Full wwPDB EM Validation Report

Oct 27, 2024 – 04:09 PM EDT

PDB ID	:	7RH6
EMDB ID	:	EMD-24456
Title	:	Mycobacterial CIII2CIV2 supercomplex, inhibitor free, -Lpqe cyt cc open
Authors	:	Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.
Deposited on	:	2021-07-16
Resolution	:	3.50 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 ⓘ symbol.

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

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

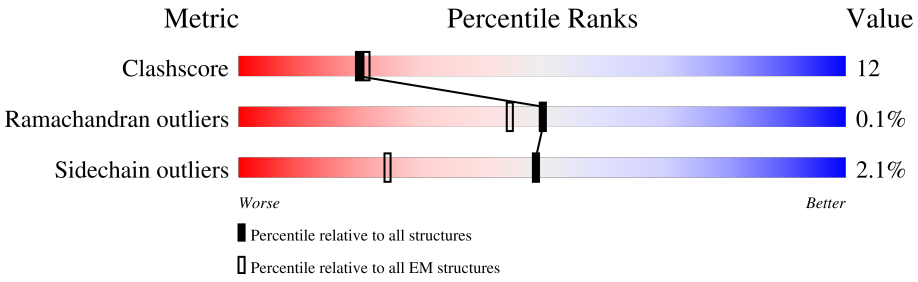
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	I	223	10% 81% 19%
1	O	223	63% 40% 42% 13% 6%
2	L	552	79% 21%
2	R	552	5% 79% 21%
3	M	382	6% 85% 15%
3	Y	382	85% 15%
4	S	203	15% 85% 15%
4	X	203	14% 84% 15%

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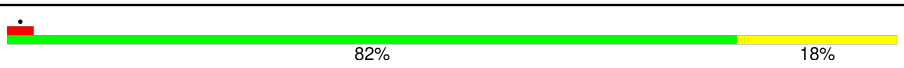
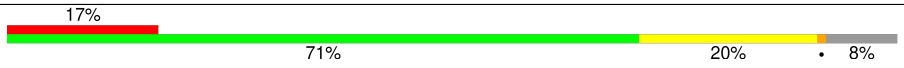
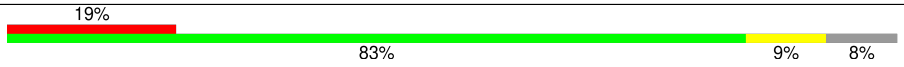
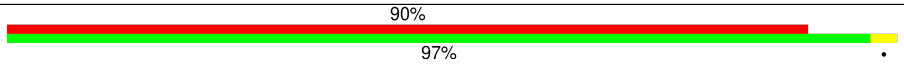
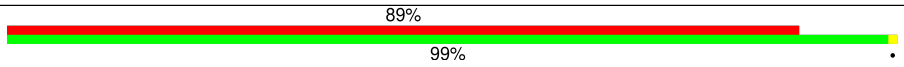
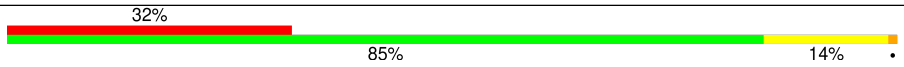
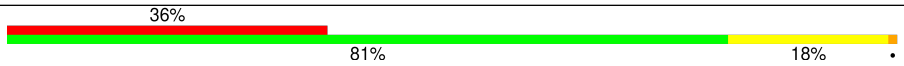
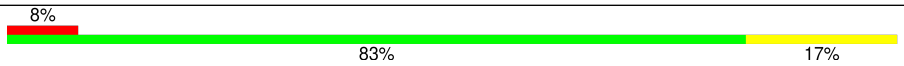
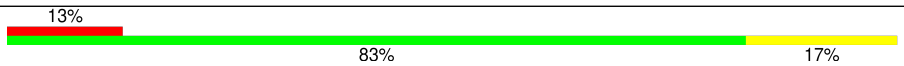
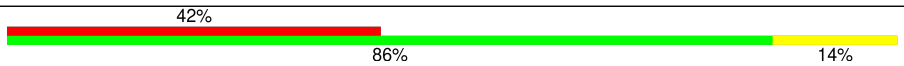
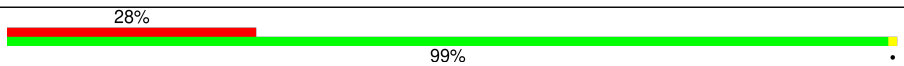
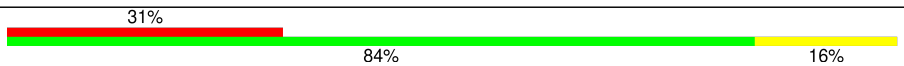
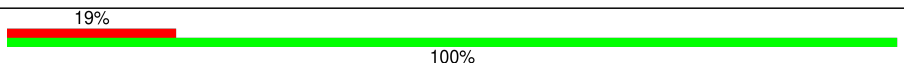
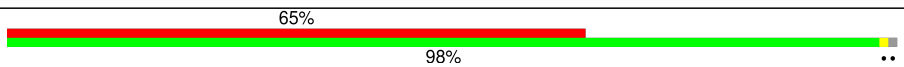
Mol	Chain	Length	Quality of chain
5	E	535	
5	F	535	
6	J	100	
6	P	100	
7	D	216	
7	G	216	
8	K	312	
8	Q	312	
9	T	139	
9	Z	139	
10	U	79	
10	a	79	
11	V	145	
11	b	145	
12	c	159	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	HEC	O	302	-	-	X	-
18	CDL	L	604	-	-	X	-
18	CDL	S	302	-	-	X	-
18	CDL	T	201	-	-	X	-
18	CDL	T	202	-	-	X	-
18	CDL	T	203	-	-	X	-
18	CDL	X	302	-	-	X	-
18	CDL	X	303	-	-	X	-
18	CDL	Z	202	-	-	X	-
18	CDL	Z	203	-	-	X	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 92757 atoms, of which 45318 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
1	O	210	Total	C	H	N	O	S	0	0
			3014	948	1483	276	295	12		
1	I	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	R	552	Total	C	H	N	O	S	0	0
			8716	2937	4346	695	712	26		
2	L	552	Total	C	H	N	O	S	0	0
			8717	2937	4347	695	712	26		

- Molecule 3 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		
3	Y	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		

- Molecule 4 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	S	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		
4	X	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		

- Molecule 5 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	535	Total	C	H	N	O	S	0	0
			8384	2751	4203	711	701	18		
5	F	535	Total	C	H	N	O	S	0	0
			8381	2751	4200	711	701	18		

- Molecule 6 is a protein called Putative conserved transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	92	Total	C	H	N	O	S	0	0
			1454	471	718	136	124	5		
6	P	92	Total	C	H	N	O	S	0	0
			1453	471	717	136	124	5		

- Molecule 7 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		
7	G	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		

- Molecule 8 is a protein called Cytochrome aa3 subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Q	312	Total	C	H	N	O	S	0	0
			4856	1592	2391	412	451	10		
8	K	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	T	139	Total	C	H	N	O	S	0	0
			2136	719	1059	167	188	3		
9	Z	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	U	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

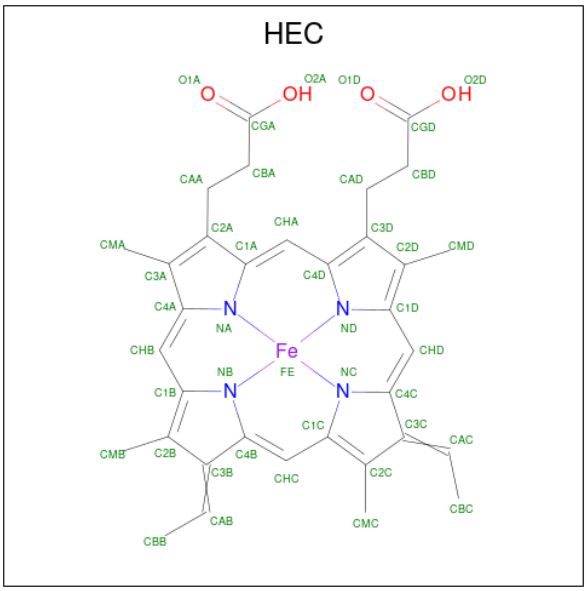
- Molecule 11 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	V	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		
11	b	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		

- Molecule 12 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	c	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
13	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
13	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
13	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

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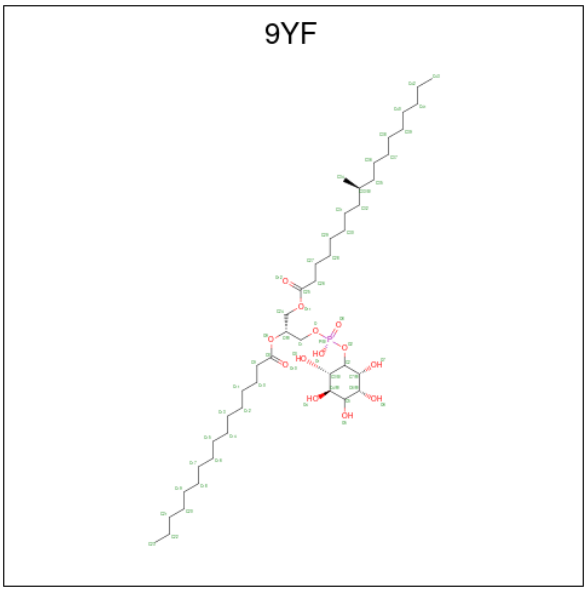
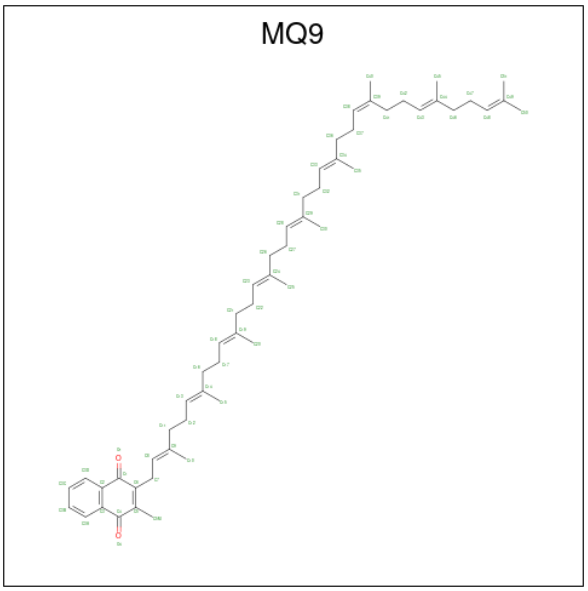
Mol	Chain	Residues	Atoms						AltConf
13	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 14 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 (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	E	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	I	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).

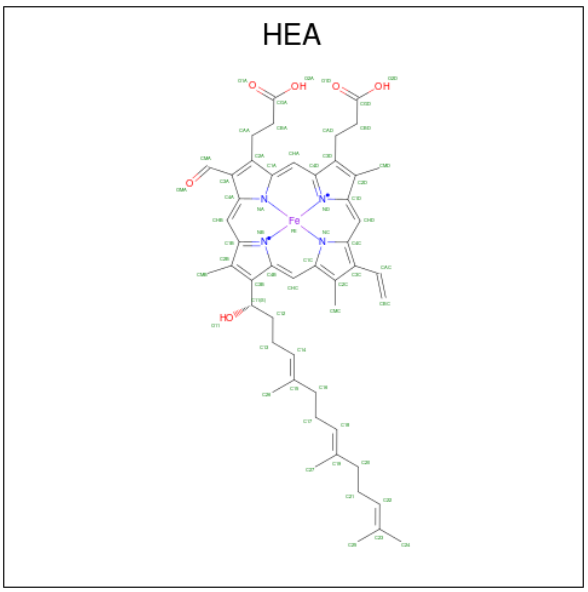


Mol	Chain	Residues	Atoms				AltConf
15	O	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	T	1	Total	C	H	O	0
			138	56	80	2	
15	Z	1	Total	C	H	O	0
			138	56	80	2	
15	I	1	Total	C	H	O	0
			138	56	80	2	

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

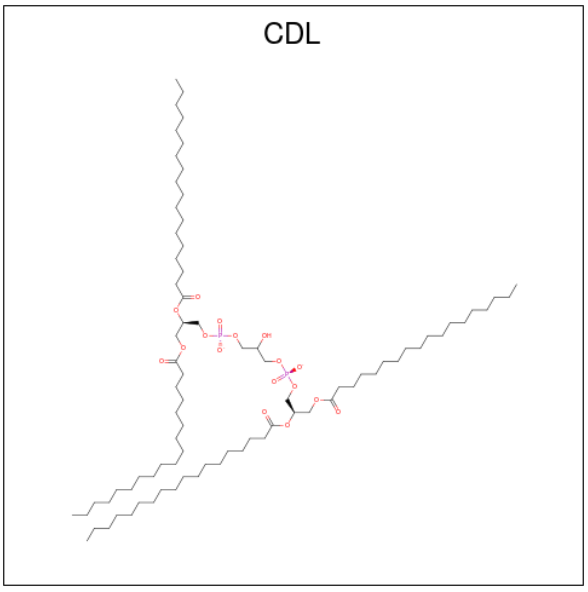
Mol	Chain	Residues	Atoms		AltConf
16	R	1	Total	Cu	0
			1	1	
16	L	1	Total	Cu	0
			1	1	
16	Q	2	Total	Cu	0
			2	2	
16	K	2	Total	Cu	0
			2	2	

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



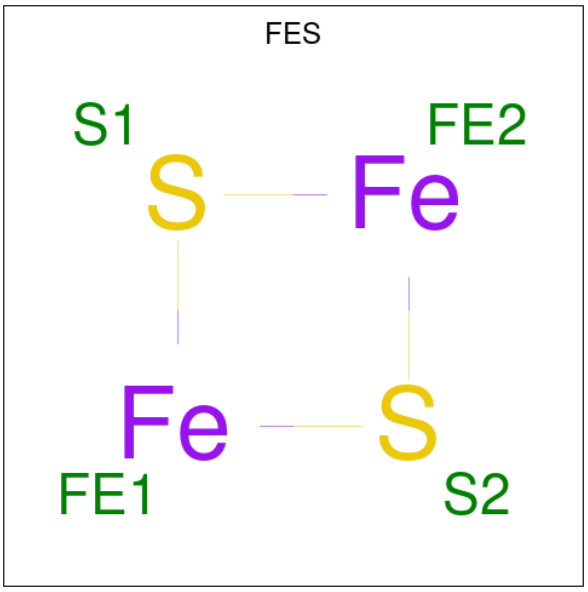
Mol	Chain	Residues	Atoms						AltConf
17	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



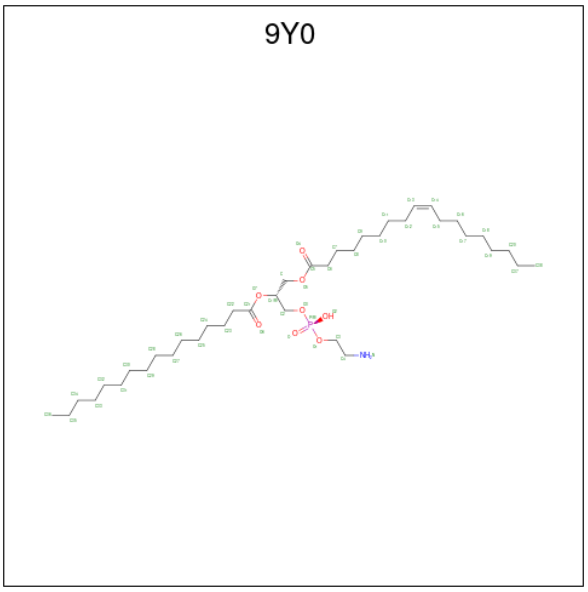
Mol	Chain	Residues	Atoms				AltConf
18	R	1	Total	C	O	P	0
			76	57	17	2	
18	S	1	Total	C	O	P	0
			76	57	17	2	
18	E	1	Total	C	O	P	0
			76	57	17	2	
18	E	1	Total	C	O	P	0
			76	57	17	2	
18	F	1	Total	C	O	P	0
			76	57	17	2	
18	F	1	Total	C	O	P	0
			76	57	17	2	
18	L	1	Total	C	O	P	0
			76	57	17	2	
18	J	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	P	1	Total	C	O	P	0
			76	57	17	2	
18	X	1	Total	C	O	P	0
			76	57	17	2	
18	X	1	Total	C	O	P	0
			76	57	17	2	
18	Z	1	Total	C	O	P	0
			76	57	17	2	
18	Z	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	Fe	S	0
			4	2	2	
19	Y	1	Total	Fe	S	0
			4	2	2	

- Molecule 20 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (three-letter code: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
20	S	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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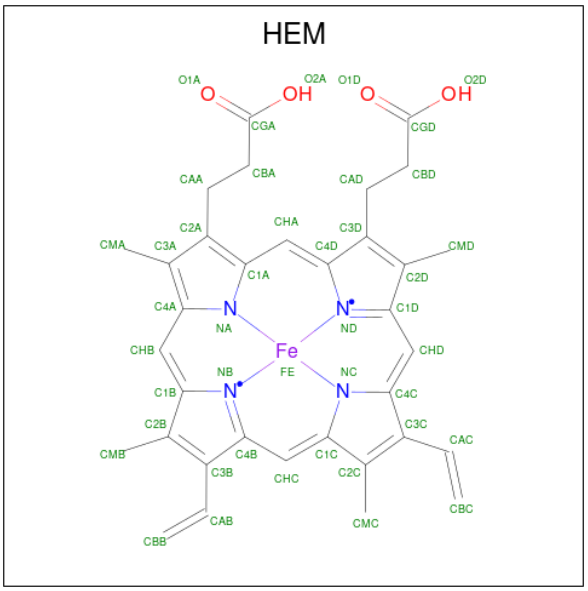
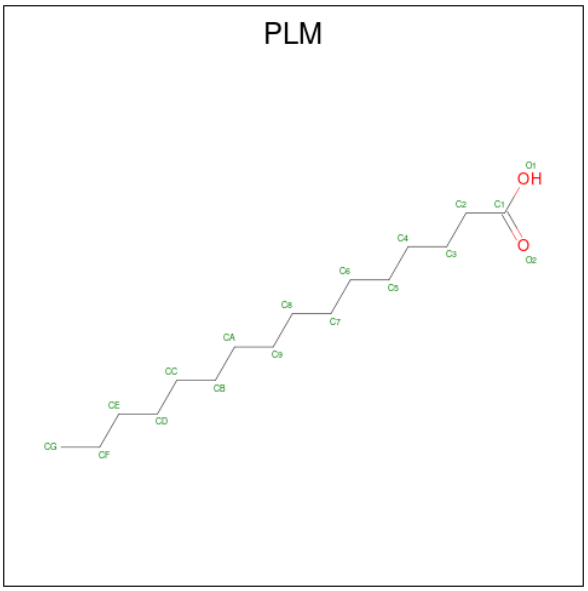
Mol	Chain	Residues	Atoms						AltConf
20	F	1	Total	C	H	N	O	P	0
			123	39	74	1	8	1	
20	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
20	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
20	X	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



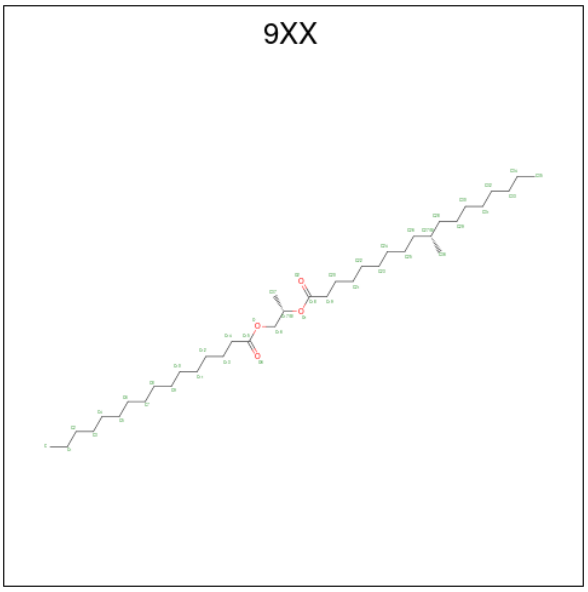
Mol	Chain	Residues	Atoms						AltConf
21	E	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
21	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
21	F	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
21	F	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 22 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	H	O	0
			27	10	16	1	
22	G	1	Total	C	H	O	0
			27	10	16	1	
22	c	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 23 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: $C_{38}H_{74}O_4$).



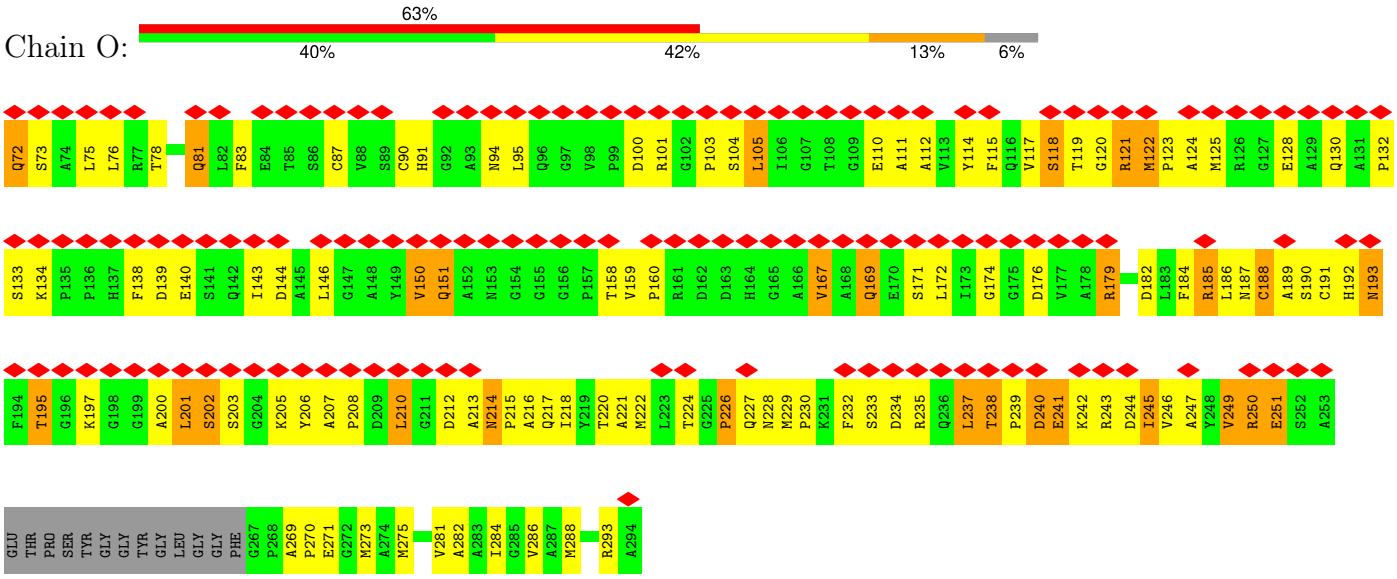
Mol	Chain	Residues	Atoms				AltConf
23	D	1	Total	C	H	O	0
			83	28	51	4	
23	G	1	Total	C	H	O	0
			83	28	51	4	
23	c	1	Total	C	H	O	0
			115	38	73	4	

3 Residue-property plots

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.

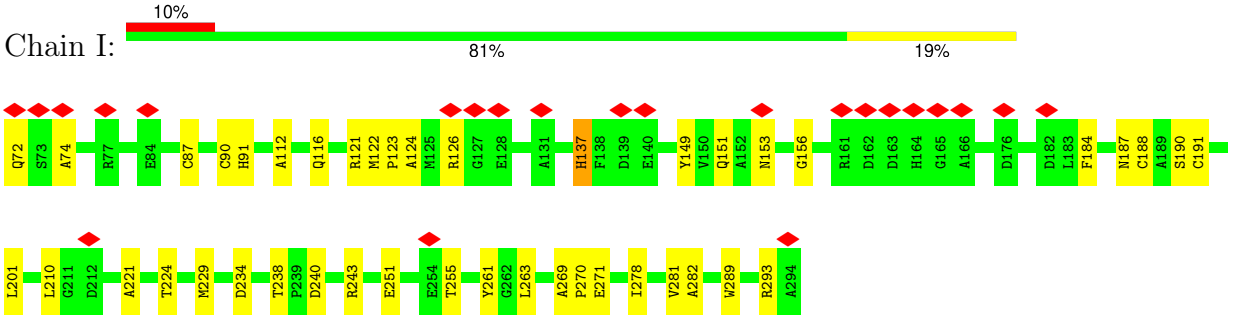
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain O:



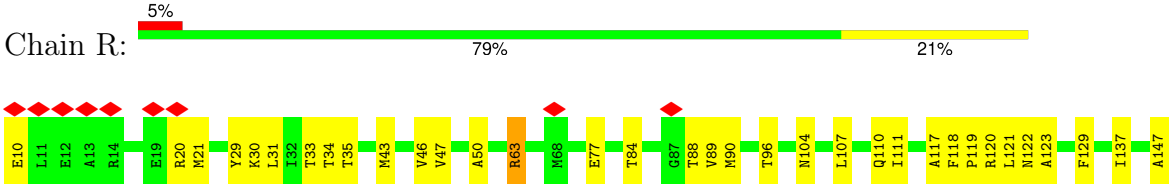
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

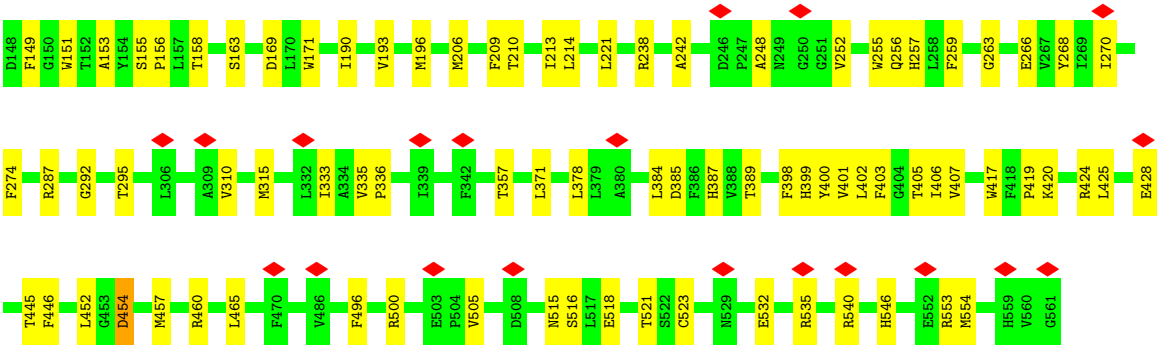
Chain I:



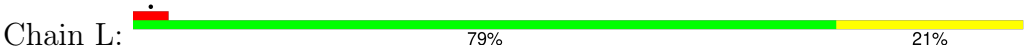
• Molecule 2: Cytochrome c oxidase subunit 1

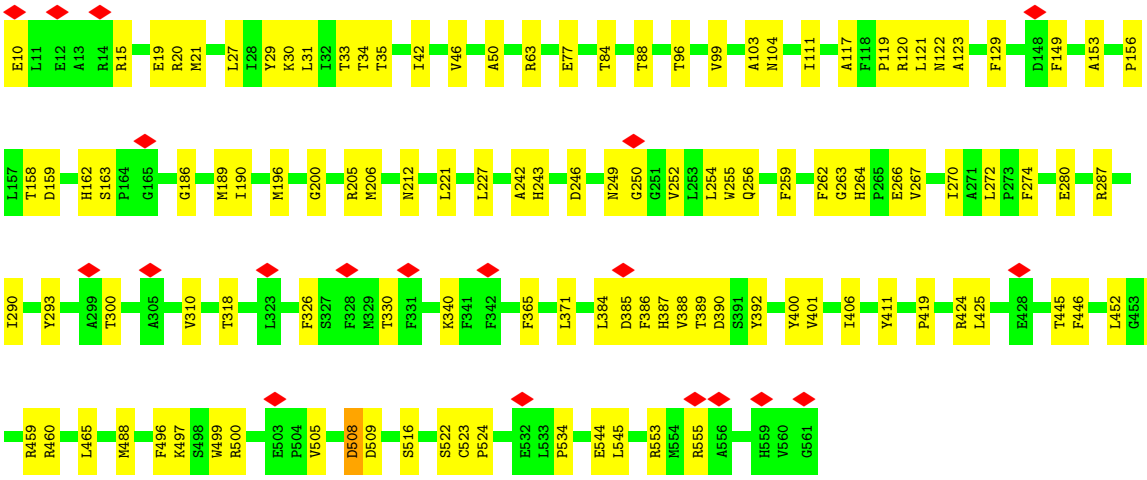
Chain R:



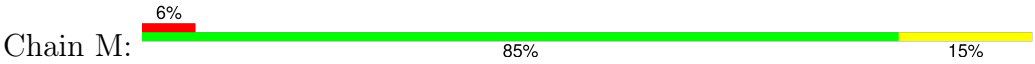


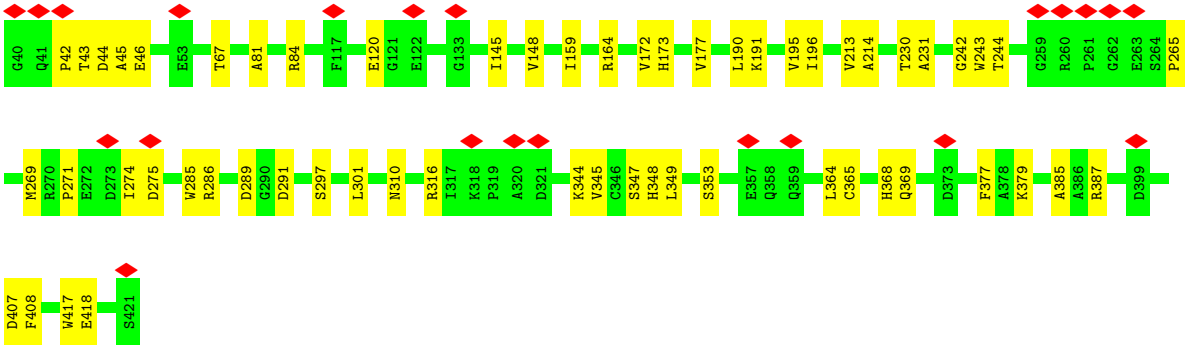
• Molecule 2: Cytochrome c oxidase subunit 1



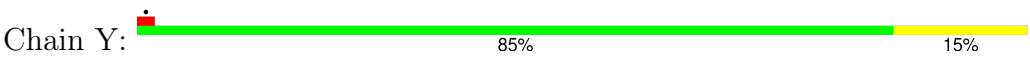


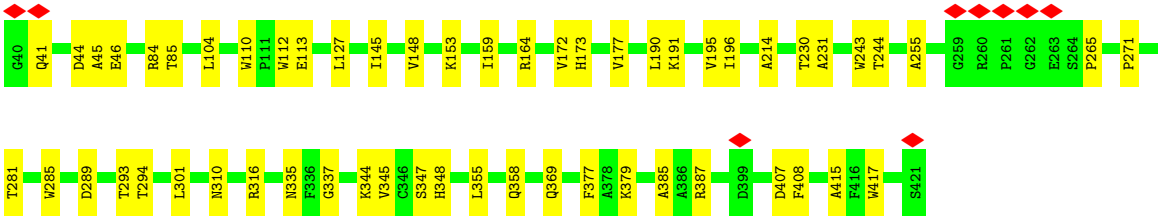
• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit



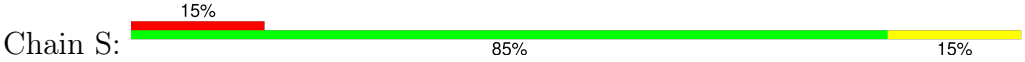


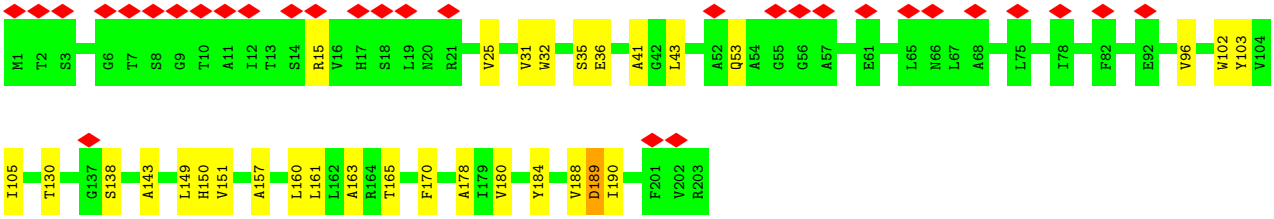
• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit



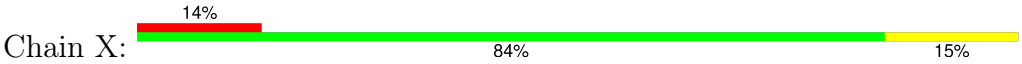


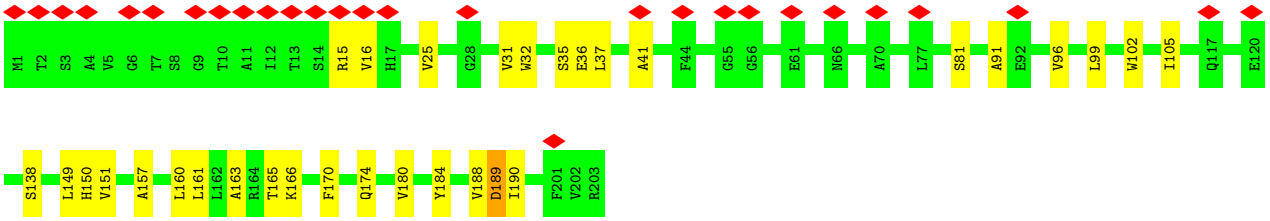
• Molecule 4: Cytochrome aa3 subunit 3



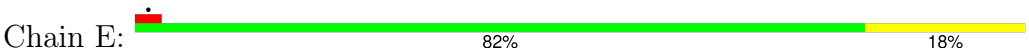


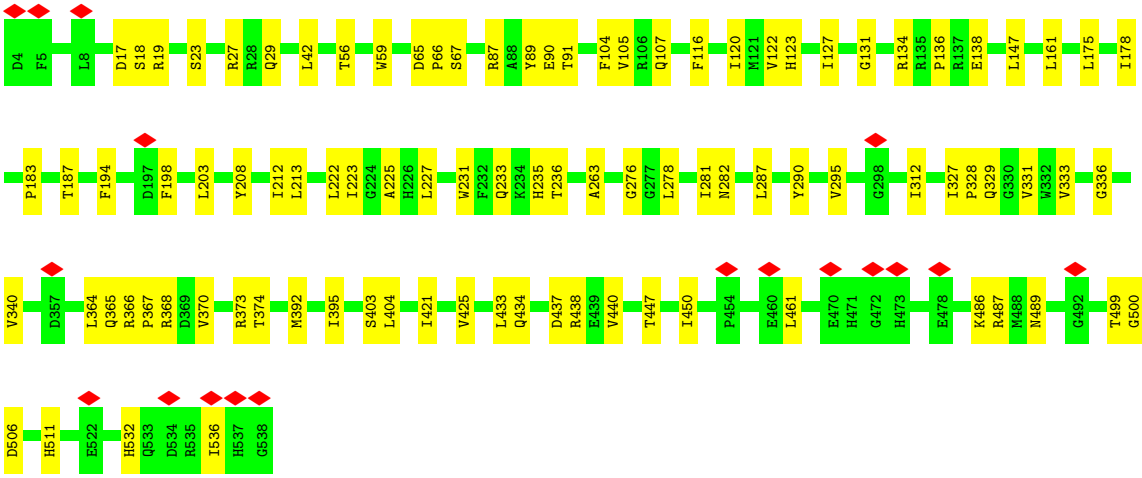
• Molecule 4: Cytochrome aa3 subunit 3





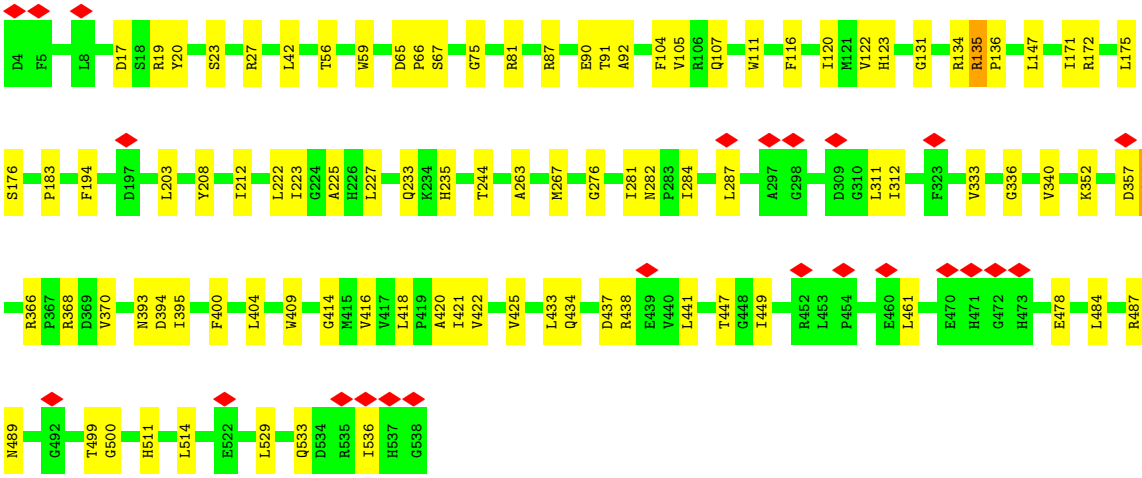
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit





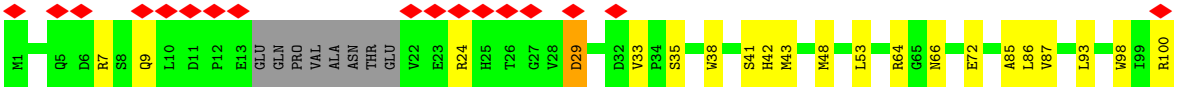
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit

Chain F:



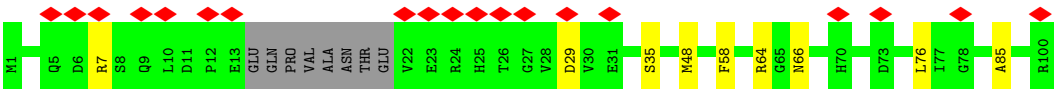
• Molecule 6: Putative conserved transmembrane protein

Chain J:



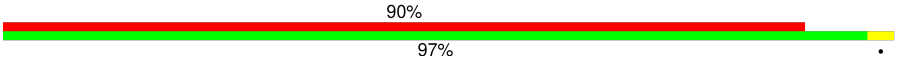
• Molecule 6: Putative conserved transmembrane protein

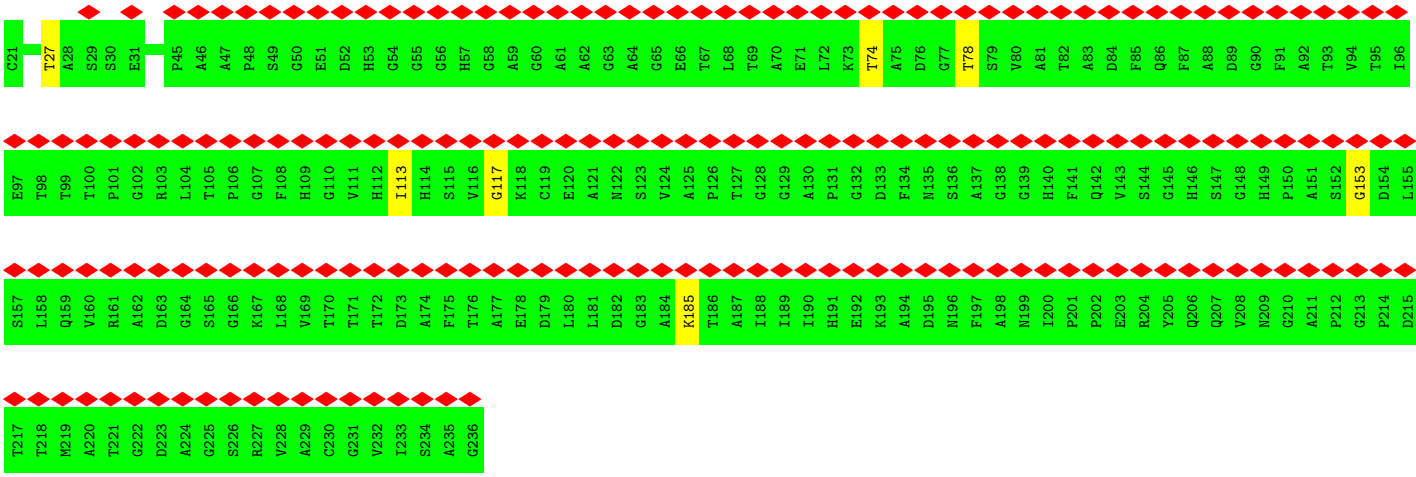
Chain P:



• Molecule 7: Superoxide dismutase [Cu-Zn]

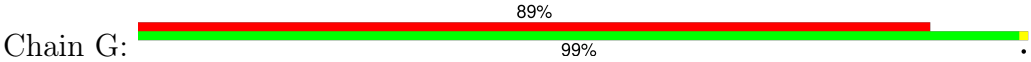
Chain D:

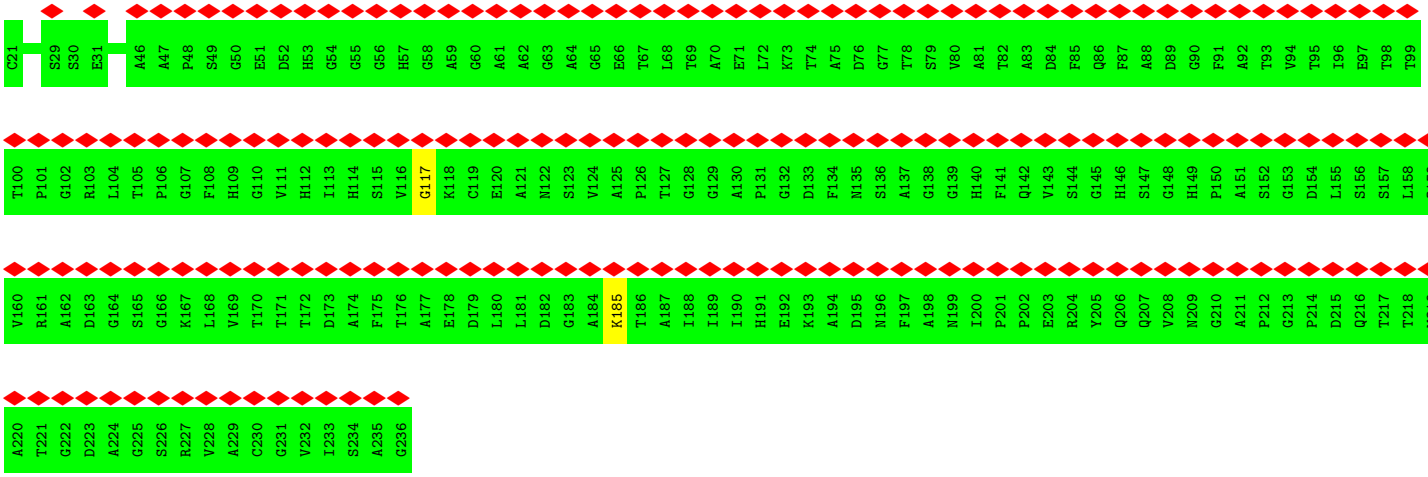




• Molecule 7: Superoxide dismutase [Cu-Zn]

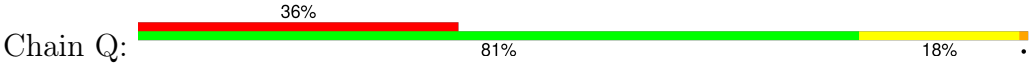
Chain G:

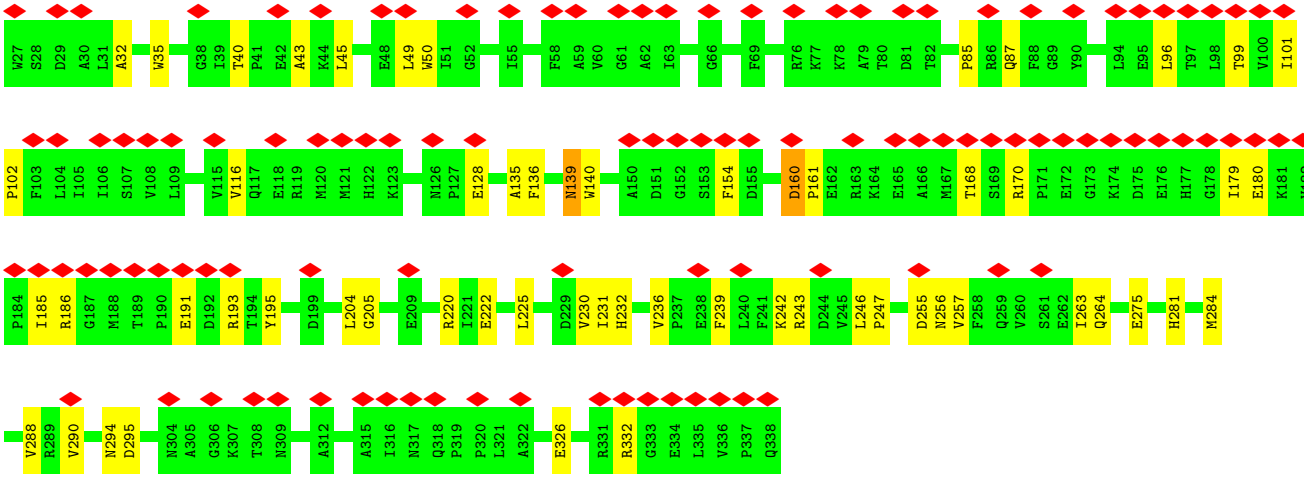




• Molecule 8: Cytochrome aa3 subunit 2

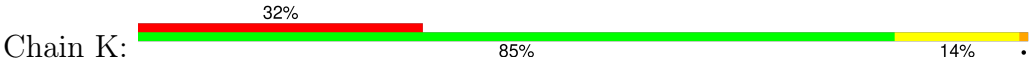
Chain Q:

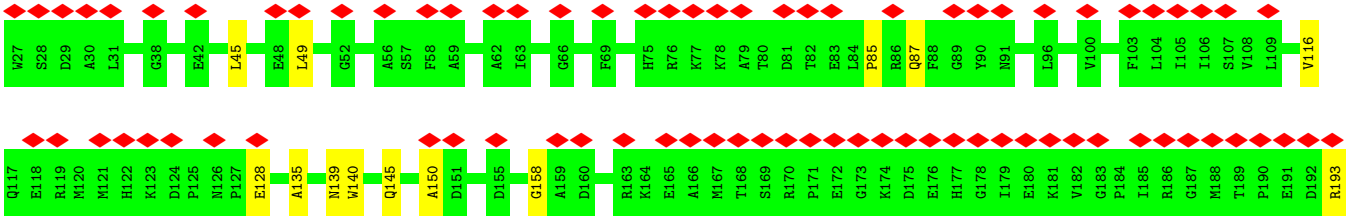


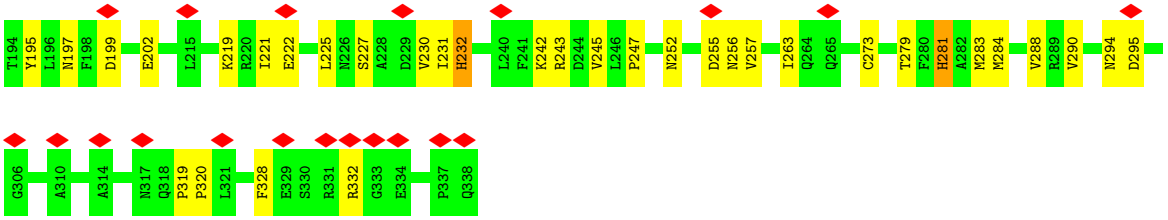


• Molecule 8: Cytochrome aa3 subunit 2

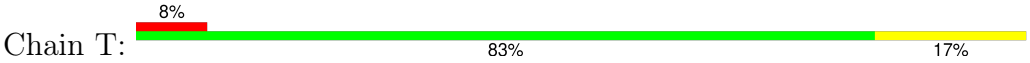
Chain K:

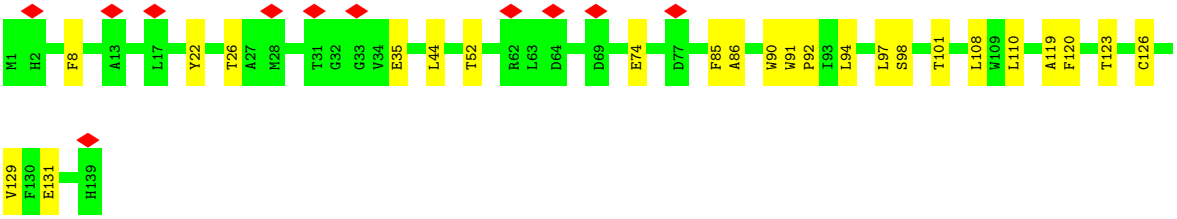




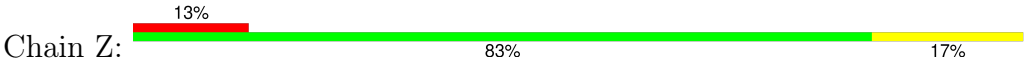


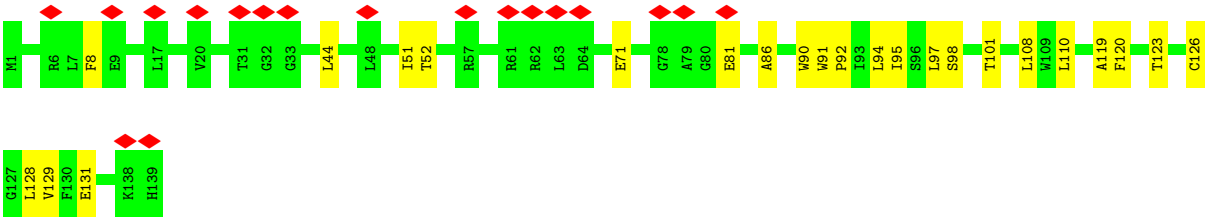
• Molecule 9: Cytochrome c oxidase polypeptide 4



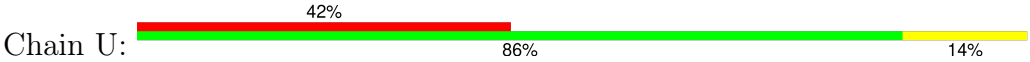


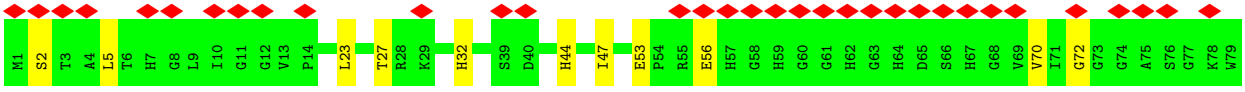
• Molecule 9: Cytochrome c oxidase polypeptide 4



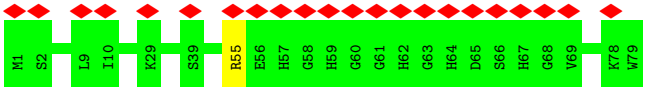


• Molecule 10: Cytochrome c oxidase subunit CtaJ

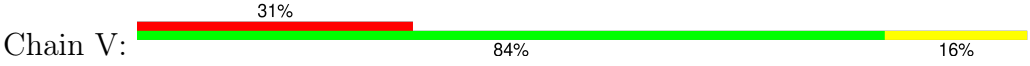


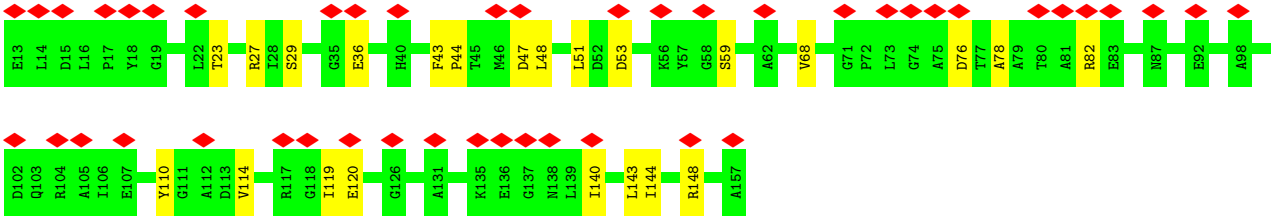


• Molecule 10: Cytochrome c oxidase subunit CtaJ



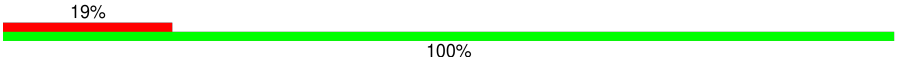
• Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

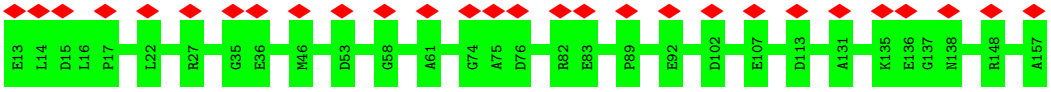




• Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

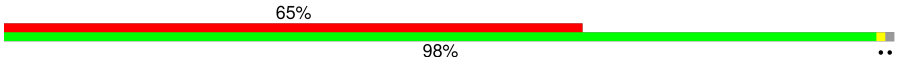
Chain b:

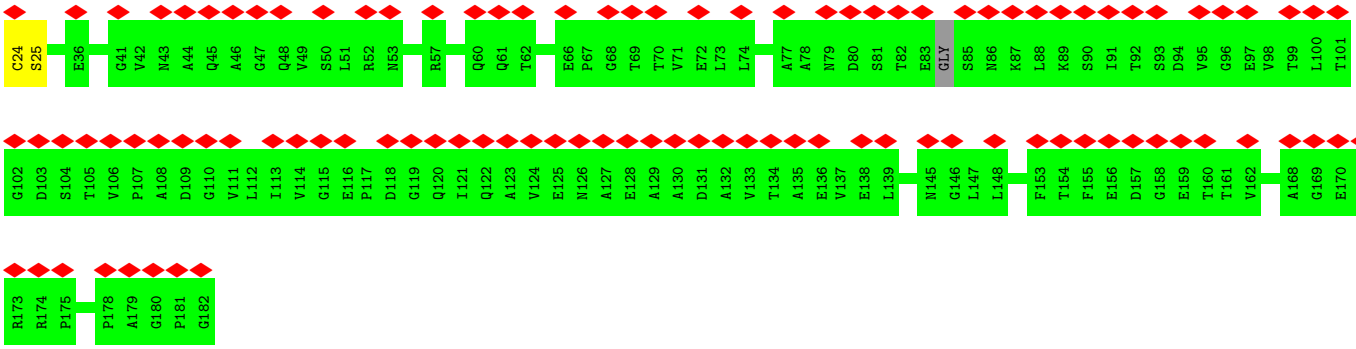




• Molecule 12: LpqE protein

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150885	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 ($e^-/Å^2$)	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.300	Depositor
Minimum map value	-1.965	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.634	Depositor
Map size (Å)	339.9, 339.9, 339.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ9, FES, HEC, HEM, CU, PLM, 9YF, HEA, 9XX, CDL, 9Y0

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	I	0.27	0/1660	0.51	0/2250
1	O	0.64	0/1563	0.89	0/2117
2	L	0.28	0/4530	0.46	0/6188
2	R	0.28	0/4530	0.46	0/6188
3	M	0.28	0/3056	0.50	0/4142
3	Y	0.28	0/3056	0.50	0/4142
4	S	0.28	0/1608	0.46	0/2195
4	X	0.29	0/1608	0.47	0/2195
5	E	0.28	0/4314	0.48	0/5882
5	F	0.27	0/4314	0.48	0/5882
6	J	0.24	0/757	0.51	0/1027
6	P	0.25	0/757	0.52	0/1027
7	D	0.26	0/1099	0.47	0/1519
7	G	0.25	0/1099	0.47	0/1519
8	K	0.27	0/2534	0.50	0/3451
8	Q	0.28	0/2534	0.51	0/3451
9	T	0.27	0/1112	0.45	0/1524
9	Z	0.28	0/1112	0.46	0/1524
10	U	0.25	0/613	0.44	0/836
10	a	0.25	0/613	0.44	0/836
11	V	0.28	0/1059	0.52	0/1446
11	b	0.28	0/1059	0.54	0/1446
12	c	0.26	0/1166	0.51	0/1599
All	All	0.29	0/45753	0.50	0/62386

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1623	1564	1564	40	0
1	O	1531	1483	1484	210	0
2	L	4370	4347	4346	95	0
2	R	4370	4346	4345	101	0
3	M	2977	2984	2984	42	0
3	Y	2977	2984	2984	42	0
4	S	1560	1548	1547	62	0
4	X	1560	1548	1547	79	0
5	E	4181	4203	4202	78	0
5	F	4181	4200	4199	80	0
6	J	736	718	717	13	0
6	P	736	717	717	9	0
7	D	1092	640	640	3	0
7	G	1092	640	640	1	0
8	K	2465	2392	2392	34	0
8	Q	2465	2391	2391	66	0
9	T	1077	1059	1058	60	0
9	Z	1077	1058	1058	63	0
10	U	591	576	576	7	0
10	a	591	576	576	0	0
11	V	1041	1052	1052	18	0
11	b	1041	1052	1052	0	0
12	c	1149	1110	1110	0	0
13	I	86	64	64	17	0
13	O	86	64	64	44	0
14	E	58	84	0	0	0
14	I	58	84	0	0	0
14	O	58	84	0	0	0
14	Y	116	168	0	0	0
15	E	116	160	160	6	0
15	F	116	160	160	4	0
15	I	58	80	80	0	0
15	O	58	80	80	2	0
15	T	58	80	80	2	0
15	Z	58	80	80	4	0
16	K	2	0	0	0	0
16	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
17	L	120	108	108	6	0
17	R	120	108	108	5	0
18	E	152	0	192	14	0
18	F	152	0	192	23	0
18	J	76	0	96	12	0
18	L	76	0	96	24	0
18	P	76	0	96	10	0
18	R	76	0	96	17	0
18	S	76	0	96	49	0
18	T	228	0	288	77	0
18	X	152	0	192	95	0
18	Z	152	0	192	78	0
19	M	4	0	0	0	0
19	Y	4	0	0	1	0
20	F	49	74	0	0	0
20	J	98	150	0	0	0
20	S	49	75	0	0	0
20	X	49	75	0	0	0
21	E	85	57	57	4	0
21	F	85	57	57	5	0
22	D	11	16	16	0	0
22	G	11	16	16	0	0
22	c	17	31	31	0	0
23	D	32	51	0	0	0
23	G	32	51	0	0	0
23	c	42	73	0	0	0
All	All	47439	45318	45878	1098	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 12.

All (1098) 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)
4:X:166:LYS:NZ	18:X:302:CDL:H112	1.28	1.48
9:T:120:PHE:CB	18:T:201:CDL:H612	1.47	1.42
1:O:203:SER:CB	8:Q:170:ARG:HG3	1.46	1.41
9:T:120:PHE:HB3	18:T:201:CDL:C61	1.50	1.41
9:Z:120:PHE:CB	18:Z:202:CDL:H612	1.53	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:120:PHE:HB3	18:Z:202:CDL:C61	1.58	1.31
9:T:94:LEU:HD21	18:T:201:CDL:C32	1.67	1.24
9:Z:94:LEU:HD21	18:Z:202:CDL:C32	1.68	1.23
18:X:302:CDL:H772	18:Z:203:CDL:C55	1.71	1.20
18:T:202:CDL:H772	18:T:203:CDL:C55	1.71	1.19
9:Z:90:TRP:CZ2	18:Z:202:CDL:HB4	1.76	1.18
4:X:149:LEU:HD22	18:X:303:CDL:C63	1.74	1.18
18:T:202:CDL:H772	18:T:203:CDL:H551	1.21	1.17
18:X:302:CDL:H721	18:Z:203:CDL:C51	1.75	1.17
1:O:203:SER:CA	8:Q:170:ARG:HG3	1.74	1.17
18:T:202:CDL:H721	18:T:203:CDL:C51	1.75	1.16
4:X:166:LYS:NZ	18:X:302:CDL:C11	2.09	1.15
9:T:90:TRP:HZ2	18:T:201:CDL:HB4	1.05	1.15
9:T:90:TRP:CZ2	18:T:201:CDL:HB4	1.82	1.15
4:X:166:LYS:HZ1	18:X:302:CDL:C11	1.60	1.15
1:O:83:PHE:CZ	1:O:95:LEU:HD23	1.82	1.14
9:T:97:LEU:HD11	18:T:201:CDL:H361	1.14	1.13
9:Z:97:LEU:HD11	18:Z:202:CDL:H361	1.18	1.12
18:X:302:CDL:H721	18:Z:203:CDL:H512	1.19	1.12
9:Z:119:ALA:HB1	18:Z:203:CDL:H411	1.23	1.12
9:Z:97:LEU:HD11	18:Z:202:CDL:C36	1.80	1.11
1:O:203:SER:HB3	8:Q:170:ARG:CG	1.79	1.11
9:T:97:LEU:HD11	18:T:201:CDL:C36	1.80	1.11
18:T:202:CDL:H721	18:T:203:CDL:H512	1.19	1.10
1:O:203:SER:CB	8:Q:170:ARG:CG	2.30	1.09
4:X:149:LEU:HD22	18:X:303:CDL:H631	1.17	1.09
18:X:302:CDL:H772	18:Z:203:CDL:H551	1.21	1.08
9:Z:94:LEU:HD21	18:Z:202:CDL:H321	1.10	1.08
9:Z:90:TRP:HZ2	18:Z:202:CDL:HB4	1.00	1.08
1:O:203:SER:HB3	8:Q:170:ARG:HG3	1.08	1.06
9:T:119:ALA:HB1	18:T:203:CDL:H411	1.32	1.06
1:O:83:PHE:CZ	1:O:95:LEU:CD2	2.40	1.05
9:T:94:LEU:HD21	18:T:201:CDL:H321	1.10	1.04
4:S:32:TRP:CZ2	18:S:302:CDL:H382	1.94	1.03
4:X:32:TRP:CZ2	18:X:303:CDL:H382	1.93	1.02
4:X:32:TRP:CE2	18:X:303:CDL:H361	1.94	1.02
9:T:120:PHE:CD2	18:T:201:CDL:H632	1.94	1.01
4:X:32:TRP:CG	18:X:303:CDL:H331	1.95	1.01
4:X:32:TRP:CB	18:X:303:CDL:H331	1.91	1.01
2:R:121:LEU:HD13	18:S:302:CDL:CA3	1.90	1.00
1:O:95:LEU:HD11	1:O:150:VAL:HA	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:32:TRP:CE2	18:S:302:CDL:H361	1.98	0.98
1:O:83:PHE:CE1	1:O:95:LEU:CD2	2.46	0.97
1:O:95:LEU:CD1	1:O:150:VAL:HB	1.94	0.97
4:S:32:TRP:CB	18:S:302:CDL:H331	1.94	0.97
2:L:121:LEU:HD13	18:X:303:CDL:CA3	1.95	0.97
9:Z:120:PHE:CD2	18:Z:202:CDL:H632	2.00	0.96
4:S:32:TRP:CG	18:S:302:CDL:H331	2.02	0.95
4:S:149:LEU:HB3	18:S:302:CDL:H801	1.44	0.95
1:O:95:LEU:HD11	1:O:150:VAL:CB	1.97	0.95
1:O:117:VAL:HA	1:O:122:MET:HG2	1.49	0.94
9:T:97:LEU:CD1	18:T:201:CDL:H361	1.96	0.94
1:O:222:MET:HG2	1:O:242:LYS:HE2	1.50	0.93
1:O:222:MET:HG3	1:O:232:PHE:HB2	1.48	0.92
1:O:215:PRO:HA	1:O:218:ILE:HD12	1.51	0.92
1:O:83:PHE:CE1	1:O:95:LEU:HD21	2.04	0.92
8:Q:231:ILE:HD13	8:Q:246:LEU:HD23	1.49	0.92
18:X:302:CDL:H761	18:Z:203:CDL:H532	1.51	0.92
3:M:385:ALA:O	6:P:66:ASN:ND2	2.03	0.91
1:O:95:LEU:HD11	1:O:150:VAL:CA	2.01	0.90
1:O:203:SER:C	8:Q:170:ARG:CG	2.37	0.90
9:T:98:SER:OG	18:T:201:CDL:H621	1.71	0.90
9:Z:97:LEU:CD1	18:Z:202:CDL:H361	2.01	0.90
18:T:202:CDL:H761	18:T:203:CDL:H532	1.51	0.90
4:X:157:ALA:HB2	18:X:303:CDL:H532	1.54	0.90
9:Z:98:SER:OG	18:Z:202:CDL:H621	1.72	0.89
2:R:121:LEU:HD13	18:S:302:CDL:HA32	1.52	0.89
2:R:121:LEU:HB2	18:S:302:CDL:OA3	1.73	0.89
2:L:121:LEU:HD13	18:X:303:CDL:HA32	1.53	0.88
1:O:202:SER:HB2	1:O:205:LYS:HD2	1.54	0.88
4:X:32:TRP:CD2	18:X:303:CDL:H352	2.10	0.87
18:Z:203:CDL:H161	1:I:281:VAL:HG11	1.57	0.86
4:S:32:TRP:NE1	18:S:302:CDL:H361	1.89	0.86
1:O:190:SER:HB2	8:Q:193:ARG:CZ	2.05	0.86
9:T:97:LEU:CD1	18:T:201:CDL:C36	2.52	0.86
9:Z:119:ALA:HB1	18:Z:203:CDL:C41	2.05	0.86
4:X:32:TRP:NE1	18:X:303:CDL:H361	1.91	0.86
4:X:149:LEU:HD22	18:X:303:CDL:C64	2.05	0.86
2:R:20:ARG:NH2	11:V:53:ASP:OD1	2.09	0.85
2:R:121:LEU:HD13	18:S:302:CDL:HA31	1.58	0.85
1:O:227:GLN:HG3	13:O:302:HEC:HBD2	1.59	0.85
4:X:149:LEU:HB3	18:X:303:CDL:H801	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:97:LEU:CD1	18:Z:202:CDL:C36	2.54	0.85
4:X:166:LYS:HZ1	18:X:302:CDL:H112	0.71	0.85
9:Z:90:TRP:HZ2	18:Z:202:CDL:CB4	1.89	0.85
1:O:95:LEU:CD1	1:O:150:VAL:HA	2.07	0.84
5:E:87:ARG:NH1	5:E:90:GLU:OE1	2.10	0.84
1:O:118:SER:HB2	1:O:143:ILE:HG21	1.58	0.84
8:Q:243:ARG:NH1	8:Q:255:ASP:O	2.11	0.84
18:X:302:CDL:C76	18:Z:203:CDL:H532	2.08	0.83
2:L:121:LEU:HB2	18:X:303:CDL:OA3	1.77	0.83
1:O:185:ARG:HA	1:O:189:ALA:CB	2.09	0.83
4:S:32:TRP:CD2	18:S:302:CDL:H352	2.13	0.83
18:T:202:CDL:H772	18:T:203:CDL:H552	1.60	0.82
2:R:389:THR:O	8:Q:242:LYS:NZ	2.11	0.82
18:X:302:CDL:H772	18:Z:203:CDL:H552	1.61	0.82
18:T:202:CDL:C76	18:T:203:CDL:H532	2.08	0.82
5:E:447:THR:OG1	5:E:461:LEU:O	1.98	0.82
4:X:166:LYS:HZ3	18:X:302:CDL:C11	1.91	0.82
9:Z:94:LEU:HD21	18:Z:202:CDL:H322	1.60	0.82
9:Z:120:PHE:CB	18:Z:202:CDL:C61	2.36	0.81
9:Z:94:LEU:CD2	18:Z:202:CDL:H321	2.04	0.81
2:L:84:THR:OG1	2:L:149:PHE:O	1.98	0.81
5:F:447:THR:OG1	5:F:461:LEU:O	1.97	0.81
11:V:23:THR:OG1	11:V:27:ARG:O	1.99	0.81
15:F:707:MQ9:H501	3:Y:214:ALA:HB1	1.62	0.81
2:L:411:TYR:OH	2:L:488:MET:SD	2.37	0.81
18:L:604:CDL:HA4	18:J:203:CDL:H312	1.62	0.81
1:O:115:PHE:CE1	1:O:119:THR:HG21	2.15	0.81
10:U:53:GLU:OE1	11:V:59:SER:OG	1.97	0.81
8:K:243:ARG:NH1	8:K:255:ASP:O	2.14	0.81
18:T:202:CDL:H721	18:T:203:CDL:H511	1.63	0.80
8:K:263:ILE:HG21	8:K:290:VAL:HG21	1.62	0.80
4:S:149:LEU:HD23	18:S:302:CDL:H631	1.61	0.80
9:T:119:ALA:HB1	18:T:203:CDL:C41	2.11	0.80
18:R:604:CDL:HA4	18:P:201:CDL:H312	1.62	0.80
9:T:94:LEU:HD21	18:T:201:CDL:H322	1.59	0.80
1:I:122:MET:O	1:I:124:ALA:N	2.14	0.80
18:T:202:CDL:C17	18:T:203:CDL:H762	2.12	0.79
1:O:95:LEU:HD11	1:O:150:VAL:HB	1.59	0.79
1:O:191:CYS:HB2	13:O:302:HEC:HBC2	1.64	0.79
4:S:157:ALA:HB2	18:S:302:CDL:H532	1.65	0.79
1:I:251:GLU:O	1:I:255:THR:OG1	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:LEU:HD23	18:L:604:CDL:H381	1.62	0.79
2:R:30:LYS:O	2:R:34:THR:N	2.15	0.79
18:X:302:CDL:C77	18:Z:203:CDL:C55	2.59	0.79
6:J:66:ASN:ND2	3:Y:385:ALA:O	2.16	0.79
18:X:302:CDL:H721	18:Z:203:CDL:H511	1.63	0.78
1:O:119:THR:HA	1:O:217:GLN:HG2	1.66	0.78
1:O:188:CYS:HB2	13:O:302:HEC:CHC	2.12	0.78
2:L:497:LYS:NZ	6:J:100:ARG:O	2.17	0.78
18:X:302:CDL:C17	18:Z:203:CDL:H762	2.12	0.78
1:O:119:THR:HG22	1:O:120:GLY:H	1.47	0.78
9:T:120:PHE:CB	18:T:201:CDL:C61	2.29	0.78
4:X:184:TYR:OH	18:X:303:CDL:H752	1.84	0.78
2:R:287:ARG:O	8:Q:87:GLN:NE2	2.17	0.77
5:E:489:ASN:ND2	9:Z:131:GLU:O	2.17	0.77
4:X:32:TRP:HB2	18:X:303:CDL:H331	1.66	0.77
4:S:32:TRP:HZ2	18:S:302:CDL:H382	1.48	0.77
9:T:94:LEU:CD2	18:T:201:CDL:H321	2.04	0.77
4:X:166:LYS:CE	18:X:302:CDL:H112	2.15	0.77
9:T:120:PHE:CA	18:T:201:CDL:H612	2.15	0.77
1:O:203:SER:C	8:Q:170:ARG:HG3	2.04	0.77
2:L:30:LYS:O	2:L:34:THR:N	2.17	0.77
2:L:205:ARG:NH1	9:Z:71:GLU:OE2	2.19	0.76
4:X:184:TYR:CZ	18:X:303:CDL:H731	2.19	0.76
2:L:121:LEU:HD13	18:X:303:CDL:HA31	1.65	0.76
1:O:95:LEU:HD13	1:O:150:VAL:HB	1.64	0.76
8:Q:263:ILE:HG21	8:Q:290:VAL:HG21	1.67	0.76
8:K:227:SER:OG	8:K:230:VAL:O	2.04	0.76
3:Y:285:TRP:NE1	3:Y:289:ASP:O	2.18	0.76
4:X:32:TRP:CZ2	18:X:303:CDL:H361	2.20	0.75
9:Z:97:LEU:CD1	18:Z:202:CDL:C35	2.64	0.75
4:X:32:TRP:HZ2	18:X:303:CDL:H382	1.51	0.75
1:O:188:CYS:HA	13:O:302:HEC:HMC3	1.67	0.75
4:X:166:LYS:HZ3	18:X:302:CDL:CA5	1.98	0.75
2:L:300:THR:OG1	2:L:340:LYS:NZ	2.16	0.75
18:T:202:CDL:C77	18:T:203:CDL:C55	2.59	0.75
4:X:32:TRP:CE2	18:X:303:CDL:C36	2.70	0.75
1:O:118:SER:HA	1:O:143:ILE:HD13	1.67	0.75
1:O:185:ARG:HA	1:O:189:ALA:HB2	1.66	0.75
1:O:245:ILE:HG21	13:O:302:HEC:HBB2	1.66	0.75
3:M:285:TRP:NE1	3:M:289:ASP:O	2.20	0.75
18:X:302:CDL:H131	18:Z:203:CDL:OB7	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:515:ASN:O	2:R:516:SER:OG	2.06	0.74
18:T:202:CDL:H131	18:T:203:CDL:OB7	1.87	0.74
11:V:47:ASP:OD1	11:V:48:LEU:N	2.20	0.74
1:O:200:ALA:O	8:Q:191:GLU:OE2	2.05	0.74
9:Z:119:ALA:CB	18:Z:203:CDL:H411	2.10	0.74
5:E:365:GLN:NE2	6:J:38:TRP:O	2.21	0.74
1:O:269:ALA:HB3	1:O:270:PRO:HD3	1.70	0.74
2:R:553:ARG:NH2	8:Q:85:PRO:O	2.21	0.74
4:S:184:TYR:OH	18:S:302:CDL:H752	1.88	0.74
5:E:138:GLU:OE2	5:F:19:ARG:NE	2.22	0.73
4:X:32:TRP:CE2	18:X:303:CDL:H352	2.23	0.73
3:M:214:ALA:HB1	15:E:604:MQ9:H501	1.69	0.73
9:Z:120:PHE:HD2	18:Z:202:CDL:H632	1.54	0.73
18:R:604:CDL:H542	18:P:201:CDL:H351	1.71	0.73
1:O:191:CYS:SG	13:O:302:HEC:HHD	2.29	0.72
5:F:489:ASN:ND2	9:T:131:GLU:O	2.22	0.72
9:T:90:TRP:HZ2	18:T:201:CDL:CB4	1.93	0.72
4:S:184:TYR:CZ	18:S:302:CDL:H731	2.24	0.72
9:T:97:LEU:CD1	18:T:201:CDL:C35	2.66	0.72
2:L:424:ARG:NH1	2:L:499:TRP:O	2.22	0.72
5:F:75:GLY:O	5:F:81:ARG:NH1	2.21	0.72
9:T:94:LEU:CD2	18:T:201:CDL:C32	2.59	0.72
1:O:119:THR:HG23	1:O:217:GLN:HG2	1.72	0.72
9:T:120:PHE:HD2	18:T:201:CDL:H632	1.47	0.72
1:O:160:PRO:HG2	1:O:172:LEU:HD21	1.70	0.72
1:O:169:GLN:HG2	1:O:215:PRO:HD2	1.71	0.71
4:S:149:LEU:CD2	18:S:302:CDL:H631	2.20	0.71
1:O:130:GLN:HG2	1:O:205:LYS:HA	1.72	0.71
8:Q:275:GLU:O	8:Q:281:HIS:NE2	2.22	0.71
9:T:120:PHE:CG	18:T:201:CDL:C61	2.73	0.71
9:Z:94:LEU:CD2	18:Z:202:CDL:C32	2.60	0.71
4:X:157:ALA:HB1	18:X:303:CDL:C51	2.20	0.71
4:S:32:TRP:CE2	18:S:302:CDL:C36	2.74	0.71
4:S:32:TRP:CE2	18:S:302:CDL:H352	2.25	0.71
2:L:385:ASP:O	2:L:389:THR:OG1	2.08	0.71
5:F:42:LEU:HD13	5:F:122:VAL:HG12	1.71	0.71
18:L:604:CDL:H542	18:J:203:CDL:H351	1.71	0.71
1:O:115:PHE:CD1	1:O:119:THR:HG21	2.26	0.71
4:X:149:LEU:CB	18:X:303:CDL:H801	2.20	0.71
2:L:385:ASP:OD1	2:L:389:THR:OG1	2.09	0.70
3:M:84:ARG:NH2	5:F:500:GLY:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:LEU:HD23	18:L:604:CDL:H412	1.72	0.70
4:X:189:ASP:OD1	4:X:190:ILE:N	2.24	0.70
9:T:120:PHE:CG	18:T:201:CDL:H611	2.25	0.70
1:O:191:CYS:CB	13:O:302:HEC:HBC2	2.21	0.70
1:O:245:ILE:HG13	13:O:302:HEC:HBB1	1.73	0.70
1:O:230:PRO:HD2	13:O:302:HEC:C3C	2.22	0.70
2:R:10:GLU:N	2:R:10:GLU:OE1	2.25	0.70
4:X:157:ALA:CB	18:X:303:CDL:H511	2.21	0.70
1:O:191:CYS:SG	1:O:207:ALA:HB2	2.31	0.69
1:O:132:PRO:HG2	1:O:134:LYS:HE3	1.74	0.69
2:R:88:THR:HG21	2:R:171:TRP:HE1	1.57	0.69
3:M:159:ILE:HG21	5:F:529:LEU:HD21	1.74	0.69
2:L:10:GLU:N	2:L:10:GLU:OE1	2.25	0.69
13:I:301:HEC:HBC3	13:I:301:HEC:HHD	1.75	0.69
8:K:128:GLU:OE1	8:K:150:ALA:N	2.24	0.69
18:X:302:CDL:H111	18:X:302:CDL:HB21	1.75	0.69
2:R:385:ASP:O	2:R:389:THR:OG1	2.10	0.69
5:E:500:GLY:O	3:Y:84:ARG:NH2	2.25	0.69
10:U:44:HIS:ND1	10:U:47:ILE:HD11	2.08	0.69
4:S:32:TRP:HB2	18:S:302:CDL:H331	1.72	0.69
2:L:270:ILE:HG23	2:L:406:ILE:HG21	1.75	0.69
18:T:202:CDL:C77	18:T:203:CDL:H551	2.14	0.69
4:X:184:TYR:CE1	18:X:303:CDL:C73	2.76	0.69
9:Z:120:PHE:CA	18:Z:202:CDL:H612	2.22	0.69
9:T:119:ALA:CB	18:T:203:CDL:H411	2.17	0.69
1:I:240:ASP:OD1	1:I:243:ARG:NH2	2.26	0.69
1:O:222:MET:HE2	13:O:302:HEC:HBB2	1.75	0.69
5:E:42:LEU:HD13	5:E:122:VAL:HG12	1.73	0.69
11:V:36:GLU:OE1	11:V:36:GLU:N	2.26	0.69
9:Z:120:PHE:CG	18:Z:202:CDL:C61	2.76	0.69
5:E:328:PRO:O	5:E:331:VAL:HG12	1.93	0.68
1:O:195:THR:HB	1:O:197:LYS:HG2	1.75	0.68
1:O:115:PHE:CZ	13:O:302:HEC:HAA1	2.29	0.68
18:T:202:CDL:C77	18:T:203:CDL:H552	2.21	0.68
4:S:32:TRP:CZ2	18:S:302:CDL:H361	2.28	0.68
4:S:157:ALA:CB	18:S:302:CDL:H511	2.24	0.68
5:E:235:HIS:O	3:Y:164:ARG:NH2	2.26	0.68
4:X:150:HIS:HA	18:X:303:CDL:H771	1.74	0.68
9:Z:123:THR:HG23	18:Z:203:CDL:H322	1.75	0.68
18:Z:203:CDL:H572	1:I:282:ALA:HA	1.73	0.68
18:L:604:CDL:H521	18:J:203:CDL:H321	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:149:LEU:CD2	18:X:303:CDL:H631	2.11	0.68
9:Z:97:LEU:CD1	18:Z:202:CDL:H351	2.24	0.68
3:M:164:ARG:NH2	5:F:235:HIS:O	2.27	0.67
4:X:184:TYR:CE1	18:X:303:CDL:H732	2.29	0.67
9:Z:120:PHE:CG	18:Z:202:CDL:H611	2.29	0.67
1:O:237:LEU:CD2	1:O:241:GLU:HB2	2.25	0.67
1:I:90:CYS:SG	13:I:301:HEC:HBC2	2.34	0.67
2:L:249:ASN:O	8:K:252:ASN:ND2	2.28	0.67
18:T:202:CDL:HB21	18:T:202:CDL:H111	1.75	0.67
1:I:151:GLN:OE1	1:I:156:GLY:N	2.27	0.67
2:L:553:ARG:NH2	8:K:85:PRO:O	2.28	0.67
2:R:96:THR:OG1	2:R:266:GLU:OE2	2.12	0.67
7:D:117:GLY:N	7:D:185:LYS:O	2.28	0.67
18:T:202:CDL:C13	18:T:203:CDL:OB7	2.43	0.67
4:X:149:LEU:CD2	18:X:303:CDL:C64	2.71	0.67
9:Z:123:THR:CG2	18:Z:203:CDL:H322	2.25	0.67
18:F:706:CDL:H771	18:F:706:CDL:H162	1.77	0.67
18:X:302:CDL:C13	18:Z:203:CDL:OB7	2.43	0.67
2:R:121:LEU:CD1	18:S:302:CDL:HA32	2.24	0.67
18:X:302:CDL:C77	18:Z:203:CDL:H552	2.22	0.67
8:K:225:LEU:O	8:K:256:ASN:ND2	2.27	0.67
3:M:377:PHE:O	3:M:379:LYS:N	2.27	0.66
4:S:150:HIS:HA	18:S:302:CDL:H771	1.77	0.66
18:X:302:CDL:C72	18:Z:203:CDL:C51	2.66	0.66
1:O:186:LEU:HD22	8:Q:204:LEU:HD13	1.77	0.66
2:R:270:ILE:HG23	2:R:406:ILE:HG21	1.76	0.66
18:R:604:CDL:H521	18:P:201:CDL:H321	1.76	0.66
5:E:329:GLN:OE1	3:Y:348:HIS:NE2	2.28	0.66
5:E:136:PRO:O	5:E:233:GLN:NE2	2.28	0.66
18:R:604:CDL:H531	18:R:604:CDL:H731	1.76	0.66
4:X:157:ALA:CB	18:X:303:CDL:C51	2.73	0.66
1:O:115:PHE:HZ	13:O:302:HEC:HAA1	1.61	0.66
1:O:288:MET:SD	18:F:706:CDL:H511	2.35	0.66
1:O:119:THR:HA	1:O:217:GLN:NE2	2.10	0.66
3:Y:377:PHE:O	3:Y:379:LYS:N	2.28	0.66
1:O:203:SER:HB3	8:Q:170:ARG:N	2.11	0.65
1:O:218:ILE:HB	1:O:246:VAL:HG22	1.77	0.65
4:S:184:TYR:CE1	18:S:302:CDL:C73	2.79	0.65
18:T:202:CDL:C72	18:T:203:CDL:C51	2.66	0.65
18:L:604:CDL:H731	18:L:604:CDL:H531	1.76	0.65
18:T:202:CDL:C14	18:T:203:CDL:OB7	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:425:VAL:HG11	18:F:706:CDL:H371	1.77	0.65
1:O:215:PRO:HB3	1:O:246:VAL:HG11	1.77	0.65
5:F:131:GLY:O	5:F:134:ARG:NH1	2.29	0.65
9:Z:90:TRP:CZ2	18:Z:202:CDL:CB4	2.68	0.65
1:O:191:CYS:SG	13:O:302:HEC:HBC2	2.37	0.64
2:L:96:THR:OG1	2:L:266:GLU:OE2	2.13	0.64
1:O:95:LEU:CD1	1:O:150:VAL:CB	2.64	0.64
18:X:302:CDL:C14	18:Z:203:CDL:OB7	2.44	0.64
1:O:282:ALA:HA	18:T:203:CDL:H572	1.79	0.64
21:E:602:HEM:HBB2	21:E:602:HEM:HHC	1.79	0.64
2:L:206:MET:O	2:L:293:TYR:OH	2.12	0.64
5:E:450:ILE:HG21	5:E:461:LEU:HD13	1.79	0.64
9:Z:120:PHE:HB3	18:Z:202:CDL:H612	0.72	0.64
1:O:119:THR:CB	1:O:217:GLN:HG2	2.28	0.64
1:O:237:LEU:HD23	1:O:241:GLU:HB2	1.79	0.64
18:X:302:CDL:C77	18:Z:203:CDL:H551	2.14	0.64
18:X:302:CDL:H141	18:Z:203:CDL:OB7	1.97	0.64
1:O:119:THR:HG22	1:O:120:GLY:N	2.12	0.64
18:F:705:CDL:H111	18:F:705:CDL:H311	1.79	0.64
8:K:256:ASN:OD1	8:K:257:VAL:N	2.31	0.64
4:S:189:ASP:OD1	4:S:190:ILE:N	2.30	0.64
18:E:607:CDL:H771	18:E:607:CDL:H162	1.80	0.64
4:S:157:ALA:HB1	18:S:302:CDL:C51	2.28	0.63
18:E:606:CDL:H311	18:E:606:CDL:H111	1.79	0.63
4:X:157:ALA:HB1	18:X:303:CDL:H511	1.80	0.63
1:O:192:HIS:CG	1:O:210:LEU:HD21	2.34	0.63
9:T:97:LEU:CD1	18:T:201:CDL:H351	2.29	0.63
4:X:157:ALA:HB1	18:X:303:CDL:H512	1.80	0.63
2:L:190:ILE:HD11	9:Z:8:PHE:HZ	1.63	0.63
2:R:387:HIS:NE2	2:R:454:ASP:O	2.29	0.63
7:G:117:GLY:N	7:G:185:LYS:O	2.31	0.63
4:X:184:TYR:CE2	18:X:303:CDL:H731	2.33	0.63
1:O:115:PHE:CE2	1:O:226:PRO:HB3	2.34	0.63
2:R:120:ARG:HB2	18:S:302:CDL:OA4	1.98	0.63
4:X:184:TYR:CZ	18:X:303:CDL:H752	2.33	0.63
2:R:274:PHE:CD2	2:R:406:ILE:HG22	2.33	0.63
2:R:335:VAL:HG13	2:R:336:PRO:HD3	1.81	0.63
4:S:184:TYR:CE1	18:S:302:CDL:H732	2.34	0.63
18:T:202:CDL:H141	18:T:203:CDL:OB7	1.98	0.63
1:O:176:ASP:HB3	1:O:179:ARG:HG2	1.80	0.63
2:R:117:ALA:O	4:S:15:ARG:NH2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:604:CDL:H731	18:R:604:CDL:H512	1.81	0.63
4:S:43:LEU:HD23	4:S:143:ALA:HA	1.80	0.62
4:S:157:ALA:CB	18:S:302:CDL:C51	2.77	0.62
18:L:604:CDL:H512	18:L:604:CDL:C73	2.29	0.62
18:R:604:CDL:H512	18:R:604:CDL:C73	2.29	0.62
1:I:269:ALA:HB3	1:I:270:PRO:HD3	1.81	0.62
1:O:191:CYS:SG	1:O:201:LEU:HG	2.40	0.62
9:Z:126:CYS:HB2	18:Z:203:CDL:H321	1.82	0.62
8:Q:225:LEU:O	8:Q:256:ASN:ND2	2.32	0.62
8:Q:45:LEU:HD21	8:Q:116:VAL:HG22	1.82	0.62
5:E:161:LEU:HD21	5:E:208:TYR:HA	1.81	0.62
1:I:229:MET:O	3:Y:358:GLN:NE2	2.33	0.62
1:O:115:PHE:CE1	1:O:221:ALA:HB2	2.34	0.61
2:R:454:ASP:OD1	8:Q:35:TRP:NE1	2.33	0.61
2:L:250:GLY:O	2:L:254:LEU:N	2.29	0.61
1:O:188:CYS:HB2	13:O:302:HEC:C4B	2.30	0.61
2:R:401:VAL:O	2:R:405:THR:OG1	2.08	0.61
3:M:148:VAL:HG23	5:F:263:ALA:HB1	1.81	0.61
2:L:252:VAL:HB	8:K:231:ILE:HD11	1.83	0.61
1:O:119:THR:HA	1:O:217:GLN:CG	2.30	0.61
2:L:120:ARG:HB2	18:X:303:CDL:OA4	2.00	0.61
9:T:123:THR:HG23	18:T:203:CDL:H322	1.82	0.61
11:V:140:ILE:O	11:V:144:ILE:HD12	2.01	0.61
5:F:87:ARG:NH1	5:F:90:GLU:OE1	2.34	0.61
18:L:604:CDL:H731	18:L:604:CDL:H512	1.81	0.61
1:O:186:LEU:HB2	8:Q:136:PHE:CG	2.35	0.61
4:S:102:TRP:CE3	4:S:105:ILE:HD11	2.35	0.61
1:O:203:SER:HB3	8:Q:170:ARG:CA	2.30	0.61
2:L:274:PHE:CD2	2:L:406:ILE:HG22	2.35	0.61
18:T:202:CDL:H792	18:T:203:CDL:H581	1.83	0.61
4:X:32:TRP:CZ2	18:X:303:CDL:C38	2.78	0.61
1:O:118:SER:CA	1:O:143:ILE:HD13	2.31	0.60
1:O:114:TYR:CZ	1:O:167:VAL:HG21	2.36	0.60
4:S:184:TYR:CZ	18:S:302:CDL:H752	2.35	0.60
4:X:32:TRP:CE2	18:X:303:CDL:C35	2.83	0.60
9:Z:97:LEU:HD11	18:Z:202:CDL:C37	2.30	0.60
2:L:227:LEU:HD22	2:L:262:PHE:CZ	2.37	0.60
8:Q:256:ASN:OD1	8:Q:257:VAL:N	2.34	0.60
9:T:90:TRP:CZ2	18:T:201:CDL:CB4	2.73	0.60
1:O:118:SER:CB	1:O:143:ILE:HG21	2.30	0.60
1:O:119:THR:HG23	1:O:217:GLN:CG	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:MET:HE3	13:O:302:HEC:CHC	2.31	0.60
5:E:29:GLN:OE1	5:E:231:TRP:NE1	2.32	0.60
4:X:81:SER:OG	4:X:189:ASP:OD2	2.14	0.60
4:X:91:ALA:HB2	4:X:99:LEU:HD12	1.84	0.60
1:O:210:LEU:HD12	13:O:302:HEC:C3A	2.32	0.60
3:M:369:GLN:CG	5:F:404:LEU:HD21	2.32	0.60
9:T:126:CYS:HB2	18:T:203:CDL:H321	1.83	0.60
18:T:202:CDL:C72	18:T:203:CDL:H511	2.31	0.60
1:O:115:PHE:O	1:O:119:THR:HB	2.01	0.60
5:F:487:ARG:NH1	9:T:131:GLU:O	2.33	0.60
9:T:97:LEU:HD11	18:T:201:CDL:C37	2.31	0.60
18:X:302:CDL:H792	18:Z:203:CDL:H581	1.83	0.60
1:O:195:THR:HB	1:O:197:LYS:HE2	1.83	0.60
6:P:48:MET:SD	18:P:201:CDL:HB61	2.42	0.59
5:F:533:GLN:OE1	6:P:7:ARG:N	2.36	0.59
1:O:105:LEU:HD21	13:O:301:HEC:HHB	1.83	0.59
1:O:119:THR:CA	1:O:217:GLN:HG2	2.32	0.59
5:E:263:ALA:HB1	3:Y:148:VAL:HG23	1.84	0.59
4:X:161:LEU:O	4:X:165:THR:HG23	2.02	0.59
7:D:113:ILE:N	7:D:153:GLY:O	2.34	0.59
9:T:123:THR:CG2	18:T:203:CDL:H322	2.33	0.59
1:O:190:SER:HB2	8:Q:193:ARG:NH2	2.17	0.59
1:O:111:ALA:HB1	1:O:220:THR:HG22	1.84	0.59
18:X:302:CDL:C72	18:Z:203:CDL:H511	2.31	0.59
1:O:105:LEU:HD21	13:O:301:HEC:CHB	2.33	0.59
2:L:35:THR:HG21	9:Z:86:ALA:O	2.03	0.58
8:K:45:LEU:CD2	8:K:116:VAL:HG22	2.33	0.58
4:X:41:ALA:HA	9:Z:44:LEU:HD22	1.85	0.58
5:E:65:ASP:HB3	5:E:91:THR:HG21	1.84	0.58
5:E:438:ARG:NH2	6:J:35:SER:OG	2.36	0.58
2:R:378:LEU:HD23	8:Q:50:TRP:CZ3	2.38	0.58
18:T:202:CDL:HB22	18:T:202:CDL:HB4	1.84	0.58
1:O:247:ALA:O	1:O:251:GLU:HB3	2.03	0.58
9:Z:101:THR:HG22	15:Z:201:MQ9:C18	2.33	0.58
1:O:120:GLY:O	1:O:133:SER:HA	2.02	0.58
1:O:185:ARG:HA	1:O:189:ALA:HB3	1.84	0.58
4:S:32:TRP:CE2	18:S:302:CDL:C35	2.87	0.58
2:L:84:THR:O	2:L:88:THR:OG1	2.18	0.58
9:T:120:PHE:HB3	18:T:201:CDL:H612	0.67	0.58
5:E:312:ILE:HD13	5:E:333:VAL:HG21	1.85	0.58
6:P:29:ASP:N	6:P:29:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:302:CDL:HB4	18:X:302:CDL:HB22	1.84	0.58
1:O:115:PHE:HE2	1:O:226:PRO:HB3	1.68	0.58
4:S:184:TYR:CE2	18:S:302:CDL:H731	2.39	0.58
18:Z:203:CDL:C16	1:I:281:VAL:HG11	2.33	0.58
2:R:540:ARG:NH2	2:R:554:MET:SD	2.77	0.58
18:E:606:CDL:H371	18:E:606:CDL:H152	1.86	0.58
2:R:88:THR:HG22	2:R:151:TRP:HD1	1.68	0.57
5:E:370:VAL:O	5:E:370:VAL:HG13	2.03	0.57
2:L:200:GLY:O	2:L:205:ARG:NH2	2.36	0.57
9:T:94:LEU:CD2	18:T:201:CDL:H322	2.30	0.57
2:R:268:TYR:OH	2:R:333:ILE:HD12	2.03	0.57
18:F:705:CDL:H371	18:F:705:CDL:H152	1.86	0.57
1:O:119:THR:HA	1:O:217:GLN:HE21	1.69	0.57
2:R:274:PHE:CE2	2:R:406:ILE:HG22	2.40	0.57
1:O:202:SER:HB2	1:O:205:LYS:CD	2.31	0.57
1:O:203:SER:HB3	8:Q:170:ARG:CB	2.35	0.57
5:E:66:PRO:O	5:E:67:SER:OG	2.23	0.57
2:L:330:THR:HG22	17:L:602:HEA:HMB2	1.87	0.57
1:O:119:THR:CG2	1:O:217:GLN:HG2	2.34	0.57
4:S:157:ALA:HA	18:S:302:CDL:H511	1.87	0.57
4:X:184:TYR:CE1	18:X:303:CDL:H731	2.39	0.57
2:R:465:LEU:HD11	8:Q:326:GLU:O	2.05	0.57
4:S:157:ALA:HB1	18:S:302:CDL:H512	1.87	0.57
2:L:256:GLN:OE1	2:L:318:THR:HG21	2.05	0.56
9:T:98:SER:HG	18:T:201:CDL:H621	1.68	0.56
2:L:122:ASN:OD1	2:L:123:ALA:N	2.38	0.56
4:S:25:VAL:HG12	4:S:180:VAL:HG11	1.86	0.56
2:L:460:ARG:N	17:L:603:HEA:O2A	2.37	0.56
2:L:544:GLU:OE2	2:L:555:ARG:NH2	2.39	0.56
1:O:110:GLU:H	1:O:151:GLN:HG3	1.69	0.56
1:O:110:GLU:HG2	1:O:159:VAL:HG12	1.88	0.56
5:E:65:ASP:OD1	5:F:67:SER:OG	2.23	0.56
8:K:45:LEU:HD21	8:K:116:VAL:HG22	1.87	0.56
4:X:184:TYR:CD1	18:X:303:CDL:H732	2.41	0.56
1:O:119:THR:HG23	1:O:217:GLN:HB3	1.87	0.56
1:O:169:GLN:CG	1:O:215:PRO:HD2	2.36	0.56
4:S:157:ALA:HB1	18:S:302:CDL:H511	1.88	0.56
2:L:387:HIS:NE2	2:L:454:ASP:O	2.38	0.56
9:T:120:PHE:HB3	18:T:201:CDL:C62	2.29	0.56
1:O:234:ASP:O	1:O:238:THR:HA	2.06	0.56
2:L:77:GLU:OE1	8:K:332:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:45:LEU:CD2	8:Q:116:VAL:HG22	2.35	0.56
4:X:149:LEU:CD2	18:X:303:CDL:C63	2.68	0.56
2:R:357:THR:N	2:R:428:GLU:OE2	2.38	0.56
2:L:274:PHE:CE2	2:L:406:ILE:HG22	2.41	0.56
1:O:130:GLN:HG3	1:O:206:TYR:H	1.70	0.56
1:O:210:LEU:HG	13:O:302:HEC:HHB	1.88	0.56
18:L:604:CDL:HB61	18:L:604:CDL:OB4	2.06	0.56
8:K:279:THR:HG21	1:I:126:ARG:HA	1.87	0.56
3:M:84:ARG:CZ	5:F:500:GLY:O	2.54	0.56
5:E:213:LEU:HD21	21:F:703:HEM:CBC	2.36	0.56
2:L:121:LEU:CD1	18:X:303:CDL:HA32	2.29	0.56
18:T:202:CDL:H572	18:T:202:CDL:H742	1.88	0.56
1:O:117:VAL:HG11	1:O:138:PHE:HB2	1.88	0.55
5:E:89:TYR:OH	5:E:287:LEU:O	2.22	0.55
5:F:422:VAL:HG22	18:F:706:CDL:H402	1.87	0.55
5:E:161:LEU:HD21	5:E:208:TYR:CA	2.37	0.55
5:E:487:ARG:NH1	9:Z:131:GLU:O	2.39	0.55
1:O:191:CYS:HB2	13:O:302:HEC:CBC	2.35	0.55
5:E:17:ASP:OD1	5:E:23:SER:OG	2.18	0.55
2:L:27:LEU:HD22	18:L:604:CDL:OA5	2.05	0.55
2:L:35:THR:HG22	2:L:119:PRO:HB2	1.88	0.55
7:D:74:THR:N	7:D:78:THR:O	2.38	0.55
9:Z:123:THR:HG23	18:Z:203:CDL:H331	1.88	0.55
2:R:156:PRO:HG3	2:R:252:VAL:HG12	1.88	0.55
5:E:104:PHE:HD2	15:E:604:MQ9:H502	1.72	0.55
5:F:116:PHE:CZ	5:F:120:ILE:HD11	2.41	0.55
2:R:252:VAL:HG21	8:Q:246:LEU:HD22	1.89	0.55
10:U:72:GLY:N	11:V:110:TYR:O	2.39	0.55
2:R:122:ASN:OD1	2:R:123:ALA:N	2.40	0.55
18:R:604:CDL:HB61	18:R:604:CDL:OB4	2.06	0.55
21:F:703:HEM:HHC	21:F:703:HEM:HBB2	1.88	0.55
2:R:209:PHE:CZ	2:R:213:ILE:HD11	2.42	0.55
4:S:184:TYR:CE1	18:S:302:CDL:H731	2.41	0.55
5:E:282:ASN:ND2	21:E:602:HEM:O1A	2.38	0.55
18:Z:203:CDL:H161	1:I:281:VAL:CG1	2.33	0.55
1:O:172:LEU:HA	1:O:243:ARG:NE	2.21	0.55
1:O:238:THR:HG23	1:O:240:ASP:H	1.71	0.55
1:O:293:ARG:HH12	18:T:203:CDL:HB22	1.71	0.55
8:K:288:VAL:HG23	8:K:288:VAL:O	2.07	0.55
1:O:186:LEU:HB2	8:Q:136:PHE:CD2	2.42	0.54
1:O:192:HIS:CE1	1:O:207:ALA:HB1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:284:ILE:HD13	18:F:706:CDL:H552	1.89	0.54
5:F:194:PHE:CE2	5:F:203:LEU:HD22	2.42	0.54
4:X:15:ARG:O	4:X:16:VAL:HG23	2.07	0.54
4:X:32:TRP:CH2	18:X:303:CDL:H382	2.42	0.54
18:R:604:CDL:H792	18:F:706:CDL:H391	1.90	0.54
18:X:302:CDL:H742	18:X:302:CDL:H572	1.88	0.54
1:O:245:ILE:HG21	13:O:302:HEC:CBB	2.35	0.54
1:O:245:ILE:HG13	13:O:302:HEC:CBB	2.36	0.54
5:E:19:ARG:O	5:F:233:GLN:NE2	2.37	0.54
6:J:29:ASP:OD1	6:J:29:ASP:N	2.40	0.54
9:Z:90:TRP:HH2	18:Z:202:CDL:OB7	1.90	0.54
2:R:398:PHE:HA	2:R:401:VAL:HG22	1.90	0.54
9:Z:123:THR:HG23	18:Z:203:CDL:C32	2.37	0.54
1:I:87:CYS:SG	13:I:301:HEC:HAB	2.47	0.54
1:O:271:GLU:CG	5:F:281:ILE:HD12	2.38	0.54
3:M:369:GLN:HG2	5:F:404:LEU:HD21	1.90	0.54
5:E:368:ARG:O	5:E:434:GLN:NE2	2.39	0.54
1:O:119:THR:CG2	1:O:120:GLY:H	2.20	0.54
1:O:210:LEU:HD12	13:O:302:HEC:CMA	2.37	0.54
1:O:226:PRO:HG2	1:O:229:MET:HB3	1.90	0.54
8:Q:40:THR:HG23	8:Q:43:ALA:H	1.73	0.54
9:Z:98:SER:OG	18:Z:202:CDL:C62	2.53	0.54
2:R:89:VAL:CG2	2:R:137:ILE:HD11	2.37	0.53
2:L:117:ALA:O	4:X:15:ARG:NH2	2.42	0.53
2:L:259:PHE:O	2:L:263:GLY:N	2.38	0.53
2:R:46:VAL:CG1	18:P:201:CDL:H371	2.38	0.53
5:F:393:ASN:OD1	5:F:394:ASP:N	2.41	0.53
9:T:22:TYR:O	9:T:26:THR:OG1	2.20	0.53
1:O:282:ALA:O	1:O:286:VAL:HG23	2.08	0.53
5:E:278:LEU:O	1:I:261:TYR:N	2.40	0.53
5:F:172:ARG:NH1	5:F:176:SER:OG	2.42	0.53
4:X:32:TRP:NE1	18:X:303:CDL:C36	2.68	0.53
5:E:116:PHE:CZ	5:E:120:ILE:HD11	2.42	0.53
2:R:21:MET:HG2	18:R:604:CDL:HA22	1.90	0.53
8:Q:294:ASN:OD1	8:Q:295:ASP:N	2.41	0.53
2:L:419:PRO:HG3	2:L:425:LEU:HD23	1.90	0.53
1:I:121:ARG:NE	13:I:302:HEC:O1D	2.41	0.53
1:O:281:VAL:HG11	18:T:203:CDL:H161	1.91	0.53
2:R:460:ARG:N	17:R:603:HEA:O2A	2.39	0.53
5:E:312:ILE:HA	5:E:333:VAL:HG21	1.90	0.53
18:E:606:CDL:OB7	18:F:705:CDL:H112	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:184:TYR:CD1	18:S:302:CDL:H732	2.44	0.52
5:E:365:GLN:OE1	5:E:373:ARG:NH2	2.42	0.52
5:E:499:THR:HG22	5:E:511:HIS:ND1	2.25	0.52
4:X:157:ALA:HA	18:X:303:CDL:H511	1.90	0.52
5:E:425:VAL:HG22	18:L:604:CDL:H722	1.91	0.52
6:J:93:LEU:O	6:J:98:TRP:N	2.40	0.52
8:K:245:VAL:HG23	8:K:245:VAL:O	2.09	0.52
2:R:84:THR:OG1	2:R:149:PHE:O	2.25	0.52
5:E:404:LEU:HD21	3:Y:369:GLN:CG	2.39	0.52
2:L:243:HIS:ND1	2:L:246:ASP:OD2	2.42	0.52
18:T:202:CDL:H741	18:T:202:CDL:H611	1.92	0.52
9:Z:97:LEU:HD12	18:Z:202:CDL:C35	2.38	0.52
5:F:27:ARG:HB2	3:Y:177:VAL:HG22	1.92	0.52
3:M:67:THR:HG23	3:M:67:THR:O	2.10	0.52
5:E:421:ILE:HG13	18:J:203:CDL:H572	1.92	0.52
17:L:603:HEA:HMC1	17:L:603:HEA:HBC1	1.91	0.52
8:K:294:ASN:OD1	8:K:295:ASP:N	2.43	0.52
2:R:419:PRO:HG3	2:R:425:LEU:HD23	1.91	0.52
2:L:15:ARG:NH1	2:L:19:GLU:OE1	2.43	0.52
8:Q:140:TRP:NE1	8:Q:284:MET:O	2.38	0.52
4:X:166:LYS:NZ	18:X:302:CDL:CA5	2.62	0.52
18:X:302:CDL:H611	18:X:302:CDL:H741	1.92	0.52
2:R:169:ASP:OD1	2:R:238:ARG:NE	2.42	0.52
2:L:42:ILE:HG22	18:L:604:CDL:H332	1.92	0.52
9:T:94:LEU:HD23	18:T:201:CDL:H352	1.91	0.52
9:T:97:LEU:HD12	18:T:201:CDL:C35	2.39	0.52
2:R:398:PHE:O	2:R:402:LEU:HD12	2.10	0.51
4:S:149:LEU:CB	18:S:302:CDL:H801	2.29	0.51
5:F:65:ASP:HB3	5:F:91:THR:HG21	1.91	0.51
1:I:187:ASN:O	13:I:302:HEC:HMC3	2.09	0.51
2:R:163:SER:OG	2:R:163:SER:O	2.26	0.51
5:E:327:ILE:CG2	5:E:331:VAL:HG11	2.40	0.51
5:E:336:GLY:O	5:E:340:VAL:HG23	2.09	0.51
4:X:32:TRP:CZ2	18:X:303:CDL:C36	2.93	0.51
10:U:56:GLU:N	10:U:56:GLU:OE1	2.43	0.51
4:X:157:ALA:CA	18:X:303:CDL:H511	2.40	0.51
9:Z:94:LEU:CD2	18:Z:202:CDL:H322	2.31	0.51
2:R:158:THR:O	2:R:238:ARG:NH1	2.42	0.51
5:E:236:THR:HG21	5:E:364:LEU:HD21	1.92	0.51
5:F:438:ARG:NH2	6:P:35:SER:OG	2.39	0.51
9:T:98:SER:O	9:T:101:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:203:SER:HB2	8:Q:170:ARG:CG	2.34	0.51
3:M:347:SER:O	3:M:387:ARG:NH1	2.41	0.51
5:F:368:ARG:O	5:F:434:GLN:NE2	2.38	0.51
2:L:445:THR:HG23	2:L:446:PHE:CD2	2.45	0.51
9:T:123:THR:HG23	18:T:203:CDL:H331	1.93	0.51
1:O:232:PHE:HE2	13:O:302:HEC:HHC	1.76	0.51
5:E:395:ILE:HG22	15:Z:201:MQ9:H5M1	1.93	0.51
9:T:98:SER:OG	18:T:201:CDL:C62	2.53	0.51
3:Y:407:ASP:OD1	3:Y:408:PHE:N	2.42	0.51
2:R:104:ASN:OD1	2:R:122:ASN:ND2	2.43	0.51
5:E:366:ARG:NH1	5:E:437:ASP:OD2	2.42	0.51
5:F:478:GLU:OE2	6:P:7:ARG:NH1	2.44	0.51
5:F:433:LEU:CD1	18:F:706:CDL:HA61	2.41	0.51
2:L:29:TYR:OH	18:Z:202:CDL:OA4	2.23	0.51
2:L:508:ASP:N	2:L:508:ASP:OD1	2.44	0.51
9:T:120:PHE:CD2	18:T:201:CDL:C63	2.81	0.51
11:V:51:LEU:HB2	11:V:144:ILE:HD11	1.93	0.51
2:R:257:HIS:NE2	9:T:35:GLU:OE1	2.43	0.50
4:S:157:ALA:CA	18:S:302:CDL:H511	2.41	0.50
2:L:534:PRO:HB3	2:L:545:LEU:HD12	1.93	0.50
6:J:87:VAL:HG22	18:J:203:CDL:H511	1.94	0.50
1:O:117:VAL:HA	1:O:122:MET:CG	2.33	0.50
3:M:145:ILE:HD13	18:T:202:CDL:H732	1.92	0.50
4:S:32:TRP:CZ2	18:S:302:CDL:C38	2.81	0.50
1:O:115:PHE:HA	1:O:119:THR:OG1	2.11	0.50
1:O:119:THR:HG23	1:O:217:GLN:CB	2.40	0.50
1:O:222:MET:CG	1:O:232:PHE:HB2	2.31	0.50
1:O:174:GLY:HA3	1:O:244:ASP:HA	1.93	0.50
2:R:445:THR:HG23	2:R:446:PHE:CD2	2.47	0.50
6:J:53:LEU:CD1	6:J:87:VAL:HG11	2.41	0.50
9:Z:108:LEU:O	9:Z:110:LEU:N	2.45	0.50
1:O:273:MET:HE3	15:O:304:MQ9:C10	2.41	0.50
2:R:496:PHE:O	2:R:500:ARG:NH2	2.44	0.50
2:L:35:THR:HG22	2:L:35:THR:O	2.12	0.50
4:X:157:ALA:HB2	18:X:303:CDL:C53	2.36	0.50
2:R:515:ASN:N	2:R:515:ASN:OD1	2.44	0.50
3:M:275:ASP:OD1	3:M:275:ASP:N	2.44	0.50
4:S:32:TRP:NE1	18:S:302:CDL:C36	2.69	0.50
3:M:159:ILE:O	3:M:159:ILE:HG22	2.12	0.50
5:E:433:LEU:CD1	18:E:607:CDL:HA61	2.42	0.50
5:F:135:ARG:HB3	5:F:136:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:202:CDL:C17	18:T:203:CDL:H731	2.42	0.50
8:K:135:ALA:HB3	8:K:245:VAL:HG21	1.94	0.50
3:Y:265:PRO:CG	3:Y:301:LEU:HD23	2.42	0.50
2:R:35:THR:HG21	9:T:86:ALA:O	2.12	0.49
2:R:406:ILE:HD11	17:R:603:HEA:CBC	2.42	0.49
5:E:227:LEU:HD22	18:E:606:CDL:H782	1.93	0.49
6:J:86:LEU:HD23	18:J:203:CDL:H162	1.94	0.49
9:T:108:LEU:O	9:T:110:LEU:N	2.45	0.49
9:Z:98:SER:O	9:Z:101:THR:OG1	2.26	0.49
9:Z:101:THR:HG22	15:Z:201:MQ9:H18	1.94	0.49
1:O:213:ALA:HA	1:O:217:GLN:OE1	2.12	0.49
1:O:232:PHE:CZ	13:O:302:HEC:HMC2	2.47	0.49
18:E:607:CDL:H412	18:L:604:CDL:H792	1.93	0.49
5:F:336:GLY:O	5:F:340:VAL:HG23	2.12	0.49
3:M:407:ASP:OD1	3:M:408:PHE:N	2.43	0.49
5:F:312:ILE:HG13	5:F:333:VAL:HG21	1.94	0.49
2:L:386:PHE:O	8:K:242:LYS:NZ	2.32	0.49
5:E:395:ILE:CG2	15:Z:201:MQ9:H5M1	2.42	0.49
5:E:131:GLY:O	5:E:134:ARG:NE	2.41	0.49
5:F:395:ILE:CG2	15:T:204:MQ9:H5M1	2.43	0.49
2:L:496:PHE:O	2:L:500:ARG:NH2	2.43	0.49
5:E:127:ILE:HD11	21:E:601:HEM:CAC	2.43	0.49
15:E:604:MQ9:H511	15:E:604:MQ9:H453	1.94	0.49
5:F:65:ASP:CB	5:F:91:THR:HG21	2.43	0.49
18:R:604:CDL:H722	5:F:425:VAL:HG22	1.93	0.49
18:E:606:CDL:H112	18:F:705:CDL:OB7	2.12	0.49
5:F:104:PHE:HD2	15:F:707:MQ9:H502	1.78	0.49
2:L:156:PRO:HG3	2:L:252:VAL:HG12	1.94	0.49
2:L:392:TYR:HD2	2:L:452:LEU:HD23	1.76	0.49
18:E:606:CDL:OB7	18:F:705:CDL:C11	2.61	0.49
4:X:81:SER:HG	4:X:189:ASP:CG	2.13	0.49
4:X:99:LEU:C	4:X:99:LEU:HD23	2.33	0.49
18:X:302:CDL:C17	18:Z:203:CDL:H731	2.42	0.49
3:Y:110:TRP:HZ2	3:Y:127:LEU:HD11	1.78	0.49
1:O:188:CYS:CA	13:O:302:HEC:HMC3	2.40	0.49
2:R:34:THR:HG21	2:R:43:MET:CE	2.43	0.49
2:R:89:VAL:HG21	2:R:137:ILE:HD11	1.93	0.49
3:M:177:VAL:HG22	5:E:27:ARG:HB2	1.95	0.49
2:L:401:VAL:HG11	17:L:602:HEA:C2C	2.42	0.49
1:O:95:LEU:HD11	1:O:150:VAL:CG1	2.42	0.48
5:E:65:ASP:CB	5:E:91:THR:HG21	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:275:GLU:O	8:Q:281:HIS:CE1	2.66	0.48
9:T:90:TRP:HH2	18:T:201:CDL:OB7	1.95	0.48
18:Z:203:CDL:C57	1:I:282:ALA:HA	2.42	0.48
5:F:227:LEU:HD22	18:F:705:CDL:H782	1.95	0.48
1:I:124:ALA:O	13:I:301:HEC:HAC	2.12	0.48
5:F:370:VAL:O	5:F:370:VAL:HG13	2.13	0.48
9:Z:120:PHE:HB3	18:Z:202:CDL:C62	2.38	0.48
1:O:124:ALA:HB2	1:O:134:LYS:HZ1	1.79	0.48
2:R:292:GLY:O	2:R:295:THR:OG1	2.25	0.48
5:E:123:HIS:NE2	21:E:601:HEM:ND	2.62	0.48
2:L:371:LEU:HD23	2:L:400:TYR:CE2	2.48	0.48
8:Q:160:ASP:N	8:Q:161:PRO:CD	2.76	0.48
9:Z:94:LEU:HD23	18:Z:202:CDL:H352	1.95	0.48
2:R:107:LEU:HD12	2:R:210:THR:HG22	1.94	0.48
4:S:149:LEU:CG	18:S:302:CDL:H631	2.43	0.48
18:X:302:CDL:H732	3:Y:145:ILE:HD13	1.95	0.48
2:R:335:VAL:HG13	2:R:336:PRO:CD	2.43	0.48
5:F:421:ILE:HG13	18:P:201:CDL:H572	1.94	0.48
2:L:96:THR:O	2:L:99:VAL:HG22	2.14	0.48
2:L:221:LEU:HD22	4:X:35:SER:OG	2.14	0.48
5:F:282:ASN:ND2	21:F:703:HEM:O1A	2.43	0.48
1:O:90:CYS:SG	13:O:301:HEC:HBC2	2.54	0.47
2:R:221:LEU:HD22	4:S:35:SER:OG	2.14	0.47
2:R:77:GLU:OE2	8:Q:332:ARG:NH1	2.43	0.47
2:R:378:LEU:HD23	8:Q:50:TRP:CH2	2.49	0.47
5:E:107:GLN:NE2	5:E:276:GLY:O	2.46	0.47
3:M:44:ASP:OD1	3:M:45:ALA:N	2.46	0.47
4:S:161:LEU:O	4:S:165:THR:HG23	2.14	0.47
5:F:147:LEU:HD13	5:F:222:LEU:HB2	1.96	0.47
1:O:203:SER:O	8:Q:170:ARG:HD3	1.93	0.47
2:L:33:THR:HG22	9:Z:90:TRP:HB3	1.97	0.47
1:O:78:THR:O	1:O:81:GLN:HG3	2.14	0.47
2:R:50:ALA:CB	18:P:201:CDL:H401	2.44	0.47
5:E:212:ILE:HD11	5:F:212:ILE:HD11	1.95	0.47
8:Q:222:GLU:OE2	8:Q:257:VAL:HG21	2.14	0.47
1:O:222:MET:CE	13:O:302:HEC:HBB2	2.43	0.47
2:L:392:TYR:CD2	2:L:452:LEU:HD23	2.49	0.47
8:K:197:ASN:OD1	8:K:197:ASN:N	2.48	0.47
3:Y:293:THR:HG23	3:Y:294:THR:HG23	1.96	0.47
1:O:117:VAL:CG1	1:O:138:PHE:HB2	2.44	0.47
1:O:275:MET:HE2	5:F:111:TRP:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:29:TYR:O	2:R:33:THR:OG1	2.32	0.47
2:R:35:THR:O	2:R:35:THR:HG22	2.15	0.47
2:R:546:HIS:NE2	11:V:29:SER:OG	2.42	0.47
3:M:230:THR:HG22	3:M:231:ALA:N	2.30	0.47
3:M:265:PRO:CG	3:M:301:LEU:HD23	2.44	0.47
3:M:271:PRO:O	3:M:316:ARG:NH1	2.48	0.47
18:E:606:CDL:C11	18:F:705:CDL:OB7	2.63	0.47
5:F:244:THR:HG21	5:F:536:ILE:HG21	1.97	0.47
2:L:326:PHE:O	2:L:330:THR:OG1	2.18	0.47
9:T:123:THR:HG23	18:T:203:CDL:C32	2.45	0.47
1:I:210:LEU:HD21	13:I:302:HEC:HHB	1.96	0.47
3:Y:230:THR:HG23	3:Y:244:THR:HG22	1.96	0.47
5:E:147:LEU:HD13	5:E:222:LEU:CB	2.44	0.47
1:O:95:LEU:HD22	1:O:105:LEU:HD23	1.97	0.47
1:O:210:LEU:HD12	13:O:302:HEC:HMA3	1.96	0.47
4:X:41:ALA:CA	9:Z:44:LEU:HD22	2.45	0.47
1:I:234:ASP:O	1:I:238:THR:HA	2.15	0.47
1:O:95:LEU:CD1	1:O:150:VAL:CA	2.75	0.47
1:O:169:GLN:HG3	1:O:216:ALA:H	1.80	0.47
1:O:218:ILE:HG23	13:O:302:HEC:HMB2	1.97	0.47
2:R:193:VAL:HG13	2:R:206:MET:HE1	1.97	0.47
18:L:604:CDL:H522	18:L:604:CDL:H552	1.43	0.47
4:X:91:ALA:CB	4:X:99:LEU:HD12	2.45	0.47
2:R:406:ILE:HD11	17:R:603:HEA:HBC2	1.95	0.46
8:K:230:VAL:HG22	8:K:231:ILE:N	2.29	0.46
4:X:184:TYR:CZ	18:X:303:CDL:C73	2.91	0.46
4:X:184:TYR:CD1	18:X:303:CDL:C73	2.99	0.46
1:O:273:MET:SD	15:O:304:MQ9:H3D	2.55	0.46
4:S:160:LEU:CD2	9:T:129:VAL:HG11	2.46	0.46
5:E:42:LEU:HD13	5:E:122:VAL:CG1	2.43	0.46
1:O:203:SER:CA	8:Q:170:ARG:CG	2.58	0.46
1:O:245:ILE:HD13	1:O:245:ILE:HA	1.75	0.46
2:R:118:PHE:HB3	18:S:302:CDL:OA3	2.16	0.46
4:S:184:TYR:CZ	18:S:302:CDL:C73	2.97	0.46
5:E:327:ILE:HG23	5:E:331:VAL:HG11	1.96	0.46
5:E:392:MET:SD	1:I:269:ALA:HB1	2.55	0.46
1:O:284:ILE:O	1:O:288:MET:HG3	2.15	0.46
2:R:310:VAL:HG11	2:R:333:ILE:HD13	1.98	0.46
5:E:440:VAL:HG21	5:E:486:LYS:HG2	1.97	0.46
5:F:17:ASP:OD2	5:F:23:SER:OG	2.18	0.46
2:L:46:VAL:CG1	18:J:203:CDL:H371	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:120:ARG:NH1	9:Z:131:GLU:OE1	2.44	0.46
9:Z:123:THR:HG23	18:Z:203:CDL:C33	2.45	0.46
13:O:302:HEC:CMA	13:O:302:HEC:HBA1	2.44	0.46
2:R:35:THR:HG22	2:R:119:PRO:HB2	1.97	0.46
2:L:104:ASN:OD1	2:L:122:ASN:ND2	2.48	0.46
2:L:186:GLY:O	2:L:190:ILE:HG22	2.16	0.46
2:R:403:PHE:CZ	2:R:407:VAL:HG11	2.50	0.46
5:E:194:PHE:CE2	5:E:203:LEU:HD22	2.51	0.46
11:V:44:PRO:O	11:V:47:ASP:OD1	2.34	0.46
1:I:112:ALA:HB2	1:I:224:THR:HG21	1.97	0.46
1:O:130:GLN:HE21	1:O:205:LYS:HG2	1.81	0.46
1:O:203:SER:N	8:Q:168:THR:HA	2.31	0.46
13:O:302:HEC:HHA	13:O:302:HEC:O2D	2.16	0.46
3:M:243:TRP:NE1	3:M:310:ASN:O	2.41	0.46
5:F:499:THR:HG22	5:F:511:HIS:ND1	2.30	0.46
10:U:32:HIS:NE2	11:V:43:PHE:O	2.47	0.46
1:I:184:PHE:O	1:I:188:CYS:N	2.46	0.46
13:I:302:HEC:CBB	13:I:302:HEC:HHC	2.45	0.46
3:Y:44:ASP:OD1	3:Y:45:ALA:N	2.48	0.46
2:R:190:ILE:HD11	9:T:8:PHE:HZ	1.81	0.46
2:R:532:GLU:OE2	11:V:23:THR:OG1	2.33	0.46
18:R:604:CDL:H552	18:R:604:CDL:H522	1.43	0.46
2:L:310:VAL:O	2:L:310:VAL:HG13	2.16	0.46
1:O:282:ALA:HA	18:T:203:CDL:C57	2.45	0.46
3:M:230:THR:HG23	3:M:244:THR:HG22	1.98	0.46
5:E:450:ILE:HD12	9:Z:81:GLU:OE2	2.16	0.46
2:L:419:PRO:CG	2:L:425:LEU:HD23	2.46	0.46
9:T:8:PHE:CE1	9:T:52:THR:HG21	2.51	0.46
18:X:302:CDL:H792	18:Z:203:CDL:C58	2.46	0.46
1:O:239:PRO:O	1:O:243:ARG:HG2	2.17	0.45
2:R:266:GLU:OE1	2:R:270:ILE:HD12	2.15	0.45
5:E:213:LEU:HD21	21:F:703:HEM:HBC1	1.98	0.45
2:R:417:TRP:NE1	2:R:518:GLU:OE2	2.46	0.45
2:L:21:MET:HG2	18:L:604:CDL:HA22	1.97	0.45
4:X:189:ASP:OD1	4:X:189:ASP:C	2.54	0.45
18:X:302:CDL:H791	18:X:302:CDL:H622	1.99	0.45
1:O:119:THR:OG1	1:O:217:GLN:HG2	2.15	0.45
1:O:121:ARG:HG3	13:O:302:HEC:O2D	2.15	0.45
3:M:81:ALA:HB3	5:F:514:LEU:HD11	1.99	0.45
2:L:465:LEU:HD21	8:K:328:PHE:CD1	2.51	0.45
13:I:301:HEC:HMB1	13:I:301:HEC:HBB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:335:ASN:ND2	3:Y:337:GLY:O	2.49	0.45
1:O:232:PHE:HZ	13:O:302:HEC:HMC2	1.82	0.45
1:O:119:THR:CG2	1:O:120:GLY:N	2.79	0.45
2:R:84:THR:O	2:R:88:THR:HG23	2.16	0.45
3:M:242:GLY:O	3:M:286:ARG:NH1	2.45	0.45
4:S:41:ALA:HA	9:T:44:LEU:HD22	1.98	0.45
8:K:145:GLN:O	8:K:158:GLY:N	2.49	0.45
4:X:25:VAL:HG12	4:X:180:VAL:HG11	1.99	0.45
3:M:364:LEU:HD12	3:M:365:CYS:H	1.82	0.45
4:S:163:ALA:HB1	18:T:202:CDL:HA61	1.98	0.45
5:E:116:PHE:CE1	5:E:120:ILE:HD11	2.51	0.45
2:L:264:HIS:O	2:L:267:VAL:HG22	2.16	0.45
15:F:707:MQ9:H453	15:F:707:MQ9:H511	1.98	0.45
9:Z:91:TRP:N	9:Z:92:PRO:CD	2.80	0.45
1:I:72:GLN:OE1	1:I:74:ALA:N	2.50	0.45
18:E:606:CDL:H551	18:E:606:CDL:H581	1.70	0.45
5:F:147:LEU:HD13	5:F:222:LEU:CB	2.47	0.45
5:F:414:GLY:O	5:F:418:LEU:N	2.48	0.45
8:Q:32:ALA:HB1	8:Q:35:TRP:HB2	1.98	0.45
4:X:37:LEU:HD22	9:Z:51:ILE:HD12	1.99	0.45
9:Z:97:LEU:HD13	18:Z:202:CDL:H351	1.98	0.45
1:O:115:PHE:HE2	1:O:226:PRO:CB	2.29	0.45
4:S:36:GLU:OE1	4:S:150:HIS:NE2	2.41	0.45
4:S:157:ALA:CB	18:S:302:CDL:H512	2.46	0.45
5:E:198:PHE:HE2	5:E:290:TYR:HH	1.63	0.45
2:L:406:ILE:HD11	17:L:603:HEA:CBC	2.47	0.45
4:X:157:ALA:CB	18:X:303:CDL:H512	2.43	0.45
3:Y:230:THR:HG22	3:Y:231:ALA:N	2.32	0.45
2:L:27:LEU:HD22	18:L:604:CDL:PA1	2.57	0.45
2:L:505:VAL:HG13	2:L:505:VAL:O	2.15	0.45
10:U:23:LEU:O	10:U:27:THR:OG1	2.24	0.45
1:O:176:ASP:CB	1:O:179:ARG:HG2	2.45	0.44
8:Q:231:ILE:HD13	8:Q:246:LEU:CD2	2.35	0.44
3:Y:355:LEU:N	3:Y:355:LEU:HD12	2.32	0.44
1:O:184:PHE:CE2	1:O:189:ALA:HA	2.53	0.44
5:E:506:ASP:OD2	3:Y:84:ARG:NH2	2.45	0.44
2:L:212:ASN:ND2	2:L:272:LEU:O	2.45	0.44
8:Q:195:TYR:CE2	8:Q:247:PRO:O	2.70	0.44
13:I:302:HEC:HBC3	13:I:302:HEC:HHD	1.99	0.44
13:I:302:HEC:HHD	13:I:302:HEC:CBC	2.46	0.44
5:E:56:THR:HG22	15:E:604:MQ9:H451	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:183:PRO:O	3:Y:417:TRP:CG	2.71	0.44
5:E:404:LEU:HD21	3:Y:369:GLN:HG2	1.99	0.44
5:F:147:LEU:HD21	5:F:223:ILE:HG13	1.99	0.44
5:F:409:TRP:CZ3	6:P:76:LEU:HD11	2.52	0.44
8:Q:230:VAL:O	8:Q:232:HIS:ND1	2.51	0.44
11:V:68:VAL:HG13	11:V:143:LEU:HD22	1.99	0.44
1:I:201:LEU:HD11	13:I:302:HEC:HMD3	1.98	0.44
1:O:130:GLN:CG	1:O:205:LYS:HA	2.46	0.44
1:O:169:GLN:HE21	1:O:216:ALA:HB3	1.82	0.44
1:O:172:LEU:CD2	1:O:216:ALA:HA	2.48	0.44
3:M:269:MET:HE1	3:M:274:ILE:HD11	1.99	0.44
3:M:349:LEU:HD12	3:M:368:HIS:CE1	2.52	0.44
2:L:111:ILE:HD12	2:L:196:MET:O	2.16	0.44
2:L:270:ILE:CG2	2:L:406:ILE:HG21	2.47	0.44
18:E:606:CDL:H332	18:E:606:CDL:H362	1.67	0.44
18:F:706:CDL:H542	18:F:706:CDL:H712	2.00	0.44
17:L:602:HEA:C18	17:L:602:HEA:H261	2.48	0.44
18:L:604:CDL:HA4	18:J:203:CDL:C31	2.43	0.44
1:O:115:PHE:CE2	1:O:226:PRO:HG3	2.52	0.44
2:R:153:ALA:O	2:R:255:TRP:NE1	2.50	0.44
3:M:172:VAL:HG13	3:M:173:HIS:N	2.33	0.44
3:M:418:GLU:OE1	3:M:418:GLU:N	2.48	0.44
4:S:184:TYR:CD1	18:S:302:CDL:C73	3.01	0.44
1:O:186:LEU:HD13	8:Q:136:PHE:CD1	2.53	0.44
2:R:242:ALA:O	4:S:138:SER:CB	2.66	0.44
6:J:33:VAL:HG11	6:J:41:SER:OG	2.18	0.44
18:T:202:CDL:H622	18:T:202:CDL:H791	1.99	0.44
4:X:32:TRP:HB2	18:X:303:CDL:C33	2.44	0.44
4:S:151:VAL:HG22	4:S:188:VAL:HG11	2.00	0.44
5:E:500:GLY:O	3:Y:84:ARG:CZ	2.66	0.44
3:Y:243:TRP:NE1	3:Y:310:ASN:O	2.42	0.44
5:E:235:HIS:ND1	5:E:236:THR:O	2.47	0.44
5:F:135:ARG:NH1	5:F:358:ASP:O	2.51	0.44
2:L:385:ASP:O	2:L:389:THR:CB	2.66	0.44
9:Z:8:PHE:CE2	9:Z:52:THR:HG21	2.52	0.44
13:I:302:HEC:HHC	13:I:302:HEC:HBB3	1.99	0.44
1:O:188:CYS:HB3	13:O:302:HEC:HAB	2.00	0.43
1:O:203:SER:HA	8:Q:170:ARG:HG3	1.87	0.43
1:O:271:GLU:CD	5:F:281:ILE:HD12	2.38	0.43
2:R:259:PHE:O	2:R:263:GLY:N	2.41	0.43
2:R:535:ARG:NH1	9:T:74:GLU:OE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:604:CDL:H562	18:L:604:CDL:H751	2.00	0.43
9:T:91:TRP:N	9:T:92:PRO:CD	2.81	0.43
1:O:112:ALA:HB2	1:O:224:THR:HG21	2.00	0.43
1:O:114:TYR:OH	1:O:167:VAL:HG21	2.17	0.43
2:R:248:ALA:HB3	8:Q:185:ILE:CD1	2.49	0.43
18:E:607:CDL:H722	18:Z:202:CDL:H111	2.00	0.43
2:L:163:SER:O	2:L:163:SER:OG	2.36	0.43
8:K:140:TRP:NE1	8:K:284:MET:O	2.47	0.43
2:R:84:THR:HG21	2:R:147:ALA:HB3	2.00	0.43
5:E:281:ILE:HD12	1:I:271:GLU:CD	2.39	0.43
2:L:50:ALA:CB	18:J:203:CDL:H401	2.48	0.43
18:T:202:CDL:H792	18:T:203:CDL:C58	2.46	0.43
11:V:78:ALA:O	11:V:82:ARG:NH1	2.51	0.43
11:V:114:VAL:HG12	11:V:119:ILE:HG21	2.00	0.43
3:Y:41:GLN:NE2	3:Y:46:GLU:OE2	2.51	0.43
2:R:63:ARG:HE	2:R:63:ARG:HA	1.83	0.43
4:S:189:ASP:OD1	4:S:189:ASP:C	2.57	0.43
5:F:395:ILE:HG21	15:T:204:MQ9:H5M1	1.99	0.43
8:Q:264:GLN:OE1	8:Q:264:GLN:N	2.50	0.43
8:K:195:TYR:CE1	8:K:247:PRO:O	2.72	0.43
8:K:232:HIS:HB2	8:K:273:CYS:SG	2.58	0.43
1:O:232:PHE:CE2	13:O:302:HEC:HHC	2.52	0.43
2:R:452:LEU:HD11	2:R:457:MET:SD	2.59	0.43
5:F:416:VAL:HG11	6:P:58:PHE:CD2	2.53	0.43
18:F:705:CDL:H621	18:F:705:CDL:H591	1.61	0.43
8:Q:179:ILE:HG23	8:Q:180:GLU:N	2.33	0.43
3:Y:195:VAL:HG23	3:Y:196:ILE:HD12	2.01	0.43
3:Y:271:PRO:O	3:Y:316:ARG:NH1	2.51	0.43
2:R:110:GLN:OE1	2:R:210:THR:HG23	2.18	0.43
5:E:147:LEU:HD21	5:E:223:ILE:HG13	2.00	0.43
8:K:193:ARG:NH2	1:I:137:HIS:O	2.52	0.43
1:I:191:CYS:SG	1:I:201:LEU:HD21	2.59	0.43
1:O:215:PRO:HG3	1:O:250:ARG:HD3	2.00	0.43
5:F:123:HIS:NE2	21:F:702:HEM:ND	2.67	0.43
5:F:171:ILE:HD12	5:F:175:LEU:HD12	2.00	0.43
5:F:284:ILE:O	5:F:287:LEU:O	2.35	0.43
5:F:366:ARG:NH1	5:F:437:ASP:OD2	2.46	0.43
4:X:32:TRP:CG	18:X:303:CDL:C33	2.85	0.43
1:O:122:MET:HE3	1:O:123:PRO:HD2	2.00	0.43
1:O:208:PRO:HG3	13:O:302:HEC:HAA2	2.01	0.43
4:X:151:VAL:HG22	4:X:188:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:602:HEA:HMC1	17:R:602:HEA:HBC1	2.00	0.43
10:U:2:SER:O	10:U:5:LEU:N	2.51	0.43
1:O:169:GLN:HG2	1:O:214:ASN:HB2	2.01	0.43
8:Q:139:ASN:OD1	8:Q:205:GLY:O	2.37	0.43
9:Z:98:SER:HG	18:Z:202:CDL:H621	1.79	0.43
3:Y:172:VAL:HG13	3:Y:173:HIS:N	2.33	0.43
1:O:230:PRO:HD2	13:O:302:HEC:C2C	2.48	0.42
1:O:249:VAL:HG11	13:O:302:HEC:HMB3	2.01	0.42
2:R:31:LEU:O	2:R:34:THR:HG22	2.19	0.42
2:R:47:VAL:CG2	18:R:604:CDL:H371	2.49	0.42
5:F:225:ALA:HA	18:F:705:CDL:H351	2.01	0.42
5:F:312:ILE:CG1	5:F:333:VAL:HG21	2.48	0.42
2:L:242:ALA:O	4:X:138:SER:CB	2.66	0.42
9:Z:95:ILE:CD1	9:Z:128:LEU:HD22	2.48	0.42
1:I:149:TYR:O	1:I:153:ASN:ND2	2.52	0.42
1:O:112:ALA:N	1:O:224:THR:HG21	2.34	0.42
1:O:184:PHE:HA	1:O:245:ILE:HD11	2.01	0.42
1:O:187:ASN:O	1:O:188:CYS:HB3	2.18	0.42
1:O:222:MET:CG	1:O:242:LYS:HE2	2.36	0.42
4:S:102:TRP:HE3	4:S:105:ILE:HD11	1.78	0.42
4:X:96:VAL:HG22	4:X:170:PHE:HB2	2.01	0.42
9:Z:123:THR:HG22	18:Z:203:CDL:H322	2.01	0.42
3:Y:348:HIS:O	19:Y:501:FES:S1	2.77	0.42
2:R:384:LEU:CD1	8:Q:49:LEU:HD23	2.48	0.42
18:R:604:CDL:H751	18:R:604:CDL:H562	2.00	0.42
5:F:56:THR:HA	15:F:707:MQ9:H451	2.01	0.42
3:Y:347:SER:O	3:Y:387:ARG:NH1	2.44	0.42
1:O:172:LEU:HD23	1:O:216:ALA:HA	2.01	0.42
2:L:280:GLU:OE1	2:L:516:SER:OG	2.29	0.42
18:L:604:CDL:H381	18:L:604:CDL:H412	1.39	0.42
18:T:202:CDL:C75	18:T:203:CDL:H532	2.50	0.42
11:V:76:ASP:N	11:V:76:ASP:OD1	2.52	0.42
2:R:88:THR:HG22	2:R:151:TRP:CD1	2.53	0.42
5:F:311:LEU:HD23	5:F:333:VAL:HG23	2.00	0.42
4:X:160:LEU:CD2	9:Z:129:VAL:HG11	2.49	0.42
18:X:302:CDL:H312	18:X:302:CDL:HA61	1.82	0.42
18:X:302:CDL:C75	18:Z:203:CDL:H532	2.50	0.42
1:O:286:VAL:HG13	5:F:267:MET:HE1	2.01	0.42
4:S:53:GLN:O	8:Q:186:ARG:NH1	2.45	0.42
4:S:96:VAL:HG22	4:S:170:PHE:CB	2.50	0.42
2:L:290:ILE:HG23	2:L:290:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:119:ILE:HG23	11:V:120:GLU:N	2.35	0.42
1:O:245:ILE:O	1:O:249:VAL:HG12	2.20	0.42
2:R:111:ILE:HD12	2:R:196:MET:O	2.19	0.42
2:R:424:ARG:NH1	2:R:500:ARG:O	2.52	0.42
3:M:345:VAL:HG23	3:M:345:VAL:O	2.19	0.42
18:F:705:CDL:H551	18:F:705:CDL:H581	1.70	0.42
9:T:97:LEU:HD13	18:T:201:CDL:H351	2.01	0.42
1:O:218:ILE:H	1:O:218:ILE:HG13	1.64	0.42
3:M:42:PRO:O	3:M:43:THR:OG1	2.32	0.42
3:M:364:LEU:HD12	3:M:365:CYS:N	2.35	0.42
4:S:149:LEU:HG	18:S:302:CDL:H631	2.02	0.42
5:E:175:LEU:CD2	15:E:603:MQ9:H5M2	2.50	0.42
5:E:225:ALA:HA	18:E:606:CDL:H351	2.00	0.42
5:F:422:VAL:CG2	18:F:706:CDL:H402	2.49	0.42
18:L:604:CDL:H611	18:L:604:CDL:H582	1.76	0.42
8:Q:96:LEU:HA	8:Q:99:THR:HG22	2.01	0.42
8:K:281:HIS:O	8:K:281:HIS:ND1	2.53	0.42
3:Y:387:ARG:CZ	3:Y:415:ALA:HB2	2.50	0.42
1:O:91:HIS:HD2	1:O:103:PRO:O	2.03	0.42
1:O:125:MET:HA	13:O:301:HEC:CAC	2.49	0.42
1:O:192:HIS:CD2	1:O:210:LEU:HD21	2.55	0.42
13:O:302:HEC:CBB	13:O:302:HEC:HMB1	2.49	0.42
2:R:454:ASP:OD1	8:Q:35:TRP:CD1	2.73	0.42
18:R:604:CDL:H531	18:R:604:CDL:H712	2.02	0.42
18:R:604:CDL:H612	18:P:201:CDL:H402	2.01	0.42
3:M:369:GLN:HG3	5:F:404:LEU:HD21	2.02	0.42
4:X:36:GLU:OE1	4:X:150:HIS:NE2	2.44	0.42
2:R:399:HIS:O	2:R:403:PHE:N	2.53	0.42
2:L:287:ARG:O	8:K:87:GLN:NE2	2.53	0.42
2:L:522:SER:OG	2:L:524:PRO:O	2.37	0.42
18:L:604:CDL:H531	18:L:604:CDL:H712	2.02	0.42
11:V:47:ASP:OD1	11:V:47:ASP:C	2.58	0.42
1:I:190:SER:O	3:Y:355:LEU:HD11	2.20	0.42
1:O:230:PRO:HD2	13:O:302:HEC:CAC	2.50	0.41
2:R:193:VAL:HG11	2:R:214:LEU:HD13	2.01	0.41
3:M:46:GLU:OE1	3:M:46:GLU:N	2.50	0.41
3:M:291:ASP:O	3:M:297:SER:OG	2.38	0.41
5:F:425:VAL:CG1	18:F:706:CDL:H371	2.45	0.41
3:Y:190:LEU:O	3:Y:191:LYS:CG	2.68	0.41
1:O:114:TYR:CE1	1:O:167:VAL:HG21	2.56	0.41
1:O:122:MET:O	1:O:134:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:344:LYS:O	3:M:353:SER:N	2.44	0.41
5:E:147:LEU:HD13	5:E:222:LEU:HB2	2.01	0.41
5:E:532:HIS:CD2	5:E:536:ILE:HD11	2.55	0.41
5:F:420:ALA:HB2	18:P:201:CDL:H771	2.01	0.41
8:Q:236:VAL:O	8:Q:239:PHE:N	2.49	0.41
18:Z:203:CDL:OB4	1:I:289:TRP:HD1	2.03	0.41
18:Z:203:CDL:HB22	1:I:293:ARG:HH12	1.84	0.41
1:I:191:CYS:CB	13:I:302:HEC:HBC2	2.50	0.41
1:I:269:ALA:HB3	1:I:270:PRO:CD	2.47	0.41
2:R:310:VAL:O	2:R:310:VAL:HG13	2.20	0.41
2:R:420:LYS:NZ	2:R:521:THR:O	2.53	0.41
15:E:603:MQ9:H403	15:E:603:MQ9:H421	1.82	0.41
18:F:706:CDL:H391	18:T:201:CDL:C42	2.50	0.41
8:Q:135:ALA:O	8:Q:232:HIS:NE2	2.53	0.41
1:I:263:LEU:HD12	1:I:263:LEU:H	1.85	0.41
3:Y:159:ILE:O	3:Y:159:ILE:HG22	2.20	0.41
1:O:193:ASN:OD1	1:O:197:LYS:HB2	2.21	0.41
18:R:604:CDL:H512	18:R:604:CDL:H732	2.01	0.41
5:F:449:ILE:HD13	9:T:85:PHE:HD2	1.86	0.41
2:L:27:LEU:CD2	18:L:604:CDL:HA62	2.51	0.41
8:Q:101:ILE:HG22	8:Q:102:PRO:HD3	2.03	0.41
1:O:124:ALA:HB2	1:O:134:LYS:NZ	2.35	0.41
2:R:90:MET:HB3	17:R:603:HEA:CAC	2.50	0.41
18:R:604:CDL:H381	18:R:604:CDL:H412	1.39	0.41
3:M:195:VAL:HG23	3:M:196:ILE:HD12	2.02	0.41
18:L:604:CDL:H612	18:J:203:CDL:H402	2.01	0.41
9:T:8:PHE:CZ	9:T:52:THR:HG21	2.55	0.41
4:X:102:TRP:CE3	4:X:105:ILE:HD11	2.55	0.41
1:I:210:LEU:HD21	13:I:302:HEC:CHB	2.51	0.41
3:Y:85:THR:HG21	3:Y:153:LYS:HB3	2.01	0.41
1:O:112:ALA:HB2	1:O:224:THR:CG2	2.50	0.41
1:O:192:HIS:ND1	1:O:207:ALA:HB1	2.35	0.41
1:O:238:THR:HG22	1:O:241:GLU:HG3	2.03	0.41
1:O:246:VAL:O	1:O:250:ARG:HB2	2.20	0.41
2:R:419:PRO:CG	2:R:425:LEU:HD23	2.50	0.41
3:M:190:LEU:O	3:M:191:LYS:CG	2.69	0.41
3:M:213:VAL:HG21	3:Y:104:LEU:CD1	2.51	0.41
3:M:417:TRP:CG	5:F:183:PRO:O	2.74	0.41
5:F:107:GLN:NE2	5:F:276:GLY:O	2.53	0.41
5:F:400:PHE:HA	9:T:108:LEU:HD13	2.01	0.41
18:F:705:CDL:H332	18:F:705:CDL:H362	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:221:LEU:HD13	4:X:31:VAL:HG13	2.03	0.41
8:K:199:ASP:N	8:K:202:GLU:OE2	2.51	0.41
8:K:219:LYS:O	8:K:221:ILE:HD12	2.20	0.41
18:X:302:CDL:H761	18:Z:203:CDL:C53	2.37	0.41
2:R:256:GLN:HB3	2:R:315:MET:SD	2.61	0.41
4:S:32:TRP:HB3	18:S:302:CDL:H331	1.95	0.41
5:F:441:LEU:HD21	5:F:484:LEU:HD21	2.02	0.41
18:X:302:CDL:H141	18:X:302:CDL:H712	2.03	0.41
1:O:72:GLN:O	1:O:76:LEU:HG	2.21	0.41
5:F:59:TRP:CE3	5:F:105:VAL:HG11	2.56	0.41
2:L:159:ASP:O	2:L:162:HIS:O	2.38	0.41
18:L:604:CDL:H312	18:L:604:CDL:H342	1.79	0.41
6:J:85:ALA:HB1	18:J:203:CDL:H161	2.02	0.41
8:Q:128:GLU:OE1	8:Q:220:ARG:N	2.46	0.41
8:Q:139:ASN:HD22	8:Q:139:ASN:HA	1.63	0.41
8:Q:168:THR:HG23	8:Q:168:THR:O	2.20	0.41
4:X:163:ALA:HB1	18:X:302:CDL:HA61	2.03	0.41
1:I:116:GLN:HG2	1:I:122:MET:SD	2.61	0.41
13:I:302:HEC:HBA2	13:I:302:HEC:HMA3	2.02	0.41
3:Y:112:TRP:O	3:Y:113:GLU:HB2	2.21	0.41
1:O:193:ASN:HB2	1:O:197:LYS:O	2.21	0.41
5:E:367:PRO:O	5:E:374:THR:OG1	2.25	0.41
5:F:66:PRO:O	5:F:67:SER:OG	2.38	0.41
5:F:208:TYR:CE2	5:F:212:ILE:HD13	2.55	0.41
18:F:706:CDL:H762	18:F:706:CDL:H792	1.80	0.41
2:L:162:HIS:O	2:L:163:SER:OG	2.33	0.41
6:J:48:MET:HG2	18:J:203:CDL:HB61	2.03	0.41
4:X:32:TRP:HZ2	18:X:303:CDL:C38	2.25	0.41
1:O:115:PHE:HE2	1:O:226:PRO:HG3	1.86	0.40
1:O:222:MET:SD	1:O:237:LEU:HD13	2.61	0.40
1:O:245:ILE:CG2	13:O:302:HEC:CBB	3.00	0.40
5:E:59:TRP:CE3	5:E:105:VAL:HG11	2.56	0.40
2:L:153:ALA:HB1	2:L:158:THR:HG21	2.04	0.40
2:L:252:VAL:HG11	8:K:247:PRO:HD2	2.04	0.40
2:L:384:LEU:CD1	8:K:49:LEU:HD23	2.52	0.40
8:K:319:PRO:HA	8:K:320:PRO:HD3	1.99	0.40
1:I:201:LEU:CD1	13:I:302:HEC:HMD3	2.51	0.40
3:Y:345:VAL:HG23	3:Y:345:VAL:O	2.21	0.40
2:R:221:LEU:HD13	4:S:31:VAL:HG13	2.02	0.40
2:R:371:LEU:HD23	2:R:400:TYR:HE2	1.86	0.40
2:R:401:VAL:HG23	2:R:402:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:92:ALA:HB1	5:F:284:ILE:HD13	2.03	0.40
2:L:103:ALA:HB1	2:L:189:MET:SD	2.61	0.40
2:L:153:ALA:O	2:L:255:TRP:NE1	2.54	0.40
6:J:7:ARG:NH1	6:J:9:GLN:OE1	2.55	0.40
6:P:85:ALA:HB1	18:P:201:CDL:H161	2.03	0.40
8:K:222:GLU:OE2	8:K:257:VAL:HG21	2.21	0.40
1:I:221:ALA:O	1:I:224:THR:O	2.40	0.40
3:Y:281:THR:HG23	3:Y:344:LYS:CD	2.52	0.40
1:O:90:CYS:SG	1:O:101:ARG:HB3	2.61	0.40
1:O:117:VAL:HG22	1:O:122:MET:HE3	2.04	0.40
1:O:119:THR:HA	1:O:217:GLN:CD	2.40	0.40
1:O:190:SER:HB2	8:Q:193:ARG:NH1	2.32	0.40
4:S:32:TRP:CZ2	18:S:302:CDL:C36	3.00	0.40
4:S:103:TYR:OH	4:S:178:ALA:O	2.37	0.40
5:E:178:ILE:HD11	5:E:312:ILE:HD11	2.03	0.40
5:F:116:PHE:CE1	5:F:120:ILE:HD11	2.56	0.40
18:X:302:CDL:C77	18:Z:203:CDL:H532	2.51	0.40
3:Y:255:ALA:HB2	3:Y:285:TRP:HB3	2.04	0.40
1:O:95:LEU:HD11	1:O:150:VAL:HG12	2.03	0.40
1:O:195:THR:CB	1:O:197:LYS:HG2	2.47	0.40
1:O:218:ILE:HG21	1:O:246:VAL:HA	2.03	0.40
8:Q:288:VAL:HG13	8:Q:288:VAL:O	2.21	0.40
18:Z:203:CDL:H611	1:I:278:ILE:HG23	2.02	0.40
1:O:118:SER:HA	1:O:143:ILE:CD1	2.45	0.40
1:O:188:CYS:HB3	13:O:302:HEC:CAB	2.51	0.40
1:O:203:SER:CB	8:Q:170:ARG:HG2	2.40	0.40
4:S:41:ALA:HB2	9:T:44:LEU:CB	2.52	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	I	221/223 (99%)	199 (90%)	22 (10%)	0	100 100
1	O	206/223 (92%)	187 (91%)	16 (8%)	3 (2%)	8 39
2	L	550/552 (100%)	516 (94%)	34 (6%)	0	100 100
2	R	550/552 (100%)	518 (94%)	32 (6%)	0	100 100
3	M	380/382 (100%)	344 (90%)	36 (10%)	0	100 100
3	Y	380/382 (100%)	347 (91%)	33 (9%)	0	100 100
4	S	201/203 (99%)	193 (96%)	8 (4%)	0	100 100
4	X	201/203 (99%)	192 (96%)	9 (4%)	0	100 100
5	E	533/535 (100%)	490 (92%)	43 (8%)	0	100 100
5	F	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	44 75
6	J	88/100 (88%)	85 (97%)	3 (3%)	0	100 100
6	P	88/100 (88%)	83 (94%)	5 (6%)	0	100 100
7	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	25 59
7	G	214/216 (99%)	187 (87%)	27 (13%)	0	100 100
8	K	310/312 (99%)	282 (91%)	28 (9%)	0	100 100
8	Q	310/312 (99%)	282 (91%)	28 (9%)	0	100 100
9	T	137/139 (99%)	129 (94%)	8 (6%)	0	100 100
9	Z	137/139 (99%)	130 (95%)	7 (5%)	0	100 100
10	U	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	10 41
10	a	77/79 (98%)	70 (91%)	7 (9%)	0	100 100
11	V	143/145 (99%)	139 (97%)	4 (3%)	0	100 100
11	b	143/145 (99%)	138 (96%)	5 (4%)	0	100 100
12	c	154/159 (97%)	135 (88%)	19 (12%)	0	100 100
All	All	5847/5931 (99%)	5398 (92%)	443 (8%)	6 (0%)	50 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	226	PRO
5	F	135	ARG
1	O	202	SER
1	O	249	VAL
7	D	27	THR
10	U	70	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	163/163 (100%)	160 (98%)	3 (2%)	54 74
1	O	155/163 (95%)	112 (72%)	43 (28%)	0 2
2	L	452/453 (100%)	442 (98%)	10 (2%)	47 70
2	R	452/453 (100%)	446 (99%)	6 (1%)	65 81
3	M	312/312 (100%)	310 (99%)	2 (1%)	84 91
3	Y	312/312 (100%)	312 (100%)	0	100 100
4	S	155/161 (96%)	153 (99%)	2 (1%)	65 81
4	X	155/161 (96%)	153 (99%)	2 (1%)	65 81
5	E	429/429 (100%)	425 (99%)	4 (1%)	75 86
5	F	429/429 (100%)	425 (99%)	4 (1%)	75 86
6	J	76/83 (92%)	70 (92%)	6 (8%)	10 34
6	P	76/83 (92%)	75 (99%)	1 (1%)	65 81
7	D	20/151 (13%)	20 (100%)	0	100 100
7	G	20/151 (13%)	20 (100%)	0	100 100
8	K	260/266 (98%)	256 (98%)	4 (2%)	60 77
8	Q	260/266 (98%)	257 (99%)	3 (1%)	67 82
9	T	106/106 (100%)	106 (100%)	0	100 100
9	Z	106/106 (100%)	106 (100%)	0	100 100
10	U	59/59 (100%)	59 (100%)	0	100 100
10	a	59/59 (100%)	58 (98%)	1 (2%)	56 75
11	V	107/107 (100%)	106 (99%)	1 (1%)	75 86
11	b	107/107 (100%)	107 (100%)	0	100 100
12	c	127/127 (100%)	125 (98%)	2 (2%)	58 76
All	All	4397/4707 (93%)	4303 (98%)	94 (2%)	49 71

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	72	GLN
1	O	73	SER
1	O	75	LEU
1	O	81	GLN
1	O	87	CYS
1	O	94	ASN
1	O	100	ASP
1	O	104	SER
1	O	105	LEU
1	O	118	SER
1	O	121	ARG
1	O	122	MET
1	O	128	GLU
1	O	139	ASP
1	O	140	GLU
1	O	144	ASP
1	O	146	LEU
1	O	150	VAL
1	O	151	GLN
1	O	158	THR
1	O	167	VAL
1	O	169	GLN
1	O	171	SER
1	O	179	ARG
1	O	182	ASP
1	O	185	ARG
1	O	188	CYS
1	O	193	ASN
1	O	195	THR
1	O	201	LEU
1	O	210	LEU
1	O	212	ASP
1	O	214	ASN
1	O	228	ASN
1	O	233	SER
1	O	235	ARG
1	O	237	LEU
1	O	238	THR
1	O	240	ASP
1	O	241	GLU
1	O	245	ILE
1	O	250	ARG
1	O	251	GLU

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Mol	Chain	Res	Type
2	R	63	ARG
2	R	129	PHE
2	R	155	SER
2	R	454	ASP
2	R	505	VAL
2	R	523	CYS
3	M	120	GLU
3	M	348	HIS
4	S	130	THR
4	S	189	ASP
5	E	18	SER
5	E	187	THR
5	E	295	VAL
5	E	403	SER
5	F	20	TYR
5	F	352	LYS
5	F	357	ASP
5	F	358	ASP
2	L	20	ARG
2	L	63	ARG
2	L	129	PHE
2	L	365	PHE
2	L	388	VAL
2	L	390	ASP
2	L	459	ARG
2	L	508	ASP
2	L	509	ASP
2	L	523	CYS
6	J	24	ARG
6	J	29	ASP
6	J	42	HIS
6	J	43	MET
6	J	64	ARG
6	J	72	GLU
8	Q	139	ASN
8	Q	154	PHE
8	Q	160	ASP
11	V	148	ARG
6	P	64	ARG
8	K	139	ASN
8	K	232	HIS
8	K	281	HIS

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Mol	Chain	Res	Type
8	K	283	MET
4	X	174	GLN
4	X	189	ASP
10	a	55	ARG
12	c	24	CYS
12	c	25	SER
1	I	91	HIS
1	I	123	PRO
1	I	137	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 60 ligands modelled in this entry, 6 are monoatomic - leaving 54 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	$\#\|Z\| > 2$
23	9XX	c	202	12	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	MQ9	F	707	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
19	FES	M	501	3	0,4,4	-	-	-		
18	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
21	HEM	E	601	5	41,49,50	1.24	4 (9%)	47,81,82	1.26	4 (8%)
21	HEM	E	602	5	42,50,50	1.51	5 (11%)	46,82,82	1.34	7 (15%)
15	MQ9	T	204	-	59,59,59	2.39	22 (37%)	73,75,75	1.59	16 (21%)
18	CDL	E	606	-	75,75,99	0.34	0	81,87,111	0.42	0
18	CDL	F	705	-	75,75,99	0.34	0	81,87,111	0.42	0
20	9Y0	J	202	-	48,48,48	1.16	3 (6%)	51,53,53	0.78	2 (3%)
21	HEM	F	703	5	42,50,50	1.49	4 (9%)	46,82,82	1.37	6 (13%)
18	CDL	S	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
18	CDL	T	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
19	FES	Y	501	3	0,4,4	-	-	-		
13	HEC	O	302	1	32,50,50	2.34	12 (37%)	30,82,82	2.09	5 (16%)
13	HEC	I	301	-	32,50,50	2.08	3 (9%)	30,82,82	2.22	5 (16%)
23	9XX	G	302	7	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
13	HEC	O	301	-	32,50,50	2.27	10 (31%)	30,82,82	2.13	5 (16%)
13	HEC	I	302	1	32,50,50	2.16	3 (9%)	30,82,82	2.04	8 (26%)
17	HEA	R	603	2	58,67,67	1.56	11 (18%)	63,103,103	2.02	12 (19%)
14	9YF	O	303	-	58,58,58	1.03	5 (8%)	68,71,71	1.06	3 (4%)
15	MQ9	F	701	-	59,59,59	2.45	23 (38%)	73,75,75	1.38	15 (20%)
22	PLM	c	201	12	15,16,17	0.47	0	14,15,17	0.35	0
17	HEA	R	602	2	58,67,67	1.62	10 (17%)	63,103,103	2.39	23 (36%)
18	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
20	9Y0	S	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
14	9YF	I	304	-	58,58,58	1.08	5 (8%)	68,71,71	1.07	2 (2%)
15	MQ9	E	604	-	59,59,59	2.42	22 (37%)	73,75,75	1.53	16 (21%)
18	CDL	X	303	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
22	PLM	G	301	7	9,10,17	0.54	0	8,9,17	0.43	0
23	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
18	CDL	L	604	-	75,75,99	0.33	0	81,87,111	0.60	2 (2%)
18	CDL	J	203	-	75,75,99	0.33	0	81,87,111	0.45	0
18	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
18	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
20	9Y0	F	704	-	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
20	9Y0	J	201	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	9YF	E	605	-	58,58,58	1.02	5 (8%)	68,71,71	1.32	7 (10%)
17	HEA	L	602	2	58,67,67	1.61	11 (18%)	63,103,103	2.46	23 (36%)
18	CDL	X	302	-	75,75,99	0.33	0	81,87,111	0.40	0
18	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
15	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	14 (19%)
15	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
18	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
18	CDL	F	706	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
21	HEM	F	702	5	41,49,50	1.23	2 (4%)	47,81,82	1.25	3 (6%)
15	MQ9	I	303	-	59,59,59	2.39	22 (37%)	73,75,75	1.43	17 (23%)
14	9YF	Y	503	-	58,58,58	1.13	8 (13%)	68,71,71	1.49	9 (13%)
20	9Y0	X	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.90	2 (3%)
17	HEA	L	603	2	58,67,67	1.56	11 (18%)	63,103,103	1.85	13 (20%)
18	CDL	E	607	-	75,75,99	0.36	0	81,87,111	0.42	0
22	PLM	D	301	7	9,10,17	0.53	0	8,9,17	0.43	0
15	MQ9	O	304	-	59,59,59	2.40	22 (37%)	73,75,75	1.43	17 (23%)
14	9YF	Y	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.29	9 (13%)

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
23	9XX	c	202	12	-	16/43/43/43	-
15	MQ9	F	707	-	-	12/53/73/73	0/2/2/2
19	FES	M	501	3	-	-	0/1/1/1
18	CDL	R	604	-	-	47/86/86/110	-
21	HEM	E	601	5	-	2/12/52/54	-
21	HEM	E	602	5	-	2/12/54/54	-
15	MQ9	T	204	-	-	13/53/73/73	0/2/2/2
18	CDL	E	606	-	-	49/86/86/110	-
18	CDL	F	705	-	-	49/86/86/110	-
20	9Y0	J	202	-	-	25/52/52/52	-
21	HEM	F	703	5	-	0/12/54/54	-
18	CDL	S	302	-	-	43/86/86/110	-
18	CDL	T	203	-	-	38/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FES	Y	501	3	-	-	0/1/1/1
13	HEC	O	302	1	-	5/10/54/54	-
13	HEC	I	301	-	-	0/10/54/54	-
23	9XX	G	302	7	-	10/33/33/43	-
13	HEC	O	301	-	-	3/10/54/54	-
13	HEC	I	302	1	-	0/10/54/54	-
17	HEA	R	603	2	-	3/32/76/76	-
14	9YF	O	303	-	-	29/54/78/78	0/1/1/1
15	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
22	PLM	c	201	12	-	5/14/14/15	-
17	HEA	R	602	2	-	7/32/76/76	-
18	CDL	T	202	-	-	46/86/86/110	-
20	9Y0	S	301	-	-	19/52/52/52	-
14	9YF	I	304	-	-	22/54/78/78	0/1/1/1
15	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
18	CDL	X	303	-	-	43/86/86/110	-
22	PLM	G	301	7	-	2/8/8/15	-
23	9XX	D	302	-	-	9/33/33/43	-
18	CDL	L	604	-	-	47/86/86/110	-
18	CDL	J	203	-	-	48/86/86/110	-
18	CDL	Z	203	-	-	38/86/86/110	-
18	CDL	P	201	-	-	48/86/86/110	-
20	9Y0	F	704	-	-	16/52/52/52	-
20	9Y0	J	201	-	-	19/52/52/52	-
14	9YF	E	605	-	-	17/54/78/78	0/1/1/1
17	HEA	L	602	2	-	12/32/76/76	-
18	CDL	X	302	-	-	46/86/86/110	-
18	CDL	Z	202	-	-	34/86/86/110	-
15	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
15	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
18	CDL	T	201	-	-	34/86/86/110	-
18	CDL	F	706	-	-	43/86/86/110	-
21	HEM	F	702	5	-	4/12/52/54	-
15	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
14	9YF	Y	503	-	-	22/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	9Y0	X	301	-	-	17/52/52/52	-
17	HEA	L	603	2	-	3/32/76/76	-
18	CDL	E	607	-	-	40/86/86/110	-
22	PLM	D	301	7	-	3/8/8/15	-
15	MQ9	O	304	-	-	7/53/73/73	0/2/2/2
14	9YF	Y	502	-	-	22/54/78/78	0/1/1/1

All (363) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	707	MQ9	C6-C5	8.77	1.50	1.35
15	E	604	MQ9	C6-C5	8.77	1.50	1.35
15	F	701	MQ9	C6-C5	8.59	1.50	1.35
15	E	603	MQ9	C6-C5	8.53	1.50	1.35
15	I	303	MQ9	C6-C5	8.49	1.50	1.35
15	O	304	MQ9	C6-C5	8.47	1.50	1.35
15	T	204	MQ9	C6-C5	8.38	1.50	1.35
15	Z	201	MQ9	C6-C5	8.28	1.50	1.35
13	O	301	HEC	C2B-C3B	6.78	1.48	1.40
13	I	302	HEC	C2B-C3B	-6.56	1.33	1.40
13	O	302	HEC	C2B-C3B	6.16	1.47	1.40
13	I	301	HEC	C2B-C3B	-5.97	1.34	1.40
13	I	302	HEC	C3C-C2C	-5.91	1.34	1.40
13	O	302	HEC	C3C-C2C	5.81	1.47	1.40
13	I	301	HEC	C3C-C2C	-5.73	1.34	1.40
13	I	301	HEC	C3D-C2D	5.42	1.53	1.37
13	I	302	HEC	C3D-C2D	5.31	1.53	1.37
13	O	301	HEC	C3C-C2C	5.17	1.46	1.40
15	F	707	MQ9	C2-C1	5.05	1.57	1.48
15	F	701	MQ9	C2-C1	5.01	1.57	1.48
15	E	604	MQ9	C2-C1	5.00	1.57	1.48
17	R	603	HEA	C3A-C4A	4.98	1.48	1.41
15	Z	201	MQ9	C2-C1	4.96	1.57	1.48
15	E	603	MQ9	C2-C1	4.95	1.57	1.48
17	L	603	HEA	C3A-C4A	4.94	1.48	1.41
15	O	304	MQ9	C2-C1	4.93	1.57	1.48
15	I	303	MQ9	C2-C1	4.93	1.57	1.48
15	T	204	MQ9	C2-C1	4.91	1.57	1.48
21	E	602	HEM	C3C-C2C	-4.91	1.33	1.40
15	I	303	MQ9	C3-C4	4.75	1.57	1.48
17	L	602	HEA	C3A-C4A	4.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	602	HEA	C3A-C4A	4.74	1.48	1.41
21	F	703	HEM	C3C-C2C	-4.70	1.34	1.40
15	O	304	MQ9	C3-C4	4.68	1.57	1.48
15	F	707	MQ9	C3-C4	4.66	1.57	1.48
15	E	603	MQ9	C3-C4	4.65	1.57	1.48
15	T	204	MQ9	C3-C4	4.62	1.57	1.48
15	F	701	MQ9	C3-C4	4.62	1.57	1.48
15	E	604	MQ9	C3-C4	4.61	1.57	1.48
15	F	707	MQ9	C26-C24	4.61	1.60	1.51
15	Z	201	MQ9	C3-C4	4.54	1.57	1.48
15	E	604	MQ9	C26-C24	4.52	1.60	1.51
15	E	603	MQ9	C26-C24	4.49	1.60	1.51
15	F	701	MQ9	C26-C24	4.49	1.60	1.51
15	T	204	MQ9	C26-C24	4.47	1.60	1.51
15	I	303	MQ9	C26-C24	4.46	1.60	1.51
15	O	304	MQ9	C26-C24	4.45	1.60	1.51
15	Z	201	MQ9	C26-C24	4.40	1.60	1.51
17	R	602	HEA	C3B-C2B	4.36	1.44	1.34
17	R	603	HEA	C3B-C2B	4.30	1.44	1.34
17	L	603	HEA	C3B-C2B	4.20	1.44	1.34
15	T	204	MQ9	C11-C9	4.18	1.59	1.51
17	L	602	HEA	C3B-C2B	4.13	1.44	1.34
15	E	603	MQ9	C31-C29	4.13	1.59	1.51
13	O	301	HEC	C3C-C4C	4.12	1.50	1.43
17	L	602	HEA	C3C-C2C	4.11	1.45	1.40
15	F	701	MQ9	C31-C29	4.10	1.59	1.51
15	Z	201	MQ9	C11-C9	4.05	1.59	1.51
15	E	604	MQ9	C11-C9	4.00	1.59	1.51
15	F	707	MQ9	C31-C29	3.98	1.59	1.51
15	O	304	MQ9	C11-C9	3.92	1.59	1.51
15	F	707	MQ9	C11-C9	3.92	1.59	1.51
23	G	302	9XX	O1-C17	-3.90	1.40	1.47
15	I	303	MQ9	C31-C29	3.88	1.59	1.51
17	R	603	HEA	C3C-C2C	3.88	1.45	1.40
15	I	303	MQ9	C11-C9	3.86	1.59	1.51
15	E	604	MQ9	C31-C29	3.86	1.59	1.51
15	O	304	MQ9	C31-C29	3.84	1.59	1.51
17	L	603	HEA	C3C-C2C	3.81	1.45	1.40
15	T	204	MQ9	C31-C29	3.81	1.59	1.51
17	R	602	HEA	C3C-C2C	3.81	1.45	1.40
23	D	302	9XX	O1-C17	-3.81	1.40	1.47
15	F	701	MQ9	C11-C9	3.80	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Z	201	MQ9	C31-C29	3.80	1.59	1.51
13	O	302	HEC	C2A-C3A	3.80	1.48	1.37
17	L	602	HEA	C3D-C2D	3.77	1.44	1.36
15	E	603	MQ9	C11-C9	3.75	1.59	1.51
23	c	202	9XX	O1-C17	-3.72	1.40	1.47
17	L	603	HEA	C3D-C2D	3.67	1.44	1.36
17	R	602	HEA	C3D-C2D	3.64	1.44	1.36
17	R	602	HEA	C4D-C3D	3.54	1.51	1.45
17	R	603	HEA	C3D-C2D	3.54	1.44	1.36
13	O	302	HEC	C3D-C2D	3.44	1.47	1.37
17	R	602	HEA	C3A-C2A	3.43	1.45	1.40
13	O	302	HEC	C3C-C4C	3.43	1.49	1.43
13	O	301	HEC	C3D-C2D	3.41	1.47	1.37
13	O	301	HEC	C2A-C3A	3.41	1.47	1.37
17	L	602	HEA	C3A-C2A	3.38	1.45	1.40
13	O	302	HEC	C4B-C3B	3.36	1.49	1.43
15	E	603	MQ9	C22-C23	3.29	1.60	1.50
17	L	602	HEA	C4B-C3B	3.28	1.50	1.44
20	X	301	9Y0	O7-C1	-3.28	1.38	1.46
20	S	301	9Y0	O7-C1	-3.27	1.38	1.46
15	E	604	MQ9	C22-C23	3.26	1.60	1.50
15	O	304	MQ9	C27-C28	3.26	1.60	1.50
18	T	201	CDL	OA6-CA4	-3.26	1.38	1.46
15	F	707	MQ9	C22-C23	3.26	1.60	1.50
18	Z	202	CDL	OA6-CA4	-3.25	1.38	1.46
15	E	604	MQ9	C21-C19	3.25	1.58	1.51
15	T	204	MQ9	C21-C19	3.24	1.58	1.51
15	F	701	MQ9	C22-C23	3.23	1.60	1.50
15	T	204	MQ9	C7-C8	3.23	1.55	1.50
15	F	707	MQ9	C21-C19	3.22	1.57	1.51
15	O	304	MQ9	C22-C23	3.22	1.60	1.50
15	I	303	MQ9	C27-C28	3.21	1.60	1.50
15	I	303	MQ9	C16-C14	3.20	1.57	1.51
15	I	303	MQ9	C22-C23	3.19	1.60	1.50
20	J	201	9Y0	O7-C1	-3.19	1.39	1.46
15	E	603	MQ9	C21-C19	3.19	1.57	1.51
21	F	703	HEM	C3C-CAC	3.18	1.54	1.47
20	F	704	9Y0	O7-C1	-3.17	1.39	1.46
15	F	701	MQ9	C21-C19	3.17	1.57	1.51
20	J	202	9Y0	O7-C1	-3.16	1.39	1.46
15	O	304	MQ9	C16-C14	3.15	1.57	1.51
15	E	604	MQ9	C16-C14	3.14	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	707	MQ9	C16-C14	3.14	1.57	1.51
15	E	603	MQ9	C41-C39	3.12	1.57	1.51
15	Z	201	MQ9	C21-C19	3.12	1.57	1.51
15	I	303	MQ9	C21-C19	3.11	1.57	1.51
15	Z	201	MQ9	C7-C8	3.11	1.55	1.50
15	Z	201	MQ9	C22-C23	3.10	1.59	1.50
15	E	603	MQ9	C27-C28	3.10	1.59	1.50
13	O	302	HEC	C2A-C1A	3.09	1.49	1.42
17	R	602	HEA	C4B-C3B	3.09	1.50	1.44
15	F	701	MQ9	C27-C28	3.08	1.59	1.50
18	T	203	CDL	OB8-CB7	3.08	1.42	1.33
15	T	204	MQ9	C22-C23	3.08	1.59	1.50
15	T	204	MQ9	C27-C28	3.08	1.59	1.50
15	O	304	MQ9	C21-C19	3.08	1.57	1.51
15	F	701	MQ9	C41-C39	3.08	1.57	1.51
15	Z	201	MQ9	C27-C28	3.08	1.59	1.50
17	R	602	HEA	C2A-C1A	3.08	1.49	1.42
18	Z	203	CDL	OB8-CB7	3.07	1.42	1.33
21	E	602	HEM	C3C-CAC	3.07	1.54	1.47
18	S	302	CDL	OB8-CB7	3.06	1.42	1.33
18	X	303	CDL	OB8-CB7	3.06	1.42	1.33
17	L	602	HEA	C4D-C3D	3.06	1.50	1.45
15	O	304	MQ9	C7-C8	3.05	1.55	1.50
15	F	707	MQ9	C27-C28	3.04	1.59	1.50
15	E	604	MQ9	C27-C28	3.02	1.59	1.50
15	F	701	MQ9	C7-C8	3.02	1.55	1.50
14	Y	502	9YF	O11-C25	3.00	1.42	1.33
21	E	602	HEM	CAB-C3B	3.00	1.55	1.47
15	E	603	MQ9	C7-C8	2.99	1.55	1.50
15	Z	201	MQ9	C16-C14	2.99	1.57	1.51
15	T	204	MQ9	C16-C14	2.98	1.57	1.51
17	L	602	HEA	C2A-C1A	2.97	1.49	1.42
15	I	303	MQ9	C7-C8	2.97	1.55	1.50
20	F	704	9Y0	O5-C5	2.96	1.42	1.33
15	F	701	MQ9	C16-C14	2.95	1.57	1.51
14	Y	503	9YF	O9-C8	2.95	1.42	1.34
17	L	603	HEA	C4B-C3B	2.94	1.49	1.44
20	J	201	9Y0	O5-C5	2.93	1.41	1.33
13	O	301	HEC	C3A-C4A	2.93	1.49	1.42
21	F	703	HEM	CAB-C3B	2.91	1.55	1.47
18	S	302	CDL	OA6-CA5	2.91	1.42	1.34
15	E	603	MQ9	C16-C14	2.91	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	203	CDL	OA6-CA5	2.91	1.42	1.34
15	E	604	MQ9	C7-C8	2.90	1.55	1.50
18	X	303	CDL	OA6-CA5	2.90	1.42	1.34
18	T	203	CDL	OA6-CA5	2.90	1.42	1.34
15	F	707	MQ9	C7-C8	2.89	1.55	1.50
18	X	303	CDL	CB6-CB4	2.89	1.59	1.50
18	S	302	CDL	CB6-CB4	2.89	1.59	1.50
21	F	702	HEM	CAB-C3B	2.88	1.55	1.47
18	X	303	CDL	OB6-CB5	2.88	1.42	1.34
18	S	302	CDL	OB6-CB5	2.88	1.42	1.34
21	E	601	HEM	CAB-C3B	2.87	1.55	1.47
20	J	202	9Y0	O5-C5	2.87	1.41	1.33
15	O	304	MQ9	C7-C6	2.87	1.56	1.51
18	T	203	CDL	OB6-CB5	2.87	1.42	1.34
15	F	701	MQ9	C7-C6	2.86	1.56	1.51
18	Z	203	CDL	OB6-CB5	2.86	1.42	1.34
15	E	603	MQ9	C7-C6	2.86	1.56	1.51
15	E	604	MQ9	C7-C6	2.85	1.56	1.51
15	F	707	MQ9	C7-C6	2.85	1.56	1.51
15	T	204	MQ9	C7-C6	2.84	1.56	1.51
15	F	701	MQ9	C5M-C5	2.83	1.56	1.50
14	Y	502	9YF	O9-C8	2.83	1.42	1.34
15	F	707	MQ9	C20-C19	2.82	1.57	1.50
18	T	203	CDL	OA8-CA7	2.82	1.41	1.33
15	E	603	MQ9	C5M-C5	2.82	1.56	1.50
18	Z	203	CDL	OA8-CA7	2.81	1.41	1.33
18	S	302	CDL	OA8-CA7	2.81	1.41	1.33
13	O	302	HEC	C3A-C4A	2.80	1.48	1.42
18	X	303	CDL	OA8-CA7	2.80	1.41	1.33
15	E	604	MQ9	C5M-C5	2.80	1.56	1.50
20	X	301	9Y0	O5-C5	2.80	1.41	1.33
15	E	604	MQ9	C20-C19	2.79	1.57	1.50
18	X	303	CDL	CB3-CB4	2.79	1.59	1.50
15	I	303	MQ9	C7-C6	2.78	1.56	1.51
18	S	302	CDL	CB3-CB4	2.78	1.59	1.50
13	O	301	HEC	C2A-C1A	2.78	1.48	1.42
15	O	304	MQ9	C20-C19	2.78	1.57	1.50
14	I	304	9YF	O9-C8	2.78	1.42	1.34
15	T	204	MQ9	C20-C19	2.77	1.57	1.50
20	J	201	9Y0	O7-C21	2.77	1.42	1.34
15	F	707	MQ9	C5M-C5	2.77	1.56	1.50
18	Z	203	CDL	CB6-CB4	2.76	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	301	9Y0	O5-C5	2.76	1.41	1.33
20	J	202	9Y0	O7-C21	2.76	1.42	1.34
15	I	303	MQ9	C20-C19	2.76	1.57	1.50
15	Z	201	MQ9	C7-C6	2.76	1.56	1.51
18	T	203	CDL	CB6-CB4	2.76	1.59	1.50
18	Z	202	CDL	CB6-CB4	2.74	1.59	1.50
18	T	203	CDL	CB3-CB4	2.74	1.59	1.50
18	T	201	CDL	CB6-CB4	2.74	1.59	1.50
15	E	603	MQ9	C20-C19	2.74	1.57	1.50
20	F	704	9Y0	O7-C21	2.74	1.42	1.34
15	F	701	MQ9	C20-C19	2.73	1.57	1.50
18	Z	203	CDL	CB3-CB4	2.73	1.59	1.50
15	Z	201	MQ9	C20-C19	2.73	1.57	1.50
18	Z	202	CDL	OB8-CB7	2.72	1.41	1.33
20	S	301	9Y0	O7-C21	2.71	1.41	1.34
20	X	301	9Y0	O7-C21	2.71	1.41	1.34
18	T	201	CDL	OB8-CB7	2.69	1.41	1.33
14	E	605	9YF	O9-C	-2.67	1.40	1.46
15	O	304	MQ9	C5M-C5	2.66	1.56	1.50
18	X	303	CDL	OA6-CA4	-2.66	1.40	1.46
13	O	302	HEC	C1C-CHC	2.66	1.48	1.41
13	O	301	HEC	C1D-CHD	2.66	1.48	1.41
14	E	605	9YF	O11-C25	2.65	1.41	1.33
18	S	302	CDL	OA6-CA4	-2.64	1.40	1.46
18	Z	203	CDL	OA6-CA4	-2.64	1.40	1.46
15	I	303	MQ9	C5M-C5	2.64	1.56	1.50
18	T	203	CDL	OA6-CA4	-2.63	1.40	1.46
17	R	603	HEA	C4B-C3B	2.63	1.49	1.44
15	F	701	MQ9	C42-C43	2.62	1.58	1.50
17	L	603	HEA	C3A-C2A	2.61	1.43	1.40
15	E	603	MQ9	C42-C43	2.60	1.58	1.50
15	O	304	MQ9	C42-C43	2.57	1.58	1.50
18	T	201	CDL	OB6-CB5	2.57	1.41	1.34
14	O	303	9YF	O9-C	-2.57	1.40	1.46
13	O	301	HEC	C4D-CHA	2.57	1.48	1.41
18	Z	202	CDL	OB6-CB5	2.57	1.41	1.34
23	c	202	9XX	O-C15	2.56	1.40	1.33
15	I	303	MQ9	C42-C43	2.56	1.58	1.50
14	E	605	9YF	O9-C8	2.56	1.41	1.34
15	E	604	MQ9	C46-C44	2.56	1.56	1.51
13	O	302	HEC	C4D-CHA	2.56	1.48	1.41
15	T	204	MQ9	C5M-C5	2.55	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	707	MQ9	C41-C39	2.55	1.56	1.51
14	O	303	9YF	O11-C25	2.53	1.40	1.33
15	F	707	MQ9	C46-C44	2.50	1.56	1.51
15	O	304	MQ9	C41-C39	2.49	1.56	1.51
15	I	303	MQ9	C41-C39	2.49	1.56	1.51
23	D	302	9XX	O-C15	2.49	1.40	1.33
14	I	304	9YF	O11-C24	-2.49	1.39	1.45
14	Y	503	9YF	O9-C	-2.49	1.40	1.46
15	F	701	MQ9	C46-C44	2.49	1.56	1.51
15	E	603	MQ9	C46-C44	2.47	1.56	1.51
15	E	604	MQ9	C41-C39	2.47	1.56	1.51
15	Z	201	MQ9	C5M-C5	2.46	1.55	1.50
17	L	603	HEA	C2A-C1A	2.44	1.48	1.42
17	R	603	HEA	C2A-C1A	2.43	1.47	1.42
15	E	603	MQ9	C12-C13	2.43	1.57	1.50
15	F	701	MQ9	C12-C13	2.43	1.57	1.50
23	G	302	9XX	O-C15	2.43	1.40	1.33
21	E	601	HEM	C2C-C3C	-2.42	1.33	1.41
14	Y	502	9YF	P-O2	2.41	1.66	1.59
13	O	302	HEC	C1D-CHD	2.40	1.47	1.41
17	R	603	HEA	C1D-ND	-2.40	1.36	1.40
14	O	303	9YF	O9-C8	2.40	1.41	1.34
15	T	204	MQ9	C41-C39	2.40	1.56	1.51
15	F	707	MQ9	C42-C43	2.39	1.57	1.50
15	T	204	MQ9	C12-C13	2.39	1.57	1.50
15	T	204	MQ9	C42-C43	2.39	1.57	1.50
14	I	304	9YF	O9-C	-2.39	1.41	1.46
17	R	603	HEA	C3A-C2A	2.39	1.43	1.40
14	O	303	9YF	O11-C24	-2.38	1.39	1.45
15	Z	201	MQ9	C46-C44	2.38	1.56	1.51
15	O	304	MQ9	C12-C13	2.38	1.57	1.50
14	E	605	9YF	O11-C24	-2.37	1.39	1.45
15	Z	201	MQ9	C42-C43	2.37	1.57	1.50
14	I	304	9YF	O11-C25	2.37	1.40	1.33
17	R	602	HEA	C1B-C2B	2.37	1.49	1.44
15	F	701	MQ9	C43-C44	2.37	1.38	1.33
15	F	707	MQ9	C12-C13	2.36	1.57	1.50
21	F	702	HEM	C2C-C3C	-2.36	1.33	1.41
15	I	303	MQ9	C12-C13	2.36	1.57	1.50
17	L	602	HEA	C1B-C2B	2.36	1.49	1.44
15	E	604	MQ9	C12-C13	2.35	1.57	1.50
17	L	603	HEA	C1D-ND	-2.34	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	701	MQ9	C28-C29	2.34	1.38	1.33
14	Y	503	9YF	O12-C25	-2.34	1.15	1.22
15	E	603	MQ9	C43-C44	2.33	1.38	1.33
15	E	604	MQ9	C42-C43	2.33	1.57	1.50
15	O	304	MQ9	C43-C44	2.33	1.38	1.33
15	E	603	MQ9	C28-C29	2.32	1.38	1.33
15	Z	201	MQ9	C41-C39	2.32	1.56	1.51
14	Y	503	9YF	O11-C25	2.32	1.40	1.33
15	I	303	MQ9	C43-C44	2.31	1.38	1.33
15	F	707	MQ9	O4-C4	-2.31	1.18	1.23
15	Z	201	MQ9	O4-C4	-2.30	1.18	1.23
14	Y	503	9YF	O11-C24	-2.30	1.40	1.45
15	O	304	MQ9	C28-C29	2.30	1.38	1.33
15	Z	201	MQ9	C12-C13	2.29	1.57	1.50
15	E	604	MQ9	O4-C4	-2.29	1.18	1.23
23	G	302	9XX	O1-C18	2.29	1.40	1.34
13	O	301	HEC	C1B-CHB	2.29	1.47	1.41
15	I	303	MQ9	C28-C29	2.28	1.38	1.33
21	F	703	HEM	C3C-C4C	2.28	1.44	1.41
15	T	204	MQ9	O4-C4	-2.28	1.18	1.23
14	O	303	9YF	P-O2	2.28	1.66	1.59
15	T	204	MQ9	C46-C44	2.28	1.56	1.51
15	O	304	MQ9	O4-C4	-2.27	1.18	1.23
15	E	603	MQ9	O4-C4	-2.27	1.18	1.23
15	I	303	MQ9	O4-C4	-2.27	1.18	1.23
23	D	302	9XX	O1-C18	2.26	1.40	1.34
15	F	701	MQ9	O4-C4	-2.26	1.18	1.23
15	F	707	MQ9	C43-C44	2.26	1.38	1.33
18	T	201	CDL	PA1-OA4	-2.25	1.44	1.55
15	E	604	MQ9	C43-C44	2.25	1.38	1.33
18	Z	202	CDL	PA1-OA4	-2.24	1.44	1.55
18	T	201	CDL	CB3-CB4	2.23	1.57	1.50
18	Z	202	CDL	CB3-CB4	2.23	1.57	1.50
17	R	602	HEA	C1D-ND	-2.20	1.36	1.40
17	L	602	HEA	C1D-ND	-2.20	1.36	1.40
15	O	304	MQ9	C46-C44	2.20	1.55	1.51
17	R	603	HEA	C4D-C3D	2.19	1.48	1.45
14	Y	502	9YF	O9-C	-2.19	1.41	1.46
15	E	604	MQ9	C28-C29	2.18	1.38	1.33
15	I	303	MQ9	C46-C44	2.18	1.55	1.51
13	O	302	HEC	C1B-CHB	2.18	1.47	1.41
15	T	204	MQ9	C43-C44	2.18	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	603	HEA	C1B-C2B	2.17	1.48	1.44
14	Y	502	9YF	O11-C24	-2.16	1.40	1.45
15	T	204	MQ9	C28-C29	2.15	1.38	1.33
15	Z	201	MQ9	C28-C29	2.14	1.38	1.33
15	T	204	MQ9	C3C-C3B	2.14	1.42	1.38
15	E	603	MQ9	C3C-C3B	2.14	1.42	1.38
14	Y	503	9YF	O6-C6	-2.14	1.37	1.43
15	Z	201	MQ9	C43-C44	2.12	1.38	1.33
15	E	604	MQ9	C3C-C3B	2.12	1.42	1.38
15	F	701	MQ9	C3C-C3B	2.12	1.42	1.38
14	Y	503	9YF	P-O	2.12	1.67	1.59
21	E	602	HEM	C3C-C4C	2.11	1.44	1.41
14	I	304	9YF	P-O2	2.11	1.65	1.59
17	L	603	HEA	C1B-C2B	2.10	1.48	1.44
15	F	707	MQ9	C28-C29	2.10	1.37	1.33
14	Y	502	9YF	P-O	2.09	1.67	1.59
15	Z	201	MQ9	C3C-C3B	2.08	1.42	1.38
15	F	707	MQ9	C3C-C3B	2.07	1.42	1.38
21	E	602	HEM	CMB-C2B	2.07	1.55	1.50
18	Z	202	CDL	OA8-CA7	2.07	1.39	1.33
15	E	603	MQ9	C5-C4	2.06	1.52	1.47
17	R	603	HEA	C1D-C2D	2.06	1.48	1.44
18	T	201	CDL	OA8-CA7	2.05	1.39	1.33
14	E	605	9YF	P-O2	2.04	1.65	1.59
18	T	201	CDL	OA6-CA5	2.04	1.40	1.34
21	E	601	HEM	CMD-C2D	2.04	1.55	1.50
17	L	602	HEA	C1D-C2D	2.04	1.48	1.44
18	Z	202	CDL	OA6-CA5	2.04	1.40	1.34
23	c	202	9XX	O1-C18	2.04	1.40	1.34
21	E	601	HEM	CMB-C2B	2.02	1.54	1.50
15	O	304	MQ9	C3C-C3B	2.02	1.42	1.38
15	F	701	MQ9	C5-C4	2.02	1.52	1.47
18	T	201	CDL	PB2-OB5	2.02	1.67	1.59
18	Z	202	CDL	PB2-OB5	2.02	1.67	1.59
17	L	603	HEA	C1D-C2D	2.02	1.48	1.44
15	I	303	MQ9	C3C-C3B	2.01	1.42	1.38
14	Y	503	9YF	O4-C4	-2.01	1.38	1.43
17	L	603	HEA	C4D-C3D	2.00	1.48	1.45

All (364) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	203	CDL	CB6-CB4-CB3	-9.91	88.68	111.78
18	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
18	X	303	CDL	CB6-CB4-CB3	-9.67	89.23	111.78
18	S	302	CDL	CB6-CB4-CB3	-9.66	89.26	111.78
18	T	201	CDL	OB6-CB4-CB6	9.23	141.46	108.34
18	Z	202	CDL	OB6-CB4-CB6	9.23	141.46	108.34
18	T	203	CDL	OB6-CB4-CB3	-8.36	78.36	108.34
18	Z	203	CDL	OB6-CB4-CB3	-8.35	78.39	108.34
17	L	602	HEA	C12-C11-C3B	8.17	124.90	112.12
17	R	602	HEA	CAD-C3D-C4D	8.13	138.87	124.70
18	X	303	CDL	OB6-CB4-CB3	-8.00	79.66	108.34
18	S	302	CDL	OB6-CB4-CB3	-7.99	79.68	108.34
13	I	301	HEC	CBB-CAB-C3B	-7.59	109.74	127.49
18	S	302	CDL	OB6-CB4-CB6	7.22	134.25	108.34
18	X	303	CDL	OB6-CB4-CB6	7.22	134.24	108.34
18	T	203	CDL	OB6-CB4-CB6	6.87	132.98	108.34
18	Z	203	CDL	OB6-CB4-CB6	6.87	132.98	108.34
13	O	302	HEC	C1D-C2D-C3D	-6.70	102.33	107.00
13	O	301	HEC	CMB-C2B-C3B	6.64	133.62	125.82
17	L	602	HEA	CMC-C2C-C1C	-6.14	119.45	128.46
17	L	602	HEA	CMC-C2C-C3C	6.09	136.85	124.68
17	L	602	HEA	CAD-C3D-C4D	5.95	135.07	124.70
17	R	603	HEA	CMC-C2C-C1C	-5.87	119.85	128.46
17	R	603	HEA	CMC-C2C-C3C	5.82	136.32	124.68
13	O	301	HEC	C1D-C2D-C3D	-5.75	103.00	107.00
17	R	602	HEA	CMC-C2C-C3C	5.74	136.15	124.68
13	I	301	HEC	CBC-CAC-C3C	-5.69	114.16	127.49
17	R	602	HEA	CMC-C2C-C1C	-5.50	120.40	128.46
17	R	602	HEA	C12-C11-C3B	5.48	120.68	112.12
13	I	302	HEC	CBC-CAC-C3C	-5.45	114.73	127.49
14	Y	502	9YF	O9-C8-C9	5.29	122.94	111.48
13	I	302	HEC	CBB-CAB-C3B	-5.29	115.12	127.49
13	O	302	HEC	CMB-C2B-C3B	5.15	131.88	125.82
14	Y	503	9YF	O9-C8-C9	5.06	122.43	111.48
14	Y	503	9YF	O11-C25-C26	4.93	126.85	111.83
23	G	302	9XX	O1-C18-C19	4.91	122.10	111.48
17	R	603	HEA	C3D-C4D-ND	4.71	114.91	110.35
17	L	602	HEA	O11-C11-C3B	-4.67	102.70	111.26
14	E	605	9YF	O9-C8-C9	4.66	121.56	111.48
18	T	201	CDL	OB6-CB4-CB3	-4.65	91.66	108.34
15	Z	201	MQ9	C7-C8-C9	-4.65	118.83	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	202	CDL	OB6-CB4-CB3	-4.64	91.69	108.34
17	L	603	HEA	CMC-C2C-C3C	4.64	133.96	124.68
23	D	302	9XX	O1-C18-C19	4.64	121.52	111.48
14	I	304	9YF	O9-C8-C9	4.60	121.43	111.48
18	T	203	CDL	OA6-CA5-C11	4.53	121.28	111.48
18	Z	203	CDL	OA6-CA5-C11	4.52	121.25	111.48
18	T	201	CDL	OB6-CB5-C51	4.49	121.20	111.48
18	Z	202	CDL	OB6-CB5-C51	4.48	121.18	111.48
17	L	603	HEA	C3D-C4D-ND	4.44	114.64	110.35
18	Z	202	CDL	OA6-CA5-C11	4.37	120.94	111.48
18	T	201	CDL	OA6-CA5-C11	4.37	120.93	111.48
15	T	204	MQ9	C7-C8-C9	-4.27	119.48	126.83
17	R	602	HEA	CAD-C3D-C2D	-4.24	119.92	127.87
14	Y	503	9YF	C7-C6-C5	4.18	118.16	110.83
14	O	303	9YF	O9-C8-C9	4.18	120.52	111.48
20	J	201	9Y0	O7-C21-C22	4.18	120.52	111.48
18	S	302	CDL	OB6-CB5-C51	4.13	120.42	111.48
18	X	303	CDL	OB6-CB5-C51	4.12	120.40	111.48
17	L	603	HEA	CMC-C2C-C1C	-4.09	122.46	128.46
17	R	603	HEA	CHA-C4D-C3D	-4.05	118.86	124.77
17	L	602	HEA	C3D-C4D-ND	4.00	114.21	110.35
17	R	603	HEA	C12-C11-C3B	-3.98	105.91	112.12
20	X	301	9Y0	O7-C21-C22	3.94	120.01	111.48
17	R	602	HEA	C4D-C3D-C2D	-3.91	101.20	106.89
17	L	603	HEA	CHA-C4D-C3D	-3.90	119.09	124.77
20	F	704	9Y0	O7-C21-C22	3.89	119.90	111.48
20	S	301	9Y0	O7-C21-C22	3.83	119.76	111.48
18	Z	203	CDL	OB6-CB5-C51	3.78	119.65	111.48
18	T	203	CDL	OB6-CB5-C51	3.76	119.61	111.48
18	X	303	CDL	OA6-CA5-C11	3.71	119.52	111.48
17	L	602	HEA	C4D-C3D-C2D	-3.70	101.50	106.89
18	S	302	CDL	OA6-CA5-C11	3.70	119.49	111.48
13	I	302	HEC	CMC-C2C-C1C	-3.67	123.08	128.46
23	c	202	9XX	O1-C18-C19	3.65	119.39	111.48
17	R	602	HEA	C3D-C4D-ND	3.64	113.87	110.35
17	R	603	HEA	CAD-C3D-C4D	3.60	130.97	124.70
17	R	603	HEA	C4D-C3D-C2D	-3.56	101.71	106.89
17	R	602	HEA	C26-C15-C14	-3.55	114.50	123.63
14	O	303	9YF	O11-C25-C26	3.54	122.63	111.83
14	E	605	9YF	C7-C6-C5	3.54	117.04	110.83
13	O	302	HEC	CMA-C3A-C2A	3.53	131.59	124.94
13	O	301	HEC	CMC-C2C-C3C	3.48	129.91	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	602	HEA	C26-C15-C16	3.47	121.24	115.23
15	E	604	MQ9	C12-C13-C14	-3.45	119.72	127.62
15	F	707	MQ9	C12-C13-C14	-3.41	119.81	127.62
15	F	707	MQ9	C30-C29-C31	3.36	121.06	115.23
17	L	603	HEA	C4D-C3D-C2D	-3.35	102.01	106.89
14	Y	502	9YF	O11-C25-C26	3.34	122.02	111.83
15	F	707	MQ9	C17-C18-C19	-3.30	120.07	127.62
18	Z	202	CDL	CB6-CB4-CB3	-3.30	104.09	111.78
15	E	604	MQ9	C17-C18-C19	-3.29	120.08	127.62
15	Z	201	MQ9	C40-C39-C41	-3.29	109.52	115.23
18	T	201	CDL	CB6-CB4-CB3	-3.29	104.12	111.78
17	R	602	HEA	C26-C15-C16	3.28	120.93	115.23
18	T	201	CDL	CA4-OA6-CA5	-3.27	109.96	117.80
18	Z	202	CDL	CA4-OA6-CA5	-3.26	109.99	117.80
15	E	604	MQ9	C32-C33-C34	-3.18	120.34	127.62
15	T	204	MQ9	C42-C43-C44	-3.18	120.36	127.62
15	Z	201	MQ9	C42-C43-C44	-3.17	120.36	127.62
17	L	602	HEA	C26-C15-C14	-3.17	115.48	123.63
15	E	603	MQ9	C17-C18-C19	-3.17	120.37	127.62
15	T	204	MQ9	C40-C39-C41	-3.16	109.75	115.23
17	L	603	HEA	CAD-C3D-C4D	3.15	130.19	124.70
15	F	707	MQ9	C32-C33-C34	-3.14	120.43	127.62
20	J	202	9Y0	O7-C21-C22	3.14	118.27	111.48
15	F	701	MQ9	C17-C18-C19	-3.13	120.45	127.62
17	R	603	HEA	CAA-CBA-CGA	-3.06	105.59	113.83
15	F	707	MQ9	C35-C34-C36	3.05	120.52	115.23
23	G	302	9XX	O-C15-C14	3.05	121.13	111.83
15	T	204	MQ9	C17-C18-C19	-3.05	120.65	127.62
15	E	604	MQ9	C30-C29-C31	3.04	120.50	115.23
15	Z	201	MQ9	C17-C18-C19	-3.03	120.68	127.62
14	Y	503	9YF	C6-C5-C4	3.02	116.14	110.83
13	I	301	HEC	CMC-C2C-C1C	-3.02	124.03	128.46
15	T	204	MQ9	C12-C13-C14	-3.01	120.73	127.62
23	D	302	9XX	O-C15-C14	3.00	120.97	111.83
15	Z	201	MQ9	C12-C13-C14	-2.96	120.85	127.62
14	E	605	9YF	C6-C5-C4	2.96	116.02	110.83
17	L	602	HEA	OMA-CMA-C3A	-2.92	117.88	124.80
14	I	304	9YF	O11-C25-C26	2.91	120.72	111.83
18	T	201	CDL	OB8-CB7-C71	2.91	120.71	111.83
15	O	304	MQ9	C5M-C5-C6	-2.91	119.67	124.45
18	Z	202	CDL	OB8-CB7-C71	2.90	120.69	111.83
15	T	204	MQ9	C22-C23-C24	-2.90	120.99	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	201	MQ9	C5M-C5-C6	-2.89	119.70	124.45
15	E	604	MQ9	C35-C34-C36	2.88	120.22	115.23
17	L	603	HEA	CMD-C2D-C1D	-2.86	120.56	125.03
18	Z	203	CDL	OB8-CB7-C71	2.86	120.55	111.83
18	T	203	CDL	OB8-CB7-C71	2.85	120.53	111.83
15	F	701	MQ9	C42-C43-C44	-2.84	121.11	127.62
15	E	604	MQ9	C15-C14-C16	2.84	120.16	115.23
17	L	602	HEA	C17-C18-C19	-2.84	121.12	127.62
20	X	301	9Y0	O5-C5-C6	2.84	120.50	111.83
15	F	707	MQ9	C27-C28-C29	-2.84	121.12	127.62
15	F	707	MQ9	C15-C14-C16	2.84	120.15	115.23
17	R	602	HEA	OMA-CMA-C3A	-2.84	118.08	124.80
15	E	604	MQ9	C27-C28-C29	-2.83	121.14	127.62
17	L	602	HEA	CHA-C4D-C3D	-2.83	120.65	124.77
17	R	602	HEA	C3B-C4B-NB	2.82	113.08	109.84
15	I	303	MQ9	C7-C8-C9	-2.82	121.98	126.83
15	Z	201	MQ9	C22-C23-C24	-2.81	121.18	127.62
14	Y	502	9YF	O11-C24-C	2.80	116.48	108.40
15	E	603	MQ9	C42-C43-C44	-2.80	121.22	127.62
18	T	201	CDL	OA8-CA7-C31	2.80	120.37	111.83
14	E	605	9YF	C6-C7-C2	2.79	116.02	109.68
20	J	201	9Y0	O5-C5-C6	2.79	120.34	111.83
15	E	604	MQ9	C7-C8-C9	-2.79	122.03	126.83
18	Z	202	CDL	OA8-CA7-C31	2.78	120.31	111.83
18	X	303	CDL	OB8-CB7-C71	2.78	120.30	111.83
21	E	602	HEM	C3B-C2B-C1B	2.77	108.49	106.41
20	F	704	9Y0	O5-C5-C6	2.77	120.27	111.83
21	F	703	HEM	C3B-C2B-C1B	2.76	108.49	106.41
18	T	201	CDL	OA6-CA5-OA7	-2.76	117.24	123.70
18	S	302	CDL	OB8-CB7-C71	2.76	120.27	111.83
18	Z	202	CDL	OA6-CA5-OA7	-2.76	117.24	123.70
15	Z	201	MQ9	C32-C33-C34	-2.76	121.30	127.62
15	I	303	MQ9	C5M-C5-C6	-2.76	119.92	124.45
15	O	304	MQ9	C7-C8-C9	-2.75	122.10	126.83
15	F	707	MQ9	C7-C8-C9	-2.74	122.11	126.83
18	T	203	CDL	OA8-CA7-C31	2.74	120.20	111.83
18	Z	203	CDL	OA8-CA7-C31	2.74	120.19	111.83
15	Z	201	MQ9	C7-C6-C5	-2.74	120.20	124.89
14	Y	503	9YF	O2-P-O8	-2.72	101.11	109.81
17	L	603	HEA	CAA-CBA-CGA	-2.72	106.50	113.83
20	S	301	9Y0	O5-C5-C6	2.71	120.10	111.83
15	E	603	MQ9	C20-C19-C21	2.71	119.93	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	701	MQ9	C20-C19-C21	2.70	119.91	115.23
15	T	204	MQ9	C32-C33-C34	-2.68	121.48	127.62
18	X	303	CDL	OA8-CA7-C31	2.68	120.01	111.83
23	c	202	9XX	O-C15-C14	2.67	119.99	111.83
18	S	302	CDL	OA8-CA7-C31	2.67	119.97	111.83
13	I	302	HEC	CBD-CAD-C3D	-2.67	108.06	112.54
20	J	202	9Y0	O5-C5-C6	2.66	119.95	111.83
17	L	603	HEA	CMD-C2D-C3D	2.66	133.34	126.15
17	L	602	HEA	C27-C19-C20	2.63	119.80	115.23
13	O	302	HEC	CBD-CAD-C3D	-2.63	108.12	112.54
14	Y	502	9YF	O9-C8-O10	-2.62	117.59	123.70
15	Z	201	MQ9	C35-C34-C36	2.61	119.76	115.23
15	T	204	MQ9	C5M-C5-C6	-2.60	120.17	124.45
15	Z	201	MQ9	C30-C29-C31	2.59	119.73	115.23
13	I	301	HEC	CBA-CAA-C2A	-2.57	108.31	112.55
15	I	303	MQ9	C12-C13-C14	-2.57	121.74	127.62
18	X	303	CDL	OB4-PB2-OB3	-2.57	100.49	112.44
18	S	302	CDL	OB4-PB2-OB3	-2.57	100.50	112.44
17	R	602	HEA	CMD-C2D-C1D	-2.56	121.03	125.03
17	R	602	HEA	C27-C19-C20	2.55	119.66	115.23
17	L	602	HEA	CAD-CBD-CGD	-2.55	106.91	113.67
17	L	602	HEA	C3B-C4B-NB	2.55	112.77	109.84
15	E	604	MQ9	C20-C19-C21	2.54	119.64	115.23
18	Z	203	CDL	OA4-PA1-OA3	-2.54	100.62	112.44
15	Z	201	MQ9	C25-C24-C26	2.54	119.64	115.23
18	T	203	CDL	OA4-PA1-OA3	-2.54	100.65	112.44
14	Y	503	9YF	O12-C25-C26	-2.53	113.87	123.78
23	G	302	9XX	C17-O1-C18	-2.53	114.13	117.78
15	T	204	MQ9	C30-C29-C31	2.53	119.61	115.23
14	Y	502	9YF	C30-C31-C32	2.53	123.14	113.62
14	Y	503	9YF	C6-C7-C2	2.53	115.41	109.68
15	O	304	MQ9	C12-C13-C14	-2.52	121.85	127.62
15	I	303	MQ9	C32-C33-C34	-2.52	121.85	127.62
15	F	707	MQ9	C20-C19-C21	2.52	119.60	115.23
17	L	602	HEA	CMD-C2D-C1D	-2.52	121.10	125.03
18	T	201	CDL	OB6-CB5-OB7	-2.52	117.82	123.70
18	Z	202	CDL	OB6-CB5-OB7	-2.52	117.82	123.70
15	T	204	MQ9	C11-C9-C8	2.52	126.82	121.17
15	Z	201	MQ9	C11-C9-C8	2.51	126.81	121.17
15	T	204	MQ9	C7-C6-C5	-2.51	120.58	124.89
15	E	604	MQ9	C40-C39-C41	-2.51	110.87	115.23
18	T	201	CDL	OA8-CA7-OA9	-2.51	117.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	304	MQ9	C30-C29-C28	-2.50	117.20	123.63
15	I	303	MQ9	C30-C29-C28	-2.50	117.20	123.63
18	Z	202	CDL	OA8-CA7-OA9	-2.50	117.37	123.63
15	T	204	MQ9	C25-C24-C26	2.50	119.57	115.23
17	R	603	HEA	CMD-C2D-C1D	-2.50	121.13	125.03
15	F	701	MQ9	C27-C28-C29	-2.50	121.91	127.62
15	O	304	MQ9	C32-C33-C34	-2.49	121.93	127.62
15	F	701	MQ9	C5M-C5-C6	-2.48	120.37	124.45
15	T	204	MQ9	C35-C34-C36	2.48	119.53	115.23
15	E	603	MQ9	C27-C28-C29	-2.48	121.95	127.62
13	I	302	HEC	CMB-C2B-C1B	-2.47	124.83	128.46
18	T	201	CDL	OA4-PA1-OA3	-2.47	100.95	112.44
17	R	602	HEA	C17-C18-C19	-2.47	121.97	127.62
18	Z	202	CDL	OA4-PA1-OA3	-2.47	100.95	112.44
14	Y	503	9YF	O6-C6-C5	-2.46	104.57	110.38
17	R	602	HEA	C4B-C3B-C2B	-2.46	103.30	107.44
15	E	604	MQ9	C45-C44-C43	-2.46	117.30	123.63
15	E	603	MQ9	C5M-C5-C6	-2.46	120.41	124.45
15	E	603	MQ9	C7-C6-C5	-2.46	120.67	124.89
18	T	203	CDL	OB4-PB2-OB3	-2.46	101.00	112.44
18	Z	203	CDL	OB4-PB2-OB3	-2.46	101.01	112.44
15	O	304	MQ9	C22-C23-C24	-2.45	122.02	127.62
15	E	603	MQ9	C22-C23-C24	-2.44	122.03	127.62
15	Z	201	MQ9	C45-C44-C46	2.43	119.45	115.23
15	F	701	MQ9	C7-C6-C5	-2.43	120.73	124.89
15	I	303	MQ9	C20-C19-C21	2.43	119.44	115.23
21	F	703	HEM	C3B-C4B-NB	-2.42	107.73	109.47
15	F	701	MQ9	C32-C33-C34	-2.41	122.10	127.62
15	O	304	MQ9	C20-C19-C21	2.41	119.41	115.23
21	F	703	HEM	C1B-NB-C4B	2.41	108.06	105.21
15	F	701	MQ9	C22-C23-C24	-2.40	122.13	127.62
15	T	204	MQ9	C45-C44-C46	2.40	119.39	115.23
15	Z	201	MQ9	C15-C14-C16	2.39	119.37	115.23
21	F	703	HEM	C4C-CHD-C1D	2.39	125.71	122.56
14	Y	503	9YF	O9-C8-O10	-2.39	118.13	123.70
21	E	602	HEM	C1B-NB-C4B	2.38	108.03	105.21
17	R	603	HEA	CMD-C2D-C3D	2.38	132.58	126.15
17	L	602	HEA	CAD-C3D-C2D	-2.38	123.42	127.87
17	L	602	HEA	C4B-C3B-C2B	-2.38	103.44	107.44
15	I	303	MQ9	C22-C23-C24	-2.37	122.20	127.62
15	E	603	MQ9	C32-C33-C34	-2.36	122.22	127.62
13	I	302	HEC	C1D-C2D-C3D	-2.36	105.36	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	603	MQ9	C7-C8-C9	-2.35	122.77	126.83
21	F	703	HEM	C4B-CHC-C1C	2.35	125.66	122.56
15	O	304	MQ9	C15-C14-C16	2.34	119.30	115.23
15	F	707	MQ9	C22-C23-C24	-2.34	122.27	127.62
15	I	303	MQ9	C51-C49-C50	2.34	119.97	114.59
14	E	605	9YF	O4-C4-C3	-2.33	104.89	110.38
18	S	302	CDL	OA4-PA1-OA3	-2.33	101.62	112.44
15	E	604	MQ9	C22-C23-C24	-2.32	122.30	127.62
18	X	303	CDL	OA4-PA1-OA3	-2.32	101.63	112.44
15	I	303	MQ9	C15-C14-C16	2.32	119.26	115.23
15	F	701	MQ9	C25-C24-C26	2.32	119.25	115.23
15	F	707	MQ9	C45-C44-C43	-2.31	117.68	123.63
15	O	304	MQ9	C25-C24-C26	2.31	119.23	115.23
18	T	201	CDL	OB4-PB2-OB3	-2.31	101.71	112.44
17	R	602	HEA	CHD-C1D-ND	2.31	127.23	124.37
15	O	304	MQ9	C35-C34-C36	2.30	119.23	115.23
13	O	301	HEC	CAD-CBD-CGD	-2.30	107.62	113.83
18	Z	202	CDL	OB4-PB2-OB3	-2.30	101.75	112.44
15	T	204	MQ9	C15-C14-C16	2.30	119.22	115.23
21	E	602	HEM	C3B-C4B-NB	-2.30	107.82	109.47
14	E	605	9YF	O11-C25-C26	2.30	118.84	111.83
17	R	603	HEA	C3C-C4C-NC	2.29	112.17	109.21
17	R	602	HEA	CAA-CBA-CGA	-2.29	107.66	113.83
15	F	701	MQ9	C7-C8-C9	-2.29	122.89	126.83
15	O	304	MQ9	C7-C6-C5	-2.29	120.97	124.89
17	L	603	HEA	C25-C23-C24	2.28	119.84	114.59
15	I	303	MQ9	C7-C6-C5	-2.28	120.98	124.89
23	D	302	9XX	C17-O1-C18	-2.28	114.50	117.78
17	R	602	HEA	CBD-CAD-C3D	2.27	118.81	112.53
15	E	603	MQ9	C25-C24-C26	2.27	119.16	115.23
15	F	701	MQ9	C15-C14-C16	2.26	119.15	115.23
15	I	303	MQ9	C35-C34-C36	2.25	119.13	115.23
23	c	202	9XX	O1-C17-C37	2.25	112.99	107.96
15	F	707	MQ9	C40-C39-C41	-2.24	111.34	115.23
21	E	602	HEM	C4B-CHC-C1C	2.23	125.51	122.56
17	L	603	HEA	C3C-C4C-NC	2.23	112.09	109.21
14	O	303	9YF	O11-C25-O12	-2.23	118.06	123.63
15	E	603	MQ9	C15-C14-C16	2.21	119.06	115.23
17	L	602	HEA	C3C-C4C-NC	2.21	112.07	109.21
17	R	603	HEA	C25-C23-C24	2.21	119.67	114.59
21	F	702	HEM	C4D-ND-C1D	2.21	107.82	105.21
13	I	301	HEC	C1D-C2D-C3D	-2.20	105.46	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	201	MQ9	C20-C19-C21	2.20	119.04	115.23
15	E	604	MQ9	C42-C43-C44	-2.19	122.60	127.62
13	I	302	HEC	CMC-C2C-C3C	-2.19	123.24	125.82
17	R	602	HEA	C3C-C4C-NC	2.19	112.04	109.21
21	E	601	HEM	C4D-ND-C1D	2.19	107.80	105.21
21	E	601	HEM	C3D-C4D-ND	-2.18	107.78	110.17
14	Y	502	9YF	O3-C3-C4	-2.18	105.24	110.38
13	O	302	HEC	CBB-CAB-C3B	-2.17	122.41	127.49
13	I	302	HEC	CBA-CAA-C2A	-2.17	108.97	112.55
15	I	303	MQ9	C32-C31-C29	-2.17	106.00	113.19
15	I	303	MQ9	C42-C43-C44	-2.17	122.66	127.62
13	O	301	HEC	CAA-CBA-CGA	-2.17	107.99	113.83
15	O	304	MQ9	C51-C49-C50	2.17	119.58	114.59
15	I	303	MQ9	C25-C24-C26	2.17	118.99	115.23
17	R	602	HEA	C25-C23-C24	2.16	119.56	114.59
17	L	602	HEA	CAA-CBA-CGA	-2.16	108.01	113.83
15	O	304	MQ9	C42-C43-C44	-2.15	122.69	127.62
15	O	304	MQ9	C32-C31-C29	-2.15	106.05	113.19
15	F	701	MQ9	C12-C13-C14	-2.15	122.70	127.62
17	L	602	HEA	CMD-C2D-C3D	2.14	131.95	126.15
23	D	302	9XX	O1-C17-C16	2.14	111.12	106.21
15	I	303	MQ9	C40-C39-C41	-2.13	111.53	115.23
15	I	303	MQ9	C10-C9-C11	2.13	118.93	115.23
17	L	602	HEA	C25-C23-C24	2.13	119.49	114.59
21	F	702	HEM	C3D-C4D-ND	-2.13	107.84	110.17
17	L	602	HEA	CBD-CAD-C3D	2.13	118.41	112.53
17	L	603	HEA	C12-C11-C3B	-2.12	108.80	112.12
23	G	302	9XX	O1-C17-C16	2.12	111.08	106.21
21	F	702	HEM	C4B-CHC-C1C	2.11	125.35	122.56
15	E	603	MQ9	C12-C13-C14	-2.11	122.80	127.62
21	E	602	HEM	C4C-CHD-C1D	2.10	125.33	122.56
15	O	304	MQ9	C40-C39-C41	-2.10	111.59	115.23
15	F	707	MQ9	C7-C6-C5	-2.10	121.30	124.89
18	R	604	CDL	OB4-PB2-OB5	-2.09	98.08	107.57
18	L	604	CDL	OB4-PB2-OB5	-2.09	98.10	107.57
21	E	602	HEM	CHC-C4B-C3B	2.09	127.77	124.57
14	E	605	9YF	O5-C5-C6	-2.09	105.46	110.38
15	I	303	MQ9	C17-C18-C19	-2.09	122.85	127.62
21	E	601	HEM	C3C-C2C-C1C	2.08	108.28	106.85
15	T	204	MQ9	C20-C19-C21	2.08	118.84	115.23
18	L	604	CDL	OA5-PA1-OA3	-2.07	100.72	108.94
18	R	604	CDL	OA5-PA1-OA3	-2.07	100.72	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	304	MQ9	C17-C18-C19	-2.07	122.88	127.62
17	R	602	HEA	CHD-C1D-C2D	-2.07	121.08	126.94
14	Y	502	9YF	O4-C4-C3	-2.07	105.50	110.38
23	c	202	9XX	C25-C26-C27	-2.06	109.12	115.97
15	O	304	MQ9	C10-C9-C11	2.06	118.80	115.23
18	Z	202	CDL	C58-C57-C56	-2.05	103.99	114.37
15	F	707	MQ9	C10-C9-C11	2.05	118.79	115.23
15	F	701	MQ9	C35-C34-C36	2.05	118.79	115.23
15	E	604	MQ9	C10-C9-C11	2.05	118.79	115.23
17	R	602	HEA	CHB-C1B-C2B	-2.05	121.79	125.03
18	T	201	CDL	C58-C57-C56	-2.05	104.02	114.37
21	E	601	HEM	CMA-C3A-C4A	-2.05	125.46	128.46
17	L	603	HEA	CHB-C1B-C2B	-2.04	121.80	125.03
15	F	701	MQ9	C30-C29-C31	2.04	118.77	115.23
15	E	603	MQ9	C30-C29-C28	-2.04	118.39	123.63
21	F	703	HEM	CMA-C3A-C4A	-2.03	125.48	128.46
18	T	201	CDL	C56-C55-C54	-2.03	104.10	114.37
18	Z	202	CDL	C56-C55-C54	-2.03	104.10	114.37
14	Y	502	9YF	C7-C2-C3	-2.03	108.05	110.86
15	E	604	MQ9	C7-C6-C5	-2.03	121.42	124.89
15	E	604	MQ9	C5M-C5-C6	-2.02	121.13	124.45
21	E	602	HEM	CMA-C3A-C4A	-2.02	125.50	128.46
15	F	701	MQ9	C30-C29-C28	-2.02	118.45	123.63
17	R	602	HEA	O11-C11-C3B	-2.02	107.56	111.26
15	E	603	MQ9	C35-C34-C36	2.01	118.72	115.23
15	F	707	MQ9	C42-C43-C44	-2.01	123.03	127.62
23	G	302	9XX	O1-C18-O2	-2.01	119.01	123.70
14	Y	502	9YF	O11-C25-O12	-2.01	118.61	123.63
18	F	706	CDL	OA6-CA5-C11	2.00	115.81	111.48

There are no chirality outliers.

All (1061) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	302	HEC	C1A-C2A-CAA-CBA
13	O	302	HEC	C3A-C2A-CAA-CBA
14	O	303	9YF	C-C1-O-P
14	O	303	9YF	C9-C8-O9-C
14	E	605	9YF	C1-O-P-O1
14	E	605	9YF	C1-O-P-O8
14	E	605	9YF	C9-C8-O9-C
14	I	304	9YF	C-C1-O-P

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Mol	Chain	Res	Type	Atoms
14	I	304	9YF	C9-C8-O9-C
14	Y	502	9YF	C9-C8-O9-C
14	Y	503	9YF	C1-O-P-O1
14	Y	503	9YF	C1-O-P-O2
14	Y	503	9YF	C9-C8-O9-C
15	E	603	MQ9	C9-C11-C12-C13
15	T	204	MQ9	C44-C46-C47-C48
17	R	602	HEA	C2D-C3D-CAD-CBD
17	R	602	HEA	C4D-C3D-CAD-CBD
17	L	602	HEA	C12-C11-C3B-C2B
18	R	604	CDL	CA3-OA5-PA1-OA2
18	R	604	CDL	CA3-OA5-PA1-OA3
18	R	604	CDL	CA3-OA5-PA1-OA4
18	R	604	CDL	C11-CA5-OA6-CA4
18	R	604	CDL	CB2-OB2-PB2-OB3
18	R	604	CDL	C51-CB5-OB6-CB4
18	S	302	CDL	CA3-OA5-PA1-OA2
18	S	302	CDL	CA3-OA5-PA1-OA3
18	S	302	CDL	CB2-OB2-PB2-OB3
18	S	302	CDL	CB2-OB2-PB2-OB4
18	S	302	CDL	CB2-OB2-PB2-OB5
18	S	302	CDL	CB3-OB5-PB2-OB2
18	S	302	CDL	CB3-OB5-PB2-OB3
18	S	302	CDL	CB3-OB5-PB2-OB4
18	S	302	CDL	OB7-CB5-OB6-CB4
18	E	606	CDL	O1-C1-CB2-OB2
18	E	606	CDL	CA2-C1-CB2-OB2
18	E	606	CDL	CA2-OA2-PA1-OA3
18	E	606	CDL	CA2-OA2-PA1-OA5
18	E	606	CDL	CA3-OA5-PA1-OA2
18	E	606	CDL	C1-CB2-OB2-PB2
18	E	606	CDL	CB2-OB2-PB2-OB3
18	E	606	CDL	CB2-OB2-PB2-OB4
18	E	606	CDL	CB2-OB2-PB2-OB5
18	E	606	CDL	CB3-OB5-PB2-OB2
18	E	606	CDL	CB3-OB5-PB2-OB3
18	E	606	CDL	CB4-CB3-OB5-PB2
18	E	607	CDL	CA2-OA2-PA1-OA5
18	E	607	CDL	CA3-OA5-PA1-OA2
18	E	607	CDL	CA3-OA5-PA1-OA4
18	E	607	CDL	CB2-OB2-PB2-OB4
18	E	607	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
18	E	607	CDL	CB3-OB5-PB2-OB4
18	F	705	CDL	O1-C1-CB2-OB2
18	F	705	CDL	CA2-C1-CB2-OB2
18	F	705	CDL	CA2-OA2-PA1-OA3
18	F	705	CDL	CA2-OA2-PA1-OA5
18	F	705	CDL	CA3-OA5-PA1-OA2
18	F	705	CDL	C1-CB2-OB2-PB2
18	F	705	CDL	CB2-OB2-PB2-OB3
18	F	705	CDL	CB2-OB2-PB2-OB4
18	F	705	CDL	CB2-OB2-PB2-OB5
18	F	705	CDL	CB3-OB5-PB2-OB2
18	F	705	CDL	CB3-OB5-PB2-OB3
18	F	705	CDL	CB4-CB3-OB5-PB2
18	F	706	CDL	CA2-OA2-PA1-OA3
18	F	706	CDL	CA2-OA2-PA1-OA4
18	F	706	CDL	CA2-OA2-PA1-OA5
18	F	706	CDL	CA3-OA5-PA1-OA2
18	F	706	CDL	CA3-OA5-PA1-OA4
18	F	706	CDL	CB3-OB5-PB2-OB2
18	F	706	CDL	CB3-OB5-PB2-OB3
18	F	706	CDL	CB3-OB5-PB2-OB4
18	L	604	CDL	CA3-OA5-PA1-OA2
18	L	604	CDL	CA3-OA5-PA1-OA3
18	L	604	CDL	CA3-OA5-PA1-OA4
18	L	604	CDL	C11-CA5-OA6-CA4
18	L	604	CDL	CB2-OB2-PB2-OB3
18	L	604	CDL	C51-CB5-OB6-CB4
18	J	203	CDL	CA2-OA2-PA1-OA3
18	J	203	CDL	CA2-OA2-PA1-OA4
18	J	203	CDL	CA2-OA2-PA1-OA5
18	J	203	CDL	CB2-OB2-PB2-OB3
18	J	203	CDL	CB2-OB2-PB2-OB4
18	J	203	CDL	CB2-OB2-PB2-OB5
18	T	201	CDL	CA3-OA5-PA1-OA2
18	T	201	CDL	CA3-OA5-PA1-OA3
18	T	201	CDL	OA6-CA4-CA6-OA8
18	T	201	CDL	C11-CA5-OA6-CA4
18	T	201	CDL	C51-CB5-OB6-CB4
18	T	202	CDL	CA2-OA2-PA1-OA4
18	T	202	CDL	CA2-OA2-PA1-OA5
18	T	202	CDL	OA6-CA4-CA6-OA8
18	T	202	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
18	T	202	CDL	CB3-OB5-PB2-OB4
18	T	202	CDL	C51-CB5-OB6-CB4
18	T	203	CDL	O1-C1-CB2-OB2
18	T	203	CDL	CA2-OA2-PA1-OA3
18	T	203	CDL	CA2-OA2-PA1-OA4
18	T	203	CDL	CA2-OA2-PA1-OA5
18	T	203	CDL	OA7-CA5-OA6-CA4
18	T	203	CDL	C11-CA5-OA6-CA4
18	P	201	CDL	CA2-OA2-PA1-OA3
18	P	201	CDL	CA2-OA2-PA1-OA4
18	P	201	CDL	CA2-OA2-PA1-OA5
18	P	201	CDL	CB2-OB2-PB2-OB3
18	P	201	CDL	CB2-OB2-PB2-OB4
18	P	201	CDL	CB2-OB2-PB2-OB5
18	X	302	CDL	CA2-OA2-PA1-OA4
18	X	302	CDL	CA2-OA2-PA1-OA5
18	X	302	CDL	OA6-CA4-CA6-OA8
18	X	302	CDL	CB3-OB5-PB2-OB2
18	X	302	CDL	CB3-OB5-PB2-OB4
18	X	302	CDL	C51-CB5-OB6-CB4
18	X	303	CDL	CA3-OA5-PA1-OA2
18	X	303	CDL	CA3-OA5-PA1-OA3
18	X	303	CDL	CB2-OB2-PB2-OB3
18	X	303	CDL	CB2-OB2-PB2-OB4
18	X	303	CDL	CB2-OB2-PB2-OB5
18	X	303	CDL	CB3-OB5-PB2-OB2
18	X	303	CDL	CB3-OB5-PB2-OB3
18	X	303	CDL	CB3-OB5-PB2-OB4
18	X	303	CDL	OB7-CB5-OB6-CB4
18	Z	202	CDL	CA3-OA5-PA1-OA2
18	Z	202	CDL	CA3-OA5-PA1-OA3
18	Z	202	CDL	OA6-CA4-CA6-OA8
18	Z	202	CDL	C11-CA5-OA6-CA4
18	Z	202	CDL	C51-CB5-OB6-CB4
18	Z	203	CDL	O1-C1-CB2-OB2
18	Z	203	CDL	CA2-OA2-PA1-OA3
18	Z	203	CDL	CA2-OA2-PA1-OA4
18	Z	203	CDL	CA2-OA2-PA1-OA5
18	Z	203	CDL	OA7-CA5-OA6-CA4
18	Z	203	CDL	C11-CA5-OA6-CA4
20	S	301	9Y0	O1-C3-C4-N
20	F	704	9Y0	C22-C21-O7-C1

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Mol	Chain	Res	Type	Atoms
20	F	704	9Y0	O6-C21-O7-C1
20	J	201	9Y0	C22-C21-O7-C1
20	J	201	9Y0	O6-C21-O7-C1
20	J	201	9Y0	C2-O3-P-O
20	J	201	9Y0	C2-O3-P-O1
20	J	201	9Y0	C2-O3-P-O2
20	J	202	9Y0	O1-C3-C4-N
20	X	301	9Y0	O1-C3-C4-N
23	D	302	9XX	C19-C18-O1-C17
23	G	302	9XX	C19-C18-O1-C17
23	c	202	9XX	O-C16-C17-O1
23	c	202	9XX	C37-C17-O1-C18
23	c	202	9XX	C19-C18-O1-C17
23	c	202	9XX	O2-C18-O1-C17
18	R	604	CDL	OA9-CA7-OA8-CA6
18	L	604	CDL	OA9-CA7-OA8-CA6
14	I	304	9YF	C26-C25-O11-C24
18	R	604	CDL	C31-CA7-OA8-CA6
18	L	604	CDL	C31-CA7-OA8-CA6
14	O	303	9YF	O12-C25-O11-C24
14	I	304	9YF	O12-C25-O11-C24
14	Y	502	9YF	O12-C25-O11-C24
18	T	201	CDL	OA9-CA7-OA8-CA6
18	T	202	CDL	OA9-CA7-OA8-CA6
18	T	203	CDL	OA9-CA7-OA8-CA6
18	T	203	CDL	OB9-CB7-OB8-CB6
18	X	302	CDL	OA9-CA7-OA8-CA6
18	Z	202	CDL	OA9-CA7-OA8-CA6
18	Z	203	CDL	OA9-CA7-OA8-CA6
18	Z	203	CDL	OB9-CB7-OB8-CB6
14	O	303	9YF	O10-C8-O9-C
14	E	605	9YF	O10-C8-O9-C
14	I	304	9YF	O10-C8-O9-C
14	Y	502	9YF	O10-C8-O9-C
18	R	604	CDL	OA7-CA5-OA6-CA4
18	R	604	CDL	OB7-CB5-OB6-CB4
18	E	606	CDL	OB7-CB5-OB6-CB4
18	E	607	CDL	OB7-CB5-OB6-CB4
18	F	705	CDL	OB7-CB5-OB6-CB4
18	F	706	CDL	OA7-CA5-OA6-CA4
18	L	604	CDL	OA7-CA5-OA6-CA4
18	L	604	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	T	201	CDL	OA7-CA5-OA6-CA4
18	T	201	CDL	OB7-CB5-OB6-CB4
18	T	202	CDL	OB7-CB5-OB6-CB4
18	X	302	CDL	OB7-CB5-OB6-CB4
18	Z	202	CDL	OA7-CA5-OA6-CA4
18	Z	202	CDL	OB7-CB5-OB6-CB4
23	D	302	9XX	O2-C18-O1-C17
23	G	302	9XX	O2-C18-O1-C17
14	O	303	9YF	C26-C25-O11-C24
14	Y	502	9YF	C26-C25-O11-C24
18	T	202	CDL	C31-CA7-OA8-CA6
18	T	203	CDL	C71-CB7-OB8-CB6
18	X	302	CDL	C31-CA7-OA8-CA6
18	Z	203	CDL	C71-CB7-OB8-CB6
20	J	201	9Y0	C6-C5-O5-C
20	X	301	9Y0	C6-C5-O5-C
18	S	302	CDL	C51-CB5-OB6-CB4
18	E	606	CDL	C51-CB5-OB6-CB4
18	F	705	CDL	C51-CB5-OB6-CB4
18	F	706	CDL	C11-CA5-OA6-CA4
18	X	303	CDL	C51-CB5-OB6-CB4
17	L	602	HEA	C26-C15-C16-C17
17	L	602	HEA	C14-C15-C16-C17
14	Y	503	9YF	C26-C25-O11-C24
18	T	201	CDL	C31-CA7-OA8-CA6
18	T	203	CDL	C31-CA7-OA8-CA6
18	Z	202	CDL	C31-CA7-OA8-CA6
18	Z	203	CDL	C31-CA7-OA8-CA6
20	S	301	9Y0	C6-C5-O5-C
20	F	704	9Y0	C6-C5-O5-C
20	F	704	9Y0	O4-C5-O5-C
20	J	201	9Y0	O4-C5-O5-C
20	X	301	9Y0	O4-C5-O5-C
14	Y	503	9YF	O10-C8-O9-C
20	S	301	9Y0	O6-C21-O7-C1
18	E	607	CDL	O1-C1-CB2-OB2
18	J	203	CDL	O1-C1-CA2-OA2
18	J	203	CDL	O1-C1-CB2-OB2
18	T	201	CDL	O1-C1-CB2-OB2
18	P	201	CDL	O1-C1-CA2-OA2
18	P	201	CDL	O1-C1-CB2-OB2
18	Z	202	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
14	E	605	9YF	C26-C25-O11-C24
14	E	605	9YF	O12-C25-O11-C24
20	S	301	9Y0	O4-C5-O5-C
18	E	607	CDL	C51-CB5-OB6-CB4
18	T	202	CDL	C11-CA5-OA6-CA4
18	X	302	CDL	C11-CA5-OA6-CA4
20	S	301	9Y0	C22-C21-O7-C1
20	X	301	9Y0	C22-C21-O7-C1
14	Y	503	9YF	O12-C25-O11-C24
18	T	202	CDL	OA7-CA5-OA6-CA4
18	X	302	CDL	OA7-CA5-OA6-CA4
15	O	304	MQ9	C14-C16-C17-C18
15	E	603	MQ9	C44-C46-C47-C48
15	E	604	MQ9	C29-C31-C32-C33
15	E	604	MQ9	C39-C41-C42-C43
15	F	701	MQ9	C9-C11-C12-C13
15	F	701	MQ9	C44-C46-C47-C48
15	F	707	MQ9	C29-C31-C32-C33
15	F	707	MQ9	C39-C41-C42-C43
15	T	204	MQ9	C39-C41-C42-C43
15	Z	201	MQ9	C9-C11-C12-C13
15	Z	201	MQ9	C14-C16-C17-C18
15	Z	201	MQ9	C29-C31-C32-C33
15	Z	201	MQ9	C44-C46-C47-C48
15	I	303	MQ9	C14-C16-C17-C18
17	R	603	HEA	C15-C16-C17-C18
17	L	603	HEA	C15-C16-C17-C18
14	Y	502	9YF	C11-C10-C9-C8
18	J	203	CDL	C1-CA2-OA2-PA1
18	P	201	CDL	C1-CA2-OA2-PA1
17	L	602	HEA	C3D-CAD-CBD-CGD
18	F	706	CDL	C76-C77-C78-C79
20	J	201	9Y0	C22-C23-C24-C25
18	E	606	CDL	C31-CA7-OA8-CA6
18	F	705	CDL	C31-CA7-OA8-CA6
18	R	604	CDL	C38-C39-C40-C41
18	L	604	CDL	C38-C39-C40-C41
18	E	606	CDL	C59-C60-C61-C62
18	F	705	CDL	C59-C60-C61-C62
18	E	607	CDL	C76-C77-C78-C79
18	E	606	CDL	OA9-CA7-OA8-CA6
18	F	705	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
20	X	301	9Y0	O6-C21-O7-C1
18	J	203	CDL	CA2-C1-CB2-OB2
18	T	201	CDL	CA2-C1-CB2-OB2
18	T	203	CDL	CA2-C1-CB2-OB2
18	P	201	CDL	CA2-C1-CB2-OB2
18	Z	202	CDL	CA2-C1-CB2-OB2
18	Z	203	CDL	CA2-C1-CB2-OB2
18	R	604	CDL	C71-CB7-OB8-CB6
18	S	302	CDL	C31-CA7-OA8-CA6
18	L	604	CDL	C71-CB7-OB8-CB6
18	X	303	CDL	C31-CA7-OA8-CA6
20	J	202	9Y0	C6-C5-O5-C
18	R	604	CDL	C52-C53-C54-C55
18	L	604	CDL	C52-C53-C54-C55
18	J	203	CDL	C55-C56-C57-C58
18	P	201	CDL	C55-C56-C57-C58
18	E	607	CDL	C58-C59-C60-C61
18	F	706	CDL	C57-C58-C59-C60
18	T	201	CDL	O1-C1-CA2-OA2
18	Z	202	CDL	O1-C1-CA2-OA2
18	E	606	CDL	C33-C34-C35-C36
18	F	705	CDL	C33-C34-C35-C36
18	E	607	CDL	C11-CA5-OA6-CA4
18	J	203	CDL	C51-CB5-OB6-CB4
18	P	201	CDL	C51-CB5-OB6-CB4
18	J	203	CDL	OB6-CB4-CB6-OB8
18	T	201	CDL	OB6-CB4-CB6-OB8
18	P	201	CDL	OB6-CB4-CB6-OB8
18	Z	202	CDL	OB6-CB4-CB6-OB8
18	Z	203	CDL	CB7-C71-C72-C73
13	O	301	HEC	C3D-CAD-CBD-CGD
13	O	302	HEC	C3D-CAD-CBD-CGD
14	E	605	9YF	C33-C35-C36-C37
18	T	203	CDL	CB7-C71-C72-C73
15	E	603	MQ9	C40-C39-C41-C42
18	S	302	CDL	CB7-C71-C72-C73
18	X	303	CDL	CB7-C71-C72-C73
17	L	602	HEA	C4D-C3D-CAD-CBD
15	E	604	MQ9	C9-C11-C12-C13
15	E	604	MQ9	C44-C46-C47-C48
15	F	707	MQ9	C9-C11-C12-C13
15	F	707	MQ9	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
15	T	204	MQ9	C9-C11-C12-C13
15	T	204	MQ9	C14-C16-C17-C18
15	T	204	MQ9	C29-C31-C32-C33
15	Z	201	MQ9	C39-C41-C42-C43
18	R	604	CDL	CB7-C71-C72-C73
18	L	604	CDL	CB7-C71-C72-C73
18	T	201	CDL	CA5-C11-C12-C13
18	Z	202	CDL	CA5-C11-C12-C13
20	J	202	9Y0	C21-C22-C23-C24
18	R	604	CDL	OB9-CB7-OB8-CB6
18	S	302	CDL	OA9-CA7-OA8-CA6
18	L	604	CDL	OB9-CB7-OB8-CB6
18	X	303	CDL	OA9-CA7-OA8-CA6
18	S	302	CDL	CA5-C11-C12-C13
18	T	202	CDL	CB7-C71-C72-C73
18	X	302	CDL	CB7-C71-C72-C73
18	X	303	CDL	CA5-C11-C12-C13
20	J	202	9Y0	O4-C5-O5-C
18	R	604	CDL	C31-C32-C33-C34
18	R	604	CDL	C58-C59-C60-C61
18	L	604	CDL	C31-C32-C33-C34
18	L	604	CDL	C58-C59-C60-C61
14	Y	503	9YF	C25-C26-C27-C28
18	E	607	CDL	OA7-CA5-OA6-CA4
18	J	203	CDL	OB7-CB5-OB6-CB4
18	P	201	CDL	OB7-CB5-OB6-CB4
18	J	203	CDL	CB2-C1-CA2-OA2
18	P	201	CDL	CB2-C1-CA2-OA2
18	T	203	CDL	CB5-C51-C52-C53
18	Z	203	CDL	CB5-C51-C52-C53
18	F	706	CDL	C78-C79-C80-C81
15	I	303	MQ9	C34-C36-C37-C38
17	L	602	HEA	C2D-C3D-CAD-CBD
20	X	301	9Y0	C21-C22-C23-C24
18	T	201	CDL	CB6-CB4-OB6-CB5
18	Z	202	CDL	CB6-CB4-OB6-CB5
18	E	607	CDL	C78-C79-C80-C81
20	F	704	9Y0	C22-C23-C24-C25
18	E	606	CDL	C11-CA5-OA6-CA4
18	F	705	CDL	C11-CA5-OA6-CA4
15	E	603	MQ9	C38-C39-C41-C42
18	E	606	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
18	F	705	CDL	C55-C56-C57-C58
23	G	302	9XX	C17-C16-O-C15
14	I	304	9YF	C35-C36-C37-C38
18	L	604	CDL	C35-C36-C37-C38
18	T	201	CDL	C12-C13-C14-C15
18	Z	202	CDL	C12-C13-C14-C15
20	J	202	9Y0	C9-C10-C11-C12
14	O	303	9YF	C9-C10-C11-C12
14	Y	503	9YF	C35-C36-C37-C38
14	Y	503	9YF	C37-C38-C39-C40
18	R	604	CDL	C35-C36-C37-C38
18	R	604	CDL	C55-C56-C57-C58
18	L	604	CDL	C55-C56-C57-C58
14	O	303	9YF	C39-C40-C41-C42
14	E	605	9YF	C9-C10-C11-C12
18	J	203	CDL	C60-C61-C62-C63
18	P	201	CDL	C60-C61-C62-C63
23	c	202	9XX	C31-C32-C33-C34
18	S	302	CDL	C71-CB7-OB8-CB6
18	X	303	CDL	C71-CB7-OB8-CB6
14	O	303	9YF	C26-C27-C28-C29
14	I	304	9YF	C26-C27-C28-C29
18	E	606	CDL	OA7-CA5-OA6-CA4
18	F	705	CDL	OA7-CA5-OA6-CA4
18	R	604	CDL	C75-C76-C77-C78
18	L	604	CDL	C75-C76-C77-C78
18	E	606	CDL	C56-C57-C58-C59
18	T	203	CDL	C37-C38-C39-C40
18	Z	203	CDL	C37-C38-C39-C40
18	F	705	CDL	C56-C57-C58-C59
18	F	706	CDL	C51-CB5-OB6-CB4
18	J	203	CDL	C11-CA5-OA6-CA4
18	P	201	CDL	C11-CA5-OA6-CA4
18	T	203	CDL	C52-C53-C54-C55
18	Z	203	CDL	C52-C53-C54-C55
20	S	301	9Y0	C21-C22-C23-C24
18	S	302	CDL	C35-C36-C37-C38
18	E	606	CDL	C75-C76-C77-C78
18	F	705	CDL	C75-C76-C77-C78
18	J	203	CDL	C75-C76-C77-C78
18	T	202	CDL	C59-C60-C61-C62
18	T	203	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
18	P	201	CDL	C75-C76-C77-C78
18	X	302	CDL	C59-C60-C61-C62
18	X	303	CDL	C35-C36-C37-C38
18	Z	203	CDL	C31-C32-C33-C34
20	J	202	9Y0	C6-C7-C8-C9
18	R	604	CDL	C53-C54-C55-C56
18	J	203	CDL	C32-C33-C34-C35
18	P	201	CDL	C32-C33-C34-C35
20	J	201	9Y0	C16-C17-C18-C19
18	S	302	CDL	C74-C75-C76-C77
18	L	604	CDL	C53-C54-C55-C56
18	X	303	CDL	C74-C75-C76-C77
20	F	704	9Y0	C15-C16-C17-C18
23	D	302	9XX	C14-C15-O-C16
15	O	304	MQ9	C34-C36-C37-C38
18	E	606	CDL	CA3-CA4-CA6-OA8
18	F	705	CDL	CA3-CA4-CA6-OA8
18	F	706	CDL	C34-C35-C36-C37
18	J	203	CDL	C31-C32-C33-C34
18	T	201	CDL	C51-C52-C53-C54
18	T	203	CDL	C32-C33-C34-C35
18	P	201	CDL	C31-C32-C33-C34
18	Z	202	CDL	C51-C52-C53-C54
18	Z	203	CDL	C32-C33-C34-C35
20	J	201	9Y0	C15-C16-C17-C18
14	O	303	9YF	C35-C36-C37-C38
14	E	605	9YF	C15-C16-C17-C18
18	F	706	CDL	C52-C53-C54-C55
18	T	203	CDL	C35-C36-C37-C38
18	Z	203	CDL	C35-C36-C37-C38
18	S	302	CDL	C31-C32-C33-C34
18	X	303	CDL	C31-C32-C33-C34
18	J	203	CDL	CB7-C71-C72-C73
18	P	201	CDL	CB7-C71-C72-C73
18	S	302	CDL	C72-C73-C74-C75
18	E	607	CDL	C34-C35-C36-C37
18	F	706	CDL	C37-C38-C39-C40
18	X	303	CDL	C72-C73-C74-C75
21	E	602	HEM	C3D-CAD-CBD-CGD
18	L	604	CDL	C32-C33-C34-C35
18	J	203	CDL	C56-C57-C58-C59
18	P	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
18	P	201	CDL	C56-C57-C58-C59
18	R	604	CDL	C32-C33-C34-C35
18	E	607	CDL	C52-C53-C54-C55
18	F	706	CDL	C12-C13-C14-C15
18	J	203	CDL	C54-C55-C56-C57
18	T	203	CDL	C11-C12-C13-C14
18	T	203	CDL	C59-C60-C61-C62
18	Z	203	CDL	C11-C12-C13-C14
18	Z	203	CDL	C59-C60-C61-C62
18	S	302	CDL	OB9-CB7-OB8-CB6
18	X	303	CDL	OB9-CB7-OB8-CB6
18	J	203	CDL	OA7-CA5-OA6-CA4
18	P	201	CDL	OA7-CA5-OA6-CA4
15	F	701	MQ9	C40-C39-C41-C42
14	E	605	9YF	C17-C18-C19-C20
18	R	604	CDL	C37-C38-C39-C40
18	E	607	CDL	C37-C38-C39-C40
18	E	607	CDL	C53-C54-C55-C56
18	L	604	CDL	C37-C38-C39-C40
18	T	201	CDL	C76-C77-C78-C79
18	F	706	CDL	C31-CA7-OA8-CA6
14	Y	503	9YF	C26-C27-C28-C29
18	Z	202	CDL	C76-C77-C78-C79
18	S	302	CDL	C11-C12-C13-C14
18	X	303	CDL	C11-C12-C13-C14
18	T	202	CDL	C11-C12-C13-C14
18	X	302	CDL	C11-C12-C13-C14
14	Y	502	9YF	C28-C29-C30-C31
14	Y	503	9YF	C14-C15-C16-C17
18	X	302	CDL	C52-C53-C54-C55
20	F	704	9Y0	C29-C30-C31-C32
18	T	202	CDL	C52-C53-C54-C55
20	J	202	9Y0	C22-C23-C24-C25
18	E	607	CDL	CB5-C51-C52-C53
18	J	203	CDL	CA7-C31-C32-C33
20	J	202	9Y0	C24-C25-C26-C27
18	F	706	CDL	OB7-CB5-OB6-CB4
20	F	704	9Y0	C16-C17-C18-C19
14	I	304	9YF	C39-C40-C41-C42
18	E	606	CDL	CA7-C31-C32-C33
18	F	705	CDL	CA7-C31-C32-C33
18	P	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
18	S	302	CDL	C60-C61-C62-C63
18	T	203	CDL	C73-C74-C75-C76
18	X	303	CDL	C60-C61-C62-C63
18	Z	203	CDL	C73-C74-C75-C76
18	T	201	CDL	C31-C32-C33-C34
18	Z	202	CDL	C31-C32-C33-C34
18	F	706	CDL	C59-C60-C61-C62
14	Y	502	9YF	C33-C35-C36-C37
22	c	201	PLM	C5-C6-C7-C8
18	E	606	CDL	CB7-C71-C72-C73
14	Y	503	9YF	C16-C17-C18-C19
20	S	301	9Y0	C18-C19-C20-C37
15	E	603	MQ9	C39-C41-C42-C43
18	P	201	CDL	C52-C53-C54-C55
18	F	705	CDL	CB7-C71-C72-C73
18	J	203	CDL	C52-C53-C54-C55
18	S	302	CDL	OA6-CA4-CA6-OA8
18	X	303	CDL	OA6-CA4-CA6-OA8
18	E	606	CDL	C12-C13-C14-C15
18	F	705	CDL	C12-C13-C14-C15
18	J	203	CDL	C57-C58-C59-C60
18	T	203	CDL	C56-C57-C58-C59
18	P	201	CDL	C57-C58-C59-C60
18	Z	203	CDL	C56-C57-C58-C59
18	F	706	CDL	C56-C57-C58-C59
20	J	201	9Y0	C6-C7-C8-C9
18	E	606	CDL	C34-C35-C36-C37
18	F	705	CDL	C34-C35-C36-C37
18	T	202	CDL	C55-C56-C57-C58
18	X	302	CDL	C55-C56-C57-C58
18	J	203	CDL	C74-C75-C76-C77
18	P	201	CDL	C74-C75-C76-C77
18	E	607	CDL	CA2-C1-CB2-OB2
18	F	706	CDL	OA9-CA7-OA8-CA6
14	Y	502	9YF	C10-C11-C12-C13
23	c	202	9XX	C1-C2-C3-C4
18	T	201	CDL	C59-C60-C61-C62
18	Z	202	CDL	C59-C60-C61-C62
18	T	202	CDL	C75-C76-C77-C78
18	X	302	CDL	C75-C76-C77-C78
20	F	704	9Y0	C6-C7-C8-C9
14	I	304	9YF	C24-C-C1-O

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Mol	Chain	Res	Type	Atoms
18	E	606	CDL	OB5-CB3-CB4-CB6
18	F	705	CDL	OB5-CB3-CB4-CB6
18	F	705	CDL	C32-C33-C34-C35
18	J	203	CDL	C73-C74-C75-C76
18	P	201	CDL	C73-C74-C75-C76
18	X	302	CDL	C38-C39-C40-C41
14	Y	503	9YF	C32-C33-C35-C36
18	E	606	CDL	C32-C33-C34-C35
18	T	202	CDL	C38-C39-C40-C41
20	J	201	9Y0	C29-C30-C31-C32
23	D	302	9XX	O6-C15-O-C16
18	T	202	CDL	CA5-C11-C12-C13
18	X	302	CDL	CA5-C11-C12-C13
18	S	302	CDL	C76-C77-C78-C79
18	X	303	CDL	C76-C77-C78-C79
14	Y	503	9YF	C27-C28-C29-C30
20	J	202	9Y0	C16-C17-C18-C19
14	Y	503	9YF	C34-C33-C35-C36
18	F	705	CDL	C71-C72-C73-C74
18	E	606	CDL	C71-C72-C73-C74
14	I	304	9YF	C18-C19-C20-C21
14	E	605	9YF	C1-C-C24-O11
14	I	304	9YF	C1-C-C24-O11
18	S	302	CDL	CB3-CB4-CB6-OB8
18	E	606	CDL	CB3-CB4-CB6-OB8
18	F	705	CDL	CB3-CB4-CB6-OB8
18	J	203	CDL	CA3-CA4-CA6-OA8
18	J	203	CDL	CB3-CB4-CB6-OB8
18	T	202	CDL	CA3-CA4-CA6-OA8
18	P	201	CDL	CA3-CA4-CA6-OA8
18	P	201	CDL	CB3-CB4-CB6-OB8
18	X	302	CDL	CA3-CA4-CA6-OA8
18	X	303	CDL	CB3-CB4-CB6-OB8
20	X	301	9Y0	O5-C-C1-C2
18	R	604	CDL	C72-C73-C74-C75
18	L	604	CDL	C72-C73-C74-C75
23	G	302	9XX	C14-C15-O-C16
18	T	203	CDL	C72-C73-C74-C75
18	Z	203	CDL	C72-C73-C74-C75
18	J	203	CDL	C76-C77-C78-C79
18	P	201	CDL	C76-C77-C78-C79
18	T	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
18	T	203	CDL	CA7-C31-C32-C33
18	Z	202	CDL	CB5-C51-C52-C53
18	Z	203	CDL	CA7-C31-C32-C33
15	F	701	MQ9	C38-C39-C41-C42
15	Z	201	MQ9	C12-C11-C9-C8
18	E	606	CDL	C72-C73-C74-C75
18	F	705	CDL	C72-C73-C74-C75
18	X	303	CDL	C34-C35-C36-C37
18	S	302	CDL	C34-C35-C36-C37
18	T	202	CDL	C72-C73-C74-C75
18	X	302	CDL	C72-C73-C74-C75
18	E	606	CDL	CB6-CB4-OB6-CB5
18	F	705	CDL	CB6-CB4-OB6-CB5
23	c	202	9XX	C28-C29-C30-C31
23	c	202	9XX	C24-C25-C26-C27
20	X	301	9Y0	C14-C15-C16-C17
14	Y	502	9YF	C25-C26-C27-C28
18	S	302	CDL	OA5-CA3-CA4-OA6
18	E	606	CDL	OA5-CA3-CA4-OA6
18	E	607	CDL	OA5-CA3-CA4-OA6
18	F	705	CDL	OA5-CA3-CA4-OA6
18	X	303	CDL	OA5-CA3-CA4-OA6
20	F	704	9Y0	O7-C1-C2-O3
18	E	607	CDL	C54-C55-C56-C57
23	c	202	9XX	C7-C8-C9-C10
18	J	203	CDL	C59-C60-C61-C62
18	X	303	CDL	C77-C78-C79-C80
18	R	604	CDL	C59-C60-C61-C62
18	S	302	CDL	C77-C78-C79-C80
18	L	604	CDL	C59-C60-C61-C62
18	J	203	CDL	C34-C35-C36-C37
18	T	202	CDL	C36-C37-C38-C39
18	P	201	CDL	C34-C35-C36-C37
18	P	201	CDL	C59-C60-C61-C62
18	X	302	CDL	C36-C37-C38-C39
18	F	706	CDL	OB6-CB4-CB6-OB8
18	T	203	CDL	OB6-CB4-CB6-OB8
18	Z	203	CDL	OB6-CB4-CB6-OB8
20	J	202	9Y0	O5-C-C1-O7
20	X	301	9Y0	O5-C-C1-O7
18	R	604	CDL	C11-C12-C13-C14
18	L	604	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	J	202	9Y0	C32-C33-C34-C35
18	X	302	CDL	C14-C15-C16-C17
14	E	605	9YF	C28-C29-C30-C31
22	G	301	PLM	C4-C5-C6-C7
18	T	202	CDL	C14-C15-C16-C17
18	T	202	CDL	C54-C55-C56-C57
18	X	302	CDL	C54-C55-C56-C57
18	J	203	CDL	C61-C62-C63-C64
18	P	201	CDL	C61-C62-C63-C64
20	X	301	9Y0	C6-C7-C8-C9
18	L	604	CDL	C39-C40-C41-C42
14	Y	503	9YF	C19-C20-C21-C22
18	R	604	CDL	C39-C40-C41-C42
14	Y	503	9YF	C40-C41-C42-C43
14	Y	503	9YF	C30-C31-C32-C33
15	O	304	MQ9	C15-C14-C16-C17
15	T	204	MQ9	C20-C19-C21-C22
15	I	303	MQ9	C15-C14-C16-C17
15	T	204	MQ9	C12-C11-C9-C8
14	I	304	9YF	C16-C17-C18-C19
18	T	201	CDL	CB4-CB3-OB5-PB2
18	T	202	CDL	C1-CB2-OB2-PB2
18	X	302	CDL	C1-CB2-OB2-PB2
18	Z	202	CDL	CB4-CB3-OB5-PB2
18	R	604	CDL	C54-C55-C56-C57
18	L	604	CDL	C54-C55-C56-C57
20	J	202	9Y0	C26-C27-C28-C29
20	X	301	9Y0	C18-C19-C20-C37
18	Z	202	CDL	C33-C34-C35-C36
18	E	607	CDL	C39-C40-C41-C42
18	F	706	CDL	C58-C59-C60-C61
18	T	201	CDL	C33-C34-C35-C36
20	S	301	9Y0	C6-C7-C8-C9
20	X	301	9Y0	C27-C28-C29-C30
14	Y	502	9YF	C12-C13-C14-C15
18	X	302	CDL	C76-C77-C78-C79
18	R	604	CDL	C78-C79-C80-C81
18	S	302	CDL	C39-C40-C41-C42
18	L	604	CDL	C78-C79-C80-C81
18	X	303	CDL	C39-C40-C41-C42
18	E	607	CDL	OA5-CA3-CA4-CA6
18	T	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
18	X	302	CDL	OB5-CB3-CB4-CB6
18	R	604	CDL	C60-C61-C62-C63
18	L	604	CDL	C60-C61-C62-C63
18	T	202	CDL	C76-C77-C78-C79
23	c	202	9XX	O1-C18-C19-C20
23	G	302	9XX	C26-C27-C28-C29
18	E	606	CDL	C78-C79-C80-C81
18	F	705	CDL	C78-C79-C80-C81
18	T	201	CDL	C36-C37-C38-C39
18	Z	202	CDL	C36-C37-C38-C39
18	T	203	CDL	C38-C39-C40-C41
18	Z	203	CDL	C38-C39-C40-C41
15	T	204	MQ9	C12-C11-C9-C10
15	Z	201	MQ9	C12-C11-C9-C10
18	R	604	CDL	C72-C71-CB7-OB8
18	L	604	CDL	C72-C71-CB7-OB8
23	c	202	9XX	O-C16-C17-C37
18	R	604	CDL	C77-C78-C79-C80
18	L	604	CDL	C77-C78-C79-C80
14	E	605	9YF	C20-C21-C22-C23
14	O	303	9YF	C11-C12-C13-C14
14	O	303	9YF	C19-C20-C21-C22
14	I	304	9YF	C29-C30-C31-C32
14	O	303	9YF	C1-C-C24-O11
15	F	701	MQ9	C39-C41-C42-C43
17	R	602	HEA	C15-C16-C17-C18
18	S	302	CDL	CA3-CA4-CA6-OA8
18	X	303	CDL	CA3-CA4-CA6-OA8
20	S	301	9Y0	O5-C-C1-C2
20	J	202	9Y0	O5-C-C1-C2
18	F	705	CDL	C53-C54-C55-C56
18	E	607	CDL	CA5-C11-C12-C13
18	T	202	CDL	CA7-C31-C32-C33
18	X	302	CDL	CA7-C31-C32-C33
18	F	705	CDL	C76-C77-C78-C79
18	S	302	CDL	C59-C60-C61-C62
18	E	606	CDL	C53-C54-C55-C56
18	X	303	CDL	C59-C60-C61-C62
18	E	606	CDL	C76-C77-C78-C79
14	Y	502	9YF	C19-C20-C21-C22
18	R	604	CDL	CB5-C51-C52-C53
18	L	604	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
14	O	303	9YF	O9-C-C1-O
18	R	604	CDL	OA5-CA3-CA4-OA6
18	F	706	CDL	OA5-CA3-CA4-OA6
18	L	604	CDL	OA5-CA3-CA4-OA6
20	S	301	9Y0	C14-C15-C16-C17
18	S	302	CDL	C61-C62-C63-C64
18	X	303	CDL	C61-C62-C63-C64
14	O	303	9YF	C17-C18-C19-C20
18	T	201	CDL	CB7-C71-C72-C73
18	Z	202	CDL	CB7-C71-C72-C73
14	I	304	9YF	O9-C-C24-O11
18	E	607	CDL	OB6-CB4-CB6-OB8
20	S	301	9Y0	O5-C-C1-O7
18	E	606	CDL	C31-C32-C33-C34
18	F	705	CDL	C31-C32-C33-C34
20	X	301	9Y0	C29-C30-C31-C32
18	R	604	CDL	C73-C74-C75-C76
18	L	604	CDL	C73-C74-C75-C76
14	O	303	9YF	C33-C35-C36-C37
15	T	204	MQ9	C18-C19-C21-C22
15	I	303	MQ9	C13-C14-C16-C17
22	c	201	PLM	CA-CB-CC-CD
18	R	604	CDL	C51-C52-C53-C54
18	L	604	CDL	C51-C52-C53-C54
23	G	302	9XX	O6-C15-O-C16
18	E	606	CDL	C61-C62-C63-C64
18	F	705	CDL	C61-C62-C63-C64
18	F	706	CDL	C61-C62-C63-C64
14	Y	502	9YF	C18-C19-C20-C21
15	O	304	MQ9	C13-C14-C16-C17
20	S	301	9Y0	C29-C30-C31-C32
18	E	607	CDL	C57-C58-C59-C60
20	S	301	9Y0	C27-C28-C29-C30
18	T	201	CDL	CB2-C1-CA2-OA2
18	Z	202	CDL	CB2-C1-CA2-OA2
18	P	201	CDL	C36-C37-C38-C39
14	O	303	9YF	C24-C-C1-O
18	J	203	CDL	C36-C37-C38-C39
18	R	604	CDL	C12-C13-C14-C15
18	S	302	CDL	C71-C72-C73-C74
18	L	604	CDL	C12-C13-C14-C15
18	X	303	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
18	F	706	CDL	C52-C51-CB5-OB6
18	T	203	CDL	C54-C55-C56-C57
18	P	201	CDL	C12-C13-C14-C15
18	Z	203	CDL	C54-C55-C56-C57
15	Z	201	MQ9	C20-C19-C21-C22
18	J	203	CDL	C12-C13-C14-C15
22	D	301	PLM	C4-C5-C6-C7
18	T	202	CDL	OB5-CB3-CB4-OB6
18	X	302	CDL	OB5-CB3-CB4-OB6
18	F	706	CDL	C39-C40-C41-C42
18	R	604	CDL	CB3-CB4-CB6-OB8
18	F	706	CDL	CB3-CB4-CB6-OB8
18	L	604	CDL	CB3-CB4-CB6-OB8
18	T	201	CDL	CA3-CA4-CA6-OA8
18	T	201	CDL	CB3-CB4-CB6-OB8
18	Z	202	CDL	CA3-CA4-CA6-OA8
18	Z	202	CDL	CB3-CB4-CB6-OB8
21	E	602	HEM	C4B-C3B-CAB-CBB
20	J	201	9Y0	C19-C20-C37-C38
14	I	304	9YF	C33-C35-C36-C37
14	O	303	9YF	O9-C-C24-O11
14	E	605	9YF	O9-C-C24-O11
18	E	606	CDL	OB6-CB4-CB6-OB8
18	F	705	CDL	OB6-CB4-CB6-OB8
18	T	203	CDL	C78-C79-C80-C81
18	Z	203	CDL	C78-C79-C80-C81
18	X	302	CDL	C73-C74-C75-C76
14	O	303	9YF	C16-C17-C18-C19
18	T	202	CDL	C73-C74-C75-C76
20	J	201	9Y0	C5-C6-C7-C8
14	O	303	9YF	C29-C30-C31-C32
23	c	202	9XX	C19-C20-C21-C22
23	G	302	9XX	C5-C6-C7-C8
14	E	605	9YF	C2-O2-P-O8
18	F	706	CDL	O1-C1-CB2-OB2
18	S	302	CDL	C33-C34-C35-C36
18	X	303	CDL	C33-C34-C35-C36
18	E	607	CDL	C51-C52-C53-C54
23	D	302	9XX	C17-C16-O-C15
18	S	302	CDL	OA5-CA3-CA4-CA6
18	E	606	CDL	OA5-CA3-CA4-CA6
18	F	705	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
18	X	303	CDL	OA5-CA3-CA4-CA6
14	O	303	9YF	C32-C33-C35-C36
23	D	302	9XX	C26-C27-C28-C29
14	Y	503	9YF	C15-C16-C17-C18
20	J	202	9Y0	C30-C31-C32-C33
23	c	202	9XX	C6-C7-C8-C9
18	T	202	CDL	CB4-CB3-OB5-PB2
18	X	302	CDL	CB4-CB3-OB5-PB2
18	E	607	CDL	C77-C78-C79-C80
18	E	607	CDL	C59-C60-C61-C62
18	E	606	CDL	OB5-CB3-CB4-OB6
18	F	705	CDL	OB5-CB3-CB4-OB6
23	D	302	9XX	C20-C21-C22-C23
18	R	604	CDL	OB6-CB4-CB6-OB8
18	S	302	CDL	OB6-CB4-CB6-OB8
18	E	606	CDL	OA6-CA4-CA6-OA8
18	F	705	CDL	OA6-CA4-CA6-OA8
18	L	604	CDL	OB6-CB4-CB6-OB8
18	J	203	CDL	OA6-CA4-CA6-OA8
18	P	201	CDL	OA6-CA4-CA6-OA8
18	X	303	CDL	OB6-CB4-CB6-OB8
18	T	202	CDL	C33-C34-C35-C36
18	X	302	CDL	C33-C34-C35-C36
22	G	301	PLM	C7-C8-C9-CA
18	E	607	CDL	C61-C62-C63-C64
14	O	303	9YF	C1-O-P-O1
14	E	605	9YF	C1-O-P-O2
14	I	304	9YF	C1-O-P-O1
14	Y	503	9YF	C1-O-P-O8
18	R	604	CDL	CB2-OB2-PB2-OB5
18	S	302	CDL	CA3-OA5-PA1-OA4
18	E	606	CDL	CB3-OB5-PB2-OB4
18	E	607	CDL	CA2-OA2-PA1-OA3
18	F	705	CDL	CB3-OB5-PB2-OB4
18	F	706	CDL	CB2-OB2-PB2-OB4
18	L	604	CDL	CB2-OB2-PB2-OB5
18	T	201	CDL	CA2-OA2-PA1-OA3
18	T	201	CDL	CB2-OB2-PB2-OB3
18	T	202	CDL	CB2-OB2-PB2-OB3
18	T	202	CDL	CB2-OB2-PB2-OB4
18	T	202	CDL	CB2-OB2-PB2-OB5
18	T	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	T	203	CDL	CA3-OA5-PA1-OA2
18	T	203	CDL	CA3-OA5-PA1-OA3
18	T	203	CDL	CA3-OA5-PA1-OA4
18	X	302	CDL	CB2-OB2-PB2-OB3
18	X	302	CDL	CB2-OB2-PB2-OB4
18	X	302	CDL	CB2-OB2-PB2-OB5
18	X	302	CDL	CB3-OB5-PB2-OB3
18	X	303	CDL	CA3-OA5-PA1-OA4
18	Z	202	CDL	CA2-OA2-PA1-OA3
18	Z	202	CDL	CB2-OB2-PB2-OB3
18	Z	203	CDL	CA3-OA5-PA1-OA2
18	Z	203	CDL	CA3-OA5-PA1-OA3
18	Z	203	CDL	CA3-OA5-PA1-OA4
20	J	202	9Y0	C2-O3-P-O
15	Z	201	MQ9	C18-C19-C21-C22
18	R	604	CDL	C1-CA2-OA2-PA1
18	S	302	CDL	C1-CA2-OA2-PA1
18	S	302	CDL	C1-CB2-OB2-PB2
18	E	607	CDL	C1-CA2-OA2-PA1
18	E	607	CDL	C1-CB2-OB2-PB2
18	F	706	CDL	C1-CA2-OA2-PA1
18	L	604	CDL	C1-CA2-OA2-PA1
18	T	203	CDL	C1-CA2-OA2-PA1
18	X	303	CDL	C1-CA2-OA2-PA1
18	X	303	CDL	C1-CB2-OB2-PB2
18	Z	203	CDL	C1-CA2-OA2-PA1
20	F	704	9Y0	C30-C31-C32-C33
22	c	201	PLM	CC-CD-CE-CF
17	L	602	HEA	C12-C11-C3B-C4B
18	F	706	CDL	C73-C74-C75-C76
18	E	606	CDL	C60-C61-C62-C63
18	F	705	CDL	C60-C61-C62-C63
20	S	301	9Y0	C22-C23-C24-C25
20	S	301	9Y0	C13-C14-C15-C16
18	T	202	CDL	C35-C36-C37-C38
18	X	302	CDL	C35-C36-C37-C38
18	R	604	CDL	OA5-CA3-CA4-CA6
18	L	604	CDL	OA5-CA3-CA4-CA6
20	F	704	9Y0	C-C1-C2-O3
23	G	302	9XX	C36-C27-C28-C29
20	J	202	9Y0	C11-C12-C13-C14
20	X	301	9Y0	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
14	I	304	9YF	O9-C-C1-O
14	Y	502	9YF	O9-C-C1-O
14	Y	502	9YF	C26-C27-C28-C29
18	F	706	CDL	C1-CB2-OB2-PB2
22	D	301	PLM	C7-C8-C9-CA
15	F	707	MQ9	C35-C34-C36-C37
18	L	604	CDL	C71-C72-C73-C74
15	I	303	MQ9	C29-C31-C32-C33
18	R	604	CDL	C71-C72-C73-C74
20	F	704	9Y0	C19-C20-C37-C38
18	F	706	CDL	C54-C55-C56-C57
23	G	302	9XX	C20-C21-C22-C23
14	Y	502	9YF	C16-C17-C18-C19
18	F	706	CDL	C38-C39-C40-C41
15	F	707	MQ9	C40-C39-C41-C42
18	X	302	CDL	C53-C54-C55-C56
18	T	202	CDL	C53-C54-C55-C56
23	D	302	9XX	C36-C27-C28-C29
18	P	201	CDL	C37-C38-C39-C40
18	J	203	CDL	C37-C38-C39-C40
20	J	202	9Y0	C14-C15-C16-C17
18	J	203	CDL	C12-C11-CA5-OA6
18	P	201	CDL	C12-C11-CA5-OA6
18	T	201	CDL	OB5-CB3-CB4-OB6
18	Z	202	CDL	OB5-CB3-CB4-OB6
20	X	301	9Y0	C22-C23-C24-C25
14	O	303	9YF	C14-C15-C16-C17
18	Z	203	CDL	C57-C58-C59-C60
20	J	201	9Y0	C7-C8-C9-C10
18	T	203	CDL	C57-C58-C59-C60
14	O	303	9YF	C36-C37-C38-C39
15	F	707	MQ9	C33-C34-C36-C37
20	S	301	9Y0	C5-C6-C7-C8
18	S	302	CDL	C57-C58-C59-C60
18	J	203	CDL	C38-C39-C40-C41
18	P	201	CDL	C38-C39-C40-C41
18	X	303	CDL	C57-C58-C59-C60
14	Y	502	9YF	C35-C36-C37-C38
14	Y	502	9YF	C-C1-O-P
13	O	301	HEC	CAA-CBA-CGA-O1A
14	I	304	9YF	C27-C28-C29-C30
18	X	302	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	T	202	CDL	C13-C14-C15-C16
14	Y	503	9YF	C36-C37-C38-C39
15	O	304	MQ9	C29-C31-C32-C33
18	R	604	CDL	C33-C34-C35-C36
18	F	706	CDL	C77-C78-C79-C80
18	L	604	CDL	C33-C34-C35-C36
13	O	302	HEC	CAA-CBA-CGA-O2A
17	R	602	HEA	CAA-CBA-CGA-O1A
15	F	707	MQ9	C38-C39-C41-C42
17	L	602	HEA	CAD-CBD-CGD-O1D
17	L	603	HEA	CAA-CBA-CGA-O1A
20	J	201	9Y0	O7-C1-C2-O3
18	E	606	CDL	CB5-C51-C52-C53
18	F	705	CDL	CB5-C51-C52-C53
13	O	301	HEC	CAA-CBA-CGA-O2A
17	R	602	HEA	CAD-CBD-CGD-O1D
23	c	202	9XX	O2-C18-C19-C20
14	I	304	9YF	C15-C16-C17-C18
15	E	604	MQ9	C40-C39-C41-C42
18	T	202	CDL	OA5-CA3-CA4-CA6
18	X	302	CDL	OA5-CA3-CA4-CA6
20	F	704	9Y0	C7-C8-C9-C10
13	O	302	HEC	CAA-CBA-CGA-O1A
17	R	602	HEA	CAA-CBA-CGA-O2A
17	L	602	HEA	CAA-CBA-CGA-O1A
18	P	201	CDL	C11-C12-C13-C14
18	J	203	CDL	C11-C12-C13-C14
14	Y	502	9YF	C37-C38-C39-C40
18	F	705	CDL	C11-C12-C13-C14
18	E	606	CDL	C11-C12-C13-C14
20	S	301	9Y0	C7-C8-C9-C10
17	R	603	HEA	CAA-CBA-CGA-O1A
15	F	701	MQ9	C15-C14-C16-C17
15	Z	201	MQ9	C30-C29-C31-C32
22	D	301	PLM	C2-C3-C4-C5
22	c	201	PLM	C7-C8-C9-CA
14	E	605	9YF	C39-C40-C41-C42
18	T	203	CDL	C14-C15-C16-C17
18	Z	203	CDL	C14-C15-C16-C17
18	X	303	CDL	C55-C56-C57-C58
18	S	302	CDL	C55-C56-C57-C58
20	J	202	9Y0	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	c	201	PLM	C8-C9-CA-CB
17	L	602	HEA	CAD-CBD-CGD-O2D
15	E	604	MQ9	C35-C34-C36-C37
17	R	602	HEA	CAD-CBD-CGD-O2D
17	L	602	HEA	CAA-CBA-CGA-O2A
14	O	303	9YF	C13-C14-C15-C16
17	L	603	HEA	CAA-CBA-CGA-O2A
18	F	706	CDL	CB7-C71-C72-C73
15	I	303	MQ9	C9-C11-C12-C13
18	E	607	CDL	CB3-CB4-CB6-OB8
17	R	603	HEA	CAA-CBA-CGA-O2A
18	T	202	CDL	OA5-CA3-CA4-OA6
18	X	302	CDL	OA5-CA3-CA4-OA6
15	F	707	MQ9	C30-C29-C31-C32
15	T	204	MQ9	C30-C29-C31-C32
18	R	604	CDL	C72-C71-CB7-OB9
18	L	604	CDL	C72-C71-CB7-OB9
14	Y	503	9YF	O11-C25-C26-C27
18	X	302	CDL	C56-C57-C58-C59
20	F	704	9Y0	C11-C12-C13-C14
18	F	706	CDL	C60-C61-C62-C63
18	T	202	CDL	C56-C57-C58-C59
18	T	203	CDL	C13-C14-C15-C16
18	Z	203	CDL	C13-C14-C15-C16
21	F	702	HEM	CAD-CBD-CGD-O2D
18	F	706	CDL	OA5-CA3-CA4-CA6
15	O	304	MQ9	C12-C11-C9-C10
15	T	204	MQ9	C28-C29-C31-C32
15	Z	201	MQ9	C28-C29-C31-C32
18	R	604	CDL	CB4-CB3-OB5-PB2
18	E	606	CDL	C1-CA2-OA2-PA1
18	F	705	CDL	C1-CA2-OA2-PA1
18	L	604	CDL	CB4-CB3-OB5-PB2
18	J	203	CDL	CA4-CA3-OA5-PA1
18	P	201	CDL	CA4-CA3-OA5-PA1
18	Z	202	CDL	C78-C79-C80-C81
20	J	201	9Y0	C24-C25-C26-C27
18	T	201	CDL	C78-C79-C80-C81
14	O	303	9YF	C34-C33-C35-C36
18	J	203	CDL	C14-C15-C16-C17
18	P	201	CDL	C14-C15-C16-C17
20	S	301	9Y0	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	F	706	CDL	C33-C34-C35-C36
15	E	604	MQ9	C20-C19-C21-C22
18	E	607	CDL	C72-C73-C74-C75
18	T	201	CDL	C32-C33-C34-C35
18	Z	202	CDL	C32-C33-C34-C35
15	I	303	MQ9	C12-C11-C9-C10
20	J	202	9Y0	O7-C1-C2-O3
15	F	707	MQ9	C24-C26-C27-C28
15	F	707	MQ9	C20-C19-C21-C22
15	T	204	MQ9	C15-C14-C16-C17
21	F	702	HEM	CAD-CBD-CGD-O1D
14	I	304	9YF	C36-C37-C38-C39
14	O	303	9YF	O11-C25-C26-C27
20	J	201	9Y0	C11-C12-C13-C14
20	J	202	9Y0	C13-C14-C15-C16
20	J	202	9Y0	C23-C24-C25-C26
15	O	304	MQ9	C9-C11-C12-C13
15	E	604	MQ9	C24-C26-C27-C28
18	T	203	CDL	C58-C59-C60-C61
18	Z	203	CDL	C58-C59-C60-C61
18	X	302	CDL	O1-C1-CB2-OB2
18	E	607	CDL	OA9-CA7-OA8-CA6
14	I	304	9YF	O11-C25-C26-C27
18	T	203	CDL	C71-C72-C73-C74
18	Z	203	CDL	C71-C72-C73-C74
18	S	302	CDL	C12-C11-CA5-OA6
18	X	303	CDL	C12-C11-CA5-OA6
15	E	603	MQ9	C15-C14-C16-C17
18	T	201	CDL	C74-C75-C76-C77
18	Z	202	CDL	C74-C75-C76-C77
15	T	204	MQ9	C31-C32-C33-C34
21	E	601	HEM	CAA-CBA-CGA-O2A
18	T	202	CDL	O1-C1-CB2-OB2
20	F	704	9Y0	C31-C32-C33-C34
15	E	604	MQ9	C12-C11-C9-C10
21	E	601	HEM	CAA-CBA-CGA-O1A
21	F	702	HEM	CAA-CBA-CGA-O1A
14	Y	502	9YF	O9-C8-C9-C10
18	J	203	CDL	C32-C31-CA7-OA8
18	P	201	CDL	C32-C31-CA7-OA8
20	J	202	9Y0	C18-C19-C20-C37
23	c	202	9XX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	T	202	CDL	CA2-C1-CB2-OB2
18	X	302	CDL	CA2-C1-CB2-OB2
14	Y	502	9YF	C40-C41-C42-C43
23	c	202	9XX	C26-C27-C28-C29
18	T	202	CDL	CB3-CB4-OB6-CB5
18	T	202	CDL	CB6-CB4-OB6-CB5
18	X	302	CDL	CB3-CB4-OB6-CB5
18	X	302	CDL	CB6-CB4-OB6-CB5
18	E	607	CDL	C31-CA7-OA8-CA6
18	L	604	CDL	C57-C58-C59-C60
14	I	304	9YF	O12-C25-C26-C27
18	R	604	CDL	C57-C58-C59-C60
15	F	707	MQ9	C12-C11-C9-C10
18	S	302	CDL	C12-C11-CA5-OA7
18	X	303	CDL	C12-C11-CA5-OA7
18	T	203	CDL	CB4-CB6-OB8-CB7
18	J	203	CDL	C32-C31-CA7-OA9
18	P	201	CDL	C32-C31-CA7-OA9
18	J	203	CDL	C52-C51-CB5-OB6
18	P	201	CDL	C52-C51-CB5-OB6
20	X	301	9Y0	C32-C33-C34-C35
18	Z	203	CDL	CB4-CB6-OB8-CB7
20	J	202	9Y0	O5-C5-C6-C7
21	F	702	HEM	CAA-CBA-CGA-O2A
18	E	607	CDL	C36-C37-C38-C39
14	O	303	9YF	O12-C25-C26-C27
15	E	604	MQ9	C11-C12-C13-C14
15	I	303	MQ9	C31-C32-C33-C34
20	J	202	9Y0	C1-C2-O3-P
15	E	604	MQ9	C33-C34-C36-C37
17	L	602	HEA	O11-C11-C3B-C4B
20	S	301	9Y0	O7-C21-C22-C23
14	Y	502	9YF	O10-C8-C9-C10
18	F	706	CDL	O1-C1-CA2-OA2
14	Y	502	9YF	C17-C18-C19-C20
23	D	302	9XX	C11-C12-C13-C14
14	O	303	9YF	O9-C8-C9-C10
20	J	201	9Y0	C11-C10-C9-C8
14	O	303	9YF	O10-C8-C9-C10
20	J	202	9Y0	O4-C5-C6-C7
23	G	302	9XX	C12-C13-C14-C15
18	E	607	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
20	X	301	9Y0	O7-C21-C22-C23
18	J	203	CDL	C52-C51-CB5-OB7
18	P	201	CDL	C52-C51-CB5-OB7

There are no ring outliers.

35 monomers are involved in 458 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	707	MQ9	4	0
18	R	604	CDL	17	0
21	E	601	HEM	2	0
21	E	602	HEM	2	0
15	T	204	MQ9	2	0
18	E	606	CDL	10	0
18	F	705	CDL	11	0
21	F	703	HEM	4	0
18	S	302	CDL	49	0
18	T	203	CDL	34	0
19	Y	501	FES	1	0
13	O	302	HEC	40	0
13	I	301	HEC	5	0
13	O	301	HEC	4	0
13	I	302	HEC	12	0
17	R	603	HEA	4	0
17	R	602	HEA	1	0
18	T	202	CDL	29	0
15	E	604	MQ9	4	0
18	X	303	CDL	54	0
18	L	604	CDL	24	0
18	J	203	CDL	12	0
18	Z	203	CDL	42	0
18	P	201	CDL	10	0
17	L	602	HEA	3	0
18	X	302	CDL	41	0
18	Z	202	CDL	36	0
15	E	603	MQ9	2	0
15	Z	201	MQ9	4	0
18	T	201	CDL	36	0
18	F	706	CDL	12	0
21	F	702	HEM	1	0
17	L	603	HEA	3	0
18	E	607	CDL	4	0

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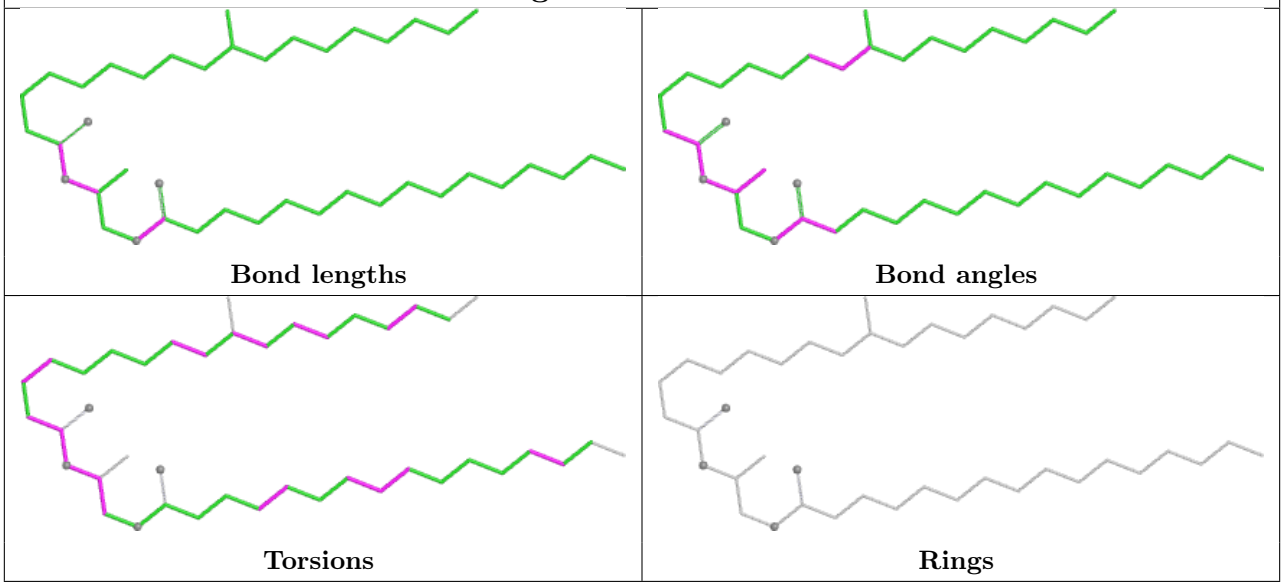
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	304	MQ9	2	0

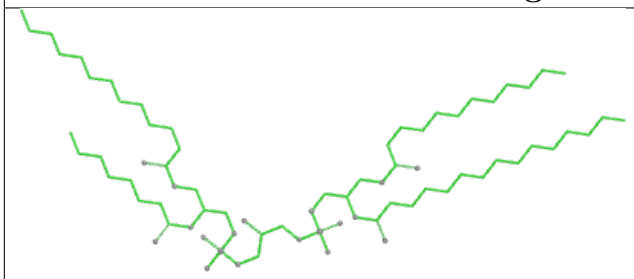
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 9XX c 202

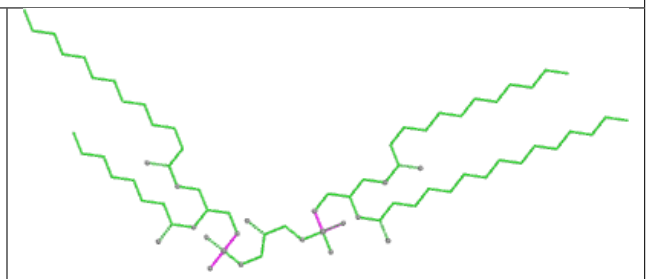


Ligand MQ9 F 707

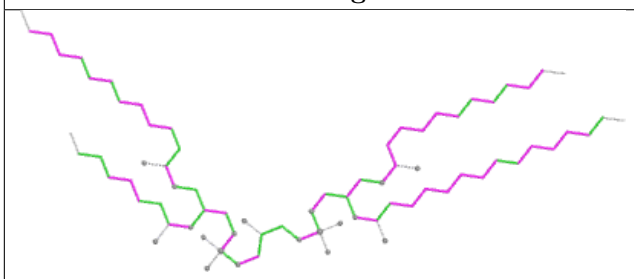
Ligand CDL R 604



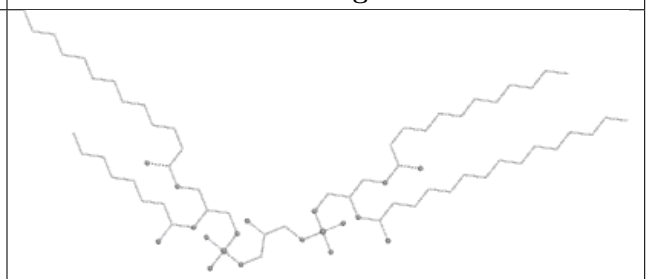
Bond lengths



Bond angles

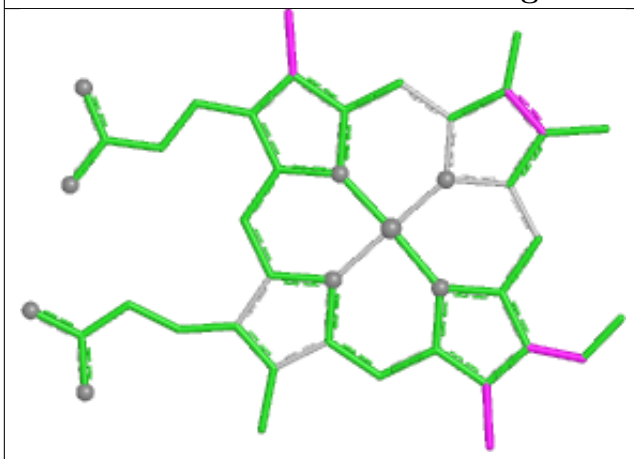


Torsions

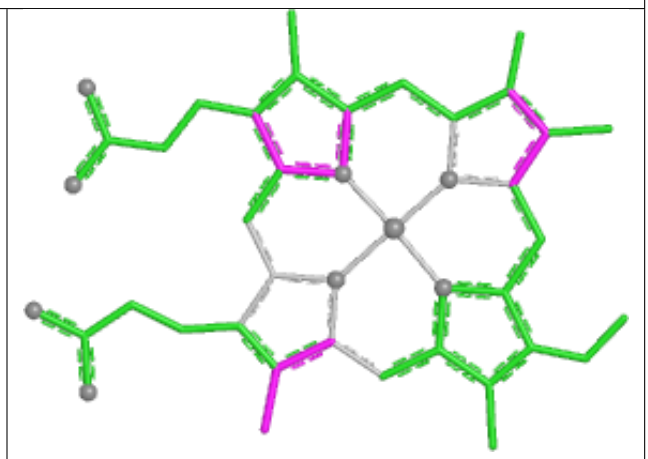


Rings

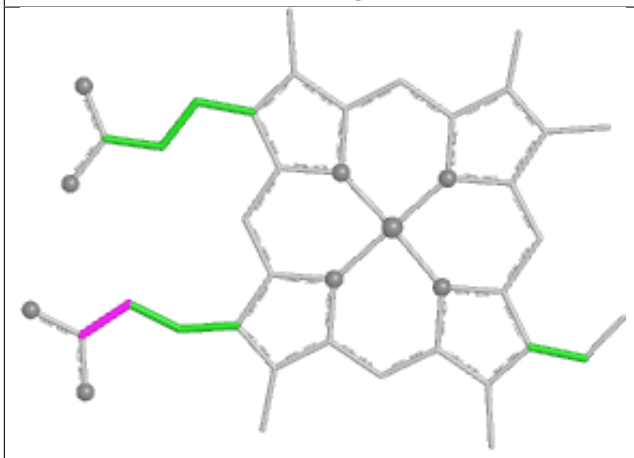
Ligand HEM E 601



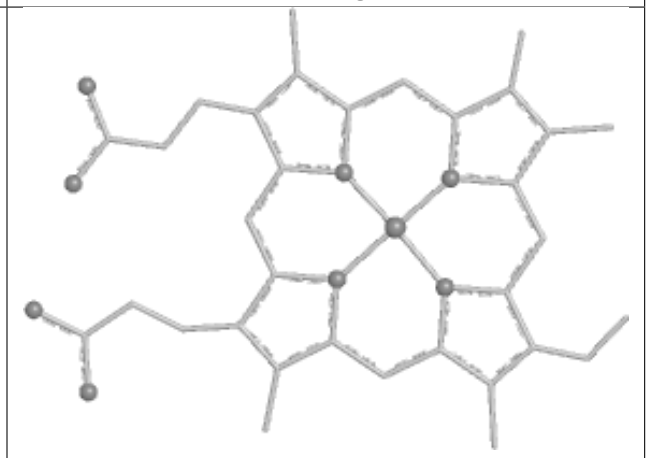
Bond lengths



Bond angles



Torsions



Rings

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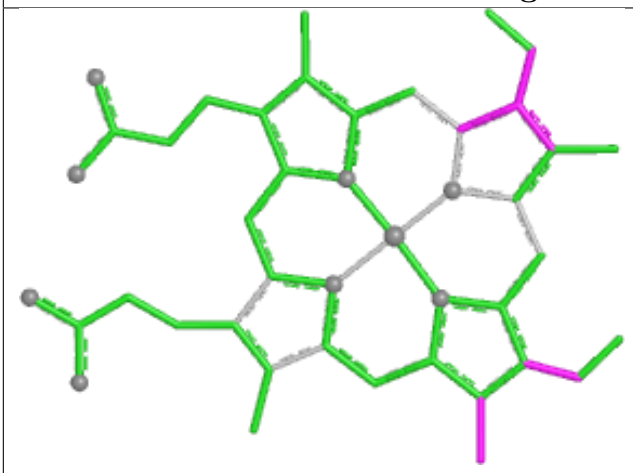
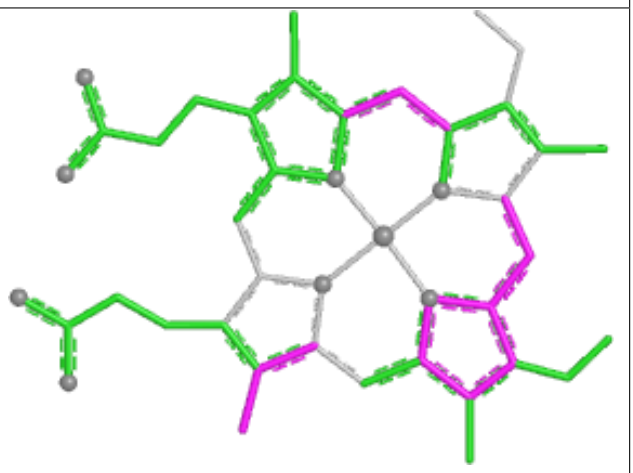
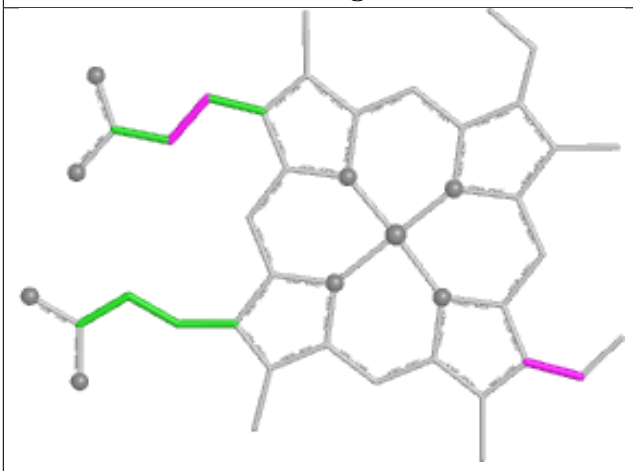


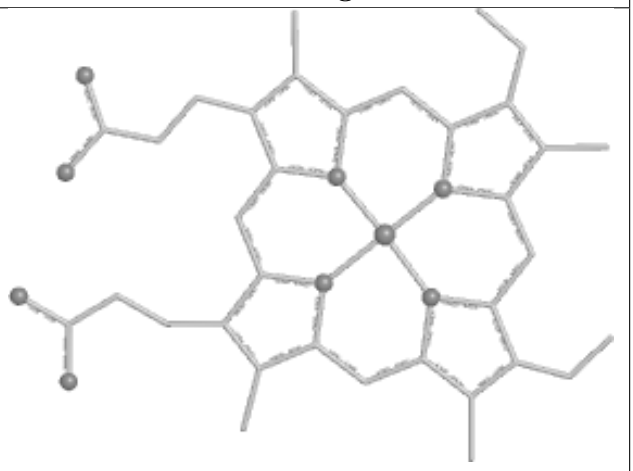
Bond lengths



Bond angles

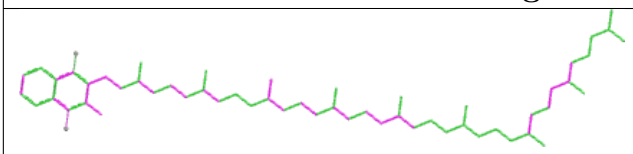


Torsions

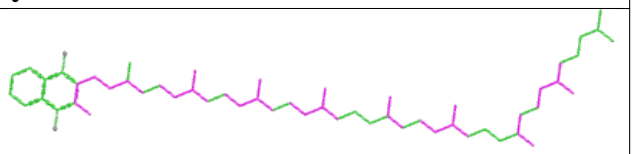


Rings

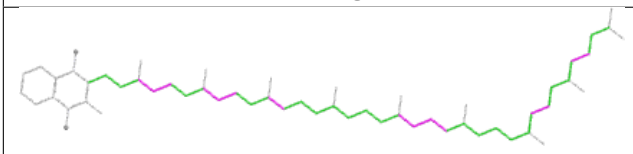
Ligand MQ9 T 204



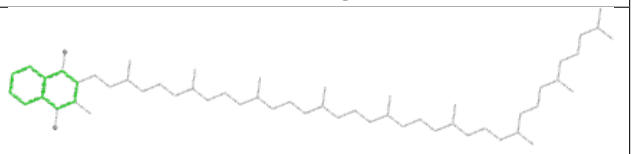
Bond lengths



Bond angles

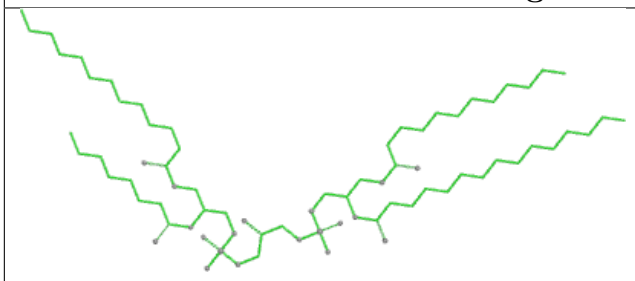


Torsions

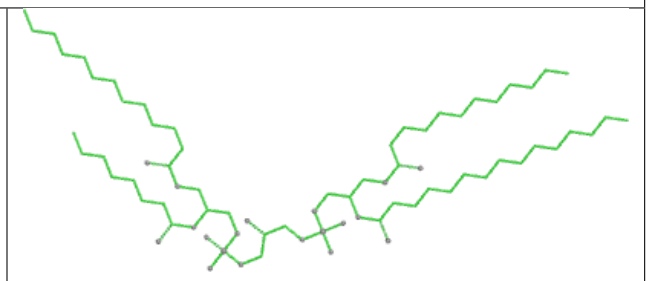


Rings

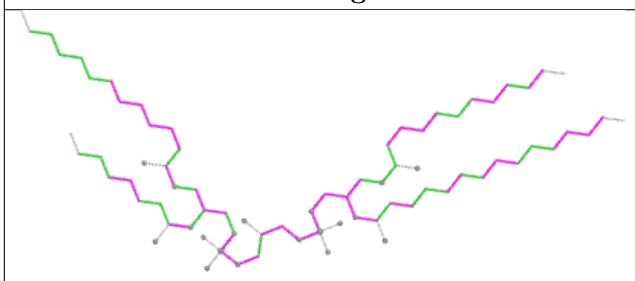
Ligand CDL E 606



Bond lengths



Bond angles



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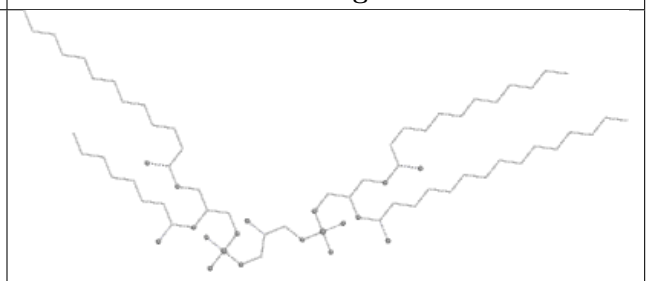
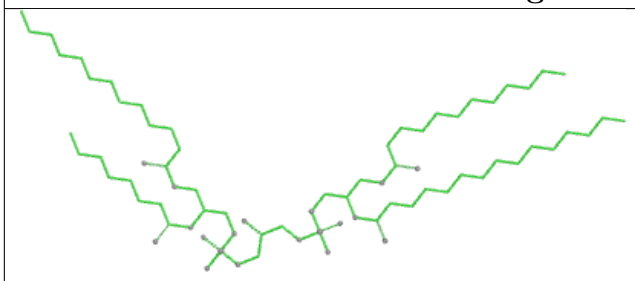
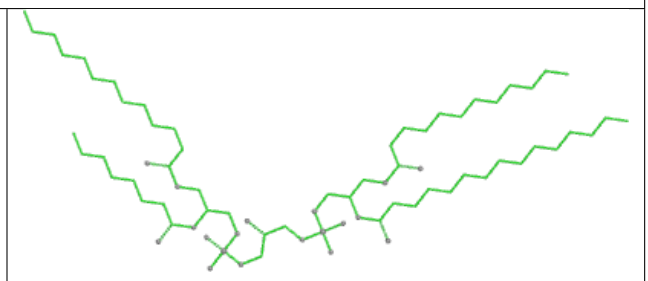


Rings

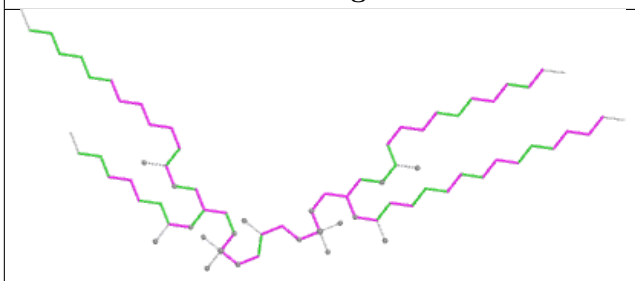
Ligand CDL F 705



Bond lengths



Bond angles



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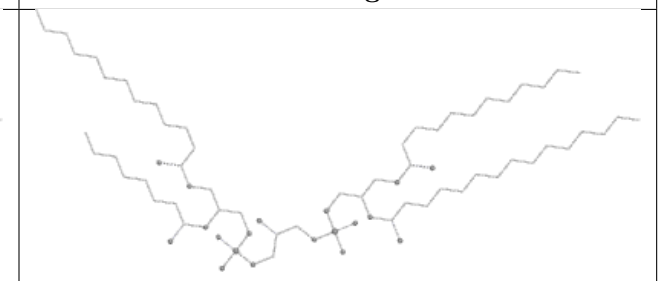
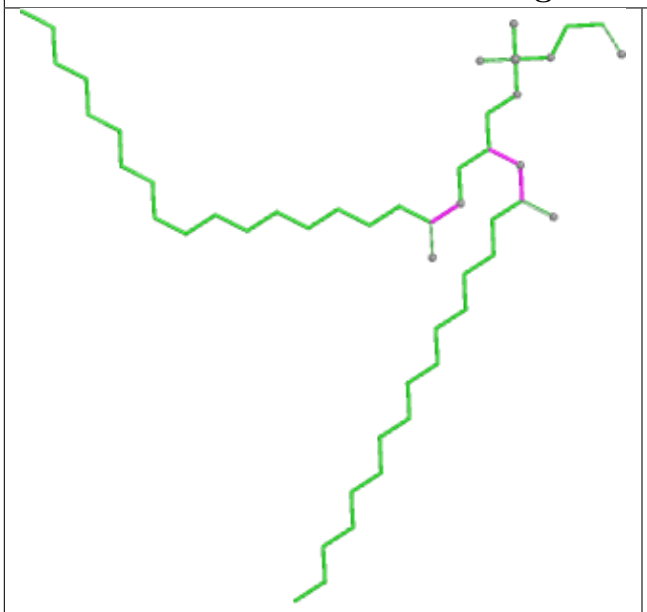


Rings

Ligand 9Y0 J 202



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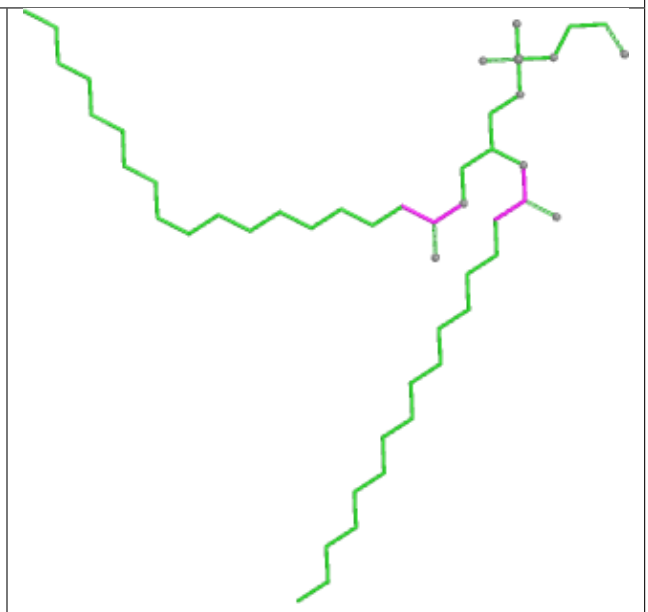
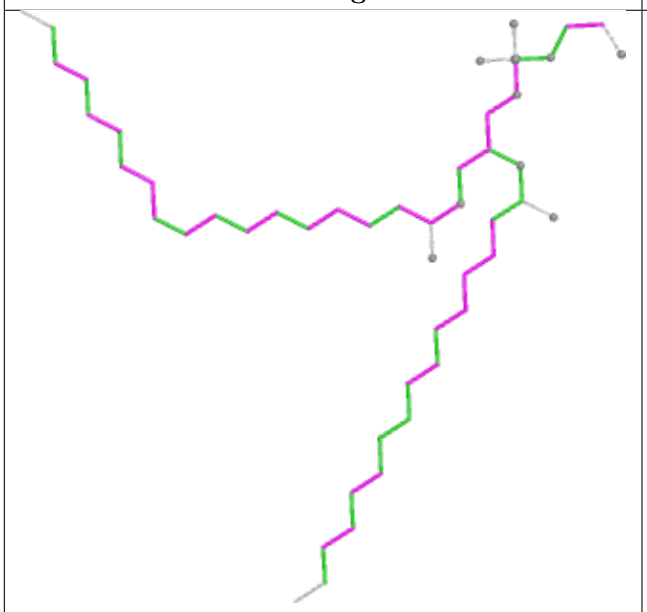


Bond angles



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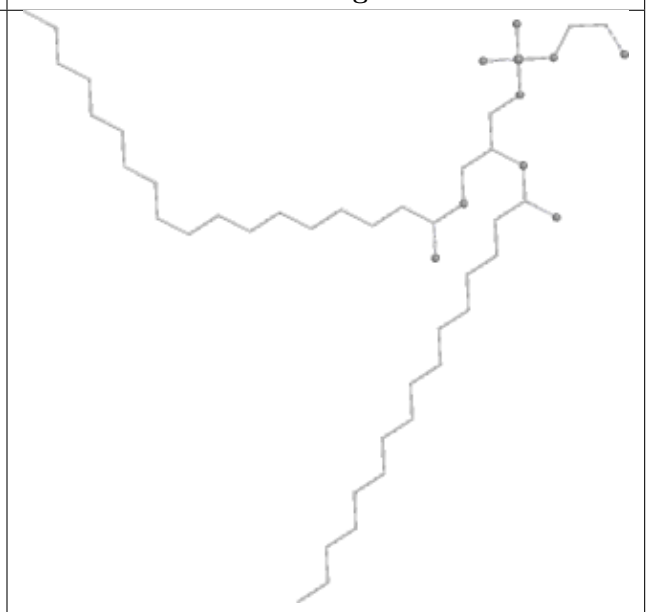
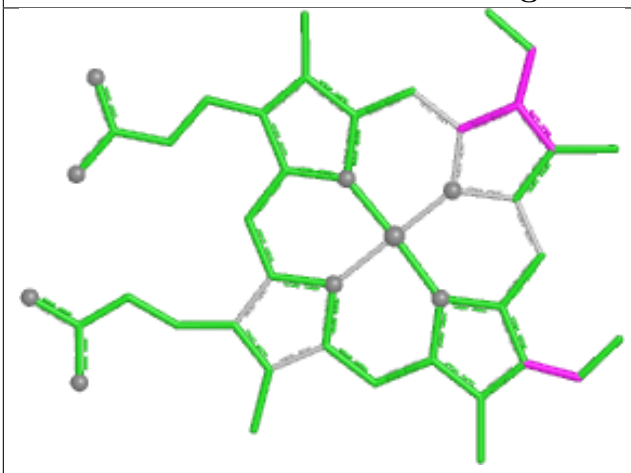


Rings

Ligand HEM F 703



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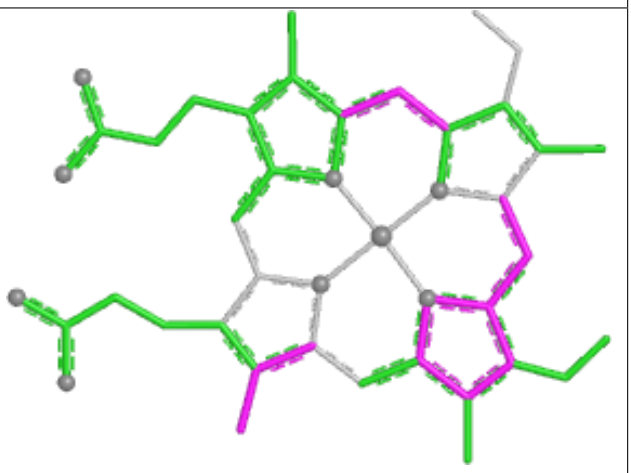
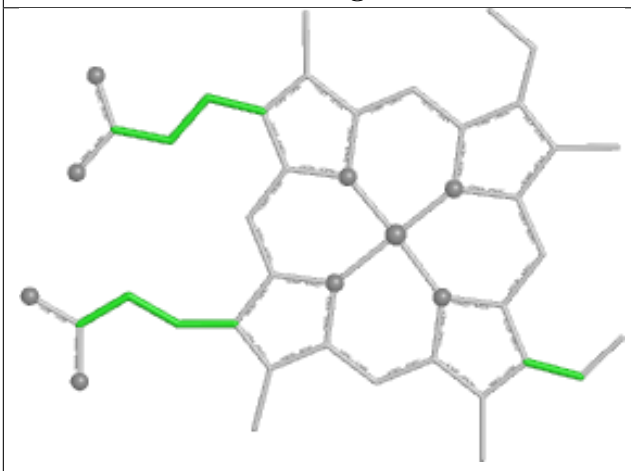
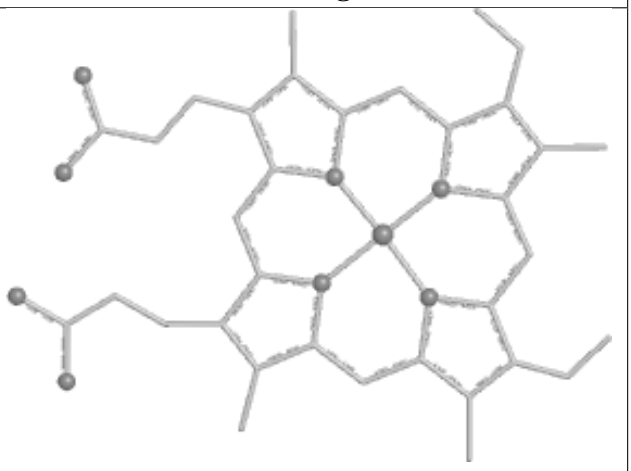


Bond angles

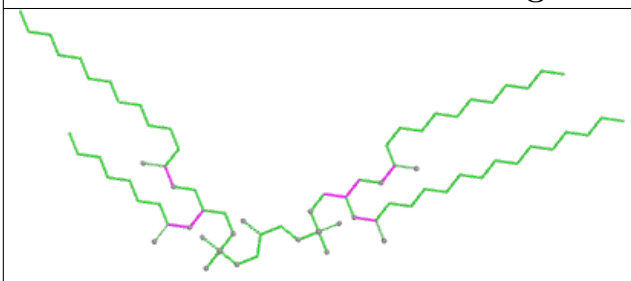


Torsions

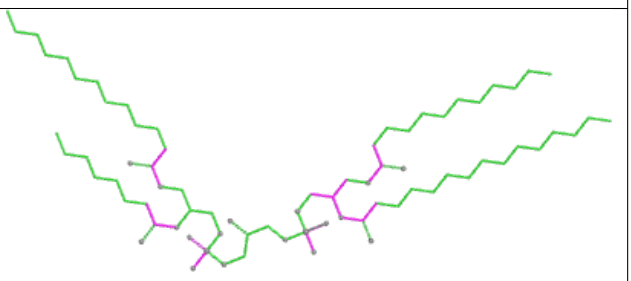


Rings

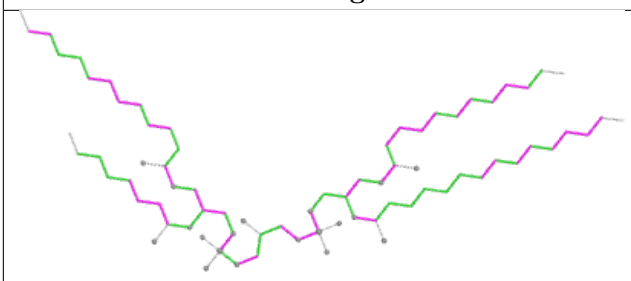
Ligand CDL S 302



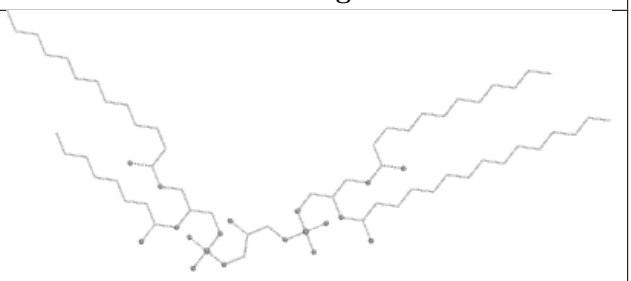
Bond lengths



Bond angles

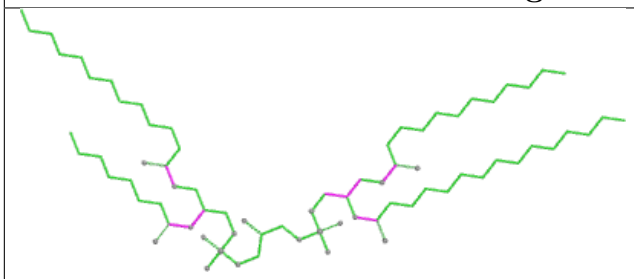


Torsions

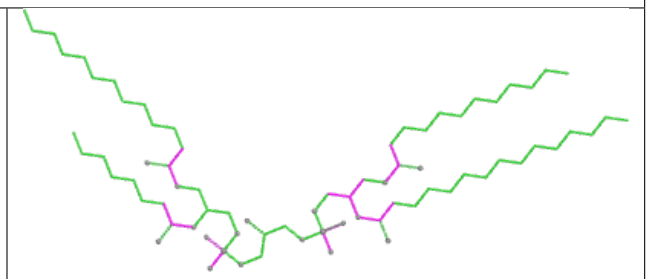


Rings

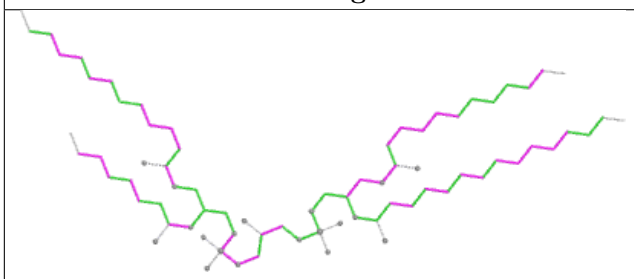
Ligand CDL T 203



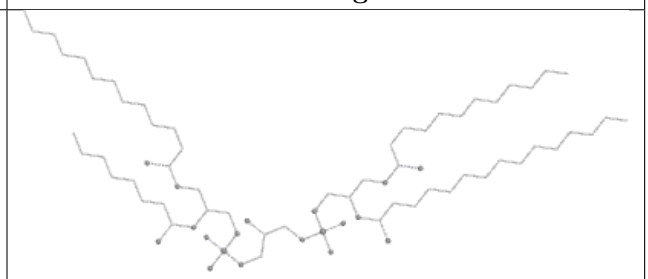
Bond lengths



Bond angles

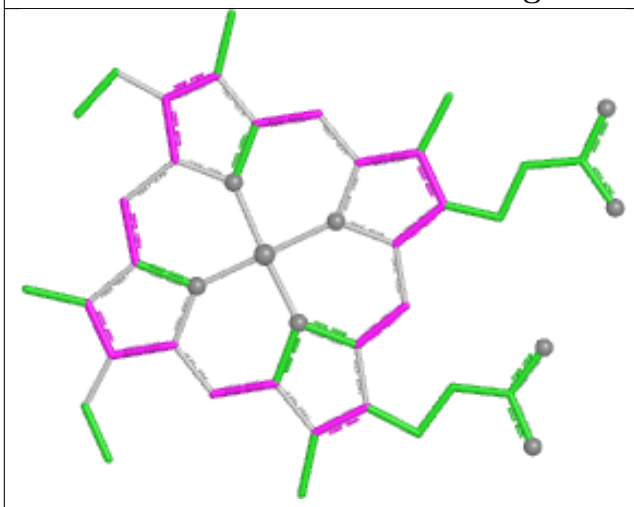


Torsions

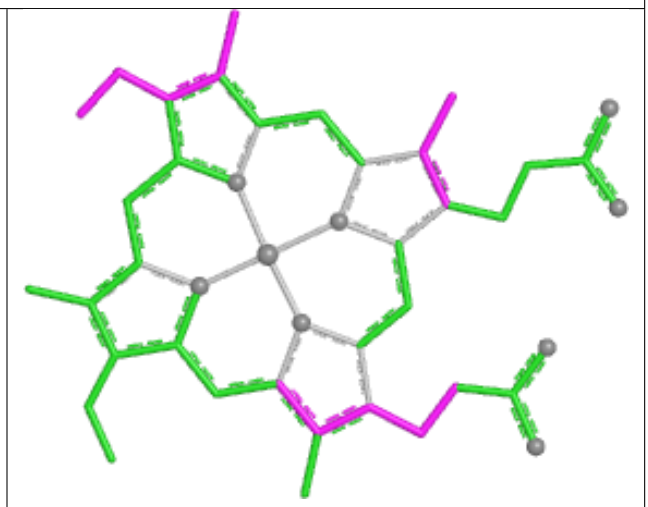


Rings

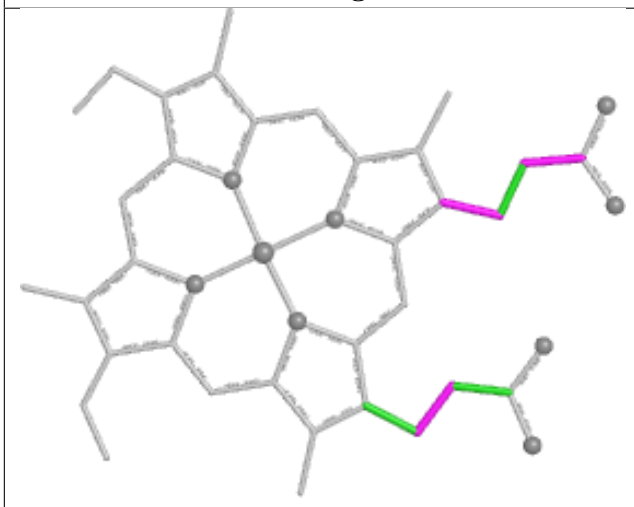
Ligand HEC O 302



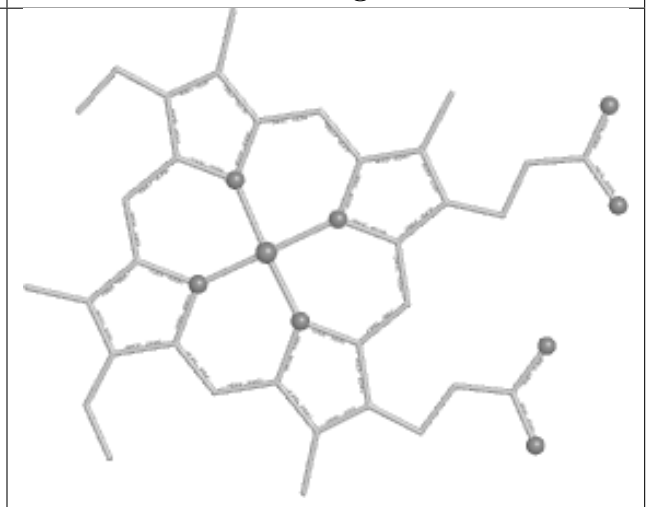
Bond lengths



Bond angles

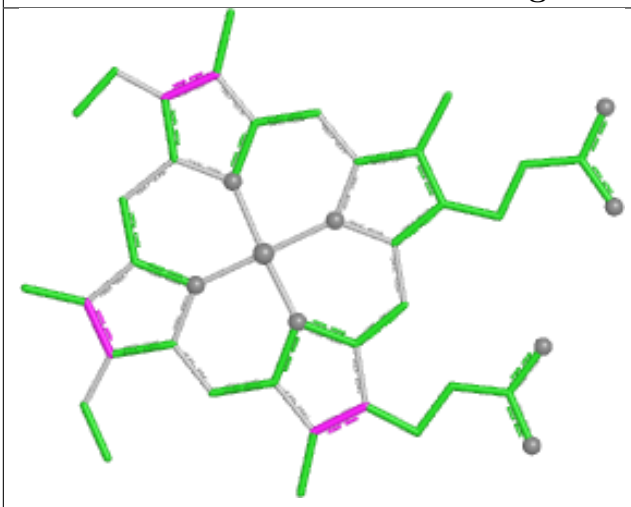


Torsions



Rings

Ligand HEC I 301



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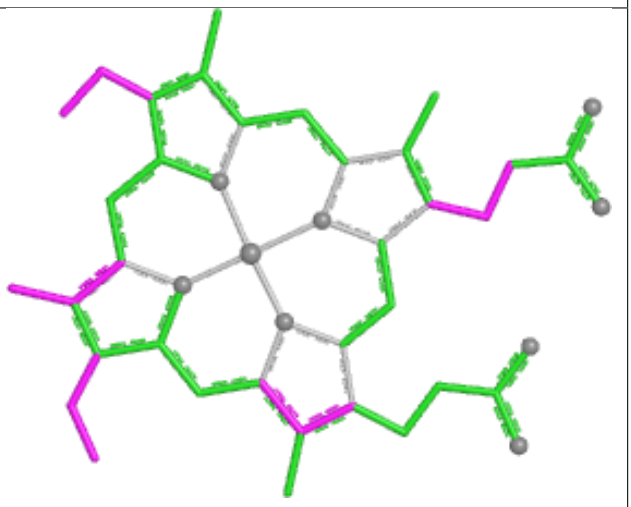
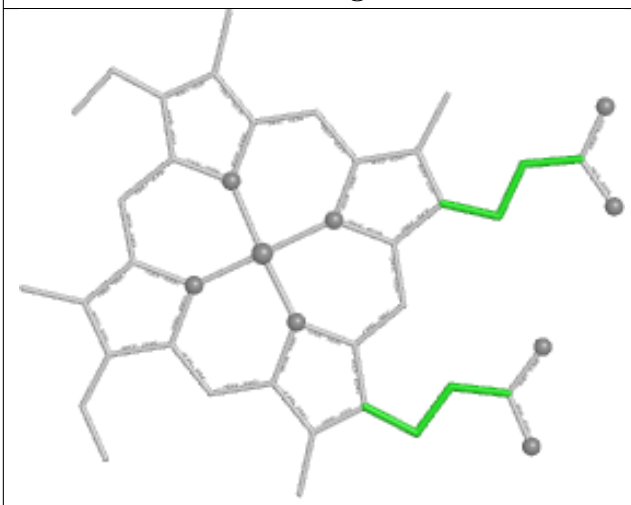
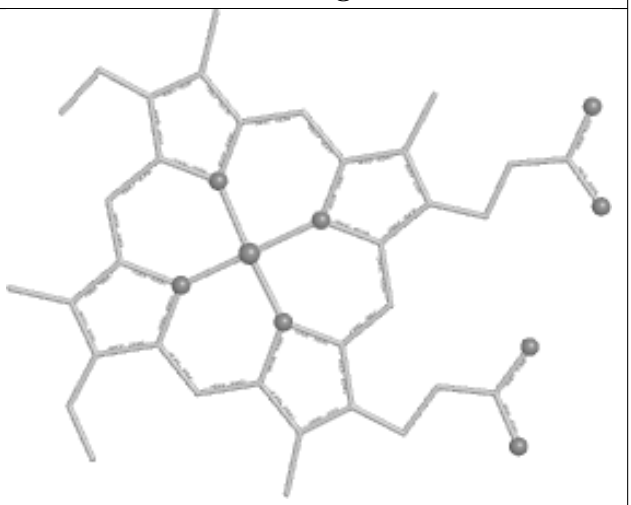


Bond angles

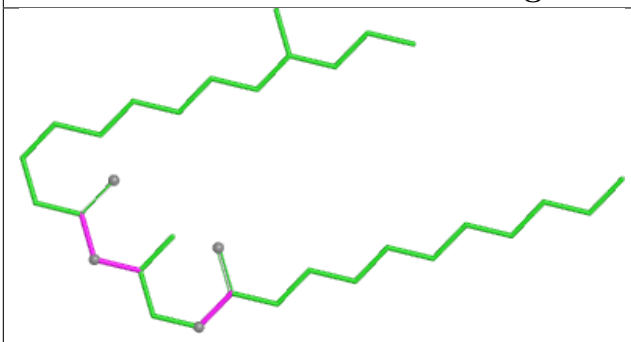


Torsions



Rings

Ligand 9XX G 302



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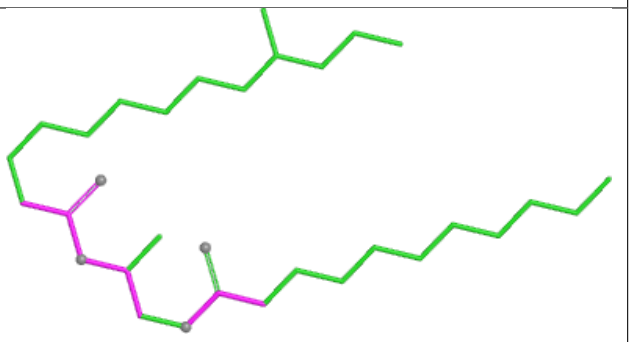
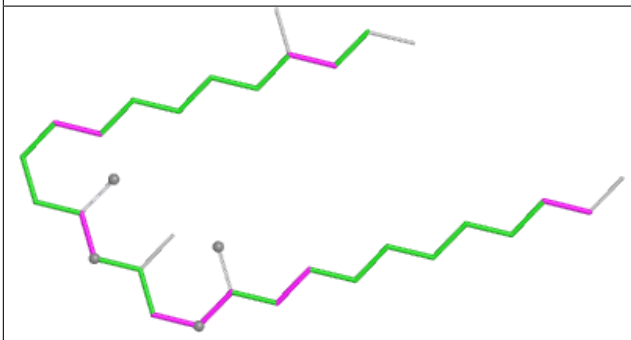


Bond angles



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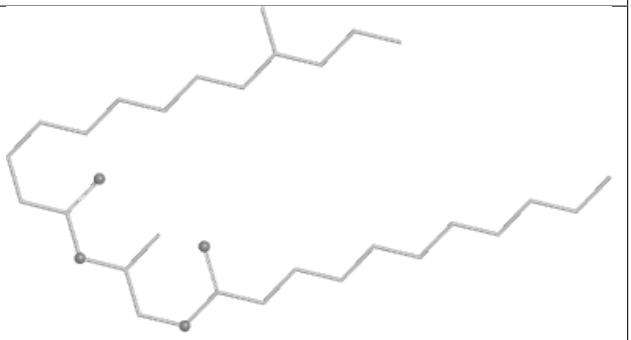
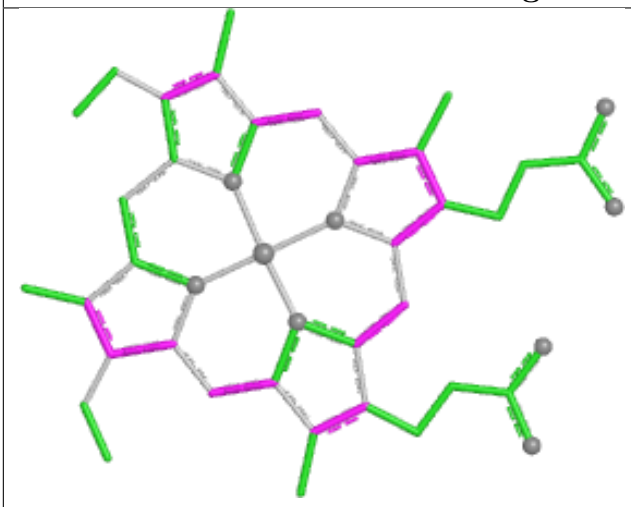
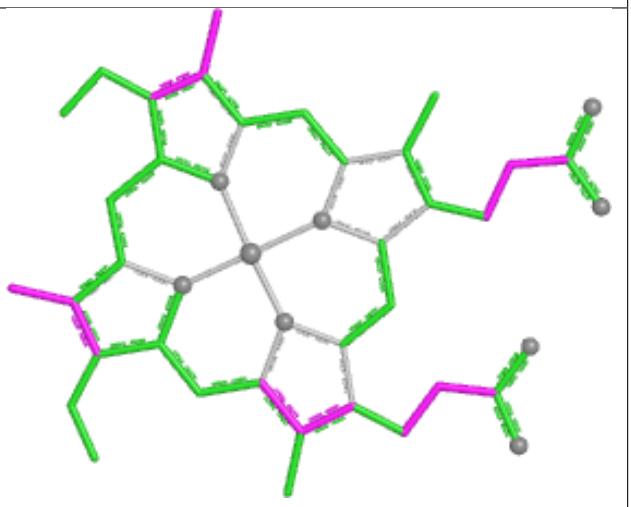


Rings

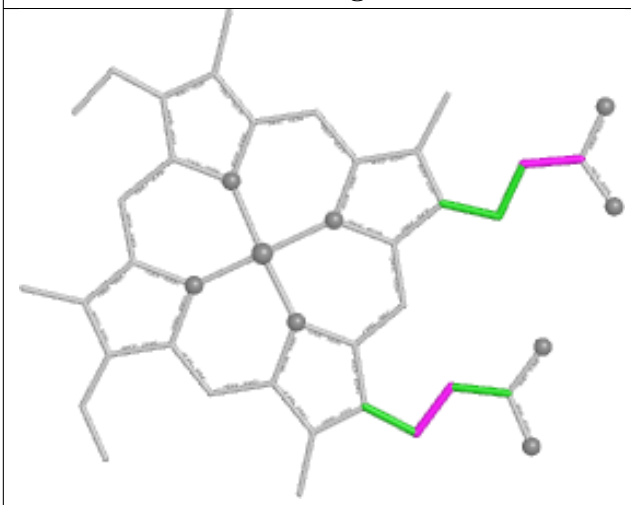
Ligand HEC O 301



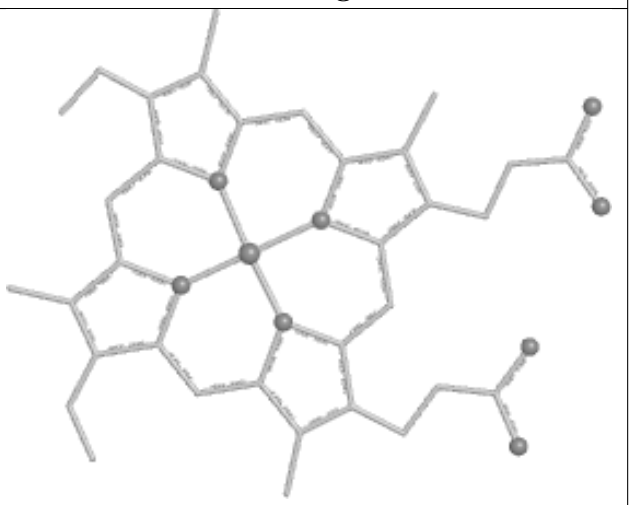
Bond lengths



Bond angles

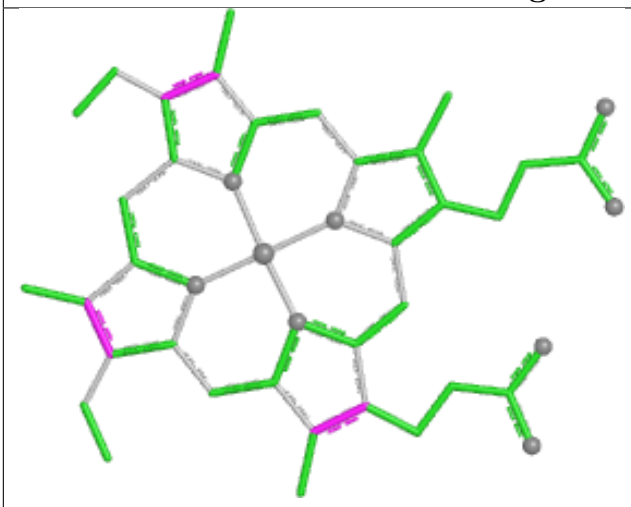


Torsions

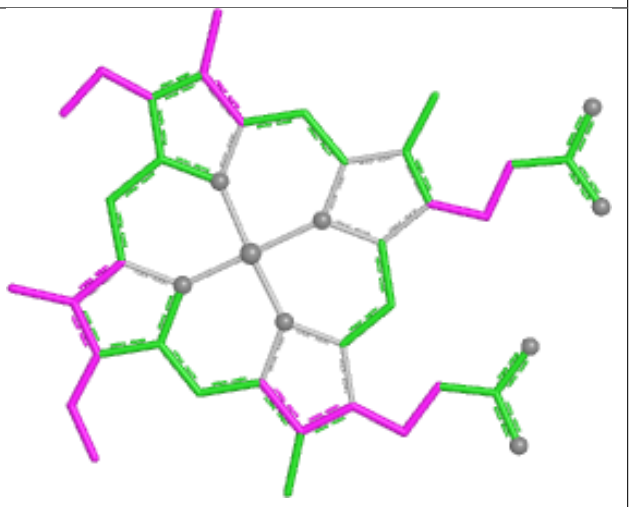


Rings

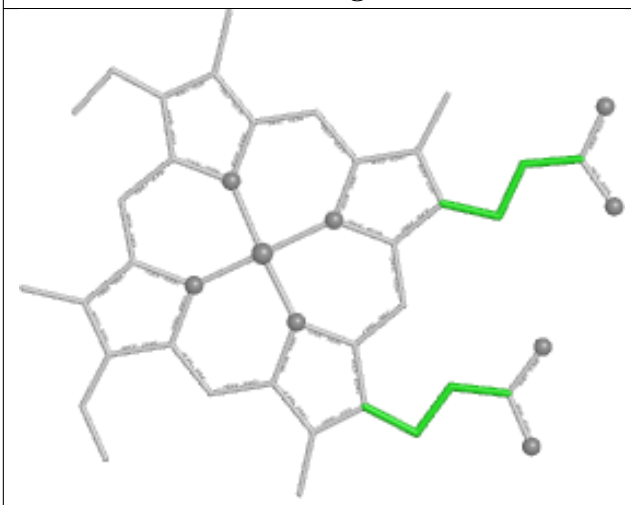
Ligand HEC I 302



Bond lengths



Bond angles



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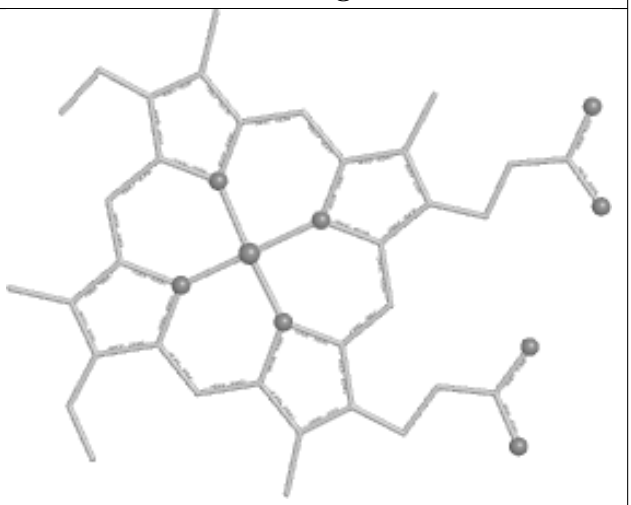
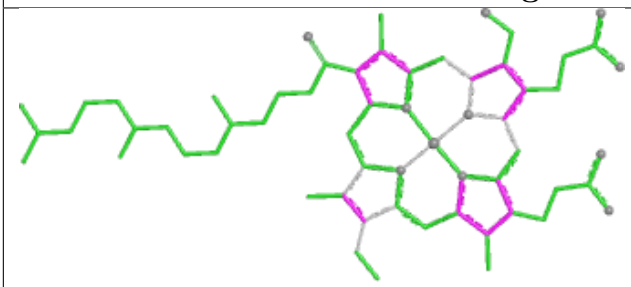
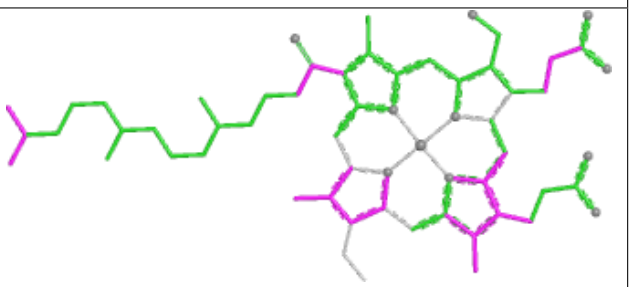


Rings

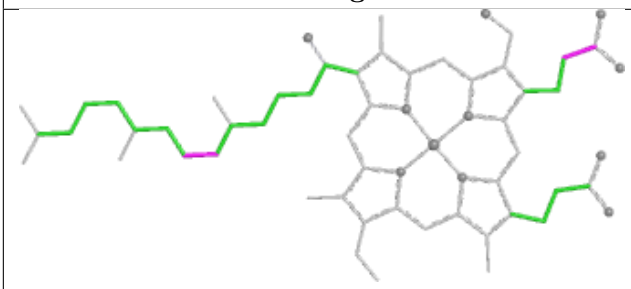
Ligand HEA R 603



Bond lengths



Bond angles



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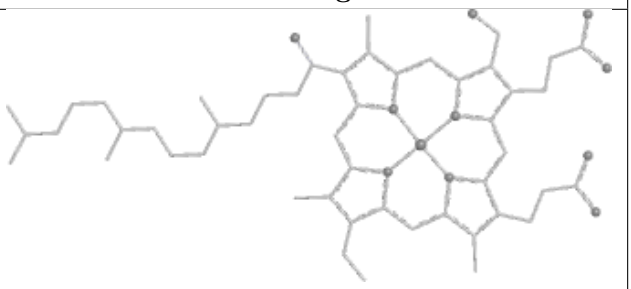
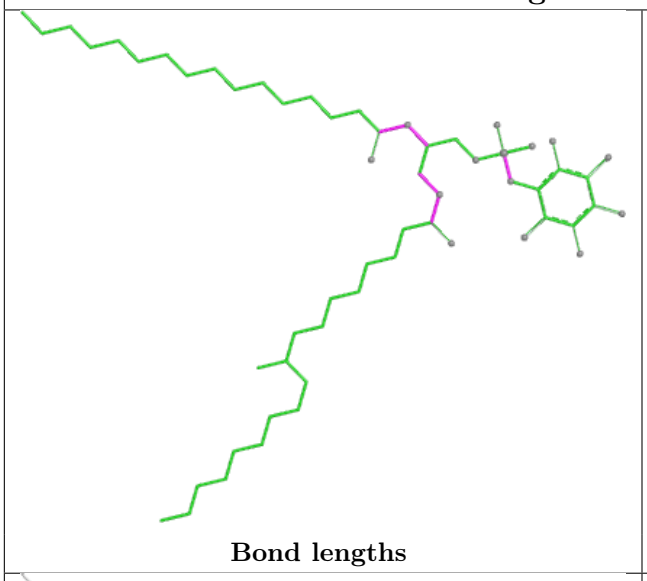


Rings

Ligand 9YF O 303



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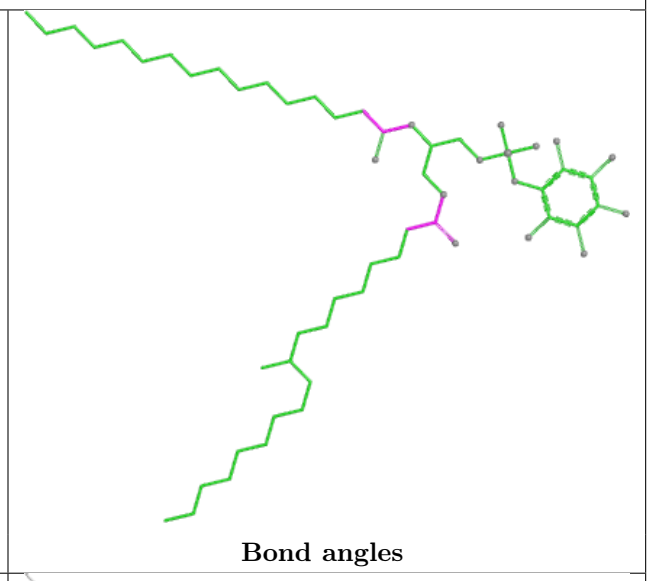
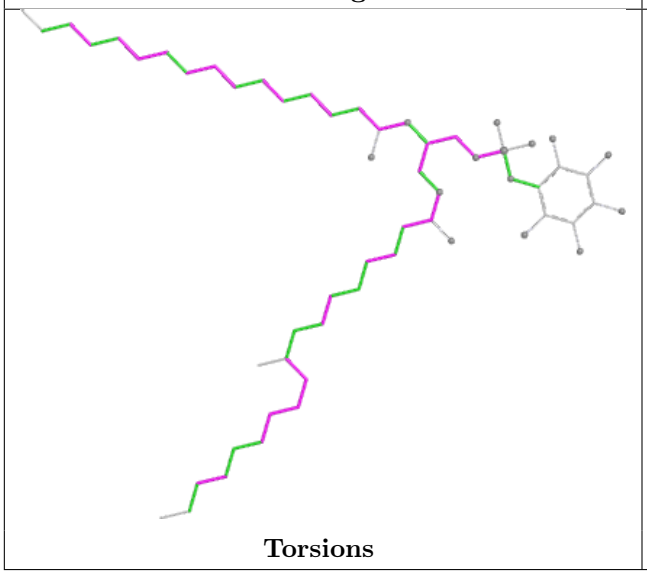
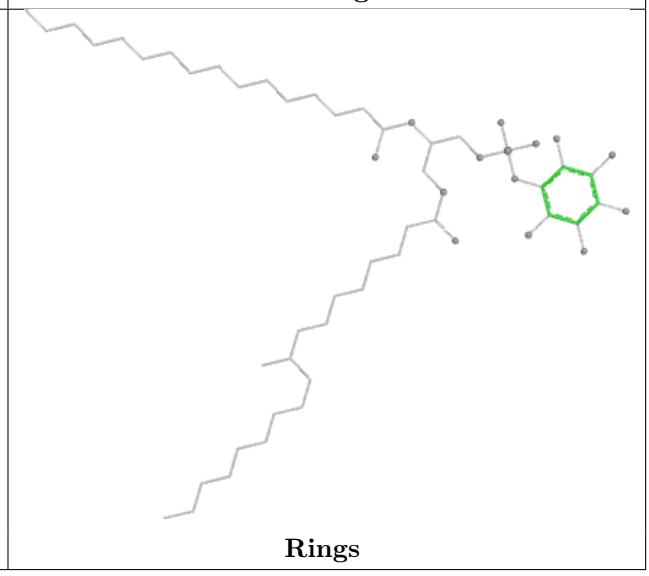


Bond angles

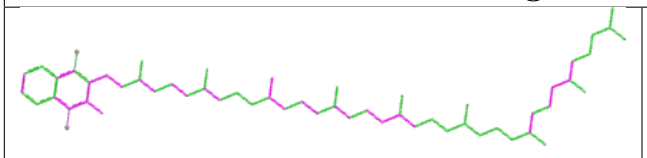


Torsions

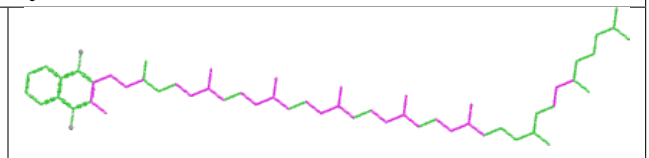


Rings

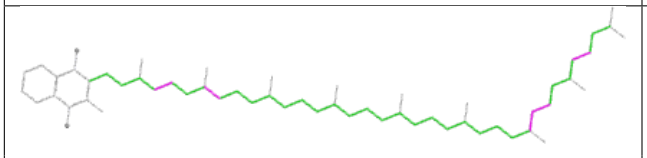
Ligand MQ9 F 701



Bond lengths



Bond angles



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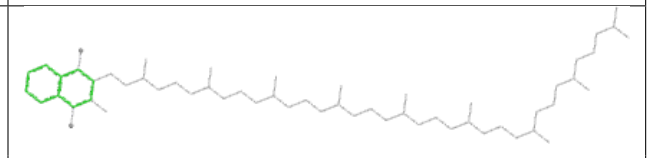
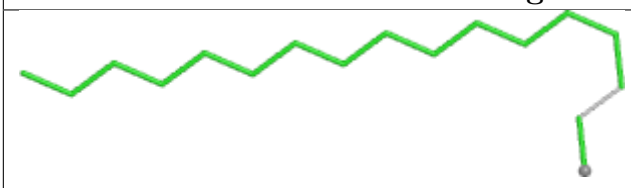
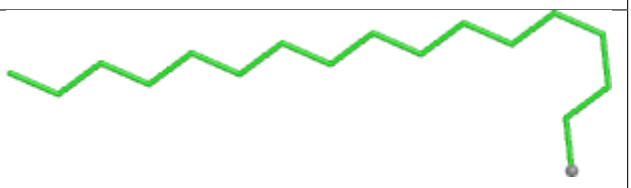


Rings

Ligand PLM c 201

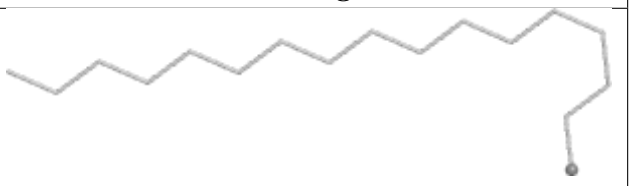


Bond lengths



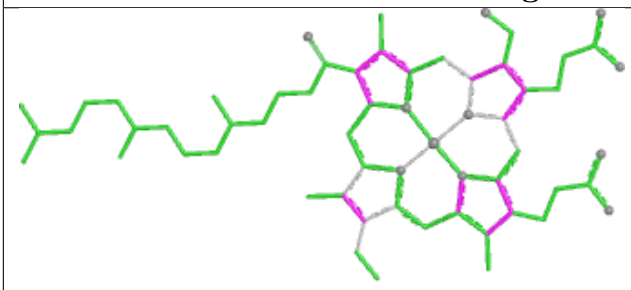
Bond angles

Torsions

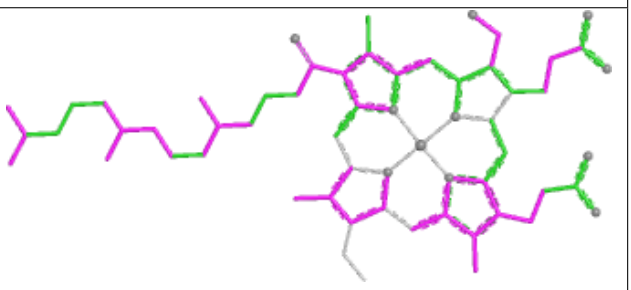


Rings

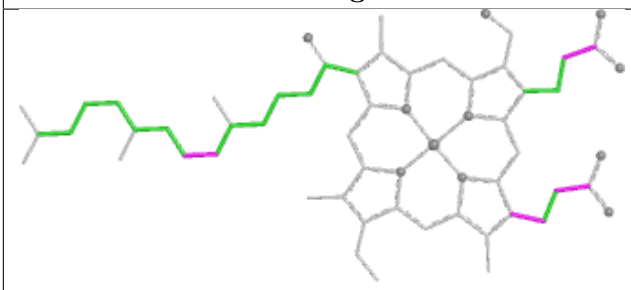
Ligand HEA R 602



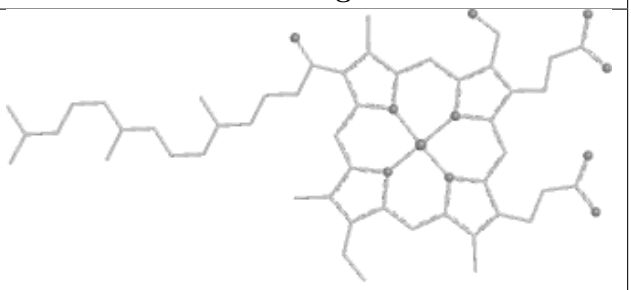
Bond lengths



Bond angles

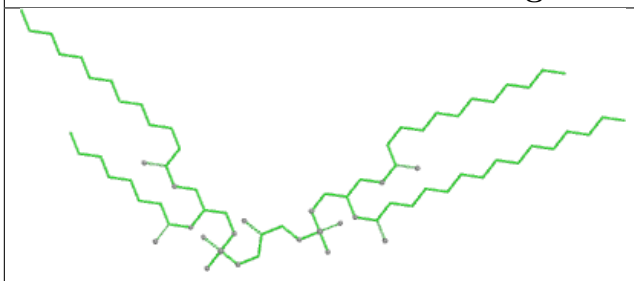


Torsions

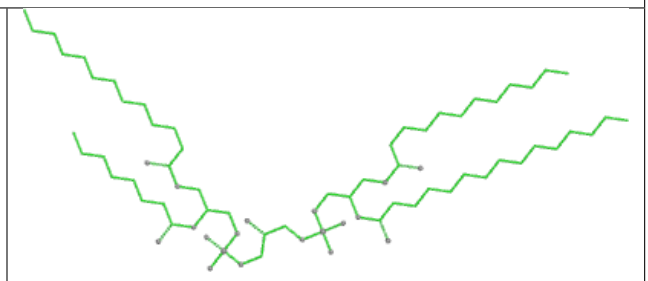


Rings

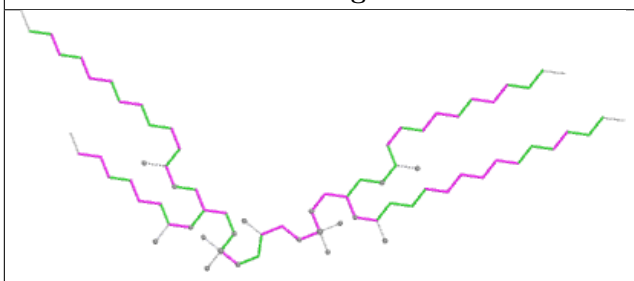
Ligand CDL T 202



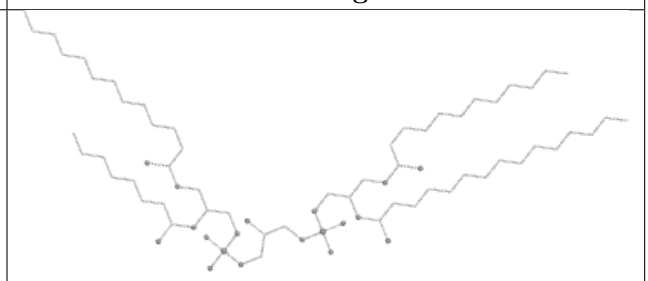
Bond lengths



Bond angles

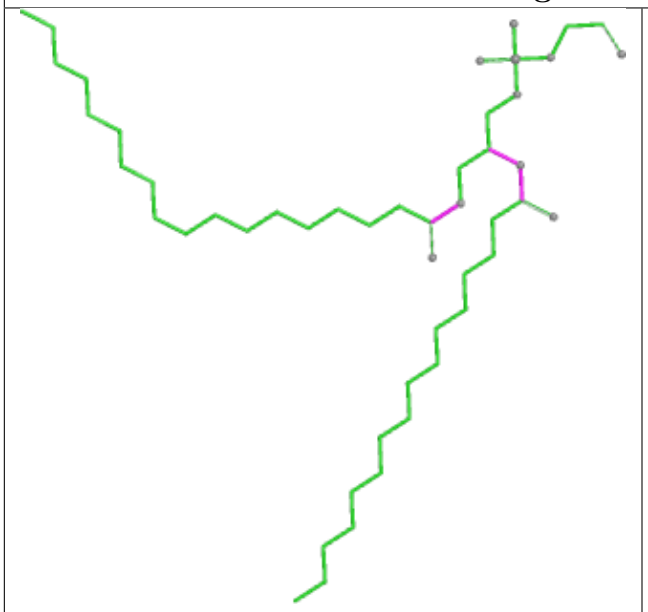


Torsions

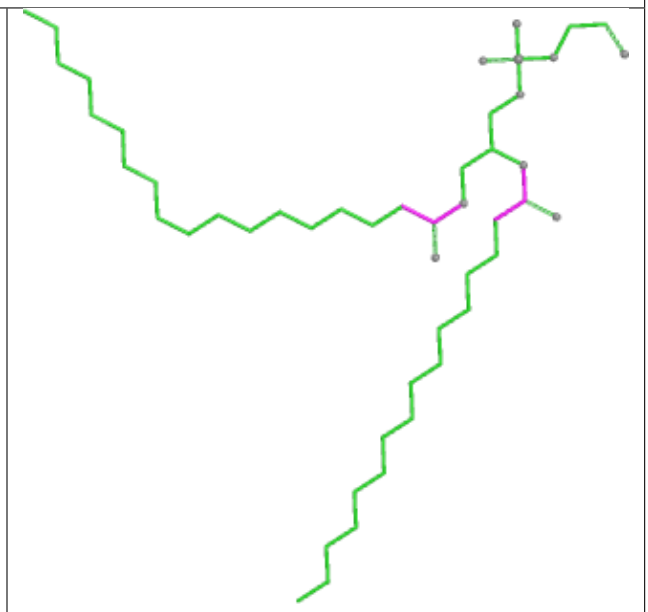


Rings

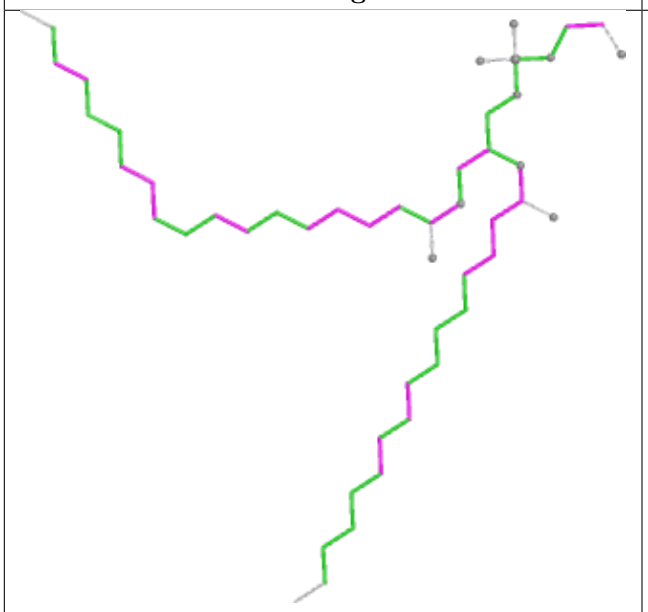
Ligand 9Y0 S 301



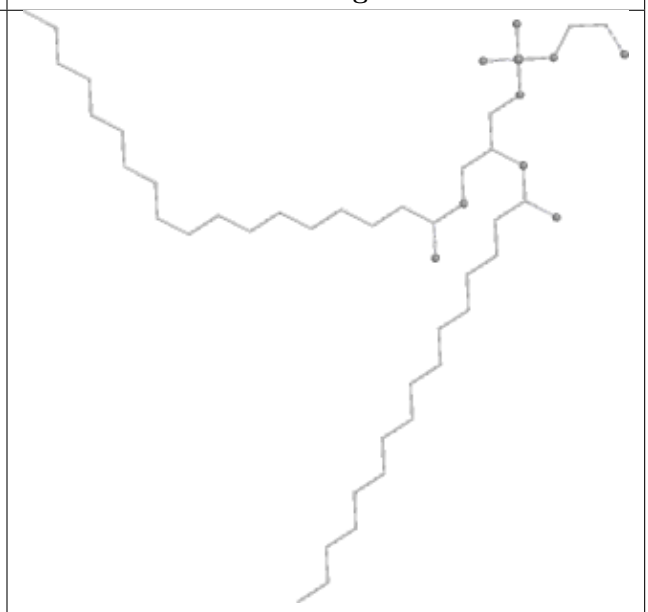
Bond lengths



Bond angles

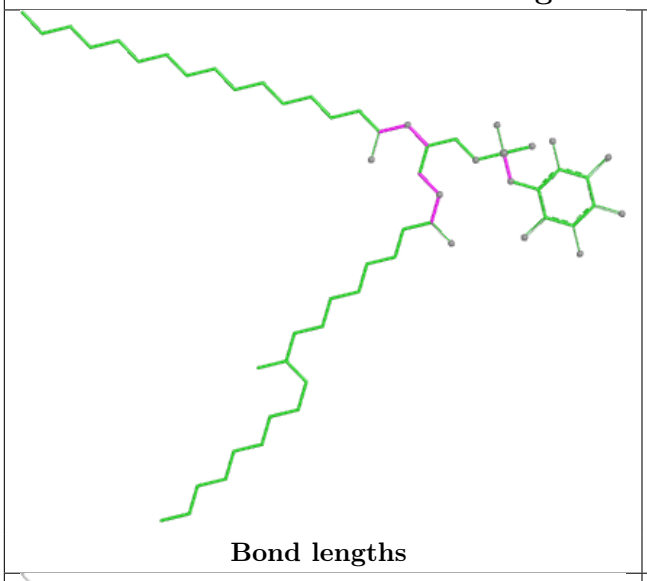


Torsions

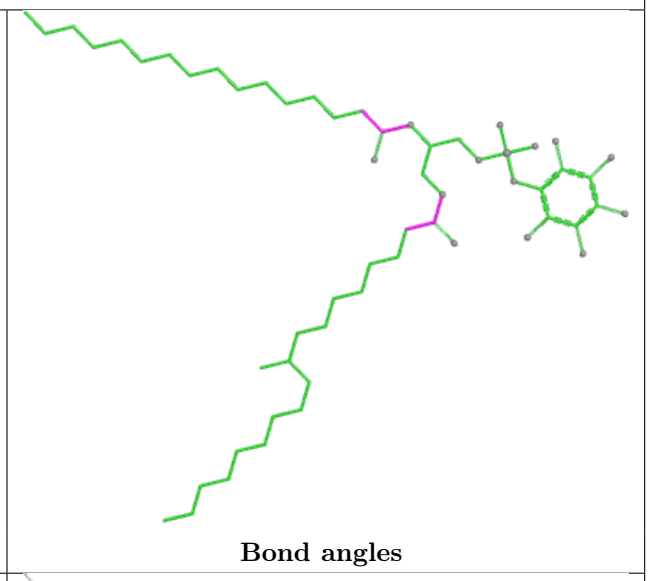


Rings

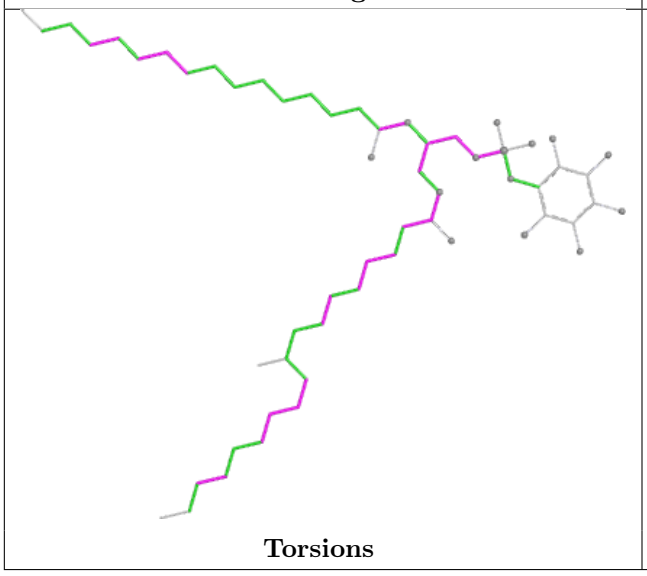
Ligand 9YF I 304



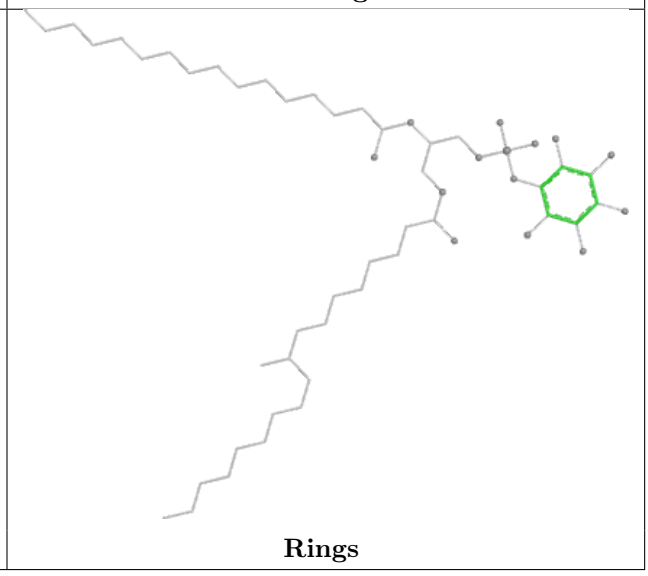
Bond lengths



Bond angles

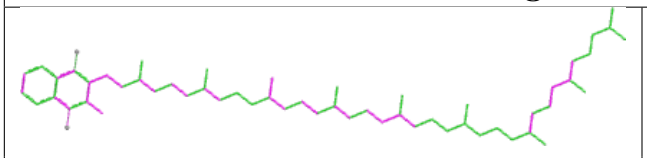


Torsions

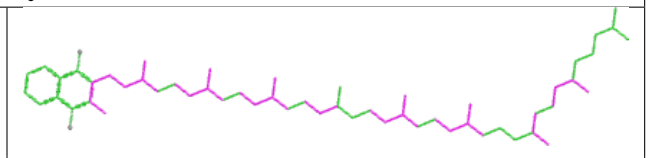


Rings

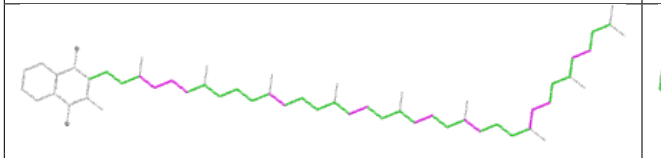
Ligand MQ9 E 604



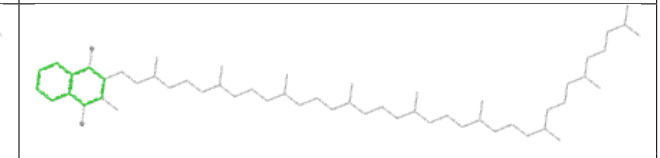
Bond lengths



Bond angles

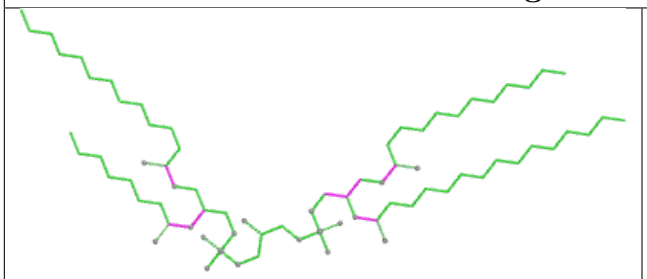


Torsions

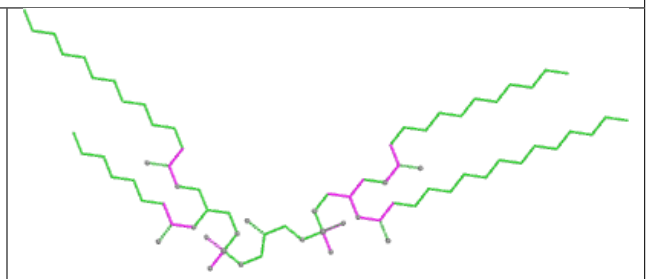


Rings

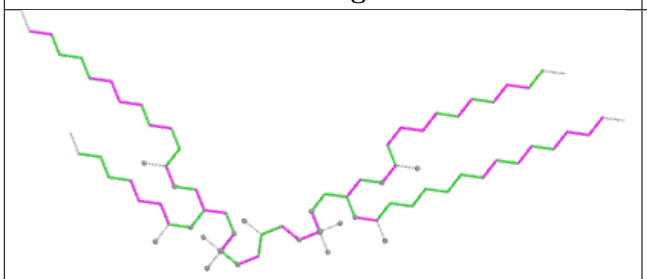
Ligand CDL X 303



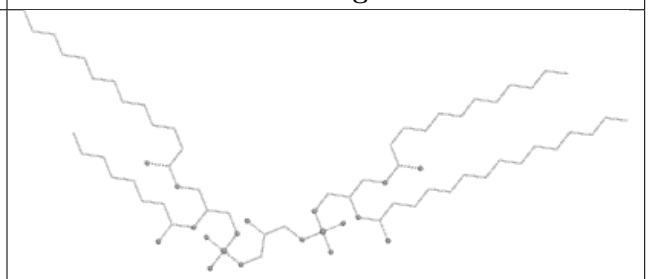
Bond lengths



Bond angles



Torsions

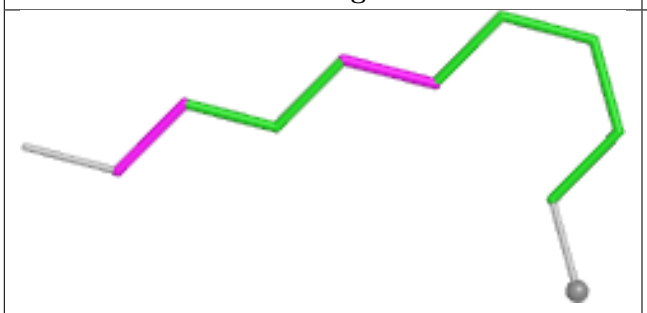


Rings

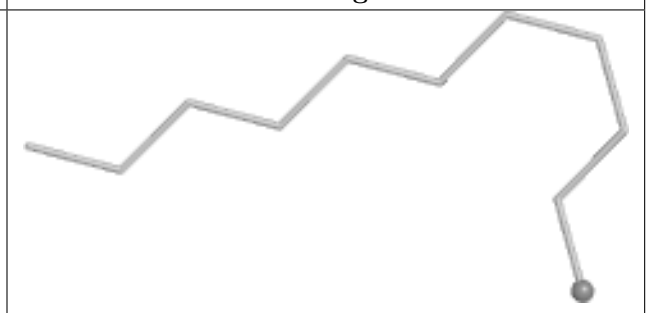
Ligand PLM G 301

Bond lengths

Bond angles

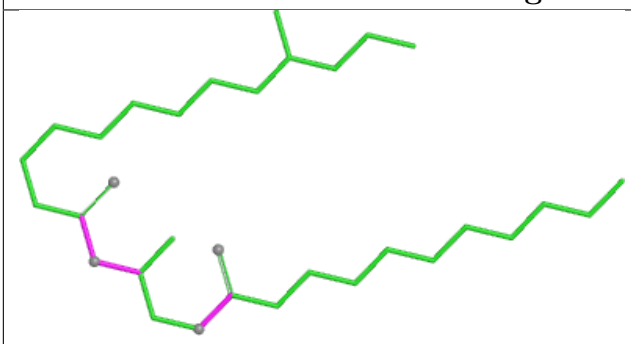


Torsions

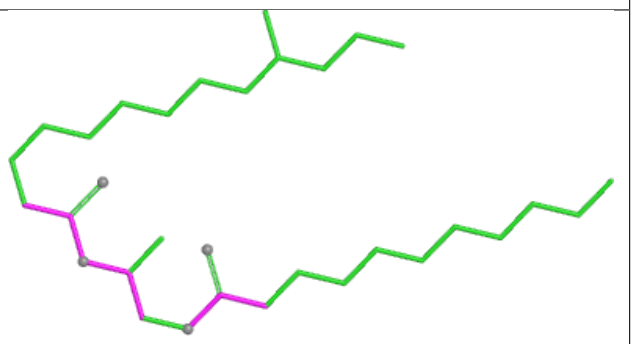


Rings

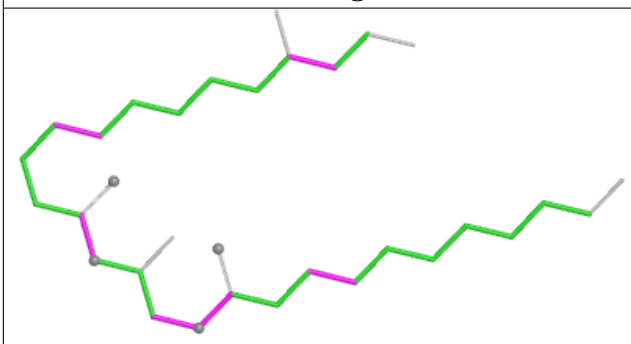
Ligand 9XX D 302



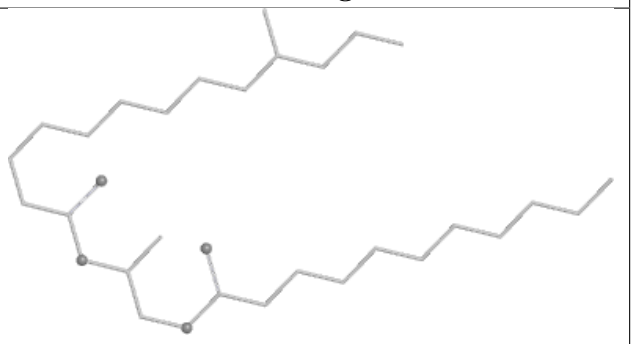
Bond lengths



Bond angles

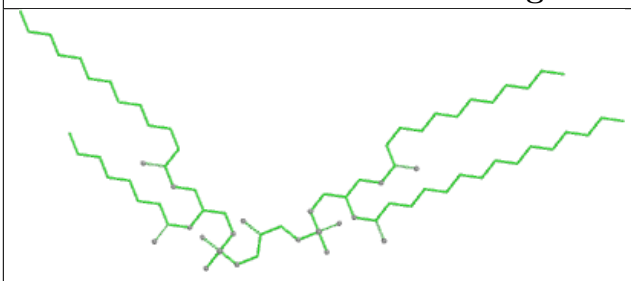


Torsions

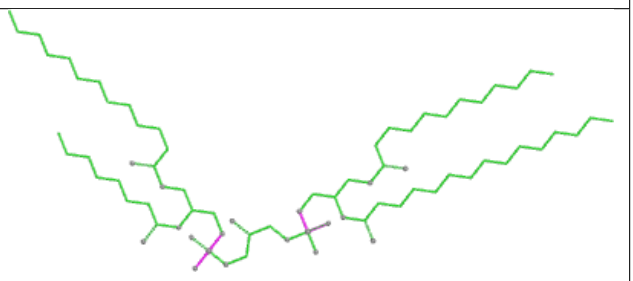


Rings

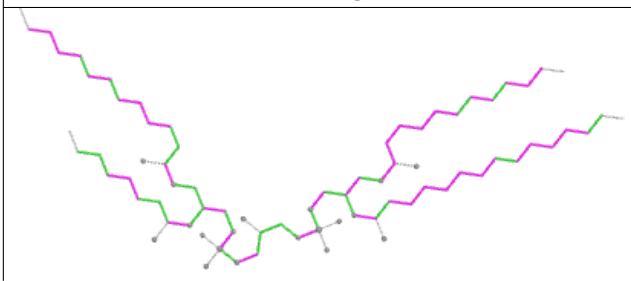
Ligand CDL L 604



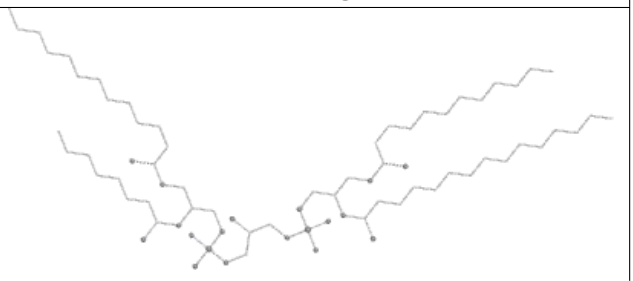
Bond lengths



Bond angles

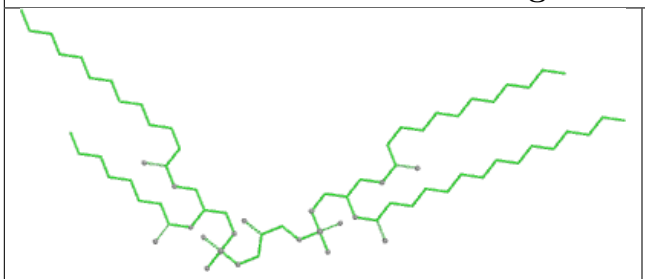


Torsions

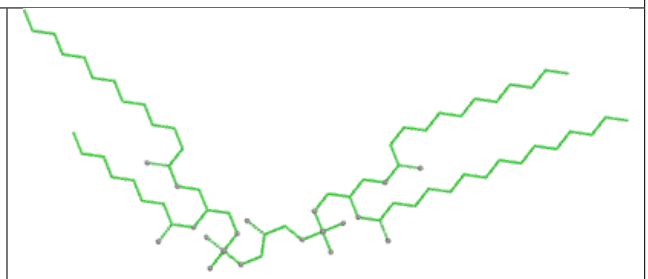


Rings

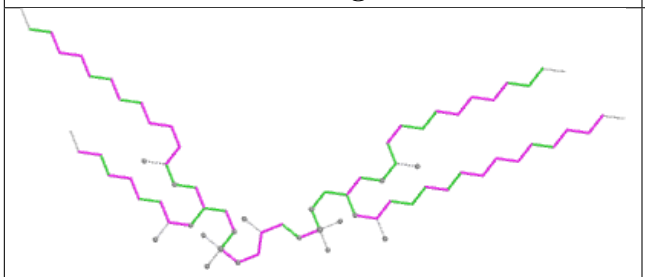
Ligand CDL J 203



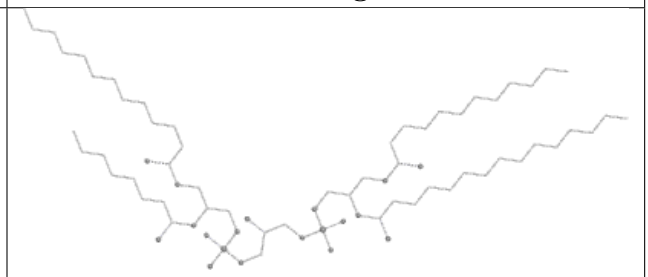
Bond lengths



Bond angles

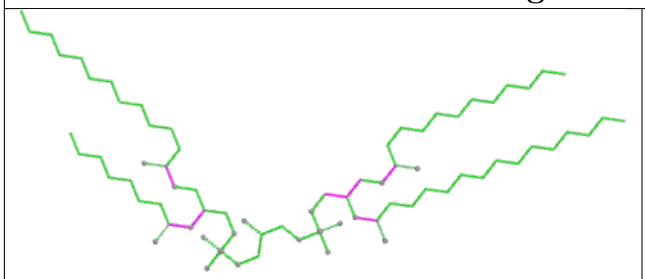


Torsions

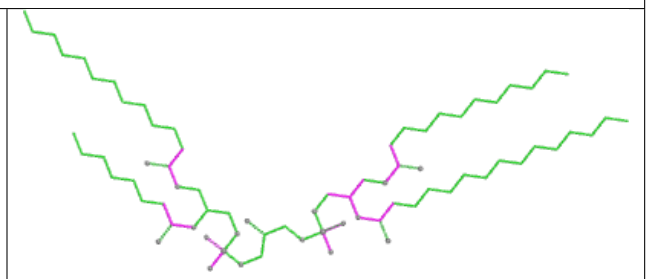


Rings

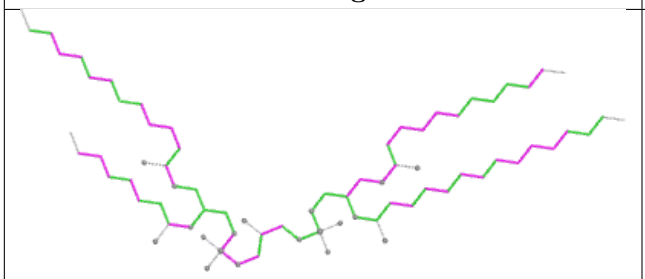
Ligand CDL Z 203



Bond lengths



Bond angles



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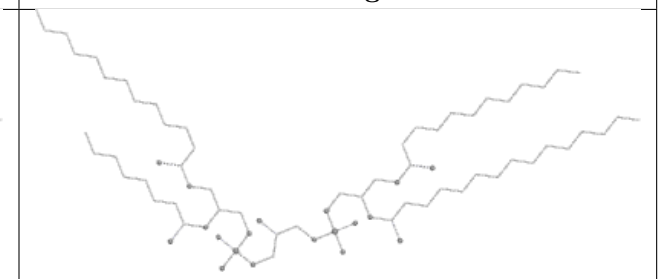
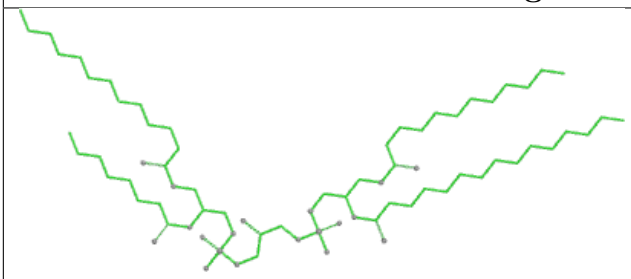
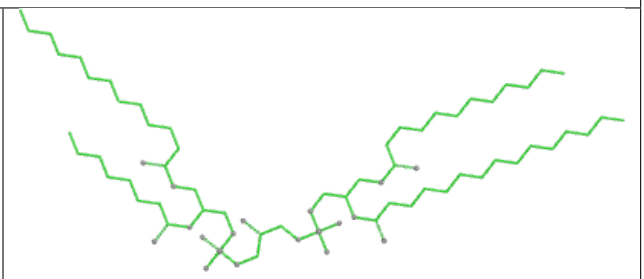


Rings

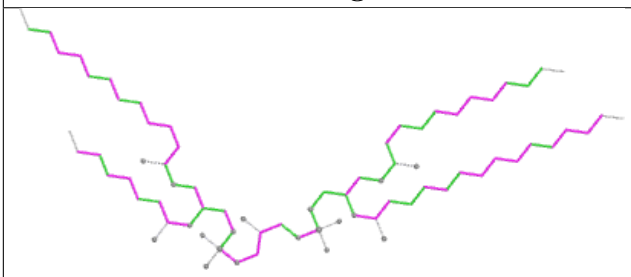
Ligand CDL P 201



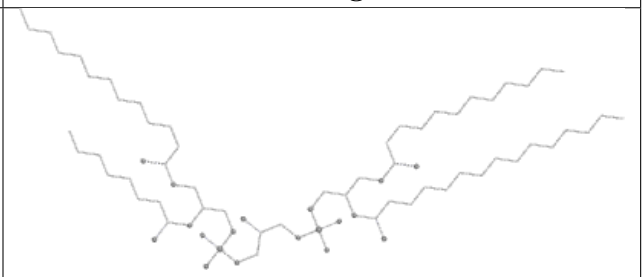
Bond lengths



Bond angles

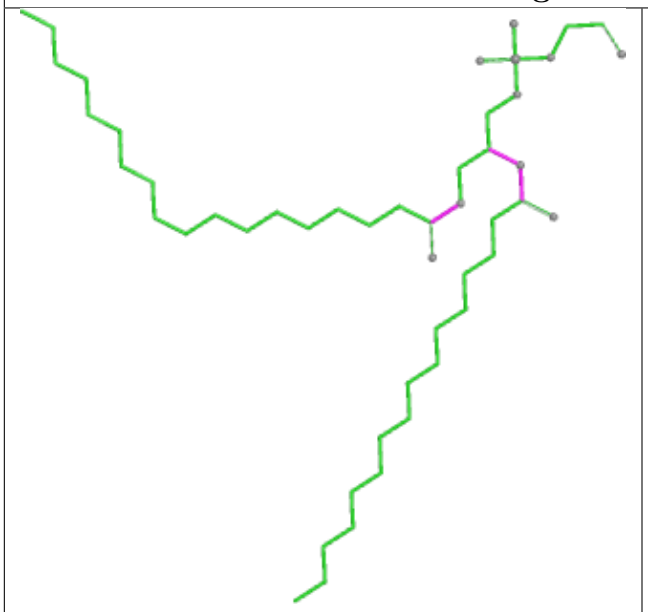


Torsions

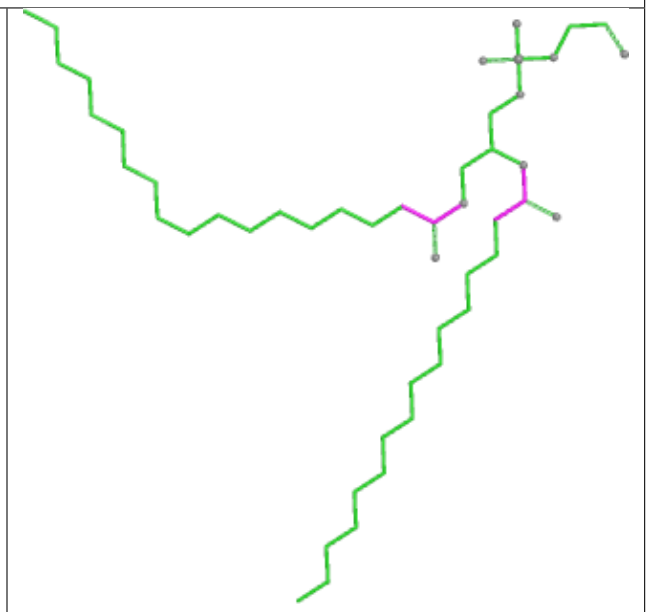


Rings

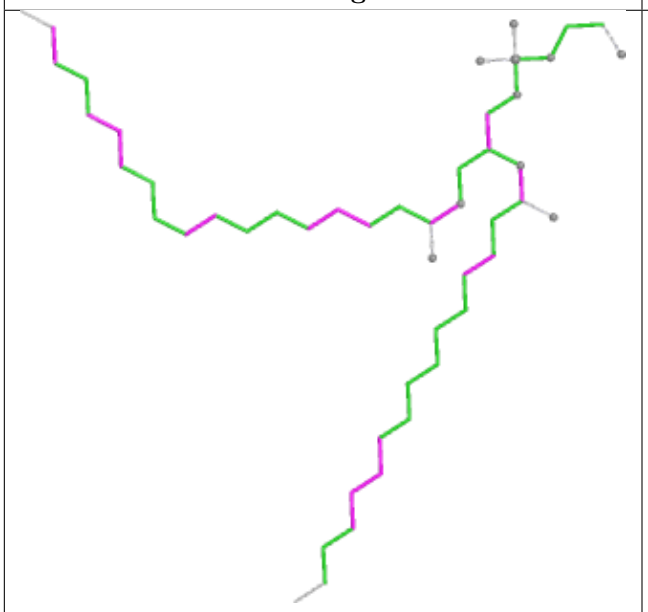
Ligand 9Y0 F 704



Bond lengths



Bond angles



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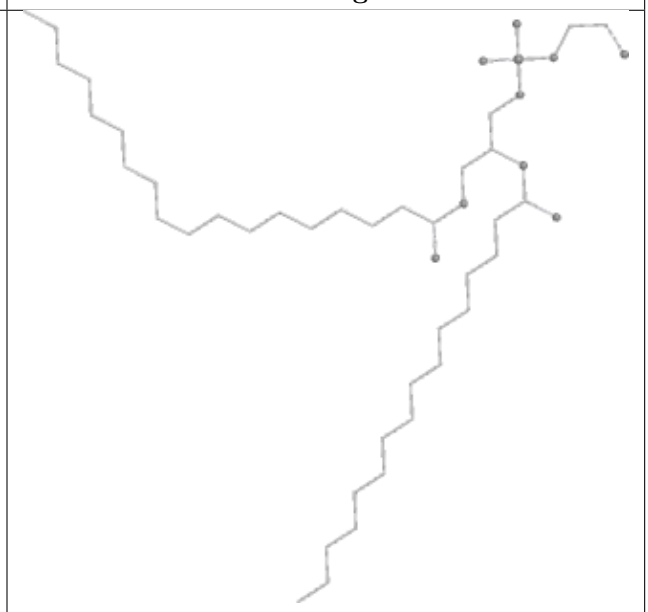
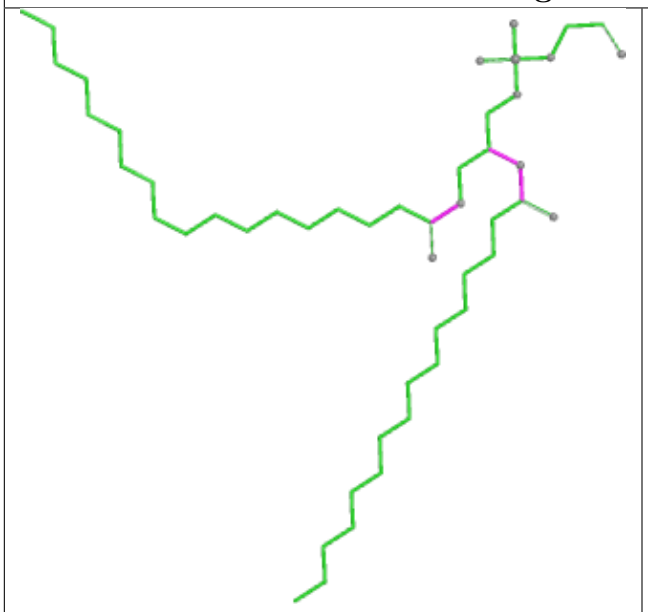


Rings

Ligand 9Y0 J 201



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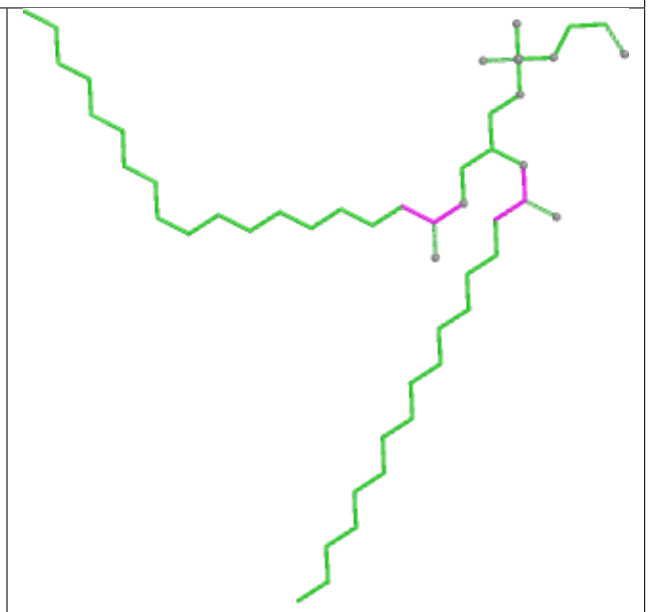
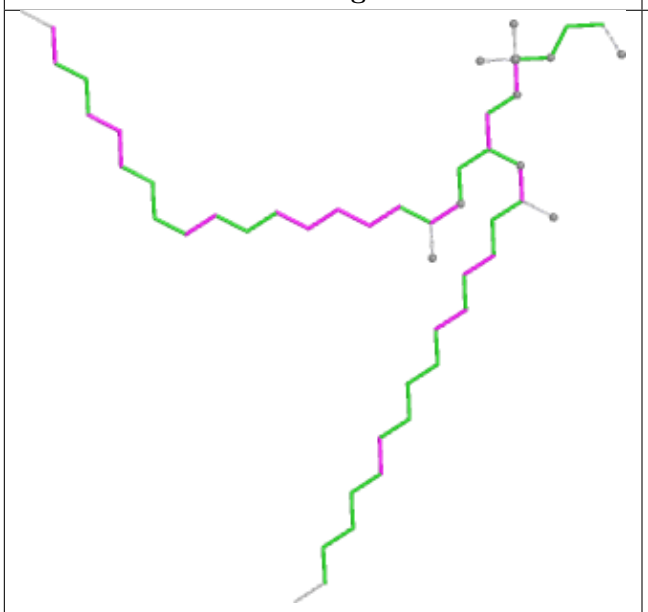


Bond angles



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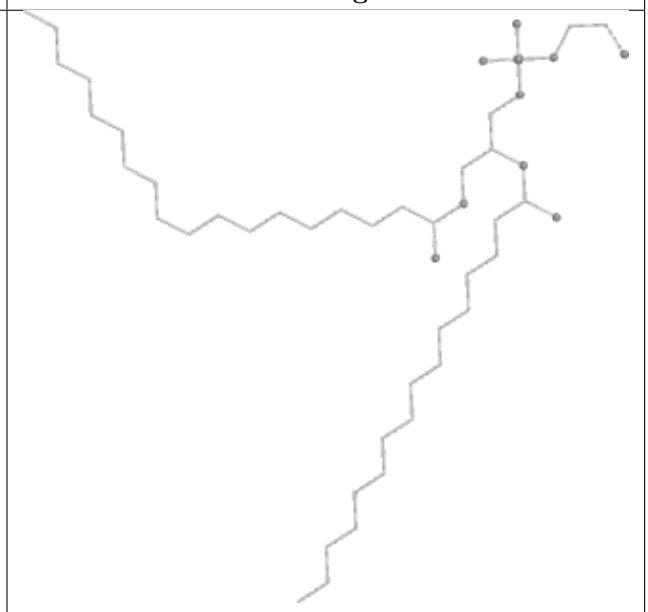
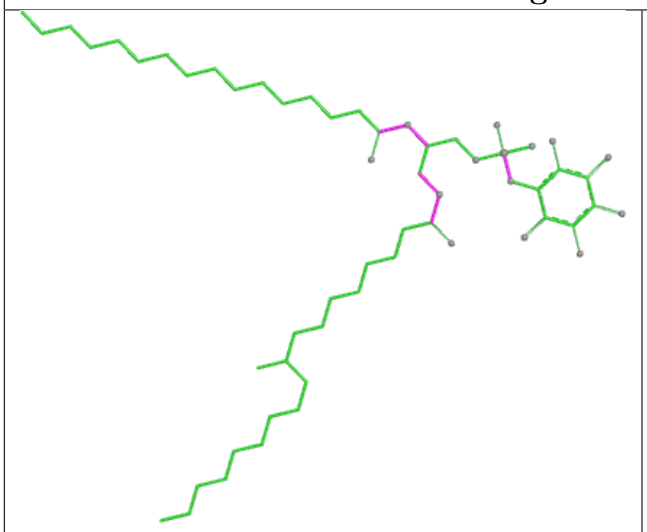
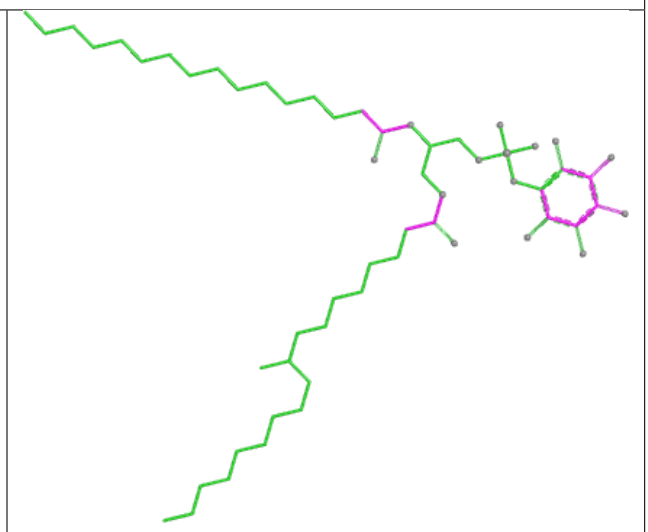


Rings

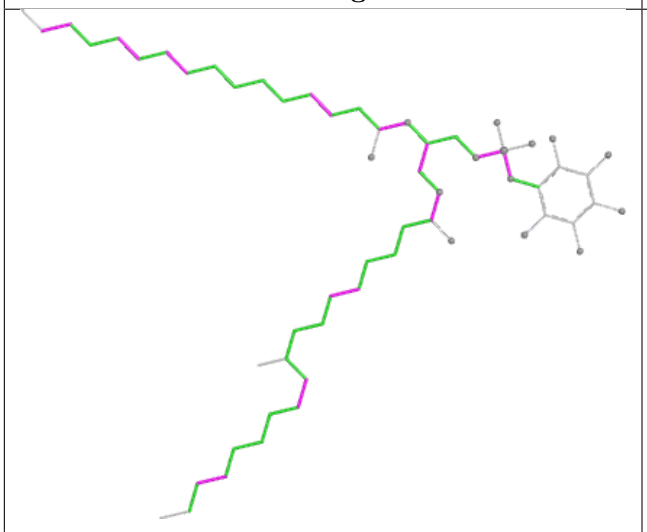
Ligand 9YF E 605



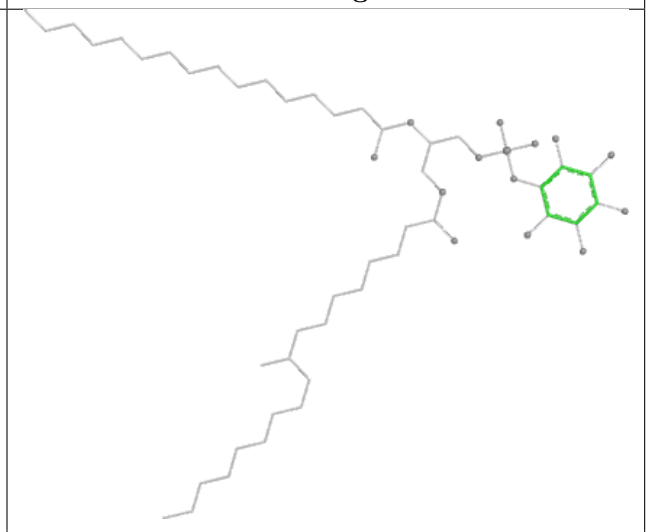
Bond lengths



Bond angles

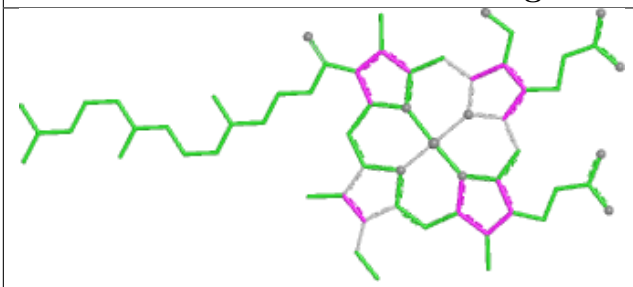


Torsions

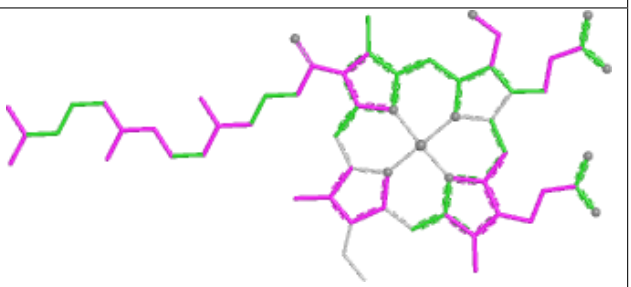


Rings

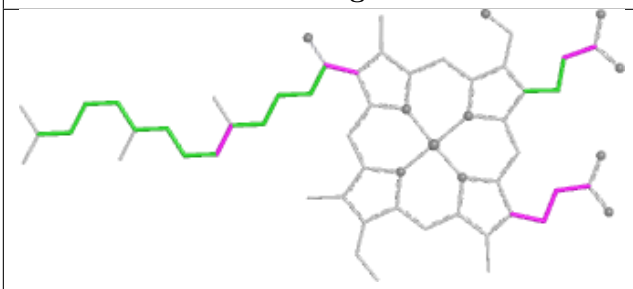
Ligand HEA L 602



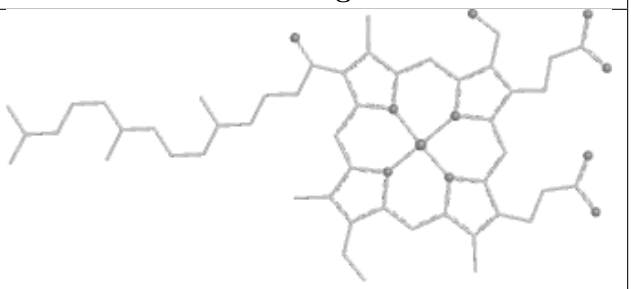
Bond lengths



Bond angles

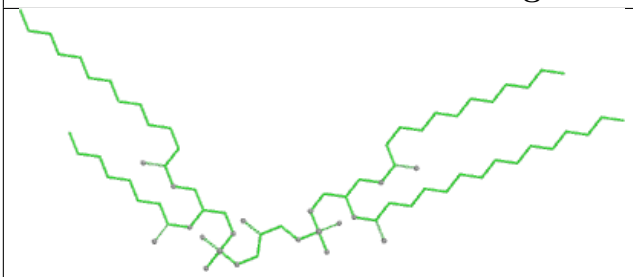


Torsions

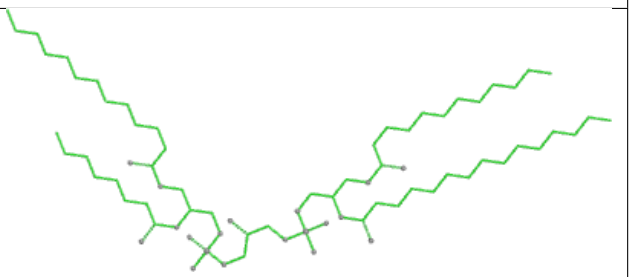


Rings

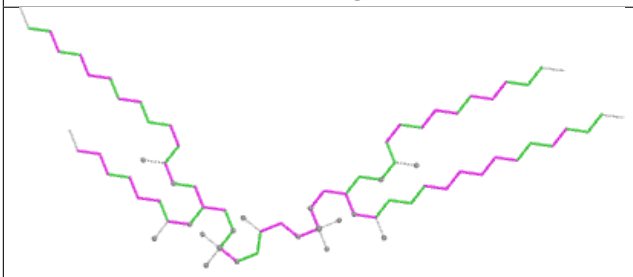
Ligand CDL X 302



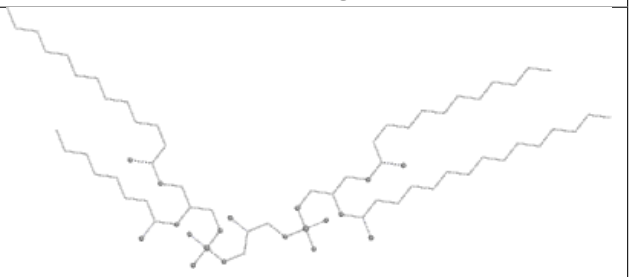
Bond lengths



Bond angles

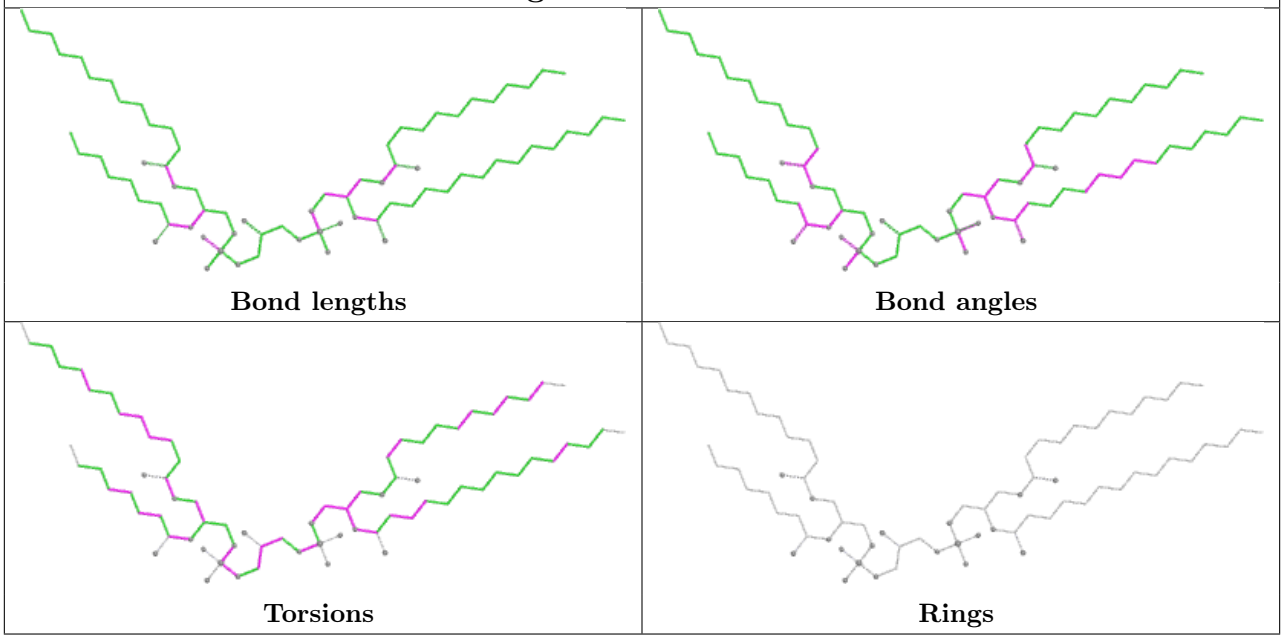


Torsions

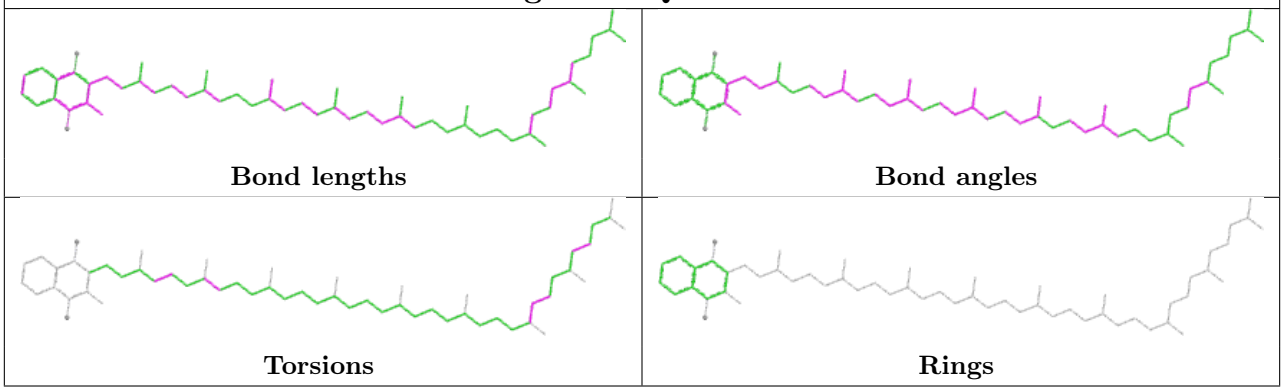


Rings

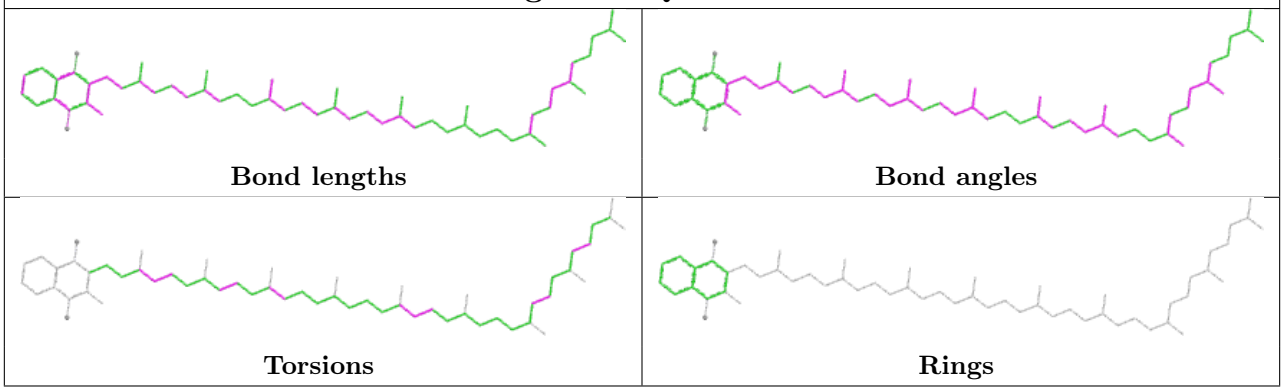
Ligand CDL Z 202



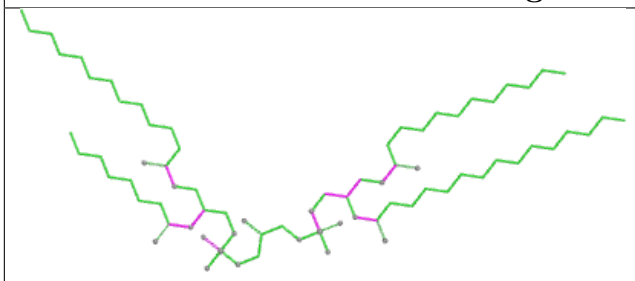
Ligand MQ9 E 603



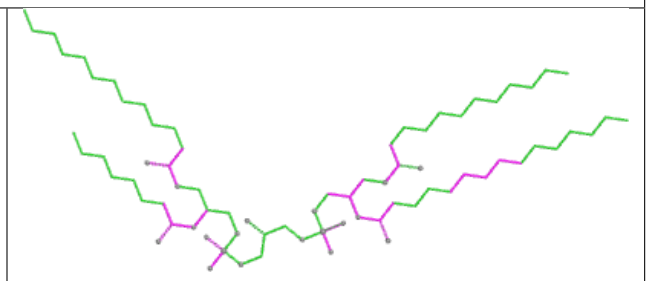
Ligand MQ9 Z 201



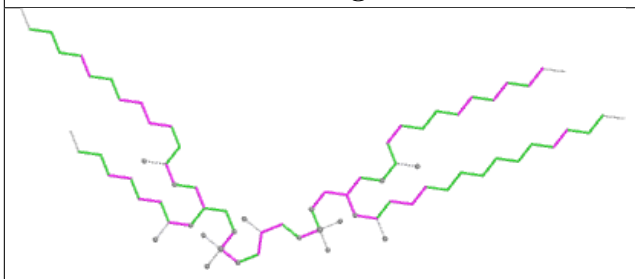
Ligand CDL T 201



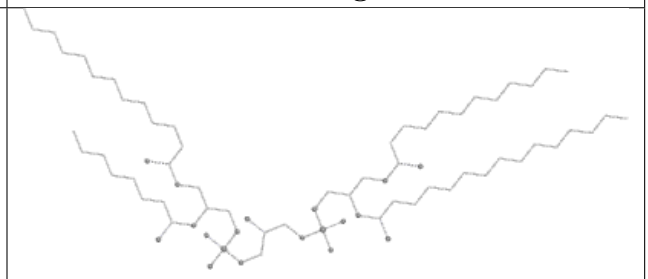
Bond lengths



Bond angles

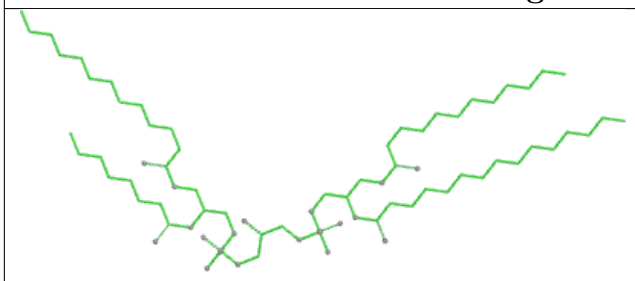


Torsions

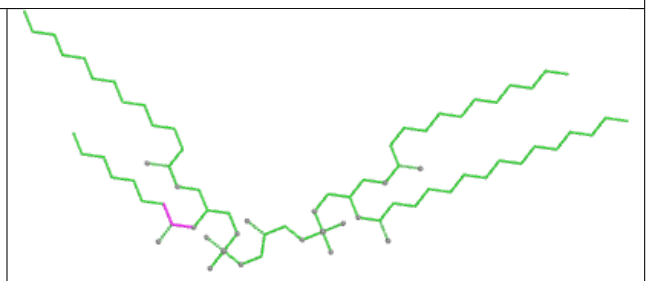


Rings

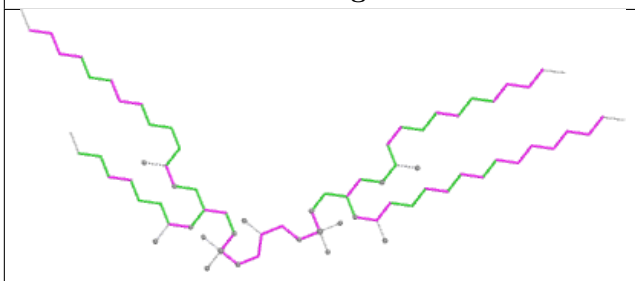
Ligand CDL F 706



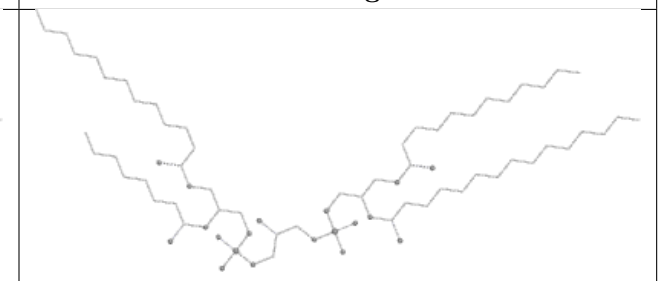
Bond lengths



Bond angles

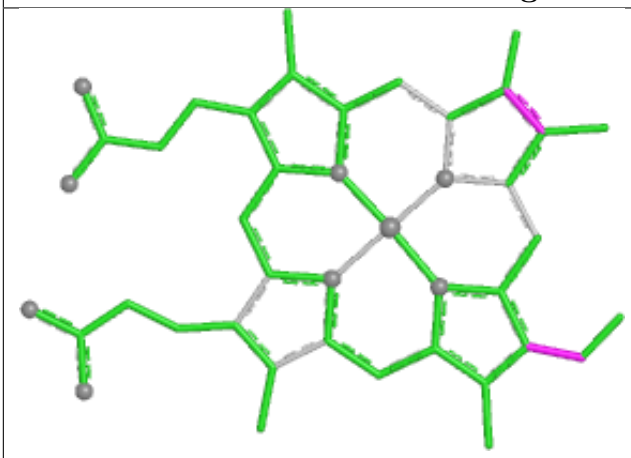


Torsions

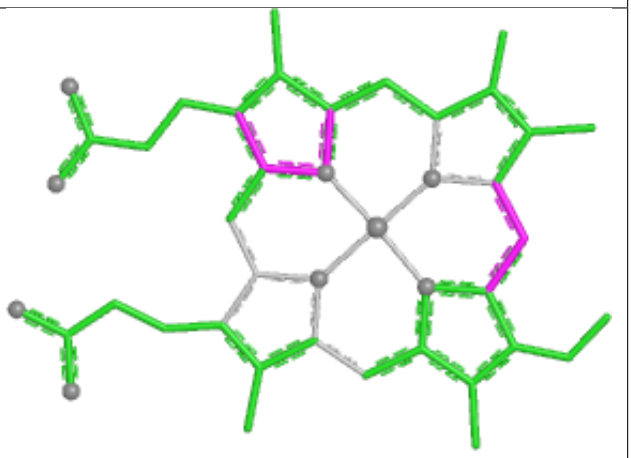


Rings

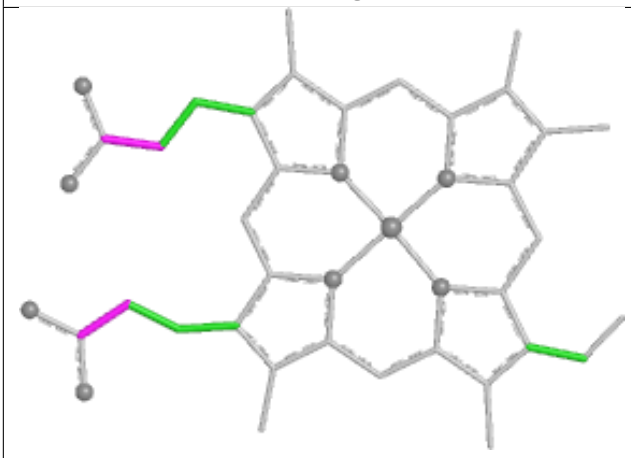
Ligand HEM F 702



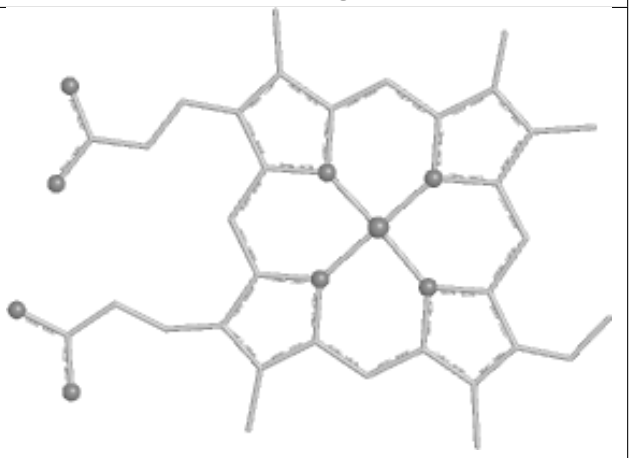
Bond lengths



Bond angles

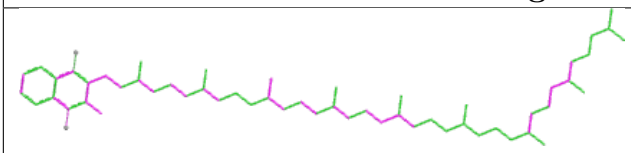


Torsions

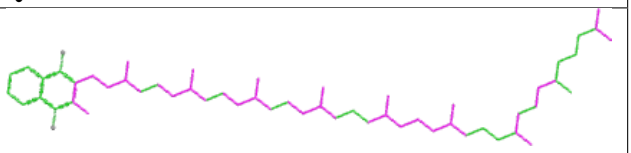


Rings

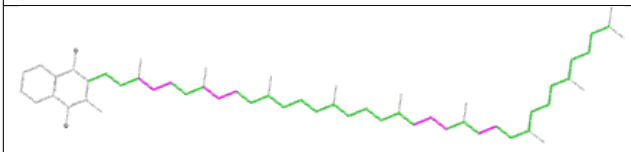
Ligand MQ9 I 303



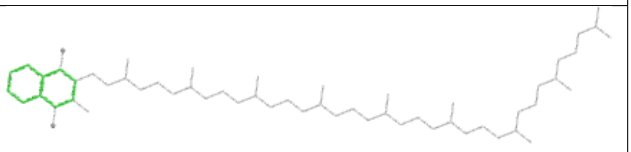
Bond lengths



Bond angles

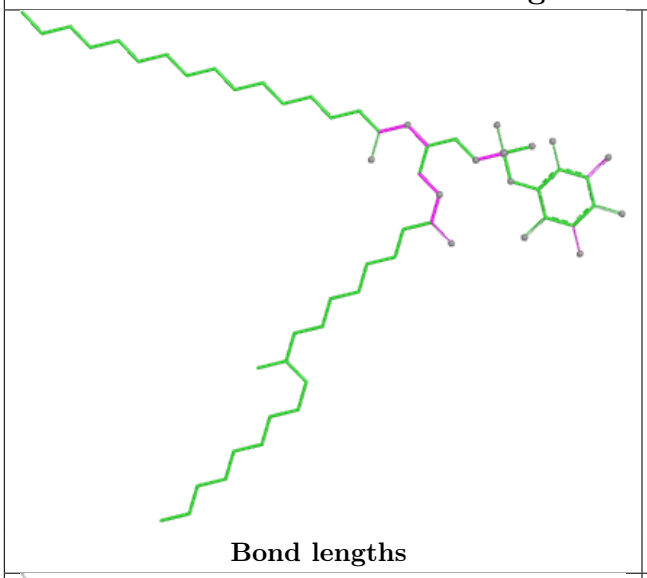


Torsions

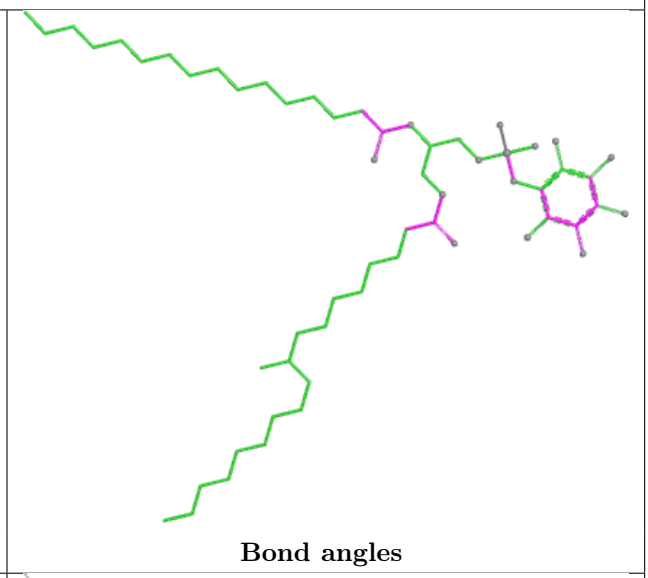


Rings

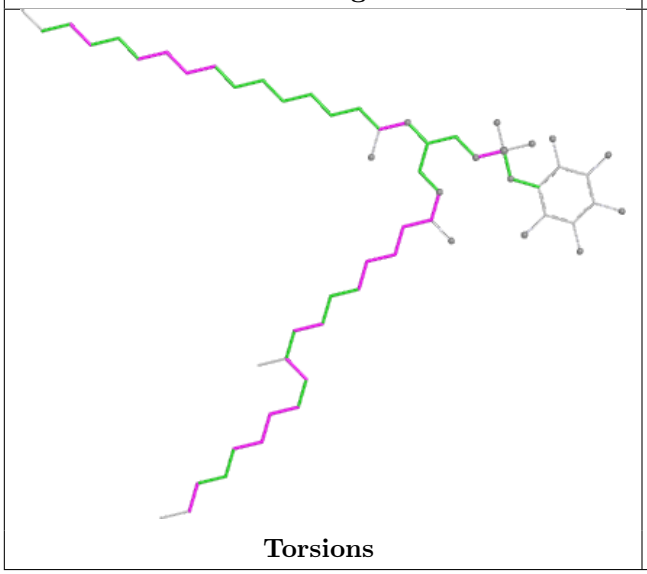
Ligand 9YF Y 503



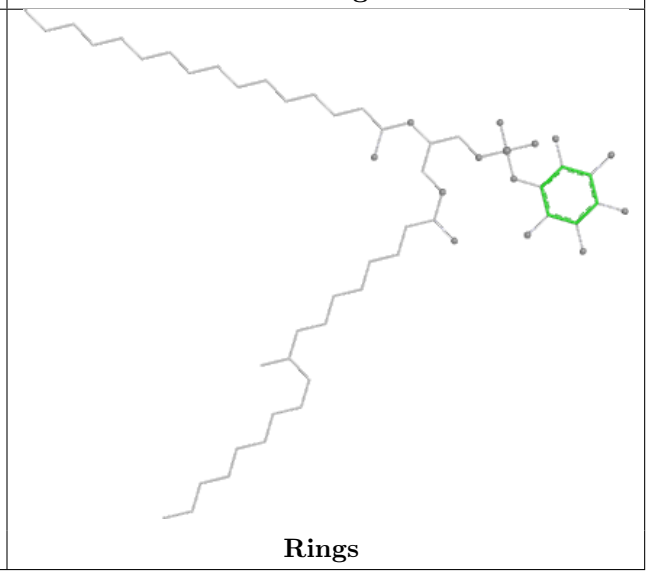
Bond lengths



Bond angles

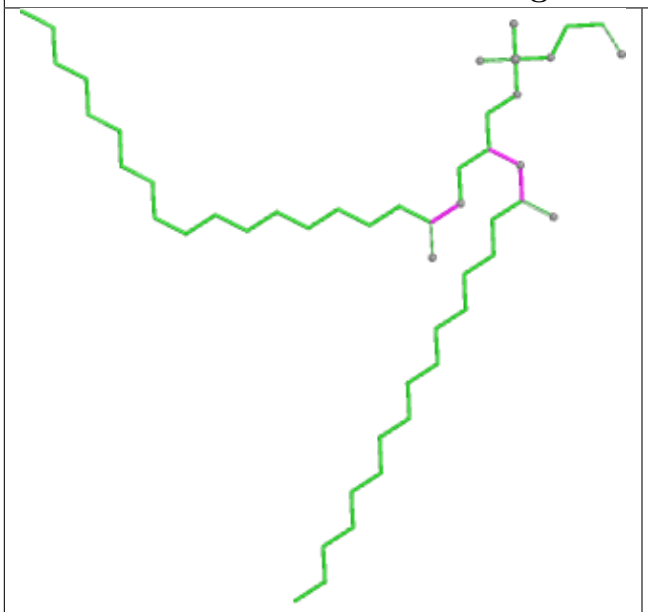


Torsions

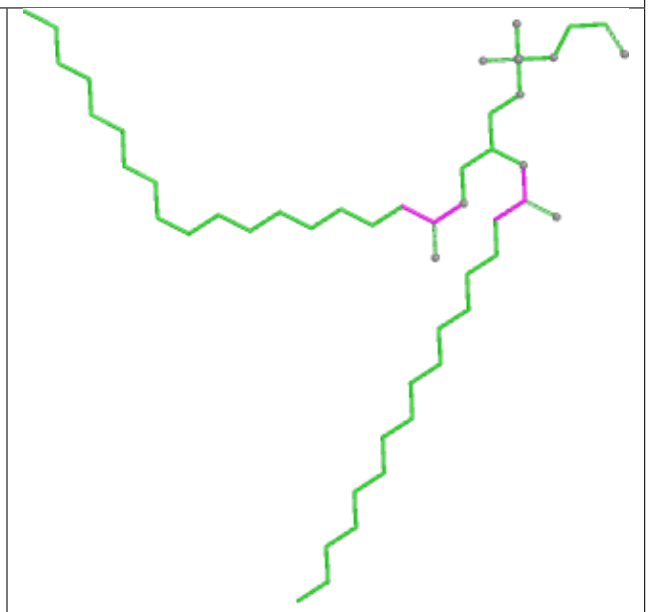


Rings

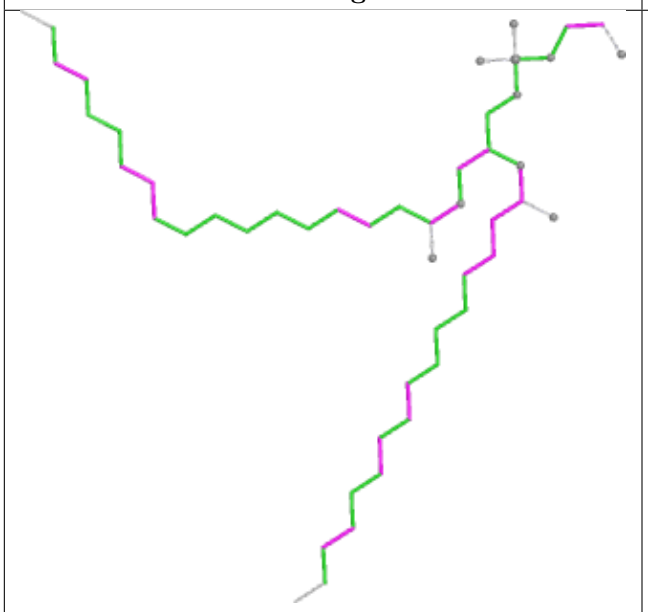
Ligand 9Y0 X 301



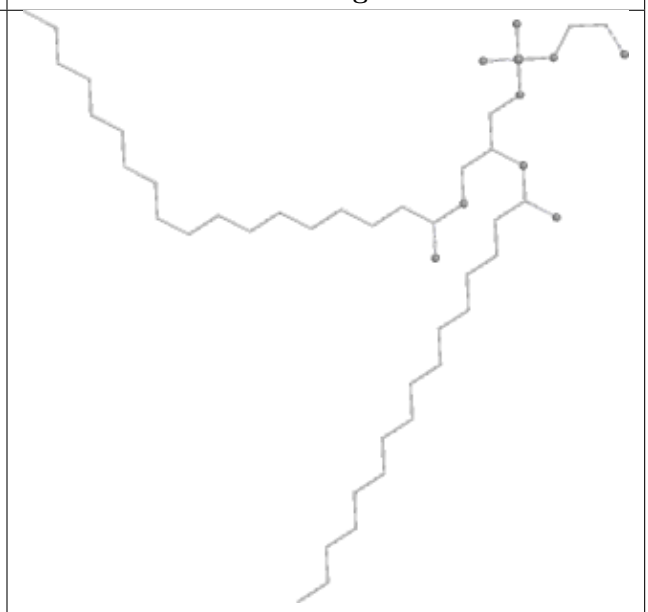
Bond lengths



Bond angles

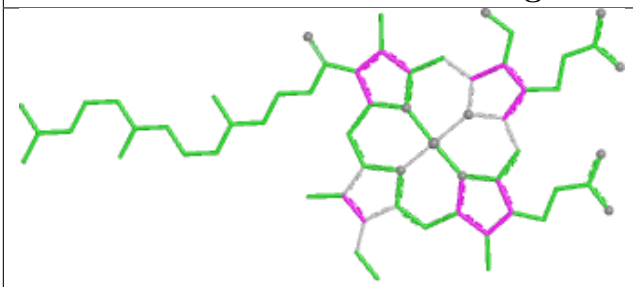


Torsions

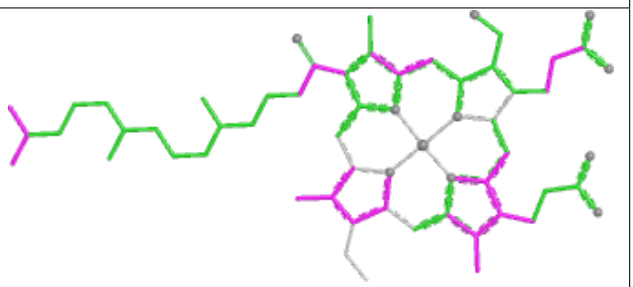


Rings

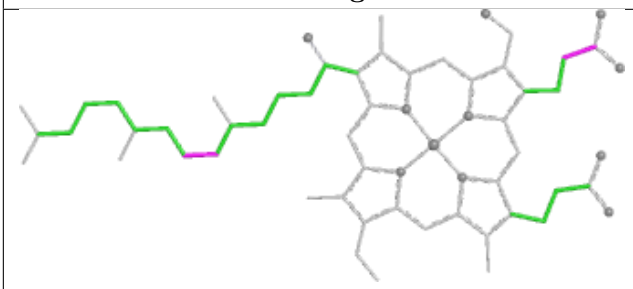
Ligand HEA L 603



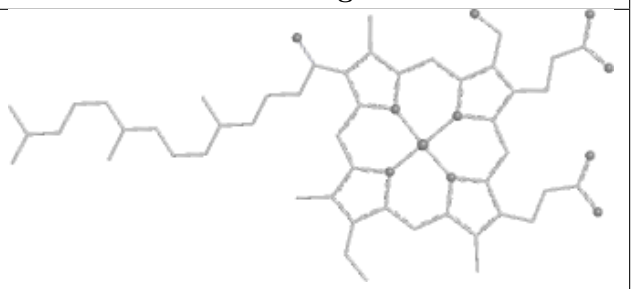
Bond lengths



Bond angles

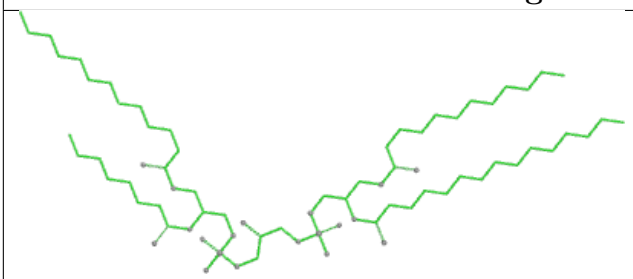


Torsions

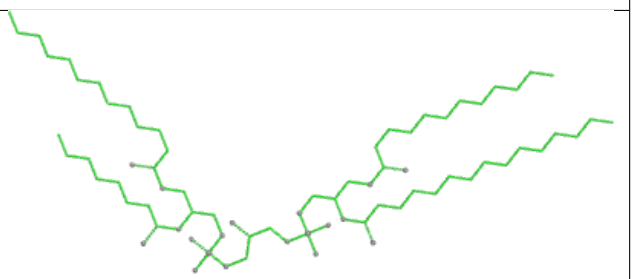


Rings

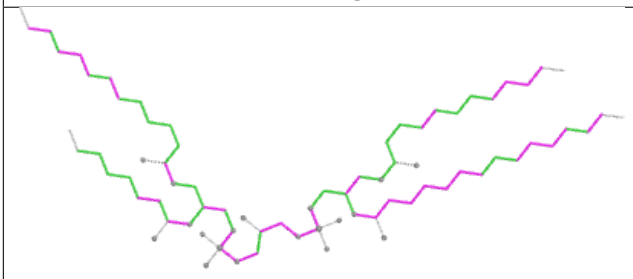
Ligand CDL E 607



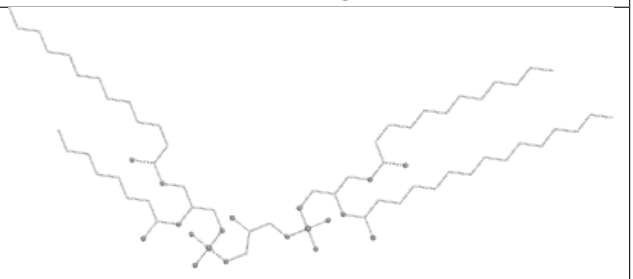
Bond lengths



Bond angles

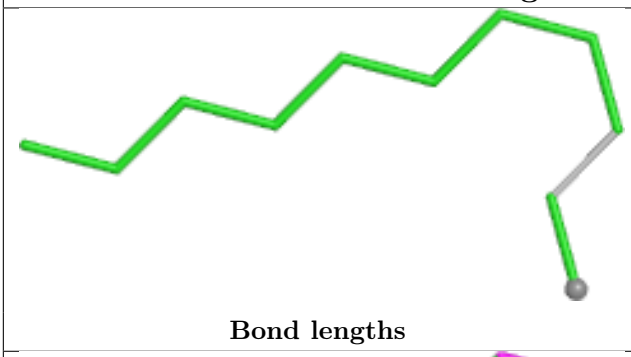


Torsions

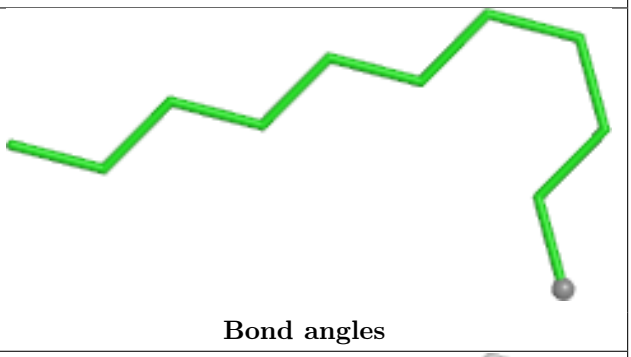


Rings

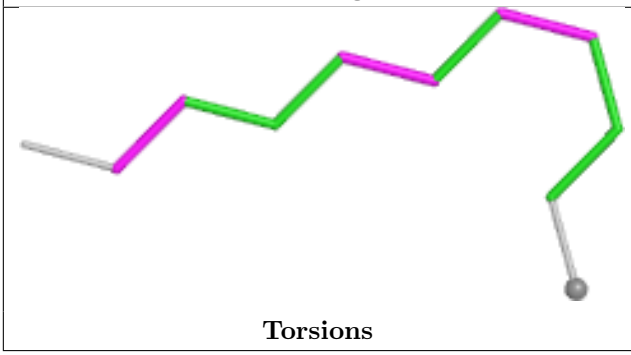
Ligand PLM D 301



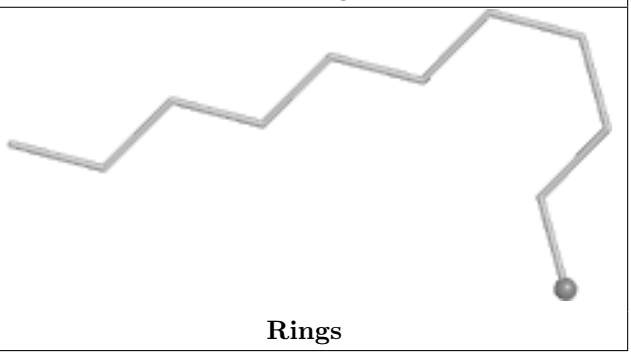
Bond lengths



Bond angles

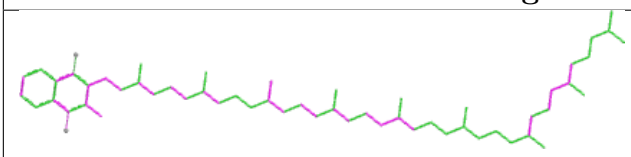


Torsions

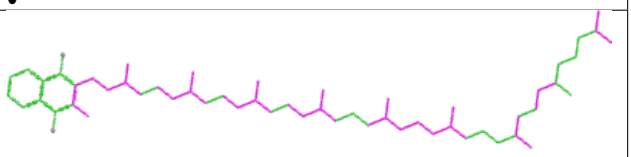


Rings

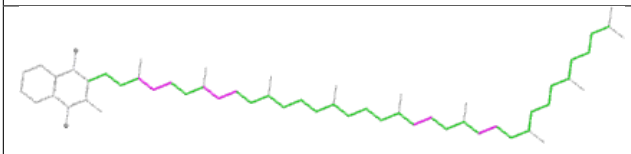
Ligand MQ9 O 304



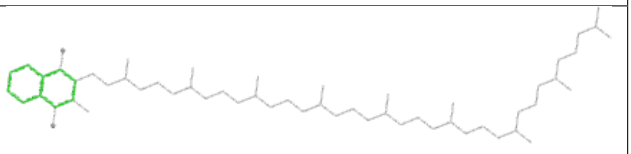
Bond lengths



Bond angles

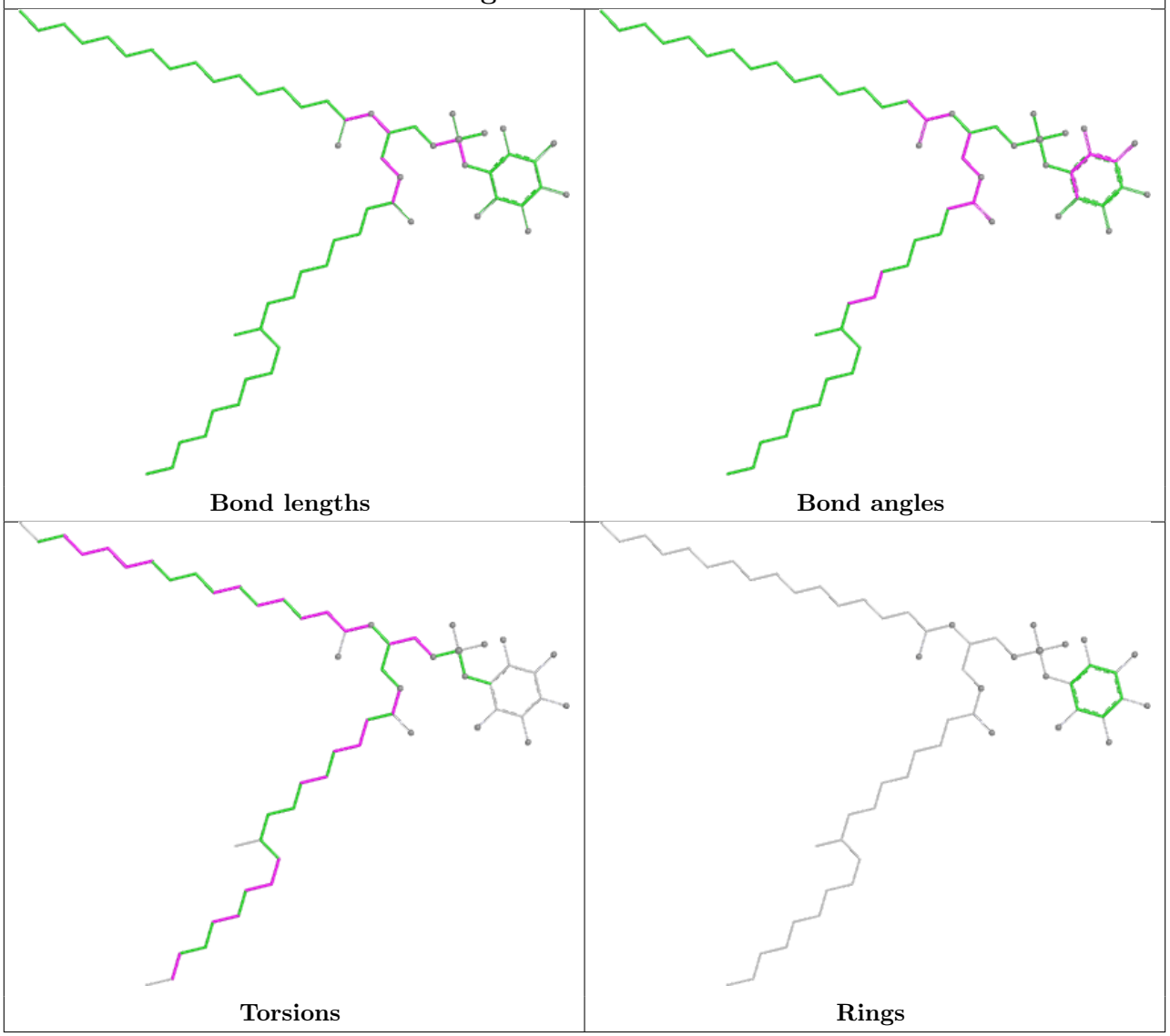


Torsions



Rings

Ligand 9YF Y 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

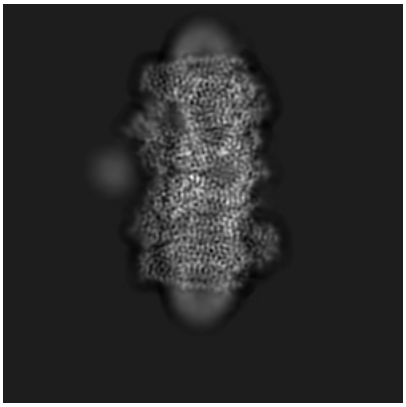
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24456. These allow visual inspection of the internal detail of the map and identification of artifacts.

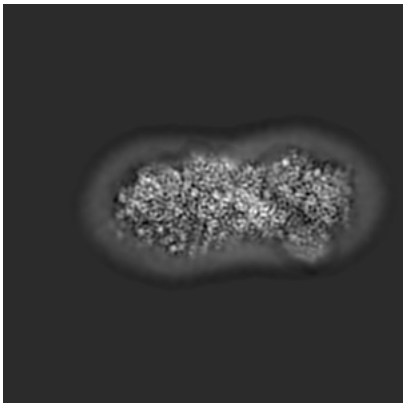
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

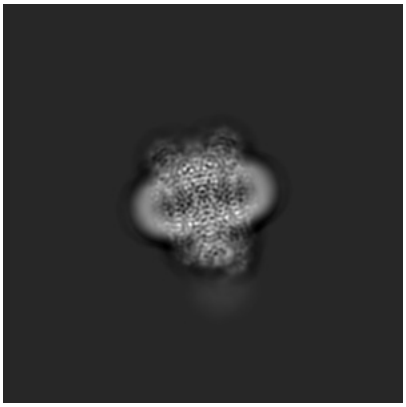
6.1.1 Primary map



X



Y

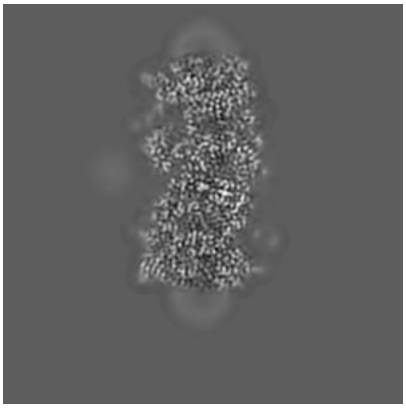


Z

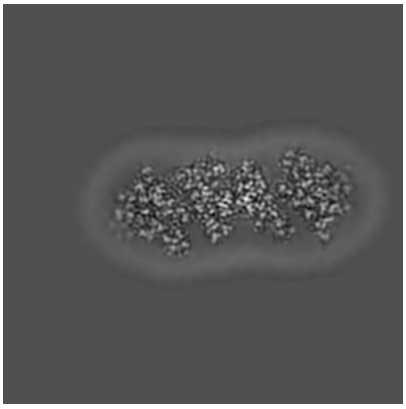
The images above show the map projected in three orthogonal directions.

6.2 Central slices

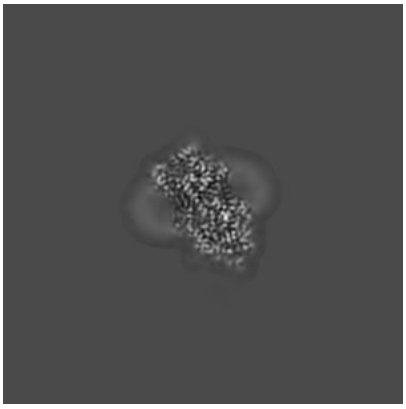
6.2.1 Primary map



X Index: 165



Y Index: 165

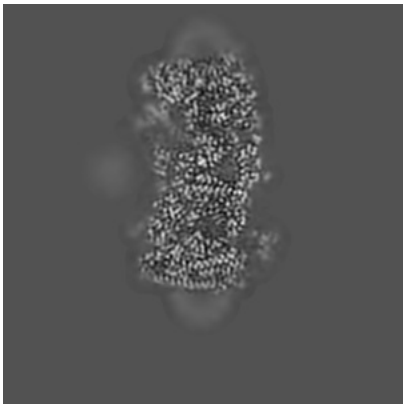


Z Index: 165

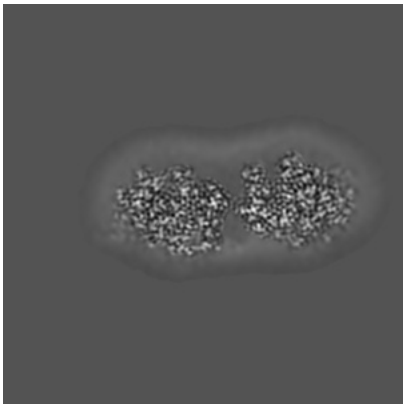
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

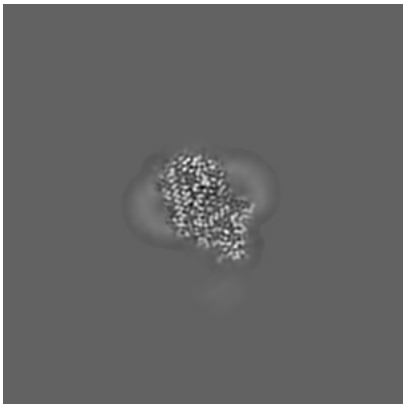
6.3.1 Primary map



X Index: 170



Y Index: 182

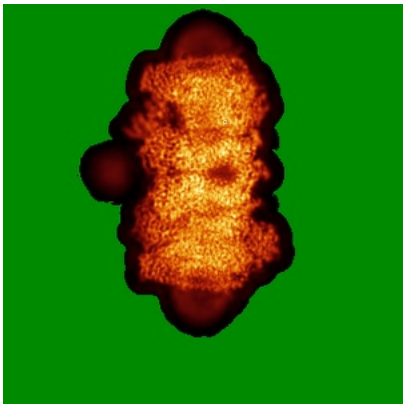


Z Index: 172

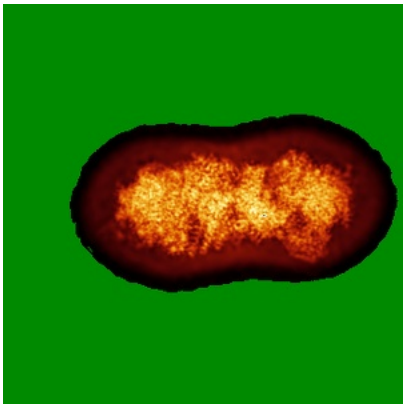
The images above show the largest variance slices of the map in three orthogonal directions.

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

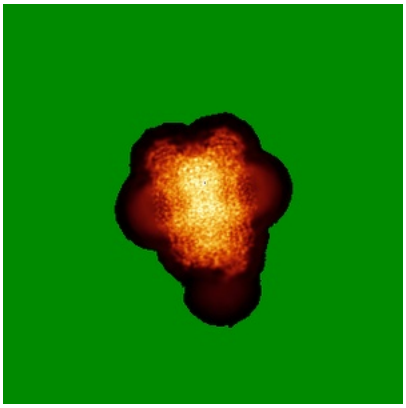
6.4.1 Primary map



X



Y



Z

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 0.634. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

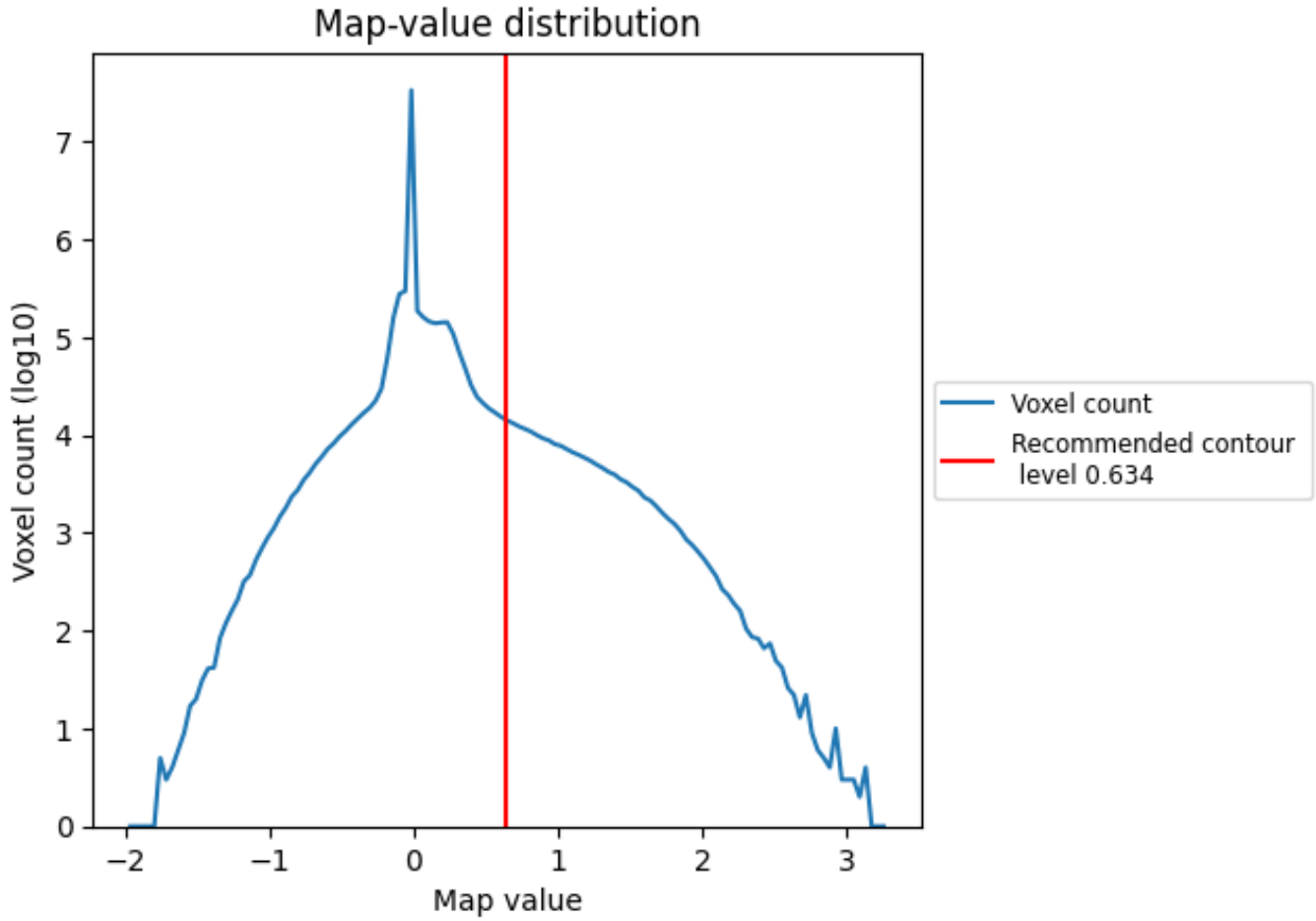
6.6 Mask visualisation (i)

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

7 Map analysis

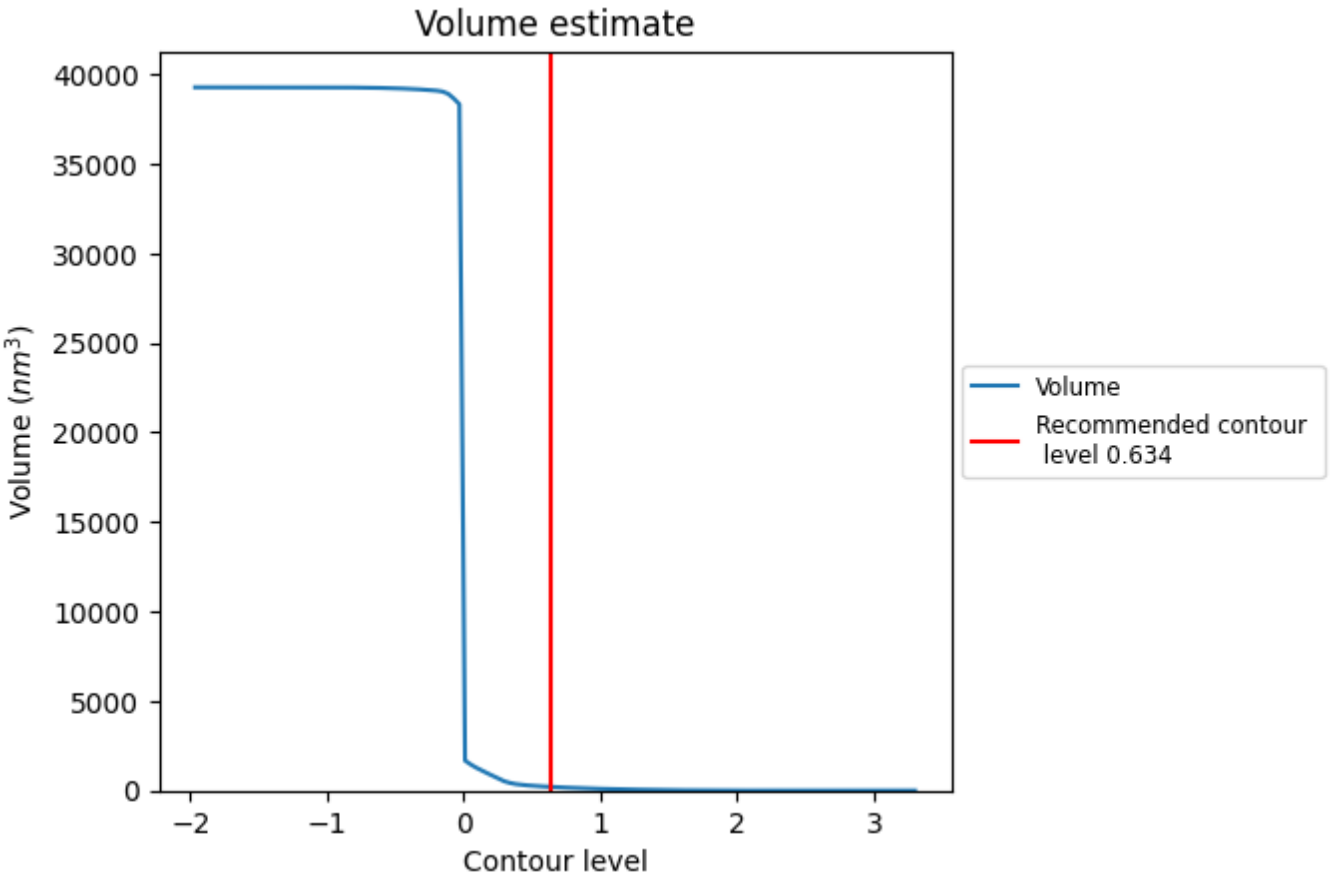
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

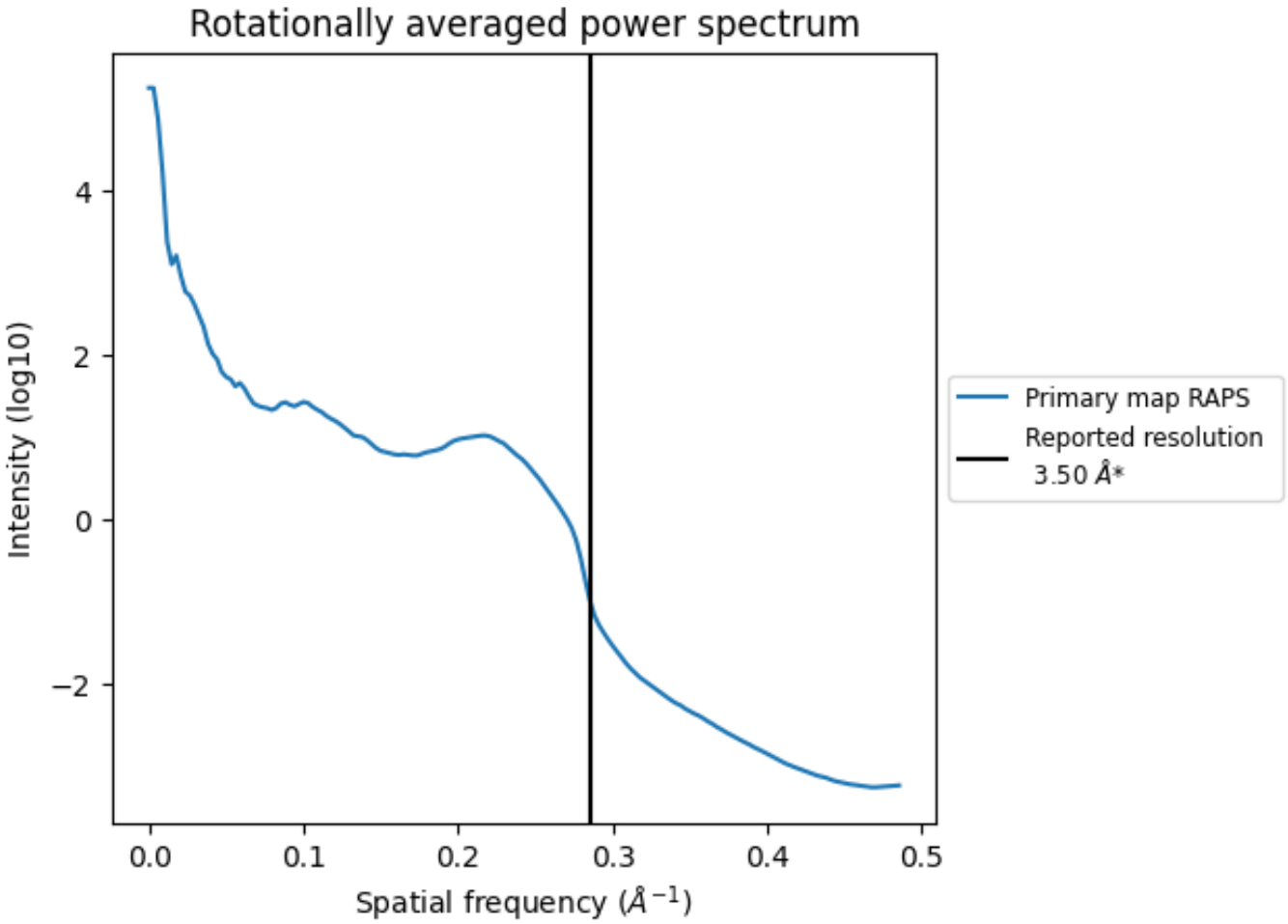
7.2 Volume estimate



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 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 0.286 $Å^{-1}$

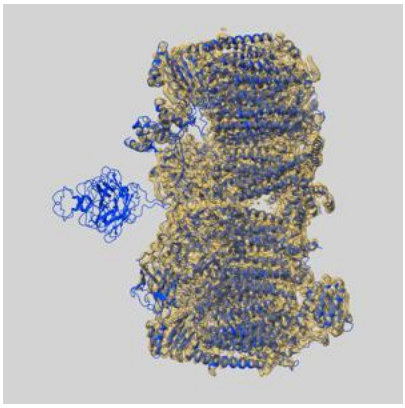
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

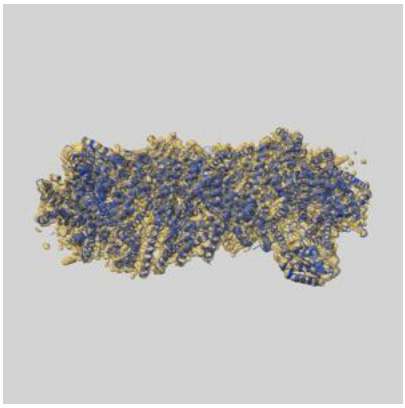
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24456 and PDB model 7RH6. Per-residue inclusion information can be found in section 3 on page 15.

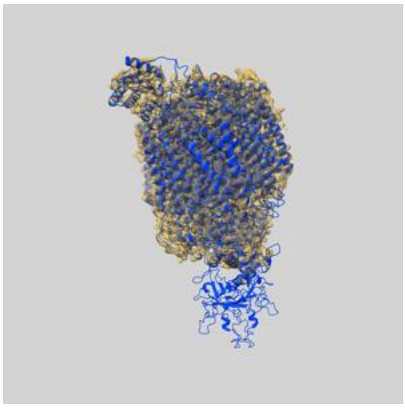
9.1 Map-model overlay



X



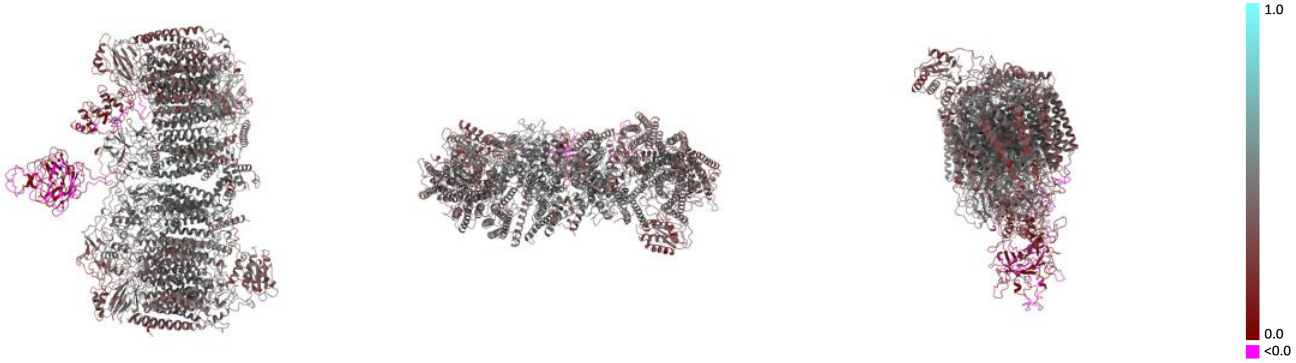
Y



Z

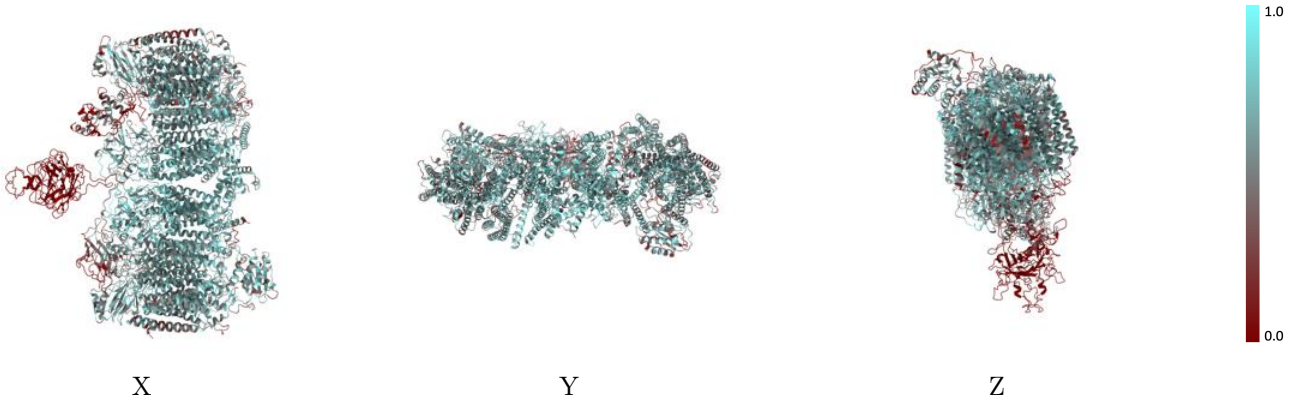
The images above show the 3D surface view of the map at the recommended contour level 0.634 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



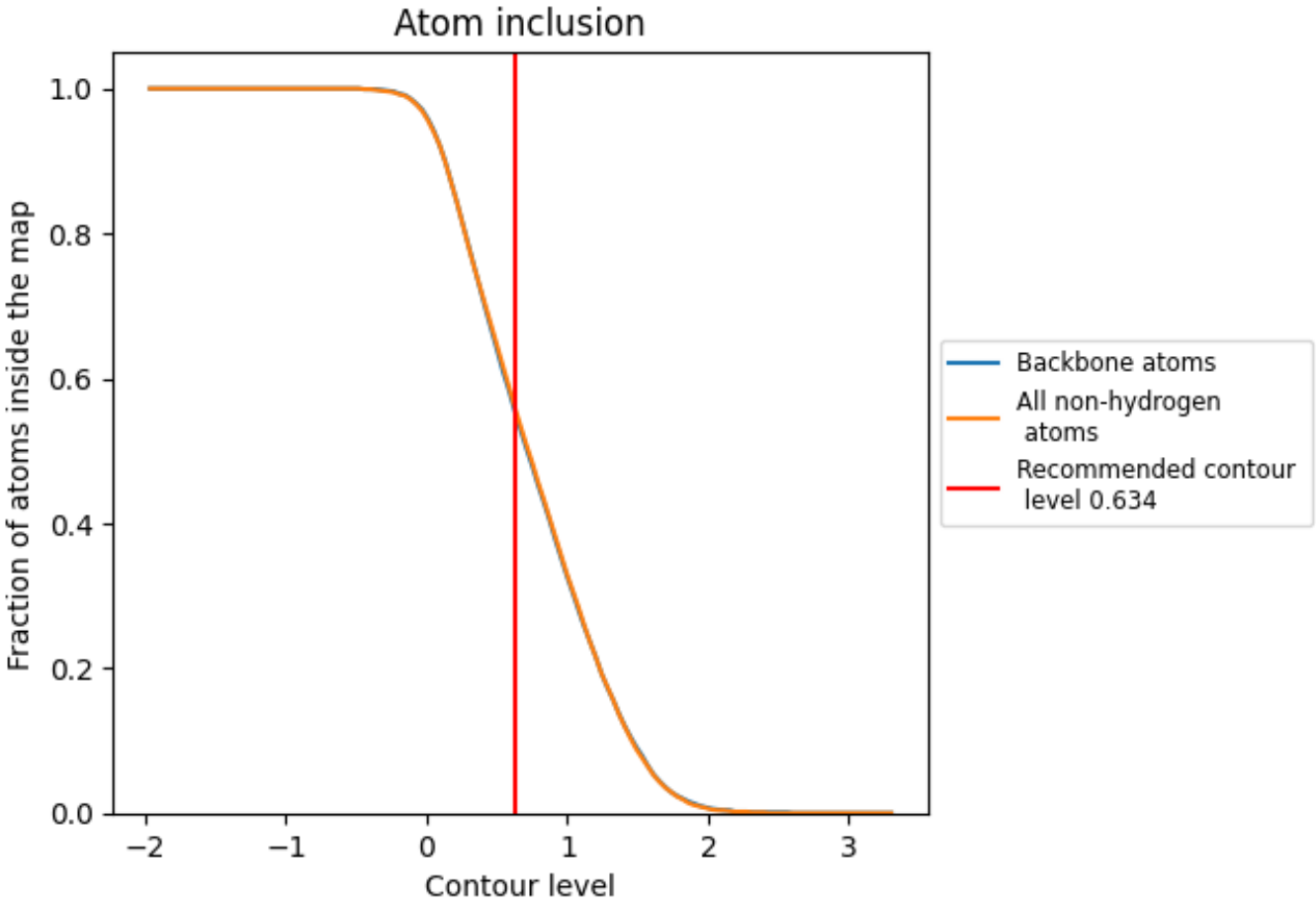
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.634).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.634) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5550	0.3950
D	0.1060	0.1100
E	0.6900	0.4680
F	0.6820	0.4590
G	0.1050	0.1110
I	0.6220	0.4400
J	0.4940	0.3960
K	0.5250	0.3690
L	0.6430	0.4400
M	0.6780	0.4330
O	0.2780	0.2240
P	0.5060	0.3970
Q	0.4680	0.3200
R	0.6210	0.4240
S	0.5620	0.3930
T	0.5170	0.3960
U	0.3950	0.3330
V	0.5040	0.3380
X	0.5640	0.4150
Y	0.6940	0.4470
Z	0.5570	0.4110
a	0.4750	0.3570
b	0.5690	0.3640
c	0.2700	0.3450