Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 05:38 AM JST

PDB ID	:	9WCX / pdb_00009wcx
EMDB ID	:	EMD-65878
Title	:	Cryo-EM structure of the Mycobacterium abscessus cytochrome bcc:aa3 supercomplex
Authors	:	Mathiyazakan, V.; Gruber, G.
Deposited on	:	2025-08-18
Resolution	:	2.66 Å(reported)

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

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

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

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

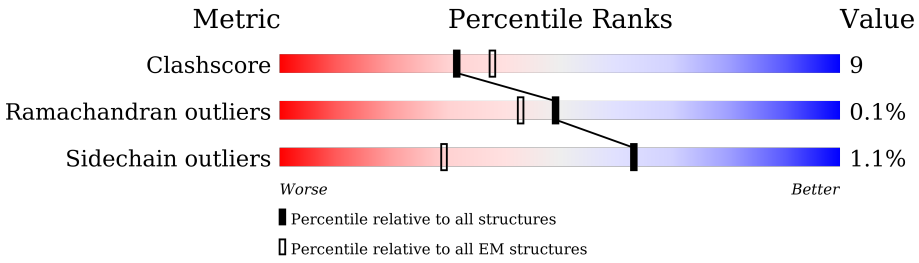
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

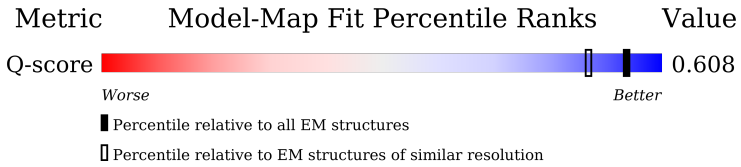
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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	G	99	74% · 23%
1	b	99	75% · 23%
2	I	564	81% 16% ·
2	L	564	83% 15% ·

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Mol	Chain	Length	Quality of chain
3	J	86	9% 63% 14% 21%
3	h	86	12% 70% 9% 21%
4	U	295	63% 10% 25%
4	o	295	68% 7% 25%
5	V	391	91% 6%
5	p	391	90% 8%
6	X	238	9% 89%
6	a	238	9% 89%
7	d	349	80% 9% 11%
7	e	349	82% 7% 11%
8	f	206	84% 14%
8	g	206	86% 13%
9	i	546	81% 15%
9	j	546	84% 12%
10	k	175	7% 70% 12% 18%
10	l	175	5% 72% 10% 18%
11	m	139	91% 9%
11	n	139	88% 12%
12	q	227	57% 12% 31%
12	r	227	55% 12% 31%

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
14	CDL	b	103	-	-	X	-
23	MQ9	i	610	-	-	X	-
24	HEC	o	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	HEC	o	602	X	-	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 46750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Prokaryotic respiratory supercomplex associate factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	76	Total	C	N	O	S	0	0
			575	372	103	98	2		
1	b	76	Total	C	N	O	S	0	0
			575	372	103	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		
2	L	551	Total	C	N	O	S	0	0
			4363	2936	696	707	24		

- Molecule 3 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	68	Total	C	N	O	S	0	0
			509	333	86	87	3		
3	h	68	Total	C	N	O	S	0	0
			509	333	86	87	3		

- Molecule 4 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		
4	o	221	Total	C	N	O	S	0	0
			1639	1015	296	318	10		

- Molecule 5 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		
5	p	381	Total	C	N	O	S	0	0
			2957	1900	511	534	12		

- Molecule 6 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	25	Total	C	N	O	S	0	0
			171	104	28	38	1		
6	a	25	Total	C	N	O	S	0	0
			171	104	28	38	1		

- Molecule 7 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		
7	e	312	Total	C	N	O	S	0	0
			2476	1604	418	445	9		

- Molecule 8 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		
8	g	206	Total	C	N	O	S	0	0
			1595	1053	259	275	8		

- Molecule 9 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		
9	j	527	Total	C	N	O	S	0	0
			4127	2716	693	696	22		

- Molecule 10 is a protein called DUF5130 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	144	Total	C	N	O	S	0	0
			1063	669	184	209	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	144	Total	C	N	O	S	0	0
			1063	669	184	209	1		

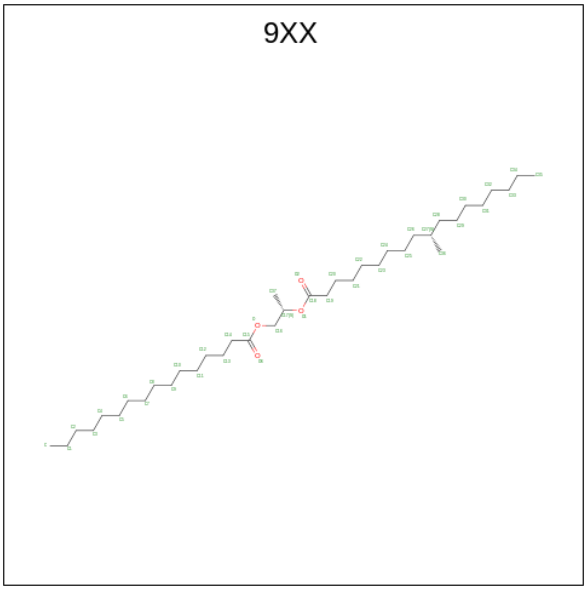
- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		
11	n	139	Total	C	N	O	S	0	0
			1066	704	169	188	5		

- Molecule 12 is a protein called Lipoprotein lpqE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		
12	r	156	Total	C	N	O	S	0	0
			1129	696	201	231	1		

- Molecule 13 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			42	38	4	

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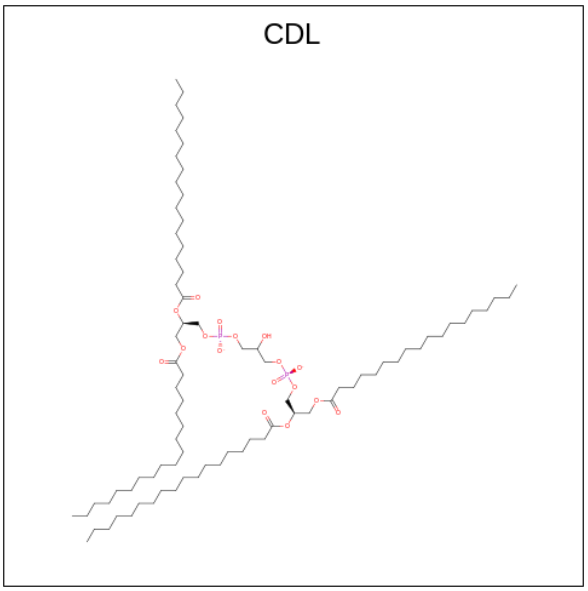
Mol	Chain	Residues	Atoms	AltConf
13	b	1	Total C O 42 38 4	0
13	i	1	Total C O 32 28 4	0
13	j	1	Total C O 32 28 4	0

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
14	G	1	Total C O P 88 69 17 2	0
14	I	1	Total C O P 76 57 17 2	0
14	I	1	Total C O P 81 62 17 2	0
14	L	1	Total C O P 76 57 17 2	0
14	L	1	Total C O P 81 62 17 2	0
14	U	1	Total C O P 79 60 17 2	0
14	b	1	Total C O P 88 69 17 2	0
14	g	1	Total C O P 95 76 17 2	0

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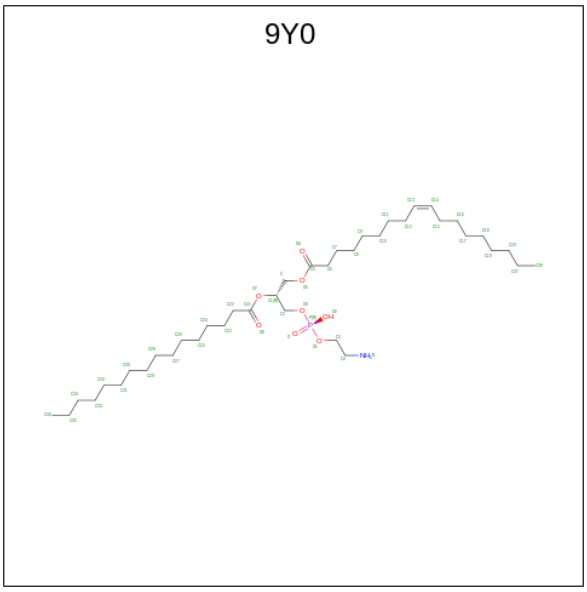
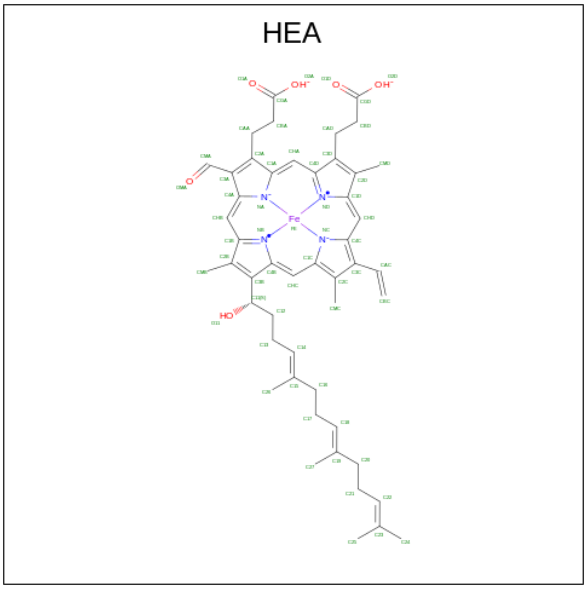
Mol	Chain	Residues	Atoms				AltConf
14	i	1	Total	C	O	P	0
			66	47	17	2	
14	i	1	Total	C	O	P	0
			74	55	17	2	
14	i	1	Total	C	O	P	0
			77	58	17	2	
14	i	1	Total	C	O	P	0
			79	60	17	2	
14	i	1	Total	C	O	P	0
			74	55	17	2	
14	j	1	Total	C	O	P	0
			77	58	17	2	
14	j	1	Total	C	O	P	0
			79	60	17	2	
14	j	1	Total	C	O	P	0
			66	47	17	2	
14	m	1	Total	C	O	P	0
			79	60	17	2	
14	p	1	Total	C	O	P	0
			95	76	17	2	

- Molecule 15 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	b	1	Total	C	N	O	P	0
			38	28	1	8	1	
15	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	f	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	q	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 16 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

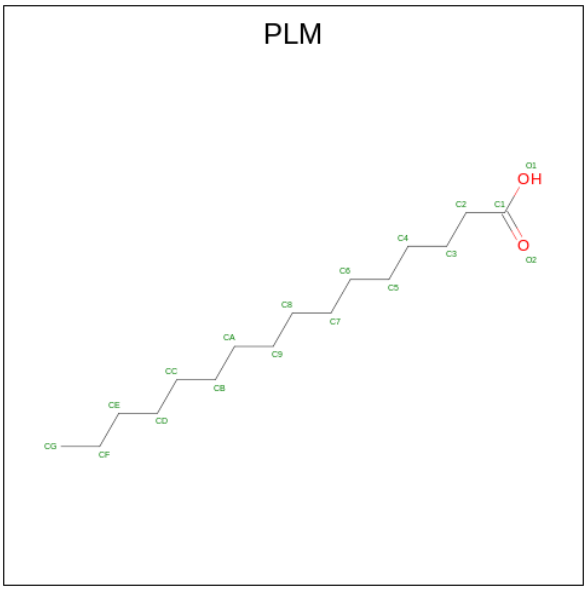


Mol	Chain	Residues	Atoms					AltConf
16	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	I	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	L	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

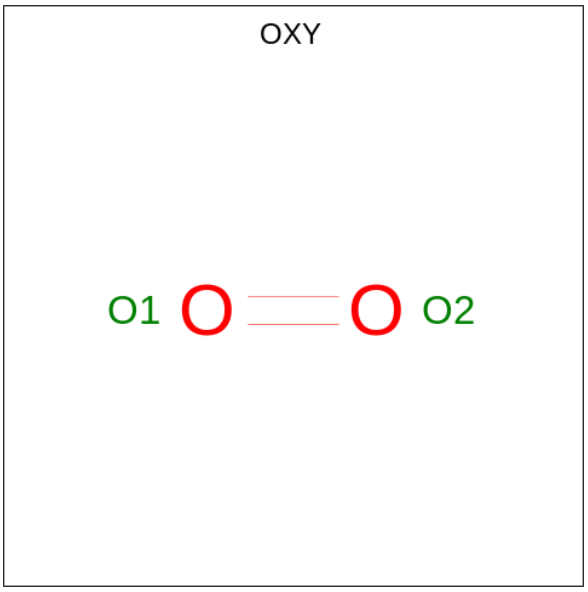
Mol	Chain	Residues	Atoms	AltConf
17	I	2	Total Cu 2 2	0
17	L	2	Total Cu 2 2	0
17	d	2	Total Cu 2 2	0
17	e	2	Total Cu 2 2	0

- Molecule 18 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



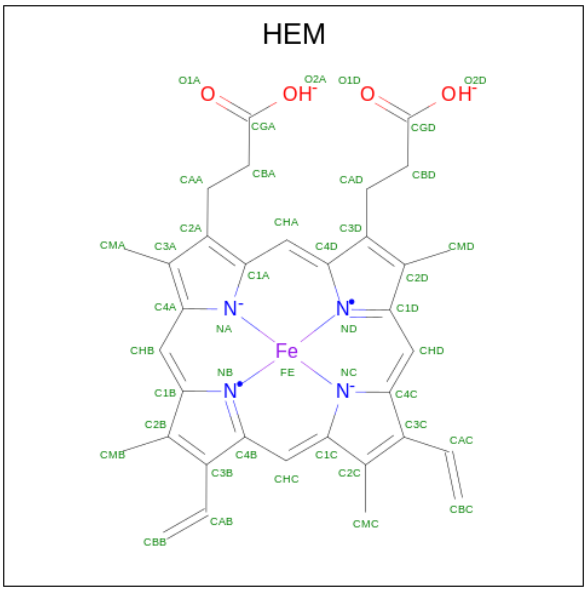
Mol	Chain	Residues	Atoms	AltConf
18	I	1	Total C O 17 16 1	0
18	q	1	Total C O 17 16 1	0

- Molecule 19 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	I	1	Total O 2 2	0
19	L	1	Total O 2 2	0

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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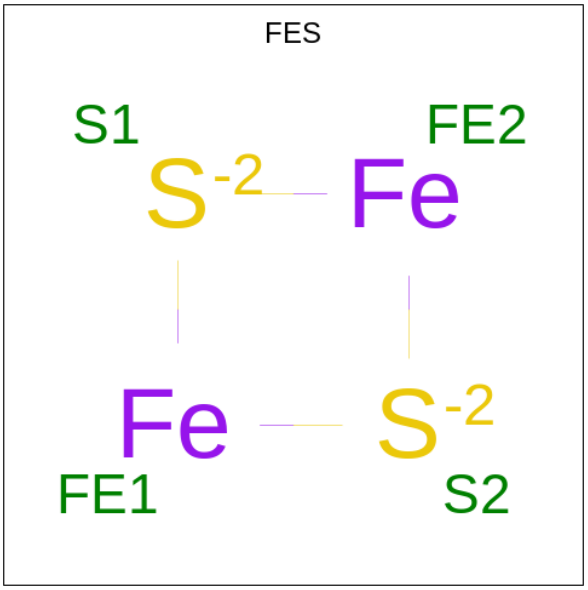
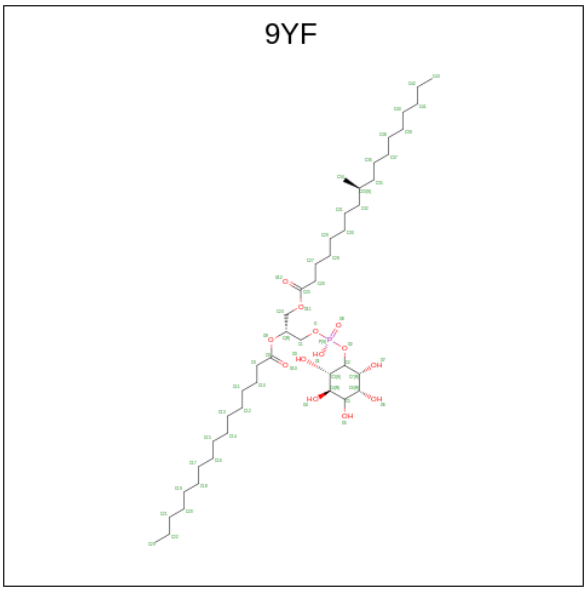
Mol	Chain	Residues	Atoms					AltConf
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	i	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	i	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	j	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



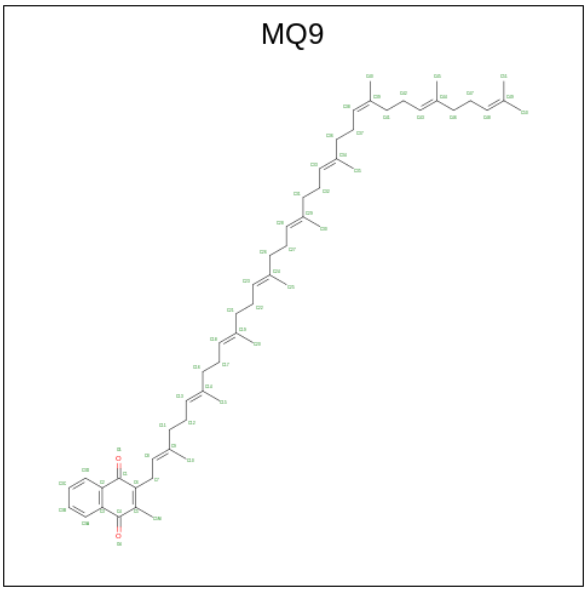
Mol	Chain	Residues	Atoms			AltConf
21	V	1	Total	Fe	S	0
			4	2	2	
21	p	1	Total	Fe	S	0
			4	2	2	

- Molecule 22 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: $C_{44}H_{85}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



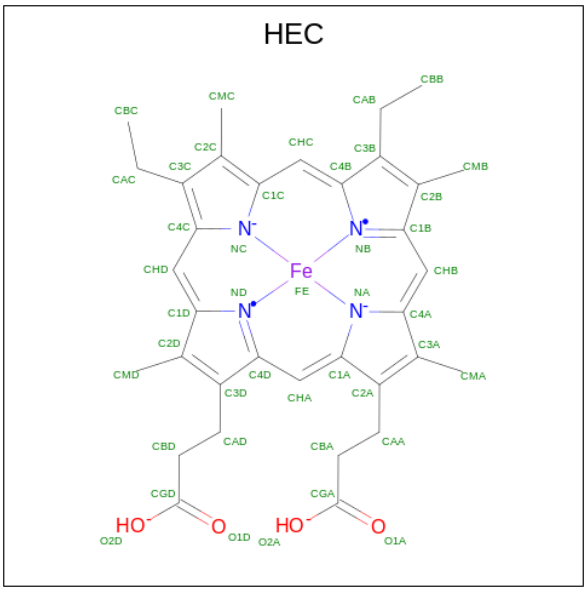
Mol	Chain	Residues	Atoms				AltConf
22	V	1	Total	C	O	P	0
			58	44	13	1	
22	i	1	Total	C	O	P	0
			58	44	13	1	
22	j	1	Total	C	O	P	0
			58	44	13	1	
22	n	1	Total	C	O	P	0
			58	44	13	1	
22	o	1	Total	C	O	P	0
			58	44	13	1	
22	p	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 23 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	i	1	Total C O 58 56 2	0
23	i	1	Total C O 58 56 2	0
23	i	1	Total C O 43 41 2	0
23	i	1	Total C O 48 46 2	0
23	i	1	Total C O 58 56 2	0
23	j	1	Total C O 58 56 2	0
23	j	1	Total C O 43 41 2	0
23	j	1	Total C O 58 56 2	0
23	j	1	Total C O 58 56 2	0
23	m	1	Total C O 48 46 2	0

- Molecule 24 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	I	18	Total	O	0
			18	18	
25	L	18	Total	O	0
			18	18	
25	U	3	Total	O	0
			3	3	
25	V	2	Total	O	0
			2	2	
25	d	1	Total	O	0
			1	1	
25	e	1	Total	O	0
			1	1	
25	i	9	Total	O	0
			9	9	
25	j	10	Total	O	0
			10	10	
25	m	2	Total	O	0
			2	2	
25	n	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms	AltConf
25	o	4	Total O 4 4	0
25	p	3	Total O 3 3	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: Prokaryotic respiratory supercomplex associate factor 1

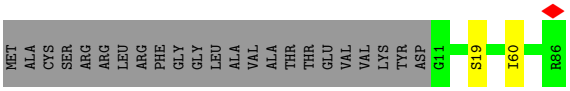
Chain G:



• Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

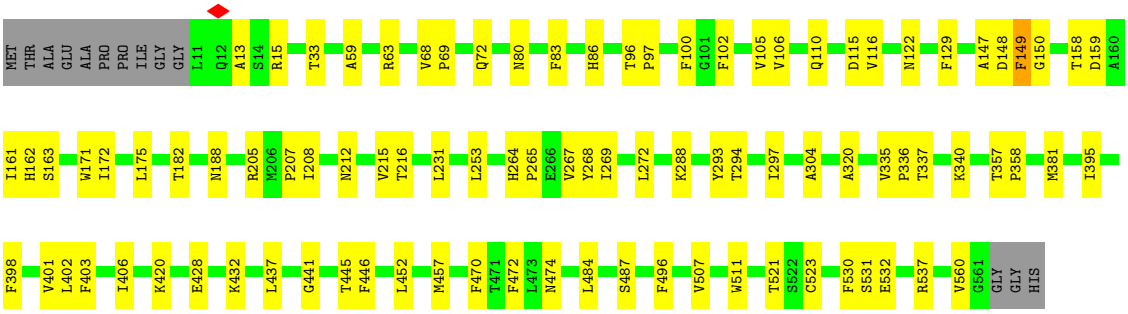
Chain b:





• Molecule 2: Cytochrome c oxidase subunit 1

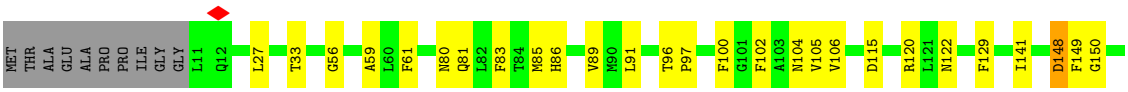
Chain I:

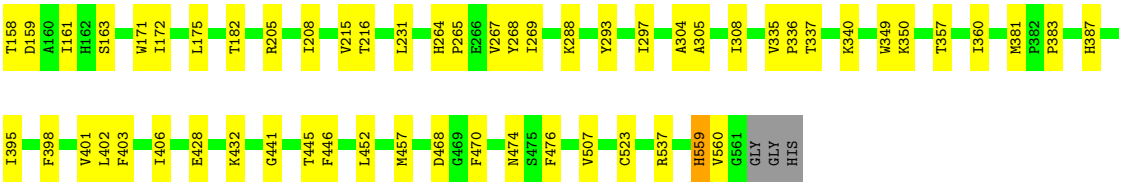


• Molecule 2: Cytochrome c oxidase subunit 1

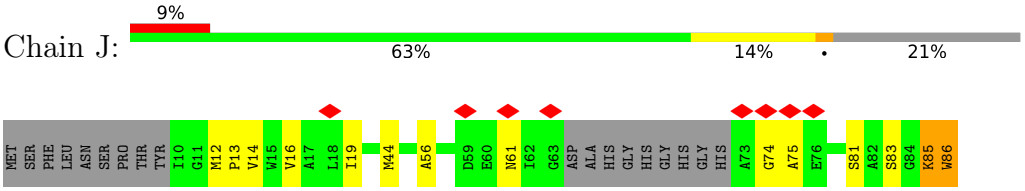
Chain L:



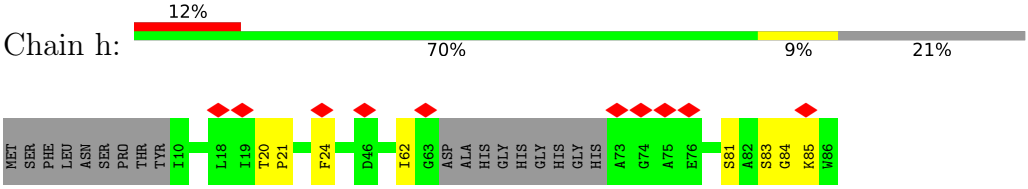




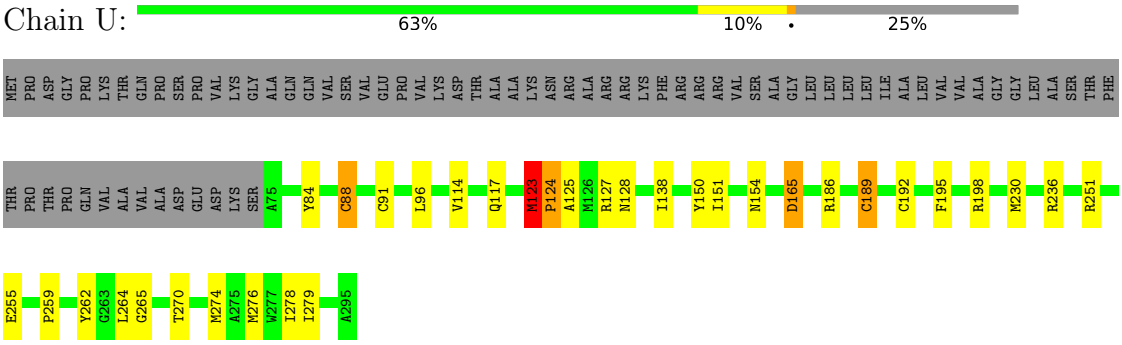
• Molecule 3: Cytochrome c oxidase subunit CtaJ



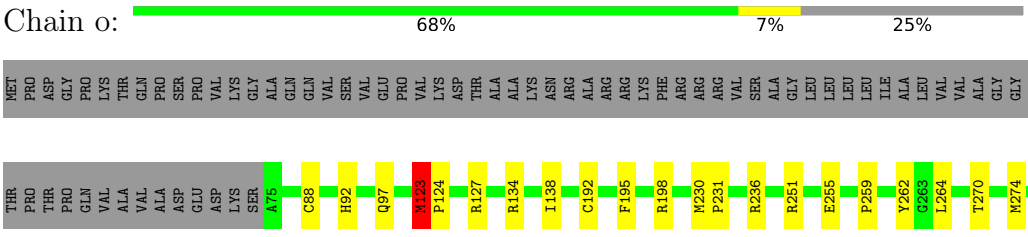
• Molecule 3: Cytochrome c oxidase subunit CtaJ



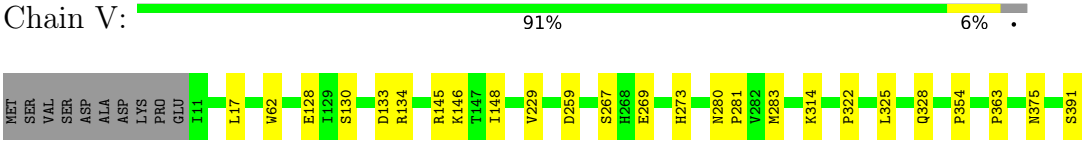
• Molecule 4: Cytochrome bc1 complex cytochrome c subunit



• Molecule 4: Cytochrome bc1 complex cytochrome c subunit

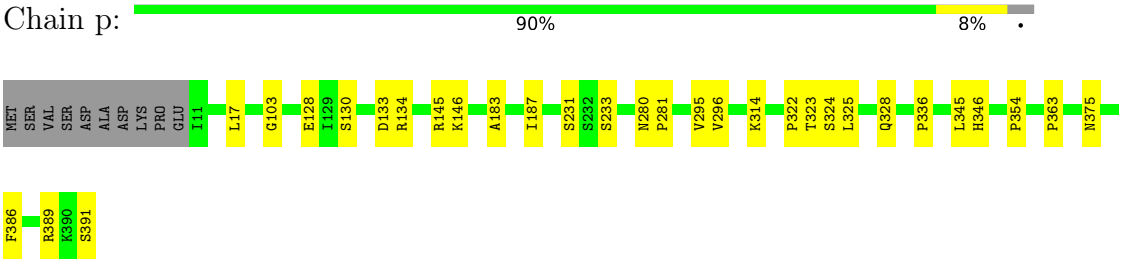


• Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit



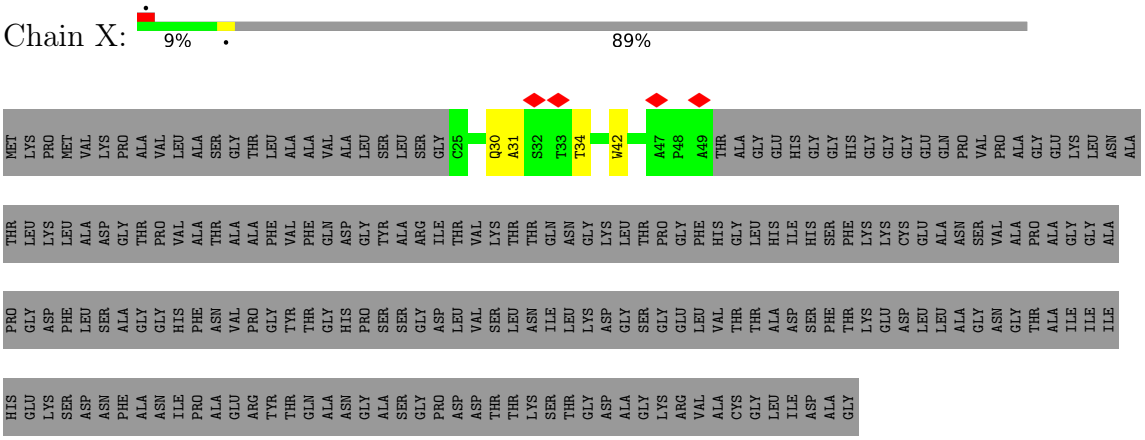
• Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain p:



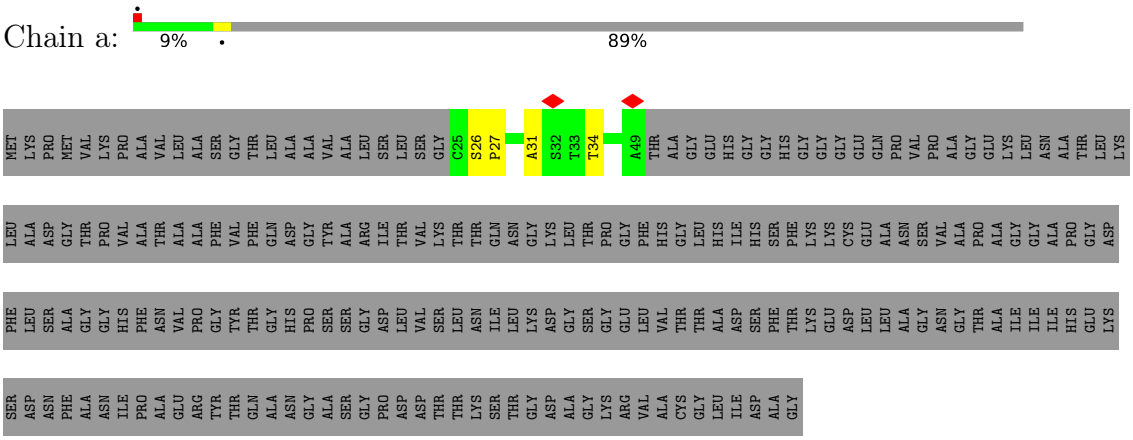
• Molecule 6: Superoxide dismutase [Cu-Zn]

Chain X:



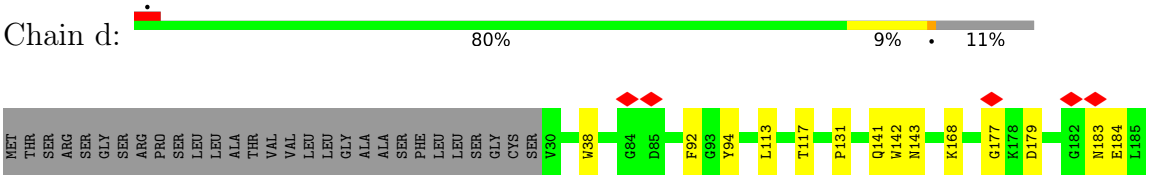
• Molecule 6: Superoxide dismutase [Cu-Zn]

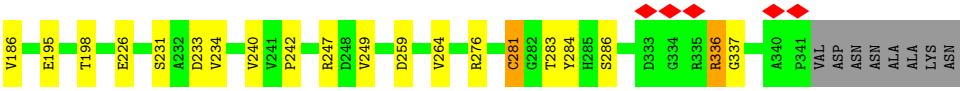
Chain a:



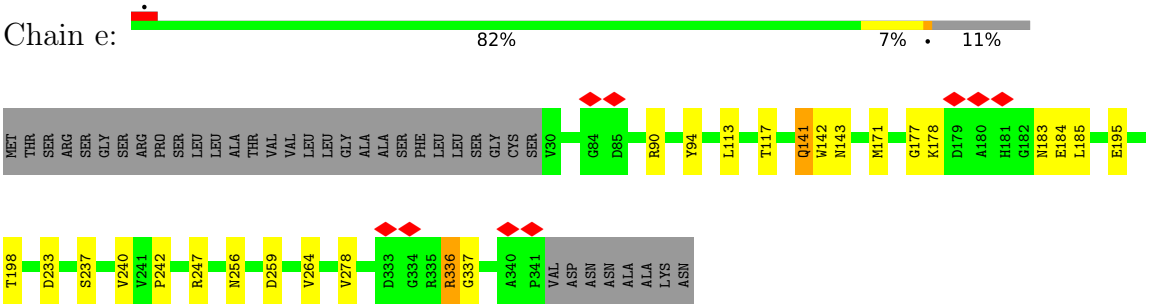
• Molecule 7: cytochrome-c oxidase

Chain d:

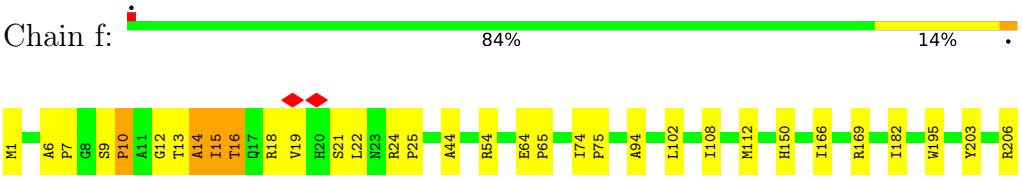




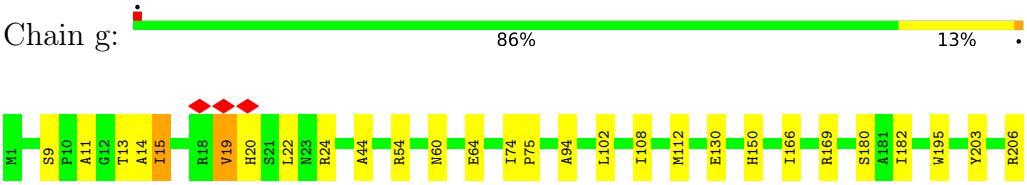
• Molecule 7: cytochrome-c oxidase



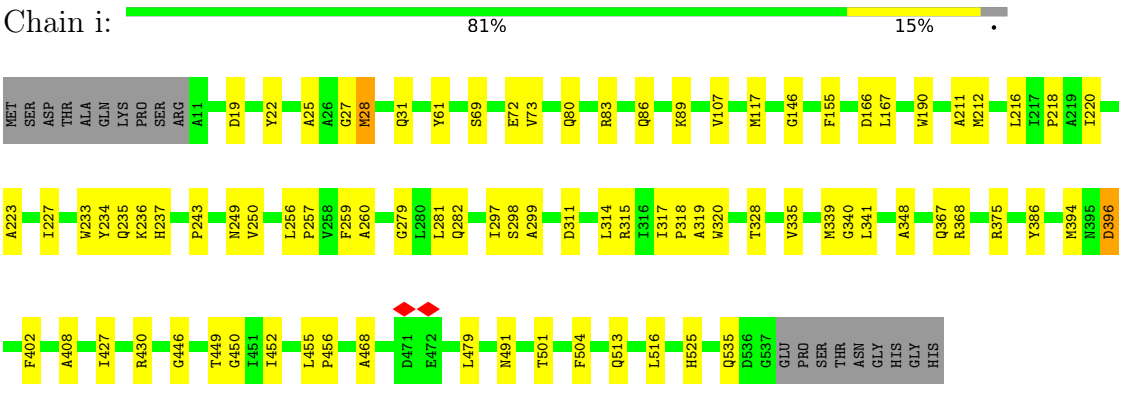
• Molecule 8: Probable cytochrome c oxidase subunit 3



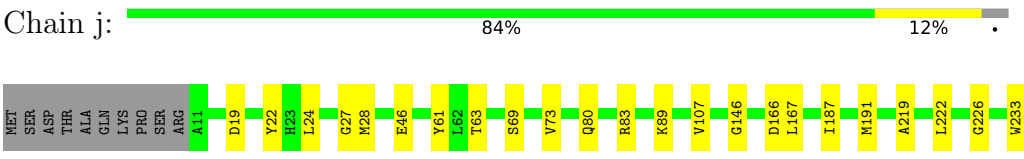
• Molecule 8: Probable cytochrome c oxidase subunit 3

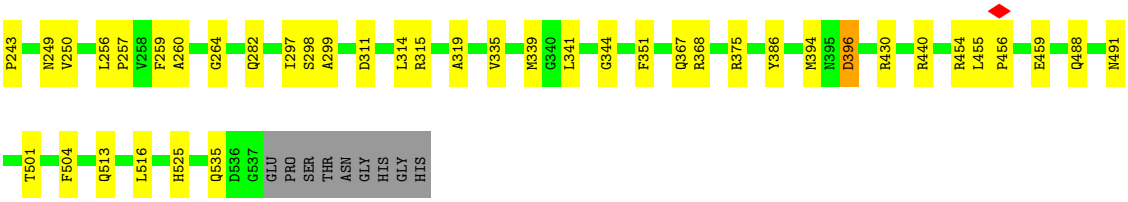


• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

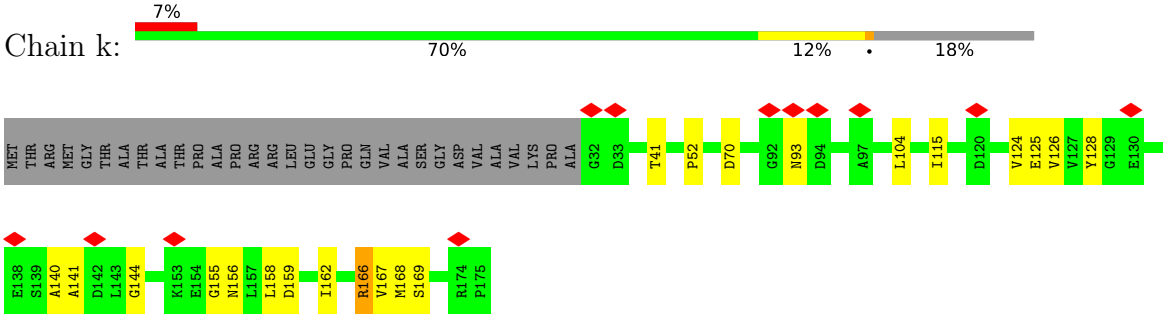


• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

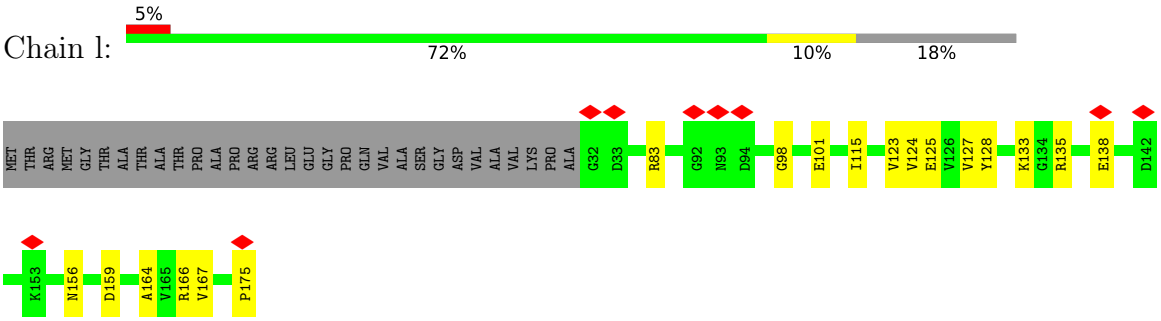




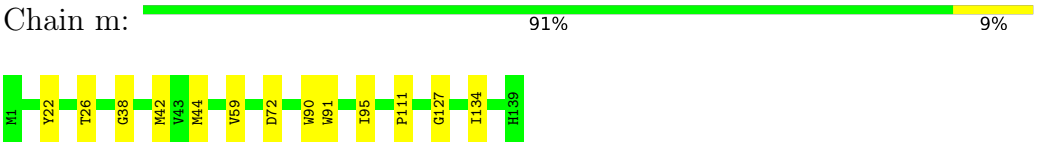
• Molecule 10: DUF5130 domain-containing protein



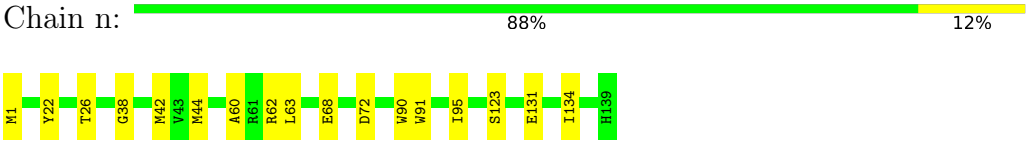
• Molecule 10: DUF5130 domain-containing protein



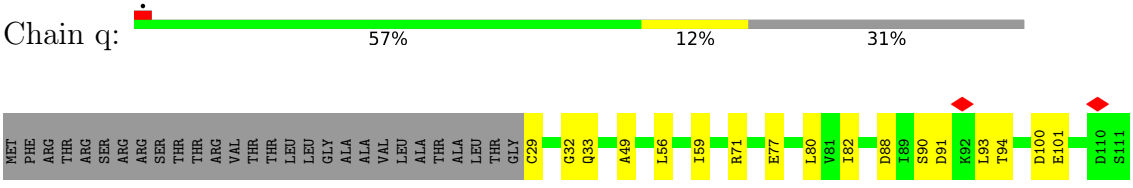
• Molecule 11: Cytochrome c oxidase polypeptide 4

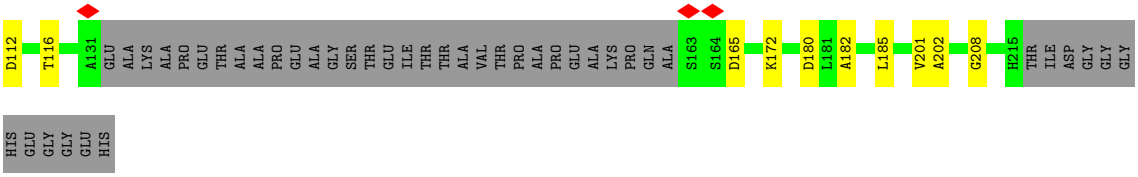


• Molecule 11: Cytochrome c oxidase polypeptide 4



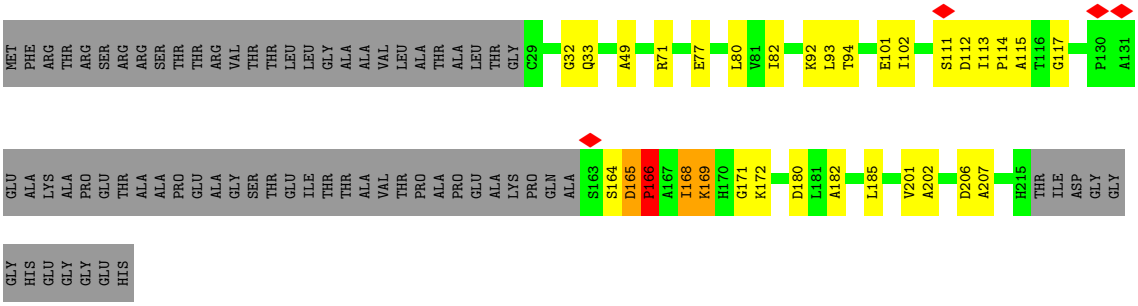
• Molecule 12: Lipoprotein lpqE





• Molecule 12: Lipoprotein lpqE





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194219	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.818	Depositor
Minimum map value	-1.707	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	402.6, 402.6, 402.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.671, 0.671, 0.671	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: FES, 9YF, HEA, HEC, CU, HEM, 9XX, MQ9, OXY, CDL, 9Y0, PLM

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	G	0.16	0/585	0.25	0/789
1	b	0.16	0/585	0.27	0/789
2	I	0.27	0/4526	0.47	2/6181 (0.0%)
2	L	0.32	1/4526 (0.0%)	0.48	4/6181 (0.1%)
3	J	0.18	0/526	0.35	0/718
3	h	0.14	0/526	0.36	0/718
4	U	0.42	0/1669	0.62	3/2257 (0.1%)
4	o	0.38	0/1669	0.59	4/2257 (0.2%)
5	V	0.17	0/3033	0.33	0/4120
5	p	0.17	0/3033	0.32	0/4120
6	X	0.46	0/177	0.85	1/248 (0.4%)
6	a	0.16	0/177	0.43	0/248
7	d	0.35	1/2547 (0.0%)	0.45	3/3466 (0.1%)
7	e	0.51	2/2547 (0.1%)	0.39	0/3466
8	f	0.35	1/1644 (0.1%)	0.46	2/2244 (0.1%)
8	g	0.31	1/1644 (0.1%)	0.42	2/2244 (0.1%)
9	i	0.26	1/4252 (0.0%)	0.42	3/5785 (0.1%)
9	j	0.19	0/4252	0.34	0/5785
10	k	0.21	0/1083	0.33	0/1474
10	l	0.17	0/1083	0.31	0/1474
11	m	0.16	0/1097	0.29	0/1499
11	n	0.58	2/1097 (0.2%)	0.48	4/1499 (0.3%)
12	q	0.14	0/1144	0.32	0/1551
12	r	0.37	1/1144 (0.1%)	0.54	4/1551 (0.3%)
All	All	0.30	10/44566 (0.0%)	0.43	32/60664 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	U	0	1
7	d	0	1
10	k	0	1
10	l	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	n	131	GLU	C-O	17.25	1.44	1.24
7	e	336	ARG	CA-CB	16.80	1.79	1.53
7	e	336	ARG	C-N	14.64	1.49	1.33
7	d	336	ARG	CA-CB	13.09	1.75	1.53
2	L	559	HIS	CA-C	-11.38	1.38	1.52
8	f	203	TYR	CA-C	-10.68	1.38	1.52
8	g	203	TYR	CA-C	-8.75	1.41	1.52
12	r	206	ASP	N-CA	8.54	1.56	1.46
9	i	450	GLY	N-CA	5.78	1.50	1.44
11	n	131	GLU	CA-CB	-5.56	1.44	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	n	131	GLU	O-C-N	-11.07	109.53	122.15
4	o	124	PRO	N-CA-C	-10.25	91.35	112.47
4	U	124	PRO	N-CA-C	-9.07	93.78	112.47
2	L	559	HIS	CB-CA-C	7.65	122.46	109.53
4	U	124	PRO	CB-CA-C	7.09	123.26	111.56
7	d	336	ARG	CA-C-N	-6.70	111.04	120.56
7	d	336	ARG	C-N-CA	-6.70	111.04	120.56
6	X	42	TRP	N-CA-C	6.62	120.61	109.76
8	f	14	ALA	N-CA-C	-6.59	102.29	111.52
2	L	150	GLY	CA-C-O	-6.54	117.35	122.52
12	r	169	LYS	CB-CA-C	6.41	120.80	110.29
2	I	150	GLY	CA-C-O	-6.40	117.46	122.52
7	d	336	ARG	O-C-N	6.11	129.78	122.27
4	o	123	MET	N-CA-C	6.04	123.15	109.81
12	r	166	PRO	N-CA-CB	-5.98	96.97	103.25
9	i	446	GLY	CA-C-O	-5.97	118.01	122.37
2	I	205	ARG	N-CA-C	-5.97	103.65	113.50
2	L	205	ARG	N-CA-C	-5.84	103.87	113.50
8	g	203	TYR	CB-CA-C	5.80	119.86	109.29
4	o	124	PRO	CB-CA-C	5.69	120.95	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	203	TYR	CB-CA-C	5.58	120.88	109.55
12	r	168	ILE	CA-C-N	-5.43	113.84	121.72
12	r	168	ILE	C-N-CA	-5.43	113.84	121.72
4	o	123	MET	CA-C-O	-5.38	112.78	120.16
11	n	131	GLU	N-CA-CB	5.36	118.09	110.16
4	U	123	MET	N-CA-C	5.26	121.43	109.81
2	L	148	ASP	CA-CB-CG	5.23	117.83	112.60
8	g	203	TYR	CA-C-O	-5.19	113.43	119.14
11	n	131	GLU	CA-C-N	5.16	130.87	122.67
11	n	131	GLU	C-N-CA	5.16	130.87	122.67
9	i	449	THR	CA-C-N	5.07	128.25	122.67
9	i	449	THR	C-N-CA	5.07	128.25	122.67

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	U	186	ARG	Sidechain
7	d	276	ARG	Sidechain
10	k	166	ARG	Sidechain
10	l	166	ARG	Sidechain

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	G	575	0	591	5	0
1	b	575	0	591	2	0
2	I	4363	0	4322	80	0
2	L	4363	0	4322	64	0
3	J	509	0	500	17	0
3	h	509	0	500	15	0
4	U	1639	0	1600	41	0
4	o	1639	0	1598	24	0
5	V	2957	0	2964	30	0
5	p	2957	0	2964	25	0
6	X	171	0	156	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	a	171	0	156	4	0
7	d	2476	0	2445	34	0
7	e	2476	0	2445	28	0
8	f	1595	0	1581	40	0
8	g	1595	0	1581	40	0
9	i	4127	0	4158	84	0
9	j	4127	0	4158	77	0
10	k	1063	0	1049	28	0
10	l	1063	0	1049	18	0
11	m	1066	0	1052	15	0
11	n	1066	0	1052	14	0
12	q	1129	0	1126	22	0
12	r	1129	0	1126	31	0
13	G	42	0	0	1	0
13	b	42	0	0	1	0
13	i	32	0	0	2	0
13	j	32	0	0	0	0
14	G	88	0	126	13	0
14	I	157	0	208	14	0
14	L	157	0	208	11	0
14	U	79	0	105	3	0
14	b	88	0	126	33	0
14	g	95	0	143	13	0
14	i	370	0	463	34	0
14	j	222	0	279	11	0
14	m	79	0	105	8	0
14	p	95	0	143	19	0
15	G	41	0	0	0	0
15	b	79	0	0	0	0
15	f	43	0	0	1	0
15	g	43	0	0	0	0
15	q	38	0	0	1	0
16	I	120	0	108	9	0
16	L	120	0	108	8	0
17	I	2	0	0	0	0
17	L	2	0	0	0	0
17	d	2	0	0	1	0
17	e	2	0	0	0	0
18	I	17	0	31	0	0
18	q	17	0	31	5	0
19	I	2	0	0	0	0
19	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	U	86	0	60	12	0
20	i	85	0	57	1	0
20	j	85	0	57	4	0
21	V	4	0	0	0	0
21	p	4	0	0	0	0
22	V	58	0	0	1	0
22	i	58	0	0	1	0
22	j	58	0	0	0	0
22	n	58	0	0	1	0
22	o	58	0	0	4	0
22	p	58	0	0	1	0
23	i	265	0	349	71	0
23	j	217	0	293	37	0
23	m	48	0	61	9	0
24	o	86	0	62	10	0
25	I	18	0	0	2	0
25	L	18	0	0	3	0
25	U	3	0	0	0	0
25	V	2	0	0	0	0
25	d	1	0	0	0	0
25	e	1	0	0	0	0
25	i	9	0	0	0	0
25	j	10	0	0	0	0
25	m	2	0	0	0	0
25	n	3	0	0	0	0
25	o	4	0	0	0	0
25	p	3	0	0	0	0
All	All	46750	0	46209	812	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 9.

All (812) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:336:ARG:CA	7:d:336:ARG:CB	1.75	1.60
23:i:610:MQ9:C26	23:i:610:MQ9:C20	1.74	1.54
7:e:336:ARG:CB	7:e:336:ARG:CA	1.80	1.54
23:i:610:MQ9:C27	23:i:610:MQ9:C19	1.99	1.40
8:g:169:ARG:HD3	9:j:504:PHE:CE1	1.55	1.39
8:f:169:ARG:HD3	9:i:504:PHE:CE1	1.59	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:402:PHE:HB3	23:i:611:MQ9:C41	1.52	1.35
14:b:103:CDL:C57	14:b:103:CDL:H741	1.62	1.30
14:b:103:CDL:C74	14:b:103:CDL:H572	1.60	1.29
9:i:402:PHE:CB	23:i:611:MQ9:C41	2.07	1.29
23:i:610:MQ9:H18	23:i:610:MQ9:C30	1.76	1.15
23:i:610:MQ9:H301	23:i:610:MQ9:C18	1.76	1.15
8:g:169:ARG:HD3	9:j:504:PHE:CD1	1.83	1.13
7:d:183:ASN:O	7:d:184:GLU:HG3	1.48	1.13
23:i:610:MQ9:H211	23:i:610:MQ9:C16	1.79	1.10
23:i:610:MQ9:H162	23:i:610:MQ9:C21	1.80	1.09
23:i:610:MQ9:C20	23:i:610:MQ9:C24	2.29	1.09
8:f:169:ARG:HD3	9:i:504:PHE:CD1	1.86	1.09
8:g:169:ARG:CD	9:j:504:PHE:CE1	2.34	1.08
9:i:402:PHE:CG	23:i:611:MQ9:C41	2.37	1.08
14:b:103:CDL:H712	14:b:103:CDL:C81	1.83	1.07
8:f:169:ARG:CD	9:i:504:PHE:CE1	2.37	1.07
23:i:610:MQ9:C20	23:i:610:MQ9:C28	2.32	1.06
8:g:166:ILE:HG12	8:g:169:ARG:NH2	1.69	1.06
8:f:166:ILE:HG12	8:f:169:ARG:NH2	1.70	1.04
8:g:11:ALA:HB3	8:g:22:LEU:CD2	1.86	1.03
14:G:102:CDL:H761	14:G:102:CDL:H812	1.40	1.02
14:b:103:CDL:H581	14:b:103:CDL:H752	1.38	1.01
2:L:141:ILE:HD11	23:i:611:MQ9:H353	1.42	1.00
8:f:169:ARG:CG	9:i:504:PHE:HE1	1.77	0.98
8:g:169:ARG:CD	9:j:504:PHE:HE1	1.73	0.97
8:g:169:ARG:CG	9:j:504:PHE:HE1	1.78	0.95
14:b:103:CDL:H742	14:b:103:CDL:H592	1.47	0.94
14:b:103:CDL:H741	14:b:103:CDL:H572	0.95	0.94
14:b:103:CDL:C57	14:b:103:CDL:C74	2.34	0.92
8:f:169:ARG:CD	9:i:504:PHE:HE1	1.77	0.92
23:j:602:MQ9:H111	23:j:602:MQ9:H5M3	1.51	0.92
2:I:171:TRP:O	2:I:175:LEU:HD13	1.71	0.91
2:L:171:TRP:O	2:L:175:LEU:HD13	1.71	0.91
8:g:169:ARG:HD3	9:j:504:PHE:HE1	1.30	0.90
23:i:610:MQ9:C20	23:i:610:MQ9:C27	0.89	0.89
7:d:233:ASP:OD1	7:d:234:VAL:N	2.05	0.88
9:j:187:ILE:HD12	9:j:187:ILE:O	1.74	0.88
8:g:54:ARG:NE	8:g:206:ARG:O	2.05	0.88
8:g:60:ASN:OD1	8:g:60:ASN:O	1.91	0.88
9:j:501:THR:HG22	9:j:513:GLN:HG2	1.55	0.88
8:f:54:ARG:NE	8:f:206:ARG:O	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:610:MQ9:H18	23:i:610:MQ9:H301	0.90	0.87
6:X:31:ALA:HB1	6:X:34:THR:OG1	1.74	0.87
8:g:11:ALA:HB3	8:g:22:LEU:HD22	1.57	0.87
14:b:103:CDL:H712	14:b:103:CDL:H812	1.54	0.86
4:U:114:VAL:HG21	4:U:151:ILE:HD12	1.57	0.85
14:b:103:CDL:H581	14:b:103:CDL:C75	2.06	0.85
14:b:103:CDL:C74	14:b:103:CDL:C58	2.55	0.84
8:g:169:ARG:NH1	9:j:504:PHE:CZ	2.45	0.84
23:i:610:MQ9:C30	23:i:610:MQ9:C18	2.45	0.84
5:V:229:VAL:HG12	5:V:229:VAL:O	1.78	0.83
9:i:260:ALA:HA	23:i:610:MQ9:H111	1.60	0.83
5:V:391:SER:OXT	6:a:26:SER:HB2	1.76	0.83
5:V:269:GLU:HG2	5:V:273:HIS:NE2	1.94	0.83
8:g:11:ALA:CB	8:g:22:LEU:HD22	2.09	0.83
5:V:148:ILE:HD11	9:i:28:MET:HG2	1.61	0.83
14:p:603:CDL:H231	14:p:603:CDL:H662	1.58	0.83
2:I:72:GLN:HG2	3:J:12:MET:HG2	1.61	0.83
14:m:202:CDL:H161	14:m:202:CDL:H332	1.58	0.82
6:a:31:ALA:HB1	6:a:34:THR:OG1	1.78	0.82
2:I:253:LEU:HD13	7:e:256:ASN:HB3	1.61	0.81
5:V:269:GLU:O	5:V:273:HIS:CD2	2.33	0.81
3:J:74:GLY:HA3	10:k:104:LEU:HD13	1.62	0.81
2:L:141:ILE:CD1	23:i:611:MQ9:H353	2.10	0.81
8:f:169:ARG:CG	9:i:504:PHE:CE1	2.64	0.81
8:f:169:ARG:NH1	9:i:504:PHE:CZ	2.49	0.81
7:e:336:ARG:HE	12:r:33:GLN:HA	1.46	0.80
7:d:183:ASN:O	7:d:184:GLU:CG	2.30	0.80
7:e:336:ARG:NH2	12:r:32:GLY:O	2.14	0.79
8:g:11:ALA:CB	8:g:22:LEU:CD2	2.61	0.79
14:b:103:CDL:H712	14:b:103:CDL:H811	1.64	0.78
8:g:169:ARG:CG	9:j:504:PHE:CE1	2.64	0.78
23:i:612:MQ9:H412	23:i:612:MQ9:C45	2.13	0.78
2:I:507:VAL:O	2:I:523:CYS:SG	2.42	0.78
14:b:103:CDL:H122	14:b:103:CDL:H161	1.66	0.77
2:L:215:VAL:HG11	2:L:304:ALA:HB2	1.67	0.77
14:G:102:CDL:H401	14:L:606:CDL:H671	1.67	0.77
14:b:103:CDL:H572	14:b:103:CDL:H742	1.65	0.76
23:i:610:MQ9:H211	23:i:610:MQ9:H162	0.88	0.76
4:U:88:CYS:SG	20:U:601:HEM:CBB	2.75	0.75
9:i:402:PHE:CD2	23:i:611:MQ9:C41	2.70	0.74
7:d:281:CYS:SG	17:d:602:CU:CU	1.78	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:q:302:PLM:H82	18:q:302:PLM:H32	1.68	0.74
4:U:189:CYS:SG	20:U:602:HEM:CBB	2.75	0.74
9:i:501:THR:HG22	9:i:513:GLN:HG2	1.69	0.74
14:G:102:CDL:H171	14:G:102:CDL:H132	1.68	0.74
2:I:215:VAL:HG11	2:I:304:ALA:HB2	1.67	0.74
8:f:13:THR:O	8:f:14:ALA:HB3	1.86	0.74
14:b:103:CDL:H192	14:b:103:CDL:H152	1.69	0.74
8:g:11:ALA:HB3	8:g:22:LEU:HD23	1.68	0.73
3:J:19:ILE:HG22	3:J:19:ILE:O	1.89	0.73
6:X:30:GLN:HE21	5:p:346:HIS:CE1	2.07	0.73
23:m:201:MQ9:H112	23:m:201:MQ9:H5M3	1.70	0.73
7:d:336:ARG:CB	7:d:336:ARG:C	2.61	0.73
8:g:13:THR:HG21	11:m:59:VAL:HG22	1.69	0.73
9:j:396:ASP:N	9:j:396:ASP:OD1	2.21	0.73
14:G:102:CDL:H151	14:G:102:CDL:H112	1.71	0.73
2:L:115:ASP:OD2	25:L:701:HOH:O	2.07	0.73
14:p:603:CDL:H191	14:p:603:CDL:H602	1.70	0.72
14:b:103:CDL:H742	14:b:103:CDL:C59	2.18	0.72
10:k:144:GLY:HA3	10:k:168:MET:SD	2.29	0.72
2:L:470:PHE:O	2:L:474:ASN:ND2	2.22	0.72
14:p:603:CDL:H192	14:p:603:CDL:H232	1.70	0.71
2:I:532:GLU:OE1	10:k:41:THR:HB	1.89	0.71
7:d:336:ARG:CA	7:d:336:ARG:CG	2.66	0.71
8:f:12:GLY:O	8:f:15:ILE:HG22	1.90	0.71
9:j:260:ALA:HA	23:j:607:MQ9:H122	1.73	0.71
2:L:337:THR:HG21	16:L:601:HEA:H263	1.73	0.71
9:j:501:THR:CG2	9:j:513:GLN:HG2	2.19	0.71
9:i:396:ASP:OD1	9:i:396:ASP:N	2.23	0.71
12:q:94:THR:HG22	12:q:112:ASP:HB2	1.73	0.71
1:G:29:GLN:CG	1:G:34:PHE:HE2	2.04	0.70
4:U:123:MET:O	4:U:125:ALA:N	2.24	0.70
9:j:46:GLU:OE2	23:j:607:MQ9:H5M2	1.91	0.70
23:j:602:MQ9:H453	23:j:602:MQ9:H48	1.73	0.70
8:g:166:ILE:HG12	8:g:169:ARG:HH22	1.55	0.70
5:V:269:GLU:CG	5:V:273:HIS:NE2	2.54	0.69
14:i:614:CDL:OB7	23:j:608:MQ9:H3A	1.91	0.69
1:G:29:GLN:HG3	1:G:34:PHE:HE2	1.56	0.69
2:L:215:VAL:CG1	2:L:304:ALA:HB2	2.22	0.69
12:q:90:SER:OG	12:q:116:THR:HG23	1.91	0.69
9:i:339:MET:HE1	23:i:603:MQ9:C3A	2.22	0.69
14:j:606:CDL:H181	14:m:202:CDL:H152	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:605:CDL:H591	14:I:605:CDL:H552	1.74	0.69
23:i:612:MQ9:H362	23:j:608:MQ9:H503	1.74	0.69
12:r:92:LYS:HA	12:r:114:PRO:HD2	1.75	0.69
14:G:102:CDL:H112	14:G:102:CDL:HA62	1.74	0.69
4:U:114:VAL:CG2	4:U:151:ILE:HD12	2.23	0.69
2:I:337:THR:HG21	16:I:601:HEA:H263	1.74	0.68
5:V:269:GLU:HG2	5:V:273:HIS:CD2	2.27	0.68
8:g:169:ARG:NH1	9:j:504:PHE:CE1	2.55	0.68
14:p:603:CDL:H782	14:p:603:CDL:H181	1.76	0.68
2:L:507:VAL:O	2:L:523:CYS:SG	2.52	0.68
4:o:88:CYS:SG	24:o:601:HEC:HBB3	2.33	0.68
2:I:215:VAL:CG1	2:I:304:ALA:HB2	2.22	0.68
8:f:169:ARG:HG3	9:i:504:PHE:HE1	1.56	0.68
9:i:501:THR:CG2	9:i:513:GLN:HG2	2.24	0.68
23:j:607:MQ9:H3D	23:j:608:MQ9:H3C	1.75	0.68
7:e:177:GLY:O	7:e:185:LEU:HD12	1.93	0.68
7:e:336:ARG:CB	7:e:336:ARG:C	2.67	0.68
8:g:169:ARG:HG3	9:j:504:PHE:HE1	1.58	0.68
23:j:607:MQ9:H3D	23:j:608:MQ9:C3C	2.24	0.68
14:j:609:CDL:H541	14:j:609:CDL:H582	1.76	0.68
3:J:75:ALA:H	10:k:104:LEU:HD11	1.60	0.67
14:b:103:CDL:H752	14:b:103:CDL:C58	2.21	0.67
2:I:470:PHE:O	2:I:474:ASN:ND2	2.23	0.67
8:f:166:ILE:HG12	8:f:169:ARG:HH21	1.58	0.67
9:i:368:ARG:HE	14:i:608:CDL:HA22	1.59	0.66
14:p:603:CDL:H231	14:p:603:CDL:H631	1.77	0.66
5:V:148:ILE:CD1	9:i:28:MET:HG2	2.24	0.66
12:r:117:GLY:HA3	12:r:166:PRO:O	1.95	0.66
4:U:114:VAL:HG21	4:U:151:ILE:CD1	2.23	0.66
3:h:62:ILE:CD1	10:l:83:ARG:HB2	2.25	0.66
9:i:233:TRP:CD1	14:i:607:CDL:H511	2.31	0.66
9:j:368:ARG:HE	14:j:605:CDL:HA22	1.59	0.66
4:o:262:TYR:CE2	4:o:264:LEU:HD23	2.31	0.66
8:f:166:ILE:HG12	8:f:169:ARG:HH22	1.56	0.66
18:q:302:PLM:H82	18:q:302:PLM:C3	2.25	0.66
8:f:15:ILE:HG21	11:n:62:ARG:NH2	2.11	0.65
9:i:341:LEU:HD12	23:i:603:MQ9:H401	1.78	0.65
2:I:122:ASN:HD21	2:I:188:ASN:HD21	1.42	0.65
14:L:606:CDL:H152	14:L:606:CDL:C32	2.25	0.65
1:G:29:GLN:HE22	14:G:102:CDL:HA32	1.61	0.65
23:i:610:MQ9:C27	23:i:610:MQ9:C18	2.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:116:VAL:HG21	2:I:122:ASN:ND2	2.11	0.65
7:d:141:GLN:CD	7:d:233:ASP:OD2	2.40	0.65
2:I:357:THR:OG1	2:I:358:PRO:HD3	1.97	0.65
12:r:111:SER:HB3	12:r:171:GLY:HA3	1.79	0.64
8:g:166:ILE:HG12	8:g:169:ARG:HH21	1.57	0.64
23:j:608:MQ9:H222	23:j:608:MQ9:H372	1.79	0.64
14:b:103:CDL:H721	14:b:103:CDL:H542	1.79	0.64
14:i:608:CDL:H591	14:i:608:CDL:H162	1.79	0.64
9:i:340:GLY:HA3	23:i:603:MQ9:H311	1.78	0.64
3:h:62:ILE:HD13	10:l:83:ARG:N	2.12	0.64
12:q:100:ASP:OD1	12:q:101:GLU:N	2.29	0.64
11:m:127:GLY:HA2	14:m:202:CDL:H121	1.79	0.64
2:I:15:ARG:NH2	10:k:70:ASP:OD2	2.24	0.64
7:e:336:ARG:CA	7:e:336:ARG:CG	2.73	0.64
12:r:101:GLU:HG2	12:r:102:ILE:HG23	1.80	0.64
2:I:496:PHE:HE2	14:b:103:CDL:H822	1.61	0.64
7:d:247:ARG:NH1	7:d:259:ASP:O	2.31	0.64
14:i:607:CDL:HA62	9:j:27:GLY:HA3	1.80	0.64
14:b:103:CDL:H741	14:b:103:CDL:C56	2.27	0.63
14:i:604:CDL:H111	9:j:351:PHE:CE2	2.33	0.63
14:b:103:CDL:H811	14:b:103:CDL:C71	2.28	0.63
2:L:264:HIS:O	2:L:267:VAL:HG22	1.97	0.63
5:V:354:PRO:HA	9:j:319:ALA:HB2	1.81	0.63
7:e:247:ARG:NH1	7:e:259:ASP:O	2.31	0.63
14:i:604:CDL:HA61	23:j:602:MQ9:H512	1.80	0.63
9:j:367:GLN:OE1	9:j:375:ARG:NH2	2.32	0.62
9:i:402:PHE:HB2	23:i:611:MQ9:C41	2.21	0.62
14:i:607:CDL:H172	14:j:609:CDL:H532	1.80	0.62
3:h:83:SER:OG	10:l:125:GLU:OE1	2.13	0.62
9:i:339:MET:HE1	23:i:603:MQ9:H3A	1.81	0.62
2:I:496:PHE:CE2	14:b:103:CDL:H822	2.35	0.62
9:i:22:TYR:CE2	14:i:614:CDL:H181	2.35	0.62
9:i:237:HIS:O	5:p:134:ARG:NH2	2.32	0.62
5:V:328:GLN:NE2	4:o:230:MET:O	2.33	0.62
12:q:29:CYS:N	18:q:302:PLM:O2	2.32	0.62
12:r:93:LEU:HD23	12:r:112:ASP:HB3	1.81	0.62
2:I:395:ILE:HD13	16:I:602:HEA:CAA	2.30	0.62
4:U:230:MET:O	5:p:328:GLN:NE2	2.33	0.62
8:g:169:ARG:CD	9:j:504:PHE:CD1	2.71	0.62
12:q:77:GLU:OE2	12:q:172:LYS:NZ	2.27	0.62
14:I:604:CDL:H511	8:g:180:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:398:PHE:HA	2:I:401:VAL:HG22	1.82	0.61
9:i:319:ALA:HB2	5:p:354:PRO:HA	1.81	0.61
2:L:120:ARG:NE	14:L:605:CDL:OA4	2.31	0.61
14:b:103:CDL:H731	14:b:103:CDL:H791	1.82	0.61
9:j:243:PRO:O	9:j:535:GLN:NE2	2.34	0.61
14:p:603:CDL:H202	14:p:603:CDL:H791	1.83	0.61
2:L:395:ILE:HD13	16:L:602:HEA:CAA	2.30	0.61
14:p:603:CDL:H751	14:p:603:CDL:H712	1.81	0.61
12:r:92:LYS:HG2	12:r:113:ILE:HG23	1.82	0.61
4:U:114:VAL:CG2	4:U:151:ILE:CD1	2.79	0.61
9:i:243:PRO:O	9:i:535:GLN:NE2	2.34	0.61
3:J:83:SER:OG	10:k:125:GLU:OE1	2.15	0.61
2:L:381:MET:SD	7:d:117:THR:OG1	2.59	0.60
2:I:532:GLU:OE2	10:k:41:THR:HG21	2.01	0.60
12:q:71:ARG:HA	12:q:180:ASP:OD1	2.02	0.60
2:L:161:ILE:HG21	4:U:138:ILE:HD11	1.83	0.60
2:L:81:GLN:HG3	2:L:148:ASP:OD1	2.01	0.60
4:U:262:TYR:CE2	4:U:264:LEU:HD23	2.37	0.60
2:L:398:PHE:HA	2:L:401:VAL:HG22	1.82	0.60
8:f:169:ARG:CD	9:i:504:PHE:CD1	2.73	0.60
3:h:62:ILE:HD12	10:l:83:ARG:HB2	1.83	0.60
5:V:134:ARG:NH2	9:j:237:HIS:O	2.35	0.60
9:i:367:GLN:OE1	9:i:375:ARG:NH2	2.33	0.60
9:i:386:TYR:CD1	23:i:602:MQ9:H312	2.36	0.60
9:j:187:ILE:O	9:j:187:ILE:CD1	2.48	0.60
23:m:201:MQ9:H5M3	23:m:201:MQ9:C8	2.31	0.60
5:p:314:LYS:HE3	5:p:324:SER:HB3	1.82	0.60
12:r:94:THR:HG23	12:r:94:THR:O	2.01	0.60
23:i:612:MQ9:H412	23:i:612:MQ9:H452	1.84	0.60
14:g:301:CDL:HA21	14:g:301:CDL:OB9	2.02	0.59
9:i:190:TRP:HB3	22:p:601:9YF:C34	2.32	0.59
23:i:610:MQ9:C20	23:i:610:MQ9:H262	2.15	0.59
23:i:611:MQ9:H13	23:i:611:MQ9:H103	1.83	0.59
2:I:253:LEU:HD22	7:e:256:ASN:O	2.02	0.59
7:d:179:ASP:O	7:d:183:ASN:N	2.34	0.59
2:L:395:ILE:HD13	16:L:602:HEA:HAA2	1.84	0.59
8:f:18:ARG:O	8:f:18:ARG:HG3	2.03	0.59
14:p:603:CDL:H802	14:p:603:CDL:H591	1.84	0.59
7:d:231:SER:HB2	7:d:249:VAL:HG12	1.85	0.59
2:I:171:TRP:O	2:I:175:LEU:CD1	2.49	0.58
5:V:391:SER:OXT	6:a:27:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:27:GLY:O	9:i:31:GLN:HG2	2.02	0.58
14:b:103:CDL:H742	14:b:103:CDL:C58	2.32	0.58
14:i:607:CDL:H812	23:i:612:MQ9:H18	1.85	0.58
23:j:602:MQ9:H5M3	23:j:602:MQ9:C11	2.30	0.58
4:o:88:CYS:HB3	24:o:601:HEC:CAB	2.33	0.58
2:I:532:GLU:CD	10:k:41:THR:HB	2.29	0.58
4:U:236:ARG:NH2	12:q:208:GLY:O	2.36	0.58
14:I:604:CDL:HA62	14:I:604:CDL:HA22	1.86	0.58
4:o:123:MET:HG3	24:o:601:HEC:C4A	2.33	0.58
1:G:29:GLN:HG3	1:G:34:PHE:CE2	2.38	0.58
2:I:395:ILE:HD13	16:I:602:HEA:HAA2	1.84	0.58
2:L:171:TRP:O	2:L:175:LEU:CD1	2.49	0.58
7:e:177:GLY:O	7:e:185:LEU:CD1	2.52	0.58
9:j:282:GLN:NE2	4:o:259:PRO:O	2.36	0.58
6:X:30:GLN:NE2	5:p:296:VAL:HG11	2.17	0.58
12:r:71:ARG:HA	12:r:180:ASP:OD1	2.04	0.58
14:g:301:CDL:H191	14:g:301:CDL:H602	1.84	0.58
14:b:103:CDL:C74	14:b:103:CDL:H581	2.31	0.58
8:f:169:ARG:NH1	9:i:504:PHE:CE1	2.59	0.58
4:U:84:TYR:OH	4:U:96:LEU:HD23	2.04	0.57
23:i:611:MQ9:O1	23:i:611:MQ9:H8	2.03	0.57
23:i:611:MQ9:H5M1	22:n:201:9YF:C37	2.34	0.57
9:j:260:ALA:O	23:j:607:MQ9:H161	2.04	0.57
12:r:168:ILE:HG22	12:r:168:ILE:O	2.04	0.57
2:I:560:VAL:HG11	7:e:90:ARG:HH21	1.69	0.57
4:U:150:TYR:O	4:U:154:ASN:ND2	2.37	0.57
7:d:336:ARG:NH2	12:q:32:GLY:O	2.36	0.57
4:U:259:PRO:O	9:i:282:GLN:NE2	2.37	0.57
22:V:602:9YF:C34	9:j:187:ILE:HD13	2.35	0.57
2:I:357:THR:HG23	2:I:428:GLU:OE1	2.04	0.57
2:L:402:LEU:HD13	16:L:602:HEA:HAC	1.85	0.57
2:I:402:LEU:HD13	16:I:602:HEA:HAC	1.86	0.57
7:e:337:GLY:HA3	12:r:33:GLN:NE2	2.20	0.57
3:J:75:ALA:N	10:k:104:LEU:HD11	2.19	0.56
14:p:603:CDL:H181	14:p:603:CDL:C78	2.34	0.56
2:I:161:ILE:HG21	4:o:138:ILE:HD11	1.85	0.56
23:j:602:MQ9:H453	23:j:602:MQ9:C48	2.35	0.56
8:g:150:HIS:CE1	8:g:195:TRP:HB2	2.40	0.56
4:U:88:CYS:SG	20:U:601:HEM:CAB	2.94	0.56
8:f:44:ALA:HB2	11:n:44:MET:HG3	1.88	0.56
8:f:94:ALA:HB2	8:f:102:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:274:MET:O	4:U:278:ILE:HG22	2.04	0.56
4:o:251:ARG:O	4:o:255:GLU:HG2	2.06	0.56
7:e:141:GLN:HB2	7:e:233:ASP:OD2	2.05	0.56
9:j:491:ASN:ND2	11:m:134:ILE:O	2.37	0.56
2:I:264:HIS:NE2	2:I:268:TYR:HE2	2.05	0.55
14:i:609:CDL:H772	14:i:609:CDL:H811	1.87	0.55
23:i:611:MQ9:H303	23:i:611:MQ9:C33	2.36	0.55
2:I:437:LEU:HD13	2:I:487:SER:HA	1.88	0.55
4:U:123:MET:O	4:U:123:MET:SD	2.64	0.55
14:j:605:CDL:H591	14:j:605:CDL:H162	1.87	0.55
10:k:140:ALA:O	10:k:168:MET:HE3	2.05	0.55
10:l:133:LYS:NZ	10:l:138:GLU:OE2	2.39	0.55
2:L:122:ASN:OD1	25:L:702:HOH:O	2.18	0.55
4:U:84:TYR:CZ	4:U:96:LEU:HD23	2.41	0.55
8:g:94:ALA:HB2	8:g:102:LEU:HD13	1.88	0.55
9:i:249:ASN:HA	5:p:133:ASP:HA	1.88	0.55
8:f:150:HIS:CE1	8:f:195:TRP:HB2	2.41	0.55
9:j:386:TYR:CD1	23:j:611:MQ9:H312	2.41	0.55
2:I:381:MET:SD	7:e:117:THR:OG1	2.65	0.55
14:U:603:CDL:CB7	14:p:603:CDL:H522	2.36	0.55
12:r:93:LEU:N	12:r:112:ASP:O	2.39	0.55
12:r:165:ASP:N	12:r:166:PRO:CD	2.69	0.55
23:i:612:MQ9:H412	23:i:612:MQ9:H451	1.89	0.55
14:p:603:CDL:H781	14:p:603:CDL:H561	1.89	0.55
14:g:301:CDL:H561	14:g:301:CDL:H161	1.89	0.55
9:i:328:THR:OG1	5:p:386:PHE:O	2.25	0.55
12:r:77:GLU:OE2	12:r:172:LYS:NZ	2.33	0.55
4:U:251:ARG:O	4:U:255:GLU:HG2	2.06	0.54
7:d:183:ASN:C	7:d:184:GLU:HG3	2.28	0.54
14:j:606:CDL:OA7	14:j:606:CDL:HA62	2.06	0.54
5:V:17:LEU:HB3	5:p:146:LYS:HD3	1.88	0.54
3:J:19:ILE:O	3:J:19:ILE:CG2	2.56	0.54
2:L:264:HIS:NE2	2:L:268:TYR:HE2	2.04	0.54
4:U:230:MET:HE3	20:U:602:HEM:C4B	2.42	0.54
23:i:612:MQ9:H362	23:j:608:MQ9:C50	2.37	0.54
9:j:488:GLN:HG3	14:j:606:CDL:HA22	1.89	0.54
2:L:305:ALA:O	2:L:308:ILE:HG22	2.07	0.54
15:q:301:9Y0:O2	15:q:301:9Y0:N	2.41	0.54
2:I:33:THR:HG22	11:m:90:TRP:HB3	1.90	0.54
2:I:115:ASP:OD2	25:I:701:HOH:O	2.18	0.54
14:b:103:CDL:H712	14:b:103:CDL:C80	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:231:PRO:HD3	24:o:602:HEC:HBC2	1.89	0.54
4:U:189:CYS:SG	20:U:602:HEM:CAB	2.96	0.54
10:k:128:TYR:CE2	10:k:141:ALA:HB2	2.43	0.54
5:V:229:VAL:O	5:V:229:VAL:CG1	2.51	0.53
14:i:607:CDL:H161	9:j:22:TYR:CE1	2.42	0.53
14:i:608:CDL:H361	14:i:608:CDL:H172	1.91	0.53
14:i:614:CDL:H122	14:i:614:CDL:H711	1.89	0.53
9:i:256:LEU:HB3	9:i:257:PRO:HD3	1.89	0.53
9:i:259:PHE:HZ	23:i:610:MQ9:H3D	1.73	0.53
3:J:81:SER:HA	10:k:126:VAL:O	2.08	0.53
14:b:103:CDL:C75	14:b:103:CDL:C58	2.79	0.53
14:L:605:CDL:HA62	14:L:605:CDL:HA22	1.89	0.53
7:d:233:ASP:OD1	7:d:234:VAL:HG22	2.07	0.53
5:p:389:ARG:NH1	5:p:391:SER:OG	2.39	0.53
12:q:201:VAL:HG12	12:q:202:ALA:N	2.23	0.53
8:f:19:VAL:O	8:f:21:SER:N	2.42	0.53
9:j:256:LEU:HB3	9:j:257:PRO:HD3	1.89	0.53
23:m:201:MQ9:H5M3	23:m:201:MQ9:C11	2.38	0.53
14:p:603:CDL:H621	14:p:603:CDL:H212	1.89	0.53
14:L:606:CDL:H152	14:L:606:CDL:H322	1.91	0.53
4:U:123:MET:HG3	20:U:601:HEM:C4A	2.44	0.53
7:e:171:MET:O	7:e:198:THR:CG2	2.57	0.53
23:m:201:MQ9:H5M2	4:o:274:MET:HG2	1.89	0.53
12:r:113:ILE:O	12:r:169:LYS:HG3	2.08	0.53
2:L:33:THR:HG22	11:n:90:TRP:HB3	1.89	0.53
8:f:9:SER:N	8:f:10:PRO:HD3	2.23	0.53
12:q:49:ALA:HB2	12:q:201:VAL:CG2	2.39	0.53
14:I:604:CDL:H552	14:I:604:CDL:CB5	2.39	0.52
23:i:612:MQ9:H222	23:j:608:MQ9:H171	1.90	0.52
12:r:201:VAL:HG12	12:r:202:ALA:N	2.24	0.52
2:I:294:THR:HG23	7:e:94:TYR:OH	2.09	0.52
8:f:25:PRO:HD3	11:n:63:LEU:HD21	1.91	0.52
5:V:269:GLU:O	5:V:273:HIS:HD2	1.90	0.52
9:j:259:PHE:CE2	23:j:607:MQ9:H5M1	2.44	0.52
9:j:24:LEU:HD13	9:j:28:MET:HG3	1.91	0.52
7:d:141:GLN:HG3	7:d:142:TRP:CD2	2.45	0.52
14:m:202:CDL:CA6	14:m:202:CDL:HA22	2.40	0.52
8:g:44:ALA:HB2	11:m:44:MET:HG3	1.92	0.52
9:i:320:TRP:HB3	13:i:613:9XX:C14	2.40	0.52
14:L:606:CDL:H152	14:L:606:CDL:H321	1.91	0.51
8:g:169:ARG:HE	14:g:301:CDL:H521	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:116:VAL:HG21	2:I:122:ASN:HD21	1.72	0.51
14:b:103:CDL:OA3	9:j:430:ARG:NH2	2.43	0.51
2:I:68:VAL:HG13	2:I:69:PRO:HD2	1.91	0.51
14:g:301:CDL:H631	14:g:301:CDL:H591	1.92	0.51
9:i:491:ASN:ND2	11:n:134:ILE:O	2.41	0.51
5:V:322:PRO:HD2	9:j:297:ILE:HD12	1.93	0.51
5:V:148:ILE:HD11	9:i:28:MET:CG	2.38	0.51
4:o:88:CYS:SG	24:o:601:HEC:CBB	2.99	0.51
2:I:102:PHE:O	2:I:106:VAL:HG22	2.11	0.51
14:U:603:CDL:H151	14:i:609:CDL:H191	1.93	0.51
9:i:220:ILE:HD11	23:i:612:MQ9:H38	1.93	0.51
23:i:612:MQ9:H272	9:j:222:LEU:HD21	1.93	0.51
4:o:123:MET:O	24:o:601:HEC:C4B	2.59	0.51
2:I:149:PHE:CD2	2:I:158:THR:HG22	2.46	0.51
8:g:19:VAL:HG22	8:g:20:HIS:H	1.75	0.51
3:J:74:GLY:CA	10:k:104:LEU:HD13	2.38	0.50
14:L:606:CDL:H322	14:L:606:CDL:H121	1.93	0.50
7:e:336:ARG:HD3	12:r:33:GLN:O	2.11	0.50
23:m:201:MQ9:H5M3	23:m:201:MQ9:C9	2.40	0.50
2:L:441:GLY:O	2:L:445:THR:HG22	2.11	0.50
14:U:603:CDL:H151	11:n:123:SER:HB3	1.93	0.50
2:I:441:GLY:O	2:I:445:THR:HG22	2.12	0.50
14:i:607:CDL:CA6	9:j:27:GLY:HA3	2.41	0.50
9:j:488:GLN:CG	14:j:606:CDL:HA22	2.42	0.50
11:m:127:GLY:CA	14:m:202:CDL:H121	2.41	0.50
14:p:603:CDL:H662	14:p:603:CDL:C23	2.36	0.50
16:I:601:HEA:HBC1	16:I:601:HEA:HMC3	1.94	0.50
7:e:177:GLY:O	7:e:185:LEU:HG	2.12	0.50
9:j:19:ASP:OD2	5:p:145:ARG:NH1	2.44	0.50
14:G:102:CDL:OA3	9:i:430:ARG:NH2	2.45	0.50
2:L:102:PHE:O	2:L:106:VAL:HG22	2.12	0.50
14:G:102:CDL:H821	14:G:102:CDL:H871	1.94	0.50
9:i:155:PHE:CE2	23:i:603:MQ9:H18	2.47	0.50
5:p:231:SER:OG	5:p:233:SER:O	2.25	0.50
12:r:164:SER:HB3	12:r:168:ILE:HG12	1.94	0.50
16:L:601:HEA:HBC1	16:L:601:HEA:HMC3	1.93	0.50
4:o:92:HIS:O	4:o:97:GLN:O	2.30	0.50
8:f:18:ARG:HA	8:f:22:LEU:HD21	1.93	0.49
23:i:610:MQ9:C18	23:i:610:MQ9:H302	2.40	0.49
2:I:122:ASN:ND2	2:I:188:ASN:HD21	2.10	0.49
1:b:60:ILE:HG22	13:b:102:9XX:C9	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:612:MQ9:C22	23:j:608:MQ9:H171	2.42	0.49
9:j:187:ILE:HD12	9:j:191:MET:HG3	1.94	0.49
9:j:339:MET:HE1	23:j:602:MQ9:C3C	2.42	0.49
14:m:202:CDL:HA22	14:m:202:CDL:HA61	1.92	0.49
14:p:603:CDL:OB7	14:p:603:CDL:HB31	2.10	0.49
14:I:604:CDL:HA62	14:I:604:CDL:CA2	2.42	0.49
2:L:208:ILE:HG12	2:L:297:ILE:HD11	1.94	0.49
2:I:59:ALA:HB2	2:I:86:HIS:CE1	2.48	0.49
12:q:29:CYS:N	18:q:302:PLM:C1	2.75	0.49
2:I:496:PHE:CE1	14:I:605:CDL:H712	2.47	0.49
4:U:165:ASP:OD1	4:U:165:ASP:N	2.40	0.49
8:g:13:THR:HG21	11:m:59:VAL:HG13	1.94	0.49
9:i:25:ALA:HA	9:i:28:MET:HB3	1.94	0.49
5:p:363:PRO:HB2	5:p:375:ASN:HB3	1.94	0.49
14:L:605:CDL:H761	14:L:605:CDL:H582	1.93	0.49
9:i:341:LEU:HD12	23:i:603:MQ9:C40	2.42	0.49
12:q:49:ALA:HB2	12:q:201:VAL:HG21	1.94	0.49
14:G:102:CDL:HA62	14:G:102:CDL:C11	2.43	0.49
3:J:74:GLY:HA2	10:k:104:LEU:HD22	1.95	0.49
2:L:80:ASN:HA	2:L:83:PHE:CE2	2.47	0.49
7:d:336:ARG:CB	7:d:336:ARG:N	2.67	0.49
3:h:62:ILE:CD1	10:l:83:ARG:CB	2.91	0.49
2:I:215:VAL:CG1	2:I:304:ALA:CB	2.91	0.49
7:d:179:ASP:HA	7:d:184:GLU:HA	1.95	0.49
7:e:171:MET:O	7:e:198:THR:HG23	2.12	0.49
8:f:15:ILE:O	8:f:16:THR:HG23	2.13	0.49
2:I:80:ASN:HA	2:I:83:PHE:CE2	2.48	0.48
2:L:381:MET:HE1	7:d:113:LEU:HD11	1.94	0.48
5:V:134:ARG:HB3	9:j:236:LYS:HD2	1.95	0.48
14:I:604:CDL:C57	14:I:604:CDL:H612	2.43	0.48
7:e:177:GLY:O	7:e:185:LEU:CG	2.62	0.48
4:o:88:CYS:SG	24:o:601:HEC:CAB	3.01	0.48
2:I:216:THR:HG23	2:I:269:ILE:HG23	1.96	0.48
23:m:201:MQ9:H303	23:m:201:MQ9:H322	1.43	0.48
6:X:30:GLN:NE2	5:p:346:HIS:NE2	2.62	0.48
12:r:49:ALA:HB2	12:r:201:VAL:HG21	1.95	0.48
12:r:165:ASP:N	12:r:166:PRO:HD3	2.28	0.48
2:L:59:ALA:HB2	2:L:86:HIS:CE1	2.49	0.48
5:V:259:ASP:O	5:V:267:SER:OG	2.24	0.48
14:p:603:CDL:H232	14:p:603:CDL:C19	2.41	0.48
14:i:604:CDL:OB9	14:i:604:CDL:H732	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:609:CDL:OA4	14:i:609:CDL:HA4	2.13	0.48
2:I:208:ILE:HG12	2:I:297:ILE:HD11	1.94	0.48
2:I:511:TRP:O	10:k:52:PRO:HG3	2.14	0.48
2:I:532:GLU:CD	10:k:41:THR:CB	2.87	0.48
3:J:44:MET:SD	10:k:155:GLY:HA2	2.53	0.48
5:V:145:ARG:NH1	9:i:19:ASP:OD2	2.46	0.48
5:V:146:LYS:HD3	5:p:17:LEU:HB3	1.93	0.48
23:i:610:MQ9:C20	23:i:610:MQ9:C23	2.89	0.48
1:G:57:VAL:HG13	13:G:101:9XX:C13	2.44	0.48
2:I:13:ALA:HB1	3:J:56:ALA:HB3	1.95	0.48
2:I:395:ILE:HD13	16:I:602:HEA:HAA1	1.95	0.48
2:I:532:GLU:OE2	10:k:41:THR:CB	2.62	0.48
2:L:216:THR:HG23	2:L:269:ILE:HG23	1.95	0.48
4:U:123:MET:HG3	20:U:601:HEM:C1B	2.49	0.47
3:h:81:SER:CB	10:l:127:VAL:HG12	2.44	0.47
9:i:298:SER:OG	9:i:299:ALA:N	2.48	0.47
23:i:612:MQ9:H253	23:i:612:MQ9:C28	2.45	0.47
23:j:607:MQ9:H121	23:j:607:MQ9:H103	1.57	0.47
2:L:349:TRP:CD1	2:L:350:LYS:HG2	2.49	0.47
14:L:606:CDL:H673	9:i:427:ILE:HD11	1.96	0.47
10:k:162:ILE:O	10:k:166:ARG:HG3	2.14	0.47
2:I:212:ASN:ND2	2:I:272:LEU:O	2.40	0.47
2:I:532:GLU:OE1	10:k:41:THR:CB	2.60	0.47
14:b:103:CDL:C74	14:b:103:CDL:C59	2.88	0.47
7:d:337:GLY:HA3	12:q:33:GLN:NE2	2.29	0.47
7:d:283:THR:HG23	7:d:284:TYR:CD2	2.50	0.47
8:g:14:ALA:HB1	8:g:182:ILE:HD13	1.95	0.47
9:i:408:ALA:HA	22:i:601:9YF:O12	2.14	0.47
9:j:298:SER:OG	9:j:299:ALA:N	2.48	0.47
9:j:454:ARG:HG3	9:j:459:GLU:HB3	1.97	0.47
12:r:49:ALA:HB2	12:r:201:VAL:CG2	2.43	0.47
2:L:215:VAL:CG1	2:L:304:ALA:CB	2.91	0.47
9:j:219:ALA:HB1	23:j:608:MQ9:H23	1.96	0.47
9:j:226:GLY:HA2	23:j:608:MQ9:H72	1.97	0.47
9:j:314:LEU:HD23	9:j:335:VAL:HG21	1.97	0.47
23:j:608:MQ9:H203	23:j:608:MQ9:H221	1.43	0.47
2:I:381:MET:HE1	7:e:113:LEU:HD11	1.97	0.47
4:U:117:GLN:HB3	4:U:123:MET:HG2	1.97	0.47
8:f:24:ARG:NH1	11:n:68:GLU:OE2	2.48	0.47
23:j:607:MQ9:H321	23:j:607:MQ9:H303	1.67	0.47
23:i:612:MQ9:H203	23:i:612:MQ9:H221	1.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:240:VAL:HG12	7:e:242:PRO:HD2	1.96	0.46
9:i:455:LEU:HB2	9:i:456:PRO:HD3	1.97	0.46
23:i:611:MQ9:H311	23:i:611:MQ9:H23	1.97	0.46
10:k:166:ARG:O	10:k:169:SER:N	2.47	0.46
4:U:264:LEU:HD21	9:i:281:LEU:HD22	1.97	0.46
5:V:363:PRO:HB2	5:V:375:ASN:HB3	1.96	0.46
8:f:15:ILE:HD12	8:f:16:THR:N	2.30	0.46
12:q:80:LEU:CD1	12:q:82:ILE:HG13	2.45	0.46
14:b:103:CDL:H592	14:b:103:CDL:H772	1.97	0.46
3:h:62:ILE:HD13	10:l:83:ARG:CA	2.45	0.46
9:i:236:LYS:HD2	5:p:134:ARG:HB3	1.96	0.46
7:d:240:VAL:HG12	7:d:242:PRO:HD2	1.97	0.46
9:j:311:ASP:O	9:j:315:ARG:HG3	2.16	0.46
14:b:103:CDL:H741	14:b:103:CDL:C58	2.24	0.46
14:j:605:CDL:H581	23:j:611:MQ9:H201	1.97	0.46
11:m:134:ILE:HD13	14:m:202:CDL:HA31	1.97	0.46
2:I:253:LEU:HD21	2:I:320:ALA:CB	2.46	0.46
14:I:605:CDL:H321	14:b:103:CDL:H552	1.97	0.46
20:U:601:HEM:HBB2	20:U:601:HEM:HMB2	1.98	0.46
7:e:237:SER:HB3	7:e:278:VAL:HG23	1.96	0.46
14:I:605:CDL:CA5	14:I:605:CDL:CA7	2.94	0.46
9:i:314:LEU:HD23	9:i:335:VAL:HG21	1.97	0.46
14:i:604:CDL:H332	9:j:344:GLY:HA2	1.98	0.46
23:i:611:MQ9:H23	23:i:611:MQ9:H203	1.97	0.46
14:i:614:CDL:H711	14:i:614:CDL:C12	2.46	0.46
4:o:134:ARG:NH1	24:o:602:HEC:O1A	2.49	0.46
12:r:80:LEU:C	12:r:80:LEU:HD12	2.41	0.46
3:J:12:MET:HB2	3:J:13:PRO:HD3	1.97	0.46
9:i:166:ASP:OD1	9:i:166:ASP:N	2.45	0.46
20:j:604:HEM:CMB	20:j:604:HEM:HBB2	2.46	0.46
10:l:164:ALA:HA	10:l:167:VAL:HG22	1.98	0.46
10:k:166:ARG:O	10:k:167:VAL:C	2.59	0.46
12:r:182:ALA:HB3	12:r:185:LEU:HD12	1.98	0.46
7:e:183:ASN:ND2	8:g:130:GLU:O	2.48	0.46
8:f:44:ALA:CB	11:n:44:MET:HG3	2.46	0.46
3:h:62:ILE:HD13	10:l:83:ARG:HB2	1.97	0.46
9:j:187:ILE:O	9:j:187:ILE:CG1	2.64	0.46
2:I:163:SER:HA	4:o:127:ARG:NH2	2.31	0.45
2:I:288:LYS:HB3	2:I:288:LYS:HE2	1.67	0.45
2:L:395:ILE:HD13	16:L:602:HEA:HAA1	1.97	0.45
3:h:62:ILE:CD1	10:l:83:ARG:CA	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:234:TYR:HB2	14:i:607:CDL:HB62	1.97	0.45
9:j:187:ILE:HD12	9:j:191:MET:SD	2.57	0.45
12:q:80:LEU:HD12	12:q:80:LEU:C	2.41	0.45
2:L:308:ILE:HG13	2:L:308:ILE:O	2.17	0.45
3:h:20:THR:HB	3:h:21:PRO:HD3	1.97	0.45
9:i:311:ASP:O	9:i:315:ARG:HG3	2.16	0.45
14:i:607:CDL:OB7	23:i:612:MQ9:H3D	2.16	0.45
14:I:605:CDL:H132	14:I:605:CDL:HB62	1.99	0.45
7:d:141:GLN:NE2	7:d:233:ASP:OD2	2.48	0.45
8:g:150:HIS:NE2	8:g:195:TRP:HB2	2.32	0.45
5:V:283:MET:HE3	5:V:314:LYS:HG2	1.97	0.45
9:j:394:MET:SD	4:o:270:THR:HG23	2.57	0.45
23:j:607:MQ9:C3D	23:j:608:MQ9:H3C	2.45	0.45
23:j:611:MQ9:H253	23:j:611:MQ9:H271	1.49	0.45
5:V:391:SER:OXT	6:a:26:SER:CB	2.58	0.45
9:i:73:VAL:CG1	9:i:89:LYS:HD3	2.47	0.45
9:i:279:GLY:HA3	5:p:103:GLY:HA3	1.98	0.45
23:j:611:MQ9:H172	23:j:611:MQ9:H153	1.33	0.45
10:k:93:ASN:OD1	10:k:93:ASN:N	2.50	0.45
23:m:201:MQ9:H121	23:m:201:MQ9:H103	1.61	0.45
12:q:201:VAL:CG1	12:q:202:ALA:N	2.80	0.45
14:i:614:CDL:HA62	14:i:614:CDL:H312	1.23	0.45
9:j:233:TRP:CD2	23:j:608:MQ9:H3B	2.51	0.45
8:f:10:PRO:HG2	8:f:24:ARG:H	1.82	0.45
4:o:123:MET:O	4:o:123:MET:SD	2.75	0.45
14:I:604:CDL:OB7	14:I:604:CDL:HB32	2.16	0.45
4:U:270:THR:HG23	9:i:394:MET:SD	2.57	0.45
8:f:15:ILE:HD12	8:f:15:ILE:C	2.41	0.45
10:k:158:LEU:HD23	10:k:158:LEU:HA	1.81	0.45
10:l:156:ASN:HB3	10:l:159:ASP:HB2	1.99	0.45
14:I:605:CDL:HA32	9:j:430:ARG:HD3	1.98	0.45
1:b:19:SER:OG	9:j:440:ARG:NH2	2.41	0.45
7:e:141:GLN:HG2	7:e:142:TRP:CE2	2.52	0.45
14:i:609:CDL:OA7	14:i:609:CDL:HA62	2.16	0.45
23:i:602:MQ9:H271	23:i:602:MQ9:H253	1.31	0.45
2:L:27:LEU:N	14:L:606:CDL:OA4	2.46	0.44
7:d:168:LYS:NZ	7:d:198:THR:O	2.49	0.44
12:r:113:ILE:HG22	12:r:115:ALA:HB2	1.99	0.44
2:I:402:LEU:O	2:I:406:ILE:HG22	2.17	0.44
2:L:149:PHE:CD2	2:L:158:THR:HG22	2.51	0.44
2:L:402:LEU:O	2:L:406:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:128:ASN:HB2	7:d:336:ARG:HH12	1.82	0.44
23:i:603:MQ9:H303	23:i:603:MQ9:H321	1.64	0.44
14:i:607:CDL:H112	14:i:607:CDL:H722	1.99	0.44
14:I:604:CDL:H552	14:I:604:CDL:OB7	2.17	0.44
12:q:88:ASP:OD1	12:q:88:ASP:N	2.49	0.44
3:h:85:LYS:HD2	10:l:123:VAL:HG12	1.99	0.44
3:J:14:VAL:HG22	3:J:16:VAL:HG22	1.99	0.44
2:L:163:SER:HA	4:U:127:ARG:HH22	1.83	0.44
16:L:601:HEA:HBC1	16:L:601:HEA:CMC	2.48	0.44
5:V:133:ASP:HA	9:j:249:ASN:HA	1.99	0.44
14:g:301:CDL:H361	14:g:301:CDL:H321	1.99	0.44
10:k:156:ASN:HB3	10:k:159:ASP:HB2	2.00	0.44
12:q:182:ALA:HB3	12:q:185:LEU:HD12	1.98	0.44
12:r:101:GLU:N	12:r:101:GLU:OE1	2.50	0.44
2:I:293:TYR:O	2:I:297:ILE:HG12	2.17	0.44
23:j:611:MQ9:H303	23:j:611:MQ9:H322	1.43	0.44
12:r:80:LEU:CD1	12:r:82:ILE:HG13	2.48	0.44
2:I:105:VAL:HG12	2:I:106:VAL:HG13	1.99	0.44
7:d:336:ARG:HE	12:q:33:GLN:HA	1.83	0.44
9:i:227:ILE:HG12	23:i:612:MQ9:H153	2.00	0.44
9:j:73:VAL:CG1	9:j:89:LYS:HD3	2.48	0.44
12:r:201:VAL:CG1	12:r:202:ALA:N	2.80	0.44
4:U:195:PHE:HE1	9:i:167:LEU:HD23	1.82	0.44
8:g:11:ALA:HB1	8:g:22:LEU:HD22	1.93	0.44
9:j:166:ASP:OD1	9:j:166:ASP:N	2.45	0.44
14:G:102:CDL:H332	14:G:102:CDL:H362	1.82	0.43
2:L:293:TYR:O	2:L:297:ILE:HG12	2.18	0.43
14:i:614:CDL:H761	14:i:614:CDL:H792	1.83	0.43
2:I:68:VAL:CG1	2:I:69:PRO:HD2	2.48	0.43
20:U:601:HEM:HBC2	20:U:601:HEM:HMC2	2.00	0.43
14:g:301:CDL:HA32	14:g:301:CDL:OA7	2.16	0.43
9:i:223:ALA:HA	23:i:612:MQ9:H212	2.00	0.43
7:d:141:GLN:HA	7:d:233:ASP:OD2	2.18	0.43
8:f:14:ALA:HB1	8:f:182:ILE:HG21	2.01	0.43
2:I:122:ASN:ND2	2:I:188:ASN:ND2	2.66	0.43
4:U:278:ILE:HG13	4:U:278:ILE:O	2.18	0.43
9:i:220:ILE:HG12	23:i:612:MQ9:H33	2.00	0.43
14:i:607:CDL:H212	14:i:607:CDL:H181	1.86	0.43
23:i:610:MQ9:H321	23:i:610:MQ9:H303	1.76	0.43
14:i:614:CDL:H112	14:i:614:CDL:H321	2.00	0.43
10:l:128:TYR:OH	10:l:138:GLU:OE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:56:LEU:HB3	12:q:59:ILE:HD11	2.01	0.43
14:G:102:CDL:H551	14:G:102:CDL:H741	2.01	0.43
14:I:604:CDL:HA61	14:I:604:CDL:HB31	2.00	0.43
14:g:301:CDL:C53	14:g:301:CDL:HB61	2.48	0.43
3:J:61:ASN:OD1	3:J:61:ASN:N	2.47	0.43
9:i:317:ILE:HA	9:i:318:PRO:HD3	1.84	0.43
23:i:610:MQ9:H303	23:i:610:MQ9:C33	2.45	0.43
9:j:455:LEU:HB3	9:j:456:PRO:HD3	2.01	0.43
22:o:603:9YF:O1	22:o:603:9YF:C8	2.67	0.43
2:I:428:GLU:O	2:I:432:LYS:HG2	2.19	0.43
16:I:601:HEA:HBC1	16:I:601:HEA:CMC	2.48	0.43
5:V:128:GLU:OE1	5:V:130:SER:OG	2.37	0.43
2:I:335:VAL:HB	2:I:336:PRO:HD3	2.00	0.43
2:L:100:PHE:HE2	2:L:182:THR:HG23	1.83	0.43
2:L:105:VAL:HG12	2:L:106:VAL:HG13	2.01	0.43
4:U:123:MET:O	4:U:124:PRO:C	2.54	0.43
8:f:150:HIS:NE2	8:f:195:TRP:HB2	2.33	0.43
9:i:73:VAL:HG11	9:i:89:LYS:HD3	2.01	0.43
9:i:212:MET:HG2	9:i:216:LEU:HD12	2.01	0.43
23:i:612:MQ9:H5M3	23:i:612:MQ9:H72	1.86	0.43
2:L:149:PHE:CG	2:L:158:THR:HG22	2.54	0.43
8:g:44:ALA:CB	11:m:44:MET:HG3	2.49	0.43
23:i:602:MQ9:H303	23:i:602:MQ9:H322	1.46	0.43
11:m:22:TYR:O	11:m:26:THR:HG23	2.18	0.43
11:m:111:PRO:HB2	22:o:603:9YF:C27	2.49	0.43
11:n:1:MET:HB2	11:n:60:ALA:HB2	2.01	0.43
2:I:100:PHE:HE2	2:I:182:THR:HG23	1.83	0.43
14:b:103:CDL:H572	14:b:103:CDL:H542	1.92	0.43
8:f:15:ILE:HG21	11:n:62:ARG:HH22	1.80	0.43
8:g:13:THR:CG2	11:m:59:VAL:HG13	2.49	0.43
14:g:301:CDL:HB61	14:g:301:CDL:H532	2.01	0.43
23:i:602:MQ9:H71	23:i:602:MQ9:H5M3	1.87	0.43
23:i:611:MQ9:O1	23:i:611:MQ9:C8	2.67	0.43
9:j:339:MET:HB2	9:j:339:MET:HE3	1.73	0.43
2:I:484:LEU:O	2:I:487:SER:OG	2.24	0.42
2:L:159:ASP:OD1	2:L:159:ASP:N	2.51	0.42
2:L:335:VAL:HB	2:L:336:PRO:HD3	2.01	0.42
15:f:601:9Y0:O3	15:f:601:9Y0:C21	2.65	0.42
23:i:602:MQ9:H372	23:i:602:MQ9:H353	1.27	0.42
9:j:187:ILE:CD1	9:j:191:MET:HG3	2.49	0.42
4:o:236:ARG:HH12	12:r:207:ALA:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:149:PHE:CG	2:I:158:THR:HG22	2.53	0.42
2:I:445:THR:HG23	2:I:446:PHE:CD2	2.54	0.42
2:L:172:ILE:HG23	2:L:231:LEU:HD22	2.01	0.42
2:L:559:HIS:HB2	7:d:94:TYR:CZ	2.54	0.42
2:L:560:VAL:HG22	7:d:92:PHE:HB2	2.01	0.42
4:U:274:MET:HB3	23:i:611:MQ9:H5M3	2.01	0.42
14:b:103:CDL:C81	14:b:103:CDL:C71	2.72	0.42
3:h:84:GLY:N	10:l:124:VAL:O	2.52	0.42
9:i:72:GLU:OE2	9:i:86:GLN:NE2	2.52	0.42
9:j:61:TYR:CD1	9:j:107:VAL:HG11	2.54	0.42
2:I:264:HIS:HB3	2:I:265:PRO:HD3	2.02	0.42
14:L:606:CDL:C32	14:L:606:CDL:H121	2.49	0.42
8:g:13:THR:C	8:g:15:ILE:H	2.26	0.42
9:i:69:SER:HB3	9:i:89:LYS:HB2	2.02	0.42
23:j:602:MQ9:H172	23:j:602:MQ9:H121	2.02	0.42
4:o:262:TYR:CD2	4:o:264:LEU:HD23	2.53	0.42
14:p:603:CDL:H212	14:p:603:CDL:C62	2.48	0.42
3:J:85:LYS:C	3:J:86:TRP:CD1	2.97	0.42
2:L:81:GLN:OE1	18:q:302:PLM:H41	2.20	0.42
7:d:131:PRO:HG3	7:d:226:GLU:OE1	2.20	0.42
7:d:177:GLY:C	7:d:179:ASP:H	2.27	0.42
23:i:611:MQ9:H5M3	23:i:611:MQ9:H72	1.79	0.42
14:j:609:CDL:H721	14:j:609:CDL:H542	2.01	0.42
11:n:22:TYR:O	11:n:26:THR:HG23	2.19	0.42
11:n:38:GLY:O	11:n:42:MET:HG3	2.19	0.42
12:r:94:THR:O	12:r:94:THR:CG2	2.66	0.42
2:L:91:LEU:HD23	2:L:91:LEU:HA	1.89	0.42
2:L:445:THR:HG23	2:L:446:PHE:CD2	2.54	0.42
2:L:537:ARG:CZ	11:n:72:ASP:HA	2.50	0.42
9:i:61:TYR:CD1	9:i:107:VAL:HG11	2.54	0.42
23:i:612:MQ9:C8	23:i:612:MQ9:O1	2.67	0.42
5:p:128:GLU:OE1	5:p:130:SER:OG	2.37	0.42
2:I:159:ASP:OD1	2:I:159:ASP:N	2.51	0.42
2:I:264:HIS:O	2:I:267:VAL:HG22	2.20	0.42
4:U:192:CYS:SG	5:p:325:LEU:HG	2.59	0.42
5:V:325:LEU:HG	4:o:192:CYS:SG	2.60	0.42
9:i:297:ILE:HD12	5:p:322:PRO:HD2	2.02	0.42
14:i:614:CDL:H142	14:i:614:CDL:H111	1.91	0.42
9:j:501:THR:HG21	9:j:516:LEU:HD12	2.01	0.42
16:I:602:HEA:HBC1	16:I:602:HEA:HMC3	2.01	0.42
2:L:288:LYS:HB3	2:L:288:LYS:HE2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:123:MET:HG3	20:U:601:HEM:CHB	2.49	0.42
7:e:142:TRP:HZ3	24:o:601:HEC:CBC	2.32	0.42
14:g:301:CDL:H162	14:g:301:CDL:H192	1.88	0.42
14:i:609:CDL:H121	14:i:609:CDL:H152	1.96	0.42
2:L:428:GLU:O	2:L:432:LYS:HG2	2.20	0.42
3:h:21:PRO:HA	3:h:24:PHE:HD2	1.84	0.42
14:p:603:CDL:H631	14:p:603:CDL:C23	2.48	0.42
14:p:603:CDL:H712	14:p:603:CDL:C75	2.45	0.42
12:q:165:ASP:OD1	12:q:165:ASP:N	2.52	0.42
7:e:178:LYS:HD2	7:e:184:GLU:HG3	2.02	0.42
8:f:18:ARG:O	8:f:18:ARG:CG	2.67	0.42
9:i:501:THR:CG2	9:i:513:GLN:HA	2.50	0.42
23:i:610:MQ9:C16	23:i:610:MQ9:C21	2.61	0.42
9:j:69:SER:HB3	9:j:89:LYS:HB2	2.02	0.42
4:U:91:CYS:SG	20:U:601:HEM:CBC	3.08	0.42
8:g:64:GLU:N	8:g:64:GLU:OE1	2.53	0.42
9:j:73:VAL:HG11	9:j:89:LYS:HD3	2.02	0.42
2:I:96:THR:HB	2:I:97:PRO:HD3	2.02	0.41
2:L:104:ASN:OD1	2:L:122:ASN:ND2	2.48	0.41
5:V:62:TRP:CZ2	14:g:301:CDL:H312	2.55	0.41
23:i:611:MQ9:H203	23:i:611:MQ9:C23	2.50	0.41
23:i:612:MQ9:H28	23:i:612:MQ9:H322	1.93	0.41
20:j:604:HEM:HBB2	20:j:604:HEM:HMB1	2.01	0.41
10:l:135:ARG:NE	10:l:175:PRO:HD2	2.34	0.41
4:U:192:CYS:SG	20:U:602:HEM:CBC	3.08	0.41
4:U:276:MET:HE1	9:i:117:MET:HE3	2.02	0.41
9:i:297:ILE:HD13	5:p:336:PRO:HG2	2.02	0.41
20:j:603:HEM:HBD1	20:j:603:HEM:HHA	2.02	0.41
23:m:201:MQ9:C8	23:m:201:MQ9:C5M	2.94	0.41
22:o:603:9YF:O9	22:o:603:9YF:P	2.78	0.41
2:I:147:ALA:HB1	2:I:149:PHE:CZ	2.56	0.41
2:L:163:SER:HA	4:U:127:ARG:NH2	2.35	0.41
14:i:604:CDL:CB7	14:i:604:CDL:H531	2.50	0.41
14:i:614:CDL:H532	9:j:233:TRP:CE2	2.55	0.41
9:j:146:GLY:HA3	20:j:603:HEM:C2C	2.55	0.41
2:I:110:GLN:HB3	2:I:207:PRO:HG2	2.02	0.41
2:I:537:ARG:CZ	11:m:72:ASP:HA	2.50	0.41
3:J:83:SER:HA	10:k:124:VAL:O	2.19	0.41
2:L:264:HIS:HB3	2:L:265:PRO:HD3	2.02	0.41
2:L:452:LEU:HD13	2:L:457:MET:HE1	2.03	0.41
7:d:186:VAL:HG21	8:f:65:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:614:CDL:H132	9:j:234:TYR:CE2	2.55	0.41
23:j:602:MQ9:H172	23:j:602:MQ9:C12	2.51	0.41
23:m:201:MQ9:H3B	4:o:262:TYR:OH	2.20	0.41
12:r:165:ASP:N	12:r:165:ASP:OD1	2.49	0.41
2:I:531:SER:HA	9:j:459:GLU:HG3	2.03	0.41
4:U:278:ILE:HG23	4:U:279:ILE:HG13	2.01	0.41
8:f:6:ALA:HB1	8:f:7:PRO:HD2	2.02	0.41
8:f:74:ILE:HB	8:f:75:PRO:HD3	2.03	0.41
8:f:108:ILE:O	8:f:112:MET:HG3	2.21	0.41
13:i:613:9XX:O	13:i:613:9XX:C18	2.69	0.41
4:o:88:CYS:HB3	24:o:601:HEC:C3B	2.50	0.41
5:p:295:VAL:HG22	5:p:345:LEU:HD22	2.03	0.41
2:I:420:LYS:HD3	2:I:523:CYS:O	2.21	0.41
3:h:81:SER:HB2	10:l:127:VAL:HG12	2.02	0.41
9:i:501:THR:HG22	9:i:513:GLN:CG	2.45	0.41
14:i:607:CDL:OA9	14:i:607:CDL:HA31	2.20	0.41
11:m:38:GLY:O	11:m:42:MET:HG3	2.20	0.41
5:V:280:ASN:N	5:V:281:PRO:HD2	2.36	0.41
8:g:74:ILE:HB	8:g:75:PRO:HD3	2.03	0.41
9:j:80:GLN:HA	9:j:83:ARG:HG3	2.03	0.41
11:m:91:TRP:O	11:m:95:ILE:HG13	2.21	0.41
14:G:102:CDL:H761	14:G:102:CDL:C81	2.30	0.41
2:I:172:ILE:HG23	2:I:231:LEU:HD22	2.03	0.41
2:I:521:THR:CG2	2:I:530:PHE:CE1	3.04	0.41
8:f:64:GLU:N	8:f:64:GLU:OE1	2.54	0.41
8:g:9:SER:HB3	8:g:24:ARG:HB2	2.02	0.41
8:g:108:ILE:O	8:g:112:MET:HG3	2.21	0.41
14:g:301:CDL:OB9	14:g:301:CDL:H731	2.21	0.41
9:i:211:ALA:HB1	9:j:63:THR:CG2	2.51	0.41
12:q:91:ASP:O	12:q:93:LEU:N	2.54	0.41
14:G:102:CDL:OB8	14:G:102:CDL:H731	2.21	0.41
16:I:602:HEA:H171	16:I:602:HEA:H261	1.69	0.41
2:L:85:MET:O	2:L:89:VAL:HG22	2.21	0.41
9:i:146:GLY:HA3	20:i:605:HEM:C2C	2.56	0.41
9:i:501:THR:HG21	9:i:516:LEU:HD12	2.03	0.41
10:k:128:TYR:OH	10:k:141:ALA:N	2.54	0.41
10:l:98:GLY:HA2	10:l:101:GLU:HG2	2.03	0.41
4:U:265:GLY:HA3	23:i:611:MQ9:C3B	2.51	0.40
7:e:237:SER:HB3	7:e:278:VAL:CG2	2.51	0.40
14:g:301:CDL:H361	14:g:301:CDL:C32	2.51	0.40
9:j:167:LEU:HD23	4:o:195:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:91:TRP:O	11:n:95:ILE:HG13	2.21	0.40
2:L:56:GLY:C	16:L:602:HEA:H162	2.46	0.40
2:L:96:THR:HB	2:L:97:PRO:HD3	2.03	0.40
2:L:340:LYS:NZ	25:L:704:HOH:O	2.54	0.40
9:i:80:GLN:HA	9:i:83:ARG:HG3	2.02	0.40
9:i:218:PRO:HB2	23:j:608:MQ9:H403	2.03	0.40
9:i:348:ALA:HB3	23:i:603:MQ9:H451	2.03	0.40
9:i:468:ALA:HB2	9:i:479:LEU:HD11	2.03	0.40
9:j:233:TRP:HE3	23:j:607:MQ9:C3C	2.34	0.40
14:j:606:CDL:OB7	14:j:606:CDL:HB32	2.20	0.40
14:p:603:CDL:H251	14:p:603:CDL:H673	2.03	0.40
2:L:357:THR:HA	2:L:360:ILE:HG12	2.04	0.40
5:V:314:LYS:O	5:V:322:PRO:HA	2.22	0.40
2:I:340:LYS:NZ	25:I:705:HOH:O	2.54	0.40
2:L:383:PRO:HD2	7:d:117:THR:HG23	2.03	0.40
3:h:21:PRO:HA	3:h:24:PHE:CD2	2.56	0.40
9:j:264:GLY:HA3	23:j:607:MQ9:H18	2.02	0.40
23:j:611:MQ9:H71	23:j:611:MQ9:H5M3	1.86	0.40
2:I:452:LEU:HD13	2:I:457:MET:HE1	2.02	0.40
2:I:532:GLU:OE2	10:k:41:THR:CG2	2.68	0.40
2:L:387:HIS:HD2	7:d:38:TRP:CE2	2.38	0.40
9:j:341:LEU:HA	23:j:602:MQ9:H411	2.03	0.40
14:m:202:CDL:OB7	14:m:202:CDL:HB32	2.20	0.40
22:o:603:9YF:P	22:o:603:9YF:O3	2.80	0.40
5:p:183:ALA:O	5:p:187:ILE:HG13	2.22	0.40
5:p:280:ASN:N	5:p:281:PRO:HD2	2.37	0.40
5:p:325:LEU:HD13	5:p:336:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
1	b	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
2	I	549/564 (97%)	520 (95%)	29 (5%)	0	100	100
2	L	549/564 (97%)	521 (95%)	28 (5%)	0	100	100
3	J	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
3	h	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
4	U	219/295 (74%)	205 (94%)	14 (6%)	0	100	100
4	o	219/295 (74%)	204 (93%)	15 (7%)	0	100	100
5	V	379/391 (97%)	370 (98%)	9 (2%)	0	100	100
5	p	379/391 (97%)	367 (97%)	12 (3%)	0	100	100
6	X	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
6	a	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
7	d	310/349 (89%)	295 (95%)	15 (5%)	0	100	100
7	e	310/349 (89%)	296 (96%)	14 (4%)	0	100	100
8	f	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	24	39
8	g	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	12	20
9	i	525/546 (96%)	494 (94%)	31 (6%)	0	100	100
9	j	525/546 (96%)	497 (95%)	28 (5%)	0	100	100
10	k	142/175 (81%)	139 (98%)	3 (2%)	0	100	100
10	l	142/175 (81%)	137 (96%)	5 (4%)	0	100	100
11	m	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	n	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
12	q	152/227 (67%)	144 (95%)	8 (5%)	0	100	100
12	r	152/227 (67%)	140 (92%)	11 (7%)	1 (1%)	18	30
All	All	5556/6630 (84%)	5282 (95%)	270 (5%)	4 (0%)	49	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	f	10	PRO
8	g	19	VAL
8	g	15	ILE
12	r	166	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	59/77 (77%)	59 (100%)	0	100	100
1	b	59/77 (77%)	59 (100%)	0	100	100
2	I	448/455 (98%)	441 (98%)	7 (2%)	55	74
2	L	448/455 (98%)	443 (99%)	5 (1%)	65	80
3	J	49/63 (78%)	47 (96%)	2 (4%)	27	46
3	h	49/63 (78%)	49 (100%)	0	100	100
4	U	164/223 (74%)	159 (97%)	5 (3%)	36	57
4	o	164/223 (74%)	162 (99%)	2 (1%)	63	79
5	V	312/321 (97%)	312 (100%)	0	100	100
5	p	312/321 (97%)	311 (100%)	1 (0%)	86	94
6	X	20/173 (12%)	20 (100%)	0	100	100
6	a	20/173 (12%)	20 (100%)	0	100	100
7	d	269/298 (90%)	264 (98%)	5 (2%)	50	71
7	e	269/298 (90%)	265 (98%)	4 (2%)	57	75
8	f	163/163 (100%)	160 (98%)	3 (2%)	51	72
8	g	163/163 (100%)	163 (100%)	0	100	100
9	i	421/437 (96%)	415 (99%)	6 (1%)	59	76
9	j	421/437 (96%)	417 (99%)	4 (1%)	68	81
10	k	108/130 (83%)	107 (99%)	1 (1%)	70	82
10	l	108/130 (83%)	107 (99%)	1 (1%)	70	82
11	m	103/103 (100%)	103 (100%)	0	100	100
11	n	103/103 (100%)	103 (100%)	0	100	100
12	q	121/171 (71%)	121 (100%)	0	100	100
12	r	121/171 (71%)	119 (98%)	2 (2%)	53	73
All	All	4474/5228 (86%)	4426 (99%)	48 (1%)	63	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	63	ARG
2	I	129	PHE
2	I	148	ASP
2	I	149	PHE
2	I	162	HIS
2	I	403	PHE
2	I	472	PHE
3	J	85	LYS
3	J	86	TRP
2	L	61	PHE
2	L	129	PHE
2	L	403	PHE
2	L	468	ASP
2	L	476	PHE
4	U	88	CYS
4	U	123	MET
4	U	165	ASP
4	U	189	CYS
4	U	198	ARG
7	d	143	ASN
7	d	195	GLU
7	d	264	VAL
7	d	281	CYS
7	d	286	SER
7	e	141	GLN
7	e	143	ASN
7	e	195	GLU
7	e	264	VAL
8	f	1	MET
8	f	15	ILE
8	f	16	THR
9	i	28	MET
9	i	235	GLN
9	i	250	VAL
9	i	396	ASP
9	i	452	ILE
9	i	525	HIS
9	j	235	GLN
9	j	250	VAL
9	j	396	ASP
9	j	525	HIS
10	k	115	ILE
10	l	115	ILE

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Mol	Chain	Res	Type
4	o	123	MET
4	o	198	ARG
5	p	323	THR
12	r	165	ASP
12	r	166	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	76	ASN
2	I	86	HIS
2	I	122	ASN
2	I	188	ASN
2	I	387	HIS
2	I	434	HIS
2	I	455	GLN
2	L	76	ASN
2	L	243	HIS
2	L	387	HIS
2	L	434	HIS
2	L	455	GLN
4	U	82	GLN
4	U	95	ASN
4	U	194	ASN
4	U	229	ASN
5	V	31	ASN
5	V	92	ASN
5	V	96	ASN
5	V	206	GLN
6	X	30	GLN
6	a	29	GLN
1	b	75	ASN
7	d	31	GLN
7	d	81	HIS
7	d	141	GLN
7	d	181	HIS
7	d	263	GLN
7	d	285	HIS
7	e	141	GLN
7	e	149	GLN
7	e	181	HIS
7	e	183	ASN

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Mol	Chain	Res	Type
8	g	60	ASN
9	i	76	ASN
9	i	80	GLN
9	i	86	GLN
9	i	331	GLN
9	i	535	GLN
9	j	76	ASN
9	j	80	GLN
9	j	525	HIS
9	j	535	GLN
10	l	58	HIS
11	m	88	HIS
11	n	88	HIS
11	n	133	HIS
4	o	128	ASN
4	o	143	GLN
5	p	16	GLN
5	p	92	ASN
5	p	96	ASN
5	p	206	GLN
12	q	50	ASN
12	q	60	HIS
12	q	64	ASN
12	q	215	HIS
12	r	33	GLN
12	r	50	ASN
12	r	60	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 8 are monoatomic - leaving 62 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	$\#\|Z\| > 2$
22	9YF	V	602	-	58,58,58	1.61	6 (10%)	69,71,71	1.63	9 (13%)
23	MQ9	j	607	-	44,44,59	0.34	0	54,57,75	0.52	0
14	CDL	i	607	-	73,73,99	0.33	0	79,85,111	0.37	0
16	HEA	I	602	2	66,67,67	2.40	23 (34%)	78,103,103	2.53	36 (46%)
14	CDL	L	605	-	75,75,99	0.38	0	81,87,111	0.24	0
23	MQ9	j	608	-	59,59,59	0.34	0	72,75,75	0.40	0
13	9XX	i	613	-	31,31,41	0.32	0	34,34,44	0.33	0
22	9YF	n	201	-	58,58,58	0.26	0	69,71,71	0.38	0
14	CDL	I	605	-	80,80,99	0.31	0	86,92,111	0.41	0
15	9Y0	b	101	-	37,37,48	0.35	0	40,42,53	0.41	0
14	CDL	j	606	-	78,78,99	0.35	0	84,90,111	0.47	0
15	9Y0	b	104	-	40,40,48	0.35	0	43,45,53	0.40	0
14	CDL	I	604	-	75,75,99	0.33	0	81,87,111	0.40	0
23	MQ9	i	610	-	44,44,59	0.33	0	54,57,75	0.39	0
18	PLM	I	606	-	16,16,17	0.34	0	15,15,17	0.37	0
22	9YF	o	603	-	58,58,58	0.29	0	69,71,71	0.41	0
16	HEA	L	601	2	66,67,67	2.37	22 (33%)	78,103,103	2.60	31 (39%)
19	OXY	L	607	-	1,1,1	0.15	0	-		
21	FES	p	602	5	0,4,4	-	-	-		
20	HEM	j	604	9	50,50,50	1.71	12 (24%)	66,82,82	1.94	16 (24%)
14	CDL	i	609	-	78,78,99	0.36	0	84,90,111	0.38	0
15	9Y0	f	601	-	42,42,48	0.34	0	44,47,53	0.39	0
14	CDL	i	614	-	73,73,99	0.34	0	79,85,111	0.42	0
13	9XX	j	610	-	31,31,41	0.31	0	34,34,44	0.40	0
13	9XX	b	102	-	41,41,41	0.28	0	44,44,44	0.22	0
14	CDL	j	609	-	65,65,99	0.34	0	71,77,111	0.39	0
16	HEA	I	601	2	66,67,67	2.38	22 (33%)	78,103,103	2.59	31 (39%)
21	FES	V	601	5	0,4,4	-	-	-		
15	9Y0	G	103	-	40,40,48	0.32	0	43,45,53	0.42	0
14	CDL	b	103	-	87,87,99	0.31	0	93,99,111	0.34	0
23	MQ9	i	612	-	59,59,59	0.35	0	72,75,75	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CDL	U	603	-	78,78,99	0.97	3 (3%)	84,90,111	0.45	0
22	9YF	i	601	-	58,58,58	0.32	0	69,71,71	0.42	0
20	HEM	j	603	9	49,49,50	1.66	9 (18%)	66,81,82	1.63	12 (18%)
14	CDL	j	605	-	76,76,99	0.35	0	82,88,111	0.37	0
20	HEM	i	606	9	50,50,50	1.68	11 (22%)	66,82,82	1.91	18 (27%)
24	HEC	o	601	4	50,50,50	2.94	24 (48%)	68,82,82	2.29	27 (39%)
22	9YF	j	601	-	58,58,58	0.31	0	69,71,71	0.43	0
23	MQ9	j	611	-	59,59,59	0.36	0	72,75,75	0.39	0
24	HEC	o	602	4	50,50,50	1.76	5 (10%)	68,82,82	1.54	11 (16%)
14	CDL	p	603	-	94,94,99	0.29	0	100,106,111	0.34	0
23	MQ9	i	611	-	49,49,59	0.34	0	60,63,75	0.54	1 (1%)
14	CDL	G	102	-	87,87,99	0.31	0	93,99,111	0.41	0
13	9XX	G	101	-	41,41,41	0.27	0	44,44,44	0.57	1 (2%)
23	MQ9	i	602	-	59,59,59	0.35	0	72,75,75	0.42	0
18	PLM	q	302	-	16,16,17	0.35	0	15,15,17	0.39	0
23	MQ9	j	602	-	59,59,59	0.32	0	72,75,75	0.45	0
14	CDL	i	608	-	76,76,99	0.36	0	82,88,111	0.43	0
20	HEM	i	605	9	49,49,50	1.68	10 (20%)	66,81,82	1.62	12 (18%)
14	CDL	L	606	-	80,80,99	0.31	0	86,92,111	0.39	0
15	9Y0	g	302	-	42,42,48	0.35	0	44,47,53	0.42	0
23	MQ9	m	201	-	49,49,59	0.39	0	60,63,75	0.42	0
22	9YF	p	601	-	58,58,58	0.31	0	69,71,71	0.54	1 (1%)
14	CDL	i	604	-	65,65,99	0.33	0	71,77,111	0.39	0
19	OXY	I	607	-	1,1,1	0.15	0	-		
23	MQ9	i	603	-	59,59,59	0.35	0	72,75,75	0.41	0
15	9Y0	q	301	-	37,37,48	0.37	0	40,42,53	0.38	0
20	HEM	U	602	4	50,50,50	2.86	28 (56%)	66,82,82	2.42	22 (33%)
14	CDL	g	301	-	94,94,99	0.29	0	100,106,111	0.32	0
20	HEM	U	601	4	50,50,50	2.88	25 (50%)	66,82,82	2.29	20 (30%)
14	CDL	m	202	-	78,78,99	0.33	0	84,90,111	0.38	0
16	HEA	L	602	2	66,67,67	2.40	23 (34%)	78,103,103	2.53	35 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	9YF	V	602	-	-	23/54/78/78	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	MQ9	j	607	-	-	19/35/55/73	0/2/2/2
14	CDL	i	607	-	-	22/84/84/110	-
16	HEA	I	602	2	-	6/36/76/76	-
14	CDL	L	605	-	-	44/86/86/110	-
23	MQ9	j	608	-	-	23/53/73/73	0/2/2/2
13	9XX	i	613	-	-	6/33/33/43	-
22	9YF	n	201	-	-	20/54/78/78	0/1/1/1
14	CDL	I	605	-	-	24/91/91/110	-
15	9Y0	b	101	-	-	9/41/41/52	-
14	CDL	j	606	-	-	27/89/89/110	-
15	9Y0	b	104	-	-	4/44/44/52	-
14	CDL	I	604	-	-	22/86/86/110	-
23	MQ9	i	610	-	-	14/35/55/73	0/2/2/2
18	PLM	I	606	-	-	1/13/14/15	-
22	9YF	o	603	-	-	12/54/78/78	0/1/1/1
16	HEA	L	601	2	-	5/36/76/76	-
21	FES	p	602	5	-	-	0/1/1/1
20	HEM	j	604	9	-	1/14/54/54	-
14	CDL	i	609	-	-	24/89/89/110	-
15	9Y0	f	601	-	-	15/46/46/52	-
14	CDL	i	614	-	-	25/84/84/110	-
13	9XX	j	610	-	-	6/33/33/43	-
13	9XX	b	102	-	-	15/43/43/43	-
14	CDL	j	609	-	-	22/76/76/110	-
16	HEA	I	601	2	-	5/36/76/76	-
21	FES	V	601	5	-	-	0/1/1/1
15	9Y0	G	103	-	-	10/44/44/52	-
14	CDL	b	103	-	-	25/98/98/110	-
23	MQ9	i	612	-	-	36/53/73/73	0/2/2/2
14	CDL	U	603	-	-	55/89/89/110	-
22	9YF	i	601	-	-	9/54/78/78	0/1/1/1
20	HEM	j	603	9	-	6/12/52/54	-
14	CDL	j	605	-	-	17/87/87/110	-
20	HEM	i	606	9	-	1/14/54/54	-
24	HEC	o	601	4	1/1/3/7	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	9YF	j	601	-	-	9/54/78/78	0/1/1/1
24	HEC	o	602	4	1/1/3/7	4/14/54/54	-
23	MQ9	j	611	-	-	31/53/73/73	0/2/2/2
14	CDL	p	603	-	-	30/105/105/110	-
23	MQ9	i	611	-	-	15/41/61/73	0/2/2/2
13	9XX	G	101	-	-	10/43/43/43	-
14	CDL	G	102	-	-	38/98/98/110	-
23	MQ9	i	602	-	-	30/53/73/73	0/2/2/2
18	PLM	q	302	-	-	4/13/14/15	-
23	MQ9	j	602	-	-	24/53/73/73	0/2/2/2
14	CDL	i	608	-	-	22/87/87/110	-
20	HEM	i	605	9	-	6/12/52/54	-
14	CDL	L	606	-	-	21/91/91/110	-
15	9Y0	g	302	-	-	15/46/46/52	-
23	MQ9	m	201	-	-	21/41/61/73	0/2/2/2
22	9YF	p	601	-	-	13/54/78/78	0/1/1/1
14	CDL	i	604	-	-	17/76/76/110	-
23	MQ9	i	603	-	-	24/53/73/73	0/2/2/2
15	9Y0	q	301	-	-	16/41/41/52	-
20	HEM	U	602	4	-	2/14/54/54	-
14	CDL	g	301	-	-	28/105/105/110	-
20	HEM	U	601	4	-	3/14/54/54	-
14	CDL	m	202	-	-	20/89/89/110	-
16	HEA	L	602	2	-	6/36/76/76	-

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	o	602	HEC	C3D-C2D	7.88	1.53	1.36
14	U	603	CDL	CB3-CB4	6.23	1.69	1.50
22	V	602	9YF	C7-C2	5.89	1.68	1.52
16	I	602	HEA	FE-NB	5.50	2.11	1.94
16	L	602	HEA	FE-NB	5.50	2.11	1.94
16	I	602	HEA	FE-ND	5.39	2.11	1.94
16	L	602	HEA	FE-ND	5.39	2.11	1.94
24	o	601	HEC	CHD-C1D	5.39	1.49	1.38
16	I	601	HEA	FE-NB	5.34	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	601	HEA	FE-NB	5.32	2.11	1.94
24	o	601	HEC	FE-NC	5.32	2.13	1.95
20	U	601	HEM	FE-ND	5.32	2.11	1.94
16	L	601	HEA	FE-ND	5.30	2.11	1.94
16	I	601	HEA	FE-ND	5.28	2.11	1.94
20	i	606	HEM	FE-NB	5.22	2.11	1.94
24	o	601	HEC	CHA-C1A	5.21	1.48	1.38
16	L	602	HEA	C3B-C2B	5.17	1.46	1.34
16	I	602	HEA	C3B-C2B	5.17	1.46	1.34
20	U	602	HEM	C3C-C2C	5.16	1.47	1.37
16	L	601	HEA	C3B-C2B	5.15	1.46	1.34
20	U	602	HEM	C3B-C2B	5.12	1.47	1.37
16	I	601	HEA	C3B-C2B	5.12	1.46	1.34
24	o	601	HEC	FE-ND	5.09	2.10	1.94
24	o	601	HEC	C3B-C2B	5.07	1.47	1.36
22	V	602	9YF	P-O	5.06	1.79	1.59
20	i	605	HEM	FE-NB	5.06	2.10	1.94
20	U	601	HEM	C3B-C2B	5.05	1.47	1.37
20	j	604	HEM	FE-NB	4.98	2.10	1.94
20	j	603	HEM	FE-NB	4.98	2.10	1.94
20	U	601	HEM	CHC-C1C	4.95	1.48	1.38
24	o	601	HEC	FE-NA	4.89	2.11	1.95
24	o	601	HEC	C3D-C2D	4.89	1.47	1.36
24	o	601	HEC	CHC-C4B	4.86	1.48	1.38
20	U	602	HEM	CHC-C1C	4.82	1.47	1.38
16	I	601	HEA	C1A-NA	4.80	1.49	1.39
20	U	601	HEM	FE-NA	4.79	2.11	1.95
20	U	601	HEM	C3C-C2C	4.79	1.47	1.37
16	L	601	HEA	C3D-C2D	4.78	1.46	1.36
16	L	602	HEA	C3D-C2D	4.78	1.46	1.36
24	o	601	HEC	FE-NB	4.77	2.09	1.94
16	L	601	HEA	C1A-NA	4.77	1.49	1.39
16	I	602	HEA	C3D-C2D	4.77	1.46	1.36
16	I	601	HEA	C3D-C2D	4.76	1.46	1.36
20	U	601	HEM	FE-NB	4.73	2.09	1.94
20	U	602	HEM	FE-ND	4.73	2.09	1.94
20	U	602	HEM	C3D-C2D	4.71	1.46	1.36
16	I	602	HEA	C1A-NA	4.69	1.48	1.39
16	L	602	HEA	C1A-NA	4.65	1.48	1.39
20	U	602	HEM	CHA-C4D	4.64	1.47	1.38
16	I	601	HEA	C4A-NA	4.64	1.48	1.39
20	U	601	HEM	CHA-C4D	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	601	HEA	C4A-NA	4.58	1.48	1.39
16	I	602	HEA	FE-NC	4.58	2.10	1.95
20	U	601	HEM	C3D-C2D	4.57	1.46	1.36
16	L	602	HEA	FE-NC	4.55	2.10	1.95
16	I	601	HEA	FE-NC	4.53	2.10	1.95
16	I	602	HEA	C3A-C2A	4.53	1.46	1.36
16	L	602	HEA	C3A-C2A	4.52	1.46	1.36
20	U	602	HEM	FE-NA	4.52	2.10	1.95
16	L	601	HEA	FE-NC	4.52	2.10	1.95
16	I	601	HEA	CHC-C4B	4.46	1.47	1.38
24	o	601	HEC	C2A-C3A	4.45	1.46	1.36
16	L	601	HEA	CHC-C4B	4.45	1.47	1.38
16	L	602	HEA	CHC-C4B	4.44	1.47	1.38
20	U	601	HEM	FE-NC	4.44	2.10	1.95
16	I	601	HEA	C3A-C2A	4.43	1.46	1.36
16	L	601	HEA	C3A-C2A	4.43	1.46	1.36
16	I	602	HEA	CHC-C4B	4.42	1.47	1.38
22	V	602	9YF	O2-C2	-4.41	1.28	1.44
24	o	602	HEC	FE-ND	4.39	2.08	1.94
20	U	602	HEM	FE-NB	4.39	2.08	1.94
20	U	601	HEM	CHD-C4C	4.38	1.46	1.38
20	i	606	HEM	FE-NC	4.38	2.10	1.95
20	U	602	HEM	CHB-C1B	4.31	1.47	1.38
16	I	602	HEA	CHA-C1A	4.29	1.46	1.38
20	j	603	HEM	FE-NC	4.28	2.09	1.95
24	o	601	HEC	CHB-C4A	4.27	1.46	1.38
16	I	602	HEA	CHD-C1D	4.25	1.47	1.38
16	L	602	HEA	CHA-C1A	4.25	1.46	1.38
16	L	602	HEA	CHD-C1D	4.23	1.47	1.38
20	U	601	HEM	CHB-C1B	4.20	1.47	1.38
16	L	602	HEA	C4A-NA	4.20	1.47	1.39
20	i	605	HEM	FE-NC	4.20	2.09	1.95
16	I	602	HEA	C4A-NA	4.19	1.47	1.39
20	j	604	HEM	FE-NC	4.17	2.09	1.95
20	U	602	HEM	FE-NC	4.15	2.09	1.95
24	o	601	HEC	CHC-C1C	4.11	1.48	1.39
20	j	604	HEM	C1B-NB	-4.07	1.33	1.40
20	U	601	HEM	CBC-CAC	4.03	1.50	1.30
20	U	602	HEM	CBC-CAC	4.02	1.50	1.30
20	U	601	HEM	CBB-CAB	4.00	1.50	1.30
20	U	602	HEM	CBB-CAB	3.98	1.50	1.30
14	U	603	CDL	CA2-C1	3.95	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	601	HEA	CHD-C1D	3.95	1.46	1.38
24	o	601	HEC	CHD-C4C	3.94	1.48	1.39
24	o	602	HEC	FE-NB	3.93	2.07	1.94
16	L	601	HEA	CHD-C1D	3.90	1.46	1.38
16	L	601	HEA	CHB-C4A	3.89	1.46	1.38
16	I	601	HEA	CHB-C4A	3.87	1.45	1.38
20	U	602	HEM	CHA-C1A	3.86	1.48	1.39
20	i	605	HEM	C1B-NB	-3.85	1.33	1.40
24	o	601	HEC	CHA-C4D	3.84	1.48	1.39
20	U	601	HEM	CHA-C1A	3.82	1.48	1.39
16	L	601	HEA	CHA-C1A	3.79	1.45	1.38
16	I	601	HEA	CHA-C1A	3.78	1.45	1.38
20	U	602	HEM	CHD-C4C	3.77	1.45	1.38
16	I	602	HEA	CHB-C4A	3.75	1.45	1.38
16	L	602	HEA	CHB-C4A	3.74	1.45	1.38
20	j	603	HEM	C1B-NB	-3.72	1.33	1.40
24	o	601	HEC	C3C-C2C	3.68	1.48	1.38
20	i	606	HEM	C1B-NB	-3.67	1.34	1.40
22	V	602	9YF	O11-C25	3.64	1.44	1.33
20	U	601	HEM	CHC-C4B	3.55	1.47	1.39
22	V	602	9YF	P-O2	3.54	1.69	1.60
20	U	602	HEM	C4D-ND	-3.53	1.34	1.40
24	o	601	HEC	CHB-C1B	3.52	1.47	1.39
16	L	602	HEA	CHC-C1C	3.49	1.47	1.39
24	o	601	HEC	C4B-NB	-3.49	1.34	1.40
20	U	601	HEM	CHD-C1D	3.48	1.47	1.39
16	I	602	HEA	CHC-C1C	3.48	1.47	1.39
16	I	602	HEA	CHA-C4D	3.45	1.47	1.39
16	L	601	HEA	CHC-C1C	3.44	1.47	1.39
16	I	601	HEA	CHC-C1C	3.44	1.47	1.39
20	i	605	HEM	C4D-ND	-3.43	1.34	1.40
16	L	602	HEA	CHA-C4D	3.41	1.47	1.39
24	o	601	HEC	C4C-C3C	3.41	1.51	1.44
20	U	602	HEM	C4C-NC	-3.38	1.33	1.39
20	U	602	HEM	CHD-C1D	3.38	1.46	1.39
16	L	602	HEA	CHD-C4C	3.36	1.46	1.39
20	U	602	HEM	CHC-C4B	3.34	1.46	1.39
16	I	602	HEA	CHD-C4C	3.34	1.46	1.39
16	I	601	HEA	C1D-ND	-3.32	1.34	1.40
16	L	601	HEA	C1D-ND	-3.32	1.34	1.40
20	j	603	HEM	C4D-ND	-3.28	1.34	1.40
20	i	606	HEM	C4D-ND	-3.25	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	j	604	HEM	C4D-ND	-3.23	1.34	1.40
16	L	602	HEA	C1D-ND	-3.22	1.34	1.40
16	L	601	HEA	CHD-C4C	3.21	1.46	1.39
16	I	601	HEA	CHD-C4C	3.20	1.46	1.39
20	U	601	HEM	CHB-C4A	3.19	1.46	1.39
16	I	602	HEA	C1D-ND	-3.19	1.34	1.40
20	U	602	HEM	CHB-C4A	3.16	1.46	1.39
16	I	601	HEA	CHB-C1B	3.16	1.46	1.39
16	L	601	HEA	CHB-C1B	3.15	1.46	1.39
20	j	604	HEM	C1C-C2C	-3.14	1.39	1.45
24	o	601	HEC	C1D-ND	-3.11	1.34	1.40
20	i	605	HEM	C1C-C2C	-3.09	1.39	1.45
20	j	603	HEM	C1C-C2C	-3.09	1.39	1.45
24	o	602	HEC	FE-NC	3.08	2.05	1.95
20	U	601	HEM	C4D-ND	-3.07	1.35	1.40
20	U	601	HEM	C1B-NB	-3.03	1.35	1.40
16	I	601	HEA	CHA-C4D	3.02	1.46	1.39
16	L	601	HEA	C4B-NB	-3.01	1.35	1.40
16	L	601	HEA	CHA-C4D	3.00	1.46	1.39
16	I	601	HEA	C4B-NB	-2.99	1.35	1.40
20	U	602	HEM	C1B-NB	-2.99	1.35	1.40
16	I	602	HEA	C4B-NB	-2.95	1.35	1.40
20	i	606	HEM	C3C-C4C	-2.95	1.40	1.46
20	U	601	HEM	C4C-NC	-2.95	1.34	1.39
24	o	602	HEC	FE-NA	2.94	2.05	1.95
20	j	604	HEM	C3C-C4C	-2.92	1.40	1.46
16	L	602	HEA	C4B-NB	-2.90	1.35	1.40
20	U	602	HEM	C2A-C3A	2.90	1.46	1.38
20	U	601	HEM	C4A-NA	-2.90	1.34	1.39
20	U	602	HEM	C4B-NB	-2.89	1.32	1.38
16	I	602	HEA	CHB-C1B	2.81	1.45	1.39
16	L	602	HEA	CHB-C1B	2.79	1.45	1.39
16	L	602	HEA	C4C-NC	-2.77	1.34	1.39
20	i	606	HEM	C1C-C2C	-2.77	1.39	1.45
16	I	602	HEA	C4C-NC	-2.74	1.34	1.39
20	j	604	HEM	C4B-NB	-2.73	1.33	1.38
20	U	601	HEM	C2A-C3A	2.73	1.46	1.38
14	U	603	CDL	OB5-CB3	-2.69	1.34	1.44
20	U	602	HEM	C1A-NA	-2.68	1.34	1.39
20	U	602	HEM	C1C-NC	-2.65	1.34	1.39
16	I	601	HEA	C4C-NC	-2.60	1.34	1.39
16	L	601	HEA	C4C-NC	-2.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	i	606	HEM	C1A-C2A	-2.59	1.39	1.44
20	j	604	HEM	C1A-C2A	-2.58	1.39	1.44
24	o	601	HEC	C4A-NA	-2.58	1.34	1.39
20	U	601	HEM	C1A-NA	-2.57	1.34	1.39
20	U	602	HEM	C4A-NA	-2.51	1.34	1.39
20	i	605	HEM	FE-ND	-2.50	1.87	1.94
20	i	606	HEM	C4B-NB	-2.48	1.33	1.38
20	j	603	HEM	FE-ND	-2.48	1.87	1.94
16	I	602	HEA	C4B-C3B	2.44	1.48	1.44
24	o	601	HEC	C1C-NC	-2.42	1.35	1.39
20	j	604	HEM	O2D-CGD	-2.40	1.22	1.30
24	o	601	HEC	C1A-NA	-2.39	1.35	1.39
16	L	602	HEA	C4B-C3B	2.39	1.48	1.44
16	I	601	HEA	C1C-NC	-2.38	1.35	1.39
20	i	605	HEM	C4B-NB	-2.37	1.33	1.38
20	U	602	HEM	C1D-ND	-2.36	1.33	1.38
16	L	601	HEA	C1C-NC	-2.36	1.35	1.39
20	i	606	HEM	O2D-CGD	-2.35	1.22	1.30
20	j	604	HEM	FE-ND	-2.33	1.87	1.94
20	i	606	HEM	O2A-CGA	-2.31	1.23	1.30
20	j	603	HEM	C4B-NB	-2.31	1.34	1.38
20	U	601	HEM	C4B-NB	-2.28	1.34	1.38
20	i	606	HEM	FE-ND	-2.27	1.87	1.94
22	V	602	9YF	O9-C	2.25	1.52	1.46
16	I	601	HEA	C4B-C3B	2.24	1.48	1.44
16	L	601	HEA	C4B-C3B	2.24	1.48	1.44
16	I	601	HEA	C1C-C2C	2.22	1.48	1.43
20	j	603	HEM	C1D-ND	-2.20	1.34	1.38
20	j	604	HEM	O2A-CGA	-2.19	1.23	1.30
20	i	605	HEM	C1A-C2A	-2.17	1.40	1.44
16	L	601	HEA	C1C-C2C	2.17	1.48	1.43
20	i	605	HEM	C1D-ND	-2.17	1.34	1.38
16	L	602	HEA	O2D-CGD	-2.16	1.23	1.30
20	U	601	HEM	C1C-NC	-2.14	1.35	1.39
20	j	603	HEM	C1A-C2A	-2.13	1.40	1.44
24	o	601	HEC	C1D-C2D	2.12	1.48	1.44
16	I	602	HEA	O2D-CGD	-2.11	1.23	1.30
24	o	601	HEC	O2D-CGD	-2.09	1.23	1.30
16	L	602	HEA	C1C-C2C	2.07	1.48	1.43
16	I	602	HEA	C1C-C2C	2.07	1.48	1.43
16	I	602	HEA	C1C-NC	-2.04	1.35	1.39
20	U	602	HEM	O2A-CGA	-2.04	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	j	604	HEM	C1B-C2B	-2.03	1.40	1.44
16	L	602	HEA	C1C-NC	-2.02	1.35	1.39
20	i	605	HEM	O2D-CGD	-2.01	1.24	1.30
20	U	602	HEM	O2D-CGD	-2.01	1.24	1.30

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	602	HEM	C3B-C2B-C1B	-9.55	99.40	106.49
20	U	601	HEM	C3B-C2B-C1B	-7.98	100.57	106.49
20	j	604	HEM	CHC-C4B-NB	7.05	132.08	124.42
16	L	601	HEA	C3C-C4C-NC	7.00	114.56	110.25
16	I	601	HEA	C3C-C4C-NC	6.86	114.47	110.25
20	i	606	HEM	CHC-C4B-NB	6.65	131.65	124.42
20	U	601	HEM	C3C-C2C-C1C	-6.52	100.85	107.08
24	o	602	HEC	C1D-ND-C4D	6.38	111.66	105.07
20	U	602	HEM	C3C-C2C-C1C	-6.34	101.02	107.08
24	o	601	HEC	C1B-C2B-C3B	-6.19	100.45	106.96
16	L	602	HEA	C3C-C4C-NC	6.19	114.05	110.25
16	I	601	HEA	C3D-C4D-ND	6.17	116.33	110.36
16	L	601	HEA	C3D-C4D-ND	6.14	116.31	110.36
16	I	602	HEA	C3C-C4C-NC	5.99	113.93	110.25
16	L	602	HEA	C2B-C1B-NB	5.94	116.99	109.88
22	V	602	9YF	C14-C13-C12	-5.92	84.37	114.42
16	I	602	HEA	C2B-C1B-NB	5.90	116.95	109.88
16	I	601	HEA	C4A-NA-C1A	-5.80	99.67	105.35
16	L	601	HEA	C4A-NA-C1A	-5.77	99.69	105.35
16	L	601	HEA	C2D-C1D-ND	5.59	116.47	109.84
16	I	602	HEA	C3D-C4D-ND	5.57	115.75	110.36
16	L	602	HEA	C3D-C4D-ND	5.56	115.74	110.36
16	I	601	HEA	C2D-C1D-ND	5.56	116.43	109.84
20	j	604	HEM	CHD-C1D-ND	5.39	130.27	124.42
16	I	602	HEA	C3C-C2C-C1C	-5.25	100.82	107.16
22	V	602	9YF	O2-C2-C3	5.25	120.88	108.66
16	L	601	HEA	C2B-C1B-NB	5.23	116.15	109.88
16	L	602	HEA	C3C-C2C-C1C	-5.21	100.87	107.16
16	I	601	HEA	C2B-C1B-NB	5.21	116.13	109.88
16	I	601	HEA	C3C-C2C-C1C	-5.15	100.94	107.16
16	L	601	HEA	C3C-C2C-C1C	-5.14	100.96	107.16
16	I	602	HEA	C4A-NA-C1A	-5.10	100.35	105.35
16	L	602	HEA	C4A-NA-C1A	-5.08	100.37	105.35
20	i	606	HEM	CHD-C1D-ND	4.98	129.83	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	602	HEA	C2D-C1D-ND	4.96	115.72	109.84
24	o	601	HEC	CAC-C3C-C4C	4.96	131.80	124.92
16	I	602	HEA	C2D-C1D-ND	4.95	115.71	109.84
24	o	601	HEC	C2B-C1B-NB	4.89	115.74	109.88
16	I	601	HEA	C3B-C4B-NB	4.82	115.56	109.84
16	L	601	HEA	C3B-C4B-NB	4.81	115.54	109.84
20	U	601	HEM	C2B-C1B-NB	4.80	115.53	109.84
20	i	605	HEM	CHC-C4B-NB	4.73	129.55	124.42
20	j	603	HEM	CHC-C4B-NB	4.70	129.52	124.42
16	L	601	HEA	C1D-C2D-C3D	-4.67	102.05	106.96
16	I	602	HEA	C3B-C4B-NB	4.66	115.37	109.84
16	L	602	HEA	C3B-C4B-NB	4.65	115.35	109.84
20	j	603	HEM	CHD-C1D-ND	4.64	129.46	124.42
16	I	601	HEA	C1D-C2D-C3D	-4.59	102.14	106.96
20	j	604	HEM	C1B-NB-C4B	4.56	109.79	105.07
20	U	602	HEM	C1D-C2D-C3D	-4.56	102.16	106.96
24	o	601	HEC	C3D-C4D-ND	4.53	114.75	110.36
20	j	604	HEM	CAD-CBD-CGD	-4.52	103.88	113.60
20	i	606	HEM	C1B-NB-C4B	4.51	109.73	105.07
20	U	602	HEM	C2D-C1D-ND	4.50	115.27	109.88
20	i	605	HEM	CHD-C1D-ND	4.47	129.28	124.42
20	U	602	HEM	C2B-C1B-NB	4.46	115.13	109.84
16	I	601	HEA	C2A-C1A-NA	4.41	114.62	110.32
16	L	601	HEA	C2A-C1A-NA	4.41	114.61	110.32
20	U	601	HEM	C2D-C1D-ND	4.39	115.14	109.88
20	i	606	HEM	CAD-CBD-CGD	-4.32	104.30	113.60
24	o	601	HEC	C3C-C4C-NC	4.24	114.89	110.15
22	V	602	9YF	O9-C8-C9	4.12	120.38	111.50
20	U	602	HEM	C4A-C3A-C2A	-4.10	102.04	106.83
20	U	601	HEM	C3D-C4D-ND	4.06	114.69	110.17
16	I	602	HEA	C1D-C2D-C3D	-4.02	102.73	106.96
16	L	601	HEA	C2C-C1C-NC	4.02	116.19	110.08
22	V	602	9YF	C7-C2-C3	-4.00	105.08	110.85
16	L	602	HEA	C1D-C2D-C3D	-4.00	102.75	106.96
16	I	601	HEA	C2C-C1C-NC	3.98	116.15	110.08
16	I	602	HEA	C2A-C1A-NA	3.90	114.12	110.32
24	o	601	HEC	C2A-C1A-NA	3.88	114.10	110.32
20	j	603	HEM	C1B-NB-C4B	3.87	109.07	105.07
16	I	602	HEA	C2C-C1C-NC	3.87	115.97	110.08
16	L	602	HEA	C1B-C2B-C3B	-3.84	102.21	106.80
20	U	601	HEM	C2A-C1A-NA	3.84	114.44	110.15
16	L	602	HEA	C2C-C1C-NC	3.84	115.92	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	602	HEA	C2A-C1A-NA	3.84	114.06	110.32
20	i	605	HEM	C1B-NB-C4B	3.82	109.02	105.07
16	I	602	HEA	C1B-C2B-C3B	-3.78	102.28	106.80
16	I	601	HEA	C13-C12-C11	-3.74	108.73	114.35
16	L	601	HEA	C13-C12-C11	-3.71	108.77	114.35
20	U	601	HEM	C1D-C2D-C3D	-3.69	103.08	106.96
20	j	604	HEM	CHD-C1D-C2D	-3.60	119.36	124.98
20	U	602	HEM	C3A-C4A-NA	3.58	115.54	110.08
16	L	601	HEA	CBA-CAA-C2A	-3.58	102.68	112.63
16	I	601	HEA	C13-C14-C15	-3.58	119.04	127.66
16	I	601	HEA	CBA-CAA-C2A	-3.57	102.70	112.63
16	L	601	HEA	C13-C14-C15	-3.57	119.07	127.66
20	U	602	HEM	C3D-C4D-ND	3.55	114.12	110.17
24	o	601	HEC	C2C-C1C-NC	3.54	115.48	110.08
20	U	602	HEM	CBA-CAA-C2A	-3.53	102.83	112.63
22	V	602	9YF	C-O9-C8	-3.51	109.15	117.79
16	L	601	HEA	C1B-C2B-C3B	-3.50	102.61	106.80
16	I	601	HEA	C1B-C2B-C3B	-3.50	102.61	106.80
24	o	601	HEC	C4C-C3C-C2C	-3.49	101.40	106.89
24	o	601	HEC	CBB-CAB-C3B	3.49	122.04	112.43
20	U	601	HEM	C3A-C4A-NA	3.47	115.37	110.08
16	L	601	HEA	C27-C19-C20	3.44	121.06	115.27
24	o	601	HEC	CAA-C2A-C1A	3.43	131.36	124.89
16	I	601	HEA	C27-C19-C20	3.43	121.03	115.27
16	I	602	HEA	CHA-C1A-NA	-3.42	120.74	124.44
20	U	601	HEM	C4A-C3A-C2A	-3.41	102.84	106.83
22	V	602	9YF	C6-C7-C2	3.39	117.43	109.68
16	L	602	HEA	CHA-C1A-NA	-3.37	120.80	124.44
16	L	602	HEA	OMA-CMA-C3A	-3.36	118.09	125.69
22	V	602	9YF	C4-C3-C2	3.35	117.34	109.68
16	I	602	HEA	OMA-CMA-C3A	-3.35	118.11	125.69
20	i	606	HEM	CHD-C1D-C2D	-3.34	119.76	124.98
20	j	603	HEM	CHA-C4D-ND	3.27	128.40	124.37
20	j	603	HEM	CHB-C1B-NB	3.25	128.38	124.37
16	I	602	HEA	C3A-C2A-C1A	-3.25	103.98	107.08
24	o	601	HEC	CBA-CAA-C2A	-3.23	103.65	112.63
20	U	602	HEM	CHC-C1C-NC	-3.21	120.97	124.44
16	L	602	HEA	C3A-C2A-C1A	-3.18	104.04	107.08
20	U	602	HEM	C2A-C1A-NA	3.17	113.69	110.15
24	o	601	HEC	C3A-C4A-NA	3.16	115.51	109.69
20	i	605	HEM	CHB-C1B-NB	3.13	128.23	124.37
20	i	605	HEM	CHA-C4D-ND	3.11	128.21	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	601	HEA	C3A-C2A-C1A	-3.10	104.11	107.08
24	o	601	HEC	CMD-C2D-C1D	3.06	129.71	125.04
16	I	601	HEA	C3A-C2A-C1A	-3.06	104.15	107.08
20	U	601	HEM	C2C-C1C-NC	3.05	115.31	109.69
20	U	601	HEM	CAD-C3D-C4D	3.04	129.97	124.66
24	o	601	HEC	C4D-C3D-C2D	-2.98	102.55	106.90
20	U	601	HEM	CBA-CAA-C2A	-2.97	104.39	112.63
24	o	602	HEC	C4B-NB-C1B	2.96	108.13	105.07
16	L	602	HEA	C4D-C3D-C2D	-2.96	102.58	106.90
16	I	602	HEA	CAD-CBD-CGD	-2.96	107.23	113.60
16	I	602	HEA	C4D-C3D-C2D	-2.94	102.61	106.90
16	I	601	HEA	C4D-C3D-C2D	-2.92	102.64	106.90
16	I	602	HEA	CMD-C2D-C1D	2.90	129.46	125.04
16	L	601	HEA	C4D-C3D-C2D	-2.89	102.69	106.90
16	L	602	HEA	CMD-C2D-C1D	2.88	129.43	125.04
20	j	603	HEM	CHD-C1D-C2D	-2.88	120.47	124.98
24	o	601	HEC	C4A-C3A-C2A	-2.88	102.73	106.94
24	o	601	HEC	C1A-C2A-C3A	-2.87	103.39	107.13
24	o	602	HEC	C2A-C1A-NA	-2.86	107.54	110.32
20	i	605	HEM	C4C-NC-C1C	2.84	108.13	105.35
16	I	602	HEA	C27-C19-C20	2.84	120.04	115.27
20	U	602	HEM	C2C-C1C-NC	2.82	114.88	109.69
20	U	601	HEM	CAA-C2A-C1A	2.81	130.42	124.89
16	I	602	HEA	C17-C18-C19	-2.81	120.89	127.66
16	L	602	HEA	C17-C18-C19	-2.81	120.90	127.66
20	i	605	HEM	CHD-C1D-C2D	-2.80	120.61	124.98
16	I	602	HEA	C13-C12-C11	-2.80	110.15	114.35
20	j	604	HEM	CHA-C4D-ND	2.79	127.82	124.37
20	i	606	HEM	CHA-C4D-ND	2.79	127.81	124.37
13	G	101	9XX	O1-C17-C16	2.79	112.59	106.13
16	L	602	HEA	C27-C19-C20	2.79	119.96	115.27
16	L	602	HEA	CHA-C4D-ND	-2.79	121.39	124.42
24	o	602	HEC	C4A-NA-C1A	2.78	108.07	105.35
24	o	601	HEC	C1D-C2D-C3D	-2.77	104.05	106.96
20	i	605	HEM	O2A-CGA-CBA	2.75	122.88	114.03
16	I	602	HEA	CHA-C4D-ND	-2.75	121.43	124.42
20	U	601	HEM	C4D-C3D-C2D	-2.75	102.89	106.90
16	L	601	HEA	C4B-C3B-C2B	-2.72	102.76	107.41
16	L	602	HEA	CBA-CAA-C2A	-2.71	105.11	112.63
16	I	601	HEA	C4B-C3B-C2B	-2.70	102.79	107.41
16	L	602	HEA	CAD-CBD-CGD	-2.70	107.79	113.60
16	L	602	HEA	CHB-C1B-C2B	-2.70	120.76	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	602	HEM	CHB-C1B-NB	-2.69	121.05	124.37
16	I	602	HEA	C4B-C3B-C2B	-2.69	102.81	107.41
20	j	603	HEM	C4C-NC-C1C	2.68	107.98	105.35
20	i	606	HEM	CHD-C4C-NC	2.68	127.34	124.44
16	L	602	HEA	C13-C12-C11	-2.68	110.33	114.35
20	U	602	HEM	CMA-C3A-C4A	2.66	129.42	125.37
16	I	602	HEA	CHB-C1B-C2B	-2.66	120.83	124.98
20	i	606	HEM	CAA-CBA-CGA	-2.66	107.89	113.60
20	j	604	HEM	CHD-C4C-NC	2.65	127.31	124.44
16	I	602	HEA	CBA-CAA-C2A	-2.65	105.26	112.63
16	L	602	HEA	C4B-C3B-C2B	-2.64	102.90	107.41
24	o	601	HEC	C2D-C1D-ND	2.64	112.97	109.84
20	U	601	HEM	CMA-C3A-C4A	2.63	129.37	125.37
16	L	602	HEA	CAD-C3D-C4D	2.63	129.25	124.66
24	o	601	HEC	CHD-C4C-NC	-2.62	119.03	123.85
16	I	602	HEA	CAD-C3D-C4D	2.62	129.23	124.66
16	L	601	HEA	CMB-C2B-C1B	2.62	129.02	125.04
24	o	601	HEC	CMA-C3A-C4A	2.60	129.30	124.71
20	j	604	HEM	CAA-CBA-CGA	-2.60	108.00	113.60
20	j	603	HEM	O2A-CGA-CBA	2.60	122.39	114.03
20	i	606	HEM	CHB-C1B-NB	2.59	127.57	124.37
16	I	601	HEA	CMC-C2C-C1C	2.59	129.32	125.37
16	I	601	HEA	CMB-C2B-C1B	2.59	128.99	125.04
16	L	602	HEA	C25-C23-C24	2.59	120.32	114.60
22	V	602	9YF	O11-C25-C26	2.58	120.01	111.91
24	o	601	HEC	CBC-CAC-C3C	2.58	119.54	112.43
16	L	601	HEA	CMC-C2C-C1C	2.58	129.30	125.37
24	o	602	HEC	C4C-NC-C1C	2.58	107.87	105.35
20	j	604	HEM	CHB-C1B-NB	2.57	127.55	124.37
20	U	602	HEM	C4C-C3C-C2C	-2.57	104.64	106.75
24	o	601	HEC	CHA-C1A-NA	-2.55	121.68	124.44
20	i	606	HEM	CBA-CAA-C2A	-2.55	105.53	112.63
24	o	602	HEC	CAC-C3C-C2C	2.54	130.94	126.86
24	o	602	HEC	CAD-CBD-CGD	-2.54	108.13	113.60
20	U	601	HEM	CMD-C2D-C1D	2.53	128.90	125.04
20	U	602	HEM	CAA-C2A-C1A	2.53	129.86	124.89
16	I	601	HEA	C1D-ND-C4D	-2.52	102.47	105.07
16	L	601	HEA	CAD-CBD-CGD	-2.51	108.20	113.60
24	o	601	HEC	C1C-C2C-C3C	-2.50	103.90	106.83
16	I	602	HEA	CAA-C2A-C1A	2.50	129.61	124.89
16	L	601	HEA	C1D-ND-C4D	-2.50	102.49	105.07
16	I	602	HEA	C25-C23-C24	2.50	120.12	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	602	HEA	CAA-C2A-C1A	2.47	129.56	124.89
20	U	602	HEM	CHD-C1D-ND	-2.45	121.75	124.42
16	L	602	HEA	C4B-NB-C1B	-2.45	102.54	105.07
20	U	601	HEM	C1A-C2A-C3A	-2.45	103.04	106.89
20	i	606	HEM	C4A-NA-C1A	2.44	107.74	105.35
16	I	601	HEA	CAD-CBD-CGD	-2.44	108.35	113.60
16	L	602	HEA	C21-C22-C23	-2.44	119.43	127.75
24	o	601	HEC	CHB-C1B-C2B	-2.43	121.17	124.98
16	L	601	HEA	CHA-C4D-C3D	-2.43	121.26	124.84
24	o	601	HEC	CAD-C3D-C4D	2.42	128.90	124.66
16	I	601	HEA	CHA-C4D-C3D	-2.41	121.29	124.84
20	i	606	HEM	C4C-NC-C1C	2.41	107.71	105.35
16	I	602	HEA	C4B-NB-C1B	-2.41	102.58	105.07
20	i	606	HEM	CHA-C1A-NA	2.40	128.26	123.85
22	p	601	9YF	P-O2-C2	2.39	128.09	119.41
24	o	602	HEC	CAC-C3C-C4C	-2.37	121.62	124.92
16	L	602	HEA	C13-C14-C15	-2.37	121.95	127.66
20	i	606	HEM	O2A-CGA-CBA	2.37	121.63	114.03
20	U	602	HEM	CBD-CAD-C3D	-2.36	106.08	112.63
20	j	604	HEM	C4A-NA-C1A	2.35	107.65	105.35
16	L	601	HEA	CHD-C1D-C2D	-2.35	120.20	126.73
16	L	601	HEA	C26-C15-C16	2.35	119.22	115.27
16	L	602	HEA	CMB-C2B-C1B	2.34	128.61	125.04
16	I	602	HEA	C13-C14-C15	-2.34	122.02	127.66
20	U	601	HEM	CHC-C1C-NC	-2.34	121.91	124.44
16	I	601	HEA	C26-C15-C16	2.33	119.19	115.27
16	I	601	HEA	CHD-C1D-C2D	-2.32	120.28	126.73
16	L	601	HEA	CHB-C1B-C2B	-2.32	121.36	124.98
16	L	601	HEA	C17-C18-C19	-2.31	122.09	127.66
16	I	601	HEA	C17-C18-C19	-2.31	122.10	127.66
16	I	602	HEA	CMC-C2C-C1C	2.31	128.88	125.37
16	I	602	HEA	CMB-C2B-C1B	2.31	128.55	125.04
20	i	606	HEM	C1A-CHA-C4D	-2.30	120.89	126.34
16	I	601	HEA	CHB-C1B-C2B	-2.29	121.40	124.98
24	o	602	HEC	C3B-C4B-NB	-2.28	107.62	110.17
23	i	611	MQ9	C7-C6-C1	2.28	120.94	118.50
16	I	601	HEA	C25-C23-C24	2.27	119.62	114.60
20	j	603	HEM	C4D-ND-C1D	2.27	107.42	105.07
20	j	604	HEM	C1A-CHA-C4D	-2.27	120.95	126.34
16	L	602	HEA	CMC-C2C-C1C	2.26	128.81	125.37
16	L	601	HEA	C25-C23-C24	2.26	119.60	114.60
20	j	604	HEM	O2A-CGA-CBA	2.26	121.28	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	602	HEM	CMD-C2D-C1D	2.23	128.43	125.04
20	j	603	HEM	O2D-CGD-CBD	2.23	121.19	114.03
20	U	602	HEM	C4D-C3D-C2D	-2.22	103.66	106.90
20	U	602	HEM	CMB-C2B-C1B	2.22	128.41	125.04
20	j	604	HEM	C4C-CHD-C1D	-2.20	121.31	126.06
16	I	602	HEA	C21-C22-C23	-2.19	120.27	127.75
20	i	605	HEM	O2A-CGA-O1A	-2.19	117.85	123.30
24	o	601	HEC	CMC-C2C-C3C	2.18	130.33	125.61
24	o	601	HEC	CMB-C2B-C3B	2.18	132.03	126.12
20	j	604	HEM	CHA-C1A-NA	2.17	127.83	123.85
16	I	601	HEA	OMA-CMA-C3A	-2.16	120.79	125.69
20	i	605	HEM	O2D-CGD-CBD	2.16	120.96	114.03
16	L	601	HEA	OMA-CMA-C3A	-2.16	120.81	125.69
20	U	601	HEM	CMC-C2C-C1C	2.15	128.51	124.71
20	i	605	HEM	C4D-ND-C1D	2.14	107.28	105.07
20	U	601	HEM	CHD-C1D-ND	-2.11	122.12	124.42
20	j	604	HEM	CHC-C4B-C3B	-2.11	120.58	125.13
24	o	602	HEC	C3D-C4D-ND	-2.11	108.31	110.36
16	I	601	HEA	C4B-NB-C1B	-2.10	102.91	105.07
20	j	603	HEM	C4C-CHD-C1D	-2.10	121.54	126.06
16	I	602	HEA	CHC-C1C-C2C	-2.09	121.34	127.24
20	j	604	HEM	CBA-CAA-C2A	-2.09	106.83	112.63
20	i	606	HEM	C2A-C1A-NA	-2.08	107.82	110.15
16	L	601	HEA	C4B-NB-C1B	-2.08	102.93	105.07
20	i	606	HEM	O2D-CGD-CBD	2.07	120.68	114.03
20	j	603	HEM	O2A-CGA-O1A	-2.07	118.15	123.30
22	V	602	9YF	O3-C3-C2	-2.06	104.49	109.94
16	L	602	HEA	CHC-C1C-C2C	-2.06	121.43	127.24
20	i	605	HEM	C4C-CHD-C1D	-2.04	121.66	126.06
20	i	606	HEM	O2A-CGA-O1A	-2.03	118.24	123.30
16	I	602	HEA	C26-C15-C16	2.03	118.69	115.27
24	o	602	HEC	CHB-C1B-NB	2.03	126.62	124.42
20	U	602	HEM	CMC-C2C-C1C	2.02	128.28	124.71
16	I	601	HEA	CHC-C1C-C2C	-2.02	121.52	127.24
16	I	602	HEA	CHB-C1B-NB	-2.02	122.22	124.42
16	L	601	HEA	CHC-C1C-C2C	-2.02	121.54	127.24
16	L	602	HEA	C26-C15-C16	2.01	118.65	115.27
16	I	602	HEA	C1A-CHA-C4D	-2.01	121.73	126.06
16	L	602	HEA	CHB-C1B-NB	-2.00	122.24	124.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	o	601	HEC	NA
24	o	602	HEC	NA

All (970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	b	102	9XX	O-C16-C17-C37
13	b	102	9XX	O-C16-C17-O1
13	b	102	9XX	C36-C27-C28-C29
13	j	610	9XX	O-C16-C17-C37
14	G	102	CDL	CA3-OA5-PA1-OA4
14	G	102	CDL	C11-CA5-OA6-CA4
14	G	102	CDL	CB2-OB2-PB2-OB5
14	I	605	CDL	O1-C1-CB2-OB2
14	I	605	CDL	CA2-OA2-PA1-OA5
14	L	605	CDL	CB2-OB2-PB2-OB3
14	L	605	CDL	CB2-OB2-PB2-OB4
14	L	605	CDL	CB2-OB2-PB2-OB5
14	L	606	CDL	CA2-OA2-PA1-OA3
14	U	603	CDL	CA2-OA2-PA1-OA3
14	U	603	CDL	CA3-OA5-PA1-OA4
14	U	603	CDL	C11-CA5-OA6-CA4
14	U	603	CDL	CB2-OB2-PB2-OB3
14	U	603	CDL	CB2-OB2-PB2-OB4
14	U	603	CDL	CB3-OB5-PB2-OB2
14	U	603	CDL	CB3-OB5-PB2-OB3
14	U	603	CDL	CB3-OB5-PB2-OB4
14	b	103	CDL	CA3-OA5-PA1-OA2
14	b	103	CDL	CA3-OA5-PA1-OA3
14	b	103	CDL	CA3-OA5-PA1-OA4
14	b	103	CDL	CB3-OB5-PB2-OB2
14	i	604	CDL	C11-CA5-OA6-CA4
14	i	604	CDL	OB6-CB4-CB6-OB8
14	i	607	CDL	CB3-OB5-PB2-OB3
14	i	607	CDL	CB3-OB5-PB2-OB4
14	i	607	CDL	C51-CB5-OB6-CB4
14	i	608	CDL	CB3-OB5-PB2-OB4
14	i	609	CDL	CA3-OA5-PA1-OA2
14	i	609	CDL	CA3-OA5-PA1-OA3
14	i	609	CDL	CB2-OB2-PB2-OB5
14	i	614	CDL	OA9-CA7-OA8-CA6
14	i	614	CDL	C31-CA7-OA8-CA6
14	i	614	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
14	j	606	CDL	CA2-OA2-PA1-OA5
14	j	606	CDL	CA3-OA5-PA1-OA3
14	j	606	CDL	C11-CA5-OA6-CA4
14	j	606	CDL	CB2-OB2-PB2-OB5
14	j	606	CDL	C51-CB5-OB6-CB4
14	j	609	CDL	CB2-OB2-PB2-OB3
14	j	609	CDL	CB3-OB5-PB2-OB2
14	j	609	CDL	C51-CB5-OB6-CB4
14	m	202	CDL	C11-CA5-OA6-CA4
14	p	603	CDL	CA2-OA2-PA1-OA4
14	p	603	CDL	OA7-CA5-OA6-CA4
14	p	603	CDL	C11-CA5-OA6-CA4
15	b	101	9Y0	O4-C5-O5-C
15	b	101	9Y0	C2-O3-P-O
15	b	104	9Y0	O1-C3-C4-N
15	f	601	9Y0	C22-C21-O7-C1
15	f	601	9Y0	C3-O1-P-O2
15	f	601	9Y0	C2-O3-P-O2
15	g	302	9Y0	C22-C21-O7-C1
15	q	301	9Y0	C3-O1-P-O3
16	I	601	HEA	C15-C16-C17-C18
16	I	602	HEA	C2A-C3A-CMA-OMA
16	I	602	HEA	C4A-C3A-CMA-OMA
16	I	602	HEA	C19-C20-C21-C22
16	L	601	HEA	C15-C16-C17-C18
16	L	602	HEA	C2A-C3A-CMA-OMA
16	L	602	HEA	C4A-C3A-CMA-OMA
20	j	604	HEM	C3D-CAD-CBD-CGD
22	n	201	9YF	C3-C2-O2-P
22	n	201	9YF	C7-C2-O2-P
22	n	201	9YF	C-C1-O-P
22	o	603	9YF	C1-O-P-O2
22	o	603	9YF	C3-C2-O2-P
22	o	603	9YF	C-C1-O-P
22	o	603	9YF	C26-C25-O11-C24
22	o	603	9YF	O12-C25-O11-C24
23	i	602	MQ9	C12-C13-C14-C15
23	i	602	MQ9	C12-C13-C14-C16
23	i	602	MQ9	C27-C28-C29-C30
23	i	602	MQ9	C27-C28-C29-C31
23	i	602	MQ9	C29-C31-C32-C33
23	i	602	MQ9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
23	i	602	MQ9	C34-C36-C37-C38
23	i	602	MQ9	C37-C38-C39-C40
23	i	602	MQ9	C37-C38-C39-C41
23	i	603	MQ9	C5-C6-C7-C8
23	i	603	MQ9	C1-C6-C7-C8
23	i	603	MQ9	C12-C13-C14-C15
23	i	603	MQ9	C12-C13-C14-C16
23	i	603	MQ9	C14-C16-C17-C18
23	i	603	MQ9	C32-C33-C34-C35
23	i	603	MQ9	C32-C33-C34-C36
23	i	610	MQ9	C16-C17-C18-C19
23	i	610	MQ9	C21-C22-C23-C24
23	i	610	MQ9	C22-C23-C24-C25
23	i	610	MQ9	C22-C23-C24-C26
23	i	611	MQ9	C5-C6-C7-C8
23	i	611	MQ9	C1-C6-C7-C8
23	i	611	MQ9	C26-C27-C28-C29
23	i	611	MQ9	C27-C28-C29-C30
23	i	611	MQ9	C27-C28-C29-C31
23	i	611	MQ9	C37-C38-C39-C41
23	i	612	MQ9	C5-C6-C7-C8
23	i	612	MQ9	C1-C6-C7-C8
23	i	612	MQ9	C7-C8-C9-C10
23	i	612	MQ9	C7-C8-C9-C11
23	i	612	MQ9	C12-C13-C14-C15
23	i	612	MQ9	C12-C13-C14-C16
23	i	612	MQ9	C19-C21-C22-C23
23	i	612	MQ9	C27-C28-C29-C30
23	i	612	MQ9	C27-C28-C29-C31
23	i	612	MQ9	C29-C31-C32-C33
23	i	612	MQ9	C32-C33-C34-C36
23	i	612	MQ9	C41-C42-C43-C44
23	j	602	MQ9	C12-C13-C14-C15
23	j	602	MQ9	C12-C13-C14-C16
23	j	602	MQ9	C27-C28-C29-C30
23	j	602	MQ9	C32-C33-C34-C35
23	j	602	MQ9	C32-C33-C34-C36
23	j	602	MQ9	C37-C38-C39-C40
23	j	602	MQ9	C37-C38-C39-C41
23	j	607	MQ9	C12-C11-C9-C10
23	j	607	MQ9	C17-C18-C19-C20
23	j	607	MQ9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
23	j	607	MQ9	C22-C23-C24-C26
23	j	608	MQ9	C7-C8-C9-C10
23	j	608	MQ9	C7-C8-C9-C11
23	j	608	MQ9	C12-C13-C14-C16
23	j	608	MQ9	C20-C19-C21-C22
23	j	611	MQ9	C27-C28-C29-C30
23	j	611	MQ9	C27-C28-C29-C31
23	j	611	MQ9	C29-C31-C32-C33
23	j	611	MQ9	C37-C38-C39-C40
23	j	611	MQ9	C37-C38-C39-C41
23	j	611	MQ9	C42-C43-C44-C45
23	j	611	MQ9	C42-C43-C44-C46
23	m	201	MQ9	C5-C6-C7-C8
23	m	201	MQ9	C1-C6-C7-C8
23	m	201	MQ9	C27-C28-C29-C31
14	g	301	CDL	OB9-CB7-OB8-CB6
14	g	301	CDL	C71-CB7-OB8-CB6
23	i	611	MQ9	C37-C38-C39-C40
24	o	601	HEC	C2B-C3B-CAB-CBB
24	o	601	HEC	C4B-C3B-CAB-CBB
14	i	607	CDL	OB9-CB7-OB8-CB6
24	o	601	HEC	C4C-C3C-CAC-CBC
24	o	601	HEC	C2C-C3C-CAC-CBC
14	G	102	CDL	OA7-CA5-OA6-CA4
14	U	603	CDL	OA7-CA5-OA6-CA4
14	i	604	CDL	OA7-CA5-OA6-CA4
14	i	607	CDL	OB7-CB5-OB6-CB4
14	j	606	CDL	OA7-CA5-OA6-CA4
14	j	606	CDL	OB7-CB5-OB6-CB4
14	j	609	CDL	OB7-CB5-OB6-CB4
14	m	202	CDL	OA7-CA5-OA6-CA4
14	p	603	CDL	OB7-CB5-OB6-CB4
15	f	601	9Y0	O6-C21-O7-C1
15	g	302	9Y0	O6-C21-O7-C1
14	i	607	CDL	C71-CB7-OB8-CB6
15	b	101	9Y0	C6-C5-O5-C
14	i	614	CDL	C11-CA5-OA6-CA4
23	j	611	MQ9	C47-C48-C49-C51
23	i	602	MQ9	C33-C34-C36-C37
15	g	302	9Y0	C12-C13-C14-C15
23	i	610	MQ9	C7-C8-C9-C10
23	i	611	MQ9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	i	611	MQ9	C17-C18-C19-C20
23	i	611	MQ9	C32-C33-C34-C35
23	i	612	MQ9	C22-C23-C24-C25
23	i	612	MQ9	C32-C33-C34-C35
23	j	602	MQ9	C7-C8-C9-C10
23	j	602	MQ9	C17-C18-C19-C20
23	j	607	MQ9	C7-C8-C9-C10
23	j	607	MQ9	C22-C23-C24-C25
23	j	607	MQ9	C27-C28-C29-C30
23	j	608	MQ9	C12-C13-C14-C15
23	m	201	MQ9	C27-C28-C29-C30
23	m	201	MQ9	C32-C33-C34-C35
14	i	614	CDL	OA7-CA5-OA6-CA4
23	i	611	MQ9	C12-C13-C14-C16
23	i	611	MQ9	C17-C18-C19-C21
23	i	611	MQ9	C32-C33-C34-C36
23	i	612	MQ9	C22-C23-C24-C26
23	j	602	MQ9	C7-C8-C9-C11
23	j	602	MQ9	C17-C18-C19-C21
23	j	602	MQ9	C27-C28-C29-C31
23	j	607	MQ9	C7-C8-C9-C11
23	j	607	MQ9	C27-C28-C29-C31
23	m	201	MQ9	C32-C33-C34-C36
14	U	603	CDL	O1-C1-CB2-OB2
13	G	101	9XX	C19-C18-O1-C17
14	i	609	CDL	C51-CB5-OB6-CB4
14	p	603	CDL	C51-CB5-OB6-CB4
14	p	603	CDL	C71-C72-C73-C74
14	L	605	CDL	C59-C60-C61-C62
14	i	609	CDL	CA4-CA3-OA5-PA1
20	i	606	HEM	C3D-CAD-CBD-CGD
23	j	607	MQ9	C32-C33-C34-C36
23	j	611	MQ9	C47-C48-C49-C50
16	I	602	HEA	C26-C15-C16-C17
16	L	602	HEA	C26-C15-C16-C17
23	i	602	MQ9	C15-C14-C16-C17
23	i	602	MQ9	C25-C24-C26-C27
23	i	602	MQ9	C30-C29-C31-C32
23	i	602	MQ9	C40-C39-C41-C42
23	i	603	MQ9	C30-C29-C31-C32
23	i	603	MQ9	C40-C39-C41-C42
23	i	603	MQ9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
23	i	610	MQ9	C30-C29-C31-C32
23	i	612	MQ9	C20-C19-C21-C22
23	i	612	MQ9	C25-C24-C26-C27
23	i	612	MQ9	C40-C39-C41-C42
23	j	607	MQ9	C15-C14-C16-C17
23	j	607	MQ9	C30-C29-C31-C32
23	j	611	MQ9	C15-C14-C16-C17
23	j	611	MQ9	C25-C24-C26-C27
23	j	611	MQ9	C30-C29-C31-C32
23	j	611	MQ9	C40-C39-C41-C42
23	m	201	MQ9	C12-C11-C9-C10
23	m	201	MQ9	C15-C14-C16-C17
23	m	201	MQ9	C30-C29-C31-C32
16	I	602	HEA	C14-C15-C16-C17
16	L	602	HEA	C14-C15-C16-C17
23	i	602	MQ9	C13-C14-C16-C17
23	i	602	MQ9	C23-C24-C26-C27
23	i	602	MQ9	C28-C29-C31-C32
23	i	602	MQ9	C38-C39-C41-C42
23	i	603	MQ9	C28-C29-C31-C32
23	i	603	MQ9	C38-C39-C41-C42
23	i	603	MQ9	C43-C44-C46-C47
23	i	610	MQ9	C28-C29-C31-C32
23	i	612	MQ9	C18-C19-C21-C22
23	i	612	MQ9	C23-C24-C26-C27
23	i	612	MQ9	C38-C39-C41-C42
23	j	607	MQ9	C12-C11-C9-C8
23	j	607	MQ9	C13-C14-C16-C17
23	j	607	MQ9	C28-C29-C31-C32
23	j	608	MQ9	C18-C19-C21-C22
23	j	611	MQ9	C13-C14-C16-C17
23	j	611	MQ9	C23-C24-C26-C27
23	j	611	MQ9	C28-C29-C31-C32
23	j	611	MQ9	C38-C39-C41-C42
23	m	201	MQ9	C12-C11-C9-C8
23	m	201	MQ9	C13-C14-C16-C17
23	m	201	MQ9	C28-C29-C31-C32
23	i	602	MQ9	C14-C16-C17-C18
23	i	602	MQ9	C39-C41-C42-C43
23	i	610	MQ9	C14-C16-C17-C18
23	i	612	MQ9	C39-C41-C42-C43
23	j	602	MQ9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	j	608	MQ9	C14-C16-C17-C18
23	j	611	MQ9	C9-C11-C12-C13
23	j	611	MQ9	C14-C16-C17-C18
23	j	611	MQ9	C19-C21-C22-C23
23	j	611	MQ9	C24-C26-C27-C28
23	j	611	MQ9	C39-C41-C42-C43
14	g	301	CDL	C16-C17-C18-C19
14	i	608	CDL	C51-CB5-OB6-CB4
23	m	201	MQ9	C7-C8-C9-C10
14	I	605	CDL	CA2-C1-CB2-OB2
14	L	605	CDL	CA2-C1-CB2-OB2
14	i	608	CDL	CB2-C1-CA2-OA2
14	j	605	CDL	CB2-C1-CA2-OA2
13	G	101	9XX	O2-C18-O1-C17
23	i	610	MQ9	C7-C8-C9-C11
23	j	607	MQ9	C12-C13-C14-C16
23	m	201	MQ9	C7-C8-C9-C11
23	m	201	MQ9	C22-C23-C24-C26
14	G	102	CDL	C31-CA7-OA8-CA6
14	i	604	CDL	C71-CB7-OB8-CB6
22	n	201	9YF	C2-O2-P-O
13	b	102	9XX	C16-C17-O1-C18
14	m	202	CDL	CB5-C51-C52-C53
14	L	606	CDL	OA6-CA4-CA6-OA8
14	i	609	CDL	OB7-CB5-OB6-CB4
14	p	603	CDL	C74-C75-C76-C77
14	L	605	CDL	CA5-C11-C12-C13
14	i	604	CDL	OB9-CB7-OB8-CB6
14	L	605	CDL	CA7-C31-C32-C33
22	i	601	9YF	C33-C35-C36-C37
23	j	602	MQ9	C47-C48-C49-C51
23	m	201	MQ9	C22-C23-C24-C25
13	b	102	9XX	C12-C13-C14-C15
13	j	610	9XX	C12-C13-C14-C15
14	L	605	CDL	CB7-C71-C72-C73
14	j	609	CDL	CB7-C71-C72-C73
22	p	601	9YF	C11-C10-C9-C8
13	i	613	9XX	C14-C15-O-C16
14	i	614	CDL	C71-CB7-OB8-CB6
14	g	301	CDL	C1-CB2-OB2-PB2
13	G	101	9XX	C26-C27-C28-C29
14	G	102	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	L	602	HEA	C19-C20-C21-C22
23	i	602	MQ9	C9-C11-C12-C13
23	i	602	MQ9	C24-C26-C27-C28
23	i	611	MQ9	C24-C26-C27-C28
23	j	608	MQ9	C24-C26-C27-C28
23	j	608	MQ9	C29-C31-C32-C33
13	G	101	9XX	C12-C13-C14-C15
23	j	607	MQ9	C32-C33-C34-C35
14	p	603	CDL	C76-C77-C78-C79
22	i	601	9YF	C10-C11-C12-C13
14	L	605	CDL	O1-C1-CB2-OB2
14	b	103	CDL	O1-C1-CB2-OB2
15	q	301	9Y0	C5-C6-C7-C8
13	i	613	9XX	O6-C15-O-C16
14	g	301	CDL	C51-CB5-OB6-CB4
14	G	102	CDL	CA3-OA5-PA1-OA2
14	I	604	CDL	CA3-OA5-PA1-OA2
14	L	605	CDL	CA3-OA5-PA1-OA2
14	U	603	CDL	CA2-OA2-PA1-OA5
14	U	603	CDL	CB2-OB2-PB2-OB5
14	i	607	CDL	CB3-OB5-PB2-OB2
14	i	608	CDL	CB3-OB5-PB2-OB2
14	i	614	CDL	CB2-OB2-PB2-OB5
14	j	605	CDL	CB3-OB5-PB2-OB2
14	j	609	CDL	CA2-OA2-PA1-OA5
15	f	601	9Y0	C2-O3-P-O1
22	n	201	9YF	C1-O-P-O2
14	L	606	CDL	CB5-C51-C52-C53
14	I	605	CDL	C53-C54-C55-C56
14	U	603	CDL	CA2-C1-CB2-OB2
14	b	103	CDL	CA2-C1-CB2-OB2
14	g	301	CDL	OB7-CB5-OB6-CB4
14	i	608	CDL	OB7-CB5-OB6-CB4
23	j	611	MQ9	C12-C13-C14-C16
22	j	601	9YF	C30-C31-C32-C33
15	q	301	9Y0	C6-C5-O5-C
22	V	602	9YF	C25-C26-C27-C28
14	i	604	CDL	C52-C53-C54-C55
14	L	605	CDL	C51-CB5-OB6-CB4
14	U	603	CDL	C11-C12-C13-C14
14	U	603	CDL	C54-C55-C56-C57
14	U	603	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
14	i	608	CDL	C16-C17-C18-C19
14	L	605	CDL	OB7-CB5-OB6-CB4
14	I	604	CDL	C31-C32-C33-C34
14	U	603	CDL	C78-C79-C80-C81
14	g	301	CDL	C72-C73-C74-C75
18	q	302	PLM	C4-C5-C6-C7
14	i	608	CDL	O1-C1-CA2-OA2
14	i	609	CDL	O1-C1-CB2-OB2
14	j	605	CDL	O1-C1-CA2-OA2
14	m	202	CDL	O1-C1-CA2-OA2
14	m	202	CDL	O1-C1-CB2-OB2
14	L	606	CDL	C60-C61-C62-C63
14	p	603	CDL	CB5-C51-C52-C53
22	V	602	9YF	C11-C10-C9-C8
14	b	103	CDL	C31-CA7-OA8-CA6
14	G	102	CDL	C83-C84-C85-C86
14	L	605	CDL	C55-C56-C57-C58
14	i	614	CDL	OB9-CB7-OB8-CB6
14	L	605	CDL	C37-C38-C39-C40
14	j	606	CDL	C73-C74-C75-C76
14	U	603	CDL	C12-C13-C14-C15
14	U	603	CDL	C74-C75-C76-C77
13	G	101	9XX	C31-C32-C33-C34
13	j	610	9XX	C11-C12-C13-C14
14	L	605	CDL	C31-C32-C33-C34
22	V	602	9YF	C18-C19-C20-C21
23	j	602	MQ9	C47-C48-C49-C50
14	I	605	CDL	C71-C72-C73-C74
14	U	603	CDL	C57-C58-C59-C60
14	j	606	CDL	C74-C75-C76-C77
15	G	103	9Y0	C26-C27-C28-C29
22	j	601	9YF	C15-C16-C17-C18
14	L	605	CDL	C56-C57-C58-C59
14	L	605	CDL	C77-C78-C79-C80
14	U	603	CDL	C32-C33-C34-C35
22	V	602	9YF	C17-C18-C19-C20
14	i	614	CDL	C56-C57-C58-C59
22	V	602	9YF	C39-C40-C41-C42
14	i	607	CDL	CB7-C71-C72-C73
14	U	603	CDL	C82-C83-C84-C85
14	j	605	CDL	C56-C57-C58-C59
15	g	302	9Y0	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	b	103	CDL	C79-C80-C81-C82
14	G	102	CDL	C34-C35-C36-C37
22	p	601	9YF	C9-C10-C11-C12
14	L	605	CDL	C51-C52-C53-C54
14	i	607	CDL	CA7-C31-C32-C33
13	b	102	9XX	C37-C17-O1-C18
14	L	605	CDL	C32-C33-C34-C35
18	q	302	PLM	C6-C7-C8-C9
22	o	603	9YF	C28-C29-C30-C31
15	G	103	9Y0	C10-C11-C12-C13
23	j	607	MQ9	C12-C13-C14-C15
15	q	301	9Y0	O4-C5-O5-C
14	i	609	CDL	C31-CA7-OA8-CA6
14	p	603	CDL	C13-C14-C15-C16
23	i	612	MQ9	C17-C18-C19-C21
14	p	603	CDL	C36-C37-C38-C39
22	V	602	9YF	C37-C38-C39-C40
22	n	201	9YF	C35-C36-C37-C38
14	i	609	CDL	C54-C55-C56-C57
22	p	601	9YF	C15-C16-C17-C18
14	i	607	CDL	C51-C52-C53-C54
14	i	614	CDL	C53-C54-C55-C56
14	b	103	CDL	OA9-CA7-OA8-CA6
22	p	601	9YF	C26-C25-O11-C24
14	m	202	CDL	C34-C35-C36-C37
22	V	602	9YF	C13-C14-C15-C16
14	I	604	CDL	CA7-C31-C32-C33
15	f	601	9Y0	C21-C22-C23-C24
24	o	602	HEC	C2C-C3C-CAC-CBC
14	I	605	CDL	C57-C58-C59-C60
14	L	605	CDL	C57-C58-C59-C60
14	i	614	CDL	C71-C72-C73-C74
22	V	602	9YF	C29-C30-C31-C32
22	j	601	9YF	C29-C30-C31-C32
20	i	605	HEM	C2B-C3B-CAB-CBB
13	j	610	9XX	C37-C17-O1-C18
14	I	605	CDL	C77-C78-C79-C80
23	m	201	MQ9	C29-C31-C32-C33
14	m	202	CDL	C11-C12-C13-C14
13	b	102	9XX	C19-C18-O1-C17
14	U	603	CDL	C51-CB5-OB6-CB4
15	G	103	9Y0	C22-C21-O7-C1

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Mol	Chain	Res	Type	Atoms
22	p	601	9YF	C28-C29-C30-C31
14	U	603	CDL	C77-C78-C79-C80
13	b	102	9XX	O2-C18-O1-C17
15	G	103	9Y0	O6-C21-O7-C1
14	G	102	CDL	OB6-CB4-CB6-OB8
14	i	607	CDL	OA6-CA4-CA6-OA8
14	j	609	CDL	OA6-CA4-CA6-OA8
14	G	102	CDL	C77-C78-C79-C80
14	i	609	CDL	OA9-CA7-OA8-CA6
15	b	101	9Y0	C6-C7-C8-C9
14	L	605	CDL	C71-C72-C73-C74
13	G	101	9XX	C36-C27-C28-C29
14	I	604	CDL	C51-C52-C53-C54
14	I	605	CDL	C74-C75-C76-C77
14	L	606	CDL	C71-CB7-OB8-CB6
14	L	606	CDL	C51-CB5-OB6-CB4
14	G	102	CDL	CA2-OA2-PA1-OA5
14	L	605	CDL	CA2-OA2-PA1-OA5
14	U	603	CDL	CA3-OA5-PA1-OA2
15	f	601	9Y0	C3-O1-P-O3
14	U	603	CDL	CB5-C51-C52-C53
14	G	102	CDL	C1-CA2-OA2-PA1
14	i	614	CDL	C1-CA2-OA2-PA1
14	G	102	CDL	OB5-CB3-CB4-CB6
14	L	605	CDL	OB5-CB3-CB4-CB6
15	g	302	9Y0	C-C1-C2-O3
23	j	611	MQ9	C12-C13-C14-C15
14	i	609	CDL	C57-C58-C59-C60
14	b	103	CDL	C53-C54-C55-C56
22	p	601	9YF	C27-C28-C29-C30
15	q	301	9Y0	C10-C11-C12-C13
14	m	202	CDL	C82-C83-C84-C85
14	U	603	CDL	C31-C32-C33-C34
14	i	608	CDL	C56-C57-C58-C59
23	i	612	MQ9	C36-C37-C38-C39
14	g	301	CDL	C74-C75-C76-C77
14	G	102	CDL	CB3-CB4-CB6-OB8
14	L	605	CDL	C73-C74-C75-C76
14	L	606	CDL	CA3-CA4-CA6-OA8
14	U	603	CDL	C34-C35-C36-C37
14	g	301	CDL	CA3-CA4-CA6-OA8
14	j	605	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
14	j	606	CDL	CA3-CA4-CA6-OA8
14	j	609	CDL	CA3-CA4-CA6-OA8
14	p	603	CDL	CA3-CA4-CA6-OA8
14	L	605	CDL	C11-C12-C13-C14
14	i	609	CDL	C16-C17-C18-C19
22	n	201	9YF	C15-C16-C17-C18
16	L	601	HEA	C4D-C3D-CAD-CBD
14	L	605	CDL	C61-C62-C63-C64
14	i	614	CDL	C77-C78-C79-C80
22	p	601	9YF	C29-C30-C31-C32
13	i	613	9XX	C13-C14-C15-O
22	p	601	9YF	O12-C25-O11-C24
14	p	603	CDL	C11-C12-C13-C14
23	j	608	MQ9	C19-C21-C22-C23
14	U	603	CDL	C17-C18-C19-C20
14	U	603	CDL	C84-C85-C86-C87
15	g	302	9Y0	C6-C5-O5-C
15	q	301	9Y0	C14-C15-C16-C17
23	i	612	MQ9	C17-C18-C19-C20
14	L	606	CDL	OB9-CB7-OB8-CB6
14	b	103	CDL	C14-C15-C16-C17
15	g	302	9Y0	C30-C31-C32-C33
14	U	603	CDL	C73-C74-C75-C76
13	j	610	9XX	C16-C17-O1-C18
14	L	606	CDL	C56-C57-C58-C59
14	i	607	CDL	C76-C77-C78-C79
14	j	609	CDL	C71-C72-C73-C74
14	p	603	CDL	C71-CB7-OB8-CB6
14	i	604	CDL	C52-C51-CB5-OB6
14	j	609	CDL	C32-C31-CA7-OA8
14	i	614	CDL	C72-C71-CB7-OB8
14	g	301	CDL	OA6-CA4-CA6-OA8
14	U	603	CDL	OB7-CB5-OB6-CB4
23	i	612	MQ9	C30-C29-C31-C32
14	i	614	CDL	C16-C17-C18-C19
22	V	602	9YF	C38-C39-C40-C41
14	I	604	CDL	C71-CB7-OB8-CB6
16	I	601	HEA	C4D-C3D-CAD-CBD
14	U	603	CDL	C52-C53-C54-C55
15	g	302	9Y0	O1-C3-C4-N
24	o	602	HEC	C4C-C3C-CAC-CBC
14	U	603	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
14	i	608	CDL	C37-C38-C39-C40
14	m	202	CDL	C78-C79-C80-C81
14	p	603	CDL	C35-C36-C37-C38
15	G	103	9Y0	C6-C5-O5-C
15	q	301	9Y0	O5-C5-C6-C7
23	i	603	MQ9	C41-C42-C43-C44
23	i	612	MQ9	C26-C27-C28-C29
23	j	608	MQ9	C31-C32-C33-C34
23	m	201	MQ9	C26-C27-C28-C29
22	V	602	9YF	C36-C37-C38-C39
14	i	607	CDL	CA4-CA3-OA5-PA1
14	i	607	CDL	C1-CB2-OB2-PB2
14	i	607	CDL	CB4-CB3-OB5-PB2
14	b	103	CDL	C75-C76-C77-C78
14	L	605	CDL	C38-C39-C40-C41
22	V	602	9YF	C16-C17-C18-C19
14	g	301	CDL	CB3-CB4-CB6-OB8
14	i	607	CDL	CA3-CA4-CA6-OA8
22	n	201	9YF	C1-C-C24-O11
14	i	604	CDL	C32-C33-C34-C35
22	n	201	9YF	C2-O2-P-O1
23	i	602	MQ9	C11-C12-C13-C14
23	i	612	MQ9	C11-C12-C13-C14
14	i	614	CDL	CB3-OB5-PB2-OB2
14	j	606	CDL	CA3-OA5-PA1-OA2
15	g	302	9Y0	O4-C5-O5-C
14	I	604	CDL	OA5-CA3-CA4-OA6
14	L	605	CDL	OB5-CB3-CB4-OB6
23	i	603	MQ9	C37-C38-C39-C40
23	i	610	MQ9	C27-C28-C29-C30
14	i	614	CDL	CB5-C51-C52-C53
14	m	202	CDL	C17-C18-C19-C20
14	p	603	CDL	C52-C53-C54-C55
13	j	610	9XX	O-C16-C17-O1
22	p	601	9YF	C10-C11-C12-C13
14	j	606	CDL	OA6-CA4-CA6-OA8
22	i	601	9YF	O9-C-C24-O11
22	n	201	9YF	O9-C-C24-O11
14	U	603	CDL	C71-CB7-OB8-CB6
14	j	605	CDL	C37-C38-C39-C40
16	L	601	HEA	C2D-C3D-CAD-CBD
14	L	606	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
23	i	612	MQ9	C28-C29-C31-C32
14	I	604	CDL	C52-C53-C54-C55
14	L	606	CDL	C1-CB2-OB2-PB2
14	b	103	CDL	CA4-CA3-OA5-PA1
14	I	605	CDL	C78-C79-C80-C81
14	L	605	CDL	C72-C73-C74-C75
14	j	606	CDL	C13-C14-C15-C16
14	g	301	CDL	C64-C65-C66-C67
14	I	605	CDL	C72-C71-CB7-OB8
14	U	603	CDL	C72-C71-CB7-OB8
14	L	605	CDL	C58-C59-C60-C61
14	g	301	CDL	C75-C76-C77-C78
15	f	601	9Y0	C13-C14-C15-C16
14	g	301	CDL	C11-C12-C13-C14
14	I	604	CDL	OA5-CA3-CA4-CA6
22	n	201	9YF	C24-C-C1-O
14	i	608	CDL	C17-C18-C19-C20
13	b	102	9XX	C26-C27-C28-C29
14	p	603	CDL	OB9-CB7-OB8-CB6
14	U	603	CDL	C55-C56-C57-C58
15	f	601	9Y0	C9-C10-C11-C12
22	V	602	9YF	C35-C36-C37-C38
22	n	201	9YF	C11-C10-C9-C8
13	b	102	9XX	C14-C15-O-C16
14	L	606	CDL	C31-CA7-OA8-CA6
14	m	202	CDL	C71-CB7-OB8-CB6
22	n	201	9YF	C26-C25-O11-C24
14	I	604	CDL	CB3-CB4-OB6-CB5
14	L	605	CDL	CB3-CB4-OB6-CB5
14	L	606	CDL	CB3-CB4-OB6-CB5
14	j	606	CDL	CA6-CA4-OA6-CA5
20	j	603	HEM	C2B-C3B-CAB-CBB
14	p	603	CDL	C51-C52-C53-C54
14	b	103	CDL	C71-CB7-OB8-CB6
23	j	602	MQ9	C35-C34-C36-C37
18	q	302	PLM	C7-C8-C9-CA
14	G	102	CDL	CA3-CA4-CA6-OA8
14	b	103	CDL	C1-CB2-OB2-PB2
14	g	301	CDL	C1-CA2-OA2-PA1
14	i	604	CDL	CB3-CB4-CB6-OB8
14	i	608	CDL	CB3-CB4-CB6-OB8
14	L	605	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
14	p	603	CDL	OB5-CB3-CB4-OB6
14	i	609	CDL	C77-C78-C79-C80
22	i	601	9YF	C28-C29-C30-C31
14	L	606	CDL	C12-C13-C14-C15
14	j	606	CDL	C55-C56-C57-C58
15	b	101	9Y0	C11-C12-C13-C14
22	p	601	9YF	C40-C41-C42-C43
14	I	604	CDL	OB9-CB7-OB8-CB6
15	G	103	9Y0	O4-C5-O5-C
16	I	601	HEA	C2D-C3D-CAD-CBD
14	G	102	CDL	OA6-CA4-CA6-OA8
14	g	301	CDL	OB6-CB4-CB6-OB8
14	m	202	CDL	OB6-CB4-CB6-OB8
14	p	603	CDL	OA6-CA4-CA6-OA8
14	i	614	CDL	C31-C32-C33-C34
14	I	605	CDL	C52-C51-CB5-OB6
14	i	604	CDL	C33-C34-C35-C36
22	o	603	9YF	C7-C2-O2-P
22	i	601	9YF	C16-C17-C18-C19
23	i	612	MQ9	C31-C32-C33-C34
23	j	602	MQ9	C26-C27-C28-C29
14	i	614	CDL	C11-C12-C13-C14
14	m	202	CDL	C54-C55-C56-C57
14	U	603	CDL	OB9-CB7-OB8-CB6
14	I	605	CDL	C32-C31-CA7-OA8
13	b	102	9XX	O6-C15-O-C16
14	L	606	CDL	OA9-CA7-OA8-CA6
14	i	609	CDL	C13-C14-C15-C16
22	i	601	9YF	C18-C19-C20-C21
14	j	605	CDL	C35-C36-C37-C38
14	p	603	CDL	C60-C61-C62-C63
14	U	603	CDL	C33-C34-C35-C36
14	L	606	CDL	CA2-OA2-PA1-OA5
14	g	301	CDL	CB2-OB2-PB2-OB5
14	i	607	CDL	CA2-OA2-PA1-OA5
14	p	603	CDL	CA2-OA2-PA1-OA5
15	b	101	9Y0	C2-O3-P-O1
14	G	102	CDL	C31-C32-C33-C34
14	L	605	CDL	C52-C53-C54-C55
14	G	102	CDL	CB2-OB2-PB2-OB4
14	I	604	CDL	CA3-OA5-PA1-OA3
14	I	605	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
14	L	605	CDL	CA2-OA2-PA1-OA4
14	L	605	CDL	CA3-OA5-PA1-OA3
14	U	603	CDL	CA2-OA2-PA1-OA4
14	U	603	CDL	CA3-OA5-PA1-OA3
14	b	103	CDL	CB3-OB5-PB2-OB4
14	i	609	CDL	CB2-OB2-PB2-OB4
14	j	605	CDL	CB3-OB5-PB2-OB4
14	j	606	CDL	CA2-OA2-PA1-OA4
14	j	606	CDL	CB2-OB2-PB2-OB4
14	j	609	CDL	CA2-OA2-PA1-OA3
14	j	609	CDL	CB3-OB5-PB2-OB4
14	p	603	CDL	CA2-OA2-PA1-OA3
15	b	101	9Y0	C2-O3-P-O2
15	f	601	9Y0	C3-O1-P-O
15	f	601	9Y0	C2-O3-P-O
15	q	301	9Y0	C3-O1-P-O
22	V	602	9YF	C1-O-P-O1
22	n	201	9YF	C1-O-P-O1
22	o	603	9YF	C1-O-P-O1
14	L	605	CDL	OA5-CA3-CA4-CA6
14	j	606	CDL	OB5-CB3-CB4-CB6
14	p	603	CDL	OB5-CB3-CB4-CB6
23	j	602	MQ9	C22-C23-C24-C25
14	m	202	CDL	OB9-CB7-OB8-CB6
14	G	102	CDL	C32-C31-CA7-OA8
15	f	601	9Y0	C6-C7-C8-C9
23	i	603	MQ9	C21-C22-C23-C24
23	i	612	MQ9	C16-C17-C18-C19
23	j	608	MQ9	C26-C27-C28-C29
15	f	601	9Y0	C4-C3-O1-P
15	g	302	9Y0	C4-C3-O1-P
15	q	301	9Y0	C11-C10-C9-C8
14	I	605	CDL	C72-C73-C74-C75
23	j	608	MQ9	C27-C28-C29-C31
15	g	302	9Y0	O7-C1-C2-O3
22	n	201	9YF	O9-C-C1-O
14	b	103	CDL	OB9-CB7-OB8-CB6
22	n	201	9YF	O12-C25-O11-C24
14	i	604	CDL	CA5-C11-C12-C13
14	g	301	CDL	C80-C81-C82-C83
14	j	606	CDL	C18-C19-C20-C21
14	i	614	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	U	603	CDL	C79-C80-C81-C82
14	i	607	CDL	C53-C54-C55-C56
14	i	608	CDL	OB6-CB4-CB6-OB8
14	j	605	CDL	OB6-CB4-CB6-OB8
22	i	601	9YF	C29-C30-C31-C32
23	i	602	MQ9	C45-C44-C46-C47
23	i	612	MQ9	C35-C34-C36-C37
14	j	606	CDL	C31-CA7-OA8-CA6
14	I	605	CDL	C12-C13-C14-C15
14	b	103	CDL	C54-C55-C56-C57
18	I	606	PLM	CB-CC-CD-CE
23	i	602	MQ9	C19-C21-C22-C23
14	G	102	CDL	C33-C34-C35-C36
14	I	604	CDL	C34-C35-C36-C37
14	i	614	CDL	C76-C77-C78-C79
14	G	102	CDL	C81-C82-C83-C84
14	I	604	CDL	C54-C55-C56-C57
23	j	602	MQ9	C33-C34-C36-C37
22	j	601	9YF	C25-C26-C27-C28
14	I	605	CDL	C60-C61-C62-C63
14	i	609	CDL	CB6-CB4-OB6-CB5
14	p	603	CDL	C15-C16-C17-C18
23	j	608	MQ9	C16-C17-C18-C19
14	L	605	CDL	C34-C35-C36-C37
14	G	102	CDL	OB5-CB3-CB4-OB6
13	G	101	9XX	C23-C24-C25-C26
23	i	610	MQ9	C25-C24-C26-C27
14	i	608	CDL	C35-C36-C37-C38
14	U	603	CDL	C13-C14-C15-C16
22	V	602	9YF	C14-C15-C16-C17
14	i	609	CDL	C12-C13-C14-C15
15	g	302	9Y0	C11-C12-C13-C14
23	i	603	MQ9	C19-C21-C22-C23
14	I	605	CDL	CB2-OB2-PB2-OB5
14	i	604	CDL	CA2-OA2-PA1-OA5
14	i	608	CDL	CA2-OA2-PA1-OA5
14	i	608	CDL	CB2-OB2-PB2-OB5
14	i	609	CDL	CB3-OB5-PB2-OB2
14	j	605	CDL	CA2-OA2-PA1-OA5
14	j	606	CDL	CB3-OB5-PB2-OB2
14	j	609	CDL	CA3-OA5-PA1-OA2
14	j	609	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
15	G	103	9Y0	C2-O3-P-O1
22	V	602	9YF	C20-C21-C22-C23
22	i	601	9YF	C1-C-C24-O11
23	i	603	MQ9	C15-C14-C16-C17
23	j	611	MQ9	C20-C19-C21-C22
14	j	609	CDL	C12-C13-C14-C15
22	V	602	9YF	C31-C32-C33-C35
23	j	611	MQ9	C31-C32-C33-C34
14	L	606	CDL	C75-C76-C77-C78
13	i	613	9XX	C13-C14-C15-O6
14	j	605	CDL	CB5-C51-C52-C53
14	b	103	CDL	C11-C12-C13-C14
14	p	603	CDL	C1-CB2-OB2-PB2
14	U	603	CDL	C56-C57-C58-C59
14	j	605	CDL	C34-C35-C36-C37
15	q	301	9Y0	C7-C8-C9-C10
15	G	103	9Y0	C13-C14-C15-C16
14	b	103	CDL	C81-C82-C83-C84
14	i	609	CDL	CA2-C1-CB2-OB2
23	j	608	MQ9	C36-C37-C38-C39
14	j	606	CDL	C72-C73-C74-C75
15	G	103	9Y0	C22-C23-C24-C25
14	I	604	CDL	CB5-C51-C52-C53
14	i	604	CDL	C52-C51-CB5-OB7
14	i	608	CDL	C15-C16-C17-C18
15	g	302	9Y0	C6-C7-C8-C9
14	G	102	CDL	C71-CB7-OB8-CB6
14	g	301	CDL	C51-C52-C53-C54
16	L	601	HEA	CAD-CBD-CGD-O1D
23	m	201	MQ9	C9-C11-C12-C13
14	G	102	CDL	C78-C79-C80-C81
22	V	602	9YF	O9-C-C1-O
23	i	602	MQ9	C31-C32-C33-C34
20	i	605	HEM	C4B-C3B-CAB-CBB
20	j	603	HEM	C4B-C3B-CAB-CBB
14	G	102	CDL	C23-C24-C25-C26
23	i	603	MQ9	C12-C11-C9-C10
23	i	612	MQ9	C45-C44-C46-C47
23	j	611	MQ9	C45-C44-C46-C47
14	I	604	CDL	C32-C33-C34-C35
22	p	601	9YF	C16-C17-C18-C19
14	I	604	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
15	q	301	9Y0	C11-C12-C13-C14
14	U	603	CDL	C36-C37-C38-C39
23	i	602	MQ9	C20-C19-C21-C22
14	g	301	CDL	C73-C74-C75-C76
23	i	612	MQ9	C33-C34-C36-C37
14	g	301	CDL	C33-C34-C35-C36
22	p	601	9YF	C37-C38-C39-C40
13	b	102	9XX	C5-C6-C7-C8
14	b	103	CDL	C83-C84-C85-C86
14	g	301	CDL	CB2-C1-CA2-OA2
14	G	102	CDL	C74-C75-C76-C77
16	I	601	HEA	CAD-CBD-CGD-O1D
14	j	606	CDL	OA9-CA7-OA8-CA6
13	b	102	9XX	C-C1-C2-C3
20	j	603	HEM	CAA-CBA-CGA-O2A
23	i	611	MQ9	C29-C31-C32-C33
14	U	603	CDL	C81-C82-C83-C84
14	i	608	CDL	C34-C35-C36-C37
20	i	605	HEM	CAA-CBA-CGA-O2A
14	I	605	CDL	CB3-CB4-OB6-CB5
14	i	609	CDL	CA6-CA4-OA6-CA5
14	j	609	CDL	CA3-CA4-OA6-CA5
14	m	202	CDL	CB3-CB4-OB6-CB5
13	i	613	9XX	C11-C12-C13-C14
16	I	601	HEA	CAD-CBD-CGD-O2D
20	i	605	HEM	CAA-CBA-CGA-O1A
20	j	603	HEM	CAA-CBA-CGA-O1A
20	U	601	HEM	CAD-CBD-CGD-O2D
14	G	102	CDL	C76-C77-C78-C79
14	g	301	CDL	C78-C79-C80-C81
23	j	608	MQ9	C27-C28-C29-C30
20	U	601	HEM	CAD-CBD-CGD-O1D
14	b	103	CDL	C73-C74-C75-C76
22	o	603	9YF	C36-C37-C38-C39
23	j	602	MQ9	C15-C14-C16-C17
23	j	608	MQ9	C12-C11-C9-C10
23	j	608	MQ9	C45-C44-C46-C47
14	j	609	CDL	C31-C32-C33-C34
22	j	601	9YF	C27-C28-C29-C30
14	I	604	CDL	CA5-C11-C12-C13
14	i	604	CDL	CA7-C31-C32-C33
23	i	610	MQ9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
23	j	611	MQ9	C18-C19-C21-C22
14	L	606	CDL	CA5-C11-C12-C13
14	I	605	CDL	OA6-CA4-CA6-OA8
22	j	601	9YF	C12-C13-C14-C15
13	G	101	9XX	C16-C17-O1-C18
15	b	104	9Y0	C12-C13-C14-C15
23	i	612	MQ9	C14-C16-C17-C18
23	j	602	MQ9	C39-C41-C42-C43
16	L	601	HEA	CAD-CBD-CGD-O2D
14	g	301	CDL	C62-C63-C64-C65
22	n	201	9YF	C27-C28-C29-C30
23	i	602	MQ9	C18-C19-C21-C22
23	i	603	MQ9	C12-C11-C9-C8
23	i	612	MQ9	C43-C44-C46-C47
23	j	608	MQ9	C43-C44-C46-C47
23	j	611	MQ9	C43-C44-C46-C47
22	n	201	9YF	C36-C37-C38-C39
14	j	609	CDL	C32-C31-CA7-OA9
13	G	101	9XX	C24-C25-C26-C27
14	i	614	CDL	C72-C71-CB7-OB9
22	V	602	9YF	O12-C25-O11-C24
20	j	603	HEM	CAD-CBD-CGD-O1D
14	I	605	CDL	C59-C60-C61-C62
14	L	605	CDL	C13-C14-C15-C16
14	m	202	CDL	C81-C82-C83-C84
23	i	602	MQ9	C43-C44-C46-C47
23	i	603	MQ9	C13-C14-C16-C17
24	o	601	HEC	CAD-CBD-CGD-O2D
14	I	605	CDL	C76-C77-C78-C79
14	I	605	CDL	C56-C57-C58-C59
14	U	603	CDL	C35-C36-C37-C38
14	j	606	CDL	C31-C32-C33-C34
14	b	103	CDL	OA5-CA3-CA4-OA6
14	g	301	CDL	OB5-CB3-CB4-OB6
14	I	605	CDL	C52-C53-C54-C55
14	i	607	CDL	C18-C19-C20-C21
14	G	102	CDL	C80-C81-C82-C83
22	j	601	9YF	C35-C36-C37-C38
14	U	603	CDL	OB5-CB3-CB4-CB6
16	L	602	HEA	C27-C19-C20-C21
23	j	611	MQ9	C12-C11-C9-C10
23	i	603	MQ9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	i	603	MQ9	C16-C17-C18-C19
23	j	608	MQ9	C12-C11-C9-C8
15	q	301	9Y0	C12-C13-C14-C15
22	n	201	9YF	C13-C14-C15-C16
15	q	301	9Y0	O4-C5-C6-C7
14	I	604	CDL	CA2-C1-CB2-OB2
14	i	607	CDL	C71-C72-C73-C74
14	G	102	CDL	C51-CB5-OB6-CB4
22	V	602	9YF	C26-C25-O11-C24
14	G	102	CDL	OB9-CB7-OB8-CB6
14	I	604	CDL	CA2-OA2-PA1-OA5
23	j	602	MQ9	C13-C14-C16-C17
22	V	602	9YF	O9-C8-C9-C10
22	V	602	9YF	C31-C32-C33-C34
14	p	603	CDL	C22-C23-C24-C25
22	o	603	9YF	C35-C36-C37-C38
14	j	606	CDL	CB6-CB4-OB6-CB5
14	j	609	CDL	CB3-CB4-OB6-CB5
14	p	603	CDL	CB3-CB4-OB6-CB5
15	b	104	9Y0	C-C1-O7-C21
15	q	301	9Y0	C2-C1-O7-C21
14	b	103	CDL	C12-C13-C14-C15
22	V	602	9YF	C12-C13-C14-C15
14	G	102	CDL	OB7-CB5-OB6-CB4
14	j	605	CDL	OB7-CB5-OB6-CB4
20	j	603	HEM	CAD-CBD-CGD-O2D
22	o	603	9YF	C40-C41-C42-C43
20	U	602	HEM	CAA-CBA-CGA-O2A
24	o	601	HEC	CAA-CBA-CGA-O2A
24	o	601	HEC	CAD-CBD-CGD-O1D
23	j	608	MQ9	C34-C36-C37-C38
15	b	101	9Y0	C10-C11-C12-C13
14	U	603	CDL	C15-C16-C17-C18
20	i	605	HEM	CAD-CBD-CGD-O1D
14	i	614	CDL	C15-C16-C17-C18
14	U	603	CDL	OB5-CB3-CB4-OB6
14	U	603	CDL	C12-C11-CA5-OA6
24	o	602	HEC	C2B-C3B-CAB-CBB
14	i	608	CDL	C71-CB7-OB8-CB6
14	j	605	CDL	C31-CA7-OA8-CA6
15	f	601	9Y0	O4-C5-O5-C
24	o	601	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	U	603	CDL	O1-C1-CA2-OA2
16	I	602	HEA	C27-C19-C20-C21
15	b	101	9Y0	C23-C24-C25-C26
14	b	103	CDL	OA5-CA3-CA4-CA6
14	g	301	CDL	C60-C61-C62-C63
14	L	606	CDL	OB6-CB4-CB6-OB8
14	i	608	CDL	C54-C55-C56-C57
20	i	605	HEM	CAD-CBD-CGD-O2D
14	U	603	CDL	C16-C17-C18-C19
23	j	611	MQ9	C12-C11-C9-C8
15	b	104	9Y0	C25-C26-C27-C28
13	b	102	9XX	C25-C26-C27-C36
23	m	201	MQ9	C24-C26-C27-C28
14	j	609	CDL	C55-C56-C57-C58
14	i	604	CDL	C54-C55-C56-C57
22	o	603	9YF	C10-C11-C12-C13
14	j	605	CDL	OA9-CA7-OA8-CA6
14	L	605	CDL	CB5-C51-C52-C53
14	G	102	CDL	C72-C73-C74-C75
14	i	614	CDL	C17-C18-C19-C20
14	j	605	CDL	C51-CB5-OB6-CB4
20	U	602	HEM	CAA-CBA-CGA-O1A
23	i	602	MQ9	C46-C47-C48-C49
23	i	603	MQ9	C46-C47-C48-C49
23	j	602	MQ9	C41-C42-C43-C44
23	m	201	MQ9	C36-C37-C38-C39
14	U	603	CDL	C72-C71-CB7-OB9
22	j	601	9YF	C14-C15-C16-C17
14	p	603	CDL	C37-C38-C39-C40
22	n	201	9YF	C16-C17-C18-C19
15	f	601	9Y0	C6-C5-O5-C
14	I	604	CDL	C57-C58-C59-C60
14	U	603	CDL	C12-C11-CA5-OA7
14	i	604	CDL	C51-C52-C53-C54
14	G	102	CDL	C13-C14-C15-C16
14	i	608	CDL	C31-CA7-OA8-CA6
14	j	609	CDL	O1-C1-CA2-OA2
14	g	301	CDL	C76-C77-C78-C79
22	V	602	9YF	O10-C8-C9-C10
18	q	302	PLM	C9-CA-CB-CC
14	G	102	CDL	CA2-OA2-PA1-OA3
14	G	102	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
14	L	605	CDL	CA2-OA2-PA1-OA3
14	L	605	CDL	CB3-OB5-PB2-OB4
14	i	604	CDL	CA2-OA2-PA1-OA3
14	i	614	CDL	CB3-OB5-PB2-OB3
15	G	103	9Y0	C2-O3-P-O
23	j	608	MQ9	C6-C7-C8-C9
14	j	606	CDL	C14-C15-C16-C17
14	m	202	CDL	C72-C71-CB7-OB8
22	i	601	9YF	O9-C8-C9-C10
22	j	601	9YF	O9-C8-C9-C10
14	i	608	CDL	OA9-CA7-OA8-CA6
14	i	609	CDL	OB5-CB3-CB4-CB6
14	g	301	CDL	C19-C20-C21-C22
14	p	603	CDL	C53-C54-C55-C56
13	i	613	9XX	C19-C20-C21-C22
14	i	607	CDL	C15-C16-C17-C18
14	i	609	CDL	C53-C54-C55-C56
14	I	605	CDL	C72-C71-CB7-OB9
14	i	608	CDL	OB9-CB7-OB8-CB6
14	L	605	CDL	C72-C71-CB7-OB8
23	j	602	MQ9	C11-C12-C13-C14
14	j	606	CDL	CB3-CB4-OB6-CB5
15	q	301	9Y0	C-C1-O7-C21
15	q	301	9Y0	C4-C3-O1-P
14	L	606	CDL	C32-C31-CA7-OA8
13	G	101	9XX	C37-C17-O1-C18
14	L	605	CDL	C32-C31-CA7-OA8
14	m	202	CDL	C12-C11-CA5-OA6
24	o	602	HEC	C4B-C3B-CAB-CBB
14	I	604	CDL	C72-C71-CB7-OB8
14	i	609	CDL	C12-C11-CA5-OA6
14	m	202	CDL	C32-C31-CA7-OA8
15	g	302	9Y0	O5-C5-C6-C7
23	i	610	MQ9	C26-C27-C28-C29
14	m	202	CDL	CB2-C1-CA2-OA2
13	b	102	9XX	C11-C12-C13-C14
14	G	102	CDL	C22-C23-C24-C25
14	G	102	CDL	C37-C38-C39-C40
14	i	609	CDL	C12-C11-CA5-OA7
14	j	609	CDL	C12-C11-CA5-OA6
14	j	605	CDL	C58-C59-C60-C61
14	L	605	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
14	L	606	CDL	C32-C31-CA7-OA9
15	g	302	9Y0	O4-C5-C6-C7
23	i	610	MQ9	C24-C26-C27-C28
23	j	608	MQ9	C9-C11-C12-C13
23	j	607	MQ9	C11-C12-C13-C14
14	i	607	CDL	C32-C31-CA7-OA8
22	p	601	9YF	C30-C31-C32-C33
14	I	604	CDL	C55-C56-C57-C58
20	U	601	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

50 monomers are involved in 323 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	V	602	9YF	1	0
23	j	607	MQ9	11	0
14	i	607	CDL	11	0
16	I	602	HEA	6	0
14	L	605	CDL	3	0
23	j	608	MQ9	14	0
13	i	613	9XX	2	0
22	n	201	9YF	1	0
14	I	605	CDL	6	0
14	j	606	CDL	5	0
14	I	604	CDL	8	0
23	i	610	MQ9	21	0
22	o	603	9YF	4	0
16	L	601	HEA	3	0
20	j	604	HEM	2	0
14	i	609	CDL	5	0
15	f	601	9Y0	1	0
14	i	614	CDL	10	0
13	b	102	9XX	1	0
14	j	609	CDL	3	0
16	I	601	HEA	3	0
14	b	103	CDL	33	0
23	i	612	MQ9	19	0
14	U	603	CDL	3	0
22	i	601	9YF	1	0
20	j	603	HEM	2	0
14	j	605	CDL	3	0
24	o	601	HEC	8	0

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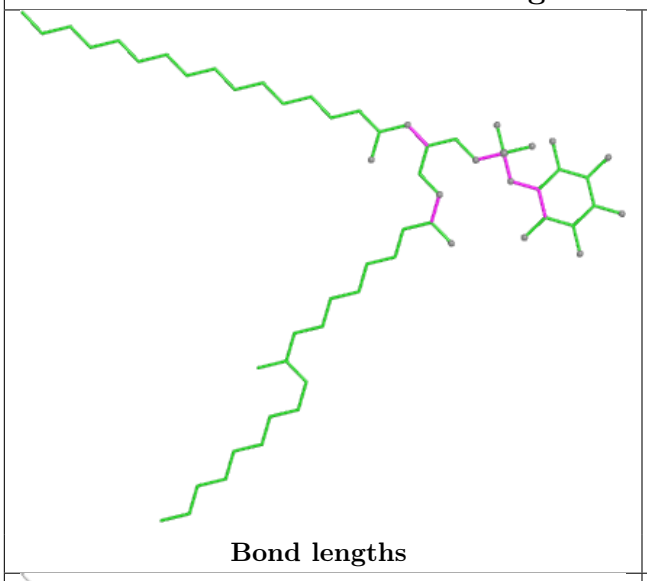
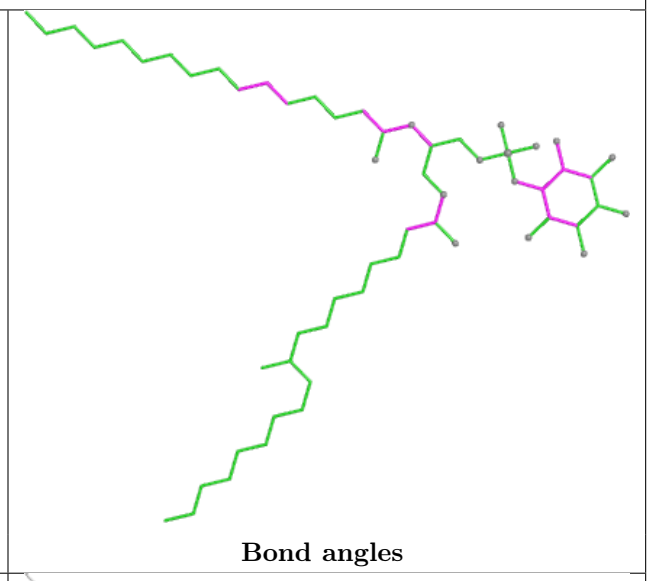
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	j	611	MQ9	6	0
24	o	602	HEC	2	0
14	p	603	CDL	19	0
23	i	611	MQ9	18	0
14	G	102	CDL	13	0
13	G	101	9XX	1	0
23	i	602	MQ9	5	0
18	q	302	PLM	5	0
23	j	602	MQ9	9	0
14	i	608	CDL	3	0
20	i	605	HEM	1	0
14	L	606	CDL	8	0
23	m	201	MQ9	9	0
22	p	601	9YF	1	0
14	i	604	CDL	5	0
23	i	603	MQ9	8	0
15	q	301	9Y0	1	0
20	U	602	HEM	4	0
14	g	301	CDL	13	0
20	U	601	HEM	8	0
14	m	202	CDL	8	0
16	L	602	HEA	5	0

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

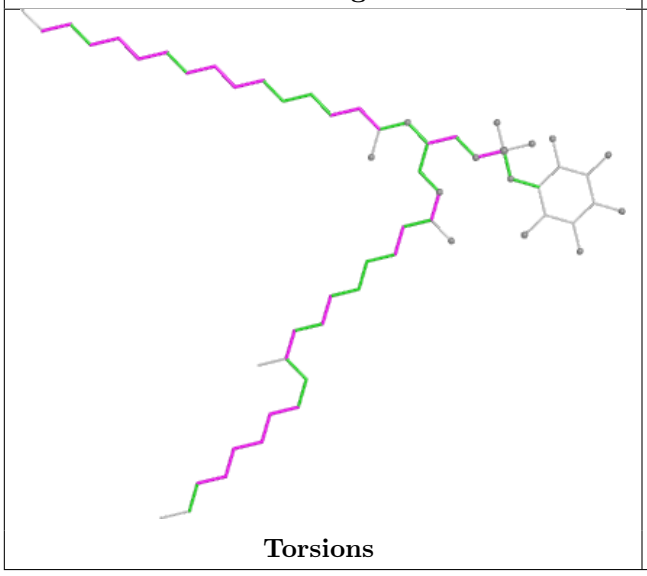
Ligand 9YF V 602



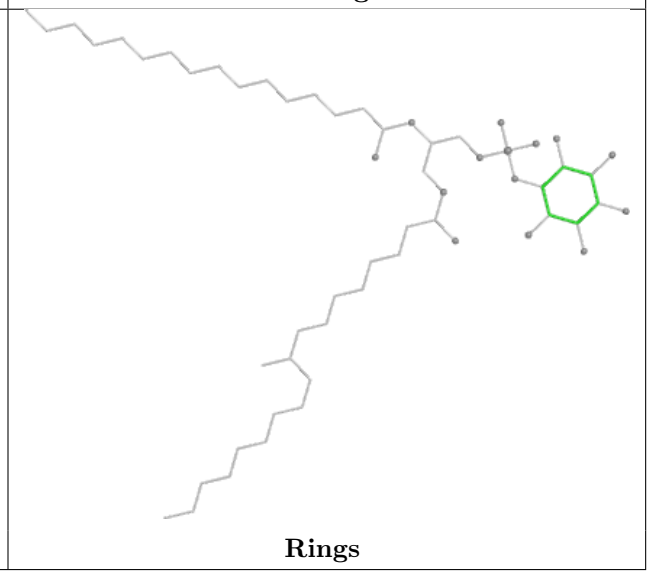
Bond lengths



Bond angles

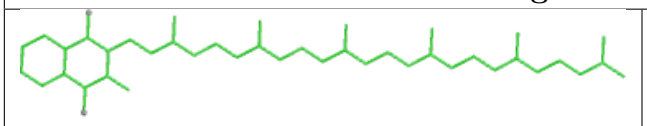


Torsions



Rings

Ligand MQ9 j 607



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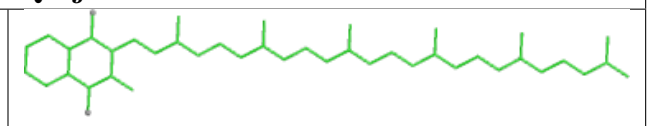

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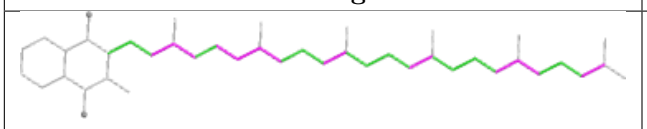

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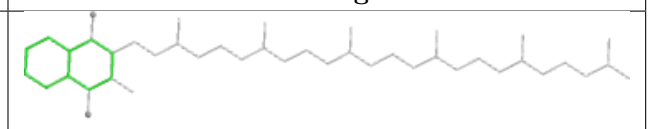
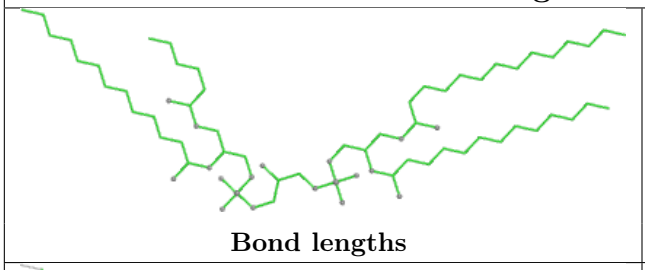


Rings

Ligand CDL i 607



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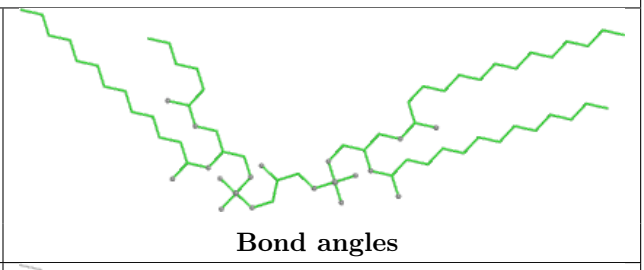

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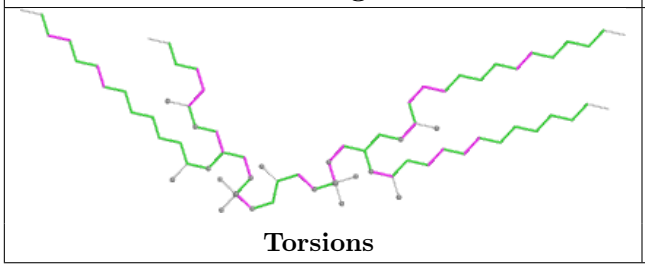

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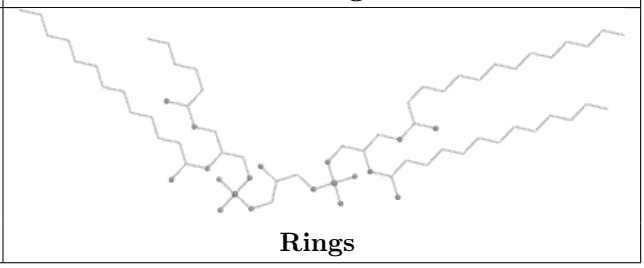
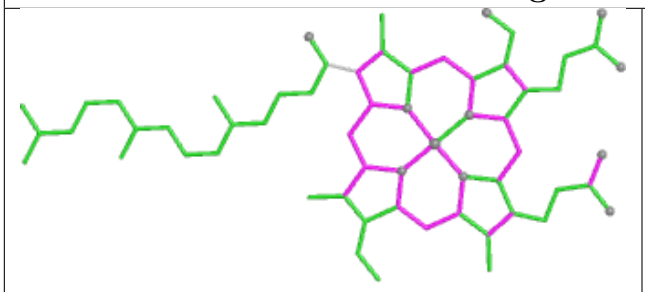


Rings

Ligand HEA I 602



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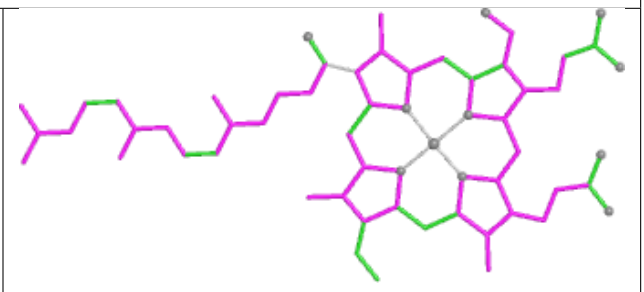

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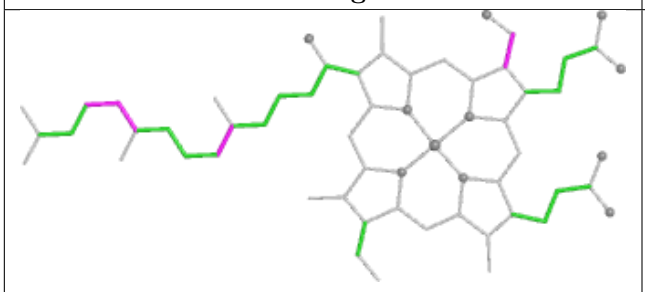

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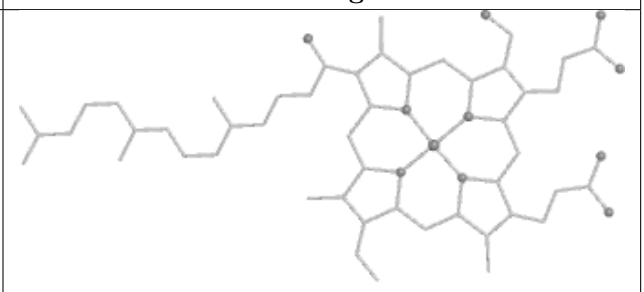
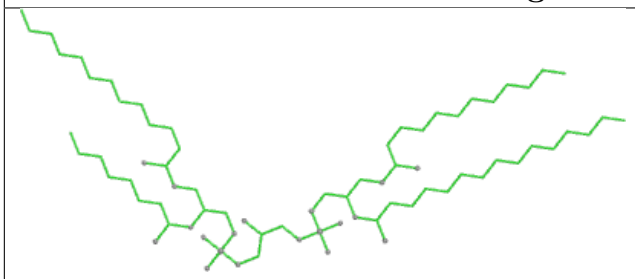


Rings

Ligand CDL L 605



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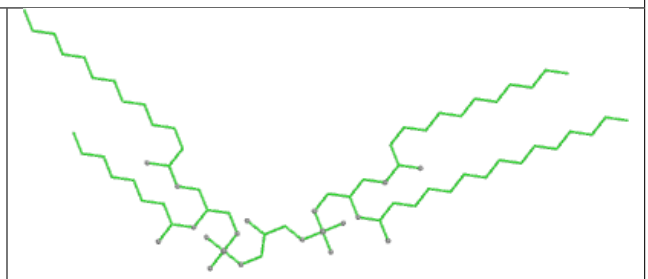

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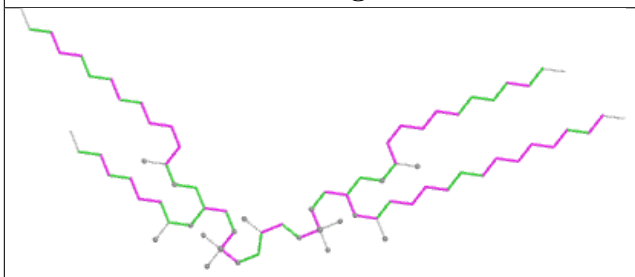

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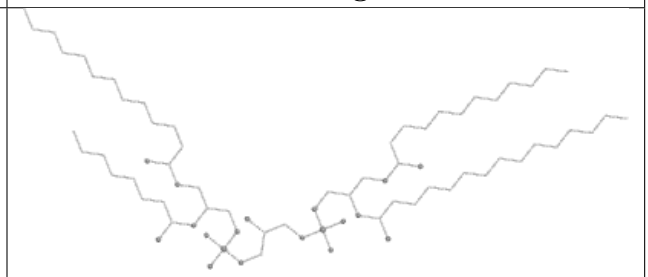
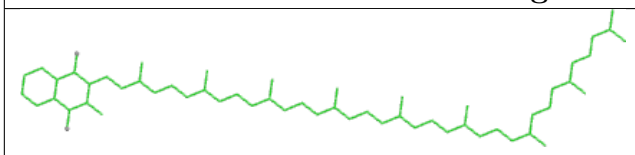


Rings

Ligand MQ9 j 608



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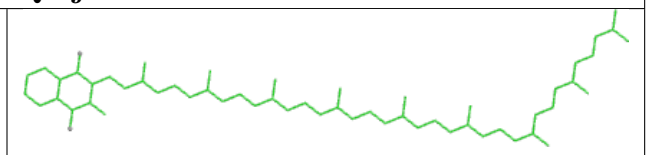

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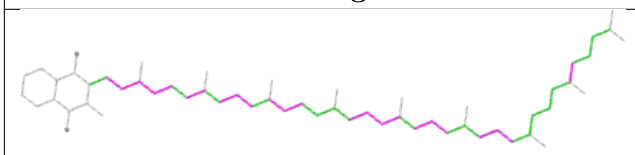

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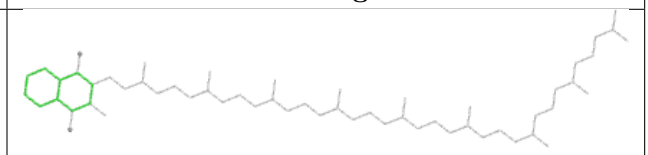
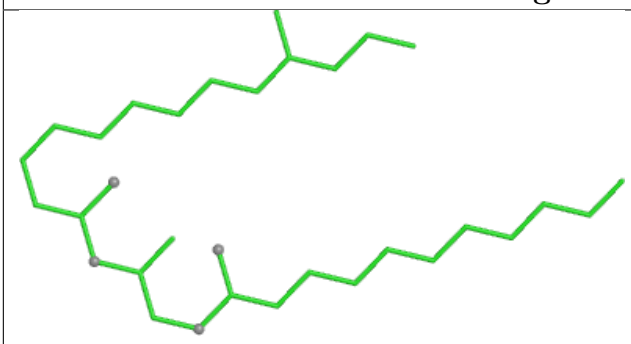


Rings

Ligand 9XX i 613



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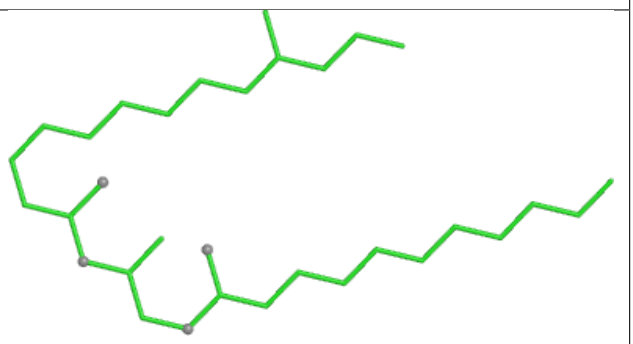

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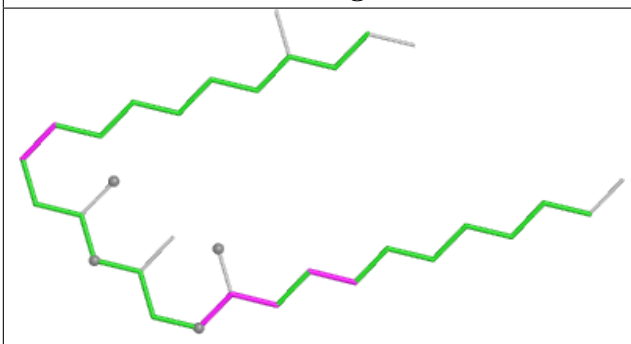

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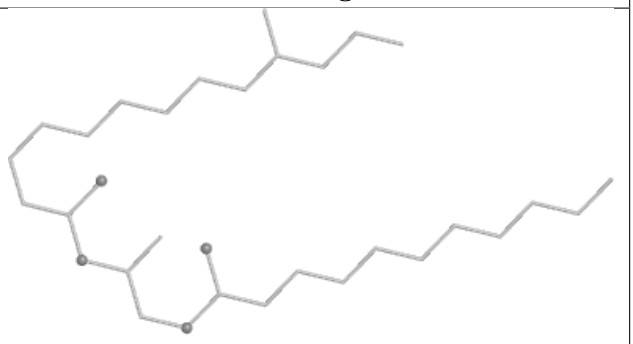
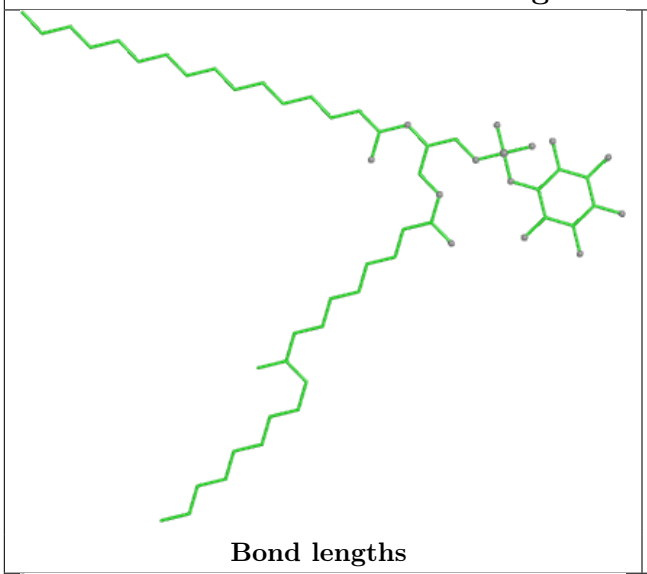


Rings

Ligand 9YF n 201



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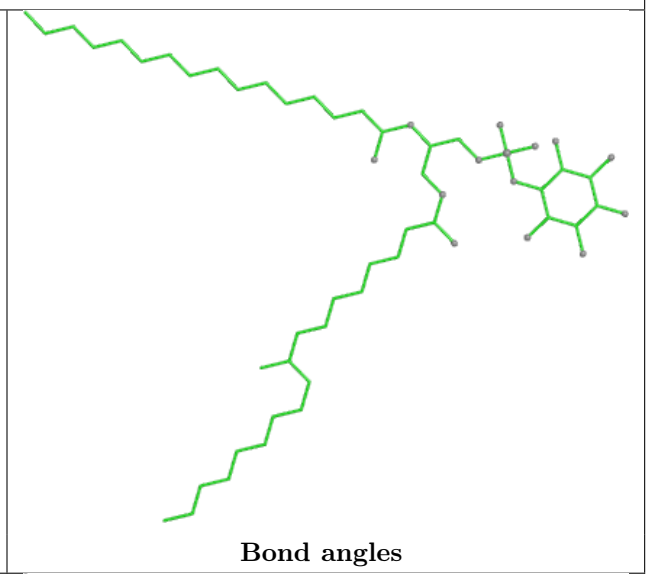

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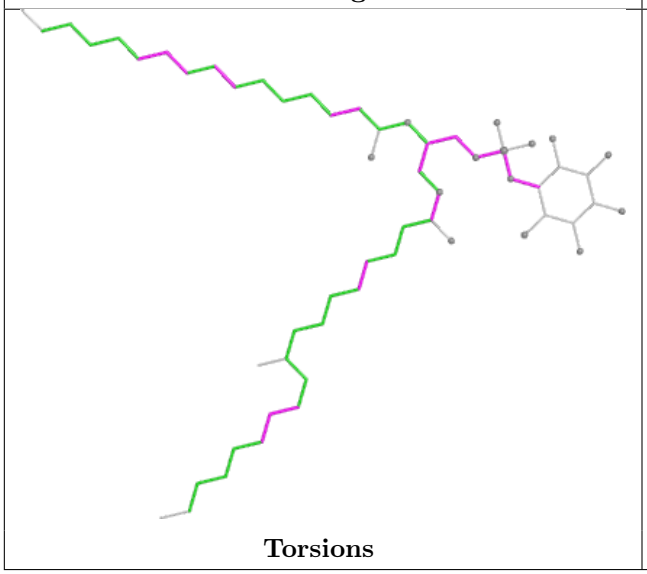

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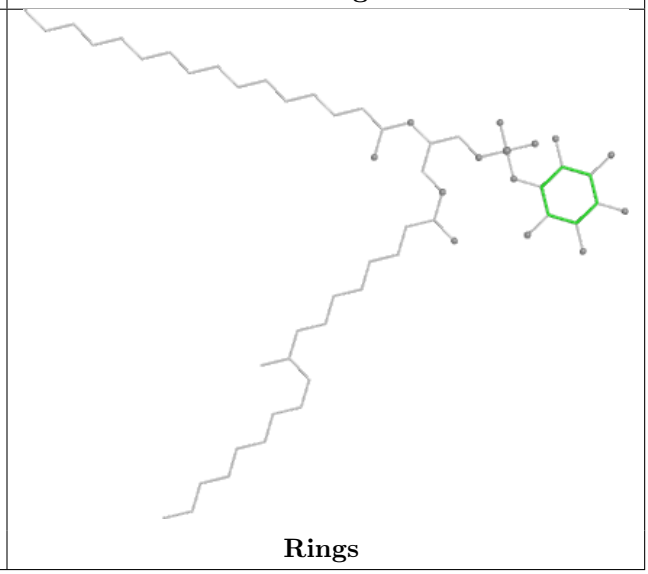
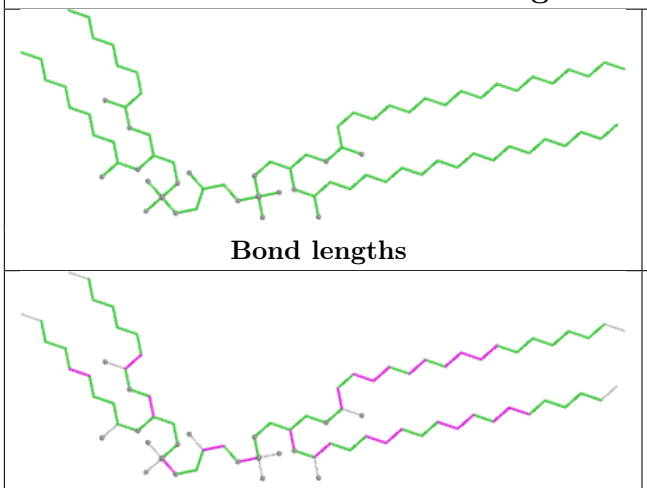


Rings

Ligand CDL I 605



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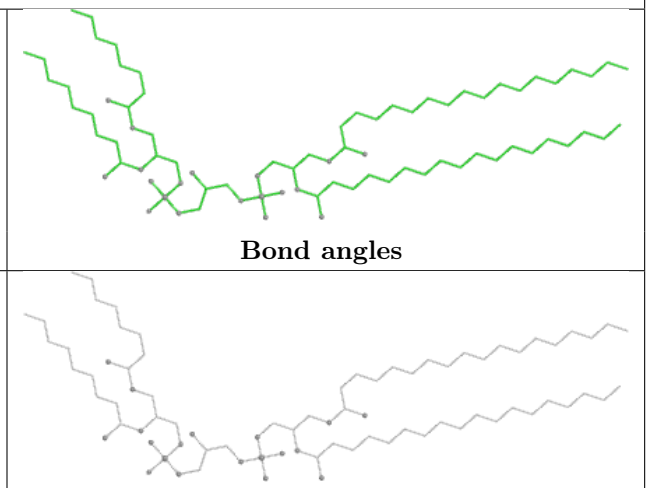
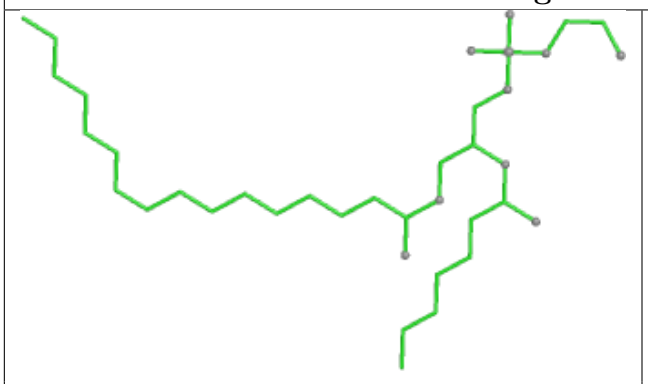


Bond angles

Torsions

Rings

Ligand 9Y0 b 101



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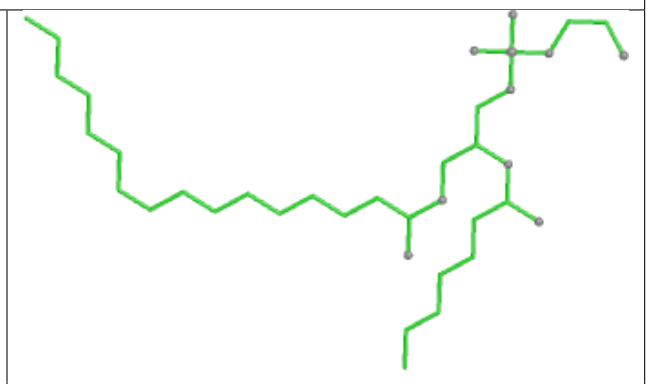

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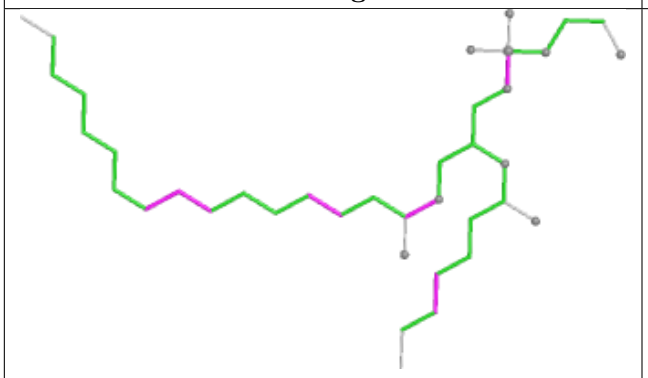

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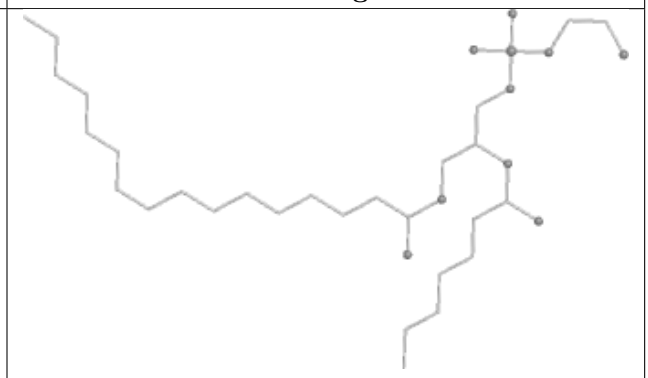
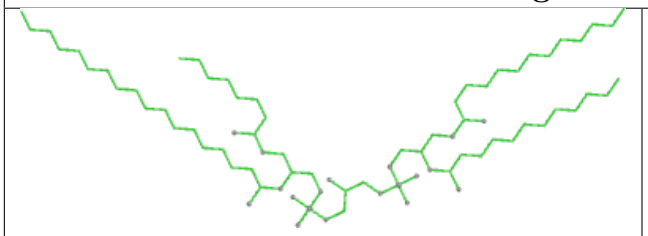


Rings

Ligand CDL j 606



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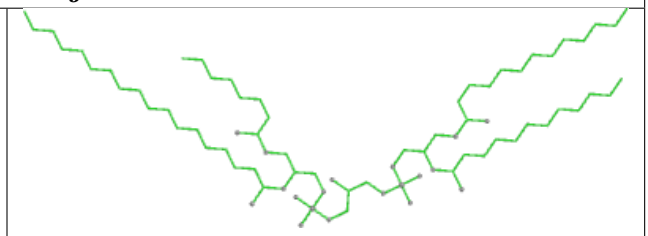

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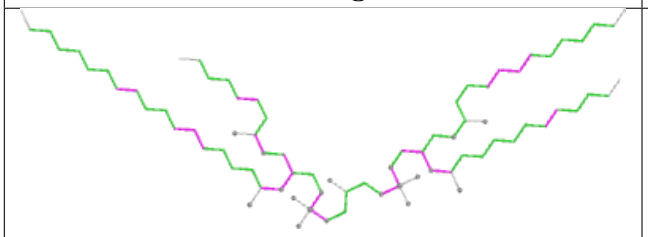

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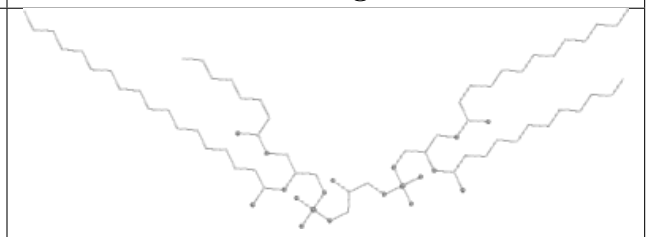
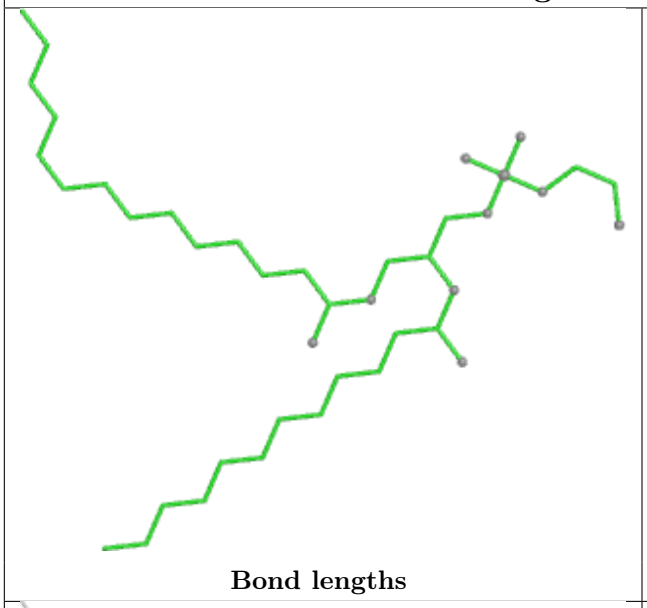


Rings

Ligand 9Y0 b 104



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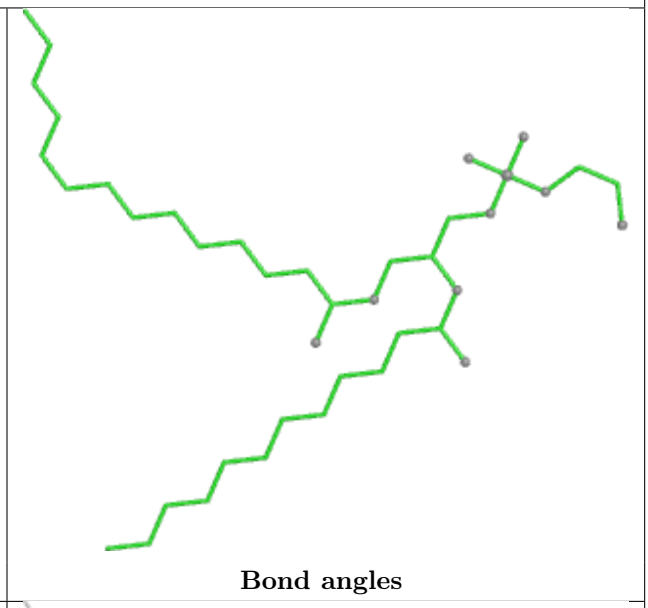

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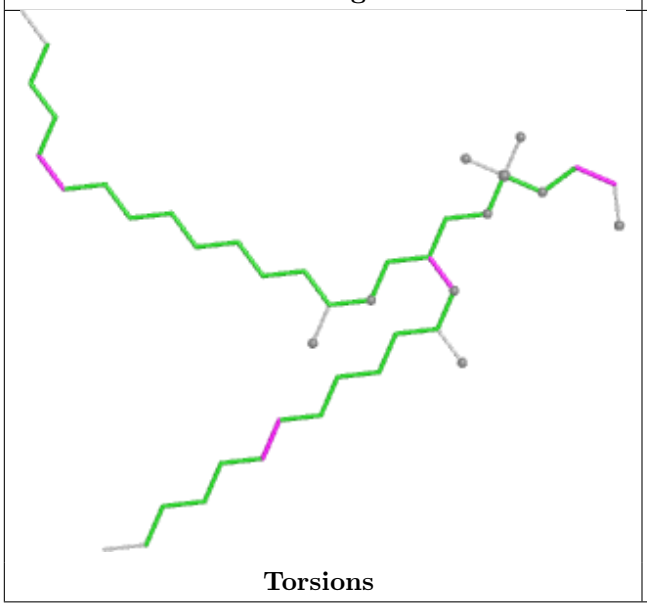

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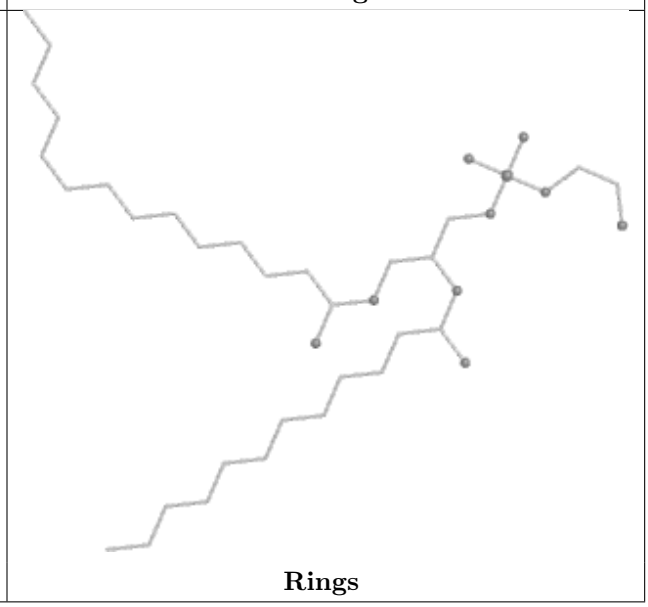
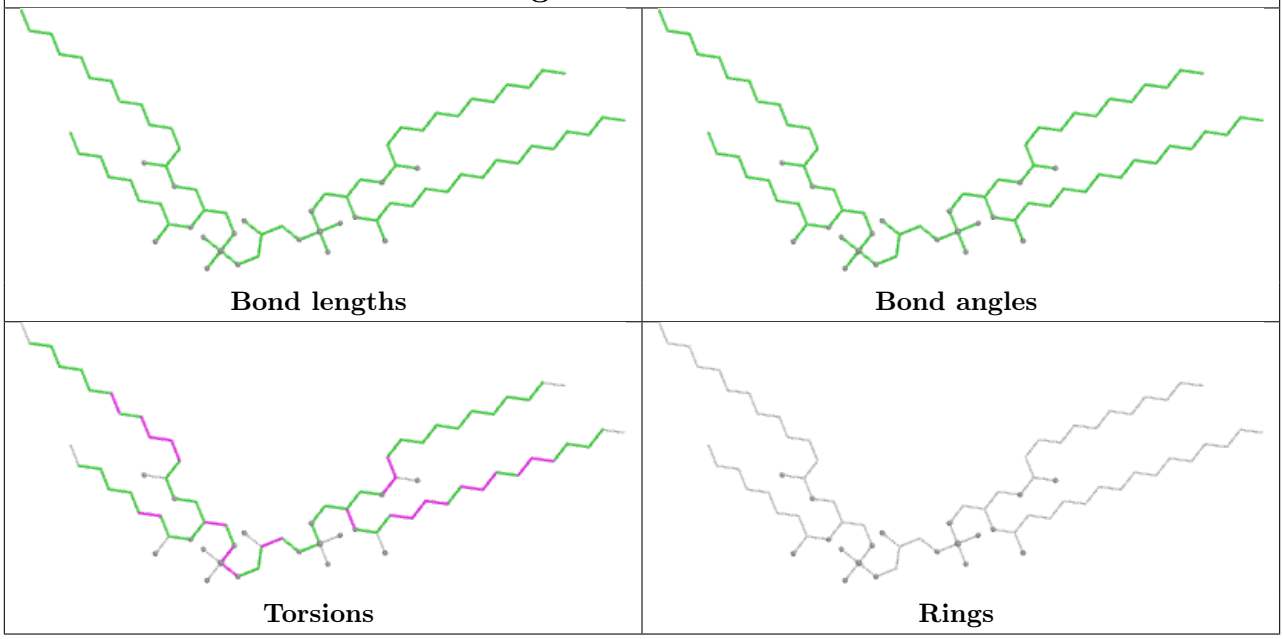


Rings

Ligand CDL I 604



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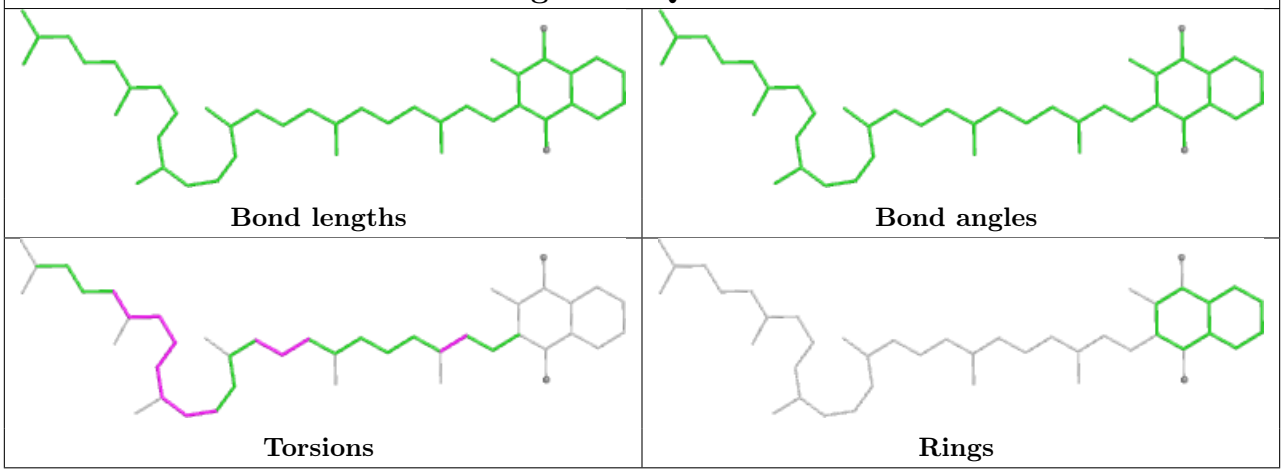
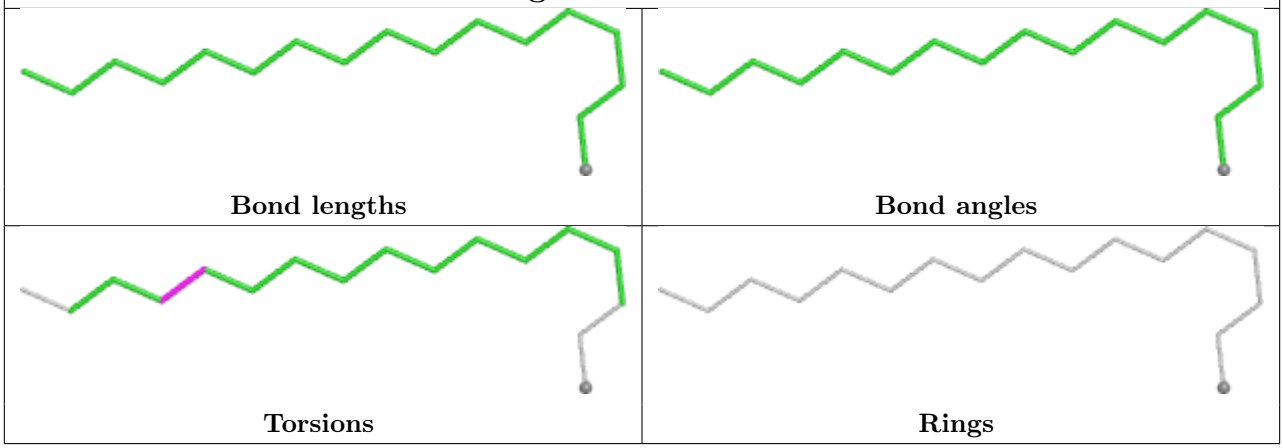
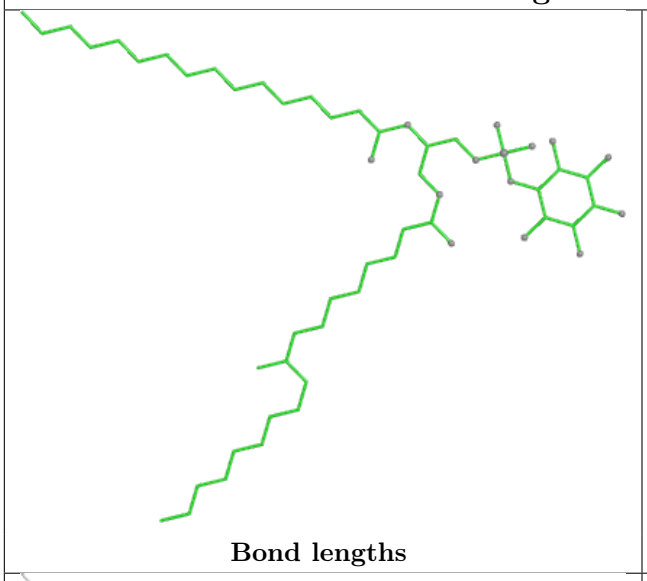


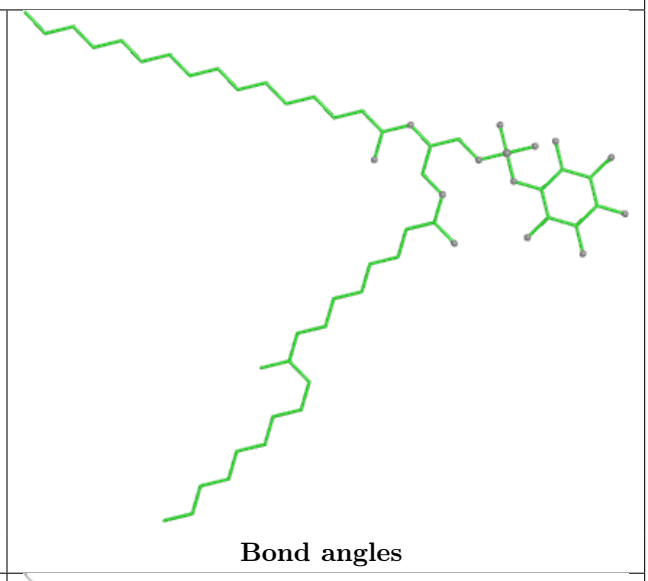
Ligand PLM I 606



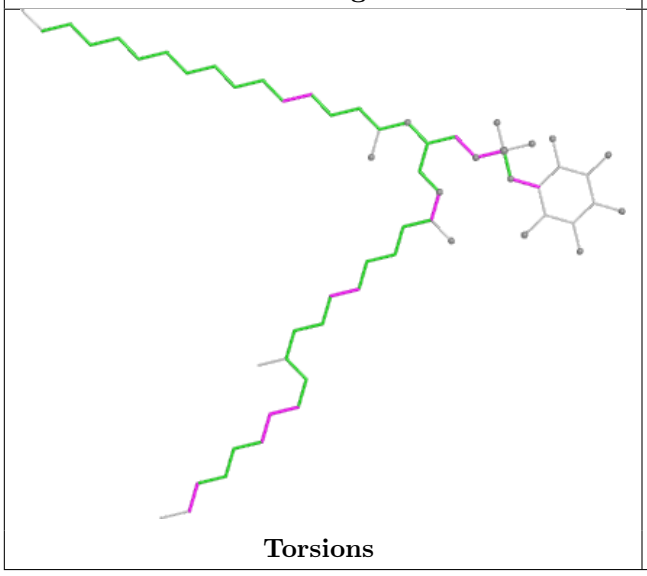
Ligand 9YF o 603



Bond lengths



Bond angles



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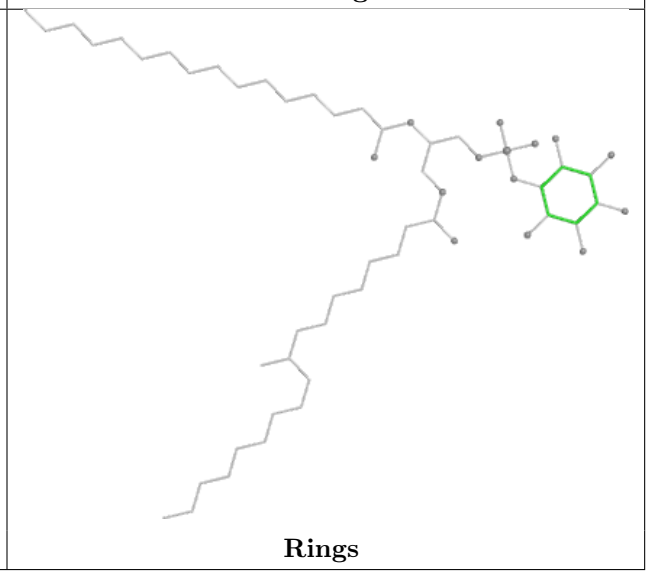
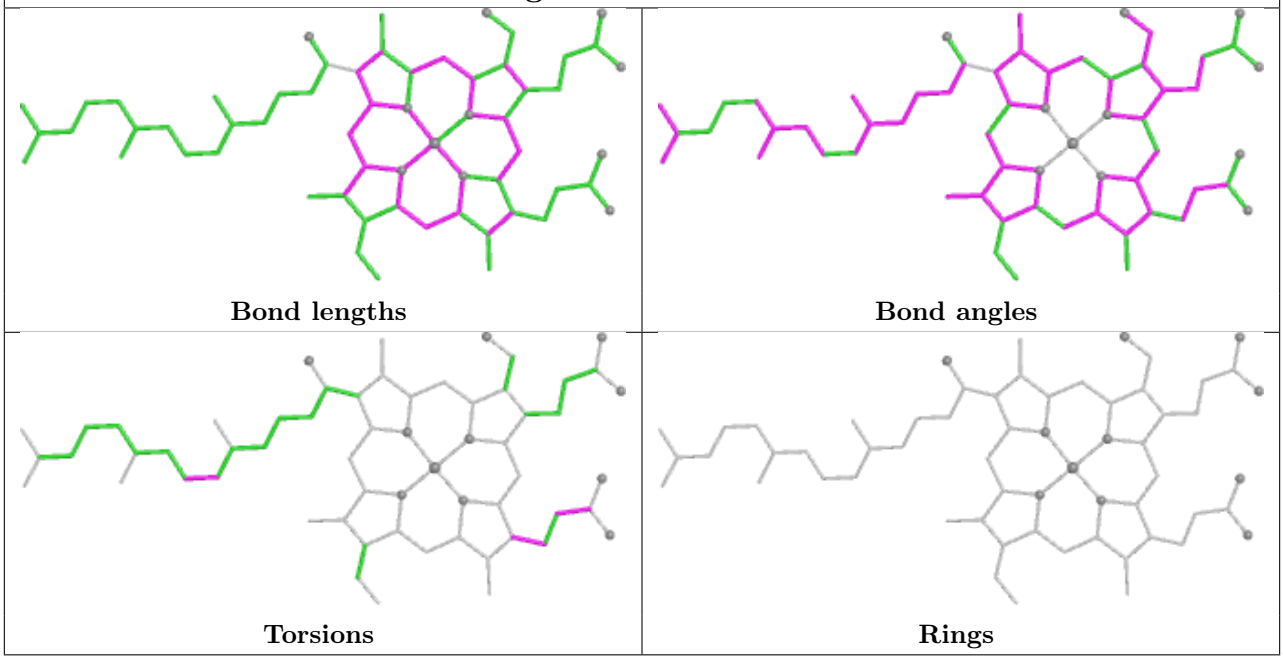
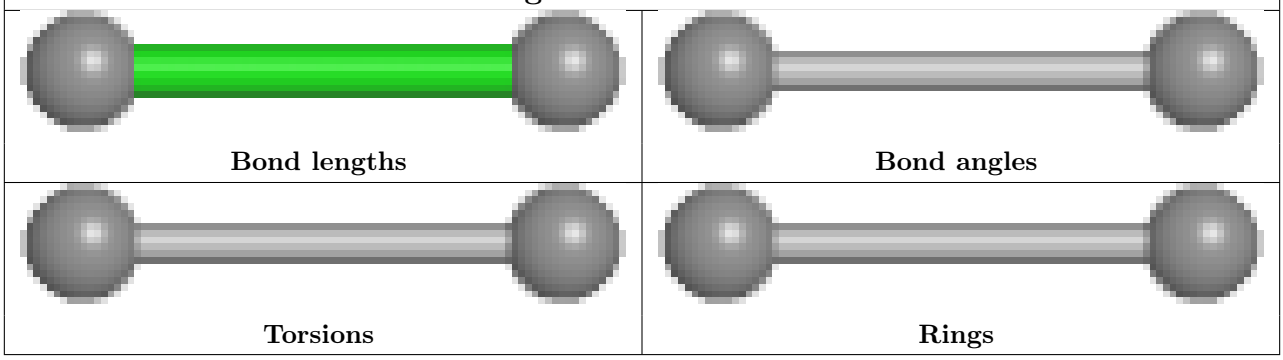


Rings

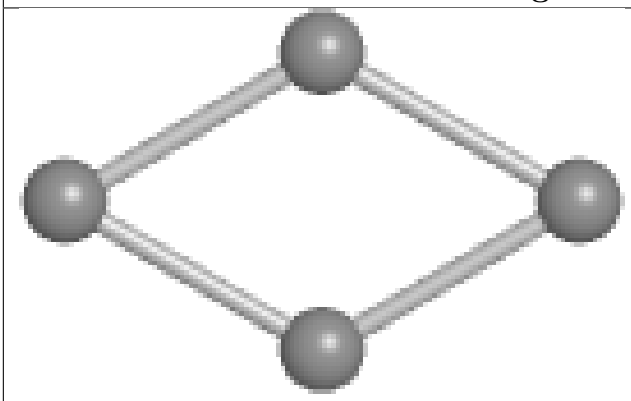
Ligand HEA L 601



Ligand OXY L 607



Ligand FES p 602



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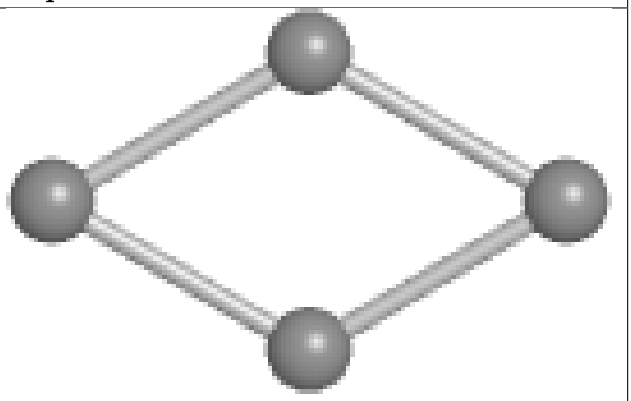
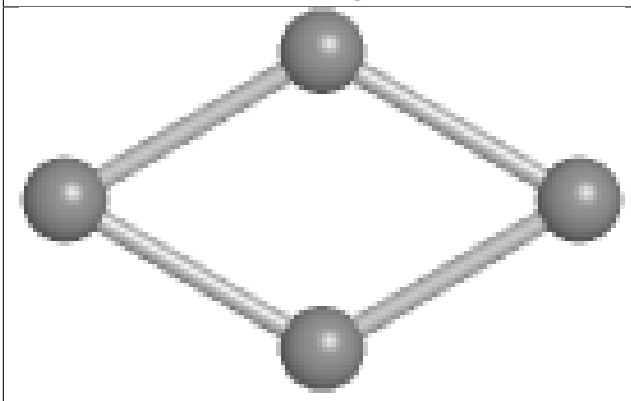
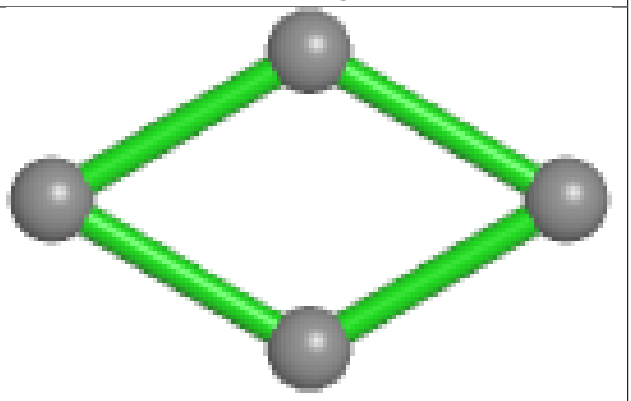


Bond angles

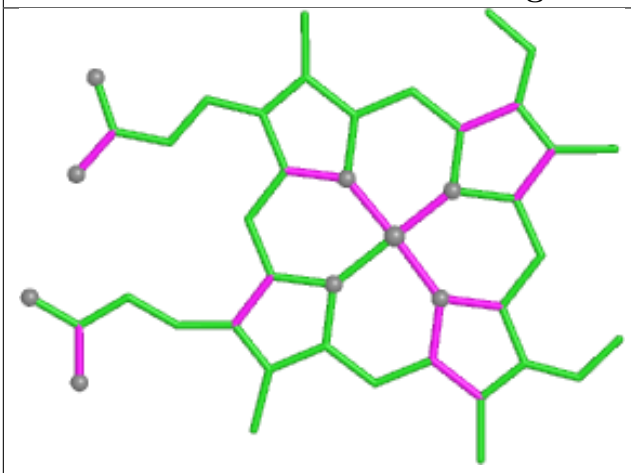


Torsions



Rings

Ligand HEM j 604



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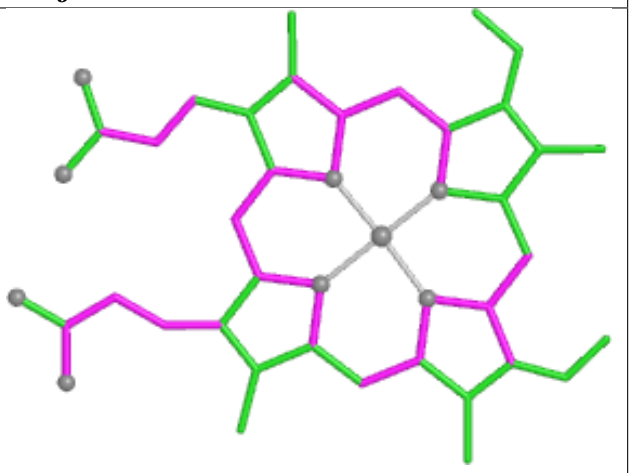
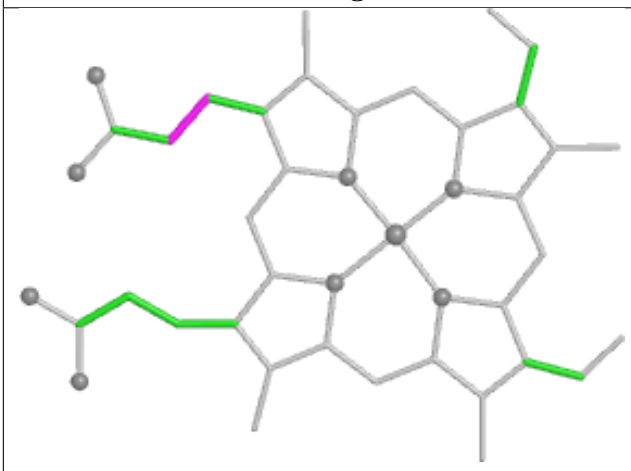


Bond angles



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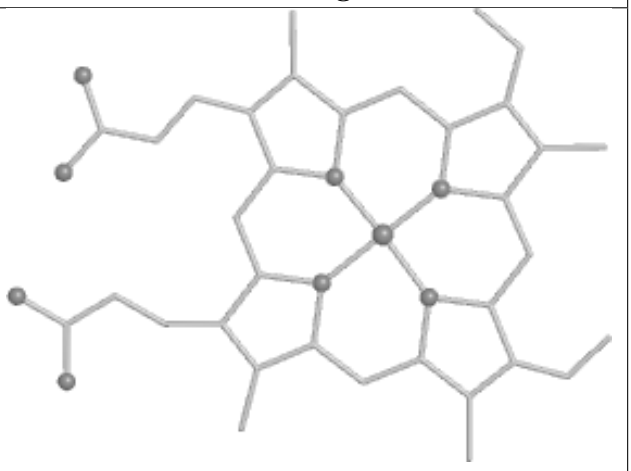
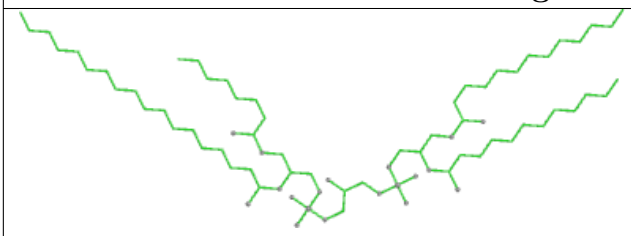


Rings

Ligand CDL i 609



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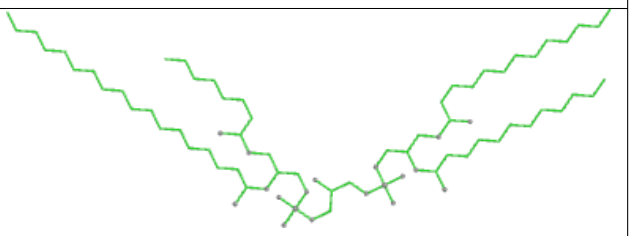

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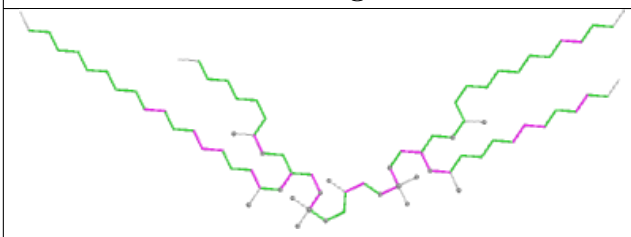

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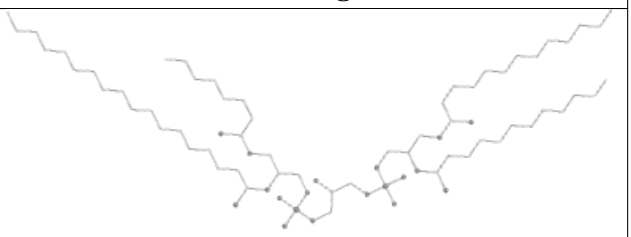
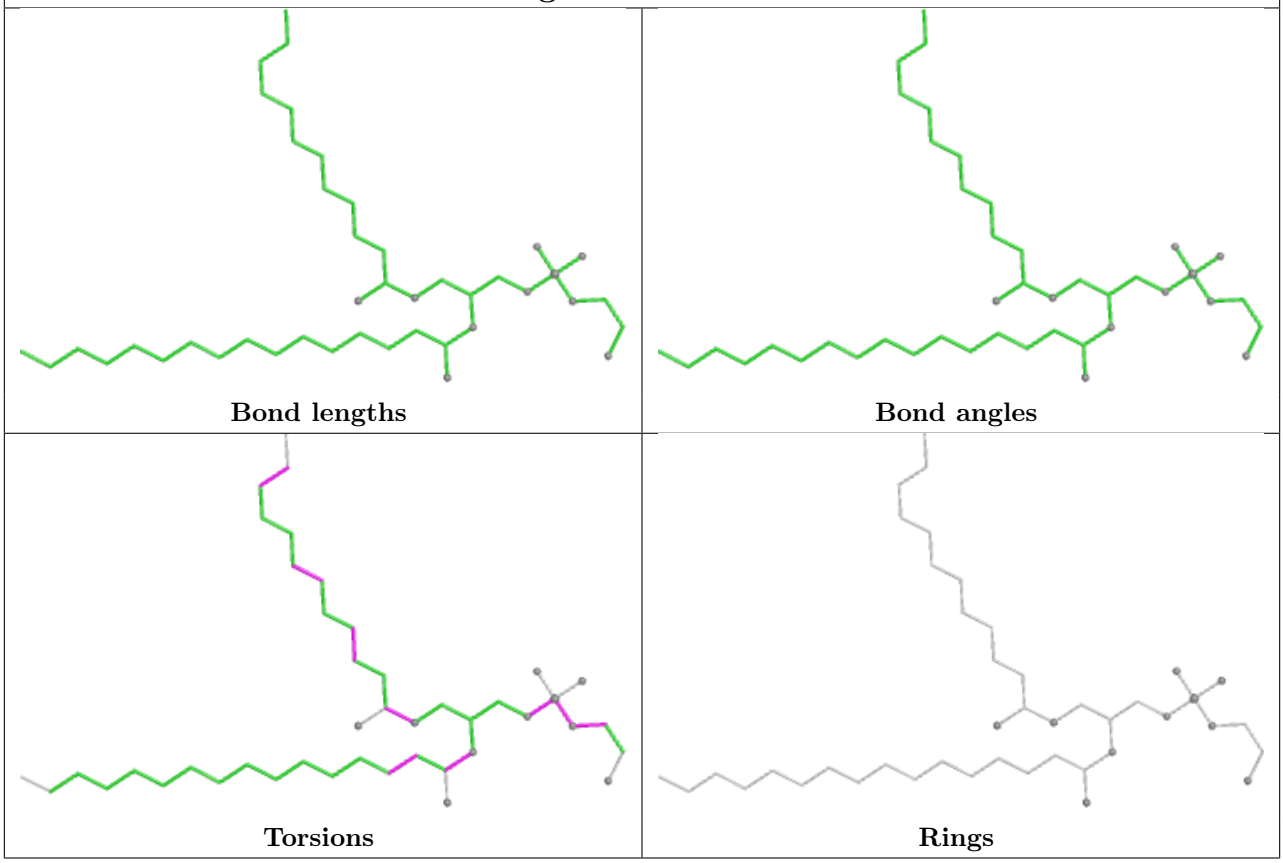


Rings

Ligand 9Y0 f 601



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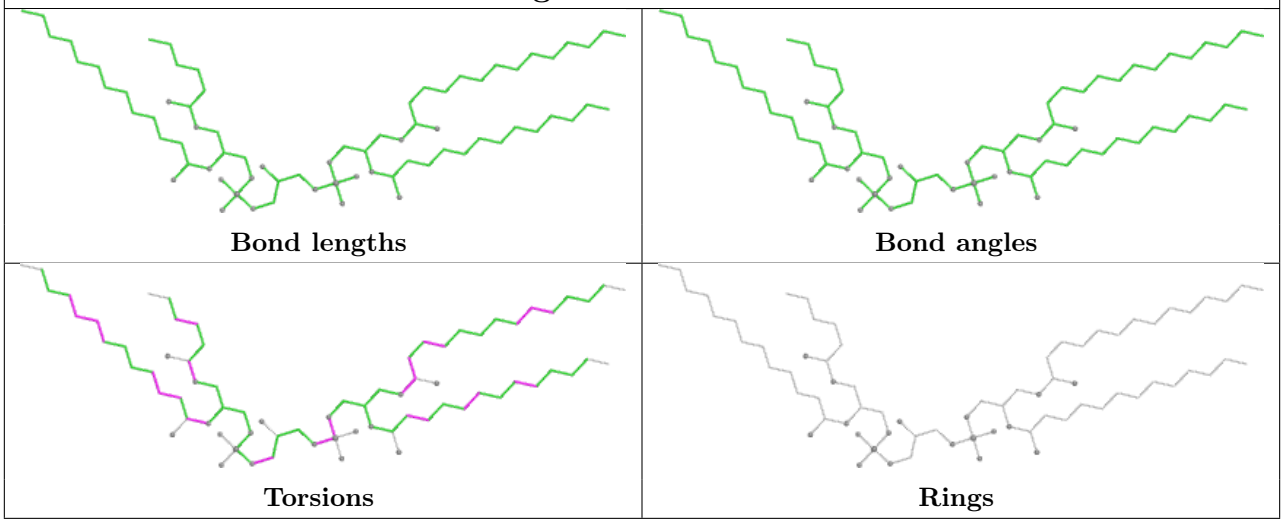
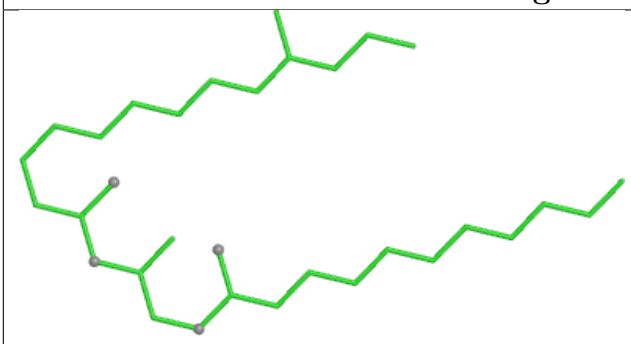


Ligand 9XX j 610



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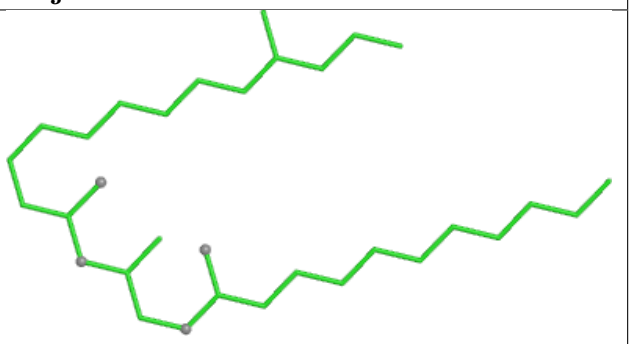
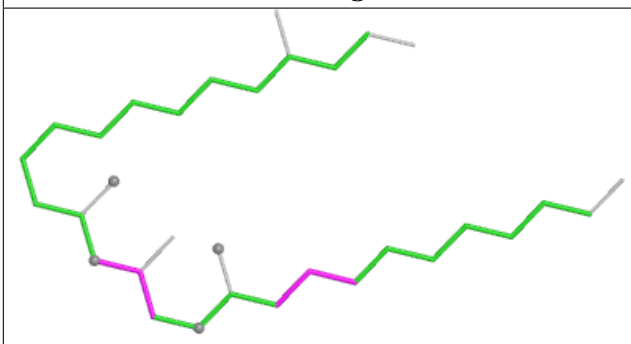


Bond angles



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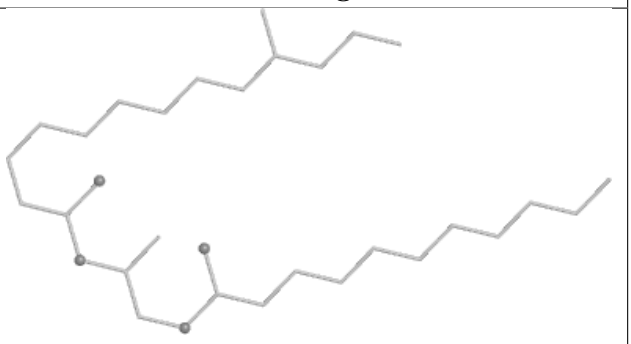
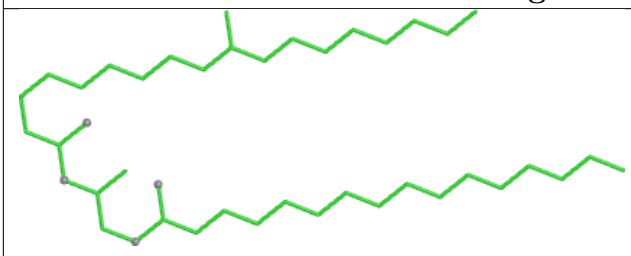


Rings

Ligand 9XX b 102



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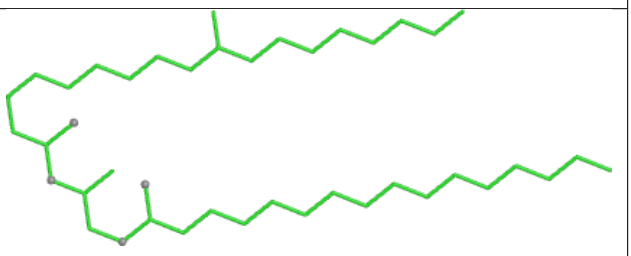
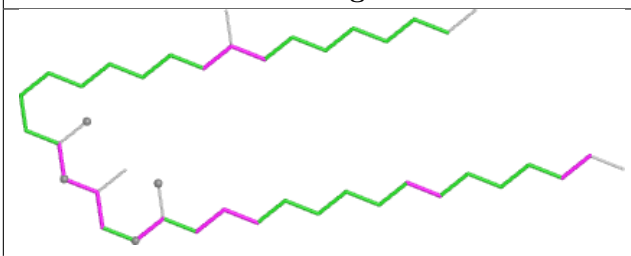


Bond angles



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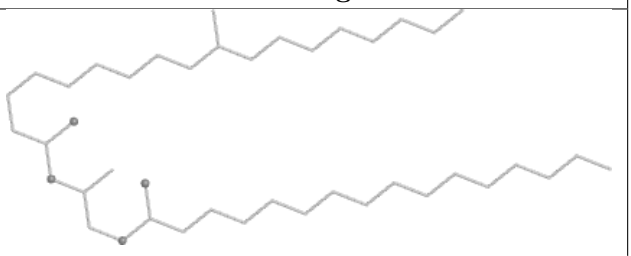
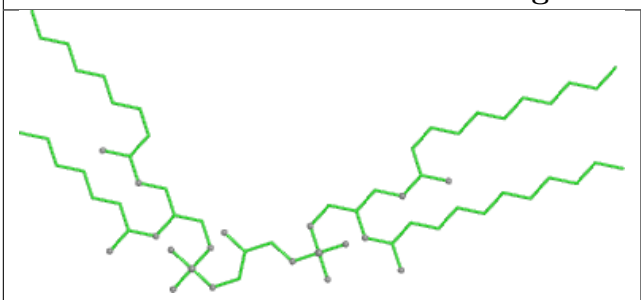


Rings

Ligand CDL j 609



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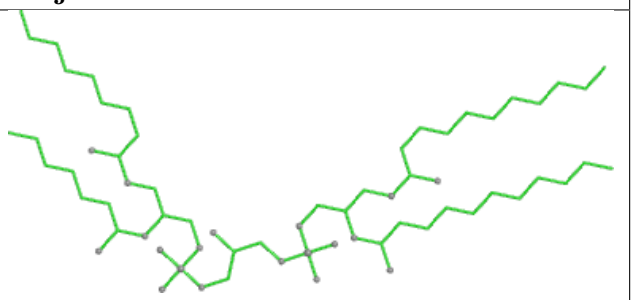
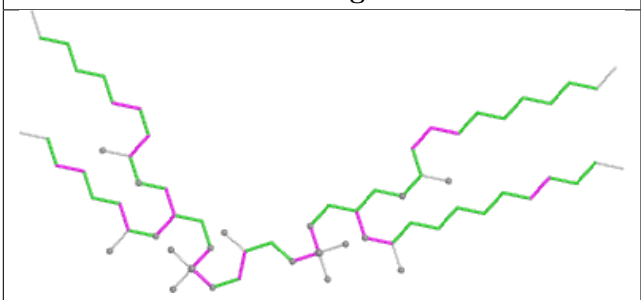


Bond angles



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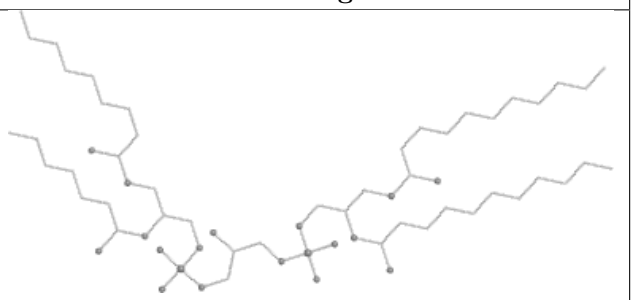
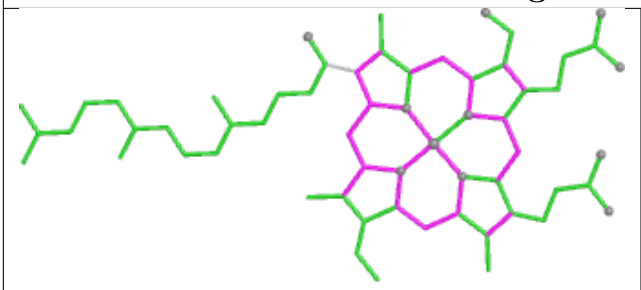


Rings

Ligand HEA I 601



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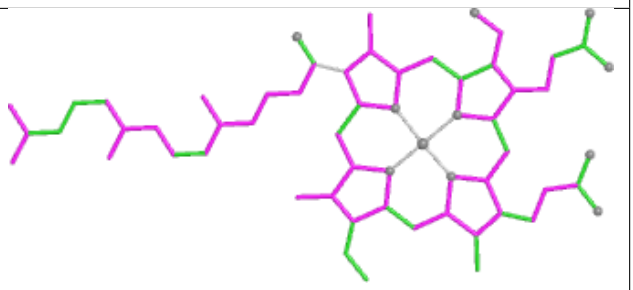
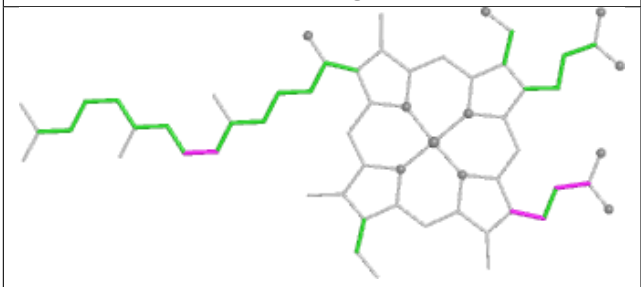


Bond angles



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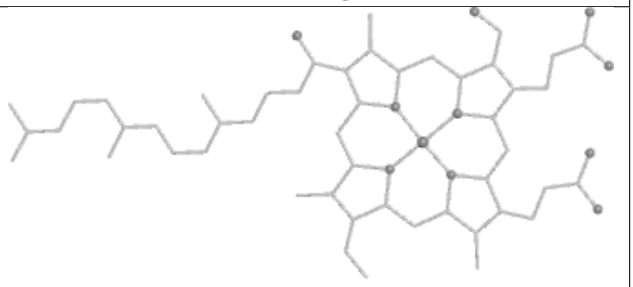
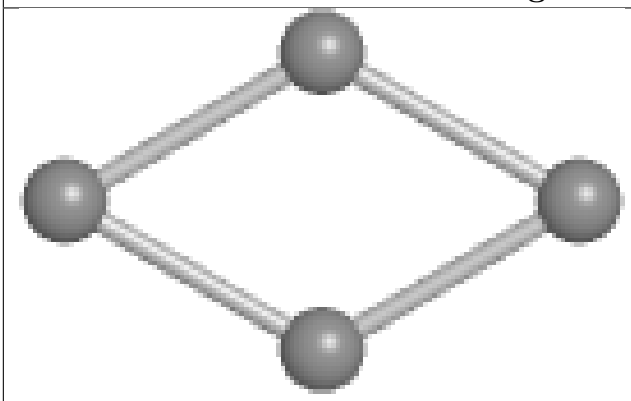


Rings

Ligand FES V 601



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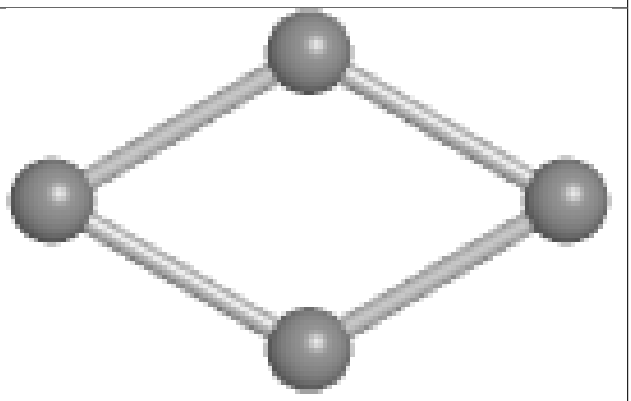
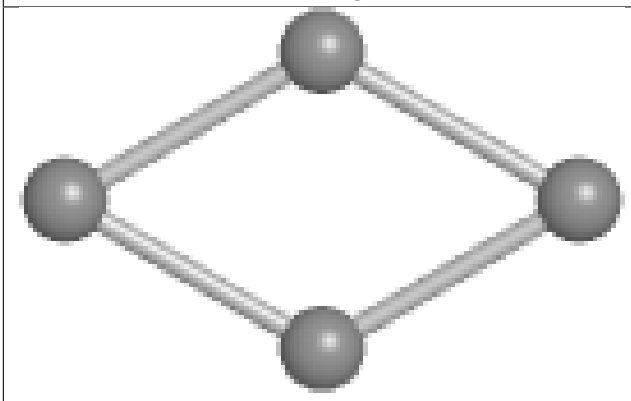


Bond angles



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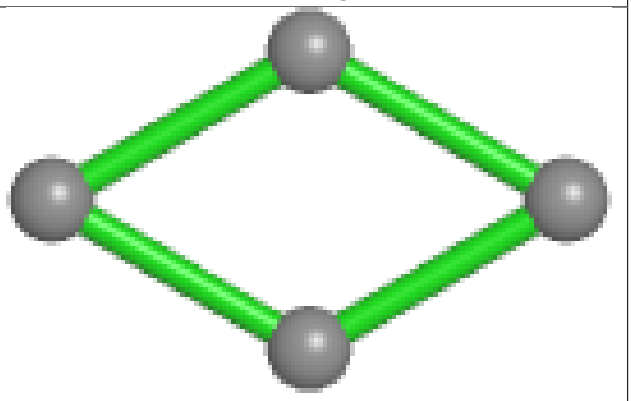
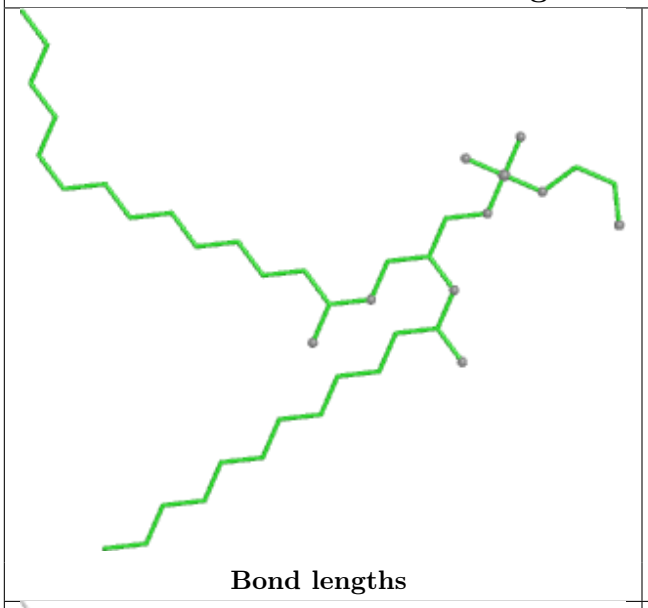


Rings

Ligand 9Y0 G 103



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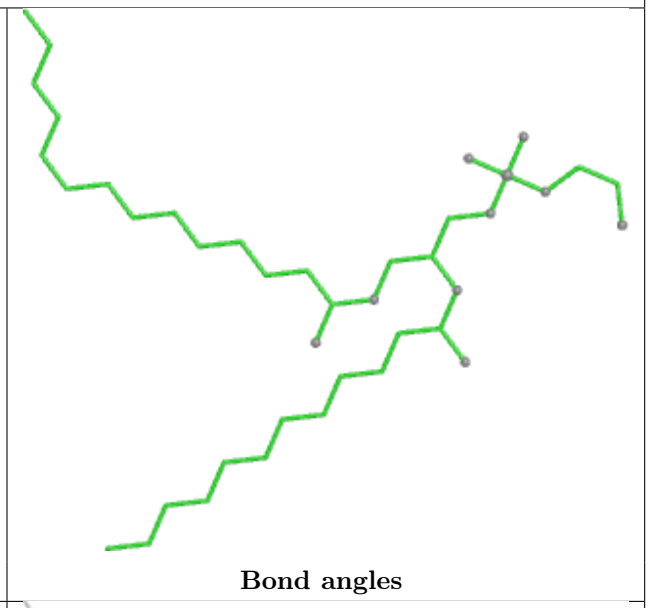
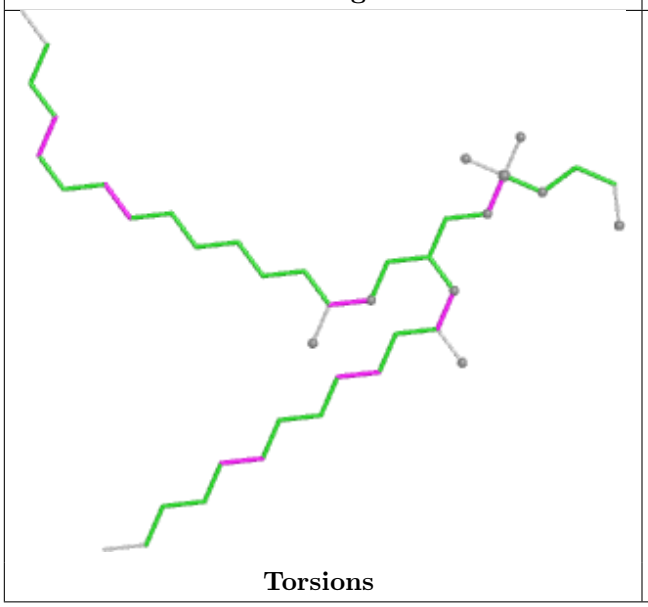


Bond angles



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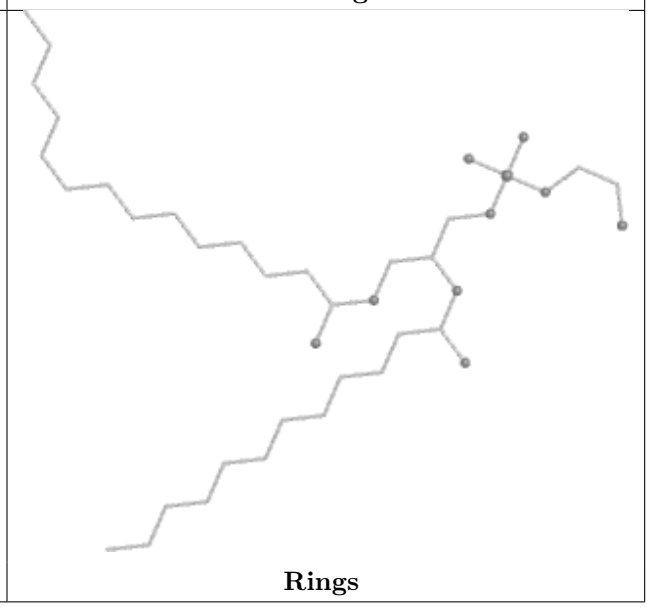
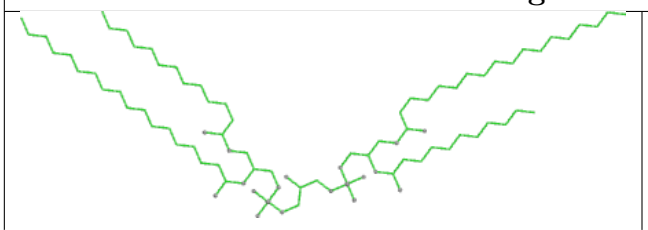


Rings

Ligand CDL b 103



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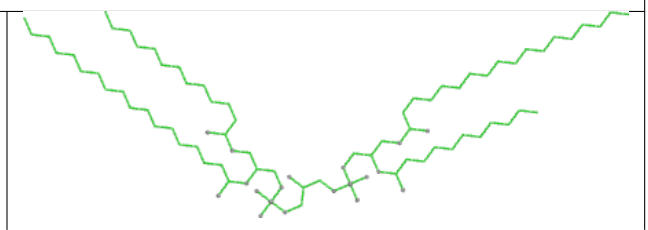
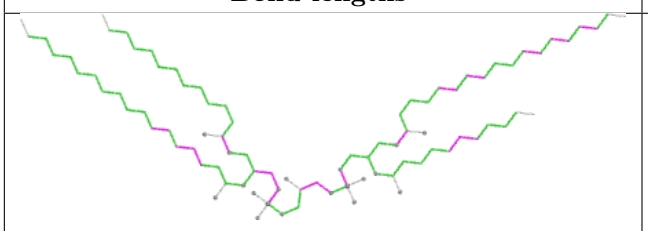


Bond angles



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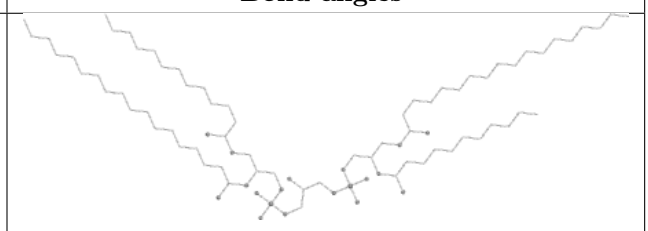
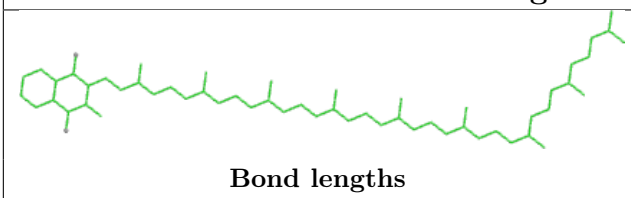


Rings

Ligand MQ9 i 612



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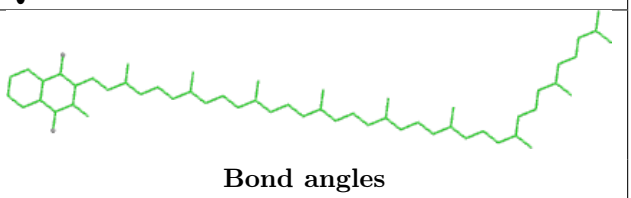
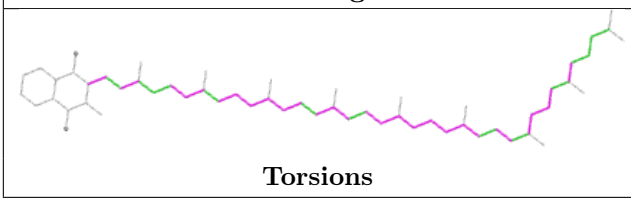


Bond angles



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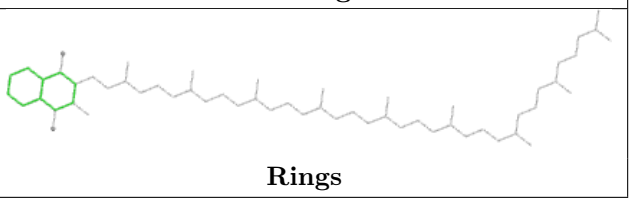
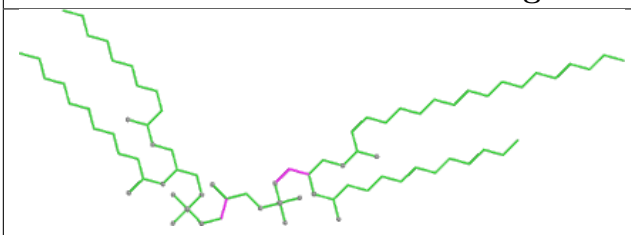


Rings

Ligand CDL U 603



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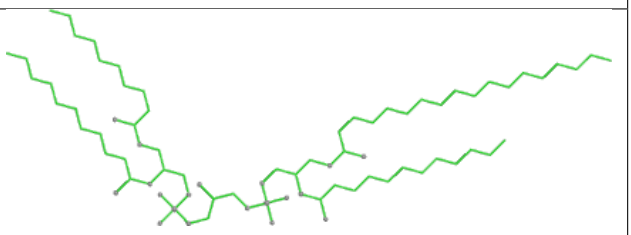
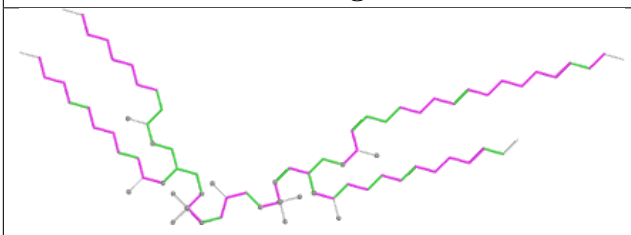


Bond angles



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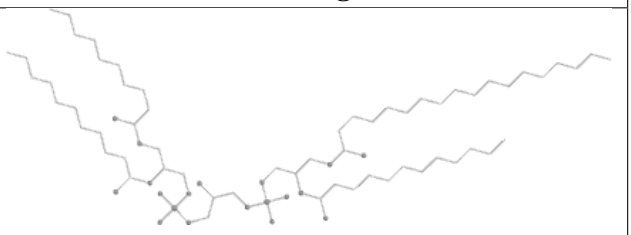
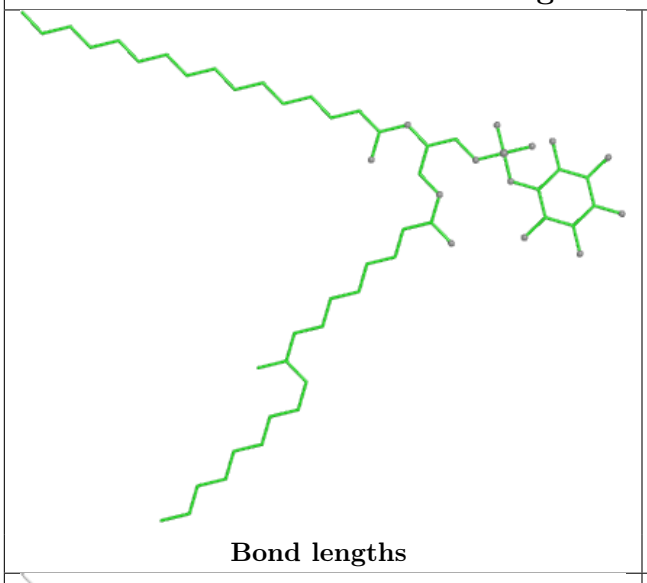


Rings

Ligand 9YF i 601



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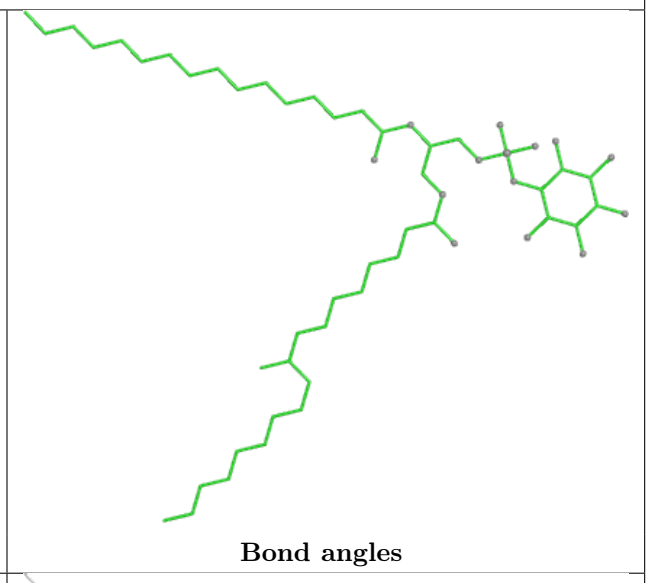
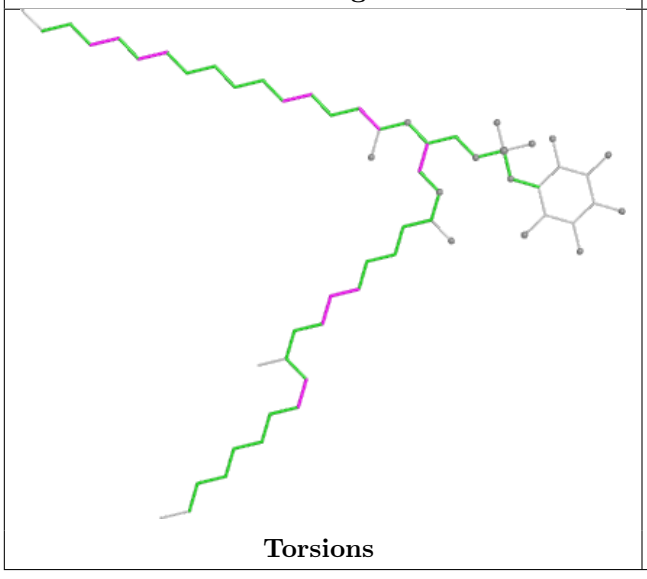


Bond angles



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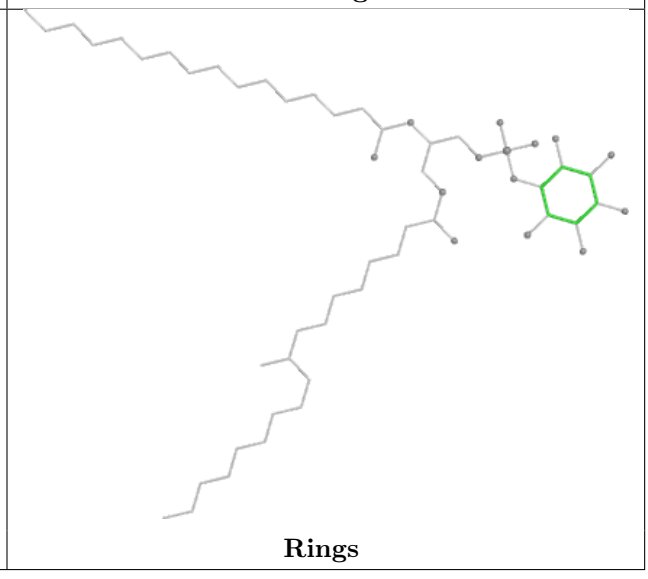
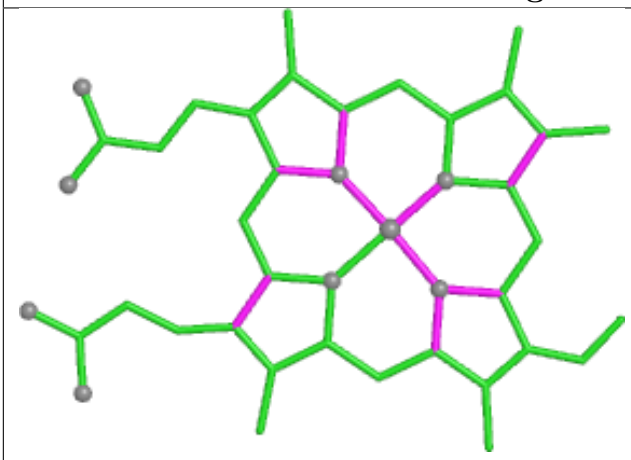


Rings

Ligand HEM j 603



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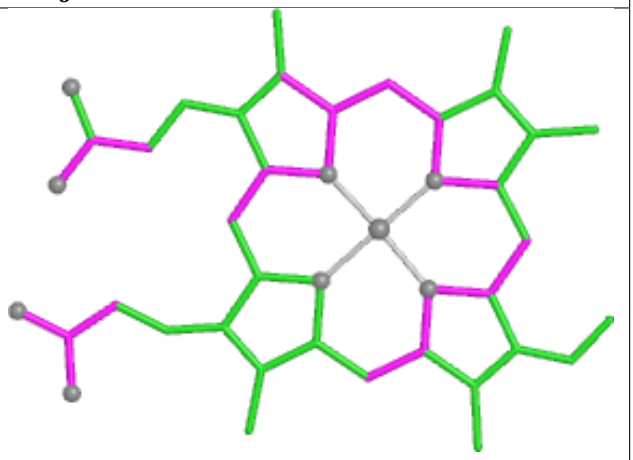
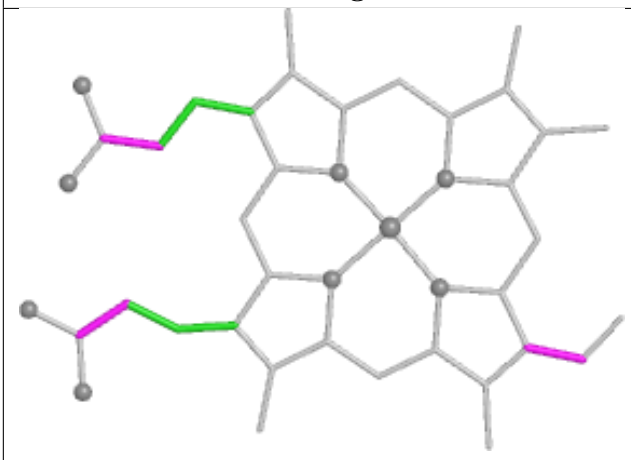


Bond angles



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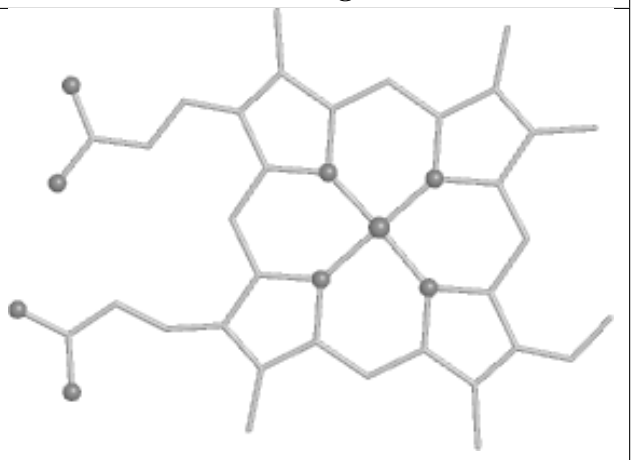
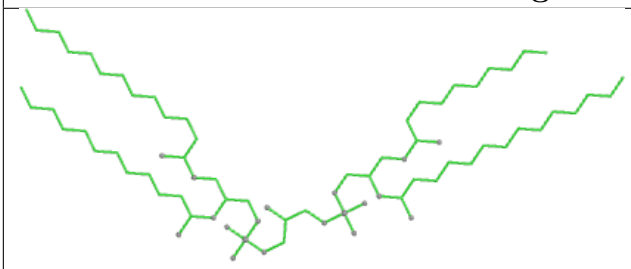


Rings

Ligand CDL j 605



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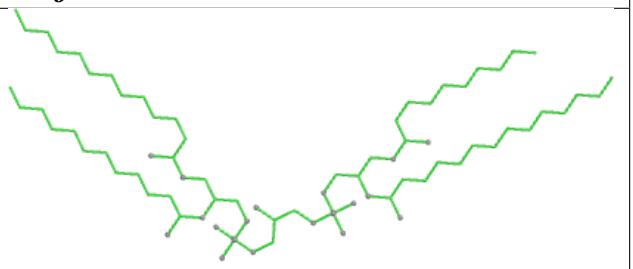
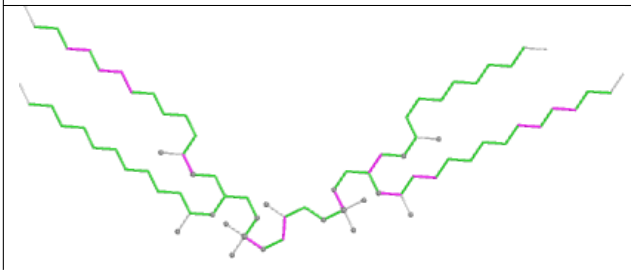
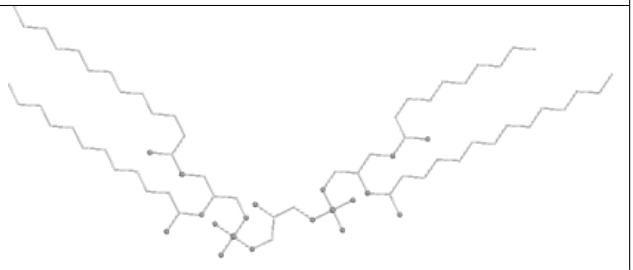


Bond angles

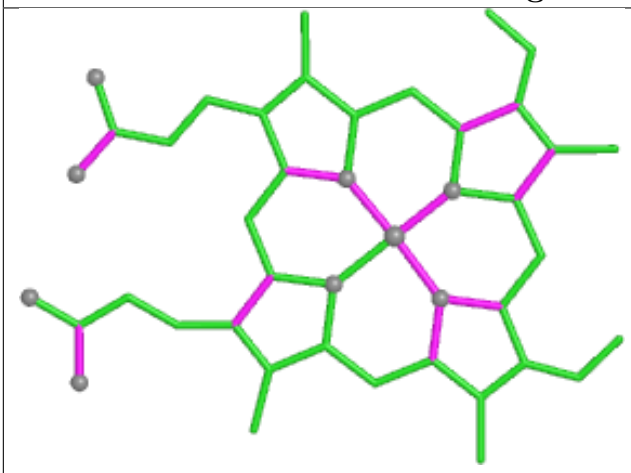


Torsions

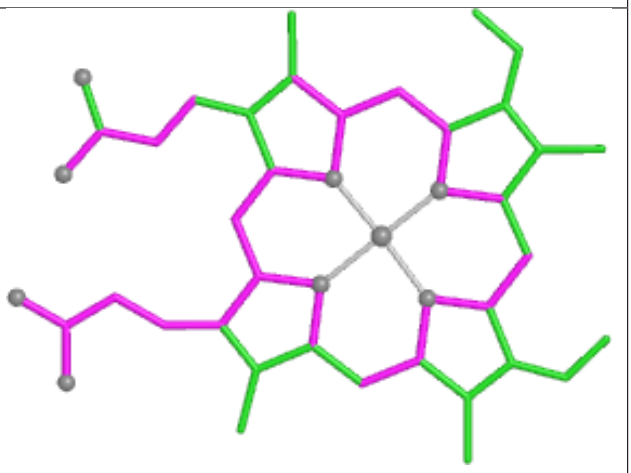


Rings

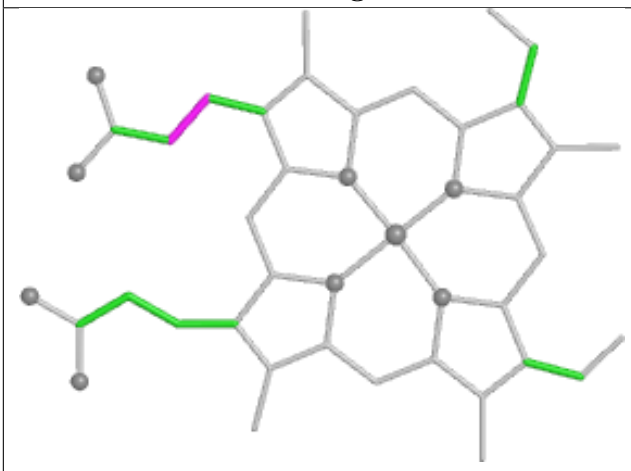
Ligand HEM i 606



Bond lengths



Bond angles



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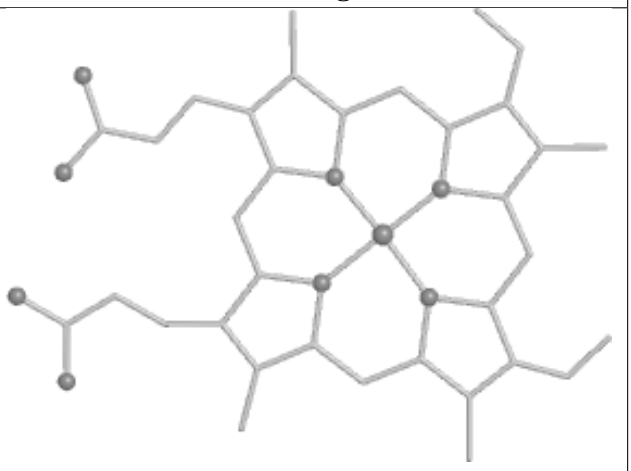
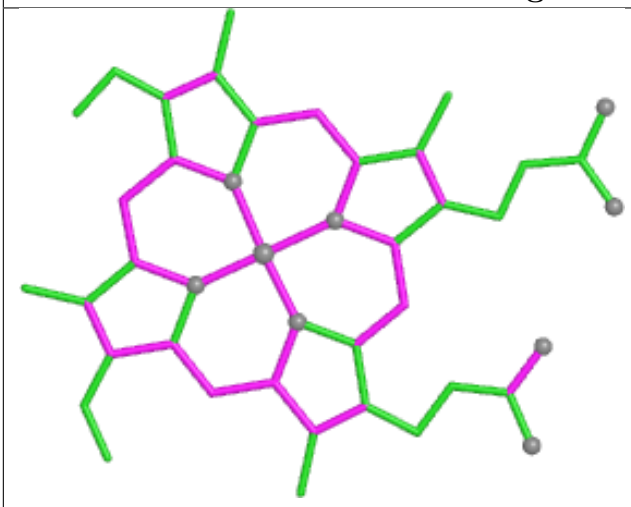
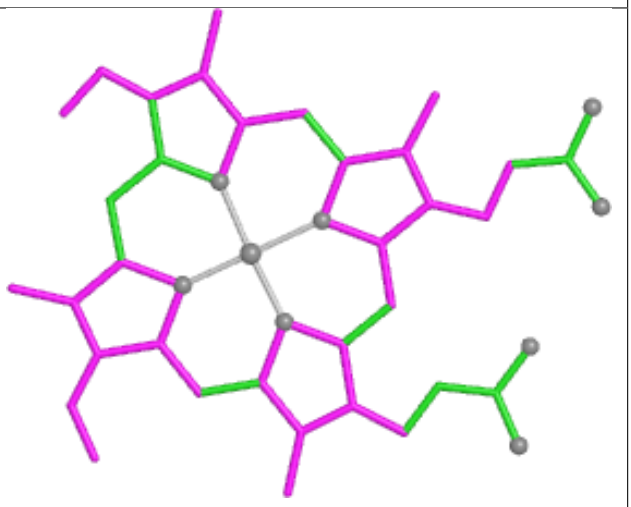


Rings

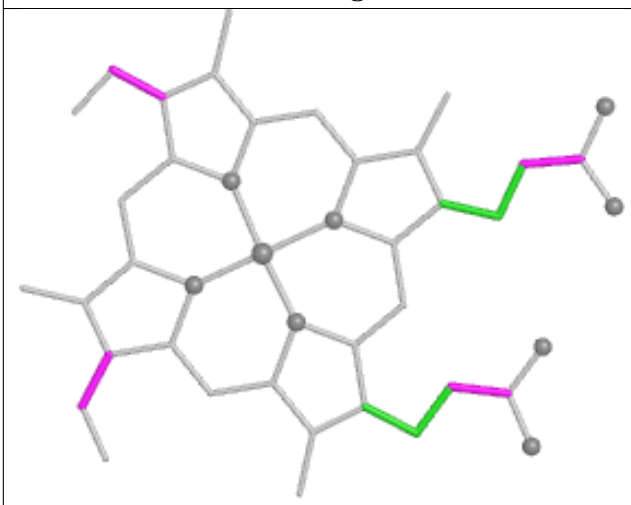
Ligand HEC o 601



Bond lengths



Bond angles



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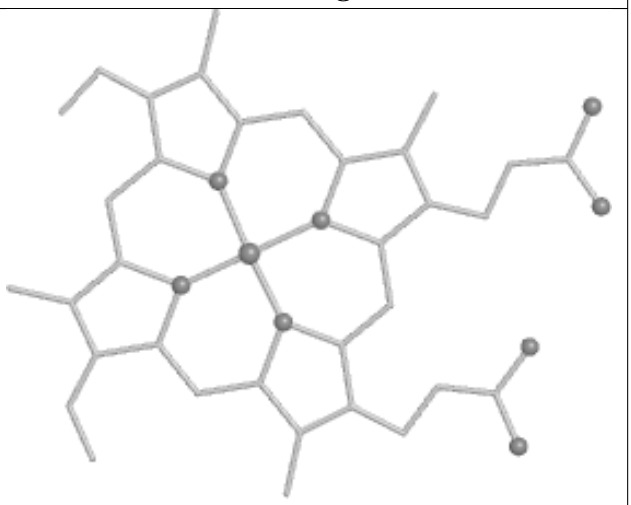
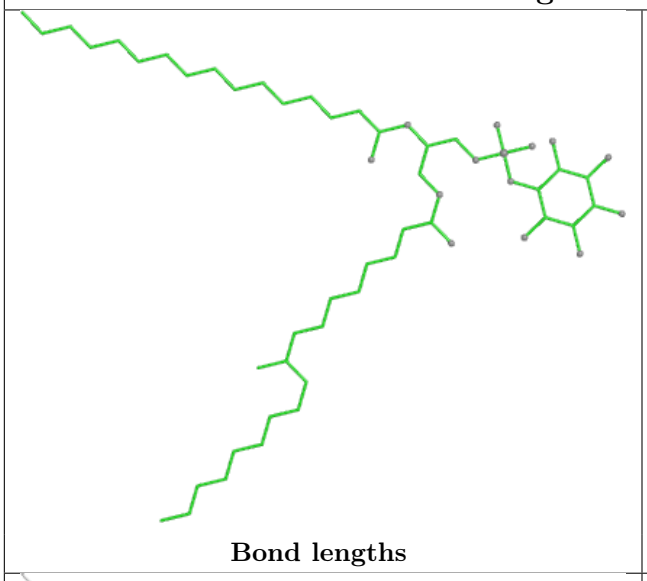


Rings

Ligand 9YF j 601



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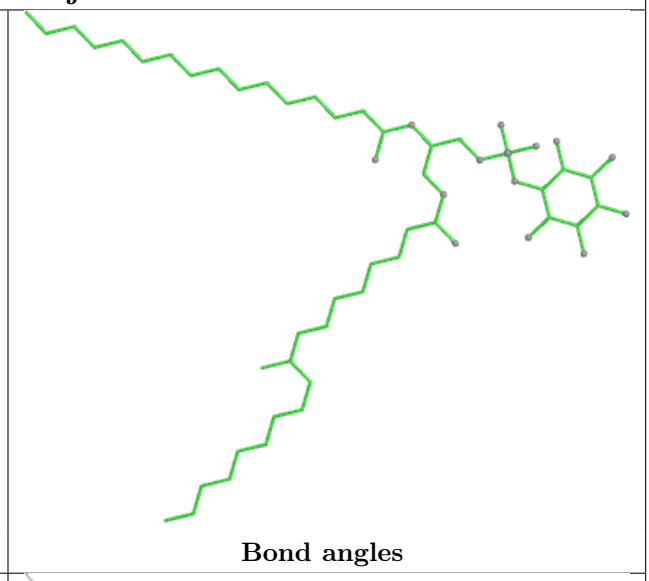
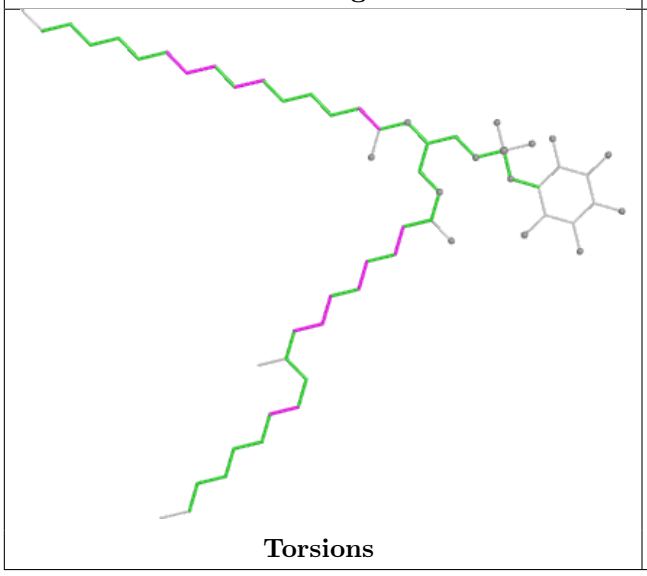


Bond angles



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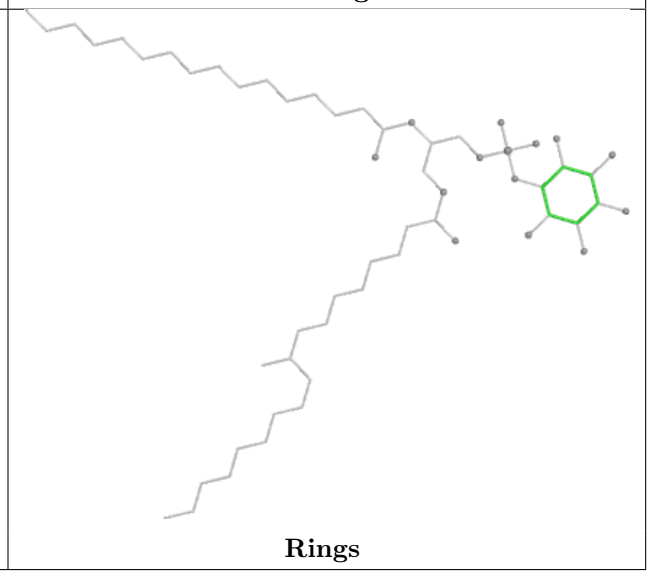
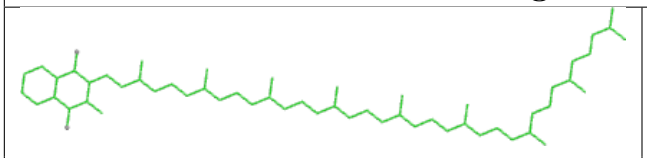


Rings

Ligand MQ9 j 611



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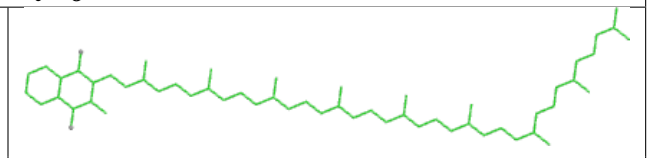
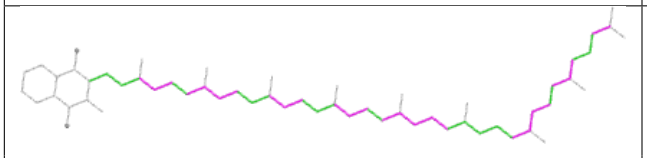


Bond angles



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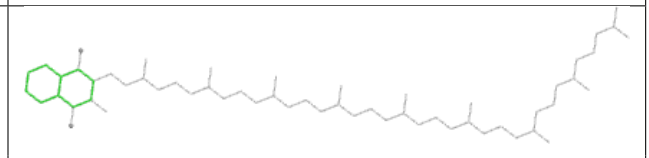
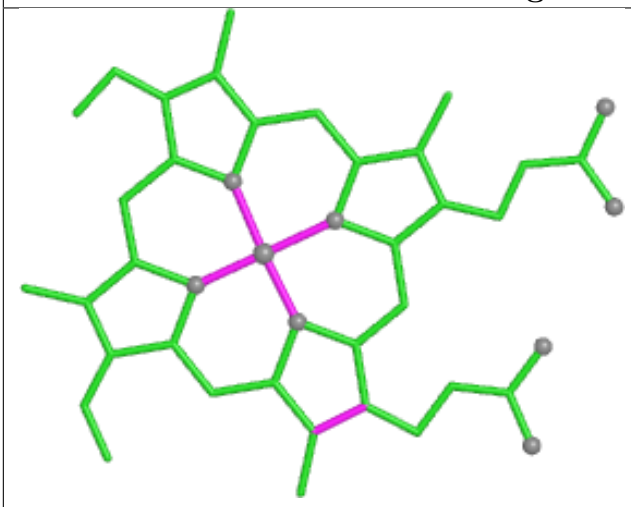


Rings

Ligand HEC o 602



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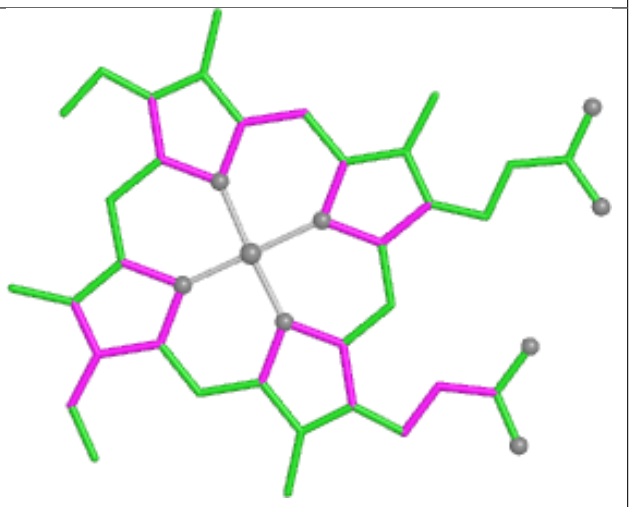
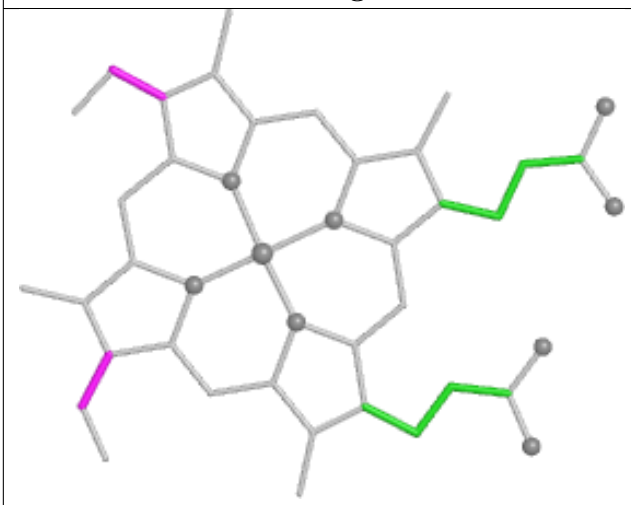


Bond angles



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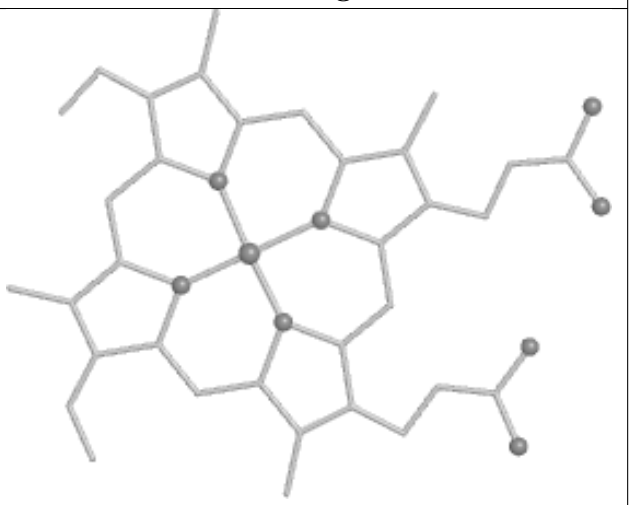
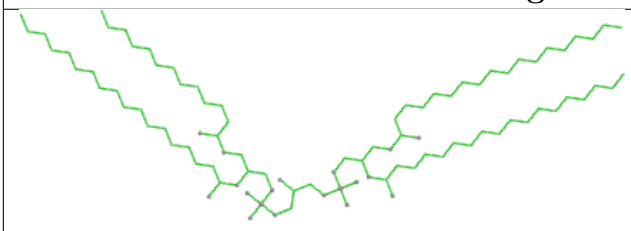
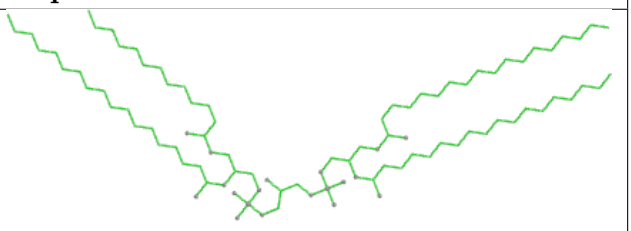


Rings

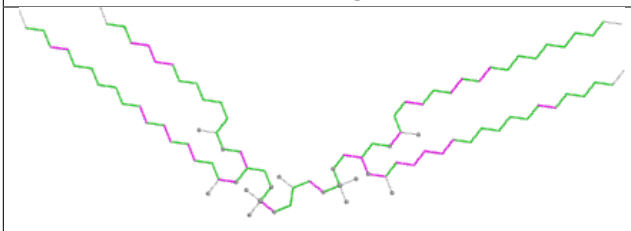
Ligand CDL p 603



Bond lengths



Bond angles



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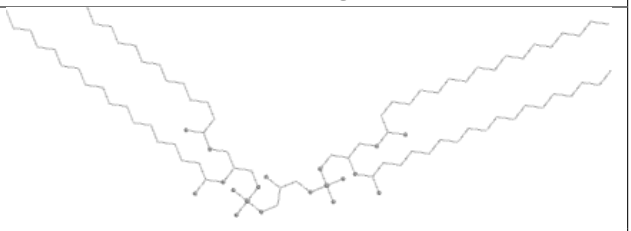
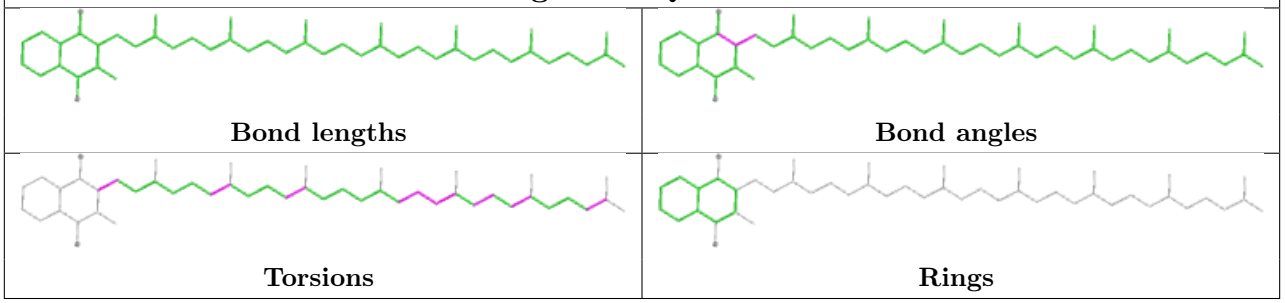
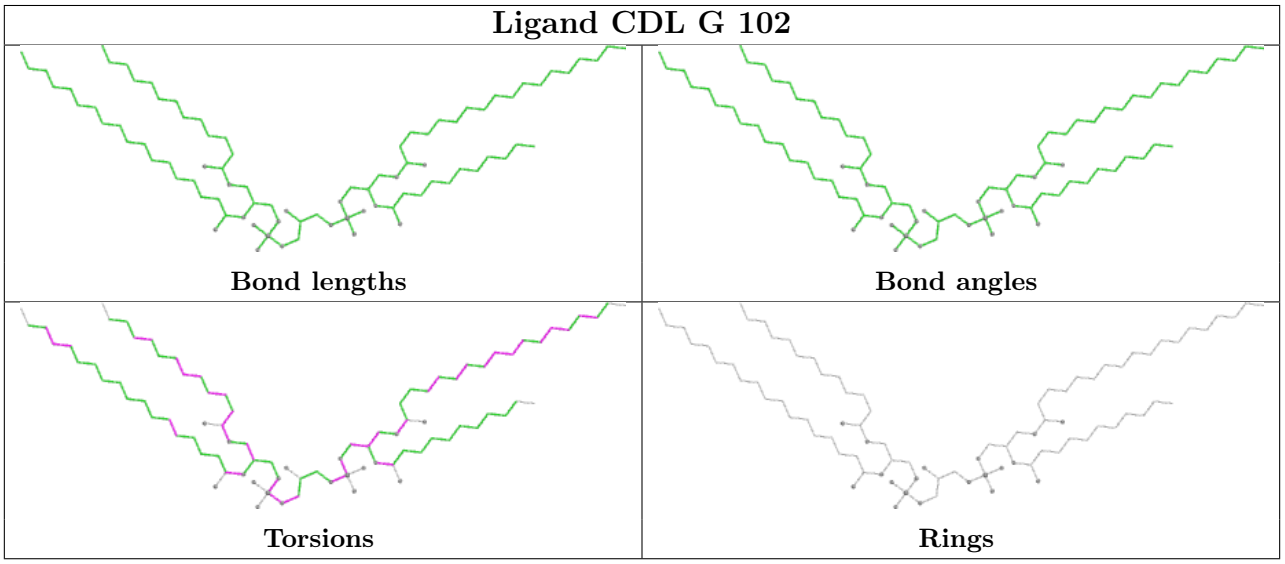


Rings

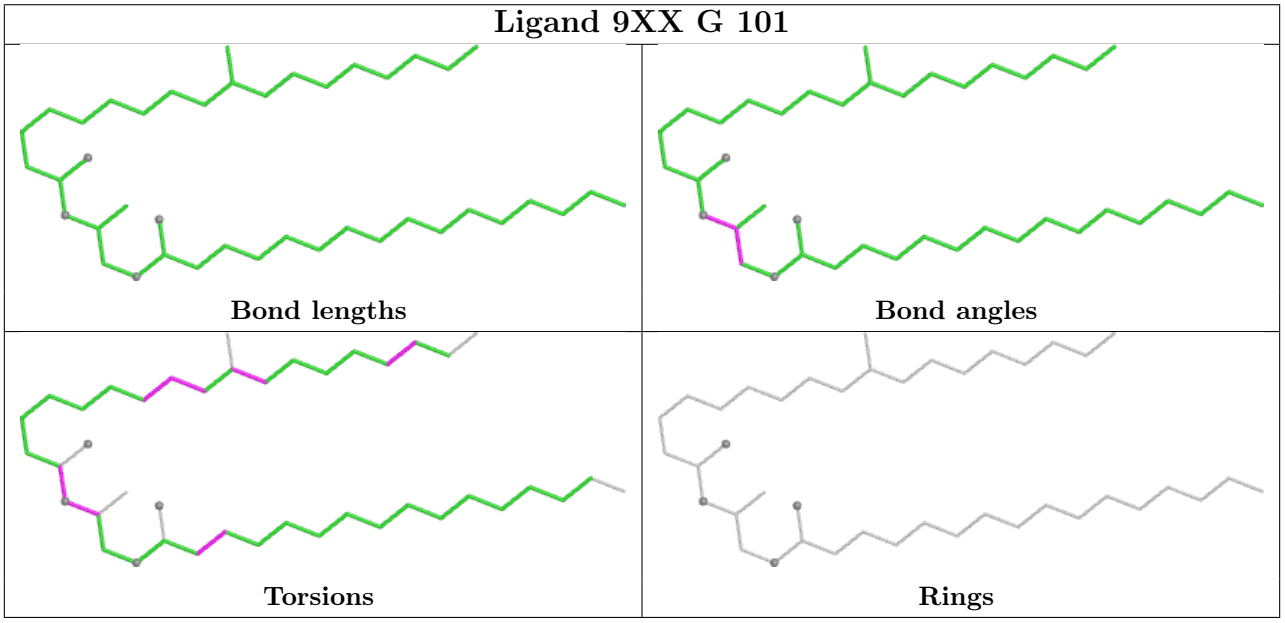
Ligand MQ9 i 611



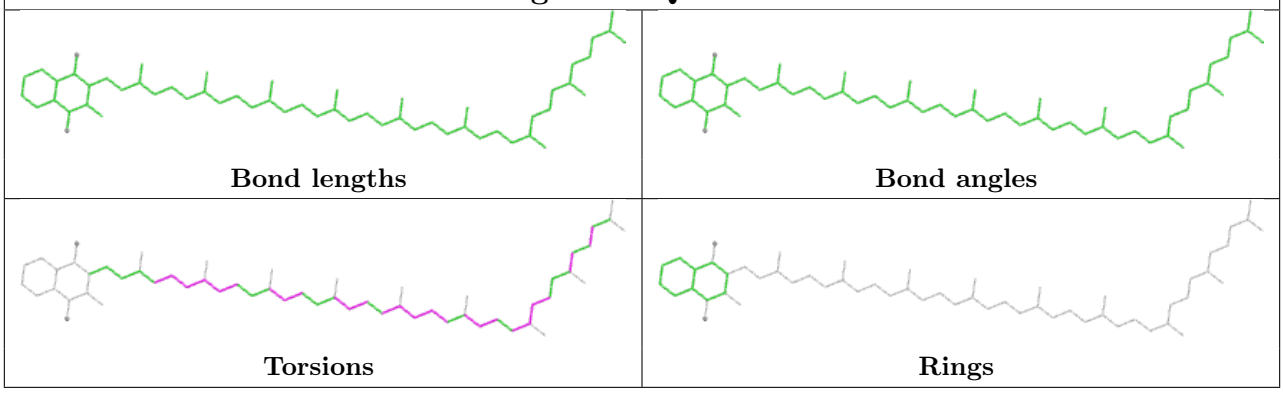
Ligand CDL G 102



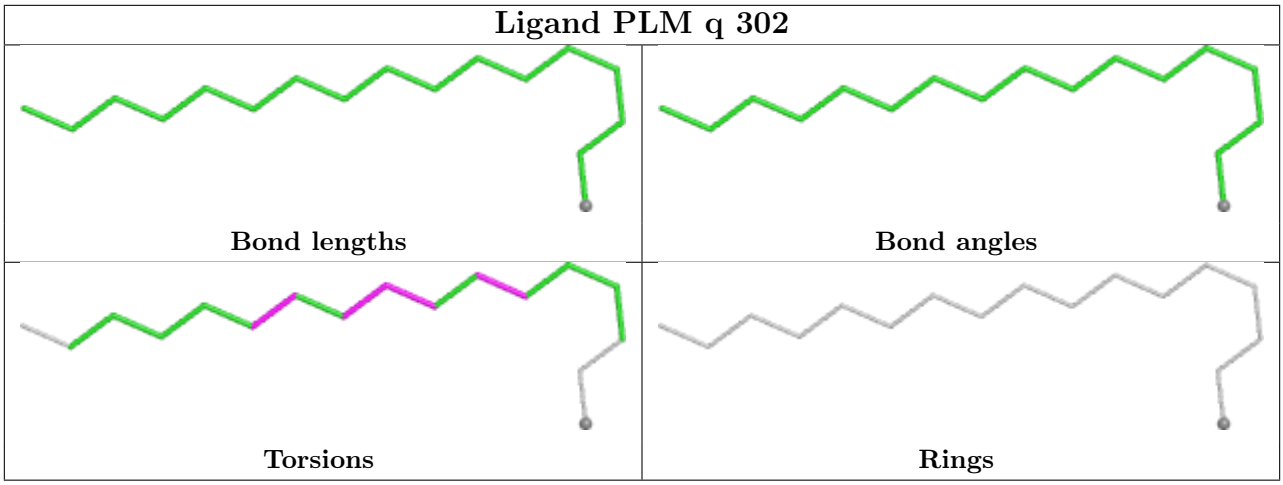
Ligand 9XX G 101



Ligand MQ9 i 602



Ligand PLM q 302



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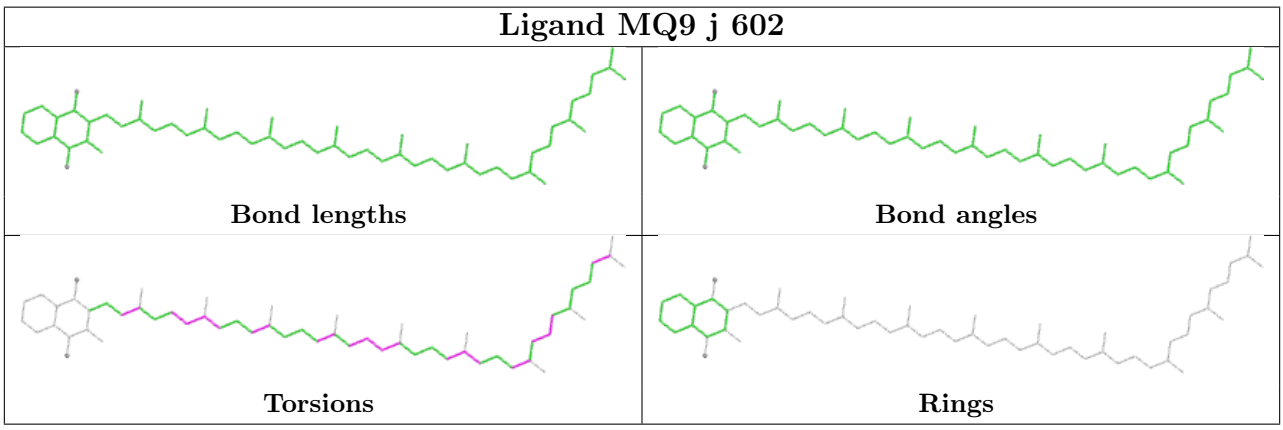
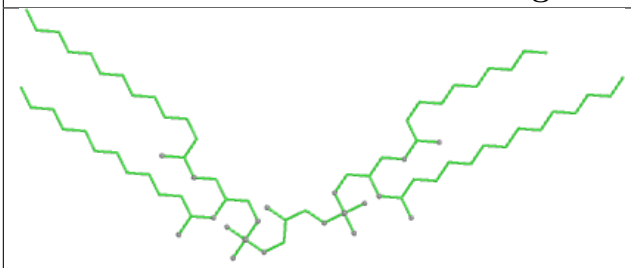
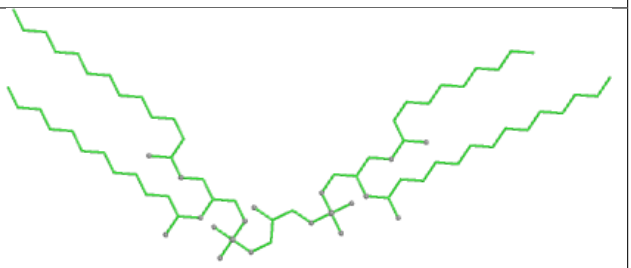


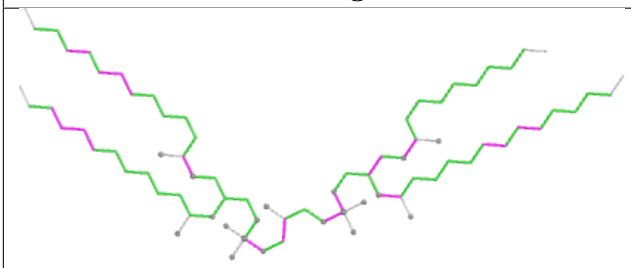
Ligand CDL i 608



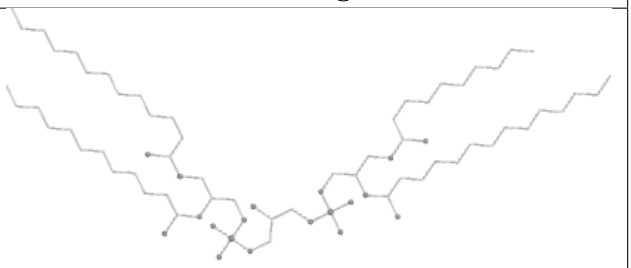
Bond lengths



Bond angles

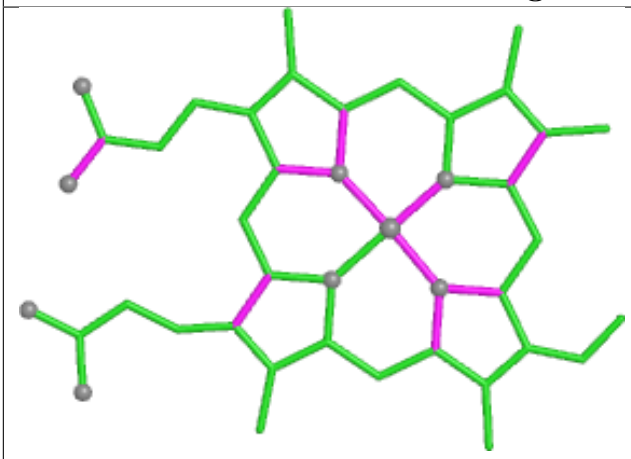


Torsions



Rings

Ligand HEM i 605



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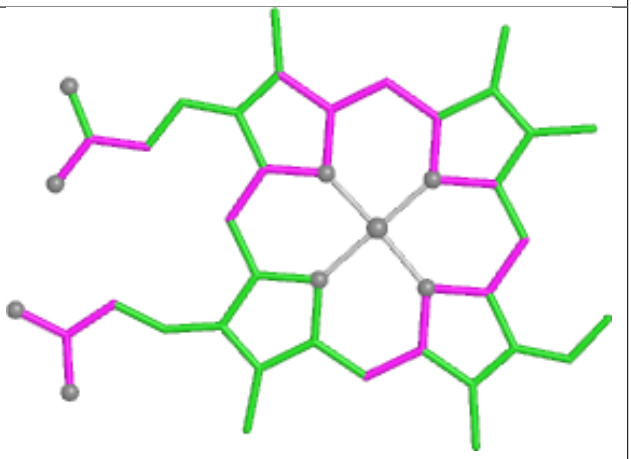
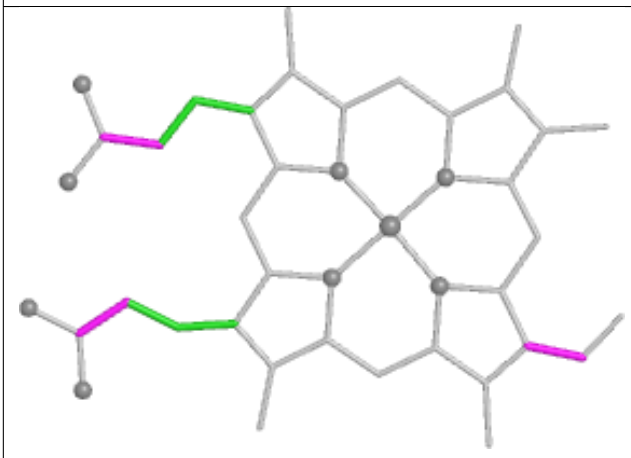


Bond angles



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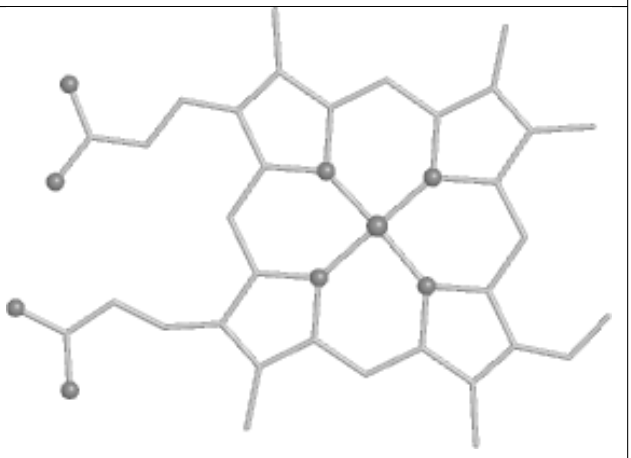
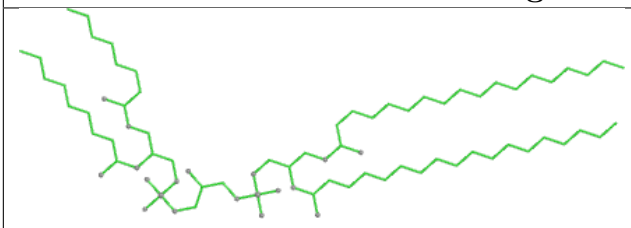


Rings

Ligand CDL L 606



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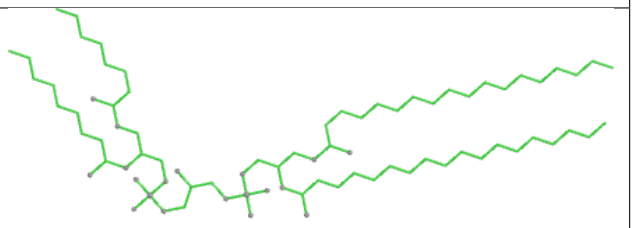
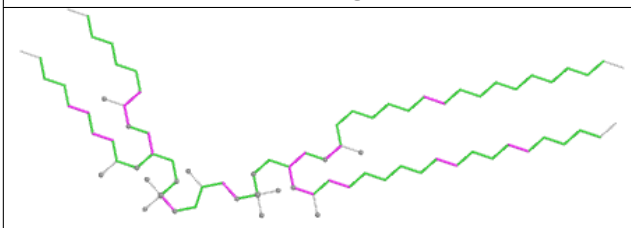


Bond angles



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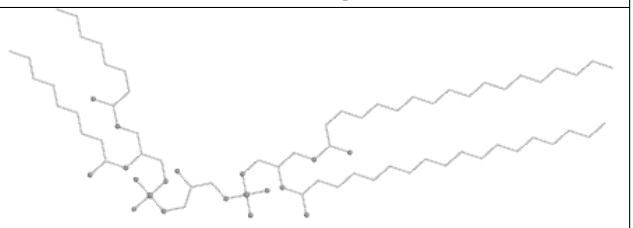
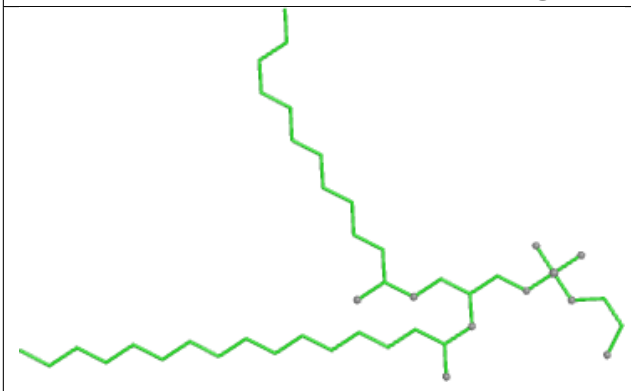


Rings

Ligand 9Y0 g 302



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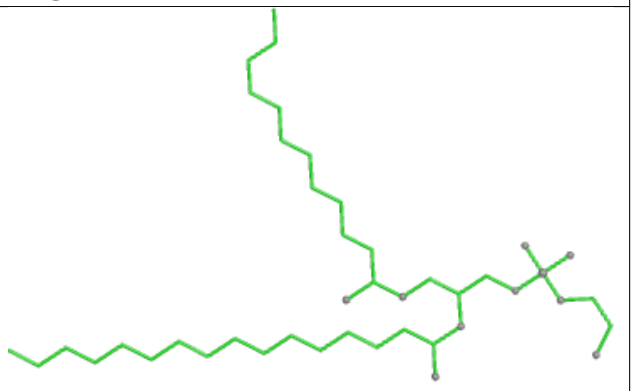
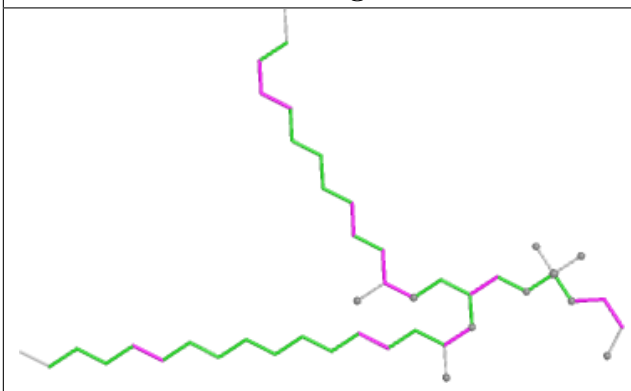


Bond angles



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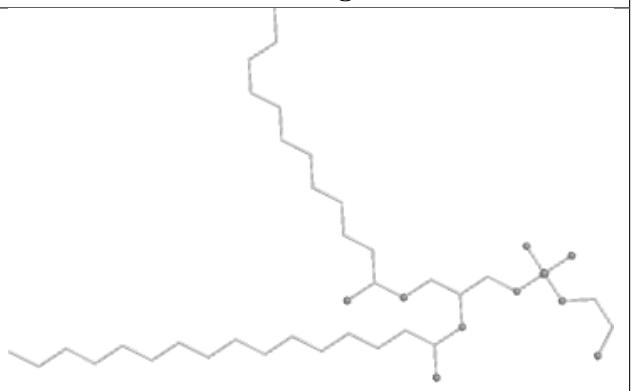
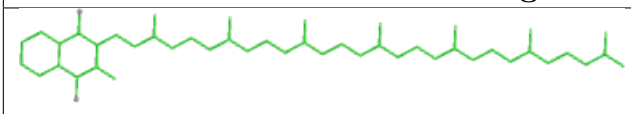
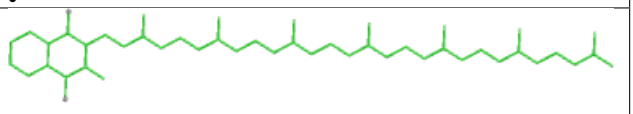


Rings

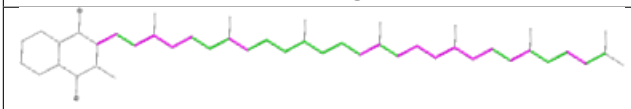
Ligand MQ9 m 201



Bond lengths



Bond angles



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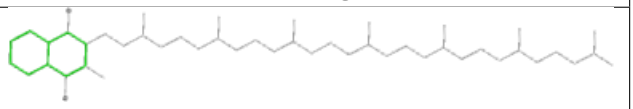
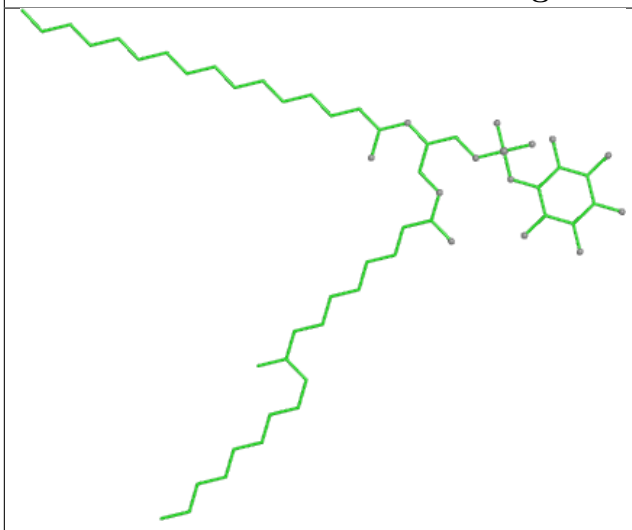


Rings

Ligand 9YF p 601



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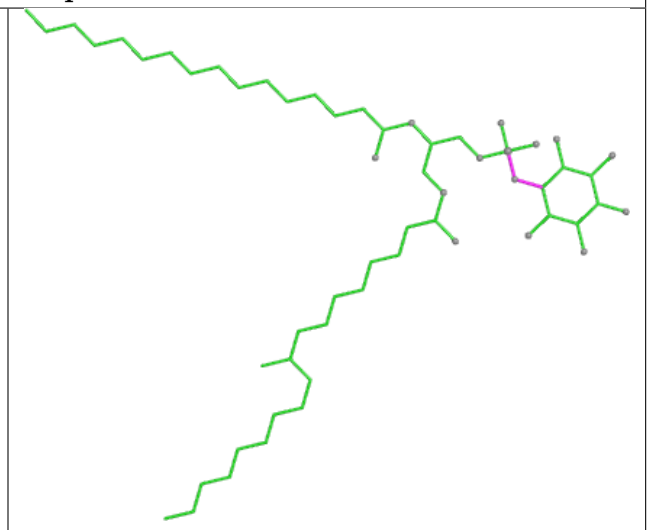
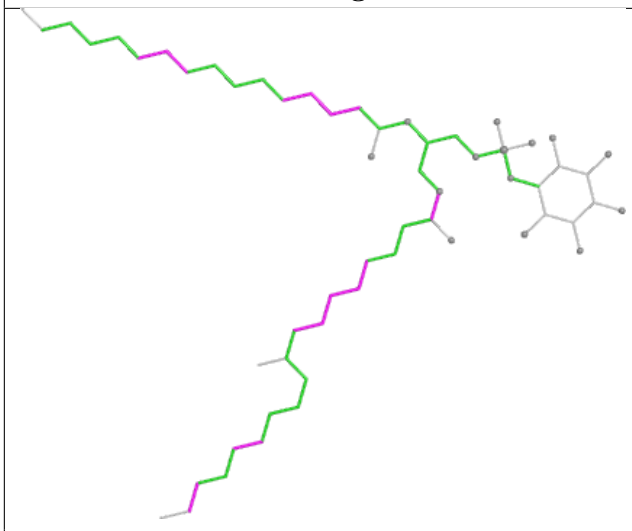


Bond angles



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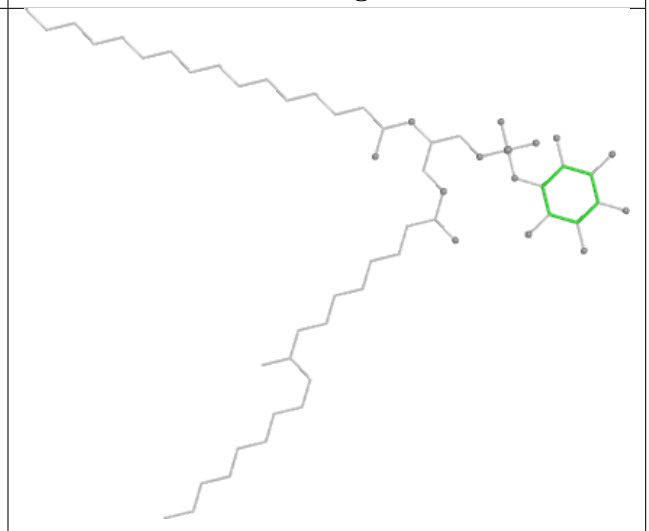
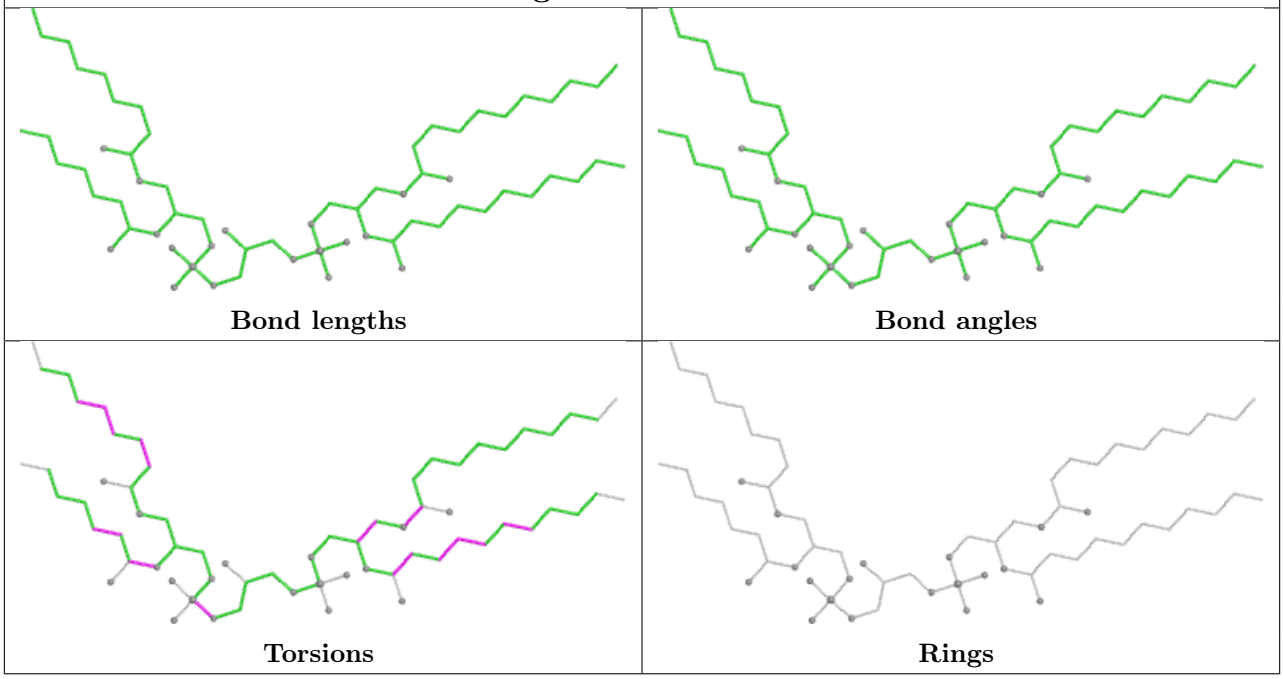
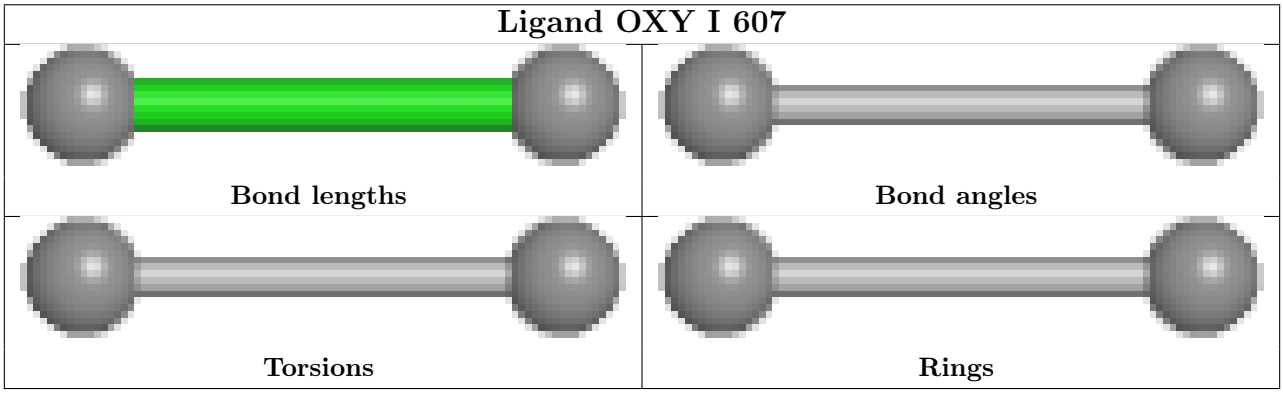


Rings

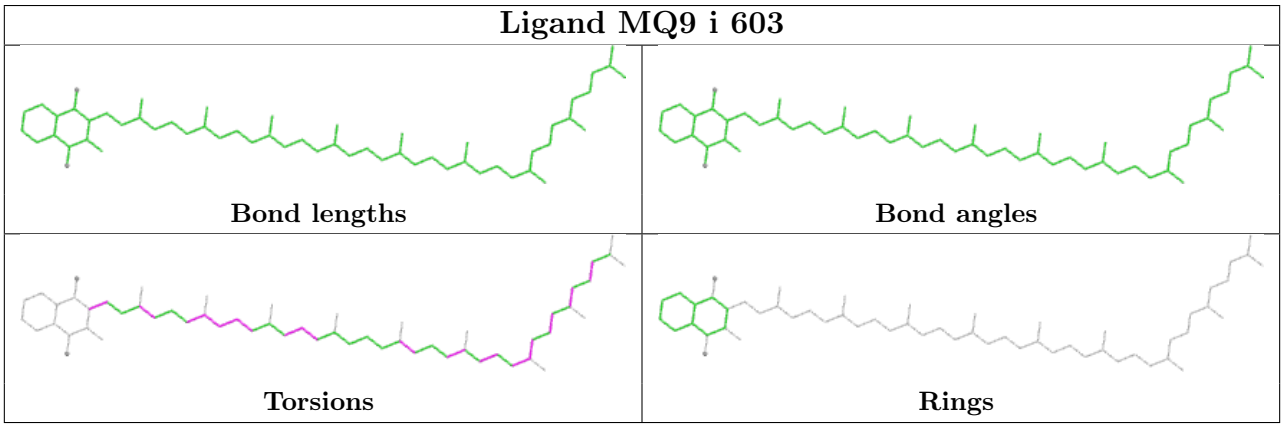
Ligand CDL i 604



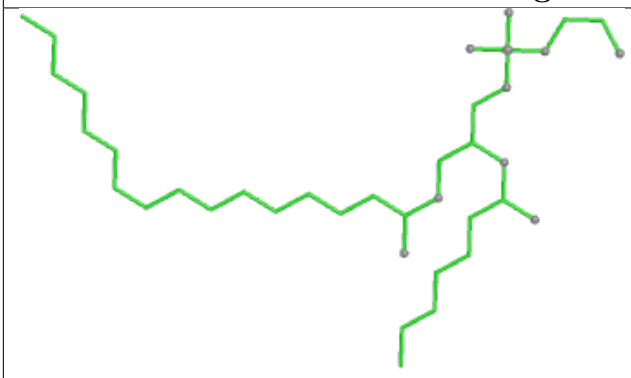
Ligand OXY I 607



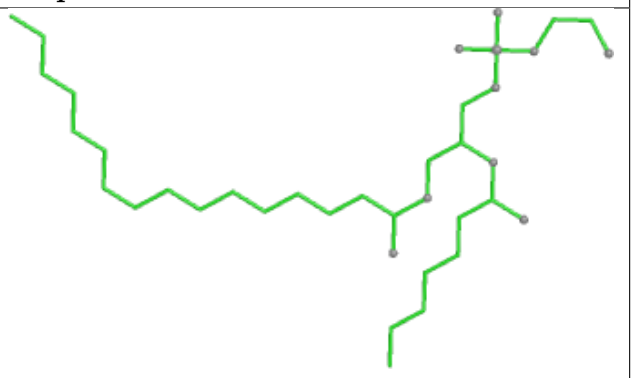
Ligand MQ9 i 603



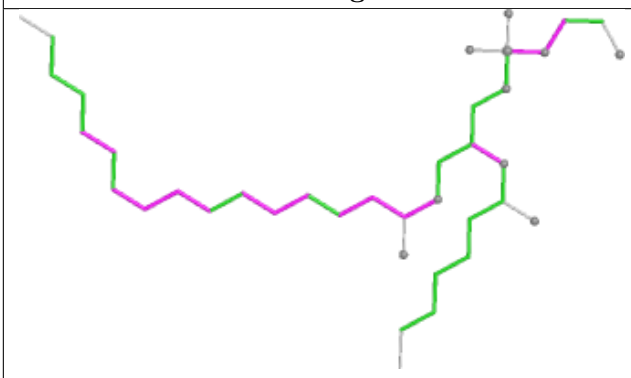
Ligand 9Y0 q 301



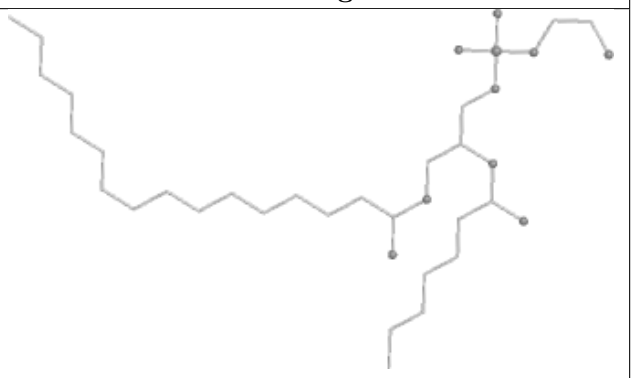
Bond lengths



Bond angles

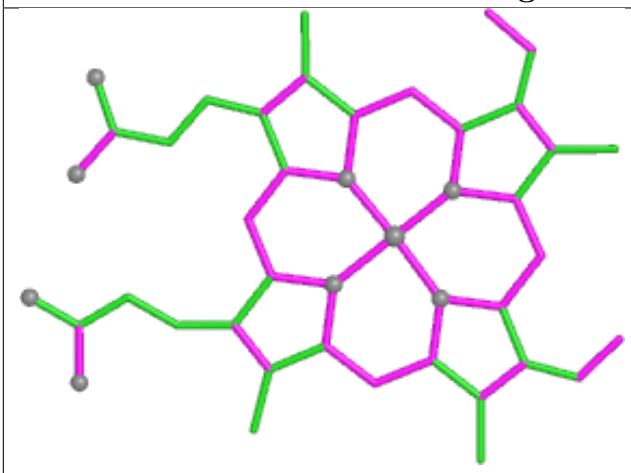


Torsions

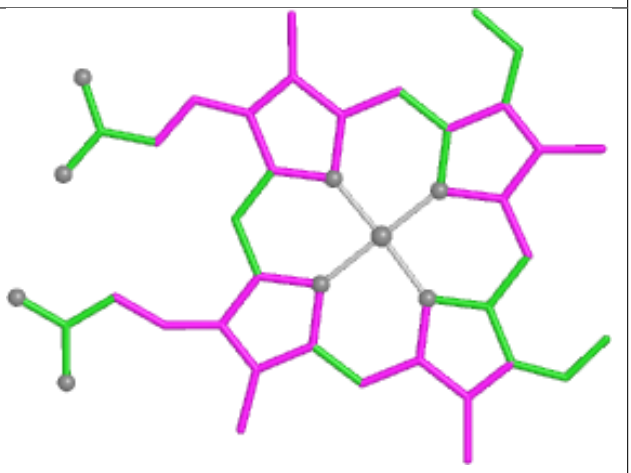


Rings

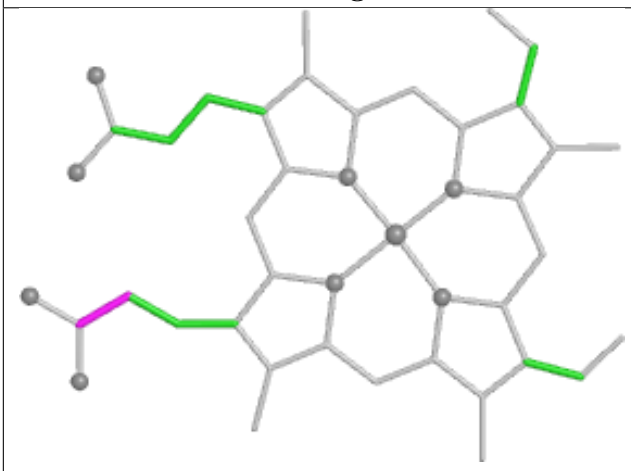
Ligand HEM U 602



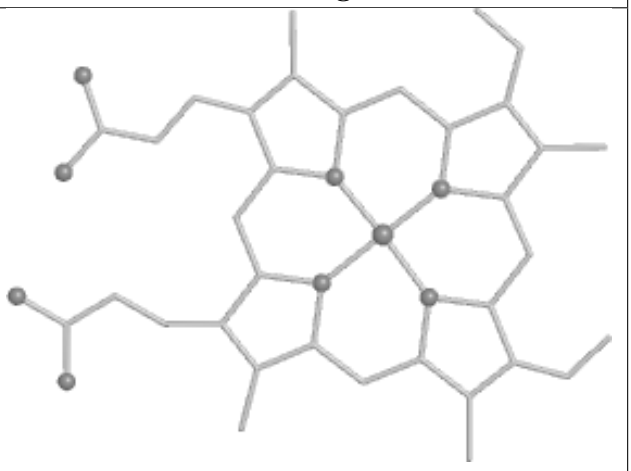
Bond lengths



Bond angles

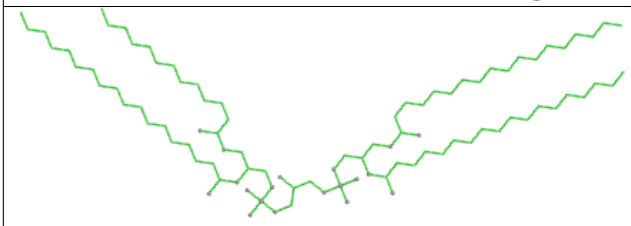


Torsions

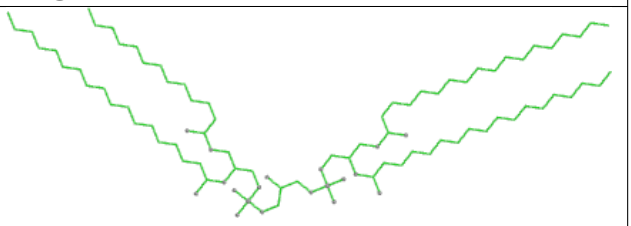


Rings

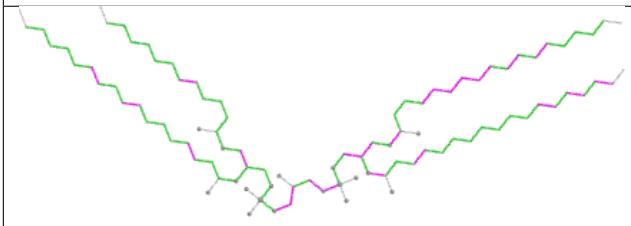
Ligand CDL g 301



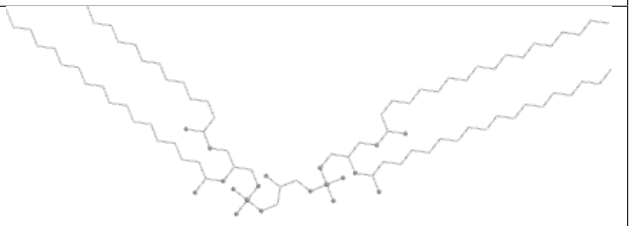
Bond lengths



Bond angles

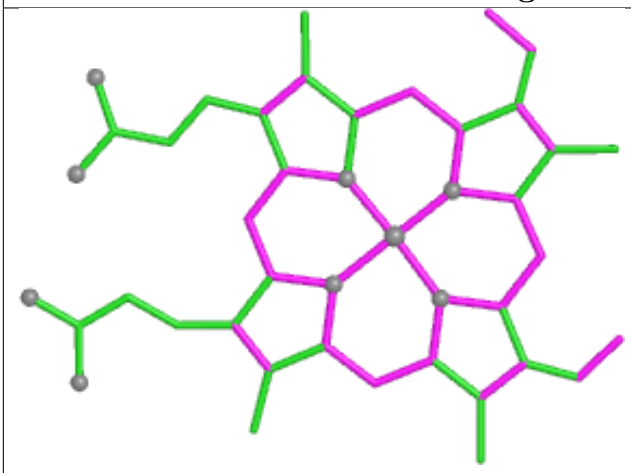


Torsions

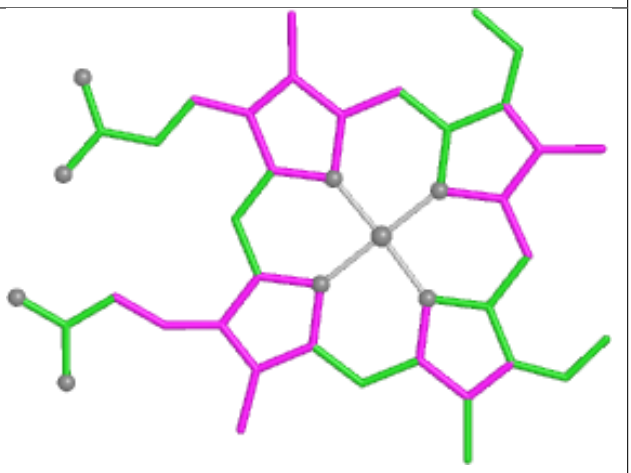


Rings

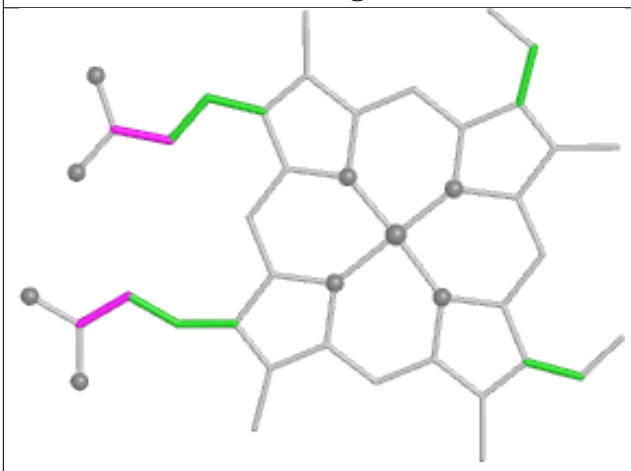
Ligand HEM U 601



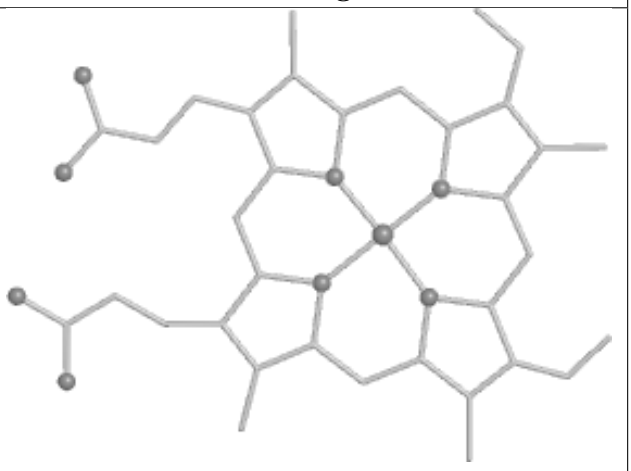
Bond lengths



Bond angles

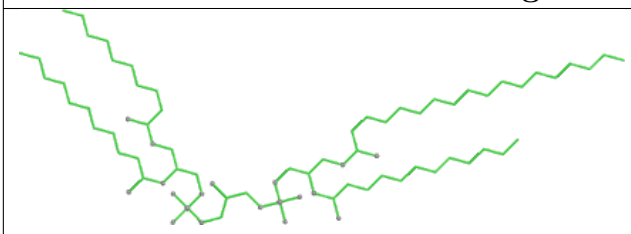


Torsions

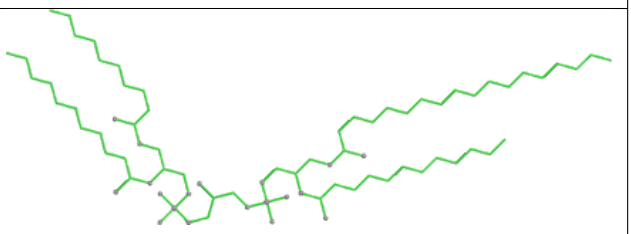


Rings

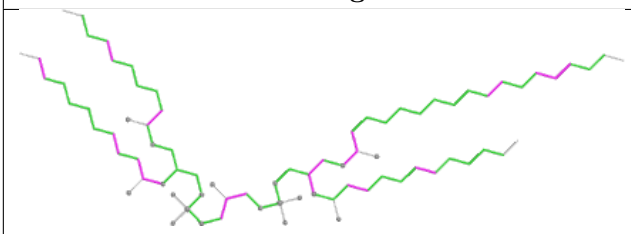
Ligand CDL m 202



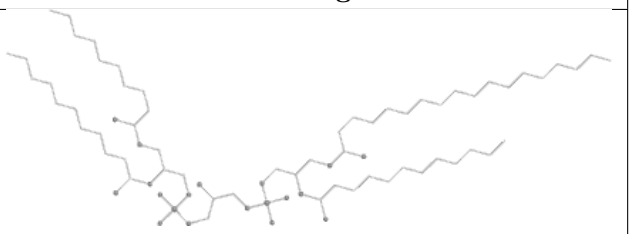
Bond lengths



Bond angles

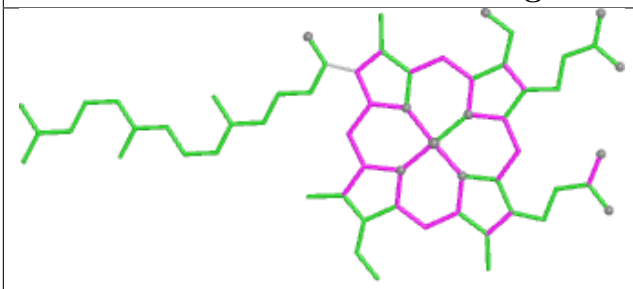


Torsions

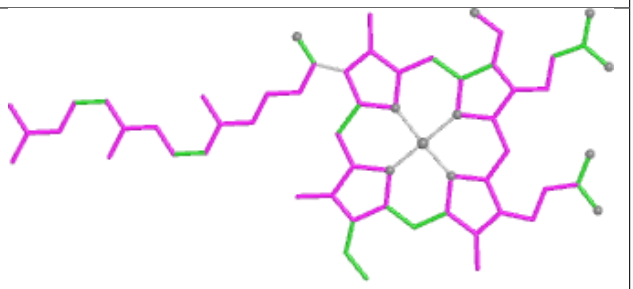


Rings

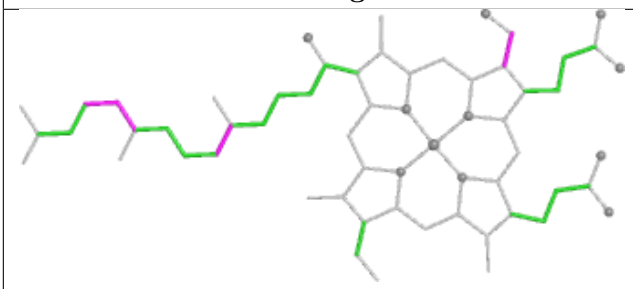
Ligand HEA L 602



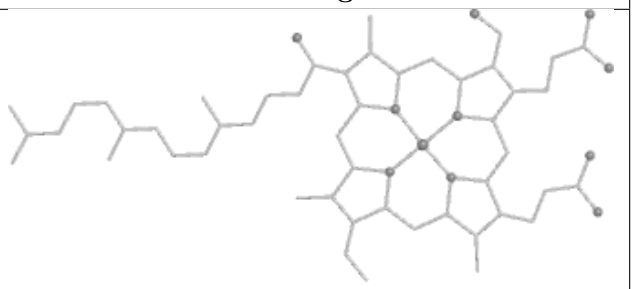
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

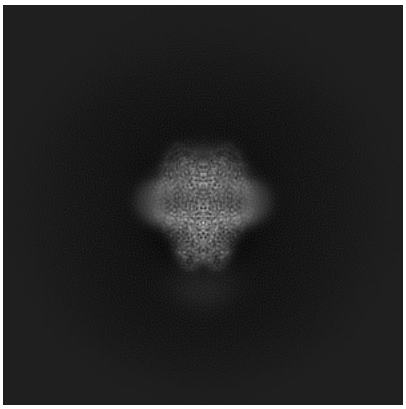
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65878. These allow visual inspection of the internal detail of the map and identification of artifacts.

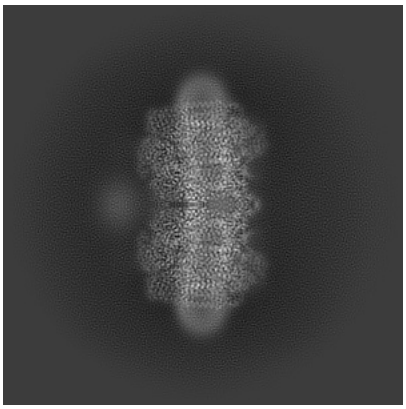
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

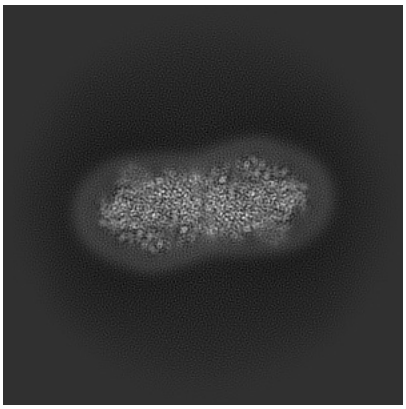
6.1.1 Primary map



X

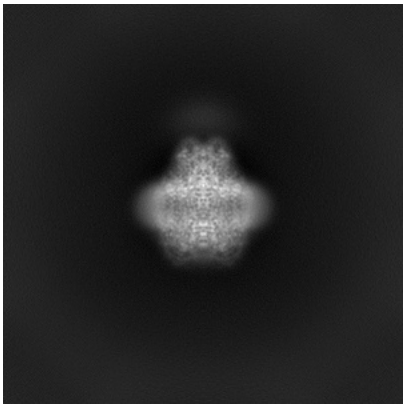


Y

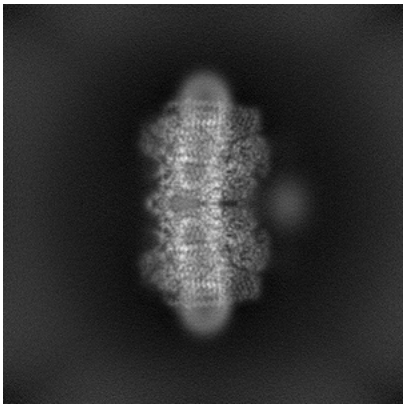


Z

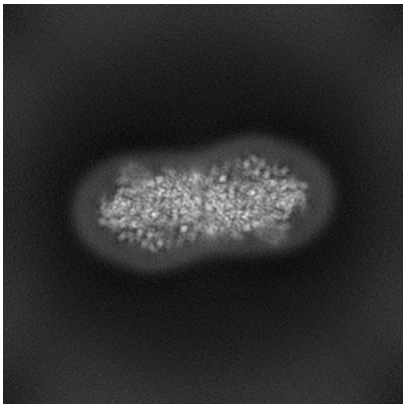
6.1.2 Raw map



X



Y

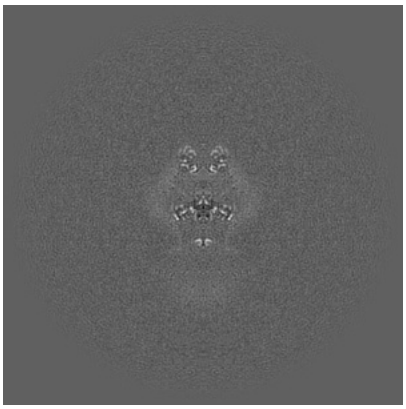


Z

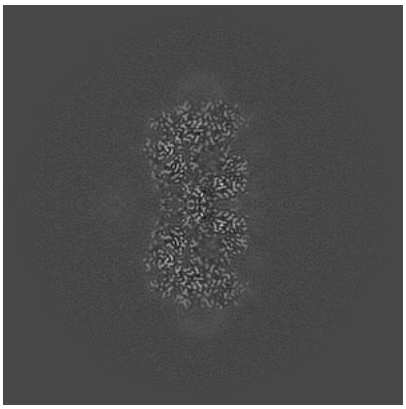
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

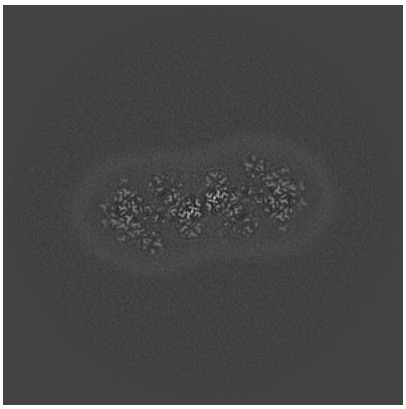
6.2.1 Primary map



X Index: 300

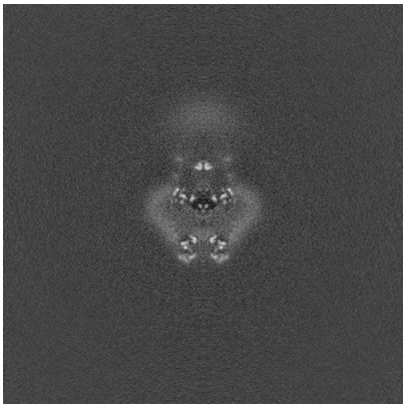


Y Index: 300

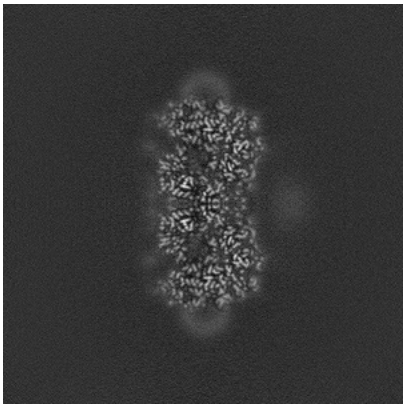


Z Index: 300

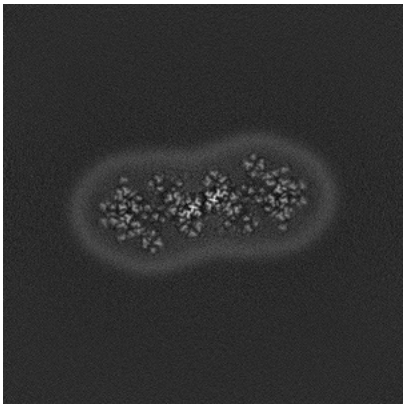
6.2.2 Raw map



X Index: 300



Y Index: 300

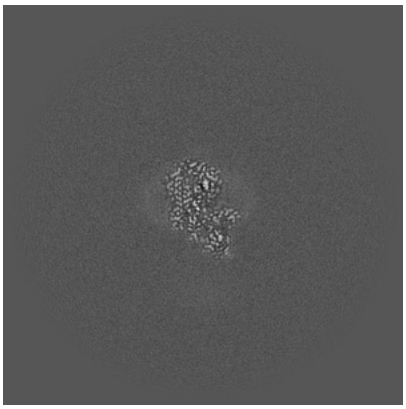


Z Index: 300

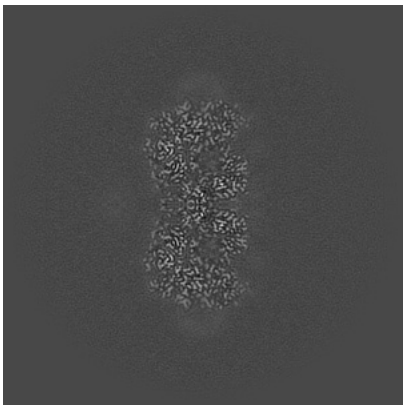
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

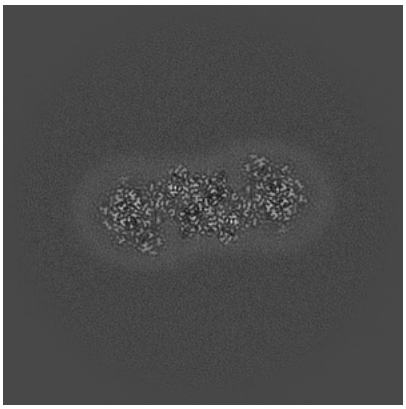
6.3.1 Primary map



X Index: 272

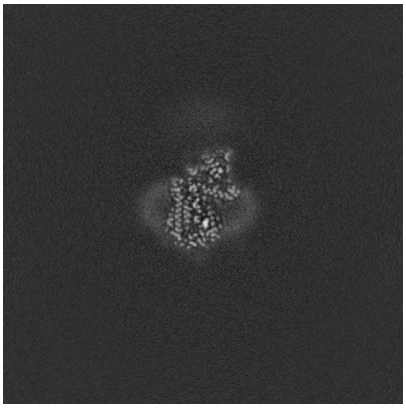


Y Index: 300

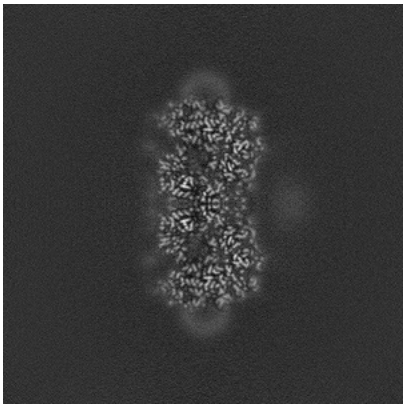


Z Index: 283

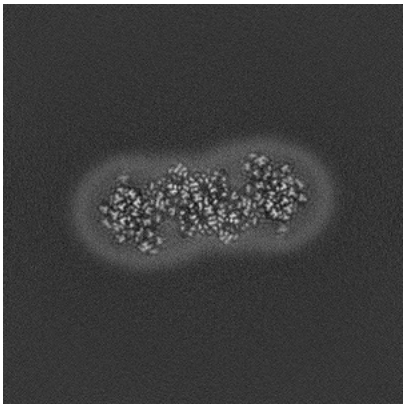
6.3.2 Raw map



X Index: 272



Y Index: 300

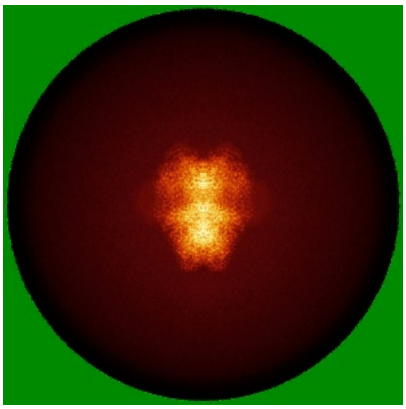


Z Index: 317

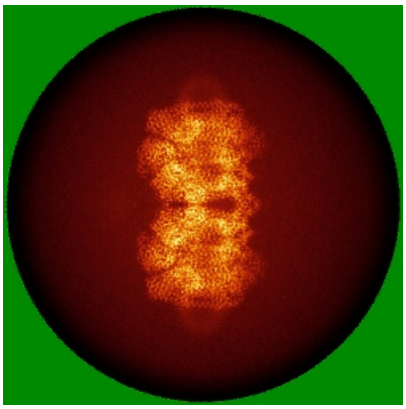
The images above show the largest variance slices of the map in three orthogonal directions.

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

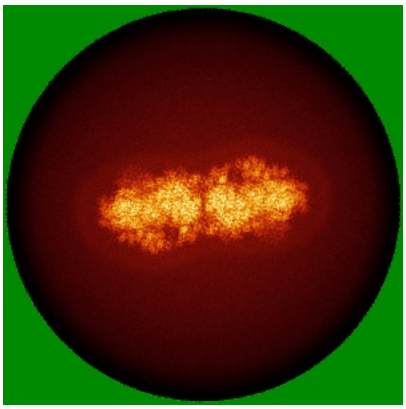
6.4.1 Primary map



X

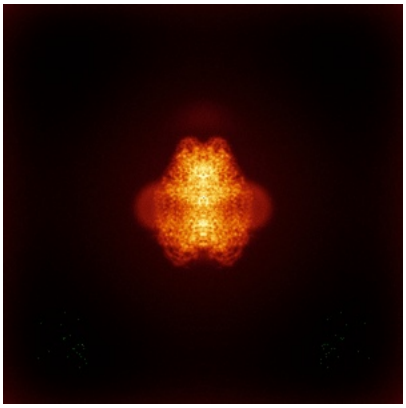


Y

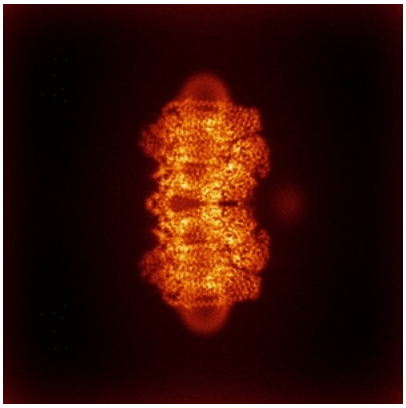


Z

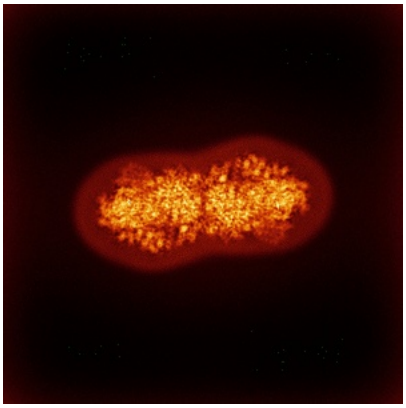
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

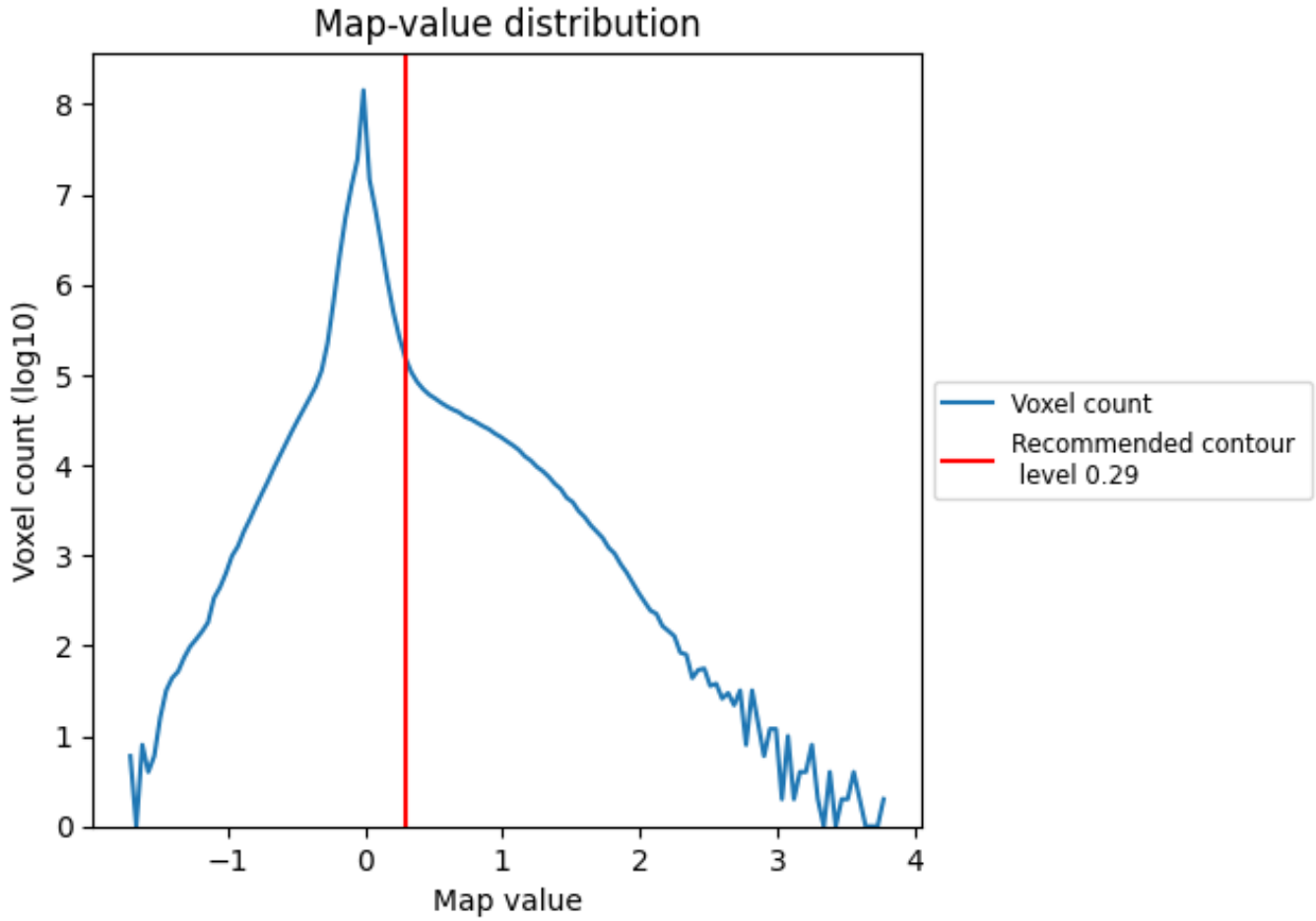
6.6 Mask visualisation (i)

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

7 Map analysis

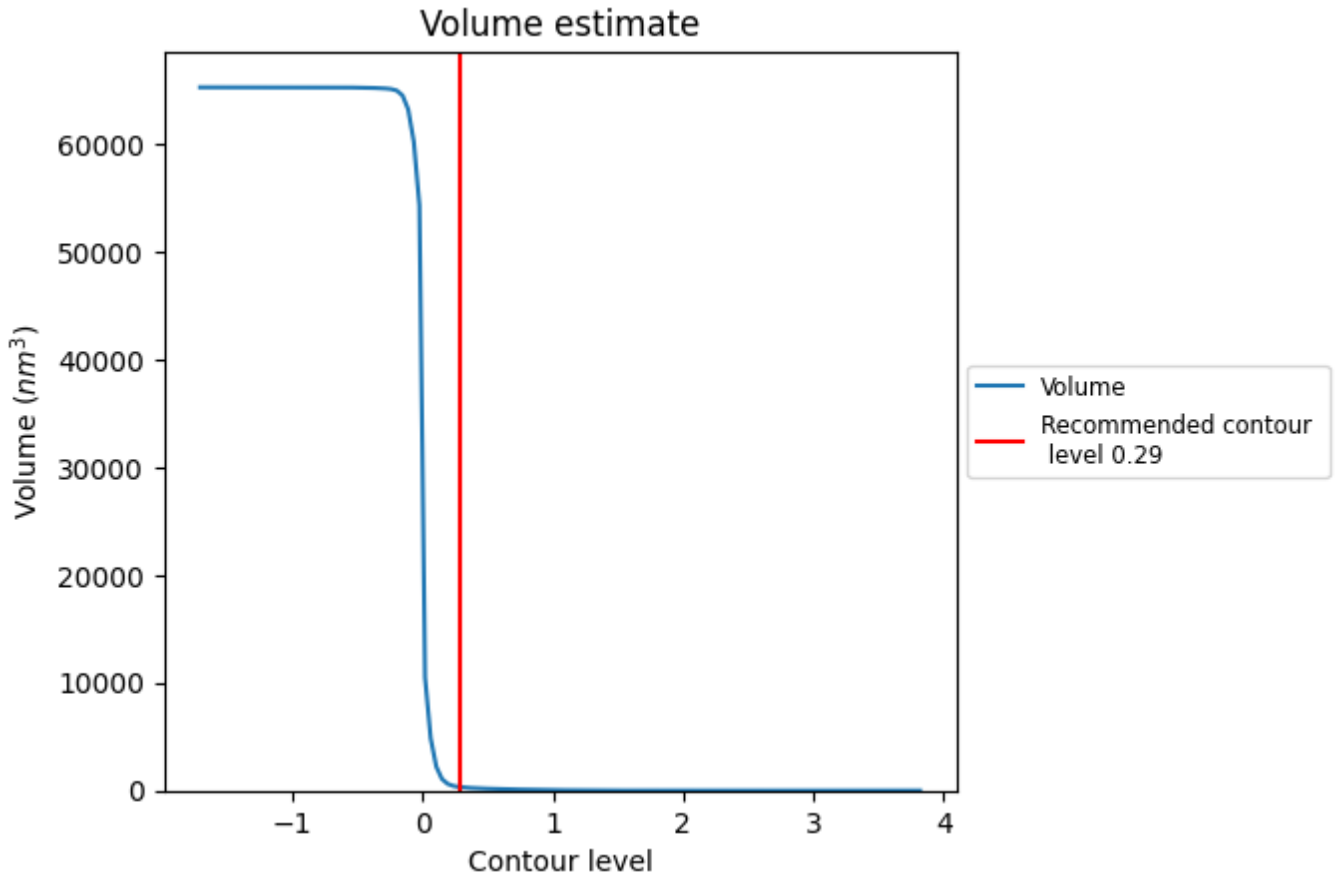
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

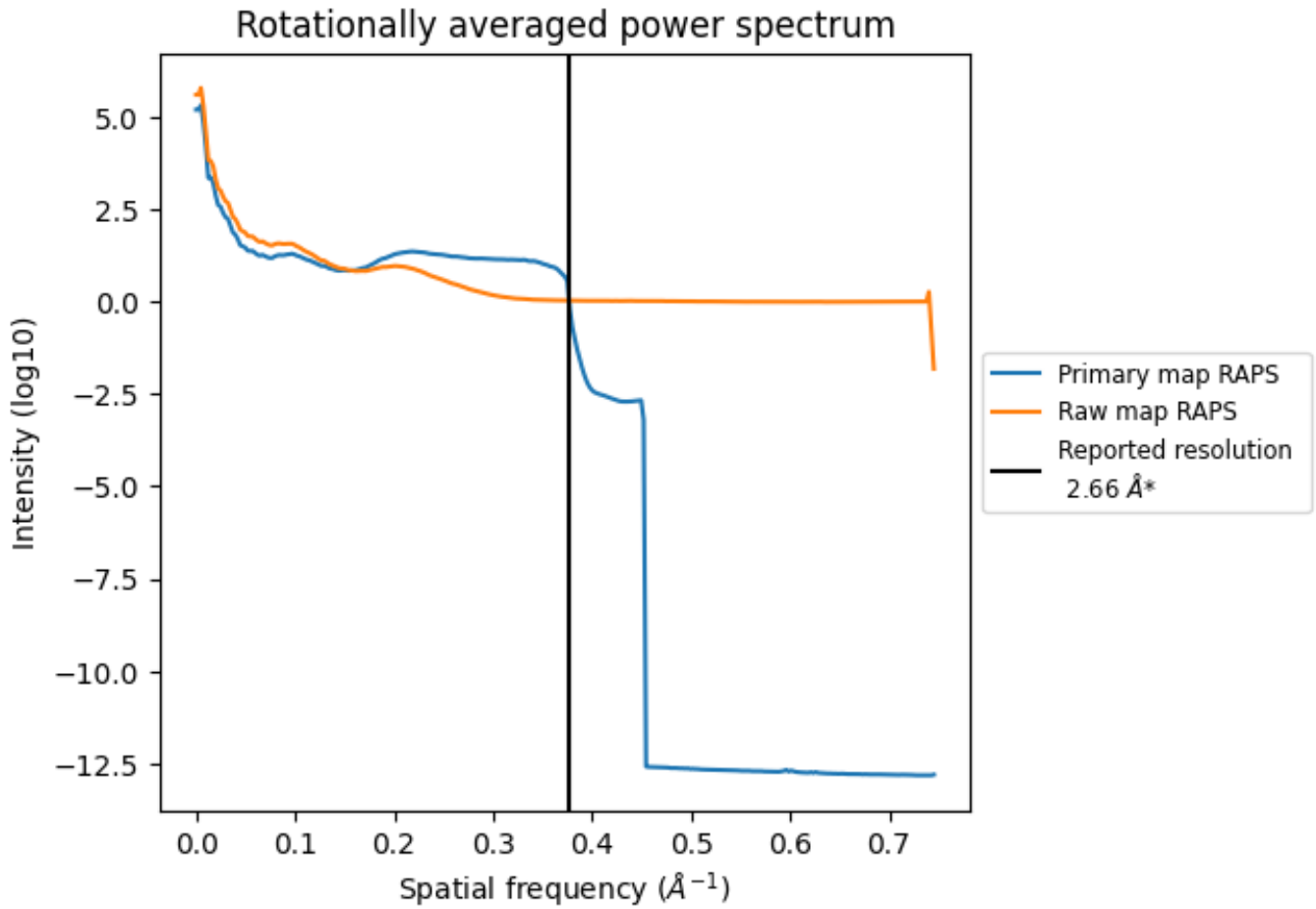
7.2 Volume estimate



The volume at the recommended contour level is 320 nm^3; this corresponds to an approximate mass of 289 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)

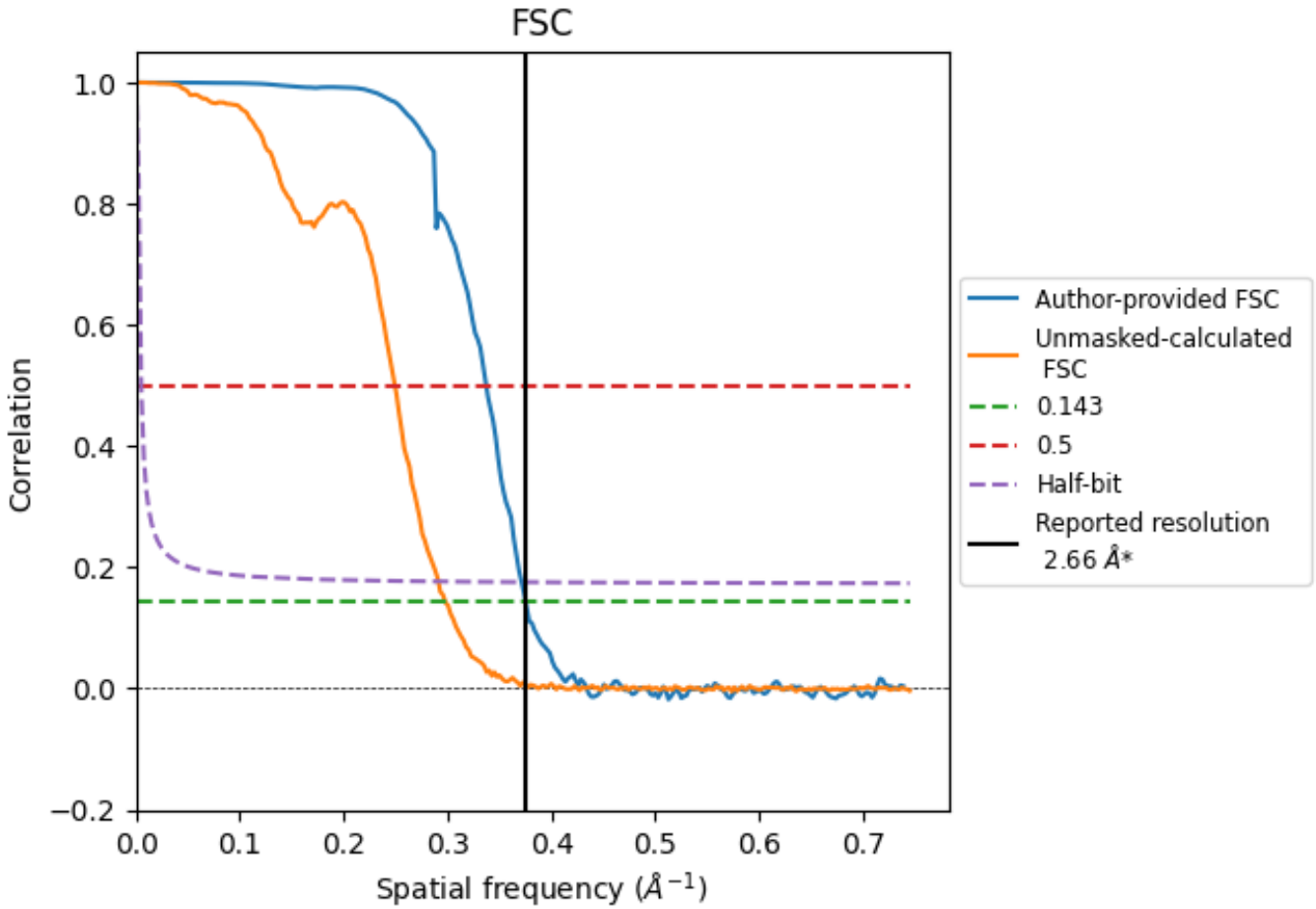


*Reported resolution corresponds to spatial frequency of 0.376 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.376 $Å^{-1}$

8.2 Resolution estimates (i)

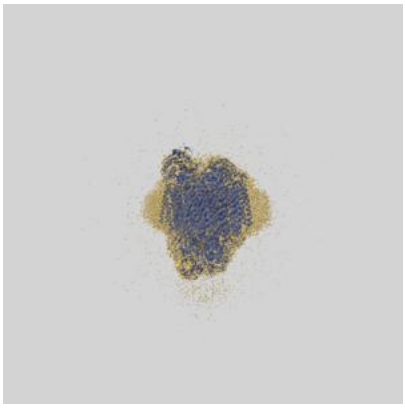
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	2.97	2.69
Unmasked-calculated*	3.36	4.01	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.66 by more than 10 %

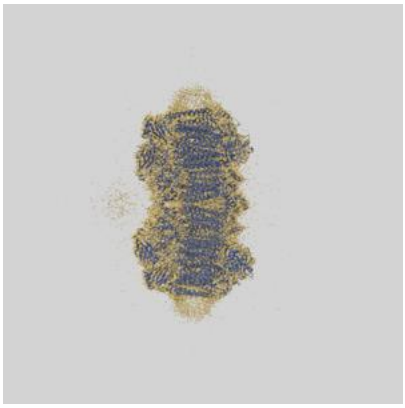
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65878 and PDB model 9WCX. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay



X



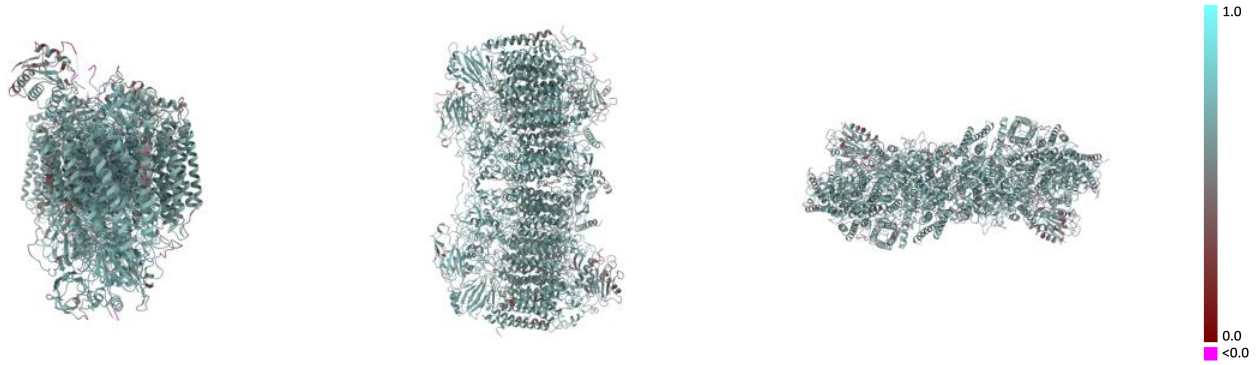
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29 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.

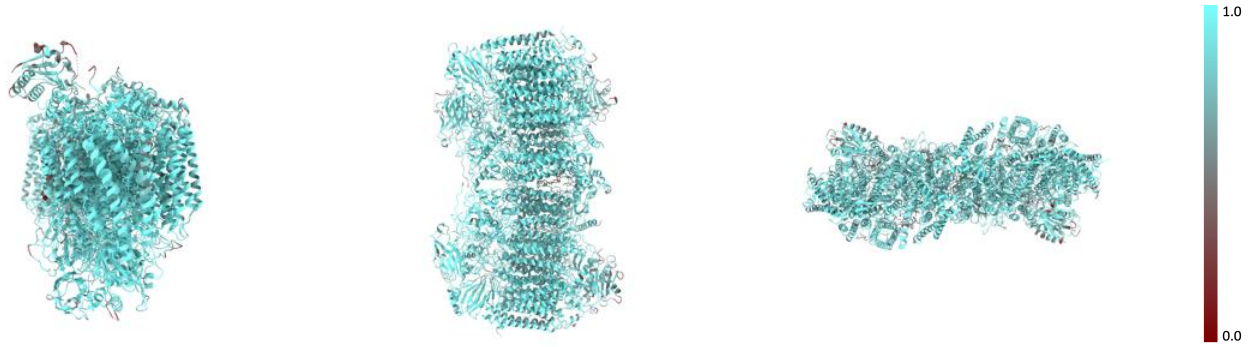
9.2 Q-score mapped to coordinate model (i)



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.

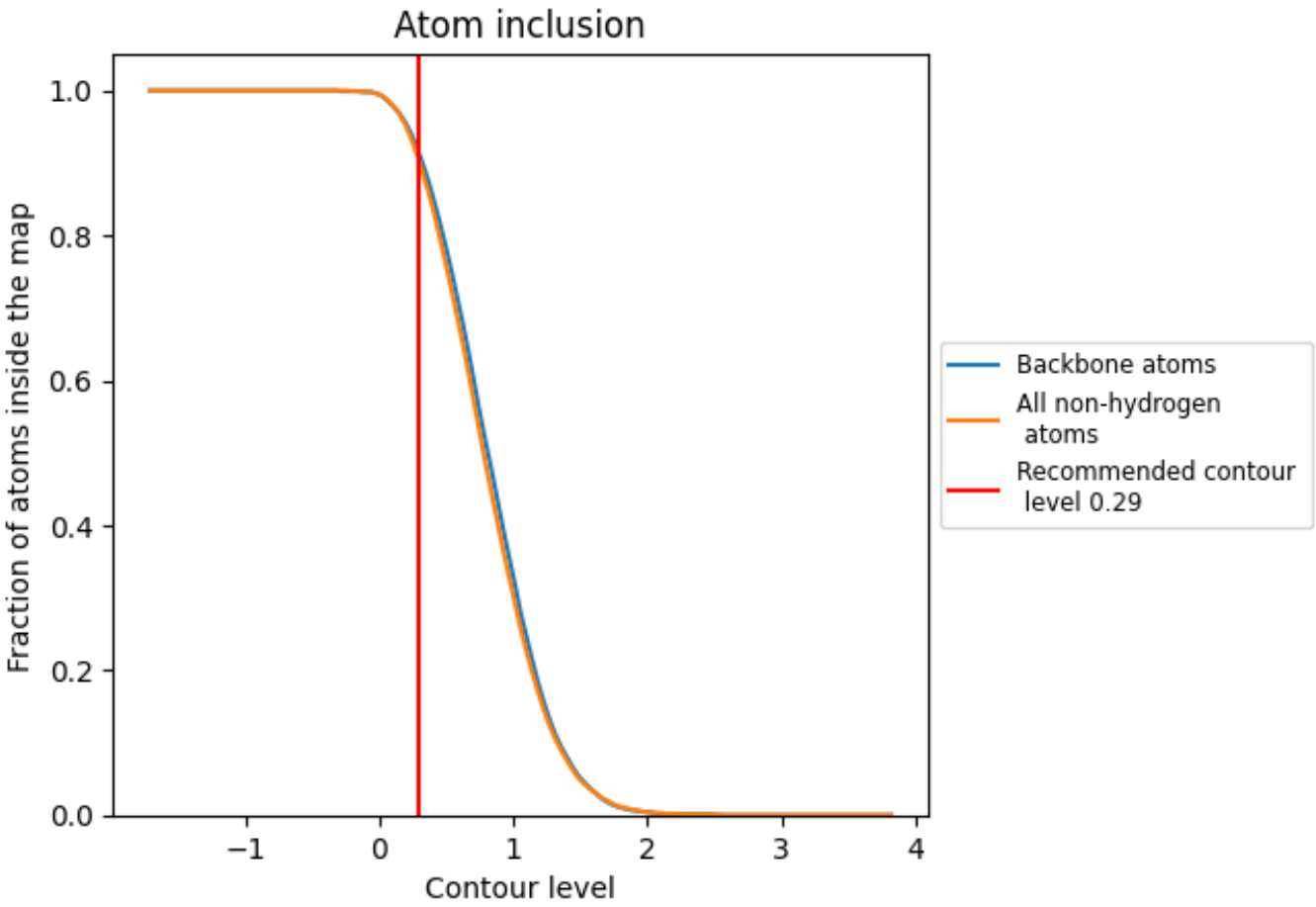
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.29).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.6080
G	0.8600	0.5990
I	0.9510	0.6290
J	0.6970	0.4740
L	0.9500	0.6280
U	0.9510	0.6370
V	0.9500	0.6310
X	0.7820	0.4980
a	0.8290	0.5120
b	0.8500	0.5940
d	0.8910	0.5920
e	0.8890	0.5930
f	0.9160	0.5860
g	0.8870	0.5800
h	0.6930	0.4890
i	0.9200	0.6270
j	0.9340	0.6290
k	0.7220	0.5070
l	0.7410	0.5150
m	0.9080	0.6010
n	0.9120	0.6010
o	0.9480	0.6350
p	0.9360	0.6280
q	0.8720	0.5830
r	0.8640	0.5790

