Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 03:57 AM JST

PDB ID	:	7E1X / pdb_00007e1x
EMDB ID	:	EMD-30945
Title	:	Cryo-EM structure of hybrid respiratory supercomplex consisting of Mycobacterium tuberculosis complexIII and Mycobacterium smegmatis complexIV in presence of TB47
Authors	:	Zhou, S.; Wang, W.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on	:	2021-02-03
Resolution	:	2.93 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 (1)) were used in the production of this report:

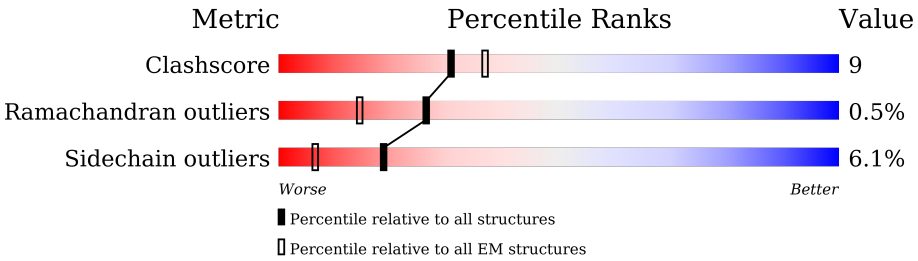
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

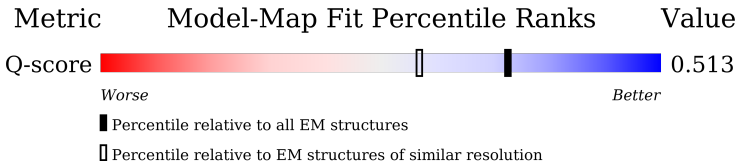
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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	13037 (2.43 - 3.43)

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	67% 14% 19%
1	Q	341	67% 16% 17%
2	F	575	77% 18%
2	R	575	76% 19%

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Mol	Chain	Length	Quality of chain
3	G	203	76% 15% 8%
3	S	203	80% 11% 9%
4	H	139	82% 16%
4	T	139	81% 17%
5	I	79	52% 29% 15%
5	U	79	53% 29% 15%
6	J	157	69% 19% 8%
6	V	157	68% 20% 8%
7	D	100	66% 10% 24%
7	P	100	64% 10% 25%
8	B	549	71% 23% 5%
8	N	549	74% 21% 5%
9	A	429	67% 18% 12%
9	M	429	70% 15% 12%
10	C	280	25% 57% 17% 22%
10	O	280	34% 61% 14% 20%

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
19	FES	A	501	-	-	X	-
21	HEC	C	301	X	-	-	-
21	HEC	C	302	X	-	-	-
21	HEC	O	304	X	-	-	-
21	HEC	O	305	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 42679 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	2242	1459	370	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	1077	719	167	188	3	0	0
4	T	139	1077	719	167	188	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	507	334	85	86	2	0	0
5	U	67	507	334	85	86	2	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	1041	658	176	205	2	0	0
6	V	145	1041	658	176	205	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	605	395	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	4140	2734	707	682	17	0	0
8	B	524	4140	2734	707	682	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	2943	1900	501	531	11	0	0
9	A	378	2943	1900	501	531	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	223	1621	1015	291	304	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	218	1584	995	283	297	9	0	0

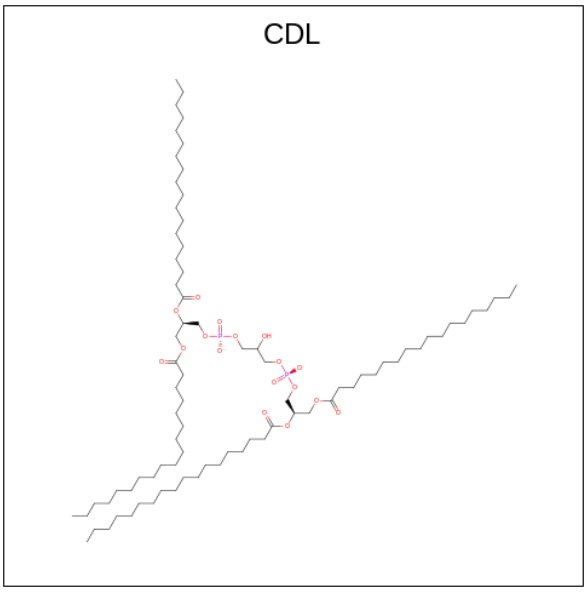
There are 2 discrepancies between the modelled and reference sequences:

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	2	2	2	0
11	R	2	2	2	0

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	F	1	76	57	17	2	0

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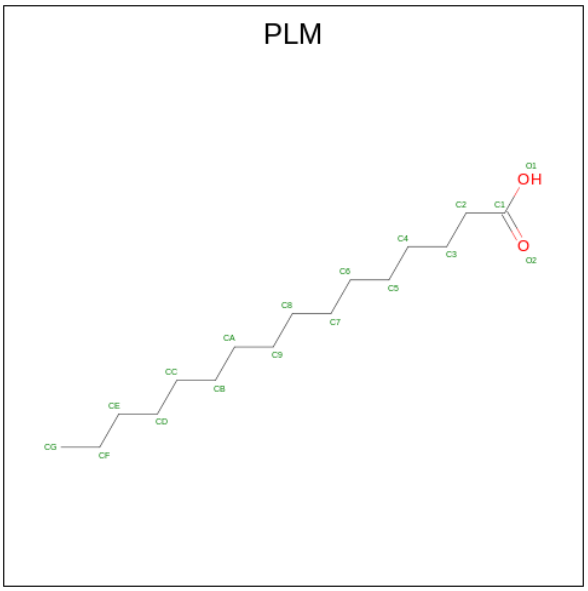
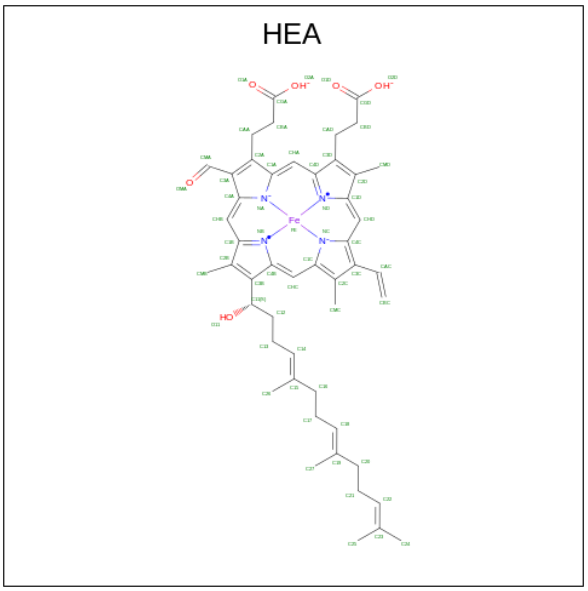
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	F	1	81	62	17	2	0
12	D	1	88	69	17	2	0
12	R	1	76	57	17	2	0
12	R	1	81	62	17	2	0
12	P	1	88	69	17	2	0
12	N	1	74	55	17	2	0
12	N	1	77	58	17	2	0
12	N	1	79	60	17	2	0
12	M	1	95	76	17	2	0
12	O	1	79	60	17	2	0
12	B	1	79	60	17	2	0
12	B	1	66	47	17	2	0
12	B	1	74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



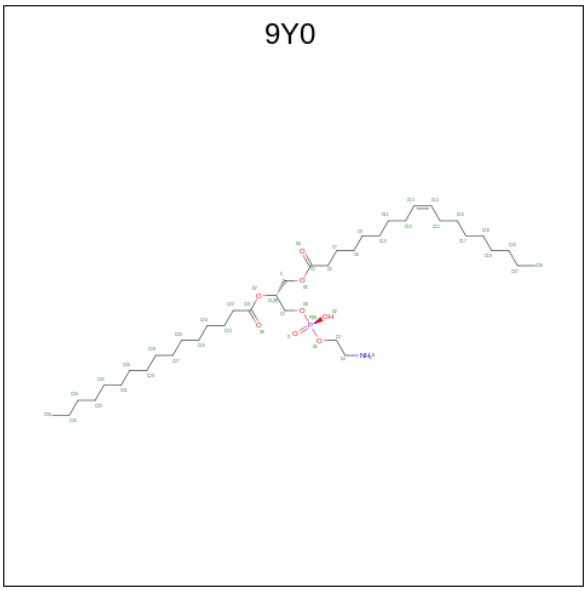
Mol	Chain	Residues	Atoms			AltConf
13	F	1	Total	C	O	0
			17	16	1	
13	R	1	Total	C	O	0
			17	16	1	
13	N	1	Total	C	O	0
			11	10	1	
13	B	1	Total	C	O	0
			11	10	1	

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



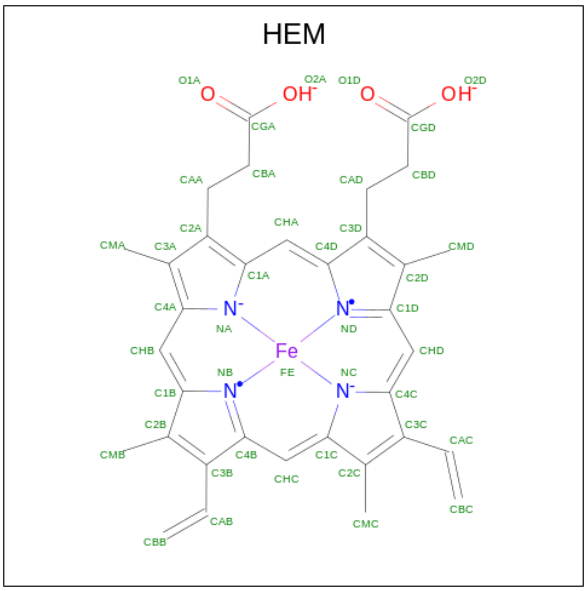
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- 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).



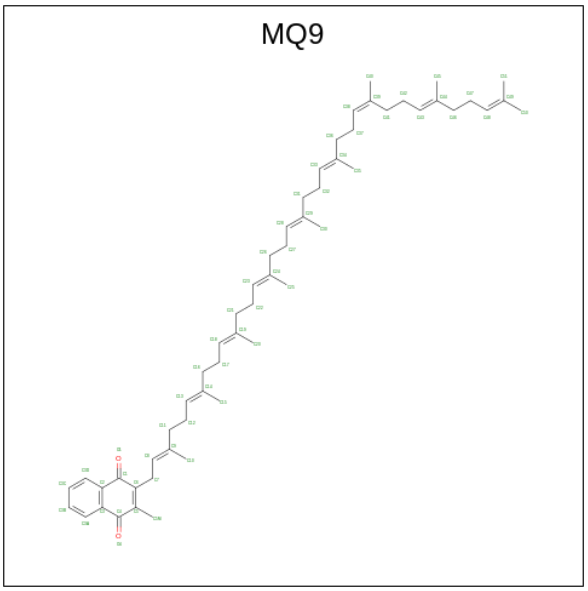
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
15	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- 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).



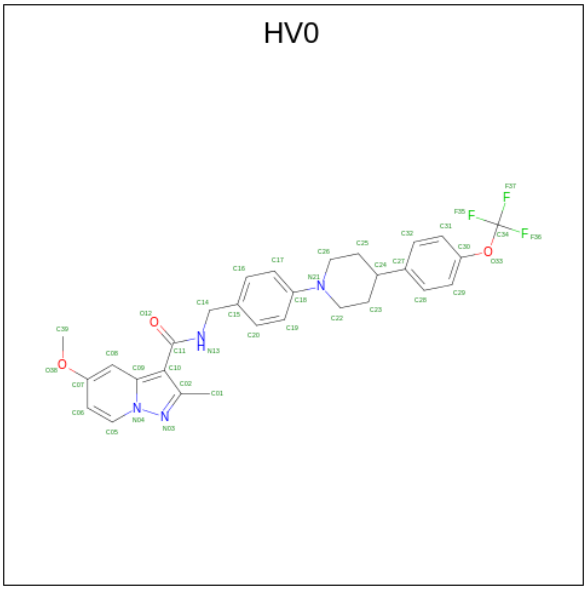
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
16	N	1	42	33	1	4	4	0
			Total	C	Fe	N	O	
16	N	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
16	B	1	42	33	1	4	4	0
			Total	C	Fe	N	O	
16	B	1	43	34	1	4	4	0

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



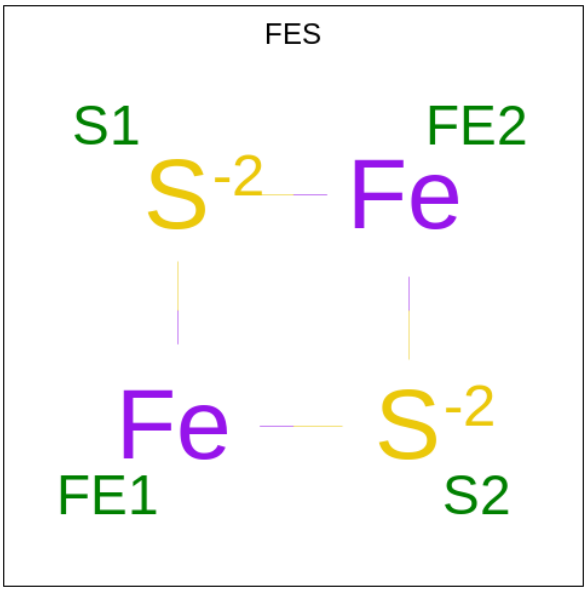
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	N	1	58	56	2	0
			Total	C	O	
17	N	1	58	56	2	0
			Total	C	O	
17	O	1	48	46	2	0
			Total	C	O	
17	O	1	58	56	2	0
			Total	C	O	
17	B	1	43	41	2	0
			Total	C	O	
17	B	1	58	56	2	0
			Total	C	O	
17	A	1	43	41	2	0
			Total	C	O	
17	C	1	48	46	2	0

- Molecule 18 is 5-methoxy-2-methyl- {N}-[[4-[4-[4-(trifluoromethyloxy)phenyl]piperidin-1-yl]phenyl]methyl]pyrazolo[1,5-a]pyridine-3-carboxamide (CCD ID: HV0) (formula: $C_{29}H_{29}F_3N_4O_3$) (labeled as "Ligand of Interest" by depositor).



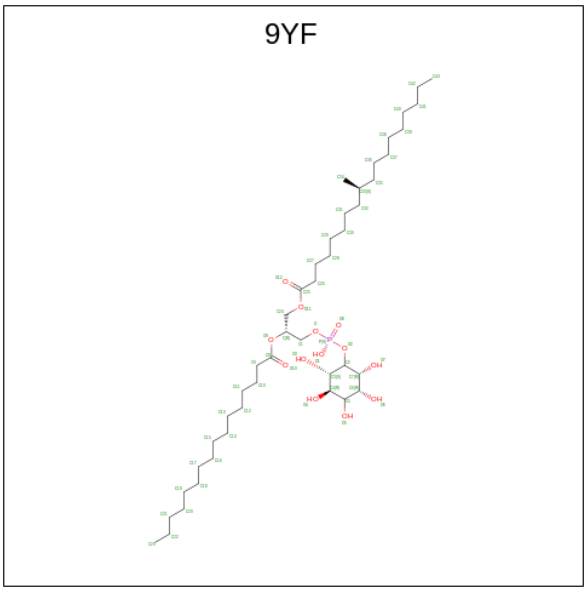
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
18	N	1	39	29	3	4	3	0
			Total	C	F	N	O	
18	B	1	39	29	3	4	3	0

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



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

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	44	30	13	1	0

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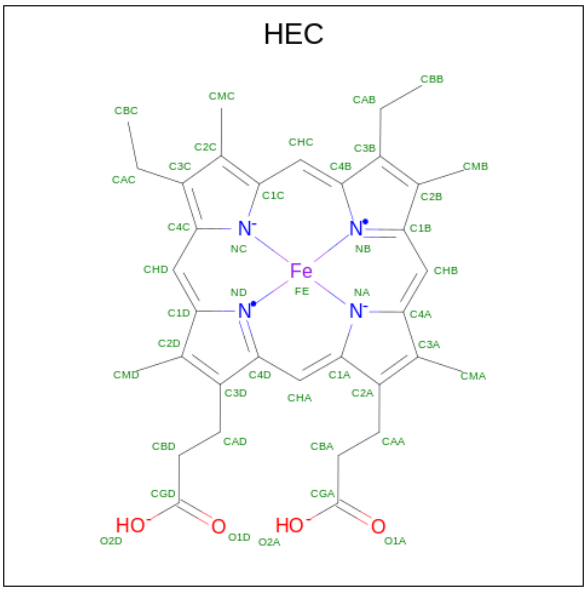
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	40	26	13	1	0
			Total	C	O	P	
20	A	1	51	37	13	1	0
			Total	C	O	P	
20	A	1	42	28	13	1	0

- Molecule 21 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



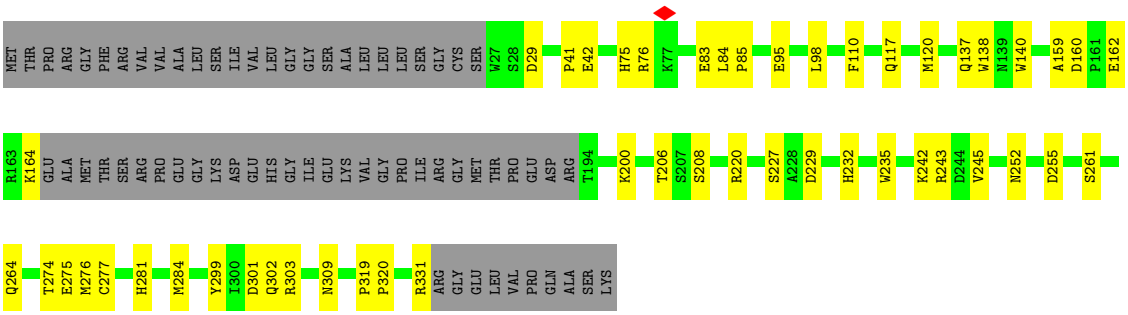
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
21	O	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
21	O	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
21	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
21	C	1	43	34	1	4	4	0

3 Residue-property plots (i)

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

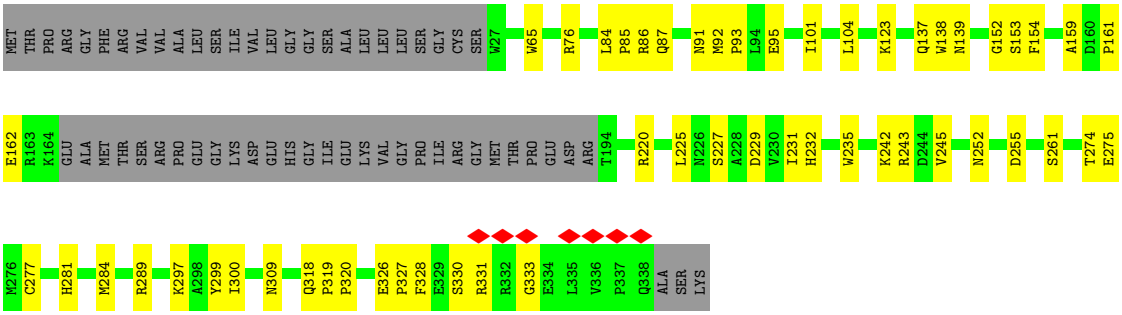
• Molecule 1: Cytochrome c oxidase subunit 2

Chain E:



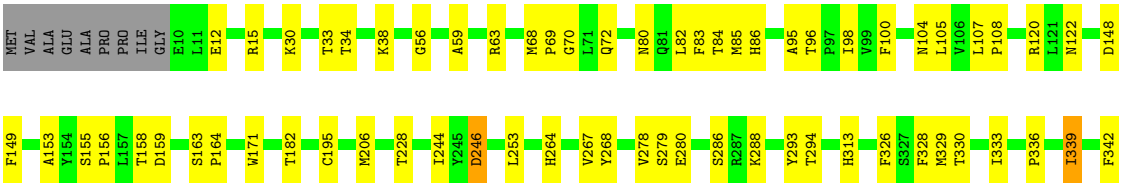
• Molecule 1: Cytochrome c oxidase subunit 2

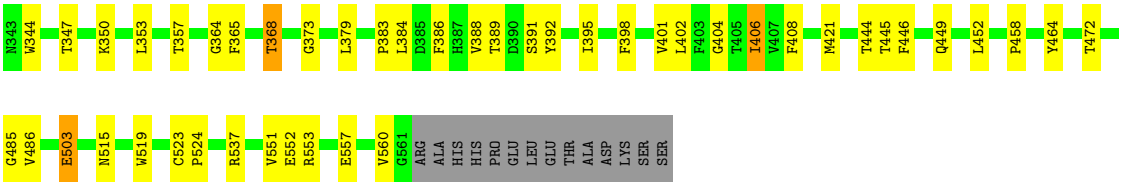
Chain Q:



• Molecule 2: Cytochrome c oxidase subunit 1

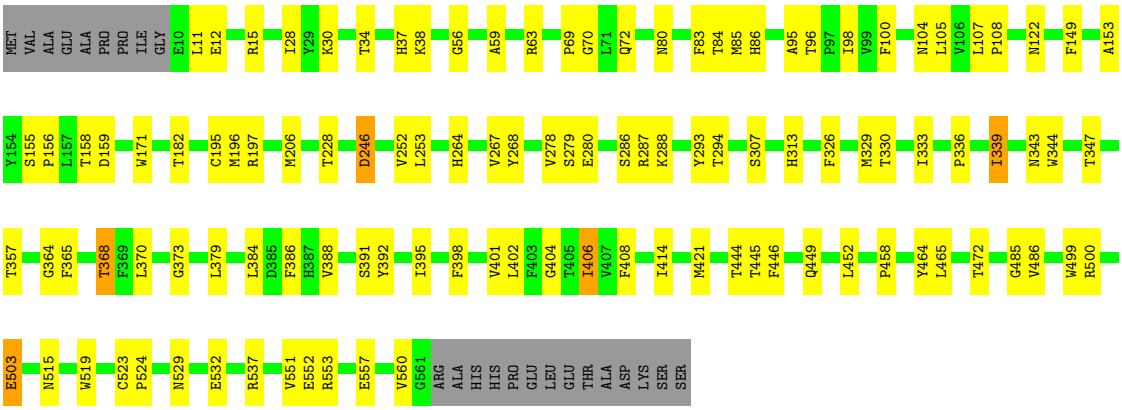
Chain F:





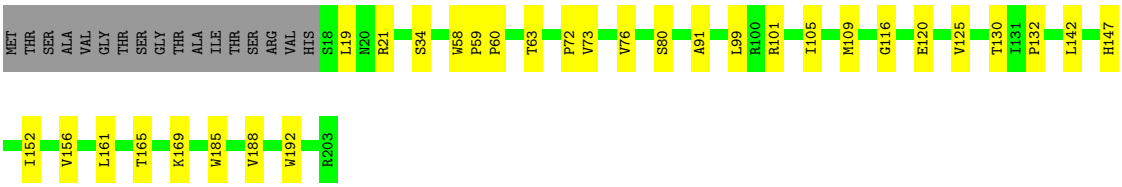
• Molecule 2: Cytochrome c oxidase subunit 1

Chain R:



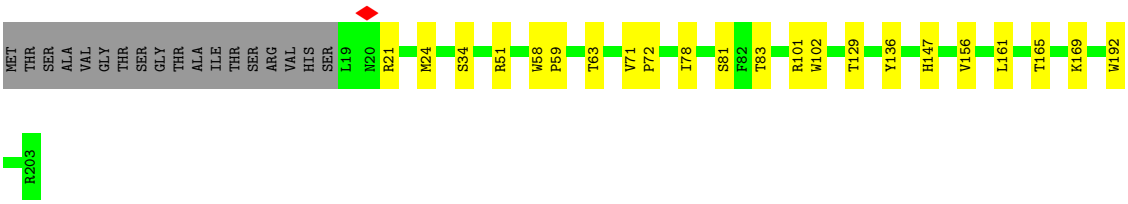
• Molecule 3: Cytochrome c oxidase subunit 3

Chain G:



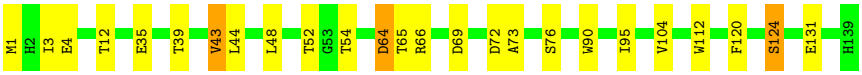
• Molecule 3: Cytochrome c oxidase subunit 3

Chain S:



• Molecule 4: Cytochrome c oxidase polypeptide 4

Chain H:

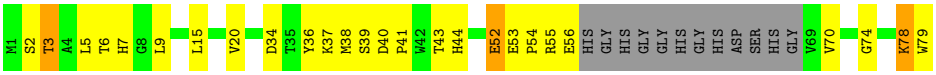


• Molecule 4: Cytochrome c oxidase polypeptide 4

Chain T:

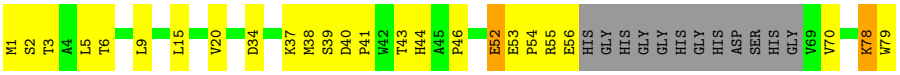
• Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain I:



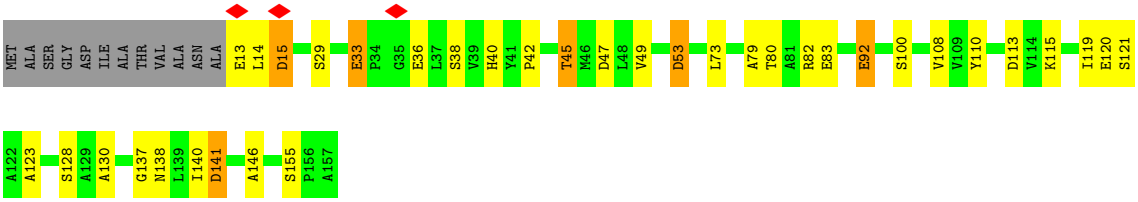
• Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain U:



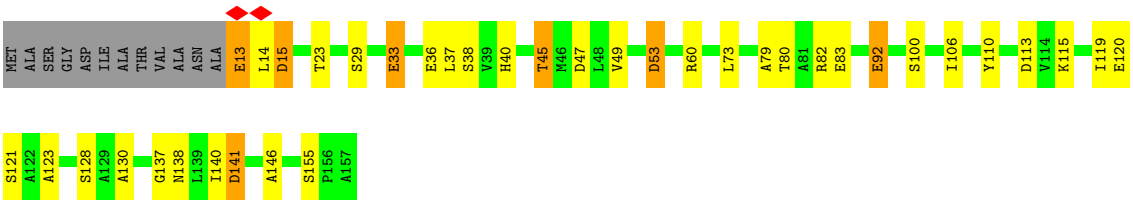
• Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain J:



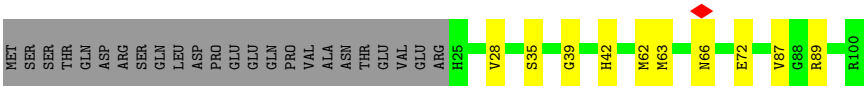
• Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:



• Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain D:



• Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

Chain P: 64% 10% • 25%

MET SER SER THR GLN ASP ARG SER GLN LEU ASP PRO GLU GLU GLN PRO VAL ALA ASN THR GLU VAL GLU ARG HIS T26 G27 V28 D29 G39 H42 L60 V61 M62 H67 V68 E72 D73 R89 R100

• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain N: 74% 21% • 5%

MET SER PRO LYS LEU SER PRO PRO ASN ILE GLY GLU VAL L14 Q17 D20 I21 D22 T23 R24 Y25 H26 P27 S28 A29 A30 L31 R32 R33 Q34 V38 H42 W43 S44 L47 Y53 Y64 S72 M73 V74 T77 G80 V81 Y82 Q83 P84 L85 R86 F109

V110 I113 W116 V127 R140 E143 S150 I154 Y161 Y164 D169 L170 L171 S172 G173 R177 S181 T184 I190 G191 L194 D202 F203 P204 L215 L218 L219 H231 T249 V253 V258 M259 P260 V261 F262 A263 S266

I273 G281 G282 Q285 P288 L292 Y295 S301 A302 G303 S304 E314 H329 H330 P335 V340 V347 E356 Q370 V375 R378 M384 F388 D399 L409 W414 R417 M420 V421 I422 L423 P424 T431 Y432 R433

S441 D442 R443 E447 H448 T452 K456 R457 L458 P459 H460 L466 V473 D474 E475 H476 I480 R492 G500 S501 G505 L508 D516 R520 E527 Q528 R529 A530 L531 R535 E536 H537 GLN ASP SER ILE MET GLY SER PRO ASP GLY GLU HIS

• Molecule 8: Cytochrome bc1 complex cytochrome b subunit

Chain B: 71% 23% • 5%

MET SER PRO LYS LEU SER PRO PRO ASN ILE GLY GLU VAL L14 Q17 D20 I21 D22 T23 R24 Y25 H26 P27 S28 A29 A30 L31 R32 R33 Q34 L35 N36 H42 W43 S44 L47 Y53 S54 F55 Y64 S72 M73 V74 T77 G80 V81 Y82 Q83 P84 L85 R86

F109 V110 I113 W116 M120 A123 M126 V127 R140 E143 T144 S150 I154 Y161 Y164 D169 L170 L171 S172 G173 R177 A178 S181 S182 I183 T184 I190 G191 L194 D202 L215 L218 L219 T249 V253 V258 M259

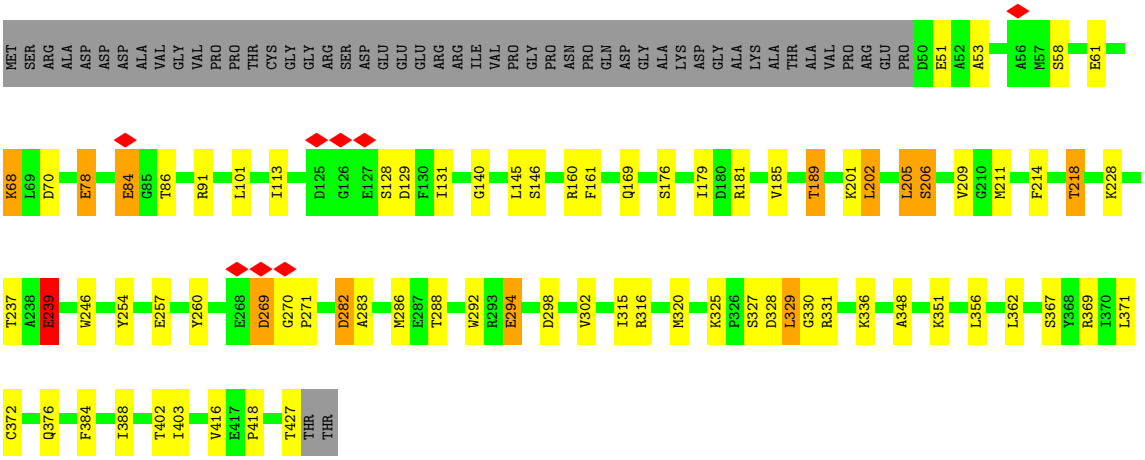
P260 V261 F262 A263 F264 K265 S266 A271 A272 I273 G281 G282 Q285 I286 N287 P288 L292 Y295 K296 P297 S301 A302 G303 S304 Q305 P306 T313 E314 W320 P321 P322 H329 H330 P335 V340 V347 E356 Q370 R371 P372 V375 R378 M384

F388 M397 N398 D399 L409 W414 N420 V421 I422 L423 P424 I430 T431 S441 E447 H448 T452 I455 K456 R457 L458 P459 H460 L466 V473 D474 E475 H476 I480 G500 S501 L508 D516 R520 E527 Q528 R529 A530 L531 R535 E536

H537 GLN ASP SER ILE MET GLY SER PRO ASP GLY GLU HIS

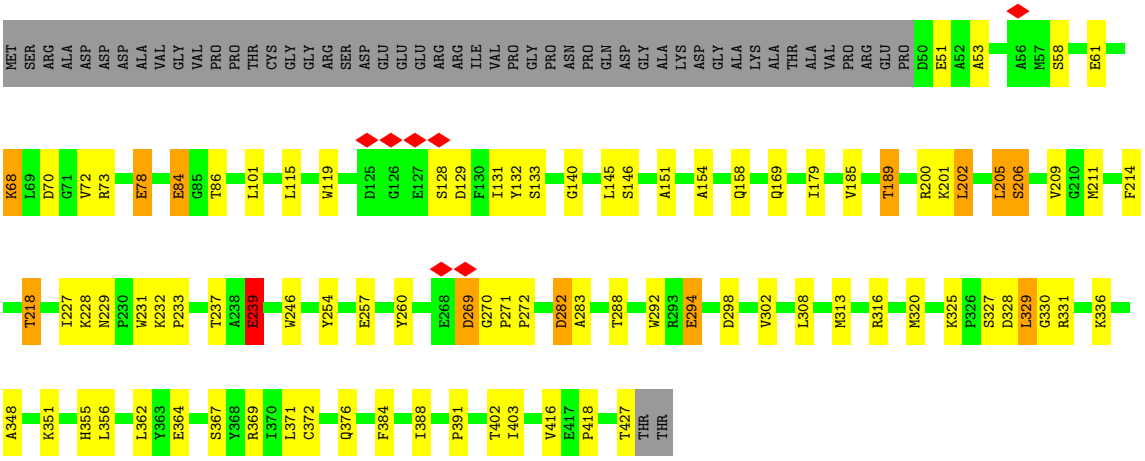
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M: • 70% 15% • 12%



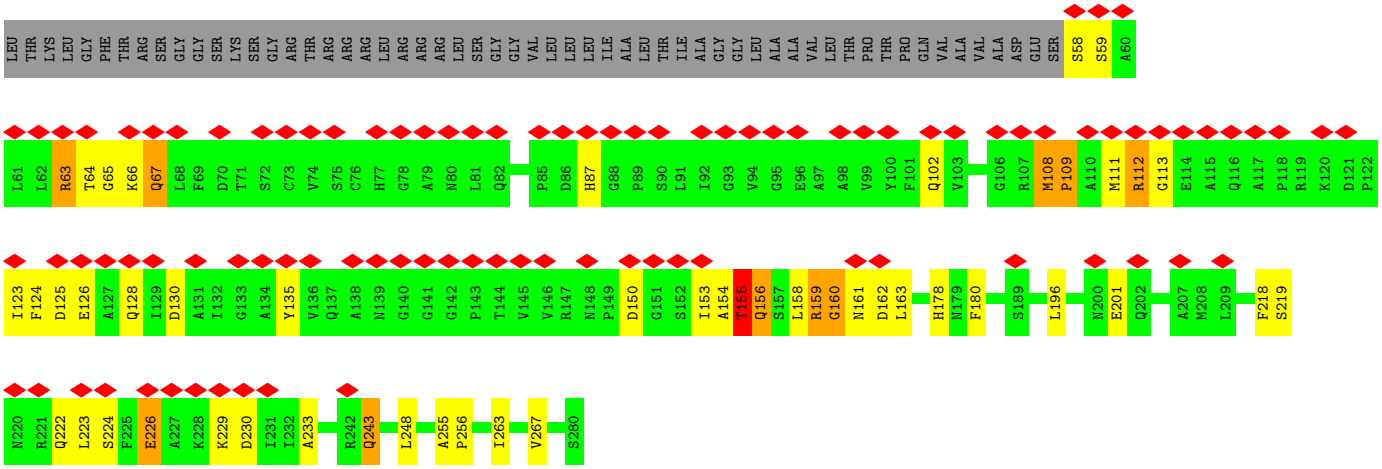
• Molecule 9: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A:



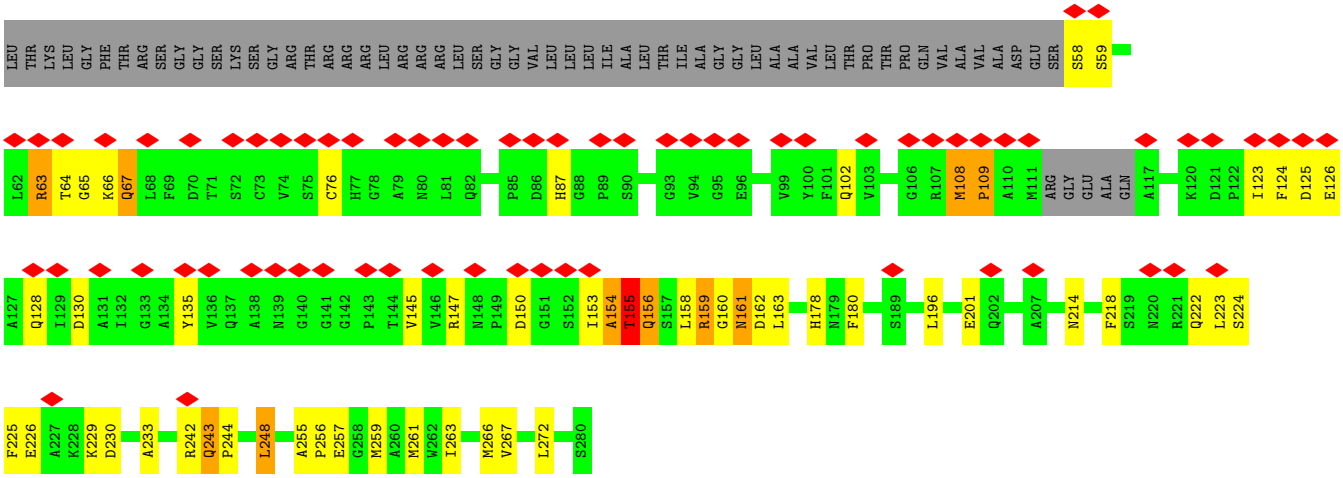
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

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	169988	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	3.778	Depositor
Minimum map value	-2.364	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.089	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: MQ9, CU, FES, HEA, HEC, PLM, 9Y0, HEM, HV0, 9YF, CDL

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	0.21	0/2254	0.39	0/3072
1	Q	0.23	0/2306	0.42	0/3144
2	F	0.25	0/4533	0.44	0/6192
2	R	0.26	0/4533	0.44	0/6192
3	G	0.23	0/1502	0.47	0/2051
3	S	0.24	0/1496	0.43	0/2043
4	H	0.22	0/1112	0.44	0/1524
4	T	0.22	0/1112	0.44	0/1524
5	I	0.21	0/523	0.54	0/714
5	U	0.21	0/523	0.54	0/714
6	J	0.24	0/1059	0.52	0/1446
6	V	0.24	0/1059	0.52	0/1446
7	D	0.19	0/626	0.37	0/852
7	P	0.22	0/617	0.42	1/840 (0.1%)
8	B	0.25	0/4276	0.55	3/5833 (0.1%)
8	N	0.25	0/4276	0.48	2/5833 (0.0%)
9	A	0.28	1/3020 (0.0%)	0.48	1/4094 (0.0%)
9	M	0.25	0/3020	0.48	1/4094 (0.0%)
10	C	0.41	1/1616 (0.1%)	0.74	6/2188 (0.3%)
10	O	0.34	1/1654 (0.1%)	0.65	5/2239 (0.2%)
All	All	0.26	3/41117 (0.0%)	0.49	19/56035 (0.0%)

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
10	C	0	1
10	O	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	355	HIS	CA-C	-6.81	1.48	1.52
10	O	154	ALA	N-CA	6.53	1.54	1.45
10	C	161	ASN	CA-C	-6.18	1.44	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	304	SER	CB-CA-C	18.68	147.60	110.42
8	B	305	GLN	N-CA-CB	11.79	131.37	110.37
10	O	154	ALA	N-CA-C	11.40	124.33	110.19
10	C	161	ASN	CA-C-N	-10.91	105.28	121.76
10	C	161	ASN	C-N-CA	-10.91	105.28	121.76
8	N	304	SER	N-CA-CB	-9.14	97.65	111.64
8	N	303	GLY	N-CA-C	-8.95	91.98	113.18
8	B	304	SER	N-CA-C	-8.33	93.05	110.80
10	C	156	GLN	N-CA-C	7.46	126.69	110.80
10	O	155	THR	N-CA-C	6.38	124.39	110.80
10	O	67	GLN	N-CA-C	-6.19	107.56	114.62
10	C	67	GLN	N-CA-C	-6.14	107.62	114.62
7	P	67	HIS	CA-C-O	-6.03	108.45	119.36
10	O	156	GLN	N-CA-C	6.02	120.36	113.19
10	C	155	THR	N-CA-C	5.78	123.12	110.80
10	O	153	ILE	O-C-N	-5.63	116.56	122.81
10	C	154	ALA	N-CA-C	5.63	122.79	110.80
9	M	239	GLU	CA-CB-CG	5.42	124.95	114.10
9	A	239	GLU	CA-CB-CG	5.42	124.93	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	C	108	MET	Peptide
10	O	108	MET	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	40	0
1	Q	2242	0	2175	44	0
2	F	4373	0	4347	72	0
2	R	4373	0	4347	88	0
3	G	1455	0	1455	21	0
3	S	1449	0	1450	17	0
4	H	1077	0	1058	14	0
4	T	1077	0	1058	16	0
5	I	507	0	516	12	0
5	U	507	0	516	12	0
6	J	1041	0	1052	21	0
6	V	1041	0	1052	24	0
7	D	605	0	587	9	0
7	P	597	0	586	10	0
8	B	4140	0	4163	89	0
8	N	4140	0	4165	71	0
9	A	2943	0	2931	85	0
9	M	2943	0	2931	61	0
10	C	1584	0	1562	53	0
10	O	1621	0	1598	42	0
11	E	2	0	0	0	0
11	F	2	0	0	0	0
11	Q	2	0	0	0	0
11	R	2	0	0	0	0
12	A	95	0	143	5	0
12	B	375	0	476	13	0
12	D	88	0	126	6	0
12	F	157	0	208	3	0
12	M	95	0	143	1	0
12	N	230	0	295	9	0
12	O	79	0	105	2	0
12	P	88	0	126	8	0
12	R	157	0	208	5	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	104	14	0
14	R	120	0	104	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	43	0	53	6	0
17	B	101	0	133	13	0
17	C	48	0	61	4	0
17	N	116	0	158	5	0
17	O	106	0	141	7	0
18	B	39	0	0	0	0
18	N	39	0	0	0	0
19	A	4	0	0	3	0
19	M	4	0	0	1	0
20	A	93	0	0	24	0
20	M	84	0	0	10	0
21	C	86	0	62	3	0
21	O	86	0	58	1	0
All	All	42679	0	42590	761	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (761) 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)
10:C:76:CYS:CB	21:C:301:HEC:HBC2	1.30	1.54
2:R:264:HIS:NE2	2:R:268:TYR:CE2	2.06	1.24
10:C:76:CYS:CB	21:C:301:HEC:CBC	2.18	1.20
2:R:268:TYR:OH	2:R:333:ILE:HD13	1.38	1.17
2:R:268:TYR:CD2	2:R:307:SER:HB2	1.82	1.15
20:M:504:9YF:O4	9:A:119:TRP:HZ2	1.34	1.09
9:M:246:TRP:HH2	20:M:503:9YF:C2	1.65	1.09
20:M:504:9YF:O4	9:A:119:TRP:CZ2	2.05	1.08
9:A:228:LYS:NZ	20:A:503:9YF:O4	1.86	1.08
2:R:264:HIS:CD2	2:R:268:TYR:CE2	2.44	1.06
9:M:246:TRP:CH2	20:M:503:9YF:C2	2.41	1.03
2:R:268:TYR:OH	2:R:333:ILE:CD1	2.07	1.00
9:A:246:TRP:CZ3	20:A:505:9YF:O1	2.15	1.00
9:A:246:TRP:HZ3	20:A:505:9YF:O1	1.45	0.99
9:M:228:LYS:HG2	20:M:504:9YF:O7	1.66	0.95
10:C:145:VAL:HG11	10:C:153:ILE:HD13	1.45	0.94
8:N:74:VAL:HG21	8:B:74:VAL:HG21	1.52	0.92
9:A:372:CYS:SG	19:A:501:FES:FE2	1.63	0.90
9:A:246:TRP:CZ3	20:A:505:9YF:O3	2.25	0.89
9:M:372:CYS:HG	19:M:501:FES:FE1	0.84	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:264:HIS:CD2	2:R:268:TYR:CD2	2.61	0.87
2:R:264:HIS:NE2	2:R:268:TYR:HE2	1.74	0.85
9:A:372:CYS:HG	19:A:501:FES:FE2	0.56	0.84
9:M:246:TRP:HH2	20:M:503:9YF:O2	1.61	0.84
1:E:331:ARG:HG2	10:O:87:HIS:HE1	1.42	0.82
10:C:160:GLY:C	10:C:162:ASP:H	1.89	0.80
9:A:246:TRP:CH2	20:A:505:9YF:C2	2.65	0.79
9:A:246:TRP:CH2	20:A:505:9YF:O3	2.36	0.79
9:M:269:ASP:OD1	9:M:269:ASP:N	2.17	0.78
9:A:269:ASP:OD1	9:A:269:ASP:N	2.16	0.78
2:F:373:GLY:HA3	14:F:606:HEA:H262	1.66	0.78
2:R:373:GLY:HA3	14:R:606:HEA:H262	1.66	0.78
8:B:24:ARG:NH1	12:B:605:CDL:OB7	2.18	0.77
16:N:602:HEM:HHC	16:N:602:HEM:HBB2	1.66	0.76
2:F:246:ASP:OD1	2:F:246:ASP:N	2.14	0.75
2:R:264:HIS:CD2	2:R:268:TYR:HE2	1.99	0.75
16:B:602:HEM:HHC	16:B:602:HEM:HBB2	1.66	0.75
6:J:15:ASP:N	6:J:15:ASP:OD1	2.17	0.75
2:R:246:ASP:OD1	2:R:246:ASP:N	2.15	0.75
3:S:58:TRP:CD1	3:S:59:PRO:HD3	2.21	0.75
6:V:15:ASP:OD1	6:V:15:ASP:N	2.17	0.74
9:A:239:GLU:N	9:A:239:GLU:OE1	2.21	0.74
10:C:145:VAL:HG11	10:C:153:ILE:CD1	2.17	0.73
9:M:239:GLU:N	9:M:239:GLU:OE1	2.21	0.73
3:G:58:TRP:CD1	3:G:59:PRO:HD3	2.22	0.73
1:E:76:ARG:HA	2:F:353:LEU:HB2	1.69	0.73
2:R:268:TYR:CE2	2:R:307:SER:HB2	2.23	0.72
8:N:409:LEU:HD21	9:M:376:GLN:HG2	1.71	0.72
9:M:214:PHE:O	9:M:218:THR:OG1	2.07	0.72
12:R:602:CDL:H121	12:P:201:CDL:H512	1.71	0.71
6:V:33:GLU:N	6:V:33:GLU:OE1	2.23	0.71
9:A:185:VAL:O	9:A:189:THR:OG1	2.08	0.71
9:A:202:LEU:O	9:A:206:SER:OG	2.08	0.71
9:M:185:VAL:O	9:M:189:THR:OG1	2.08	0.71
9:A:214:PHE:O	9:A:218:THR:OG1	2.07	0.71
6:J:33:GLU:N	6:J:33:GLU:OE1	2.23	0.71
9:M:181:ARG:NH1	8:B:22:ASP:OD2	2.24	0.71
5:I:38:MET:HE2	6:J:137:GLY:HA2	1.72	0.71
9:M:202:LEU:O	9:M:206:SER:OG	2.08	0.71
10:O:158:LEU:HA	10:O:229:LYS:HE3	1.73	0.71
10:C:160:GLY:C	10:C:162:ASP:N	2.46	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:282:ASP:N	9:A:282:ASP:OD1	2.22	0.71
9:M:282:ASP:N	9:M:282:ASP:OD1	2.22	0.70
10:O:109:PRO:HD3	21:O:304:HEC:HAB	1.73	0.70
1:Q:243:ARG:NH1	1:Q:255:ASP:O	2.25	0.69
2:R:63:ARG:HD3	14:R:607:HEA:HMA	1.75	0.69
2:F:63:ARG:HD3	14:F:607:HEA:HMA	1.74	0.69
8:B:32:ARG:NH2	9:A:70:ASP:OD2	2.24	0.69
1:E:41:PRO:HD3	1:E:264:GLN:HE22	1.58	0.69
10:C:102:GLN:HB3	10:C:108:MET:HG2	1.74	0.69
10:C:109:PRO:HD3	21:C:301:HEC:HAB	1.73	0.69
10:O:102:GLN:HB3	10:O:108:MET:HG2	1.74	0.69
3:S:34:SER:HB3	4:T:48:LEU:HG	1.74	0.68
5:U:38:MET:HE2	6:V:137:GLY:HA2	1.74	0.68
8:N:27:PRO:O	8:N:29:ALA:N	2.27	0.68
8:B:27:PRO:O	8:B:29:ALA:N	2.27	0.68
8:N:529:ARG:NH2	9:M:78:GLU:OE2	2.24	0.67
1:Q:289:ARG:NH1	1:Q:318:GLN:OE1	2.27	0.67
1:Q:137:GLN:HG2	1:Q:229:ASP:OD2	1.95	0.67
8:B:260:PRO:HG2	8:B:261:VAL:HG23	1.77	0.67
8:N:260:PRO:HG2	8:N:261:VAL:HG23	1.77	0.67
9:M:302:VAL:HG12	9:A:302:VAL:HG12	1.77	0.67
9:A:246:TRP:CE3	20:A:505:9YF:O3	2.47	0.67
8:B:306:PRO:HD3	8:B:314:GLU:OE1	1.95	0.67
10:C:153:ILE:HG22	10:C:153:ILE:O	1.96	0.66
12:P:201:CDL:H182	8:B:384:MET:HE1	1.77	0.65
2:R:268:TYR:CD2	2:R:307:SER:CB	2.72	0.65
8:N:384:MET:HG3	8:N:424:PRO:HB3	1.78	0.65
9:A:227:ILE:HD12	20:A:503:9YF:C13	2.27	0.65
8:B:384:MET:HG3	8:B:424:PRO:HB3	1.77	0.65
1:E:331:ARG:HG2	10:O:87:HIS:CE1	2.28	0.64
3:G:101:ARG:NH1	8:N:508:LEU:O	2.30	0.64
1:Q:84:LEU:O	2:R:553:ARG:NH2	2.29	0.64
8:N:33:ARG:NH1	12:N:604:CDL:OB3	2.30	0.64
17:N:607:MQ9:H101	17:A:502:MQ9:H3B	1.79	0.64
6:J:138:ASN:HB3	6:J:141:ASP:HB2	1.79	0.64
6:V:138:ASN:HB3	6:V:141:ASP:HB2	1.79	0.64
9:M:282:ASP:OD1	10:O:219:SER:HB3	1.97	0.64
2:F:206:MET:O	2:F:293:TYR:OH	2.13	0.64
1:E:275:GLU:HG3	1:E:276:MET:H	1.63	0.64
8:B:30:ALA:O	8:B:34:GLN:NE2	2.31	0.64
8:N:30:ALA:O	8:N:34:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:124:PHE:HB3	10:C:128:GLN:HG3	1.80	0.64
1:Q:76:ARG:HD2	2:R:287:ARG:HH12	1.62	0.63
8:B:282:GLY:HA3	9:A:140:GLY:HA3	1.79	0.63
8:B:409:LEU:HD21	9:A:376:GLN:HG2	1.80	0.63
2:R:206:MET:O	2:R:293:TYR:OH	2.14	0.63
10:O:124:PHE:HB3	10:O:128:GLN:HG3	1.80	0.63
10:O:218:PHE:HA	10:O:222:GLN:HE21	1.63	0.63
1:Q:227:SER:HB2	1:Q:245:VAL:HG12	1.80	0.62
4:H:120:PHE:HZ	10:O:263:ILE:HD11	1.65	0.62
16:N:602:HEM:HMC1	16:N:602:HEM:HBC2	1.82	0.62
10:O:160:GLY:O	10:O:162:ASP:N	2.33	0.62
9:M:78:GLU:HA	9:M:78:GLU:OE1	1.99	0.62
10:C:218:PHE:HA	10:C:222:GLN:HE21	1.63	0.62
8:N:253:VAL:HB	9:M:169:GLN:HB3	1.82	0.62
17:O:303:MQ9:C9	17:O:303:MQ9:H151	2.29	0.62
16:B:602:HEM:HMC1	16:B:602:HEM:HBC2	1.82	0.62
10:C:145:VAL:CG1	10:C:153:ILE:HD13	2.26	0.62
17:B:610:MQ9:H412	17:B:610:MQ9:H353	1.82	0.61
4:H:104:VAL:HG11	17:O:302:MQ9:H203	1.81	0.61
2:R:523:CYS:HB3	2:R:524:PRO:HD3	1.82	0.61
9:A:78:GLU:HA	9:A:78:GLU:OE1	1.99	0.61
3:G:34:SER:HB3	4:H:48:LEU:HG	1.83	0.61
2:F:523:CYS:HB3	2:F:524:PRO:HD3	1.83	0.61
7:P:67:HIS:HB3	7:P:72:GLU:OE2	2.00	0.61
8:B:529:ARG:NH2	9:A:78:GLU:OE2	2.26	0.61
10:C:125:ASP:O	10:C:128:GLN:NE2	2.33	0.61
8:N:458:LEU:O	8:N:460:HIS:N	2.34	0.61
8:B:262:PHE:O	8:B:266:SER:OG	2.18	0.61
9:A:229:ASN:HB2	20:A:503:9YF:C1	2.30	0.61
2:F:164:PRO:HD2	10:O:112:ARG:HH22	1.65	0.61
4:T:120:PHE:O	4:T:124:SER:OG	2.18	0.61
10:O:160:GLY:C	10:O:162:ASP:H	2.09	0.61
4:H:120:PHE:O	4:H:124:SER:OG	2.18	0.61
8:N:262:PHE:O	8:N:266:SER:OG	2.18	0.61
10:O:125:ASP:O	10:O:128:GLN:NE2	2.33	0.61
8:B:458:LEU:O	8:B:460:HIS:N	2.34	0.61
16:B:601:HEM:HMB2	16:B:601:HEM:HBB2	1.83	0.61
3:G:147:HIS:CE1	3:G:192:TRP:HB2	2.36	0.60
1:Q:225:LEU:HD23	1:Q:245:VAL:HG22	1.81	0.60
4:T:39:THR:O	4:T:43:VAL:HG22	2.01	0.60
1:E:299:TYR:OH	1:E:303:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:160:GLY:HA3	10:O:230:ASP:HA	1.82	0.60
4:H:39:THR:O	4:H:43:VAL:HG22	2.01	0.60
3:S:21:ARG:HB3	4:T:63:LEU:HD11	1.82	0.60
8:N:202:ASP:OD1	9:M:316:ARG:NH1	2.35	0.59
4:H:95:ILE:HG12	4:H:124:SER:HB2	1.84	0.59
5:I:44:HIS:NE2	6:J:40:HIS:O	2.35	0.59
2:R:264:HIS:HD2	2:R:268:TYR:CD2	2.15	0.59
8:B:431:THR:HG23	12:B:607:CDL:H332	1.83	0.59
2:R:56:GLY:HA3	14:R:607:HEA:H161	1.83	0.59
8:B:170:LEU:HD23	10:C:180:PHE:HE1	1.67	0.59
12:B:605:CDL:H552	12:B:606:CDL:H602	1.84	0.59
2:F:56:GLY:HA3	14:F:607:HEA:H161	1.83	0.59
8:N:431:THR:HG23	12:N:605:CDL:H331	1.84	0.59
2:F:364:GLY:O	2:F:368:THR:OG1	2.21	0.59
2:R:364:GLY:O	2:R:368:THR:OG1	2.21	0.58
4:T:95:ILE:HG12	4:T:124:SER:HB2	1.84	0.58
8:B:335:PRO:HG2	9:A:356:LEU:HD21	1.84	0.58
5:I:78:LYS:NZ	5:I:78:LYS:HB3	2.17	0.58
1:E:252:ASN:HB3	2:F:253:LEU:HD23	1.85	0.58
2:R:268:TYR:HH	2:R:333:ILE:HD13	1.60	0.58
5:U:78:LYS:NZ	5:U:78:LYS:HB3	2.17	0.58
6:V:33:GLU:HB2	6:V:36:GLU:OE1	2.04	0.58
9:M:320:MET:HG3	9:M:351:LYS:HG3	1.86	0.58
4:T:120:PHE:HZ	10:C:263:ILE:HD11	1.68	0.58
8:N:475:GLU:OE2	8:N:476:HIS:ND1	2.30	0.58
9:A:320:MET:HG3	9:A:351:LYS:HG3	1.86	0.58
2:F:84:THR:OG1	2:F:149:PHE:O	2.14	0.58
6:J:33:GLU:HB2	6:J:36:GLU:OE1	2.04	0.58
8:N:80:GLY:O	8:N:86:ARG:NH1	2.37	0.58
2:F:105:LEU:HD22	2:F:421:MET:HE2	1.85	0.57
2:R:105:LEU:HD22	2:R:421:MET:HE2	1.85	0.57
10:C:158:LEU:HA	10:C:229:LYS:HE3	1.85	0.57
2:F:68:MET:SD	5:I:3:THR:OG1	2.62	0.57
8:B:80:GLY:O	8:B:86:ARG:NH1	2.37	0.57
6:V:53:ASP:OD1	6:V:53:ASP:N	2.38	0.57
9:M:246:TRP:CH2	20:M:503:9YF:O2	2.50	0.57
8:B:301:SER:OG	8:B:302:ALA:N	2.36	0.57
6:V:110:TYR:CZ	6:V:119:ILE:HB	2.39	0.57
8:N:301:SER:OG	8:N:302:ALA:N	2.36	0.57
17:O:302:MQ9:H153	17:O:302:MQ9:C41	2.34	0.57
12:B:606:CDL:H311	12:B:606:CDL:H111	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:53:ASP:OD1	6:J:53:ASP:N	2.38	0.57
6:J:110:TYR:CZ	6:J:119:ILE:HB	2.39	0.57
1:Q:328:PHE:HB3	2:R:465:LEU:HD21	1.85	0.57
8:N:170:LEU:HD23	10:O:180:PHE:HE1	1.69	0.57
8:B:475:GLU:OE2	8:B:476:HIS:ND1	2.30	0.57
1:Q:92:MET:O	1:Q:95:GLU:HG2	2.06	0.56
1:Q:159:ALA:C	1:Q:161:PRO:HD3	2.31	0.56
2:R:499:TRP:NE1	12:R:602:CDL:HB4	2.21	0.56
17:B:610:MQ9:H353	17:B:610:MQ9:C41	2.36	0.56
3:S:101:ARG:NH1	8:B:508:LEU:O	2.39	0.56
17:C:303:MQ9:H261	17:C:303:MQ9:H212	1.88	0.56
8:N:47:LEU:HD13	8:N:127:VAL:HG12	1.88	0.56
2:R:537:ARG:NH2	4:T:73:ALA:O	2.39	0.56
2:F:398:PHE:HA	2:F:401:VAL:HG22	1.88	0.56
7:D:72:GLU:HG2	8:N:414:TRP:NE1	2.21	0.56
8:B:27:PRO:C	8:B:29:ALA:H	2.14	0.56
8:B:33:ARG:HA	9:A:70:ASP:OD1	2.06	0.56
8:B:47:LEU:HD13	8:B:127:VAL:HG12	1.88	0.56
1:E:232:HIS:ND1	1:E:277:CYS:SG	2.79	0.56
5:U:53:GLU:HB3	5:U:54:PRO:HD3	1.88	0.56
8:N:27:PRO:C	8:N:29:ALA:H	2.14	0.56
3:S:63:THR:OG1	3:S:129:THR:OG1	2.18	0.55
10:O:201:GLU:OE2	10:O:201:GLU:N	2.38	0.55
10:C:201:GLU:OE2	10:C:201:GLU:N	2.38	0.55
5:I:53:GLU:HB3	5:I:54:PRO:HD3	1.88	0.55
3:G:105:ILE:O	3:G:109:MET:HG2	2.06	0.55
3:G:169:LYS:HB2	8:N:500:GLY:O	2.05	0.55
2:R:326:PHE:O	2:R:330:THR:HG23	2.07	0.55
2:R:398:PHE:HA	2:R:401:VAL:HG22	1.88	0.55
8:N:218:LEU:HD21	16:B:602:HEM:HBC1	1.88	0.55
2:F:326:PHE:O	2:F:330:THR:HG23	2.07	0.55
14:F:607:HEA:H261	14:F:607:HEA:C18	2.31	0.55
9:A:229:ASN:N	20:A:503:9YF:O8	2.32	0.55
16:N:601:HEM:HMB1	16:N:601:HEM:HBB2	1.87	0.55
9:A:328:ASP:O	9:A:330:GLY:N	2.40	0.55
1:Q:154:PHE:CZ	1:Q:297:LYS:HB2	2.42	0.55
8:B:388:PHE:HE1	8:B:420:MET:HG3	1.72	0.55
9:A:133:SER:HB3	10:C:242:ARG:HG3	1.89	0.55
2:F:449:GLN:HA	2:F:452:LEU:HB3	1.88	0.55
8:N:388:PHE:HE1	8:N:420:MET:HG3	1.72	0.55
10:O:243:GLN:H	10:O:243:GLN:CD	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:449:GLN:HA	2:R:452:LEU:HB3	1.88	0.54
8:B:55:PHE:HE1	16:B:602:HEM:HBB1	1.72	0.54
8:N:282:GLY:HA3	9:M:140:GLY:HA3	1.88	0.54
9:M:328:ASP:O	9:M:330:GLY:N	2.40	0.54
1:Q:101:ILE:O	1:Q:104:LEU:HG	2.08	0.54
12:N:605:CDL:H112	12:N:605:CDL:H311	1.89	0.54
8:B:372:PRO:HB2	12:B:607:CDL:HA61	1.89	0.54
2:F:80:ASN:HA	2:F:83:PHE:CE1	2.43	0.54
12:D:201:CDL:H231	12:D:201:CDL:H412	1.89	0.54
9:M:51:GLU:CD	9:M:53:ALA:HB3	2.33	0.54
9:M:418:PRO:HD2	9:M:427:THR:HG23	1.89	0.54
3:G:91:ALA:HB2	3:G:99:LEU:HD12	1.89	0.54
7:D:89:ARG:NH1	12:D:201:CDL:OB3	2.41	0.54
1:Q:330:SER:CB	10:C:87:HIS:HE1	2.21	0.54
9:A:51:GLU:CD	9:A:53:ALA:HB3	2.33	0.54
9:M:160:ARG:HH22	12:M:502:CDL:H112	1.72	0.54
14:R:607:HEA:H261	14:R:607:HEA:C18	2.31	0.54
10:C:154:ALA:O	10:C:155:THR:OG1	2.20	0.54
1:E:275:GLU:O	1:E:281:HIS:NE2	2.41	0.53
3:G:147:HIS:NE2	3:G:192:TRP:HB2	2.23	0.53
9:A:418:PRO:HD2	9:A:427:THR:HG23	1.89	0.53
3:S:83:THR:HG23	3:S:102:TRP:HE3	1.73	0.53
12:N:605:CDL:H152	12:N:605:CDL:H582	1.91	0.53
2:R:80:ASN:HA	2:R:83:PHE:CE1	2.43	0.53
8:B:264:PHE:HE2	9:A:154:ALA:O	1.90	0.53
20:A:505:9YF:C11	20:A:505:9YF:C17	2.85	0.53
2:F:404:GLY:HA2	2:F:408:PHE:HD2	1.74	0.53
1:Q:330:SER:HB2	10:C:87:HIS:HE1	1.73	0.53
2:F:15:ARG:HD2	5:I:52:GLU:OE1	2.09	0.53
7:D:28:VAL:HG13	7:D:42:HIS:HB2	1.89	0.53
8:N:259:MET:HB3	8:N:260:PRO:HD3	1.90	0.53
10:C:159:ARG:HA	10:C:233:ALA:HB2	1.91	0.53
1:Q:275:GLU:O	1:Q:281:HIS:NE2	2.42	0.53
8:B:259:MET:HB3	8:B:260:PRO:HD3	1.90	0.53
2:R:268:TYR:CZ	2:R:333:ILE:CD1	2.90	0.53
2:R:404:GLY:HA2	2:R:408:PHE:HD2	1.74	0.53
10:C:158:LEU:HA	10:C:229:LYS:HG2	1.91	0.53
2:R:84:THR:OG1	2:R:149:PHE:O	2.14	0.52
3:S:147:HIS:CE1	3:S:192:TRP:HB2	2.44	0.52
2:R:104:ASN:ND2	2:R:122:ASN:HD21	2.07	0.52
8:B:537:HIS:CD2	9:A:73:ARG:HH21	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:160:GLY:O	10:C:162:ASP:N	2.41	0.52
3:G:185:TRP:O	3:G:188:VAL:HG12	2.09	0.52
2:R:500:ARG:HH22	12:P:201:CDL:H801	1.74	0.52
20:M:504:9YF:O3	20:M:504:9YF:O5	2.26	0.52
2:F:104:ASN:ND2	2:F:122:ASN:HD21	2.07	0.52
10:O:160:GLY:C	10:O:162:ASP:N	2.66	0.52
10:C:147:ARG:NH2	10:C:153:ILE:HD11	2.25	0.52
7:P:89:ARG:HH21	12:P:201:CDL:H802	1.74	0.52
1:E:303:ARG:NH1	1:E:309:ASN:OD1	2.43	0.52
2:F:59:ALA:HB2	2:F:86:HIS:CE1	2.45	0.52
6:V:79:ALA:O	6:V:82:ARG:HG2	2.09	0.52
9:M:369:ARG:HD3	9:M:388:ILE:HD11	1.90	0.52
10:C:243:GLN:CD	10:C:243:GLN:H	2.15	0.52
8:N:169:ASP:OD1	8:N:169:ASP:N	2.43	0.52
8:B:322:PRO:HB3	9:A:391:PRO:HA	1.92	0.52
8:B:370:GLN:OE1	8:B:378:ARG:NH2	2.40	0.52
1:E:164:LYS:NZ	10:O:126:GLU:OE1	2.38	0.52
3:G:60:PRO:O	3:G:63:THR:HG22	2.09	0.52
1:Q:331:ARG:HE	1:Q:333:GLY:H	1.56	0.52
8:B:190:ILE:HG13	8:B:191:GLY:H	1.75	0.52
9:A:51:GLU:HG3	9:A:53:ALA:H	1.74	0.52
9:A:246:TRP:HZ3	20:A:505:9YF:P	2.32	0.52
6:J:79:ALA:O	6:J:82:ARG:HG2	2.09	0.52
5:U:44:HIS:NE2	6:V:40:HIS:O	2.43	0.52
9:M:51:GLU:HG3	9:M:53:ALA:H	1.74	0.52
8:B:169:ASP:OD1	8:B:169:ASP:N	2.43	0.52
9:A:246:TRP:CH2	20:A:505:9YF:O1	2.63	0.52
9:A:369:ARG:HD3	9:A:388:ILE:HD11	1.90	0.52
10:C:158:LEU:CA	10:C:229:LYS:HG2	2.40	0.52
2:R:336:PRO:HA	2:R:339:ILE:HG13	1.90	0.51
4:T:82:LEU:N	8:B:455:ILE:O	2.42	0.51
8:N:190:ILE:HG13	8:N:191:GLY:H	1.75	0.51
8:N:258:VAL:HA	8:N:262:PHE:HB3	1.92	0.51
8:N:370:GLN:OE1	8:N:378:ARG:NH2	2.40	0.51
9:M:176:SER:OG	8:B:26:HIS:HB2	2.09	0.51
2:R:155:SER:HB2	2:R:156:PRO:HD3	1.92	0.51
2:R:268:TYR:CZ	2:R:333:ILE:HD11	2.45	0.51
2:R:59:ALA:HB2	2:R:86:HIS:CE1	2.45	0.51
12:N:605:CDL:H312	12:N:606:CDL:H512	1.92	0.51
20:A:505:9YF:C11	20:A:505:9YF:C16	2.89	0.51
2:F:69:PRO:HG3	2:F:464:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:SER:HB2	2:F:156:PRO:HD3	1.92	0.51
8:B:258:VAL:HA	8:B:262:PHE:HB3	1.92	0.51
9:A:246:TRP:CZ3	20:A:505:9YF:C2	2.93	0.51
2:F:336:PRO:HA	2:F:339:ILE:HG13	1.91	0.51
2:R:69:PRO:HG3	2:R:464:TYR:CE2	2.45	0.51
8:B:285:GLN:CD	10:C:248:LEU:HD12	2.35	0.51
8:B:297:PRO:HD3	9:A:313:MET:HE3	1.92	0.51
17:B:610:MQ9:H351	17:B:610:MQ9:H301	1.92	0.51
2:R:63:ARG:CD	14:R:607:HEA:HMA	2.41	0.51
1:E:75:HIS:CD2	2:F:350:LYS:H	2.29	0.51
1:E:275:GLU:H	1:E:281:HIS:CE1	2.29	0.51
1:Q:231:ILE:HG22	1:Q:275:GLU:HG2	1.93	0.51
12:R:602:CDL:HB62	12:P:201:CDL:H552	1.92	0.51
2:R:197:ARG:HB3	4:T:68:GLU:HG2	1.93	0.50
2:R:268:TYR:CE2	2:R:307:SER:CB	2.94	0.50
2:R:388:VAL:O	2:R:391:SER:OG	2.29	0.50
8:B:320:TRP:O	9:A:391:PRO:HG3	2.11	0.50
20:A:505:9YF:O7	20:A:505:9YF:O	2.29	0.50
2:F:395:ILE:HA	2:F:398:PHE:CE1	2.47	0.50
1:Q:252:ASN:HB3	2:R:253:LEU:HD23	1.91	0.50
2:R:395:ILE:HA	2:R:398:PHE:CE1	2.47	0.50
8:N:329:HIS:O	8:N:330:HIS:ND1	2.43	0.50
2:F:63:ARG:CD	14:F:607:HEA:HMA	2.41	0.50
12:F:602:CDL:OA3	8:N:433:ARG:NH1	2.39	0.50
10:O:162:ASP:HB3	10:O:230:ASP:OD1	2.11	0.50
1:E:229:ASP:OD1	1:E:229:ASP:N	2.45	0.50
8:B:329:HIS:O	8:B:330:HIS:ND1	2.43	0.50
10:C:162:ASP:HB3	10:C:230:ASP:OD1	2.12	0.50
2:F:100:PHE:HE2	2:F:182:THR:HG23	1.75	0.50
8:B:399:ASP:OD1	8:B:399:ASP:N	2.45	0.50
3:G:72:PRO:O	3:G:76:VAL:HG13	2.12	0.50
8:N:399:ASP:OD1	8:N:399:ASP:N	2.45	0.50
2:F:33:THR:HG22	4:H:90:TRP:HB3	1.94	0.50
2:F:379:LEU:HD21	14:F:606:HEA:HBA2	1.93	0.50
4:T:66:ARG:NH1	4:T:69:ASP:OD2	2.45	0.50
9:M:260:TYR:HB2	9:M:292:TRP:HB3	1.94	0.50
2:F:537:ARG:NH2	4:H:73:ALA:O	2.45	0.49
6:V:119:ILE:HG13	6:V:120:GLU:N	2.26	0.49
10:O:125:ASP:O	10:O:126:GLU:HB3	2.12	0.49
10:C:125:ASP:O	10:C:126:GLU:HB3	2.12	0.49
4:H:66:ARG:NH1	4:H:69:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:138:TRP:O	1:Q:139:ASN:HB2	2.12	0.49
1:Q:232:HIS:ND1	1:Q:277:CYS:SG	2.86	0.49
2:R:70:GLY:O	2:R:72:GLN:NE2	2.45	0.49
2:R:100:PHE:HE2	2:R:182:THR:HG23	1.75	0.49
1:E:29:ASP:OD2	1:E:29:ASP:N	2.42	0.49
8:B:516:ASP:OD2	8:B:520:ARG:NH1	2.45	0.49
10:C:65:GLY:C	10:C:67:GLN:H	2.20	0.49
2:R:379:LEU:HD21	14:R:606:HEA:HBA2	1.93	0.49
8:N:516:ASP:OD2	8:N:520:ARG:NH1	2.45	0.49
9:M:320:MET:O	9:M:348:ALA:HA	2.13	0.49
9:A:237:THR:OG1	9:A:239:GLU:OE1	2.14	0.49
9:A:260:TYR:HB2	9:A:292:TRP:HB3	1.94	0.49
6:J:119:ILE:HG13	6:J:120:GLU:N	2.26	0.49
7:D:35:SER:OG	8:N:443:ARG:NH1	2.39	0.49
12:P:201:CDL:H402	8:B:422:ILE:HG22	1.94	0.49
8:N:231:HIS:NE2	16:N:601:HEM:NA	2.61	0.49
9:A:320:MET:O	9:A:348:ALA:HA	2.13	0.49
10:C:243:GLN:OE1	10:C:243:GLN:N	2.38	0.49
10:O:65:GLY:C	10:O:67:GLN:H	2.20	0.49
2:R:30:LYS:O	2:R:34:THR:HB	2.13	0.49
1:E:206:THR:HG23	1:E:208:SER:H	1.78	0.49
2:F:70:GLY:O	2:F:72:GLN:NE2	2.45	0.49
2:R:532:GLU:HG3	6:V:23:THR:HB	1.95	0.49
6:V:73:LEU:HG	6:V:100:SER:HB2	1.95	0.49
1:E:235:TRP:CD1	1:E:242:LYS:HB3	2.47	0.48
2:F:30:LYS:O	2:F:34:THR:HB	2.13	0.48
1:Q:326:GLU:HG2	1:Q:327:PRO:HD2	1.93	0.48
9:M:328:ASP:OD2	9:M:331:ARG:NH1	2.46	0.48
9:A:364:GLU:HB3	10:C:214:ASN:OD1	2.13	0.48
6:J:45:THR:O	6:J:49:VAL:HG23	2.13	0.48
6:J:73:LEU:HG	6:J:100:SER:HB2	1.95	0.48
12:B:603:CDL:OB4	12:A:504:CDL:O1	2.31	0.48
9:A:328:ASP:OD2	9:A:331:ARG:NH1	2.45	0.48
1:Q:162:GLU:HB3	10:C:67:GLN:HE22	1.78	0.48
2:F:313:HIS:ND1	14:F:606:HEA:OMA	2.46	0.48
2:R:15:ARG:HD2	5:U:52:GLU:OE1	2.13	0.48
2:R:196:MET:HE3	3:S:24:MET:SD	2.53	0.48
6:V:45:THR:O	6:V:49:VAL:HG23	2.13	0.48
8:B:126:MET:SD	17:B:610:MQ9:H28	2.53	0.48
8:B:253:VAL:HB	9:A:169:GLN:HB3	1.95	0.48
1:E:98:LEU:HD13	2:F:342:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:264:HIS:CD2	2:F:268:TYR:HE2	2.31	0.48
1:Q:85:PRO:O	1:Q:87:GLN:HG2	2.13	0.48
10:C:63:ARG:HG2	10:C:64:THR:N	2.28	0.48
12:N:605:CDL:HA61	12:N:606:CDL:H512	1.95	0.48
8:B:537:HIS:HD2	9:A:73:ARG:HH21	1.61	0.48
2:R:313:HIS:ND1	14:R:606:HEA:OMA	2.46	0.48
8:N:38:VAL:HB	9:M:169:GLN:HB2	1.96	0.48
10:O:63:ARG:HG2	10:O:64:THR:N	2.28	0.48
10:O:109:PRO:HG2	10:O:123:ILE:HD12	1.95	0.48
1:E:137:GLN:HG3	1:E:138:TRP:CD2	2.49	0.48
8:B:194:LEU:HD23	20:A:503:9YF:C34	2.44	0.48
1:Q:154:PHE:HZ	1:Q:297:LYS:HB2	1.78	0.48
9:M:237:THR:OG1	9:M:239:GLU:OE1	2.14	0.48
2:F:85:MET:HE1	2:F:171:TRP:HD1	1.80	0.47
4:H:44:LEU:HD23	4:H:44:LEU:HA	1.68	0.47
6:J:47:ASP:HB3	6:J:140:ILE:HG21	1.96	0.47
9:A:372:CYS:SG	19:A:501:FES:S2	3.12	0.47
2:F:244:ILE:HD11	3:G:142:LEU:HD13	1.96	0.47
7:D:72:GLU:HG2	8:N:414:TRP:CE2	2.50	0.47
2:R:56:GLY:HA3	14:R:607:HEA:C16	2.45	0.47
2:R:85:MET:HE1	2:R:171:TRP:HD1	1.80	0.47
3:S:147:HIS:NE2	3:S:192:TRP:HB2	2.29	0.47
9:A:51:GLU:HG3	9:A:53:ALA:N	2.28	0.47
9:A:132:TYR:HE2	10:C:242:ARG:HH21	1.61	0.47
5:I:36:TYR:HB2	6:J:42:PRO:HB2	1.96	0.47
2:R:515:ASN:O	2:R:519:TRP:HD1	1.97	0.47
10:C:109:PRO:HG2	10:C:123:ILE:HD12	1.95	0.47
1:E:138:TRP:HA	1:E:284:MET:HG2	1.97	0.47
1:E:242:LYS:HG2	2:F:386:PHE:O	2.15	0.47
2:F:56:GLY:HA3	14:F:607:HEA:C16	2.45	0.47
6:V:47:ASP:HB3	6:V:140:ILE:HG21	1.96	0.47
9:M:51:GLU:HG3	9:M:53:ALA:N	2.28	0.47
9:M:205:LEU:O	9:M:209:VAL:HG13	2.14	0.47
8:B:26:HIS:O	8:B:26:HIS:ND1	2.48	0.47
1:Q:242:LYS:HG2	2:R:386:PHE:O	2.15	0.47
8:N:109:PHE:CZ	8:N:113:ILE:HD11	2.49	0.47
8:B:286:ILE:HG13	10:C:257:GLU:CD	2.39	0.47
10:C:159:ARG:HG2	10:C:233:ALA:HA	1.97	0.47
8:N:505:GLY:O	9:M:91:ARG:NH2	2.47	0.47
8:B:447:GLU:HG2	8:B:448:HIS:CD2	2.50	0.47
9:A:246:TRP:CH2	20:A:505:9YF:C3	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:26:HIS:O	8:N:26:HIS:ND1	2.48	0.47
9:M:205:LEU:HD23	9:M:206:SER:N	2.30	0.47
12:B:608:CDL:H121	12:B:608:CDL:H151	1.72	0.47
9:A:205:LEU:O	9:A:209:VAL:HG13	2.14	0.47
2:F:515:ASN:O	2:F:519:TRP:HD1	1.97	0.46
20:A:505:9YF:C16	20:A:505:9YF:C12	2.92	0.46
8:N:64:TYR:CD2	8:N:110:VAL:HG11	2.50	0.46
8:N:356:GLU:OE2	8:N:378:ARG:NH1	2.48	0.46
9:M:283:ALA:HB1	9:M:325:LYS:HA	1.96	0.46
17:O:302:MQ9:H72	17:O:302:MQ9:H101	1.62	0.46
8:B:356:GLU:OE2	8:B:378:ARG:NH1	2.48	0.46
9:A:205:LEU:HD23	9:A:206:SER:N	2.31	0.46
2:F:288:LYS:HB3	2:F:288:LYS:HE2	1.62	0.46
12:N:604:CDL:CA5	12:B:606:CDL:H511	2.46	0.46
8:B:109:PHE:CZ	8:B:113:ILE:HD11	2.49	0.46
12:D:201:CDL:H372	12:D:201:CDL:H131	1.97	0.46
1:Q:331:ARG:NE	1:Q:333:GLY:H	2.14	0.46
7:P:72:GLU:HG3	8:B:414:TRP:CZ2	2.50	0.46
8:N:447:GLU:HG2	8:N:448:HIS:CD2	2.50	0.46
1:Q:138:TRP:HA	1:Q:284:MET:HG2	1.97	0.46
7:P:29:ASP:N	7:P:29:ASP:OD1	2.49	0.46
7:P:62:MET:O	7:P:67:HIS:HE1	1.98	0.46
9:M:129:ASP:C	9:M:131:ILE:H	2.23	0.46
9:A:246:TRP:CZ2	20:A:505:9YF:O3	2.68	0.46
2:F:330:THR:O	2:F:333:ILE:HG22	2.16	0.46
2:R:330:THR:O	2:R:333:ILE:HG22	2.16	0.46
2:R:402:LEU:HD23	14:R:606:HEA:HBC1	1.98	0.46
8:N:53:TYR:HD2	8:N:273:ILE:HD12	1.81	0.46
8:B:64:TYR:CD2	8:B:110:VAL:HG11	2.50	0.46
17:B:610:MQ9:H3D	10:C:259:MET:SD	2.56	0.46
2:F:148:ASP:OD2	10:O:112:ARG:NH1	2.48	0.46
6:J:110:TYR:OH	6:J:123:ALA:HB2	2.16	0.46
7:P:28:VAL:HG23	7:P:42:HIS:HB2	1.97	0.46
8:N:204:PRO:HG3	9:M:315:ILE:HG23	1.98	0.46
9:A:283:ALA:HB1	9:A:325:LYS:HA	1.96	0.46
7:D:39:GLY:HA3	8:N:375:VAL:HG22	1.98	0.46
10:O:243:GLN:CD	10:O:243:GLN:N	2.74	0.46
8:B:53:TYR:HD2	8:B:273:ILE:HD12	1.81	0.46
17:B:609:MQ9:H202	17:B:609:MQ9:H171	1.74	0.46
17:B:609:MQ9:H261	17:B:609:MQ9:H302	1.98	0.46
2:F:264:HIS:O	2:F:267:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:63:MET:O	7:D:66:ASN:ND2	2.49	0.46
4:T:78:GLY:HA3	8:B:457:ARG:HH11	1.80	0.46
8:B:272:ALA:HB1	10:C:272:LEU:HD13	1.98	0.46
2:F:153:ALA:HB1	2:F:158:THR:HG21	1.98	0.45
2:F:388:VAL:O	2:F:391:SER:OG	2.29	0.45
6:V:110:TYR:OH	6:V:123:ALA:HB2	2.16	0.45
7:P:39:GLY:HA3	8:B:375:VAL:HG22	1.98	0.45
8:N:263:ALA:HB1	17:A:502:MQ9:H3D	1.98	0.45
9:A:231:TRP:HE1	20:A:505:9YF:C13	2.29	0.45
5:U:79:TRP:HE1	6:V:106:ILE:HD11	1.81	0.45
9:M:282:ASP:CG	10:O:219:SER:HB3	2.40	0.45
17:O:302:MQ9:H261	17:O:302:MQ9:H221	1.66	0.45
8:B:397:MET:SD	17:C:303:MQ9:H103	2.56	0.45
9:A:329:LEU:HD23	9:A:329:LEU:HA	1.79	0.45
10:C:243:GLN:CD	10:C:243:GLN:N	2.74	0.45
8:N:190:ILE:HD12	8:N:194:LEU:HD11	1.97	0.45
8:B:190:ILE:HD12	8:B:194:LEU:HD11	1.97	0.45
8:B:264:PHE:CD2	9:A:158:GLN:HB2	2.51	0.45
9:A:129:ASP:C	9:A:131:ILE:H	2.23	0.45
9:A:246:TRP:CZ3	20:A:505:9YF:P	3.09	0.45
17:A:502:MQ9:H251	17:A:502:MQ9:H222	1.84	0.45
2:F:95:ALA:O	2:F:98:ILE:HG22	2.17	0.45
2:F:384:LEU:O	2:F:388:VAL:HG22	2.17	0.45
2:R:384:LEU:O	2:R:388:VAL:HG22	2.17	0.45
14:F:607:HEA:HHA	14:F:607:HEA:HAD1	1.62	0.45
2:R:153:ALA:HB1	2:R:158:THR:HG21	1.98	0.45
9:M:294:GLU:OE1	9:M:294:GLU:N	2.48	0.45
4:T:44:LEU:HD23	4:T:44:LEU:HA	1.68	0.45
8:B:55:PHE:CE1	16:B:602:HEM:HBB1	2.50	0.45
8:B:123:ALA:HB3	10:C:266:MET:HE3	1.98	0.45
12:A:504:CDL:HA62	12:A:504:CDL:H132	1.99	0.45
10:C:255:ALA:HB3	10:C:256:PRO:HD3	1.99	0.45
1:E:243:ARG:NH1	1:E:255:ASP:O	2.50	0.45
2:F:163:SER:HA	10:O:112:ARG:HH12	1.81	0.45
2:R:485:GLY:HA2	14:R:607:HEA:H262	1.97	0.45
9:A:294:GLU:OE1	9:A:294:GLU:N	2.48	0.45
2:F:402:LEU:HD23	14:F:606:HEA:HBC1	1.99	0.45
2:F:485:GLY:HA2	14:F:607:HEA:H262	1.97	0.45
12:F:602:CDL:H512	12:F:602:CDL:H542	1.64	0.45
2:R:95:ALA:O	2:R:98:ILE:HG22	2.17	0.45
9:M:270:GLY:H	9:M:271:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:329:LEU:HD23	9:M:329:LEU:HA	1.79	0.45
10:O:255:ALA:HB3	10:O:256:PRO:HD3	1.99	0.45
9:A:270:GLY:H	9:A:271:PRO:HD2	1.82	0.45
12:F:601:CDL:H342	12:F:601:CDL:H312	1.44	0.44
2:R:28:ILE:HD11	8:B:430:ILE:HG23	1.99	0.44
17:A:502:MQ9:H112	17:A:502:MQ9:H71	1.65	0.44
1:E:220:ARG:HD2	1:E:261:SER:O	2.18	0.44
12:N:606:CDL:H131	12:N:606:CDL:H161	1.71	0.44
17:N:607:MQ9:H203	17:N:607:MQ9:H222	1.79	0.44
9:M:84:GLU:CD	9:M:84:GLU:H	2.24	0.44
12:B:605:CDL:H712	12:B:605:CDL:H121	1.99	0.44
9:A:84:GLU:H	9:A:84:GLU:CD	2.24	0.44
1:E:159:ALA:O	1:E:200:LYS:NZ	2.49	0.44
1:Q:229:ASP:OD1	1:Q:229:ASP:N	2.45	0.44
9:A:58:SER:HB3	9:A:61:GLU:OE1	2.17	0.44
17:A:502:MQ9:H302	17:A:502:MQ9:H272	1.74	0.44
1:Q:284:MET:HE2	1:Q:284:MET:HB3	1.87	0.44
2:R:414:ILE:HD12	12:R:602:CDL:H852	1.99	0.44
2:R:553:ARG:O	2:R:557:GLU:HG2	2.17	0.44
14:R:606:HEA:H261	14:R:606:HEA:H172	1.28	0.44
8:N:32:ARG:NH2	9:M:70:ASP:OD2	2.49	0.44
8:N:116:TRP:CD1	8:N:281:GLY:HA2	2.52	0.44
9:M:58:SER:HB3	9:M:61:GLU:OE1	2.17	0.44
8:B:116:TRP:CD1	8:B:281:GLY:HA2	2.52	0.44
2:F:120:ARG:NH1	4:H:131:GLU:OE1	2.51	0.44
2:F:553:ARG:O	2:F:557:GLU:HG2	2.17	0.44
2:R:288:LYS:HE2	2:R:288:LYS:HB3	1.62	0.44
2:R:503:GLU:N	2:R:503:GLU:OE1	2.50	0.44
8:B:202:ASP:OD1	9:A:316:ARG:NH1	2.50	0.44
1:E:242:LYS:HD3	2:F:389:THR:HG22	1.98	0.44
1:Q:220:ARG:HD2	1:Q:261:SER:HA	2.00	0.44
14:R:607:HEA:HHA	14:R:607:HEA:HAD1	1.62	0.44
3:S:156:VAL:HG22	12:A:504:CDL:H822	2.00	0.44
1:E:42:GLU:HB3	1:E:120:MET:HG2	1.99	0.44
1:Q:86:ARG:NH2	2:R:557:GLU:OE1	2.48	0.44
3:S:169:LYS:HB3	8:B:500:GLY:O	2.17	0.44
2:F:503:GLU:N	2:F:503:GLU:OE1	2.50	0.44
1:Q:123:LYS:NZ	1:Q:255:ASP:OD1	2.50	0.44
9:A:362:LEU:HD22	9:A:371:LEU:HD23	2.00	0.44
3:G:116:GLY:O	3:G:120:GLU:HG3	2.18	0.43
1:Q:319:PRO:HA	1:Q:320:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:107:LEU:HB3	2:R:108:PRO:HD3	1.99	0.43
8:N:285:GLN:HE21	8:N:288:PRO:HB3	1.83	0.43
9:M:362:LEU:HD22	9:M:371:LEU:HD23	2.00	0.43
2:R:503:GLU:HG3	6:V:37:LEU:HD13	1.98	0.43
12:P:201:CDL:H361	12:P:201:CDL:H331	1.60	0.43
8:N:529:ARG:HH22	9:M:78:GLU:CD	2.20	0.43
8:B:17:GLN:O	8:B:21:ILE:HG13	2.18	0.43
8:B:120:MET:HE3	10:C:261:MET:HE1	2.00	0.43
8:B:285:GLN:HE21	8:B:288:PRO:HB3	1.83	0.43
1:E:274:THR:HG22	2:F:458:PRO:HB3	1.99	0.43
14:F:606:HEA:HBD1	14:F:606:HEA:HMD3	2.00	0.43
3:G:130:THR:HB	3:G:132:PRO:HD2	2.01	0.43
1:Q:252:ASN:HD21	2:R:252:VAL:H	1.65	0.43
12:N:606:CDL:H222	12:N:606:CDL:H191	1.94	0.43
1:E:140:TRP:NE1	1:E:284:MET:O	2.48	0.43
6:J:92:GLU:H	6:J:92:GLU:HG3	1.44	0.43
3:S:71:VAL:HB	3:S:72:PRO:HD3	2.00	0.43
8:N:17:GLN:O	8:N:21:ILE:HG13	2.18	0.43
8:N:335:PRO:HG2	9:M:356:LEU:HD21	1.99	0.43
8:B:452:THR:OG1	8:B:466:LEU:O	2.28	0.43
1:E:117:GLN:HB3	2:F:383:PRO:HD3	2.00	0.43
1:E:137:GLN:HG3	1:E:138:TRP:CE2	2.54	0.43
1:Q:152:GLY:O	1:Q:153:SER:OG	2.31	0.43
1:E:319:PRO:HA	1:E:320:PRO:HD3	1.88	0.43
17:O:303:MQ9:H101	17:O:303:MQ9:H72	1.51	0.43
2:F:107:LEU:HB3	2:F:108:PRO:HD3	1.99	0.43
2:F:445:THR:HG23	2:F:446:PHE:CD2	2.53	0.43
6:J:119:ILE:HG13	6:J:120:GLU:H	1.83	0.43
2:F:68:MET:HE1	5:I:7:HIS:CD2	2.53	0.43
3:G:19:LEU:HD22	3:G:21:ARG:NH2	2.33	0.43
5:U:53:GLU:HG3	6:V:60:ARG:HG3	2.00	0.43
12:B:608:CDL:H581	12:B:608:CDL:H551	1.84	0.43
12:A:504:CDL:H632	12:A:504:CDL:H661	1.81	0.43
3:G:80:SER:HB2	3:G:185:TRP:CH2	2.54	0.43
12:D:201:CDL:H811	12:D:201:CDL:H841	1.85	0.43
17:N:607:MQ9:H253	17:N:607:MQ9:H272	1.89	0.43
12:O:301:CDL:H762	12:O:301:CDL:H791	1.53	0.43
17:B:609:MQ9:H121	17:B:609:MQ9:H103	1.67	0.43
8:B:173:GLY:HA3	8:B:295:TYR:CD1	2.54	0.43
8:B:271:ALA:HB3	9:A:151:ALA:HB2	2.01	0.43
17:B:610:MQ9:H102	17:B:610:MQ9:H72	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:GLU:O	1:E:84:LEU:HG	2.18	0.42
2:F:38:LYS:HG2	2:F:421:MET:HE1	2.01	0.42
7:D:62:MET:SD	8:N:417:ARG:HG2	2.59	0.42
2:R:38:LYS:HG2	2:R:421:MET:HE1	2.01	0.42
2:R:445:THR:HG23	2:R:446:PHE:CD2	2.53	0.42
12:B:603:CDL:H831	12:B:603:CDL:H862	1.65	0.42
10:C:158:LEU:HD22	10:C:225:PHE:CZ	2.53	0.42
3:G:161:LEU:O	3:G:165:THR:HG23	2.19	0.42
2:R:392:TYR:CD1	2:R:395:ILE:HD12	2.54	0.42
4:T:104:VAL:HG11	17:C:303:MQ9:C20	2.49	0.42
12:P:201:CDL:H821	12:P:201:CDL:H791	1.33	0.42
8:N:173:GLY:HA3	8:N:295:TYR:CD1	2.54	0.42
8:N:177:ARG:O	8:N:181:SER:HB3	2.19	0.42
9:M:336:LYS:H	9:M:336:LYS:HD2	1.85	0.42
2:F:552:GLU:HG2	2:F:553:ARG:N	2.35	0.42
6:J:49:VAL:O	6:J:53:ASP:OD1	2.37	0.42
1:E:84:LEU:O	2:F:553:ARG:NH2	2.47	0.42
3:G:152:ILE:O	3:G:156:VAL:HG23	2.20	0.42
8:N:219:LEU:HB3	17:N:608:MQ9:H352	1.48	0.42
10:O:159:ARG:HA	10:O:233:ALA:HB2	2.01	0.42
10:O:178:HIS:CE1	10:O:196:LEU:HD21	2.55	0.42
8:B:177:ARG:O	8:B:181:SER:HB3	2.19	0.42
17:B:610:MQ9:H102	17:B:610:MQ9:O1	2.19	0.42
2:F:392:TYR:CD1	2:F:395:ILE:HD12	2.54	0.42
1:Q:299:TYR:OH	1:Q:309:ASN:OD1	2.24	0.42
12:R:602:CDL:H512	12:R:602:CDL:H542	1.64	0.42
6:V:119:ILE:HG13	6:V:120:GLU:H	1.83	0.42
8:N:452:THR:OG1	8:N:466:LEU:O	2.28	0.42
17:N:608:MQ9:H5M2	17:N:608:MQ9:C9	2.50	0.42
10:O:158:LEU:CB	10:O:229:LYS:HG2	2.49	0.42
12:A:504:CDL:H722	12:A:504:CDL:H752	1.50	0.42
1:E:301:ASP:OD2	1:E:302:GLN:N	2.53	0.42
10:O:102:GLN:HB3	10:O:108:MET:CG	2.48	0.42
10:O:223:LEU:HD12	10:O:223:LEU:HA	1.91	0.42
8:B:36:ASN:HB3	9:A:72:VAL:HG21	2.02	0.42
9:A:336:LYS:H	9:A:336:LYS:HD2	1.85	0.42
10:C:178:HIS:CE1	10:C:196:LEU:HD21	2.55	0.42
2:R:105:LEU:HD23	2:R:105:LEU:HA	1.84	0.42
2:R:552:GLU:HG2	2:R:553:ARG:N	2.35	0.42
8:N:109:PHE:HE2	17:A:502:MQ9:H352	1.84	0.42
1:Q:235:TRP:CD1	1:Q:242:LYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:330:SER:HB2	10:C:87:HIS:CE1	2.54	0.42
9:M:68:LYS:HB3	9:M:68:LYS:HE3	1.31	0.42
12:B:603:CDL:HA4	12:B:608:CDL:H132	2.01	0.42
9:A:254:TYR:CZ	9:A:257:GLU:HB3	2.55	0.42
5:U:1:MET:HE2	5:U:1:MET:HB3	1.90	0.42
8:N:25:TYR:OH	8:B:144:THR:HG21	2.20	0.42
8:N:42:HIS:ND1	8:N:44:SER:HB3	2.35	0.42
9:M:129:ASP:OD1	9:M:129:ASP:N	2.52	0.42
9:M:254:TYR:CZ	9:M:257:GLU:HB3	2.55	0.42
1:Q:91:ASN:OD1	1:Q:93:PRO:HD2	2.20	0.41
3:S:58:TRP:CG	3:S:59:PRO:HD3	2.53	0.41
6:V:49:VAL:O	6:V:53:ASP:OD1	2.37	0.41
8:N:150:SER:O	8:N:154:ILE:HG12	2.19	0.41
8:N:492:ARG:NH2	12:O:301:CDL:OA4	2.43	0.41
8:B:140:ARG:HA	8:B:143:GLU:OE2	2.20	0.41
17:B:610:MQ9:H221	17:B:610:MQ9:H251	1.76	0.41
2:F:105:LEU:HD23	2:F:105:LEU:HA	1.84	0.41
2:R:406:ILE:H	2:R:406:ILE:HG12	1.39	0.41
3:S:161:LEU:O	3:S:165:THR:HG23	2.20	0.41
6:V:92:GLU:H	6:V:92:GLU:HG3	1.44	0.41
7:P:67:HIS:O	7:P:68:VAL:C	2.63	0.41
10:O:243:GLN:N	10:O:243:GLN:OE1	2.38	0.41
20:A:503:9YF:P	20:A:503:9YF:O3	2.78	0.41
10:C:66:LYS:HB2	10:C:135:TYR:CE1	2.55	0.41
10:C:259:MET:HB3	17:C:303:MQ9:H5M2	2.02	0.41
2:R:264:HIS:HD2	2:R:268:TYR:HD2	1.63	0.41
8:N:215:LEU:HD23	8:N:219:LEU:HD22	2.01	0.41
8:B:178:ALA:O	8:B:182:SER:OG	2.34	0.41
9:A:129:ASP:OD1	9:A:129:ASP:N	2.52	0.41
10:C:102:GLN:HB3	10:C:108:MET:CG	2.48	0.41
2:F:82:LEU:HD23	2:F:82:LEU:HA	1.90	0.41
1:Q:65:TRP:NE1	2:R:370:LEU:HD23	2.35	0.41
1:Q:300:ILE:HD13	1:Q:300:ILE:HA	1.94	0.41
6:V:110:TYR:CE1	6:V:119:ILE:HB	2.55	0.41
16:N:602:HEM:HBC1	8:B:218:LEU:HD21	2.01	0.41
10:O:158:LEU:CA	10:O:229:LYS:HG2	2.50	0.41
8:B:215:LEU:HD23	8:B:219:LEU:HD22	2.01	0.41
8:B:456:LYS:HE2	8:B:456:LYS:HB3	1.77	0.41
10:C:223:LEU:HD12	10:C:223:LEU:HA	1.91	0.41
3:G:125:VAL:HG23	3:G:130:THR:HG22	2.02	0.41
1:Q:274:THR:HG22	2:R:458:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:275:GLU:O	1:Q:281:HIS:CE1	2.73	0.41
9:M:270:GLY:O	9:M:298:ASP:HB2	2.21	0.41
20:M:503:9YF:O7	20:M:503:9YF:O3	2.38	0.41
8:B:150:SER:O	8:B:154:ILE:HG12	2.19	0.41
17:B:610:MQ9:H451	17:B:610:MQ9:H422	1.64	0.41
9:A:270:GLY:O	9:A:298:ASP:HB2	2.21	0.41
4:H:64:ASP:OD1	4:H:64:ASP:N	2.54	0.41
4:H:112:TRP:CD1	4:H:112:TRP:H	2.37	0.41
3:S:58:TRP:CZ3	3:S:136:TYR:HD1	2.39	0.41
8:N:140:ARG:HA	8:N:143:GLU:OE2	2.20	0.41
9:M:51:GLU:OE2	9:M:53:ALA:HB3	2.21	0.41
20:M:503:9YF:O7	20:M:503:9YF:P	2.78	0.41
17:O:302:MQ9:H13	17:O:302:MQ9:H172	1.75	0.41
8:B:42:HIS:ND1	8:B:44:SER:HB3	2.35	0.41
8:B:171:LEU:HB2	8:B:292:LEU:HD21	2.02	0.41
17:B:610:MQ9:H353	17:B:610:MQ9:C38	2.50	0.41
3:G:58:TRP:CG	3:G:59:PRO:HD3	2.54	0.41
2:R:11:LEU:HD21	5:U:46:PRO:HB2	2.03	0.41
2:R:264:HIS:O	2:R:267:VAL:HG22	2.20	0.41
4:T:64:ASP:OD1	4:T:64:ASP:N	2.54	0.41
9:M:113:ILE:HD13	9:M:113:ILE:HA	1.95	0.41
10:O:66:LYS:HB2	10:O:135:TYR:CE1	2.55	0.41
10:O:111:MET:O	10:O:112:ARG:C	2.64	0.41
12:B:603:CDL:H382	12:B:603:CDL:H351	1.93	0.41
9:A:51:GLU:OE2	9:A:53:ALA:HB3	2.21	0.41
5:I:79:TRP:N	5:I:79:TRP:CD1	2.89	0.41
4:T:112:TRP:H	4:T:112:TRP:CD1	2.37	0.41
10:O:226:GLU:H	10:O:226:GLU:HG2	1.64	0.41
1:E:98:LEU:HD13	2:F:342:PHE:HD2	1.86	0.41
1:E:275:GLU:HG3	1:E:276:MET:N	2.34	0.41
2:F:278:VAL:HG21	2:F:365:PHE:CE2	2.56	0.41
2:F:406:ILE:H	2:F:406:ILE:HG12	1.39	0.41
4:H:1:MET:HB2	4:H:4:GLU:CD	2.46	0.41
6:J:110:TYR:CE1	6:J:119:ILE:HB	2.55	0.41
2:R:279:SER:HB3	2:R:344:TRP:HE1	1.85	0.41
4:T:1:MET:HB2	4:T:4:GLU:CD	2.46	0.41
6:V:13:GLU:C	6:V:13:GLU:OE1	2.64	0.41
8:N:82:TYR:CE2	8:N:84:PRO:HG2	2.55	0.41
8:N:171:LEU:HB2	8:N:292:LEU:HD21	2.02	0.41
10:O:111:MET:O	10:O:113:GLY:N	2.54	0.41
10:O:126:GLU:O	10:O:126:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:82:TYR:CE2	8:B:84:PRO:HG2	2.55	0.41
9:A:68:LYS:HB3	9:A:68:LYS:HE3	1.31	0.41
9:A:232:LYS:HA	9:A:233:PRO:HD3	1.96	0.41
1:E:110:PHE:CZ	2:F:328:PHE:HB2	2.56	0.41
1:E:227:SER:HB2	1:E:245:VAL:HG12	2.03	0.41
3:S:78:ILE:O	3:S:81:SER:OG	2.35	0.41
5:U:78:LYS:HB3	5:U:78:LYS:HZ2	1.84	0.41
10:O:155:THR:HB	10:O:156:GLN:H	1.68	0.41
9:A:115:LEU:HD23	9:A:115:LEU:HA	1.89	0.41
14:F:606:HEA:H261	14:F:606:HEA:H172	1.28	0.40
2:R:37:HIS:HE1	2:R:529:ASN:HD21	1.68	0.40
6:V:130:ALA:HB2	6:V:146:ALA:HB2	2.03	0.40
9:M:286:MET:HE3	9:M:286:MET:HB3	2.01	0.40
2:R:343:ASN:HD22	2:R:343:ASN:HA	1.72	0.40
14:R:607:HEA:HHA	14:R:607:HEA:HBA1	2.03	0.40
3:S:51:ARG:HG3	3:S:58:TRP:CE2	2.56	0.40
5:U:40:ASP:HB3	5:U:41:PRO:HD2	2.02	0.40
7:P:60:LEU:HD23	7:P:60:LEU:HA	1.87	0.40
9:M:161:PHE:HE1	9:A:200:ARG:HH21	1.69	0.40
8:B:537:HIS:HD2	9:A:73:ARG:NH2	2.19	0.40
9:A:402:THR:OG1	9:A:403:ILE:N	2.54	0.40
1:E:95:GLU:HA	1:E:98:LEU:HG	2.03	0.40
1:E:160:ASP:OD1	1:E:162:GLU:HB2	2.21	0.40
2:F:279:SER:HB3	2:F:344:TRP:HE1	1.85	0.40
3:G:73:VAL:O	3:G:76:VAL:HG22	2.22	0.40
5:U:79:TRP:N	5:U:79:TRP:CD1	2.89	0.40
8:N:456:LYS:HE2	8:N:456:LYS:HB3	1.77	0.40
8:B:161:TYR:HA	8:B:164:TYR:CE2	2.57	0.40
9:A:246:TRP:HH2	20:A:505:9YF:C2	2.31	0.40
10:C:242:ARG:NH2	10:C:244:PRO:HG3	2.36	0.40
5:I:40:ASP:HB3	5:I:41:PRO:HD2	2.02	0.40
5:I:74:GLY:HA2	6:J:108:VAL:O	2.21	0.40
6:J:130:ALA:HB2	6:J:146:ALA:HB2	2.03	0.40
2:R:278:VAL:HG21	2:R:365:PHE:CE2	2.56	0.40
7:P:72:GLU:HG2	7:P:73:ASP:N	2.37	0.40
8:N:161:TYR:HA	8:N:164:TYR:CE2	2.57	0.40
9:M:402:THR:OG1	9:M:403:ILE:N	2.54	0.40
9:A:272:PRO:HG2	9:A:308:LEU:HD13	2.02	0.40
14:F:607:HEA:HHA	14:F:607:HEA:HBA1	2.03	0.40
5:I:78:LYS:HB3	5:I:78:LYS:HZ2	1.85	0.40
7:D:87:VAL:HG22	12:D:201:CDL:H321	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:201:CDL:H352	12:D:201:CDL:H322	1.78	0.40
1:Q:76:ARG:HD2	2:R:287:ARG:NH1	2.34	0.40
9:A:298:ASP:OD1	9:A:298:ASP:N	2.55	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%)	243 (89%)	28 (10%)	1 (0%)	30	54
1	Q	279/341 (82%)	246 (88%)	33 (12%)	0	100	100
2	F	550/575 (96%)	517 (94%)	33 (6%)	0	100	100
2	R	550/575 (96%)	518 (94%)	32 (6%)	0	100	100
3	G	184/203 (91%)	177 (96%)	7 (4%)	0	100	100
3	S	183/203 (90%)	176 (96%)	7 (4%)	0	100	100
4	H	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
4	T	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
5	I	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
5	U	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
6	J	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
6	V	143/157 (91%)	134 (94%)	9 (6%)	0	100	100
7	D	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
7	P	73/100 (73%)	71 (97%)	2 (3%)	0	100	100
8	B	522/549 (95%)	475 (91%)	41 (8%)	6 (1%)	11	29
8	N	522/549 (95%)	477 (91%)	41 (8%)	4 (1%)	16	36
9	A	376/429 (88%)	334 (89%)	39 (10%)	3 (1%)	16	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	M	376/429 (88%)	336 (89%)	37 (10%)	3 (1%)	16	36
10	C	214/280 (76%)	182 (85%)	29 (14%)	3 (1%)	9	24
10	O	221/280 (79%)	186 (84%)	30 (14%)	5 (2%)	5	14
All	All	5082/5704 (89%)	4655 (92%)	402 (8%)	25 (0%)	26	49

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	28	SER
9	M	329	LEU
8	B	28	SER
9	A	329	LEU
10	C	155	THR
10	O	161	ASN
8	B	304	SER
8	N	27	PRO
9	M	384	PHE
10	O	109	PRO
10	O	160	GLY
8	B	27	PRO
9	A	384	PHE
10	C	109	PRO
1	E	85	PRO
8	N	459	PRO
9	M	294	GLU
8	B	305	GLN
8	B	459	PRO
9	A	294	GLU
10	C	156	GLN
10	O	112	ARG
10	O	155	THR
8	N	260	PRO
8	B	260	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	236/288 (82%)	236 (100%)	0	100	100
2	F	453/471 (96%)	432 (95%)	21 (5%)	24	49
2	R	453/471 (96%)	432 (95%)	21 (5%)	24	49
3	G	148/161 (92%)	148 (100%)	0	100	100
3	S	147/161 (91%)	147 (100%)	0	100	100
4	H	106/106 (100%)	95 (90%)	11 (10%)	7	18
4	T	106/106 (100%)	95 (90%)	11 (10%)	7	18
5	I	52/59 (88%)	36 (69%)	16 (31%)	0	0
5	U	52/59 (88%)	36 (69%)	16 (31%)	0	0
6	J	107/114 (94%)	90 (84%)	17 (16%)	2	7
6	V	107/114 (94%)	90 (84%)	17 (16%)	2	7
7	D	59/83 (71%)	59 (100%)	0	100	100
7	P	59/83 (71%)	59 (100%)	0	100	100
8	B	424/446 (95%)	399 (94%)	25 (6%)	18	39
8	N	424/446 (95%)	401 (95%)	23 (5%)	20	42
9	A	304/343 (89%)	281 (92%)	23 (8%)	12	29
9	M	304/343 (89%)	281 (92%)	23 (8%)	12	29
10	C	158/207 (76%)	145 (92%)	13 (8%)	10	26
10	O	162/207 (78%)	149 (92%)	13 (8%)	11	27
All	All	4092/4556 (90%)	3842 (94%)	250 (6%)	19	38

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	12	GLU
2	F	96	THR
2	F	159	ASP
2	F	195	CYS
2	F	228	THR
2	F	246	ASP
2	F	280	GLU
2	F	286	SER
2	F	294	THR

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Mol	Chain	Res	Type
2	F	329	MET
2	F	339	ILE
2	F	347	THR
2	F	357	THR
2	F	368	THR
2	F	406	ILE
2	F	444	THR
2	F	472	THR
2	F	486	VAL
2	F	503	GLU
2	F	551	VAL
2	F	560	VAL
4	H	3	ILE
4	H	12	THR
4	H	35	GLU
4	H	43	VAL
4	H	52	THR
4	H	54	THR
4	H	64	ASP
4	H	65	THR
4	H	72	ASP
4	H	76	SER
4	H	124	SER
5	I	2	SER
5	I	3	THR
5	I	5	LEU
5	I	6	THR
5	I	9	LEU
5	I	15	LEU
5	I	20	VAL
5	I	34	ASP
5	I	37	LYS
5	I	39	SER
5	I	43	THR
5	I	52	GLU
5	I	55	ARG
5	I	56	GLU
5	I	70	VAL
5	I	78	LYS
6	J	13	GLU
6	J	14	LEU
6	J	15	ASP

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Mol	Chain	Res	Type
6	J	29	SER
6	J	33	GLU
6	J	38	SER
6	J	45	THR
6	J	53	ASP
6	J	80	THR
6	J	83	GLU
6	J	92	GLU
6	J	113	ASP
6	J	115	LYS
6	J	121	SER
6	J	128	SER
6	J	141	ASP
6	J	155	SER
2	R	12	GLU
2	R	96	THR
2	R	159	ASP
2	R	195	CYS
2	R	228	THR
2	R	246	ASP
2	R	280	GLU
2	R	286	SER
2	R	294	THR
2	R	329	MET
2	R	339	ILE
2	R	347	THR
2	R	357	THR
2	R	368	THR
2	R	406	ILE
2	R	444	THR
2	R	472	THR
2	R	486	VAL
2	R	503	GLU
2	R	551	VAL
2	R	560	VAL
4	T	3	ILE
4	T	12	THR
4	T	35	GLU
4	T	43	VAL
4	T	52	THR
4	T	54	THR
4	T	64	ASP

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Mol	Chain	Res	Type
4	T	65	THR
4	T	72	ASP
4	T	76	SER
4	T	124	SER
5	U	2	SER
5	U	3	THR
5	U	5	LEU
5	U	6	THR
5	U	9	LEU
5	U	15	LEU
5	U	20	VAL
5	U	34	ASP
5	U	37	LYS
5	U	39	SER
5	U	43	THR
5	U	52	GLU
5	U	55	ARG
5	U	56	GLU
5	U	70	VAL
5	U	78	LYS
6	V	13	GLU
6	V	14	LEU
6	V	15	ASP
6	V	29	SER
6	V	33	GLU
6	V	38	SER
6	V	45	THR
6	V	53	ASP
6	V	80	THR
6	V	83	GLU
6	V	92	GLU
6	V	113	ASP
6	V	115	LYS
6	V	121	SER
6	V	128	SER
6	V	141	ASP
6	V	155	SER
8	N	14	LEU
8	N	17	GLN
8	N	20	ASP
8	N	23	THR
8	N	72	SER

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Mol	Chain	Res	Type
8	N	77	THR
8	N	184	THR
8	N	249	THR
8	N	266	SER
8	N	301	SER
8	N	314	GLU
8	N	340	VAL
8	N	347	VAL
8	N	399	ASP
8	N	422	ILE
8	N	441	SER
8	N	447	GLU
8	N	473	VAL
8	N	480	ILE
8	N	501	SER
8	N	527	GLU
8	N	531	LEU
8	N	535	ARG
9	M	68	LYS
9	M	78	GLU
9	M	84	GLU
9	M	86	THR
9	M	101	LEU
9	M	128	SER
9	M	145	LEU
9	M	146	SER
9	M	179	ILE
9	M	189	THR
9	M	201	LYS
9	M	202	LEU
9	M	205	LEU
9	M	206	SER
9	M	211	MET
9	M	218	THR
9	M	239	GLU
9	M	269	ASP
9	M	282	ASP
9	M	288	THR
9	M	327	SER
9	M	367	SER
9	M	416	VAL
10	O	58	SER

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Mol	Chain	Res	Type
10	O	59	SER
10	O	63	ARG
10	O	130	ASP
10	O	150	ASP
10	O	155	THR
10	O	159	ARG
10	O	163	LEU
10	O	224	SER
10	O	226	GLU
10	O	243	GLN
10	O	248	LEU
10	O	267	VAL
8	B	14	LEU
8	B	17	GLN
8	B	20	ASP
8	B	23	THR
8	B	72	SER
8	B	77	THR
8	B	184	THR
8	B	249	THR
8	B	266	SER
8	B	301	SER
8	B	304	SER
8	B	313	THR
8	B	314	GLU
8	B	340	VAL
8	B	347	VAL
8	B	399	ASP
8	B	422	ILE
8	B	441	SER
8	B	447	GLU
8	B	473	VAL
8	B	480	ILE
8	B	501	SER
8	B	527	GLU
8	B	531	LEU
8	B	535	ARG
9	A	68	LYS
9	A	78	GLU
9	A	84	GLU
9	A	86	THR
9	A	101	LEU

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Mol	Chain	Res	Type
9	A	128	SER
9	A	145	LEU
9	A	146	SER
9	A	179	ILE
9	A	189	THR
9	A	201	LYS
9	A	202	LEU
9	A	205	LEU
9	A	206	SER
9	A	211	MET
9	A	218	THR
9	A	239	GLU
9	A	269	ASP
9	A	282	ASP
9	A	288	THR
9	A	327	SER
9	A	367	SER
9	A	416	VAL
10	C	58	SER
10	C	59	SER
10	C	63	ARG
10	C	130	ASP
10	C	150	ASP
10	C	159	ARG
10	C	161	ASN
10	C	163	LEU
10	C	224	SER
10	C	226	GLU
10	C	243	GLN
10	C	248	LEU
10	C	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	75	HIS
1	E	145	GLN
1	E	259	GLN
1	E	302	GLN
1	E	318	GLN
2	F	37	HIS
2	F	72	GLN

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Mol	Chain	Res	Type
2	F	80	ASN
2	F	104	ASN
2	F	162	HIS
2	F	212	ASN
2	F	239	HIS
2	F	343	ASN
2	F	397	HIS
2	F	449	GLN
2	F	450	HIS
2	F	474	ASN
3	G	123	HIS
3	G	147	HIS
3	G	150	HIS
3	G	186	HIS
6	J	40	HIS
6	J	103	GLN
7	D	42	HIS
7	D	66	ASN
7	D	90	ASN
1	Q	122	HIS
1	Q	252	ASN
1	Q	265	GLN
2	R	37	HIS
2	R	72	GLN
2	R	80	ASN
2	R	104	ASN
2	R	162	HIS
2	R	343	ASN
2	R	397	HIS
2	R	450	HIS
2	R	474	ASN
3	S	150	HIS
3	S	186	HIS
4	T	139	HIS
6	V	40	HIS
6	V	103	GLN
7	P	42	HIS
7	P	67	HIS
8	N	34	GLN
8	N	115	HIS
8	N	285	GLN
8	N	366	HIS

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Mol	Chain	Res	Type
8	N	406	HIS
8	N	537	HIS
9	M	158	GLN
9	M	398	GLN
10	O	87	HIS
10	O	128	GLN
10	O	178	HIS
8	B	34	GLN
8	B	36	ASN
8	B	366	HIS
8	B	406	HIS
8	B	537	HIS
9	A	158	GLN
9	A	398	GLN
10	C	67	GLN
10	C	87	HIS
10	C	128	GLN
10	C	178	HIS
10	C	222	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	$\#\|Z\| > 2$
12	CDL	B	606	8	73,73,99	1.16	7 (9%)	79,85,111	1.01	4 (5%)
12	CDL	B	608	-	78,78,99	1.12	7 (8%)	84,90,111	1.03	4 (4%)
14	HEA	R	607	2	66,67,67	2.67	35 (53%)	78,103,103	3.31	45 (57%)
20	9YF	M	504	-	40,40,58	1.01	3 (7%)	50,52,71	1.38	7 (14%)
21	HEC	O	305	10	50,50,50	1.66	6 (12%)	68,82,82	1.38	6 (8%)
21	HEC	C	302	10	50,50,50	1.66	5 (10%)	68,82,82	1.38	6 (8%)
12	CDL	B	603	-	78,78,99	1.14	8 (10%)	84,90,111	0.99	4 (4%)
18	HV0	B	611	-	43,43,43	1.99	11 (25%)	57,62,62	2.00	8 (14%)
20	9YF	A	505	-	42,42,58	1.03	4 (9%)	52,54,71	1.27	6 (11%)
12	CDL	B	605	-	65,65,99	1.22	8 (12%)	71,77,111	0.98	4 (5%)
14	HEA	F	607	2	66,67,67	2.67	35 (53%)	78,103,103	3.31	45 (57%)
12	CDL	N	604	-	73,73,99	1.16	7 (9%)	79,85,111	1.03	4 (5%)
16	HEM	N	602	8	50,50,50	1.35	8 (16%)	66,82,82	1.16	4 (6%)
12	CDL	N	606	-	78,78,99	1.11	8 (10%)	84,90,111	0.99	4 (4%)
21	HEC	C	301	10	50,50,50	1.74	5 (10%)	68,82,82	1.44	8 (11%)
12	CDL	P	201	7	87,87,99	1.07	6 (6%)	93,99,111	0.94	4 (4%)
17	MQ9	A	502	-	44,44,59	3.90	15 (34%)	54,57,75	3.22	24 (44%)
16	HEM	N	601	8	49,49,50	1.31	5 (10%)	66,81,82	1.05	3 (4%)
14	HEA	F	606	2	66,67,67	2.66	35 (53%)	78,103,103	3.40	44 (56%)
17	MQ9	N	607	-	59,59,59	3.94	18 (30%)	72,75,75	3.30	31 (43%)
18	HV0	N	609	-	43,43,43	1.94	11 (25%)	57,62,62	2.08	12 (21%)
13	PLM	N	603	-	10,10,17	0.62	0	9,9,17	0.55	0
12	CDL	D	201	7	87,87,99	1.07	6 (6%)	93,99,111	0.96	4 (4%)
15	9Y0	G	301	-	42,42,48	0.94	4 (9%)	44,47,53	0.91	2 (4%)
13	PLM	F	603	-	16,16,17	0.56	0	15,15,17	0.42	0
17	MQ9	B	610	-	59,59,59	3.86	18 (30%)	72,75,75	3.40	33 (45%)
19	FES	A	501	9	0,4,4	-	-	-		
17	MQ9	C	303	-	49,49,59	3.96	16 (32%)	60,63,75	3.16	26 (43%)
12	CDL	R	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
12	CDL	O	301	-	78,78,99	1.12	7 (8%)	84,90,111	0.97	5 (5%)
12	CDL	N	605	-	76,76,99	1.13	7 (9%)	82,88,111	0.98	4 (4%)
16	HEM	B	601	8	49,49,50	1.31	5 (10%)	66,81,82	1.06	3 (4%)
21	HEC	O	304	10	50,50,50	1.73	5 (10%)	68,82,82	1.44	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	PLM	B	604	-	10,10,17	0.62	0	9,9,17	0.55	0
13	PLM	R	603	-	16,16,17	0.56	0	15,15,17	0.42	0
19	FES	M	501	9	0,4,4	-	-	-		
17	MQ9	O	303	-	59,59,59	3.87	18 (30%)	72,75,75	3.38	33 (45%)
12	CDL	A	504	-	94,94,99	1.05	7 (7%)	100,106,111	0.91	4 (4%)
14	HEA	R	606	2	66,67,67	2.65	35 (53%)	78,103,103	3.40	44 (56%)
15	9Y0	S	301	-	42,42,48	0.95	4 (9%)	44,47,53	0.91	2 (4%)
12	CDL	F	602	-	80,80,99	1.11	7 (8%)	86,92,111	0.97	4 (4%)
16	HEM	B	602	8	50,50,50	1.34	8 (16%)	66,82,82	1.15	5 (7%)
12	CDL	M	502	-	94,94,99	1.05	7 (7%)	100,106,111	0.85	4 (4%)
17	MQ9	B	609	-	44,44,59	3.89	15 (34%)	54,57,75	3.16	22 (40%)
17	MQ9	O	302	-	49,49,59	3.90	16 (32%)	60,63,75	3.25	25 (41%)
12	CDL	F	601	-	75,75,99	1.14	7 (9%)	81,87,111	1.00	4 (4%)
20	9YF	M	503	-	44,44,58	0.99	4 (9%)	55,57,71	1.10	5 (9%)
12	CDL	B	607	-	76,76,99	1.13	7 (9%)	82,88,111	1.03	4 (4%)
17	MQ9	N	608	8	59,59,59	3.96	19 (32%)	72,75,75	3.33	33 (45%)
20	9YF	A	503	-	51,51,58	0.95	5 (9%)	62,64,71	1.01	4 (6%)
12	CDL	R	602	-	80,80,99	1.11	7 (8%)	86,92,111	0.97	4 (4%)

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
12	CDL	B	606	8	-	39/84/84/110	-
12	CDL	B	608	-	-	45/89/89/110	-
14	HEA	R	607	2	-	19/36/76/76	-
21	HEC	O	305	10	1/1/3/7	2/14/54/54	-
20	9YF	M	504	-	-	18/35/59/78	0/1/1/1
21	HEC	C	302	10	1/1/3/7	2/14/54/54	-
12	CDL	B	603	-	-	53/89/89/110	-
18	HV0	B	611	-	-	4/24/34/34	0/5/5/5
20	9YF	A	505	-	-	15/37/61/78	0/1/1/1
12	CDL	B	605	-	-	48/76/76/110	-
14	HEA	F	607	2	-	18/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	N	604	-	-	51/84/84/110	-
21	HEC	C	301	10	1/1/3/7	8/14/54/54	-
12	CDL	N	606	-	-	46/89/89/110	-
16	HEM	N	602	8	-	3/14/54/54	-
12	CDL	P	201	7	-	63/98/98/110	-
17	MQ9	A	502	-	-	21/35/55/73	0/2/2/2
16	HEM	N	601	8	-	1/12/52/54	-
14	HEA	F	606	2	-	16/36/76/76	-
17	MQ9	N	607	-	-	30/53/73/73	0/2/2/2
18	HV0	N	609	-	-	4/24/34/34	0/5/5/5
13	PLM	N	603	-	-	1/7/8/15	-
12	CDL	D	201	7	-	49/98/98/110	-
15	9Y0	G	301	-	-	29/46/46/52	-
13	PLM	F	603	-	-	5/13/14/15	-
17	MQ9	B	610	-	-	24/53/73/73	0/2/2/2
19	FES	A	501	9	-	-	0/1/1/1
17	MQ9	C	303	-	-	24/41/61/73	0/2/2/2
12	CDL	R	601	-	-	42/86/86/110	-
12	CDL	O	301	-	-	47/89/89/110	-
12	CDL	N	605	-	-	40/87/87/110	-
21	HEC	O	304	10	1/1/3/7	8/14/54/54	-
16	HEM	B	601	8	-	2/12/52/54	-
13	PLM	B	604	-	-	1/7/8/15	-
13	PLM	R	603	-	-	4/13/14/15	-
19	FES	M	501	9	-	-	0/1/1/1
17	MQ9	O	303	-	-	26/53/73/73	0/2/2/2
12	CDL	A	504	-	-	57/105/105/110	-
14	HEA	R	606	2	-	16/36/76/76	-
15	9Y0	S	301	-	-	29/46/46/52	-
12	CDL	F	602	-	-	58/91/91/110	-
16	HEM	B	602	8	-	3/14/54/54	-
12	CDL	M	502	-	-	65/105/105/110	-
17	MQ9	B	609	-	-	20/35/55/73	0/2/2/2
17	MQ9	O	302	-	-	26/41/61/73	0/2/2/2
12	CDL	F	601	-	-	42/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	9YF	M	503	-	-	19/39/63/78	0/1/1/1
12	CDL	B	607	-	-	38/87/87/110	-
17	MQ9	N	608	8	-	30/53/73/73	0/2/2/2
20	9YF	A	503	-	-	30/47/71/78	0/1/1/1
12	CDL	R	602	-	-	58/91/91/110	-

All (488) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	607	MQ9	C18-C19	9.34	1.55	1.33
17	C	303	MQ9	C23-C24	9.34	1.55	1.33
17	N	608	MQ9	C18-C19	9.29	1.55	1.33
17	N	608	MQ9	C33-C34	9.29	1.55	1.33
17	A	502	MQ9	C23-C24	9.28	1.55	1.33
17	N	607	MQ9	C23-C24	9.27	1.55	1.33
17	C	303	MQ9	C18-C19	9.26	1.55	1.33
17	B	609	MQ9	C18-C19	9.24	1.55	1.33
17	N	608	MQ9	C23-C24	9.23	1.55	1.33
17	A	502	MQ9	C18-C19	9.22	1.55	1.33
17	O	302	MQ9	C23-C24	9.21	1.55	1.33
17	O	303	MQ9	C18-C19	9.20	1.55	1.33
17	O	302	MQ9	C18-C19	9.19	1.55	1.33
17	B	609	MQ9	C23-C24	9.19	1.55	1.33
17	C	303	MQ9	C28-C29	9.16	1.54	1.33
17	C	303	MQ9	C33-C34	9.12	1.54	1.33
17	N	607	MQ9	C33-C34	9.11	1.54	1.33
17	O	303	MQ9	C23-C24	9.09	1.54	1.33
17	N	607	MQ9	C28-C29	9.09	1.54	1.33
17	B	610	MQ9	C18-C19	9.07	1.54	1.33
17	B	610	MQ9	C23-C24	9.04	1.54	1.33
17	O	302	MQ9	C33-C34	9.02	1.54	1.33
17	N	608	MQ9	C28-C29	9.02	1.54	1.33
17	O	303	MQ9	C33-C34	9.00	1.54	1.33
17	N	607	MQ9	C38-C39	8.96	1.54	1.33
17	O	303	MQ9	C28-C29	8.93	1.54	1.33
17	O	302	MQ9	C28-C29	8.92	1.54	1.33
17	B	610	MQ9	C33-C34	8.91	1.54	1.33
17	A	502	MQ9	C28-C29	8.89	1.54	1.33
17	B	610	MQ9	C28-C29	8.89	1.54	1.33
17	B	609	MQ9	C28-C29	8.87	1.54	1.33
17	N	608	MQ9	C38-C39	8.84	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	610	MQ9	C38-C39	8.80	1.54	1.33
17	O	303	MQ9	C38-C39	8.75	1.54	1.33
17	N	608	MQ9	C13-C14	8.65	1.53	1.33
17	C	303	MQ9	C13-C14	8.57	1.53	1.33
17	A	502	MQ9	C13-C14	8.56	1.53	1.33
17	B	609	MQ9	C13-C14	8.56	1.53	1.33
17	O	302	MQ9	C13-C14	8.52	1.53	1.33
17	N	607	MQ9	C13-C14	8.49	1.53	1.33
17	N	607	MQ9	C43-C44	8.49	1.53	1.33
17	O	303	MQ9	C13-C14	8.47	1.53	1.33
17	B	610	MQ9	C13-C14	8.46	1.53	1.33
17	N	608	MQ9	C43-C44	8.45	1.53	1.33
17	B	610	MQ9	C43-C44	8.44	1.53	1.33
17	O	303	MQ9	C43-C44	8.27	1.52	1.33
17	N	608	MQ9	C8-C9	8.22	1.52	1.33
17	B	609	MQ9	C8-C9	8.12	1.52	1.33
17	N	607	MQ9	C8-C9	8.08	1.52	1.33
17	A	502	MQ9	C8-C9	8.06	1.52	1.33
17	C	303	MQ9	C8-C9	7.98	1.52	1.33
17	B	610	MQ9	C8-C9	7.96	1.52	1.33
17	O	303	MQ9	C8-C9	7.94	1.52	1.33
17	O	302	MQ9	C8-C9	7.93	1.52	1.33
21	O	304	HEC	C3D-C2D	7.76	1.53	1.36
21	C	301	HEC	C3D-C2D	7.74	1.53	1.36
21	O	305	HEC	C3D-C2D	7.73	1.53	1.36
21	C	302	HEC	C3D-C2D	7.69	1.53	1.36
17	A	502	MQ9	C33-C34	7.68	1.54	1.32
17	C	303	MQ9	C38-C39	7.66	1.54	1.32
17	B	609	MQ9	C33-C34	7.64	1.54	1.32
17	A	502	MQ9	O1-C1	7.57	1.39	1.23
17	O	302	MQ9	C38-C39	7.54	1.54	1.32
17	B	609	MQ9	O1-C1	7.54	1.39	1.23
17	N	607	MQ9	O1-C1	7.54	1.39	1.23
17	N	608	MQ9	O1-C1	7.53	1.39	1.23
17	B	609	MQ9	O4-C4	7.50	1.39	1.23
17	A	502	MQ9	O4-C4	7.49	1.39	1.23
17	B	610	MQ9	O4-C4	7.48	1.39	1.23
17	O	303	MQ9	O1-C1	7.47	1.39	1.23
17	O	302	MQ9	O1-C1	7.46	1.39	1.23
17	O	303	MQ9	O4-C4	7.46	1.39	1.23
17	C	303	MQ9	O1-C1	7.45	1.39	1.23
17	N	608	MQ9	O4-C4	7.45	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	610	MQ9	O1-C1	7.43	1.38	1.23
17	N	607	MQ9	O4-C4	7.43	1.38	1.23
17	C	303	MQ9	O4-C4	7.41	1.38	1.23
17	O	302	MQ9	O4-C4	7.35	1.38	1.23
18	N	609	HV0	C11-N13	7.19	1.46	1.33
17	N	608	MQ9	C48-C49	7.13	1.52	1.32
18	B	611	HV0	C11-N13	7.10	1.45	1.33
17	N	607	MQ9	C48-C49	7.10	1.52	1.32
17	O	303	MQ9	C48-C49	7.00	1.52	1.32
17	B	610	MQ9	C48-C49	6.99	1.52	1.32
14	F	606	HEA	C1D-ND	-6.70	1.28	1.40
14	R	607	HEA	C1D-ND	-6.66	1.28	1.40
14	R	606	HEA	C1D-ND	-6.64	1.28	1.40
14	F	607	HEA	C1D-ND	-6.61	1.28	1.40
14	F	607	HEA	C1C-NC	-5.74	1.28	1.39
14	R	607	HEA	C1C-NC	-5.73	1.28	1.39
14	F	606	HEA	C1C-NC	-5.72	1.28	1.39
14	R	606	HEA	C1C-NC	-5.66	1.28	1.39
14	R	607	HEA	C4B-NB	-5.35	1.31	1.40
14	F	607	HEA	C4B-NB	-5.28	1.31	1.40
14	R	606	HEA	C4B-NB	-5.14	1.31	1.40
14	F	606	HEA	C3A-C4A	-5.11	1.37	1.46
14	F	606	HEA	C4B-NB	-5.10	1.31	1.40
14	F	607	HEA	C3A-C4A	-5.09	1.37	1.46
14	R	606	HEA	C3A-C4A	-5.09	1.37	1.46
14	R	607	HEA	C3A-C4A	-5.08	1.37	1.46
17	C	303	MQ9	C5-C4	-4.83	1.37	1.48
21	C	301	HEC	FE-NB	4.81	2.09	1.94
21	O	304	HEC	FE-NB	4.79	2.09	1.94
17	O	302	MQ9	C5-C4	-4.74	1.37	1.48
17	N	607	MQ9	C5-C4	-4.68	1.38	1.48
17	O	303	MQ9	C5-C4	-4.60	1.38	1.48
17	B	610	MQ9	C5-C4	-4.60	1.38	1.48
14	F	607	HEA	C1B-NB	-4.59	1.29	1.38
17	N	608	MQ9	C5-C4	-4.57	1.38	1.48
17	A	502	MQ9	C5-C4	-4.56	1.38	1.48
14	R	607	HEA	C1B-NB	-4.55	1.29	1.38
17	B	609	MQ9	C5-C4	-4.53	1.38	1.48
14	F	606	HEA	C1B-NB	-4.52	1.29	1.38
14	R	606	HEA	C1B-NB	-4.48	1.29	1.38
14	F	606	HEA	FE-NB	4.48	2.08	1.94
14	R	606	HEA	FE-NB	4.48	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	607	HEA	FE-NB	4.45	2.08	1.94
14	R	607	HEA	FE-NB	4.42	2.08	1.94
14	R	607	HEA	O2A-CGA	-4.32	1.16	1.30
14	F	607	HEA	C4C-NC	-4.31	1.31	1.39
14	R	606	HEA	O2A-CGA	-4.30	1.16	1.30
14	F	607	HEA	O2A-CGA	-4.29	1.16	1.30
14	F	606	HEA	O2A-CGA	-4.27	1.16	1.30
14	F	606	HEA	C4C-NC	-4.21	1.31	1.39
14	R	607	HEA	C4C-NC	-4.21	1.31	1.39
14	R	606	HEA	C4C-NC	-4.14	1.31	1.39
18	B	611	HV0	C22-N21	4.10	1.53	1.46
18	B	611	HV0	C26-N21	4.09	1.53	1.46
14	F	607	HEA	O2D-CGD	-4.05	1.17	1.30
14	R	607	HEA	C3A-C2A	4.03	1.45	1.36
14	R	607	HEA	O2D-CGD	-4.03	1.17	1.30
14	F	607	HEA	C3A-C2A	4.00	1.45	1.36
14	R	606	HEA	O2D-CGD	-3.98	1.17	1.30
14	F	606	HEA	O2D-CGD	-3.97	1.17	1.30
17	C	303	MQ9	C3-C4	-3.90	1.40	1.48
14	F	606	HEA	C16-C15	-3.86	1.43	1.51
14	F	607	HEA	C16-C15	-3.85	1.43	1.51
14	R	606	HEA	C3A-C2A	3.85	1.45	1.36
18	N	609	HV0	C26-N21	3.84	1.52	1.46
14	R	607	HEA	C16-C15	-3.84	1.43	1.51
14	R	606	HEA	C16-C15	-3.82	1.43	1.51
17	N	607	MQ9	C6-C1	-3.82	1.37	1.47
17	C	303	MQ9	C6-C1	-3.82	1.37	1.47
14	F	606	HEA	C3A-C2A	3.82	1.45	1.36
14	F	606	HEA	C4D-ND	-3.75	1.31	1.38
14	R	607	HEA	C4D-ND	-3.75	1.31	1.38
14	F	607	HEA	C4D-ND	-3.75	1.31	1.38
17	O	303	MQ9	C6-C1	-3.74	1.37	1.47
21	C	302	HEC	FE-ND	3.73	2.06	1.94
18	B	611	HV0	N04-N03	3.73	1.41	1.37
17	O	302	MQ9	C6-C1	-3.71	1.37	1.47
14	R	606	HEA	C4D-ND	-3.70	1.31	1.38
21	O	305	HEC	FE-ND	3.69	2.06	1.94
17	B	610	MQ9	C6-C1	-3.66	1.38	1.47
17	N	608	MQ9	C6-C1	-3.64	1.38	1.47
17	O	302	MQ9	C3-C4	-3.58	1.41	1.48
18	N	609	HV0	C22-N21	3.54	1.52	1.46
17	N	608	MQ9	C3-C4	-3.53	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	502	MQ9	C3-C4	-3.51	1.41	1.48
17	O	303	MQ9	C3-C4	-3.46	1.41	1.48
14	R	607	HEA	C4D-C3D	-3.46	1.39	1.45
17	B	610	MQ9	C3-C4	-3.43	1.41	1.48
17	B	609	MQ9	C6-C1	-3.42	1.38	1.47
14	F	607	HEA	C4D-C3D	-3.41	1.39	1.45
18	N	609	HV0	N04-N03	3.41	1.41	1.37
14	R	606	HEA	C4D-C3D	-3.41	1.39	1.45
17	N	607	MQ9	C3-C4	-3.40	1.41	1.48
14	F	606	HEA	CBA-CGA	-3.38	1.42	1.50
21	O	304	HEC	FE-ND	3.36	2.05	1.94
14	R	606	HEA	CBA-CGA	-3.36	1.42	1.50
14	F	607	HEA	CBA-CGA	-3.36	1.42	1.50
14	R	607	HEA	CBA-CGA	-3.35	1.42	1.50
21	C	301	HEC	FE-ND	3.35	2.05	1.94
14	F	606	HEA	C4D-C3D	-3.34	1.39	1.45
17	B	609	MQ9	C3-C4	-3.34	1.41	1.48
12	F	602	CDL	OA8-CA7	3.33	1.43	1.33
12	R	602	CDL	OA8-CA7	3.33	1.43	1.33
16	B	602	HEM	FE-ND	3.32	2.05	1.94
16	N	602	HEM	FE-ND	3.27	2.05	1.94
12	B	605	CDL	OA8-CA7	3.26	1.42	1.33
17	A	502	MQ9	C2-C3	-3.26	1.35	1.40
17	N	608	MQ9	C2-C3	-3.25	1.35	1.40
12	N	604	CDL	OA8-CA7	3.24	1.42	1.33
12	A	504	CDL	OA8-CA7	3.23	1.42	1.33
17	C	303	MQ9	C2-C3	-3.23	1.35	1.40
12	P	201	CDL	OA8-CA7	3.22	1.42	1.33
17	O	303	MQ9	C2-C3	-3.22	1.35	1.40
12	O	301	CDL	OA8-CA7	3.22	1.42	1.33
14	F	607	HEA	CBD-CGD	-3.22	1.43	1.50
17	B	610	MQ9	C2-C3	-3.22	1.35	1.40
17	A	502	MQ9	C6-C1	-3.20	1.39	1.47
14	R	606	HEA	CBD-CGD	-3.20	1.43	1.50
12	B	606	CDL	OA8-CA7	3.19	1.42	1.33
12	M	502	CDL	OA8-CA7	3.19	1.42	1.33
14	R	607	HEA	CBD-CGD	-3.18	1.43	1.50
17	O	302	MQ9	C2-C3	-3.17	1.35	1.40
12	B	603	CDL	OA8-CA7	3.17	1.42	1.33
21	O	305	HEC	FE-NB	3.16	2.04	1.94
21	C	302	HEC	FE-NB	3.15	2.04	1.94
14	F	606	HEA	CBD-CGD	-3.14	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	601	CDL	OA8-CA7	3.14	1.42	1.33
17	B	609	MQ9	C2-C3	-3.13	1.35	1.40
12	B	608	CDL	OA8-CA7	3.12	1.42	1.33
12	D	201	CDL	OA8-CA7	3.09	1.42	1.33
12	F	601	CDL	OA8-CA7	3.09	1.42	1.33
14	R	606	HEA	C3D-C2D	3.07	1.43	1.36
12	N	606	CDL	OA8-CA7	3.06	1.42	1.33
17	N	607	MQ9	C2-C3	-3.05	1.35	1.40
12	N	605	CDL	OA8-CA7	3.02	1.42	1.33
14	F	606	HEA	C3D-C2D	3.01	1.43	1.36
12	D	201	CDL	OB6-CB5	3.01	1.42	1.34
14	F	606	HEA	FE-NC	3.00	2.05	1.95
12	B	607	CDL	OA8-CA7	3.00	1.42	1.33
14	R	606	HEA	FE-NC	3.00	2.05	1.95
18	N	609	HV0	C25-C24	-2.97	1.45	1.53
12	P	201	CDL	OB6-CB5	2.97	1.42	1.34
14	R	607	HEA	FE-NC	2.97	2.05	1.95
14	F	607	HEA	FE-NC	2.96	2.05	1.95
14	R	607	HEA	C3D-C2D	2.96	1.43	1.36
12	N	604	CDL	OB6-CB5	2.95	1.42	1.34
16	B	601	HEM	FE-ND	2.94	2.03	1.94
12	M	502	CDL	OB6-CB5	2.94	1.42	1.34
12	B	603	CDL	OB6-CB5	2.94	1.42	1.34
14	F	607	HEA	O11-C11	-2.93	1.36	1.42
12	B	606	CDL	OB6-CB5	2.92	1.42	1.34
14	F	606	HEA	O11-C11	-2.90	1.36	1.42
16	N	601	HEM	FE-ND	2.90	2.03	1.94
14	F	607	HEA	C3D-C2D	2.89	1.42	1.36
12	A	504	CDL	OB6-CB5	2.89	1.42	1.34
14	R	607	HEA	O11-C11	-2.89	1.36	1.42
14	R	606	HEA	CHC-C4B	2.87	1.44	1.38
14	F	606	HEA	CHC-C4B	2.87	1.44	1.38
12	R	601	CDL	OB6-CB5	2.87	1.42	1.34
17	O	303	MQ9	C2-C1	-2.86	1.42	1.48
17	C	303	MQ9	C2-C1	-2.86	1.42	1.48
17	B	610	MQ9	C2-C1	-2.85	1.42	1.48
12	R	602	CDL	OB6-CB5	2.85	1.42	1.34
12	F	602	CDL	OB6-CB5	2.84	1.42	1.34
14	R	606	HEA	O11-C11	-2.84	1.36	1.42
12	F	601	CDL	OB6-CB5	2.84	1.42	1.34
12	B	608	CDL	OB6-CB5	2.84	1.42	1.34
18	B	611	HV0	C23-C24	-2.82	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	302	MQ9	C2-C1	-2.82	1.42	1.48
21	O	304	HEC	FE-NA	2.81	2.04	1.95
12	B	605	CDL	OB6-CB5	2.81	1.42	1.34
12	B	606	CDL	OA6-CA5	2.81	1.42	1.34
16	N	602	HEM	FE-NB	2.79	2.03	1.94
17	N	608	MQ9	C2-C1	-2.79	1.42	1.48
16	B	601	HEM	CAB-C3B	2.79	1.55	1.47
14	F	606	HEA	C3B-C2B	2.79	1.41	1.34
21	C	301	HEC	FE-NA	2.78	2.04	1.95
16	N	601	HEM	CAB-C3B	2.78	1.55	1.47
16	B	602	HEM	FE-NB	2.78	2.03	1.94
16	B	602	HEM	CAC-C3C	2.78	1.55	1.47
18	B	611	HV0	C25-C24	-2.77	1.45	1.53
18	N	609	HV0	C23-C24	-2.77	1.45	1.53
17	N	607	MQ9	C2-C1	-2.77	1.42	1.48
16	N	602	HEM	CAC-C3C	2.77	1.55	1.47
12	N	606	CDL	OB6-CB5	2.75	1.42	1.34
12	A	504	CDL	OA6-CA5	2.75	1.42	1.34
14	R	607	HEA	C3B-C2B	2.74	1.40	1.34
14	R	606	HEA	C3B-C2B	2.73	1.40	1.34
12	N	605	CDL	OB6-CB5	2.72	1.42	1.34
12	B	607	CDL	OB6-CB5	2.72	1.42	1.34
14	F	607	HEA	C3B-C2B	2.71	1.40	1.34
14	F	606	HEA	CHD-C4C	2.71	1.45	1.39
14	F	607	HEA	CHC-C4B	2.71	1.44	1.38
17	B	609	MQ9	C2-C1	-2.71	1.43	1.48
12	O	301	CDL	OB6-CB5	2.71	1.41	1.34
14	R	607	HEA	CHC-C4B	2.71	1.44	1.38
20	A	505	9YF	O9-C	-2.70	1.39	1.46
16	B	601	HEM	FE-NA	2.70	2.04	1.95
18	B	611	HV0	C10-C11	2.70	1.53	1.48
17	N	608	MQ9	C6-C5	2.70	1.40	1.35
18	N	609	HV0	C10-C11	2.69	1.53	1.48
12	P	201	CDL	OA6-CA5	2.68	1.41	1.34
16	N	601	HEM	FE-NA	2.68	2.04	1.95
12	B	607	CDL	OA6-CA5	2.67	1.41	1.34
14	F	606	HEA	FE-ND	2.67	2.03	1.94
14	R	606	HEA	CHD-C4C	2.67	1.45	1.39
14	R	606	HEA	FE-ND	2.67	2.03	1.94
14	F	606	HEA	CBD-CAD	-2.66	1.43	1.52
15	G	301	9Y0	O7-C1	-2.66	1.39	1.46
17	A	502	MQ9	C2-C1	-2.66	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	608	CDL	OA6-CA5	2.66	1.41	1.34
14	F	607	HEA	CHD-C4C	2.66	1.45	1.39
12	N	604	CDL	OA6-CA5	2.66	1.41	1.34
12	M	502	CDL	OA6-CA5	2.66	1.41	1.34
16	N	602	HEM	CAB-C3B	2.65	1.54	1.47
18	B	611	HV0	C18-N21	2.65	1.46	1.38
12	F	602	CDL	OA6-CA5	2.65	1.41	1.34
20	M	504	9YF	O9-C	-2.65	1.40	1.46
14	R	607	HEA	C20-C19	-2.65	1.45	1.51
12	B	603	CDL	OA6-CA5	2.64	1.41	1.34
12	D	201	CDL	OA6-CA5	2.64	1.41	1.34
12	R	602	CDL	OA6-CA5	2.63	1.41	1.34
21	O	305	HEC	FE-NC	2.63	2.04	1.95
14	R	606	HEA	CBD-CAD	-2.62	1.43	1.52
12	B	605	CDL	OA6-CA5	2.62	1.41	1.34
15	S	301	9Y0	O7-C1	-2.61	1.40	1.46
14	F	607	HEA	C20-C19	-2.61	1.45	1.51
14	F	607	HEA	C1A-NA	2.61	1.44	1.39
16	N	601	HEM	FE-NB	2.60	2.02	1.94
16	B	602	HEM	CAB-C3B	2.60	1.54	1.47
21	C	302	HEC	FE-NC	2.60	2.03	1.95
14	F	607	HEA	CBD-CAD	-2.60	1.43	1.52
21	C	301	HEC	FE-NC	2.59	2.03	1.95
14	R	606	HEA	C1A-NA	2.59	1.44	1.39
14	F	606	HEA	C1A-NA	2.59	1.44	1.39
18	N	609	HV0	O12-C11	-2.59	1.18	1.23
14	F	607	HEA	CMC-C2C	-2.59	1.45	1.50
14	R	607	HEA	CHD-C4C	2.58	1.45	1.39
14	R	607	HEA	CMC-C2C	-2.58	1.45	1.50
16	B	601	HEM	FE-NB	2.58	2.02	1.94
14	R	606	HEA	C20-C19	-2.58	1.45	1.51
12	O	301	CDL	OA6-CA5	2.57	1.41	1.34
14	F	606	HEA	C20-C19	-2.57	1.45	1.51
14	R	607	HEA	CBD-CAD	-2.56	1.43	1.52
21	C	302	HEC	FE-NA	2.56	2.03	1.95
12	N	606	CDL	OA6-CA5	2.56	1.41	1.34
14	R	607	HEA	C12-C11	-2.56	1.48	1.52
12	N	605	CDL	OA6-CA4	-2.56	1.40	1.46
18	N	609	HV0	C09-N04	-2.55	1.31	1.37
14	R	607	HEA	FE-ND	2.55	2.02	1.94
21	O	304	HEC	FE-NC	2.55	2.03	1.95
14	F	607	HEA	C12-C11	-2.55	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	606	CDL	OA6-CA4	-2.54	1.40	1.46
14	F	606	HEA	O1A-CGA	-2.53	1.13	1.22
12	R	601	CDL	OA6-CA5	2.53	1.41	1.34
21	O	305	HEC	FE-NA	2.52	2.03	1.95
12	F	601	CDL	OA6-CA5	2.52	1.41	1.34
14	F	606	HEA	CMC-C2C	-2.52	1.45	1.50
14	R	607	HEA	C1A-NA	2.51	1.44	1.39
12	O	301	CDL	OA6-CA4	-2.51	1.40	1.46
14	F	606	HEA	CHD-C1D	2.51	1.43	1.38
14	R	606	HEA	CMC-C2C	-2.50	1.45	1.50
14	F	607	HEA	FE-ND	2.50	2.02	1.94
12	R	601	CDL	OA6-CA4	-2.50	1.40	1.46
12	N	605	CDL	OA6-CA5	2.50	1.41	1.34
12	F	601	CDL	OA6-CA4	-2.50	1.40	1.46
14	F	606	HEA	C12-C11	-2.49	1.48	1.52
18	B	611	HV0	O12-C11	-2.49	1.18	1.23
14	R	606	HEA	O1A-CGA	-2.48	1.13	1.22
17	A	502	MQ9	C6-C5	2.48	1.39	1.35
14	R	607	HEA	O1A-CGA	-2.48	1.13	1.22
14	F	607	HEA	O1A-CGA	-2.48	1.14	1.22
20	A	503	9YF	O9-C	-2.48	1.40	1.46
12	D	201	CDL	OB8-CB7	2.47	1.40	1.33
14	R	606	HEA	CHD-C1D	2.47	1.43	1.38
14	R	607	HEA	CHD-C1D	2.47	1.43	1.38
12	B	607	CDL	OB8-CB7	2.46	1.40	1.33
14	R	606	HEA	C12-C11	-2.45	1.48	1.52
16	B	602	HEM	FE-NC	2.45	2.03	1.95
14	F	606	HEA	C18-C19	-2.44	1.27	1.33
16	N	602	HEM	FE-NC	2.44	2.03	1.95
14	R	606	HEA	C18-C19	-2.44	1.27	1.33
14	F	607	HEA	CHD-C1D	2.44	1.43	1.38
20	A	503	9YF	O11-C25	2.43	1.40	1.33
12	N	605	CDL	OB8-CB7	2.42	1.40	1.33
20	A	505	9YF	O11-C25	2.42	1.40	1.33
12	B	605	CDL	OB8-CB7	2.42	1.40	1.33
12	B	608	CDL	OA6-CA4	-2.41	1.40	1.46
17	B	609	MQ9	C6-C5	2.41	1.39	1.35
18	B	611	HV0	C09-N04	-2.41	1.31	1.37
12	B	603	CDL	OA6-CA4	-2.41	1.40	1.46
12	B	603	CDL	OB8-CB7	2.41	1.40	1.33
20	M	504	9YF	O11-C25	2.40	1.40	1.33
16	N	601	HEM	FE-NC	2.40	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	301	CDL	OB6-CB4	-2.40	1.40	1.46
12	N	606	CDL	OB6-CB4	-2.40	1.40	1.46
12	M	502	CDL	OA6-CA4	-2.40	1.40	1.46
20	M	503	9YF	O11-C25	2.40	1.40	1.33
14	F	607	HEA	C18-C19	-2.40	1.27	1.33
20	M	503	9YF	O9-C	-2.39	1.40	1.46
16	B	601	HEM	FE-NC	2.39	2.03	1.95
12	B	607	CDL	OB6-CB4	-2.39	1.40	1.46
12	N	605	CDL	OB6-CB4	-2.39	1.40	1.46
12	N	604	CDL	OA6-CA4	-2.38	1.40	1.46
15	S	301	9Y0	O5-C5	2.37	1.40	1.33
14	R	607	HEA	C18-C19	-2.36	1.27	1.33
12	P	201	CDL	OA6-CA4	-2.36	1.40	1.46
12	D	201	CDL	OA6-CA4	-2.35	1.40	1.46
18	N	609	HV0	C18-N21	2.35	1.45	1.38
12	R	602	CDL	OA6-CA4	-2.34	1.40	1.46
17	B	609	MQ9	C21-C19	2.34	1.56	1.51
20	A	503	9YF	P-O2	2.34	1.66	1.60
12	R	601	CDL	OB6-CB4	-2.34	1.40	1.46
12	F	602	CDL	OB6-CB4	-2.34	1.40	1.46
12	A	504	CDL	OB6-CB4	-2.34	1.40	1.46
12	N	604	CDL	OB8-CB7	2.34	1.40	1.33
12	F	602	CDL	OA6-CA4	-2.33	1.40	1.46
12	B	606	CDL	OB8-CB7	2.33	1.40	1.33
12	B	605	CDL	OA6-CA4	-2.33	1.40	1.46
12	P	201	CDL	OB8-CB7	2.33	1.40	1.33
12	R	602	CDL	OB6-CB4	-2.33	1.40	1.46
12	F	601	CDL	OB6-CB4	-2.33	1.40	1.46
12	F	601	CDL	OB8-CB7	2.33	1.40	1.33
15	G	301	9Y0	O5-C5	2.33	1.40	1.33
12	B	608	CDL	OB8-CB6	-2.32	1.39	1.45
17	N	607	MQ9	C21-C19	2.31	1.56	1.51
17	N	608	MQ9	C21-C19	2.31	1.56	1.51
12	B	607	CDL	OA6-CA4	-2.31	1.40	1.46
17	C	303	MQ9	C21-C19	2.30	1.56	1.51
12	B	606	CDL	OB6-CB4	-2.30	1.40	1.46
12	O	301	CDL	OB8-CB7	2.30	1.40	1.33
14	R	607	HEA	O1D-CGD	-2.29	1.14	1.22
20	M	504	9YF	O11-C24	-2.29	1.39	1.45
12	R	602	CDL	OB8-CB7	2.29	1.40	1.33
17	A	502	MQ9	C21-C19	2.29	1.56	1.51
12	R	601	CDL	OB8-CB7	2.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	607	HEA	C1C-C2C	-2.28	1.37	1.43
14	R	607	HEA	CHA-C1A	2.28	1.42	1.38
12	F	602	CDL	OB8-CB7	2.28	1.40	1.33
14	R	606	HEA	C1C-C2C	-2.28	1.37	1.43
12	M	502	CDL	OB8-CB6	-2.27	1.40	1.45
14	F	607	HEA	CHA-C1A	2.27	1.42	1.38
17	N	607	MQ9	C6-C5	2.27	1.39	1.35
14	R	607	HEA	CHA-C4D	2.27	1.44	1.39
14	F	607	HEA	CHA-C4D	2.26	1.44	1.39
15	S	301	9Y0	O5-C	-2.26	1.40	1.45
17	O	302	MQ9	C21-C19	2.26	1.56	1.51
14	R	606	HEA	CHA-C4D	2.26	1.44	1.39
14	R	607	HEA	C1C-C2C	-2.26	1.37	1.43
12	N	606	CDL	OB8-CB7	2.26	1.39	1.33
14	F	606	HEA	CHA-C4D	2.25	1.44	1.39
14	F	607	HEA	O1D-CGD	-2.25	1.14	1.22
14	F	606	HEA	O1D-CGD	-2.25	1.14	1.22
12	B	608	CDL	OB6-CB4	-2.25	1.41	1.46
12	M	502	CDL	OB8-CB7	2.24	1.39	1.33
17	O	303	MQ9	C6-C5	2.23	1.39	1.35
14	R	607	HEA	C1B-C2B	-2.23	1.40	1.44
12	B	603	CDL	OB6-CB4	-2.23	1.41	1.46
14	F	606	HEA	C1C-C2C	-2.22	1.38	1.43
12	A	504	CDL	OB8-CB6	-2.22	1.40	1.45
14	R	606	HEA	O1D-CGD	-2.22	1.14	1.22
12	N	604	CDL	OB6-CB4	-2.22	1.41	1.46
12	A	504	CDL	OA6-CA4	-2.22	1.41	1.46
14	F	607	HEA	C1B-C2B	-2.22	1.40	1.44
16	N	602	HEM	FE-NA	2.22	2.02	1.95
12	B	606	CDL	OA6-CA4	-2.22	1.41	1.46
17	O	303	MQ9	C21-C19	2.21	1.55	1.51
12	A	504	CDL	OB8-CB7	2.21	1.39	1.33
20	M	503	9YF	O11-C24	-2.21	1.40	1.45
12	R	602	CDL	OB8-CB6	-2.21	1.40	1.45
14	R	606	HEA	C1B-C2B	-2.21	1.40	1.44
12	N	606	CDL	OB8-CB6	-2.19	1.40	1.45
16	B	602	HEM	FE-NA	2.19	2.02	1.95
15	G	301	9Y0	O5-C	-2.17	1.40	1.45
17	B	610	MQ9	C21-C19	2.17	1.55	1.51
12	F	602	CDL	OB8-CB6	-2.16	1.40	1.45
17	B	610	MQ9	C6-C5	2.15	1.39	1.35
12	B	608	CDL	OB8-CB7	2.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	502	CDL	OB6-CB4	-2.14	1.41	1.46
12	F	601	CDL	OB8-CB6	-2.14	1.40	1.45
14	F	606	HEA	C1B-C2B	-2.14	1.40	1.44
16	N	602	HEM	C3B-C2B	-2.12	1.33	1.37
18	B	611	HV0	O38-C39	-2.12	1.40	1.45
20	A	505	9YF	O11-C24	-2.12	1.40	1.45
20	A	503	9YF	O11-C24	-2.12	1.40	1.45
20	M	503	9YF	O9-C8	2.11	1.40	1.34
20	A	503	9YF	O9-C8	2.11	1.40	1.34
12	R	601	CDL	OB8-CB6	-2.11	1.40	1.45
12	O	301	CDL	OB8-CB6	-2.11	1.40	1.45
18	N	609	HV0	O38-C39	-2.11	1.40	1.45
12	B	605	CDL	OB6-CB4	-2.10	1.41	1.46
12	B	603	CDL	OB8-CB6	-2.09	1.40	1.45
15	S	301	9Y0	O7-C21	2.09	1.40	1.34
12	B	607	CDL	OB8-CB6	-2.09	1.40	1.45
20	A	505	9YF	P-O2	2.09	1.66	1.60
17	N	608	MQ9	C36-C34	2.08	1.55	1.51
12	N	604	CDL	OB8-CB6	-2.08	1.40	1.45
16	N	602	HEM	C2A-C3A	-2.07	1.33	1.38
12	D	201	CDL	OB6-CB4	-2.06	1.41	1.46
12	N	605	CDL	OB8-CB6	-2.06	1.40	1.45
16	B	602	HEM	C3B-C2B	-2.06	1.33	1.37
16	B	602	HEM	C2A-C3A	-2.05	1.33	1.38
15	G	301	9Y0	O7-C21	2.05	1.40	1.34
14	F	606	HEA	CHA-C1A	2.05	1.42	1.38
12	B	606	CDL	OB8-CB6	-2.03	1.40	1.45
12	P	201	CDL	OB8-CB6	-2.02	1.40	1.45
12	B	603	CDL	PA1-OA2	2.02	1.67	1.59
21	O	305	HEC	C3C-C2C	-2.02	1.33	1.38
12	B	605	CDL	PA1-OA2	2.02	1.67	1.59
12	N	606	CDL	PA1-OA2	2.01	1.67	1.59
14	R	606	HEA	CHA-C1A	2.01	1.42	1.38
12	B	605	CDL	PB2-OB5	2.01	1.67	1.59
17	O	302	MQ9	C6-C5	2.00	1.38	1.35
17	C	303	MQ9	C6-C5	2.00	1.38	1.35

All (563) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	R	607	HEA	CBC-CAC-C3C	10.44	179.54	127.62
14	F	607	HEA	CBC-CAC-C3C	10.43	179.51	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	606	HEA	CBC-CAC-C3C	10.43	179.50	127.62
14	R	606	HEA	CBC-CAC-C3C	10.42	179.46	127.62
17	N	608	MQ9	C7-C8-C9	-10.15	109.89	126.79
18	B	611	HV0	C25-C24-C27	-9.96	89.45	112.79
17	O	303	MQ9	C7-C8-C9	-9.88	110.34	126.79
17	B	610	MQ9	C7-C8-C9	-9.82	110.44	126.79
17	O	302	MQ9	C7-C8-C9	-9.82	110.45	126.79
17	N	607	MQ9	C7-C8-C9	-9.68	110.67	126.79
17	C	303	MQ9	C7-C8-C9	-9.58	110.85	126.79
18	N	609	HV0	C25-C24-C27	-9.36	90.85	112.79
17	A	502	MQ9	C7-C8-C9	-8.68	112.34	126.79
17	B	609	MQ9	C7-C8-C9	-8.43	112.76	126.79
14	R	606	HEA	C2B-C1B-NB	7.51	118.87	109.88
14	F	606	HEA	C2B-C1B-NB	7.49	118.86	109.88
14	F	607	HEA	C2B-C1B-NB	7.46	118.81	109.88
14	R	607	HEA	C2B-C1B-NB	7.41	118.76	109.88
14	R	606	HEA	CHB-C4A-NA	7.06	132.07	124.44
14	R	607	HEA	CHB-C4A-NA	7.05	132.07	124.44
14	F	606	HEA	CHB-C4A-NA	6.98	131.99	124.44
17	O	303	MQ9	C12-C13-C14	-6.93	110.97	127.66
14	F	607	HEA	CHB-C4A-NA	6.92	131.93	124.44
17	B	610	MQ9	C12-C13-C14	-6.79	111.30	127.66
17	N	607	MQ9	C12-C13-C14	-6.77	111.36	127.66
17	A	502	MQ9	C27-C28-C29	-6.76	111.39	127.66
14	R	606	HEA	C3B-C4B-NB	6.65	117.71	109.84
14	F	606	HEA	C3B-C4B-NB	6.64	117.71	109.84
14	R	607	HEA	C3B-C4B-NB	6.62	117.69	109.84
17	C	303	MQ9	C12-C13-C14	-6.62	111.72	127.66
17	O	302	MQ9	C12-C13-C14	-6.60	111.76	127.66
17	A	502	MQ9	C12-C13-C14	-6.59	111.78	127.66
14	F	607	HEA	C3B-C4B-NB	6.58	117.63	109.84
14	F	606	HEA	CHA-C4D-C3D	-6.55	115.22	124.84
14	R	606	HEA	CHA-C4D-C3D	-6.55	115.22	124.84
17	B	609	MQ9	C12-C13-C14	-6.53	111.94	127.66
17	O	303	MQ9	C42-C43-C44	-6.51	111.98	127.66
17	B	609	MQ9	C27-C28-C29	-6.51	111.98	127.66
17	N	608	MQ9	C42-C43-C44	-6.47	112.08	127.66
14	F	606	HEA	C4A-C3A-C2A	6.43	112.03	106.75
17	N	608	MQ9	C12-C13-C14	-6.40	112.25	127.66
14	R	606	HEA	C4A-C3A-C2A	6.38	111.99	106.75
17	B	610	MQ9	C27-C28-C29	-6.33	112.41	127.66
17	N	607	MQ9	C42-C43-C44	-6.33	112.42	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	303	MQ9	C27-C28-C29	-6.31	112.46	127.66
17	N	608	MQ9	C27-C28-C29	-6.30	112.50	127.66
17	O	302	MQ9	C17-C18-C19	-6.25	112.60	127.66
21	C	302	HEC	C1D-ND-C4D	6.23	111.50	105.07
21	O	304	HEC	C1D-ND-C4D	6.22	111.50	105.07
21	O	305	HEC	C1D-ND-C4D	6.20	111.47	105.07
17	C	303	MQ9	C17-C18-C19	-6.19	112.75	127.66
21	C	301	HEC	C1D-ND-C4D	6.19	111.47	105.07
17	B	610	MQ9	C17-C18-C19	-6.18	112.77	127.66
17	O	302	MQ9	C27-C28-C29	-6.16	112.82	127.66
17	B	609	MQ9	C17-C18-C19	-6.10	112.97	127.66
17	B	609	MQ9	C15-C14-C13	-6.08	108.09	123.68
17	O	302	MQ9	C11-C9-C8	-6.07	108.83	121.12
17	N	607	MQ9	C27-C28-C29	-6.06	113.06	127.66
17	B	610	MQ9	C42-C43-C44	-6.04	113.12	127.66
14	F	607	HEA	CHA-C4D-C3D	-6.03	115.97	124.84
14	R	607	HEA	CHA-C4D-C3D	-6.03	115.97	124.84
17	C	303	MQ9	C10-C9-C8	-6.01	108.27	123.68
17	N	607	MQ9	C17-C18-C19	-6.00	113.22	127.66
17	A	502	MQ9	C17-C18-C19	-6.00	113.22	127.66
17	B	610	MQ9	C11-C9-C8	-5.94	109.09	121.12
17	B	609	MQ9	C10-C9-C8	-5.92	108.49	123.68
14	R	607	HEA	C4A-C3A-C2A	5.90	111.60	106.75
17	C	303	MQ9	C15-C14-C13	-5.88	108.59	123.68
17	O	302	MQ9	C10-C9-C8	-5.87	108.62	123.68
17	A	502	MQ9	C15-C14-C13	-5.86	108.64	123.68
17	O	303	MQ9	C11-C9-C8	-5.86	109.27	121.12
17	N	607	MQ9	C15-C14-C13	-5.85	108.66	123.68
17	O	303	MQ9	C15-C14-C13	-5.85	108.66	123.68
17	N	608	MQ9	C17-C18-C19	-5.85	113.57	127.66
14	F	607	HEA	C4A-C3A-C2A	5.84	111.55	106.75
17	N	608	MQ9	C15-C14-C13	-5.81	108.77	123.68
17	O	303	MQ9	C17-C18-C19	-5.80	113.70	127.66
14	R	606	HEA	C3D-C4D-ND	5.80	115.97	110.36
17	O	302	MQ9	C15-C14-C13	-5.77	108.88	123.68
17	N	607	MQ9	C11-C9-C8	-5.75	109.49	121.12
14	F	606	HEA	C3D-C4D-ND	5.74	115.91	110.36
17	B	610	MQ9	C10-C9-C8	-5.73	108.98	123.68
17	C	303	MQ9	C27-C28-C29	-5.72	113.88	127.66
17	O	303	MQ9	C37-C38-C39	-5.71	113.90	127.66
17	B	610	MQ9	C15-C14-C13	-5.69	109.07	123.68
17	B	610	MQ9	C22-C23-C24	-5.69	113.95	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	502	MQ9	C10-C9-C8	-5.68	109.11	123.68
17	O	303	MQ9	C10-C9-C8	-5.66	109.15	123.68
17	N	607	MQ9	C10-C9-C8	-5.64	109.22	123.68
17	A	502	MQ9	C11-C9-C8	-5.60	109.79	121.12
14	R	606	HEA	CAD-C3D-C2D	5.56	138.24	127.88
14	F	606	HEA	CAD-C3D-C2D	5.56	138.23	127.88
17	C	303	MQ9	C11-C9-C8	-5.55	109.88	121.12
17	O	303	MQ9	C45-C44-C43	-5.48	109.63	123.68
17	B	609	MQ9	C11-C9-C8	-5.45	110.08	121.12
17	N	608	MQ9	C10-C9-C8	-5.45	109.70	123.68
17	O	303	MQ9	C22-C23-C24	-5.41	114.64	127.66
17	O	303	MQ9	C36-C34-C33	-5.40	110.18	121.12
17	N	607	MQ9	C37-C38-C39	-5.38	114.71	127.66
17	B	609	MQ9	C22-C23-C24	-5.35	114.78	127.66
17	N	608	MQ9	C36-C34-C33	-5.35	110.29	121.12
17	N	608	MQ9	C22-C23-C24	-5.33	114.84	127.66
17	O	302	MQ9	C36-C34-C33	-5.32	110.34	121.12
18	B	611	HV0	C23-C24-C27	5.31	125.24	112.79
17	B	610	MQ9	C46-C44-C43	-5.28	110.44	121.12
17	N	608	MQ9	C37-C38-C39	-5.27	114.96	127.66
17	B	610	MQ9	C32-C33-C34	-5.27	114.97	127.66
17	N	608	MQ9	C11-C9-C8	-5.24	110.50	121.12
17	O	302	MQ9	C22-C23-C24	-5.23	115.06	127.66
17	B	610	MQ9	C45-C44-C43	-5.23	110.26	123.68
17	A	502	MQ9	C22-C23-C24	-5.21	115.12	127.66
14	F	607	HEA	C27-C19-C20	5.21	124.03	115.27
14	R	606	HEA	C4B-NB-C1B	-5.20	99.71	105.07
17	N	607	MQ9	C22-C23-C24	-5.19	115.17	127.66
14	R	607	HEA	C27-C19-C20	5.18	123.98	115.27
14	F	606	HEA	C3A-C2A-C1A	-5.18	102.13	107.08
17	B	610	MQ9	C37-C38-C39	-5.16	115.24	127.66
14	F	606	HEA	C4B-NB-C1B	-5.15	99.75	105.07
14	F	606	HEA	C27-C19-C20	5.15	123.93	115.27
17	N	607	MQ9	C45-C44-C43	-5.12	110.55	123.68
14	R	606	HEA	C27-C19-C20	5.12	123.88	115.27
14	R	606	HEA	C3A-C2A-C1A	-5.11	102.19	107.08
17	O	303	MQ9	C46-C44-C43	-5.11	110.78	121.12
14	R	607	HEA	C3D-C4D-ND	5.09	115.29	110.36
14	F	607	HEA	C3D-C4D-ND	5.08	115.27	110.36
17	N	607	MQ9	C36-C34-C33	-5.07	110.85	121.12
14	F	607	HEA	C4B-NB-C1B	-5.06	99.84	105.07
14	R	607	HEA	C4B-NB-C1B	-5.04	99.87	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	303	MQ9	C22-C23-C24	-5.03	115.56	127.66
14	R	606	HEA	CHC-C4B-NB	-5.03	118.18	124.37
14	F	606	HEA	CHC-C4B-NB	-5.02	118.19	124.37
17	N	608	MQ9	C45-C44-C43	-5.02	110.81	123.68
17	N	608	MQ9	C46-C44-C43	-5.01	110.98	121.12
17	A	502	MQ9	C7-C6-C1	5.00	123.85	118.50
17	N	607	MQ9	C46-C44-C43	-5.00	111.00	121.12
14	F	607	HEA	CHC-C4B-NB	-4.99	118.22	124.37
18	N	609	HV0	C23-C24-C27	4.99	124.49	112.79
14	R	607	HEA	CHC-C4B-NB	-4.97	118.25	124.37
17	C	303	MQ9	C36-C34-C33	-4.97	111.06	121.12
14	F	607	HEA	CAD-C3D-C2D	4.95	137.10	127.88
17	B	610	MQ9	C40-C39-C38	-4.93	111.02	123.68
17	B	610	MQ9	C36-C34-C33	-4.93	111.13	121.12
14	R	607	HEA	CAD-C3D-C2D	4.92	137.03	127.88
17	N	608	MQ9	C40-C39-C38	-4.91	111.08	123.68
17	O	302	MQ9	C16-C14-C13	-4.90	111.19	121.12
17	B	610	MQ9	C16-C14-C13	-4.86	111.29	121.12
17	O	303	MQ9	C40-C39-C38	-4.84	111.27	123.68
17	N	607	MQ9	C32-C33-C34	-4.81	116.08	127.66
14	R	607	HEA	C3A-C2A-C1A	-4.80	102.49	107.08
17	O	302	MQ9	C32-C33-C34	-4.80	116.11	127.66
17	N	607	MQ9	C41-C39-C38	-4.79	111.43	121.12
17	O	303	MQ9	C41-C39-C38	-4.77	111.47	121.12
17	N	607	MQ9	C40-C39-C38	-4.76	111.45	123.68
17	O	303	MQ9	C32-C33-C34	-4.76	116.20	127.66
14	F	607	HEA	C3A-C2A-C1A	-4.75	102.54	107.08
17	B	610	MQ9	C25-C24-C23	-4.72	111.56	123.68
14	F	606	HEA	C20-C19-C18	-4.72	111.57	121.12
17	N	608	MQ9	C32-C33-C34	-4.71	116.32	127.66
14	R	606	HEA	C20-C19-C18	-4.70	111.60	121.12
14	F	606	HEA	C13-C14-C15	4.67	138.90	127.66
17	N	608	MQ9	C16-C14-C13	-4.65	111.70	121.12
12	B	608	CDL	OB6-CB5-C51	4.65	121.53	111.50
14	R	606	HEA	C13-C14-C15	4.65	138.85	127.66
17	N	607	MQ9	C16-C14-C13	-4.63	111.74	121.12
17	A	502	MQ9	C30-C29-C28	-4.63	111.81	123.68
17	N	608	MQ9	C41-C39-C38	-4.62	111.78	121.12
17	C	303	MQ9	C16-C14-C13	-4.58	111.85	121.12
17	B	609	MQ9	C16-C14-C13	-4.58	111.85	121.12
12	B	607	CDL	OA6-CA5-C11	4.55	121.31	111.50
17	A	502	MQ9	C16-C14-C13	-4.54	111.93	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	609	MQ9	C36-C34-C33	-4.53	109.56	122.65
17	B	610	MQ9	C35-C34-C33	-4.53	112.07	123.68
12	N	604	CDL	OB6-CB5-C51	4.44	121.08	111.50
18	N	609	HV0	C19-C18-N21	-4.44	115.26	121.38
17	B	609	MQ9	C25-C24-C23	-4.44	112.29	123.68
17	C	303	MQ9	C20-C19-C18	-4.43	112.32	123.68
17	O	302	MQ9	C30-C29-C28	-4.39	112.41	123.68
17	O	302	MQ9	C25-C24-C23	-4.37	112.46	123.68
17	A	502	MQ9	C36-C34-C33	-4.37	110.02	122.65
17	O	303	MQ9	C47-C48-C49	-4.37	112.83	127.75
17	B	609	MQ9	C20-C19-C18	-4.35	112.52	123.68
17	O	302	MQ9	C20-C19-C18	-4.34	112.55	123.68
12	P	201	CDL	OB6-CB5-C51	4.33	120.84	111.50
14	F	607	HEA	C20-C19-C18	-4.33	112.35	121.12
17	C	303	MQ9	C25-C24-C23	-4.33	112.58	123.68
17	O	303	MQ9	C25-C24-C23	-4.33	112.58	123.68
17	N	608	MQ9	C30-C29-C28	-4.32	112.61	123.68
17	B	609	MQ9	C30-C29-C28	-4.32	112.61	123.68
12	B	603	CDL	OA6-CA5-C11	4.31	120.80	111.50
17	N	608	MQ9	C25-C24-C23	-4.31	112.62	123.68
17	N	607	MQ9	C25-C24-C23	-4.30	112.65	123.68
14	R	607	HEA	C20-C19-C18	-4.30	112.42	121.12
17	O	303	MQ9	C16-C14-C13	-4.30	112.42	121.12
12	B	606	CDL	OA6-CA5-C11	4.30	120.76	111.50
17	B	610	MQ9	C47-C48-C49	-4.30	113.06	127.75
17	B	610	MQ9	C30-C29-C28	-4.29	112.66	123.68
20	M	504	9YF	C6-C7-C2	4.29	119.48	109.68
17	B	610	MQ9	C20-C19-C18	-4.29	112.68	123.68
14	F	606	HEA	CHB-C1B-C2B	-4.28	118.29	124.98
17	A	502	MQ9	C20-C19-C18	-4.28	112.70	123.68
12	D	201	CDL	OB6-CB5-C51	4.27	120.70	111.50
17	A	502	MQ9	C25-C24-C23	-4.27	112.73	123.68
12	D	201	CDL	OA6-CA5-C11	4.26	120.69	111.50
17	B	610	MQ9	C41-C39-C38	-4.25	112.52	121.12
14	R	606	HEA	CHB-C1B-C2B	-4.25	118.34	124.98
12	N	604	CDL	OA6-CA5-C11	4.23	120.62	111.50
17	C	303	MQ9	C30-C29-C28	-4.23	112.82	123.68
12	B	603	CDL	OB6-CB5-C51	4.23	120.61	111.50
17	O	303	MQ9	C30-C29-C28	-4.23	112.84	123.68
17	N	607	MQ9	C47-C48-C49	-4.22	113.31	127.75
17	N	608	MQ9	C47-C48-C49	-4.21	113.36	127.75
12	N	605	CDL	OB6-CB5-C51	4.20	120.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	607	HEA	CHB-C1B-C2B	-4.18	118.45	124.98
20	A	503	9YF	O9-C8-C9	4.17	120.49	111.50
12	R	601	CDL	OB6-CB5-C51	4.17	120.48	111.50
12	P	201	CDL	OA6-CA5-C11	4.16	120.47	111.50
17	C	303	MQ9	C32-C33-C34	-4.16	117.66	127.66
17	N	607	MQ9	C30-C29-C28	-4.13	113.08	123.68
14	R	606	HEA	C4B-C3B-C2B	-4.13	100.35	107.41
12	O	301	CDL	OB6-CB5-C51	4.13	120.40	111.50
14	F	606	HEA	C4B-C3B-C2B	-4.13	100.36	107.41
14	R	607	HEA	CHB-C1B-C2B	-4.13	118.53	124.98
12	B	606	CDL	OB6-CB5-C51	4.12	120.38	111.50
12	R	602	CDL	OA6-CA5-C11	4.12	120.37	111.50
12	F	601	CDL	OB6-CB5-C51	4.12	120.37	111.50
12	F	602	CDL	OA6-CA5-C11	4.11	120.37	111.50
12	B	608	CDL	OA6-CA5-C11	4.11	120.36	111.50
20	M	504	9YF	O9-C8-C9	4.11	120.35	111.50
14	F	606	HEA	CHA-C4D-ND	4.10	128.87	124.42
12	R	601	CDL	OA6-CA5-C11	4.08	120.28	111.50
12	F	601	CDL	OA6-CA5-C11	4.07	120.28	111.50
20	A	505	9YF	C4-C3-C2	4.07	118.98	109.68
12	A	504	CDL	OB6-CB5-C51	4.07	120.27	111.50
17	O	302	MQ9	C31-C29-C28	-4.07	112.89	121.12
17	O	302	MQ9	C40-C39-C38	-4.06	110.91	122.65
14	R	607	HEA	C4B-C3B-C2B	-4.05	100.49	107.41
12	A	504	CDL	OA6-CA5-C11	4.05	120.22	111.50
14	R	606	HEA	CHA-C4D-ND	4.04	128.81	124.42
14	R	606	HEA	OMA-CMA-C3A	-4.04	116.56	125.69
14	F	606	HEA	OMA-CMA-C3A	-4.03	116.57	125.69
12	B	607	CDL	OB6-CB5-C51	4.02	120.17	111.50
17	B	609	MQ9	C31-C29-C28	-4.02	112.98	121.12
17	N	608	MQ9	C26-C24-C23	-4.02	112.99	121.12
14	F	607	HEA	C4B-C3B-C2B	-4.00	100.58	107.41
17	O	303	MQ9	C20-C19-C18	-4.00	113.42	123.68
17	N	608	MQ9	C31-C29-C28	-4.00	113.03	121.12
14	F	606	HEA	C21-C20-C19	-3.99	99.84	112.98
12	N	605	CDL	OA6-CA5-C11	3.99	120.10	111.50
17	C	303	MQ9	C31-C29-C28	-3.98	113.05	121.12
14	F	607	HEA	CHA-C4D-ND	3.98	128.75	124.42
14	R	606	HEA	C21-C20-C19	-3.98	99.90	112.98
14	R	607	HEA	C13-C14-C15	3.98	137.23	127.66
12	N	606	CDL	OA6-CA5-C11	3.98	120.07	111.50
14	R	607	HEA	CHA-C4D-ND	3.97	128.73	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	O	302	MQ9	C35-C34-C33	-3.96	113.52	123.68
14	F	607	HEA	C13-C14-C15	3.95	137.18	127.66
12	N	606	CDL	OB6-CB5-C51	3.95	120.01	111.50
20	A	505	9YF	O9-C8-C9	3.95	120.01	111.50
17	O	302	MQ9	C37-C38-C39	-3.94	114.27	127.75
20	M	503	9YF	O9-C8-C9	3.94	119.99	111.50
14	F	607	HEA	CHB-C4A-C3A	-3.93	118.54	125.26
14	R	607	HEA	CHB-C4A-C3A	-3.92	118.55	125.26
17	O	303	MQ9	C50-C49-C48	-3.92	111.31	122.65
12	B	605	CDL	OA6-CA5-C11	3.91	119.92	111.50
12	R	602	CDL	OB6-CB5-C51	3.89	119.89	111.50
17	N	608	MQ9	C20-C19-C18	-3.89	113.69	123.68
12	F	602	CDL	OB6-CB5-C51	3.89	119.89	111.50
12	M	502	CDL	OB6-CB5-C51	3.89	119.88	111.50
17	N	607	MQ9	C31-C29-C28	-3.88	113.26	121.12
17	B	610	MQ9	C50-C49-C48	-3.88	111.44	122.65
17	N	607	MQ9	C26-C24-C23	-3.87	113.28	121.12
14	F	607	HEA	C21-C20-C19	-3.87	100.25	112.98
14	F	607	HEA	C26-C15-C16	-3.85	108.79	115.27
17	N	607	MQ9	C20-C19-C18	-3.85	113.79	123.68
17	O	302	MQ9	C41-C39-C38	-3.85	111.51	122.65
14	R	607	HEA	C21-C20-C19	-3.85	100.33	112.98
17	O	303	MQ9	C31-C29-C28	-3.84	113.34	121.12
14	R	607	HEA	C26-C15-C16	-3.83	108.82	115.27
17	B	610	MQ9	C31-C29-C28	-3.83	113.36	121.12
14	R	606	HEA	CHB-C4A-C3A	-3.83	118.71	125.26
17	A	502	MQ9	C26-C24-C23	-3.82	113.38	121.12
15	G	301	9Y0	O7-C21-C22	3.82	119.73	111.50
17	O	303	MQ9	C35-C34-C33	-3.81	113.90	123.68
17	N	607	MQ9	C51-C49-C48	-3.80	111.65	122.65
17	O	303	MQ9	C26-C24-C23	-3.80	113.43	121.12
15	S	301	9Y0	O7-C21-C22	3.79	119.67	111.50
17	A	502	MQ9	C31-C29-C28	-3.79	113.45	121.12
17	B	610	MQ9	C51-C49-C48	-3.79	111.70	122.65
14	F	606	HEA	CHB-C4A-C3A	-3.79	118.78	125.26
17	C	303	MQ9	C41-C39-C38	-3.78	111.73	122.65
17	O	303	MQ9	C51-C49-C48	-3.77	111.74	122.65
17	N	608	MQ9	C50-C49-C48	-3.76	111.78	122.65
17	N	608	MQ9	C35-C34-C33	-3.76	114.03	123.68
12	O	301	CDL	OA6-CA5-C11	3.76	119.60	111.50
17	N	608	MQ9	C51-C49-C48	-3.74	111.83	122.65
17	C	303	MQ9	C26-C24-C23	-3.72	113.60	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	303	MQ9	C35-C34-C33	-3.71	114.15	123.68
17	N	607	MQ9	C50-C49-C48	-3.71	111.92	122.65
17	N	607	MQ9	C35-C34-C33	-3.69	114.20	123.68
17	B	609	MQ9	C26-C24-C23	-3.69	113.64	121.12
17	B	610	MQ9	C45-C44-C46	-3.69	109.07	115.27
17	C	303	MQ9	C40-C39-C38	-3.69	111.99	122.65
20	M	504	9YF	C7-C6-C5	3.66	117.22	110.82
17	C	303	MQ9	C37-C38-C39	-3.66	115.24	127.75
14	F	607	HEA	C16-C15-C14	3.65	128.51	121.12
17	O	302	MQ9	C26-C24-C23	-3.64	113.74	121.12
14	R	607	HEA	C16-C15-C14	3.63	128.47	121.12
12	M	502	CDL	OA6-CA5-C11	3.62	119.31	111.50
17	B	610	MQ9	C26-C24-C23	-3.61	113.82	121.12
12	B	605	CDL	OB6-CB5-C51	3.60	119.27	111.50
17	B	609	MQ9	C32-C33-C34	-3.60	115.45	127.75
14	R	606	HEA	C2C-C1C-NC	3.59	115.55	110.08
14	F	606	HEA	C2C-C1C-NC	3.58	115.53	110.08
17	O	303	MQ9	C21-C19-C18	-3.55	113.93	121.12
18	B	611	HV0	C09-N04-N03	-3.55	109.81	112.86
14	F	607	HEA	C2C-C1C-NC	3.55	115.48	110.08
14	R	606	HEA	C25-C23-C22	-3.55	112.40	122.65
14	F	606	HEA	C25-C23-C22	-3.54	112.40	122.65
14	R	607	HEA	C2C-C1C-NC	3.54	115.47	110.08
14	R	607	HEA	CAA-C2A-C1A	3.53	131.56	124.89
20	A	505	9YF	C5-C4-C3	3.53	116.99	110.82
20	M	503	9YF	C6-C5-C4	3.51	116.95	110.82
14	F	607	HEA	CAA-C2A-C1A	3.48	131.46	124.89
17	N	608	MQ9	C21-C19-C18	-3.48	114.08	121.12
14	R	606	HEA	O2A-CGA-CBA	3.47	125.18	114.03
14	R	606	HEA	C4D-C3D-C2D	-3.47	101.84	106.90
14	F	606	HEA	C4D-C3D-C2D	-3.45	101.86	106.90
14	F	606	HEA	O2A-CGA-CBA	3.44	125.09	114.03
14	R	606	HEA	C16-C15-C14	3.44	128.07	121.12
14	F	606	HEA	C16-C15-C14	3.43	128.07	121.12
18	B	611	HV0	C01-C02-N03	3.43	126.15	119.33
14	F	606	HEA	CAA-C2A-C1A	3.43	131.35	124.89
17	B	609	MQ9	C21-C19-C18	-3.42	114.20	121.12
17	B	610	MQ9	C21-C19-C18	-3.41	114.21	121.12
14	R	606	HEA	CAA-C2A-C1A	3.41	131.32	124.89
14	R	607	HEA	C25-C23-C22	-3.39	112.85	122.65
14	F	606	HEA	C2D-C1D-ND	3.39	113.85	109.84
17	A	502	MQ9	C21-C19-C18	-3.38	114.28	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	611	HV0	C10-C02-N03	-3.37	107.60	111.58
14	F	607	HEA	C25-C23-C22	-3.37	112.90	122.65
14	R	606	HEA	C2D-C1D-ND	3.36	113.83	109.84
17	O	303	MQ9	C45-C44-C46	-3.36	109.61	115.27
14	F	607	HEA	CHA-C1A-NA	-3.33	120.83	124.44
17	A	502	MQ9	C32-C33-C34	-3.33	116.36	127.75
14	F	607	HEA	O2A-CGA-CBA	3.33	124.72	114.03
14	R	607	HEA	O2A-CGA-CBA	3.32	124.69	114.03
18	N	609	HV0	C09-N04-N03	-3.30	110.03	112.86
18	N	609	HV0	C10-C02-N03	-3.29	107.70	111.58
14	R	607	HEA	CHA-C1A-NA	-3.28	120.89	124.44
17	N	608	MQ9	C45-C44-C46	-3.28	109.75	115.27
14	R	607	HEA	C2D-C1D-ND	3.25	113.69	109.84
17	O	302	MQ9	C21-C19-C18	-3.24	114.56	121.12
14	F	607	HEA	C2D-C1D-ND	3.23	113.67	109.84
17	N	607	MQ9	C45-C44-C46	-3.20	109.88	115.27
14	R	607	HEA	C3C-C2C-C1C	-3.18	103.32	107.16
18	N	609	HV0	C01-C02-N03	3.18	125.64	119.33
14	F	607	HEA	C3C-C2C-C1C	-3.17	103.33	107.16
14	F	606	HEA	C3C-C2C-C1C	-3.16	103.35	107.16
17	N	607	MQ9	C21-C19-C18	-3.15	114.73	121.12
14	R	606	HEA	C3C-C2C-C1C	-3.15	103.36	107.16
14	R	607	HEA	C4D-C3D-C2D	-3.15	102.31	106.90
14	F	607	HEA	C4D-C3D-C2D	-3.14	102.32	106.90
17	A	502	MQ9	C35-C34-C33	-3.14	113.57	122.65
17	B	610	MQ9	C40-C39-C41	-3.12	110.02	115.27
14	F	607	HEA	CAA-CBA-CGA	-3.12	106.89	113.60
14	F	606	HEA	C26-C15-C16	-3.12	110.03	115.27
14	R	607	HEA	C1D-C2D-C3D	-3.11	103.69	106.96
17	B	609	MQ9	C35-C34-C33	-3.10	113.68	122.65
14	R	606	HEA	C26-C15-C16	-3.10	110.05	115.27
14	R	607	HEA	CAA-CBA-CGA	-3.09	106.96	113.60
14	F	607	HEA	C1B-C2B-C3B	-3.07	103.13	106.80
14	F	607	HEA	C1D-C2D-C3D	-3.06	103.74	106.96
17	O	303	MQ9	C35-C34-C36	-3.04	110.15	115.27
14	F	606	HEA	C1D-C2D-C3D	-3.04	103.76	106.96
14	R	606	HEA	C1D-C2D-C3D	-3.02	103.79	106.96
14	R	607	HEA	C1B-C2B-C3B	-3.01	103.20	106.80
20	A	505	9YF	C7-C2-C3	3.00	115.18	110.85
17	N	608	MQ9	C40-C39-C41	-2.97	110.27	115.27
12	D	201	CDL	OB8-CB7-C71	2.95	121.15	111.91
17	B	610	MQ9	C35-C34-C36	-2.94	110.32	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	606	CDL	OB8-CB7-C71	2.92	121.08	111.91
17	O	303	MQ9	C40-C39-C41	-2.92	110.36	115.27
14	F	606	HEA	C1B-C2B-C3B	-2.91	103.32	106.80
18	N	609	HV0	C22-N21-C18	2.90	125.92	118.09
18	N	609	HV0	C17-C18-N21	2.89	125.37	121.38
14	F	606	HEA	CHA-C1A-NA	-2.89	121.31	124.44
14	R	606	HEA	C1B-C2B-C3B	-2.88	103.36	106.80
12	N	604	CDL	OB8-CB7-C71	2.88	120.93	111.91
17	N	608	MQ9	C25-C24-C26	-2.87	110.45	115.27
20	M	504	9YF	C7-C2-C3	2.86	114.98	110.85
12	B	605	CDL	OB8-CB7-C71	2.86	120.89	111.91
14	R	606	HEA	CHA-C1A-NA	-2.86	121.35	124.44
17	C	303	MQ9	C21-C19-C18	-2.84	115.37	121.12
12	F	602	CDL	OB8-CB7-C71	2.82	120.77	111.91
14	R	606	HEA	CAA-CBA-CGA	-2.82	107.54	113.60
17	B	610	MQ9	C25-C24-C26	-2.81	110.54	115.27
12	R	602	CDL	OB8-CB7-C71	2.81	120.73	111.91
17	C	303	MQ9	C35-C34-C36	-2.80	110.56	115.27
17	B	609	MQ9	C25-C24-C26	-2.79	110.58	115.27
20	A	503	9YF	O4-C4-C5	2.79	116.80	110.35
14	F	606	HEA	CAA-CBA-CGA	-2.79	107.61	113.60
12	P	201	CDL	OB8-CB7-C71	2.78	120.64	111.91
14	R	606	HEA	C12-C13-C14	-2.78	104.90	112.23
14	F	606	HEA	C12-C13-C14	-2.77	104.93	112.23
14	R	607	HEA	C17-C16-C15	-2.76	103.89	112.98
14	F	607	HEA	C12-C13-C14	-2.76	104.94	112.23
16	N	602	HEM	C1B-NB-C4B	2.76	107.92	105.07
17	N	607	MQ9	C40-C39-C41	-2.76	110.64	115.27
12	B	608	CDL	OA8-CA7-C31	2.76	120.56	111.91
17	O	302	MQ9	C35-C34-C36	-2.75	110.65	115.27
14	R	606	HEA	O2A-CGA-O1A	-2.75	116.45	123.30
12	B	607	CDL	OA8-CA7-C31	2.74	120.51	111.91
12	B	607	CDL	OB8-CB7-C71	2.74	120.50	111.91
14	F	607	HEA	C17-C16-C15	-2.74	103.98	112.98
14	F	607	HEA	O2A-CGA-O1A	-2.73	116.48	123.30
12	N	606	CDL	OA8-CA7-C31	2.73	120.49	111.91
14	R	607	HEA	C12-C13-C14	-2.73	105.02	112.23
12	A	504	CDL	OA8-CA7-C31	2.72	120.45	111.91
16	B	602	HEM	C1B-NB-C4B	2.72	107.88	105.07
14	F	606	HEA	O2A-CGA-O1A	-2.72	116.52	123.30
14	F	606	HEA	CAD-C3D-C4D	-2.72	119.91	124.66
14	R	606	HEA	CAD-C3D-C4D	-2.71	119.91	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	609	MQ9	C10-C9-C11	-2.71	110.71	115.27
14	F	606	HEA	CHC-C1C-C2C	-2.70	119.60	127.24
12	R	601	CDL	OB8-CB7-C71	2.70	120.39	111.91
12	F	601	CDL	OB8-CB7-C71	2.70	120.38	111.91
14	R	607	HEA	O2A-CGA-O1A	-2.70	116.58	123.30
17	O	303	MQ9	C25-C24-C26	-2.69	110.74	115.27
14	R	606	HEA	CHC-C1C-C2C	-2.69	119.64	127.24
12	B	606	CDL	OA8-CA7-C31	2.69	120.35	111.91
12	B	603	CDL	OA8-CA7-C31	2.68	120.32	111.91
12	O	301	CDL	OA8-CA7-C31	2.68	120.32	111.91
12	N	605	CDL	OA8-CA7-C31	2.67	120.30	111.91
12	B	606	CDL	OB8-CB7-C71	2.67	120.30	111.91
15	G	301	9Y0	O5-C5-C6	2.67	120.28	111.91
12	B	608	CDL	OB8-CB7-C71	2.67	120.27	111.91
12	F	601	CDL	OA8-CA7-C31	2.66	120.27	111.91
12	R	601	CDL	OA8-CA7-C31	2.66	120.27	111.91
15	S	301	9Y0	O5-C5-C6	2.64	120.19	111.91
17	B	609	MQ9	C7-C6-C1	2.63	121.32	118.50
17	A	502	MQ9	C8-C7-C6	2.63	119.13	112.05
21	O	304	HEC	CAB-C3B-C4B	2.63	128.22	124.81
14	F	607	HEA	CHC-C1C-C2C	-2.62	119.83	127.24
12	A	504	CDL	OB8-CB7-C71	2.62	120.14	111.91
14	R	607	HEA	CHC-C1C-C2C	-2.62	119.83	127.24
17	O	302	MQ9	C25-C24-C26	-2.62	110.87	115.27
21	C	301	HEC	CAB-C3B-C4B	2.61	128.20	124.81
12	B	603	CDL	OB8-CB7-C71	2.61	120.08	111.91
17	A	502	MQ9	C25-C24-C26	-2.60	110.89	115.27
20	A	505	9YF	O11-C25-C26	2.60	120.06	111.91
12	M	502	CDL	OA8-CA7-C31	2.60	120.06	111.91
17	N	607	MQ9	C35-C34-C36	-2.58	110.93	115.27
12	B	605	CDL	OA8-CA7-C31	2.58	120.00	111.91
20	M	503	9YF	O11-C25-C26	2.58	120.00	111.91
20	A	503	9YF	O11-C25-C26	2.58	120.00	111.91
12	M	502	CDL	OB8-CB7-C71	2.58	119.99	111.91
17	N	607	MQ9	C25-C24-C26	-2.57	110.94	115.27
20	M	504	9YF	O11-C25-C26	2.57	119.97	111.91
17	C	303	MQ9	C25-C24-C26	-2.56	110.96	115.27
12	P	201	CDL	OA8-CA7-C31	2.54	119.88	111.91
20	A	503	9YF	C4-C3-C2	2.54	115.47	109.68
12	D	201	CDL	OA8-CA7-C31	2.54	119.87	111.91
14	F	606	HEA	C17-C16-C15	-2.53	104.67	112.98
14	R	606	HEA	C17-C16-C15	-2.53	104.67	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	605	CDL	OB8-CB7-C71	2.53	119.83	111.91
14	R	607	HEA	CMC-C2C-C1C	2.52	129.21	125.37
14	F	607	HEA	CMC-C2C-C1C	2.51	129.20	125.37
12	O	301	CDL	OB8-CB7-C71	2.50	119.75	111.91
12	N	604	CDL	OA8-CA7-C31	2.50	119.75	111.91
17	B	610	MQ9	C10-C9-C11	-2.49	111.08	115.27
21	C	301	HEC	C4C-NC-C1C	2.49	107.78	105.35
16	N	602	HEM	C3B-C2B-C1B	2.49	108.33	106.49
17	O	303	MQ9	C15-C14-C16	-2.47	111.11	115.27
14	R	606	HEA	O1A-CGA-CBA	-2.47	115.16	123.08
21	O	304	HEC	C4C-NC-C1C	2.47	107.76	105.35
18	N	609	HV0	C15-C14-N13	-2.46	107.77	113.05
21	O	305	HEC	C2A-C1A-NA	-2.46	107.93	110.32
14	F	606	HEA	O1A-CGA-CBA	-2.45	115.21	123.08
16	B	602	HEM	C3B-C2B-C1B	2.45	108.30	106.49
21	C	302	HEC	C2A-C1A-NA	-2.45	107.94	110.32
12	F	602	CDL	OA8-CA7-C31	2.42	119.51	111.91
12	R	602	CDL	OA8-CA7-C31	2.41	119.48	111.91
14	R	607	HEA	O1A-CGA-CBA	-2.41	115.34	123.08
14	R	606	HEA	CMC-C2C-C1C	2.41	129.03	125.37
14	F	606	HEA	CMC-C2C-C1C	2.39	129.01	125.37
17	N	608	MQ9	C35-C34-C36	-2.38	111.26	115.27
14	F	607	HEA	O1A-CGA-CBA	-2.38	115.43	123.08
21	O	304	HEC	C4A-NA-C1A	2.37	107.67	105.35
21	C	301	HEC	C4A-NA-C1A	2.36	107.66	105.35
14	R	607	HEA	C13-C12-C11	2.35	117.88	114.35
17	C	303	MQ9	C15-C14-C16	-2.34	111.33	115.27
21	C	302	HEC	CAD-CBD-CGD	-2.34	108.56	113.60
14	F	607	HEA	CAD-C3D-C4D	-2.34	120.57	124.66
21	O	305	HEC	CAD-CBD-CGD	-2.34	108.57	113.60
16	B	601	HEM	C4D-ND-C1D	2.34	107.49	105.07
14	F	607	HEA	O11-C11-C12	-2.34	102.89	109.42
14	F	607	HEA	O2D-CGD-O1D	-2.34	117.48	123.30
17	B	609	MQ9	C15-C14-C16	-2.33	111.34	115.27
16	N	602	HEM	C4A-NA-C1A	2.33	107.63	105.35
16	B	601	HEM	C4C-NC-C1C	2.32	107.62	105.35
20	A	505	9YF	C-O9-C8	-2.32	112.07	117.79
14	R	607	HEA	O11-C11-C12	-2.32	102.93	109.42
21	C	302	HEC	C4C-NC-C1C	2.32	107.62	105.35
14	R	607	HEA	O2D-CGD-O1D	-2.32	117.53	123.30
12	O	301	CDL	CB4-OB6-CB5	-2.32	112.09	117.79
21	C	301	HEC	CAD-C3D-C4D	2.30	128.68	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	607	HEA	C13-C12-C11	2.30	117.81	114.35
21	O	305	HEC	C4A-NA-C1A	2.30	107.60	105.35
17	C	303	MQ9	C10-C9-C11	-2.30	111.41	115.27
14	R	607	HEA	CAD-C3D-C4D	-2.30	120.64	124.66
21	O	304	HEC	CAD-C3D-C4D	2.28	128.65	124.66
16	N	602	HEM	CAD-CBD-CGD	-2.28	108.69	113.60
21	O	305	HEC	C4C-NC-C1C	2.28	107.58	105.35
16	B	602	HEM	CAD-CBD-CGD	-2.28	108.70	113.60
21	C	302	HEC	C4A-NA-C1A	2.27	107.57	105.35
16	N	601	HEM	C4C-NC-C1C	2.27	107.57	105.35
21	C	301	HEC	C2A-C1A-NA	-2.27	108.12	110.32
17	A	502	MQ9	C15-C14-C16	-2.27	111.46	115.27
17	A	502	MQ9	C10-C9-C11	-2.26	111.47	115.27
18	B	611	HV0	C01-C02-C10	-2.26	126.25	130.01
14	R	606	HEA	O2D-CGD-O1D	-2.26	117.67	123.30
21	O	304	HEC	C2A-C1A-NA	-2.25	108.13	110.32
14	F	606	HEA	O2D-CGD-O1D	-2.24	117.72	123.30
16	B	602	HEM	C4A-NA-C1A	2.24	107.54	105.35
17	O	303	MQ9	C10-C9-C11	-2.23	111.52	115.27
16	N	601	HEM	C4D-ND-C1D	2.22	107.37	105.07
20	M	504	9YF	O7-C7-C2	2.21	115.80	109.94
20	M	504	9YF	C-O9-C8	-2.20	112.36	117.79
20	M	503	9YF	C5-C4-C3	2.20	114.67	110.82
21	C	302	HEC	C4B-NB-C1B	2.19	107.33	105.07
17	C	303	MQ9	C3A-C3-C2	2.17	121.67	119.26
14	R	606	HEA	C4A-CHB-C1B	-2.17	121.38	126.06
14	R	607	HEA	CMD-C2D-C1D	2.17	128.34	125.04
14	F	606	HEA	C4A-CHB-C1B	-2.16	121.40	126.06
20	M	503	9YF	O7-C7-C6	-2.16	105.36	110.35
18	N	609	HV0	C22-C23-C24	2.16	113.59	111.04
21	C	301	HEC	C4B-NB-C1B	2.15	107.30	105.07
18	B	611	HV0	O38-C07-C08	-2.15	120.23	124.63
17	N	608	MQ9	C8-C7-C6	2.15	117.84	112.05
17	O	302	MQ9	C7-C6-C1	2.15	120.80	118.50
18	N	609	HV0	C25-C24-C23	2.14	114.01	109.56
21	O	304	HEC	C4B-NB-C1B	2.13	107.27	105.07
14	F	607	HEA	CMD-C2D-C1D	2.12	128.28	125.04
14	F	607	HEA	C4A-CHB-C1B	-2.12	121.47	126.06
14	R	607	HEA	C4A-CHB-C1B	-2.12	121.48	126.06
14	R	606	HEA	O11-C11-C12	-2.12	103.49	109.42
14	F	606	HEA	O11-C11-C12	-2.11	103.52	109.42
14	F	607	HEA	CHA-C1A-C2A	2.10	128.34	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	305	HEC	C4B-NB-C1B	2.10	107.24	105.07
16	N	601	HEM	C1B-NB-C4B	2.10	107.24	105.07
17	O	302	MQ9	C15-C14-C16	-2.09	111.76	115.27
17	B	610	MQ9	C15-C14-C16	-2.09	111.76	115.27
18	B	611	HV0	O38-C07-C06	2.09	120.09	113.74
17	N	608	MQ9	C15-C14-C16	-2.08	111.77	115.27
14	R	606	HEA	C1A-CHA-C4D	-2.08	121.57	126.06
21	C	301	HEC	CAD-CBD-CGD	-2.08	109.13	113.60
14	F	606	HEA	C1A-CHA-C4D	-2.08	121.58	126.06
14	R	607	HEA	CHA-C1A-C2A	2.06	128.27	124.94
16	B	602	HEM	C4D-ND-C1D	2.05	107.19	105.07
16	B	601	HEM	C1B-NB-C4B	2.04	107.18	105.07
21	O	304	HEC	CAD-CBD-CGD	-2.03	109.23	113.60
17	A	502	MQ9	C5M-C5-C6	-2.03	121.10	124.40
18	N	609	HV0	C01-C02-C10	-2.02	126.66	130.01

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	O	304	HEC	NA
21	O	305	HEC	NA
21	C	301	HEC	NA
21	C	302	HEC	NA

All (1299) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	CDL	CB2-OB2-PB2-OB3
12	F	601	CDL	OB5-CB3-CB4-OB6
12	F	602	CDL	CA3-OA5-PA1-OA4
12	F	602	CDL	CB3-OB5-PB2-OB3
12	F	602	CDL	CB3-OB5-PB2-OB4
12	F	602	CDL	OB5-CB3-CB4-OB6
12	D	201	CDL	OA7-CA5-OA6-CA4
12	D	201	CDL	C11-CA5-OA6-CA4
12	R	601	CDL	CB2-OB2-PB2-OB3
12	R	601	CDL	OB5-CB3-CB4-OB6
12	R	602	CDL	CA3-OA5-PA1-OA4
12	R	602	CDL	CB3-OB5-PB2-OB3
12	R	602	CDL	CB3-OB5-PB2-OB4
12	R	602	CDL	OB5-CB3-CB4-OB6
12	P	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
12	P	201	CDL	CB3-OB5-PB2-OB3
12	P	201	CDL	C51-CB5-OB6-CB4
12	N	604	CDL	CA2-OA2-PA1-OA3
12	N	604	CDL	CA2-OA2-PA1-OA4
12	N	604	CDL	CA2-OA2-PA1-OA5
12	N	604	CDL	C11-CA5-OA6-CA4
12	N	604	CDL	CB2-OB2-PB2-OB3
12	N	604	CDL	CB2-OB2-PB2-OB4
12	N	604	CDL	CB3-OB5-PB2-OB3
12	N	604	CDL	OB7-CB5-OB6-CB4
12	N	605	CDL	CA3-OA5-PA1-OA3
12	N	605	CDL	CA3-OA5-PA1-OA4
12	N	605	CDL	C11-CA5-OA6-CA4
12	N	605	CDL	CB2-OB2-PB2-OB3
12	N	605	CDL	CB2-OB2-PB2-OB4
12	N	605	CDL	C51-CB5-OB6-CB4
12	N	606	CDL	CA2-OA2-PA1-OA3
12	N	606	CDL	CA3-OA5-PA1-OA3
12	N	606	CDL	OA7-CA5-OA6-CA4
12	M	502	CDL	CA3-OA5-PA1-OA3
12	M	502	CDL	CB2-OB2-PB2-OB3
12	M	502	CDL	CB2-OB2-PB2-OB4
12	M	502	CDL	CB2-OB2-PB2-OB5
12	M	502	CDL	CB3-OB5-PB2-OB3
12	M	502	CDL	CB3-OB5-PB2-OB4
12	O	301	CDL	CB2-C1-CA2-OA2
12	O	301	CDL	CA2-OA2-PA1-OA3
12	B	603	CDL	CB2-OB2-PB2-OB3
12	B	603	CDL	CB3-OB5-PB2-OB3
12	B	603	CDL	CB3-OB5-PB2-OB4
12	B	603	CDL	C51-CB5-OB6-CB4
12	B	605	CDL	CB2-OB2-PB2-OB3
12	B	605	CDL	CB2-OB2-PB2-OB4
12	B	605	CDL	CB3-OB5-PB2-OB3
12	B	605	CDL	CB3-OB5-PB2-OB4
12	B	606	CDL	CA2-OA2-PA1-OA3
12	B	606	CDL	CA2-OA2-PA1-OA4
12	B	606	CDL	CA3-OA5-PA1-OA2
12	B	606	CDL	CA3-OA5-PA1-OA3
12	B	606	CDL	CA3-OA5-PA1-OA4
12	B	606	CDL	C11-CA5-OA6-CA4
12	B	607	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
12	B	607	CDL	C11-CA5-OA6-CA4
12	B	607	CDL	CB3-OB5-PB2-OB3
12	B	608	CDL	OA7-CA5-OA6-CA4
12	B	608	CDL	C11-CA5-OA6-CA4
12	B	608	CDL	C51-CB5-OB6-CB4
12	A	504	CDL	CB2-C1-CA2-OA2
12	A	504	CDL	C11-CA5-OA6-CA4
12	A	504	CDL	CB2-OB2-PB2-OB4
12	A	504	CDL	CB2-OB2-PB2-OB5
12	A	504	CDL	CB3-OB5-PB2-OB3
14	F	606	HEA	C2A-C3A-CMA-OMA
14	F	606	HEA	C4A-C3A-CMA-OMA
14	F	606	HEA	C4D-C3D-CAD-CBD
14	F	606	HEA	O11-C11-C12-C13
14	F	606	HEA	C14-C15-C16-C17
14	F	606	HEA	C26-C15-C16-C17
14	F	606	HEA	C17-C18-C19-C20
14	F	607	HEA	C2A-C3A-CMA-OMA
14	F	607	HEA	C4A-C3A-CMA-OMA
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	606	HEA	C2A-C3A-CMA-OMA
14	R	606	HEA	C4A-C3A-CMA-OMA
14	R	606	HEA	C4D-C3D-CAD-CBD
14	R	606	HEA	O11-C11-C12-C13
14	R	606	HEA	C14-C15-C16-C17
14	R	606	HEA	C26-C15-C16-C17
14	R	606	HEA	C17-C18-C19-C20
14	R	607	HEA	C2A-C3A-CMA-OMA
14	R	607	HEA	C4A-C3A-CMA-OMA
14	R	607	HEA	O11-C11-C12-C13
14	R	607	HEA	C14-C15-C16-C17
14	R	607	HEA	C15-C16-C17-C18
15	G	301	9Y0	O1-C3-C4-N
15	G	301	9Y0	C3-O1-P-O
15	G	301	9Y0	C3-O1-P-O2
15	S	301	9Y0	O1-C3-C4-N
15	S	301	9Y0	C3-O1-P-O
15	S	301	9Y0	C3-O1-P-O2
17	N	607	MQ9	C7-C8-C9-C10
17	N	607	MQ9	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
17	N	607	MQ9	C12-C13-C14-C15
17	N	607	MQ9	C12-C13-C14-C16
17	N	607	MQ9	C19-C21-C22-C23
17	N	607	MQ9	C22-C23-C24-C25
17	N	607	MQ9	C24-C26-C27-C28
17	N	607	MQ9	C32-C33-C34-C35
17	N	607	MQ9	C33-C34-C36-C37
17	N	607	MQ9	C37-C38-C39-C41
17	N	607	MQ9	C42-C43-C44-C45
17	N	607	MQ9	C42-C43-C44-C46
17	N	608	MQ9	C5-C6-C7-C8
17	N	608	MQ9	C1-C6-C7-C8
17	N	608	MQ9	C7-C8-C9-C11
17	N	608	MQ9	C12-C13-C14-C15
17	N	608	MQ9	C12-C13-C14-C16
17	N	608	MQ9	C13-C14-C16-C17
17	N	608	MQ9	C17-C18-C19-C20
17	N	608	MQ9	C17-C18-C19-C21
17	N	608	MQ9	C19-C21-C22-C23
17	N	608	MQ9	C22-C23-C24-C25
17	N	608	MQ9	C22-C23-C24-C26
17	N	608	MQ9	C25-C24-C26-C27
17	N	608	MQ9	C29-C31-C32-C33
17	N	608	MQ9	C32-C33-C34-C36
17	N	608	MQ9	C41-C42-C43-C44
17	N	608	MQ9	C42-C43-C44-C45
17	N	608	MQ9	C42-C43-C44-C46
17	O	302	MQ9	C7-C8-C9-C10
17	O	302	MQ9	C12-C13-C14-C15
17	O	302	MQ9	C17-C18-C19-C20
17	O	302	MQ9	C18-C19-C21-C22
17	O	302	MQ9	C20-C19-C21-C22
17	O	302	MQ9	C22-C23-C24-C25
17	O	302	MQ9	C23-C24-C26-C27
17	O	302	MQ9	C27-C28-C29-C30
17	O	302	MQ9	C27-C28-C29-C31
17	O	302	MQ9	C28-C29-C31-C32
17	O	302	MQ9	C32-C33-C34-C36
17	O	302	MQ9	C34-C36-C37-C38
17	O	302	MQ9	C37-C38-C39-C41
17	O	303	MQ9	C7-C8-C9-C10
17	O	303	MQ9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	O	303	MQ9	C20-C19-C21-C22
17	O	303	MQ9	C22-C23-C24-C25
17	O	303	MQ9	C34-C36-C37-C38
17	O	303	MQ9	C37-C38-C39-C41
17	O	303	MQ9	C40-C39-C41-C42
17	O	303	MQ9	C42-C43-C44-C45
17	O	303	MQ9	C44-C46-C47-C48
17	B	609	MQ9	C1-C6-C7-C8
17	B	609	MQ9	C7-C8-C9-C11
17	B	609	MQ9	C12-C11-C9-C8
17	B	609	MQ9	C9-C11-C12-C13
17	B	609	MQ9	C12-C13-C14-C15
17	B	609	MQ9	C12-C13-C14-C16
17	B	609	MQ9	C18-C19-C21-C22
17	B	609	MQ9	C22-C23-C24-C26
17	B	609	MQ9	C23-C24-C26-C27
17	B	609	MQ9	C25-C24-C26-C27
17	B	609	MQ9	C27-C28-C29-C31
17	B	609	MQ9	C32-C33-C34-C35
17	B	610	MQ9	C12-C13-C14-C16
17	B	610	MQ9	C17-C18-C19-C21
17	B	610	MQ9	C22-C23-C24-C26
17	B	610	MQ9	C27-C28-C29-C31
17	B	610	MQ9	C37-C38-C39-C41
17	B	610	MQ9	C42-C43-C44-C46
17	B	610	MQ9	C47-C48-C49-C50
17	A	502	MQ9	C5-C6-C7-C8
17	A	502	MQ9	C1-C6-C7-C8
17	A	502	MQ9	C7-C8-C9-C11
17	A	502	MQ9	C12-C13-C14-C15
17	A	502	MQ9	C12-C13-C14-C16
17	A	502	MQ9	C17-C18-C19-C20
17	A	502	MQ9	C22-C23-C24-C25
17	A	502	MQ9	C27-C28-C29-C31
17	C	303	MQ9	C7-C8-C9-C10
17	C	303	MQ9	C12-C13-C14-C15
17	C	303	MQ9	C12-C13-C14-C16
17	C	303	MQ9	C13-C14-C16-C17
17	C	303	MQ9	C14-C16-C17-C18
17	C	303	MQ9	C17-C18-C19-C20
17	C	303	MQ9	C18-C19-C21-C22
17	C	303	MQ9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	C	303	MQ9	C24-C26-C27-C28
17	C	303	MQ9	C26-C27-C28-C29
17	C	303	MQ9	C28-C29-C31-C32
17	C	303	MQ9	C31-C32-C33-C34
17	C	303	MQ9	C32-C33-C34-C35
20	M	503	9YF	C7-C2-O2-P
20	M	503	9YF	C26-C25-O11-C24
20	M	503	9YF	O12-C25-O11-C24
20	M	504	9YF	C2-O2-P-O1
20	A	503	9YF	C3-C2-O2-P
20	A	503	9YF	C7-C2-O2-P
20	A	505	9YF	C1-O-P-O2
20	A	505	9YF	C1-O-P-O8
20	A	505	9YF	C9-C8-O9-C
20	A	505	9YF	O10-C8-O9-C
12	B	608	CDL	OA9-CA7-OA8-CA6
20	A	503	9YF	O12-C25-O11-C24
12	B	608	CDL	C31-CA7-OA8-CA6
20	A	503	9YF	C26-C25-O11-C24
17	N	607	MQ9	C47-C48-C49-C50
17	N	608	MQ9	C47-C48-C49-C50
17	O	303	MQ9	C47-C48-C49-C50
12	D	201	CDL	OB9-CB7-OB8-CB6
12	N	605	CDL	OA9-CA7-OA8-CA6
12	B	603	CDL	OA9-CA7-OA8-CA6
12	P	201	CDL	OA7-CA5-OA6-CA4
12	P	201	CDL	OB7-CB5-OB6-CB4
12	N	604	CDL	OA7-CA5-OA6-CA4
12	N	605	CDL	OA7-CA5-OA6-CA4
12	N	605	CDL	OB7-CB5-OB6-CB4
12	M	502	CDL	OB7-CB5-OB6-CB4
12	B	603	CDL	OB7-CB5-OB6-CB4
12	B	606	CDL	OA7-CA5-OA6-CA4
12	B	608	CDL	OB7-CB5-OB6-CB4
12	A	504	CDL	OA7-CA5-OA6-CA4
12	N	605	CDL	C31-CA7-OA8-CA6
12	B	603	CDL	C31-CA7-OA8-CA6
12	N	604	CDL	C51-CB5-OB6-CB4
12	N	606	CDL	C11-CA5-OA6-CA4
17	B	610	MQ9	C47-C48-C49-C51
14	F	606	HEA	C2D-C3D-CAD-CBD
14	R	606	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
17	O	302	MQ9	C12-C11-C9-C10
17	O	302	MQ9	C25-C24-C26-C27
17	C	303	MQ9	C20-C19-C21-C22
17	O	302	MQ9	C12-C11-C9-C8
17	B	610	MQ9	C23-C24-C26-C27
17	A	502	MQ9	C18-C19-C21-C22
12	B	603	CDL	OB9-CB7-OB8-CB6
12	B	607	CDL	OA9-CA7-OA8-CA6
12	F	601	CDL	C71-CB7-OB8-CB6
12	D	201	CDL	C71-CB7-OB8-CB6
12	R	601	CDL	C71-CB7-OB8-CB6
12	N	606	CDL	C31-CA7-OA8-CA6
12	B	606	CDL	C31-CA7-OA8-CA6
12	B	607	CDL	C31-CA7-OA8-CA6
20	M	504	9YF	C26-C25-O11-C24
17	A	502	MQ9	C32-C33-C34-C35
17	C	303	MQ9	C37-C38-C39-C41
14	F	607	HEA	C13-C14-C15-C26
14	R	607	HEA	C13-C14-C15-C26
17	N	607	MQ9	C17-C18-C19-C20
17	N	607	MQ9	C27-C28-C29-C30
17	N	608	MQ9	C27-C28-C29-C30
17	N	608	MQ9	C37-C38-C39-C40
17	O	303	MQ9	C17-C18-C19-C20
17	O	303	MQ9	C27-C28-C29-C30
17	O	303	MQ9	C32-C33-C34-C35
17	B	610	MQ9	C12-C13-C14-C15
17	C	303	MQ9	C27-C28-C29-C30
17	N	607	MQ9	C22-C23-C24-C26
17	O	302	MQ9	C22-C23-C24-C26
12	F	601	CDL	OB9-CB7-OB8-CB6
12	R	601	CDL	OB9-CB7-OB8-CB6
12	B	606	CDL	OA9-CA7-OA8-CA6
12	P	201	CDL	C33-C34-C35-C36
12	F	602	CDL	CA5-C11-C12-C13
12	R	602	CDL	CA5-C11-C12-C13
12	D	201	CDL	O1-C1-CB2-OB2
12	P	201	CDL	O1-C1-CB2-OB2
12	M	502	CDL	O1-C1-CA2-OA2
12	O	301	CDL	O1-C1-CA2-OA2
12	B	603	CDL	O1-C1-CB2-OB2
12	B	605	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
12	B	607	CDL	O1-C1-CB2-OB2
12	D	201	CDL	C31-CA7-OA8-CA6
12	B	605	CDL	C31-CA7-OA8-CA6
12	M	502	CDL	C51-CB5-OB6-CB4
12	B	603	CDL	C11-CA5-OA6-CA4
12	B	607	CDL	C51-CB5-OB6-CB4
12	F	602	CDL	C51-C52-C53-C54
12	D	201	CDL	C79-C80-C81-C82
12	R	602	CDL	C51-C52-C53-C54
12	P	201	CDL	C79-C80-C81-C82
12	O	301	CDL	C76-C77-C78-C79
12	B	608	CDL	C57-C58-C59-C60
12	A	504	CDL	C72-C73-C74-C75
20	A	505	9YF	C10-C11-C12-C13
12	B	603	CDL	C71-CB7-OB8-CB6
12	F	602	CDL	C75-C76-C77-C78
12	D	201	CDL	C81-C82-C83-C84
12	R	602	CDL	C75-C76-C77-C78
12	B	605	CDL	OA9-CA7-OA8-CA6
20	M	504	9YF	O12-C25-O11-C24
16	N	602	HEM	C3D-CAD-CBD-CGD
16	B	602	HEM	C3D-CAD-CBD-CGD
12	R	601	CDL	C31-C32-C33-C34
12	P	201	CDL	C51-C52-C53-C54
12	N	604	CDL	C72-C73-C74-C75
20	A	503	9YF	C28-C29-C30-C31
14	F	607	HEA	C21-C22-C23-C25
14	R	607	HEA	C21-C22-C23-C25
17	O	302	MQ9	C37-C38-C39-C40
17	N	607	MQ9	C12-C11-C9-C10
17	N	607	MQ9	C20-C19-C21-C22
17	N	608	MQ9	C20-C19-C21-C22
17	O	303	MQ9	C25-C24-C26-C27
17	B	610	MQ9	C20-C19-C21-C22
17	B	610	MQ9	C30-C29-C31-C32
17	B	610	MQ9	C35-C34-C36-C37
17	A	502	MQ9	C12-C11-C9-C10
17	C	303	MQ9	C35-C34-C36-C37
17	N	607	MQ9	C23-C24-C26-C27
17	N	608	MQ9	C12-C11-C9-C8
17	O	303	MQ9	C13-C14-C16-C17
17	B	609	MQ9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
17	B	610	MQ9	C38-C39-C41-C42
17	C	303	MQ9	C23-C24-C26-C27
12	F	601	CDL	C31-C32-C33-C34
12	D	201	CDL	OA9-CA7-OA8-CA6
12	N	606	CDL	OA9-CA7-OA8-CA6
14	F	607	HEA	C19-C20-C21-C22
14	R	607	HEA	C19-C20-C21-C22
17	N	607	MQ9	C44-C46-C47-C48
17	O	302	MQ9	C19-C21-C22-C23
17	O	302	MQ9	C29-C31-C32-C33
17	B	610	MQ9	C39-C41-C42-C43
17	B	610	MQ9	C44-C46-C47-C48
12	B	603	CDL	C83-C84-C85-C86
12	O	301	CDL	C51-CB5-OB6-CB4
17	N	608	MQ9	C7-C8-C9-C10
17	B	610	MQ9	C7-C8-C9-C10
17	B	610	MQ9	C32-C33-C34-C35
12	B	605	CDL	CA2-C1-CB2-OB2
12	F	601	CDL	C31-CA7-OA8-CA6
12	F	602	CDL	C71-CB7-OB8-CB6
12	R	601	CDL	C31-CA7-OA8-CA6
12	R	602	CDL	C71-CB7-OB8-CB6
12	N	605	CDL	C71-CB7-OB8-CB6
12	M	502	CDL	C71-CB7-OB8-CB6
12	B	605	CDL	C71-CB7-OB8-CB6
15	G	301	9Y0	C6-C5-O5-C
15	S	301	9Y0	C6-C5-O5-C
20	A	503	9YF	C2-O2-P-O
12	F	602	CDL	C57-C58-C59-C60
12	D	201	CDL	C52-C53-C54-C55
12	R	602	CDL	C57-C58-C59-C60
12	B	608	CDL	C12-C13-C14-C15
12	B	606	CDL	O1-C1-CA2-OA2
12	A	504	CDL	O1-C1-CA2-OA2
12	N	605	CDL	CA5-C11-C12-C13
12	N	605	CDL	OA6-CA4-CA6-OA8
12	D	201	CDL	C32-C33-C34-C35
12	O	301	CDL	C57-C58-C59-C60
15	G	301	9Y0	O4-C5-O5-C
15	S	301	9Y0	O4-C5-O5-C
20	A	503	9YF	C34-C33-C35-C36
12	B	603	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	A	503	9YF	C9-C8-O9-C
20	A	505	9YF	C26-C25-O11-C24
12	P	201	CDL	CB7-C71-C72-C73
12	O	301	CDL	CB5-C51-C52-C53
12	B	608	CDL	CB5-C51-C52-C53
12	F	602	CDL	OB9-CB7-OB8-CB6
17	O	303	MQ9	C37-C38-C39-C40
12	R	602	CDL	OB9-CB7-OB8-CB6
12	M	502	CDL	OB9-CB7-OB8-CB6
12	O	301	CDL	CA5-C11-C12-C13
12	B	606	CDL	CA7-C31-C32-C33
12	B	607	CDL	CA5-C11-C12-C13
12	N	606	CDL	C19-C20-C21-C22
12	B	607	CDL	OB7-CB5-OB6-CB4
12	F	601	CDL	CA7-C31-C32-C33
12	R	601	CDL	CA7-C31-C32-C33
12	N	605	CDL	CA7-C31-C32-C33
12	B	605	CDL	CA5-C11-C12-C13
20	A	503	9YF	C31-C32-C33-C35
12	N	605	CDL	OB9-CB7-OB8-CB6
12	B	605	CDL	OB9-CB7-OB8-CB6
12	F	601	CDL	OA9-CA7-OA8-CA6
12	R	601	CDL	OA9-CA7-OA8-CA6
14	F	606	HEA	C15-C16-C17-C18
14	R	606	HEA	C15-C16-C17-C18
17	N	607	MQ9	C39-C41-C42-C43
17	O	303	MQ9	C29-C31-C32-C33
17	B	609	MQ9	C14-C16-C17-C18
17	B	609	MQ9	C19-C21-C22-C23
17	A	502	MQ9	C9-C11-C12-C13
17	A	502	MQ9	C14-C16-C17-C18
17	C	303	MQ9	C34-C36-C37-C38
12	F	601	CDL	CA5-C11-C12-C13
12	R	601	CDL	CA5-C11-C12-C13
12	B	603	CDL	O1-C1-CA2-OA2
12	M	502	CDL	C31-CA7-OA8-CA6
20	A	505	9YF	O12-C25-O11-C24
20	M	504	9YF	C9-C8-O9-C
20	A	503	9YF	C30-C31-C32-C33
12	F	601	CDL	CB2-OB2-PB2-OB5
12	F	602	CDL	CA3-OA5-PA1-OA2
12	F	602	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
12	F	602	CDL	CB3-OB5-PB2-OB2
12	D	201	CDL	CB3-OB5-PB2-OB2
12	R	601	CDL	CB2-OB2-PB2-OB5
12	R	602	CDL	CA3-OA5-PA1-OA2
12	R	602	CDL	CB2-OB2-PB2-OB5
12	R	602	CDL	CB3-OB5-PB2-OB2
12	P	201	CDL	CA3-OA5-PA1-OA2
12	P	201	CDL	CB3-OB5-PB2-OB2
12	N	604	CDL	CB2-OB2-PB2-OB5
12	N	605	CDL	CA3-OA5-PA1-OA2
12	N	605	CDL	CB2-OB2-PB2-OB5
12	N	606	CDL	CA2-OA2-PA1-OA5
12	N	606	CDL	CA3-OA5-PA1-OA2
12	M	502	CDL	CA2-OA2-PA1-OA5
12	M	502	CDL	CB3-OB5-PB2-OB2
12	O	301	CDL	CA3-OA5-PA1-OA2
12	B	603	CDL	CA2-OA2-PA1-OA5
12	B	603	CDL	CB3-OB5-PB2-OB2
12	B	605	CDL	CA3-OA5-PA1-OA2
12	B	605	CDL	CB2-OB2-PB2-OB5
12	B	605	CDL	CB3-OB5-PB2-OB2
12	B	606	CDL	CA2-OA2-PA1-OA5
12	B	608	CDL	CA2-OA2-PA1-OA5
12	B	608	CDL	CA3-OA5-PA1-OA2
15	G	301	9Y0	C3-O1-P-O3
15	S	301	9Y0	C3-O1-P-O3
20	M	504	9YF	C1-O-P-O2
14	F	606	HEA	C21-C22-C23-C25
12	F	602	CDL	CB7-C71-C72-C73
12	R	602	CDL	CB7-C71-C72-C73
12	D	201	CDL	CA2-C1-CB2-OB2
12	M	502	CDL	CB2-C1-CA2-OA2
12	B	603	CDL	CB2-C1-CA2-OA2
12	O	301	CDL	OB7-CB5-OB6-CB4
20	M	504	9YF	O10-C8-O9-C
20	A	503	9YF	O10-C8-O9-C
17	A	502	MQ9	C20-C19-C21-C22
17	C	303	MQ9	C32-C33-C34-C36
14	R	606	HEA	C21-C22-C23-C25
12	P	201	CDL	C31-CA7-OA8-CA6
12	A	504	CDL	C31-CA7-OA8-CA6
20	M	504	9YF	C2-O2-P-O

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Mol	Chain	Res	Type	Atoms
12	B	606	CDL	CA5-C11-C12-C13
12	R	601	CDL	C32-C33-C34-C35
12	R	601	CDL	C71-C72-C73-C74
12	P	201	CDL	C19-C20-C21-C22
12	P	201	CDL	C31-C32-C33-C34
20	M	503	9YF	C9-C8-O9-C
12	F	601	CDL	C32-C33-C34-C35
12	F	601	CDL	C71-C72-C73-C74
12	F	601	CDL	C77-C78-C79-C80
12	R	601	CDL	C77-C78-C79-C80
12	P	201	CDL	C75-C76-C77-C78
12	P	201	CDL	C78-C79-C80-C81
12	B	605	CDL	C71-C72-C73-C74
12	A	504	CDL	C71-C72-C73-C74
12	F	601	CDL	C37-C38-C39-C40
12	F	602	CDL	C81-C82-C83-C84
12	R	602	CDL	C81-C82-C83-C84
12	N	604	CDL	C74-C75-C76-C77
12	N	605	CDL	C31-C32-C33-C34
12	M	502	CDL	C23-C24-C25-C26
12	M	502	CDL	C75-C76-C77-C78
12	O	301	CDL	C11-C12-C13-C14
12	B	603	CDL	C76-C77-C78-C79
12	B	606	CDL	C31-C32-C33-C34
12	B	608	CDL	C21-C22-C23-C24
20	M	503	9YF	O10-C8-O9-C
12	B	605	CDL	CA7-C31-C32-C33
12	B	605	CDL	CB5-C51-C52-C53
12	R	601	CDL	C37-C38-C39-C40
12	P	201	CDL	C23-C24-C25-C26
12	N	604	CDL	C79-C80-C81-C82
12	N	605	CDL	C72-C73-C74-C75
12	N	604	CDL	C12-C13-C14-C15
12	N	604	CDL	C31-C32-C33-C34
12	N	604	CDL	C52-C53-C54-C55
12	N	606	CDL	C71-C72-C73-C74
12	M	502	CDL	C59-C60-C61-C62
12	B	606	CDL	C78-C79-C80-C81
12	B	607	CDL	C33-C34-C35-C36
12	B	608	CDL	C33-C34-C35-C36
12	B	605	CDL	O1-C1-CA2-OA2
21	O	304	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
21	C	301	HEC	C3D-CAD-CBD-CGD
12	M	502	CDL	C31-C32-C33-C34
12	B	605	CDL	C31-C32-C33-C34
15	G	301	9Y0	C25-C26-C27-C28
15	S	301	9Y0	C25-C26-C27-C28
20	M	503	9YF	C13-C14-C15-C16
20	A	503	9YF	C37-C38-C39-C40
12	D	201	CDL	CA5-C11-C12-C13
12	N	604	CDL	C14-C15-C16-C17
12	N	604	CDL	C51-C52-C53-C54
12	B	603	CDL	C52-C53-C54-C55
12	B	605	CDL	C75-C76-C77-C78
12	A	504	CDL	C21-C22-C23-C24
12	A	504	CDL	OA9-CA7-OA8-CA6
17	O	302	MQ9	C15-C14-C16-C17
12	O	301	CDL	C72-C73-C74-C75
12	B	606	CDL	C79-C80-C81-C82
12	A	504	CDL	C19-C20-C21-C22
12	A	504	CDL	C75-C76-C77-C78
13	F	603	PLM	C5-C6-C7-C8
13	R	603	PLM	C5-C6-C7-C8
20	A	503	9YF	C9-C10-C11-C12
20	A	503	9YF	C29-C30-C31-C32
17	O	303	MQ9	C33-C34-C36-C37
12	M	502	CDL	C72-C73-C74-C75
12	B	608	CDL	C52-C53-C54-C55
12	B	608	CDL	C54-C55-C56-C57
20	M	504	9YF	C26-C27-C28-C29
12	M	502	CDL	C21-C22-C23-C24
12	O	301	CDL	C14-C15-C16-C17
12	B	605	CDL	C12-C13-C14-C15
12	B	606	CDL	C72-C73-C74-C75
12	B	607	CDL	C11-C12-C13-C14
12	A	504	CDL	C14-C15-C16-C17
12	A	504	CDL	C38-C39-C40-C41
12	N	606	CDL	C51-CB5-OB6-CB4
12	P	201	CDL	C83-C84-C85-C86
12	N	606	CDL	C56-C57-C58-C59
12	B	603	CDL	C13-C14-C15-C16
12	B	605	CDL	C55-C56-C57-C58
12	B	607	CDL	C37-C38-C39-C40
17	O	303	MQ9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
12	N	604	CDL	CB5-C51-C52-C53
12	F	601	CDL	C13-C14-C15-C16
12	F	601	CDL	C57-C58-C59-C60
12	F	601	CDL	C72-C73-C74-C75
12	F	602	CDL	C59-C60-C61-C62
12	F	602	CDL	C72-C73-C74-C75
12	R	601	CDL	C57-C58-C59-C60
12	R	601	CDL	C72-C73-C74-C75
12	R	602	CDL	C59-C60-C61-C62
12	R	602	CDL	C72-C73-C74-C75
12	N	606	CDL	C75-C76-C77-C78
12	M	502	CDL	C71-C72-C73-C74
12	B	603	CDL	C55-C56-C57-C58
12	B	607	CDL	C57-C58-C59-C60
12	A	504	CDL	C13-C14-C15-C16
12	A	504	CDL	C59-C60-C61-C62
15	G	301	9Y0	C23-C24-C25-C26
15	S	301	9Y0	C23-C24-C25-C26
20	M	503	9YF	C29-C30-C31-C32
20	A	503	9YF	C36-C37-C38-C39
12	A	504	CDL	CA4-CA6-OA8-CA7
17	O	303	MQ9	C24-C26-C27-C28
12	F	602	CDL	C32-C33-C34-C35
12	F	602	CDL	C71-C72-C73-C74
12	R	601	CDL	C13-C14-C15-C16
12	R	602	CDL	C32-C33-C34-C35
12	P	201	CDL	C76-C77-C78-C79
12	N	605	CDL	C55-C56-C57-C58
12	B	606	CDL	C75-C76-C77-C78
12	B	607	CDL	C51-C52-C53-C54
12	B	608	CDL	C20-C21-C22-C23
12	F	602	CDL	C11-C12-C13-C14
12	D	201	CDL	C38-C39-C40-C41
12	R	602	CDL	C11-C12-C13-C14
12	R	602	CDL	C71-C72-C73-C74
12	N	605	CDL	C71-C72-C73-C74
12	M	502	CDL	C14-C15-C16-C17
12	M	502	CDL	C52-C53-C54-C55
12	M	502	CDL	C57-C58-C59-C60
12	B	608	CDL	C13-C14-C15-C16
12	B	608	CDL	C77-C78-C79-C80
20	A	503	9YF	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
12	M	502	CDL	C80-C81-C82-C83
12	O	301	CDL	C80-C81-C82-C83
12	B	607	CDL	C52-C53-C54-C55
12	A	504	CDL	C23-C24-C25-C26
12	F	602	CDL	C31-C32-C33-C34
12	R	602	CDL	C31-C32-C33-C34
12	P	201	CDL	C34-C35-C36-C37
12	F	602	CDL	C78-C79-C80-C81
12	D	201	CDL	C54-C55-C56-C57
12	M	502	CDL	C74-C75-C76-C77
12	M	502	CDL	C79-C80-C81-C82
12	O	301	CDL	C78-C79-C80-C81
12	R	602	CDL	C78-C79-C80-C81
12	N	605	CDL	C57-C58-C59-C60
12	M	502	CDL	C77-C78-C79-C80
20	M	503	9YF	C12-C13-C14-C15
12	O	301	CDL	CA3-CA4-CA6-OA8
12	B	603	CDL	C77-C78-C79-C80
12	B	607	CDL	C74-C75-C76-C77
12	O	301	CDL	C34-C35-C36-C37
12	M	502	CDL	OA9-CA7-OA8-CA6
17	A	502	MQ9	C13-C14-C16-C17
12	F	601	CDL	C51-CB5-OB6-CB4
12	R	601	CDL	C51-CB5-OB6-CB4
12	M	502	CDL	C11-CA5-OA6-CA4
12	M	502	CDL	C76-C77-C78-C79
12	M	502	CDL	C83-C84-C85-C86
12	O	301	CDL	C52-C53-C54-C55
12	P	201	CDL	C82-C83-C84-C85
12	N	604	CDL	C57-C58-C59-C60
12	M	502	CDL	C11-C12-C13-C14
12	B	606	CDL	C14-C15-C16-C17
12	P	201	CDL	OA9-CA7-OA8-CA6
12	A	504	CDL	CB5-C51-C52-C53
12	O	301	CDL	C79-C80-C81-C82
12	B	603	CDL	C57-C58-C59-C60
12	N	606	CDL	C77-C78-C79-C80
12	N	606	CDL	C53-C54-C55-C56
12	R	602	CDL	C14-C15-C16-C17
12	P	201	CDL	C14-C15-C16-C17
12	B	607	CDL	C59-C60-C61-C62
12	B	608	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
12	F	602	CDL	OB7-CB5-OB6-CB4
12	N	606	CDL	OB7-CB5-OB6-CB4
12	M	502	CDL	OA7-CA5-OA6-CA4
17	N	608	MQ9	C47-C48-C49-C51
12	F	602	CDL	C14-C15-C16-C17
12	P	201	CDL	C16-C17-C18-C19
12	P	201	CDL	C77-C78-C79-C80
12	N	604	CDL	C77-C78-C79-C80
12	B	607	CDL	C72-C73-C74-C75
15	G	301	9Y0	C6-C7-C8-C9
15	S	301	9Y0	C6-C7-C8-C9
20	M	503	9YF	C-C1-O-P
12	F	602	CDL	C12-C13-C14-C15
12	R	602	CDL	C12-C13-C14-C15
12	N	605	CDL	C59-C60-C61-C62
12	B	606	CDL	C77-C78-C79-C80
15	G	301	9Y0	C22-C23-C24-C25
15	S	301	9Y0	C22-C23-C24-C25
20	M	503	9YF	C11-C12-C13-C14
20	M	504	9YF	C10-C11-C12-C13
20	A	505	9YF	C27-C28-C29-C30
12	O	301	CDL	CB7-C71-C72-C73
12	N	605	CDL	C75-C76-C77-C78
12	N	606	CDL	C23-C24-C25-C26
12	N	606	CDL	C71-CB7-OB8-CB6
12	F	602	CDL	C51-CB5-OB6-CB4
12	R	602	CDL	C51-CB5-OB6-CB4
12	P	201	CDL	C52-C53-C54-C55
12	B	603	CDL	C14-C15-C16-C17
12	B	607	CDL	C14-C15-C16-C17
12	N	606	CDL	C57-C58-C59-C60
12	B	606	CDL	C51-C52-C53-C54
12	P	201	CDL	C71-C72-C73-C74
12	B	606	CDL	C13-C14-C15-C16
12	B	608	CDL	C24-C25-C26-C27
17	O	302	MQ9	C35-C34-C36-C37
17	O	302	MQ9	C13-C14-C16-C17
12	D	201	CDL	C24-C25-C26-C27
12	M	502	CDL	C22-C23-C24-C25
14	F	607	HEA	C1A-C2A-CAA-CBA
14	R	607	HEA	C1A-C2A-CAA-CBA
12	F	601	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
12	R	601	CDL	OB7-CB5-OB6-CB4
12	R	602	CDL	OB7-CB5-OB6-CB4
12	N	606	CDL	C72-C73-C74-C75
12	B	607	CDL	C31-C32-C33-C34
15	S	301	9Y0	C29-C30-C31-C32
12	M	502	CDL	C51-C52-C53-C54
15	G	301	9Y0	C29-C30-C31-C32
20	A	505	9YF	C26-C27-C28-C29
17	C	303	MQ9	C9-C11-C12-C13
12	F	602	CDL	C80-C81-C82-C83
12	R	602	CDL	C80-C81-C82-C83
12	M	502	CDL	C58-C59-C60-C61
12	B	606	CDL	C76-C77-C78-C79
12	B	608	CDL	C55-C56-C57-C58
12	A	504	CDL	C54-C55-C56-C57
12	F	602	CDL	C11-CA5-OA6-CA4
12	R	602	CDL	C11-CA5-OA6-CA4
12	P	201	CDL	OA5-CA3-CA4-OA6
12	B	606	CDL	OA5-CA3-CA4-OA6
12	O	301	CDL	C77-C78-C79-C80
16	B	602	HEM	C4B-C3B-CAB-CBB
12	M	502	CDL	C37-C38-C39-C40
12	N	606	CDL	O1-C1-CB2-OB2
12	B	605	CDL	OB7-CB5-OB6-CB4
20	M	503	9YF	C11-C10-C9-C8
12	N	606	CDL	C51-C52-C53-C54
12	N	605	CDL	C32-C33-C34-C35
12	M	502	CDL	C20-C21-C22-C23
12	A	504	CDL	C53-C54-C55-C56
12	N	604	CDL	C75-C76-C77-C78
21	O	304	HEC	C4D-C3D-CAD-CBD
21	C	301	HEC	C4D-C3D-CAD-CBD
12	N	606	CDL	C22-C23-C24-C25
12	N	606	CDL	OB9-CB7-OB8-CB6
12	B	605	CDL	C51-CB5-OB6-CB4
13	R	603	PLM	CA-CB-CC-CD
12	N	604	CDL	CB3-OB5-PB2-OB2
12	B	603	CDL	CB2-OB2-PB2-OB5
12	F	601	CDL	OB5-CB3-CB4-CB6
12	F	602	CDL	OB5-CB3-CB4-CB6
12	R	601	CDL	OB5-CB3-CB4-CB6
12	R	602	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
12	N	604	CDL	OA5-CA3-CA4-CA6
12	N	604	CDL	OB5-CB3-CB4-CB6
12	P	201	CDL	C20-C21-C22-C23
12	N	605	CDL	C74-C75-C76-C77
12	A	504	CDL	C83-C84-C85-C86
12	B	603	CDL	CA2-C1-CB2-OB2
12	B	607	CDL	CB2-C1-CA2-OA2
17	B	609	MQ9	C15-C14-C16-C17
12	N	606	CDL	C31-C32-C33-C34
12	A	504	CDL	C12-C13-C14-C15
12	F	602	CDL	C77-C78-C79-C80
12	D	201	CDL	C71-C72-C73-C74
12	P	201	CDL	C73-C74-C75-C76
12	R	602	CDL	C77-C78-C79-C80
12	A	504	CDL	C78-C79-C80-C81
12	F	602	CDL	CB3-CB4-CB6-OB8
12	R	602	CDL	CB3-CB4-CB6-OB8
12	P	201	CDL	CA3-CA4-CA6-OA8
12	N	605	CDL	CB3-CB4-CB6-OB8
12	M	502	CDL	C24-C25-C26-C27
12	O	301	CDL	CB3-CB4-CB6-OB8
12	B	605	CDL	C77-C78-C79-C80
12	B	607	CDL	CB3-CB4-CB6-OB8
12	A	504	CDL	C63-C64-C65-C66
15	G	301	9Y0	O5-C-C1-C2
15	S	301	9Y0	O5-C-C1-C2
20	M	504	9YF	C1-C-C24-O11
12	B	608	CDL	C79-C80-C81-C82
14	F	606	HEA	C1A-C2A-CAA-CBA
14	R	606	HEA	C1A-C2A-CAA-CBA
17	B	609	MQ9	C5-C6-C7-C8
12	B	606	CDL	C80-C81-C82-C83
12	P	201	CDL	C18-C19-C20-C21
12	A	504	CDL	C76-C77-C78-C79
12	A	504	CDL	C84-C85-C86-C87
12	B	603	CDL	C11-C12-C13-C14
12	A	504	CDL	C37-C38-C39-C40
17	A	502	MQ9	C32-C33-C34-C36
12	B	606	CDL	C59-C60-C61-C62
20	A	505	9YF	C30-C31-C32-C33
12	D	201	CDL	C11-C12-C13-C14
12	A	504	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
12	P	201	CDL	C32-C33-C34-C35
17	O	302	MQ9	C26-C27-C28-C29
12	F	602	CDL	CB5-C51-C52-C53
12	R	602	CDL	CB5-C51-C52-C53
12	B	603	CDL	C74-C75-C76-C77
12	P	201	CDL	CB6-CB4-OB6-CB5
12	N	606	CDL	C12-C13-C14-C15
12	D	201	CDL	C53-C54-C55-C56
12	R	601	CDL	C78-C79-C80-C81
12	M	502	CDL	C64-C65-C66-C67
12	N	604	CDL	C71-CB7-OB8-CB6
12	B	603	CDL	OA5-CA3-CA4-OA6
12	M	502	CDL	CB5-C51-C52-C53
15	G	301	9Y0	C21-C22-C23-C24
15	S	301	9Y0	C21-C22-C23-C24
12	F	601	CDL	C78-C79-C80-C81
12	N	604	CDL	C59-C60-C61-C62
12	A	504	CDL	C77-C78-C79-C80
20	M	503	9YF	C9-C10-C11-C12
12	F	601	CDL	C59-C60-C61-C62
12	B	607	CDL	C53-C54-C55-C56
12	A	504	CDL	C24-C25-C26-C27
12	R	601	CDL	C59-C60-C61-C62
12	P	201	CDL	C36-C37-C38-C39
12	O	301	CDL	OA6-CA4-CA6-OA8
12	B	605	CDL	OB6-CB4-CB6-OB8
20	A	503	9YF	O9-C-C24-O11
12	D	201	CDL	C77-C78-C79-C80
12	R	602	CDL	C84-C85-C86-C87
12	B	608	CDL	C18-C19-C20-C21
17	B	609	MQ9	C17-C18-C19-C20
12	F	602	CDL	C84-C85-C86-C87
12	N	604	CDL	C76-C77-C78-C79
20	A	503	9YF	C32-C33-C35-C36
14	F	607	HEA	C3A-C2A-CAA-CBA
14	R	607	HEA	C3A-C2A-CAA-CBA
21	O	304	HEC	C2D-C3D-CAD-CBD
21	C	301	HEC	C2D-C3D-CAD-CBD
12	F	602	CDL	C64-C65-C66-C67
12	P	201	CDL	C80-C81-C82-C83
12	R	602	CDL	C64-C65-C66-C67
12	P	201	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
17	N	607	MQ9	C47-C48-C49-C51
12	B	608	CDL	C34-C35-C36-C37
12	M	502	CDL	C32-C33-C34-C35
12	P	201	CDL	CA2-C1-CB2-OB2
12	B	607	CDL	CA2-C1-CB2-OB2
12	N	606	CDL	C18-C19-C20-C21
12	B	603	CDL	C81-C82-C83-C84
12	B	606	CDL	C74-C75-C76-C77
12	D	201	CDL	CB5-C51-C52-C53
12	F	601	CDL	OA5-CA3-CA4-CA6
12	F	602	CDL	OA5-CA3-CA4-CA6
12	R	601	CDL	OA5-CA3-CA4-CA6
12	R	602	CDL	OA5-CA3-CA4-CA6
17	B	610	MQ9	C29-C31-C32-C33
12	O	301	CDL	C74-C75-C76-C77
12	A	504	CDL	CB7-C71-C72-C73
12	D	201	CDL	C33-C34-C35-C36
20	A	505	9YF	C11-C12-C13-C14
17	B	609	MQ9	C12-C11-C9-C10
17	N	608	MQ9	C38-C39-C41-C42
20	A	505	9YF	C28-C29-C30-C31
12	O	301	CDL	C75-C76-C77-C78
12	A	504	CDL	C15-C16-C17-C18
12	N	606	CDL	C52-C53-C54-C55
12	M	502	CDL	C62-C63-C64-C65
12	N	606	CDL	CA7-C31-C32-C33
12	D	201	CDL	C72-C73-C74-C75
12	N	605	CDL	C11-C12-C13-C14
12	N	606	CDL	C74-C75-C76-C77
12	O	301	CDL	C31-C32-C33-C34
12	M	502	CDL	C81-C82-C83-C84
12	B	603	CDL	C80-C81-C82-C83
12	D	201	CDL	C82-C83-C84-C85
12	B	605	CDL	C57-C58-C59-C60
20	M	503	9YF	C14-C15-C16-C17
12	F	601	CDL	CB3-CB4-CB6-OB8
12	F	602	CDL	CA3-CA4-CA6-OA8
12	R	601	CDL	CB3-CB4-CB6-OB8
12	R	602	CDL	CA3-CA4-CA6-OA8
12	N	604	CDL	CB3-CB4-CB6-OB8
12	N	605	CDL	CA3-CA4-CA6-OA8
12	B	605	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
12	B	605	CDL	CB3-CB4-CB6-OB8
12	B	606	CDL	CA3-CA4-CA6-OA8
12	A	504	CDL	CA3-CA4-CA6-OA8
20	M	503	9YF	C1-C-C24-O11
20	A	503	9YF	C1-C-C24-O11
12	F	602	CDL	OA7-CA5-OA6-CA4
12	R	602	CDL	OA7-CA5-OA6-CA4
12	A	504	CDL	C79-C80-C81-C82
12	F	601	CDL	C74-C75-C76-C77
12	R	601	CDL	C74-C75-C76-C77
12	D	201	CDL	C39-C40-C41-C42
12	N	605	CDL	C60-C61-C62-C63
12	B	603	CDL	C72-C73-C74-C75
20	M	504	9YF	C2-O2-P-O8
12	D	201	CDL	CB7-C71-C72-C73
17	N	608	MQ9	C23-C24-C26-C27
12	D	201	CDL	C14-C15-C16-C17
20	M	504	9YF	C13-C14-C15-C16
12	B	605	CDL	C73-C74-C75-C76
12	B	605	CDL	C74-C75-C76-C77
12	M	502	CDL	CA3-OA5-PA1-OA2
12	D	201	CDL	OA5-CA3-CA4-OA6
12	P	201	CDL	OB5-CB3-CB4-OB6
12	N	604	CDL	OA5-CA3-CA4-OA6
12	O	301	CDL	OA5-CA3-CA4-OA6
12	O	301	CDL	OB5-CB3-CB4-OB6
12	B	605	CDL	OA5-CA3-CA4-OA6
12	B	608	CDL	OA5-CA3-CA4-OA6
12	D	201	CDL	C37-C38-C39-C40
12	N	604	CDL	OB9-CB7-OB8-CB6
15	G	301	9Y0	C7-C8-C9-C10
12	N	605	CDL	C14-C15-C16-C17
12	O	301	CDL	C51-C52-C53-C54
15	S	301	9Y0	C7-C8-C9-C10
20	A	503	9YF	C38-C39-C40-C41
20	M	504	9YF	C28-C29-C30-C31
12	N	604	CDL	OB6-CB4-CB6-OB8
12	N	606	CDL	OB6-CB4-CB6-OB8
12	B	606	CDL	OA6-CA4-CA6-OA8
12	B	608	CDL	OB6-CB4-CB6-OB8
12	A	504	CDL	OA6-CA4-CA6-OA8
20	M	503	9YF	O9-C-C24-O11

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Mol	Chain	Res	Type	Atoms
12	O	301	CDL	C32-C33-C34-C35
12	P	201	CDL	C13-C14-C15-C16
12	N	606	CDL	C24-C25-C26-C27
17	A	502	MQ9	C29-C31-C32-C33
12	B	605	CDL	C11-C12-C13-C14
15	G	301	9Y0	C33-C34-C35-C36
15	S	301	9Y0	C33-C34-C35-C36
17	A	502	MQ9	C25-C24-C26-C27
12	N	606	CDL	C79-C80-C81-C82
12	F	601	CDL	C61-C62-C63-C64
12	R	601	CDL	C61-C62-C63-C64
12	N	604	CDL	C15-C16-C17-C18
12	B	608	CDL	C76-C77-C78-C79
12	P	201	CDL	C57-C58-C59-C60
12	B	605	CDL	CB4-CB3-OB5-PB2
12	B	605	CDL	C72-C73-C74-C75
12	B	605	CDL	C56-C57-C58-C59
12	D	201	CDL	C17-C18-C19-C20
13	F	603	PLM	C6-C7-C8-C9
12	N	606	CDL	C13-C14-C15-C16
14	F	606	HEA	C3A-C2A-CAA-CBA
14	R	606	HEA	C3A-C2A-CAA-CBA
12	R	601	CDL	C14-C15-C16-C17
15	G	301	9Y0	C13-C14-C15-C16
15	S	301	9Y0	C13-C14-C15-C16
12	F	601	CDL	C14-C15-C16-C17
12	B	608	CDL	C23-C24-C25-C26
12	O	301	CDL	OA5-CA3-CA4-CA6
12	O	301	CDL	OB5-CB3-CB4-CB6
12	B	603	CDL	OA5-CA3-CA4-CA6
12	B	603	CDL	OB5-CB3-CB4-CB6
12	B	605	CDL	OA5-CA3-CA4-CA6
12	B	606	CDL	OA5-CA3-CA4-CA6
18	N	609	HV0	C23-C24-C27-C32
15	G	301	9Y0	C31-C32-C33-C34
15	S	301	9Y0	C31-C32-C33-C34
13	F	603	PLM	CB-CC-CD-CE
12	M	502	CDL	C78-C79-C80-C81
12	N	604	CDL	C78-C79-C80-C81
12	N	605	CDL	C33-C34-C35-C36
12	N	606	CDL	C33-C34-C35-C36
12	D	201	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
15	G	301	9Y0	C28-C29-C30-C31
18	N	609	HV0	C23-C24-C27-C28
15	S	301	9Y0	C28-C29-C30-C31
12	F	601	CDL	C75-C76-C77-C78
13	F	603	PLM	C2-C3-C4-C5
12	F	602	CDL	C79-C80-C81-C82
12	R	601	CDL	C75-C76-C77-C78
12	R	602	CDL	C79-C80-C81-C82
12	B	608	CDL	C51-C52-C53-C54
12	A	504	CDL	C31-C32-C33-C34
15	G	301	9Y0	C27-C28-C29-C30
15	S	301	9Y0	C27-C28-C29-C30
12	N	606	CDL	C58-C59-C60-C61
12	B	603	CDL	C35-C36-C37-C38
12	B	606	CDL	C32-C33-C34-C35
12	M	502	CDL	CB6-CB4-OB6-CB5
20	A	503	9YF	C24-C-O9-C8
17	A	502	MQ9	C7-C8-C9-C10
17	B	610	MQ9	C45-C44-C46-C47
17	N	607	MQ9	C14-C16-C17-C18
17	B	610	MQ9	C9-C11-C12-C13
15	G	301	9Y0	C24-C25-C26-C27
12	P	201	CDL	C1-CA2-OA2-PA1
12	P	201	CDL	CB3-CB4-CB6-OB8
12	N	606	CDL	CB3-CB4-CB6-OB8
12	B	608	CDL	CB3-CB4-CB6-OB8
12	A	504	CDL	C51-CB5-OB6-CB4
15	S	301	9Y0	C24-C25-C26-C27
12	F	601	CDL	OA5-CA3-CA4-OA6
12	F	602	CDL	OA5-CA3-CA4-OA6
12	R	601	CDL	OA5-CA3-CA4-OA6
12	R	602	CDL	OA5-CA3-CA4-OA6
12	B	608	CDL	OB5-CB3-CB4-OB6
16	N	602	HEM	C4B-C3B-CAB-CBB
12	B	603	CDL	C54-C55-C56-C57
12	B	607	CDL	O1-C1-CA2-OA2
12	R	602	CDL	C74-C75-C76-C77
12	F	602	CDL	C74-C75-C76-C77
12	F	601	CDL	OB6-CB4-CB6-OB8
12	F	602	CDL	OB6-CB4-CB6-OB8
12	R	601	CDL	OB6-CB4-CB6-OB8
12	R	602	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
12	P	201	CDL	OA6-CA4-CA6-OA8
15	G	301	9Y0	O5-C-C1-O7
15	S	301	9Y0	O5-C-C1-O7
12	A	504	CDL	C64-C65-C66-C67
12	O	301	CDL	C36-C37-C38-C39
12	B	606	CDL	C71-C72-C73-C74
12	P	201	CDL	C37-C38-C39-C40
14	F	607	HEA	C2D-C3D-CAD-CBD
14	R	607	HEA	C2D-C3D-CAD-CBD
12	B	607	CDL	C58-C59-C60-C61
12	A	504	CDL	OB7-CB5-OB6-CB4
12	O	301	CDL	C55-C56-C57-C58
12	N	604	CDL	C19-C20-C21-C22
12	B	605	CDL	C52-C53-C54-C55
12	B	606	CDL	C52-C53-C54-C55
12	B	607	CDL	C16-C17-C18-C19
12	P	201	CDL	CA2-OA2-PA1-OA5
12	N	604	CDL	CA3-OA5-PA1-OA2
12	O	301	CDL	CA2-OA2-PA1-OA5
12	B	607	CDL	CA2-OA2-PA1-OA5
12	B	607	CDL	CB3-OB5-PB2-OB2
12	D	201	CDL	C13-C14-C15-C16
20	A	503	9YF	C39-C40-C41-C42
12	N	604	CDL	C1-CB2-OB2-PB2
12	M	502	CDL	C1-CA2-OA2-PA1
17	O	303	MQ9	C28-C29-C31-C32
12	R	601	CDL	C12-C13-C14-C15
12	M	502	CDL	C15-C16-C17-C18
12	F	602	CDL	CA3-OA5-PA1-OA3
12	F	602	CDL	CB2-OB2-PB2-OB3
12	F	602	CDL	CB2-OB2-PB2-OB4
12	D	201	CDL	CB3-OB5-PB2-OB4
12	R	602	CDL	CA3-OA5-PA1-OA3
12	R	602	CDL	CB2-OB2-PB2-OB3
12	R	602	CDL	CB2-OB2-PB2-OB4
12	P	201	CDL	CA3-OA5-PA1-OA3
12	P	201	CDL	CB3-OB5-PB2-OB4
12	N	604	CDL	CA3-OA5-PA1-OA3
12	N	604	CDL	CA3-OA5-PA1-OA4
12	N	606	CDL	CA2-OA2-PA1-OA4
12	M	502	CDL	CA2-OA2-PA1-OA4
12	M	502	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
12	O	301	CDL	CA2-OA2-PA1-OA4
12	O	301	CDL	CA3-OA5-PA1-OA3
12	O	301	CDL	CA3-OA5-PA1-OA4
12	B	603	CDL	CA2-OA2-PA1-OA3
12	B	603	CDL	CA2-OA2-PA1-OA4
12	B	603	CDL	CA3-OA5-PA1-OA4
12	B	605	CDL	CA3-OA5-PA1-OA3
12	B	606	CDL	CB2-OB2-PB2-OB3
12	B	608	CDL	CA2-OA2-PA1-OA3
12	B	608	CDL	CA3-OA5-PA1-OA3
12	B	608	CDL	CA3-OA5-PA1-OA4
12	B	608	CDL	CB2-OB2-PB2-OB4
12	A	504	CDL	CA3-OA5-PA1-OA3
12	A	504	CDL	CB2-OB2-PB2-OB3
20	M	504	9YF	C1-O-P-O1
12	B	603	CDL	CA5-C11-C12-C13
12	F	601	CDL	C12-C13-C14-C15
12	D	201	CDL	OA5-CA3-CA4-CA6
12	N	606	CDL	OB5-CB3-CB4-CB6
12	B	607	CDL	OA5-CA3-CA4-CA6
12	B	608	CDL	OA5-CA3-CA4-CA6
12	B	608	CDL	OB5-CB3-CB4-CB6
12	B	603	CDL	C71-C72-C73-C74
12	D	201	CDL	C21-C22-C23-C24
14	F	606	HEA	C3B-C11-C12-C13
14	F	607	HEA	C3B-C11-C12-C13
14	R	606	HEA	C3B-C11-C12-C13
14	R	607	HEA	C3B-C11-C12-C13
13	R	603	PLM	C6-C7-C8-C9
12	B	603	CDL	C16-C17-C18-C19
12	F	601	CDL	C76-C77-C78-C79
12	R	601	CDL	C76-C77-C78-C79
20	M	503	9YF	C26-C27-C28-C29
12	B	603	CDL	OB5-CB3-CB4-OB6
12	B	607	CDL	OA5-CA3-CA4-OA6
12	R	602	CDL	C34-C35-C36-C37
12	M	502	CDL	C19-C20-C21-C22
20	M	503	9YF	C25-C26-C27-C28
12	F	601	CDL	C11-CA5-OA6-CA4
12	R	601	CDL	C11-CA5-OA6-CA4
12	F	602	CDL	C34-C35-C36-C37
12	N	604	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	F	602	CDL	C13-C14-C15-C16
12	R	602	CDL	C13-C14-C15-C16
20	A	505	9YF	C14-C15-C16-C17
13	R	603	PLM	C1-C2-C3-C4
12	F	602	CDL	OA6-CA4-CA6-OA8
12	R	602	CDL	OA6-CA4-CA6-OA8
12	P	201	CDL	OB6-CB4-CB6-OB8
12	N	605	CDL	OB6-CB4-CB6-OB8
12	N	606	CDL	OA6-CA4-CA6-OA8
12	B	603	CDL	OB6-CB4-CB6-OB8
12	B	605	CDL	OA6-CA4-CA6-OA8
12	M	502	CDL	C12-C13-C14-C15
12	A	504	CDL	C35-C36-C37-C38
12	N	605	CDL	C51-C52-C53-C54
12	P	201	CDL	C17-C18-C19-C20
12	B	605	CDL	C1-CA2-OA2-PA1
20	M	504	9YF	C-C1-O-P
17	B	610	MQ9	C15-C14-C16-C17
12	N	605	CDL	C34-C35-C36-C37
12	O	301	CDL	C83-C84-C85-C86
20	A	503	9YF	C13-C14-C15-C16
17	N	608	MQ9	C18-C19-C21-C22
20	A	503	9YF	C31-C32-C33-C34
12	M	502	CDL	C84-C85-C86-C87
12	B	606	CDL	CB5-C51-C52-C53
15	G	301	9Y0	C10-C11-C12-C13
15	S	301	9Y0	C10-C11-C12-C13
12	A	504	CDL	C74-C75-C76-C77
12	N	604	CDL	O1-C1-CA2-OA2
12	F	601	CDL	C73-C74-C75-C76
12	R	601	CDL	C73-C74-C75-C76
12	B	608	CDL	C14-C15-C16-C17
18	N	609	HV0	C31-C30-O33-C34
17	C	303	MQ9	C1-C6-C7-C8
12	B	605	CDL	C76-C77-C78-C79
12	N	606	CDL	C34-C35-C36-C37
12	B	603	CDL	C56-C57-C58-C59
20	M	503	9YF	C30-C31-C32-C33
12	B	603	CDL	CA6-CA4-OA6-CA5
12	B	607	CDL	CA6-CA4-OA6-CA5
12	B	608	CDL	CA6-CA4-OA6-CA5
20	M	504	9YF	C24-C-O9-C8

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Mol	Chain	Res	Type	Atoms
12	P	201	CDL	OA5-CA3-CA4-CA6
12	F	601	CDL	OA7-CA5-OA6-CA4
12	R	601	CDL	OA7-CA5-OA6-CA4
12	F	601	CDL	C52-C53-C54-C55
12	R	601	CDL	C52-C53-C54-C55
12	P	201	CDL	C84-C85-C86-C87
12	N	606	CDL	C55-C56-C57-C58
12	N	604	CDL	OB5-CB3-CB4-OB6
12	N	606	CDL	OB5-CB3-CB4-OB6
17	N	607	MQ9	C18-C19-C21-C22
17	N	607	MQ9	C38-C39-C41-C42
12	D	201	CDL	C83-C84-C85-C86
12	A	504	CDL	C34-C35-C36-C37
12	B	603	CDL	C78-C79-C80-C81
12	O	301	CDL	OB6-CB4-CB6-OB8
12	B	607	CDL	OB6-CB4-CB6-OB8
20	M	504	9YF	O9-C-C24-O11
12	D	201	CDL	CA2-OA2-PA1-OA5
12	P	201	CDL	CB2-OB2-PB2-OB5
12	N	605	CDL	CB3-OB5-PB2-OB2
12	B	605	CDL	CA2-OA2-PA1-OA5
12	A	504	CDL	CB3-OB5-PB2-OB2
12	N	605	CDL	C16-C17-C18-C19
12	N	606	CDL	C15-C16-C17-C18
12	M	502	CDL	CA3-CA4-CA6-OA8
12	B	603	CDL	C58-C59-C60-C61
14	F	607	HEA	C4D-C3D-CAD-CBD
14	R	607	HEA	C4D-C3D-CAD-CBD
12	B	603	CDL	C34-C35-C36-C37
12	B	605	CDL	C51-C52-C53-C54
12	R	602	CDL	C62-C63-C64-C65
18	B	611	HV0	C31-C30-O33-C34
12	P	201	CDL	C1-CB2-OB2-PB2
12	F	602	CDL	C62-C63-C64-C65
12	B	606	CDL	CB2-C1-CA2-OA2
15	G	301	9Y0	O6-C21-O7-C1
17	O	302	MQ9	C16-C17-C18-C19
21	O	304	HEC	C2C-C3C-CAC-CBC
21	C	301	HEC	C2C-C3C-CAC-CBC
12	M	502	CDL	C18-C19-C20-C21
20	A	503	9YF	C26-C27-C28-C29
15	S	301	9Y0	O6-C21-O7-C1

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Mol	Chain	Res	Type	Atoms
17	N	607	MQ9	C34-C36-C37-C38
12	B	603	CDL	C33-C34-C35-C36
12	F	602	CDL	C52-C53-C54-C55
12	A	504	CDL	C61-C62-C63-C64
14	F	607	HEA	CAA-CBA-CGA-O2A
14	R	607	HEA	CAA-CBA-CGA-O2A
12	R	602	CDL	C52-C53-C54-C55
12	B	603	CDL	C79-C80-C81-C82
18	N	609	HV0	C29-C30-O33-C34
18	B	611	HV0	C29-C30-O33-C34
12	M	502	CDL	C63-C64-C65-C66
12	O	301	CDL	C71-C72-C73-C74
12	D	201	CDL	OA6-CA4-CA6-OA8
12	R	602	CDL	C83-C84-C85-C86
12	N	604	CDL	C17-C18-C19-C20
12	B	605	CDL	C32-C33-C34-C35
12	F	602	CDL	C83-C84-C85-C86
12	D	201	CDL	C35-C36-C37-C38
12	O	301	CDL	C81-C82-C83-C84
17	N	608	MQ9	C40-C39-C41-C42
12	F	602	CDL	C82-C83-C84-C85
12	R	602	CDL	C82-C83-C84-C85
12	D	201	CDL	C75-C76-C77-C78
17	N	607	MQ9	C29-C31-C32-C33
12	D	201	CDL	C22-C23-C24-C25
20	A	503	9YF	C2-O2-P-O1
20	A	503	9YF	C2-O2-P-O8
12	B	608	CDL	CB6-CB4-OB6-CB5
17	O	303	MQ9	C12-C11-C9-C10
17	O	303	MQ9	C45-C44-C46-C47
12	A	504	CDL	C18-C19-C20-C21
12	B	608	CDL	CB2-OB2-PB2-OB5
12	P	201	CDL	C21-C22-C23-C24
12	B	607	CDL	C36-C37-C38-C39
12	P	201	CDL	C12-C13-C14-C15
12	M	502	CDL	OB5-CB3-CB4-OB6
12	D	201	CDL	OB5-CB3-CB4-CB6
17	O	303	MQ9	C12-C13-C14-C15
17	A	502	MQ9	C28-C29-C31-C32
12	M	502	CDL	C16-C17-C18-C19
12	O	301	CDL	C84-C85-C86-C87
12	F	601	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
12	R	602	CDL	C56-C57-C58-C59
12	P	201	CDL	C72-C73-C74-C75
12	F	602	CDL	C56-C57-C58-C59
12	O	301	CDL	C73-C74-C75-C76
12	F	601	CDL	OA6-CA4-CA6-OA8
12	R	601	CDL	OA6-CA4-CA6-OA8
12	B	606	CDL	C16-C17-C18-C19
12	R	601	CDL	C60-C61-C62-C63
14	F	607	HEA	CAA-CBA-CGA-O1A
14	R	607	HEA	CAA-CBA-CGA-O1A
12	B	607	CDL	C39-C40-C41-C42
12	F	602	CDL	CA2-C1-CB2-OB2
12	R	602	CDL	CA2-C1-CB2-OB2
17	N	608	MQ9	C43-C44-C46-C47
17	C	303	MQ9	C12-C11-C9-C8
12	B	606	CDL	C12-C13-C14-C15
12	B	603	CDL	C84-C85-C86-C87
14	F	606	HEA	CAA-CBA-CGA-O2A
14	R	606	HEA	CAA-CBA-CGA-O2A
15	G	301	9Y0	C22-C21-O7-C1
15	S	301	9Y0	C22-C21-O7-C1
12	N	604	CDL	C71-C72-C73-C74
12	A	504	CDL	C20-C21-C22-C23
17	N	607	MQ9	C15-C14-C16-C17
12	D	201	CDL	C19-C20-C21-C22
12	D	201	CDL	C52-C51-CB5-OB6
17	B	610	MQ9	C25-C24-C26-C27
18	B	611	HV0	C23-C24-C27-C28
20	A	503	9YF	C25-C26-C27-C28
12	O	301	CDL	C72-C71-CB7-OB8
12	P	201	CDL	CB4-CB3-OB5-PB2
12	N	604	CDL	C80-C81-C82-C83
12	N	604	CDL	C16-C17-C18-C19
13	N	603	PLM	C4-C5-C6-C7
13	B	604	PLM	C4-C5-C6-C7
17	N	607	MQ9	C30-C29-C31-C32
17	B	610	MQ9	C12-C11-C9-C10
12	N	604	CDL	C58-C59-C60-C61
12	D	201	CDL	C76-C77-C78-C79
12	N	605	CDL	C76-C77-C78-C79
16	N	602	HEM	C1A-C2A-CAA-CBA
20	M	503	9YF	C24-C-O9-C8

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Mol	Chain	Res	Type	Atoms
17	C	303	MQ9	C7-C8-C9-C11
21	O	304	HEC	CAA-CBA-CGA-O2A
12	P	201	CDL	C32-C31-CA7-OA8
12	N	605	CDL	C52-C51-CB5-OB6
15	G	301	9Y0	C9-C10-C11-C12
21	C	301	HEC	CAA-CBA-CGA-O2A
15	S	301	9Y0	C9-C10-C11-C12
17	N	607	MQ9	C43-C44-C46-C47
12	P	201	CDL	C72-C71-CB7-OB8
12	R	601	CDL	C36-C37-C38-C39
17	O	303	MQ9	C39-C41-C42-C43
15	G	301	9Y0	C11-C12-C13-C14
15	S	301	9Y0	C11-C12-C13-C14
12	F	601	CDL	C36-C37-C38-C39
12	B	608	CDL	C22-C23-C24-C25
12	N	606	CDL	CA3-CA4-CA6-OA8
12	B	603	CDL	CB3-CB4-CB6-OB8
12	M	502	CDL	C34-C35-C36-C37
12	B	607	CDL	OB5-CB3-CB4-OB6
12	N	604	CDL	C32-C31-CA7-OA8
12	D	201	CDL	C84-C85-C86-C87
12	A	504	CDL	C52-C53-C54-C55
14	F	606	HEA	CAA-CBA-CGA-O1A
12	A	504	CDL	OB6-CB4-CB6-OB8
12	N	604	CDL	CB7-C71-C72-C73
16	B	602	HEM	C1A-C2A-CAA-CBA
20	A	503	9YF	C40-C41-C42-C43
14	R	606	HEA	CAA-CBA-CGA-O1A
12	F	601	CDL	C12-C11-CA5-OA6
12	R	601	CDL	C12-C11-CA5-OA6
20	A	505	9YF	O9-C8-C9-C10
12	F	602	CDL	C12-C11-CA5-OA6
12	R	602	CDL	C12-C11-CA5-OA6
12	B	605	CDL	C72-C71-CB7-OB8
12	M	502	CDL	C55-C56-C57-C58
12	D	201	CDL	C57-C58-C59-C60
14	R	607	HEA	C2C-C3C-CAC-CBC
12	B	608	CDL	C31-C32-C33-C34
15	S	301	9Y0	C11-C10-C9-C8
12	A	504	CDL	C39-C40-C41-C42
12	M	502	CDL	C38-C39-C40-C41
15	G	301	9Y0	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	N	608	MQ9	C35-C34-C36-C37
12	O	301	CDL	C33-C34-C35-C36
12	B	608	CDL	C73-C74-C75-C76
12	O	301	CDL	C72-C71-CB7-OB9
14	F	607	HEA	C17-C18-C19-C27
14	R	607	HEA	C17-C18-C19-C27
12	P	201	CDL	C72-C71-CB7-OB9
12	B	607	CDL	C75-C76-C77-C78
12	B	605	CDL	C72-C71-CB7-OB9
12	F	601	CDL	CA3-CA4-CA6-OA8
12	D	201	CDL	CA3-CA4-CA6-OA8
12	R	601	CDL	CA3-CA4-CA6-OA8
21	O	305	HEC	C2C-C3C-CAC-CBC
12	B	605	CDL	C52-C51-CB5-OB6
12	N	605	CDL	C52-C51-CB5-OB7
21	C	301	HEC	CAA-CBA-CGA-O1A
12	N	606	CDL	C11-C12-C13-C14
12	F	602	CDL	C12-C11-CA5-OA7
12	F	602	CDL	CA2-OA2-PA1-OA4
12	R	602	CDL	CA2-OA2-PA1-OA4
12	P	201	CDL	CA2-OA2-PA1-OA3
12	B	608	CDL	CA2-OA2-PA1-OA4
12	A	504	CDL	CA2-OA2-PA1-OA3
15	G	301	9Y0	C2-O3-P-O
15	S	301	9Y0	C2-O3-P-O
17	B	609	MQ9	C6-C7-C8-C9
20	M	504	9YF	C1-O-P-O8
12	R	602	CDL	C63-C64-C65-C66
12	R	602	CDL	C12-C11-CA5-OA7
12	M	502	CDL	C33-C34-C35-C36
21	O	304	HEC	CAA-CBA-CGA-O1A
21	C	302	HEC	C2C-C3C-CAC-CBC
12	F	602	CDL	C63-C64-C65-C66
21	O	305	HEC	C2B-C3B-CAB-CBB
12	N	604	CDL	C32-C31-CA7-OA9
12	A	504	CDL	C11-C12-C13-C14
20	A	503	9YF	C11-C12-C13-C14
21	C	302	HEC	C2B-C3B-CAB-CBB
12	B	606	CDL	C15-C16-C17-C18
18	B	611	HV0	C23-C24-C27-C32
13	F	603	PLM	CD-CE-CF-CG
16	N	601	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	601	HEM	CAA-CBA-CGA-O2A
12	B	607	CDL	C72-C71-CB7-OB8
15	G	301	9Y0	O7-C21-C22-C23
15	S	301	9Y0	O7-C21-C22-C23
12	F	601	CDL	C12-C11-CA5-OA7
12	R	601	CDL	C12-C11-CA5-OA7
14	F	607	HEA	C27-C19-C20-C21
14	R	607	HEA	C27-C19-C20-C21
17	O	303	MQ9	C38-C39-C41-C42
21	O	304	HEC	CAD-CBD-CGD-O2D
21	C	301	HEC	CAD-CBD-CGD-O2D
12	A	504	CDL	C36-C37-C38-C39
20	A	505	9YF	O10-C8-C9-C10
14	F	606	HEA	C19-C20-C21-C22
14	R	606	HEA	C19-C20-C21-C22
17	O	302	MQ9	C14-C16-C17-C18
17	A	502	MQ9	C19-C21-C22-C23
14	F	607	HEA	C16-C17-C18-C19
14	R	607	HEA	C16-C17-C18-C19
12	F	602	CDL	O1-C1-CB2-OB2
12	R	602	CDL	O1-C1-CB2-OB2
16	B	601	HEM	CAA-CBA-CGA-O1A
21	O	304	HEC	CAD-CBD-CGD-O1D
21	C	301	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

40 monomers are involved in 162 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	606	CDL	3	0
12	B	608	CDL	3	0
14	R	607	HEA	8	0
20	M	504	9YF	4	0
12	B	603	CDL	4	0
20	A	505	9YF	18	0
12	B	605	CDL	3	0
14	F	607	HEA	8	0
12	N	604	CDL	2	0
16	N	602	HEM	3	0
12	N	606	CDL	4	0
21	C	301	HEC	3	0
12	P	201	CDL	8	0

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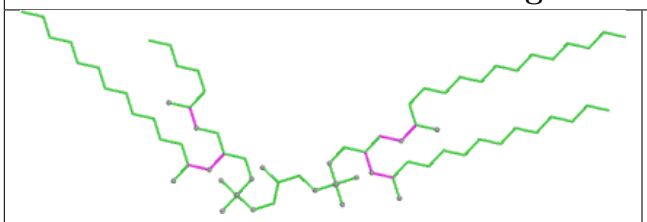
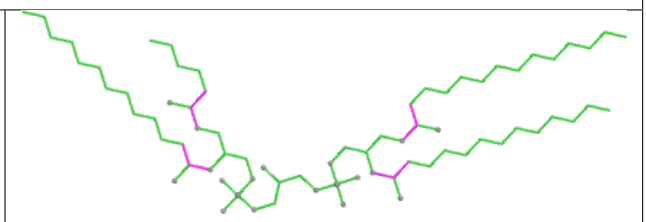
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	502	MQ9	6	0
16	N	601	HEM	2	0
14	F	606	HEA	6	0
17	N	607	MQ9	3	0
12	D	201	CDL	6	0
17	B	610	MQ9	10	0
19	A	501	FES	3	0
17	C	303	MQ9	4	0
12	O	301	CDL	2	0
12	N	605	CDL	5	0
16	B	601	HEM	1	0
21	O	304	HEC	1	0
19	M	501	FES	1	0
17	O	303	MQ9	2	0
12	A	504	CDL	5	0
14	R	606	HEA	5	0
12	F	602	CDL	2	0
16	B	602	HEM	5	0
12	M	502	CDL	1	0
17	B	609	MQ9	3	0
17	O	302	MQ9	5	0
12	F	601	CDL	1	0
20	M	503	9YF	6	0
12	B	607	CDL	2	0
17	N	608	MQ9	2	0
20	A	503	9YF	6	0
12	R	602	CDL	5	0

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

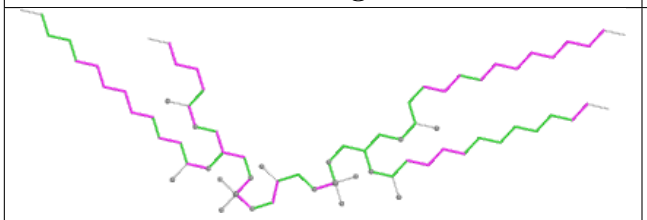
Ligand CDL B 606



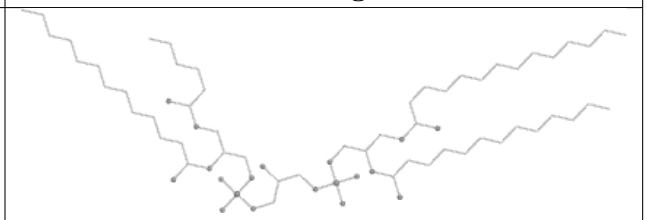
Bond lengths



Bond angles

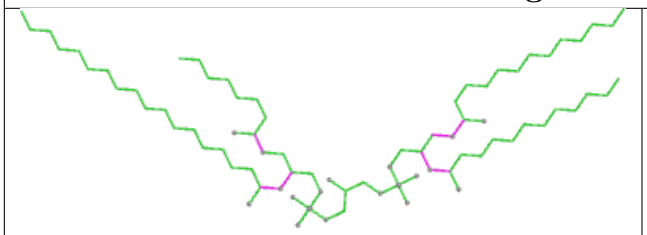


Torsions

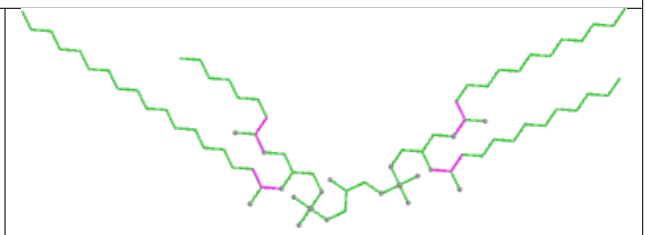


Rings

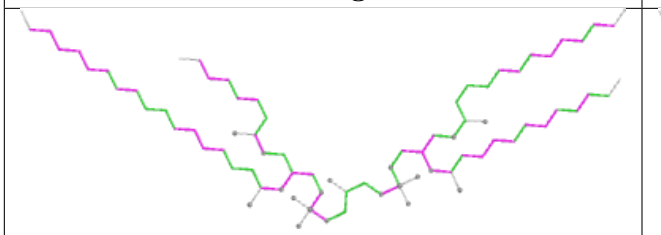
Ligand CDL B 608



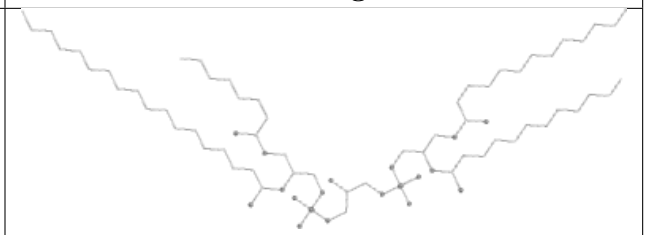
Bond lengths



Bond angles

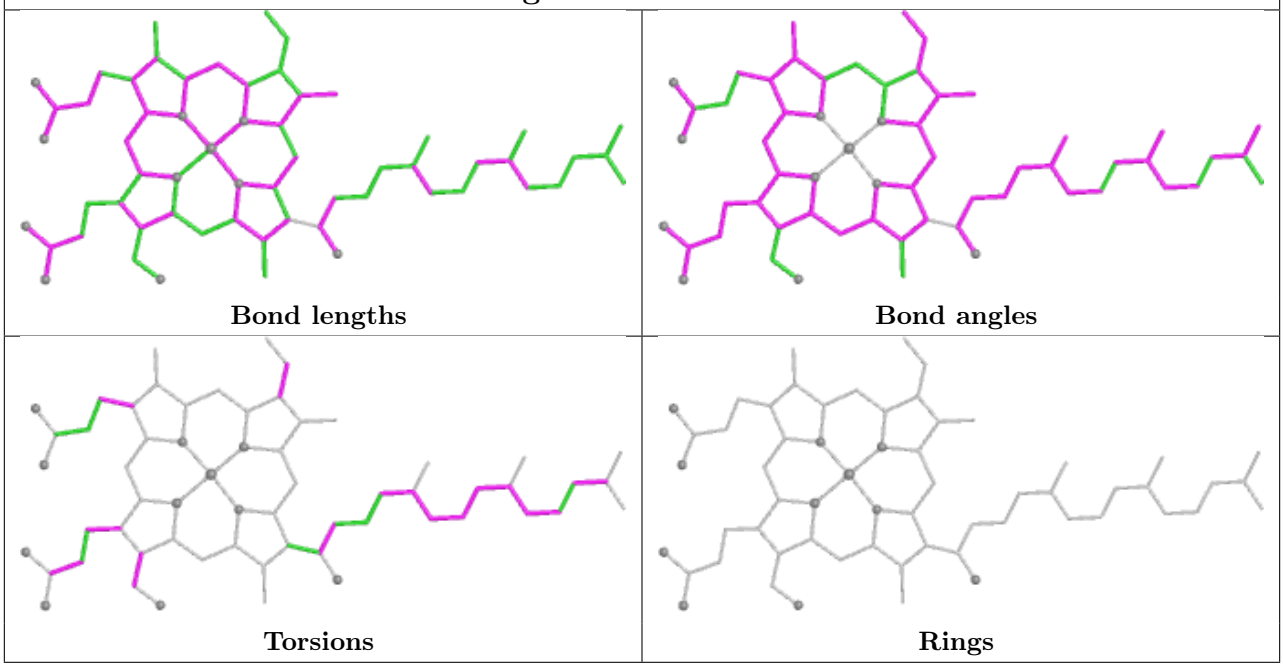


Torsions

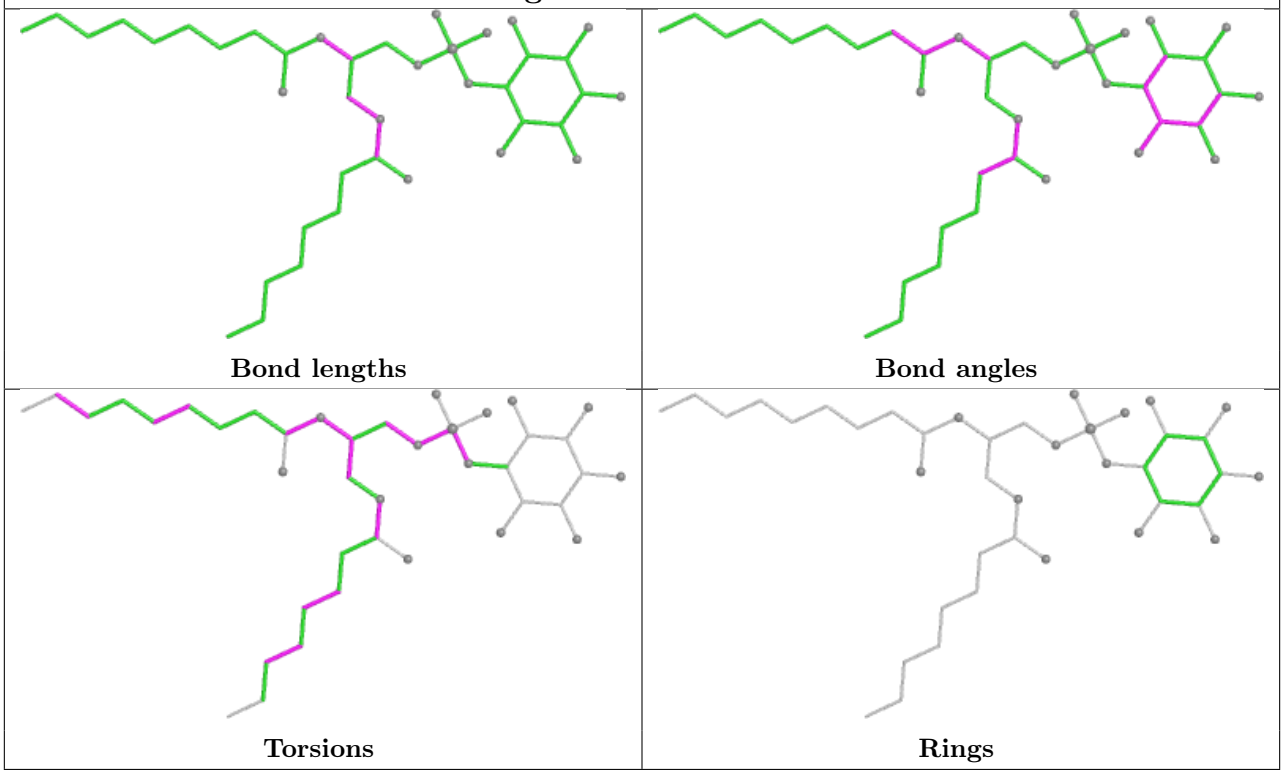


Rings

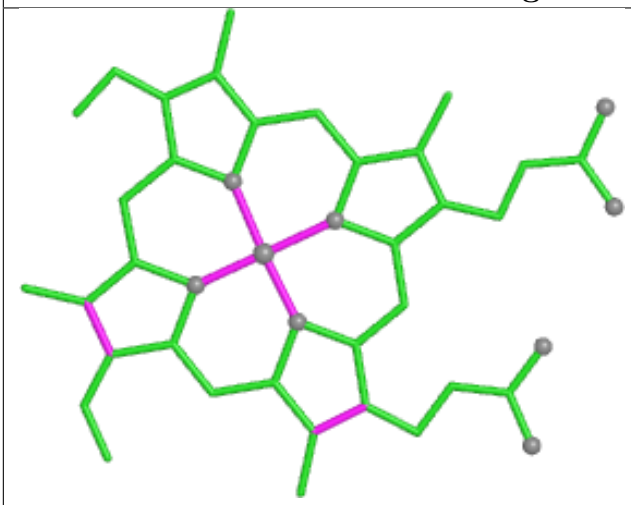
Ligand HEA R 607



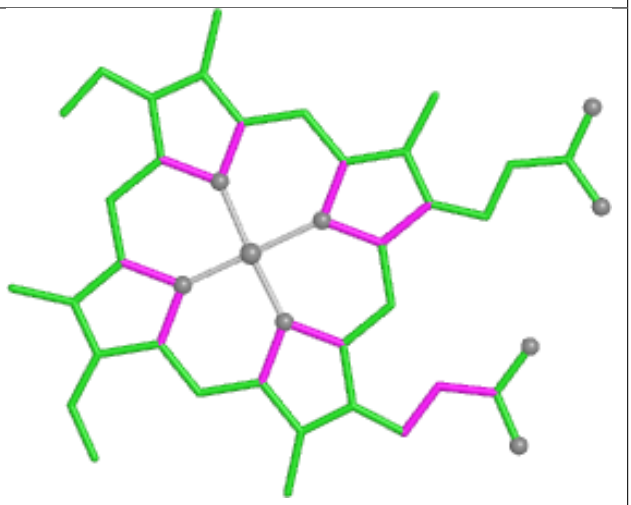
Ligand 9YF M 504



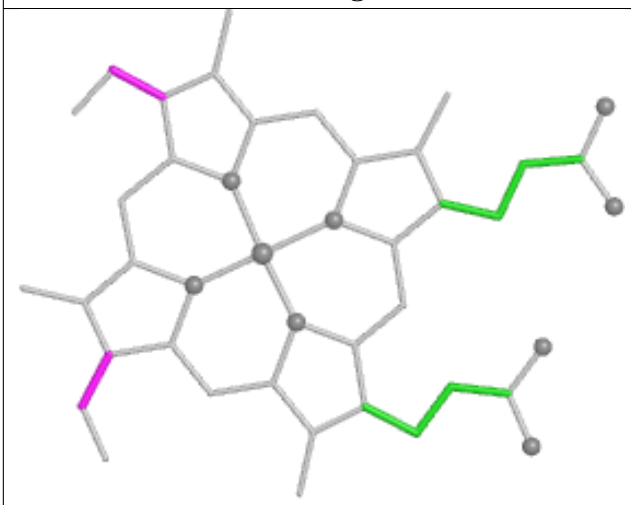
Ligand HEC O 305



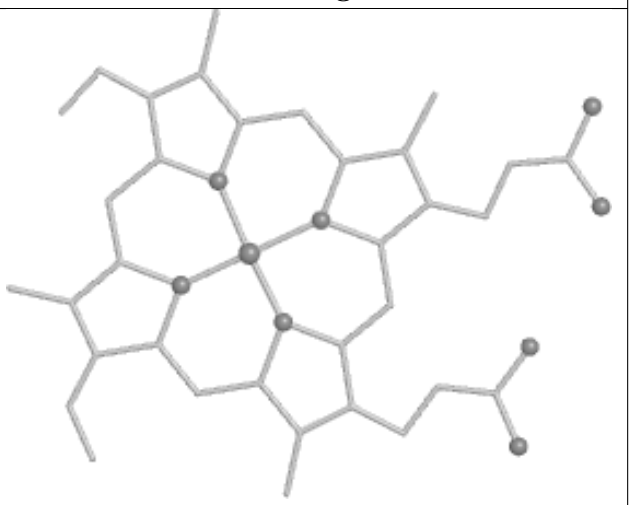
Bond lengths



Bond angles

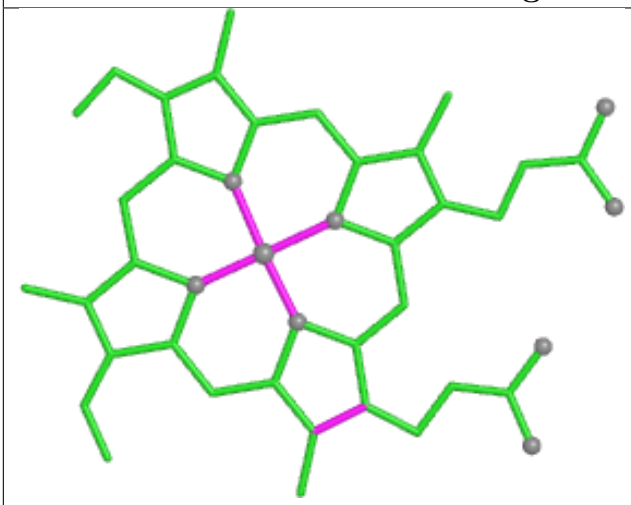


Torsions

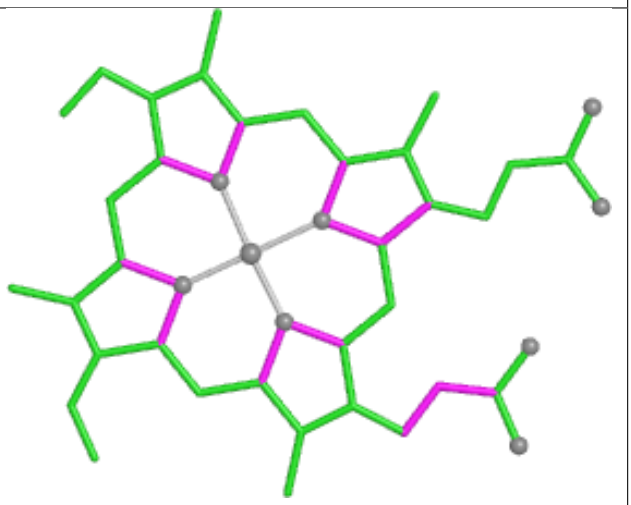


Rings

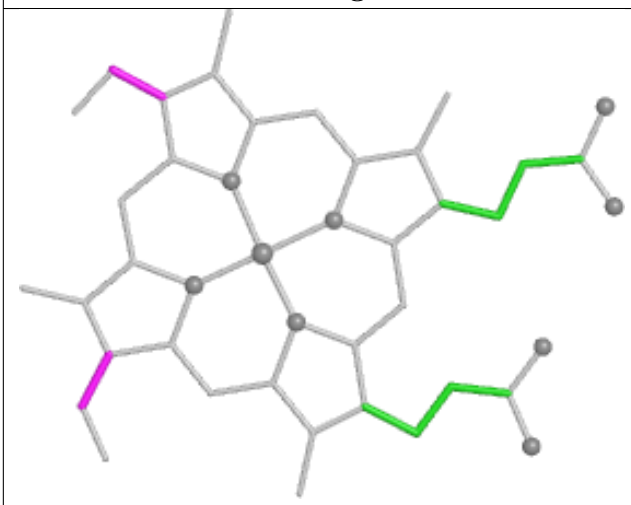
Ligand HEC C 302



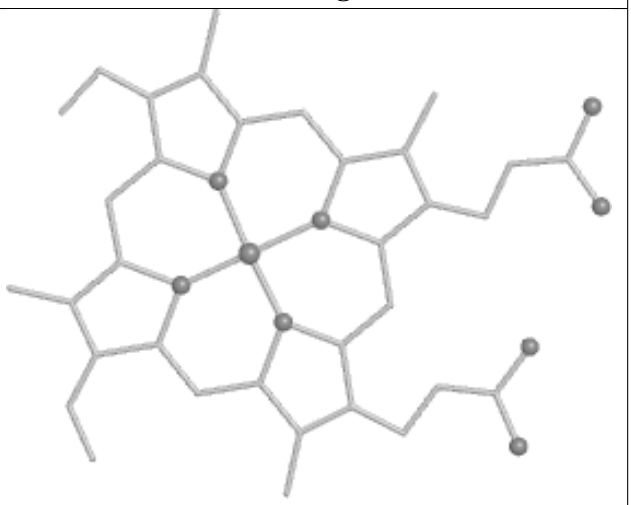
Bond lengths



Bond angles

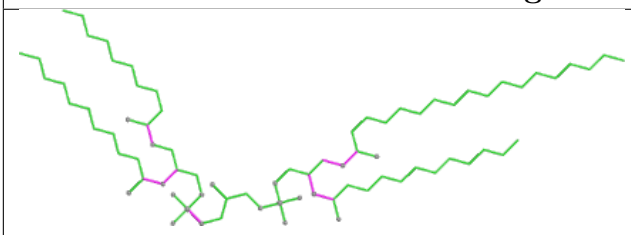


Torsions

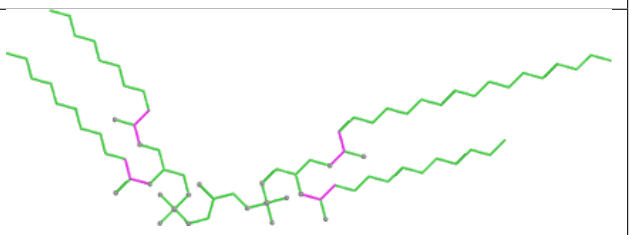


Rings

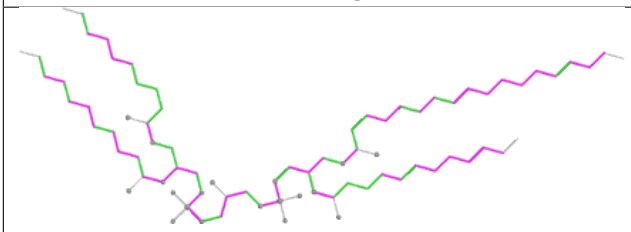
Ligand CDL B 603



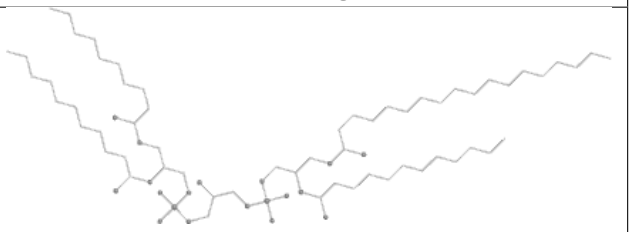
Bond lengths



Bond angles

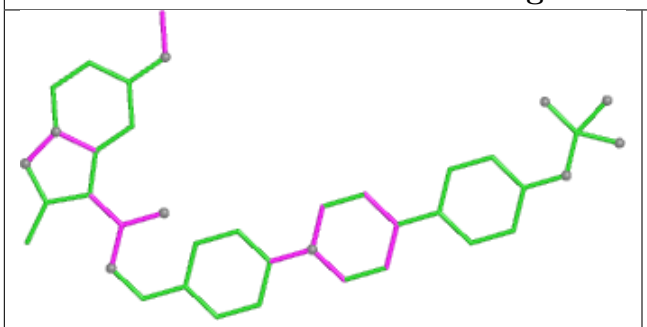


Torsions

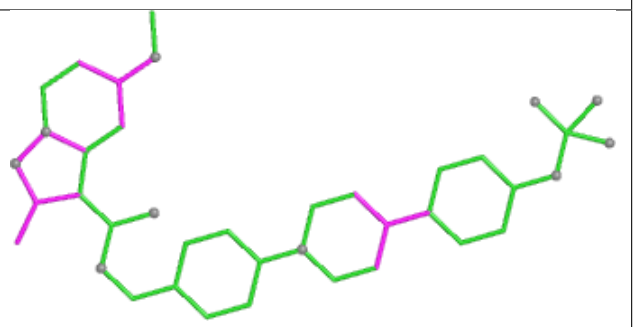


Rings

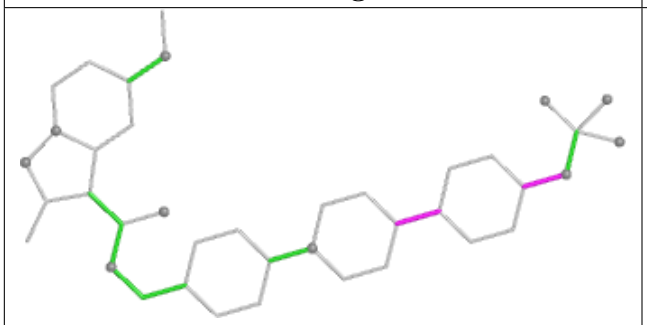
Ligand HV0 B 611



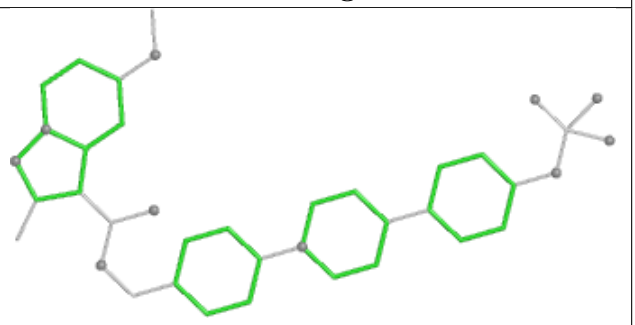
Bond lengths



Bond angles

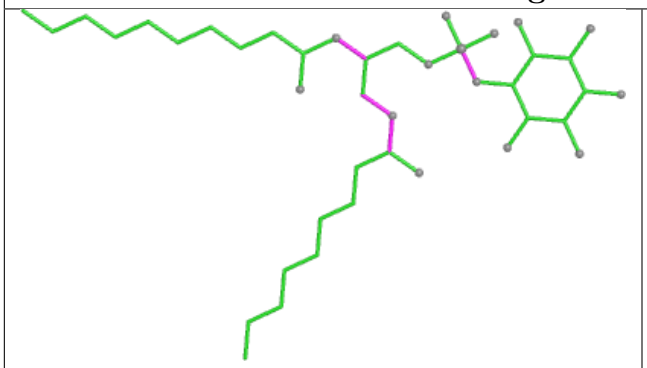


Torsions

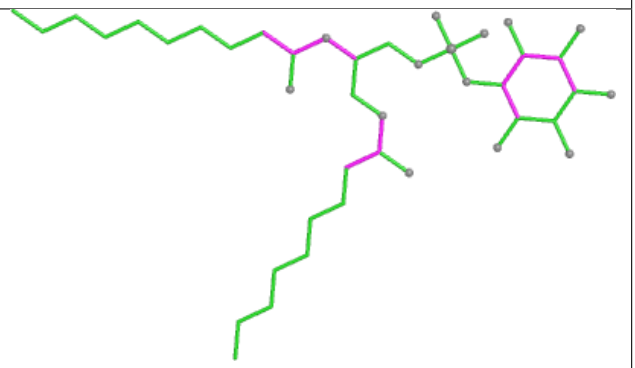


Rings

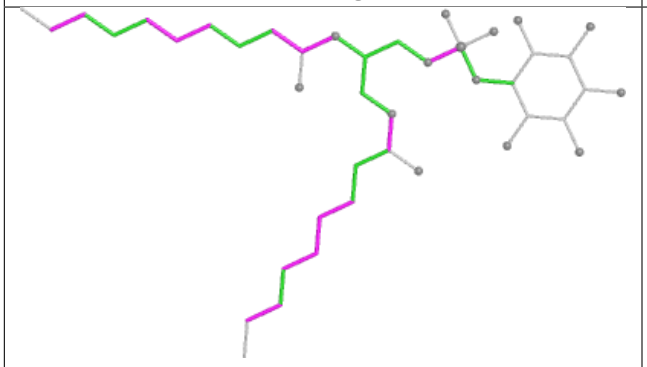
Ligand 9YF A 505



Bond lengths



Bond angles



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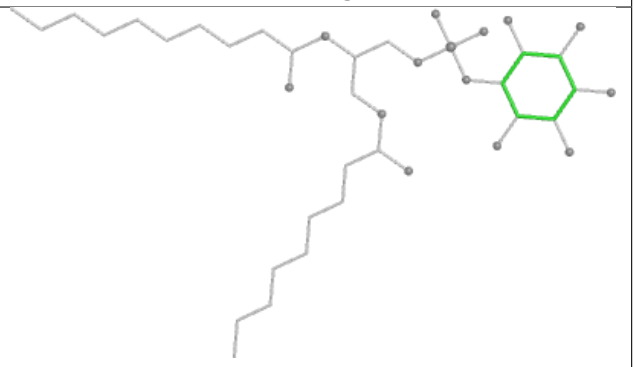
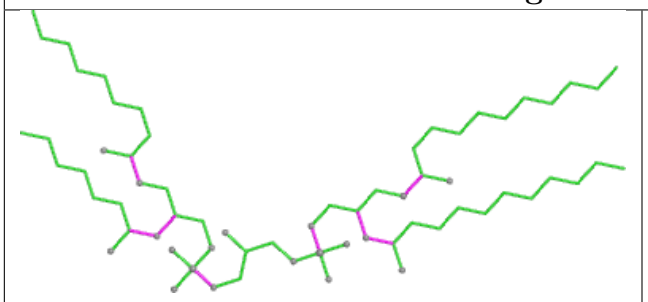
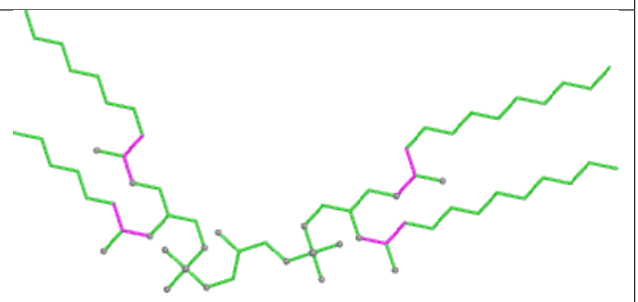


Rings

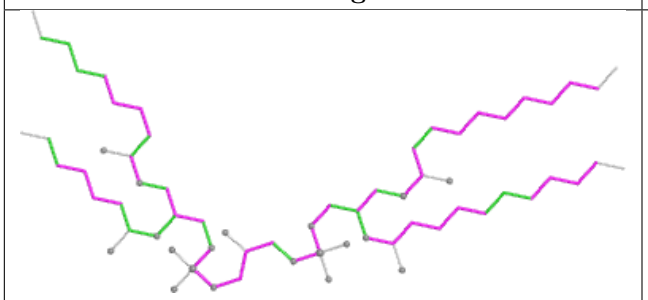
Ligand CDL B 605



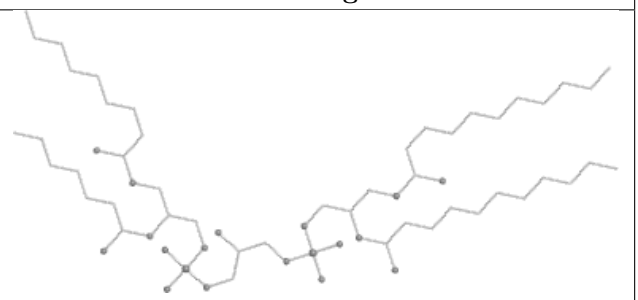
Bond lengths



Bond angles

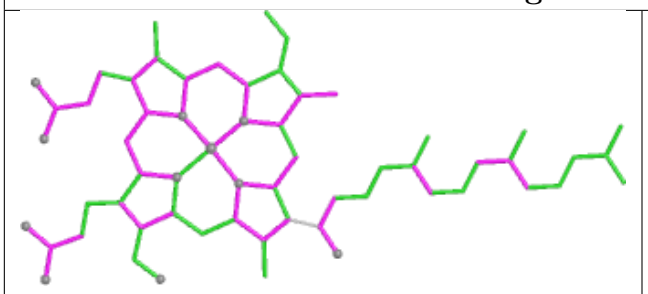


Torsions

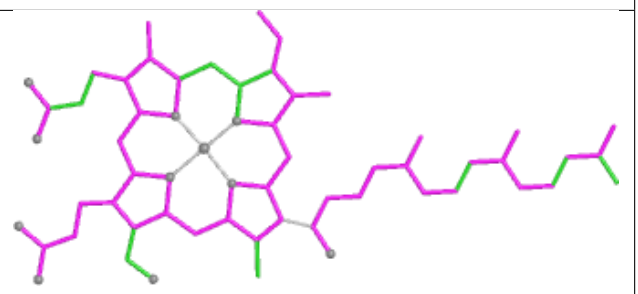


Rings

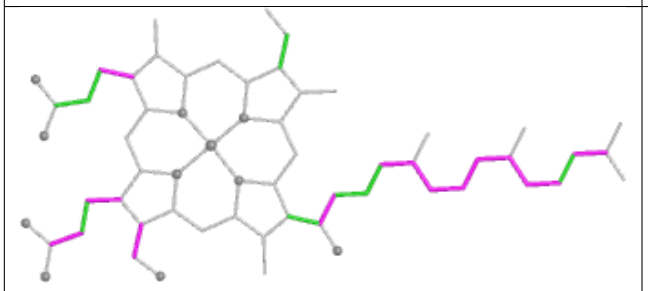
Ligand HEA F 607



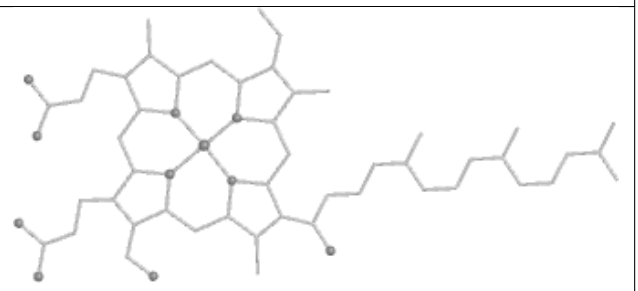
Bond lengths



Bond angles

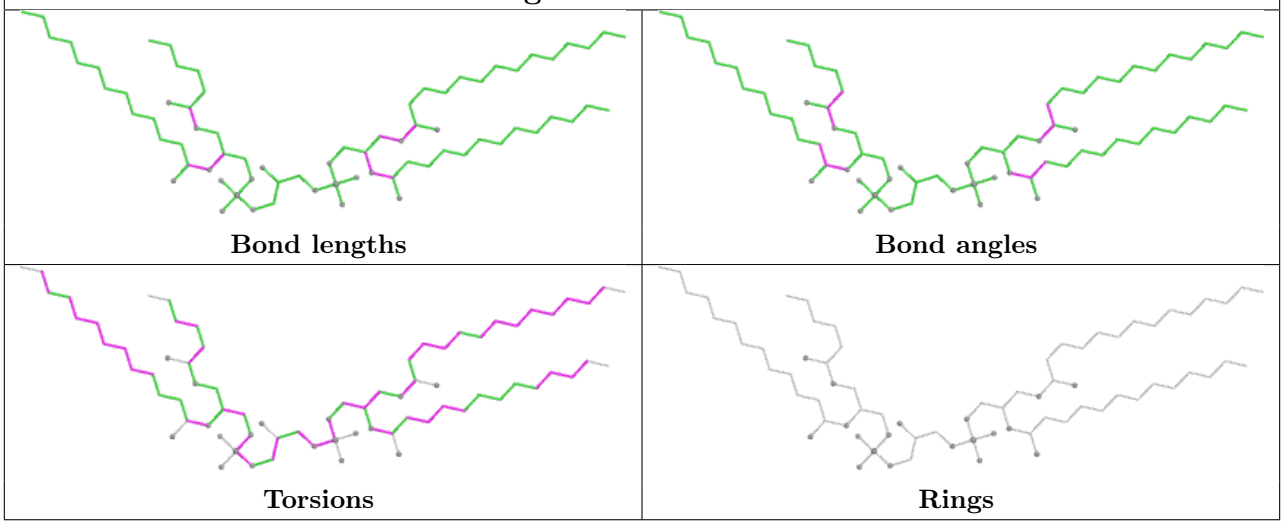


Torsions

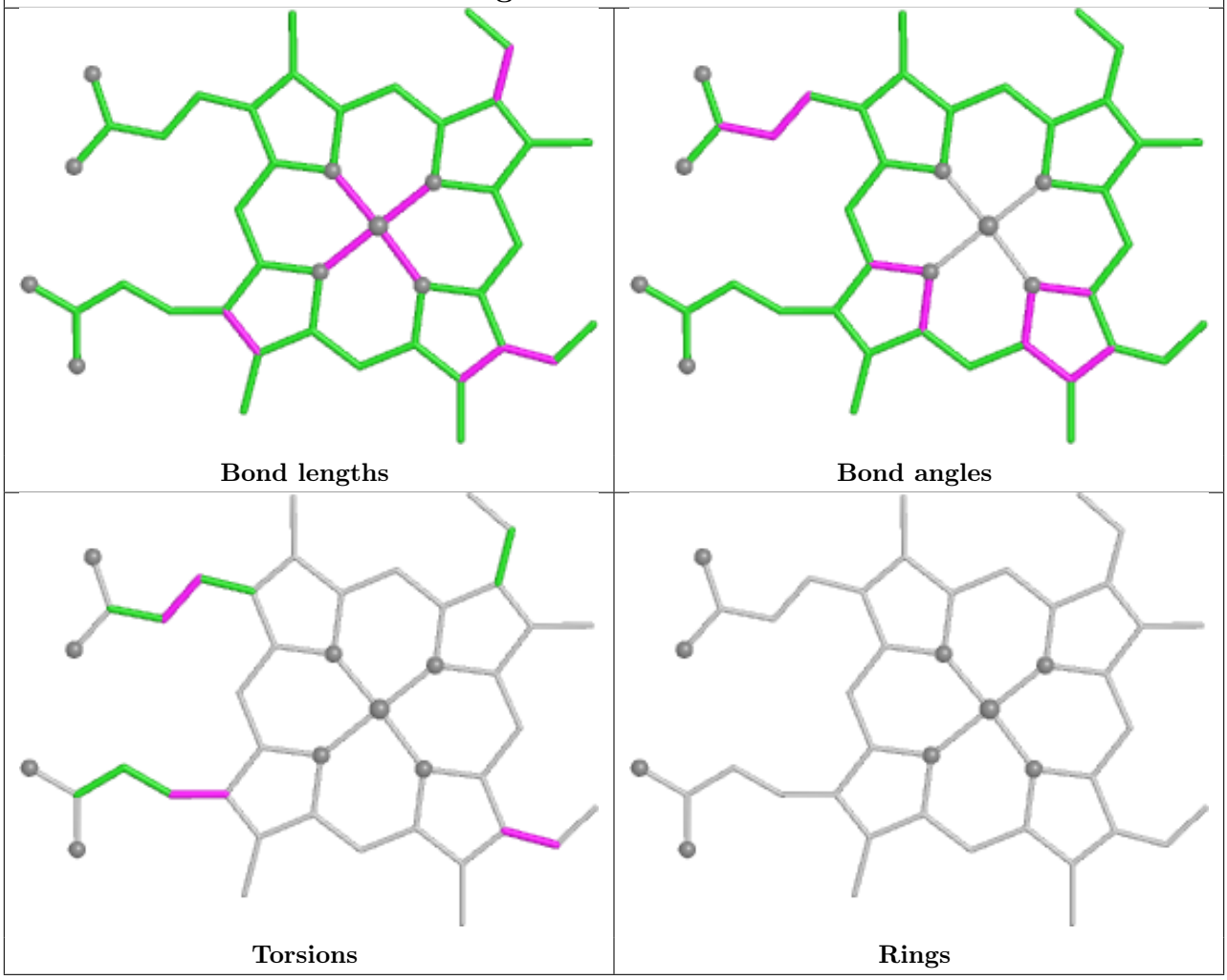


Rings

Ligand CDL N 604



Ligand HEM N 602



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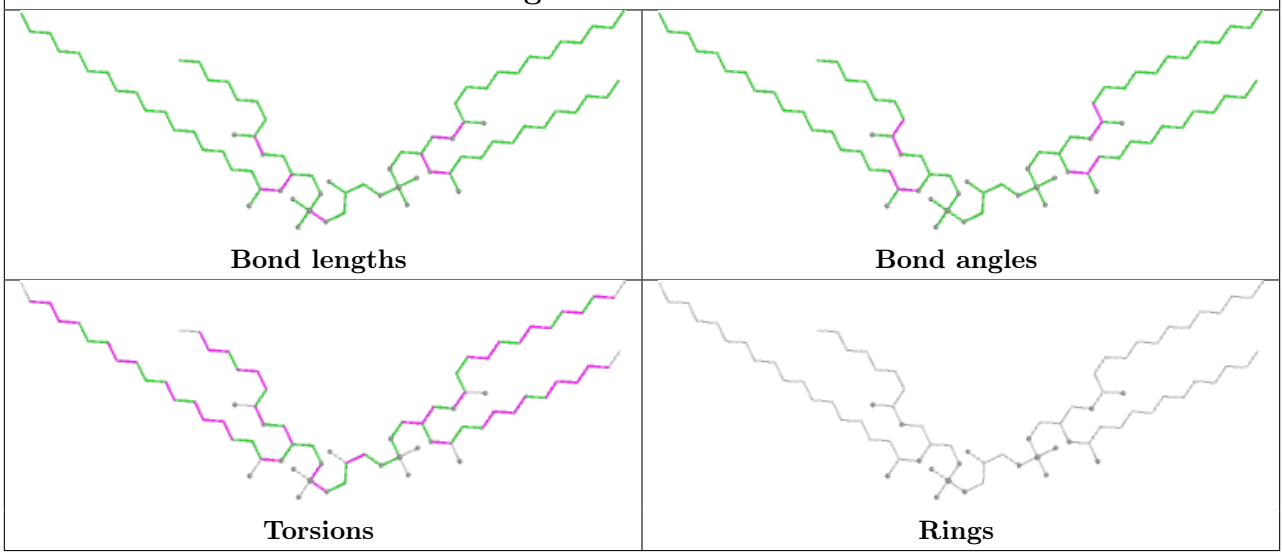
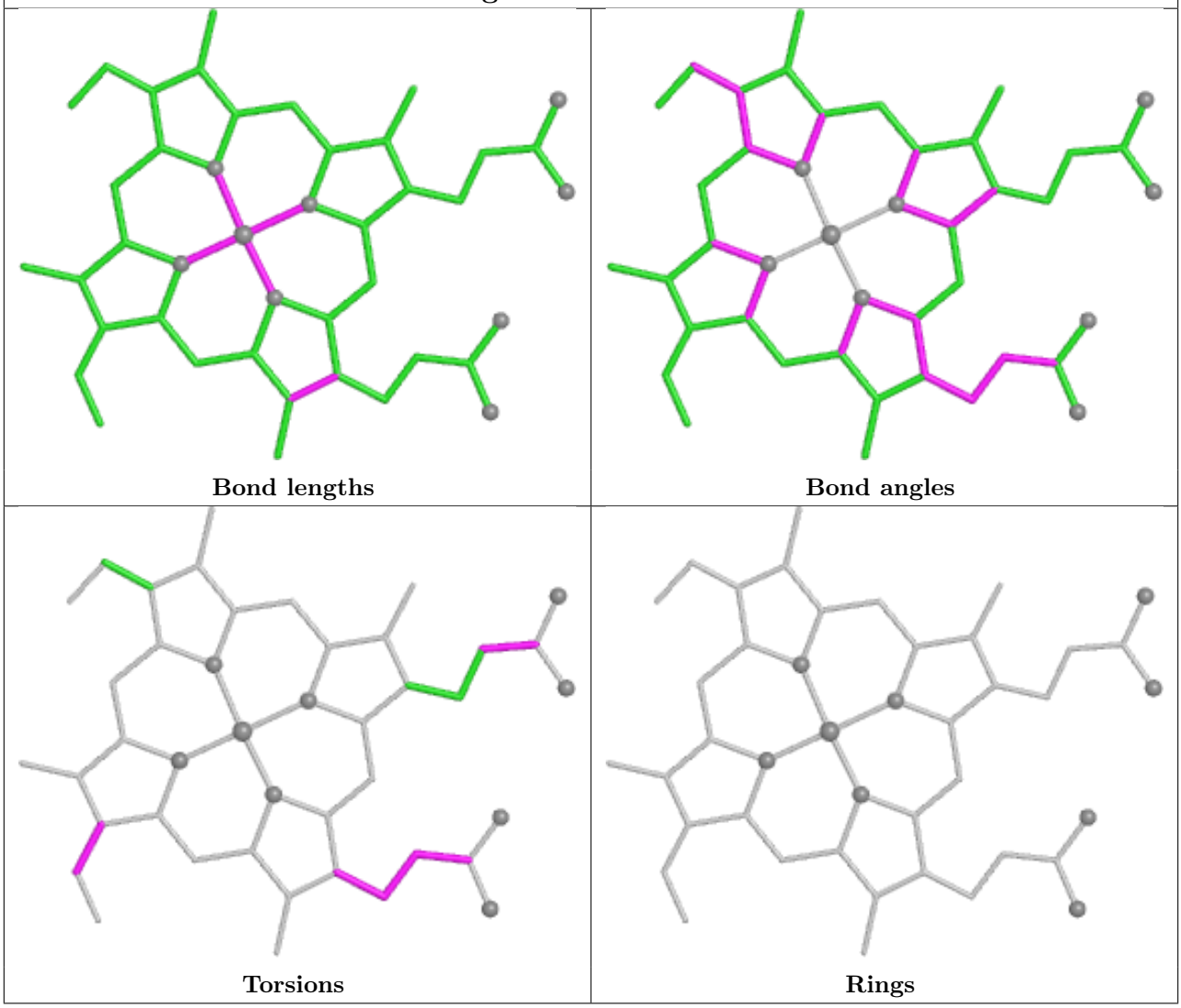
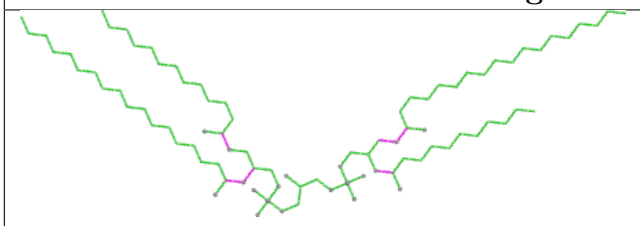
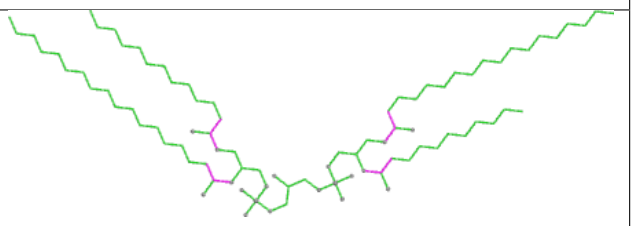
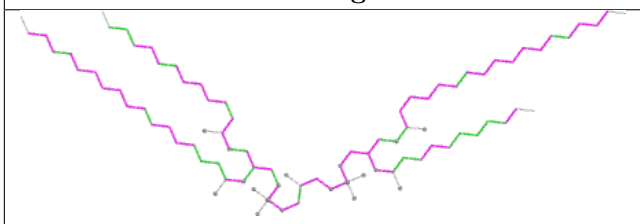
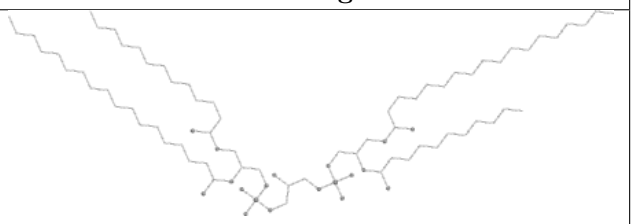
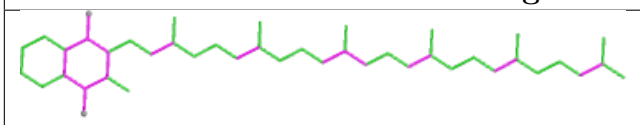
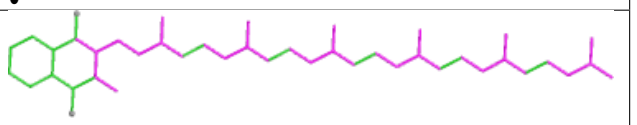
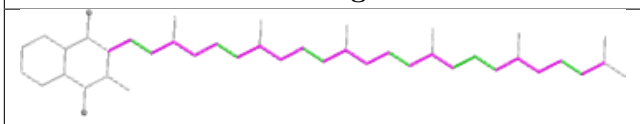
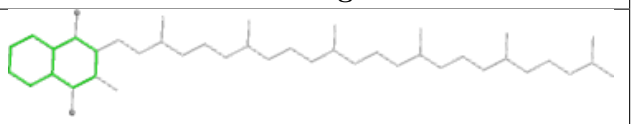


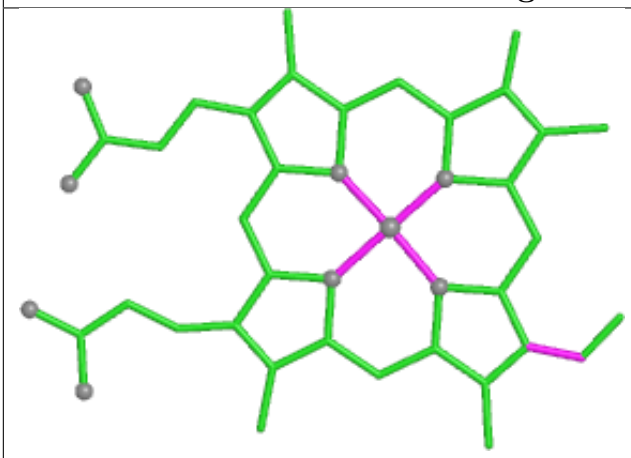
Ligand HEC C 301



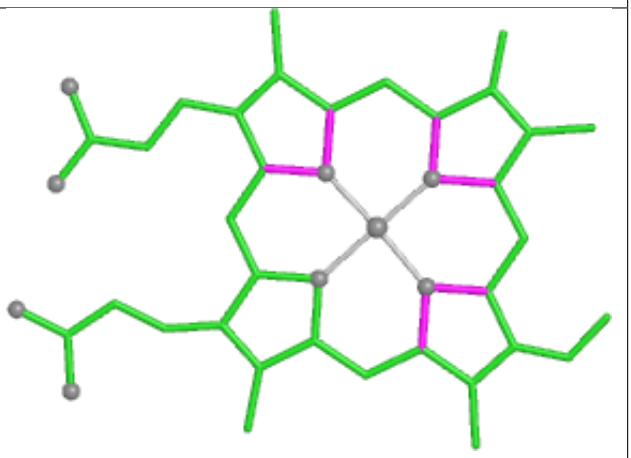
Ligand CDL P 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 A 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

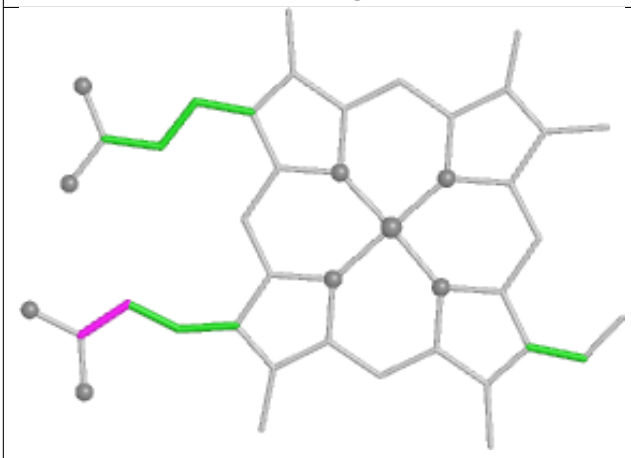
Ligand HEM N 601



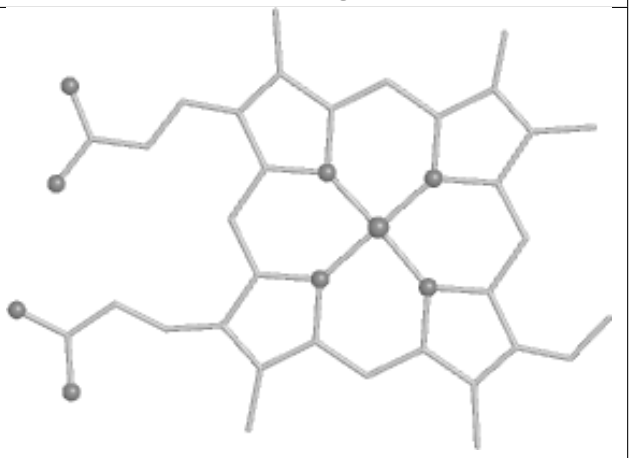
Bond lengths



Bond angles

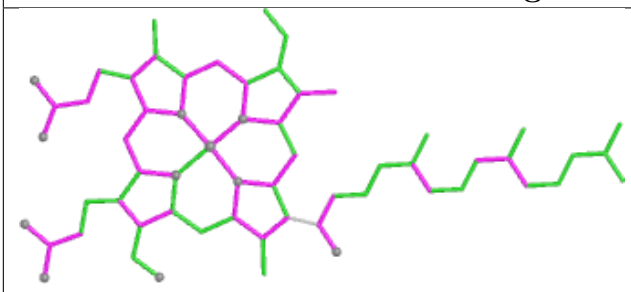


Torsions

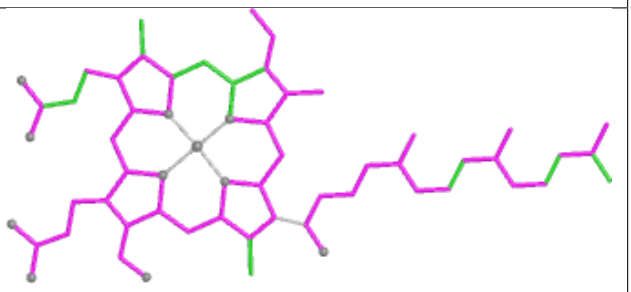


Rings

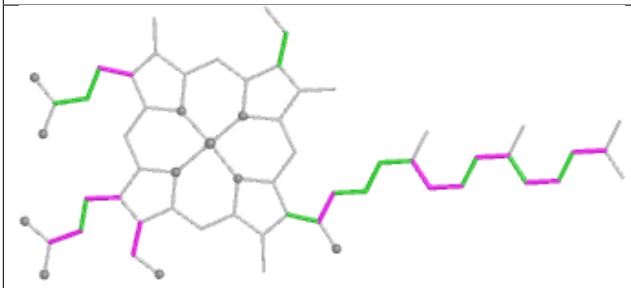
Ligand HEA F 606



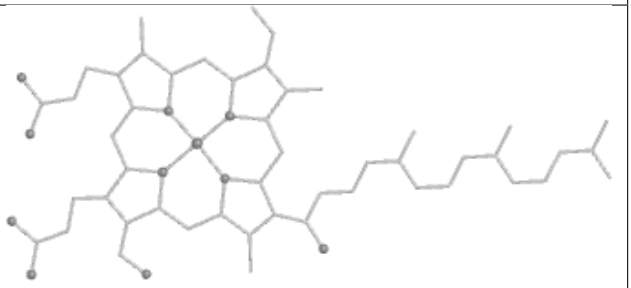
Bond lengths



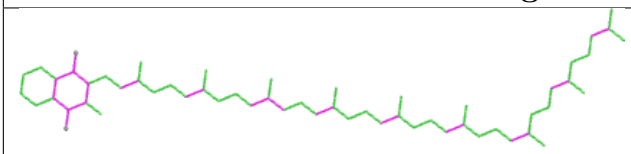
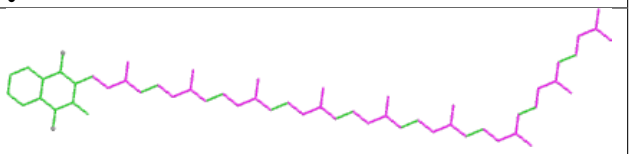
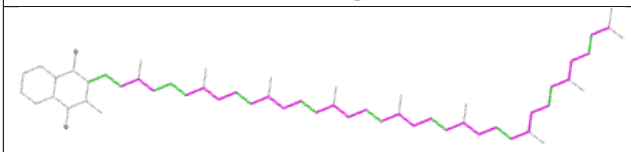
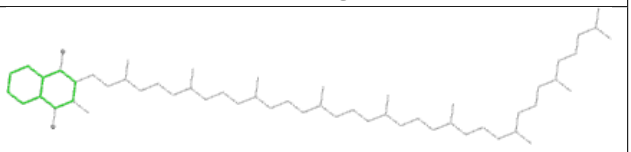
Bond angles

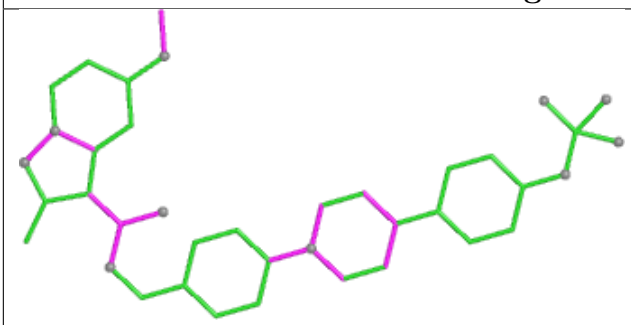
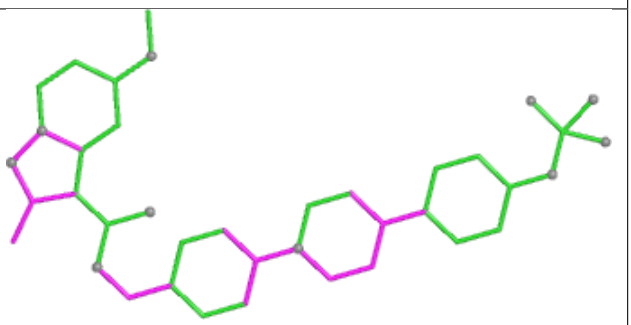
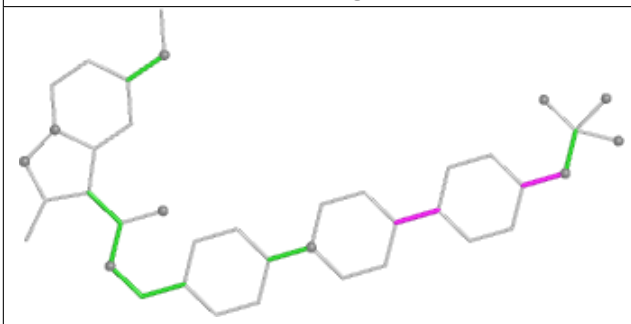
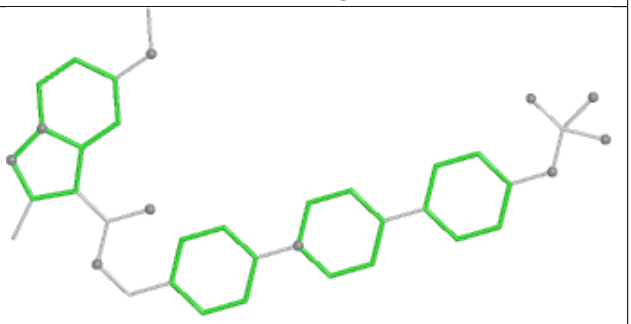


Torsions

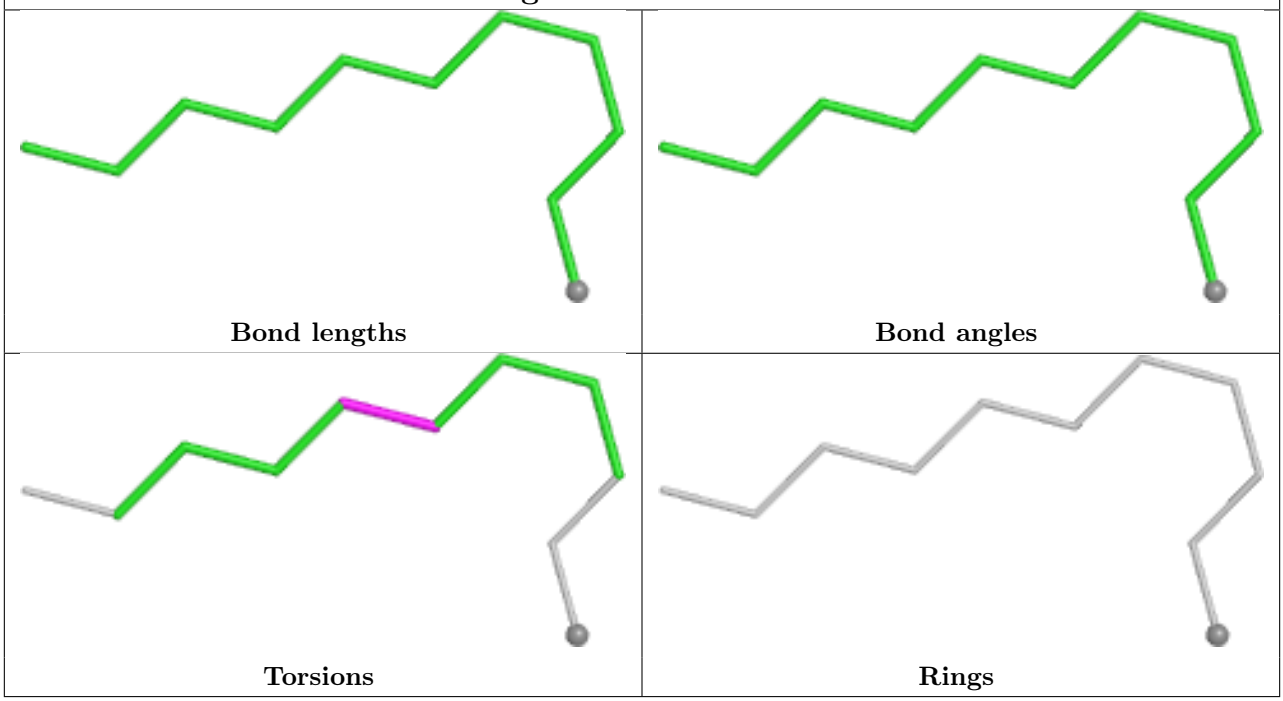


Rings

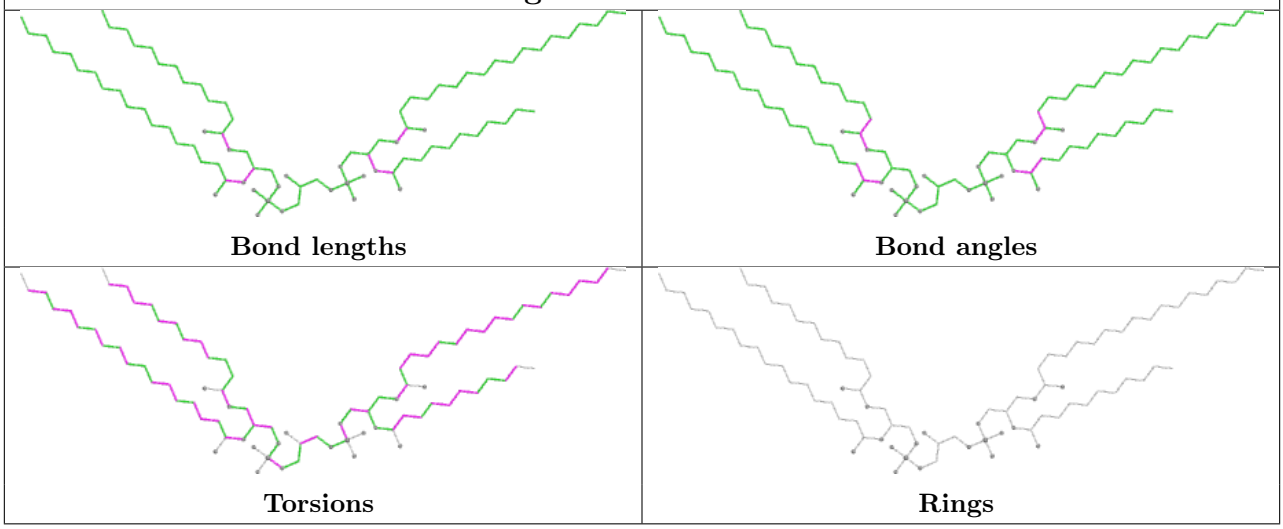
Ligand MQ9 N 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HV0 N 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

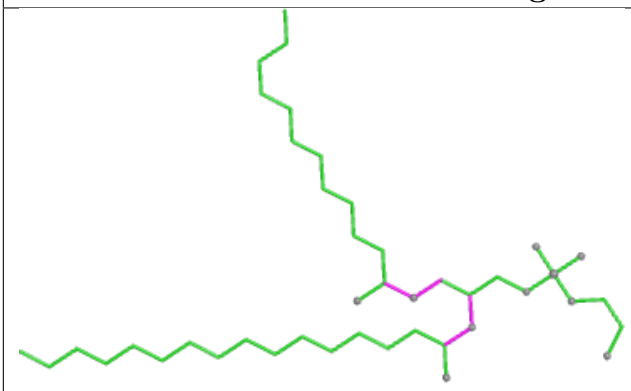
Ligand PLM N 603



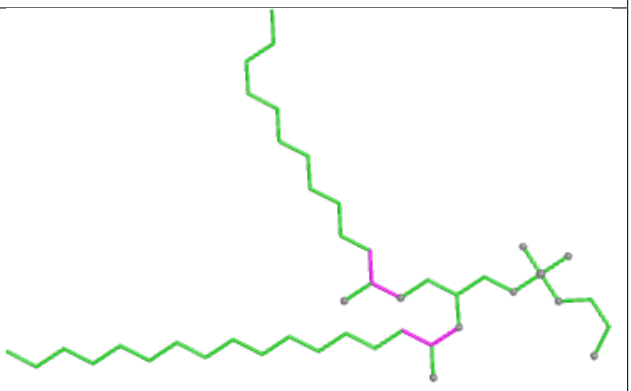
Ligand CDL D 201



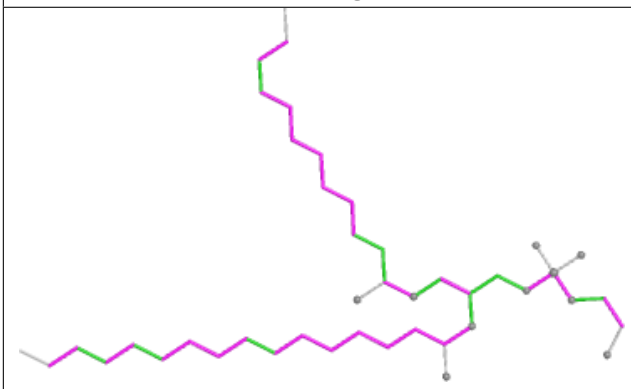
Ligand 9Y0 G 301



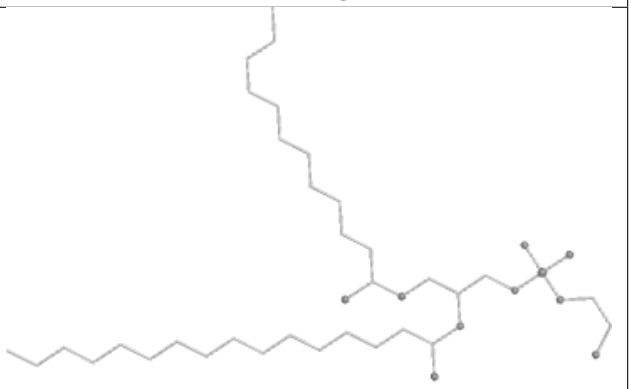
Bond lengths



Bond angles

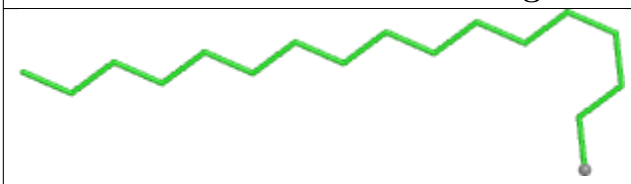


Torsions

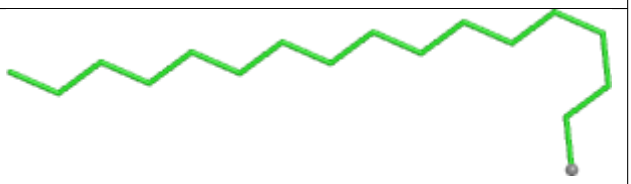


Rings

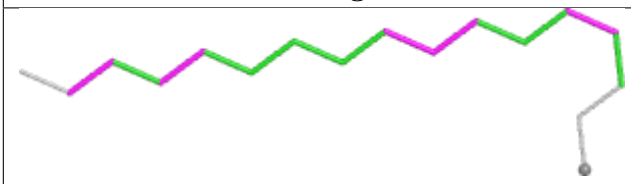
Ligand PLM F 603



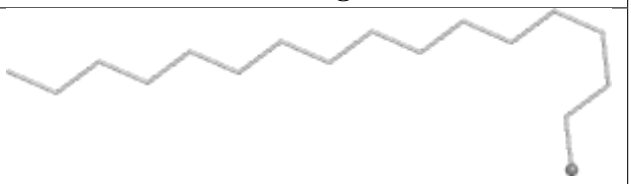
Bond lengths



Bond angles

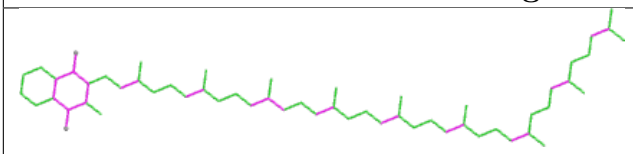


Torsions



Rings

Ligand MQ9 B 610



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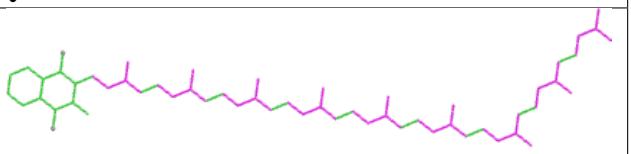
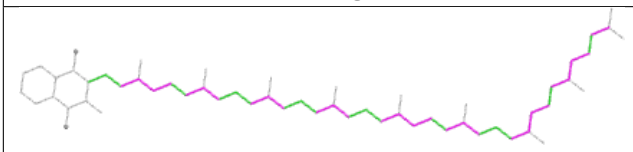


Bond angles



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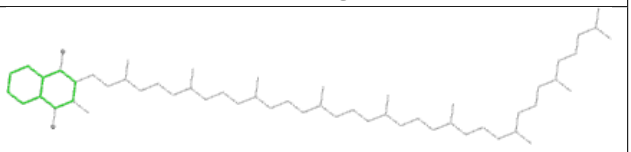
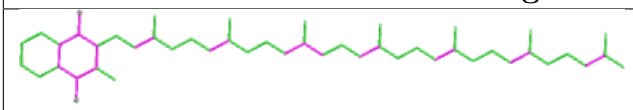


Rings

Ligand MQ9 C 303



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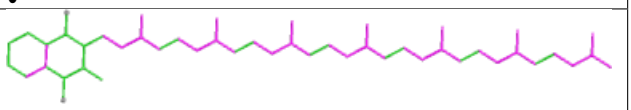
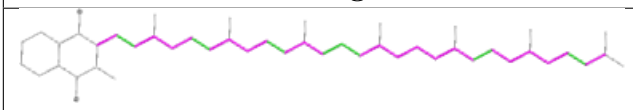


Bond angles



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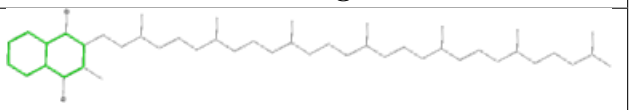
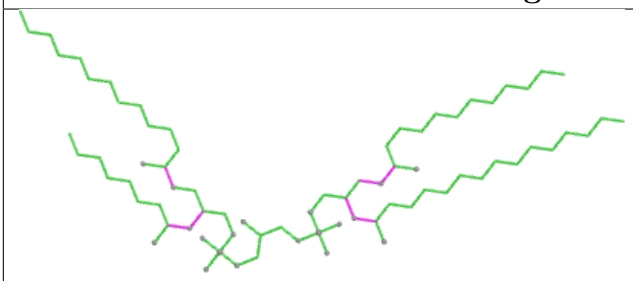


Rings

Ligand CDL R 601



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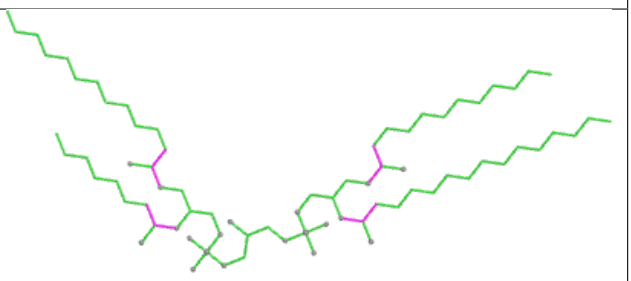
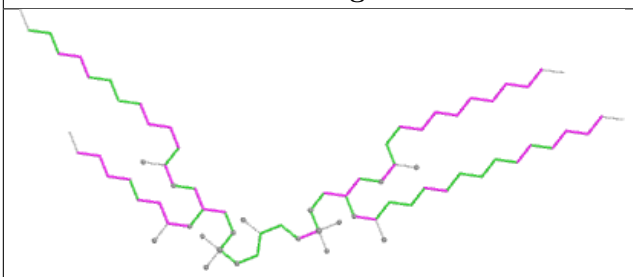


Bond angles



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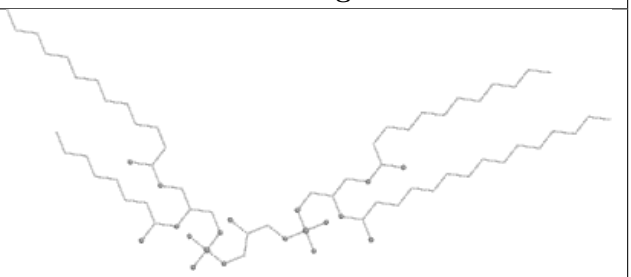
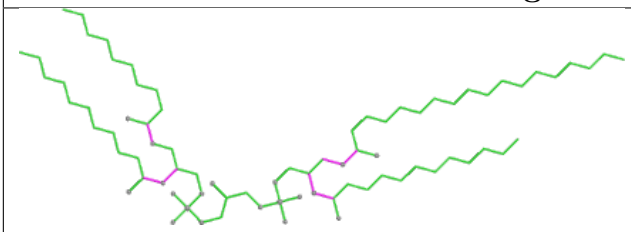
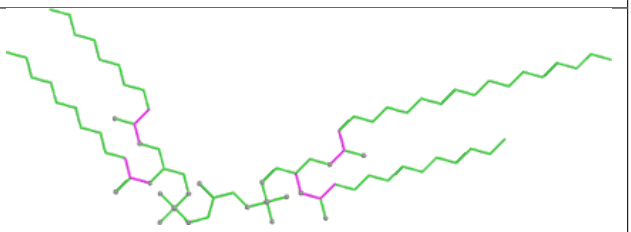
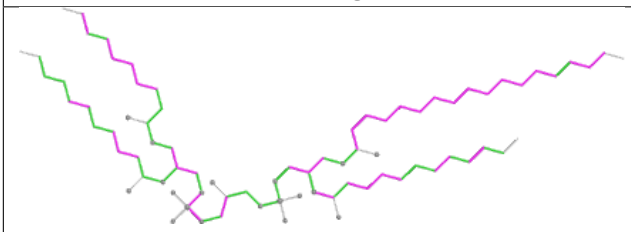
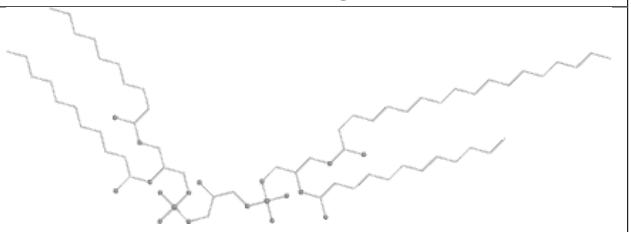
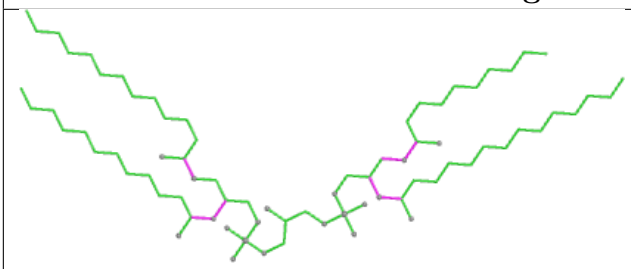
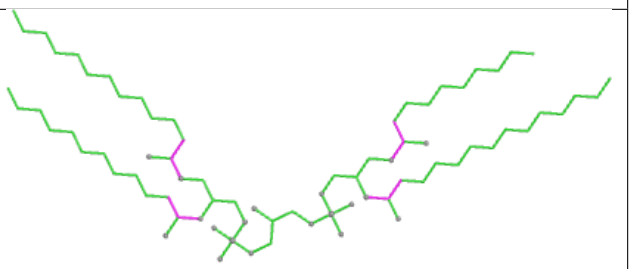
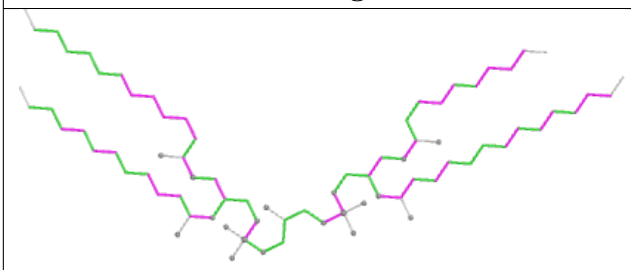
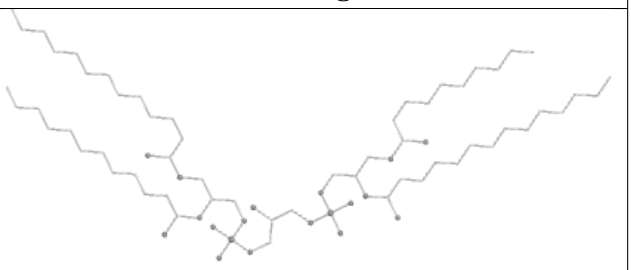
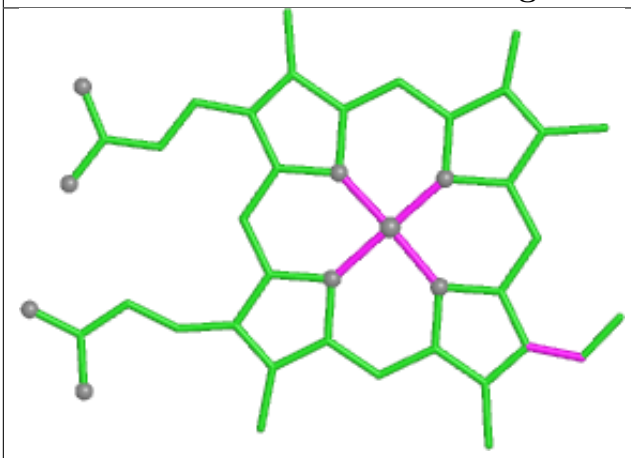


Rings

Ligand CDL O 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM B 601



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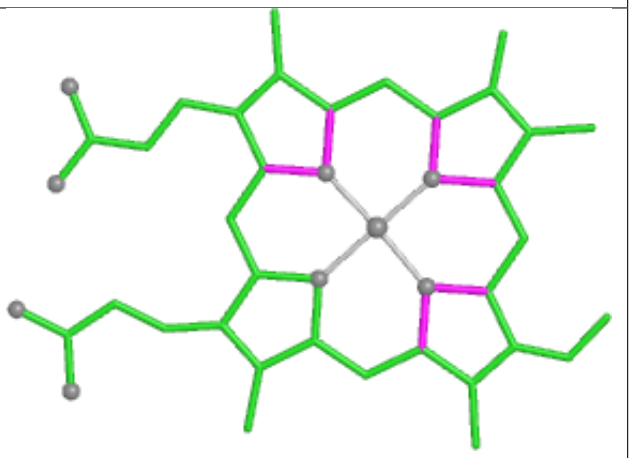
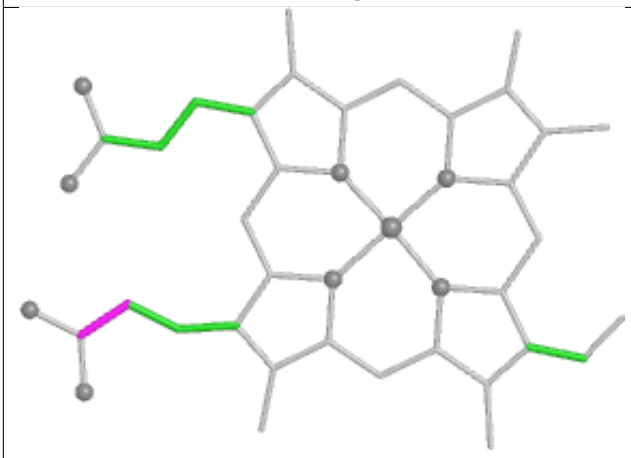


Bond angles



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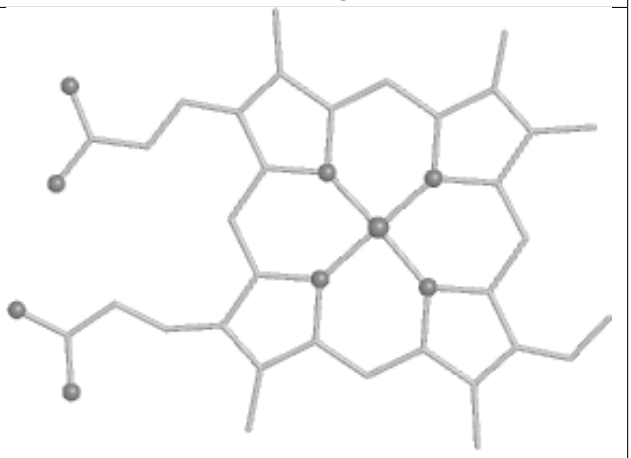
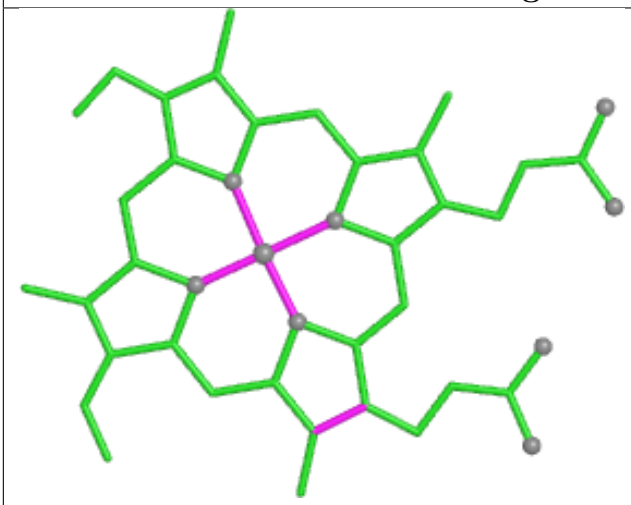


Rings

Ligand HEC O 304



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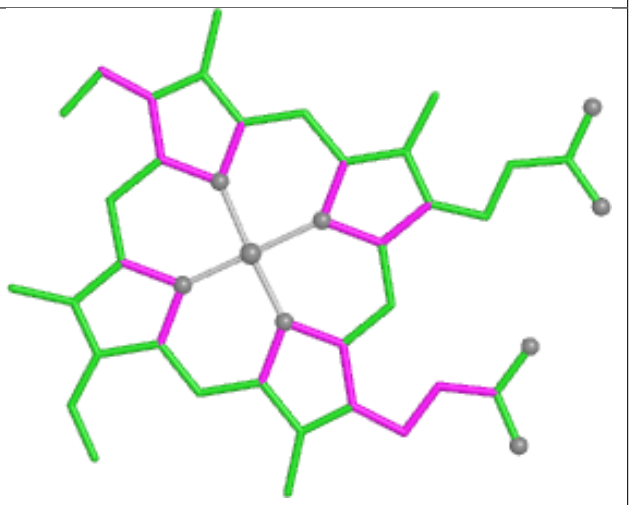
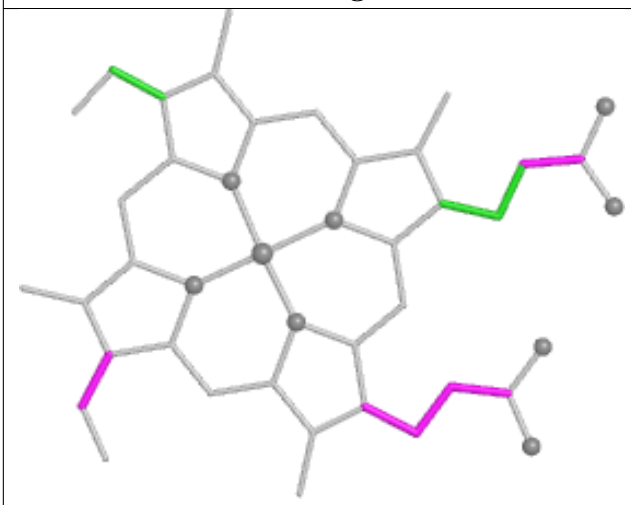
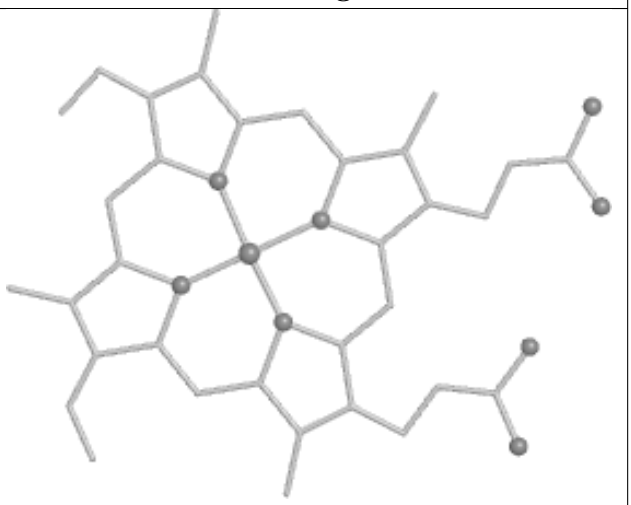


Bond angles

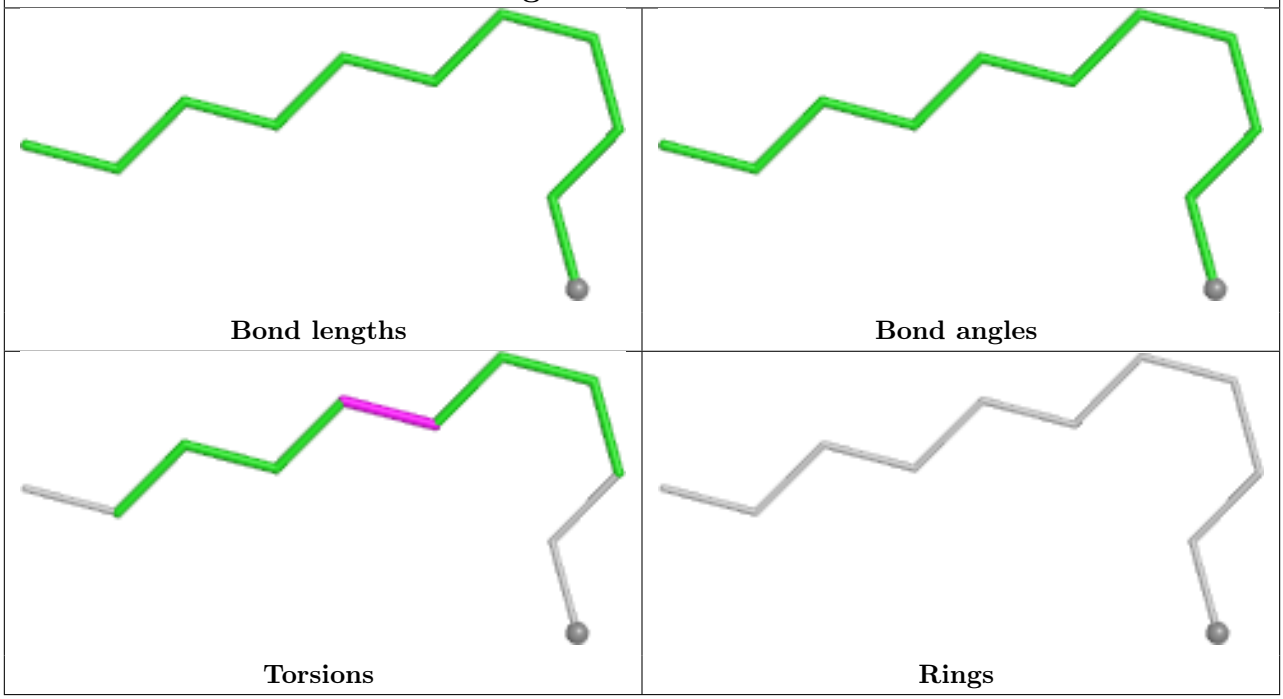


Torsions

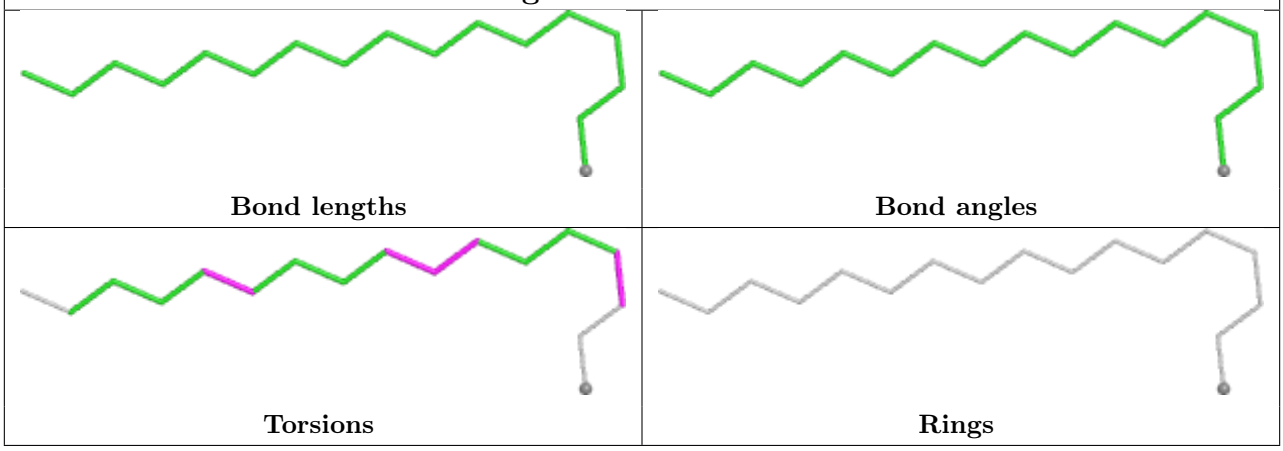


Rings

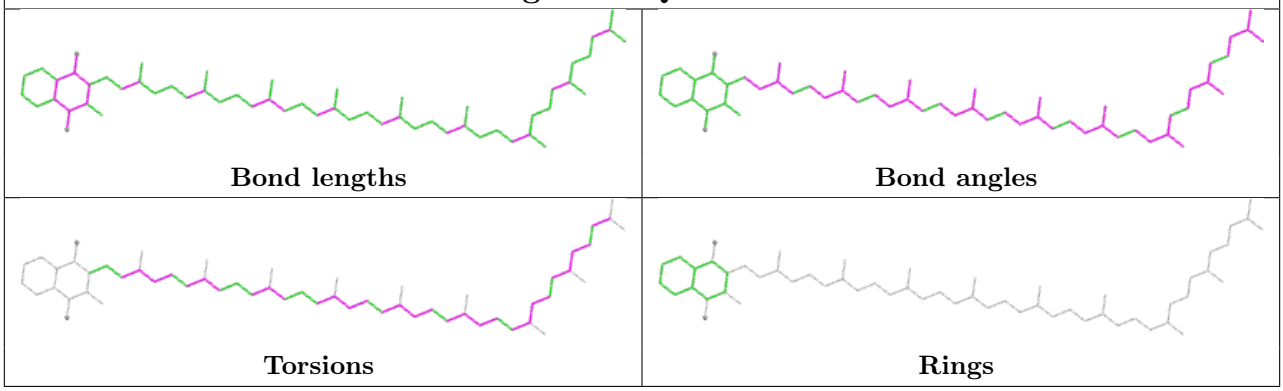
Ligand PLM B 604



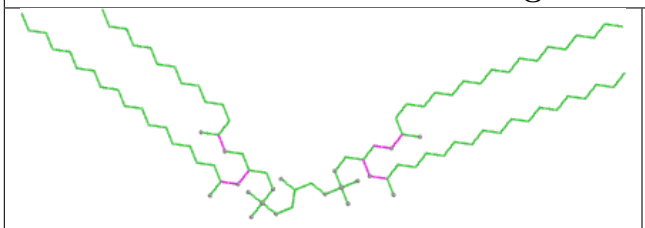
Ligand PLM R 603



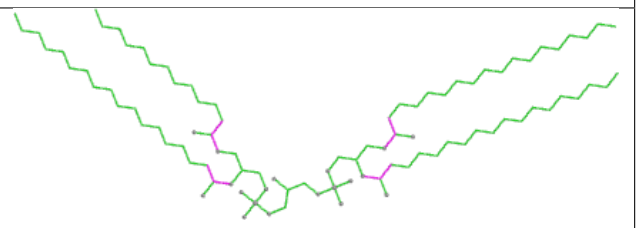
Ligand MQ9 O 303



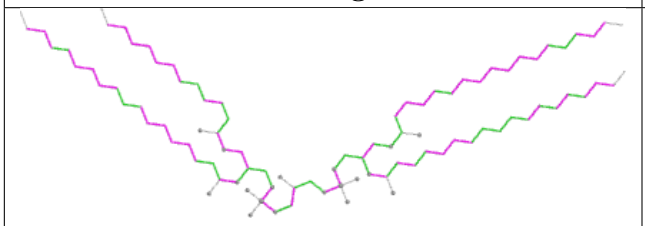
Ligand CDL A 504



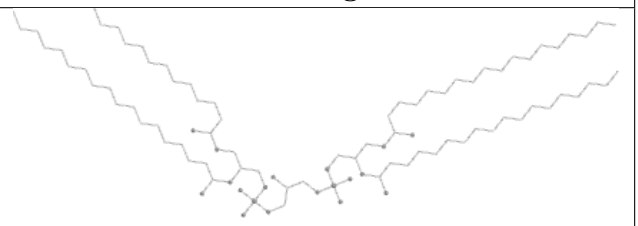
Bond lengths



Bond angles

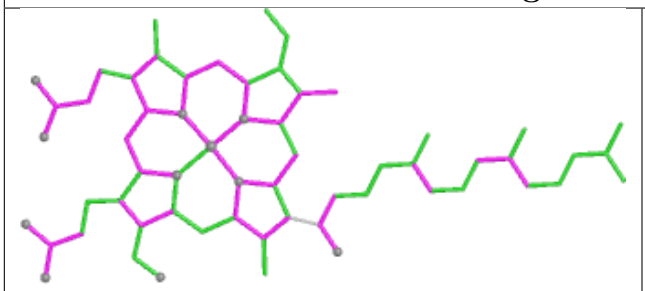


Torsions



Rings

Ligand HEA R 606



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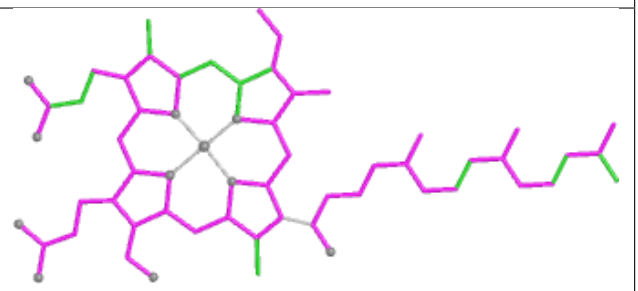
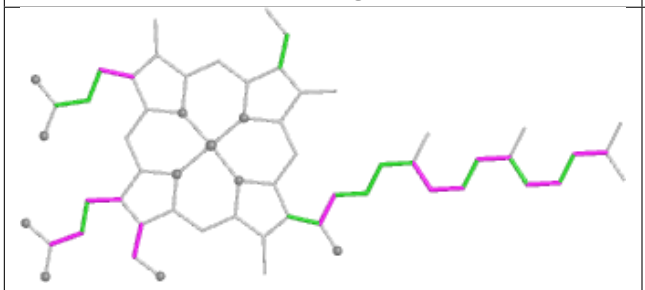
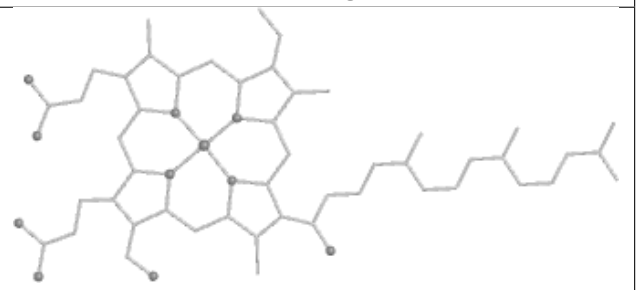


Bond angles

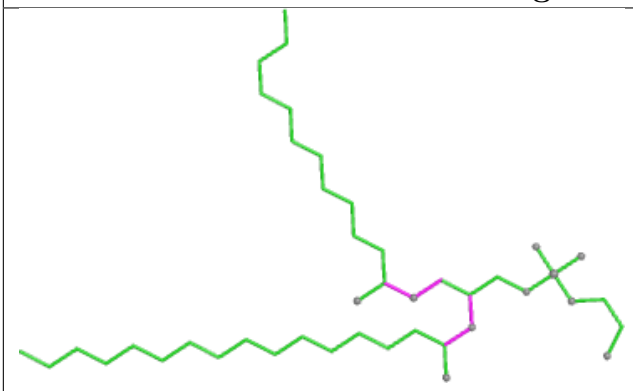


Torsions

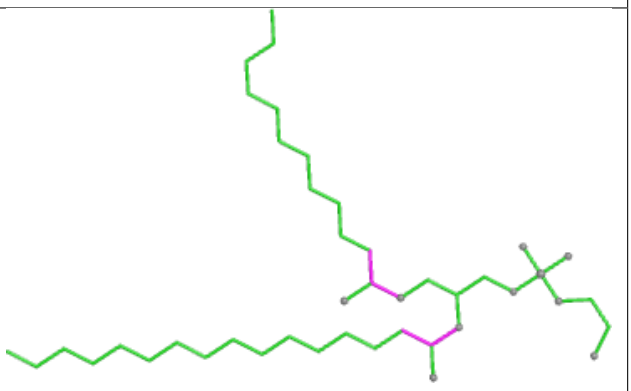


Rings

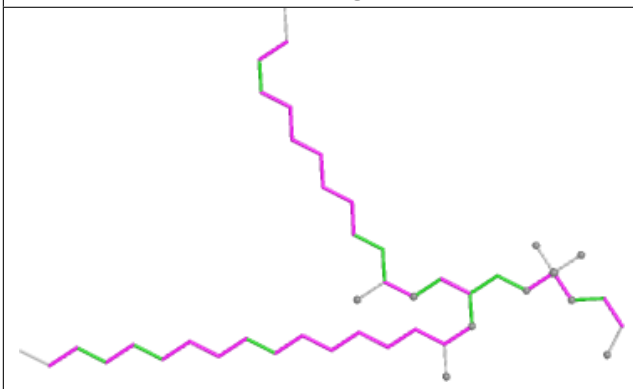
Ligand 9Y0 S 301



Bond lengths



Bond angles



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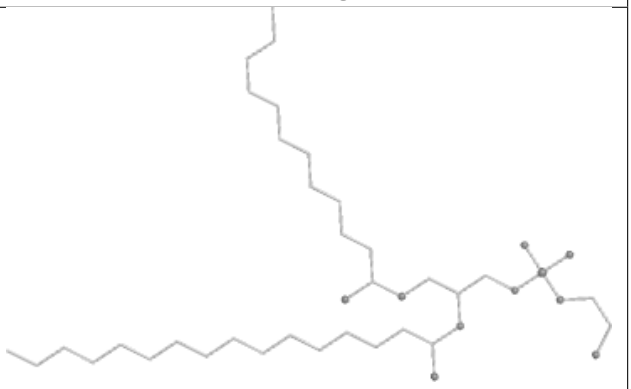
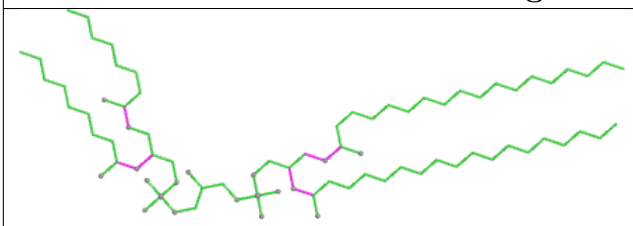


Rings

Ligand CDL F 602



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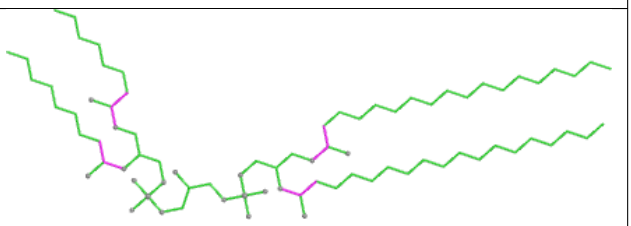
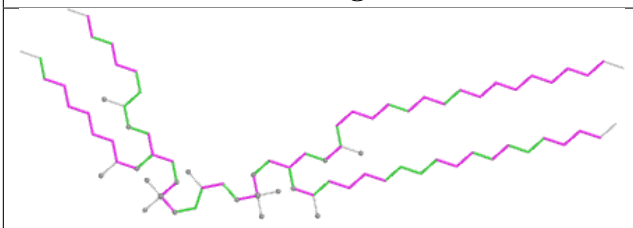
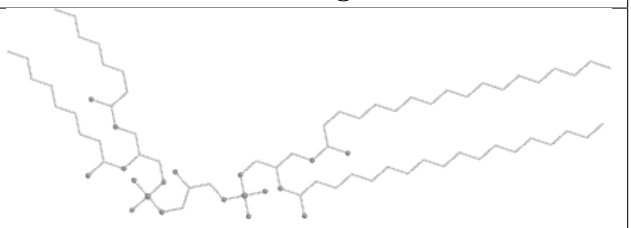


Bond angles

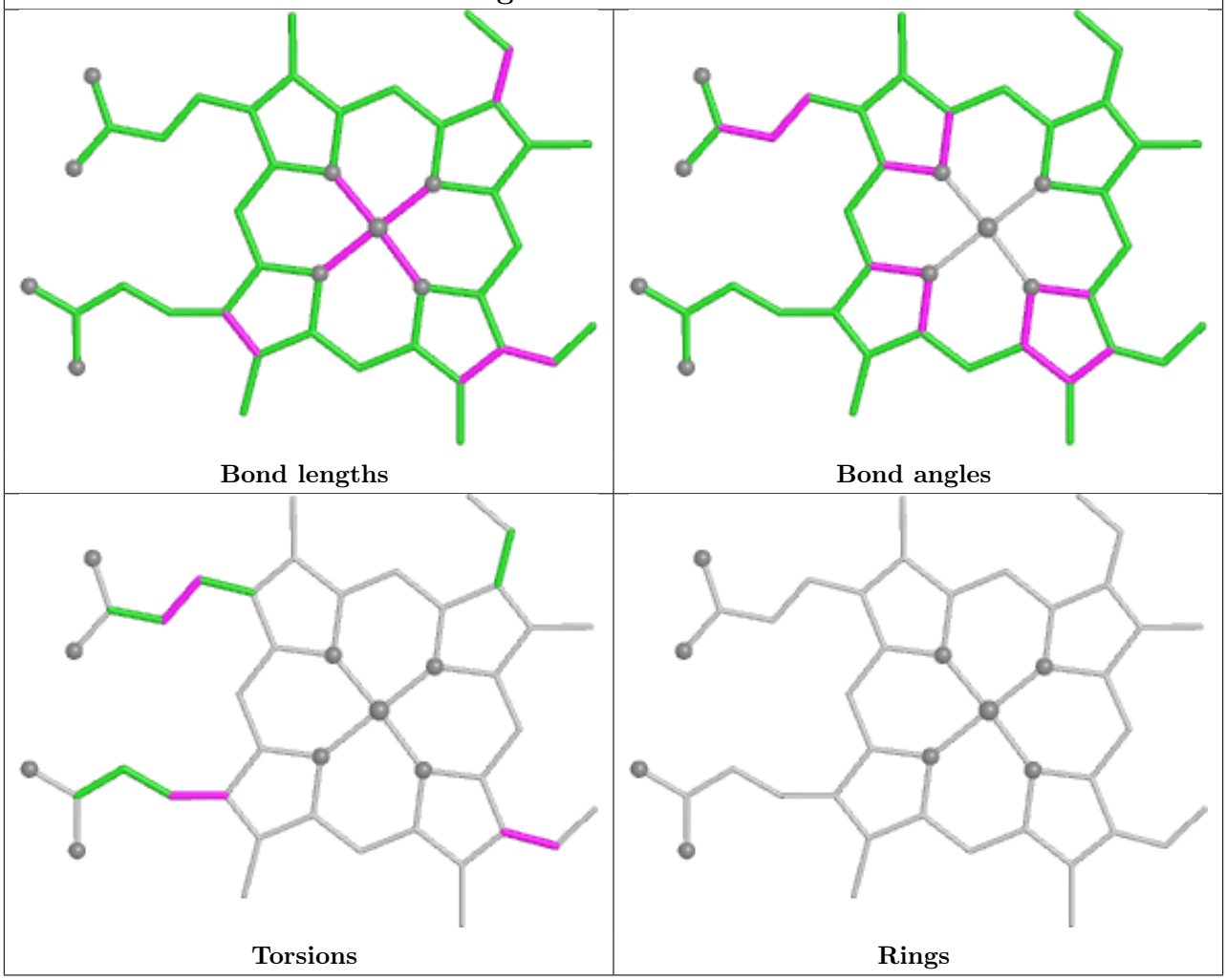


Torsions

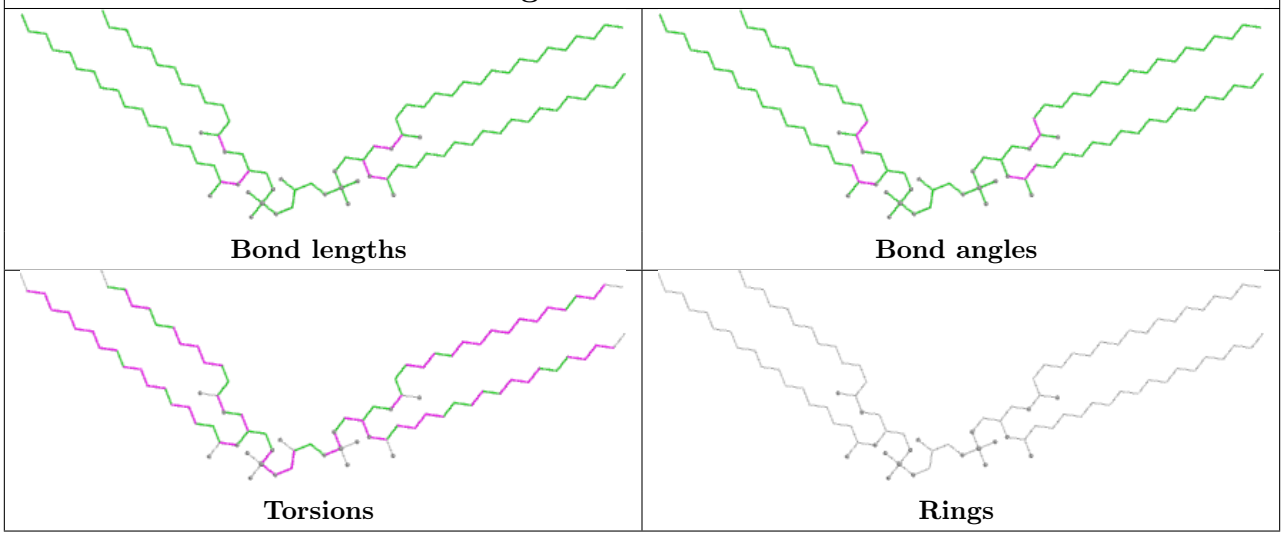


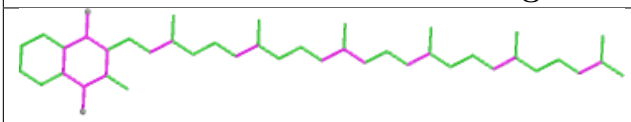
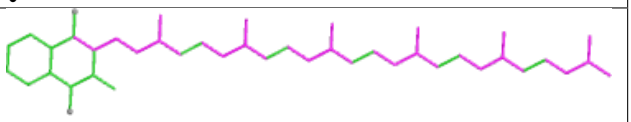
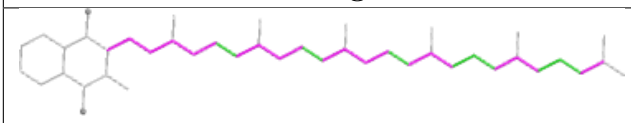
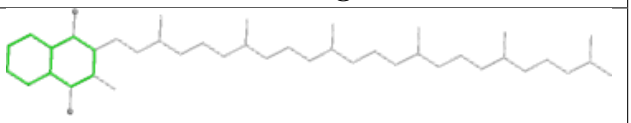
Rings

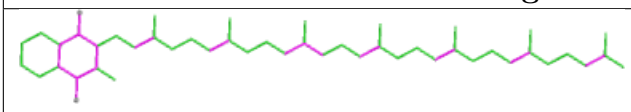
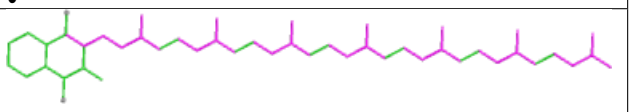
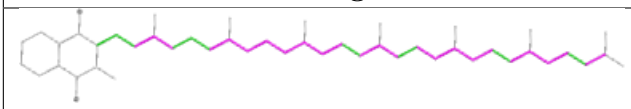
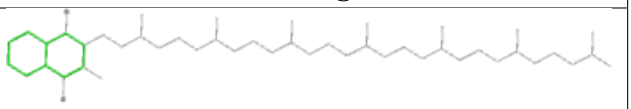
Ligand HEM B 602

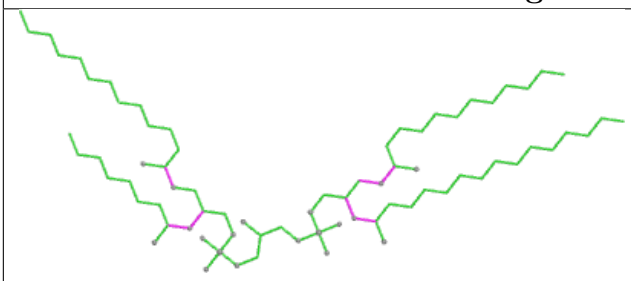
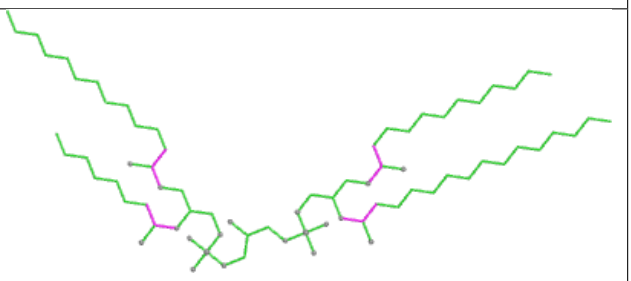
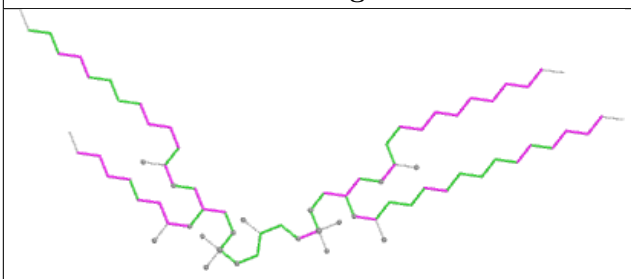
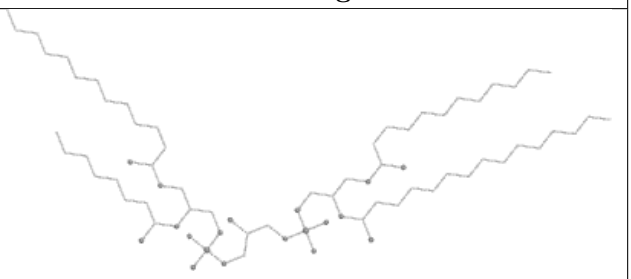


Ligand CDL M 502

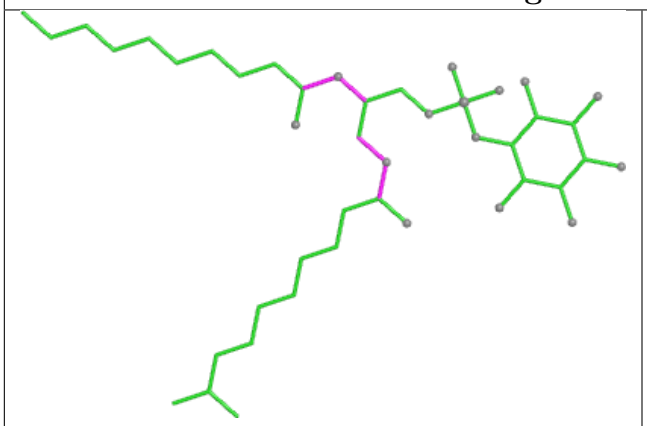


Ligand MQ9 B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

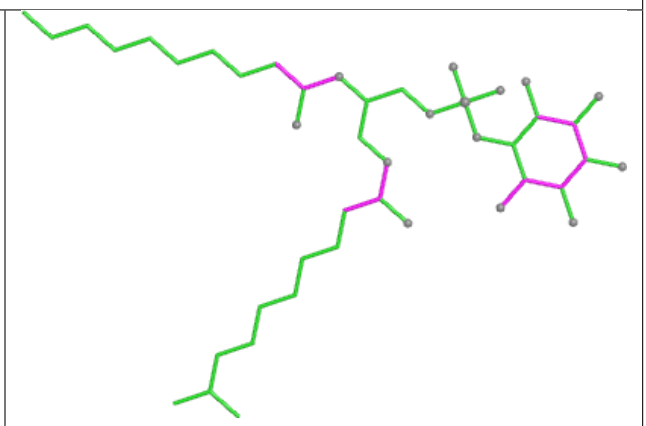
Ligand MQ9 O 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL F 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

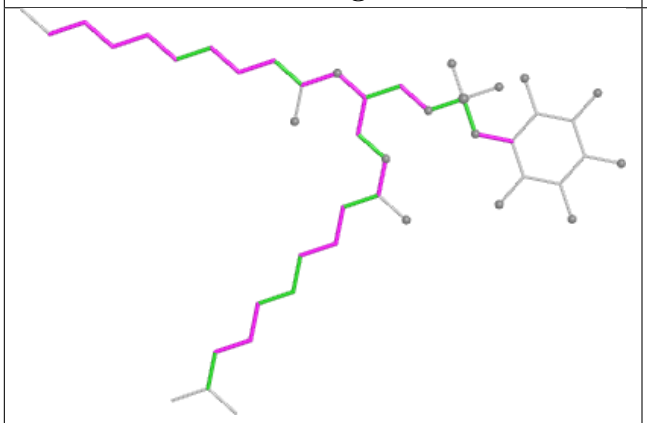
Ligand 9YF M 503



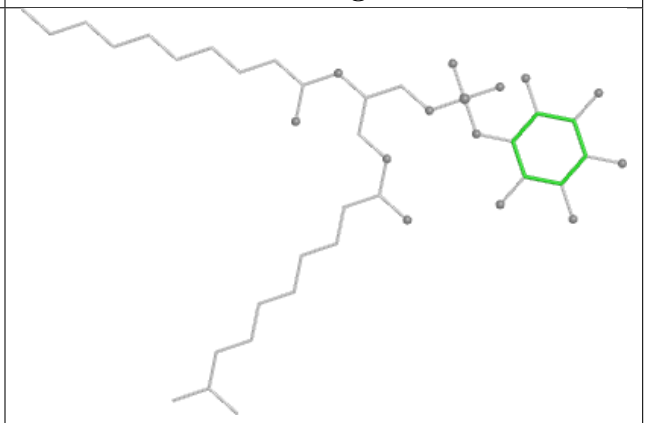
Bond lengths



Bond angles

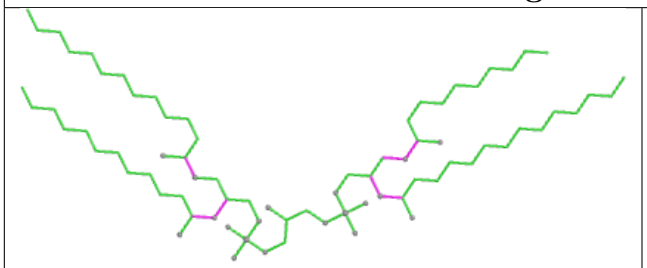


Torsions

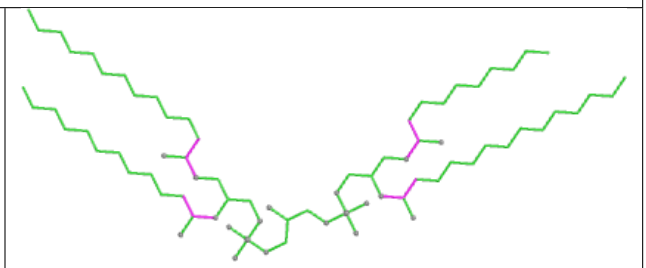


Rings

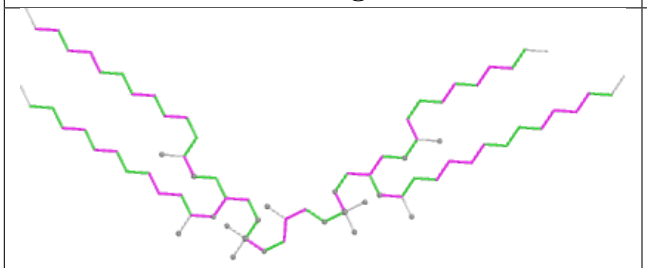
Ligand CDL B 607



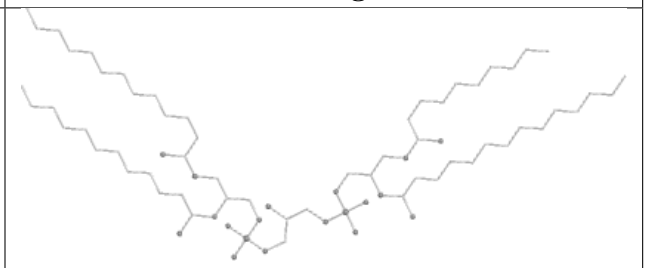
Bond lengths



Bond angles

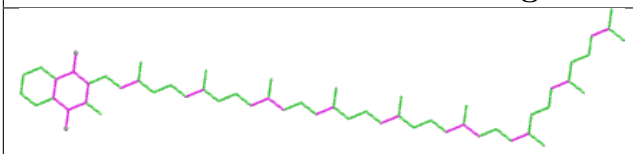


Torsions

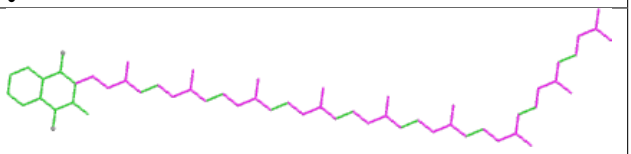


Rings

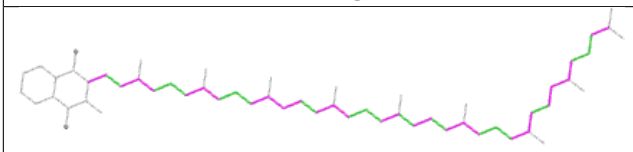
Ligand MQ9 N 608



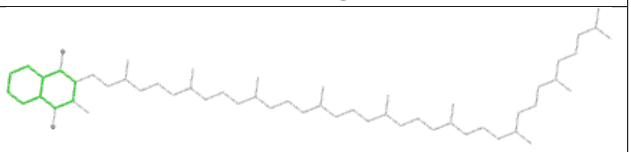
Bond lengths



Bond angles

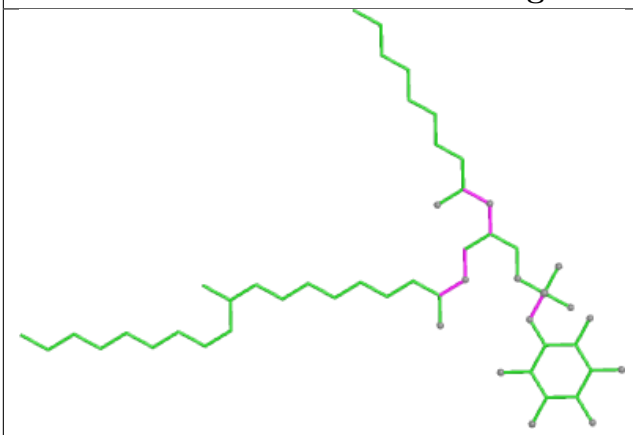


Torsions

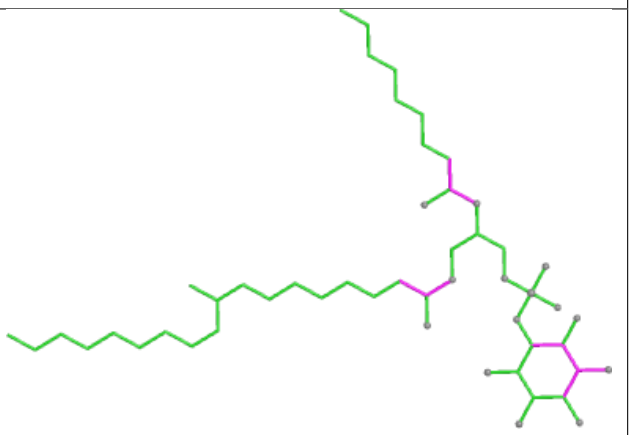


Rings

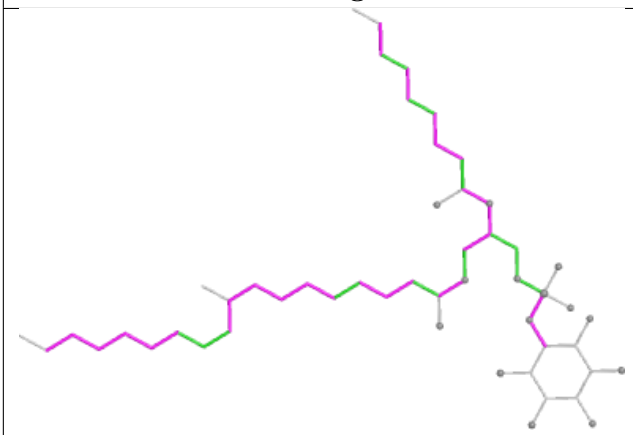
Ligand 9YF A 503



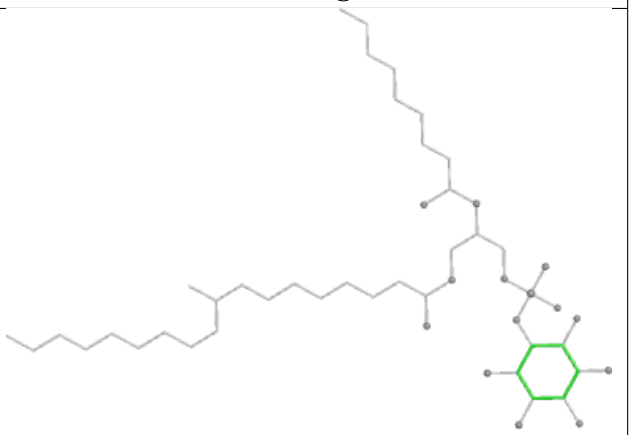
Bond lengths



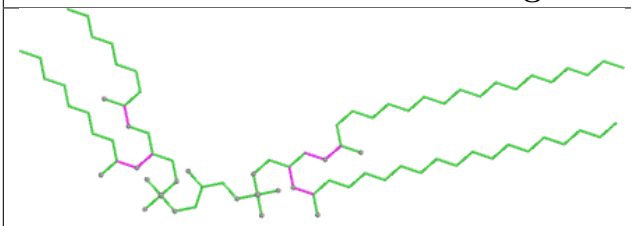
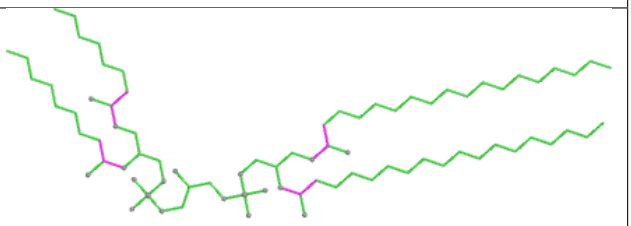
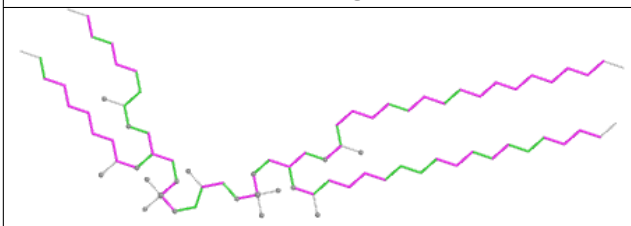
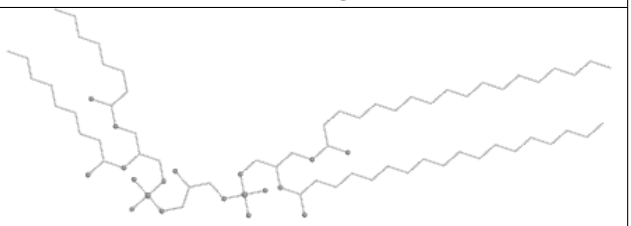
Bond angles



Torsions



Rings

Ligand CDL R 602	
 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.

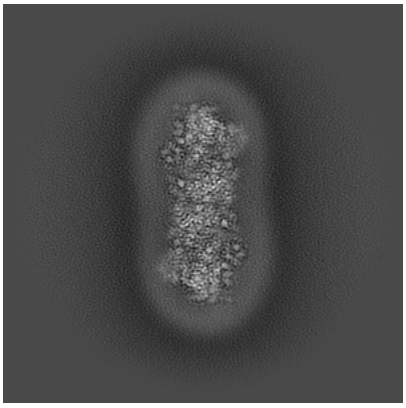
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30945. These allow visual inspection of the internal detail of the map and identification of artifacts.

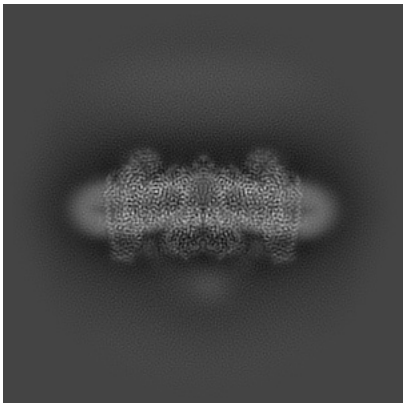
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

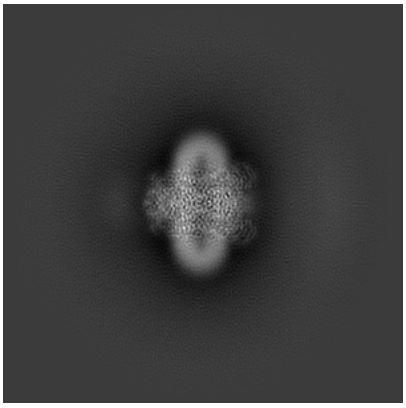
6.1.1 Primary map



X



Y

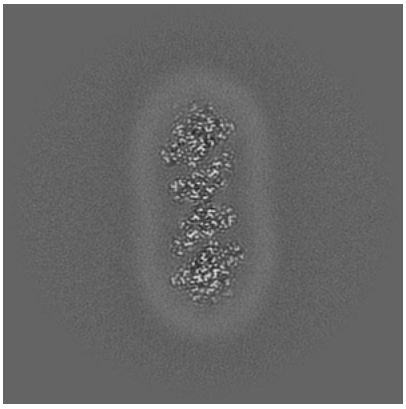


Z

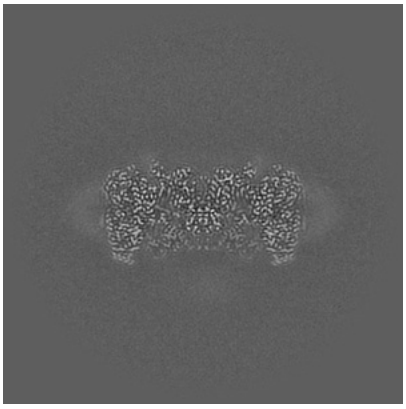
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

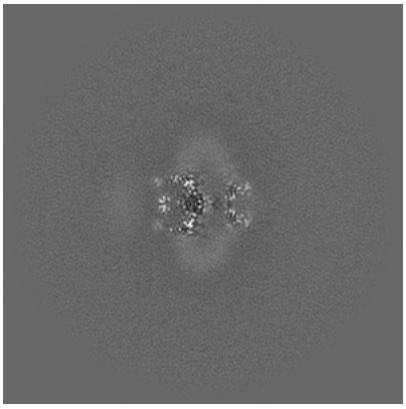
6.2.1 Primary map



X Index: 256



Y Index: 256

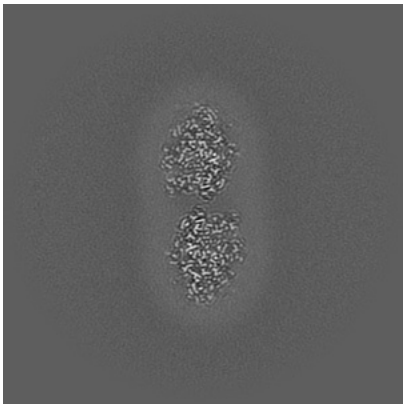


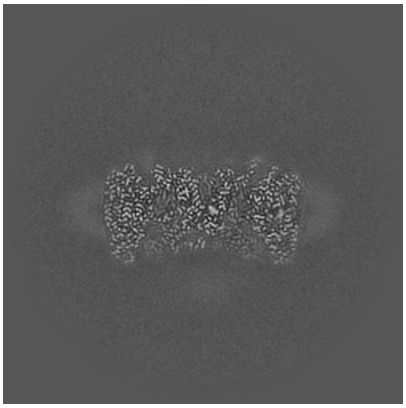
Z Index: 256

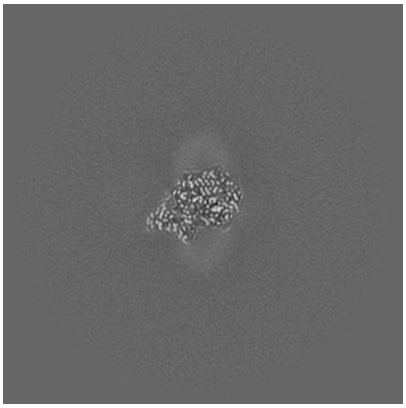
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 275

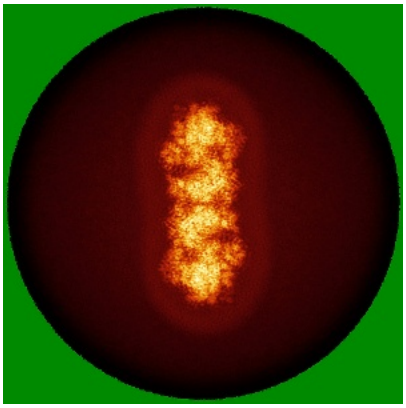

Y Index: 252

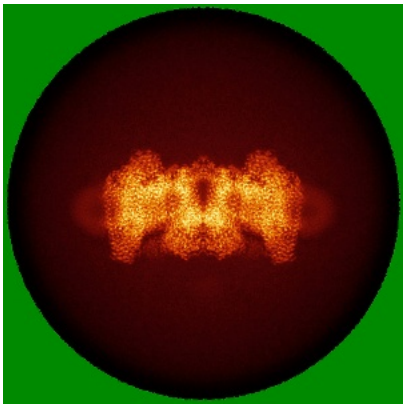

Z Index: 233

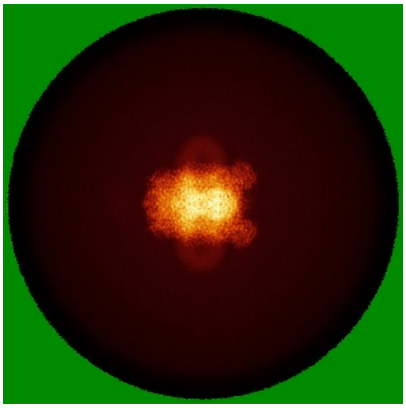
The images above show the largest variance slices of the map in three orthogonal directions.

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.

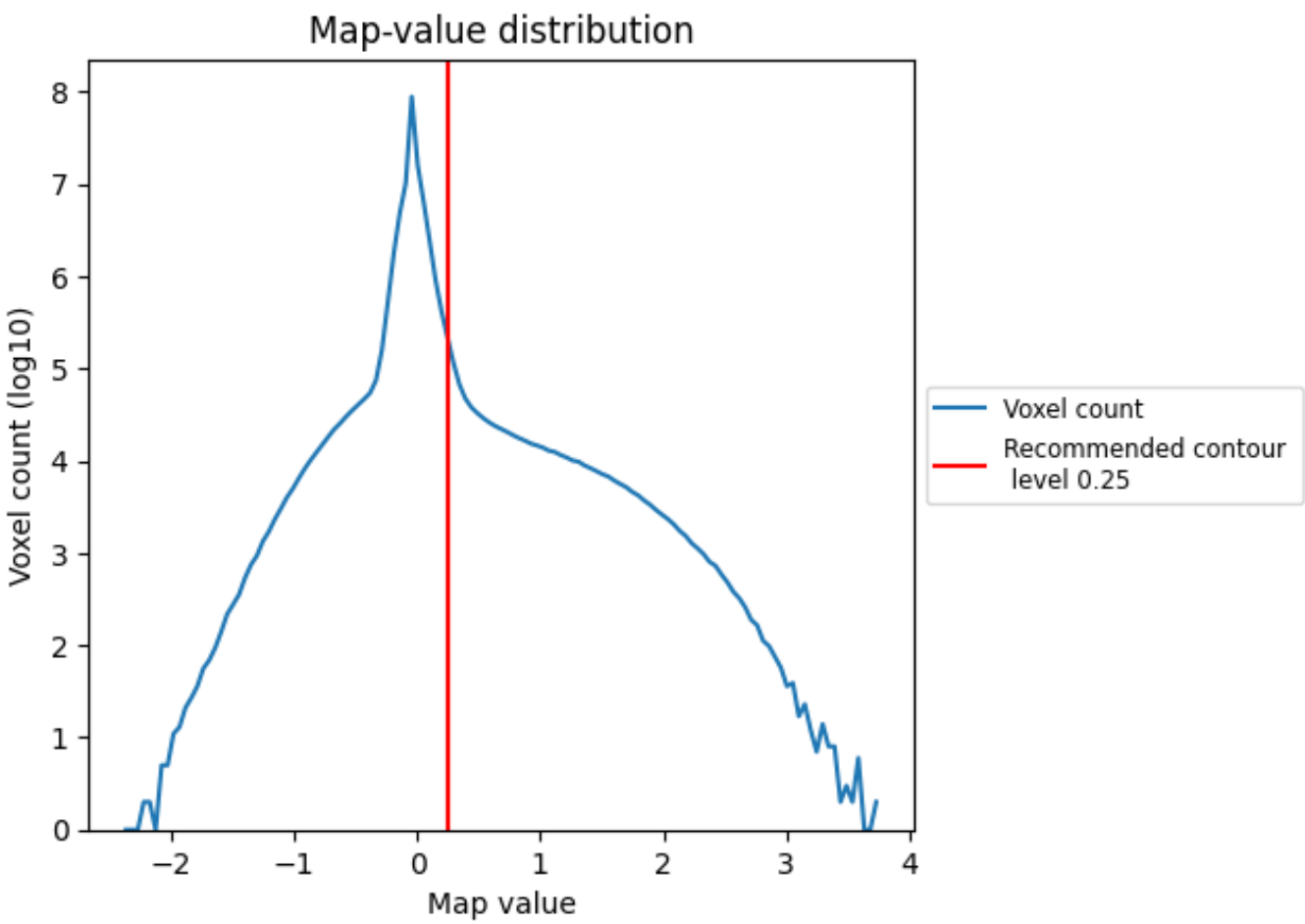
6.6 Mask visualisation (i)

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

7 Map analysis (i)

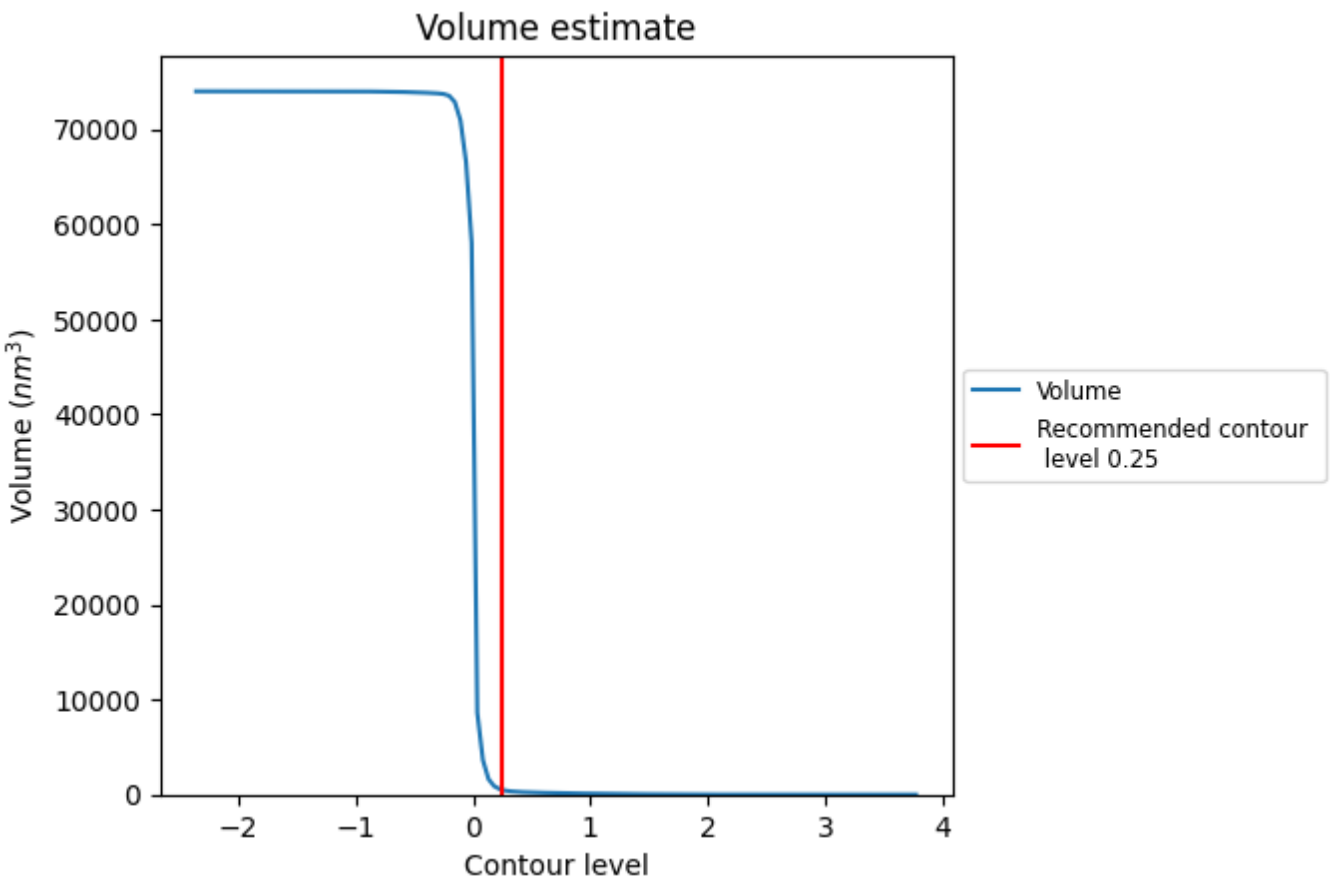
This section contains the results of statistical analysis of the map.

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.

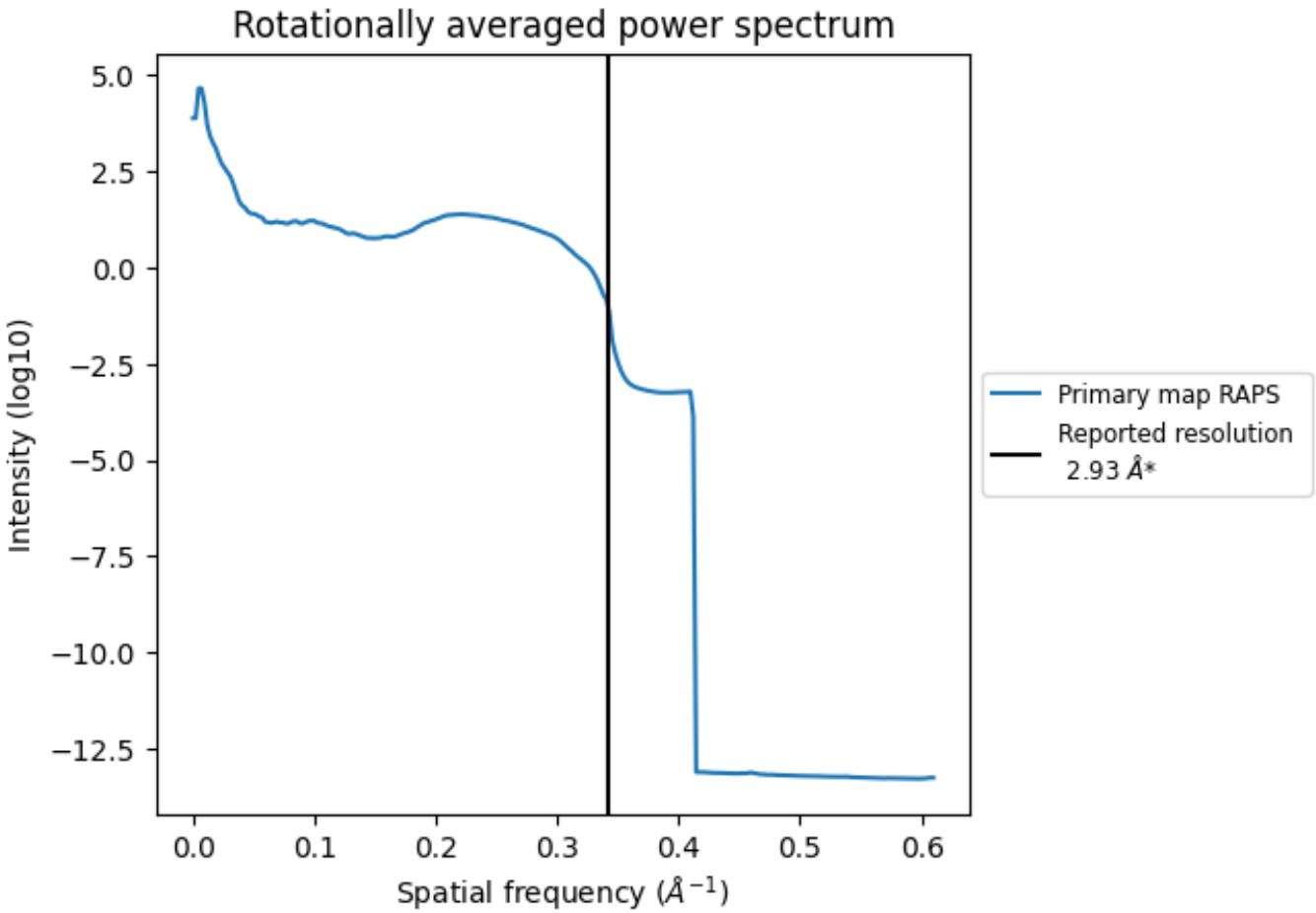
7.2 Volume estimate (i)



The volume at the recommended contour level is 502 nm^3; this corresponds to an approximate mass of 453 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 0.341 Å^{-1}

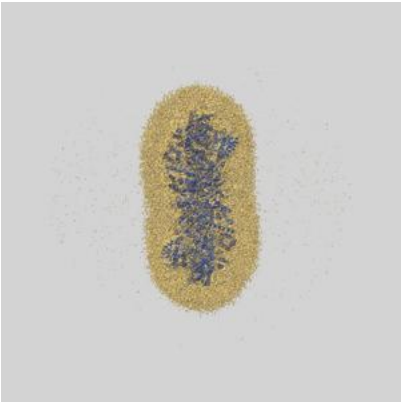
8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

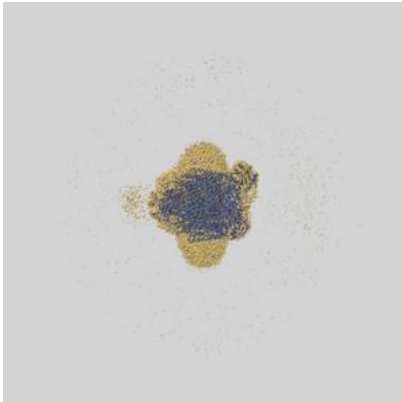
This section contains information regarding the fit between EMDB map EMD-30945 and PDB model 7E1X. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)



X

Y



Z

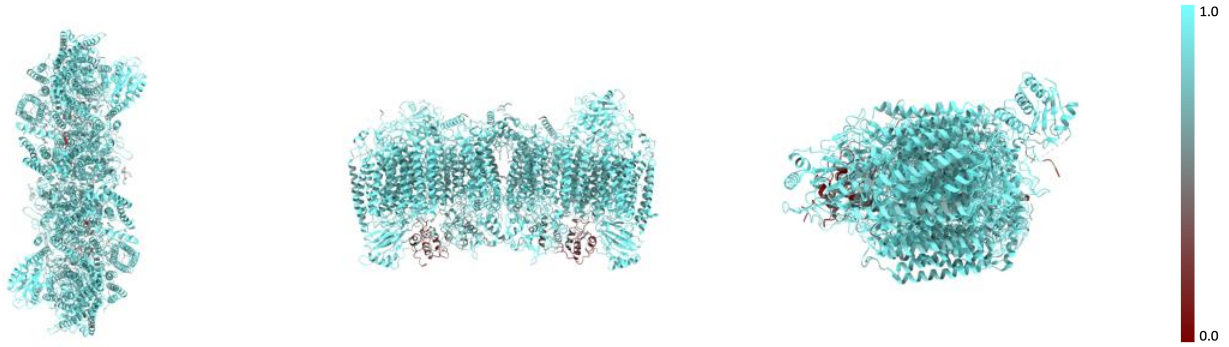
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

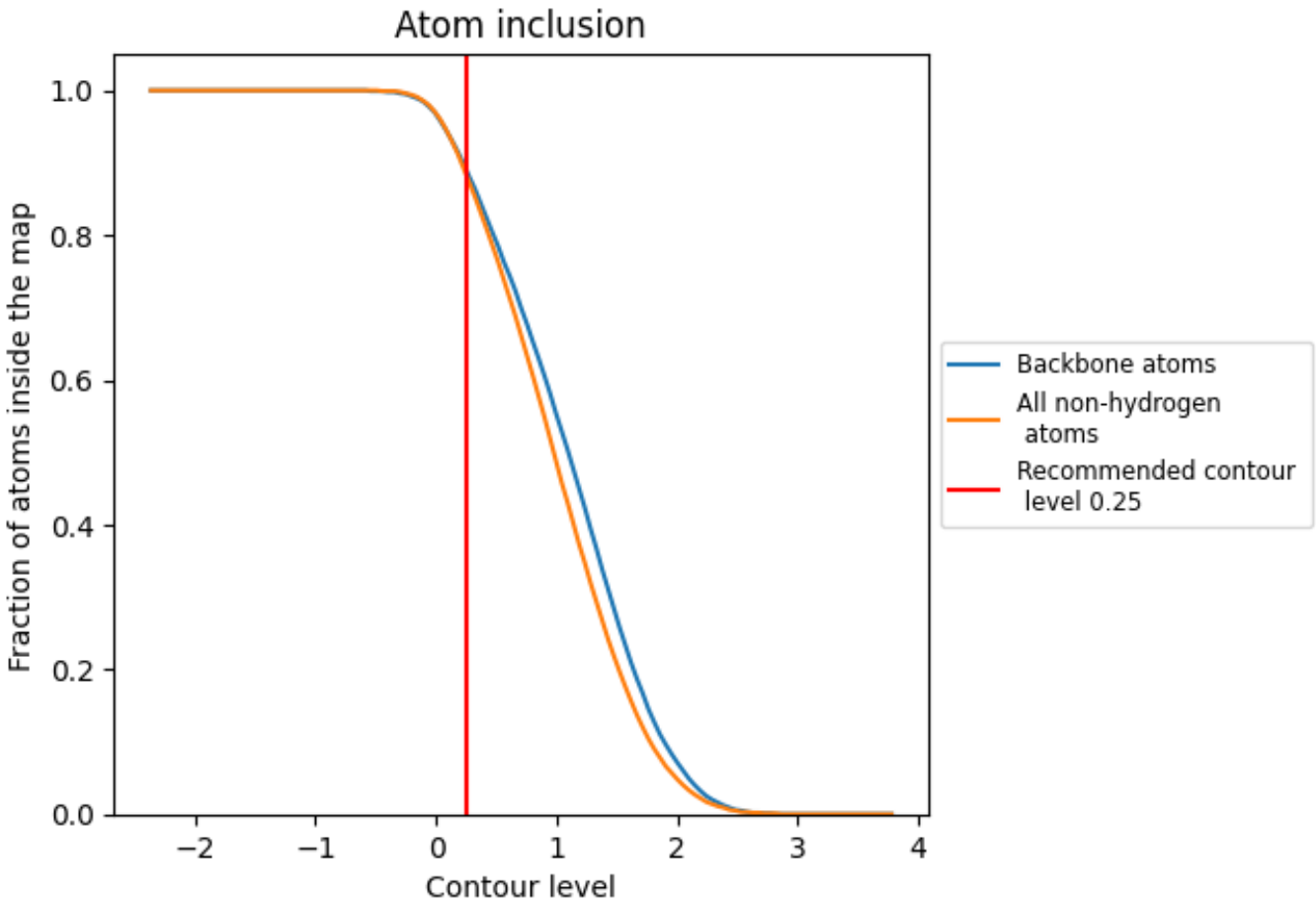
9.3 Atom inclusion mapped to coordinate model (i)



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, 89% of all backbone atoms, 88% 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	0.8840	0.5130
A	0.8980	0.5180
B	0.9240	0.5540
C	0.5870	0.2820
D	0.8960	0.5370
E	0.9000	0.4980
F	0.9360	0.5570
G	0.9000	0.5120
H	0.8900	0.5050
I	0.8860	0.4890
J	0.9000	0.4820
M	0.8960	0.5280
N	0.9270	0.5680
O	0.5560	0.2890
P	0.9190	0.5490
Q	0.8750	0.4790
R	0.9380	0.5610
S	0.9000	0.5020
T	0.9080	0.5330
U	0.8880	0.5010
V	0.9080	0.5080