CA3-OA5-PA1-OA4
23	L	609	CDL	CB2-OB2-PB2-OB3
27	J	602	3PE	C1-O11-P-O12
23	R	601	CDL	OA5-CA3-CA4-CA6
23	H	1005	CDL	OA5-CA3-CA4-CA6
23	L	609	CDL	OA5-CA3-CA4-CA6
23	L	609	CDL	OB5-CB3-CB4-CB6
16	C	305	MQ9	C9-C11-C12-C13
17	O	304	WUO	C66-C67-C68-C69
19	G	502	IZL	C51-C52-C53-C54
23	R	601	CDL	C32-C31-CA7-OA8
20	b	201	9YF	C37-C38-C39-C40
21	H	1001	7PH	C32-C33-C34-C35
25	b	202	9XX	C12-C13-C14-C15
23	K	201	CDL	C72-C71-CB7-OB8
23	R	601	CDL	OA7-CA5-OA6-CA4
23	N	604	CDL	C23-C24-C25-C26
16	H	1006	MQ9	C40-C39-C41-C42
17	O	304	WUO	C87-C88-C90-C91
17	C	304	WUO	O55-C56-C57-O58
17	C	304	WUO	C86-C87-C88-C90
19	M	502	IZL	C54-C55-C56-C58
20	b	201	9YF	C32-C33-C35-C36
23	N	602	CDL	OB5-CB3-CB4-OB6
23	P	301	CDL	OB5-CB3-CB4-OB6
23	R	601	CDL	OA5-CA3-CA4-OA6
23	L	609	CDL	OB5-CB3-CB4-OB6
23	R	605	CDL	C53-C54-C55-C56
23	P	301	CDL	C12-C11-CA5-OA6
20	b	201	9YF	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	I	302	CDL	C11-CA5-OA6-CA4
23	N	602	CDL	C32-C33-C34-C35
23	R	601	CDL	C16-C17-C18-C19
23	K	201	CDL	C71-C72-C73-C74
23	G	506	CDL	O1-C1-CB2-OB2
23	I	301	CDL	C59-C60-C61-C62
23	L	601	CDL	C16-C17-C18-C19
23	N	604	CDL	CA3-CA4-CA6-OA8
23	R	601	CDL	CB3-CB4-CB6-OB8
23	G	506	CDL	CB3-CB4-CB6-OB8
23	I	301	CDL	CA3-CA4-CA6-OA8
23	L	609	CDL	CB3-CB4-CB6-OB8
28	R	603	HEA	C4A-C3A-CMA-OMA
28	R	603	HEA	O11-C11-C3B-C4B
28	L	603	HEA	O11-C11-C3B-C4B
23	I	302	CDL	OA7-CA5-OA6-CA4
19	G	502	IZL	O34-C45-C46-O32
20	b	201	9YF	O9-C-C24-O11
21	H	1001	7PH	O21-C2-C3-O31
23	N	604	CDL	OA6-CA4-CA6-OA8
23	T	1302	CDL	OB6-CB4-CB6-OB8
23	R	601	CDL	OB6-CB4-CB6-OB8
23	G	506	CDL	OA6-CA4-CA6-OA8
23	H	1004	CDL	OA6-CA4-CA6-OA8
23	I	302	CDL	OB6-CB4-CB6-OB8
23	K	201	CDL	OB6-CB4-CB6-OB8
23	L	609	CDL	OB6-CB4-CB6-OB8
23	L	609	CDL	C12-C13-C14-C15
17	P	302	WUO	C68-C69-C70-C71
16	N	607	MQ9	C5-C6-C7-C8
19	M	502	IZL	C23-C24-O11-C25
21	M	504	7PH	O31-C31-C32-C33
21	H	1001	7PH	C31-C32-C33-C34
21	G	505	7PH	C38-C39-C3A-C3B
25	W	202	9XX	C25-C26-C27-C36
23	R	601	CDL	C57-C58-C59-C60
16	N	605	MQ9	C44-C46-C47-C48
20	G	503	9YF	C19-C20-C21-C22
23	H	1004	CDL	C17-C18-C19-C20
23	L	601	CDL	C72-C71-CB7-OB8
17	P	302	WUO	C23-C24-C25-C26
17	C	304	WUO	O40-C41-C48-O49

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Mol	Chain	Res	Type	Atoms
28	R	602	HEA	C2C-C3C-CAC-CBC
28	L	602	HEA	C2C-C3C-CAC-CBC
23	N	604	CDL	C71-C72-C73-C74
23	N	604	CDL	C78-C79-C80-C81
23	N	603	CDL	C32-C31-CA7-OA8
20	W	201	9YF	C19-C20-C21-C22
23	P	303	CDL	C31-C32-C33-C34
28	R	603	HEA	C18-C19-C20-C21
23	P	303	CDL	C33-C34-C35-C36
23	G	506	CDL	C72-C73-C74-C75
23	L	609	CDL	C53-C54-C55-C56
17	O	304	WUO	C31-C01-O02-C03
23	P	301	CDL	C55-C56-C57-C58
17	O	304	WUO	C81-C82-C83-C84
19	M	502	IZL	C68-C69-C70-C74
23	N	602	CDL	C56-C57-C58-C59
21	H	1001	7PH	C3-C2-O21-C21
19	M	502	IZL	O31-C44-C45-C46
23	I	301	CDL	C74-C75-C76-C77
17	I	303	WUO	C59-C61-C62-C63
23	P	303	CDL	C32-C33-C34-C35
23	H	1005	CDL	C32-C31-CA7-OA8
24	L	610	PLM	C3-C4-C5-C6
23	R	605	CDL	OA5-CA3-CA4-OA6
23	H	1005	CDL	OA5-CA3-CA4-OA6
23	L	609	CDL	OA5-CA3-CA4-OA6
16	C	305	MQ9	C15-C14-C16-C17
21	M	504	7PH	C21-C22-C23-C24
23	N	604	CDL	C58-C59-C60-C61
23	T	1302	CDL	C83-C84-C85-C86
16	O	303	MQ9	C29-C31-C32-C33
23	H	1003	CDL	OB6-CB4-CB6-OB8
23	H	1004	CDL	OB6-CB4-CB6-OB8
23	N	603	CDL	C15-C16-C17-C18
23	R	605	CDL	C58-C59-C60-C61
23	R	605	CDL	C75-C76-C77-C78
23	H	1004	CDL	CA2-OA2-PA1-OA5
23	R	605	CDL	C52-C53-C54-C55
20	G	503	9YF	C7-C2-O2-P
23	H	1003	CDL	C58-C59-C60-C61
23	I	301	CDL	C58-C59-C60-C61
23	K	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
23	I	301	CDL	C76-C77-C78-C79
19	G	502	IZL	C44-C45-C46-O32
20	b	201	9YF	C2-O2-P-O
23	H	1003	CDL	C32-C31-CA7-OA8
23	L	601	CDL	C54-C55-C56-C57
20	b	201	9YF	C34-C33-C35-C36
20	G	503	9YF	C20-C21-C22-C23
23	R	605	CDL	C52-C51-CB5-OB7
23	R	605	CDL	C14-C15-C16-C17
24	L	610	PLM	C4-C5-C6-C7
20	b	201	9YF	C-C1-O-P
23	N	604	CDL	CA4-CA3-OA5-PA1
17	C	304	WUO	C26-C27-C28-C29
23	L	609	CDL	C73-C74-C75-C76
25	b	202	9XX	C9-C10-C11-C12
23	K	201	CDL	CB2-C1-CA2-OA2
16	C	303	MQ9	C30-C29-C31-C32
20	W	201	9YF	C25-C26-C27-C28
23	R	601	CDL	C52-C51-CB5-OB6
23	L	601	CDL	C12-C13-C14-C15
17	C	304	WUO	C16-C14-O13-C12
28	L	602	HEA	C4C-C3C-CAC-CBC
28	L	603	HEA	CAA-CBA-CGA-O1A
23	L	601	CDL	C78-C79-C80-C81
23	L	609	CDL	C51-C52-C53-C54
17	I	303	WUO	O55-C56-C57-C76
16	O	303	MQ9	C14-C16-C17-C18
16	N	605	MQ9	C24-C26-C27-C28
23	R	601	CDL	C55-C56-C57-C58
23	I	301	CDL	C31-C32-C33-C34
16	C	305	MQ9	C25-C24-C26-C27
23	H	1004	CDL	C60-C61-C62-C63
28	R	602	HEA	CAA-CBA-CGA-O1A
20	G	503	9YF	C12-C13-C14-C15
27	S	503	3PE	C23-C24-C25-C26
17	P	302	WUO	C80-C81-C82-C83
23	P	303	CDL	C52-C53-C54-C55
22	H	1007	HEM	CAA-CBA-CGA-O1A
23	R	605	CDL	OB6-CB4-CB6-OB8
23	G	506	CDL	C17-C18-C19-C20
19	G	502	IZL	C49-C50-C51-C52
23	I	302	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
23	N	603	CDL	CA4-CA3-OA5-PA1
23	G	506	CDL	C1-CB2-OB2-PB2
25	W	202	9XX	C5-C6-C7-C8
20	G	503	9YF	C2-O2-P-O
23	T	1302	CDL	C79-C80-C81-C82
17	P	302	WUO	C81-C82-C83-C84
17	O	304	WUO	C68-C69-C70-C71
17	C	304	WUO	C16-C17-C18-C19
15	O	301	HEC	CAD-CBD-CGD-O2D
15	C	301	HEC	CAD-CBD-CGD-O2D
28	L	602	HEA	CAD-CBD-CGD-O2D
26	R	609	TRD	C3-C4-C5-C6
28	L	602	HEA	C18-C19-C20-C21
17	P	302	WUO	C89-C88-C90-C91
17	I	303	WUO	C89-C88-C90-C91
23	I	301	CDL	C13-C14-C15-C16
15	O	302	HEC	CAA-CBA-CGA-O2A
15	C	302	HEC	CAA-CBA-CGA-O2A
28	R	602	HEA	CAD-CBD-CGD-O1D
17	P	302	WUO	C26-C27-C28-C29
17	C	304	WUO	C63-C64-C65-C66
17	I	303	WUO	C25-C26-C27-C28
23	K	201	CDL	C83-C84-C85-C86
23	N	603	CDL	CA2-C1-CB2-OB2
22	N	606	HEM	CAA-CBA-CGA-O1A
17	C	304	WUO	C31-C01-O02-C03
23	K	201	CDL	C35-C36-C37-C38
28	L	602	HEA	CAD-CBD-CGD-O1D
23	T	1302	CDL	C58-C59-C60-C61
19	M	502	IZL	O17-C31-O16-C30
23	I	302	CDL	CA5-C11-C12-C13
25	W	202	9XX	C31-C32-C33-C34
28	R	603	HEA	CAD-CBD-CGD-O1D
28	L	603	HEA	CAA-CBA-CGA-O2A
19	M	502	IZL	C46-C45-O34-C60
20	G	503	9YF	C1-C-O9-C8
23	R	605	CDL	CA6-CA4-OA6-CA5
16	H	1006	MQ9	C15-C14-C16-C17
23	R	605	CDL	C32-C31-CA7-OA9
23	N	602	CDL	OB7-CB5-OB6-CB4
17	I	303	WUO	C86-C87-C88-C90
21	S	501	7PH	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
19	G	502	IZL	C3-C4-C5-C6
23	L	609	CDL	C31-C32-C33-C34
20	G	503	9YF	C26-C27-C28-C29
23	N	602	CDL	C19-C20-C21-C22
28	R	603	HEA	CAA-CBA-CGA-O1A
17	C	304	WUO	O15-C14-O13-C12
23	T	1302	CDL	OB5-CB3-CB4-OB6
23	N	602	CDL	C32-C31-CA7-OA8
17	C	304	WUO	C42-C41-C48-O49
28	R	603	HEA	CAA-CBA-CGA-O2A
20	b	201	9YF	C40-C41-C42-C43
25	W	202	9XX	C11-C10-C9-C8
23	N	602	CDL	OA5-CA3-CA4-CA6
23	P	303	CDL	C55-C56-C57-C58
23	G	506	CDL	C83-C84-C85-C86
22	N	606	HEM	CAA-CBA-CGA-O2A
22	H	1007	HEM	CAA-CBA-CGA-O2A
28	R	602	HEA	CAA-CBA-CGA-O2A
20	b	201	9YF	C19-C20-C21-C22
17	C	304	WUO	C06-C05-C12-O13
16	N	605	MQ9	C12-C11-C9-C10
19	M	502	IZL	C2-C1-C7-C8
23	P	303	CDL	C36-C37-C38-C39
19	M	502	IZL	C36-C31-O16-C30
22	N	606	HEM	CAD-CBD-CGD-O2D
15	O	301	HEC	CAD-CBD-CGD-O1D
15	C	301	HEC	CAD-CBD-CGD-O1D
23	L	609	CDL	C33-C34-C35-C36
26	T	1303	TRD	C5-C6-C7-C8
16	N	607	MQ9	C29-C31-C32-C33
16	H	1006	MQ9	C39-C41-C42-C43
23	I	301	CDL	C36-C37-C38-C39
16	C	303	MQ9	C28-C29-C31-C32
28	R	602	HEA	CAD-CBD-CGD-O2D
28	R	603	HEA	CAD-CBD-CGD-O2D
23	N	602	CDL	C58-C59-C60-C61
23	H	1004	CDL	C13-C14-C15-C16
23	P	303	CDL	C1-CB2-OB2-PB2
23	T	1302	CDL	C72-C71-CB7-OB8
25	W	202	9XX	C-C1-C2-C3
23	P	301	CDL	C52-C51-CB5-OB7
23	L	601	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
21	M	504	7PH	C25-C26-C27-C28
23	H	1004	CDL	C59-C60-C61-C62
23	I	302	CDL	C53-C54-C55-C56
23	N	603	CDL	C53-C54-C55-C56
16	O	303	MQ9	C45-C44-C46-C47
28	L	602	HEA	C27-C19-C20-C21
23	T	1302	CDL	C54-C55-C56-C57
23	L	609	CDL	C55-C56-C57-C58
16	C	305	MQ9	C13-C14-C16-C17
22	N	606	HEM	CAD-CBD-CGD-O1D
19	G	502	IZL	C23-C24-O11-C25
17	O	304	WUO	C50-C01-O02-C03
23	K	201	CDL	C33-C34-C35-C36
23	H	1005	CDL	C12-C11-CA5-OA6
32	H	1008	DCQ	C7-C8-C9-C10
19	M	502	IZL	O8-C20-C21-O9
24	W	203	PLM	C6-C7-C8-C9
23	H	1004	CDL	C38-C39-C40-C41
23	I	302	CDL	C31-C32-C33-C34
25	W	202	9XX	C21-C22-C23-C24
23	T	1302	CDL	OB5-CB3-CB4-CB6
16	O	303	MQ9	C30-C29-C31-C32
16	T	1301	MQ9	C25-C24-C26-C27
28	L	602	HEA	C26-C15-C16-C17
23	R	605	CDL	C35-C36-C37-C38
16	H	1006	MQ9	C13-C14-C16-C17
15	O	302	HEC	CAA-CBA-CGA-O1A
15	C	302	HEC	CAA-CBA-CGA-O1A
20	M	503	9YF	C26-C27-C28-C29
23	H	1005	CDL	C78-C79-C80-C81
23	T	1302	CDL	C32-C31-CA7-OA9
20	G	503	9YF	C36-C37-C38-C39
17	P	302	WUO	O13-C14-C16-C17
17	C	304	WUO	C70-C71-C72-C73
20	W	201	9YF	C18-C19-C20-C21
23	K	201	CDL	C32-C33-C34-C35
23	L	609	CDL	C35-C36-C37-C38
25	W	202	9XX	C3-C4-C5-C6
23	L	601	CDL	C73-C74-C75-C76
19	G	502	IZL	O32-C47-C48-C49
16	N	605	MQ9	C25-C24-C26-C27
23	P	303	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	L	609	CDL	C12-C11-CA5-OA6
23	N	604	CDL	C15-C16-C17-C18
20	G	503	9YF	C24-C-O9-C8
23	R	605	CDL	CA3-CA4-OA6-CA5
28	L	602	HEA	C11-C12-C13-C14
26	J	601	TRD	C6-C7-C8-C9
23	R	601	CDL	C12-C11-CA5-OA6
23	N	603	CDL	C13-C14-C15-C16
16	T	1301	MQ9	C15-C14-C16-C17
17	C	304	WUO	C71-C72-C73-C74
16	N	605	MQ9	C12-C11-C9-C8
23	K	201	CDL	C12-C11-CA5-OA6
23	L	609	CDL	C72-C71-CB7-OB8
23	H	1004	CDL	C12-C13-C14-C15
23	L	609	CDL	C58-C59-C60-C61
19	M	502	IZL	C44-C45-C46-O32
23	R	605	CDL	CB3-CB4-CB6-OB8
23	H	1004	CDL	CB3-CB4-CB6-OB8
17	P	302	WUO	C31-C01-O02-C03
23	N	603	CDL	OB5-CB3-CB4-OB6
23	P	303	CDL	OA5-CA3-CA4-OA6
21	G	505	7PH	O21-C21-C22-C23
23	N	602	CDL	C80-C81-C82-C83
23	N	602	CDL	C12-C13-C14-C15
21	G	505	7PH	C36-C37-C38-C39
23	P	301	CDL	C72-C71-CB7-OB8
25	N	609	9XX	C13-C14-C15-O
28	L	602	HEA	CAA-CBA-CGA-O2A
23	K	201	CDL	O1-C1-CB2-OB2
23	I	301	CDL	C39-C40-C41-C42
23	I	302	CDL	C60-C61-C62-C63
28	L	602	HEA	CAA-CBA-CGA-O1A
17	O	304	WUO	O58-C59-C61-C62
16	O	303	MQ9	C43-C44-C46-C47
23	H	1003	CDL	C19-C20-C21-C22
25	c	302	9XX	C22-C23-C24-C25
23	R	605	CDL	OA5-CA3-CA4-CA6
23	I	302	CDL	OA5-CA3-CA4-CA6
15	O	301	HEC	CAA-CBA-CGA-O1A
15	C	301	HEC	CAA-CBA-CGA-O1A
17	C	304	WUO	C81-C82-C83-C84
23	G	506	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	T	1302	CDL	C75-C76-C77-C78
27	S	503	3PE	C24-C25-C26-C27
23	L	601	CDL	OB9-CB7-OB8-CB6
20	G	503	9YF	O11-C25-C26-C27
17	O	304	WUO	C63-C64-C65-C66
23	N	603	CDL	C31-C32-C33-C34
23	L	601	CDL	C71-CB7-OB8-CB6
20	M	503	9YF	O9-C8-C9-C10
20	W	201	9YF	C36-C37-C38-C39
20	b	201	9YF	C36-C37-C38-C39
16	H	1006	MQ9	C38-C39-C41-C42
23	T	1302	CDL	C35-C36-C37-C38
23	L	609	CDL	C32-C31-CA7-OA8
25	W	202	9XX	C11-C12-C13-C14
23	N	604	CDL	C33-C34-C35-C36
32	H	1008	DCQ	C2-C3-O3-C3M
23	N	602	CDL	C51-CB5-OB6-CB4
16	C	303	MQ9	C36-C37-C38-C39
23	L	609	CDL	C12-C11-CA5-OA7
23	R	601	CDL	C37-C38-C39-C40
22	H	1002	HEM	C3D-CAD-CBD-CGD
17	P	302	WUO	O15-C14-C16-C17
23	L	601	CDL	C77-C78-C79-C80
21	G	504	7PH	C27-C28-C29-C2A
17	P	302	WUO	C50-O51-P52-O55
19	G	502	IZL	C43-O28-P-O31
16	O	303	MQ9	C31-C32-C33-C34
16	N	605	MQ9	C21-C22-C23-C24
17	O	304	WUO	O60-C59-C61-C62
19	G	502	IZL	O33-C47-C48-C49
23	K	201	CDL	C12-C11-CA5-OA7
23	P	303	CDL	C52-C51-CB5-OB6
23	T	1302	CDL	C12-C11-CA5-OA6
23	P	301	CDL	CA2-OA2-PA1-OA5
23	R	601	CDL	C72-C71-CB7-OB8
20	G	503	9YF	O12-C25-C26-C27
23	L	609	CDL	C72-C71-CB7-OB9
15	O	302	HEC	CAD-CBD-CGD-O2D
15	C	302	HEC	CAD-CBD-CGD-O2D
20	M	503	9YF	C1-O-P-O1
23	R	601	CDL	CA3-OA5-PA1-OA3
23	L	601	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
27	S	503	3PE	C11-O13-P-O14
27	J	602	3PE	C11-O13-P-O14
25	N	609	9XX	C13-C14-C15-O6
17	O	304	WUO	O55-C56-C57-C76
15	O	301	HEC	CAA-CBA-CGA-O2A
15	C	301	HEC	CAA-CBA-CGA-O2A
17	I	303	WUO	C68-C69-C70-C71
23	R	601	CDL	C12-C11-CA5-OA7
17	I	303	WUO	C31-C01-O02-C03
25	W	202	9XX	C13-C14-C15-O
27	S	503	3PE	O31-C31-C32-C33
21	G	504	7PH	O32-C31-C32-C33
21	G	505	7PH	O22-C21-C22-C23
28	L	603	HEA	C3B-C11-C12-C13
20	M	503	9YF	O10-C8-C9-C10
23	I	302	CDL	C71-C72-C73-C74
17	O	304	WUO	C06-C05-C12-O13
23	N	603	CDL	O1-C1-CB2-OB2
23	N	604	CDL	C32-C31-CA7-OA8
23	P	303	CDL	C72-C71-CB7-OB8
23	H	1005	CDL	C72-C71-CB7-OB8
23	I	301	CDL	C32-C31-CA7-OA8
23	L	601	CDL	C84-C85-C86-C87
17	I	303	WUO	C80-C81-C82-C83
23	L	609	CDL	C32-C31-CA7-OA9
26	T	1303	TRD	C6-C7-C8-C9
23	N	603	CDL	C52-C51-CB5-OB6
23	P	301	CDL	C32-C31-CA7-OA8
23	G	506	CDL	C52-C51-CB5-OB6
25	c	302	9XX	C13-C14-C15-O
23	H	1005	CDL	C33-C34-C35-C36
17	I	303	WUO	C57-C56-O55-P52
16	C	305	MQ9	C23-C24-C26-C27
17	P	302	WUO	C86-C87-C88-C90
23	P	301	CDL	C72-C71-CB7-OB9
22	H	1002	HEM	CAA-CBA-CGA-O2A
22	H	1007	HEM	CAD-CBD-CGD-O2D
23	H	1004	CDL	C32-C31-CA7-OA8
15	O	302	HEC	C4C-C3C-CAC-CBC
15	C	302	HEC	C4C-C3C-CAC-CBC
21	G	505	7PH	C22-C23-C24-C25
23	N	603	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	I	302	CDL	C75-C76-C77-C78
23	G	506	CDL	C33-C34-C35-C36
23	N	603	CDL	C52-C51-CB5-OB7
23	P	303	CDL	C52-C51-CB5-OB7
23	T	1302	CDL	C12-C11-CA5-OA7
23	R	601	CDL	C72-C71-CB7-OB9
23	G	506	CDL	C52-C51-CB5-OB7
23	H	1005	CDL	C72-C71-CB7-OB9
26	S	502	TRD	C7-C8-C9-C10
17	C	304	WUO	O58-C59-C61-C62
23	I	301	CDL	C72-C71-CB7-OB8
19	G	502	IZL	C7-C1-C2-C3
19	G	502	IZL	O12-C25-O11-C24
23	P	301	CDL	C39-C40-C41-C42
23	P	301	CDL	C32-C31-CA7-OA9
23	P	303	CDL	C72-C71-CB7-OB9
25	c	302	9XX	C13-C14-C15-O6
16	N	607	MQ9	C44-C46-C47-C48
16	H	1006	MQ9	C44-C46-C47-C48
21	G	505	7PH	C32-C33-C34-C35
23	N	604	CDL	C32-C31-CA7-OA9
23	I	301	CDL	C32-C31-CA7-OA9
25	W	202	9XX	C13-C14-C15-O6
25	W	202	9XX	C27-C28-C29-C30

There are no ring outliers.

41 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	O	303	MQ9	3	0
15	O	302	HEC	4	0
23	G	506	CDL	1	0
23	H	1003	CDL	1	0
15	C	302	HEC	5	0
23	I	302	CDL	2	0
28	L	602	HEA	10	0
21	H	1001	7PH	1	0
23	H	1005	CDL	5	0
23	L	601	CDL	3	0
21	S	501	7PH	2	0
22	N	601	HEM	3	0
24	N	608	PLM	1	0

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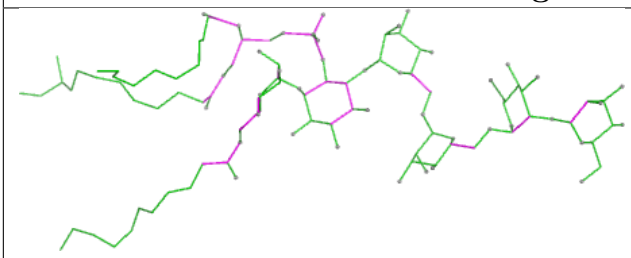
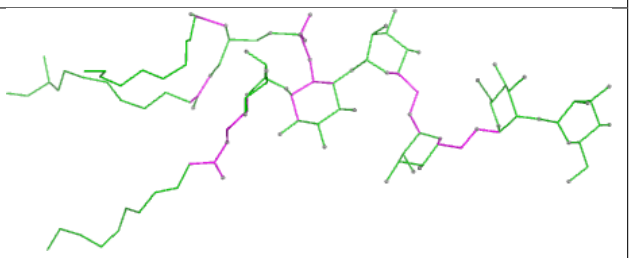
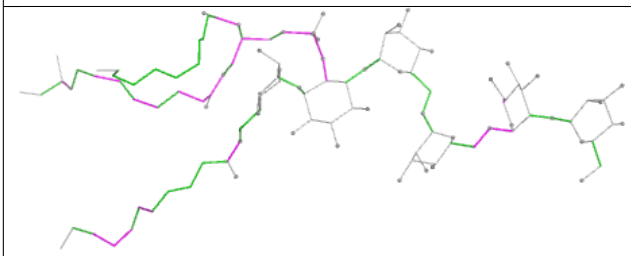
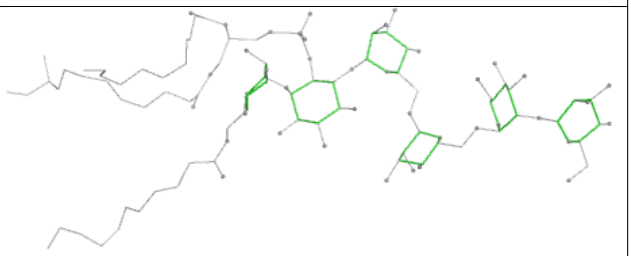
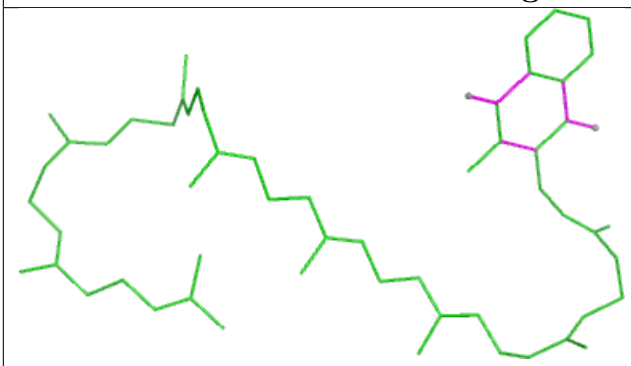
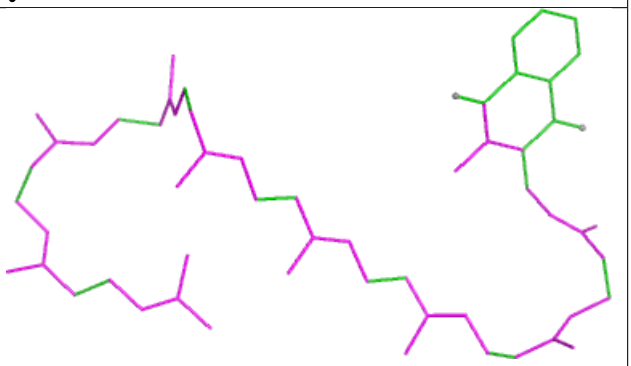
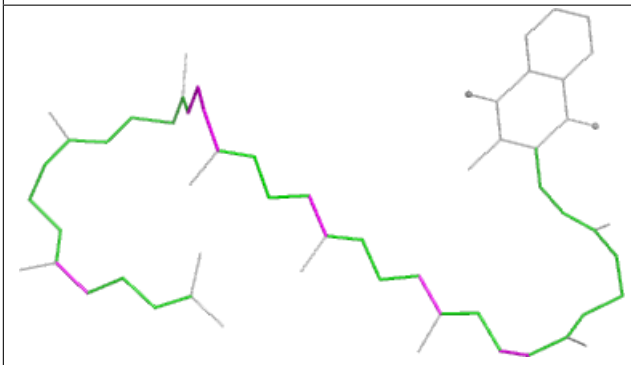
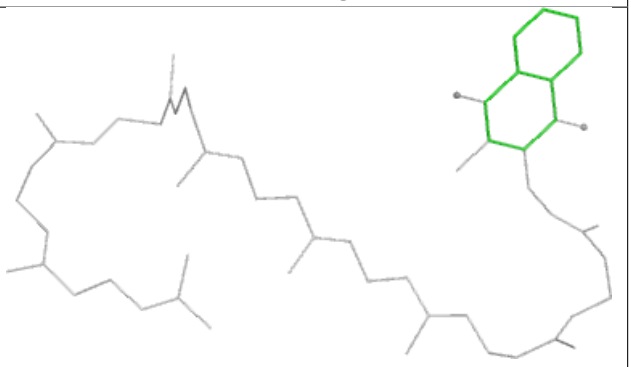
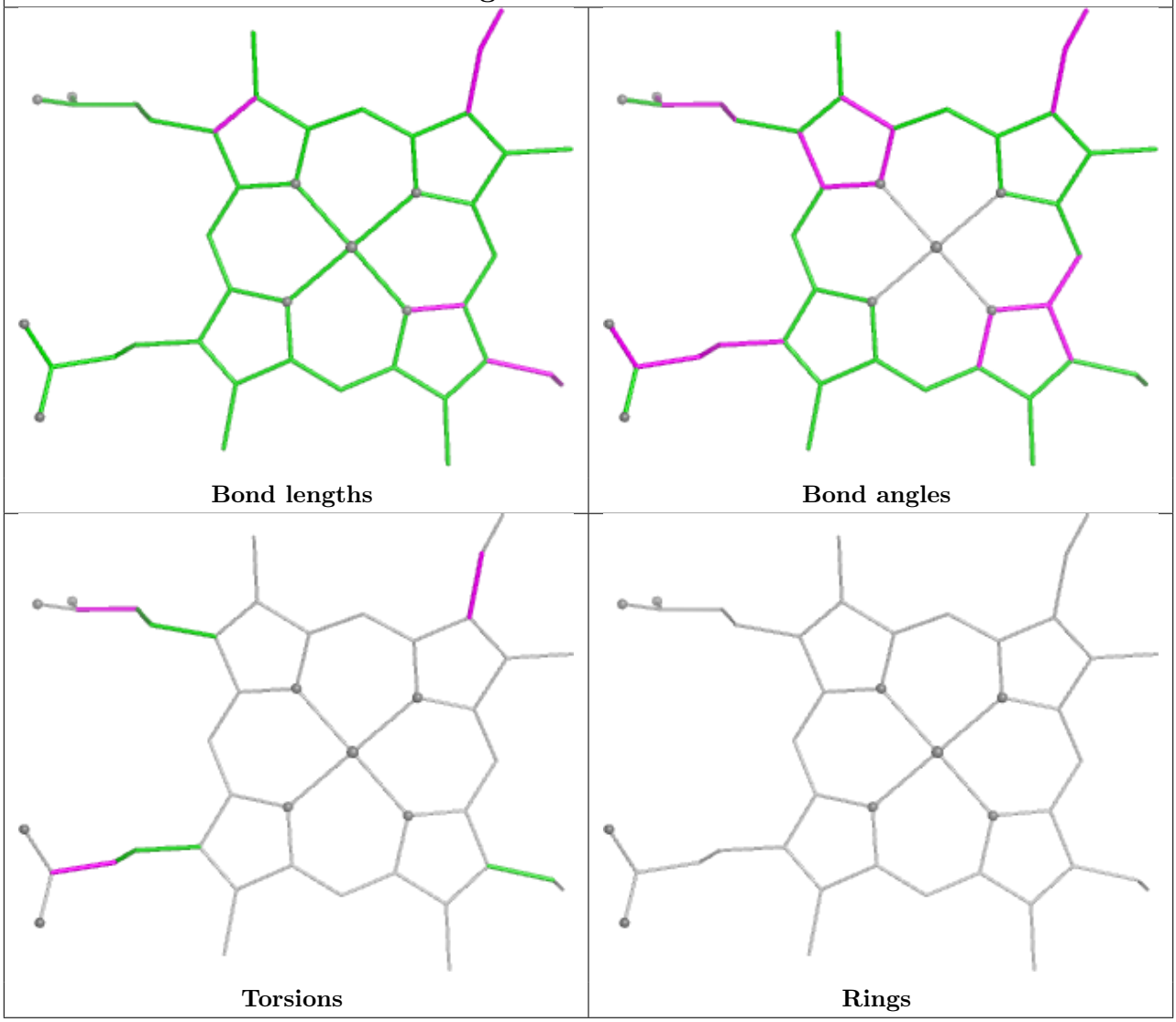
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Q	403	TRD	1	0
16	C	305	MQ9	3	0
23	L	609	CDL	3	0
23	I	301	CDL	5	0
23	T	1302	CDL	5	0
23	P	303	CDL	7	0
16	N	605	MQ9	3	0
16	C	303	MQ9	1	0
16	T	1301	MQ9	7	0
22	N	606	HEM	2	0
15	C	301	HEC	1	0
23	P	301	CDL	6	0
21	M	504	7PH	3	0
28	L	603	HEA	2	0
22	H	1002	HEM	2	0
23	H	1004	CDL	1	0
23	R	605	CDL	4	0
22	H	1007	HEM	4	0
28	R	602	HEA	7	0
16	N	607	MQ9	5	0
21	G	504	7PH	3	0
23	N	604	CDL	5	0
23	K	201	CDL	2	0
28	R	603	HEA	31	0
23	R	601	CDL	2	0
23	N	603	CDL	5	0
26	J	601	TRD	1	0
16	H	1006	MQ9	10	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 IZL G 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 O 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC O 302



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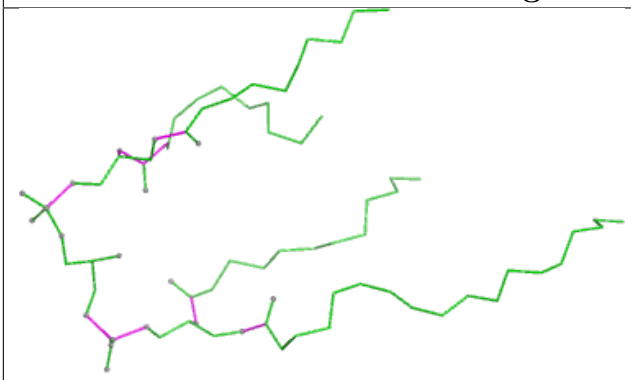
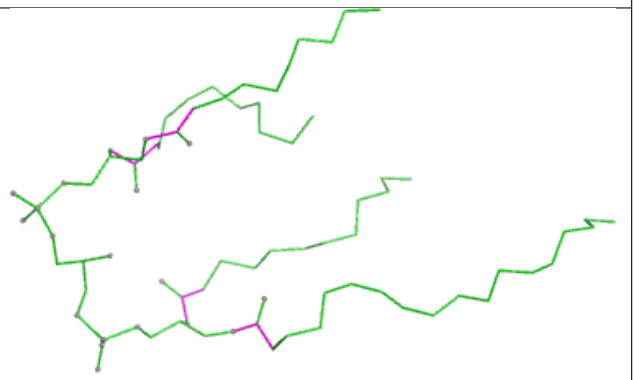
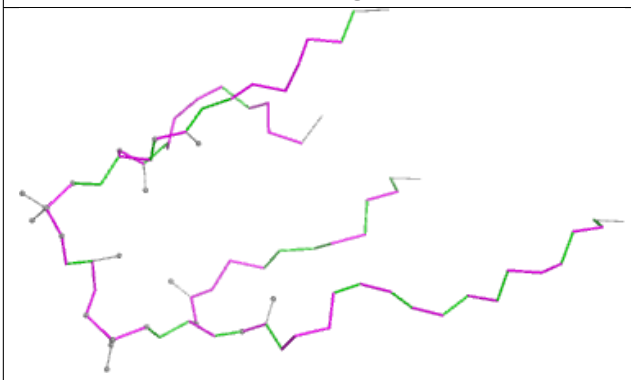
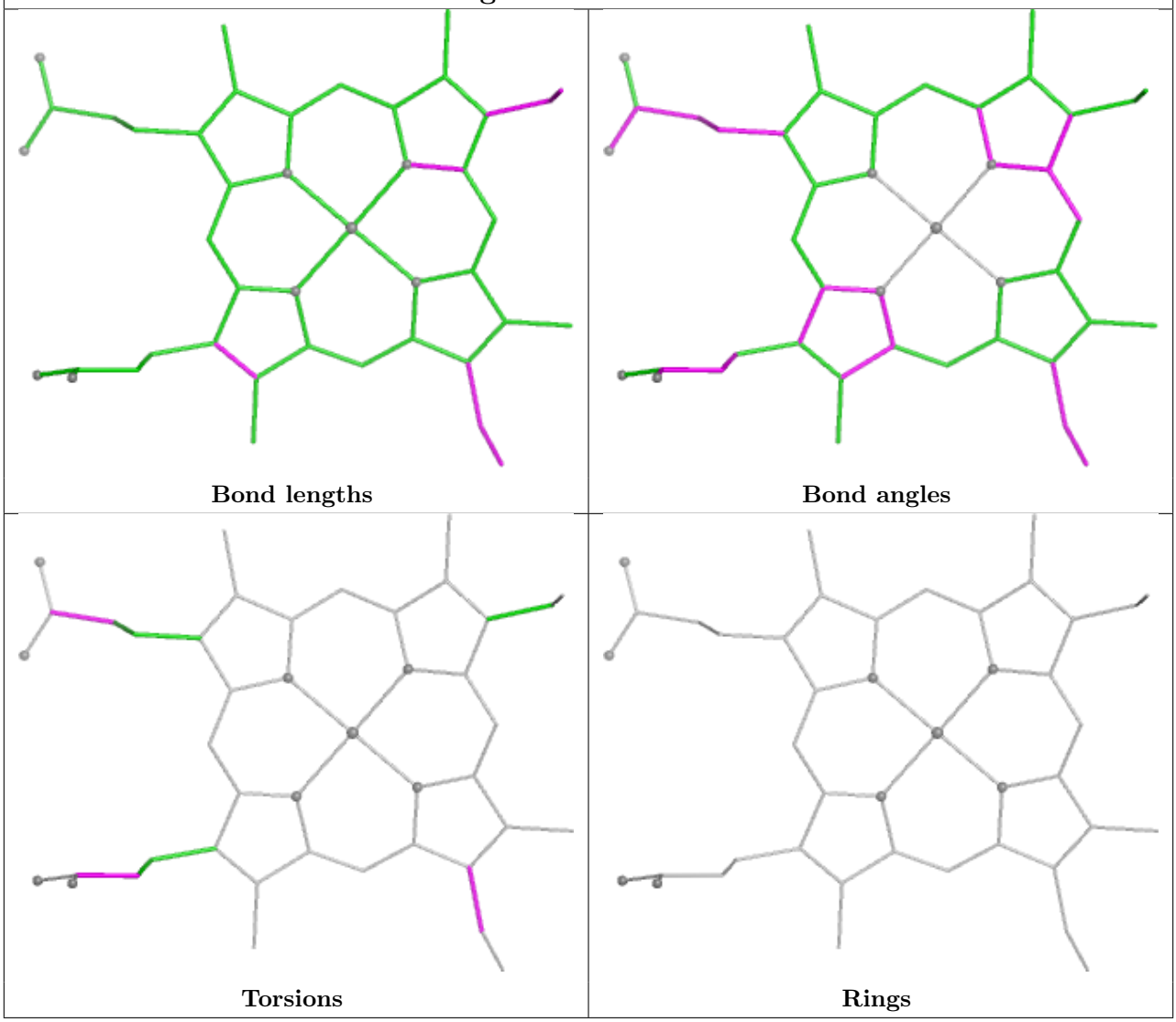
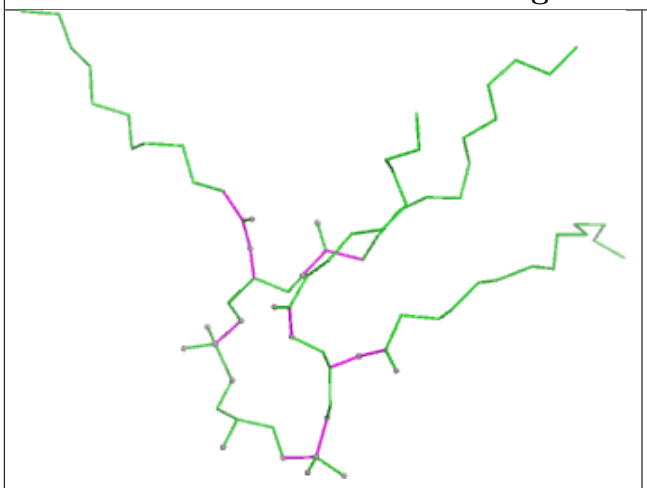
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL H 1003	
Bond lengths	Bond angles
Torsions	Rings

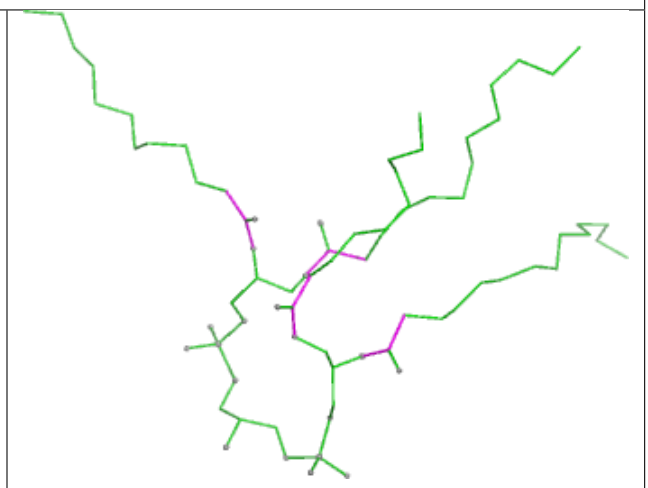
Ligand HEC C 302



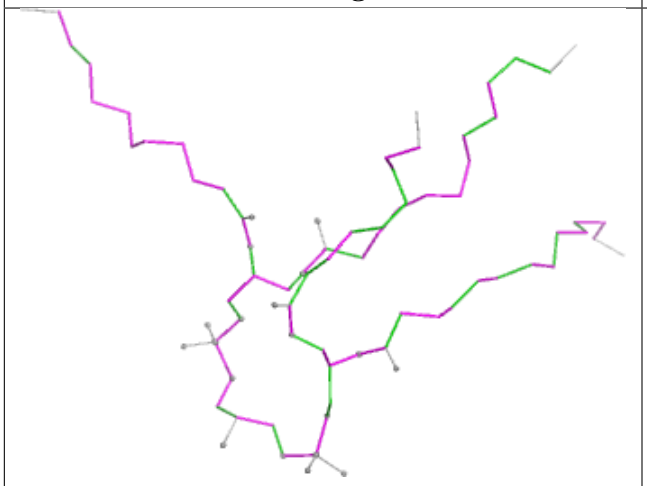
Ligand CDL I 302



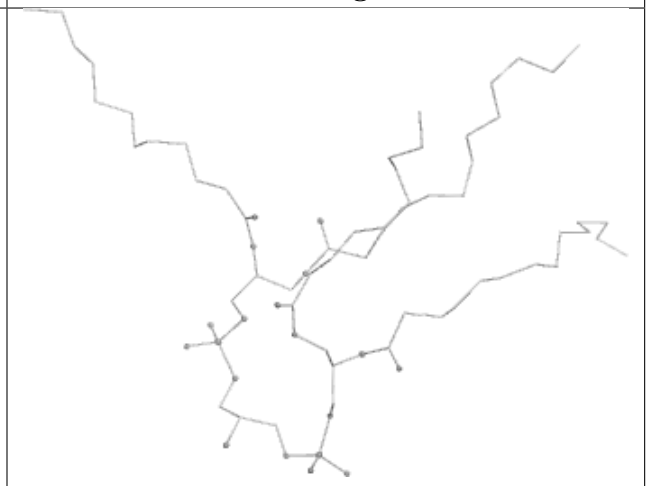
Bond lengths



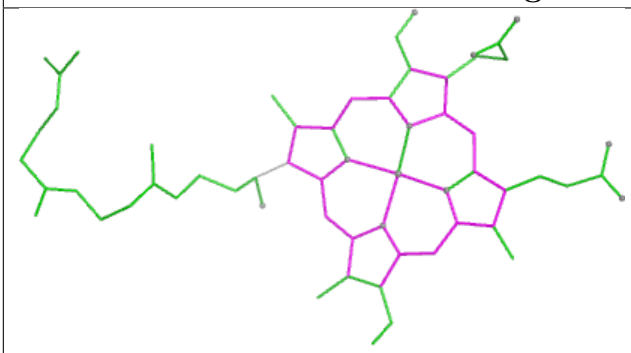
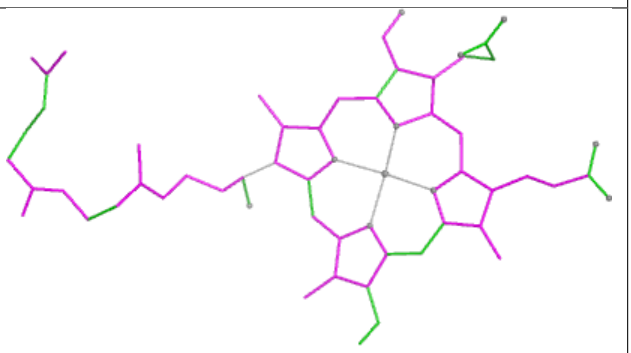
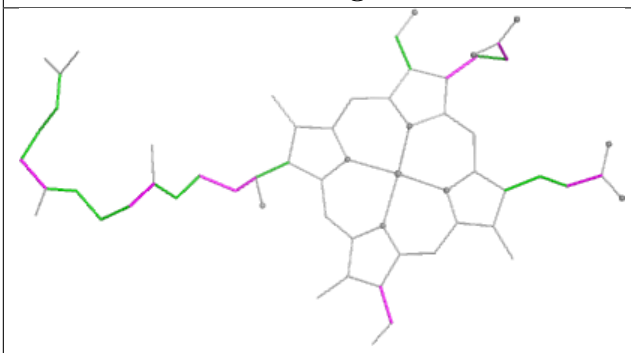
Bond angles



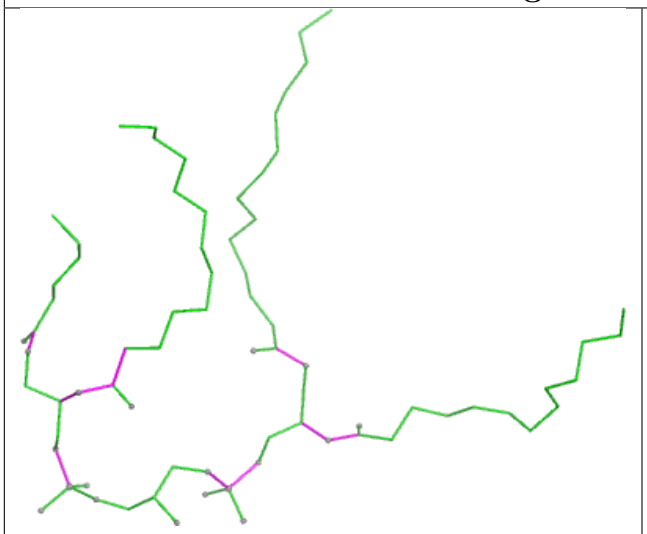
Torsions



Rings

Ligand HEA L 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CDL N 602

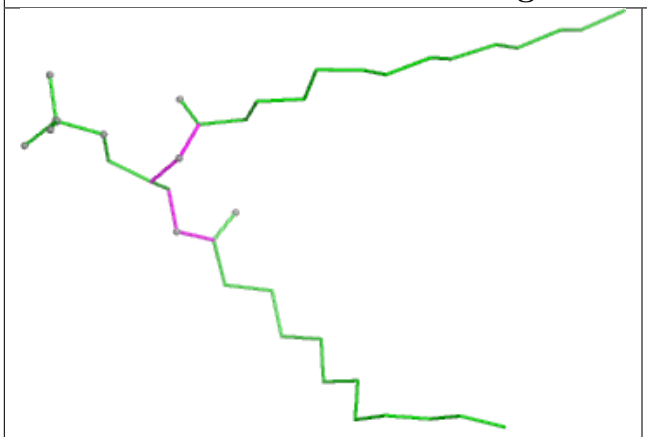
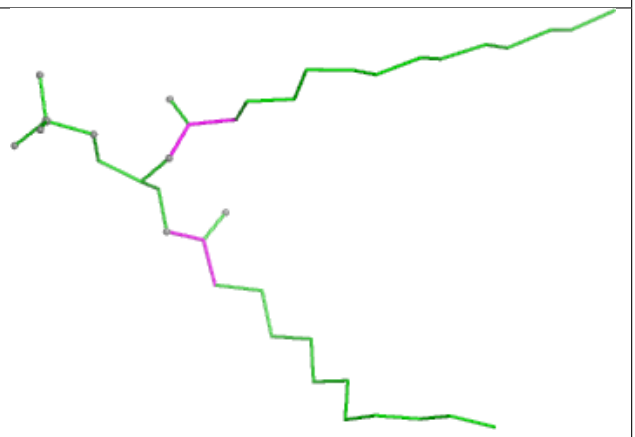
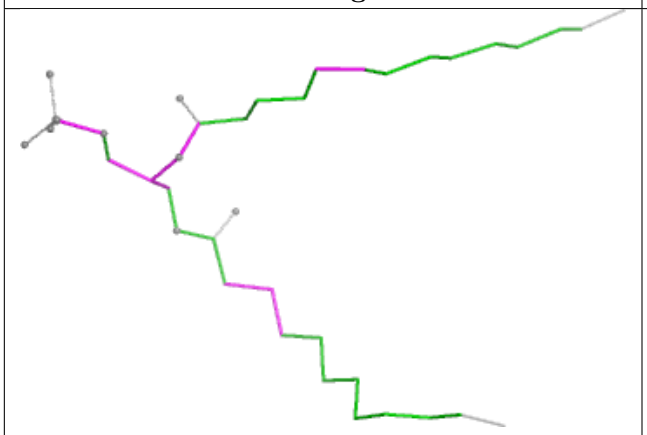
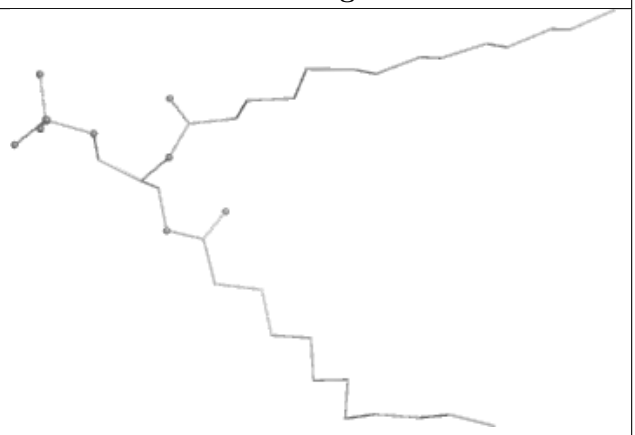


Bond lengths

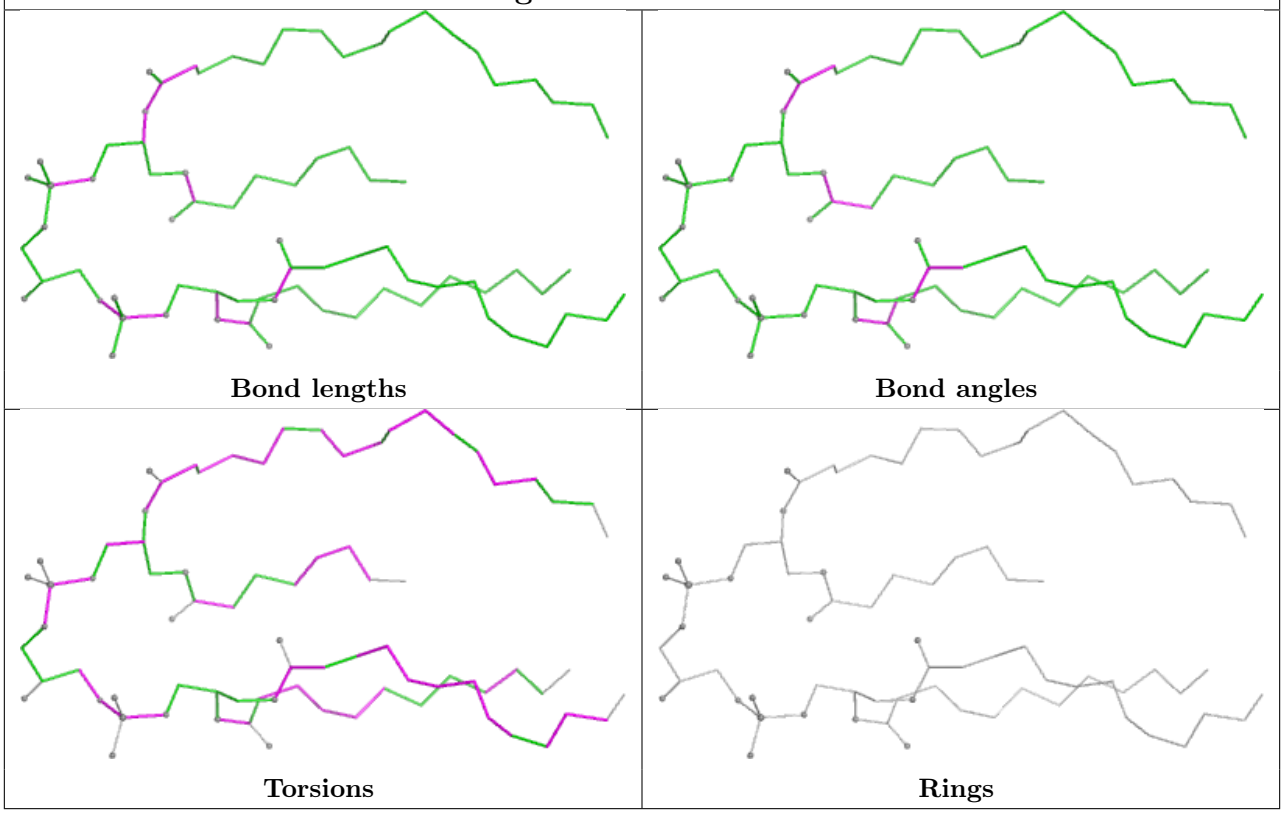
Bond angles

Torsions

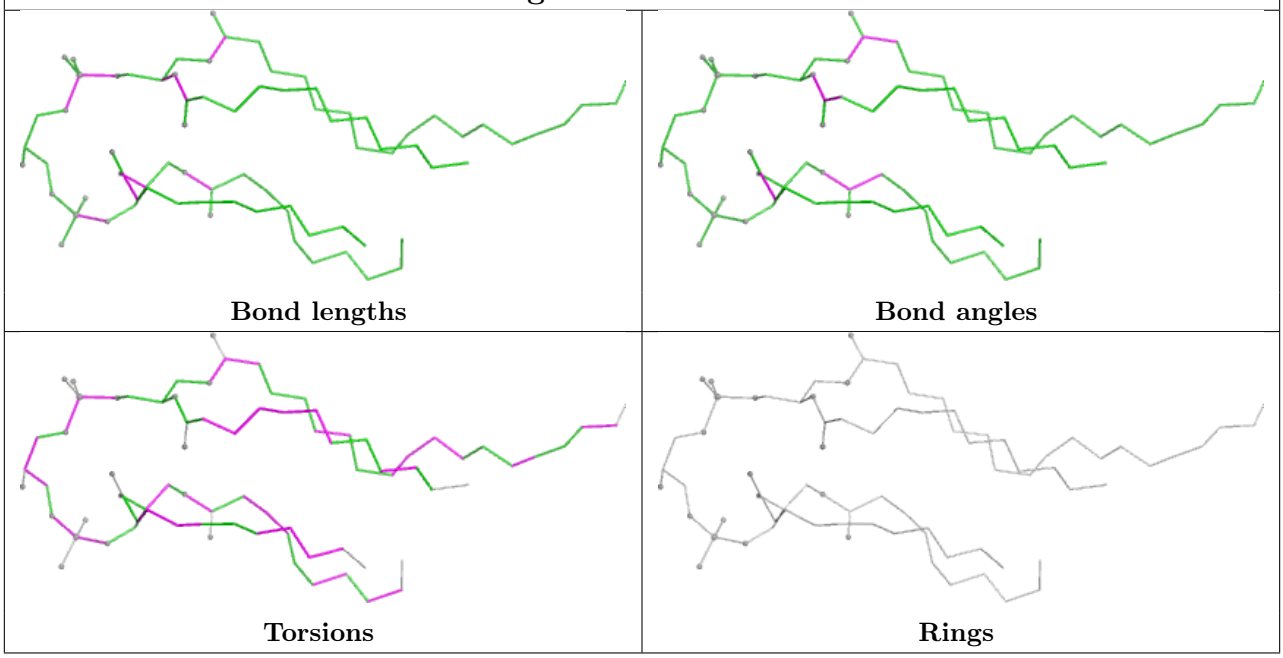
Rings

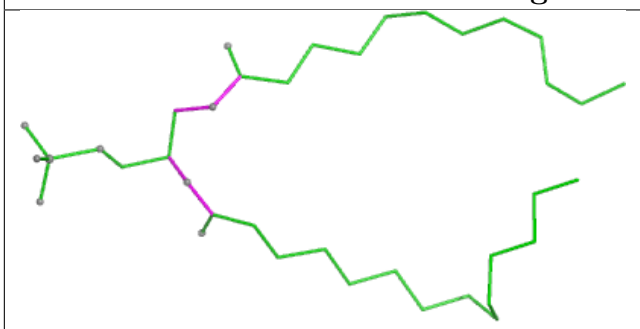
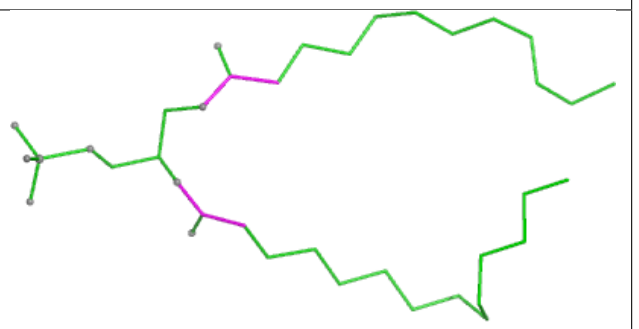
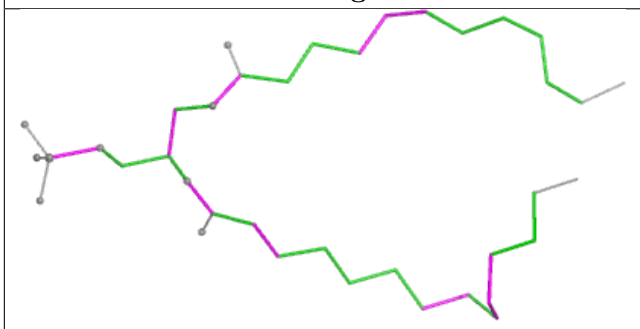
Ligand 7PH H 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

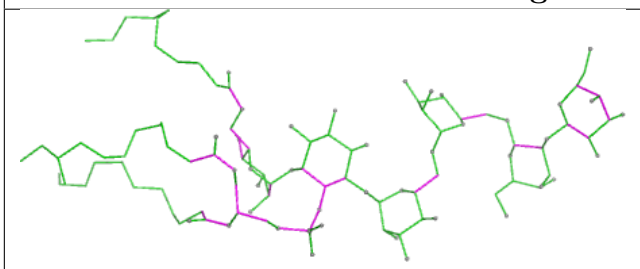
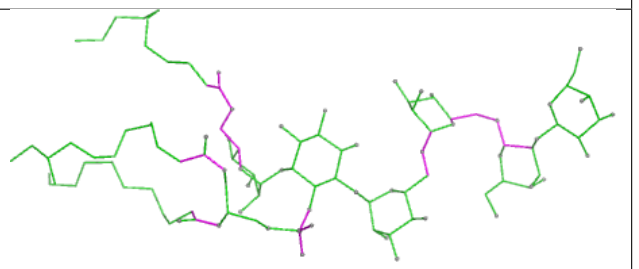
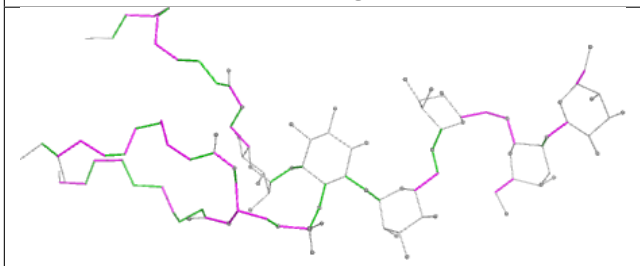
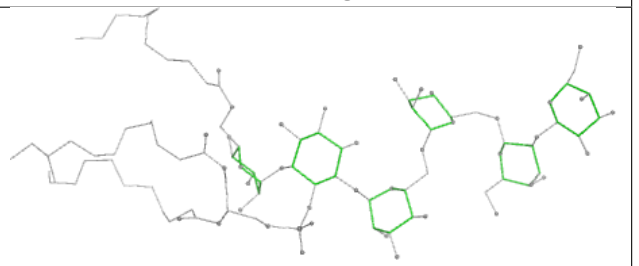
Ligand CDL H 1005



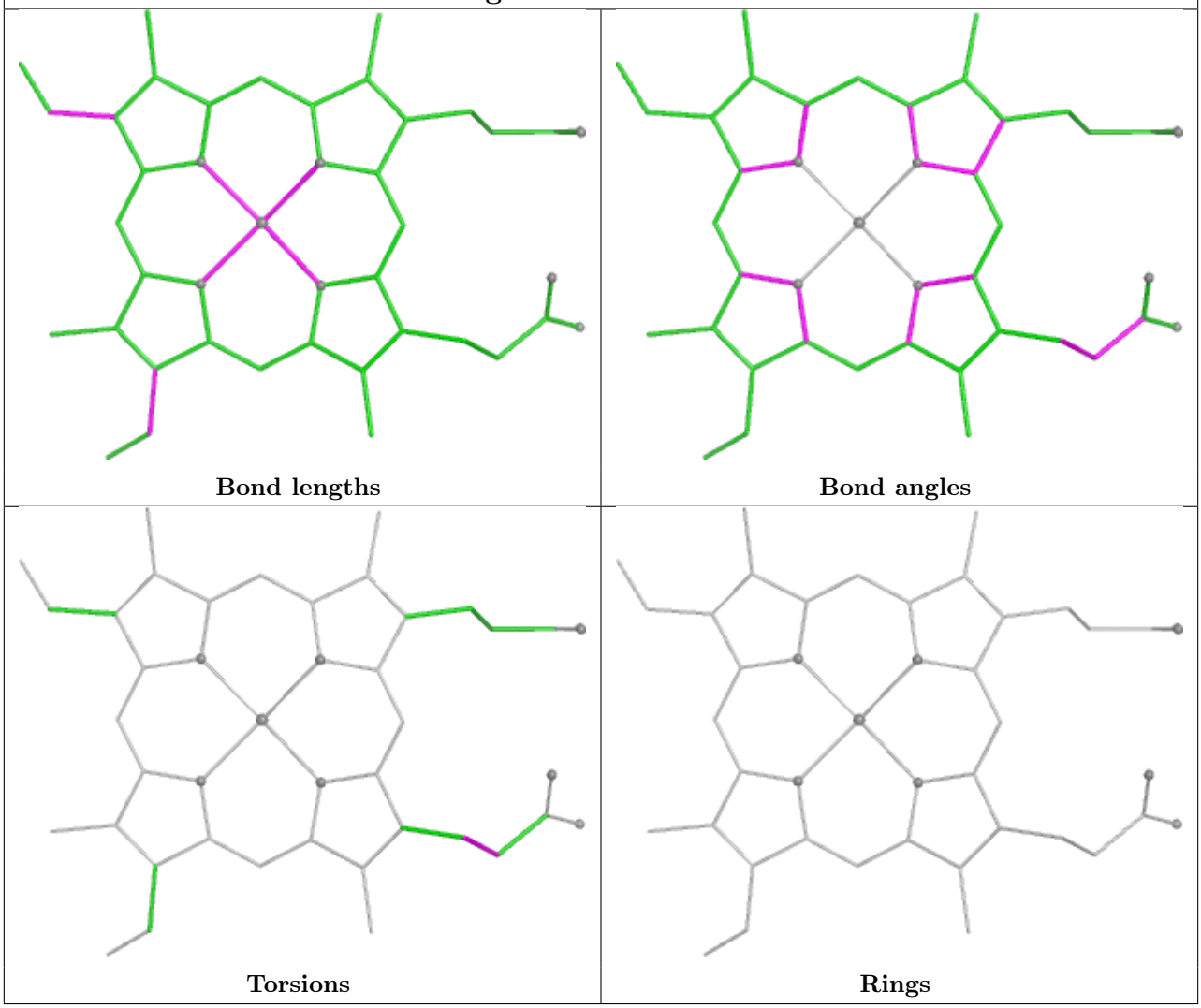
Ligand CDL L 601



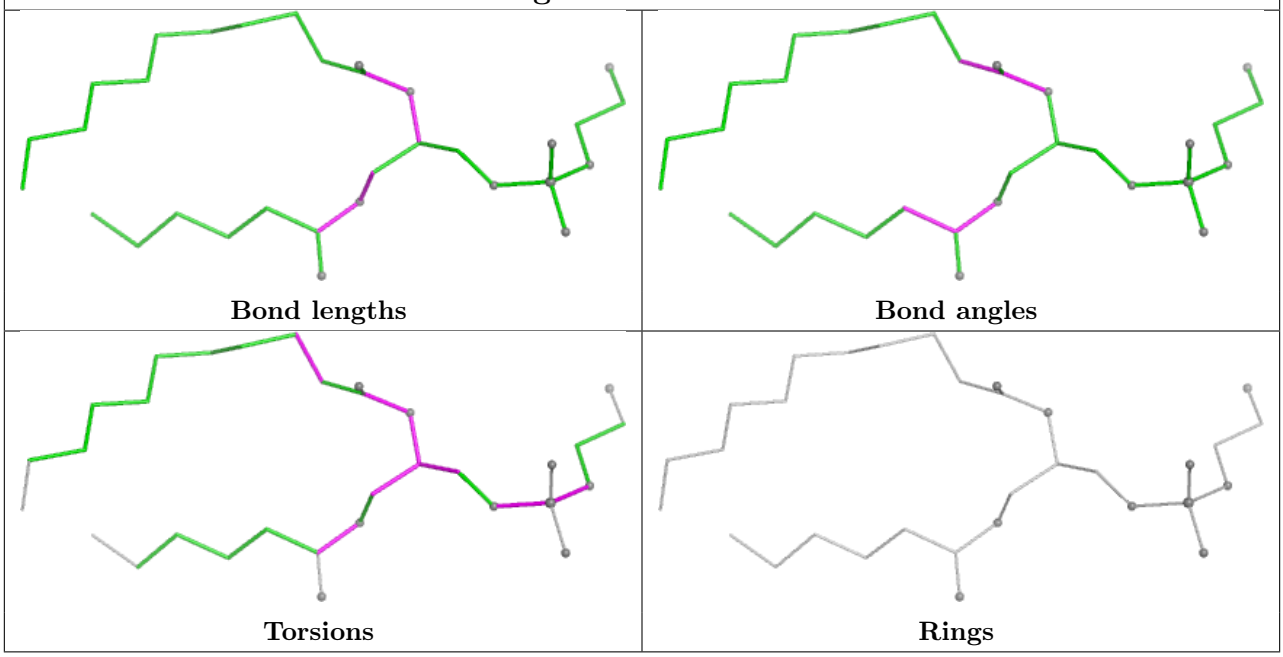
Ligand 7PH S 501	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand IZL M 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

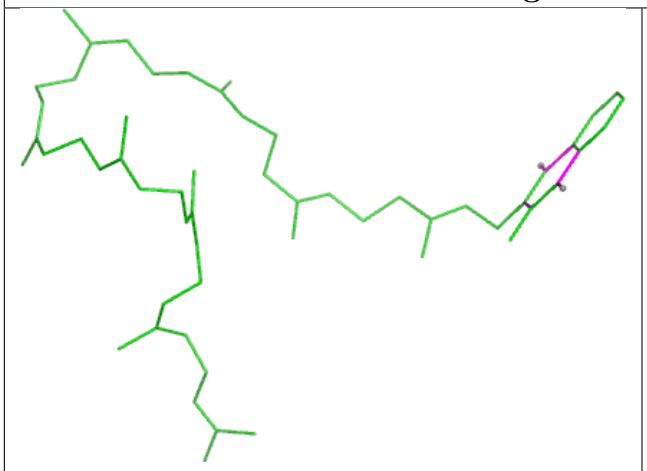
Ligand HEM N 601



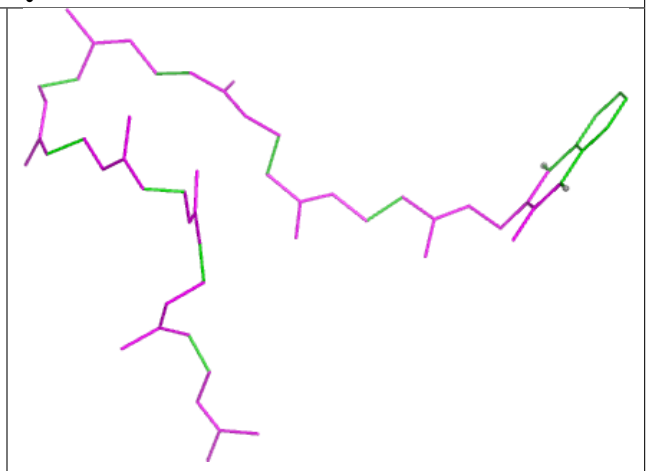
Ligand 3PE J 602



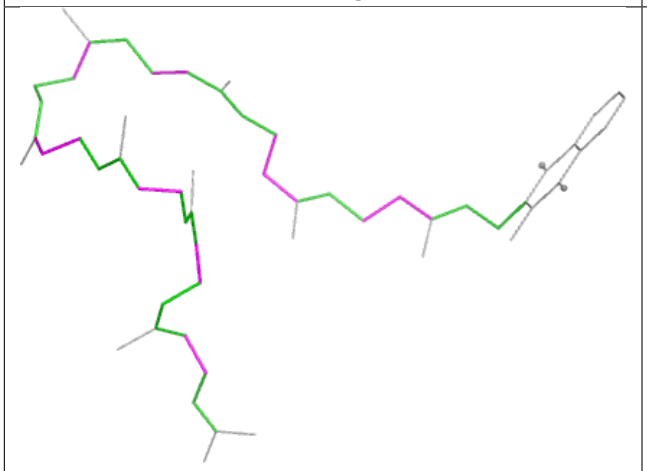
Ligand MQ9 C 305



Bond lengths



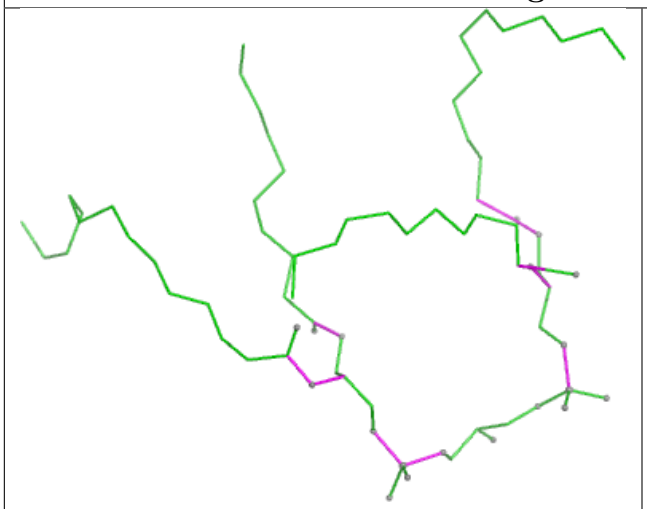
Bond angles



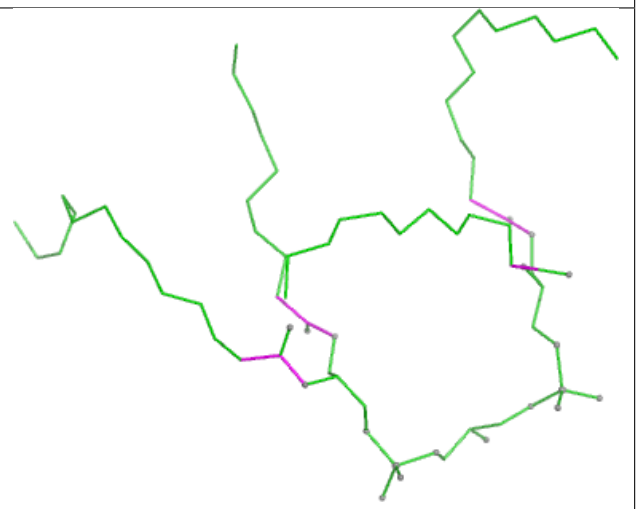
Torsions

Rings

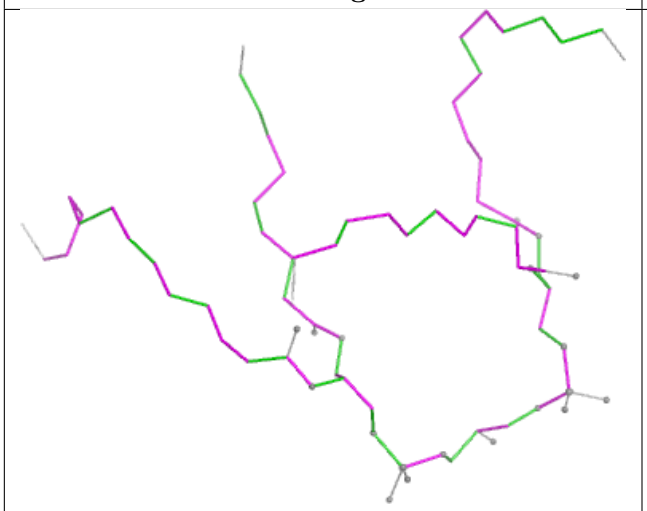
Ligand CDL L 609



Bond lengths

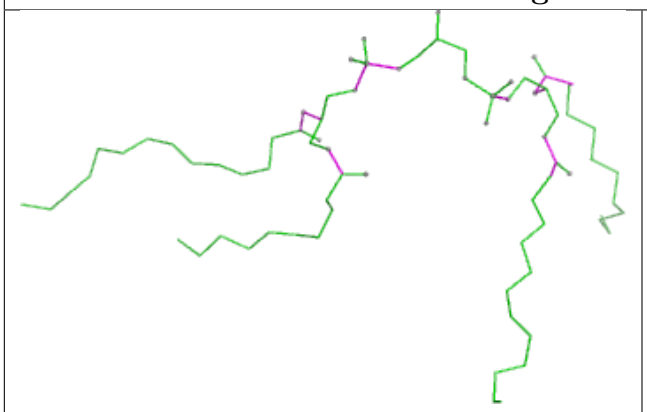
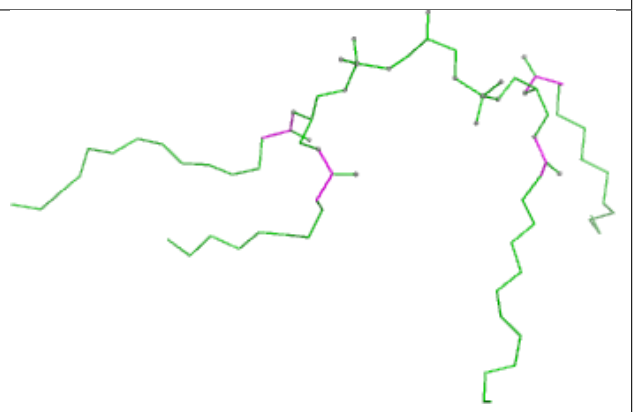
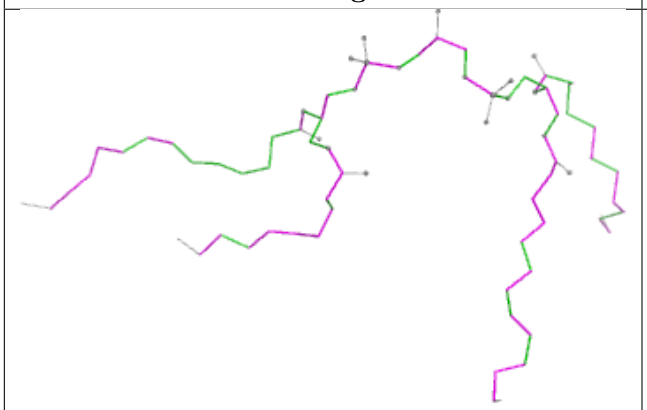
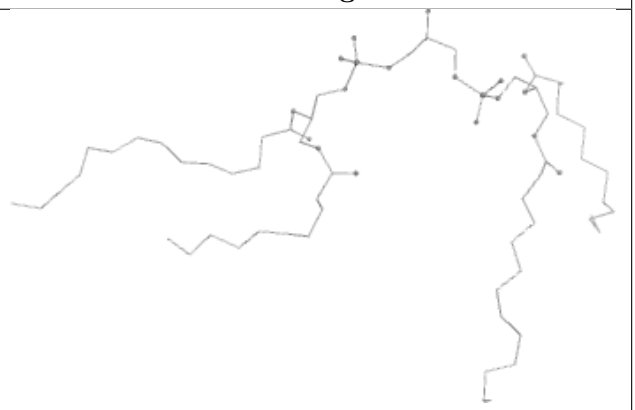


Bond angles

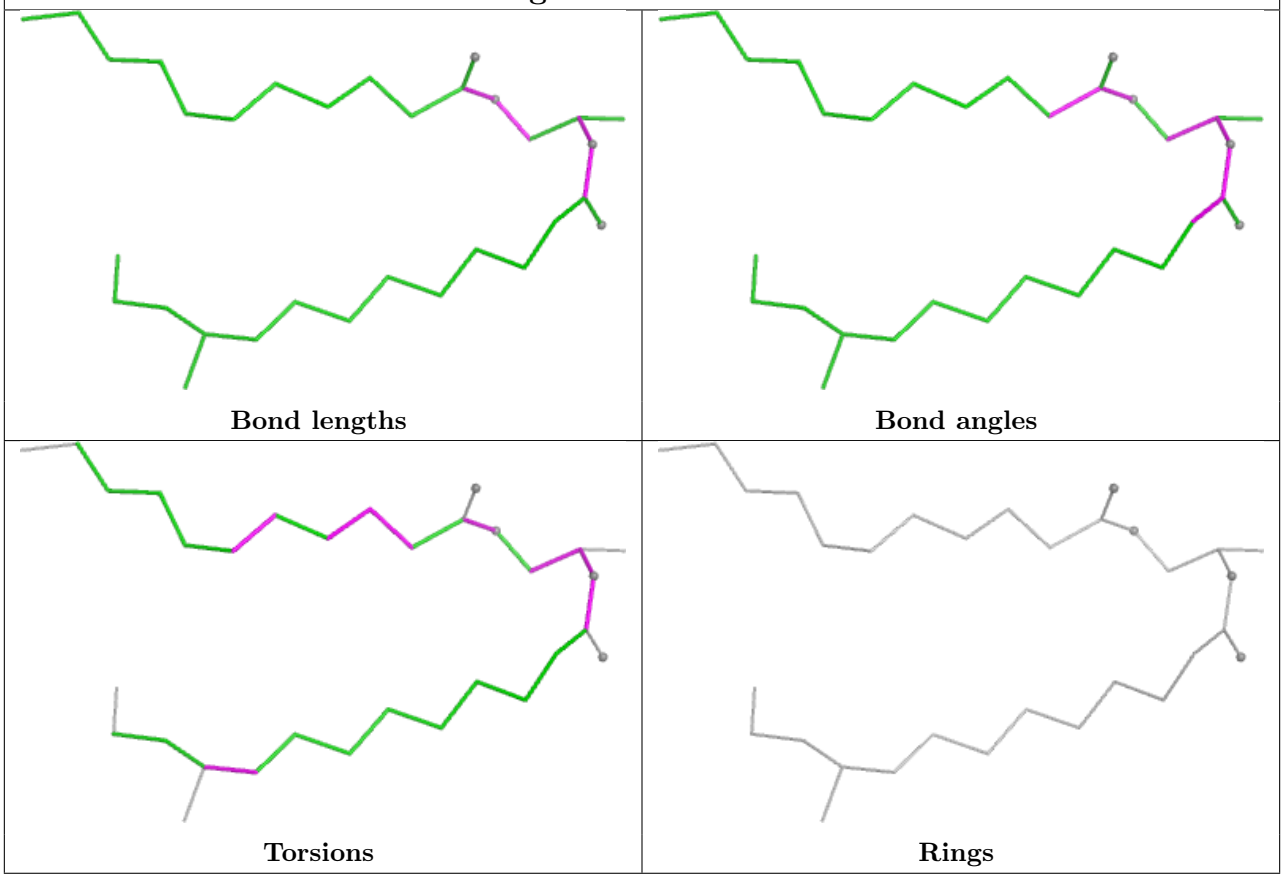


Torsions

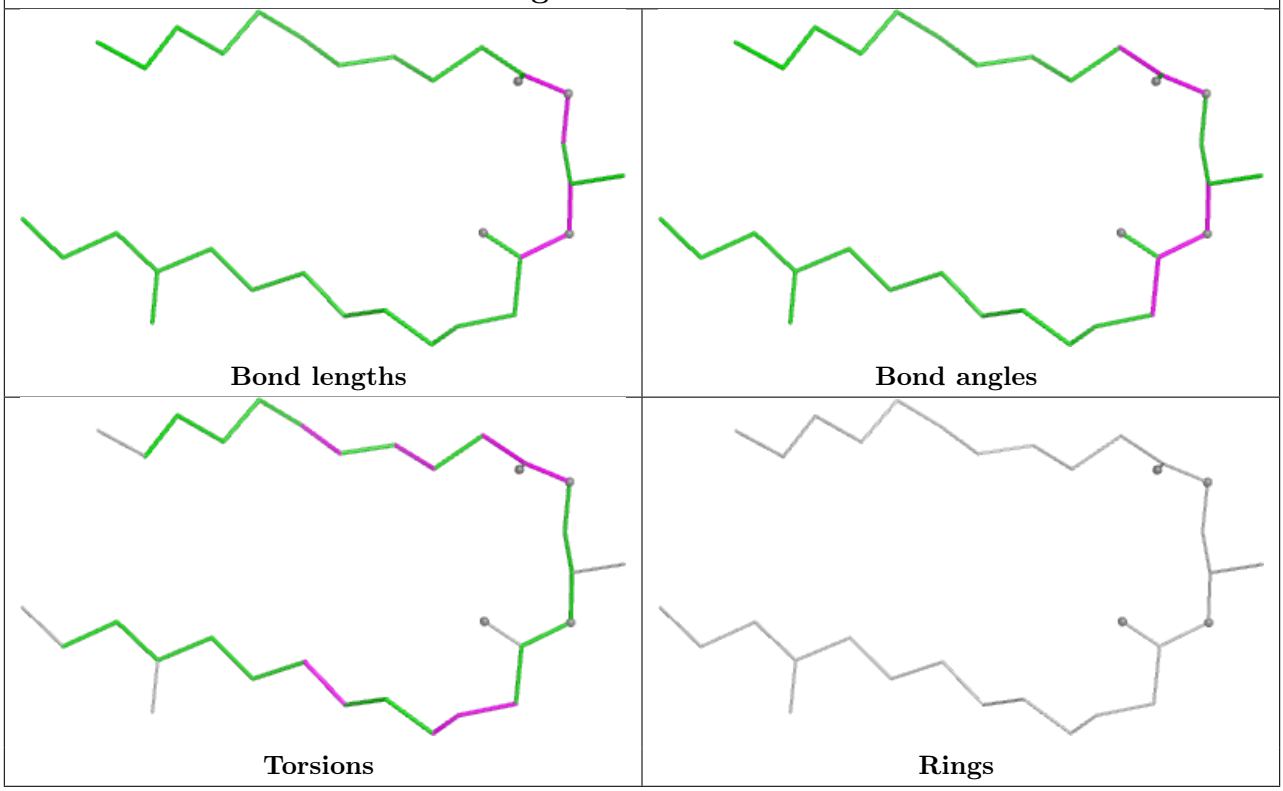
Rings

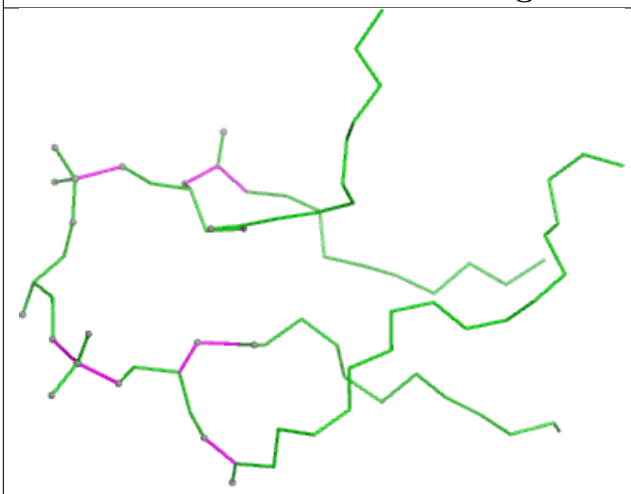
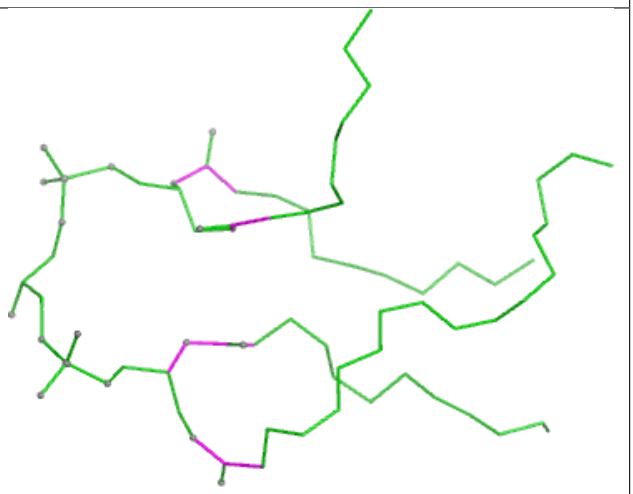
Ligand CDL I 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

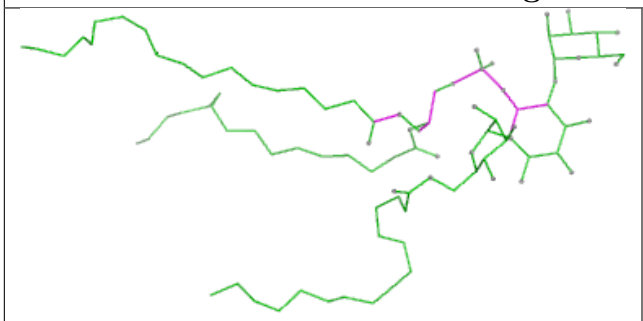
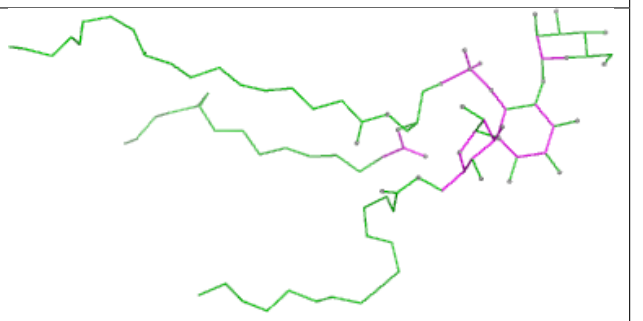
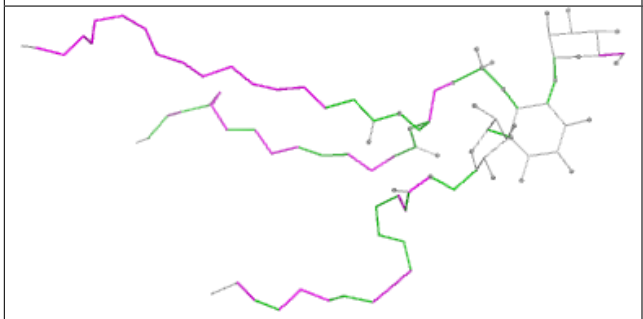
Ligand 9XX b 202



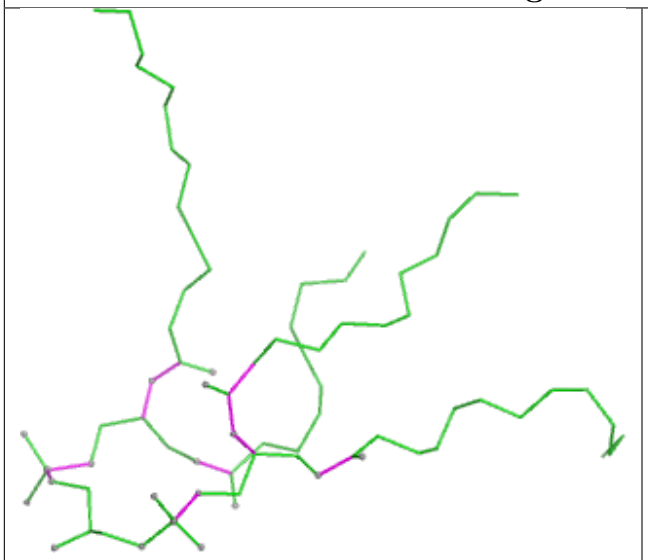
Ligand 9XX c 302



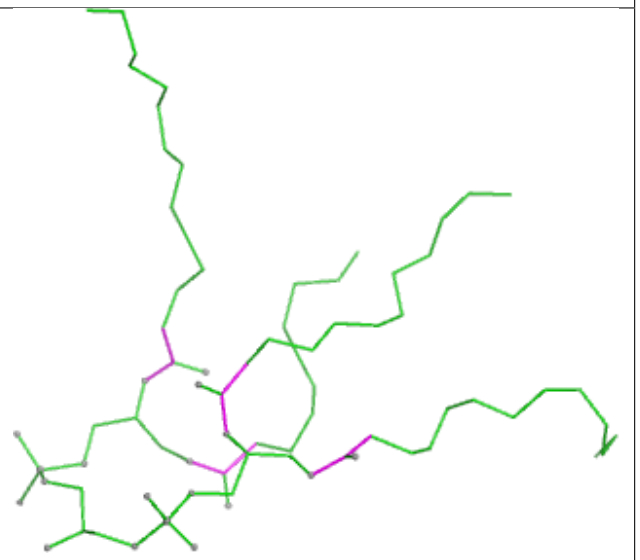
Ligand CDL T 1302	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand WUO I 303	
 Bond lengths	 Bond angles
 Torsions	Rings

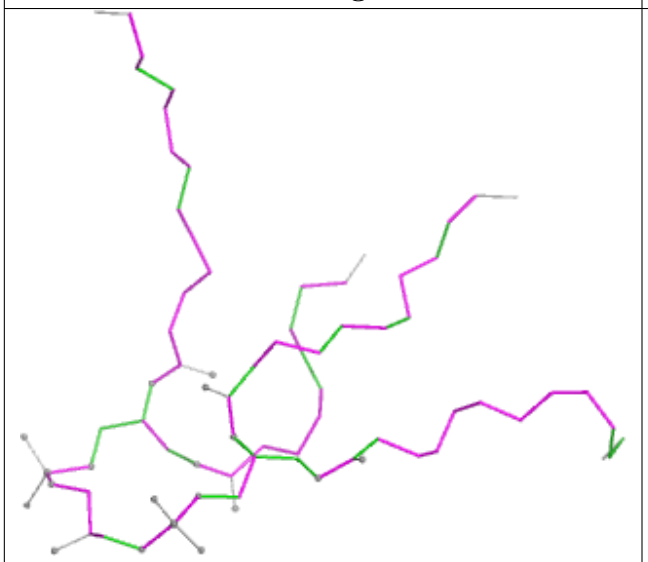
Ligand CDL P 303



Bond lengths



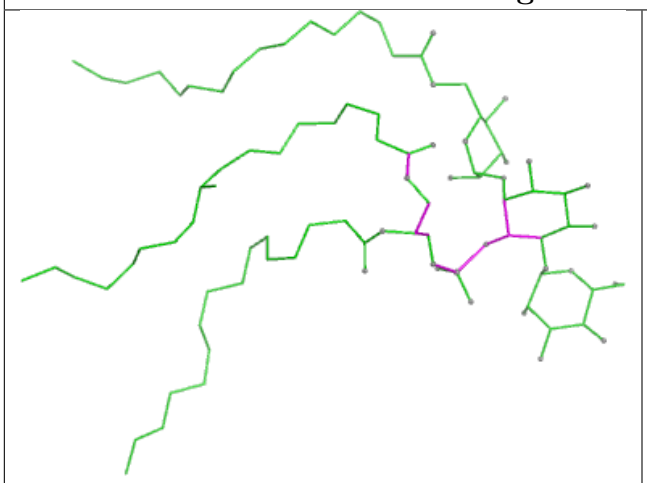
Bond angles



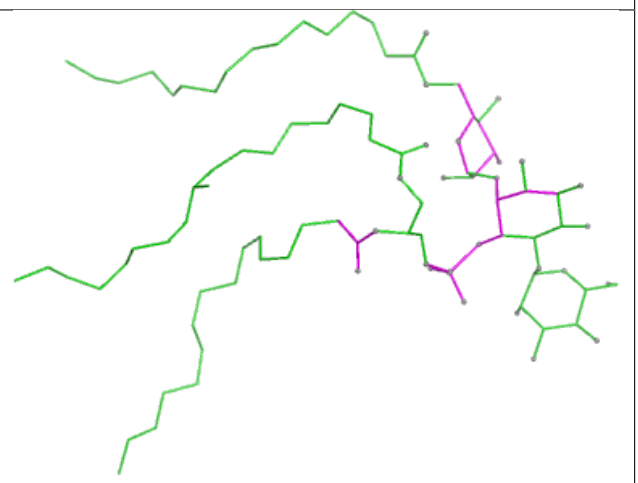
Torsions

Rings

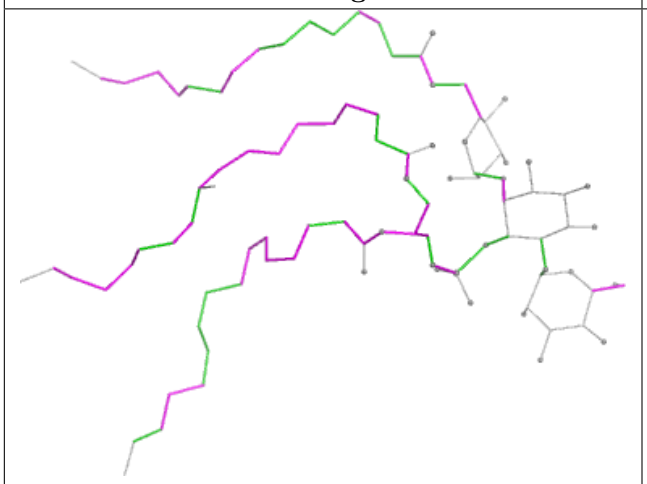
Ligand WUO C 304



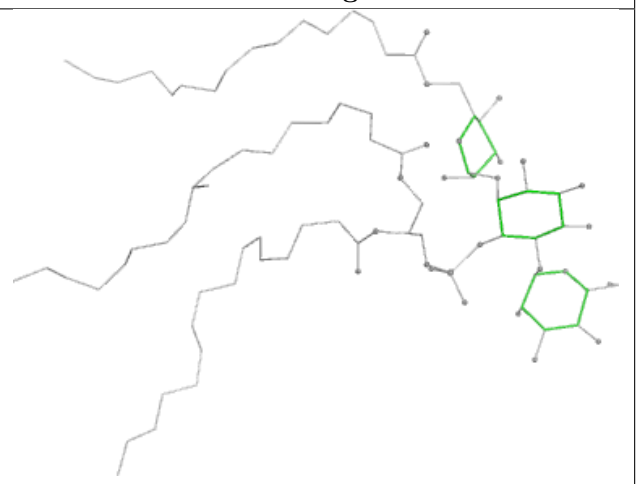
Bond lengths



Bond angles

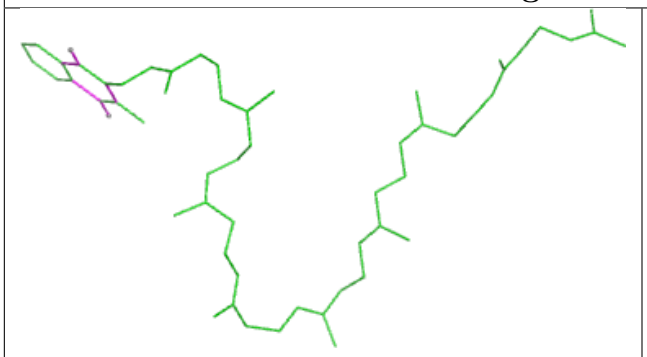


Torsions



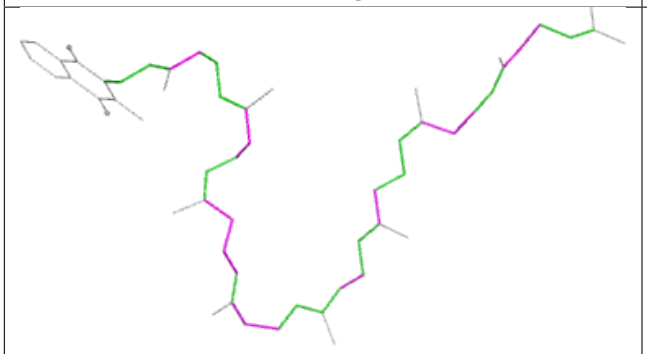
Rings

Ligand MQ9 N 605

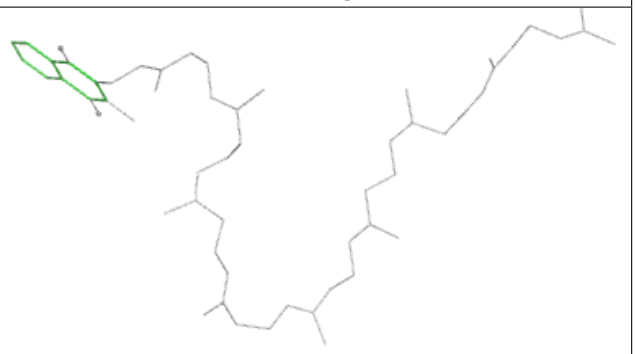


Bond lengths

Bond angles

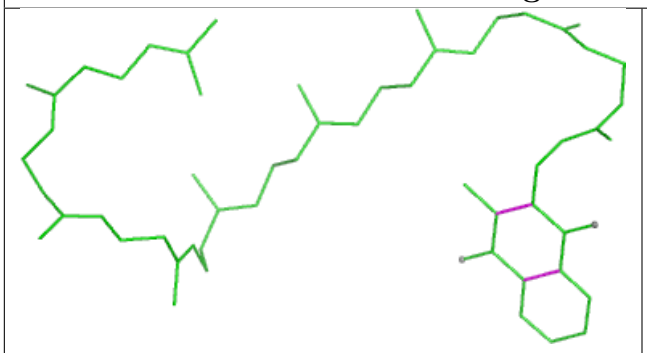


Torsions

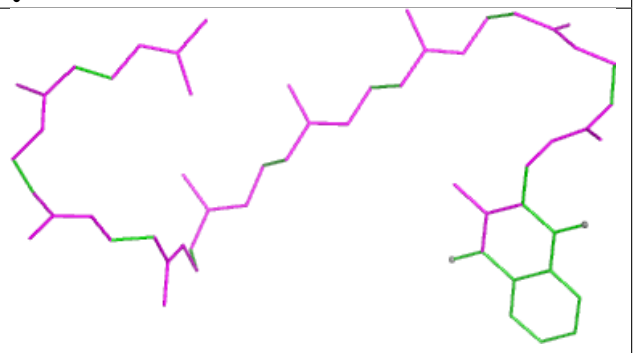


Rings

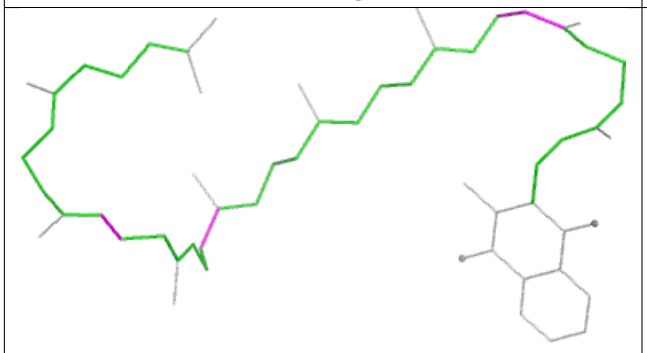
Ligand MQ9 C 303



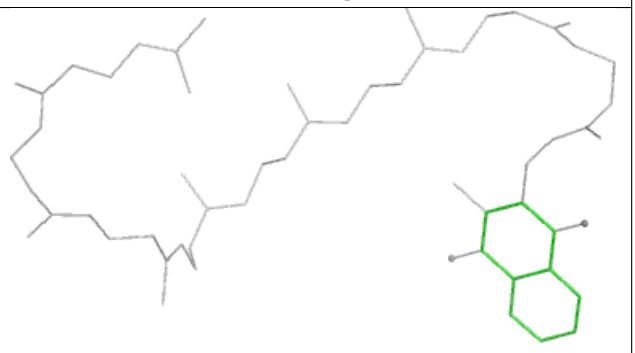
Bond lengths



Bond angles

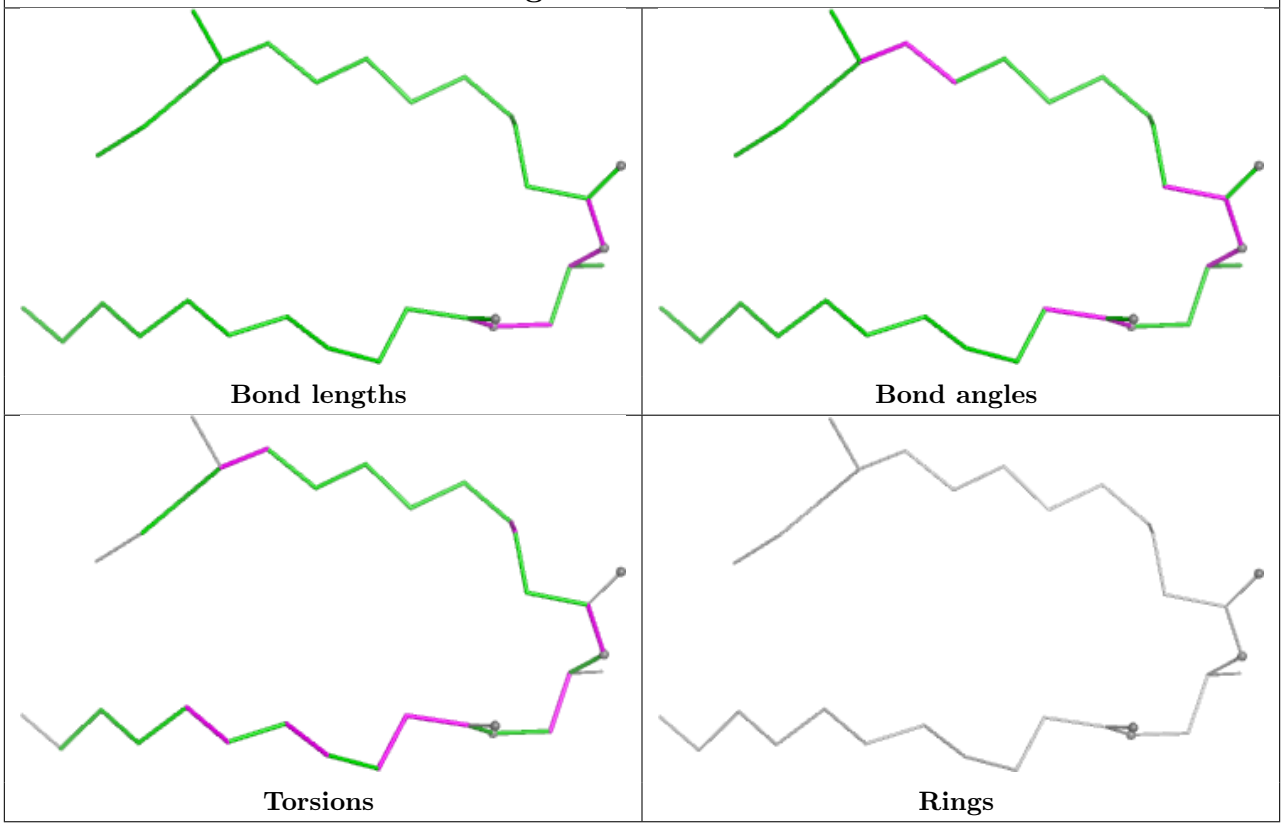


Torsions

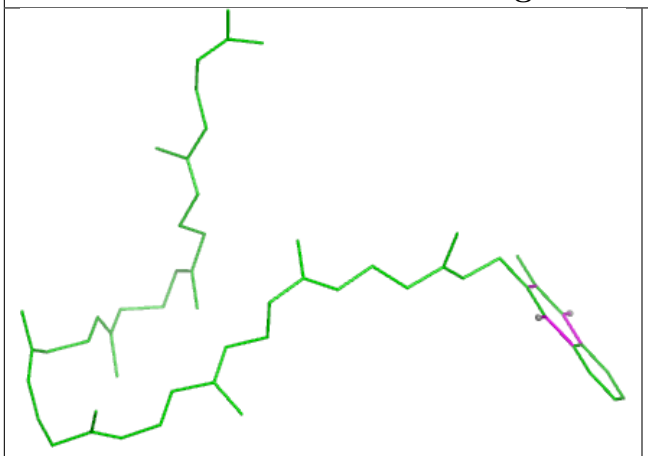


Rings

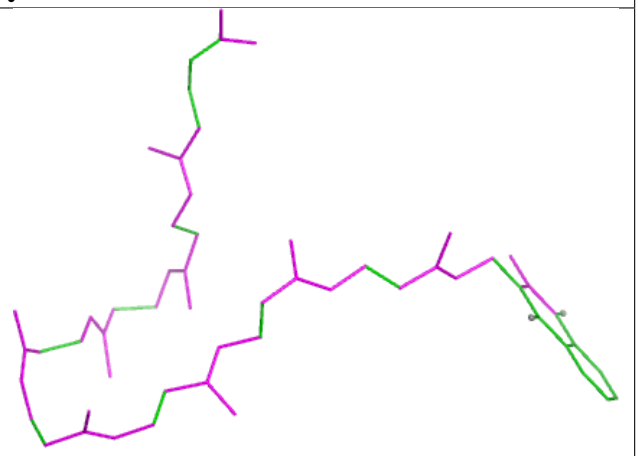
Ligand 9XX N 609



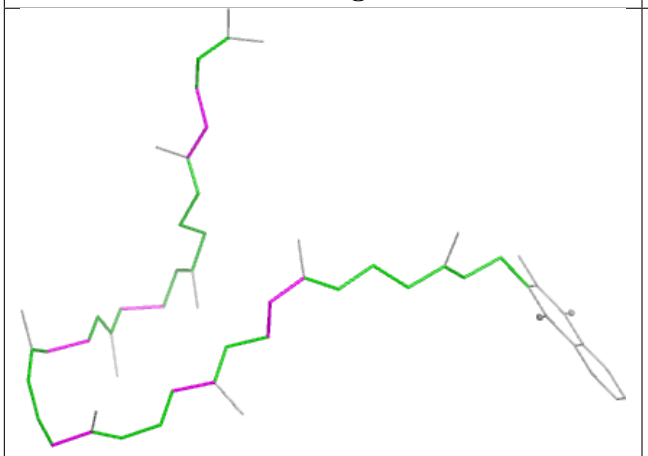
Ligand MQ9 T 1301



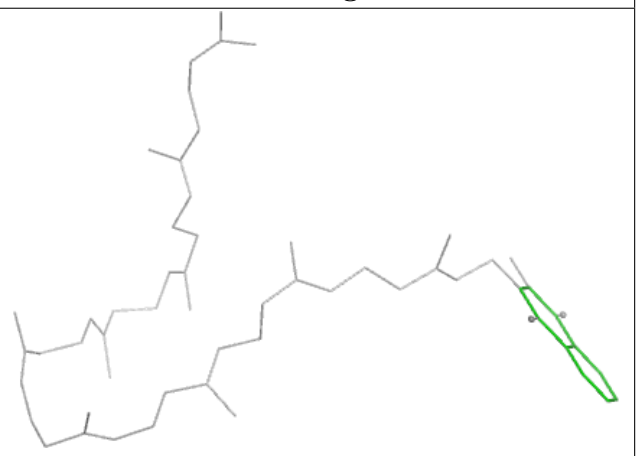
Bond lengths



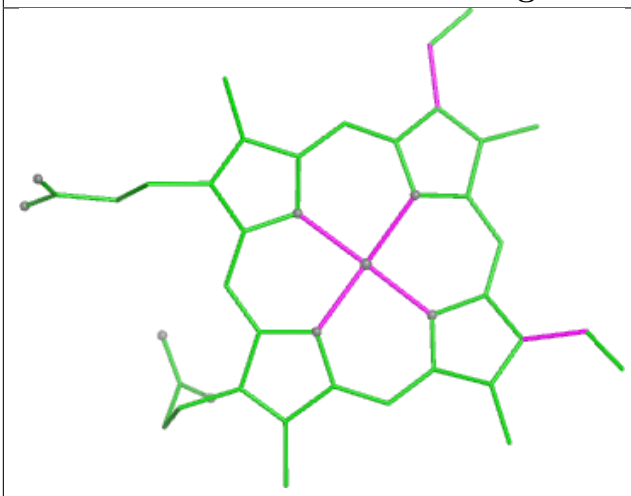
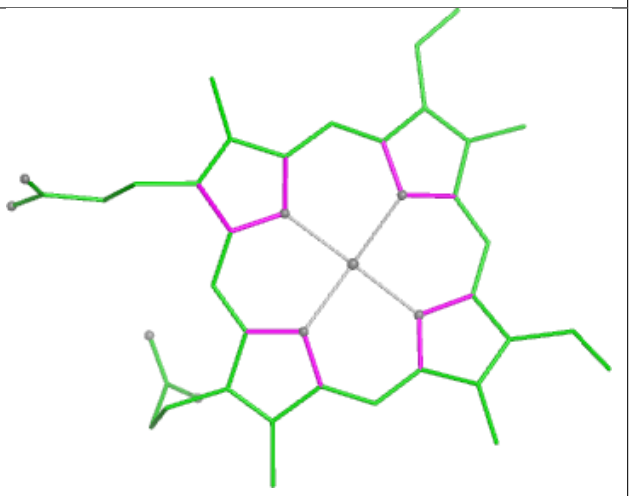
Bond angles



Torsions



Rings

Ligand HEM N 606	
	
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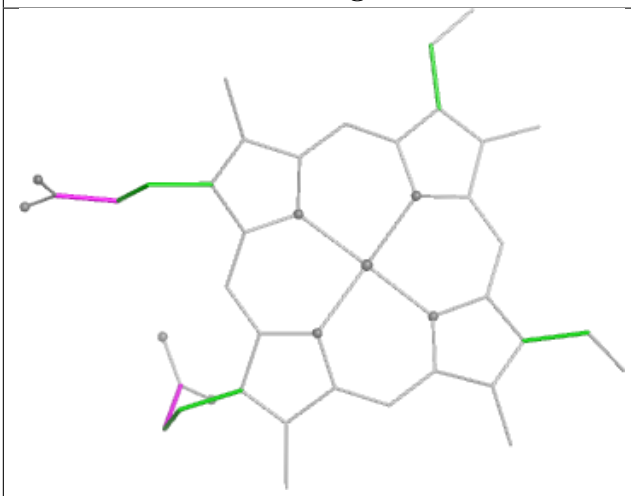
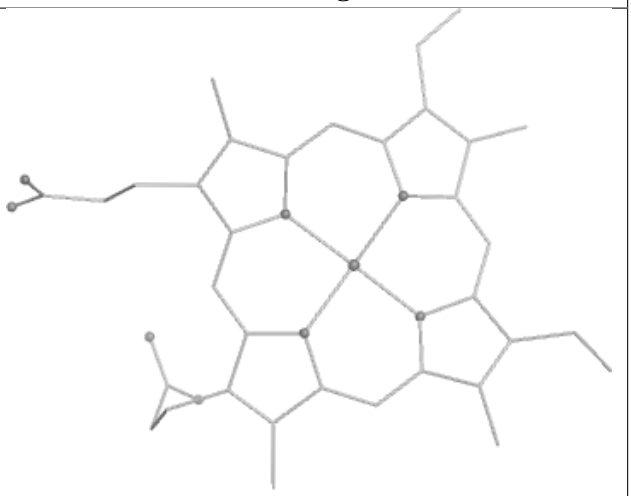
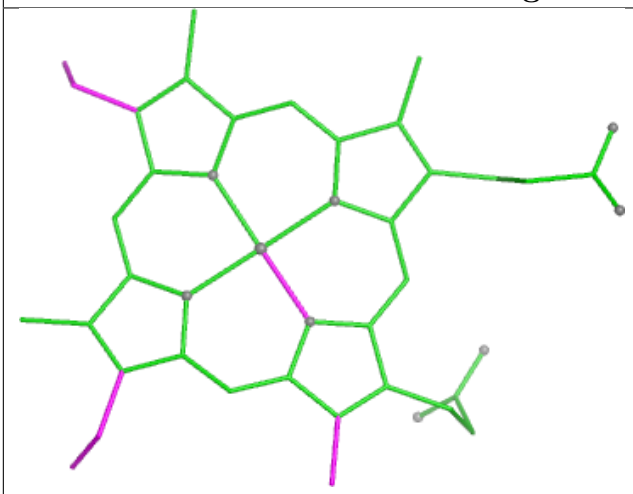
	
Torsions	**Rings**

Ligand HEC C 301



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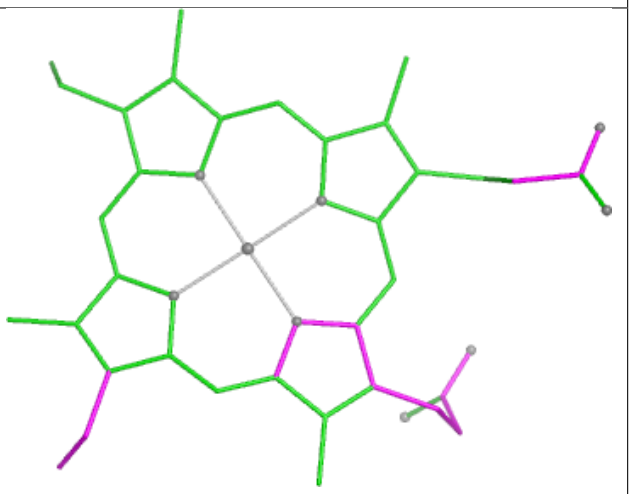

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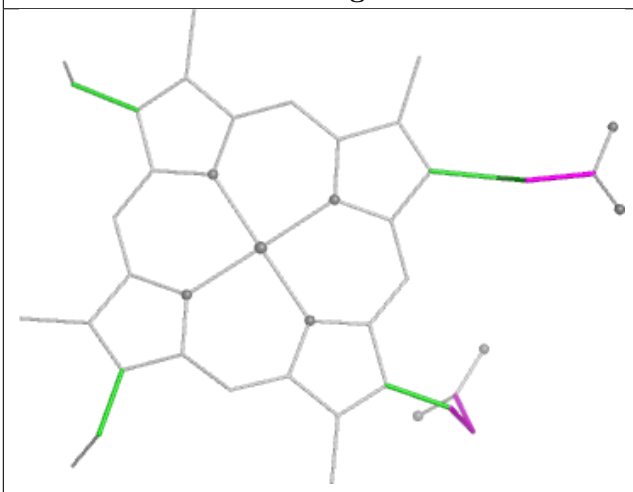

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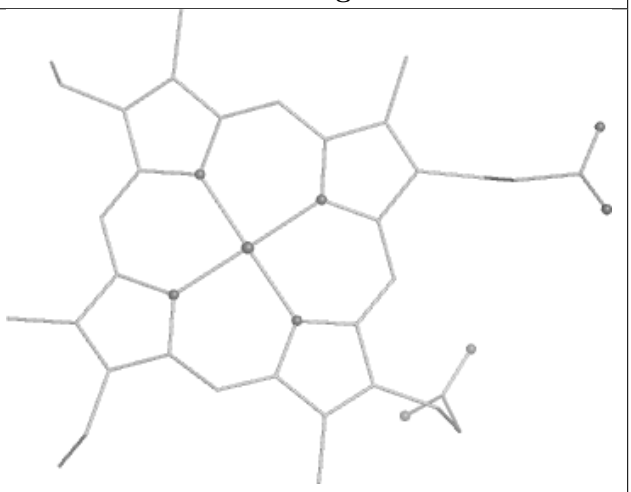
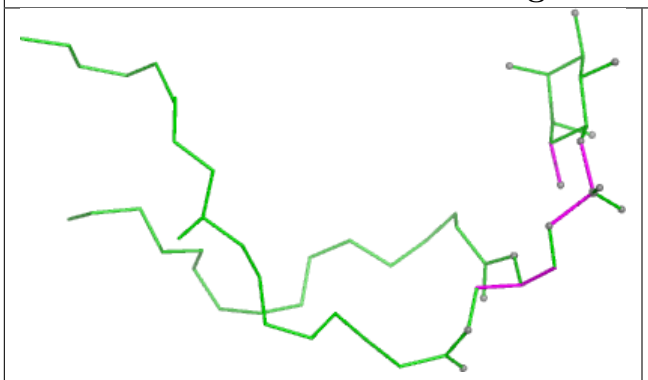


Rings

Ligand 9YF G 503



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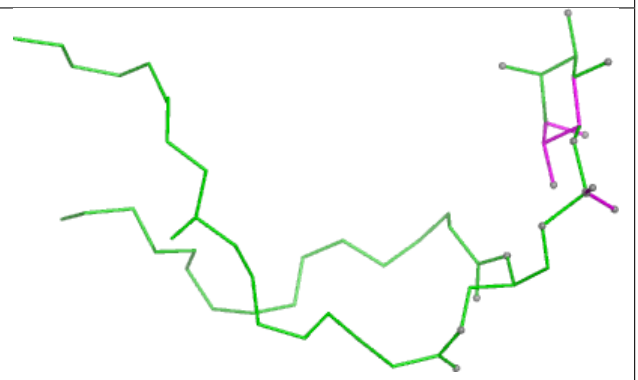

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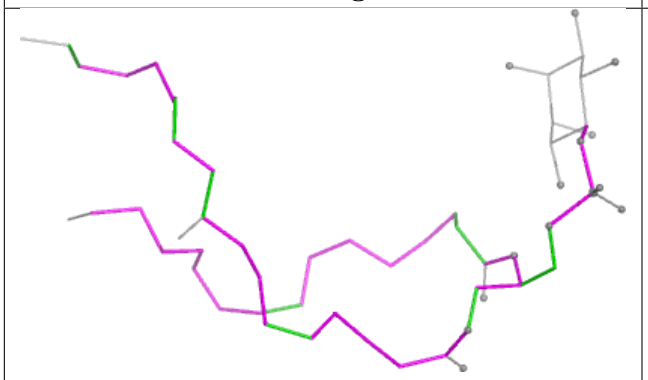

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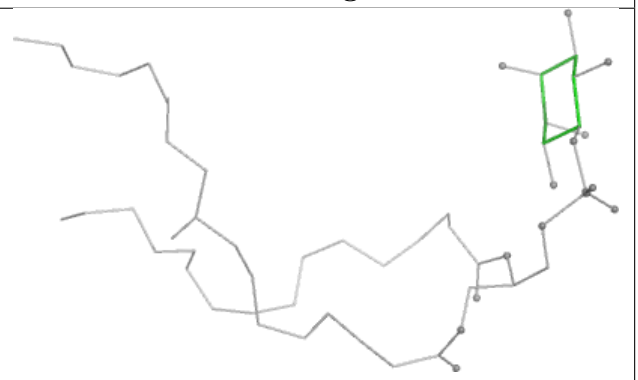
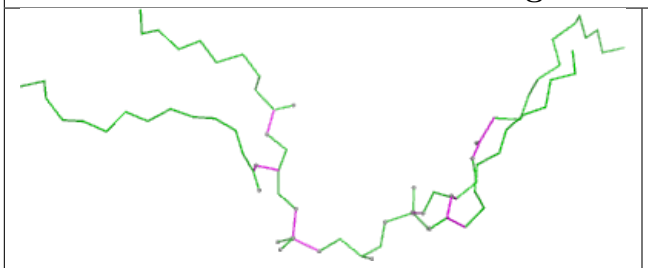


Rings

Ligand CDL P 301



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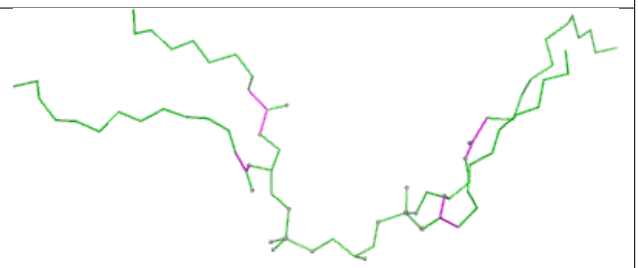

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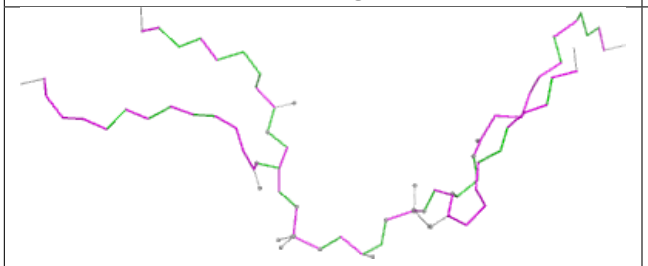

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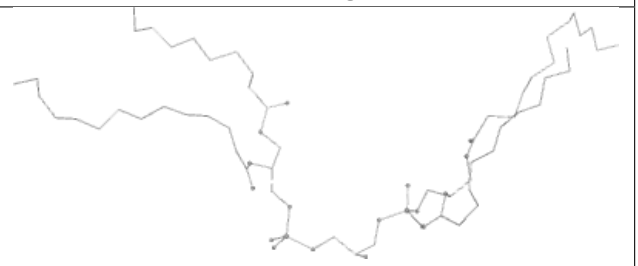
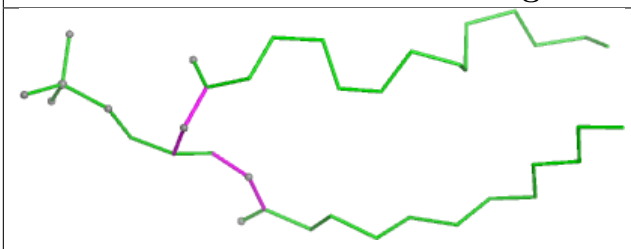
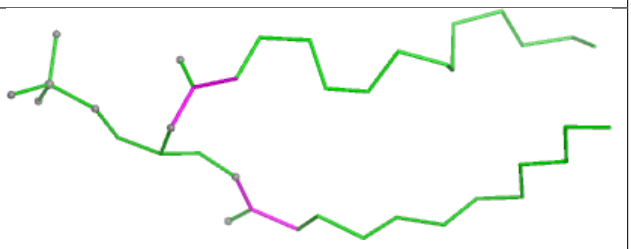
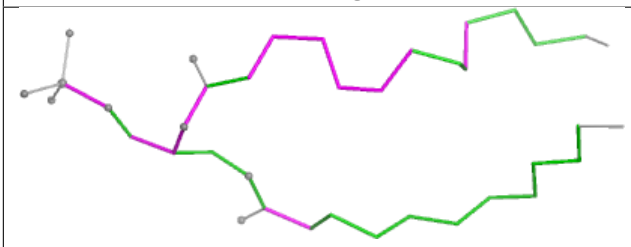
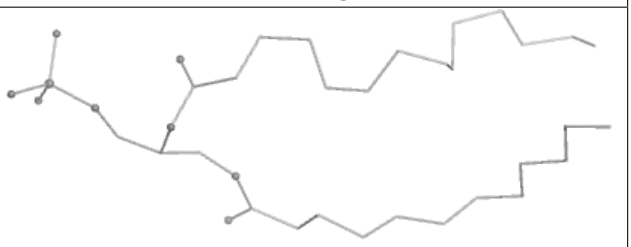
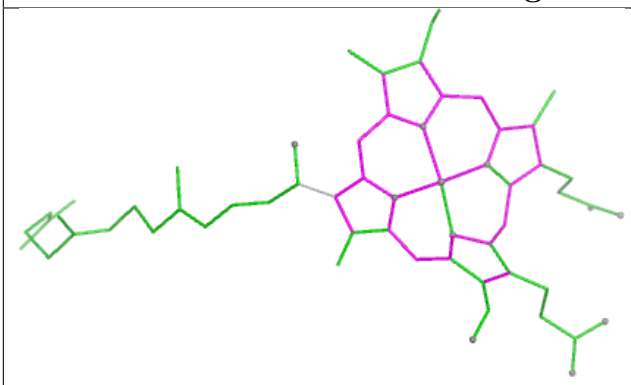
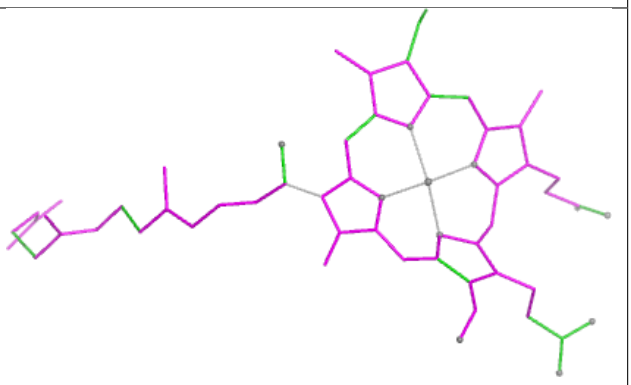
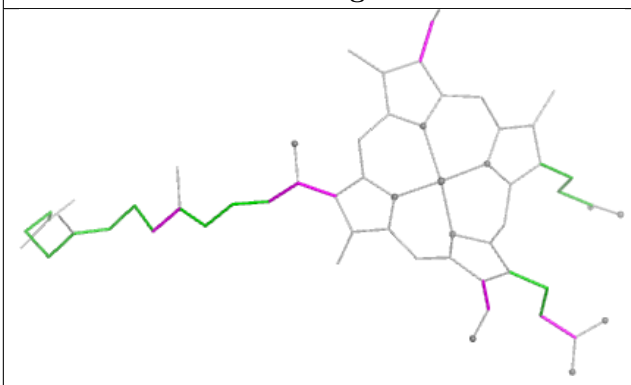
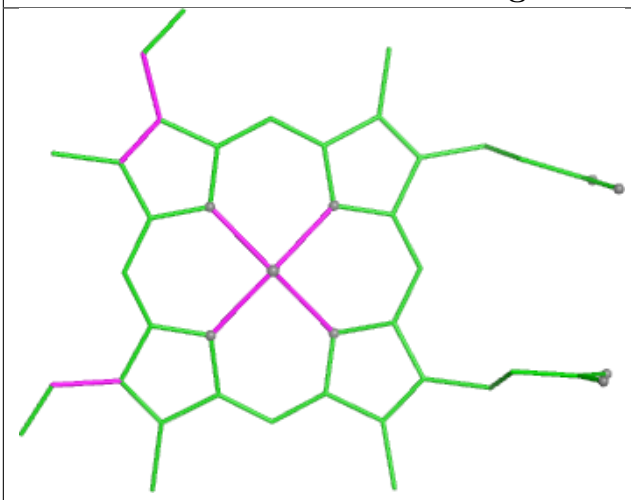


Rings

Ligand 7PH M 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA L 603	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand HEM H 1002



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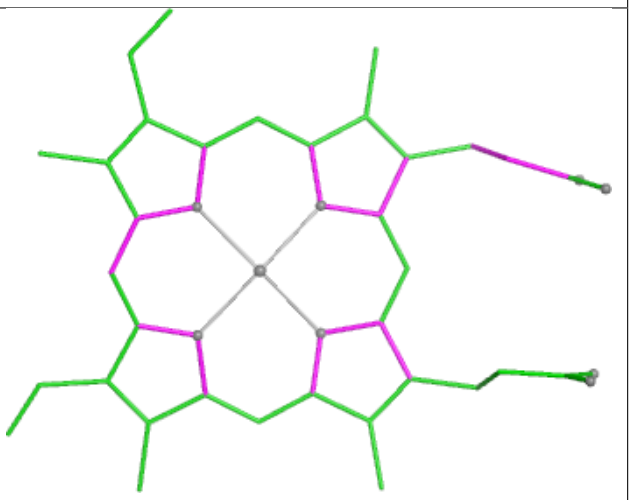
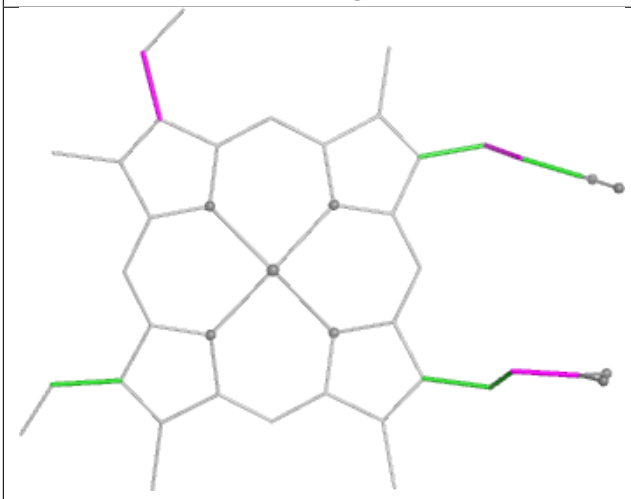
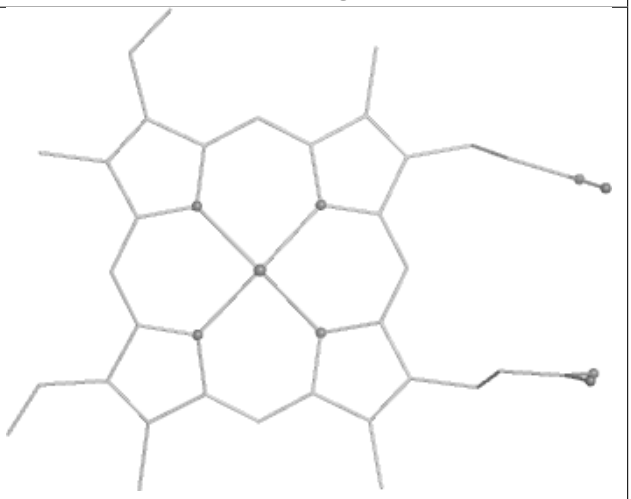


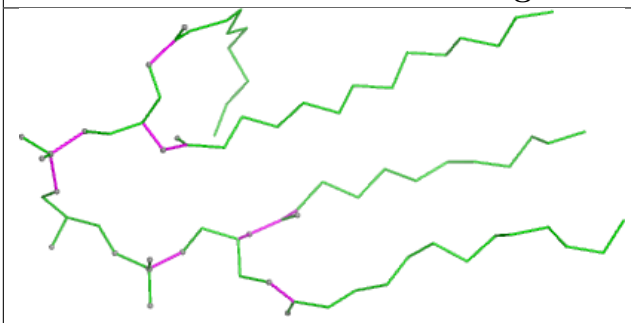
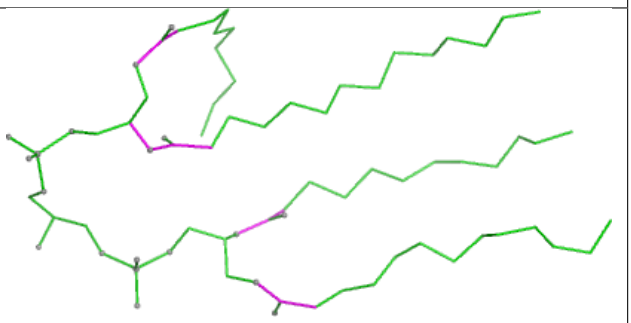
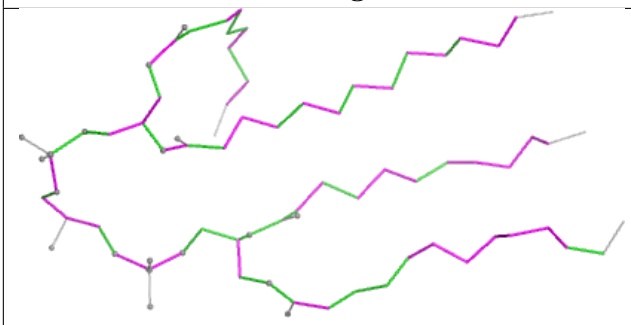
Bond angles



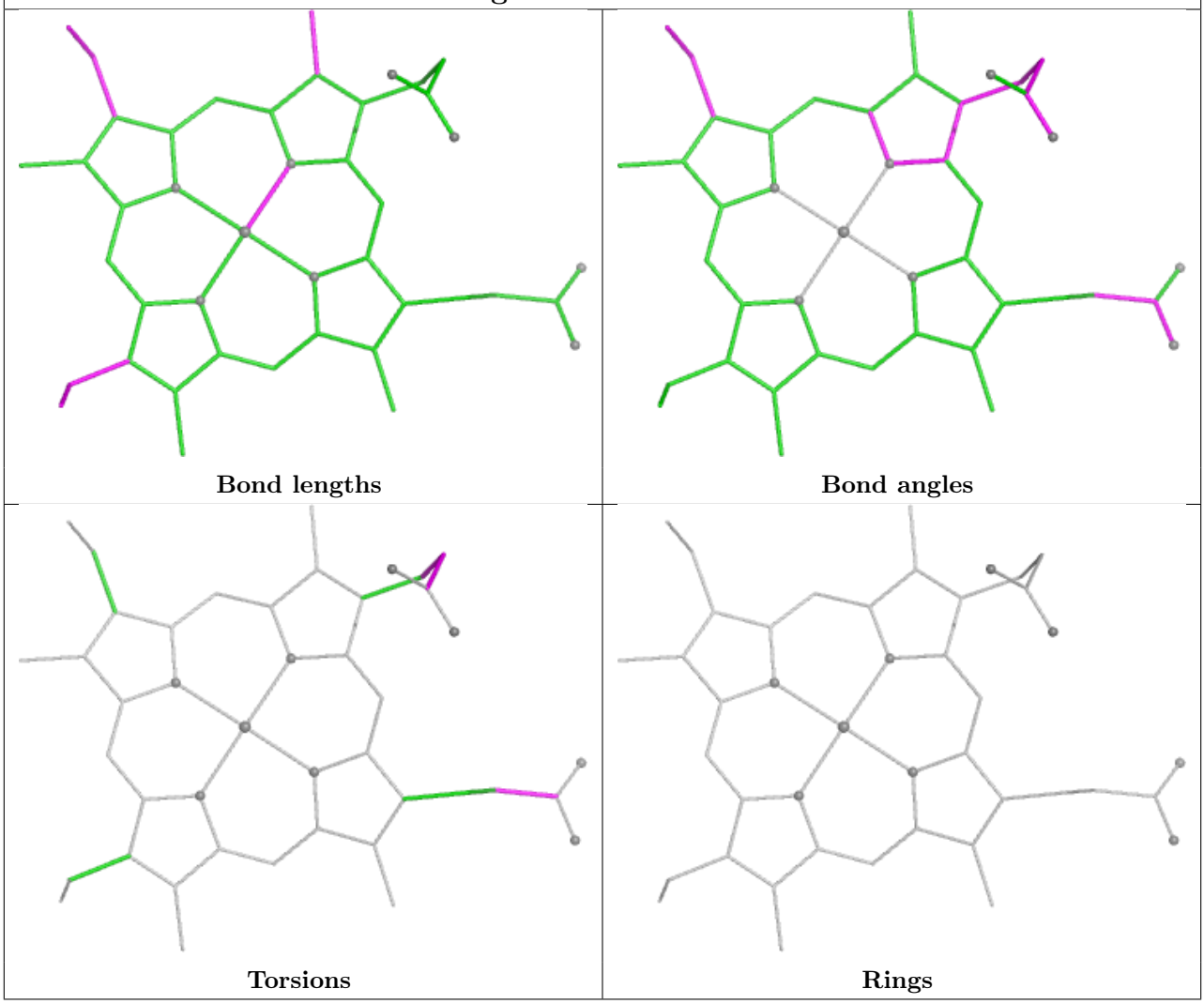
Torsions



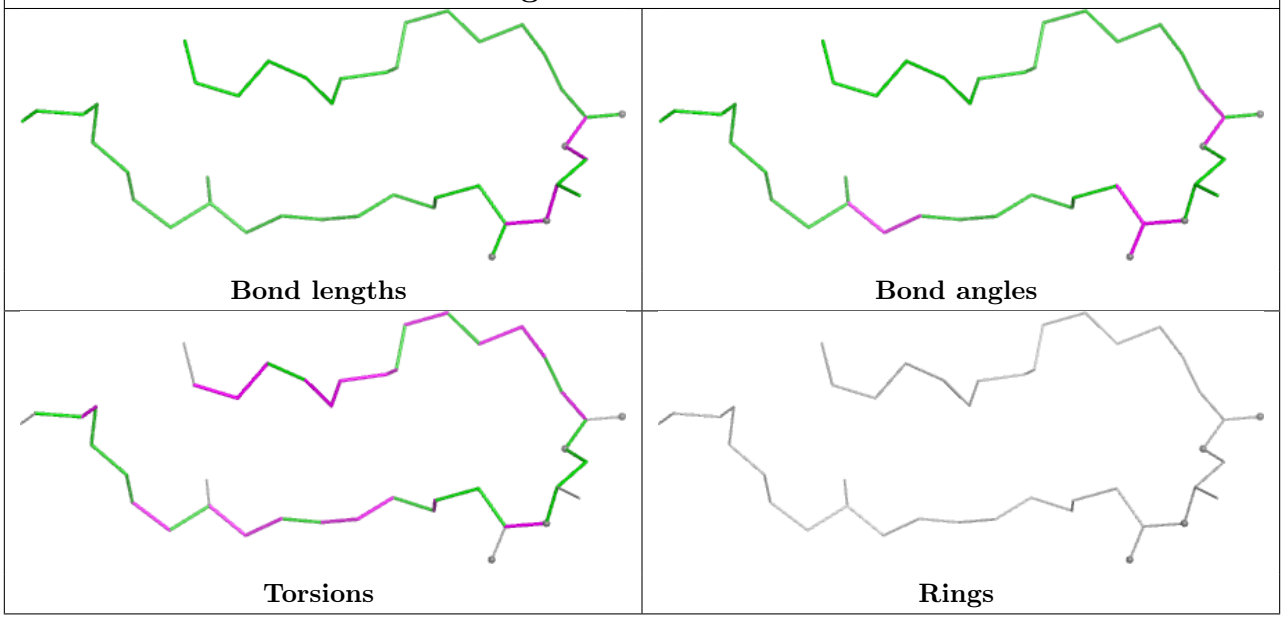
Rings

Ligand CDL H 1004	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand HEC O 301



Ligand 9XX W 202



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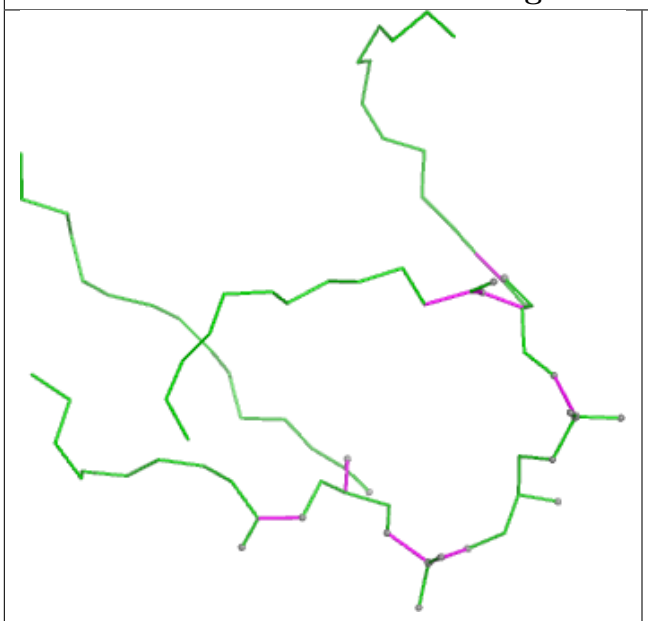
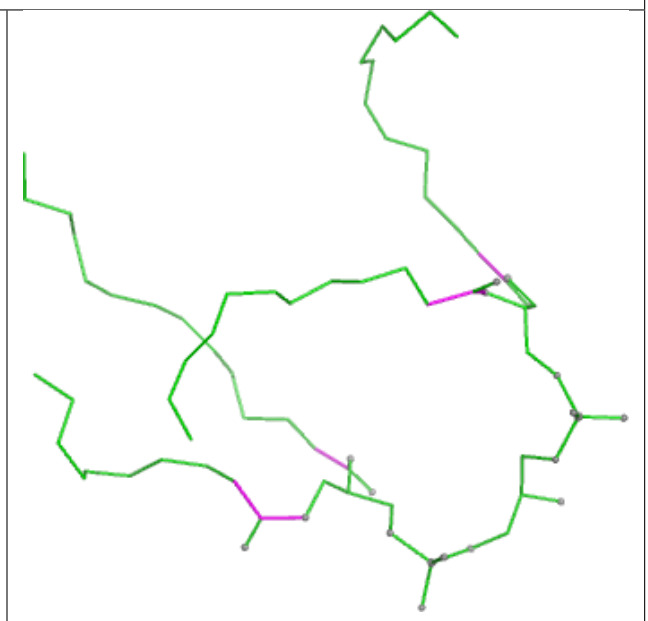
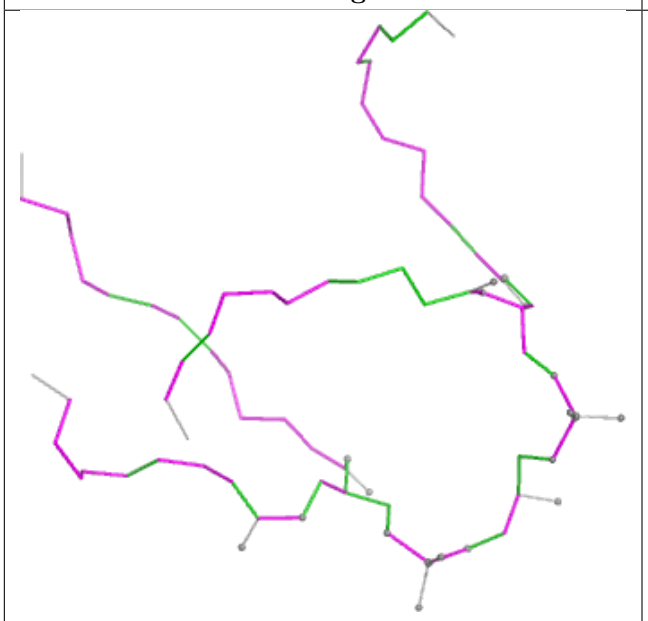


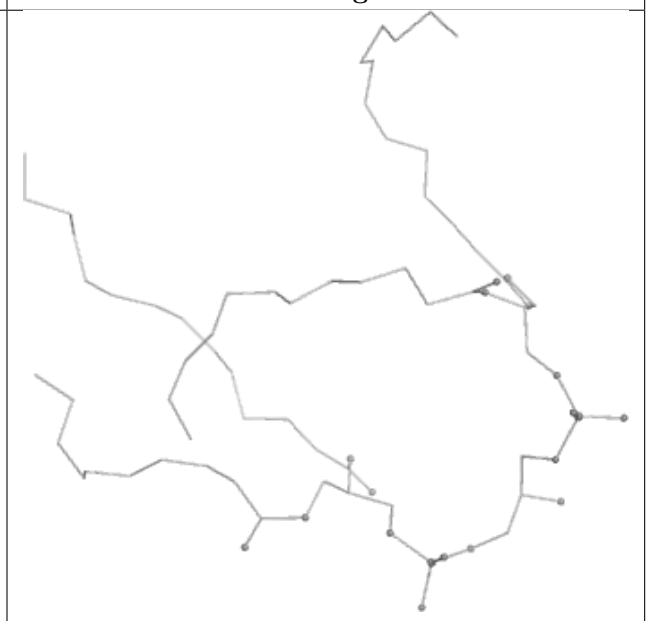
Bond lengths



Bond angles

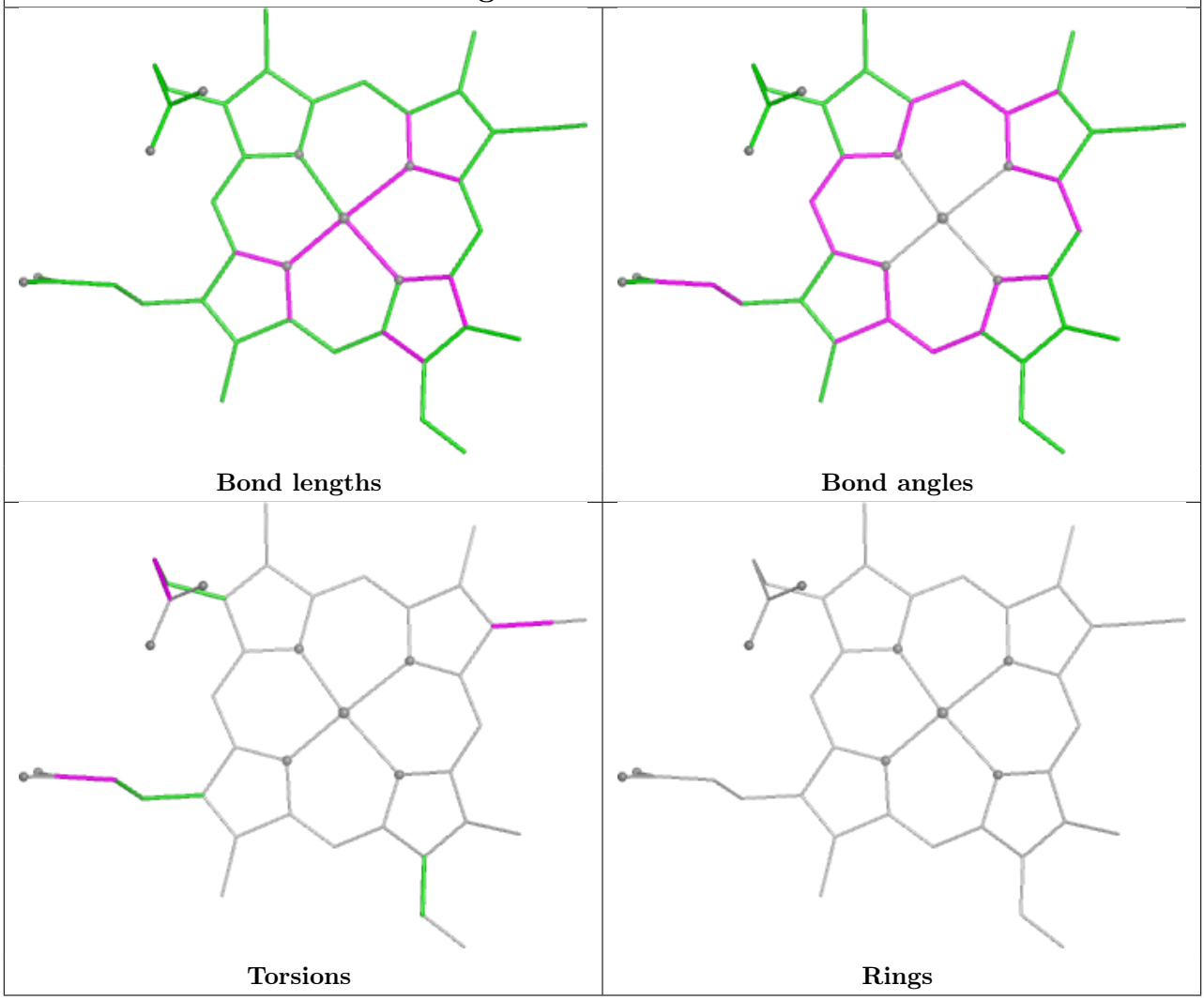


Torsions



Rings

Ligand HEM H 1007



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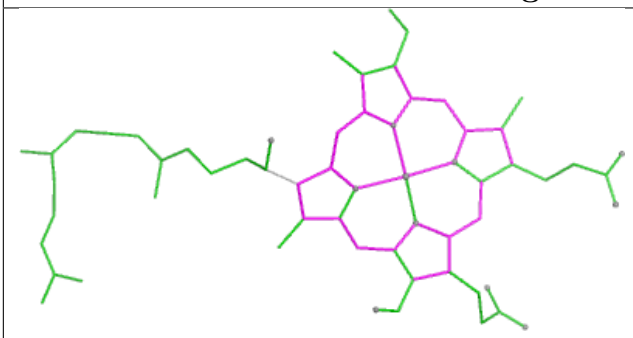
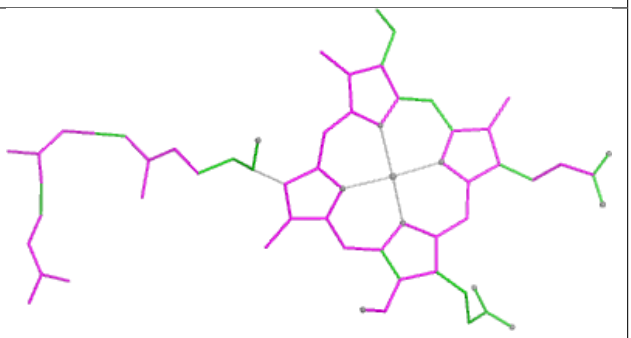
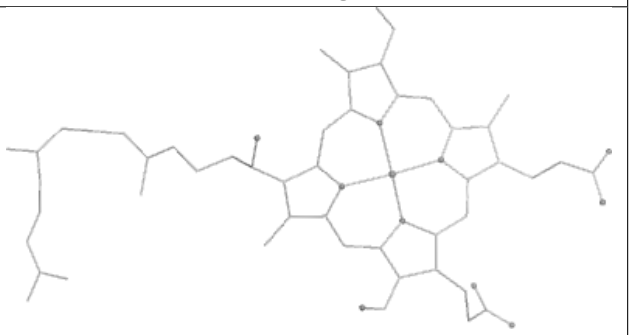


Bond lengths



Bond angles

Torsions

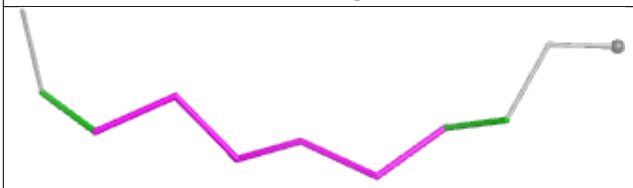


Rings

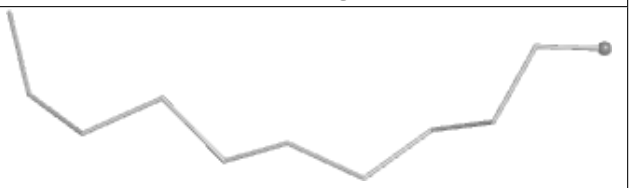
Ligand PLM L 610

Bond lengths

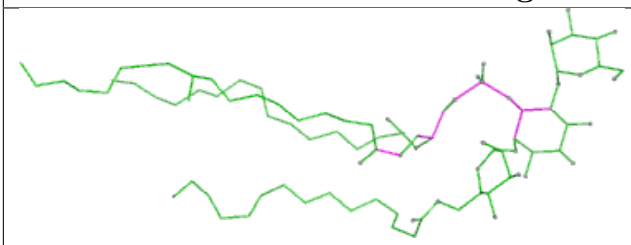
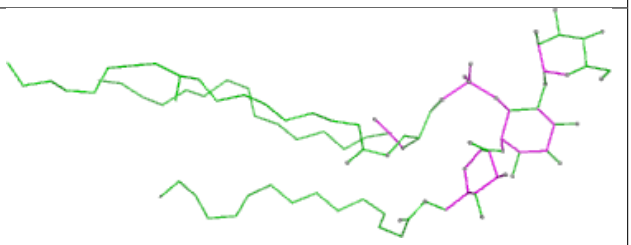
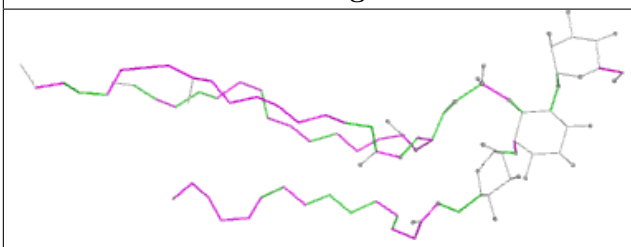
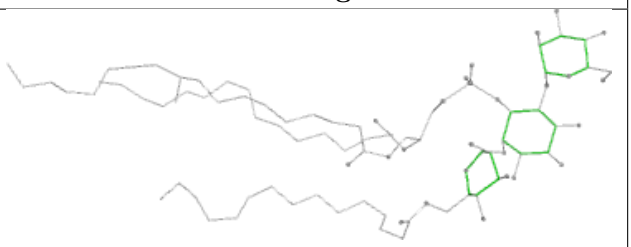
Bond angles

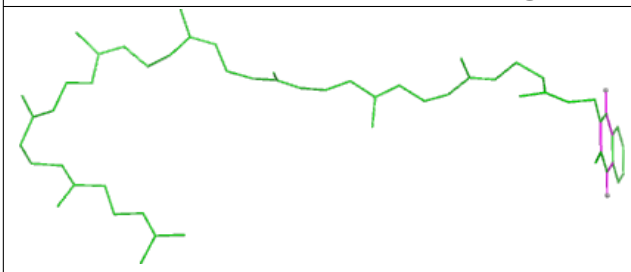
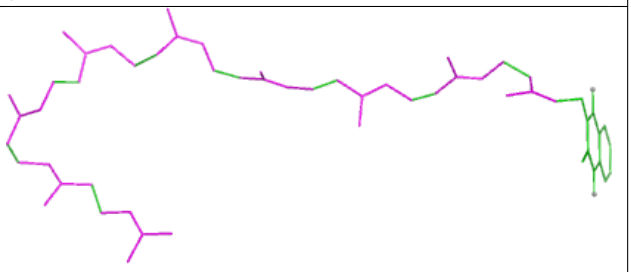
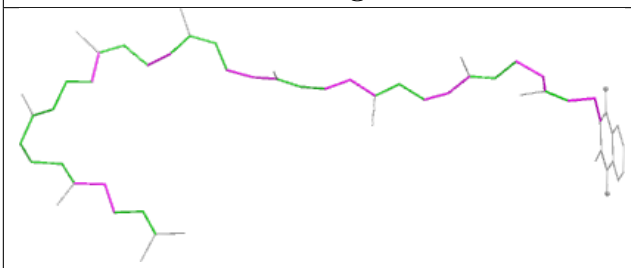
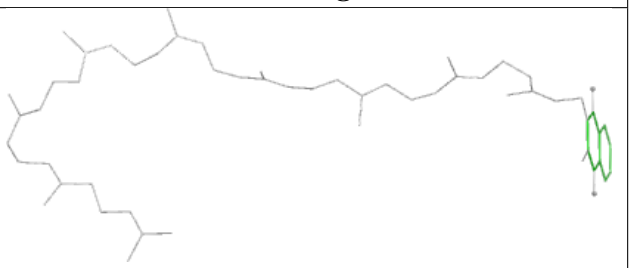


Torsions

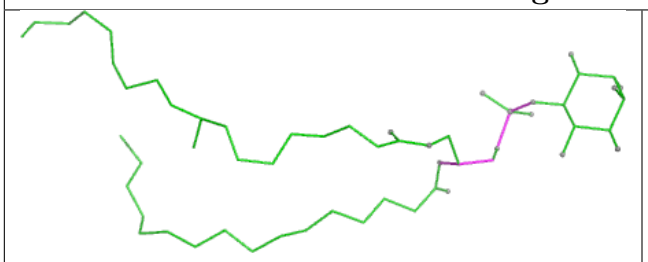


Rings

Ligand WUO P 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 N 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9YF b 201



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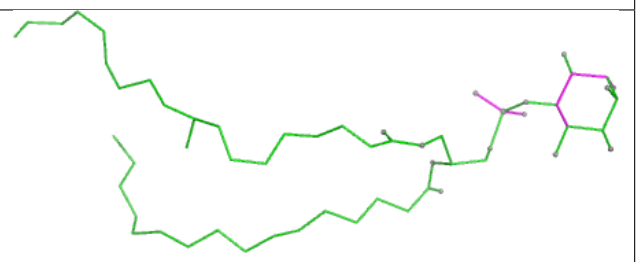
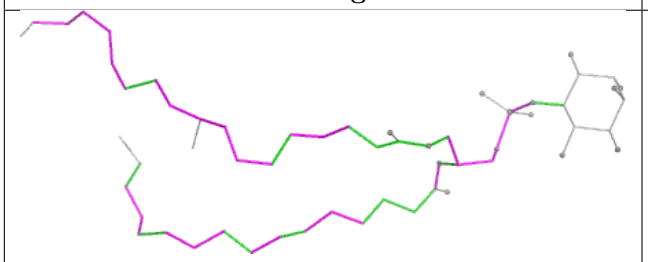


Bond angles



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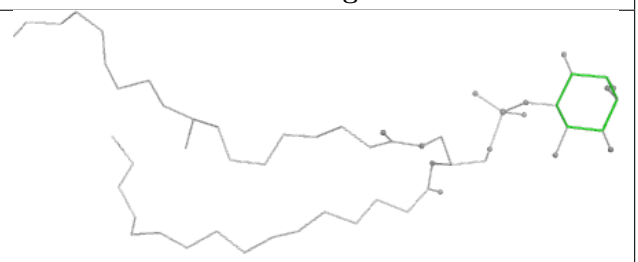
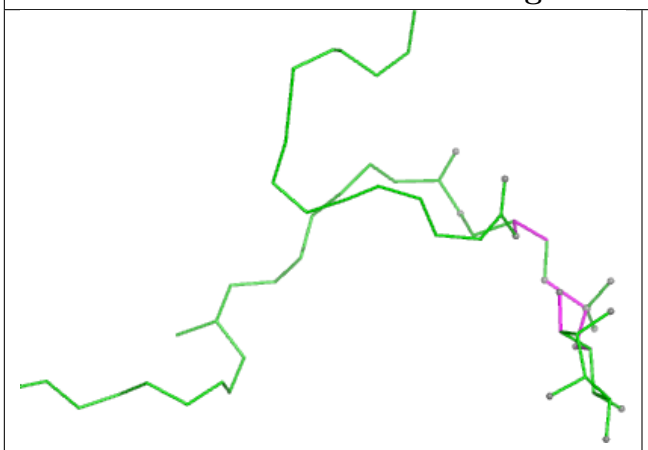
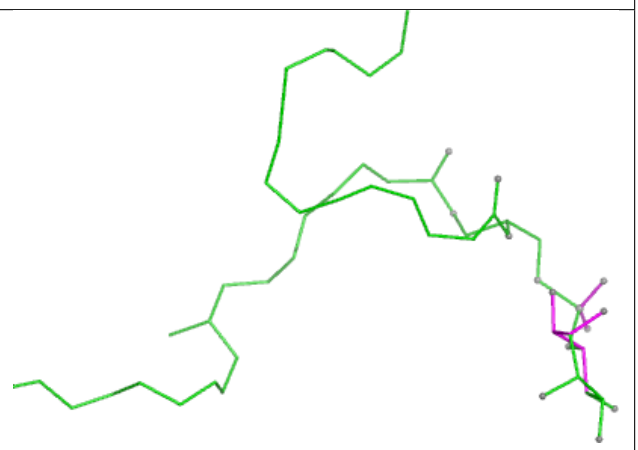


Rings

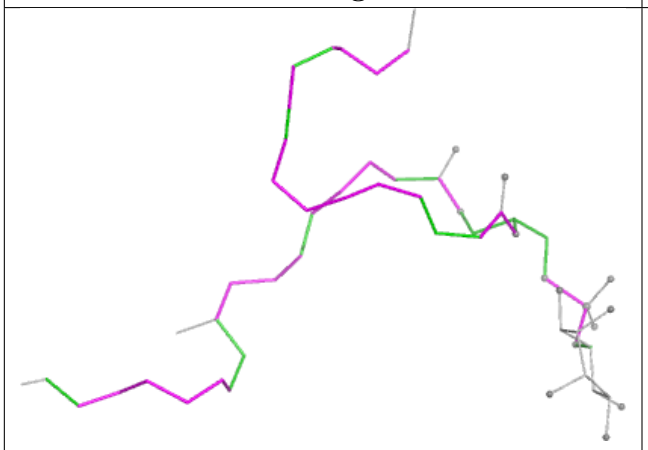
Ligand 9YF M 503



Bond lengths



Bond angles



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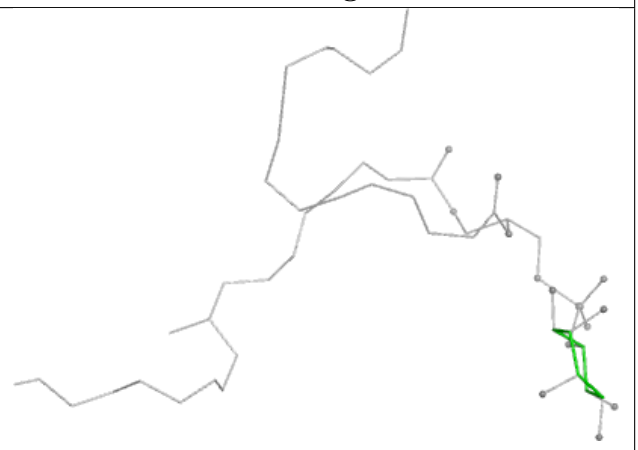
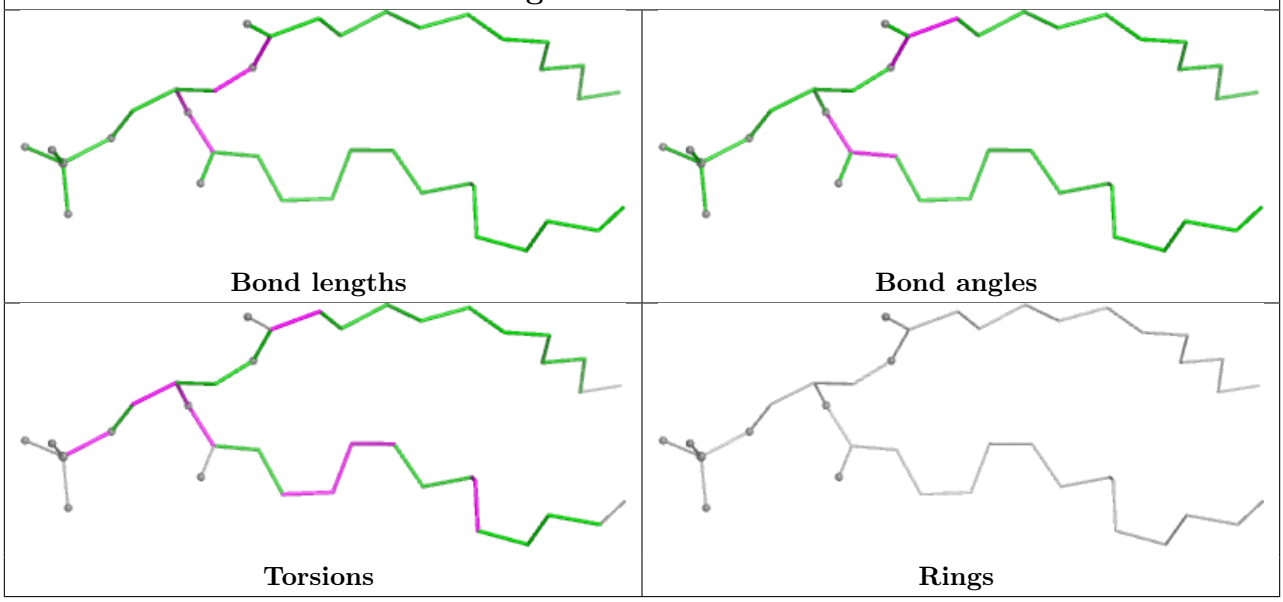
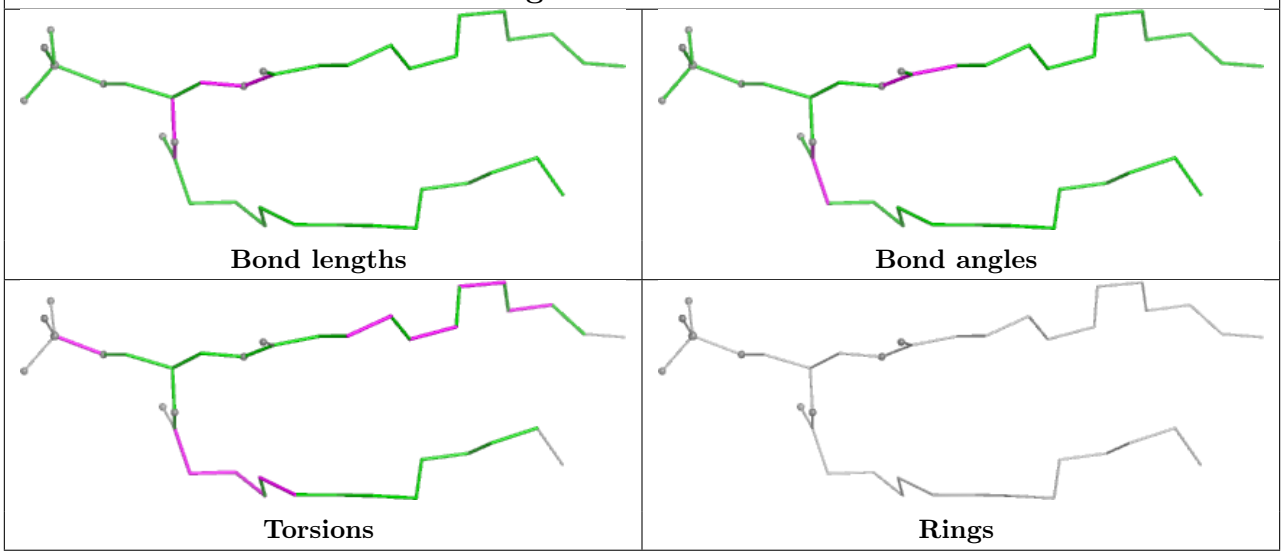


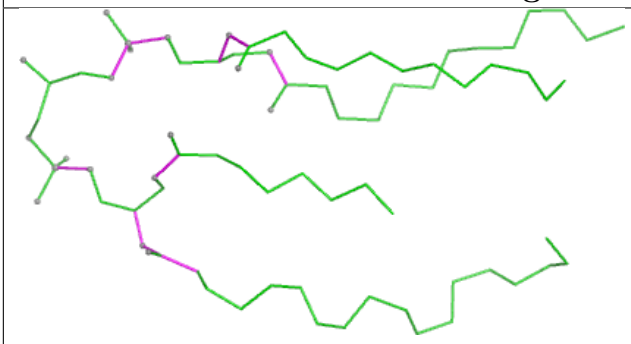
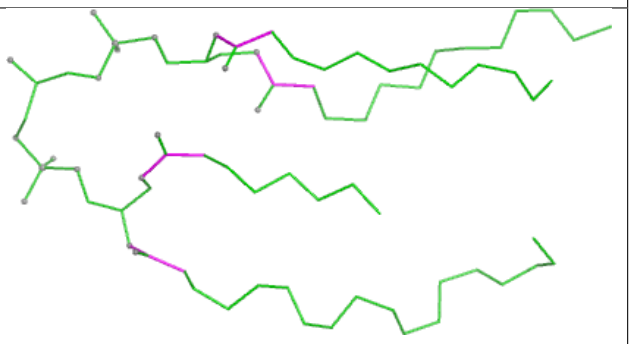
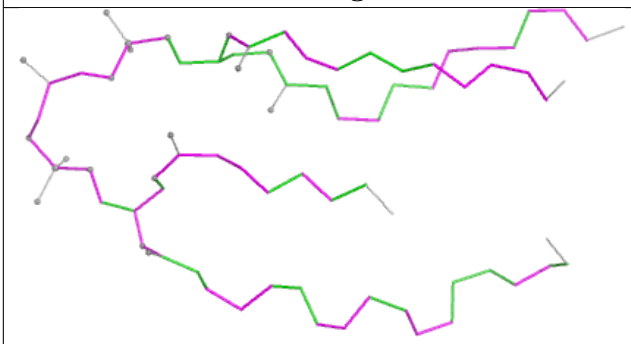
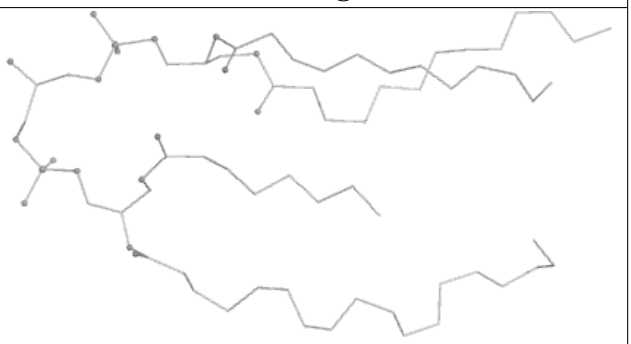
Rings

Ligand 7PH G 504

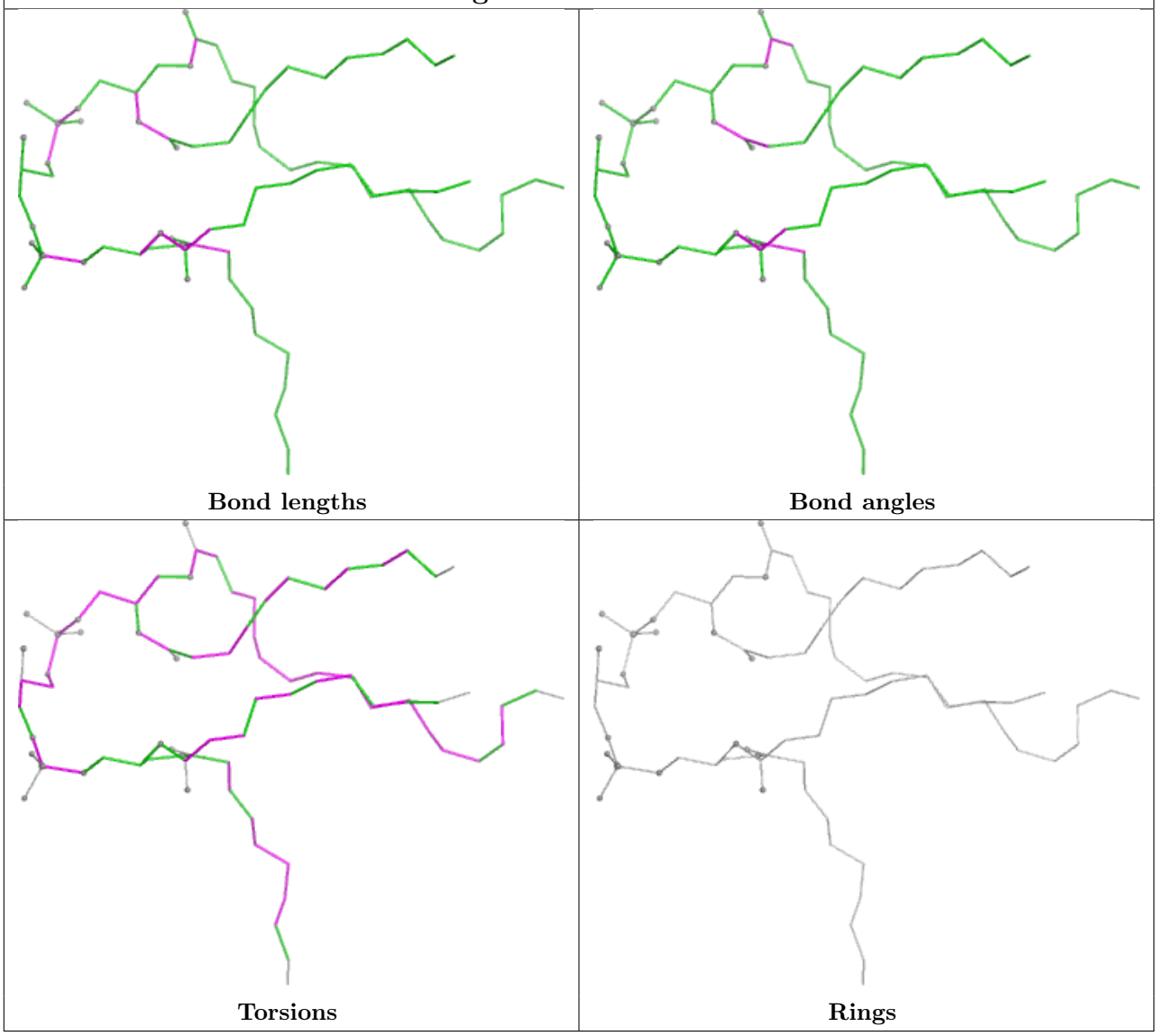


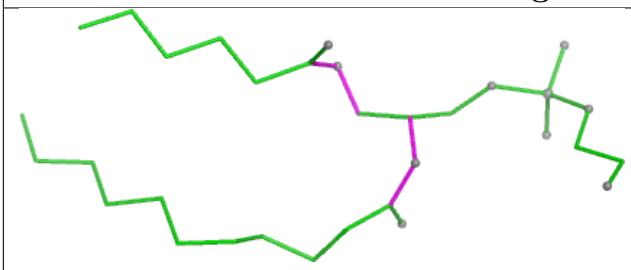
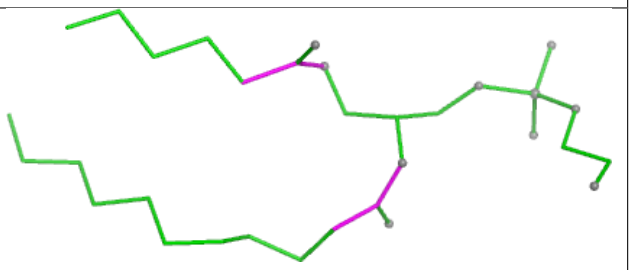
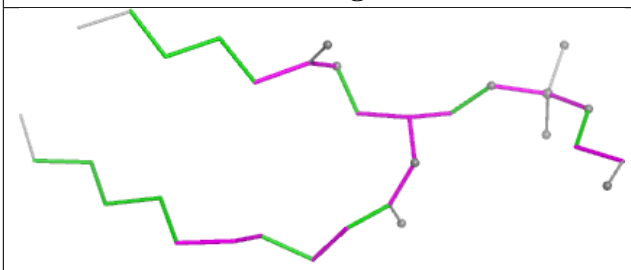
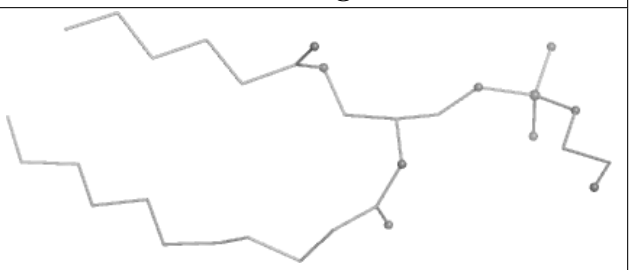
Ligand 7PH G 505

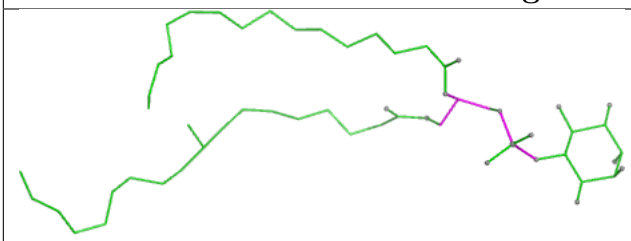
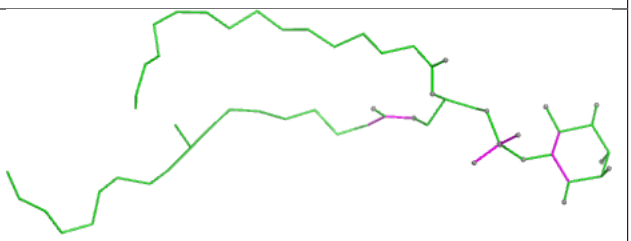
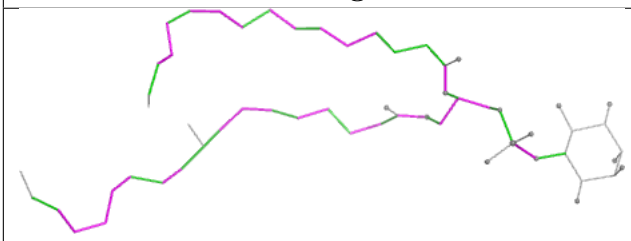
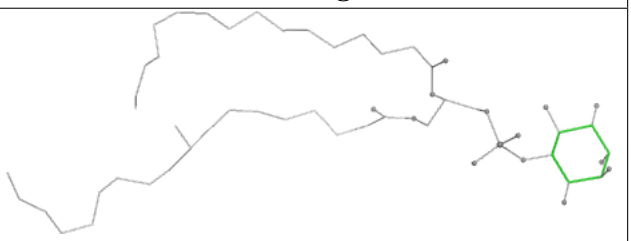


Ligand CDL N 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

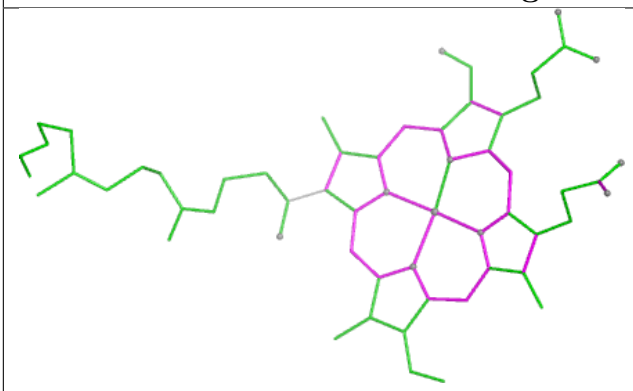
Ligand CDL K 201



Ligand 3PE S 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9YF W 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA R 603



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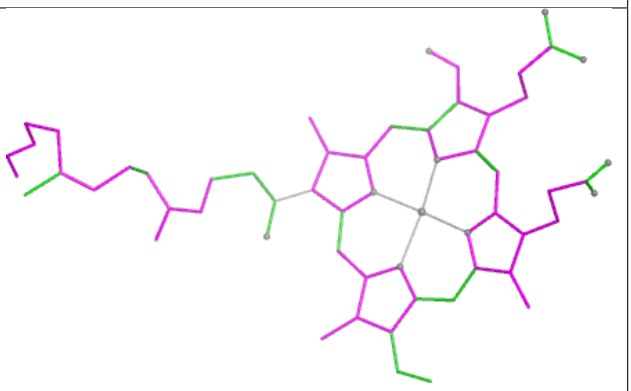
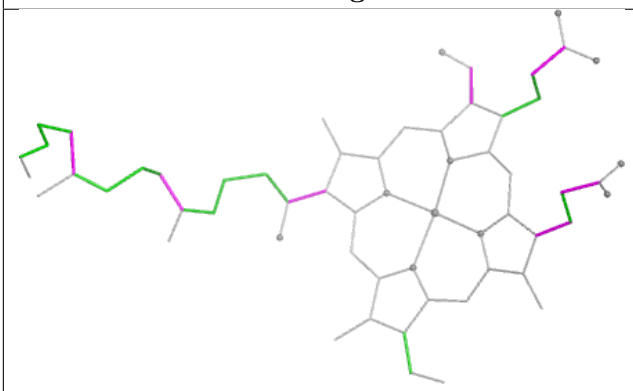


Bond angles



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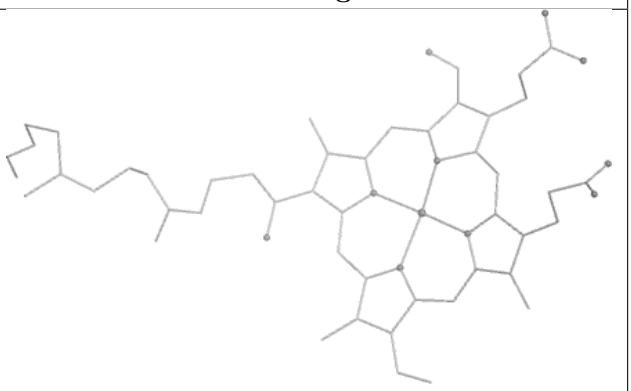
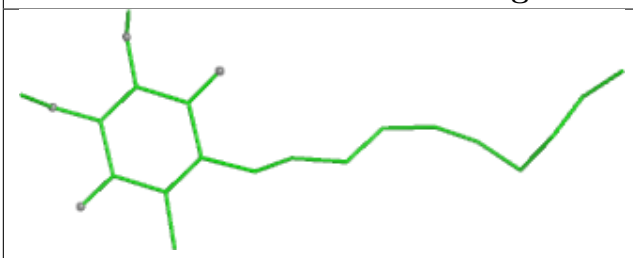
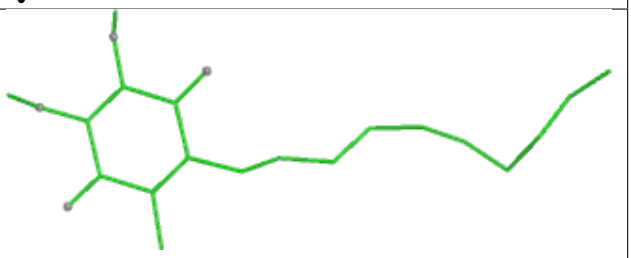


Rings

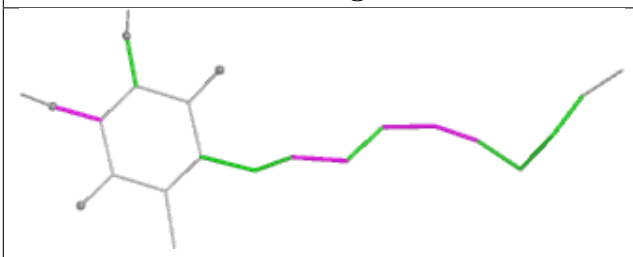
Ligand DCQ H 1008



Bond lengths



Bond angles



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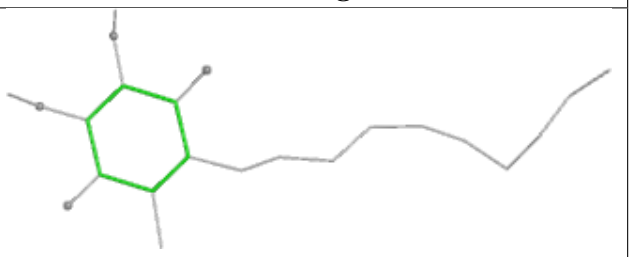
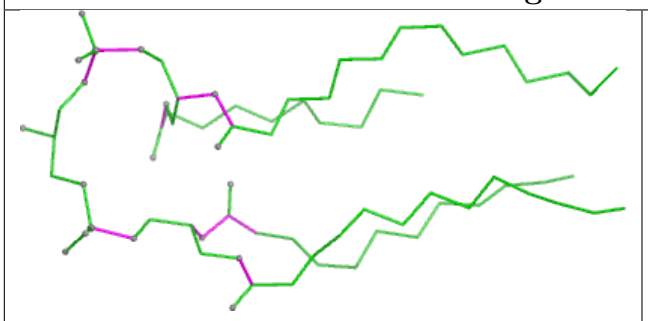
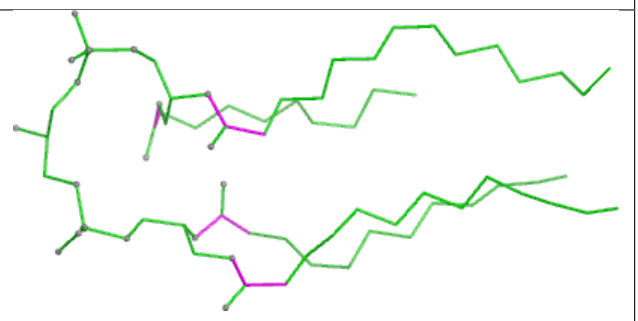


Rings

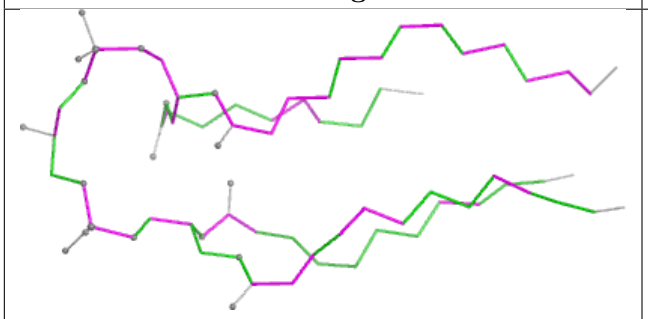
Ligand CDL R 601



Bond lengths



Bond angles



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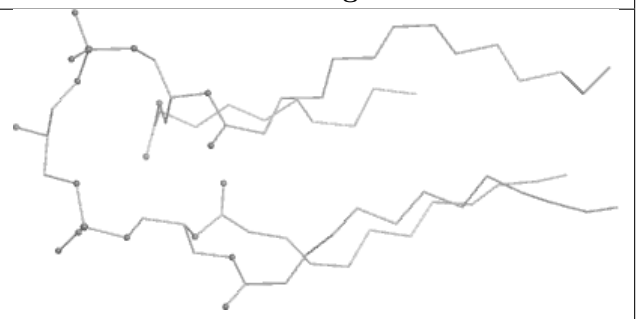
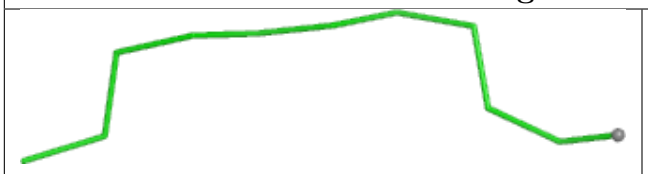


Rings

Ligand PLM W 203



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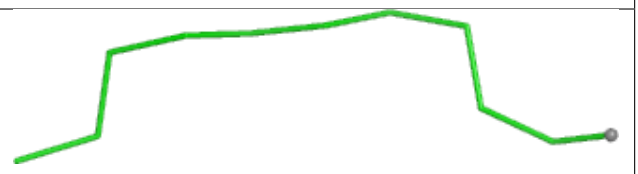

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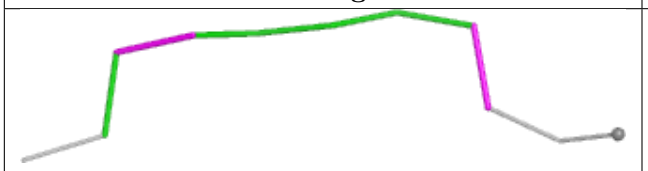

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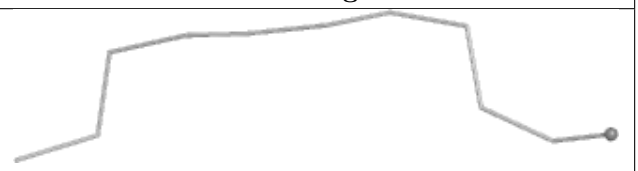
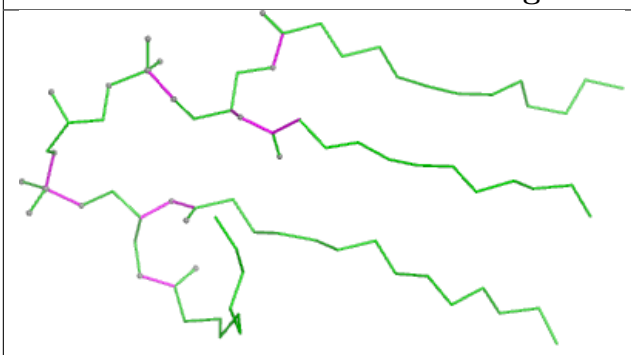
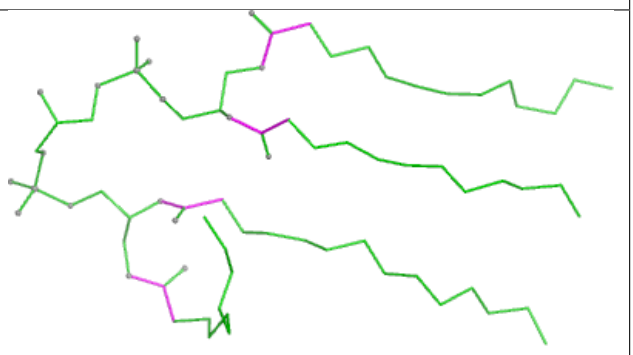
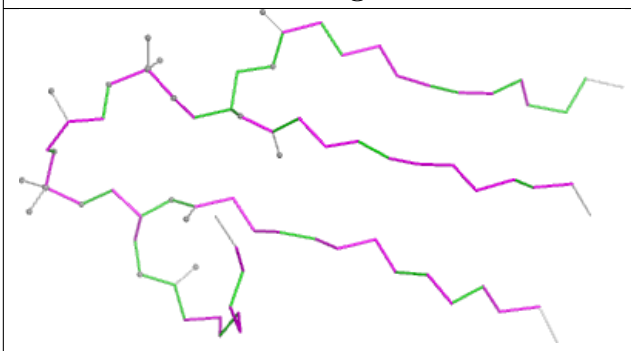
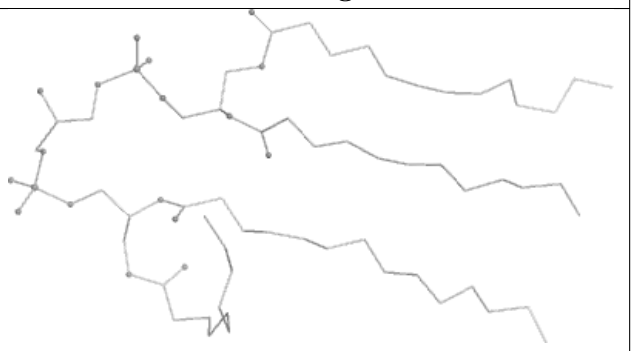
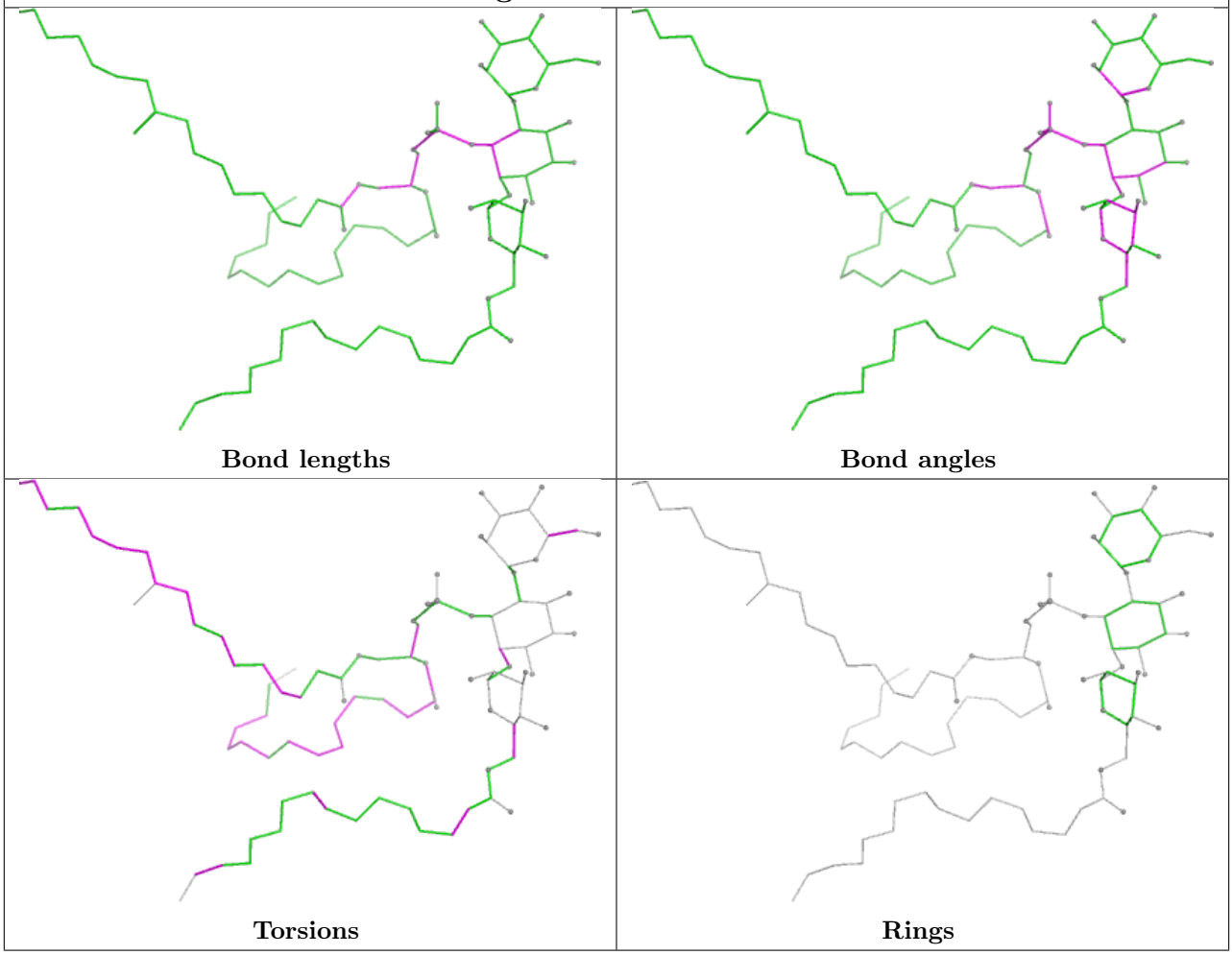
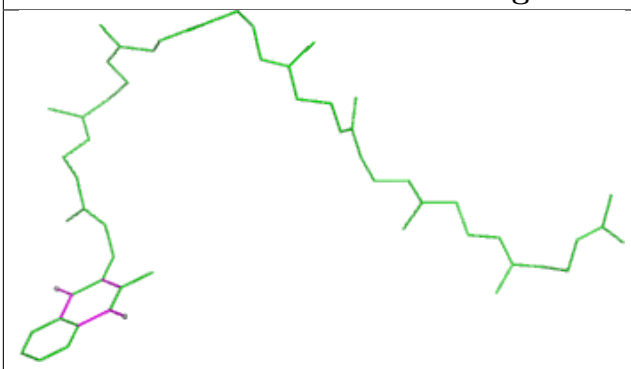
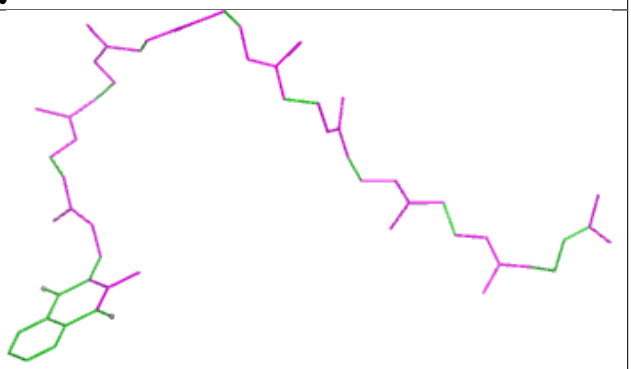
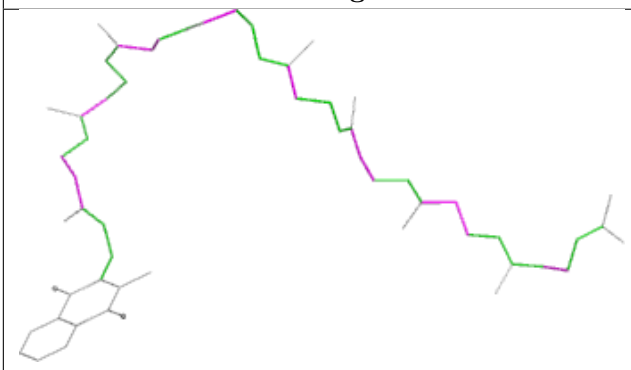
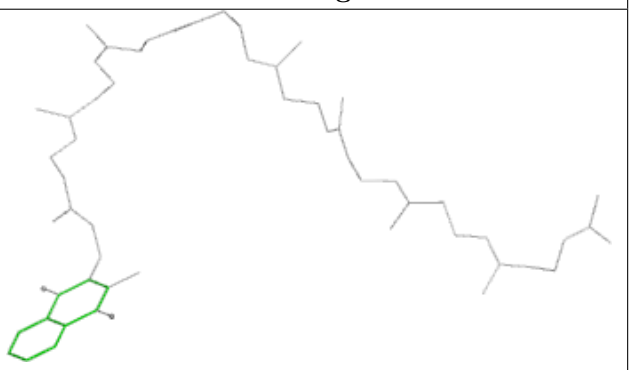


Rings

Ligand CDL N 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WUO O 304



Ligand MQ9 H 1006	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

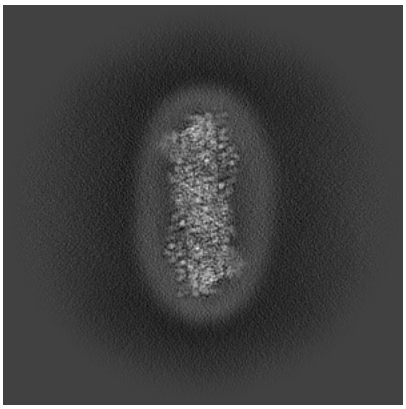
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-53065. These allow visual inspection of the internal detail of the map and identification of artifacts.

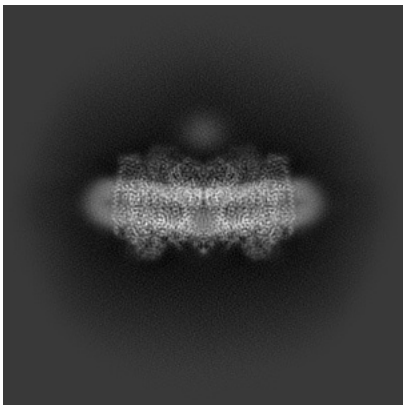
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

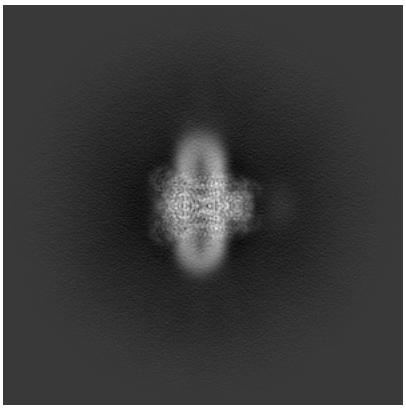
6.1.1 Primary map



X

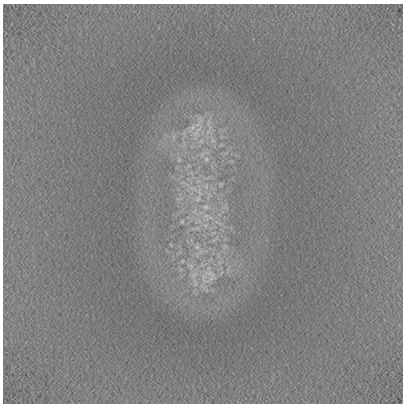


Y

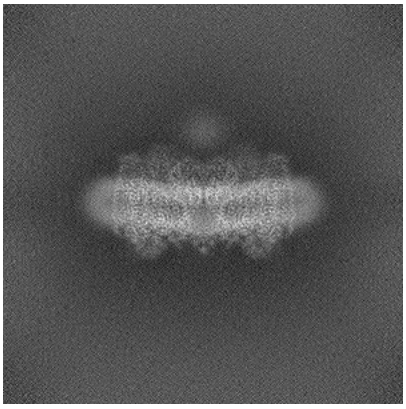


Z

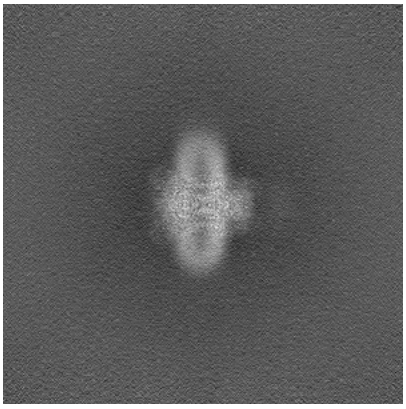
6.1.2 Raw map



X



Y

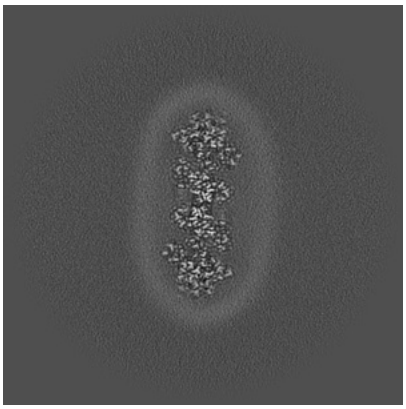


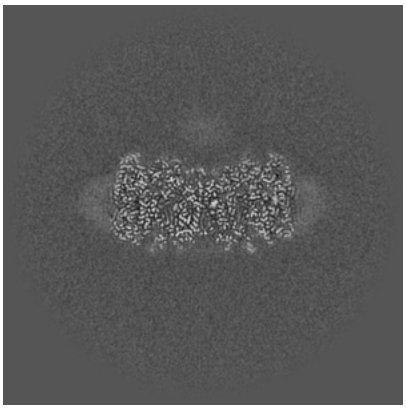
Z

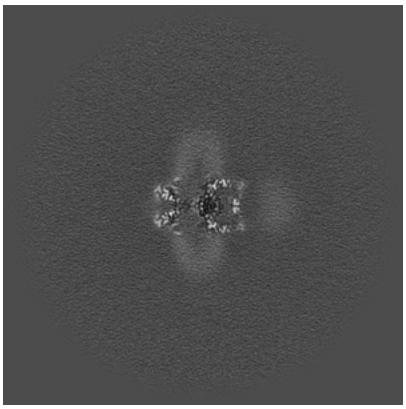
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

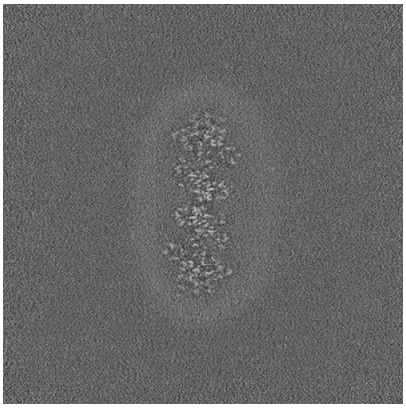
6.2.1 Primary map

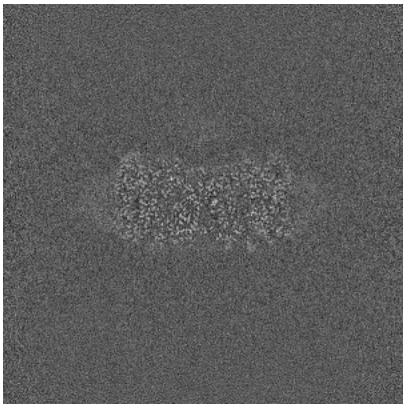

X Index: 270

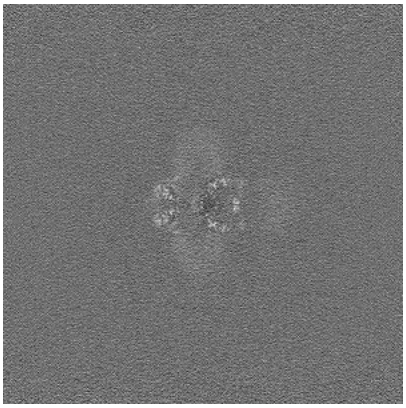

Y Index: 270


Z Index: 270

6.2.2 Raw map


X Index: 270

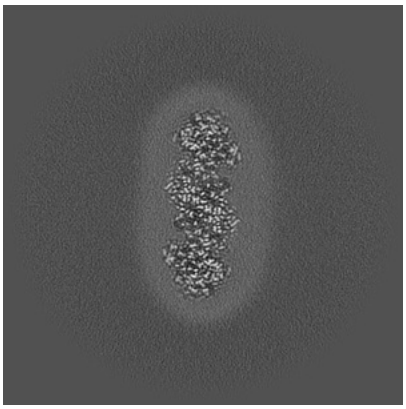

Y Index: 270

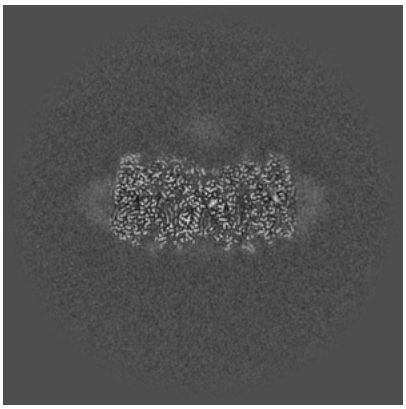

Z Index: 270

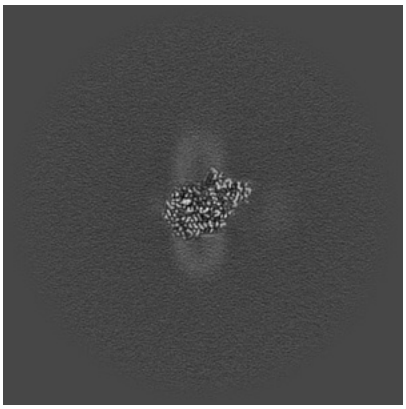
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

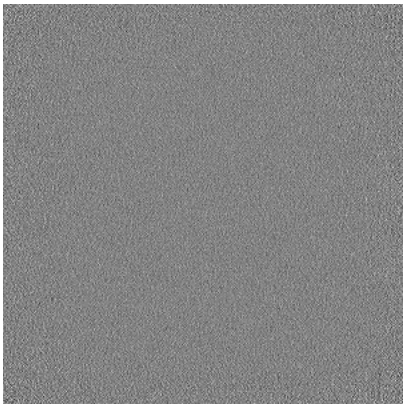
6.3.1 Primary map

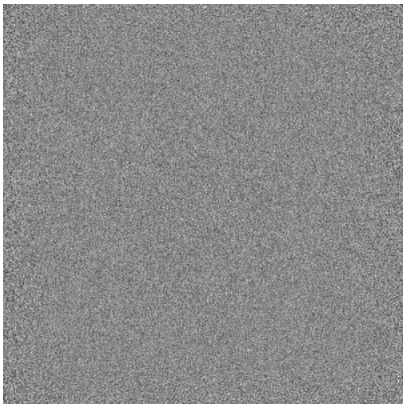

X Index: 284

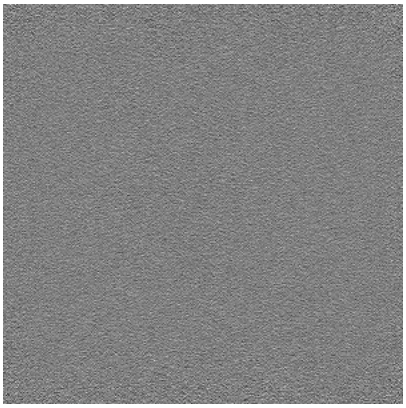

Y Index: 271


Z Index: 248

6.3.2 Raw map


X Index: 0

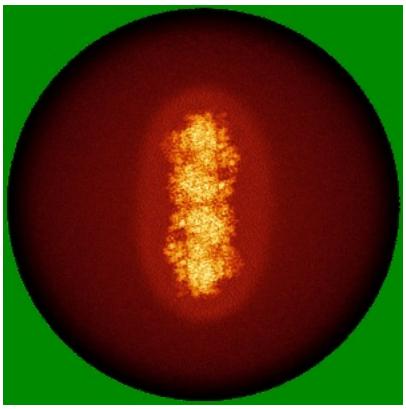

Y Index: 0

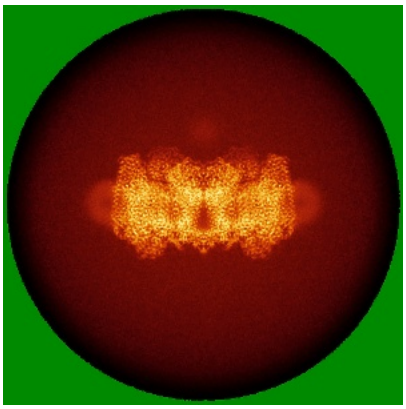

Z Index: 0

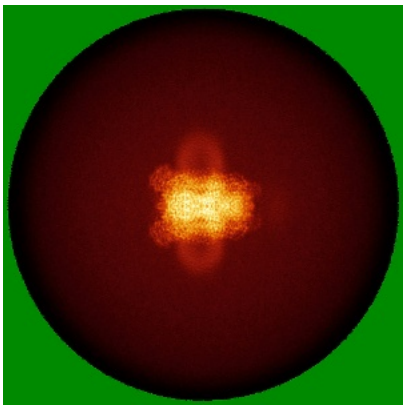
The images above show the largest variance slices of the map in three orthogonal directions.

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

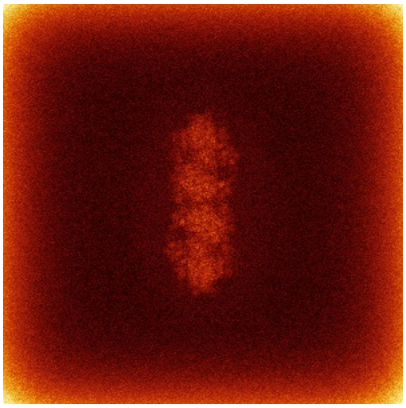
6.4.1 Primary map

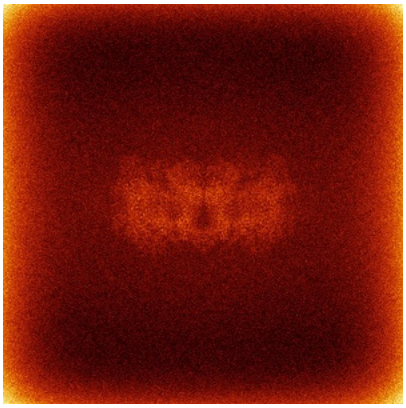

X

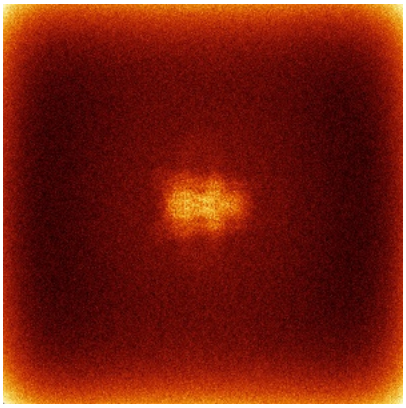

Y


Z

6.4.2 Raw map


X

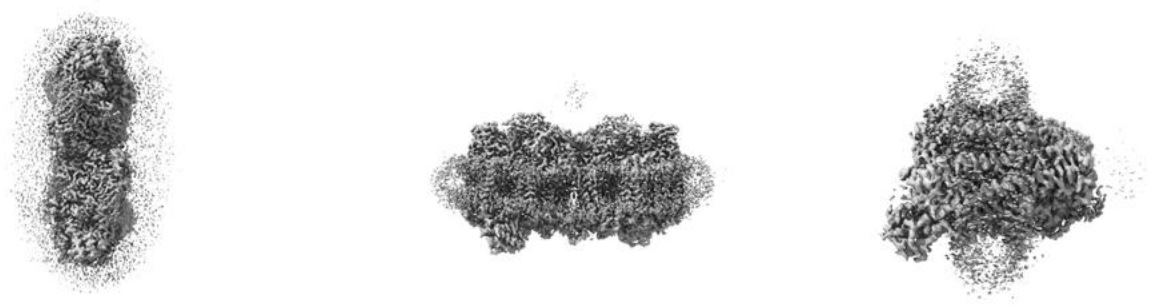

Y


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)

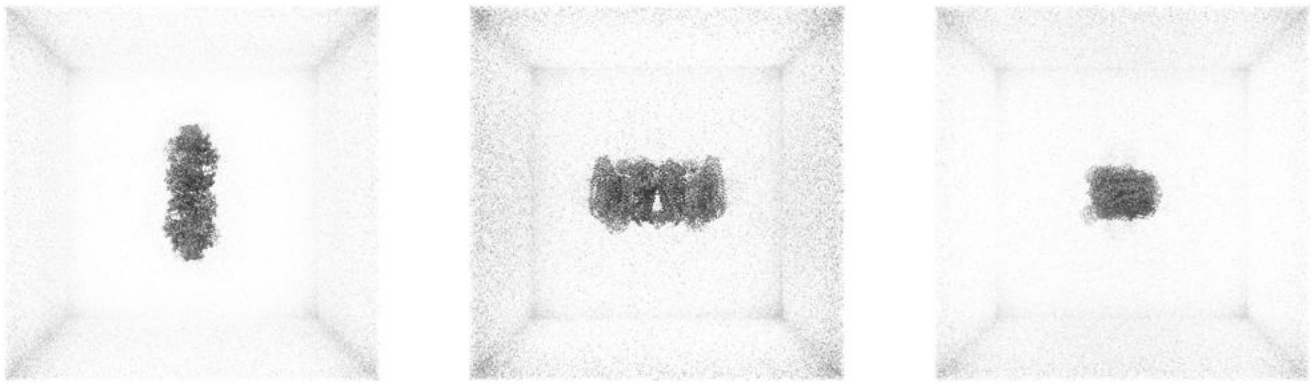
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.129. 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.

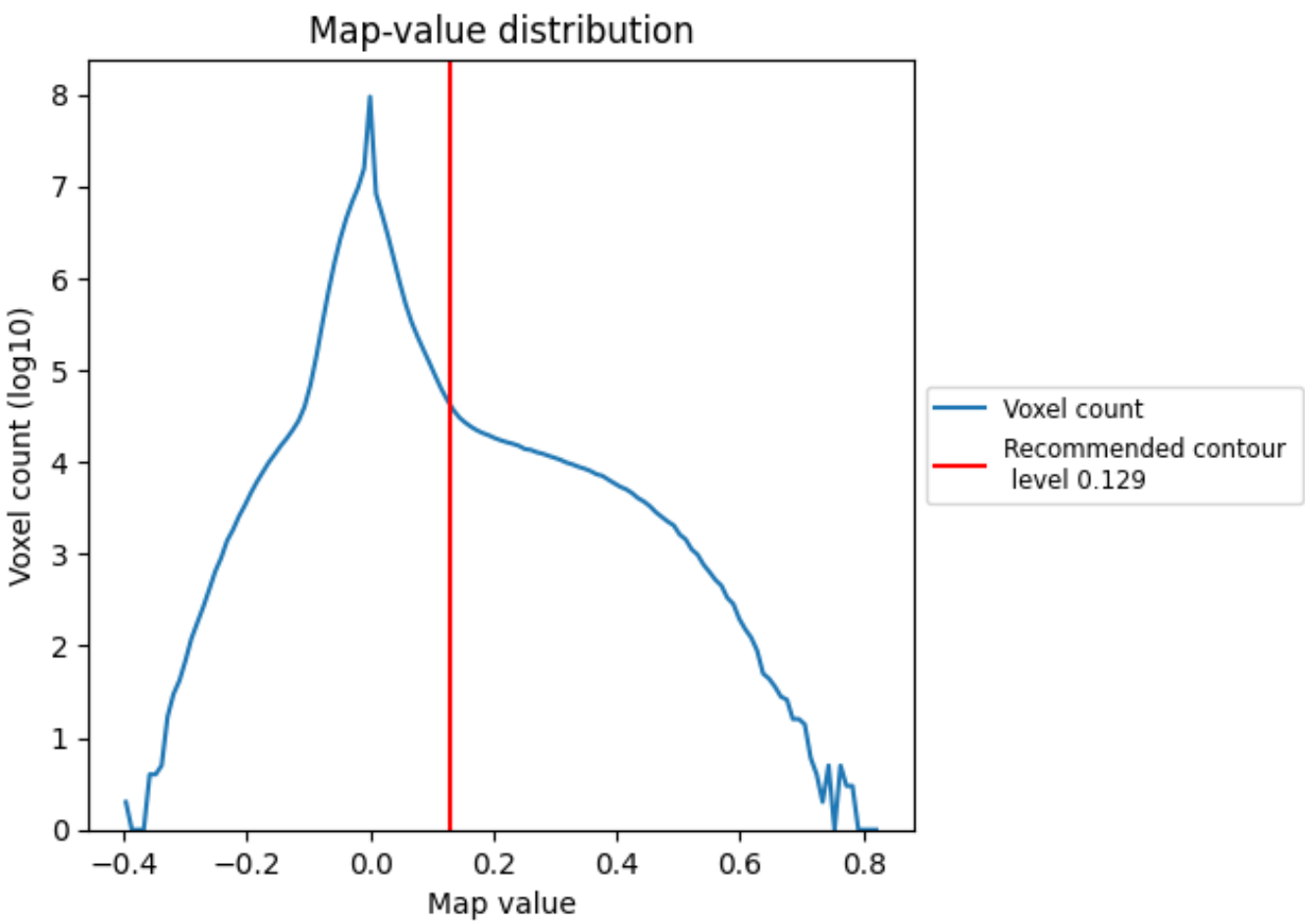
6.6 Mask visualisation (i)

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

7 Map analysis (i)

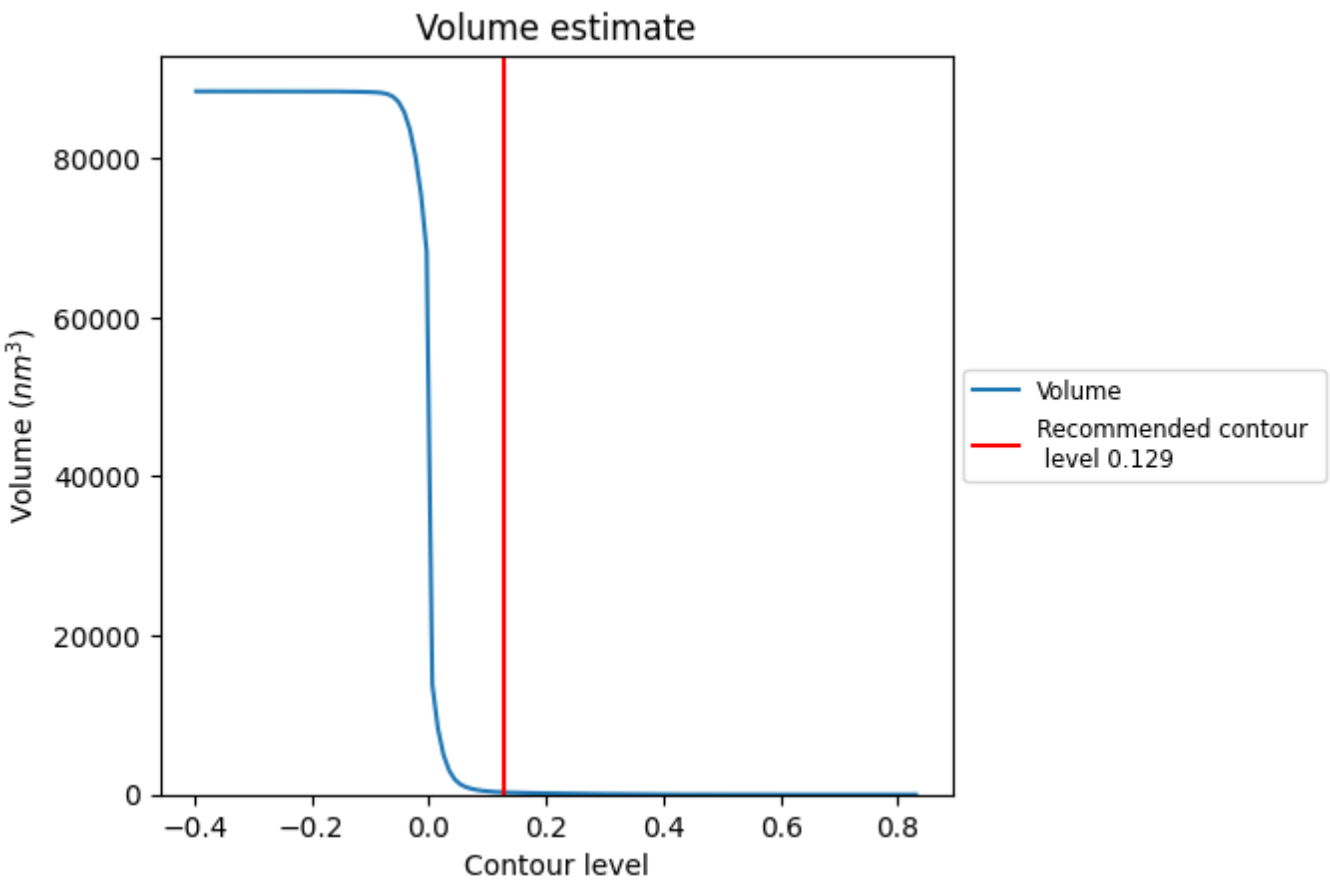
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

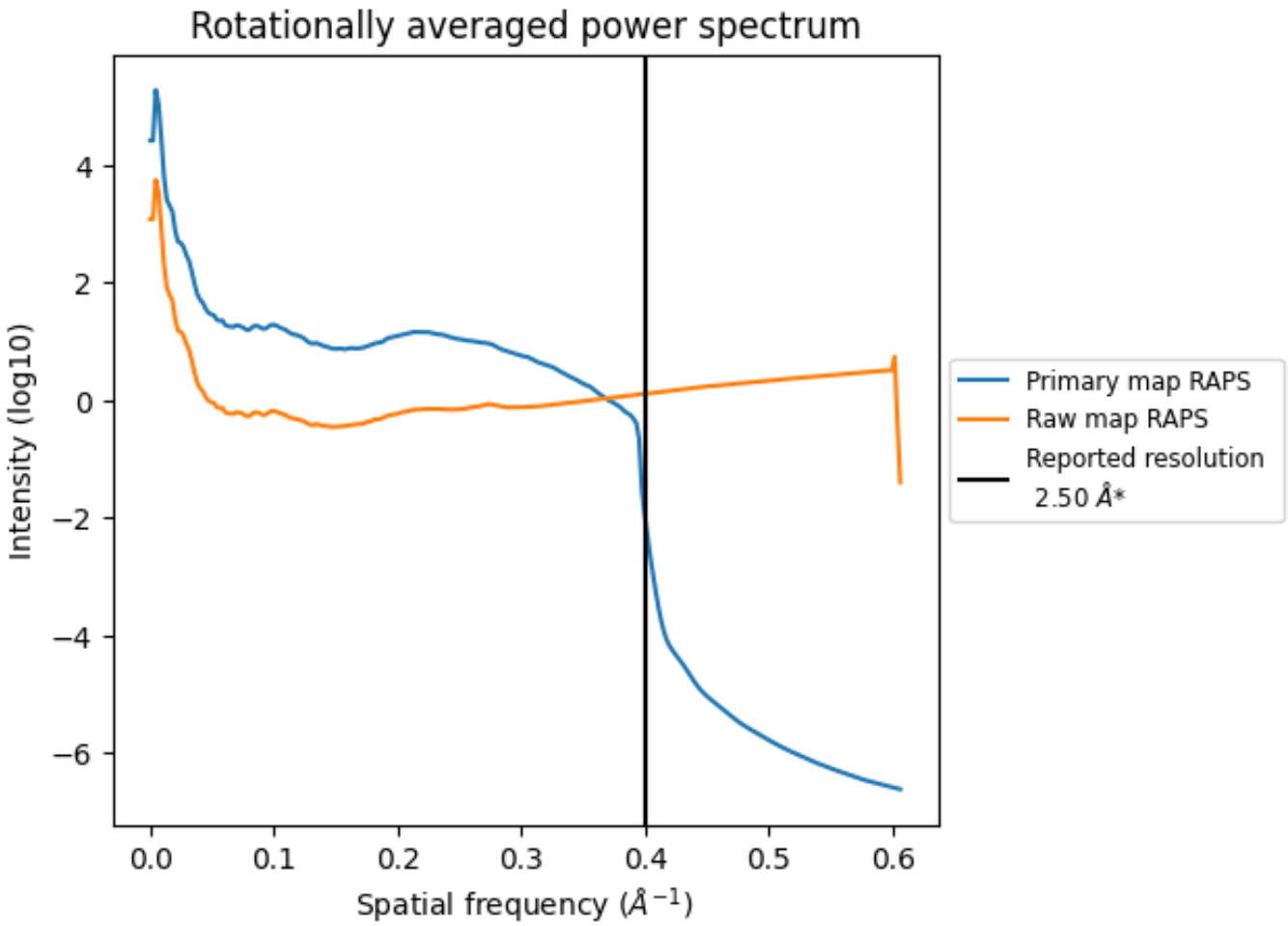
7.2 Volume estimate (i)



The volume at the recommended contour level is 277 nm^3; this corresponds to an approximate mass of 250 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)

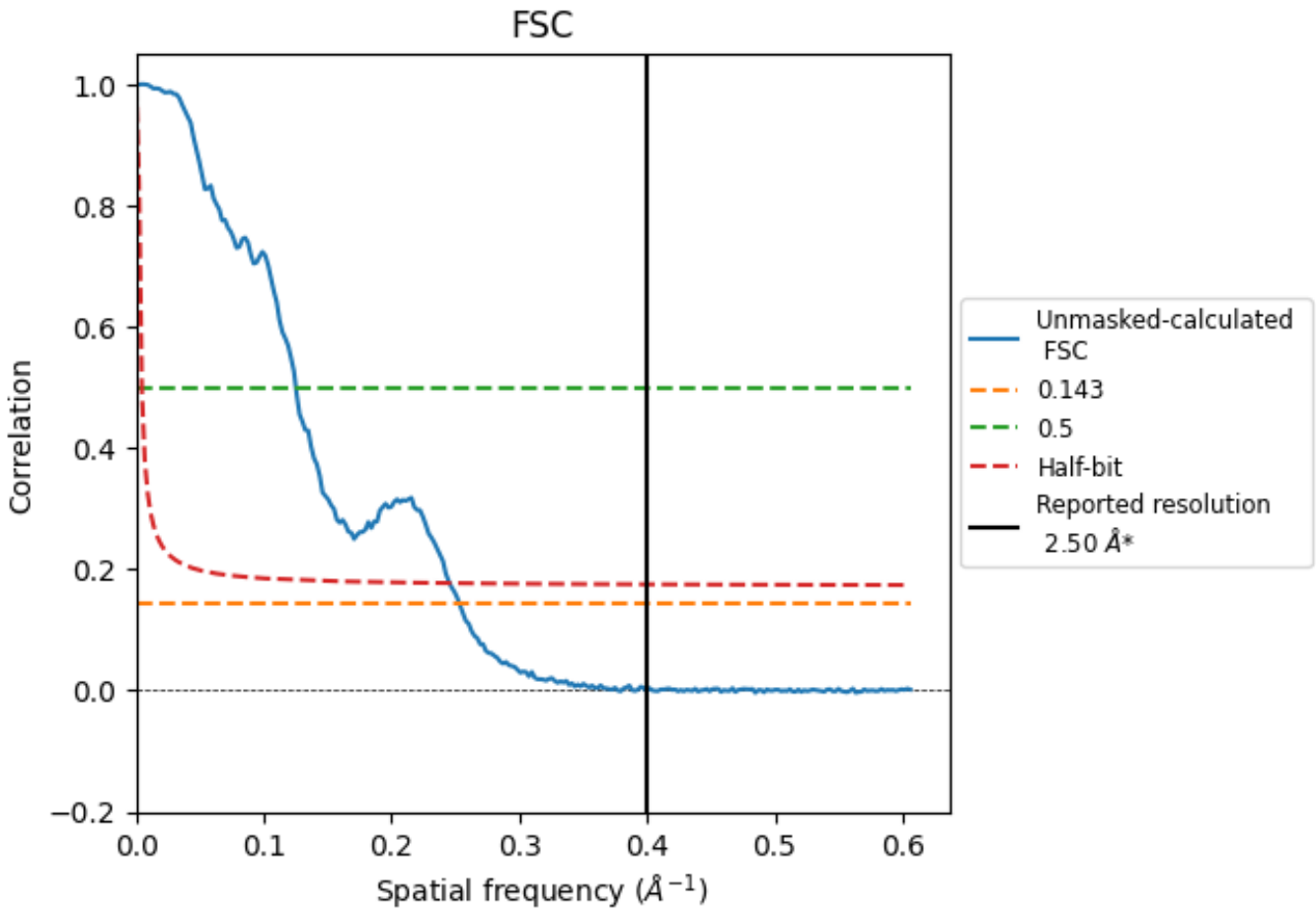


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

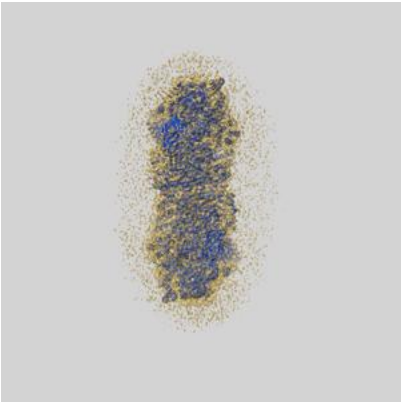
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	8.00	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.5 by more than 10 %

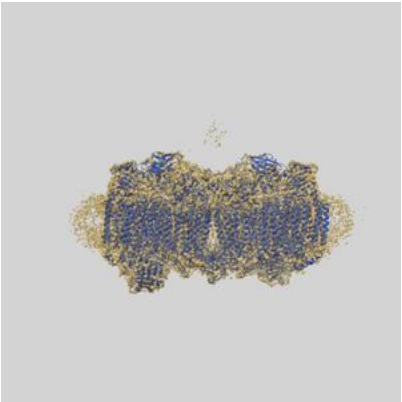
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-53065 and PDB model 9QEF. Per-residue inclusion information can be found in section 3 on page 24.

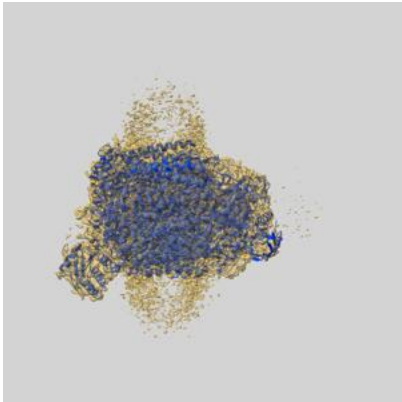
9.1 Map-model overlay (i)



X



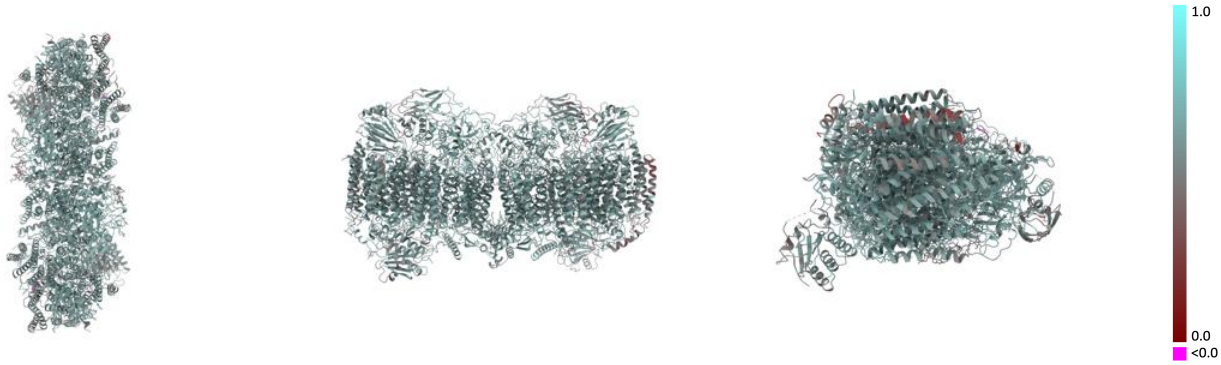
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.129 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.

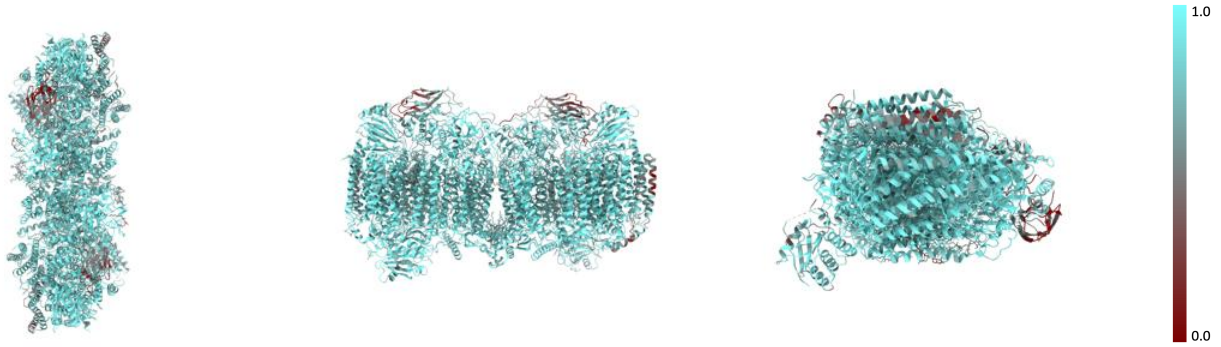
9.2 Q-score mapped to coordinate model (i)



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.

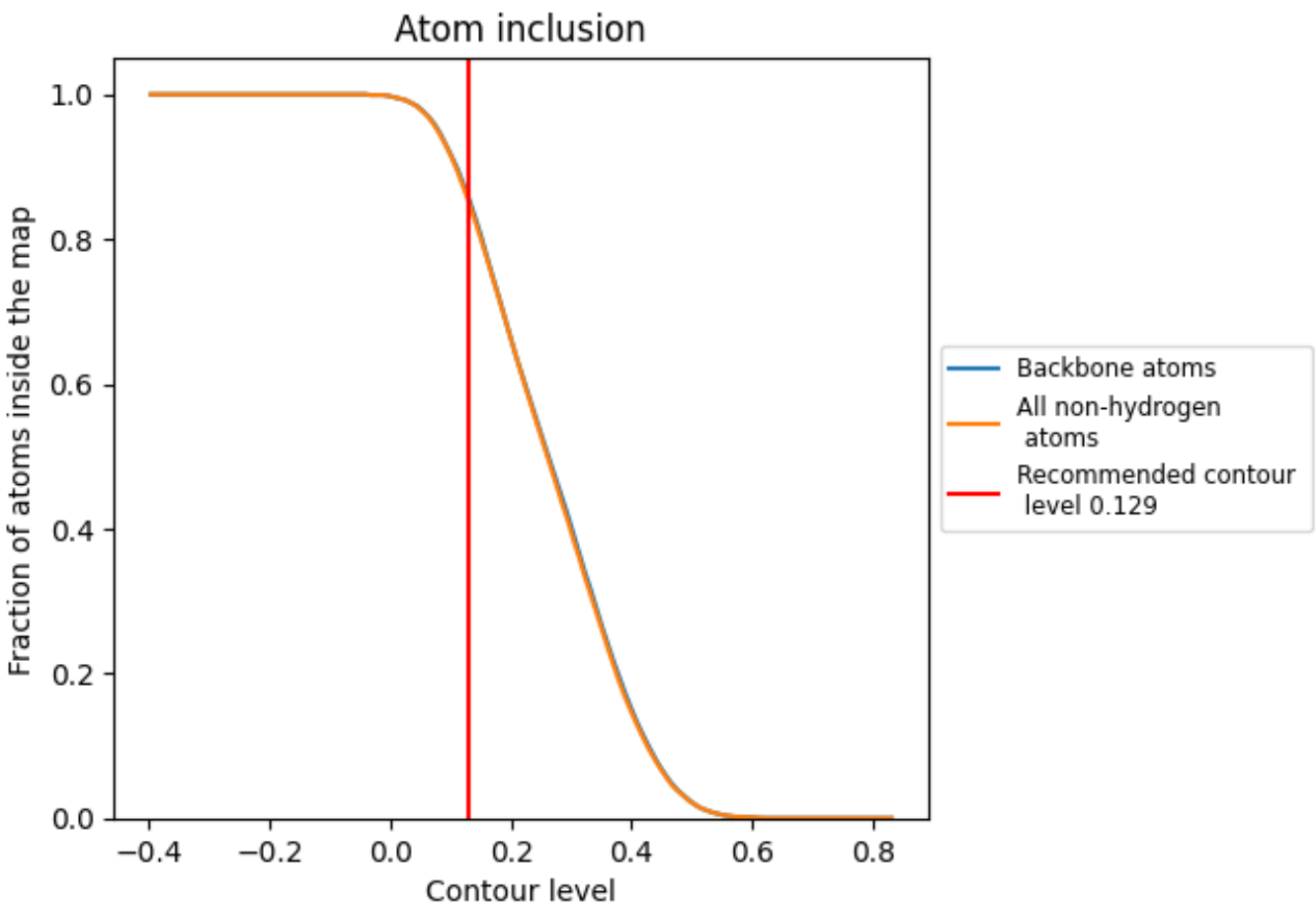
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.129).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.5890
A	0.5220	0.4510
B	0.7760	0.5530
C	0.8540	0.6060
E	0.5720	0.4720
F	0.8370	0.5770
G	0.8840	0.6010
H	0.9270	0.6190
I	0.8030	0.5890
J	0.8580	0.5810
K	0.8880	0.5970
L	0.9080	0.5970
M	0.8990	0.6080
N	0.9260	0.6210
O	0.8870	0.6050
P	0.8080	0.5870
Q	0.8520	0.5670
R	0.9250	0.6040
S	0.8960	0.5900
T	0.8960	0.5990
U	0.8190	0.5560
V	0.8590	0.5600
W	0.5290	0.5440
X	0.8260	0.5640
Y	0.8800	0.5710
Z	0.7760	0.5440
a	0.8070	0.5480
b	0.4120	0.5220
c	0.7860	0.5480