Full wwPDB EM Validation Report ⓘ

Oct 18, 2021 – 10:19 am BST

PDB ID	:	7O3H
EMDB ID	:	EMD-12706
Title	:	Murine CIII2 focus-refined from supercomplex CICIII2
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2021-04-01
Resolution	:	2.60 Å(reported)
Based on initial models	:	1NTZ, 3L75

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

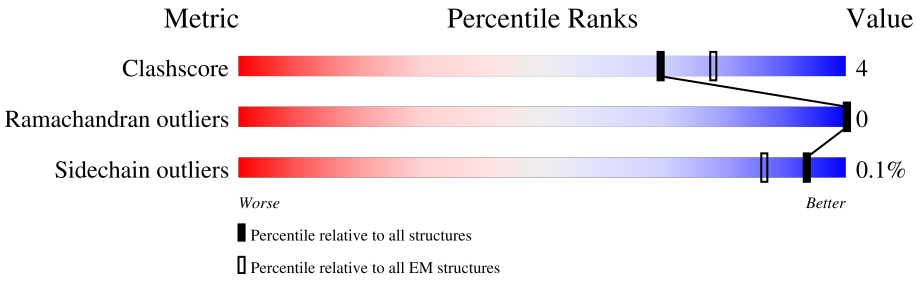
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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.



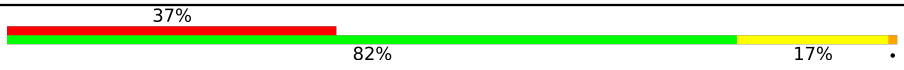
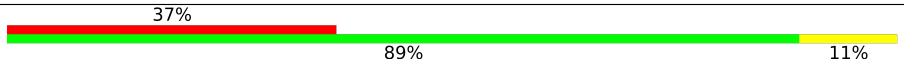
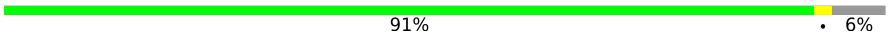
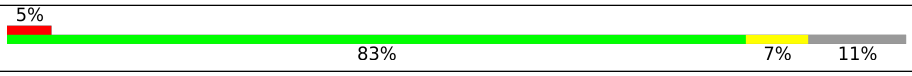
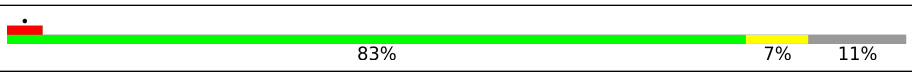
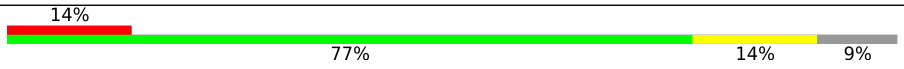
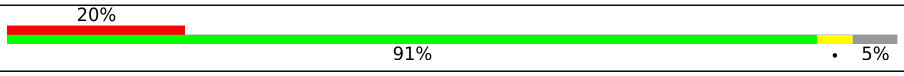
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	446	87% 13%
1	L	446	89% 11%
2	B	439	85% 11%
2	M	439	88% 8%
3	C	381	91% 8%
3	N	381	90% 9%
4	D	241	91% 9%
4	O	241	89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	196	
5	P	196	
6	F	110	
6	Q	110	
7	G	81	
7	R	81	
8	H	76	
8	S	76	
9	J	63	
9	U	63	
10	K	56	
10	V	56	
11	T	78	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3466	2167	611	671	17		
1	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
3	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
4	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1512	952	263	290	7		
5	P	196	Total	C	N	O	S	0	0
			1512	952	263	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		
6	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			674	434	124	115	1		
7	R	76	Total	C	N	O	S	0	0
			637	412	119	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	68	Total	C	N	O	S	0	0
			563	343	103	112	5		
8	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- 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	0	0
			495	323	86	86		
9	U	60	Total	C	N	O	0	0
			495	323	86	86		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

Continued on next page...

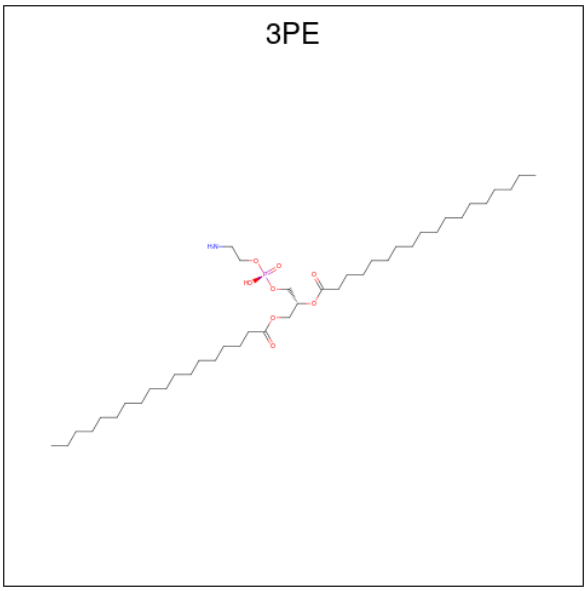
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



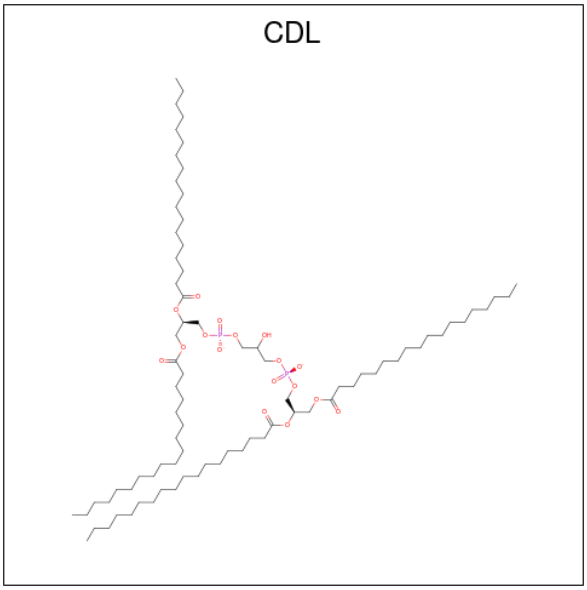
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
12	O	1	Total	C	N	O	P	0
			23	13	1	8	1	

Continued on next page...

Continued from previous page...

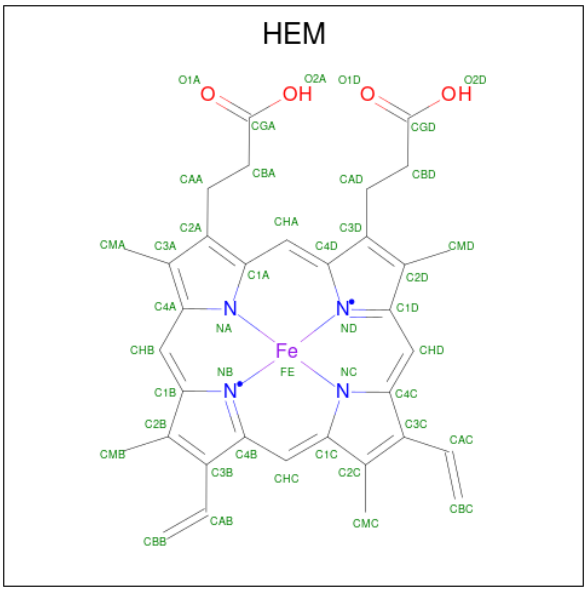
Mol	Chain	Residues	Atoms					AltConf
12	R	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



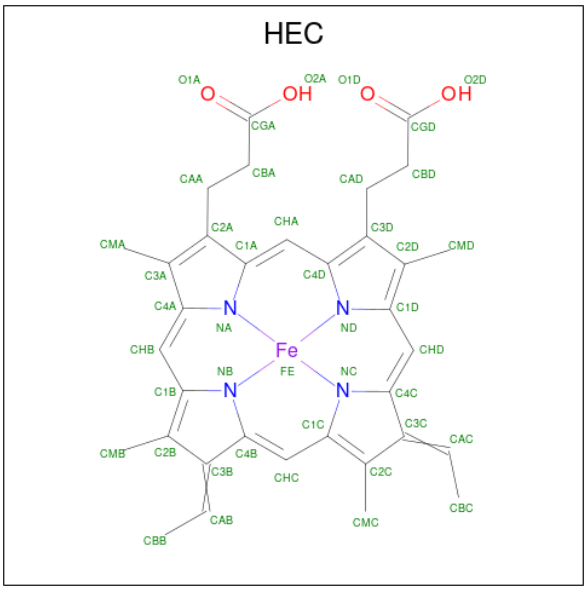
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			46	27	17	2	
13	G	1	Total	C	O	P	0
			98	60	34	4	
13	G	1	Total	C	O	P	0
			98	60	34	4	
13	N	1	Total	C	O	P	0
			46	27	17	2	
13	O	1	Total	C	O	P	0
			57	38	17	2	
13	R	1	Total	C	O	P	0
			41	22	17	2	

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



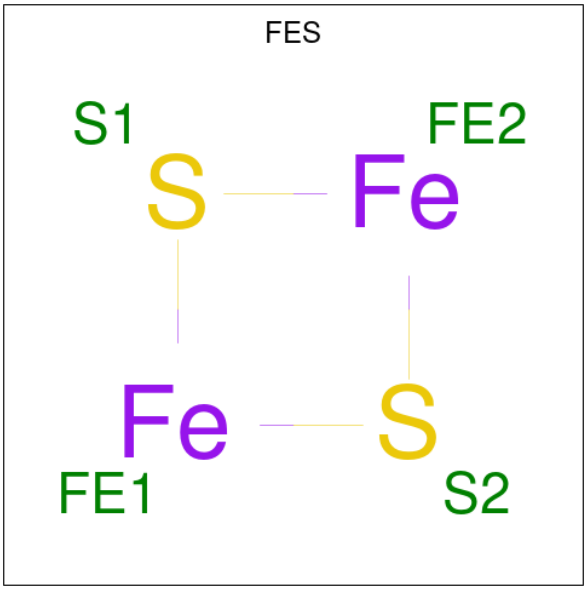
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
14	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



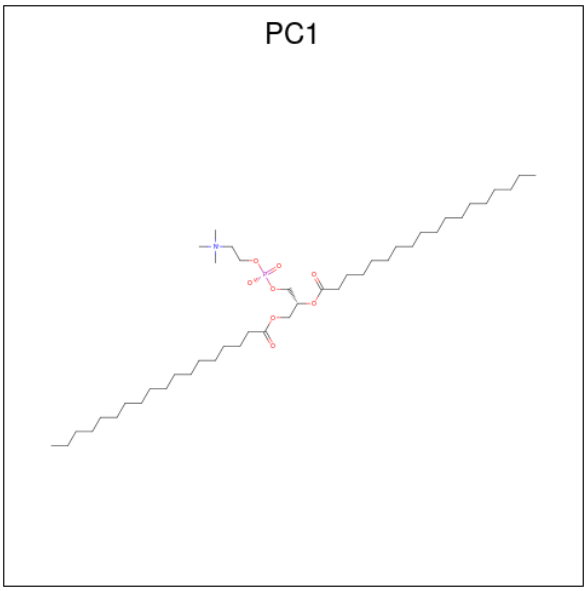
Mol	Chain	Residues	Atoms					AltConf
15	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
16	E	1	Total	Fe	S	0
			4	2	2	
16	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



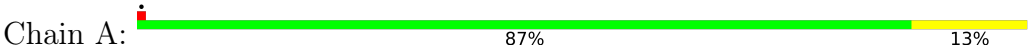
Mol	Chain	Residues	Atoms					AltConf
17	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
17	P	1	Total	C	N	O	P	0
			24	14	1	8	1	

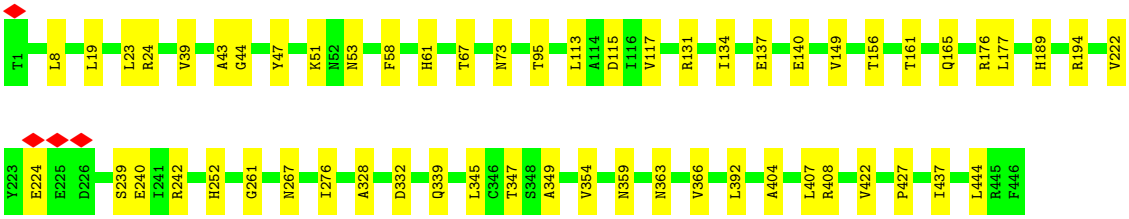
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

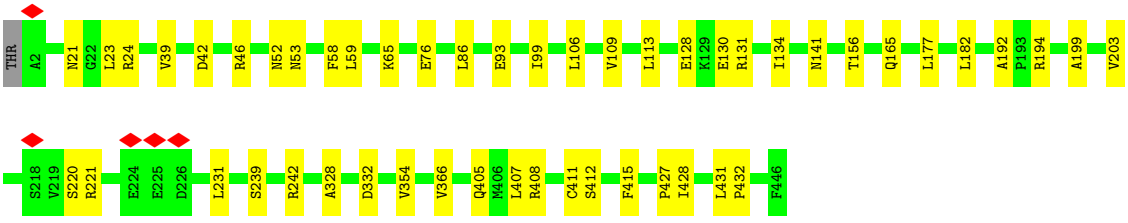
Chain A:





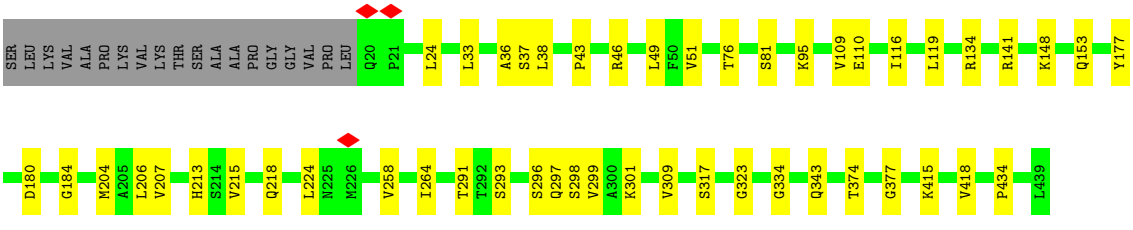
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



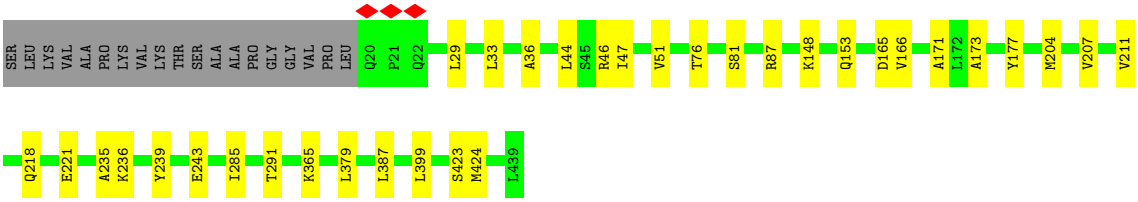
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:

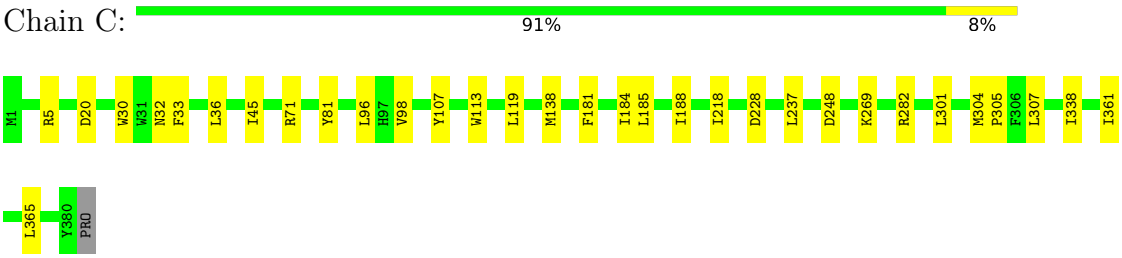


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

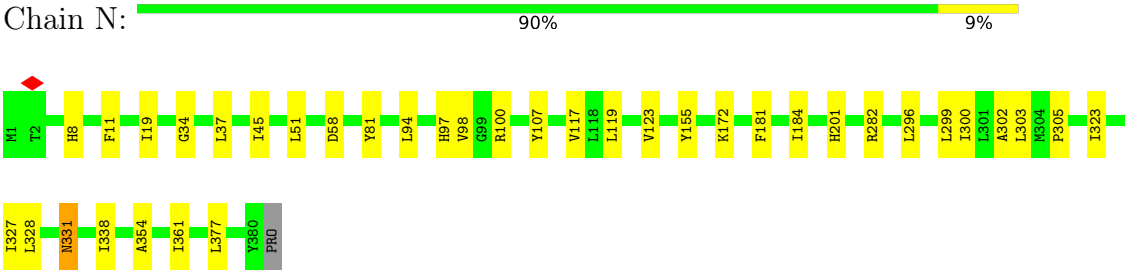
Chain M:



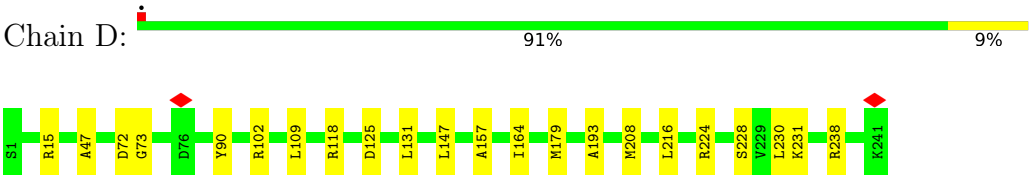
• Molecule 3: Cytochrome b



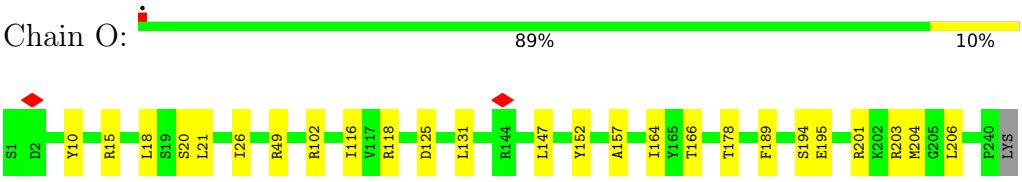
• Molecule 3: Cytochrome b



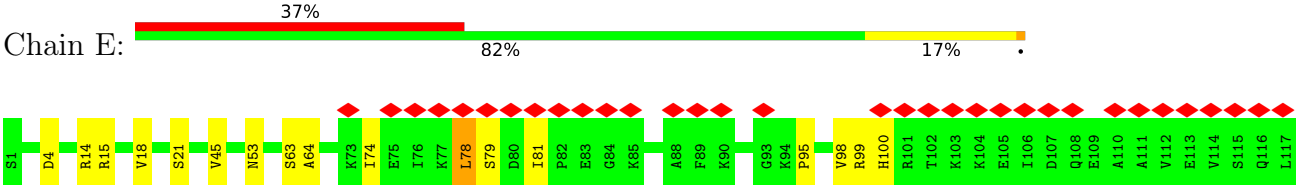
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

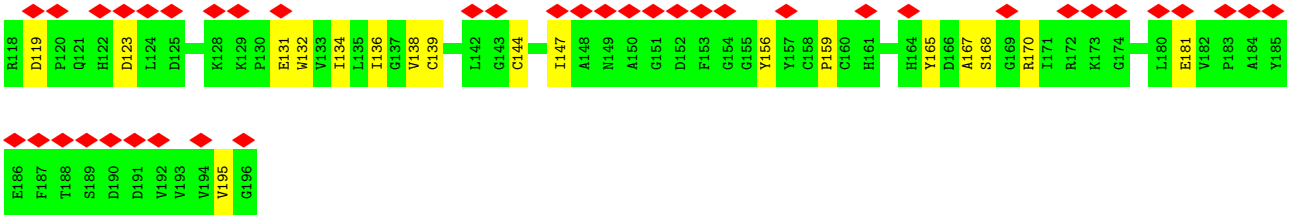


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

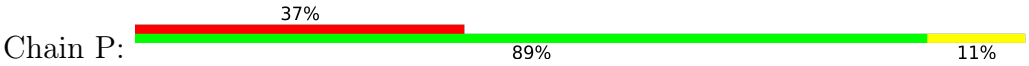


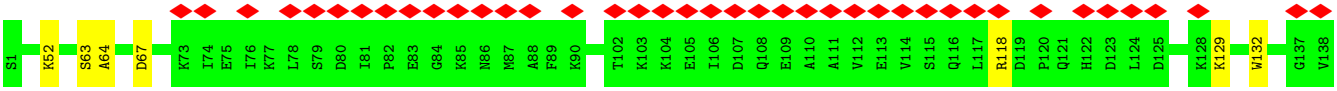
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

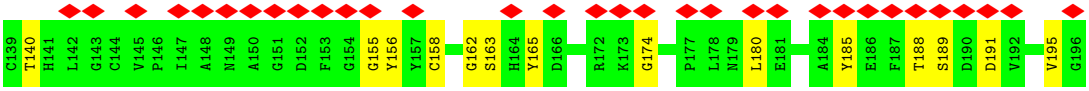




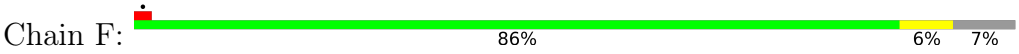
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



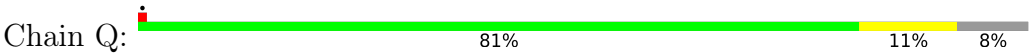


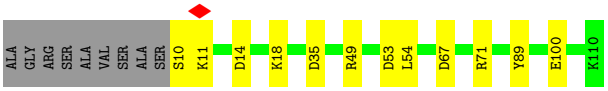


• Molecule 6: Cytochrome b-c1 complex subunit 7

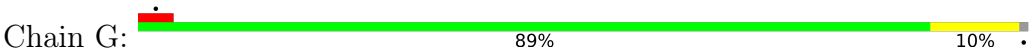


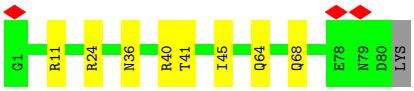
• Molecule 6: Cytochrome b-c1 complex subunit 7



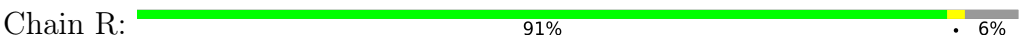


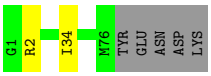
• Molecule 7: Cytochrome b-c1 complex subunit 8





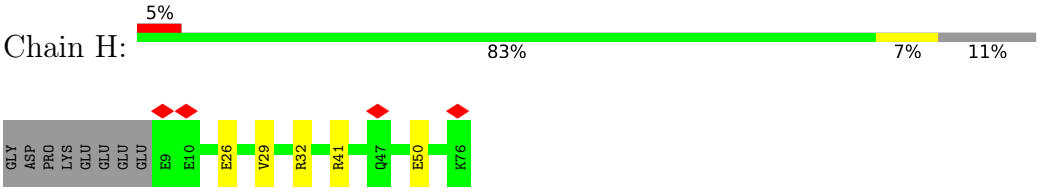
• Molecule 7: Cytochrome b-c1 complex subunit 8





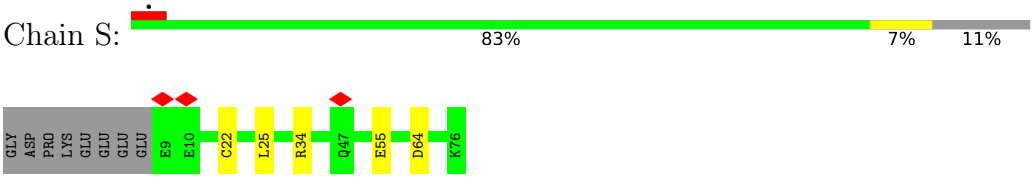
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



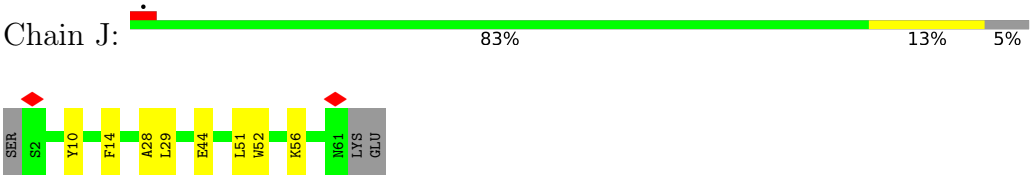
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S:



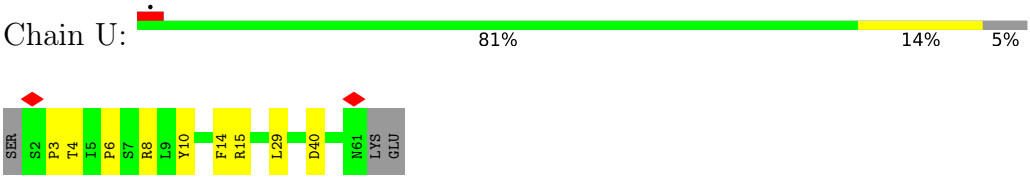
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain J:



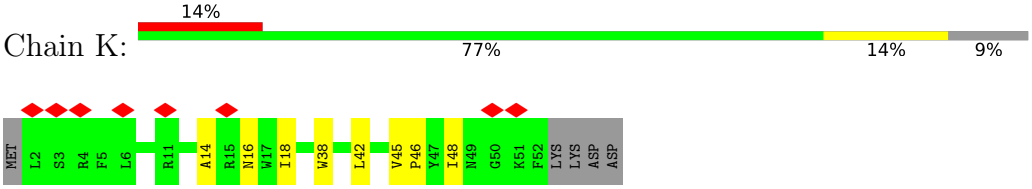
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain U:



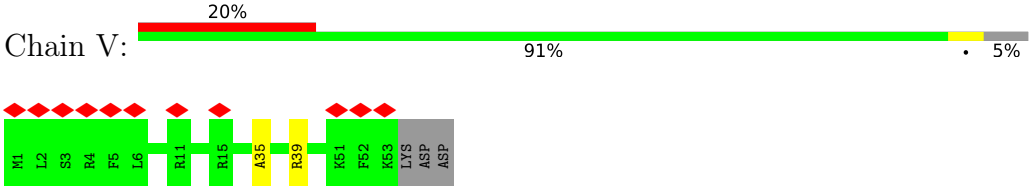
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain K:



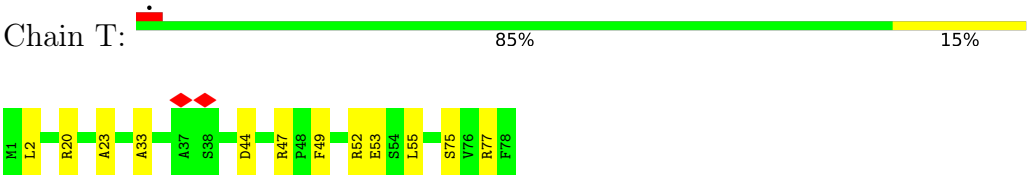
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain V:



• Molecule 11: Cytochrome b-c1 complex subunit 9

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129	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 ($e^-/Å^2$)	90.66	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	121.4548, 128.4522, 162.43954	wwPDB
Map dimensions	325, 257, 243	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.499814, 0.49981397, 0.49981397	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3536	0.59	1/4803 (0.0%)
1	L	0.29	0/3530	0.61	2/4793 (0.0%)
2	B	0.28	0/3205	0.55	0/4332
2	M	0.30	0/3205	0.55	0/4332
3	C	0.30	0/3147	0.54	0/4297
3	N	0.30	0/3147	0.56	1/4297 (0.0%)
4	D	0.29	0/1978	0.53	0/2685
4	O	0.28	0/1968	0.53	0/2674
5	E	0.26	0/1545	0.58	1/2091 (0.0%)
5	P	0.28	0/1545	0.56	0/2091
6	F	0.27	0/922	0.55	0/1234
6	Q	0.28	0/916	0.57	0/1226
7	G	0.33	0/693	0.63	0/936
7	R	0.36	0/655	0.68	0/884
8	H	0.32	0/570	0.68	0/763
8	S	0.27	0/570	0.59	0/763
9	J	0.32	0/509	0.59	1/687 (0.1%)
9	U	0.29	0/509	0.59	1/687 (0.1%)
10	K	0.26	0/437	0.54	0/598
10	V	0.26	0/454	0.56	0/619
11	T	0.32	0/565	0.65	0/772
All	All	0.29	0/33606	0.57	7/45564 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	332	ASP	CB-CG-OD1	9.51	126.86	118.30
1	L	332	ASP	CB-CG-OD1	8.58	126.02	118.30
5	E	78	LEU	CA-CB-CG	8.20	134.17	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	29	LEU	CA-CB-CG	6.10	129.33	115.30
3	N	377	LEU	CA-CB-CG	5.74	128.50	115.30
9	J	29	LEU	CA-CB-CG	5.36	127.64	115.30
1	L	23	LEU	CA-CB-CG	5.26	127.41	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	3466	0	3377	33	0
1	L	3460	0	3367	30	0
2	B	3154	0	3158	29	0
2	M	3154	0	3158	23	0
3	C	3046	0	3112	20	0
3	N	3046	0	3112	23	0
4	D	1919	0	1867	17	0
4	O	1909	0	1854	18	0
5	E	1512	0	1495	21	0
5	P	1512	0	1495	13	0
6	F	900	0	887	5	0
6	Q	894	0	882	7	0
7	G	674	0	672	7	0
7	R	637	0	647	2	0
8	H	563	0	543	3	0
8	S	563	0	541	3	0
9	J	495	0	489	4	0
9	U	495	0	489	5	0
10	K	421	0	418	5	0
10	V	438	0	443	1	0
11	T	554	0	590	8	0
12	A	23	0	20	1	0
12	C	35	0	44	0	0
12	E	32	0	38	2	0
12	G	51	0	82	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	23	0	20	1	0
12	N	37	0	48	0	0
12	O	23	0	20	1	0
12	R	51	0	82	2	0
13	A	46	0	36	0	0
13	G	98	0	84	2	0
13	N	46	0	36	3	0
13	O	57	0	58	1	0
13	R	41	0	26	0	0
14	C	86	0	60	3	0
14	N	86	0	60	4	0
15	D	43	0	30	1	0
15	O	43	0	30	2	0
16	E	4	0	0	0	0
16	P	4	0	0	1	0
17	J	35	0	44	0	0
17	P	24	0	22	0	0
All	All	33700	0	33436	246	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 4.

All (246) 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)
3:N:98:VAL:HG22	14:N:402:HEM:HBC2	1.71	0.71
1:L:411:CYS:O	1:L:415:PHE:HB2	1.93	0.68
9:U:4:THR:HG22	9:U:6:PRO:HD2	1.76	0.67
3:C:98:VAL:HG22	14:C:402:HEM:HBC2	1.78	0.65
4:D:102:ARG:HE	4:D:109:LEU:HB2	1.62	0.64
1:A:354:VAL:HG22	1:A:407:LEU:HD13	1.81	0.63
1:L:53:ASN:HD21	1:L:165:GLN:HB2	1.63	0.62
3:C:282:ARG:NH2	3:C:338:ILE:O	2.32	0.62
3:C:45:ILE:HA	14:C:401:HEM:HAB	1.82	0.61
9:U:10:TYR:HA	9:U:14:PHE:HB2	1.81	0.61
1:A:444:LEU:HD11	12:A:501:3PE:H11	1.83	0.60
4:D:224:ARG:O	4:D:228:SER:HB3	2.02	0.60
5:P:155:GLY:HA3	5:P:165:TYR:O	2.01	0.60
2:B:33:LEU:HD22	2:B:224:LEU:HD11	1.83	0.60
9:J:10:TYR:HA	9:J:14:PHE:HB2	1.82	0.60
3:N:45:ILE:HA	14:N:401:HEM:HAB	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:ILE:HD12	5:E:195:VAL:HG13	1.83	0.59
2:B:299:VAL:HG21	2:B:309:VAL:HG21	1.83	0.59
1:L:65:LYS:NZ	1:L:130:GLU:OE2	2.36	0.59
2:B:153:GLN:NE2	11:T:33:ALA:O	2.36	0.58
3:N:107:TYR:HB2	3:N:305:PRO:HG3	1.86	0.58
7:G:64:GLN:O	7:G:68:GLN:NE2	2.36	0.58
3:N:296:LEU:HA	3:N:299:LEU:HB2	1.86	0.58
9:J:52:TRP:O	9:J:56:LYS:HB2	2.04	0.58
1:L:76:GLU:HG2	2:M:285:ILE:HD12	1.85	0.58
1:A:261:GLY:O	1:A:267:ASN:ND2	2.35	0.57
2:M:153:GLN:NE2	11:T:44:ASP:O	2.37	0.57
6:Q:14:ASP:OD2	6:Q:18:LYS:NZ	2.37	0.57
1:A:53:ASN:HD21	1:A:165:GLN:HB2	1.69	0.57
1:A:240:GLU:HG3	1:A:422:VAL:HB	1.87	0.57
1:A:222:VAL:HG12	1:A:224:GLU:H	1.70	0.57
5:P:158:CYS:O	5:P:162:GLY:N	2.34	0.57
2:B:134:ARG:NH2	6:Q:49:ARG:O	2.39	0.56
2:B:148:LYS:NZ	2:B:180:ASP:OD1	2.38	0.56
3:N:51:LEU:HD13	14:N:401:HEM:HBA1	1.87	0.56
3:C:119:LEU:HD22	14:C:402:HEM:HBB2	1.87	0.55
6:F:14:ASP:OD2	6:F:18:LYS:NZ	2.39	0.55
1:A:61:HIS:NE2	1:A:137:GLU:OE2	2.39	0.55
4:D:238:ARG:HH22	5:E:4:ASP:HB2	1.72	0.55
8:H:41:ARG:NH2	8:H:50:GLU:OE2	2.40	0.55
5:E:53:ASN:ND2	12:E:201:3PE:O22	2.39	0.55
6:Q:67:ASP:OD2	6:Q:71:ARG:NH1	2.36	0.55
4:O:49:ARG:NH2	5:P:67:ASP:OD1	2.39	0.55
4:O:147:LEU:HD13	4:O:157:ALA:HB1	1.88	0.55
2:M:46:ARG:HG2	2:M:379:LEU:HD13	1.88	0.55
2:B:46:ARG:HG3	2:B:110:GLU:HB3	1.88	0.54
1:A:347:THR:O	10:K:16:ASN:ND2	2.39	0.54
11:T:52:ARG:NH2	11:T:53:GLU:OE2	2.39	0.54
1:A:131:ARG:NH2	1:A:177:LEU:O	2.41	0.54
1:L:21:ASN:HA	1:L:221:ARG:HD3	1.90	0.54
3:N:8:HIS:HB3	3:N:11:PHE:HB2	1.89	0.54
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.89	0.54
1:A:137:GLU:HA	1:A:140:GLU:HG2	1.89	0.54
9:U:3:PRO:O	9:U:8:ARG:NH1	2.41	0.53
11:T:75:SER:OG	11:T:77:ARG:NH1	2.41	0.53
2:B:415:LYS:HA	2:B:418:VAL:HG12	1.89	0.53
3:C:138:MET:HE2	3:C:269:LYS:H	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:VAL:HG12	5:E:134:ILE:HG12	1.91	0.53
2:M:29:LEU:HD12	2:M:33:LEU:HD23	1.90	0.53
4:O:166:THR:HG23	4:O:178:THR:HA	1.90	0.53
1:L:131:ARG:NH2	1:L:177:LEU:O	2.42	0.53
1:L:59:LEU:HD21	1:L:182:LEU:HB3	1.90	0.53
4:D:231:LYS:O	6:F:71:ARG:NH1	2.39	0.53
7:G:64:GLN:OE1	7:G:68:GLN:NE2	2.41	0.53
2:M:365:LYS:HG2	2:M:399:LEU:HD22	1.91	0.52
5:E:119:ASP:O	5:E:170:ARG:NH2	2.42	0.52
3:N:119:LEU:HD22	14:N:402:HEM:HBB2	1.91	0.52
8:S:22:CYS:HA	8:S:25:LEU:HD23	1.89	0.52
2:B:36:ALA:HB3	2:B:207:VAL:HG22	1.90	0.52
6:Q:49:ARG:NH2	6:Q:100:GLU:OE2	2.43	0.52
1:A:58:PHE:HD1	1:A:134:ILE:HD12	1.73	0.52
1:A:161:THR:HG22	5:E:21:SER:HB2	1.92	0.52
1:L:412:SER:O	9:U:15:ARG:NH2	2.43	0.52
3:N:323:ILE:HD11	12:R:102:3PE:H12	1.92	0.52
9:J:44:GLU:HG3	9:J:51:LEU:HD12	1.92	0.52
5:E:99:ARG:NH2	5:E:167:ALA:O	2.41	0.52
2:B:291:THR:O	2:B:297:GLN:NE2	2.43	0.52
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.91	0.52
1:A:189:HIS:HA	1:A:194:ARG:HH22	1.75	0.51
5:P:63:SER:OG	5:P:64:ALA:N	2.43	0.51
1:A:19:LEU:HD12	1:A:23:LEU:HD23	1.91	0.51
1:L:354:VAL:HG22	1:L:407:LEU:HD13	1.92	0.51
1:L:141:ASN:OD1	11:T:47:ARG:NH1	2.44	0.51
3:N:282:ARG:NH2	3:N:338:ILE:O	2.44	0.51
5:P:156:TYR:HB2	5:P:165:TYR:HB2	1.93	0.50
6:Q:10:SER:OG	6:Q:11:LYS:N	2.43	0.50
1:A:359:ASN:O	1:A:363:ASN:ND2	2.44	0.50
4:D:208:MET:HA	12:E:201:3PE:H231	1.93	0.50
1:A:39:VAL:HG23	1:A:113:LEU:HD13	1.93	0.50
3:N:201:HIS:O	7:R:2:ARG:NH2	2.44	0.50
1:L:76:GLU:OE1	2:M:291:THR:OG1	2.29	0.50
3:N:181:PHE:HA	3:N:184:ILE:HG22	1.94	0.50
1:L:58:PHE:HD1	1:L:134:ILE:HD12	1.76	0.50
4:D:131:LEU:HD11	15:D:301:HEC:HMB2	1.94	0.49
3:N:58:ASP:HA	3:N:172:LYS:HE3	1.93	0.49
3:N:327:ILE:HG12	12:R:102:3PE:H2A2	1.95	0.49
2:B:37:SER:HB3	2:B:213:HIS:HD1	1.76	0.49
2:B:374:THR:HG23	2:B:377:GLY:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HG21	1:A:115:ASP:HB3	1.94	0.49
5:E:63:SER:OG	5:E:64:ALA:N	2.45	0.49
4:O:131:LEU:HD11	15:O:303:HEC:HMB2	1.95	0.49
5:E:78:LEU:HD23	5:E:79:SER:H	1.77	0.49
2:M:76:THR:HG23	2:M:81:SER:HA	1.93	0.49
3:C:218:ILE:HG21	4:D:230:LEU:HD11	1.94	0.49
1:L:39:VAL:HG23	1:L:113:LEU:HD13	1.95	0.49
3:C:304:MET:HA	3:C:307:LEU:HD12	1.96	0.48
3:C:32:ASN:ND2	3:C:228:ASP:OD1	2.47	0.48
2:B:76:THR:HG23	2:B:81:SER:HA	1.95	0.48
2:B:95:LYS:O	2:B:109:VAL:HA	2.14	0.48
1:L:199:ALA:HB1	1:L:203:VAL:HG21	1.96	0.48
3:N:117:VAL:HG11	3:N:302:ALA:HB2	1.95	0.48
5:E:139:CYS:SG	5:E:165:TYR:OH	2.70	0.48
3:C:361:ILE:HA	3:C:365:LEU:HB2	1.95	0.48
1:L:106:LEU:HD11	1:L:203:VAL:HG13	1.96	0.47
2:B:298:SER:OG	2:B:343:GLN:NE2	2.40	0.47
1:A:328:ALA:HB2	1:A:427:PRO:HB2	1.95	0.47
4:O:26:ILE:HG23	4:O:189:PHE:HA	1.96	0.47
4:O:131:LEU:HB3	4:O:164:ILE:HD11	1.96	0.47
4:D:164:ILE:HG22	4:D:179:MET:HG3	1.97	0.47
10:K:38:TRP:HE1	3:N:155:TYR:HH	1.62	0.47
10:K:42:LEU:HD22	10:K:48:ILE:HG21	1.96	0.47
1:A:156:THR:O	1:A:239:SER:OG	2.30	0.47
3:N:81:TYR:OH	4:O:118:ARG:NH2	2.48	0.47
4:O:15:ARG:NH2	4:O:125:ASP:OD2	2.48	0.47
3:C:185:LEU:HD23	3:C:188:ILE:HD12	1.95	0.47
2:M:171:ALA:HB2	2:M:235:ALA:HB3	1.96	0.47
1:A:276:ILE:HG21	1:A:345:LEU:HD21	1.97	0.46
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.96	0.46
1:L:86:LEU:HD13	1:L:99:ILE:HG12	1.96	0.46
1:A:349:ALA:O	1:A:408:ARG:NH1	2.48	0.46
3:C:81:TYR:OH	4:D:118:ARG:NH1	2.47	0.46
4:O:118:ARG:HG3	4:O:194:SER:HB3	1.97	0.46
4:O:203:ARG:NH1	9:U:40:ASP:OD1	2.47	0.46
2:B:215:VAL:HA	2:B:218:GLN:HG2	1.98	0.46
4:D:72:ASP:OD2	4:D:73:GLY:N	2.48	0.46
1:L:156:THR:O	1:L:239:SER:OG	2.32	0.46
3:C:30:TRP:HZ3	3:C:96:LEU:HD22	1.81	0.46
1:L:128:GLU:OE2	1:L:131:ARG:NH1	2.49	0.46
13:N:404:CDL:HB31	13:N:404:CDL:H112	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ILE:HB	2:B:317:SER:HA	1.98	0.46
6:F:73:GLN:OE1	7:G:36:ASN:ND2	2.49	0.46
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.42	0.46
4:D:15:ARG:NH2	4:D:125:ASP:OD2	2.49	0.46
1:L:328:ALA:HB2	1:L:427:PRO:HB2	1.98	0.46
1:L:242:ARG:HB2	1:L:428:ILE:HD12	1.98	0.45
2:M:243:GLU:HA	2:M:424:MET:O	2.16	0.45
3:N:94:LEU:HD11	3:N:123:VAL:HG11	1.98	0.45
1:A:134:ILE:HA	1:A:137:GLU:HG2	1.98	0.45
3:C:113:TRP:NE1	3:C:301:LEU:O	2.37	0.45
5:P:191:ASP:N	5:P:191:ASP:OD1	2.43	0.45
11:T:20:ARG:HD3	11:T:23:ALA:HA	1.99	0.45
1:A:44:GLY:H	1:A:47:TYR:HD2	1.65	0.45
5:P:118:ARG:HH22	5:P:174:GLY:H	1.65	0.45
5:E:15:ARG:HG2	7:G:24:ARG:HG3	1.98	0.45
5:E:147:ILE:HG13	5:E:159:PRO:HD3	1.98	0.44
1:A:240:GLU:OE2	1:A:242:ARG:NH1	2.45	0.44
2:B:264:ILE:HG23	11:T:2:LEU:HD22	1.98	0.44
4:O:18:LEU:HD22	4:O:206:LEU:HB2	1.99	0.44
8:S:34:ARG:HG2	8:S:55:GLU:HG2	1.99	0.44
2:B:141:ARG:HD2	2:B:184:GLY:H	1.83	0.44
4:O:152:TYR:OH	8:S:64:ASP:OD2	2.29	0.44
5:E:136:ILE:HD12	5:E:181:GLU:HG3	2.00	0.44
3:C:237:LEU:HD22	4:D:216:LEU:HD11	1.99	0.44
3:C:248:ASP:OD2	4:D:118:ARG:NH1	2.50	0.44
2:M:239:TYR:OH	2:M:423:SER:OG	2.33	0.44
1:L:86:LEU:HB3	2:M:285:ILE:HG12	1.98	0.44
2:B:116:ILE:HA	2:B:119:LEU:HB2	2.00	0.43
5:E:144:CYS:SG	4:O:102:ARG:NH1	2.91	0.43
3:N:300:ILE:HA	3:N:303:LEU:HB3	2.00	0.43
5:E:156:TYR:HB2	5:E:165:TYR:HB2	2.00	0.43
2:M:51:VAL:HG22	2:M:204:MET:HG2	2.00	0.43
2:B:49:LEU:HD12	2:B:206:LEU:HD13	1.99	0.43
2:M:87:ARG:HA	2:M:87:ARG:HD3	1.86	0.43
1:A:8:LEU:HD22	1:A:392:LEU:HB3	2.00	0.43
4:D:224:ARG:NH1	13:G:102:CDL:O1	2.52	0.43
4:O:10:TYR:O	4:O:15:ARG:NE	2.51	0.43
2:B:298:SER:HA	2:B:301:LYS:HE3	1.99	0.43
1:L:366:VAL:HG12	2:M:44:LEU:HD22	2.00	0.43
2:M:166:VAL:HG12	2:M:423:SER:HB3	2.00	0.43
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:ILE:HB	5:E:132:TRP:HZ3	1.84	0.43
1:A:73:ASN:HB2	2:B:291:THR:HG21	2.01	0.43
1:L:42:ASP:HB3	1:L:194:ARG:HB3	1.99	0.43
1:A:339:GLN:NE2	1:A:437:ILE:O	2.49	0.43
1:L:405:GLN:OE1	1:L:408:ARG:NH2	2.48	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43
8:H:29:VAL:HG23	8:H:32:ARG:HH21	1.84	0.43
1:L:99:ILE:HD12	1:L:109:VAL:HG13	2.00	0.43
2:M:36:ALA:O	2:M:207:VAL:HA	2.19	0.43
2:M:236:LYS:HA	2:M:236:LYS:HD3	1.90	0.43
4:O:116:ILE:HG12	15:O:303:HEC:HMA3	2.00	0.42
10:K:14:ALA:O	10:K:18:ILE:HG12	2.18	0.42
3:N:331:ASN:HD21	3:N:354:ALA:HB1	1.84	0.42
5:E:123:ASP:OD1	5:E:168:SER:OG	2.33	0.42
8:H:26:GLU:HA	8:H:29:VAL:HG12	2.02	0.42
2:M:239:TYR:HH	2:M:423:SER:HG	1.65	0.42
5:P:185:TYR:HB3	5:P:195:VAL:HG13	2.01	0.42
1:A:149:VAL:HG21	1:A:252:HIS:HB2	2.02	0.42
3:C:181:PHE:HA	3:C:184:ILE:HG22	2.00	0.42
5:P:188:THR:HG22	5:P:189:SER:H	1.85	0.42
4:O:20:SER:OG	4:O:21:LEU:N	2.52	0.42
2:B:24:LEU:HD13	2:B:38:LEU:HB2	2.02	0.42
7:G:41:THR:O	7:G:45:ILE:HB	2.19	0.42
1:L:192:ALA:N	1:L:220:SER:OG	2.49	0.42
2:B:258:VAL:HA	2:B:323:GLY:HA3	2.02	0.42
3:C:5:ARG:NH1	3:C:20:ASP:OD2	2.49	0.42
2:M:218:GLN:HA	2:M:221:GLU:HG3	2.02	0.42
3:N:97:HIS:CE1	3:N:100:ARG:HH22	2.38	0.42
3:N:328:LEU:HB2	3:N:361:ILE:HG21	2.01	0.42
4:O:204:MET:HG2	12:O:302:3PE:H11	2.02	0.42
3:C:33:PHE:O	3:C:36:LEU:HB2	2.19	0.41
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.30	0.41
1:L:231:LEU:HD12	1:L:231:LEU:HA	1.90	0.41
3:N:19:ILE:HG12	13:N:404:CDL:H331	2.01	0.41
5:P:52:LYS:HD2	10:V:35:ALA:HA	2.01	0.41
5:P:129:LYS:HD2	5:P:132:TRP:HB2	2.01	0.41
6:Q:53:ASP:OD1	6:Q:54:LEU:N	2.52	0.41
3:C:71:ARG:NH2	4:D:193:ALA:O	2.50	0.41
1:L:46:ARG:NH1	1:L:93:GLU:OE2	2.52	0.41
5:E:45:VAL:HG13	9:J:28:ALA:HA	2.02	0.41
5:E:100:HIS:NE2	5:E:131:GLU:OE2	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:148:LYS:HG3	2:M:177:TYR:HB3	2.02	0.41
1:A:39:VAL:HG11	1:A:117:VAL:HG11	2.03	0.41
1:A:43:ALA:O	1:A:95:THR:OG1	2.38	0.41
5:E:14:ARG:HG2	5:E:18:VAL:HG23	2.01	0.41
1:L:431:LEU:HA	1:L:432:PRO:HD3	1.96	0.41
4:O:195:GLU:OE2	4:O:201:ARG:NE	2.54	0.41
13:O:301:CDL:H311	7:R:34:ILE:HD13	2.02	0.41
4:D:147:LEU:HD13	4:D:157:ALA:HB1	2.03	0.41
5:P:140:THR:HG23	5:P:180:LEU:HD23	2.03	0.41
11:T:49:PHE:HB3	11:T:55:LEU:HG	2.02	0.41
2:B:293:SER:HB2	2:B:296:SER:HB2	2.02	0.41
12:L:501:3PE:H32	13:N:404:CDL:H312	2.03	0.41
1:A:354:VAL:HG21	1:A:404:ALA:HA	2.02	0.41
2:B:51:VAL:HG22	2:B:204:MET:HG2	2.03	0.41
5:E:95:PRO:HD2	5:E:138:VAL:HG22	2.03	0.41
2:M:47:ILE:HD11	2:M:211:VAL:HG11	2.02	0.41
2:M:165:ASP:HA	2:M:173:ALA:HB1	2.03	0.41
3:N:34:GLY:O	3:N:37:LEU:HB2	2.21	0.41
7:G:40:ARG:NE	13:G:101:CDL:OB4	2.45	0.41
5:P:163:SER:OG	16:P:201:FES:S1	2.69	0.40
6:Q:35:ASP:OD1	6:Q:89:TYR:OH	2.29	0.40
1:A:51:LYS:O	1:A:176:ARG:NH2	2.50	0.40
1:L:52:ASN:OD1	1:L:52:ASN:N	2.54	0.40
10:K:45:VAL:HA	10:K:46:PRO:HD3	1.95	0.40
2:M:387:LEU:HD23	2:M:387:LEU:HA	1.92	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	444/446 (100%)	428 (96%)	16 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	443/446 (99%)	432 (98%)	11 (2%)	0	100	100
2	B	418/439 (95%)	405 (97%)	13 (3%)	0	100	100
2	M	418/439 (95%)	402 (96%)	16 (4%)	0	100	100
3	C	378/381 (99%)	371 (98%)	7 (2%)	0	100	100
3	N	378/381 (99%)	370 (98%)	8 (2%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
4	O	238/241 (99%)	234 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
5	P	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
6	F	100/110 (91%)	100 (100%)	0	0	100	100
6	Q	99/110 (90%)	99 (100%)	0	0	100	100
7	G	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
7	R	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
8	H	66/76 (87%)	65 (98%)	1 (2%)	0	100	100
8	S	66/76 (87%)	62 (94%)	4 (6%)	0	100	100
9	J	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
9	U	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
10	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
10	V	51/56 (91%)	51 (100%)	0	0	100	100
11	T	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
All	All	4119/4256 (97%)	4004 (97%)	115 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	373/373 (100%)	372 (100%)	1 (0%)	92	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	372/373 (100%)	371 (100%)	1 (0%)	92 98
2	B	330/344 (96%)	330 (100%)	0	100 100
2	M	330/344 (96%)	330 (100%)	0	100 100
3	C	332/333 (100%)	332 (100%)	0	100 100
3	N	332/333 (100%)	331 (100%)	1 (0%)	92 98
4	D	206/206 (100%)	206 (100%)	0	100 100
4	O	205/206 (100%)	205 (100%)	0	100 100
5	E	166/166 (100%)	166 (100%)	0	100 100
5	P	166/166 (100%)	166 (100%)	0	100 100
6	F	94/98 (96%)	94 (100%)	0	100 100
6	Q	93/98 (95%)	93 (100%)	0	100 100
7	G	72/73 (99%)	72 (100%)	0	100 100
7	R	68/73 (93%)	68 (100%)	0	100 100
8	H	65/72 (90%)	65 (100%)	0	100 100
8	S	65/72 (90%)	65 (100%)	0	100 100
9	J	51/54 (94%)	51 (100%)	0	100 100
9	U	51/54 (94%)	51 (100%)	0	100 100
10	K	41/46 (89%)	41 (100%)	0	100 100
10	V	43/46 (94%)	42 (98%)	1 (2%)	50 75
11	T	58/58 (100%)	58 (100%)	0	100 100
All	All	3513/3588 (98%)	3509 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	L	24	ARG
3	N	331	ASN
10	V	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	53	ASN
7	G	36	ASN
7	G	68	GLN
1	L	53	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	3PE	A	501	-	22,22,50	0.46	0	25,27,55	0.73	1 (4%)
14	HEM	N	401	3	27,50,50	0.96	2 (7%)	17,82,82	1.25	2 (11%)
16	FES	P	201	5	0,4,4	-	-	-		
16	FES	E	202	5	0,4,4	-	-	-		
14	HEM	N	402	3	27,50,50	0.99	2 (7%)	17,82,82	1.16	1 (5%)
13	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.37	0
12	3PE	O	302	-	22,22,50	0.44	0	25,27,55	0.40	0
14	HEM	C	401	3	27,50,50	0.95	2 (7%)	17,82,82	1.24	2 (11%)
12	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CDL	N	404	-	45,45,99	0.44	0	51,57,111	0.55	1 (1%)
17	PC1	P	202	-	23,23,53	0.45	0	29,31,61	0.70	1 (3%)
12	3PE	G	103	-	50,50,50	0.31	0	53,55,55	0.29	0
12	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.32	0
12	3PE	E	201	-	31,31,50	0.38	0	34,36,55	0.38	0
14	HEM	C	402	3	27,50,50	0.99	2 (7%)	17,82,82	1.17	0
17	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.37	0
13	CDL	G	102	-	55,55,99	0.39	0	61,67,111	0.33	0
13	CDL	R	101	-	40,40,99	0.47	0	46,52,111	0.58	1 (2%)
13	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.32	0
12	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.40	0
12	3PE	R	102	-	50,50,50	0.33	0	53,55,55	0.59	1 (1%)
15	HEC	D	301	4	26,50,50	2.36	3 (11%)	18,82,82	1.81	5 (27%)
15	HEC	O	303	4	26,50,50	2.35	3 (11%)	18,82,82	1.87	5 (27%)
13	CDL	G	101	-	41,41,99	0.45	0	47,53,111	0.35	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
12	3PE	A	501	-	-	7/26/26/54	-
14	HEM	N	401	3	-	1/6/54/54	-
16	FES	P	201	5	-	-	0/1/1/1
16	FES	E	202	5	-	-	0/1/1/1
14	HEM	N	402	3	-	0/6/54/54	-
13	CDL	A	502	-	-	17/56/56/110	-
12	3PE	O	302	-	-	10/26/26/54	-
14	HEM	C	401	3	-	1/6/54/54	-
12	3PE	C	403	-	-	2/38/38/54	-
13	CDL	N	404	-	-	5/56/56/110	-
17	PC1	P	202	-	-	12/27/27/57	-
12	3PE	G	103	-	-	10/54/54/54	-
12	3PE	N	403	-	-	4/40/40/54	-
12	3PE	E	201	-	-	8/35/35/54	-
14	HEM	C	402	3	-	0/6/54/54	-
17	PC1	J	101	-	-	7/38/38/57	-
13	CDL	G	102	-	-	13/66/66/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	R	101	-	-	10/51/51/110	-
13	CDL	O	301	-	-	19/67/67/110	-
12	3PE	L	501	-	-	7/26/26/54	-
12	3PE	R	102	-	-	10/54/54/54	-
15	HEC	D	301	4	-	0/6/54/54	-
15	HEC	O	303	4	-	0/6/54/54	-
13	CDL	G	101	-	-	14/52/52/110	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	301	HEC	C3C-C2C	-6.35	1.34	1.40
15	O	303	HEC	C3C-C2C	-6.35	1.34	1.40
15	D	301	HEC	C3B-C2B	-6.31	1.34	1.40
15	O	303	HEC	C3B-C2B	-6.26	1.34	1.40
15	D	301	HEC	C3D-C2D	5.39	1.53	1.37
15	O	303	HEC	C3D-C2D	5.34	1.53	1.37
14	N	402	HEM	C3B-C2B	-3.07	1.36	1.40
14	C	402	HEM	C3B-C2B	-2.98	1.36	1.40
14	N	401	HEM	C3B-C2B	-2.88	1.36	1.40
14	C	401	HEM	C3B-C2B	-2.83	1.36	1.40
14	C	402	HEM	C4D-C3D	2.29	1.47	1.42
14	N	402	HEM	C4D-C3D	2.25	1.47	1.42
14	C	401	HEM	C4D-C3D	2.06	1.47	1.42
14	N	401	HEM	C4D-C3D	2.03	1.47	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	301	HEC	CMC-C2C-C1C	-3.82	122.60	128.46
15	O	303	HEC	CMC-C2C-C1C	-3.59	122.95	128.46
15	O	303	HEC	CBD-CAD-C3D	-3.23	106.54	112.49
15	D	301	HEC	CMB-C2B-C1B	-2.78	124.19	128.46
15	D	301	HEC	CAA-CBA-CGA	-2.72	108.11	112.67
15	O	303	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
15	O	303	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
15	O	303	HEC	CAA-CBA-CGA	-2.63	108.25	112.67
14	C	401	HEM	CBD-CAD-C3D	-2.48	107.91	112.48
14	N	401	HEM	CAA-CBA-CGA	-2.37	108.69	112.67
15	D	301	HEC	C1D-C2D-C3D	-2.33	105.37	107.00
13	N	404	CDL	CB4-OB6-CB5	2.31	123.47	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	501	3PE	C2-O21-C21	2.24	123.31	117.79
17	P	202	PC1	C2-O21-C21	2.23	123.27	117.79
13	R	101	CDL	CA4-OA6-CA5	2.20	123.21	117.79
14	N	402	HEM	CMC-C2C-C3C	2.16	128.72	124.68
12	R	102	3PE	C2-O21-C21	2.16	123.10	117.79
15	D	301	HEC	CBD-CAD-C3D	-2.13	108.56	112.49
14	C	401	HEM	CAA-CBA-CGA	-2.08	109.18	112.67
14	N	401	HEM	CBD-CAD-C3D	-2.06	108.69	112.48

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	3PE	C11-O13-P-O12
12	A	501	3PE	O13-C11-C12-N
12	C	403	3PE	C11-O13-P-O14
12	G	103	3PE	C1-O11-P-O12
12	G	103	3PE	C1-O11-P-O14
12	G	103	3PE	C11-O13-P-O11
12	G	103	3PE	O13-C11-C12-N
12	L	501	3PE	C11-O13-P-O11
12	L	501	3PE	C11-O13-P-O12
12	L	501	3PE	C11-O13-P-O14
12	N	403	3PE	O13-C11-C12-N
12	O	302	3PE	C1-O11-P-O14
12	O	302	3PE	C11-O13-P-O14
12	O	302	3PE	O13-C11-C12-N
12	R	102	3PE	C11-O13-P-O11
12	R	102	3PE	C11-O13-P-O14
12	R	102	3PE	O13-C11-C12-N
13	A	502	CDL	CA2-OA2-PA1-OA3
13	A	502	CDL	CA2-OA2-PA1-OA4
13	A	502	CDL	CA2-OA2-PA1-OA5
13	A	502	CDL	CB2-OB2-PB2-OB4
13	G	101	CDL	CA2-OA2-PA1-OA3
13	G	101	CDL	CA2-OA2-PA1-OA4
13	G	101	CDL	CB2-OB2-PB2-OB3
13	G	101	CDL	CB2-OB2-PB2-OB4
13	G	101	CDL	CB2-OB2-PB2-OB5
13	G	101	CDL	CB3-OB5-PB2-OB2
13	G	101	CDL	CB3-OB5-PB2-OB3
13	G	101	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	102	CDL	CB2-OB2-PB2-OB5
13	G	102	CDL	CB3-OB5-PB2-OB4
13	O	301	CDL	CB2-OB2-PB2-OB3
13	O	301	CDL	CB3-OB5-PB2-OB4
13	R	101	CDL	CA2-OA2-PA1-OA3
13	R	101	CDL	CA2-OA2-PA1-OA4
13	R	101	CDL	CA2-OA2-PA1-OA5
13	R	101	CDL	CB2-OB2-PB2-OB3
14	C	401	HEM	C2A-CAA-CBA-CGA
14	N	401	HEM	C2A-CAA-CBA-CGA
17	P	202	PC1	C11-O13-P-O14
17	P	202	PC1	C1-O11-P-O12
17	P	202	PC1	C1-O11-P-O13
17	P	202	PC1	O13-C11-C12-N
12	R	102	3PE	C32-C33-C34-C35
12	G	103	3PE	C32-C33-C34-C35
13	O	301	CDL	CB4-CB3-OB5-PB2
12	A	501	3PE	C11-O13-P-O11
12	G	103	3PE	C1-O11-P-O13
12	O	302	3PE	C1-O11-P-O13
12	R	102	3PE	C1-O11-P-O13
13	A	502	CDL	CB2-OB2-PB2-OB5
13	A	502	CDL	CB3-OB5-PB2-OB2
13	G	101	CDL	CA2-OA2-PA1-OA5
13	G	102	CDL	CB3-OB5-PB2-OB2
13	O	301	CDL	CA2-OA2-PA1-OA5
13	O	301	CDL	CB3-OB5-PB2-OB2
17	J	101	PC1	C11-O13-P-O11
17	J	101	PC1	C1-O11-P-O13
17	P	202	PC1	C11-O13-P-O11
12	G	103	3PE	C3C-C3D-C3E-C3F
12	R	102	3PE	C3C-C3D-C3E-C3F
12	G	103	3PE	C37-C38-C39-C3A
12	N	403	3PE	C25-C26-C27-C28
13	G	102	CDL	C74-C75-C76-C77
12	R	102	3PE	C38-C39-C3A-C3B
13	G	101	CDL	OB5-CB3-CB4-OB6
12	E	201	3PE	C11-O13-P-O11
12	L	501	3PE	C1-O11-P-O13
13	O	301	CDL	CB2-OB2-PB2-OB5
13	G	102	CDL	C1-CB2-OB2-PB2
13	O	301	CDL	C52-C51-CB5-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	501	3PE	C32-C33-C34-C35
13	G	101	CDL	OB5-CB3-CB4-CB6
13	G	102	CDL	OB5-CB3-CB4-CB6
12	E	201	3PE	O13-C11-C12-N
12	O	302	3PE	C1-C2-C3-O31
17	P	202	PC1	C1-C2-C3-O31
13	G	102	CDL	OB5-CB3-CB4-OB6
12	O	302	3PE	O21-C2-C3-O31
12	E	201	3PE	O11-C1-C2-C3
13	G	102	CDL	CB4-CB3-OB5-PB2
13	N	404	CDL	CB4-CB3-OB5-PB2
17	J	101	PC1	C2-C1-O11-P
13	A	502	CDL	OB5-CB3-CB4-OB6
12	E	201	3PE	C1-O11-P-O13
13	R	101	CDL	CB2-OB2-PB2-OB5
13	R	101	CDL	CA4-CA3-OA5-PA1
12	A	501	3PE	C11-O13-P-O14
12	G	103	3PE	C11-O13-P-O12
12	O	302	3PE	C1-O11-P-O12
12	R	102	3PE	C1-O11-P-O14
13	A	502	CDL	CB2-OB2-PB2-OB3
13	A	502	CDL	CB3-OB5-PB2-OB3
13	A	502	CDL	CB3-OB5-PB2-OB4
13	G	102	CDL	CB2-OB2-PB2-OB4
13	O	301	CDL	CA2-OA2-PA1-OA3
13	O	301	CDL	CA2-OA2-PA1-OA4
13	O	301	CDL	CB2-OB2-PB2-OB4
17	J	101	PC1	C11-O13-P-O14
17	J	101	PC1	C1-O11-P-O12
17	J	101	PC1	C1-O11-P-O14
17	P	202	PC1	C11-O13-P-O12
17	P	202	PC1	C1-O11-P-O14
13	A	502	CDL	OB5-CB3-CB4-CB6
13	R	101	CDL	OB5-CB3-CB4-CB6
12	E	201	3PE	O11-C1-C2-O21
17	J	101	PC1	O13-C11-C12-N
13	G	102	CDL	C1-CA2-OA2-PA1
13	O	301	CDL	C1-CA2-OA2-PA1
13	R	101	CDL	OB5-CB3-CB4-OB6
12	G	103	3PE	C35-C36-C37-C38
12	L	501	3PE	C31-C32-C33-C34
13	N	404	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	O	301	CDL	CA3-OA5-PA1-OA2
13	R	101	CDL	C52-C51-CB5-OB6
13	O	301	CDL	C52-C51-CB5-OB7
13	R	101	CDL	C52-C51-CB5-OB7
12	R	102	3PE	C2B-C2C-C2D-C2E
13	G	102	CDL	C72-C73-C74-C75
13	O	301	CDL	C75-C76-C77-C78
13	G	102	CDL	C52-C51-CB5-OB6
17	P	202	PC1	O11-C1-C2-O21
13	O	301	CDL	O1-C1-CA2-OA2
13	G	101	CDL	C72-C71-CB7-OB8
13	A	502	CDL	C32-C31-CA7-OA8
12	C	403	3PE	C11-O13-P-O11
12	O	302	3PE	O21-C21-C22-C23
12	E	201	3PE	C21-C22-C23-C24
12	N	403	3PE	O31-C31-C32-C33
13	G	101	CDL	C72-C71-CB7-OB9
13	O	301	CDL	C12-C11-CA5-OA6
12	A	501	3PE	O31-C31-C32-C33
17	P	202	PC1	O21-C21-C22-C23
17	P	202	PC1	O31-C31-C32-C33
13	A	502	CDL	C32-C31-CA7-OA9
12	O	302	3PE	O22-C21-C22-C23
17	P	202	PC1	O32-C31-C32-C33
13	A	502	CDL	CB3-CB4-CB6-OB8
12	N	403	3PE	O32-C31-C32-C33
12	E	201	3PE	C11-O13-P-O14
12	L	501	3PE	C1-O11-P-O14
13	O	301	CDL	C12-C11-CA5-OA7
13	G	101	CDL	C32-C31-CA7-OA8
12	O	302	3PE	C12-C11-O13-P
12	R	102	3PE	C3-C2-O21-C21
13	N	404	CDL	CB6-CB4-OB6-CB5
13	A	502	CDL	C12-C11-CA5-OA6
13	O	301	CDL	C72-C71-CB7-OB8
13	G	102	CDL	CB2-C1-CA2-OA2
12	A	501	3PE	O21-C21-C22-C23
13	A	502	CDL	C72-C71-CB7-OB8
13	N	404	CDL	C52-C51-CB5-OB6
13	N	404	CDL	C72-C71-CB7-OB8
13	A	502	CDL	C12-C11-CA5-OA7
12	A	501	3PE	O32-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	O	301	CDL	C72-C71-CB7-OB9
12	E	201	3PE	O31-C31-C32-C33

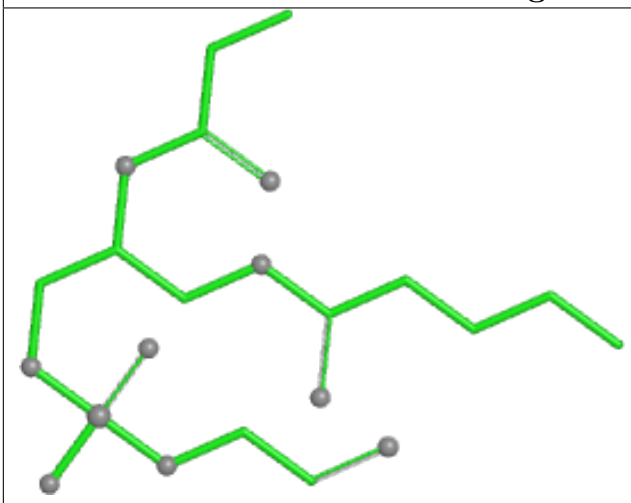
There are no ring outliers.

16 monomers are involved in 23 short contacts:

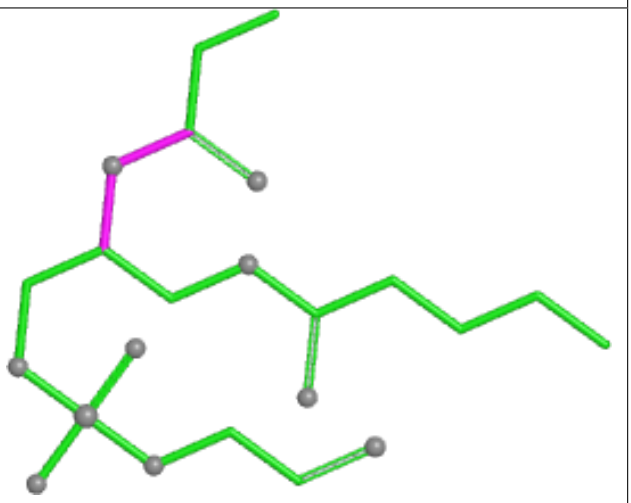
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	501	3PE	1	0
14	N	401	HEM	2	0
16	P	201	FES	1	0
14	N	402	HEM	2	0
12	O	302	3PE	1	0
14	C	401	HEM	1	0
13	N	404	CDL	3	0
12	E	201	3PE	2	0
14	C	402	HEM	2	0
13	G	102	CDL	1	0
13	O	301	CDL	1	0
12	L	501	3PE	1	0
12	R	102	3PE	2	0
15	D	301	HEC	1	0
15	O	303	HEC	2	0
13	G	101	CDL	1	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.

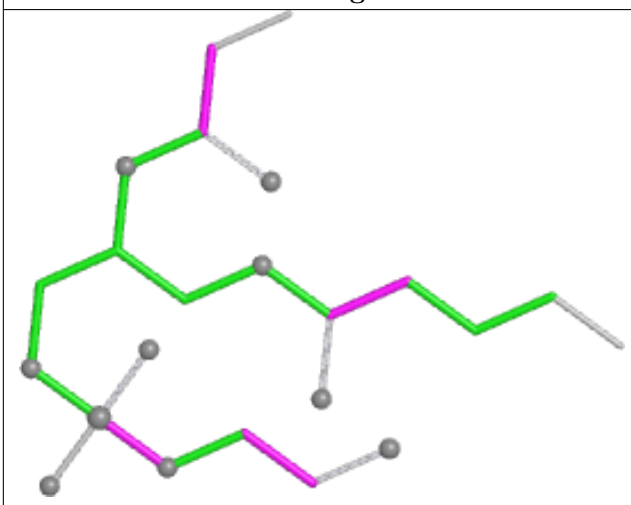
Ligand 3PE A 501



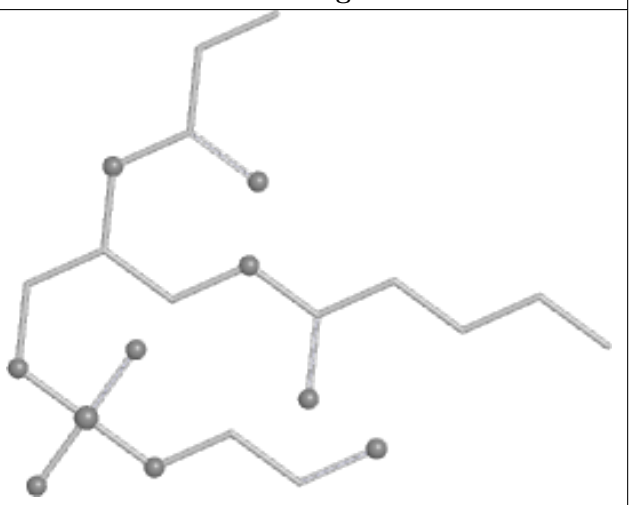
Bond lengths



Bond angles

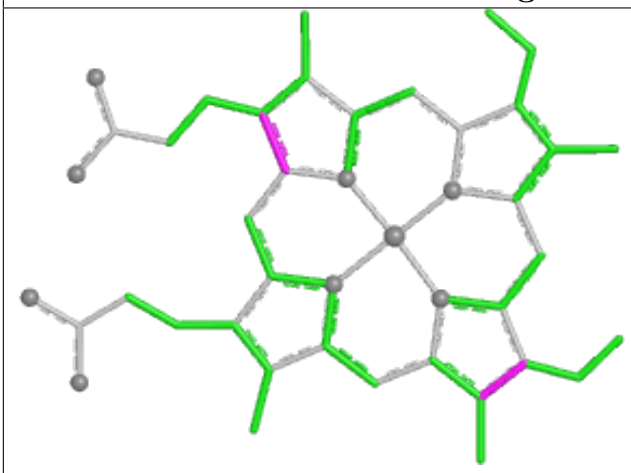


Torsions

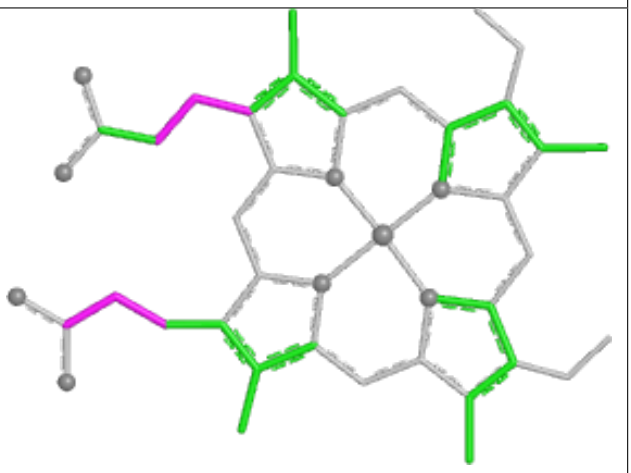


Rings

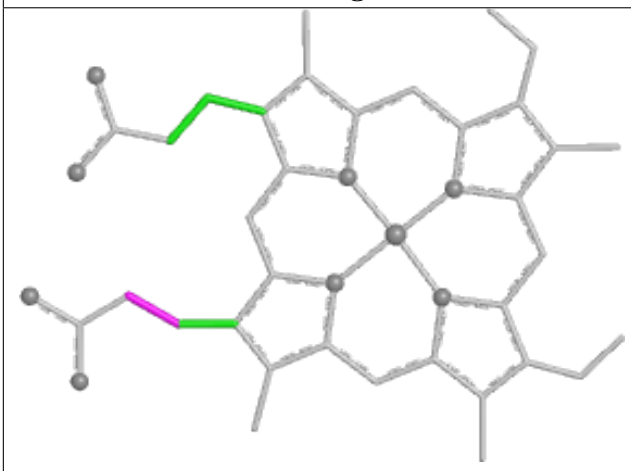
Ligand HEM N 401



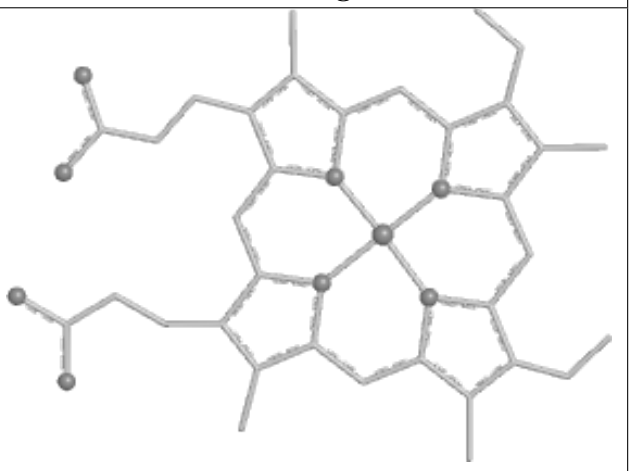
Bond lengths



Bond angles

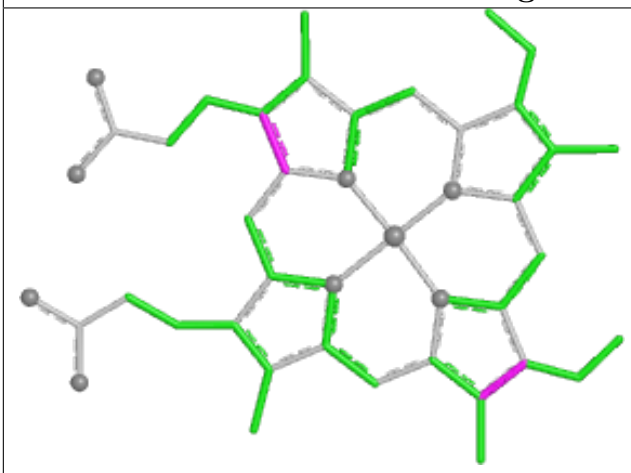


Torsions

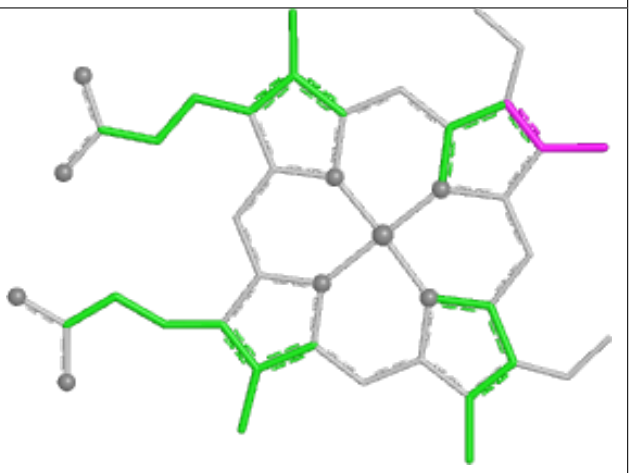


Rings

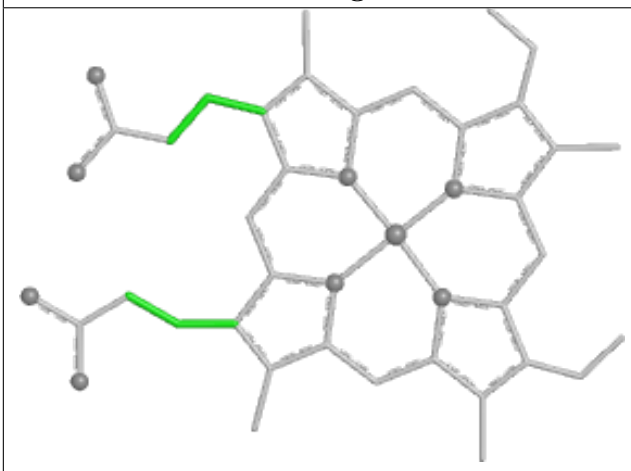
Ligand HEM N 402



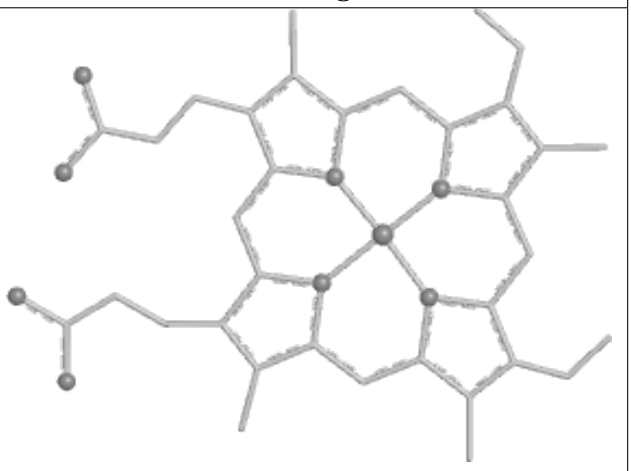
Bond lengths



Bond angles

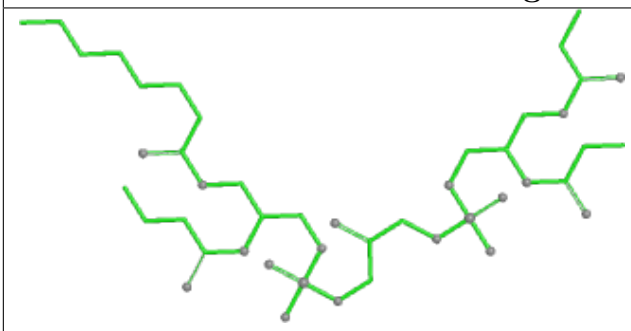


Torsions

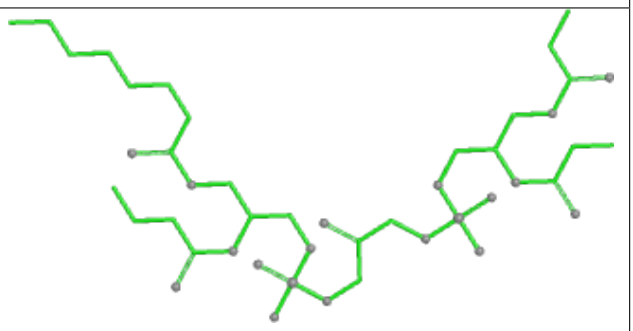


Rings

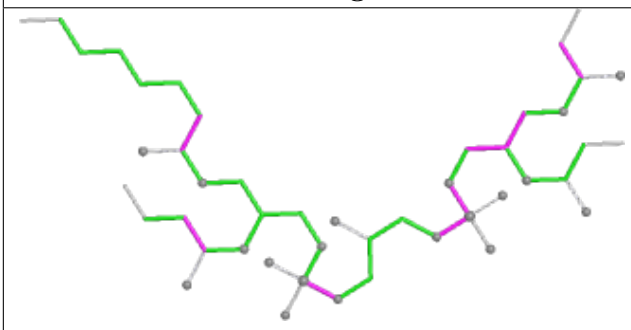
Ligand CDL A 502



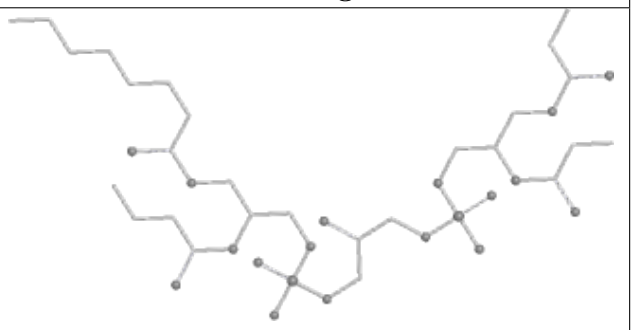
Bond lengths



Bond angles

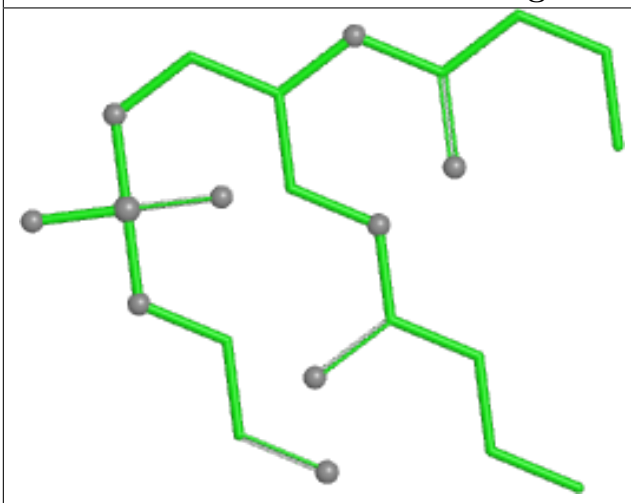


Torsions

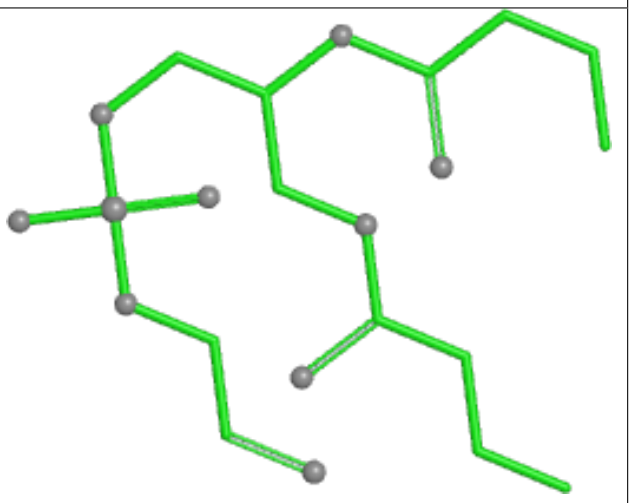


Rings

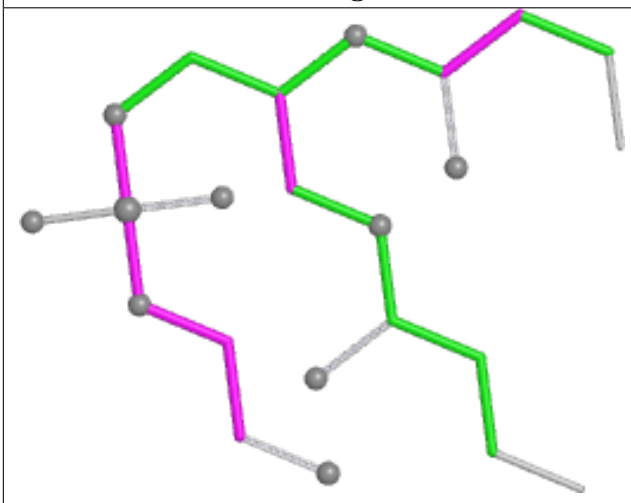
Ligand 3PE O 302



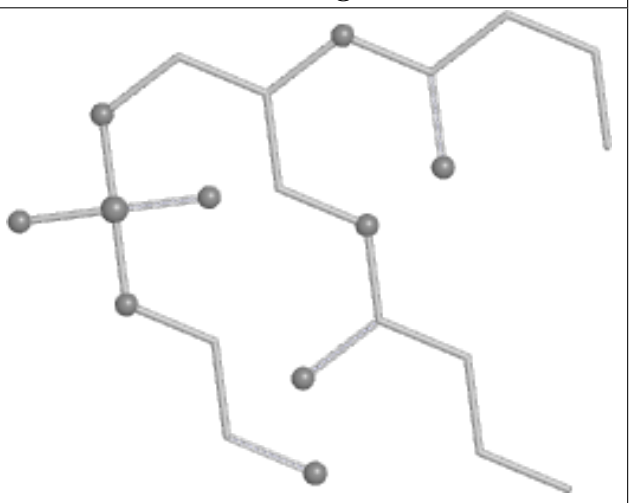
Bond lengths



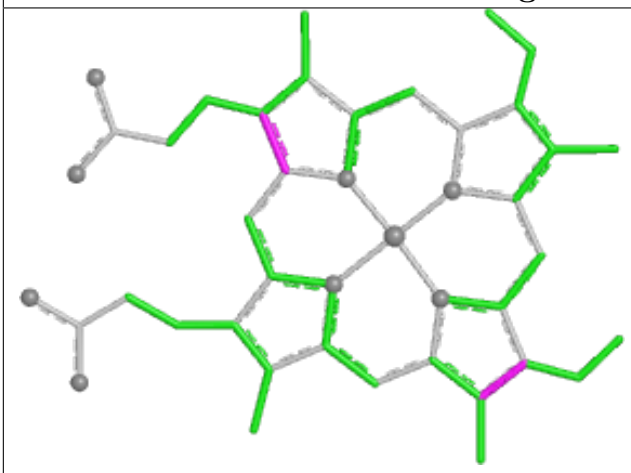
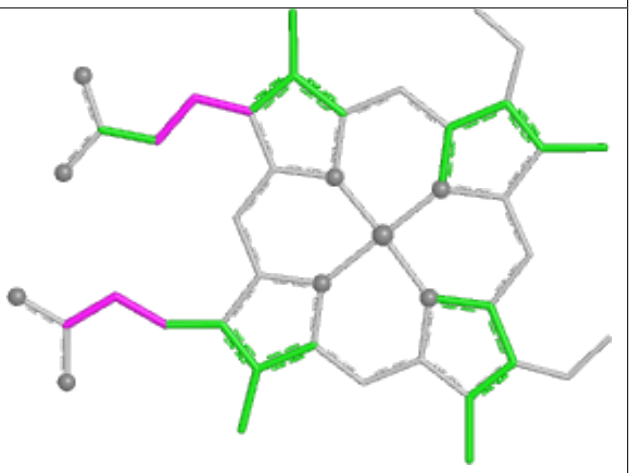
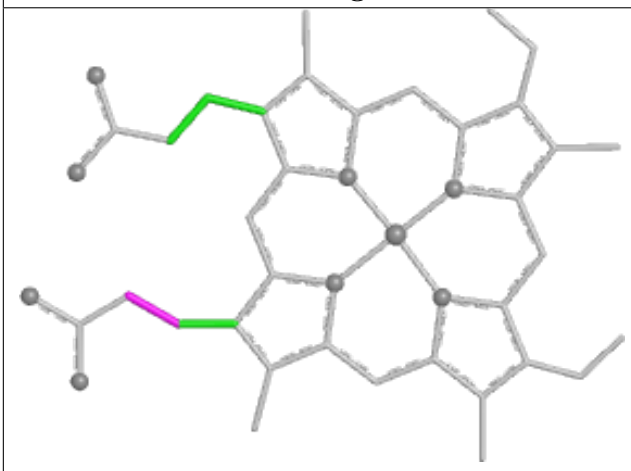
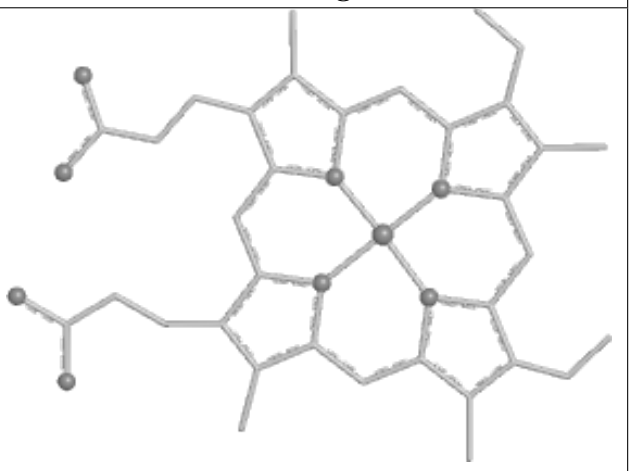
Bond angles

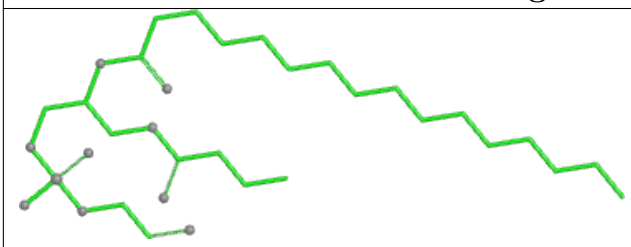
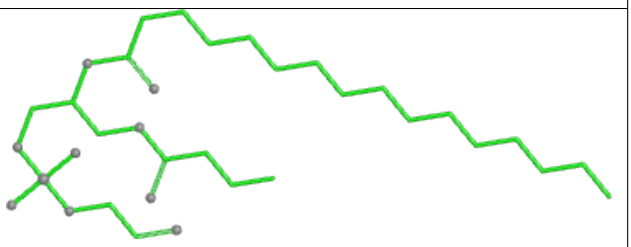
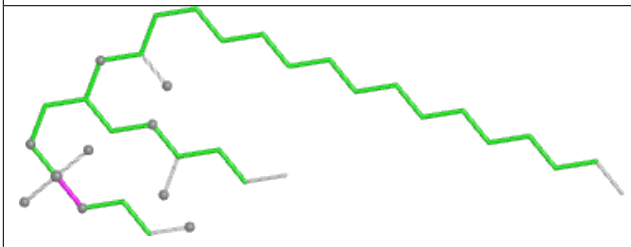
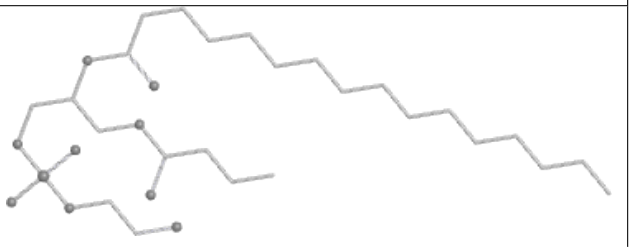


Torsions

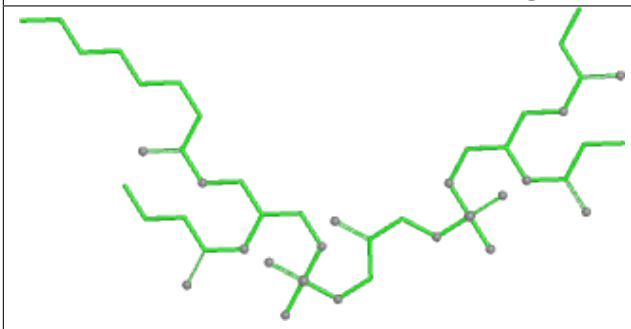


Rings

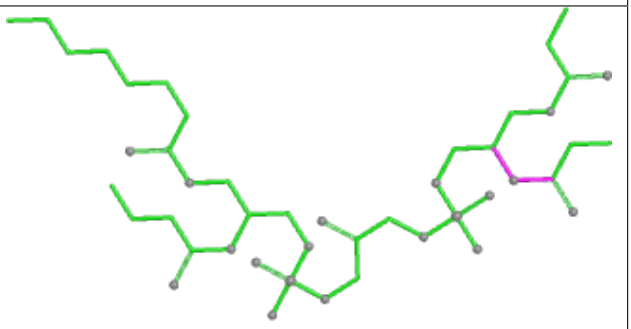
Ligand HEM C 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE C 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

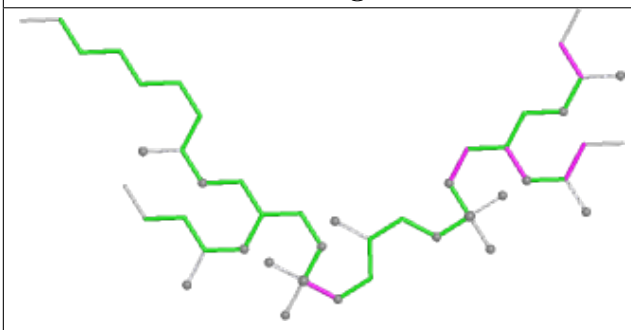
Ligand CDL N 404



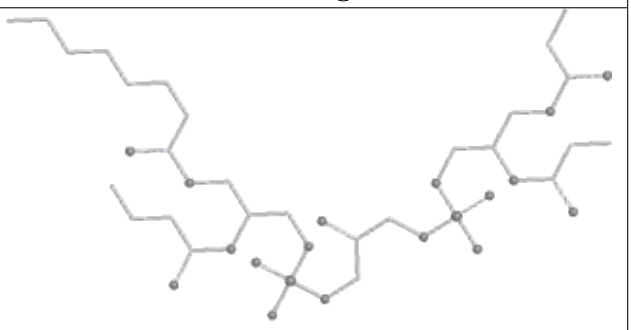
Bond lengths



Bond angles

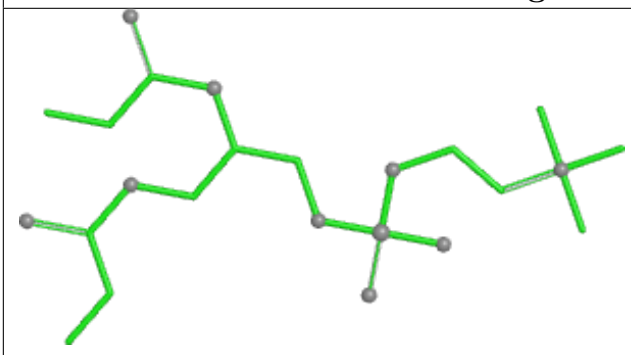


Torsions

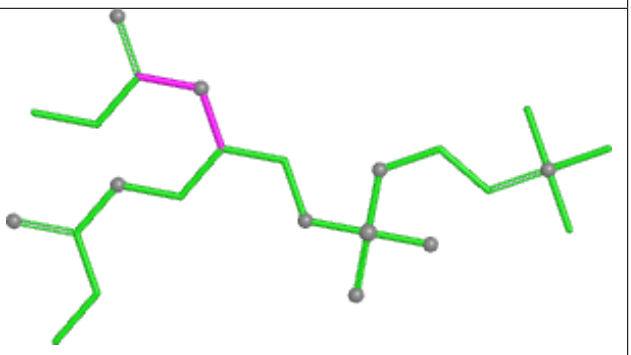


Rings

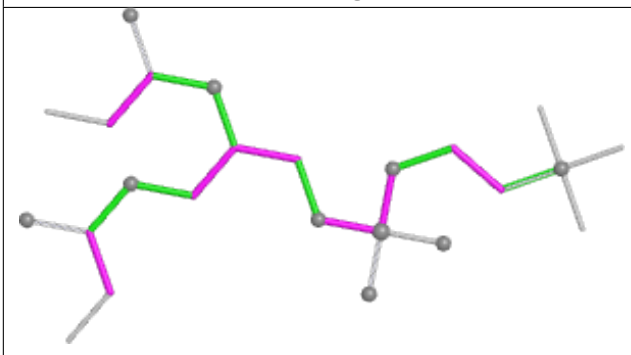
Ligand PC1 P 202



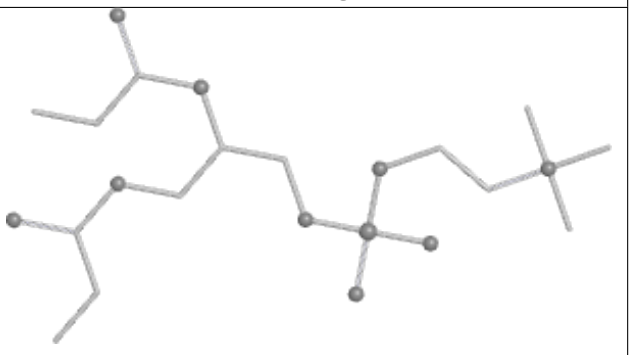
Bond lengths



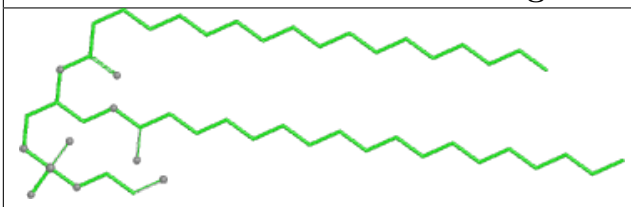
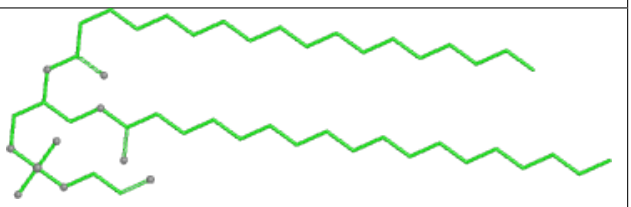
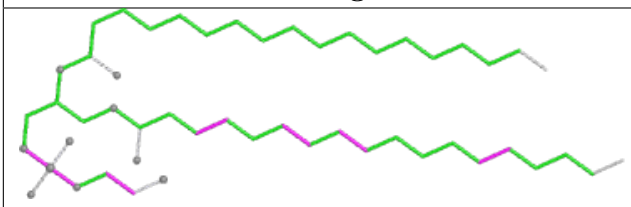
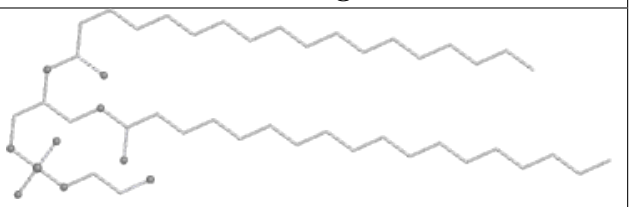
Bond angles

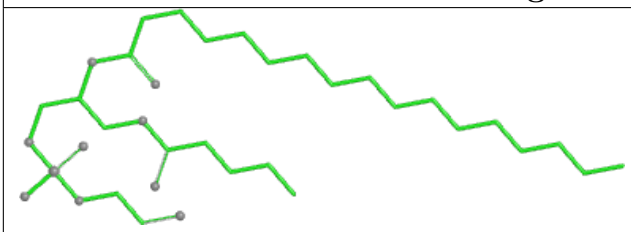
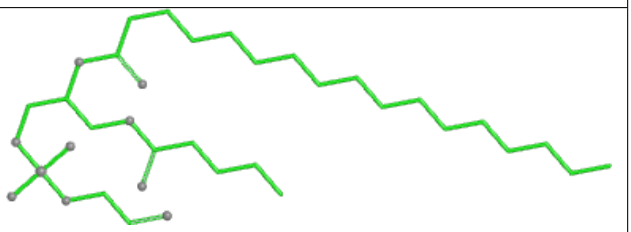
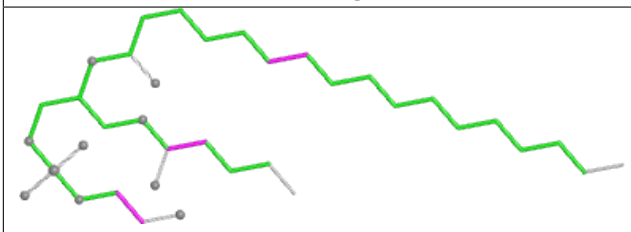
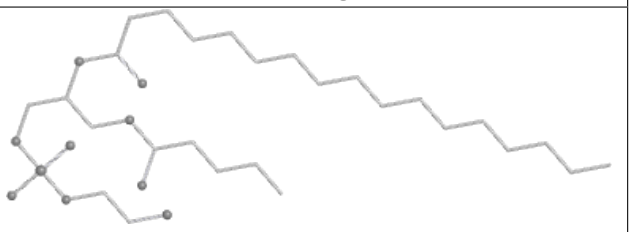


Torsions

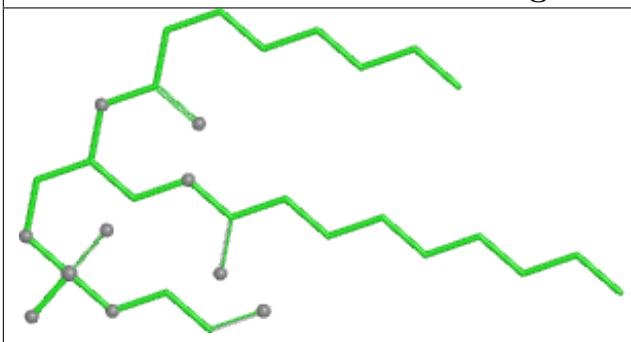


Rings

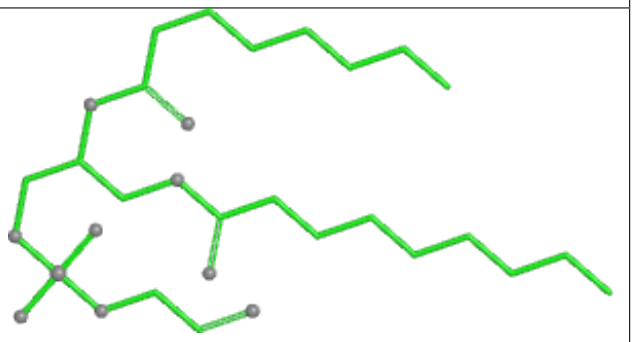
Ligand 3PE G 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE N 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

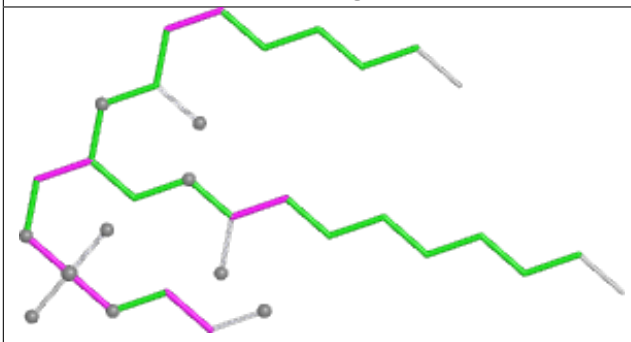
Ligand 3PE E 201



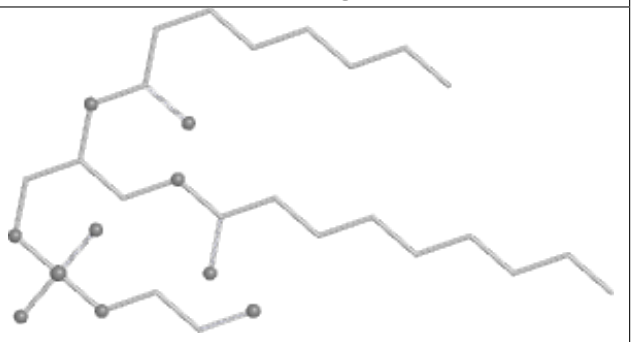
Bond lengths



Bond angles

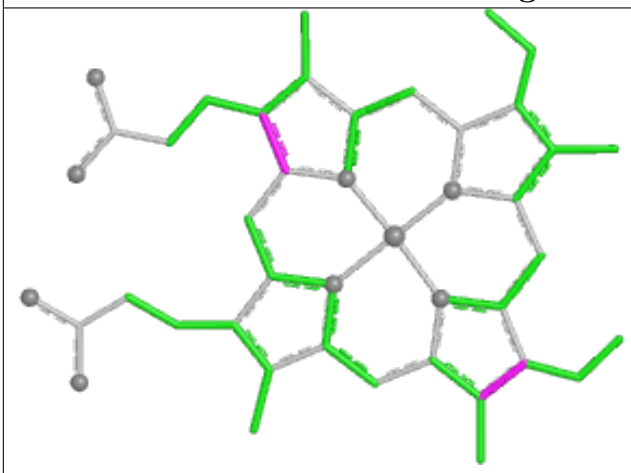


Torsions

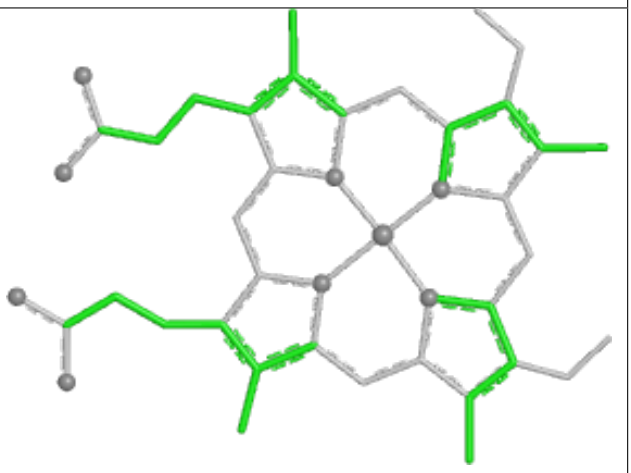


Rings

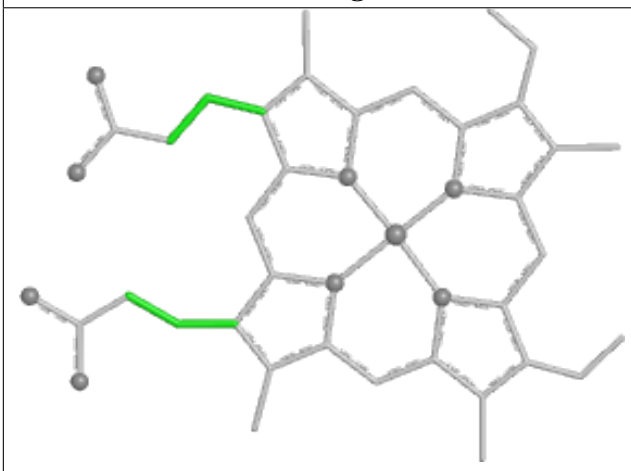
Ligand HEM C 402



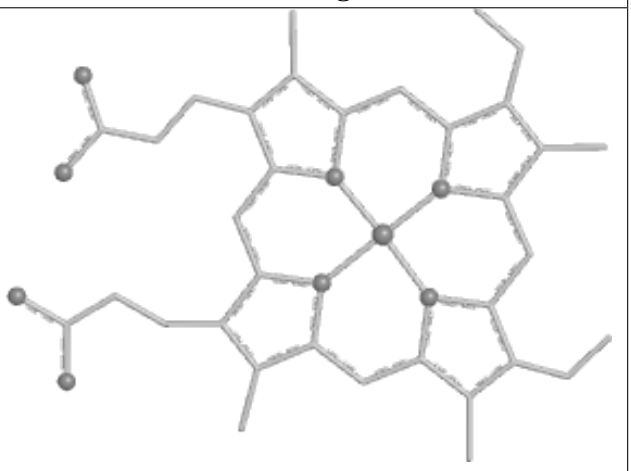
Bond lengths



Bond angles

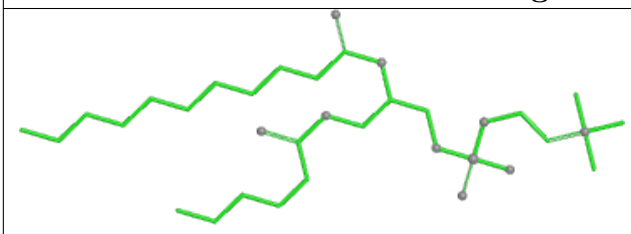


Torsions

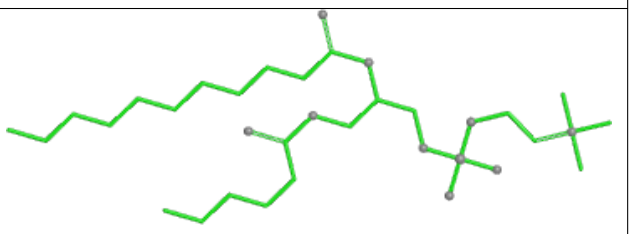


Rings

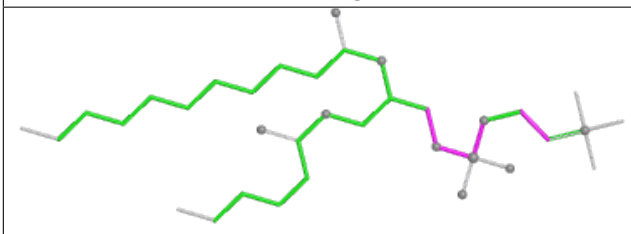
Ligand PC1 J 101



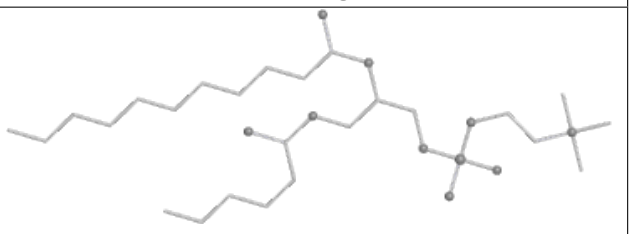
Bond lengths



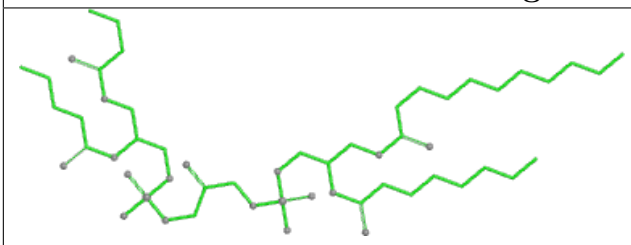
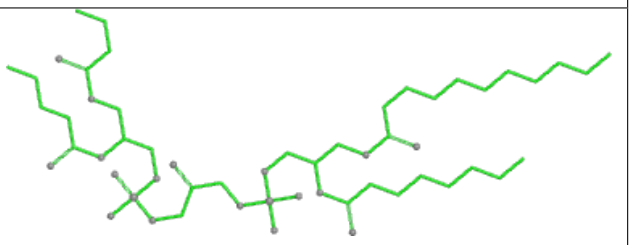
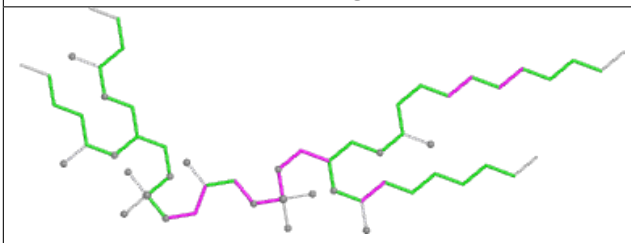
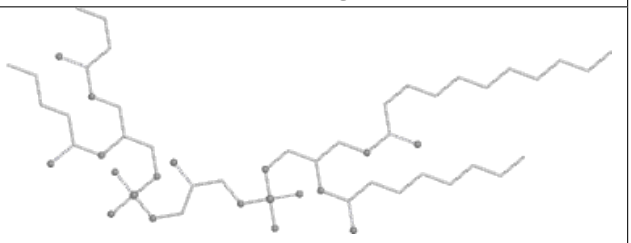
Bond angles

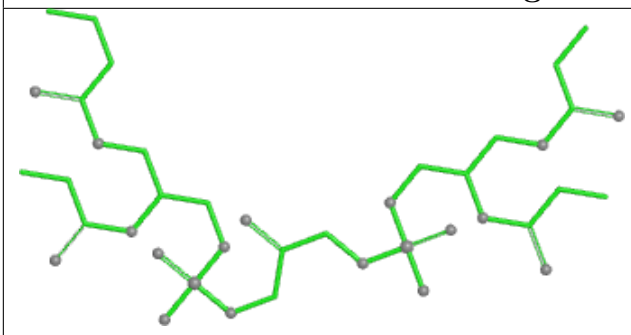
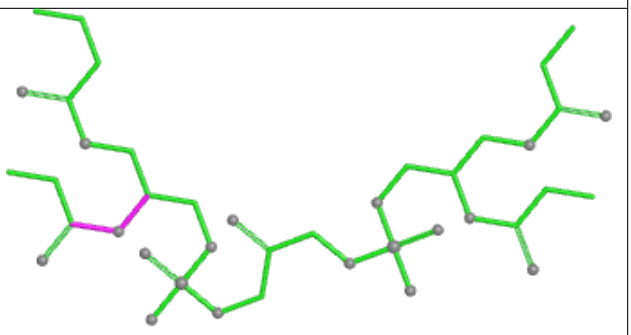
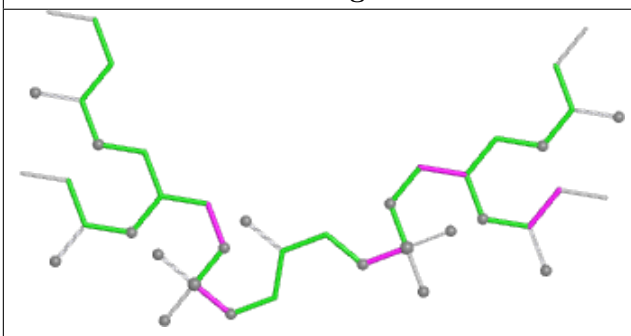
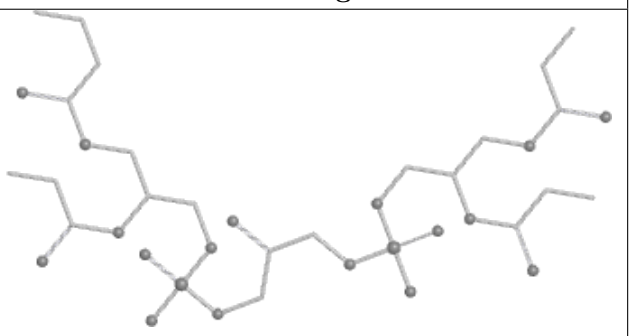


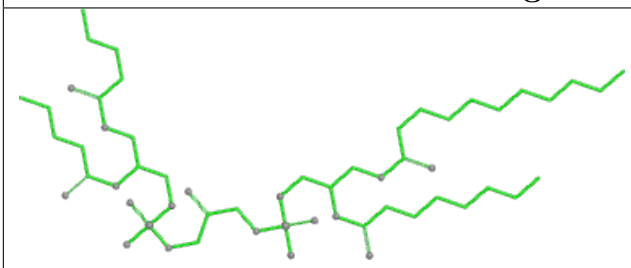
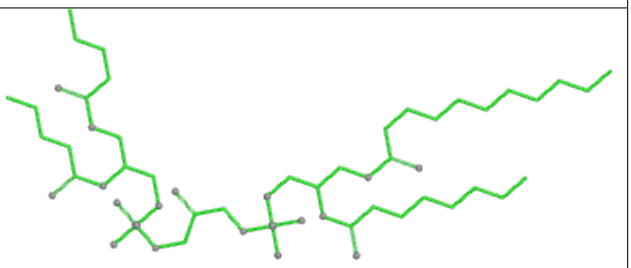
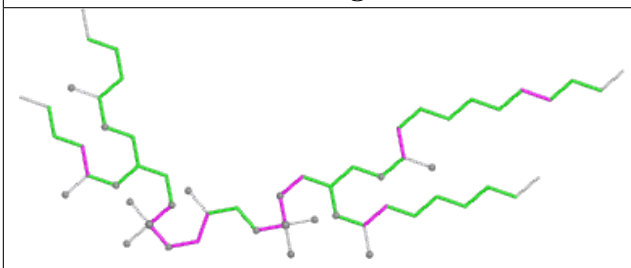
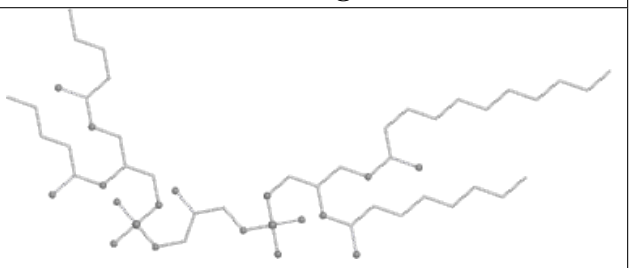
Torsions

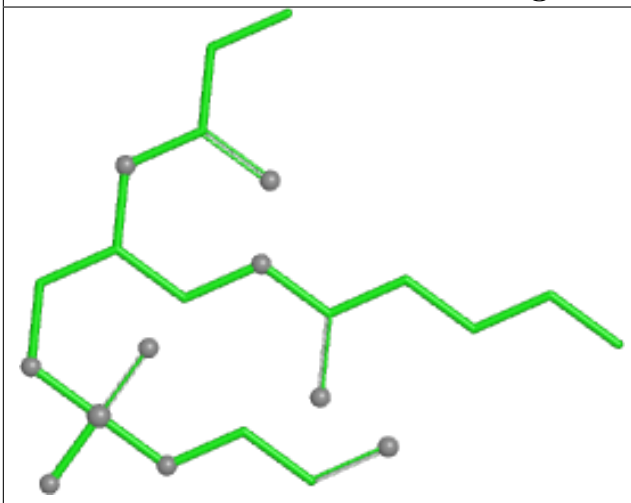
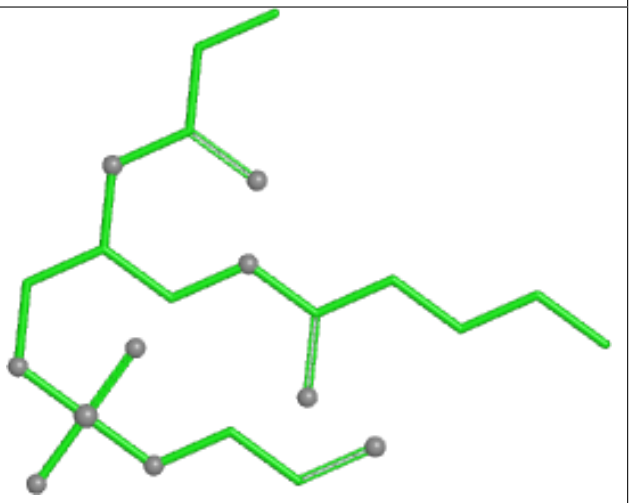
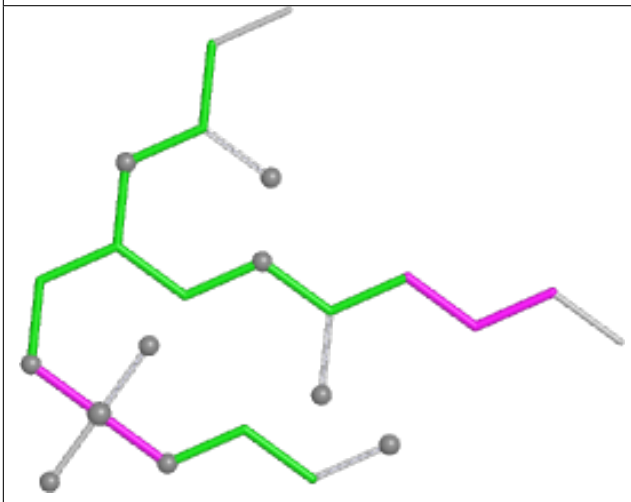
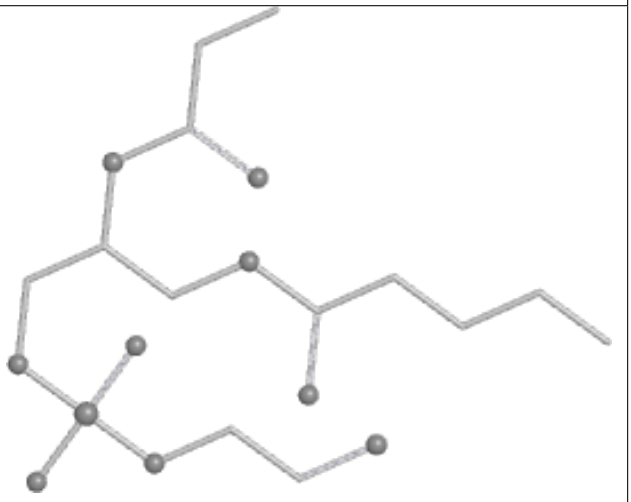


Rings

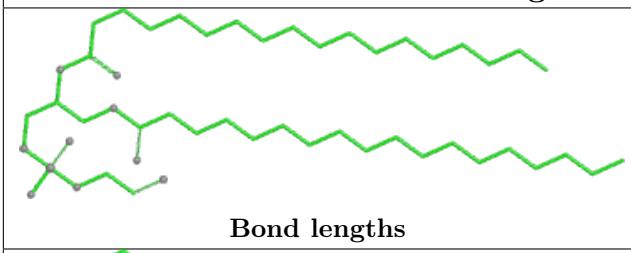
Ligand CDL G 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL R 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

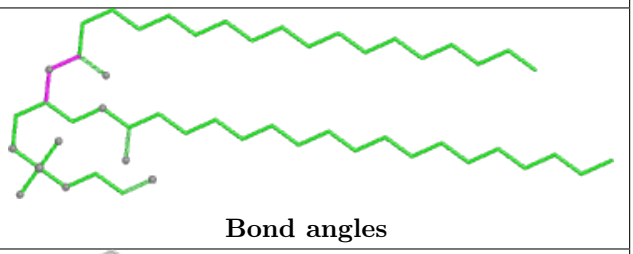
Ligand CDL O 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

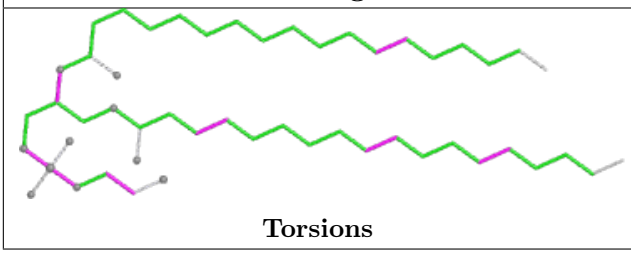
Ligand 3PE R 102



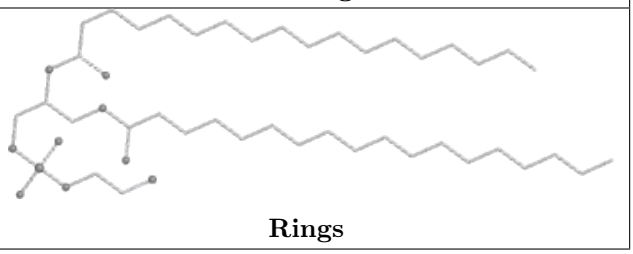
Bond lengths



Bond angles

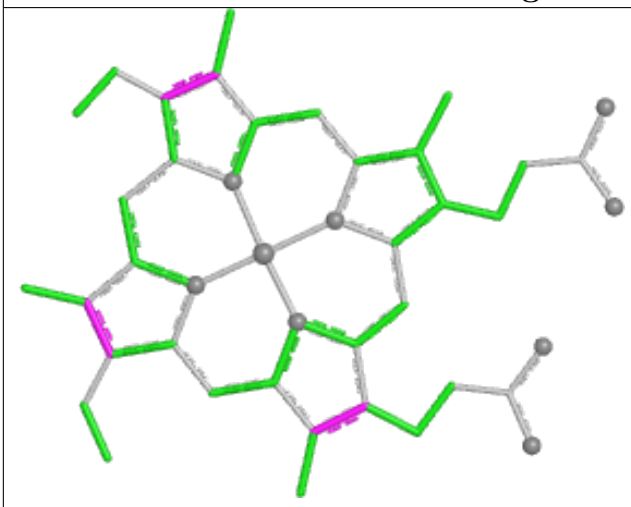


Torsions

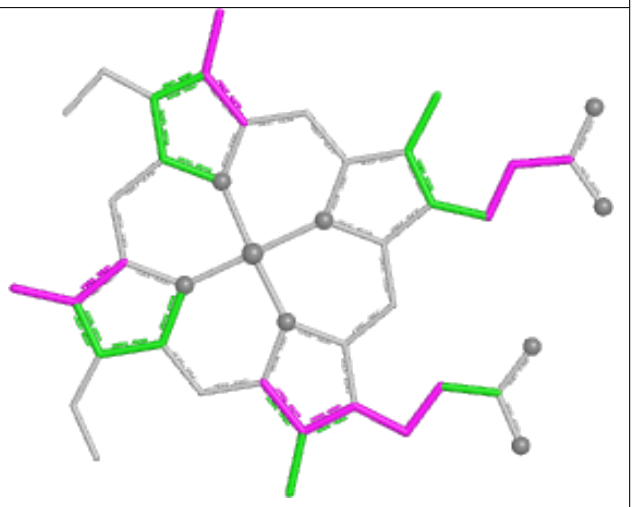


Rings

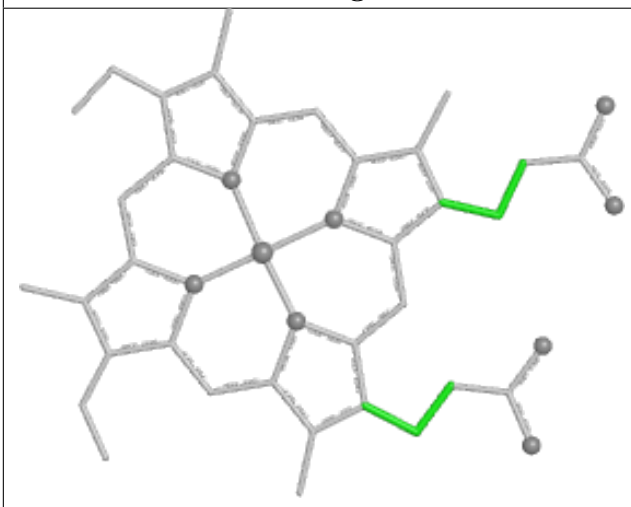
Ligand HEC D 301



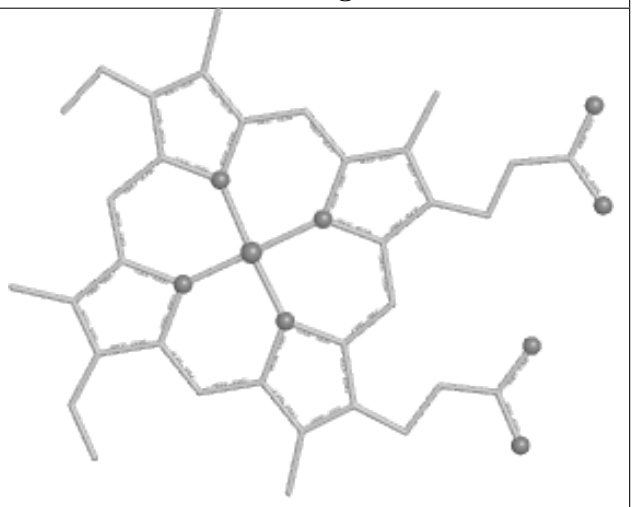
Bond lengths



Bond angles

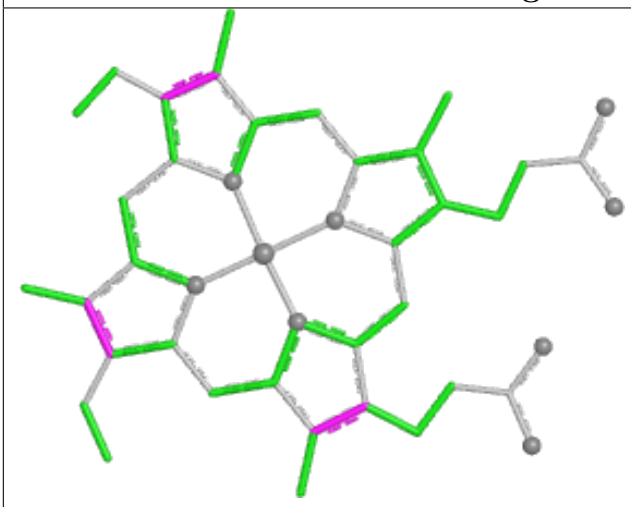


Torsions

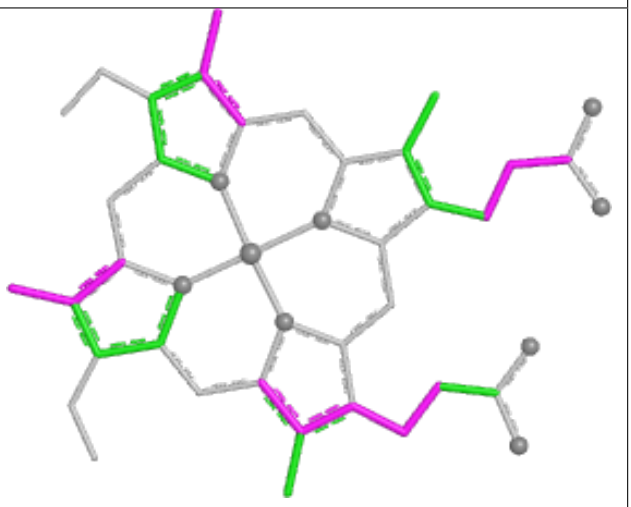


Rings

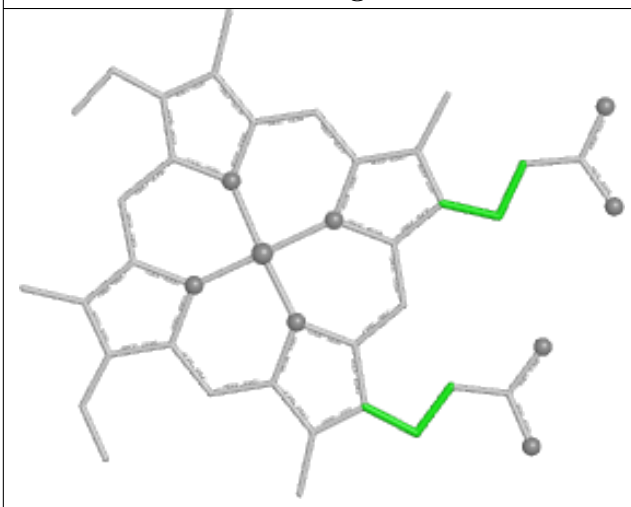
Ligand HEC O 303



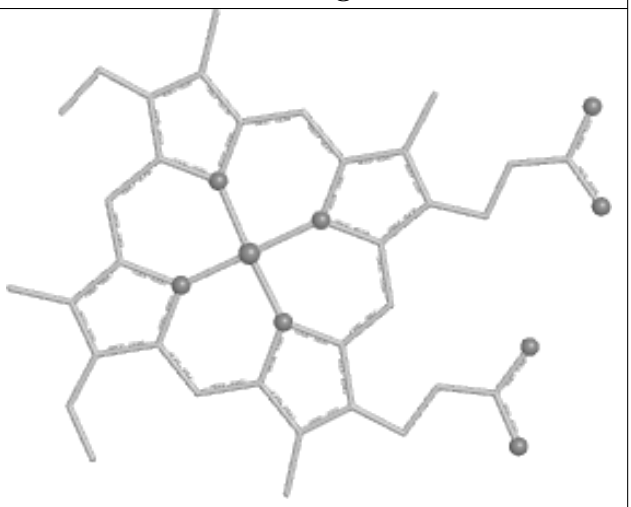
Bond lengths



Bond angles

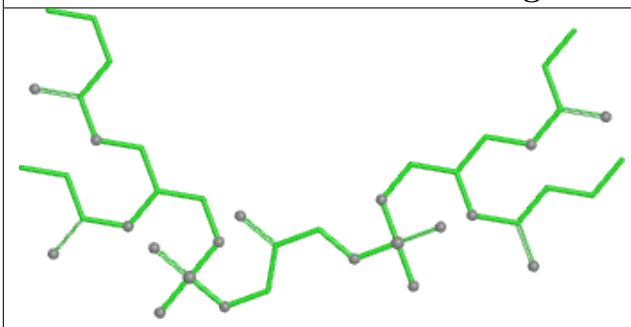


Torsions

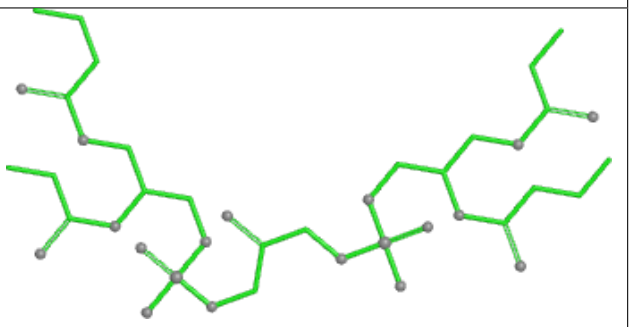


Rings

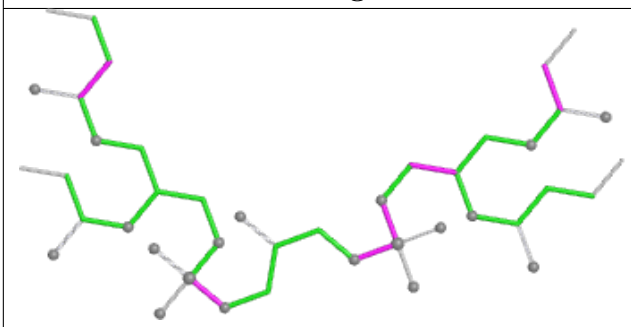
Ligand CDL G 101



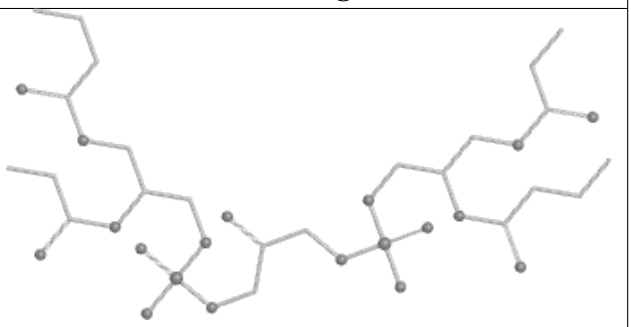
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

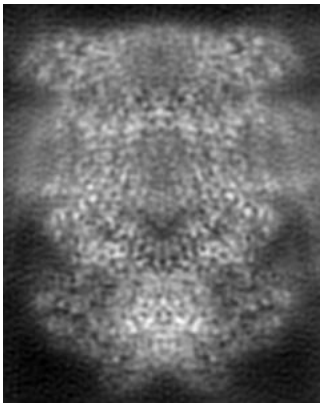
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12706. These allow visual inspection of the internal detail of the map and identification of artifacts.

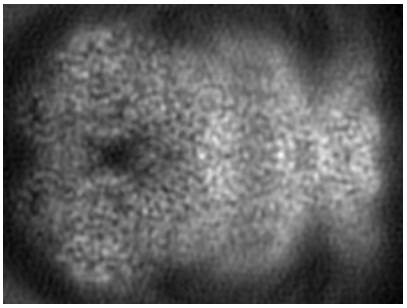
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

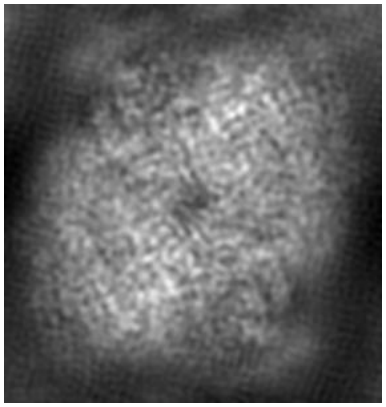
6.1.1 Primary map



X



Y

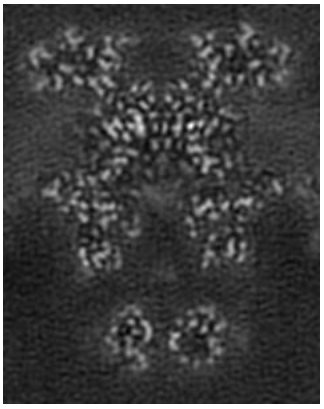


Z

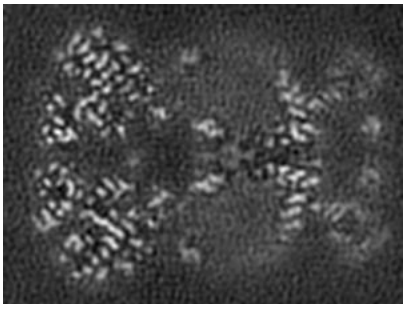
The images above show the map projected in three orthogonal directions.

6.2 Central slices

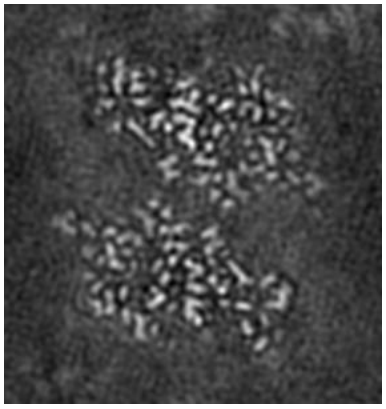
6.2.1 Primary map



X Index: 121



Y Index: 128



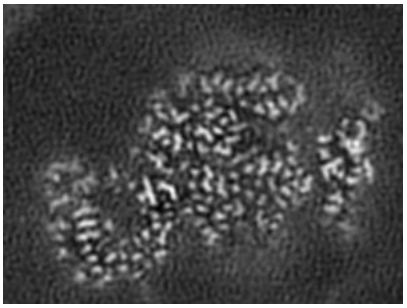
Z Index: 162

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

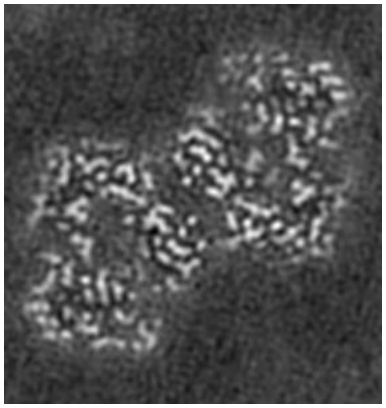
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134



Y Index: 72



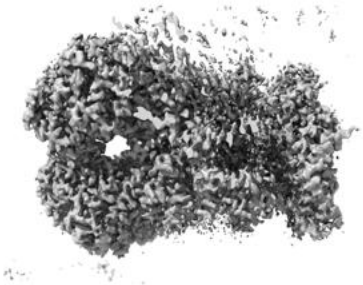
Z Index: 61

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

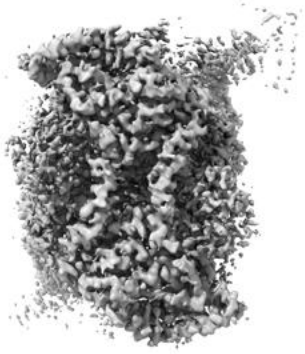
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

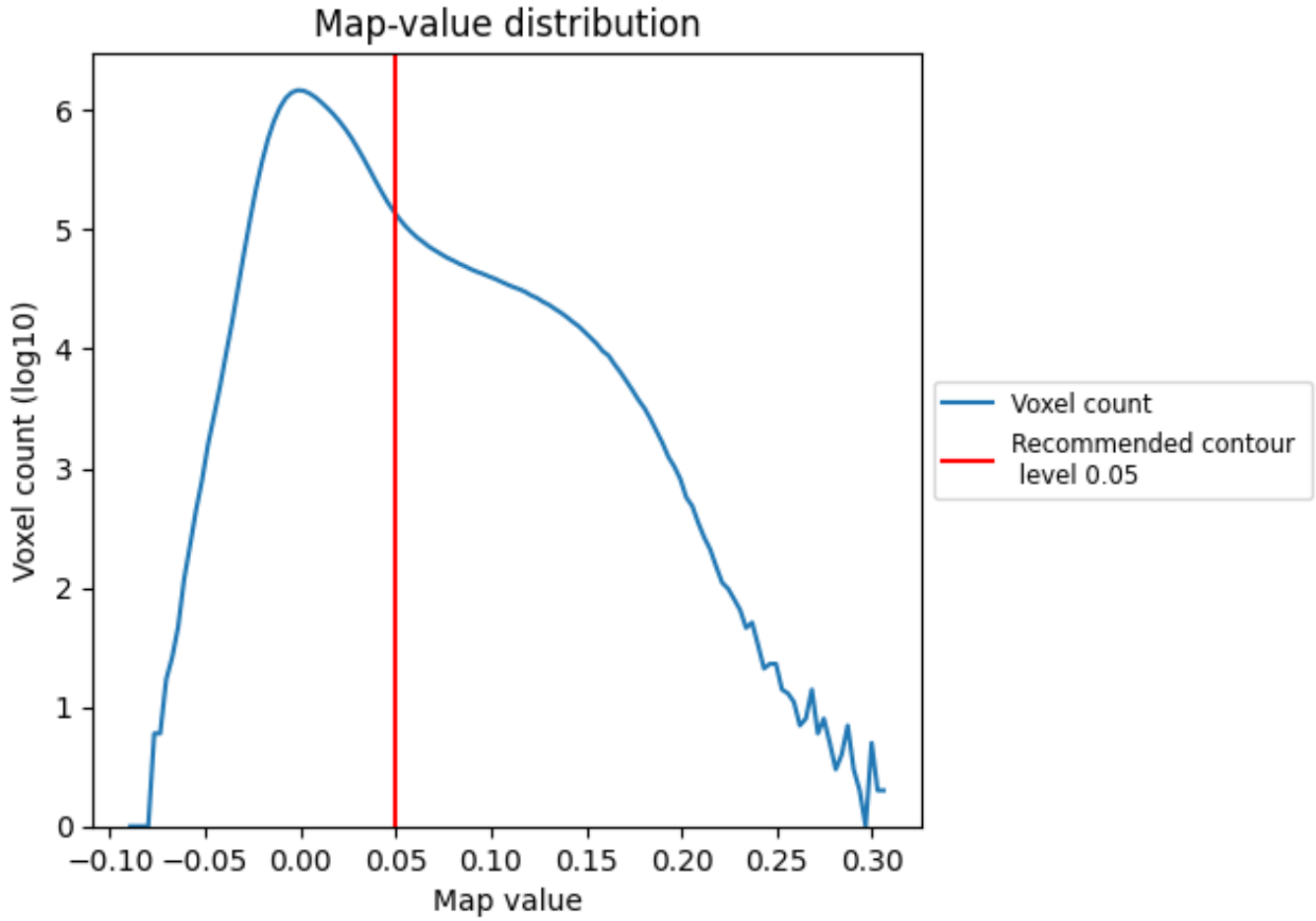
6.5 Mask visualisation (i)

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

7 Map analysis

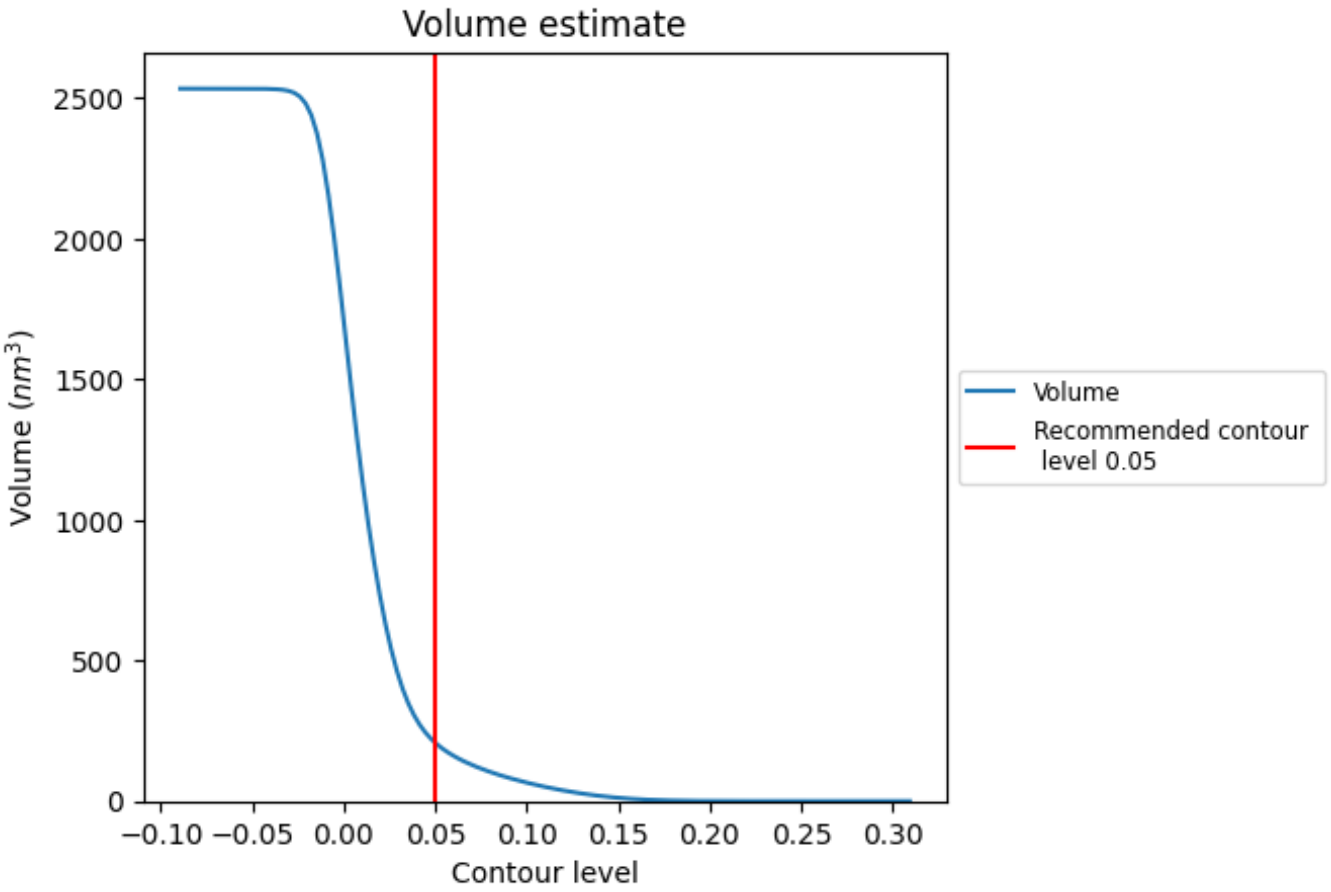
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 208 nm^3; this corresponds to an approximate mass of 188 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.

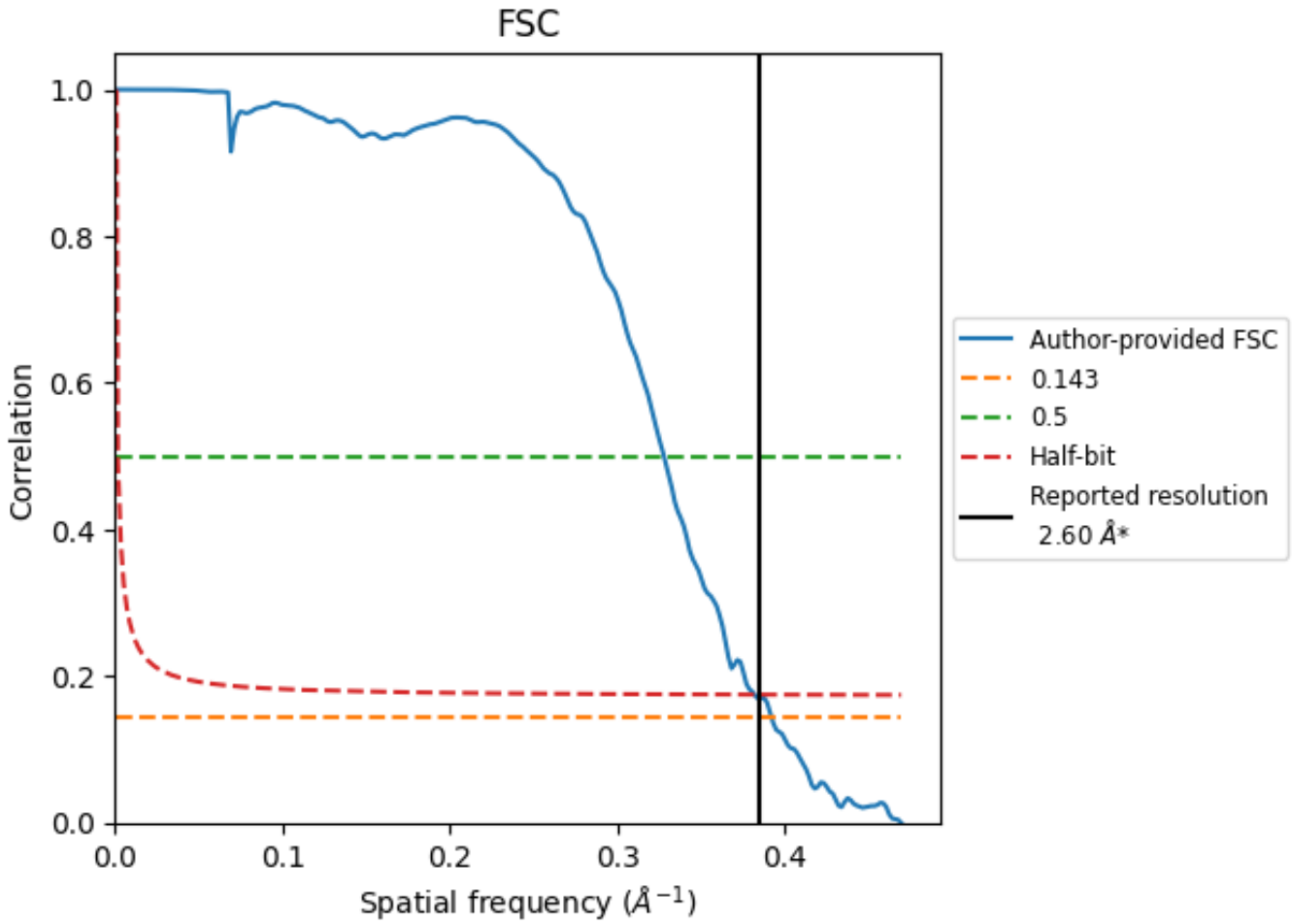
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

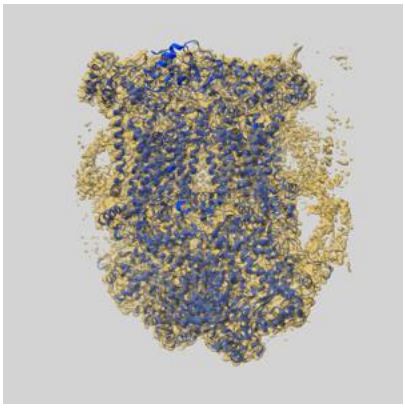
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.55	3.05	2.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

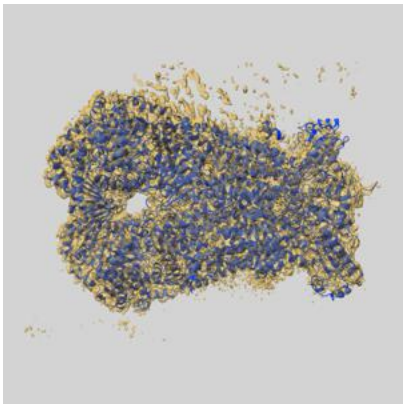
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12706 and PDB model 7O3H. Per-residue inclusion information can be found in section 3 on page 11.

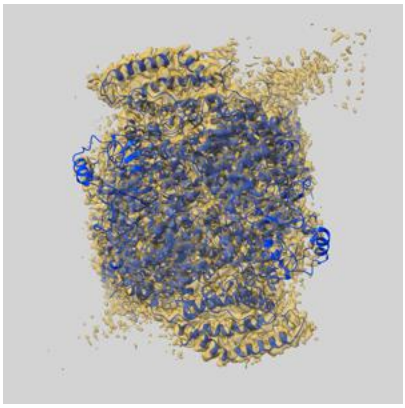
9.1 Map-model overlay



X



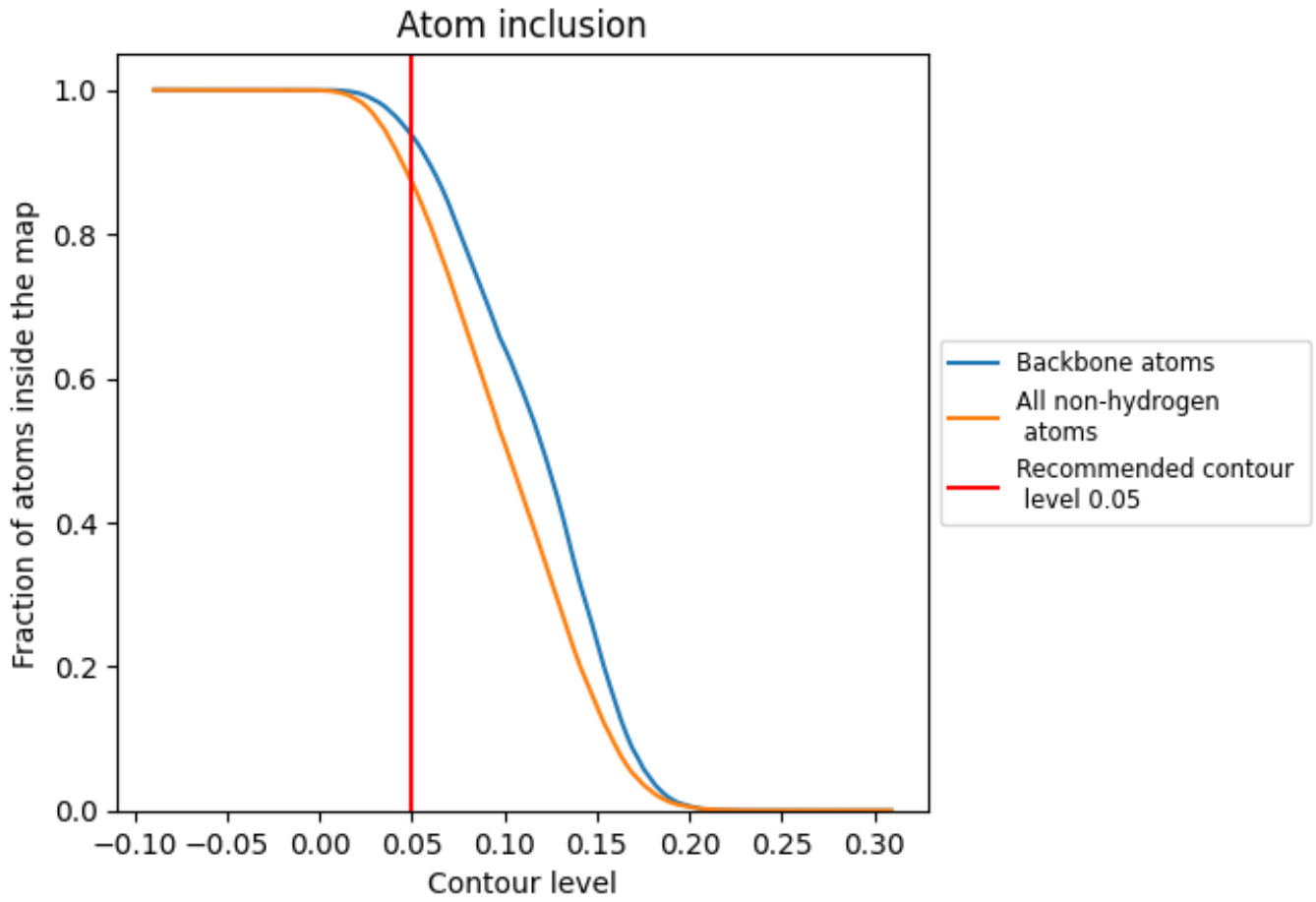
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.