Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 02:16 AM EDT

PDB ID	:	7RH6 / pdb_00007rh6
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 (i) symbol.

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

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

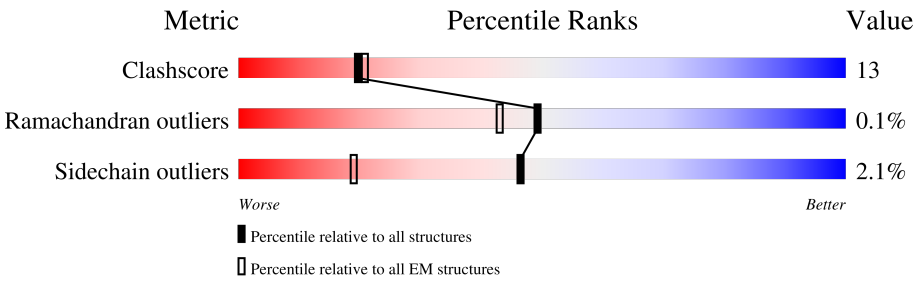
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

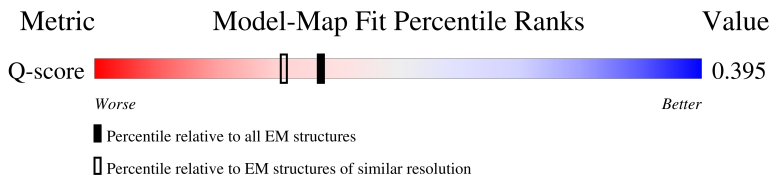
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	I	223	10% 80% 19% •
1	O	223	63% 39% 39% 15% • 6%
2	L	552	• 78% 22%
2	R	552	5% 79% 20% •

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Mol	Chain	Length	Quality of chain
3	M	382	6% 85% 15%
3	Y	382	84% 16%
4	S	203	15% 84% 16%
4	X	203	14% 82% 17%
5	E	535	82% 18%
5	F	535	81% 19%
6	J	100	17% 72% 20% 8%
6	P	100	19% 83% 8% 8%
7	D	216	90% 97%
7	G	216	89% 99%
8	K	312	32% 83% 17%
8	Q	312	36% 80% 19%
9	T	139	8% 81% 19%
9	Z	139	13% 81% 19%
10	U	79	42% 81% 19%
10	a	79	28% 92% 8%
11	V	145	31% 84% 15%
11	b	145	19% 83% 17%
12	c	159	65% 84% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	HEC	I	302	X	-	-	-
13	HEC	O	301	X	-	-	-
13	HEC	O	302	X	-	X	-
18	CDL	L	604	-	-	X	-
18	CDL	S	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
			Total	C	H	N	O	S		
1	O	210	3014	948	1483	276	295	12	0	0
1	I	223	3187	1008	1564	289	314	12	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

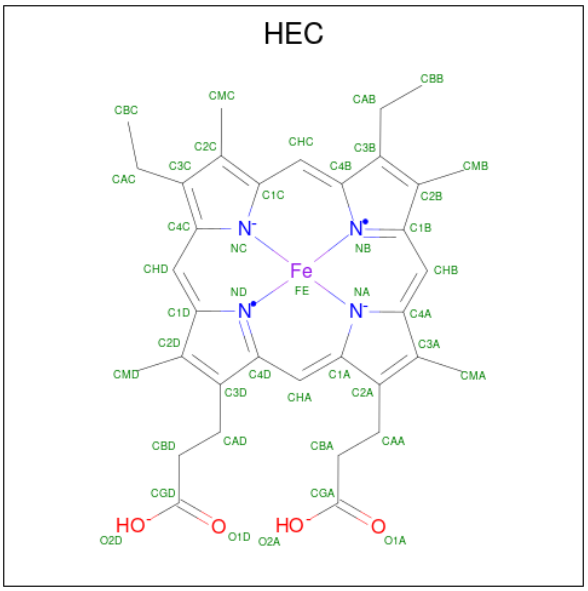
- Molecule 11 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

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

- Molecule 12 is a protein called LpqE protein.

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

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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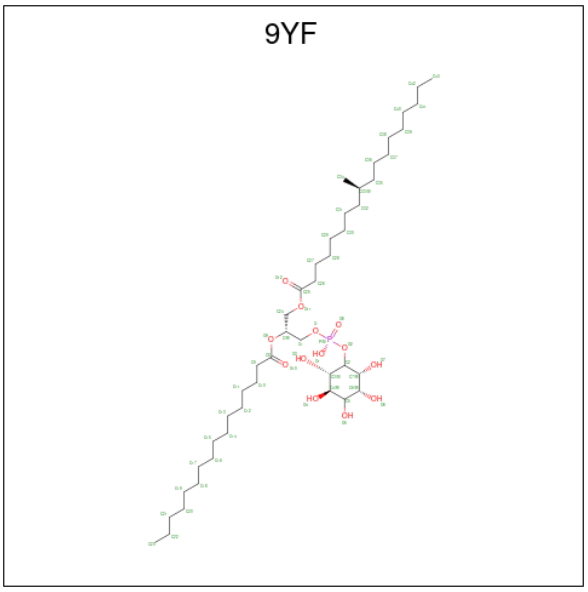
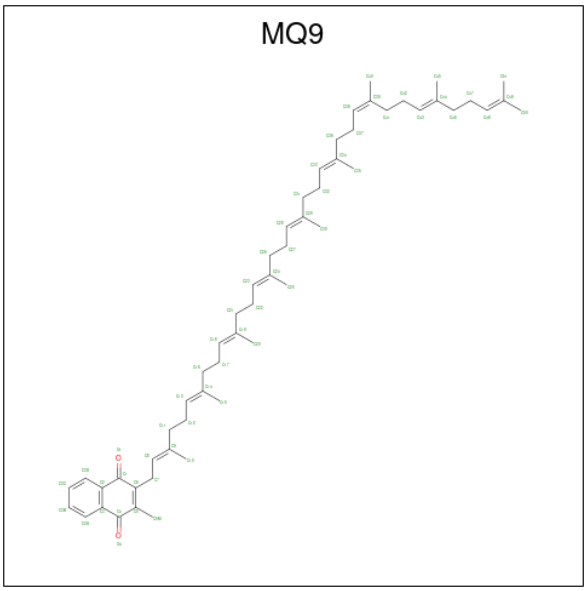
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
13	I	1	75	34	1	32	4	4	0

- 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 (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



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

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

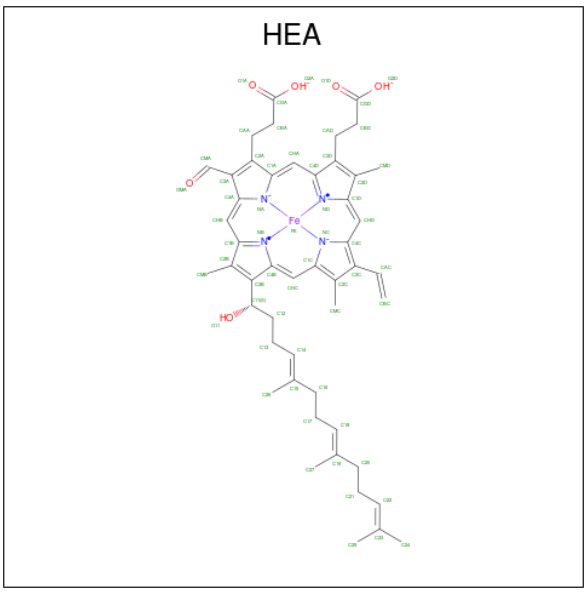


Mol	Chain	Residues	Atoms				AltConf
15	O	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	T	1	Total	C	H	O	0
			138	56	80	2	
15	Z	1	Total	C	H	O	0
			138	56	80	2	
15	I	1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

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

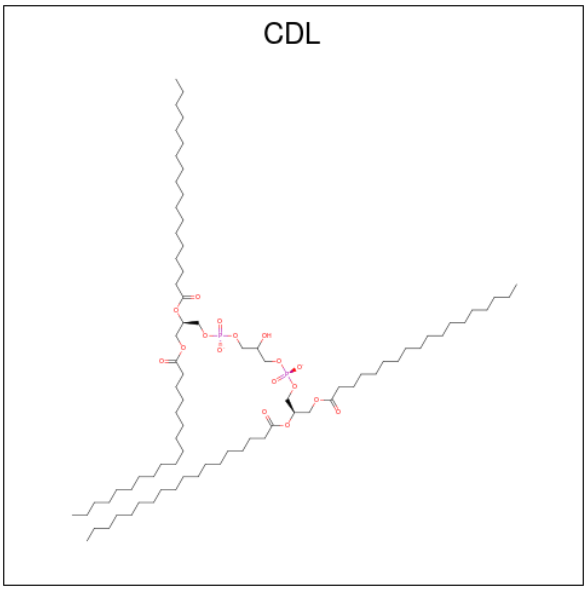
Mol	Chain	Residues	Atoms		AltConf
16	R	1	Total	Cu	0
			1	1	
16	L	1	Total	Cu	0
			1	1	
16	Q	2	Total	Cu	0
			2	2	
16	K	2	Total	Cu	0
			2	2	

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



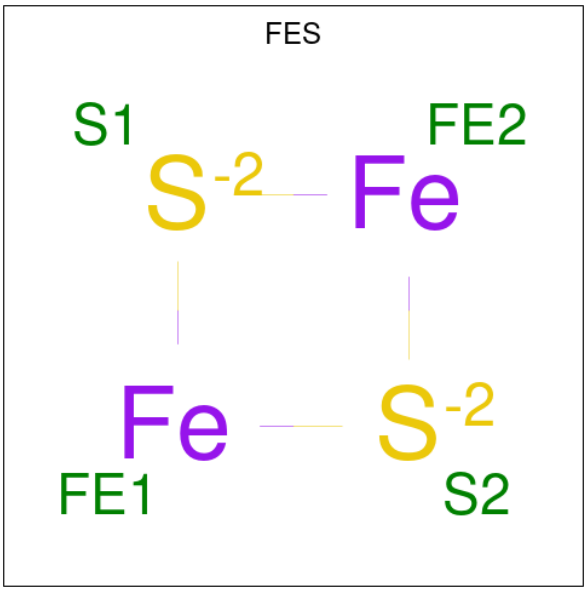
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
17	R	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
17	R	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
17	L	1	114	49	1	54	4	6	0
			Total	C	Fe	H	N	O	
17	L	1	114	49	1	54	4	6	0

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



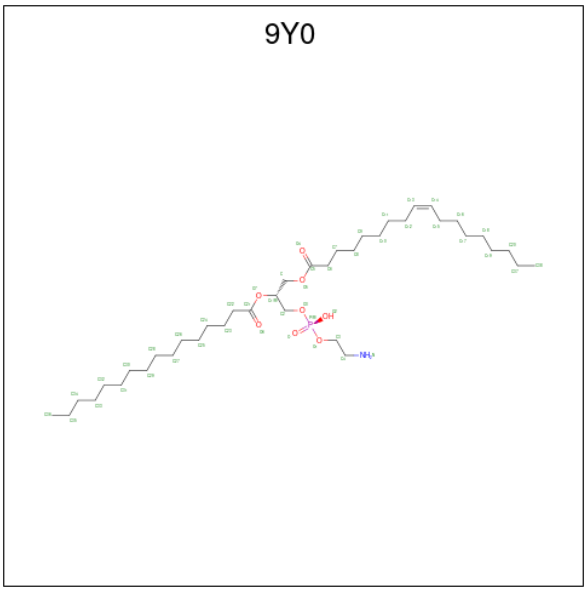
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	R	1	76	57	17	2	0
18	S	1	76	57	17	2	0
18	E	1	76	57	17	2	0
18	E	1	76	57	17	2	0
18	F	1	76	57	17	2	0
18	F	1	76	57	17	2	0
18	L	1	76	57	17	2	0
18	J	1	76	57	17	2	0
18	T	1	76	57	17	2	0
18	T	1	76	57	17	2	0
18	T	1	76	57	17	2	0
18	P	1	76	57	17	2	0
18	X	1	76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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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



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

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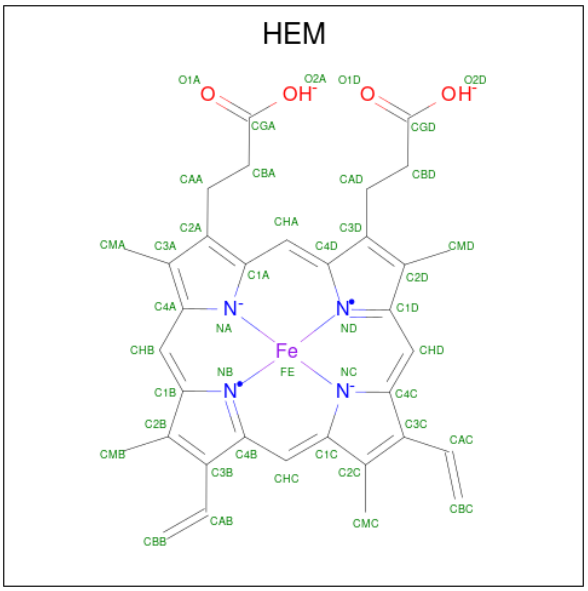
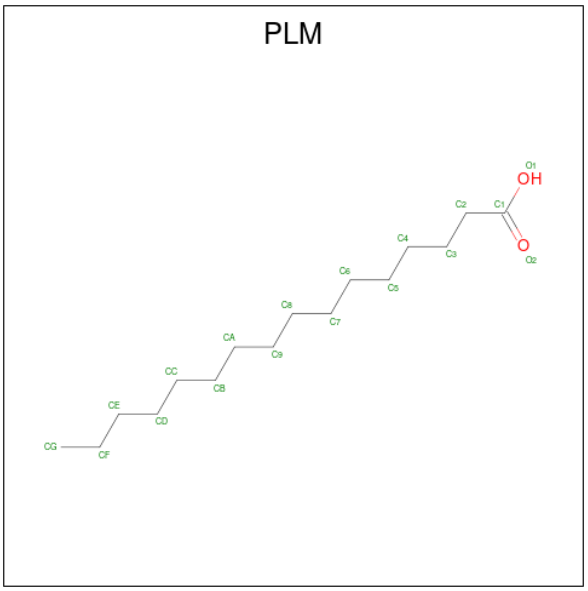
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
20	F	1	123	39	74	1	8	1	0
			Total	C	H	N	O	P	
20	J	1	124	39	75	1	8	1	0
			Total	C	H	N	O	P	
20	J	1	124	39	75	1	8	1	0
			Total	C	H	N	O	P	
20	X	1	124	39	75	1	8	1	0

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



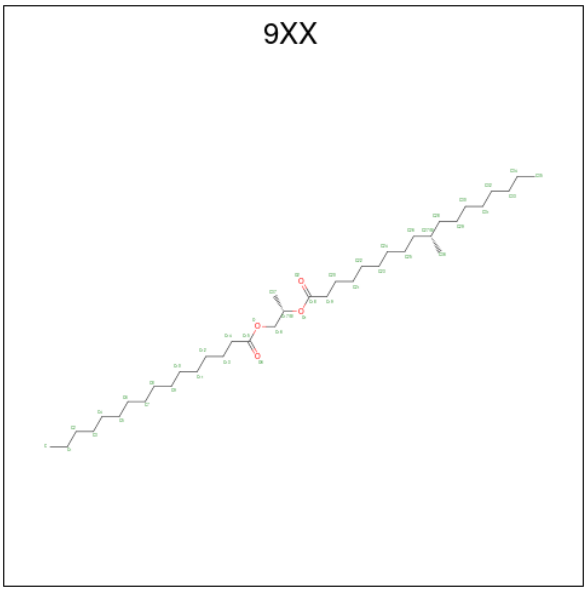
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
21	E	1	69	33	1	27	4	4	0
			Total	C	Fe	H	N	O	
21	E	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
21	F	1	69	33	1	27	4	4	0
			Total	C	Fe	H	N	O	
21	F	1	73	34	1	30	4	4	0

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



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

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



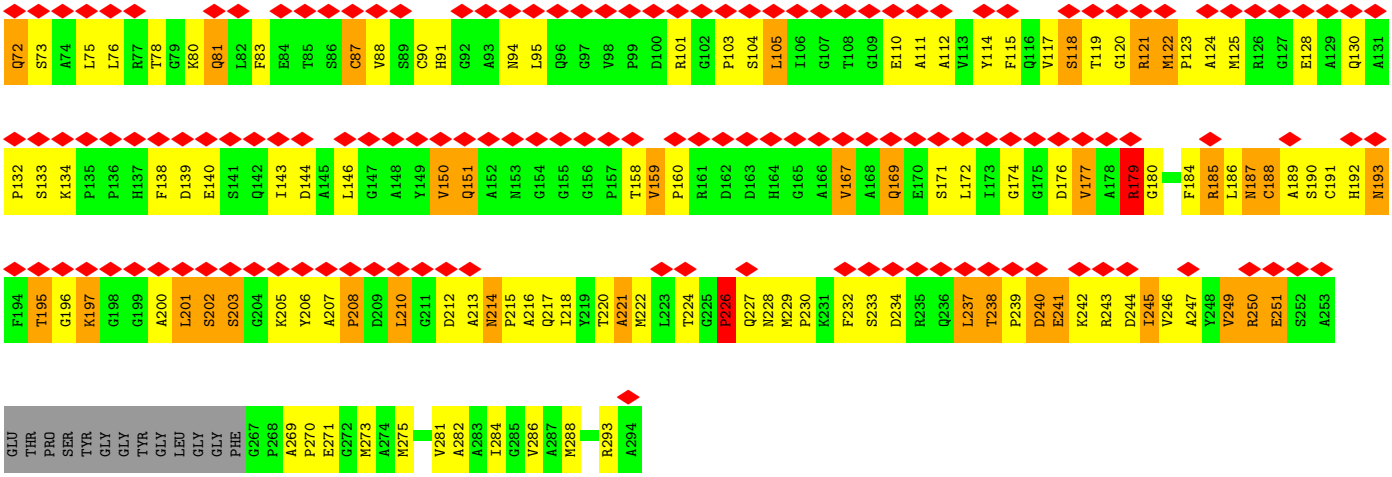
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
23	D	1	83	28	51	4	0
			Total	C	H	O	
23	G	1	83	28	51	4	0
			Total	C	H	O	
23	c	1	115	38	73	4	0

3 Residue-property plots (i)

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

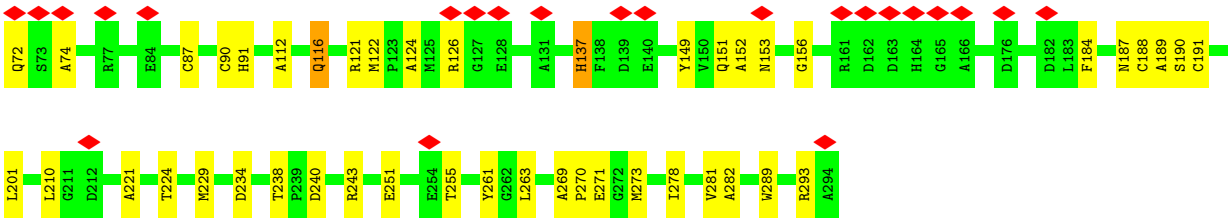
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain O:



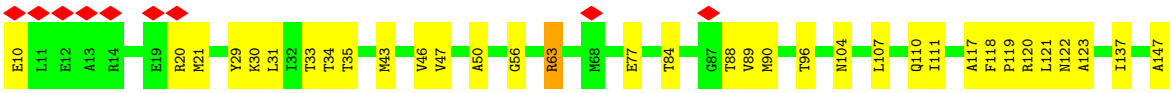
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

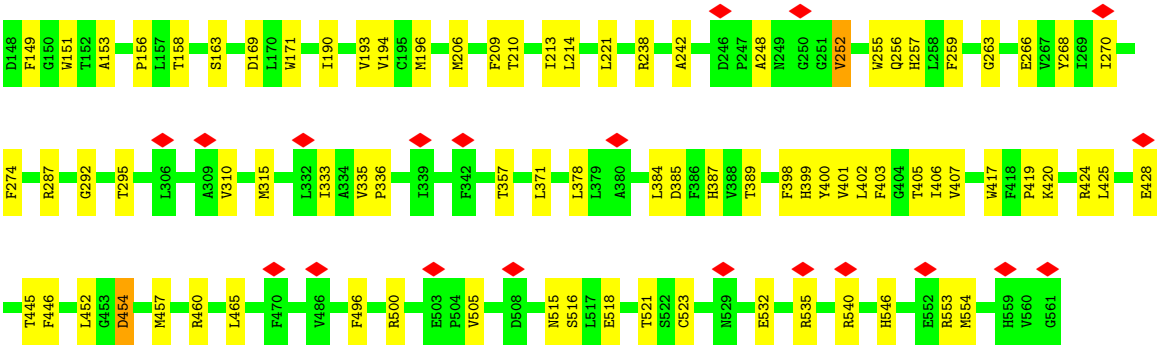
Chain I:



• Molecule 2: Cytochrome c oxidase subunit 1

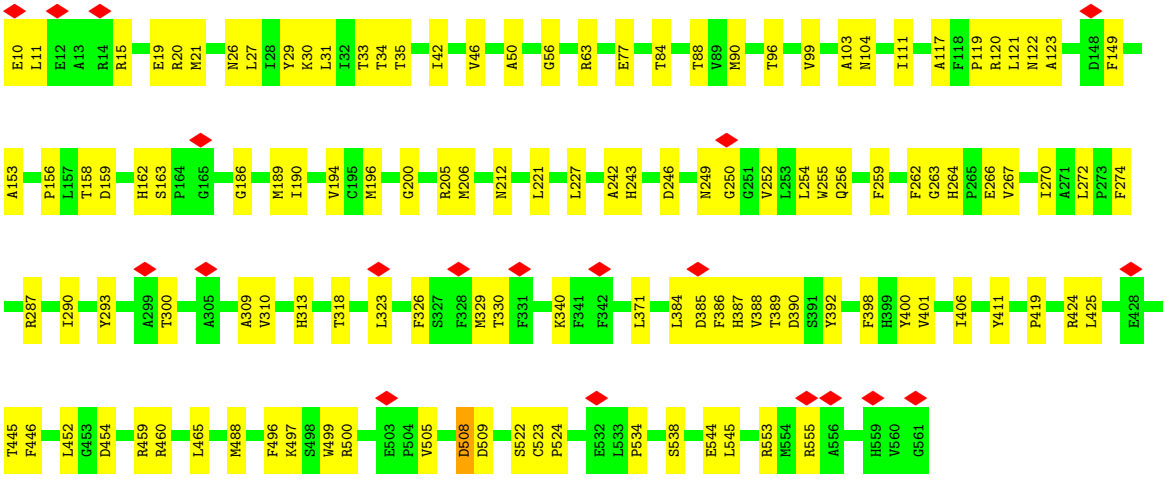
Chain R:





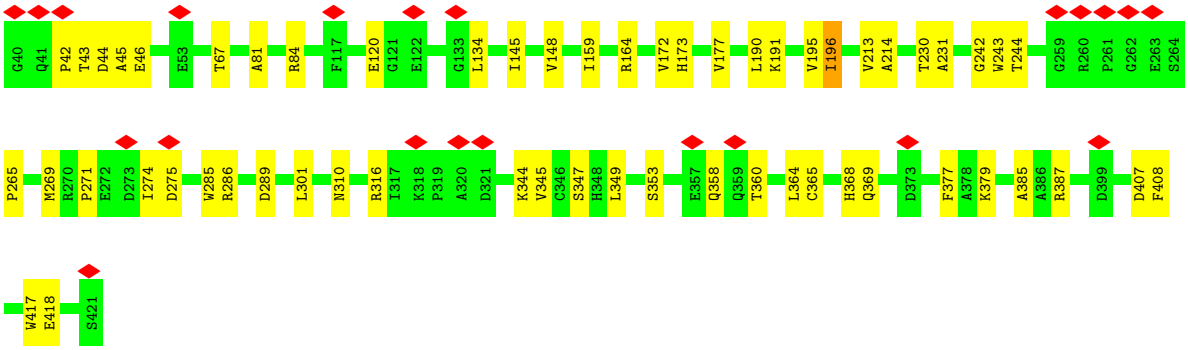
• Molecule 2: Cytochrome c oxidase subunit 1

Chain L:



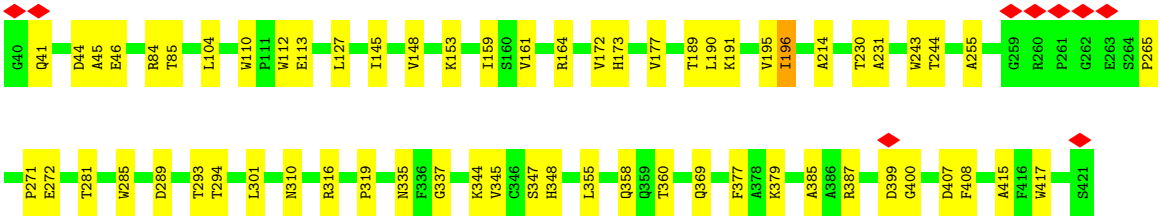
• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M:



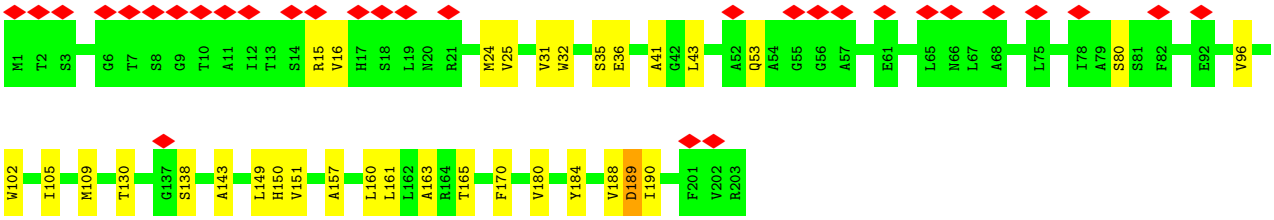
• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain Y:



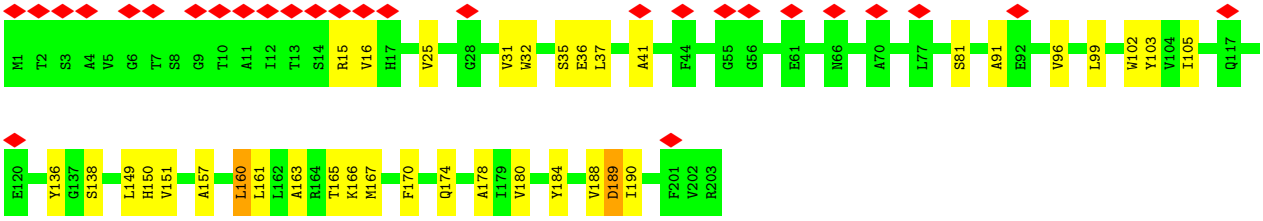
• Molecule 4: Cytochrome aa3 subunit 3

Chain S:



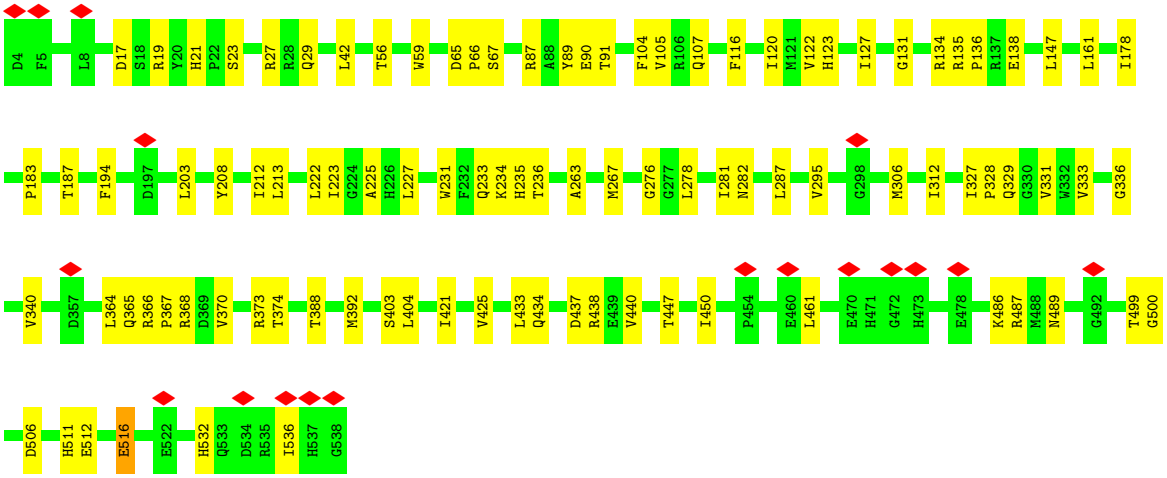
• Molecule 4: Cytochrome aa3 subunit 3

Chain X:



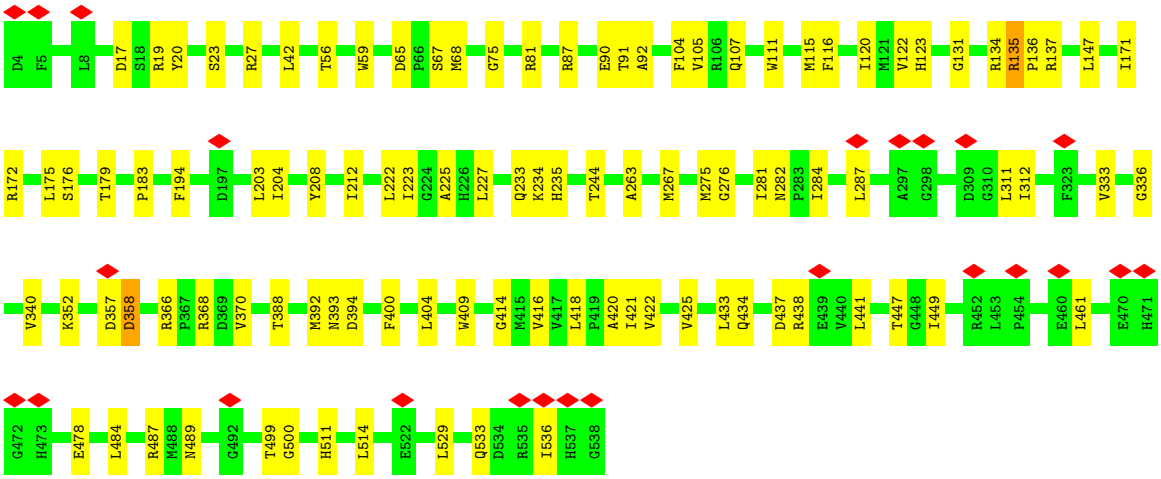
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit

Chain E:



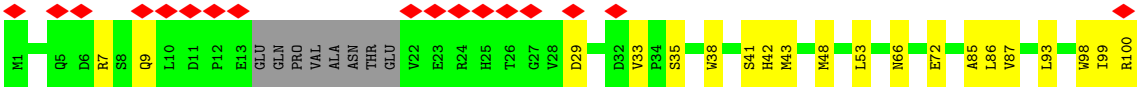
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit

Chain F:



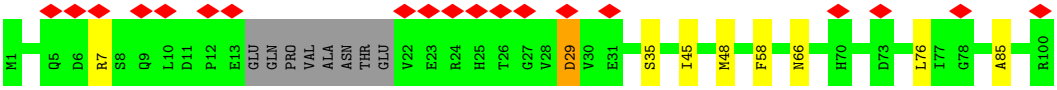
- Molecule 6: Putative conserved transmembrane protein

Chain J:



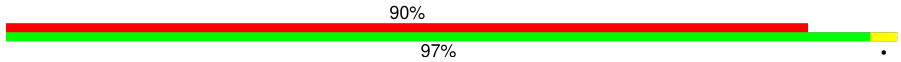
- Molecule 6: Putative conserved transmembrane protein

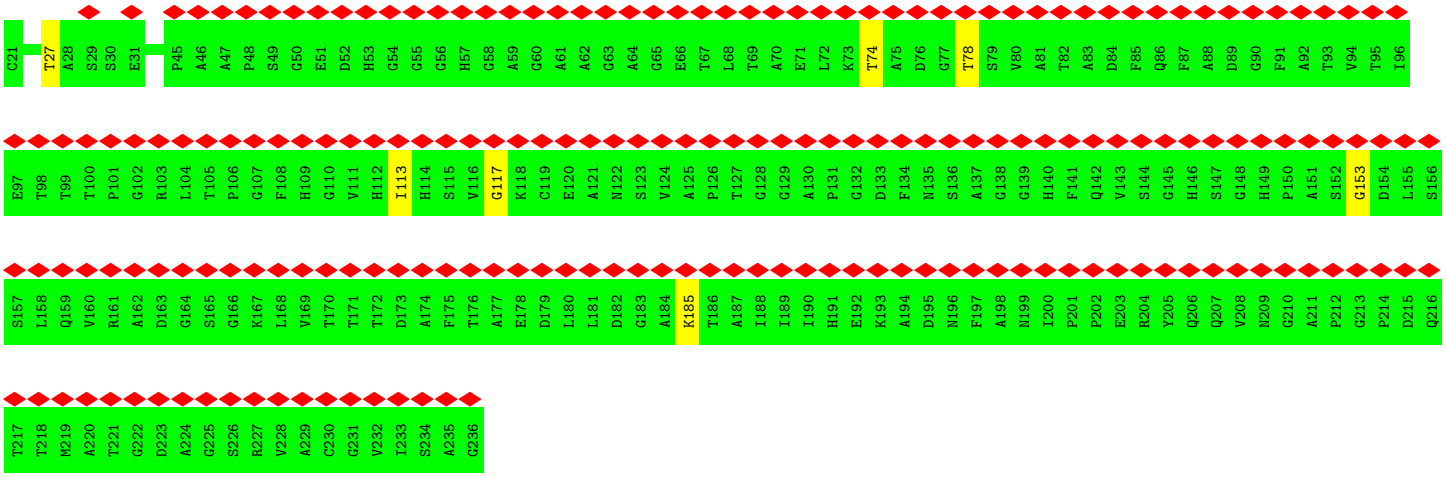
Chain P:



- Molecule 7: Superoxide dismutase [Cu-Zn]

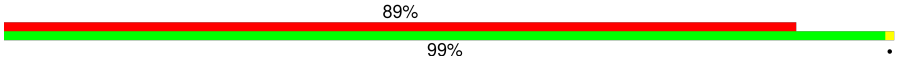
Chain D:

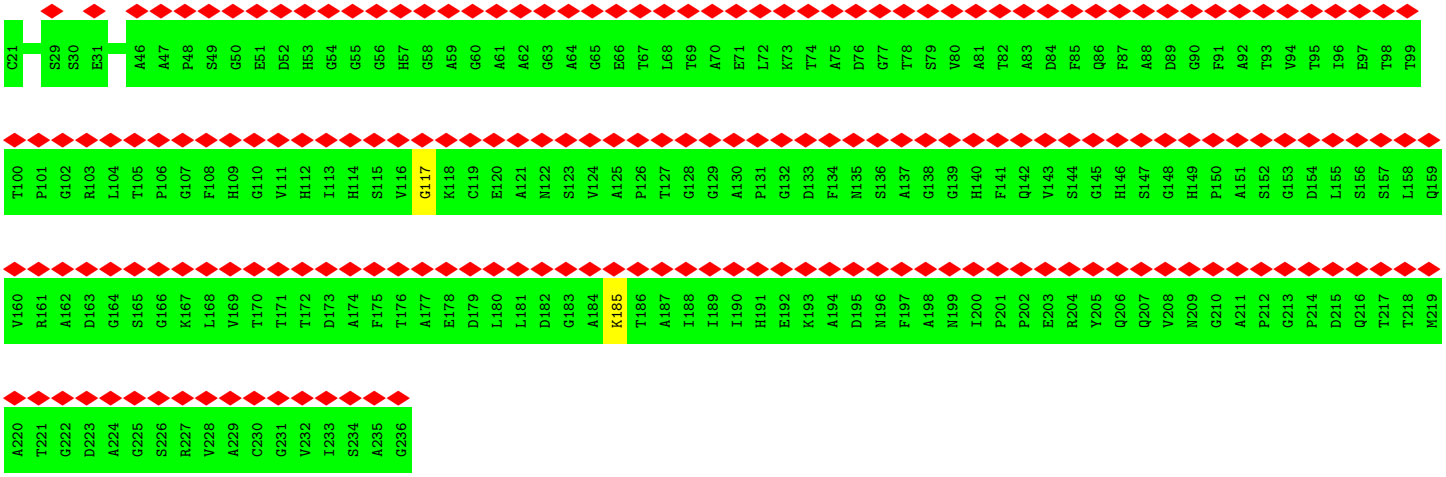




• Molecule 7: Superoxide dismutase [Cu-Zn]

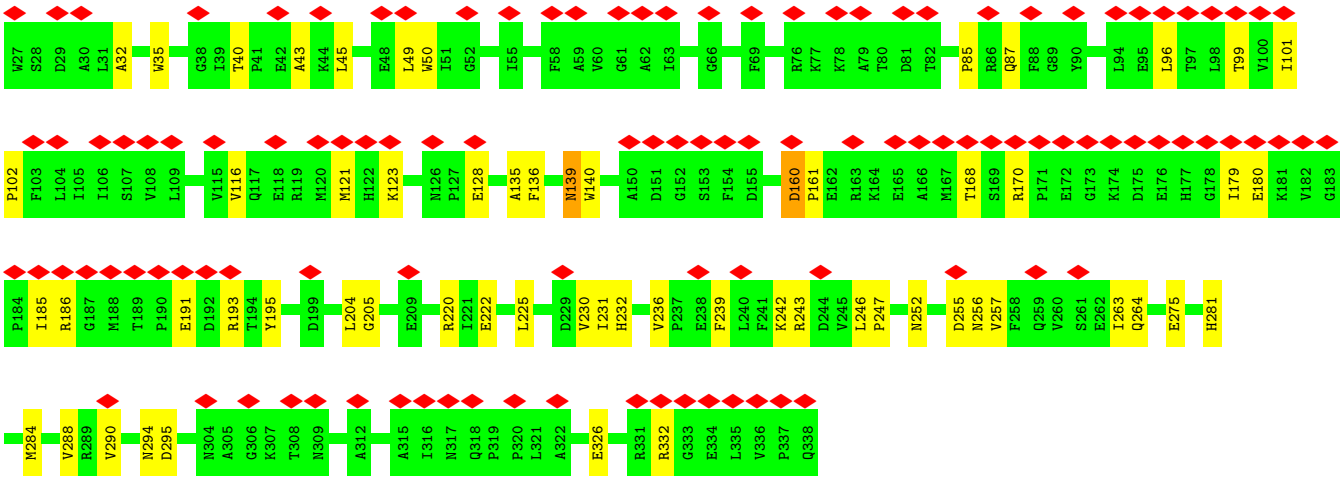
Chain G:





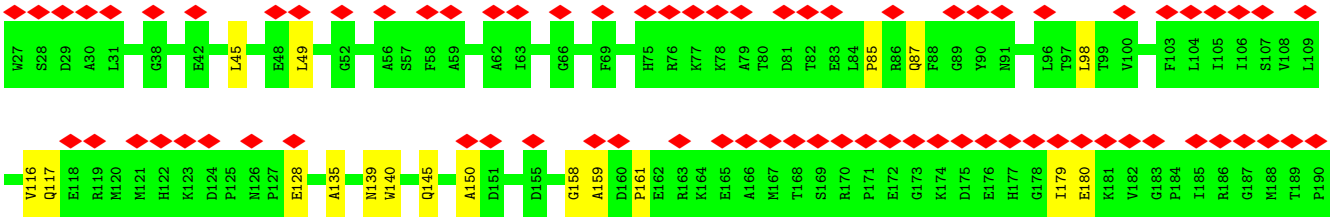
• Molecule 8: Cytochrome aa3 subunit 2

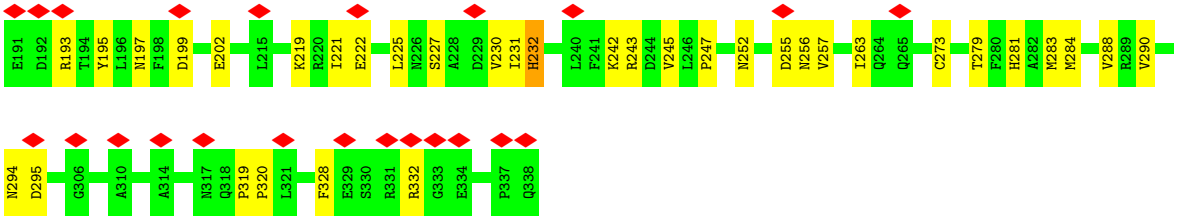
Chain Q:



• Molecule 8: Cytochrome aa3 subunit 2

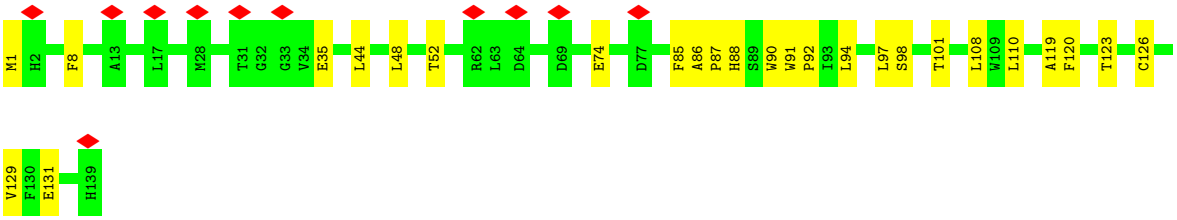
Chain K:





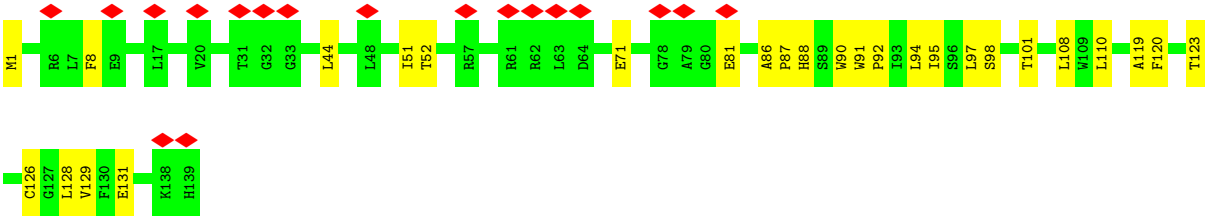
• Molecule 9: Cytochrome c oxidase polypeptide 4

Chain T:



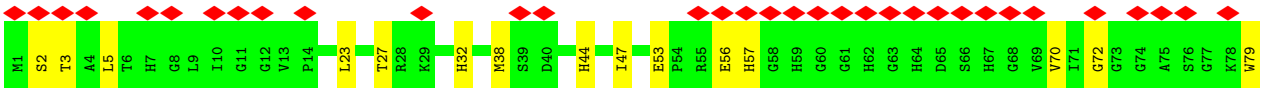
• Molecule 9: Cytochrome c oxidase polypeptide 4

Chain Z:



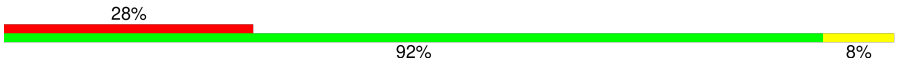
• Molecule 10: Cytochrome c oxidase subunit CtaJ

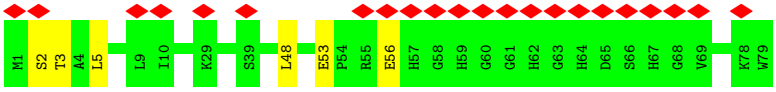
Chain U:



• Molecule 10: Cytochrome c oxidase subunit CtaJ

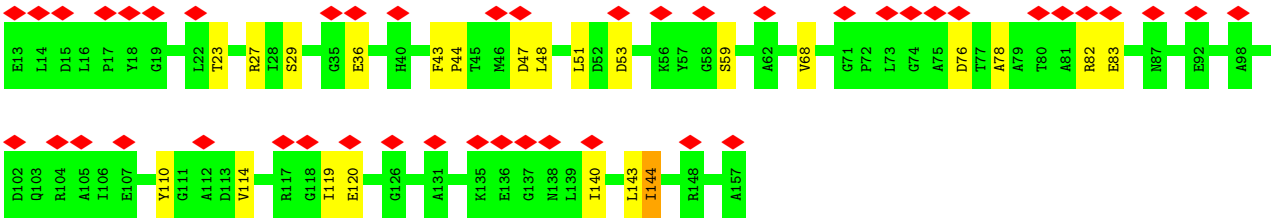
Chain a:





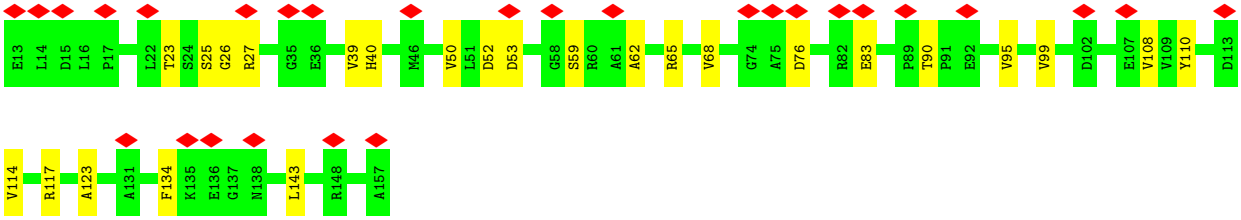
• Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:



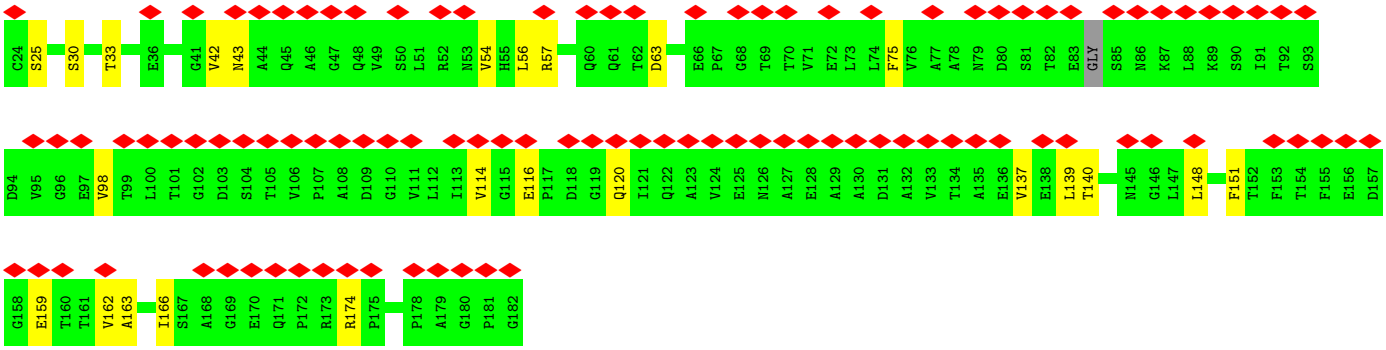
- Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9XX, HEM, 9YF, CDL, HEA, HEC, MQ9, PLM, FES, CU, 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	0.18	0/1660	0.39	0/2250
1	O	0.95	1/1563 (0.1%)	1.49	12/2117 (0.6%)
2	L	0.17	0/4530	0.34	0/6188
2	R	0.17	0/4530	0.33	0/6188
3	M	0.17	0/3056	0.34	0/4142
3	Y	0.18	0/3056	0.33	0/4142
4	S	0.17	0/1608	0.32	0/2195
4	X	0.18	0/1608	0.32	0/2195
5	E	0.19	0/4314	0.35	0/5882
5	F	0.18	0/4314	0.34	0/5882
6	J	0.15	0/757	0.29	0/1027
6	P	0.15	0/757	0.29	0/1027
7	D	0.14	0/1099	0.33	0/1519
7	G	0.13	0/1099	0.34	0/1519
8	K	0.18	0/2534	0.37	0/3451
8	Q	0.19	0/2534	0.36	0/3451
9	T	0.15	0/1112	0.31	0/1524
9	Z	0.17	0/1112	0.31	0/1524
10	U	0.12	0/613	0.27	0/836
10	a	0.12	0/613	0.28	0/836
11	V	0.16	0/1059	0.34	0/1446
11	b	0.15	0/1059	0.35	0/1446
12	c	0.13	0/1166	0.33	0/1599
All	All	0.24	1/45753 (0.0%)	0.43	12/62386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	C-O	-5.37	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	177	VAL	N-CA-C	-8.02	104.94	112.96
1	O	221	ALA	N-CA-C	-7.99	101.87	111.69
1	O	88	VAL	N-CA-C	-7.66	102.66	113.07
1	O	196	GLY	N-CA-C	-6.42	106.06	115.63
1	O	87	CYS	CB-CA-C	-5.89	101.48	111.02
1	O	179	ARG	N-CA-C	-5.72	105.79	112.89
1	O	180	GLY	N-CA-C	-5.53	106.91	113.99
1	O	208	PRO	N-CA-C	5.49	119.64	111.41
1	O	197	LYS	N-CA-C	-5.39	102.77	110.59
1	O	226	PRO	CA-C-N	-5.16	115.72	123.00
1	O	226	PRO	C-N-CA	-5.16	115.72	123.00
1	O	187	ASN	CA-C-O	-5.14	114.84	120.70

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	43	0
1	O	1531	1483	1484	208	0
2	L	4370	4347	4346	104	0
2	R	4370	4346	4345	106	0
3	M	2977	2984	2984	44	0
3	Y	2977	2984	2984	48	0
4	S	1560	1548	1547	64	0
4	X	1560	1548	1547	82	0
5	E	4181	4203	4202	81	0
5	F	4181	4200	4199	85	0
6	J	736	718	717	14	0
6	P	736	717	717	10	0
7	D	1092	640	640	3	0
7	G	1092	640	640	1	0
8	K	2465	2392	2392	39	0
8	Q	2465	2391	2391	70	0
9	T	1077	1059	1058	62	0
9	Z	1077	1058	1058	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	U	591	576	576	10	0
10	a	591	576	576	5	0
11	V	1041	1052	1052	18	0
11	b	1041	1052	1052	18	0
12	c	1149	1110	1110	20	0
13	I	86	64	64	13	0
13	O	86	64	64	39	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	5	0
15	F	116	160	160	4	0
15	I	58	80	80	1	0
15	O	58	80	80	1	0
15	T	58	80	80	0	0
15	Z	58	80	80	3	0
16	K	2	0	0	0	0
16	L	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
17	L	120	108	108	4	0
17	R	120	108	108	4	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	25	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	76	0
18	X	152	0	192	96	0
18	Z	152	0	192	77	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	G	11	16	16	0	0
22	c	17	31	31	1	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	1170	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 13.

All (1170) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:203:SER:C	8:Q:170:ARG:CG	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:a:53:GLU:OE1	11:b:59:SER:OG	1.93	0.87
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
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
2:L:20:ARG:NH2	11:b:53:ASP:OD1	2.10	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
1:O:203:SER:C	8:Q:170:ARG:HG3	2.04	0.81
9:Z:94:LEU:CD2	18:Z:202:CDL:H321	2.04	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:84:THR:OG1	2:L:149:PHE:O	1.98	0.81
12:c:30:SER:HG	12:c:33:THR:HG1	1.16	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
2:L:31:LEU:HD23	18:L:604:CDL:H381	1.62	0.79
2:L:300:THR:OG1	2:L:340:LYS:NZ	2.16	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
12:c:98:VAL:HG22	12:c:137:VAL:HG12	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:X:166:LYS:HZ3	18:X:302:CDL:CA5	1.98	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
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
12:c:63:ASP:OD1	3:Y:399:ASP:N	2.22	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:c:148:LEU:HD11	3:Y:319:PRO:HB3	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:117:VAL:HG22	1:O:122:MET:HE3	1.74	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
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
11:b:23:THR:OG1	11:b:27:ARG:O	2.11	0.68
18:L:604:CDL:H521	18:J:203:CDL:H321	1.76	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:MET:HE3	13:O:302:HEC:CHC	2.24	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
2:R:515:ASN:O	2:R:516:SER:OG	2.06	0.66
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
11:b:65:ARG:NH1	11:b:90:THR:OG1	2.27	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
12:c:98:VAL:HG22	12:c:137:VAL:CG1	2.26	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
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
4:S:16:VAL:HG23	4:S:24:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:c:120:GLN:NE2	1:I:152:ALA:O	2.30	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
1:O:124:ALA:HB2	1:O:134:LYS:HZ1	1.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:c:54:VAL:HG11	12:c:162:VAL:HG11	1.82	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
2:L:326:PHE:O	2:L:330:THR:OG1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:c:139:LEU:O	12:c:140:THR:OG1	2.16	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
1:O:275:MET:CE	5:F:275:MET:HE1	2.32	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
1:O:222:MET:HE2	13:O:302:HEC:HBB2	1.86	0.58
2:R:378:LEU:HD23	8:Q:50:TRP:CZ3	2.38	0.58
2:L:386:PHE:O	8:K:242:LYS:NZ	2.32	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
13:O:302:HEC:HBA1	13:O:302:HEC:HMA3	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:c:56:LEU:HD12	12:c:166:ILE:CD1	2.33	0.57
11:b:68:VAL:HG11	11:b:143:LEU:HD13	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
5:E:370:VAL:O	5:E:370:VAL:HG13	2.03	0.56
2:L:256:GLN:OE1	2:L:318:THR:HG21	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:c:42:VAL:HG12	12:c:54:VAL:HG13	1.89	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
12:c:148:LEU:HD12	12:c:163:ALA:O	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:X:99:LEU:C	4:X:99:LEU:HD23	2.33	0.54
4:X:81:SER:HG	4:X:189:ASP:CG	2.13	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
12:c:159:GLU:N	12:c:159:GLU:OE1	2.40	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
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:L:194:VAL:HG13	9:Z:1:MET:HE3	1.91	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:R:193:VAL:HG13	2:R:206:MET:HE1	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:606:CDL:OB7	18:F:705:CDL:H112	2.09	0.53
4:S:184:TYR:CD1	18:S:302:CDL:H732	2.44	0.52
8:Q:121:MET:HE1	8:Q:257:VAL:HG13	1.89	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
11:b:114:VAL:O	11:b:114:VAL:HG13	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:P:45:ILE:HD12	6:P:48:MET:HE3	1.91	0.51
1:O:232:PHE:HE2	13:O:302:HEC:HHC	1.76	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
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
5:F:175:LEU:O	5:F:179:THR:OG1	2.27	0.50
11:b:95:VAL:HG13	11:b:110:TYR:CE1	2.46	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
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
4:X:189:ASP:OD1	4:X:189:ASP:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:S:15:ARG:HB3	4:S:24:MET:HE3	1.94	0.50
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
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
11:b:25:SER:OG	11:b:26:GLY:N	2.44	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
1:O:275:MET:HE3	5:F:115:MET:N	2.27	0.49
2:R:515:ASN:N	2:R:515:ASN:OD1	2.44	0.49
5:E:131:GLY:O	5:E:134:ARG:NE	2.41	0.49
2:L:496:PHE:O	2:L:500:ARG:NH2	2.43	0.49
10:a:56:GLU:OE1	10:a:56:GLU:N	2.45	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
3:M:269:MET:HE1	3:M:274:ILE:HD11	1.95	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
12:c:63:ASP:OD1	3:Y:400:GLY:N	2.46	0.49
1:O:275:MET:HE1	5:F:275:MET:HE1	1.93	0.49
10:U:23:LEU:O	10:U:27:THR:OG1	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:b:76:ASP:OD1	11:b:76:ASP:N	2.46	0.49
1:O:95:LEU:HD11	1:O:150:VAL:CG1	2.42	0.48
1:O:275:MET:SD	5:F:275:MET:HE1	2.52	0.48
5:E:65:ASP:CB	5:E:91:THR:HG21	2.41	0.48
2:L:508:ASP:N	2:L:508:ASP:OD1	2.44	0.48
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
10:U:38:MET:HE3	10:U:79:TRP:CH2	2.48	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:188:CYS:HA	13:O:302:HEC:HMC3	1.95	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
5:E:281:ILE:HD12	1:I:271:GLU:CD	2.39	0.48
4:S:189:ASP:OD1	4:S:189:ASP:C	2.57	0.48
5:E:388:THR:HG22	5:E:392:MET:HE2	1.95	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
1:O:271:GLU:CD	5:F:281:ILE:HD12	2.38	0.48
2:L:221:LEU:HD22	4:X:35:SER:OG	2.14	0.48
1:O:222:MET:CE	13:O:302:HEC:HBB2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:275:MET:HE2	5:F:111:TRP:HE3	1.80	0.47
2:R:194:VAL:CG1	9:T:1:MET:HE3	2.44	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
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
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
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
4:X:167:MET:HE2	18:X:302:CDL:HA31	1.95	0.47
1:O:95:LEU:HD22	1:O:105:LEU:HD23	1.97	0.47
1:O:188:CYS:HA	13:O:302:HEC:CMC	2.45	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
5:F:388:THR:HG22	5:F:392:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:LEU:HD13	5:E:122:VAL:CG1	2.43	0.46
11:V:47:ASP:OD1	11:V:47:ASP:C	2.58	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
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:HBA1	13:O:302:HEC:CMA	2.44	0.46
2:R:35:THR:HG22	2:R:119:PRO:HB2	1.97	0.46
11:b:110:TYR:OH	11:b:123:ALA:HB2	2.16	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
11:b:99:VAL:HG21	11:b:134:PHE:CE2	2.51	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
12:c:75:PHE:CZ	12:c:114:VAL:HG11	2.50	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
12:c:56:LEU:HD12	12:c:166:ILE:HD13	1.95	0.46
1:O:282:ALA:HA	18:T:203:CDL:C57	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:Z:201:MQ9:H152	1:I:273:MET:HE3	1.97	0.45
2:R:56:GLY:N	2:R:90:MET:HE2	2.30	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
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
3:Y:335:ASN:ND2	3:Y:337:GLY:O	2.49	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
1:O:119:THR:HA	1:O:217:GLN:CD	2.40	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
2:L:309:ALA:HB3	2:L:329:MET:HE1	1.98	0.45
11:b:95:VAL:HG13	11:b:110:TYR:HE1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:c:42:VAL:O	12:c:54:VAL:HG12	2.16	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
1:O:176:ASP:CB	1:O:179:ARG:HG2	2.45	0.44
18:L:604:CDL:C64	22:c:201:PLM:HG2	2.47	0.44
8:Q:231:ILE:HD13	8:Q:246:LEU:CD2	2.35	0.44
8:K:159:ALA:C	8:K:161:PRO:HD3	2.43	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
1:O:288:MET:HE3	1:O:293:ARG:NH2	2.33	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
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: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: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
1:O:123:PRO:C	1:O:134:LYS:HZ3	2.25	0.44
5:E:392:MET:HE1	15:I:303:MQ9:C3C	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
2:L:20:ARG:NH1	11:b:52:ASP:OD1	2.45	0.44
2:L:538:SER:OG	2:L:544:GLU:OE2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:306:MET:HE1	1:I:269:ALA:HA	2.00	0.44
2:L:11:LEU:CD1	10:a:48:LEU:HD22	2.47	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
3:M:148:VAL:HG21	5:F:267:MET:HE2	1.99	0.44
3:M:358:GLN:C	3:M:360:THR:H	2.25	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
5:E:512:GLU:O	5:E:516:GLU:CD	2.61	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:323:LEU:HD23	8:K:117:GLN:CD	2.42	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
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
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
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
2:R:252:VAL:HG22	8:Q:252:ASN:CG	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:233:GLN:O	5:F:234:LYS:C	2.60	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
12:c:57:ARG:NH1	12:c:116:GLU:O	2.46	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:E:233:GLN:O	5:E:234:LYS:C	2.62	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
2:L:313:HIS:CD2	2:L:313:HIS:C	2.96	0.43
8:K:193:ARG:NH2	1:I:137:HIS:O	2.52	0.43
12:c:174:ARG:NH1	3:Y:272:GLU:OE2	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:208:PRO:HG3	13:O:302:HEC:HAA2	2.01	0.43
3:M:134:LEU:HD23	3:M:134:LEU:C	2.44	0.43
5:E:134:ARG:O	5:E:135:ARG:C	2.62	0.43
4:X:151:VAL:HG22	4:X:188:VAL:HG11	2.00	0.43
10:U:2:SER:O	10:U:5:LEU:N	2.51	0.43
4:X:136:TYR:CD1	4:X:136:TYR:C	2.96	0.43
12:c:56:LEU:HD11	12:c:151:PHE:HE2	1.84	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
10:a:2:SER:O	10:a:5:LEU:N	2.51	0.43
1:I:189:ALA:O	1:I:190:SER:C	2.62	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
2:R:31:LEU:O	2:R:34:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:K:98:LEU:HD12	8:K:98:LEU:C	2.44	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
3:Y:358:GLN:C	3:Y:360:THR:H	2.26	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
8:Q:179:ILE:O	8:Q:180:GLU:C	2.62	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
18:L:604:CDL:H381	18:L:604:CDL:H412	1.39	0.42
8:Q:121:MET:HE2	8:Q:123:LYS:HG3	2.02	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
11:b:62:ALA:O	11:b:117:ARG:NH2	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:97:LEU:HD13	18:T:201:CDL:H351	2.01	0.42
4:X:103:TYR:OH	4:X:178:ALA:O	2.38	0.42
11:b:68:VAL:HG13	11:b:143:LEU:HD22	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: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
6:J:99:ILE:HD11	11:b:50:VAL:HG22	2.00	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
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
5:F:68:MET:HE1	5:F:204:ILE:H	1.85	0.42
8:K:179:ILE:O	8:K:180:GLU:C	2.62	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:194:VAL:CG1	9:Z:1:MET:HE3	2.49	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
12:c:42:VAL:HG22	12:c:43:ASN:N	2.34	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
5:F:425:VAL:CG1	18:F:706:CDL:H371	2.45	0.41
2:L:26:ASN:OD1	2:L:26:ASN:C	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:b:108:VAL:HG12	11:b:110:TYR:CE1	2.55	0.41
1:I:122:MET:HE3	1:I:122:MET:HA	2.01	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
9:T:48:LEU:HD23	9:T:48:LEU:C	2.46	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
2:L:56:GLY:HA2	2:L:90:MET:HE2	2.02	0.41
1:O:238:THR:H	1:O:241:GLU:CD	2.28	0.41
3:M:417:TRP:CG	5:F:183:PRO:O	2.74	0.41
4:S:80:SER:HA	4:S:109:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:163:SER:O	2:L:163:SER:OG	2.36	0.41
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:E:267:MET:HE2	3:Y:148:VAL:HG21	2.03	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
2:R:194:VAL:HG13	9:T:1:MET:HE3	2.03	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
10:a:2:SER:O	10:a:3:THR:C	2.64	0.41
1:I:116:GLN:HG2	1:I:122:MET:SD	2.61	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: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
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
10:U:2:SER:O	10:U:3:THR:C	2.64	0.40
8:K:319:PRO:HA	8:K:320:PRO:HD3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:T:87:PRO:O	9:T:88:HIS:C	2.64	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: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
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
8:K:135:ALA:C	8:K:232:HIS:HE2	2.28	0.40
18:X:302:CDL:C77	18:Z:203:CDL:H532	2.51	0.40
9:Z:87:PRO:O	9:Z:88:HIS:C	2.62	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
2:L:398:PHE:CD1	2:L:398:PHE:C	2.99	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
11:b:39:VAL:HG23	11:b:40:HIS:N	2.37	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
2:R:122:ASN:OD1	2:R:122:ASN:C	2.65	0.40
4:S:41:ALA:HB2	9:T:44:LEU:CB	2.52	0.40
10:U:56:GLU:O	10:U:57:HIS:C	2.63	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	37
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%)	43	74
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%)	24	57
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%)	9	39
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%)	49	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%)	51	69
1	O	155/163 (95%)	111 (72%)	44 (28%)	0	2
2	L	452/453 (100%)	445 (98%)	7 (2%)	57	71
2	R	452/453 (100%)	447 (99%)	5 (1%)	65	74
3	M	312/312 (100%)	310 (99%)	2 (1%)	78	79
3	Y	312/312 (100%)	309 (99%)	3 (1%)	68	75
4	S	155/161 (96%)	153 (99%)	2 (1%)	61	72
4	X	155/161 (96%)	152 (98%)	3 (2%)	50	68
5	E	429/429 (100%)	424 (99%)	5 (1%)	63	73
5	F	429/429 (100%)	424 (99%)	5 (1%)	63	73
6	J	76/83 (92%)	73 (96%)	3 (4%)	28	54
6	P	76/83 (92%)	75 (99%)	1 (1%)	61	72
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%)	257 (99%)	3 (1%)	63	73
8	Q	260/266 (98%)	258 (99%)	2 (1%)	73	77
9	T	106/106 (100%)	106 (100%)	0	100	100
9	Z	106/106 (100%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	U	59/59 (100%)	59 (100%)	0	100	100
10	a	59/59 (100%)	59 (100%)	0	100	100
11	V	107/107 (100%)	105 (98%)	2 (2%)	50	68
11	b	107/107 (100%)	106 (99%)	1 (1%)	70	76
12	c	127/127 (100%)	126 (99%)	1 (1%)	73	77
All	All	4397/4707 (93%)	4305 (98%)	92 (2%)	46	66

All (92) 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	80	LYS
1	O	81	GLN
1	O	87	CYS
1	O	94	ASN
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	159	VAL
1	O	167	VAL
1	O	169	GLN
1	O	171	SER
1	O	177	VAL
1	O	179	ARG
1	O	185	ARG
1	O	188	CYS
1	O	193	ASN
1	O	195	THR

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Mol	Chain	Res	Type
1	O	201	LEU
1	O	203	SER
1	O	210	LEU
1	O	212	ASP
1	O	214	ASN
1	O	228	ASN
1	O	233	SER
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
2	R	63	ARG
2	R	252	VAL
2	R	454	ASP
2	R	505	VAL
2	R	523	CYS
3	M	120	GLU
3	M	196	ILE
4	S	130	THR
4	S	189	ASP
5	E	21	HIS
5	E	187	THR
5	E	295	VAL
5	E	403	SER
5	E	516	GLU
5	F	20	TYR
5	F	137	ARG
5	F	352	LYS
5	F	357	ASP
5	F	358	ASP
2	L	63	ARG
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	42	HIS
6	J	43	MET

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Mol	Chain	Res	Type
6	J	72	GLU
8	Q	139	ASN
8	Q	160	ASP
11	V	83	GLU
11	V	144	ILE
6	P	29	ASP
8	K	139	ASN
8	K	232	HIS
8	K	283	MET
4	X	160	LEU
4	X	174	GLN
4	X	189	ASP
11	b	83	GLU
12	c	25	SER
1	I	91	HIS
1	I	116	GLN
1	I	137	HIS
3	Y	161	VAL
3	Y	189	THR
3	Y	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	130	GLN
1	O	228	ASN
2	R	80	ASN
3	M	331	GLN
5	E	21	HIS
5	E	443	HIS
5	F	110	HIS
5	F	532	HIS
2	L	76	ASN
2	L	249	ASN
8	Q	145	GLN
8	Q	265	GLN
10	U	64	HIS
8	K	145	GLN
8	K	265	GLN
4	X	127	HIS
9	Z	139	HIS
10	a	64	HIS

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Mol	Chain	Res	Type
12	c	31	GLN
1	I	81	GLN
1	I	137	HIS
1	I	169	GLN
3	Y	180	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
13	HEC	O	302	1	50,50,50	2.95	30 (60%)	68,82,82	2.58	29 (42%)
15	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
18	CDL	E	606	-	75,75,99	0.34	0	81,87,111	0.42	0
15	MQ9	F	707	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
17	HEA	L	602	2	67,67,67	1.42	11 (16%)	81,103,103	2.38	30 (37%)
15	MQ9	F	701	-	59,59,59	2.45	23 (38%)	73,75,75	1.38	15 (20%)
18	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	9YF	Y	503	-	58,58,58	1.13	8 (13%)	68,71,71	1.49	9 (13%)
18	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
23	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
15	MQ9	I	303	-	59,59,59	2.39	22 (37%)	73,75,75	1.43	17 (23%)
14	9YF	I	304	-	58,58,58	1.08	5 (8%)	68,71,71	1.07	2 (2%)
18	CDL	J	203	-	75,75,99	0.33	0	81,87,111	0.45	0
15	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	14 (19%)
18	CDL	F	706	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
22	PLM	G	301	7	9,10,17	0.54	0	8,9,17	0.43	0
20	9Y0	S	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
18	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
23	9XX	c	202	18,12	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
21	HEM	F	703	5	50,50,50	1.40	6 (12%)	67,82,82	1.11	3 (4%)
20	9Y0	J	201	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
22	PLM	D	301	7	9,10,17	0.53	0	8,9,17	0.43	0
14	9YF	O	303	-	58,58,58	1.03	5 (8%)	68,71,71	1.06	3 (4%)
15	MQ9	E	604	-	59,59,59	2.42	22 (37%)	73,75,75	1.53	16 (21%)
15	MQ9	T	204	-	59,59,59	2.39	22 (37%)	73,75,75	1.59	16 (21%)
17	HEA	R	603	2	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
19	FES	M	501	3	0,4,4	-	-	-		
18	CDL	F	705	-	75,75,99	0.34	0	81,87,111	0.42	0
19	FES	Y	501	3	0,4,4	-	-	-		
13	HEC	O	301	-	50,50,50	2.90	27 (54%)	68,82,82	2.73	34 (50%)
18	CDL	T	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
21	HEM	E	601	5	49,49,50	1.38	7 (14%)	67,81,82	1.05	2 (2%)
17	HEA	L	603	2	67,67,67	1.37	10 (14%)	81,103,103	1.92	19 (23%)
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%)
20	9Y0	F	704	5	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
20	9Y0	J	202	-	48,48,48	1.16	3 (6%)	51,53,53	0.78	2 (3%)
15	MQ9	O	304	-	59,59,59	2.40	22 (37%)	73,75,75	1.43	17 (23%)
18	CDL	E	607	-	75,75,99	0.36	0	81,87,111	0.42	0
17	HEA	R	602	2	67,67,67	1.44	10 (14%)	81,103,103	2.33	31 (38%)
13	HEC	I	301	-	50,50,50	1.78	5 (10%)	68,82,82	1.32	5 (7%)
18	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
18	CDL	L	604	23	75,75,99	0.33	0	81,87,111	0.60	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	HEC	I	302	1	50,50,50	1.73	6 (12%)	68,82,82	1.65	11 (16%)
20	9Y0	X	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.90	2 (3%)
22	PLM	c	201	12	15,16,17	0.47	0	14,15,17	0.35	0
14	9YF	Y	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.29	9 (13%)
21	HEM	F	702	5	49,49,50	1.37	5 (10%)	67,81,82	1.03	2 (2%)
18	CDL	S	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
18	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
14	9YF	E	605	-	58,58,58	1.02	5 (8%)	68,71,71	1.32	7 (10%)
18	CDL	X	303	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
23	9XX	G	302	7	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
21	HEM	E	602	5	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)

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
13	HEC	O	302	1	1/1/7/7	10/14/54/54	-
15	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
18	CDL	E	606	-	-	49/86/86/110	-
15	MQ9	F	707	-	-	12/53/73/73	0/2/2/2
17	HEA	L	602	2	-	12/36/76/76	-
15	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
18	CDL	T	201	-	-	34/86/86/110	-
14	9YF	Y	503	-	-	22/54/78/78	0/1/1/1
18	CDL	T	202	-	-	46/86/86/110	-
23	9XX	D	302	-	-	9/33/33/43	-
15	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
14	9YF	I	304	-	-	22/54/78/78	0/1/1/1
18	CDL	J	203	-	-	48/86/86/110	-
15	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
18	CDL	F	706	-	-	43/86/86/110	-
22	PLM	G	301	7	-	2/8/8/15	-
20	9Y0	S	301	-	-	19/52/52/52	-
18	CDL	Z	203	-	-	38/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	9XX	c	202	18,12	-	16/43/43/43	-
21	HEM	F	703	5	-	0/14/54/54	-
20	9Y0	J	201	-	-	19/52/52/52	-
22	PLM	D	301	7	-	3/8/8/15	-
14	9YF	O	303	-	-	29/54/78/78	0/1/1/1
15	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
15	MQ9	T	204	-	-	13/53/73/73	0/2/2/2
17	HEA	R	603	2	-	3/36/76/76	-
21	HEM	E	601	5	-	2/12/52/54	-
18	CDL	F	705	-	-	49/86/86/110	-
19	FES	M	501	3	-	-	0/1/1/1
13	HEC	O	301	-	1/1/7/7	7/14/54/54	-
18	CDL	T	203	-	-	38/86/86/110	-
19	FES	Y	501	3	-	-	0/1/1/1
17	HEA	L	603	2	-	3/36/76/76	-
18	CDL	X	302	-	-	46/86/86/110	-
18	CDL	Z	202	-	-	34/86/86/110	-
20	9Y0	F	704	5	-	16/52/52/52	-
20	9Y0	J	202	-	-	25/52/52/52	-
15	MQ9	O	304	-	-	7/53/73/73	0/2/2/2
18	CDL	E	607	-	-	40/86/86/110	-
17	HEA	R	602	2	-	7/36/76/76	-
13	HEC	I	301	-	-	6/14/54/54	-
18	CDL	R	604	-	-	47/86/86/110	-
18	CDL	L	604	23	-	47/86/86/110	-
13	HEC	I	302	1	1/1/7/7	5/14/54/54	-
20	9Y0	X	301	-	-	17/52/52/52	-
22	PLM	c	201	12	-	5/14/14/15	-
14	9YF	Y	502	-	-	22/54/78/78	0/1/1/1
21	HEM	F	702	5	-	4/12/52/54	-
18	CDL	S	302	-	-	43/86/86/110	-
18	CDL	P	201	-	-	48/86/86/110	-
14	9YF	E	605	-	-	17/54/78/78	0/1/1/1
18	CDL	X	303	-	-	43/86/86/110	-
23	9XX	G	302	7	-	10/33/33/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	HEM	E	602	5	-	2/14/54/54	-

All (411) 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	I	301	HEC	C3D-C2D	7.86	1.53	1.36
13	I	302	HEC	C3D-C2D	7.71	1.53	1.36
13	O	302	HEC	C2A-C3A	5.64	1.48	1.36
13	O	301	HEC	C3B-C2B	5.36	1.48	1.36
13	O	302	HEC	C3D-C2D	5.14	1.47	1.36
13	O	302	HEC	CHC-C4B	5.14	1.48	1.38
13	O	301	HEC	C3D-C2D	5.11	1.47	1.36
13	O	301	HEC	C2A-C3A	5.10	1.47	1.36
15	F	707	MQ9	C2-C1	5.05	1.57	1.48
13	O	302	HEC	C3B-C2B	5.04	1.47	1.36
15	F	701	MQ9	C2-C1	5.01	1.57	1.48
15	E	604	MQ9	C2-C1	5.00	1.57	1.48
15	Z	201	MQ9	C2-C1	4.96	1.57	1.48
15	E	603	MQ9	C2-C1	4.95	1.57	1.48
13	O	301	HEC	CHD-C1D	4.94	1.48	1.38
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
13	O	301	HEC	FE-NC	4.80	2.11	1.95
13	O	302	HEC	CHA-C1A	4.80	1.47	1.38
13	O	301	HEC	CHB-C4A	4.76	1.47	1.38
13	O	301	HEC	FE-NA	4.76	2.10	1.95
15	I	303	MQ9	C3-C4	4.75	1.57	1.48
13	O	302	HEC	CHB-C4A	4.74	1.47	1.38
13	O	301	HEC	FE-ND	4.73	2.09	1.94
15	O	304	MQ9	C3-C4	4.68	1.57	1.48
13	O	301	HEC	CHA-C1A	4.67	1.47	1.38
15	F	707	MQ9	C3-C4	4.66	1.57	1.48
15	E	603	MQ9	C3-C4	4.65	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	301	HEC	FE-NB	4.64	2.09	1.94
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
13	O	302	HEC	CHD-C1D	4.59	1.47	1.38
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
13	O	302	HEC	FE-NB	4.34	2.08	1.94
13	I	301	HEC	FE-ND	4.30	2.08	1.94
13	O	302	HEC	FE-ND	4.30	2.08	1.94
17	R	603	HEA	C3B-C2B	4.30	1.44	1.34
13	O	302	HEC	FE-NA	4.22	2.09	1.95
17	L	603	HEA	C3B-C2B	4.20	1.44	1.34
15	T	204	MQ9	C11-C9	4.18	1.59	1.51
13	O	302	HEC	FE-NC	4.18	2.09	1.95
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	CHC-C4B	4.12	1.46	1.38
13	I	301	HEC	FE-NB	4.12	2.07	1.94
15	F	701	MQ9	C31-C29	4.10	1.59	1.51
15	Z	201	MQ9	C11-C9	4.05	1.59	1.51
13	O	301	HEC	CHD-C4C	4.03	1.48	1.39
15	E	604	MQ9	C11-C9	4.00	1.59	1.51
13	O	302	HEC	CHC-C1C	3.99	1.48	1.39
15	F	707	MQ9	C31-C29	3.98	1.59	1.51
13	O	301	HEC	C4B-NB	-3.96	1.33	1.40
13	O	301	HEC	CHA-C4D	3.93	1.48	1.39
21	E	602	HEM	FE-ND	3.92	2.07	1.94
15	O	304	MQ9	C11-C9	3.92	1.59	1.51
15	F	707	MQ9	C11-C9	3.92	1.59	1.51
13	O	302	HEC	CHA-C4D	3.91	1.48	1.39
23	G	302	9XX	O1-C17	-3.90	1.40	1.47
15	I	303	MQ9	C31-C29	3.88	1.59	1.51
13	I	302	HEC	FE-NB	3.86	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
13	O	302	HEC	C4B-NB	-3.84	1.33	1.40
15	T	204	MQ9	C31-C29	3.81	1.59	1.51
23	D	302	9XX	O1-C17	-3.81	1.40	1.47
15	F	701	MQ9	C11-C9	3.80	1.59	1.51
15	Z	201	MQ9	C31-C29	3.80	1.59	1.51
21	F	703	HEM	FE-ND	3.78	2.06	1.94
17	L	602	HEA	C3D-C2D	3.77	1.44	1.36
15	E	603	MQ9	C11-C9	3.75	1.59	1.51
13	O	302	HEC	CHD-C4C	3.75	1.47	1.39
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
21	E	602	HEM	FE-NB	3.59	2.05	1.94
13	O	301	HEC	CHB-C1B	3.58	1.47	1.39
13	I	302	HEC	FE-ND	3.56	2.05	1.94
17	R	602	HEA	C4D-C3D	3.54	1.51	1.45
13	O	302	HEC	C1D-ND	-3.54	1.34	1.40
17	R	603	HEA	C3D-C2D	3.54	1.44	1.36
17	R	602	HEA	C3A-C2A	3.45	1.45	1.37
13	O	302	HEC	CHB-C1B	3.45	1.47	1.39
17	L	602	HEA	C3A-C2A	3.42	1.45	1.37
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
21	E	601	HEM	FE-ND	3.22	2.04	1.94
21	E	601	HEM	FE-NB	3.21	2.04	1.94
15	I	303	MQ9	C27-C28	3.21	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	703	HEM	FE-NB	3.21	2.04	1.94
13	O	302	HEC	C3C-C2C	3.20	1.47	1.38
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
20	F	704	9Y0	O7-C1	-3.17	1.39	1.46
15	F	701	MQ9	C21-C19	3.17	1.57	1.51
13	O	301	HEC	CHC-C1C	3.17	1.46	1.39
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
15	F	707	MQ9	C16-C14	3.14	1.57	1.51
13	O	302	HEC	C1A-NA	-3.14	1.33	1.39
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
17	R	602	HEA	C4B-C3B	3.09	1.50	1.44
21	F	702	HEM	FE-NA	3.09	2.05	1.95
13	I	301	HEC	FE-NC	3.09	2.05	1.95
21	E	601	HEM	FE-NA	3.09	2.05	1.95
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
18	Z	203	CDL	OB8-CB7	3.07	1.42	1.33
18	S	302	CDL	OB8-CB7	3.06	1.42	1.33
21	F	702	HEM	FE-NB	3.06	2.04	1.94
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
17	L	603	HEA	C1C-C2C	3.05	1.50	1.43
15	F	707	MQ9	C27-C28	3.04	1.59	1.50
13	I	301	HEC	FE-NA	3.04	2.05	1.95
21	F	702	HEM	FE-ND	3.03	2.04	1.94
15	E	604	MQ9	C27-C28	3.02	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	701	MQ9	C7-C8	3.02	1.55	1.50
13	O	301	HEC	C1D-ND	-3.01	1.35	1.40
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
15	I	303	MQ9	C7-C8	2.97	1.55	1.50
17	L	603	HEA	C3A-C2A	2.97	1.43	1.37
13	O	301	HEC	C4C-C3C	2.97	1.50	1.44
21	F	702	HEM	FE-NC	2.97	2.04	1.95
13	O	302	HEC	C4A-NA	-2.96	1.34	1.39
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
13	I	302	HEC	FE-NC	2.94	2.04	1.95
20	J	201	9Y0	O5-C5	2.93	1.41	1.33
13	I	302	HEC	FE-NA	2.93	2.04	1.95
13	O	301	HEC	C3C-C2C	2.93	1.46	1.38
17	R	603	HEA	C1C-C2C	2.92	1.50	1.43
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
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
21	E	601	HEM	FE-NC	2.89	2.04	1.95
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
17	R	603	HEA	C3A-C2A	2.84	1.43	1.37
17	R	602	HEA	C1C-C2C	2.83	1.49	1.43
15	F	701	MQ9	C5M-C5	2.83	1.56	1.50
14	Y	502	9YF	O9-C8	2.83	1.42	1.34
17	L	602	HEA	C1C-C2C	2.83	1.49	1.43
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
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
15	O	304	MQ9	C20-C19	2.78	1.57	1.50
14	I	304	9YF	O9-C8	2.78	1.42	1.34
21	F	703	HEM	CAC-C3C	2.77	1.54	1.47
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	X	301	9Y0	O7-C21	2.71	1.41	1.34
18	T	201	CDL	OB8-CB7	2.69	1.41	1.33
21	E	602	HEM	CAC-C3C	2.68	1.54	1.47
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
21	F	703	HEM	FE-NA	2.65	2.03	1.95
13	O	302	HEC	C4D-ND	-2.65	1.33	1.38
13	O	301	HEC	C1A-NA	-2.65	1.34	1.39
14	E	605	9YF	O11-C25	2.65	1.41	1.33
18	S	302	CDL	OA6-CA4	-2.64	1.40	1.46
13	O	302	HEC	C1C-NC	-2.64	1.34	1.39
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
15	E	603	MQ9	C42-C43	2.60	1.58	1.50
13	O	302	HEC	C1C-C2C	2.59	1.49	1.43
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
18	Z	202	CDL	OB6-CB5	2.57	1.41	1.34
23	c	202	9XX	O-C15	2.56	1.40	1.33
13	O	301	HEC	C4A-NA	-2.56	1.34	1.39
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
15	T	204	MQ9	C5M-C5	2.55	1.56	1.50
15	F	707	MQ9	C41-C39	2.55	1.56	1.51
14	O	303	9YF	O11-C25	2.53	1.40	1.33
21	E	602	HEM	FE-NA	2.50	2.03	1.95
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
13	O	302	HEC	C4B-C3B	2.43	1.49	1.45
13	O	302	HEC	C1A-C2A	2.41	1.49	1.45
14	Y	502	9YF	P-O2	2.41	1.66	1.59
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	602	HEA	C1A-C2A	2.39	1.49	1.45
14	O	303	9YF	O11-C24	-2.38	1.39	1.45
13	O	302	HEC	C4C-NC	-2.38	1.35	1.39
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
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	R	602	HEA	C3C-C4C	2.35	1.49	1.42
13	O	301	HEC	C4D-C3D	2.35	1.49	1.45
13	O	302	HEC	C4C-C3C	2.34	1.49	1.44
17	L	603	HEA	C1D-ND	-2.34	1.36	1.40
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
17	L	602	HEA	C3C-C4C	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
15	I	303	MQ9	C28-C29	2.28	1.38	1.33
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
13	O	301	HEC	C1C-NC	-2.28	1.35	1.39
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
21	F	703	HEM	FE-NC	2.27	2.02	1.95
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
13	O	301	HEC	C1B-C2B	2.26	1.49	1.44
17	L	602	HEA	C1A-C2A	2.26	1.49	1.45
17	R	603	HEA	C3C-C4C	2.25	1.49	1.42
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
13	O	302	HEC	C1B-NB	-2.23	1.34	1.38
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
15	T	204	MQ9	C43-C44	2.18	1.38	1.33
17	R	603	HEA	C1B-C2B	2.17	1.48	1.44
13	O	302	HEC	C4D-C3D	2.17	1.48	1.45
14	Y	502	9YF	O11-C24	-2.16	1.40	1.45
17	L	603	HEA	C3C-C4C	2.16	1.49	1.42
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	603	MQ9	C3C-C3B	2.14	1.42	1.38
14	Y	503	9YF	O6-C6	-2.14	1.37	1.43
13	O	301	HEC	C4D-ND	-2.13	1.34	1.38
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
13	O	301	HEC	C1D-C2D	2.11	1.48	1.44
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
21	E	602	HEM	FE-NC	2.09	2.02	1.95
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
13	I	302	HEC	CMC-C2C	2.04	1.55	1.50
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
13	O	302	HEC	C1D-C2D	2.04	1.48	1.44
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
13	O	301	HEC	C1A-C2A	2.01	1.48	1.45
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 (439) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

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	O	301	HEC	CAC-C3C-C4C	7.37	135.06	124.91
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
13	O	301	HEC	C1B-C2B-C3B	-6.92	99.70	106.98
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
17	L	602	HEA	C3A-C2A-C1A	-6.20	101.18	107.05
13	O	302	HEC	CAC-C3C-C4C	6.17	133.41	124.91
13	O	302	HEC	C1B-C2B-C3B	-6.02	100.65	106.98
17	L	602	HEA	CAD-C3D-C4D	5.95	135.07	124.70
17	R	602	HEA	C3A-C2A-C1A	-5.94	101.42	107.05
13	O	302	HEC	CBC-CAC-C3C	5.65	127.74	112.42
17	R	603	HEA	C3A-C2A-C1A	-5.57	101.77	107.05
13	O	301	HEC	CBC-CAC-C3C	5.57	127.52	112.42
17	L	603	HEA	C3A-C2A-C1A	-5.52	101.82	107.05
13	I	302	HEC	C1D-ND-C4D	5.50	111.72	105.21
17	R	602	HEA	C12-C11-C3B	5.48	120.68	112.12
13	I	301	HEC	C1D-ND-C4D	5.37	111.56	105.21
14	Y	502	9YF	O9-C8-C9	5.29	122.94	111.48
13	O	301	HEC	C2B-C1B-NB	5.23	115.95	109.90
13	O	302	HEC	C2B-C1B-NB	5.13	115.83	109.90
13	I	302	HEC	CAB-C3B-C4B	5.13	131.47	124.79
14	Y	503	9YF	O9-C8-C9	5.06	122.43	111.48
13	O	302	HEC	C2A-C1A-NA	5.04	115.18	110.32
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
13	O	301	HEC	C1C-C2C-C3C	-4.86	101.25	106.82
17	R	603	HEA	C3D-C4D-ND	4.71	114.91	110.35
13	O	301	HEC	C2A-C1A-NA	4.70	114.86	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
18	Z	202	CDL	OB6-CB4-CB3	-4.64	91.69	108.34
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
13	O	301	HEC	CAC-C3C-C2C	-4.43	119.88	126.89
13	O	302	HEC	C1D-C2D-C3D	-4.42	102.33	106.98
17	L	602	HEA	CMC-C2C-C3C	4.38	136.85	126.55
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
13	O	302	HEC	CHA-C1A-NA	-4.36	119.71	124.45
17	L	603	HEA	C2A-C1A-NA	4.31	114.48	110.32
17	L	602	HEA	C2A-C1A-NA	4.29	114.46	110.32
13	O	301	HEC	C3D-C4D-ND	4.28	114.49	110.35
17	R	603	HEA	C2A-C1A-NA	4.27	114.44	110.32
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
17	R	603	HEA	CMC-C2C-C3C	4.15	136.32	126.55
13	O	301	HEC	C2C-C1C-NC	4.14	116.78	110.14
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	R	603	HEA	CHA-C1A-C2A	-4.11	118.38	124.86
13	O	302	HEC	C1C-C2C-C3C	-4.09	102.13	106.82
17	R	602	HEA	CMC-C2C-C3C	4.08	136.15	126.55
13	O	302	HEC	C2D-C1D-ND	4.07	114.52	109.84
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
13	O	301	HEC	C2D-C1D-ND	3.93	114.36	109.84
17	L	602	HEA	CMC-C2C-C1C	-3.92	119.45	125.42
17	R	602	HEA	C4D-C3D-C2D	-3.91	101.20	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
17	L	603	HEA	CHA-C1A-C2A	-3.89	118.72	124.86
13	O	301	HEC	CBB-CAB-C3B	3.88	122.95	112.42
17	R	602	HEA	C2A-C1A-NA	3.87	114.06	110.32
13	O	301	HEC	CAB-C3B-C2B	3.87	134.67	127.56
13	O	302	HEC	C1A-C2A-C3A	-3.84	102.05	107.11
13	O	301	HEC	CAB-C3B-C4B	-3.84	119.79	124.79
20	S	301	9Y0	O7-C21-C22	3.83	119.76	111.48
13	O	302	HEC	C3D-C4D-ND	3.81	114.03	110.35
13	O	301	HEC	C1D-C2D-C3D	-3.79	103.00	106.98
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
17	L	602	HEA	CHA-C1A-C2A	-3.74	118.96	124.86
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	O	302	HEC	CBB-CAB-C3B	3.68	122.41	112.42
17	R	602	HEA	CHA-C1A-C2A	-3.68	119.05	124.86
17	R	603	HEA	CMC-C2C-C1C	-3.66	119.85	125.42
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	I	302	HEC	CAB-C3B-C2B	-3.50	121.12	127.56
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
17	L	602	HEA	OMA-CMA-C3A	-3.43	117.88	125.62
13	O	302	HEC	CMC-C2C-C1C	3.42	130.63	125.42
15	F	707	MQ9	C12-C13-C14	-3.41	119.81	127.62
13	O	301	HEC	C3B-C4B-NB	3.40	113.91	110.17
13	I	302	HEC	CAC-C3C-C4C	3.38	129.57	124.91
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
17	R	602	HEA	OMA-CMA-C3A	-3.34	118.08	125.62
14	Y	502	9YF	O11-C25-C26	3.34	122.02	111.83
13	O	302	HEC	CHC-C4B-NB	-3.33	120.25	124.37
13	O	302	HEC	CHB-C4A-NA	-3.31	120.84	124.45
13	O	302	HEC	CHA-C4D-ND	-3.30	120.87	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
17	R	603	HEA	CAA-C2A-C1A	3.30	131.56	124.85
17	R	602	HEA	CMC-C2C-C1C	-3.30	120.40	125.42
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
13	O	301	HEC	C1A-C2A-C3A	-3.21	102.88	107.11
17	L	603	HEA	CAA-C2A-C1A	3.18	131.33	124.85
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	R	602	HEA	C3C-C2C-C1C	-3.15	103.46	107.17
17	L	603	HEA	CMC-C2C-C3C	3.15	133.96	126.55
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
13	O	301	HEC	CHB-C1B-NB	-3.05	121.14	124.42
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
17	R	603	HEA	CAA-CBA-CGA	-3.05	105.59	113.67
17	L	603	HEA	C3C-C2C-C1C	-3.04	103.58	107.17
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
13	O	302	HEC	CHD-C1D-ND	-3.02	120.63	124.37
14	Y	503	9YF	C6-C5-C4	3.02	116.14	110.83
13	O	302	HEC	CAC-C3C-C2C	-3.02	122.12	126.89
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
13	O	301	HEC	C4A-C3A-C2A	-2.96	102.58	106.97
15	Z	201	MQ9	C12-C13-C14	-2.96	120.85	127.62
13	O	302	HEC	C4A-C3A-C2A	-2.96	102.58	106.97
14	E	605	9YF	C6-C5-C4	2.96	116.02	110.83
17	L	602	HEA	C3C-C2C-C1C	-2.95	103.69	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	302	HEC	CHB-C1B-NB	-2.94	121.25	124.42
13	O	302	HEC	C3A-C4A-NA	2.93	115.05	109.64
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
13	I	302	HEC	CAC-C3C-C2C	-2.91	122.29	126.89
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
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
13	O	301	HEC	CHB-C4A-NA	-2.87	121.32	124.45
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
15	E	604	MQ9	C27-C28-C29	-2.83	121.14	127.62
17	R	603	HEA	C3C-C2C-C1C	-2.83	103.83	107.17
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
17	R	603	HEA	C3C-C4C-NC	2.82	112.17	109.80
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
13	O	301	HEC	C3A-C4A-NA	2.81	114.83	109.64
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
13	O	301	HEC	C4D-C3D-C2D	-2.79	102.83	106.89
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	202	CDL	OA6-CA5-OA7	-2.76	117.24	123.70
13	O	301	HEC	CMB-C2B-C3B	2.76	133.62	126.15
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
17	L	603	HEA	C3C-C4C-NC	2.73	112.09	109.80
13	I	301	HEC	C4B-NB-C1B	2.72	108.43	105.21
14	Y	503	9YF	O2-P-O8	-2.72	101.11	109.81
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
17	L	603	HEA	CAA-CBA-CGA	-2.70	106.50	113.67
15	F	701	MQ9	C20-C19-C21	2.70	119.91	115.23
17	L	602	HEA	C3C-C4C-NC	2.69	112.07	109.80
17	R	602	HEA	CAA-C2A-C1A	2.69	130.32	124.85
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
17	R	602	HEA	C3C-C4C-NC	2.66	112.04	109.80
17	L	602	HEA	CAA-C2A-C1A	2.66	130.27	124.85
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
13	O	302	HEC	C2C-C1C-NC	2.65	114.39	110.14
17	L	602	HEA	C27-C19-C20	2.63	119.80	115.23
13	O	301	HEC	CHA-C1A-NA	-2.62	121.60	124.45
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
13	O	301	HEC	CHC-C1C-C2C	-2.60	119.89	127.43
15	Z	201	MQ9	C30-C29-C31	2.59	119.73	115.23
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
13	I	302	HEC	C3C-C4C-NC	-2.56	107.31	110.15
17	R	602	HEA	C27-C19-C20	2.55	119.66	115.23
13	O	302	HEC	CMD-C2D-C1D	2.55	129.02	125.03
17	L	602	HEA	CAD-CBD-CGD	-2.55	106.91	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
13	O	301	HEC	CAD-C3D-C4D	2.53	129.11	124.70
21	E	602	HEM	CHD-C4C-NC	2.53	127.21	124.45
23	G	302	9XX	C17-O1-C18	-2.53	114.13	117.78
13	O	302	HEC	C4D-C3D-C2D	-2.53	103.21	106.89
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
15	O	304	MQ9	C30-C29-C28	-2.50	117.20	123.63
17	R	603	HEA	CHA-C1A-NA	2.50	127.18	124.45
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
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
13	I	301	HEC	C2A-C1A-NA	-2.47	107.94	110.32
13	I	302	HEC	C4B-NB-C1B	2.47	108.13	105.21
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
13	O	301	HEC	CMD-C2D-C1D	2.46	128.87	125.03
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
13	I	301	HEC	C3B-C4B-NB	-2.42	107.52	110.17
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
13	I	302	HEC	C3B-C4B-NB	-2.39	107.56	110.17
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
15	E	603	MQ9	C7-C8-C9	-2.35	122.77	126.83
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
17	R	602	HEA	CHD-C1D-ND	2.32	127.23	124.37
15	F	707	MQ9	C45-C44-C43	-2.31	117.68	123.63
13	I	302	HEC	C2A-C1A-NA	-2.31	108.09	110.32
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	301	HEC	CMA-C3A-C4A	2.30	128.79	124.73
15	O	304	MQ9	C35-C34-C36	2.30	119.23	115.23
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
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
13	O	301	HEC	CAD-CBD-CGD	-2.28	107.62	113.67
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
13	I	302	HEC	CHC-C4B-C3B	2.26	129.40	125.23
13	I	302	HEC	CHB-C1B-NB	2.26	126.86	124.42
17	R	602	HEA	CAA-CBA-CGA	-2.26	107.66	113.67
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
13	O	301	HEC	CMC-C2C-C1C	2.25	128.84	125.42
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
17	R	602	HEA	CHA-C1A-NA	2.24	126.89	124.45
14	O	303	9YF	O11-C25-O12	-2.23	118.06	123.63
13	O	301	HEC	CHD-C4C-NC	-2.22	119.83	123.86
17	R	602	HEA	CHB-C4A-NA	2.21	126.86	124.45
15	E	603	MQ9	C15-C14-C16	2.21	119.06	115.23
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	O	302	HEC	CHD-C4C-NC	-2.20	119.87	123.86
13	O	302	HEC	C3C-C4C-NC	2.20	112.59	110.15
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
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
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
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
15	O	304	MQ9	C42-C43-C44	-2.15	122.69	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	304	MQ9	C32-C31-C29	-2.15	106.05	113.19
17	L	603	HEA	CHA-C1A-NA	2.15	126.80	124.45
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
13	O	301	HEC	CAA-CBA-CGA	-2.14	107.99	113.67
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
13	O	302	HEC	C3B-C4B-NB	2.13	112.51	110.17
15	I	303	MQ9	C10-C9-C11	2.13	118.93	115.23
17	L	602	HEA	CAA-CBA-CGA	-2.13	108.01	113.67
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
13	O	302	HEC	CMB-C2B-C3B	2.12	131.88	126.15
23	G	302	9XX	O1-C17-C16	2.12	111.08	106.21
15	E	603	MQ9	C12-C13-C14	-2.11	122.80	127.62
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
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
15	T	204	MQ9	C20-C19-C21	2.08	118.84	115.23
17	R	602	HEA	CHC-C1C-C2C	-2.08	121.39	127.43
17	L	602	HEA	CHC-C1C-C2C	-2.07	121.40	127.43
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
15	O	304	MQ9	C17-C18-C19	-2.07	122.88	127.62
14	Y	502	9YF	O4-C4-C3	-2.07	105.50	110.38
17	R	602	HEA	CHD-C1D-C2D	-2.07	121.08	126.95
23	c	202	9XX	C25-C26-C27	-2.06	109.12	115.97
17	L	602	HEA	CHB-C4A-NA	2.06	126.69	124.45
15	O	304	MQ9	C10-C9-C11	2.06	118.80	115.23
13	O	301	HEC	C3C-C4C-NC	2.05	112.43	110.15
21	E	602	HEM	CHC-C1C-NC	2.05	126.69	124.45
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
13	O	301	HEC	CHA-C4D-ND	-2.05	122.22	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	201	CDL	C58-C57-C56	-2.05	104.02	114.37
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
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
17	L	603	HEA	OMA-CMA-C3A	-2.03	121.04	125.62
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
13	I	301	HEC	C3C-C4C-NC	-2.03	107.90	110.15
13	O	301	HEC	CMC-C2C-C3C	2.02	129.91	125.62
15	E	604	MQ9	C5M-C5-C6	-2.02	121.13	124.45
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
13	O	302	HEC	CMA-C3A-C2A	2.01	131.59	126.15
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

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	O	301	HEC	NA
13	O	302	HEC	NA
13	I	302	HEC	NA

All (1081) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	302	HEC	C1A-C2A-CAA-CBA
13	I	302	HEC	C2B-C3B-CAB-CBB
13	I	302	HEC	C4B-C3B-CAB-CBB
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
14	I	304	9YF	C9-C8-O9-C
14	Y	502	9YF	C9-C8-O9-C

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Mol	Chain	Res	Type	Atoms
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
18	E	607	CDL	CB3-OB5-PB2-OB4
18	F	705	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
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
18	T	202	CDL	CB3-OB5-PB2-OB4
18	T	202	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
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
20	F	704	9Y0	O6-C21-O7-C1
20	J	201	9Y0	C22-C21-O7-C1

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Mol	Chain	Res	Type	Atoms
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
13	I	302	HEC	C4C-C3C-CAC-CBC
18	R	604	CDL	OA9-CA7-OA8-CA6
18	L	604	CDL	OA9-CA7-OA8-CA6
13	O	301	HEC	C2C-C3C-CAC-CBC
13	I	302	HEC	C2C-C3C-CAC-CBC
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
13	O	302	HEC	C2C-C3C-CAC-CBC
13	O	301	HEC	C4C-C3C-CAC-CBC
13	O	302	HEC	C4C-C3C-CAC-CBC
13	O	301	HEC	C4B-C3B-CAB-CBB
13	O	302	HEC	C4B-C3B-CAB-CBB
13	O	301	HEC	C2B-C3B-CAB-CBB
13	O	302	HEC	C2B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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
13	O	302	HEC	C3A-C2A-CAA-CBA
17	L	602	HEA	C3D-CAD-CBD-CGD
18	F	706	CDL	C76-C77-C78-C79
20	J	201	9Y0	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
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
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
13	I	301	HEC	C4C-C3C-CAC-CBC
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
13	I	301	HEC	C2C-C3C-CAC-CBC
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
14	E	605	9YF	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
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
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
13	O	302	HEC	C3D-CAD-CBD-CGD
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

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Mol	Chain	Res	Type	Atoms
17	L	602	HEA	C2D-C3D-CAD-CBD
13	O	301	HEC	C3D-CAD-CBD-CGD
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
13	I	301	HEC	C2B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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
13	I	301	HEC	C4B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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
13	I	301	HEC	C2D-C3D-CAD-CBD
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

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Mol	Chain	Res	Type	Atoms
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
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
13	O	302	HEC	C2A-CAA-CBA-CGA
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

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Mol	Chain	Res	Type	Atoms
15	E	603	MQ9	C15-C14-C16-C17
13	I	302	HEC	C3A-C2A-CAA-CBA
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
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
13	I	301	HEC	C4D-C3D-CAD-CBD
21	F	702	HEM	CAA-CBA-CGA-O2A
18	E	607	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
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
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 442 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	O	302	HEC	35	0
15	Z	201	MQ9	3	0
18	E	606	CDL	10	0
15	F	707	MQ9	4	0
17	L	602	HEA	2	0
18	T	201	CDL	35	0
18	T	202	CDL	29	0
15	I	303	MQ9	1	0
18	J	203	CDL	12	0
15	E	603	MQ9	1	0
18	F	706	CDL	12	0
18	Z	203	CDL	42	0
21	F	703	HEM	4	0
15	E	604	MQ9	4	0
17	R	603	HEA	4	0
18	F	705	CDL	11	0
19	Y	501	FES	1	0

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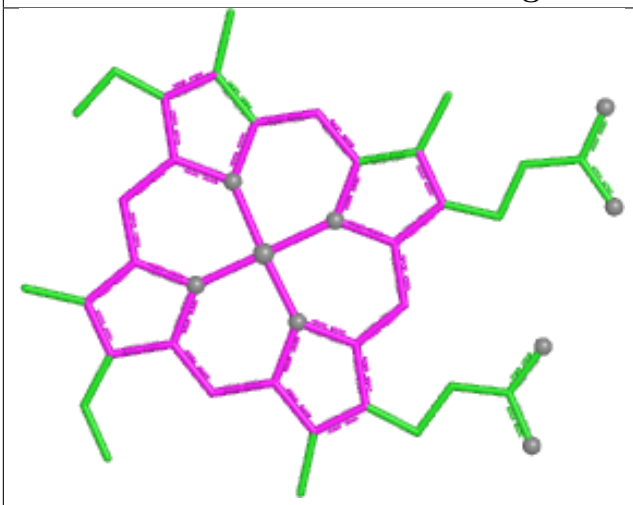
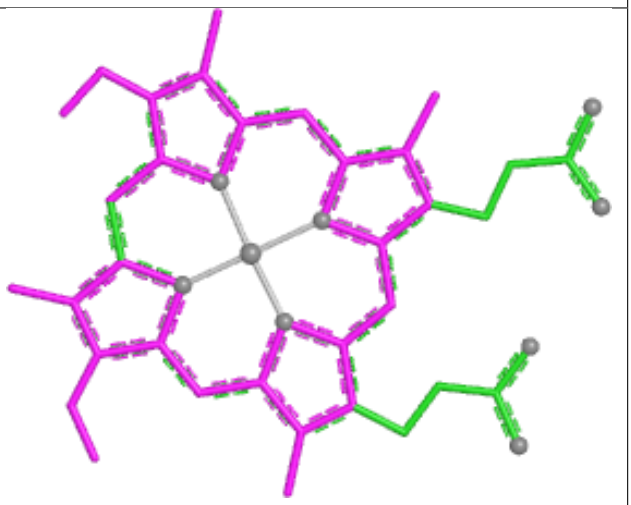
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	O	301	HEC	4	0
18	T	203	CDL	34	0
21	E	601	HEM	2	0
17	L	603	HEA	2	0
18	X	302	CDL	42	0
18	Z	202	CDL	35	0
15	O	304	MQ9	1	0
18	E	607	CDL	4	0
13	I	301	HEC	4	0
18	R	604	CDL	17	0
18	L	604	CDL	25	0
13	I	302	HEC	9	0
22	c	201	PLM	1	0
21	F	702	HEM	1	0
18	S	302	CDL	49	0
18	P	201	CDL	10	0
18	X	303	CDL	54	0
21	E	602	HEM	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.

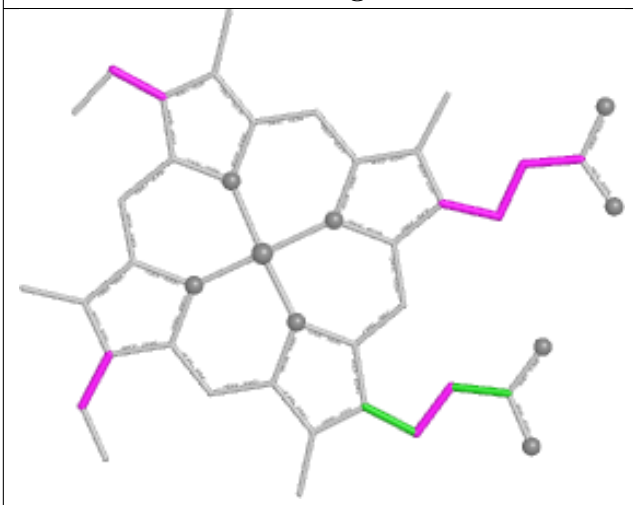
Ligand HEC O 302



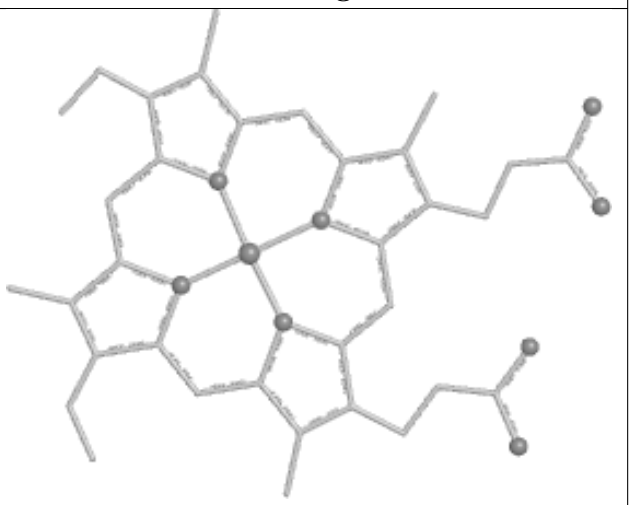
Bond lengths



Bond angles

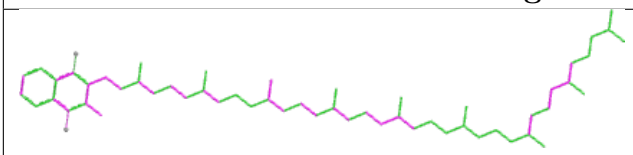


Torsions

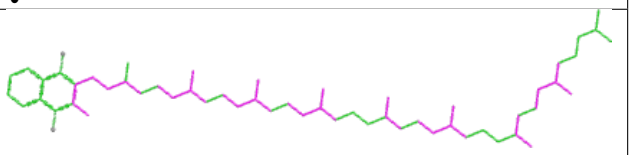


Rings

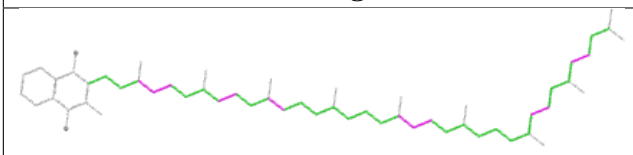
Ligand MQ9 Z 201



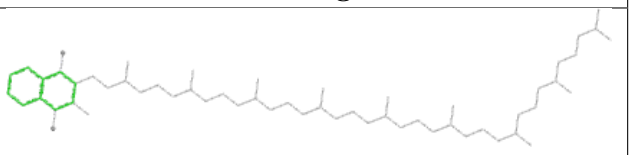
Bond lengths



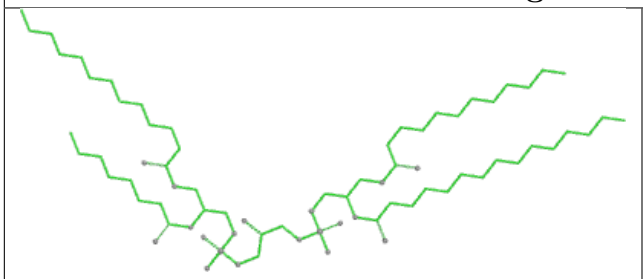
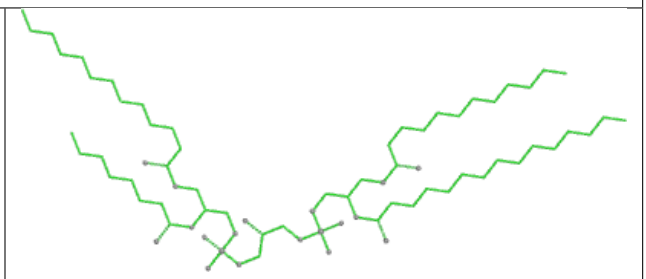
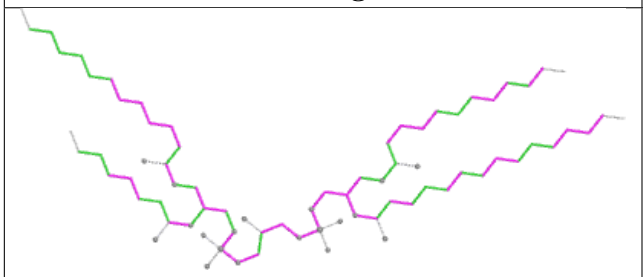
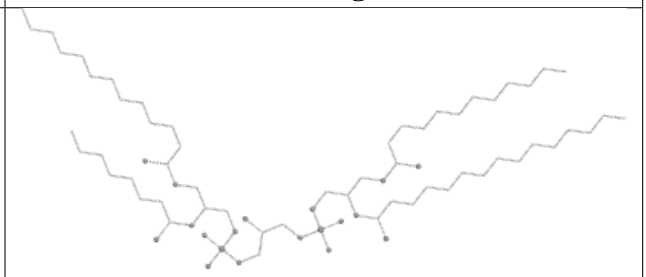
Bond angles

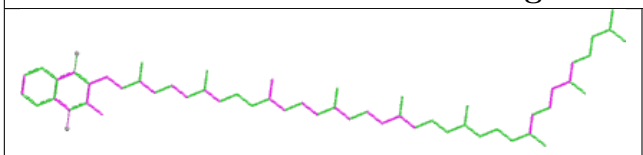
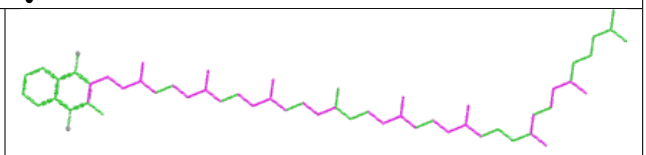
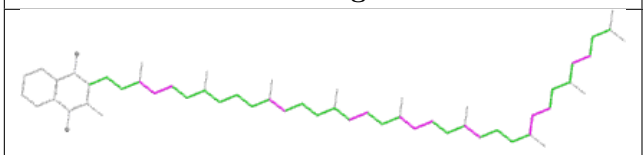


Torsions

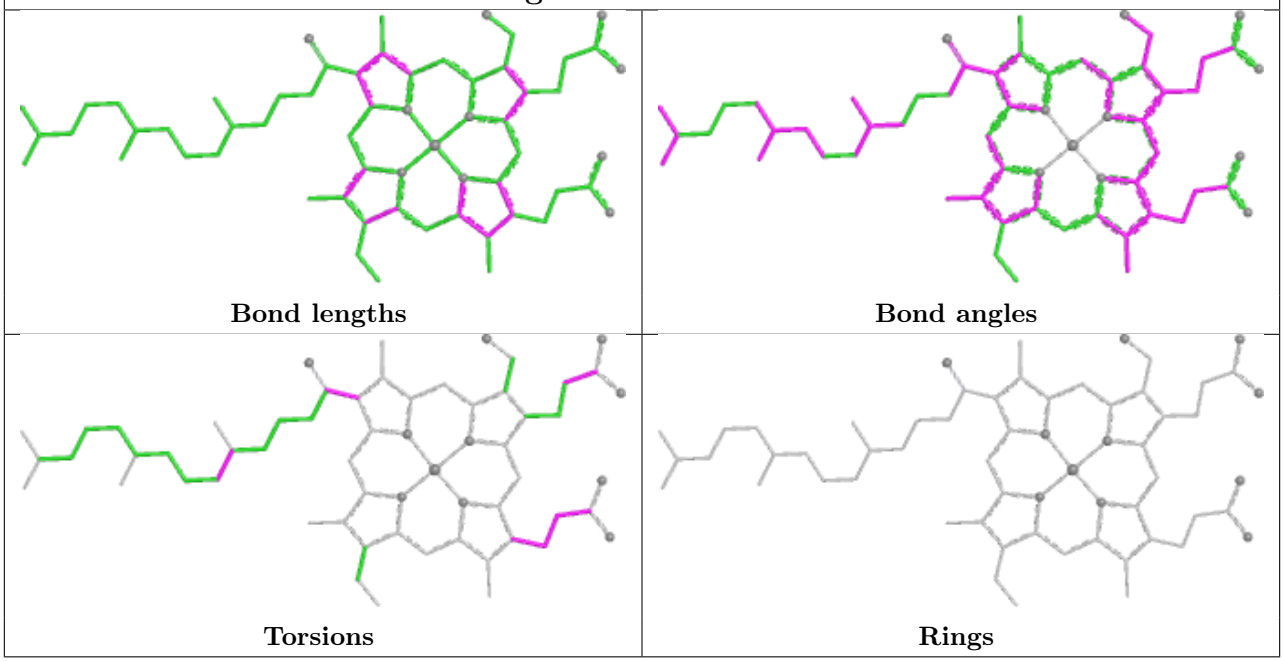


Rings

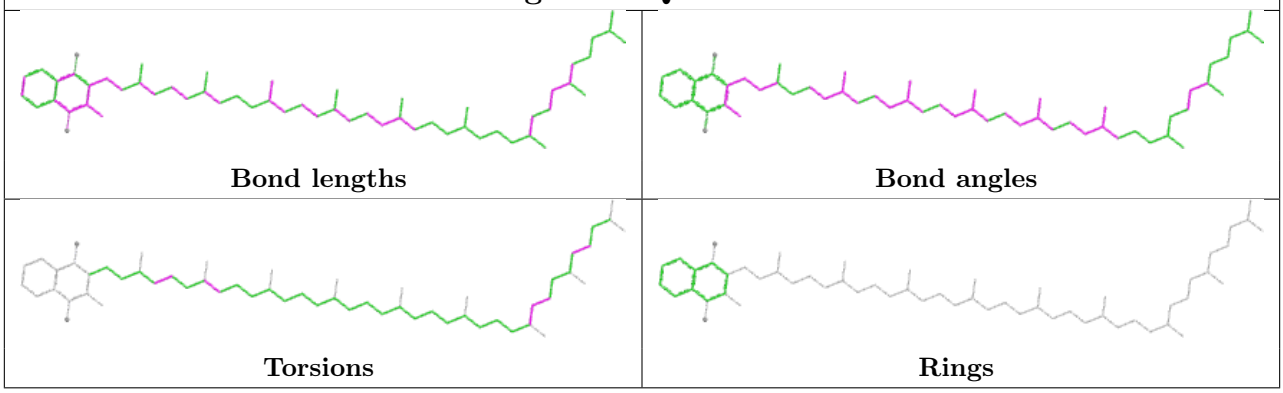
Ligand CDL E 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

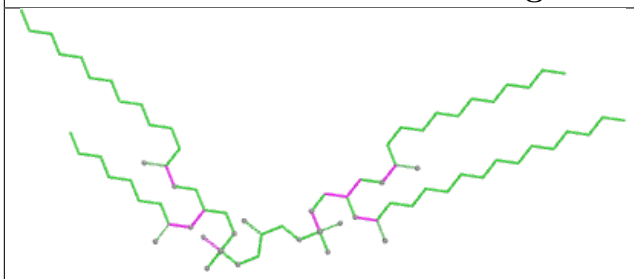
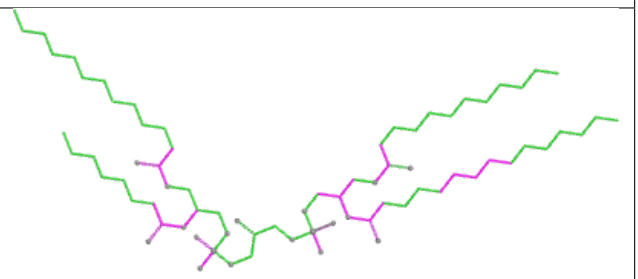
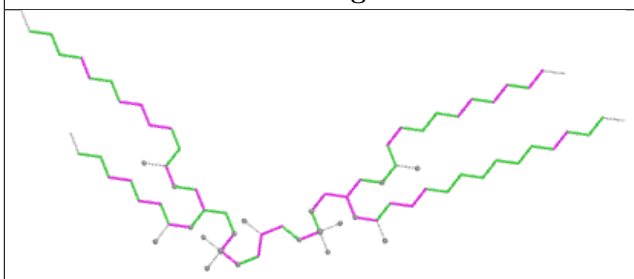
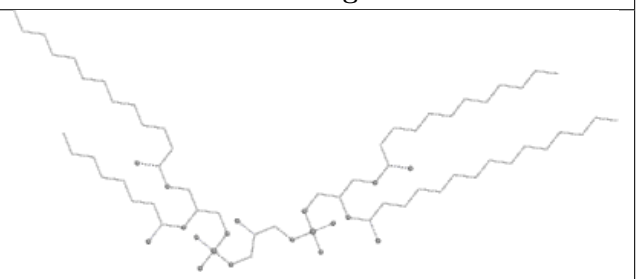
Ligand MQ9 F 707	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand HEA L 602

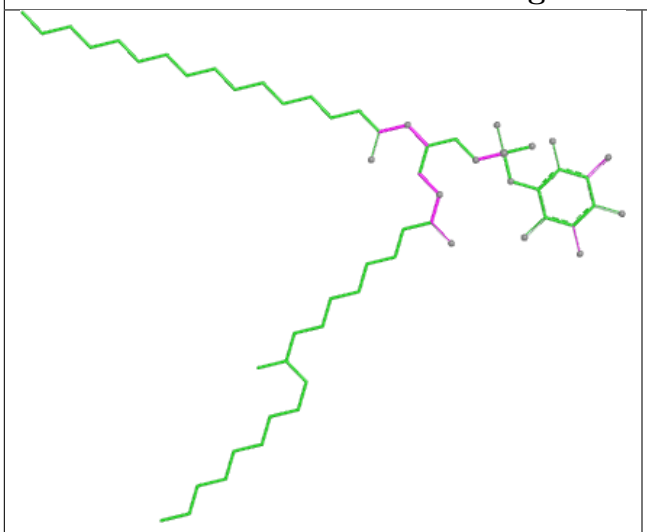


Ligand MQ9 F 701

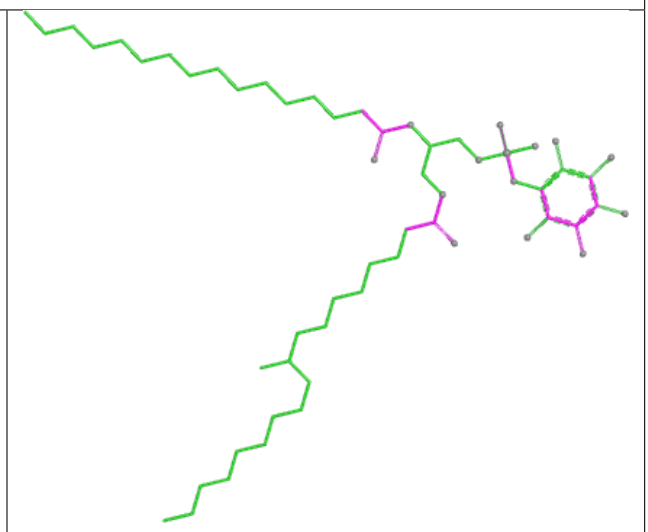


Ligand CDL T 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

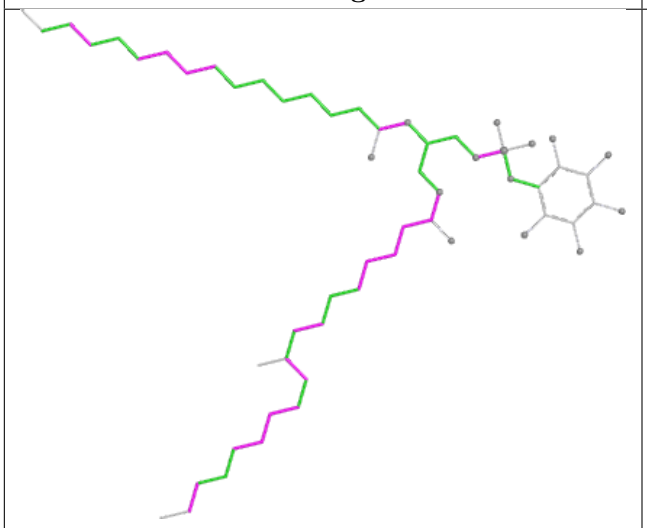
Ligand 9YF Y 503



Bond lengths



Bond angles



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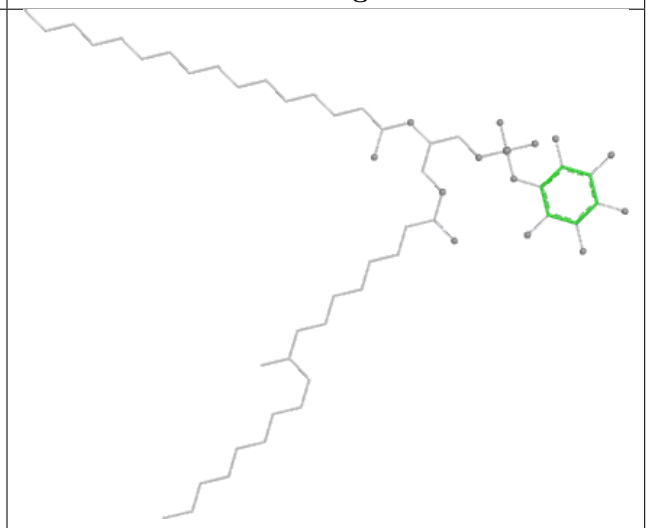
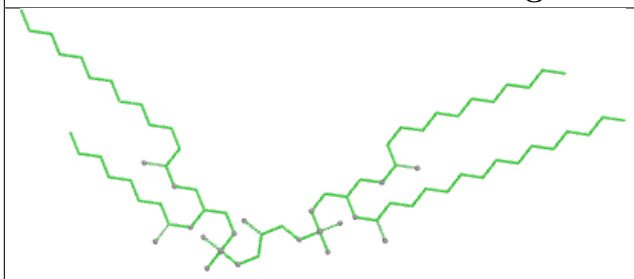


Rings

Ligand CDL T 202



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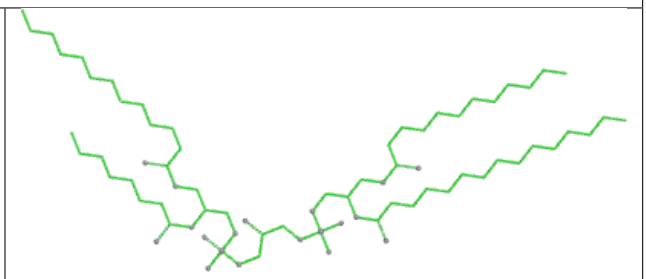
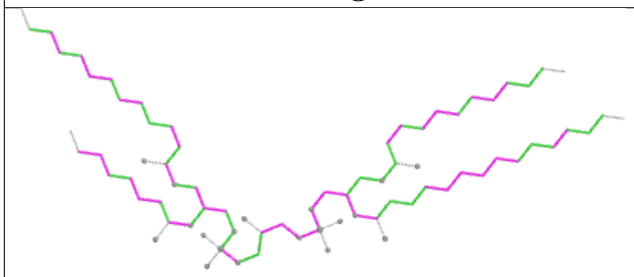


Bond angles



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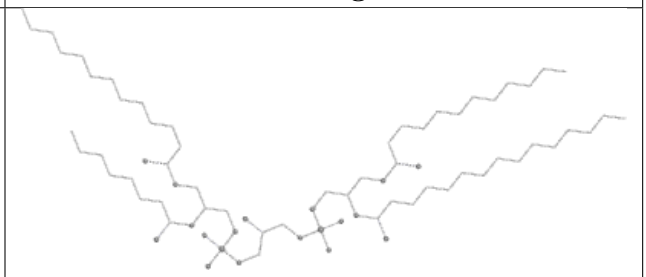
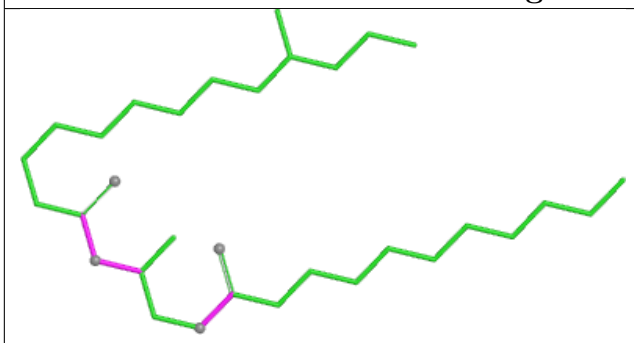


Rings

Ligand 9XX D 302



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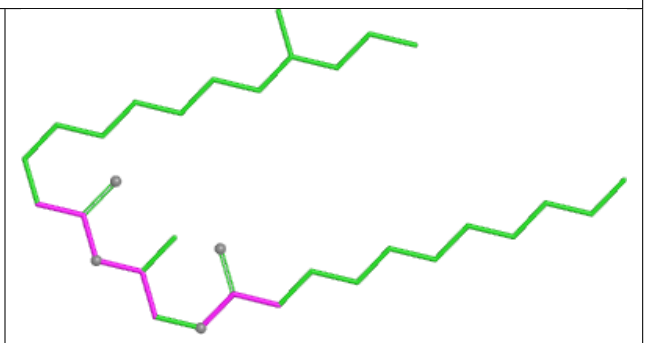
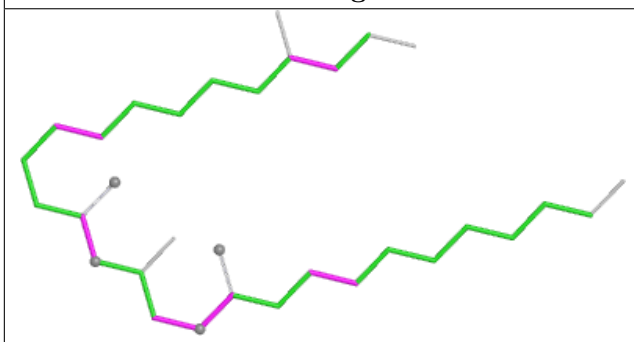


Bond angles



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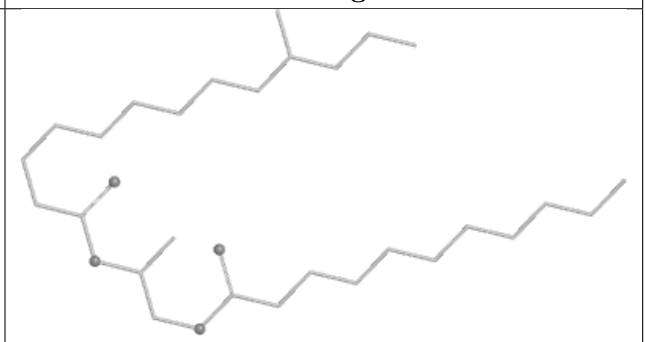
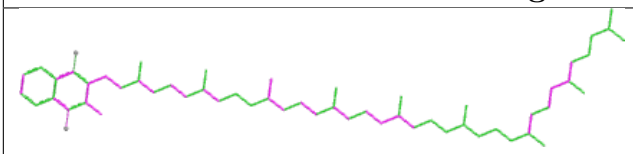


Rings

Ligand MQ9 I 303



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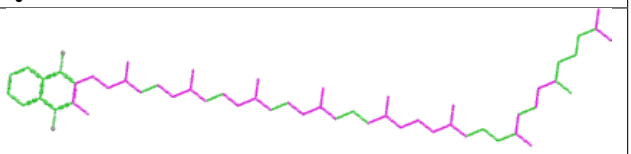
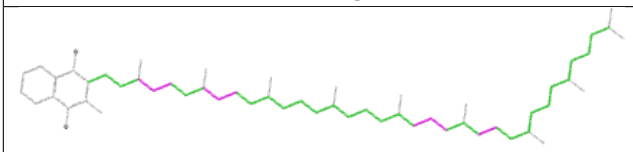
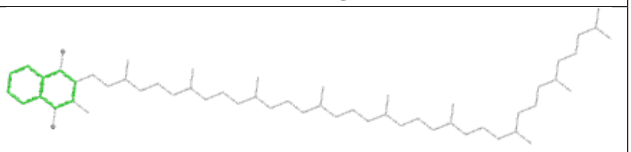


Bond angles

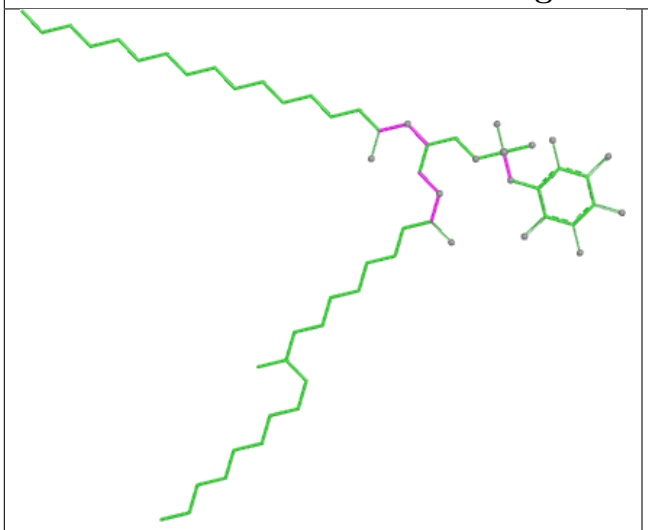


Torsions



Rings

Ligand 9YF I 304



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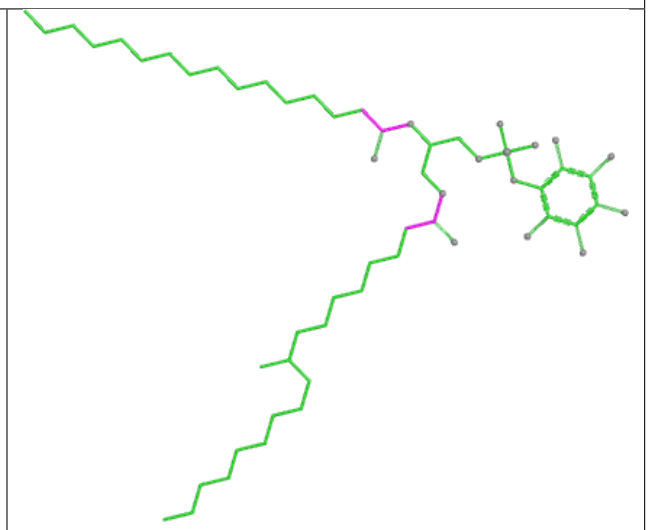

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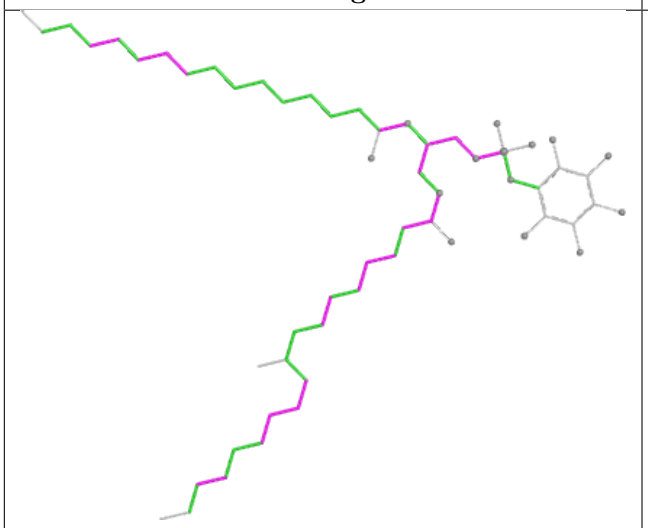

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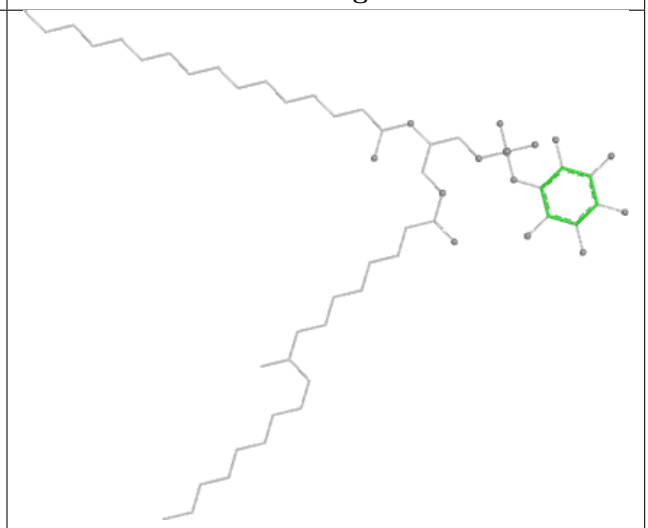
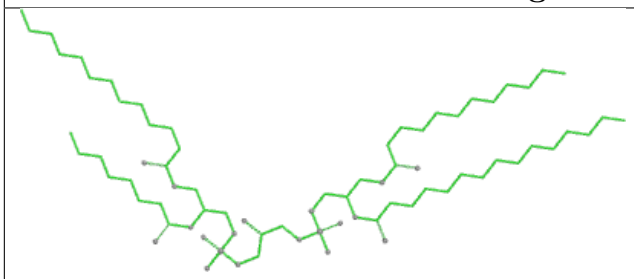


Rings

Ligand CDL J 203



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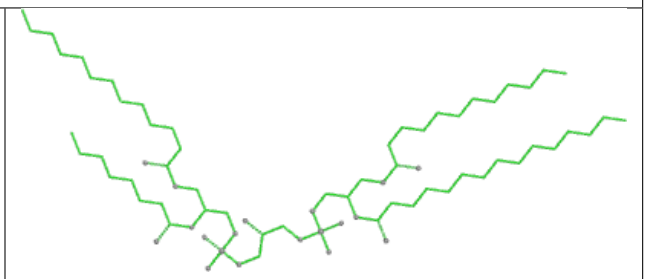

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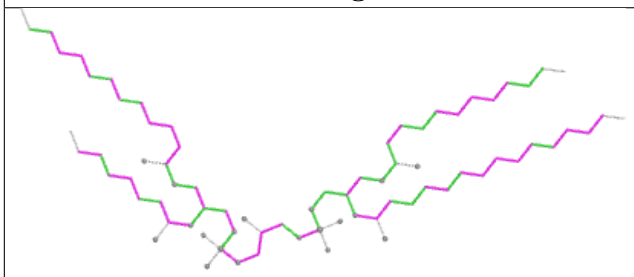

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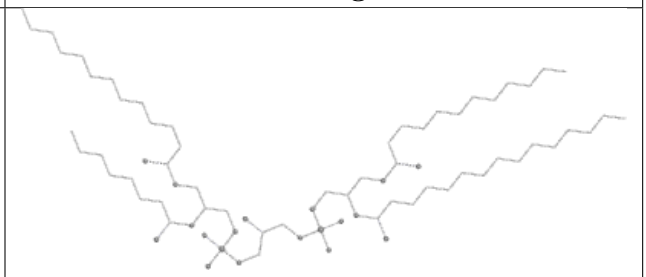
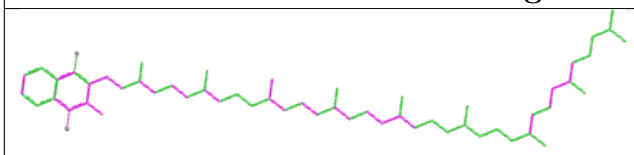


Rings

Ligand MQ9 E 603



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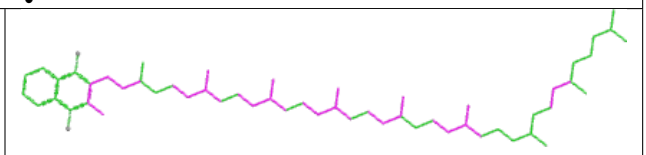
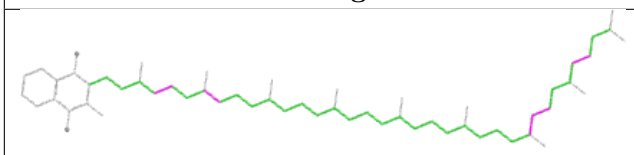


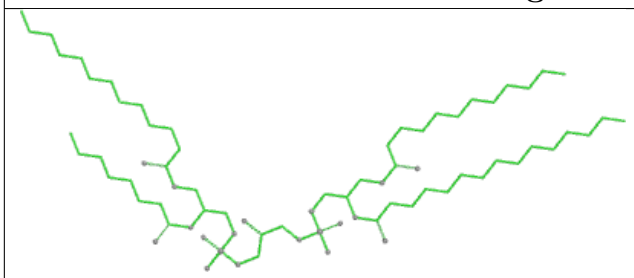
Bond angles



Torsions

Rings

Ligand CDL F 706



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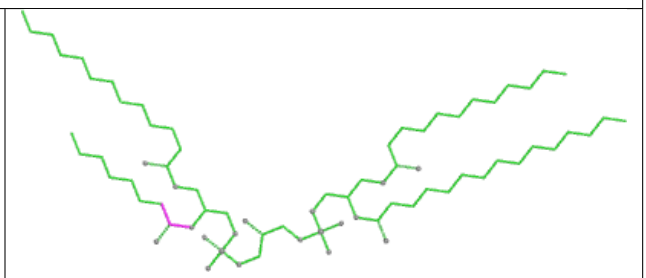
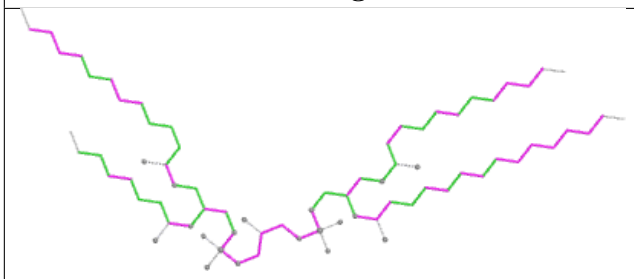
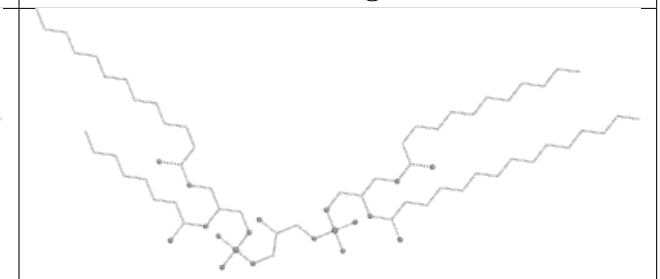


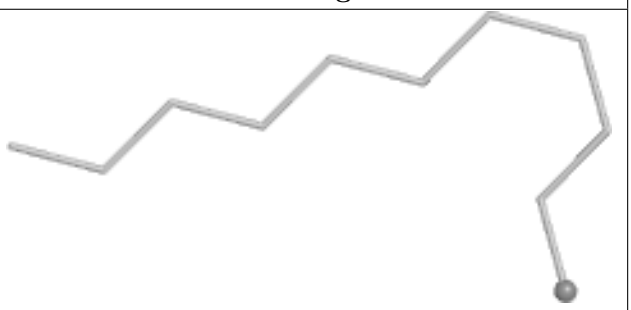
Bond angles



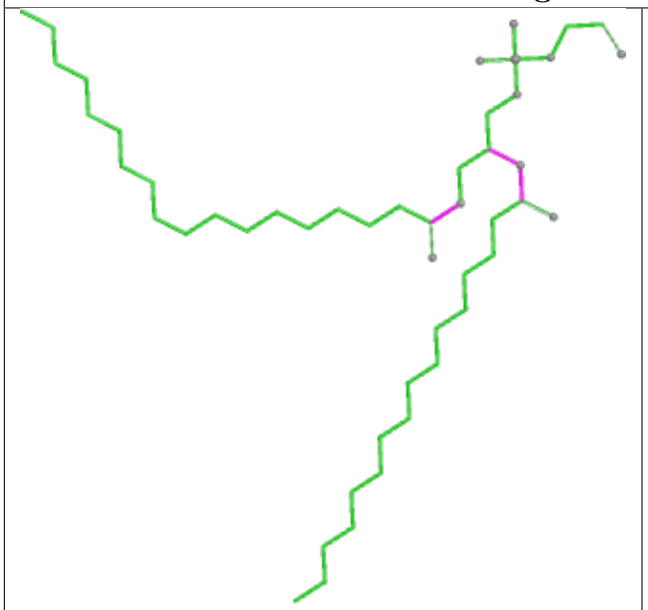
Torsions



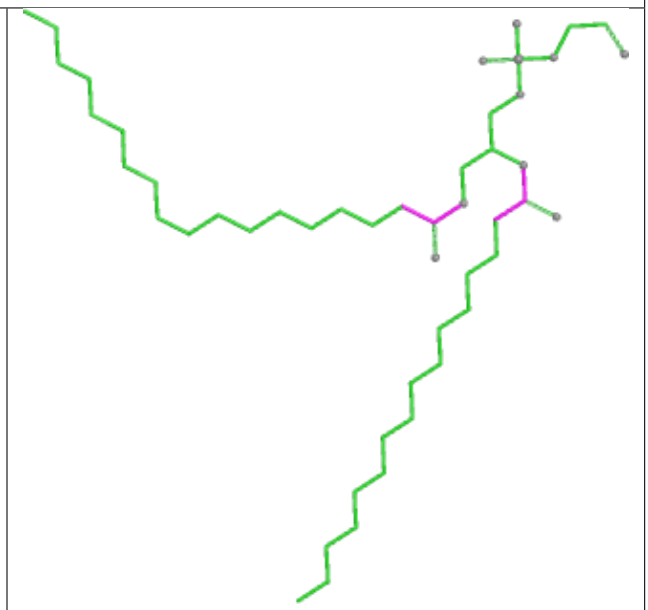
Rings

Ligand PLM G 301	
Bond lengths	Bond angles
Torsions	 Rings

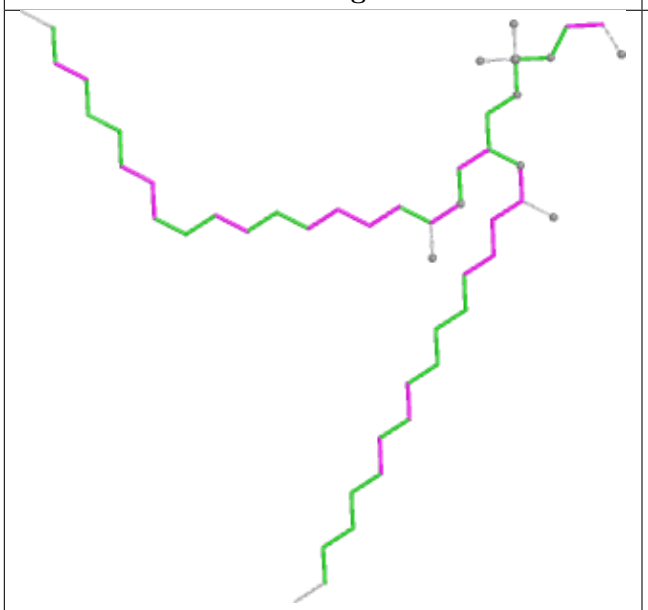
Ligand 9Y0 S 301



Bond lengths



Bond angles



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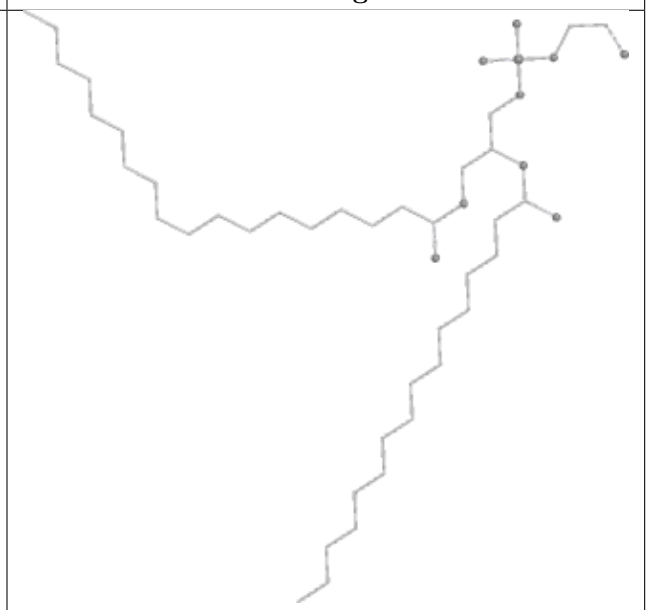
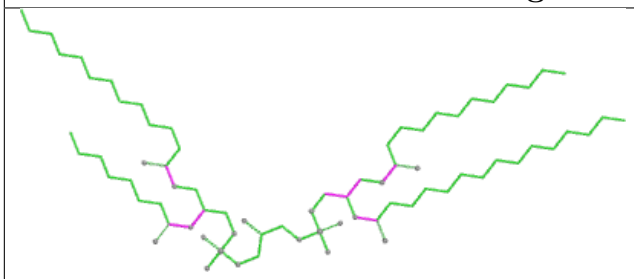
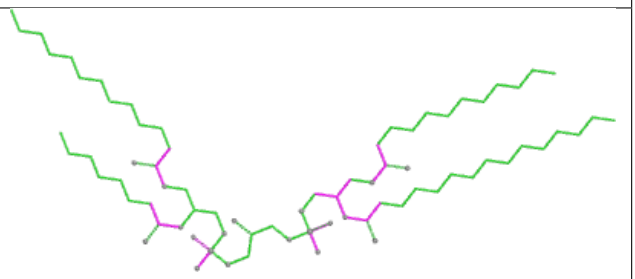
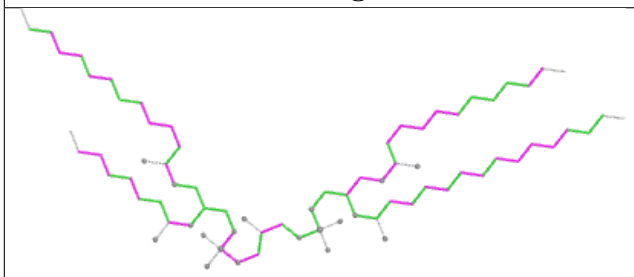
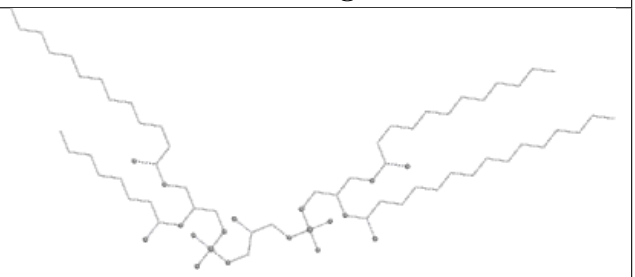
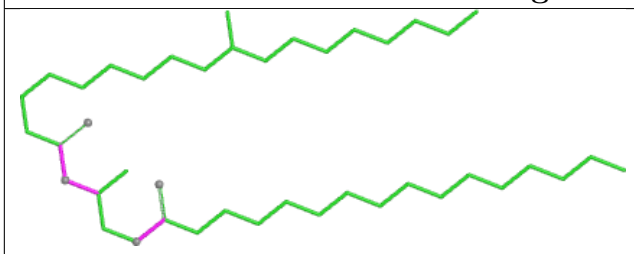
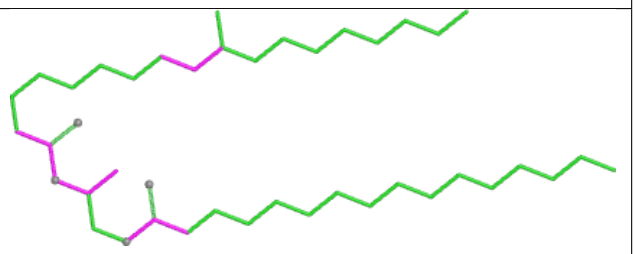
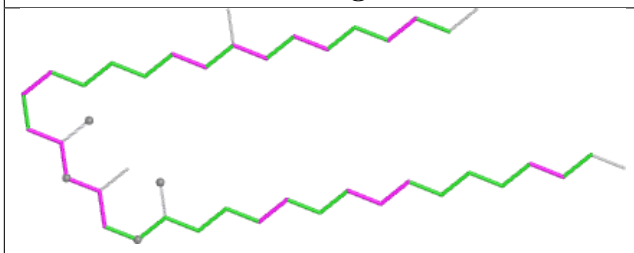
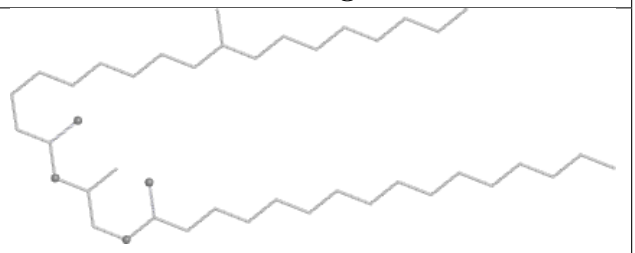
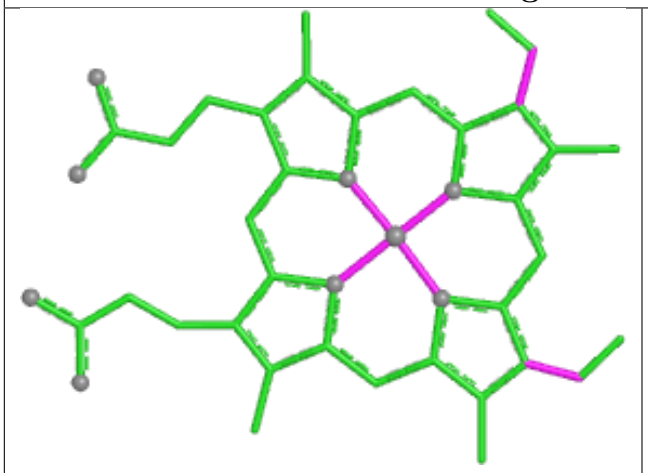


Rings

Ligand CDL Z 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9XX c 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM F 703



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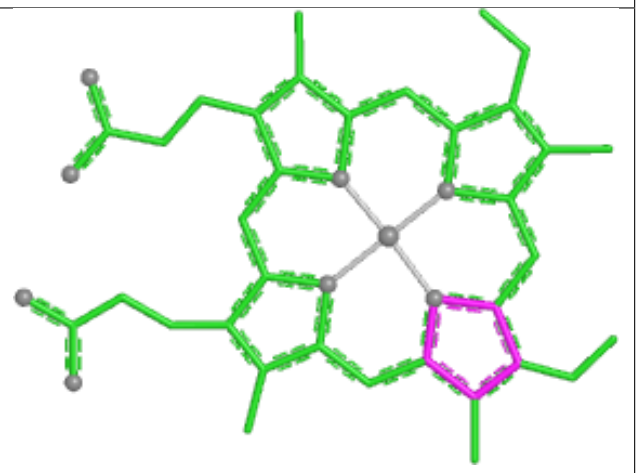

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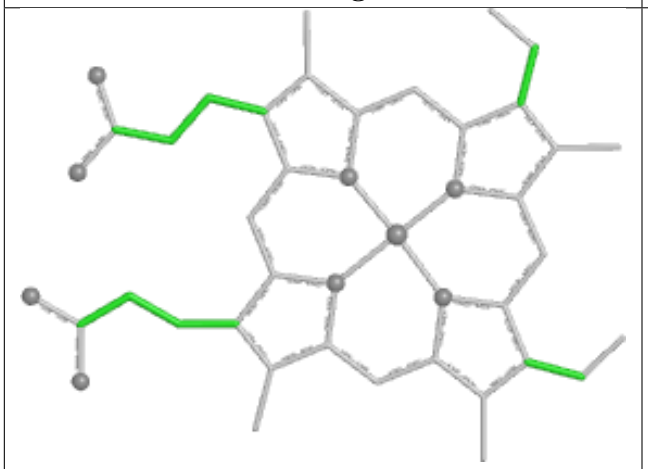

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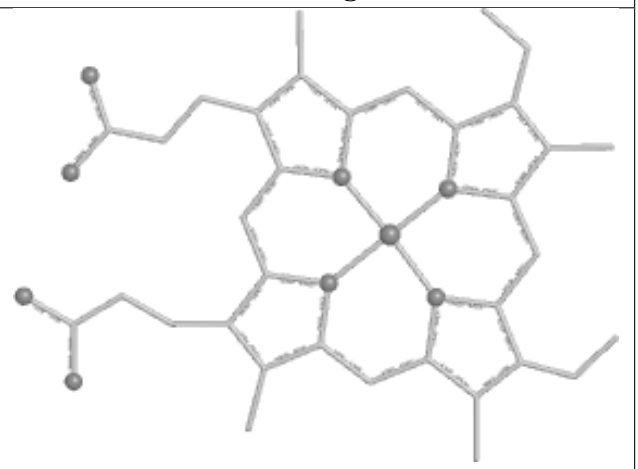
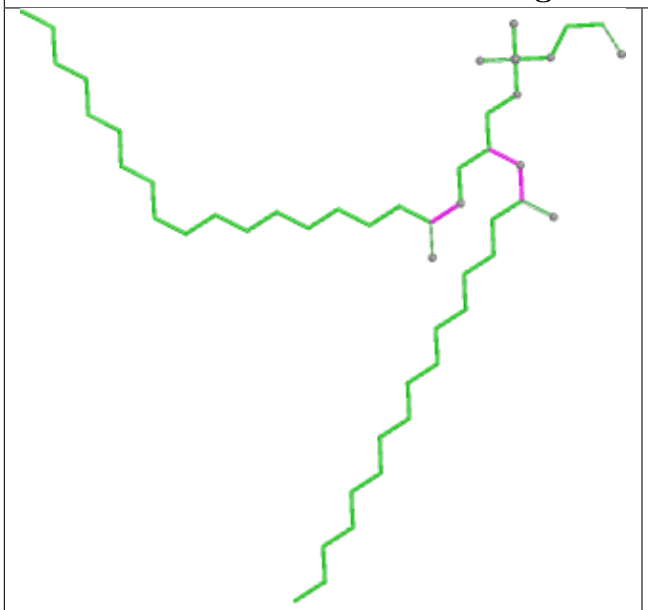


Rings

Ligand 9Y0 J 201



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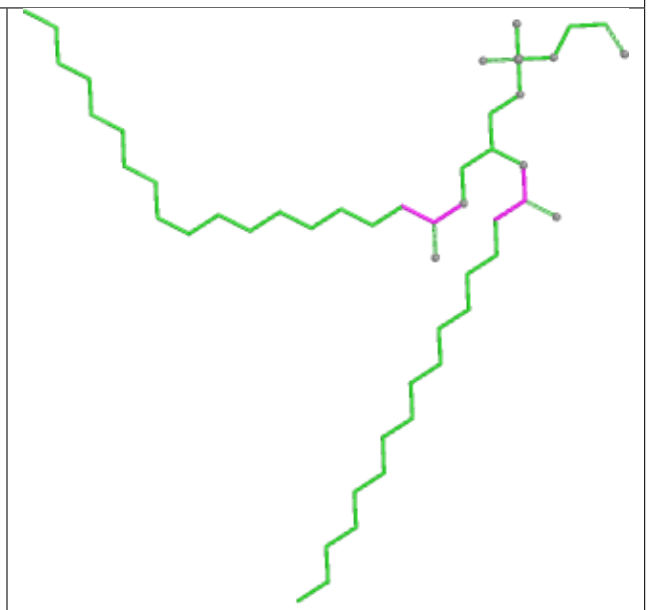

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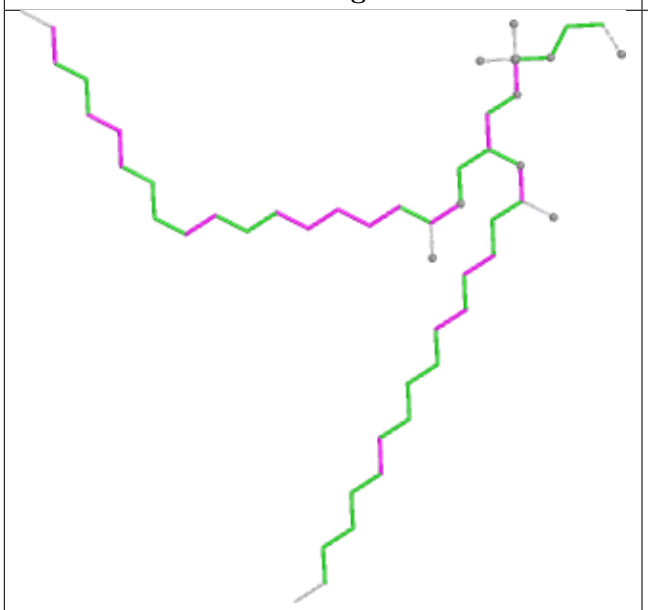

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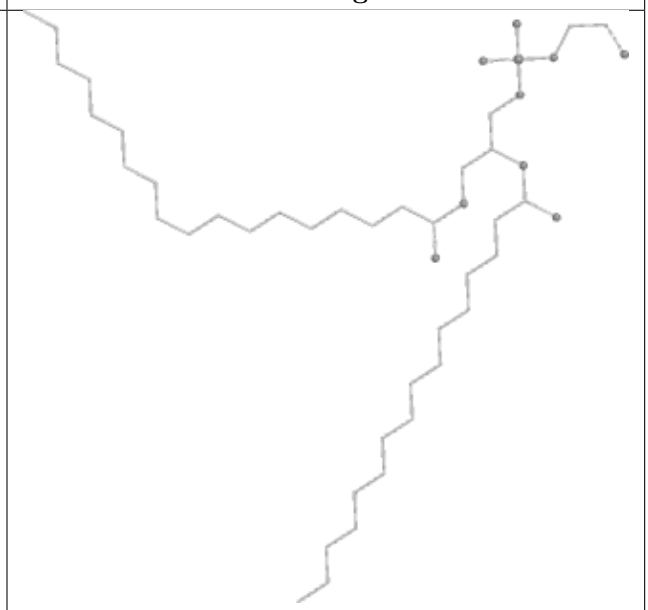
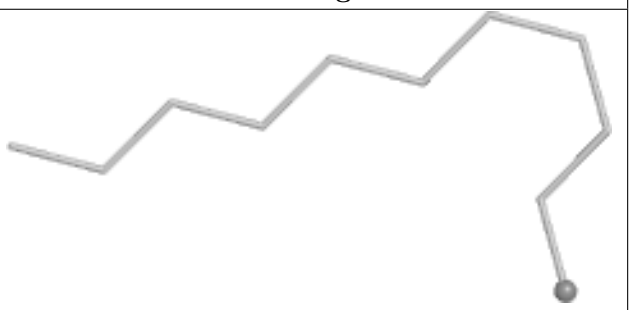
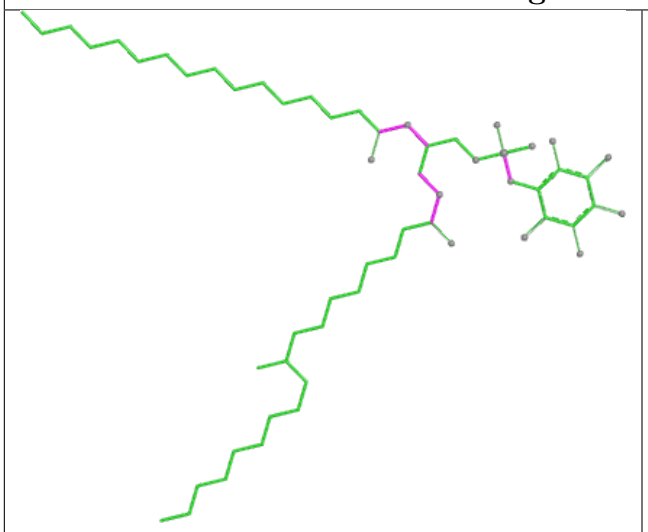


Rings

Ligand PLM D 301	
Bond lengths	Bond angles
Torsions	 Rings

Ligand 9YF O 303



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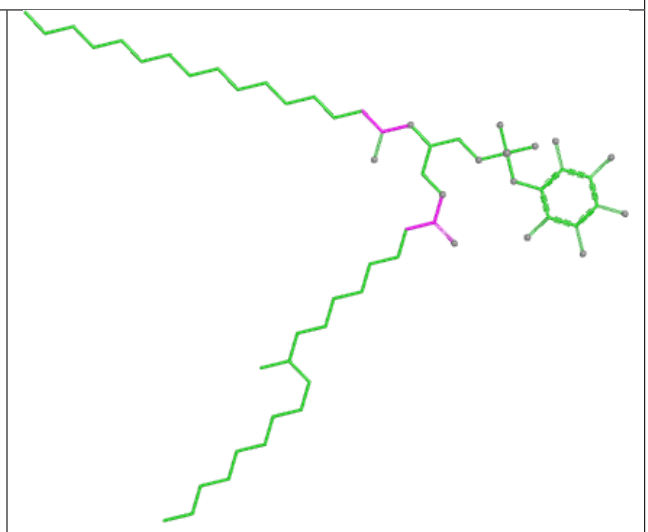
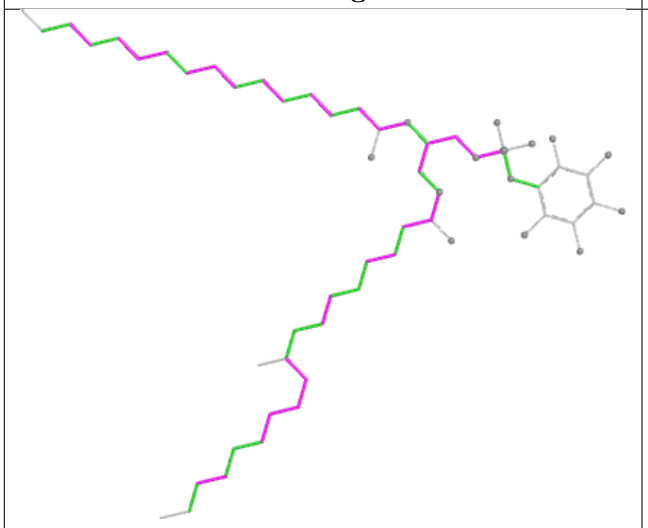


Bond angles



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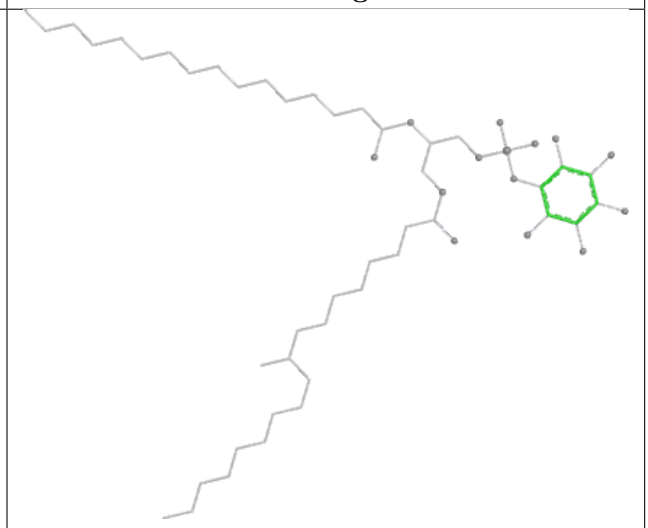
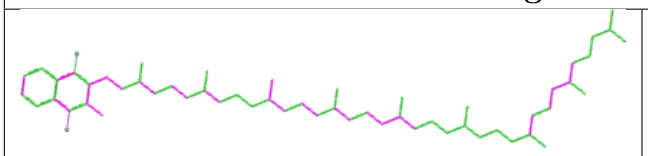


Rings

Ligand MQ9 E 604



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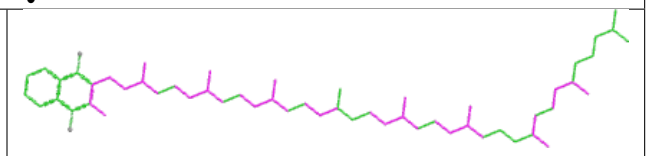
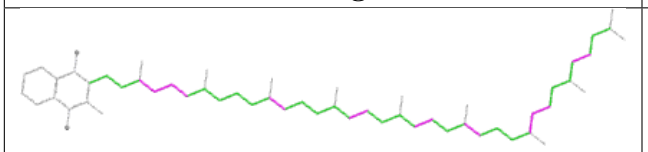


Bond angles



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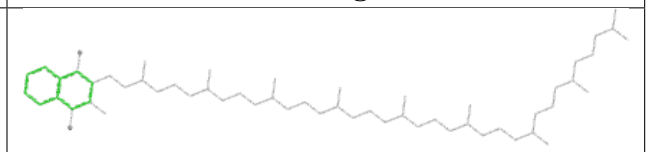
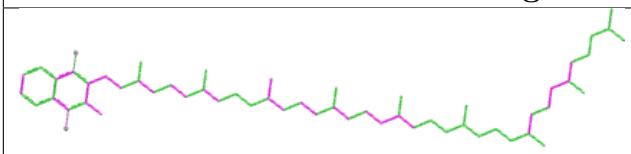
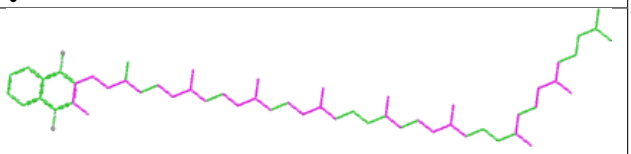
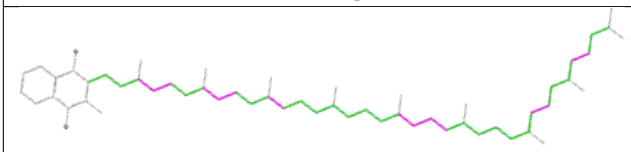
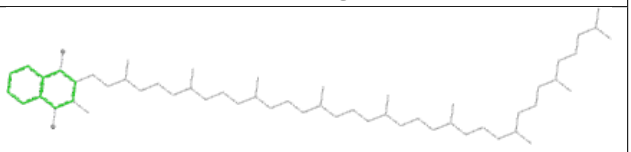
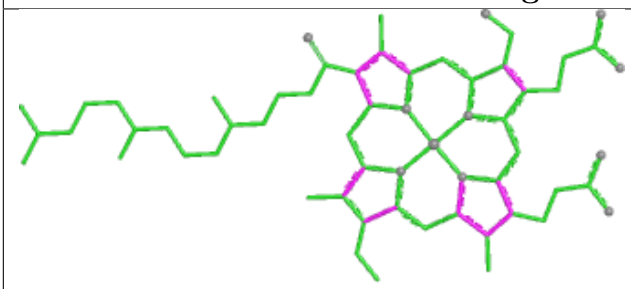
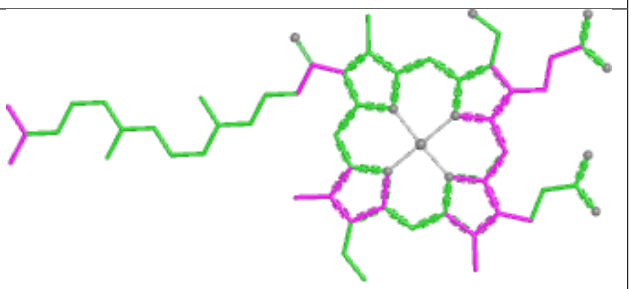
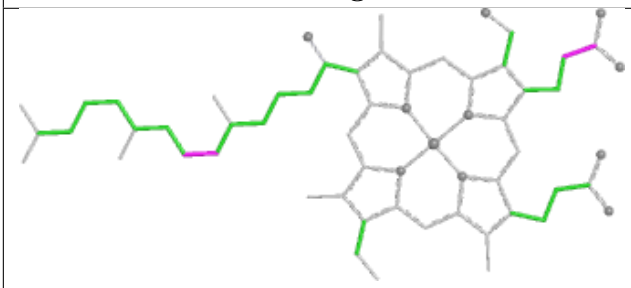
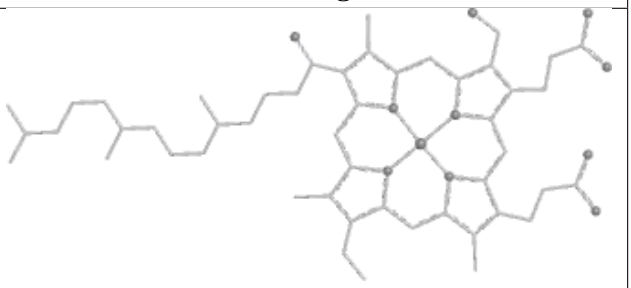
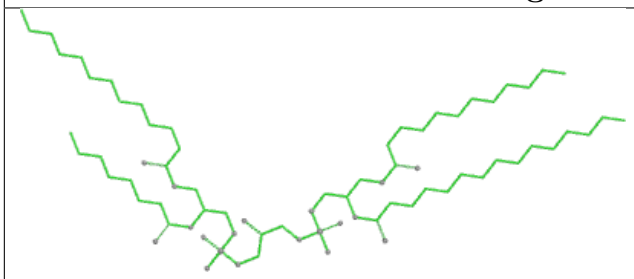


Rings

Ligand MQ9 T 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA R 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL F 705



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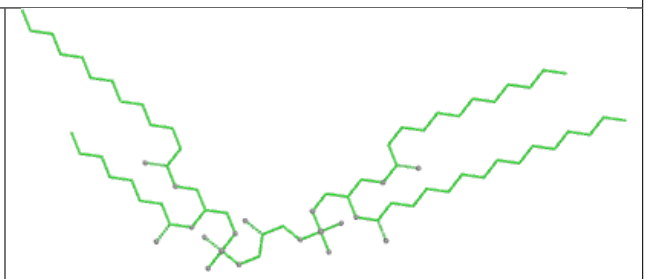

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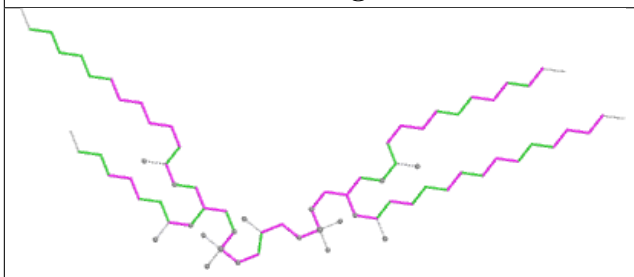

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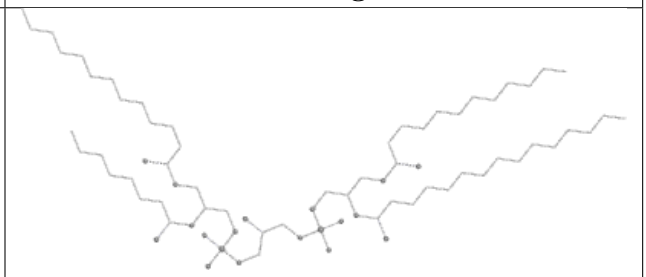
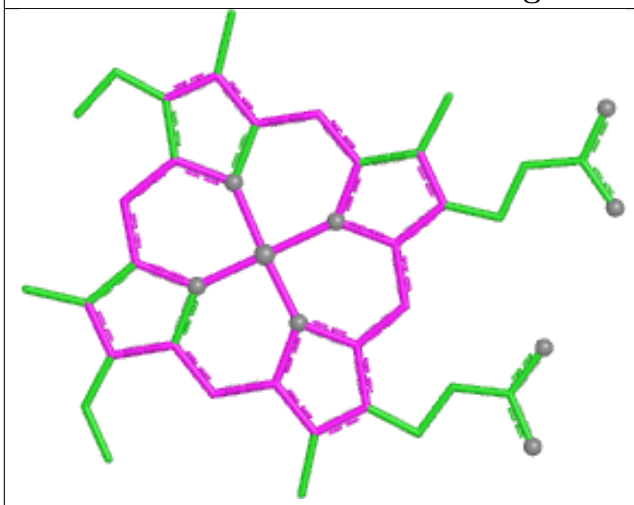


Rings

Ligand HEC O 301



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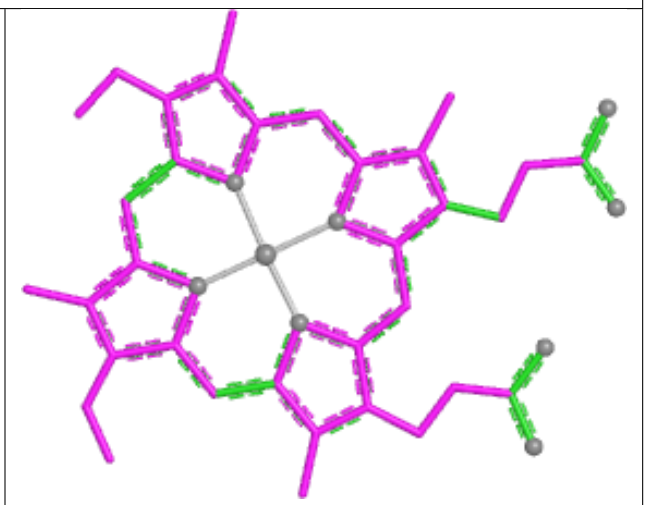

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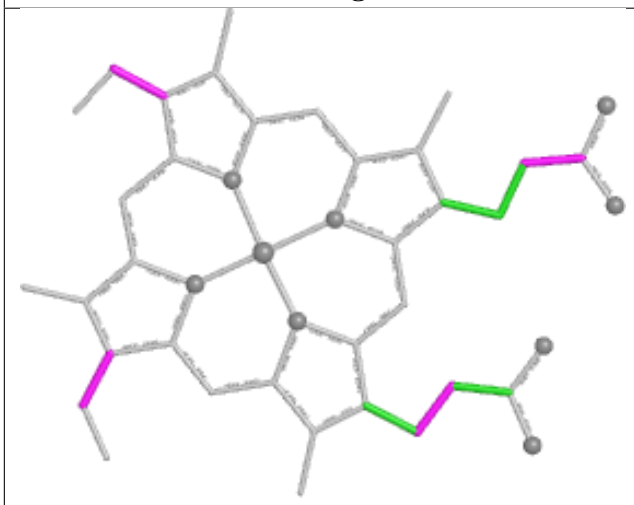

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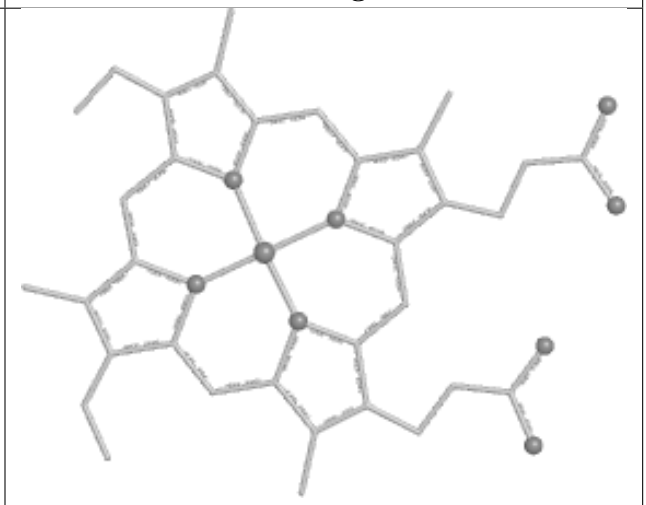
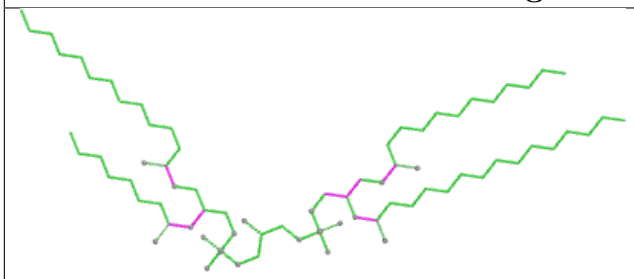


Rings

Ligand CDL T 203



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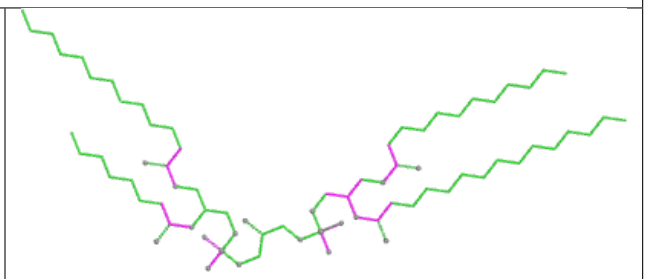
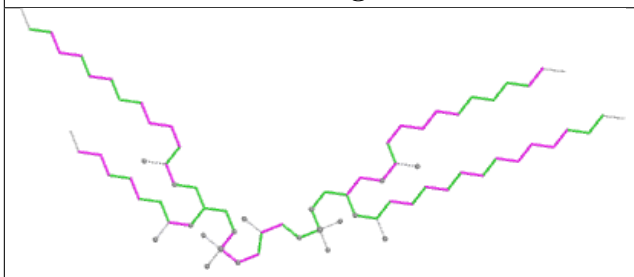


Bond angles



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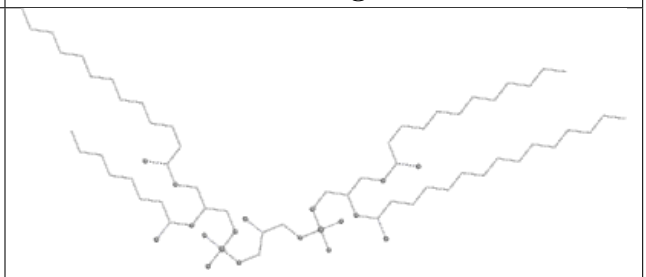
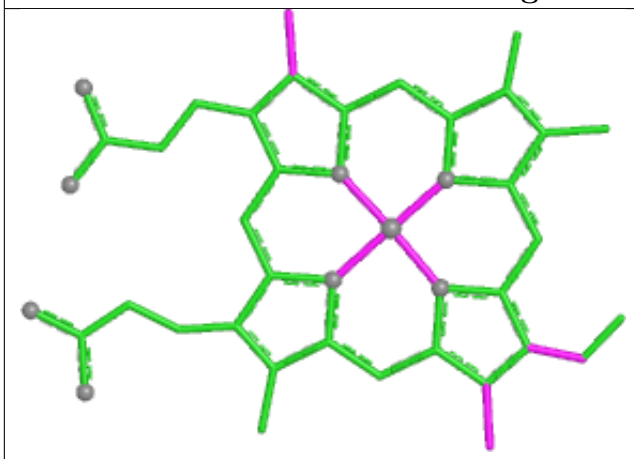


Rings

Ligand HEM E 601



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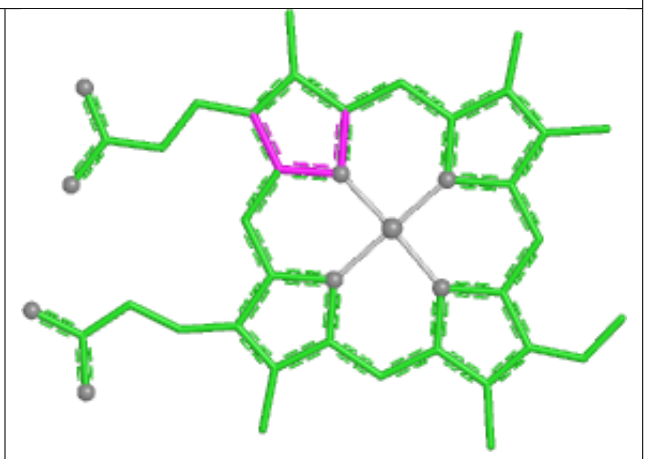

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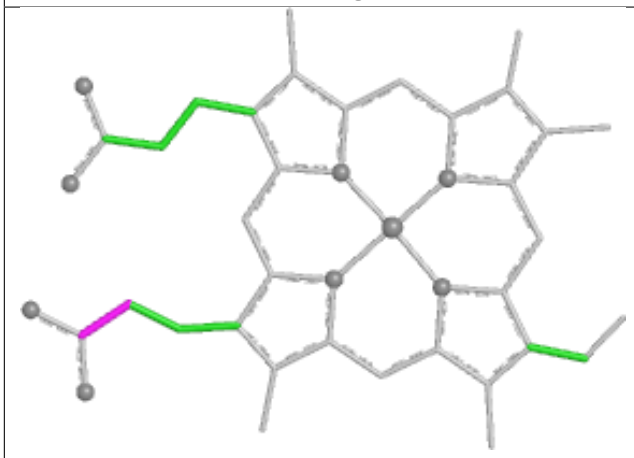

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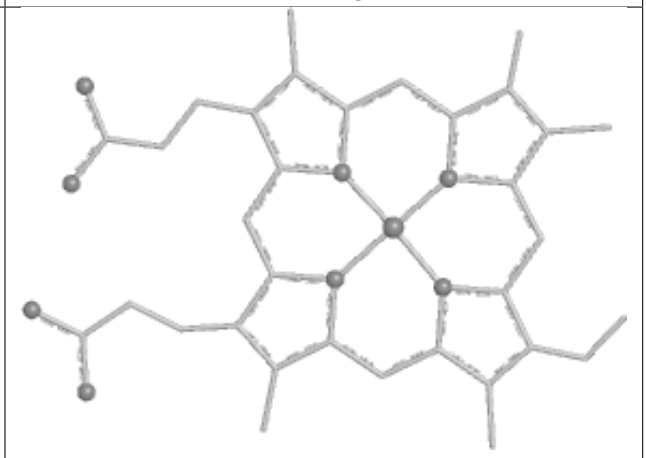
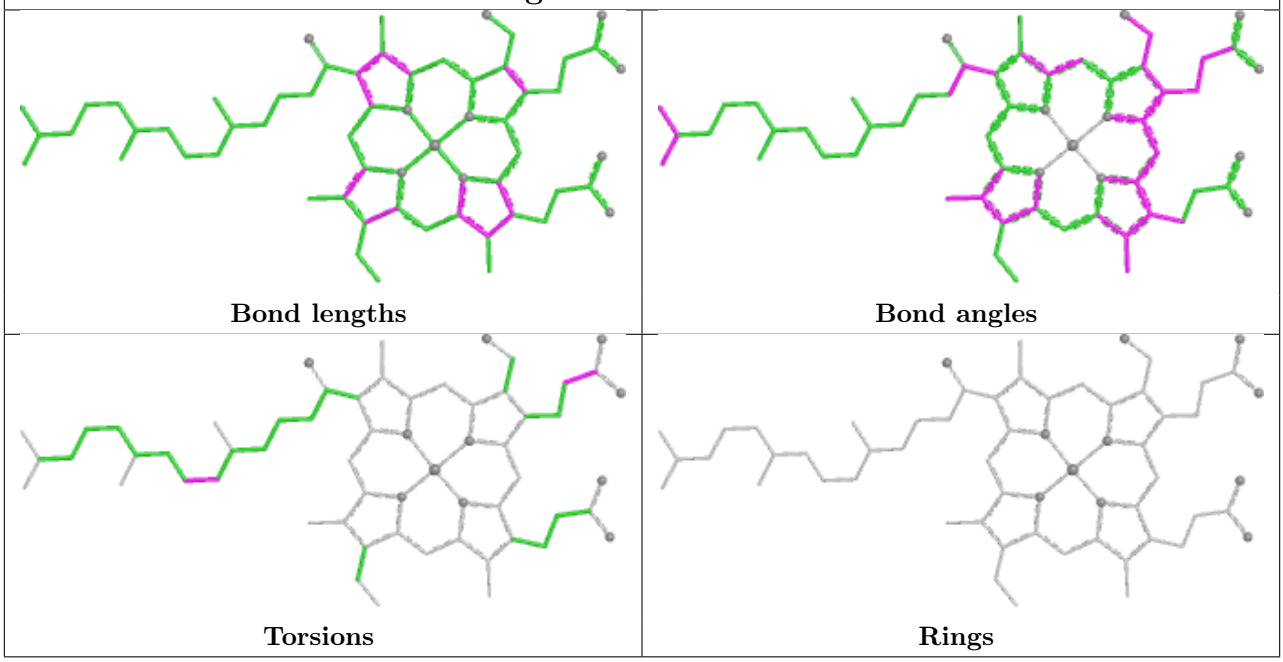
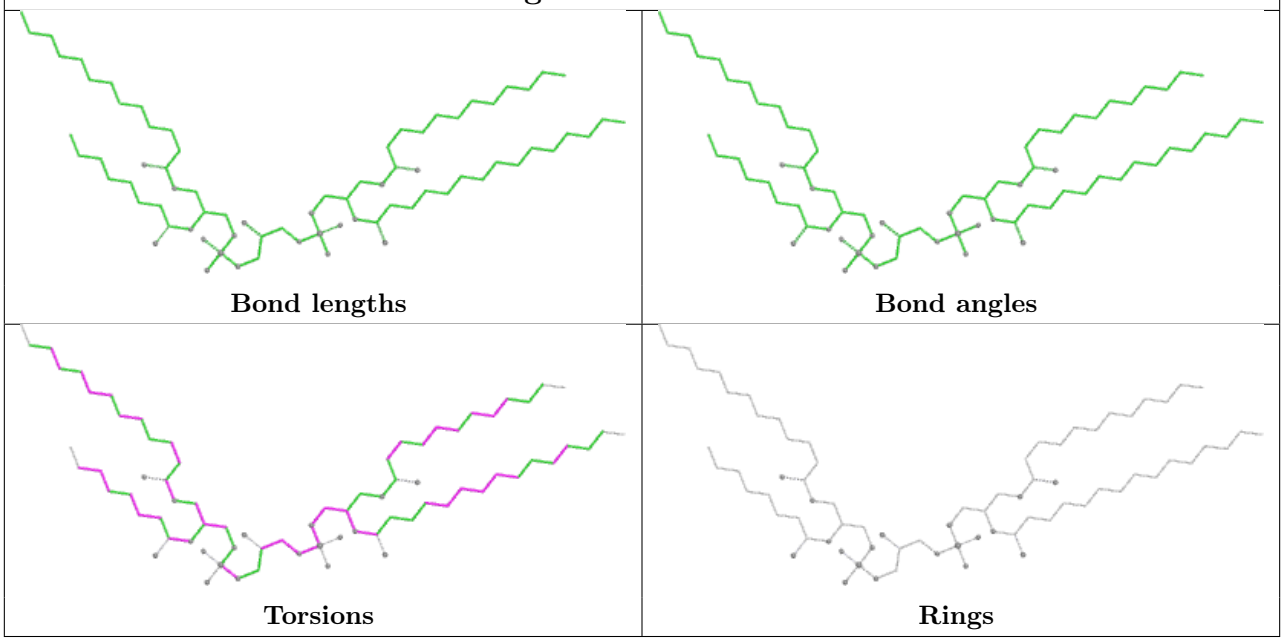


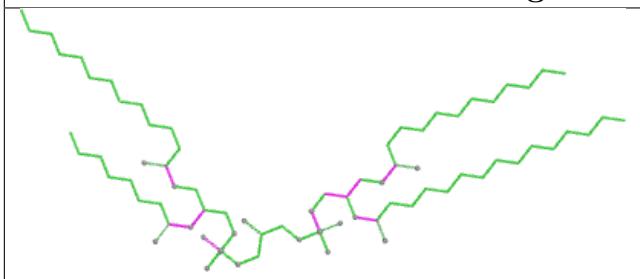
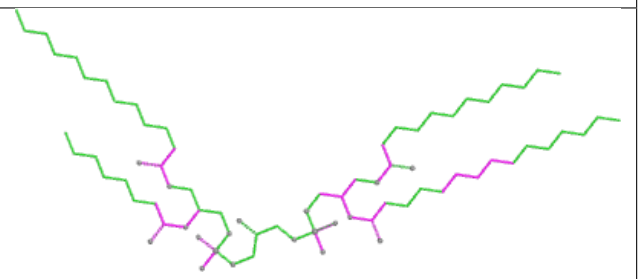
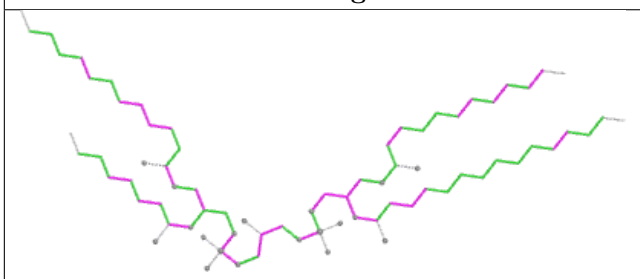
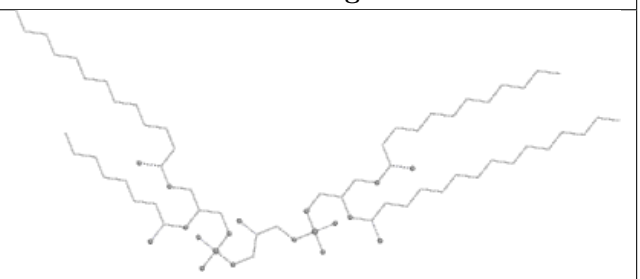
Rings

Ligand HEA L 603

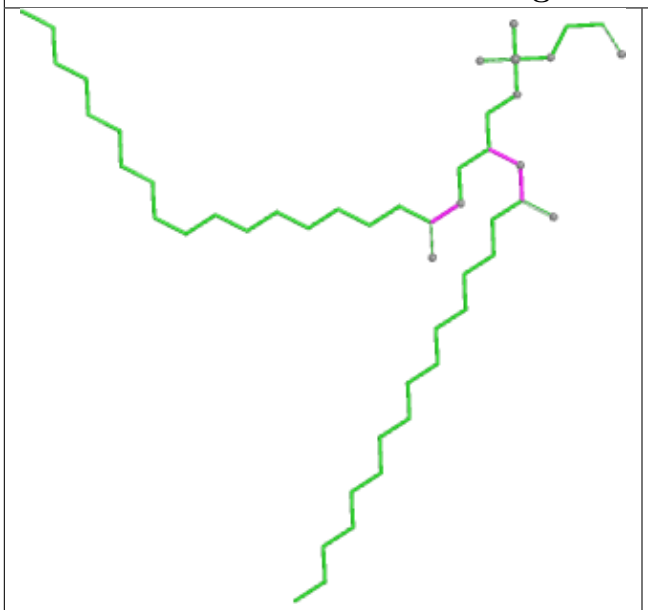


Ligand CDL X 302

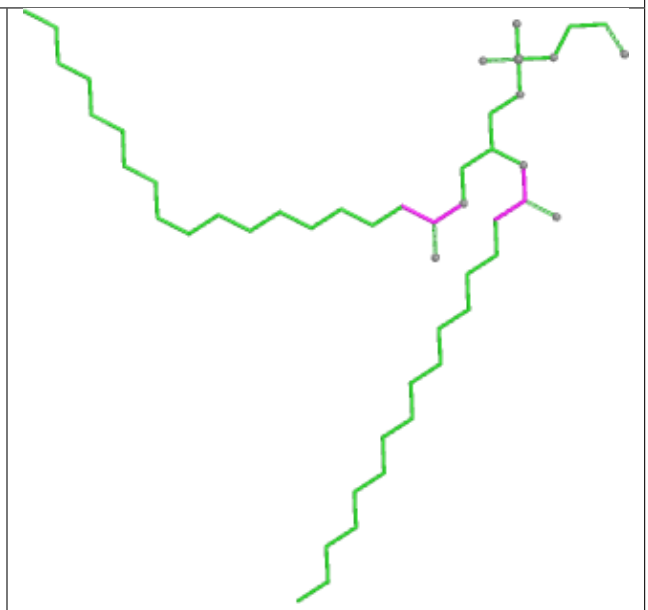


Ligand CDL Z 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

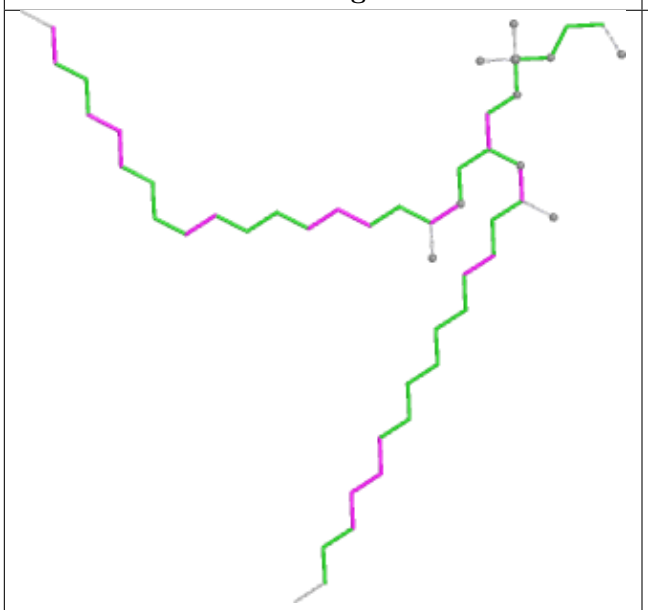
Ligand 9Y0 F 704



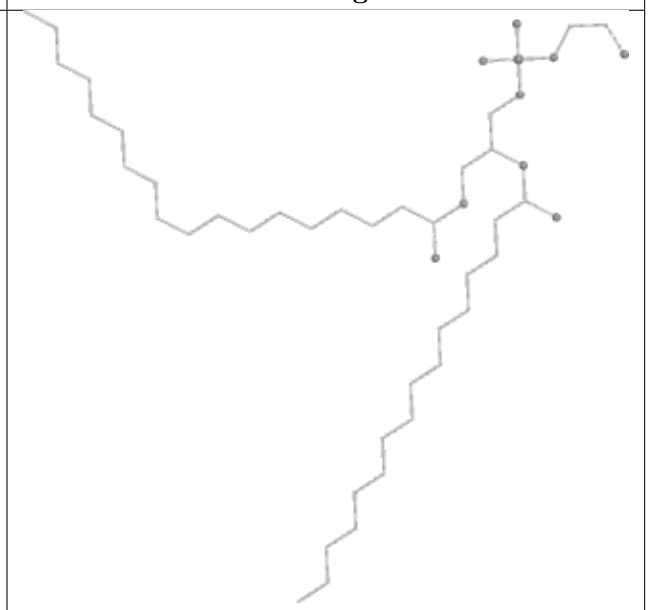
Bond lengths



Bond angles

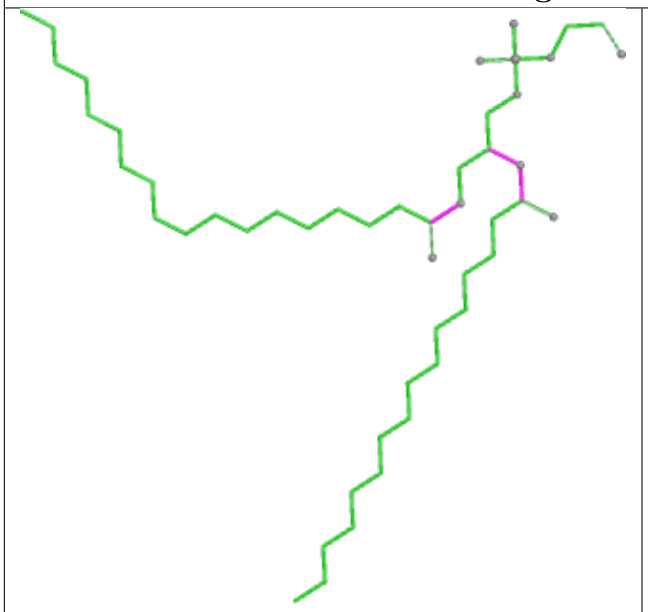


Torsions

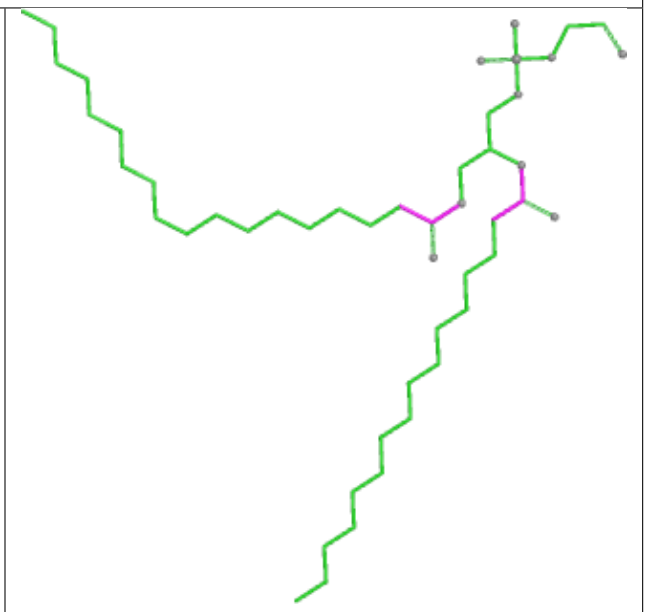


Rings

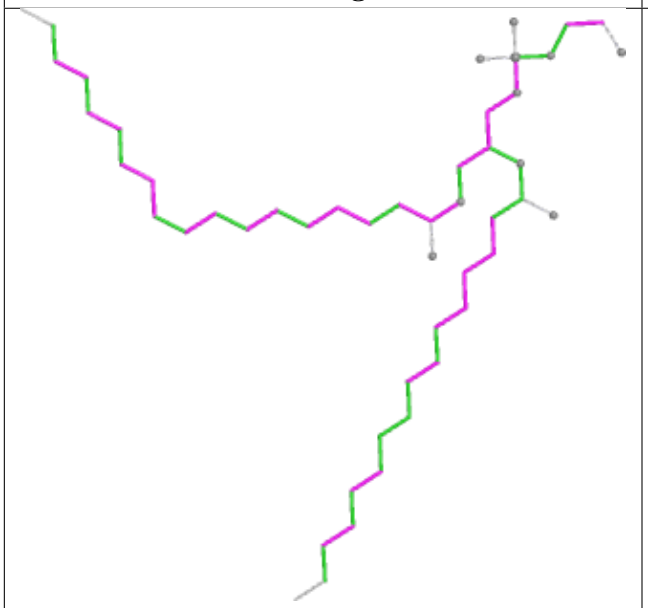
Ligand 9Y0 J 202



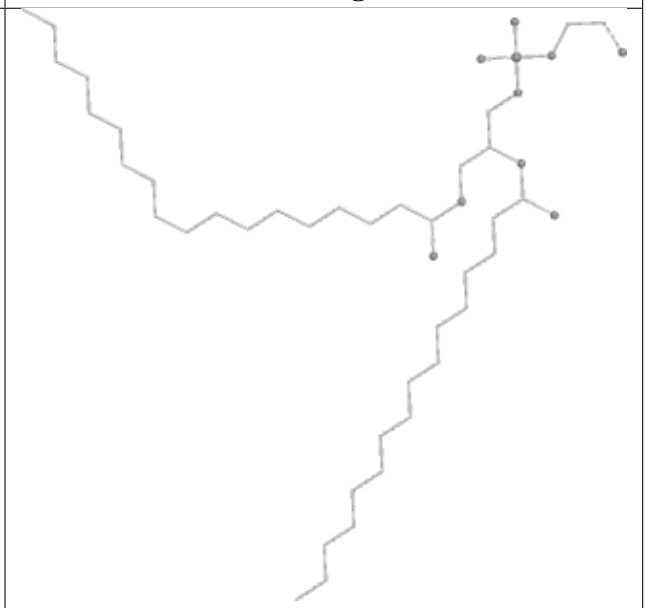
Bond lengths



Bond angles



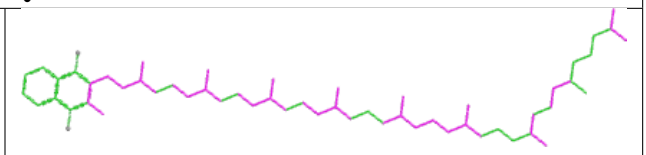
Torsions



Rings

Ligand MQ9 O 304

Bond lengths



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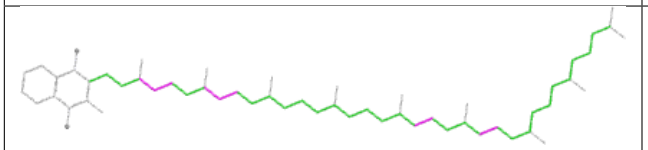

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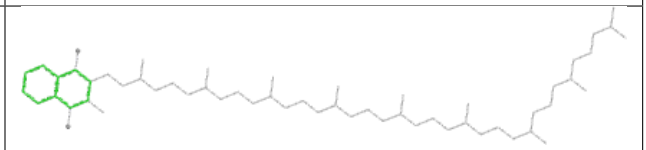
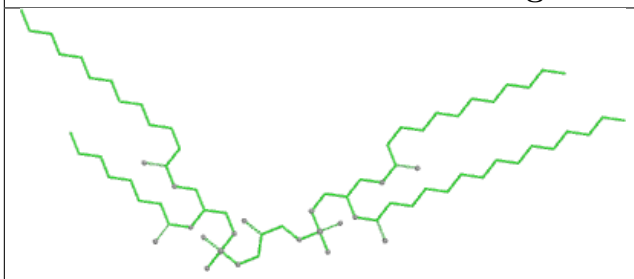


Rings

Ligand CDL E 607



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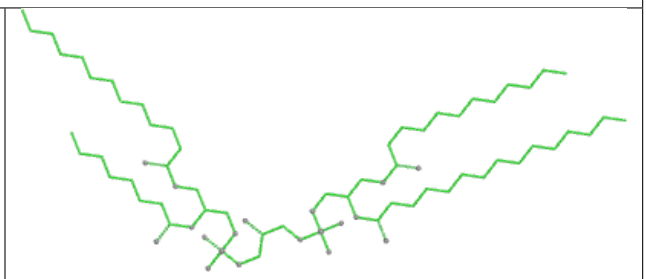

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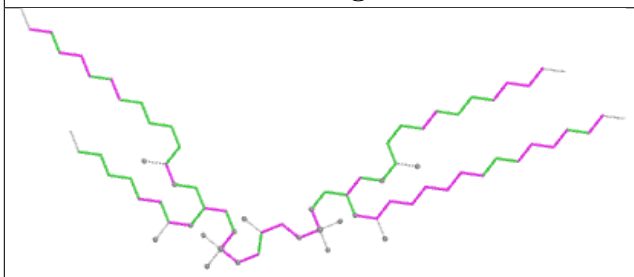

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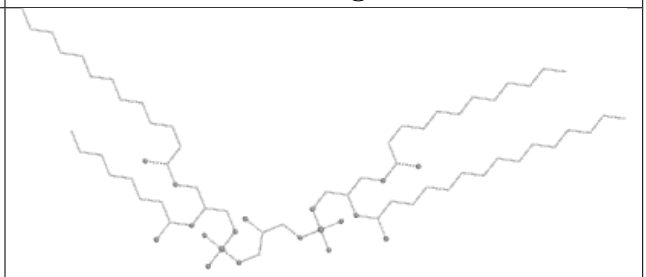
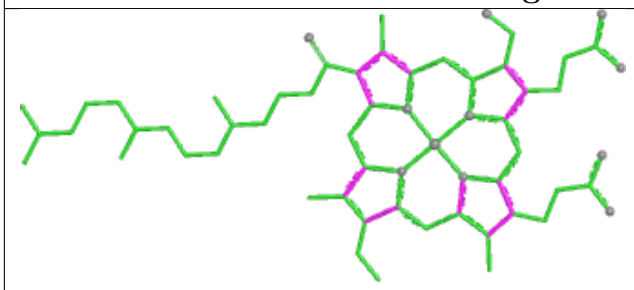


Rings

Ligand HEA R 602



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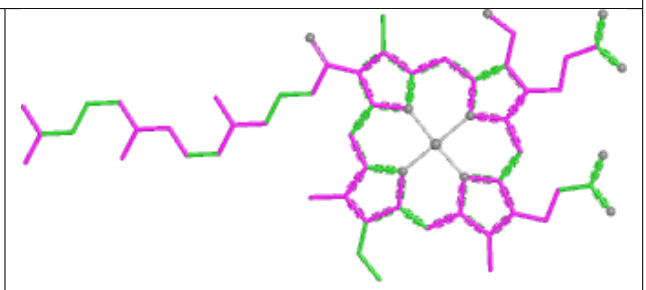

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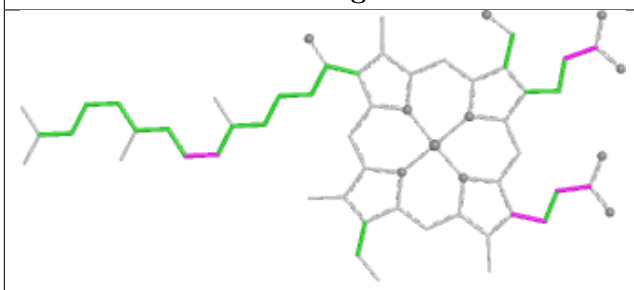

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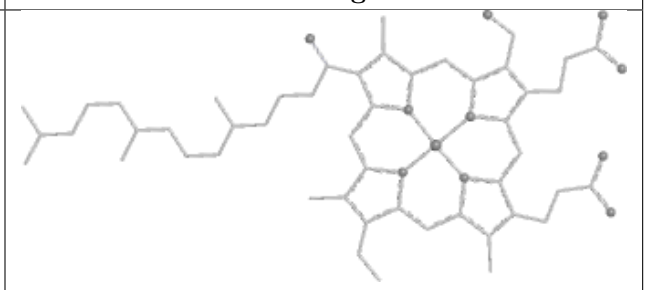
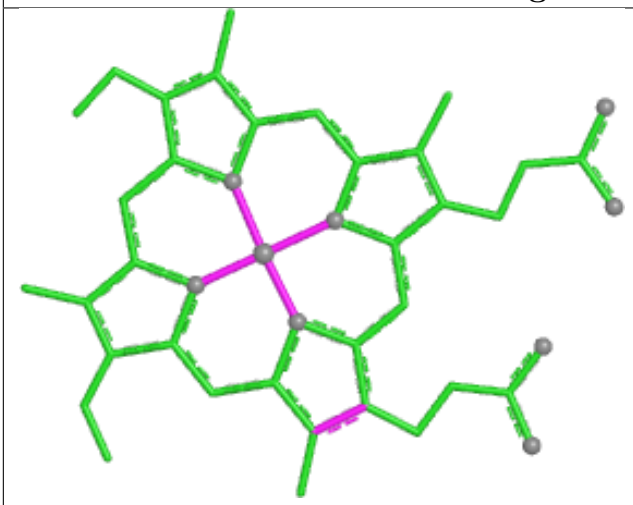


Rings

Ligand HEC I 301



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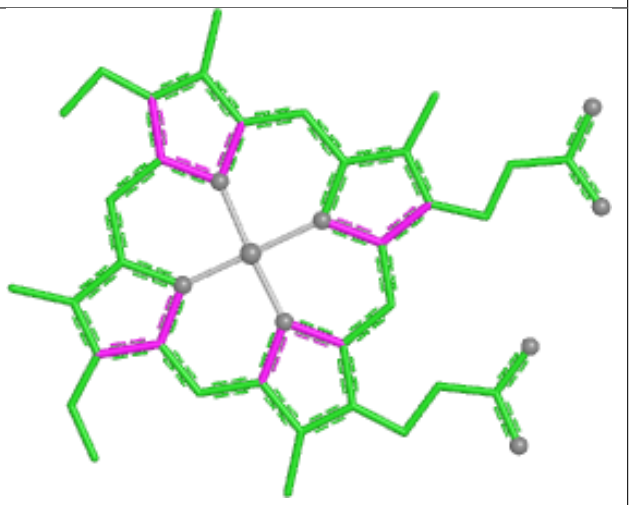

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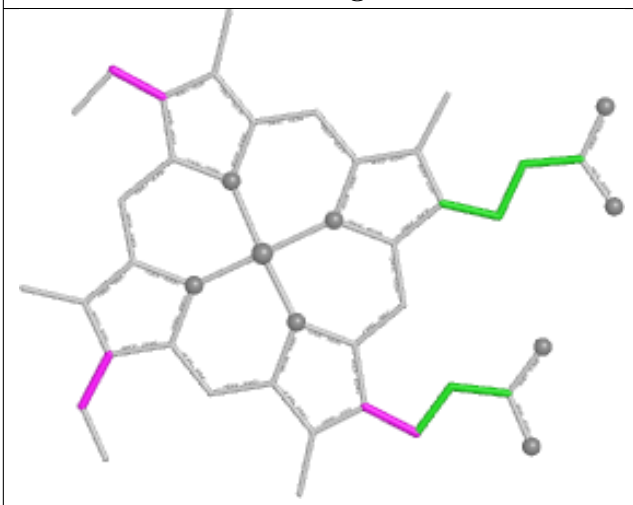

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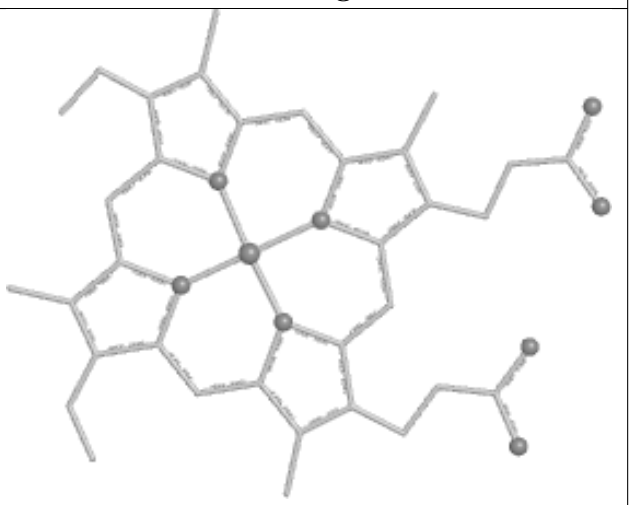
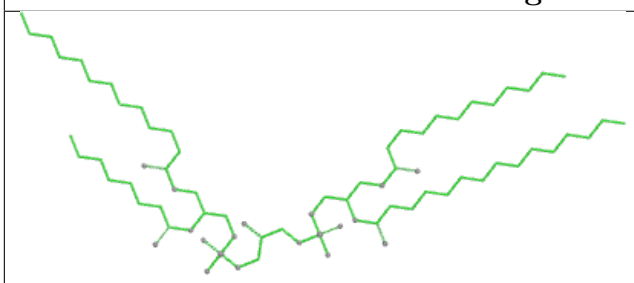


Rings

Ligand CDL R 604



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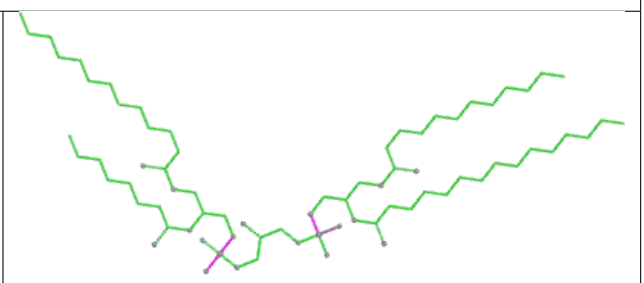

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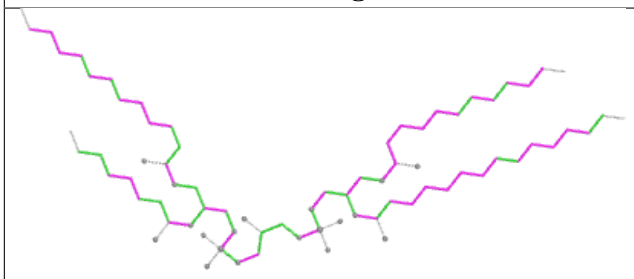

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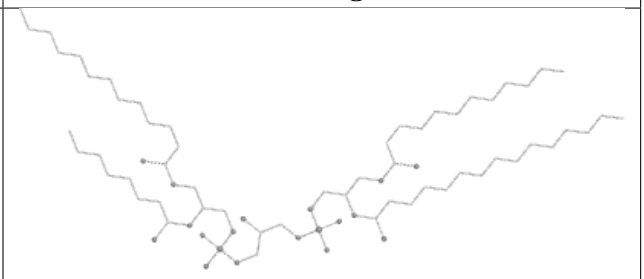
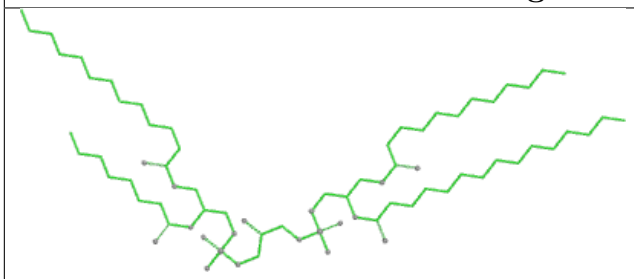


Rings

Ligand CDL L 604



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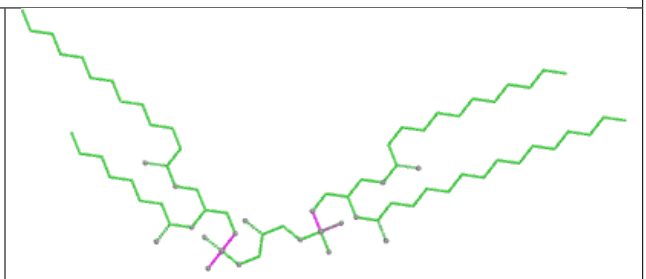

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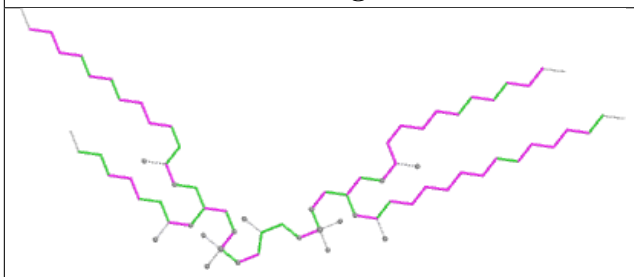

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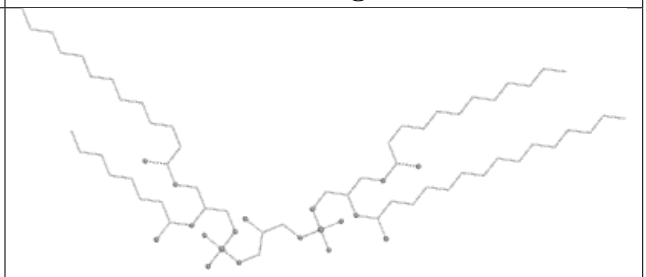
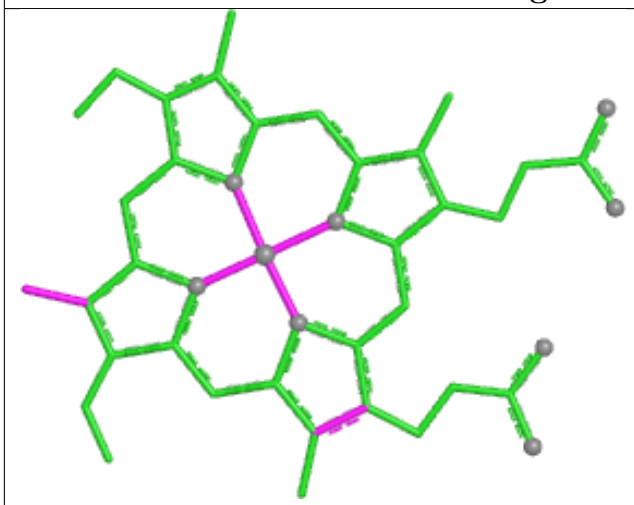


Rings

Ligand HEC I 302



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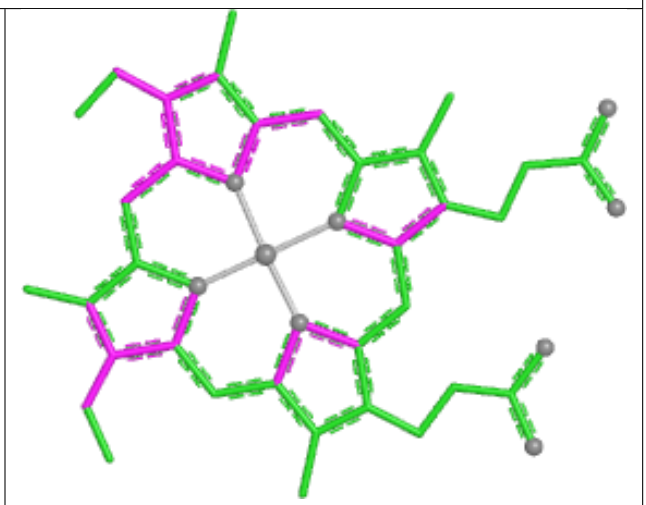

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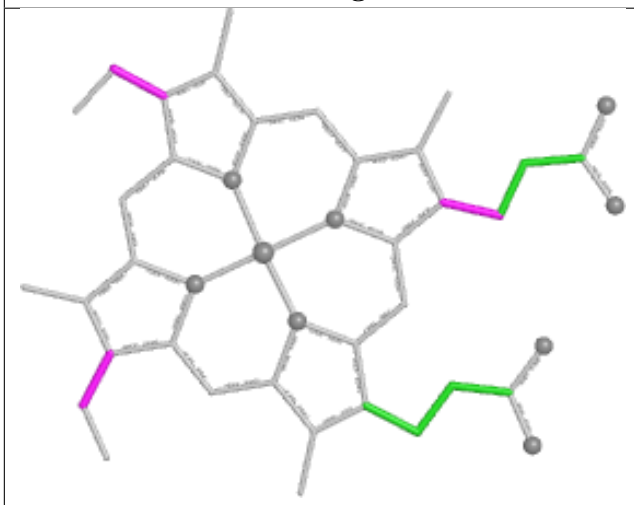

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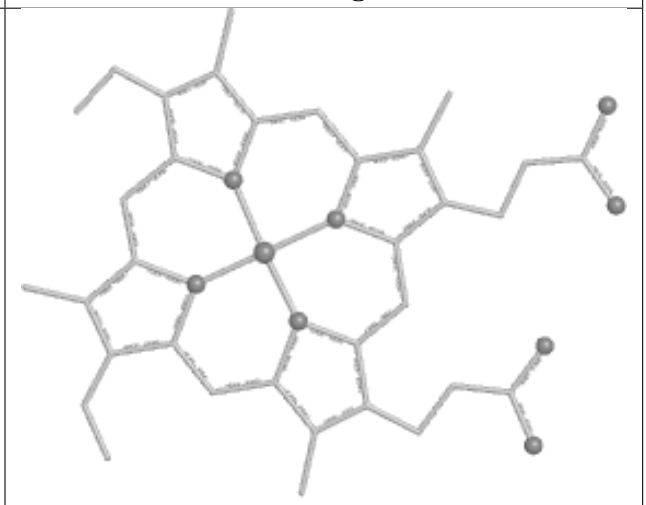
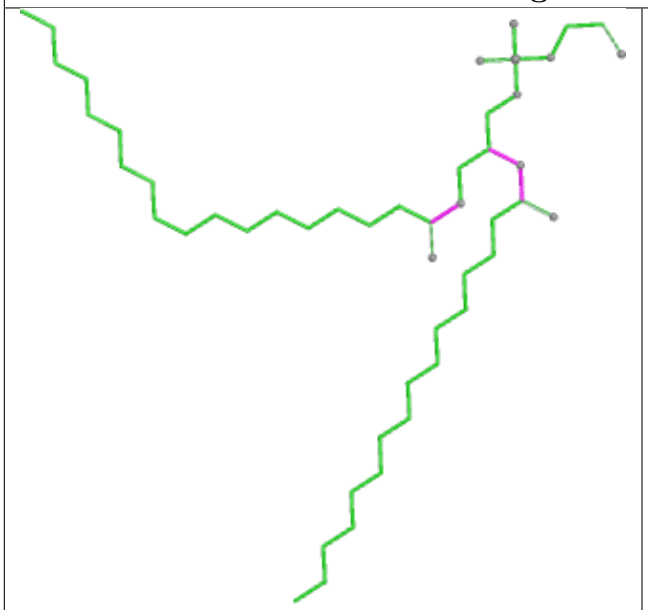


Rings

Ligand 9Y0 X 301



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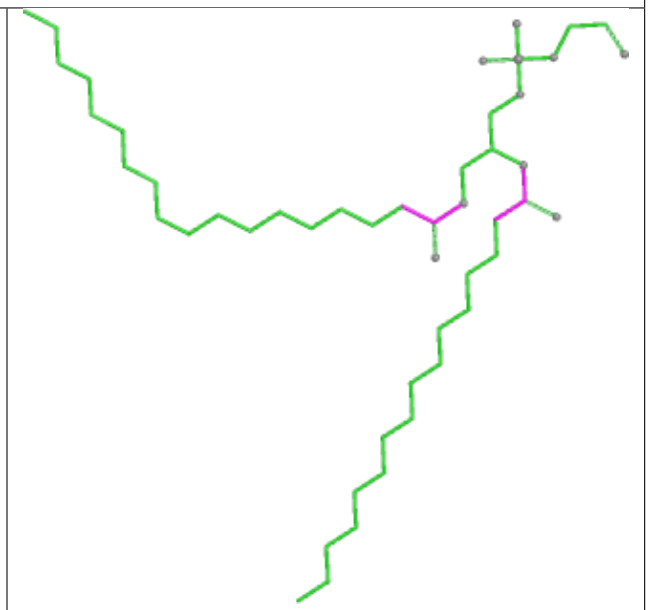

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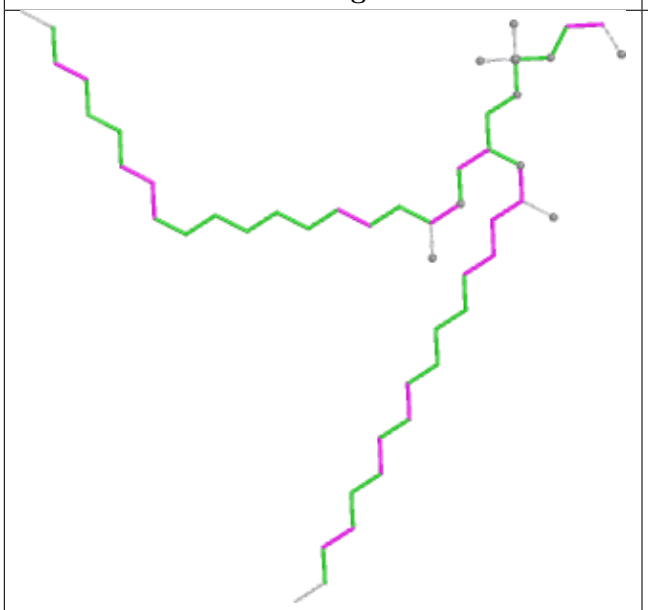

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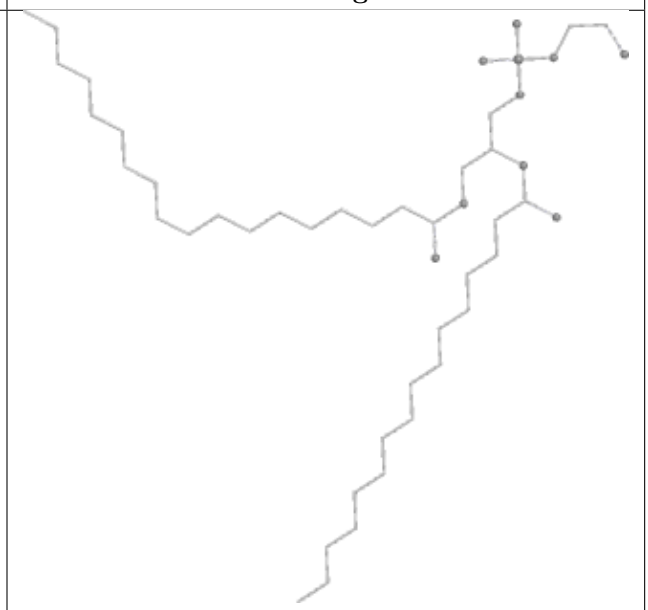
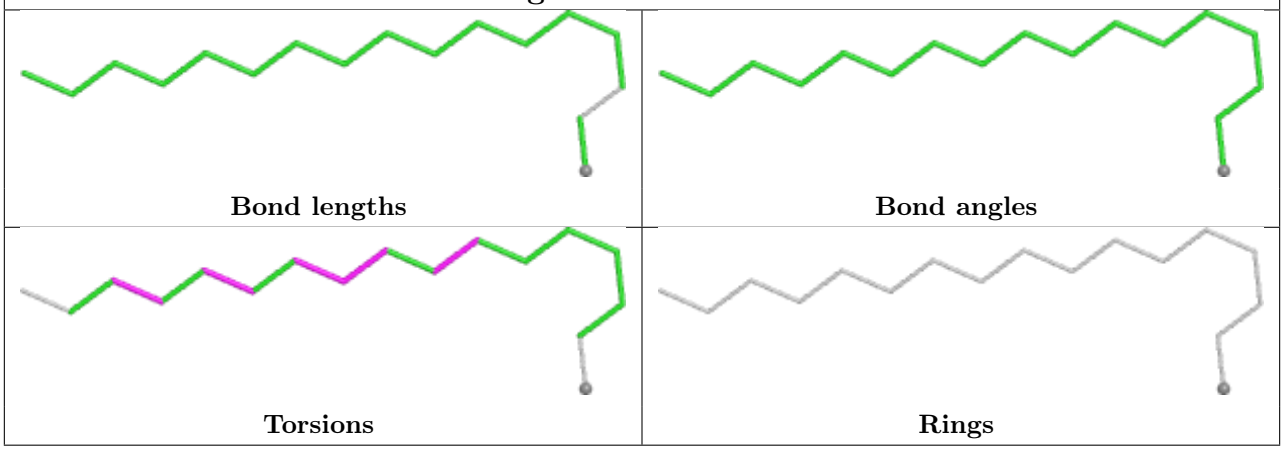
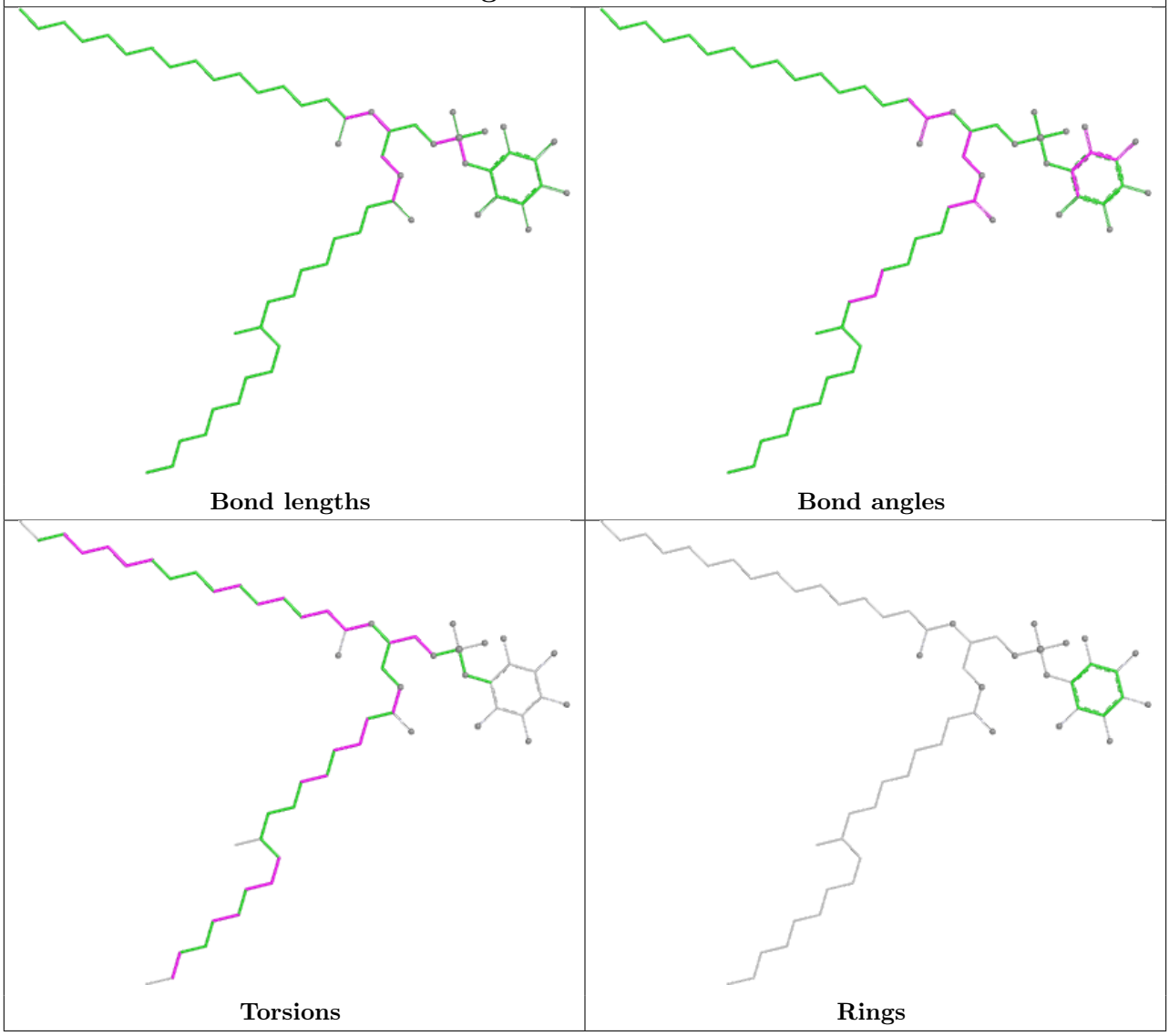


Rings

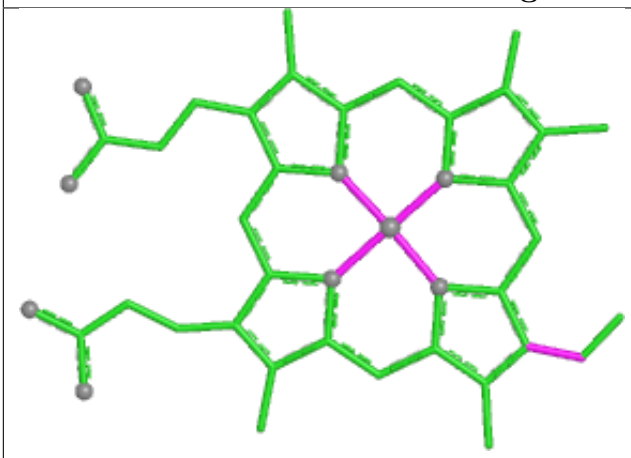
Ligand PLM c 201



Ligand 9YF Y 502



Ligand HEM F 702



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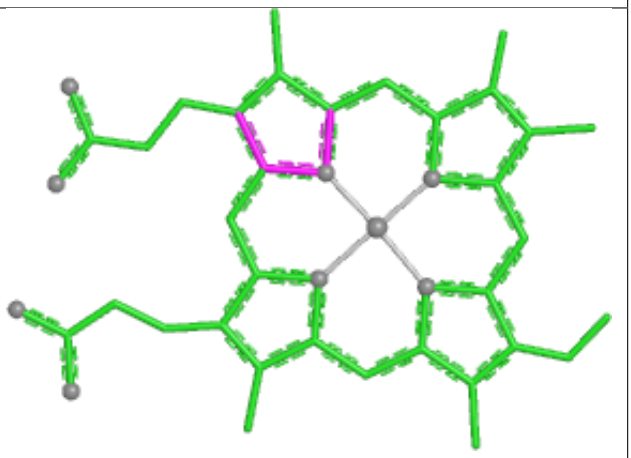
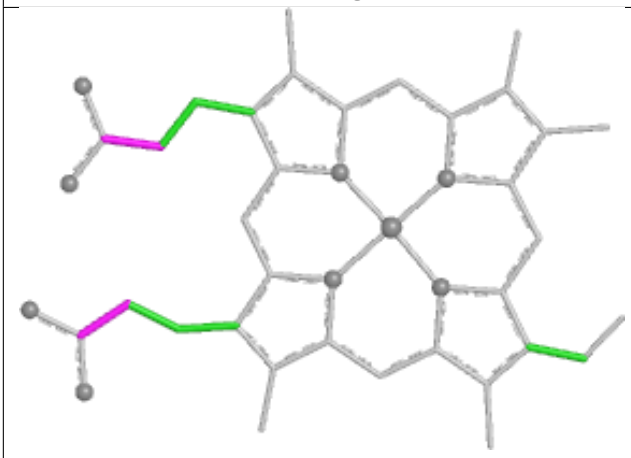


Bond angles



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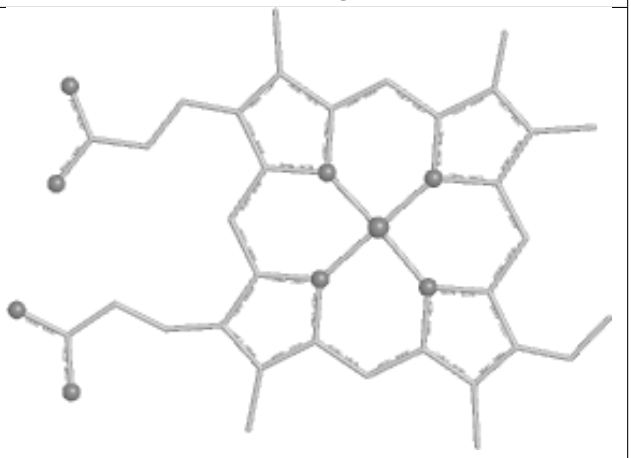
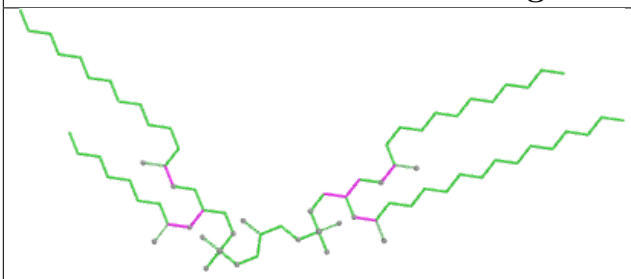


Rings

Ligand CDL S 302



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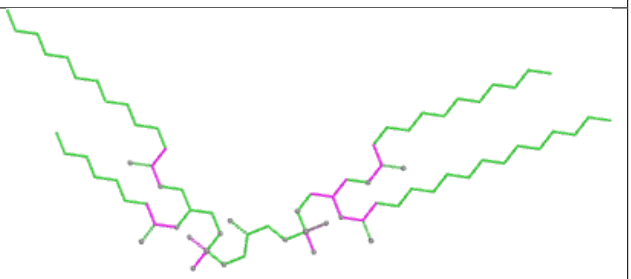

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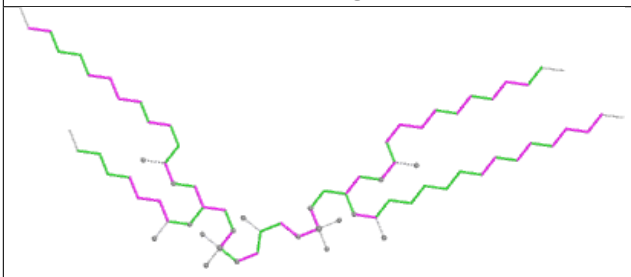

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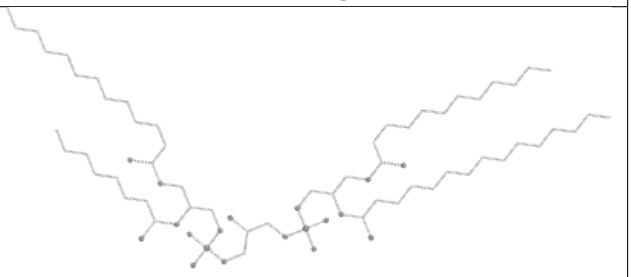
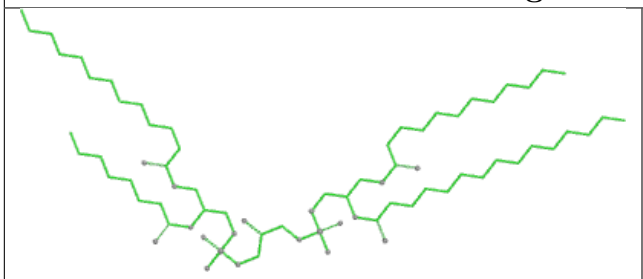
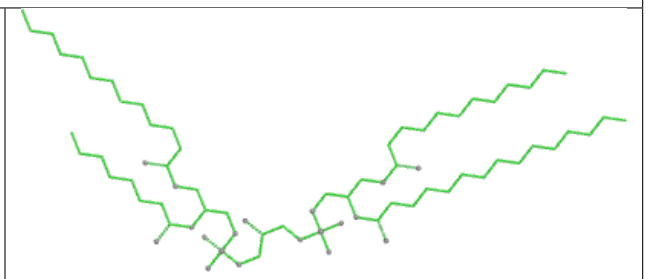
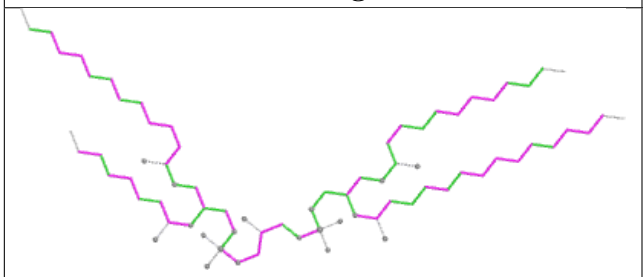
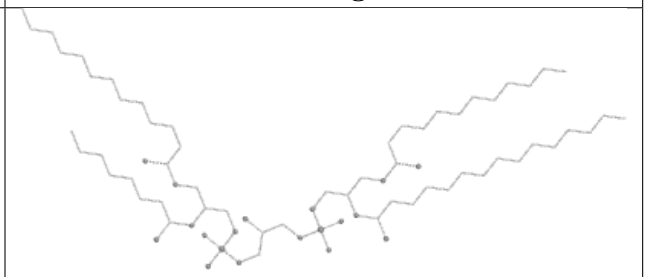
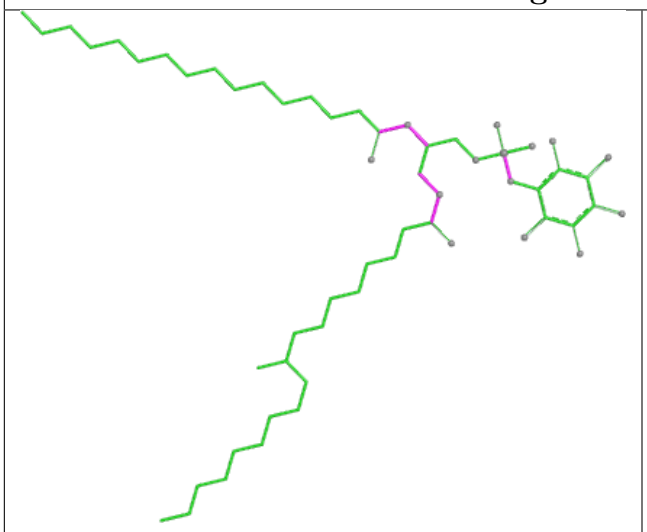


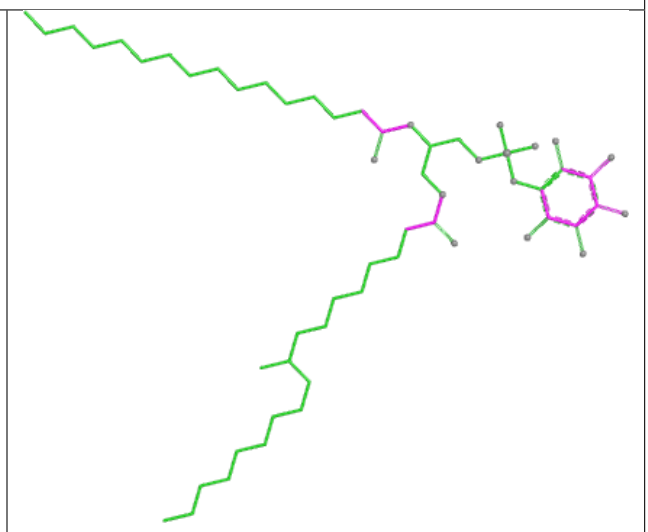
Rings

Ligand CDL P 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

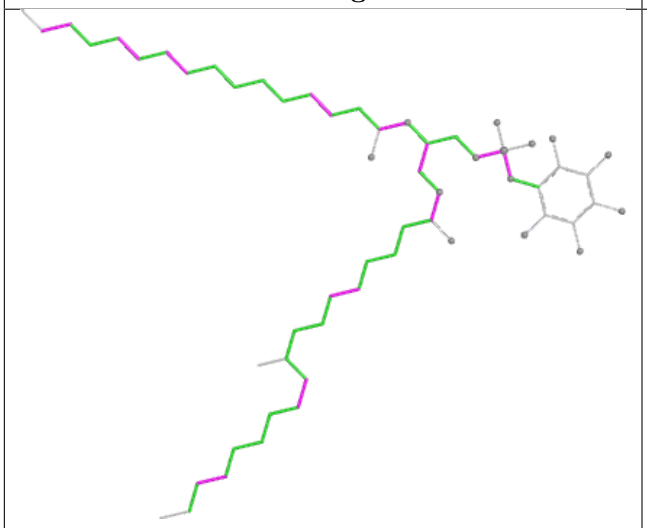
Ligand 9YF E 605



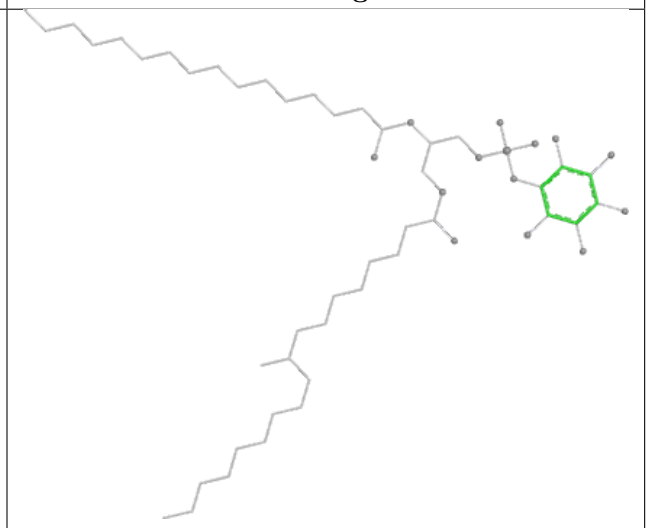
Bond lengths



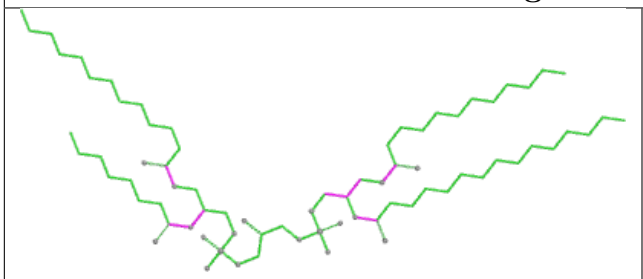
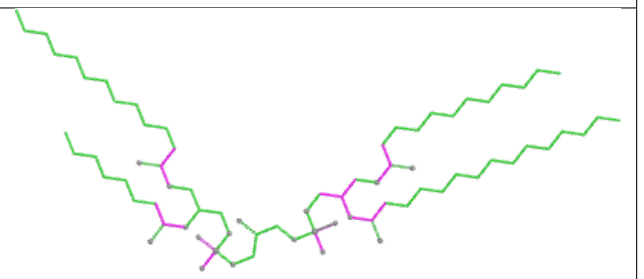
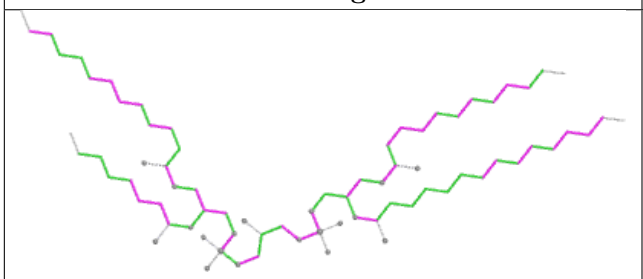
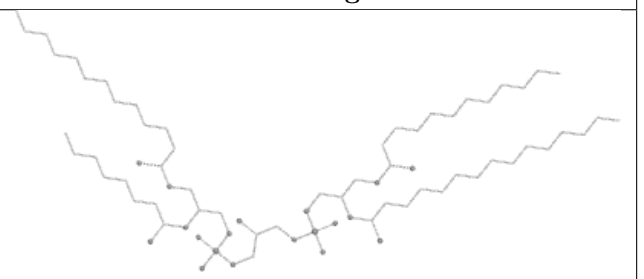
Bond angles

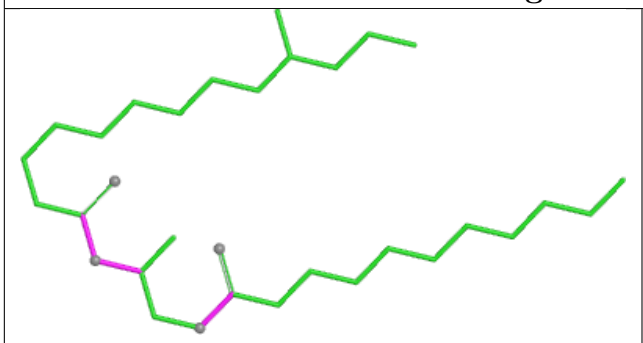
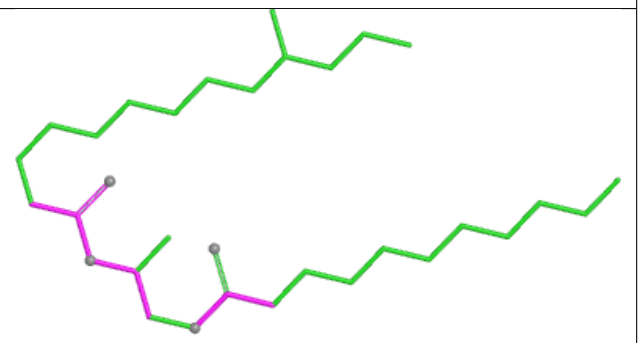
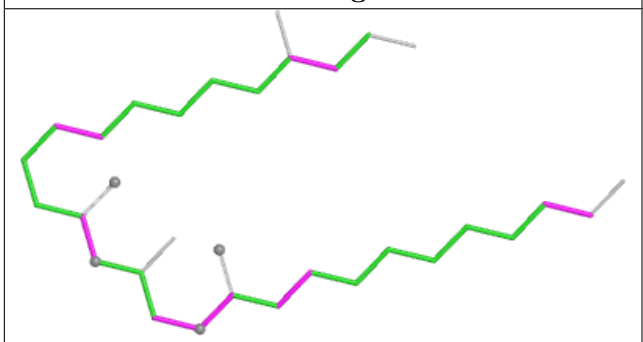
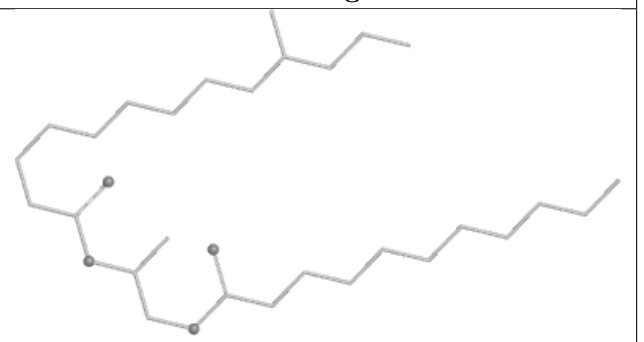


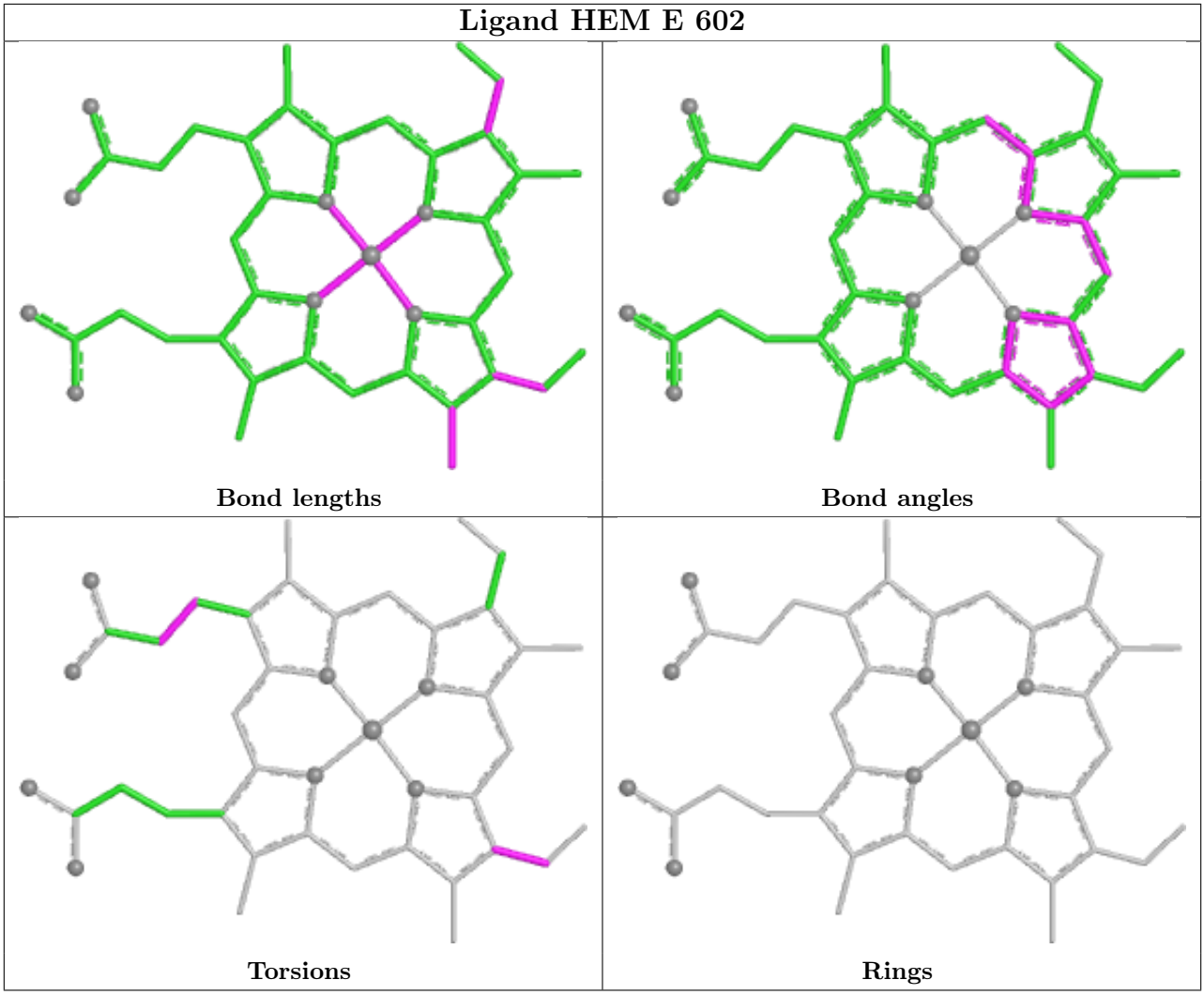
Torsions



Rings

Ligand CDL X 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9XX G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

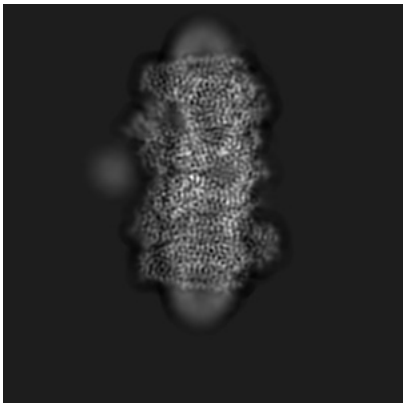
6 Map visualisation (i)

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

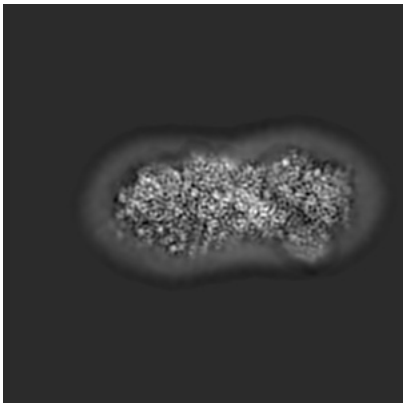
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

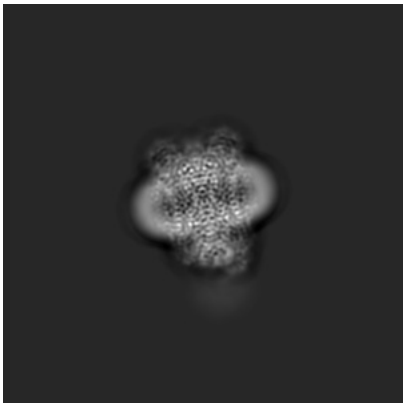
6.1.1 Primary map



X



Y

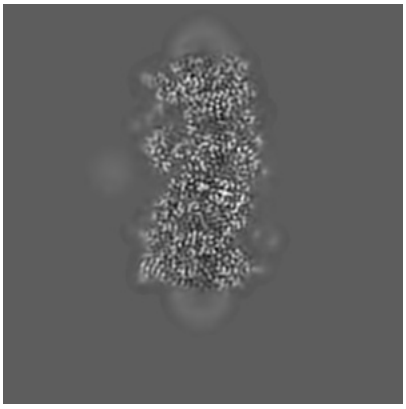


Z

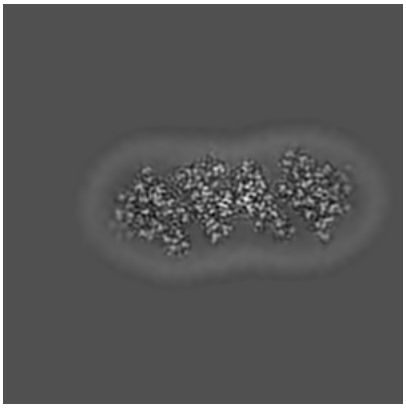
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

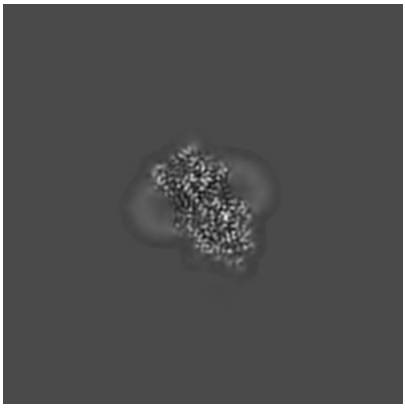
6.2.1 Primary map



X Index: 165



Y Index: 165

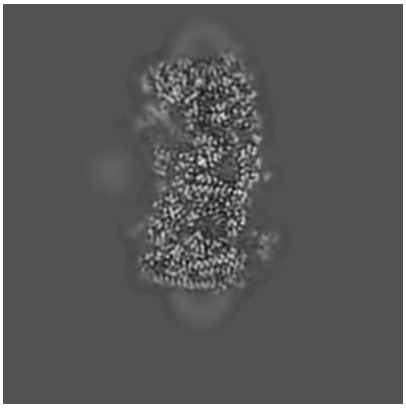


Z Index: 165

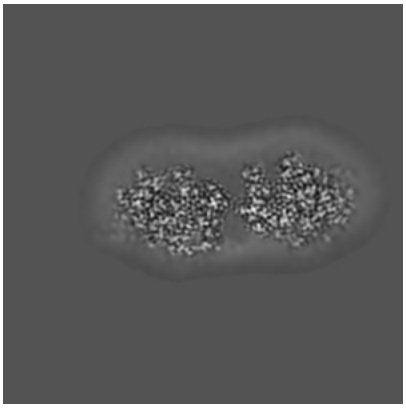
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

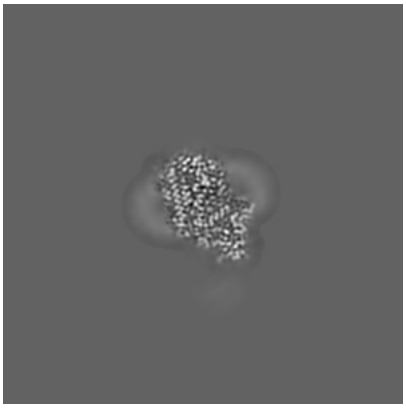
6.3.1 Primary map



X Index: 170



Y Index: 182

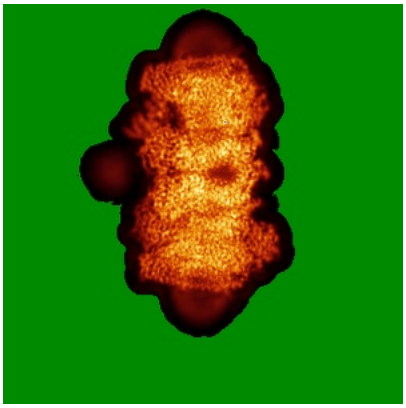


Z Index: 172

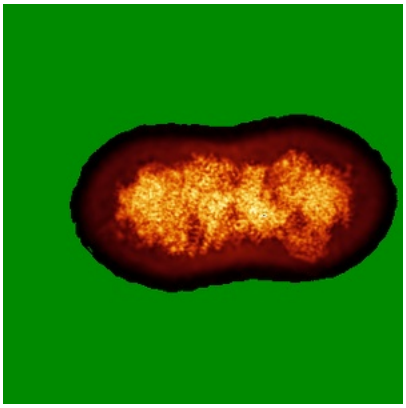
The images above show the largest variance slices of the map in three orthogonal directions.

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

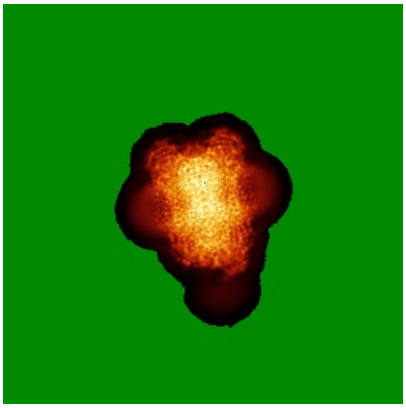
6.4.1 Primary map



X



Y

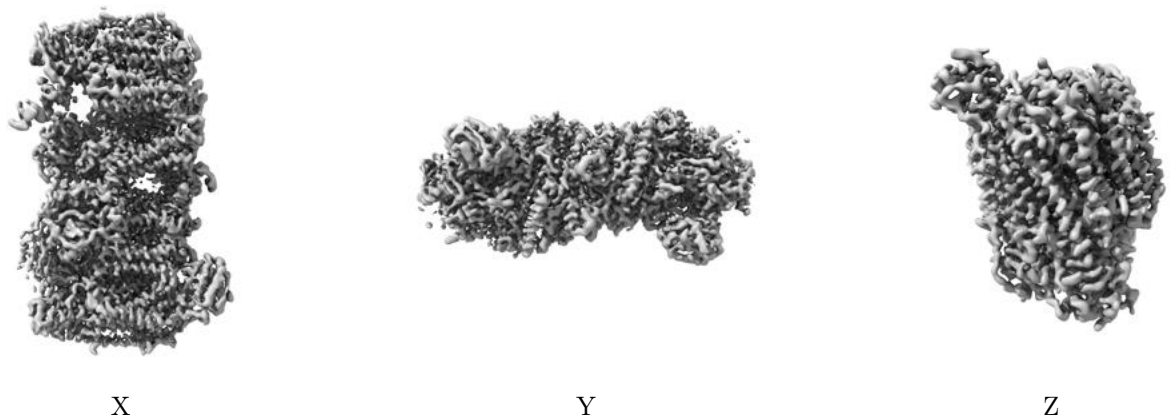


Z

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



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.

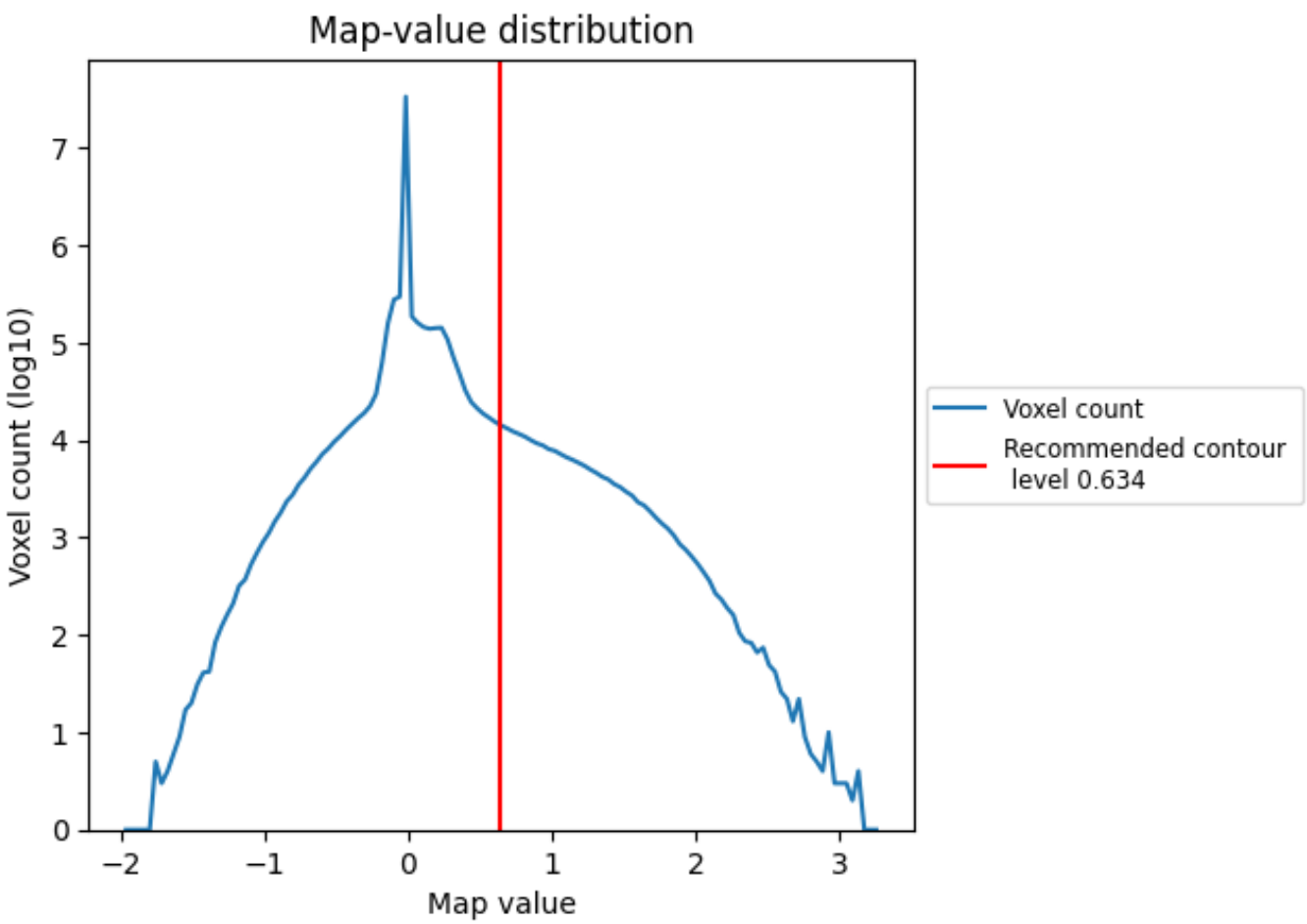
6.6 Mask visualisation (i)

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

7 Map analysis (i)

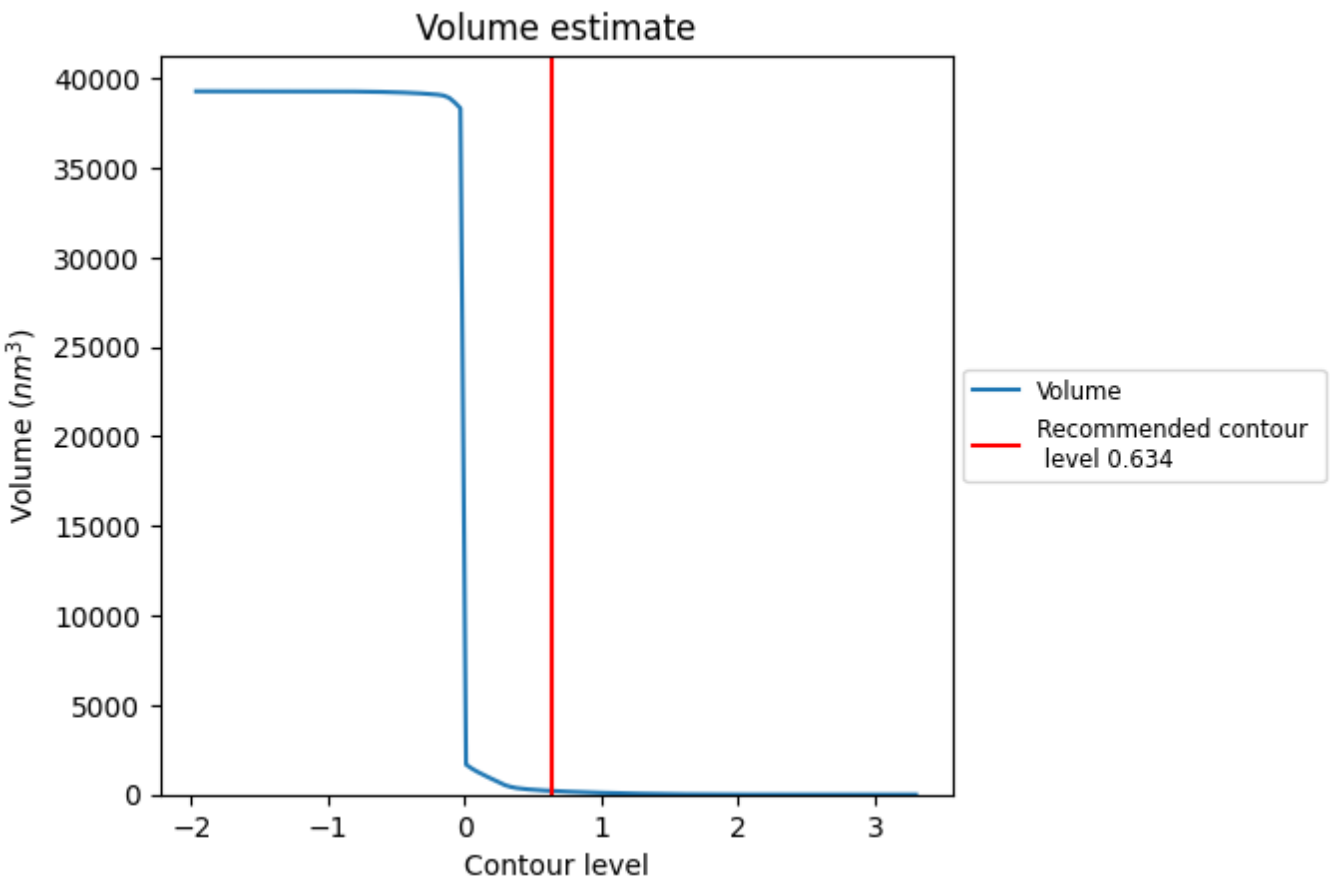
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

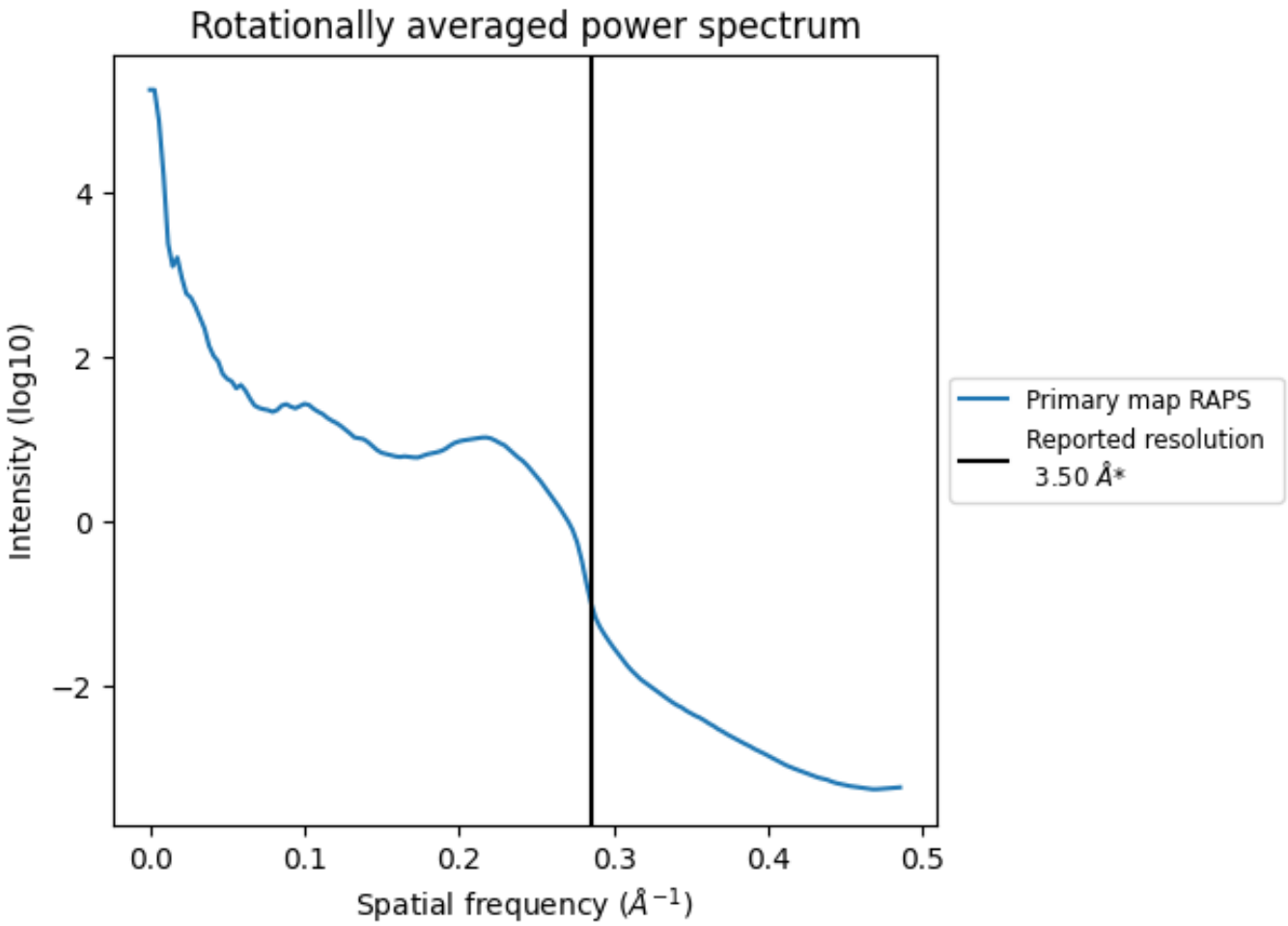
7.2 Volume estimate (i)



The volume at the recommended contour level is 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}

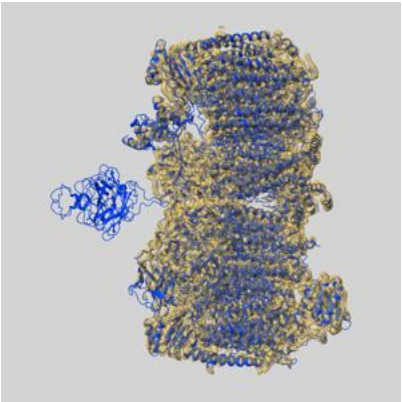
8 Fourier-Shell correlation (i)

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

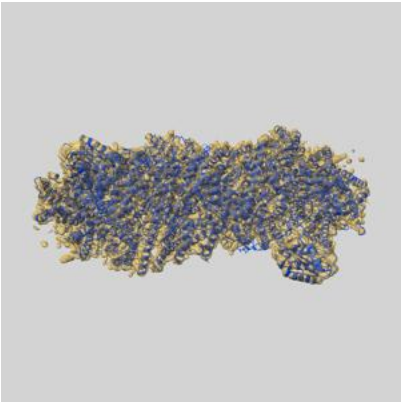
9 Map-model fit (i)

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 16.

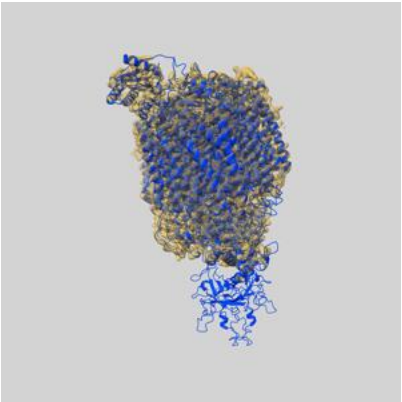
9.1 Map-model overlay (i)



X



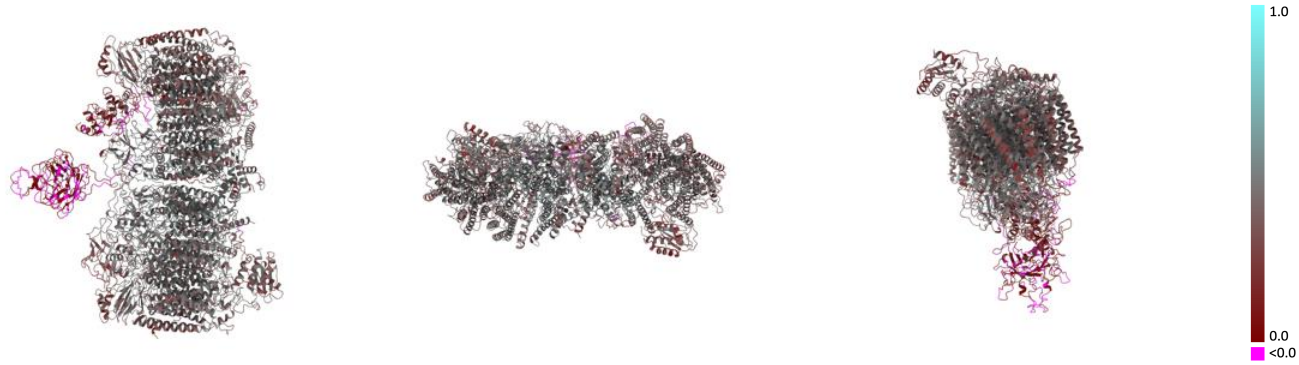
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.634 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.

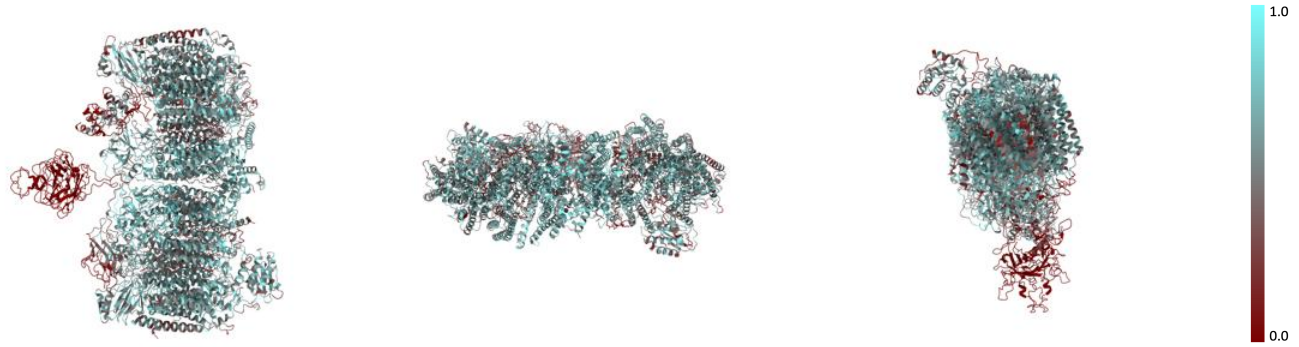
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

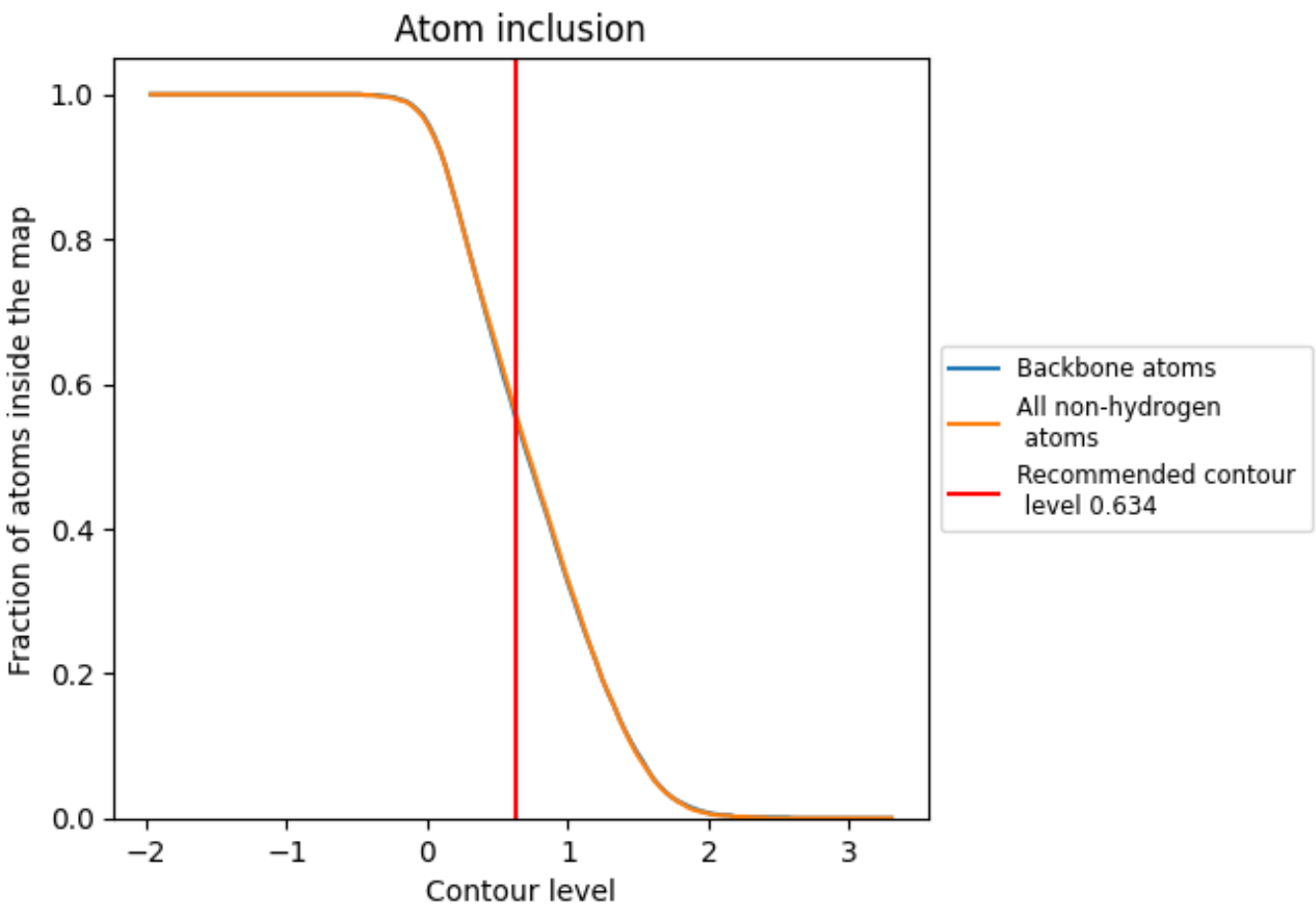
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.634).

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 (i)

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