Full wwPDB EM Validation Report ⓘ

Jan 16, 2023 – 05:09 pm GMT

PDB ID	:	7ZYV
EMDB ID	:	EMD-15027
Title	:	Cryo-EM structure of catalytically active Spinacia oleracea cytochrome b6f in complex with endogenous plastoquinones at 2.13 A resolution
Authors	:	Sarewicz, M.; Szwalec, M.; Pintscher, S.; Indyka, P.; Rawski, M.; Pietras, R.; Mielecki, B.; Koziej, L.; Jaciuk, M.; Glatt, S.; Osyczka, A.
Deposited on	:	2022-05-25
Resolution	:	2.13 Å(reported)
Based on initial model	:	7QRM

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:

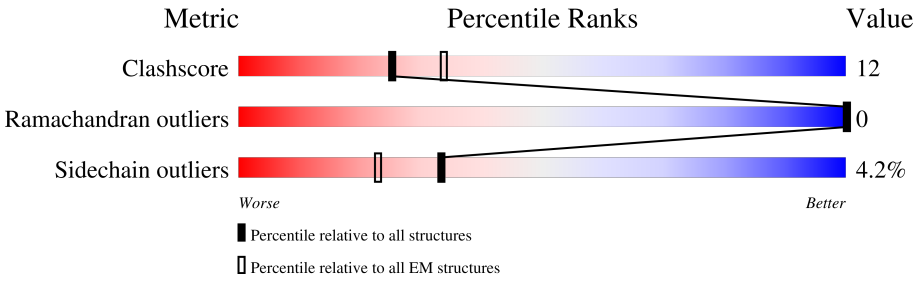
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.13 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.



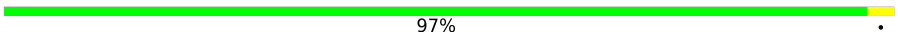
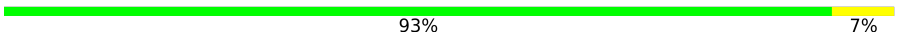
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	215	86% 13%
1	I	215	85% 14%
2	B	160	85% 13% ••
2	J	160	86% 12% ••
3	C	320	66% 18% • 13%
3	K	320	67% 18% • 13%
4	D	230	60% 11% • 28%
4	L	230	59% 12% • 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	31	
5	M	31	
6	F	131	
6	N	131	
7	G	37	
7	O	37	
8	H	29	
8	P	29	
9	Q	103	
9	R	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	304	X	-	-	-
12	CLA	I	304	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 16892 atoms, of which 440 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 b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		
1	I	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	159	Total	C	N	O	S	0	0
			1225	820	193	208	4		
2	J	159	Total	C	N	O	S	0	0
			1226	820	193	209	4		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	278	Total	C	N	O	S	0	0
			2158	1391	365	396	6		
3	K	279	Total	C	N	O	S	0	0
			2167	1396	366	399	6		

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1259	807	212	233	7		
4	L	165	Total	C	N	O	S	0	0
			1254	804	211	232	7		

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	31	Total	C	N	O	S	0	0
			243	167	36	39	1		
5	M	31	Total	C	N	O	S	0	0
			243	167	36	39	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	37	Total	C	N	O	S	0	0
			269	174	45	49	1		
6	N	36	Total	C	N	O	S	0	0
			264	171	44	48	1		

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	34	Total	C	N	O	S	0	0
			266	181	41	43	1		
7	O	33	Total	C	N	O	S	0	0
			261	178	40	42	1		

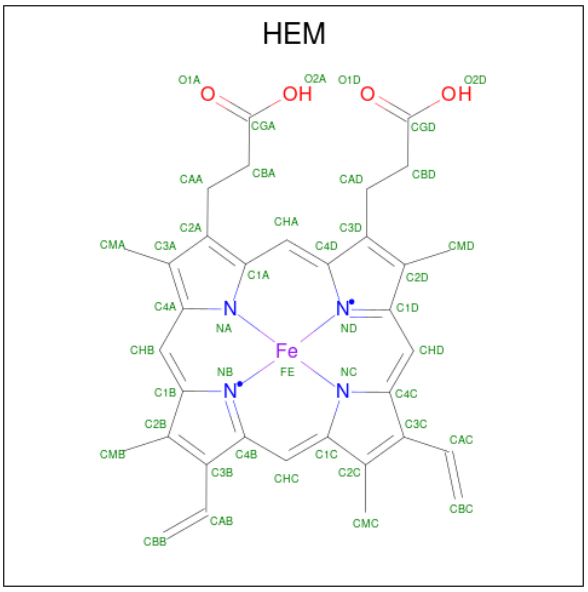
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			222	150	34	36	2		
8	P	29	Total	C	N	O	S	0	0
			223	150	34	37	2		

- Molecule 9 is a protein called Thylakoid soluble phosphoprotein.

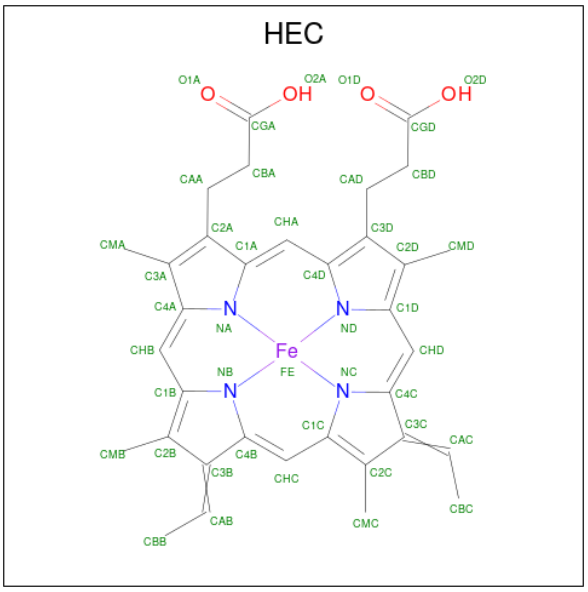
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	26	Total	C	N	O	0	0
			219	144	34	41		
9	Q	26	Total	C	N	O	0	0
			219	144	34	41		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



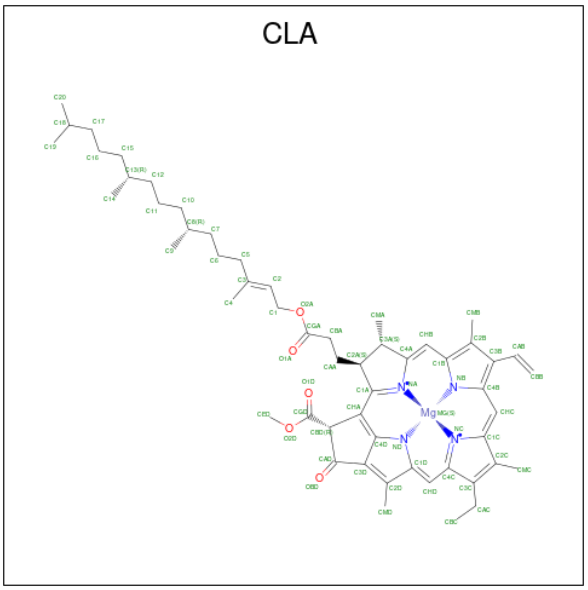
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	I	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	I	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 11 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



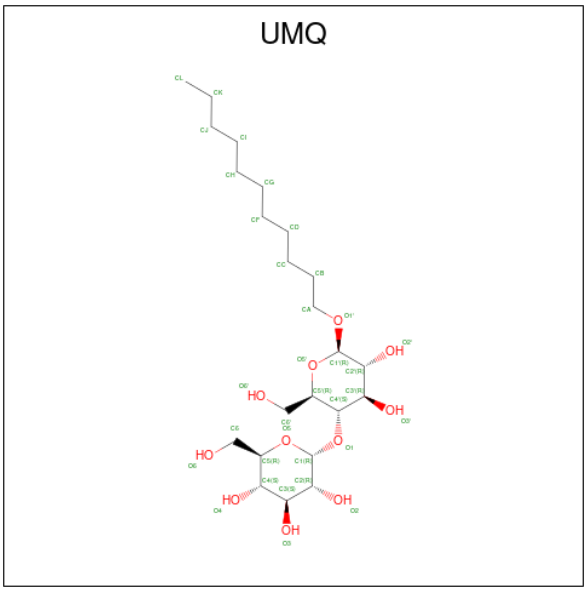
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



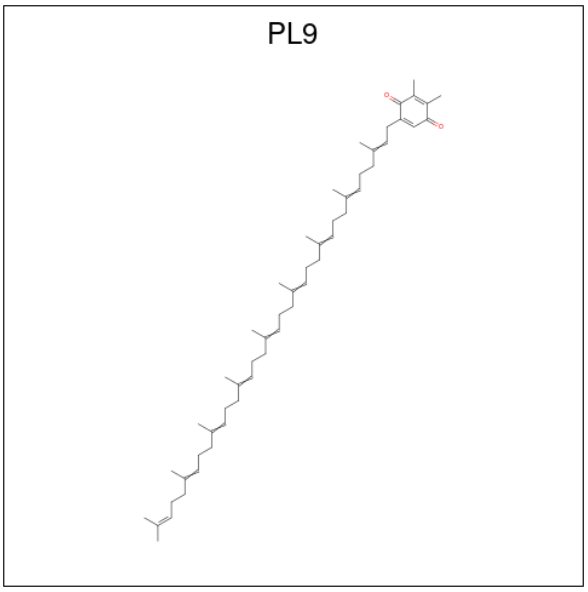
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$) (labeled as "Ligand of Interest" by depositor).



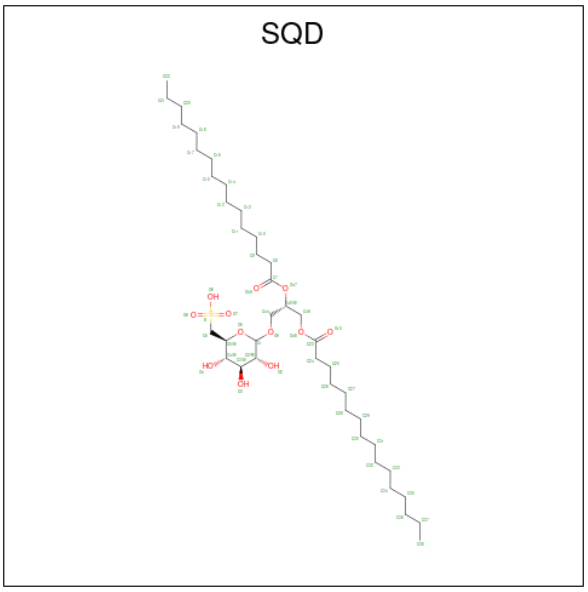
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	H	O	0
			156	46	88	22	
13	A	1	Total	C	H	O	0
			156	46	88	22	
13	B	1	Total	C	H	O	0
			156	46	88	22	
13	B	1	Total	C	H	O	0
			156	46	88	22	
13	H	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			156	46	88	22	
13	I	1	Total	C	H	O	0
			156	46	88	22	
13	J	1	Total	C	H	O	0
			156	46	88	22	
13	J	1	Total	C	H	O	0
			156	46	88	22	
13	P	1	Total	C	H	O	0
			78	23	44	11	

- Molecule 14 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



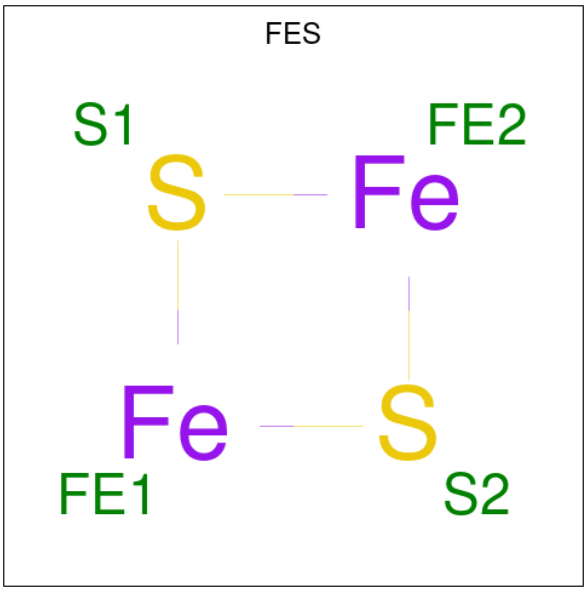
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total 55	C 53	O 2	0
14	B	1	Total 110	C 106	O 4	0
14	B	1	Total 110	C 106	O 4	0
14	J	1	Total 110	C 106	O 4	0
14	J	1	Total 110	C 106	O 4	0
14	K	1	Total 55	C 53	O 2	0

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	D	1	Total	C	O	S	0
			54	41	12	1	
15	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



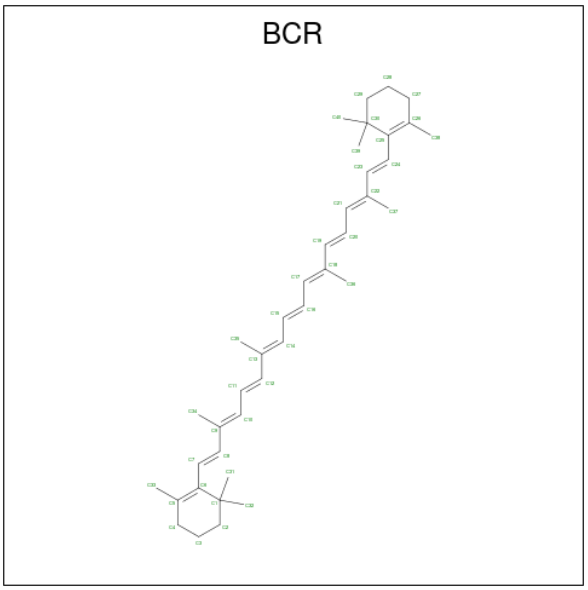
Mol	Chain	Residues	Atoms			AltConf
16	D	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



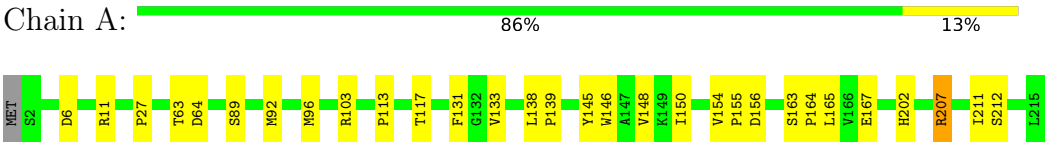
Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	P	1	Total C 40 40	0

3 Residue-property plots (i)

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

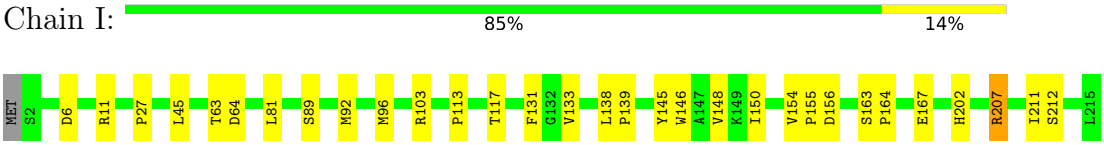
• Molecule 1: Cytochrome b6

Chain A:



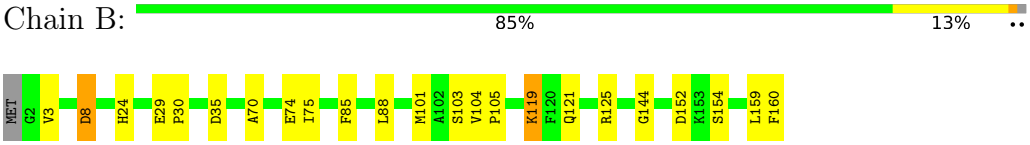
• Molecule 1: Cytochrome b6

Chain I:



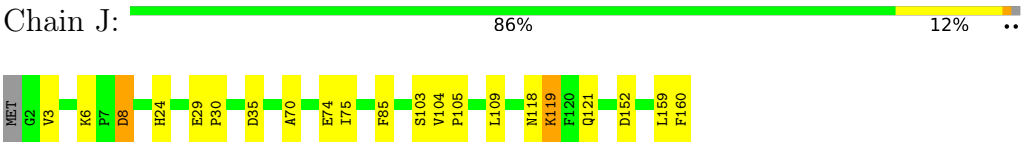
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:



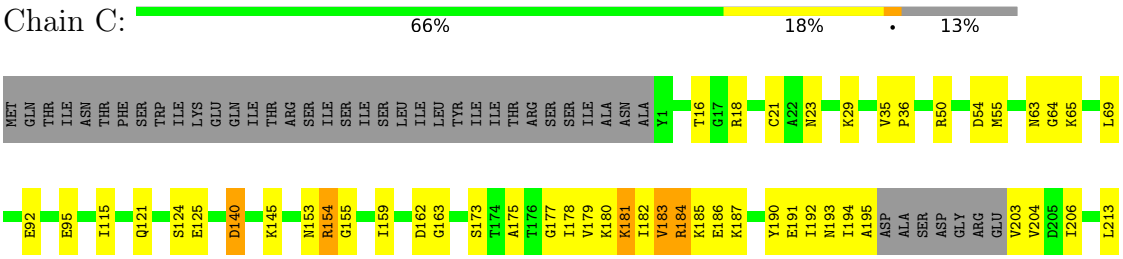
• Molecule 2: Cytochrome b6-f complex subunit 4

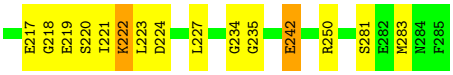
Chain J:



• Molecule 3: Cytochrome f

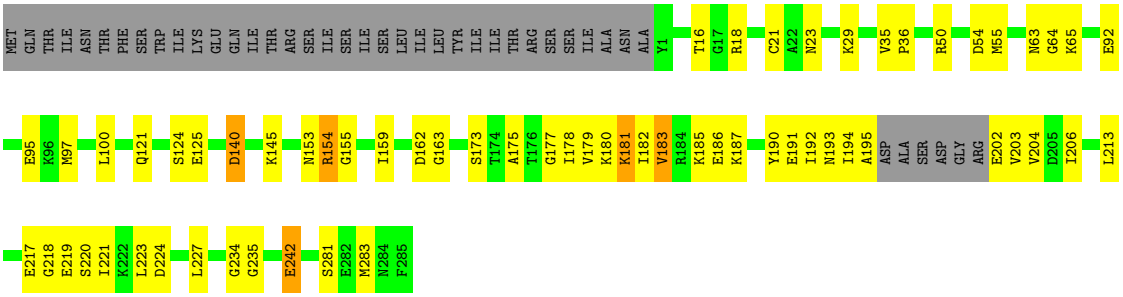
Chain C:





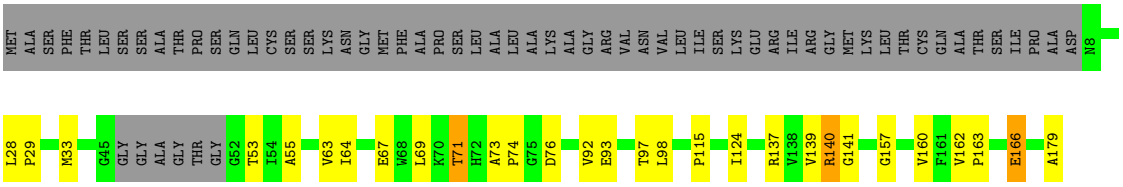
• Molecule 3: Cytochrome f

Chain K:



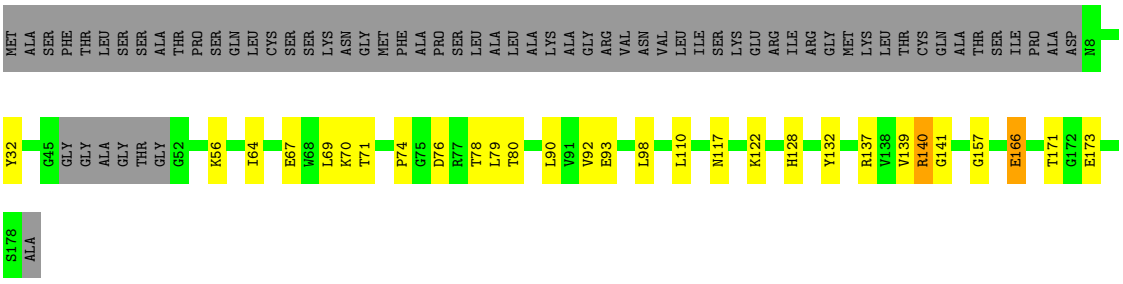
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain D:



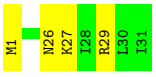
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain L:



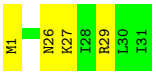
• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



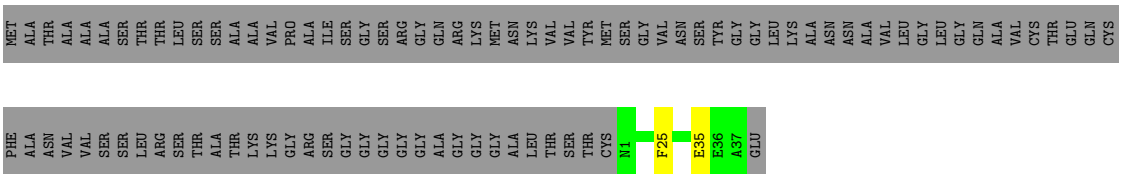
• Molecule 5: Cytochrome b6-f complex subunit 6

Chain M:



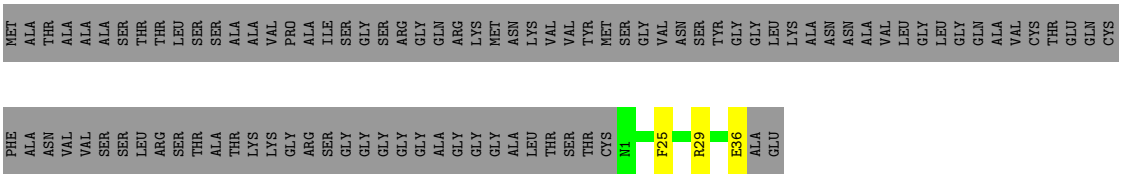
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



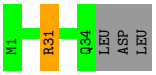
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain N:



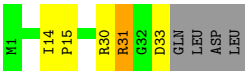
• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:



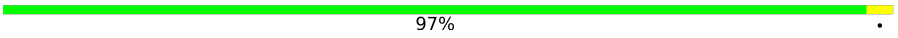
• Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:



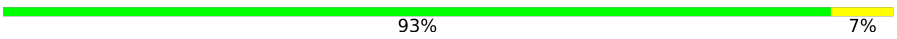
• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:



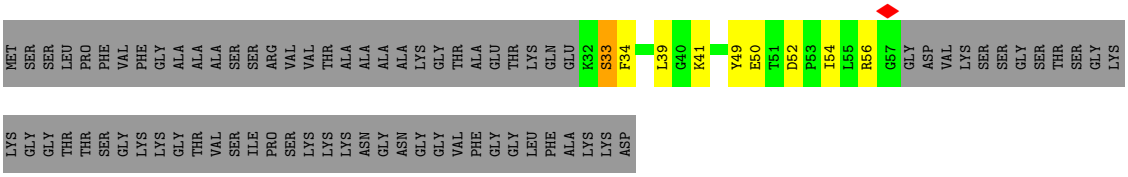
• Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:



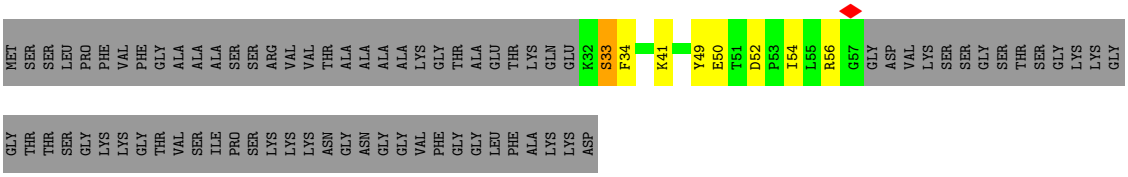
• Molecule 9: Thylakoid soluble phosphoprotein

Chain R:



• Molecule 9: Thylakoid soluble phosphoprotein

Chain Q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	685979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Non-uniform Refinement with iterative global CTF refinement and anisotropic magnification fitting	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.455	Depositor
Minimum map value	-0.577	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.208	Depositor
Map size (Å)	319.92, 319.92, 319.92	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SQD, UMQ, PL9, BCR, HEM, HEC, CLA

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	0.26	0/1747	0.42	0/2382
1	I	0.26	0/1747	0.42	0/2382
2	B	0.25	0/1262	0.43	0/1733
2	J	0.25	0/1263	0.43	0/1733
3	C	0.26	0/2204	0.44	0/2987
3	K	0.27	0/2213	0.44	0/2999
4	D	0.24	0/1293	0.44	0/1769
4	L	0.24	0/1288	0.44	0/1762
5	E	0.26	0/247	0.41	0/333
5	M	0.26	0/247	0.40	0/333
6	F	0.28	0/270	0.40	0/366
6	N	0.29	0/265	0.41	0/359
7	G	0.27	0/271	0.41	0/367
7	O	0.27	0/266	0.40	0/360
8	H	0.26	0/227	0.39	0/309
8	P	0.27	0/228	0.40	0/309
9	Q	0.24	0/224	0.35	0/301
9	R	0.23	0/224	0.35	0/301
All	All	0.26	0/15486	0.43	0/21085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1697	0	1724	18	0
1	I	1697	0	1724	20	0
2	B	1225	0	1276	28	0
2	J	1226	0	1276	23	0
3	C	2158	0	2212	84	0
3	K	2167	0	2218	78	0
4	D	1259	0	1232	23	0
4	L	1254	0	1227	23	0
5	E	243	0	268	1	0
5	M	243	0	268	4	0
6	F	269	0	287	2	0
6	N	264	0	282	2	0
7	G	266	0	282	1	0
7	O	261	0	280	3	0
8	H	222	0	234	1	0
8	P	223	0	234	1	0
9	Q	219	0	216	7	0
9	R	219	0	216	8	0
10	A	86	0	60	9	0
10	I	86	0	60	10	0
11	A	43	0	31	2	0
11	C	43	0	31	6	0
11	I	43	0	31	2	0
11	K	43	0	31	5	0
12	A	65	0	72	4	0
12	I	65	0	72	5	0
13	A	68	88	88	0	0
13	B	68	88	88	3	0
13	H	34	44	44	1	0
13	I	68	88	88	2	0
13	J	68	88	88	1	0
13	P	34	44	44	1	0
14	A	55	0	80	10	0
14	B	110	0	158	27	0
14	J	110	0	160	28	0
14	K	55	0	77	4	0
15	D	54	0	77	5	0
15	L	54	0	77	1	0
16	D	4	0	0	0	0
16	L	4	0	0	0	0
17	F	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	40	0	56	5	0
All	All	16452	440	17025	386	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 12.

All (386) 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:K:180:LYS:HG2	3:K:194:ILE:HA	1.39	1.04
3:K:180:LYS:HE2	3:K:195:ALA:H	1.22	1.03
3:C:180:LYS:HE2	3:C:195:ALA:H	1.22	1.01
3:C:180:LYS:HG2	3:C:194:ILE:HA	1.39	1.00
3:C:179:VAL:HA	3:C:194:ILE:HG22	1.44	0.99
3:K:179:VAL:HA	3:K:194:ILE:HG22	1.44	0.99
3:C:178:ILE:HA	3:C:220:SER:HA	1.44	0.97
3:K:178:ILE:HA	3:K:220:SER:HA	1.44	0.97
3:K:21:CYS:HB2	11:K:301:HEC:HAB	1.47	0.97
3:C:222:LYS:HB3	3:C:222:LYS:HZ2	1.31	0.94
3:C:222:LYS:HB3	3:C:222:LYS:NZ	1.79	0.94
3:C:21:CYS:HB2	11:C:301:HEC:HAB	1.47	0.94
3:C:29:LYS:HG3	3:C:235:GLY:HA3	1.50	0.92
3:K:29:LYS:HG3	3:K:235:GLY:HA3	1.50	0.91
3:C:182:ILE:HG12	3:C:192:ILE:HD12	1.54	0.90
3:K:182:ILE:HG12	3:K:192:ILE:HD12	1.54	0.89
10:A:301:HEM:HBC2	10:A:301:HEM:HMC2	1.58	0.85
10:I:302:HEM:HBC2	10:I:302:HEM:HMC2	1.60	0.84
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.60	0.83
14:A:307:PL9:H453	15:D:201:SQD:H202	1.59	0.83
10:I:301:HEM:HBC2	10:I:301:HEM:HMC2	1.59	0.83
10:I:301:HEM:HMB1	10:I:301:HEM:HBB2	1.61	0.82
3:K:178:ILE:HG22	3:K:220:SER:HB2	1.61	0.82
3:C:178:ILE:HG22	3:C:220:SER:HB2	1.61	0.82
4:D:64:ILE:HG23	4:D:157:GLY:O	1.81	0.81
10:A:301:HEM:HMB1	10:A:301:HEM:HBB2	1.61	0.81
13:B:403:UMQ:O3'	13:B:403:UMQ:O2	1.93	0.80
3:C:177:GLY:O	3:C:220:SER:OG	2.00	0.79
3:K:180:LYS:HE2	3:K:195:ALA:N	1.98	0.79
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	1.63	0.78
3:K:177:GLY:O	3:K:220:SER:OG	2.00	0.78
3:K:178:ILE:HG13	3:K:180:LYS:NZ	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:ILE:HG13	3:C:180:LYS:NZ	1.99	0.78
10:I:302:HEM:HMB1	10:I:302:HEM:HBB2	1.63	0.78
3:C:180:LYS:HE2	3:C:195:ALA:N	1.98	0.77
3:C:179:VAL:HA	3:C:194:ILE:CG2	2.15	0.77
3:K:175:ALA:O	3:K:221:ILE:HD11	1.86	0.76
3:K:179:VAL:HA	3:K:194:ILE:CG2	2.15	0.76
3:C:175:ALA:O	3:C:221:ILE:HD11	1.86	0.75
3:K:195:ALA:HB2	3:K:202:GLU:HG3	1.68	0.74
2:J:121:GLN:N	9:R:50:GLU:OE2	2.21	0.74
4:L:122:LYS:HB2	4:L:132:TYR:O	1.87	0.74
3:C:179:VAL:HG13	3:C:218:GLY:H	1.53	0.74
3:C:173:SER:HB3	3:C:227:LEU:HD11	1.70	0.74
1:I:150:ILE:HG21	14:J:401:PL9:H502	1.70	0.73
3:K:179:VAL:HG13	3:K:218:GLY:H	1.53	0.72
3:K:173:SER:HB3	3:K:227:LEU:HD11	1.70	0.72
2:J:74:GLU:HB3	14:J:402:PL9:H121	1.70	0.72
3:C:178:ILE:HG13	3:C:180:LYS:HZ3	1.52	0.72
14:B:402:PL9:HC72	14:B:402:PL9:H122	1.71	0.71
3:C:63:ASN:OD1	3:C:65:LYS:HG2	1.91	0.71
12:I:304:CLA:H151	14:J:401:PL9:H312	1.71	0.71
1:I:27:PRO:HG3	2:J:24:HIS:O	1.90	0.71
3:K:63:ASN:OD1	3:K:65:LYS:HG2	1.91	0.70
3:K:283:MET:HE3	3:K:283:MET:HA	1.73	0.69
3:K:162:ASP:OD1	3:K:163:GLY:N	2.26	0.69
3:K:178:ILE:HG13	3:K:180:LYS:HZ3	1.56	0.69
3:K:181:LYS:HZ1	3:K:183:VAL:HG12	1.56	0.69
4:D:28:LEU:HB2	4:D:29:PRO:HD3	1.74	0.68
3:C:162:ASP:OD1	3:C:163:GLY:N	2.26	0.68
2:B:121:GLN:N	9:Q:50:GLU:OE2	2.22	0.68
3:C:184:ARG:NH2	3:C:186:GLU:HA	2.08	0.68
1:A:27:PRO:HG3	2:B:24:HIS:O	1.93	0.68
8:P:2:ASP:OD2	13:P:102:UMQ:O4	2.07	0.68
1:A:150:ILE:HD13	14:B:401:PL9:H512	1.75	0.68
2:B:74:GLU:OE1	2:B:74:GLU:N	2.27	0.68
14:J:402:PL9:H252	14:J:402:PL9:H201	1.75	0.68
5:M:29:ARG:HG3	5:M:29:ARG:HH11	1.57	0.67
3:K:121:GLN:HA	3:K:121:GLN:OE1	1.93	0.67
17:P:101:BCR:H401	9:R:39:LEU:HD21	1.76	0.67
2:J:74:GLU:N	2:J:74:GLU:OE1	2.27	0.67
3:C:283:MET:HE3	3:C:283:MET:HA	1.74	0.67
3:C:121:GLN:OE1	3:C:121:GLN:HA	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:HB2	2:B:101:MET:CE	2.25	0.67
3:C:184:ARG:HH22	3:C:186:GLU:HA	1.59	0.67
4:L:93:GLU:OE2	4:L:93:GLU:HA	1.95	0.67
12:A:304:CLA:O1D	14:B:402:PL9:H502	1.95	0.67
3:C:182:ILE:HG12	3:C:192:ILE:CD1	2.24	0.67
7:G:31:ARG:HG2	9:Q:49:TYR:OH	1.95	0.67
3:K:182:ILE:HG12	3:K:192:ILE:CD1	2.24	0.66
4:L:137:ARG:HG2	4:L:137:ARG:HH21	1.60	0.66
3:C:185:LYS:HD2	3:C:186:GLU:H	1.61	0.66
10:I:302:HEM:HBA1	10:I:302:HEM:HHA	1.78	0.66
4:L:67:GLU:O	4:L:71:THR:HG22	1.96	0.66
3:K:185:LYS:HD2	3:K:186:GLU:H	1.61	0.65
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.78	0.65
3:C:185:LYS:HZ3	3:C:187:LYS:H	1.45	0.65
12:I:304:CLA:HBB1	12:I:304:CLA:HMB1	1.78	0.65
3:C:63:ASN:OD1	3:C:64:GLY:N	2.30	0.65
12:A:304:CLA:HMB1	12:A:304:CLA:HBB1	1.79	0.65
2:J:85:PHE:CE1	14:J:401:PL9:H503	2.33	0.64
3:K:185:LYS:HZ3	3:K:187:LYS:H	1.45	0.64
3:K:63:ASN:OD1	3:K:64:GLY:N	2.30	0.64
3:C:178:ILE:HG22	3:C:220:SER:CB	2.28	0.64
7:O:31:ARG:HG2	9:R:49:TYR:OH	1.97	0.64
4:L:64:ILE:HB	4:L:67:GLU:OE1	1.98	0.63
2:J:74:GLU:HA	14:J:402:PL9:O2	1.99	0.63
2:J:75:ILE:HG12	14:J:401:PL9:C51	2.29	0.63
2:B:75:ILE:HG12	14:B:401:PL9:H501	1.81	0.63
4:L:140:ARG:HD2	4:L:141:GLY:N	2.14	0.63
3:K:181:LYS:NZ	3:K:183:VAL:HG12	2.14	0.62
4:D:140:ARG:HD2	4:D:141:GLY:N	2.14	0.62
10:A:301:HEM:HBC2	10:A:301:HEM:CMC	2.30	0.62
3:C:181:LYS:NZ	3:C:183:VAL:HG12	2.14	0.62
14:J:402:PL9:H153	14:J:402:PL9:H101	1.81	0.62
3:K:178:ILE:HG22	3:K:220:SER:CB	2.28	0.62
11:C:301:HEC:HBC3	11:C:301:HEC:HHD	1.82	0.61
3:C:181:LYS:HG2	3:C:182:ILE:N	2.15	0.61
10:I:301:HEM:HBB2	10:I:301:HEM:CMB	2.31	0.61
1:I:145:TYR:O	1:I:148:VAL:HG12	2.00	0.61
10:I:301:HEM:HBC2	10:I:301:HEM:CMC	2.30	0.61
3:K:181:LYS:HG2	3:K:182:ILE:N	2.15	0.61
4:D:64:ILE:HB	4:D:67:GLU:OE1	2.01	0.61
10:I:302:HEM:HBC2	10:I:302:HEM:CMC	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	2.31	0.61
2:B:75:ILE:HG12	14:B:401:PL9:C50	2.31	0.61
1:A:145:TYR:O	1:A:148:VAL:HG12	2.01	0.60
3:C:191:GLU:O	3:C:192:ILE:HD13	2.01	0.60
17:P:101:BCR:H401	9:R:39:LEU:CD2	2.30	0.60
10:I:302:HEM:HBB2	10:I:302:HEM:CMB	2.31	0.60
3:K:194:ILE:O	3:K:203:VAL:HG22	2.01	0.60
11:K:301:HEC:HBC3	11:K:301:HEC:HHD	1.82	0.60
2:J:121:GLN:HB2	9:R:50:GLU:OE2	2.01	0.60
4:D:163:PRO:HB3	4:D:179:ALA:O	2.01	0.60
3:K:92:GLU:O	3:K:95:GLU:HG3	2.02	0.60
2:B:74:GLU:HA	14:B:402:PL9:O2	2.01	0.60
3:C:194:ILE:O	3:C:203:VAL:HG22	2.01	0.60
10:A:302:HEM:HBC2	10:A:302:HEM:CMC	2.31	0.60
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.31	0.59
3:C:92:GLU:O	3:C:95:GLU:HG3	2.02	0.59
4:D:67:GLU:O	4:D:71:THR:HG22	2.01	0.59
4:L:64:ILE:HG23	4:L:157:GLY:O	2.02	0.59
3:K:191:GLU:O	3:K:192:ILE:HD13	2.01	0.59
14:A:307:PL9:H453	15:D:201:SQD:H223	1.86	0.58
2:B:88:LEU:HB2	2:B:101:MET:HE1	1.85	0.58
8:H:2:ASP:OD2	13:H:201:UMQ:O4	2.19	0.58
3:K:185:LYS:NZ	3:K:186:GLU:HG3	2.18	0.58
3:K:202:GLU:OE1	3:K:202:GLU:N	2.36	0.58
3:C:185:LYS:NZ	3:C:186:GLU:HG3	2.18	0.58
4:D:64:ILE:HB	4:D:67:GLU:OE2	2.04	0.58
3:K:180:LYS:HG2	3:K:194:ILE:CA	2.26	0.57
3:C:181:LYS:HZ1	3:C:183:VAL:HG12	1.68	0.57
3:K:193:ASN:OD1	3:K:204:VAL:HG22	2.05	0.57
4:L:70:LYS:HB2	4:L:70:LYS:NZ	2.20	0.57
3:C:193:ASN:OD1	3:C:204:VAL:HG22	2.04	0.57
3:K:195:ALA:HB2	3:K:202:GLU:CG	2.34	0.56
3:K:173:SER:OG	3:K:224:ASP:N	2.39	0.56
12:A:304:CLA:H151	14:B:401:PL9:H28	1.88	0.56
3:C:173:SER:OG	3:C:224:ASP:N	2.39	0.56
14:A:307:PL9:H453	15:D:201:SQD:C20	2.34	0.56
3:C:179:VAL:HG22	3:C:217:GLU:OE1	2.06	0.56
4:L:171:THR:HB	4:L:173:GLU:OE1	2.06	0.56
14:J:402:PL9:H201	14:J:402:PL9:C25	2.36	0.55
1:A:113:PRO:HB2	1:I:11:ARG:HG2	1.88	0.55
3:C:180:LYS:HG2	3:C:194:ILE:CA	2.26	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:ARG:NH1	3:C:185:LYS:O	2.39	0.55
3:C:221:ILE:C	3:C:221:ILE:HD12	2.27	0.55
3:K:221:ILE:HD12	3:K:221:ILE:C	2.27	0.55
14:A:307:PL9:H451	14:A:307:PL9:C48	2.36	0.55
12:I:304:CLA:HMA3	14:J:402:PL9:H513	1.88	0.55
3:K:179:VAL:HG12	3:K:219:GLU:O	2.07	0.55
3:C:179:VAL:HG12	3:C:219:GLU:O	2.07	0.55
11:I:303:HEC:HBC3	11:I:303:HEC:HMC1	1.89	0.55
4:D:64:ILE:HB	4:D:67:GLU:CD	2.28	0.54
3:C:183:VAL:HG13	3:C:191:GLU:CB	2.38	0.54
4:L:74:PRO:HA	4:L:92:VAL:HG12	1.88	0.54
3:K:179:VAL:HG22	3:K:217:GLU:OE1	2.06	0.54
14:A:307:PL9:C35	14:J:401:PL9:H532	2.37	0.54
2:B:154:SER:OG	13:B:404:UMQ:O2'	2.25	0.54
4:L:137:ARG:HG2	4:L:137:ARG:NH2	2.20	0.54
3:C:179:VAL:HG12	3:C:219:GLU:H	1.73	0.54
2:J:74:GLU:HA	14:J:402:PL9:C1	2.38	0.54
3:K:183:VAL:HG13	3:K:191:GLU:CB	2.37	0.54
4:D:166:GLU:OE1	4:D:166:GLU:N	2.41	0.54
14:K:302:PL9:H301	14:K:302:PL9:H33	1.90	0.54
13:I:306:UMQ:O3'	13:I:306:UMQ:O2	2.21	0.53
11:A:303:HEC:HMC1	11:A:303:HEC:HBC3	1.89	0.53
3:K:179:VAL:HG12	3:K:219:GLU:H	1.73	0.53
2:B:88:LEU:HB2	2:B:101:MET:HE2	1.90	0.53
14:B:402:PL9:C38	14:B:402:PL9:H351	2.38	0.53
3:K:179:VAL:CG1	3:K:219:GLU:H	2.21	0.53
5:M:29:ARG:HG3	5:M:29:ARG:NH1	2.23	0.53
2:J:70:ALA:HB1	3:K:16:THR:HG22	1.89	0.53
2:B:29:GLU:HG2	2:B:30:PRO:HD2	1.90	0.53
3:C:179:VAL:CG1	3:C:219:GLU:H	2.21	0.53
4:D:74:PRO:HA	4:D:92:VAL:HG12	1.90	0.53
3:K:155:GLY:O	11:K:301:HEC:HBA1	2.09	0.53
3:K:29:LYS:HB2	3:K:154:ARG:NH1	2.24	0.53
4:L:64:ILE:HB	4:L:67:GLU:CD	2.29	0.53
2:J:29:GLU:HG2	2:J:30:PRO:HD2	1.90	0.53
3:C:29:LYS:HE2	3:C:234:GLY:O	2.09	0.52
3:C:185:LYS:HD2	3:C:186:GLU:N	2.24	0.52
3:C:29:LYS:HB2	3:C:154:ARG:NH1	2.24	0.52
1:I:150:ILE:HD13	14:J:401:PL9:C50	2.39	0.52
3:C:155:GLY:O	11:C:301:HEC:HBA1	2.09	0.52
3:K:185:LYS:HD2	3:K:186:GLU:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:401:PL9:H101	14:B:401:PL9:H13	1.92	0.52
4:L:64:ILE:HB	4:L:67:GLU:OE2	2.10	0.52
3:K:283:MET:HE3	3:K:283:MET:CA	2.40	0.52
14:B:402:PL9:H523	4:L:128:HIS:NE2	2.25	0.52
3:C:173:SER:O	3:C:224:ASP:HA	2.10	0.52
11:C:301:HEC:HMB1	11:C:301:HEC:HBB3	1.92	0.52
3:K:183:VAL:HG13	3:K:191:GLU:HB3	1.92	0.52
3:C:179:VAL:CG1	3:C:218:GLY:H	2.23	0.51
11:K:301:HEC:HBB3	11:K:301:HEC:HMB1	1.93	0.51
4:D:29:PRO:O	4:D:33:MET:HG2	2.10	0.51
14:J:402:PL9:H252	14:J:402:PL9:C20	2.40	0.51
3:K:140:ASP:OD1	3:K:140:ASP:N	2.43	0.51
3:K:173:SER:O	3:K:224:ASP:HA	2.10	0.51
13:I:305:UMQ:HJ2	15:L:401:SQD:H301	1.92	0.51
3:K:29:LYS:HE2	3:K:234:GLY:O	2.09	0.51
2:J:118:ASN:OD1	2:J:119:LYS:N	2.43	0.51
4:L:74:PRO:HA	4:L:92:VAL:CG1	2.41	0.51
3:C:183:VAL:HG13	3:C:191:GLU:HB3	1.92	0.51
3:K:173:SER:HG	3:K:224:ASP:H	1.58	0.51
3:K:190:TYR:CE2	3:K:213:LEU:HG	2.46	0.51
3:C:140:ASP:OD1	3:C:140:ASP:N	2.43	0.51
1:I:117:THR:HG22	1:I:202:HIS:CE1	2.46	0.51
3:K:178:ILE:HG13	3:K:180:LYS:HZ2	1.72	0.51
1:A:117:THR:HG22	1:A:202:HIS:CE1	2.46	0.50
2:B:85:PHE:CE1	14:B:401:PL9:H513	2.47	0.50
3:C:190:TYR:CE2	3:C:213:LEU:HG	2.46	0.50
9:R:33:SER:O	9:R:34:PHE:HB3	2.12	0.50
9:Q:33:SER:O	9:Q:34:PHE:HB3	2.12	0.50
3:K:179:VAL:CG1	3:K:218:GLY:H	2.23	0.49
14:A:307:PL9:H13	3:C:250:ARG:HA	1.94	0.49
2:B:75:ILE:HG22	14:B:402:PL9:H531	1.94	0.49
6:F:25:PHE:HE1	9:Q:41:LYS:HB3	1.78	0.49
4:D:115:PRO:HD2	4:D:124:ILE:O	2.10	0.49
14:B:402:PL9:H251	14:B:402:PL9:H272	1.55	0.49
3:C:222:LYS:NZ	3:C:222:LYS:CB	2.66	0.49
2:J:70:ALA:HB1	3:K:16:THR:CG2	2.42	0.49
2:B:74:GLU:HG3	14:B:402:PL9:H152	1.94	0.49
3:C:185:LYS:HZ3	3:C:186:GLU:HG3	1.76	0.49
1:I:81:LEU:HD21	14:K:302:PL9:H221	1.95	0.49
3:K:185:LYS:HZ3	3:K:186:GLU:HG3	1.78	0.49
2:B:74:GLU:HA	14:B:402:PL9:C1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:GLY:HA3	14:B:402:PL9:H422	1.95	0.48
3:C:283:MET:HE3	3:C:283:MET:CA	2.42	0.48
3:C:194:ILE:O	3:C:194:ILE:HD12	2.14	0.48
3:C:178:ILE:HG13	3:C:180:LYS:HZ2	1.76	0.48
4:D:93:GLU:N	4:D:97:THR:O	2.43	0.48
14:B:402:PL9:H451	14:B:402:PL9:H471	1.56	0.47
6:N:25:PHE:HE1	9:R:41:LYS:HB3	1.79	0.47
4:L:166:GLU:OE1	4:L:166:GLU:N	2.47	0.47
14:A:307:PL9:C45	15:D:201:SQD:H223	2.44	0.47
3:C:184:ARG:NH2	3:C:185:LYS:O	2.47	0.47
2:J:74:GLU:HB3	14:J:402:PL9:C12	2.42	0.47
14:B:402:PL9:H121	14:B:402:PL9:H172	1.96	0.47
3:K:194:ILE:O	3:K:194:ILE:HD12	2.14	0.47
1:A:150:ILE:HG21	14:B:401:PL9:H512	1.97	0.47
1:A:11:ARG:HG2	1:I:113:PRO:HB2	1.97	0.47
14:A:307:PL9:H322	14:A:307:PL9:H301	1.68	0.47
3:K:54:ASP:OD2	3:K:55:MET:N	2.49	0.46
4:L:67:GLU:OE1	4:L:67:GLU:N	2.38	0.46
2:B:125:ARG:NH1	9:Q:50:GLU:OE1	2.48	0.46
4:D:93:GLU:OE1	4:D:93:GLU:HA	2.16	0.46
2:B:85:PHE:CD1	14:B:401:PL9:H472	2.50	0.46
3:C:54:ASP:OD2	3:C:55:MET:N	2.49	0.46
17:F:101:BCR:C8	17:F:101:BCR:H331	2.45	0.46
1:A:150:ILE:HD13	14:B:401:PL9:C51	2.42	0.46
3:C:178:ILE:HB	3:C:219:GLU:O	2.16	0.46
14:B:401:PL9:H471	14:B:401:PL9:H451	1.70	0.46
3:C:180:LYS:CE	3:C:195:ALA:H	2.11	0.46
3:K:159:ILE:O	11:K:301:HEC:HBC3	2.16	0.46
3:K:178:ILE:HB	3:K:219:GLU:O	2.16	0.46
13:B:403:UMQ:O3'	13:B:403:UMQ:C2	2.64	0.46
1:I:207:ARG:HD2	11:I:303:HEC:O2D	2.15	0.46
3:K:145:LYS:HE3	3:K:242:GLU:HG3	1.98	0.46
1:A:207:ARG:HD2	11:A:303:HEC:O2D	2.15	0.45
2:J:74:GLU:HA	14:J:402:PL9:C2	2.46	0.45
1:A:103:ARG:HD2	1:A:103:ARG:C	2.37	0.45
3:C:145:LYS:HE3	3:C:242:GLU:HG3	1.98	0.45
3:C:159:ILE:O	11:C:301:HEC:HBC3	2.16	0.45
1:I:146:TRP:HB2	2:J:75:ILE:HD13	1.97	0.45
6:N:36:GLU:OE2	6:N:36:GLU:N	2.48	0.45
14:A:307:PL9:H151	14:A:307:PL9:H172	1.66	0.45
14:J:402:PL9:C38	14:J:402:PL9:H351	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:18:ARG:NH2	3:K:23:ASN:OD1	2.50	0.45
2:B:104:VAL:HB	2:B:105:PRO:CD	2.47	0.45
3:C:184:ARG:HH22	3:C:186:GLU:CA	2.28	0.45
2:J:104:VAL:HB	2:J:105:PRO:CD	2.47	0.45
3:K:206:ILE:H	3:K:206:ILE:HD12	1.82	0.45
14:B:402:PL9:H212	14:B:402:PL9:H161	1.99	0.45
1:I:103:ARG:C	1:I:103:ARG:HD2	2.37	0.45
5:E:27:LYS:CA	5:E:27:LYS:HE2	2.47	0.45
17:P:101:BCR:H20C	17:P:101:BCR:H361	1.84	0.45
3:C:206:ILE:HD12	3:C:206:ILE:H	1.82	0.45
3:K:180:LYS:CE	3:K:195:ALA:H	2.11	0.45
14:J:401:PL9:H23	14:J:401:PL9:C18	2.47	0.44
4:D:55:ALA:O	4:D:63:VAL:HG23	2.17	0.44
4:D:73:ALA:HB1	4:D:74:PRO:HD2	1.98	0.44
1:A:211:ILE:HG13	1:A:212:SER:H	1.81	0.44
3:C:18:ARG:NH2	3:C:23:ASN:OD1	2.50	0.44
1:I:150:ILE:HD13	14:J:401:PL9:H502	1.98	0.44
17:P:101:BCR:H24C	17:P:101:BCR:H371	1.83	0.44
1:I:211:ILE:HG13	1:I:212:SER:H	1.81	0.44
3:C:223:LEU:O	3:C:224:ASP:HB2	2.18	0.44
1:I:63:THR:HG22	1:I:64:ASP:OD2	2.17	0.44
17:P:101:BCR:C8	17:P:101:BCR:H331	2.48	0.44
1:A:63:THR:HG22	1:A:64:ASP:OD2	2.18	0.44
9:R:54:ILE:HD12	9:R:54:ILE:H	1.83	0.44
1:I:163:SER:HB2	1:I:164:PRO:HD3	2.00	0.44
5:M:27:LYS:CA	5:M:27:LYS:HE2	2.47	0.44
1:A:163:SER:HB2	1:A:164:PRO:HD3	2.00	0.43
4:D:74:PRO:HA	4:D:92:VAL:CG1	2.48	0.43
1:I:138:LEU:N	1:I:139:PRO:CD	2.81	0.43
1:A:138:LEU:N	1:A:139:PRO:CD	2.81	0.43
3:K:35:VAL:HB	3:K:36:PRO:HD2	1.99	0.43
4:L:110:LEU:HD23	4:L:110:LEU:HA	1.85	0.43
14:J:401:PL9:H422	14:J:401:PL9:H401	1.58	0.43
3:K:223:LEU:O	3:K:224:ASP:HB2	2.18	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.86	0.43
2:B:159:LEU:O	2:B:160:PHE:C	2.57	0.43
6:F:25:PHE:CE1	9:Q:41:LYS:HB3	2.54	0.43
3:K:191:GLU:C	3:K:192:ILE:HD13	2.39	0.43
3:C:35:VAL:HB	3:C:36:PRO:HD2	1.99	0.43
3:C:191:GLU:C	3:C:192:ILE:HD13	2.39	0.43
4:D:69:LEU:HD21	4:D:98:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:159:LEU:O	2:J:160:PHE:C	2.57	0.43
7:O:30:ARG:HA	7:O:30:ARG:HD2	1.77	0.43
9:Q:54:ILE:H	9:Q:54:ILE:HD12	1.83	0.43
14:B:402:PL9:HC72	14:B:402:PL9:C12	2.39	0.43
3:K:178:ILE:O	3:K:180:LYS:HD3	2.19	0.43
14:J:402:PL9:H201	14:J:402:PL9:H221	1.64	0.43
3:K:283:MET:HA	3:K:283:MET:CE	2.45	0.43
4:L:69:LEU:HD21	4:L:98:LEU:HD23	2.01	0.43
1:A:154:VAL:N	1:A:155:PRO:HD2	2.34	0.42
15:D:201:SQD:H102	15:D:201:SQD:H132	1.87	0.42
1:I:154:VAL:N	1:I:155:PRO:HD2	2.34	0.42
10:I:302:HEM:HBA1	10:I:302:HEM:CHA	2.48	0.42
2:J:8:ASP:O	2:J:8:ASP:CG	2.58	0.42
3:K:100:LEU:HD23	3:K:100:LEU:HA	1.93	0.42
4:D:139:VAL:O	4:D:140:ARG:HB2	2.20	0.42
3:C:178:ILE:O	3:C:180:LYS:HD3	2.19	0.42
4:D:97:THR:OG1	4:D:98:LEU:N	2.51	0.42
4:D:162:VAL:HG13	4:D:163:PRO:HD2	2.01	0.42
17:F:101:BCR:H24C	17:F:101:BCR:H371	1.82	0.42
1:I:45:LEU:HD12	14:K:302:PL9:H403	2.01	0.42
2:B:119:LYS:HB3	2:B:119:LYS:HE3	1.18	0.42
14:B:402:PL9:H351	14:B:402:PL9:H38	2.00	0.42
3:C:283:MET:HA	3:C:283:MET:CE	2.45	0.42
2:J:109:LEU:HD12	2:J:109:LEU:HA	1.86	0.42
5:M:29:ARG:HD2	5:M:29:ARG:N	2.34	0.42
3:C:50:ARG:NH2	3:C:125:GLU:OE1	2.53	0.42
14:J:401:PL9:H361	14:J:401:PL9:H321	1.67	0.42
4:L:78:THR:HG22	4:L:79:LEU:N	2.35	0.42
3:C:153:ASN:ND2	3:C:235:GLY:O	2.53	0.42
14:K:302:PL9:H422	14:K:302:PL9:H401	1.40	0.42
4:L:90:LEU:HD23	4:L:90:LEU:HA	1.83	0.42
2:B:70:ALA:HB1	3:C:16:THR:HG22	2.00	0.42
3:K:50:ARG:NH2	3:K:125:GLU:OE1	2.53	0.42
3:K:181:LYS:HE3	3:K:181:LYS:HB3	1.98	0.42
3:C:184:ARG:HG2	3:C:184:ARG:HH11	1.83	0.41
4:D:140:ARG:CD	4:D:141:GLY:N	2.83	0.41
2:J:29:GLU:HG2	2:J:30:PRO:CD	2.50	0.41
12:I:304:CLA:C20	14:J:401:PL9:H221	2.51	0.41
2:B:29:GLU:HG2	2:B:30:PRO:CD	2.50	0.41
1:I:150:ILE:HD13	14:J:401:PL9:H501	2.02	0.41
12:I:304:CLA:H61	12:I:304:CLA:H101	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:402:PL9:HC72	14:J:402:PL9:H112	1.70	0.41
4:L:139:VAL:O	4:L:140:ARG:HB2	2.20	0.41
2:B:144:GLY:HA3	14:B:402:PL9:C42	2.50	0.41
4:D:53:THR:O	4:D:160:VAL:HA	2.21	0.41
3:K:191:GLU:OE2	3:K:206:ILE:HG13	2.21	0.41
3:K:153:ASN:ND2	3:K:235:GLY:O	2.53	0.41
1:A:146:TRP:HB2	2:B:75:ILE:HD13	2.02	0.41
14:A:307:PL9:H112	3:C:250:ARG:HA	2.02	0.41
2:B:8:ASP:O	2:B:8:ASP:CG	2.58	0.41
1:I:92:MET:O	1:I:96:MET:HG2	2.21	0.41
13:J:403:UMQ:O5	13:J:403:UMQ:O6'	2.30	0.41
2:B:119:LYS:H	2:B:119:LYS:HG2	1.69	0.41
2:B:74:GLU:HA	14:B:402:PL9:C2	2.51	0.40
3:C:191:GLU:OE2	3:C:206:ILE:HG13	2.21	0.40
2:J:6:LYS:HE3	2:J:6:LYS:HB3	1.74	0.40
14:J:402:PL9:H401	14:J:402:PL9:H422	1.74	0.40
4:L:56:LYS:O	4:L:80:THR:HB	2.21	0.40
12:A:304:CLA:H61	12:A:304:CLA:H101	1.74	0.40
3:C:21:CYS:HB2	11:C:301:HEC:CAB	2.35	0.40
2:J:85:PHE:HE1	14:J:401:PL9:H503	1.84	0.40
14:J:401:PL9:H301	14:J:401:PL9:H322	1.59	0.40
7:O:14:ILE:N	7:O:15:PRO:HD2	2.36	0.40
1:A:92:MET:O	1:A:96:MET:HG2	2.21	0.40
3:C:115:ILE:HG23	3:C:115:ILE:O	2.21	0.40
3:C:69:LEU:N	3:C:69:LEU:HD12	2.37	0.40
3:K:97:MET:HE2	3:K:97:MET:HB2	1.91	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	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
2	J	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	274/320 (86%)	263 (96%)	11 (4%)	0	100	100
3	K	275/320 (86%)	264 (96%)	11 (4%)	0	100	100
4	D	162/230 (70%)	151 (93%)	11 (7%)	0	100	100
4	L	161/230 (70%)	152 (94%)	9 (6%)	0	100	100
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	35/131 (27%)	35 (100%)	0	0	100	100
6	N	34/131 (26%)	34 (100%)	0	0	100	100
7	G	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
7	O	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
9	Q	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
9	R	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
All	All	1902/2512 (76%)	1828 (96%)	74 (4%)	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	185/186 (100%)	178 (96%)	7 (4%)	33	30
1	I	185/186 (100%)	178 (96%)	7 (4%)	33	30
2	B	134/135 (99%)	128 (96%)	6 (4%)	27	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	134/135 (99%)	128 (96%)	6 (4%)	27 23
3	C	237/275 (86%)	228 (96%)	9 (4%)	33 30
3	K	238/275 (86%)	231 (97%)	7 (3%)	42 40
4	D	135/183 (74%)	130 (96%)	5 (4%)	34 31
4	L	135/183 (74%)	130 (96%)	5 (4%)	34 31
5	E	26/26 (100%)	23 (88%)	3 (12%)	5 2
5	M	26/26 (100%)	24 (92%)	2 (8%)	13 7
6	F	26/90 (29%)	25 (96%)	1 (4%)	33 30
6	N	26/90 (29%)	25 (96%)	1 (4%)	33 30
7	G	27/31 (87%)	26 (96%)	1 (4%)	34 31
7	O	27/31 (87%)	25 (93%)	2 (7%)	13 8
8	H	24/24 (100%)	24 (100%)	0	100 100
8	P	24/24 (100%)	23 (96%)	1 (4%)	30 26
9	Q	24/78 (31%)	21 (88%)	3 (12%)	4 1
9	R	24/78 (31%)	21 (88%)	3 (12%)	4 1
All	All	1637/2056 (80%)	1568 (96%)	69 (4%)	33 26

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	89	SER
1	A	131	PHE
1	A	133	VAL
1	A	156	ASP
1	A	167	GLU
1	A	207	ARG
2	B	3	VAL
2	B	8	ASP
2	B	35	ASP
2	B	103	SER
2	B	119	LYS
2	B	152	ASP
3	C	124	SER
3	C	140	ASP
3	C	154	ARG
3	C	181	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	183	VAL
3	C	184	ARG
3	C	222	LYS
3	C	242	GLU
3	C	281	SER
4	D	71	THR
4	D	76	ASP
4	D	137	ARG
4	D	140	ARG
4	D	166	GLU
5	E	1	MET
5	E	26	ASN
5	E	29	ARG
6	F	35	GLU
7	G	31	ARG
1	I	6	ASP
1	I	89	SER
1	I	131	PHE
1	I	133	VAL
1	I	156	ASP
1	I	167	GLU
1	I	207	ARG
2	J	3	VAL
2	J	8	ASP
2	J	35	ASP
2	J	103	SER
2	J	119	LYS
2	J	152	ASP
3	K	124	SER
3	K	140	ASP
3	K	154	ARG
3	K	181	LYS
3	K	183	VAL
3	K	242	GLU
3	K	281	SER
4	L	32	TYR
4	L	76	ASP
4	L	117	ASN
4	L	140	ARG
4	L	166	GLU
5	M	1	MET
5	M	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	29	ARG
7	O	31	ARG
7	O	33	ASP
8	P	1	MET
9	R	33	SER
9	R	52	ASP
9	R	56	ARG
9	Q	33	SER
9	Q	52	ASP
9	Q	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

32 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	$\#\|Z\| > 2$
13	UMQ	I	305	-	35,35,35	1.15	1 (2%)	46,46,46	0.96	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	FES	D	202	4	0,4,4	-	-	-		
17	BCR	F	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	7 (12%)
13	UMQ	A	306	-	35,35,35	1.15	1 (2%)	46,46,46	0.96	3 (6%)
13	UMQ	I	306	-	35,35,35	1.13	1 (2%)	46,46,46	0.97	1 (2%)
10	HEM	A	301	1	41,50,50	1.47	3 (7%)	45,82,82	1.41	6 (13%)
12	CLA	A	304	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	9 (11%)
13	UMQ	H	201	-	35,35,35	1.12	1 (2%)	46,46,46	0.94	3 (6%)
14	PL9	B	402	-	55,55,55	1.08	4 (7%)	68,69,69	1.53	16 (23%)
12	CLA	I	304	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	9 (11%)
13	UMQ	B	404	-	35,35,35	1.14	2 (5%)	46,46,46	1.05	4 (8%)
14	PL9	A	307	-	55,55,55	1.03	4 (7%)	68,69,69	1.54	10 (14%)
16	FES	L	402	4	0,4,4	-	-	-		
11	HEC	I	303	1	32,50,50	2.28	3 (9%)	24,82,82	1.37	2 (8%)
14	PL9	J	401	-	55,55,55	1.03	4 (7%)	68,69,69	1.55	12 (17%)
10	HEM	I	302	1	41,50,50	1.47	3 (7%)	45,82,82	1.33	6 (13%)
10	HEM	I	301	1	41,50,50	1.46	3 (7%)	45,82,82	1.40	6 (13%)
13	UMQ	J	403	-	35,35,35	1.18	3 (8%)	46,46,46	0.92	2 (4%)
14	PL9	K	302	14	55,55,55	1.02	3 (5%)	68,69,69	1.52	10 (14%)
13	UMQ	P	102	-	35,35,35	1.12	1 (2%)	46,46,46	1.09	3 (6%)
15	SQD	L	401	-	53,54,54	0.98	5 (9%)	62,65,65	1.46	8 (12%)
11	HEC	K	301	3	32,50,50	2.26	3 (9%)	24,82,82	1.32	1 (4%)
11	HEC	C	301	3	32,50,50	2.25	3 (9%)	24,82,82	1.32	1 (4%)
13	UMQ	A	305	-	35,35,35	1.15	2 (5%)	46,46,46	0.85	0
14	PL9	B	401	14	55,55,55	1.03	4 (7%)	68,69,69	1.55	13 (19%)
17	BCR	P	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	9 (16%)
13	UMQ	B	403	-	35,35,35	1.23	3 (8%)	46,46,46	1.40	7 (15%)
14	PL9	J	402	-	55,55,55	1.05	4 (7%)	68,69,69	1.53	11 (16%)
10	HEM	A	302	1	41,50,50	1.47	3 (7%)	45,82,82	1.33	6 (13%)
15	SQD	D	201	-	53,54,54	0.97	5 (9%)	62,65,65	1.53	8 (12%)
13	UMQ	J	404	-	35,35,35	1.23	4 (11%)	46,46,46	1.40	7 (15%)
11	HEC	A	303	1	32,50,50	2.27	3 (9%)	24,82,82	1.36	2 (8%)

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	UMQ	I	305	-	-	9/20/60/60	0/2/2/2
16	FES	D	202	4	-	-	0/1/1/1
17	BCR	F	101	-	-	4/29/63/63	0/2/2/2
13	UMQ	A	306	-	-	9/20/60/60	0/2/2/2
13	UMQ	I	306	-	-	12/20/60/60	0/2/2/2
12	CLA	A	304	-	1/1/15/20	16/37/115/115	-
10	HEM	A	301	1	-	3/12/54/54	-
13	UMQ	H	201	-	-	5/20/60/60	0/2/2/2
14	PL9	B	402	-	-	24/53/73/73	0/1/1/1
12	CLA	I	304	-	1/1/15/20	16/37/115/115	-
13	UMQ	B	404	-	-	11/20/60/60	0/2/2/2
14	PL9	A	307	-	-	19/53/73/73	0/1/1/1
16	FES	L	402	4	-	-	0/1/1/1
11	HEC	I	303	1	-	4/10/54/54	-
14	PL9	J	401	-	-	21/53/73/73	0/1/1/1
10	HEM	I	301	1	-	3/12/54/54	-
10	HEM	I	302	1	-	2/12/54/54	-
13	UMQ	J	403	-	-	12/20/60/60	0/2/2/2
14	PL9	K	302	14	-	21/53/73/73	0/1/1/1
13	UMQ	P	102	-	-	8/20/60/60	0/2/2/2
15	SQD	L	401	-	-	20/49/69/69	0/1/1/1
11	HEC	K	301	3	-	2/10/54/54	-
11	HEC	C	301	3	-	2/10/54/54	-
13	UMQ	A	305	-	-	7/20/60/60	0/2/2/2
14	PL9	B	401	14	-	18/53/73/73	0/1/1/1
17	BCR	P	101	-	-	2/29/63/63	0/2/2/2
13	UMQ	B	403	-	-	8/20/60/60	0/2/2/2
14	PL9	J	402	-	-	21/53/73/73	0/1/1/1
10	HEM	A	302	1	-	2/12/54/54	-
15	SQD	D	201	-	-	15/49/69/69	0/1/1/1
13	UMQ	J	404	-	-	8/20/60/60	0/2/2/2
11	HEC	A	303	1	-	4/10/54/54	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	304	CLA	C4B-NB	7.39	1.41	1.35
12	I	304	CLA	C4B-NB	7.34	1.41	1.35
11	I	303	HEC	C2B-C3B	-6.94	1.33	1.40
11	A	303	HEC	C2B-C3B	-6.88	1.33	1.40
11	I	303	HEC	C3C-C2C	-6.76	1.33	1.40
11	K	301	HEC	C2B-C3B	-6.74	1.33	1.40
11	K	301	HEC	C3C-C2C	-6.72	1.33	1.40
11	A	303	HEC	C3C-C2C	-6.71	1.33	1.40
11	C	301	HEC	C3C-C2C	-6.71	1.33	1.40
11	C	301	HEC	C2B-C3B	-6.67	1.33	1.40
11	K	301	HEC	C3D-C2D	5.40	1.53	1.37
11	C	301	HEC	C3D-C2D	5.38	1.53	1.37
11	I	303	HEC	C3D-C2D	5.38	1.53	1.37
11	A	303	HEC	C3D-C2D	5.37	1.53	1.37
10	I	302	HEM	C3C-C2C	-4.38	1.34	1.40
10	A	301	HEM	C3C-C2C	-4.38	1.34	1.40
10	A	302	HEM	C3C-C2C	-4.37	1.34	1.40
10	I	301	HEM	C3C-C2C	-4.35	1.34	1.40
12	A	304	CLA	C1D-ND	3.80	1.42	1.37
12	I	304	CLA	C1D-ND	3.80	1.42	1.37
14	B	401	PL9	C7-C3	-3.67	1.47	1.51
17	F	101	BCR	C1-C6	-3.63	1.48	1.53
14	A	307	PL9	C7-C3	-3.57	1.47	1.51
10	A	302	HEM	C3C-CAC	3.53	1.55	1.47
10	A	301	HEM	C3C-CAC	3.53	1.55	1.47
10	I	301	HEM	C3C-CAC	3.51	1.55	1.47
10	I	302	HEM	C3C-CAC	3.51	1.55	1.47
14	B	402	PL9	C7-C3	-3.51	1.47	1.51
14	J	402	PL9	C7-C3	-3.44	1.47	1.51
17	P	101	BCR	C30-C25	-3.40	1.49	1.53
14	K	302	PL9	C7-C3	-3.39	1.47	1.51
14	J	401	PL9	C7-C3	-3.36	1.47	1.51
17	F	101	BCR	C30-C25	-3.29	1.49	1.53
17	P	101	BCR	C1-C6	-3.26	1.49	1.53
12	A	304	CLA	CHC-C1C	3.12	1.43	1.35
15	D	201	SQD	O48-C23	3.10	1.42	1.33
15	L	401	SQD	O48-C23	3.09	1.42	1.33
12	I	304	CLA	CHC-C1C	3.08	1.42	1.35
12	A	304	CLA	C4D-ND	-3.02	1.33	1.37
12	I	304	CLA	C4D-ND	-2.98	1.33	1.37
15	D	201	SQD	O47-C7	2.82	1.42	1.34
10	I	301	HEM	CAB-C3B	2.82	1.55	1.47
10	A	302	HEM	CAB-C3B	2.82	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	301	HEM	CAB-C3B	2.81	1.55	1.47
15	L	401	SQD	O47-C7	2.80	1.42	1.34
10	I	302	HEM	CAB-C3B	2.80	1.55	1.47
14	B	402	PL9	C3-C4	-2.78	1.45	1.49
14	J	402	PL9	C3-C4	-2.73	1.45	1.49
13	B	403	UMQ	O5'-C5'	2.68	1.50	1.44
13	J	404	UMQ	O5'-C5'	2.68	1.50	1.44
14	K	302	PL9	C3-C4	-2.62	1.45	1.49
13	B	403	UMQ	O5'-C1'	2.57	1.48	1.41
13	J	404	UMQ	O5'-C1'	2.55	1.48	1.41
14	A	307	PL9	C3-C4	-2.50	1.45	1.49
14	J	401	PL9	C3-C4	-2.47	1.45	1.49
14	B	401	PL9	C3-C4	-2.47	1.45	1.49
12	I	304	CLA	CMB-C2B	-2.43	1.46	1.51
12	A	304	CLA	CMB-C2B	-2.42	1.46	1.51
14	J	402	PL9	C6-C1	-2.36	1.44	1.48
13	I	305	UMQ	C3-C4	-2.32	1.46	1.52
13	A	306	UMQ	C3-C4	-2.30	1.46	1.52
15	D	201	SQD	O2-C2	-2.29	1.37	1.43
15	L	401	SQD	O2-C2	-2.28	1.37	1.43
13	A	305	UMQ	C3-C4	-2.24	1.46	1.52
14	J	401	PL9	C53-C6	-2.22	1.46	1.50
13	J	403	UMQ	C3-C4	-2.16	1.46	1.52
15	L	401	SQD	O4-C4	-2.14	1.37	1.43
15	D	201	SQD	O3-C3	-2.14	1.37	1.43
13	J	403	UMQ	O5'-C1'	2.14	1.47	1.41
14	B	402	PL9	C6-C1	-2.13	1.44	1.48
13	H	201	UMQ	C3-C4	-2.13	1.46	1.52
15	L	401	SQD	O3-C3	-2.12	1.38	1.43
13	I	306	UMQ	C3-C4	-2.12	1.46	1.52
14	A	307	PL9	C6-C1	-2.12	1.44	1.48
13	B	404	UMQ	O5'-C5'	2.10	1.49	1.44
13	J	404	UMQ	C3'-C4'	-2.10	1.46	1.52
14	J	402	PL9	C53-C6	-2.09	1.46	1.50
13	B	403	UMQ	C3'-C4'	-2.09	1.46	1.52
15	D	201	SQD	O4-C4	-2.09	1.38	1.43
14	K	302	PL9	C53-C6	-2.08	1.46	1.50
13	P	102	UMQ	C3-C4	-2.07	1.47	1.52
14	A	307	PL9	C53-C6	-2.07	1.46	1.50
14	J	401	PL9	C6-C1	-2.06	1.44	1.48
13	J	403	UMQ	O5'-C5'	2.05	1.49	1.44
14	B	401	PL9	C53-C6	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	304	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	402	PL9	C53-C6	-2.02	1.46	1.50
14	B	401	PL9	C6-C1	-2.02	1.45	1.48
13	B	404	UMQ	C3-C2	-2.02	1.47	1.52
13	A	305	UMQ	O5'-C5'	2.01	1.49	1.44
12	I	304	CLA	CMD-C2D	-2.01	1.46	1.50
13	J	404	UMQ	O5-C1	2.01	1.47	1.41

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	304	CLA	C4A-NA-C1A	6.36	109.56	106.71
12	I	304	CLA	C4A-NA-C1A	6.30	109.54	106.71
14	J	401	PL9	C7-C3-C4	5.60	121.43	116.88
14	A	307	PL9	C7-C3-C4	5.55	121.39	116.88
14	B	401	PL9	C7-C3-C4	5.39	121.25	116.88
14	K	302	PL9	C7-C3-C4	5.31	121.19	116.88
14	J	402	PL9	C7-C3-C4	5.27	121.16	116.88
14	B	402	PL9	C7-C3-C4	5.02	120.96	116.88
15	D	201	SQD	O6-C1-C2	4.24	114.92	108.30
13	P	102	UMQ	CA-O1'-C1'	-4.12	107.01	113.84
15	D	201	SQD	O9-S-C6	4.08	111.78	106.94
15	L	401	SQD	O9-S-C6	4.05	111.75	106.94
15	L	401	SQD	O7-S-C6	3.80	111.45	106.94
15	D	201	SQD	O7-S-C6	3.79	111.45	106.94
15	D	201	SQD	O47-C7-C8	3.75	119.59	111.50
14	J	401	PL9	C7-C3-C2	-3.74	118.38	123.30
14	A	307	PL9	C7-C3-C2	-3.72	118.41	123.30
15	L	401	SQD	O9-S-O7	-3.71	101.09	113.95
15	D	201	SQD	O9-S-O7	-3.70	101.16	113.95
14	B	401	PL9	C7-C3-C2	-3.64	118.51	123.30
14	K	302	PL9	C7-C3-C2	-3.54	118.64	123.30
13	J	404	UMQ	O1-C1-C2	3.49	117.14	108.10
13	B	403	UMQ	O1-C1-C2	3.48	117.12	108.10
14	J	402	PL9	C7-C3-C2	-3.47	118.73	123.30
12	A	304	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
12	I	304	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
15	L	401	SQD	O6-C1-C2	3.36	113.55	108.30
14	B	402	PL9	C7-C3-C2	-3.35	118.89	123.30
15	L	401	SQD	O47-C7-C8	3.27	118.54	111.50
13	J	403	UMQ	O1-C4'-C5'	3.17	118.13	109.45
13	J	404	UMQ	C1'-O5'-C5'	3.13	119.83	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	403	UMQ	C1'-O5'-C5'	3.12	119.81	113.69
14	A	307	PL9	C40-C39-C41	3.05	120.40	115.27
14	K	302	PL9	C40-C39-C41	2.99	120.31	115.27
13	B	403	UMQ	O5-C1-C2	2.96	116.61	110.35
13	I	305	UMQ	C1-O1-C4'	-2.95	110.66	117.96
12	A	304	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	J	404	UMQ	O5-C1-C2	2.94	116.58	110.35
12	I	304	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	A	306	UMQ	C1-O1-C4'	-2.92	110.74	117.96
13	B	403	UMQ	C1-C2-C3	2.90	116.04	110.00
13	J	404	UMQ	C1-C2-C3	2.90	116.03	110.00
15	L	401	SQD	O8-S-C6	2.89	110.34	105.74
10	I	302	HEM	C4D-ND-C1D	2.87	108.04	105.07
15	D	201	SQD	O8-S-C6	2.86	110.30	105.74
12	A	304	CLA	CMB-C2B-C3B	2.86	130.04	124.68
14	J	402	PL9	C40-C39-C41	2.86	120.08	115.27
10	A	301	HEM	C4D-ND-C1D	2.86	108.02	105.07
12	I	304	CLA	CMB-C2B-C3B	2.85	130.01	124.68
13	H	201	UMQ	CA-O1'-C1'	-2.83	109.14	113.84
10	A	302	HEM	C4D-ND-C1D	2.82	107.99	105.07
10	I	301	HEM	C4D-ND-C1D	2.81	107.97	105.07
10	A	301	HEM	C1B-NB-C4B	2.79	107.95	105.07
10	I	301	HEM	C4B-CHC-C1C	2.78	126.22	122.56
10	I	301	HEM	C1B-NB-C4B	2.78	107.94	105.07
15	D	201	SQD	O5-C5-C4	2.77	114.72	109.69
14	B	401	PL9	C7-C8-C9	-2.75	122.21	126.79
10	A	301	HEM	C4B-CHC-C1C	2.73	126.17	122.56
14	B	402	PL9	C27-C28-C29	-2.73	121.09	127.66
17	F	101	BCR	C33-C5-C6	-2.72	121.48	124.53
10	A	302	HEM	C1B-NB-C4B	2.72	107.88	105.07
10	I	302	HEM	C1B-NB-C4B	2.71	107.88	105.07
14	B	402	PL9	C22-C23-C24	-2.70	121.15	127.66
13	B	403	UMQ	C4-C3-C2	2.69	115.51	110.82
13	J	404	UMQ	C4-C3-C2	2.68	115.50	110.82
14	J	402	PL9	C22-C23-C24	-2.67	121.22	127.66
14	J	402	PL9	C27-C28-C29	-2.66	121.25	127.66
13	P	102	UMQ	O1'-C1'-C2'	2.66	112.46	108.30
17	P	101	BCR	C15-C16-C17	-2.66	118.02	123.47
15	L	401	SQD	O5-C5-C4	2.66	114.53	109.69
14	J	401	PL9	C27-C28-C29	-2.64	121.30	127.66
14	J	401	PL9	C40-C39-C41	2.64	119.71	115.27
13	P	102	UMQ	C1'-O5'-C5'	-2.63	108.53	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	101	BCR	C15-C16-C17	-2.62	118.11	123.47
14	B	401	PL9	C22-C23-C24	-2.61	121.37	127.66
14	K	302	PL9	C7-C8-C9	-2.60	122.46	126.79
13	B	404	UMQ	C1-O1-C4'	-2.59	111.54	117.96
17	P	101	BCR	C2-C1-C6	2.59	114.47	110.48
14	K	302	PL9	C22-C23-C24	-2.53	121.56	127.66
17	P	101	BCR	C27-C26-C25	2.52	126.39	122.73
14	J	402	PL9	C20-C19-C21	2.52	119.50	115.27
14	B	401	PL9	C27-C28-C29	-2.52	121.60	127.66
14	J	402	PL9	C7-C8-C9	-2.51	122.62	126.79
14	B	402	PL9	C7-C8-C9	-2.50	122.62	126.79
17	F	101	BCR	C27-C26-C25	2.50	126.36	122.73
14	A	307	PL9	C7-C8-C9	-2.49	122.65	126.79
14	J	401	PL9	C20-C19-C21	2.47	119.43	115.27
10	A	301	HEM	C4C-CHD-C1D	2.46	125.81	122.56
14	J	401	PL9	C7-C8-C9	-2.45	122.71	126.79
10	I	301	HEM	C4C-CHD-C1D	2.42	125.75	122.56
14	K	302	PL9	C27-C28-C29	-2.41	121.85	127.66
10	A	302	HEM	C4B-CHC-C1C	2.41	125.74	122.56
14	A	307	PL9	C27-C28-C29	-2.41	121.86	127.66
14	A	307	PL9	C22-C23-C24	-2.40	121.88	127.66
14	J	401	PL9	C22-C23-C24	-2.39	121.90	127.66
10	I	302	HEM	C4B-CHC-C1C	2.39	125.71	122.56
17	P	101	BCR	C33-C5-C6	-2.37	121.87	124.53
13	A	306	UMQ	CA-O1'-C1'	-2.35	109.94	113.84
13	I	305	UMQ	CA-O1'-C1'	-2.35	109.94	113.84
15	D	201	SQD	O48-C23-C24	2.35	119.28	111.91
14	B	401	PL9	C40-C39-C41	2.34	119.20	115.27
12	I	304	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
12	A	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
13	H	201	UMQ	O1'-C1'-C2'	2.31	111.91	108.30
13	J	404	UMQ	C3-C4-C5	2.31	114.36	110.24
14	B	401	PL9	C20-C19-C21	2.31	119.16	115.27
12	I	304	CLA	CHB-C4A-NA	2.31	127.70	124.51
12	A	304	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	P	101	BCR	C15-C14-C13	-2.30	124.03	127.31
11	I	303	HEC	C1D-C2D-C3D	-2.29	105.40	107.00
17	F	101	BCR	C15-C14-C13	-2.29	124.05	127.31
13	B	403	UMQ	C3-C4-C5	2.28	114.30	110.24
11	A	303	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
17	P	101	BCR	C7-C8-C9	-2.27	122.81	126.23
17	F	101	BCR	C38-C26-C25	-2.25	122.00	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	101	BCR	C3-C4-C5	-2.24	110.07	114.08
14	B	402	PL9	C32-C33-C34	-2.24	122.27	127.66
17	P	101	BCR	C24-C23-C22	-2.21	122.89	126.23
13	B	404	UMQ	O5'-C5'-C4'	2.20	114.40	109.75
10	A	301	HEM	C3B-C2B-C1B	2.20	108.12	106.49
11	K	301	HEC	C1D-C2D-C3D	-2.20	105.47	107.00
14	B	402	PL9	C40-C39-C41	2.20	118.97	115.27
11	C	301	HEC	C1D-C2D-C3D	-2.19	105.47	107.00
14	B	402	PL9	C37-C38-C39	-2.19	122.39	127.66
14	B	402	PL9	C36-C34-C33	-2.19	116.69	121.12
17	F	101	BCR	C7-C8-C9	-2.17	122.95	126.23
13	B	404	UMQ	C3'-C4'-C5'	2.17	115.91	110.93
10	A	302	HEM	C4C-CHD-C1D	2.17	125.42	122.56
14	B	402	PL9	C20-C19-C21	2.17	118.92	115.27
17	P	101	BCR	C38-C26-C25	-2.17	122.09	124.53
14	B	402	PL9	O1-C4-C3	-2.17	118.33	120.72
14	K	302	PL9	C37-C38-C39	-2.16	122.45	127.66
15	L	401	SQD	O48-C23-C24	2.16	118.69	111.91
14	B	401	PL9	C37-C38-C39	-2.16	122.46	127.66
14	B	402	PL9	C31-C32-C33	-2.15	104.81	111.88
10	I	302	HEM	C4C-CHD-C1D	2.15	125.40	122.56
14	A	307	PL9	C37-C38-C39	-2.15	122.48	127.66
10	I	301	HEM	C3B-C2B-C1B	2.14	108.07	106.49
14	K	302	PL9	O2-C1-C6	2.13	124.28	120.59
13	B	403	UMQ	O5'-C5'-C4'	2.13	114.24	109.75
13	J	404	UMQ	O5'-C5'-C4'	2.13	114.24	109.75
14	B	401	PL9	O2-C1-C6	2.12	124.27	120.59
14	K	302	PL9	O1-C4-C3	-2.12	118.39	120.72
12	A	304	CLA	C1-C2-C3	-2.12	122.38	126.04
12	I	304	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
14	A	307	PL9	O2-C1-C2	-2.11	116.94	121.78
14	B	401	PL9	O2-C1-C2	-2.11	116.94	121.78
10	I	302	HEM	C3D-C4D-ND	-2.11	107.82	110.17
14	J	402	PL9	O1-C4-C3	-2.11	118.40	120.72
14	J	402	PL9	C32-C33-C34	-2.11	122.59	127.66
12	A	304	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
14	J	401	PL9	O2-C1-C6	2.11	124.24	120.59
14	A	307	PL9	O2-C1-C6	2.10	124.23	120.59
12	I	304	CLA	C1-C2-C3	-2.09	122.42	126.04
14	B	402	PL9	O2-C1-C6	2.09	124.21	120.59
17	F	101	BCR	C24-C23-C22	-2.09	123.08	126.23
14	J	401	PL9	C12-C13-C14	-2.09	122.63	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	302	PL9	O2-C1-C2	-2.09	117.00	121.78
14	B	401	PL9	C31-C32-C33	-2.08	105.06	111.88
13	J	403	UMQ	O5'-C1'-C2'	2.07	114.74	110.35
14	B	402	PL9	C41-C39-C38	-2.07	116.93	121.12
14	B	401	PL9	O1-C4-C3	-2.07	118.44	120.72
13	B	404	UMQ	O5-C5-C4	2.07	113.45	109.69
10	A	302	HEM	C3D-C4D-ND	-2.07	107.87	110.17
13	I	305	UMQ	O1'-C1'-C2'	2.06	111.53	108.30
10	I	302	HEM	C3B-C2B-C1B	2.06	108.02	106.49
13	A	306	UMQ	O1'-C1'-C2'	2.06	111.52	108.30
10	A	301	HEM	CBA-CAA-C2A	-2.06	109.11	112.62
14	B	402	PL9	O2-C1-C2	-2.06	117.06	121.78
14	B	401	PL9	C36-C34-C33	-2.05	116.96	121.12
14	J	401	PL9	O2-C1-C2	-2.05	117.08	121.78
13	H	201	UMQ	C1'-O5'-C5'	-2.05	109.66	113.69
12	I	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
10	I	301	HEM	CBA-CAA-C2A	-2.04	109.14	112.62
14	A	307	PL9	C50-C49-C48	-2.04	116.75	122.65
13	I	306	UMQ	C2'-C3'-C4'	2.03	114.33	109.68
12	A	304	CLA	CHD-C1D-ND	-2.03	122.58	124.45
11	A	303	HEC	CBD-CAD-C3D	-2.03	109.16	112.62
14	J	402	PL9	O2-C1-C6	2.03	124.11	120.59
14	B	402	PL9	C42-C43-C44	-2.03	122.78	127.66
14	J	401	PL9	C37-C38-C39	-2.02	122.79	127.66
11	I	303	HEC	CBD-CAD-C3D	-2.02	109.17	112.62
14	J	401	PL9	C31-C32-C33	-2.02	105.25	111.88
14	J	402	PL9	O2-C1-C2	-2.02	117.16	121.78
10	A	302	HEM	C3B-C2B-C1B	2.01	107.98	106.49

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	304	CLA	ND
12	I	304	CLA	ND

All (308) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	302	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	C3A-C2A-CAA-CBA
10	I	302	HEM	C1A-C2A-CAA-CBA
10	I	302	HEM	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	303	HEC	C1A-C2A-CAA-CBA
11	A	303	HEC	C3A-C2A-CAA-CBA
11	I	303	HEC	C1A-C2A-CAA-CBA
11	I	303	HEC	C3A-C2A-CAA-CBA
12	A	304	CLA	C1A-C2A-CAA-CBA
12	A	304	CLA	C3A-C2A-CAA-CBA
12	I	304	CLA	C1A-C2A-CAA-CBA
12	I	304	CLA	C3A-C2A-CAA-CBA
13	B	403	UMQ	O5'-C1'-O1'-CA
13	J	404	UMQ	O5'-C1'-O1'-CA
14	A	307	PL9	C12-C13-C14-C16
14	A	307	PL9	C13-C14-C16-C17
14	A	307	PL9	C14-C16-C17-C18
14	A	307	PL9	C27-C28-C29-C30
14	A	307	PL9	C27-C28-C29-C31
14	A	307	PL9	C30-C29-C31-C32
14	A	307	PL9	C47-C48-C49-C50
14	A	307	PL9	C47-C48-C49-C51
14	B	401	PL9	C22-C23-C24-C26
14	B	401	PL9	C34-C36-C37-C38
14	B	401	PL9	C37-C38-C39-C41
14	B	401	PL9	C40-C39-C41-C42
14	B	401	PL9	C43-C44-C46-C47
14	B	401	PL9	C45-C44-C46-C47
14	B	402	PL9	C7-C8-C9-C11
14	B	402	PL9	C19-C21-C22-C23
14	B	402	PL9	C25-C24-C26-C27
14	B	402	PL9	C29-C31-C32-C33
14	B	402	PL9	C35-C34-C36-C37
14	B	402	PL9	C37-C38-C39-C41
14	B	402	PL9	C42-C43-C44-C46
14	B	402	PL9	C45-C44-C46-C47
14	J	401	PL9	C4-C3-C7-C8
14	J	401	PL9	C15-C14-C16-C17
14	J	401	PL9	C14-C16-C17-C18
14	J	401	PL9	C22-C23-C24-C25
14	J	401	PL9	C22-C23-C24-C26
14	J	401	PL9	C24-C26-C27-C28
14	J	402	PL9	C9-C11-C12-C13
14	J	402	PL9	C22-C23-C24-C26
14	J	402	PL9	C27-C28-C29-C31
14	J	402	PL9	C33-C34-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	J	402	PL9	C38-C39-C41-C42
14	K	302	PL9	C12-C11-C9-C10
14	K	302	PL9	C32-C33-C34-C35
14	K	302	PL9	C32-C33-C34-C36
14	K	302	PL9	C42-C43-C44-C45
14	K	302	PL9	C42-C43-C44-C46
14	K	302	PL9	C44-C46-C47-C48
15	D	201	SQD	O6-C44-C45-O47
15	L	401	SQD	O49-C7-O47-C45
15	L	401	SQD	C8-C7-O47-C45
13	J	403	UMQ	C5'-C4'-O1-C1
13	B	403	UMQ	C2-C1-O1-C4'
13	J	404	UMQ	C2-C1-O1-C4'
13	B	403	UMQ	O5-C1-O1-C4'
13	J	404	UMQ	O5-C1-O1-C4'
12	A	304	CLA	O1A-CGA-O2A-C1
12	I	304	CLA	O1A-CGA-O2A-C1
12	A	304	CLA	CBA-CGA-O2A-C1
12	I	304	CLA	CBA-CGA-O2A-C1
14	J	401	PL9	C40-C39-C41-C42
14	J	401	PL9	C28-C29-C31-C32
14	J	401	PL9	C38-C39-C41-C42
14	B	402	PL9	C42-C43-C44-C45
14	K	302	PL9	C27-C28-C29-C30
14	B	402	PL9	C12-C13-C14-C16
14	K	302	PL9	C27-C28-C29-C31
13	J	403	UMQ	O5-C5-C6-O6
13	J	403	UMQ	C4-C5-C6-O6
13	A	306	UMQ	O5-C5-C6-O6
13	I	305	UMQ	O5-C5-C6-O6
15	D	201	SQD	C10-C11-C12-C13
14	J	401	PL9	C47-C48-C49-C51
14	A	307	PL9	C15-C14-C16-C17
14	J	401	PL9	C30-C29-C31-C32
14	J	402	PL9	C20-C19-C21-C22
14	J	402	PL9	C35-C34-C36-C37
14	K	302	PL9	C40-C39-C41-C42
14	J	402	PL9	C18-C19-C21-C22
14	K	302	PL9	C12-C11-C9-C8
14	K	302	PL9	C38-C39-C41-C42
13	J	403	UMQ	O5'-C5'-C6'-O6'
13	A	306	UMQ	O5'-C1'-O1'-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	I	305	UMQ	O5'-C1'-O1'-CA
14	A	307	PL9	C34-C36-C37-C38
14	B	401	PL9	C24-C26-C27-C28
14	B	402	PL9	C24-C26-C27-C28
14	J	401	PL9	C39-C41-C42-C43
14	J	402	PL9	C24-C26-C27-C28
14	A	307	PL9	C12-C13-C14-C15
14	J	401	PL9	C27-C28-C29-C30
14	B	402	PL9	C17-C18-C19-C21
14	J	401	PL9	C7-C8-C9-C11
14	J	401	PL9	C2-C3-C7-C8
13	J	403	UMQ	C4'-C5'-C6'-O6'
12	A	304	CLA	C13-C15-C16-C17
12	I	304	CLA	C13-C15-C16-C17
15	D	201	SQD	O47-C45-C46-O48
15	D	201	SQD	O10-C23-O48-C46
14	B	402	PL9	C43-C44-C46-C47
15	D	201	SQD	C11-C10-C9-C8
15	D	201	SQD	C24-C23-O48-C46
10	A	301	HEM	C2A-CAA-CBA-CGA
10	I	301	HEM	C2A-CAA-CBA-CGA
11	A	303	HEC	C3D-CAD-CBD-CGD
11	I	303	HEC	C3D-CAD-CBD-CGD
15	D	201	SQD	C23-C24-C25-C26
13	A	306	UMQ	C4-C5-C6-O6
13	I	305	UMQ	C4-C5-C6-O6
13	I	306	UMQ	O1'-CA-CB-CC
14	A	307	PL9	C44-C46-C47-C48
14	B	401	PL9	C29-C31-C32-C33
14	J	401	PL9	C9-C11-C12-C13
14	J	401	PL9	C34-C36-C37-C38
14	J	402	PL9	C44-C46-C47-C48
14	K	302	PL9	C39-C41-C42-C43
14	K	302	PL9	C20-C19-C21-C22
13	B	403	UMQ	CB-CC-CD-CF
13	I	306	UMQ	CC-CD-CF-CG
13	I	306	UMQ	CD-CF-CG-CH
13	J	404	UMQ	CB-CC-CD-CF
13	P	102	UMQ	CB-CC-CD-CF
13	B	404	UMQ	CH-CI-CJ-CK
15	L	401	SQD	C28-C29-C30-C31
13	B	403	UMQ	C2'-C1'-O1'-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	J	404	UMQ	C2'-C1'-O1'-CA
14	B	401	PL9	C37-C38-C39-C40
13	A	306	UMQ	CC-CD-CF-CG
13	I	305	UMQ	CC-CD-CF-CG
15	D	201	SQD	C24-C25-C26-C27
15	L	401	SQD	C31-C32-C33-C34
15	L	401	SQD	C27-C28-C29-C30
13	B	403	UMQ	CB-CA-O1'-C1'
13	J	404	UMQ	CB-CA-O1'-C1'
12	A	304	CLA	C15-C16-C17-C18
12	I	304	CLA	C15-C16-C17-C18
13	P	102	UMQ	CC-CD-CF-CG
14	K	302	PL9	C12-C13-C14-C16
13	I	306	UMQ	CH-CI-CJ-CK
13	B	403	UMQ	CC-CD-CF-CG
17	F	101	BCR	C23-C24-C25-C26
17	F	101	BCR	C23-C24-C25-C30
13	J	404	UMQ	CC-CD-CF-CG
14	K	302	PL9	C47-C48-C49-C50
14	K	302	PL9	C15-C14-C16-C17
15	L	401	SQD	C10-C11-C12-C13
13	I	306	UMQ	O5-C5-C6-O6
13	B	404	UMQ	CD-CF-CG-CH
14	B	402	PL9	C34-C36-C37-C38
13	H	201	UMQ	CF-CG-CH-CI
14	J	402	PL9	C47-C48-C49-C51
13	J	403	UMQ	CH-CI-CJ-CK
12	A	304	CLA	C4-C3-C5-C6
12	I	304	CLA	C4-C3-C5-C6
14	A	307	PL9	C28-C29-C31-C32
14	B	402	PL9	C4-C3-C7-C8
14	J	402	PL9	C4-C3-C7-C8
13	A	305	UMQ	O5-C5-C6-O6
12	A	304	CLA	C2A-CAA-CBA-CGA
12	I	304	CLA	C2A-CAA-CBA-CGA
13	B	404	UMQ	O5'-C5'-C6'-O6'
14	B	402	PL9	C7-C8-C9-C10
14	B	402	PL9	C12-C13-C14-C15
13	H	201	UMQ	CA-CB-CC-CD
15	D	201	SQD	C11-C12-C13-C14
14	B	401	PL9	C42-C43-C44-C46
13	P	102	UMQ	CA-CB-CC-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	I	306	UMQ	CF-CG-CH-CI
13	I	306	UMQ	O5'-C5'-C6'-O6'
14	A	307	PL9	C24-C26-C27-C28
14	K	302	PL9	C29-C31-C32-C33
15	L	401	SQD	C24-C25-C26-C27
13	A	305	UMQ	O1'-CA-CB-CC
13	B	403	UMQ	O5'-C5'-C6'-O6'
13	J	404	UMQ	O5'-C5'-C6'-O6'
13	I	306	UMQ	C2-C1-O1-C4'
12	A	304	CLA	C2-C1-O2A-CGA
12	I	304	CLA	C2-C1-O2A-CGA
13	P	102	UMQ	C4-C5-C6-O6
13	I	306	UMQ	O5-C1-O1-C4'
13	A	305	UMQ	CF-CG-CH-CI
15	D	201	SQD	C12-C13-C14-C15
13	P	102	UMQ	CG-CH-CI-CJ
13	A	306	UMQ	CH-CI-CJ-CK
13	I	305	UMQ	CH-CI-CJ-CK
13	H	201	UMQ	CH-CI-CJ-CK
13	A	306	UMQ	CB-CC-CD-CF
13	I	305	UMQ	CB-CC-CD-CF
14	J	402	PL9	C25-C24-C26-C27
12	A	304	CLA	C2-C3-C5-C6
12	I	304	CLA	C2-C3-C5-C6
15	L	401	SQD	C29-C30-C31-C32
13	A	305	UMQ	CB-CA-O1'-C1'
13	I	306	UMQ	CB-CA-O1'-C1'
13	A	306	UMQ	CG-CH-CI-CJ
13	I	305	UMQ	CG-CH-CI-CJ
15	D	201	SQD	O6-C44-C45-C46
15	D	201	SQD	C44-C45-C46-O48
15	L	401	SQD	C44-C45-C46-O48
14	J	402	PL9	C42-C43-C44-C45
13	I	306	UMQ	CB-CC-CD-CF
15	D	201	SQD	C13-C14-C15-C16
14	A	307	PL9	C9-C11-C12-C13
13	J	403	UMQ	CD-CF-CG-CH
15	L	401	SQD	C19-C20-C21-C22
14	B	401	PL9	C47-C48-C49-C50
12	A	304	CLA	C11-C12-C13-C15
12	I	304	CLA	C11-C12-C13-C15
13	J	403	UMQ	O1'-CA-CB-CC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	402	PL9	C32-C33-C34-C36
13	A	305	UMQ	CH-CI-CJ-CK
14	J	402	PL9	C12-C13-C14-C15
15	L	401	SQD	O47-C45-C46-O48
13	B	404	UMQ	CF-CG-CH-CI
14	A	307	PL9	C43-C44-C46-C47
13	H	201	UMQ	C4-C5-C6-O6
13	A	305	UMQ	CB-CC-CD-CF
13	I	306	UMQ	CG-CH-CI-CJ
13	P	102	UMQ	CD-CF-CG-CH
13	J	403	UMQ	CC-CD-CF-CG
13	P	102	UMQ	O5-C5-C6-O6
13	B	404	UMQ	C3'-C4'-O1-C1
12	A	304	CLA	C11-C12-C13-C14
12	I	304	CLA	C11-C12-C13-C14
14	A	307	PL9	C25-C24-C26-C27
15	L	401	SQD	C14-C15-C16-C17
14	J	402	PL9	C7-C8-C9-C11
14	J	401	PL9	C13-C14-C16-C17
15	D	201	SQD	C33-C34-C35-C36
14	K	302	PL9	C24-C26-C27-C28
15	L	401	SQD	C2-C1-O6-C44
14	J	401	PL9	C37-C38-C39-C41
14	K	302	PL9	C7-C8-C9-C11
12	A	304	CLA	C11-C10-C8-C9
12	I	304	CLA	C11-C10-C8-C9
14	J	401	PL9	C43-C44-C46-C47
14	B	401	PL9	C47-C48-C49-C51
14	J	402	PL9	C19-C21-C22-C23
14	J	402	PL9	C34-C36-C37-C38
14	B	402	PL9	C15-C14-C16-C17
14	J	402	PL9	C12-C11-C9-C10
15	L	401	SQD	C18-C19-C20-C21
13	I	305	UMQ	CD-CF-CG-CH
13	A	306	UMQ	CD-CF-CG-CH
13	J	403	UMQ	CG-CH-CI-CJ
17	F	101	BCR	C11-C10-C9-C34
17	P	101	BCR	C11-C10-C9-C34
14	B	401	PL9	C12-C13-C14-C15
14	J	402	PL9	C2-C3-C7-C8
13	A	305	UMQ	CC-CD-CF-CG
14	B	401	PL9	C15-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	K	302	PL9	C25-C24-C26-C27
14	B	402	PL9	C12-C11-C9-C10
13	P	102	UMQ	CF-CG-CH-CI
17	F	101	BCR	C11-C10-C9-C8
17	P	101	BCR	C11-C10-C9-C8
13	B	404	UMQ	O5-C1-O1-C4'
13	I	305	UMQ	CI-CJ-CK-CL
13	A	306	UMQ	CI-CJ-CK-CL
14	B	402	PL9	C27-C28-C29-C30
13	B	404	UMQ	C5'-C4'-O1-C1
14	B	402	PL9	C40-C39-C41-C42
14	B	402	PL9	C23-C24-C26-C27
15	L	401	SQD	C33-C34-C35-C36
13	B	404	UMQ	C2-C1-O1-C4'
14	B	401	PL9	C30-C29-C31-C32
14	J	402	PL9	C40-C39-C41-C42
11	C	301	HEC	CAA-CBA-CGA-O2A
13	H	201	UMQ	O5-C5-C6-O6
11	K	301	HEC	CAA-CBA-CGA-O2A
15	L	401	SQD	C11-C12-C13-C14
14	B	401	PL9	C20-C19-C21-C22
12	A	304	CLA	CAA-CBA-CGA-O2A
12	I	304	CLA	CAA-CBA-CGA-O2A
14	B	401	PL9	C39-C41-C42-C43
15	L	401	SQD	C34-C35-C36-C37
15	L	401	SQD	O6-C44-C45-O47
14	A	307	PL9	C4-C3-C7-C8
15	D	201	SQD	C9-C10-C11-C12
14	B	401	PL9	C13-C14-C16-C17
13	J	403	UMQ	CA-CB-CC-CD
12	A	304	CLA	CAA-CBA-CGA-O1A
12	I	304	CLA	CAA-CBA-CGA-O1A
11	C	301	HEC	CAA-CBA-CGA-O1A
11	K	301	HEC	CAA-CBA-CGA-O1A
15	L	401	SQD	C11-C10-C9-C8
13	B	404	UMQ	CG-CH-CI-CJ
10	A	301	HEM	CAD-CBD-CGD-O2D
10	I	301	HEM	CAD-CBD-CGD-O2D
13	B	404	UMQ	O5-C5-C6-O6
12	A	304	CLA	CAD-CBD-CGD-O1D
12	I	304	CLA	CAD-CBD-CGD-O1D
10	I	301	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	301	HEM	CAD-CBD-CGD-O1D
11	A	303	HEC	C2A-CAA-CBA-CGA
11	I	303	HEC	C2A-CAA-CBA-CGA
14	B	402	PL9	C28-C29-C31-C32
13	B	404	UMQ	CB-CC-CD-CF
15	L	401	SQD	C32-C33-C34-C35
13	J	403	UMQ	CB-CA-O1'-C1'
14	K	302	PL9	C9-C11-C12-C13
14	A	307	PL9	C21-C22-C23-C24
14	J	401	PL9	C41-C42-C43-C44

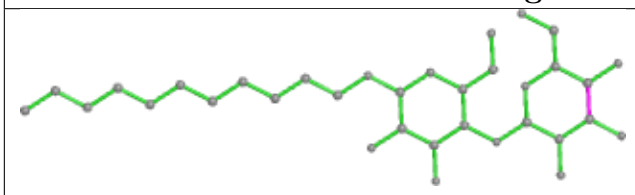
There are no ring outliers.

27 monomers are involved in 122 short contacts:

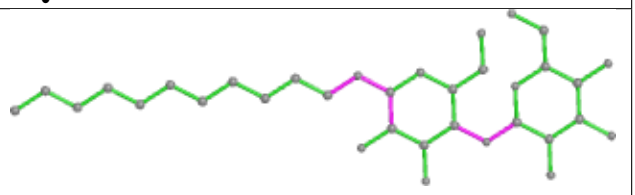
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	305	UMQ	1	0
17	F	101	BCR	2	0
13	I	306	UMQ	1	0
10	A	301	HEM	4	0
12	A	304	CLA	4	0
13	H	201	UMQ	1	0
14	B	402	PL9	17	0
12	I	304	CLA	5	0
13	B	404	UMQ	1	0
14	A	307	PL9	10	0
11	I	303	HEC	2	0
14	J	401	PL9	14	0
10	I	302	HEM	6	0
10	I	301	HEM	4	0
13	J	403	UMQ	1	0
14	K	302	PL9	4	0
13	P	102	UMQ	1	0
15	L	401	SQD	1	0
11	K	301	HEC	5	0
11	C	301	HEC	6	0
14	B	401	PL9	10	0
17	P	101	BCR	5	0
13	B	403	UMQ	2	0
14	J	402	PL9	14	0
10	A	302	HEM	5	0
15	D	201	SQD	5	0
11	A	303	HEC	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.

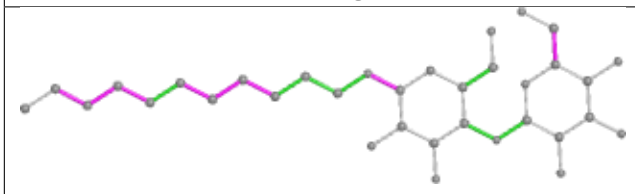
Ligand UMQ I 305



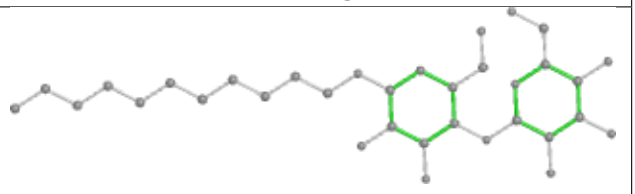
Bond lengths



Bond angles

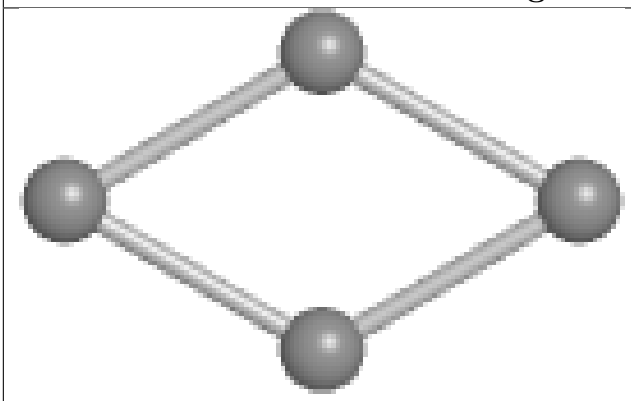


Torsions

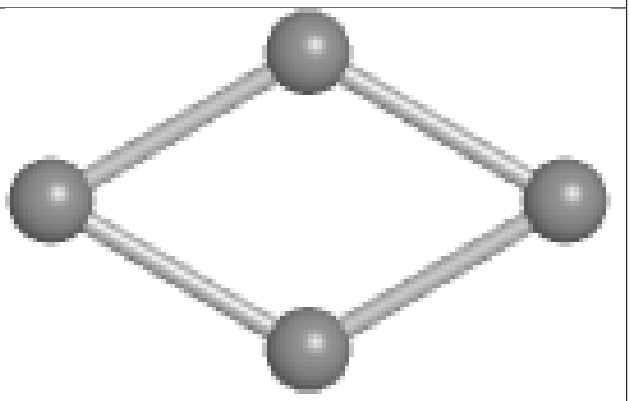


Rings

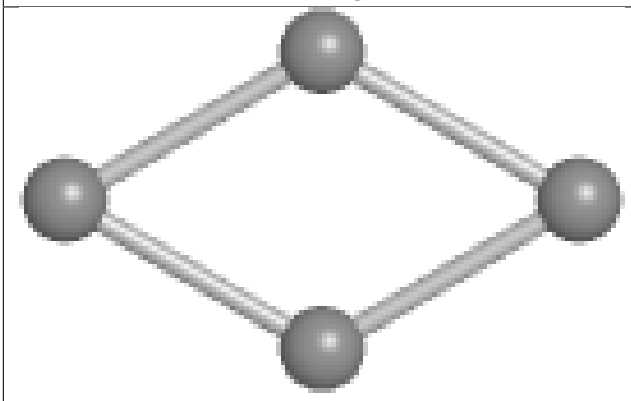
Ligand FES D 202



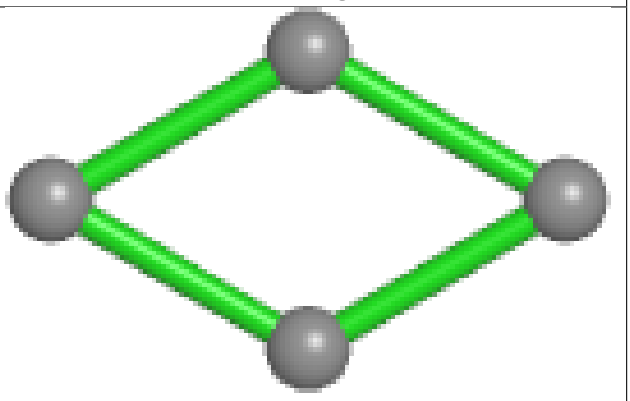
Bond lengths



Bond angles

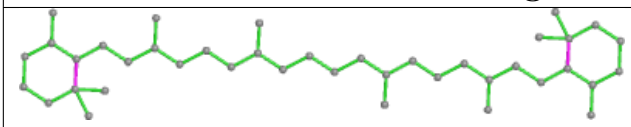


Torsions

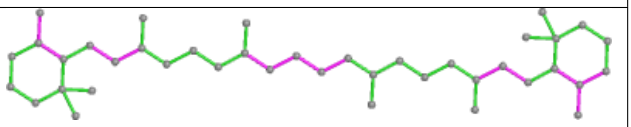


Rings

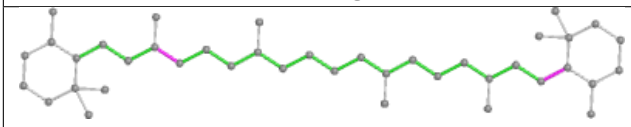
Ligand BCR F 101



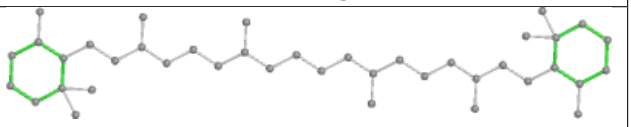
Bond lengths



Bond angles

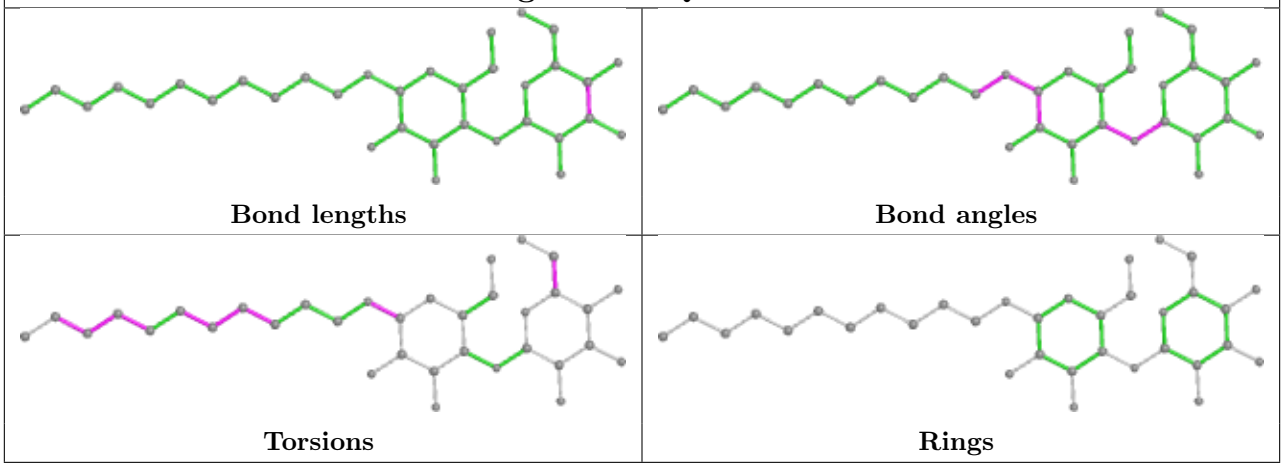


Torsions

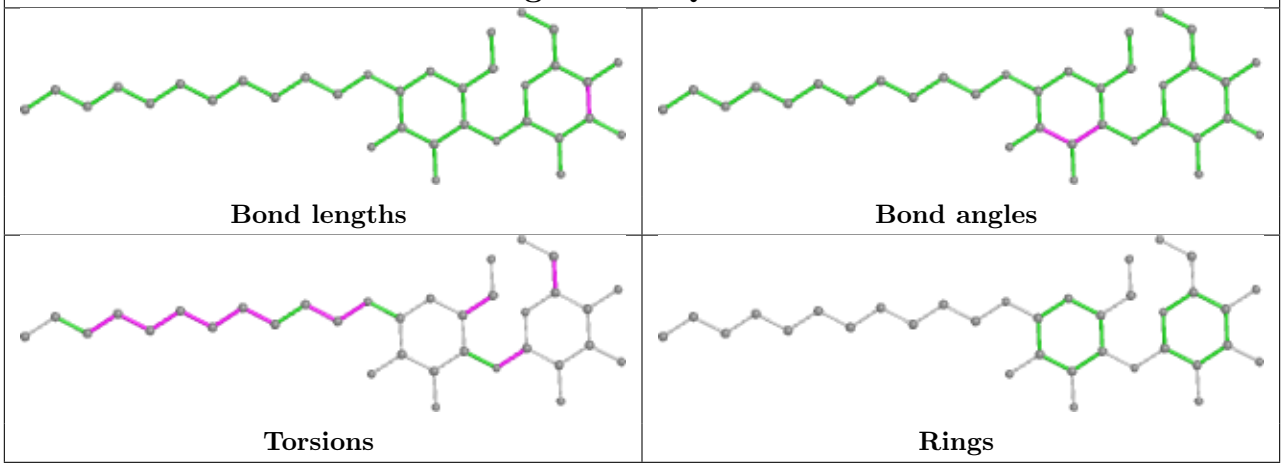


Rings

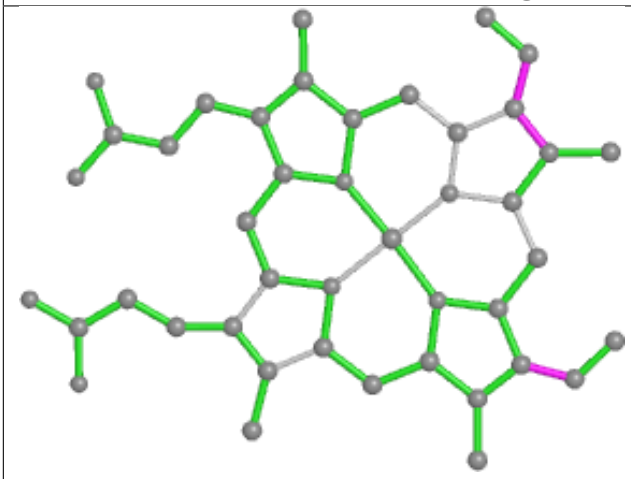
Ligand UMQ A 306



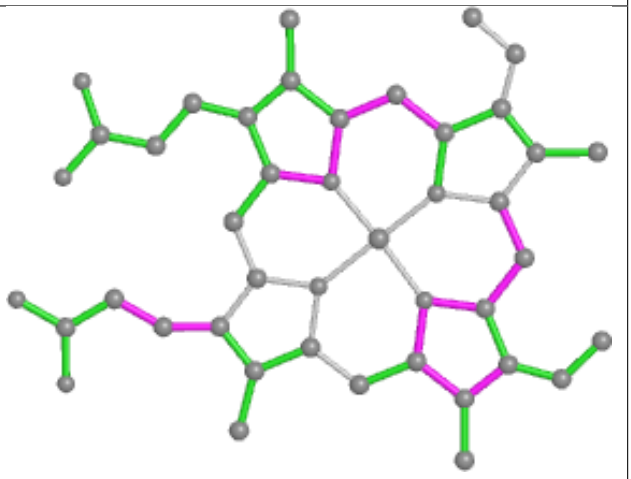
Ligand UMQ I 306



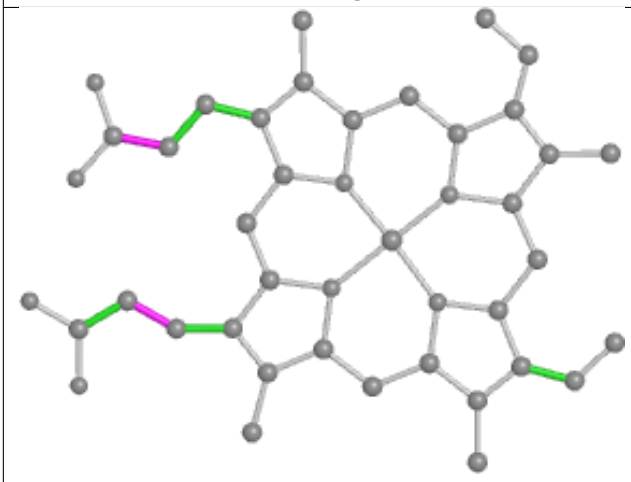
Ligand HEM A 301



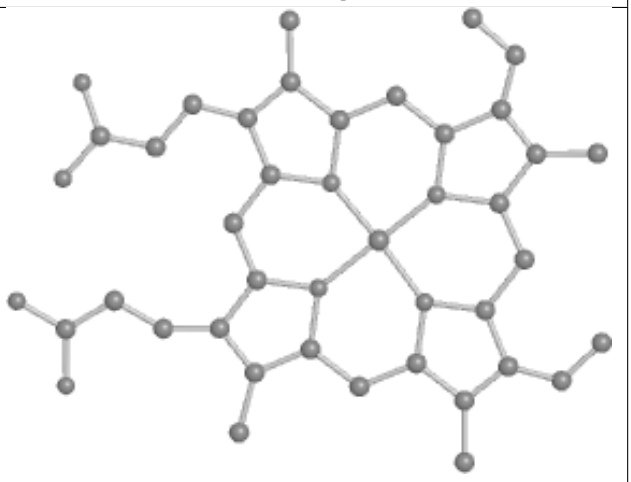
Bond lengths



Bond angles

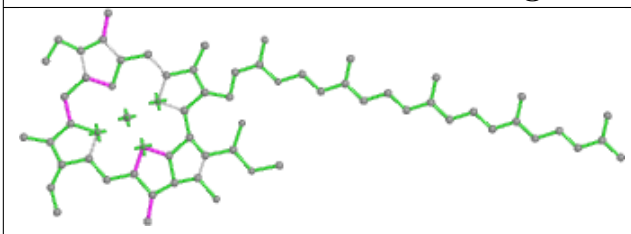


Torsions

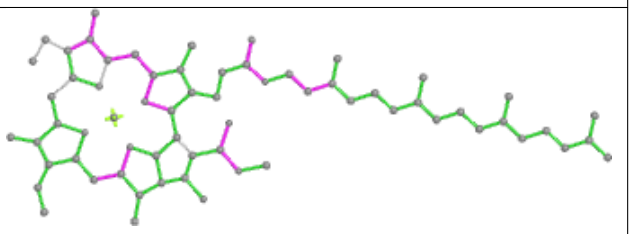


Rings

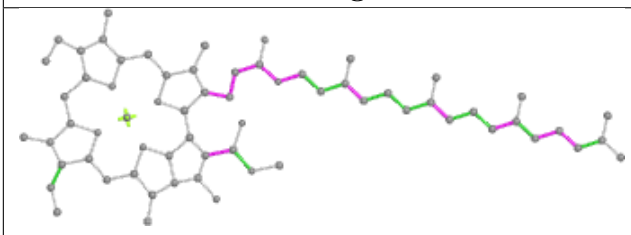
Ligand CLA A 304



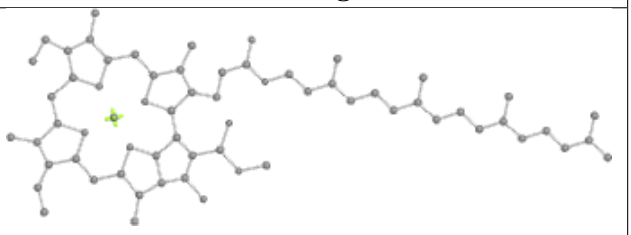
Bond lengths



Bond angles

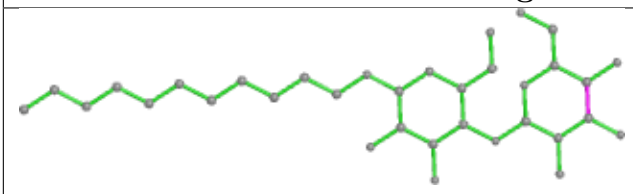


Torsions

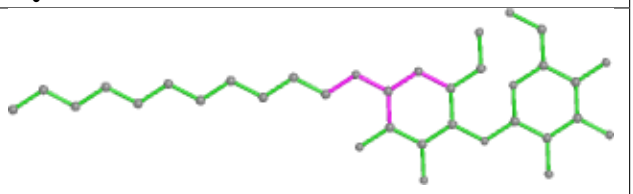


Rings

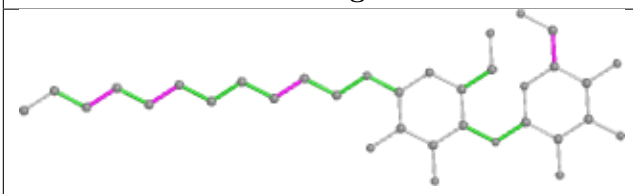
Ligand UMQ H 201



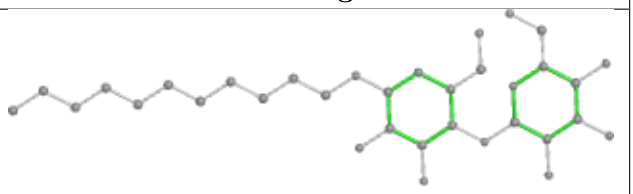
Bond lengths



Bond angles

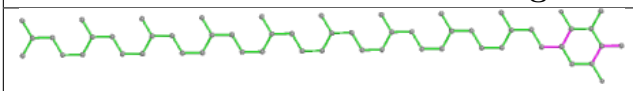


Torsions

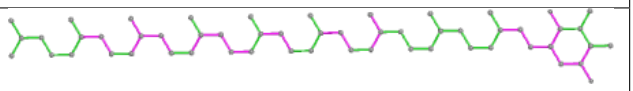


Rings

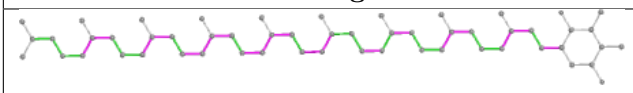
Ligand PL9 B 402



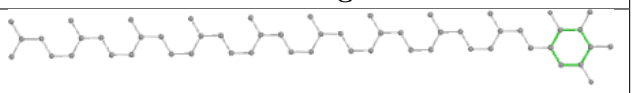
Bond lengths



Bond angles

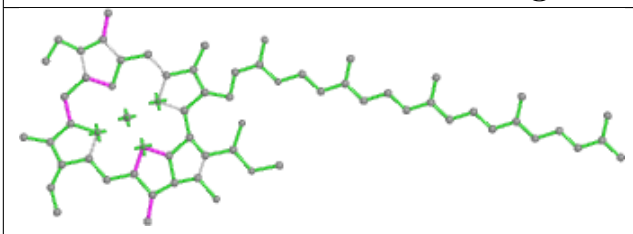


Torsions

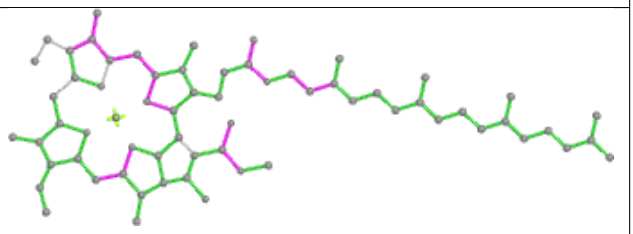


Rings

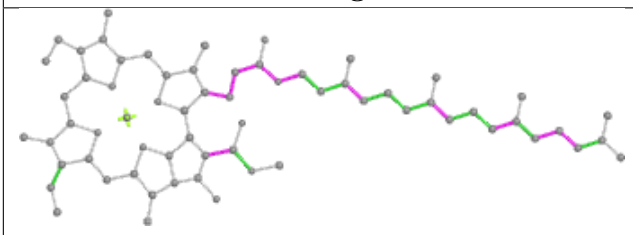
Ligand CLA I 304



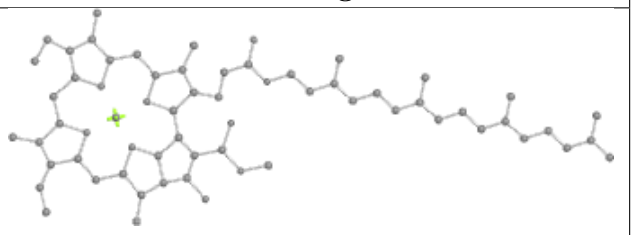
Bond lengths



Bond angles

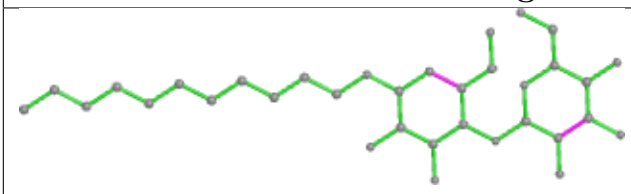


Torsions

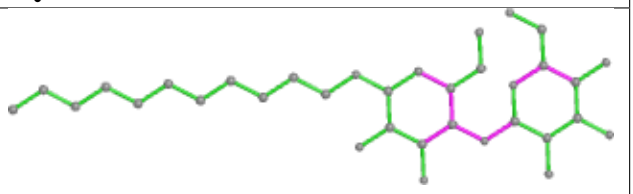


Rings

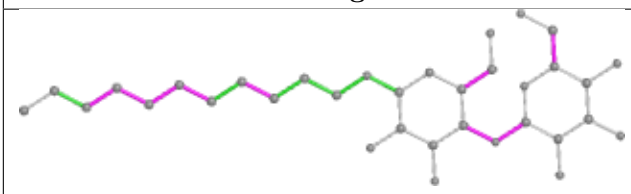
Ligand UMQ B 404



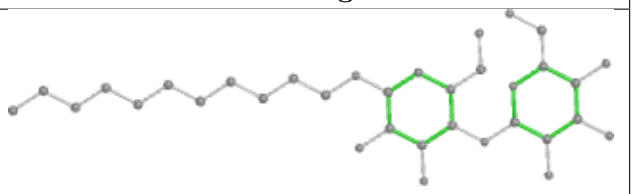
Bond lengths



Bond angles

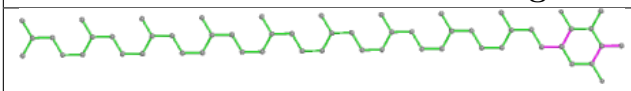


Torsions

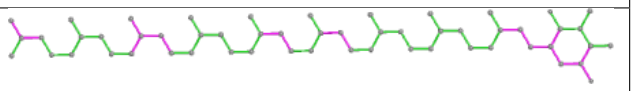


Rings

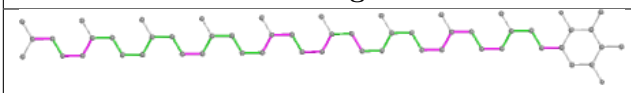
Ligand PL9 A 307



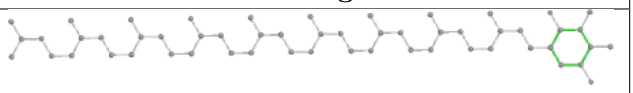
Bond lengths



Bond angles

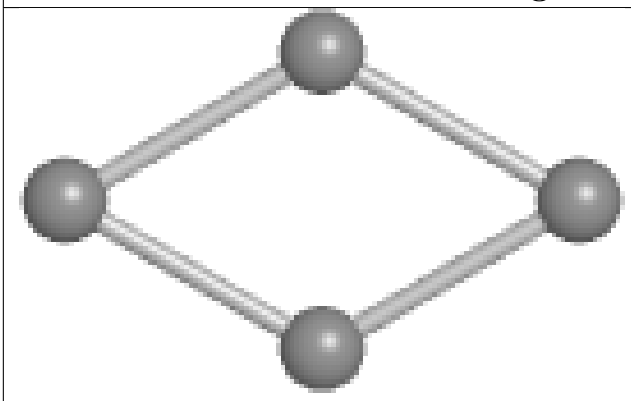


Torsions

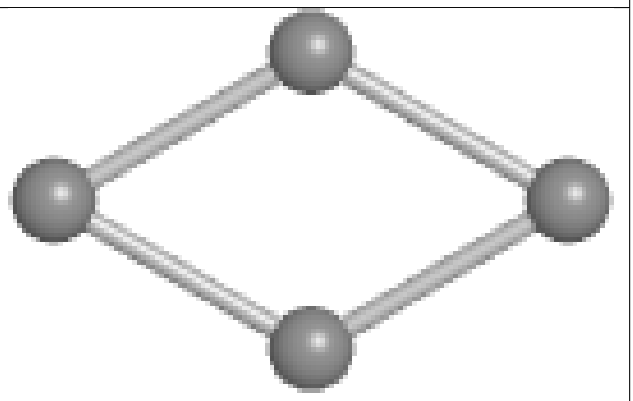


Rings

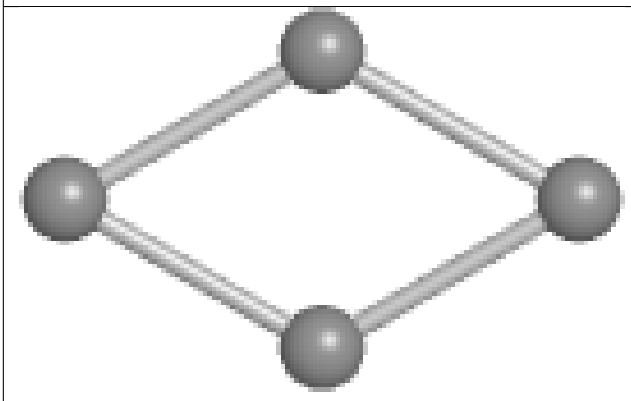
Ligand FES L 402



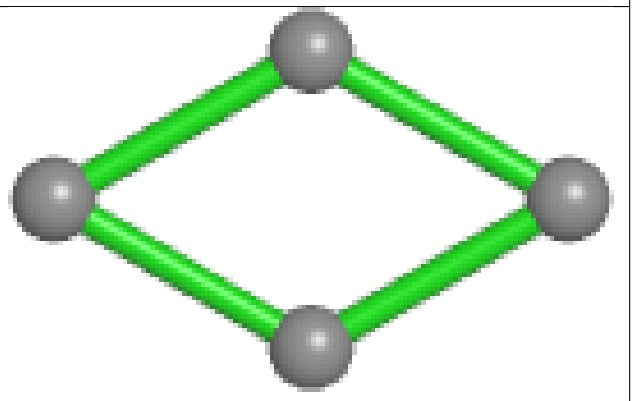
Bond lengths



Bond angles

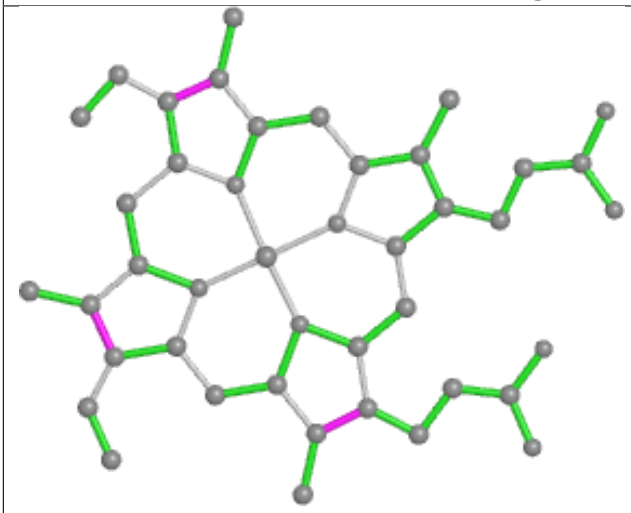


Torsions

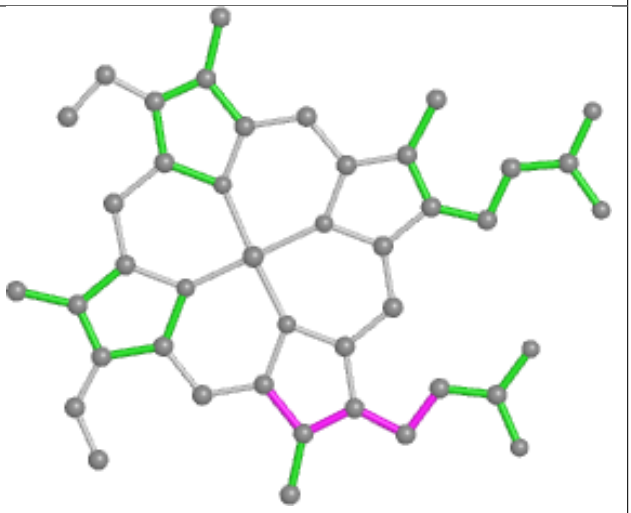


Rings

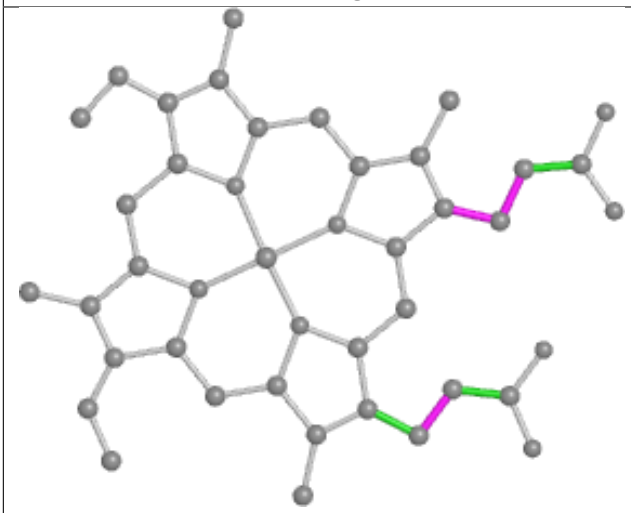
Ligand HEC I 303



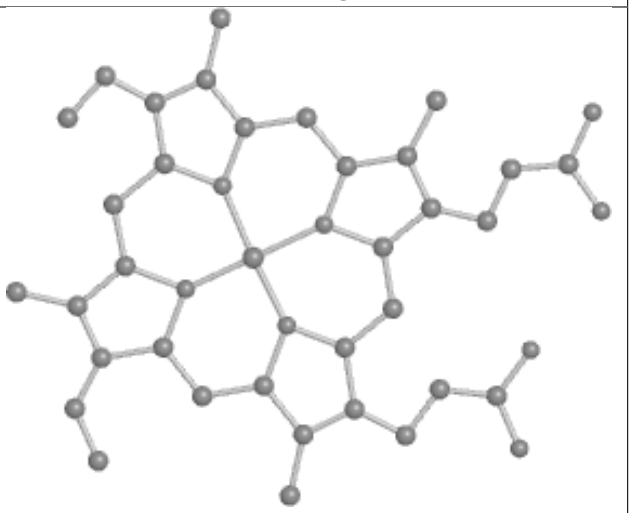
Bond lengths



Bond angles

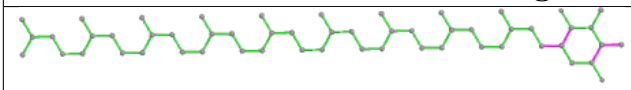


Torsions

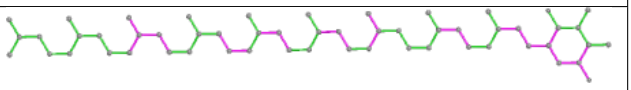


Rings

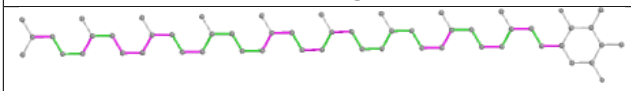
Ligand PL9 J 401



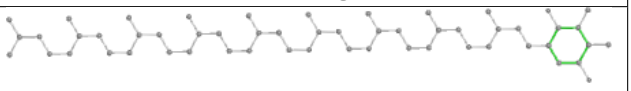
Bond lengths



Bond angles

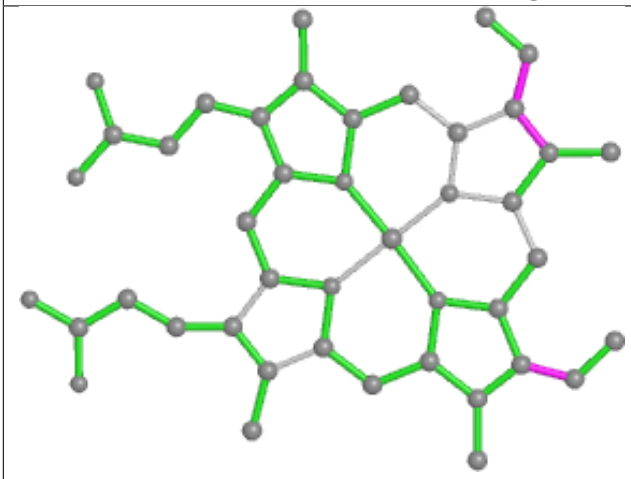


Torsions

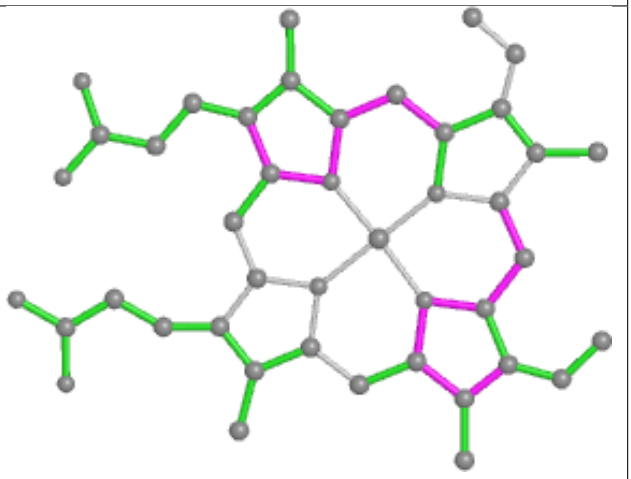


Rings

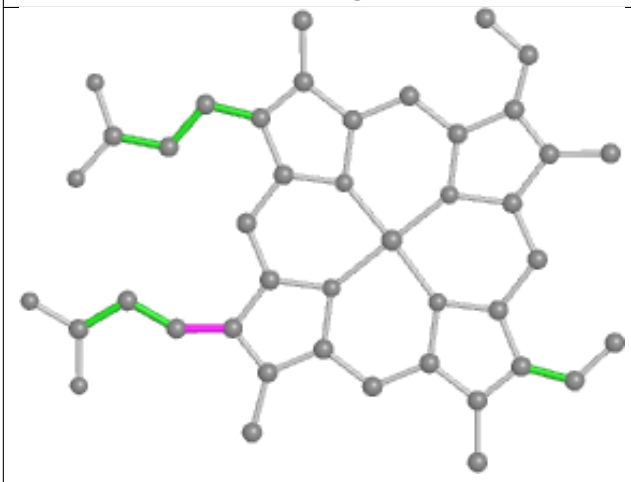
Ligand HEM I 302



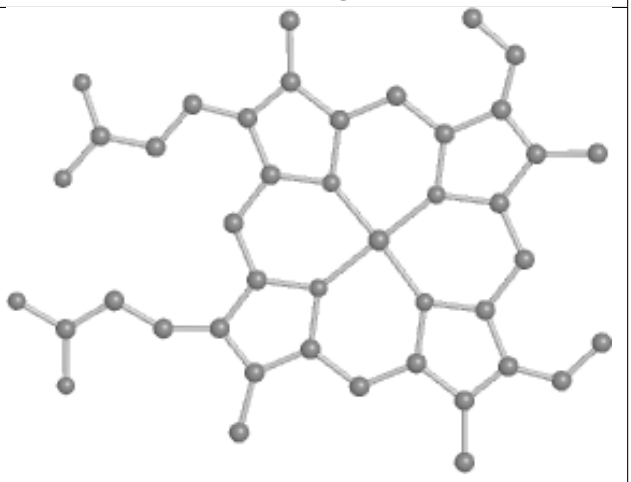
Bond lengths



Bond angles

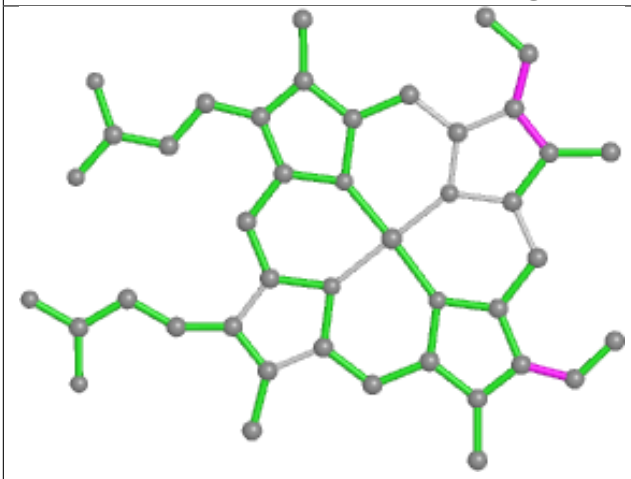


Torsions

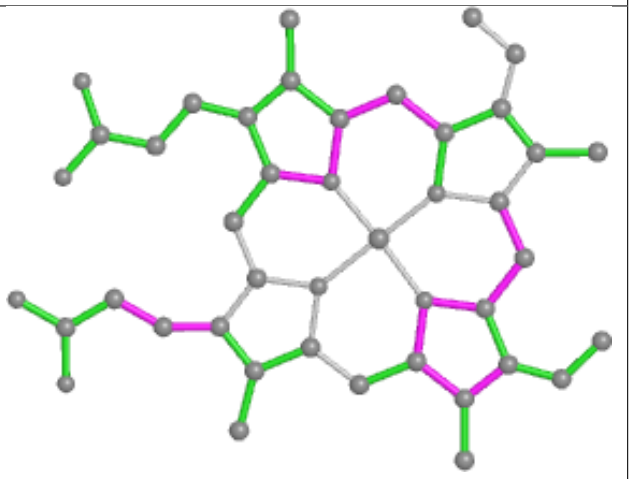


Rings

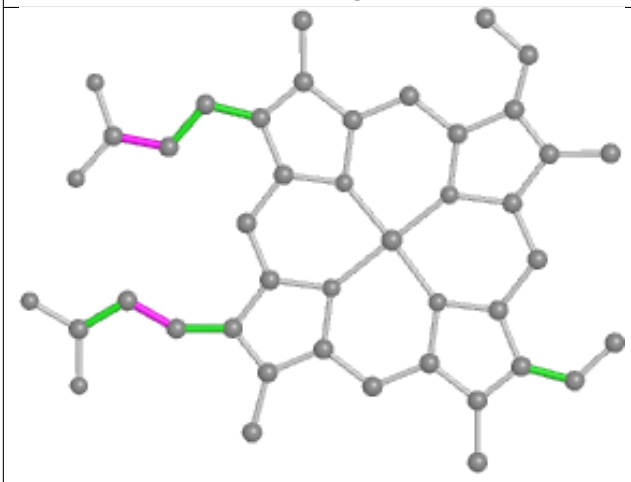
Ligand HEM I 301



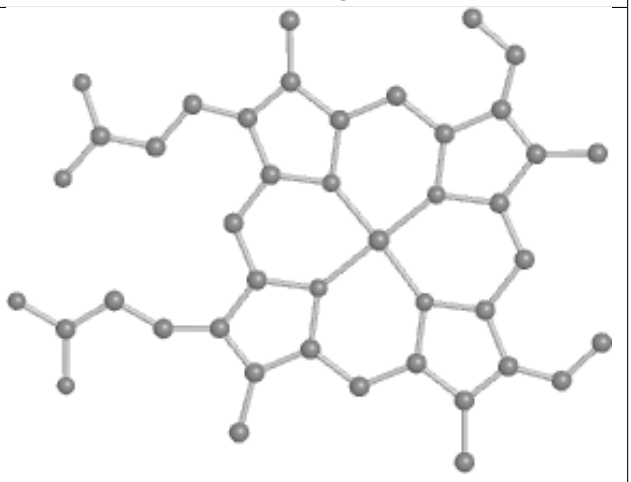
Bond lengths



Bond angles

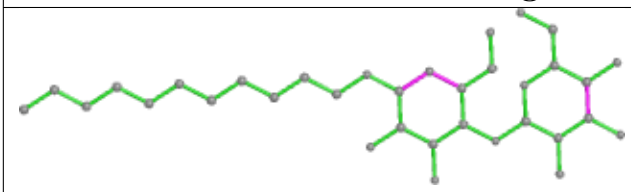


Torsions

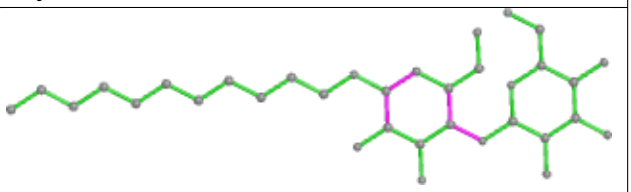


Rings

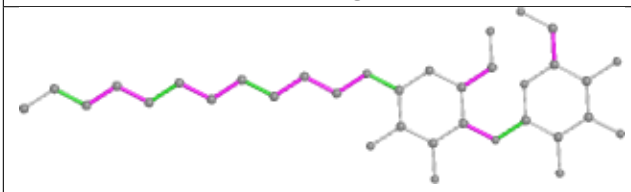
Ligand UMQ J 403



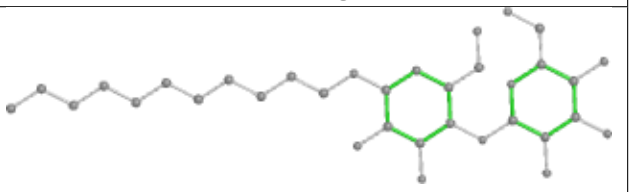
Bond lengths



Bond angles

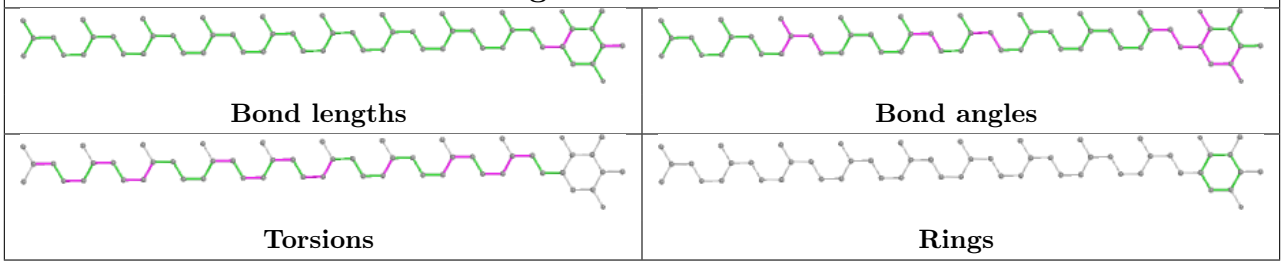


Torsions

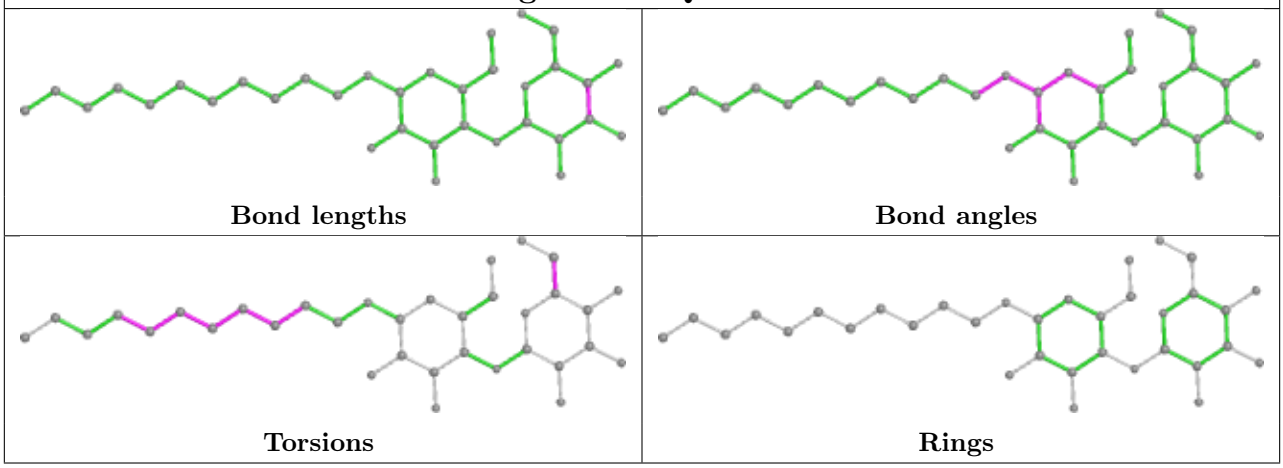


Rings

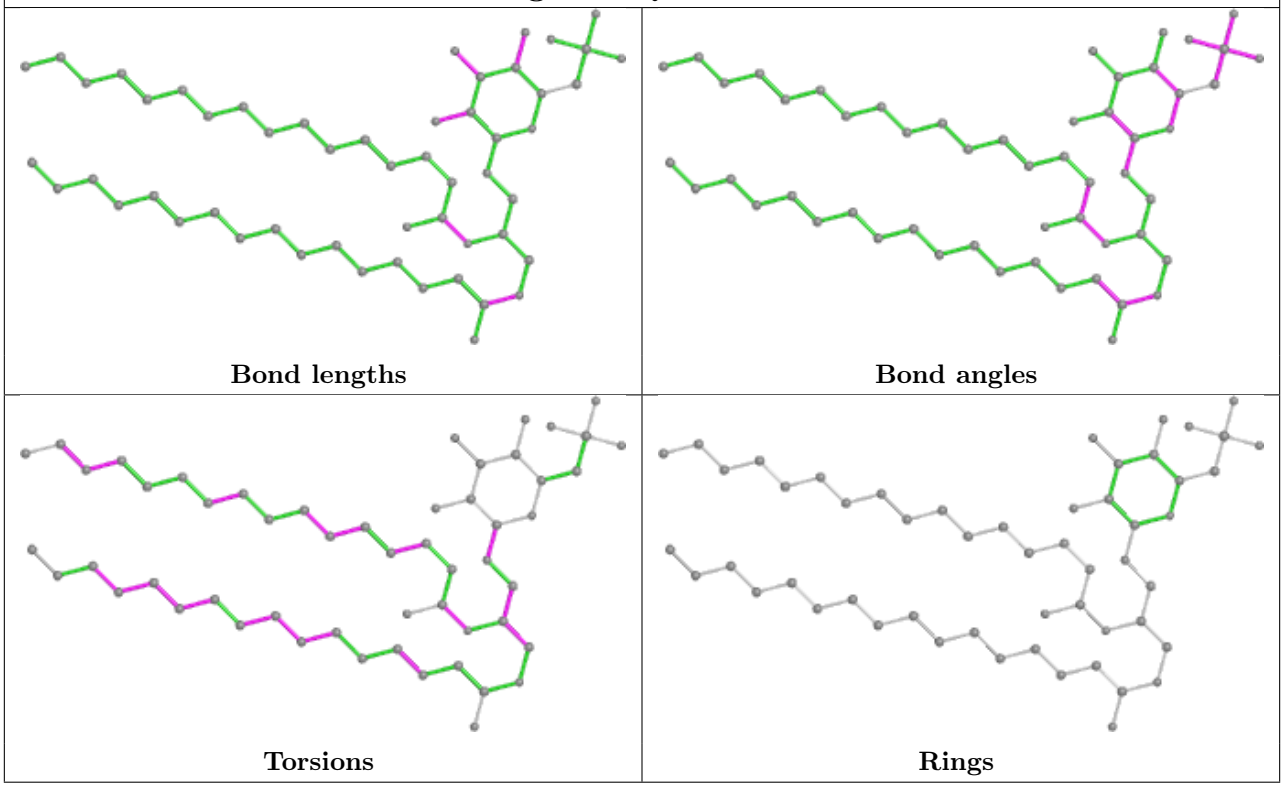
Ligand PL9 K 302



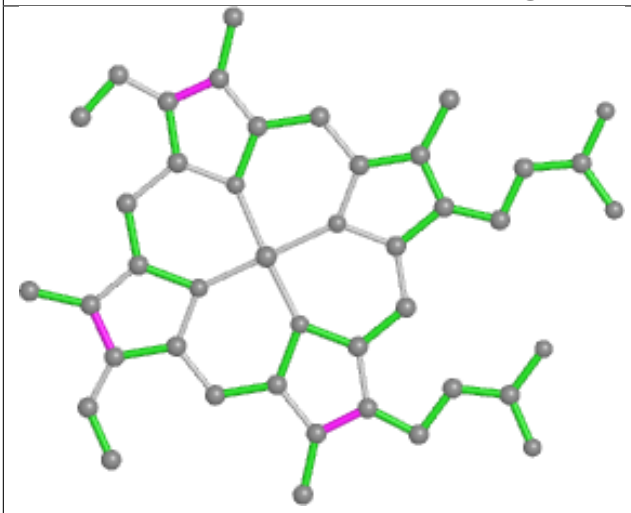
Ligand UMQ P 102



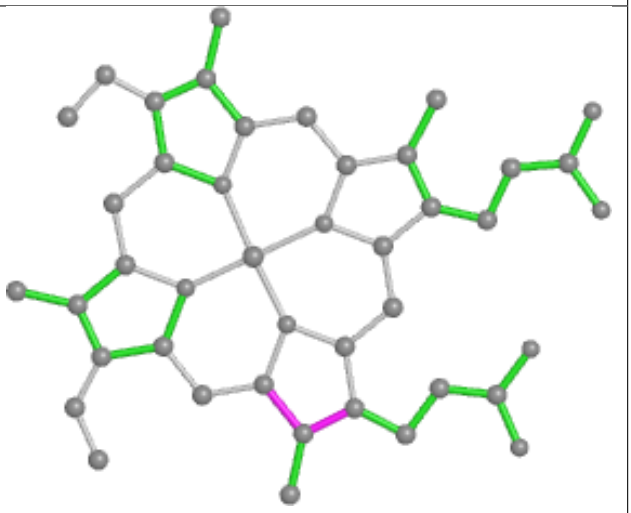
Ligand SQD L 401



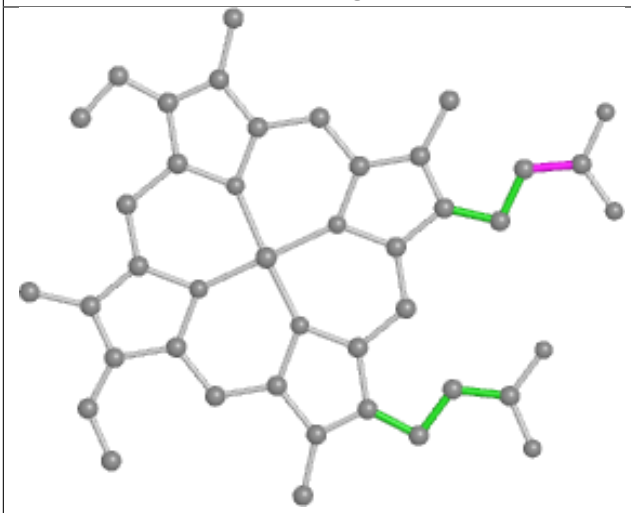
Ligand HEC K 301



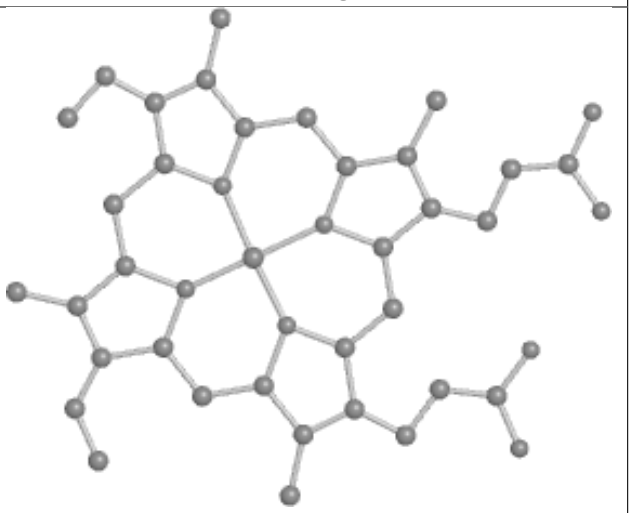
Bond lengths



Bond angles

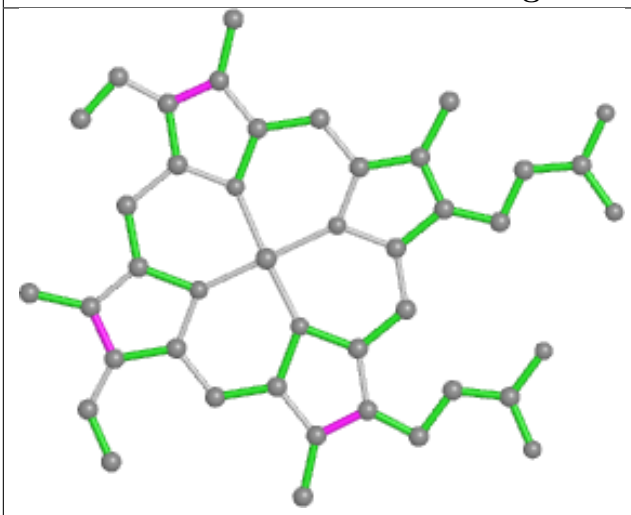


Torsions

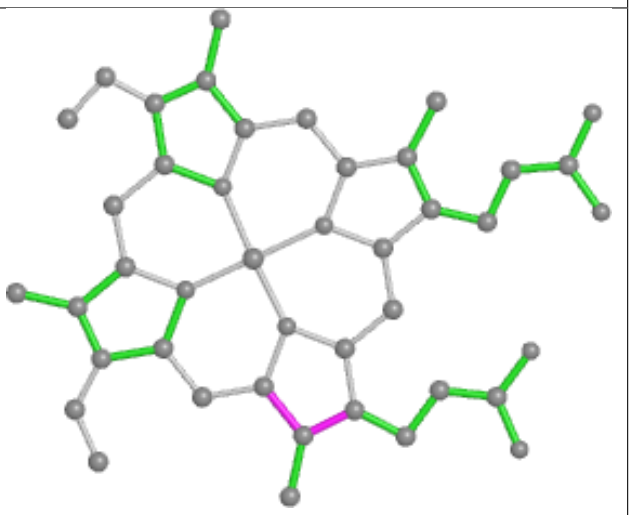


Rings

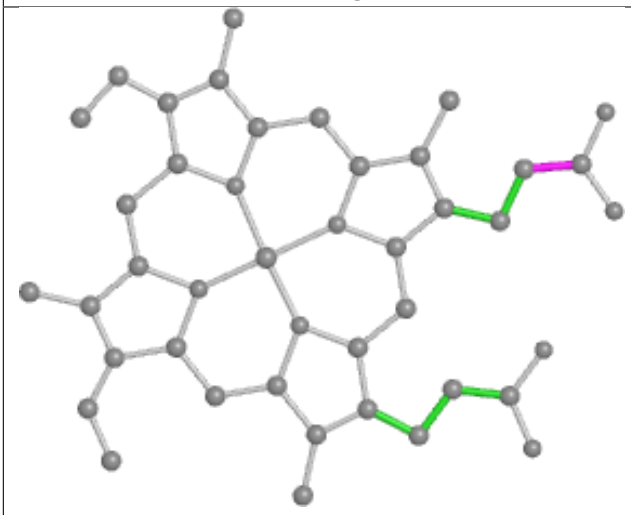
Ligand HEC C 301



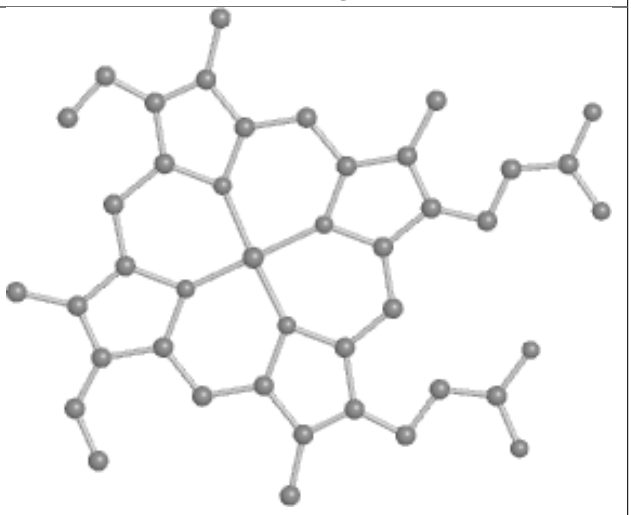
Bond lengths



Bond angles

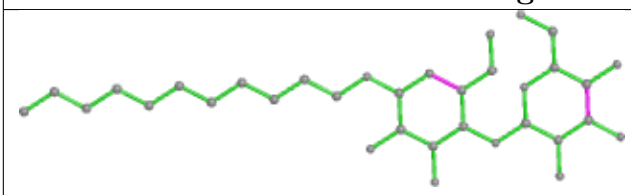


Torsions

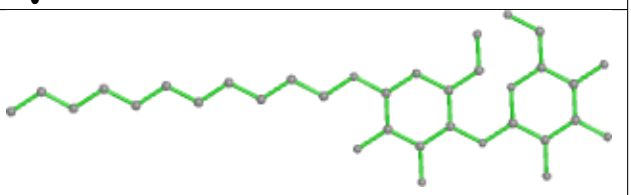


Rings

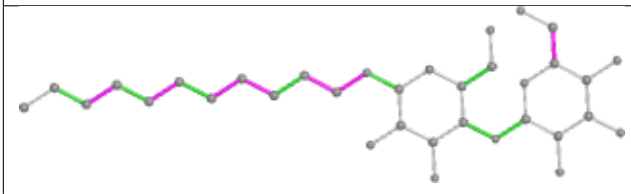
Ligand UMQ A 305



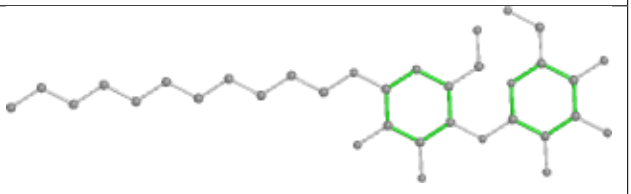
Bond lengths



Bond angles

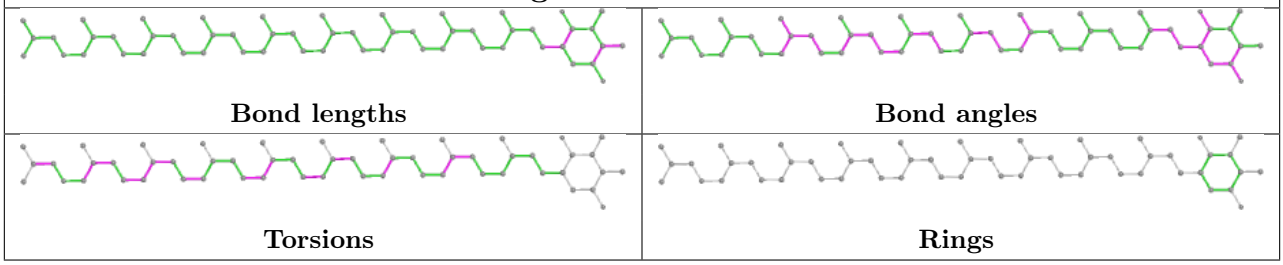


Torsions

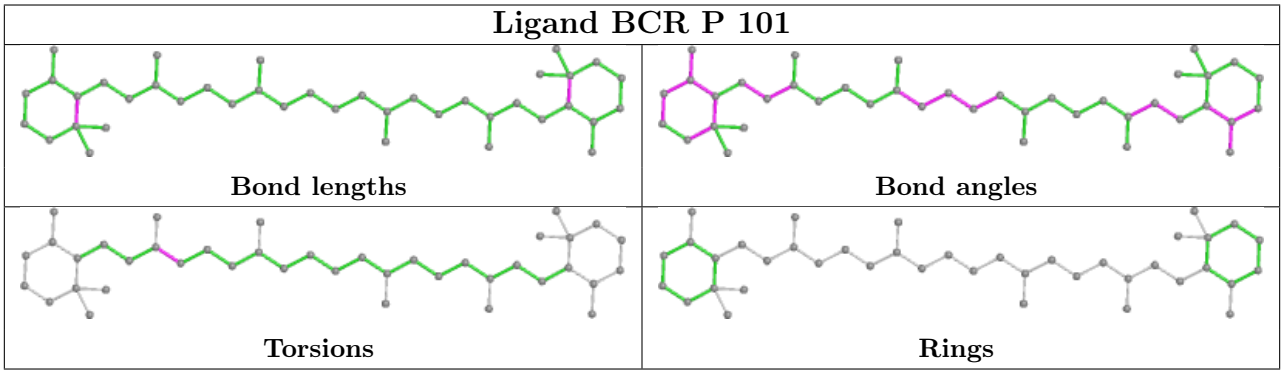


Rings

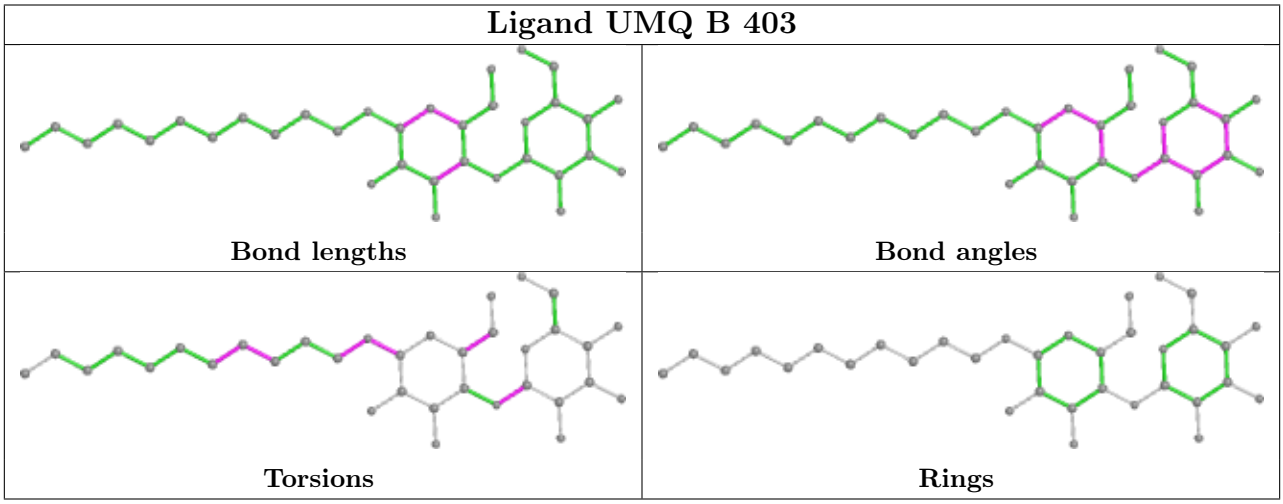
Ligand PL9 B 401



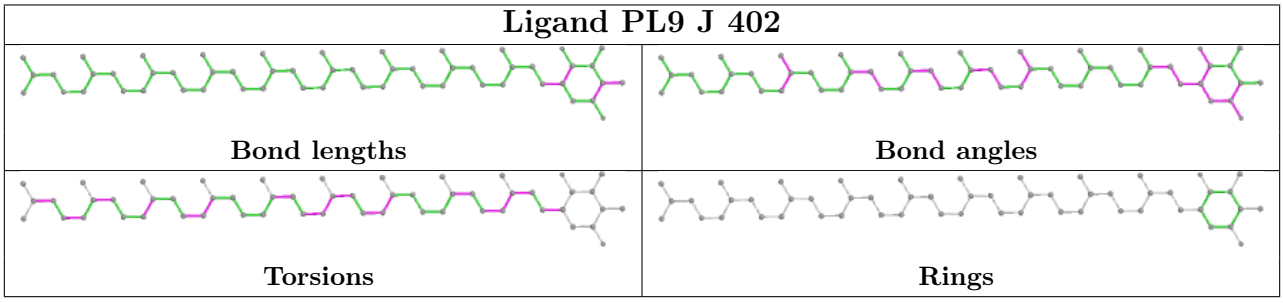
Ligand BCR P 101



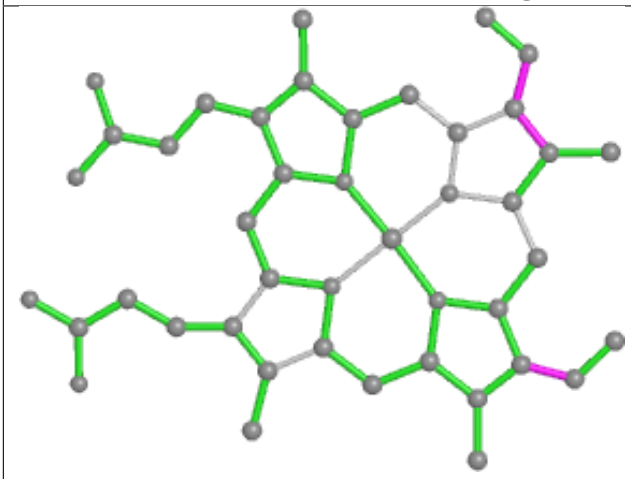
Ligand UMQ B 403



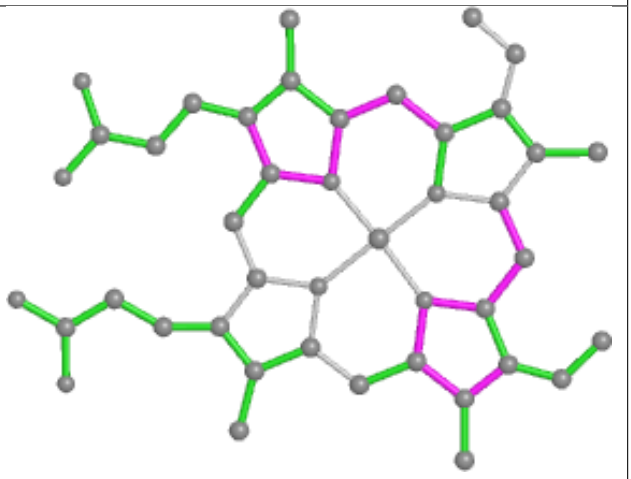
Ligand PL9 J 402



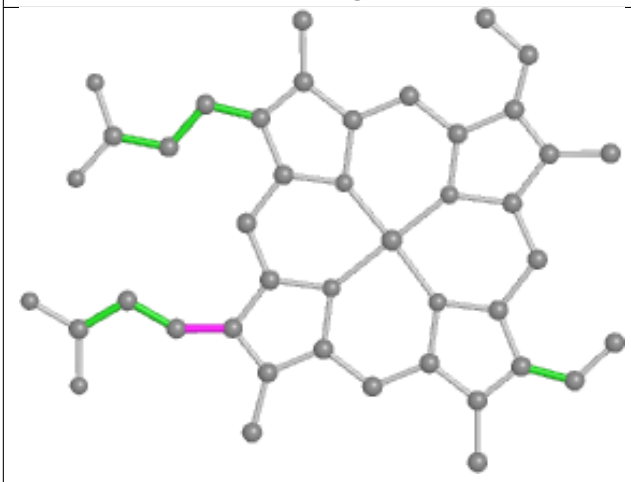
Ligand HEM A 302



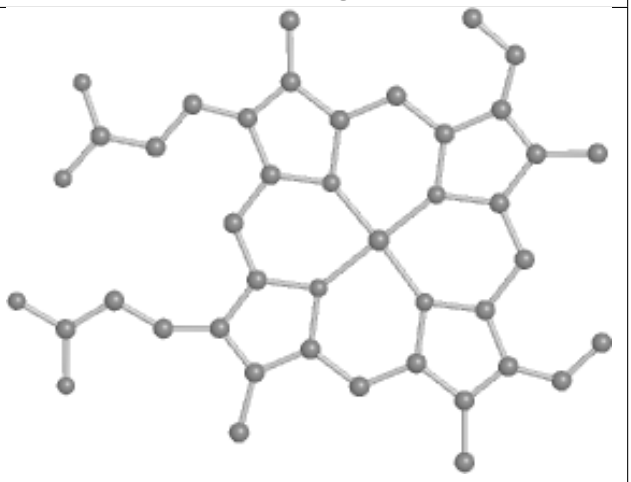
Bond lengths



Bond angles

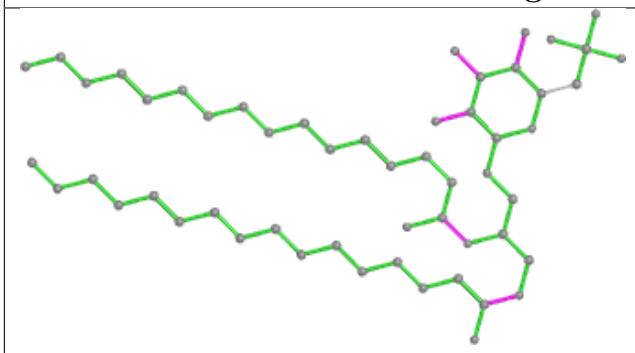


Torsions

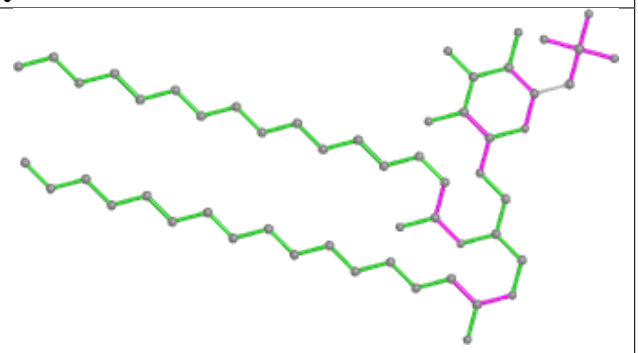


Rings

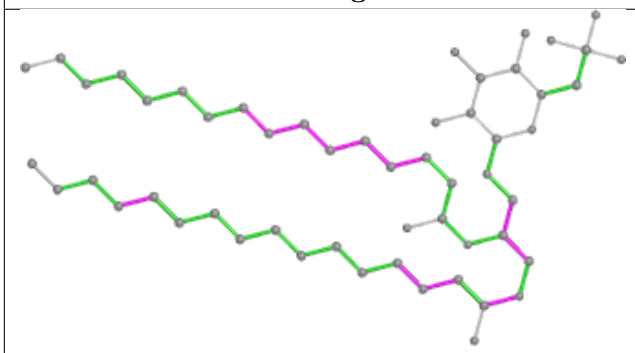
Ligand SQD D 201



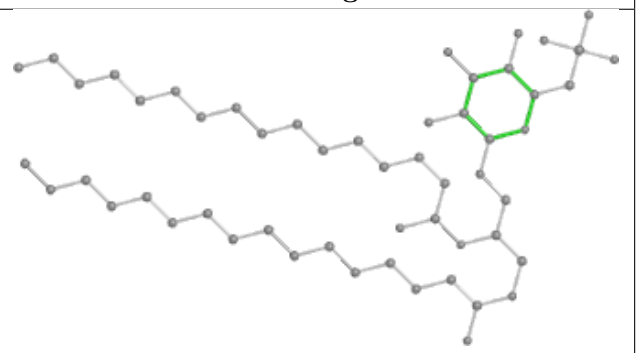
Bond lengths



Bond angles

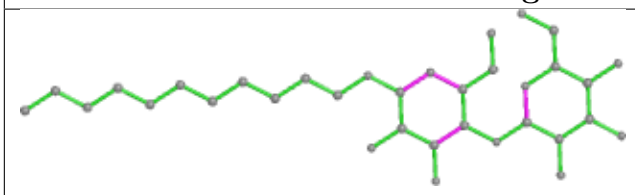


Torsions

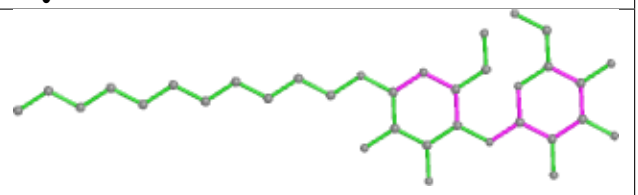


Rings

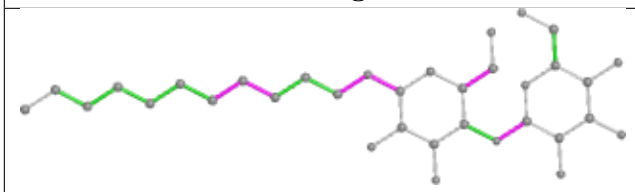
Ligand UMQ J 404



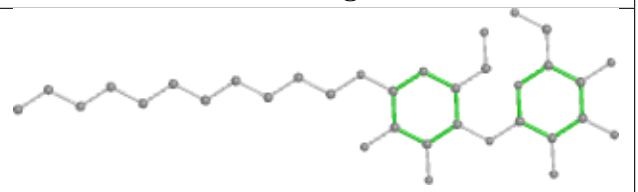
Bond lengths



Bond angles

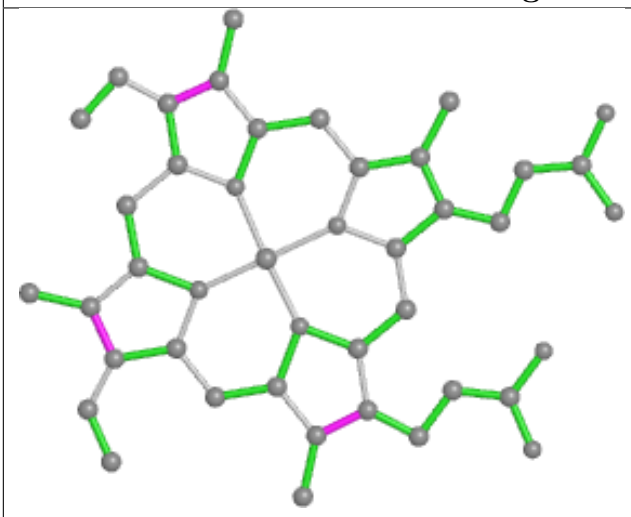


Torsions

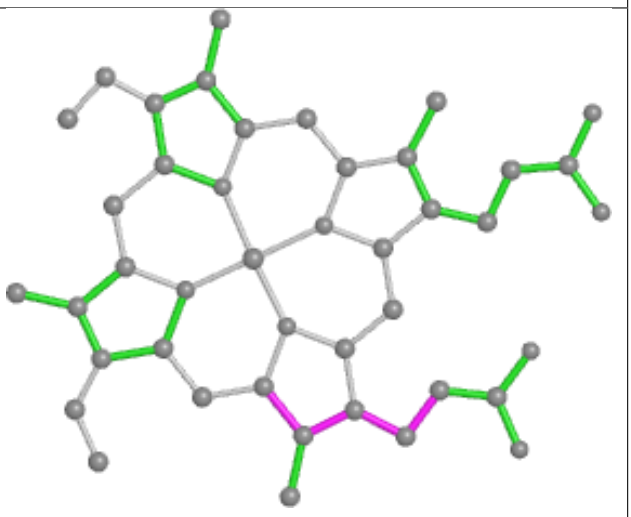


Rings

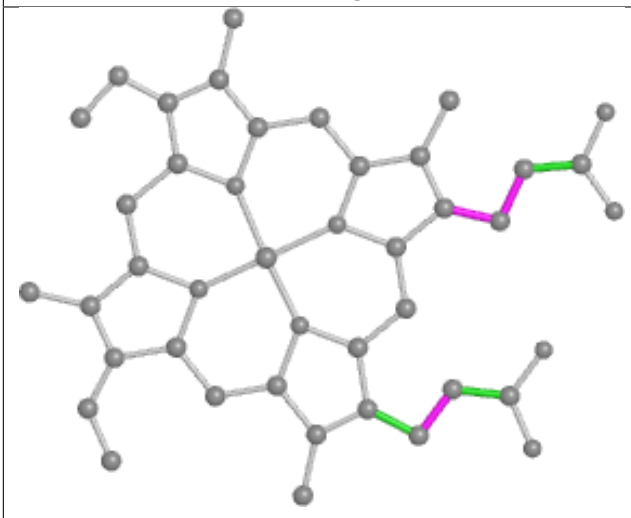
Ligand HEC A 303



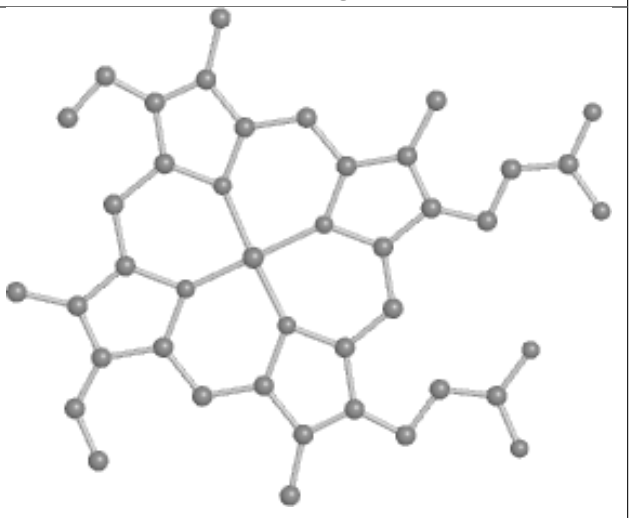
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

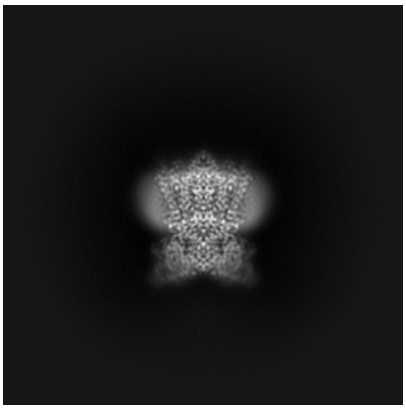
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15027. These allow visual inspection of the internal detail of the map and identification of artifacts.

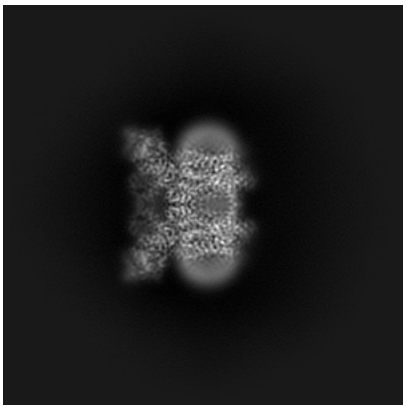
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

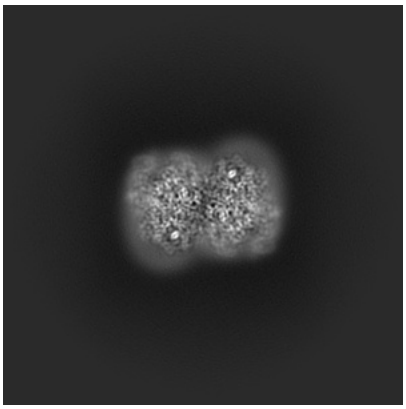
6.1.1 Primary map



X

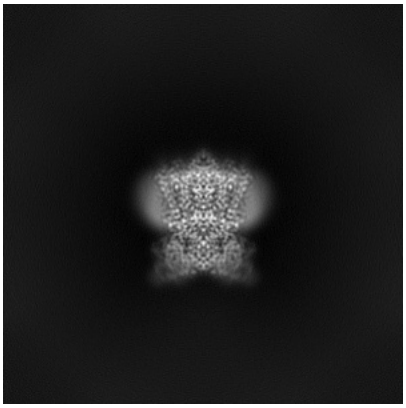


Y

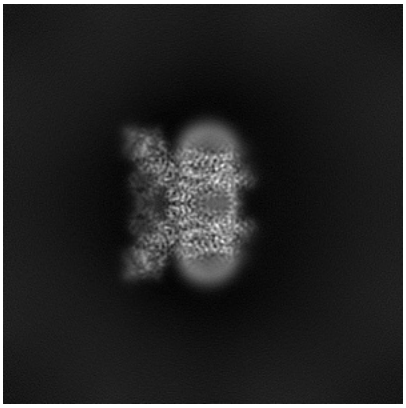


Z

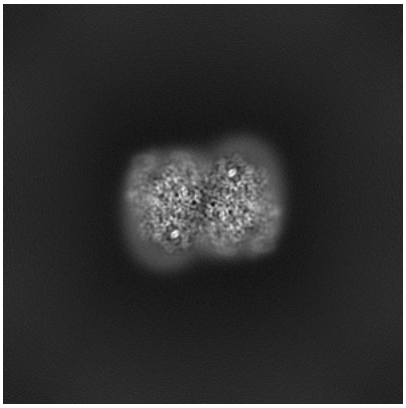
6.1.2 Raw map



X



Y

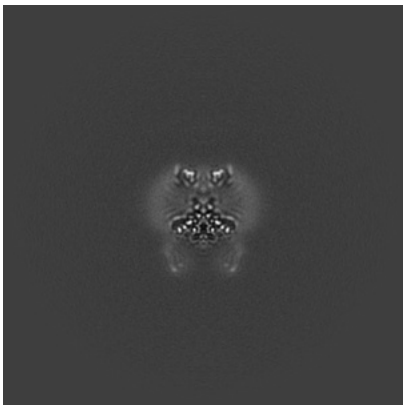


Z

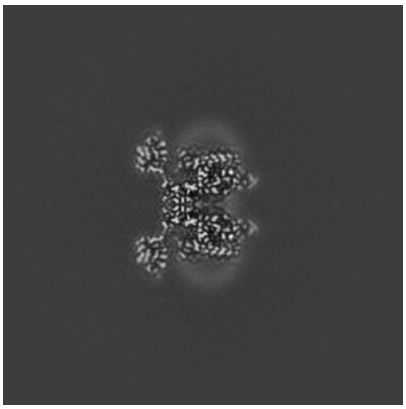
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

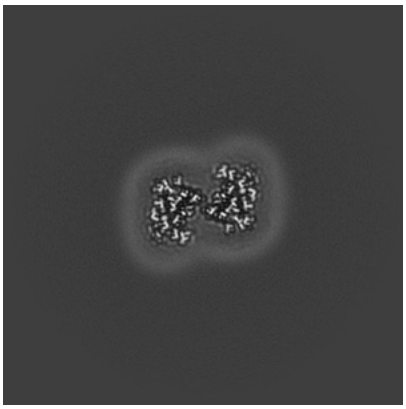
6.2.1 Primary map



X Index: 186

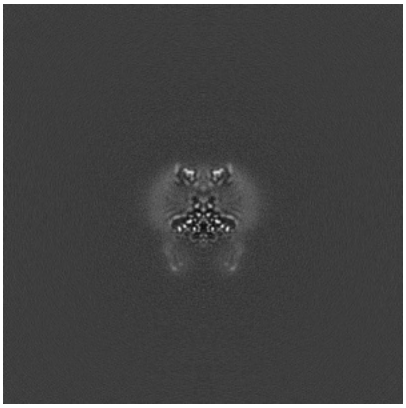


Y Index: 186

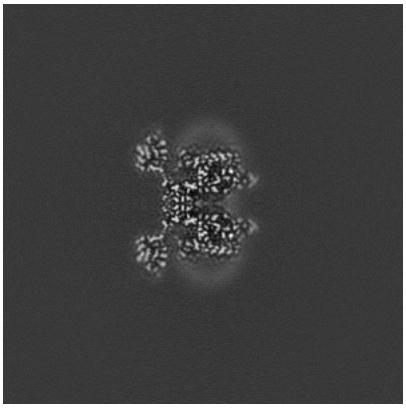


Z Index: 186

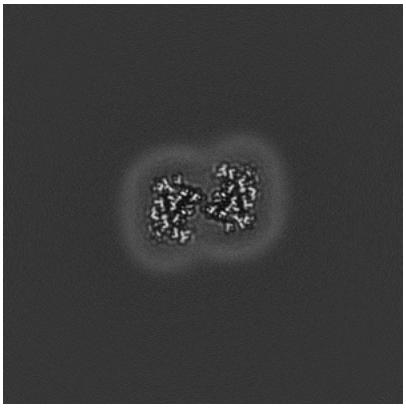
6.2.2 Raw map



X Index: 186



Y Index: 186

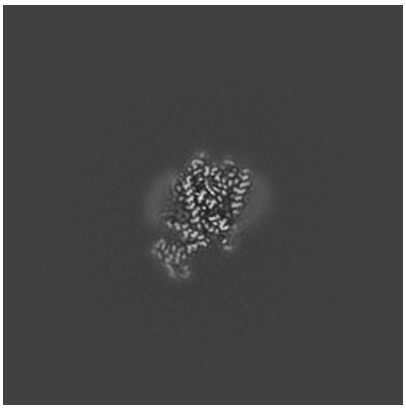


Z Index: 186

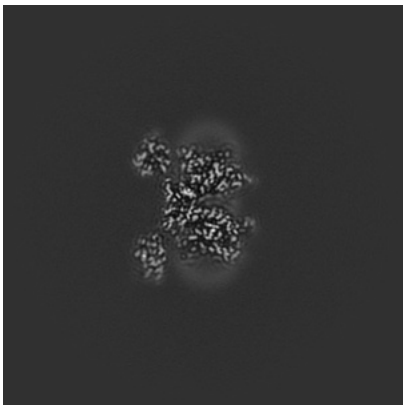
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

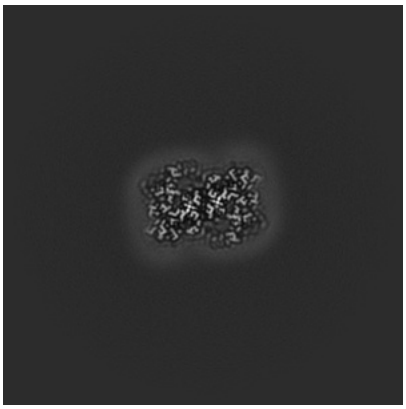
6.3.1 Primary map



X Index: 205

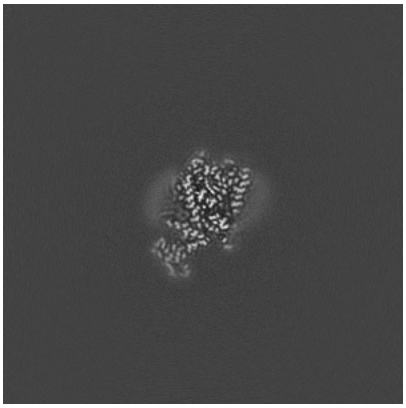


Y Index: 189

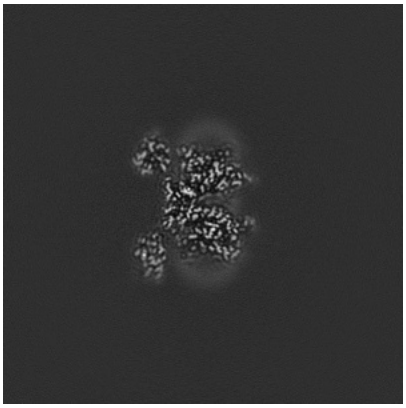


Z Index: 173

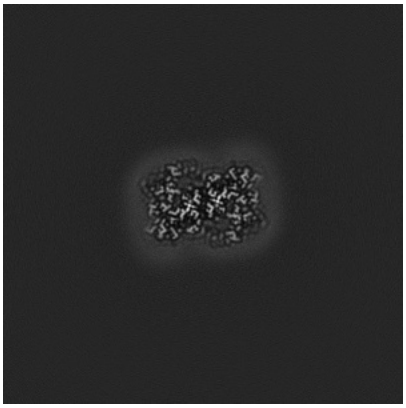
6.3.2 Raw map



X Index: 205



Y Index: 189

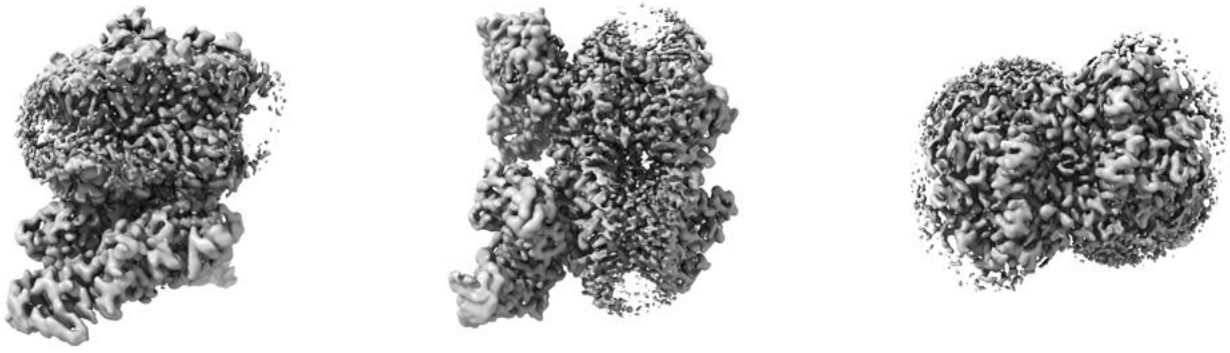


Z Index: 173

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

6.4 Orthogonal surface views (i)

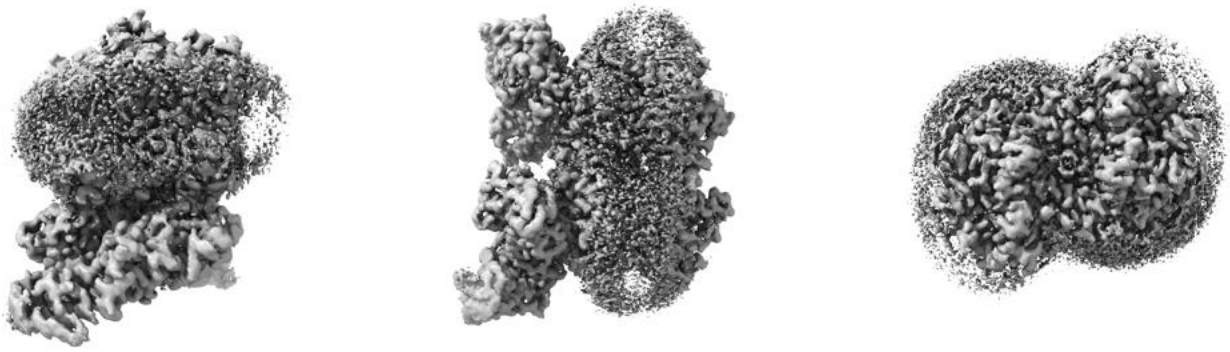
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.208. 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.

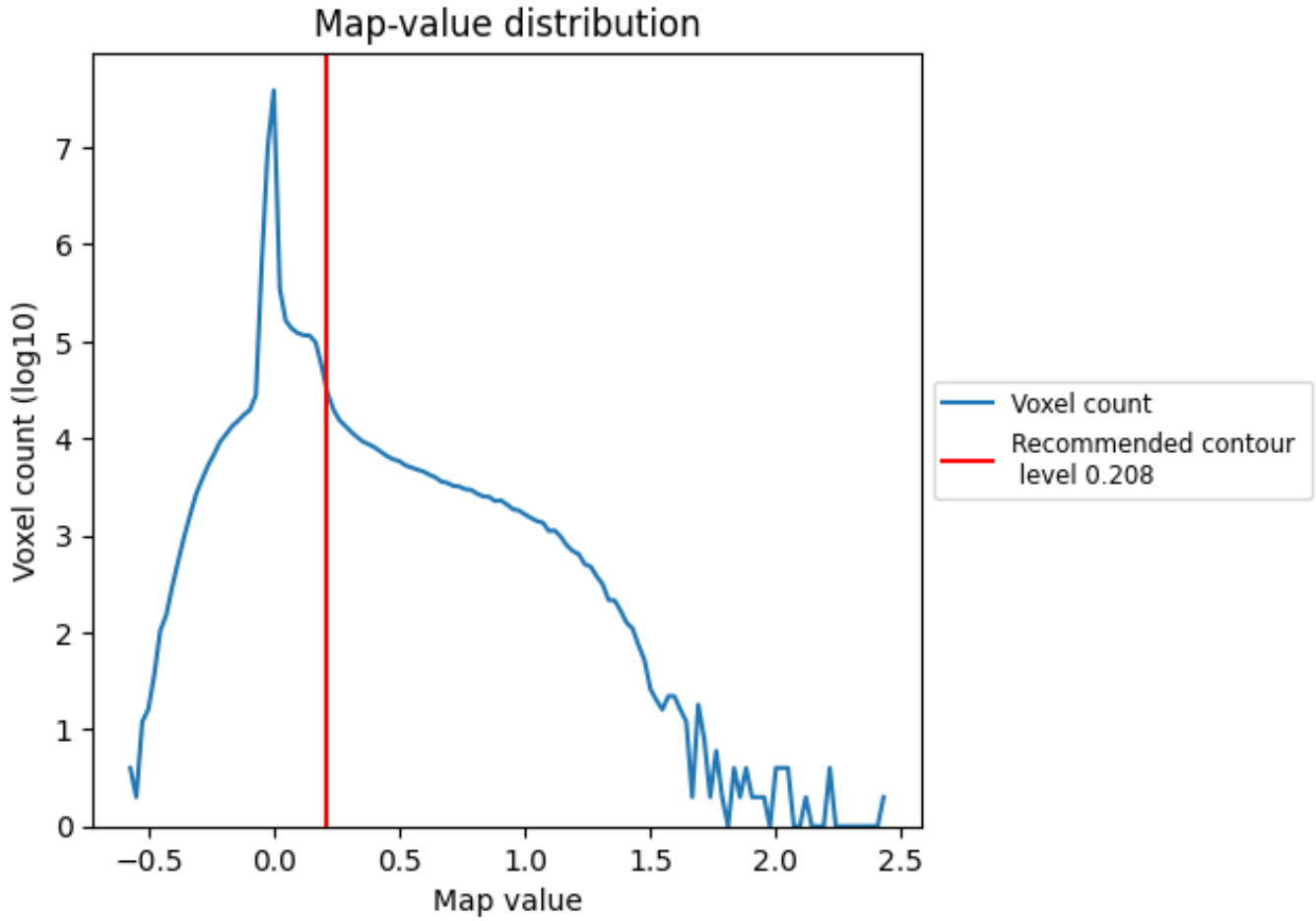
6.5 Mask visualisation (i)

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

7 Map analysis

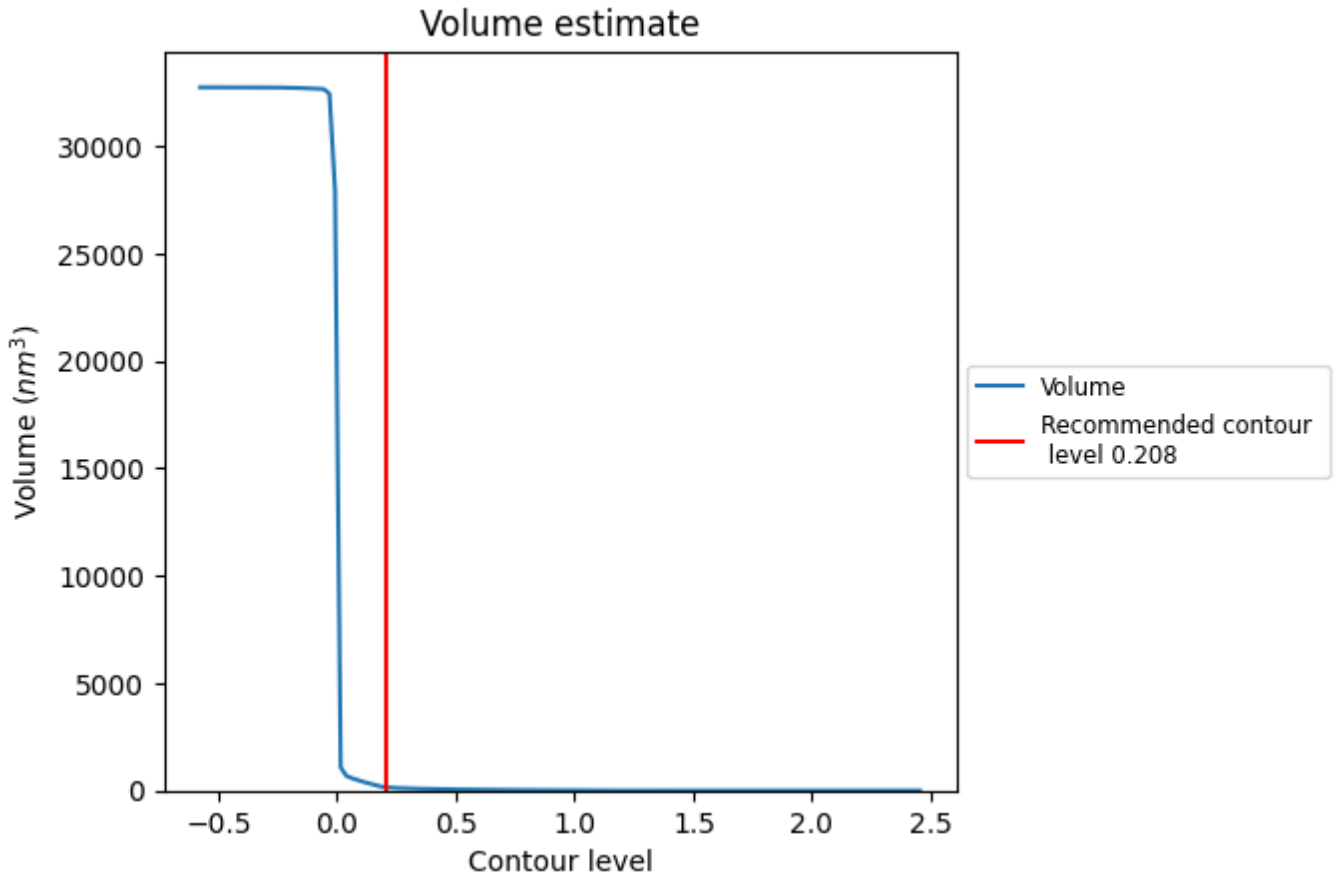
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

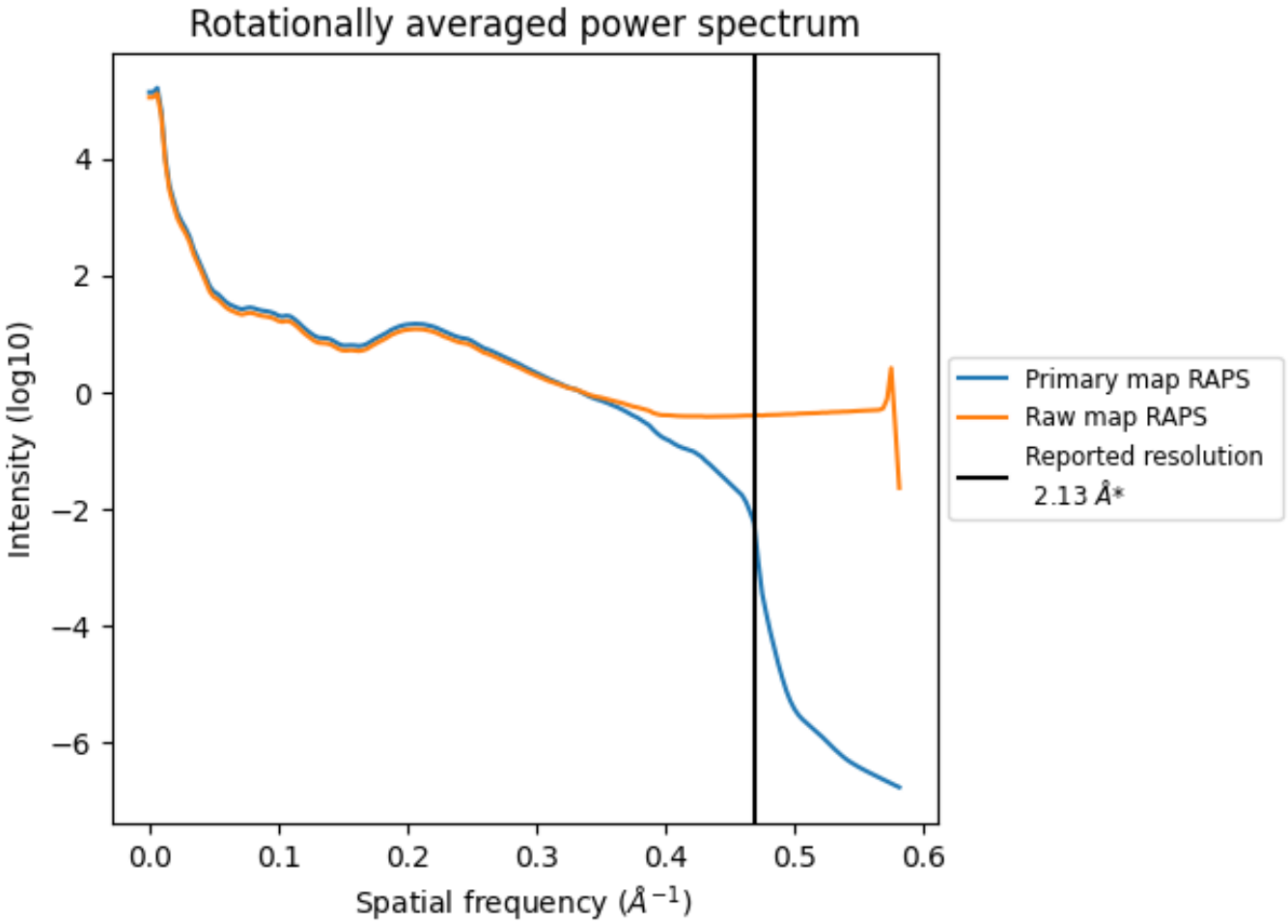
7.2 Volume estimate



The volume at the recommended contour level is 150 nm^3; this corresponds to an approximate mass of 136 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)

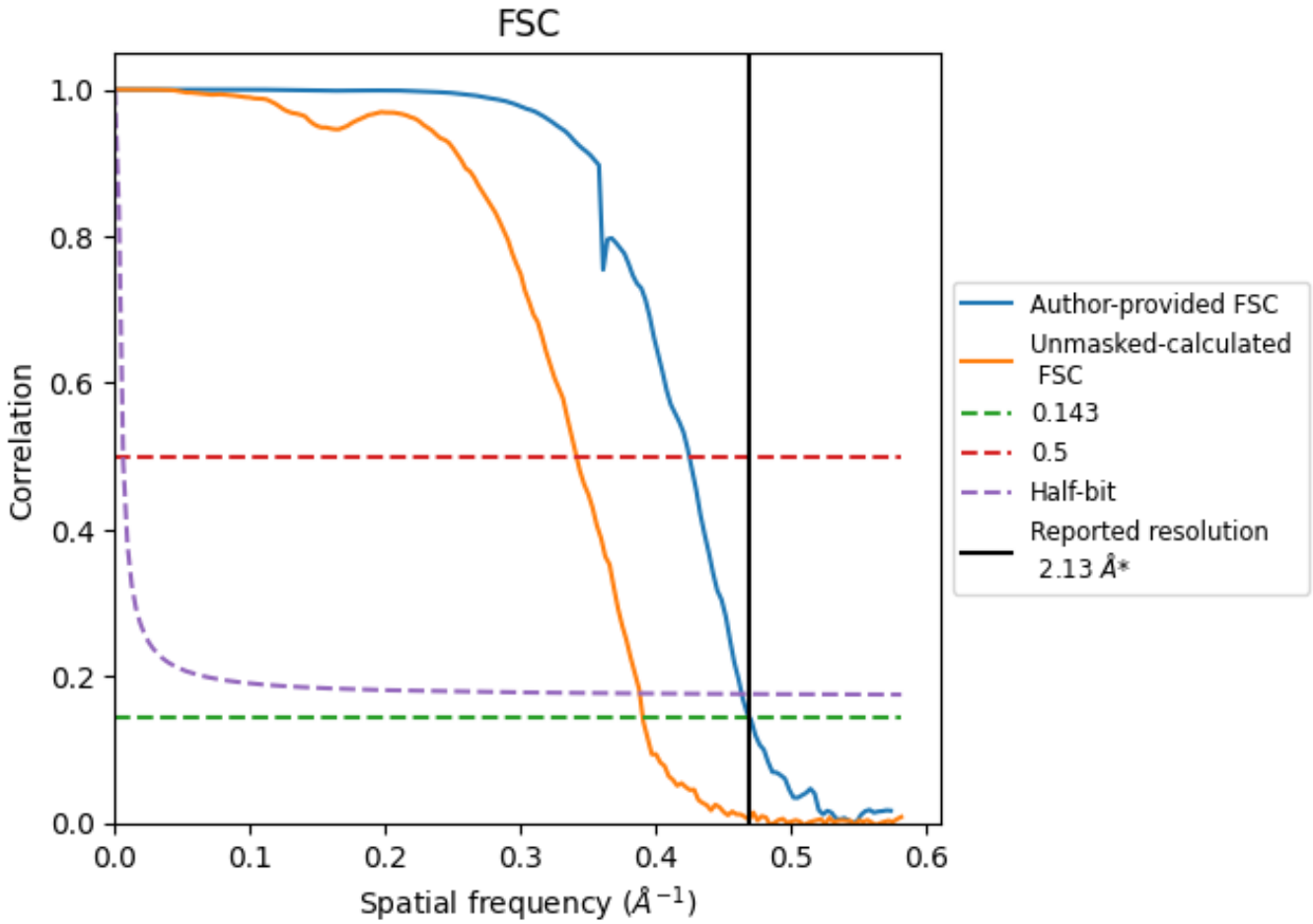


*Reported resolution corresponds to spatial frequency of 0.469 Å^{-1}

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 0.469 $Å^{-1}$

8.2 Resolution estimates (i)

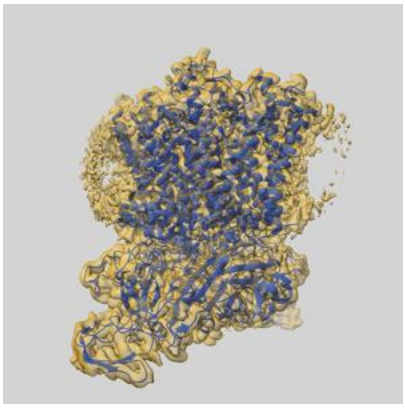
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.36	2.16
Unmasked-calculated*	2.56	2.93	2.58

*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 2.56 differs from the reported value 2.13 by more than 10 %

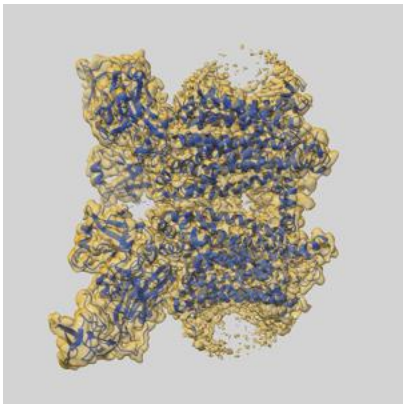
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15027 and PDB model 7ZYV. Per-residue inclusion information can be found in section 3 on page 12.

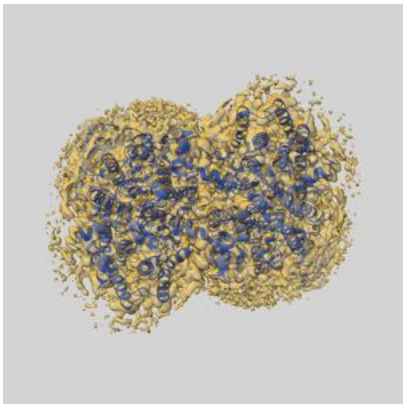
9.1 Map-model overlay



X



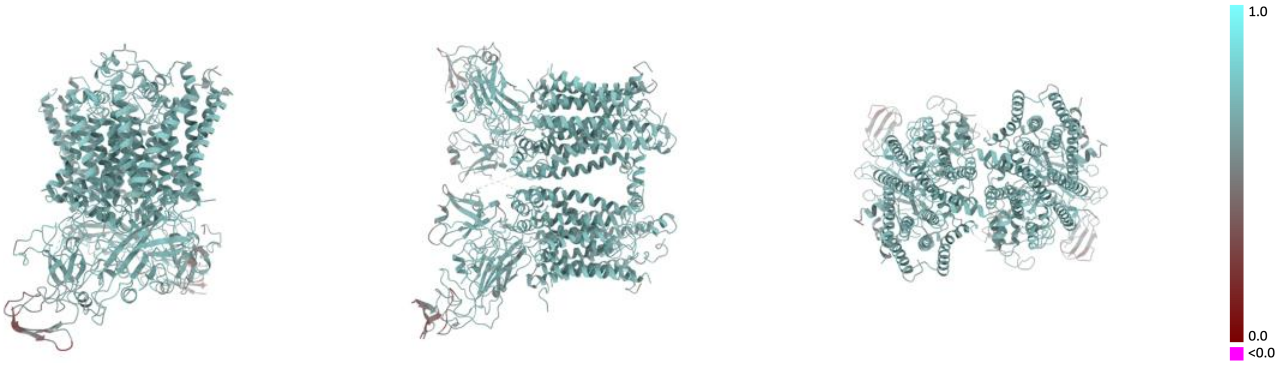
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.208 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.

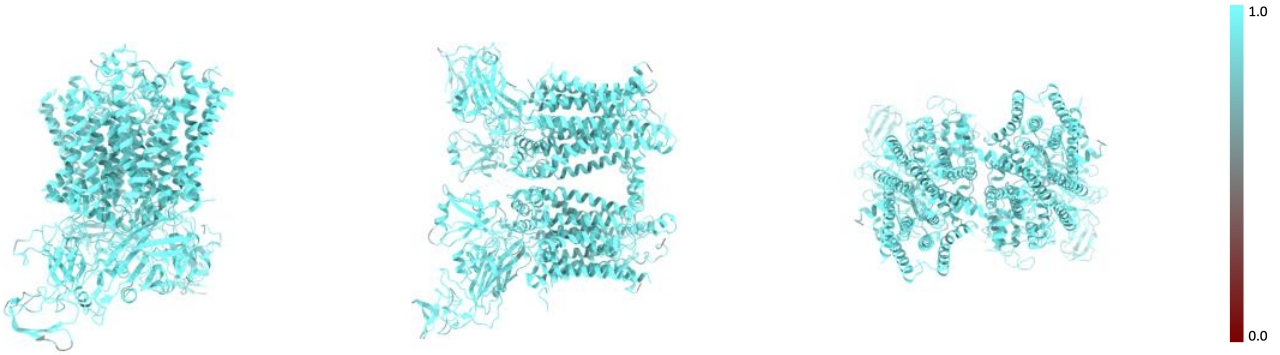
9.2 Q-score mapped to coordinate model (i)



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.

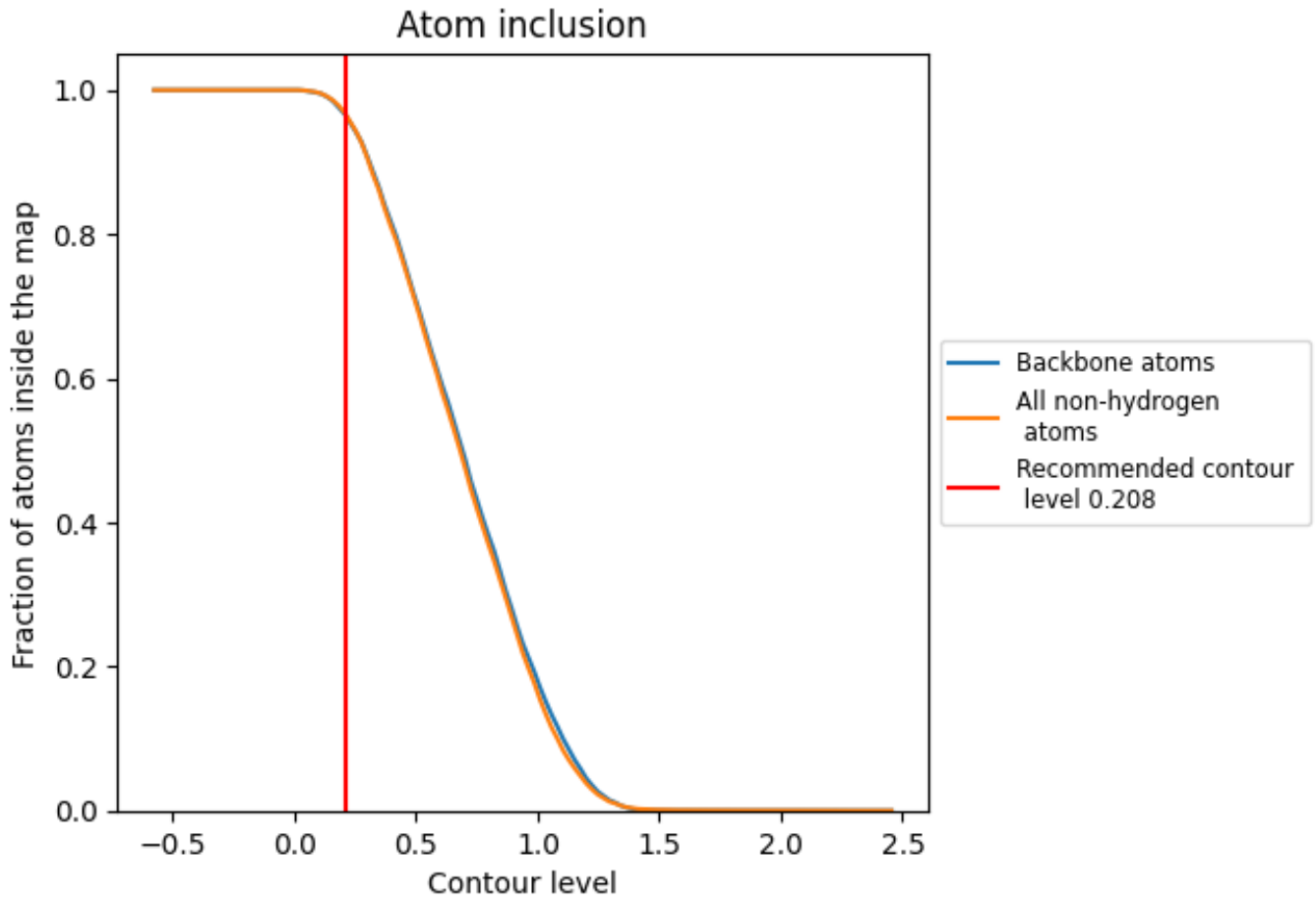
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.208).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9675	0.6440
A	0.9873	0.6780
B	0.9646	0.6510
C	0.9571	0.6120
D	0.9654	0.6270
E	0.9917	0.6400
F	0.9639	0.6470
G	0.9885	0.6670
H	0.9920	0.6740
I	0.9885	0.6820
J	0.9640	0.6510
K	0.9543	0.6110
L	0.9606	0.6300
M	0.9958	0.6480
N	0.9808	0.6500
O	0.9961	0.6730
P	0.9829	0.6700
Q	0.8930	0.6110
R	0.8884	0.5990