Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:32 PM EST

PDB ID	:	7JRG
EMDB ID	:	EMD-22445
Title	:	Plant Mitochondrial complex III2 from Vigna radiata
Authors	:	Maldonado, M.; Letts, J.A.
Deposited on	:	2020-08-12
Resolution	:	3.20 Å(reported)
Based on initial models	:	6Q9E, 6HU9

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

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

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

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

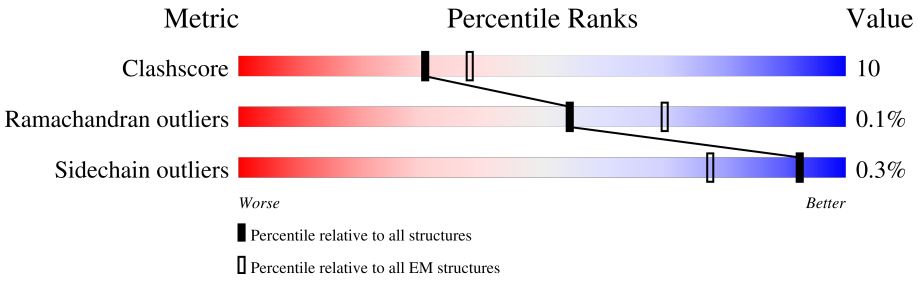
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	527	74% 19% 8%
1	M	527	68% 24% 8%
2	B	506	7% 65% 26% 10%
2	N	506	6% 67% 23% 10%
3	C	393	82% 16%
3	O	393	77% 21%
4	D	306	5% 63% 17% 20%
4	P	306	64% 15% 20%

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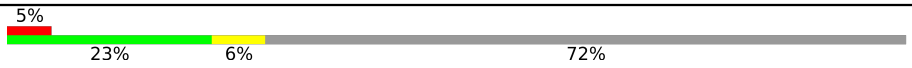
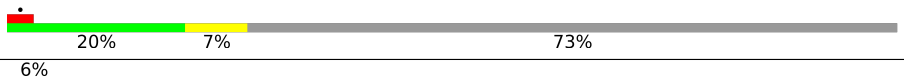
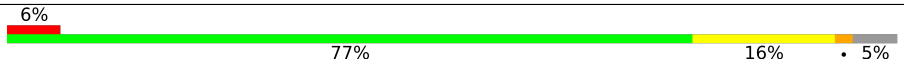
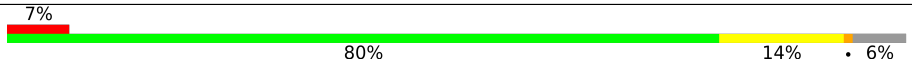
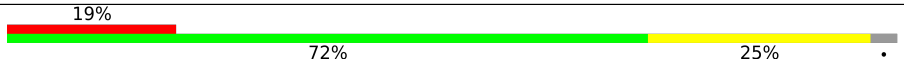
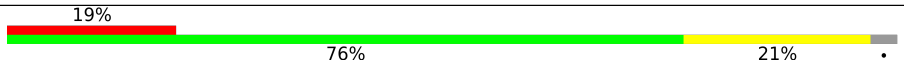
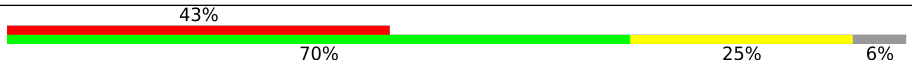
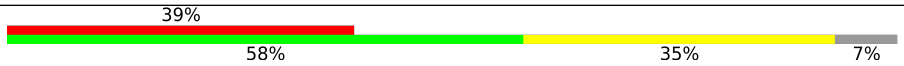
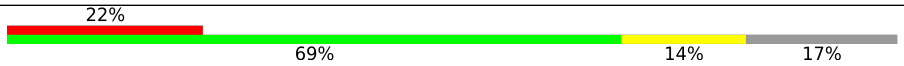
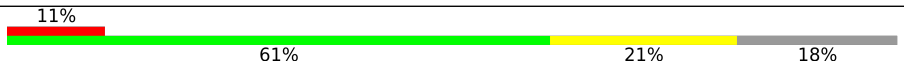
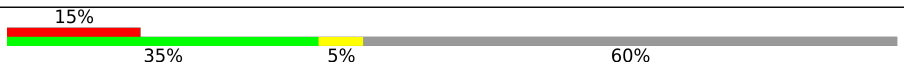
Mol	Chain	Length	Quality of chain
5	E	271	
5	Q	271	
6	F	122	
6	R	122	
7	G	72	
7	S	72	
8	H	69	
8	T	69	
9	J	72	
9	V	72	
10	K	81	
10	W	81	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 32930 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 Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		
1	M	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		

- Molecule 2 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	457	Total	C	N	O	S	0	0
			3471	2196	588	675	12		
2	N	455	Total	C	N	O	S	0	0
			3456	2187	585	672	12		

- Molecule 3 is a protein called COB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		
3	O	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		

- Molecule 4 is a protein called cytochrome c1-2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		
4	P	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	77	Total	C	N	O	S	0	0
			597	392	100	104	1		
5	Q	74	Total	C	N	O	S	0	0
			574	375	97	101	1		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	116	Total	C	N	O	S	0	0
			965	616	173	172	4		
6	R	115	Total	C	N	O	S	0	0
			959	613	172	170	4		

- Molecule 7 is a protein called cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			578	382	97	98	1		
7	S	70	Total	C	N	O	S	0	0
			578	382	97	98	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			536	344	90	96	6		
8	T	64	Total	C	N	O	S	0	0
			527	339	89	93	6		

- Molecule 9 is a protein called cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			480	313	83	83	1		
9	V	59	Total	C	N	O	S	0	0
			476	311	82	82	1		

- Molecule 10 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	31	Total	C	N	O	S	0	0
			218	144	35	38	1		

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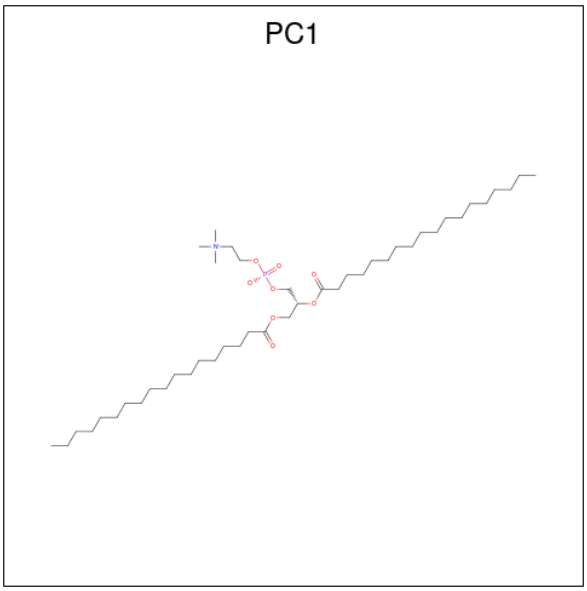
Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	32	Total	C	N	O	S	0	0
			226	150	36	39	1		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

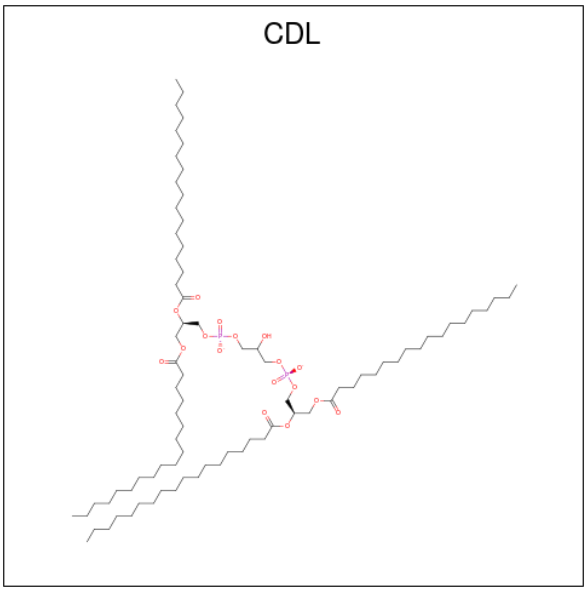
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Zn	0
			1	1	
11	M	1	Total	Zn	0
			1	1	

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



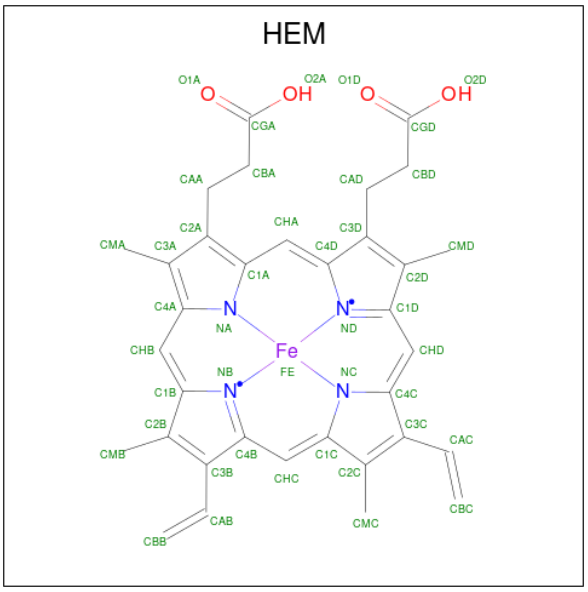
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
12	S	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



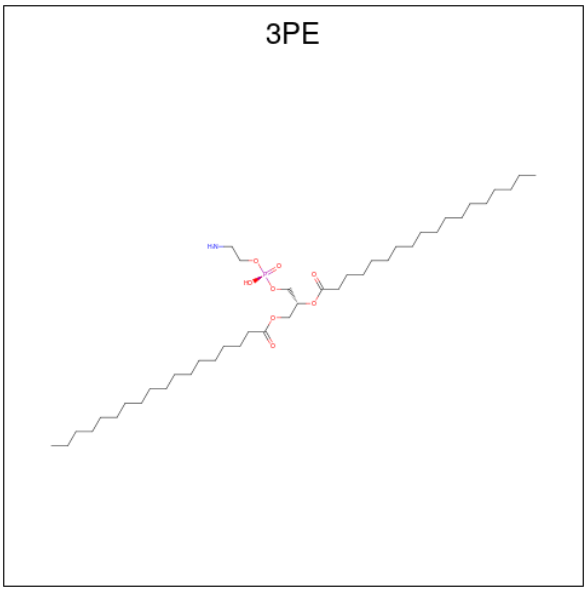
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			69	50	17	2	
13	C	1	Total	C	O	P	0
			123	85	34	4	
13	C	1	Total	C	O	P	0
			123	85	34	4	
13	D	1	Total	C	O	P	0
			68	49	17	2	
13	M	1	Total	C	O	P	0
			70	51	17	2	
13	O	1	Total	C	O	P	0
			145	107	34	4	
13	O	1	Total	C	O	P	0
			145	107	34	4	
13	P	1	Total	C	O	P	0
			63	44	17	2	
13	S	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



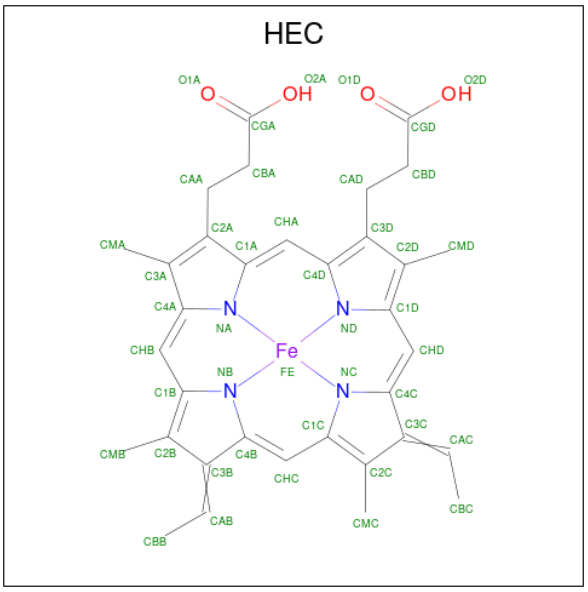
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	O	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	O	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 15 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	C	1	Total 206	C 146	N 6	O 48	P 6	0
15	F	1	Total 83	C 63	N 2	O 16	P 2	0
15	F	1	Total 83	C 63	N 2	O 16	P 2	0
15	G	1	Total 37	C 27	N 1	O 8	P 1	0
15	M	1	Total 45	C 35	N 1	O 8	P 1	0
15	O	1	Total 189	C 139	N 5	O 40	P 5	0
15	O	1	Total 189	C 139	N 5	O 40	P 5	0
15	O	1	Total 189	C 139	N 5	O 40	P 5	0
15	O	1	Total 189	C 139	N 5	O 40	P 5	0
15	O	1	Total 189	C 139	N 5	O 40	P 5	0
15	W	1	Total 56	C 36	N 2	O 16	P 2	0
15	W	1	Total 56	C 36	N 2	O 16	P 2	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



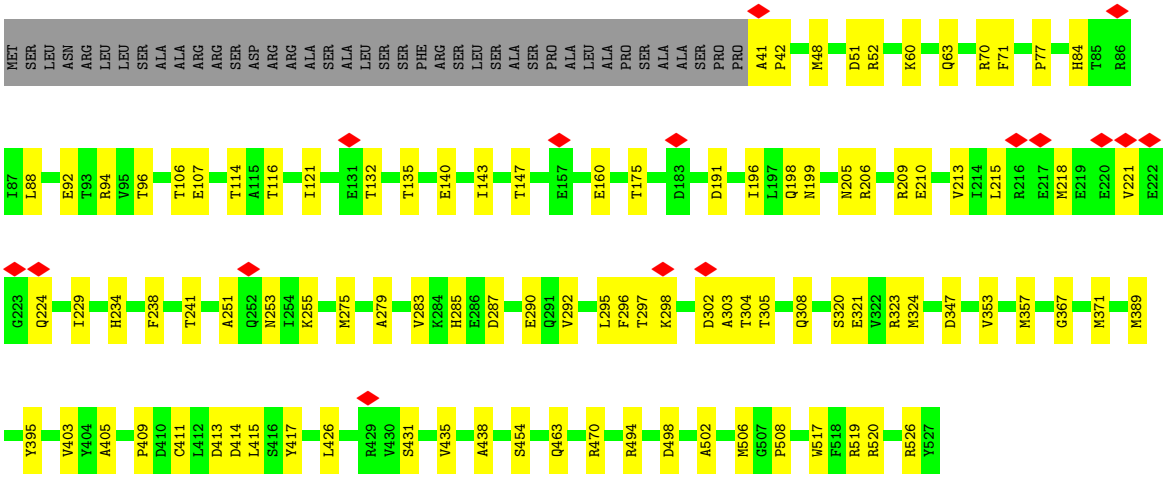
Mol	Chain	Residues	Atoms					AltConf
16	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

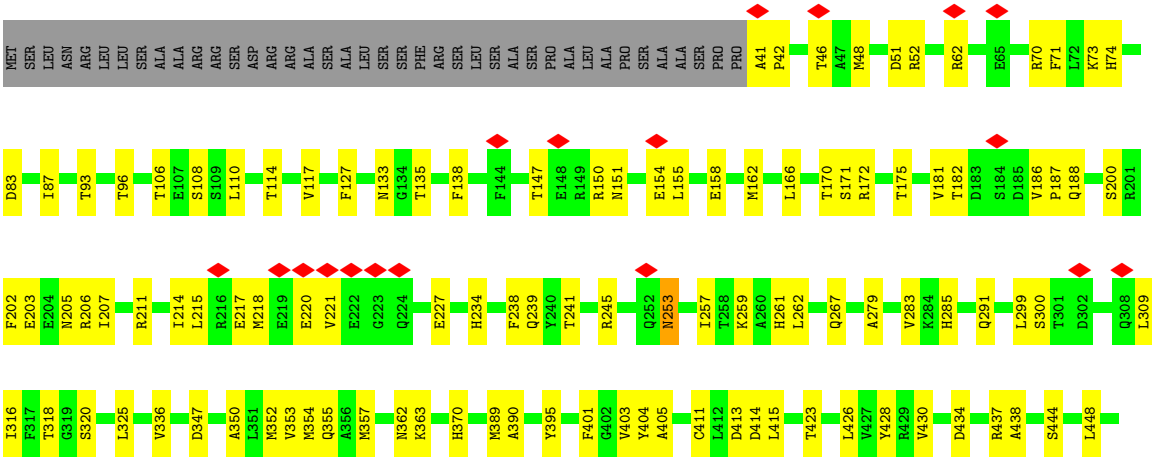
• Molecule 1: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

Chain A:



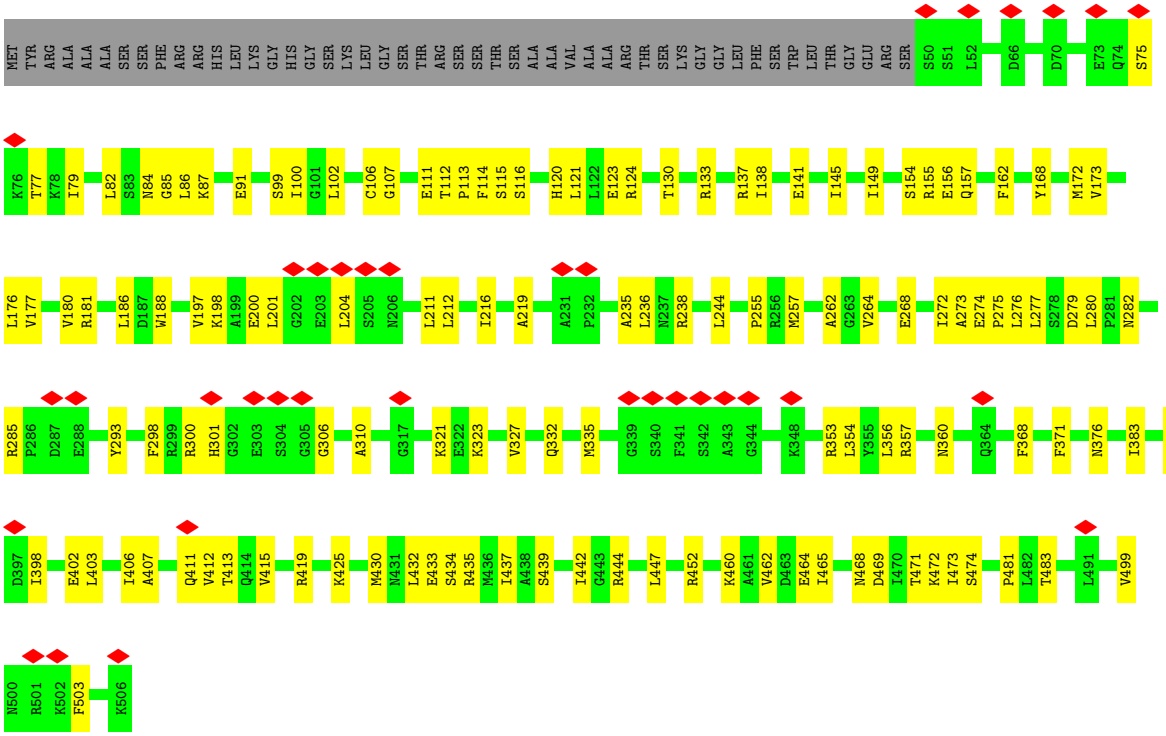
• Molecule 1: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

Chain M:



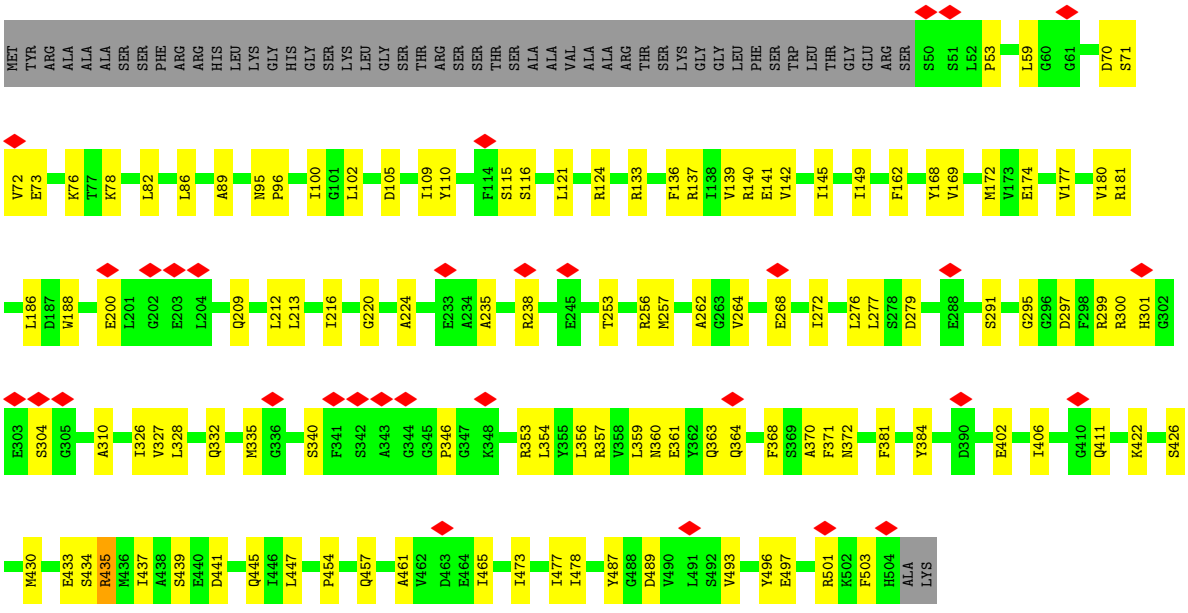
• Molecule 2: Alpha-MPP

Chain B:



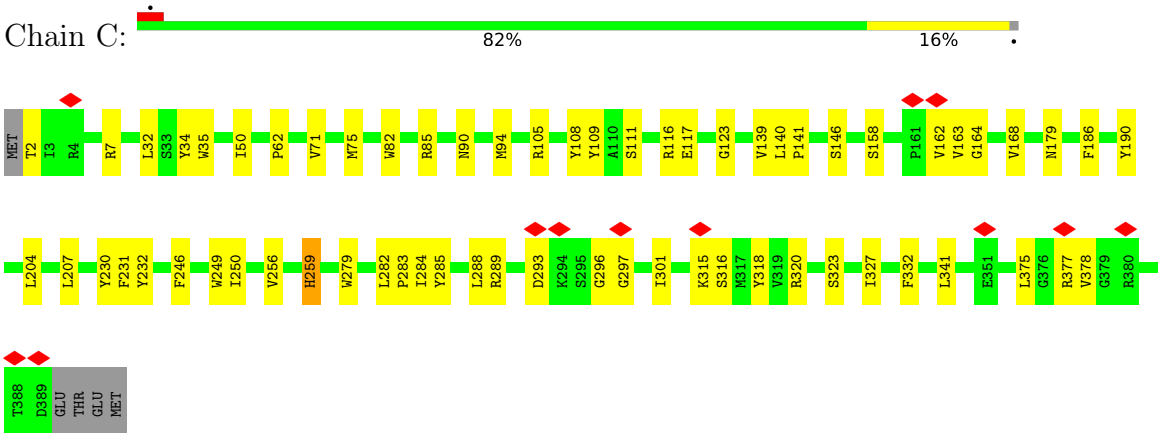
• Molecule 2: Alpha-MPP

Chain N:



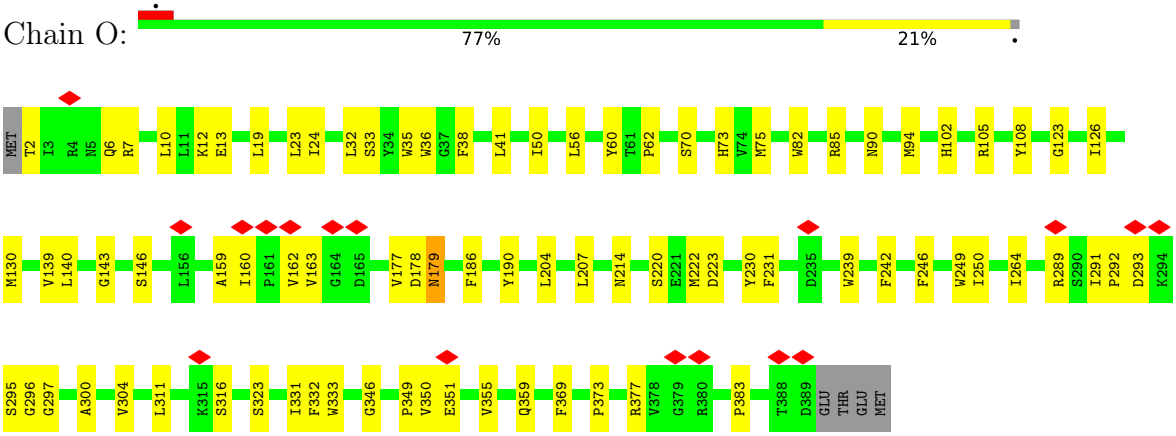
• Molecule 3: COB

Chain C:



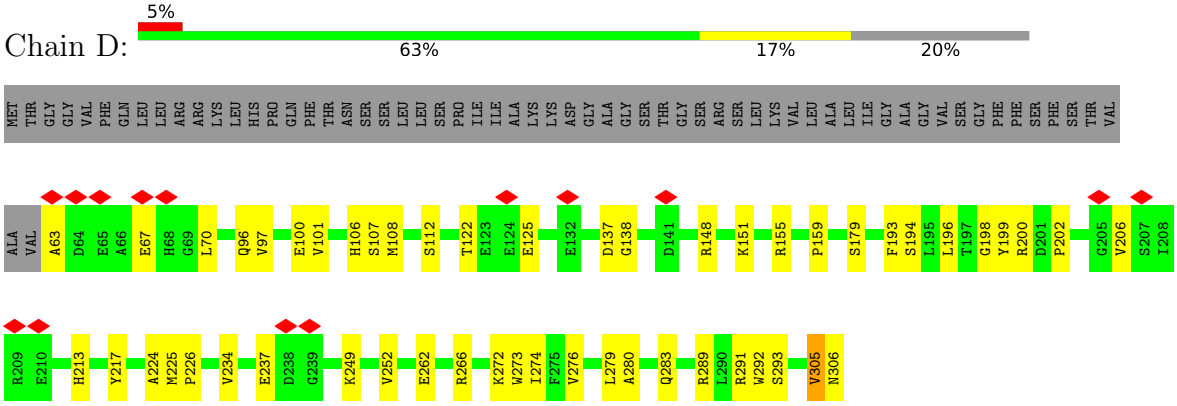
• Molecule 3: COB

Chain O:



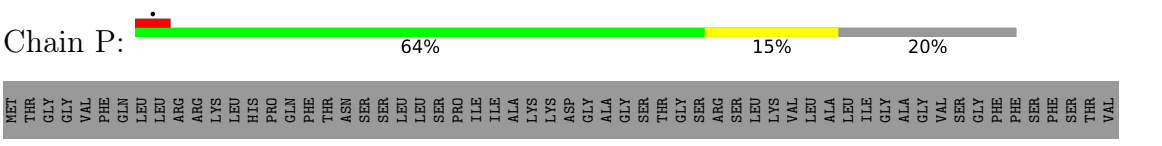
• Molecule 4: cytochrome c1-2, heme protein, mitochondrial

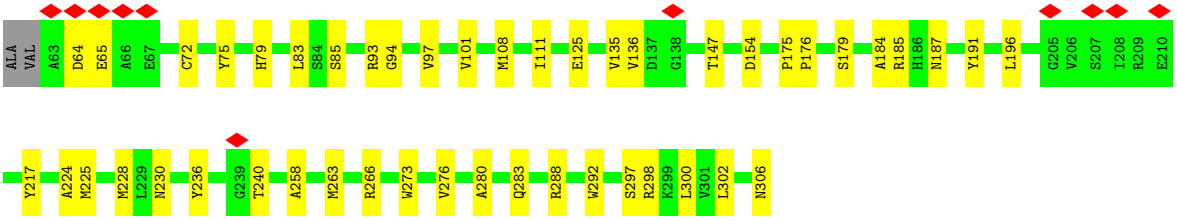
Chain D:



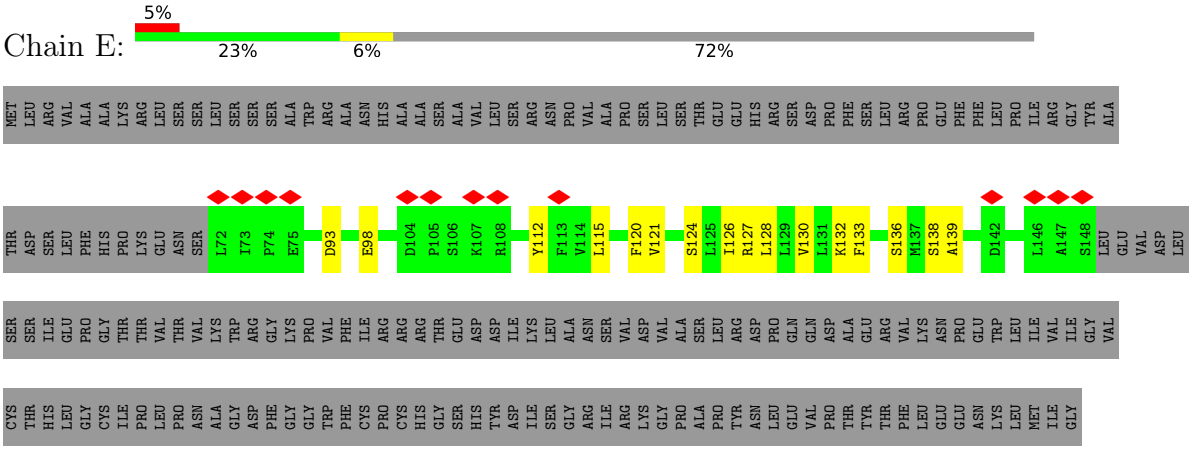
• Molecule 4: cytochrome c1-2, heme protein, mitochondrial

Chain P:

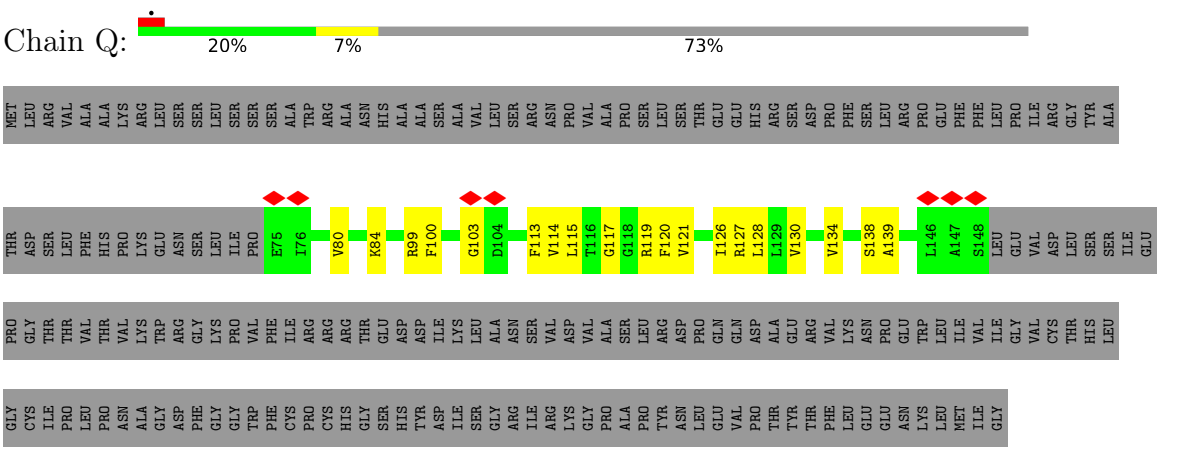




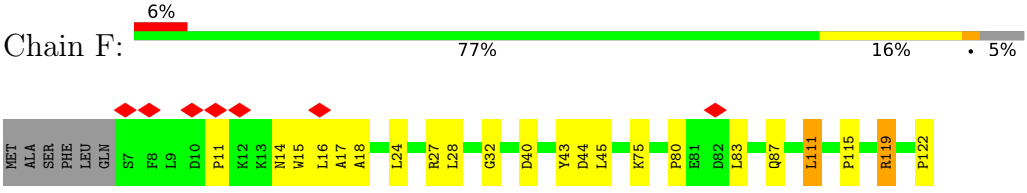
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 7



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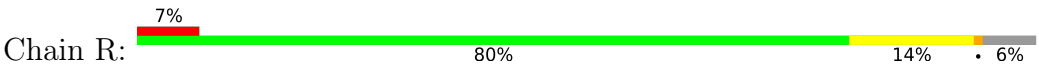
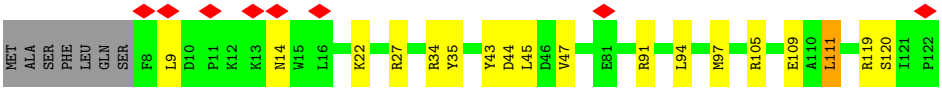
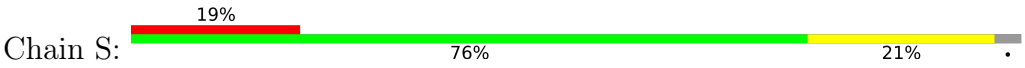


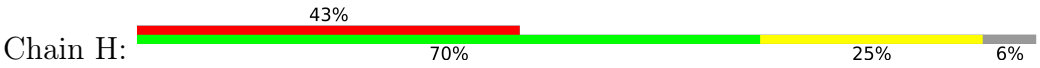


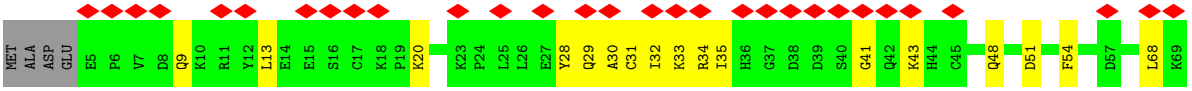
• Molecule 7: cytochrome b-c1 complex subunit 8

• Molecule 7: cytochrome b-c1 complex subunit 8

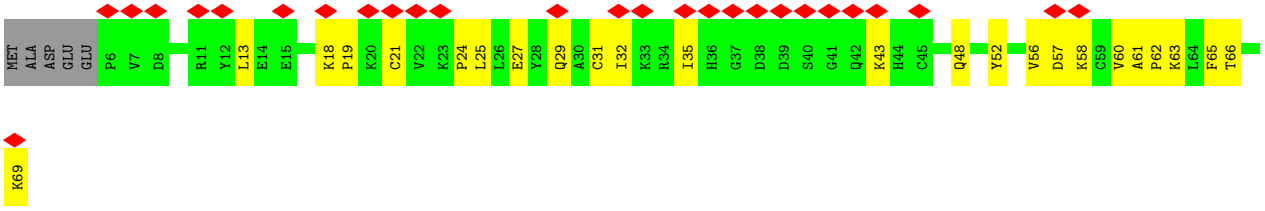


• Molecule 8: Cytochrome b-c1 complex subunit 6

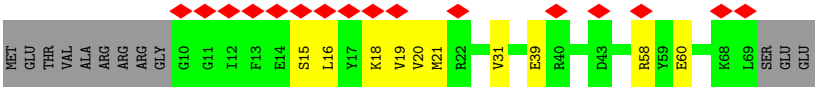




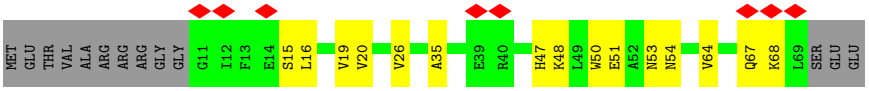
• Molecule 8: Cytochrome b-c1 complex subunit 6



• Molecule 9: cytochrome b-c1 complex subunit 9

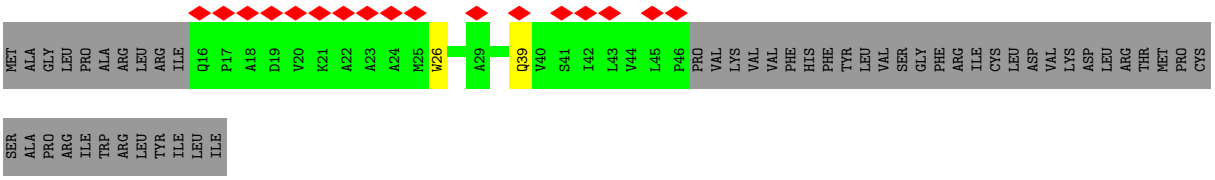


• Molecule 9: cytochrome b-c1 complex subunit 9



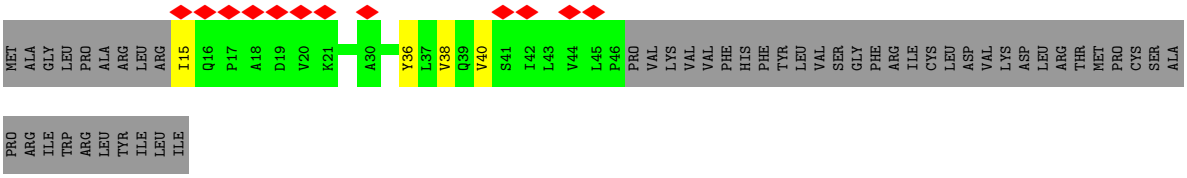
• Molecule 10: QCR10

Chain K:



• Molecule 10: QCR10

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48111	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 ($e^-/Å^2$)	86.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60010	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.820	Depositor
Minimum map value	-0.839	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, ZN, HEM, HEC, CDL, PC1

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	A	0.33	0/3914	0.48	0/5309
1	M	0.32	0/3914	0.49	0/5309
2	B	0.30	0/3541	0.48	0/4803
2	N	0.30	0/3526	0.49	0/4785
3	C	0.38	0/3220	0.46	0/4413
3	O	0.38	0/3220	0.47	0/4413
4	D	0.33	0/1962	0.45	0/2663
4	P	0.34	0/1962	0.45	0/2663
5	E	0.33	0/612	0.45	0/831
5	Q	0.34	0/588	0.46	0/797
6	F	0.35	0/986	0.46	1/1326 (0.1%)
6	R	0.35	0/980	0.46	1/1318 (0.1%)
7	G	0.29	0/595	0.42	0/807
7	S	0.29	0/595	0.44	0/807
8	H	0.30	0/550	0.44	0/737
8	T	0.29	0/541	0.52	0/724
9	J	0.30	0/490	0.43	0/660
9	V	0.30	0/486	0.41	0/655
10	K	0.27	0/222	0.41	0/305
10	W	0.31	0/230	0.45	0/316
All	All	0.33	0/32134	0.47	2/43641 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	111	LEU	CA-CB-CG	5.48	127.91	115.30
6	R	111	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3838	0	3797	67	0
1	M	3838	0	3797	95	0
2	B	3471	0	3471	97	0
2	N	3456	0	3453	90	0
3	C	3104	0	3070	57	0
3	O	3104	0	3070	67	0
4	D	1910	0	1843	43	0
4	P	1910	0	1843	36	0
5	E	597	0	620	16	0
5	Q	574	0	591	17	0
6	F	965	0	982	21	0
6	R	959	0	977	15	0
7	G	578	0	599	18	0
7	S	578	0	599	13	0
8	H	536	0	528	15	0
8	T	527	0	521	19	0
9	J	480	0	486	8	0
9	V	476	0	483	11	0
10	K	218	0	230	2	0
10	W	226	0	241	3	0
11	A	1	0	0	0	0
11	M	1	0	0	0	0
12	A	38	0	50	3	0
12	M	40	0	54	6	0
12	S	38	0	50	2	0
13	A	69	0	85	1	0
13	C	123	0	134	5	0
13	D	68	0	83	2	0
13	M	70	0	87	6	0
13	O	145	0	184	10	0
13	P	63	0	70	2	0
13	S	55	0	54	2	0
14	C	86	0	60	8	0
14	O	86	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	206	0	259	13	0
15	F	83	0	120	3	0
15	G	37	0	48	1	0
15	M	45	0	67	2	0
15	O	189	0	254	5	0
15	W	56	0	60	0	0
16	D	43	0	30	6	0
16	P	43	0	30	4	0
All	All	32930	0	33040	645	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 10.

All (645) 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)
1:M:187:PRO:HB3	1:M:291:GLN:HE22	1.40	0.86
3:C:75:MET:HE1	3:C:82:TRP:HA	1.60	0.84
6:F:16:LEU:HD12	15:F:201:3PE:H352	1.65	0.79
3:C:315:LYS:HE3	3:C:377:ARG:HH21	1.47	0.79
3:O:162:VAL:HG13	3:O:163:VAL:HG13	1.64	0.79
4:D:280:ALA:HB2	5:E:121:VAL:HG11	1.67	0.76
1:M:106:THR:HG22	1:M:279:ALA:HB3	1.67	0.76
2:B:84:ASN:HD21	2:B:280:LEU:HB2	1.52	0.74
12:M:604:PC1:H3C1	13:O:402:CDL:H192	1.69	0.74
7:G:71:ARG:NH1	8:H:51:ASP:OD2	2.20	0.74
3:O:35:TRP:HA	3:O:38:PHE:HD2	1.53	0.74
2:B:293:TYR:HH	2:B:483:THR:HG1	1.37	0.73
2:N:212:LEU:HD12	2:N:384:TYR:HE1	1.53	0.73
1:A:526:ARG:O	10:K:26:TRP:NE1	2.22	0.72
12:M:604:PC1:H371	13:O:402:CDL:H741	1.73	0.71
2:B:204:LEU:HD13	2:B:211:LEU:HD21	1.73	0.70
2:N:326:ILE:HG22	2:N:465:ILE:HD11	1.73	0.70
4:P:280:ALA:HB2	5:Q:121:VAL:HG11	1.72	0.70
4:D:225:MET:HE3	16:D:501:HEC:NC	2.07	0.70
2:N:357:ARG:O	2:N:361:GLU:HB2	1.91	0.69
3:C:62:PRO:HD2	3:O:62:PRO:HD2	1.73	0.69
15:O:409:3PE:H292	15:O:409:3PE:H371	1.75	0.69
1:A:121:ILE:HG12	1:A:275:MET:HG2	1.76	0.68
3:O:293:ASP:O	3:O:296:GLY:N	2.26	0.68
2:B:301:HIS:H	2:N:300:ARG:HH12	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:THR:O	1:M:52:ARG:NH1	2.27	0.67
6:F:119:ARG:NH1	6:F:122:PRO:OXT	2.26	0.67
2:B:468:ASN:HB2	2:B:472:LYS:NZ	2.09	0.67
3:C:259:HIS:HE1	15:C:408:3PE:H11	1.60	0.67
2:N:354:LEU:HD22	2:N:368:PHE:HE2	1.60	0.67
3:C:293:ASP:O	3:C:296:GLY:N	2.28	0.67
2:N:162:PHE:CE2	2:N:172:MET:HG2	2.29	0.67
6:R:119:ARG:NH1	6:R:120:SER:O	2.28	0.67
5:E:124:SER:OG	9:J:39:GLU:OE1	2.13	0.66
4:P:83:LEU:O	9:V:53:ASN:ND2	2.28	0.66
1:M:70:ARG:HA	1:M:73:LYS:HE3	1.77	0.66
2:N:137:ARG:NH2	2:N:141:GLU:OE2	2.28	0.66
3:O:105:ARG:HH12	14:O:404:HEM:HBD2	1.60	0.66
3:O:94:MET:HG3	3:O:246:PHE:HD1	1.60	0.66
1:A:107:GLU:OE1	1:A:470:ARG:NH1	2.23	0.66
8:T:35:ILE:HG23	8:T:43:LYS:HB2	1.78	0.66
1:M:110:LEU:HB2	2:N:71:SER:HB2	1.78	0.65
4:P:283:GLN:HE21	5:Q:115:LEU:HA	1.61	0.65
1:A:71:PHE:O	2:B:133:ARG:NH2	2.30	0.64
3:C:327:ILE:HD11	15:F:201:3PE:H341	1.79	0.64
13:O:402:CDL:H712	5:Q:126:ILE:HD12	1.78	0.64
4:D:289:ARG:HH12	7:G:26:LEU:HG	1.63	0.64
3:C:323:SER:O	6:F:27:ARG:NH1	2.31	0.64
10:W:38:VAL:HG12	10:W:40:VAL:HG13	1.80	0.64
6:F:80:PRO:HG2	6:F:83:LEU:HD13	1.80	0.64
6:F:119:ARG:O	3:O:7:ARG:NH1	2.30	0.64
2:B:357:ARG:NH2	2:B:402:GLU:OE1	2.31	0.64
4:P:224:ALA:HB3	16:P:501:HEC:HBD2	1.79	0.64
1:M:162:MET:SD	1:M:188:GLN:NE2	2.70	0.64
3:C:117:GLU:OE1	6:F:119:ARG:NH2	2.31	0.63
1:M:411:CYS:SG	3:O:2:THR:OG1	2.52	0.63
2:N:363:GLN:HG2	2:N:364:GLN:OE1	1.98	0.63
2:B:84:ASN:O	2:B:282:ASN:ND2	2.28	0.63
3:C:7:ARG:NH1	6:R:119:ARG:O	2.31	0.63
2:N:381:PHE:HB3	2:N:477:ILE:HD11	1.80	0.63
7:S:71:ARG:HD3	8:T:48:GLN:HE22	1.64	0.63
1:A:302:ASP:OD1	1:A:303:ALA:N	2.32	0.62
3:O:291:ILE:HD12	3:O:292:PRO:HD2	1.78	0.62
3:O:36:TRP:NE1	14:O:404:HEM:O2D	2.29	0.62
3:O:331:ILE:HD11	15:O:409:3PE:H2A1	1.80	0.62
8:T:21:CYS:O	8:T:24:PRO:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:OE2	1:A:94:ARG:NH1	2.32	0.62
3:C:320:ARG:NH1	6:F:40:ASP:OD2	2.32	0.62
1:M:170:THR:HG22	1:M:175:THR:HG23	1.81	0.62
4:P:125:GLU:HG2	9:V:68:LYS:HB3	1.81	0.62
1:M:257:ILE:HG22	1:M:259:LYS:H	1.65	0.61
2:N:297:ASP:OD2	2:N:299:ARG:NH1	2.33	0.61
1:M:257:ILE:O	1:M:261:HIS:ND1	2.32	0.61
2:B:137:ARG:NH2	2:B:141:GLU:OE2	2.33	0.61
15:C:407:3PE:H382	4:D:274:ILE:HG21	1.81	0.61
1:M:106:THR:OG1	1:M:285:HIS:ND1	2.31	0.61
1:M:405:ALA:HB1	1:M:415:LEU:HD21	1.82	0.61
2:N:332:GLN:NE2	2:N:370:ALA:O	2.33	0.61
3:O:126:ILE:O	3:O:130:MET:HG3	2.01	0.61
1:M:347:ASP:OD2	1:M:494:ARG:NH1	2.33	0.60
3:C:163:VAL:HG23	3:C:164:GLY:H	1.65	0.60
3:O:323:SER:O	6:R:27:ARG:NH1	2.34	0.60
1:M:267:GLN:O	1:M:300:SER:OG	2.18	0.60
3:O:90:ASN:O	3:O:94:MET:HG2	2.02	0.60
1:A:70:ARG:NH1	2:B:275:PRO:O	2.28	0.60
2:B:434:SER:O	2:B:437:ILE:N	2.33	0.60
2:B:353:ARG:NH2	2:B:411:GLN:O	2.32	0.60
8:T:29:GLN:HA	8:T:32:ILE:HD12	1.83	0.60
1:A:106:THR:HG22	1:A:279:ALA:HB3	1.84	0.60
2:N:124:ARG:NH2	2:N:200:GLU:OE2	2.33	0.60
1:A:70:ARG:NH2	2:B:279:ASP:OD2	2.31	0.60
2:N:262:ALA:HB2	2:N:439:SER:HB3	1.82	0.60
2:B:162:PHE:CE2	2:B:172:MET:HG2	2.36	0.60
3:C:230:TYR:O	4:D:292:TRP:NE1	2.34	0.60
3:C:249:TRP:HZ3	3:C:256:VAL:HB	1.65	0.60
3:O:223:ASP:OD2	4:P:298:ARG:NH1	2.35	0.60
2:B:293:TYR:OH	2:B:481:PRO:O	2.20	0.60
2:B:177:VAL:HG11	2:B:276:LEU:HB3	1.84	0.59
3:O:41:LEU:HD21	3:O:242:PHE:HB2	1.83	0.59
7:S:56:TYR:O	7:S:60:GLN:HG2	2.01	0.59
13:A:603:CDL:H131	13:C:401:CDL:HB4	1.84	0.59
15:C:406:3PE:H3C2	15:C:406:3PE:H3H2	1.83	0.59
9:V:20:VAL:HG23	9:V:26:VAL:HG12	1.84	0.59
1:A:198:GLN:HE22	1:A:296:PHE:HA	1.68	0.59
15:C:405:3PE:H111	6:F:24:LEU:HD11	1.85	0.59
2:N:162:PHE:CD2	2:N:172:MET:HG2	2.37	0.59
1:A:321:GLU:HG2	7:G:14:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:ASN:OD1	2:B:469:ASP:N	2.36	0.59
1:A:405:ALA:HB1	1:A:415:LEU:HD21	1.84	0.58
4:D:276:VAL:HG12	5:E:121:VAL:HG13	1.85	0.58
2:B:121:LEU:HD23	2:B:244:LEU:HD11	1.85	0.58
2:B:332:GLN:HE21	2:B:371:PHE:HA	1.68	0.58
7:G:67:LYS:O	7:G:71:ARG:HB2	2.02	0.58
1:M:525:ASN:N	13:M:603:CDL:OB3	2.27	0.58
3:O:289:ARG:HD3	3:O:350:VAL:HG12	1.85	0.58
1:M:205:ASN:OD1	1:M:206:ARG:N	2.36	0.58
13:M:603:CDL:H142	13:O:402:CDL:HA4	1.86	0.58
2:B:168:TYR:O	2:B:172:MET:HG3	2.04	0.58
1:A:48:MET:O	1:A:52:ARG:NE	2.32	0.58
4:D:225:MET:CE	16:D:501:HEC:NC	2.66	0.58
4:D:224:ALA:HB3	16:D:501:HEC:HBD2	1.85	0.58
1:M:234:HIS:NE2	1:M:395:TYR:OH	2.27	0.58
7:S:41:ASN:HB2	13:S:102:CDL:H712	1.85	0.58
2:B:79:ILE:HD11	2:B:87:LYS:HD2	1.86	0.57
7:S:15:LEU:HB3	7:S:20:GLN:HE21	1.69	0.57
5:E:138:SER:OG	5:E:139:ALA:N	2.35	0.57
2:B:100:ILE:HD11	2:B:264:VAL:HG21	1.85	0.57
3:C:288:LEU:HD12	3:C:301:ILE:HG13	1.86	0.57
13:C:401:CDL:HA22	13:C:401:CDL:HB32	1.85	0.57
1:M:93:THR:HG21	1:M:470:ARG:HD3	1.86	0.57
2:N:327:VAL:HG11	2:N:473:ILE:HG13	1.87	0.57
8:T:35:ILE:HD12	8:T:43:LYS:HB2	1.87	0.57
3:C:116:ARG:HH22	3:C:320:ARG:HH22	1.53	0.56
5:E:126:ILE:O	5:E:130:VAL:HG23	2.05	0.56
1:M:211:ARG:HH21	1:M:257:ILE:H	1.51	0.56
4:D:305:VAL:CG1	1:M:48:MET:SD	2.93	0.56
1:M:138:PHE:HZ	1:M:207:ILE:HG23	1.70	0.56
4:D:137:ASP:OD1	4:D:138:GLY:N	2.39	0.56
1:M:350:ALA:O	1:M:354:MET:HG3	2.06	0.56
2:B:77:THR:HG21	2:B:452:ARG:HD2	1.87	0.56
1:A:199:ASN:OD1	1:A:298:LYS:NZ	2.39	0.56
2:N:224:ALA:HB3	2:N:291:SER:HB3	1.87	0.56
1:M:354:MET:HE3	1:M:426:LEU:HD23	1.88	0.55
2:B:468:ASN:HB2	2:B:472:LYS:HZ3	1.69	0.55
1:M:514:ASP:OD1	1:M:514:ASP:N	2.37	0.55
7:G:22:VAL:HG12	7:G:23:MET:HG2	1.88	0.55
1:M:48:MET:O	1:M:51:ASP:N	2.38	0.55
9:V:50:TRP:O	9:V:54:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:MET:HE3	2:B:354:LEU:HG	1.88	0.55
1:M:166:LEU:HB3	2:N:346:PRO:HG2	1.87	0.55
3:O:159:ALA:HB1	3:O:295:SER:HA	1.88	0.55
4:P:72:CYS:SG	4:P:187:ASN:ND2	2.71	0.55
4:P:184:ALA:O	4:P:185:ARG:NH2	2.33	0.55
1:A:347:ASP:OD2	1:A:494:ARG:NH1	2.39	0.55
2:B:156:GLU:OE1	2:B:376:ASN:ND2	2.37	0.55
1:M:147:THR:HG22	1:M:200:SER:HA	1.89	0.55
2:N:335:MET:HE3	2:N:406:ILE:HD13	1.88	0.54
1:M:413:ASP:OD1	1:M:414:ASP:N	2.39	0.54
3:O:246:PHE:CE2	3:O:250:ILE:HD11	2.43	0.54
6:R:47:VAL:HG13	6:R:94:LEU:HD21	1.89	0.54
2:B:86:LEU:HG	2:B:257:MET:HB2	1.89	0.54
1:A:198:GLN:NE2	1:A:297:THR:O	2.40	0.54
4:D:96:GLN:HE22	4:D:237:GLU:HG2	1.72	0.54
12:M:604:PC1:H272	13:O:402:CDL:H731	1.90	0.54
1:A:229:ILE:HD11	1:A:506:MET:HG2	1.90	0.54
2:B:99:SER:H	2:B:262:ALA:HB3	1.72	0.54
2:B:114:PHE:O	2:B:238:ARG:NH1	2.41	0.54
4:D:273:TRP:CE2	5:E:128:LEU:HD22	2.43	0.54
2:N:142:VAL:HG13	2:N:162:PHE:HE1	1.72	0.54
2:B:75:SER:OG	2:B:91:GLU:HB2	2.09	0.53
2:N:53:PRO:HG3	2:N:59:LEU:HA	1.89	0.53
8:T:31:CYS:O	8:T:35:ILE:HG12	2.07	0.53
3:O:123:GLY:C	14:O:404:HEM:HBC2	2.29	0.53
1:M:413:ASP:OD2	1:M:511:ARG:NH2	2.42	0.53
2:N:212:LEU:HD12	2:N:384:TYR:CE1	2.40	0.53
3:O:50:ILE:HA	14:O:403:HEM:HAB	1.89	0.53
2:B:216:ILE:HD11	2:B:310:ALA:HB1	1.91	0.53
2:B:354:LEU:HD13	2:B:368:PHE:CE2	2.43	0.53
12:M:604:PC1:H341	13:O:402:CDL:H111	1.90	0.53
2:N:441:ASP:OD1	2:N:445:GLN:NE2	2.40	0.53
4:P:135:VAL:HG21	4:P:154:ASP:OD2	2.09	0.53
1:M:71:PHE:O	2:N:133:ARG:NH2	2.40	0.53
2:N:133:ARG:NH1	2:N:141:GLU:OE2	2.42	0.53
1:A:413:ASP:OD1	1:A:414:ASP:N	2.41	0.53
2:B:86:LEU:HD13	2:B:277:LEU:HB3	1.89	0.53
2:B:186:LEU:HD13	2:B:188:TRP:CZ2	2.43	0.53
4:D:289:ARG:NH1	7:G:26:LEU:HG	2.23	0.53
2:N:168:TYR:O	2:N:172:MET:HG3	2.08	0.53
4:P:228:MET:O	4:P:230:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:33:LYS:O	7:S:37:LYS:HG2	2.09	0.53
2:B:162:PHE:CD2	2:B:172:MET:HG2	2.44	0.53
2:B:262:ALA:HB2	2:B:439:SER:HB3	1.91	0.53
2:B:154:SER:OG	2:B:155:ARG:N	2.41	0.52
1:A:210:GLU:HA	1:A:213:VAL:HG12	1.91	0.52
1:A:305:THR:HB	1:A:308:GLN:HG2	1.91	0.52
4:P:302:LEU:HD23	7:S:10:SER:HB3	1.91	0.52
1:M:138:PHE:HD1	1:M:214:ILE:HD12	1.74	0.52
9:V:47:HIS:NE2	9:V:51:GLU:OE2	2.43	0.52
2:N:105:ASP:O	2:N:256:ARG:NH2	2.43	0.52
2:N:434:SER:O	2:N:437:ILE:N	2.40	0.52
4:P:217:TYR:OH	8:T:57:ASP:OD2	2.19	0.52
2:N:169:VAL:HA	2:N:172:MET:HE3	1.92	0.52
2:N:353:ARG:NH2	2:N:411:GLN:O	2.34	0.52
2:B:323:LYS:O	2:B:327:VAL:HG23	2.10	0.52
4:D:283:GLN:HE21	5:E:115:LEU:HA	1.75	0.52
8:H:35:ILE:HD12	8:H:43:LYS:HG3	1.91	0.52
8:T:25:LEU:HD12	8:T:52:TYR:CZ	2.45	0.52
1:A:389:MET:O	1:A:403:VAL:O	2.28	0.52
3:C:158:SER:HB3	3:C:168:VAL:HG21	1.92	0.52
8:H:41:GLY:H	8:H:43:LYS:NZ	2.08	0.52
1:M:336:VAL:HG12	1:M:503:ILE:HG12	1.92	0.52
5:Q:127:ARG:HD3	10:W:36:TYR:CZ	2.45	0.52
1:M:389:MET:O	1:M:403:VAL:O	2.28	0.51
4:P:191:TYR:OH	16:P:501:HEC:O2A	2.20	0.51
2:B:112:THR:O	2:B:114:PHE:N	2.43	0.51
4:D:108:MET:O	4:D:179:SER:OG	2.29	0.51
4:P:273:TRP:CE2	5:Q:128:LEU:HD22	2.46	0.51
1:A:143:ILE:HG12	1:A:196:ILE:HG23	1.93	0.51
2:N:78:LYS:O	2:N:89:ALA:HA	2.11	0.51
5:Q:120:PHE:HB2	9:V:35:ALA:HB2	1.92	0.51
4:D:225:MET:HE3	16:D:501:HEC:C4C	2.40	0.51
1:M:171:SER:OG	1:M:172:ARG:N	2.44	0.51
5:Q:99:ARG:NH1	5:Q:100:PHE:O	2.40	0.51
8:T:27:GLU:HG3	8:T:48:GLN:HG3	1.92	0.51
1:M:181:VAL:HG22	1:M:182:THR:H	1.74	0.51
13:M:603:CDL:H132	3:O:24:ILE:HG12	1.93	0.51
1:A:292:VAL:HG13	1:A:296:PHE:CD2	2.45	0.51
3:C:316:SER:O	6:F:43:TYR:OH	2.11	0.51
8:H:29:GLN:HA	8:H:32:ILE:HD12	1.93	0.51
1:M:151:ASN:HB3	1:M:154:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:VAL:HG11	1:M:186:VAL:HA	1.93	0.51
2:B:106:CYS:SG	2:B:107:GLY:N	2.84	0.50
3:C:259:HIS:CE1	15:C:408:3PE:H11	2.42	0.50
1:M:434:ASP:OD1	1:M:437:ARG:NH2	2.44	0.50
1:A:77:PRO:HG3	2:B:137:ARG:HG3	1.91	0.50
3:C:109:TYR:OH	15:C:409:3PE:O12	2.24	0.50
4:D:262:GLU:O	4:D:266:ARG:HB2	2.11	0.50
1:A:238:PHE:O	1:A:241:THR:OG1	2.30	0.50
4:P:93:ARG:HG2	4:P:236:TYR:CE1	2.46	0.50
4:P:108:MET:O	4:P:179:SER:OG	2.25	0.50
5:E:120:PHE:HE1	9:J:31:VAL:HA	1.76	0.50
6:R:34:ARG:NH1	6:R:91:ARG:O	2.44	0.50
1:A:411:CYS:SG	3:C:2:THR:OG1	2.69	0.50
1:M:316:ILE:HD13	5:Q:103:GLY:HA2	1.93	0.50
1:A:357:MET:HB3	1:A:438:ALA:HB2	1.94	0.50
2:B:327:VAL:HG22	2:B:465:ILE:HD12	1.94	0.50
2:N:328:LEU:HD11	2:N:381:PHE:HB2	1.93	0.50
1:A:320:SER:O	1:A:502:ALA:HA	2.12	0.50
2:B:306:GLY:HA2	2:B:389:PRO:HD3	1.94	0.50
4:D:70:LEU:HD11	8:H:54:PHE:HB2	1.94	0.50
2:B:407:ALA:HA	2:B:474:SER:OG	2.12	0.49
13:P:502:CDL:O1	13:S:102:CDL:OA4	2.20	0.49
2:N:268:GLU:O	2:N:272:ILE:HG12	2.11	0.49
3:O:94:MET:HG3	3:O:246:PHE:CD1	2.43	0.49
15:O:401:3PE:H372	15:O:401:3PE:H272	1.94	0.49
8:T:13:LEU:HD13	8:T:63:LYS:HB2	1.94	0.49
1:M:203:GLU:N	1:M:203:GLU:OE1	2.45	0.49
2:N:461:ALA:O	2:N:465:ILE:HG13	2.12	0.49
3:O:75:MET:SD	3:O:85:ARG:HD3	2.52	0.49
2:B:335:MET:SD	2:B:406:ILE:HG21	2.52	0.49
6:F:111:LEU:HD12	6:F:111:LEU:O	2.13	0.49
1:M:127:PHE:HD2	1:M:309:LEU:HD22	1.77	0.49
2:N:177:VAL:HG11	2:N:276:LEU:HB3	1.95	0.49
4:P:288:ARG:NH1	13:P:502:CDL:OA4	2.45	0.49
2:N:70:ASP:O	2:N:71:SER:HB3	2.13	0.49
2:N:426:SER:O	2:N:430:MET:HG3	2.12	0.49
1:M:454:SER:OG	1:M:455:PRO:HD3	2.12	0.49
3:C:282:LEU:HD12	15:C:406:3PE:H321	1.94	0.49
4:D:196:LEU:HD11	16:D:501:HEC:HMB2	1.94	0.49
1:M:74:HIS:HB2	2:N:174:GLU:OE1	2.13	0.49
2:N:162:PHE:HE2	2:N:172:MET:HG2	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:497:GLU:HB3	2:N:501:ARG:HH12	1.77	0.49
4:P:111:ILE:HD11	4:P:258:ALA:HB1	1.95	0.49
7:S:61:ASN:O	7:S:65:LYS:HG3	2.13	0.49
3:C:34:TYR:HB2	13:C:410:CDL:HB32	1.95	0.48
3:C:94:MET:HG3	3:C:246:PHE:CD1	2.48	0.48
3:O:177:VAL:HG12	3:O:177:VAL:O	2.13	0.48
2:B:145:ILE:HD11	2:B:162:PHE:CZ	2.48	0.48
3:C:316:SER:HB2	3:C:318:TYR:CE2	2.48	0.48
4:D:198:GLY:HA3	4:D:217:TYR:HE2	1.78	0.48
1:M:218:MET:O	1:M:221:VAL:HG12	2.13	0.48
3:O:249:TRP:CH2	15:O:407:3PE:H342	2.48	0.48
1:A:224:GLN:N	1:A:224:GLN:OE1	2.46	0.48
1:A:116:THR:HG21	1:A:454:SER:HA	1.94	0.48
1:A:147:THR:OG1	1:A:196:ILE:HD13	2.13	0.48
1:A:292:VAL:HG13	1:A:296:PHE:HD2	1.78	0.48
15:C:407:3PE:H111	15:C:408:3PE:H241	1.93	0.48
13:C:410:CDL:H352	7:G:42:TRP:HA	1.96	0.48
2:N:145:ILE:HD11	2:N:162:PHE:CZ	2.48	0.48
3:O:143:GLY:H	3:O:146:SER:HB3	1.78	0.48
2:B:84:ASN:ND2	2:B:277:LEU:O	2.47	0.48
2:B:353:ARG:NH2	2:B:412:VAL:HA	2.29	0.48
1:A:160:GLU:HB3	2:B:419:ARG:HD2	1.94	0.48
1:A:215:LEU:HD11	1:A:255:LYS:HE2	1.95	0.48
2:B:468:ASN:HB2	2:B:472:LYS:HZ1	1.78	0.48
2:N:220:GLY:HA2	2:N:295:GLY:HA3	1.95	0.48
6:F:40:ASP:HB3	6:F:43:TYR:HB2	1.94	0.48
1:M:444:SER:O	1:M:448:LEU:HG	2.14	0.48
2:N:454:PRO:HG2	2:N:457:GLN:HG2	1.96	0.48
3:C:116:ARG:HH22	3:C:320:ARG:NH2	2.10	0.48
4:D:107:SER:HB3	4:D:159:PRO:HD2	1.94	0.48
4:D:200:ARG:NH1	4:D:217:TYR:OH	2.34	0.48
2:B:111:GLU:O	2:B:115:SER:HB2	2.13	0.48
2:B:327:VAL:HG11	2:B:473:ILE:HG13	1.96	0.48
5:E:133:PHE:O	5:E:136:SER:OG	2.22	0.48
8:T:63:LYS:HA	8:T:66:THR:HG22	1.96	0.48
8:H:9:GLN:OE1	8:H:9:GLN:N	2.46	0.47
2:N:72:VAL:HG13	2:N:73:GLU:H	1.79	0.47
3:O:207:LEU:CD2	14:O:404:HEM:HAA1	2.44	0.47
1:A:48:MET:HB2	1:A:51:ASP:HB2	1.95	0.47
1:A:140:GLU:O	1:A:143:ILE:HG22	2.14	0.47
4:D:213:HIS:NE2	4:D:226:PRO:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:311:LEU:HD11	3:O:369:PHE:HE1	1.79	0.47
4:P:75:TYR:HB3	8:T:65:PHE:CE2	2.48	0.47
3:C:35:TRP:HB3	3:C:105:ARG:HD3	1.95	0.47
6:R:111:LEU:HD12	6:R:111:LEU:O	2.13	0.47
1:A:191:ASP:HA	1:A:295:LEU:HD21	1.96	0.47
3:O:33:SER:HG	3:O:35:TRP:HD1	1.60	0.47
4:P:297:SER:OG	7:S:20:GLN:NE2	2.46	0.47
5:E:98:GLU:HB3	7:G:21:LYS:HD2	1.97	0.47
2:N:72:VAL:HG13	2:N:73:GLU:N	2.29	0.47
2:N:357:ARG:NH1	2:N:402:GLU:OE1	2.48	0.47
3:O:349:PRO:HB2	3:O:351:GLU:HG2	1.97	0.47
2:B:149:ILE:HG22	2:B:162:PHE:CD1	2.49	0.47
2:B:468:ASN:HA	2:B:471:THR:HG22	1.97	0.47
3:C:32:LEU:HB2	3:C:231:PHE:HE1	1.79	0.47
4:D:148:ARG:NH2	4:D:151:LYS:HG3	2.29	0.47
2:N:100:ILE:HD11	2:N:264:VAL:HG21	1.96	0.47
3:C:123:GLY:C	14:C:403:HEM:HBC2	2.34	0.47
3:C:378:VAL:HB	15:C:405:3PE:H32	1.96	0.47
1:M:355:GLN:HB3	1:M:401:PHE:HE2	1.79	0.47
1:M:390:ALA:HA	1:M:403:VAL:HA	1.95	0.47
2:N:76:LYS:HE3	2:N:78:LYS:HE3	1.96	0.47
1:A:498:ASP:OD1	1:A:519:ARG:NH2	2.43	0.47
2:B:300:ARG:HH12	2:N:301:HIS:H	1.63	0.47
3:C:139:VAL:HA	3:C:146:SER:HB2	1.96	0.47
4:D:293:SER:OG	7:G:20:GLN:OE1	2.33	0.47
2:N:149:ILE:HG22	2:N:162:PHE:HD1	1.80	0.47
2:N:497:GLU:O	2:N:501:ARG:HG2	2.15	0.47
4:P:64:ASP:OD1	4:P:65:GLU:N	2.48	0.47
8:T:58:LYS:HB3	8:T:58:LYS:HE2	1.61	0.47
3:C:34:TYR:OH	13:D:502:CDL:OB4	2.15	0.47
1:A:302:ASP:OD1	1:A:304:THR:HG23	2.15	0.47
1:M:430:VAL:O	10:W:15:ILE:HD11	2.15	0.47
5:Q:130:VAL:O	5:Q:134:VAL:HG23	2.15	0.47
3:C:190:TYR:CD2	3:O:190:TYR:CD2	3.04	0.46
3:C:283:PRO:HG2	15:C:406:3PE:H3B2	1.96	0.46
1:M:362:ASN:OD1	1:M:363:LYS:N	2.48	0.46
7:G:32:THR:O	7:G:36:HIS:ND1	2.40	0.46
2:B:301:HIS:H	2:N:300:ARG:NH1	2.10	0.46
4:D:97:VAL:O	4:D:101:VAL:HG22	2.15	0.46
1:M:238:PHE:O	1:M:241:THR:OG1	2.33	0.46
6:R:22:LYS:HE3	6:R:22:LYS:HB2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:HIS:NE2	1:A:395:TYR:OH	2.31	0.46
3:C:207:LEU:CD2	14:C:403:HEM:HAA1	2.46	0.46
7:G:71:ARG:HD2	8:H:48:GLN:HE22	1.81	0.46
5:Q:114:VAL:HG22	12:S:101:PC1:H252	1.98	0.46
3:C:105:ARG:HH22	14:C:403:HEM:HBD2	1.81	0.46
1:M:135:THR:HG23	1:M:262:LEU:HD23	1.97	0.46
2:N:209:GLN:O	2:N:213:LEU:HD23	2.16	0.46
1:A:114:THR:HG21	2:B:430:MET:HG3	1.98	0.46
1:M:117:VAL:HG21	1:M:186:VAL:HG13	1.97	0.46
2:N:335:MET:CE	2:N:406:ILE:HG21	2.45	0.46
5:E:127:ARG:NH2	10:K:39:GLN:HG3	2.29	0.46
1:M:83:ASP:OD1	1:M:83:ASP:N	2.45	0.46
2:N:86:LEU:HD11	2:N:277:LEU:HD13	1.98	0.46
4:P:94:GLY:HA2	4:P:97:VAL:HG12	1.97	0.46
2:B:383:ILE:CD1	2:B:403:LEU:HD11	2.46	0.46
6:F:15:TRP:HE3	6:F:16:LEU:HD22	1.81	0.46
1:A:96:THR:OG1	1:A:285:HIS:NE2	2.32	0.46
3:C:162:VAL:HG23	3:C:163:VAL:HG13	1.97	0.46
6:F:83:LEU:HD12	6:F:83:LEU:H	1.80	0.46
2:N:335:MET:HE1	2:N:406:ILE:HG21	1.97	0.46
3:O:60:TYR:OH	3:O:140:LEU:O	2.24	0.46
2:B:173:VAL:HG11	2:B:273:ALA:HB2	1.98	0.46
1:M:108:SER:OG	1:M:283:VAL:O	2.30	0.46
7:S:15:LEU:HB3	7:S:20:GLN:NE2	2.31	0.46
3:C:285:TYR:CE2	3:C:289:ARG:HD3	2.50	0.45
3:O:35:TRP:CB	3:O:105:ARG:HG3	2.46	0.45
1:M:87:ILE:HG22	2:N:96:PRO:HB3	1.99	0.45
1:A:321:GLU:OE1	1:A:323:ARG:NE	2.50	0.45
4:D:106:HIS:CD2	16:D:501:HEC:NC	2.84	0.45
1:M:357:MET:HB3	1:M:438:ALA:HB2	1.99	0.45
1:M:448:LEU:HD22	2:N:435:ARG:NH2	2.31	0.45
2:N:186:LEU:HD13	2:N:188:TRP:CZ2	2.51	0.45
5:Q:117:GLY:HA2	5:Q:120:PHE:CZ	2.51	0.45
2:B:124:ARG:HA	2:B:124:ARG:HD3	1.70	0.45
2:B:468:ASN:O	2:B:472:LYS:HE2	2.16	0.45
3:O:289:ARG:NH1	3:O:346:GLY:O	2.49	0.45
1:A:279:ALA:HB1	1:A:283:VAL:HG21	1.99	0.45
2:B:268:GLU:O	2:B:272:ILE:HG12	2.16	0.45
6:F:28:LEU:O	6:F:32:GLY:N	2.50	0.45
7:G:33:LYS:O	7:G:37:LYS:HG2	2.17	0.45
8:H:33:LYS:HB2	8:H:33:LYS:HE2	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:602:3PE:H3A2	13:M:603:CDL:H721	1.99	0.45
1:A:60:LYS:O	1:A:63:GLN:HG3	2.17	0.45
1:A:367:GLY:HA3	1:A:371:MET:HE2	1.99	0.45
13:M:603:CDL:H712	13:O:402:CDL:H332	1.98	0.45
3:O:56:LEU:HD13	14:O:403:HEM:HBA1	1.97	0.45
1:A:205:ASN:HB2	1:A:209:ARG:HH21	1.82	0.45
2:B:102:LEU:HD23	2:B:180:VAL:HG21	1.99	0.45
2:N:102:LEU:HD23	2:N:180:VAL:HG21	1.99	0.45
2:N:181:ARG:NH2	2:N:279:ASP:OD1	2.48	0.45
1:A:251:ALA:O	1:A:255:LYS:HG2	2.17	0.45
2:B:198:LYS:HB2	2:B:236:LEU:HD21	1.99	0.45
4:D:202:PRO:HB2	4:D:206:VAL:HG23	1.98	0.45
1:M:114:THR:OG1	2:N:433:GLU:OE2	2.31	0.45
2:N:478:ILE:HD11	2:N:503:PHE:HD1	1.81	0.45
8:T:60:VAL:HG12	8:T:60:VAL:O	2.15	0.45
4:D:276:VAL:CG1	5:E:121:VAL:HG13	2.47	0.45
8:H:30:ALA:O	8:H:34:ARG:HG3	2.16	0.45
3:O:82:TRP:CZ3	4:P:266:ARG:HG3	2.51	0.45
13:O:406:CDL:H241	13:O:406:CDL:H212	1.77	0.45
13:M:603:CDL:H122	13:O:402:CDL:HA32	1.98	0.45
1:A:417:TYR:HA	1:A:517:TRP:HH2	1.81	0.44
4:D:112:SER:HA	4:D:155:ARG:HA	2.00	0.44
7:G:56:TYR:O	7:G:60:GLN:HG2	2.16	0.44
1:M:239:GLN:HE21	1:M:318:THR:HG21	1.82	0.44
1:M:389:MET:O	1:M:403:VAL:C	2.55	0.44
1:M:460:ILE:HG12	1:M:470:ARG:HD2	1.97	0.44
12:M:604:PC1:O14	5:Q:119:ARG:NH2	2.50	0.44
3:O:222:MET:SD	3:O:222:MET:N	2.89	0.44
4:P:276:VAL:CG1	5:Q:121:VAL:HG13	2.47	0.44
2:N:299:ARG:HH21	2:N:493:VAL:HG23	1.83	0.44
3:O:230:TYR:O	4:P:292:TRP:NE1	2.46	0.44
4:P:300:LEU:HD13	4:P:302:LEU:HG	1.99	0.44
1:A:298:LYS:O	1:A:298:LYS:HG2	2.18	0.44
4:D:63:ALA:O	4:D:67:GLU:HG2	2.17	0.44
1:M:138:PHE:CE2	1:M:257:ILE:HG21	2.53	0.44
1:M:370:HIS:HB3	2:N:136:PHE:HD1	1.82	0.44
1:M:465:LEU:HD23	1:M:465:LEU:HA	1.85	0.44
4:P:240:THR:HG23	8:T:69:LYS:HD3	1.99	0.44
2:B:442:ILE:HG12	2:B:452:ARG:HE	1.83	0.44
3:C:105:ARG:HH12	14:C:403:HEM:HBD2	1.82	0.44
3:C:279:TRP:HA	3:C:282:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:ASP:O	6:F:45:LEU:HB2	2.17	0.44
4:P:175:PRO:HA	4:P:176:PRO:HD3	1.90	0.44
7:S:67:LYS:HB3	7:S:67:LYS:HE2	1.75	0.44
1:A:353:VAL:O	1:A:357:MET:HG2	2.18	0.44
3:C:284:ILE:HG23	3:C:301:ILE:HD12	1.99	0.44
9:J:18:LYS:HE2	9:J:18:LYS:HB3	1.82	0.44
1:M:464:LEU:HD23	1:M:464:LEU:HA	1.84	0.44
3:O:190:TYR:CD1	14:O:403:HEM:HMB3	2.53	0.44
4:D:291:ARG:HA	4:D:291:ARG:HD3	1.82	0.44
1:M:217:GLU:O	1:M:220:GLU:HG3	2.16	0.44
1:M:423:THR:HG22	1:M:496:ILE:HD13	2.00	0.44
5:Q:113:PHE:CZ	9:V:16:LEU:HB3	2.53	0.44
1:A:389:MET:O	1:A:403:VAL:C	2.56	0.44
2:B:201:LEU:HA	2:B:204:LEU:HD23	2.00	0.44
15:C:405:3PE:H251	6:F:16:LEU:HB3	2.00	0.44
3:O:300:ALA:O	3:O:304:VAL:HG23	2.18	0.44
5:Q:117:GLY:HA2	5:Q:120:PHE:CE1	2.52	0.44
3:O:102:HIS:HD2	14:O:404:HEM:C1C	2.36	0.44
2:B:398:ILE:O	2:B:402:GLU:HG2	2.18	0.43
2:N:115:SER:O	2:N:238:ARG:NH2	2.48	0.43
3:O:41:LEU:HD13	3:O:239:TRP:HD1	1.82	0.43
2:B:473:ILE:HD13	2:B:473:ILE:HA	1.90	0.43
3:C:50:ILE:HA	14:C:402:HEM:HAB	1.99	0.43
4:P:79:HIS:HB2	4:P:263:MET:HE1	1.99	0.43
8:T:13:LEU:HD23	8:T:13:LEU:HA	1.85	0.43
1:A:121:ILE:HB	1:A:175:THR:OG1	2.17	0.43
2:B:383:ILE:HD13	2:B:403:LEU:HD11	1.99	0.43
4:D:280:ALA:HB2	5:E:121:VAL:CG1	2.44	0.43
5:E:93:ASP:OD2	6:F:75:LYS:HD3	2.18	0.43
1:M:150:ARG:HA	1:M:150:ARG:HD3	1.66	0.43
1:M:451:ASP:O	1:M:455:PRO:HG2	2.19	0.43
3:O:35:TRP:HB2	3:O:105:ARG:HG3	2.00	0.43
3:O:383:PRO:HG3	6:R:35:TYR:CE2	2.54	0.43
2:B:130:THR:HG23	2:B:138:ILE:HD11	2.00	0.43
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.43
4:D:194:SER:O	4:D:198:GLY:N	2.43	0.43
1:M:479:ARG:HH22	2:N:53:PRO:HG2	1.83	0.43
7:S:42:TRP:O	7:S:46:THR:HG23	2.18	0.43
9:V:48:LYS:HA	9:V:48:LYS:HD3	1.60	0.43
1:A:132:THR:HB	1:A:135:THR:OG1	2.18	0.43
2:B:354:LEU:HB3	2:B:368:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:297:ASP:HB2	2:N:496:TYR:HB2	2.00	0.43
3:C:375:LEU:HD23	15:C:405:3PE:O32	2.19	0.43
4:D:225:MET:HE2	4:D:225:MET:HB2	1.72	0.43
13:D:502:CDL:HA62	7:G:26:LEU:O	2.19	0.43
7:G:72:TYR:HE2	8:H:43:LYS:HA	1.83	0.43
1:M:127:PHE:CD2	1:M:309:LEU:HD22	2.52	0.43
2:N:372:ASN:HB3	2:N:381:PHE:HD1	1.84	0.43
3:O:214:ASN:ND2	3:O:220:SER:HB3	2.34	0.43
1:A:287:ASP:O	1:A:290:GLU:HG3	2.18	0.43
1:A:324:MET:HG2	7:G:11:VAL:HG22	2.01	0.43
2:B:425:LYS:HG3	2:B:462:VAL:HG11	1.99	0.43
4:D:198:GLY:HA3	4:D:217:TYR:CE2	2.54	0.43
6:F:11:PRO:HB3	6:F:18:ALA:HA	2.00	0.43
2:B:157:GLN:HG3	2:B:444:ARG:NH1	2.33	0.43
6:R:105:ARG:O	6:R:109:GLU:HG2	2.19	0.43
1:A:84:HIS:O	1:A:88:LEU:HG	2.19	0.43
1:M:215:LEU:HD23	1:M:215:LEU:HA	1.89	0.43
1:M:320:SER:O	1:M:502:ALA:HA	2.19	0.43
12:A:602:PC1:H143	9:J:21:MET:HB3	2.01	0.42
2:B:300:ARG:HD3	2:N:300:ARG:HH11	1.84	0.42
3:C:232:TYR:OH	13:C:401:CDL:HA32	2.18	0.42
3:O:32:LEU:HB2	3:O:231:PHE:HE1	1.84	0.42
1:A:205:ASN:OD1	1:A:206:ARG:N	2.52	0.42
1:A:357:MET:HB2	1:A:357:MET:HE2	1.82	0.42
2:B:82:LEU:O	2:B:85:GLY:N	2.33	0.42
2:B:255:PRO:O	2:B:285:ARG:NH1	2.52	0.42
1:M:62:ARG:NH1	1:M:62:ARG:HB2	2.34	0.42
1:M:133:ASN:HD21	1:M:245:ARG:HB2	1.84	0.42
1:A:431:SER:O	1:A:435:VAL:HG23	2.19	0.42
1:M:253:ASN:O	1:M:253:ASN:ND2	2.50	0.42
3:O:70:SER:O	3:O:73:HIS:HB3	2.19	0.42
3:O:264:ILE:HD11	4:P:185:ARG:HH22	1.83	0.42
2:B:413:THR:HG22	2:B:415:VAL:H	1.85	0.42
3:C:186:PHE:HE2	3:O:186:PHE:HE2	1.67	0.42
9:J:16:LEU:O	9:J:20:VAL:HG12	2.20	0.42
9:V:15:SER:O	9:V:19:VAL:HG23	2.20	0.42
2:B:121:LEU:HD12	2:B:121:LEU:HA	1.92	0.42
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.91	0.42
8:H:28:TYR:CE2	8:H:32:ILE:HD11	2.55	0.42
1:M:353:VAL:O	1:M:357:MET:HG2	2.19	0.42
2:N:109:ILE:HG13	2:N:110:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:340:SER:HB2	2:N:359:LEU:HD13	2.02	0.42
4:P:85:SER:HB2	9:V:50:TRP:CZ2	2.55	0.42
3:C:108:TYR:HD2	3:C:332:PHE:CD2	2.38	0.42
4:D:122:THR:OG1	4:D:125:GLU:HG3	2.20	0.42
2:N:121:LEU:HD12	2:N:121:LEU:HA	1.82	0.42
5:Q:138:SER:OG	5:Q:139:ALA:N	2.52	0.42
1:A:96:THR:HG1	1:A:285:HIS:HE2	1.61	0.42
3:C:204:LEU:HD12	3:C:204:LEU:HA	1.86	0.42
8:H:13:LEU:HD23	8:H:13:LEU:HA	1.82	0.42
2:N:149:ILE:HG22	2:N:162:PHE:CD1	2.55	0.42
1:A:114:THR:OG1	2:B:433:GLU:OE2	2.36	0.42
3:O:204:LEU:HD12	3:O:204:LEU:HA	1.87	0.42
9:V:64:VAL:HG13	9:V:67:GLN:HB2	2.01	0.42
2:B:356:LEU:O	2:B:360:ASN:HB2	2.20	0.42
3:C:111:SER:OG	14:C:403:HEM:O1D	2.23	0.42
1:M:227:GLU:OE1	1:M:227:GLU:HA	2.20	0.42
2:N:212:LEU:HD23	2:N:212:LEU:HA	1.75	0.42
2:B:149:ILE:HG22	2:B:162:PHE:HD1	1.84	0.41
3:C:85:ARG:NH1	14:C:402:HEM:O2D	2.53	0.41
4:D:199:TYR:OH	4:D:225:MET:HG3	2.19	0.41
1:M:96:THR:OG1	1:M:285:HIS:NE2	2.39	0.41
1:M:299:LEU:HD23	1:M:299:LEU:HA	1.84	0.41
2:N:332:GLN:HE21	2:N:371:PHE:HA	1.84	0.41
7:S:56:TYR:CE1	7:S:60:GLN:NE2	2.88	0.41
1:A:41:ALA:N	1:A:42:PRO:HD2	2.35	0.41
1:A:463:GLN:OE1	1:A:470:ARG:HG3	2.20	0.41
4:D:272:LYS:NZ	9:J:39:GLU:OE2	2.34	0.41
8:H:31:CYS:O	8:H:35:ILE:HG12	2.20	0.41
1:M:370:HIS:O	2:N:139:VAL:HG11	2.20	0.41
2:N:140:ARG:HD3	2:N:140:ARG:HA	1.67	0.41
2:N:253:THR:O	2:N:257:MET:HG3	2.19	0.41
3:C:140:LEU:HD23	3:C:140:LEU:HA	1.83	0.41
9:J:15:SER:O	9:J:19:VAL:HG23	2.21	0.41
1:M:96:THR:HG1	1:M:285:HIS:HE2	1.65	0.41
1:M:325:LEU:HD11	1:M:510:GLN:NE2	2.35	0.41
3:O:36:TRP:HE3	3:O:36:TRP:H	1.69	0.41
3:O:333:TRP:CE3	7:S:48:LEU:HD12	2.55	0.41
8:T:61:ALA:HB3	8:T:62:PRO:HD3	2.02	0.41
2:B:197:VAL:HA	2:B:200:GLU:HG2	2.02	0.41
2:B:432:LEU:HD23	2:B:432:LEU:HA	1.74	0.41
2:B:460:LYS:O	2:B:464:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:LYS:HA	5:E:132:LYS:HD3	1.85	0.41
1:A:409:PRO:HB3	1:A:508:PRO:HB2	2.03	0.41
2:B:177:VAL:O	2:B:181:ARG:HG2	2.21	0.41
1:M:428:TYR:CE1	1:M:524:TRP:HB2	2.56	0.41
2:N:116:SER:O	2:N:235:ALA:HB1	2.21	0.41
3:O:178:ASP:CG	3:O:179:ASN:H	2.24	0.41
4:P:136:VAL:HG12	4:P:147:THR:HG22	2.02	0.41
6:R:44:ASP:HB3	6:R:47:VAL:HG23	2.01	0.41
8:T:52:TYR:O	8:T:56:VAL:HG23	2.21	0.41
2:B:100:ILE:HG22	2:B:176:LEU:HD12	2.03	0.41
3:C:327:ILE:HD12	15:F:201:3PE:H362	2.03	0.41
6:F:14:ASN:HB3	6:F:17:ALA:HB3	2.02	0.41
1:M:133:ASN:ND2	1:M:245:ARG:HB2	2.35	0.41
1:M:138:PHE:HD2	1:M:262:LEU:HD21	1.85	0.41
3:O:12:LYS:HE2	3:O:12:LYS:HB3	1.96	0.41
2:B:145:ILE:HD11	2:B:162:PHE:HZ	1.84	0.41
2:B:219:ALA:HB2	2:B:298:PHE:HB2	2.03	0.41
8:H:20:LYS:NZ	8:H:20:LYS:HB3	2.36	0.41
1:M:526:ARG:HE	15:M:602:3PE:H221	1.86	0.41
2:N:304:SER:HA	2:N:489:ASP:OD1	2.21	0.41
4:P:97:VAL:O	4:P:101:VAL:HG12	2.20	0.41
4:P:225:MET:HB3	16:P:501:HEC:C1D	2.50	0.41
2:B:120:HIS:O	2:B:123:GLU:HG2	2.21	0.41
2:B:354:LEU:HD23	2:B:354:LEU:HA	1.84	0.41
4:D:249:LYS:HD2	8:H:68:LEU:HD23	2.03	0.41
1:M:352:MET:O	1:M:355:GLN:HG3	2.20	0.41
12:M:604:PC1:H361	13:O:402:CDL:H122	2.01	0.41
2:N:447:LEU:HA	2:N:447:LEU:HD23	1.85	0.41
3:O:108:TYR:HD2	3:O:332:PHE:CD2	2.38	0.41
3:O:316:SER:O	6:R:43:TYR:OH	2.34	0.41
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.90	0.41
2:B:162:PHE:HE2	2:B:172:MET:HG2	1.83	0.41
2:B:321:LYS:HE3	2:B:321:LYS:HB3	1.81	0.41
4:D:100:GLU:OE1	4:D:234:VAL:HG23	2.21	0.41
4:D:279:LEU:HD13	15:G:101:3PE:H2B1	2.03	0.41
6:F:83:LEU:O	6:F:87:GLN:HG2	2.20	0.41
1:M:138:PHE:CE2	1:M:262:LEU:HD11	2.55	0.41
1:M:202:PHE:HB2	1:M:259:LYS:HG3	2.03	0.41
2:N:95:ASN:HA	2:N:96:PRO:HD3	1.93	0.41
2:N:145:ILE:HD11	2:N:162:PHE:CE2	2.56	0.41
15:O:409:3PE:H282	15:O:409:3PE:H2B2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:80:VAL:O	5:Q:84:LYS:HG3	2.20	0.41
2:N:82:LEU:HD23	2:N:82:LEU:HA	1.91	0.41
2:N:216:ILE:HD11	2:N:310:ALA:CB	2.52	0.41
3:O:179:ASN:O	3:O:179:ASN:ND2	2.54	0.41
6:R:97:MET:HE2	6:R:97:MET:HB2	1.92	0.41
12:S:101:PC1:H153	12:S:101:PC1:H112	1.88	0.41
8:T:18:LYS:HB3	8:T:19:PRO:HD3	2.03	0.41
2:B:116:SER:O	2:B:235:ALA:HB1	2.21	0.40
3:C:71:VAL:CG1	3:C:85:ARG:HE	2.35	0.40
3:C:297:GLY:O	3:C:301:ILE:HG12	2.19	0.40
15:C:406:3PE:H3B2	15:C:406:3PE:H381	1.95	0.40
1:M:41:ALA:N	1:M:42:PRO:HD2	2.36	0.40
1:M:138:PHE:CZ	1:M:207:ILE:HG23	2.54	0.40
6:R:9:LEU:O	6:R:14:ASN:HB2	2.20	0.40
1:A:218:MET:O	1:A:221:VAL:HG12	2.21	0.40
2:B:274:GLU:HB3	2:B:275:PRO:HD3	2.03	0.40
3:C:141:PRO:HG3	14:C:402:HEM:O1A	2.21	0.40
2:N:300:ARG:O	2:N:487:TYR:HA	2.21	0.40
3:O:19:LEU:HG	3:O:23:LEU:HD12	2.03	0.40
3:O:291:ILE:HG23	3:O:297:GLY:HA2	2.03	0.40
3:O:355:VAL:O	3:O:359:GLN:HG3	2.21	0.40
4:P:306:ASN:ND2	6:R:34:ARG:HH21	2.19	0.40
2:B:499:VAL:O	2:B:503:PHE:HD1	2.05	0.40
3:C:90:ASN:O	3:C:94:MET:HG2	2.22	0.40
3:C:246:PHE:CZ	3:C:250:ILE:HD11	2.55	0.40
1:M:150:ARG:HB3	1:M:155:LEU:HB2	2.03	0.40
1:M:389:MET:O	1:M:404:TYR:HB3	2.21	0.40
2:N:422:LYS:HD2	2:N:422:LYS:HA	1.89	0.40
3:O:160:ILE:H	3:O:160:ILE:HG12	1.72	0.40
6:R:45:LEU:HD23	6:R:45:LEU:HA	1.93	0.40
12:A:602:PC1:H131	5:E:112:TYR:CE2	2.56	0.40
3:C:341:LEU:HD11	7:G:55:THR:HG21	2.03	0.40
4:D:193:PHE:HB2	4:D:252:VAL:HG21	2.03	0.40
6:F:115:PRO:O	3:O:6:GLN:NE2	2.54	0.40
9:J:58:ARG:HH12	9:J:60:GLU:HG2	1.85	0.40
2:N:356:LEU:O	2:N:360:ASN:HB2	2.21	0.40
3:O:105:ARG:NH1	14:O:404:HEM:HBD2	2.31	0.40
3:O:139:VAL:HA	3:O:146:SER:OG	2.20	0.40
3:O:373:PRO:O	3:O:377:ARG:HG3	2.21	0.40
12:A:602:PC1:H252	12:A:602:PC1:H321	2.02	0.40
2:B:447:LEU:HD23	2:B:447:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:282:LEU:HD23	3:C:282:LEU:HA	1.86	0.40
1:M:150:ARG:NH1	1:M:158:GLU:OE2	2.54	0.40
2:N:363:GLN:OE1	2:N:363:GLN:N	2.49	0.40
3:O:10:LEU:HA	3:O:13:GLU:HG2	2.04	0.40
4:P:196:LEU:HD11	16:P:501:HEC:HMB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/527 (92%)	450 (93%)	35 (7%)	0	100	100
1	M	485/527 (92%)	451 (93%)	34 (7%)	0	100	100
2	B	455/506 (90%)	411 (90%)	42 (9%)	2 (0%)	34	69
2	N	453/506 (90%)	406 (90%)	47 (10%)	0	100	100
3	C	386/393 (98%)	365 (95%)	21 (5%)	0	100	100
3	O	386/393 (98%)	363 (94%)	23 (6%)	0	100	100
4	D	242/306 (79%)	233 (96%)	9 (4%)	0	100	100
4	P	242/306 (79%)	229 (95%)	13 (5%)	0	100	100
5	E	75/271 (28%)	68 (91%)	7 (9%)	0	100	100
5	Q	72/271 (27%)	66 (92%)	6 (8%)	0	100	100
6	F	114/122 (93%)	111 (97%)	3 (3%)	0	100	100
6	R	113/122 (93%)	109 (96%)	4 (4%)	0	100	100
7	G	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
7	S	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
8	H	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
8	T	62/69 (90%)	55 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	58/72 (81%)	54 (93%)	4 (7%)	0	100	100
9	V	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
10	K	29/81 (36%)	25 (86%)	4 (14%)	0	100	100
10	W	30/81 (37%)	28 (93%)	2 (7%)	0	100	100
All	All	3943/4838 (82%)	3671 (93%)	270 (7%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	435	ARG
2	B	113	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	A	407/438 (93%)	405 (100%)	2 (0%)	88	95
1	M	407/438 (93%)	405 (100%)	2 (0%)	88	95
2	B	378/414 (91%)	378 (100%)	0	100	100
2	N	377/414 (91%)	376 (100%)	1 (0%)	92	96
3	C	333/338 (98%)	331 (99%)	2 (1%)	86	94
3	O	333/338 (98%)	332 (100%)	1 (0%)	92	96
4	D	198/247 (80%)	196 (99%)	2 (1%)	76	90
4	P	198/247 (80%)	198 (100%)	0	100	100
5	E	65/233 (28%)	65 (100%)	0	100	100
5	Q	62/233 (27%)	62 (100%)	0	100	100
6	F	102/107 (95%)	101 (99%)	1 (1%)	76	90
6	R	101/107 (94%)	101 (100%)	0	100	100
7	G	64/65 (98%)	64 (100%)	0	100	100
7	S	64/65 (98%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	60/63 (95%)	60 (100%)	0	100 100
8	T	59/63 (94%)	59 (100%)	0	100 100
9	J	49/59 (83%)	49 (100%)	0	100 100
9	V	49/59 (83%)	49 (100%)	0	100 100
10	K	21/66 (32%)	21 (100%)	0	100 100
10	W	22/66 (33%)	22 (100%)	0	100 100
All	All	3349/4060 (82%)	3338 (100%)	11 (0%)	92 96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	520	ARG
3	C	179	ASN
3	C	259	HIS
4	D	305	VAL
4	D	306	ASN
6	F	119	ARG
1	M	253	ASN
1	M	520	ARG
2	N	435	ARG
3	O	179	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
2	B	84	ASN
2	B	332	GLN
4	D	95	HIS
4	D	96	GLN
7	S	20	GLN
8	T	48	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CDL	P	502	-	62,62,99	0.37	0	68,74,111	0.44	0
15	3PE	W	101	-	27,27,50	0.40	0	30,32,55	0.40	0
12	PC1	M	604	-	39,39,53	0.34	0	45,47,61	0.37	0
13	CDL	A	603	-	68,68,99	0.35	0	74,80,111	0.32	0
13	CDL	C	401	-	63,63,99	0.37	0	69,75,111	0.34	0
15	3PE	C	407	-	32,32,50	0.37	0	35,37,55	0.32	0
13	CDL	M	603	-	69,69,99	0.36	0	75,81,111	0.38	0
15	3PE	O	407	-	38,38,50	0.34	0	41,43,55	0.35	0
14	HEM	C	403	3	41,50,50	1.30	4 (9%)	45,82,82	1.76	9 (20%)
15	3PE	O	401	-	35,35,50	0.36	0	38,40,55	0.40	0
15	3PE	C	405	-	28,28,50	0.40	0	31,33,55	0.41	0
15	3PE	F	202	-	50,50,50	0.31	0	53,55,55	0.31	0
15	3PE	O	405	-	29,29,50	0.38	0	32,34,55	0.34	0
14	HEM	C	402	3	41,50,50	1.29	4 (9%)	45,82,82	1.82	11 (24%)
15	3PE	C	408	-	26,26,50	0.40	0	29,31,55	0.34	0
15	3PE	M	602	-	44,44,50	0.32	0	47,49,55	0.33	0
13	CDL	O	406	-	63,63,99	0.37	0	69,75,111	0.41	0
15	3PE	O	408	-	32,32,50	0.37	0	35,37,55	0.34	0
15	3PE	G	101	-	36,36,50	0.35	0	39,41,55	0.31	0
15	3PE	C	406	-	44,44,50	0.32	0	47,49,55	0.37	0
13	CDL	S	102	-	54,54,99	0.39	0	60,66,111	0.38	0
15	3PE	O	409	-	50,50,50	0.30	0	53,55,55	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	HEC	P	501	4	32,50,50	2.08	4 (12%)	24,82,82	2.31	14 (58%)
15	3PE	F	201	-	31,31,50	0.39	0	34,36,55	0.54	0
13	CDL	C	410	-	58,58,99	0.38	0	64,70,111	0.33	0
12	PC1	A	602	-	37,37,53	0.35	0	43,45,61	0.28	0
15	3PE	C	409	-	33,33,50	0.37	0	36,38,55	0.33	0
13	CDL	D	502	-	67,67,99	0.36	0	73,79,111	0.36	0
13	CDL	O	402	-	80,80,99	0.34	0	86,92,111	0.38	0
14	HEM	O	403	3	41,50,50	1.33	4 (9%)	45,82,82	1.84	11 (24%)
14	HEM	O	404	3	41,50,50	1.33	4 (9%)	45,82,82	1.74	8 (17%)
15	3PE	W	102	-	27,27,50	0.40	0	30,32,55	0.36	0
16	HEC	D	501	4	32,50,50	2.13	4 (12%)	24,82,82	2.32	14 (58%)
12	PC1	S	101	-	37,37,53	0.34	0	43,45,61	0.34	0
15	3PE	C	404	-	37,37,50	0.35	0	40,42,55	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	P	502	-	-	16/73/73/110	-
15	3PE	W	101	-	-	7/31/31/54	-
12	PC1	M	604	-	-	6/43/43/57	-
13	CDL	A	603	-	-	17/79/79/110	-
13	CDL	C	401	-	-	11/74/74/110	-
15	3PE	C	407	-	-	8/36/36/54	-
13	CDL	M	603	-	-	10/80/80/110	-
15	3PE	O	407	-	-	10/42/42/54	-
14	HEM	C	403	3	-	6/12/54/54	-
15	3PE	O	401	-	-	13/39/39/54	-
15	3PE	C	405	-	-	8/32/32/54	-
15	3PE	F	202	-	-	13/54/54/54	-
15	3PE	O	405	-	-	5/33/33/54	-
14	HEM	C	402	3	-	3/12/54/54	-
15	3PE	C	408	-	-	11/30/30/54	-
15	3PE	M	602	-	-	16/48/48/54	-
13	CDL	O	406	-	-	17/74/74/110	-
15	3PE	O	408	-	-	7/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	3PE	G	101	-	-	6/40/40/54	-
15	3PE	C	406	-	-	15/48/48/54	-
13	CDL	S	102	-	-	17/65/65/110	-
15	3PE	O	409	-	-	6/54/54/54	-
16	HEC	P	501	4	-	2/10/54/54	-
15	3PE	F	201	-	-	9/35/35/54	-
13	CDL	C	410	-	-	8/69/69/110	-
12	PC1	A	602	-	-	6/41/41/57	-
15	3PE	C	409	-	-	5/37/37/54	-
13	CDL	D	502	-	-	19/78/78/110	-
13	CDL	O	402	-	-	16/91/91/110	-
14	HEM	O	403	3	-	8/12/54/54	-
14	HEM	O	404	3	-	7/12/54/54	-
15	3PE	W	102	-	-	9/31/31/54	-
16	HEC	D	501	4	-	2/10/54/54	-
12	PC1	S	101	-	-	7/41/41/57	-
15	3PE	C	404	-	-	10/41/41/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3C-C2C	-6.87	1.33	1.40
16	P	501	HEC	C3C-C2C	-6.77	1.33	1.40
16	D	501	HEC	C2B-C3B	-6.75	1.33	1.40
16	P	501	HEC	C2B-C3B	-6.58	1.33	1.40
14	O	403	HEM	C4D-ND	-3.96	1.33	1.40
14	C	402	HEM	C4D-ND	-3.88	1.33	1.40
14	C	403	HEM	C4D-ND	-3.75	1.33	1.40
14	O	404	HEM	C4D-ND	-3.72	1.33	1.40
14	O	403	HEM	C1B-NB	-3.56	1.34	1.40
14	C	402	HEM	C1B-NB	-3.52	1.34	1.40
14	O	404	HEM	C1B-NB	-3.49	1.34	1.40
16	P	501	HEC	CBC-CAC	-3.46	1.36	1.49
14	C	403	HEM	C1B-NB	-3.45	1.34	1.40
16	D	501	HEC	CBC-CAC	-3.42	1.36	1.49
14	O	404	HEM	C1D-ND	-2.76	1.33	1.38
14	O	403	HEM	C1D-ND	-2.76	1.33	1.38
14	C	402	HEM	C1D-ND	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	403	HEM	C1D-ND	-2.64	1.33	1.38
16	D	501	HEC	CBB-CAB	-2.35	1.40	1.49
16	P	501	HEC	CBB-CAB	-2.34	1.40	1.49
14	O	403	HEM	C4B-NB	-2.21	1.34	1.38
14	C	402	HEM	C4B-NB	-2.14	1.34	1.38
14	O	404	HEM	C4B-NB	-2.11	1.34	1.38
14	C	403	HEM	C4B-NB	-2.06	1.34	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	403	HEM	CHC-C4B-NB	4.83	129.68	124.43
14	C	402	HEM	CHC-C4B-NB	4.76	129.60	124.43
14	C	402	HEM	CHB-C1B-NB	4.42	129.85	124.38
16	D	501	HEC	CMD-C2D-C1D	-4.38	121.72	128.46
14	O	404	HEM	CHB-C1B-NB	4.34	129.74	124.38
16	P	501	HEC	CMD-C2D-C1D	-4.33	121.81	128.46
14	O	403	HEM	CHB-C1B-NB	4.29	129.68	124.38
14	C	403	HEM	CHB-C1B-NB	4.22	129.59	124.38
14	O	404	HEM	CHC-C4B-NB	4.21	129.01	124.43
14	C	403	HEM	CHC-C4B-NB	4.14	128.93	124.43
14	C	403	HEM	C4D-ND-C1D	4.04	109.24	105.07
14	O	404	HEM	C4D-ND-C1D	3.95	109.15	105.07
14	O	403	HEM	C4D-ND-C1D	3.72	108.92	105.07
14	C	402	HEM	C4D-ND-C1D	3.54	108.73	105.07
14	O	403	HEM	C1B-NB-C4B	3.25	108.44	105.07
16	D	501	HEC	CMB-C2B-C1B	-3.23	123.50	128.46
14	O	403	HEM	CHA-C4D-ND	3.20	128.33	124.38
16	P	501	HEC	CMB-C2B-C1B	-3.20	123.55	128.46
14	C	402	HEM	CHA-C4D-ND	3.15	128.28	124.38
16	D	501	HEC	CMC-C2C-C3C	3.14	129.51	125.82
14	C	402	HEM	C1B-NB-C4B	3.13	108.31	105.07
16	P	501	HEC	CMC-C2C-C3C	3.12	129.49	125.82
16	P	501	HEC	CMB-C2B-C3B	3.10	129.46	125.82
16	P	501	HEC	CBA-CAA-C2A	3.07	117.78	112.60
16	D	501	HEC	CMB-C2B-C3B	2.97	129.31	125.82
16	D	501	HEC	C4C-C3C-C2C	2.90	109.48	106.35
14	C	402	HEM	CHD-C1D-ND	2.89	127.57	124.43
14	C	403	HEM	CHD-C1D-ND	2.89	127.57	124.43
16	P	501	HEC	O1D-CGD-CBD	-2.86	113.88	123.08
14	O	404	HEM	CHD-C1D-ND	2.86	127.53	124.43
16	D	501	HEC	O1D-CGD-CBD	-2.85	113.92	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	404	HEM	CHB-C1B-C2B	-2.83	118.89	126.72
16	D	501	HEC	CBD-CAD-C3D	2.78	117.37	112.62
16	P	501	HEC	C4C-C3C-C2C	2.77	109.34	106.35
14	C	403	HEM	CHB-C1B-C2B	-2.76	119.08	126.72
16	P	501	HEC	CBD-CAD-C3D	2.75	117.31	112.62
16	D	501	HEC	CBA-CAA-C2A	2.69	117.14	112.60
16	D	501	HEC	CMD-C2D-C3D	2.69	130.01	124.94
14	C	403	HEM	CHA-C4D-ND	2.67	127.68	124.38
14	O	403	HEM	CHD-C1D-ND	2.64	127.30	124.43
16	D	501	HEC	CMC-C2C-C1C	-2.62	124.44	128.46
16	P	501	HEC	CMD-C2D-C3D	2.58	129.81	124.94
14	O	403	HEM	C4B-C3B-C2B	-2.57	105.08	107.11
14	O	404	HEM	C1B-NB-C4B	2.56	107.72	105.07
16	P	501	HEC	CMC-C2C-C1C	-2.56	124.53	128.46
14	C	403	HEM	CBA-CAA-C2A	-2.55	108.27	112.62
14	C	403	HEM	C1B-NB-C4B	2.51	107.67	105.07
14	O	404	HEM	CAD-C3D-C4D	2.48	129.00	124.66
14	C	402	HEM	C4B-C3B-C2B	-2.48	105.15	107.11
14	C	402	HEM	CHB-C1B-C2B	-2.45	119.94	126.72
14	O	403	HEM	CBA-CAA-C2A	-2.44	108.46	112.62
16	D	501	HEC	CMA-C3A-C2A	2.42	129.51	124.94
16	D	501	HEC	C2B-C3B-C4B	2.41	108.95	106.35
14	O	403	HEM	CHB-C1B-C2B	-2.31	120.34	126.72
14	O	404	HEM	CHA-C4D-ND	2.28	127.20	124.38
16	P	501	HEC	C2B-C3B-C4B	2.27	108.81	106.35
16	D	501	HEC	O1A-CGA-CBA	-2.26	115.81	123.08
14	O	403	HEM	CAA-CBA-CGA	-2.25	107.46	113.76
14	C	402	HEM	CAA-CBA-CGA	-2.22	107.53	113.76
16	P	501	HEC	O1A-CGA-CBA	-2.22	115.94	123.08
14	C	402	HEM	CBA-CAA-C2A	-2.10	109.04	112.62
16	P	501	HEC	CMA-C3A-C2A	2.08	128.86	124.94
14	C	403	HEM	O2A-CGA-CBA	2.06	120.66	114.03
14	C	402	HEM	O2A-CGA-CBA	2.06	120.64	114.03
16	P	501	HEC	O2A-CGA-O1A	2.06	128.42	123.30
16	D	501	HEC	O2A-CGA-O1A	2.04	128.40	123.30
14	O	403	HEM	CAD-CBD-CGD	-2.00	109.29	113.60

There are no chirality outliers.

All (336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	602	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
12	S	101	PC1	C1-O11-P-O12
12	S	101	PC1	C1-O11-P-O14
12	S	101	PC1	C1-O11-P-O13
13	A	603	CDL	CB2-OB2-PB2-OB3
13	A	603	CDL	CB2-OB2-PB2-OB4
13	A	603	CDL	CB2-OB2-PB2-OB5
13	A	603	CDL	CB3-OB5-PB2-OB2
13	A	603	CDL	CB3-OB5-PB2-OB3
13	A	603	CDL	CB3-OB5-PB2-OB4
13	C	401	CDL	CA3-OA5-PA1-OA3
13	C	401	CDL	CB2-OB2-PB2-OB4
13	C	401	CDL	CB3-OB5-PB2-OB2
13	C	401	CDL	CB3-OB5-PB2-OB3
13	C	401	CDL	CB3-OB5-PB2-OB4
13	C	410	CDL	CA3-OA5-PA1-OA3
13	C	410	CDL	CB3-OB5-PB2-OB3
13	C	410	CDL	CB3-OB5-PB2-OB4
13	D	502	CDL	CA2-OA2-PA1-OA3
13	D	502	CDL	CB2-OB2-PB2-OB4
13	D	502	CDL	CB2-OB2-PB2-OB5
13	D	502	CDL	CB3-OB5-PB2-OB2
13	D	502	CDL	CB3-OB5-PB2-OB3
13	D	502	CDL	CB3-OB5-PB2-OB4
13	O	402	CDL	CA3-OA5-PA1-OA3
13	O	402	CDL	CB2-OB2-PB2-OB3
13	O	402	CDL	CB3-OB5-PB2-OB4
13	O	406	CDL	CA3-OA5-PA1-OA3
13	O	406	CDL	CB3-OB5-PB2-OB3
13	P	502	CDL	CA2-OA2-PA1-OA5
13	P	502	CDL	CA3-OA5-PA1-OA4
13	P	502	CDL	CB2-OB2-PB2-OB3
13	P	502	CDL	CB2-OB2-PB2-OB4
13	S	102	CDL	CA2-OA2-PA1-OA4
13	S	102	CDL	CA3-OA5-PA1-OA4
14	O	403	HEM	C2A-CAA-CBA-CGA
15	C	404	3PE	C11-O13-P-O14
15	C	404	3PE	O13-C11-C12-N
15	C	405	3PE	O13-C11-C12-N
15	C	405	3PE	O21-C2-C3-O31
15	C	406	3PE	C1-O11-P-O14
15	C	407	3PE	C1-O11-P-O12
15	C	407	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
15	C	407	3PE	C1-O11-P-O14
15	C	407	3PE	O13-C11-C12-N
15	C	408	3PE	C1-O11-P-O12
15	C	408	3PE	C11-O13-P-O14
15	C	409	3PE	C1-O11-P-O12
15	C	409	3PE	C1-O11-P-O13
15	C	409	3PE	C1-O11-P-O14
15	F	201	3PE	C1-O11-P-O14
15	F	201	3PE	C12-C11-O13-P
15	F	202	3PE	C11-O13-P-O11
15	F	202	3PE	O13-C11-C12-N
15	G	101	3PE	C1-O11-P-O12
15	G	101	3PE	C11-O13-P-O11
15	G	101	3PE	C11-O13-P-O12
15	G	101	3PE	C11-O13-P-O14
15	M	602	3PE	C1-O11-P-O12
15	M	602	3PE	C1-O11-P-O14
15	M	602	3PE	O13-C11-C12-N
15	O	405	3PE	C11-O13-P-O11
15	O	405	3PE	C11-O13-P-O12
15	O	405	3PE	C11-O13-P-O14
15	O	407	3PE	C11-O13-P-O11
15	O	407	3PE	C11-O13-P-O12
15	O	407	3PE	C11-O13-P-O14
15	O	407	3PE	O13-C11-C12-N
15	O	408	3PE	O13-C11-C12-N
15	W	101	3PE	C1-O11-P-O12
15	W	101	3PE	C11-O13-P-O14
15	W	101	3PE	C2-C1-O11-P
15	W	101	3PE	O13-C11-C12-N
15	W	102	3PE	C1-O11-P-O14
15	W	102	3PE	C11-O13-P-O14
15	W	102	3PE	O13-C11-C12-N
13	C	401	CDL	O1-C1-CA2-OA2
14	C	402	HEM	C2A-CAA-CBA-CGA
12	M	604	PC1	C31-C32-C33-C34
13	C	401	CDL	CA3-OA5-PA1-OA2
13	C	401	CDL	CB2-OB2-PB2-OB5
13	C	410	CDL	CB3-OB5-PB2-OB2
13	D	502	CDL	CA2-OA2-PA1-OA5
13	M	603	CDL	CB2-OB2-PB2-OB5
13	O	402	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
13	O	406	CDL	CA2-OA2-PA1-OA5
13	O	406	CDL	CA3-OA5-PA1-OA2
13	P	502	CDL	CB2-OB2-PB2-OB5
13	S	102	CDL	CA2-OA2-PA1-OA5
15	C	404	3PE	C11-O13-P-O11
15	C	406	3PE	C1-O11-P-O13
15	C	406	3PE	C11-O13-P-O11
15	C	407	3PE	C11-O13-P-O11
15	C	408	3PE	C1-O11-P-O13
15	F	201	3PE	C11-O13-P-O11
15	G	101	3PE	C1-O11-P-O13
15	M	602	3PE	C1-O11-P-O13
15	M	602	3PE	C11-O13-P-O11
15	O	401	3PE	C1-O11-P-O13
15	O	401	3PE	C11-O13-P-O11
15	W	101	3PE	C1-O11-P-O13
15	W	101	3PE	C11-O13-P-O11
15	W	102	3PE	C1-O11-P-O13
15	W	102	3PE	C11-O13-P-O11
15	O	407	3PE	C21-C22-C23-C24
15	C	406	3PE	C28-C29-C2A-C2B
15	C	408	3PE	C21-C22-C23-C24
13	P	502	CDL	C53-C54-C55-C56
13	D	502	CDL	CB7-C71-C72-C73
13	A	603	CDL	C16-C17-C18-C19
13	O	406	CDL	C11-C12-C13-C14
15	C	405	3PE	C23-C24-C25-C26
15	C	406	3PE	C3E-C3F-C3G-C3H
15	F	202	3PE	C31-C32-C33-C34
13	O	402	CDL	C22-C23-C24-C25
15	C	405	3PE	C21-C22-C23-C24
15	F	202	3PE	C33-C34-C35-C36
13	O	402	CDL	C53-C54-C55-C56
13	O	406	CDL	OB5-CB3-CB4-OB6
13	S	102	CDL	OB5-CB3-CB4-OB6
13	O	402	CDL	C57-C58-C59-C60
13	O	402	CDL	C62-C63-C64-C65
12	A	602	PC1	C11-O13-P-O11
13	C	410	CDL	CA3-OA5-PA1-OA2
13	S	102	CDL	CA3-OA5-PA1-OA2
15	C	408	3PE	C11-O13-P-O11
15	F	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
13	S	102	CDL	OB5-CB3-CB4-CB6
15	C	406	3PE	O11-C1-C2-C3
13	C	401	CDL	CB2-C1-CA2-OA2
14	O	404	HEM	C4D-C3D-CAD-CBD
15	C	408	3PE	C2-C1-O11-P
15	C	408	3PE	O11-C1-C2-O21
13	D	502	CDL	OA6-CA4-CA6-OA8
13	M	603	CDL	CA7-C31-C32-C33
15	M	602	3PE	C21-C22-C23-C24
13	A	603	CDL	OA5-CA3-CA4-CA6
13	D	502	CDL	OB5-CB3-CB4-CB6
13	O	406	CDL	OB5-CB3-CB4-CB6
15	C	404	3PE	O11-C1-C2-C3
15	C	408	3PE	O11-C1-C2-C3
15	O	408	3PE	O11-C1-C2-C3
15	O	401	3PE	O13-C11-C12-N
15	O	408	3PE	O21-C21-C22-C23
15	F	202	3PE	C3F-C3G-C3H-C3I
13	M	603	CDL	CA4-CA3-OA5-PA1
15	C	406	3PE	C2-C1-O11-P
15	M	602	3PE	C2B-C2C-C2D-C2E
13	D	502	CDL	CA3-CA4-CA6-OA8
13	P	502	CDL	CA3-OA5-PA1-OA2
13	A	603	CDL	OB5-CB3-CB4-OB6
15	C	409	3PE	O11-C1-C2-O21
13	M	603	CDL	C52-C53-C54-C55
13	A	603	CDL	CA4-CA3-OA5-PA1
15	F	201	3PE	C2-C1-O11-P
13	P	502	CDL	C32-C31-CA7-OA8
12	A	602	PC1	C24-C25-C26-C27
14	O	404	HEM	C2D-C3D-CAD-CBD
15	O	401	3PE	O11-C1-C2-C3
14	C	403	HEM	C2B-C3B-CAB-CBB
14	O	403	HEM	C2B-C3B-CAB-CBB
14	O	404	HEM	C2B-C3B-CAB-CBB
13	C	401	CDL	C1-CB2-OB2-PB2
15	C	405	3PE	C1-C2-C3-O31
13	O	402	CDL	OB5-CB3-CB4-OB6
15	O	407	3PE	O31-C31-C32-C33
13	S	102	CDL	OB6-CB4-CB6-OB8
12	S	101	PC1	C23-C24-C25-C26
13	O	402	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
15	M	602	3PE	C24-C25-C26-C27
13	P	502	CDL	C1-CB2-OB2-PB2
15	C	404	3PE	C2-C1-O11-P
15	O	401	3PE	C2-C1-O11-P
12	A	602	PC1	C11-O13-P-O14
13	C	410	CDL	CA3-OA5-PA1-OA4
13	D	502	CDL	CA2-OA2-PA1-OA4
13	D	502	CDL	CB2-OB2-PB2-OB3
13	M	603	CDL	CB2-OB2-PB2-OB3
13	O	402	CDL	CB2-OB2-PB2-OB4
13	O	402	CDL	CB3-OB5-PB2-OB3
13	O	406	CDL	CA2-OA2-PA1-OA3
13	O	406	CDL	CA3-OA5-PA1-OA4
13	O	406	CDL	CB3-OB5-PB2-OB4
13	P	502	CDL	CA2-OA2-PA1-OA4
13	P	502	CDL	CA3-OA5-PA1-OA3
13	S	102	CDL	CA2-OA2-PA1-OA3
13	S	102	CDL	CA3-OA5-PA1-OA3
15	C	404	3PE	C11-O13-P-O12
15	C	406	3PE	C1-O11-P-O12
15	C	406	3PE	C11-O13-P-O14
15	C	407	3PE	C11-O13-P-O12
15	C	407	3PE	C11-O13-P-O14
15	C	408	3PE	C11-O13-P-O12
15	F	201	3PE	C1-O11-P-O12
15	F	201	3PE	C11-O13-P-O14
15	F	202	3PE	C11-O13-P-O12
15	M	602	3PE	C11-O13-P-O12
15	M	602	3PE	C11-O13-P-O14
15	O	401	3PE	C1-O11-P-O12
15	O	401	3PE	C1-O11-P-O14
15	O	401	3PE	C11-O13-P-O14
15	W	102	3PE	C1-O11-P-O12
15	W	102	3PE	C11-O13-P-O12
15	O	409	3PE	C31-C32-C33-C34
15	O	409	3PE	O13-C11-C12-N
15	W	101	3PE	C12-C11-O13-P
13	A	603	CDL	OA5-CA3-CA4-OA6
13	D	502	CDL	OB5-CB3-CB4-OB6
13	P	502	CDL	OB5-CB3-CB4-OB6
15	C	404	3PE	O11-C1-C2-O21
15	C	406	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
15	O	401	3PE	O11-C1-C2-O21
15	O	408	3PE	O11-C1-C2-O21
13	C	401	CDL	C1-CA2-OA2-PA1
15	F	202	3PE	C2C-C2D-C2E-C2F
15	O	408	3PE	C24-C25-C26-C27
15	F	201	3PE	C1-C2-O21-C21
13	O	402	CDL	OB5-CB3-CB4-CB6
13	P	502	CDL	OB5-CB3-CB4-CB6
15	C	409	3PE	O11-C1-C2-C3
12	S	101	PC1	C22-C23-C24-C25
15	M	602	3PE	C25-C26-C27-C28
13	A	603	CDL	CA2-OA2-PA1-OA5
13	O	406	CDL	CB3-OB5-PB2-OB2
13	S	102	CDL	CB3-OB5-PB2-OB2
15	C	405	3PE	C1-O11-P-O13
15	F	202	3PE	C1-O11-P-O13
15	O	409	3PE	C11-O13-P-O11
15	F	202	3PE	C36-C37-C38-C39
15	O	401	3PE	C1-C2-C3-O31
15	F	202	3PE	C34-C35-C36-C37
15	C	407	3PE	C2-C1-O11-P
15	F	202	3PE	C39-C3A-C3B-C3C
15	C	408	3PE	O13-C11-C12-N
14	O	404	HEM	C4B-C3B-CAB-CBB
13	M	603	CDL	C20-C21-C22-C23
14	O	403	HEM	CAD-CBD-CGD-O1D
15	C	404	3PE	O21-C2-C3-O31
15	O	401	3PE	O21-C2-C3-O31
13	O	406	CDL	C1-CB2-OB2-PB2
15	M	602	3PE	C2-C1-O11-P
15	O	405	3PE	O31-C31-C32-C33
13	O	402	CDL	C75-C76-C77-C78
15	C	404	3PE	C1-C2-C3-O31
13	C	410	CDL	C55-C56-C57-C58
14	O	403	HEM	CAD-CBD-CGD-O2D
13	M	603	CDL	CA6-CA4-OA6-CA5
13	O	406	CDL	CB6-CB4-OB6-CB5
13	P	502	CDL	CA6-CA4-OA6-CA5
13	S	102	CDL	CA3-CA4-OA6-CA5
15	O	408	3PE	C23-C24-C25-C26
15	M	602	3PE	C2A-C2B-C2C-C2D
15	C	406	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
13	A	603	CDL	C32-C31-CA7-OA8
15	O	409	3PE	C3C-C3D-C3E-C3F
15	W	102	3PE	C1-C2-C3-O31
14	O	403	HEM	C3D-CAD-CBD-CGD
15	W	102	3PE	O21-C21-C22-C23
15	O	409	3PE	C28-C29-C2A-C2B
13	P	502	CDL	C12-C13-C14-C15
14	C	402	HEM	CAD-CBD-CGD-O2D
16	P	501	HEC	CAD-CBD-CGD-O2D
13	A	603	CDL	OB5-CB3-CB4-CB6
14	C	403	HEM	CAD-CBD-CGD-O1D
14	C	403	HEM	CAD-CBD-CGD-O2D
15	O	409	3PE	C39-C3A-C3B-C3C
14	C	403	HEM	CAA-CBA-CGA-O2A
12	A	602	PC1	C1-O11-P-O13
15	C	406	3PE	C3-C2-O21-C21
13	O	406	CDL	C21-C22-C23-C24
14	O	403	HEM	CAA-CBA-CGA-O2A
12	S	101	PC1	O31-C31-C32-C33
15	O	407	3PE	C26-C27-C28-C29
14	C	402	HEM	CAD-CBD-CGD-O1D
13	O	402	CDL	C1-CB2-OB2-PB2
13	O	406	CDL	CA3-CA4-CA6-OA8
16	P	501	HEC	CAD-CBD-CGD-O1D
13	D	502	CDL	C32-C31-CA7-OA8
13	S	102	CDL	C32-C31-CA7-OA8
15	O	408	3PE	O22-C21-C22-C23
14	O	404	HEM	CAA-CBA-CGA-O2A
14	C	403	HEM	C4B-C3B-CAB-CBB
14	O	403	HEM	C4B-C3B-CAB-CBB
15	O	401	3PE	O31-C31-C32-C33
14	O	403	HEM	CAA-CBA-CGA-O1A
14	O	404	HEM	CAA-CBA-CGA-O1A
13	O	406	CDL	OA6-CA4-CA6-OA8
14	C	403	HEM	CAA-CBA-CGA-O1A
12	M	604	PC1	O31-C31-C32-C33
13	A	603	CDL	C72-C71-CB7-OB8
14	O	404	HEM	C3D-CAD-CBD-CGD
12	M	604	PC1	C32-C33-C34-C35
15	O	407	3PE	C33-C34-C35-C36
13	D	502	CDL	C32-C31-CA7-OA9
15	O	401	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
13	A	603	CDL	C20-C21-C22-C23
15	O	407	3PE	C25-C26-C27-C28
15	O	405	3PE	C2-C1-O11-P
12	S	101	PC1	O32-C31-C32-C33
12	M	604	PC1	C1-O11-P-O14
13	M	603	CDL	CA2-OA2-PA1-OA3
13	O	402	CDL	CA2-OA2-PA1-OA3
15	F	202	3PE	C1-O11-P-O14
15	M	602	3PE	O21-C21-C22-C23
16	D	501	HEC	CAD-CBD-CGD-O2D
15	C	406	3PE	O13-C11-C12-N
15	F	201	3PE	O13-C11-C12-N
13	S	102	CDL	C32-C31-CA7-OA9
13	P	502	CDL	C32-C31-CA7-OA9
13	O	406	CDL	CB3-CB4-OB6-CB5
13	S	102	CDL	CA6-CA4-OA6-CA5
15	C	404	3PE	C12-C11-O13-P
15	C	405	3PE	C12-C11-O13-P
15	C	406	3PE	C1-C2-O21-C21
15	C	408	3PE	C12-C11-O13-P
15	F	202	3PE	C12-C11-O13-P
15	M	602	3PE	C12-C11-O13-P
15	G	101	3PE	C21-C22-C23-C24
15	O	407	3PE	O32-C31-C32-C33
12	A	602	PC1	C22-C23-C24-C25
16	D	501	HEC	CAD-CBD-CGD-O1D
13	C	410	CDL	CA5-C11-C12-C13
13	M	603	CDL	C12-C11-CA5-OA6
13	S	102	CDL	C33-C34-C35-C36
13	A	603	CDL	C1-CB2-OB2-PB2
12	M	604	PC1	O32-C31-C32-C33
13	D	502	CDL	C72-C71-CB7-OB8
13	S	102	CDL	C12-C11-CA5-OA6
13	M	603	CDL	C12-C11-CA5-OA7
13	S	102	CDL	C12-C11-CA5-OA7
12	M	604	PC1	O21-C21-C22-C23
13	D	502	CDL	C52-C51-CB5-OB6
13	D	502	CDL	C72-C71-CB7-OB9
15	M	602	3PE	O22-C21-C22-C23
15	C	405	3PE	C22-C23-C24-C25
15	C	406	3PE	O31-C31-C32-C33

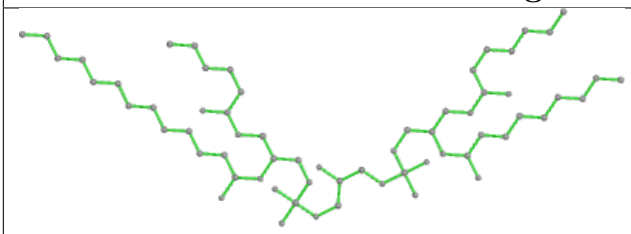
There are no ring outliers.

29 monomers are involved in 79 short contacts:

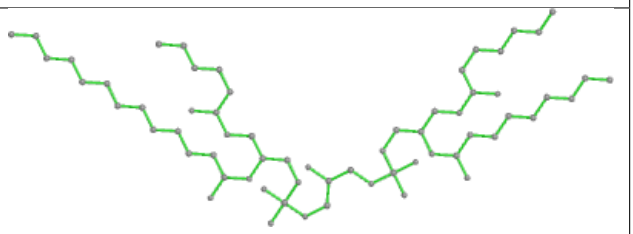
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	502	CDL	2	0
12	M	604	PC1	6	0
13	A	603	CDL	1	0
13	C	401	CDL	3	0
15	C	407	3PE	2	0
13	M	603	CDL	6	0
15	O	407	3PE	1	0
14	C	403	HEM	5	0
15	O	401	3PE	1	0
15	C	405	3PE	4	0
14	C	402	HEM	3	0
15	C	408	3PE	3	0
15	M	602	3PE	2	0
13	O	406	CDL	1	0
15	G	101	3PE	1	0
15	C	406	3PE	4	0
13	S	102	CDL	2	0
15	O	409	3PE	3	0
16	P	501	HEC	4	0
15	F	201	3PE	3	0
13	C	410	CDL	2	0
12	A	602	PC1	3	0
15	C	409	3PE	1	0
13	D	502	CDL	2	0
13	O	402	CDL	9	0
14	O	403	HEM	3	0
14	O	404	HEM	6	0
16	D	501	HEC	6	0
12	S	101	PC1	2	0

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

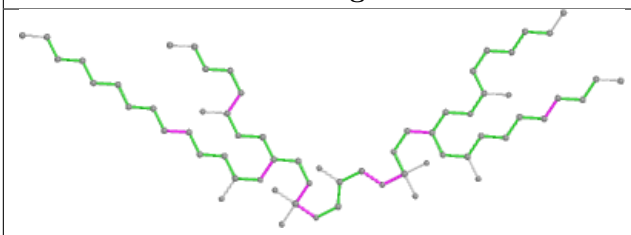
Ligand CDL P 502



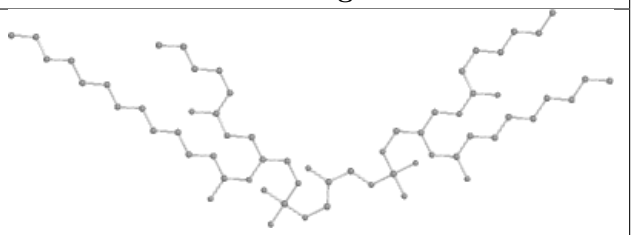
Bond lengths



Bond angles

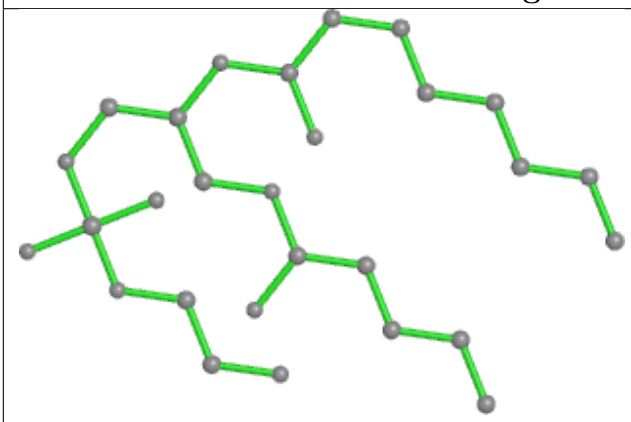


Torsions

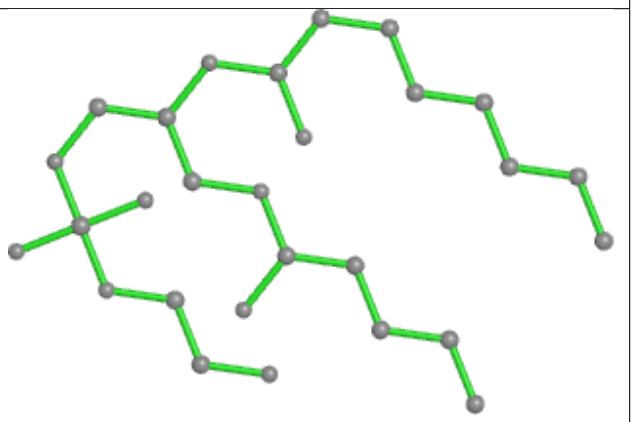


Rings

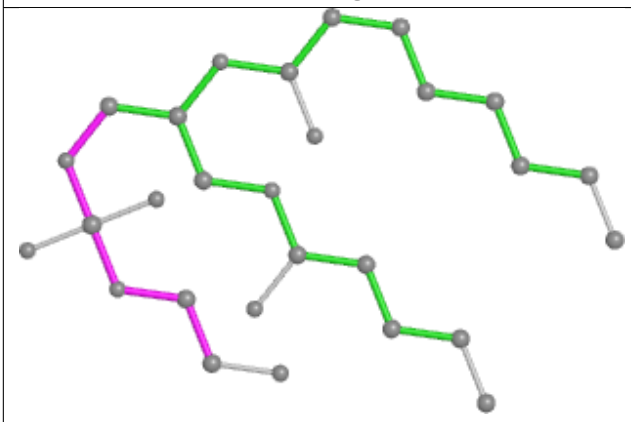
Ligand 3PE W 101



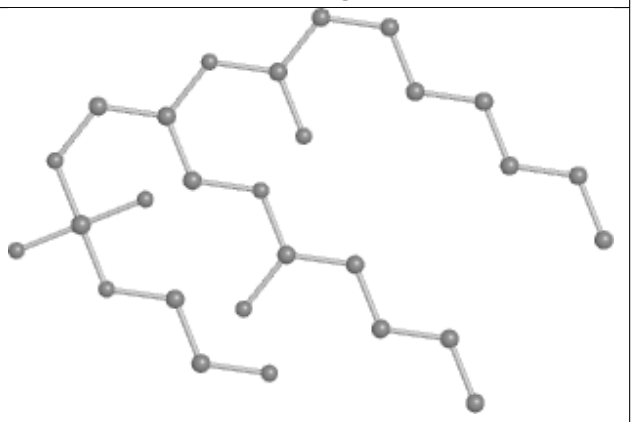
Bond lengths



Bond angles

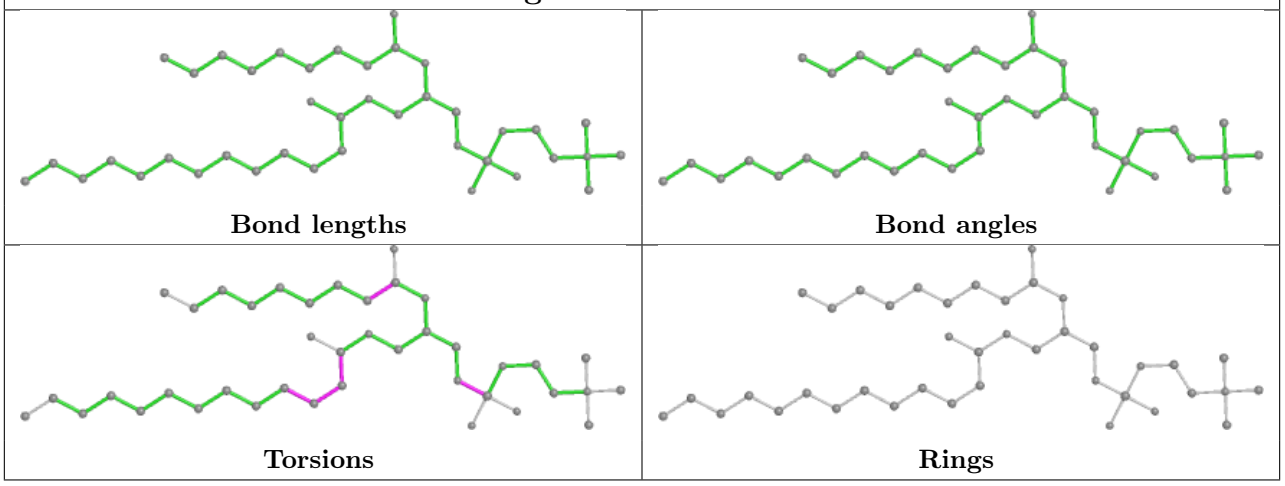


Torsions

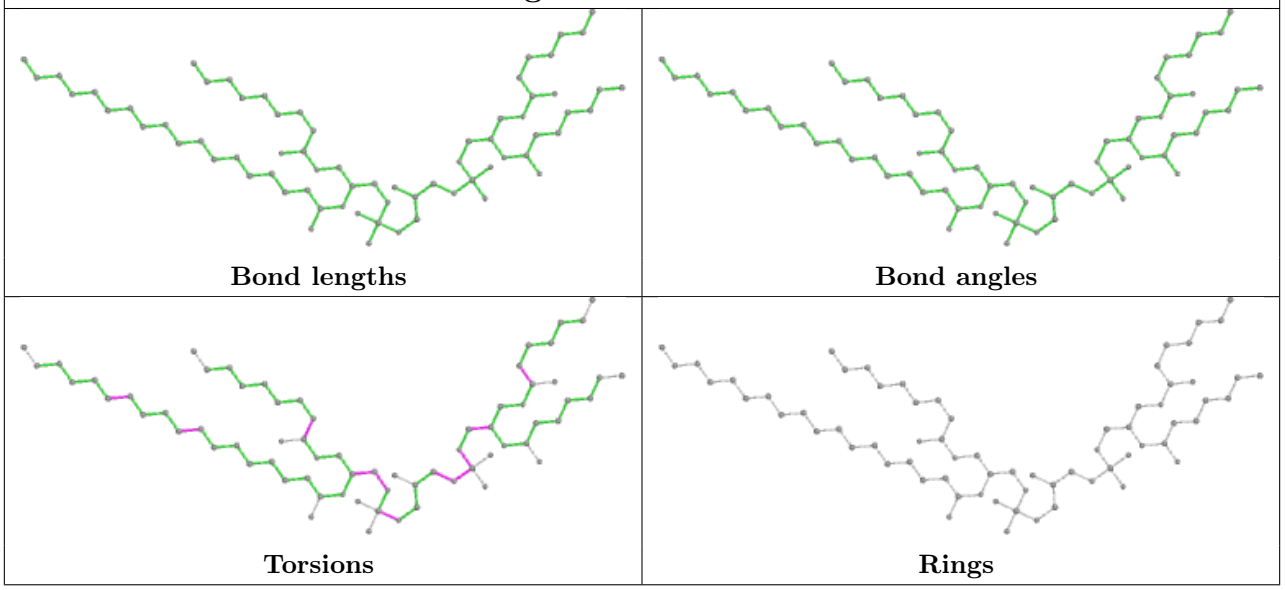


Rings

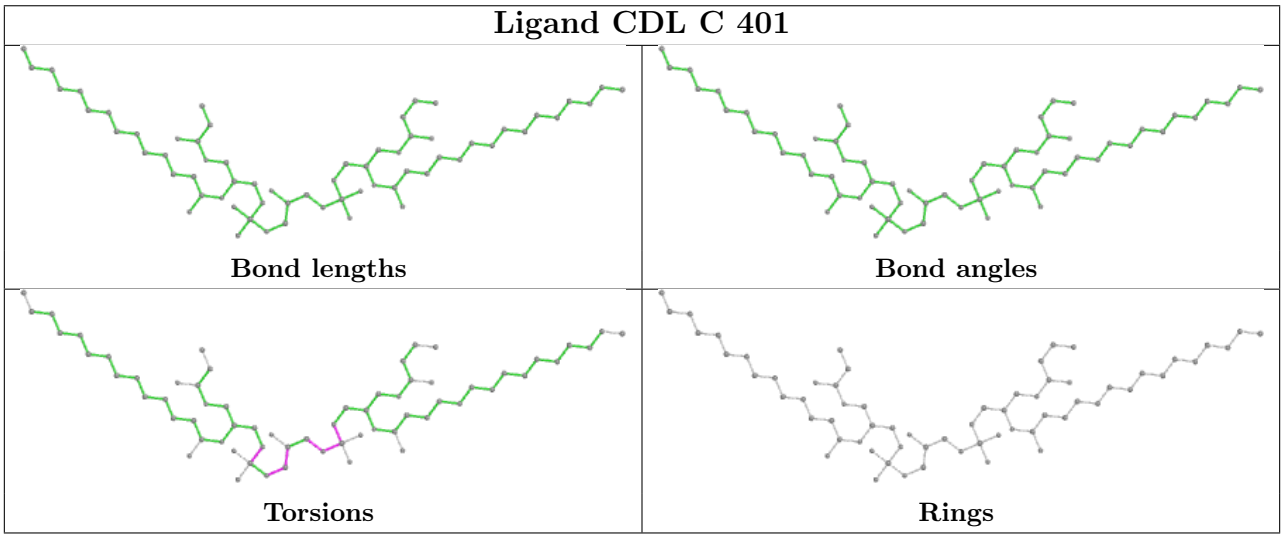
Ligand PC1 M 604



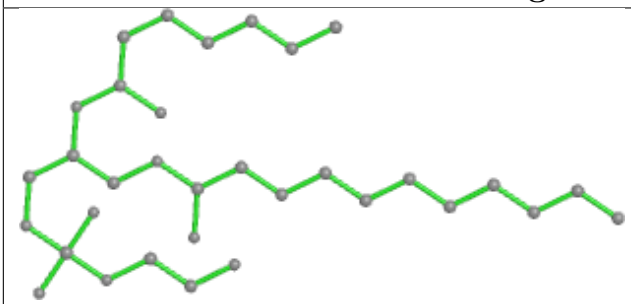
Ligand CDL A 603



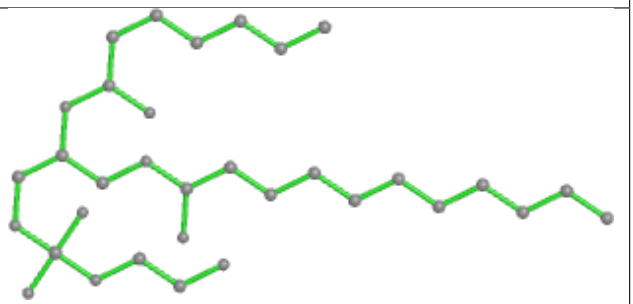
Ligand CDL C 401



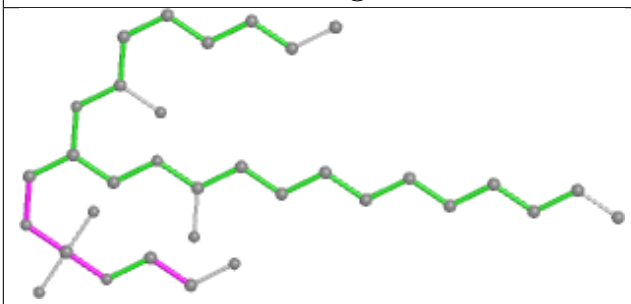
Ligand 3PE C 407



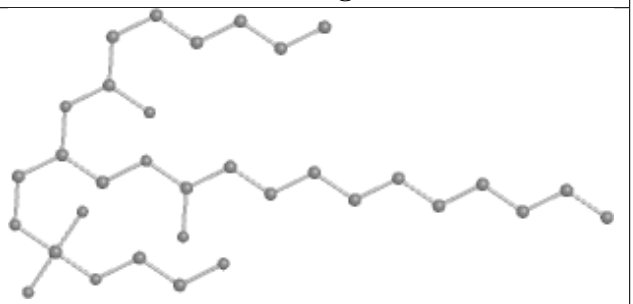
Bond lengths



Bond angles

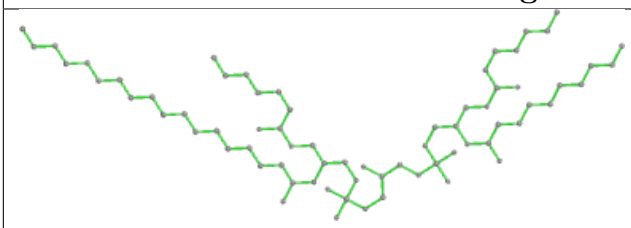


Torsions



Rings

Ligand CDL M 603



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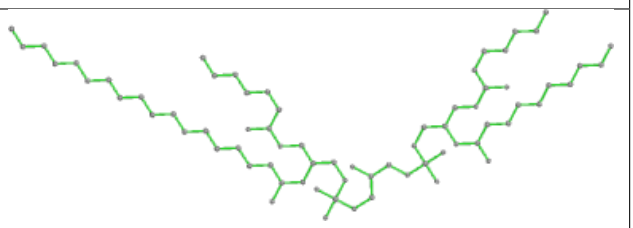
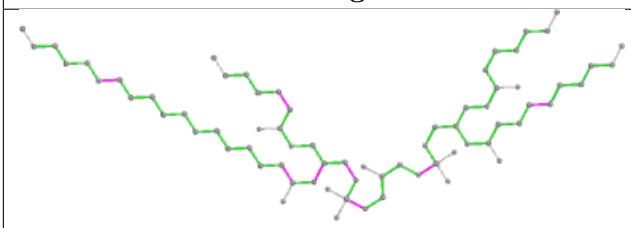


Bond angles



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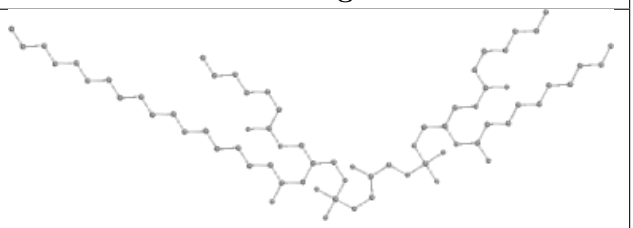
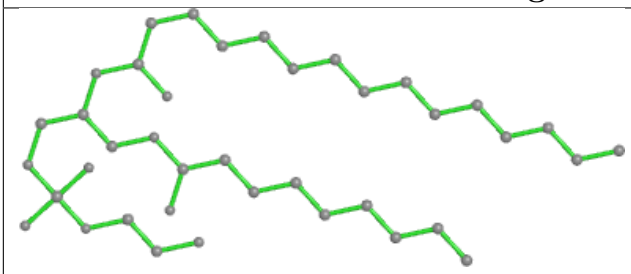


Rings

Ligand 3PE O 407



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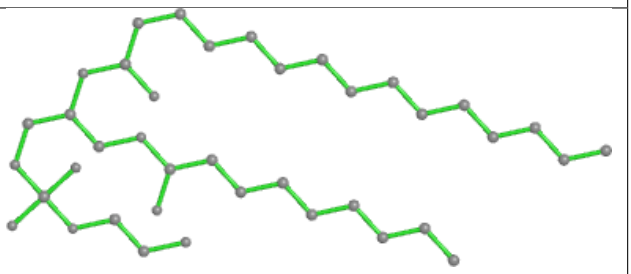
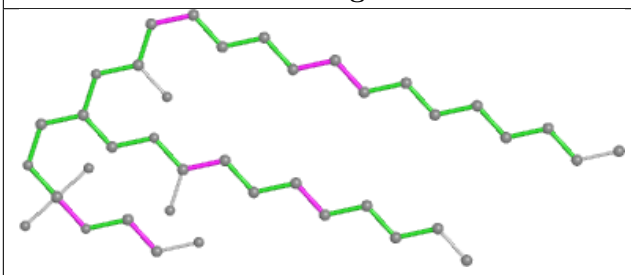


Bond angles



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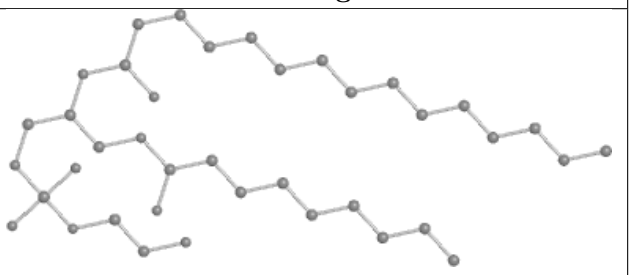
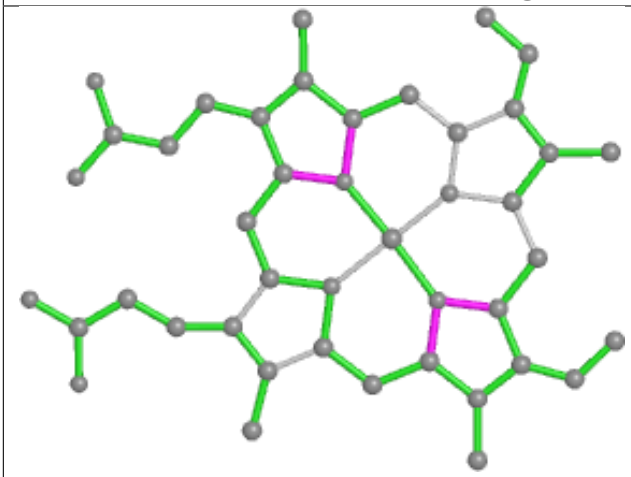


Rings

Ligand HEM C 403



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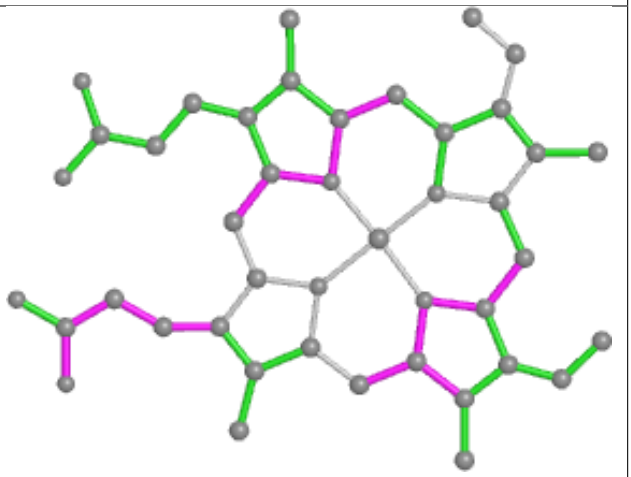
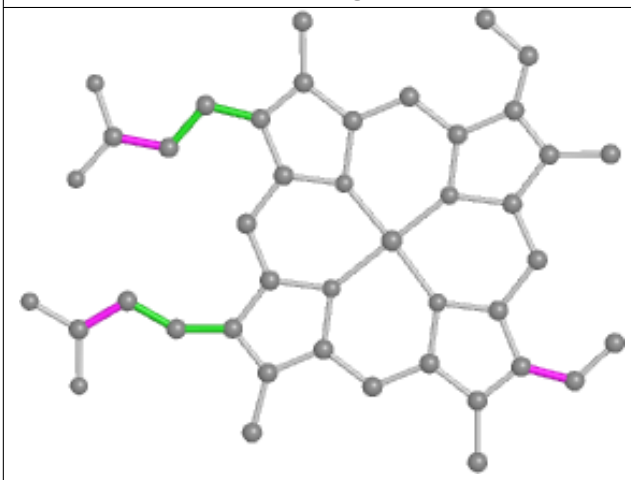


Bond angles



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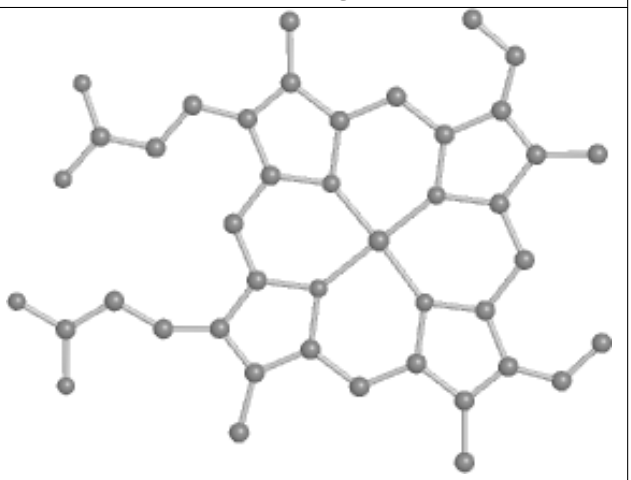
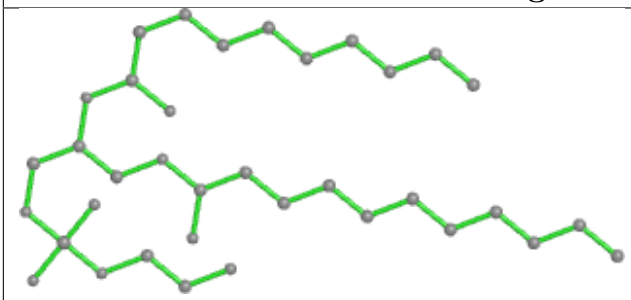


Rings

Ligand 3PE O 401



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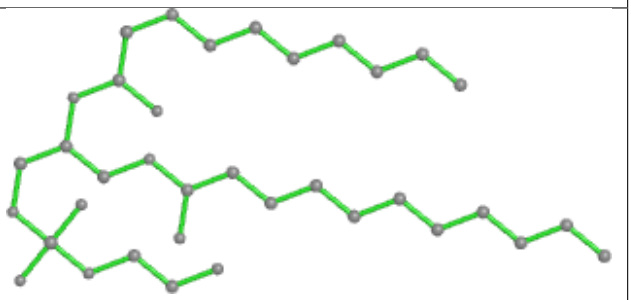
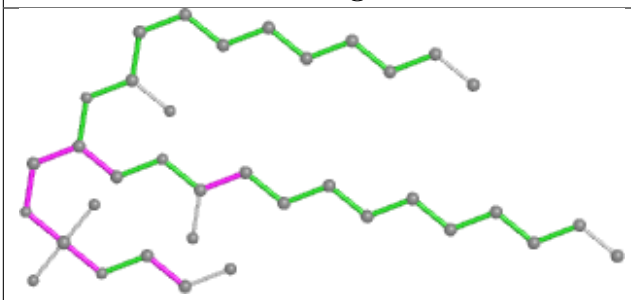


Bond angles



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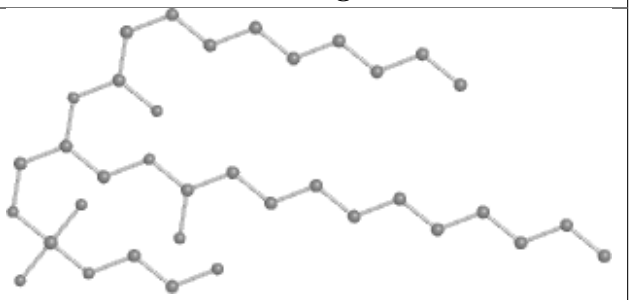
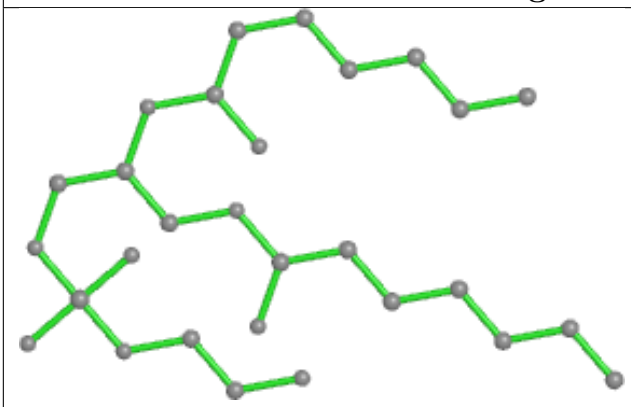


Rings

Ligand 3PE C 405



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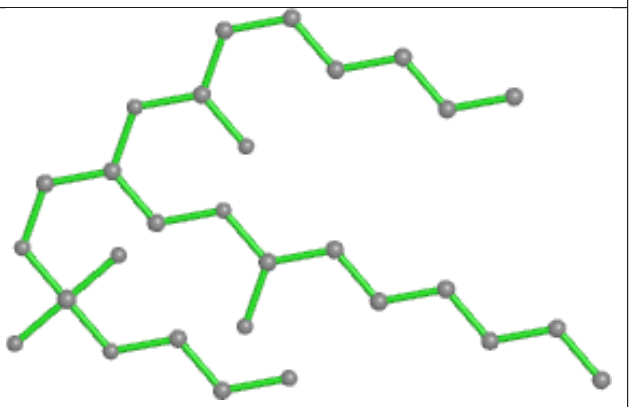
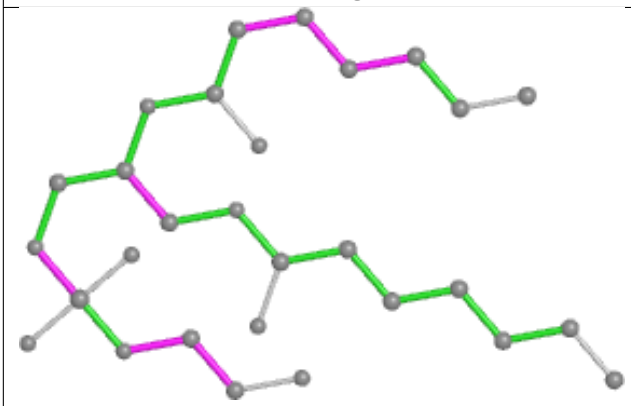


Bond angles



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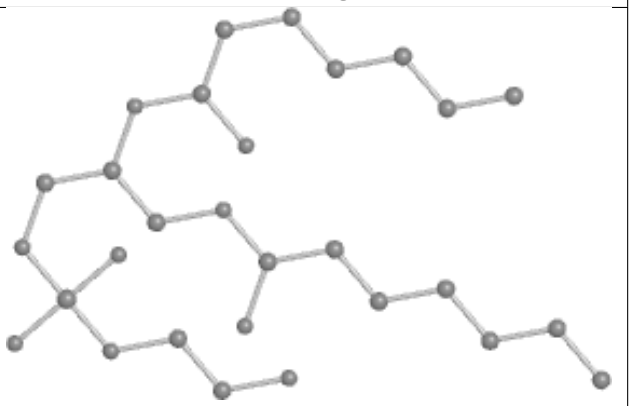
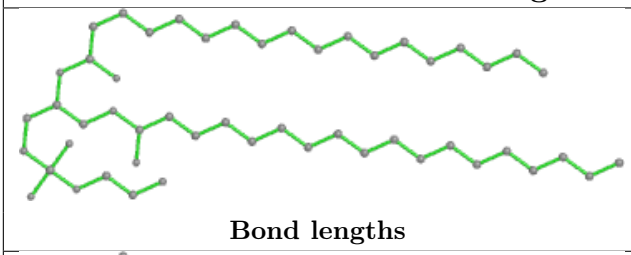


Rings

Ligand 3PE F 202



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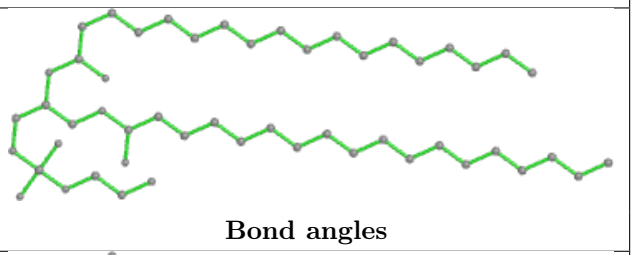
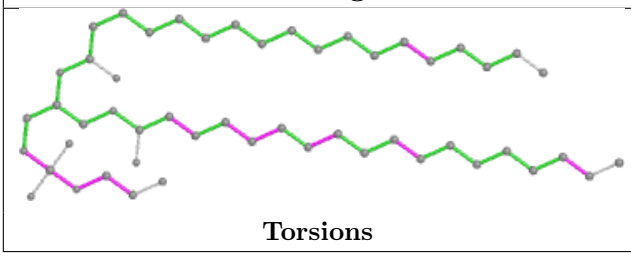
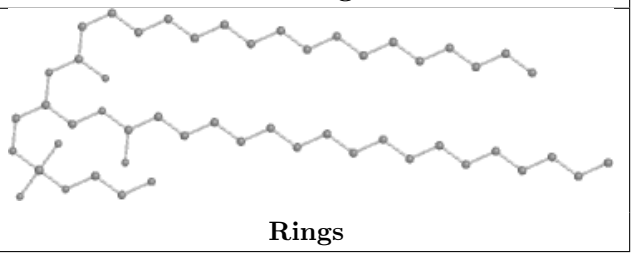


Bond angles

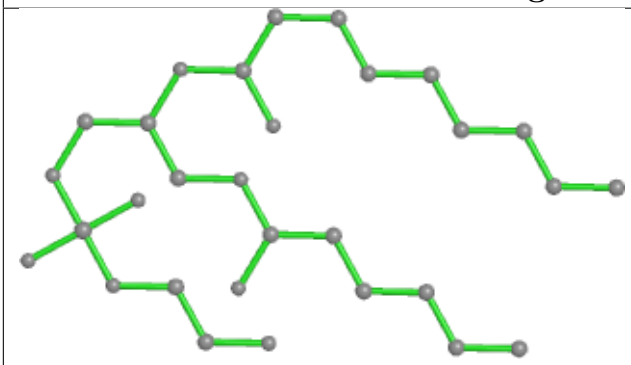


Torsions



Rings

Ligand 3PE O 405



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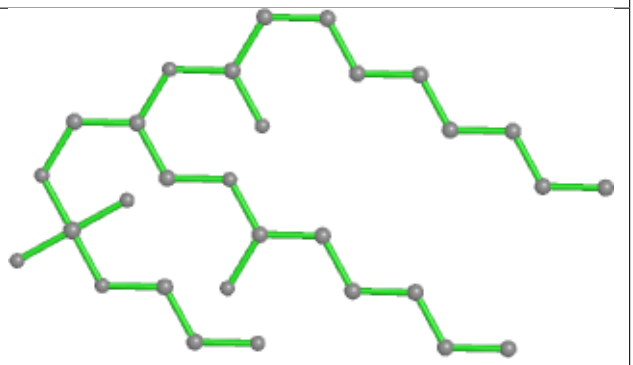
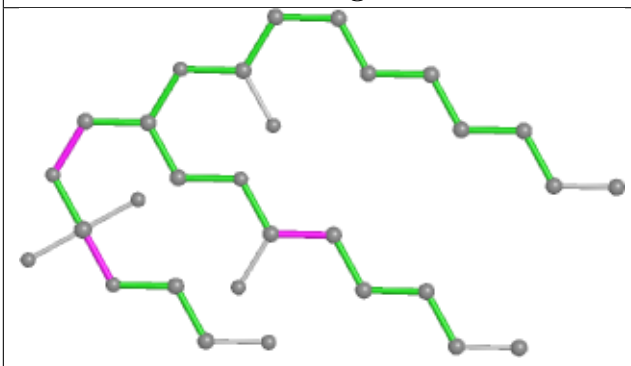
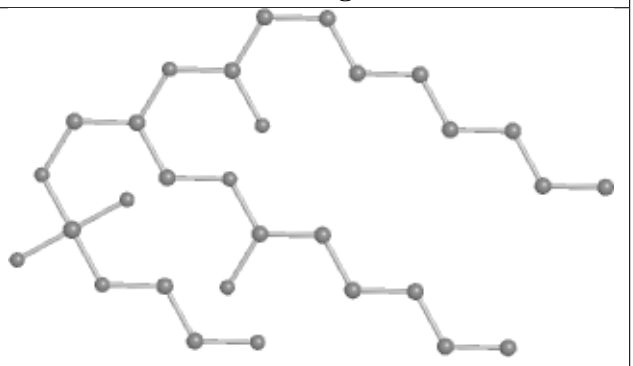


Bond angles

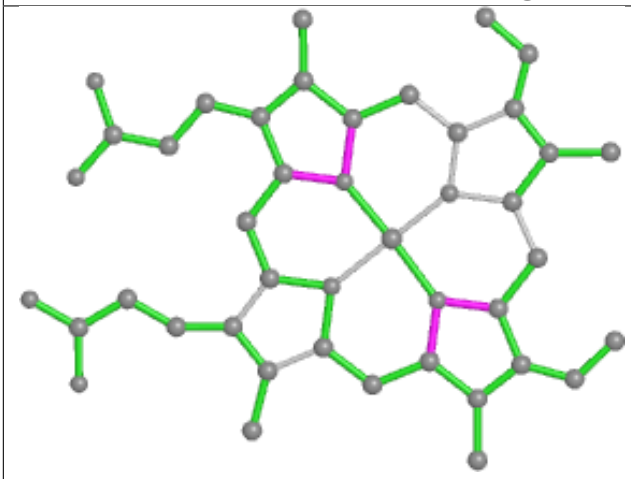


Torsions



Rings

Ligand HEM C 402



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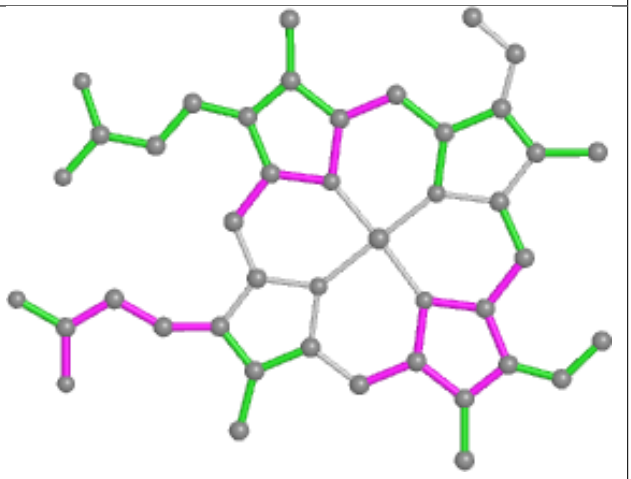
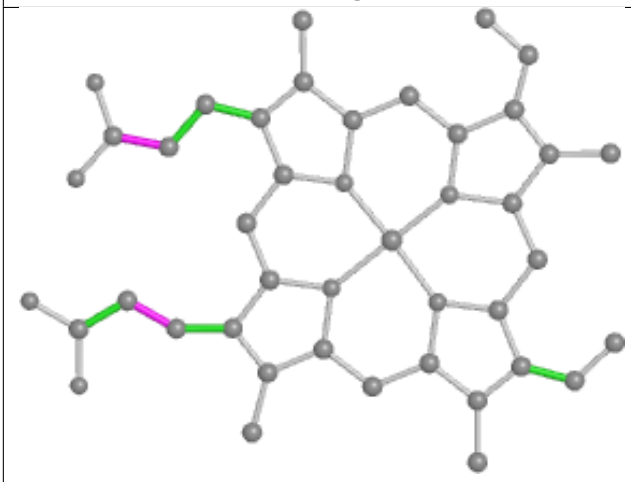
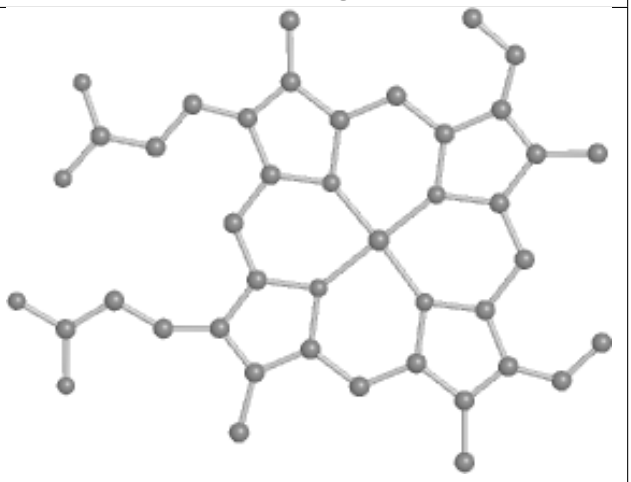


Bond angles

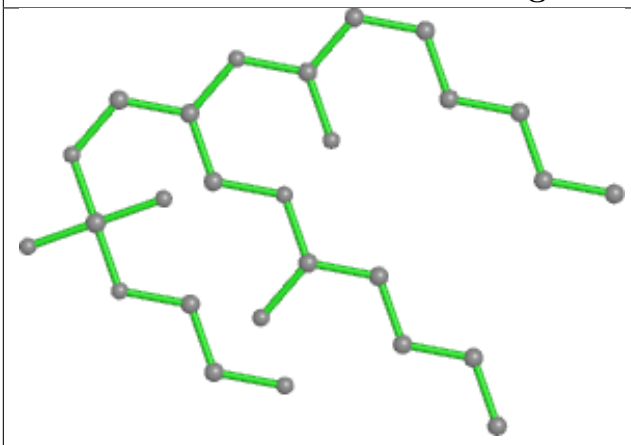


Torsions



Rings

Ligand 3PE C 408



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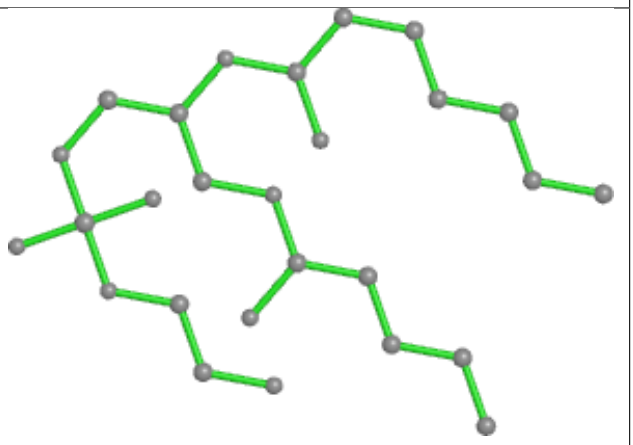
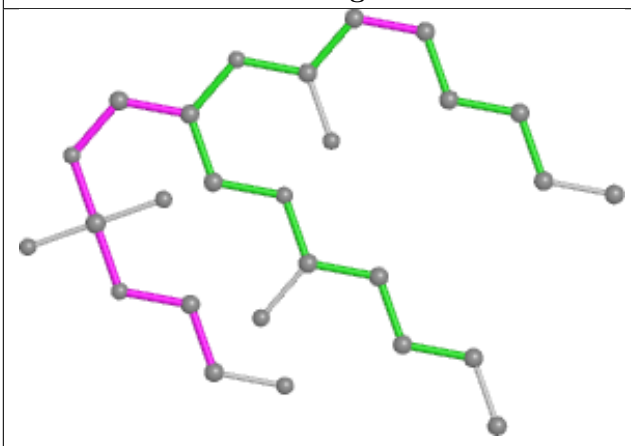
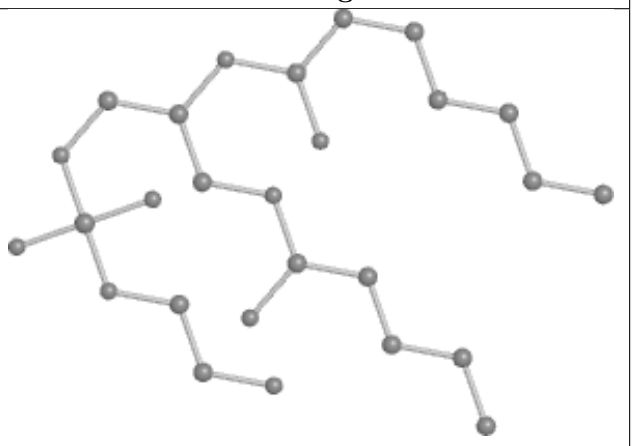


Bond angles

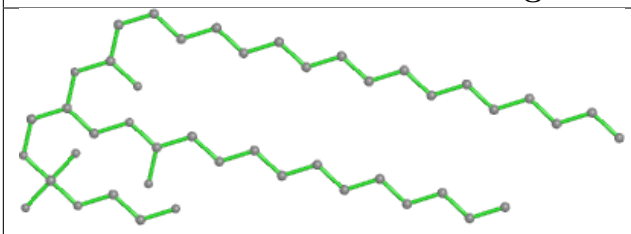


Torsions



Rings

Ligand 3PE M 602



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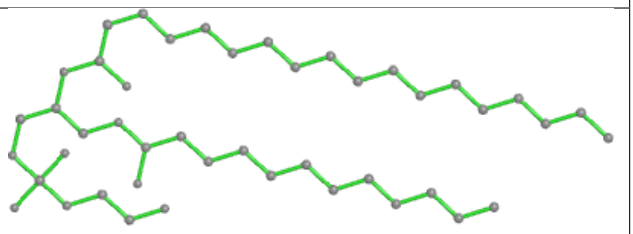
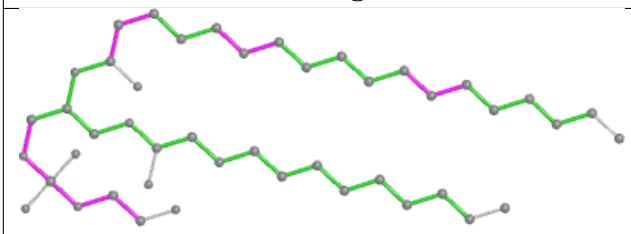


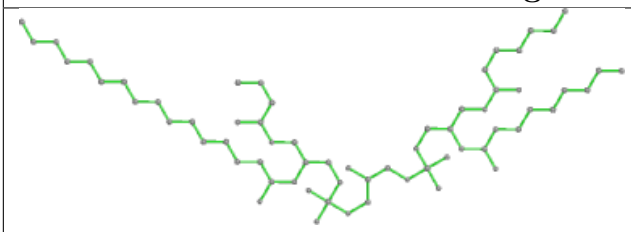
Bond angles



Torsions

Rings

Ligand CDL O 406



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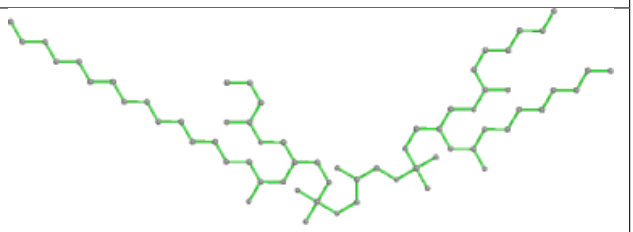
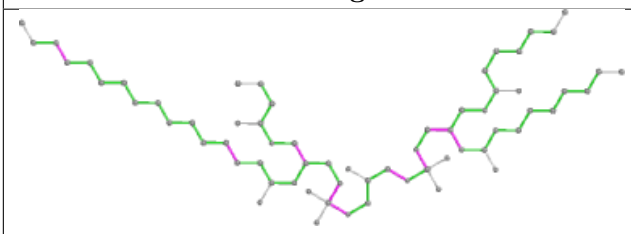
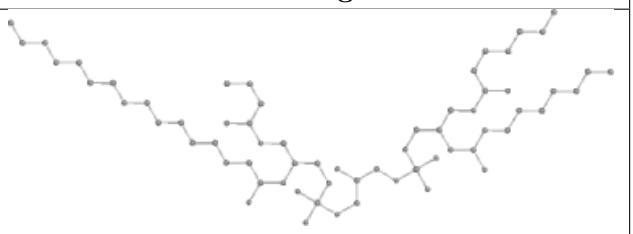


Bond angles

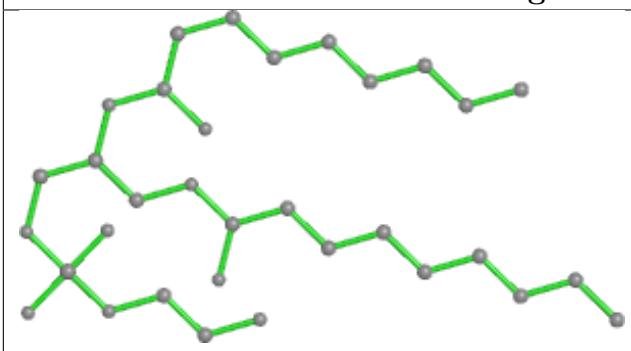


Torsions

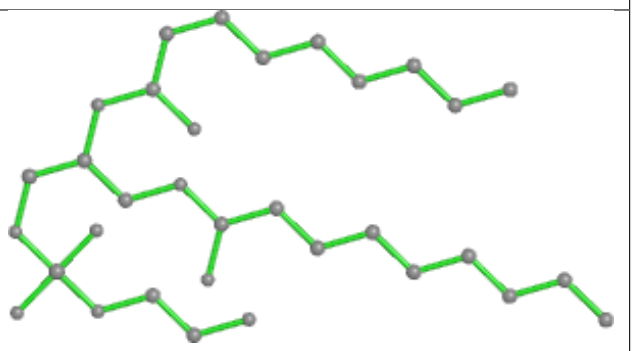


Rings

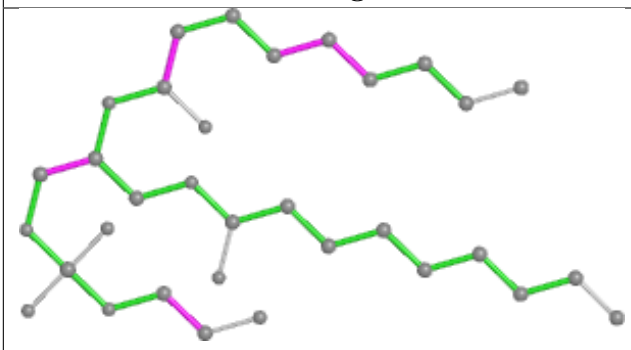
Ligand 3PE O 408



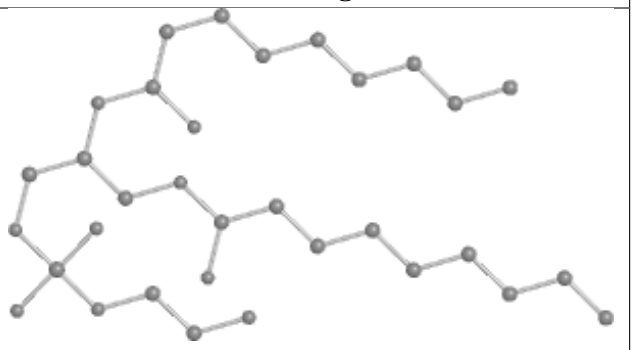
Bond lengths



Bond angles

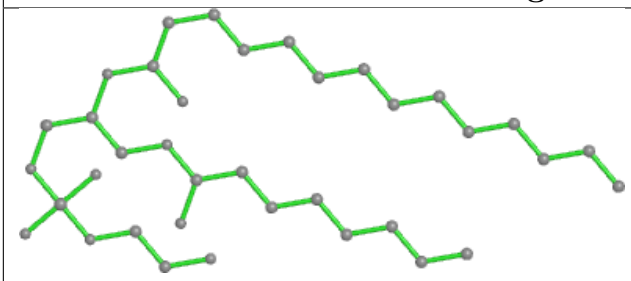


Torsions

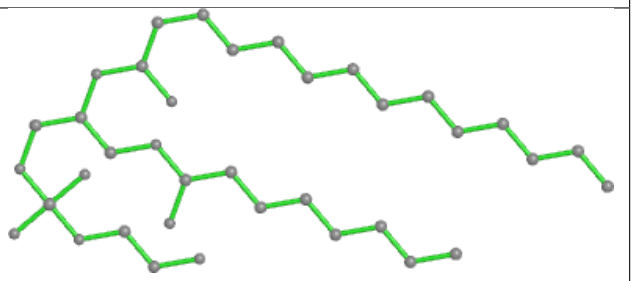


Rings

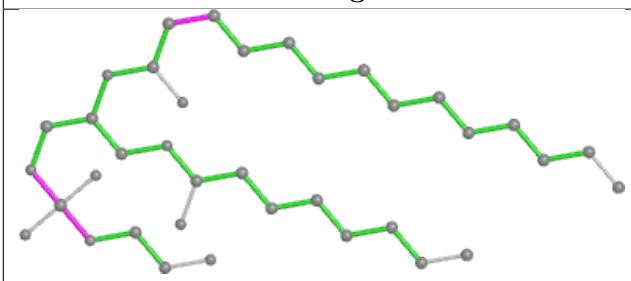
Ligand 3PE G 101



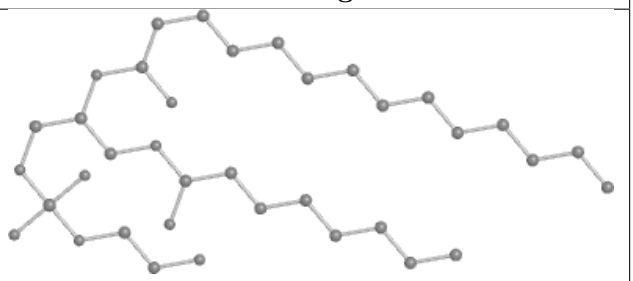
Bond lengths



Bond angles

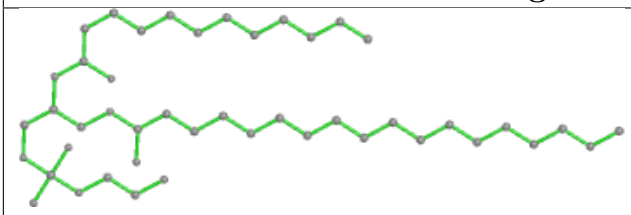


Torsions



Rings

Ligand 3PE C 406



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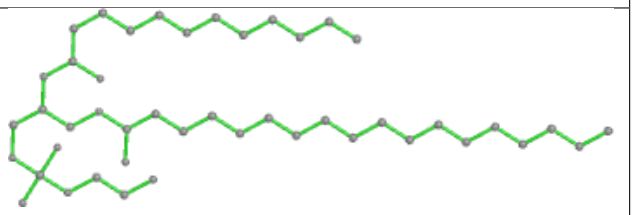

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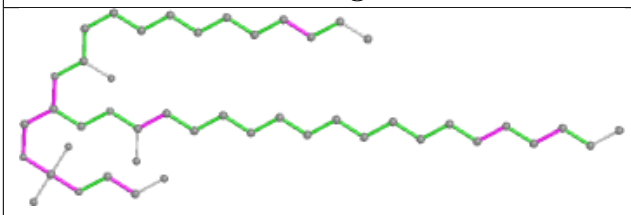

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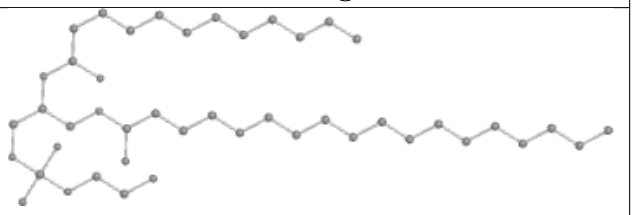
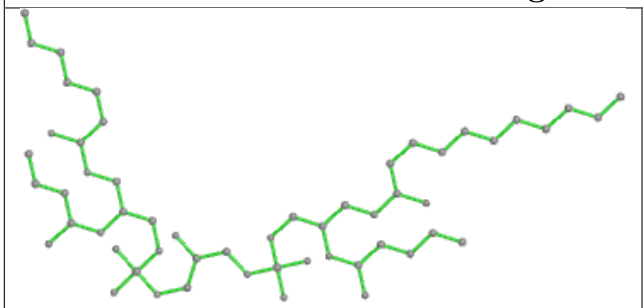


Rings

Ligand CDL S 102



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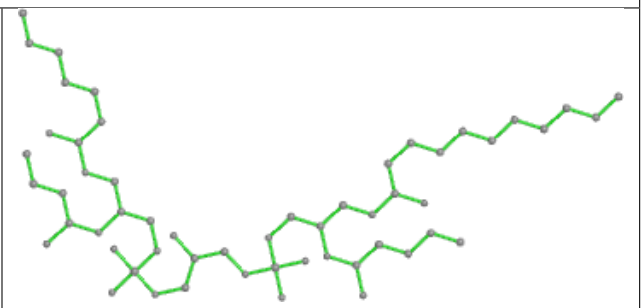
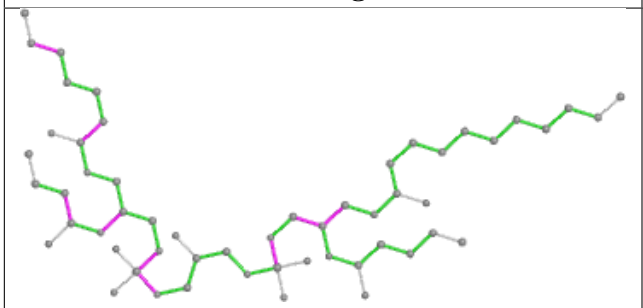


Bond angles



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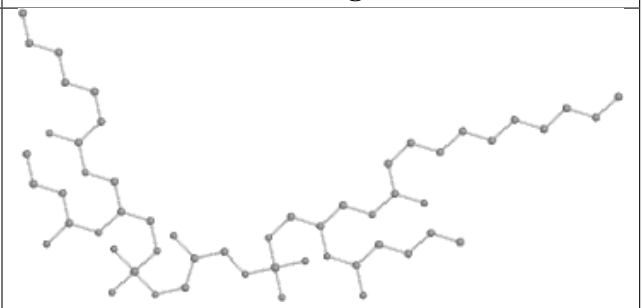
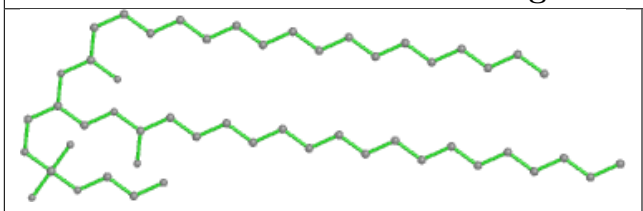


Rings

Ligand 3PE O 409



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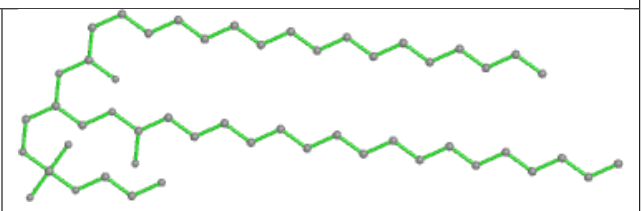
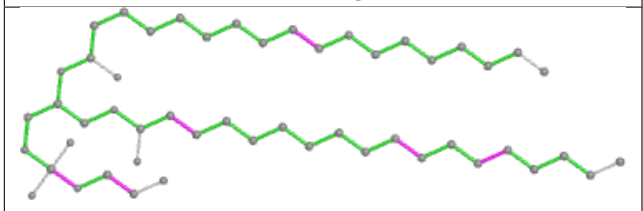


Bond angles



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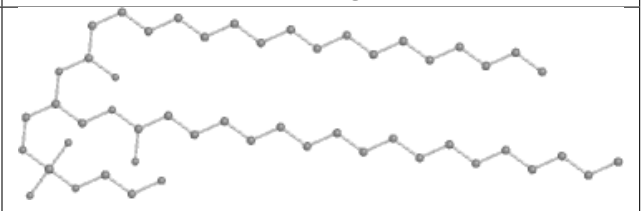
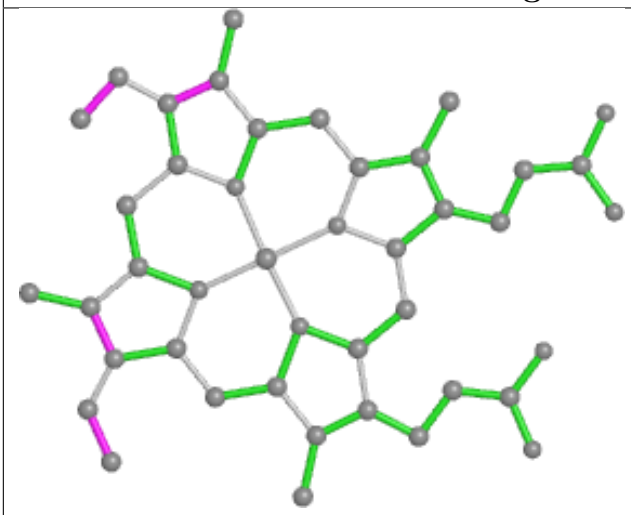


Rings

Ligand HEC P 501



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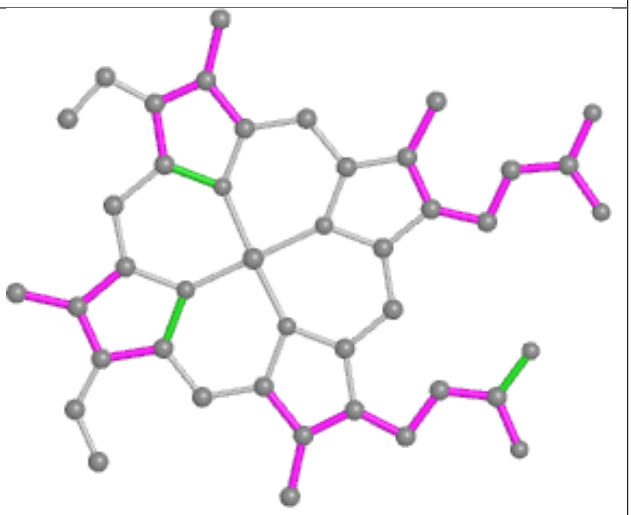
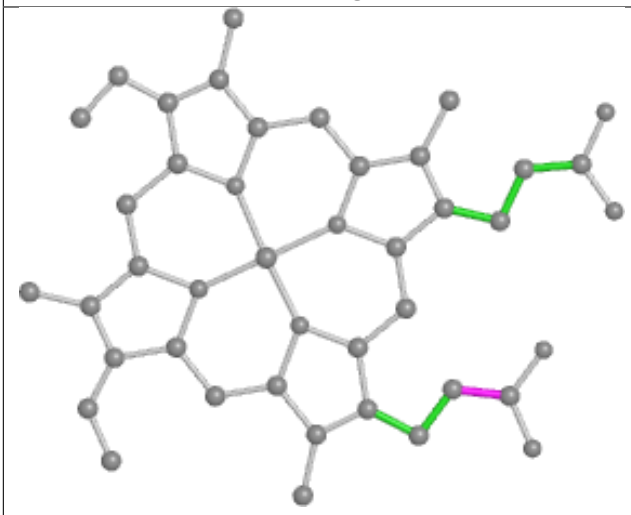


Bond angles



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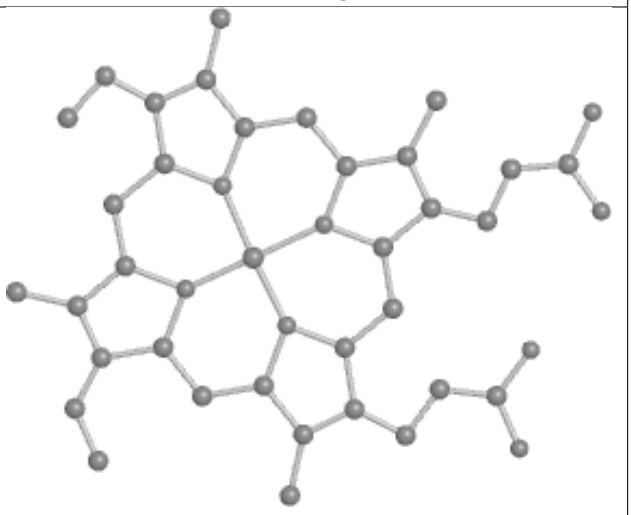
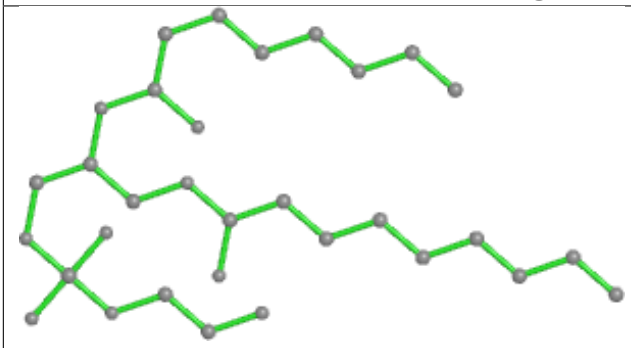


Rings

Ligand 3PE F 201



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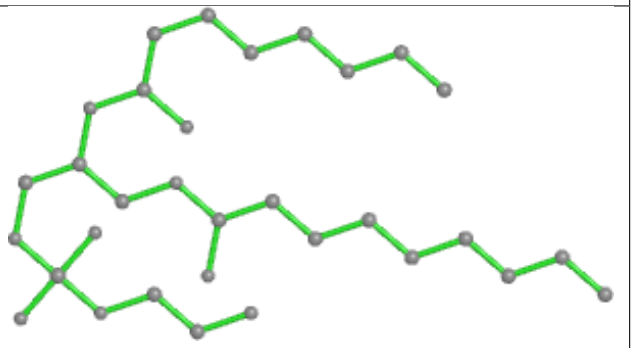

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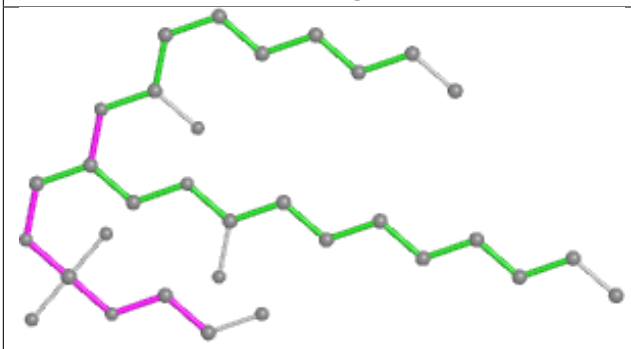

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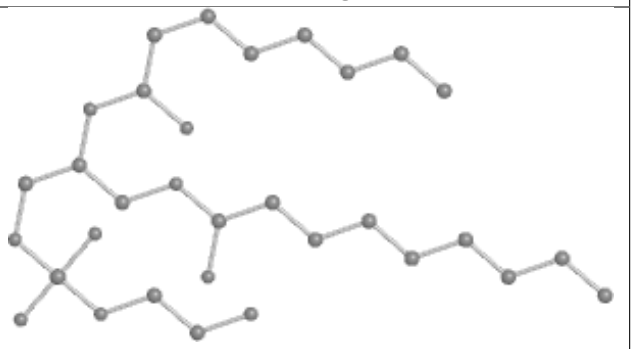
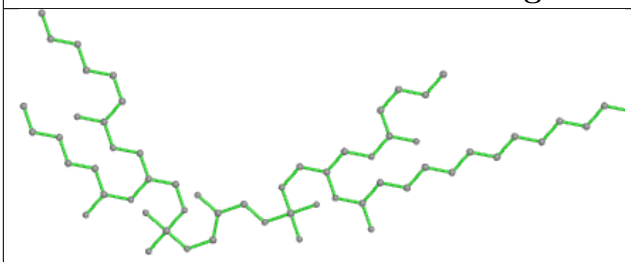


Rings

Ligand CDL C 410



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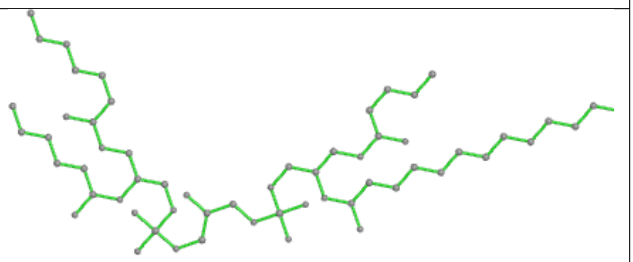
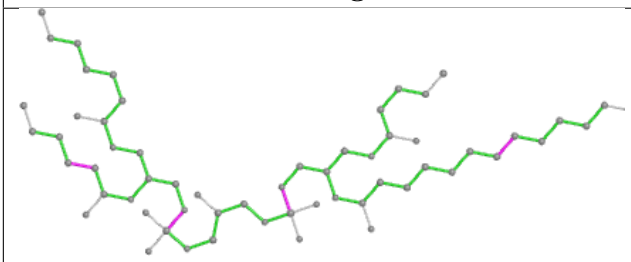


Bond angles



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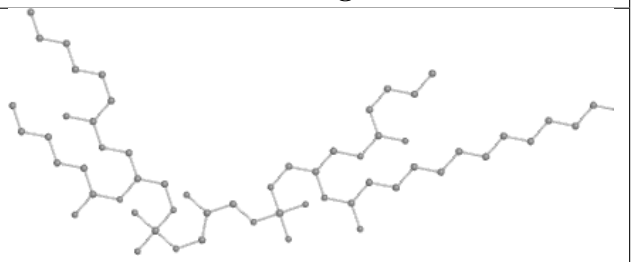
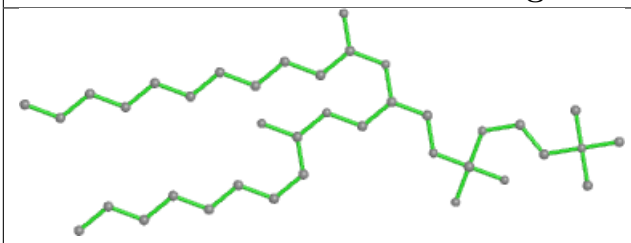


Rings

Ligand PC1 A 602



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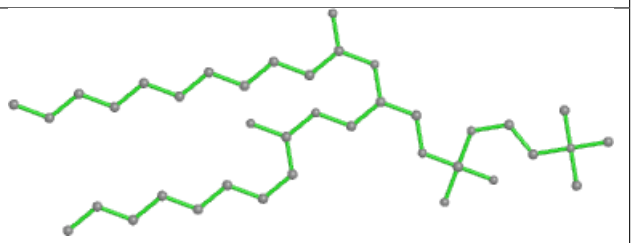
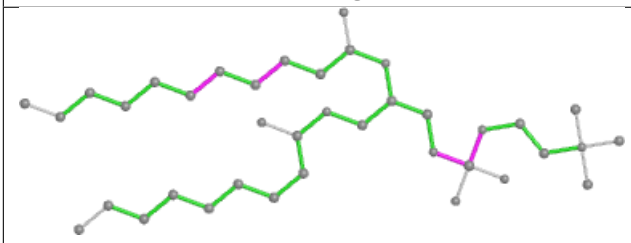


Bond angles



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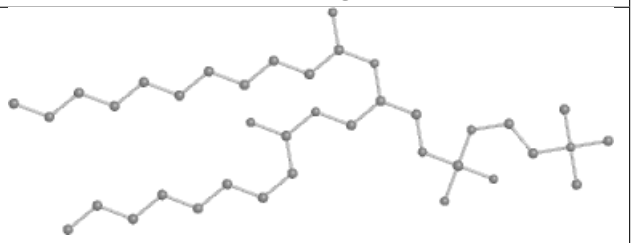
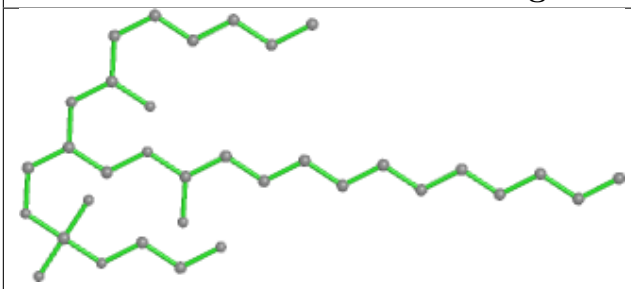


Rings

Ligand 3PE C 409



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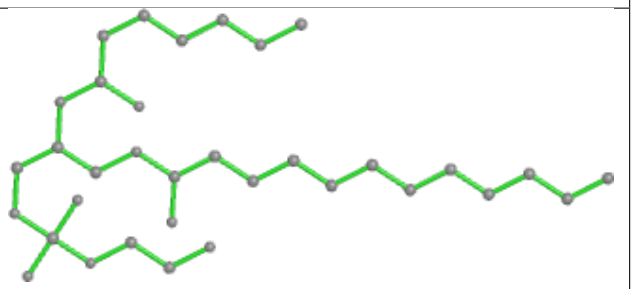

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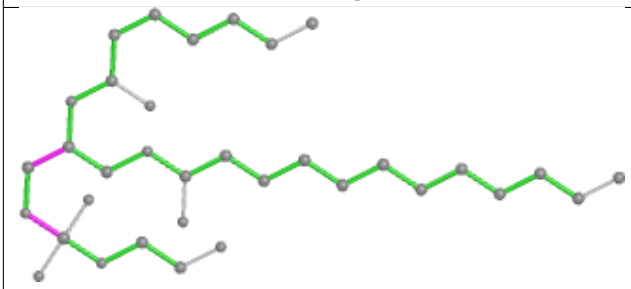
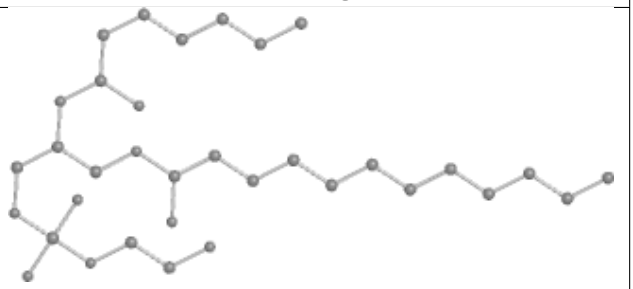
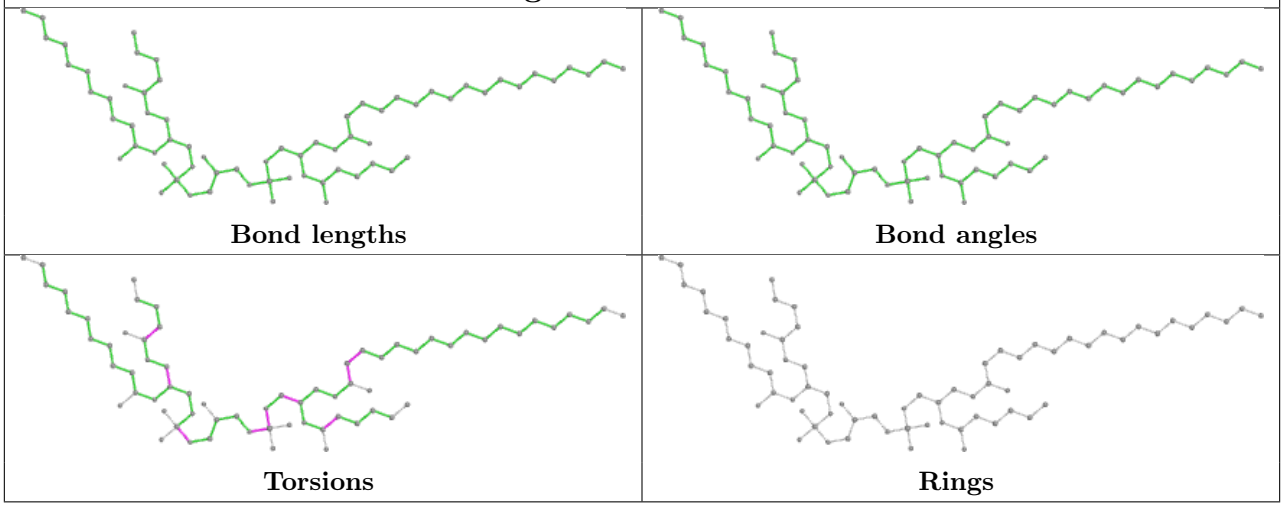


Torsions

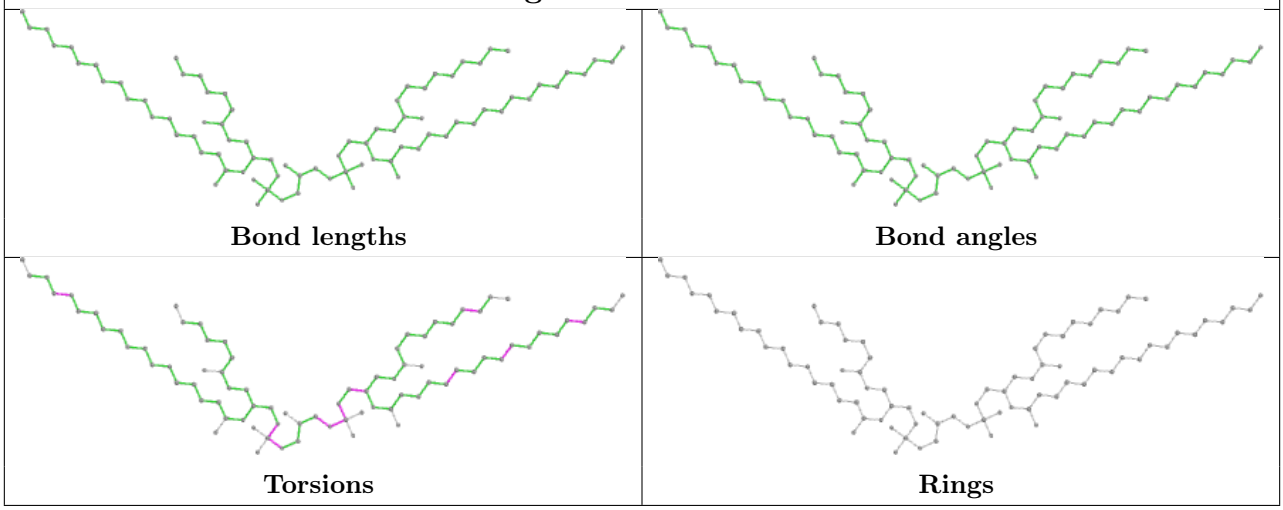


Rings

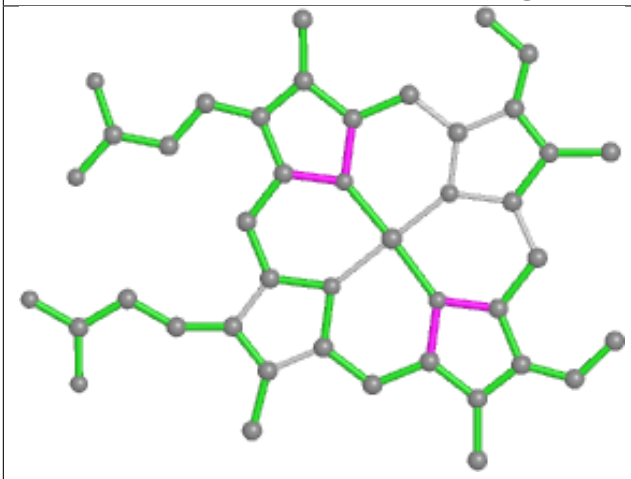
Ligand CDL D 502



Ligand CDL O 402



Ligand HEM O 403



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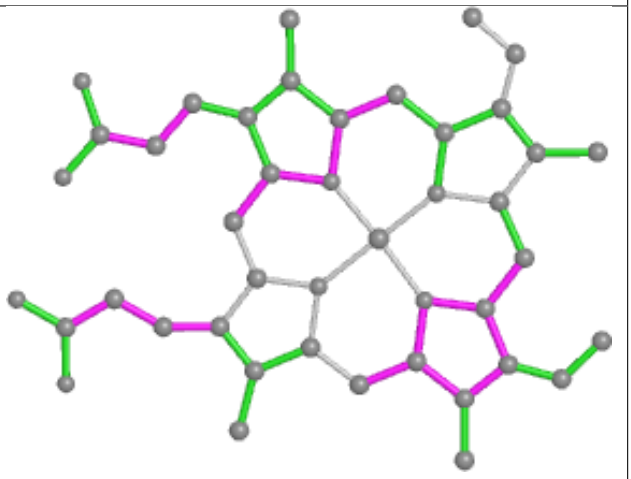
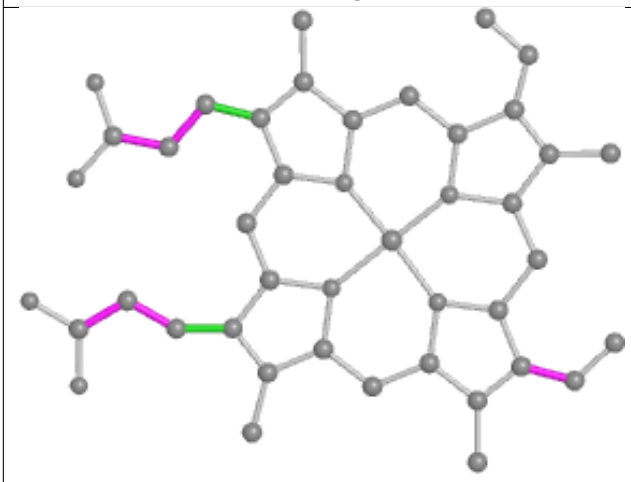
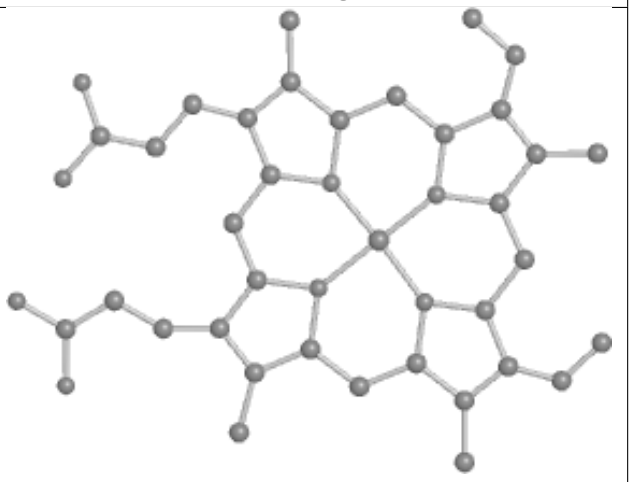


Bond angles

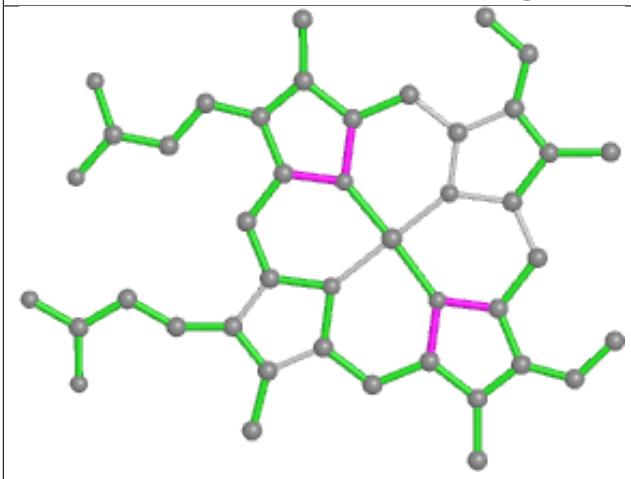


Torsions



Rings

Ligand HEM O 404



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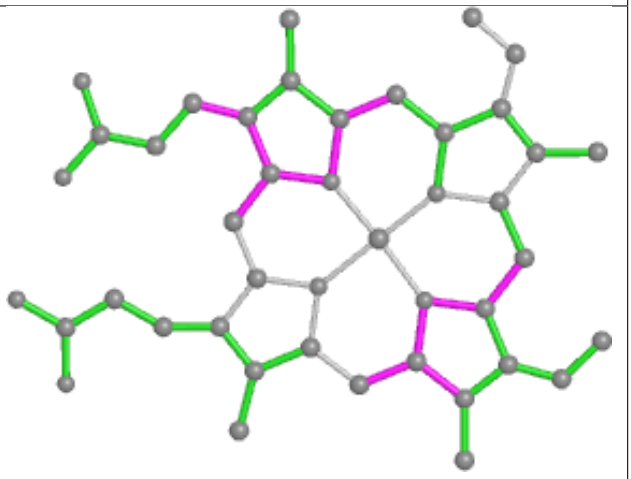
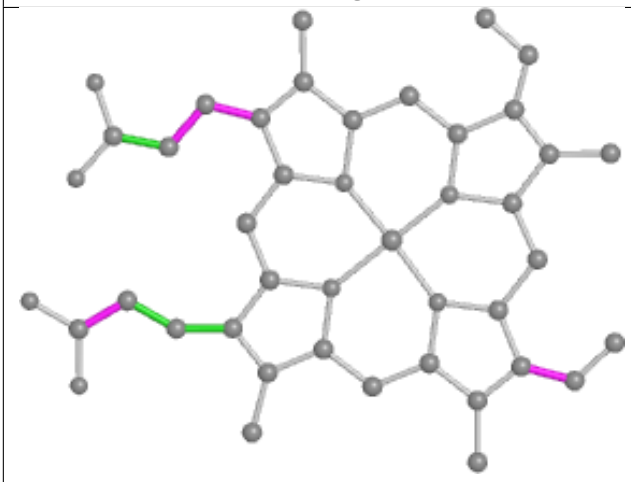
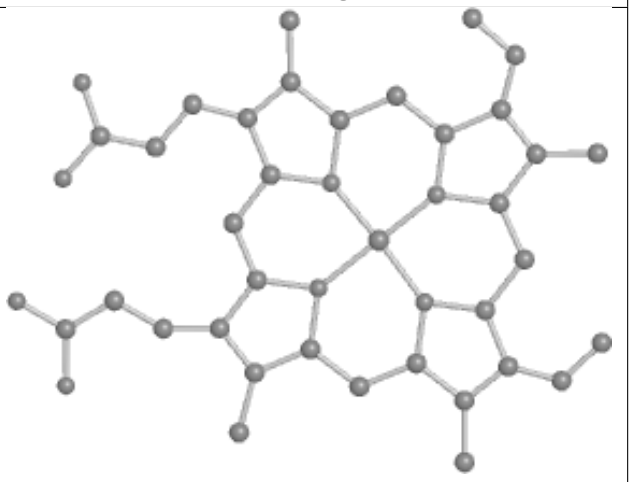


Bond angles

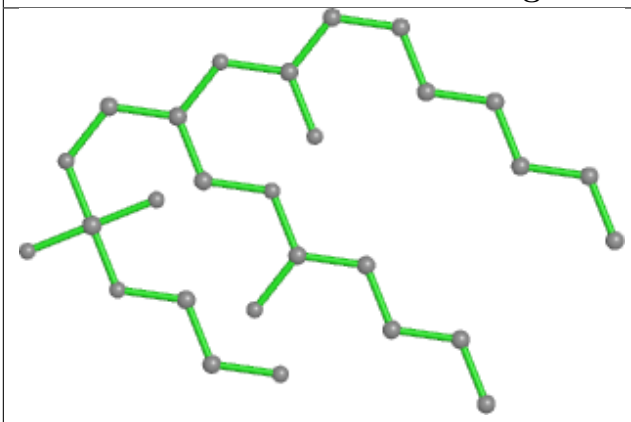


Torsions



Rings

Ligand 3PE W 102



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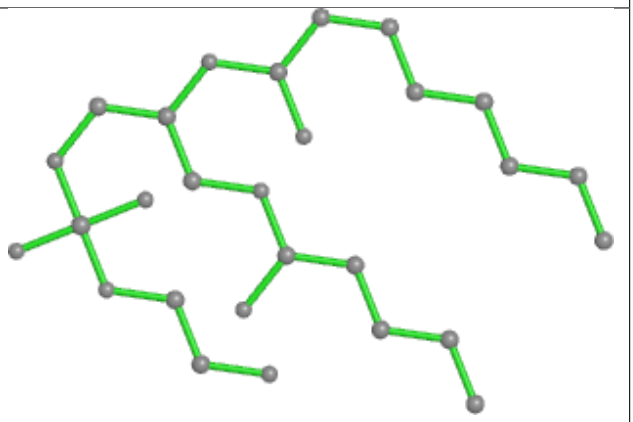
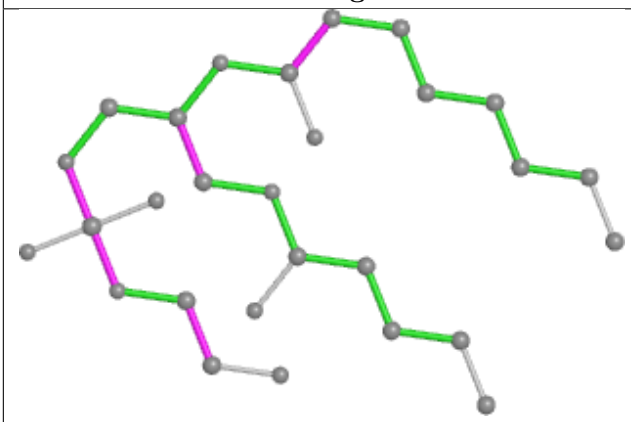
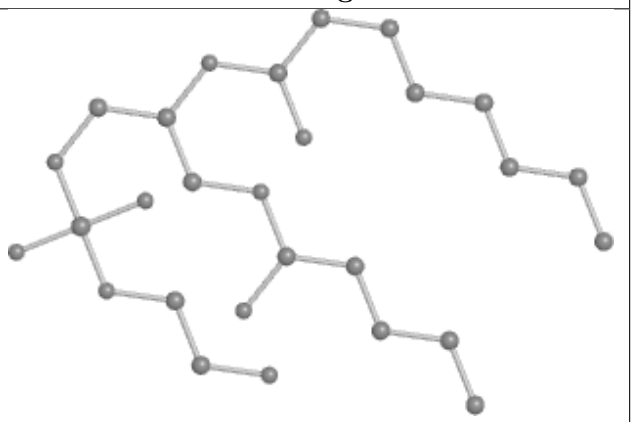


Bond angles

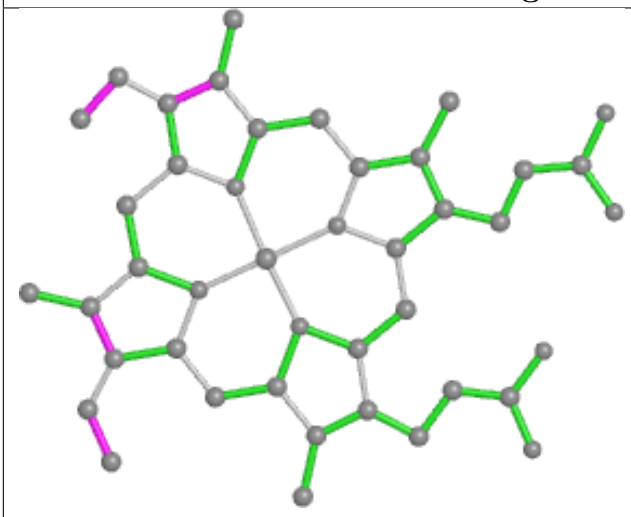


Torsions



Rings

Ligand HEC D 501



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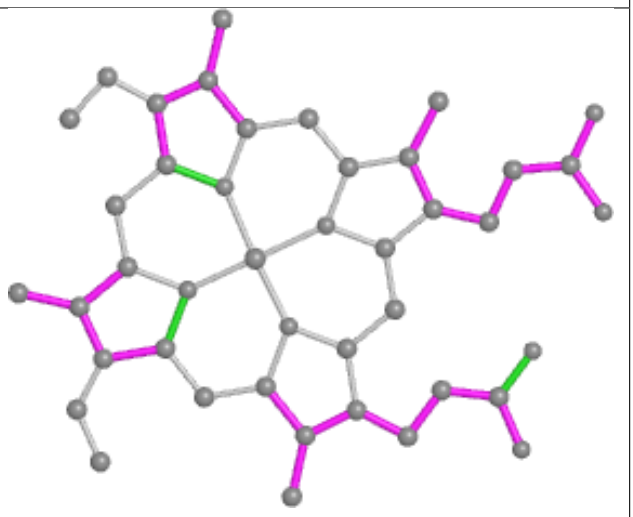
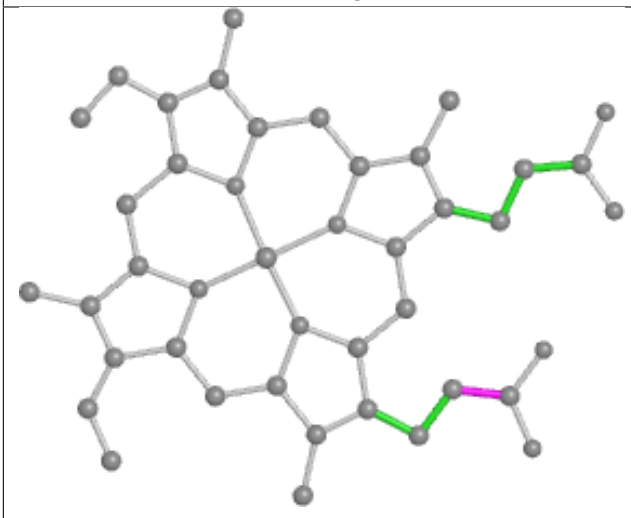
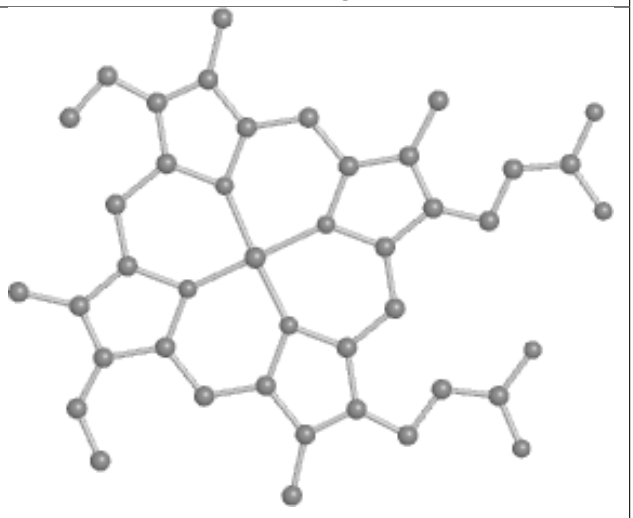


Bond angles

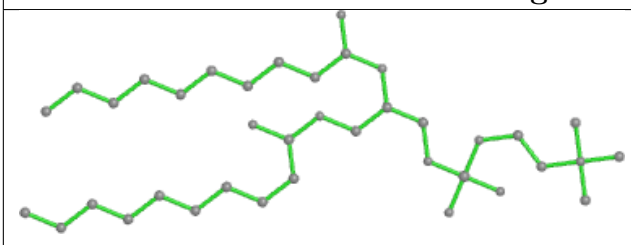


Torsions



Rings

Ligand PC1 S 101



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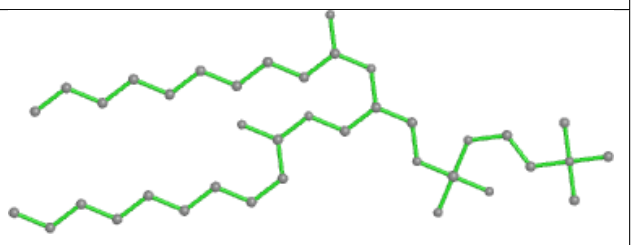
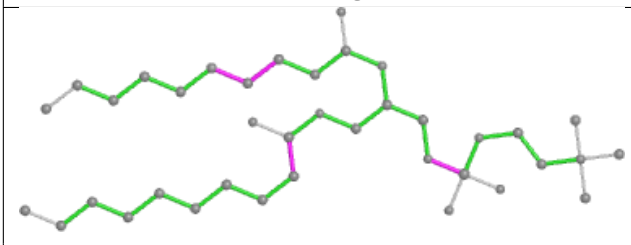


Bond angles



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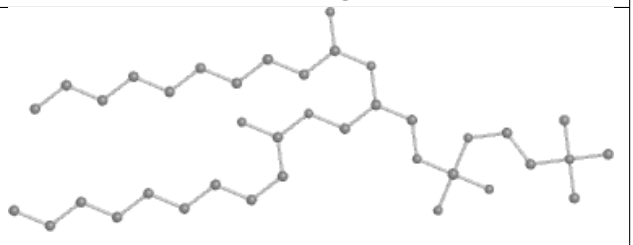
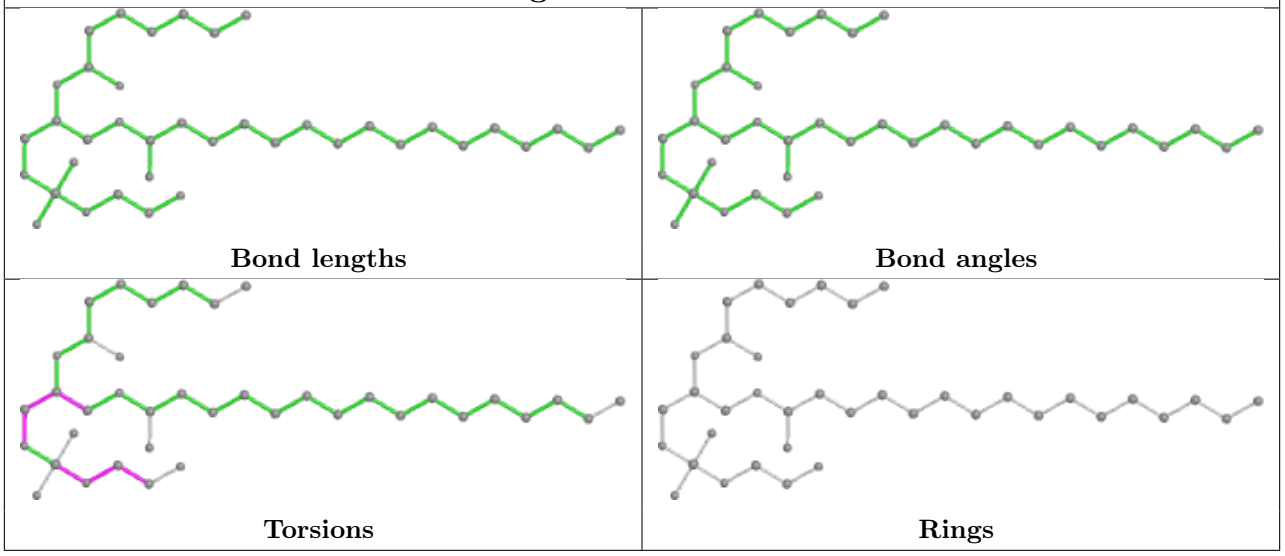


Rings

Ligand 3PE C 404



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

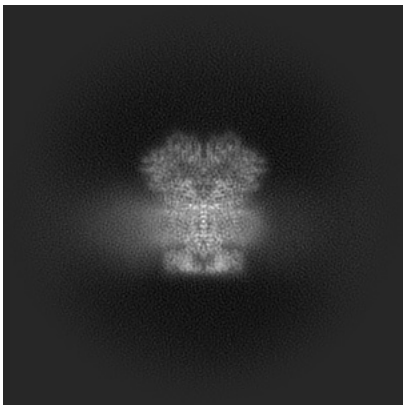
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22445. These allow visual inspection of the internal detail of the map and identification of artifacts.

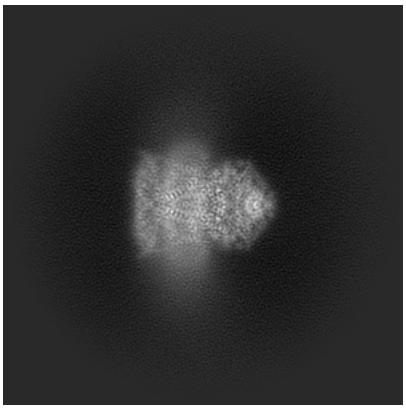
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

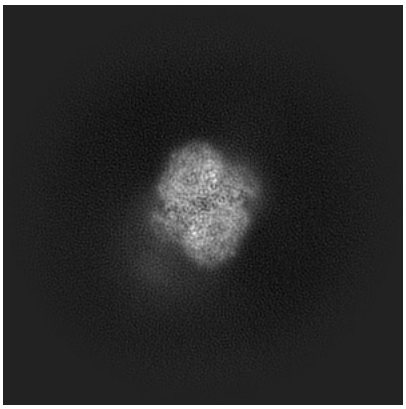
6.1.1 Primary map



X

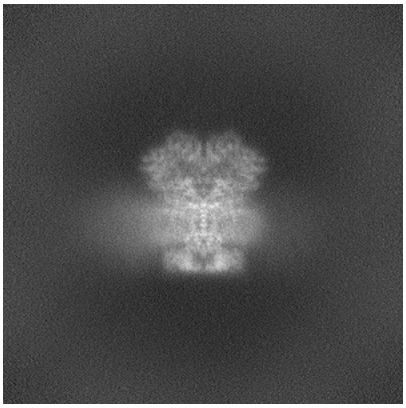


Y

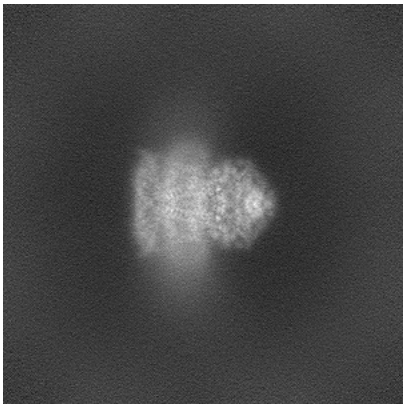


Z

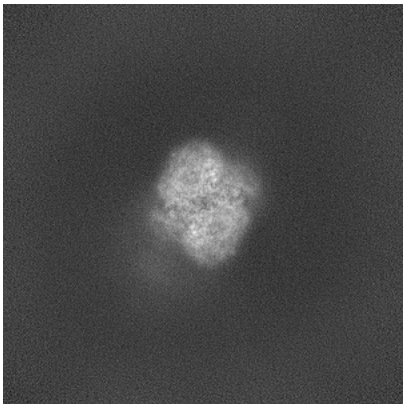
6.1.2 Raw map



X



Y

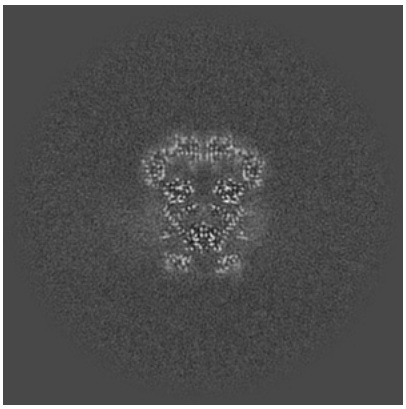


Z

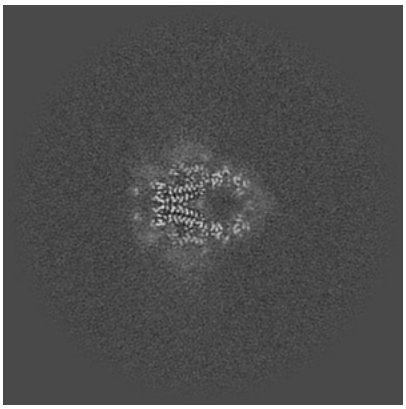
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

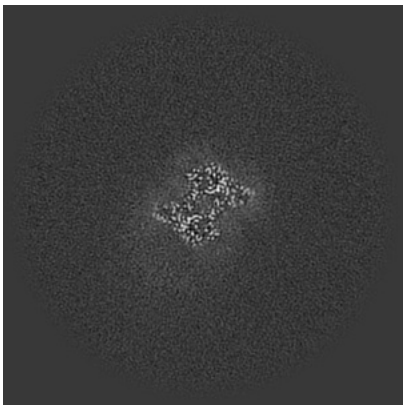
6.2.1 Primary map



X Index: 256

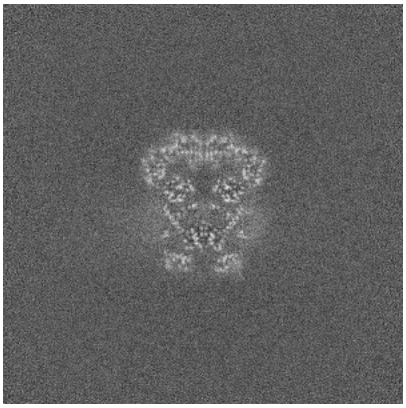


Y Index: 256

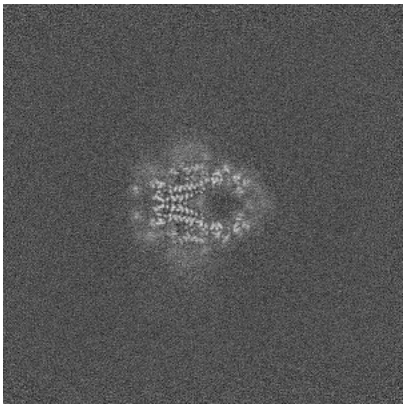


Z Index: 256

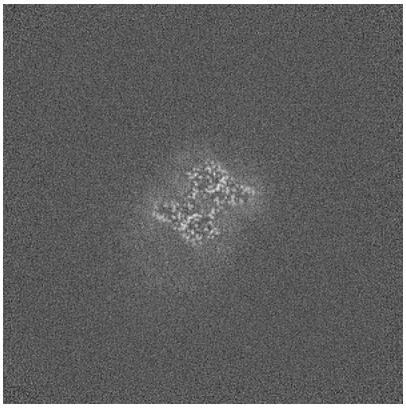
6.2.2 Raw map



X Index: 256



Y Index: 256

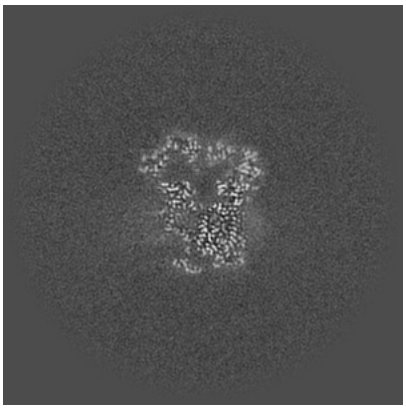


Z Index: 256

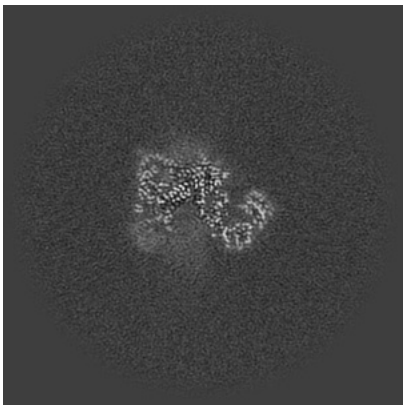
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

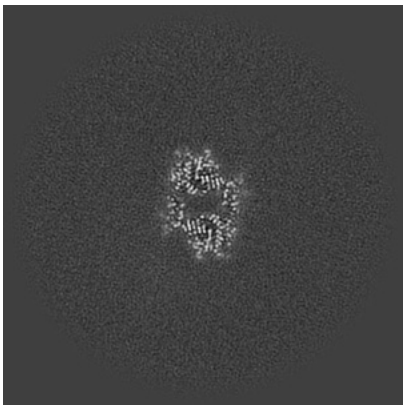
6.3.1 Primary map



X Index: 264

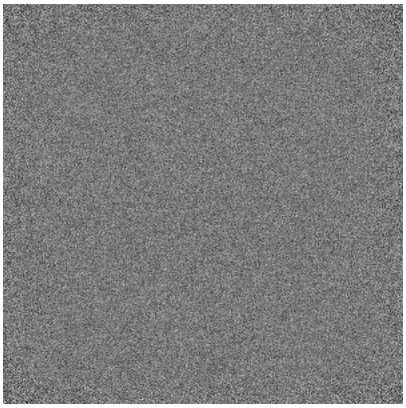


Y Index: 273

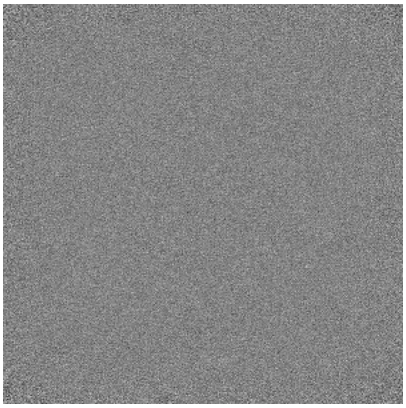


Z Index: 276

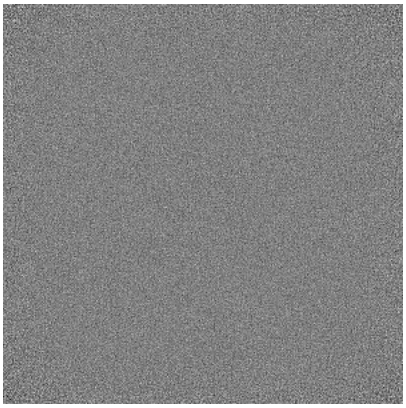
6.3.2 Raw map



X Index: 0



Y Index: 0

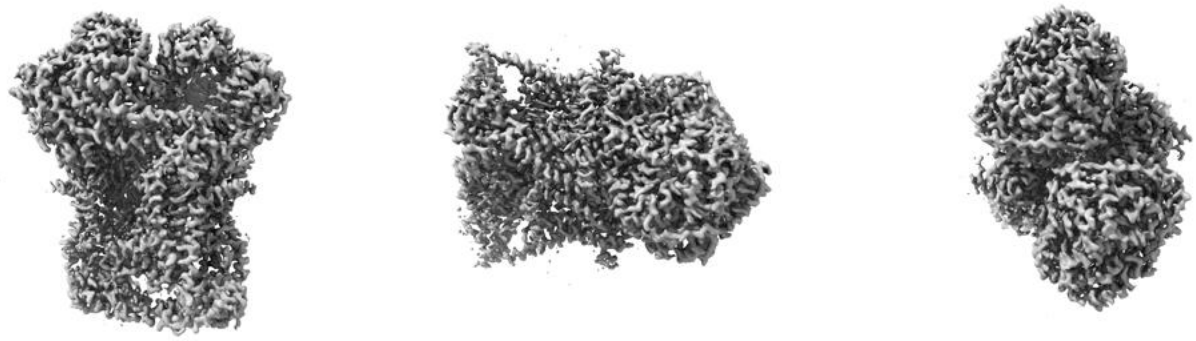


Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

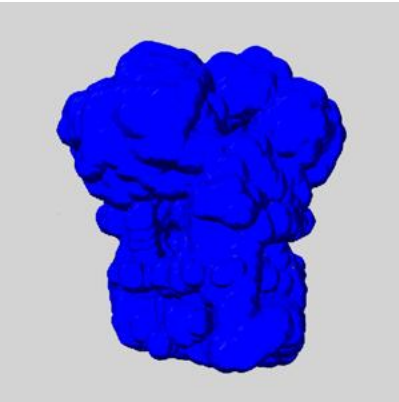
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

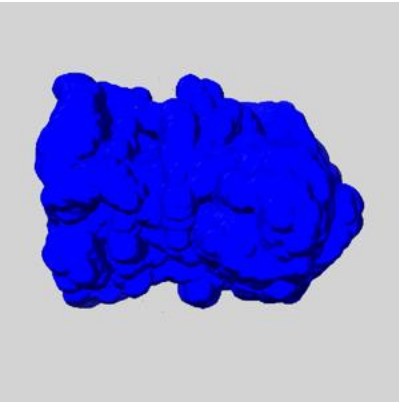
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

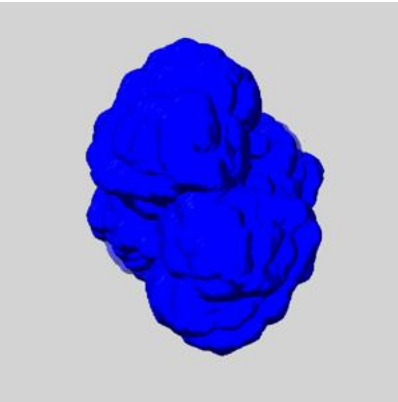
6.5.1 emd_22445_msk_1.map (i)



X



Y

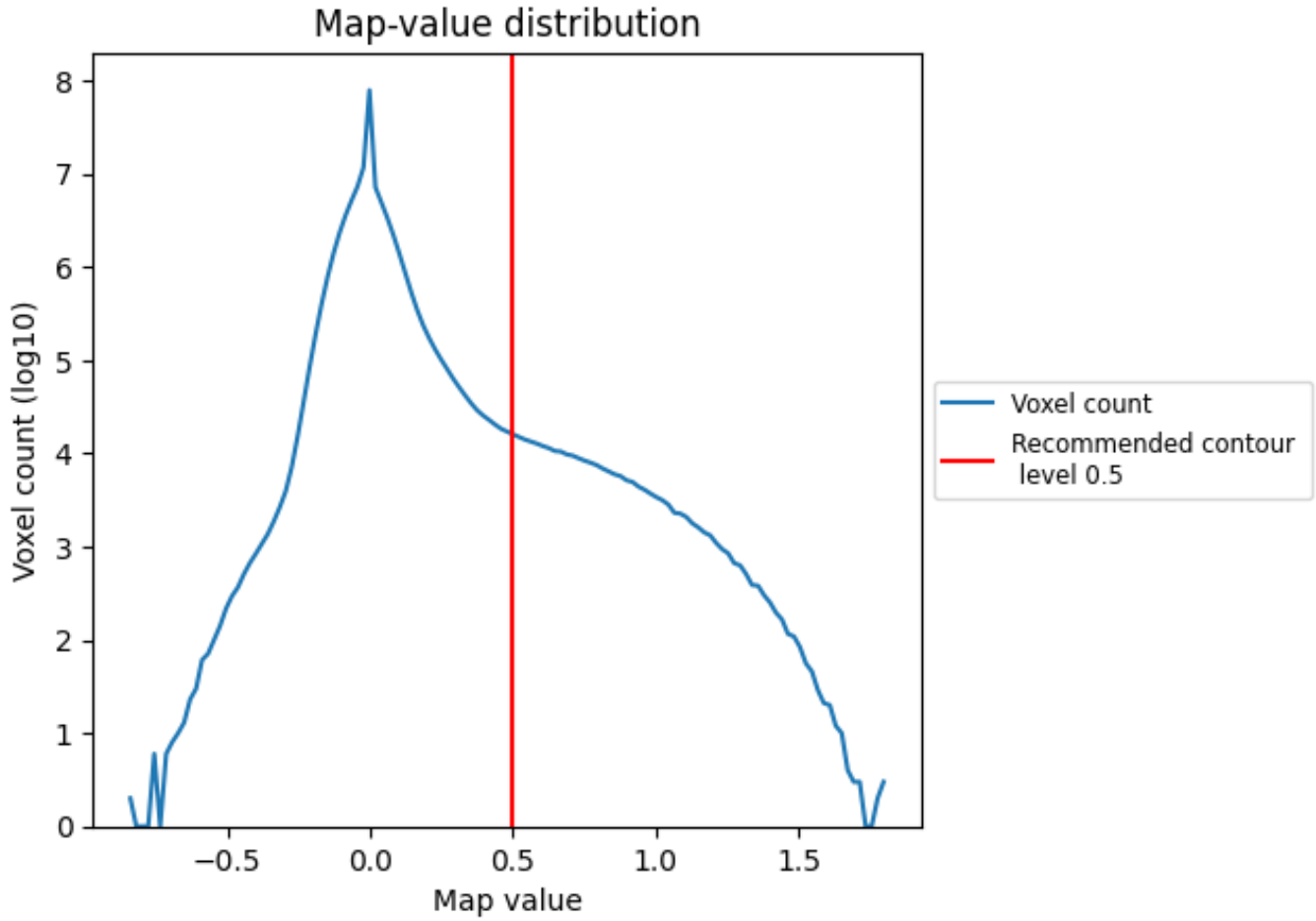


Z

7 Map analysis

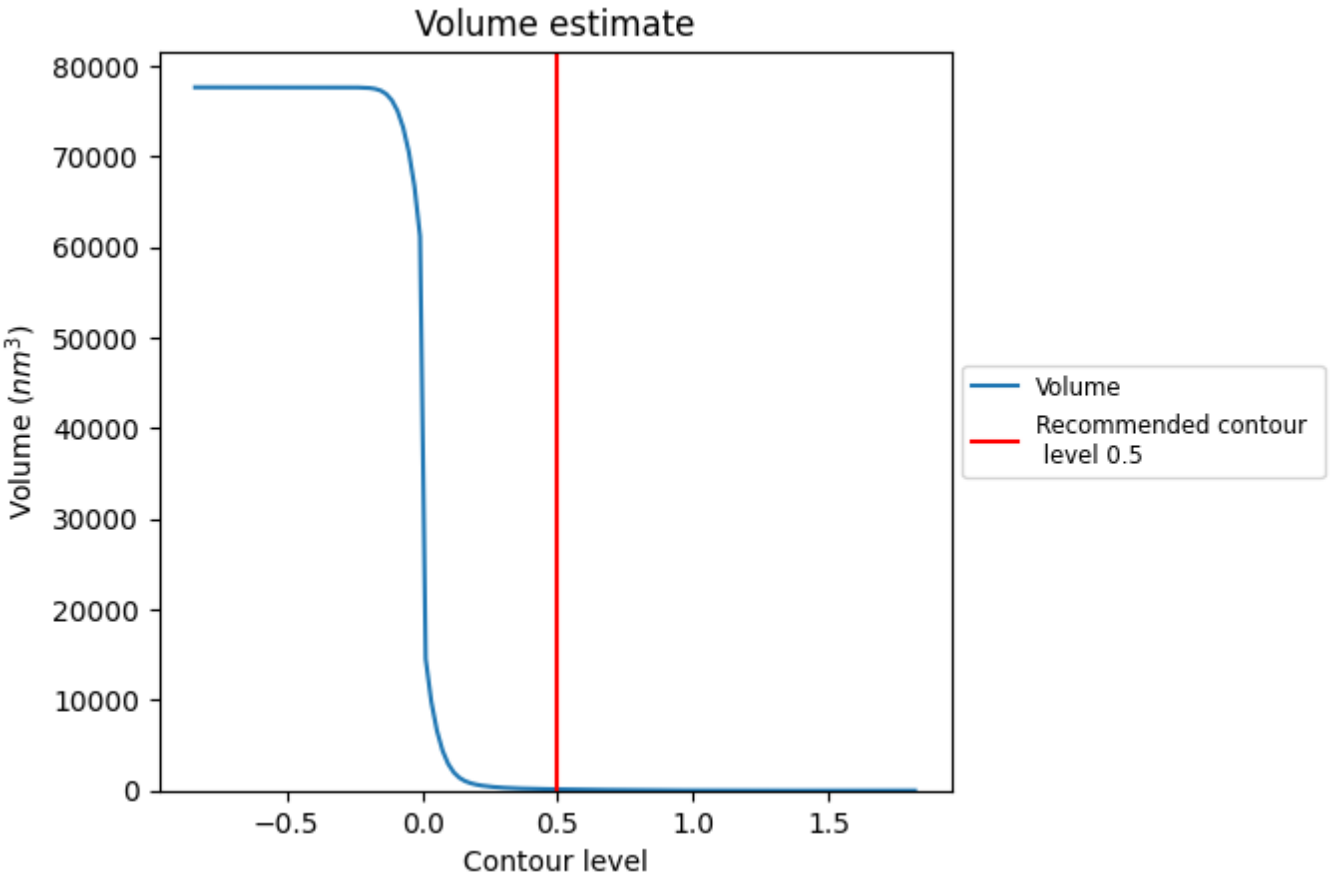
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

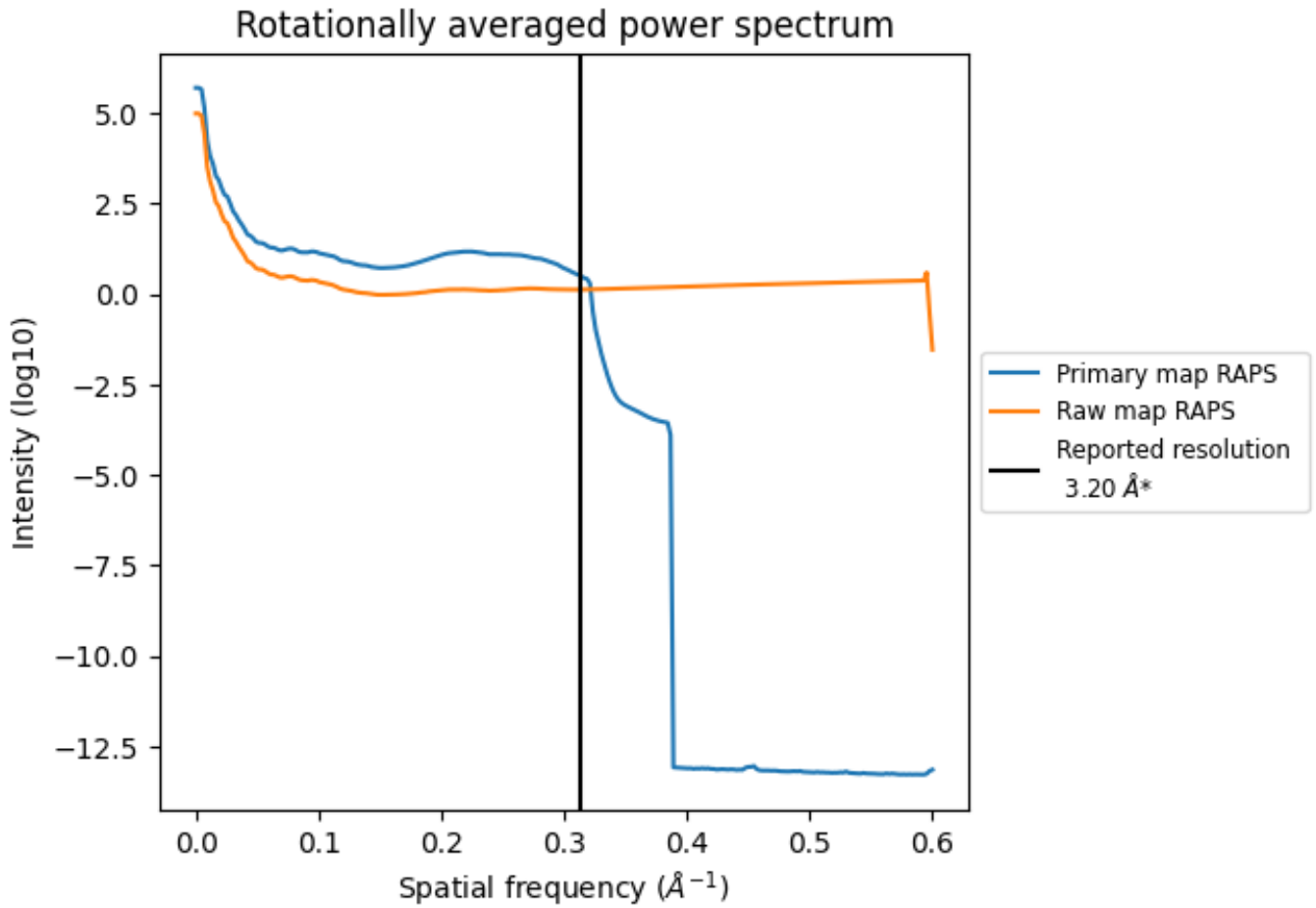
7.2 Volume estimate (i)



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 128 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)

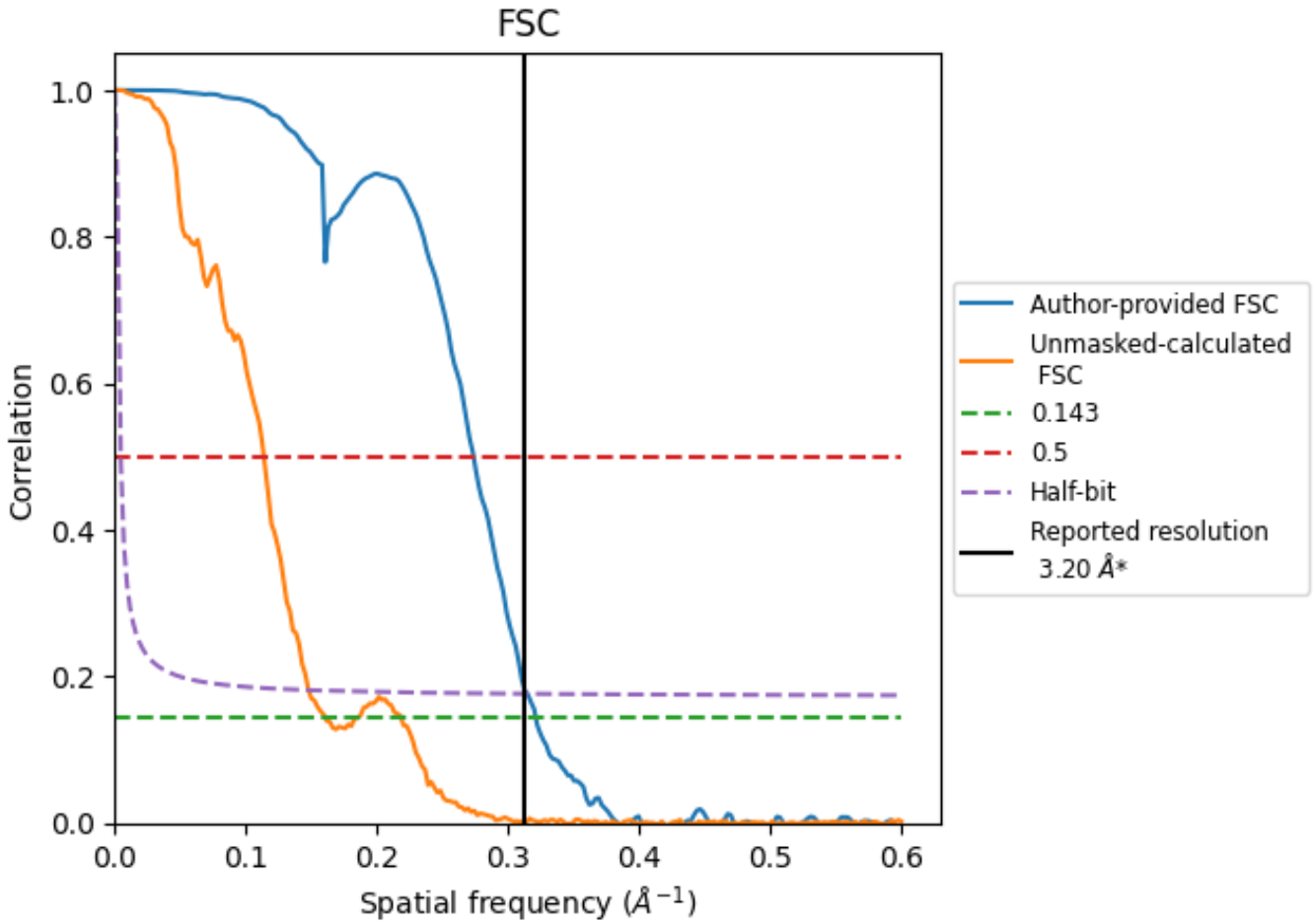


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

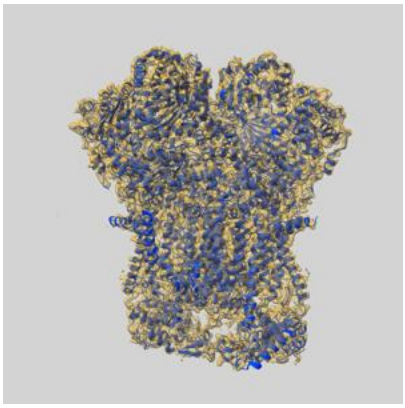
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.11	3.65	3.18
Unmasked-calculated*	6.23	8.79	6.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.23 differs from the reported value 3.2 by more than 10 %

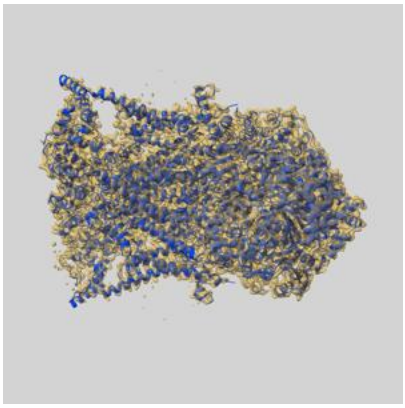
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22445 and PDB model 7JRG. Per-residue inclusion information can be found in section 3 on page 11.

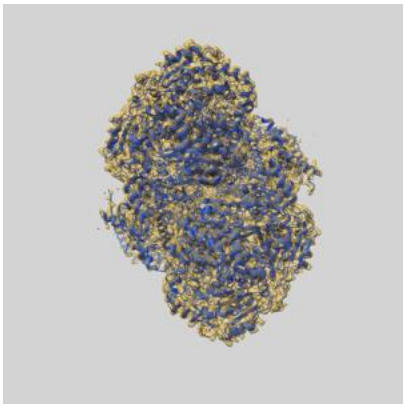
9.1 Map-model overlay



X



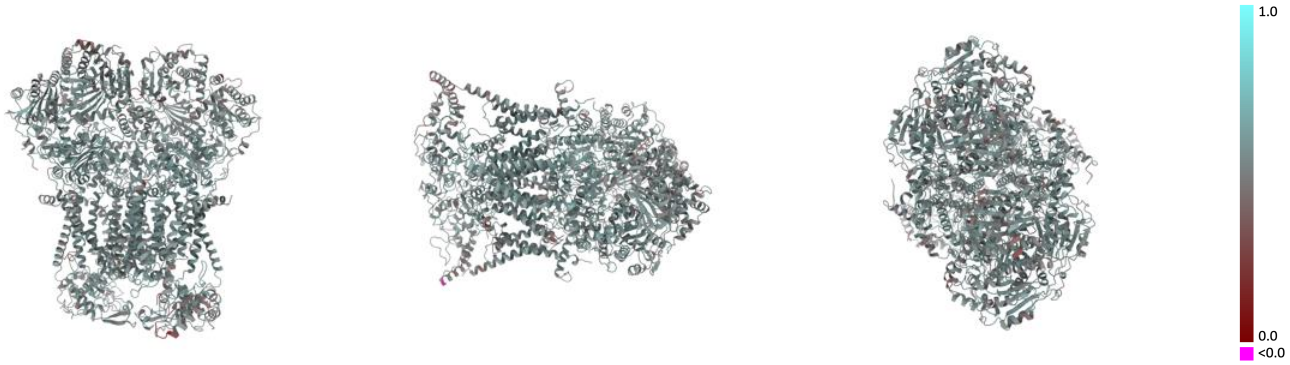
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

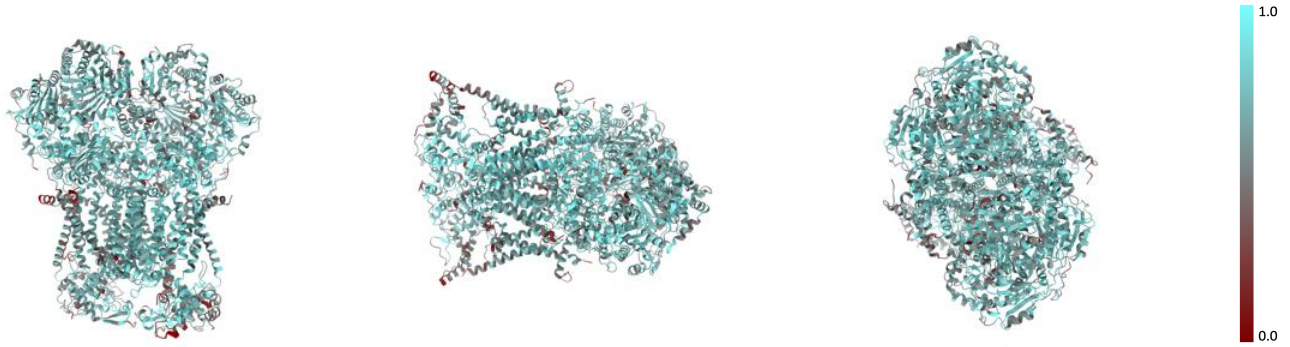
9.2 Q-score mapped to coordinate model (i)



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.

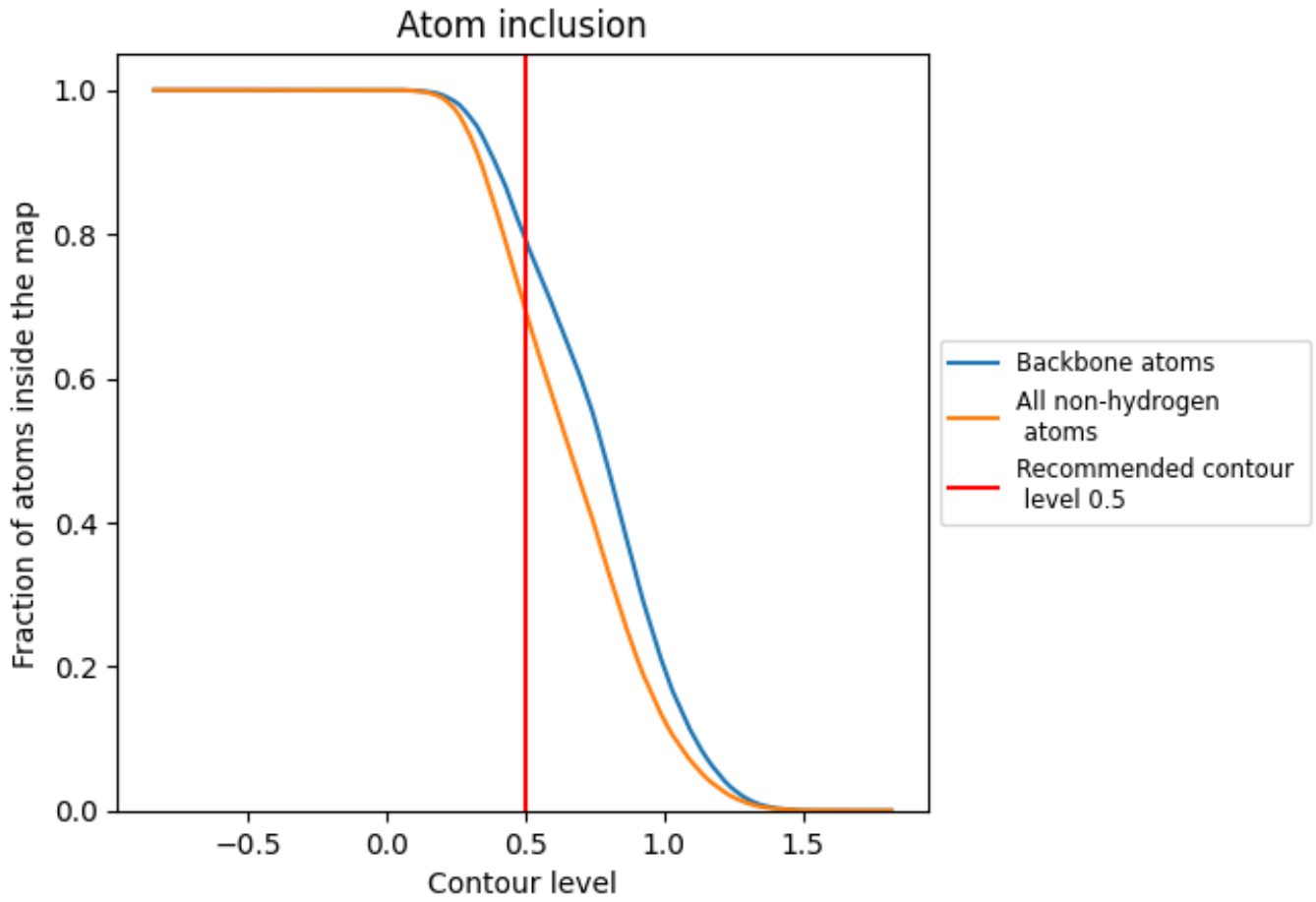
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6953	0.5430
A	0.7396	0.5500
B	0.6734	0.5180
C	0.7381	0.5670
D	0.7235	0.5520
E	0.5819	0.5370
F	0.6995	0.5660
G	0.5429	0.5240
H	0.4288	0.4610
J	0.5139	0.5210
K	0.3843	0.4960
M	0.7330	0.5490
N	0.6914	0.5220
O	0.7459	0.5690
P	0.7558	0.5530
Q	0.6661	0.5420
R	0.7608	0.5620
S	0.5393	0.5330
T	0.4556	0.4520
V	0.6199	0.5390
W	0.4714	0.5040