Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 01:02 PM JST

PDB ID	:	8YIL
EMDB ID	:	EMD-39322
Title	:	Cryo-EM structure of Saccharomyces cerevisiae bc1 complex in YF24228-bound state
Authors	:	Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on	:	2024-02-29
Resolution	:	2.58 Å(reported)
Based on initial model	:	6YMX

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:

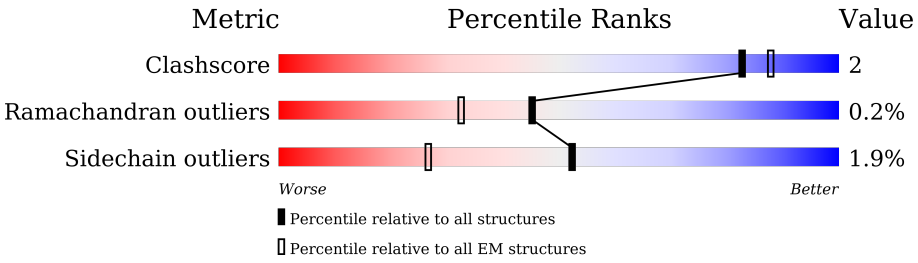
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.58 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	431	94% 6%
1	L	431	95% 5%
2	C	385	96%
2	N	385	95%
3	B	352	97%
3	M	352	97%
4	D	248	97%
4	O	248	99%

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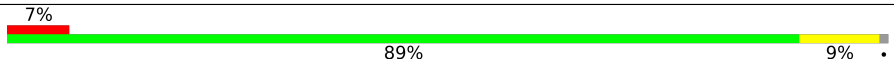
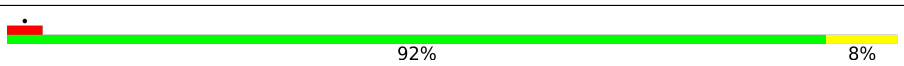
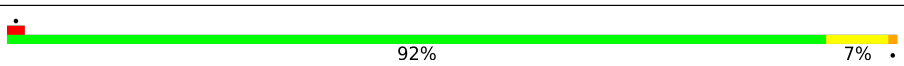
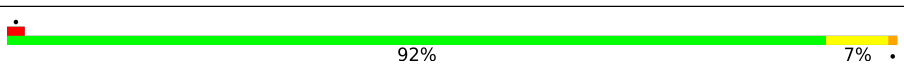
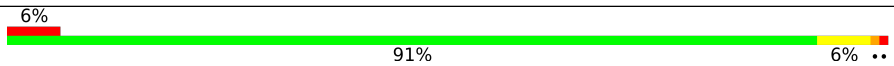
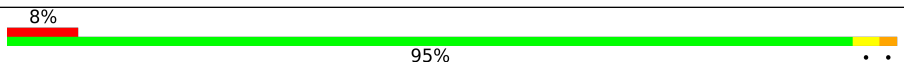
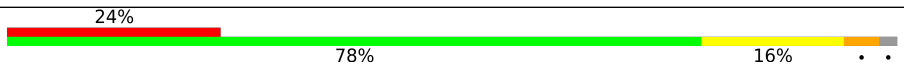
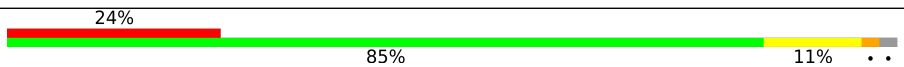
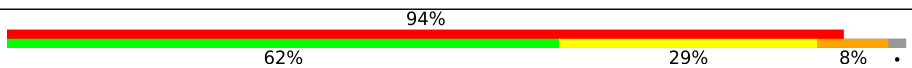
Mol	Chain	Length	Quality of chain
5	E	185	
5	P	185	
6	F	75	
6	Q	75	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	55	
9	T	55	
10	U	52	
10	V	52	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 32326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
1	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
2	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
3	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
4	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called QCR6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	54	Total	C	N	O	0	0
			442	295	74	73		
9	T	54	Total	C	N	O	0	0
			443	295	74	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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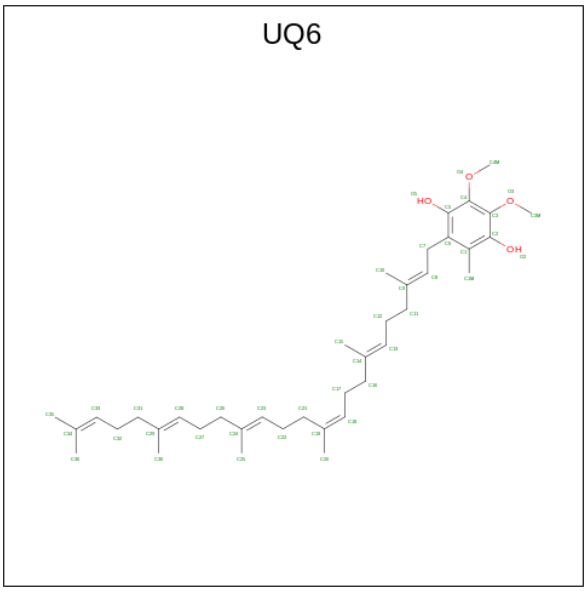
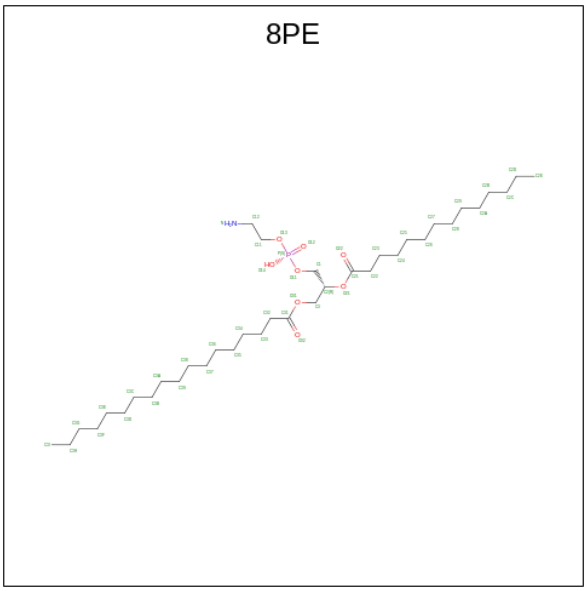
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



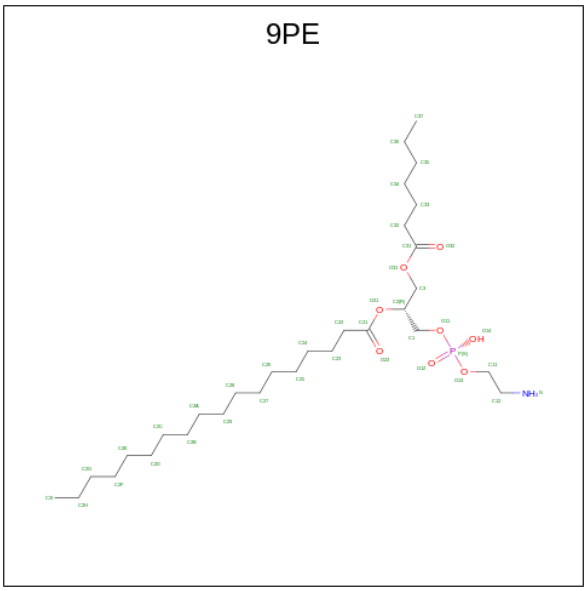
Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O		0
			43	39	4		
11	N	1	Total	C	O		0
			43	39	4		

- Molecule 12 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
12	S	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 13 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (three-letter code: 9PE) (formula: $C_{30}H_{60}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

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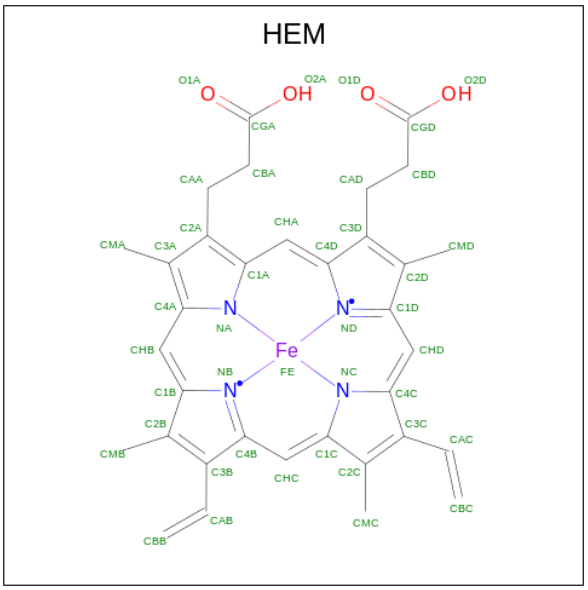
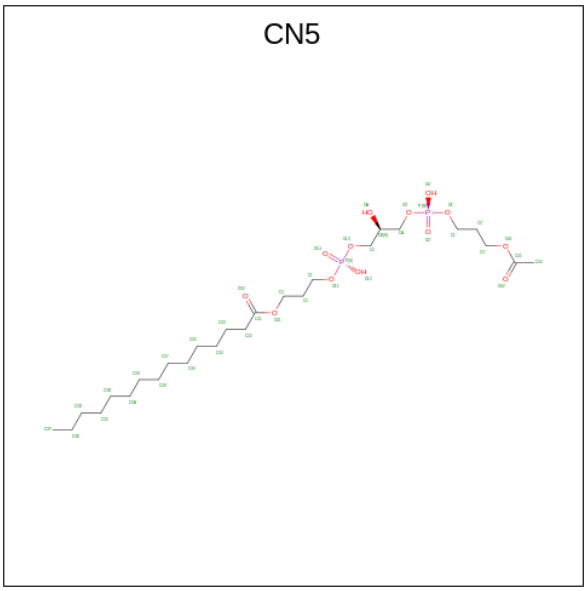
Mol	Chain	Residues	Atoms					AltConf
13	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



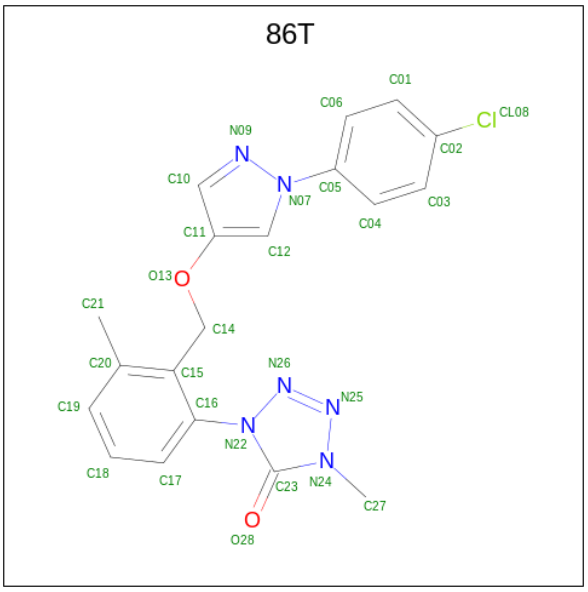
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (three-letter code: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



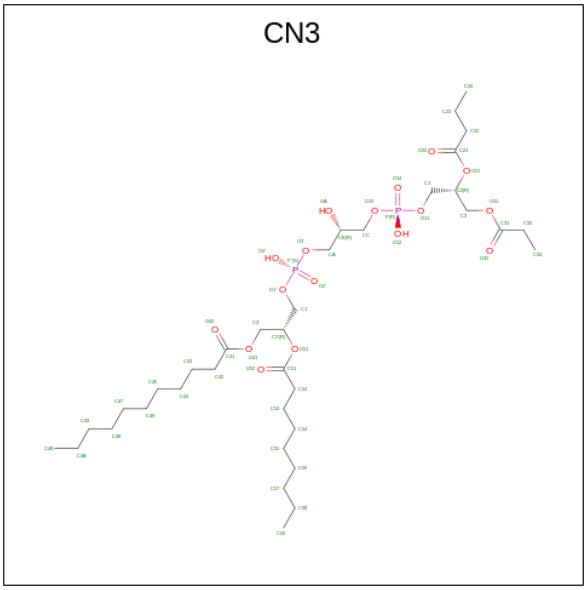
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 16 is metyltetraprole (three-letter code: 86T) (formula: $C_{19}H_{17}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



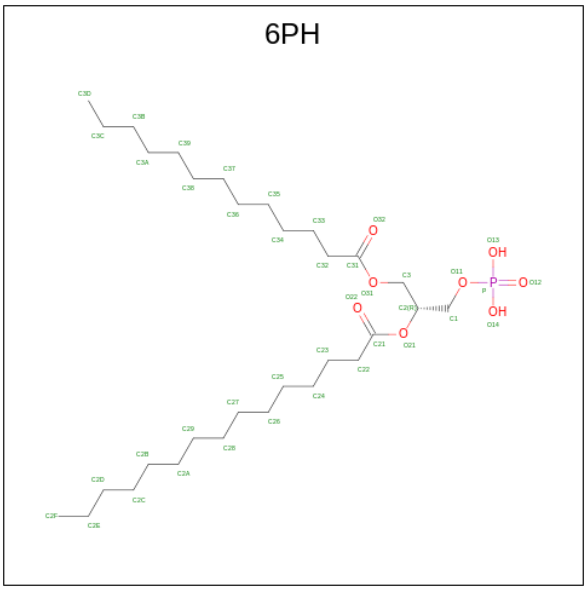
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
16	N	1	Total	C	Cl	N	O	0
			28	19	1	6	2	

- Molecule 17 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (three-letter code: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
17	C	1	Total	C	O	P	0
			55	36	17	2	
17	N	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 18 is (1R)-2-(phosphonooxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (three-letter code: 6PH) (formula: $C_{31}H_{61}O_8P$).

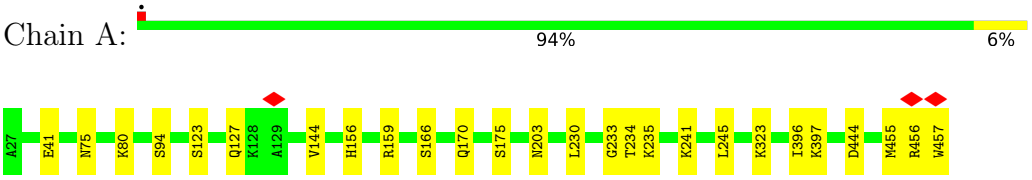


Mol	Chain	Residues	Atoms				AltConf
18	O	1	Total	C	O	P	0
			40	31	8	1	

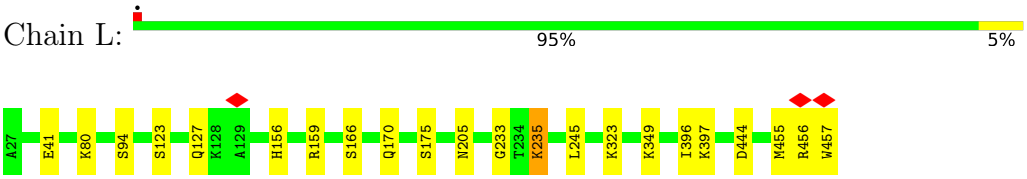
3 Residue-property plots (i)

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

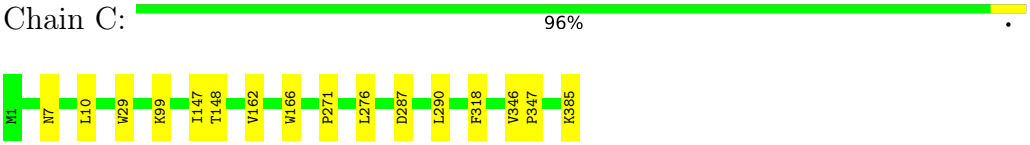
• Molecule 1: COR1 isoform 1



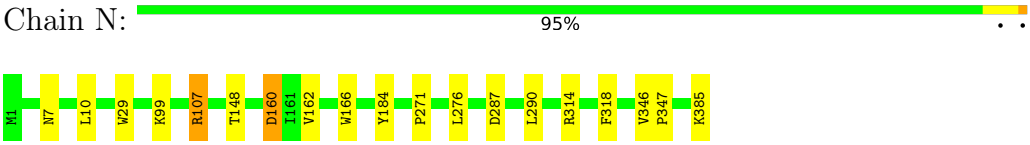
• Molecule 1: COR1 isoform 1



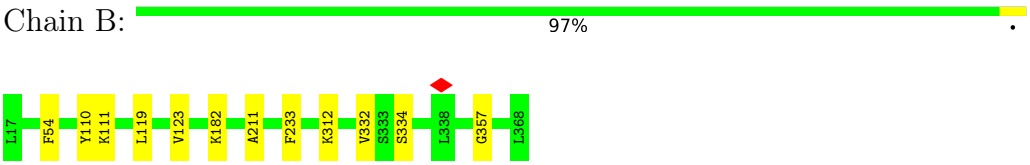
• Molecule 2: Cytochrome b



• Molecule 2: Cytochrome b

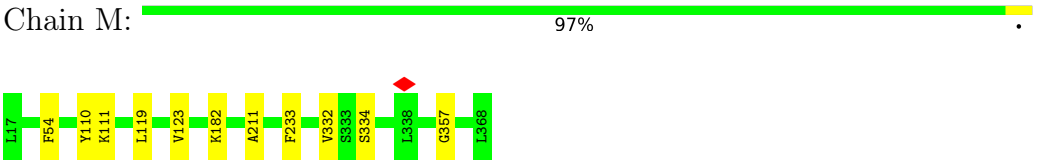


• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial



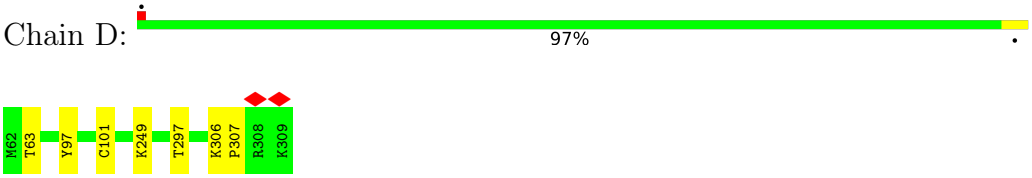
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



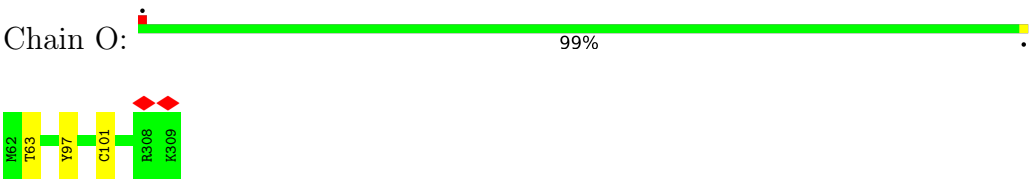
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



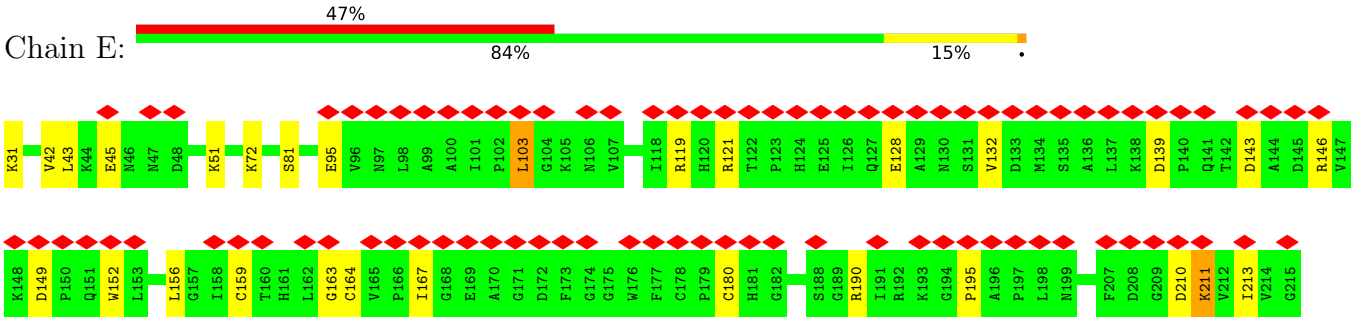
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



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

Chain E:

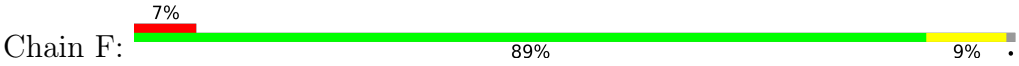


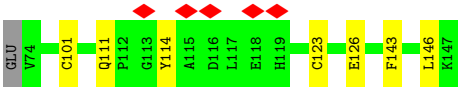
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:

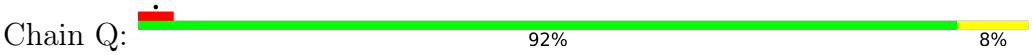
• Molecule 6: QCR6 isoform 1

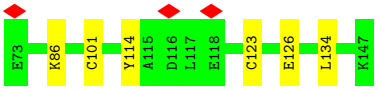
Chain F:



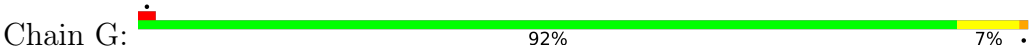


• Molecule 6: QCR6 isoform 1

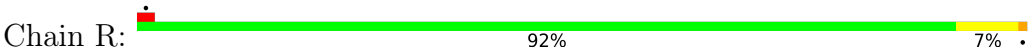




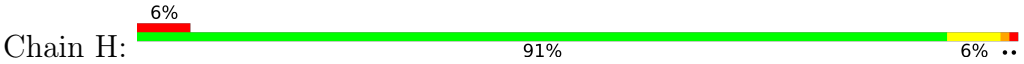
• Molecule 7: Cytochrome b-c1 complex subunit 7

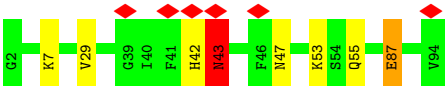


• Molecule 7: Cytochrome b-c1 complex subunit 7

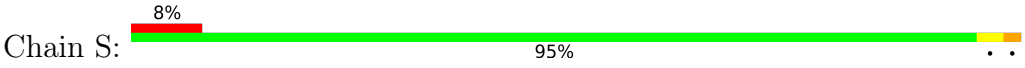


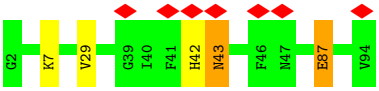
• Molecule 8: Cytochrome b-c1 complex subunit 8



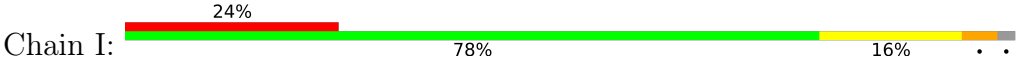


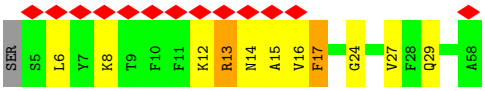
• Molecule 8: Cytochrome b-c1 complex subunit 8





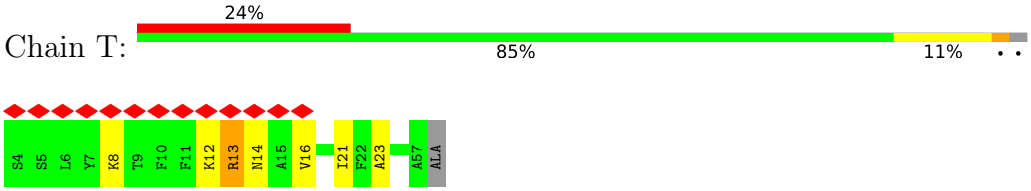
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial





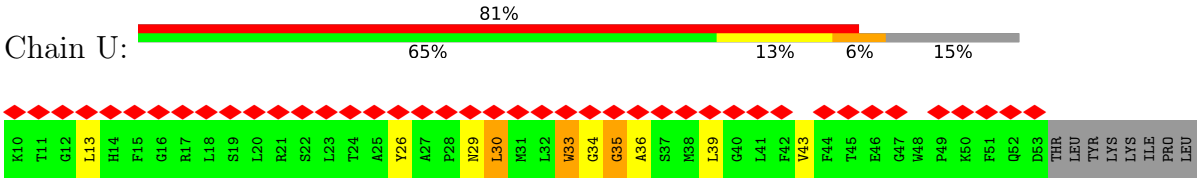
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain T:



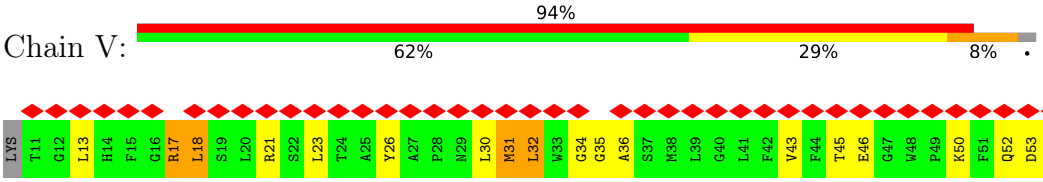
• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain U:



• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.48	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.808	Depositor
Minimum map value	-3.244	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 9PE, 8PE, CN3, CN5, 6PH, UQ6, 86T

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	0.39	2/3405 (0.1%)	0.56	0/4615
1	L	0.39	1/3405 (0.0%)	0.56	0/4615
2	C	0.38	0/3192	0.53	0/4354
2	N	0.38	0/3192	0.53	0/4354
3	B	0.36	0/2781	0.50	0/3764
3	M	0.36	0/2781	0.50	0/3764
4	D	0.34	0/2022	0.47	0/2751
4	O	0.34	0/2022	0.47	0/2751
5	E	0.40	1/1444 (0.1%)	0.72	3/1957 (0.2%)
5	P	0.48	2/1444 (0.1%)	0.73	3/1957 (0.2%)
6	F	0.31	0/638	0.55	0/858
6	Q	0.34	0/647	0.63	0/870
7	G	0.41	1/1040 (0.1%)	0.65	4/1408 (0.3%)
7	R	0.39	0/1040	0.57	1/1408 (0.1%)
8	H	0.49	1/804 (0.1%)	0.84	4/1088 (0.4%)
8	S	0.45	0/804	0.72	4/1088 (0.4%)
9	I	0.41	0/455	0.53	0/614
9	T	0.33	0/456	0.58	0/615
10	U	0.44	0/358	0.95	2/483 (0.4%)
10	V	0.53	1/419 (0.2%)	0.78	0/567
All	All	0.39	9/32349 (0.0%)	0.58	21/43881 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	L	0	1
2	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	2
6	Q	0	1
8	H	0	1
8	S	0	1
9	I	0	1
9	T	0	1
10	V	0	1
All	All	0	11

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	233	GLY	C-N	11.06	1.59	1.34
5	P	102	PRO	C-N	10.54	1.58	1.34
1	A	233	GLY	C-N	8.60	1.53	1.34
1	A	234	THR	C-N	7.89	1.52	1.34
8	H	43	ASN	C-N	7.56	1.51	1.34
7	G	2	PRO	C-N	7.20	1.50	1.34
5	E	103	LEU	C-N	6.88	1.45	1.33
10	V	53	ASP	C-N	6.43	1.48	1.34
5	P	196	ALA	C-N	5.66	1.45	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	43	ASN	O-C-N	-15.85	97.34	122.70
8	H	43	ASN	CA-C-N	10.13	139.48	117.20
8	S	43	ASN	O-C-N	-9.76	107.09	122.70
5	P	210	ASP	CB-CG-OD1	7.62	125.16	118.30
5	E	210	ASP	CB-CG-OD1	7.57	125.11	118.30
7	G	3	GLN	C-N-CA	7.54	140.55	121.70
8	S	43	ASN	CA-C-N	7.37	133.41	117.20
8	S	43	ASN	C-N-CA	7.01	139.24	121.70
8	S	87	GLU	CA-CB-CG	6.43	127.54	113.40
8	H	87	GLU	CA-CB-CG	6.39	127.45	113.40
7	G	2	PRO	C-N-CA	-6.24	106.10	121.70
7	G	3	GLN	O-C-N	-6.22	112.75	122.70
7	R	3	GLN	C-N-CA	6.13	137.02	121.70
8	H	42	HIS	O-C-N	-5.99	113.12	122.70
5	E	132	VAL	C-N-CA	5.83	136.27	121.70
10	U	30	LEU	CA-CB-CG	5.60	128.18	115.30
7	G	2	PRO	O-C-N	5.44	131.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	13	LEU	CA-CB-CG	5.37	127.65	115.30
5	P	103	LEU	O-C-N	-5.35	114.10	123.20
5	E	211	LYS	CD-CE-NZ	5.15	123.55	111.70
5	P	211	LYS	CD-CE-NZ	5.15	123.55	111.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Peptide
2	C	346	VAL	Peptide
8	H	43	ASN	Mainchain
9	I	6	LEU	Peptide
1	L	456	ARG	Peptide
2	N	107	ARG	Sidechain
2	N	346	VAL	Peptide
6	Q	114	TYR	Peptide
8	S	43	ASN	Mainchain
9	T	13	ARG	Sidechain
10	V	17	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3323	12	0
1	L	3344	0	3323	11	0
2	C	3090	0	3129	11	0
2	N	3090	0	3129	14	0
3	B	2735	0	2774	6	0
3	M	2735	0	2774	5	0
4	D	1961	0	1890	7	0
4	O	1961	0	1890	1	0
5	E	1411	0	1390	11	0
5	P	1411	0	1390	12	0
6	F	624	0	583	10	0
6	Q	633	0	589	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1019	0	1034	5	0
7	R	1019	0	1034	6	0
8	H	773	0	736	4	0
8	S	773	0	736	1	0
9	I	442	0	439	8	0
9	T	443	0	440	6	0
10	U	347	0	345	11	0
10	V	406	0	414	15	0
11	C	43	0	60	4	0
11	N	43	0	60	4	0
12	C	47	0	73	3	0
12	S	47	0	73	1	0
13	C	40	0	59	1	0
13	N	40	0	59	1	0
14	C	86	0	60	0	0
14	D	43	0	30	0	0
14	N	86	0	60	2	0
14	O	43	0	30	1	0
15	C	41	0	50	4	0
16	C	28	0	0	0	0
16	N	28	0	0	0	0
17	C	55	0	66	0	0
17	N	55	0	66	0	0
18	O	40	0	59	1	0
All	All	32326	0	32167	151	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 2.

All (151) 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)
5:E:164:CYS:HB3	5:E:180:CYS:SG	1.89	1.13
5:P:164:CYS:HB3	5:P:180:CYS:SG	1.89	1.13
6:F:101:CYS:HB3	6:F:123:CYS:SG	2.29	0.72
10:V:46:GLU:HA	10:V:52:GLN:HE21	1.54	0.72
1:A:75:ASN:HD22	1:A:144:VAL:CG2	2.04	0.70
6:Q:101:CYS:HB3	6:Q:123:CYS:SG	2.31	0.70
1:A:75:ASN:ND2	1:A:144:VAL:HG22	2.06	0.69
1:A:170:GLN:HE21	1:A:245:LEU:HD23	1.58	0.69
5:E:159:CYS:H	5:E:163:GLY:HA2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:GLN:HE21	1:L:245:LEU:HD23	1.58	0.69
9:I:13:ARG:HB3	9:I:16:VAL:HG23	1.76	0.68
2:C:385:LYS:HZ1	7:G:17:LYS:HE3	1.58	0.67
5:E:164:CYS:CB	5:E:180:CYS:SG	2.77	0.67
5:P:159:CYS:H	5:P:163:GLY:HA2	1.58	0.67
6:Q:101:CYS:SG	6:Q:126:GLU:HG2	2.36	0.65
10:U:33:TRP:HA	10:U:33:TRP:CE3	2.32	0.64
2:N:385:LYS:HZ1	7:R:17:LYS:HE3	1.62	0.64
6:F:101:CYS:SG	6:F:126:GLU:HG2	2.37	0.64
5:P:164:CYS:CB	5:P:180:CYS:SG	2.77	0.62
1:A:323:LYS:HB3	1:A:396:ILE:HD11	1.82	0.61
11:C:401:UQ6:H103	15:C:405:CN5:H33	1.80	0.61
5:E:164:CYS:SG	5:E:180:CYS:HB3	2.41	0.61
5:P:164:CYS:SG	5:P:180:CYS:HB3	2.41	0.61
1:L:323:LYS:HB3	1:L:396:ILE:HD11	1.82	0.60
5:E:72:LYS:HE2	9:I:29:GLN:HE22	1.67	0.60
1:A:75:ASN:HD22	1:A:144:VAL:HG21	1.66	0.58
10:U:30:LEU:HA	10:U:33:TRP:CB	2.34	0.57
7:G:55:ILE:HD13	7:G:111:GLU:HG2	1.87	0.56
2:N:148:THR:HG22	2:N:162:VAL:HG23	1.87	0.56
10:U:33:TRP:HA	10:U:33:TRP:HE3	1.69	0.56
4:D:249:LYS:HD2	6:F:146:LEU:HD12	1.87	0.56
14:N:404:HEM:HBC2	14:N:404:HEM:HHD	1.88	0.56
7:R:55:ILE:HD13	7:R:111:GLU:HG2	1.87	0.56
2:C:148:THR:HG22	2:C:162:VAL:HG23	1.87	0.55
5:P:164:CYS:HB3	5:P:180:CYS:HG	1.67	0.55
4:D:249:LYS:HE2	6:F:143:PHE:CE2	2.43	0.54
1:L:205:ASN:ND2	1:L:235:LYS:HE2	2.22	0.54
7:R:51:GLU:HA	7:R:56:MET:HG2	1.90	0.54
10:V:45:THR:HG22	10:V:52:GLN:HA	1.89	0.54
2:N:29:TRP:HB3	2:N:99:LYS:HG3	1.89	0.53
2:C:29:TRP:HB3	2:C:99:LYS:HG3	1.89	0.53
1:L:455:MET:HG2	9:T:14:ASN:OD1	2.10	0.52
11:C:401:UQ6:C10	15:C:405:CN5:H33	2.40	0.52
7:G:51:GLU:HA	7:G:56:MET:HG2	1.90	0.52
5:E:164:CYS:SG	5:E:180:CYS:CB	2.99	0.51
9:I:13:ARG:NH1	9:I:14:ASN:HB2	2.26	0.51
1:A:123:SER:H	1:A:127:GLN:HG3	1.76	0.51
2:N:287:ASP:HB3	2:N:290:LEU:HB2	1.92	0.51
5:P:164:CYS:SG	5:P:180:CYS:CB	2.99	0.51
5:P:72:LYS:HD2	10:U:43:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:287:ASP:HB3	2:C:290:LEU:HB2	1.92	0.50
5:E:72:LYS:HD2	10:V:43:VAL:O	2.12	0.50
10:V:32:LEU:O	10:V:36:ALA:N	2.45	0.49
1:L:123:SER:H	1:L:127:GLN:HG3	1.76	0.49
6:Q:101:CYS:SG	6:Q:126:GLU:CG	3.00	0.49
2:C:385:LYS:HB3	7:G:16:LEU:HD13	1.94	0.49
10:V:31:MET:O	10:V:35:GLY:N	2.38	0.49
5:P:65:LEU:HD12	9:T:21:ILE:HA	1.93	0.49
2:C:29:TRP:CH2	12:C:402:8PE:H33A	2.48	0.48
2:N:148:THR:HG21	2:N:166:TRP:NE1	2.28	0.48
2:N:385:LYS:HB3	7:R:16:LEU:HD13	1.96	0.48
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.62	0.48
2:C:148:THR:HG21	2:C:166:TRP:NE1	2.28	0.48
6:F:101:CYS:SG	6:F:126:GLU:CG	3.01	0.48
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.62	0.48
4:D:249:LYS:HE2	6:F:143:PHE:CD2	2.49	0.48
10:U:34:GLY:O	10:U:35:GLY:C	2.49	0.47
6:Q:101:CYS:SG	6:Q:126:GLU:CD	2.92	0.47
10:U:36:ALA:HA	10:U:39:LEU:HB3	1.96	0.47
8:H:43:ASN:HA	8:H:47:ASN:HB2	1.96	0.47
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.96	0.47
3:B:119:LEU:HA	3:B:123:VAL:HB	1.97	0.47
10:U:30:LEU:HA	10:U:33:TRP:HB2	1.97	0.46
10:U:26:TYR:HA	10:U:29:ASN:HB2	1.96	0.46
5:P:95:GLU:HG2	5:P:213:ILE:HG22	1.96	0.46
10:V:18:LEU:HD12	10:V:23:LEU:HB2	1.96	0.46
11:N:406:UQ6:H151	11:N:406:UQ6:H172	1.66	0.46
3:M:119:LEU:HA	3:M:123:VAL:HB	1.97	0.46
15:C:405:CN5:H3AB	15:C:405:CN5:H3DA	1.55	0.46
3:M:110:TYR:HD2	3:M:111:LYS:HG3	1.81	0.46
3:B:110:TYR:HD2	3:B:111:LYS:HG3	1.81	0.46
11:N:406:UQ6:H1M1	11:N:406:UQ6:H71	1.62	0.46
14:O:401:HEM:HBC2	14:O:401:HEM:HHD	1.97	0.46
10:V:45:THR:O	10:V:52:GLN:HG2	2.15	0.46
2:N:160:ASP:CG	10:V:50:LYS:HB2	2.36	0.45
1:A:241:LYS:HD3	1:A:241:LYS:HA	1.82	0.45
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.99	0.45
6:Q:86:LYS:HE3	6:Q:134:LEU:HD21	1.98	0.45
2:N:7:ASN:HA	13:N:403:9PE:H11	1.99	0.45
3:M:182:LYS:HE2	3:M:211:ALA:HB2	1.99	0.45
4:D:249:LYS:HD2	6:F:146:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:TYR:CE2	14:N:404:HEM:HBC1	2.53	0.44
1:L:396:ILE:HG23	1:L:397:LYS:HG3	2.00	0.44
4:D:97:TYR:HA	4:D:101:CYS:HB3	1.99	0.44
6:F:111:GLN:HG3	6:F:114:TYR:HB3	2.00	0.44
8:S:29:VAL:HG11	5:P:43:LEU:HD21	2.00	0.44
1:A:396:ILE:HG23	1:A:397:LYS:HG3	2.00	0.44
1:L:205:ASN:HD21	1:L:235:LYS:HE2	1.83	0.44
6:F:101:CYS:SG	6:F:126:GLU:CD	2.96	0.43
12:S:101:8PE:H25	12:S:101:8PE:H22A	1.86	0.43
3:B:182:LYS:HE2	3:B:211:ALA:HB2	1.99	0.43
9:T:23:ALA:HA	10:U:39:LEU:HD11	2.01	0.43
9:I:13:ARG:HD3	9:I:15:ALA:H	1.84	0.43
1:A:455:MET:HG2	9:I:14:ASN:HD21	1.83	0.43
11:C:401:UQ6:H301	11:C:401:UQ6:H322	1.86	0.43
4:O:97:TYR:HA	4:O:101:CYS:HB3	1.99	0.43
10:U:30:LEU:HA	10:U:33:TRP:HB3	2.01	0.43
1:L:349:LYS:HD3	1:L:349:LYS:HA	1.84	0.43
10:V:18:LEU:HD13	10:V:18:LEU:HA	1.85	0.43
3:B:332:VAL:HB	3:B:334:SER:H	1.84	0.43
2:C:271:PRO:HG2	2:C:276:LEU:HD23	2.01	0.42
3:B:233:PHE:HB3	3:B:357:GLY:HA2	2.01	0.42
10:V:31:MET:O	10:V:34:GLY:N	2.52	0.42
6:F:101:CYS:CB	6:F:123:CYS:SG	3.06	0.42
9:T:23:ALA:HB2	10:U:39:LEU:HD21	2.02	0.42
12:C:402:8PE:H1A	8:H:55:GLN:HE22	1.84	0.42
13:C:403:9PE:H2B	13:C:403:9PE:H2E	1.69	0.42
10:V:13:LEU:HD12	10:V:13:LEU:HA	1.92	0.42
2:N:160:ASP:OD1	10:V:50:LYS:HB2	2.20	0.42
9:I:17:PHE:HD1	9:I:17:PHE:HA	1.75	0.41
2:N:107:ARG:HH21	2:N:314:ARG:HA	1.84	0.41
11:N:406:UQ6:H321	11:N:406:UQ6:H301	1.94	0.41
2:N:271:PRO:HG2	2:N:276:LEU:HD23	2.01	0.41
11:N:406:UQ6:H251	11:N:406:UQ6:H272	1.82	0.41
9:I:24:GLY:HA2	9:I:27:VAL:HG22	2.01	0.41
2:C:147:ILE:HD13	2:C:147:ILE:HA	1.94	0.41
18:O:402:6PH:H38A	18:O:402:6PH:H3B	1.80	0.41
3:M:233:PHE:HB3	3:M:357:GLY:HA2	2.01	0.41
3:M:332:VAL:HB	3:M:334:SER:H	1.84	0.41
3:B:312:LYS:HD3	3:B:312:LYS:HA	1.87	0.41
4:D:297:THR:HG21	5:E:42:VAL:HG21	2.02	0.41
5:E:149:ASP:HB3	5:E:152:TRP:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:7:ASN:HB3	2:N:10:LEU:HB2	2.03	0.41
2:N:318:PHE:HB3	7:R:36:ALA:HB1	2.03	0.41
1:L:455:MET:O	9:T:14:ASN:ND2	2.54	0.41
5:P:149:ASP:HB3	5:P:152:TRP:HE3	1.86	0.41
1:A:203:ASN:HB2	1:A:230:LEU:HB2	2.03	0.41
2:C:7:ASN:HB3	2:C:10:LEU:HB2	2.03	0.41
4:D:306:LYS:HA	4:D:307:PRO:HD3	1.98	0.40
1:L:166:SER:HA	1:L:175:SER:HB2	2.03	0.40
8:H:53:LYS:HA	8:H:53:LYS:HD3	1.95	0.40
7:R:123:ILE:H	10:V:21:ARG:NH2	2.19	0.40
1:A:166:SER:HA	1:A:175:SER:HB2	2.03	0.40
5:P:79:ILE:HD13	5:P:79:ILE:HA	1.96	0.40
10:V:46:GLU:HA	10:V:52:GLN:NE2	2.30	0.40
2:C:318:PHE:HB3	7:G:36:ALA:HB1	2.03	0.40
11:C:401:UQ6:H102	15:C:405:CN5:H35A	2.02	0.40
12:C:402:8PE:H35	12:C:402:8PE:H38A	1.59	0.40
9:I:8:LYS:HA	9:I:12:LYS:HB3	2.03	0.40
9:T:8:LYS:HG2	9:T:12:LYS:HG2	2.03	0.40
10:V:26:TYR:CD2	10:V:30:LEU:HB2	2.56	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	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
1	L	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
2	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	37	57
2	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	37	57
3	B	350/352 (99%)	336 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
4	D	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
4	O	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
5	E	183/185 (99%)	152 (83%)	30 (16%)	1 (0%)	25	45
5	P	183/185 (99%)	154 (84%)	29 (16%)	0	100	100
6	F	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
6	Q	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
7	G	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
7	R	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/93 (98%)	79 (87%)	12 (13%)	0	100	100
8	S	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
9	I	52/55 (94%)	48 (92%)	4 (8%)	0	100	100
9	T	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
10	U	42/52 (81%)	32 (76%)	9 (21%)	1 (2%)	5	8
10	V	49/52 (94%)	36 (74%)	11 (22%)	2 (4%)	2	3
All	All	3952/4004 (99%)	3677 (93%)	269 (7%)	6 (0%)	45	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	V	17	ARG
10	V	54	THR
2	N	347	PRO
10	U	35	GLY
2	C	347	PRO
5	E	195	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	364 (98%)	6 (2%)	58 78
1	L	370/370 (100%)	364 (98%)	6 (2%)	58 78
2	C	338/338 (100%)	338 (100%)	0	100 100
2	N	338/338 (100%)	337 (100%)	1 (0%)	91 97
3	B	301/301 (100%)	300 (100%)	1 (0%)	91 97
3	M	301/301 (100%)	300 (100%)	1 (0%)	91 97
4	D	206/206 (100%)	205 (100%)	1 (0%)	86 95
4	O	206/206 (100%)	205 (100%)	1 (0%)	86 95
5	E	151/151 (100%)	136 (90%)	15 (10%)	6 12
5	P	151/151 (100%)	136 (90%)	15 (10%)	6 12
6	F	67/68 (98%)	67 (100%)	0	100 100
6	Q	68/68 (100%)	68 (100%)	0	100 100
7	G	110/110 (100%)	108 (98%)	2 (2%)	54 75
7	R	110/110 (100%)	108 (98%)	2 (2%)	54 75
8	H	77/77 (100%)	75 (97%)	2 (3%)	41 65
8	S	77/77 (100%)	74 (96%)	3 (4%)	27 51
9	I	44/45 (98%)	42 (96%)	2 (4%)	23 45
9	T	45/45 (100%)	43 (96%)	2 (4%)	24 46
10	U	35/43 (81%)	34 (97%)	1 (3%)	37 62
10	V	42/43 (98%)	39 (93%)	3 (7%)	12 25
All	All	3407/3418 (100%)	3343 (98%)	64 (2%)	52 74

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	80	LYS
1	A	94	SER
1	A	235	LYS
1	A	444	ASP
1	A	457	TRP
3	B	54	PHE
4	D	63	THR
5	E	31	LYS
5	E	45	GLU
5	E	51	LYS

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Mol	Chain	Res	Type
5	E	81	SER
5	E	103	LEU
5	E	119	ARG
5	E	121	ARG
5	E	128	GLU
5	E	139	ASP
5	E	143	ASP
5	E	146	ARG
5	E	156	LEU
5	E	167	ILE
5	E	190	ARG
5	E	211	LYS
2	N	160	ASP
7	G	17	LYS
7	G	100	VAL
8	H	7	LYS
8	H	87	GLU
9	I	13	ARG
9	I	17	PHE
1	L	41	GLU
1	L	80	LYS
1	L	94	SER
1	L	235	LYS
1	L	444	ASP
1	L	457	TRP
4	O	63	THR
3	M	54	PHE
8	S	7	LYS
8	S	42	HIS
8	S	87	GLU
5	P	31	LYS
5	P	45	GLU
5	P	51	LYS
5	P	81	SER
5	P	103	LEU
5	P	119	ARG
5	P	121	ARG
5	P	128	GLU
5	P	139	ASP
5	P	143	ASP
5	P	146	ARG
5	P	156	LEU

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Mol	Chain	Res	Type
5	P	167	ILE
5	P	190	ARG
5	P	211	LYS
7	R	17	LYS
7	R	100	VAL
9	T	13	ARG
9	T	16	VAL
10	U	33	TRP
10	V	18	LEU
10	V	31	MET
10	V	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	102	GLN
1	A	122	GLN
1	A	149	GLN
1	A	156	HIS
1	A	170	GLN
1	A	274	ASN
1	A	283	GLN
1	A	317	HIS
1	A	350	GLN
1	A	352	ASN
1	A	376	GLN
1	A	388	ASN
2	C	22	GLN
3	B	57	GLN
3	B	328	GLN
4	D	79	ASN
4	D	127	ASN
4	D	185	HIS
5	E	106	ASN
5	E	184	HIS
2	N	22	GLN
7	G	3	GLN
8	H	21	GLN
8	H	74	ASN
9	I	14	ASN
9	I	29	GLN

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Mol	Chain	Res	Type
1	L	102	GLN
1	L	122	GLN
1	L	149	GLN
1	L	156	HIS
1	L	170	GLN
1	L	274	ASN
1	L	283	GLN
1	L	317	HIS
1	L	350	GLN
1	L	352	ASN
1	L	376	GLN
1	L	388	ASN
4	O	79	ASN
4	O	127	ASN
4	O	185	HIS
3	M	57	GLN
3	M	328	GLN
8	S	21	GLN
8	S	74	ASN
5	P	106	ASN
7	R	3	GLN
9	T	44	ASN
10	V	52	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
17	CN3	C	407	-	54,54,54	1.16	8 (14%)	60,66,66	1.19	4 (6%)
16	86T	N	401	-	30,31,31	0.55	0	32,44,44	1.67	3 (9%)
11	UQ6	C	401	-	43,43,43	1.57	8 (18%)	51,55,55	1.52	10 (19%)
14	HEM	C	408	2	41,50,50	1.41	3 (7%)	45,82,82	1.44	8 (17%)
14	HEM	D	401	4	41,50,50	1.39	3 (7%)	45,82,82	1.42	7 (15%)
14	HEM	N	404	2	41,50,50	1.60	3 (7%)	45,82,82	1.94	13 (28%)
15	CN5	C	405	-	40,40,40	0.35	0	44,48,48	0.42	0
18	6PH	O	402	-	39,39,39	0.93	3 (7%)	43,44,44	1.16	2 (4%)
12	8PE	S	101	-	46,46,46	0.90	4 (8%)	49,51,51	1.07	2 (4%)
11	UQ6	N	406	-	43,43,43	1.68	11 (25%)	51,55,55	1.48	8 (15%)
14	HEM	N	405	2	41,50,50	1.44	4 (9%)	45,82,82	1.44	6 (13%)
12	8PE	C	402	-	46,46,46	0.48	0	49,51,51	0.49	0
13	9PE	N	403	-	39,39,39	0.94	4 (10%)	42,44,44	1.11	2 (4%)
13	9PE	C	403	-	39,39,39	0.93	4 (10%)	42,44,44	1.02	2 (4%)
14	HEM	O	401	4	41,50,50	1.53	4 (9%)	45,82,82	1.59	10 (22%)
16	86T	C	406	-	30,31,31	0.54	0	32,44,44	1.67	2 (6%)
14	HEM	C	404	2	41,50,50	1.51	4 (9%)	45,82,82	1.94	13 (28%)
17	CN3	N	402	-	54,54,54	1.16	7 (12%)	60,66,66	1.27	4 (6%)

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
17	CN3	C	407	-	-	25/65/65/65	-
16	86T	N	401	-	-	2/11/13/13	0/4/4/4
11	UQ6	C	401	-	-	6/39/39/39	0/1/1/1
14	HEM	C	408	2	-	3/12/54/54	-
14	HEM	D	401	4	-	0/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEM	N	404	2	-	4/12/54/54	-
15	CN5	C	405	-	-	27/44/44/44	-
18	6PH	O	402	-	-	26/41/41/41	-
12	8PE	S	101	-	-	18/50/50/50	-
11	UQ6	N	406	-	-	13/39/39/39	0/1/1/1
14	HEM	N	405	2	-	4/12/54/54	-
12	8PE	C	402	-	-	30/50/50/50	-
13	9PE	N	403	-	-	23/43/43/43	-
13	9PE	C	403	-	-	17/43/43/43	-
14	HEM	O	401	4	-	2/12/54/54	-
16	86T	C	406	-	-	2/11/13/13	0/4/4/4
14	HEM	C	404	2	-	4/12/54/54	-
17	CN3	N	402	-	-	36/65/65/65	-

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	404	HEM	C3C-C2C	-5.61	1.32	1.40
14	O	401	HEM	C3C-C2C	-5.26	1.33	1.40
11	N	406	UQ6	C7-C6	5.24	1.57	1.51
11	C	401	UQ6	C7-C6	4.76	1.56	1.51
14	C	404	HEM	C3C-C2C	-4.09	1.34	1.40
14	D	401	HEM	C3C-CAC	3.80	1.55	1.47
14	C	408	HEM	C3C-CAC	3.75	1.55	1.47
14	N	405	HEM	C3C-CAC	3.73	1.55	1.47
11	N	406	UQ6	C16-C14	3.70	1.59	1.51
14	O	401	HEM	C3C-CAC	3.68	1.55	1.47
14	N	405	HEM	C3C-C2C	-3.62	1.35	1.40
14	D	401	HEM	C3C-C2C	-3.52	1.35	1.40
14	C	408	HEM	C3C-C2C	-3.51	1.35	1.40
14	C	404	HEM	C3C-CAC	3.46	1.54	1.47
11	C	401	UQ6	C16-C14	3.36	1.58	1.51
14	N	404	HEM	C3C-CAC	3.17	1.54	1.47
14	N	405	HEM	CAB-C3B	3.14	1.56	1.47
14	C	408	HEM	CAB-C3B	3.12	1.55	1.47
14	C	404	HEM	CAB-C3B	2.99	1.55	1.47
14	N	404	HEM	CAB-C3B	2.99	1.55	1.47
14	D	401	HEM	CAB-C3B	2.83	1.55	1.47
12	S	101	8PE	O21-C2	-2.80	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	402	CN3	O21-C2	-2.76	1.39	1.46
11	C	401	UQ6	O3-C3	2.75	1.43	1.38
14	O	401	HEM	CAB-C3B	2.72	1.54	1.47
11	N	406	UQ6	C12-C13	2.66	1.59	1.50
11	N	406	UQ6	C11-C9	2.66	1.56	1.51
11	N	406	UQ6	C7-C8	2.58	1.56	1.50
17	C	407	CN3	O21-C2	-2.58	1.40	1.46
18	O	402	6PH	O21-C2	-2.55	1.40	1.46
17	N	402	CN3	O51-C2'	-2.53	1.40	1.46
17	C	407	CN3	O51-C2'	-2.48	1.40	1.46
17	C	407	CN3	O41-C3'	-2.46	1.39	1.45
11	C	401	UQ6	C7-C8	2.46	1.56	1.50
11	C	401	UQ6	C12-C13	2.43	1.58	1.50
11	N	406	UQ6	O3-C3	2.42	1.42	1.38
11	C	401	UQ6	C11-C9	2.40	1.56	1.51
12	S	101	8PE	O31-C3	-2.37	1.39	1.45
13	N	403	9PE	O31-C31	2.34	1.40	1.33
17	C	407	CN3	O31-C3	-2.34	1.39	1.45
17	N	402	CN3	O31-C3	-2.33	1.39	1.45
18	O	402	6PH	O31-C31	2.32	1.40	1.33
17	C	407	CN3	O51-C51	2.30	1.40	1.34
17	N	402	CN3	O41-C41	2.27	1.40	1.33
12	S	101	8PE	O31-C31	2.26	1.39	1.33
17	C	407	CN3	O41-C41	2.26	1.39	1.33
13	C	403	9PE	O21-C21	2.26	1.40	1.34
17	N	402	CN3	O31-C31	2.25	1.39	1.33
13	N	403	9PE	O21-C21	2.24	1.40	1.34
17	N	402	CN3	O41-C3'	-2.24	1.40	1.45
14	N	405	HEM	CAA-C2A	2.22	1.55	1.52
11	N	406	UQ6	C26-C24	2.22	1.55	1.51
13	C	403	9PE	O31-C31	2.21	1.39	1.33
18	O	402	6PH	O31-C3	-2.20	1.40	1.45
11	N	406	UQ6	C17-C18	2.20	1.57	1.50
17	N	402	CN3	O51-C51	2.19	1.40	1.34
17	C	407	CN3	O31-C31	2.19	1.39	1.33
11	N	406	UQ6	C31-C29	2.16	1.55	1.51
11	N	406	UQ6	C21-C19	2.14	1.55	1.51
13	C	403	9PE	O31-C3	-2.13	1.40	1.45
14	C	404	HEM	FE-ND	2.12	2.07	1.96
13	N	403	9PE	O21-C2	-2.11	1.41	1.46
17	C	407	CN3	O21-C21	2.11	1.40	1.34
13	N	403	9PE	O31-C3	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	401	UQ6	C26-C24	2.09	1.55	1.51
13	C	403	9PE	O21-C2	-2.07	1.41	1.46
11	N	406	UQ6	O4-C4	2.07	1.42	1.38
12	S	101	8PE	O21-C21	2.07	1.40	1.34
11	C	401	UQ6	C17-C18	2.05	1.57	1.50
14	O	401	HEM	C3B-C2B	-2.05	1.33	1.37

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	406	86T	C05-N07-N09	8.02	125.92	118.80
16	N	401	86T	C05-N07-N09	8.00	125.90	118.80
14	C	404	HEM	CAD-C3D-C4D	5.76	134.73	124.66
14	N	404	HEM	CAD-C3D-C4D	5.36	134.03	124.66
14	C	404	HEM	CAD-C3D-C2D	-5.10	118.37	127.88
14	N	404	HEM	CAD-C3D-C2D	-4.75	119.03	127.88
14	N	404	HEM	C4C-CHD-C1D	4.73	128.80	122.56
11	C	401	UQ6	C7-C8-C9	-4.40	120.41	127.24
17	N	402	CN3	O21-C21-C22	3.97	120.06	111.50
17	C	407	CN3	O51-C51-C52	3.96	120.04	111.50
17	N	402	CN3	O51-C51-C52	3.94	119.98	111.50
18	O	402	6PH	O21-C21-C22	3.89	119.88	111.50
17	C	407	CN3	O21-C21-C22	3.75	119.58	111.50
17	N	402	CN3	O31-C31-C32	3.65	120.95	111.38
14	O	401	HEM	C3B-C2B-C1B	3.45	109.04	106.49
14	O	401	HEM	C4B-CHC-C1C	3.43	127.08	122.56
12	S	101	8PE	O21-C21-C22	3.40	118.83	111.50
13	N	403	9PE	O21-C21-C22	3.36	118.75	111.50
17	C	407	CN3	O31-C31-C32	3.31	120.07	111.38
13	C	403	9PE	O21-C21-C22	3.27	118.55	111.50
14	C	408	HEM	CMC-C2C-C3C	3.19	130.65	124.68
14	N	405	HEM	CMC-C2C-C3C	3.13	130.53	124.68
14	C	404	HEM	C4C-CHD-C1D	3.13	126.68	122.56
14	D	401	HEM	CMC-C2C-C3C	3.11	130.49	124.68
11	N	406	UQ6	C10-C9-C11	3.04	120.39	115.27
14	C	404	HEM	CHA-C4D-C3D	3.03	131.02	125.33
11	N	406	UQ6	C15-C14-C16	2.98	120.28	115.27
14	D	401	HEM	CMB-C2B-C1B	-2.98	120.50	125.04
11	C	401	UQ6	C12-C13-C14	-2.97	120.50	127.66
14	O	401	HEM	C4C-CHD-C1D	2.94	126.44	122.56
11	N	406	UQ6	C2-C1-C6	2.93	121.93	118.75
14	C	404	HEM	C4D-ND-C1D	2.92	108.08	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	401	HEM	CHC-C4B-C3B	2.90	129.01	124.57
14	N	404	HEM	CBD-CAD-C3D	2.90	120.67	112.63
14	O	401	HEM	C1B-NB-C4B	2.89	108.06	105.07
11	N	406	UQ6	C30-C29-C31	2.88	120.11	115.27
14	C	408	HEM	C4D-ND-C1D	2.87	108.04	105.07
14	D	401	HEM	CAA-CBA-CGA	-2.82	105.86	113.76
14	C	404	HEM	CBD-CAD-C3D	2.81	120.42	112.63
14	N	404	HEM	CHA-C4D-C3D	2.78	130.55	125.33
18	O	402	6PH	O31-C31-C32	2.78	120.64	111.91
14	C	408	HEM	CMB-C2B-C1B	-2.78	120.81	125.04
11	C	401	UQ6	C17-C18-C19	-2.77	120.98	127.66
14	O	401	HEM	CAA-CBA-CGA	-2.75	106.06	113.76
13	N	403	9PE	O31-C31-C32	2.75	120.52	111.91
11	N	406	UQ6	C27-C28-C29	-2.70	121.15	127.66
11	C	401	UQ6	C20-C19-C21	2.69	119.80	115.27
14	O	401	HEM	CHB-C1B-NB	2.69	127.70	124.38
14	N	405	HEM	CMB-C2B-C1B	-2.67	120.97	125.04
12	S	101	8PE	O31-C31-C32	2.67	120.28	111.91
11	C	401	UQ6	C25-C24-C26	2.66	119.74	115.27
11	N	406	UQ6	C25-C24-C26	2.65	119.74	115.27
11	C	401	UQ6	C22-C23-C24	-2.65	121.28	127.66
14	N	404	HEM	C4D-ND-C1D	2.64	107.80	105.07
11	N	406	UQ6	C22-C23-C24	-2.63	121.33	127.66
14	C	404	HEM	CHD-C1D-ND	2.62	127.28	124.43
11	N	406	UQ6	C17-C18-C19	-2.57	121.48	127.66
14	N	405	HEM	C4D-ND-C1D	2.57	107.72	105.07
14	N	405	HEM	C4B-CHC-C1C	2.56	125.94	122.56
16	N	401	86T	C10-N09-N07	2.48	105.50	103.70
14	N	404	HEM	CHD-C1D-ND	2.48	127.12	124.43
11	C	401	UQ6	C10-C9-C11	2.47	119.43	115.27
14	N	405	HEM	C4A-C3A-C2A	2.47	108.71	107.00
16	C	406	86T	C10-N09-N07	2.44	105.47	103.70
14	C	408	HEM	C4B-CHC-C1C	2.43	125.76	122.56
14	C	404	HEM	CBA-CAA-C2A	-2.41	108.51	112.62
17	C	407	CN3	O41-C41-C42	2.41	119.46	111.91
17	N	402	CN3	O41-C41-C42	2.40	119.45	111.91
14	N	404	HEM	CBA-CAA-C2A	-2.39	108.55	112.62
14	C	404	HEM	C3D-C4D-ND	-2.38	107.51	110.17
11	C	401	UQ6	C36-C34-C35	2.38	119.87	114.60
11	C	401	UQ6	C15-C14-C16	2.38	119.28	115.27
14	C	404	HEM	CHA-C4D-ND	-2.36	121.47	124.38
14	C	408	HEM	CMA-C3A-C4A	-2.34	124.86	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	D	401	HEM	C4B-CHC-C1C	2.27	125.55	122.56
14	D	401	HEM	C1B-NB-C4B	2.25	107.39	105.07
14	C	404	HEM	C1D-C2D-C3D	2.23	109.30	106.96
14	N	405	HEM	C1B-NB-C4B	2.22	107.37	105.07
14	C	404	HEM	C1B-NB-C4B	2.21	107.36	105.07
14	N	404	HEM	CHA-C4D-ND	-2.20	121.67	124.38
11	C	401	UQ6	C30-C29-C31	2.18	118.95	115.27
14	O	401	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
14	O	401	HEM	CAB-C3B-C2B	-2.16	121.49	128.60
14	C	408	HEM	C1B-NB-C4B	2.15	107.29	105.07
14	N	404	HEM	C3D-C4D-ND	-2.15	107.78	110.17
14	C	408	HEM	C3D-C4D-ND	-2.11	107.82	110.17
14	D	401	HEM	C4C-CHD-C1D	2.09	125.31	122.56
14	O	401	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
14	D	401	HEM	CAD-CBD-CGD	-2.07	109.15	113.60
14	N	404	HEM	C4B-CHC-C1C	2.06	125.28	122.56
14	N	404	HEM	C1B-NB-C4B	2.04	107.18	105.07
14	C	404	HEM	CMC-C2C-C3C	2.03	128.47	124.68
14	C	408	HEM	C4C-CHD-C1D	2.02	125.22	122.56
13	C	403	9PE	O31-C31-C32	2.02	118.24	111.91
14	N	404	HEM	C2C-C3C-C4C	2.01	108.30	106.90
16	N	401	86T	C06-C05-N07	2.01	120.91	119.15

There are no chirality outliers.

All (242) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	UQ6	C9-C11-C12-C13
11	C	401	UQ6	C19-C21-C22-C23
11	N	406	UQ6	C1-C6-C7-C8
11	N	406	UQ6	C23-C24-C26-C27
11	N	406	UQ6	C25-C24-C26-C27
11	N	406	UQ6	C28-C29-C31-C32
11	N	406	UQ6	C30-C29-C31-C32
12	C	402	8PE	C1-O11-P-O13
12	C	402	8PE	C1-O11-P-O14
12	C	402	8PE	C11-O13-P-O12
12	C	402	8PE	C11-O13-P-O14
12	C	402	8PE	O11-C1-C2-O21
12	C	402	8PE	O22-C21-O21-C2
12	S	101	8PE	C1-O11-P-O12
12	S	101	8PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
13	C	403	9PE	C1-O11-P-O12
13	C	403	9PE	C1-O11-P-O13
13	C	403	9PE	C1-O11-P-O14
13	C	403	9PE	O13-C11-C12-N
13	N	403	9PE	C11-O13-P-O11
13	N	403	9PE	C11-O13-P-O14
14	C	404	HEM	C2D-C3D-CAD-CBD
14	C	404	HEM	C4D-C3D-CAD-CBD
14	N	404	HEM	C2D-C3D-CAD-CBD
14	N	404	HEM	C4D-C3D-CAD-CBD
14	N	405	HEM	C1A-C2A-CAA-CBA
14	N	405	HEM	C3A-C2A-CAA-CBA
15	C	405	CN5	C1-O11-P-O13
15	C	405	CN5	C1-O11-P-O14
15	C	405	CN5	C2-C1-O11-P
15	C	405	CN5	O11-C1-C2-C3
15	C	405	CN5	C1'-O1'-P'-O4'
15	C	405	CN5	CB-CA-O3'-P'
17	C	407	CN3	O3'-CA-CB-OA
17	C	407	CN3	O3'-CA-CB-CC
17	N	402	CN3	C1-O11-P-O12
17	N	402	CN3	C1-O11-P-O14
17	N	402	CN3	CC-O13-P-O12
17	N	402	CN3	C1'-O1'-P'-O2'
17	N	402	CN3	C1'-O1'-P'-O4'
17	N	402	CN3	CA-O3'-P'-O2'
17	N	402	CN3	O3'-CA-CB-CC
18	O	402	6PH	C1-O11-P-O13
18	O	402	6PH	C1-O11-P-O14
12	S	101	8PE	C32-C31-O31-C3
12	S	101	8PE	O32-C31-O31-C3
13	N	403	9PE	O32-C31-O31-C3
13	N	403	9PE	O22-C21-O21-C2
13	N	403	9PE	C32-C31-O31-C3
15	C	405	CN5	C42-C41-O41-C3'
12	C	402	8PE	C22-C21-O21-C2
11	C	401	UQ6	C12-C11-C9-C10
11	C	401	UQ6	C12-C11-C9-C8
17	N	402	CN3	O3'-CA-CB-OA
12	C	402	8PE	C3B-C3C-C3D-C3E
13	C	403	9PE	C22-C21-O21-C2
13	N	403	9PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
13	C	403	9PE	O22-C21-O21-C2
15	C	405	CN5	C3A-C3B-C3C-C3D
11	N	406	UQ6	C15-C14-C16-C17
11	N	406	UQ6	C13-C14-C16-C17
11	N	406	UQ6	C9-C11-C12-C13
18	O	402	6PH	C32-C31-O31-C3
17	N	402	CN3	C32-C31-O31-C3
17	C	407	CN3	O51-C2'-C3'-O41
15	C	405	CN5	O42-C41-O41-C3'
12	C	402	8PE	C35-C36-C37-C38
15	C	405	CN5	C31-C32-C33-C34
18	O	402	6PH	C31-C32-C33-C34
17	C	407	CN3	C42-C41-O41-C3'
17	N	402	CN3	C51-C52-C53-C54
15	C	405	CN5	C1-C2-C3-O31
17	N	402	CN3	O32-C31-O31-C3
11	N	406	UQ6	C14-C16-C17-C18
11	N	406	UQ6	C19-C21-C22-C23
18	O	402	6PH	O32-C31-O31-C3
12	C	402	8PE	C11-O13-P-O11
12	S	101	8PE	C1-O11-P-O13
15	C	405	CN5	CC-O13-P-O11
15	C	405	CN5	C1'-O1'-P'-O3'
17	C	407	CN3	CC-O13-P-O11
17	N	402	CN3	C1-O11-P-O13
17	N	402	CN3	C1'-O1'-P'-O3'
17	N	402	CN3	CA-O3'-P'-O1'
12	C	402	8PE	C31-C32-C33-C34
15	C	405	CN5	C32-C31-O31-C3
17	N	402	CN3	C22-C21-O21-C2
12	C	402	8PE	C38-C39-C3A-C3B
18	O	402	6PH	C23-C24-C25-C26
18	O	402	6PH	C26-C27-C28-C29
12	C	402	8PE	C34-C35-C36-C37
15	C	405	CN5	C39-C3A-C3B-C3C
17	N	402	CN3	C52-C53-C54-C55
12	S	101	8PE	C36-C37-C38-C39
13	C	403	9PE	C2E-C2F-C2G-C2H
15	C	405	CN5	C34-C35-C36-C37
12	C	402	8PE	C27-C28-C29-C2A
17	N	402	CN3	C41-C42-C43-C44
13	N	403	9PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
18	O	402	6PH	C25-C26-C27-C28
17	C	407	CN3	O42-C41-O41-C3'
17	N	402	CN3	O22-C21-O21-C2
17	N	402	CN3	C52-C51-O51-C2'
12	S	101	8PE	C38-C39-C3A-C3B
12	S	101	8PE	C3A-C3B-C3C-C3D
18	O	402	6PH	C33-C34-C35-C36
12	C	402	8PE	O13-C11-C12-N
12	C	402	8PE	C22-C23-C24-C25
12	C	402	8PE	C2A-C2B-C2C-C2D
12	S	101	8PE	C35-C36-C37-C38
15	C	405	CN5	C32-C33-C34-C35
18	O	402	6PH	C36-C37-C38-C39
17	C	407	CN3	C51-C52-C53-C54
15	C	405	CN5	O32-C31-O31-C3
13	C	403	9PE	C24-C25-C26-C27
15	C	405	CN5	C33-C34-C35-C36
13	N	403	9PE	C2E-C2F-C2G-C2H
18	O	402	6PH	C22-C23-C24-C25
12	C	402	8PE	C23-C24-C25-C26
17	N	402	CN3	O52-C51-O51-C2'
18	O	402	6PH	C37-C38-C39-C3A
12	S	101	8PE	C3E-C3F-C3G-C3H
12	C	402	8PE	C21-C22-C23-C24
17	C	407	CN3	C47-C48-C49-C4A
13	N	403	9PE	C26-C27-C28-C29
15	C	405	CN5	C3C-C3D-C3E-C3F
18	O	402	6PH	C27-C28-C29-C2A
18	O	402	6PH	C24-C25-C26-C27
11	N	406	UQ6	C12-C11-C9-C10
11	N	406	UQ6	C12-C11-C9-C8
13	C	403	9PE	C28-C29-C2A-C2B
12	C	402	8PE	C24-C25-C26-C27
18	O	402	6PH	C35-C36-C37-C38
17	C	407	CN3	C43-C44-C45-C46
17	N	402	CN3	C42-C43-C44-C45
17	N	402	CN3	CC-O13-P-O11
12	C	402	8PE	C3C-C3D-C3E-C3F
18	O	402	6PH	C29-C2A-C2B-C2C
12	C	402	8PE	C29-C2A-C2B-C2C
12	S	101	8PE	C28-C29-C2A-C2B
13	N	403	9PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
17	C	407	CN3	C1'-C2'-C3'-O41
13	N	403	9PE	C21-C22-C23-C24
17	C	407	CN3	C32-C31-O31-C3
13	N	403	9PE	C3-C2-O21-C21
18	O	402	6PH	C1-O11-P-O12
17	C	407	CN3	C45-C46-C47-C48
12	C	402	8PE	C39-C3A-C3B-C3C
13	N	403	9PE	C25-C26-C27-C28
13	C	403	9PE	C23-C24-C25-C26
17	N	402	CN3	C56-C57-C58-C59
12	S	101	8PE	O11-C1-C2-C3
13	C	403	9PE	O11-C1-C2-C3
13	N	403	9PE	O11-C1-C2-C3
11	C	401	UQ6	C24-C26-C27-C28
18	O	402	6PH	C32-C33-C34-C35
15	C	405	CN5	O1'-C1'-C2'-C3'
13	C	403	9PE	C31-C32-C33-C34
17	C	407	CN3	C1-C2-C3-O31
17	N	402	CN3	C1'-C2'-C3'-O41
17	C	407	CN3	O32-C31-O31-C3
18	O	402	6PH	O11-C1-C2-O21
17	C	407	CN3	O51-C51-C52-C53
17	N	402	CN3	O51-C2'-C3'-O41
13	N	403	9PE	C2A-C2B-C2C-C2D
15	C	405	CN5	C1'-C2'-C3'-O41
13	N	403	9PE	C24-C25-C26-C27
15	C	405	CN5	C36-C37-C38-C39
12	C	402	8PE	O11-C1-C2-C3
18	O	402	6PH	O11-C1-C2-C3
12	C	402	8PE	C32-C33-C34-C35
13	N	403	9PE	C29-C2A-C2B-C2C
18	O	402	6PH	C22-C21-O21-C2
13	C	403	9PE	C3-C2-O21-C21
17	N	402	CN3	C2-C1-O11-P
13	C	403	9PE	O11-C1-C2-O21
13	N	403	9PE	O11-C1-C2-O21
17	C	407	CN3	C52-C53-C54-C55
17	N	402	CN3	C55-C56-C57-C58
18	O	402	6PH	O22-C21-O21-C2
18	O	402	6PH	C2A-C2B-C2C-C2D
15	C	405	CN5	CA-O3'-P'-O1'
12	C	402	8PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
13	N	403	9PE	C11-O13-P-O12
15	C	405	CN5	CC-O13-P-O14
17	C	407	CN3	CC-O13-P-O12
17	N	402	CN3	CC-O13-P-O14
17	N	402	CN3	CA-O3'-P'-O4'
13	C	403	9PE	C2A-C2B-C2C-C2D
17	N	402	CN3	C45-C46-C47-C48
17	C	407	CN3	C42-C43-C44-C45
12	S	101	8PE	O11-C1-C2-O21
18	O	402	6PH	C34-C35-C36-C37
17	C	407	CN3	C41-C42-C43-C44
13	N	403	9PE	O21-C2-C3-O31
17	C	407	CN3	O21-C2-C3-O31
11	N	406	UQ6	C5-C6-C7-C8
17	N	402	CN3	C46-C47-C48-C49
15	C	405	CN5	C38-C39-C3A-C3B
12	C	402	8PE	C2B-C2C-C2D-C2E
17	C	407	CN3	C2-C1-O11-P
17	N	402	CN3	O42-C41-O41-C3'
15	C	405	CN5	C3B-C3C-C3D-C3E
12	S	101	8PE	C34-C35-C36-C37
17	N	402	CN3	C42-C41-O41-C3'
13	N	403	9PE	C28-C29-C2A-C2B
13	N	403	9PE	C2F-C2G-C2H-C2I
18	O	402	6PH	O21-C2-C3-O31
13	C	403	9PE	C32-C33-C34-C35
17	C	407	CN3	C44-C45-C46-C47
14	N	405	HEM	CAA-CBA-CGA-O1A
12	C	402	8PE	C3F-C3G-C3H-C3I
12	C	402	8PE	C36-C37-C38-C39
17	N	402	CN3	C53-C54-C55-C56
12	S	101	8PE	O21-C2-C3-O31
11	C	401	UQ6	C30-C29-C31-C32
17	C	407	CN3	O41-C41-C42-C43
14	N	405	HEM	CAA-CBA-CGA-O2A
17	C	407	CN3	O52-C51-C52-C53
17	N	402	CN3	O41-C41-C42-C43
12	C	402	8PE	O21-C2-C3-O31
14	C	404	HEM	CAA-CBA-CGA-O1A
14	O	401	HEM	CAA-CBA-CGA-O1A
14	C	408	HEM	CAA-CBA-CGA-O2A
13	C	403	9PE	O31-C31-C32-C33

Continued on next page...

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Mol	Chain	Res	Type	Atoms
12	S	101	8PE	C37-C38-C39-C3A
16	C	406	86T	C04-C05-N07-C12
16	C	406	86T	C06-C05-N07-C12
16	N	401	86T	C04-C05-N07-C12
16	N	401	86T	C06-C05-N07-C12
14	C	408	HEM	CAD-CBD-CGD-O2D
17	C	407	CN3	O42-C41-C42-C43
14	C	408	HEM	CAA-CBA-CGA-O1A
12	S	101	8PE	C12-C11-O13-P
17	N	402	CN3	O42-C41-C42-C43
14	N	404	HEM	CAD-CBD-CGD-O1D
14	C	404	HEM	CAA-CBA-CGA-O2A
13	N	403	9PE	C23-C24-C25-C26
14	O	401	HEM	CAA-CBA-CGA-O2A
14	N	404	HEM	CAD-CBD-CGD-O2D
18	O	402	6PH	C38-C39-C3A-C3B
12	S	101	8PE	C3D-C3E-C3F-C3G

There are no ring outliers.

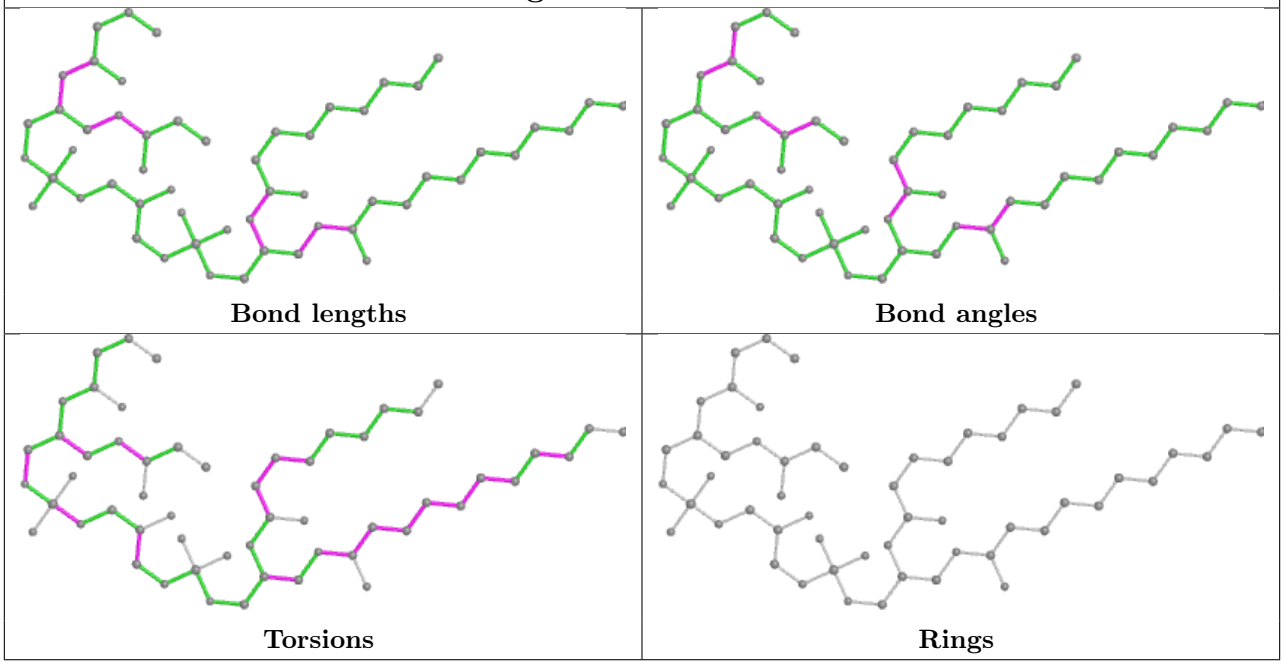
10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	401	UQ6	4	0
14	N	404	HEM	2	0
15	C	405	CN5	4	0
18	O	402	6PH	1	0
12	S	101	8PE	1	0
11	N	406	UQ6	4	0
12	C	402	8PE	3	0
13	N	403	9PE	1	0
13	C	403	9PE	1	0
14	O	401	HEM	1	0

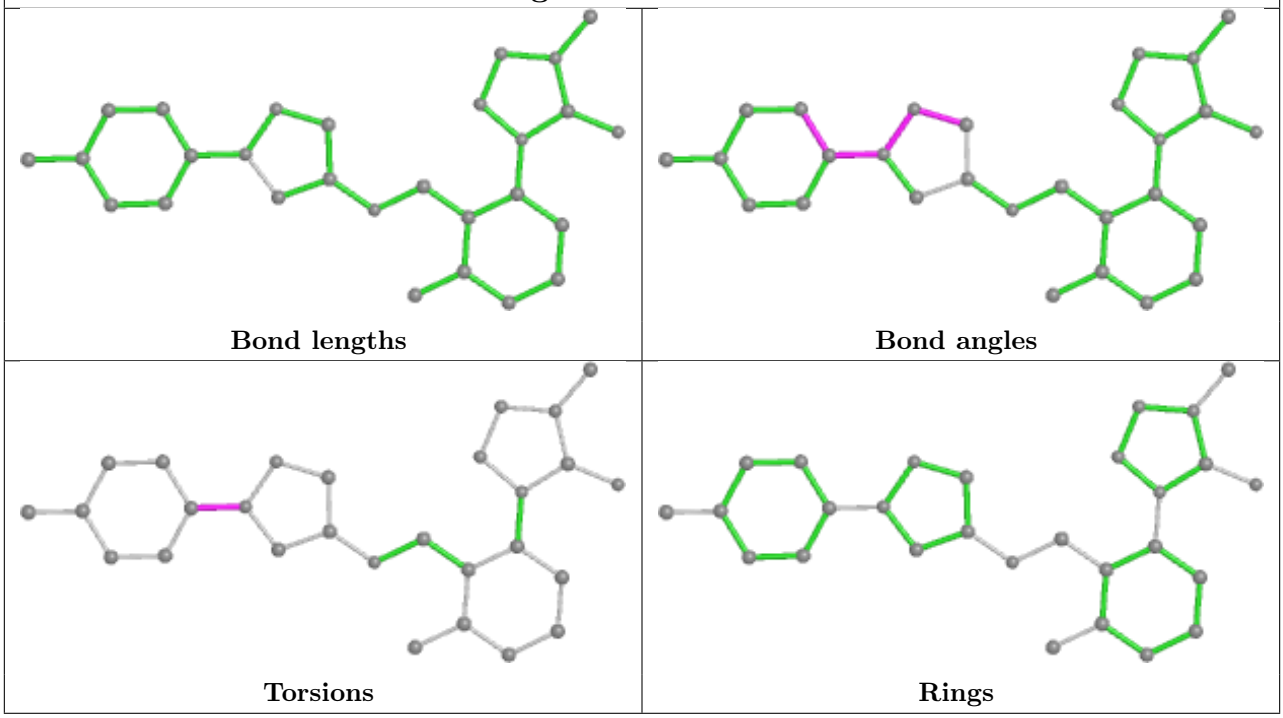
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

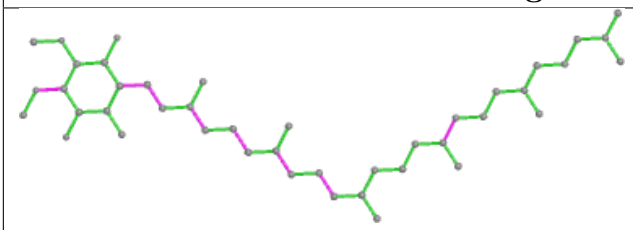
Ligand CN3 C 407



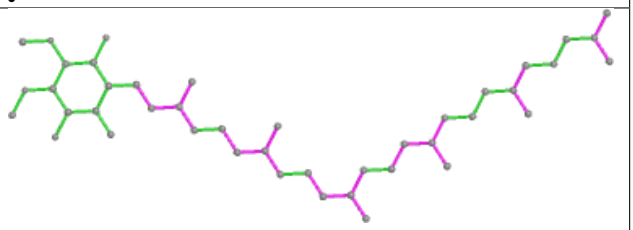
Ligand 86T N 401



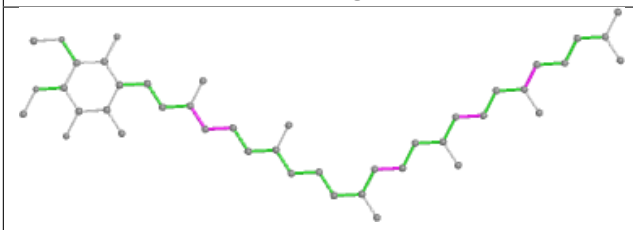
Ligand UQ6 C 401



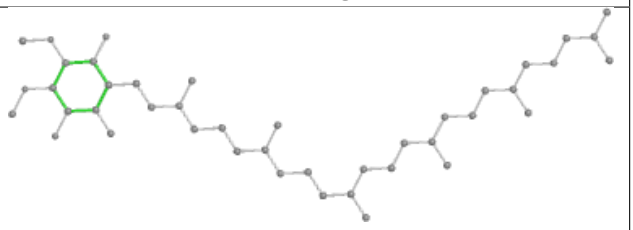
Bond lengths



Bond angles

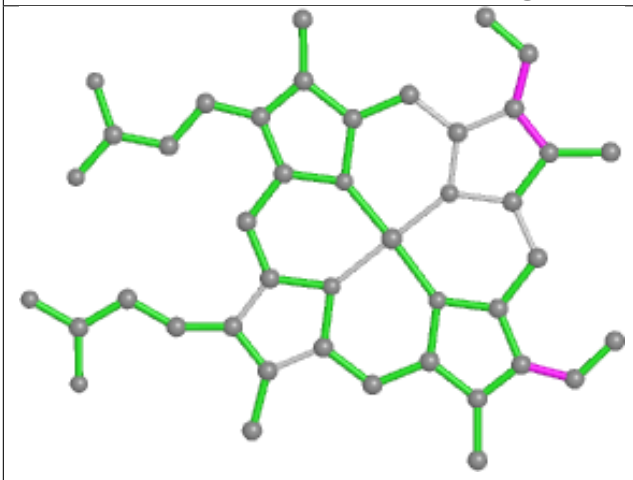


Torsions

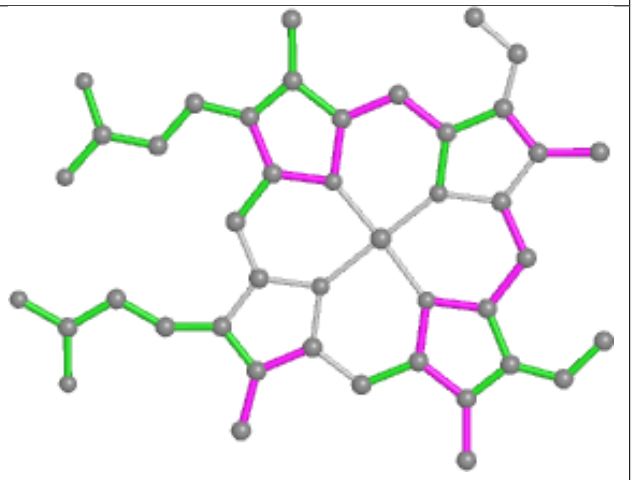


Rings

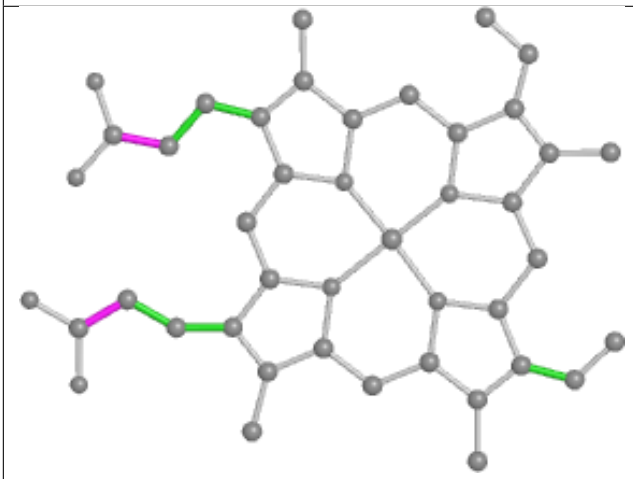
Ligand HEM C 408



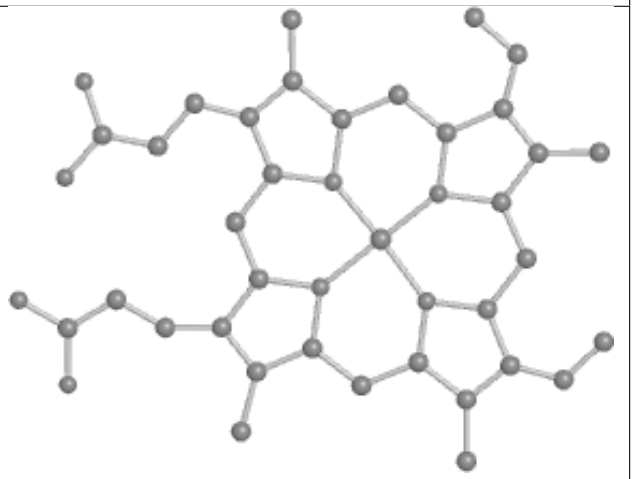
Bond lengths



Bond angles

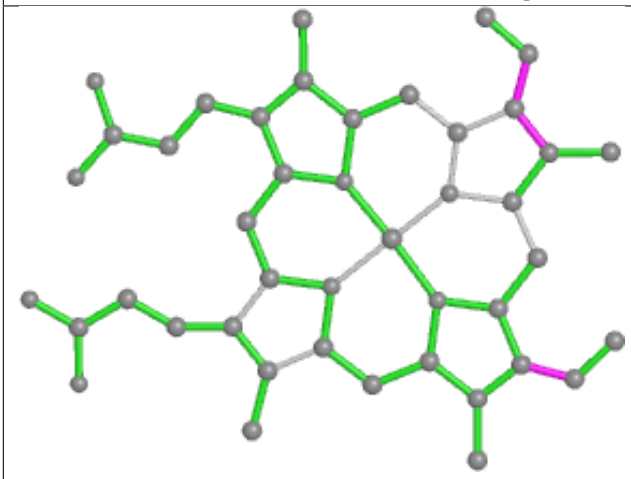


Torsions

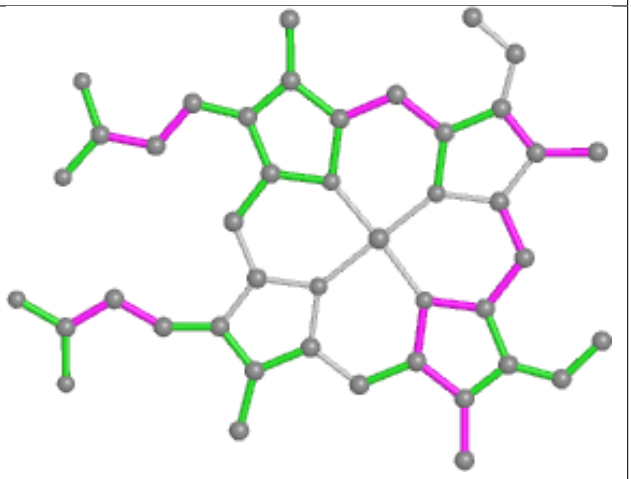


Rings

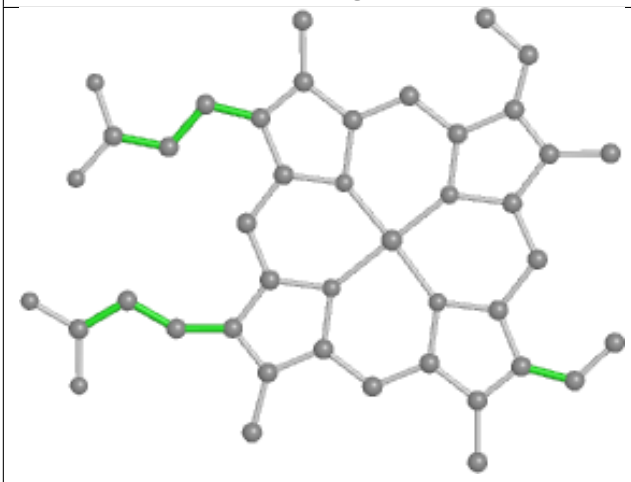
Ligand HEM D 401



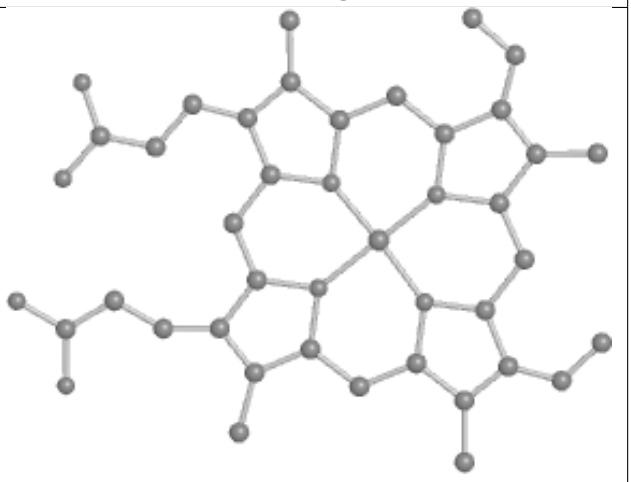
Bond lengths



Bond angles

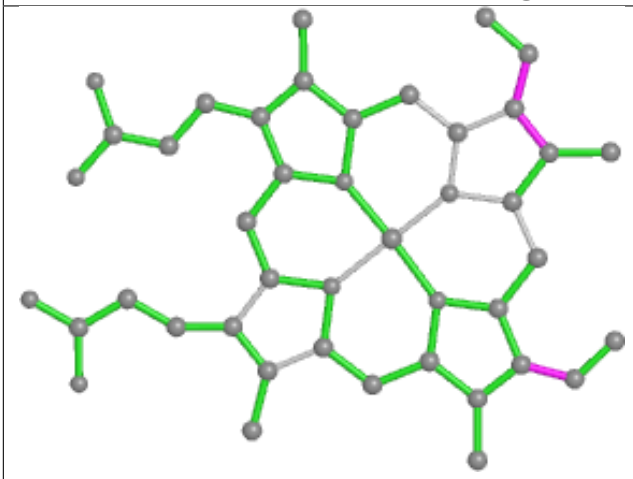


Torsions



Rings

Ligand HEM N 404



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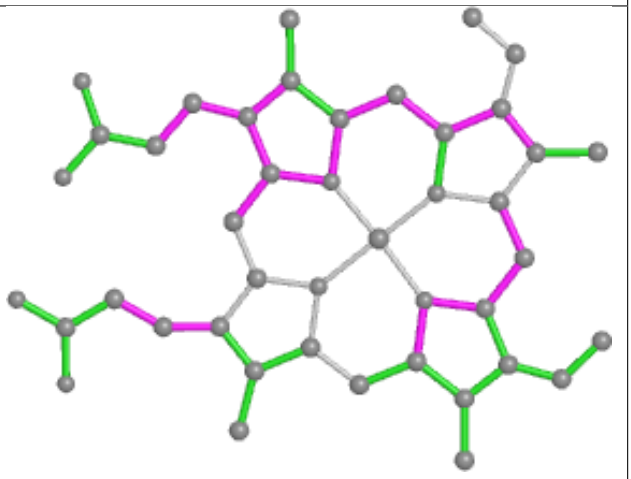
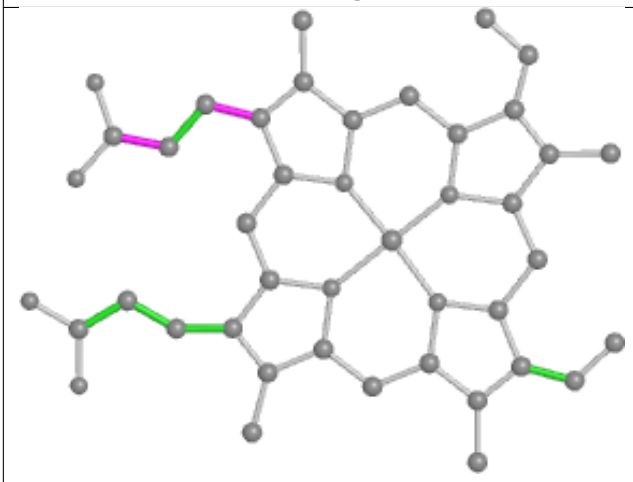
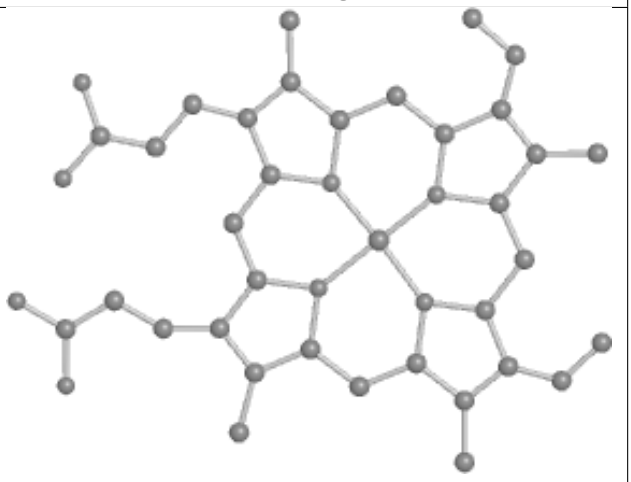


Bond angles

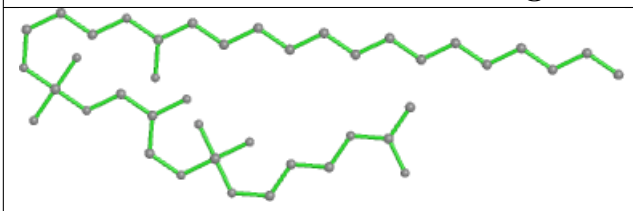


Torsions



Rings

Ligand CN5 C 405



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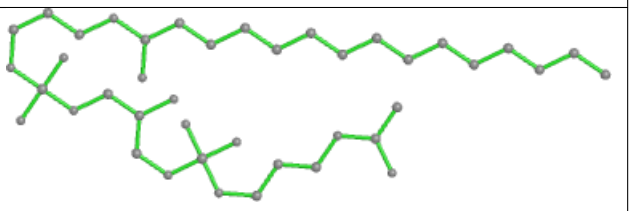
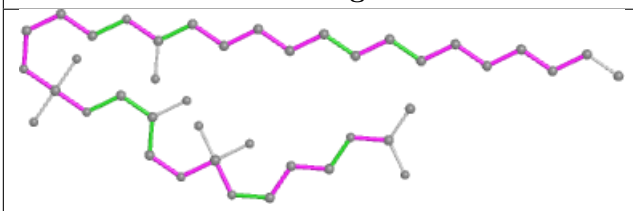


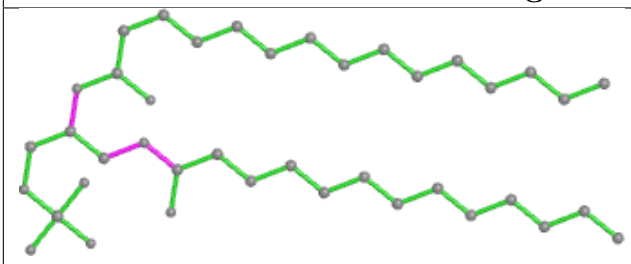
Bond angles



Torsions

Rings

Ligand 6PH O 402



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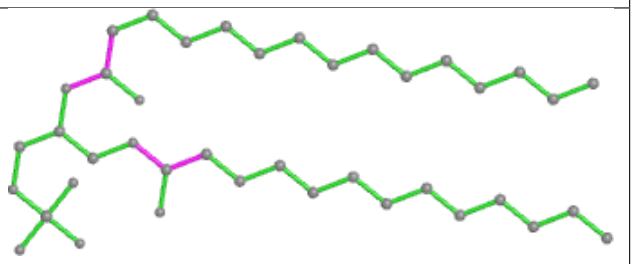

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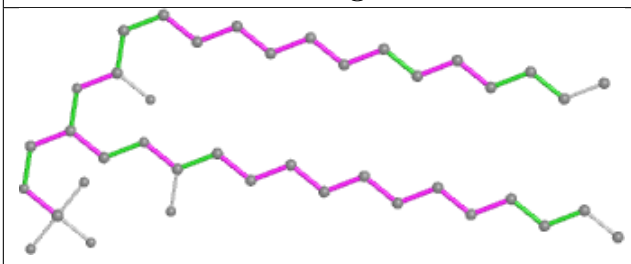
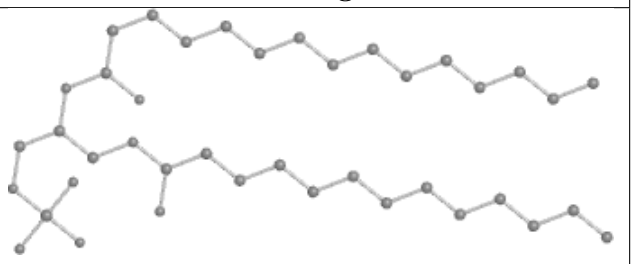
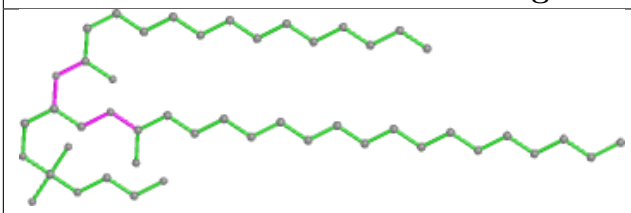


Torsions



Rings

Ligand 8PE S 101



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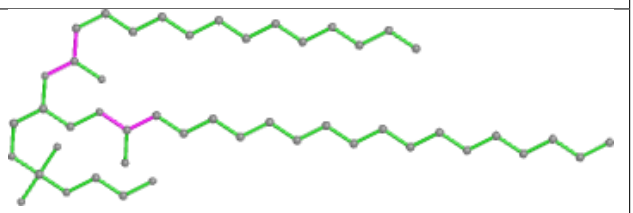
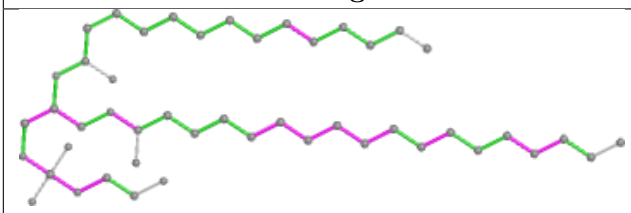


Bond angles



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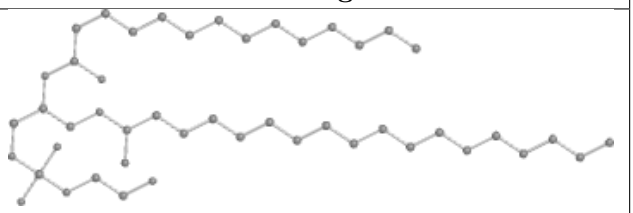
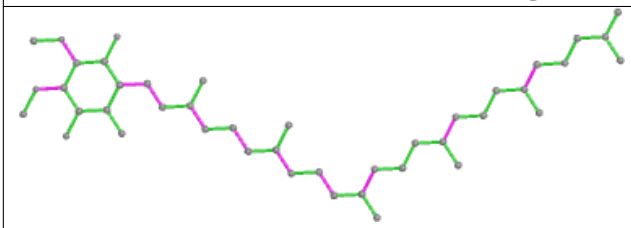


Rings

Ligand UQ6 N 406



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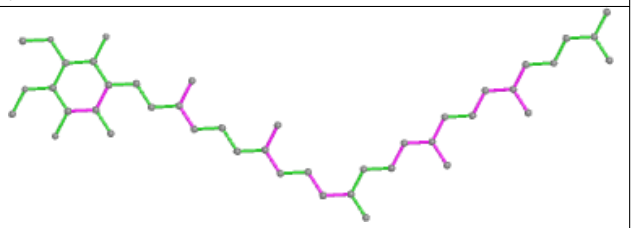
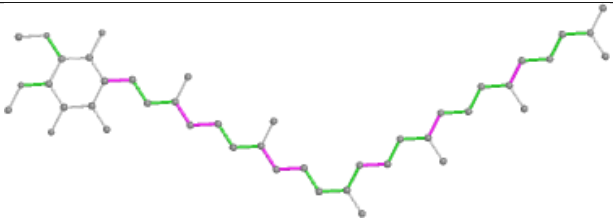


Bond angles



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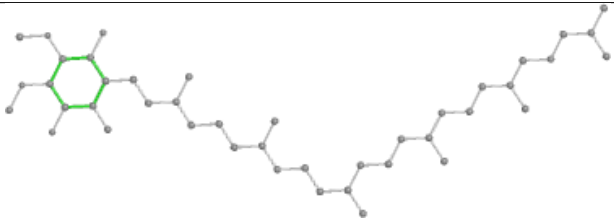
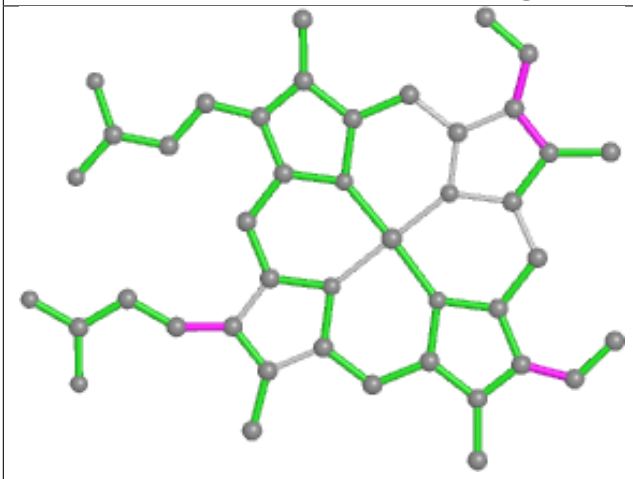


Rings

Ligand HEM N 405



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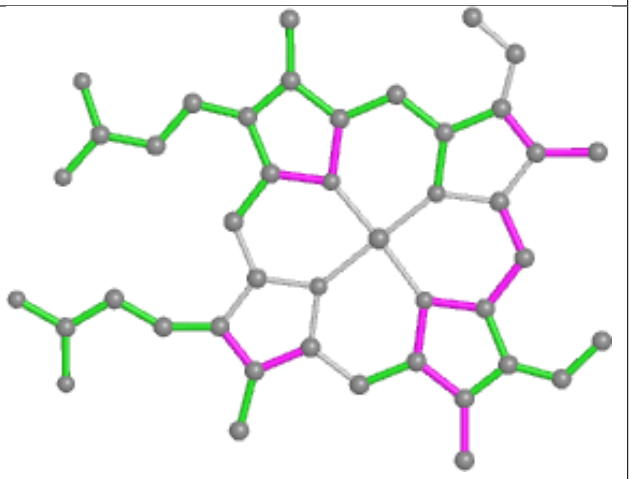
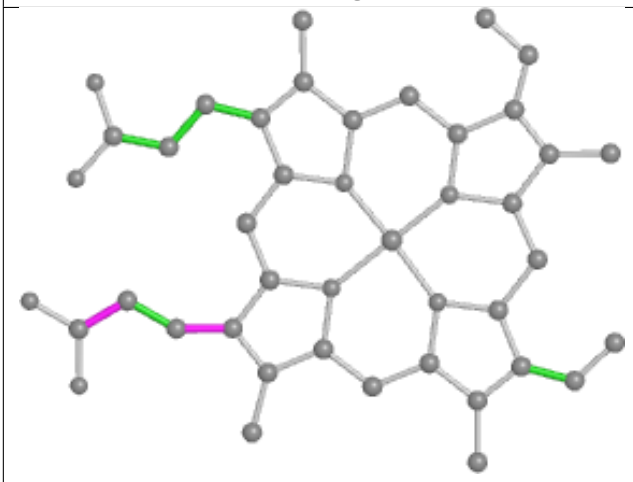
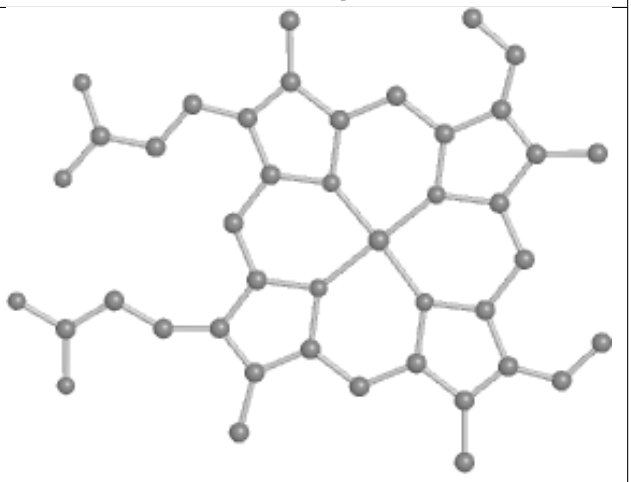


Bond angles

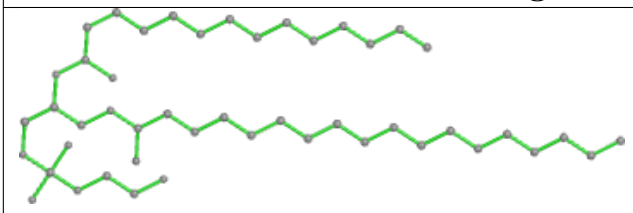


Torsions

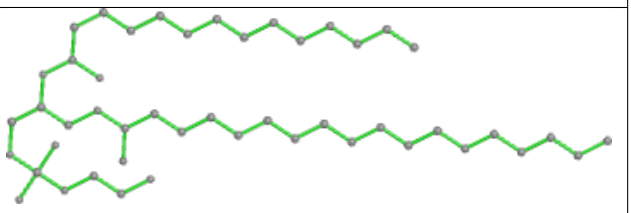


Rings

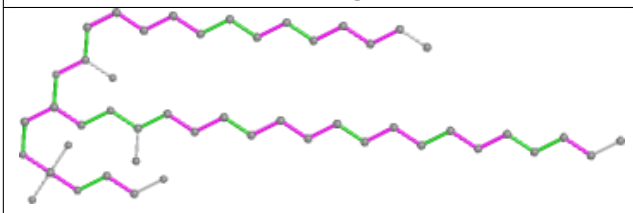
Ligand 8PE C 402



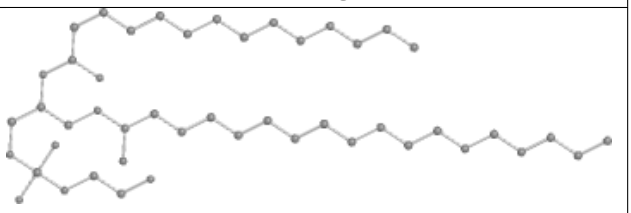
Bond lengths



Bond angles

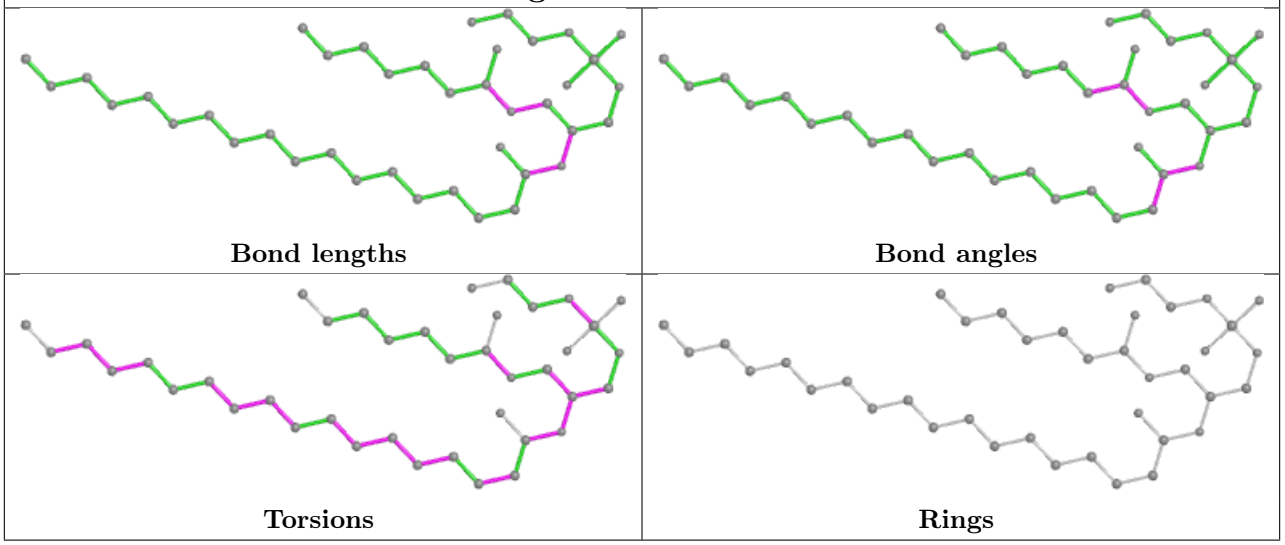


Torsions



Rings

Ligand 9PE N 403



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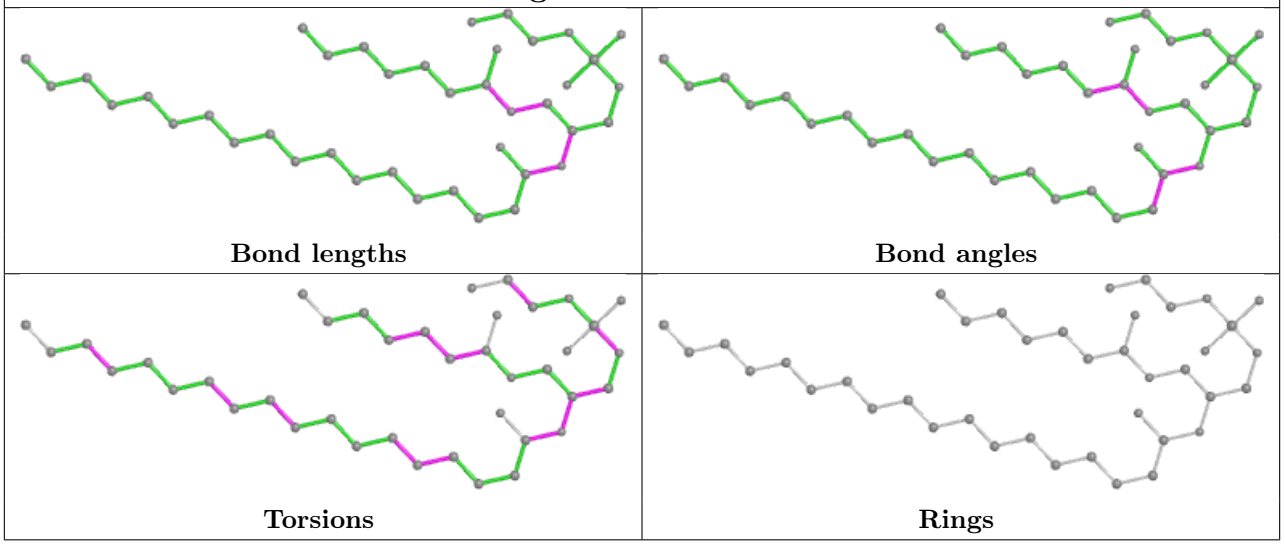
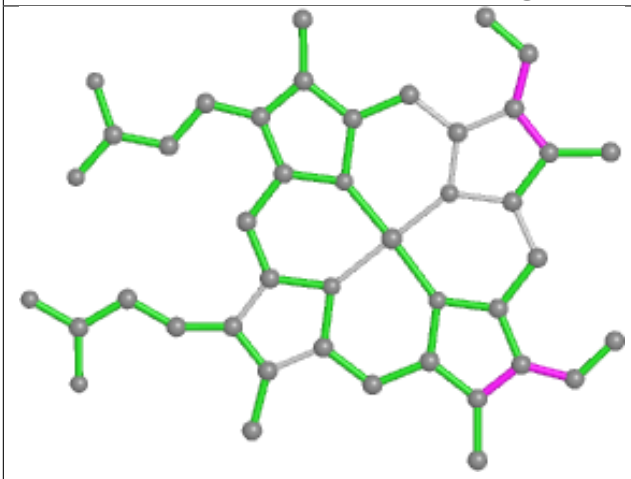
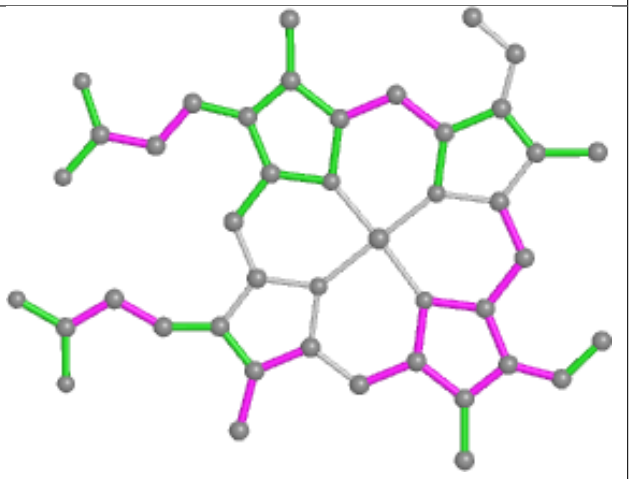


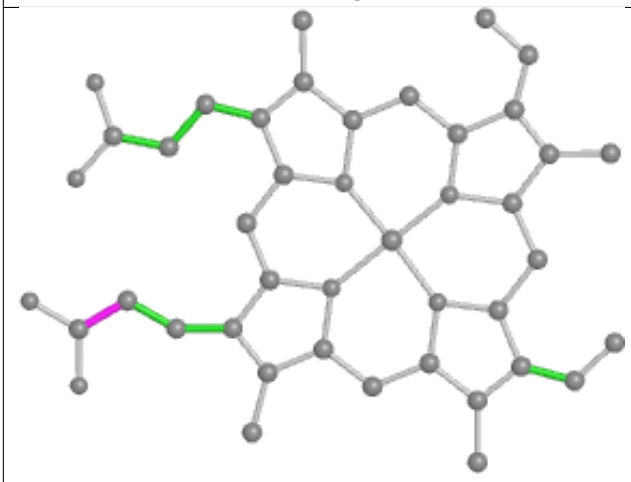
Ligand HEM O 401



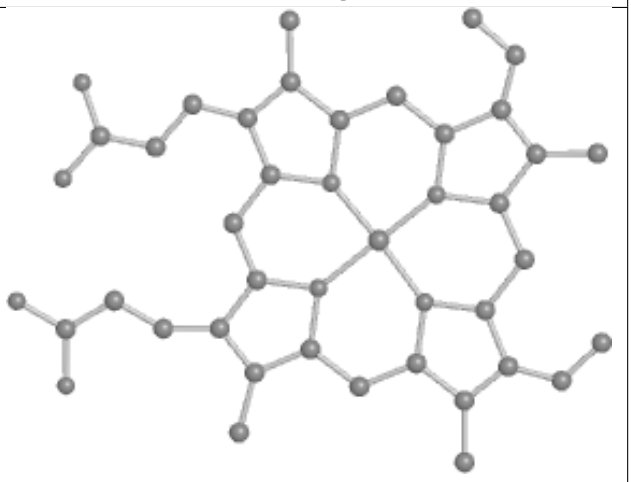
Bond lengths



Bond angles

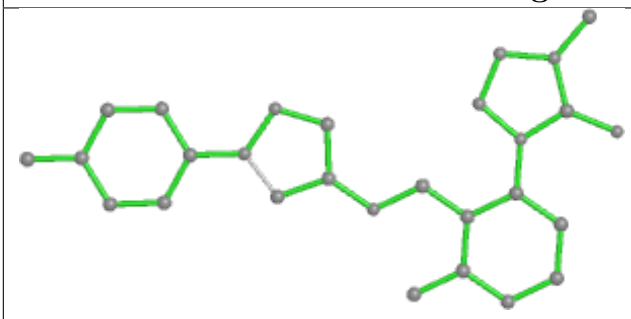


Torsions

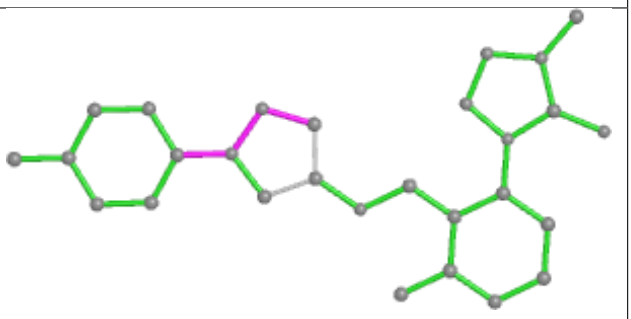


Rings

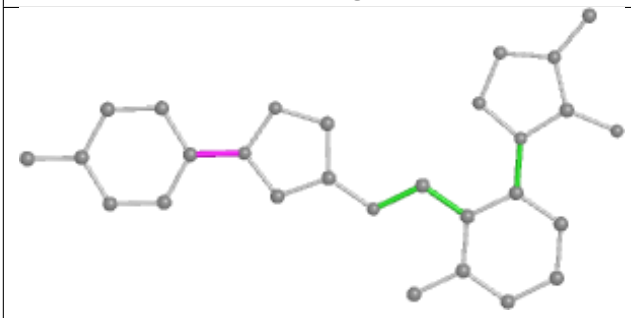
Ligand 86T C 406



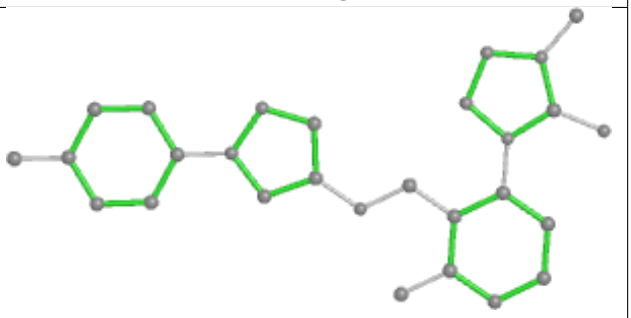
Bond lengths



Bond angles

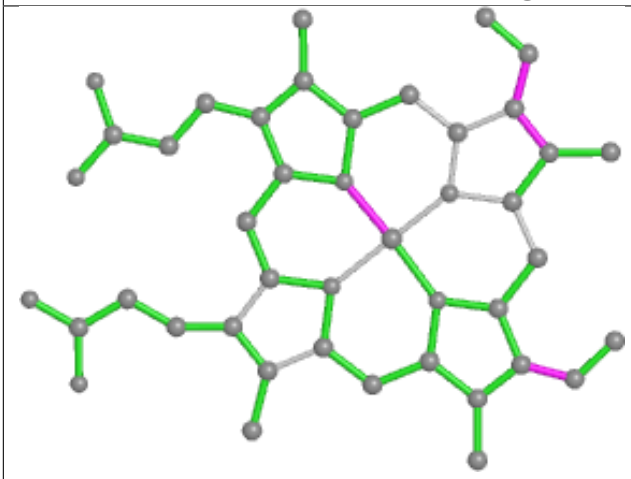


Torsions

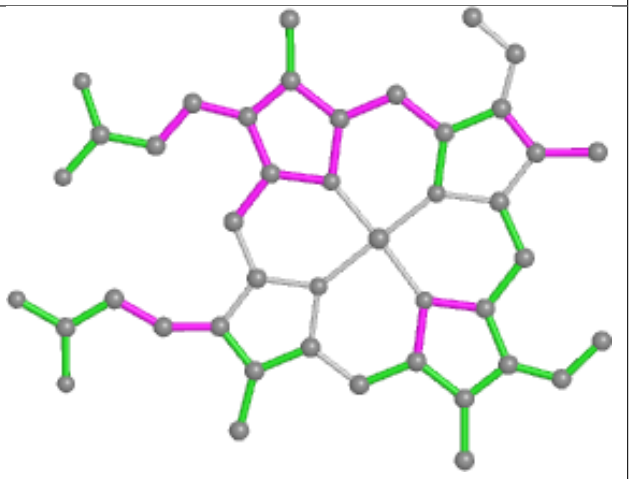


Rings

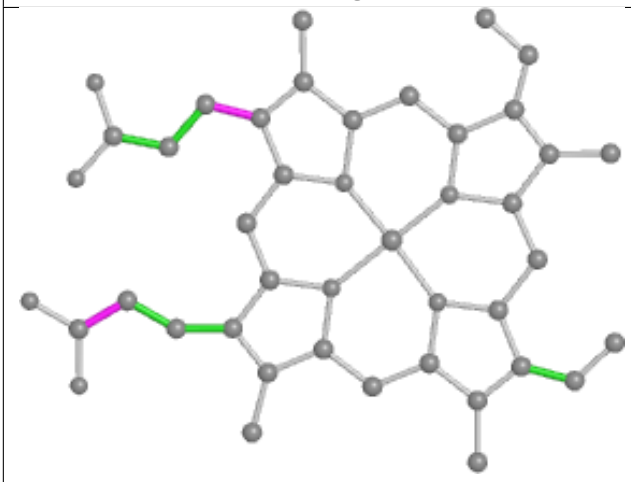
Ligand HEM C 404



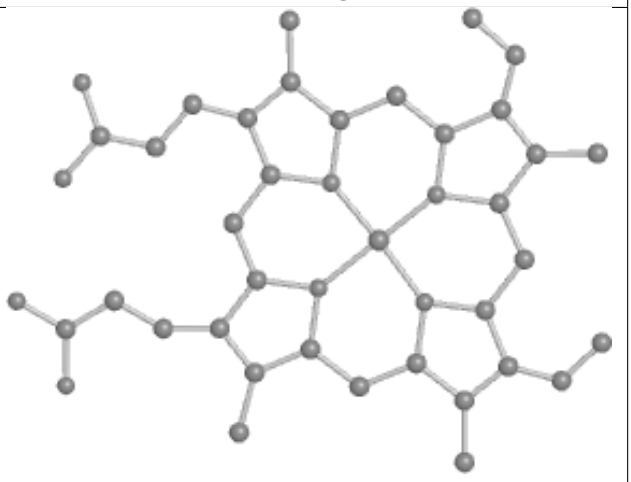
Bond lengths



Bond angles

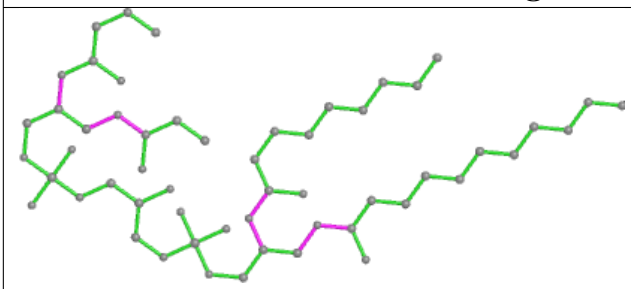


Torsions

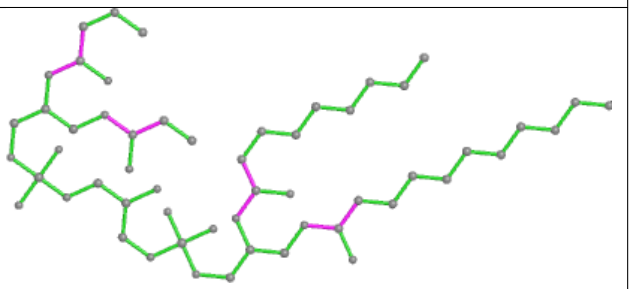


Rings

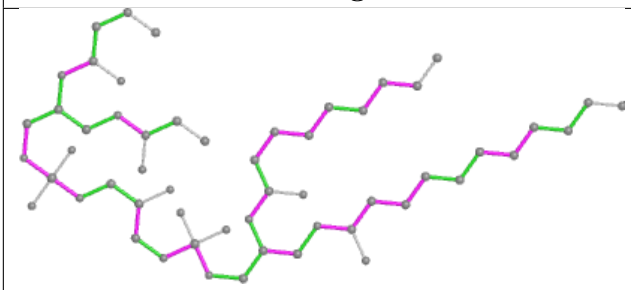
Ligand CN3 N 402



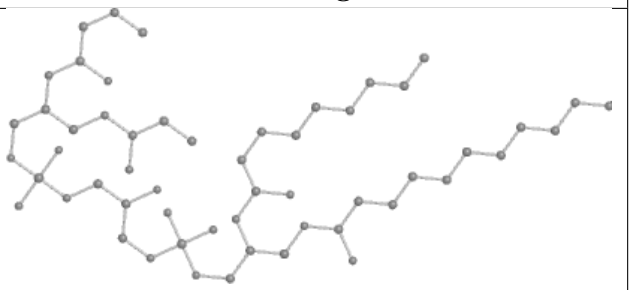
Bond lengths



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.

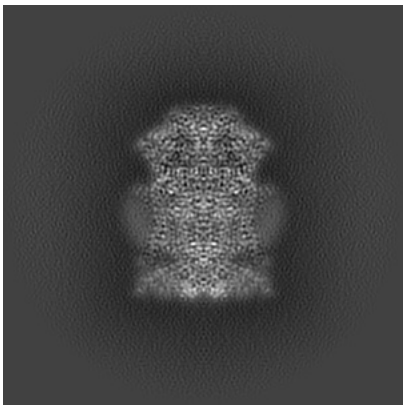
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39322. These allow visual inspection of the internal detail of the map and identification of artifacts.

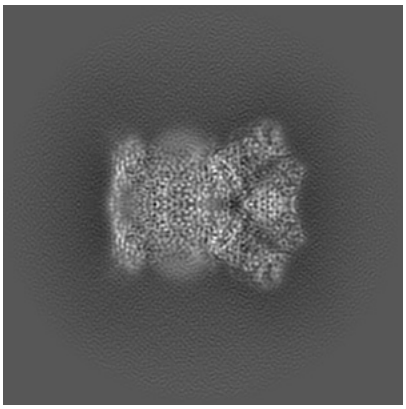
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

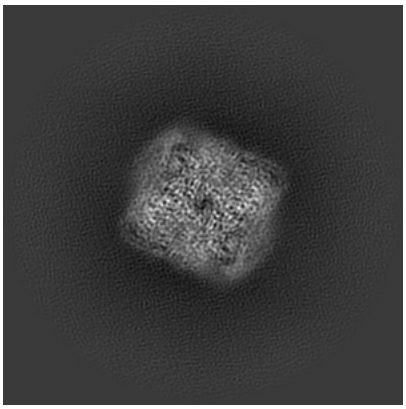
6.1.1 Primary map



X

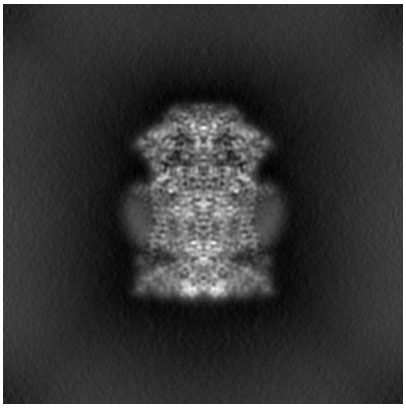


Y

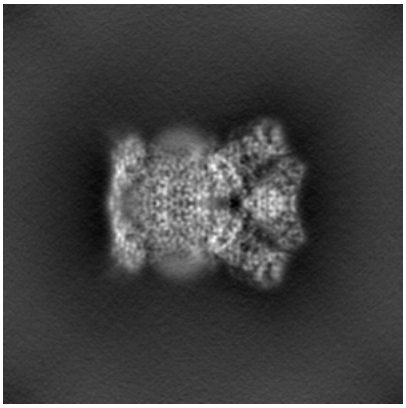


Z

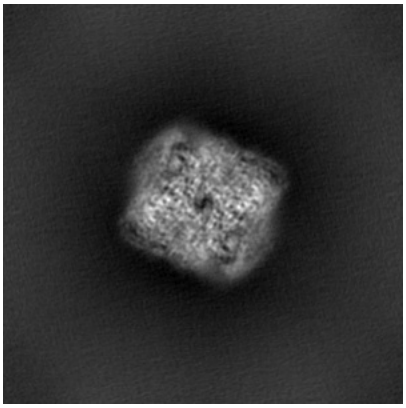
6.1.2 Raw map



X



Y

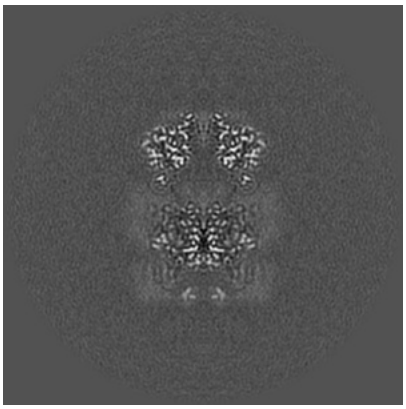


Z

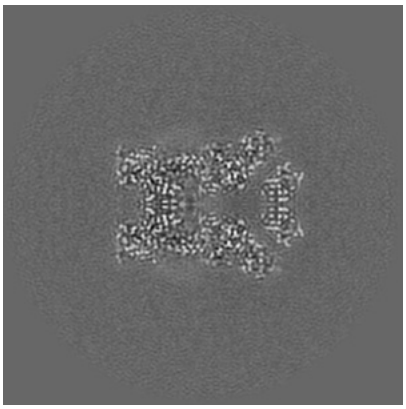
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

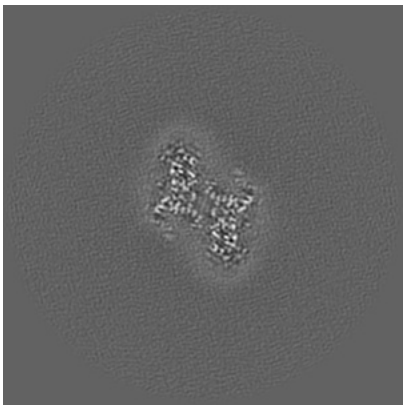
6.2.1 Primary map



X Index: 160

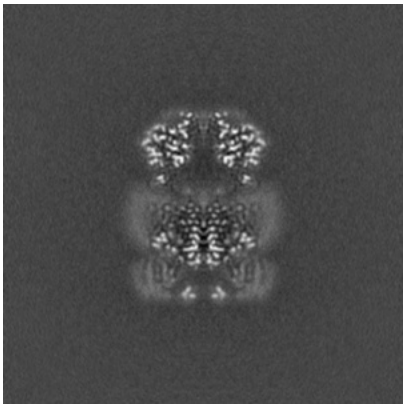


Y Index: 160

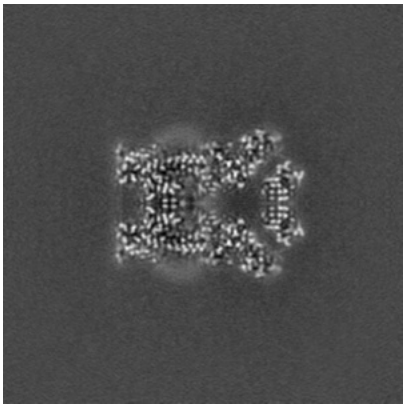


Z Index: 160

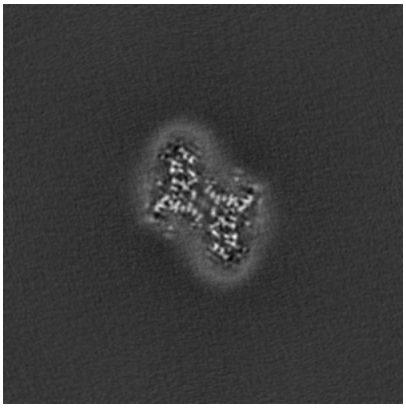
6.2.2 Raw map



X Index: 160



Y Index: 160

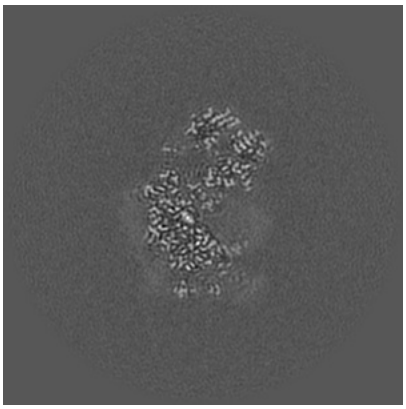


Z Index: 160

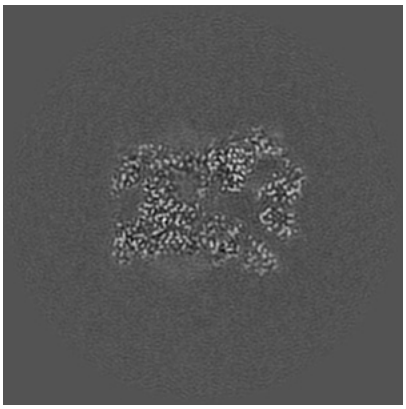
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

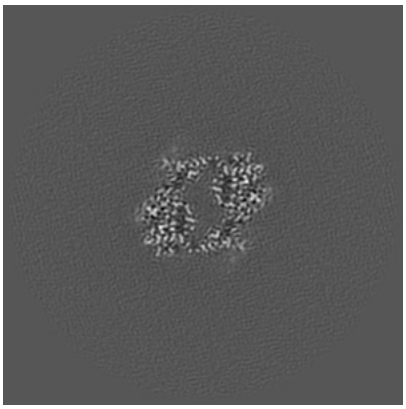
6.3.1 Primary map



X Index: 172

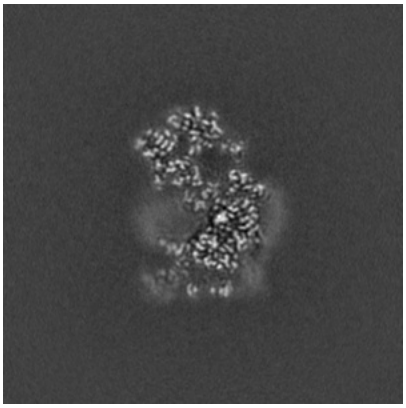


Y Index: 165

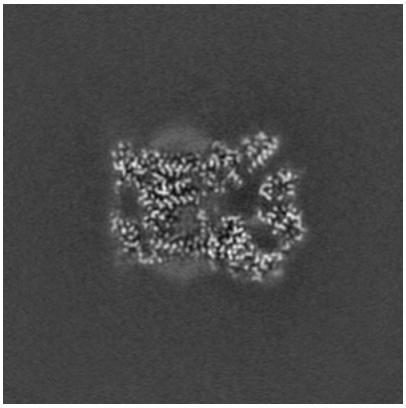


Z Index: 181

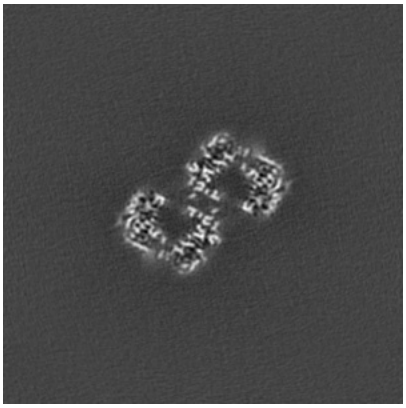
6.3.2 Raw map



X Index: 149



Y Index: 155

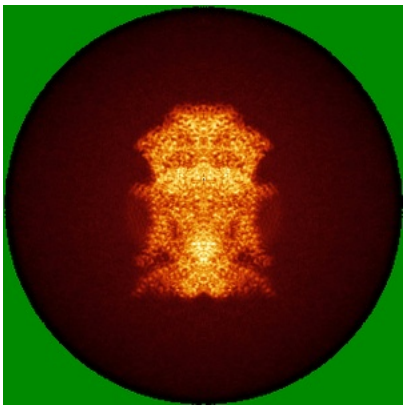


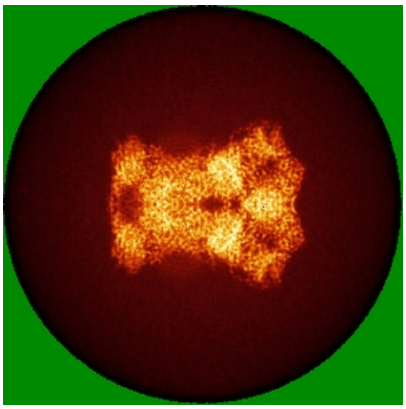
Z Index: 205

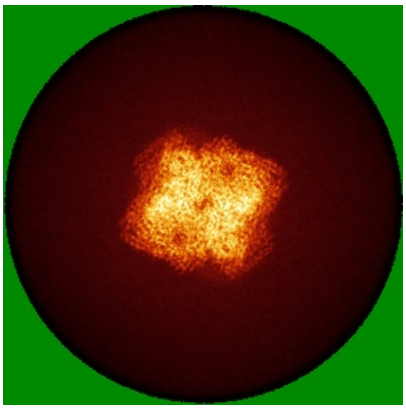
The images above show the largest variance slices of the map in three orthogonal directions.

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

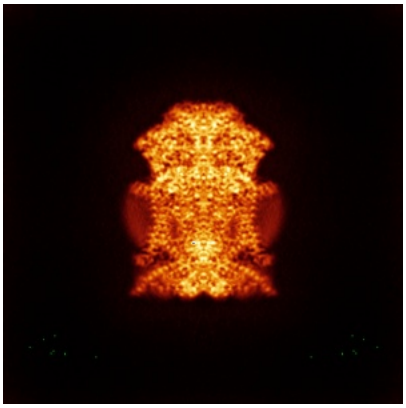
6.4.1 Primary map

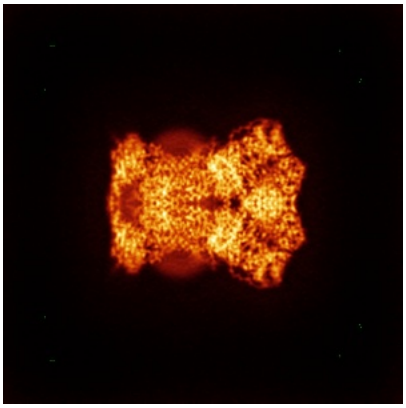

X

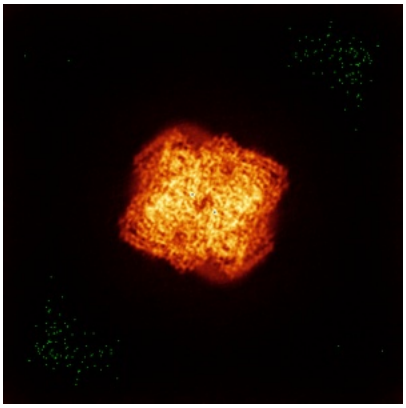

Y


Z

6.4.2 Raw map


X


Y

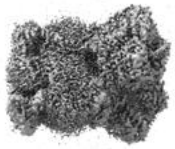

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

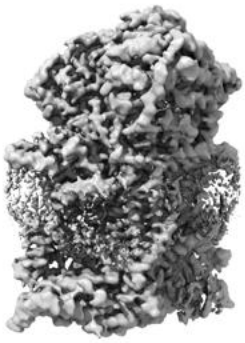


Y

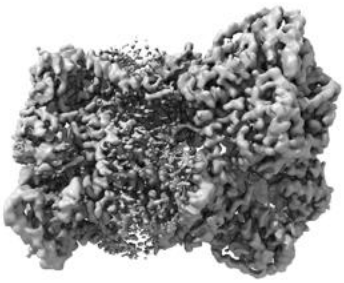
Z

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

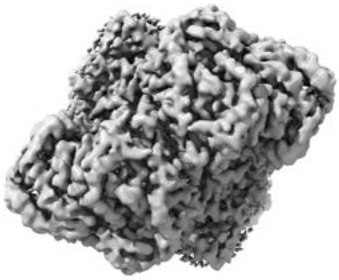
6.5.2 Raw map



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.

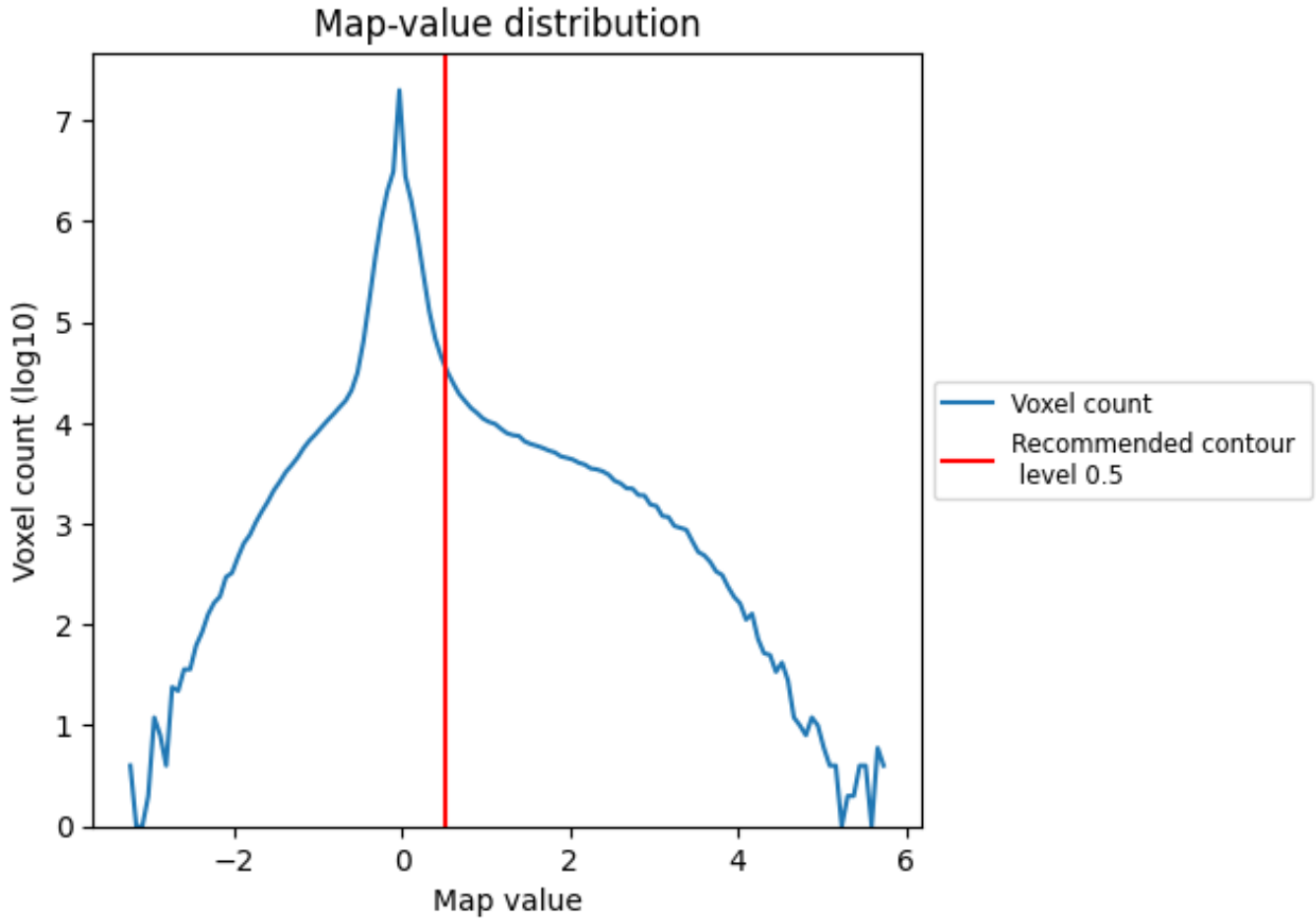
6.6 Mask visualisation (i)

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

7 Map analysis

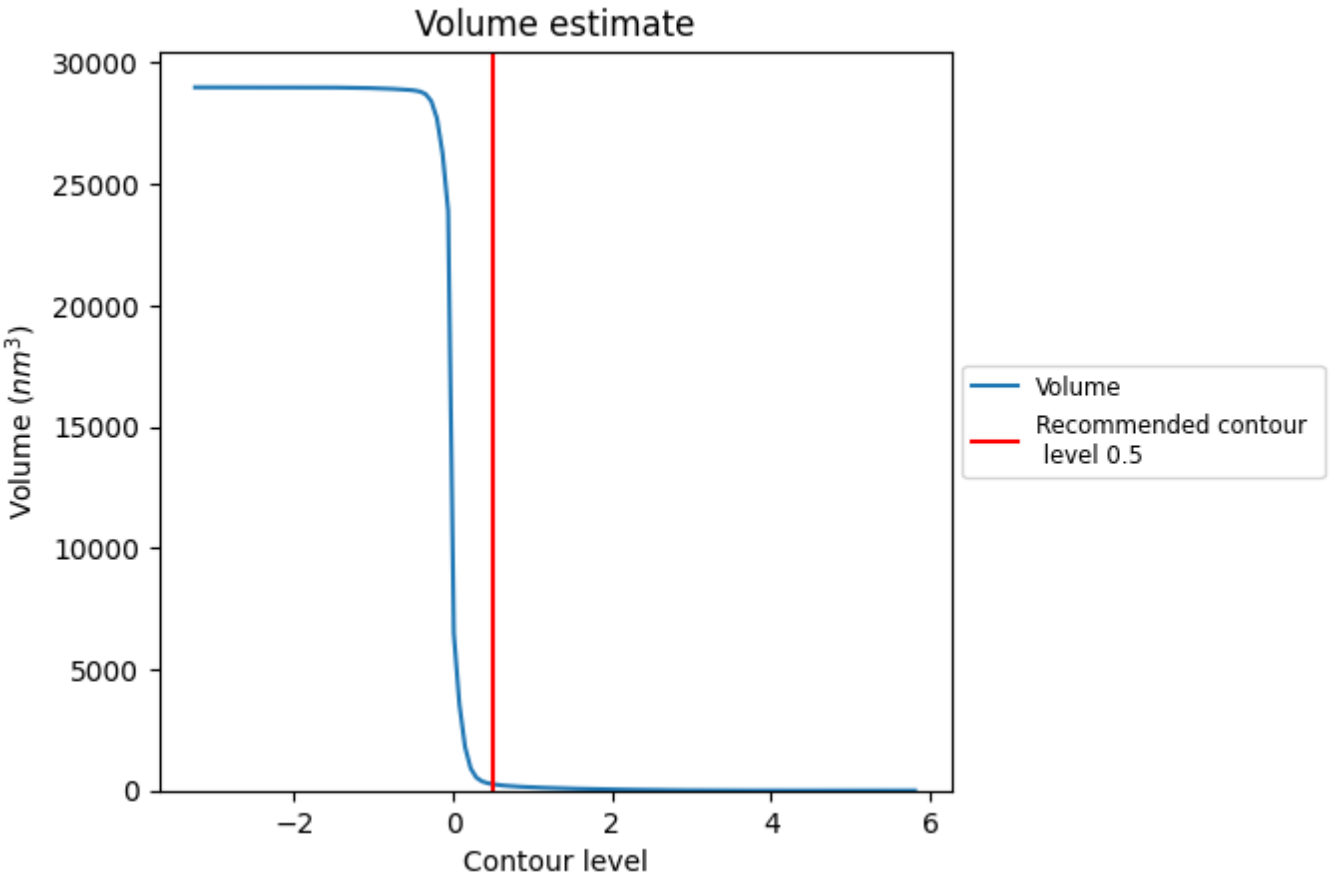
This section contains the results of statistical analysis of the map.

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.

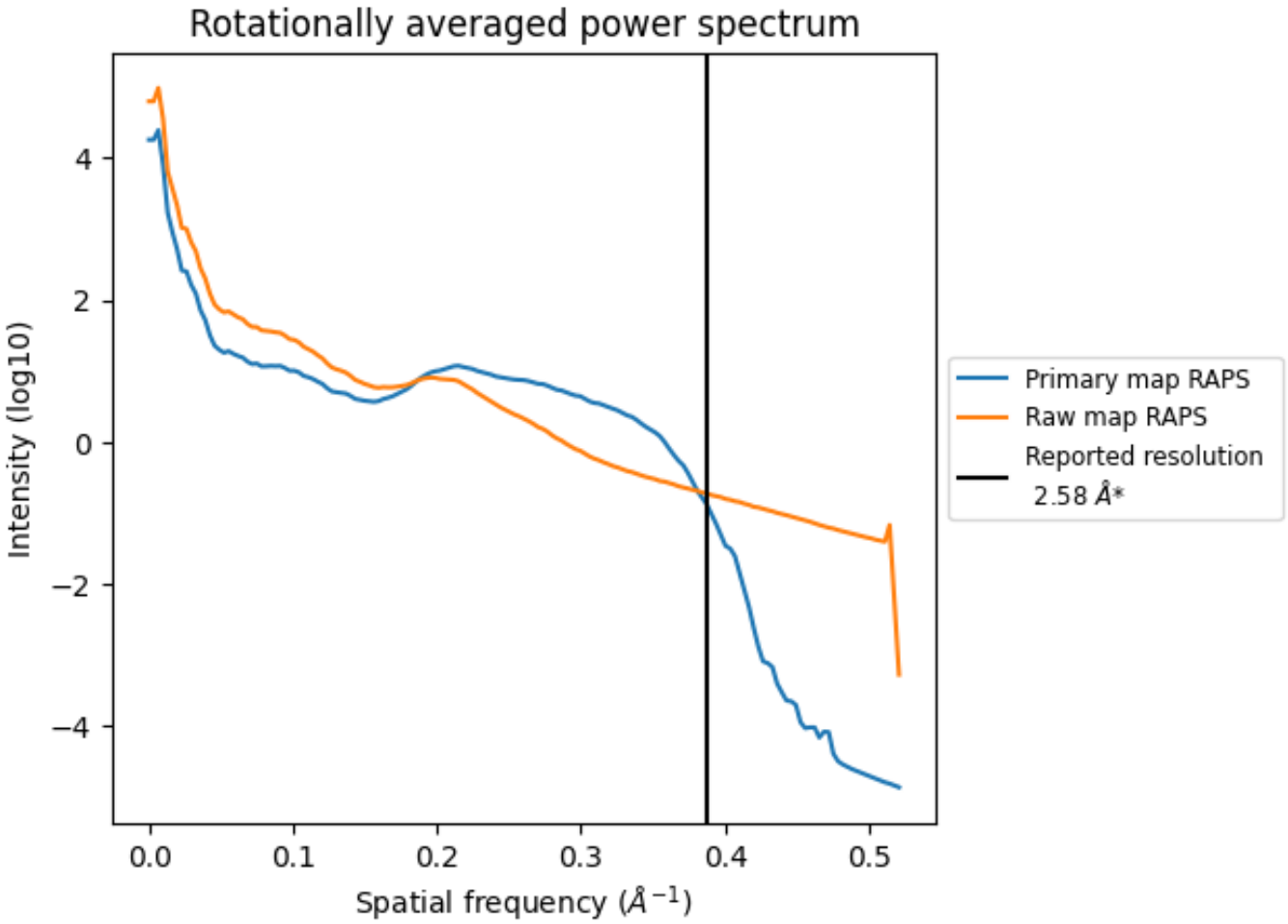
7.2 Volume estimate



The volume at the recommended contour level is 262 nm^3; this corresponds to an approximate mass of 237 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)

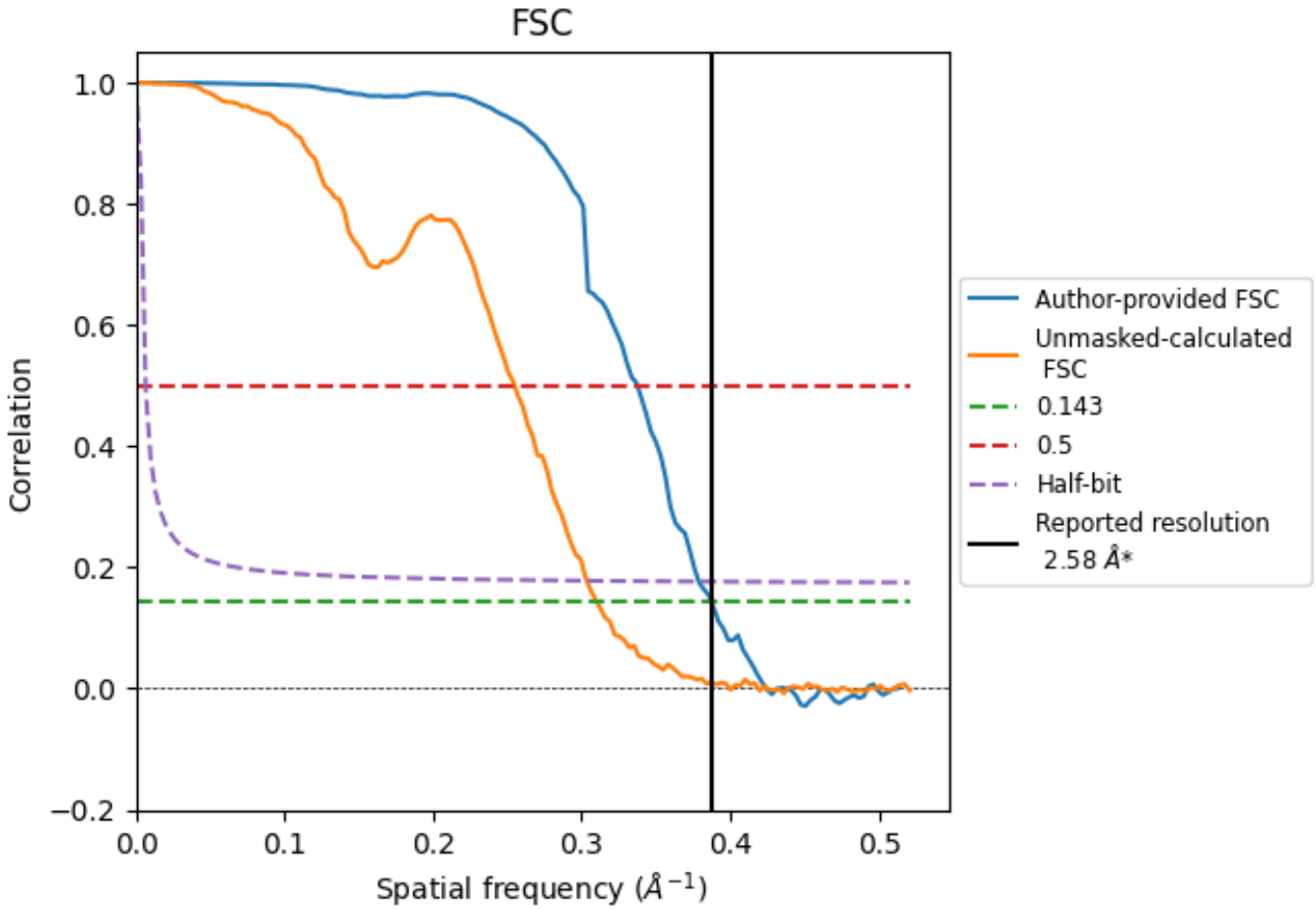


*Reported resolution corresponds to spatial frequency of 0.388 $Å^{-1}$

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 0.388 Å^{-1}

8.2 Resolution estimates (i)

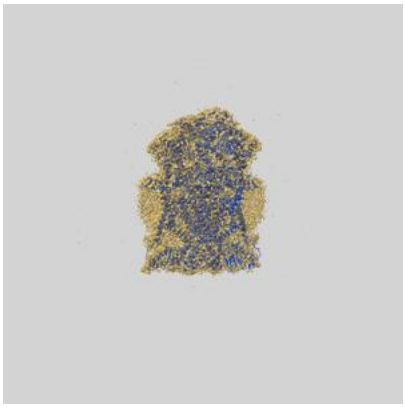
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.96	2.64
Unmasked-calculated*	3.22	3.92	3.29

*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 3.22 differs from the reported value 2.58 by more than 10 %

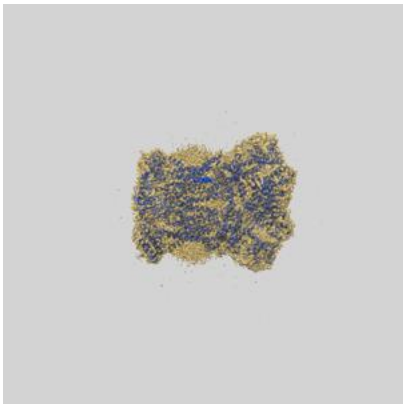
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39322 and PDB model 8YIL. Per-residue inclusion information can be found in section 3 on page 12.

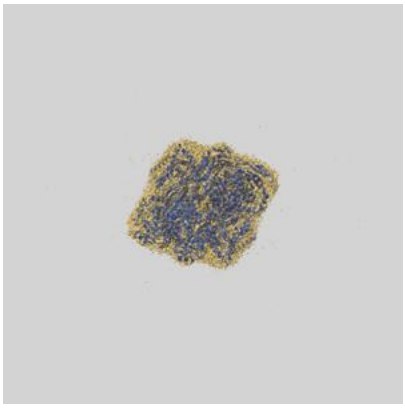
9.1 Map-model overlay



X



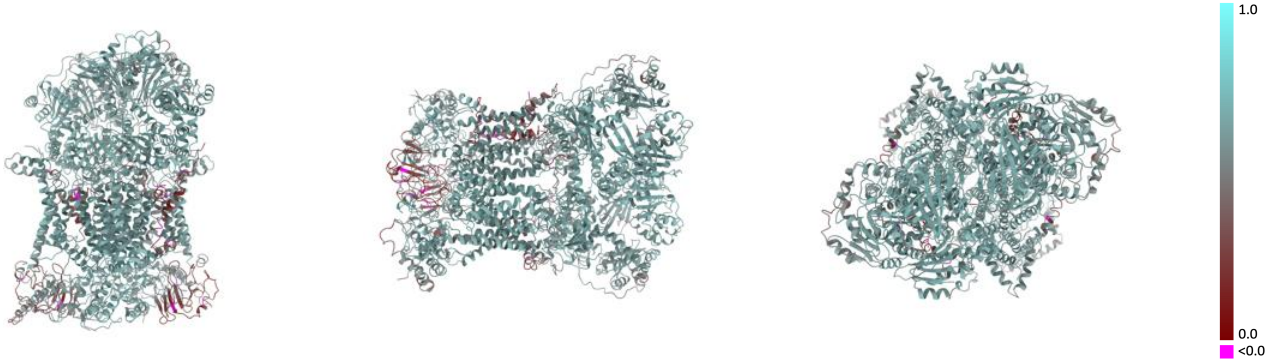
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

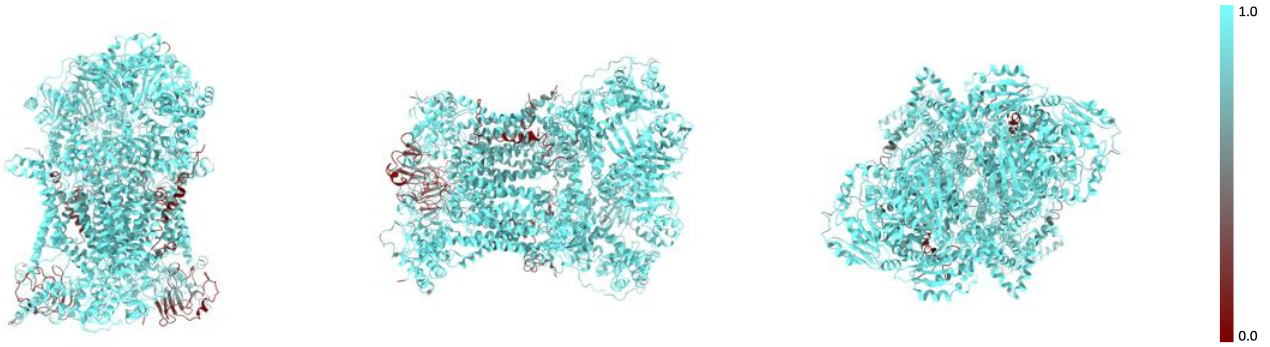
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

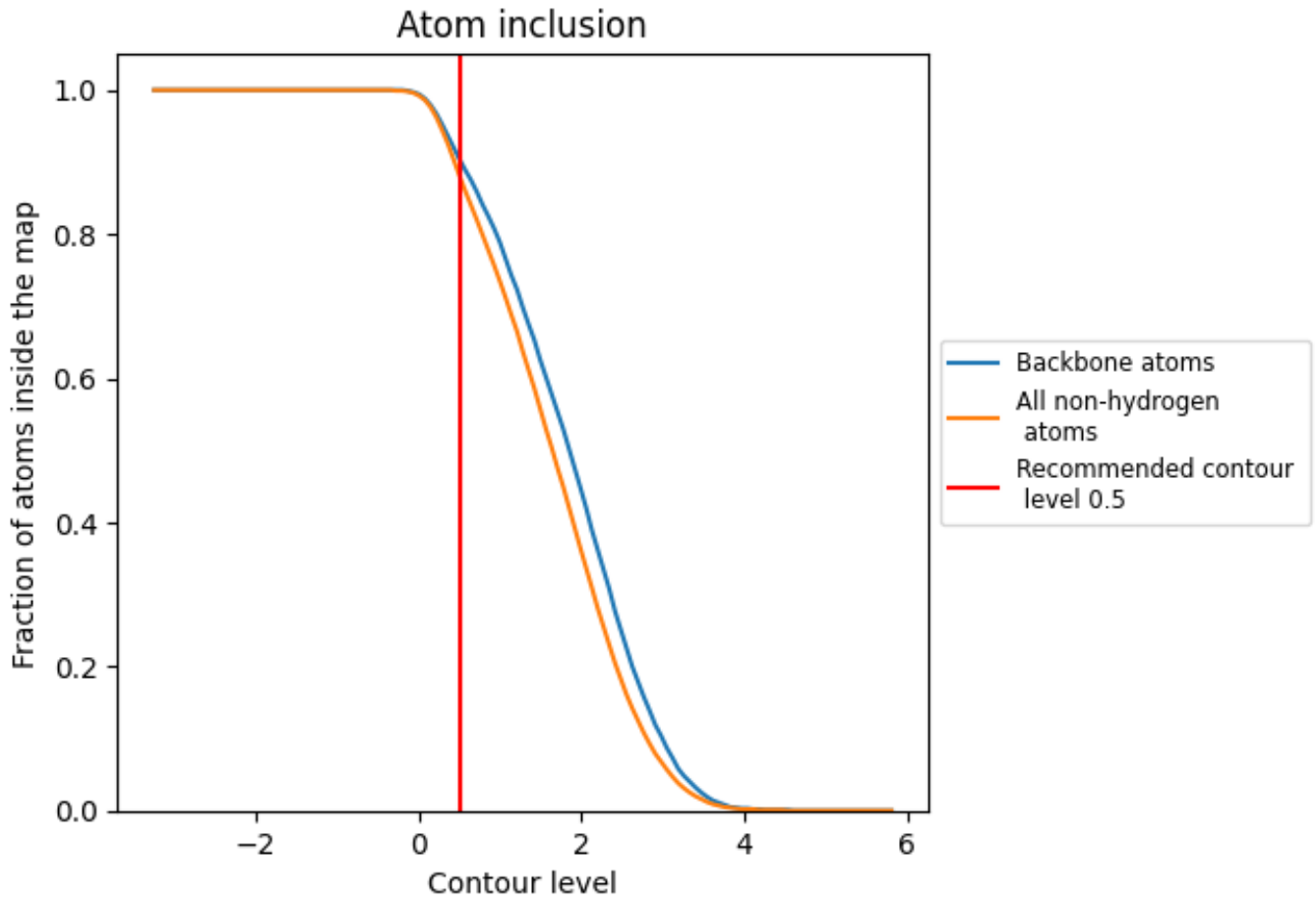
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.8820	0.5760
A	0.9560	0.6000
B	0.9720	0.6290
C	0.9720	0.6370
D	0.9650	0.6160
E	0.4880	0.3830
F	0.8210	0.5030
G	0.9370	0.6040
H	0.8440	0.5370
I	0.6700	0.4430
L	0.9560	0.6010
M	0.9710	0.6290
N	0.9740	0.6390
O	0.9660	0.6190
P	0.4760	0.3770
Q	0.8290	0.4980
R	0.9380	0.6030
S	0.8400	0.5340
T	0.6690	0.4720
U	0.1030	0.2300
V	0.0850	0.1980