Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 05:33 PM JST

PDB ID	:	8JAX / pdb_00008jax
EMDB ID	:	EMD-36137
Title	:	Cryo-EM structure of Holo form of ScBfr with O symmetry
Authors	:	Jobichen, C.; Sivaraman, J.
Deposited on	:	2023-05-07
Resolution	:	3.27 Å(reported)

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

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

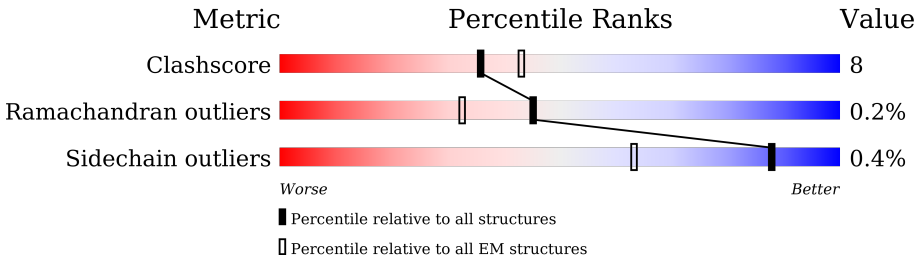
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.27 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	162	84% 16%
1	B	162	80% 19%
1	C	162	82% 18%
1	D	162	78% 22%
1	E	162	81% 18%
1	F	162	75% 24%
1	G	162	83% 16%
1	H	162	83% 17%

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Mol	Chain	Length	Quality of chain
1	I	162	
1	J	162	
1	K	162	
1	L	162	
1	M	162	
1	N	162	
1	O	162	
1	P	162	
1	Q	162	
1	R	162	
1	S	162	
1	T	162	
1	U	162	
1	V	162	
1	W	162	
1	X	162	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31889 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	162	Total	C	N	O	S	0	0
			1313	827	227	255	4		
1	B	160	Total	C	N	O	S	0	0
			1293	814	224	251	4		
1	C	162	Total	C	N	O	S	0	0
			1318	832	226	256	4		
1	D	161	Total	C	N	O	S	0	0
			1305	823	225	253	4		
1	F	161	Total	C	N	O	S	0	0
			1310	826	225	255	4		
1	E	161	Total	C	N	O	S	0	0
			1304	823	225	252	4		
1	G	161	Total	C	N	O	S	0	0
			1304	823	225	252	4		
1	H	161	Total	C	N	O	S	0	0
			1304	823	225	252	4		
1	I	160	Total	C	N	O	S	0	0
			1299	820	224	251	4		
1	J	162	Total	C	N	O	S	0	0
			1318	831	227	256	4		
1	K	157	Total	C	N	O	S	0	0
			1285	811	221	249	4		
1	L	162	Total	C	N	O	S	0	0
			1318	832	226	256	4		
1	M	162	Total	C	N	O	S	0	0
			1307	825	226	252	4		
1	N	161	Total	C	N	O	S	0	0
			1310	826	225	255	4		
1	O	162	Total	C	N	O	S	0	0
			1315	828	227	256	4		
1	P	161	Total	C	N	O	S	0	0
			1305	823	225	253	4		
1	Q	162	Total	C	N	O	S	0	0
			1318	832	226	256	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	157	Total	C	N	O	S	0	0
			1285	811	221	249	4		
1	S	161	Total	C	N	O	S	0	0
			1310	826	225	255	4		
1	T	162	Total	C	N	O	S	0	0
			1315	828	227	256	4		
1	U	157	Total	C	N	O	S	0	0
			1285	811	221	249	4		
1	V	162	Total	C	N	O	S	0	0
			1318	832	226	256	4		
1	W	160	Total	C	N	O	S	0	0
			1300	820	224	252	4		
1	X	161	Total	C	N	O	S	0	0
			1310	826	225	255	4		

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Fe	0
			1	1	
2	B	1	Total	Fe	0
			1	1	
2	C	1	Total	Fe	0
			1	1	
2	D	1	Total	Fe	0
			1	1	
2	F	1	Total	Fe	0
			1	1	
2	E	1	Total	Fe	0
			1	1	
2	G	1	Total	Fe	0
			1	1	
2	H	1	Total	Fe	0
			1	1	
2	I	1	Total	Fe	0
			1	1	
2	J	1	Total	Fe	0
			1	1	
2	K	1	Total	Fe	0
			1	1	
2	L	1	Total	Fe	0
			1	1	

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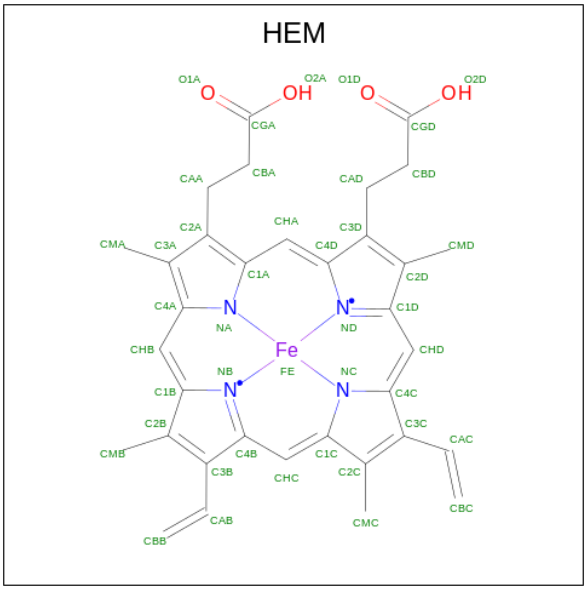
Mol	Chain	Residues	Atoms	AltConf
2	M	1	Total Fe 1 1	0
2	N	1	Total Fe 1 1	0
2	O	1	Total Fe 1 1	0
2	P	1	Total Fe 1 1	0
2	Q	1	Total Fe 1 1	0
2	R	1	Total Fe 1 1	0
2	S	1	Total Fe 1 1	0
2	T	1	Total Fe 1 1	0
2	U	1	Total Fe 1 1	0
2	V	1	Total Fe 1 1	0
2	W	1	Total Fe 1 1	0
2	X	1	Total Fe 1 1	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



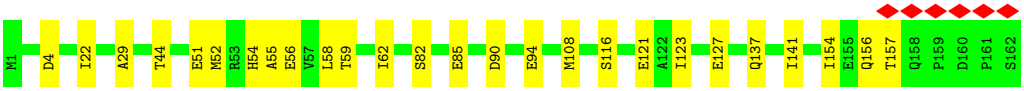
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	R	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	S	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	X	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

• Molecule 1: Bacterioferritin

Chain A:



• Molecule 1: Bacterioferritin

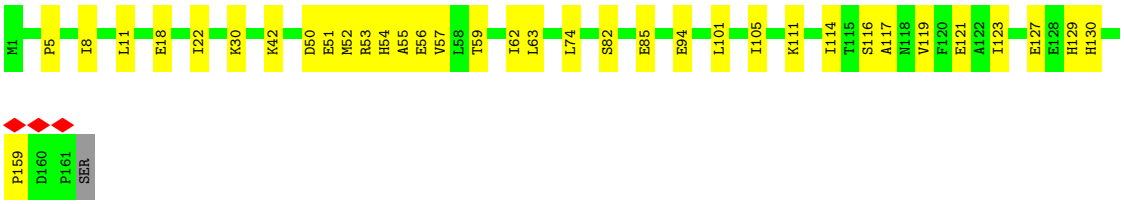
Chain B:

• Molecule 1: Bacterioferritin

Chain C:

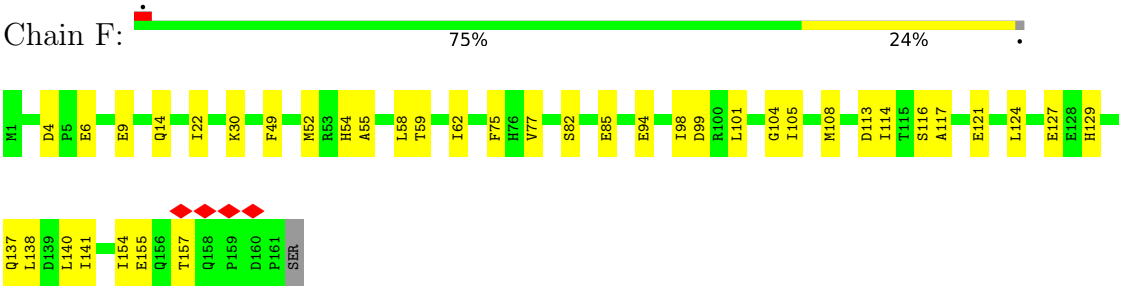
• Molecule 1: Bacterioferritin

Chain D:



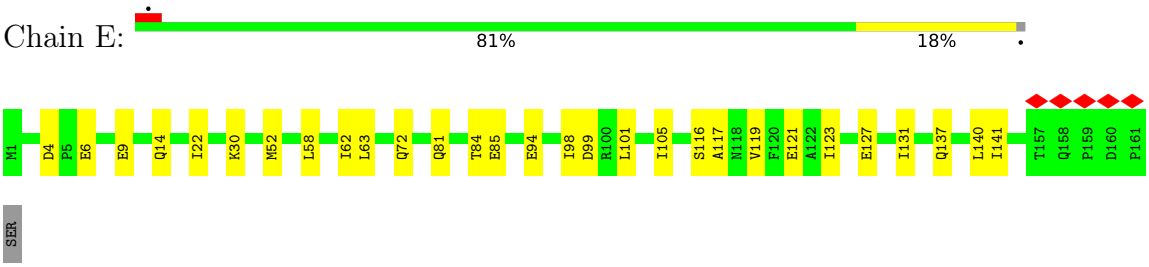
• Molecule 1: Bacterioferritin

Chain F:



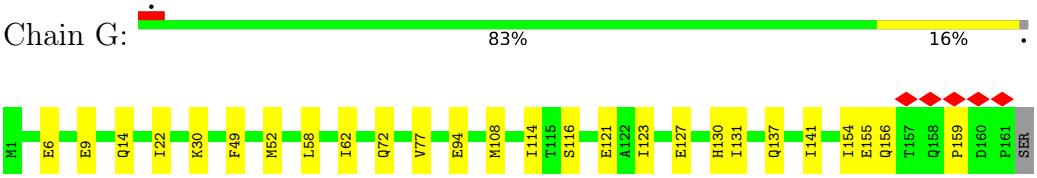
• Molecule 1: Bacterioferritin

Chain E:



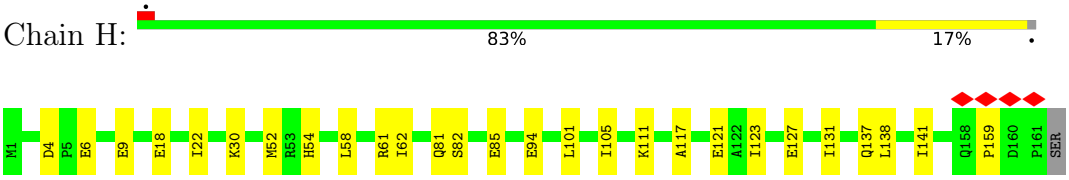
• Molecule 1: Bacterioferritin

Chain G:



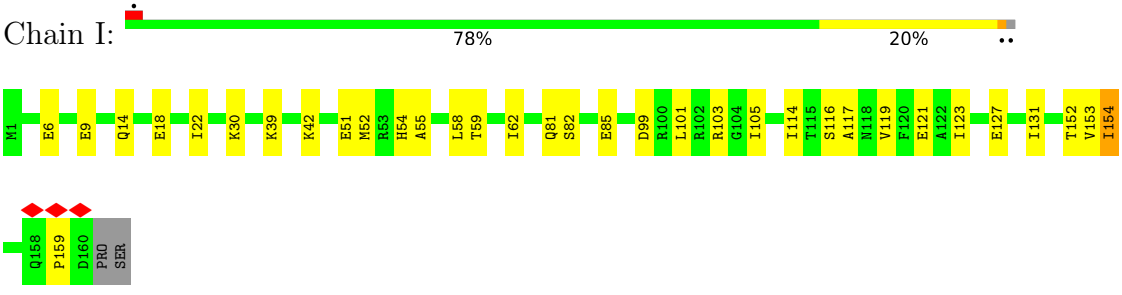
• Molecule 1: Bacterioferritin

Chain H:



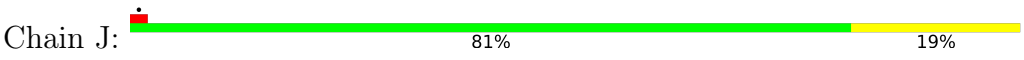
• Molecule 1: Bacterioferritin

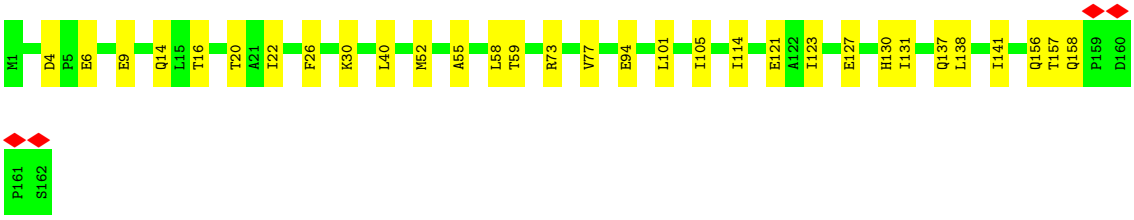
Chain I:



• Molecule 1: Bacterioferritin

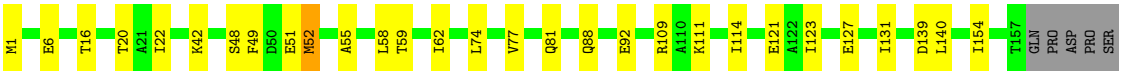
Chain J:





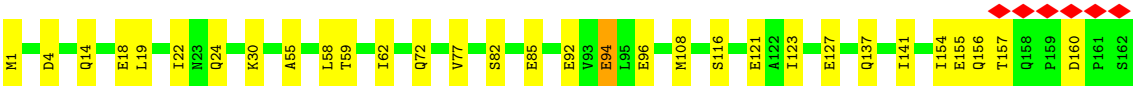
• Molecule 1: Bacterioferritin

Chain K:



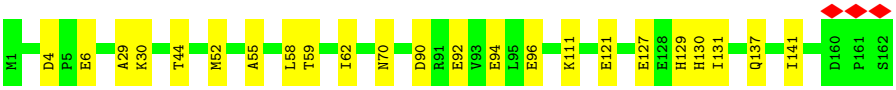
• Molecule 1: Bacterioferritin

Chain L:



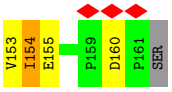
• Molecule 1: Bacterioferritin

Chain M:



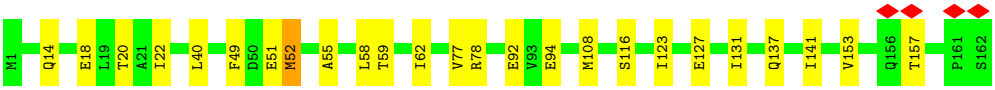
• Molecule 1: Bacterioferritin

Chain N:



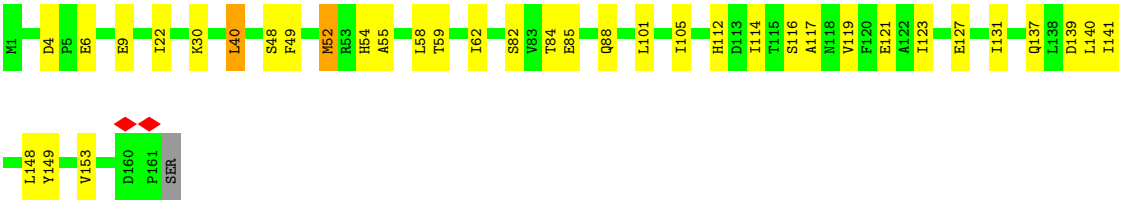
• Molecule 1: Bacterioferritin

Chain O:



• Molecule 1: Bacterioferritin

Chain P:

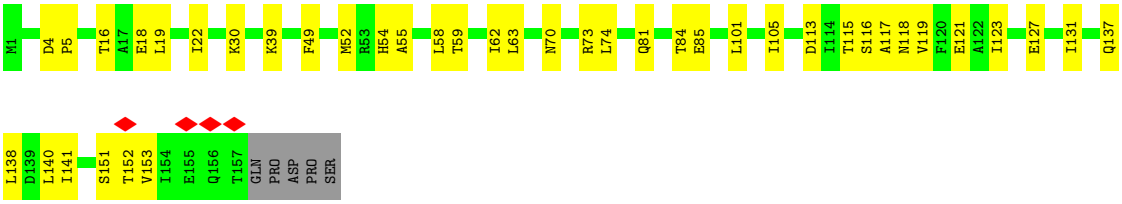


• Molecule 1: Bacterioferritin

Chain Q:

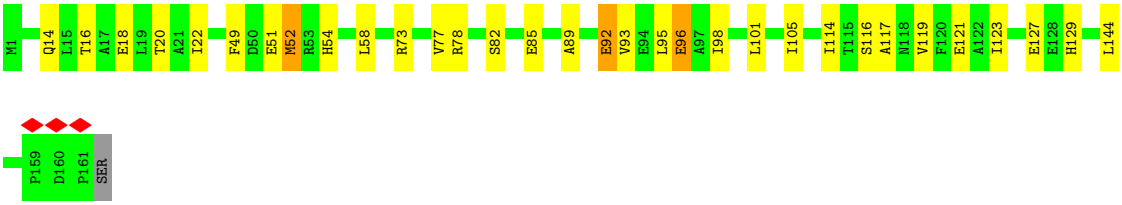
• Molecule 1: Bacterioferritin

Chain R:



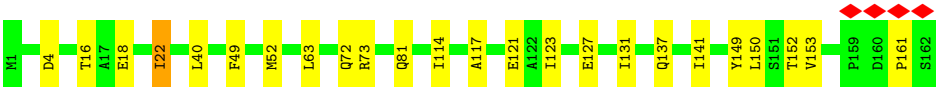
• Molecule 1: Bacterioferritin

Chain S:



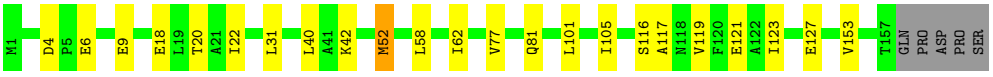
• Molecule 1: Bacterioferritin

Chain T:



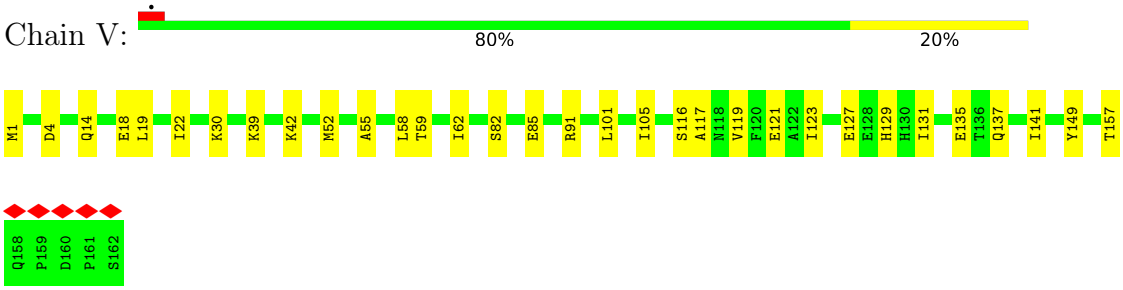
• Molecule 1: Bacterioferritin

Chain U:



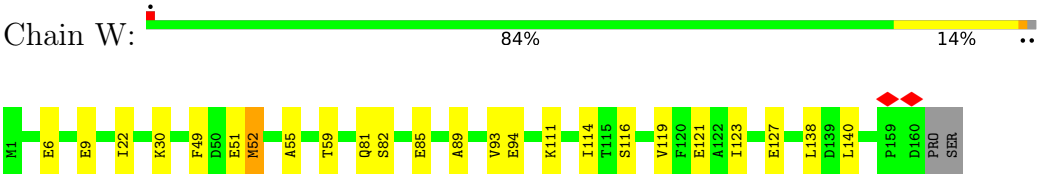
• Molecule 1: Bacterioferritin

Chain V:



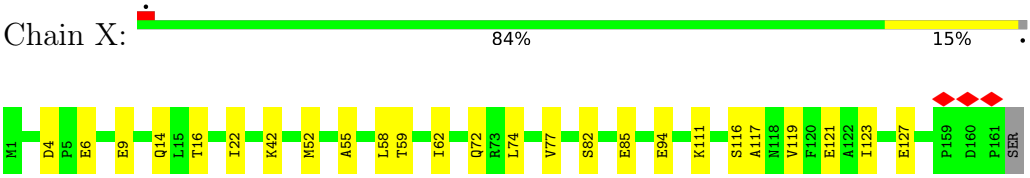
• Molecule 1: Bacterioferritin

Chain W:



• Molecule 1: Bacterioferritin

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11617	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 ($e^-/Å^2$)	1.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0061	Depositor
Map size (Å)	219.648, 219.648, 219.648	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	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, FE2

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	0.20	0/1334	0.33	0/1802
1	B	0.21	0/1313	0.40	1/1774 (0.1%)
1	C	0.18	0/1341	0.32	0/1814
1	D	0.19	0/1326	0.39	1/1792 (0.1%)
1	E	0.19	0/1325	0.32	0/1790
1	F	0.21	0/1332	0.41	0/1801
1	G	0.20	0/1325	0.33	0/1790
1	H	0.20	0/1325	0.33	0/1790
1	I	0.20	0/1320	0.36	1/1784 (0.1%)
1	J	0.19	0/1340	0.34	0/1812
1	K	0.20	0/1306	0.50	4/1764 (0.2%)
1	L	0.19	0/1341	0.32	0/1814
1	M	0.19	0/1328	0.34	0/1795
1	N	0.22	0/1332	0.39	0/1801
1	O	0.21	0/1336	0.41	1/1805 (0.1%)
1	P	0.21	0/1326	0.37	1/1792 (0.1%)
1	Q	0.19	0/1341	0.34	1/1814 (0.1%)
1	R	0.19	0/1306	0.32	0/1764
1	S	0.21	0/1332	0.39	1/1801 (0.1%)
1	T	0.21	0/1336	0.33	0/1805
1	U	0.20	0/1306	0.37	1/1764 (0.1%)
1	V	0.19	0/1341	0.32	0/1814
1	W	0.20	0/1321	0.42	1/1785 (0.1%)
1	X	0.20	0/1332	0.36	0/1801
All	All	0.20	0/31865	0.36	13/43068 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	52	MET	CB-CG-SD	-9.75	83.45	112.70
1	K	52	MET	CB-CG-SD	9.50	141.19	112.70
1	U	52	MET	CB-CG-SD	-7.69	89.62	112.70
1	W	52	MET	CB-CG-SD	-6.96	91.82	112.70
1	B	52	MET	CB-CG-SD	-6.54	93.10	112.70
1	K	52	MET	CA-CB-CG	6.52	127.14	114.10
1	S	52	MET	CA-CB-CG	6.36	126.81	114.10
1	K	51	GLU	CA-C-N	-6.24	111.09	122.38
1	K	51	GLU	C-N-CA	-6.24	111.09	122.38
1	D	52	MET	CA-CB-CG	5.84	125.79	114.10
1	I	52	MET	CB-CG-SD	-5.74	95.47	112.70
1	Q	52	MET	CB-CG-SD	-5.57	95.99	112.70
1	P	52	MET	CG-SD-CE	-5.36	89.12	100.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1313	0	1281	21	0
1	B	1293	0	1260	19	0
1	C	1318	0	1289	20	0
1	D	1305	0	1268	23	0
1	E	1304	0	1268	22	0
1	F	1310	0	1276	29	0
1	G	1304	0	1268	17	0
1	H	1304	0	1266	22	0
1	I	1299	0	1267	28	0
1	J	1318	0	1287	21	0
1	K	1285	0	1262	24	0
1	L	1318	0	1289	21	0
1	M	1307	0	1268	16	0
1	N	1310	0	1276	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1315	0	1280	19	0
1	P	1305	0	1268	26	0
1	Q	1318	0	1289	17	0
1	R	1285	0	1262	28	0
1	S	1310	0	1276	22	0
1	T	1315	0	1280	15	0
1	U	1285	0	1262	15	0
1	V	1318	0	1289	23	0
1	W	1300	0	1267	18	0
1	X	1310	0	1276	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	B	43	0	30	0	0
3	D	43	0	30	0	0
3	F	43	0	30	0	0
3	H	43	0	30	0	0
3	K	43	0	30	4	0
3	M	43	0	30	3	0
3	P	43	0	30	3	0
3	R	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	43	0	30	0	0
3	U	43	0	30	0	0
3	V	43	0	30	4	0
3	X	43	0	30	0	0
All	All	31889	0	30934	475	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 8.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:GLU:OE2	1:H:127:GLU:OE1	1.59	1.19
1:Q:94:GLU:OE1	1:Q:127:GLU:OE1	1.62	1.15
1:N:18:GLU:OE2	1:N:51:GLU:OE1	1.69	1.08
1:N:94:GLU:OE1	1:N:127:GLU:OE1	1.71	1.07
1:S:18:GLU:CD	1:S:54:HIS:HD1	1.63	1.05
1:B:94:GLU:OE1	1:B:127:GLU:OE1	1.70	1.05
1:V:52:MET:SD	3:V:202:HEM:NA	2.29	1.05
1:B:18:GLU:OE1	1:B:51:GLU:OE1	1.78	1.00
1:O:94:GLU:OE1	1:O:127:GLU:OE1	1.76	1.00
1:L:94:GLU:OE2	1:L:127:GLU:OE2	1.82	0.97
1:A:94:GLU:OE1	1:A:127:GLU:OE2	1.89	0.90
1:I:51:GLU:OE2	1:I:54:HIS:ND1	2.04	0.89
1:W:94:GLU:OE2	1:W:127:GLU:OE1	1.94	0.85
1:P:52:MET:HE1	3:P:202:HEM:C1B	2.17	0.80
1:F:54:HIS:CE1	1:F:127:GLU:OE1	2.38	0.76
1:W:22:ILE:HD11	1:W:52:MET:HA	1.69	0.75
1:I:54:HIS:CE1	1:I:127:GLU:OE2	2.39	0.75
1:P:54:HIS:CE1	1:P:127:GLU:OE2	2.40	0.74
1:J:22:ILE:HD11	1:J:52:MET:HA	1.70	0.73
1:O:18:GLU:OE1	1:O:51:GLU:CD	2.32	0.72
1:A:54:HIS:CE1	1:A:127:GLU:OE1	2.43	0.71
1:Q:22:ILE:HD11	1:Q:52:MET:HA	1.72	0.70
1:H:54:HIS:HE1	1:H:127:GLU:OE2	1.73	0.70
1:J:26:PHE:CE1	3:K:201:HEM:HBC1	2.26	0.70
1:A:22:ILE:HD11	1:A:52:MET:HA	1.72	0.70
1:O:22:ILE:HD11	1:O:52:MET:HA	1.72	0.70
1:P:22:ILE:HD11	1:P:52:MET:HA	1.74	0.69
1:N:22:ILE:HD11	1:N:52:MET:HA	1.76	0.68
1:K:52:MET:HE2	3:K:201:HEM:CHC	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:52:MET:SD	3:V:202:HEM:C4A	2.84	0.67
1:H:94:GLU:CD	1:H:127:GLU:OE1	2.36	0.67
1:O:49:PHE:HA	1:O:52:MET:SD	2.35	0.67
1:H:54:HIS:CE1	1:H:127:GLU:OE2	2.48	0.66
1:Q:94:GLU:CD	1:Q:127:GLU:OE1	2.38	0.66
1:R:54:HIS:CE1	1:R:127:GLU:OE2	2.49	0.66
1:F:154:ILE:HG21	1:R:140:LEU:HD21	1.76	0.65
1:X:22:ILE:HD11	1:X:52:MET:HA	1.79	0.65
1:J:26:PHE:CZ	3:K:201:HEM:HBC1	2.32	0.65
1:C:22:ILE:HD11	1:C:52:MET:HA	1.78	0.65
1:P:84:THR:O	1:P:88:GLN:HG2	1.97	0.64
1:H:117:ALA:O	1:H:121:GLU:HG2	1.98	0.64
1:E:22:ILE:HD11	1:E:52:MET:HA	1.80	0.64
1:E:117:ALA:O	1:E:121:GLU:HG2	1.99	0.63
1:I:123:ILE:O	1:I:127:GLU:HG2	1.98	0.63
1:F:82:SER:OG	1:F:85:GLU:OE1	2.16	0.63
1:G:22:ILE:HD11	1:G:52:MET:HA	1.79	0.62
1:X:82:SER:OG	1:X:85:GLU:OE1	2.16	0.62
1:S:117:ALA:O	1:S:121:GLU:HG3	2.00	0.62
1:T:4:ASP:OD1	1:T:4:ASP:N	2.33	0.62
1:M:94:GLU:OE2	1:M:130:HIS:ND1	2.27	0.61
1:B:22:ILE:HD11	1:B:52:MET:HA	1.83	0.61
1:I:54:HIS:HE1	1:I:127:GLU:OE2	1.84	0.60
1:K:81:GLN:OE1	1:K:81:GLN:N	2.34	0.60
1:M:52:MET:SD	3:M:202:HEM:C4A	2.94	0.60
1:I:81:GLN:N	1:I:81:GLN:OE1	2.34	0.60
1:T:81:GLN:N	1:T:81:GLN:OE1	2.34	0.60
1:E:14:GLN:HG3	1:E:58:LEU:HD11	1.84	0.60
1:S:49:PHE:HA	1:S:52:MET:HG2	1.82	0.60
1:V:117:ALA:O	1:V:121:GLU:HG3	2.01	0.60
1:V:101:LEU:O	1:V:105:ILE:HG22	2.02	0.60
1:X:6:GLU:OE2	1:X:111:LYS:NZ	2.35	0.60
1:U:18:GLU:O	1:U:22:ILE:HG23	2.02	0.60
1:D:18:GLU:O	1:D:22:ILE:HG23	2.02	0.59
1:S:22:ILE:HD11	1:S:52:MET:HA	1.83	0.59
1:C:40:LEU:HD23	1:C:153:VAL:HG21	1.84	0.59
1:F:54:HIS:ND1	1:F:127:GLU:OE1	2.34	0.59
1:W:89:ALA:O	1:W:93:VAL:HG13	2.03	0.59
1:A:156:GLN:HB3	1:C:39:LYS:HZ2	1.66	0.59
1:D:117:ALA:O	1:D:121:GLU:HG3	2.02	0.59
1:W:82:SER:OG	1:W:85:GLU:OE1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ILE:HD11	1:F:124:LEU:HD23	1.82	0.59
1:V:82:SER:OG	1:V:85:GLU:OE1	2.21	0.59
1:S:92:GLU:HA	1:S:95:LEU:HD12	1.83	0.59
1:M:6:GLU:OE2	1:M:111:LYS:NZ	2.36	0.58
1:S:123:ILE:O	1:S:127:GLU:HG2	2.02	0.58
1:K:6:GLU:OE2	1:K:111:LYS:NZ	2.36	0.58
1:R:49:PHE:HA	1:R:52:MET:HE2	1.86	0.58
1:D:50:ASP:OD1	1:D:53:ARG:NH2	2.37	0.58
1:D:82:SER:OG	1:D:85:GLU:OE1	2.18	0.58
1:U:101:LEU:O	1:U:105:ILE:HG22	2.03	0.58
1:H:4:ASP:OD1	1:H:4:ASP:N	2.37	0.58
1:I:117:ALA:O	1:I:121:GLU:HG3	2.04	0.58
1:P:4:ASP:OD1	1:P:4:ASP:N	2.36	0.58
1:P:40:LEU:HD13	1:P:153:VAL:HG21	1.85	0.58
1:E:101:LEU:O	1:E:105:ILE:HG22	2.03	0.58
1:T:49:PHE:O	1:T:52:MET:HB2	2.04	0.58
1:I:39:LYS:HB2	1:I:153:VAL:HG23	1.84	0.58
1:I:101:LEU:O	1:I:105:ILE:HG22	2.04	0.58
1:B:123:ILE:O	1:B:127:GLU:HG2	2.04	0.57
1:C:101:LEU:O	1:C:105:ILE:HG22	2.04	0.57
1:F:94:GLU:O	1:F:98:ILE:HG23	2.04	0.57
1:K:22:ILE:HG13	1:K:52:MET:HB3	1.86	0.57
1:F:104:GLY:O	1:F:108:MET:HG3	2.05	0.57
1:O:18:GLU:OE1	1:O:51:GLU:OE1	2.22	0.57
1:P:54:HIS:HE1	1:P:127:GLU:OE2	1.85	0.57
1:R:101:LEU:O	1:R:105:ILE:HG22	2.05	0.57
1:H:18:GLU:OE1	1:H:54:HIS:ND1	2.31	0.57
1:U:117:ALA:O	1:U:121:GLU:HG3	2.04	0.57
1:I:18:GLU:O	1:I:22:ILE:HG23	2.05	0.56
1:C:117:ALA:O	1:C:121:GLU:HG3	2.05	0.56
1:R:113:ASP:OD2	1:R:116:SER:OG	2.22	0.56
1:G:49:PHE:O	1:G:52:MET:HB2	2.05	0.56
1:F:113:ASP:OD2	1:F:116:SER:OG	2.24	0.56
1:H:22:ILE:HD11	1:H:52:MET:HA	1.87	0.56
1:B:16:THR:OG1	1:B:73:ARG:NH1	2.38	0.56
1:E:94:GLU:O	1:E:98:ILE:HG23	2.06	0.56
1:K:49:PHE:HD1	1:K:52:MET:HE1	1.70	0.56
1:E:4:ASP:N	1:E:4:ASP:OD1	2.38	0.55
3:M:202:HEM:HMB2	3:M:202:HEM:HBB2	1.88	0.55
1:J:4:ASP:N	1:J:4:ASP:OD1	2.39	0.55
1:P:117:ALA:O	1:P:121:GLU:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:82:SER:OG	1:N:85:GLU:OE1	2.23	0.55
1:R:18:GLU:O	1:R:22:ILE:HG23	2.07	0.55
1:O:78:ARG:NH1	1:O:92:GLU:OE2	2.39	0.55
1:F:101:LEU:O	1:F:105:ILE:HG22	2.07	0.55
1:P:52:MET:HE1	3:P:202:HEM:NB	2.21	0.55
1:X:94:GLU:OE2	1:X:127:GLU:OE1	2.24	0.55
1:U:81:GLN:N	1:U:81:GLN:OE1	2.40	0.55
1:U:123:ILE:O	1:U:127:GLU:HG2	2.06	0.55
1:C:4:ASP:OD1	1:C:4:ASP:N	2.35	0.54
1:S:101:LEU:O	1:S:105:ILE:HG22	2.07	0.54
1:P:48:SER:O	1:P:52:MET:HG3	2.07	0.54
1:V:4:ASP:N	1:V:4:ASP:OD1	2.40	0.54
1:W:81:GLN:OE1	1:W:81:GLN:N	2.41	0.54
1:E:123:ILE:O	1:E:127:GLU:HG2	2.07	0.54
1:O:40:LEU:HG	1:O:153:VAL:HG21	1.88	0.54
1:R:81:GLN:OE1	1:R:81:GLN:N	2.40	0.54
1:L:123:ILE:O	1:L:127:GLU:HG2	2.07	0.54
1:S:51:GLU:O	1:S:54:HIS:HB2	2.07	0.54
1:H:81:GLN:OE1	1:H:81:GLN:N	2.40	0.54
1:U:58:LEU:O	1:U:62:ILE:HG22	2.08	0.54
1:L:4:ASP:N	1:L:4:ASP:OD1	2.41	0.53
1:L:155:GLU:OE1	1:L:155:GLU:N	2.35	0.53
1:V:123:ILE:O	1:V:127:GLU:HG2	2.08	0.53
1:A:56:GLU:OE2	1:B:45:ARG:NH2	2.41	0.53
1:B:18:GLU:OE1	1:B:54:HIS:ND1	2.31	0.53
1:G:121:GLU:HG2	1:N:114:ILE:HG21	1.91	0.53
1:J:123:ILE:O	1:J:127:GLU:HG2	2.08	0.53
1:F:117:ALA:O	1:F:121:GLU:HG3	2.09	0.53
1:G:72:GLN:HG2	1:X:77:VAL:HG12	1.90	0.53
1:G:123:ILE:O	1:G:127:GLU:HG2	2.07	0.53
1:A:123:ILE:O	1:A:127:GLU:HG2	2.08	0.53
1:F:75:PHE:O	1:E:72:GLN:NE2	2.41	0.53
1:O:18:GLU:OE1	1:O:51:GLU:OE2	2.26	0.53
1:D:101:LEU:O	1:D:105:ILE:HG22	2.08	0.53
1:P:123:ILE:O	1:P:127:GLU:HG2	2.09	0.53
1:P:82:SER:OG	1:P:85:GLU:OE1	2.16	0.53
1:I:51:GLU:OE2	1:I:54:HIS:CE1	2.61	0.53
1:D:123:ILE:O	1:D:127:GLU:HG2	2.08	0.53
1:P:139:ASP:OD1	1:P:140:LEU:N	2.42	0.53
1:B:82:SER:OG	1:B:85:GLU:OE1	2.19	0.52
1:C:81:GLN:OE1	1:C:81:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:GLN:O	1:K:92:GLU:HG3	2.09	0.52
1:U:20:THR:HG23	1:U:77:VAL:HG12	1.91	0.52
1:K:114:ILE:HG21	1:L:121:GLU:HG2	1.92	0.52
1:X:4:ASP:N	1:X:4:ASP:OD1	2.42	0.52
1:W:6:GLU:O	1:W:9:GLU:HG3	2.10	0.52
1:F:155:GLU:HG2	1:F:157:THR:H	1.75	0.52
1:C:58:LEU:O	1:C:62:ILE:HG22	2.08	0.52
1:P:101:LEU:O	1:P:105:ILE:HG22	2.10	0.52
1:S:89:ALA:O	1:S:92:GLU:HG2	2.10	0.52
1:B:55:ALA:O	1:B:59:THR:HG22	2.10	0.52
1:C:123:ILE:O	1:C:127:GLU:HG2	2.10	0.52
1:O:157:THR:HA	1:Q:39:LYS:HG2	1.90	0.52
1:R:117:ALA:O	1:R:121:GLU:HG3	2.10	0.52
1:B:58:LEU:O	1:B:62:ILE:HG22	2.10	0.52
1:Q:101:LEU:O	1:Q:105:ILE:HG22	2.09	0.52
1:W:111:LYS:O	1:W:111:LYS:HG2	2.09	0.52
1:F:137:GLN:O	1:F:141:ILE:HG22	2.11	0.51
1:P:58:LEU:O	1:P:62:ILE:HG22	2.10	0.51
1:S:18:GLU:CD	1:S:54:HIS:ND1	2.43	0.51
1:U:22:ILE:HD12	1:U:52:MET:HG2	1.92	0.51
1:V:14:GLN:HG3	1:V:58:LEU:HD11	1.91	0.51
1:V:18:GLU:O	1:V:22:ILE:HG23	2.10	0.51
1:G:154:ILE:HD11	1:I:152:THR:HG21	1.92	0.51
1:R:123:ILE:O	1:R:127:GLU:HG2	2.10	0.51
1:M:92:GLU:O	1:M:96:GLU:HG3	2.10	0.51
1:R:19:LEU:O	1:R:22:ILE:HG12	2.10	0.51
1:U:4:ASP:OD1	1:U:4:ASP:N	2.37	0.51
1:H:58:LEU:O	1:H:62:ILE:HG22	2.11	0.51
1:C:137:GLN:O	1:C:141:ILE:HG22	2.11	0.51
1:D:94:GLU:OE2	1:D:130:HIS:ND1	2.44	0.51
1:N:137:GLN:O	1:N:141:ILE:HG22	2.11	0.51
1:X:55:ALA:O	1:X:59:THR:HG22	2.10	0.51
1:K:139:ASP:OD1	1:K:140:LEU:N	2.44	0.50
1:M:58:LEU:O	1:M:62:ILE:HG22	2.12	0.50
1:G:114:ILE:HG21	1:M:121:GLU:HG2	1.93	0.50
1:K:123:ILE:O	1:K:127:GLU:HG2	2.11	0.50
1:L:18:GLU:O	1:L:22:ILE:HG23	2.11	0.50
1:O:108:MET:SD	1:O:116:SER:HB2	2.51	0.50
1:Q:58:LEU:O	1:Q:62:ILE:HG22	2.11	0.50
1:Q:31:LEU:HD12	1:R:63:LEU:HD11	1.94	0.50
1:R:39:LYS:HE3	1:R:153:VAL:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ILE:O	1:H:127:GLU:HG2	2.11	0.50
1:G:58:LEU:O	1:G:62:ILE:HG22	2.11	0.50
1:P:127:GLU:O	1:P:131:ILE:HG22	2.11	0.50
1:T:127:GLU:O	1:T:131:ILE:HG22	2.11	0.50
1:A:55:ALA:O	1:A:59:THR:HG22	2.12	0.50
1:F:14:GLN:HB3	1:F:58:LEU:HD21	1.93	0.50
1:E:85:GLU:OE1	1:E:85:GLU:N	2.44	0.50
1:G:6:GLU:O	1:G:9:GLU:HG3	2.12	0.50
1:H:101:LEU:O	1:H:105:ILE:HG22	2.12	0.50
1:M:129:HIS:C	1:M:129:HIS:HD1	2.20	0.50
1:O:137:GLN:O	1:O:141:ILE:HG22	2.12	0.50
1:V:55:ALA:O	1:V:59:THR:HG22	2.12	0.50
1:V:58:LEU:O	1:V:62:ILE:HG22	2.11	0.50
1:D:55:ALA:O	1:D:59:THR:HG22	2.12	0.50
1:I:99:ASP:OD2	1:I:103:ARG:NH1	2.45	0.50
1:J:127:GLU:O	1:J:131:ILE:HG22	2.11	0.50
1:K:16:THR:HG23	1:K:74:LEU:HA	1.94	0.50
1:N:70:ASN:HD21	1:N:73:ARG:HE	1.58	0.50
1:W:123:ILE:O	1:W:127:GLU:HG2	2.12	0.50
1:W:114:ILE:HG21	1:X:121:GLU:HG2	1.94	0.50
1:X:58:LEU:O	1:X:62:ILE:HG22	2.12	0.50
1:G:108:MET:HE3	1:G:116:SER:HB2	1.94	0.49
1:I:55:ALA:O	1:I:59:THR:HG22	2.11	0.49
1:L:55:ALA:O	1:L:59:THR:HG22	2.12	0.49
1:R:58:LEU:O	1:R:62:ILE:HG22	2.13	0.49
1:A:121:GLU:HG2	1:Q:114:ILE:HG21	1.92	0.49
1:S:82:SER:OG	1:S:85:GLU:OE1	2.23	0.49
1:U:6:GLU:O	1:U:9:GLU:HG3	2.11	0.49
1:E:58:LEU:O	1:E:62:ILE:HG22	2.13	0.49
1:E:84:THR:OG1	1:E:85:GLU:OE1	2.30	0.49
1:P:49:PHE:O	1:P:52:MET:HB2	2.12	0.49
1:D:111:LYS:O	1:D:111:LYS:HG2	2.12	0.49
1:F:129:HIS:C	1:F:129:HIS:HD1	2.20	0.49
1:L:58:LEU:O	1:L:62:ILE:HG22	2.13	0.49
1:O:58:LEU:O	1:O:62:ILE:HG22	2.12	0.49
1:R:54:HIS:HE1	1:R:127:GLU:OE2	1.95	0.49
1:T:137:GLN:O	1:T:141:ILE:HG22	2.12	0.49
1:A:54:HIS:HE1	1:A:127:GLU:OE1	1.95	0.49
1:F:55:ALA:O	1:F:59:THR:HG22	2.12	0.49
1:I:14:GLN:NE2	1:I:18:GLU:OE2	2.46	0.49
1:L:157:THR:HG23	1:N:39:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:GLU:O	1:J:9:GLU:HG3	2.13	0.49
1:J:55:ALA:O	1:J:59:THR:HG22	2.13	0.49
1:K:55:ALA:O	1:K:59:THR:HG22	2.13	0.49
1:L:82:SER:OG	1:L:85:GLU:OE1	2.22	0.49
1:T:117:ALA:O	1:T:121:GLU:HG2	2.13	0.49
1:A:58:LEU:O	1:A:62:ILE:HG22	2.13	0.48
1:H:6:GLU:O	1:H:9:GLU:HG3	2.13	0.48
1:R:55:ALA:O	1:R:59:THR:HG22	2.13	0.48
1:R:70:ASN:HD21	1:R:73:ARG:HE	1.61	0.48
1:E:81:GLN:N	1:E:81:GLN:OE1	2.47	0.48
1:B:137:GLN:O	1:B:141:ILE:HG22	2.13	0.48
1:B:155:GLU:HG3	1:B:157:THR:H	1.79	0.48
1:K:22:ILE:CD1	1:K:52:MET:HB3	2.43	0.48
1:N:36:GLY:O	1:N:154:ILE:HG22	2.14	0.48
1:O:55:ALA:O	1:O:59:THR:HG22	2.13	0.48
1:F:58:LEU:O	1:F:62:ILE:HG22	2.13	0.48
1:I:114:ILE:HG21	1:W:121:GLU:HG2	1.95	0.48
1:L:24:GLN:HB2	1:L:77:VAL:HG23	1.95	0.48
1:P:55:ALA:O	1:P:59:THR:HG22	2.13	0.48
1:K:58:LEU:O	1:K:62:ILE:HG22	2.12	0.48
1:A:82:SER:OG	1:A:85:GLU:OE1	2.24	0.48
1:I:39:LYS:HE2	1:I:153:VAL:HG23	1.95	0.48
1:L:108:MET:HE3	1:L:116:SER:HB2	1.95	0.48
1:S:78:ARG:HD2	1:S:92:GLU:OE2	2.14	0.48
1:B:121:GLU:HG2	1:J:114:ILE:HG21	1.96	0.48
1:F:77:VAL:HG23	1:E:72:GLN:HE21	1.79	0.48
1:H:137:GLN:O	1:H:141:ILE:HG22	2.13	0.48
1:J:16:THR:HG21	1:J:73:ARG:HE	1.79	0.48
1:L:1:MET:HE2	1:L:1:MET:HA	1.94	0.48
1:M:55:ALA:O	1:M:59:THR:HG22	2.14	0.48
1:P:6:GLU:O	1:P:9:GLU:HG3	2.14	0.48
1:Q:117:ALA:O	1:Q:121:GLU:HG3	2.14	0.48
1:R:4:ASP:OD2	1:R:5:PRO:HD2	2.14	0.48
1:J:94:GLU:OE2	1:J:130:HIS:ND1	2.42	0.48
1:A:94:GLU:CD	1:A:127:GLU:OE2	2.56	0.48
1:T:40:LEU:HD13	1:T:153:VAL:HG21	1.95	0.48
1:I:6:GLU:O	1:I:9:GLU:HG3	2.14	0.48
1:R:84:THR:OG1	1:R:85:GLU:OE1	2.29	0.48
1:K:121:GLU:HG2	1:T:114:ILE:HG21	1.95	0.47
1:V:137:GLN:OE1	1:V:149:TYR:OH	2.21	0.47
1:G:127:GLU:O	1:G:131:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:LEU:O	1:L:22:ILE:HG12	2.15	0.47
1:R:85:GLU:OE1	1:R:85:GLU:N	2.46	0.47
1:B:30:LYS:HD2	1:B:30:LYS:HA	1.69	0.47
1:C:114:ILE:HG21	1:J:121:GLU:HG2	1.95	0.47
1:E:137:GLN:O	1:E:141:ILE:HG22	2.14	0.47
1:H:85:GLU:N	1:H:85:GLU:OE1	2.46	0.47
1:L:154:ILE:HG21	1:N:140:LEU:HD21	1.97	0.47
1:T:72:GLN:HG2	1:U:77:VAL:HG22	1.97	0.47
1:F:114:ILE:HG21	1:H:121:GLU:OE2	2.15	0.47
1:J:137:GLN:O	1:J:141:ILE:HG22	2.15	0.47
1:P:137:GLN:O	1:P:141:ILE:HG22	2.14	0.47
1:W:49:PHE:O	1:W:52:MET:HB3	2.14	0.47
1:F:98:ILE:HG13	1:F:99:ASP:N	2.29	0.47
1:I:101:LEU:HD11	1:I:123:ILE:HG22	1.97	0.47
1:P:52:MET:HB3	1:P:52:MET:HE2	1.65	0.47
1:D:11:LEU:HB3	1:D:62:ILE:HD11	1.97	0.46
1:N:14:GLN:HB3	1:N:58:LEU:HD21	1.97	0.46
1:Q:6:GLU:O	1:Q:9:GLU:HG3	2.14	0.46
1:W:55:ALA:O	1:W:59:THR:HG22	2.15	0.46
1:L:137:GLN:O	1:L:141:ILE:HG22	2.14	0.46
1:K:127:GLU:O	1:K:131:ILE:HG22	2.16	0.46
1:M:4:ASP:OD1	1:M:4:ASP:N	2.48	0.46
1:X:123:ILE:O	1:X:127:GLU:HG2	2.15	0.46
1:D:51:GLU:O	1:D:54:HIS:HB2	2.16	0.46
1:K:22:ILE:HD11	1:K:48:SER:O	2.15	0.46
1:V:52:MET:SD	3:V:202:HEM:C1A	2.97	0.46
1:C:116:SER:O	1:C:119:VAL:HG22	2.15	0.46
1:N:25:TYR:OH	1:N:130:HIS:HE1	1.99	0.46
1:S:16:THR:HG21	1:S:73:ARG:HE	1.80	0.46
1:I:116:SER:O	1:I:119:VAL:HG22	2.15	0.46
1:L:14:GLN:HG3	1:L:58:LEU:HD11	1.98	0.46
1:E:116:SER:O	1:E:119:VAL:HG22	2.15	0.46
1:U:42:LYS:HB3	1:U:42:LYS:HE3	1.68	0.46
1:C:30:LYS:NZ	1:D:56:GLU:OE2	2.47	0.46
1:J:30:LYS:HD2	1:J:30:LYS:HA	1.66	0.46
1:M:90:ASP:N	1:M:90:ASP:OD1	2.49	0.46
1:N:40:LEU:HD13	1:N:153:VAL:HG11	1.97	0.46
1:K:20:THR:HG23	1:K:77:VAL:HG22	1.98	0.46
1:O:52:MET:HE2	3:P:202:HEM:NA	2.31	0.46
1:U:40:LEU:HG	1:U:153:VAL:HG21	1.98	0.46
1:G:94:GLU:OE2	1:G:130:HIS:ND1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:ARG:NE	1:N:135:GLU:OE2	2.50	0.45
1:T:18:GLU:O	1:T:22:ILE:HG22	2.15	0.45
1:X:6:GLU:O	1:X:9:GLU:HG3	2.16	0.45
1:P:137:GLN:OE1	1:P:149:TYR:OH	2.22	0.45
1:F:6:GLU:O	1:F:9:GLU:HG3	2.17	0.45
1:N:150:LEU:HD23	1:N:150:LEU:HA	1.84	0.45
1:C:154:ILE:HD12	1:F:140:LEU:HD21	1.99	0.45
1:Q:137:GLN:O	1:Q:141:ILE:HG22	2.16	0.45
1:M:52:MET:SD	3:M:202:HEM:CHB	2.99	0.45
1:R:151:SER:OG	1:R:152:THR:N	2.50	0.45
1:A:137:GLN:O	1:A:141:ILE:HG22	2.16	0.45
1:D:42:LYS:HB3	1:D:42:LYS:HE3	1.65	0.45
1:K:42:LYS:HE3	1:K:42:LYS:HB3	1.69	0.45
1:V:19:LEU:O	1:V:22:ILE:HG12	2.17	0.45
1:A:157:THR:HG22	1:C:157:THR:HA	1.99	0.45
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.86	0.45
1:K:109:ARG:HA	1:K:109:ARG:HD3	1.81	0.45
1:C:29:ALA:HB2	1:C:44:THR:HB	1.97	0.45
1:C:85:GLU:OE1	1:C:85:GLU:N	2.47	0.45
1:I:42:LYS:HB3	1:I:42:LYS:HE3	1.66	0.45
1:M:137:GLN:O	1:M:141:ILE:HG22	2.16	0.45
1:S:93:VAL:O	1:S:96:GLU:HG2	2.17	0.45
1:X:16:THR:HG23	1:X:74:LEU:HA	1.98	0.45
1:A:29:ALA:HB2	1:A:44:THR:HB	1.98	0.44
1:G:30:LYS:HA	1:G:30:LYS:HD2	1.74	0.44
1:Q:20:THR:HG23	1:Q:77:VAL:HG22	1.98	0.44
1:X:14:GLN:HB3	1:X:58:LEU:HD21	1.99	0.44
1:I:30:LYS:HA	1:I:30:LYS:HD2	1.67	0.44
1:L:30:LYS:HD3	1:L:30:LYS:HA	1.77	0.44
1:S:14:GLN:HB3	1:S:58:LEU:HD21	1.98	0.44
1:U:116:SER:O	1:U:119:VAL:HG22	2.16	0.44
1:F:49:PHE:O	1:F:52:MET:HB3	2.18	0.44
1:R:137:GLN:O	1:R:141:ILE:HG22	2.17	0.44
1:A:4:ASP:OD1	1:A:4:ASP:N	2.50	0.44
1:H:127:GLU:O	1:H:131:ILE:HG22	2.17	0.44
1:A:90:ASP:OD1	1:A:90:ASP:N	2.48	0.44
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.66	0.44
1:J:101:LEU:O	1:J:105:ILE:HG22	2.17	0.44
1:M:30:LYS:HA	1:M:30:LYS:HD2	1.61	0.44
1:G:14:GLN:HB3	1:G:58:LEU:HD21	1.99	0.44
1:J:20:THR:HG23	1:J:77:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:116:SER:O	1:P:119:VAL:HG22	2.18	0.44
1:B:40:LEU:HG	1:B:153:VAL:HG21	2.00	0.44
1:C:14:GLN:HG3	1:C:58:LEU:HD11	2.00	0.44
1:E:6:GLU:O	1:E:9:GLU:HG3	2.17	0.44
1:G:137:GLN:O	1:G:141:ILE:HG22	2.17	0.44
1:H:4:ASP:OD2	1:H:111:LYS:HD2	2.18	0.44
1:N:18:GLU:OE2	1:N:127:GLU:OE2	2.36	0.44
1:F:22:ILE:HD11	1:F:52:MET:HA	1.99	0.43
1:F:138:LEU:HD23	1:F:138:LEU:HA	1.90	0.43
1:V:1:MET:HE2	1:V:1:MET:HA	2.00	0.43
1:V:42:LYS:HE3	1:V:42:LYS:HB3	1.69	0.43
1:N:160:ASP:OD1	1:N:160:ASP:N	2.43	0.43
1:O:14:GLN:HG3	1:O:58:LEU:HD11	2.00	0.43
1:S:116:SER:O	1:S:119:VAL:HG22	2.18	0.43
1:H:61:ARG:HA	1:H:61:ARG:HD2	1.82	0.43
1:L:94:GLU:OE2	1:L:127:GLU:CD	2.57	0.43
1:N:123:ILE:O	1:N:127:GLU:HG2	2.18	0.43
1:O:94:GLU:CD	1:O:127:GLU:OE1	2.55	0.43
1:E:63:LEU:HD12	1:E:63:LEU:HA	1.84	0.43
1:I:58:LEU:O	1:I:62:ILE:HG22	2.19	0.43
1:I:85:GLU:OE1	1:I:85:GLU:N	2.50	0.43
1:R:116:SER:HA	1:R:119:VAL:HG12	1.99	0.43
1:V:52:MET:HE3	1:V:52:MET:HB2	1.84	0.43
1:O:127:GLU:O	1:O:131:ILE:HG22	2.19	0.43
1:D:129:HIS:HD1	1:D:129:HIS:C	2.27	0.43
1:K:111:LYS:HD3	1:K:111:LYS:HA	1.80	0.43
1:J:138:LEU:HD12	1:J:138:LEU:HA	1.88	0.43
1:V:39:LYS:H	1:V:39:LYS:HG2	1.61	0.43
1:W:138:LEU:HD12	1:W:138:LEU:HA	1.88	0.43
1:L:92:GLU:O	1:L:96:GLU:HG3	2.18	0.43
1:Q:123:ILE:O	1:Q:127:GLU:HG2	2.19	0.43
1:T:16:THR:HG21	1:T:73:ARG:HE	1.84	0.43
1:V:30:LYS:HD2	1:V:30:LYS:HA	1.68	0.43
1:E:121:GLU:OE2	1:S:114:ILE:HG21	2.19	0.43
1:A:154:ILE:HD12	1:C:140:LEU:HD21	2.01	0.42
1:O:20:THR:HG23	1:O:77:VAL:HG22	2.00	0.42
1:S:144:LEU:HD23	1:S:144:LEU:HA	1.88	0.42
1:T:149:TYR:O	1:T:152:THR:HG22	2.19	0.42
1:D:5:PRO:HA	1:D:8:ILE:HG12	2.00	0.42
1:N:155:GLU:N	1:N:155:GLU:OE1	2.51	0.42
1:Q:127:GLU:O	1:Q:131:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:150:LEU:HD23	1:T:150:LEU:HA	1.82	0.42
1:W:30:LYS:HA	1:W:30:LYS:HD2	1.67	0.42
1:B:90:ASP:HA	1:B:93:VAL:HG12	2.01	0.42
1:J:157:THR:HG23	1:J:158:GLN:O	2.19	0.42
1:H:138:LEU:HD12	1:H:138:LEU:HA	1.88	0.42
1:K:22:ILE:CG1	1:K:52:MET:HB3	2.49	0.42
1:S:129:HIS:HD1	1:S:129:HIS:C	2.27	0.42
1:U:31:LEU:HD12	1:U:31:LEU:HA	1.90	0.42
1:R:140:LEU:HD12	1:R:140:LEU:HA	1.91	0.42
1:S:20:THR:HG23	1:S:77:VAL:HG22	2.00	0.42
1:B:140:LEU:HD21	1:K:154:ILE:HG13	2.00	0.42
1:F:30:LYS:HA	1:F:30:LYS:HD2	1.72	0.42
1:E:98:ILE:HG13	1:E:99:ASP:N	2.34	0.42
1:G:77:VAL:HG12	1:X:72:GLN:OE1	2.20	0.42
1:P:112:HIS:NE2	1:Q:106:GLU:HG3	2.35	0.42
1:R:16:THR:HG23	1:R:74:LEU:HA	2.00	0.42
1:S:58:LEU:HD12	1:S:58:LEU:HA	1.89	0.42
1:J:40:LEU:HD23	1:J:40:LEU:HA	1.86	0.42
1:M:70:ASN:OD1	1:M:70:ASN:N	2.52	0.42
1:M:127:GLU:O	1:M:131:ILE:HG22	2.20	0.42
1:N:58:LEU:HD12	1:N:58:LEU:HA	1.88	0.42
1:R:115:THR:HA	1:R:118:ASN:ND2	2.35	0.42
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.87	0.42
1:N:127:GLU:O	1:N:131:ILE:HG22	2.20	0.42
1:O:123:ILE:O	1:O:127:GLU:HG2	2.20	0.42
1:P:114:ILE:HG21	1:Q:121:GLU:HG2	2.02	0.42
1:V:127:GLU:O	1:V:131:ILE:HG22	2.20	0.42
1:C:127:GLU:O	1:C:131:ILE:HG22	2.20	0.42
1:E:140:LEU:HD21	1:I:154:ILE:HD12	2.01	0.41
1:N:70:ASN:ND2	1:N:73:ARG:HE	2.17	0.41
1:R:30:LYS:HA	1:R:30:LYS:HD2	1.80	0.41
1:S:101:LEU:HD12	1:S:101:LEU:HA	1.90	0.41
1:V:116:SER:O	1:V:119:VAL:HG22	2.19	0.41
1:D:101:LEU:HD11	1:D:123:ILE:HG22	2.02	0.41
1:M:29:ALA:HB2	1:M:44:THR:HB	2.02	0.41
1:V:129:HIS:C	1:V:129:HIS:HD1	2.28	0.41
1:X:116:SER:O	1:X:119:VAL:HG22	2.20	0.41
1:A:108:MET:HE3	1:A:116:SER:HB2	2.03	0.41
1:A:51:GLU:O	1:A:54:HIS:HB2	2.20	0.41
1:I:82:SER:HB2	1:I:85:GLU:OE1	2.20	0.41
3:V:202:HEM:ND	1:W:52:MET:HE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:SER:O	1:D:119:VAL:HG22	2.20	0.41
1:K:48:SER:O	1:K:52:MET:HE3	2.21	0.41
1:W:116:SER:O	1:W:119:VAL:HG22	2.19	0.41
1:F:4:ASP:HB3	1:F:6:GLU:OE1	2.21	0.41
1:H:30:LYS:HA	1:H:30:LYS:HD2	1.73	0.41
1:D:74:LEU:HD23	1:D:74:LEU:HA	1.93	0.41
1:F:6:GLU:OE1	1:F:6:GLU:N	2.36	0.41
1:K:1:MET:HE3	1:K:1:MET:HB2	1.85	0.41
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.86	0.41
1:I:127:GLU:O	1:I:131:ILE:HG22	2.21	0.41
1:R:127:GLU:O	1:R:131:ILE:HG22	2.21	0.41
1:T:63:LEU:HD12	1:T:63:LEU:HA	1.82	0.41
1:E:30:LYS:HA	1:E:30:LYS:HD3	1.83	0.41
1:H:82:SER:HB2	1:H:85:GLU:OE1	2.21	0.41
1:I:51:GLU:O	1:I:54:HIS:HB2	2.21	0.41
1:J:14:GLN:HG3	1:J:58:LEU:HD11	2.03	0.41
1:L:155:GLU:HG2	1:L:156:GLN:N	2.35	0.41
1:N:117:ALA:O	1:N:121:GLU:HG3	2.21	0.41
1:N:133:TYR:O	1:N:136:THR:HG22	2.21	0.41
1:W:140:LEU:HD12	1:W:140:LEU:HA	1.88	0.41
1:X:42:LYS:HB3	1:X:42:LYS:HE3	1.89	0.41
1:N:29:ALA:HB2	1:N:44:THR:HB	2.03	0.41
1:T:123:ILE:O	1:T:127:GLU:HG2	2.22	0.40
1:X:117:ALA:O	1:X:121:GLU:HG3	2.21	0.40
1:J:52:MET:HE2	3:K:201:HEM:NA	2.35	0.40
1:Q:14:GLN:HB3	1:Q:58:LEU:HD21	2.01	0.40
1:B:47:GLU:HG2	1:B:130:HIS:CE1	2.57	0.40
1:D:114:ILE:HD13	1:F:105:ILE:HD13	2.03	0.40
1:R:138:LEU:HD12	1:R:138:LEU:HA	1.81	0.40
1:E:127:GLU:O	1:E:131:ILE:HG22	2.22	0.40
1:G:155:GLU:CD	1:G:156:GLN:HE21	2.26	0.40
1:P:30:LYS:HA	1:P:30:LYS:HD2	1.68	0.40
1:V:91:ARG:NH2	1:V:135:GLU:OE2	2.39	0.40
1:W:51:GLU:OE2	1:W:94:GLU:OE2	2.40	0.40
1:D:54:HIS:O	1:D:57:VAL:HG12	2.22	0.40
1:I:59:THR:HA	1:I:62:ILE:HG22	2.04	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	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	B	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
1	C	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	D	159/162 (98%)	154 (97%)	4 (2%)	1 (1%)	22	52
1	E	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
1	F	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
1	G	159/162 (98%)	155 (98%)	3 (2%)	1 (1%)	22	52
1	H	159/162 (98%)	155 (98%)	3 (2%)	1 (1%)	22	52
1	I	158/162 (98%)	151 (96%)	6 (4%)	1 (1%)	22	52
1	J	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	K	155/162 (96%)	152 (98%)	3 (2%)	0	100	100
1	L	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	M	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	N	159/162 (98%)	149 (94%)	9 (6%)	1 (1%)	22	52
1	O	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	P	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
1	Q	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	R	155/162 (96%)	152 (98%)	3 (2%)	0	100	100
1	S	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
1	T	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	22	52
1	U	155/162 (96%)	152 (98%)	3 (2%)	0	100	100
1	V	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	22	52
1	W	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
1	X	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
All	All	3810/3888 (98%)	3710 (97%)	93 (2%)	7 (0%)	45	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	PRO
1	G	159	PRO
1	H	159	PRO
1	I	159	PRO
1	T	161	PRO
1	N	154	ILE
1	V	157	THR

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	140/144 (97%)	140 (100%)	0	100 100
1	B	137/144 (95%)	137 (100%)	0	100 100
1	C	142/144 (99%)	142 (100%)	0	100 100
1	D	138/144 (96%)	138 (100%)	0	100 100
1	E	138/144 (96%)	138 (100%)	0	100 100
1	F	140/144 (97%)	140 (100%)	0	100 100
1	G	138/144 (96%)	138 (100%)	0	100 100
1	H	138/144 (96%)	138 (100%)	0	100 100
1	I	138/144 (96%)	137 (99%)	1 (1%)	81 88
1	J	141/144 (98%)	140 (99%)	1 (1%)	81 88
1	K	138/144 (96%)	138 (100%)	0	100 100
1	L	142/144 (99%)	139 (98%)	3 (2%)	48 70
1	M	137/144 (95%)	137 (100%)	0	100 100
1	N	140/144 (97%)	140 (100%)	0	100 100
1	O	140/144 (97%)	140 (100%)	0	100 100
1	P	138/144 (96%)	136 (99%)	2 (1%)	62 78
1	Q	142/144 (99%)	142 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	138/144 (96%)	138 (100%)	0	100 100
1	S	140/144 (97%)	137 (98%)	3 (2%)	48 70
1	T	140/144 (97%)	139 (99%)	1 (1%)	81 88
1	U	138/144 (96%)	138 (100%)	0	100 100
1	V	142/144 (99%)	141 (99%)	1 (1%)	81 88
1	W	138/144 (96%)	138 (100%)	0	100 100
1	X	140/144 (97%)	140 (100%)	0	100 100
All	All	3343/3456 (97%)	3331 (100%)	12 (0%)	88 93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	154	ILE
1	J	156	GLN
1	L	72	GLN
1	L	94	GLU
1	L	160	ASP
1	P	40	LEU
1	P	148	LEU
1	S	92	GLU
1	S	96	GLU
1	S	98	ILE
1	T	22	ILE
1	V	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	B	24	GLN
1	B	130	HIS
1	D	28	HIS
1	E	28	HIS
1	E	118	ASN
1	H	2	GLN
1	J	2	GLN
1	K	130	HIS
1	L	28	HIS

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Mol	Chain	Res	Type
1	M	2	GLN
1	N	130	HIS
1	P	54	HIS
1	P	118	ASN
1	Q	2	GLN
1	T	130	HIS
1	T	158	GLN
1	V	28	HIS
1	X	24	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	K	201	-	41,50,50	1.70	5 (12%)	45,82,82	1.69	8 (17%)
3	HEM	X	201	-	41,50,50	1.40	3 (7%)	45,82,82	1.47	7 (15%)
3	HEM	F	202	-	41,50,50	1.55	4 (9%)	45,82,82	1.84	10 (22%)
3	HEM	S	202	1	41,50,50	1.66	5 (12%)	45,82,82	1.51	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	B	201	-	41,50,50	1.48	4 (9%)	45,82,82	1.57	9 (20%)
3	HEM	R	201	1	41,50,50	1.60	5 (12%)	45,82,82	1.36	5 (11%)
3	HEM	P	202	-	41,50,50	1.58	7 (17%)	45,82,82	1.55	6 (13%)
3	HEM	M	202	-	41,50,50	1.48	4 (9%)	45,82,82	1.39	8 (17%)
3	HEM	H	202	-	41,50,50	1.70	6 (14%)	45,82,82	1.76	8 (17%)
3	HEM	U	202	-	41,50,50	1.64	6 (14%)	45,82,82	1.69	10 (22%)
3	HEM	V	202	-	41,50,50	1.60	6 (14%)	45,82,82	1.44	6 (13%)
3	HEM	D	201	-	41,50,50	1.65	5 (12%)	45,82,82	1.51	8 (17%)

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
3	HEM	K	201	-	-	4/12/54/54	-
3	HEM	X	201	-	-	4/12/54/54	-
3	HEM	F	202	-	-	3/12/54/54	-
3	HEM	S	202	1	-	6/12/54/54	-
3	HEM	B	201	-	-	1/12/54/54	-
3	HEM	R	201	1	-	1/12/54/54	-
3	HEM	P	202	-	-	6/12/54/54	-
3	HEM	M	202	-	-	0/12/54/54	-
3	HEM	H	202	-	-	3/12/54/54	-
3	HEM	U	202	-	-	3/12/54/54	-
3	HEM	V	202	-	-	3/12/54/54	-
3	HEM	D	201	-	-	1/12/54/54	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	HEM	C3C-C2C	-5.70	1.32	1.40
3	U	202	HEM	C3C-C2C	-5.51	1.32	1.40
3	K	201	HEM	C3C-C2C	-5.09	1.33	1.40
3	P	202	HEM	C3C-C2C	-4.97	1.33	1.40
3	H	202	HEM	C3C-C2C	-4.96	1.33	1.40
3	F	202	HEM	C3C-C2C	-4.96	1.33	1.40
3	M	202	HEM	C3C-C2C	-4.89	1.33	1.40
3	V	202	HEM	C3C-C2C	-4.88	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	201	HEM	C3C-C2C	-4.84	1.33	1.40
3	S	202	HEM	C3C-C2C	-4.62	1.34	1.40
3	B	201	HEM	C3C-C2C	-4.51	1.34	1.40
3	S	202	HEM	FE-ND	4.26	2.17	1.96
3	H	202	HEM	FE-NB	3.99	2.16	1.96
3	K	201	HEM	FE-NB	3.91	2.16	1.96
3	H	202	HEM	FE-ND	3.79	2.15	1.96
3	X	201	HEM	C3C-CAC	3.71	1.55	1.47
3	X	201	HEM	C3C-C2C	-3.62	1.35	1.40
3	K	201	HEM	FE-ND	3.54	2.14	1.96
3	R	201	HEM	C3C-CAC	3.50	1.55	1.47
3	F	202	HEM	C3C-CAC	3.48	1.54	1.47
3	V	202	HEM	C3C-CAC	3.47	1.54	1.47
3	K	201	HEM	C3C-CAC	3.42	1.54	1.47
3	S	202	HEM	C3C-CAC	3.37	1.54	1.47
3	H	202	HEM	C3C-CAC	3.36	1.54	1.47
3	B	201	HEM	C3C-CAC	3.36	1.54	1.47
3	P	202	HEM	C3C-CAC	3.35	1.54	1.47
3	D	201	HEM	C3C-CAC	3.34	1.54	1.47
3	U	202	HEM	C3C-CAC	3.31	1.54	1.47
3	M	202	HEM	C3C-CAC	3.26	1.54	1.47
3	U	202	HEM	FE-NB	3.09	2.12	1.96
3	D	201	HEM	FE-NB	3.04	2.11	1.96
3	V	202	HEM	FE-NB	2.99	2.11	1.96
3	M	202	HEM	CAB-C3B	2.99	1.55	1.47
3	R	201	HEM	FE-ND	2.96	2.11	1.96
3	R	201	HEM	FE-NB	2.94	2.11	1.96
3	B	201	HEM	CAB-C3B	2.94	1.55	1.47
3	P	202	HEM	CAB-C3B	2.90	1.55	1.47
3	U	202	HEM	CAB-C3B	2.87	1.55	1.47
3	U	202	HEM	FE-ND	2.86	2.11	1.96
3	V	202	HEM	FE-ND	2.85	2.10	1.96
3	F	202	HEM	CAB-C3B	2.83	1.55	1.47
3	S	202	HEM	FE-NB	2.80	2.10	1.96
3	R	201	HEM	CAB-C3B	2.80	1.55	1.47
3	P	202	HEM	FE-NB	2.80	2.10	1.96
3	X	201	HEM	CAB-C3B	2.79	1.55	1.47
3	K	201	HEM	CAB-C3B	2.79	1.55	1.47
3	D	201	HEM	CAB-C3B	2.78	1.55	1.47
3	S	202	HEM	CAB-C3B	2.78	1.55	1.47
3	V	202	HEM	CAB-C3B	2.78	1.55	1.47
3	H	202	HEM	CAB-C3B	2.75	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	HEM	FE-ND	2.61	2.09	1.96
3	P	202	HEM	CAA-C2A	2.50	1.55	1.52
3	P	202	HEM	FE-ND	2.49	2.09	1.96
3	M	202	HEM	CAA-C2A	2.34	1.55	1.52
3	H	202	HEM	CMD-C2D	2.13	1.55	1.50
3	F	202	HEM	CMD-C2D	2.13	1.55	1.50
3	B	201	HEM	CAA-C2A	2.12	1.55	1.52
3	U	202	HEM	CMD-C2D	2.05	1.55	1.50
3	V	202	HEM	CAA-C2A	2.02	1.55	1.52
3	P	202	HEM	C3B-C2B	-2.02	1.33	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	202	HEM	CBA-CAA-C2A	-7.02	100.64	112.62
3	H	202	HEM	C4B-CHC-C1C	-6.94	113.39	122.56
3	K	201	HEM	C4B-CHC-C1C	-5.37	115.47	122.56
3	U	202	HEM	CHC-C4B-C3B	4.22	131.02	124.57
3	P	202	HEM	C3B-C2B-C1B	4.20	109.60	106.49
3	K	201	HEM	CHC-C4B-C3B	3.92	130.57	124.57
3	D	201	HEM	C3B-C2B-C1B	3.73	109.25	106.49
3	B	201	HEM	C4D-ND-C1D	3.67	108.86	105.07
3	X	201	HEM	C1B-NB-C4B	3.60	108.79	105.07
3	B	201	HEM	C3B-C2B-C1B	3.48	109.07	106.49
3	V	202	HEM	C3B-C2B-C1B	3.46	109.06	106.49
3	X	201	HEM	C3B-C2B-C1B	3.44	109.04	106.49
3	U	202	HEM	C1B-NB-C4B	3.37	108.56	105.07
3	M	202	HEM	C4D-ND-C1D	3.34	108.52	105.07
3	K	201	HEM	CHC-C4B-NB	-3.32	120.82	124.43
3	P	202	HEM	C1B-NB-C4B	3.27	108.45	105.07
3	R	201	HEM	C3B-C2B-C1B	3.25	108.90	106.49
3	U	202	HEM	CHC-C4B-NB	-3.23	120.92	124.43
3	S	202	HEM	C4C-CHD-C1D	-3.21	118.32	122.56
3	F	202	HEM	C4D-ND-C1D	3.19	108.37	105.07
3	S	202	HEM	C3B-C2B-C1B	3.02	108.72	106.49
3	H	202	HEM	C4D-ND-C1D	3.01	108.18	105.07
3	V	202	HEM	C1B-NB-C4B	3.00	108.17	105.07
3	S	202	HEM	CHA-C4D-ND	2.93	128.00	124.38
3	D	201	HEM	C1B-NB-C4B	2.89	108.06	105.07
3	U	202	HEM	C4B-CHC-C1C	-2.85	118.80	122.56
3	F	202	HEM	C3D-C4D-ND	-2.82	107.02	110.17
3	M	202	HEM	CAD-CBD-CGD	-2.82	107.53	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	202	HEM	C4D-ND-C1D	2.81	107.98	105.07
3	U	202	HEM	C3B-C2B-C1B	2.81	108.57	106.49
3	D	201	HEM	C4D-ND-C1D	2.78	107.94	105.07
3	F	202	HEM	CAD-CBD-CGD	-2.76	107.65	113.60
3	B	201	HEM	C3D-C4D-ND	-2.75	107.10	110.17
3	H	202	HEM	C3B-C2B-C1B	2.73	108.51	106.49
3	P	202	HEM	C4C-CHD-C1D	2.70	126.12	122.56
3	S	202	HEM	C1B-NB-C4B	2.69	107.85	105.07
3	R	201	HEM	C1B-NB-C4B	2.68	107.84	105.07
3	F	202	HEM	CMA-C3A-C4A	-2.66	124.37	128.46
3	P	202	HEM	C2B-C1B-NB	-2.66	106.69	109.84
3	P	202	HEM	C4D-ND-C1D	2.65	107.81	105.07
3	F	202	HEM	C1B-NB-C4B	2.64	107.80	105.07
3	F	202	HEM	C4B-CHC-C1C	2.61	126.00	122.56
3	V	202	HEM	C4D-ND-C1D	2.56	107.72	105.07
3	D	201	HEM	CHC-C4B-C3B	2.56	128.49	124.57
3	F	202	HEM	CHC-C4B-C3B	2.55	128.48	124.57
3	U	202	HEM	C2C-C3C-C4C	2.54	108.67	106.90
3	K	201	HEM	C1B-NB-C4B	2.53	107.69	105.07
3	R	201	HEM	CBA-CAA-C2A	-2.50	108.36	112.62
3	X	201	HEM	CHC-C4B-C3B	2.43	128.28	124.57
3	X	201	HEM	CMC-C2C-C3C	2.40	129.17	124.68
3	K	201	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
3	X	201	HEM	C2B-C1B-NB	-2.37	107.03	109.84
3	M	202	HEM	C3D-C4D-ND	-2.34	107.56	110.17
3	K	201	HEM	C4C-CHD-C1D	-2.33	119.48	122.56
3	U	202	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
3	M	202	HEM	C4C-CHD-C1D	2.33	125.63	122.56
3	B	201	HEM	C2D-C1D-ND	-2.32	107.11	109.88
3	R	201	HEM	C4D-ND-C1D	2.30	107.45	105.07
3	V	202	HEM	CAD-CBD-CGD	-2.30	108.66	113.60
3	M	202	HEM	C2C-C3C-C4C	2.29	108.50	106.90
3	K	201	HEM	C3B-C2B-C1B	2.29	108.19	106.49
3	B	201	HEM	CAD-CBD-CGD	-2.28	108.69	113.60
3	B	201	HEM	C1B-NB-C4B	2.28	107.42	105.07
3	H	202	HEM	C2C-C3C-C4C	2.28	108.49	106.90
3	U	202	HEM	C3D-C4D-ND	-2.27	107.64	110.17
3	B	201	HEM	C4C-CHD-C1D	2.27	125.56	122.56
3	S	202	HEM	C4A-C3A-C2A	2.27	108.58	107.00
3	M	202	HEM	C3B-C2B-C1B	2.27	108.17	106.49
3	D	201	HEM	C2B-C1B-NB	-2.22	107.20	109.84
3	F	202	HEM	C4C-CHD-C1D	2.22	125.49	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	201	HEM	CHD-C1D-C2D	2.22	128.44	124.98
3	S	202	HEM	CHD-C1D-ND	2.20	126.82	124.43
3	H	202	HEM	C3D-C4D-ND	-2.17	107.75	110.17
3	P	202	HEM	C4A-C3A-C2A	2.17	108.51	107.00
3	D	201	HEM	CAD-CBD-CGD	-2.14	108.99	113.60
3	D	201	HEM	C4A-C3A-C2A	2.14	108.48	107.00
3	V	202	HEM	C2B-C1B-NB	-2.13	107.31	109.84
3	R	201	HEM	CAD-CBD-CGD	-2.12	109.04	113.60
3	F	202	HEM	C3B-C2B-C1B	2.12	108.06	106.49
3	S	202	HEM	CAD-CBD-CGD	-2.11	109.07	113.60
3	M	202	HEM	C2D-C1D-ND	-2.10	107.36	109.88
3	U	202	HEM	CBA-CAA-C2A	-2.10	109.04	112.62
3	V	202	HEM	C4A-C3A-C2A	2.09	108.45	107.00
3	S	202	HEM	CAD-C3D-C2D	-2.09	123.99	127.88
3	B	201	HEM	C2C-C3C-C4C	2.08	108.35	106.90
3	H	202	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
3	H	202	HEM	CHC-C4B-C3B	2.07	127.73	124.57
3	M	202	HEM	CHB-C1B-NB	2.05	126.92	124.38
3	K	201	HEM	C4D-ND-C1D	2.04	107.18	105.07
3	B	201	HEM	C2B-C1B-NB	-2.04	107.42	109.84
3	X	201	HEM	CAD-CBD-CGD	-2.04	109.22	113.60
3	H	202	HEM	CAD-C3D-C2D	-2.01	124.14	127.88
3	X	201	HEM	CHD-C1D-ND	2.00	126.61	124.43

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	202	HEM	C1A-C2A-CAA-CBA
3	P	202	HEM	C3A-C2A-CAA-CBA
3	S	202	HEM	C1A-C2A-CAA-CBA
3	R	201	HEM	C4B-C3B-CAB-CBB
3	B	201	HEM	C4B-C3B-CAB-CBB
3	D	201	HEM	C4B-C3B-CAB-CBB
3	F	202	HEM	C4B-C3B-CAB-CBB
3	H	202	HEM	C4B-C3B-CAB-CBB
3	K	201	HEM	C4B-C3B-CAB-CBB
3	P	202	HEM	C4B-C3B-CAB-CBB
3	S	202	HEM	C4B-C3B-CAB-CBB
3	U	202	HEM	C4B-C3B-CAB-CBB
3	V	202	HEM	C4B-C3B-CAB-CBB
3	X	201	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	P	202	HEM	C2A-CAA-CBA-CGA
3	S	202	HEM	C3A-C2A-CAA-CBA
3	H	202	HEM	C2D-C3D-CAD-CBD
3	H	202	HEM	C4D-C3D-CAD-CBD
3	F	202	HEM	CAD-CBD-CGD-O2D
3	P	202	HEM	CAD-CBD-CGD-O2D
3	V	202	HEM	CAA-CBA-CGA-O2A
3	X	201	HEM	CAA-CBA-CGA-O2A
3	F	202	HEM	CAD-CBD-CGD-O1D
3	P	202	HEM	CAD-CBD-CGD-O1D
3	S	202	HEM	CAD-CBD-CGD-O2D
3	V	202	HEM	CAA-CBA-CGA-O1A
3	U	202	HEM	CAD-CBD-CGD-O2D
3	X	201	HEM	CAA-CBA-CGA-O1A
3	K	201	HEM	CAA-CBA-CGA-O2A
3	K	201	HEM	CAD-CBD-CGD-O2D
3	S	202	HEM	CAD-CBD-CGD-O1D
3	U	202	HEM	CAD-CBD-CGD-O1D
3	K	201	HEM	CAA-CBA-CGA-O1A
3	S	202	HEM	C2D-C3D-CAD-CBD
3	X	201	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

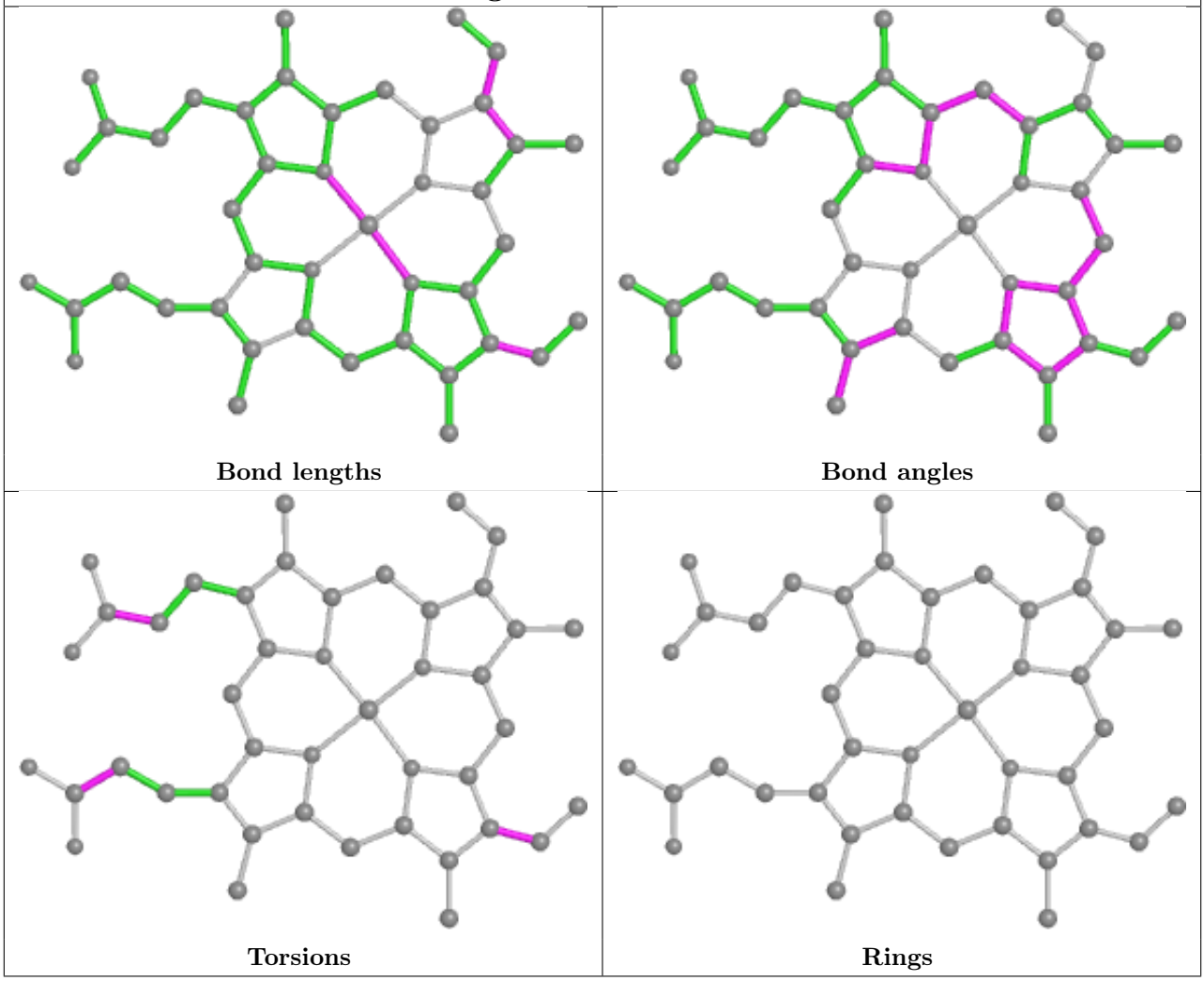
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	201	HEM	4	0
3	P	202	HEM	3	0
3	M	202	HEM	3	0
3	V	202	HEM	4	0

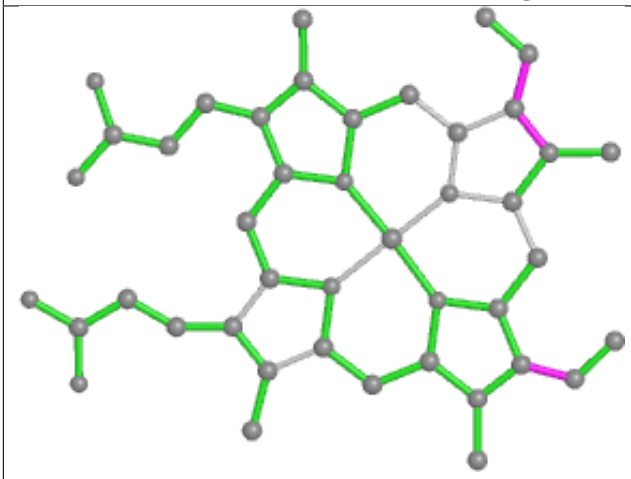
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

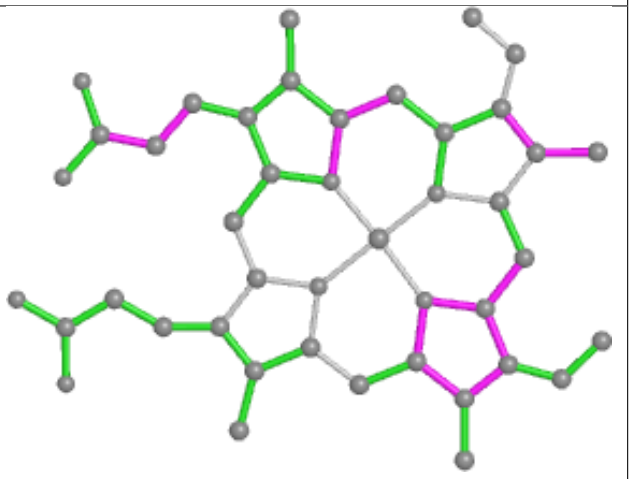
Ligand HEM K 201



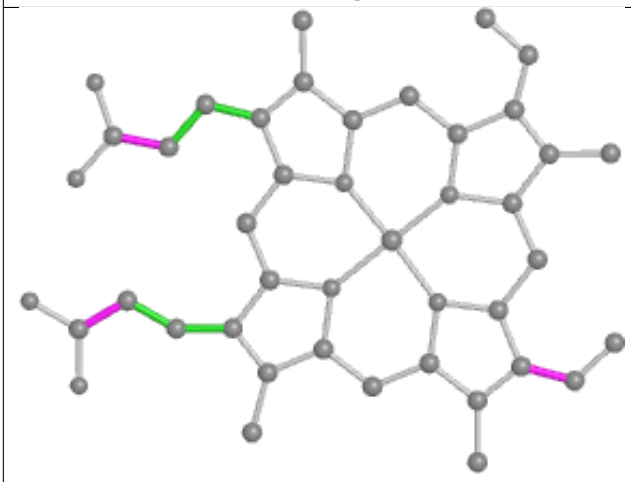
Ligand HEM X 201



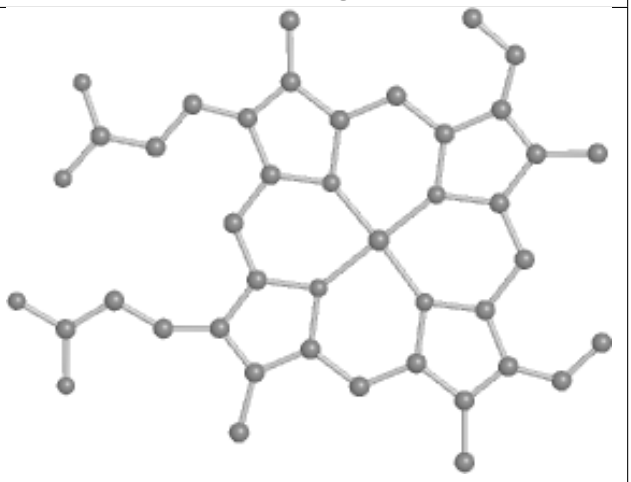
Bond lengths



Bond angles

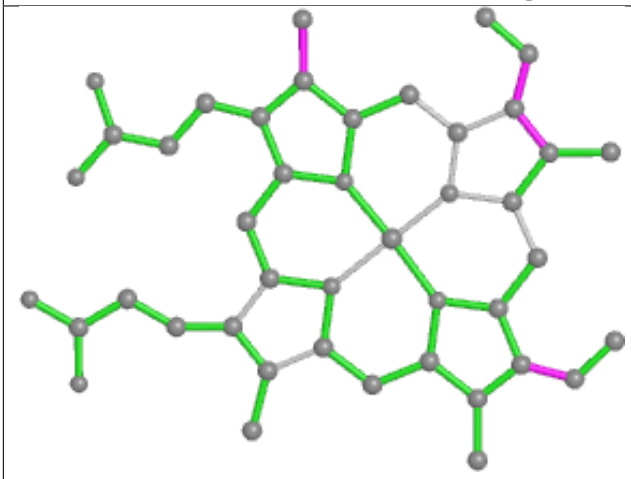


Torsions



Rings

Ligand HEM F 202



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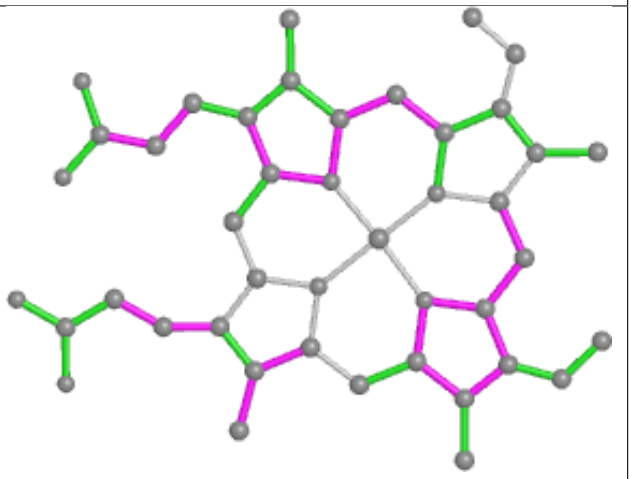
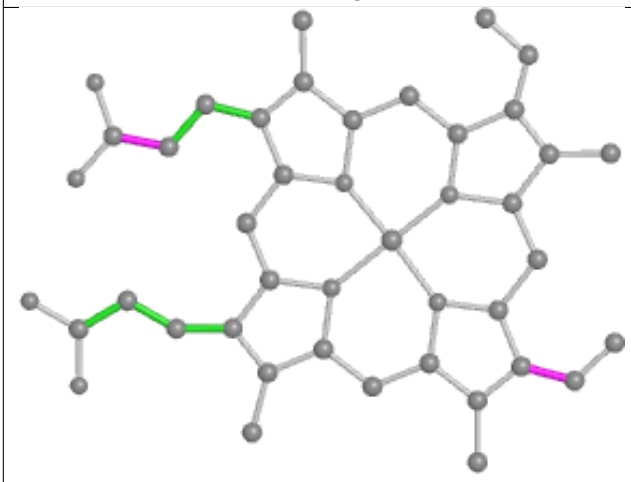


Bond angles



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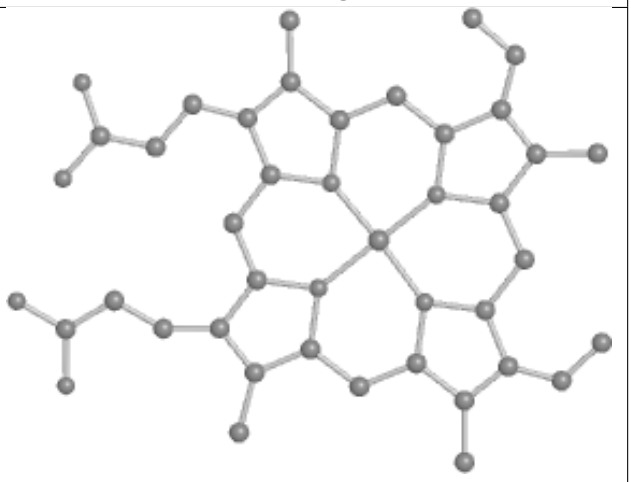
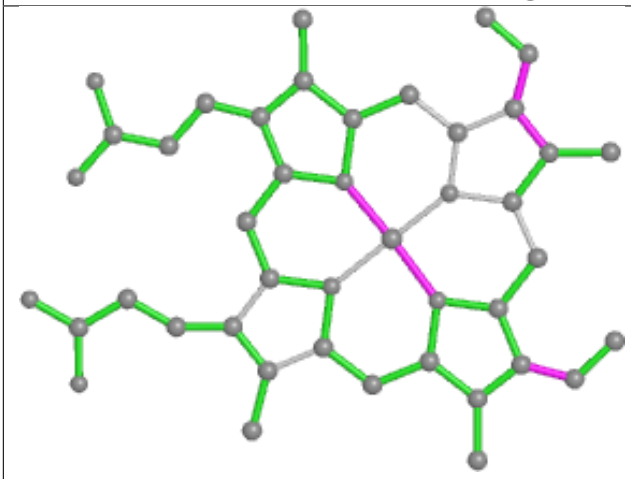


Rings

Ligand HEM S 202



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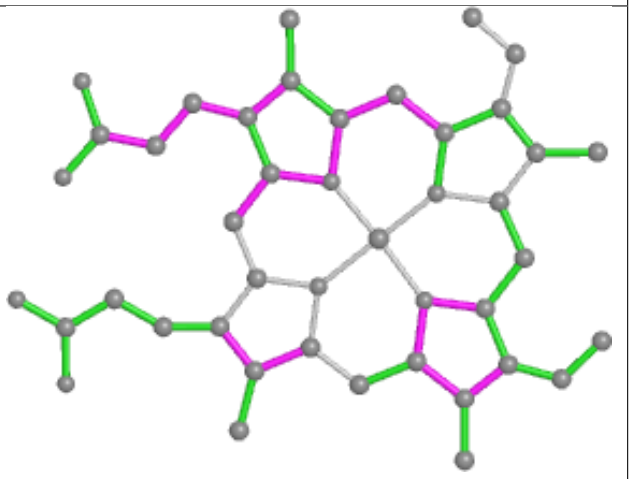
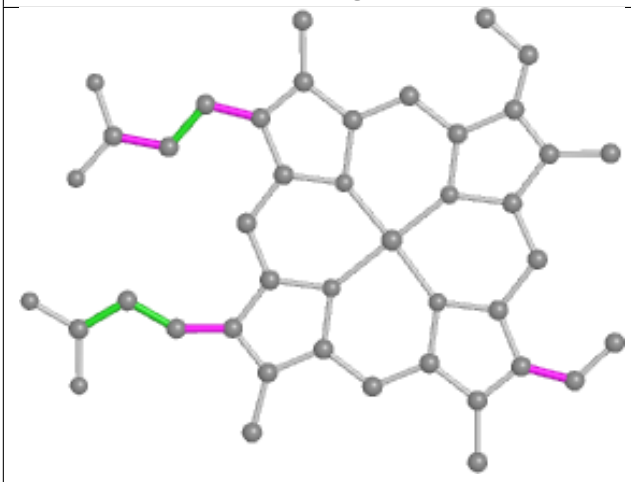


Bond angles



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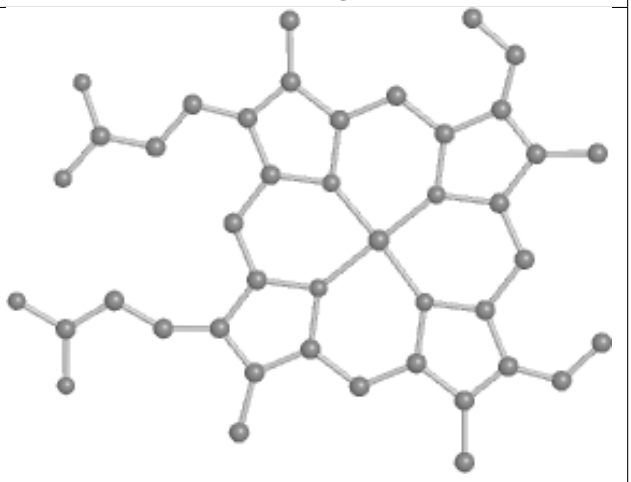
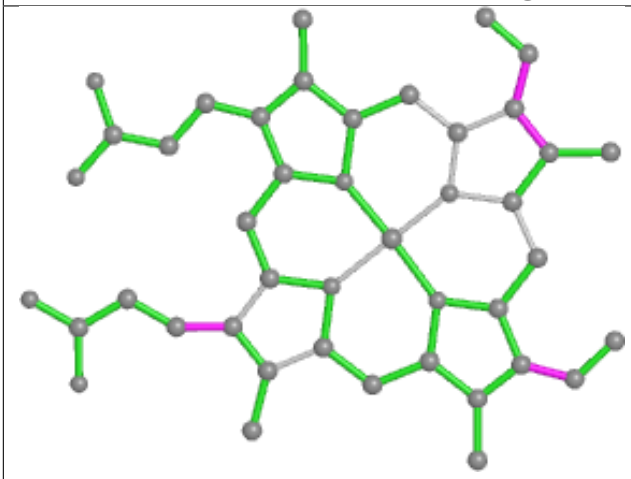


Rings

Ligand HEM B 201



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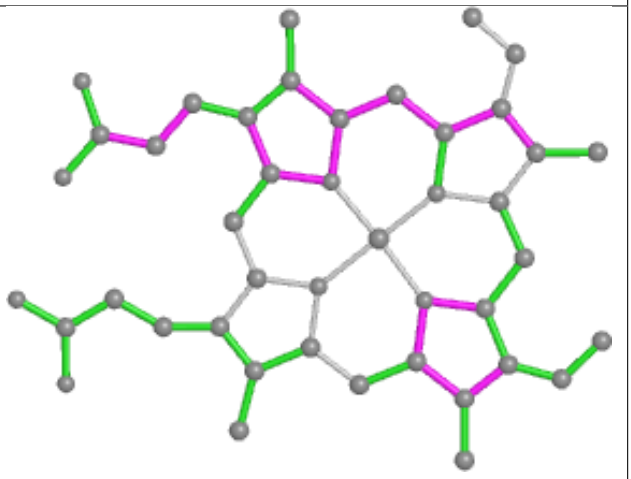
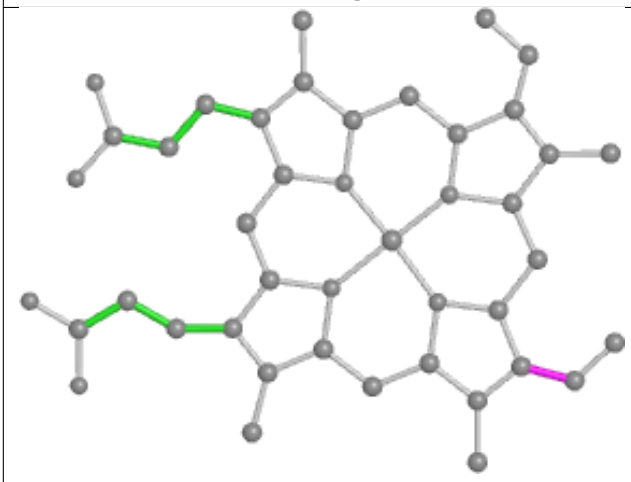


Bond angles



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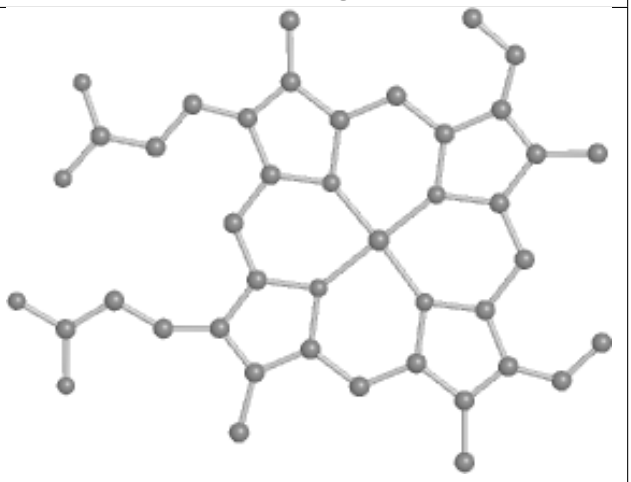
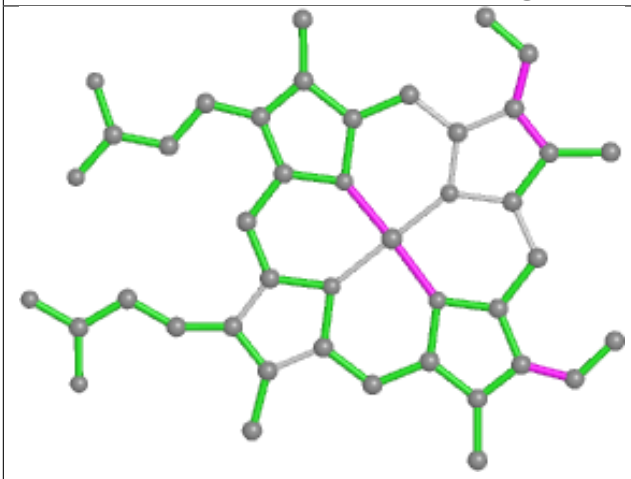


Rings

Ligand HEM R 201



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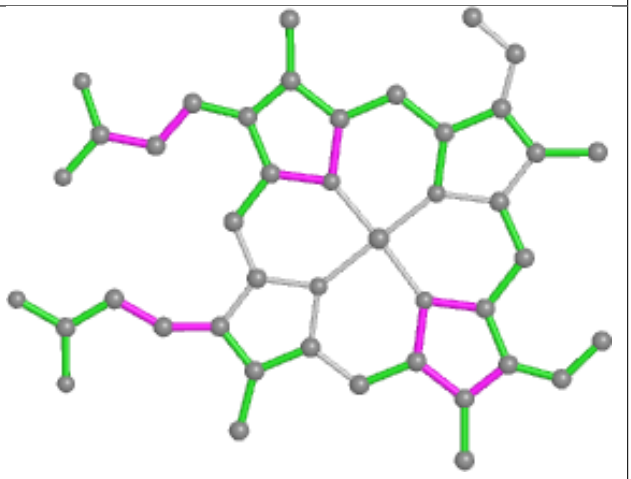

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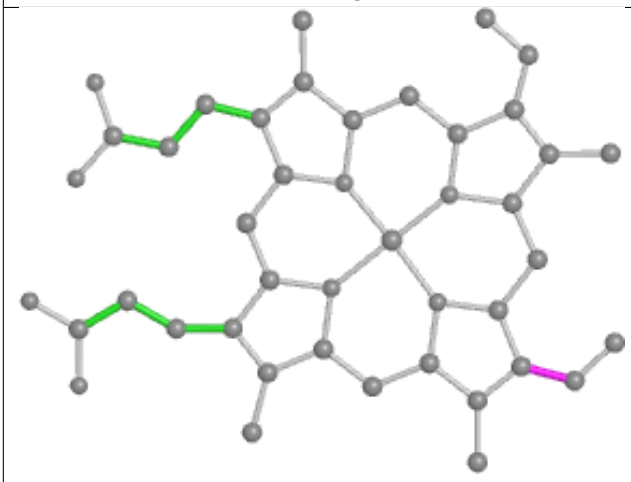

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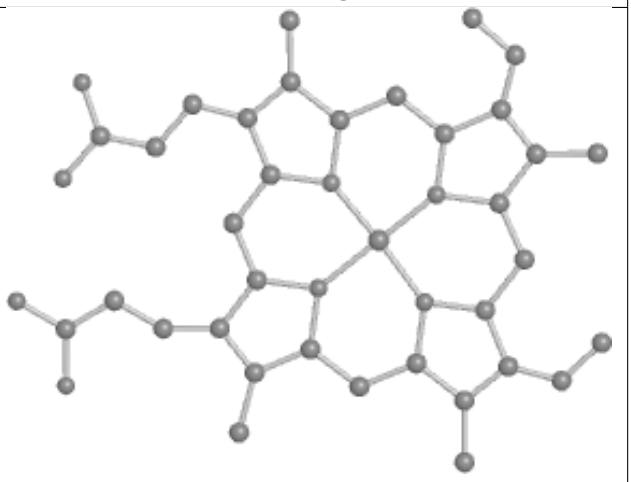

Rings

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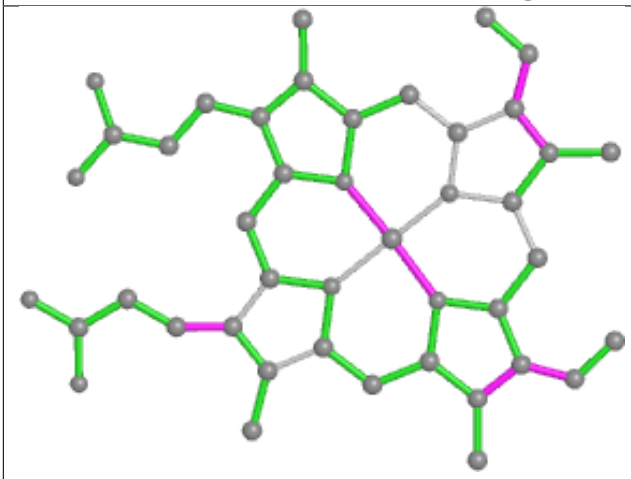

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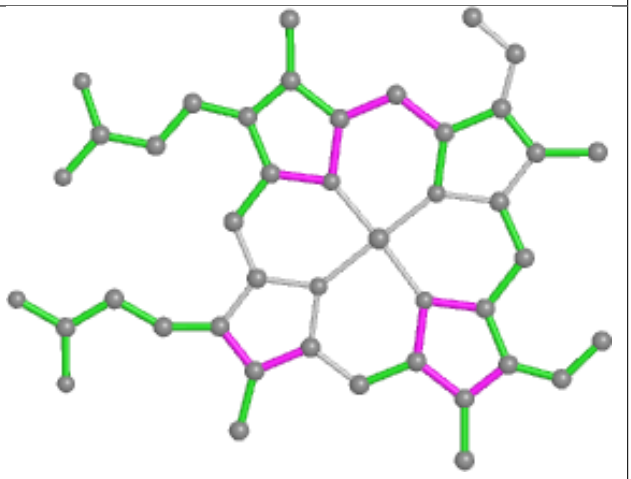
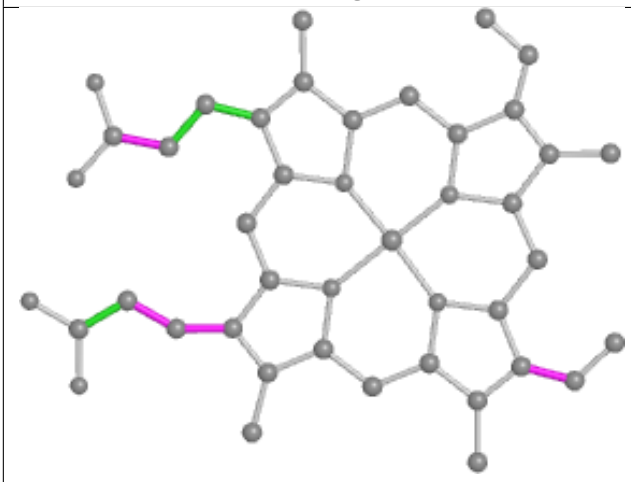


Bond angles



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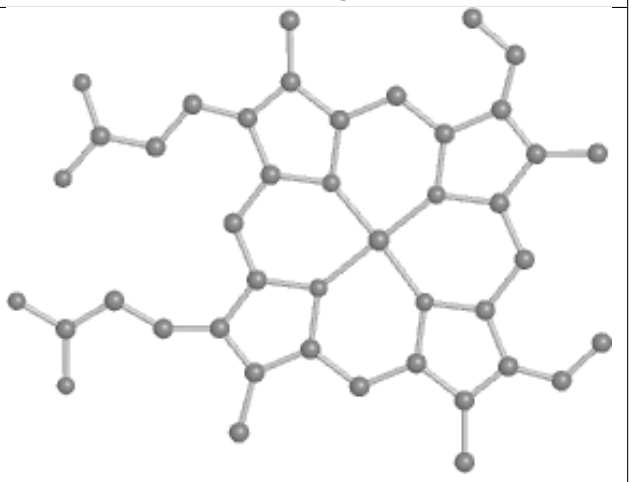
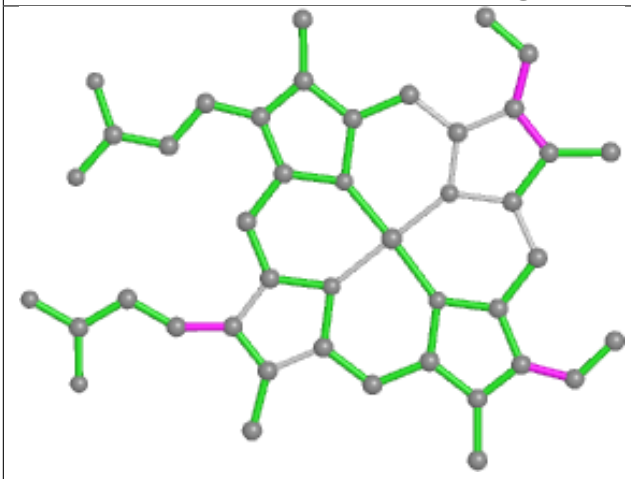


Rings

Ligand HEM M 202



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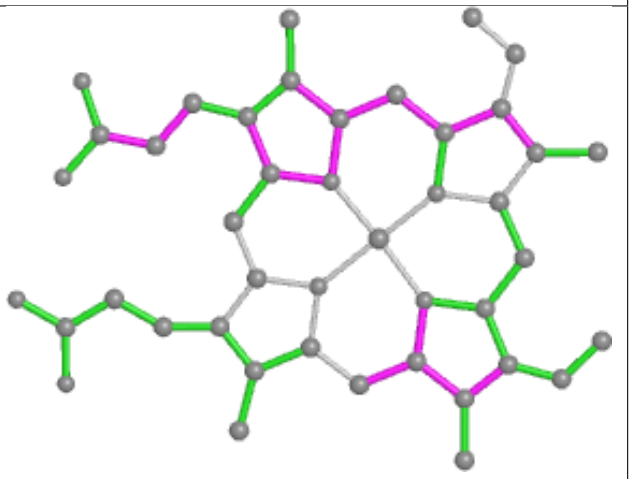

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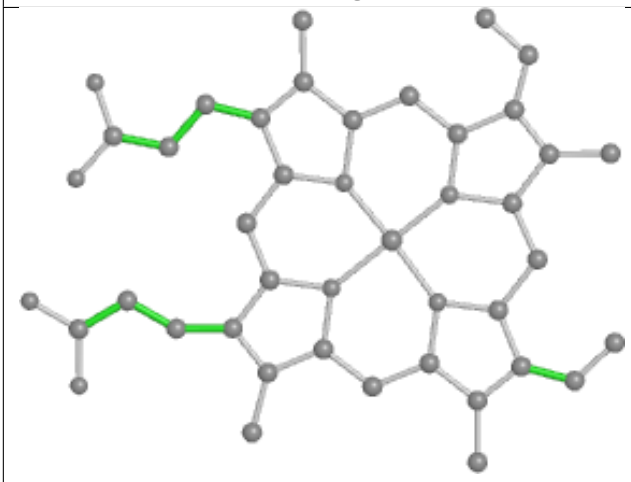

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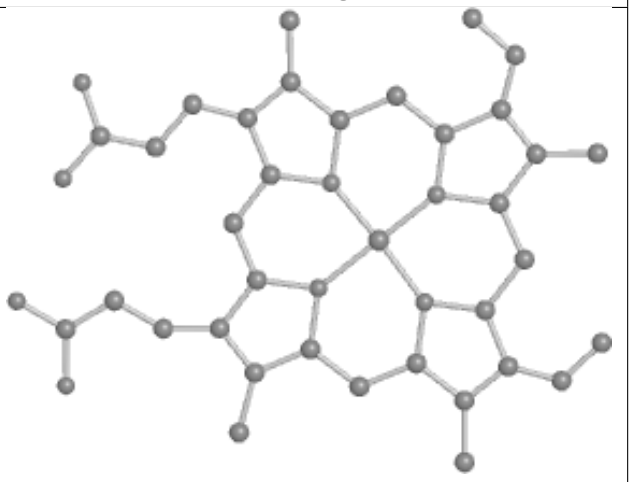

Rings

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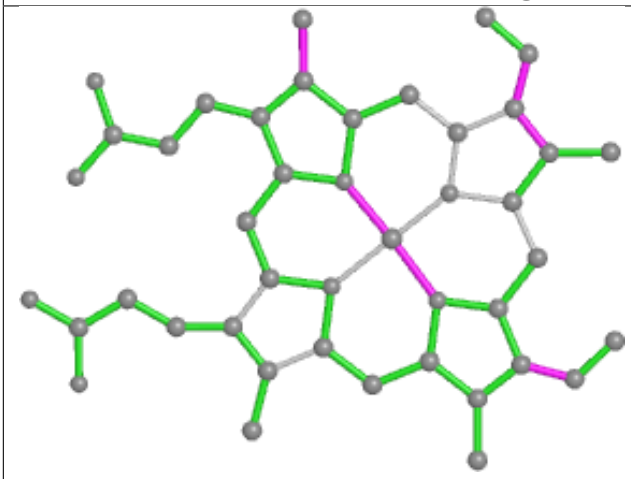

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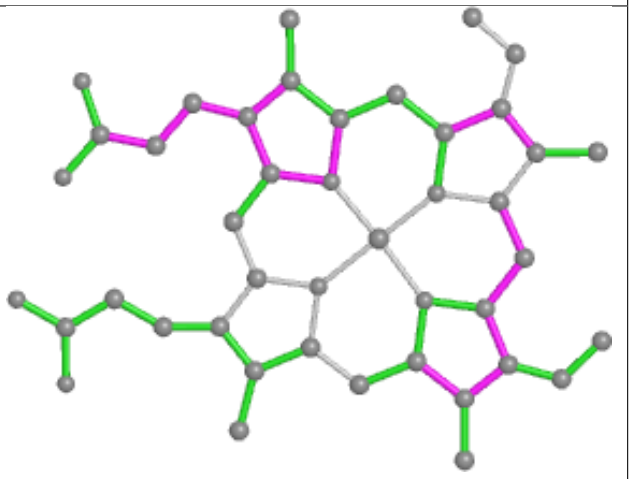
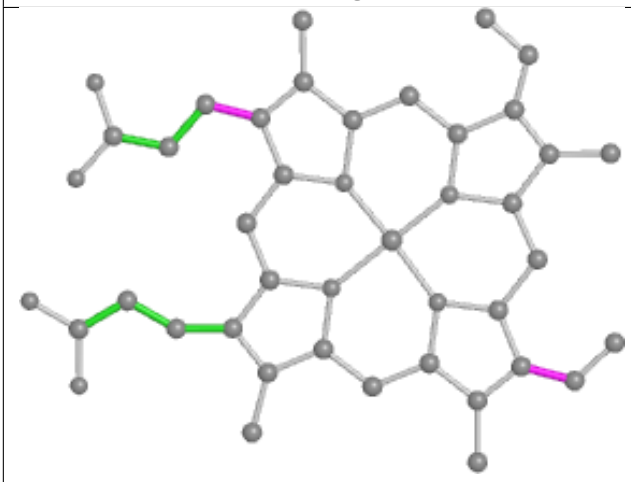


Bond angles



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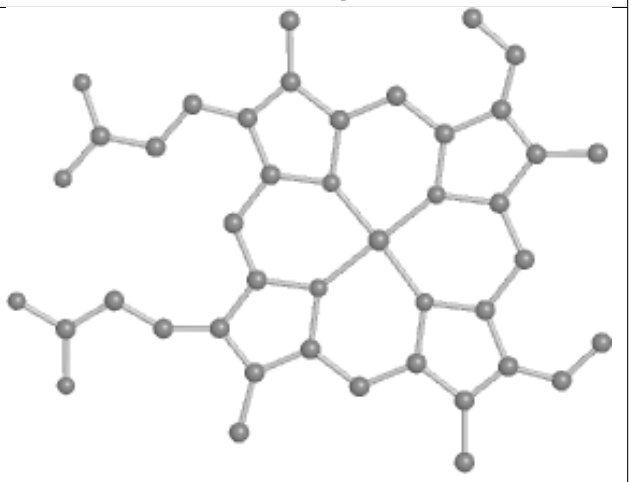
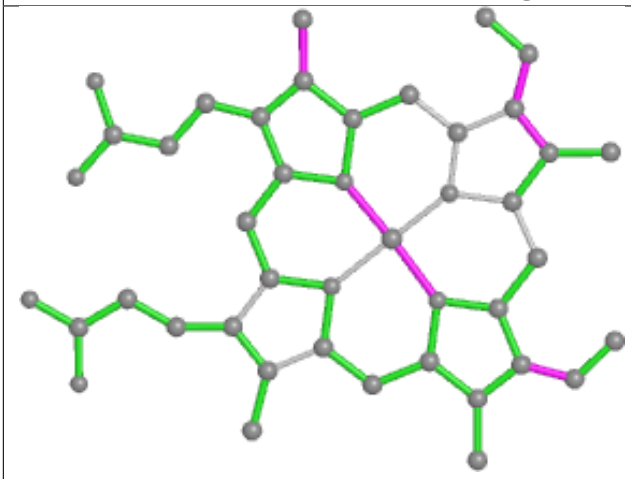


Rings

Ligand HEM U 202



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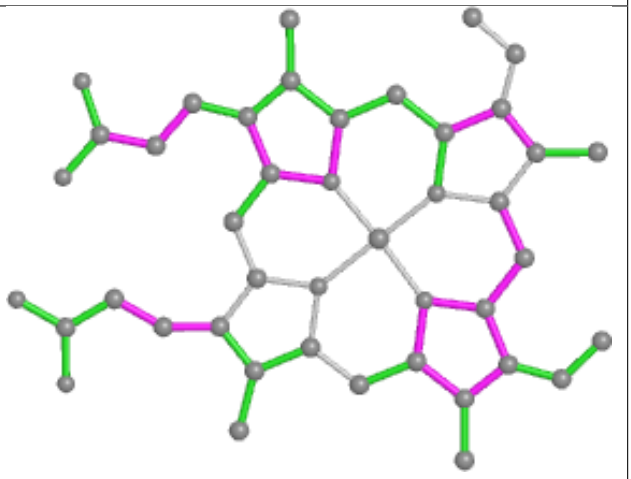
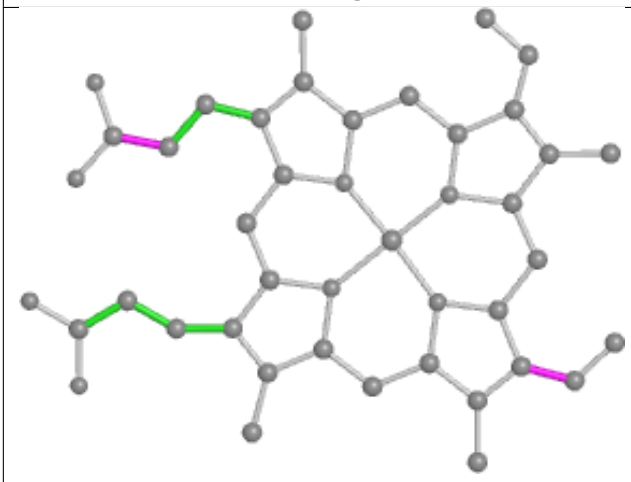


Bond angles



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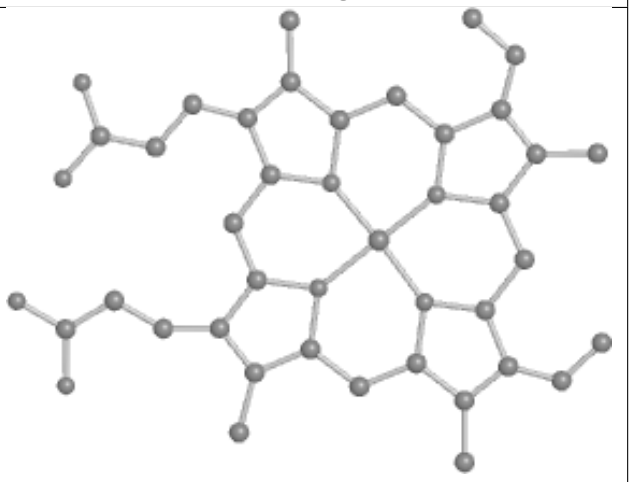
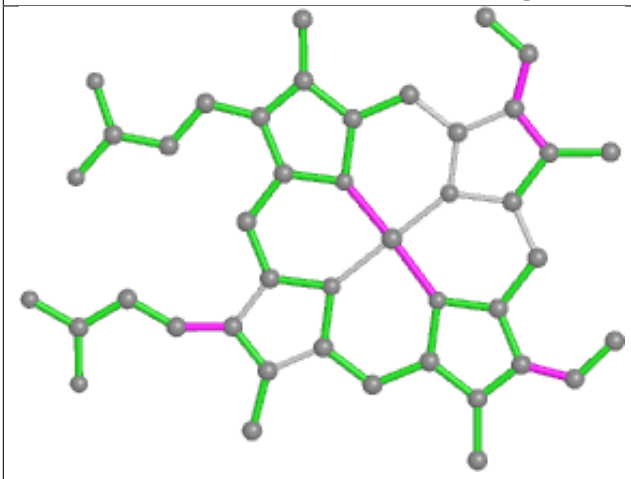


Rings

Ligand HEM V 202



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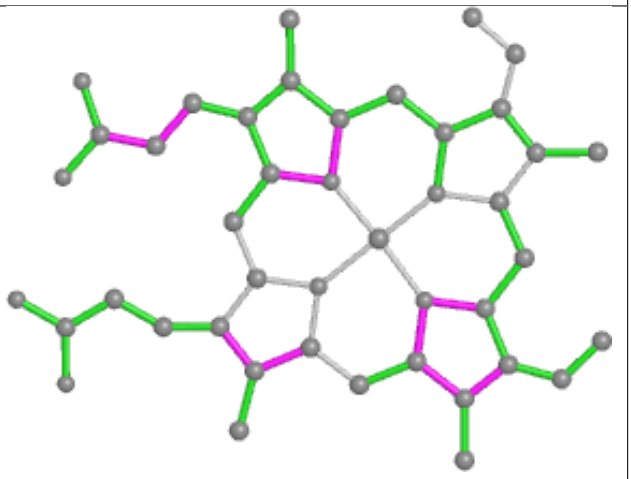
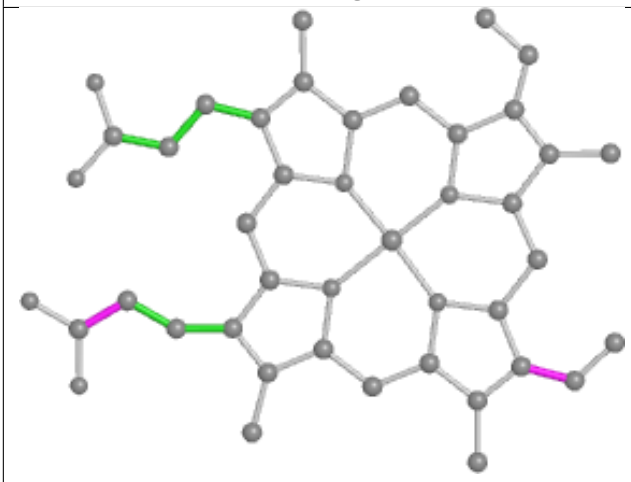


Bond angles



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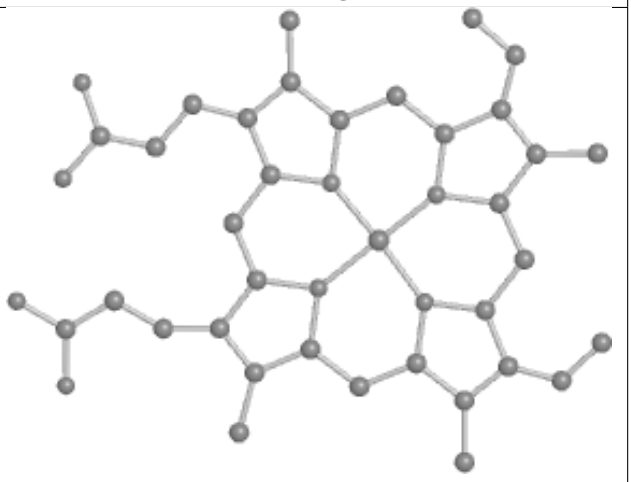
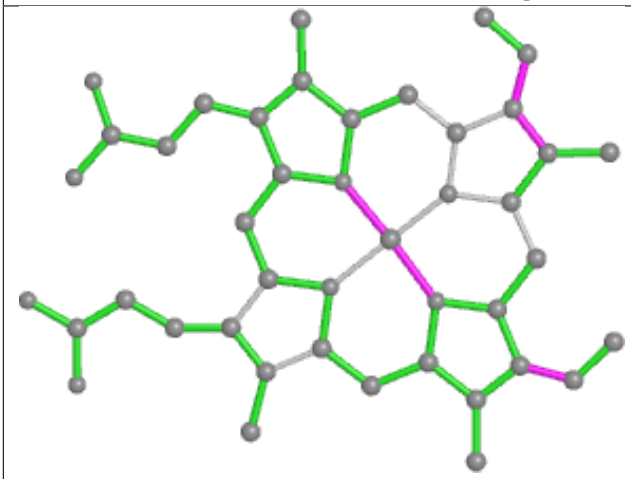
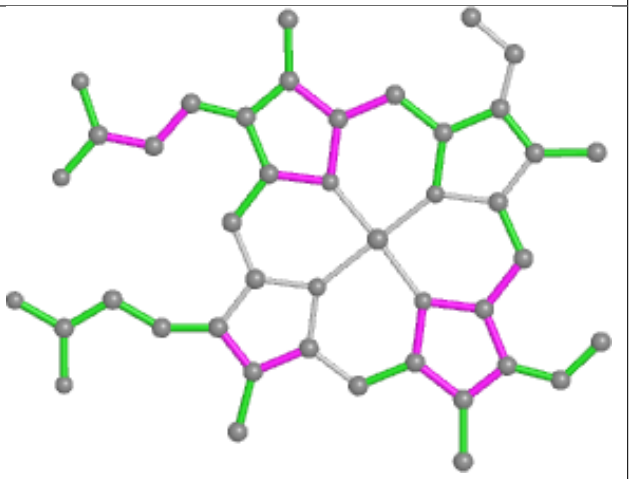


Rings

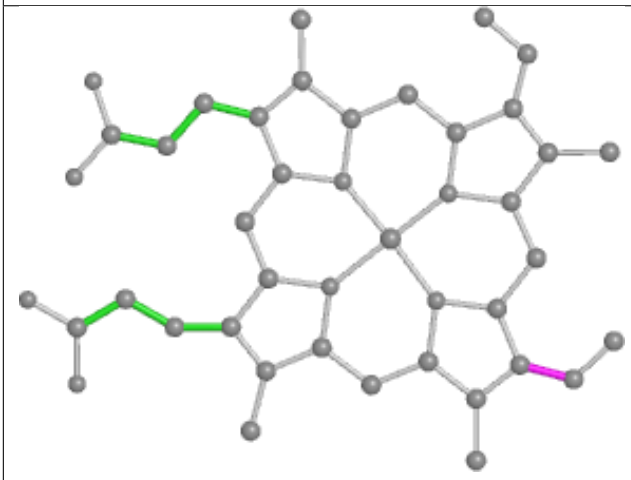
Ligand HEM D 201



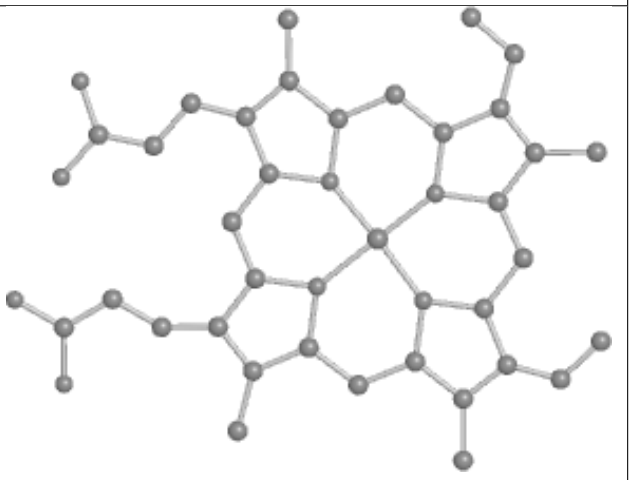
Bond lengths



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.

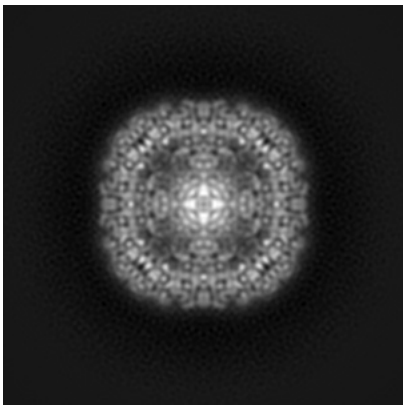
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36137. These allow visual inspection of the internal detail of the map and identification of artifacts.

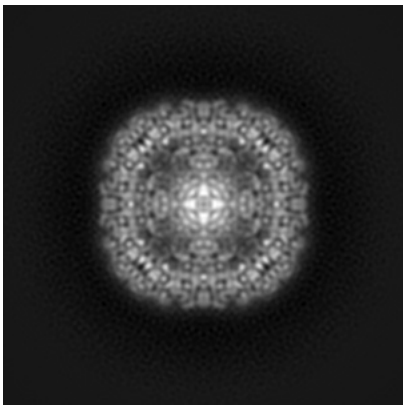
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

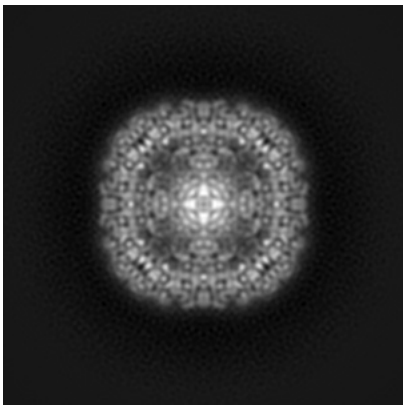
6.1.1 Primary map



X

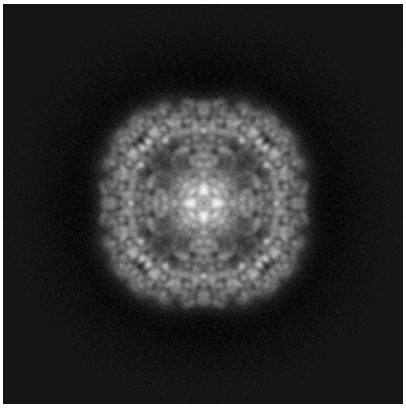


Y

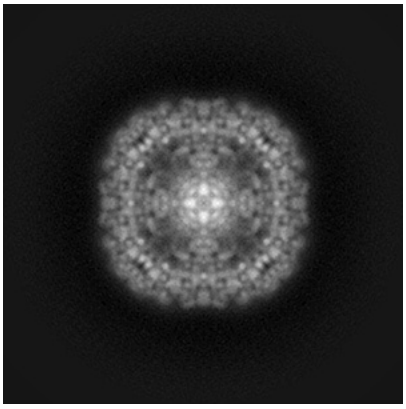


Z

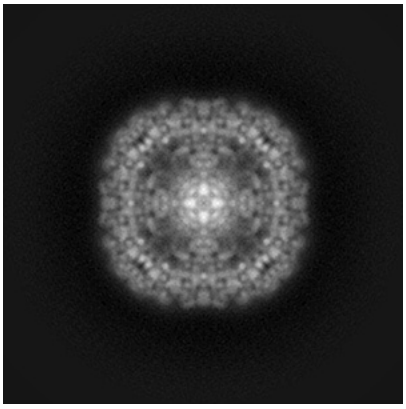
6.1.2 Raw map



X



Y

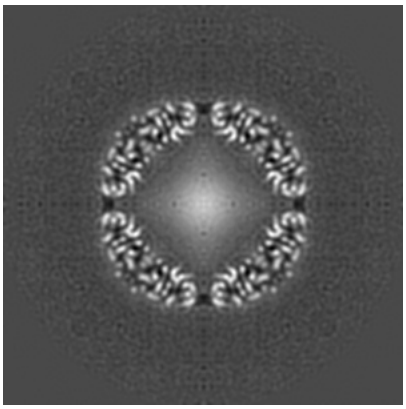


Z

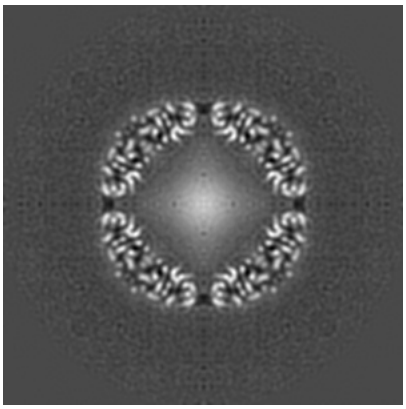
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

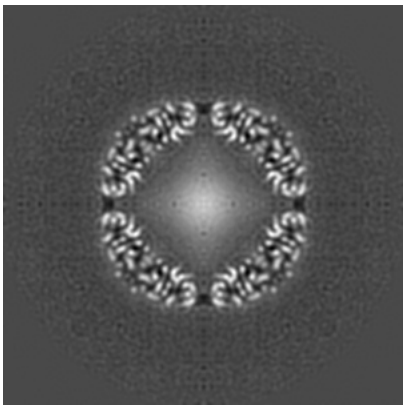
6.2.1 Primary map



X Index: 128

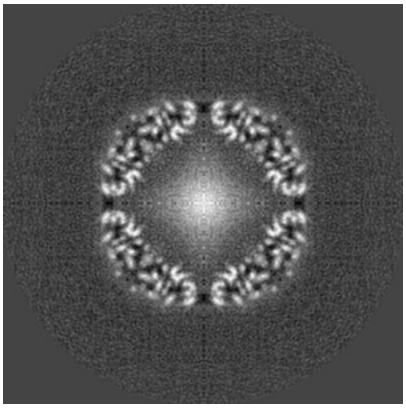


Y Index: 128

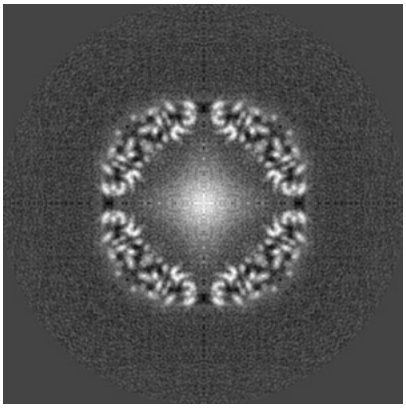


Z Index: 128

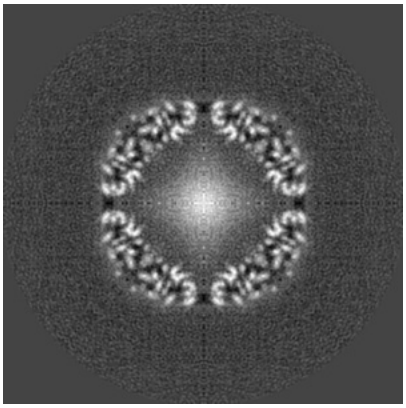
6.2.2 Raw map



X Index: 128



Y Index: 128

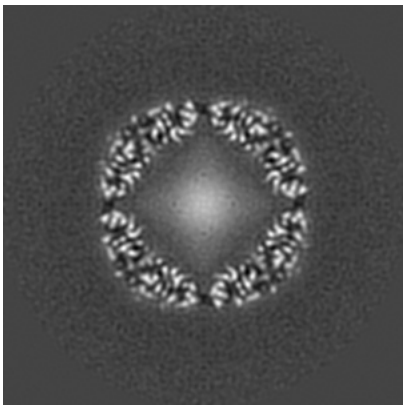


Z Index: 128

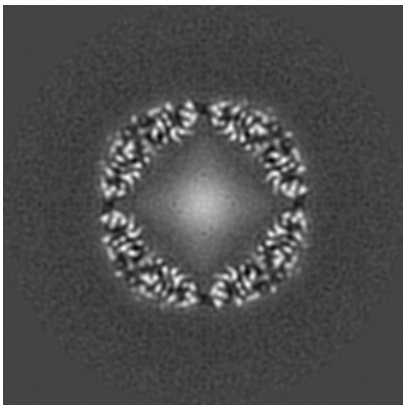
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

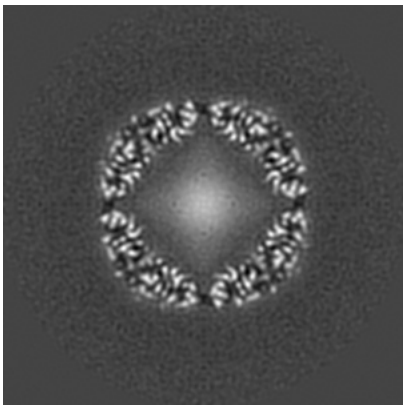
6.3.1 Primary map



X Index: 127

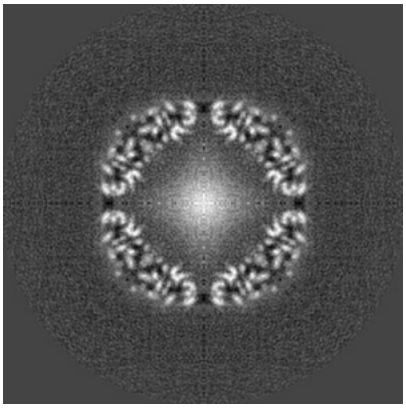


Y Index: 127

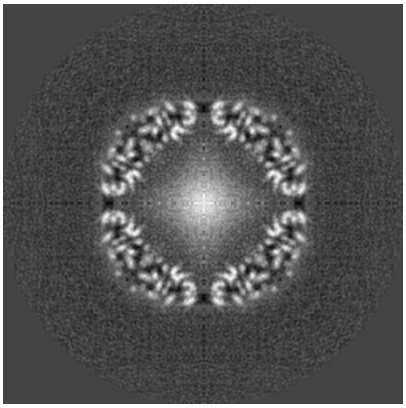


Z Index: 127

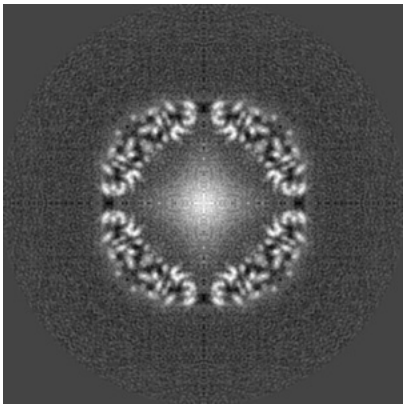
6.3.2 Raw map



X Index: 128



Y Index: 128

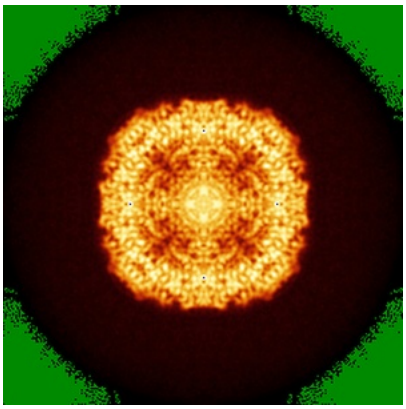


Z Index: 128

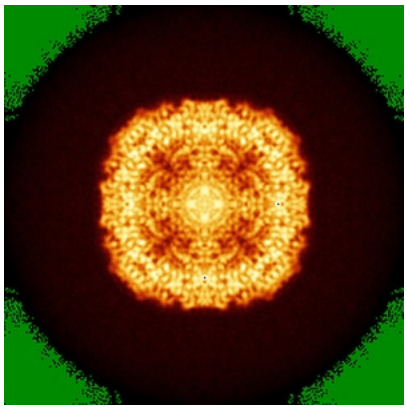
The images above show the largest variance slices of the map in three orthogonal directions.

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

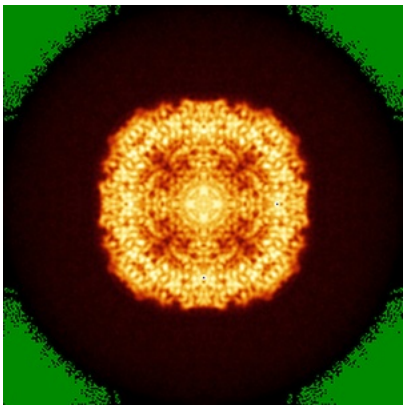
6.4.1 Primary map



X

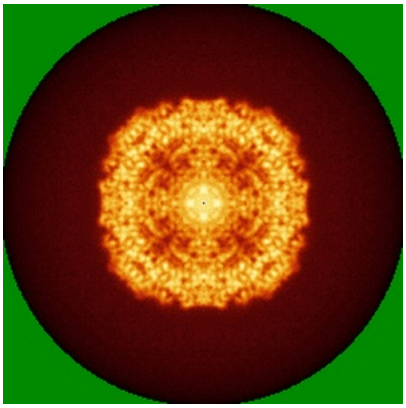


Y

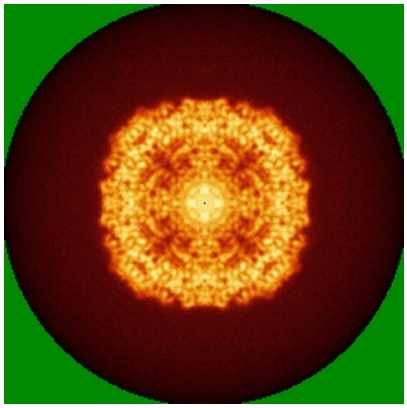


Z

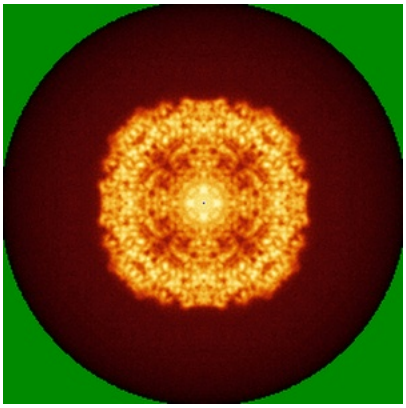
6.4.2 Raw map



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 0.0061. 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.

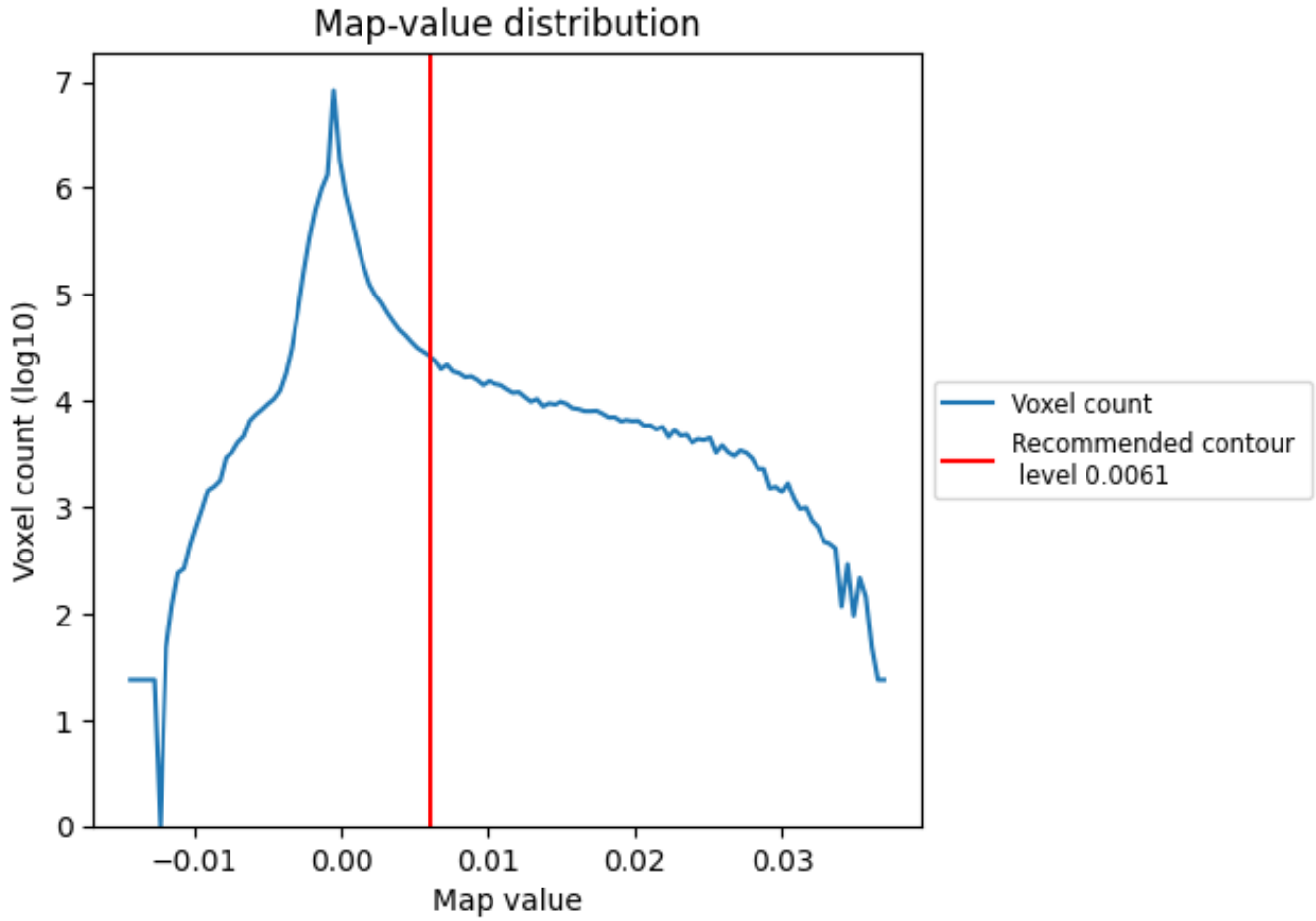
6.6 Mask visualisation (i)

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

7 Map analysis

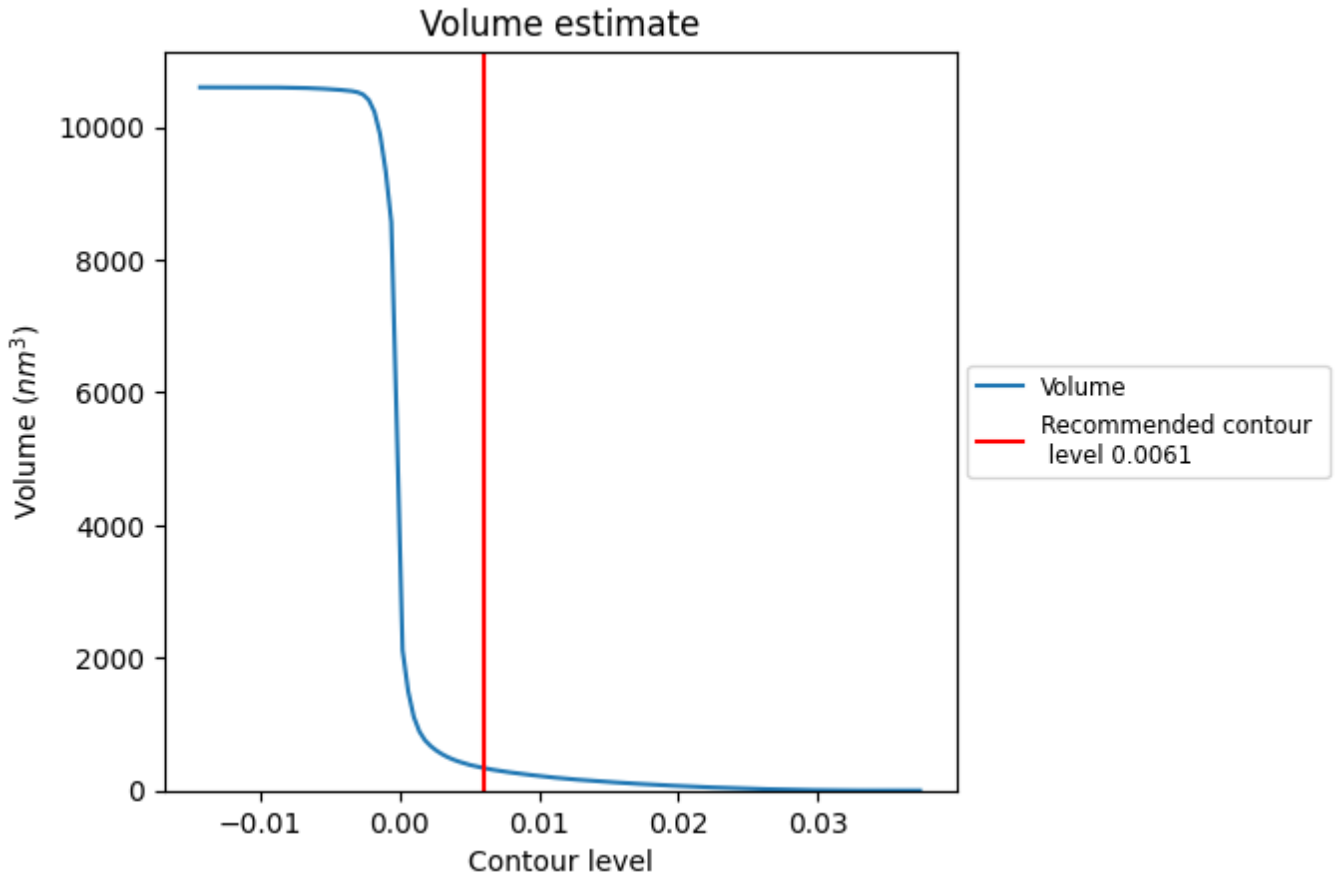
This section contains the results of statistical analysis of the map.

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.

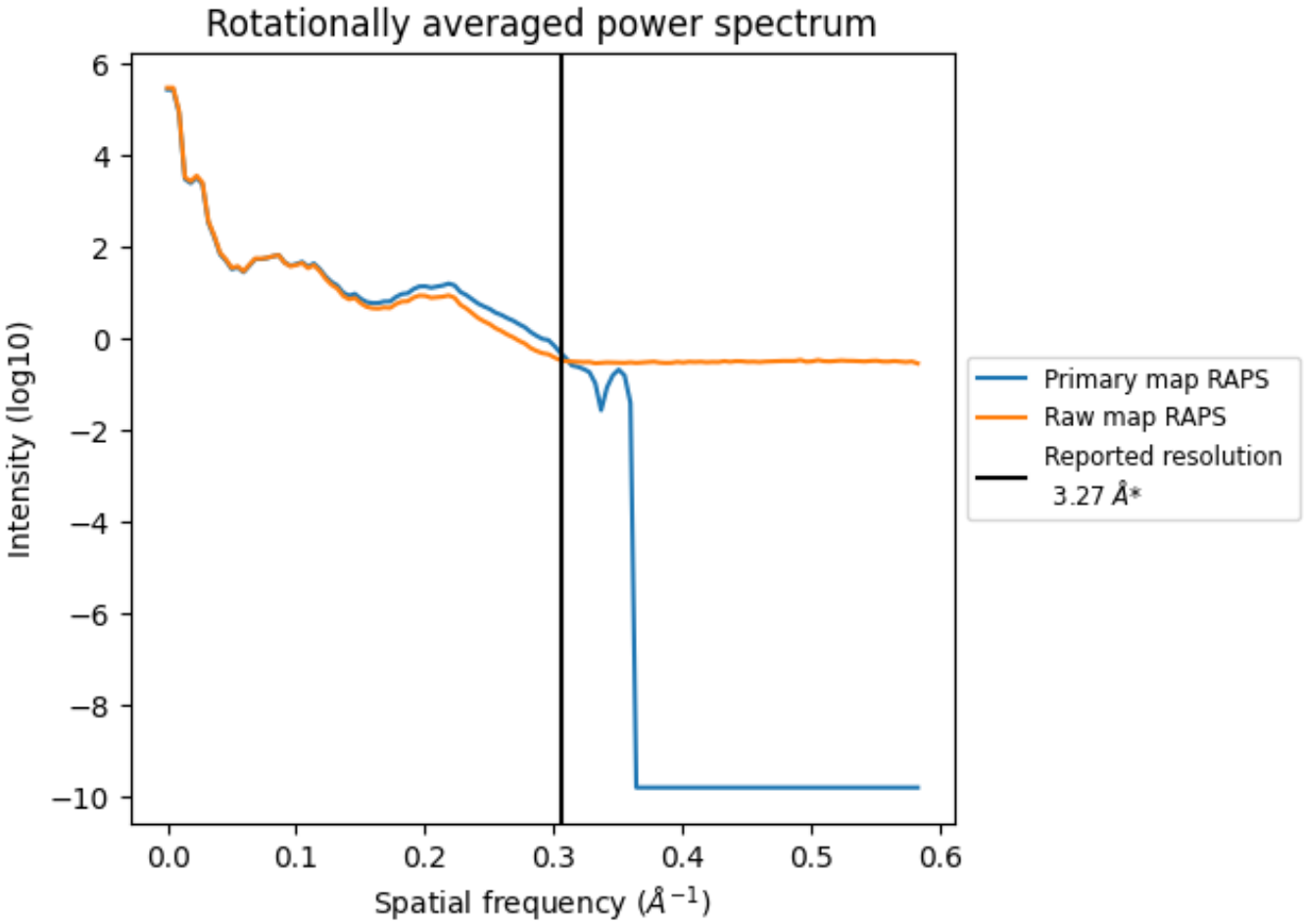
7.2 Volume estimate



The volume at the recommended contour level is 336 nm^3; this corresponds to an approximate mass of 304 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)

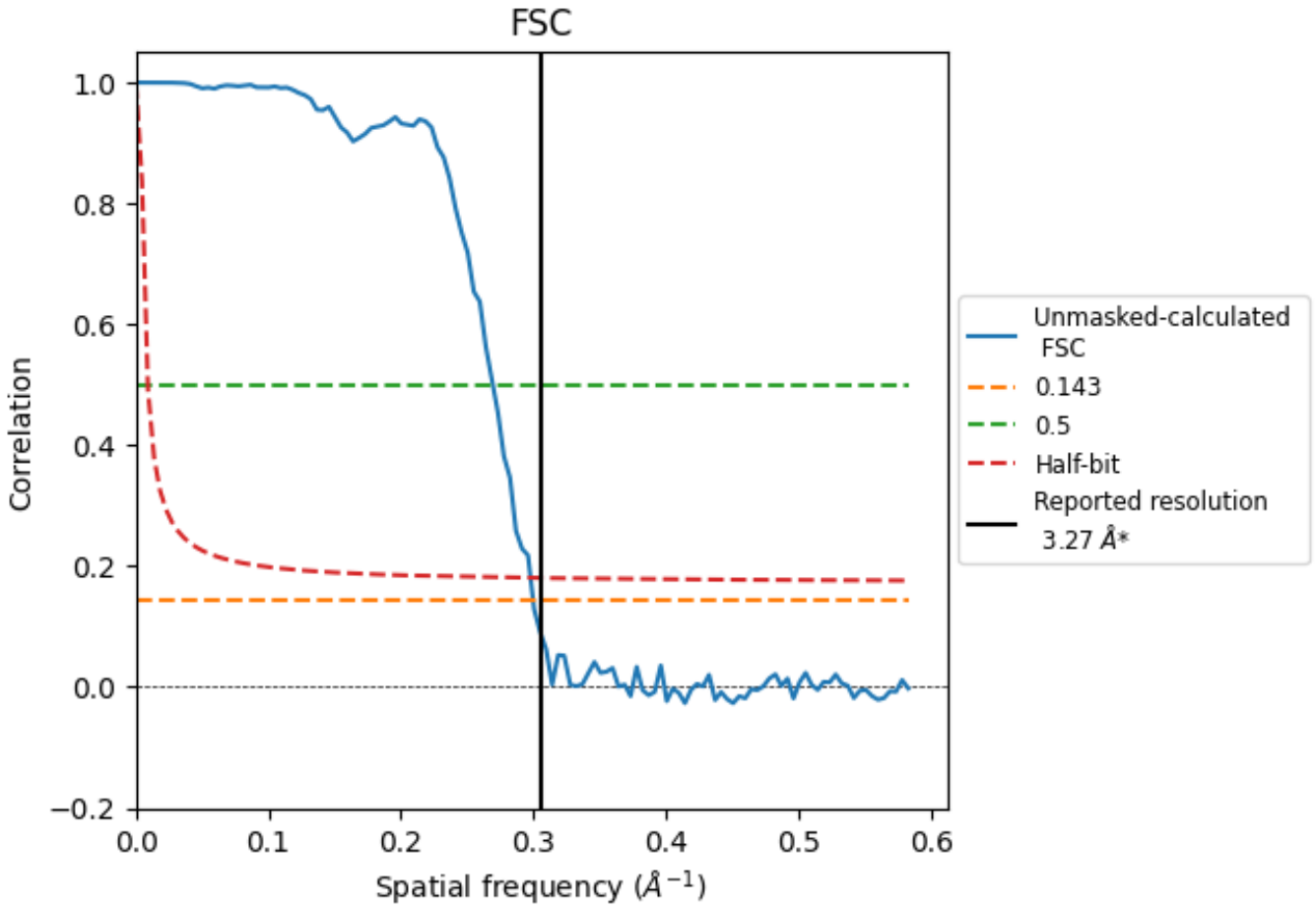


*Reported resolution corresponds to spatial frequency of 0.306 $Å^{-1}$

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 0.306 Å^{-1}

8.2 Resolution estimates (i)

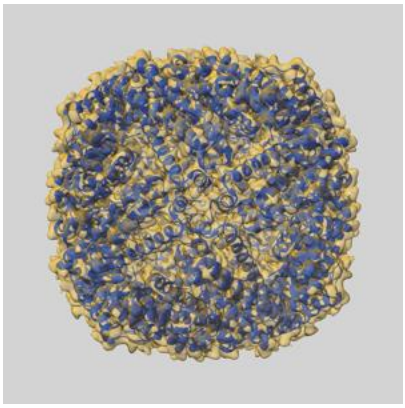
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.71	3.36

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

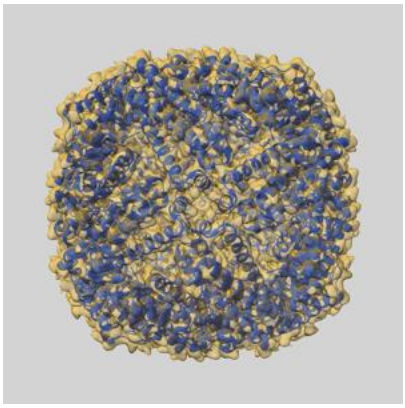
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36137 and PDB model 8JAX. Per-residue inclusion information can be found in section 3 on page 8.

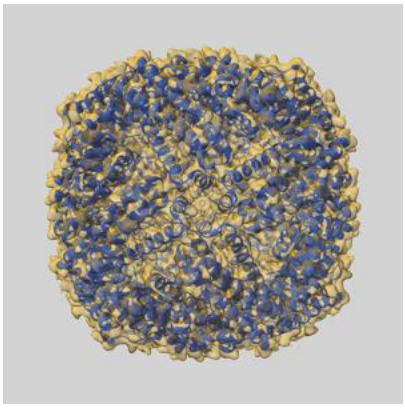
9.1 Map-model overlay



X



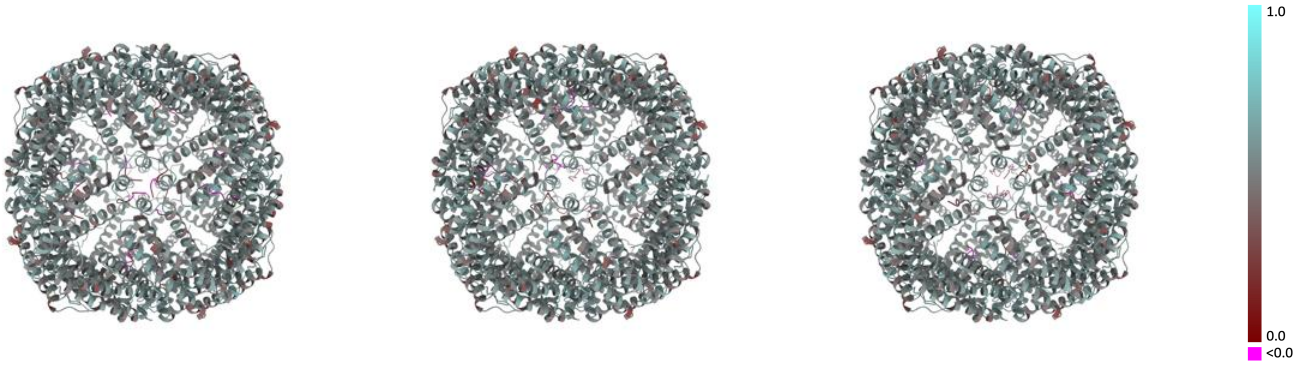
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0061 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.

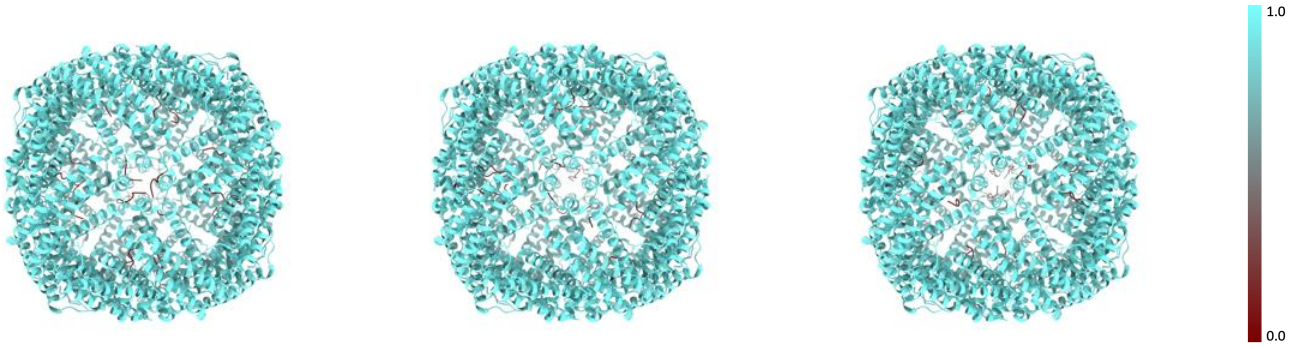
9.2 Q-score mapped to coordinate model (i)



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.

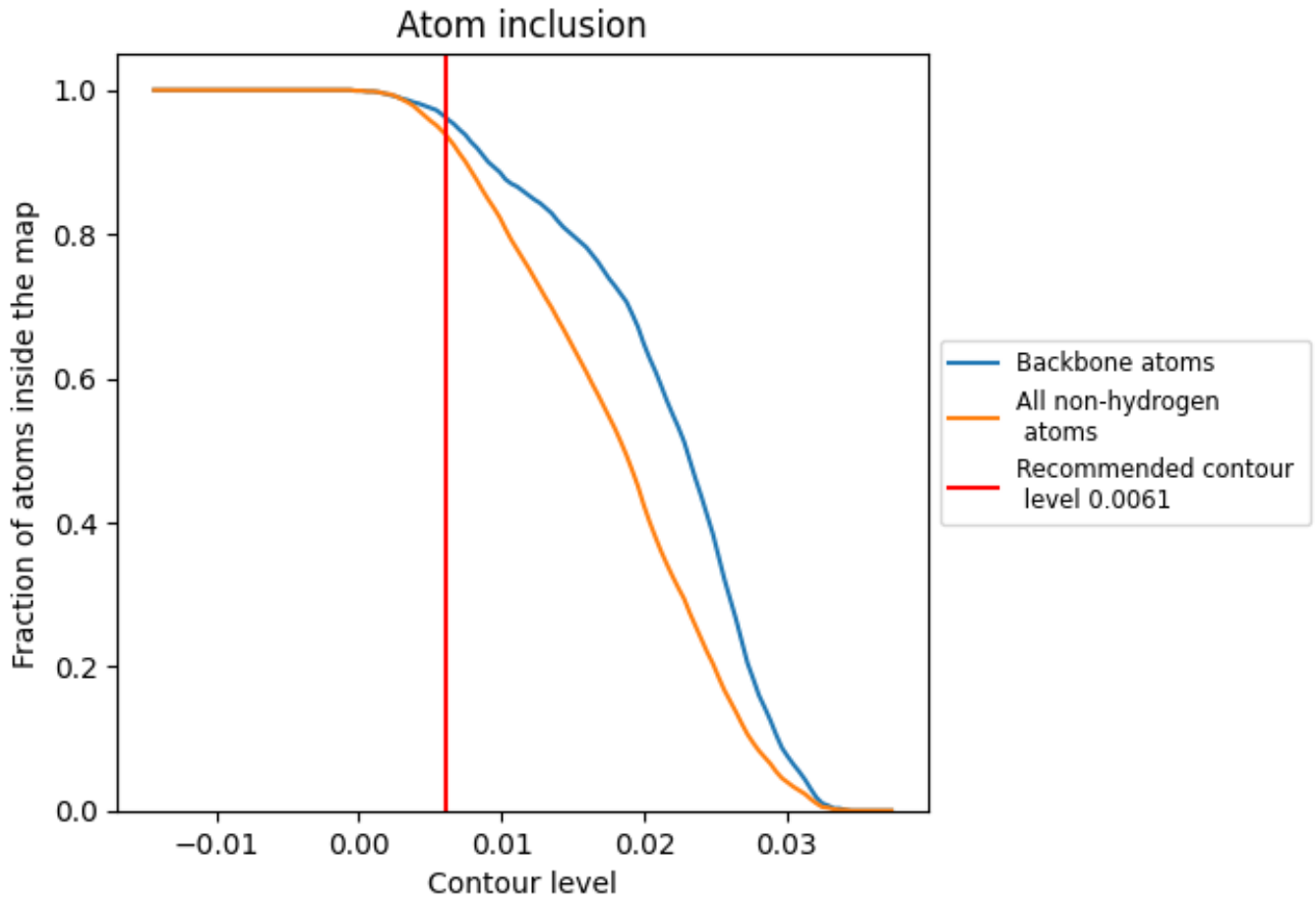
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0061).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.0061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.5220
A	0.9270	0.5140
B	0.9470	0.5220
C	0.9290	0.5170
D	0.9440	0.5240
E	0.9360	0.5230
F	0.9280	0.5170
G	0.9390	0.5250
H	0.9320	0.5150
I	0.9480	0.5260
J	0.9370	0.5290
K	0.9480	0.5230
L	0.9270	0.5200
M	0.9430	0.5240
N	0.9370	0.5230
O	0.9350	0.5230
P	0.9450	0.5270
Q	0.9330	0.5190
R	0.9260	0.5100
S	0.9330	0.5170
T	0.9400	0.5250
U	0.9510	0.5270
V	0.9350	0.5220
W	0.9450	0.5290
X	0.9400	0.5180