Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 10:06 AM JST

PDB ID	:	7E1V / pdb_00007e1v
EMDB ID	:	EMD-30943
Title	:	Cryo-EM structure of apo hybrid respiratory supercomplex consisting of Mycobacterium tuberculosis complexIII and Mycobacterium smegmatis complexIV
Authors	:	Zhou, S.; Wang, W.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on	:	2021-02-03
Resolution	:	2.68 Å(reported)

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

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

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

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

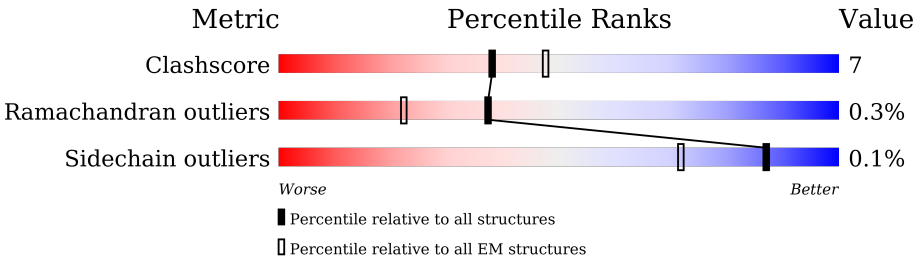
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

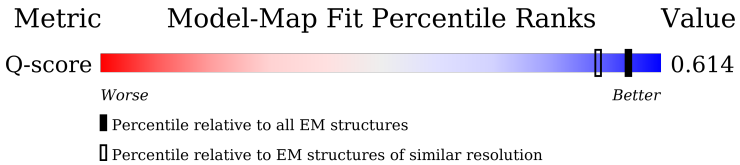
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	E	341	69% 12% 19%
1	Q	341	• 62% 21% 17%
2	F	575	76% 20% •
2	R	575	80% 16% •

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Mol	Chain	Length	Quality of chain
3	G	203	75% 17% 8%
3	S	203	73% 18% 9%
4	H	139	95% 5%
4	T	139	96%
5	I	79	73% 11% 15%
5	U	79	78% 6% 15%
6	J	157	79% 13% 8%
6	V	157	74% 18% 8%
7	D	100	65% 11% 24%
7	P	100	63% 12% 25%
8	B	549	82% 13% 5%
8	N	549	79% 16% 5%
9	A	429	75% 13% 12%
9	M	429	74% 14% 12%
10	C	280	66% 11% 22%
10	O	280	69% 6% 24%

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
17	MQ9	N	609	-	X	-	-
18	FES	A	501	-	-	X	-
20	HEC	C	301	X	-	-	-
20	HEC	C	302	X	-	-	-
20	HEC	O	303	X	-	-	-
20	HEC	O	304	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 42279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	276	2191	1428	360	395	8	0	0
1	Q	283	2236	1456	367	405	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	552	4373	2938	695	714	26	0	0
2	R	552	4373	2938	695	714	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	186	1455	976	231	241	7	0	0
3	S	185	1449	973	230	239	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	139	1071	716	164	188	3	0	0
4	T	139	1068	715	164	186	3	0	0

- Molecule 5 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	67	500	330	85	84	1	0	0
5	U	67	499	330	85	83	1	0	0

- Molecule 6 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	145	1026	651	176	197	2	0	0
6	V	145	1029	652	176	199	2	0	0

- Molecule 7 is a protein called Prokaryotic respiratory supercomplex associate factor 1 PRSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	76	607	397	112	94	4	0	0
7	P	75	597	391	109	93	4	0	0

- Molecule 8 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	524	4118	2723	701	677	17	0	0
8	B	524	4130	2729	703	681	17	0	0

- Molecule 9 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	378	2924	1890	500	523	11	0	0
9	A	378	2912	1884	499	518	11	0	0

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	O	213	1458	921	261	268	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	218	1487	930	274	274	9	0	0

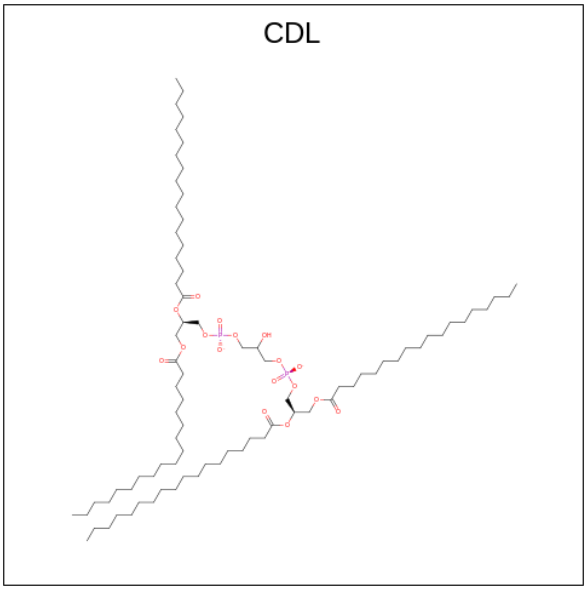
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	LEU	-	expression tag	UNP P9WP35
C	1	LEU	-	expression tag	UNP P9WP35

- Molecule 11 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
11	E	2	2	2	0
11	F	2	2	2	0
11	Q	3	3	3	0
11	R	1	1	1	0

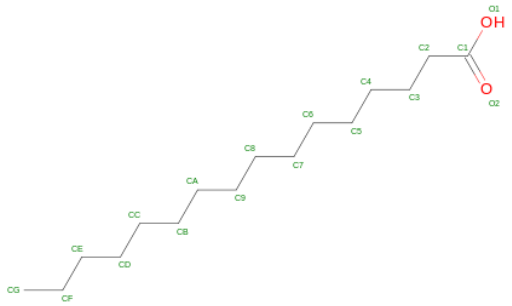
- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	F	1	76	57	17	2	0
			Total	C	O	P	
12	F	1	81	62	17	2	0
			Total	C	O	P	
12	D	1	88	69	17	2	0
			Total	C	O	P	
12	R	1	76	57	17	2	0
			Total	C	O	P	
12	R	1	81	62	17	2	0
			Total	C	O	P	
12	P	1	88	69	17	2	0
			Total	C	O	P	
12	N	1	79	60	17	2	0
			Total	C	O	P	
12	N	1	74	55	17	2	0
			Total	C	O	P	
12	N	1	77	58	17	2	0
			Total	C	O	P	
12	N	1	79	60	17	2	0
			Total	C	O	P	
12	M	1	95	76	17	2	0
			Total	C	O	P	
12	B	1	66	47	17	2	0
			Total	C	O	P	
12	B	1	74	55	17	2	0
			Total	C	O	P	
12	B	1	77	58	17	2	0
			Total	C	O	P	
12	B	1	79	60	17	2	0
			Total	C	O	P	
12	C	1	79	60	17	2	0
			Total	C	O	P	
12	C	1	95	76	17	2	0

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

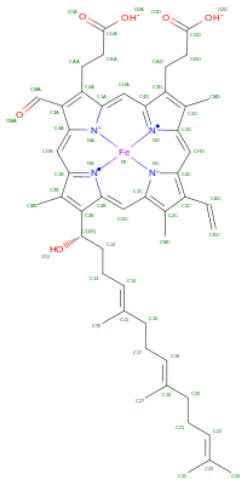
PLM



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	F	1	17	16	1	0
			Total	C	O	
13	R	1	17	16	1	0
			Total	C	O	
13	N	1	11	10	1	0
			Total	C	O	
13	B	1	11	10	1	0

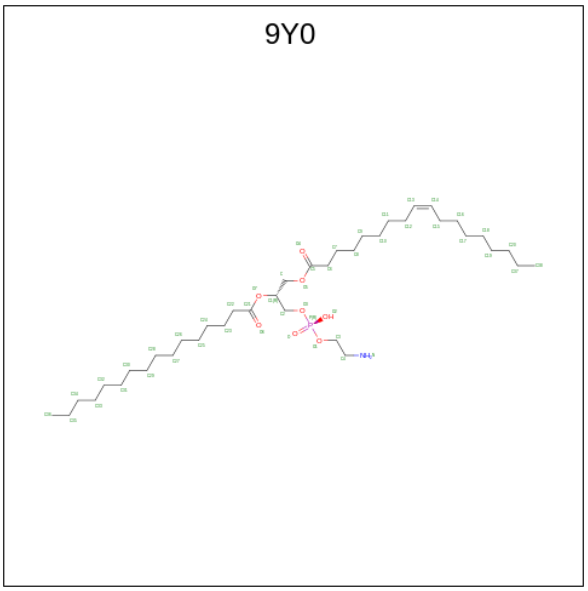
- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

HEA



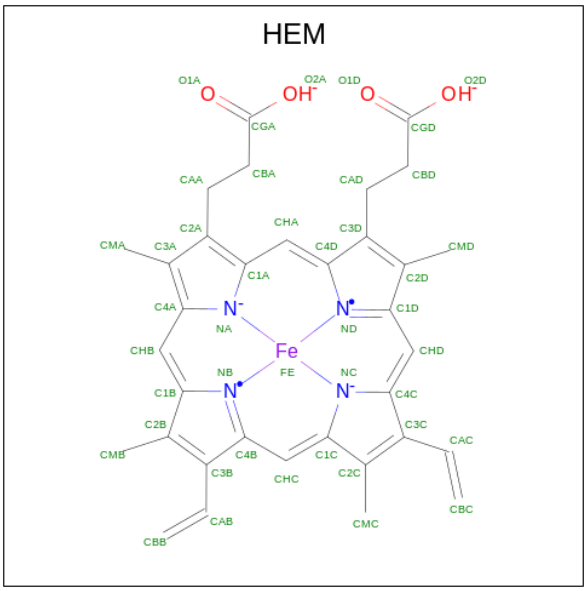
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- 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).



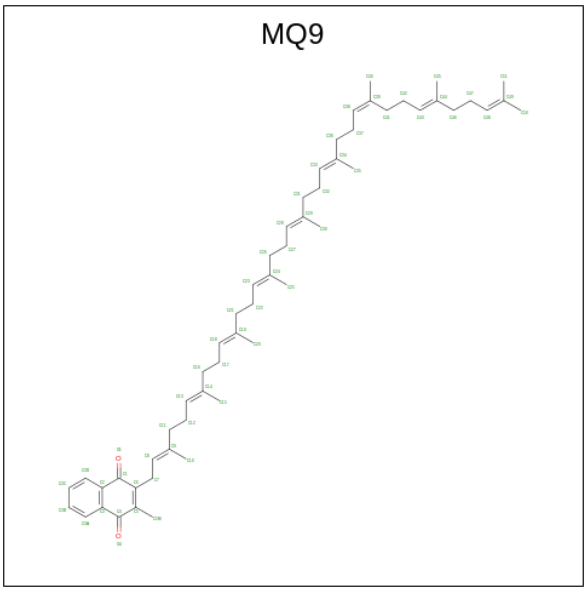
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



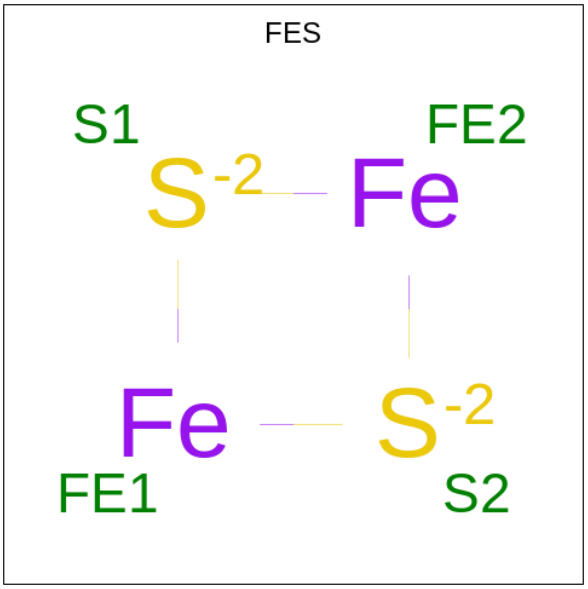
Mol	Chain	Residues	Atoms					AltConf
16	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
16	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
16	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



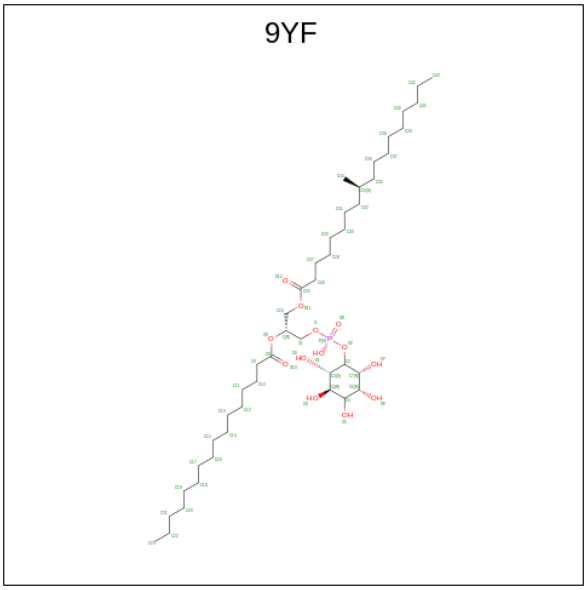
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	N	1	58	56	2	0
			Total	C	O	
17	N	1	58	56	2	0
			Total	C	O	
17	N	1	43	41	2	0
			Total	C	O	
17	N	1	43	41	2	0
			Total	C	O	
17	O	1	48	46	2	0
			Total	C	O	
17	O	1	58	56	2	0
			Total	C	O	
17	B	1	43	41	2	0
			Total	C	O	
17	B	1	38	36	2	0
			Total	C	O	
17	C	1	48	46	2	0
			Total	C	O	
17	C	1	58	56	2	0

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



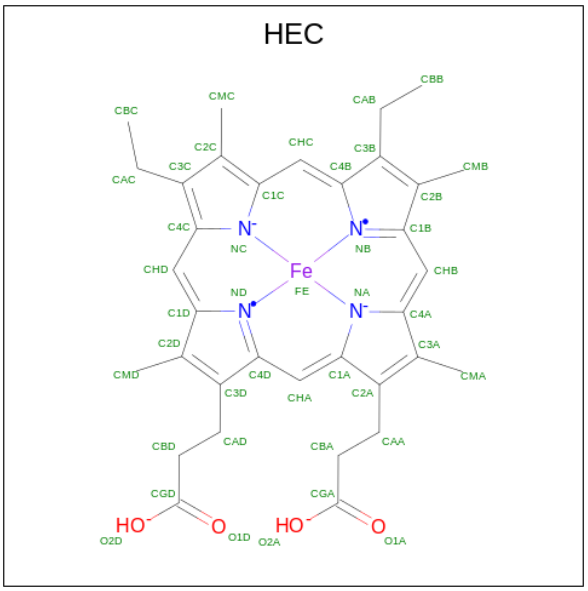
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	M	1	4	2	2	0
			Total	Fe	S	
18	A	1	4	2	2	0

- Molecule 19 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	M	1	44	30	13	1	0
			Total	C	O	P	
19	M	1	40	26	13	1	0
			Total	C	O	P	
19	A	1	51	37	13	1	0
			Total	C	O	P	
19	A	1	42	28	13	1	0

- Molecule 20 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



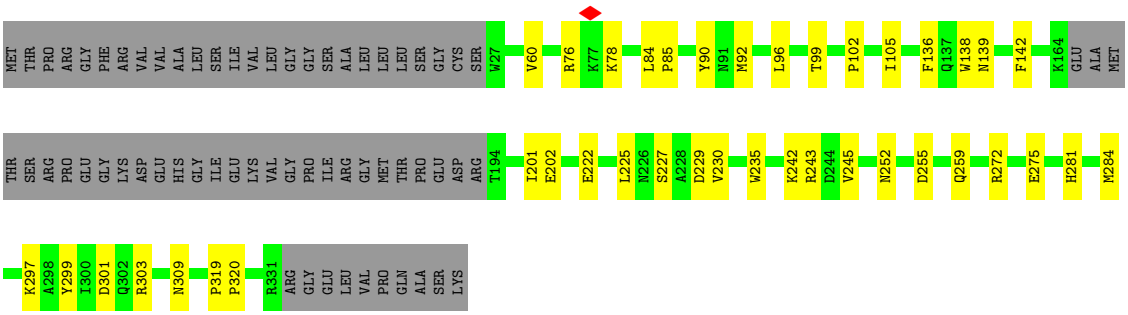
Mol	Chain	Residues	Atoms					AltConf
20	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

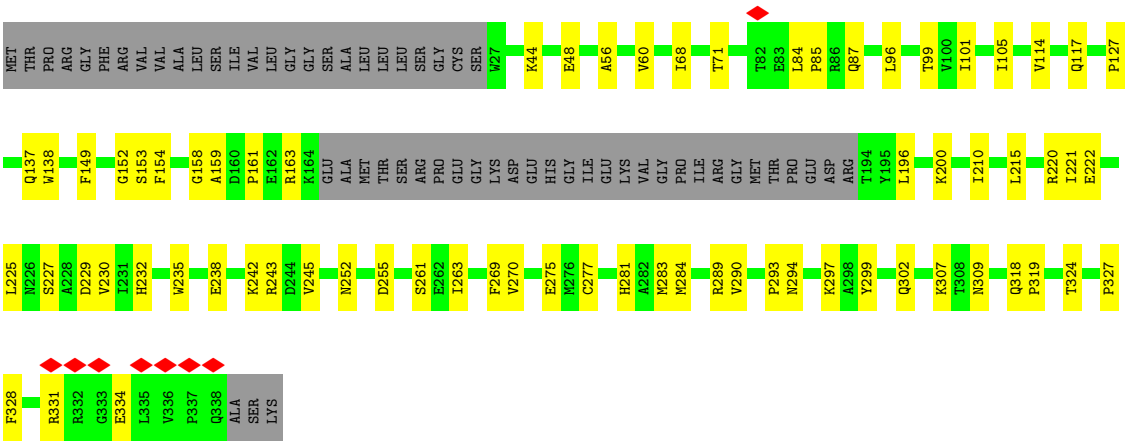
• Molecule 1: Cytochrome c oxidase subunit 2

Chain E:



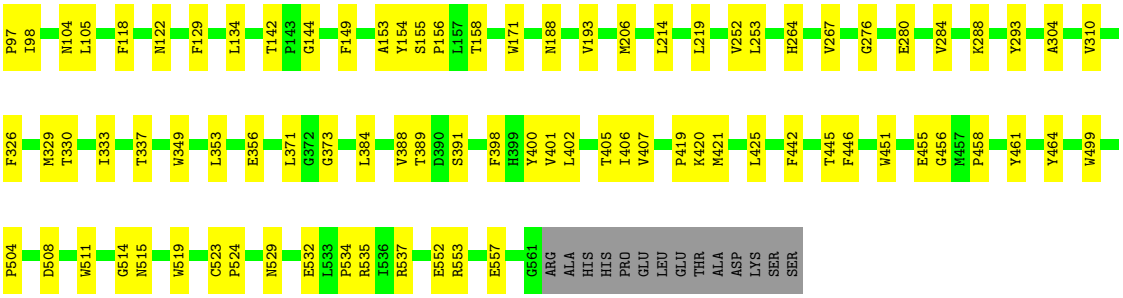
• Molecule 1: Cytochrome c oxidase subunit 2

Chain Q:



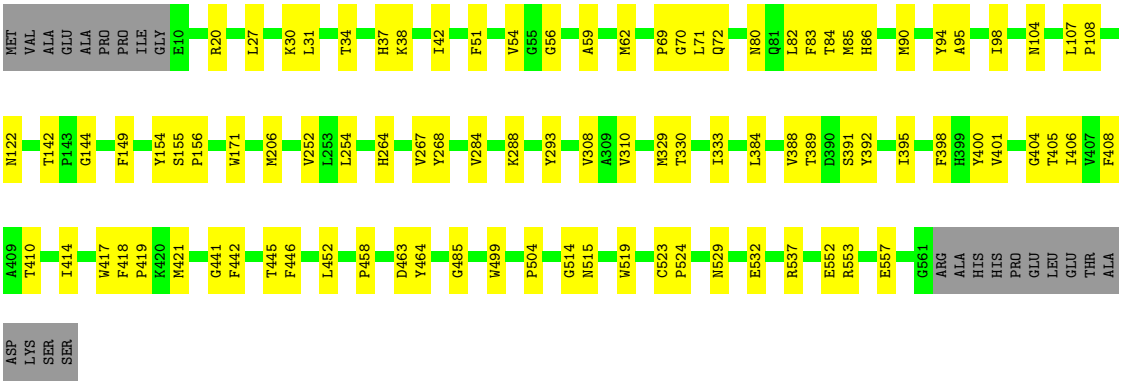
• Molecule 2: Cytochrome c oxidase subunit 1

Chain F:



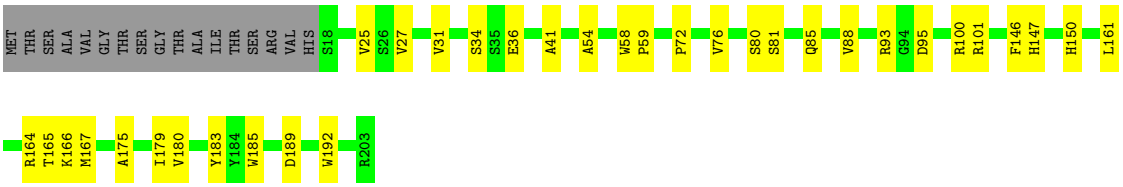
• Molecule 2: Cytochrome c oxidase subunit 1

Chain R:



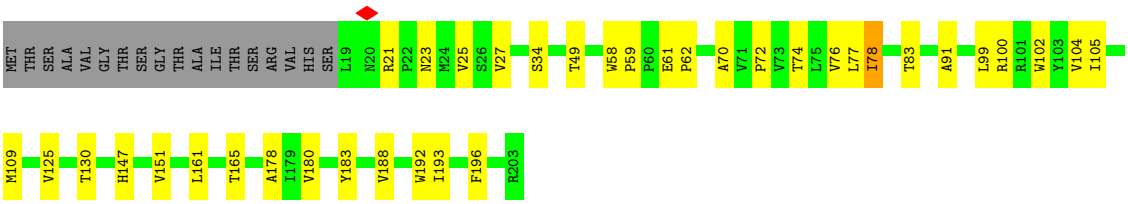
• Molecule 3: Cytochrome c oxidase subunit 3

Chain G:



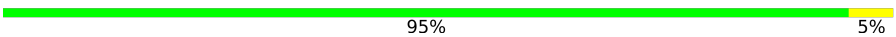
• Molecule 3: Cytochrome c oxidase subunit 3

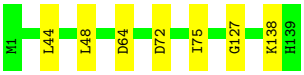
Chain S:



• Molecule 4: Cytochrome c oxidase polypeptide 4

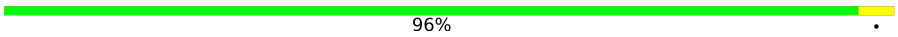
Chain H:

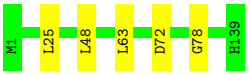




• Molecule 4: Cytochrome c oxidase polypeptide 4

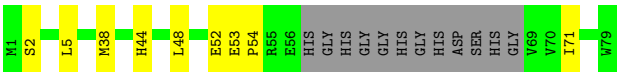
Chain T:





• Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain I:

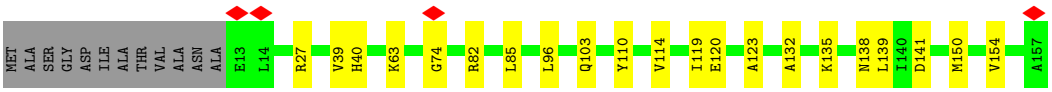


• Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain U:

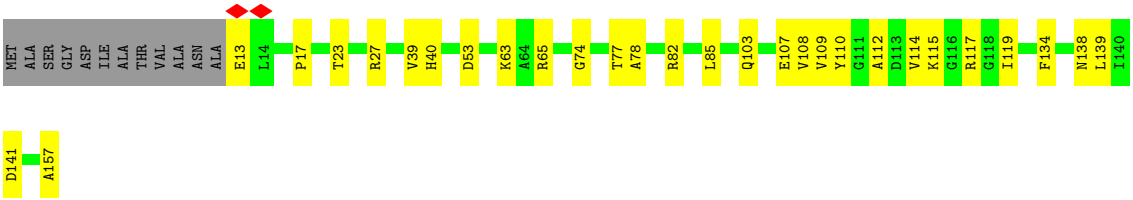
• Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain J:



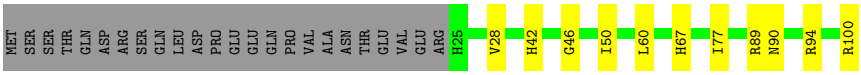
• Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:



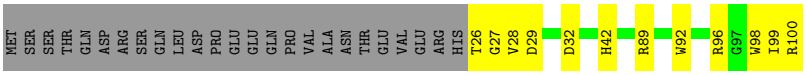
• Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain D:



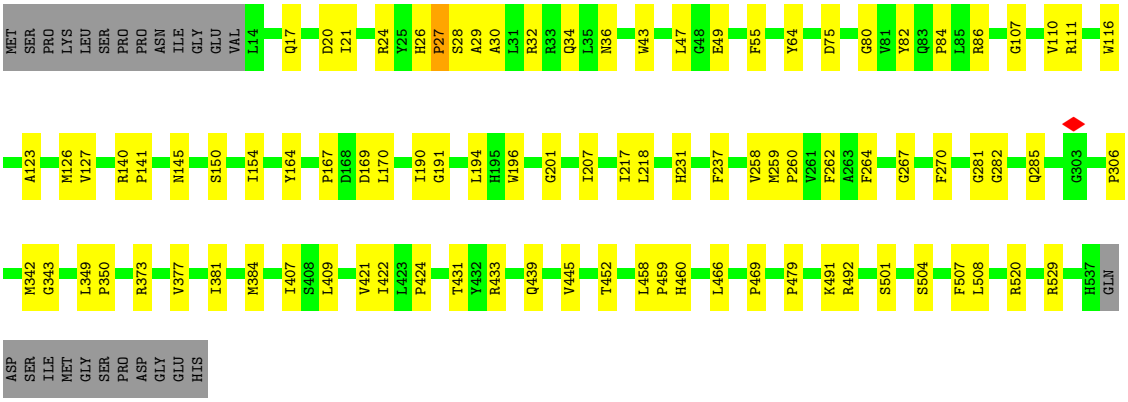
• Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain P:



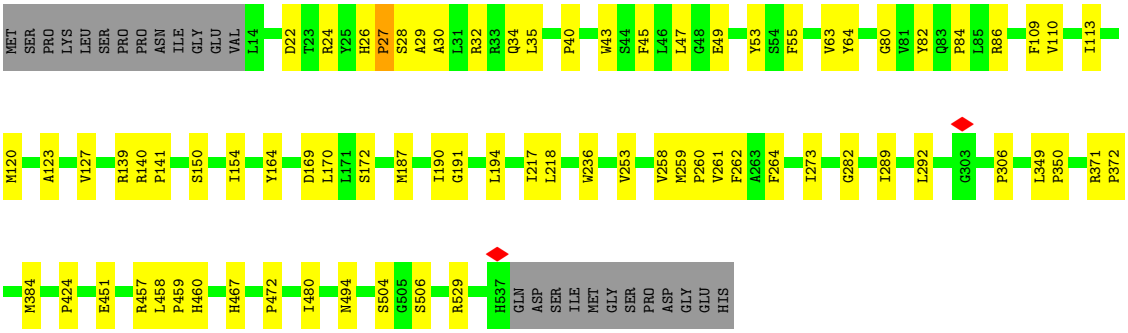
• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain N:



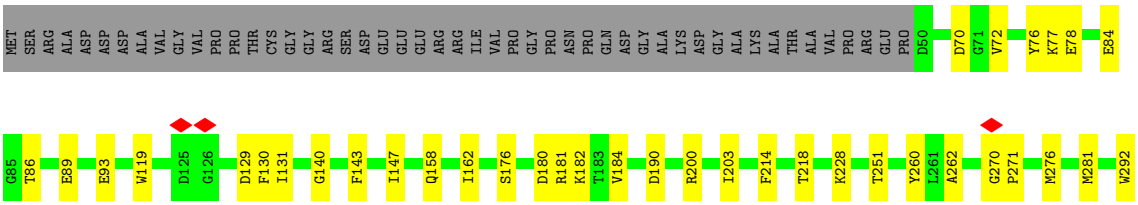
• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain B:



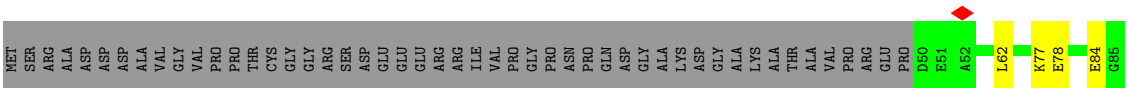
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

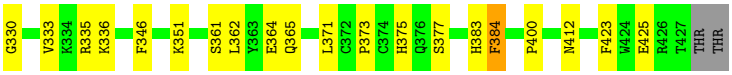
Chain M:



• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

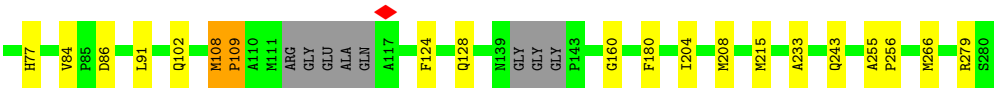
Chain A:





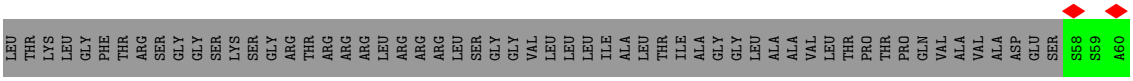
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

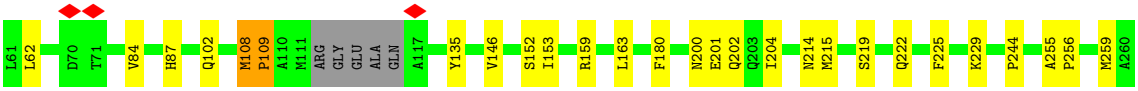
Chain O:

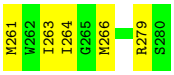


• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain C:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.664	Depositor
Minimum map value	-1.439	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: PLM, HEC, FES, 9Y0, HEM, CDL, HEA, 9YF, CU, MQ9

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	E	0.18	0/2254	0.42	0/3072
1	Q	0.18	0/2300	0.45	0/3137
2	F	0.21	0/4533	0.45	0/6192
2	R	0.20	0/4533	0.44	0/6192
3	G	0.21	0/1502	0.44	0/2051
3	S	0.21	0/1496	0.45	0/2043
4	H	0.18	0/1106	0.38	0/1517
4	T	0.16	0/1103	0.37	0/1513
5	I	0.15	0/516	0.35	0/706
5	U	0.14	0/515	0.34	0/705
6	J	0.17	0/1044	0.40	0/1427
6	V	0.17	0/1047	0.44	0/1431
7	D	0.15	0/628	0.38	0/855
7	P	0.16	0/617	0.35	0/840
8	B	0.19	0/4266	0.43	0/5821
8	N	0.20	0/4253	0.43	0/5804
9	A	0.19	0/2989	0.43	0/4056
9	M	0.19	0/3001	0.44	0/4071
10	C	0.16	0/1516	0.44	0/2061
10	O	0.16	0/1487	0.42	0/2022
All	All	0.19	0/40706	0.43	0/55516

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
2	F	0	1
2	R	0	1
8	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	C	0	1
10	O	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	139	ARG	Peptide
10	C	108	MET	Peptide
2	F	154	TYR	Peptide
10	O	108	MET	Peptide
2	R	154	TYR	Peptide

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	E	2191	0	2129	30	0
1	Q	2236	0	2164	46	0
2	F	4373	0	4347	84	0
2	R	4373	0	4347	66	0
3	G	1455	0	1455	24	0
3	S	1449	0	1450	29	0
4	H	1071	0	1047	8	0
4	T	1068	0	1045	5	0
5	I	500	0	505	8	0
5	U	499	0	502	6	0
6	J	1026	0	1038	17	0
6	V	1029	0	1040	22	0
7	D	607	0	594	7	0
7	P	597	0	586	7	0
8	B	4130	0	4145	60	0
8	N	4118	0	4137	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2912	0	2893	42	0
9	M	2924	0	2907	44	0
10	C	1487	0	1396	22	0
10	O	1458	0	1365	14	0
11	E	2	0	0	0	0
11	F	2	0	0	0	0
11	Q	3	0	0	0	0
11	R	1	0	0	0	0
12	B	296	0	371	13	0
12	C	174	0	248	9	0
12	D	88	0	126	6	0
12	F	157	0	208	5	0
12	M	95	0	143	5	0
12	N	309	0	400	16	0
12	P	88	0	126	5	0
12	R	157	0	208	6	0
13	B	11	0	16	0	0
13	F	17	0	31	0	0
13	N	11	0	16	0	0
13	R	17	0	31	0	0
14	F	120	0	108	12	0
14	R	120	0	108	8	0
15	G	43	0	0	0	0
15	S	43	0	0	0	0
16	B	85	0	57	6	0
16	N	85	0	57	5	0
17	B	81	0	98	2	0
17	C	106	0	141	11	0
17	N	202	0	264	17	0
17	O	106	0	141	10	0
18	A	4	0	0	2	0
18	M	4	0	0	0	0
19	A	93	0	0	8	0
19	M	84	0	0	6	0
20	C	86	0	61	2	0
20	O	86	0	62	4	0
All	All	42279	0	42113	621	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (621) 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)
19:M:504:9YF:O4	9:A:119:TRP:HZ2	1.36	1.05
19:M:504:9YF:O4	9:A:119:TRP:CZ2	2.13	1.00
1:E:303:ARG:HH12	1:E:309:ASN:HA	1.34	0.92
8:N:267:GLY:HA3	17:N:611:MQ9:H111	1.50	0.90
9:M:228:LYS:HG2	19:M:504:9YF:O7	1.75	0.85
3:S:74:THR:HG22	3:S:192:TRP:HE1	1.42	0.84
10:C:102:GLN:HB3	10:C:108:MET:HG2	1.62	0.79
1:E:242:LYS:NZ	2:F:389:THR:O	2.16	0.78
1:Q:154:PHE:HZ	1:Q:297:LYS:HE3	1.48	0.76
1:E:243:ARG:NH1	1:E:255:ASP:O	2.19	0.75
8:N:431:THR:HG23	12:N:606:CDL:H331	1.69	0.74
10:O:102:GLN:HB3	10:O:108:MET:HG2	1.69	0.74
8:B:282:GLY:HA3	9:A:140:GLY:HA3	1.69	0.73
1:E:60:VAL:HG11	14:F:606:HEA:H212	1.72	0.72
8:N:30:ALA:O	8:N:34:GLN:NE2	2.22	0.72
8:N:342:MET:HE2	17:N:610:MQ9:H103	1.72	0.71
9:M:320:MET:O	9:M:348:ALA:HA	1.90	0.71
1:Q:220:ARG:HD2	1:Q:261:SER:HA	1.70	0.71
6:V:74:GLY:HA2	6:V:103:GLN:HE22	1.56	0.71
1:Q:225:LEU:HD23	1:Q:245:VAL:HG22	1.72	0.71
16:N:602:HEM:HHC	16:N:602:HEM:HBB2	1.72	0.70
16:B:603:HEM:HHC	16:B:603:HEM:HBB2	1.72	0.70
8:B:506:SER:HB2	12:C:306:CDL:H212	1.72	0.70
6:J:74:GLY:HA2	6:J:103:GLN:HE22	1.56	0.70
3:S:78:ILE:HD11	3:S:193:ILE:HD11	1.73	0.69
8:N:32:ARG:NH2	9:M:70:ASP:OD2	2.26	0.69
8:N:501:SER:O	8:N:520:ARG:NH2	2.25	0.69
8:B:30:ALA:O	8:B:34:GLN:NE2	2.25	0.69
2:F:532:GLU:OE2	6:J:27:ARG:NH1	2.26	0.68
3:G:58:TRP:CD1	3:G:59:PRO:HD3	2.28	0.68
8:B:529:ARG:NH1	9:A:78:GLU:OE2	2.27	0.68
2:R:84:THR:OG1	2:R:149:PHE:O	2.11	0.68
3:G:34:SER:HB3	4:H:48:LEU:HG	1.76	0.67
1:E:76:ARG:HA	2:F:353:LEU:HB2	1.76	0.67
1:Q:243:ARG:NH1	1:Q:255:ASP:O	2.28	0.67
8:N:282:GLY:HA3	9:M:140:GLY:HA3	1.76	0.67
9:A:328:ASP:O	9:A:330:GLY:N	2.28	0.66
8:N:384:MET:HG3	8:N:424:PRO:HB3	1.76	0.66
1:Q:215:LEU:HD13	1:Q:221:ILE:HD13	1.77	0.66
10:O:160:GLY:H	10:O:233:ALA:HB2	1.60	0.66
1:E:303:ARG:NH1	1:E:309:ASN:HA	2.08	0.66
8:B:384:MET:HG3	8:B:424:PRO:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:605:HEA:HBC1	14:R:605:HEA:HMC3	1.78	0.66
9:M:184:VAL:HG22	8:B:32:ARG:HB2	1.78	0.66
17:O:301:MQ9:H311	17:O:301:MQ9:H261	1.77	0.65
12:N:605:CDL:H111	12:N:605:CDL:H321	1.78	0.65
9:M:251:THR:O	9:M:293:ARG:NH2	2.30	0.65
8:B:80:GLY:O	8:B:86:ARG:NH1	2.29	0.65
9:M:320:MET:HG3	9:M:351:LYS:HG3	1.78	0.65
8:N:264:PHE:HA	17:N:611:MQ9:H103	1.78	0.65
7:P:26:THR:HG23	7:P:27:GLY:H	1.60	0.65
1:Q:138:TRP:HA	1:Q:284:MET:HG2	1.78	0.65
3:S:58:TRP:CD1	3:S:59:PRO:HD3	2.32	0.65
3:S:21:ARG:HB3	4:T:63:LEU:HD11	1.78	0.64
2:R:532:GLU:OE2	6:V:27:ARG:NH1	2.30	0.64
2:R:30:LYS:O	2:R:34:THR:HB	1.98	0.64
6:J:132:ALA:HA	6:J:135:LYS:HE2	1.79	0.64
2:F:155:SER:HB2	2:F:156:PRO:HD3	1.80	0.63
3:S:34:SER:HB3	4:T:48:LEU:HG	1.80	0.63
2:F:30:LYS:O	2:F:34:THR:HB	1.99	0.63
1:E:138:TRP:HA	1:E:284:MET:HG2	1.79	0.63
9:A:129:ASP:OD1	9:A:130:PHE:N	2.26	0.62
7:P:28:VAL:HG13	7:P:42:HIS:HB2	1.81	0.62
1:E:102:PRO:HA	1:E:105:ILE:HG22	1.82	0.62
1:Q:294:ASN:OD1	1:Q:297:LYS:NZ	2.32	0.62
2:R:80:ASN:HA	2:R:83:PHE:CE1	2.33	0.62
8:B:187:MET:HE2	17:B:609:MQ9:H121	1.80	0.62
8:N:47:LEU:HD13	8:N:127:VAL:HG12	1.82	0.62
8:B:170:LEU:HD23	10:C:180:PHE:HE1	1.64	0.62
17:C:304:MQ9:H212	17:C:304:MQ9:H261	1.81	0.62
10:O:124:PHE:HB3	10:O:128:GLN:HB2	1.81	0.62
12:R:602:CDL:H111	12:P:201:CDL:H512	1.81	0.61
12:N:603:CDL:HB31	12:M:502:CDL:H1	1.82	0.61
2:F:310:VAL:HG12	2:F:329:MET:HB3	1.82	0.61
10:C:159:ARG:NH2	10:C:201:GLU:OE2	2.33	0.61
12:D:201:CDL:H231	12:D:201:CDL:H412	1.81	0.61
3:G:81:SER:OG	3:G:189:ASP:OD2	2.18	0.61
1:Q:137:GLN:HG2	1:Q:229:ASP:OD2	2.01	0.61
10:C:109:PRO:HD3	20:C:301:HEC:HBB2	1.82	0.60
2:F:508:ASP:OD2	6:J:27:ARG:NH2	2.34	0.60
2:R:56:GLY:HA3	14:R:606:HEA:H161	1.83	0.60
2:F:523:CYS:HB3	2:F:524:PRO:HD3	1.82	0.60
2:F:537:ARG:HH12	4:H:72:ASP:HA	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:201:CDL:H151	12:D:201:CDL:H411	1.84	0.60
8:N:458:LEU:O	8:N:460:HIS:N	2.35	0.60
2:R:537:ARG:HH12	4:T:72:ASP:HA	1.65	0.60
2:F:373:GLY:HA3	14:F:606:HEA:H262	1.84	0.60
2:F:193:VAL:HG11	2:F:214:LEU:HD12	1.82	0.59
1:E:297:LYS:NZ	1:E:301:ASP:OD2	2.35	0.59
8:B:35:LEU:HD22	8:B:259:MET:HB2	1.82	0.59
8:N:469:PRO:HB3	8:N:479:PRO:HB3	1.85	0.59
17:N:609:MQ9:H302	8:B:63:VAL:HG11	1.84	0.59
6:V:117:ARG:HG2	6:V:157:ALA:HB3	1.83	0.59
8:N:80:GLY:O	8:N:86:ARG:NH1	2.36	0.59
8:B:26:HIS:O	8:B:26:HIS:ND1	2.35	0.59
2:F:80:ASN:HA	2:F:83:PHE:CE1	2.37	0.59
2:F:398:PHE:HA	2:F:401:VAL:HG22	1.85	0.59
1:Q:289:ARG:NH1	1:Q:319:PRO:O	2.28	0.59
8:N:24:ARG:HH21	8:B:140:ARG:HG3	1.68	0.59
2:R:70:GLY:O	2:R:72:GLN:NE2	2.37	0.58
7:P:98:TRP:HE1	12:P:201:CDL:H862	1.68	0.58
9:M:77:LYS:NZ	9:A:190:ASP:OD1	2.36	0.58
8:N:170:LEU:HD23	10:O:180:PHE:HE1	1.68	0.58
9:M:129:ASP:OD1	9:M:130:PHE:N	2.34	0.58
8:B:458:LEU:O	8:B:460:HIS:N	2.37	0.58
8:B:27:PRO:O	8:B:29:ALA:N	2.36	0.57
3:G:80:SER:HB3	3:G:185:TRP:HE1	1.68	0.57
3:S:161:LEU:HD11	3:S:178:ALA:HA	1.86	0.57
9:M:260:TYR:HB2	9:M:292:TRP:HB3	1.86	0.57
1:Q:101:ILE:O	1:Q:105:ILE:HD12	2.04	0.57
3:G:58:TRP:CG	3:G:59:PRO:HD3	2.40	0.57
1:E:299:TYR:OH	1:E:303:ARG:NH1	2.38	0.57
2:F:206:MET:O	2:F:293:TYR:OH	2.18	0.57
14:F:606:HEA:HMD1	14:F:606:HEA:HBD2	1.87	0.57
12:N:606:CDL:H312	12:N:607:CDL:H512	1.86	0.57
5:U:53:GLU:HB3	5:U:54:PRO:HD3	1.87	0.56
10:O:77:HIS:NE2	20:O:303:HEC:NB	2.54	0.56
1:E:252:ASN:HD21	2:F:252:VAL:H	1.53	0.56
8:N:75:ASP:OD2	9:M:309:GLN:NE2	2.38	0.56
12:B:604:CDL:H552	12:B:605:CDL:H602	1.86	0.56
12:C:303:CDL:H522	12:C:303:CDL:H711	1.87	0.56
3:S:83:THR:HG23	3:S:102:TRP:HE3	1.69	0.56
14:R:605:HEA:HMD3	14:R:605:HEA:HBD2	1.88	0.56
6:J:110:TYR:CZ	6:J:119:ILE:HB	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:84:LEU:O	2:R:553:ARG:NH2	2.37	0.56
2:R:523:CYS:HB3	2:R:524:PRO:HD3	1.88	0.56
6:V:13:GLU:HA	6:V:17:PRO:HB3	1.87	0.56
10:C:146:VAL:O	10:C:202:GLN:NE2	2.39	0.56
3:S:58:TRP:CG	3:S:59:PRO:HD3	2.42	0.55
3:S:72:PRO:O	3:S:76:VAL:HG23	2.06	0.55
8:N:27:PRO:O	8:N:29:ALA:N	2.39	0.55
8:B:372:PRO:HB2	12:B:606:CDL:HA61	1.87	0.55
2:F:405:THR:HG23	2:F:406:ILE:HG23	1.88	0.55
1:Q:275:GLU:O	1:Q:281:HIS:NE2	2.40	0.55
2:F:56:GLY:HA3	14:F:607:HEA:H161	1.89	0.55
1:Q:334:GLU:HB2	2:R:72:GLN:HA	1.89	0.55
2:F:504:PRO:HG2	6:J:39:VAL:HG21	1.87	0.55
1:Q:227:SER:HB2	1:Q:245:VAL:HG12	1.87	0.55
8:N:217:ILE:HD11	8:B:217:ILE:HD11	1.89	0.55
2:R:155:SER:HB2	2:R:156:PRO:HD3	1.88	0.55
2:R:206:MET:O	2:R:293:TYR:OH	2.21	0.55
6:V:85:LEU:HD13	6:V:109:VAL:HG23	1.89	0.55
9:M:281:MET:O	9:M:323:ARG:NH2	2.39	0.55
2:F:59:ALA:HB2	2:F:86:HIS:CE1	2.42	0.54
12:N:606:CDL:H311	12:N:606:CDL:H112	1.90	0.54
2:F:288:LYS:NZ	2:F:349:TRP:O	2.39	0.54
3:S:125:VAL:HG23	3:S:130:THR:HG22	1.89	0.54
8:B:190:ILE:HG13	8:B:191:GLY:H	1.71	0.54
2:F:142:THR:HG22	2:F:144:GLY:H	1.72	0.54
7:D:28:VAL:HG13	7:D:42:HIS:HB2	1.90	0.54
8:N:26:HIS:O	8:N:26:HIS:ND1	2.40	0.54
16:N:601:HEM:HMB1	16:N:601:HEM:HBB2	1.88	0.54
8:B:190:ILE:HD12	8:B:194:LEU:HD11	1.90	0.54
19:A:503:9YF:C17	19:A:503:9YF:C11	2.86	0.54
1:Q:302:GLN:HG3	1:Q:307:LYS:HD2	1.90	0.54
9:A:246:TRP:CE2	19:A:503:9YF:O3	2.60	0.54
9:A:251:THR:O	9:A:293:ARG:NH2	2.41	0.54
2:F:53:LEU:HB3	14:F:607:HEA:H242	1.90	0.54
2:F:104:ASN:ND2	2:F:122:ASN:HD21	2.05	0.54
7:D:89:ARG:HD2	12:D:201:CDL:H741	1.89	0.54
9:M:328:ASP:HB3	9:M:331:ARG:HD3	1.89	0.54
9:M:328:ASP:O	9:M:330:GLY:N	2.40	0.54
2:F:535:ARG:HG2	2:F:537:ARG:HE	1.73	0.54
3:G:101:ARG:NH1	8:N:508:LEU:O	2.41	0.54
1:Q:159:ALA:C	1:Q:161:PRO:HD3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:25:VAL:HG12	3:S:180:VAL:HG11	1.89	0.53
2:F:37:HIS:CE1	2:F:529:ASN:HD21	2.26	0.53
2:F:84:THR:OG1	2:F:149:PHE:O	2.16	0.53
2:F:326:PHE:O	2:F:330:THR:HG23	2.08	0.53
3:G:25:VAL:HG12	3:G:180:VAL:HG11	1.89	0.53
3:G:27:VAL:O	3:G:31:VAL:HG23	2.08	0.53
2:R:264:HIS:NE2	2:R:268:TYR:HE2	2.06	0.53
2:R:398:PHE:HA	2:R:401:VAL:HG22	1.91	0.53
12:D:201:CDL:H182	8:N:384:MET:HE1	1.89	0.53
3:S:147:HIS:NE2	3:S:192:TRP:HB2	2.23	0.53
9:M:365:GLN:NE2	10:O:215:MET:O	2.42	0.53
2:F:97:PRO:HG3	2:F:129:PHE:CE1	2.43	0.53
16:B:602:HEM:HMB1	16:B:602:HEM:HBB2	1.89	0.53
1:Q:154:PHE:CZ	1:Q:297:LYS:HB3	2.44	0.53
7:D:90:ASN:HD21	7:D:94:ARG:HE	1.57	0.53
8:N:49:GLU:OE2	17:N:608:MQ9:H3D	2.09	0.53
5:U:44:HIS:NE2	6:V:40:HIS:O	2.42	0.53
9:M:182:LYS:HE3	9:A:62:LEU:HD11	1.90	0.53
17:C:305:MQ9:H353	17:C:305:MQ9:H411	1.89	0.53
1:Q:299:TYR:OH	1:Q:309:ASN:OD1	2.18	0.53
19:M:504:9YF:O3	19:M:504:9YF:O5	2.26	0.53
17:O:302:MQ9:H151	17:O:302:MQ9:C9	2.39	0.53
1:E:235:TRP:CG	1:E:242:LYS:HE2	2.44	0.53
3:G:72:PRO:O	3:G:76:VAL:HG23	2.09	0.53
12:N:603:CDL:HA21	10:O:279:ARG:HH12	1.73	0.53
8:B:260:PRO:HG2	8:B:261:VAL:HG23	1.90	0.53
9:A:267:THR:HG22	9:A:269:ASP:H	1.73	0.53
1:E:252:ASN:HB3	2:F:253:LEU:HD23	1.91	0.52
2:R:504:PRO:HG2	6:V:39:VAL:HG11	1.91	0.52
17:C:305:MQ9:H301	17:C:305:MQ9:H351	1.91	0.52
2:R:405:THR:HG23	2:R:406:ILE:HG13	1.91	0.52
9:A:260:TYR:HB2	9:A:292:TRP:HB3	1.91	0.52
7:D:94:ARG:HB3	7:D:100:ARG:HH11	1.73	0.52
3:G:147:HIS:CE1	3:G:192:TRP:HB2	2.45	0.52
9:M:426:ARG:HG3	9:M:427:THR:H	1.74	0.52
2:R:104:ASN:ND2	2:R:122:ASN:HD21	2.08	0.52
9:M:307:LYS:O	9:M:310:GLU:HG3	2.10	0.52
1:E:96:LEU:HA	1:E:99:THR:HG22	1.92	0.52
6:V:110:TYR:CZ	6:V:119:ILE:HB	2.45	0.52
2:F:402:LEU:O	2:F:406:ILE:HG12	2.09	0.52
8:N:190:ILE:HD12	8:N:194:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:17:GLN:O	8:N:21:ILE:HG12	2.10	0.51
8:B:529:ARG:HH12	9:A:78:GLU:HG3	1.75	0.51
2:R:254:LEU:HD13	3:S:49:THR:HG21	1.92	0.51
2:R:395:ILE:HA	2:R:398:PHE:CE1	2.46	0.51
17:O:302:MQ9:H503	17:O:302:MQ9:H253	1.92	0.51
2:R:69:PRO:HG3	2:R:464:TYR:CE2	2.45	0.51
8:B:169:ASP:OD1	8:B:172:SER:OG	2.22	0.51
19:A:503:9YF:O	19:A:503:9YF:O7	2.29	0.51
12:C:306:CDL:H261	12:C:306:CDL:H662	1.92	0.51
9:M:180:ASP:OD1	8:B:32:ARG:NH1	2.41	0.51
8:N:258:VAL:HA	8:N:262:PHE:HB3	1.92	0.51
19:A:503:9YF:C11	19:A:503:9YF:C16	2.89	0.51
2:R:532:GLU:HG3	6:V:23:THR:HB	1.92	0.51
3:S:147:HIS:CE1	3:S:192:TRP:HB2	2.46	0.51
8:B:504:SER:O	8:B:504:SER:OG	2.26	0.51
9:A:263:ARG:HE	9:A:274:ILE:HD11	1.75	0.51
8:N:407:ILE:HD11	17:O:301:MQ9:H38	1.93	0.51
17:B:608:MQ9:H302	17:B:608:MQ9:H261	1.93	0.50
2:R:142:THR:HG22	2:R:144:GLY:H	1.77	0.50
8:N:285:GLN:HE22	10:O:243:GLN:HE21	1.59	0.50
1:E:275:GLU:O	1:E:281:HIS:NE2	2.45	0.50
2:F:337:THR:HG21	14:F:606:HEA:H14	1.94	0.50
4:H:127:GLY:HA2	12:N:603:CDL:H112	1.93	0.50
6:V:138:ASN:HB3	6:V:141:ASP:HB2	1.93	0.50
8:B:27:PRO:C	8:B:29:ALA:H	2.20	0.50
2:F:284:VAL:HG22	2:F:514:GLY:HA2	1.92	0.50
8:B:258:VAL:HA	8:B:262:PHE:HB3	1.94	0.50
2:R:59:ALA:HB2	2:R:86:HIS:CE1	2.47	0.50
16:B:603:HEM:HMC2	16:B:603:HEM:HBC2	1.93	0.50
3:G:147:HIS:NE2	3:G:192:TRP:HB2	2.26	0.50
10:C:219:SER:H	10:C:222:GLN:HE21	1.60	0.50
2:F:118:PHE:HB2	2:F:188:ASN:ND2	2.27	0.49
2:F:356:GLU:HG2	2:F:511:TRP:HZ3	1.77	0.49
6:J:150:MET:O	6:J:154:VAL:HG23	2.12	0.49
8:N:529:ARG:HH12	9:M:78:GLU:CD	2.20	0.49
2:F:28:ILE:HD12	8:N:433:ARG:HB2	1.95	0.49
12:P:201:CDL:H182	8:B:384:MET:HE1	1.95	0.49
9:A:400:PRO:HB2	9:A:412:ASN:HB3	1.94	0.49
8:N:190:ILE:HG13	8:N:191:GLY:H	1.77	0.49
8:N:116:TRP:CD1	8:N:281:GLY:HA2	2.48	0.49
9:M:214:PHE:O	9:M:218:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:161:LEU:O	3:G:165:THR:HG23	2.13	0.49
9:A:377:SER:OG	18:A:501:FES:S2	2.69	0.49
2:F:515:ASN:O	2:F:519:TRP:HD1	1.96	0.49
1:Q:163:ARG:HD2	1:Q:196:LEU:O	2.13	0.48
1:Q:232:HIS:ND1	1:Q:277:CYS:SG	2.86	0.48
2:R:445:THR:HG23	2:R:446:PHE:CD2	2.48	0.48
8:N:126:MET:SD	17:O:302:MQ9:H28	2.53	0.48
10:O:109:PRO:HD3	20:O:303:HEC:HAB	1.95	0.48
5:I:44:HIS:NE2	6:J:40:HIS:O	2.46	0.48
2:R:441:GLY:O	2:R:445:THR:HG22	2.14	0.48
3:S:105:ILE:O	3:S:109:MET:HG3	2.13	0.48
8:N:445:VAL:HG21	8:N:491:LYS:HD3	1.95	0.48
9:M:336:LYS:H	9:M:336:LYS:HD2	1.77	0.48
8:B:120:MET:HE3	10:C:261:MET:HE1	1.96	0.48
2:R:310:VAL:HG12	2:R:329:MET:HB3	1.94	0.48
8:N:27:PRO:C	8:N:29:ALA:H	2.21	0.48
10:C:279:ARG:NH1	12:C:303:CDL:OA3	2.47	0.48
12:C:306:CDL:H661	12:C:306:CDL:H632	1.59	0.48
1:Q:85:PRO:O	1:Q:87:GLN:HG2	2.13	0.48
7:P:89:ARG:HH21	12:P:201:CDL:H802	1.78	0.48
8:N:349:LEU:HB3	8:N:350:PRO:HD3	1.95	0.48
12:B:607:CDL:H272	12:B:607:CDL:H242	1.70	0.48
2:F:105:LEU:HD22	2:F:421:MET:HE2	1.95	0.48
2:F:405:THR:HG23	2:F:406:ILE:N	2.29	0.48
8:N:504:SER:O	8:N:504:SER:OG	2.28	0.48
9:M:158:GLN:HA	9:M:162:ILE:HD12	1.96	0.48
1:Q:154:PHE:CZ	1:Q:297:LYS:HE3	2.37	0.48
2:R:20:ARG:NH2	6:V:53:ASP:OD1	2.47	0.48
8:N:164:TYR:OH	8:N:306:PRO:HB3	2.14	0.47
2:R:254:LEU:HD22	3:S:49:THR:HG21	1.96	0.47
12:R:601:CDL:HA61	12:R:601:CDL:HB61	1.95	0.47
8:N:24:ARG:HG2	8:B:141:PRO:HA	1.96	0.47
17:O:301:MQ9:H203	17:O:301:MQ9:H222	1.80	0.47
9:A:129:ASP:C	9:A:131:ILE:H	2.22	0.47
3:G:175:ALA:O	3:G:179:ILE:HG13	2.14	0.47
1:Q:263:ILE:HG21	1:Q:290:VAL:HG21	1.95	0.47
8:N:43:TRP:CH2	12:N:606:CDL:H712	2.49	0.47
9:A:254:TYR:CZ	9:A:257:GLU:HB3	2.49	0.47
6:J:110:TYR:OH	6:J:123:ALA:HB2	2.14	0.47
8:N:218:LEU:HD21	16:B:603:HEM:HBC1	1.97	0.47
10:O:91:LEU:HD21	20:O:303:HEC:CHB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:503:9YF:C16	19:A:503:9YF:C12	2.92	0.47
2:F:37:HIS:HE1	2:F:529:ASN:HD21	1.61	0.47
1:Q:44:LYS:O	1:Q:48:GLU:HG3	2.14	0.47
12:R:601:CDL:H132	12:R:601:CDL:H381	1.96	0.47
9:M:262:ALA:HB2	9:M:292:TRP:HB2	1.95	0.47
8:B:47:LEU:HD13	8:B:127:VAL:HG12	1.97	0.47
8:B:82:TYR:CE2	8:B:84:PRO:HG2	2.50	0.47
8:B:170:LEU:HD23	10:C:180:PHE:CE1	2.47	0.47
8:B:253:VAL:HB	9:A:169:GLN:HB3	1.97	0.47
10:C:259:MET:HB3	17:C:304:MQ9:H5M2	1.97	0.47
17:C:305:MQ9:H353	17:C:305:MQ9:C41	2.44	0.47
2:F:85:MET:HE1	2:F:171:TRP:CD1	2.50	0.47
2:F:330:THR:O	2:F:333:ILE:HG22	2.15	0.47
8:N:150:SER:O	8:N:154:ILE:HG12	2.14	0.47
8:B:109:PHE:CZ	8:B:113:ILE:HD11	2.50	0.47
1:E:84:LEU:O	2:F:553:ARG:NH2	2.35	0.47
2:R:410:THR:O	2:R:414:ILE:HG12	2.15	0.47
2:R:552:GLU:CD	2:R:552:GLU:H	2.22	0.47
2:F:288:LYS:HB3	2:F:288:LYS:HE2	1.70	0.47
14:F:607:HEA:HMC1	14:F:607:HEA:HBC1	1.97	0.47
3:G:36:GLU:OE2	3:G:150:HIS:HE1	1.98	0.47
3:G:100:ARG:HD3	8:N:507:PHE:O	2.14	0.47
2:R:392:TYR:CD2	2:R:452:LEU:HD23	2.50	0.47
2:F:371:LEU:HD23	2:F:400:TYR:CE2	2.50	0.46
2:F:552:GLU:CD	2:F:552:GLU:H	2.23	0.46
5:I:52:GLU:O	5:I:52:GLU:HG2	2.13	0.46
5:I:53:GLU:HB3	5:I:54:PRO:HD3	1.97	0.46
2:R:515:ASN:O	2:R:519:TRP:HD1	1.98	0.46
9:M:200:ARG:HB3	9:M:203:ILE:HB	1.96	0.46
8:B:34:GLN:HG3	8:B:236:TRP:HZ2	1.80	0.46
8:B:451:GLU:HG2	8:B:467:HIS:CE1	2.50	0.46
2:F:15:ARG:HD2	5:I:52:GLU:OE1	2.15	0.46
9:M:190:ASP:OD1	9:A:77:LYS:NZ	2.48	0.46
2:R:37:HIS:HD2	2:R:104:ASN:O	1.99	0.46
2:R:384:LEU:O	2:R:388:VAL:HG22	2.15	0.46
9:A:229:ASN:HB2	19:A:502:9YF:C1	2.45	0.46
9:A:335:ARG:HB2	9:A:384:PHE:CG	2.50	0.46
1:Q:152:GLY:O	1:Q:153:SER:OG	2.30	0.46
17:N:609:MQ9:H48	12:B:604:CDL:C38	2.45	0.46
1:E:225:LEU:HD23	1:E:245:VAL:HG22	1.98	0.46
2:R:405:THR:HG23	2:R:406:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:369:ARG:HD3	9:M:388:ILE:HD11	1.98	0.46
20:O:303:HEC:HBD2	20:O:303:HEC:HHA	1.97	0.46
2:F:406:ILE:HD11	14:F:607:HEA:HBC1	1.97	0.46
1:E:90:TYR:HB3	1:E:92:MET:SD	2.55	0.46
2:F:38:LYS:HG2	2:F:421:MET:HE1	1.98	0.46
3:G:41:ALA:HA	4:H:44:LEU:HD12	1.97	0.46
9:A:375:HIS:HB2	18:A:501:FES:S2	2.56	0.46
2:F:445:THR:HG23	2:F:446:PHE:CD2	2.51	0.46
14:F:606:HEA:HMC1	14:F:606:HEA:HBC1	1.96	0.46
1:Q:270:VAL:HB	1:Q:324:THR:HG21	1.98	0.46
14:R:605:HEA:HBC1	14:R:605:HEA:CMC	2.44	0.46
8:N:64:TYR:CD2	8:N:110:VAL:HG11	2.51	0.46
10:O:84:VAL:HG12	10:O:86:ASP:H	1.81	0.46
9:A:362:LEU:HB2	9:A:371:LEU:O	2.15	0.46
17:C:304:MQ9:H261	17:C:304:MQ9:C21	2.43	0.46
3:S:74:THR:HG22	3:S:192:TRP:NE1	2.21	0.46
12:P:201:CDL:H821	12:P:201:CDL:H791	1.34	0.46
16:N:602:HEM:HBC1	8:B:218:LEU:HD21	1.97	0.46
12:M:502:CDL:H582	12:M:502:CDL:H611	1.71	0.46
9:A:351:LYS:HE2	9:A:361:SER:HB3	1.98	0.46
10:C:84:VAL:HG11	10:C:87:HIS:HD2	1.80	0.46
12:C:306:CDL:H722	12:C:306:CDL:H752	1.44	0.46
2:F:553:ARG:O	2:F:557:GLU:HG2	2.16	0.45
8:N:343:GLY:HA3	17:N:610:MQ9:H161	1.98	0.45
12:N:605:CDL:H162	12:N:605:CDL:H131	1.67	0.45
17:N:610:MQ9:H253	17:N:610:MQ9:H271	1.54	0.45
10:O:255:ALA:HB3	10:O:256:PRO:HD3	1.98	0.45
3:G:85:GLN:HA	3:G:88:VAL:HG12	1.99	0.45
2:R:107:LEU:HB3	2:R:108:PRO:HD3	1.98	0.45
9:A:365:GLN:NE2	10:C:215:MET:O	2.50	0.45
2:F:69:PRO:HG3	2:F:464:TYR:CE2	2.51	0.45
2:R:90:MET:HB3	14:R:606:HEA:CAC	2.47	0.45
8:B:64:TYR:CD2	8:B:110:VAL:HG11	2.52	0.45
2:R:85:MET:HE1	2:R:171:TRP:HD1	1.81	0.45
2:R:330:THR:O	2:R:333:ILE:HG22	2.16	0.45
12:M:502:CDL:H351	12:M:502:CDL:H382	1.78	0.45
1:E:227:SER:OG	1:E:230:VAL:O	2.22	0.45
1:Q:127:PRO:HG3	1:Q:222:GLU:OE1	2.17	0.45
1:Q:210:ILE:HG13	1:Q:327:PRO:HB3	1.98	0.45
14:R:606:HEA:H211	14:R:606:HEA:H271	1.73	0.45
17:N:608:MQ9:H252	17:N:611:MQ9:H253	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:609:MQ9:H203	17:N:609:MQ9:H221	1.85	0.45
17:C:305:MQ9:H451	17:C:305:MQ9:H422	1.67	0.45
2:F:401:VAL:O	2:F:405:THR:HG22	2.17	0.45
5:I:71:ILE:HD13	6:J:82:ARG:HD3	1.98	0.45
8:N:140:ARG:HB3	8:N:141:PRO:HD3	1.99	0.45
9:M:176:SER:OG	8:B:26:HIS:HB2	2.17	0.45
9:A:336:LYS:H	9:A:336:LYS:HD2	1.82	0.45
12:F:602:CDL:H512	12:F:602:CDL:H542	1.61	0.45
8:N:237:PHE:CE2	12:N:605:CDL:H122	2.51	0.45
9:M:129:ASP:C	9:M:131:ILE:H	2.24	0.45
8:B:84:PRO:HA	10:C:163:LEU:HB3	1.99	0.45
8:B:123:ALA:HB3	10:C:266:MET:HE3	1.98	0.45
17:C:304:MQ9:H353	17:C:304:MQ9:H372	1.76	0.45
4:H:138:LYS:HE2	12:M:502:CDL:HB21	1.99	0.45
6:V:115:LYS:HA	6:V:119:ILE:HD13	1.98	0.45
16:N:602:HEM:HBC2	16:N:602:HEM:HMC2	1.99	0.45
2:F:11:LEU:HD13	5:I:48:LEU:HD12	1.98	0.45
2:R:284:VAL:HG22	2:R:514:GLY:HA2	1.99	0.45
17:N:610:MQ9:H102	17:N:610:MQ9:O1	2.17	0.45
12:B:606:CDL:H562	12:B:607:CDL:H552	1.98	0.45
12:B:607:CDL:H121	12:B:607:CDL:H151	1.75	0.45
6:J:85:LEU:HD13	6:J:96:LEU:HB2	1.99	0.45
1:Q:138:TRP:HA	1:Q:284:MET:CG	2.46	0.45
2:R:95:ALA:O	2:R:98:ILE:HG22	2.17	0.45
8:N:167:PRO:O	8:N:169:ASP:N	2.50	0.45
1:E:229:ASP:OD1	1:E:229:ASP:N	2.49	0.44
2:F:60:LEU:HG	14:F:607:HEA:H263	1.99	0.44
8:N:82:TYR:CE2	8:N:84:PRO:HG2	2.52	0.44
9:A:333:VAL:HG21	9:A:383:HIS:ND1	2.32	0.44
17:C:305:MQ9:H102	17:C:305:MQ9:H72	1.47	0.44
8:N:20:ASP:OD2	8:N:24:ARG:NH1	2.50	0.44
12:B:607:CDL:H172	12:C:303:CDL:H382	1.99	0.44
6:J:119:ILE:HG13	6:J:120:GLU:N	2.33	0.44
2:R:499:TRP:NE1	12:R:602:CDL:HB4	2.33	0.44
10:O:204:ILE:O	10:O:208:MET:HG2	2.17	0.44
2:F:18:PRO:O	2:F:20:ARG:NH1	2.51	0.44
2:F:406:ILE:HG13	2:F:407:VAL:N	2.32	0.44
5:I:2:SER:O	5:I:5:LEU:N	2.50	0.44
2:R:308:VAL:HG12	2:R:308:VAL:O	2.16	0.44
8:N:196:TRP:CE3	8:N:201:GLY:HA2	2.53	0.44
10:C:263:ILE:HG23	10:C:264:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:384:LEU:O	2:F:388:VAL:HG22	2.17	0.44
2:R:414:ILE:HD12	12:R:602:CDL:H852	2.00	0.44
2:R:59:ALA:HA	2:R:62:MET:HE2	2.00	0.44
8:N:492:ARG:NH1	12:N:607:CDL:OA4	2.50	0.44
12:C:303:CDL:H752	12:C:303:CDL:H722	1.82	0.44
12:C:303:CDL:H832	12:C:303:CDL:H862	1.65	0.44
2:F:400:TYR:HA	2:F:442:PHE:HZ	1.83	0.44
2:R:264:HIS:HE2	2:R:268:TYR:HE2	1.66	0.44
8:N:116:TRP:HD1	8:N:281:GLY:HA2	1.81	0.44
17:N:609:MQ9:H422	17:N:609:MQ9:H38	1.60	0.44
9:M:76:TYR:CE1	9:M:78:GLU:HG3	2.53	0.44
17:O:301:MQ9:H261	17:O:301:MQ9:H221	1.57	0.44
8:B:53:TYR:HD2	8:B:273:ILE:HD12	1.83	0.44
1:E:235:TRP:CH2	2:F:456:GLY:HA2	2.52	0.44
2:F:91:LEU:HD23	2:F:91:LEU:HA	1.87	0.44
12:N:605:CDL:H792	12:N:605:CDL:H762	1.65	0.44
17:N:609:MQ9:H3D	8:B:49:GLU:OE2	2.17	0.44
9:A:296:ASP:OD2	9:A:311:ILE:HD11	2.17	0.44
8:B:24:ARG:NH2	12:B:604:CDL:OB4	2.38	0.44
2:F:155:SER:HB3	2:F:252:VAL:HA	1.99	0.43
1:Q:68:ILE:O	1:Q:71:THR:HG22	2.18	0.43
5:U:74:GLY:HA2	6:V:108:VAL:O	2.17	0.43
8:N:123:ALA:HB3	10:O:266:MET:HE3	1.99	0.43
8:N:409:LEU:HD21	9:M:376:GLN:HG2	1.99	0.43
9:M:362:LEU:HB2	9:M:371:LEU:O	2.18	0.43
9:A:121:PHE:CZ	9:A:123:ALA:HB3	2.53	0.43
10:C:200:ASN:O	10:C:204:ILE:HG13	2.17	0.43
2:F:419:PRO:HG3	2:F:425:LEU:HD23	1.99	0.43
2:F:534:PRO:O	4:H:75:ILE:HD11	2.18	0.43
8:N:82:TYR:CZ	8:N:84:PRO:HG2	2.53	0.43
8:B:55:PHE:HE1	16:B:603:HEM:HBB1	1.83	0.43
8:B:150:SER:O	8:B:154:ILE:HG12	2.17	0.43
12:F:602:CDL:H352	12:F:602:CDL:H652	2.00	0.43
1:Q:96:LEU:HA	1:Q:99:THR:HG22	2.00	0.43
8:N:270:PHE:CD2	17:N:611:MQ9:H203	2.53	0.43
3:G:146:PHE:O	3:G:150:HIS:HD2	2.00	0.43
2:F:10:GLU:HG3	2:F:11:LEU:HG	2.00	0.43
2:F:57:LEU:HD13	14:F:607:HEA:H202	2.00	0.43
2:F:65:GLU:HB2	2:F:74:LEU:HD12	2.01	0.43
5:U:54:PRO:HD2	6:V:65:ARG:NH1	2.34	0.43
17:C:305:MQ9:H303	17:C:305:MQ9:H322	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:MET:HE1	2:F:171:TRP:HD1	1.84	0.43
1:Q:283:MET:HE2	1:Q:328:PHE:HE2	1.83	0.43
1:Q:289:ARG:HH11	1:Q:318:GLN:HB3	1.84	0.43
8:B:140:ARG:HB3	8:B:141:PRO:HD3	2.01	0.43
8:B:164:TYR:OH	8:B:306:PRO:HB3	2.18	0.43
1:E:272:ARG:NH1	2:F:456:GLY:O	2.51	0.43
6:J:63:LYS:HA	6:J:63:LYS:HD3	1.83	0.43
6:V:63:LYS:HD3	6:V:63:LYS:HA	1.80	0.43
9:M:362:LEU:HD22	9:M:371:LEU:HD23	2.00	0.43
10:C:225:PHE:CE2	10:C:229:LYS:HD2	2.53	0.43
2:F:264:HIS:O	2:F:267:VAL:HG22	2.18	0.43
1:Q:56:ALA:O	1:Q:60:VAL:HG23	2.18	0.43
1:Q:252:ASN:HD21	2:R:252:VAL:H	1.66	0.43
2:R:553:ARG:O	2:R:557:GLU:HG2	2.19	0.43
3:S:70:ALA:HB1	3:S:196:PHE:HE1	1.84	0.43
1:E:319:PRO:HA	1:E:320:PRO:HD3	1.88	0.43
2:F:276:GLY:O	2:F:280:GLU:HG2	2.19	0.43
3:G:180:VAL:HA	3:G:183:TYR:CE2	2.54	0.43
3:S:74:THR:O	3:S:78:ILE:HD12	2.19	0.43
3:S:91:ALA:HB2	3:S:99:LEU:HD12	2.00	0.43
6:V:78:ALA:O	6:V:82:ARG:HG2	2.18	0.43
8:N:421:VAL:HG13	8:N:422:ILE:HG23	2.01	0.43
9:M:119:TRP:CZ2	19:A:502:9YF:O7	2.71	0.43
8:B:494:ASN:OD1	8:B:494:ASN:N	2.48	0.43
9:A:321:LEU:HD11	9:A:346:PHE:HB3	1.99	0.43
2:R:38:LYS:O	2:R:42:ILE:HG12	2.19	0.43
8:N:452:THR:OG1	8:N:466:LEU:O	2.35	0.43
12:N:603:CDL:H572	12:N:603:CDL:H542	1.91	0.43
17:O:302:MQ9:H72	17:O:302:MQ9:H101	1.49	0.43
2:F:95:ALA:O	2:F:98:ILE:HG22	2.18	0.42
1:Q:227:SER:OG	1:Q:230:VAL:O	2.27	0.42
1:Q:275:GLU:O	1:Q:281:HIS:CE1	2.72	0.42
2:R:391:SER:HA	2:R:458:PRO:HA	2.01	0.42
9:M:89:GLU:O	9:M:93:GLU:HG3	2.18	0.42
3:G:54:ALA:HB3	3:G:58:TRP:HB2	2.00	0.42
2:R:82:LEU:HD23	2:R:82:LEU:HA	1.88	0.42
8:N:377:VAL:O	8:N:381:ILE:HG12	2.18	0.42
9:M:260:TYR:CD2	9:M:292:TRP:HD1	2.37	0.42
9:M:276:MET:HB3	9:M:276:MET:HE2	1.75	0.42
2:F:310:VAL:HB	2:F:330:THR:HG22	2.00	0.42
12:F:602:CDL:H782	12:F:602:CDL:H752	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:93:ARG:O	3:G:95:ASP:N	2.52	0.42
12:D:201:CDL:H372	12:D:201:CDL:H131	2.01	0.42
3:S:147:HIS:O	3:S:151:VAL:HG23	2.19	0.42
8:N:55:PHE:HE1	16:N:602:HEM:HBB1	1.85	0.42
10:C:255:ALA:HB3	10:C:256:PRO:HD3	2.01	0.42
1:Q:242:LYS:NZ	2:R:389:THR:O	2.39	0.42
2:R:51:PHE:HA	2:R:54:VAL:HG22	2.01	0.42
12:N:603:CDL:H762	12:N:603:CDL:H791	1.41	0.42
8:B:43:TRP:CH2	12:B:606:CDL:H711	2.54	0.42
9:A:200:ARG:HB3	9:A:203:ILE:HB	2.02	0.42
10:C:152:SER:OG	10:C:153:ILE:N	2.53	0.42
6:J:138:ASN:HB3	6:J:141:ASP:HB2	2.00	0.42
3:G:100:ARG:HH11	3:G:166:LYS:HA	1.84	0.42
12:D:201:CDL:H762	12:D:201:CDL:H792	1.68	0.42
7:P:29:ASP:HB2	7:P:32:ASP:OD1	2.19	0.42
8:B:55:PHE:CE1	16:B:603:HEM:HBB1	2.55	0.42
3:G:179:ILE:HG22	3:G:183:TYR:CE1	2.55	0.42
6:J:110:TYR:CD2	6:J:119:ILE:HD12	2.55	0.42
2:R:37:HIS:CE1	2:R:529:ASN:HD21	2.37	0.42
2:R:264:HIS:O	2:R:267:VAL:HG22	2.20	0.42
7:D:67:HIS:HB3	9:M:388:ILE:O	2.18	0.42
1:Q:235:TRP:CD1	1:Q:242:LYS:HB3	2.54	0.42
6:V:134:PHE:CE1	6:V:139:LEU:HA	2.55	0.42
17:N:608:MQ9:H203	17:N:608:MQ9:H222	1.91	0.42
9:A:329:LEU:HD12	9:A:329:LEU:HA	1.92	0.42
2:F:40:ILE:HA	2:F:43:MET:HE2	2.01	0.42
2:F:499:TRP:CE2	12:F:602:CDL:HB4	2.55	0.42
3:G:164:ARG:HA	3:G:167:MET:HG2	2.01	0.42
3:S:61:GLU:HB2	3:S:62:PRO:HD3	2.02	0.42
5:U:54:PRO:HD2	6:V:65:ARG:HH11	1.85	0.42
7:P:92:TRP:CZ2	7:P:96:ARG:HD2	2.55	0.42
8:B:264:PHE:CE2	9:A:158:GLN:HB2	2.55	0.42
2:R:463:ASP:OD2	2:R:464:TYR:N	2.49	0.42
3:S:83:THR:HG23	3:S:102:TRP:CE3	2.52	0.42
3:S:180:VAL:HG12	3:S:183:TYR:OH	2.20	0.42
5:U:70:VAL:HG23	6:V:112:ALA:HB2	2.00	0.42
8:N:259:MET:HB3	8:N:260:PRO:HD3	2.02	0.42
17:N:611:MQ9:H5M2	17:N:611:MQ9:H71	1.78	0.42
8:B:472:PRO:HG2	8:B:480:ILE:HD11	2.01	0.42
4:T:78:GLY:O	8:B:457:ARG:HD2	2.20	0.41
8:N:207:ILE:HD12	8:N:207:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:270:PHE:HD2	17:N:611:MQ9:H203	1.84	0.41
9:M:181:ARG:NH1	8:B:22:ASP:OD2	2.46	0.41
9:A:84:GLU:O	9:A:86:THR:HG23	2.20	0.41
9:A:362:LEU:HD13	9:A:373:PRO:HD3	2.02	0.41
19:A:502:9YF:O3	19:A:502:9YF:P	2.78	0.41
1:E:235:TRP:CD2	1:E:242:LYS:HE2	2.55	0.41
1:Q:149:PHE:HE2	1:Q:293:PRO:HB3	1.85	0.41
12:N:605:CDL:CB5	12:B:605:CDL:H112	2.50	0.41
9:A:269:ASP:CG	9:A:270:GLY:H	2.28	0.41
2:F:82:LEU:HD23	2:F:82:LEU:HA	1.92	0.41
2:F:134:LEU:HB3	17:O:301:MQ9:H28	2.01	0.41
2:R:485:GLY:HA2	14:R:606:HEA:H262	2.02	0.41
6:V:115:LYS:HG3	6:V:119:ILE:HD11	2.01	0.41
7:P:99:ILE:O	7:P:100:ARG:HB3	2.20	0.41
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.84	0.41
7:D:46:GLY:O	7:D:50:ILE:HG12	2.21	0.41
3:S:161:LEU:O	3:S:165:THR:HG23	2.20	0.41
9:M:270:GLY:H	9:M:271:PRO:HD2	1.86	0.41
12:M:502:CDL:H661	12:M:502:CDL:H632	1.82	0.41
1:E:142:PHE:O	1:E:202:GLU:HA	2.20	0.41
1:E:222:GLU:HG3	1:E:259:GLN:HG2	2.02	0.41
2:R:37:HIS:HE1	2:R:529:ASN:HD21	1.69	0.41
6:V:114:VAL:HG22	6:V:119:ILE:HG21	2.01	0.41
19:M:503:9YF:O7	19:M:503:9YF:P	2.78	0.41
1:E:201:ILE:HG23	1:E:303:ARG:HD2	2.01	0.41
2:F:153:ALA:HB1	2:F:158:THR:HG21	2.01	0.41
1:Q:331:ARG:HH11	2:R:71:LEU:H	1.68	0.41
2:R:288:LYS:HE2	2:R:288:LYS:HB3	1.79	0.41
2:R:417:TRP:O	2:R:421:MET:HG2	2.21	0.41
3:S:77:LEU:HD12	3:S:77:LEU:HA	1.92	0.41
6:V:77:THR:OG1	6:V:107:GLU:OE1	2.31	0.41
8:N:373:ARG:O	8:N:439:GLN:NE2	2.42	0.41
2:R:404:GLY:HA2	2:R:408:PHE:HD2	1.84	0.41
12:R:602:CDL:H782	12:R:602:CDL:H752	1.87	0.41
4:H:44:LEU:HD23	4:H:44:LEU:HA	1.77	0.41
5:I:38:MET:HE3	6:J:139:LEU:HD13	2.03	0.41
1:Q:238:GLU:HG3	1:Q:269:PHE:CD1	2.55	0.41
19:M:503:9YF:O7	19:M:503:9YF:O3	2.38	0.41
17:O:301:MQ9:H303	17:O:301:MQ9:H322	1.92	0.41
8:B:349:LEU:HB3	8:B:350:PRO:HD3	2.03	0.41
2:F:62:MET:SD	2:F:83:PHE:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:420:LYS:HD3	2:F:523:CYS:O	2.21	0.41
2:R:27:LEU:O	2:R:31:LEU:HB2	2.21	0.41
14:R:605:HEA:HMD3	14:R:605:HEA:CBD	2.49	0.41
3:S:23:ASN:O	3:S:27:VAL:HG23	2.21	0.41
3:S:100:ARG:O	3:S:104:VAL:HG23	2.21	0.41
8:N:145:ASN:OD1	8:N:231:HIS:ND1	2.54	0.41
12:N:607:CDL:H222	12:N:607:CDL:H191	1.72	0.41
9:M:84:GLU:O	9:M:86:THR:HG23	2.21	0.41
9:M:143:PHE:O	9:M:147:ILE:HG22	2.20	0.41
8:B:40:PRO:HB2	8:B:45:PHE:HE2	1.85	0.41
9:A:132:TYR:CE2	10:C:244:PRO:HB3	2.56	0.41
10:C:62:LEU:CB	10:C:135:TYR:HB2	2.50	0.41
17:C:305:MQ9:H251	17:C:305:MQ9:H221	1.85	0.41
2:F:90:MET:HB3	14:F:607:HEA:CAC	2.51	0.41
2:F:458:PRO:HG2	2:F:461:TYR:CZ	2.56	0.41
12:B:607:CDL:H601	12:B:607:CDL:H571	1.53	0.41
1:E:76:ARG:O	1:E:78:LYS:N	2.49	0.40
1:Q:114:VAL:HA	1:Q:117:GLN:HG2	2.03	0.40
1:Q:294:ASN:HA	1:Q:297:LYS:NZ	2.36	0.40
2:R:418:PHE:HB3	2:R:419:PRO:HD3	2.03	0.40
9:M:426:ARG:HA	9:M:426:ARG:HD2	1.81	0.40
8:B:259:MET:HB3	8:B:260:PRO:HD3	2.04	0.40
9:A:62:LEU:HD23	9:A:62:LEU:HA	1.92	0.40
1:Q:158:GLY:O	1:Q:200:LYS:NZ	2.54	0.40
2:R:94:TYR:O	2:R:98:ILE:HB	2.21	0.40
2:R:400:TYR:HA	2:R:442:PHE:HZ	1.87	0.40
4:T:25:LEU:HD23	4:T:25:LEU:HA	1.89	0.40
9:A:270:GLY:H	9:A:271:PRO:HD2	1.87	0.40
9:A:423:PHE:CE2	9:A:425:GLU:HB2	2.57	0.40
2:F:219:LEU:HD11	2:F:304:ALA:HB1	2.02	0.40
2:F:451:TRP:O	2:F:455:GLU:HG2	2.21	0.40
12:F:601:CDL:H312	12:F:601:CDL:H342	1.66	0.40
8:B:289:ILE:HA	8:B:292:LEU:HD13	2.03	0.40
8:B:371:ARG:HE	12:B:606:CDL:HA22	1.86	0.40
12:B:606:CDL:H152	12:B:606:CDL:H571	2.03	0.40
20:C:301:HEC:HBC3	20:C:301:HEC:HHD	2.04	0.40
1:E:136:PHE:CZ	1:E:139:ASN:HB3	2.56	0.40
2:F:391:SER:HA	2:F:458:PRO:HA	2.04	0.40
4:H:64:ASP:OD1	4:H:64:ASP:N	2.51	0.40
6:J:114:VAL:HG22	6:J:119:ILE:HG21	2.02	0.40
7:D:60:LEU:HD23	7:D:60:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:159:ALA:HB1	1:Q:161:PRO:HD3	2.04	0.40
3:S:147:HIS:HE1	3:S:188:VAL:O	2.05	0.40
8:N:36:ASN:HB3	9:M:72:VAL:HG21	2.03	0.40
8:N:107:GLY:O	8:N:111:ARG:HG2	2.22	0.40
9:A:364:GLU:HB3	10:C:214:ASN:OD1	2.22	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	E	272/341 (80%)	247 (91%)	24 (9%)	1 (0%)	30	51
1	Q	279/341 (82%)	248 (89%)	31 (11%)	0	100	100
2	F	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
2	R	550/575 (96%)	522 (95%)	28 (5%)	0	100	100
3	G	184/203 (91%)	176 (96%)	8 (4%)	0	100	100
3	S	183/203 (90%)	174 (95%)	9 (5%)	0	100	100
4	H	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
4	T	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
5	I	63/79 (80%)	60 (95%)	3 (5%)	0	100	100
5	U	63/79 (80%)	60 (95%)	3 (5%)	0	100	100
6	J	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
6	V	143/157 (91%)	136 (95%)	7 (5%)	0	100	100
7	D	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
7	P	73/100 (73%)	67 (92%)	6 (8%)	0	100	100
8	B	522/549 (95%)	478 (92%)	41 (8%)	3 (1%)	21	41
8	N	522/549 (95%)	480 (92%)	39 (8%)	3 (1%)	21	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	376/429 (88%)	342 (91%)	32 (8%)	2 (0%)	24	45
9	M	376/429 (88%)	343 (91%)	30 (8%)	3 (1%)	16	34
10	C	214/280 (76%)	192 (90%)	21 (10%)	1 (0%)	24	45
10	O	207/280 (74%)	191 (92%)	15 (7%)	1 (0%)	24	45
All	All	5068/5704 (89%)	4701 (93%)	353 (7%)	14 (0%)	37	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	M	329	LEU
9	A	329	LEU
8	N	28	SER
9	M	384	PHE
8	B	28	SER
8	N	27	PRO
8	B	27	PRO
9	A	384	PHE
1	E	85	PRO
10	C	109	PRO
8	N	459	PRO
9	M	294	GLU
10	O	109	PRO
8	B	459	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	E	231/288 (80%)	231 (100%)	0	100	100
1	Q	235/288 (82%)	235 (100%)	0	100	100
2	F	453/471 (96%)	453 (100%)	0	100	100
2	R	453/471 (96%)	453 (100%)	0	100	100
3	G	148/161 (92%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	147/161 (91%)	146 (99%)	1 (1%)	76	89
4	H	105/106 (99%)	105 (100%)	0	100	100
4	T	104/106 (98%)	104 (100%)	0	100	100
5	I	50/59 (85%)	50 (100%)	0	100	100
5	U	49/59 (83%)	49 (100%)	0	100	100
6	J	103/114 (90%)	103 (100%)	0	100	100
6	V	104/114 (91%)	104 (100%)	0	100	100
7	D	60/83 (72%)	59 (98%)	1 (2%)	53	77
7	P	59/83 (71%)	59 (100%)	0	100	100
8	B	422/446 (95%)	422 (100%)	0	100	100
8	N	419/446 (94%)	419 (100%)	0	100	100
9	A	296/343 (86%)	296 (100%)	0	100	100
9	M	299/343 (87%)	299 (100%)	0	100	100
10	C	131/207 (63%)	131 (100%)	0	100	100
10	O	128/207 (62%)	128 (100%)	0	100	100
All	All	3996/4556 (88%)	3994 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	77	ILE
3	S	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	75	HIS
1	E	252	ASN
1	E	259	GLN
1	E	317	ASN
1	E	318	GLN
2	F	37	HIS
2	F	72	GLN
2	F	76	ASN
2	F	80	ASN
2	F	104	ASN

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Mol	Chain	Res	Type
2	F	212	ASN
2	F	343	ASN
2	F	397	HIS
2	F	528	HIS
3	G	53	GLN
3	G	123	HIS
3	G	150	HIS
3	G	186	HIS
5	I	7	HIS
6	J	103	GLN
7	D	66	ASN
7	D	90	ASN
1	Q	197	ASN
1	Q	252	ASN
1	Q	259	GLN
1	Q	285	ASN
2	R	37	HIS
2	R	80	ASN
2	R	104	ASN
2	R	212	ASN
2	R	313	HIS
2	R	343	ASN
3	S	53	GLN
3	S	123	HIS
3	S	127	HIS
3	S	147	HIS
3	S	150	HIS
3	S	186	HIS
6	V	87	ASN
6	V	103	GLN
7	P	42	HIS
7	P	70	HIS
8	N	34	GLN
8	N	36	ASN
8	N	79	ASN
8	N	366	HIS
8	N	406	HIS
8	N	467	HIS
9	M	309	GLN
9	M	375	HIS
9	M	398	GLN
10	O	222	GLN

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Mol	Chain	Res	Type
10	O	243	GLN
8	B	34	GLN
8	B	79	ASN
8	B	299	GLN
8	B	366	HIS
8	B	367	ASN
8	B	406	HIS
8	B	467	HIS
8	B	476	HIS
8	B	528	GLN
9	A	59	ASN
9	A	306	HIS
9	A	365	GLN
9	A	375	HIS
9	A	398	GLN
10	C	102	GLN
10	C	156	GLN
10	C	243	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	9YF	M	504	-	40,40,58	1.01	3 (7%)	50,52,71	1.38	7 (14%)
12	CDL	N	607	-	78,78,99	1.18	6 (7%)	84,90,111	1.09	5 (5%)
17	MQ9	O	302	-	59,59,59	3.87	17 (28%)	72,75,75	3.31	31 (43%)
12	CDL	D	201	7	87,87,99	1.16	7 (8%)	93,99,111	1.04	5 (5%)
14	HEA	F	606	2	66,67,67	2.36	22 (33%)	78,103,103	2.39	28 (35%)
14	HEA	R	605	-	66,67,67	2.36	22 (33%)	78,103,103	2.37	27 (34%)
12	CDL	B	605	8	73,73,99	1.23	8 (10%)	79,85,111	0.99	4 (5%)
12	CDL	B	604	8	65,65,99	1.27	7 (10%)	71,77,111	1.02	4 (5%)
14	HEA	R	606	2	66,67,67	2.35	22 (33%)	78,103,103	2.35	30 (38%)
12	CDL	M	502	-	94,94,99	1.12	7 (7%)	100,106,111	0.97	5 (5%)
13	PLM	F	603	-	16,16,17	0.52	0	15,15,17	0.43	0
14	HEA	F	607	2	66,67,67	2.34	22 (33%)	78,103,103	2.34	30 (38%)
19	9YF	M	503	-	44,44,58	0.99	4 (9%)	55,57,71	1.10	5 (9%)
12	CDL	R	601	-	75,75,99	1.20	7 (9%)	81,87,111	0.98	4 (4%)
12	CDL	B	606	-	76,76,99	1.19	7 (9%)	82,88,111	1.02	4 (4%)
18	FES	M	501	9	0,4,4	-	-	-		
17	MQ9	C	305	-	59,59,59	3.89	17 (28%)	72,75,75	3.32	31 (43%)
16	HEM	B	602	8	49,49,50	1.40	5 (10%)	66,81,82	1.11	5 (7%)
12	CDL	N	606	-	76,76,99	1.20	7 (9%)	82,88,111	0.97	4 (4%)
17	MQ9	B	609	-	39,39,59	3.87	14 (35%)	48,51,75	3.00	17 (35%)
12	CDL	R	602	-	80,80,99	1.16	6 (7%)	86,92,111	1.00	5 (5%)
12	CDL	F	602	-	80,80,99	1.17	7 (8%)	86,92,111	0.96	4 (4%)
16	HEM	B	603	8	50,50,50	1.42	7 (14%)	66,82,82	1.24	7 (10%)
12	CDL	C	303	-	78,78,99	1.20	7 (8%)	84,90,111	0.99	5 (5%)
12	CDL	F	601	-	75,75,99	1.21	7 (9%)	81,87,111	0.96	4 (4%)
12	CDL	N	603	-	78,78,99	1.19	7 (8%)	84,90,111	0.94	4 (4%)
13	PLM	R	603	-	16,16,17	0.56	0	15,15,17	0.42	0
20	HEC	C	302	10	50,50,50	1.75	5 (10%)	68,82,82	1.44	8 (11%)
19	9YF	A	503	-	42,42,58	1.02	4 (9%)	52,54,71	1.27	6 (11%)
13	PLM	N	604	-	10,10,17	0.59	0	9,9,17	0.55	0
15	9Y0	G	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.93	2 (4%)
12	CDL	P	201	7	87,87,99	1.15	7 (8%)	93,99,111	1.01	5 (5%)
12	CDL	N	605	-	73,73,99	1.24	7 (9%)	79,85,111	1.03	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	HEM	N	602	8	50,50,50	1.41	6 (12%)	66,82,82	1.26	7 (10%)
17	MQ9	N	609	8	59,59,59	3.94	18 (30%)	72,75,75	3.27	32 (44%)
13	PLM	B	601	-	10,10,17	0.64	0	9,9,17	0.54	0
12	CDL	C	306	-	94,94,99	1.12	7 (7%)	100,106,111	1.01	5 (5%)
17	MQ9	O	301	-	49,49,59	3.92	15 (30%)	60,63,75	3.19	23 (38%)
17	MQ9	B	608	-	44,44,59	3.88	15 (34%)	54,57,75	3.13	21 (38%)
18	FES	A	501	9	0,4,4	-	-	-		
20	HEC	C	301	10	50,50,50	1.79	6 (12%)	68,82,82	1.47	7 (10%)
17	MQ9	N	611	-	44,44,59	3.89	15 (34%)	54,57,75	3.09	22 (40%)
16	HEM	N	601	8	49,49,50	1.41	5 (10%)	66,81,82	1.13	5 (7%)
17	MQ9	N	610	-	44,44,59	3.92	15 (34%)	54,57,75	3.10	20 (37%)
17	MQ9	C	304	-	49,49,59	3.98	15 (30%)	60,63,75	3.05	23 (38%)
20	HEC	O	304	10	50,50,50	1.74	5 (10%)	68,82,82	1.49	8 (11%)
15	9Y0	S	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.95	2 (4%)
19	9YF	A	502	-	51,51,58	0.95	5 (9%)	62,64,71	1.02	4 (6%)
17	MQ9	N	608	-	59,59,59	3.93	18 (30%)	72,75,75	3.28	31 (43%)
12	CDL	B	607	-	78,78,99	1.17	6 (7%)	84,90,111	1.10	5 (5%)
20	HEC	O	303	-	50,50,50	1.80	5 (10%)	68,82,82	1.57	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9YF	M	504	-	-	18/35/59/78	0/1/1/1
12	CDL	N	607	-	-	42/89/89/110	-
17	MQ9	O	302	-	-	26/53/73/73	0/2/2/2
12	CDL	D	201	7	-	53/98/98/110	-
14	HEA	F	606	2	-	19/36/76/76	-
14	HEA	R	605	-	-	12/36/76/76	-
12	CDL	B	605	8	-	47/84/84/110	-
12	CDL	B	604	8	-	49/76/76/110	-
14	HEA	R	606	2	-	15/36/76/76	-
12	CDL	M	502	-	-	68/105/105/110	-
13	PLM	F	603	-	-	5/13/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	F	607	2	-	12/36/76/76	-
19	9YF	M	503	-	-	19/39/63/78	0/1/1/1
12	CDL	R	601	-	-	39/86/86/110	-
12	CDL	B	606	-	-	42/87/87/110	-
18	FES	M	501	9	-	-	0/1/1/1
17	MQ9	C	305	-	-	25/53/73/73	0/2/2/2
16	HEM	B	602	8	-	2/12/52/54	-
12	CDL	N	606	-	-	40/87/87/110	-
17	MQ9	B	609	-	-	14/29/49/73	0/2/2/2
12	CDL	R	602	-	-	43/91/91/110	-
12	CDL	F	602	-	-	41/91/91/110	-
16	HEM	B	603	8	-	4/14/54/54	-
12	CDL	C	303	-	-	54/89/89/110	-
12	CDL	F	601	-	-	39/86/86/110	-
12	CDL	N	603	-	-	51/89/89/110	-
13	PLM	R	603	-	-	4/13/14/15	-
20	HEC	C	302	10	1/1/3/7	0/14/54/54	-
19	9YF	A	503	-	-	15/37/61/78	0/1/1/1
13	PLM	N	604	-	-	1/7/8/15	-
15	9Y0	G	301	-	-	24/46/46/52	-
12	CDL	P	201	7	-	58/98/98/110	-
12	CDL	N	605	-	-	44/84/84/110	-
16	HEM	N	602	8	-	4/14/54/54	-
17	MQ9	N	609	8	-	35/53/73/73	0/2/2/2
13	PLM	B	601	-	-	0/7/8/15	-
12	CDL	C	306	-	-	60/105/105/110	-
17	MQ9	O	301	-	-	23/41/61/73	0/2/2/2
17	MQ9	B	608	-	-	21/35/55/73	0/2/2/2
18	FES	A	501	9	-	-	0/1/1/1
20	HEC	C	301	10	1/1/3/7	5/14/54/54	-
17	MQ9	N	611	-	-	21/35/55/73	0/2/2/2
16	HEM	N	601	8	-	2/12/52/54	-
20	HEC	O	304	10	1/1/3/7	1/14/54/54	-
17	MQ9	N	610	-	-	21/35/55/73	0/2/2/2
17	MQ9	C	304	-	-	22/41/61/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	9Y0	S	301	-	-	27/46/46/52	-
19	9YF	A	502	-	-	30/47/71/78	0/1/1/1
17	MQ9	N	608	-	-	29/53/73/73	0/2/2/2
12	CDL	B	607	-	-	53/89/89/110	-
20	HEC	O	303	-	1/1/3/7	5/14/54/54	-

All (432) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	608	MQ9	C18-C19	9.58	1.56	1.33
17	C	304	MQ9	C18-C19	9.58	1.56	1.33
17	N	609	MQ9	C18-C19	9.52	1.55	1.33
17	N	610	MQ9	C18-C19	9.52	1.55	1.33
17	N	611	MQ9	C18-C19	9.48	1.55	1.33
17	C	304	MQ9	C23-C24	9.46	1.55	1.33
17	B	608	MQ9	C18-C19	9.45	1.55	1.33
17	O	301	MQ9	C18-C19	9.42	1.55	1.33
17	B	609	MQ9	C18-C19	9.42	1.55	1.33
17	O	302	MQ9	C18-C19	9.40	1.55	1.33
17	C	305	MQ9	C18-C19	9.38	1.55	1.33
17	N	610	MQ9	C23-C24	9.31	1.55	1.33
17	N	609	MQ9	C23-C24	9.30	1.55	1.33
17	N	608	MQ9	C23-C24	9.30	1.55	1.33
17	O	301	MQ9	C23-C24	9.30	1.55	1.33
17	B	609	MQ9	C23-C24	9.29	1.55	1.33
17	N	611	MQ9	C23-C24	9.25	1.55	1.33
17	O	302	MQ9	C23-C24	9.20	1.55	1.33
17	C	305	MQ9	C23-C24	9.16	1.54	1.33
17	C	304	MQ9	C33-C34	9.15	1.54	1.33
17	B	608	MQ9	C23-C24	9.15	1.54	1.33
17	N	608	MQ9	C33-C34	9.11	1.54	1.33
17	N	609	MQ9	C33-C34	9.08	1.54	1.33
17	O	301	MQ9	C33-C34	9.07	1.54	1.33
17	C	304	MQ9	C28-C29	9.06	1.54	1.33
17	N	609	MQ9	C28-C29	8.99	1.54	1.33
17	N	608	MQ9	C28-C29	8.99	1.54	1.33
17	N	610	MQ9	C28-C29	8.96	1.54	1.33
17	O	302	MQ9	C33-C34	8.96	1.54	1.33
17	N	609	MQ9	C38-C39	8.96	1.54	1.33
17	C	305	MQ9	C33-C34	8.94	1.54	1.33
17	C	305	MQ9	C28-C29	8.94	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	608	MQ9	C38-C39	8.94	1.54	1.33
17	N	611	MQ9	C28-C29	8.92	1.54	1.33
17	C	305	MQ9	C38-C39	8.91	1.54	1.33
17	O	301	MQ9	C28-C29	8.89	1.54	1.33
17	B	608	MQ9	C28-C29	8.85	1.54	1.33
17	O	302	MQ9	C28-C29	8.85	1.54	1.33
17	O	302	MQ9	C38-C39	8.77	1.54	1.33
17	N	609	MQ9	C13-C14	8.66	1.53	1.33
17	C	304	MQ9	C13-C14	8.64	1.53	1.33
17	N	611	MQ9	C13-C14	8.59	1.53	1.33
17	N	608	MQ9	C43-C44	8.59	1.53	1.33
17	N	608	MQ9	C13-C14	8.57	1.53	1.33
17	N	610	MQ9	C13-C14	8.55	1.53	1.33
17	B	609	MQ9	C13-C14	8.52	1.53	1.33
17	O	302	MQ9	C13-C14	8.52	1.53	1.33
17	O	301	MQ9	C13-C14	8.51	1.53	1.33
17	B	608	MQ9	C13-C14	8.50	1.53	1.33
17	N	609	MQ9	C43-C44	8.49	1.53	1.33
17	C	305	MQ9	C13-C14	8.48	1.53	1.33
17	C	305	MQ9	C43-C44	8.47	1.53	1.33
17	O	302	MQ9	C43-C44	8.42	1.53	1.33
20	O	303	HEC	C3D-C2D	8.02	1.53	1.36
17	N	609	MQ9	C8-C9	8.01	1.52	1.33
17	N	610	MQ9	C8-C9	7.97	1.52	1.33
20	C	301	HEC	C3D-C2D	7.96	1.53	1.36
20	O	304	HEC	C3D-C2D	7.96	1.53	1.36
17	C	304	MQ9	C8-C9	7.96	1.52	1.33
20	C	302	HEC	C3D-C2D	7.87	1.53	1.36
17	B	609	MQ9	C8-C9	7.84	1.51	1.33
17	C	305	MQ9	C8-C9	7.83	1.51	1.33
17	B	608	MQ9	C8-C9	7.79	1.51	1.33
17	N	611	MQ9	C8-C9	7.79	1.51	1.33
17	O	302	MQ9	C8-C9	7.77	1.51	1.33
17	O	301	MQ9	C8-C9	7.77	1.51	1.33
17	N	608	MQ9	C8-C9	7.75	1.51	1.33
17	C	304	MQ9	C38-C39	7.73	1.54	1.32
17	N	610	MQ9	C33-C34	7.72	1.54	1.32
17	B	608	MQ9	C33-C34	7.71	1.54	1.32
17	B	609	MQ9	C28-C29	7.67	1.54	1.32
17	O	301	MQ9	C38-C39	7.66	1.54	1.32
17	N	611	MQ9	C33-C34	7.65	1.54	1.32
17	B	608	MQ9	O1-C1	7.54	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	611	MQ9	O1-C1	7.52	1.39	1.23
17	B	609	MQ9	O1-C1	7.51	1.39	1.23
17	N	609	MQ9	O1-C1	7.51	1.39	1.23
17	N	608	MQ9	O1-C1	7.50	1.39	1.23
17	N	610	MQ9	O1-C1	7.46	1.39	1.23
17	C	305	MQ9	O1-C1	7.43	1.38	1.23
17	O	301	MQ9	O1-C1	7.41	1.38	1.23
17	C	304	MQ9	O1-C1	7.38	1.38	1.23
17	O	302	MQ9	O1-C1	7.31	1.38	1.23
17	N	611	MQ9	O4-C4	7.16	1.38	1.23
17	B	608	MQ9	O4-C4	7.11	1.38	1.23
17	N	609	MQ9	O4-C4	7.11	1.38	1.23
17	N	608	MQ9	O4-C4	7.11	1.38	1.23
17	N	610	MQ9	O4-C4	7.10	1.38	1.23
17	C	304	MQ9	O4-C4	7.08	1.38	1.23
17	O	301	MQ9	O4-C4	7.08	1.38	1.23
17	O	302	MQ9	O4-C4	7.07	1.38	1.23
17	B	609	MQ9	O4-C4	7.07	1.38	1.23
17	C	305	MQ9	O4-C4	7.06	1.38	1.23
17	N	609	MQ9	C48-C49	7.00	1.52	1.32
17	N	608	MQ9	C48-C49	6.97	1.52	1.32
17	C	305	MQ9	C48-C49	6.96	1.52	1.32
17	O	302	MQ9	C48-C49	6.95	1.52	1.32
14	F	606	HEA	FE-NB	5.45	2.11	1.94
14	R	605	HEA	FE-NB	5.41	2.11	1.94
14	R	606	HEA	FE-NB	5.34	2.11	1.94
14	R	606	HEA	C3B-C2B	5.30	1.46	1.34
14	F	607	HEA	C3B-C2B	5.30	1.46	1.34
14	F	607	HEA	FE-NB	5.29	2.11	1.94
14	F	606	HEA	FE-ND	5.29	2.11	1.94
14	F	606	HEA	C3B-C2B	5.27	1.46	1.34
14	R	605	HEA	C3B-C2B	5.25	1.46	1.34
14	R	605	HEA	FE-ND	5.20	2.11	1.94
14	F	607	HEA	FE-ND	5.20	2.11	1.94
14	R	606	HEA	FE-ND	5.17	2.10	1.94
14	F	607	HEA	C3A-C2A	5.02	1.47	1.36
14	R	606	HEA	C3A-C2A	5.01	1.47	1.36
17	O	301	MQ9	C5-C4	-4.99	1.37	1.48
17	N	608	MQ9	C5-C4	-4.98	1.37	1.48
17	C	304	MQ9	C5-C4	-4.96	1.37	1.48
17	C	305	MQ9	C5-C4	-4.95	1.37	1.48
17	N	610	MQ9	C5-C4	-4.94	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	609	MQ9	C5-C4	-4.94	1.37	1.48
17	N	611	MQ9	C5-C4	-4.91	1.37	1.48
17	O	302	MQ9	C5-C4	-4.90	1.37	1.48
17	N	609	MQ9	C5-C4	-4.86	1.37	1.48
14	R	605	HEA	C3D-C2D	4.85	1.47	1.36
14	R	605	HEA	C3A-C2A	4.83	1.47	1.36
17	B	608	MQ9	C5-C4	-4.82	1.37	1.48
14	F	606	HEA	C3D-C2D	4.78	1.46	1.36
14	F	606	HEA	C3A-C2A	4.73	1.46	1.36
14	R	606	HEA	C3D-C2D	4.58	1.46	1.36
20	O	303	HEC	FE-ND	4.56	2.09	1.94
14	R	605	HEA	CHC-C4B	4.55	1.47	1.38
14	F	606	HEA	CHC-C4B	4.54	1.47	1.38
14	F	607	HEA	C3D-C2D	4.51	1.46	1.36
14	F	607	HEA	CHC-C4B	4.51	1.47	1.38
14	R	605	HEA	FE-NC	4.50	2.10	1.95
14	R	606	HEA	FE-NC	4.48	2.10	1.95
14	F	607	HEA	FE-NC	4.44	2.10	1.95
14	R	606	HEA	CHC-C4B	4.43	1.47	1.38
14	F	606	HEA	FE-NC	4.43	2.10	1.95
20	O	303	HEC	FE-NB	4.36	2.08	1.94
20	C	301	HEC	FE-ND	4.32	2.08	1.94
20	C	302	HEC	FE-ND	4.25	2.08	1.94
14	R	606	HEA	CHB-C4A	4.11	1.46	1.38
14	F	607	HEA	CHA-C1A	4.04	1.46	1.38
14	R	605	HEA	CHD-C1D	4.01	1.46	1.38
17	N	608	MQ9	C6-C1	-4.01	1.37	1.47
17	O	302	MQ9	C6-C1	-4.01	1.37	1.47
14	F	606	HEA	CHB-C4A	4.00	1.46	1.38
14	R	606	HEA	CHA-C1A	4.00	1.46	1.38
17	O	301	MQ9	C6-C1	-4.00	1.37	1.47
14	R	605	HEA	CHB-C4A	3.99	1.46	1.38
17	B	609	MQ9	C6-C1	-3.97	1.37	1.47
17	C	305	MQ9	C6-C1	-3.95	1.37	1.47
14	F	607	HEA	CHB-C4A	3.95	1.46	1.38
17	C	304	MQ9	C6-C1	-3.94	1.37	1.47
14	F	606	HEA	CHD-C1D	3.93	1.46	1.38
17	N	610	MQ9	C6-C1	-3.89	1.37	1.47
17	N	609	MQ9	C6-C1	-3.89	1.37	1.47
20	O	304	HEC	FE-ND	3.85	2.06	1.94
14	R	605	HEA	CHA-C1A	3.85	1.45	1.38
14	F	606	HEA	CHA-C1A	3.84	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	606	HEA	CHD-C1D	3.82	1.46	1.38
20	C	301	HEC	FE-NB	3.81	2.06	1.94
20	C	302	HEC	FE-NB	3.81	2.06	1.94
17	C	304	MQ9	C3-C4	-3.79	1.41	1.48
14	F	606	HEA	C1A-NA	3.75	1.47	1.39
16	N	602	HEM	FE-ND	3.74	2.06	1.94
14	F	606	HEA	CHC-C1C	3.73	1.47	1.39
14	R	605	HEA	C1A-NA	3.71	1.47	1.39
14	F	607	HEA	CHD-C1D	3.70	1.46	1.38
14	R	605	HEA	CHC-C1C	3.69	1.47	1.39
17	N	611	MQ9	C6-C1	-3.69	1.37	1.47
17	B	608	MQ9	C6-C1	-3.69	1.37	1.47
16	B	603	HEM	FE-ND	3.67	2.06	1.94
14	F	607	HEA	C1A-NA	3.64	1.46	1.39
17	C	305	MQ9	C3-C4	-3.63	1.41	1.48
17	N	609	MQ9	C3-C4	-3.62	1.41	1.48
14	F	607	HEA	CHC-C1C	3.61	1.47	1.39
12	N	606	CDL	OB8-CB7	3.59	1.43	1.33
12	D	201	CDL	OB8-CB7	3.59	1.43	1.33
14	R	606	HEA	CHC-C1C	3.59	1.47	1.39
16	N	602	HEM	FE-NB	3.58	2.05	1.94
17	B	608	MQ9	C3-C4	-3.57	1.41	1.48
17	N	611	MQ9	C3-C4	-3.56	1.41	1.48
20	O	304	HEC	FE-NB	3.56	2.05	1.94
17	O	302	MQ9	C3-C4	-3.55	1.41	1.48
12	B	604	CDL	OB8-CB7	3.55	1.43	1.33
17	N	608	MQ9	C3-C4	-3.54	1.41	1.48
12	B	606	CDL	OB8-CB7	3.52	1.43	1.33
12	B	605	CDL	OB8-CB7	3.51	1.43	1.33
16	N	601	HEM	FE-NA	3.51	2.07	1.95
14	R	606	HEA	C1A-NA	3.50	1.46	1.39
17	N	610	MQ9	C3-C4	-3.50	1.41	1.48
14	R	606	HEA	C4A-NA	3.49	1.46	1.39
17	O	301	MQ9	C3-C4	-3.49	1.41	1.48
12	C	303	CDL	OB8-CB7	3.46	1.43	1.33
12	P	201	CDL	OB8-CB7	3.46	1.43	1.33
16	B	602	HEM	FE-NC	3.45	2.06	1.95
17	N	610	MQ9	C2-C3	-3.45	1.35	1.40
12	R	601	CDL	OB8-CB7	3.44	1.43	1.33
12	F	601	CDL	OB8-CB7	3.44	1.43	1.33
17	B	609	MQ9	C3-C4	-3.44	1.41	1.48
14	R	605	HEA	CHD-C4C	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	603	CDL	OB8-CB7	3.43	1.43	1.33
12	N	605	CDL	OB8-CB7	3.43	1.43	1.33
16	B	603	HEM	FE-NB	3.43	2.05	1.94
12	M	502	CDL	OB8-CB7	3.40	1.43	1.33
14	F	606	HEA	CHD-C4C	3.38	1.47	1.39
17	C	305	MQ9	C2-C3	-3.37	1.35	1.40
17	O	302	MQ9	C2-C3	-3.37	1.35	1.40
14	R	605	HEA	C4A-NA	3.36	1.46	1.39
16	B	602	HEM	FE-NA	3.36	2.06	1.95
12	C	306	CDL	OB8-CB7	3.35	1.43	1.33
20	C	301	HEC	FE-NC	3.35	2.06	1.95
16	N	601	HEM	FE-ND	3.35	2.05	1.94
12	F	602	CDL	OB8-CB7	3.35	1.43	1.33
17	B	609	MQ9	C2-C3	-3.33	1.35	1.40
12	R	602	CDL	OB8-CB7	3.32	1.43	1.33
17	N	609	MQ9	C2-C3	-3.32	1.35	1.40
17	O	301	MQ9	C2-C3	-3.32	1.35	1.40
12	N	607	CDL	OB8-CB7	3.32	1.43	1.33
14	R	606	HEA	CHB-C1B	3.31	1.46	1.39
16	B	602	HEM	FE-ND	3.30	2.05	1.94
14	F	607	HEA	C4A-NA	3.29	1.46	1.39
17	N	611	MQ9	C2-C3	-3.29	1.35	1.40
14	R	606	HEA	CHA-C4D	3.29	1.46	1.39
12	B	607	CDL	OB8-CB7	3.28	1.42	1.33
17	C	304	MQ9	C2-C3	-3.27	1.35	1.40
14	F	606	HEA	C4A-NA	3.26	1.46	1.39
17	B	608	MQ9	C2-C3	-3.25	1.35	1.40
14	F	607	HEA	CHB-C1B	3.24	1.46	1.39
14	R	605	HEA	CHA-C4D	3.24	1.46	1.39
14	F	607	HEA	C1D-ND	-3.23	1.34	1.40
16	N	601	HEM	FE-NC	3.22	2.06	1.95
17	N	608	MQ9	C2-C3	-3.22	1.35	1.40
14	F	606	HEA	CHA-C4D	3.22	1.46	1.39
14	F	606	HEA	C1D-ND	-3.21	1.34	1.40
14	F	607	HEA	CHA-C4D	3.21	1.46	1.39
14	R	606	HEA	CHD-C4C	3.19	1.46	1.39
14	F	606	HEA	CHB-C1B	3.19	1.46	1.39
14	R	605	HEA	CHB-C1B	3.19	1.46	1.39
14	R	606	HEA	C1D-ND	-3.19	1.34	1.40
14	F	607	HEA	CHD-C4C	3.18	1.46	1.39
12	P	201	CDL	OA8-CA7	3.17	1.42	1.33
12	N	605	CDL	OA8-CA7	3.12	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	306	CDL	OA8-CA7	3.10	1.42	1.33
14	R	605	HEA	C1D-ND	-3.10	1.35	1.40
12	F	602	CDL	OA8-CA7	3.07	1.42	1.33
20	O	304	HEC	FE-NA	3.05	2.05	1.95
12	C	303	CDL	OA8-CA7	3.05	1.42	1.33
12	N	605	CDL	OB6-CB5	3.04	1.42	1.34
12	M	502	CDL	OA8-CA7	3.03	1.42	1.33
12	P	201	CDL	OB6-CB5	3.03	1.42	1.34
12	F	601	CDL	OB6-CB5	3.03	1.42	1.34
12	N	603	CDL	OA8-CA7	3.02	1.42	1.33
12	D	201	CDL	OB6-CB5	3.02	1.42	1.34
12	M	502	CDL	OB6-CB5	3.02	1.42	1.34
20	C	301	HEC	FE-NA	3.01	2.05	1.95
12	R	602	CDL	OA8-CA7	3.01	1.42	1.33
12	B	605	CDL	OA8-CA7	3.01	1.42	1.33
12	B	604	CDL	OA8-CA7	3.01	1.42	1.33
16	N	601	HEM	CAB-C3B	3.00	1.55	1.47
20	C	302	HEC	FE-NC	3.00	2.05	1.95
16	B	603	HEM	FE-NA	2.98	2.05	1.95
12	N	606	CDL	OA8-CA7	2.98	1.42	1.33
20	O	304	HEC	FE-NC	2.98	2.05	1.95
12	C	303	CDL	OB6-CB5	2.97	1.42	1.34
12	B	605	CDL	OB6-CB5	2.97	1.42	1.34
12	F	601	CDL	OA8-CA7	2.96	1.42	1.33
12	N	607	CDL	OA8-CA7	2.96	1.42	1.33
16	N	601	HEM	FE-NB	2.95	2.04	1.94
14	R	606	HEA	C4B-NB	-2.95	1.35	1.40
20	O	303	HEC	FE-NA	2.95	2.05	1.95
12	R	601	CDL	OA8-CA7	2.94	1.41	1.33
12	D	201	CDL	OA8-CA7	2.94	1.41	1.33
12	N	603	CDL	OA6-CA4	-2.94	1.39	1.46
12	B	607	CDL	OA8-CA7	2.93	1.41	1.33
12	C	306	CDL	OB6-CB5	2.92	1.42	1.34
12	R	602	CDL	OB6-CB5	2.92	1.42	1.34
12	R	601	CDL	OB6-CB5	2.92	1.42	1.34
12	B	604	CDL	OB6-CB5	2.92	1.42	1.34
14	F	607	HEA	C4B-NB	-2.91	1.35	1.40
16	B	602	HEM	CAB-C3B	2.90	1.55	1.47
12	N	607	CDL	OB6-CB5	2.90	1.42	1.34
12	B	607	CDL	OB6-CB5	2.89	1.42	1.34
17	O	302	MQ9	C2-C1	-2.88	1.42	1.48
17	O	301	MQ9	C2-C1	-2.87	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	303	CDL	OA6-CA4	-2.85	1.39	1.46
16	B	603	HEM	CAC-C3C	2.85	1.55	1.47
12	N	603	CDL	OB6-CB5	2.84	1.42	1.34
12	F	602	CDL	OB6-CB5	2.84	1.42	1.34
16	B	602	HEM	FE-NB	2.82	2.03	1.94
16	N	602	HEM	CAC-C3C	2.82	1.55	1.47
12	B	606	CDL	OB6-CB5	2.82	1.42	1.34
12	N	607	CDL	OA6-CA4	-2.82	1.39	1.46
12	B	606	CDL	OA6-CA5	2.81	1.42	1.34
12	F	602	CDL	OA6-CA4	-2.81	1.39	1.46
12	R	602	CDL	OA6-CA4	-2.80	1.39	1.46
12	N	606	CDL	OB6-CB5	2.80	1.42	1.34
17	C	305	MQ9	C2-C1	-2.80	1.42	1.48
14	F	606	HEA	C4B-C3B	2.80	1.49	1.44
16	N	602	HEM	CAB-C3B	2.79	1.55	1.47
17	B	609	MQ9	C2-C1	-2.79	1.42	1.48
12	F	601	CDL	OA6-CA4	-2.79	1.39	1.46
14	F	607	HEA	C4C-NC	-2.78	1.34	1.39
12	B	606	CDL	OA8-CA7	2.78	1.41	1.33
12	R	601	CDL	OA6-CA4	-2.78	1.39	1.46
12	N	606	CDL	OA6-CA4	-2.78	1.39	1.46
17	N	610	MQ9	C2-C1	-2.77	1.42	1.48
14	R	605	HEA	C4B-C3B	2.76	1.49	1.44
14	R	605	HEA	C4B-NB	-2.75	1.35	1.40
16	B	603	HEM	FE-NC	2.75	2.04	1.95
12	M	502	CDL	OA6-CA5	2.75	1.42	1.34
12	D	201	CDL	OA6-CA4	-2.71	1.39	1.46
12	B	604	CDL	OA6-CA4	-2.71	1.39	1.46
12	P	201	CDL	OA6-CA4	-2.71	1.39	1.46
12	C	306	CDL	OA6-CA5	2.70	1.41	1.34
20	C	302	HEC	FE-NA	2.70	2.04	1.95
12	B	605	CDL	OA6-CA4	-2.70	1.39	1.46
12	D	201	CDL	OA6-CA5	2.70	1.41	1.34
19	A	503	9YF	O9-C	-2.69	1.39	1.46
16	B	603	HEM	CAB-C3B	2.69	1.54	1.47
17	N	609	MQ9	C2-C1	-2.68	1.43	1.48
12	B	607	CDL	OA6-CA4	-2.68	1.39	1.46
12	N	605	CDL	OA6-CA4	-2.68	1.39	1.46
17	C	304	MQ9	C2-C1	-2.67	1.43	1.48
14	F	606	HEA	C4B-NB	-2.66	1.35	1.40
12	P	201	CDL	OA6-CA5	2.66	1.41	1.34
12	N	605	CDL	OA6-CA5	2.65	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	606	HEA	C4C-NC	-2.65	1.34	1.39
19	M	504	9YF	O9-C	-2.65	1.40	1.46
12	M	502	CDL	OA6-CA4	-2.65	1.40	1.46
17	N	608	MQ9	C2-C1	-2.64	1.43	1.48
12	B	605	CDL	OA6-CA5	2.64	1.41	1.34
12	F	601	CDL	OA6-CA5	2.63	1.41	1.34
12	B	607	CDL	OA6-CA5	2.62	1.41	1.34
12	R	601	CDL	OA6-CA5	2.62	1.41	1.34
17	N	611	MQ9	C2-C1	-2.62	1.43	1.48
12	B	604	CDL	OA6-CA5	2.61	1.41	1.34
12	N	607	CDL	OA6-CA5	2.60	1.41	1.34
12	N	606	CDL	OA6-CA5	2.60	1.41	1.34
12	F	602	CDL	OB6-CB4	-2.60	1.40	1.46
12	F	602	CDL	OA6-CA5	2.60	1.41	1.34
15	S	301	9Y0	O7-C1	-2.59	1.40	1.46
15	G	301	9Y0	O7-C1	-2.59	1.40	1.46
12	B	606	CDL	OA6-CA4	-2.58	1.40	1.46
17	B	608	MQ9	C2-C1	-2.58	1.43	1.48
12	R	602	CDL	OB6-CB4	-2.57	1.40	1.46
12	N	607	CDL	OB6-CB4	-2.56	1.40	1.46
12	C	306	CDL	OA6-CA4	-2.56	1.40	1.46
16	N	602	HEM	FE-NA	2.56	2.03	1.95
20	O	303	HEC	FE-NC	2.56	2.03	1.95
12	C	303	CDL	OA6-CA5	2.55	1.41	1.34
14	R	605	HEA	C4C-NC	-2.54	1.34	1.39
12	R	602	CDL	OA6-CA5	2.53	1.41	1.34
14	F	606	HEA	C4C-NC	-2.53	1.34	1.39
12	N	603	CDL	OA6-CA5	2.52	1.41	1.34
17	N	608	MQ9	C21-C19	2.51	1.56	1.51
12	N	603	CDL	OB6-CB4	-2.50	1.40	1.46
17	C	304	MQ9	C21-C19	2.50	1.56	1.51
16	N	602	HEM	FE-NC	2.50	2.03	1.95
19	A	502	9YF	O9-C	-2.49	1.40	1.46
12	C	306	CDL	OB6-CB4	-2.47	1.40	1.46
12	R	601	CDL	OB6-CB4	-2.47	1.40	1.46
12	N	605	CDL	OB6-CB4	-2.47	1.40	1.46
12	B	606	CDL	OB6-CB4	-2.46	1.40	1.46
12	B	607	CDL	OB6-CB4	-2.46	1.40	1.46
17	N	609	MQ9	C6-C5	2.46	1.39	1.35
12	B	604	CDL	OB6-CB4	-2.45	1.40	1.46
12	N	606	CDL	OB6-CB4	-2.45	1.40	1.46
14	F	607	HEA	C4B-C3B	2.44	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	610	MQ9	C21-C19	2.43	1.56	1.51
12	C	303	CDL	OB6-CB4	-2.43	1.40	1.46
17	N	609	MQ9	C21-C19	2.42	1.56	1.51
19	A	503	9YF	O11-C25	2.41	1.40	1.33
19	M	504	9YF	O11-C25	2.40	1.40	1.33
19	A	502	9YF	O11-C25	2.40	1.40	1.33
17	B	609	MQ9	C21-C19	2.40	1.56	1.51
15	G	301	9Y0	O5-C5	2.40	1.40	1.33
19	M	503	9YF	O11-C25	2.39	1.40	1.33
19	M	503	9YF	O9-C	-2.39	1.40	1.46
12	D	201	CDL	OB6-CB4	-2.38	1.40	1.46
17	O	301	MQ9	C21-C19	2.38	1.56	1.51
12	F	601	CDL	OB6-CB4	-2.38	1.40	1.46
12	B	605	CDL	OB6-CB4	-2.38	1.40	1.46
14	R	606	HEA	C4B-C3B	2.36	1.48	1.44
17	B	608	MQ9	C21-C19	2.36	1.56	1.51
17	O	302	MQ9	C21-C19	2.34	1.56	1.51
19	A	502	9YF	P-O2	2.34	1.66	1.60
15	S	301	9Y0	O5-C5	2.33	1.40	1.33
17	C	305	MQ9	C21-C19	2.32	1.56	1.51
12	M	502	CDL	OB6-CB4	-2.32	1.40	1.46
17	N	611	MQ9	C21-C19	2.31	1.56	1.51
19	M	504	9YF	O11-C24	-2.27	1.40	1.45
14	R	606	HEA	C1C-C2C	2.25	1.48	1.43
14	R	605	HEA	C1C-C2C	2.24	1.48	1.43
14	F	607	HEA	C1C-C2C	2.22	1.48	1.43
14	F	606	HEA	C1C-C2C	2.22	1.48	1.43
14	F	606	HEA	C1C-NC	-2.20	1.35	1.39
19	M	503	9YF	O11-C24	-2.20	1.40	1.45
14	R	606	HEA	C1C-NC	-2.20	1.35	1.39
15	S	301	9Y0	O5-C	-2.19	1.40	1.45
17	N	611	MQ9	C6-C5	2.18	1.39	1.35
14	R	605	HEA	C1C-NC	-2.18	1.35	1.39
12	P	201	CDL	C71-CB7	2.16	1.57	1.50
14	F	607	HEA	C1C-NC	-2.16	1.35	1.39
12	N	606	CDL	C71-CB7	2.15	1.57	1.50
17	B	608	MQ9	C6-C5	2.13	1.39	1.35
19	A	502	9YF	O11-C24	-2.13	1.40	1.45
19	M	503	9YF	O9-C8	2.12	1.40	1.34
12	R	601	CDL	C71-CB7	2.11	1.56	1.50
12	P	201	CDL	OB6-CB4	-2.11	1.41	1.46
19	A	503	9YF	O11-C24	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	301	9Y0	O5-C	-2.11	1.40	1.45
19	A	502	9YF	O9-C8	2.10	1.40	1.34
12	F	601	CDL	C71-CB7	2.10	1.56	1.50
19	A	503	9YF	P-O2	2.10	1.66	1.60
17	N	608	MQ9	C6-C5	2.09	1.39	1.35
12	D	201	CDL	C71-CB7	2.08	1.56	1.50
12	B	604	CDL	C71-CB7	2.08	1.56	1.50
12	N	605	CDL	C71-CB7	2.08	1.56	1.50
12	C	303	CDL	C71-CB7	2.07	1.56	1.50
17	B	609	MQ9	C6-C5	2.07	1.39	1.35
15	S	301	9Y0	O7-C21	2.06	1.40	1.34
12	M	502	CDL	C71-CB7	2.06	1.56	1.50
12	F	602	CDL	C71-CB7	2.06	1.56	1.50
12	N	603	CDL	C71-CB7	2.05	1.56	1.50
12	C	306	CDL	C71-CB7	2.05	1.56	1.50
20	C	301	HEC	CMB-C2B	2.05	1.55	1.50
12	B	606	CDL	C71-CB7	2.04	1.56	1.50
12	B	605	CDL	PB2-OB5	2.04	1.67	1.59
12	B	605	CDL	C71-CB7	2.03	1.56	1.50
15	G	301	9Y0	O7-C21	2.01	1.40	1.34
17	N	610	MQ9	C6-C5	2.01	1.38	1.35
16	B	603	HEM	C3B-C2B	-2.00	1.33	1.37

All (525) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	301	MQ9	C7-C8-C9	-10.86	108.72	126.79
17	C	305	MQ9	C7-C8-C9	-10.67	109.03	126.79
17	N	608	MQ9	C7-C8-C9	-10.58	109.19	126.79
17	N	609	MQ9	C7-C8-C9	-10.40	109.48	126.79
17	N	610	MQ9	C7-C8-C9	-10.14	109.91	126.79
17	O	302	MQ9	C7-C8-C9	-9.92	110.28	126.79
17	C	304	MQ9	C7-C8-C9	-9.79	110.50	126.79
17	B	608	MQ9	C7-C8-C9	-9.41	111.12	126.79
17	B	609	MQ9	C7-C8-C9	-9.36	111.20	126.79
17	N	611	MQ9	C7-C8-C9	-8.57	112.52	126.79
14	R	606	HEA	C3C-C4C-NC	7.08	114.60	110.25
17	B	608	MQ9	C12-C13-C14	-6.96	110.90	127.66
17	B	608	MQ9	C27-C28-C29	-6.92	111.00	127.66
14	F	607	HEA	C3C-C4C-NC	6.92	114.50	110.25
17	O	301	MQ9	C12-C13-C14	-6.88	111.08	127.66
17	O	302	MQ9	C12-C13-C14	-6.86	111.13	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	304	MQ9	C12-C13-C14	-6.82	111.24	127.66
17	N	608	MQ9	C12-C13-C14	-6.82	111.24	127.66
17	C	305	MQ9	C12-C13-C14	-6.81	111.25	127.66
20	O	304	HEC	C1D-ND-C4D	6.73	112.03	105.07
20	C	302	HEC	C1D-ND-C4D	6.70	111.99	105.07
17	B	609	MQ9	C12-C13-C14	-6.68	111.58	127.66
17	N	611	MQ9	C12-C13-C14	-6.62	111.71	127.66
17	N	610	MQ9	C12-C13-C14	-6.62	111.73	127.66
20	O	303	HEC	C1D-ND-C4D	6.61	111.90	105.07
17	N	609	MQ9	C12-C13-C14	-6.57	111.84	127.66
17	O	302	MQ9	C27-C28-C29	-6.56	111.87	127.66
17	N	609	MQ9	C42-C43-C44	-6.55	111.90	127.66
17	N	611	MQ9	C27-C28-C29	-6.52	111.95	127.66
14	F	606	HEA	C3C-C4C-NC	6.51	114.25	110.25
17	N	609	MQ9	C27-C28-C29	-6.50	112.00	127.66
17	N	611	MQ9	C10-C9-C8	-6.49	107.03	123.68
17	C	305	MQ9	C27-C28-C29	-6.47	112.08	127.66
17	N	608	MQ9	C27-C28-C29	-6.47	112.08	127.66
17	N	610	MQ9	C27-C28-C29	-6.46	112.11	127.66
17	O	302	MQ9	C42-C43-C44	-6.40	112.25	127.66
17	O	301	MQ9	C27-C28-C29	-6.35	112.36	127.66
14	R	605	HEA	C3C-C4C-NC	6.29	114.12	110.25
17	N	608	MQ9	C42-C43-C44	-6.28	112.54	127.66
17	O	301	MQ9	C10-C9-C8	-6.24	107.67	123.68
20	C	301	HEC	C1D-ND-C4D	6.23	111.50	105.07
17	B	608	MQ9	C10-C9-C8	-6.17	107.84	123.68
14	R	605	HEA	C3D-C4D-ND	6.14	116.30	110.36
14	F	606	HEA	C3D-C4D-ND	6.13	116.29	110.36
17	C	304	MQ9	C10-C9-C8	-6.12	107.98	123.68
17	N	608	MQ9	C10-C9-C8	-6.05	108.15	123.68
17	C	305	MQ9	C42-C43-C44	-6.05	113.10	127.66
17	C	304	MQ9	C27-C28-C29	-6.04	113.12	127.66
17	B	608	MQ9	C15-C14-C13	-6.01	108.27	123.68
17	B	609	MQ9	C10-C9-C8	-6.01	108.27	123.68
17	N	610	MQ9	C10-C9-C8	-5.98	108.34	123.68
17	O	302	MQ9	C15-C14-C13	-5.95	108.42	123.68
17	C	305	MQ9	C10-C9-C8	-5.94	108.43	123.68
17	N	610	MQ9	C15-C14-C13	-5.93	108.48	123.68
17	B	609	MQ9	C15-C14-C13	-5.92	108.48	123.68
17	N	611	MQ9	C15-C14-C13	-5.92	108.49	123.68
17	C	305	MQ9	C15-C14-C13	-5.92	108.49	123.68
17	N	609	MQ9	C10-C9-C8	-5.91	108.51	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	608	MQ9	C15-C14-C13	-5.88	108.59	123.68
17	C	304	MQ9	C15-C14-C13	-5.79	108.83	123.68
17	O	301	MQ9	C15-C14-C13	-5.76	108.89	123.68
17	N	609	MQ9	C15-C14-C13	-5.76	108.91	123.68
17	O	302	MQ9	C10-C9-C8	-5.66	109.15	123.68
14	F	607	HEA	C2D-C1D-ND	5.63	116.51	109.84
17	O	302	MQ9	C37-C38-C39	-5.61	114.14	127.66
17	O	301	MQ9	C11-C9-C8	-5.55	109.88	121.12
14	R	606	HEA	C2D-C1D-ND	5.55	116.41	109.84
14	R	606	HEA	C3D-C4D-ND	5.54	115.72	110.36
14	F	606	HEA	C2D-C1D-ND	5.54	116.40	109.84
14	F	607	HEA	C3D-C4D-ND	5.52	115.70	110.36
17	O	302	MQ9	C11-C9-C8	-5.50	109.98	121.12
17	N	611	MQ9	C11-C9-C8	-5.44	110.10	121.12
17	N	608	MQ9	C11-C9-C8	-5.44	110.11	121.12
17	O	302	MQ9	C36-C34-C33	-5.44	110.12	121.12
14	F	606	HEA	C2B-C1B-NB	5.43	116.39	109.88
17	C	305	MQ9	C22-C23-C24	-5.40	114.65	127.66
14	R	605	HEA	C2B-C1B-NB	5.40	116.35	109.88
14	R	605	HEA	C2D-C1D-ND	5.39	116.22	109.84
17	B	608	MQ9	C11-C9-C8	-5.38	110.22	121.12
17	C	305	MQ9	C17-C18-C19	-5.37	114.74	127.66
17	C	305	MQ9	C11-C9-C8	-5.36	110.28	121.12
17	B	608	MQ9	C17-C18-C19	-5.34	114.80	127.66
17	N	611	MQ9	C17-C18-C19	-5.34	114.80	127.66
17	O	301	MQ9	C17-C18-C19	-5.33	114.83	127.66
17	N	608	MQ9	C36-C34-C33	-5.32	110.34	121.12
17	N	609	MQ9	C36-C34-C33	-5.31	110.37	121.12
17	N	610	MQ9	C11-C9-C8	-5.28	110.44	121.12
17	B	608	MQ9	C22-C23-C24	-5.27	114.96	127.66
17	N	608	MQ9	C37-C38-C39	-5.26	114.99	127.66
17	O	302	MQ9	C45-C44-C43	-5.26	110.19	123.68
14	F	607	HEA	C2B-C1B-NB	5.25	116.17	109.88
17	B	609	MQ9	C17-C18-C19	-5.24	115.05	127.66
17	C	304	MQ9	C11-C9-C8	-5.23	110.54	121.12
14	F	607	HEA	C3C-C2C-C1C	-5.22	100.86	107.16
14	R	606	HEA	C2B-C1B-NB	5.21	116.12	109.88
17	N	611	MQ9	C22-C23-C24	-5.20	115.15	127.66
17	N	609	MQ9	C37-C38-C39	-5.18	115.19	127.66
17	O	301	MQ9	C36-C34-C33	-5.17	110.65	121.12
17	N	609	MQ9	C22-C23-C24	-5.16	115.25	127.66
14	R	606	HEA	C3C-C2C-C1C	-5.14	100.96	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	R	605	HEA	C3C-C2C-C1C	-5.13	100.97	107.16
17	N	609	MQ9	C17-C18-C19	-5.12	115.32	127.66
17	O	302	MQ9	C17-C18-C19	-5.11	115.35	127.66
14	R	606	HEA	C3B-C4B-NB	5.11	115.89	109.84
17	B	609	MQ9	C11-C9-C8	-5.10	110.79	121.12
17	B	609	MQ9	C22-C23-C24	-5.10	115.39	127.66
17	N	608	MQ9	C22-C23-C24	-5.07	115.44	127.66
17	N	610	MQ9	C22-C23-C24	-5.06	115.48	127.66
17	O	302	MQ9	C22-C23-C24	-5.05	115.51	127.66
14	F	606	HEA	C3C-C2C-C1C	-5.04	101.07	107.16
14	R	605	HEA	C3B-C4B-NB	5.03	115.80	109.84
17	N	610	MQ9	C17-C18-C19	-5.03	115.56	127.66
17	N	608	MQ9	C17-C18-C19	-5.01	115.59	127.66
17	O	301	MQ9	C22-C23-C24	-5.00	115.62	127.66
17	N	609	MQ9	C11-C9-C8	-4.99	111.01	121.12
17	C	305	MQ9	C36-C34-C33	-4.98	111.05	121.12
17	C	305	MQ9	C46-C44-C43	-4.96	111.09	121.12
14	F	606	HEA	C3B-C4B-NB	4.96	115.71	109.84
17	O	302	MQ9	C46-C44-C43	-4.94	111.13	121.12
17	C	305	MQ9	C40-C39-C38	-4.93	111.02	123.68
14	F	607	HEA	C3B-C4B-NB	4.93	115.68	109.84
17	N	609	MQ9	C46-C44-C43	-4.92	111.16	121.12
17	C	305	MQ9	C32-C33-C34	-4.92	115.82	127.66
17	C	305	MQ9	C37-C38-C39	-4.90	115.85	127.66
17	C	305	MQ9	C45-C44-C43	-4.90	111.11	123.68
17	N	608	MQ9	C46-C44-C43	-4.88	111.25	121.12
17	C	304	MQ9	C17-C18-C19	-4.86	115.95	127.66
17	O	302	MQ9	C41-C39-C38	-4.86	111.28	121.12
17	N	608	MQ9	C45-C44-C43	-4.81	111.34	123.68
17	N	608	MQ9	C41-C39-C38	-4.79	111.43	121.12
17	O	302	MQ9	C40-C39-C38	-4.78	111.42	123.68
17	N	609	MQ9	C45-C44-C43	-4.77	111.43	123.68
17	O	302	MQ9	C32-C33-C34	-4.76	116.21	127.66
17	N	608	MQ9	C40-C39-C38	-4.75	111.50	123.68
17	C	304	MQ9	C22-C23-C24	-4.70	116.35	127.66
17	O	301	MQ9	C32-C33-C34	-4.69	116.37	127.66
17	C	304	MQ9	C36-C34-C33	-4.67	111.66	121.12
17	C	305	MQ9	C41-C39-C38	-4.66	111.69	121.12
17	B	609	MQ9	C27-C28-C29	-4.60	112.03	127.75
17	N	609	MQ9	C32-C33-C34	-4.60	116.59	127.66
17	N	609	MQ9	C41-C39-C38	-4.59	111.83	121.12
14	F	607	HEA	C1D-C2D-C3D	-4.59	102.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	606	CDL	OA6-CA5-C11	4.58	121.38	111.50
12	R	602	CDL	OA6-CA5-C11	4.57	121.36	111.50
17	N	609	MQ9	C40-C39-C38	-4.57	111.96	123.68
17	N	608	MQ9	C32-C33-C34	-4.56	116.69	127.66
17	N	610	MQ9	C16-C14-C13	-4.47	112.07	121.12
17	N	611	MQ9	C36-C34-C33	-4.47	109.73	122.65
17	B	608	MQ9	C16-C14-C13	-4.44	112.13	121.12
14	R	606	HEA	C1D-C2D-C3D	-4.44	102.29	106.96
12	F	601	CDL	OB6-CB5-C51	4.43	121.04	111.50
17	C	305	MQ9	C16-C14-C13	-4.42	112.17	121.12
17	N	608	MQ9	C47-C48-C49	-4.40	112.70	127.75
14	F	606	HEA	C1D-C2D-C3D	-4.39	102.34	106.96
12	N	605	CDL	OA6-CA5-C11	4.37	120.91	111.50
12	B	607	CDL	OB6-CB5-C51	4.35	120.88	111.50
12	P	201	CDL	C25-C24-C23	4.35	136.51	114.42
17	O	302	MQ9	C47-C48-C49	-4.35	112.90	127.75
12	D	201	CDL	OB6-CB5-C51	4.34	120.86	111.50
14	R	605	HEA	C1D-C2D-C3D	-4.34	102.39	106.96
17	B	609	MQ9	C16-C14-C13	-4.33	112.35	121.12
17	N	609	MQ9	C47-C48-C49	-4.33	112.95	127.75
12	N	605	CDL	OB6-CB5-C51	4.32	120.82	111.50
17	C	305	MQ9	C47-C48-C49	-4.32	112.98	127.75
17	O	301	MQ9	C16-C14-C13	-4.31	112.40	121.12
17	N	610	MQ9	C36-C34-C33	-4.30	110.21	122.65
19	M	504	9YF	C6-C7-C2	4.30	119.50	109.68
12	D	201	CDL	C25-C24-C23	4.29	136.22	114.42
17	O	302	MQ9	C16-C14-C13	-4.28	112.45	121.12
12	N	607	CDL	OA6-CA5-C11	4.28	120.73	111.50
12	R	601	CDL	OB6-CB5-C51	4.28	120.72	111.50
12	N	606	CDL	OB6-CB5-C51	4.27	120.71	111.50
12	B	605	CDL	OA6-CA5-C11	4.25	120.66	111.50
17	N	609	MQ9	C16-C14-C13	-4.25	112.52	121.12
17	C	305	MQ9	C35-C34-C33	-4.24	112.81	123.68
17	N	611	MQ9	C25-C24-C23	-4.23	112.82	123.68
12	M	502	CDL	C25-C24-C23	4.22	135.85	114.42
17	C	305	MQ9	C25-C24-C23	-4.22	112.85	123.68
12	D	201	CDL	OA6-CA5-C11	4.22	120.59	111.50
17	N	611	MQ9	C16-C14-C13	-4.22	112.58	121.12
12	B	607	CDL	C25-C24-C23	4.22	135.84	114.42
17	N	608	MQ9	C16-C14-C13	-4.21	112.59	121.12
17	C	304	MQ9	C32-C33-C34	-4.21	117.52	127.66
12	C	303	CDL	OA6-CA5-C11	4.21	120.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	608	MQ9	C25-C24-C23	-4.21	112.88	123.68
17	B	608	MQ9	C36-C34-C33	-4.20	110.51	122.65
17	B	609	MQ9	C25-C24-C23	-4.19	112.94	123.68
12	C	303	CDL	OB6-CB5-C51	4.19	120.52	111.50
19	A	502	9YF	O9-C8-C9	4.18	120.52	111.50
12	C	306	CDL	C25-C24-C23	4.17	135.62	114.42
12	B	604	CDL	OA6-CA5-C11	4.17	120.50	111.50
12	C	306	CDL	OA6-CA5-C11	4.16	120.47	111.50
17	O	301	MQ9	C30-C29-C28	-4.16	113.01	123.68
12	N	606	CDL	OA6-CA5-C11	4.16	120.46	111.50
17	N	611	MQ9	C30-C29-C28	-4.13	113.09	123.68
17	O	301	MQ9	C25-C24-C23	-4.12	113.12	123.68
17	N	610	MQ9	C30-C29-C28	-4.11	113.13	123.68
12	P	201	CDL	OA6-CA5-C11	4.11	120.36	111.50
17	N	609	MQ9	C25-C24-C23	-4.11	113.14	123.68
12	C	306	CDL	OB6-CB5-C51	4.11	120.35	111.50
17	B	608	MQ9	C30-C29-C28	-4.10	113.16	123.68
17	N	610	MQ9	C25-C24-C23	-4.10	113.17	123.68
17	N	609	MQ9	C35-C34-C33	-4.10	113.17	123.68
19	M	504	9YF	O9-C8-C9	4.09	120.32	111.50
12	B	605	CDL	OB6-CB5-C51	4.08	120.30	111.50
12	N	607	CDL	C25-C24-C23	4.07	135.10	114.42
12	B	607	CDL	OA6-CA5-C11	4.07	120.27	111.50
19	A	503	9YF	C4-C3-C2	4.07	118.97	109.68
17	O	302	MQ9	C30-C29-C28	-4.05	113.29	123.68
12	N	603	CDL	OB6-CB5-C51	4.05	120.23	111.50
12	B	606	CDL	OB6-CB5-C51	4.05	120.23	111.50
17	N	608	MQ9	C25-C24-C23	-4.05	113.29	123.68
15	S	301	9Y0	O7-C21-C22	4.03	120.19	111.50
17	O	302	MQ9	C25-C24-C23	-4.03	113.34	123.68
17	C	304	MQ9	C30-C29-C28	-4.02	113.36	123.68
17	C	304	MQ9	C25-C24-C23	-4.02	113.37	123.68
12	F	602	CDL	OB6-CB5-C51	4.00	120.12	111.50
12	P	201	CDL	OB6-CB5-C51	3.98	120.07	111.50
17	C	304	MQ9	C35-C34-C33	-3.96	113.52	123.68
17	O	301	MQ9	C35-C34-C33	-3.95	113.53	123.68
19	A	503	9YF	O9-C8-C9	3.95	120.01	111.50
12	M	502	CDL	OA6-CA5-C11	3.94	120.00	111.50
12	N	607	CDL	OB6-CB5-C51	3.94	120.00	111.50
19	M	503	9YF	O9-C8-C9	3.94	119.99	111.50
17	N	608	MQ9	C30-C29-C28	-3.92	113.62	123.68
17	O	302	MQ9	C35-C34-C33	-3.92	113.62	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	608	MQ9	C35-C34-C33	-3.92	113.63	123.68
12	M	502	CDL	OB6-CB5-C51	3.92	119.94	111.50
14	R	606	HEA	C2C-C1C-NC	3.91	116.04	110.08
17	C	305	MQ9	C30-C29-C28	-3.91	113.64	123.68
17	N	609	MQ9	C30-C29-C28	-3.91	113.64	123.68
12	F	602	CDL	OA6-CA5-C11	3.88	119.86	111.50
14	R	605	HEA	C2C-C1C-NC	3.87	115.97	110.08
17	O	301	MQ9	C20-C19-C18	-3.85	113.80	123.68
12	R	601	CDL	OA6-CA5-C11	3.83	119.77	111.50
14	F	606	HEA	C2C-C1C-NC	3.83	115.92	110.08
15	G	301	9Y0	O7-C21-C22	3.82	119.74	111.50
17	O	302	MQ9	C51-C49-C48	-3.78	111.73	122.65
17	O	301	MQ9	C41-C39-C38	-3.77	111.74	122.65
17	C	305	MQ9	C20-C19-C18	-3.77	114.00	123.68
17	N	608	MQ9	C51-C49-C48	-3.76	111.78	122.65
12	R	602	CDL	OB6-CB5-C51	3.76	119.60	111.50
17	B	608	MQ9	C20-C19-C18	-3.76	114.04	123.68
17	N	609	MQ9	C50-C49-C48	-3.75	111.80	122.65
17	C	304	MQ9	C16-C14-C13	-3.75	113.53	121.12
17	C	305	MQ9	C51-C49-C48	-3.74	111.82	122.65
17	O	302	MQ9	C20-C19-C18	-3.74	114.07	123.68
14	F	607	HEA	C2C-C1C-NC	3.74	115.77	110.08
17	O	302	MQ9	C50-C49-C48	-3.74	111.85	122.65
17	C	304	MQ9	C41-C39-C38	-3.72	111.89	122.65
17	C	304	MQ9	C40-C39-C38	-3.72	111.89	122.65
12	B	604	CDL	OB6-CB5-C51	3.71	119.50	111.50
12	F	601	CDL	OA6-CA5-C11	3.71	119.50	111.50
17	N	611	MQ9	C31-C29-C28	-3.70	113.63	121.12
17	O	301	MQ9	C40-C39-C38	-3.70	111.96	122.65
17	N	608	MQ9	C50-C49-C48	-3.69	111.97	122.65
17	C	305	MQ9	C50-C49-C48	-3.68	112.00	122.65
17	B	609	MQ9	C20-C19-C18	-3.67	114.25	123.68
17	O	302	MQ9	C26-C24-C23	-3.66	113.70	121.12
19	M	504	9YF	C7-C6-C5	3.66	117.22	110.82
17	N	609	MQ9	C51-C49-C48	-3.65	112.09	122.65
17	N	611	MQ9	C20-C19-C18	-3.64	114.34	123.68
17	O	301	MQ9	C31-C29-C28	-3.61	113.81	121.12
17	N	610	MQ9	C31-C29-C28	-3.60	113.83	121.12
17	N	610	MQ9	C20-C19-C18	-3.60	114.43	123.68
17	C	304	MQ9	C37-C38-C39	-3.59	115.48	127.75
17	O	302	MQ9	C45-C44-C46	-3.58	109.24	115.27
17	C	305	MQ9	C31-C29-C28	-3.58	113.88	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	609	MQ9	C20-C19-C18	-3.57	114.51	123.68
17	B	609	MQ9	C26-C24-C23	-3.56	113.91	121.12
17	C	304	MQ9	C20-C19-C18	-3.56	114.54	123.68
19	A	503	9YF	C5-C4-C3	3.55	117.02	110.82
17	O	301	MQ9	C37-C38-C39	-3.55	115.63	127.75
17	N	608	MQ9	C20-C19-C18	-3.54	114.58	123.68
17	N	608	MQ9	C45-C44-C46	-3.52	109.35	115.27
17	C	305	MQ9	C21-C19-C18	-3.51	114.01	121.12
17	N	610	MQ9	C26-C24-C23	-3.51	114.02	121.12
17	B	608	MQ9	C31-C29-C28	-3.50	114.03	121.12
19	M	503	9YF	C6-C5-C4	3.50	116.94	110.82
17	O	302	MQ9	C31-C29-C28	-3.48	114.07	121.12
17	N	611	MQ9	C32-C33-C34	-3.48	115.87	127.75
17	N	609	MQ9	C31-C29-C28	-3.47	114.09	121.12
17	O	302	MQ9	C21-C19-C18	-3.47	114.09	121.12
17	N	609	MQ9	C26-C24-C23	-3.45	114.13	121.12
12	N	603	CDL	OA6-CA5-C11	3.41	118.85	111.50
17	C	305	MQ9	C45-C44-C46	-3.41	109.54	115.27
14	R	606	HEA	C1B-C2B-C3B	-3.39	102.75	106.80
17	C	305	MQ9	C26-C24-C23	-3.38	114.28	121.12
17	N	608	MQ9	C31-C29-C28	-3.37	114.30	121.12
14	R	605	HEA	CHA-C4D-C3D	-3.36	119.90	124.84
17	B	608	MQ9	C32-C33-C34	-3.36	116.27	127.75
17	N	611	MQ9	C26-C24-C23	-3.36	114.33	121.12
17	C	304	MQ9	C31-C29-C28	-3.35	114.34	121.12
20	C	301	HEC	C4B-NB-C1B	3.34	108.52	105.07
17	B	608	MQ9	C21-C19-C18	-3.32	114.39	121.12
14	F	606	HEA	CHA-C4D-C3D	-3.32	119.96	124.84
17	N	610	MQ9	C32-C33-C34	-3.31	116.43	127.75
14	F	607	HEA	C1B-C2B-C3B	-3.31	102.84	106.80
14	R	605	HEA	C1B-C2B-C3B	-3.28	102.88	106.80
17	N	609	MQ9	C45-C44-C46	-3.28	109.76	115.27
17	N	608	MQ9	C26-C24-C23	-3.27	114.50	121.12
14	F	606	HEA	C1B-C2B-C3B	-3.26	102.90	106.80
17	O	301	MQ9	C26-C24-C23	-3.25	114.54	121.12
17	C	304	MQ9	C21-C19-C18	-3.24	114.57	121.12
17	O	301	MQ9	C21-C19-C18	-3.22	114.60	121.12
17	N	610	MQ9	C21-C19-C18	-3.22	114.61	121.12
14	F	606	HEA	C3A-C2A-C1A	-3.21	104.01	107.08
14	R	605	HEA	C27-C19-C20	3.20	120.65	115.27
17	N	609	MQ9	C21-C19-C18	-3.17	114.70	121.12
17	B	609	MQ9	C21-C19-C18	-3.17	114.71	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	R	606	HEA	C17-C18-C19	-3.16	120.05	127.66
14	F	606	HEA	CHB-C1B-C2B	-3.15	120.05	124.98
16	N	602	HEM	C1B-NB-C4B	3.14	108.32	105.07
17	B	608	MQ9	C26-C24-C23	-3.14	114.77	121.12
14	R	605	HEA	CAD-CBD-CGD	-3.12	106.89	113.60
14	R	605	HEA	CHB-C1B-C2B	-3.12	120.11	124.98
17	B	608	MQ9	C35-C34-C33	-3.12	113.63	122.65
17	B	609	MQ9	C30-C29-C28	-3.11	113.66	122.65
17	N	609	MQ9	C25-C24-C26	-3.10	110.05	115.27
16	B	603	HEM	C1B-NB-C4B	3.10	108.27	105.07
17	C	304	MQ9	C26-C24-C23	-3.08	114.89	121.12
17	N	610	MQ9	C35-C34-C33	-3.07	113.78	122.65
17	B	609	MQ9	C31-C29-C28	-3.07	113.78	122.65
20	C	301	HEC	C4C-NC-C1C	3.06	108.35	105.35
17	N	611	MQ9	C7-C6-C1	3.04	121.76	118.50
17	N	611	MQ9	C35-C34-C33	-3.04	113.87	122.65
17	N	608	MQ9	C21-C19-C18	-3.02	115.00	121.12
14	F	607	HEA	CHB-C1B-C2B	-3.02	120.26	124.98
14	F	606	HEA	C4D-C3D-C2D	-3.01	102.50	106.90
19	A	503	9YF	C7-C2-C3	3.01	115.19	110.85
14	R	605	HEA	C4D-C3D-C2D	-3.01	102.52	106.90
17	N	611	MQ9	C21-C19-C18	-3.00	115.04	121.12
14	R	605	HEA	C3A-C2A-C1A	-2.99	104.22	107.08
17	N	610	MQ9	C25-C24-C26	-2.99	110.24	115.27
17	B	608	MQ9	C25-C24-C26	-2.99	110.25	115.27
20	O	303	HEC	C4C-NC-C1C	2.98	108.27	105.35
17	N	608	MQ9	C25-C24-C26	-2.98	110.25	115.27
14	F	606	HEA	C4B-C3B-C2B	-2.97	102.34	107.41
17	C	304	MQ9	C25-C24-C26	-2.97	110.28	115.27
20	O	304	HEC	C4C-NC-C1C	2.97	108.25	105.35
14	R	606	HEA	CHB-C1B-C2B	-2.96	120.35	124.98
14	R	605	HEA	C4B-C3B-C2B	-2.96	102.36	107.41
14	F	607	HEA	C4B-C3B-C2B	-2.95	102.36	107.41
14	F	606	HEA	C2A-C1A-NA	2.95	113.19	110.32
20	O	303	HEC	C4A-NA-C1A	2.95	108.23	105.35
17	O	302	MQ9	C25-C24-C26	-2.94	110.32	115.27
14	R	605	HEA	C2A-C1A-NA	2.93	113.17	110.32
14	F	607	HEA	C17-C18-C19	-2.93	120.61	127.66
17	O	301	MQ9	C25-C24-C26	-2.93	110.35	115.27
17	N	611	MQ9	C25-C24-C26	-2.91	110.37	115.27
12	N	607	CDL	OB8-CB7-C71	2.90	121.01	111.91
14	R	606	HEA	C4B-C3B-C2B	-2.90	102.46	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	601	HEM	C1B-NB-C4B	2.88	108.05	105.07
14	R	606	HEA	C27-C19-C20	2.85	120.07	115.27
17	C	305	MQ9	C25-C24-C26	-2.85	110.47	115.27
17	C	305	MQ9	C40-C39-C41	-2.85	110.47	115.27
20	O	303	HEC	CAB-C3B-C4B	2.85	128.50	124.81
19	M	504	9YF	C7-C2-C3	2.84	114.95	110.85
20	O	303	HEC	C2A-C1A-NA	-2.83	107.57	110.32
14	F	607	HEA	C27-C19-C20	2.82	120.02	115.27
19	A	502	9YF	O4-C4-C5	2.82	116.86	110.35
15	G	301	9Y0	O5-C5-C6	2.80	120.69	111.91
14	F	606	HEA	CAD-CBD-CGD	-2.80	107.59	113.60
12	N	605	CDL	OB8-CB7-C71	2.79	120.67	111.91
17	B	609	MQ9	C25-C24-C26	-2.78	110.59	115.27
14	F	606	HEA	C27-C19-C20	2.78	119.95	115.27
12	M	502	CDL	OA8-CA7-C31	2.78	120.63	111.91
20	O	303	HEC	C4B-NB-C1B	2.78	107.94	105.07
16	N	602	HEM	C3B-C2B-C1B	2.76	108.54	106.49
12	C	306	CDL	OA8-CA7-C31	2.76	120.58	111.91
12	B	607	CDL	OB8-CB7-C71	2.76	120.56	111.91
16	B	602	HEM	C4D-ND-C1D	2.76	107.92	105.07
14	R	606	HEA	C4D-C3D-C2D	-2.75	102.89	106.90
16	B	603	HEM	C4A-NA-C1A	2.74	108.03	105.35
12	R	601	CDL	OB8-CB7-C71	2.74	120.50	111.91
12	N	603	CDL	OA8-CA7-C31	2.74	120.50	111.91
12	B	606	CDL	OA8-CA7-C31	2.73	120.47	111.91
12	D	201	CDL	OB8-CB7-C71	2.73	120.47	111.91
12	N	607	CDL	OA8-CA7-C31	2.73	120.47	111.91
14	F	606	HEA	C17-C18-C19	-2.73	121.09	127.66
12	F	601	CDL	OB8-CB7-C71	2.72	120.45	111.91
16	N	601	HEM	C4D-ND-C1D	2.71	107.87	105.07
12	C	306	CDL	OB8-CB7-C71	2.71	120.40	111.91
20	C	302	HEC	C4C-NC-C1C	2.70	108.00	105.35
16	B	603	HEM	C3B-C2B-C1B	2.70	108.49	106.49
12	B	604	CDL	OB8-CB7-C71	2.70	120.37	111.91
14	F	607	HEA	CAA-CBA-CGA	-2.69	107.80	113.60
14	F	607	HEA	C3A-C2A-C1A	-2.69	104.50	107.08
12	B	607	CDL	OA8-CA7-C31	2.69	120.36	111.91
16	N	601	HEM	C4C-NC-C1C	2.69	107.98	105.35
12	C	303	CDL	OA8-CA7-C31	2.69	120.35	111.91
16	B	602	HEM	C1B-NB-C4B	2.69	107.85	105.07
17	C	305	MQ9	C35-C34-C36	-2.68	110.75	115.27
12	N	606	CDL	OA8-CA7-C31	2.68	120.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	301	9Y0	O5-C5-C6	2.67	120.28	111.91
14	R	606	HEA	C2A-C1A-NA	2.67	112.92	110.32
14	F	607	HEA	C4D-C3D-C2D	-2.66	103.02	106.90
12	M	502	CDL	OB8-CB7-C71	2.66	120.26	111.91
12	R	602	CDL	OB8-CB7-C71	2.66	120.25	111.91
12	N	606	CDL	OB8-CB7-C71	2.66	120.24	111.91
20	O	304	HEC	C4B-NB-C1B	2.65	107.81	105.07
12	B	606	CDL	OB8-CB7-C71	2.65	120.23	111.91
14	F	607	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
14	R	606	HEA	CAA-CBA-CGA	-2.64	107.92	113.60
12	B	605	CDL	OA8-CA7-C31	2.64	120.19	111.91
12	R	601	CDL	OA8-CA7-C31	2.63	120.16	111.91
14	R	606	HEA	CHA-C4D-C3D	-2.62	120.99	124.84
12	F	602	CDL	OB8-CB7-C71	2.61	120.11	111.91
12	N	603	CDL	OB8-CB7-C71	2.61	120.11	111.91
12	F	602	CDL	OA8-CA7-C31	2.61	120.09	111.91
12	P	201	CDL	OA8-CA7-C31	2.60	120.08	111.91
12	P	201	CDL	OB8-CB7-C71	2.60	120.05	111.91
12	D	201	CDL	OA8-CA7-C31	2.59	120.05	111.91
20	O	304	HEC	C2A-C1A-NA	-2.59	107.81	110.32
19	A	503	9YF	O11-C25-C26	2.59	120.03	111.91
20	C	302	HEC	C4A-NA-C1A	2.59	107.88	105.35
19	A	502	9YF	O11-C25-C26	2.58	120.02	111.91
14	R	605	HEA	C17-C18-C19	-2.58	121.44	127.66
17	O	302	MQ9	C35-C34-C36	-2.58	110.94	115.27
20	C	302	HEC	C4B-NB-C1B	2.58	107.73	105.07
20	C	302	HEC	C2A-C1A-NA	-2.57	107.82	110.32
20	C	301	HEC	C4A-NA-C1A	2.57	107.87	105.35
19	M	504	9YF	O11-C25-C26	2.57	119.97	111.91
19	M	503	9YF	O11-C25-C26	2.57	119.97	111.91
14	F	606	HEA	OMA-CMA-C3A	-2.57	119.89	125.69
14	R	606	HEA	CMC-C2C-C1C	2.56	129.26	125.37
12	B	604	CDL	OA8-CA7-C31	2.56	119.93	111.91
16	N	602	HEM	C4C-NC-C1C	2.55	107.85	105.35
12	F	601	CDL	OA8-CA7-C31	2.55	119.92	111.91
17	C	304	MQ9	C35-C34-C36	-2.55	110.98	115.27
12	C	303	CDL	OB8-CB7-C71	2.55	119.90	111.91
16	B	602	HEM	C4C-NC-C1C	2.53	107.83	105.35
19	A	502	9YF	C4-C3-C2	2.53	115.46	109.68
12	N	605	CDL	OA8-CA7-C31	2.53	119.84	111.91
12	R	602	CDL	OA8-CA7-C31	2.53	119.84	111.91
14	F	606	HEA	C1D-ND-C4D	-2.52	102.47	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	607	HEA	CMD-C2D-C1D	2.52	128.87	125.04
14	F	607	HEA	C2A-C1A-NA	2.51	112.77	110.32
20	C	301	HEC	C3B-C4B-NB	-2.51	107.37	110.17
20	O	304	HEC	C4A-NA-C1A	2.50	107.80	105.35
14	F	607	HEA	CBD-CAD-C3D	-2.50	105.67	112.63
12	B	605	CDL	OB8-CB7-C71	2.47	119.66	111.91
16	N	602	HEM	C4A-NA-C1A	2.46	107.76	105.35
16	N	601	HEM	C4A-NA-C1A	2.46	107.75	105.35
14	F	607	HEA	CMC-C2C-C1C	2.45	129.10	125.37
14	R	606	HEA	C3A-C2A-C1A	-2.45	104.74	107.08
16	B	602	HEM	C4A-NA-C1A	2.44	107.74	105.35
20	C	301	HEC	C2A-C1A-NA	-2.44	107.95	110.32
14	R	606	HEA	CHD-C1D-C2D	-2.43	119.97	126.73
20	O	303	HEC	CAB-C3B-C2B	-2.43	123.38	127.53
14	R	605	HEA	C1D-ND-C4D	-2.42	102.57	105.07
14	R	606	HEA	C17-C16-C15	-2.40	105.07	112.98
17	B	608	MQ9	C10-C9-C11	-2.40	111.24	115.27
20	O	303	HEC	CAD-C3D-C4D	2.39	128.84	124.66
17	N	609	MQ9	C40-C39-C41	-2.39	111.25	115.27
14	R	605	HEA	OMA-CMA-C3A	-2.39	120.28	125.69
20	O	303	HEC	C3B-C4B-NB	-2.38	107.52	110.17
14	R	605	HEA	C4B-NB-C1B	-2.38	102.62	105.07
16	B	603	HEM	C4D-ND-C1D	2.38	107.53	105.07
14	F	607	HEA	C1D-ND-C4D	-2.36	102.64	105.07
16	N	602	HEM	C4D-ND-C1D	2.36	107.51	105.07
14	F	607	HEA	CHD-C1D-C2D	-2.35	120.20	126.73
14	F	606	HEA	C4B-NB-C1B	-2.34	102.66	105.07
19	A	503	9YF	C-O9-C8	-2.33	112.06	117.79
17	O	302	MQ9	C40-C39-C41	-2.31	111.38	115.27
14	R	606	HEA	C1D-ND-C4D	-2.31	102.69	105.07
14	F	606	HEA	C4A-C3A-C2A	2.30	108.64	106.75
14	F	606	HEA	CAA-C2A-C1A	2.29	129.22	124.89
17	N	608	MQ9	C40-C39-C41	-2.29	111.42	115.27
17	B	608	MQ9	C7-C6-C1	2.29	120.95	118.50
20	O	303	HEC	C3C-C4C-NC	-2.28	107.60	110.15
14	F	607	HEA	C12-C13-C14	-2.27	106.23	112.23
14	R	606	HEA	CBD-CAD-C3D	-2.26	106.33	112.63
14	R	605	HEA	CBA-CAA-C2A	-2.26	106.35	112.63
20	O	304	HEC	C3D-C4D-ND	-2.25	108.18	110.36
16	N	602	HEM	CHD-C4C-NC	2.25	126.87	124.44
14	F	607	HEA	C17-C16-C15	-2.24	105.60	112.98
17	O	301	MQ9	C35-C34-C36	-2.23	111.52	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	R	606	HEA	CMD-C2D-C1D	2.23	128.44	125.04
17	N	611	MQ9	C10-C9-C11	-2.23	111.52	115.27
14	F	606	HEA	C17-C16-C15	-2.23	105.64	112.98
19	M	503	9YF	C5-C4-C3	2.22	114.69	110.82
14	R	606	HEA	C4B-NB-C1B	-2.21	102.79	105.07
14	F	606	HEA	CHD-C1D-C2D	-2.21	120.59	126.73
19	M	504	9YF	O7-C7-C2	2.21	115.79	109.94
19	M	504	9YF	C-O9-C8	-2.20	112.36	117.79
14	R	605	HEA	CHD-C1D-C2D	-2.20	120.61	126.73
16	B	603	HEM	C4C-NC-C1C	2.20	107.50	105.35
12	R	602	CDL	CA4-OA6-CA5	-2.20	112.39	117.79
14	R	606	HEA	CAD-C3D-C4D	2.20	128.50	124.66
14	R	605	HEA	CMC-C2C-C1C	2.19	128.71	125.37
16	B	603	HEM	CHD-C4C-NC	2.19	126.81	124.44
20	C	301	HEC	CAD-CBD-CGD	-2.18	108.91	113.60
17	N	608	MQ9	C35-C34-C36	-2.18	111.60	115.27
14	R	605	HEA	CMB-C2B-C1B	2.18	128.36	125.04
14	F	606	HEA	C25-C23-C24	2.17	119.41	114.60
14	F	607	HEA	C26-C15-C14	-2.16	118.14	123.68
19	M	503	9YF	O7-C7-C6	-2.16	105.36	110.35
17	N	611	MQ9	C8-C7-C6	2.16	117.86	112.05
20	C	302	HEC	C3C-C4C-NC	-2.15	107.74	110.15
16	B	602	HEM	C3D-C4D-ND	-2.15	107.77	110.17
14	F	606	HEA	CMC-C2C-C1C	2.15	128.64	125.37
20	C	302	HEC	C3D-C4D-ND	-2.14	108.28	110.36
20	C	302	HEC	CAD-CBD-CGD	-2.13	109.02	113.60
20	O	304	HEC	C3C-C4C-NC	-2.12	107.78	110.15
12	C	303	CDL	CA4-OA6-CA5	-2.11	112.59	117.79
14	R	606	HEA	C25-C23-C24	2.09	119.23	114.60
14	F	607	HEA	CAD-C3D-C4D	2.09	128.32	124.66
14	F	607	HEA	CAA-C2A-C1A	2.09	128.84	124.89
17	N	609	MQ9	C35-C34-C36	-2.09	111.76	115.27
14	R	606	HEA	C26-C15-C14	-2.08	118.33	123.68
14	R	605	HEA	C12-C13-C14	-2.08	106.73	112.23
14	R	605	HEA	CHC-C1C-C2C	-2.08	121.37	127.24
14	F	607	HEA	C4B-NB-C1B	-2.07	102.93	105.07
17	N	610	MQ9	C10-C9-C11	-2.07	111.78	115.27
16	N	601	HEM	C3D-C4D-ND	-2.07	107.86	110.17
16	B	603	HEM	C2A-C1A-NA	-2.06	107.85	110.15
14	R	606	HEA	C12-C13-C14	-2.05	106.83	112.23
17	N	609	MQ9	O1-C1-C6	-2.04	117.27	120.56
20	O	304	HEC	C3B-C4B-NB	-2.03	107.90	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	N	602	HEM	CAD-CBD-CGD	-2.03	109.24	113.60
17	B	609	MQ9	O4-C4-C5	-2.03	117.62	120.25
14	F	607	HEA	C25-C23-C24	2.02	119.07	114.60
14	R	606	HEA	CMB-C2B-C1B	2.02	128.11	125.04
14	F	606	HEA	CMB-C2B-C1B	2.00	128.09	125.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	O	303	HEC	NA
20	O	304	HEC	NA
20	C	301	HEC	NA
20	C	302	HEC	NA

All (1284) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CB2-OB2-PB2-OB3
12	F	601	CDL	CB2-OB2-PB2-OB4
12	F	601	CDL	CB3-OB5-PB2-OB3
12	F	601	CDL	CB3-OB5-PB2-OB4
12	F	602	CDL	CB3-OB5-PB2-OB3
12	F	602	CDL	CB3-OB5-PB2-OB4
12	D	201	CDL	OA7-CA5-OA6-CA4
12	D	201	CDL	CB3-OB5-PB2-OB3
12	D	201	CDL	CB3-OB5-PB2-OB4
12	R	601	CDL	O1-C1-CA2-OA2
12	R	601	CDL	CB2-OB2-PB2-OB3
12	R	602	CDL	CA2-OA2-PA1-OA3
12	R	602	CDL	CA3-OA5-PA1-OA3
12	R	602	CDL	CA3-OA5-PA1-OA4
12	R	602	CDL	OB5-CB3-CB4-OB6
12	P	201	CDL	CA2-OA2-PA1-OA3
12	P	201	CDL	CA2-OA2-PA1-OA5
12	P	201	CDL	CA3-OA5-PA1-OA2
12	P	201	CDL	CA3-OA5-PA1-OA3
12	P	201	CDL	C11-CA5-OA6-CA4
12	P	201	CDL	CB3-OB5-PB2-OB3
12	P	201	CDL	C51-CB5-OB6-CB4
12	N	603	CDL	O1-C1-CA2-OA2
12	N	603	CDL	CB2-C1-CA2-OA2
12	N	603	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
12	N	605	CDL	CA2-OA2-PA1-OA3
12	N	605	CDL	CA2-OA2-PA1-OA4
12	N	605	CDL	CA2-OA2-PA1-OA5
12	N	605	CDL	CA3-OA5-PA1-OA4
12	N	605	CDL	CB2-OB2-PB2-OB3
12	N	605	CDL	CB2-OB2-PB2-OB4
12	N	605	CDL	CB2-OB2-PB2-OB5
12	N	605	CDL	OB7-CB5-OB6-CB4
12	N	606	CDL	CA3-OA5-PA1-OA3
12	N	606	CDL	OA6-CA4-CA6-OA8
12	N	606	CDL	C11-CA5-OA6-CA4
12	N	606	CDL	CB3-OB5-PB2-OB2
12	N	606	CDL	C51-CB5-OB6-CB4
12	N	607	CDL	CA2-OA2-PA1-OA3
12	N	607	CDL	OA7-CA5-OA6-CA4
12	M	502	CDL	CA2-OA2-PA1-OA4
12	M	502	CDL	CA3-OA5-PA1-OA3
12	M	502	CDL	CB3-OB5-PB2-OB3
12	B	604	CDL	O1-C1-CB2-OB2
12	B	604	CDL	CA3-OA5-PA1-OA2
12	B	604	CDL	CA3-OA5-PA1-OA4
12	B	604	CDL	CB2-OB2-PB2-OB3
12	B	604	CDL	CB2-OB2-PB2-OB4
12	B	604	CDL	CB3-OB5-PB2-OB4
12	B	605	CDL	O1-C1-CA2-OA2
12	B	605	CDL	CA2-OA2-PA1-OA3
12	B	605	CDL	CA2-OA2-PA1-OA4
12	B	605	CDL	CA3-OA5-PA1-OA2
12	B	605	CDL	CA3-OA5-PA1-OA3
12	B	605	CDL	CA3-OA5-PA1-OA4
12	B	605	CDL	CB2-OB2-PB2-OB3
12	B	605	CDL	CB2-OB2-PB2-OB4
12	B	606	CDL	CA2-OA2-PA1-OA5
12	B	606	CDL	OA7-CA5-OA6-CA4
12	B	606	CDL	C11-CA5-OA6-CA4
12	B	607	CDL	CA2-OA2-PA1-OA3
12	B	607	CDL	CA2-OA2-PA1-OA4
12	B	607	CDL	CA2-OA2-PA1-OA5
12	B	607	CDL	OA7-CA5-OA6-CA4
12	B	607	CDL	C11-CA5-OA6-CA4
12	B	607	CDL	OB7-CB5-OB6-CB4
12	B	607	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
12	C	303	CDL	CB2-C1-CA2-OA2
12	C	303	CDL	O1-C1-CB2-OB2
12	C	303	CDL	CA2-C1-CB2-OB2
12	C	303	CDL	CA3-OA5-PA1-OA3
12	C	303	CDL	OA5-CA3-CA4-OA6
12	C	303	CDL	OA7-CA5-OA6-CA4
12	C	303	CDL	C11-CA5-OA6-CA4
12	C	303	CDL	CB2-OB2-PB2-OB3
12	C	303	CDL	CB3-OB5-PB2-OB3
12	C	303	CDL	CB3-OB5-PB2-OB4
12	C	303	CDL	C51-CB5-OB6-CB4
12	C	306	CDL	C11-CA5-OA6-CA4
12	C	306	CDL	CB2-OB2-PB2-OB3
12	C	306	CDL	CB2-OB2-PB2-OB5
14	F	606	HEA	C2A-C3A-CMA-OMA
14	F	606	HEA	C4A-C3A-CMA-OMA
14	F	606	HEA	C2D-C3D-CAD-CBD
14	F	606	HEA	C13-C14-C15-C16
14	F	606	HEA	C26-C15-C16-C17
14	F	607	HEA	C2A-C3A-CMA-OMA
14	F	607	HEA	C4A-C3A-CMA-OMA
14	F	607	HEA	C3B-C11-C12-C13
14	F	607	HEA	O11-C11-C12-C13
14	F	607	HEA	C14-C15-C16-C17
14	F	607	HEA	C15-C16-C17-C18
14	R	605	HEA	C2A-C3A-CMA-OMA
14	R	605	HEA	C4A-C3A-CMA-OMA
14	R	605	HEA	C2D-C3D-CAD-CBD
14	R	605	HEA	C21-C22-C23-C25
14	R	606	HEA	C2A-C3A-CMA-OMA
14	R	606	HEA	C4A-C3A-CMA-OMA
14	R	606	HEA	C3B-C11-C12-C13
14	R	606	HEA	O11-C11-C12-C13
14	R	606	HEA	C15-C16-C17-C18
15	G	301	9Y0	O1-C3-C4-N
15	G	301	9Y0	C2-O3-P-O
15	S	301	9Y0	O1-C3-C4-N
15	S	301	9Y0	C2-O3-P-O
15	S	301	9Y0	C2-O3-P-O2
17	N	608	MQ9	C7-C8-C9-C11
17	N	608	MQ9	C9-C11-C12-C13
17	N	608	MQ9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	N	608	MQ9	C12-C13-C14-C16
17	N	608	MQ9	C17-C18-C19-C20
17	N	608	MQ9	C22-C23-C24-C25
17	N	608	MQ9	C24-C26-C27-C28
17	N	608	MQ9	C32-C33-C34-C35
17	N	608	MQ9	C37-C38-C39-C41
17	N	608	MQ9	C39-C41-C42-C43
17	N	608	MQ9	C42-C43-C44-C45
17	N	608	MQ9	C42-C43-C44-C46
17	N	609	MQ9	C7-C8-C9-C11
17	N	609	MQ9	C12-C13-C14-C15
17	N	609	MQ9	C12-C13-C14-C16
17	N	609	MQ9	C13-C14-C16-C17
17	N	609	MQ9	C17-C18-C19-C20
17	N	609	MQ9	C17-C18-C19-C21
17	N	609	MQ9	C22-C23-C24-C25
17	N	609	MQ9	C22-C23-C24-C26
17	N	609	MQ9	C30-C29-C31-C32
17	N	609	MQ9	C29-C31-C32-C33
17	N	609	MQ9	C37-C38-C39-C40
17	N	609	MQ9	C42-C43-C44-C45
17	N	609	MQ9	C42-C43-C44-C46
17	N	609	MQ9	C47-C48-C49-C50
17	N	610	MQ9	C6-C7-C8-C9
17	N	610	MQ9	C7-C8-C9-C10
17	N	610	MQ9	C12-C13-C14-C15
17	N	610	MQ9	C15-C14-C16-C17
17	N	610	MQ9	C16-C17-C18-C19
17	N	610	MQ9	C17-C18-C19-C20
17	N	610	MQ9	C17-C18-C19-C21
17	N	610	MQ9	C22-C23-C24-C25
17	N	610	MQ9	C25-C24-C26-C27
17	N	610	MQ9	C24-C26-C27-C28
17	N	611	MQ9	C5-C6-C7-C8
17	N	611	MQ9	C1-C6-C7-C8
17	N	611	MQ9	C6-C7-C8-C9
17	N	611	MQ9	C7-C8-C9-C11
17	N	611	MQ9	C12-C13-C14-C16
17	N	611	MQ9	C14-C16-C17-C18
17	N	611	MQ9	C17-C18-C19-C21
17	N	611	MQ9	C18-C19-C21-C22
17	N	611	MQ9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	O	301	MQ9	C12-C11-C9-C10
17	O	301	MQ9	C17-C18-C19-C20
17	O	301	MQ9	C17-C18-C19-C21
17	O	301	MQ9	C20-C19-C21-C22
17	O	301	MQ9	C22-C23-C24-C25
17	O	301	MQ9	C27-C28-C29-C30
17	O	301	MQ9	C27-C28-C29-C31
17	O	301	MQ9	C32-C33-C34-C36
17	O	301	MQ9	C37-C38-C39-C40
17	O	302	MQ9	C9-C11-C12-C13
17	O	302	MQ9	C12-C13-C14-C15
17	O	302	MQ9	C34-C36-C37-C38
17	O	302	MQ9	C37-C38-C39-C41
17	O	302	MQ9	C42-C43-C44-C45
17	B	608	MQ9	C7-C8-C9-C11
17	B	608	MQ9	C12-C11-C9-C10
17	B	608	MQ9	C9-C11-C12-C13
17	B	608	MQ9	C12-C13-C14-C15
17	B	608	MQ9	C23-C24-C26-C27
17	B	608	MQ9	C25-C24-C26-C27
17	B	608	MQ9	C28-C29-C31-C32
17	B	608	MQ9	C30-C29-C31-C32
17	B	609	MQ9	C14-C16-C17-C18
17	B	609	MQ9	C17-C18-C19-C20
17	B	609	MQ9	C17-C18-C19-C21
17	B	609	MQ9	C19-C21-C22-C23
17	C	304	MQ9	C7-C8-C9-C10
17	C	304	MQ9	C7-C8-C9-C11
17	C	304	MQ9	C12-C13-C14-C15
17	C	304	MQ9	C22-C23-C24-C25
17	C	304	MQ9	C24-C26-C27-C28
17	C	304	MQ9	C27-C28-C29-C30
17	C	304	MQ9	C32-C33-C34-C35
17	C	304	MQ9	C32-C33-C34-C36
17	C	305	MQ9	C7-C8-C9-C10
17	C	305	MQ9	C12-C13-C14-C15
17	C	305	MQ9	C12-C13-C14-C16
17	C	305	MQ9	C17-C18-C19-C20
17	C	305	MQ9	C18-C19-C21-C22
17	C	305	MQ9	C20-C19-C21-C22
17	C	305	MQ9	C22-C23-C24-C26
17	C	305	MQ9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
17	C	305	MQ9	C27-C28-C29-C31
17	C	305	MQ9	C32-C33-C34-C35
17	C	305	MQ9	C35-C34-C36-C37
17	C	305	MQ9	C37-C38-C39-C41
17	C	305	MQ9	C42-C43-C44-C46
19	M	503	9YF	C7-C2-O2-P
19	M	503	9YF	C26-C25-O11-C24
19	M	503	9YF	O12-C25-O11-C24
19	M	504	9YF	C2-O2-P-O1
19	A	502	9YF	C3-C2-O2-P
19	A	502	9YF	C7-C2-O2-P
19	A	503	9YF	C1-O-P-O2
19	A	503	9YF	C1-O-P-O8
19	A	503	9YF	C9-C8-O9-C
19	A	503	9YF	O10-C8-O9-C
12	D	201	CDL	OB9-CB7-OB8-CB6
12	N	606	CDL	OA9-CA7-OA8-CA6
12	C	303	CDL	OB9-CB7-OB8-CB6
19	A	502	9YF	O12-C25-O11-C24
19	A	502	9YF	C26-C25-O11-C24
14	F	606	HEA	C21-C22-C23-C25
17	N	608	MQ9	C47-C48-C49-C50
17	O	302	MQ9	C47-C48-C49-C50
17	C	304	MQ9	C37-C38-C39-C41
17	C	305	MQ9	C47-C48-C49-C50
12	N	607	CDL	OA9-CA7-OA8-CA6
12	B	607	CDL	OA9-CA7-OA8-CA6
12	C	303	CDL	OA9-CA7-OA8-CA6
12	P	201	CDL	OA7-CA5-OA6-CA4
12	P	201	CDL	OB7-CB5-OB6-CB4
12	N	606	CDL	OA7-CA5-OA6-CA4
12	N	606	CDL	OB7-CB5-OB6-CB4
12	M	502	CDL	OB7-CB5-OB6-CB4
12	C	303	CDL	OB7-CB5-OB6-CB4
12	C	306	CDL	OA7-CA5-OA6-CA4
12	F	601	CDL	C71-CB7-OB8-CB6
12	D	201	CDL	C71-CB7-OB8-CB6
12	N	606	CDL	C31-CA7-OA8-CA6
12	N	607	CDL	C31-CA7-OA8-CA6
12	B	607	CDL	C31-CA7-OA8-CA6
12	C	303	CDL	C31-CA7-OA8-CA6
12	C	303	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
12	D	201	CDL	C11-CA5-OA6-CA4
12	N	605	CDL	C51-CB5-OB6-CB4
12	N	607	CDL	C11-CA5-OA6-CA4
12	M	502	CDL	C51-CB5-OB6-CB4
17	N	609	MQ9	C46-C47-C48-C49
14	F	606	HEA	C21-C22-C23-C24
17	N	609	MQ9	C47-C48-C49-C51
17	N	610	MQ9	C12-C11-C9-C10
17	O	302	MQ9	C20-C19-C21-C22
17	O	302	MQ9	C13-C14-C16-C17
17	B	609	MQ9	C12-C11-C9-C8
12	N	606	CDL	C71-CB7-OB8-CB6
12	M	502	CDL	C71-CB7-OB8-CB6
12	B	606	CDL	C31-CA7-OA8-CA6
19	M	504	9YF	C26-C25-O11-C24
14	F	606	HEA	C4D-C3D-CAD-CBD
14	R	605	HEA	C4D-C3D-CAD-CBD
14	R	606	HEA	C21-C22-C23-C25
17	N	610	MQ9	C32-C33-C34-C35
17	B	609	MQ9	C27-C28-C29-C31
14	F	606	HEA	C13-C14-C15-C26
14	F	606	HEA	C17-C18-C19-C27
17	N	608	MQ9	C27-C28-C29-C30
17	N	609	MQ9	C27-C28-C29-C30
17	N	610	MQ9	C27-C28-C29-C30
17	O	301	MQ9	C7-C8-C9-C10
17	O	301	MQ9	C12-C13-C14-C15
17	O	302	MQ9	C7-C8-C9-C10
17	O	302	MQ9	C17-C18-C19-C20
17	O	302	MQ9	C22-C23-C24-C25
17	O	302	MQ9	C27-C28-C29-C30
17	O	302	MQ9	C32-C33-C34-C35
17	B	609	MQ9	C7-C8-C9-C10
17	B	609	MQ9	C12-C13-C14-C15
17	B	609	MQ9	C22-C23-C24-C25
17	C	304	MQ9	C17-C18-C19-C20
12	F	601	CDL	OB7-CB5-OB6-CB4
14	F	606	HEA	C17-C18-C19-C20
17	N	608	MQ9	C22-C23-C24-C26
17	N	610	MQ9	C12-C13-C14-C16
17	N	610	MQ9	C22-C23-C24-C26
17	B	608	MQ9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
17	B	609	MQ9	C7-C8-C9-C11
12	F	601	CDL	O1-C1-CB2-OB2
12	D	201	CDL	O1-C1-CB2-OB2
12	C	303	CDL	O1-C1-CA2-OA2
12	D	201	CDL	C31-CA7-OA8-CA6
12	B	604	CDL	C71-CB7-OB8-CB6
12	B	605	CDL	C31-CA7-OA8-CA6
12	F	602	CDL	C51-C52-C53-C54
12	P	201	CDL	C79-C80-C81-C82
12	F	601	CDL	OB9-CB7-OB8-CB6
12	F	601	CDL	C51-CB5-OB6-CB4
12	R	601	CDL	C51-CB5-OB6-CB4
12	N	603	CDL	C51-CB5-OB6-CB4
12	M	502	CDL	C11-CA5-OA6-CA4
12	B	605	CDL	C11-CA5-OA6-CA4
12	F	602	CDL	C57-C58-C59-C60
12	F	602	CDL	C75-C76-C77-C78
17	B	608	MQ9	C32-C33-C34-C36
12	D	201	CDL	C76-C77-C78-C79
12	R	602	CDL	C75-C76-C77-C78
12	B	607	CDL	C57-C58-C59-C60
12	C	303	CDL	C83-C84-C85-C86
12	N	606	CDL	OB9-CB7-OB8-CB6
12	D	201	CDL	C79-C80-C81-C82
12	N	603	CDL	C76-C77-C78-C79
12	N	605	CDL	C76-C77-C78-C79
19	A	503	9YF	C10-C11-C12-C13
12	R	602	CDL	C57-C58-C59-C60
12	C	306	CDL	C72-C73-C74-C75
12	M	502	CDL	OB9-CB7-OB8-CB6
19	M	504	9YF	O12-C25-O11-C24
12	F	601	CDL	C31-C32-C33-C34
19	A	502	9YF	C28-C29-C30-C31
17	O	301	MQ9	C37-C38-C39-C41
17	N	608	MQ9	C12-C11-C9-C10
17	N	608	MQ9	C20-C19-C21-C22
17	N	609	MQ9	C20-C19-C21-C22
17	N	609	MQ9	C25-C24-C26-C27
17	N	611	MQ9	C12-C11-C9-C10
17	O	301	MQ9	C25-C24-C26-C27
17	O	302	MQ9	C25-C24-C26-C27
17	O	302	MQ9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
17	C	304	MQ9	C12-C11-C9-C10
17	C	304	MQ9	C35-C34-C36-C37
17	C	305	MQ9	C30-C29-C31-C32
17	N	608	MQ9	C23-C24-C26-C27
17	N	609	MQ9	C12-C11-C9-C8
17	N	609	MQ9	C33-C34-C36-C37
17	O	301	MQ9	C18-C19-C21-C22
17	O	301	MQ9	C28-C29-C31-C32
17	C	304	MQ9	C18-C19-C21-C22
17	C	305	MQ9	C38-C39-C41-C42
12	C	303	CDL	C72-C73-C74-C75
12	D	201	CDL	OA9-CA7-OA8-CA6
12	B	604	CDL	OB9-CB7-OB8-CB6
12	B	606	CDL	OA9-CA7-OA8-CA6
14	F	606	HEA	C15-C16-C17-C18
14	F	607	HEA	C19-C20-C21-C22
14	R	606	HEA	C19-C20-C21-C22
17	N	608	MQ9	C19-C21-C22-C23
17	N	609	MQ9	C19-C21-C22-C23
17	N	609	MQ9	C39-C41-C42-C43
17	N	611	MQ9	C9-C11-C12-C13
17	N	611	MQ9	C19-C21-C22-C23
17	O	301	MQ9	C19-C21-C22-C23
17	O	302	MQ9	C24-C26-C27-C28
17	O	302	MQ9	C39-C41-C42-C43
17	O	302	MQ9	C44-C46-C47-C48
17	B	608	MQ9	C14-C16-C17-C18
17	B	608	MQ9	C19-C21-C22-C23
17	C	304	MQ9	C14-C16-C17-C18
17	C	304	MQ9	C19-C21-C22-C23
12	R	601	CDL	C31-C32-C33-C34
12	F	602	CDL	C31-CA7-OA8-CA6
12	F	602	CDL	C71-CB7-OB8-CB6
12	R	601	CDL	C71-CB7-OB8-CB6
12	B	604	CDL	C31-CA7-OA8-CA6
12	F	602	CDL	OB9-CB7-OB8-CB6
12	B	605	CDL	OA9-CA7-OA8-CA6
12	B	606	CDL	C51-CB5-OB6-CB4
14	R	605	HEA	C21-C22-C23-C24
17	N	608	MQ9	C7-C8-C9-C10
17	N	611	MQ9	C12-C13-C14-C15
17	O	302	MQ9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CA2-C1-CB2-OB2
12	R	601	CDL	CB2-C1-CA2-OA2
12	B	604	CDL	CA2-C1-CB2-OB2
12	B	605	CDL	CB2-C1-CA2-OA2
12	N	603	CDL	OB7-CB5-OB6-CB4
12	B	605	CDL	OA7-CA5-OA6-CA4
17	O	301	MQ9	C22-C23-C24-C26
12	F	602	CDL	OA9-CA7-OA8-CA6
12	R	601	CDL	OB9-CB7-OB8-CB6
12	B	604	CDL	OA9-CA7-OA8-CA6
12	R	602	CDL	C71-CB7-OB8-CB6
12	B	605	CDL	C71-CB7-OB8-CB6
15	S	301	9Y0	C6-C5-O5-C
19	A	502	9YF	C2-O2-P-O
12	D	201	CDL	CA5-C11-C12-C13
12	D	201	CDL	C81-C82-C83-C84
17	N	611	MQ9	C32-C33-C34-C35
17	C	305	MQ9	C47-C48-C49-C51
12	R	601	CDL	OB5-CB3-CB4-OB6
12	D	201	CDL	C32-C33-C34-C35
12	B	606	CDL	O1-C1-CA2-OA2
12	N	603	CDL	OA6-CA4-CA6-OA8
12	B	605	CDL	OB9-CB7-OB8-CB6
17	B	608	MQ9	C12-C11-C9-C8
17	C	304	MQ9	C23-C24-C26-C27
19	A	502	9YF	C34-C33-C35-C36
12	M	502	CDL	OA7-CA5-OA6-CA4
19	A	502	9YF	C9-C8-O9-C
17	N	611	MQ9	C32-C33-C34-C36
12	B	606	CDL	C71-CB7-OB8-CB6
15	G	301	9Y0	C6-C5-O5-C
19	A	503	9YF	C26-C25-O11-C24
12	M	502	CDL	C58-C59-C60-C61
12	B	607	CDL	C22-C23-C24-C25
12	F	601	CDL	CA7-C31-C32-C33
12	R	602	CDL	CB7-C71-C72-C73
12	P	201	CDL	CB7-C71-C72-C73
17	B	608	MQ9	C17-C18-C19-C20
17	C	305	MQ9	C37-C38-C39-C40
12	F	601	CDL	CB7-C71-C72-C73
12	R	601	CDL	CA7-C31-C32-C33
12	N	603	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	N	606	CDL	CB7-C71-C72-C73
12	B	606	CDL	CA5-C11-C12-C13
15	S	301	9Y0	C21-C22-C23-C24
12	P	201	CDL	C22-C23-C24-C25
12	P	201	CDL	C33-C34-C35-C36
12	N	607	CDL	C13-C14-C15-C16
12	R	601	CDL	OB7-CB5-OB6-CB4
12	D	201	CDL	CB5-C51-C52-C53
12	P	201	CDL	CB5-C51-C52-C53
16	N	602	HEM	C3D-CAD-CBD-CGD
19	A	502	9YF	C31-C32-C33-C35
12	R	602	CDL	OB9-CB7-OB8-CB6
15	S	301	9Y0	O4-C5-O5-C
14	R	605	HEA	C15-C16-C17-C18
17	N	608	MQ9	C34-C36-C37-C38
17	N	608	MQ9	C44-C46-C47-C48
17	O	301	MQ9	C29-C31-C32-C33
17	O	302	MQ9	C29-C31-C32-C33
17	C	304	MQ9	C34-C36-C37-C38
17	C	305	MQ9	C14-C16-C17-C18
17	C	305	MQ9	C39-C41-C42-C43
12	C	306	CDL	C63-C64-C65-C66
12	B	606	CDL	OB7-CB5-OB6-CB4
12	C	306	CDL	C31-CA7-OA8-CA6
12	P	201	CDL	C51-C52-C53-C54
12	B	606	CDL	OB9-CB7-OB8-CB6
15	G	301	9Y0	O4-C5-O5-C
19	A	503	9YF	O12-C25-O11-C24
19	M	504	9YF	C9-C8-O9-C
12	D	201	CDL	C52-C53-C54-C55
19	A	502	9YF	C30-C31-C32-C33
12	F	601	CDL	CB2-OB2-PB2-OB5
12	F	601	CDL	CB3-OB5-PB2-OB2
12	F	602	CDL	CB3-OB5-PB2-OB2
12	D	201	CDL	CB3-OB5-PB2-OB2
12	R	602	CDL	CA2-OA2-PA1-OA5
12	R	602	CDL	CA3-OA5-PA1-OA2
12	N	603	CDL	CA3-OA5-PA1-OA2
12	M	502	CDL	CA2-OA2-PA1-OA5
12	M	502	CDL	CA3-OA5-PA1-OA2
12	M	502	CDL	CB2-OB2-PB2-OB5
12	M	502	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
12	B	604	CDL	CB2-OB2-PB2-OB5
12	B	604	CDL	CB3-OB5-PB2-OB2
12	B	605	CDL	CA2-OA2-PA1-OA5
12	B	605	CDL	CB2-OB2-PB2-OB5
12	B	607	CDL	CA3-OA5-PA1-OA2
12	C	303	CDL	CB3-OB5-PB2-OB2
15	S	301	9Y0	C2-O3-P-O1
19	M	504	9YF	C1-O-P-O2
12	C	306	CDL	CA7-C31-C32-C33
12	F	601	CDL	C31-CA7-OA8-CA6
12	N	603	CDL	CB5-C51-C52-C53
12	D	201	CDL	CA2-C1-CB2-OB2
12	B	606	CDL	CB2-C1-CA2-OA2
19	M	504	9YF	O10-C8-O9-C
19	A	502	9YF	O10-C8-O9-C
19	M	504	9YF	C2-O2-P-O
12	D	201	CDL	CB7-C71-C72-C73
12	F	601	CDL	C13-C14-C15-C16
12	C	306	CDL	C59-C60-C61-C62
12	C	306	CDL	C83-C84-C85-C86
12	R	602	CDL	C51-CB5-OB6-CB4
15	S	301	9Y0	C22-C21-O7-C1
19	M	503	9YF	C9-C8-O9-C
12	F	602	CDL	C82-C83-C84-C85
12	R	602	CDL	C59-C60-C61-C62
12	P	201	CDL	C72-C73-C74-C75
12	P	201	CDL	C75-C76-C77-C78
12	N	603	CDL	C11-C12-C13-C14
12	N	603	CDL	C75-C76-C77-C78
12	N	607	CDL	C71-C72-C73-C74
12	N	607	CDL	C77-C78-C79-C80
12	M	502	CDL	C21-C22-C23-C24
12	M	502	CDL	C76-C77-C78-C79
12	B	605	CDL	C31-C32-C33-C34
12	B	605	CDL	C78-C79-C80-C81
12	B	607	CDL	C77-C78-C79-C80
12	C	303	CDL	C76-C77-C78-C79
12	R	601	CDL	C76-C77-C78-C79
12	N	605	CDL	C16-C17-C18-C19
12	B	604	CDL	C31-C32-C33-C34
12	B	607	CDL	C12-C13-C14-C15
12	B	607	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	C	303	CDL	C74-C75-C76-C77
12	R	602	CDL	OB7-CB5-OB6-CB4
15	S	301	9Y0	O6-C21-O7-C1
19	M	503	9YF	O10-C8-O9-C
12	R	601	CDL	CB7-C71-C72-C73
12	N	603	CDL	CB7-C71-C72-C73
12	F	601	CDL	C37-C38-C39-C40
12	R	601	CDL	C60-C61-C62-C63
12	N	605	CDL	C51-C52-C53-C54
12	N	606	CDL	C55-C56-C57-C58
12	C	306	CDL	C12-C13-C14-C15
12	C	306	CDL	C32-C33-C34-C35
15	S	301	9Y0	C25-C26-C27-C28
12	D	201	CDL	C74-C75-C76-C77
12	R	601	CDL	C37-C38-C39-C40
12	M	502	CDL	C80-C81-C82-C83
19	M	503	9YF	C13-C14-C15-C16
19	A	502	9YF	C37-C38-C39-C40
12	P	201	CDL	O1-C1-CB2-OB2
12	M	502	CDL	O1-C1-CB2-OB2
16	B	603	HEM	C3D-CAD-CBD-CGD
12	N	606	CDL	C37-C38-C39-C40
12	M	502	CDL	C57-C58-C59-C60
12	M	502	CDL	C59-C60-C61-C62
12	B	604	CDL	C55-C56-C57-C58
12	B	605	CDL	C14-C15-C16-C17
12	B	604	CDL	CA7-C31-C32-C33
12	F	601	CDL	C59-C60-C61-C62
12	F	602	CDL	C14-C15-C16-C17
12	F	602	CDL	C59-C60-C61-C62
12	R	601	CDL	C57-C58-C59-C60
12	N	605	CDL	C52-C53-C54-C55
12	N	606	CDL	C74-C75-C76-C77
12	B	606	CDL	C74-C75-C76-C77
12	B	607	CDL	C20-C21-C22-C23
17	N	611	MQ9	C27-C28-C29-C30
12	P	201	CDL	C52-C53-C54-C55
12	M	502	CDL	C83-C84-C85-C86
12	B	604	CDL	C75-C76-C77-C78
12	C	306	CDL	C71-C72-C73-C74
13	R	603	PLM	C8-C9-CA-CB
15	S	301	9Y0	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	S	301	9Y0	C23-C24-C25-C26
19	A	502	9YF	C9-C10-C11-C12
19	A	502	9YF	C29-C30-C31-C32
17	O	302	MQ9	C33-C34-C36-C37
12	B	604	CDL	CA5-C11-C12-C13
12	D	201	CDL	C54-C55-C56-C57
12	D	201	CDL	C73-C74-C75-C76
12	R	602	CDL	C52-C53-C54-C55
12	P	201	CDL	C23-C24-C25-C26
12	N	607	CDL	C75-C76-C77-C78
12	M	502	CDL	C31-C32-C33-C34
12	M	502	CDL	C75-C76-C77-C78
12	M	502	CDL	C79-C80-C81-C82
12	B	606	CDL	C37-C38-C39-C40
12	B	606	CDL	C71-C72-C73-C74
19	M	504	9YF	C26-C27-C28-C29
15	G	301	9Y0	C22-C23-C24-C25
12	N	605	CDL	OA7-CA5-OA6-CA4
12	N	605	CDL	C11-CA5-OA6-CA4
12	F	602	CDL	C77-C78-C79-C80
12	P	201	CDL	C31-C32-C33-C34
12	P	201	CDL	C80-C81-C82-C83
12	N	606	CDL	C72-C73-C74-C75
12	B	606	CDL	C11-C12-C13-C14
12	B	607	CDL	C21-C22-C23-C24
12	C	306	CDL	C74-C75-C76-C77
15	G	301	9Y0	C29-C30-C31-C32
12	B	605	CDL	CA7-C31-C32-C33
12	F	601	CDL	C55-C56-C57-C58
12	F	602	CDL	C13-C14-C15-C16
12	D	201	CDL	C72-C73-C74-C75
12	P	201	CDL	C82-C83-C84-C85
12	N	605	CDL	C73-C74-C75-C76
12	M	502	CDL	C14-C15-C16-C17
12	B	604	CDL	C56-C57-C58-C59
12	C	303	CDL	C55-C56-C57-C58
12	C	303	CDL	C57-C58-C59-C60
12	C	306	CDL	C17-C18-C19-C20
15	G	301	9Y0	C25-C26-C27-C28
19	M	503	9YF	C29-C30-C31-C32
19	A	502	9YF	C36-C37-C38-C39
17	N	609	MQ9	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
12	F	602	CDL	C31-C32-C33-C34
12	R	602	CDL	C31-C32-C33-C34
12	R	602	CDL	C77-C78-C79-C80
12	P	201	CDL	C14-C15-C16-C17
12	P	201	CDL	C21-C22-C23-C24
12	F	601	CDL	C76-C77-C78-C79
12	F	601	CDL	C77-C78-C79-C80
12	D	201	CDL	C38-C39-C40-C41
12	N	603	CDL	C83-C84-C85-C86
12	B	605	CDL	C72-C73-C74-C75
12	B	605	CDL	C75-C76-C77-C78
12	B	606	CDL	C31-C32-C33-C34
12	B	607	CDL	C33-C34-C35-C36
12	N	606	CDL	CA7-C31-C32-C33
12	C	303	CDL	CA5-C11-C12-C13
19	A	502	9YF	C11-C10-C9-C8
12	D	201	CDL	C22-C23-C24-C25
12	D	201	CDL	C37-C38-C39-C40
12	R	602	CDL	C32-C33-C34-C35
12	M	502	CDL	C37-C38-C39-C40
12	M	502	CDL	C77-C78-C79-C80
12	B	605	CDL	C74-C75-C76-C77
12	C	306	CDL	C75-C76-C77-C78
12	R	601	CDL	C71-C72-C73-C74
12	P	201	CDL	C78-C79-C80-C81
12	R	601	CDL	C77-C78-C79-C80
12	P	201	CDL	C55-C56-C57-C58
12	N	603	CDL	C14-C15-C16-C17
12	N	603	CDL	C77-C78-C79-C80
12	B	607	CDL	C72-C73-C74-C75
12	C	303	CDL	C80-C81-C82-C83
12	F	601	CDL	OA9-CA7-OA8-CA6
12	C	306	CDL	OA9-CA7-OA8-CA6
12	F	601	CDL	C57-C58-C59-C60
12	F	602	CDL	C12-C13-C14-C15
12	N	607	CDL	C23-C24-C25-C26
12	C	303	CDL	C52-C53-C54-C55
15	G	301	9Y0	C6-C7-C8-C9
19	M	503	9YF	C12-C13-C14-C15
12	N	607	CDL	CB3-CB4-CB6-OB8
12	B	604	CDL	CA3-CA4-CA6-OA8
12	F	602	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
12	B	606	CDL	C57-C58-C59-C60
12	B	607	CDL	C52-C53-C54-C55
12	N	603	CDL	C79-C80-C81-C82
12	F	602	CDL	C51-CB5-OB6-CB4
12	N	607	CDL	C51-CB5-OB6-CB4
12	F	602	CDL	C71-C72-C73-C74
12	F	602	CDL	C81-C82-C83-C84
12	N	607	CDL	C74-C75-C76-C77
12	M	502	CDL	C74-C75-C76-C77
12	B	605	CDL	C71-C72-C73-C74
12	B	605	CDL	C79-C80-C81-C82
12	B	607	CDL	C76-C77-C78-C79
12	B	605	CDL	CA5-C11-C12-C13
12	B	604	CDL	O1-C1-CA2-OA2
12	M	502	CDL	C62-C63-C64-C65
12	C	306	CDL	C54-C55-C56-C57
12	N	606	CDL	CA5-C11-C12-C13
12	P	201	CDL	C77-C78-C79-C80
12	C	303	CDL	C13-C14-C15-C16
12	F	602	CDL	OB7-CB5-OB6-CB4
12	N	607	CDL	OB7-CB5-OB6-CB4
12	B	606	CDL	C33-C34-C35-C36
12	B	607	CDL	C23-C24-C25-C26
12	B	607	CDL	C24-C25-C26-C27
19	M	503	9YF	C-C1-O-P
12	N	606	CDL	C71-C72-C73-C74
12	N	607	CDL	C22-C23-C24-C25
12	B	604	CDL	C11-C12-C13-C14
12	B	604	CDL	C77-C78-C79-C80
12	B	606	CDL	C51-C52-C53-C54
19	M	503	9YF	C11-C12-C13-C14
19	M	504	9YF	C10-C11-C12-C13
19	A	503	9YF	C27-C28-C29-C30
12	F	602	CDL	C11-C12-C13-C14
20	C	301	HEC	C3D-CAD-CBD-CGD
12	N	603	CDL	C72-C73-C74-C75
12	B	604	CDL	CB5-C51-C52-C53
12	N	605	CDL	C13-C14-C15-C16
12	N	606	CDL	C31-C32-C33-C34
12	M	502	CDL	C71-C72-C73-C74
12	N	607	CDL	C72-C73-C74-C75
14	R	606	HEA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	R	602	CDL	C80-C81-C82-C83
12	C	306	CDL	OB7-CB5-OB6-CB4
12	N	605	CDL	C71-CB7-OB8-CB6
12	N	607	CDL	C71-CB7-OB8-CB6
12	F	602	CDL	C78-C79-C80-C81
15	G	301	9Y0	C27-C28-C29-C30
12	C	303	CDL	C71-C72-C73-C74
12	F	601	CDL	C60-C61-C62-C63
12	P	201	CDL	C76-C77-C78-C79
12	C	306	CDL	C52-C53-C54-C55
12	B	606	CDL	CB5-C51-C52-C53
12	C	306	CDL	CB5-C51-C52-C53
12	R	602	CDL	C63-C64-C65-C66
12	N	603	CDL	C57-C58-C59-C60
12	C	306	CDL	C21-C22-C23-C24
12	C	306	CDL	C78-C79-C80-C81
17	N	609	MQ9	C7-C8-C9-C10
12	N	606	CDL	C57-C58-C59-C60
12	C	306	CDL	C13-C14-C15-C16
19	A	503	9YF	C26-C27-C28-C29
12	P	201	CDL	C71-C72-C73-C74
20	O	303	HEC	C2B-C3B-CAB-CBB
12	C	306	CDL	C51-CB5-OB6-CB4
15	G	301	9Y0	C22-C21-O7-C1
15	S	301	9Y0	O7-C1-C2-O3
12	N	606	CDL	C75-C76-C77-C78
12	M	502	CDL	C63-C64-C65-C66
16	B	603	HEM	C4B-C3B-CAB-CBB
12	N	607	CDL	C53-C54-C55-C56
12	B	605	CDL	C13-C14-C15-C16
15	S	301	9Y0	C29-C30-C31-C32
15	G	301	9Y0	O6-C21-O7-C1
19	M	503	9YF	C11-C10-C9-C8
12	M	502	CDL	C81-C82-C83-C84
12	N	607	CDL	OB6-CB4-CB6-OB8
12	B	604	CDL	OB6-CB4-CB6-OB8
12	D	201	CDL	C21-C22-C23-C24
17	O	301	MQ9	C15-C14-C16-C17
17	C	305	MQ9	C25-C24-C26-C27
17	C	305	MQ9	C12-C11-C9-C8
12	B	604	CDL	C73-C74-C75-C76
15	G	301	9Y0	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	F	607	HEA	C21-C22-C23-C25
12	R	601	CDL	C59-C60-C61-C62
12	B	606	CDL	C59-C60-C61-C62
12	C	306	CDL	C23-C24-C25-C26
12	P	201	CDL	C38-C39-C40-C41
12	N	603	CDL	C32-C33-C34-C35
12	N	605	CDL	C12-C13-C14-C15
12	B	607	CDL	C54-C55-C56-C57
12	B	605	CDL	C51-CB5-OB6-CB4
12	F	602	CDL	C72-C73-C74-C75
12	D	201	CDL	C83-C84-C85-C86
12	P	201	CDL	C83-C84-C85-C86
12	N	605	CDL	C74-C75-C76-C77
12	C	303	CDL	C78-C79-C80-C81
12	P	201	CDL	CB3-OB5-PB2-OB2
12	N	603	CDL	CB3-OB5-PB2-OB2
12	N	605	CDL	CA3-OA5-PA1-OA2
12	N	606	CDL	CA3-OA5-PA1-OA2
12	N	607	CDL	CA2-OA2-PA1-OA5
12	C	303	CDL	CA2-OA2-PA1-OA5
12	C	303	CDL	CA3-OA5-PA1-OA2
15	G	301	9Y0	C2-O3-P-O1
12	P	201	CDL	C32-C33-C34-C35
17	N	610	MQ9	C32-C33-C34-C36
12	R	601	CDL	OB5-CB3-CB4-CB6
12	R	602	CDL	OB5-CB3-CB4-CB6
12	N	603	CDL	OA5-CA3-CA4-CA6
12	C	303	CDL	OA5-CA3-CA4-CA6
12	N	605	CDL	C19-C20-C21-C22
12	B	606	CDL	C72-C73-C74-C75
12	N	607	CDL	C19-C20-C21-C22
12	C	306	CDL	C37-C38-C39-C40
12	N	605	CDL	C14-C15-C16-C17
12	N	605	CDL	C57-C58-C59-C60
12	F	602	CDL	C80-C81-C82-C83
12	P	201	CDL	C73-C74-C75-C76
12	C	306	CDL	C14-C15-C16-C17
12	B	607	CDL	C75-C76-C77-C78
12	N	605	CDL	C17-C18-C19-C20
12	M	502	CDL	C34-C35-C36-C37
12	R	601	CDL	C74-C75-C76-C77
12	R	602	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	S	301	9Y0	C9-C10-C11-C12
12	B	605	CDL	C77-C78-C79-C80
12	F	602	CDL	CA3-CA4-CA6-OA8
12	F	602	CDL	CB3-CB4-CB6-OB8
12	F	602	CDL	C64-C65-C66-C67
12	R	602	CDL	CA3-CA4-CA6-OA8
12	P	201	CDL	CB3-CB4-CB6-OB8
12	N	603	CDL	CA3-CA4-CA6-OA8
12	N	603	CDL	CB3-CB4-CB6-OB8
12	N	605	CDL	C77-C78-C79-C80
12	B	604	CDL	C57-C58-C59-C60
12	B	605	CDL	CA3-CA4-CA6-OA8
12	B	606	CDL	C16-C17-C18-C19
12	C	306	CDL	C31-C32-C33-C34
15	G	301	9Y0	O5-C-C1-C2
19	M	504	9YF	C1-C-C24-O11
12	C	303	CDL	C81-C82-C83-C84
12	N	607	CDL	OB9-CB7-OB8-CB6
17	N	609	MQ9	C5-C6-C7-C8
17	B	608	MQ9	C5-C6-C7-C8
12	N	605	CDL	C59-C60-C61-C62
12	B	605	CDL	C52-C53-C54-C55
12	B	605	CDL	C59-C60-C61-C62
12	M	502	CDL	C84-C85-C86-C87
12	B	605	CDL	C76-C77-C78-C79
12	C	306	CDL	C24-C25-C26-C27
12	N	605	CDL	OB9-CB7-OB8-CB6
12	N	607	CDL	C56-C57-C58-C59
15	G	301	9Y0	C33-C34-C35-C36
17	O	301	MQ9	C34-C36-C37-C38
17	B	609	MQ9	C9-C11-C12-C13
12	N	603	CDL	C31-C32-C33-C34
19	A	503	9YF	C30-C31-C32-C33
12	P	201	CDL	C20-C21-C22-C23
12	N	605	CDL	C80-C81-C82-C83
12	M	502	CDL	C52-C53-C54-C55
12	R	601	CDL	C52-C53-C54-C55
12	R	601	CDL	C78-C79-C80-C81
12	B	604	CDL	C32-C33-C34-C35
12	C	306	CDL	C79-C80-C81-C82
12	B	607	CDL	C74-C75-C76-C77
17	N	611	MQ9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
17	O	301	MQ9	C35-C34-C36-C37
17	C	305	MQ9	C15-C14-C16-C17
12	R	602	CDL	C71-C72-C73-C74
12	R	601	CDL	CB5-C51-C52-C53
12	R	601	CDL	C31-CA7-OA8-CA6
12	R	602	CDL	C64-C65-C66-C67
12	M	502	CDL	C23-C24-C25-C26
17	N	609	MQ9	C1-C6-C7-C8
17	B	608	MQ9	C1-C6-C7-C8
12	B	605	CDL	C32-C33-C34-C35
12	B	607	CDL	C79-C80-C81-C82
12	C	303	CDL	C84-C85-C86-C87
12	P	201	CDL	CB6-CB4-OB6-CB5
12	B	606	CDL	CA6-CA4-OA6-CA5
12	M	502	CDL	C55-C56-C57-C58
12	M	502	CDL	C72-C73-C74-C75
12	R	601	CDL	C34-C35-C36-C37
12	B	604	CDL	C51-C52-C53-C54
12	B	606	CDL	C14-C15-C16-C17
12	F	601	CDL	OB5-CB3-CB4-OB6
12	N	607	CDL	OB5-CB3-CB4-OB6
12	C	303	CDL	C77-C78-C79-C80
12	C	306	CDL	C80-C81-C82-C83
19	M	503	9YF	C9-C10-C11-C12
12	D	201	CDL	C39-C40-C41-C42
12	C	303	CDL	C75-C76-C77-C78
12	B	605	CDL	C80-C81-C82-C83
15	S	301	9Y0	C33-C34-C35-C36
15	S	301	9Y0	C6-C7-C8-C9
19	A	502	9YF	O9-C-C24-O11
12	B	604	CDL	C12-C13-C14-C15
12	C	306	CDL	C38-C39-C40-C41
17	N	611	MQ9	C7-C8-C9-C10
17	C	304	MQ9	C20-C19-C21-C22
19	A	502	9YF	C32-C33-C35-C36
12	R	602	CDL	C61-C62-C63-C64
12	N	607	CDL	C58-C59-C60-C61
12	C	306	CDL	C39-C40-C41-C42
17	N	608	MQ9	C47-C48-C49-C51
12	D	201	CDL	C24-C25-C26-C27
12	C	306	CDL	C64-C65-C66-C67
12	N	606	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
12	M	502	CDL	C64-C65-C66-C67
12	B	607	CDL	C19-C20-C21-C22
12	D	201	CDL	OB5-CB3-CB4-CB6
12	P	201	CDL	OA5-CA3-CA4-CA6
12	N	603	CDL	OB5-CB3-CB4-CB6
12	N	605	CDL	OA5-CA3-CA4-CA6
15	S	301	9Y0	C-C1-C2-O3
17	N	609	MQ9	C9-C11-C12-C13
19	A	503	9YF	C11-C12-C13-C14
12	F	601	CDL	C32-C33-C34-C35
12	M	502	CDL	C22-C23-C24-C25
17	N	609	MQ9	C40-C39-C41-C42
14	R	606	HEA	C21-C22-C23-C24
12	C	306	CDL	CA5-C11-C12-C13
12	B	606	CDL	C39-C40-C41-C42
19	A	503	9YF	C28-C29-C30-C31
12	B	605	CDL	OB7-CB5-OB6-CB4
17	N	609	MQ9	C41-C42-C43-C44
17	C	304	MQ9	C26-C27-C28-C29
17	C	304	MQ9	C31-C32-C33-C34
15	G	301	9Y0	C5-C6-C7-C8
12	N	603	CDL	C52-C53-C54-C55
12	B	607	CDL	C78-C79-C80-C81
12	R	601	CDL	C13-C14-C15-C16
12	N	606	CDL	C76-C77-C78-C79
12	C	306	CDL	C34-C35-C36-C37
13	F	603	PLM	C5-C6-C7-C8
12	D	201	CDL	C31-C32-C33-C34
12	R	601	CDL	C14-C15-C16-C17
12	M	502	CDL	C31-CA7-OA8-CA6
19	M	503	9YF	C14-C15-C16-C17
12	F	601	CDL	CB3-CB4-CB6-OB8
12	P	201	CDL	CA3-CA4-CA6-OA8
12	N	605	CDL	CB3-CB4-CB6-OB8
12	N	606	CDL	CA3-CA4-CA6-OA8
12	M	502	CDL	CA3-CA4-CA6-OA8
12	M	502	CDL	CB3-CB4-CB6-OB8
12	B	604	CDL	CB3-CB4-CB6-OB8
12	B	606	CDL	CB3-CB4-CB6-OB8
12	B	607	CDL	CB3-CB4-CB6-OB8
12	C	306	CDL	CA3-CA4-CA6-OA8
19	M	503	9YF	C1-C-C24-O11

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Mol	Chain	Res	Type	Atoms
19	A	502	9YF	C1-C-C24-O11
12	R	602	CDL	C55-C56-C57-C58
19	M	504	9YF	C2-O2-P-O8
19	A	502	9YF	C2-O2-P-O8
12	N	607	CDL	C57-C58-C59-C60
17	B	609	MQ9	C20-C19-C21-C22
17	B	609	MQ9	C23-C24-C26-C27
12	F	602	CDL	C84-C85-C86-C87
12	D	201	CDL	C33-C34-C35-C36
15	G	301	9Y0	C9-C10-C11-C12
19	M	504	9YF	C13-C14-C15-C16
12	N	603	CDL	CB2-OB2-PB2-OB5
12	R	601	CDL	OA9-CA7-OA8-CA6
12	D	201	CDL	C13-C14-C15-C16
12	C	303	CDL	C14-C15-C16-C17
12	P	201	CDL	C35-C36-C37-C38
12	C	303	CDL	C36-C37-C38-C39
12	C	303	CDL	C54-C55-C56-C57
12	N	603	CDL	OA5-CA3-CA4-OA6
12	N	605	CDL	OA5-CA3-CA4-OA6
12	N	606	CDL	C59-C60-C61-C62
12	M	502	CDL	C51-C52-C53-C54
19	M	504	9YF	C28-C29-C30-C31
19	A	502	9YF	C38-C39-C40-C41
12	F	601	CDL	OB6-CB4-CB6-OB8
12	R	601	CDL	OB6-CB4-CB6-OB8
12	N	603	CDL	OB6-CB4-CB6-OB8
12	B	605	CDL	OA6-CA4-CA6-OA8
15	G	301	9Y0	O5-C-C1-O7
19	M	503	9YF	O9-C-C24-O11
15	S	301	9Y0	C24-C25-C26-C27
12	C	306	CDL	C11-C12-C13-C14
17	C	304	MQ9	C15-C14-C16-C17
12	F	601	CDL	C14-C15-C16-C17
12	F	601	CDL	C71-C72-C73-C74
12	M	502	CDL	C78-C79-C80-C81
12	F	602	CDL	C74-C75-C76-C77
12	C	306	CDL	C73-C74-C75-C76
12	P	201	CDL	C1-CA2-OA2-PA1
12	B	604	CDL	C1-CA2-OA2-PA1
12	B	607	CDL	C14-C15-C16-C17
13	R	603	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	D	201	CDL	C84-C85-C86-C87
15	G	301	9Y0	C13-C14-C15-C16
15	S	301	9Y0	C13-C14-C15-C16
12	D	201	CDL	OA5-CA3-CA4-CA6
12	R	602	CDL	OA5-CA3-CA4-CA6
12	N	605	CDL	OB5-CB3-CB4-CB6
12	C	303	CDL	OB5-CB3-CB4-CB6
12	C	306	CDL	C72-C71-CB7-OB8
12	F	602	CDL	CB5-C51-C52-C53
15	G	301	9Y0	C32-C33-C34-C35
12	M	502	CDL	C38-C39-C40-C41
12	B	604	CDL	C52-C53-C54-C55
12	B	604	CDL	C74-C75-C76-C77
12	M	502	CDL	CB6-CB4-OB6-CB5
19	A	502	9YF	C24-C-O9-C8
17	N	608	MQ9	C37-C38-C39-C40
12	R	602	CDL	C84-C85-C86-C87
12	B	606	CDL	C52-C53-C54-C55
17	N	608	MQ9	C33-C34-C36-C37
17	B	609	MQ9	C13-C14-C16-C17
12	R	601	CDL	CB3-CB4-CB6-OB8
12	N	606	CDL	CB3-CB4-CB6-OB8
12	B	604	CDL	CB4-CB3-OB5-PB2
12	B	605	CDL	CB3-CB4-CB6-OB8
12	C	306	CDL	C1-CB2-OB2-PB2
12	M	502	CDL	OA9-CA7-OA8-CA6
12	F	601	CDL	OA5-CA3-CA4-OA6
12	D	201	CDL	OA5-CA3-CA4-OA6
12	R	602	CDL	OA5-CA3-CA4-OA6
12	P	201	CDL	OA5-CA3-CA4-OA6
12	N	603	CDL	OB5-CB3-CB4-OB6
12	N	605	CDL	OB5-CB3-CB4-OB6
12	B	606	CDL	OA5-CA3-CA4-OA6
12	B	607	CDL	OB5-CB3-CB4-OB6
16	N	602	HEM	C4B-C3B-CAB-CBB
12	N	606	CDL	C33-C34-C35-C36
15	S	301	9Y0	C7-C8-C9-C10
12	R	602	CDL	C51-C52-C53-C54
12	N	607	CDL	C51-C52-C53-C54
12	R	602	CDL	OA6-CA4-CA6-OA8
12	P	201	CDL	OA6-CA4-CA6-OA8
12	N	606	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
12	B	604	CDL	OA6-CA4-CA6-OA8
12	B	606	CDL	OB6-CB4-CB6-OB8
12	C	306	CDL	OA6-CA4-CA6-OA8
12	N	605	CDL	C53-C54-C55-C56
12	C	303	CDL	C56-C57-C58-C59
17	O	301	MQ9	C26-C27-C28-C29
12	R	602	CDL	C81-C82-C83-C84
12	P	201	CDL	C24-C25-C26-C27
12	N	603	CDL	C53-C54-C55-C56
12	B	604	CDL	C33-C34-C35-C36
12	N	605	CDL	C72-C73-C74-C75
20	O	303	HEC	C4D-C3D-CAD-CBD
12	N	606	CDL	C32-C33-C34-C35
12	B	607	CDL	CB5-C51-C52-C53
12	D	201	CDL	C82-C83-C84-C85
17	N	609	MQ9	C32-C33-C34-C36
12	R	601	CDL	CB2-OB2-PB2-OB5
12	B	607	CDL	CB2-OB2-PB2-OB5
12	N	605	CDL	C31-C32-C33-C34
12	N	607	CDL	C55-C56-C57-C58
12	C	303	CDL	CA7-C31-C32-C33
19	A	502	9YF	C39-C40-C41-C42
14	R	606	HEA	C27-C19-C20-C21
12	N	605	CDL	C1-CB2-OB2-PB2
12	D	201	CDL	C71-C72-C73-C74
12	R	602	CDL	CA2-OA2-PA1-OA4
12	P	201	CDL	CB3-OB5-PB2-OB4
12	N	603	CDL	CA2-OA2-PA1-OA4
12	N	603	CDL	CA3-OA5-PA1-OA3
12	N	603	CDL	CA3-OA5-PA1-OA4
12	N	603	CDL	CB2-OB2-PB2-OB3
12	N	603	CDL	CB3-OB5-PB2-OB4
12	N	605	CDL	CA3-OA5-PA1-OA3
12	N	606	CDL	CA3-OA5-PA1-OA4
12	N	606	CDL	CB3-OB5-PB2-OB4
12	N	607	CDL	CA2-OA2-PA1-OA4
12	N	607	CDL	CB3-OB5-PB2-OB4
12	M	502	CDL	CA3-OA5-PA1-OA4
12	M	502	CDL	CB2-OB2-PB2-OB4
12	B	604	CDL	CA3-OA5-PA1-OA3
12	B	604	CDL	CB3-OB5-PB2-OB3
12	B	607	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
12	B	607	CDL	CA3-OA5-PA1-OA4
12	B	607	CDL	CB2-OB2-PB2-OB4
12	C	303	CDL	CA2-OA2-PA1-OA3
12	C	303	CDL	CA3-OA5-PA1-OA4
15	G	301	9Y0	C2-O3-P-O2
19	M	504	9YF	C1-O-P-O1
12	M	502	CDL	CA7-C31-C32-C33
12	N	606	CDL	C34-C35-C36-C37
12	F	601	CDL	OB5-CB3-CB4-CB6
12	N	607	CDL	OB5-CB3-CB4-CB6
12	B	607	CDL	OB5-CB3-CB4-CB6
15	S	301	9Y0	C28-C29-C30-C31
12	R	602	CDL	C62-C63-C64-C65
12	R	602	CDL	C78-C79-C80-C81
12	N	603	CDL	C58-C59-C60-C61
12	B	606	CDL	C76-C77-C78-C79
14	F	606	HEA	C3B-C11-C12-C13
12	N	607	CDL	C31-C32-C33-C34
12	F	601	CDL	C74-C75-C76-C77
19	M	503	9YF	C26-C27-C28-C29
12	P	201	CDL	C57-C58-C59-C60
12	C	306	CDL	C16-C17-C18-C19
12	M	502	CDL	CB5-C51-C52-C53
19	M	503	9YF	C25-C26-C27-C28
12	M	502	CDL	C13-C14-C15-C16
12	D	201	CDL	C77-C78-C79-C80
12	D	201	CDL	C57-C58-C59-C60
19	A	503	9YF	C14-C15-C16-C17
12	P	201	CDL	C12-C13-C14-C15
12	P	201	CDL	C34-C35-C36-C37
13	F	603	PLM	C1-C2-C3-C4
15	S	301	9Y0	O5-C-C1-C2
12	F	602	CDL	OA6-CA4-CA6-OA8
12	F	602	CDL	OB6-CB4-CB6-OB8
12	N	605	CDL	OB6-CB4-CB6-OB8
12	M	502	CDL	OA6-CA4-CA6-OA8
12	B	605	CDL	OB6-CB4-CB6-OB8
12	B	607	CDL	OB6-CB4-CB6-OB8
12	R	601	CDL	C72-C73-C74-C75
12	R	601	CDL	C39-C40-C41-C42
19	M	504	9YF	C-C1-O-P
12	M	502	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	B	608	MQ9	C15-C14-C16-C17
19	A	502	9YF	C13-C14-C15-C16
19	A	502	9YF	C31-C32-C33-C34
12	N	605	CDL	C32-C33-C34-C35
12	C	303	CDL	C34-C35-C36-C37
12	B	605	CDL	C11-C12-C13-C14
12	B	607	CDL	C18-C19-C20-C21
12	B	607	CDL	C56-C57-C58-C59
20	O	303	HEC	C2D-C3D-CAD-CBD
17	O	301	MQ9	C24-C26-C27-C28
12	F	602	CDL	C55-C56-C57-C58
12	R	602	CDL	C72-C73-C74-C75
12	C	306	CDL	C55-C56-C57-C58
12	N	603	CDL	C74-C75-C76-C77
12	B	605	CDL	C19-C20-C21-C22
12	D	201	CDL	C52-C51-CB5-OB6
12	B	607	CDL	CB7-C71-C72-C73
12	B	607	CDL	C73-C74-C75-C76
12	D	201	CDL	C34-C35-C36-C37
12	C	306	CDL	C57-C58-C59-C60
12	N	607	CDL	C12-C13-C14-C15
12	N	607	CDL	CA6-CA4-OA6-CA5
12	B	607	CDL	CA6-CA4-OA6-CA5
19	M	504	9YF	C24-C-O9-C8
12	B	606	CDL	OA5-CA3-CA4-CA6
19	M	503	9YF	C30-C31-C32-C33
14	F	607	HEA	C11-C12-C13-C14
14	R	606	HEA	C11-C12-C13-C14
12	B	604	CDL	C35-C36-C37-C38
12	P	201	CDL	C32-C31-CA7-OA8
12	M	502	CDL	C1-CA2-OA2-PA1
12	D	201	CDL	OB5-CB3-CB4-OB6
12	B	604	CDL	OA5-CA3-CA4-OA6
17	N	610	MQ9	C30-C29-C31-C32
12	B	607	CDL	C15-C16-C17-C18
12	M	502	CDL	C19-C20-C21-C22
12	N	603	CDL	C84-C85-C86-C87
12	B	605	CDL	C15-C16-C17-C18
12	P	201	CDL	OB6-CB4-CB6-OB8
19	M	504	9YF	O9-C-C24-O11
12	D	201	CDL	CA2-OA2-PA1-OA5
12	P	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
12	N	607	CDL	CB3-OB5-PB2-OB2
12	B	604	CDL	CA2-OA2-PA1-OA5
12	B	606	CDL	CB3-OB5-PB2-OB2
12	N	605	CDL	C78-C79-C80-C81
12	D	201	CDL	C18-C19-C20-C21
12	N	607	CDL	C52-C53-C54-C55
12	M	502	CDL	C11-C12-C13-C14
13	F	603	PLM	C3-C4-C5-C6
17	C	305	MQ9	C33-C34-C36-C37
12	B	606	CDL	C75-C76-C77-C78
13	N	604	PLM	C3-C4-C5-C6
12	N	607	CDL	C78-C79-C80-C81
12	N	603	CDL	OB9-CB7-OB8-CB6
12	C	306	CDL	C71-CB7-OB8-CB6
12	B	605	CDL	CA4-CA3-OA5-PA1
12	F	601	CDL	C39-C40-C41-C42
17	O	302	MQ9	C11-C12-C13-C14
12	B	607	CDL	CA7-C31-C32-C33
14	F	606	HEA	C14-C15-C16-C17
12	N	603	CDL	C71-CB7-OB8-CB6
12	D	201	CDL	C12-C13-C14-C15
12	N	606	CDL	C38-C39-C40-C41
12	P	201	CDL	C54-C55-C56-C57
12	F	601	CDL	OA5-CA3-CA4-CA6
19	A	502	9YF	C26-C27-C28-C29
16	B	602	HEM	CAA-CBA-CGA-O1A
12	R	601	CDL	OA5-CA3-CA4-OA6
12	B	606	CDL	OB5-CB3-CB4-OB6
12	F	601	CDL	C75-C76-C77-C78
12	C	306	CDL	C82-C83-C84-C85
12	C	306	CDL	OB9-CB7-OB8-CB6
16	N	601	HEM	CAA-CBA-CGA-O1A
12	B	604	CDL	OB7-CB5-OB6-CB4
12	N	603	CDL	C80-C81-C82-C83
12	B	607	CDL	C71-C72-C73-C74
12	C	303	CDL	C58-C59-C60-C61
12	M	502	CDL	C35-C36-C37-C38
12	M	502	CDL	C82-C83-C84-C85
12	C	303	CDL	OB6-CB4-CB6-OB8
12	C	306	CDL	OB6-CB4-CB6-OB8
12	M	502	CDL	C1-CB2-OB2-PB2
12	R	601	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
12	N	607	CDL	C11-C12-C13-C14
12	N	607	CDL	C18-C19-C20-C21
12	M	502	CDL	C24-C25-C26-C27
12	B	607	CDL	C58-C59-C60-C61
12	D	201	CDL	C75-C76-C77-C78
14	F	606	HEA	CAA-CBA-CGA-O1A
16	N	602	HEM	CAA-CBA-CGA-O2A
12	B	607	CDL	C53-C54-C55-C56
12	D	201	CDL	C11-C12-C13-C14
12	M	502	CDL	CA2-C1-CB2-OB2
12	N	603	CDL	C36-C37-C38-C39
20	O	303	HEC	C4B-C3B-CAB-CBB
19	A	502	9YF	C2-O2-P-O1
14	R	605	HEA	CAA-CBA-CGA-O1A
12	B	607	CDL	CB6-CB4-OB6-CB5
14	F	607	HEA	CAA-CBA-CGA-O2A
12	C	306	CDL	C61-C62-C63-C64
12	N	603	CDL	CA2-OA2-PA1-OA5
14	F	607	HEA	CAA-CBA-CGA-O1A
14	R	606	HEA	CAA-CBA-CGA-O1A
12	R	601	CDL	C36-C37-C38-C39
12	N	603	CDL	C33-C34-C35-C36
12	P	201	CDL	C74-C75-C76-C77
15	S	301	9Y0	C31-C32-C33-C34
12	B	604	CDL	OA5-CA3-CA4-CA6
14	R	606	HEA	CAA-CBA-CGA-O2A
17	N	611	MQ9	C25-C24-C26-C27
14	R	606	HEA	C3D-CAD-CBD-CGD
16	N	601	HEM	CAA-CBA-CGA-O2A
12	B	606	CDL	C73-C74-C75-C76
12	C	306	CDL	C19-C20-C21-C22
12	C	306	CDL	C62-C63-C64-C65
12	F	601	CDL	C78-C79-C80-C81
16	B	602	HEM	CAA-CBA-CGA-O2A
14	F	606	HEA	C19-C20-C21-C22
17	N	609	MQ9	C14-C16-C17-C18
14	F	606	HEA	CAA-CBA-CGA-O2A
14	R	605	HEA	CAA-CBA-CGA-O2A
16	N	602	HEM	CAA-CBA-CGA-O1A
17	O	302	MQ9	C12-C11-C9-C10
13	F	603	PLM	CC-CD-CE-CF
17	O	302	MQ9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
12	F	601	CDL	C52-C51-CB5-OB6
12	N	607	CDL	O1-C1-CB2-OB2
12	C	306	CDL	CB3-CB4-CB6-OB8
12	P	201	CDL	CA7-C31-C32-C33
12	C	303	CDL	C35-C36-C37-C38
12	F	602	CDL	OB5-CB3-CB4-OB6
12	C	303	CDL	OB5-CB3-CB4-OB6
12	N	607	CDL	C17-C18-C19-C20
13	R	603	PLM	CA-CB-CC-CD
19	A	502	9YF	C25-C26-C27-C28
12	R	601	CDL	OA5-CA3-CA4-CA6
17	N	608	MQ9	C15-C14-C16-C17
17	N	609	MQ9	C45-C44-C46-C47
12	N	605	CDL	O1-C1-CA2-OA2
17	N	610	MQ9	C9-C11-C12-C13
12	D	201	CDL	C14-C15-C16-C17
17	N	611	MQ9	C13-C14-C16-C17
16	B	603	HEM	CAA-CBA-CGA-O2A
15	G	301	9Y0	C7-C8-C9-C10
12	N	607	CDL	C79-C80-C81-C82
12	B	604	CDL	C52-C51-CB5-OB6
17	C	304	MQ9	C30-C29-C31-C32
12	B	607	CDL	C34-C35-C36-C37
12	C	303	CDL	CB2-OB2-PB2-OB5
14	R	606	HEA	C18-C19-C20-C21
12	R	602	CDL	C72-C71-CB7-OB8
12	F	602	CDL	C53-C54-C55-C56
12	R	602	CDL	O1-C1-CA2-OA2
15	S	301	9Y0	C11-C12-C13-C14
19	M	503	9YF	C24-C-O9-C8
12	N	603	CDL	C13-C14-C15-C16
12	M	502	CDL	C73-C74-C75-C76
17	B	608	MQ9	C22-C23-C24-C26
16	B	603	HEM	CAA-CBA-CGA-O1A
12	B	606	CDL	C36-C37-C38-C39
17	N	608	MQ9	C43-C44-C46-C47
12	D	201	CDL	C32-C31-CA7-OA8
17	N	609	MQ9	C24-C26-C27-C28
17	C	305	MQ9	C29-C31-C32-C33
15	G	301	9Y0	C11-C12-C13-C14
12	B	605	CDL	C1-CB2-OB2-PB2
12	C	303	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
12	B	605	CDL	OA5-CA3-CA4-OA6
17	B	608	MQ9	C26-C27-C28-C29
15	G	301	9Y0	C24-C25-C26-C27
12	P	201	CDL	C84-C85-C86-C87
12	C	306	CDL	C76-C77-C78-C79
14	F	607	HEA	CAD-CBD-CGD-O1D
12	R	601	CDL	C54-C55-C56-C57
12	C	306	CDL	C20-C21-C22-C23
12	C	303	CDL	C15-C16-C17-C18
20	C	301	HEC	CAA-CBA-CGA-O2A
12	N	606	CDL	C12-C11-CA5-OA6
19	A	503	9YF	O9-C8-C9-C10
12	C	306	CDL	C33-C34-C35-C36
19	A	502	9YF	C40-C41-C42-C43
12	B	604	CDL	OA7-CA5-OA6-CA4
12	F	602	CDL	C12-C11-CA5-OA6
12	M	502	CDL	CB7-C71-C72-C73
12	M	502	CDL	C52-C51-CB5-OB6
17	N	610	MQ9	C29-C31-C32-C33
14	R	605	HEA	C2C-C3C-CAC-CBC
12	F	602	CDL	C33-C34-C35-C36
12	B	604	CDL	C51-CB5-OB6-CB4
14	R	605	HEA	CAD-CBD-CGD-O2D
20	C	301	HEC	C2B-C3B-CAB-CBB
12	C	306	CDL	C56-C57-C58-C59
13	R	603	PLM	CD-CE-CF-CG
17	B	608	MQ9	C22-C23-C24-C25
12	N	606	CDL	C15-C16-C17-C18
12	R	602	CDL	CB2-C1-CA2-OA2
12	R	602	CDL	CA7-C31-C32-C33
12	D	201	CDL	C32-C31-CA7-OA9
12	B	605	CDL	C51-C52-C53-C54
12	B	607	CDL	C31-C32-C33-C34
17	N	610	MQ9	C23-C24-C26-C27
12	F	602	CDL	CB2-OB2-PB2-OB3
12	D	201	CDL	CB2-OB2-PB2-OB4
12	R	602	CDL	CB3-OB5-PB2-OB3
12	P	201	CDL	CB2-OB2-PB2-OB3
12	N	603	CDL	CB3-OB5-PB2-OB3
12	N	605	CDL	CB3-OB5-PB2-OB3
12	N	606	CDL	CA2-OA2-PA1-OA4
12	B	606	CDL	CA2-OA2-PA1-OA4

Continued on next page...

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Mol	Chain	Res	Type	Atoms
12	B	606	CDL	CB3-OB5-PB2-OB3
12	B	607	CDL	CB2-OB2-PB2-OB3
12	C	303	CDL	CA2-OA2-PA1-OA4
12	C	306	CDL	CA3-OA5-PA1-OA3
19	M	504	9YF	C1-O-P-O8
20	O	303	HEC	C2C-C3C-CAC-CBC
12	R	602	CDL	C72-C71-CB7-OB9
12	M	502	CDL	C52-C51-CB5-OB7
17	N	609	MQ9	C32-C33-C34-C35
20	C	301	HEC	CAA-CBA-CGA-O1A
17	N	610	MQ9	C19-C21-C22-C23
13	F	603	PLM	C4-C5-C6-C7
14	F	606	HEA	O11-C11-C12-C13
12	N	606	CDL	C13-C14-C15-C16
12	B	604	CDL	C53-C54-C55-C56
12	C	306	CDL	C72-C71-CB7-OB9
17	O	302	MQ9	C15-C14-C16-C17
19	A	502	9YF	C11-C12-C13-C14
14	F	606	HEA	CAD-CBD-CGD-O2D
14	R	605	HEA	C3B-C11-C12-C13
15	S	301	9Y0	C4-C3-O1-P
12	F	602	CDL	C12-C11-CA5-OA7
12	N	603	CDL	C81-C82-C83-C84
20	O	304	HEC	C2B-C3B-CAB-CBB
12	B	606	CDL	C52-C51-CB5-OB6
12	N	603	CDL	C35-C36-C37-C38
12	N	606	CDL	C12-C11-CA5-OA7
12	P	201	CDL	CA4-CA3-OA5-PA1
17	O	302	MQ9	C30-C29-C31-C32
17	N	608	MQ9	C32-C33-C34-C36
17	N	608	MQ9	C28-C29-C31-C32
15	S	301	9Y0	O5-C5-C6-C7
12	M	502	CDL	C32-C33-C34-C35
12	B	604	CDL	C72-C73-C74-C75
12	R	601	CDL	C52-C51-CB5-OB6
19	A	503	9YF	O10-C8-C9-C10
17	N	611	MQ9	C29-C31-C32-C33
17	B	608	MQ9	C27-C28-C29-C30
12	N	603	CDL	CA7-C31-C32-C33
12	B	606	CDL	C52-C51-CB5-OB7
20	C	301	HEC	C4B-C3B-CAB-CBB

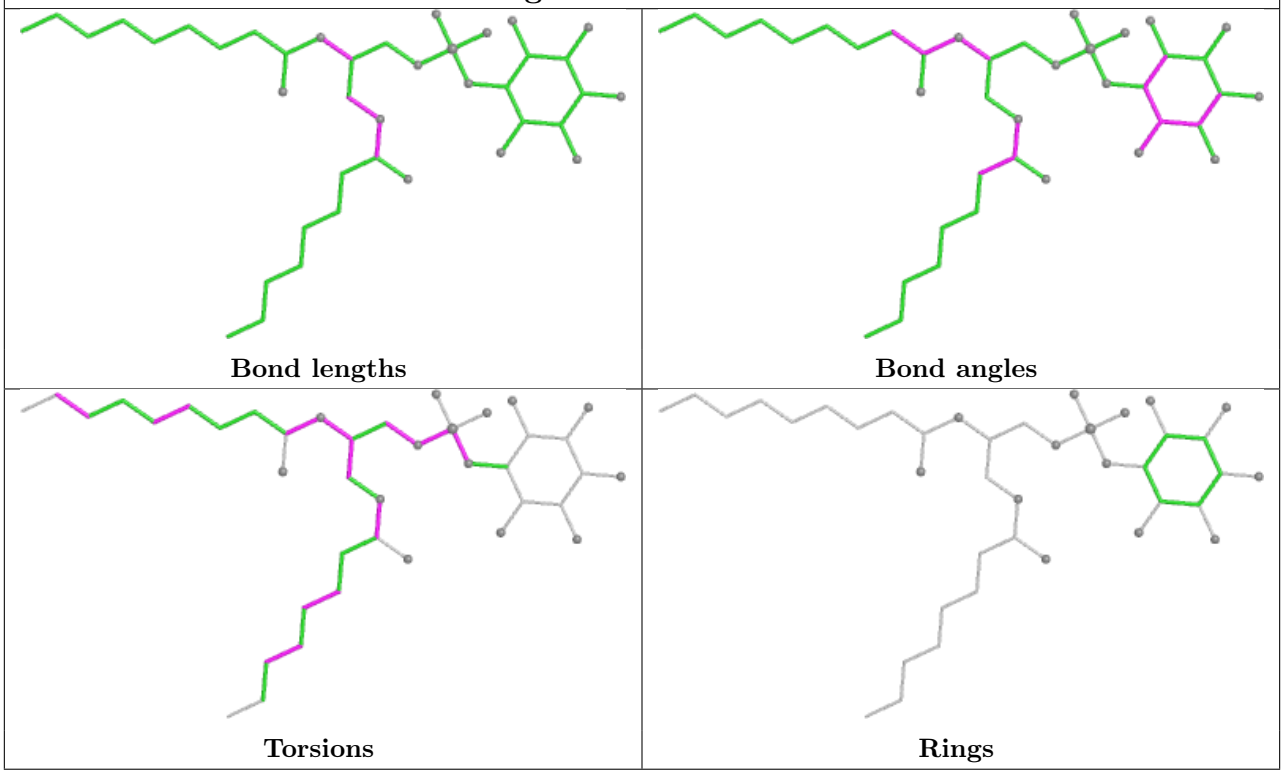
There are no ring outliers.

42 monomers are involved in 153 short contacts:

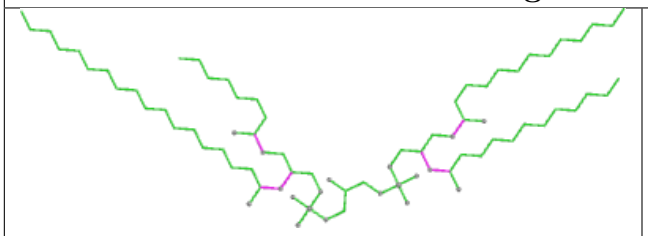
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	504	9YF	4	0
12	N	607	CDL	3	0
17	O	302	MQ9	4	0
12	D	201	CDL	6	0
14	F	606	HEA	5	0
14	R	605	HEA	4	0
12	B	605	CDL	2	0
12	B	604	CDL	3	0
14	R	606	HEA	4	0
12	M	502	CDL	5	0
14	F	607	HEA	7	0
19	M	503	9YF	2	0
12	R	601	CDL	2	0
12	B	606	CDL	5	0
17	C	305	MQ9	7	0
16	B	602	HEM	1	0
12	N	606	CDL	4	0
17	B	609	MQ9	1	0
12	R	602	CDL	4	0
12	F	602	CDL	4	0
16	B	603	HEM	5	0
12	C	303	CDL	5	0
12	F	601	CDL	1	0
12	N	603	CDL	5	0
19	A	503	9YF	5	0
12	P	201	CDL	5	0
12	N	605	CDL	5	0
16	N	602	HEM	4	0
17	N	609	MQ9	5	0
12	C	306	CDL	4	0
17	O	301	MQ9	6	0
17	B	608	MQ9	1	0
18	A	501	FES	2	0
20	C	301	HEC	2	0
17	N	611	MQ9	6	0
16	N	601	HEM	1	0
17	N	610	MQ9	4	0
17	C	304	MQ9	4	0
19	A	502	9YF	3	0
17	N	608	MQ9	3	0
12	B	607	CDL	5	0
20	O	303	HEC	4	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.

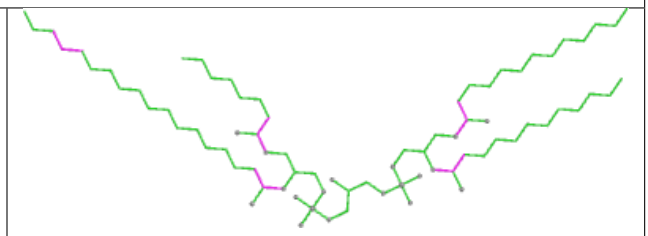
Ligand 9YF M 504



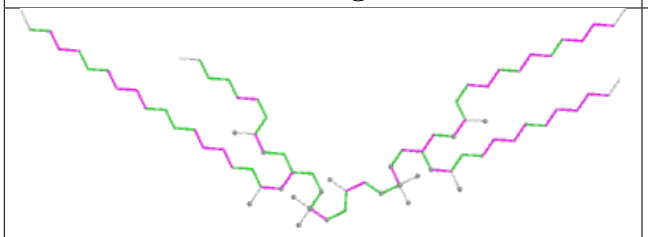
Ligand CDL N 607



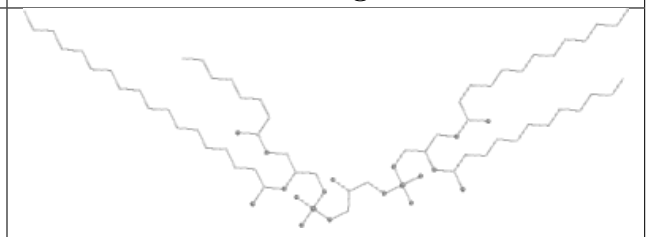
Bond lengths



Bond angles

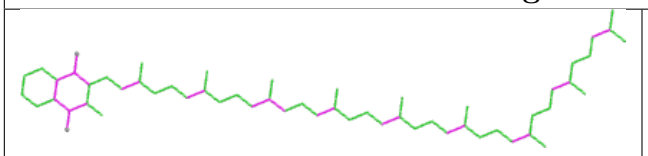


Torsions

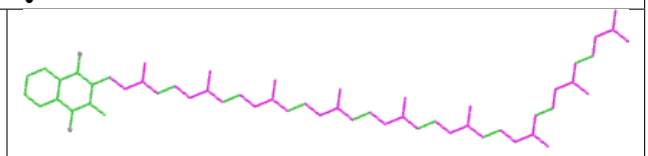


Rings

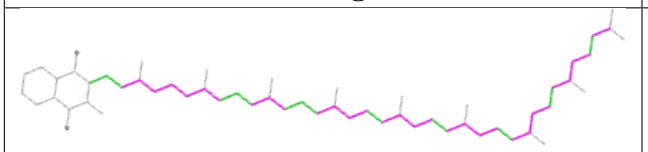
Ligand MQ9 O 302



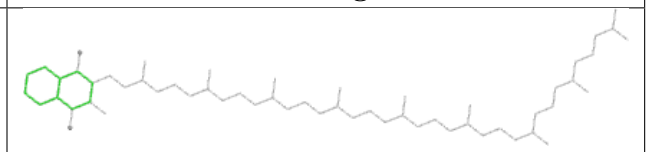
Bond lengths



Bond angles

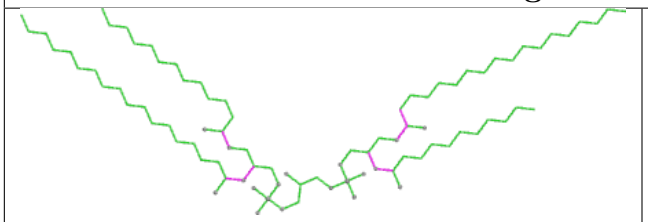


Torsions

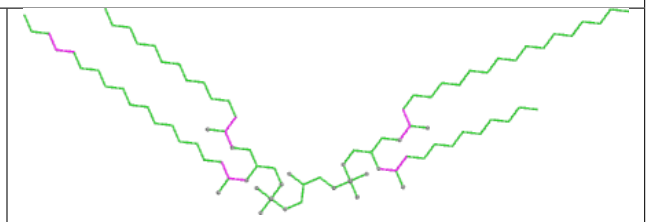


Rings

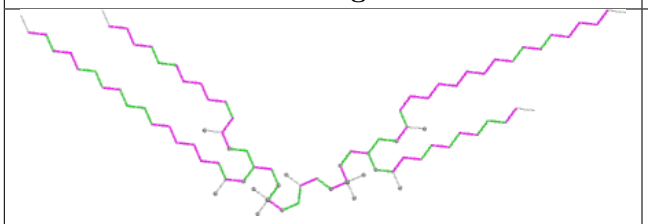
Ligand CDL D 201



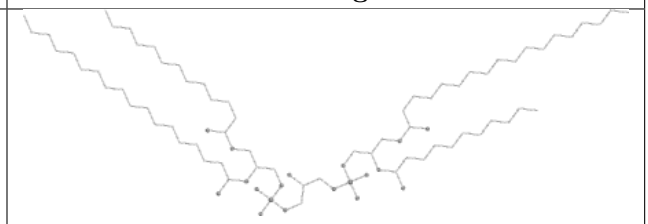
Bond lengths



Bond angles

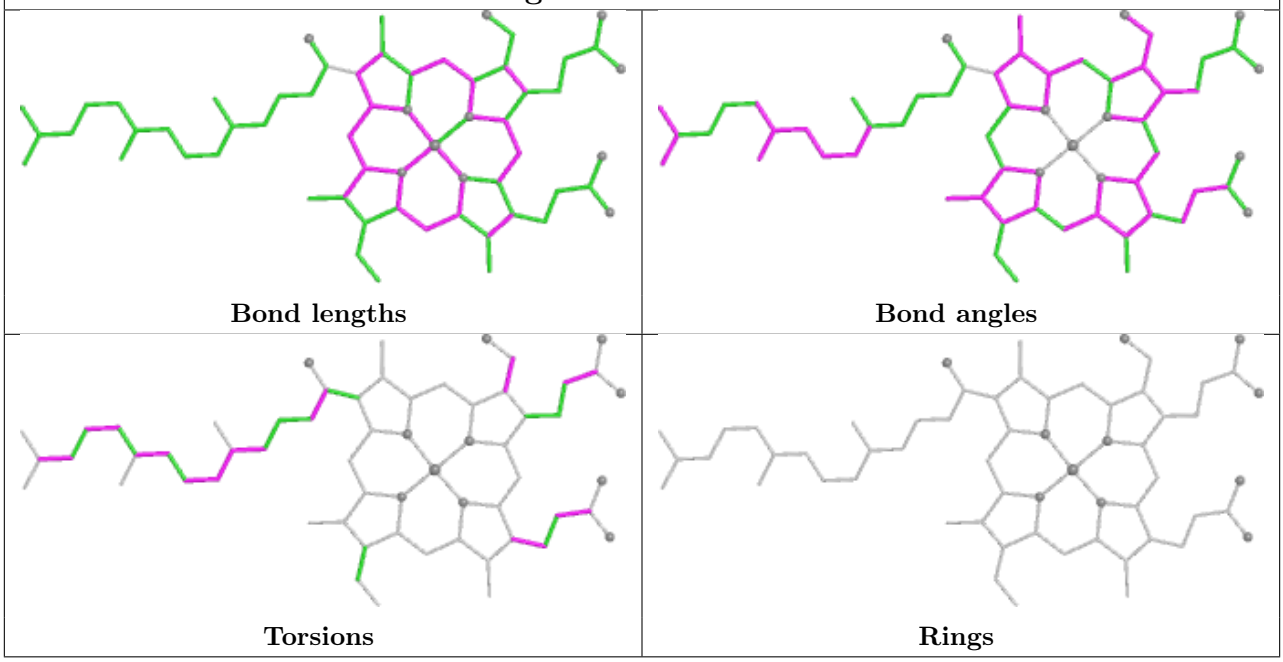


Torsions

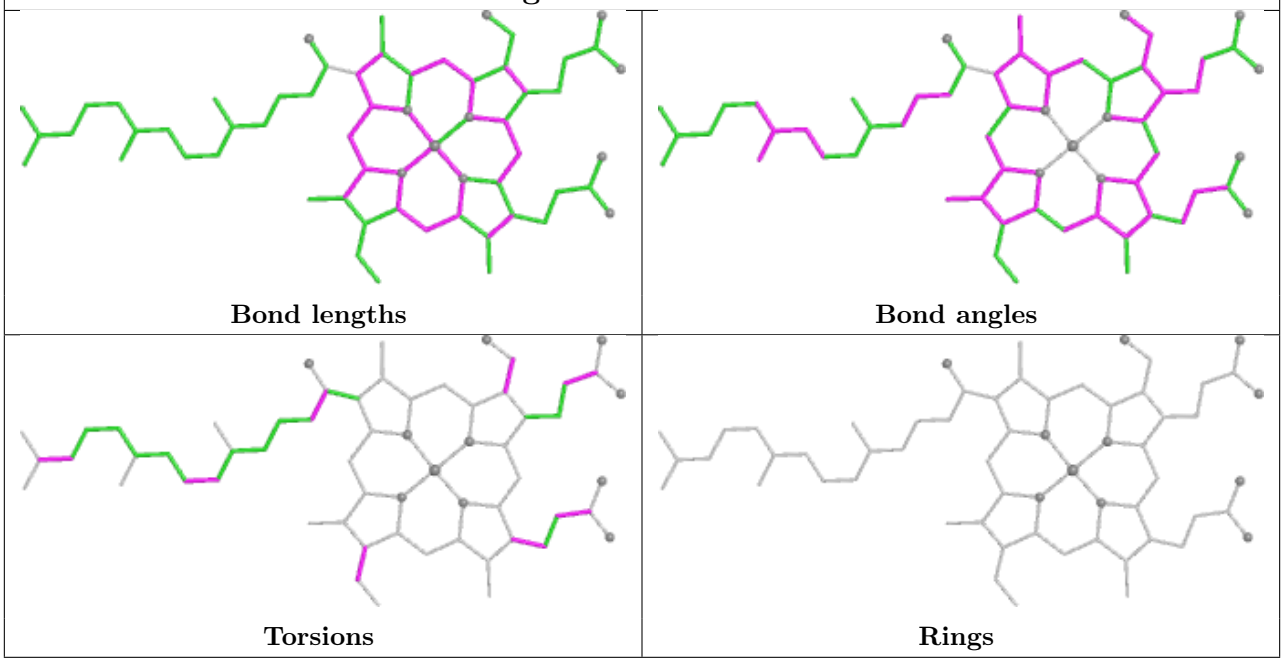


Rings

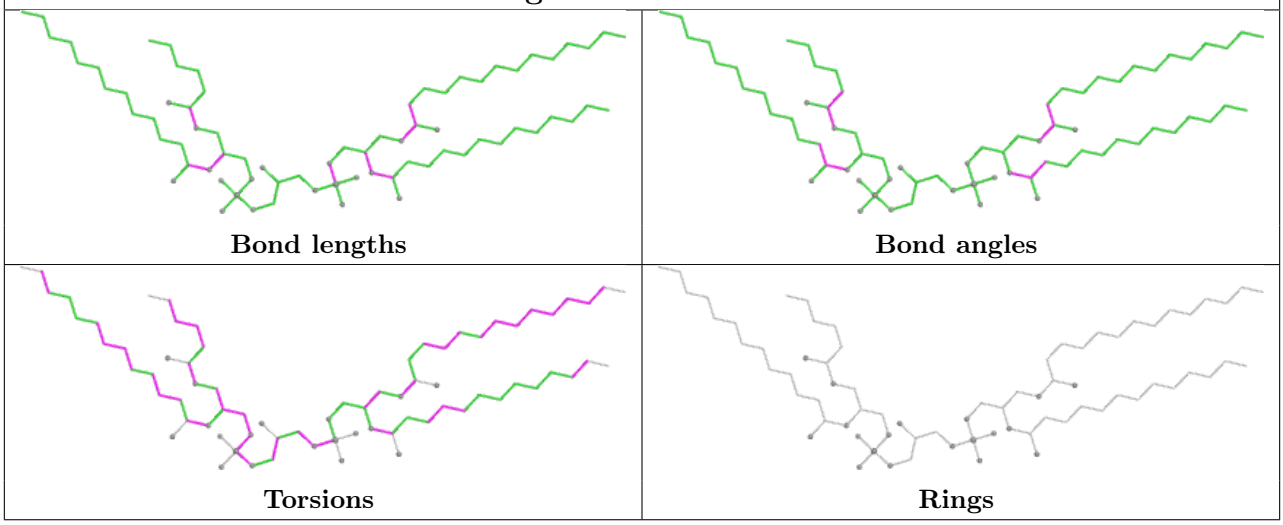
Ligand HEA F 606



Ligand HEA R 605



Ligand CDL B 605



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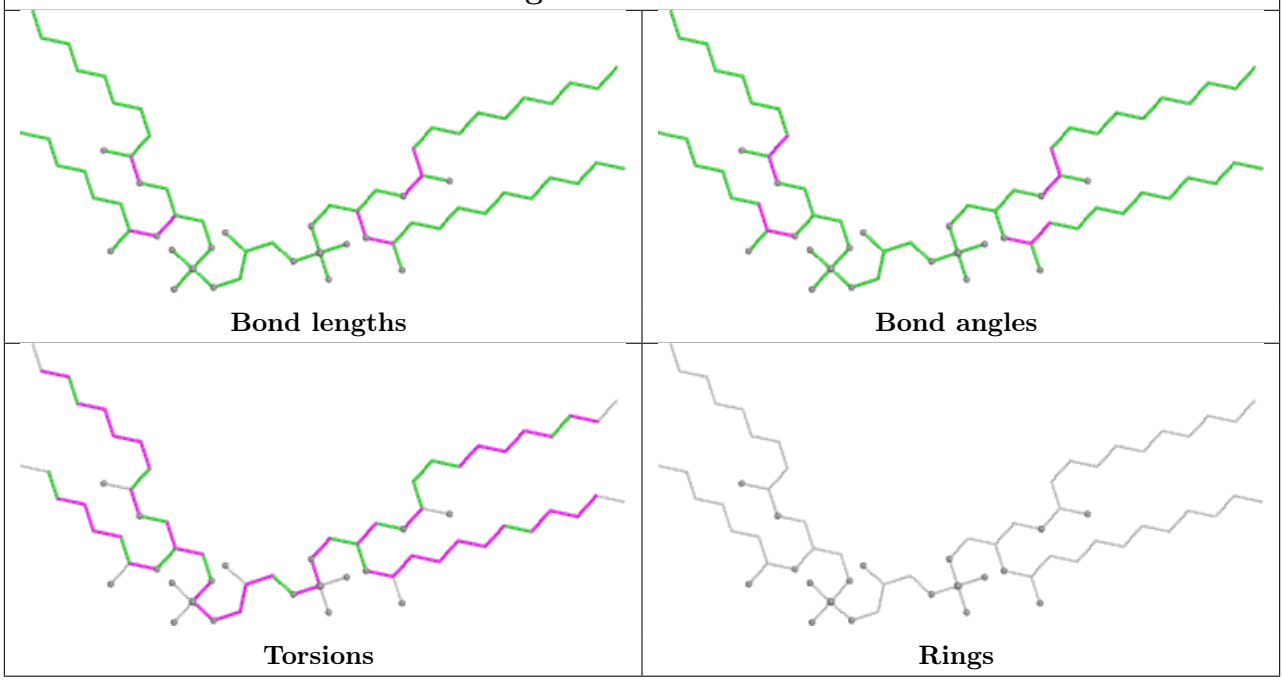

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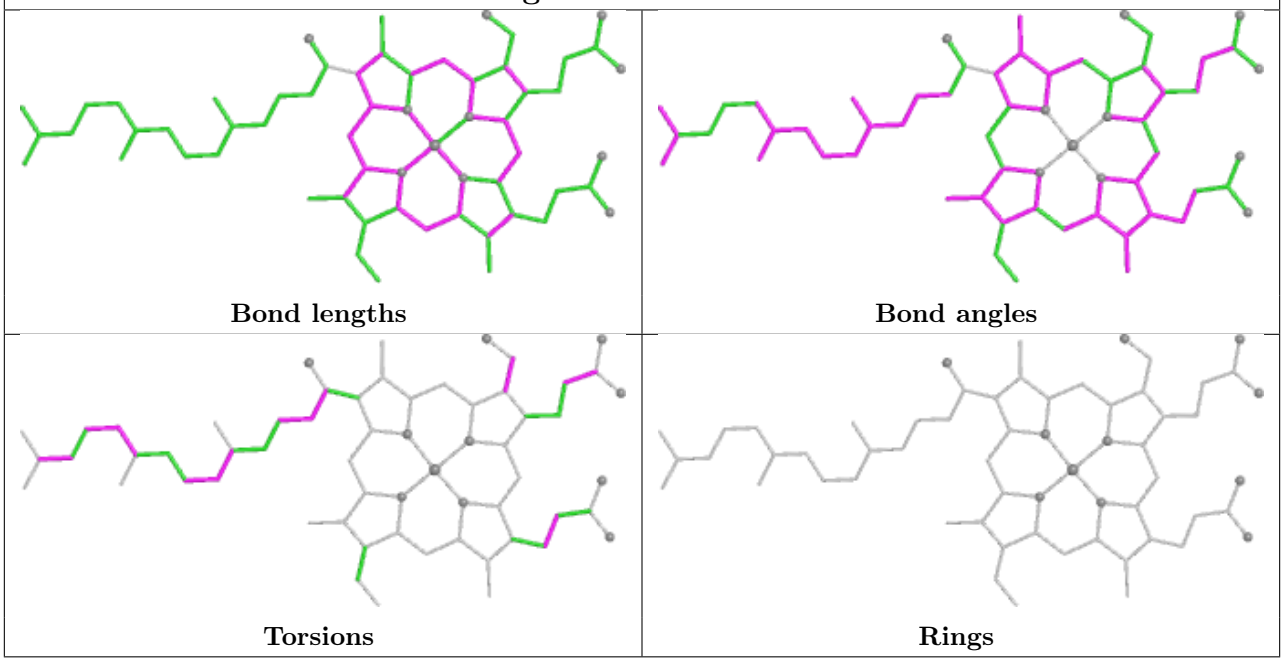
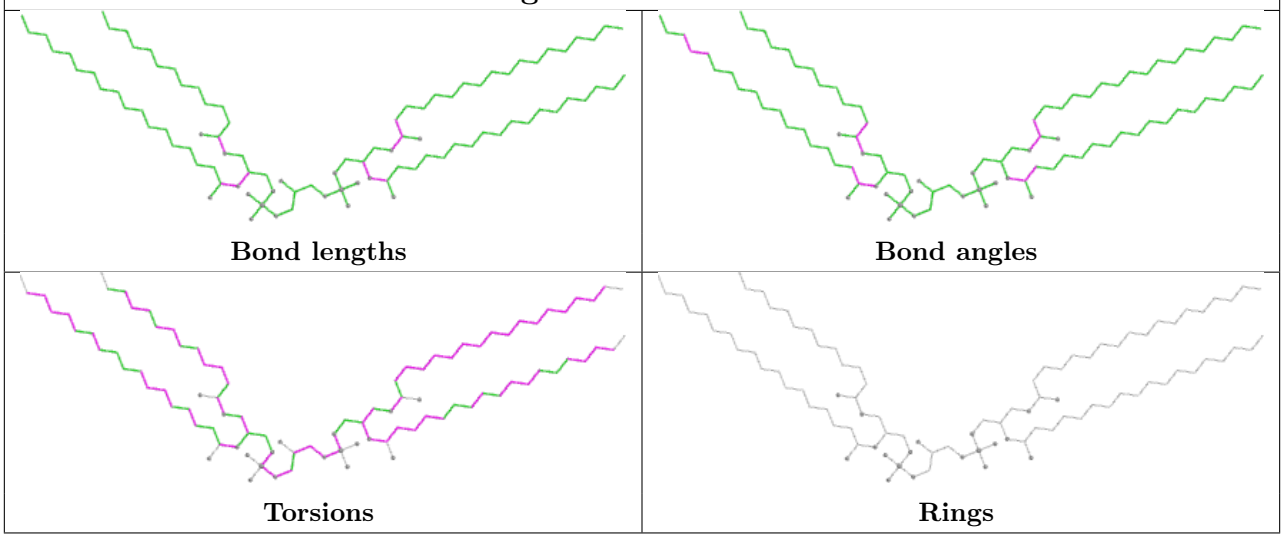
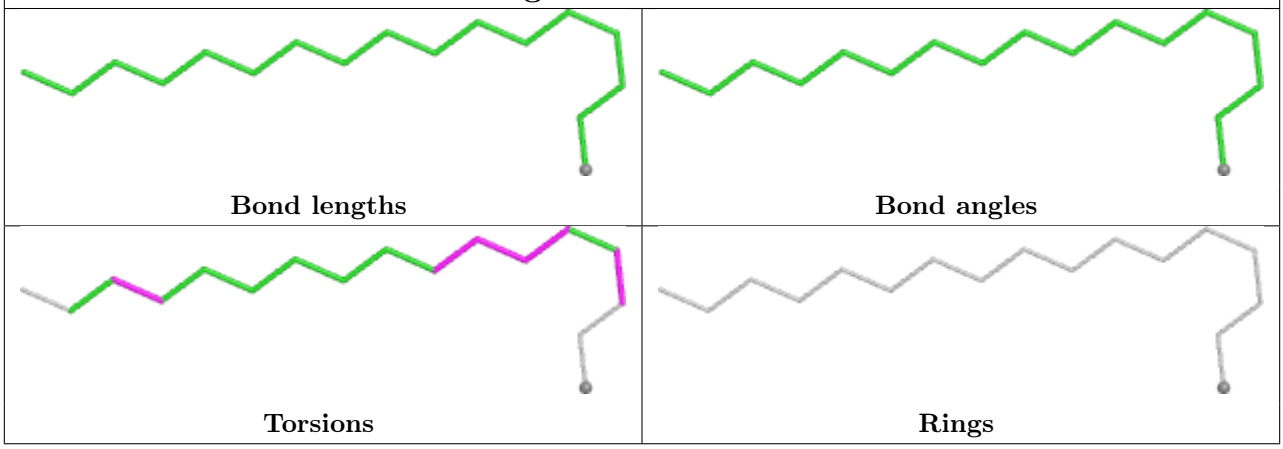


Ligand CDL M 502



Ligand PLM F 603



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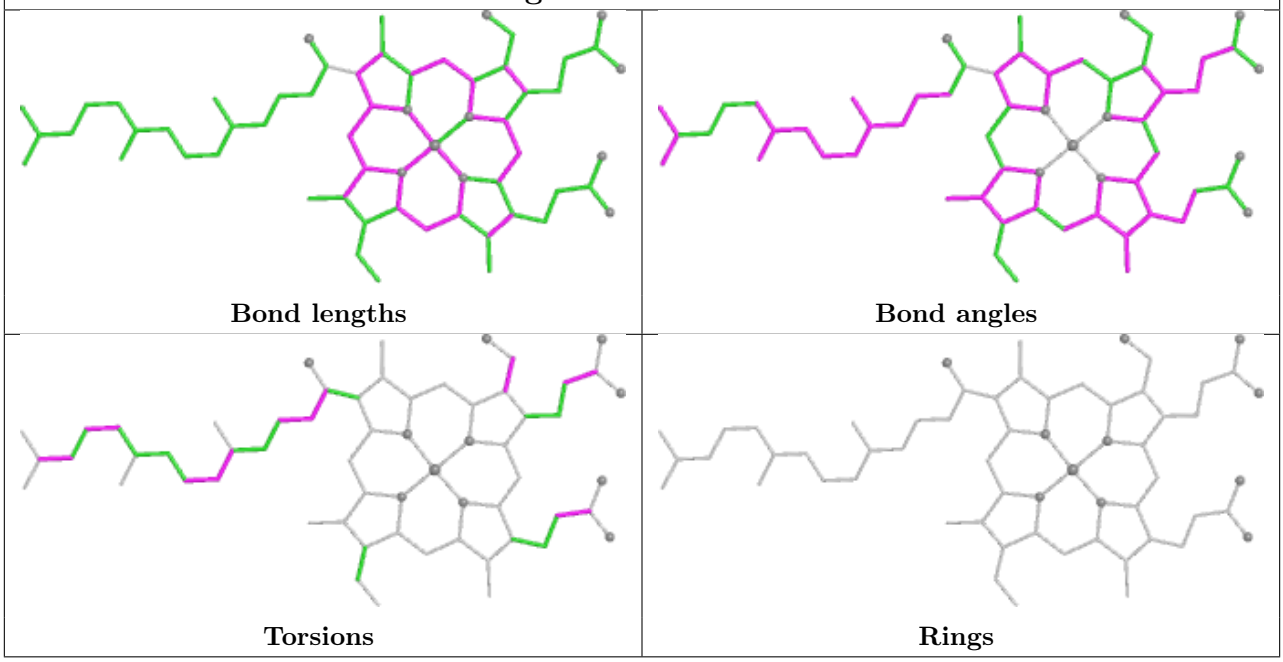
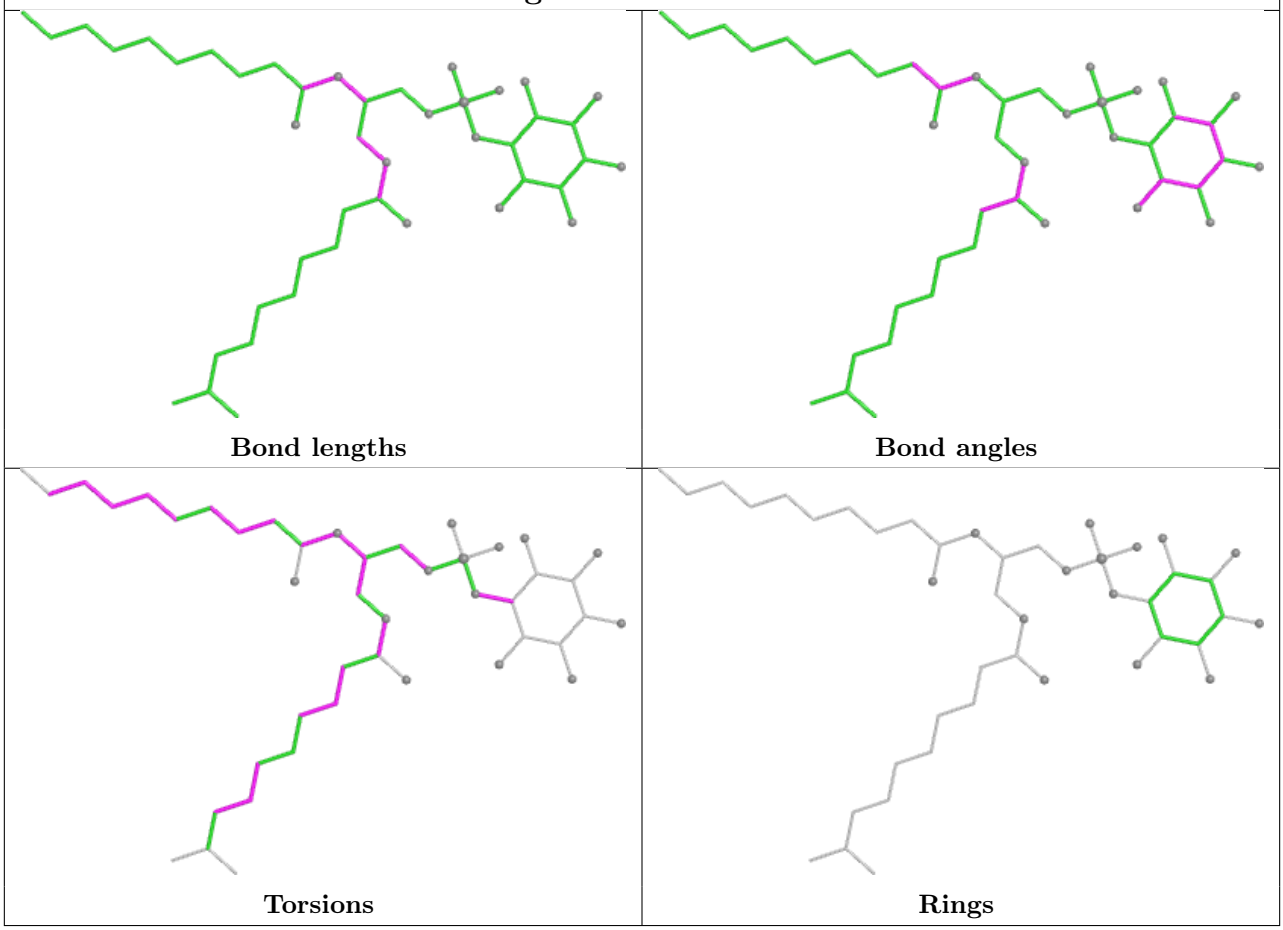


Ligand 9YF M 503



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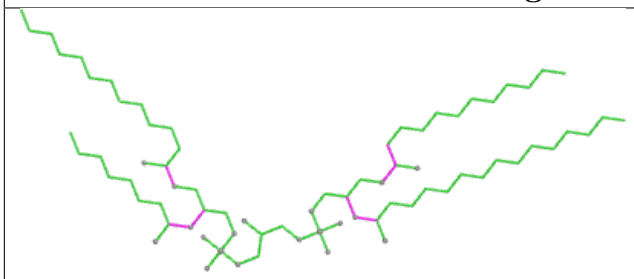
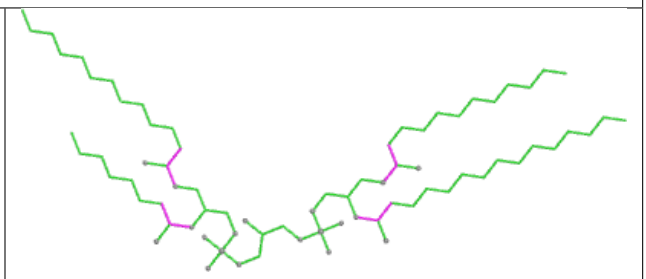
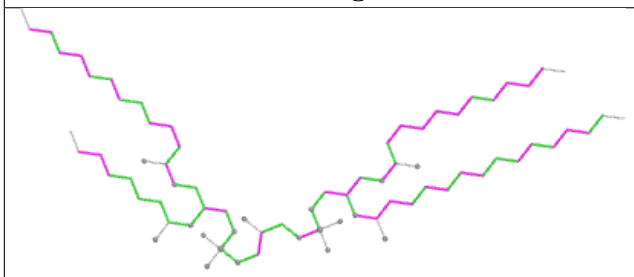


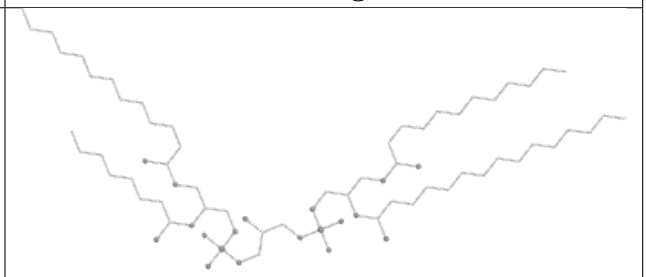
Bond lengths



Bond angles

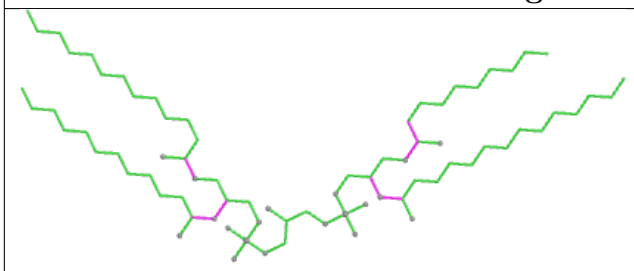


Torsions

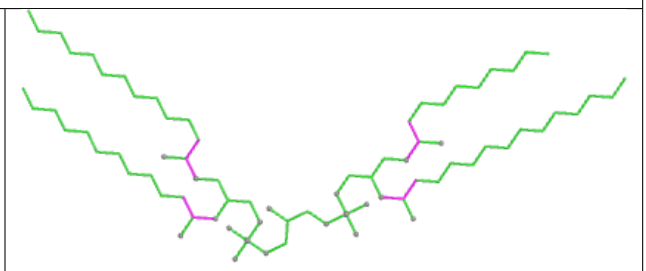


Rings

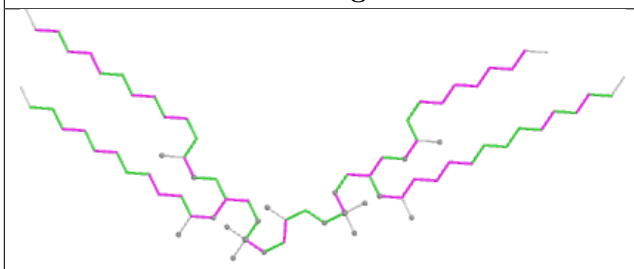
Ligand CDL B 606



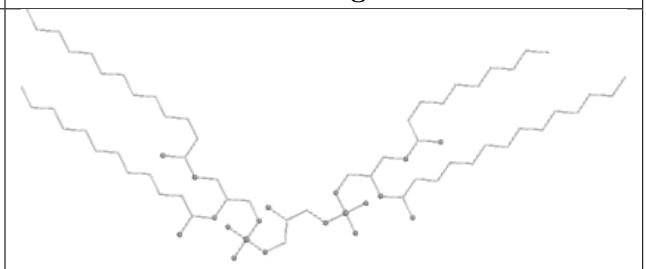
Bond lengths



Bond angles

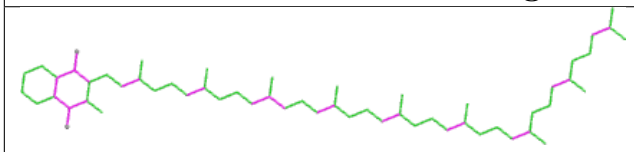


Torsions

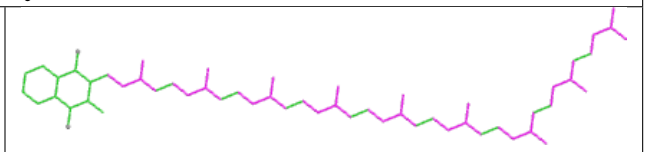


Rings

Ligand MQ9 C 305

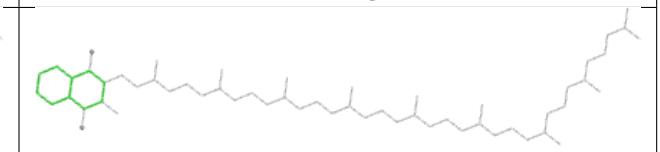


Bond lengths



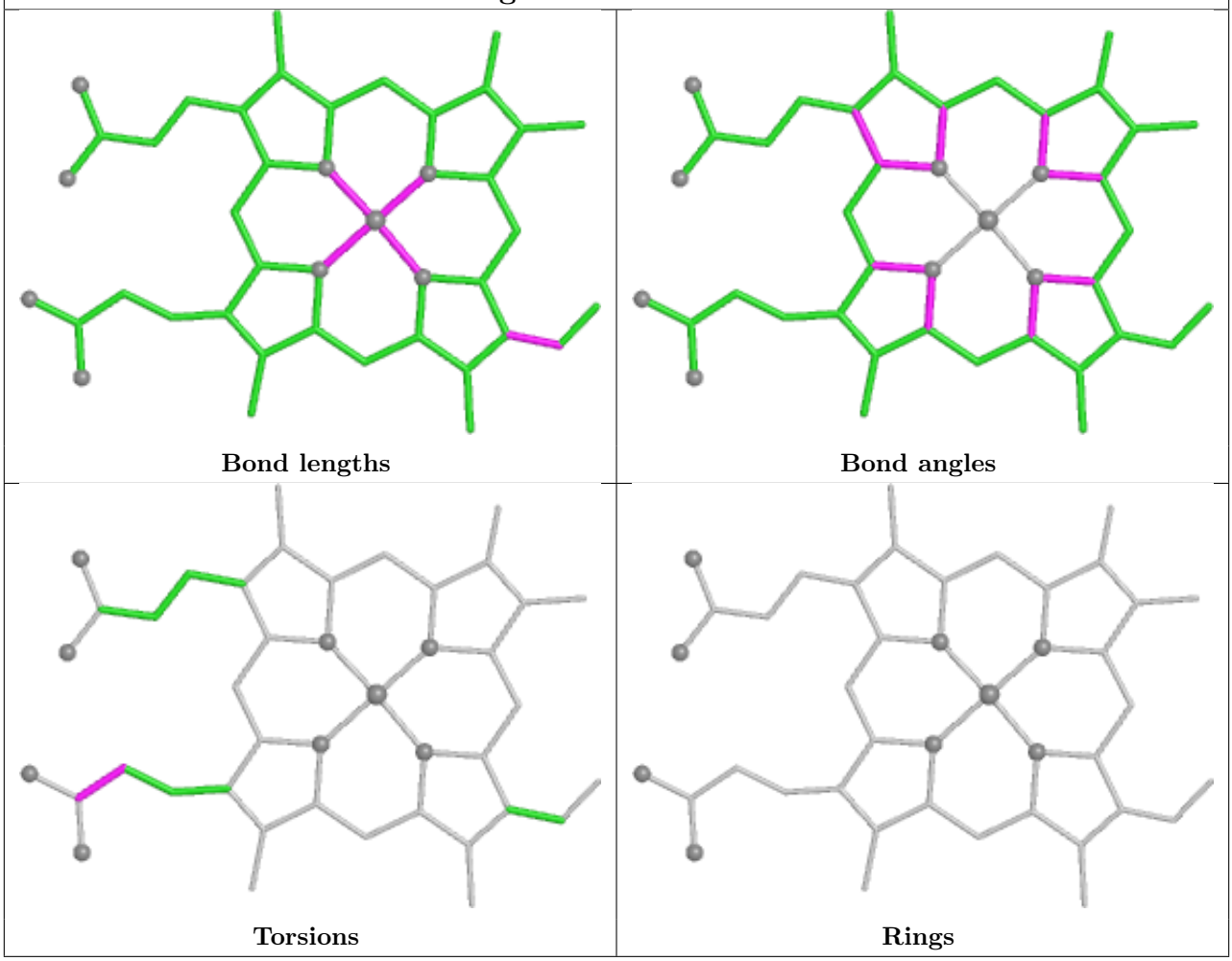
Bond angles

Torsions

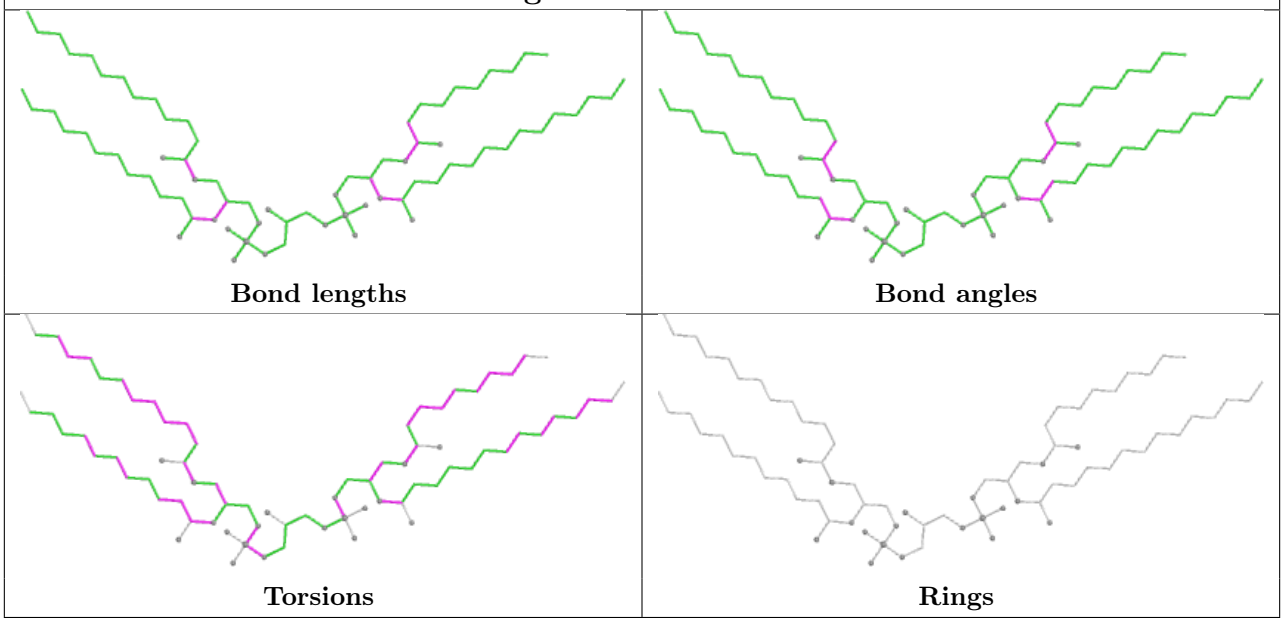


Rings

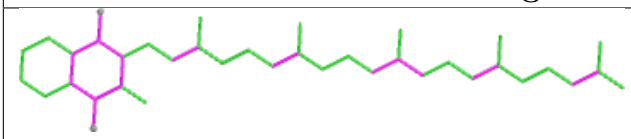
Ligand HEM B 602



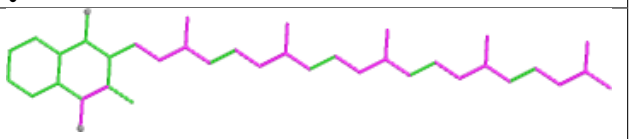
Ligand CDL N 606



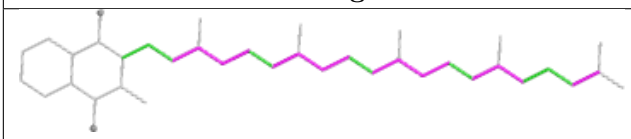
Ligand MQ9 B 609



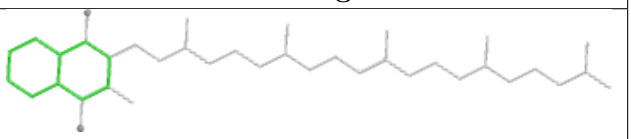
Bond lengths



Bond angles

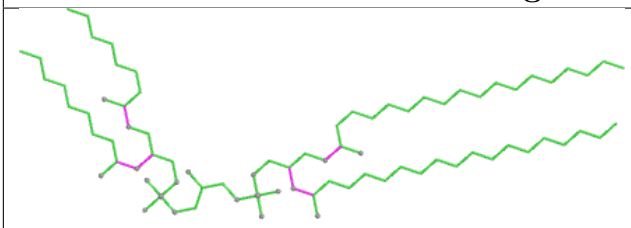


Torsions

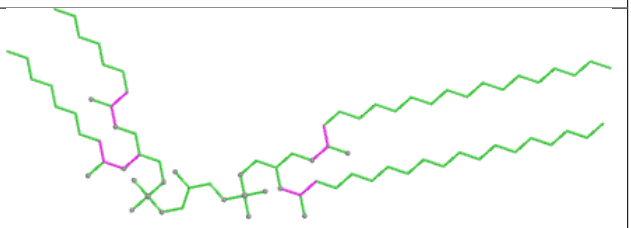


Rings

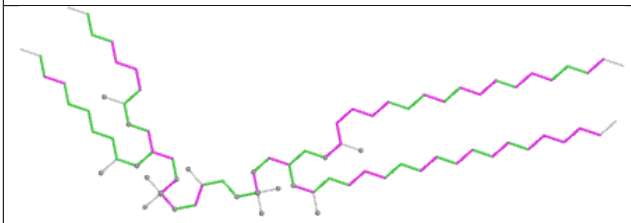
Ligand CDL R 602



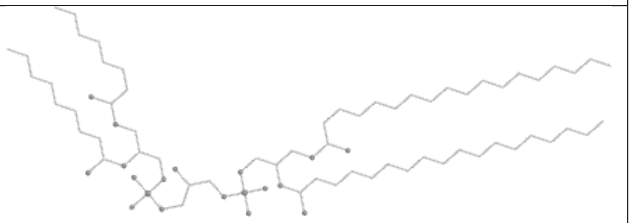
Bond lengths



Bond angles

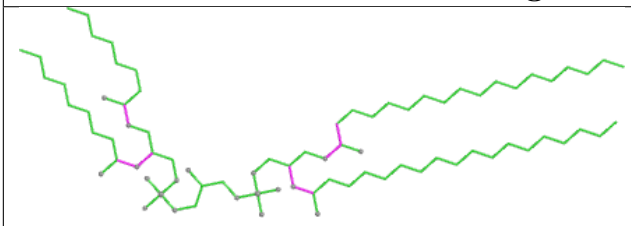


Torsions



Rings

Ligand CDL F 602



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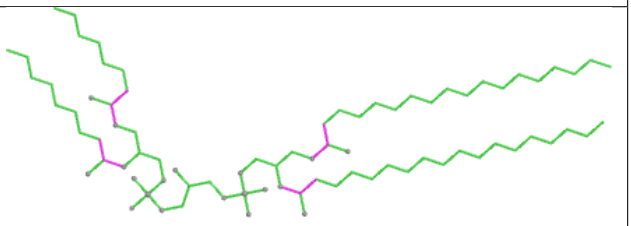
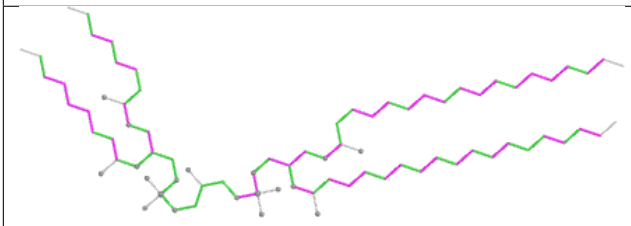


Bond angles



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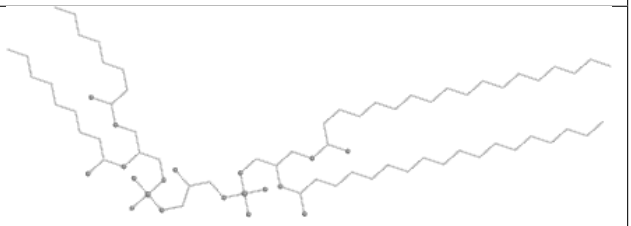
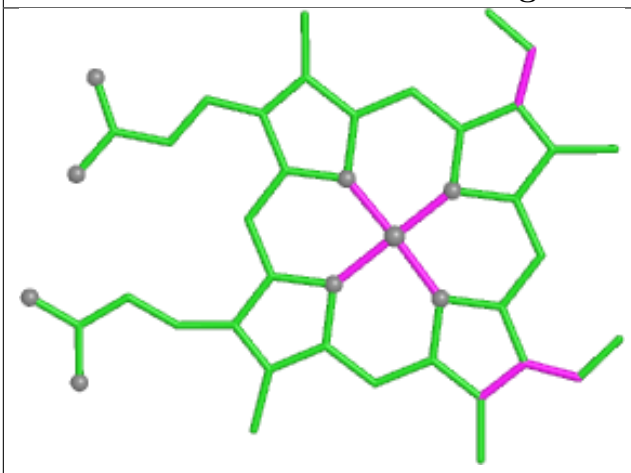


Rings

Ligand HEM B 603



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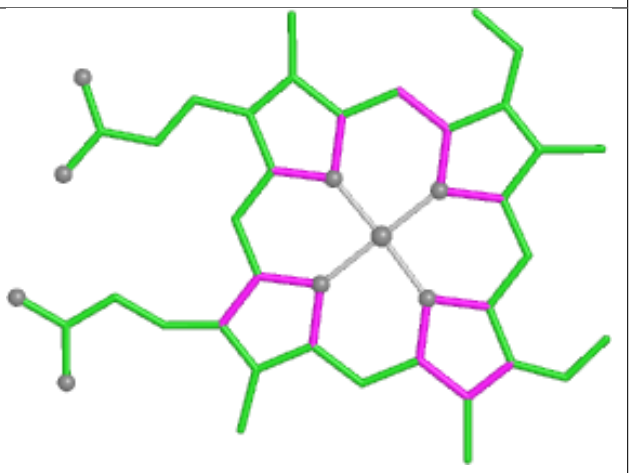
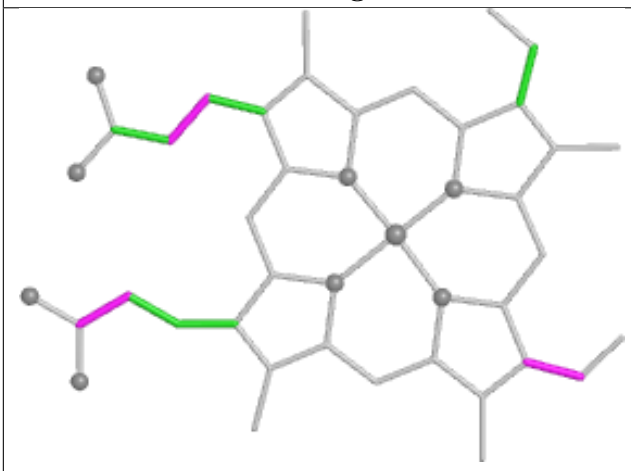


Bond angles



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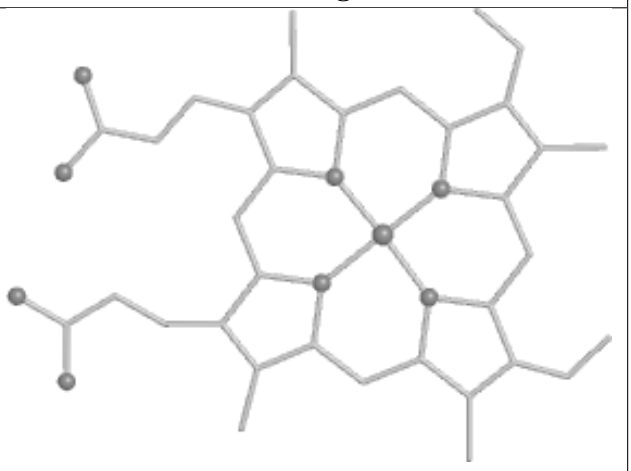
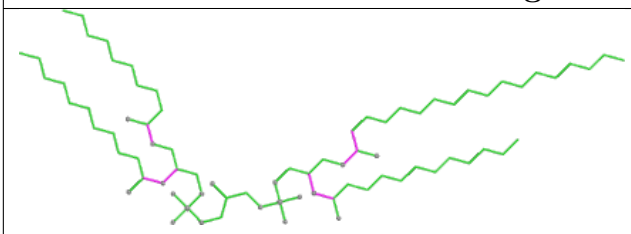


Rings

Ligand CDL C 303



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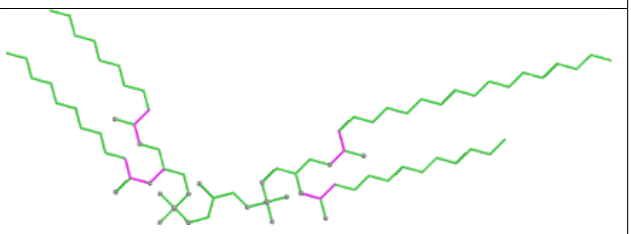
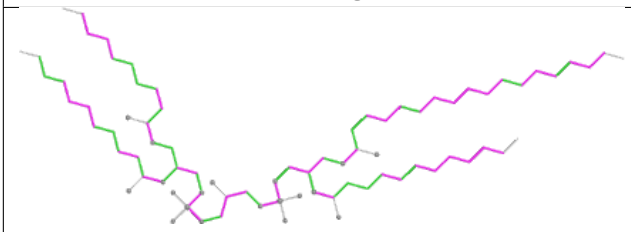
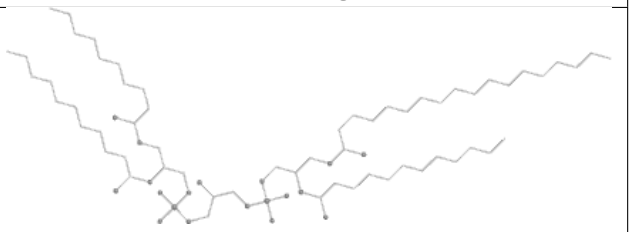


Bond angles

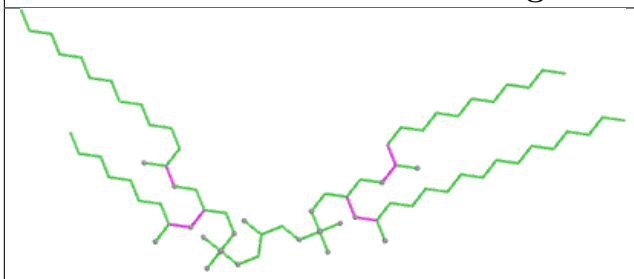


Torsions



Rings

Ligand CDL F 601



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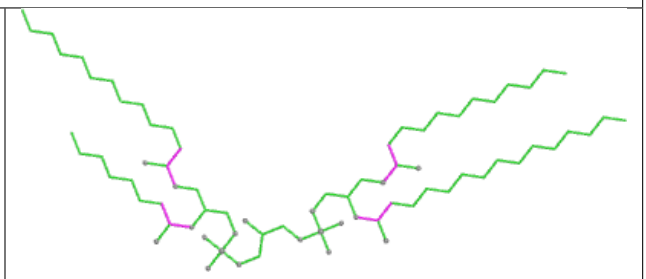
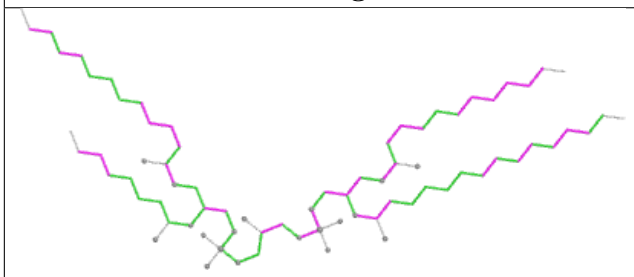


Bond angles



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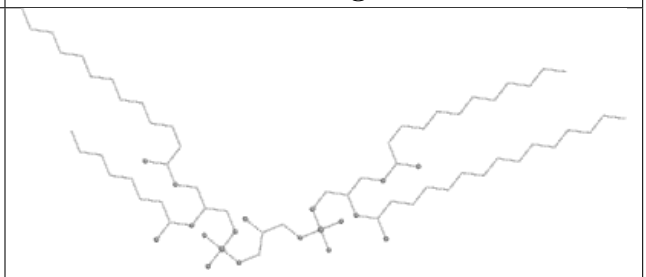
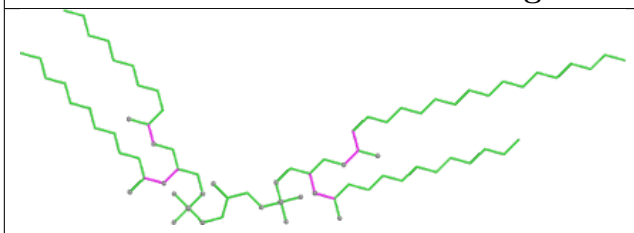


Rings

Ligand CDL N 603



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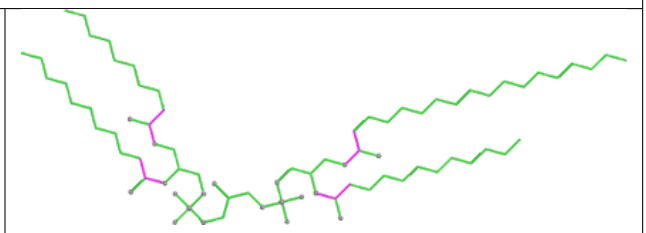
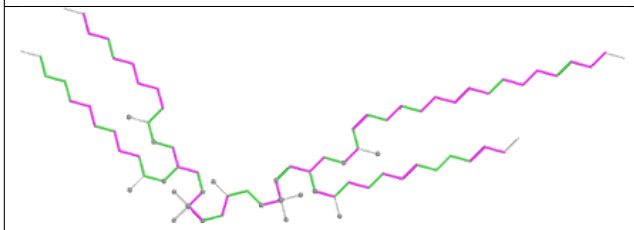
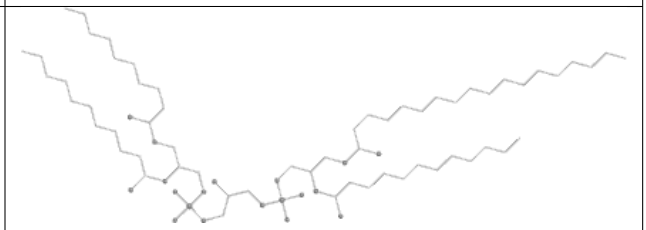


Bond angles

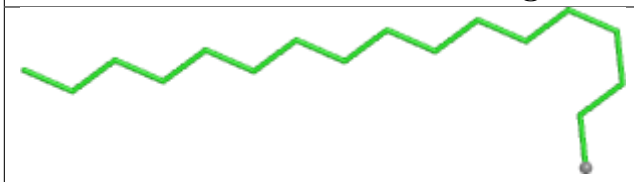


Torsions



Rings

Ligand PLM R 603



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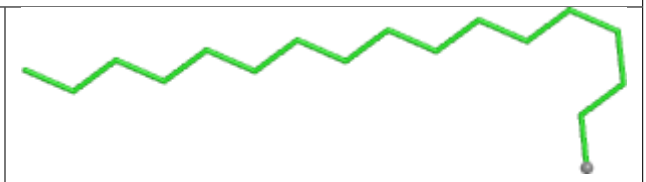
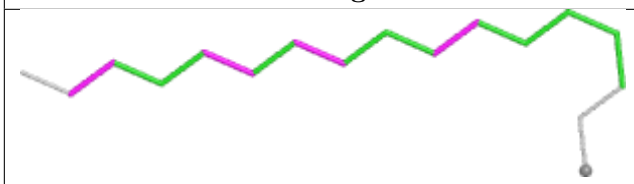


Bond angles



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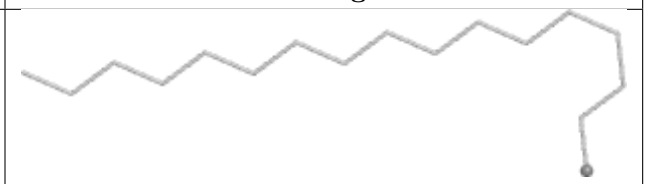
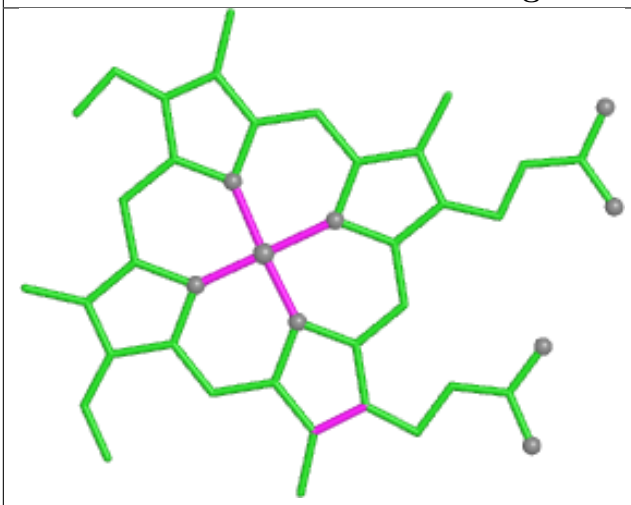


Rings

Ligand HEC C 302



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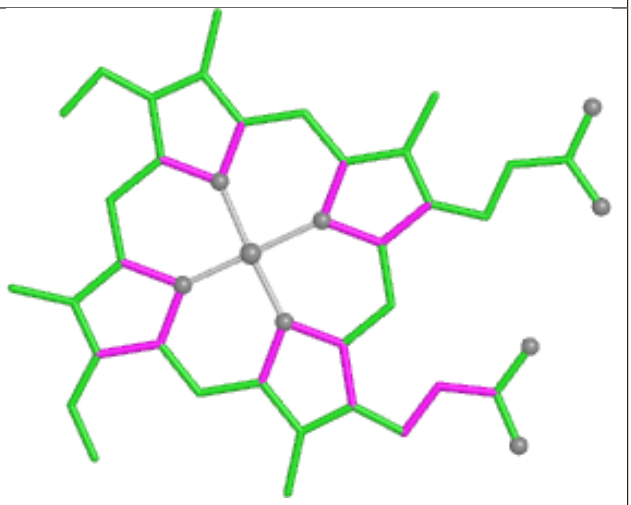
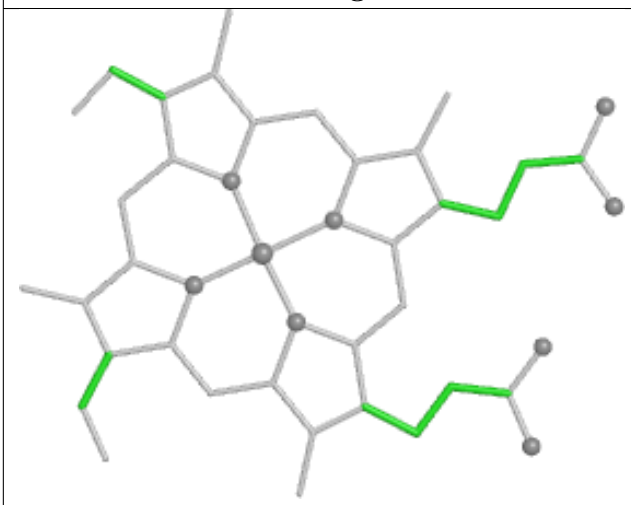
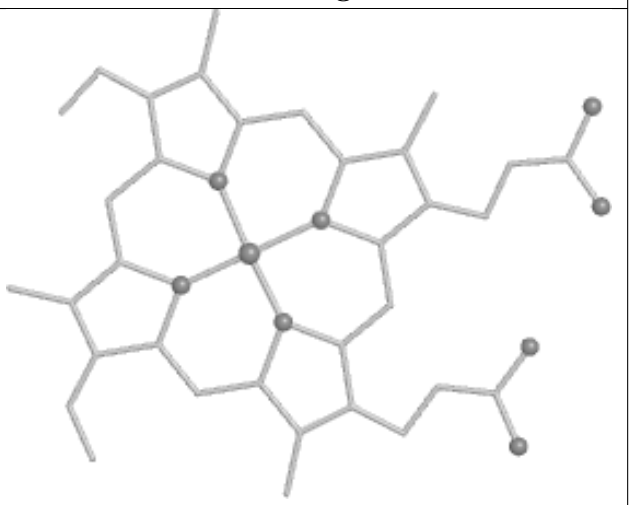


Bond angles

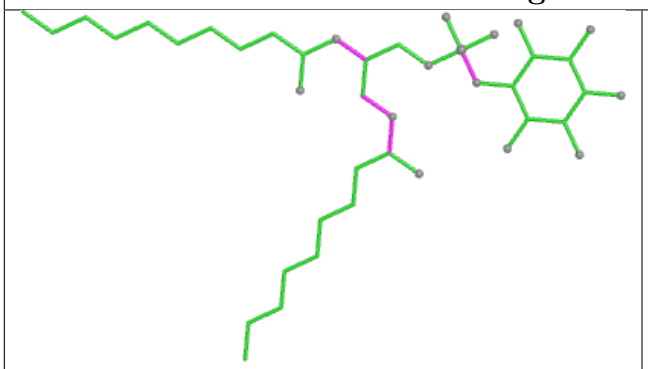


Torsions



Rings

Ligand 9YF A 503



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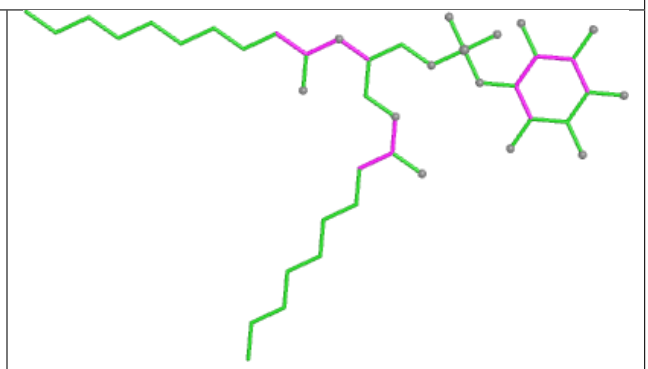
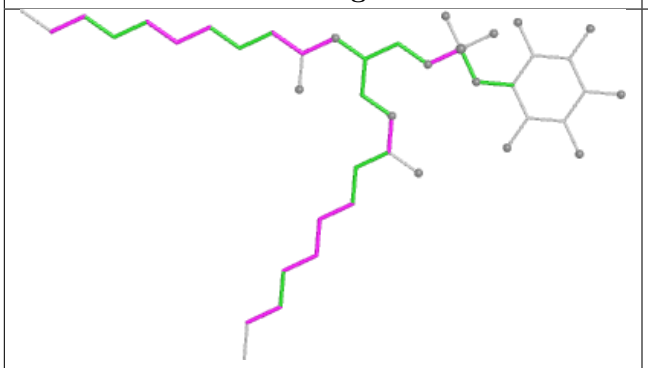
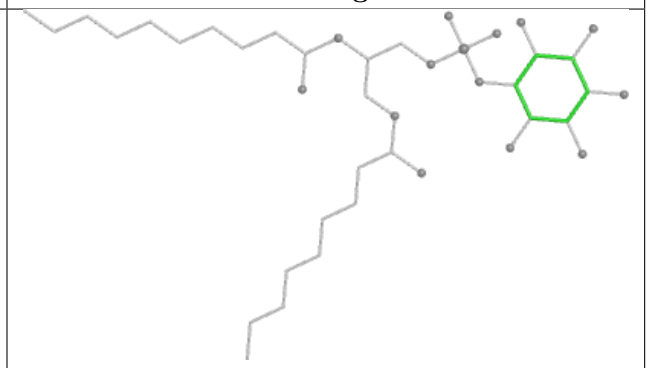


Bond angles



Torsions



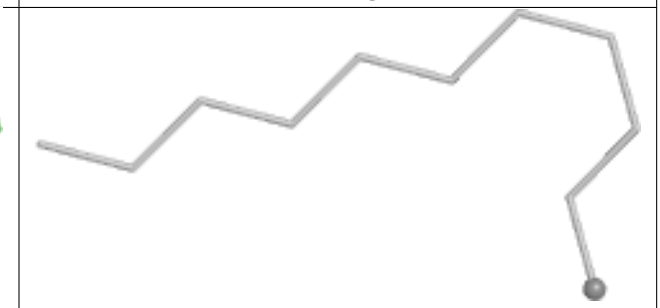
Rings

Ligand PLM N 604

Bond lengths

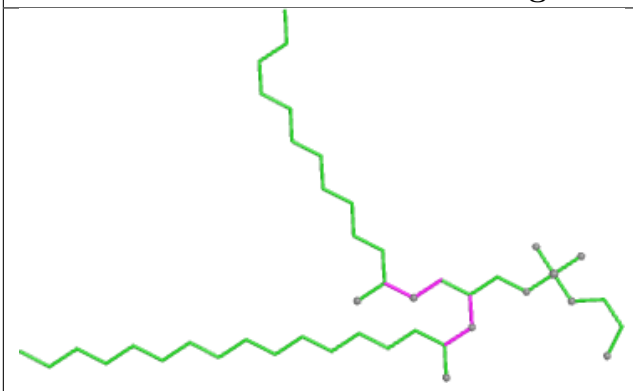
Bond angles

Torsions

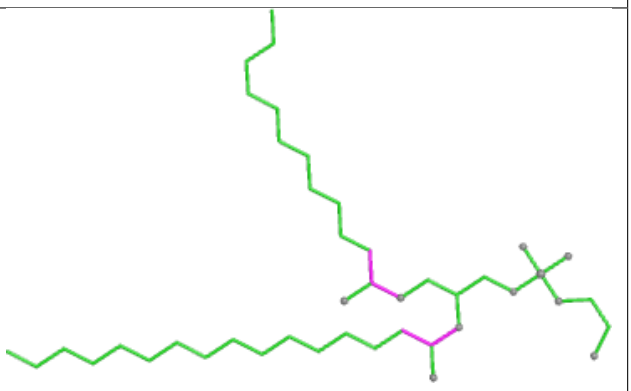


Rings

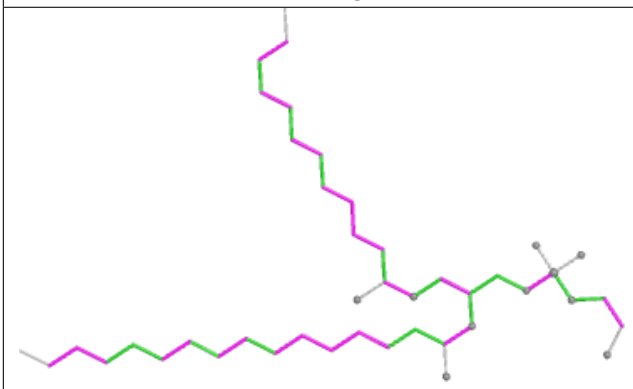
Ligand 9Y0 G 301



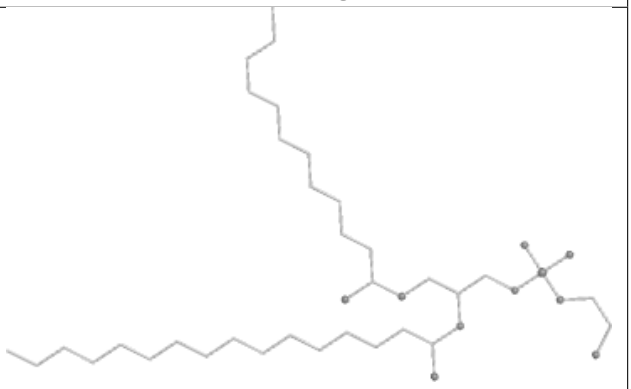
Bond lengths



Bond angles

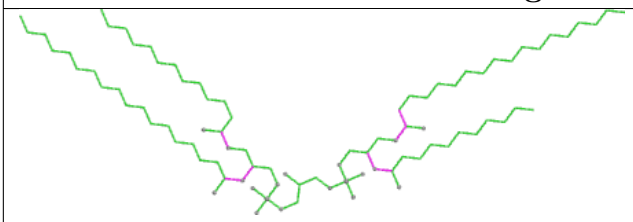


Torsions

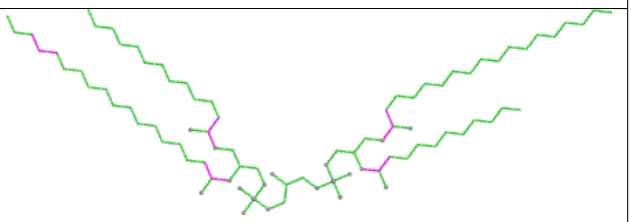


Rings

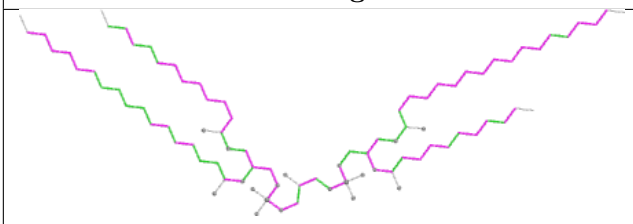
Ligand CDL P 201



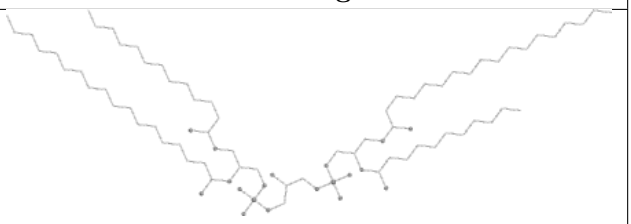
Bond lengths



Bond angles

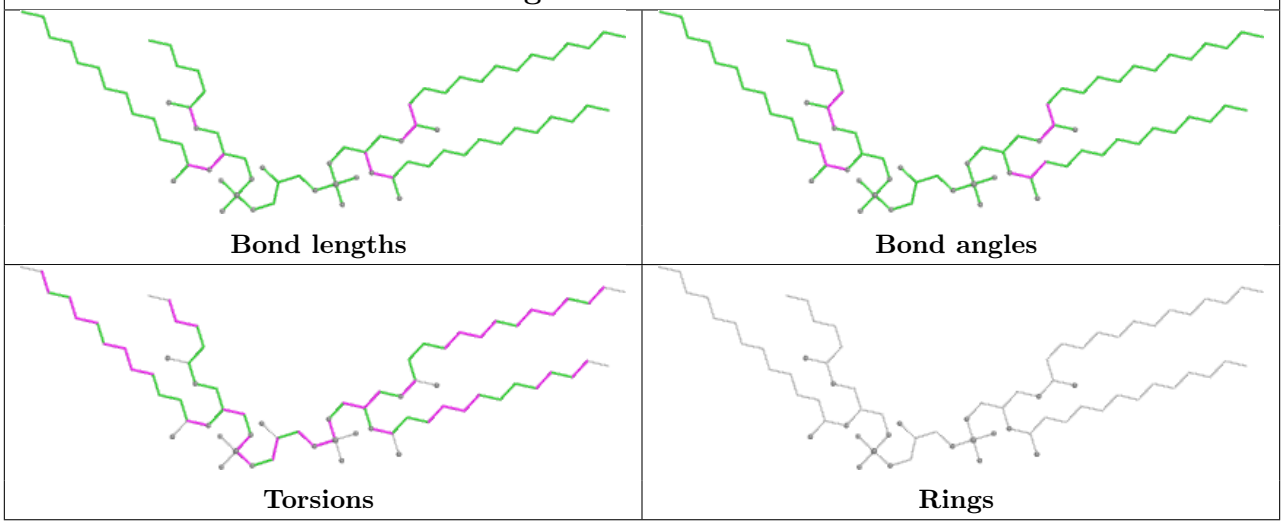


Torsions

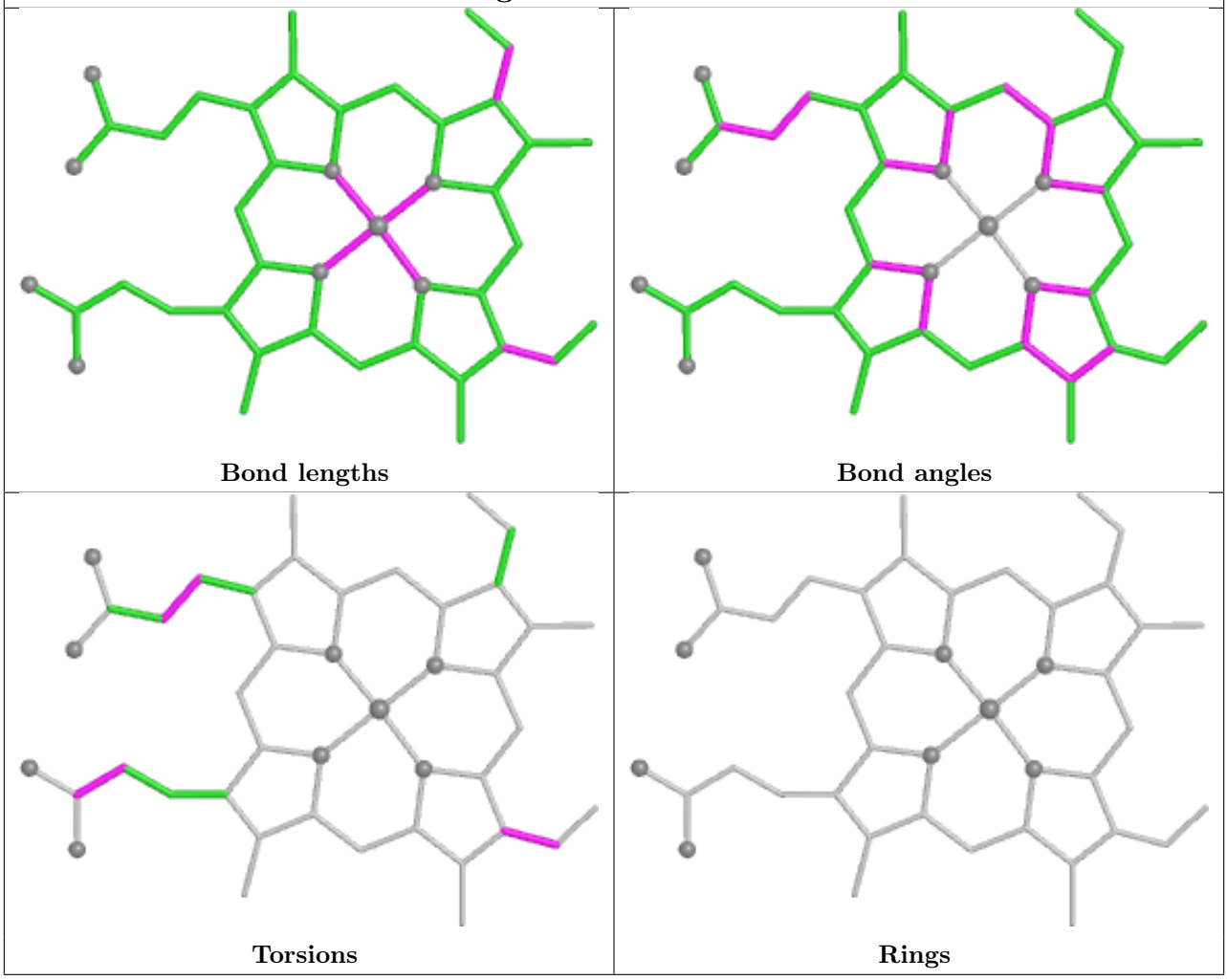


Rings

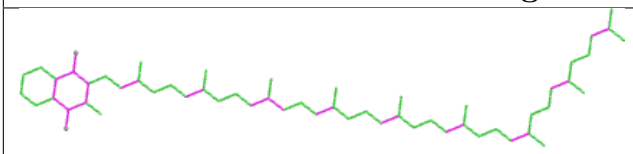
Ligand CDL N 605



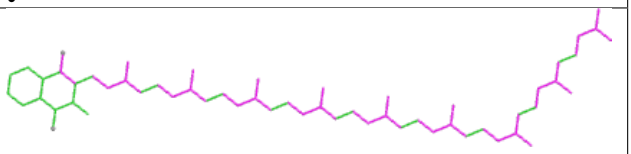
Ligand HEM N 602



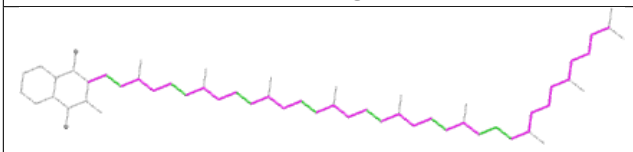
Ligand MQ9 N 609



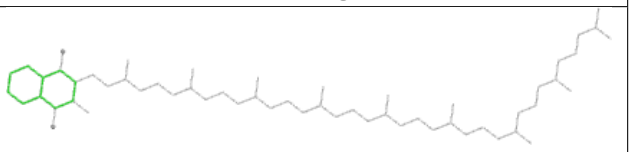
Bond lengths



Bond angles



Torsions



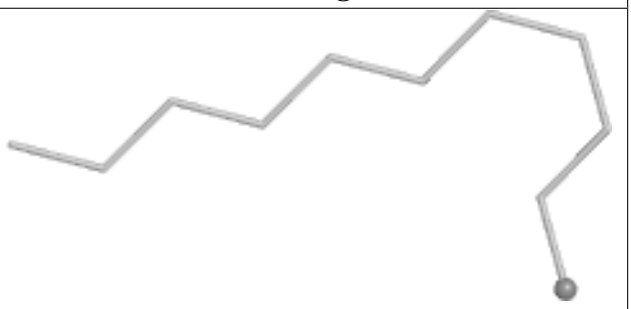
Rings

Ligand PLM B 601

Bond lengths

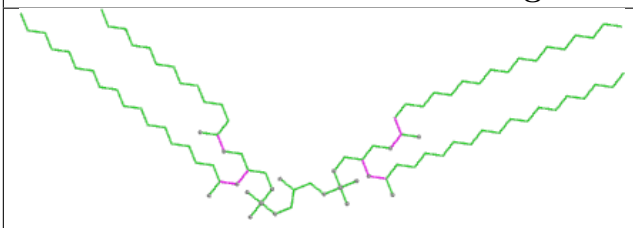
Bond angles

Torsions

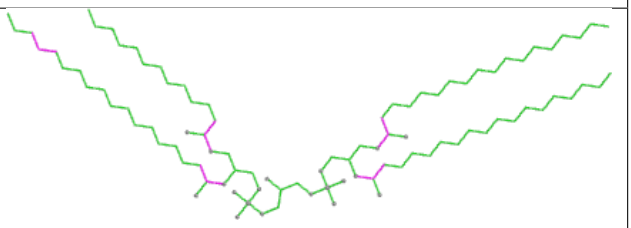


Rings

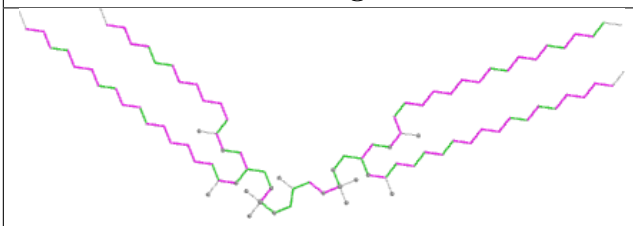
Ligand CDL C 306



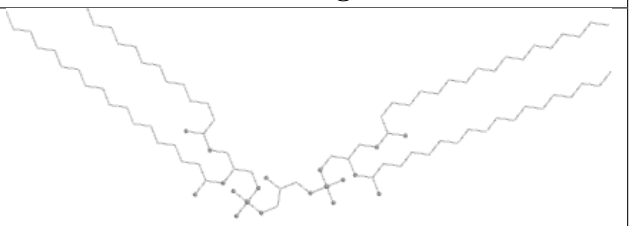
Bond lengths



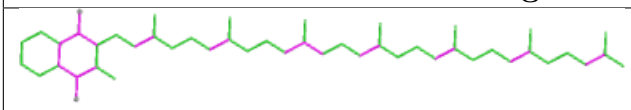
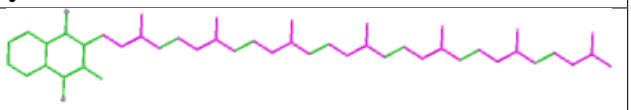
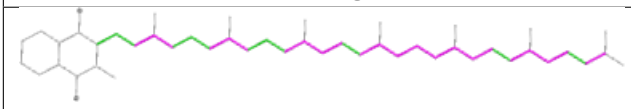
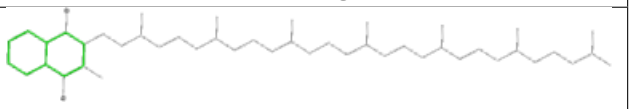
Bond angles

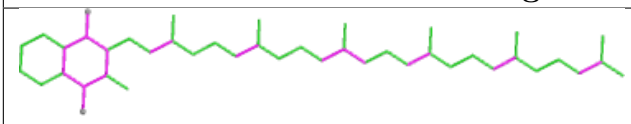
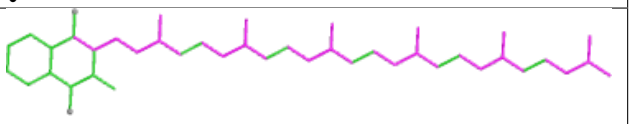
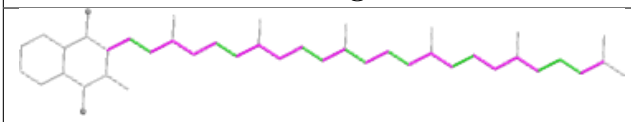
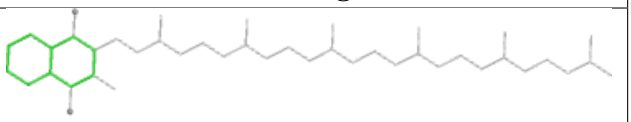


Torsions

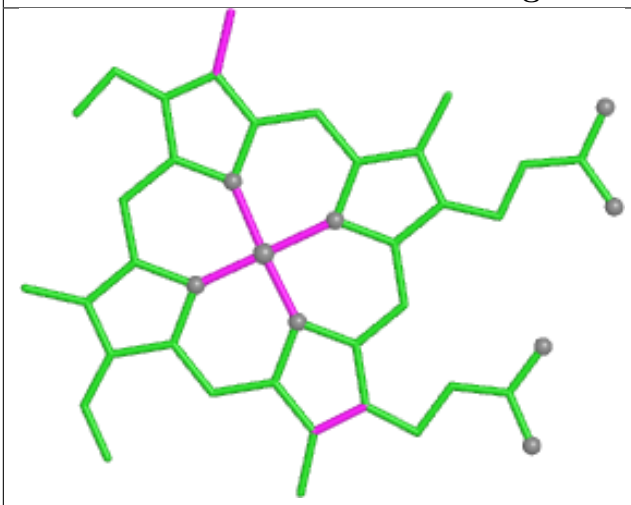


Rings

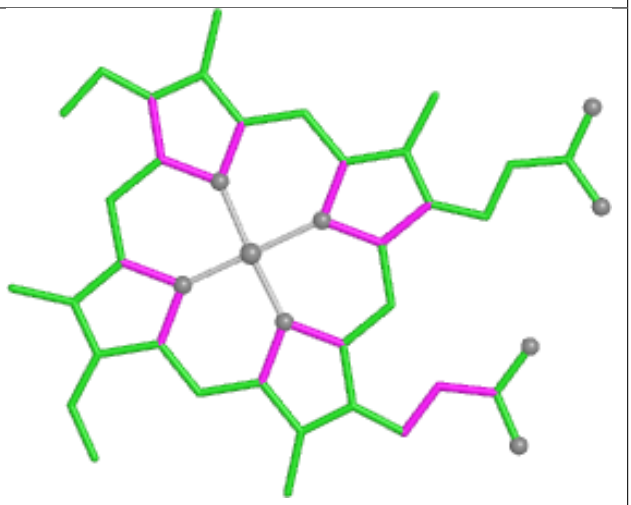
Ligand MQ9 O 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

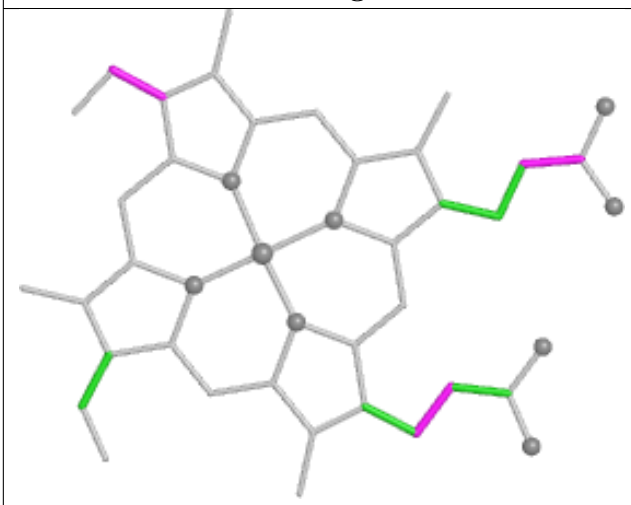
Ligand HEC C 301



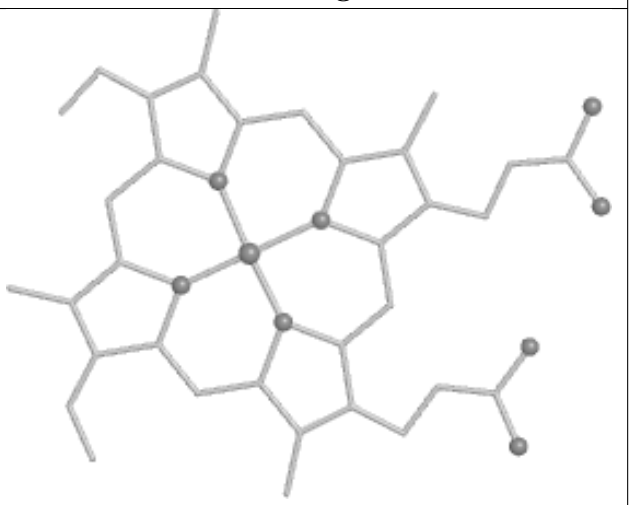
Bond lengths



Bond angles

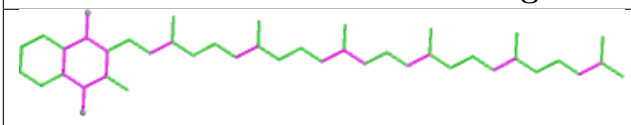


Torsions

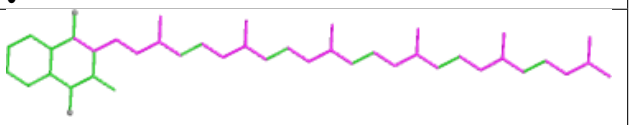


Rings

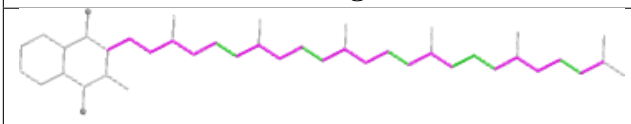
Ligand MQ9 N 611



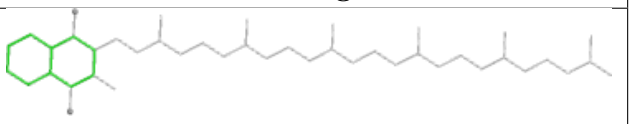
Bond lengths



Bond angles

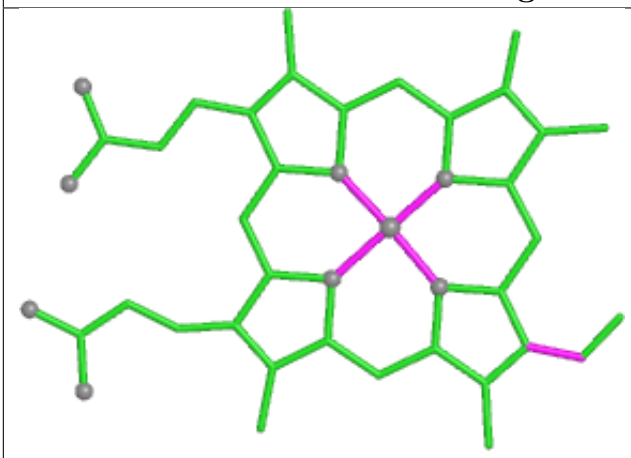


Torsions

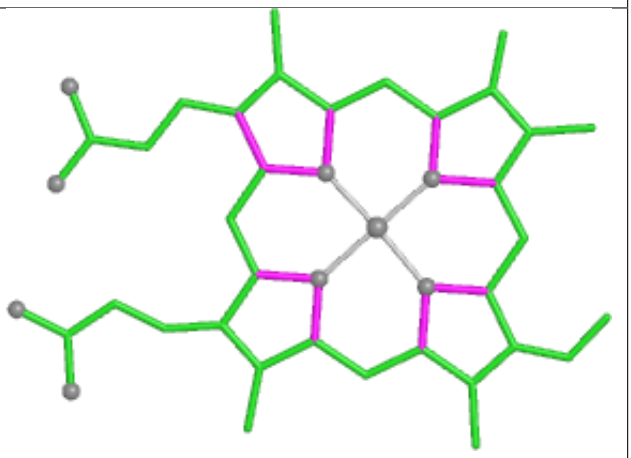


Rings

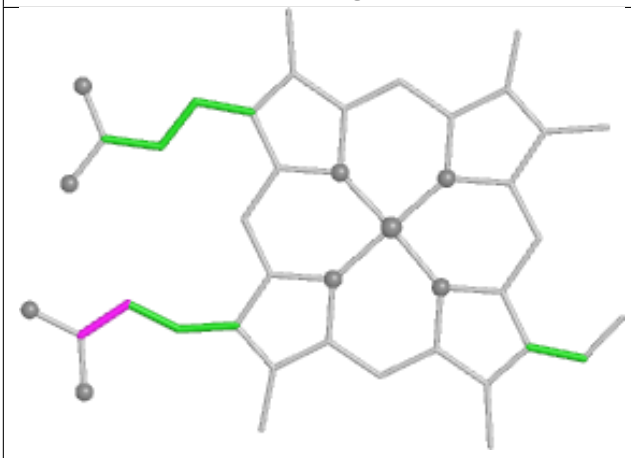
Ligand HEM N 601



Bond lengths



Bond angles



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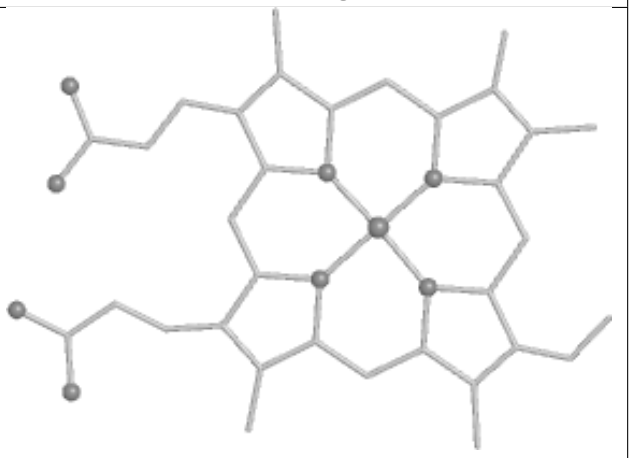
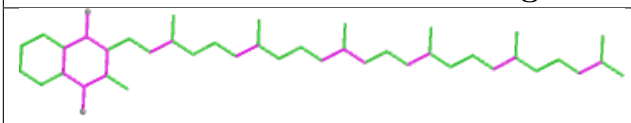
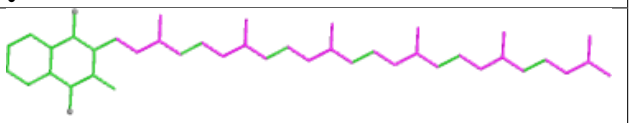


Rings

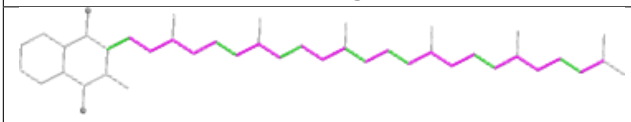
Ligand MQ9 N 610



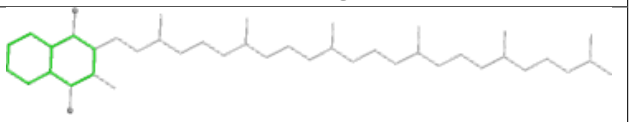
Bond lengths



Bond angles

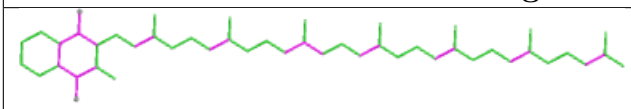


Torsions

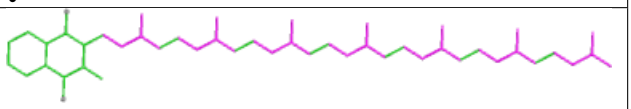


Rings

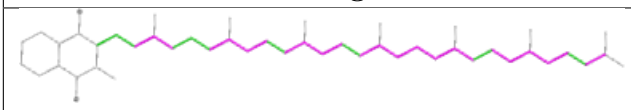
Ligand MQ9 C 304



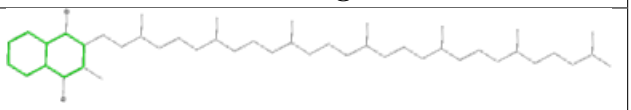
Bond lengths



Bond angles

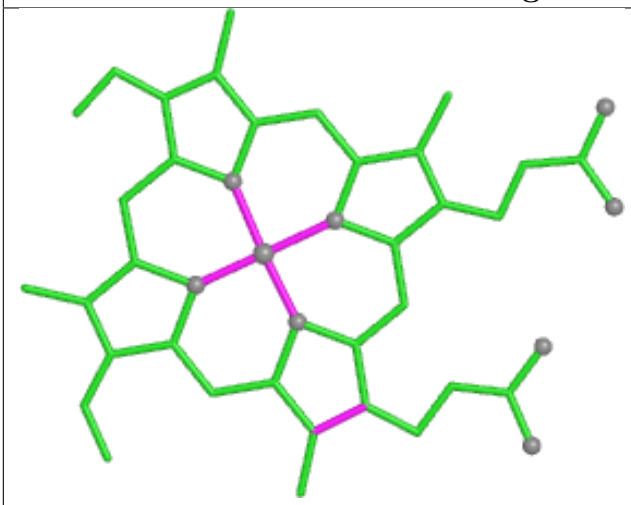


Torsions

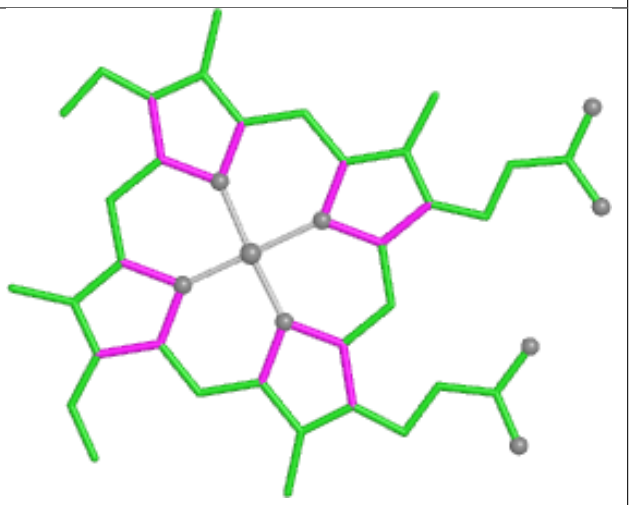


Rings

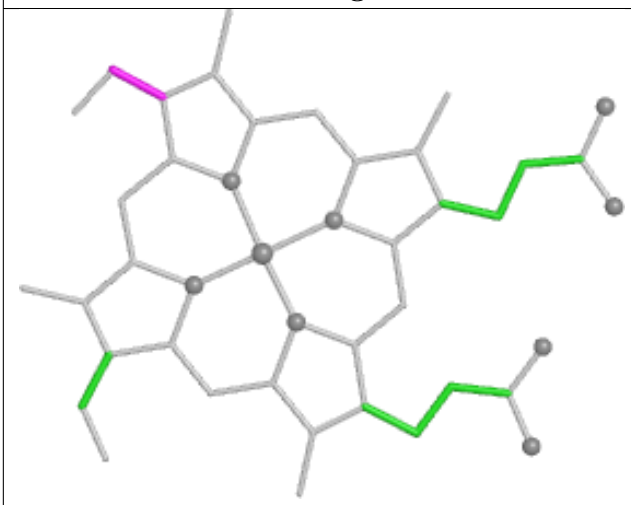
Ligand HEC O 304



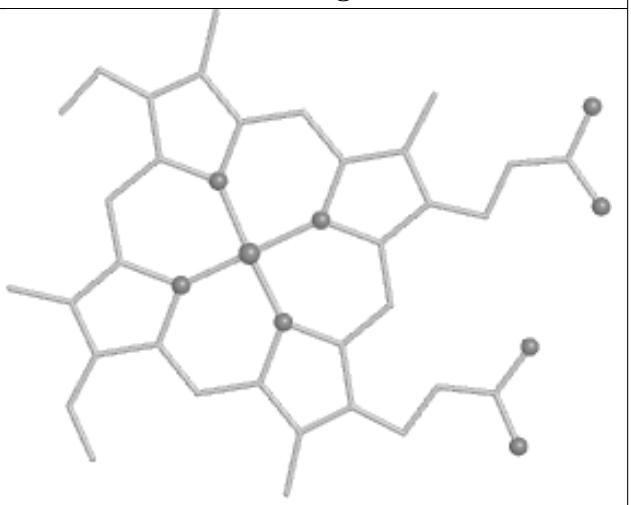
Bond lengths



Bond angles

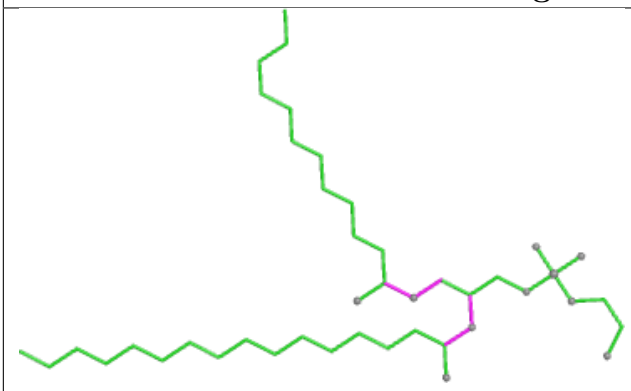


Torsions

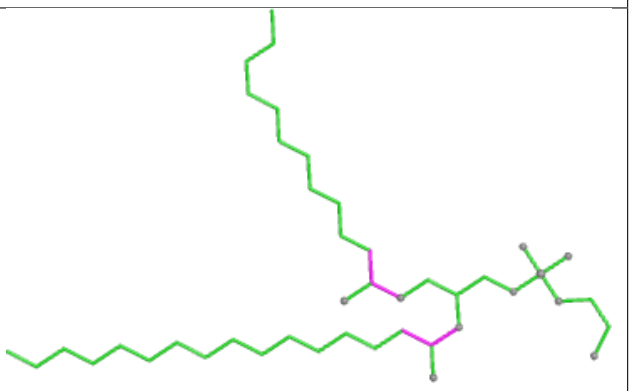


Rings

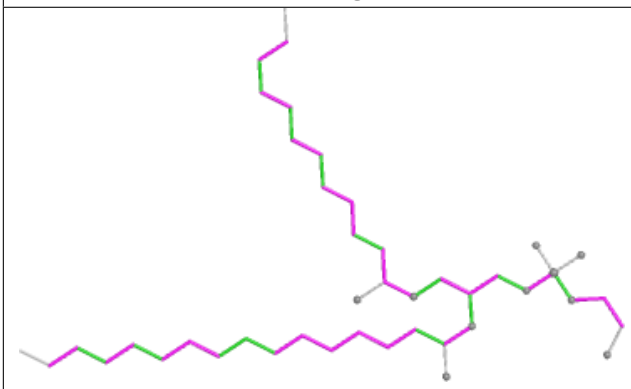
Ligand 9Y0 S 301



Bond lengths



Bond angles



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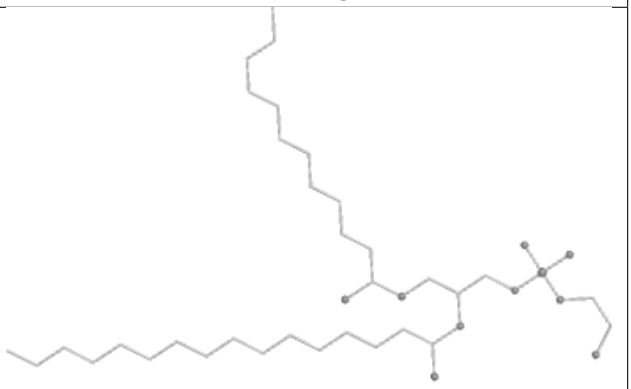
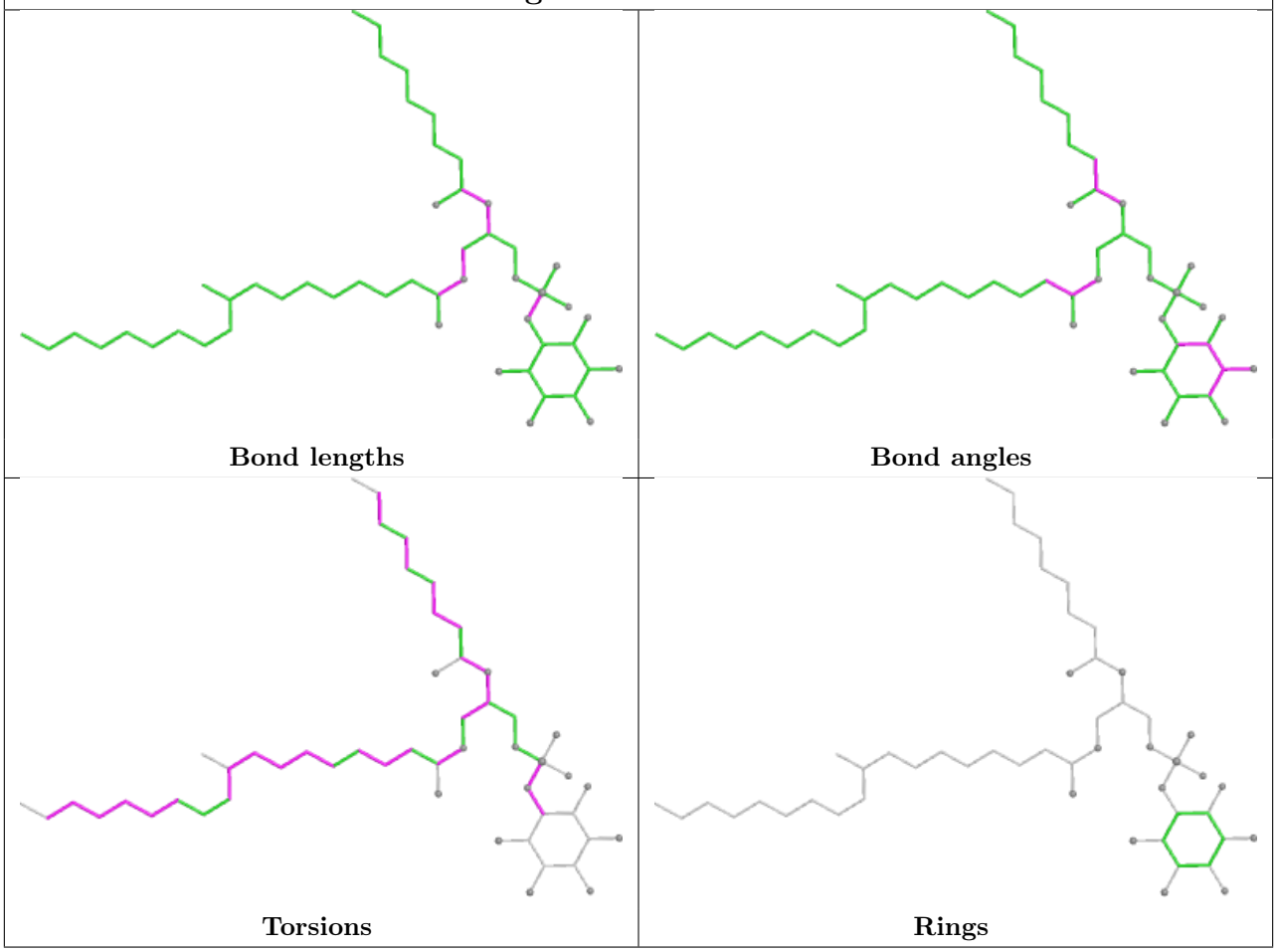
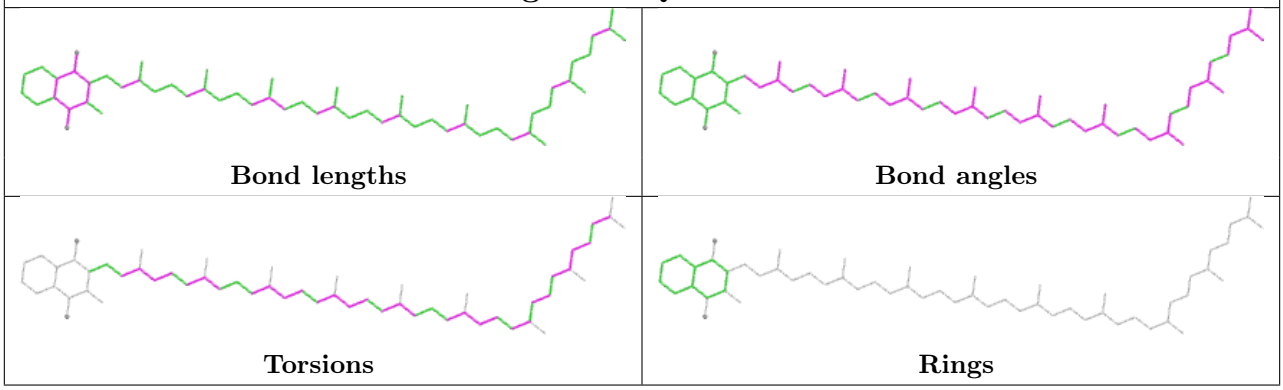


Rings

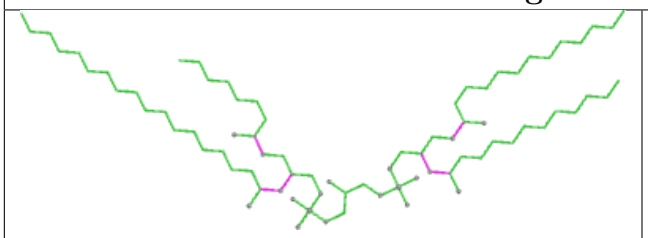
Ligand 9YF A 502



Ligand MQ9 N 608



Ligand CDL B 607



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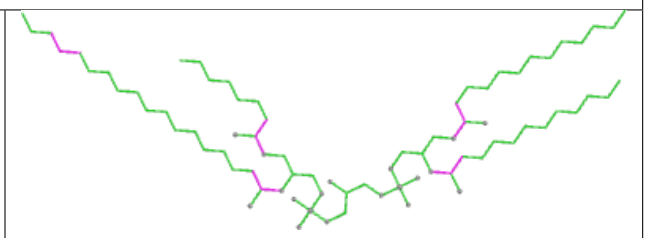
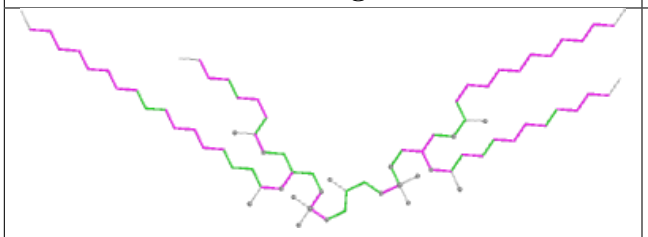
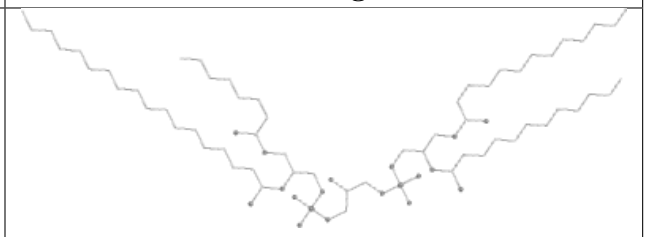


Bond angles

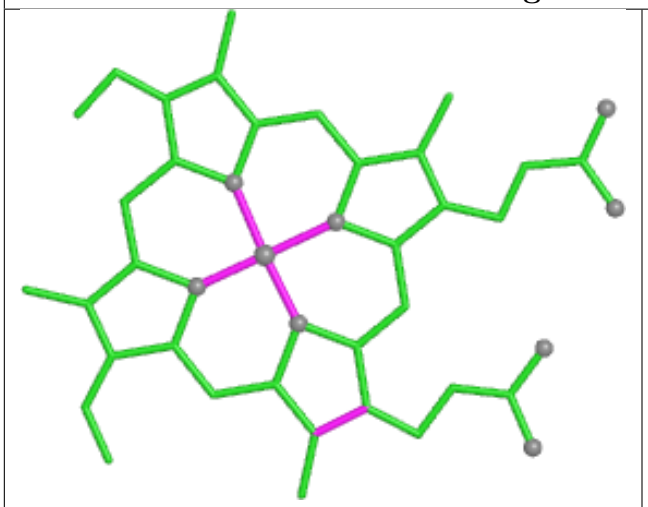


Torsions

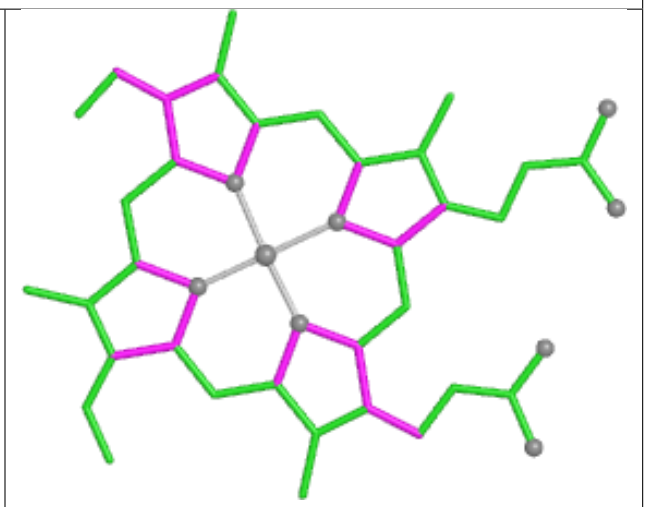


Rings

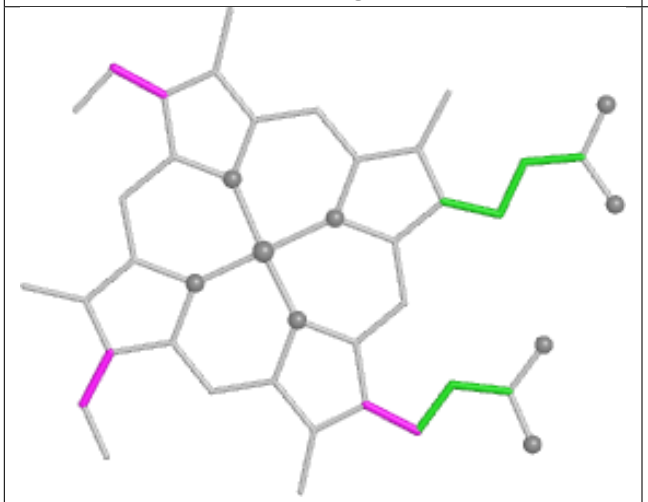
Ligand HEC O 303



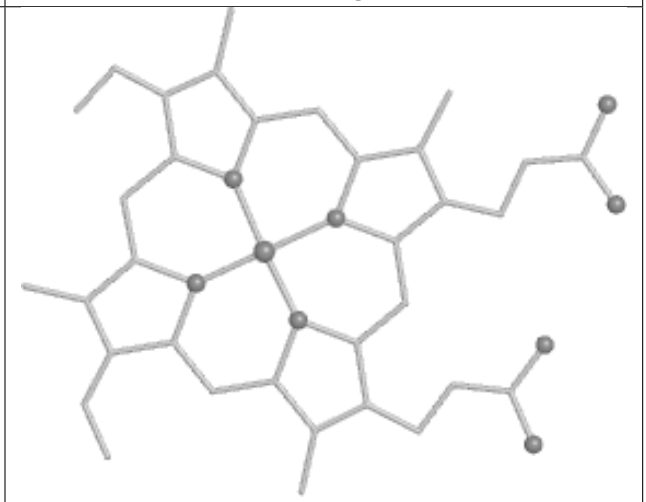
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

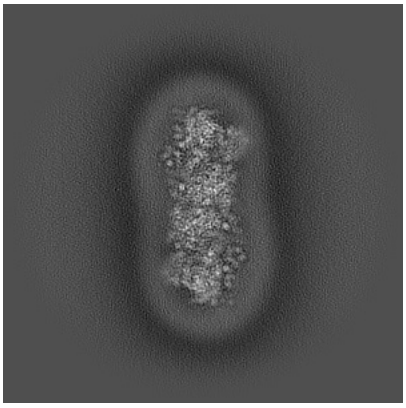
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30943. These allow visual inspection of the internal detail of the map and identification of artifacts.

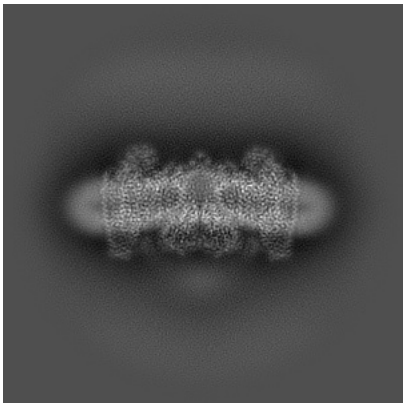
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

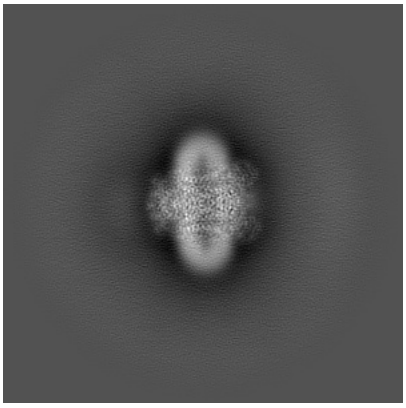
6.1.1 Primary map



X



Y

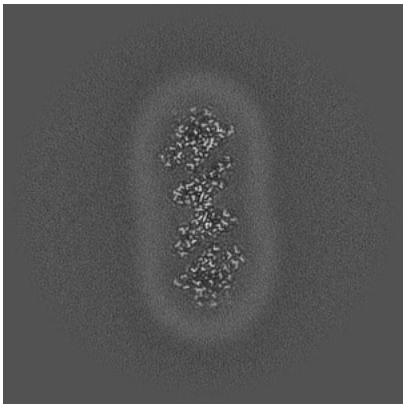


Z

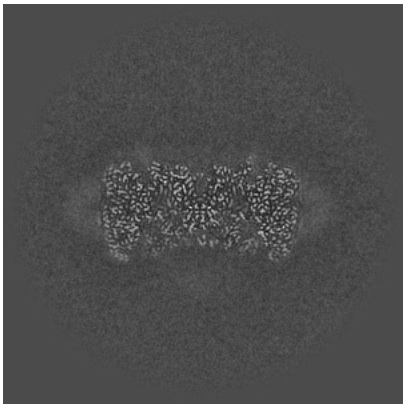
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

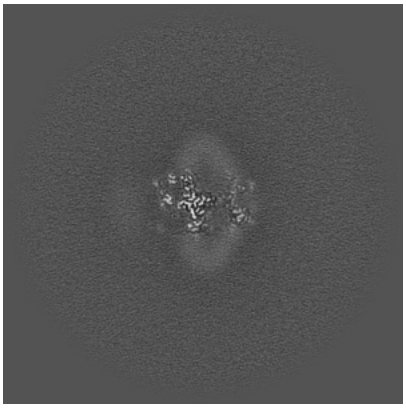
6.2.1 Primary map



X Index: 256



Y Index: 256

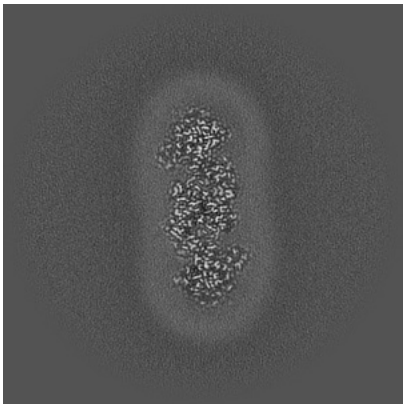


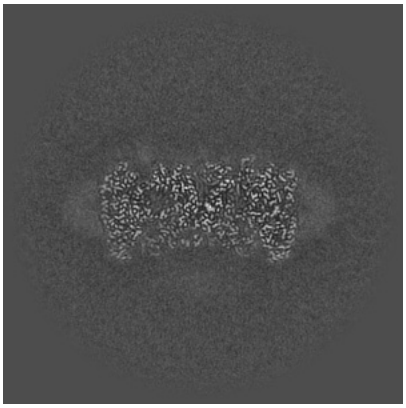
Z Index: 256

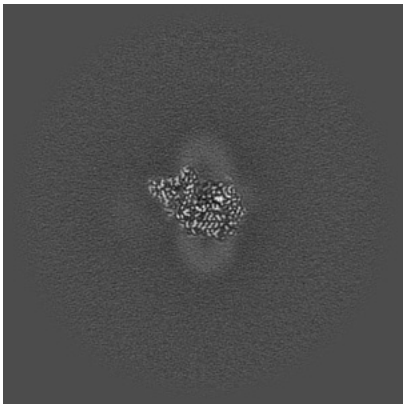
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 243

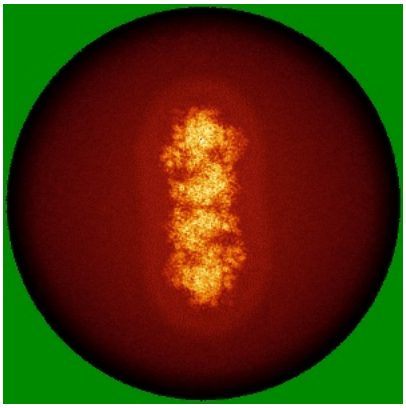

Y Index: 252

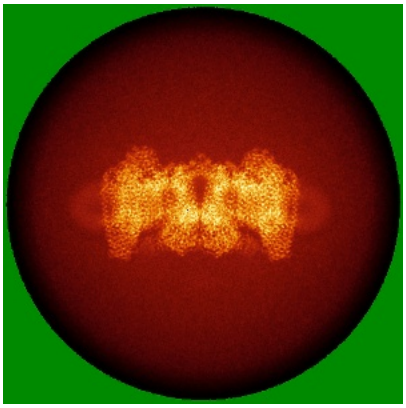

Z Index: 274

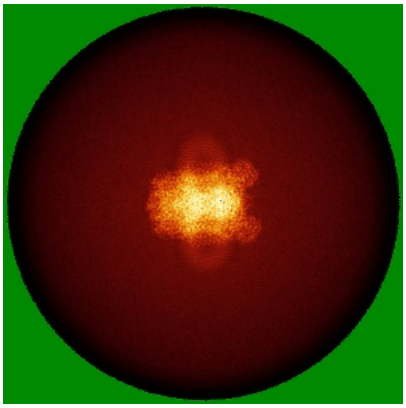
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

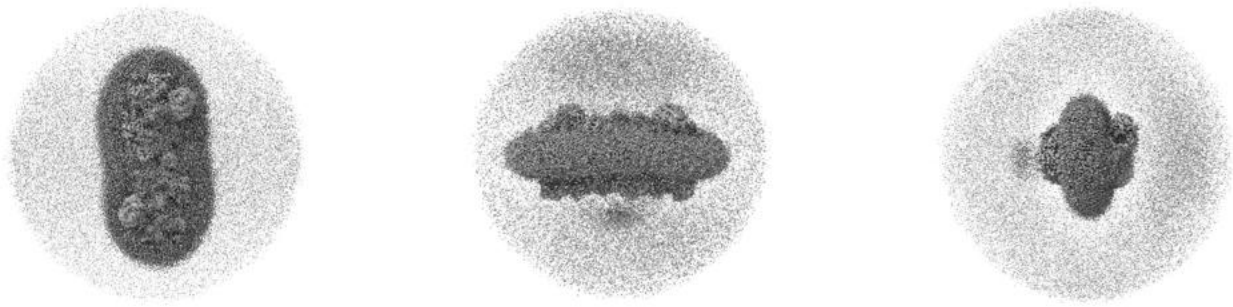

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

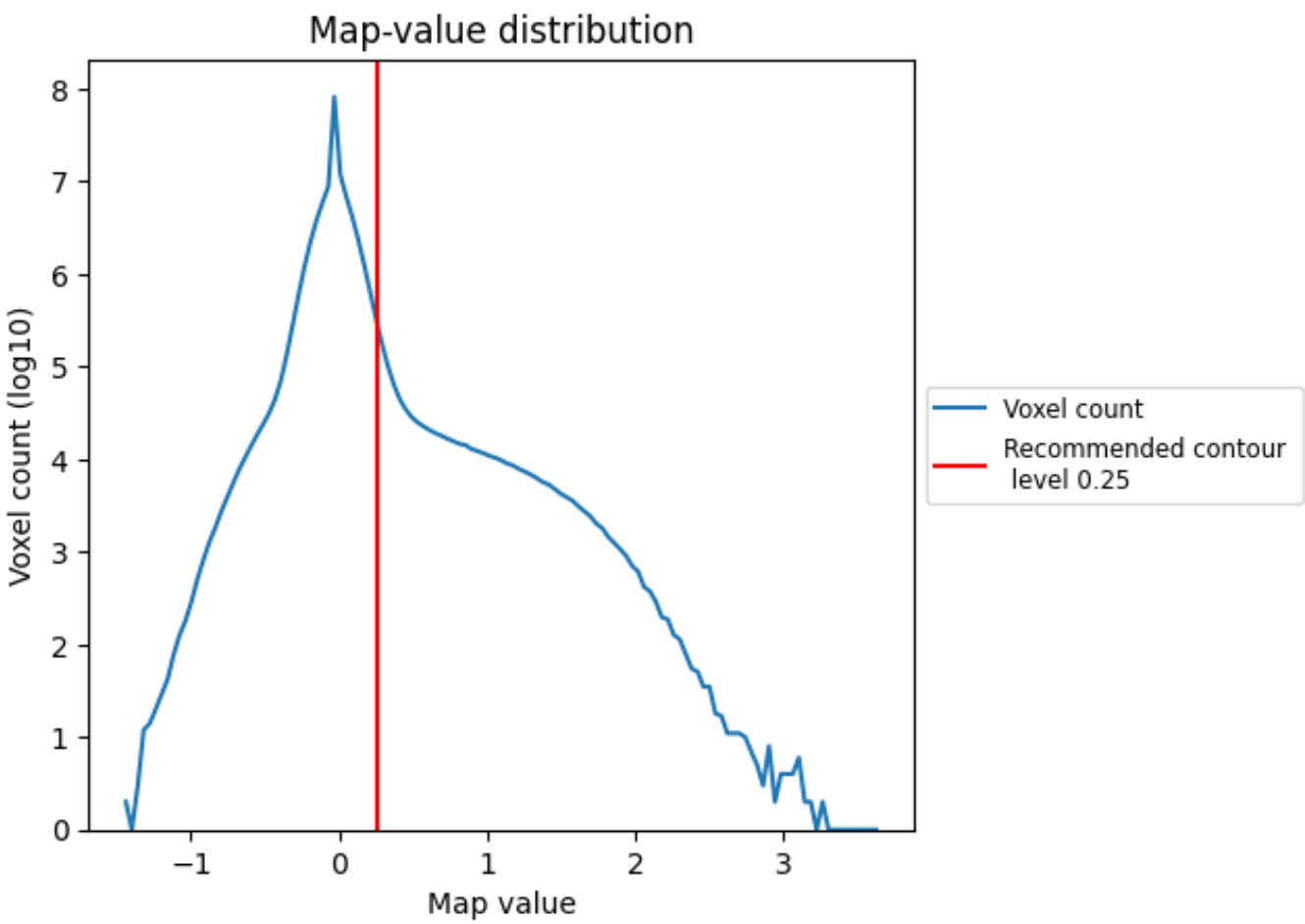
6.6 Mask visualisation (i)

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

7 Map analysis (i)

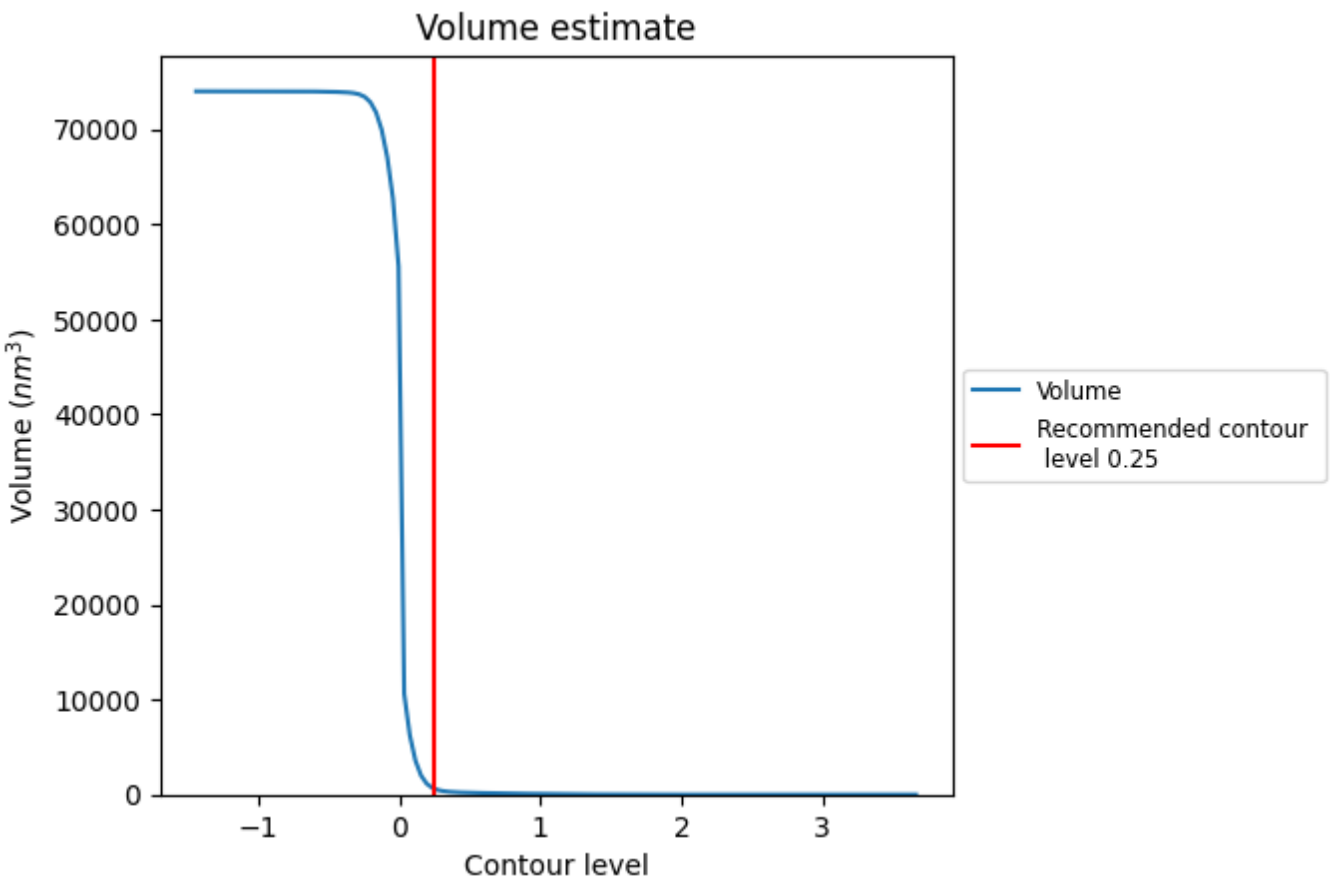
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

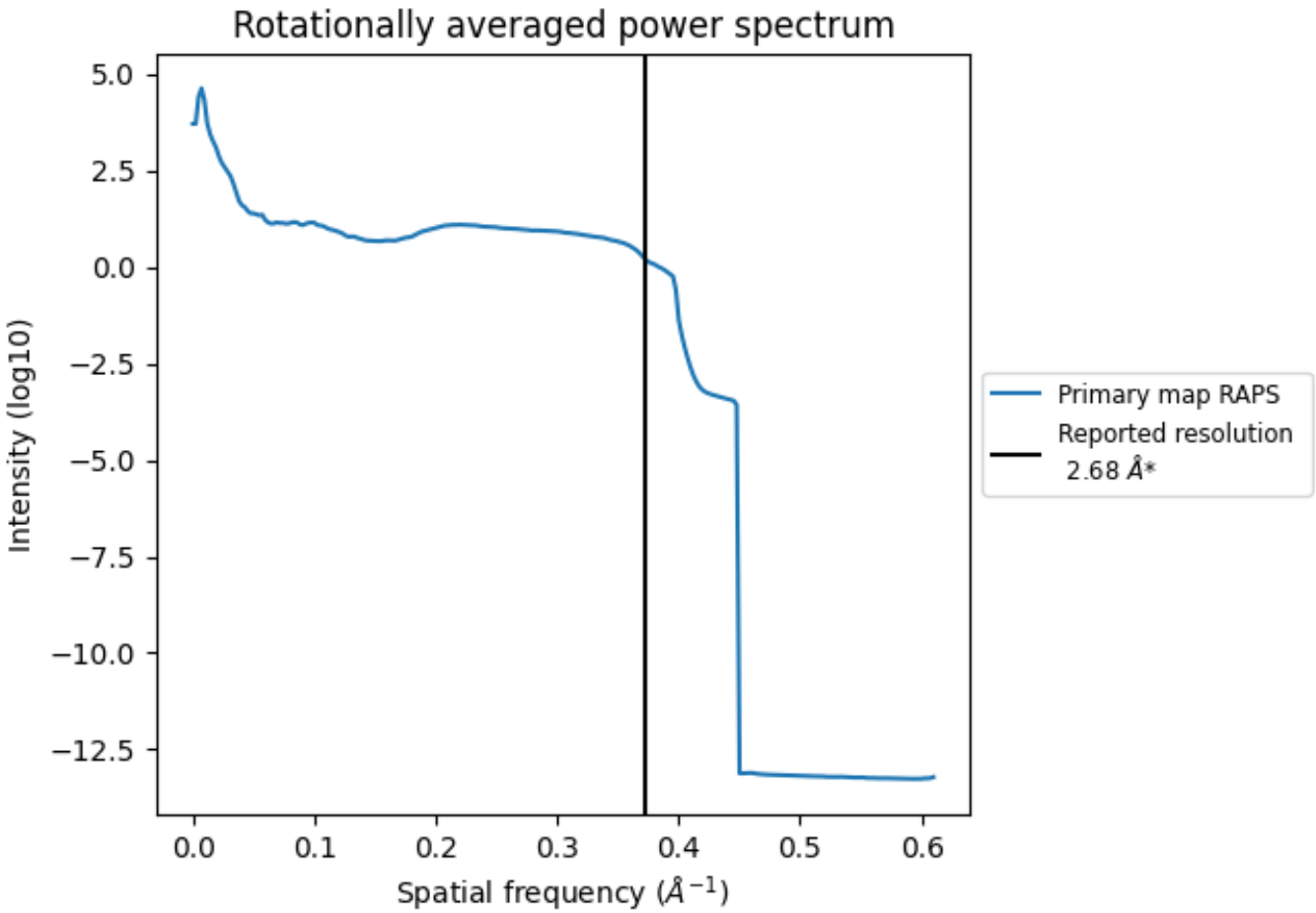
7.2 Volume estimate (i)



The volume at the recommended contour level is 620 nm^3; this corresponds to an approximate mass of 560 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 0.373 Å^{-1}

8 Fourier-Shell correlation (i)

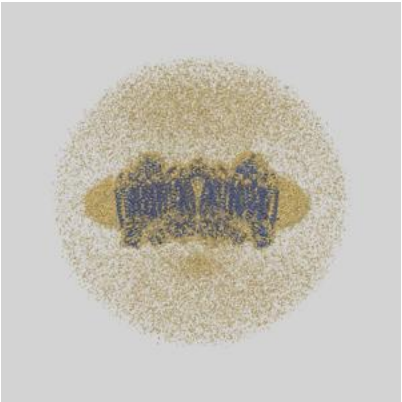
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

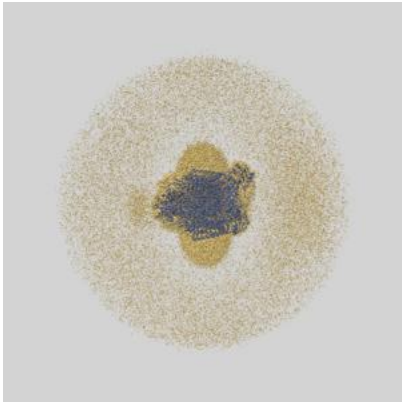
This section contains information regarding the fit between EMDB map EMD-30943 and PDB model 7E1V. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)

X



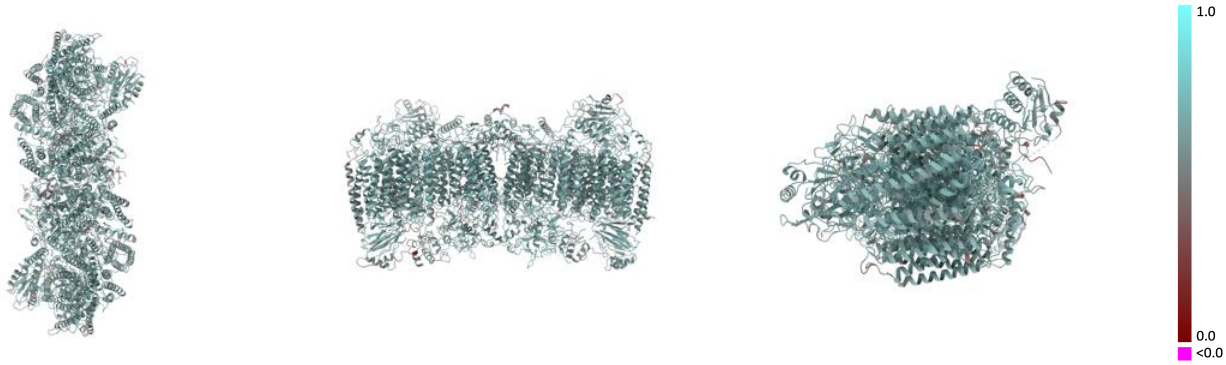
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

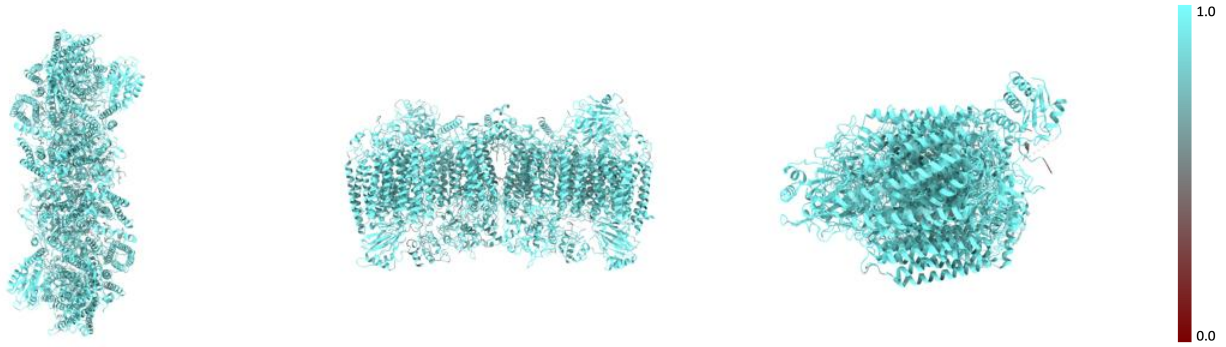
9.2 Q-score mapped to coordinate model (i)



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.

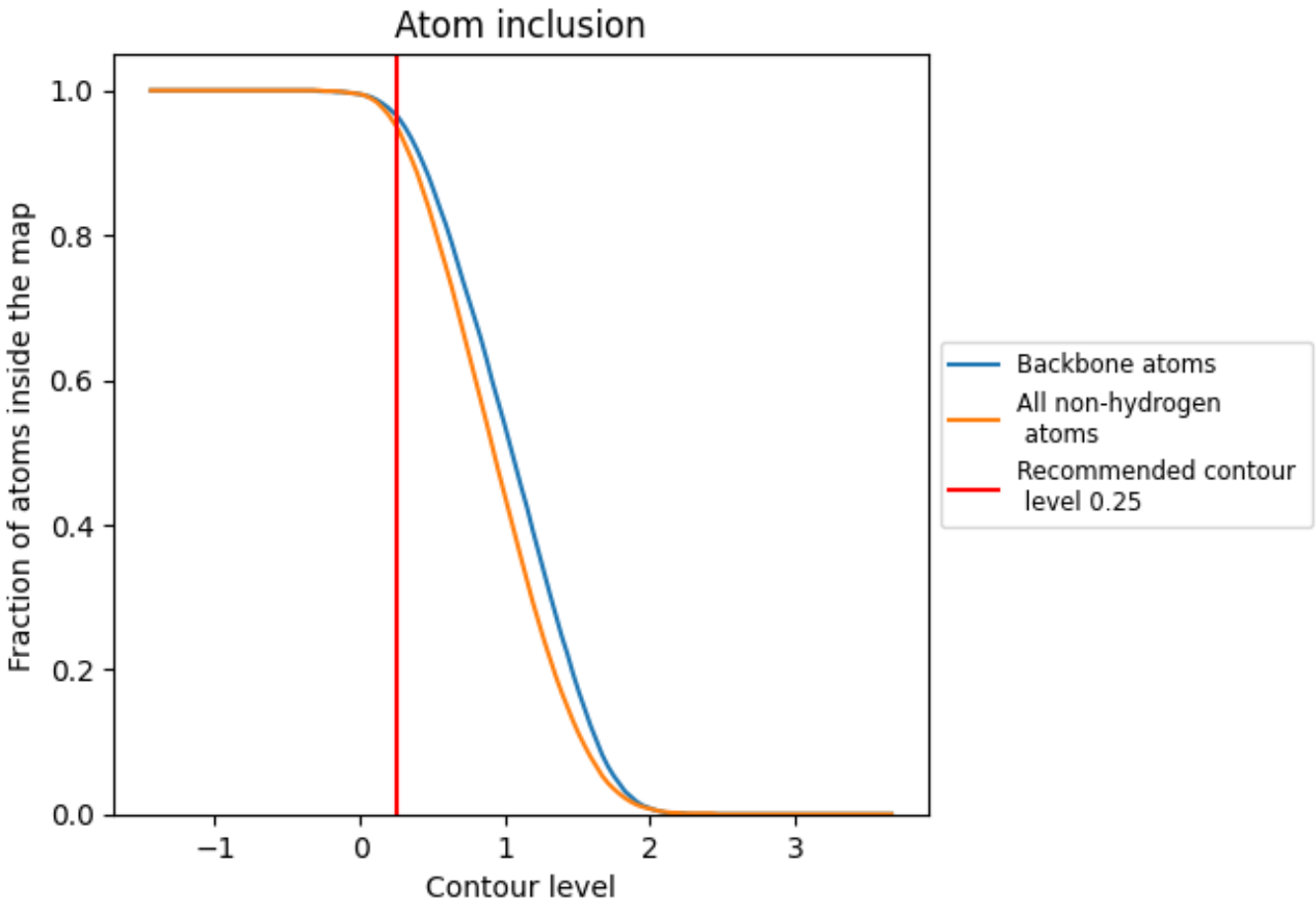
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9510	0.6140
A	0.9560	0.6130
B	0.9590	0.6310
C	0.8700	0.5840
D	0.9530	0.6060
E	0.9500	0.5980
F	0.9780	0.6410
G	0.9500	0.6020
H	0.9620	0.6210
I	0.9490	0.5830
J	0.9460	0.5790
M	0.9510	0.6140
N	0.9580	0.6330
O	0.9290	0.6060
P	0.9450	0.6030
Q	0.9120	0.5590
R	0.9690	0.6340
S	0.9390	0.5940
T	0.9610	0.6180
U	0.9230	0.5700
V	0.9360	0.5660