Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:42 PM EDT

PDB ID	:	7RJC / pdb_00007rjc
EMDB ID	:	EMD-24484
Title	:	Complex III2 from Candida albicans, inhibitor free, Rieske head domain in intermediate position
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2021-07-20
Resolution	:	3.30 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:

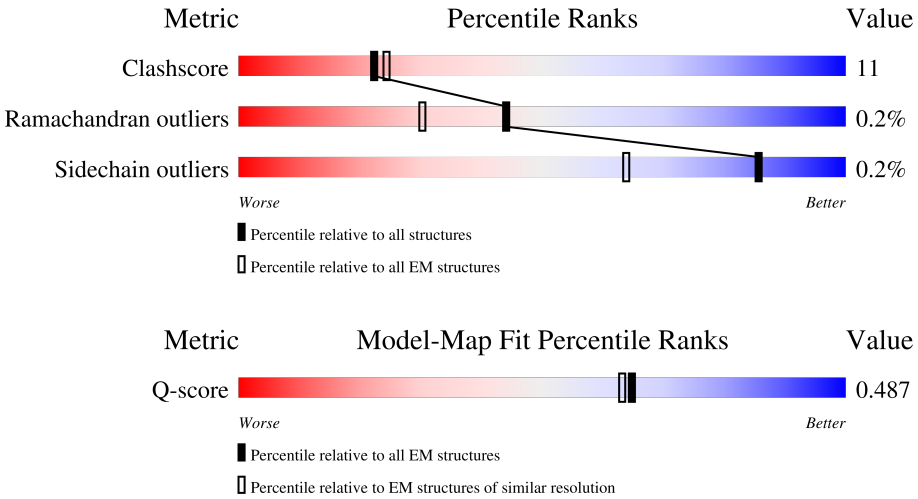
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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.



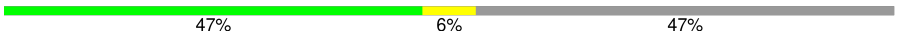
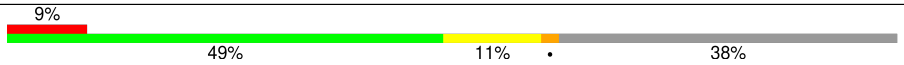
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	439	81% 14% 5%
2	K	387	72% 27%
3	D	288	70% 15% 15%
4	G	127	80% 16%

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Mol	Chain	Length	Quality of chain
5	F	95	
6	H	135	
7	I	39	
8	B	374	
9	E	213	
9	M	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FES	E	301	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 28513 atoms, of which 13804 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 Ubiquinol--cytochrome-c reductase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	416	6364	2012	3166	546	636	4	0	0

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	383	6146	2056	3090	478	505	17	0	0

- Molecule 3 is a protein called Ubiquinol--cytochrome-c reductase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	244	3736	1225	1820	333	351	7	0	0

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	G	122	1978	629	1002	161	183	3	0	0

- Molecule 5 is a protein called Ubiquinol--cytochrome-c reductase subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	85	1399	466	691	119	122	1	0	0

- Molecule 6 is a protein called Ubiquinol--cytochrome-c reductase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	H	72	1148	376	544	106	116	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	47	GLU	ASP	conflict	UNP A0A1D8PJT8

- Molecule 7 is a protein called Ubiquinol--cytochrome-c reductase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	H	N	O	0	0
			639	220	315	54	50		

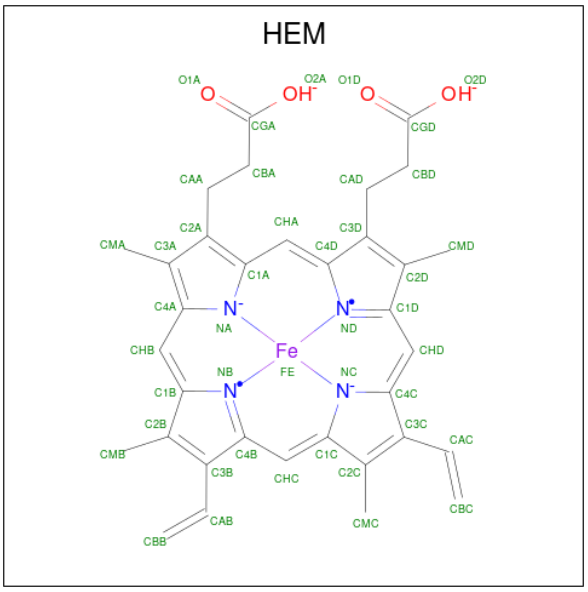
- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		

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

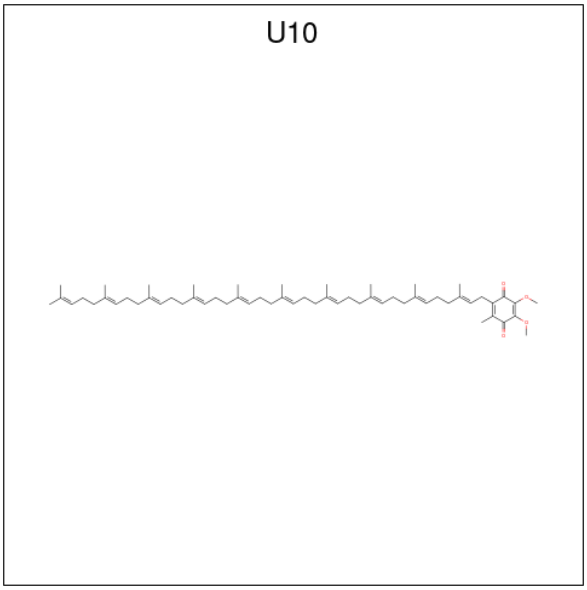
Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	50	Total	C	H	N	O	S	0	0
			723	239	344	62	76	2		
9	E	132	Total	C	N	O	S		0	0
			664	395	133	135	1			

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



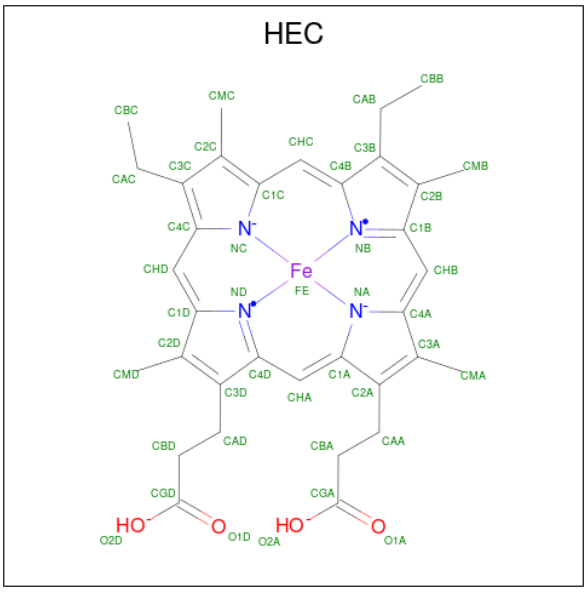
Mol	Chain	Residues	Atoms						AltConf
10	K	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
10	K	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



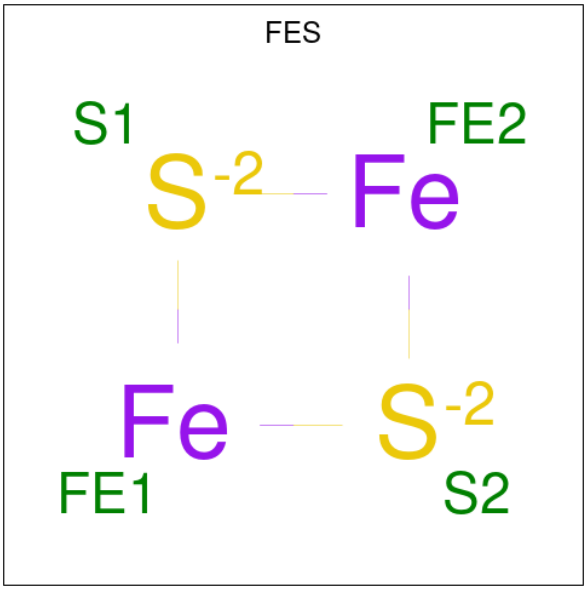
Mol	Chain	Residues	Atoms				AltConf
11	K	1	Total	C	H	O	0
			58	24	30	4	
11	K	1	Total	C	H	O	0
			43	19	20	4	

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
12	D	1	73	34	1	30	4	4	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



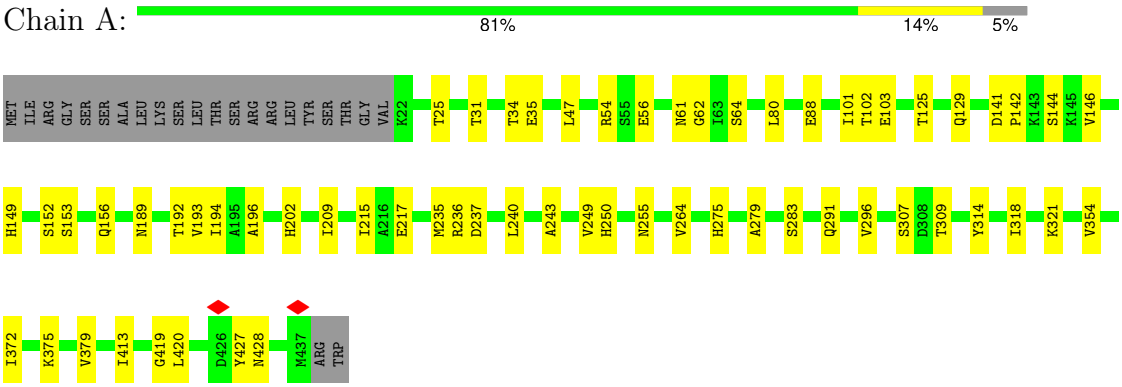
Mol	Chain	Residues	Atoms				AltConf
			Total	Fe	S		
13	E	1	4	2	2		0

3 Residue-property plots (i)

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

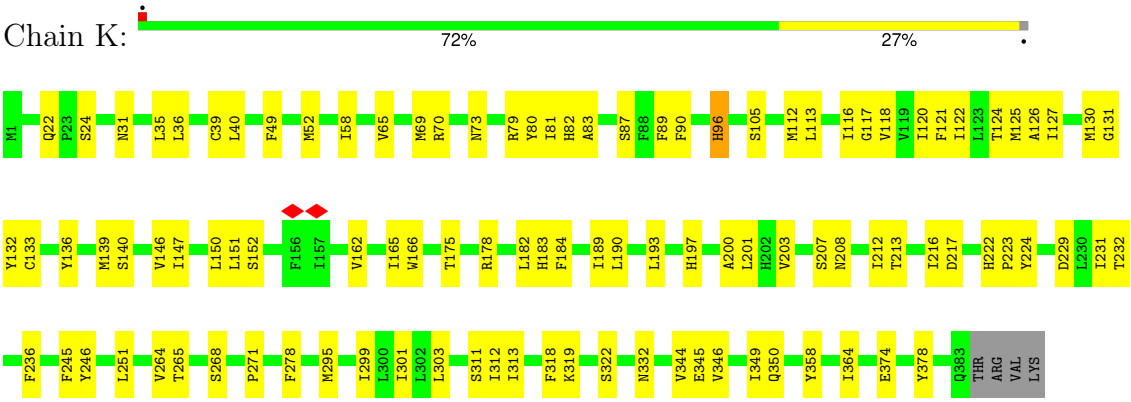
• Molecule 1: Ubiquinol--cytochrome-c reductase subunit

Chain A:



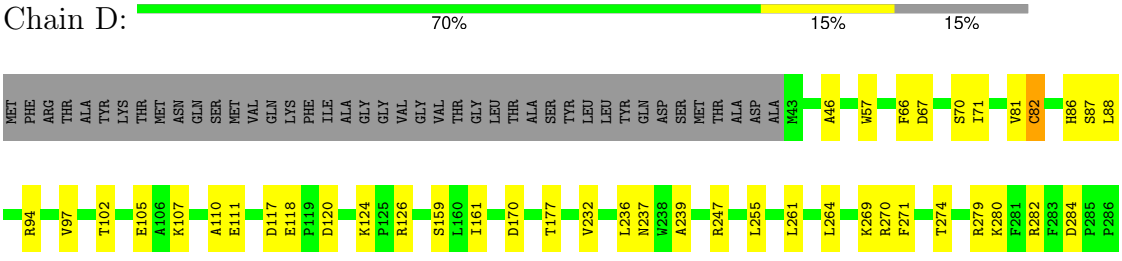
• Molecule 2: Cytochrome b

Chain K:



• Molecule 3: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain D:

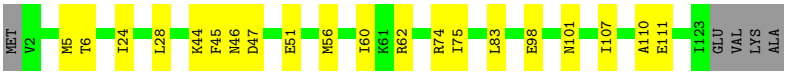




• Molecule 4: Cytochrome b-c1 complex subunit 7

Chain G:

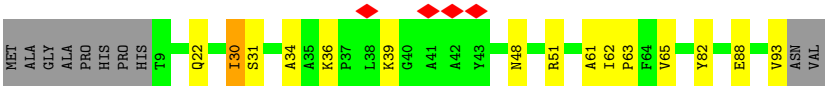




• Molecule 5: Ubiquinol--cytochrome-c reductase subunit 8

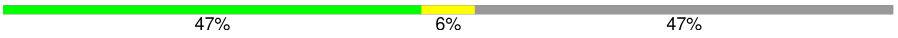
Chain F:





• Molecule 6: Ubiquinol--cytochrome-c reductase subunit 6

Chain H:



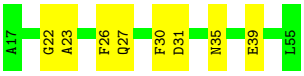




• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 9

Chain I:

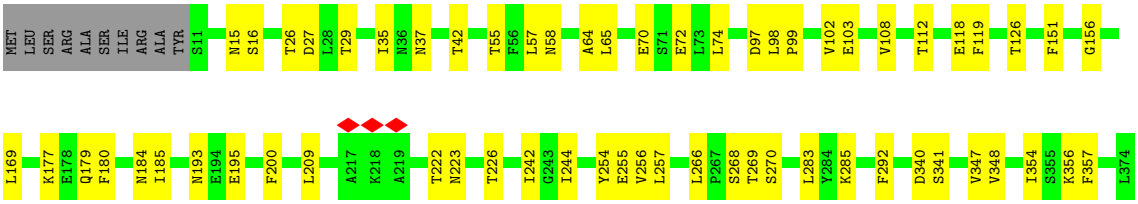




• Molecule 8: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:

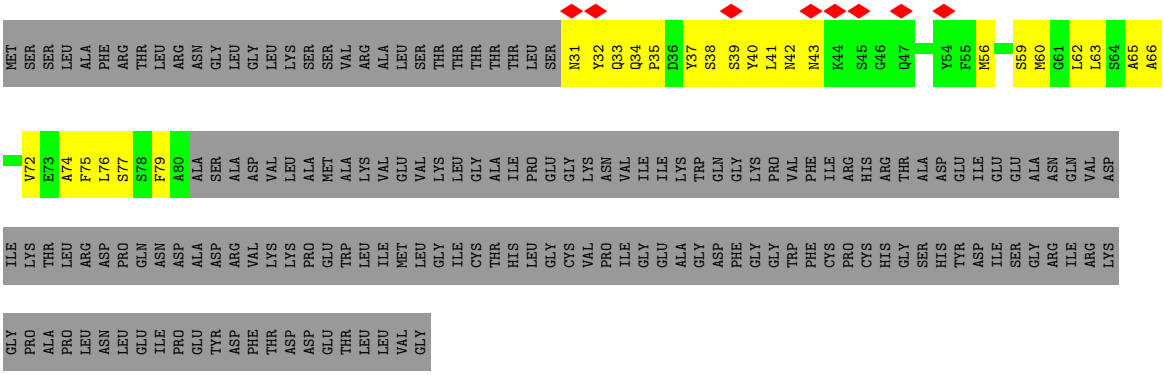




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

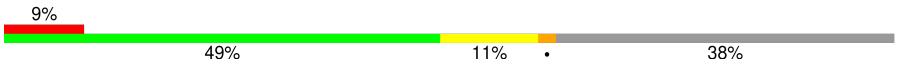
Chain M:

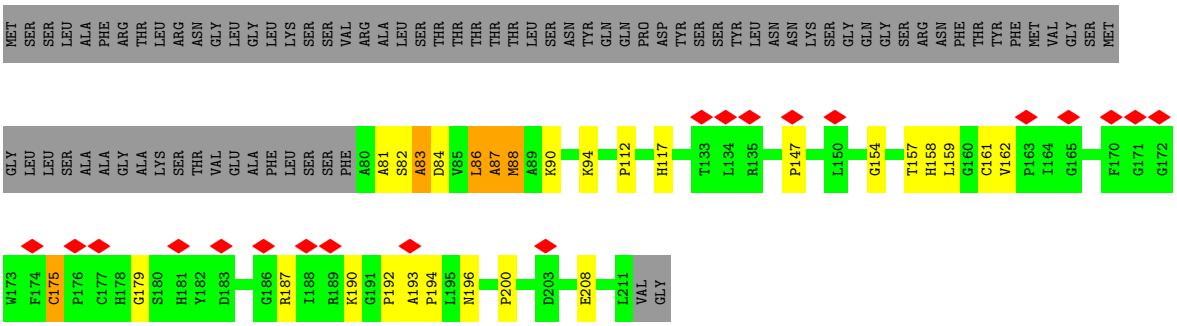




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.272	Depositor
Minimum map value	-5.441	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.63	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, U10, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.19	0/3254	0.31	0/4409
2	K	0.31	1/3158 (0.0%)	0.39	0/4317
3	D	0.37	1/1978 (0.1%)	0.40	1/2696 (0.0%)
4	G	0.19	0/994	0.29	0/1346
5	F	0.31	1/731 (0.1%)	0.33	0/994
6	H	0.14	0/621	0.32	0/840
7	I	0.16	0/336	0.25	0/451
8	B	0.20	0/2748	0.33	0/3735
9	E	1.18	0/663	1.73	6/916 (0.7%)
9	M	0.21	0/387	0.43	0/520
All	All	0.36	3/14870 (0.0%)	0.50	7/20224 (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
9	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	82	CYS	C-O	-13.76	1.08	1.24
5	F	30	ILE	C-N	-6.53	1.23	1.33
2	K	96	HIS	CD2-NE2	-6.25	1.30	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	82	CYS	CA-C-O	-10.21	109.72	120.55
9	E	117	HIS	CB-CA-C	7.79	123.19	109.72
9	E	200	PRO	N-CA-CB	-7.45	95.43	103.25
9	E	192	PRO	N-CA-C	5.70	121.45	113.53
9	E	159	LEU	N-CA-C	-5.53	100.97	109.76
9	E	194	PRO	N-CA-CB	-5.27	97.54	103.44
9	E	87	ALA	CA-C-O	-5.25	115.90	121.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	E	190	LYS	Mainchain

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	3198	3166	3168	50	0
2	K	3056	3090	3090	100	0
3	D	1916	1820	1821	48	0
4	G	976	1002	1002	20	0
5	F	708	691	692	30	0
6	H	604	544	543	6	0
7	I	324	315	314	13	0
8	B	2700	2692	2685	46	0
9	E	664	0	338	30	0
9	M	379	344	354	68	0
10	K	86	60	60	16	0
11	K	51	50	52	9	0
12	D	43	30	31	16	0
13	E	4	0	0	2	0
All	All	14709	13804	14150	329	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 11.

All (329) 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)
2:K:265:THR:HG22	9:E:162:VAL:CB	1.56	1.35
2:K:265:THR:CG2	9:E:162:VAL:H	1.55	1.18
1:A:156:GLN:HB2	9:M:34:GLN:HG3	1.18	1.16
9:E:187:ARG:HA	9:E:196:ASN:HA	1.33	1.11
2:K:265:THR:HG21	9:E:162:VAL:H	0.95	1.09
1:A:156:GLN:CB	9:M:34:GLN:HG3	1.81	1.08
5:F:36:LYS:N	9:M:40:TYR:O	1.84	1.08
3:D:261:LEU:CD1	9:M:60:MET:HG3	1.86	1.06
5:F:36:LYS:HD2	9:M:39:SER:O	1.56	1.04
2:K:265:THR:HG21	9:E:162:VAL:N	1.72	1.03
3:D:280:LYS:HD2	9:M:35:PRO:CB	1.90	1.02
3:D:261:LEU:HD11	9:M:60:MET:HG3	1.41	1.00
7:I:30:PHE:HE2	9:M:63:LEU:HD11	1.23	1.00
7:I:30:PHE:CE2	9:M:63:LEU:HD11	1.96	0.99
1:A:236:ARG:NH2	5:F:22:GLN:OE1	1.96	0.98
2:K:265:THR:CG2	9:E:162:VAL:N	2.26	0.98
10:K:401:HEM:HBC2	10:K:401:HEM:HHD	1.42	0.97
2:K:345:GLU:OE1	5:F:82:TYR:OH	1.84	0.95
2:K:49:PHE:CE2	9:M:75:PHE:HB3	2.02	0.95
5:F:34:ALA:O	9:M:41:LEU:HD13	1.70	0.92
8:B:58:ASN:ND2	8:B:118:GLU:OE2	2.05	0.90
9:M:31:ASN:OD1	9:M:32:TYR:N	2.08	0.87
2:K:318:PHE:O	2:K:378:TYR:OH	1.93	0.86
3:D:280:LYS:HD2	9:M:35:PRO:CG	2.04	0.86
1:A:156:GLN:HB2	9:M:34:GLN:CG	2.04	0.86
5:F:36:LYS:HG3	9:M:40:TYR:O	1.78	0.84
5:F:36:LYS:HG3	9:M:41:LEU:O	1.79	0.83
9:E:187:ARG:HA	9:E:196:ASN:CA	2.10	0.82
5:F:36:LYS:HG3	9:M:41:LEU:C	2.05	0.81
5:F:36:LYS:CG	9:M:41:LEU:O	2.29	0.81
2:K:184:PHE:CE1	10:K:401:HEM:HBC1	2.19	0.78
5:F:36:LYS:HE3	9:M:41:LEU:O	1.83	0.78
2:K:125:MET:HE2	11:K:403:U10:H102	1.64	0.77
5:F:36:LYS:CE	9:M:41:LEU:O	2.32	0.77
3:D:261:LEU:HD12	9:M:60:MET:HG3	1.65	0.77
7:I:31:ASP:OD1	7:I:35:ASN:ND2	2.16	0.77
8:B:15:ASN:ND2	8:B:209:LEU:O	2.18	0.77
2:K:265:THR:HG22	9:E:162:VAL:CA	2.13	0.77
5:F:36:LYS:CD	9:M:39:SER:O	2.32	0.76
1:A:194:ILE:HG21	1:A:209:ILE:HD13	1.65	0.76
9:E:161:CYS:CB	13:E:301:FES:S1	2.74	0.76
1:A:428:ASN:OD1	2:K:224:TYR:OH	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:LEU:HD11	9:M:60:MET:CG	2.16	0.75
3:D:282:ARG:NH2	3:D:284:ASP:OD2	2.20	0.75
2:K:311:SER:OG	2:K:319:LYS:NZ	2.17	0.74
3:D:280:LYS:HD2	9:M:35:PRO:HG2	1.69	0.73
9:E:81:ALA:HB3	9:E:86:LEU:HD23	1.71	0.73
9:E:112:PRO:CB	9:E:154:GLY:HA3	2.20	0.72
7:I:30:PHE:HE2	9:M:63:LEU:CD1	2.03	0.70
9:M:59:SER:O	9:M:63:LEU:HD23	1.91	0.70
2:K:295:MET:CE	11:K:403:U10:H103	2.21	0.70
1:A:189:ASN:ND2	1:A:217:GLU:OE1	2.26	0.69
1:A:156:GLN:HB3	9:M:34:GLN:HG3	1.75	0.69
3:D:57:TRP:NE1	3:D:170:ASP:OD1	2.24	0.68
4:G:56:MET:O	4:G:60:ILE:HD12	1.93	0.67
1:A:47:LEU:HD12	1:A:194:ILE:HD11	1.76	0.67
5:F:39:LYS:HE2	9:M:39:SER:O	1.95	0.67
2:K:105:SER:OG	10:K:402:HEM:O2D	2.13	0.67
3:D:177:THR:O	6:H:70:ARG:NH2	2.28	0.67
5:F:36:LYS:HG3	9:M:40:TYR:C	2.19	0.67
9:E:81:ALA:CB	9:E:86:LEU:HD23	2.25	0.67
7:I:30:PHE:CE2	9:M:63:LEU:CD1	2.76	0.66
2:K:312:ILE:HG21	4:G:5:MET:CE	2.25	0.66
3:D:161:ILE:HG12	12:D:301:HEC:CMA	2.26	0.65
8:B:108:VAL:O	8:B:112:THR:OG1	2.15	0.65
8:B:340:ASP:OD2	8:B:341:SER:N	2.31	0.64
5:F:36:LYS:CG	9:M:40:TYR:O	2.45	0.64
8:B:255:GLU:OE2	8:B:285:LYS:NZ	2.18	0.64
2:K:265:THR:H	9:E:162:VAL:CB	2.11	0.64
5:F:39:LYS:HD3	9:M:40:TYR:HA	1.79	0.64
8:B:226:THR:OG1	8:B:356:LYS:O	2.16	0.63
2:K:346:VAL:HG13	5:F:93:VAL:HG11	1.80	0.63
5:F:36:LYS:CB	9:M:40:TYR:O	2.46	0.63
3:D:118:GLU:O	3:D:126:ARG:NH1	2.32	0.63
1:A:255:ASN:ND2	1:A:307:SER:O	2.31	0.63
1:A:250:HIS:NE2	1:A:309:THR:OG1	2.33	0.62
2:K:312:ILE:HG21	4:G:5:MET:HE1	1.80	0.62
12:D:301:HEC:HBD1	12:D:301:HEC:HHA	1.82	0.61
9:E:187:ARG:HA	9:E:196:ASN:CB	2.30	0.61
3:D:67:ASP:O	3:D:70:SER:N	2.34	0.61
4:G:56:MET:HE1	4:G:107:ILE:HD13	1.83	0.61
1:A:54:ARG:NH1	1:A:88:GLU:OE2	2.32	0.60
8:B:15:ASN:O	8:B:16:SER:OG	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:280:LYS:CD	9:M:35:PRO:CB	2.75	0.60
1:A:321:LYS:HB3	1:A:420:LEU:HD23	1.85	0.59
1:A:413:ILE:O	1:A:427:TYR:OH	2.05	0.59
3:D:86:HIS:CE1	12:D:301:HEC:NA	2.69	0.59
3:D:280:LYS:HD2	9:M:35:PRO:HB3	1.80	0.59
3:D:282:ARG:HD2	9:M:32:TYR:CE2	2.38	0.59
7:I:23:ALA:HB2	9:M:65:ALA:HB3	1.85	0.59
7:I:23:ALA:HB2	9:M:65:ALA:CB	2.32	0.59
8:B:37:ASN:O	8:B:42:THR:OG1	2.11	0.59
2:K:265:THR:CG2	9:E:162:VAL:CB	2.52	0.59
4:G:6:THR:N	4:G:111:GLU:OE1	2.35	0.59
2:K:146:VAL:O	2:K:150:LEU:HD23	2.03	0.58
12:D:301:HEC:HHA	12:D:301:HEC:CBD	2.34	0.58
6:H:123:ASN:HA	6:H:126:VAL:HG22	1.85	0.58
3:D:102:THR:HG22	3:D:105:GLU:OE1	2.03	0.57
2:K:130:MET:HE1	2:K:182:LEU:CB	2.35	0.57
9:E:88:MET:O	9:E:88:MET:HG2	2.04	0.57
2:K:31:ASN:ND2	2:K:229:ASP:OD1	2.37	0.57
10:K:402:HEM:HHA	10:K:402:HEM:O2A	2.04	0.57
3:D:280:LYS:HD2	9:M:35:PRO:HB2	1.82	0.57
2:K:212:ILE:HD12	4:G:75:ILE:HG23	1.87	0.56
9:E:82:SER:O	9:E:84:ASP:N	2.38	0.56
9:E:87:ALA:O	9:E:88:MET:HB3	2.04	0.56
1:A:141:ASP:OD2	1:A:144:SER:OG	2.20	0.56
2:K:49:PHE:CD2	9:M:75:PHE:CD2	2.93	0.56
5:F:36:LYS:CE	9:M:39:SER:O	2.53	0.56
8:B:74:LEU:HD12	8:B:97:ASP:OD1	2.06	0.56
2:K:265:THR:HG22	9:E:162:VAL:N	2.05	0.56
2:K:49:PHE:CD2	9:M:75:PHE:HD2	2.24	0.56
2:K:112:MET:O	2:K:116:ILE:HD12	2.06	0.56
6:H:66:LEU:HD13	6:H:130:LEU:CD1	2.36	0.56
1:A:153:SER:HA	9:M:34:GLN:NE2	2.21	0.55
12:D:301:HEC:HHD	12:D:301:HEC:HBC3	1.89	0.55
3:D:161:ILE:HG12	12:D:301:HEC:HMA1	1.87	0.55
1:A:249:VAL:HG12	1:A:413:ILE:HG22	1.89	0.55
3:D:236:LEU:HD11	12:D:301:HEC:HMB2	1.88	0.55
3:D:232:VAL:HG11	12:D:301:HEC:HMB3	1.89	0.54
4:G:44:LYS:NZ	4:G:98:GLU:O	2.31	0.54
1:A:47:LEU:HD12	1:A:194:ILE:CD1	2.37	0.54
8:B:180:PHE:O	8:B:209:LEU:HD13	2.08	0.54
3:D:280:LYS:CD	9:M:35:PRO:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:70:GLU:O	8:B:74:LEU:HD23	2.07	0.54
3:D:161:ILE:HG12	12:D:301:HEC:HMA3	1.89	0.53
8:B:55:THR:O	8:B:108:VAL:HG13	2.08	0.53
1:A:149:HIS:ND1	1:A:235:MET:SD	2.81	0.53
3:D:271:PHE:O	3:D:274:THR:OG1	2.22	0.53
9:E:158:HIS:H	9:E:193:ALA:CB	2.22	0.53
2:K:313:ILE:HD11	4:G:45:PHE:HE1	1.74	0.53
2:K:130:MET:HE1	2:K:182:LEU:HB2	1.91	0.53
5:F:61:ALA:O	5:F:65:VAL:HG23	2.08	0.53
9:M:74:ALA:O	9:M:77:SER:OG	2.27	0.53
7:I:27:GLN:HB2	9:M:66:ALA:HB1	1.92	0.52
8:B:242:ILE:HG23	8:B:357:PHE:HB2	1.92	0.52
9:M:42:ASN:OD1	9:M:43:ASN:N	2.43	0.52
2:K:264:VAL:HG13	2:K:264:VAL:O	2.08	0.52
5:F:30:ILE:HG23	9:M:37:TYR:CE2	2.44	0.52
2:K:133:CYS:HA	2:K:140:SER:OG	2.10	0.52
10:K:401:HEM:HBB2	10:K:401:HEM:HMB2	1.90	0.52
9:E:157:THR:CB	13:E:301:FES:S2	2.96	0.52
8:B:244:ILE:HD13	8:B:357:PHE:HA	1.92	0.52
8:B:26:THR:O	8:B:27:ASP:OD1	2.28	0.52
1:A:152:SER:HB2	9:M:31:ASN:N	2.25	0.51
6:H:84:HIS:O	6:H:88:GLU:OE1	2.28	0.51
10:K:402:HEM:HMB1	10:K:402:HEM:HBB2	1.90	0.51
1:A:279:ALA:O	1:A:291:GLN:NE2	2.42	0.51
3:D:82:CYS:N	12:D:301:HEC:HBB2	2.25	0.51
10:K:402:HEM:HMC1	10:K:402:HEM:HBC2	1.93	0.51
3:D:117:ASP:OD1	3:D:118:GLU:N	2.39	0.51
12:D:301:HEC:HHC	12:D:301:HEC:HBB3	1.90	0.51
1:A:31:THR:CG2	1:A:193:VAL:HG22	2.40	0.51
8:B:354:ILE:HG22	8:B:354:ILE:O	2.10	0.51
2:K:189:ILE:O	2:K:193:LEU:HD23	2.11	0.51
6:H:66:LEU:HD13	6:H:130:LEU:HD11	1.93	0.51
8:B:57:LEU:HD23	8:B:118:GLU:HG2	1.93	0.51
8:B:255:GLU:HG2	8:B:283:LEU:HD23	1.93	0.51
2:K:201:LEU:HD11	10:K:402:HEM:HAA1	1.93	0.50
8:B:29:THR:HG21	8:B:98:LEU:HD13	1.94	0.50
9:E:157:THR:HA	9:E:193:ALA:HB2	1.94	0.50
2:K:207:SER:OG	2:K:208:ASN:N	2.44	0.50
7:I:22:GLY:C	9:M:62:LEU:HD22	2.37	0.50
2:K:58:ILE:HD11	2:K:136:TYR:CZ	2.46	0.50
10:K:401:HEM:HBB2	10:K:401:HEM:CMB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:OE1	1:A:307:SER:N	2.43	0.50
3:D:88:LEU:HD23	3:D:88:LEU:O	2.11	0.50
2:K:58:ILE:HD11	2:K:136:TYR:OH	2.11	0.49
8:B:254:TYR:HB2	8:B:283:LEU:HD22	1.93	0.49
2:K:147:ILE:HD11	11:K:403:U10:C2	2.41	0.49
3:D:107:LYS:O	3:D:111:GLU:OE1	2.31	0.49
1:A:237:ASP:HB2	1:A:240:LEU:HD13	1.94	0.49
2:K:344:VAL:O	2:K:344:VAL:HG23	2.13	0.49
1:A:275:HIS:O	8:B:126:THR:HG23	2.13	0.49
2:K:116:ILE:HD12	2:K:116:ILE:H	1.77	0.49
2:K:295:MET:HE1	11:K:403:U10:H72	1.94	0.49
2:K:120:ILE:HG23	2:K:190:LEU:HD11	1.94	0.49
2:K:332:ASN:HD22	2:K:358:TYR:HD2	1.60	0.48
8:B:269:THR:O	8:B:270:SER:OG	2.21	0.48
1:A:125:THR:O	1:A:129:GLN:OE1	2.31	0.48
12:D:301:HEC:HHD	12:D:301:HEC:CBC	2.43	0.48
8:B:151:PHE:O	8:B:156:GLY:HA3	2.13	0.48
9:E:82:SER:O	9:E:83:ALA:C	2.56	0.48
8:B:119:PHE:HB2	8:B:169:LEU:HD12	1.96	0.48
1:A:31:THR:HG22	1:A:193:VAL:HG22	1.95	0.48
1:A:192:THR:HG21	1:A:215:ILE:CD1	2.44	0.48
2:K:312:ILE:HD13	4:G:5:MET:HE1	1.95	0.48
8:B:57:LEU:O	8:B:64:ALA:N	2.47	0.48
1:A:34:THR:CG2	1:A:202:HIS:HD1	2.27	0.48
2:K:87:SER:HB3	2:K:251:LEU:HD13	1.95	0.48
2:K:216:ILE:HD12	4:G:75:ILE:HG21	1.95	0.48
1:A:283:SER:OG	8:B:72:GLU:OE1	2.14	0.47
10:K:402:HEM:HBB2	10:K:402:HEM:CMB	2.44	0.47
4:G:5:MET:HG3	4:G:107:ILE:HG21	1.95	0.47
5:F:48:ASN:OD1	5:F:51:ARG:NH2	2.45	0.47
1:A:80:LEU:HD13	8:B:266:LEU:HB3	1.97	0.47
2:K:52:MET:SD	9:M:79:PHE:CE2	3.07	0.47
4:G:46:ASN:ND2	4:G:101:ASN:HA	2.30	0.47
5:F:36:LYS:CA	9:M:40:TYR:O	2.60	0.47
2:K:246:TYR:CE2	3:D:255:LEU:HD11	2.50	0.47
8:B:65:LEU:O	8:B:65:LEU:HD23	2.14	0.47
2:K:113:LEU:HD11	2:K:197:HIS:CE1	2.49	0.47
1:A:61:ASN:OD1	1:A:62:GLY:N	2.48	0.47
1:A:80:LEU:HD11	8:B:268:SER:HB2	1.95	0.47
1:A:296:VAL:HG23	1:A:318:ILE:HG13	1.96	0.47
2:K:35:LEU:HD11	2:K:232:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:CYS:CB	2:K:89:PHE:HD1	2.27	0.47
2:K:49:PHE:CG	9:M:75:PHE:HD2	2.32	0.47
2:K:245:PHE:O	3:D:247:ARG:NH1	2.43	0.47
8:B:222:THR:HG23	8:B:223:ASN:N	2.30	0.47
1:A:243:ALA:HA	1:A:419:GLY:O	2.14	0.47
1:A:375:LYS:O	1:A:379:VAL:HG22	2.15	0.47
3:D:87:SER:OG	3:D:88:LEU:N	2.48	0.47
2:K:349:ILE:HG13	2:K:350:GLN:N	2.30	0.47
9:E:94:LYS:HA	9:E:208:GLU:CB	2.45	0.47
9:E:157:THR:CB	9:E:193:ALA:HB2	2.45	0.47
12:D:301:HEC:HHC	12:D:301:HEC:CBB	2.45	0.46
4:G:24:ILE:O	4:G:28:LEU:HD13	2.15	0.46
8:B:35:ILE:CD1	8:B:185:ILE:HG22	2.46	0.46
3:D:237:ASN:C	3:D:237:ASN:HD22	2.23	0.46
7:I:35:ASN:O	7:I:39:GLU:OE1	2.34	0.46
8:B:37:ASN:OD1	8:B:184:ASN:ND2	2.43	0.46
2:K:222:HIS:HB3	2:K:223:PRO:HD3	1.97	0.46
2:K:39:CYS:HB2	2:K:89:PHE:HD1	1.81	0.46
2:K:166:TRP:O	2:K:175:THR:OG1	2.29	0.46
2:K:322:SER:HB2	2:K:374:GLU:OE1	2.17	0.45
2:K:52:MET:SD	9:M:79:PHE:HE2	2.39	0.45
8:B:102:VAL:HG13	8:B:103:GLU:N	2.31	0.45
3:D:82:CYS:CA	12:D:301:HEC:HBB2	2.45	0.45
8:B:57:LEU:O	8:B:64:ALA:CA	2.64	0.45
9:E:187:ARG:CA	9:E:196:ASN:HA	2.23	0.45
1:A:101:ILE:HG23	1:A:102:THR:N	2.31	0.45
5:F:62:ILE:HB	5:F:63:PRO:HD3	1.97	0.45
9:E:86:LEU:HD22	9:E:86:LEU:HA	1.83	0.45
8:B:193:ASN:OD1	8:B:195:GLU:N	2.46	0.45
9:M:33:GLN:O	9:M:33:GLN:HG2	2.17	0.45
4:G:47:ASP:OD1	4:G:74:ARG:NH1	2.48	0.44
2:K:49:PHE:CG	9:M:75:PHE:CD2	3.06	0.44
3:D:66:PHE:CB	3:D:71:ILE:HD11	2.47	0.44
7:I:23:ALA:N	9:M:62:LEU:HD22	2.32	0.44
1:A:237:ASP:CB	1:A:240:LEU:HD13	2.48	0.44
7:I:26:PHE:HD2	9:M:62:LEU:HB3	1.81	0.44
8:B:169:LEU:HD23	8:B:169:LEU:C	2.43	0.44
1:A:34:THR:HG22	1:A:196:ALA:HB3	2.00	0.44
2:K:70:ARG:NH2	3:D:159:SER:O	2.50	0.44
2:K:125:MET:HE1	2:K:278:PHE:CD2	2.52	0.44
9:M:72:VAL:O	9:M:76:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:401:HEM:HBA2	10:K:401:HEM:HHA	1.99	0.43
2:K:36:LEU:CD1	2:K:96:HIS:CD2	3.01	0.43
2:K:295:MET:SD	11:K:403:U10:H1M2	2.59	0.43
3:D:120:ASP:OD1	3:D:124:LYS:N	2.50	0.43
2:K:126:ALA:O	2:K:127:ILE:C	2.60	0.43
9:E:158:HIS:H	9:E:193:ALA:HB1	1.83	0.43
1:A:102:THR:HG23	1:A:103:GLU:OE1	2.19	0.43
2:K:213:THR:HG21	4:G:51:GLU:OE1	2.19	0.43
5:F:34:ALA:O	9:M:41:LEU:CD1	2.56	0.43
2:K:231:ILE:HD11	3:D:269:LYS:CB	2.47	0.43
8:B:102:VAL:HG11	8:B:200:PHE:HB3	1.99	0.43
2:K:130:MET:HE1	2:K:182:LEU:HB3	2.00	0.43
3:D:264:LEU:HG	9:M:56:MET:HE2	2.01	0.43
5:F:88:GLU:H	5:F:88:GLU:CD	2.26	0.43
1:A:25:THR:HG23	1:A:25:THR:O	2.18	0.43
1:A:142:PRO:O	1:A:146:VAL:HG23	2.18	0.43
2:K:65:VAL:HG22	10:K:401:HEM:O2D	2.19	0.43
2:K:73:ASN:HD22	9:M:77:SER:HB2	1.84	0.43
2:K:217:ASP:OD2	3:D:279:ARG:NH2	2.40	0.43
8:B:35:ILE:HD12	8:B:185:ILE:HG22	2.01	0.43
2:K:70:ARG:NH1	3:D:239:ALA:O	2.50	0.43
2:K:184:PHE:CE1	10:K:401:HEM:CBC	2.98	0.43
2:K:200:ALA:O	2:K:203:VAL:HG12	2.19	0.43
3:D:66:PHE:HB3	3:D:71:ILE:HD11	2.01	0.43
9:E:157:THR:CA	9:E:193:ALA:HB2	2.48	0.43
2:K:40:LEU:HD12	10:K:401:HEM:HBB1	2.00	0.42
2:K:122:ILE:HG12	2:K:299:ILE:HG21	2.01	0.42
11:K:403:U10:H122	11:K:403:U10:H101	1.76	0.42
8:B:347:VAL:HG23	8:B:347:VAL:O	2.19	0.42
1:A:189:ASN:N	1:A:189:ASN:OD1	2.51	0.42
2:K:90:PHE:CZ	2:K:124:THR:HG22	2.55	0.42
2:K:131:GLY:HA3	2:K:183:HIS:CE1	2.53	0.42
2:K:132:TYR:HA	10:K:401:HEM:HAA1	2.01	0.42
3:D:81:VAL:HB	12:D:301:HEC:HBB1	2.01	0.42
2:K:81:ILE:O	2:K:83:ALA:N	2.52	0.42
2:K:125:MET:O	2:K:126:ALA:C	2.63	0.42
5:F:30:ILE:HD13	9:M:37:TYR:CD1	2.55	0.42
8:B:256:VAL:HG21	8:B:348:VAL:O	2.19	0.42
2:K:147:ILE:HD11	11:K:403:U10:C3	2.49	0.42
3:D:46:ALA:HB2	6:H:112:ILE:HG21	2.02	0.42
3:D:107:LYS:O	3:D:110:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:57:LEU:O	8:B:64:ALA:HB2	2.20	0.42
1:A:56:GLU:OE2	1:A:64:SER:OG	2.32	0.42
2:K:81:ILE:O	2:K:82:HIS:C	2.62	0.42
2:K:313:ILE:HD11	4:G:45:PHE:CE1	2.53	0.42
1:A:427:TYR:CE2	5:F:31:SER:HB2	2.54	0.42
2:K:22:GLN:OE1	11:K:404:U10:H4M2	2.20	0.41
2:K:69:MET:HE1	2:K:80:TYR:CZ	2.54	0.41
10:K:402:HEM:HBC2	10:K:402:HEM:CMC	2.49	0.41
2:K:116:ILE:O	2:K:117:GLY:C	2.62	0.41
2:K:301:ILE:HD11	2:K:364:ILE:HG23	2.02	0.41
5:F:30:ILE:HD13	9:M:37:TYR:CG	2.55	0.41
8:B:74:LEU:HB3	8:B:97:ASP:OD2	2.20	0.41
2:K:165:ILE:O	2:K:178:ARG:HD2	2.20	0.41
1:A:314:TYR:CD1	1:A:314:TYR:C	2.99	0.41
2:K:39:CYS:SG	2:K:236:PHE:CZ	3.13	0.41
2:K:120:ILE:O	2:K:121:PHE:C	2.62	0.41
3:D:94:ARG:O	3:D:97:VAL:HG22	2.19	0.41
2:K:118:VAL:HG21	2:K:303:LEU:HD23	2.03	0.41
9:M:37:TYR:O	9:M:38:SER:C	2.63	0.41
2:K:231:ILE:HD11	3:D:269:LYS:HB3	2.02	0.41
8:B:98:LEU:N	8:B:99:PRO:HD2	2.36	0.41
8:B:177:LYS:C	8:B:179:GLN:H	2.29	0.41
9:E:175:CYS:O	9:E:179:GLY:N	2.54	0.41
1:A:80:LEU:HD22	8:B:266:LEU:HD22	2.03	0.41
1:A:264:VAL:HA	1:A:354:VAL:HG21	2.03	0.41
2:K:24:SER:O	4:G:83:LEU:HD12	2.20	0.41
2:K:212:ILE:HG22	4:G:47:ASP:O	2.20	0.41
4:G:51:GLU:HA	4:G:56:MET:HG2	2.01	0.41
5:F:36:LYS:CG	9:M:41:LEU:C	2.82	0.41
7:I:23:ALA:HB2	9:M:65:ALA:HB1	2.02	0.41
2:K:147:ILE:O	2:K:151:LEU:HD13	2.21	0.41
2:K:152:SER:HB2	2:K:162:VAL:HG21	2.03	0.41
3:D:270:ARG:O	3:D:274:THR:HG23	2.21	0.41
1:A:152:SER:HG	9:M:31:ASN:N	2.18	0.40
2:K:139:MET:HE1	2:K:268:SER:O	2.21	0.40
2:K:271:PRO:HB3	11:K:403:U10:O4	2.22	0.40
4:G:62:ARG:HH21	4:G:110:ALA:HB2	1.86	0.40
1:A:35:GLU:HB2	1:A:372:ILE:HD11	2.03	0.40
8:B:257:LEU:HD22	8:B:292:PHE:CZ	2.55	0.40
2:K:69:MET:SD	2:K:79:ARG:HD3	2.61	0.40
12:D:301:HEC:CBD	12:D:301:HEC:CHA	2.98	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	414/439 (94%)	399 (96%)	15 (4%)	0	100 100
2	K	381/387 (98%)	357 (94%)	24 (6%)	0	100 100
3	D	242/288 (84%)	232 (96%)	10 (4%)	0	100 100
4	G	120/127 (94%)	119 (99%)	1 (1%)	0	100 100
5	F	83/95 (87%)	78 (94%)	5 (6%)	0	100 100
6	H	70/135 (52%)	69 (99%)	1 (1%)	0	100 100
7	I	37/39 (95%)	35 (95%)	2 (5%)	0	100 100
8	B	362/374 (97%)	346 (96%)	16 (4%)	0	100 100
9	E	130/213 (61%)	114 (88%)	13 (10%)	3 (2%)	5 25
9	M	48/213 (22%)	48 (100%)	0	0	100 100
All	All	1887/2310 (82%)	1797 (95%)	87 (5%)	3 (0%)	44 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	E	83	ALA
9	E	175	CYS
9	E	147	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	345/365 (94%)	345 (100%)	0	100 100
2	K	333/338 (98%)	333 (100%)	0	100 100
3	D	196/237 (83%)	196 (100%)	0	100 100
4	G	106/110 (96%)	106 (100%)	0	100 100
5	F	71/80 (89%)	71 (100%)	0	100 100
6	H	67/128 (52%)	67 (100%)	0	100 100
7	I	30/30 (100%)	30 (100%)	0	100 100
8	B	295/307 (96%)	295 (100%)	0	100 100
9	E	6/176 (3%)	3 (50%)	3 (50%)	0 0
9	M	40/176 (23%)	40 (100%)	0	100 100
All	All	1489/1947 (76%)	1486 (100%)	3 (0%)	85 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	E	86	LEU
9	E	88	MET
9	E	90	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	191	ASN
1	A	383	GLN
1	A	430	ASN
2	K	73	ASN
2	K	177	GLN
2	K	353	GLN
3	D	51	HIS
5	F	55	ASN
6	H	84	HIS
7	I	27	GLN
7	I	35	ASN
9	M	47	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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	HEC	D	301	3	50,50,50	1.50	6 (12%)	68,82,82	1.34	9 (13%)
13	FES	E	301	9	0,4,4	-	-	-		
11	U10	K	404	2	23,23,63	2.74	9 (39%)	30,31,79	1.51	5 (16%)
11	U10	K	403	-	28,28,63	2.81	10 (35%)	36,37,79	1.44	7 (19%)
10	HEM	K	401	2	50,50,50	1.33	8 (16%)	67,82,82	1.09	3 (4%)
10	HEM	K	402	2	50,50,50	1.35	6 (12%)	67,82,82	1.25	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEC	D	301	3	-	10/14/54/54	-
13	FES	E	301	9	-	-	0/1/1/1
11	U10	K	404	2	-	2/15/39/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	U10	K	403	-	-	3/21/45/87	0/1/1/1
10	HEM	K	401	2	-	6/14/54/54	-
10	HEM	K	402	2	-	2/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	403	U10	C13-C14	6.42	1.47	1.33
11	K	403	U10	C8-C9	6.37	1.47	1.33
11	K	404	U10	C8-C9	6.28	1.47	1.33
11	K	403	U10	O3-C3	-5.72	1.23	1.36
11	K	403	U10	O4-C4	-5.63	1.23	1.36
11	K	404	U10	O3-C3	-5.48	1.23	1.36
11	K	404	U10	O4-C4	-5.45	1.23	1.36
11	K	404	U10	C13-C14	5.17	1.47	1.32
11	K	403	U10	C18-C19	4.99	1.47	1.32
12	D	301	HEC	CBB-CAB	-4.19	1.33	1.51
12	D	301	HEC	CBC-CAC	-4.10	1.34	1.51
10	K	402	HEM	FE-NA	3.63	2.07	1.95
10	K	402	HEM	FE-NC	3.50	2.06	1.95
11	K	403	U10	C4-C5	-3.49	1.38	1.48
12	D	301	HEC	FE-NA	3.39	2.06	1.95
11	K	404	U10	C4-C5	-3.31	1.39	1.48
10	K	401	HEM	FE-ND	3.28	2.05	1.94
11	K	403	U10	C3-C2	-3.27	1.39	1.48
11	K	404	U10	C3-C2	-3.20	1.39	1.48
12	D	301	HEC	FE-ND	3.00	2.04	1.94
10	K	402	HEM	CAC-C3C	2.81	1.54	1.47
11	K	403	U10	C6-C5	-2.80	1.38	1.46
10	K	402	HEM	CAB-C3B	2.78	1.54	1.47
10	K	401	HEM	CAB-C3B	2.73	1.54	1.47
12	D	301	HEC	FE-NB	2.58	2.02	1.94
11	K	404	U10	C6-C1	2.53	1.39	1.35
11	K	404	U10	C6-C5	-2.49	1.39	1.46
10	K	401	HEM	CAC-C3C	2.44	1.53	1.47
11	K	403	U10	C6-C1	2.39	1.39	1.35
10	K	401	HEM	FE-NB	2.35	2.02	1.94
11	K	404	U10	C1-C2	-2.28	1.39	1.47
11	K	403	U10	C1-C2	-2.24	1.39	1.47
10	K	401	HEM	C3C-C2C	-2.22	1.32	1.37
10	K	401	HEM	C2A-C3A	-2.18	1.33	1.38
10	K	401	HEM	FE-NC	2.16	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	401	HEM	FE-NA	2.13	2.02	1.95
12	D	301	HEC	C3C-C2C	-2.08	1.33	1.38
10	K	402	HEM	C2A-C3A	-2.05	1.33	1.38
10	K	402	HEM	C3D-C2D	-2.01	1.32	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	404	U10	C10-C9-C11	3.92	122.04	115.23
12	D	301	HEC	CBC-CAC-C3C	3.45	121.78	112.42
12	D	301	HEC	CBB-CAB-C3B	3.35	121.50	112.42
10	K	402	HEM	CHA-C4D-ND	3.31	128.46	124.37
11	K	404	U10	C7-C8-C9	-3.23	121.27	126.83
11	K	403	U10	C12-C13-C14	-3.18	120.35	127.62
10	K	402	HEM	CHD-C1D-ND	3.14	127.80	124.42
10	K	402	HEM	CBD-CAD-C3D	-3.13	103.89	112.53
11	K	403	U10	C10-C9-C11	2.95	120.35	115.23
12	D	301	HEC	CAB-C3B-C4B	2.50	128.04	124.79
11	K	403	U10	C15-C14-C16	2.47	119.52	115.23
11	K	404	U10	C12-C13-C14	-2.46	119.45	127.64
11	K	404	U10	C7-C6-C1	-2.36	120.84	124.89
11	K	403	U10	C21-C19-C20	2.32	119.93	114.59
11	K	403	U10	C7-C8-C9	-2.31	122.86	126.83
11	K	403	U10	C1M-C1-C6	-2.29	120.68	124.45
10	K	402	HEM	CHC-C4B-NB	2.27	126.87	124.42
11	K	403	U10	C17-C18-C19	-2.21	120.28	127.64
12	D	301	HEC	C4B-NB-C1B	2.20	107.81	105.21
10	K	402	HEM	C1B-NB-C4B	2.19	107.80	105.21
12	D	301	HEC	CHB-C1B-NB	2.14	126.73	124.42
12	D	301	HEC	C3B-C4B-NB	-2.12	107.84	110.17
10	K	402	HEM	C3B-C2B-C1B	2.11	108.00	106.41
12	D	301	HEC	CAA-CBA-CGA	-2.08	108.15	113.67
12	D	301	HEC	CAC-C3C-C4C	2.05	127.74	124.91
11	K	404	U10	C16-C14-C15	2.05	119.30	114.59
10	K	402	HEM	C1A-CHA-C4D	-2.04	121.44	126.25
10	K	401	HEM	C1B-NB-C4B	2.03	107.61	105.21
12	D	301	HEC	C3D-C4D-ND	-2.01	108.41	110.35
10	K	401	HEM	C2A-C1A-NA	-2.00	107.93	110.15
10	K	401	HEM	C3B-C2B-C1B	2.00	107.91	106.41

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	401	HEM	C1A-C2A-CAA-CBA
12	D	301	HEC	C2B-C3B-CAB-CBB
12	D	301	HEC	C4B-C3B-CAB-CBB
12	D	301	HEC	C2D-C3D-CAD-CBD
12	D	301	HEC	C4D-C3D-CAD-CBD
12	D	301	HEC	C2C-C3C-CAC-CBC
12	D	301	HEC	C4C-C3C-CAC-CBC
11	K	403	U10	C12-C11-C9-C10
11	K	403	U10	C12-C11-C9-C8
10	K	401	HEM	C3D-CAD-CBD-CGD
10	K	401	HEM	C4C-C3C-CAC-CBC
10	K	401	HEM	C4D-C3D-CAD-CBD
10	K	401	HEM	C3A-C2A-CAA-CBA
10	K	401	HEM	C2D-C3D-CAD-CBD
12	D	301	HEC	C1A-C2A-CAA-CBA
11	K	403	U10	C5-C4-O4-C4M
12	D	301	HEC	C3A-C2A-CAA-CBA
11	K	404	U10	C5-C4-O4-C4M
10	K	402	HEM	CAA-CBA-CGA-O1A
11	K	404	U10	C3-C4-O4-C4M
12	D	301	HEC	CAD-CBD-CGD-O1D
12	D	301	HEC	CAD-CBD-CGD-O2D
10	K	402	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

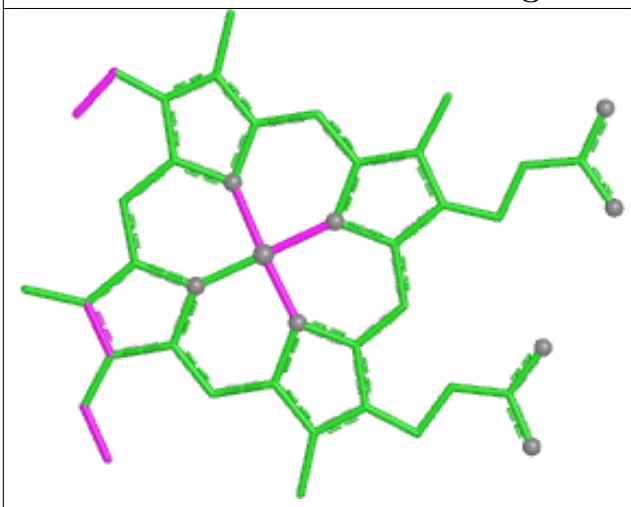
6 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	301	HEC	16	0
13	E	301	FES	2	0
11	K	404	U10	1	0
11	K	403	U10	8	0
10	K	401	HEM	9	0
10	K	402	HEM	7	0

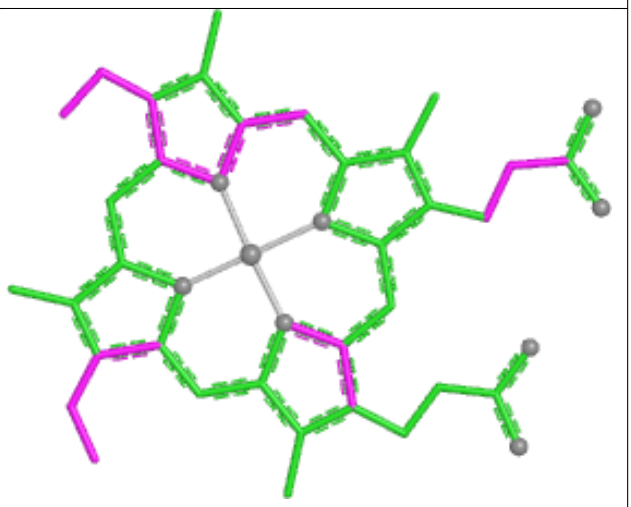
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

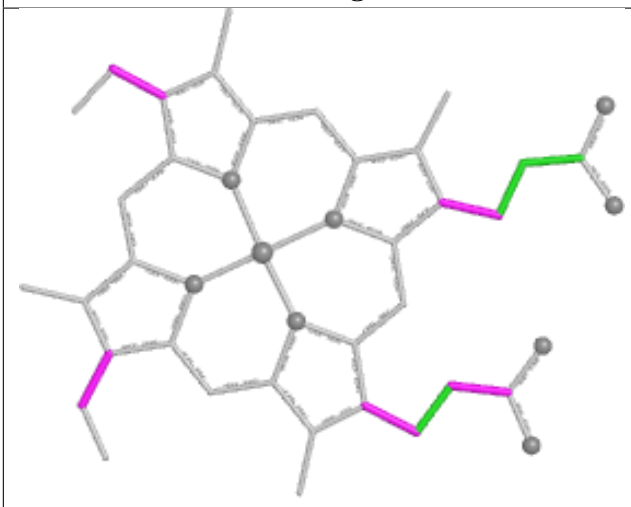
Ligand HEC D 301



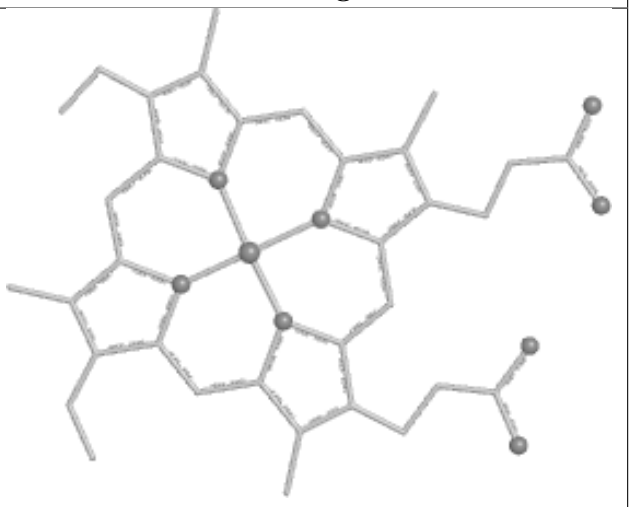
Bond lengths



Bond angles

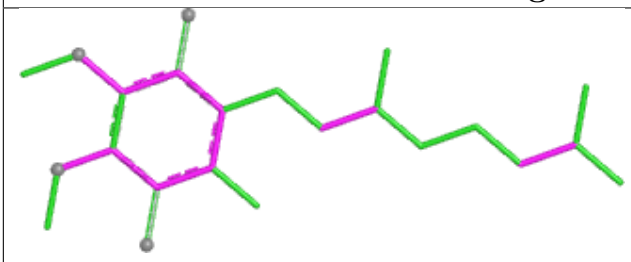


Torsions

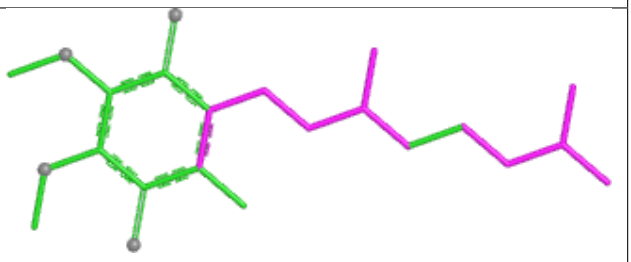


Rings

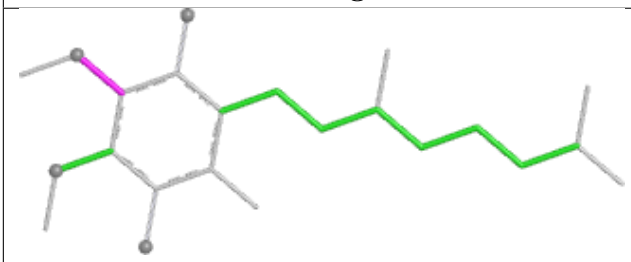
Ligand U10 K 404



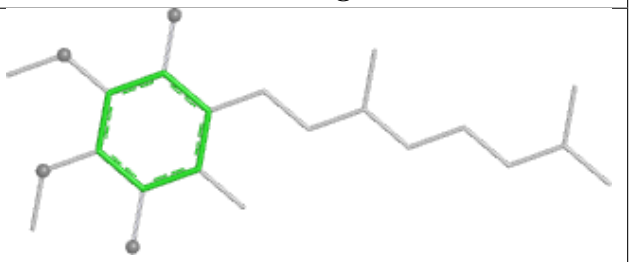
Bond lengths



Bond angles

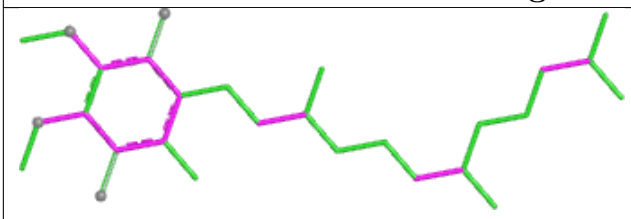


Torsions

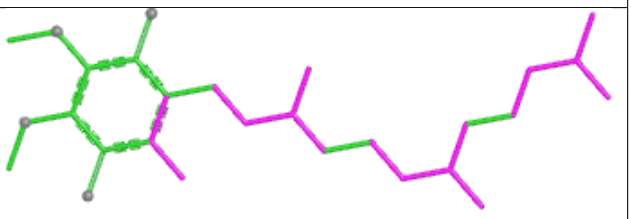


Rings

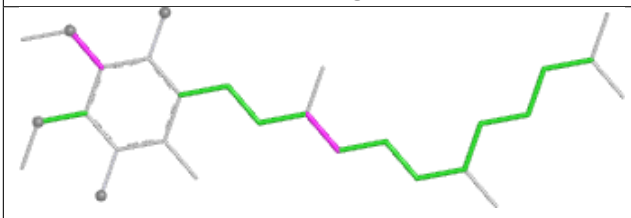
Ligand U10 K 403



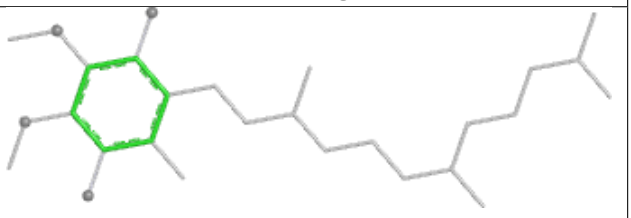
Bond lengths



Bond angles

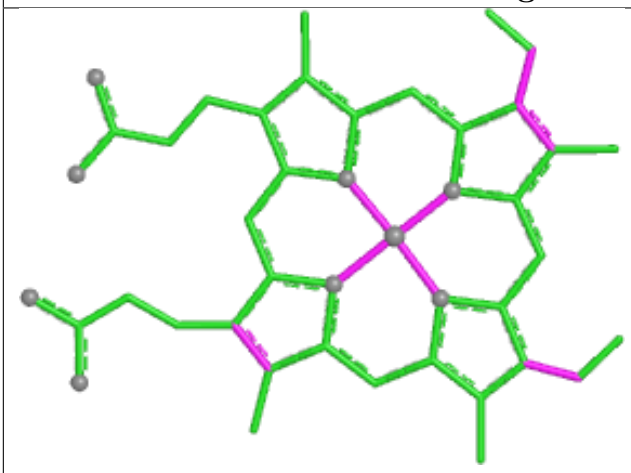


Torsions

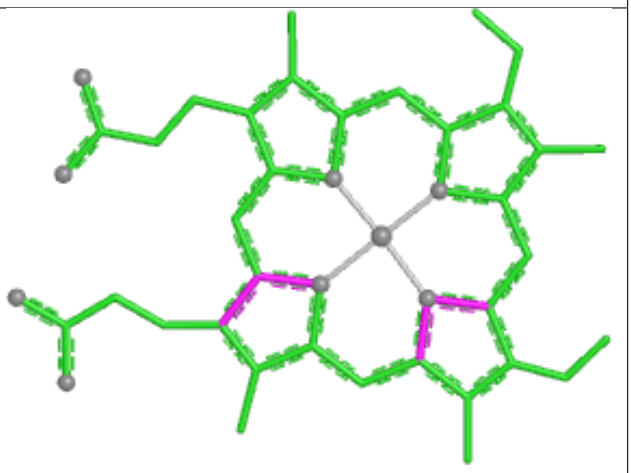


Rings

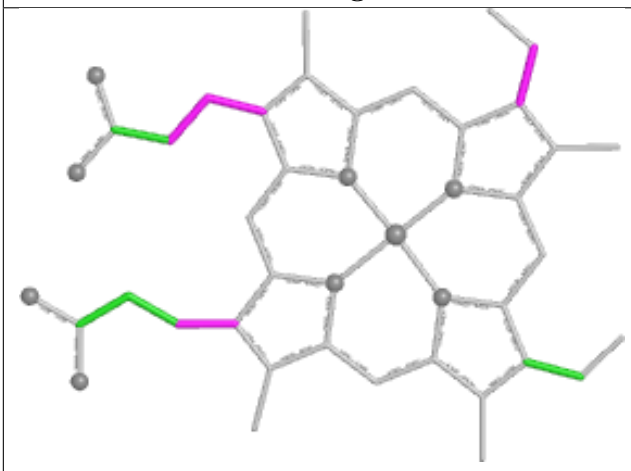
Ligand HEM K 401



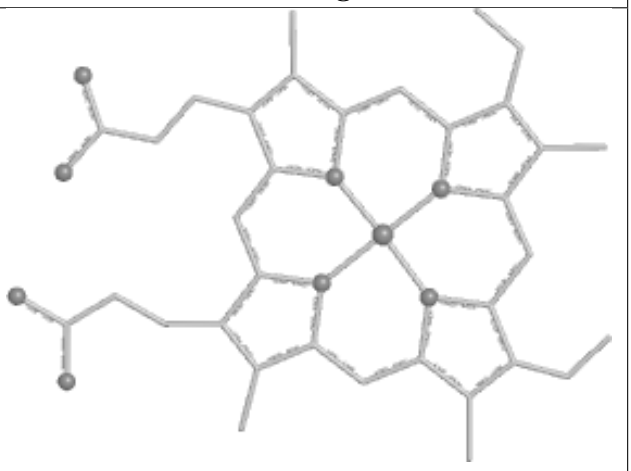
Bond lengths



Bond angles

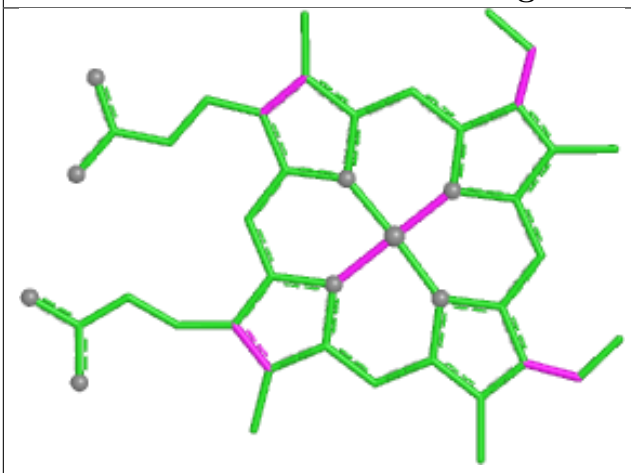


Torsions

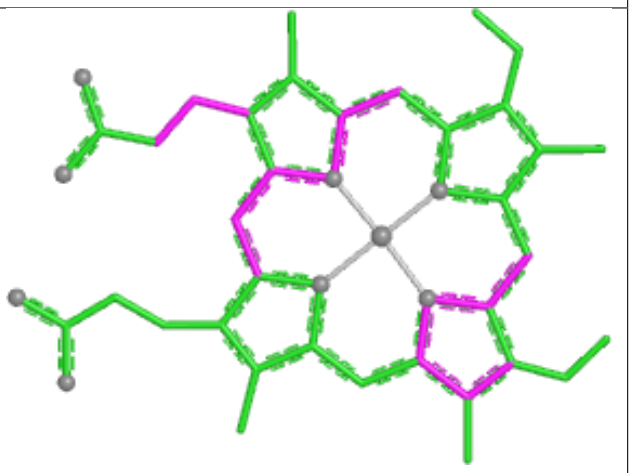


Rings

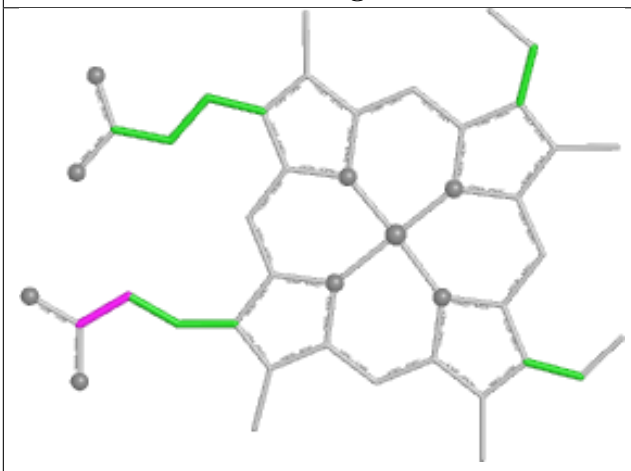
Ligand HEM K 402



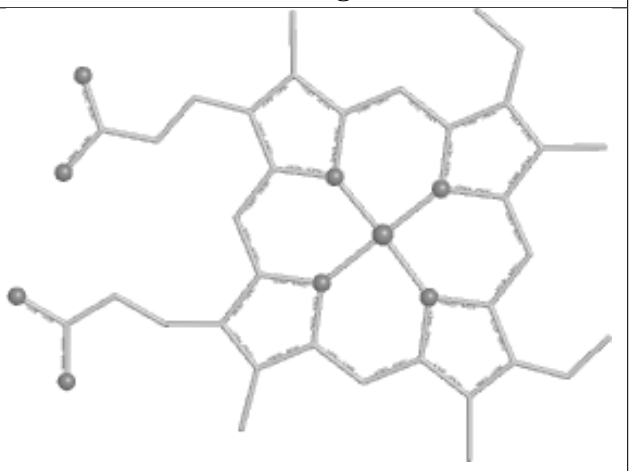
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

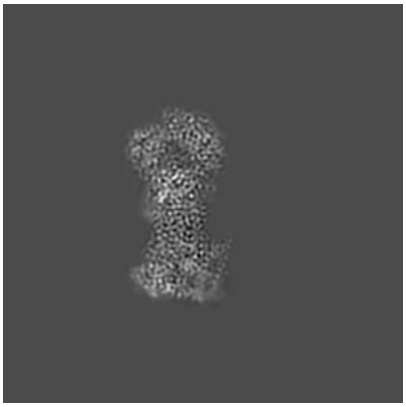
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24484. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

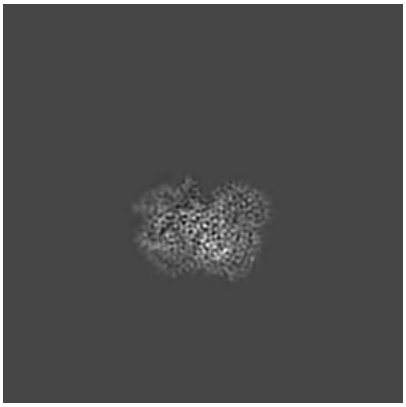
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 144



Y Index: 144



Z Index: 144

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

6.3 Largest variance slices (i)

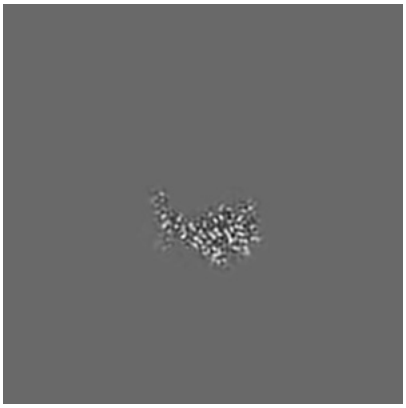
6.3.1 Primary map



X Index: 152



Y Index: 120

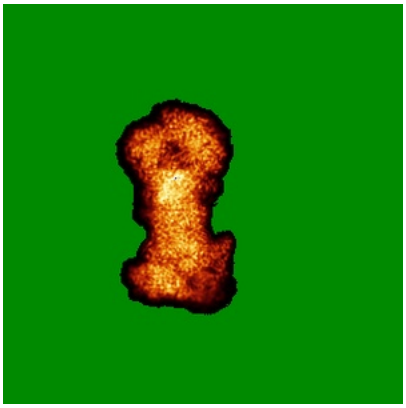


Z Index: 161

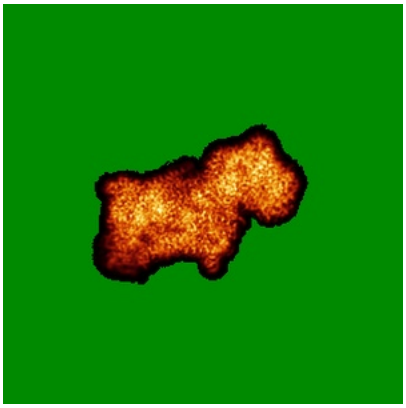
The images above show the largest variance slices of the map in three orthogonal directions.

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

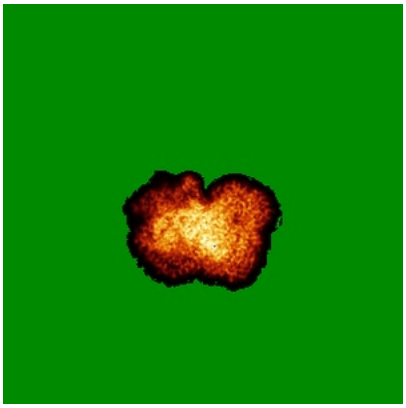
6.4.1 Primary map



X



Y



Z

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 0.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

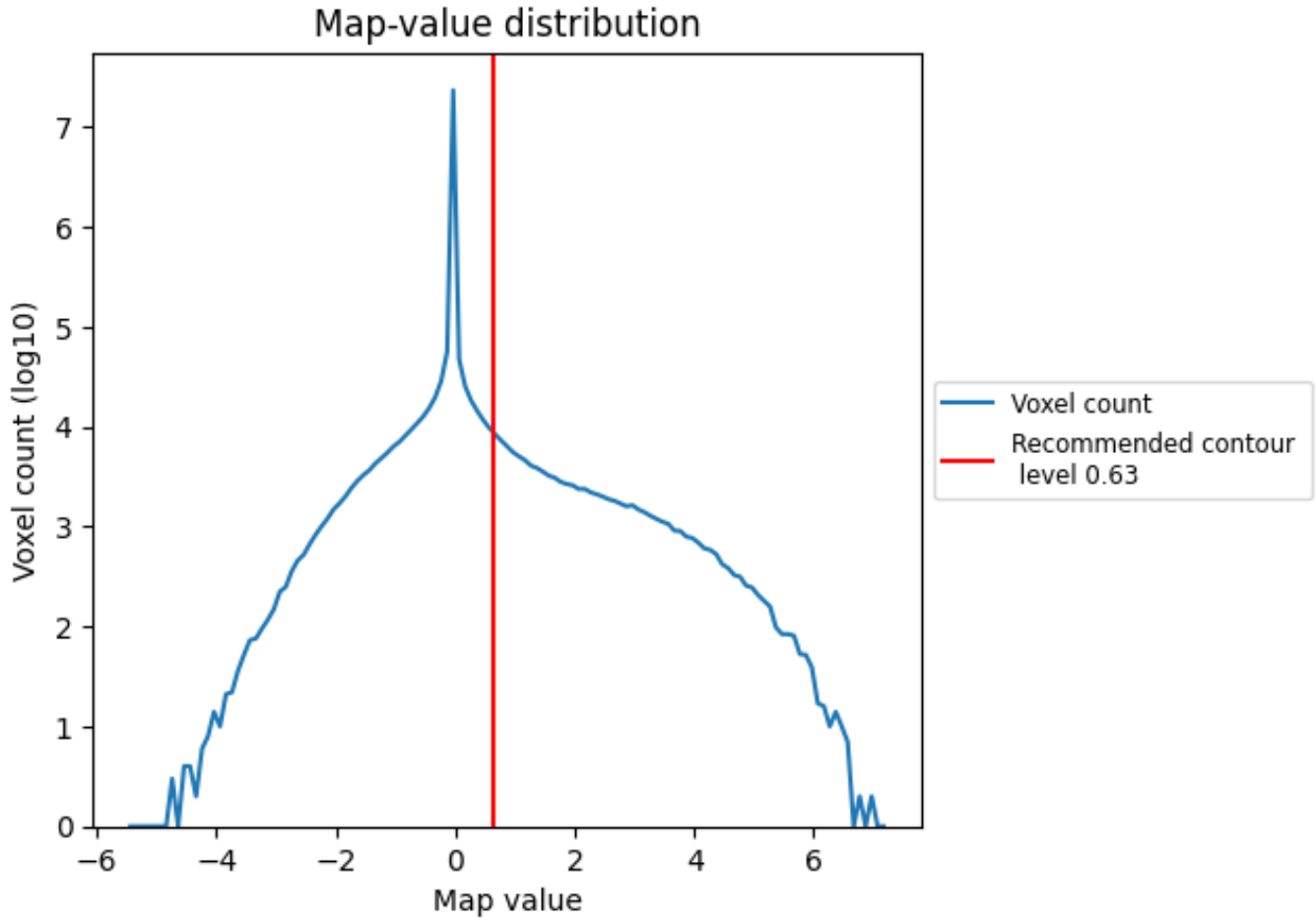
6.6 Mask visualisation (i)

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

7 Map analysis

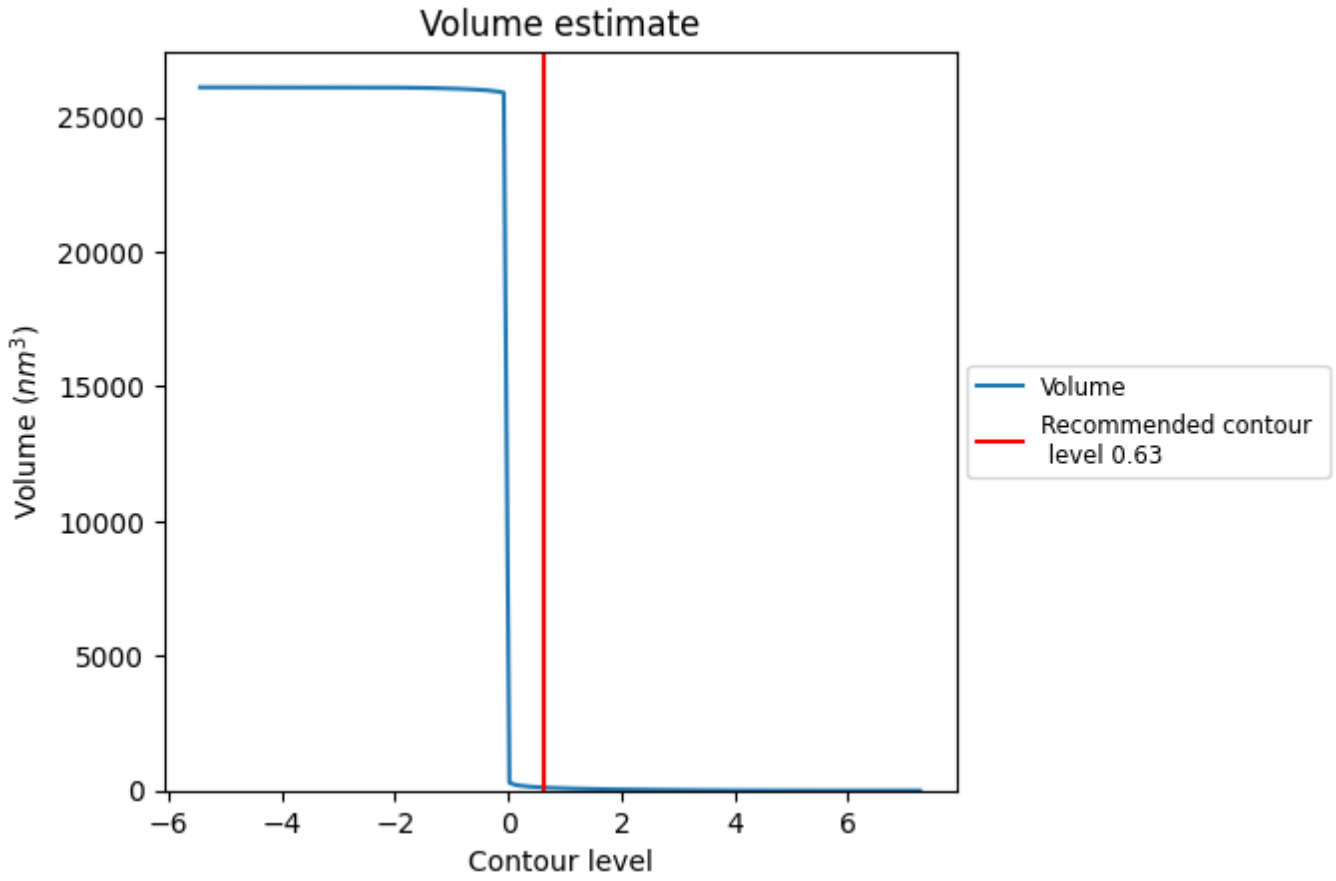
This section contains the results of statistical analysis of the map.

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.

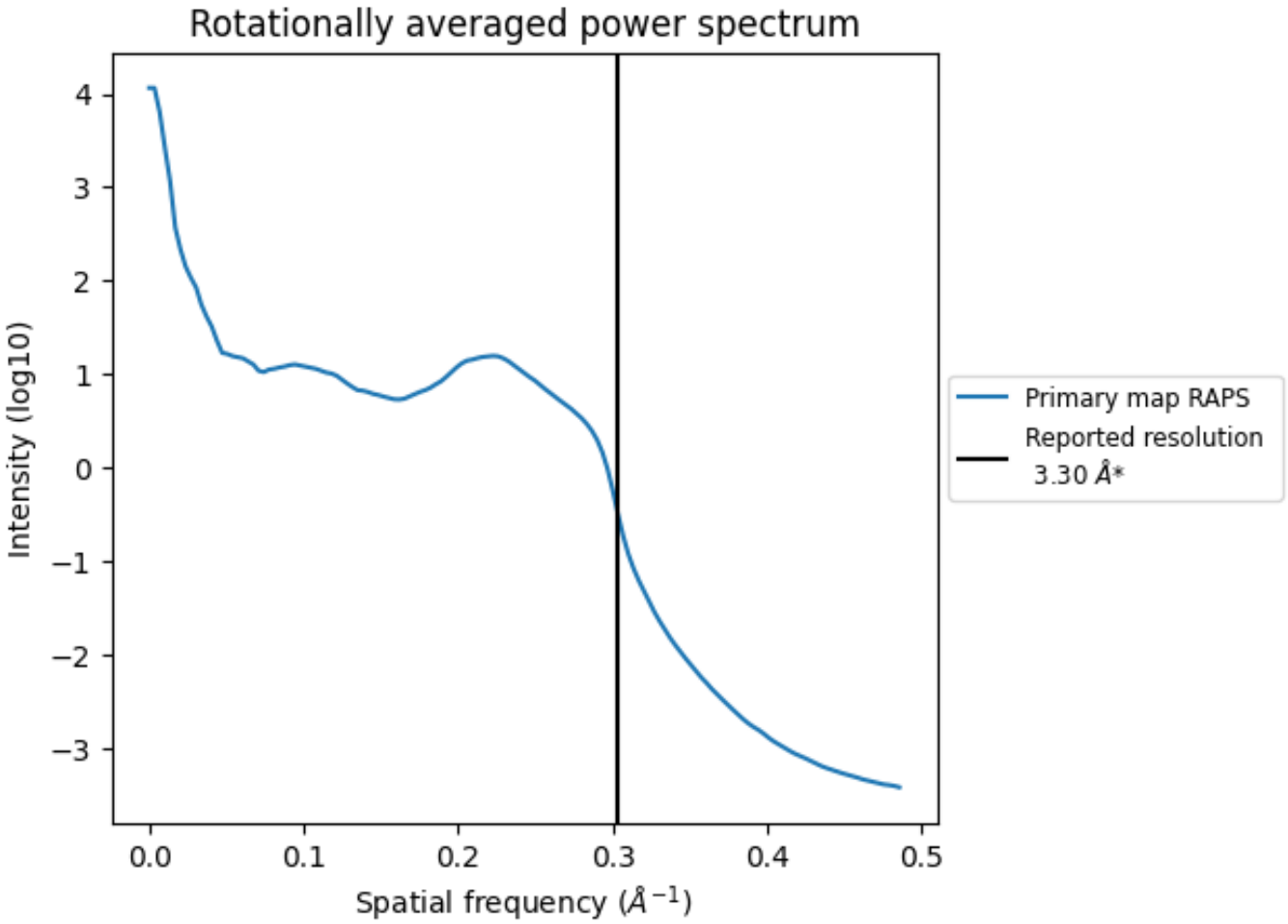
7.2 Volume estimate



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 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)

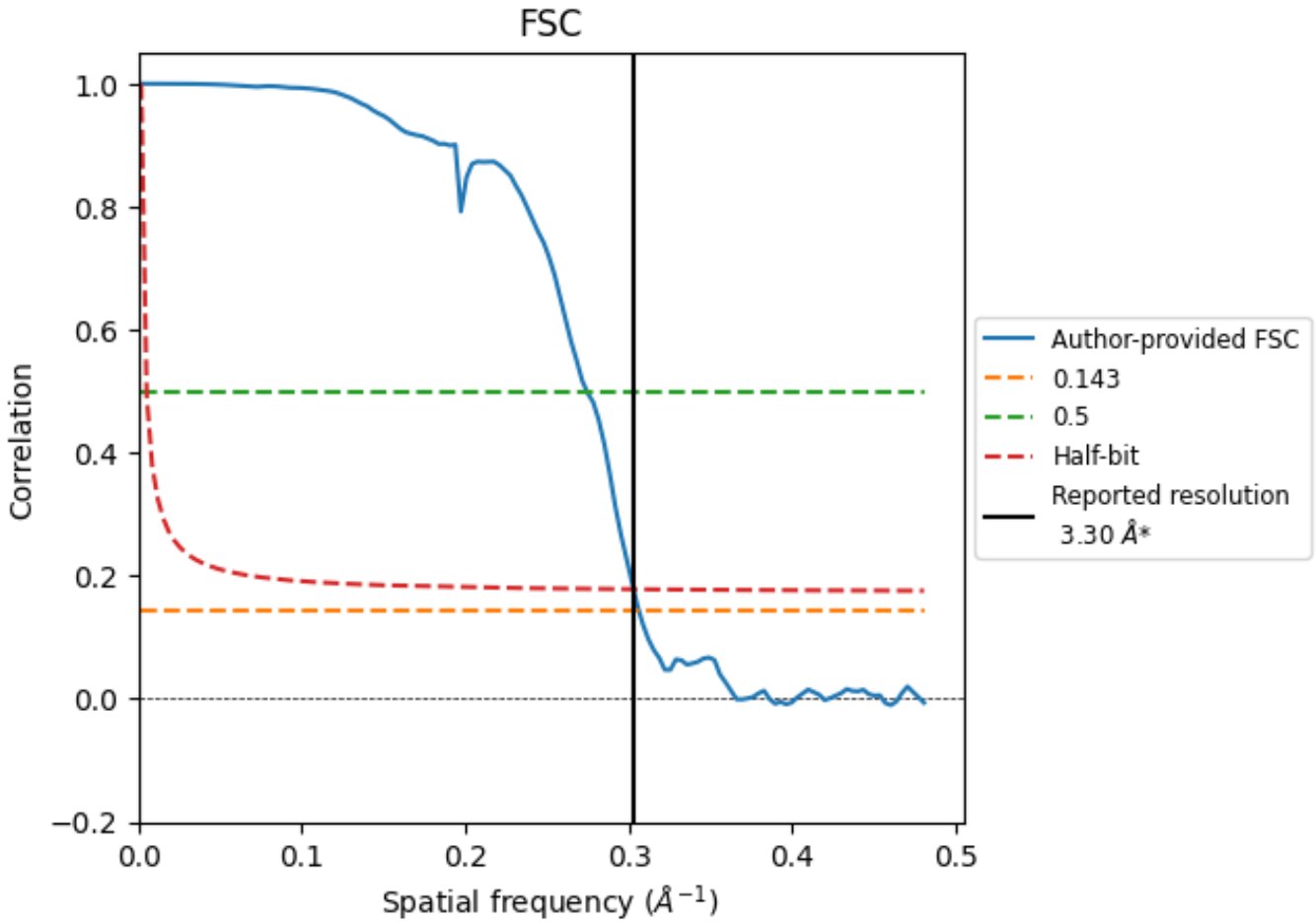


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

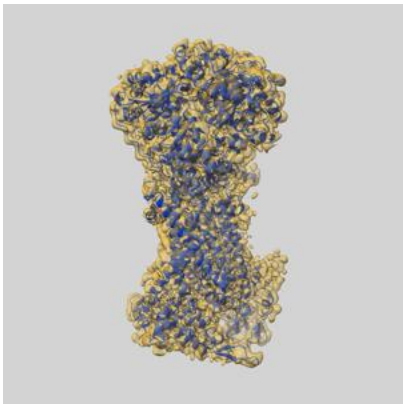
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.65	3.30
Unmasked-calculated*	-	-	-

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

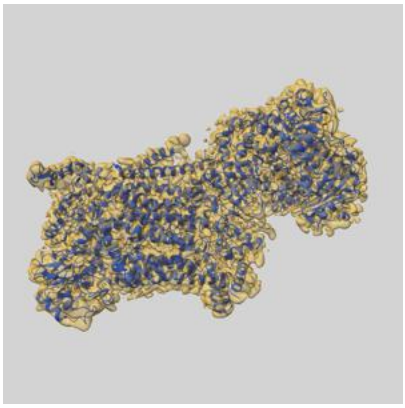
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24484 and PDB model 7RJC. Per-residue inclusion information can be found in section 3 on page 8.

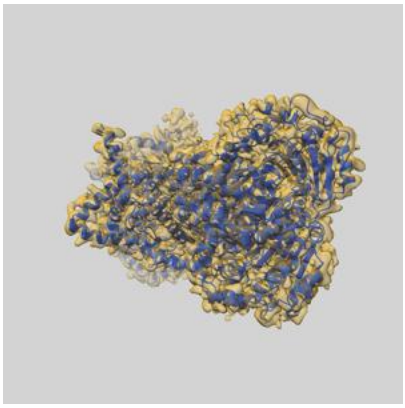
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.63 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.

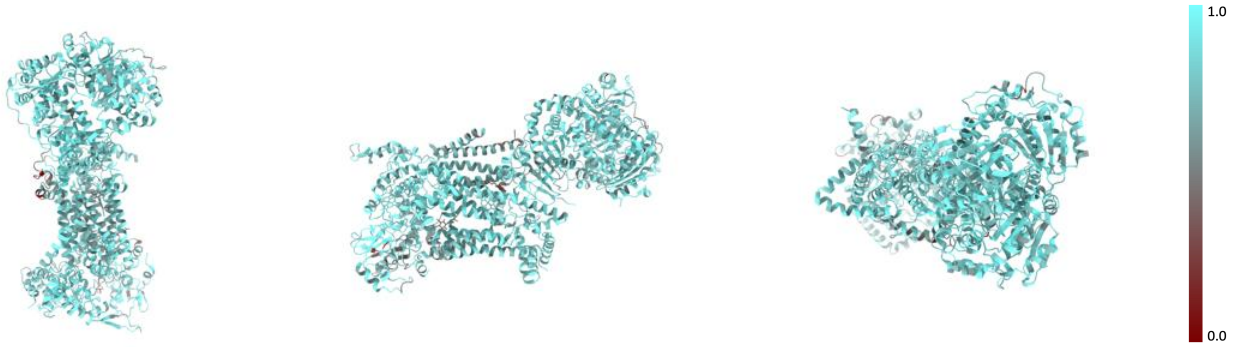
9.2 Q-score mapped to coordinate model (i)



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.

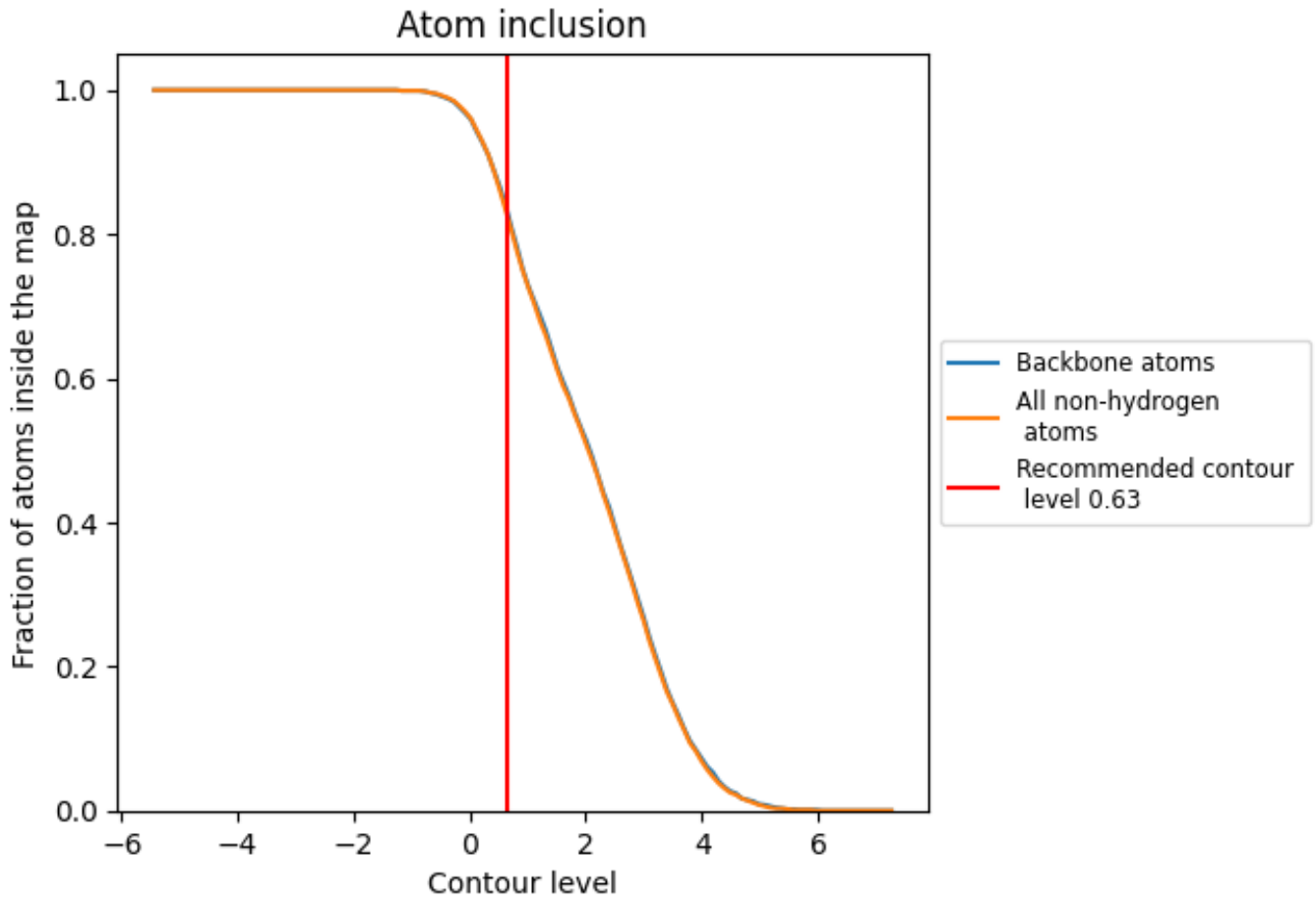
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.63).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4870
A	0.8580	0.5150
B	0.8390	0.4930
D	0.8700	0.5080
E	0.7660	0.3220
F	0.7910	0.4710
G	0.8430	0.4970
H	0.7730	0.4210
I	0.8220	0.4730
K	0.8490	0.5190
M	0.6220	0.2600

