



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:37 AM EDT

PDB ID : 7RJA / pdb_00007rja
EMDB ID : EMD-24482
Title : Complex III2 from Candida albicans, inhibitor free
Authors : Di Trani, J.M.; Rubinstein, J.L.
Deposited on : 2021-07-20
Resolution : 3.00 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:

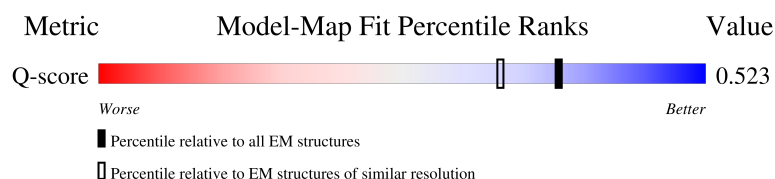
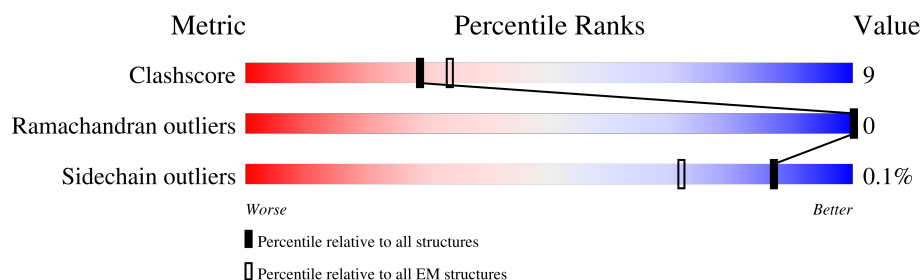
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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 $\leq 5\%$. 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	 82% 13% 5%
1	J	439	 77% 17% 5%
2	K	387	 72% 27% .
2	T	387	 78% 21% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	288	
3	N	288	
4	G	127	
4	Q	127	
5	F	95	
5	P	95	
6	H	135	
6	R	135	
7	I	65	
7	S	65	
8	C	213	
8	M	213	
9	B	374	
9	L	374	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	HEC	D	301	X	-	X	-
12	HEC	N	301	X	-	X	-
13	FES	M	301	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 57732 atoms, of which 28314 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
1	A	416	Total	C	H	N	O	S	0	0
			6364	2012	3166	546	636	4		
1	J	416	Total	C	H	N	O	S	0	0
			6364	2012	3166	546	636	4		

- Molecule 2 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	47	GLU	ASP	conflict	UNP A0A1D8PJT8
R	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			
7	S	39	Total	C	H	N	O		0	0
			639	220	315	54	50			

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

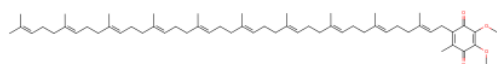
Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		
8	M	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

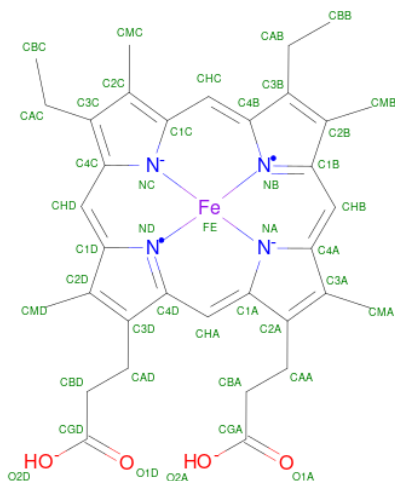
Mol	Chain	Residues	Atoms						AltConf	Trace
9	B	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		
9	L	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		

- # HEM

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

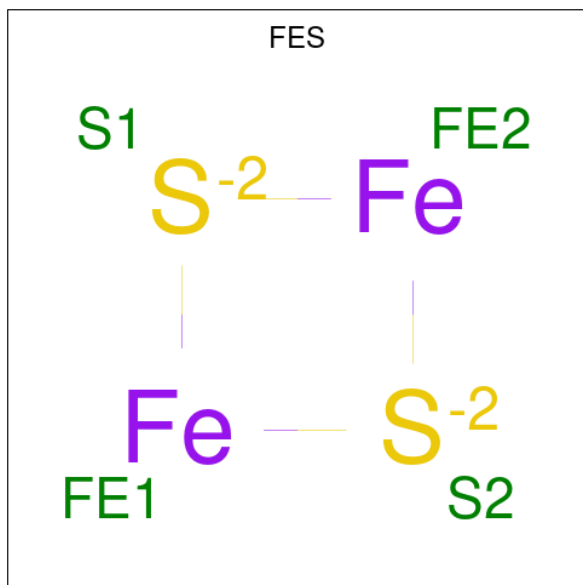


- Molecule 12 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

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

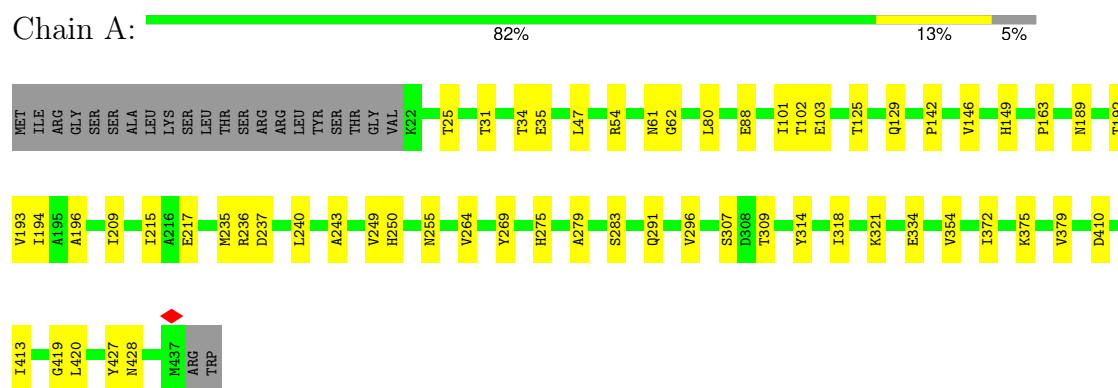


Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	M	1	Total	Fe	S	0
			4	2	2	

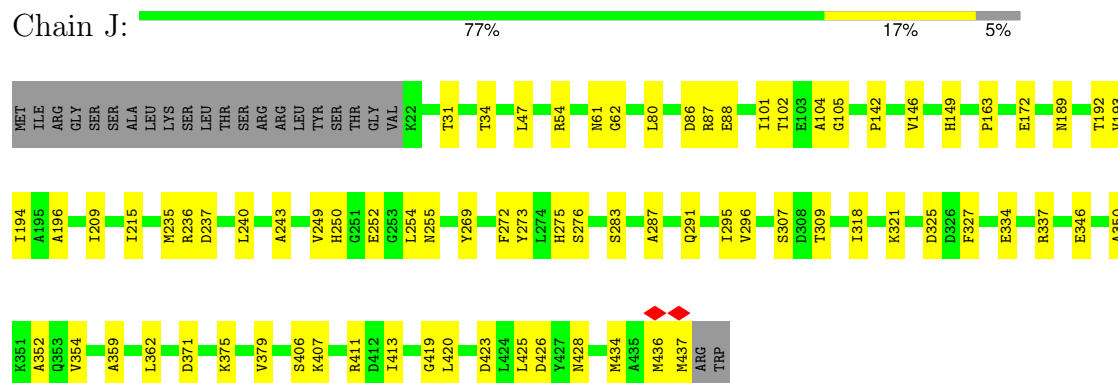
3 Residue-property plots

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.

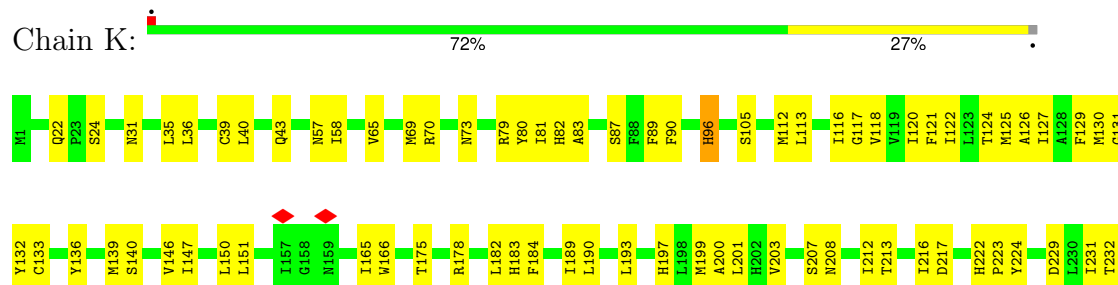
• Molecule 1: Ubiquinol--cytochrome-c reductase subunit

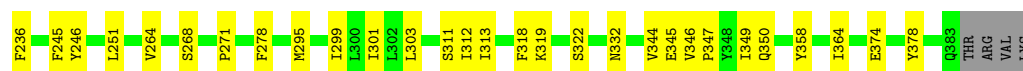


• Molecule 1: Ubiquinol--cytochrome-c reductase subunit



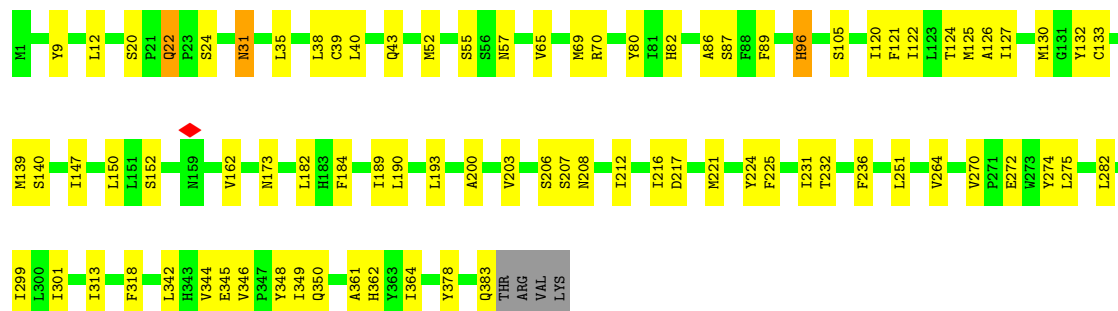
• Molecule 2: Cytochrome b





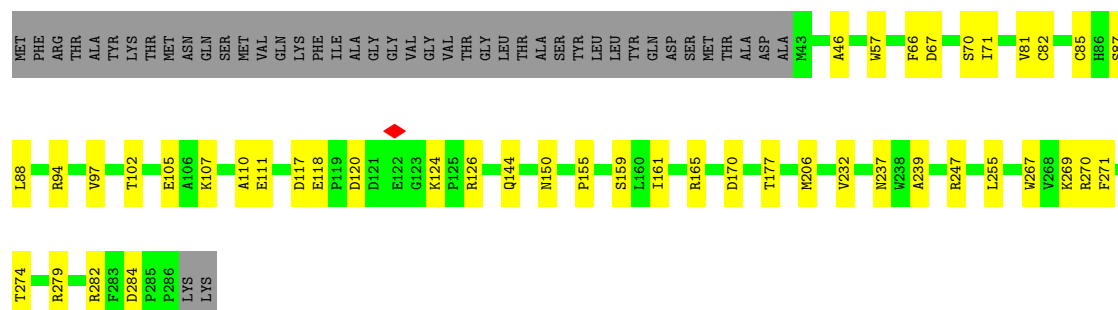
• Molecule 2: Cytochrome b

Chain T: 78% 21% ..



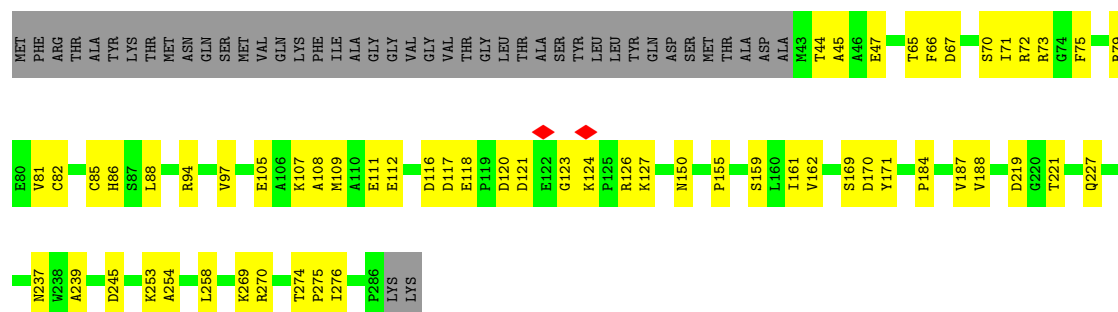
• Molecule 3: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain D: 69% 16% 15%



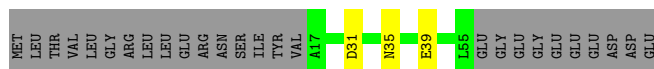
• Molecule 3: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain N: 64% 21% 15%



• Molecule 4: Cytochrome b-c1 complex subunit 7

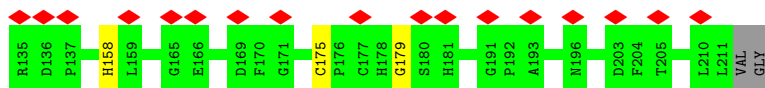
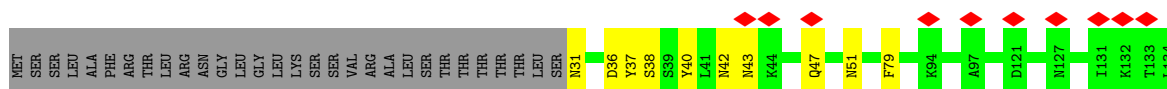
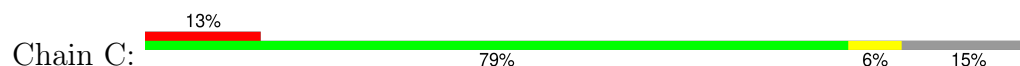
Chain G: 78% 18%



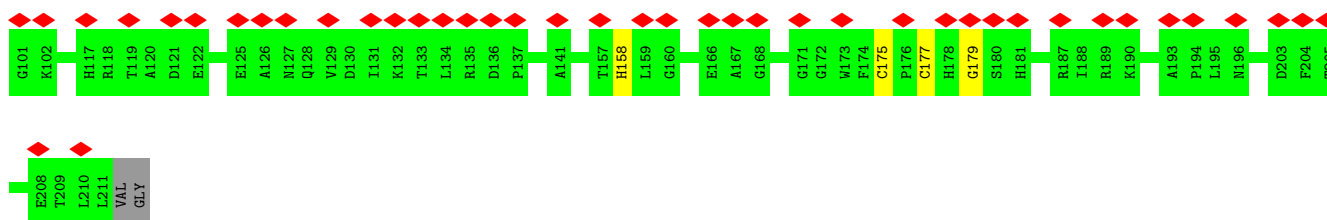
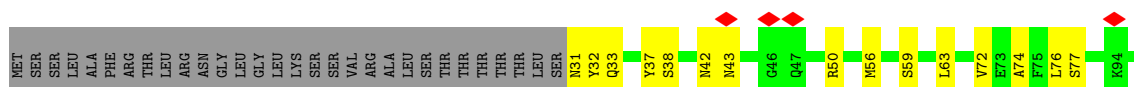
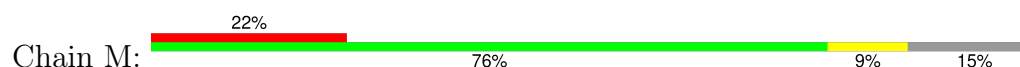
• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 9



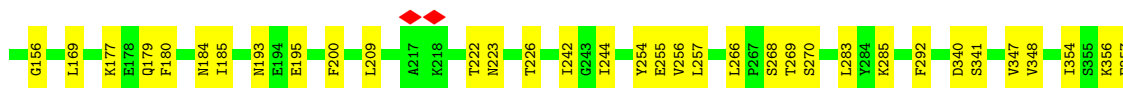
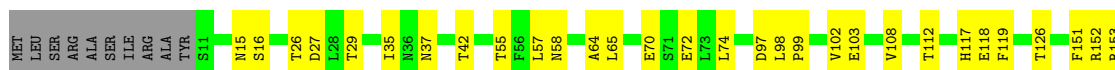
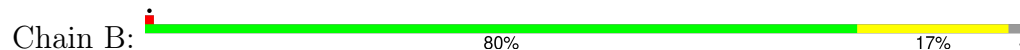
• Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



• Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial



● Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96783	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 ($e^-/\text{\AA}^2$)	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	4.587	Depositor
Minimum map value	-2.941	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.180	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 [i](#)

5.1 Standard geometry [i](#)

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

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
1	J	0.20	0/3254	0.32	0/4409
2	K	0.31	1/3158 (0.0%)	0.39	0/4317
2	T	0.31	2/3158 (0.1%)	0.39	0/4317
3	D	0.20	0/1978	0.31	0/2696
3	N	0.20	0/1978	0.33	0/2696
4	G	0.19	0/994	0.29	0/1346
4	Q	0.19	0/994	0.29	0/1346
5	F	0.31	1/731 (0.1%)	0.33	0/994
5	P	0.19	0/731	0.33	0/994
6	H	0.14	0/621	0.32	0/840
6	R	0.14	0/621	0.27	0/840
7	I	0.16	0/336	0.25	0/451
7	S	0.18	0/336	0.29	0/451
8	C	0.15	0/1051	0.28	0/1441
8	M	0.15	0/1051	0.33	0/1441
9	B	0.20	0/2748	0.33	0/3735
9	L	0.20	0/2748	0.32	0/3735
All	All	0.22	4/29742 (0.0%)	0.33	0/40458

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	30	ILE	C-N	-6.52	1.23	1.33
2	K	96	HIS	CD2-NE2	-6.28	1.30	1.37
2	T	96	HIS	CD2-NE2	-5.98	1.31	1.37
2	T	96	HIS	CB-CG	-5.11	1.43	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	3166	3168	45	0
1	J	3198	3166	3168	53	0
2	K	3056	3090	3090	92	0
2	T	3056	3090	3091	73	0
3	D	1916	1820	1821	49	0
3	N	1916	1820	1821	62	0
4	G	976	1002	1002	26	0
4	Q	976	1002	1002	24	0
5	F	708	691	692	8	0
5	P	708	691	692	7	0
6	H	604	544	543	6	0
6	R	604	544	543	4	0
7	I	324	315	314	2	0
7	S	324	315	314	3	0
8	C	1043	697	706	14	0
8	M	1043	697	706	19	0
9	B	2700	2692	2685	54	0
9	L	2700	2692	2685	60	0
10	K	86	60	60	17	0
10	T	86	60	60	17	0
11	K	51	50	52	9	0
11	T	51	50	54	5	0
12	D	43	30	30	23	0
12	N	43	30	30	28	0
13	C	4	0	0	1	0
13	M	4	0	0	4	0
All	All	29418	28314	28329	542	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 9.

All (542) 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)
8:M:158:HIS:O	13:M:301:FES:S2	1.97	1.21
3:N:82:CYS:CA	12:N:301:HEC:HBB2	1.71	1.11
3:N:82:CYS:HA	12:N:301:HEC:HBB2	1.33	1.06
3:D:82:CYS:CA	12:D:301:HEC:HBB2	1.84	1.02
10:K:401:HEM:HBC2	10:K:401:HEM:HHD	1.42	0.99
8:C:158:HIS:CB	13:C:301:FES:S2	2.51	0.99
1:A:236:ARG:NH2	5:F:22:GLN:OE1	1.96	0.97
10:T:401:HEM:HBC2	10:T:401:HEM:HHD	1.44	0.96
2:K:345:GLU:OE1	5:F:82:TYR:OH	1.84	0.95
3:D:82:CYS:N	12:D:301:HEC:HBB2	1.86	0.91
3:N:150:ASN:OD1	12:N:301:HEC:HBC2	1.70	0.90
3:D:82:CYS:HA	12:D:301:HEC:HBB2	1.53	0.90
9:B:58:ASN:ND2	9:B:118:GLU:OE2	2.05	0.90
8:M:31:ASN:OD1	8:M:32:TYR:N	2.08	0.87
2:T:318:PHE:O	2:T:378:TYR:OH	1.92	0.87
3:N:73:ARG:NH1	3:N:231:ASP:OD2	2.05	0.87
1:J:428:ASN:OD1	2:T:224:TYR:OH	1.92	0.86
2:K:318:PHE:O	2:K:378:TYR:OH	1.93	0.86
1:J:236:ARG:NH2	5:P:22:GLN:OE1	2.09	0.84
3:N:116:ASP:OD2	3:N:127:LYS:NZ	2.14	0.81
4:G:120:LEU:HD12	9:L:65:LEU:HD23	1.62	0.81
3:N:155:PRO:HB3	12:N:301:HEC:C1D	2.11	0.80
3:D:81:VAL:HB	12:D:301:HEC:HBB1	1.65	0.79
2:K:184:PHE:CE1	10:K:401:HEM:HBC1	2.19	0.78
2:T:150:LEU:HD12	2:T:282:LEU:HD21	1.65	0.78
7:I:31:ASP:OD1	7:I:35:ASN:ND2	2.16	0.78
3:N:79:ARG:NH1	3:N:109:MET:SD	2.58	0.77
9:B:15:ASN:ND2	9:B:209:LEU:O	2.18	0.77
3:N:82:CYS:N	12:N:301:HEC:HBB2	1.99	0.77
1:A:428:ASN:OD1	2:K:224:TYR:OH	2.00	0.77
1:A:194:ILE:HG21	1:A:209:ILE:HD13	1.65	0.77
2:K:125:MET:HE2	11:K:403:U10:H102	1.64	0.76
1:J:337:ARG:NH1	1:J:346:GLU:OE2	2.18	0.76
2:T:150:LEU:CD1	2:T:282:LEU:HD21	2.16	0.75
2:K:311:SER:OG	2:K:319:LYS:NZ	2.17	0.75
3:D:282:ARG:NH2	3:D:284:ASP:OD2	2.20	0.75
1:J:287:ALA:O	1:J:291:GLN:NE2	2.19	0.74
3:N:150:ASN:OD1	12:N:301:HEC:CBC	2.35	0.74
2:T:383:GLN:NE2	4:Q:101:ASN:OD1	2.21	0.74
1:J:194:ILE:HG21	1:J:209:ILE:HD13	1.70	0.74
2:T:152:SER:HB2	2:T:162:VAL:HG21	1.70	0.73
1:A:149:HIS:CG	8:M:31:ASN:HD22	2.07	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:ASN:OD1	12:D:301:HEC:HBC2	1.88	0.73
3:N:72:ARG:NH2	3:N:105:GLU:OE1	2.21	0.72
3:N:86:HIS:CD2	12:N:301:HEC:C4B	2.72	0.72
3:N:67:ASP:O	3:N:70:SER:N	2.23	0.71
1:A:413:ILE:O	1:A:427:TYR:OH	2.05	0.71
8:M:59:SER:O	8:M:63:LEU:HD23	1.91	0.70
2:K:295:MET:CE	11:K:403:U10:H103	2.21	0.70
3:N:86:HIS:HD2	12:N:301:HEC:CHC	2.04	0.70
2:T:96:HIS:NE2	10:T:402:HEM:ND	2.39	0.70
3:D:82:CYS:N	12:D:301:HEC:CBB	2.54	0.69
3:D:155:PRO:HB3	12:D:301:HEC:C1D	2.22	0.69
9:B:65:LEU:HD23	4:Q:120:LEU:HD12	1.75	0.69
3:N:82:CYS:N	12:N:301:HEC:CBB	2.55	0.69
3:N:155:PRO:HD3	12:N:301:HEC:HMD3	1.73	0.69
1:A:189:ASN:ND2	1:A:217:GLU:OE1	2.26	0.69
3:D:144:GLN:NE2	3:N:121:ASP:O	2.26	0.69
3:N:219:ASP:OD1	3:N:221:THR:OG1	2.06	0.69
3:D:161:ILE:HG12	12:D:301:HEC:HMA3	1.74	0.68
4:G:56:MET:O	4:G:60:ILE:HD12	1.93	0.68
8:M:177:CYS:CB	13:M:301:FES:S1	2.81	0.68
3:D:57:TRP:NE1	3:D:170:ASP:OD1	2.24	0.68
2:T:31:ASN:N	2:T:31:ASN:HD22	1.92	0.68
3:D:177:THR:O	6:H:70:ARG:NH2	2.28	0.67
1:J:283:SER:OG	9:L:72:GLU:OE1	2.10	0.67
3:N:82:CYS:CA	12:N:301:HEC:CBB	2.63	0.67
1:A:47:LEU:HD12	1:A:194:ILE:HD11	1.76	0.67
3:N:120:ASP:OD1	3:N:124:LYS:N	2.28	0.67
2:K:105:SER:OG	10:K:402:HEM:O2D	2.13	0.67
2:K:312:ILE:HG21	4:G:5:MET:CE	2.25	0.66
2:T:105:SER:OG	10:T:402:HEM:O2D	2.07	0.66
3:N:155:PRO:HB3	12:N:301:HEC:CHD	2.26	0.65
9:B:108:VAL:O	9:B:112:THR:OG1	2.15	0.65
1:J:86:ASP:OD1	1:J:87:ARG:N	2.28	0.65
9:L:255:GLU:OE2	9:L:285:LYS:NZ	2.26	0.65
1:J:54:ARG:NH1	1:J:88:GLU:OE2	2.30	0.64
9:B:340:ASP:OD2	9:B:341:SER:N	2.31	0.64
2:T:231:ILE:HD11	3:N:269:LYS:HB3	1.79	0.64
1:A:410:ASP:OD2	8:M:50:ARG:NE	2.31	0.64
2:K:346:VAL:HG13	5:F:93:VAL:HG11	1.80	0.63
3:D:161:ILE:HG12	12:D:301:HEC:CMA	2.28	0.63
5:P:88:GLU:OE2	5:P:88:GLU:N	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:LEU:HD12	1:J:194:ILE:HD11	1.80	0.63
3:N:86:HIS:CD2	12:N:301:HEC:CHC	2.81	0.63
2:T:22:GLN:OE1	11:T:404:U10:H3M3	1.99	0.63
2:T:35:LEU:HD11	2:T:232:THR:HG22	1.79	0.63
3:N:85:CYS:SG	12:N:301:HEC:CMC	2.86	0.63
1:A:255:ASN:ND2	1:A:307:SER:O	2.31	0.63
8:C:79:PHE:CZ	2:T:52:MET:HE1	2.33	0.63
2:K:312:ILE:HG21	4:G:5:MET:HE1	1.80	0.63
9:B:226:THR:OG1	9:B:356:LYS:O	2.16	0.62
9:B:255:GLU:OE2	9:B:285:LYS:NZ	2.18	0.62
3:D:118:GLU:O	3:D:126:ARG:NH1	2.32	0.62
11:T:403:U10:H4M3	11:T:403:U10:H3M2	1.80	0.62
1:A:54:ARG:NH1	1:A:88:GLU:OE2	2.32	0.62
9:L:15:ASN:O	9:L:16:SER:OG	2.12	0.62
2:T:20:SER:O	2:T:22:GLN:NE2	2.33	0.62
2:K:184:PHE:CD2	2:T:184:PHE:CD2	2.87	0.62
1:J:31:THR:HG23	1:J:193:VAL:HG23	1.82	0.62
1:A:250:HIS:NE2	1:A:309:THR:OG1	2.33	0.61
3:N:86:HIS:CD2	12:N:301:HEC:C1C	2.83	0.61
2:T:89:PHE:HE2	2:T:124:THR:HG21	1.66	0.61
9:L:340:ASP:OD1	9:L:341:SER:N	2.33	0.61
3:D:67:ASP:O	3:D:70:SER:N	2.34	0.61
3:D:155:PRO:HD3	12:D:301:HEC:HMD3	1.83	0.61
4:G:56:MET:HE1	4:G:107:ILE:HD13	1.83	0.60
4:G:61:LYS:NZ	9:L:121:GLU:OE2	2.31	0.60
3:N:118:GLU:O	3:N:126:ARG:NH1	2.35	0.60
2:T:212:ILE:HD12	4:Q:75:ILE:HG23	1.84	0.60
2:T:57:ASN:OD1	2:T:173:ASN:ND2	2.35	0.59
3:N:94:ARG:O	3:N:97:VAL:HG22	2.02	0.59
1:A:321:LYS:HB3	1:A:420:LEU:HD23	1.85	0.59
2:T:24:SER:OG	2:T:217:ASP:OD2	2.13	0.59
6:R:123:ASN:HA	6:R:126:VAL:HG22	1.85	0.58
2:K:146:VAL:O	2:K:150:LEU:HD23	2.03	0.58
6:H:123:ASN:HA	6:H:126:VAL:HG22	1.85	0.58
1:J:321:LYS:HB3	1:J:420:LEU:HD23	1.85	0.58
4:Q:44:LYS:NZ	4:Q:98:GLU:O	2.28	0.58
4:G:6:THR:N	4:G:111:GLU:OE1	2.35	0.58
3:D:102:THR:HG22	3:D:105:GLU:OE1	2.03	0.58
8:C:31:ASN:N	1:J:163:PRO:HG3	2.19	0.58
9:B:15:ASN:O	9:B:16:SER:OG	2.14	0.58
9:L:49:HIS:NE2	9:L:130:GLU:OE1	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:130:MET:HE1	2:K:182:LEU:CB	2.34	0.57
10:K:402:HEM:HHA	10:K:402:HEM:O2A	2.04	0.57
2:T:231:ILE:HD11	3:N:269:LYS:CB	2.33	0.57
2:K:31:ASN:ND2	2:K:229:ASP:OD1	2.37	0.57
3:D:165:ARG:NH2	12:D:301:HEC:O2A	2.30	0.57
8:M:158:HIS:C	13:M:301:FES:S2	2.82	0.57
3:N:171:TYR:OH	12:N:301:HEC:O1A	2.21	0.57
10:T:402:HEM:HHA	10:T:402:HEM:O2A	2.05	0.57
2:K:212:ILE:HD12	4:G:75:ILE:HG23	1.87	0.56
1:J:172:GLU:N	1:J:172:GLU:OE1	2.39	0.56
9:L:226:THR:OG1	9:L:356:LYS:O	2.23	0.56
9:B:74:LEU:HD12	9:B:97:ASP:OD1	2.06	0.56
2:K:112:MET:O	2:K:116:ILE:HD12	2.06	0.56
3:D:155:PRO:HD3	12:D:301:HEC:CMD	2.34	0.56
8:M:158:HIS:CB	13:M:301:FES:S2	2.93	0.56
9:L:354:ILE:O	9:L:354:ILE:HG22	2.05	0.56
6:H:66:LEU:HD13	6:H:130:LEU:CD1	2.36	0.55
1:J:362:LEU:HD21	1:J:371:ASP:OD2	2.06	0.55
3:N:88:LEU:HD23	3:N:88:LEU:O	2.07	0.55
1:J:149:HIS:ND1	1:J:235:MET:SD	2.79	0.55
1:J:296:VAL:HG23	1:J:318:ILE:HG13	1.88	0.55
3:N:161:ILE:HG12	12:N:301:HEC:CMA	2.37	0.55
3:D:271:PHE:O	3:D:274:THR:OG1	2.22	0.55
4:G:44:LYS:NZ	4:G:98:GLU:O	2.31	0.55
4:G:62:ARG:HD2	9:L:117:HIS:HB2	1.88	0.55
1:A:249:VAL:HG12	1:A:413:ILE:HG22	1.89	0.55
9:L:255:GLU:HG2	9:L:283:LEU:HD23	1.90	0.54
9:L:269:THR:O	9:L:270:SER:OG	2.17	0.54
3:D:82:CYS:HA	12:D:301:HEC:HHC	1.89	0.54
2:T:345:GLU:OE1	5:P:78:ASN:ND2	2.35	0.54
3:N:82:CYS:HA	12:N:301:HEC:HHC	1.89	0.54
3:N:117:ASP:OD1	3:N:118:GLU:N	2.40	0.54
1:A:47:LEU:HD12	1:A:194:ILE:CD1	2.37	0.54
9:B:70:GLU:O	9:B:74:LEU:HD23	2.07	0.54
1:J:359:ALA:O	9:L:26:THR:OG1	2.18	0.54
9:B:180:PHE:O	9:B:209:LEU:HD13	2.08	0.54
3:N:155:PRO:HD3	12:N:301:HEC:CMD	2.38	0.54
10:T:402:HEM:HMC1	10:T:402:HEM:HBC2	1.90	0.54
2:T:65:VAL:HG22	10:T:401:HEM:O2D	2.07	0.54
9:L:242:ILE:HG23	9:L:357:PHE:HB2	1.89	0.54
8:C:42:ASN:OD1	8:C:43:ASN:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:264:VAL:HG13	2:T:264:VAL:O	2.09	0.53
1:A:149:HIS:ND1	1:A:235:MET:SD	2.81	0.53
4:G:120:LEU:HD12	9:L:65:LEU:CD2	2.36	0.53
9:L:70:GLU:O	9:L:74:LEU:HD23	2.07	0.53
9:B:55:THR:O	9:B:108:VAL:HG13	2.08	0.53
2:T:125:MET:HE1	2:T:299:ILE:HD11	1.91	0.53
2:K:313:ILE:HD11	4:G:45:PHE:HE1	1.74	0.53
10:T:401:HEM:HBB2	10:T:401:HEM:HMB2	1.89	0.53
3:D:85:CYS:CB	12:D:301:HEC:C4C	2.87	0.53
3:N:161:ILE:HG12	12:N:301:HEC:HMA3	1.90	0.53
3:N:227:GLN:O	3:N:231:ASP:OD1	2.27	0.53
5:F:61:ALA:O	5:F:65:VAL:HG23	2.08	0.53
9:B:117:HIS:HB2	4:Q:62:ARG:HD2	1.91	0.53
1:J:88:GLU:OE1	1:J:307:SER:N	2.39	0.53
3:N:66:PHE:CB	3:N:71:ILE:HD11	2.39	0.53
3:N:120:ASP:OD1	3:N:123:GLY:N	2.41	0.53
2:K:178:ARG:HB2	2:T:52:MET:HE3	1.90	0.53
2:K:264:VAL:HG13	2:K:264:VAL:O	2.08	0.53
2:T:207:SER:OG	2:T:208:ASN:N	2.42	0.53
8:M:74:ALA:O	8:M:77:SER:OG	2.27	0.53
2:K:130:MET:HE1	2:K:182:LEU:HB2	1.91	0.53
5:P:61:ALA:O	5:P:65:VAL:HG23	2.08	0.53
9:B:242:ILE:HG23	9:B:357:PHE:HB2	1.91	0.52
4:Q:56:MET:SD	4:Q:107:ILE:HD11	2.49	0.52
10:K:402:HEM:HMB1	10:K:402:HEM:HBB2	1.90	0.52
8:M:42:ASN:OD1	8:M:43:ASN:N	2.43	0.52
3:D:150:ASN:OD1	12:D:301:HEC:CBC	2.57	0.52
9:B:244:ILE:HD13	9:B:357:PHE:HA	1.92	0.52
1:A:279:ALA:O	1:A:291:GLN:NE2	2.42	0.52
2:T:147:ILE:HD11	11:T:403:U10:C3	2.39	0.52
8:C:47:GLN:OE1	8:C:51:ASN:ND2	2.43	0.52
6:H:84:HIS:O	6:H:88:GLU:OE1	2.28	0.52
1:J:61:ASN:OD1	1:J:62:GLY:N	2.42	0.52
9:B:26:THR:O	9:B:27:ASP:OD1	2.28	0.52
2:K:133:CYS:HA	2:K:140:SER:OG	2.10	0.51
10:K:401:HEM:HBB2	10:K:401:HEM:HMB2	1.90	0.51
3:D:206:MET:SD	12:D:301:HEC:NA	2.83	0.51
10:K:402:HEM:HMC1	10:K:402:HEM:HBC2	1.93	0.51
12:D:301:HEC:HBC2	12:D:301:HEC:HHH	1.92	0.51
9:B:269:THR:O	9:B:270:SER:OG	2.21	0.51
10:T:402:HEM:HMB1	10:T:402:HEM:HBB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:CG2	1:A:193:VAL:HG22	2.40	0.51
2:K:189:ILE:O	2:K:193:LEU:HD23	2.11	0.51
2:K:201:LEU:HD11	10:K:402:HEM:HAA1	1.93	0.51
2:K:207:SER:OG	2:K:208:ASN:N	2.44	0.51
4:G:117:LYS:HA	9:L:65:LEU:HD21	1.92	0.51
2:T:189:ILE:O	2:T:193:LEU:HD23	2.11	0.51
9:B:354:ILE:HG22	9:B:354:ILE:O	2.10	0.50
3:N:86:HIS:HD2	12:N:301:HEC:C1C	2.23	0.50
2:K:58:ILE:HD11	2:K:136:TYR:CZ	2.46	0.50
2:T:70:ARG:NH1	3:N:239:ALA:O	2.38	0.50
6:H:66:LEU:HD13	6:H:130:LEU:HD11	1.93	0.50
9:L:35:ILE:CD1	9:L:185:ILE:HG22	2.40	0.50
9:L:263:THR:HG23	9:L:266:LEU:H	1.77	0.50
2:K:58:ILE:HD11	2:K:136:TYR:OH	2.11	0.50
2:K:147:ILE:HD11	11:K:403:U10:C2	2.41	0.50
1:J:80:LEU:HD22	9:L:266:LEU:HD22	1.93	0.50
2:T:346:VAL:HG13	5:P:93:VAL:HG11	1.94	0.50
9:B:255:GLU:HG2	9:B:283:LEU:HD23	1.93	0.50
9:B:29:THR:HG21	9:B:98:LEU:HD13	1.94	0.50
10:K:401:HEM:HBB2	10:K:401:HEM:CMB	2.41	0.50
3:D:117:ASP:OD1	3:D:118:GLU:N	2.39	0.50
1:J:47:LEU:HD12	1:J:194:ILE:CD1	2.41	0.50
12:N:301:HEC:HBC2	12:N:301:HEC:HHH	1.93	0.50
2:T:89:PHE:CE2	2:T:124:THR:HG21	2.47	0.50
2:T:313:ILE:HD11	4:Q:45:PHE:CE1	2.46	0.50
9:L:180:PHE:O	9:L:209:LEU:HD13	2.11	0.50
9:B:57:LEU:HD23	9:B:118:GLU:HG2	1.93	0.49
2:T:344:VAL:HG23	2:T:344:VAL:O	2.11	0.49
3:D:88:LEU:HD23	3:D:88:LEU:O	2.11	0.49
2:K:332:ASN:HD22	2:K:358:TYR:HD2	1.60	0.49
2:K:344:VAL:O	2:K:344:VAL:HG23	2.13	0.49
1:J:295:ILE:HG22	1:J:327:PHE:HB2	1.94	0.49
3:D:107:LYS:O	3:D:111:GLU:OE1	2.31	0.49
9:L:55:THR:O	9:L:108:VAL:HG13	2.12	0.49
2:T:147:ILE:HD11	11:T:403:U10:C2	2.43	0.49
10:T:401:HEM:HBB2	10:T:401:HEM:CMB	2.41	0.49
3:D:85:CYS:SG	12:D:301:HEC:CMC	2.99	0.49
1:J:249:VAL:HG12	1:J:413:ILE:HG22	1.95	0.49
9:L:338:THR:HG22	9:L:339:VAL:N	2.28	0.49
2:K:295:MET:HE1	11:K:403:U10:H72	1.94	0.49
8:C:31:ASN:OD1	1:J:149:HIS:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:ASP:HB2	1:J:240:LEU:HD13	1.93	0.49
9:B:117:HIS:CB	4:Q:62:ARG:HD2	2.43	0.49
2:K:116:ILE:HD12	2:K:116:ILE:H	1.78	0.48
9:L:37:ASN:OD1	9:L:184:ASN:ND2	2.39	0.48
2:K:73:ASN:ND2	8:M:77:SER:O	2.46	0.48
2:K:216:ILE:HD12	4:G:75:ILE:HG21	1.95	0.48
9:B:119:PHE:HB2	9:B:169:LEU:HD12	1.96	0.48
9:B:254:TYR:HB2	9:B:283:LEU:HD22	1.93	0.48
1:J:406:SER:O	1:J:411:ARG:NH1	2.46	0.48
1:A:163:PRO:HG3	8:M:31:ASN:N	2.28	0.48
2:K:87:SER:HB3	2:K:251:LEU:HD13	1.95	0.48
9:B:151:PHE:O	9:B:156:GLY:HA3	2.13	0.48
9:L:108:VAL:O	9:L:112:THR:OG1	2.31	0.48
2:K:312:ILE:HD13	4:G:5:MET:HE1	1.95	0.48
10:T:402:HEM:HBB2	10:T:402:HEM:CMB	2.44	0.48
1:A:31:THR:HG22	1:A:193:VAL:HG22	1.96	0.48
1:A:192:THR:HG21	1:A:215:ILE:CD1	2.44	0.48
1:A:275:HIS:O	9:B:126:THR:HG23	2.13	0.48
1:A:283:SER:OG	9:B:72:GLU:OE1	2.14	0.48
2:K:57:ASN:OD1	2:T:55:SER:OG	2.27	0.48
9:B:57:LEU:O	9:B:64:ALA:N	2.47	0.48
9:B:65:LEU:HD21	4:Q:117:LYS:HA	1.96	0.48
1:A:125:THR:O	1:A:129:GLN:OE1	2.31	0.48
2:K:120:ILE:HG23	2:K:190:LEU:HD11	1.94	0.48
2:K:199:MET:HE1	2:T:12:LEU:HD22	1.96	0.48
1:J:80:LEU:HD11	9:L:268:SER:HB2	1.96	0.48
3:N:66:PHE:HB3	3:N:71:ILE:HD11	1.95	0.48
1:A:237:ASP:HB2	1:A:240:LEU:HD13	1.94	0.48
10:K:402:HEM:HBB2	10:K:402:HEM:CMB	2.44	0.48
2:T:31:ASN:N	2:T:31:ASN:ND2	2.62	0.48
9:L:150:THR:OG1	9:L:358:ASN:ND2	2.46	0.48
2:K:113:LEU:HD11	2:K:197:HIS:CE1	2.49	0.47
4:G:5:MET:HG3	4:G:107:ILE:HG21	1.95	0.47
8:C:37:TYR:O	8:C:40:TYR:N	2.47	0.47
1:J:436:MET:O	1:J:436:MET:SD	2.72	0.47
2:T:378:TYR:HB3	4:Q:45:PHE:CE1	2.49	0.47
1:A:80:LEU:HD11	9:B:268:SER:HB2	1.96	0.47
9:B:65:LEU:CD2	4:Q:120:LEU:HD12	2.43	0.47
3:N:75:PHE:CE2	3:N:79:ARG:HD2	2.49	0.47
1:A:80:LEU:HD13	9:B:266:LEU:HB3	1.97	0.47
4:G:46:ASN:ND2	4:G:101:ASN:HA	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:HIS:NE2	1:J:309:THR:OG1	2.44	0.47
1:J:273:TYR:O	1:J:276:SER:OG	2.27	0.47
9:B:65:LEU:HD23	9:B:65:LEU:O	2.14	0.47
8:M:175:CYS:O	8:M:179:GLY:N	2.47	0.47
3:D:87:SER:OG	3:D:88:LEU:N	2.48	0.47
9:L:151:PHE:O	9:L:156:GLY:HA3	2.14	0.47
1:A:61:ASN:OD1	1:A:62:GLY:N	2.48	0.47
2:K:39:CYS:CB	2:K:89:PHE:HD1	2.27	0.47
2:K:349:ILE:HG13	2:K:350:GLN:N	2.30	0.47
9:B:222:THR:HG23	9:B:223:ASN:N	2.30	0.47
3:N:184:PRO:O	3:N:187:VAL:HG12	2.15	0.47
7:S:43:LYS:O	7:S:49:ASN:ND2	2.45	0.47
1:A:375:LYS:O	1:A:379:VAL:HG22	2.15	0.47
2:K:246:TYR:CE2	3:D:255:LEU:HD11	2.50	0.47
1:J:255:ASN:OD1	1:J:379:VAL:HG12	2.15	0.47
1:J:243:ALA:HA	1:J:419:GLY:O	2.14	0.47
2:T:139:MET:HE1	2:T:270:VAL:H	1.80	0.47
3:N:85:CYS:HB2	12:N:301:HEC:C2C	2.45	0.47
1:A:243:ALA:HA	1:A:419:GLY:O	2.14	0.47
1:A:296:VAL:HG23	1:A:318:ILE:HG13	1.96	0.47
9:L:21:ALA:HB1	9:L:192:ALA:O	2.15	0.47
5:F:48:ASN:OD1	5:F:51:ARG:NH2	2.45	0.46
9:B:37:ASN:OD1	9:B:184:ASN:ND2	2.43	0.46
1:J:423:ASP:O	1:J:425:LEU:HD22	2.14	0.46
2:K:222:HIS:HB3	2:K:223:PRO:HD3	1.97	0.46
4:G:24:ILE:O	4:G:28:LEU:HD13	2.15	0.46
1:J:269:TYR:OH	1:J:334:GLU:O	2.21	0.46
4:Q:62:ARG:NH2	4:Q:110:ALA:HB2	2.31	0.46
2:K:35:LEU:HD11	2:K:232:THR:HG22	1.96	0.46
3:N:65:THR:HB	3:N:245:ASP:OD2	2.16	0.46
3:N:237:ASN:C	3:N:237:ASN:HD22	2.24	0.46
4:Q:46:ASN:ND2	4:Q:101:ASN:HA	2.31	0.46
2:T:184:PHE:CD1	10:T:401:HEM:CBC	2.99	0.46
6:R:70:ARG:O	6:R:74:THR:HG23	2.14	0.46
1:J:192:THR:HG21	1:J:215:ILE:CD1	2.45	0.46
1:J:34:THR:HG22	1:J:196:ALA:HB3	1.97	0.46
2:K:39:CYS:HB2	2:K:89:PHE:HD1	1.81	0.46
5:F:62:ILE:HB	5:F:63:PRO:HD3	1.97	0.46
9:L:162:ASN:OD1	9:L:163:GLU:N	2.49	0.46
10:T:401:HEM:HBC2	10:T:401:HEM:CHD	2.26	0.46
1:A:269:TYR:OH	1:A:334:GLU:O	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:221:MET:O	2:T:224:TYR:O	2.34	0.46
9:B:35:ILE:CD1	9:B:185:ILE:HG22	2.46	0.46
2:T:184:PHE:HD1	10:T:401:HEM:CBC	2.29	0.46
3:N:276:ILE:HG21	4:Q:83:LEU:HD11	1.98	0.46
9:L:254:TYR:HB2	9:L:283:LEU:HD22	1.97	0.46
2:K:322:SER:HB2	2:K:374:GLU:OE1	2.16	0.45
7:I:35:ASN:O	7:I:39:GLU:OE1	2.34	0.45
8:C:79:PHE:CE2	2:T:52:MET:HE1	2.51	0.45
9:B:102:VAL:HG13	9:B:103:GLU:N	2.31	0.45
3:N:70:SER:OG	3:N:73:ARG:NH2	2.49	0.45
3:N:254:ALA:O	3:N:258:LEU:HD13	2.16	0.45
1:A:101:ILE:HG23	1:A:102:THR:N	2.31	0.45
2:K:166:TRP:O	2:K:175:THR:OG1	2.29	0.45
10:K:401:HEM:HHD	10:K:401:HEM:CBC	2.30	0.45
9:B:37:ASN:O	9:B:42:THR:OG1	2.11	0.45
9:B:153:ARG:HE	9:L:370:TYR:HE1	1.63	0.45
9:L:174:GLN:O	9:L:177:LYS:O	2.34	0.45
2:T:70:ARG:NH2	3:N:159:SER:O	2.49	0.45
8:C:36:ASP:OD1	8:C:36:ASP:O	2.35	0.45
4:Q:51:GLU:HA	4:Q:56:MET:HG2	1.97	0.45
9:L:35:ILE:O	9:L:86:ALA:HB1	2.17	0.45
8:C:79:PHE:CE1	2:T:52:MET:HE1	2.52	0.45
2:T:69:MET:HE1	2:T:80:TYR:CZ	2.52	0.45
2:K:245:PHE:O	3:D:247:ARG:NH1	2.43	0.45
4:G:47:ASP:OD1	4:G:74:ARG:NH1	2.48	0.45
1:A:410:ASP:CG	8:M:50:ARG:HE	2.25	0.45
2:K:200:ALA:HB2	2:T:9:TYR:OH	2.17	0.45
4:G:62:ARG:HD2	9:L:117:HIS:CB	2.46	0.45
9:B:57:LEU:O	9:B:64:ALA:CA	2.64	0.45
1:J:101:ILE:HG23	1:J:102:THR:N	2.31	0.45
3:N:108:ALA:O	3:N:112:GLU:OE1	2.34	0.45
3:N:270:ARG:O	3:N:274:THR:HG23	2.16	0.45
4:Q:56:MET:HE1	4:Q:107:ILE:CD1	2.47	0.45
9:L:17:VAL:O	9:L:19:ILE:HD12	2.17	0.45
9:L:102:VAL:HG13	9:L:103:GLU:N	2.31	0.45
2:K:217:ASP:OD2	3:D:279:ARG:NH2	2.40	0.45
1:J:275:HIS:O	9:L:126:THR:HG23	2.16	0.45
4:Q:24:ILE:O	4:Q:28:LEU:HD13	2.17	0.45
8:M:33:GLN:O	8:M:33:GLN:HG2	2.17	0.45
8:C:31:ASN:ND2	1:J:149:HIS:CE1	2.85	0.44
10:T:402:HEM:HBC2	10:T:402:HEM:CMC	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:125:MET:HE1	2:K:278:PHE:CD2	2.53	0.44
3:D:66:PHE:CB	3:D:71:ILE:HD11	2.47	0.44
6:R:114:GLU:OE1	6:R:114:GLU:N	2.46	0.44
2:T:132:TYR:CE2	2:T:272:GLU:OE2	2.71	0.44
3:N:44:THR:HB	3:N:47:GLU:OE1	2.17	0.44
5:P:62:ILE:HB	5:P:63:PRO:HD3	1.98	0.44
2:K:70:ARG:NH2	3:D:159:SER:O	2.50	0.44
2:K:184:PHE:CD2	2:T:184:PHE:CE2	3.05	0.44
2:T:40:LEU:HD12	10:T:401:HEM:HBB1	2.00	0.44
2:T:216:ILE:HD12	4:Q:75:ILE:HG21	1.99	0.44
1:A:237:ASP:CB	1:A:240:LEU:HD13	2.48	0.44
3:D:161:ILE:CG1	12:D:301:HEC:HMA3	2.45	0.44
4:Q:56:MET:O	4:Q:60:ILE:HG12	2.18	0.44
1:J:254:LEU:HB3	1:J:379:VAL:HG11	2.00	0.44
12:D:301:HEC:CBB	12:D:301:HEC:HHC	2.48	0.44
12:D:301:HEC:HBD1	12:D:301:HEC:HHA	1.99	0.44
9:B:169:LEU:HD23	9:B:169:LEU:C	2.43	0.44
4:Q:47:ASP:OD1	4:Q:74:ARG:NH1	2.51	0.44
1:A:34:THR:HG22	1:A:196:ALA:HB3	2.00	0.44
3:D:120:ASP:OD1	3:D:124:LYS:N	2.50	0.44
8:M:72:VAL:O	8:M:76:LEU:HD23	2.17	0.44
2:K:231:ILE:HD11	3:D:269:LYS:CB	2.47	0.43
1:A:102:THR:HG23	1:A:103:GLU:OE1	2.18	0.43
2:K:126:ALA:O	2:K:127:ILE:C	2.60	0.43
9:L:37:ASN:O	9:L:42:THR:OG1	2.14	0.43
9:L:109:VAL:CG2	9:L:209:LEU:HD11	2.47	0.43
9:L:332:SER:O	9:L:336:GLN:HG3	2.18	0.43
1:A:25:THR:HG23	1:A:25:THR:O	2.18	0.43
2:K:130:MET:HE1	2:K:182:LEU:HB3	2.00	0.43
1:J:375:LYS:O	1:J:379:VAL:HG22	2.18	0.43
1:J:426:ASP:OD2	2:T:224:TYR:CE2	2.71	0.43
12:N:301:HEC:CBB	12:N:301:HEC:HHC	2.48	0.43
2:K:36:LEU:CD1	2:K:96:HIS:CD2	3.01	0.43
4:Q:56:MET:HE1	4:Q:107:ILE:HD13	2.00	0.43
2:K:213:THR:HG21	4:G:51:GLU:OE1	2.19	0.43
2:T:130:MET:HE1	2:T:182:LEU:HB3	2.01	0.43
3:N:81:VAL:HB	12:N:301:HEC:HBB1	2.00	0.43
2:K:295:MET:SD	11:K:403:U10:H1M2	2.59	0.43
10:K:401:HEM:HBA2	10:K:401:HEM:HHA	1.99	0.43
3:D:237:ASN:C	3:D:237:ASN:HD22	2.23	0.43
3:N:107:LYS:O	3:N:111:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:28:GLY:O	7:S:32:VAL:HG22	2.18	0.43
1:A:142:PRO:O	1:A:146:VAL:HG23	2.18	0.43
2:K:122:ILE:HG12	2:K:299:ILE:HG21	2.01	0.43
2:K:200:ALA:O	2:K:203:VAL:HG12	2.19	0.43
9:B:193:ASN:OD1	9:B:195:GLU:N	2.46	0.43
2:T:274:TYR:CD1	2:T:275:LEU:HG	2.53	0.43
2:K:40:LEU:HD12	10:K:401:HEM:HBB1	2.00	0.43
9:B:35:ILE:HD12	9:B:185:ILE:HG22	2.01	0.43
3:N:162:VAL:HG21	3:N:237:ASN:HA	2.01	0.43
9:L:109:VAL:HG21	9:L:209:LEU:HD11	2.00	0.43
1:A:88:GLU:OE1	1:A:307:SER:N	2.43	0.43
2:K:65:VAL:HG22	10:K:401:HEM:O2D	2.19	0.43
8:C:37:TYR:HD1	8:C:40:TYR:HD2	1.66	0.43
9:B:347:VAL:HG23	9:B:347:VAL:O	2.19	0.43
3:N:85:CYS:CB	12:N:301:HEC:C4C	2.95	0.43
9:B:102:VAL:HG11	9:B:200:PHE:HB3	1.99	0.43
5:F:88:GLU:H	5:F:88:GLU:CD	2.26	0.42
2:T:133:CYS:HA	2:T:140:SER:OG	2.18	0.42
9:L:98:LEU:N	9:L:99:PRO:HD2	2.34	0.42
3:D:66:PHE:HB3	3:D:71:ILE:HD11	2.01	0.42
2:T:87:SER:HB3	2:T:251:LEU:HD13	2.01	0.42
2:T:152:SER:CB	2:T:162:VAL:HG21	2.44	0.42
2:T:224:TYR:O	2:T:225:PHE:HB2	2.20	0.42
5:P:70:ILE:O	5:P:73:ARG:HG2	2.19	0.42
9:L:177:LYS:C	9:L:179:GLN:H	2.27	0.42
9:L:193:ASN:OD1	9:L:195:GLU:N	2.50	0.42
1:A:189:ASN:N	1:A:189:ASN:OD1	2.51	0.42
2:K:69:MET:HE1	2:K:80:TYR:CZ	2.54	0.42
3:N:82:CYS:N	12:N:301:HEC:HBB1	2.35	0.42
9:L:88:ILE:HG21	9:L:340:ASP:HB2	2.01	0.42
8:C:37:TYR:O	8:C:38:SER:C	2.62	0.42
9:B:256:VAL:HG21	9:B:348:VAL:O	2.19	0.42
1:J:142:PRO:O	1:J:146:VAL:HG23	2.19	0.42
9:B:57:LEU:O	9:B:64:ALA:HB2	2.20	0.42
9:L:53:LYS:O	9:L:57:LEU:HD13	2.20	0.42
9:L:102:VAL:HG11	9:L:200:PHE:HB3	2.00	0.42
2:K:70:ARG:NH1	3:D:239:ALA:O	2.50	0.42
2:K:125:MET:O	2:K:126:ALA:C	2.63	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	2.02	0.42
3:D:282:ARG:CZ	8:M:32:TYR:CZ	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:401:HEM:HHO	10:T:401:HEM:CBC	2.29	0.42
3:N:44:THR:HG22	3:N:45:ALA:N	2.35	0.42
3:N:188:VAL:HG13	3:N:188:VAL:O	2.20	0.42
9:L:35:ILE:HD13	9:L:185:ILE:HG22	2.00	0.42
2:K:90:PHE:CZ	2:K:124:THR:HG22	2.55	0.42
9:B:370:TYR:HE2	9:L:153:ARG:HE	1.67	0.42
2:T:39:CYS:SG	2:T:236:PHE:CZ	3.13	0.42
2:T:43:GLN:NE2	2:T:82:HIS:O	2.53	0.42
6:R:110:ASP:OD2	6:R:112:ILE:HD12	2.20	0.42
1:A:427:TYR:CE2	5:F:31:SER:HB2	2.54	0.42
1:J:252:GLU:OE1	1:J:407:LYS:NZ	2.39	0.42
1:J:325:ASP:CG	1:J:425:LEU:HD23	2.45	0.42
9:L:222:THR:HG23	9:L:223:ASN:N	2.33	0.42
3:D:107:LYS:O	3:D:110:ALA:HB3	2.19	0.42
1:J:272:PHE:CZ	1:J:291:GLN:OE1	2.73	0.42
2:T:24:SER:O	4:Q:83:LEU:HD12	2.19	0.42
2:T:301:ILE:HD11	2:T:364:ILE:HG23	2.02	0.42
2:K:184:PHE:CE1	10:K:401:HEM:CBC	2.98	0.42
3:D:46:ALA:HB2	6:H:112:ILE:HG21	2.02	0.42
9:B:74:LEU:HB3	9:B:97:ASP:OD2	2.20	0.42
1:J:423:ASP:O	1:J:423:ASP:OD1	2.37	0.42
9:L:58:ASN:ND2	9:L:113:GLN:OE1	2.53	0.42
2:T:126:ALA:O	2:T:127:ILE:C	2.62	0.41
2:T:120:ILE:HG23	2:T:190:LEU:HD11	2.01	0.41
2:K:22:GLN:OE1	11:K:404:U10:H4M2	2.20	0.41
2:K:120:ILE:O	2:K:121:PHE:C	2.62	0.41
2:K:212:ILE:HG22	4:G:47:ASP:O	2.20	0.41
2:K:313:ILE:HD11	4:G:45:PHE:CE1	2.53	0.41
2:T:206:SER:HB3	11:T:404:U10:H3M1	2.02	0.41
2:T:349:ILE:HG13	2:T:350:GLN:N	2.35	0.41
3:N:274:THR:OG1	3:N:275:PRO:HD3	2.20	0.41
2:K:24:SER:O	4:G:83:LEU:HD12	2.20	0.41
2:K:81:ILE:O	2:K:83:ALA:N	2.52	0.41
2:K:116:ILE:O	2:K:117:GLY:C	2.62	0.41
2:K:165:ILE:O	2:K:178:ARG:HD2	2.20	0.41
10:K:402:HEM:HBC2	10:K:402:HEM:CMC	2.49	0.41
3:N:253:LYS:HG3	7:S:34:VAL:HG11	2.02	0.41
9:L:244:ILE:HD13	9:L:357:PHE:HA	2.01	0.41
2:T:86:ALA:HB3	10:T:401:HEM:HMA3	2.03	0.41
1:A:314:TYR:CD1	1:A:314:TYR:C	2.99	0.41
2:K:147:ILE:HD11	11:K:403:U10:C3	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:301:ILE:HD11	2:K:364:ILE:HG23	2.01	0.41
3:D:232:VAL:HG11	12:D:301:HEC:HMB1	2.00	0.41
9:L:57:LEU:O	9:L:64:ALA:CA	2.68	0.41
1:A:80:LEU:HD22	9:B:266:LEU:HD22	2.03	0.41
3:D:155:PRO:HB3	12:D:301:HEC:C2D	2.50	0.41
1:J:189:ASN:N	1:J:189:ASN:OD1	2.54	0.41
1:J:352:ALA:HB1	9:L:75:GLY:HA3	2.02	0.41
8:M:37:TYR:O	8:M:38:SER:C	2.63	0.41
9:L:35:ILE:HD12	9:L:185:ILE:HG22	2.02	0.41
2:K:81:ILE:O	2:K:82:HIS:C	2.62	0.41
3:D:94:ARG:O	3:D:97:VAL:HG22	2.19	0.41
4:G:51:GLU:HA	4:G:56:MET:HG2	2.01	0.41
9:B:152:ARG:NH1	9:L:372:ASP:OD2	2.52	0.41
4:Q:62:ARG:HH21	4:Q:110:ALA:HB2	1.85	0.41
9:L:116:PRO:HA	9:L:169:LEU:HD22	2.02	0.41
2:K:139:MET:HE1	2:K:268:SER:O	2.21	0.41
4:G:62:ARG:HH21	4:G:110:ALA:HB2	1.86	0.41
9:B:177:LYS:C	9:B:179:GLN:H	2.29	0.41
1:J:434:MET:HE3	1:J:434:MET:HB3	2.00	0.41
2:T:39:CYS:CB	2:T:89:PHE:HD1	2.33	0.41
2:T:121:PHE:O	2:T:122:ILE:C	2.62	0.41
2:T:200:ALA:O	2:T:203:VAL:HG12	2.21	0.41
2:T:342:LEU:HD23	2:T:348:TYR:CE2	2.55	0.41
2:T:361:ALA:O	2:T:362:HIS:C	2.63	0.41
2:K:118:VAL:HG21	2:K:303:LEU:HD23	2.03	0.41
2:K:231:ILE:HD11	3:D:269:LYS:HB3	2.02	0.41
3:D:270:ARG:O	3:D:274:THR:HG23	2.21	0.41
9:B:98:LEU:N	9:B:99:PRO:HD2	2.36	0.41
12:N:301:HEC:HBD1	12:N:301:HEC:HHA	2.02	0.41
2:K:39:CYS:SG	2:K:236:PHE:CZ	3.13	0.40
2:K:147:ILE:O	2:K:151:LEU:HD13	2.21	0.40
8:C:175:CYS:O	8:C:179:GLY:N	2.54	0.40
9:B:257:LEU:HD22	9:B:292:PHE:CZ	2.55	0.40
1:J:350:ALA:O	1:J:354:VAL:HG23	2.21	0.40
1:J:436:MET:O	1:J:437:MET:C	2.64	0.40
9:L:273:LEU:HD11	9:L:310:ALA:HB1	2.03	0.40
2:K:346:VAL:HB	2:K:347:PRO:HD3	2.03	0.40
1:J:104:ALA:O	1:J:105:GLY:C	2.64	0.40
2:T:38:LEU:C	2:T:38:LEU:HD23	2.46	0.40
3:N:169:SER:O	3:N:170:ASP:C	2.65	0.40
4:Q:46:ASN:ND2	4:Q:103:LEU:H	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:HB2	1:A:372:ILE:HD11	2.03	0.40
1:A:264:VAL:HA	1:A:354:VAL:HG21	2.03	0.40
2:K:69:MET:SD	2:K:79:ARG:HD3	2.61	0.40
2:K:129:PHE:CD1	11:K:403:U10:H4M2	2.57	0.40
2:K:271:PRO:HB3	11:K:403:U10:O4	2.22	0.40
9:L:257:LEU:HD22	9:L:292:PHE:CZ	2.56	0.40
2:K:43:GLN:NE2	2:K:82:HIS:O	2.54	0.40
3:D:267:TRP:CG	8:M:56:MET:HE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/439 (94%)	399 (96%)	15 (4%)	0	100	100
1	J	414/439 (94%)	398 (96%)	16 (4%)	0	100	100
2	K	381/387 (98%)	357 (94%)	24 (6%)	0	100	100
2	T	381/387 (98%)	363 (95%)	18 (5%)	0	100	100
3	D	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
3	N	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
4	G	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
4	Q	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
5	F	83/95 (87%)	78 (94%)	5 (6%)	0	100	100
5	P	83/95 (87%)	79 (95%)	4 (5%)	0	100	100
6	H	70/135 (52%)	69 (99%)	1 (1%)	0	100	100
6	R	70/135 (52%)	69 (99%)	1 (1%)	0	100	100
7	I	37/65 (57%)	36 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S	37/65 (57%)	37 (100%)	0	0	100	100
8	C	179/213 (84%)	170 (95%)	9 (5%)	0	100	100
8	M	179/213 (84%)	171 (96%)	8 (4%)	0	100	100
9	B	362/374 (97%)	347 (96%)	15 (4%)	0	100	100
9	L	362/374 (97%)	345 (95%)	17 (5%)	0	100	100
All	All	3776/4246 (89%)	3622 (96%)	154 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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
1	J	345/365 (94%)	345 (100%)	0	100	100
2	K	333/338 (98%)	333 (100%)	0	100	100
2	T	333/338 (98%)	331 (99%)	2 (1%)	78	88
3	D	196/237 (83%)	196 (100%)	0	100	100
3	N	196/237 (83%)	196 (100%)	0	100	100
4	G	106/110 (96%)	106 (100%)	0	100	100
4	Q	106/110 (96%)	106 (100%)	0	100	100
5	F	71/80 (89%)	71 (100%)	0	100	100
5	P	71/80 (89%)	71 (100%)	0	100	100
6	H	67/128 (52%)	67 (100%)	0	100	100
6	R	67/128 (52%)	67 (100%)	0	100	100
7	I	30/53 (57%)	30 (100%)	0	100	100
7	S	30/53 (57%)	30 (100%)	0	100	100
8	C	48/176 (27%)	48 (100%)	0	100	100
8	M	48/176 (27%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B	295/307 (96%)	295 (100%)	0	100	100
9	L	295/307 (96%)	295 (100%)	0	100	100
All	All	2982/3588 (83%)	2980 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	22	GLN
2	T	31	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	383	GLN
1	A	430	ASN
2	K	177	GLN
2	K	353	GLN
3	D	51	HIS
5	F	55	ASN
6	H	84	HIS
7	I	35	ASN
1	J	57	HIS
1	J	100	ASN
1	J	127	HIS
1	J	191	ASN
1	J	383	GLN
1	J	398	ASN
1	J	430	ASN
2	T	22	GLN
2	T	27	ASN
2	T	31	ASN
2	T	173	ASN
2	T	215	ASN
2	T	222	HIS
3	N	59	HIS
3	N	237	ASN
6	R	87	HIS
6	R	104	HIS
8	M	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	L	15	ASN
9	L	58	ASN
9	L	179	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	FES	M	301	8	0,4,4	-	-	-		
10	HEM	T	402	2	50,50,50	1.34	5 (10%)	67,82,82	1.27	7 (10%)
11	U10	T	404	-	23,23,63	2.73	9 (39%)	30,31,79	1.34	4 (13%)
12	HEC	N	301	3	50,50,50	1.54	6 (12%)	68,82,82	1.36	10 (14%)
13	FES	C	301	8	0,4,4	-	-	-		
11	U10	T	403	-	28,28,63	2.80	11 (39%)	36,37,79	1.31	6 (16%)
10	HEM	K	401	2	50,50,50	1.33	8 (16%)	67,82,82	1.08	1 (1%)
10	HEM	T	401	2	50,50,50	1.32	7 (14%)	67,82,82	1.01	0
10	HEM	K	402	2	50,50,50	1.35	6 (12%)	67,82,82	1.25	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	U10	K	403	-	28,28,63	2.82	10 (35%)	36,37,79	1.44	7 (19%)
12	HEC	D	301	3	50,50,50	1.54	6 (12%)	68,82,82	1.35	10 (14%)
11	U10	K	404	2	23,23,63	2.74	9 (39%)	30,31,79	1.51	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FES	M	301	8	-	-	0/1/1/1
10	HEM	T	402	2	-	2/14/54/54	-
12	HEC	N	301	3	1/1/7/7	6/14/54/54	-
11	U10	T	404	-	-	3/15/39/87	0/1/1/1
13	FES	C	301	8	-	-	0/1/1/1
11	U10	T	403	-	-	3/21/45/87	0/1/1/1
10	HEM	K	401	2	-	6/14/54/54	-
10	HEM	T	401	2	-	6/14/54/54	-
10	HEM	K	402	2	-	2/14/54/54	-
11	U10	K	403	-	-	3/21/45/87	0/1/1/1
12	HEC	D	301	3	1/1/7/7	6/14/54/54	-
11	U10	K	404	2	-	2/15/39/87	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	404	U10	C8-C9	6.50	1.48	1.33
11	T	403	U10	C13-C14	6.44	1.47	1.33
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	T	403	U10	C8-C9	6.37	1.47	1.33
11	K	404	U10	C8-C9	6.27	1.47	1.33
11	T	403	U10	O4-C4	-5.74	1.23	1.36
11	K	403	U10	O3-C3	-5.72	1.23	1.36
11	K	403	U10	O4-C4	-5.64	1.23	1.36
11	T	403	U10	O3-C3	-5.55	1.23	1.36
11	K	404	U10	O3-C3	-5.49	1.23	1.36
11	K	404	U10	O4-C4	-5.45	1.23	1.36
11	T	404	U10	O3-C3	-5.41	1.23	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	404	U10	O4-C4	-5.30	1.24	1.36
11	K	404	U10	C13-C14	5.16	1.47	1.32
11	T	404	U10	C13-C14	5.13	1.47	1.32
11	T	403	U10	C18-C19	5.03	1.47	1.32
11	K	403	U10	C18-C19	4.99	1.47	1.32
12	N	301	HEC	CBB-CAB	-4.22	1.33	1.51
12	D	301	HEC	CBB-CAB	-4.16	1.33	1.51
12	D	301	HEC	CBC-CAC	-4.09	1.34	1.51
12	N	301	HEC	CBC-CAC	-4.06	1.34	1.51
10	T	402	HEM	FE-NA	3.73	2.07	1.95
10	K	402	HEM	FE-NA	3.63	2.07	1.95
12	D	301	HEC	FE-NB	3.53	2.05	1.94
10	T	402	HEM	FE-NC	3.50	2.06	1.95
11	K	403	U10	C4-C5	-3.49	1.38	1.48
10	K	402	HEM	FE-NC	3.47	2.06	1.95
12	N	301	HEC	FE-NB	3.43	2.05	1.94
11	T	403	U10	C4-C5	-3.36	1.39	1.48
11	T	403	U10	C3-C2	-3.32	1.39	1.48
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	T	404	U10	C4-C5	-3.28	1.39	1.48
11	K	403	U10	C3-C2	-3.27	1.39	1.48
12	N	301	HEC	FE-NC	3.22	2.05	1.95
11	K	404	U10	C3-C2	-3.21	1.39	1.48
11	T	404	U10	C3-C2	-3.19	1.39	1.48
12	D	301	HEC	FE-NC	3.18	2.05	1.95
12	D	301	HEC	FE-ND	2.99	2.04	1.94
11	K	403	U10	C6-C5	-2.83	1.38	1.46
10	T	402	HEM	CAC-C3C	2.82	1.54	1.47
12	N	301	HEC	FE-ND	2.82	2.03	1.94
10	K	402	HEM	CAC-C3C	2.81	1.54	1.47
10	T	401	HEM	CAB-C3B	2.79	1.54	1.47
10	T	402	HEM	CAB-C3B	2.78	1.54	1.47
10	K	402	HEM	CAB-C3B	2.77	1.54	1.47
10	K	401	HEM	CAB-C3B	2.75	1.54	1.47
10	T	401	HEM	FE-ND	2.72	2.03	1.94
12	N	301	HEC	FE-NA	2.69	2.04	1.95
12	D	301	HEC	FE-NA	2.67	2.04	1.95
11	T	403	U10	C6-C5	-2.66	1.39	1.46
10	T	401	HEM	FE-NB	2.60	2.02	1.94
10	T	401	HEM	CAC-C3C	2.58	1.54	1.47
11	K	404	U10	C6-C1	2.57	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	404	U10	C6-C1	2.56	1.39	1.35
11	T	404	U10	C6-C5	-2.50	1.39	1.46
11	K	404	U10	C6-C5	-2.49	1.39	1.46
10	K	401	HEM	CAC-C3C	2.45	1.53	1.47
11	T	403	U10	C6-C1	2.44	1.39	1.35
10	T	401	HEM	FE-NA	2.43	2.03	1.95
11	K	403	U10	C6-C1	2.40	1.39	1.35
10	K	401	HEM	FE-NB	2.36	2.02	1.94
11	K	404	U10	C1-C2	-2.29	1.39	1.47
11	K	403	U10	C1-C2	-2.24	1.39	1.47
11	T	404	U10	C1-C2	-2.24	1.39	1.47
10	K	401	HEM	C3C-C2C	-2.21	1.32	1.37
11	T	403	U10	C1-C2	-2.20	1.39	1.47
10	K	401	HEM	C2A-C3A	-2.19	1.33	1.38
10	T	401	HEM	C2A-C3A	-2.16	1.33	1.38
10	T	401	HEM	FE-NC	2.16	2.02	1.95
10	K	401	HEM	FE-NA	2.15	2.02	1.95
10	K	401	HEM	FE-NC	2.14	2.02	1.95
10	K	402	HEM	C3D-C2D	-2.02	1.32	1.36
10	T	402	HEM	C2A-C3A	-2.02	1.33	1.38
10	K	402	HEM	C2A-C3A	-2.01	1.33	1.38
11	T	403	U10	O4-C4M	-2.00	1.40	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	404	U10	C10-C9-C11	3.95	122.09	115.23
10	T	402	HEM	CHA-C4D-ND	3.53	128.74	124.37
12	N	301	HEC	CBC-CAC-C3C	3.49	121.88	112.42
12	D	301	HEC	CBC-CAC-C3C	3.49	121.87	112.42
12	N	301	HEC	CBB-CAB-C3B	3.45	121.78	112.42
12	D	301	HEC	CBB-CAB-C3B	3.45	121.76	112.42
10	K	402	HEM	CHA-C4D-ND	3.34	128.50	124.37
10	T	402	HEM	CHD-C1D-ND	3.24	127.91	124.42
11	K	404	U10	C7-C8-C9	-3.22	121.28	126.83
11	K	403	U10	C12-C13-C14	-3.19	120.33	127.62
12	D	301	HEC	CAB-C3B-C4B	3.18	128.93	124.79
12	N	301	HEC	CAB-C3B-C4B	3.16	128.90	124.79
10	K	402	HEM	CHD-C1D-ND	3.12	127.78	124.42
10	K	402	HEM	CBD-CAD-C3D	-3.12	103.90	112.53
10	T	402	HEM	CBD-CAD-C3D	-3.06	104.08	112.53
11	T	404	U10	C10-C9-C11	2.97	120.39	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	403	U10	C10-C9-C11	2.96	120.36	115.23
11	T	403	U10	C15-C14-C16	2.52	119.61	115.23
11	T	404	U10	C7-C8-C9	-2.51	122.51	126.83
11	T	403	U10	C1M-C1-C6	-2.50	120.34	124.45
11	K	403	U10	C15-C14-C16	2.48	119.54	115.23
11	T	403	U10	C12-C13-C14	-2.46	121.99	127.62
11	K	404	U10	C12-C13-C14	-2.45	119.49	127.64
11	K	404	U10	C7-C6-C1	-2.37	120.84	124.89
11	T	404	U10	C12-C13-C14	-2.36	119.77	127.64
12	N	301	HEC	CAB-C3B-C2B	-2.34	123.25	127.56
11	K	403	U10	C7-C8-C9	-2.33	122.82	126.83
12	D	301	HEC	CAB-C3B-C2B	-2.32	123.30	127.56
11	K	403	U10	C21-C19-C20	2.30	119.87	114.59
11	K	403	U10	C1M-C1-C6	-2.28	120.70	124.45
11	T	403	U10	C21-C19-C20	2.28	119.84	114.59
10	K	402	HEM	CHC-C4B-NB	2.26	126.86	124.42
10	T	402	HEM	CHC-C4B-NB	2.26	126.85	124.42
12	N	301	HEC	C3B-C4B-NB	-2.24	107.71	110.17
10	T	402	HEM	C1B-NB-C4B	2.24	107.86	105.21
12	N	301	HEC	CAC-C3C-C4C	2.22	127.97	124.91
10	K	402	HEM	C1B-NB-C4B	2.22	107.83	105.21
11	K	403	U10	C17-C18-C19	-2.21	120.28	127.64
12	D	301	HEC	CAC-C3C-C4C	2.18	127.91	124.91
12	N	301	HEC	C1D-ND-C4D	2.17	107.78	105.21
11	T	404	U10	C16-C14-C15	2.16	119.56	114.59
12	N	301	HEC	C4B-NB-C1B	2.16	107.77	105.21
11	T	403	U10	C17-C18-C19	-2.16	120.45	127.64
10	T	402	HEM	C3B-C2B-C1B	2.16	108.03	106.41
10	T	402	HEM	C1A-CHA-C4D	-2.15	121.20	126.25
12	N	301	HEC	C3D-C4D-ND	-2.14	108.28	110.35
12	D	301	HEC	C3B-C4B-NB	-2.14	107.83	110.17
12	D	301	HEC	C1D-ND-C4D	2.13	107.73	105.21
12	N	301	HEC	CHB-C1B-NB	2.12	126.71	124.42
10	K	402	HEM	C3B-C2B-C1B	2.11	108.00	106.41
12	D	301	HEC	C4B-NB-C1B	2.10	107.69	105.21
11	T	403	U10	C10-C9-C11	2.09	118.85	115.23
10	K	402	HEM	C1A-CHA-C4D	-2.06	121.39	126.25
11	K	404	U10	C16-C14-C15	2.05	119.30	114.59
10	K	401	HEM	C1B-NB-C4B	2.04	107.62	105.21
12	D	301	HEC	C2A-C1A-NA	-2.03	108.36	110.32
12	D	301	HEC	C3D-C4D-ND	-2.02	108.40	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	D	301	HEC	NA
12	N	301	HEC	NA

All (39) 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	N	301	HEC	C2B-C3B-CAB-CBB
12	N	301	HEC	C4B-C3B-CAB-CBB
12	D	301	HEC	C2C-C3C-CAC-CBC
12	N	301	HEC	C2C-C3C-CAC-CBC
12	D	301	HEC	C4C-C3C-CAC-CBC
12	N	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	T	401	HEM	C3D-CAD-CBD-CGD
10	T	401	HEM	C1A-C2A-CAA-CBA
10	T	401	HEM	C4D-C3D-CAD-CBD
10	T	401	HEM	C2D-C3D-CAD-CBD
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
11	T	403	U10	C2-C3-O3-C3M
10	T	401	HEM	C4C-C3C-CAC-CBC
11	K	403	U10	C5-C4-O4-C4M
11	T	403	U10	C9-C11-C12-C13
10	T	401	HEM	C3A-C2A-CAA-CBA
11	T	404	U10	C5-C4-O4-C4M
11	K	404	U10	C5-C4-O4-C4M
12	D	301	HEC	CAA-CBA-CGA-O2A
10	K	402	HEM	CAA-CBA-CGA-O1A
11	K	404	U10	C3-C4-O4-C4M
12	D	301	HEC	CAA-CBA-CGA-O1A
11	T	403	U10	C5-C4-O4-C4M
12	N	301	HEC	CAA-CBA-CGA-O2A
10	T	402	HEM	CAA-CBA-CGA-O1A
10	T	402	HEM	CAA-CBA-CGA-O2A
12	N	301	HEC	CAA-CBA-CGA-O1A
11	T	404	U10	C12-C11-C9-C10

Continued on next page...

Continued from previous page...

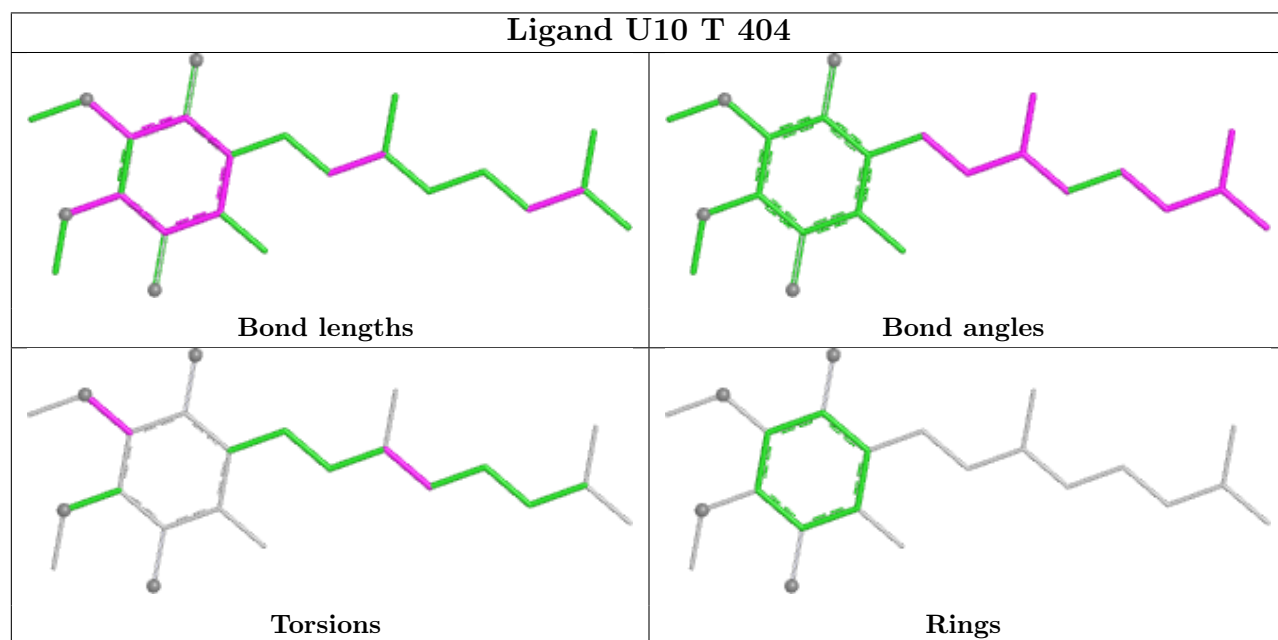
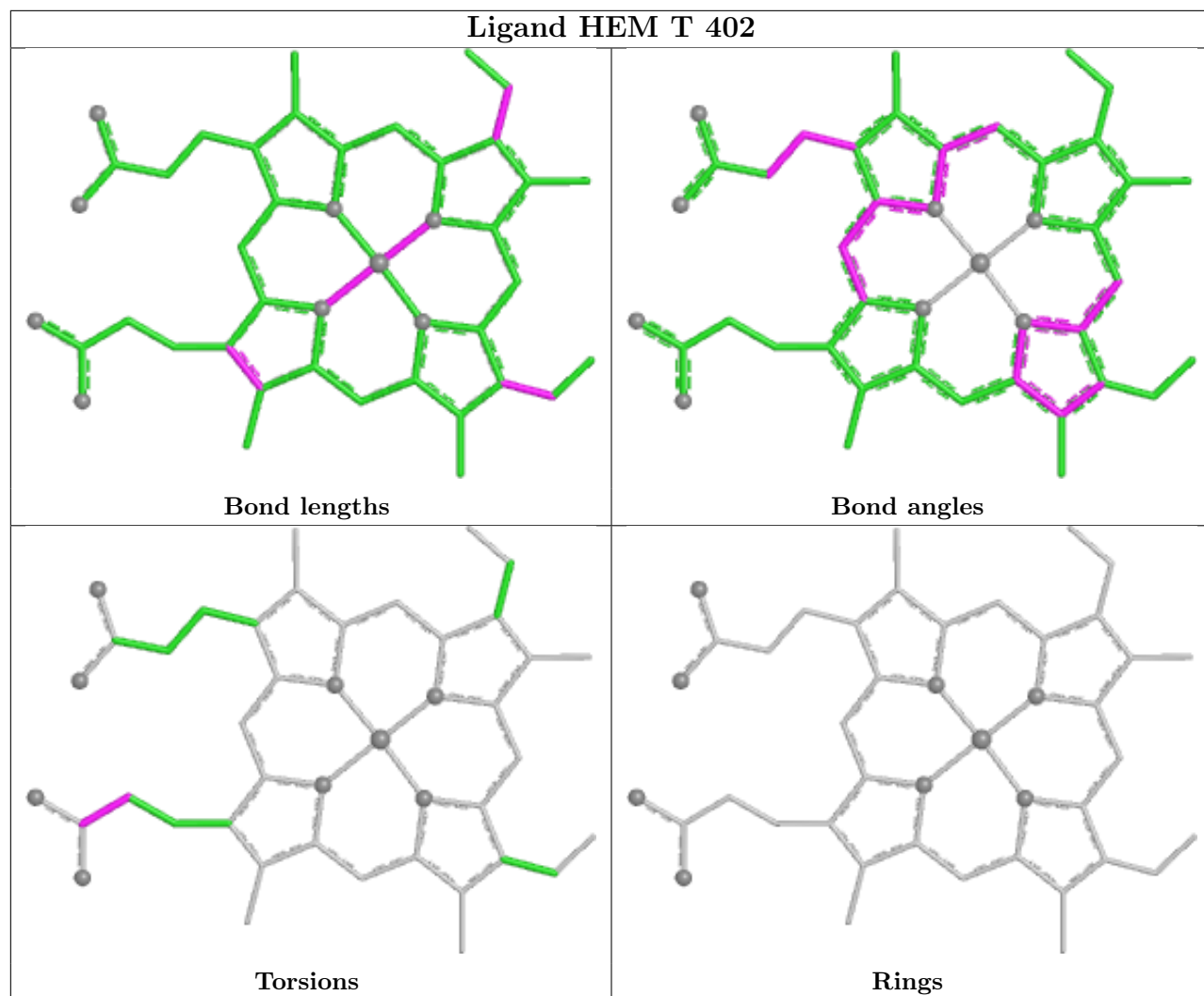
Mol	Chain	Res	Type	Atoms
11	T	404	U10	C12-C11-C9-C8
10	K	402	HEM	CAA-CBA-CGA-O2A

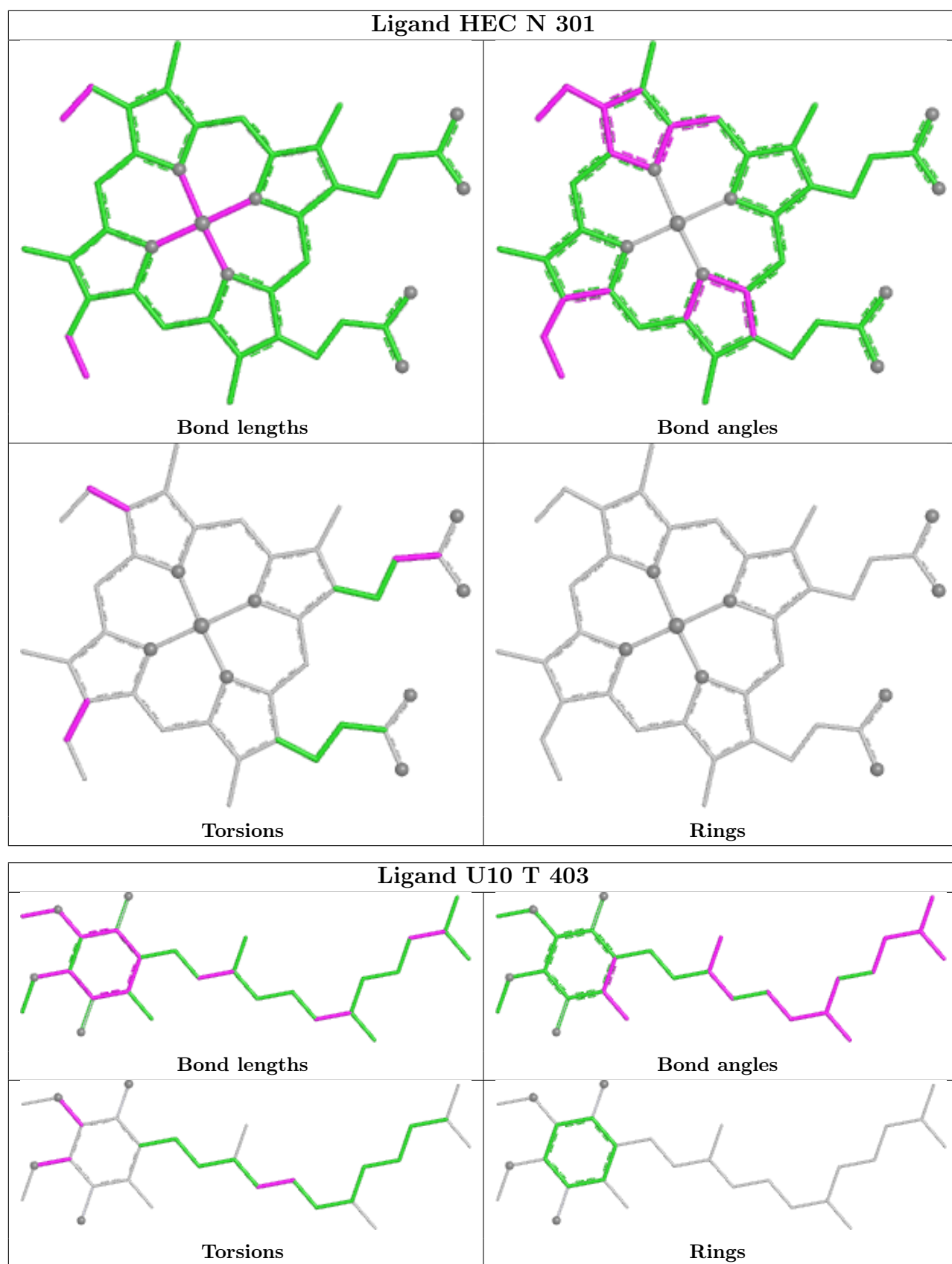
There are no ring outliers.

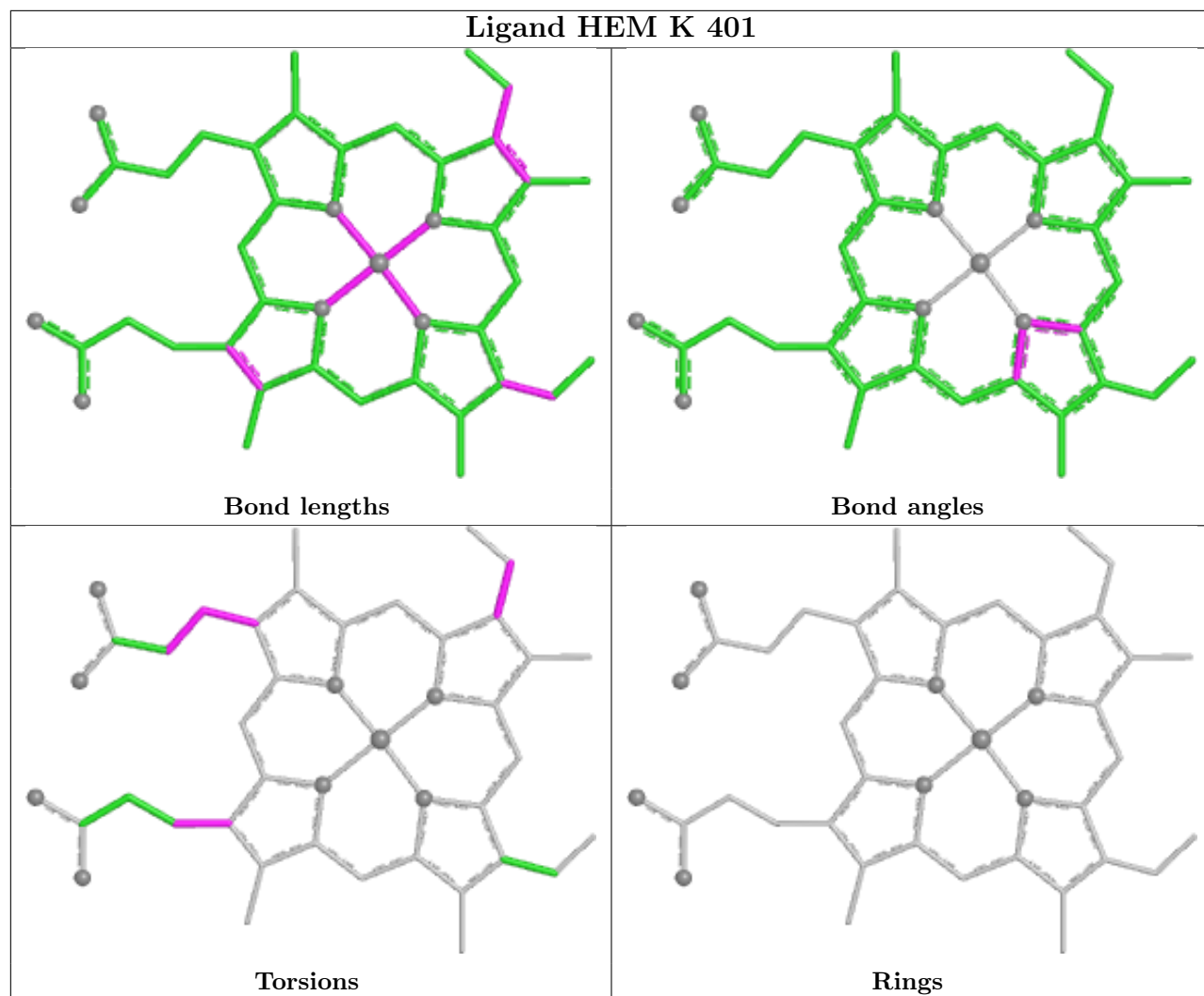
12 monomers are involved in 104 short contacts:

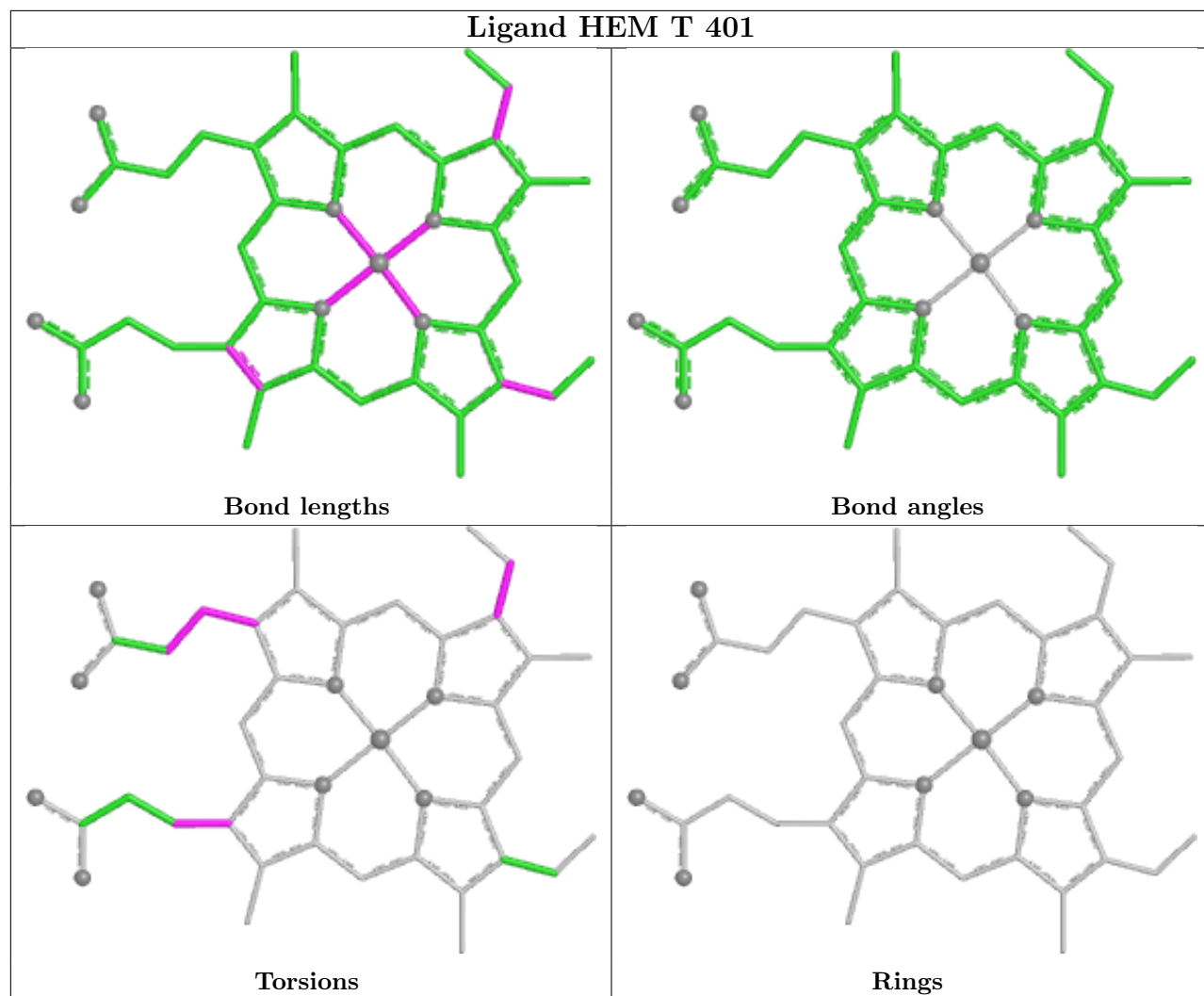
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	301	FES	4	0
10	T	402	HEM	7	0
11	T	404	U10	2	0
12	N	301	HEC	28	0
13	C	301	FES	1	0
11	T	403	U10	3	0
10	K	401	HEM	10	0
10	T	401	HEM	10	0
10	K	402	HEM	7	0
11	K	403	U10	8	0
12	D	301	HEC	23	0
11	K	404	U10	1	0

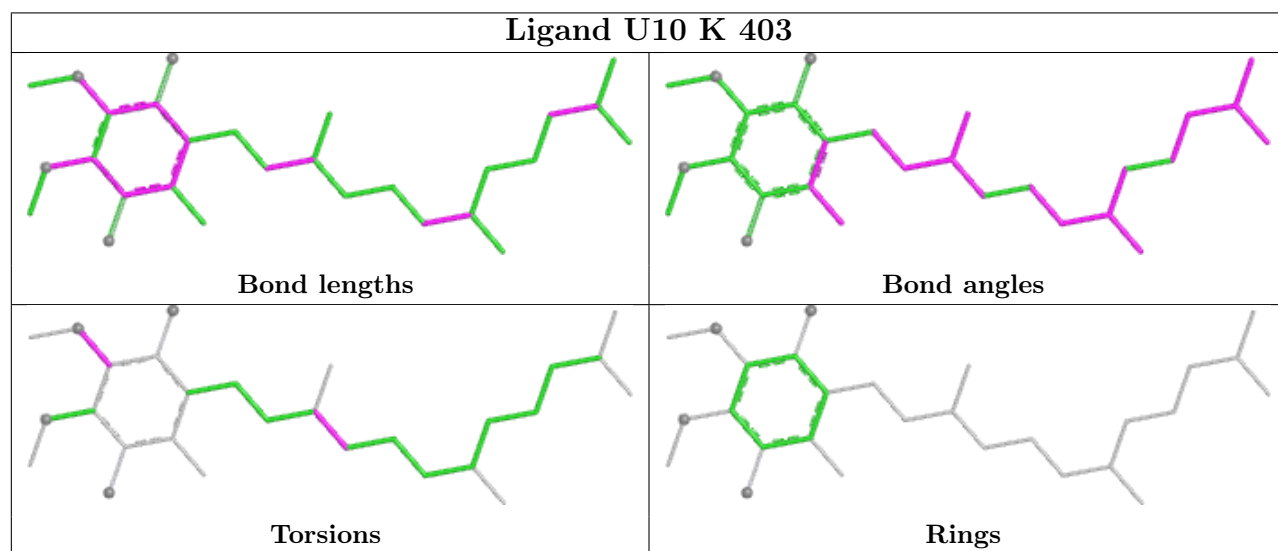
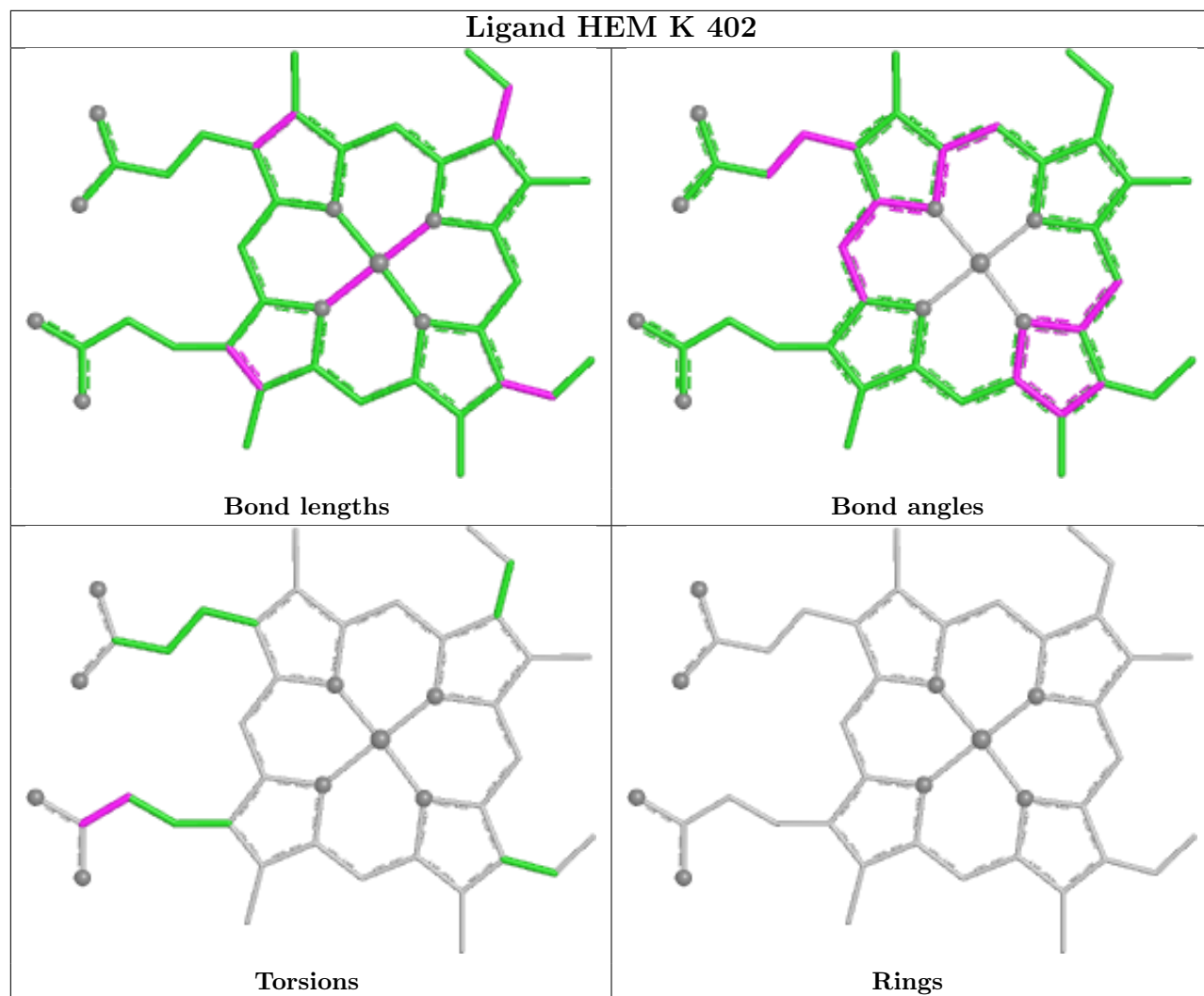
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



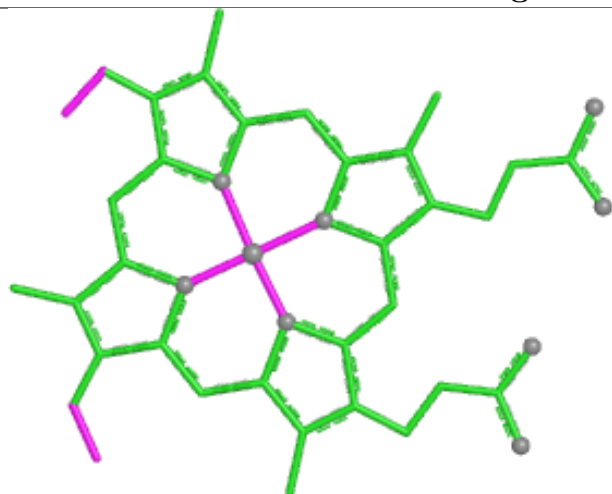




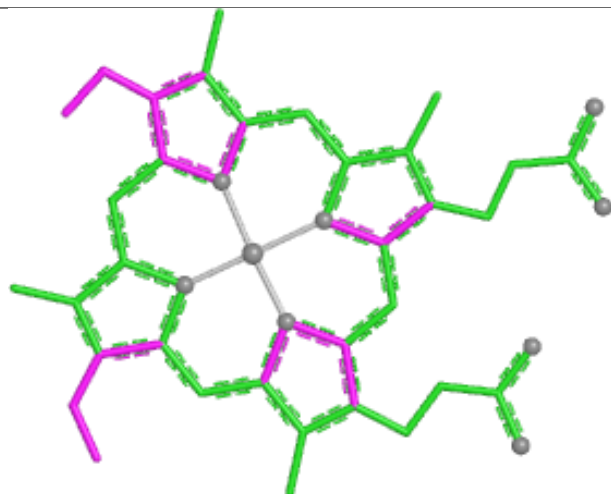




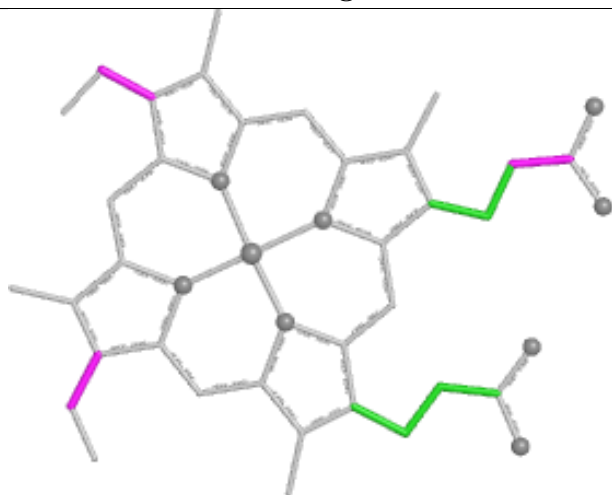
Ligand HEC D 301



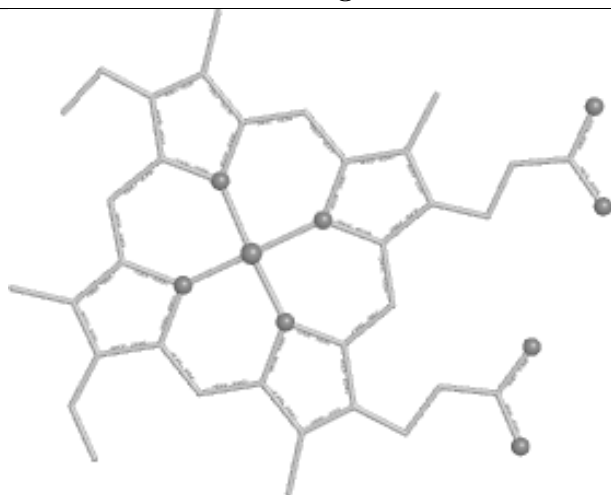
Bond lengths



Bond angles

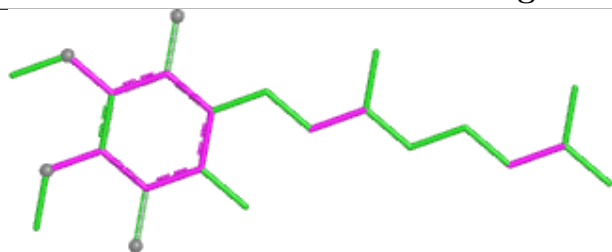


Torsions

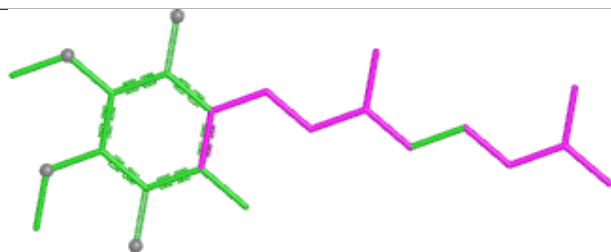


Rings

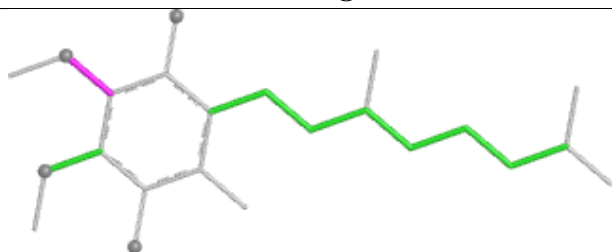
Ligand U10 K 404



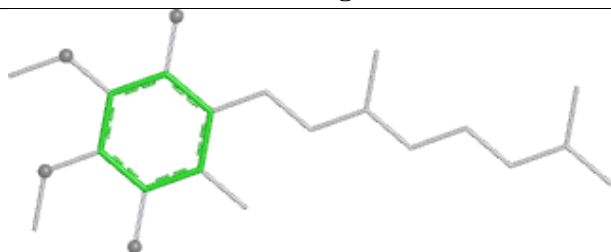
Bond lengths



Bond angles



Torsions



Rings

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.

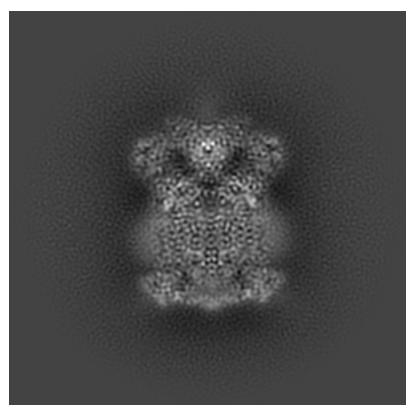
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24482. These allow visual inspection of the internal detail of the map and identification of artifacts.

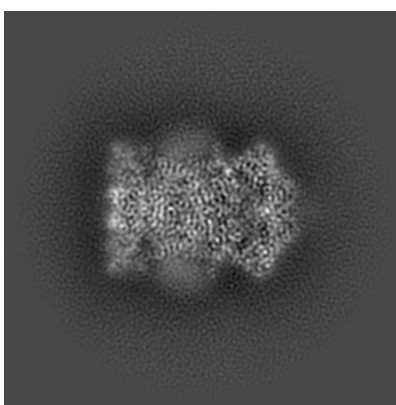
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

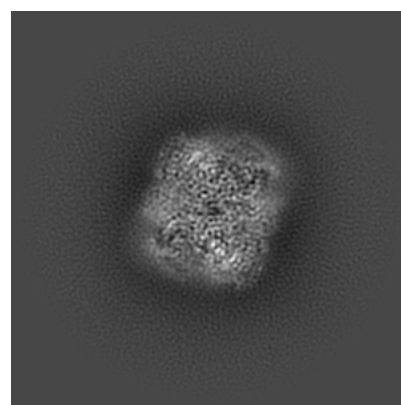
6.1.1 Primary map



X



Y

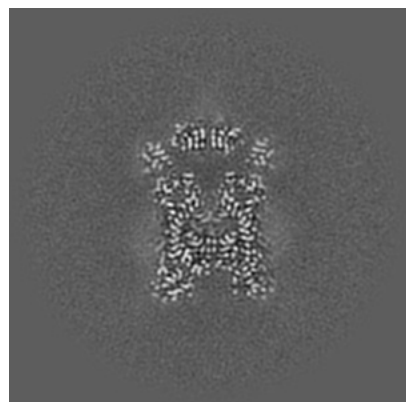


Z

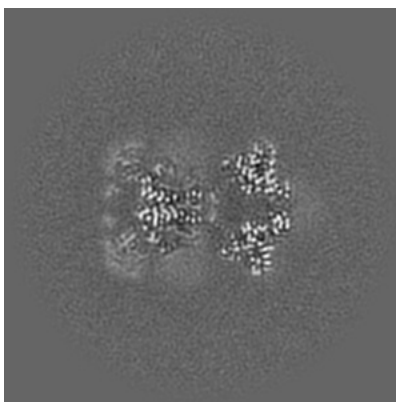
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

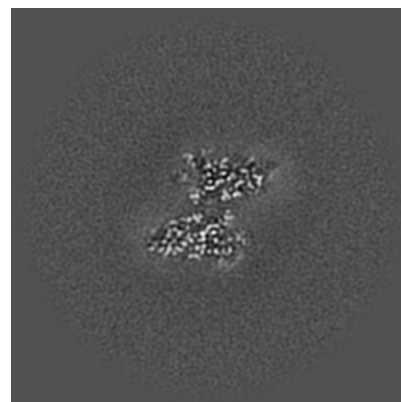
6.2.1 Primary map



X Index: 144



Y Index: 144

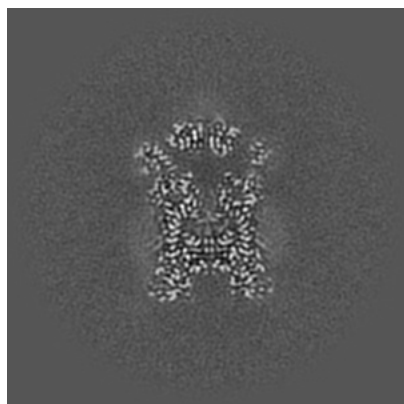


Z Index: 144

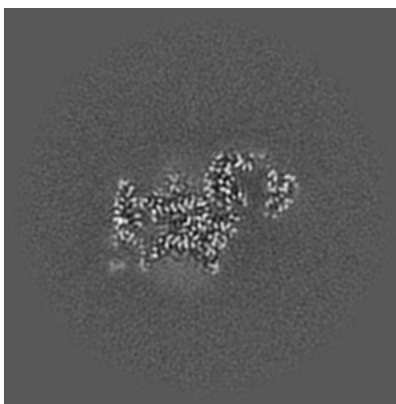
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

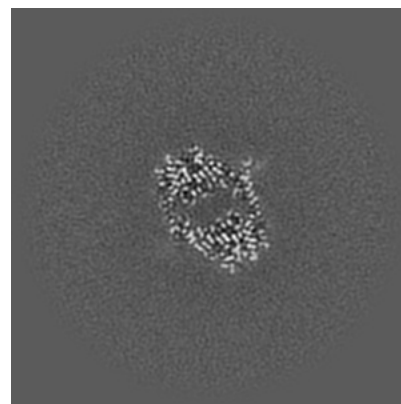
6.3.1 Primary map



X Index: 145



Y Index: 121

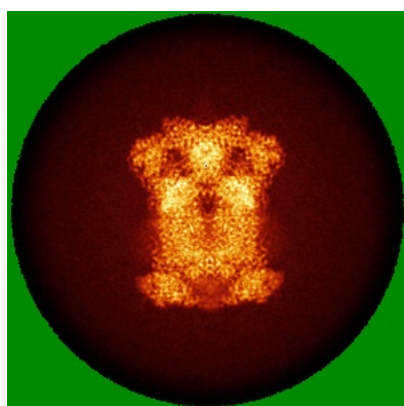


Z Index: 161

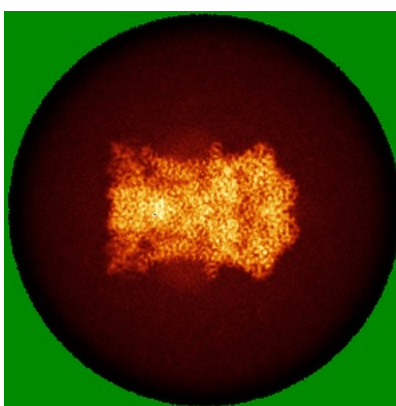
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

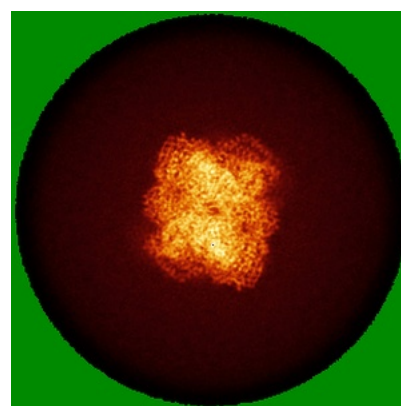
6.4.1 Primary map



X



Y

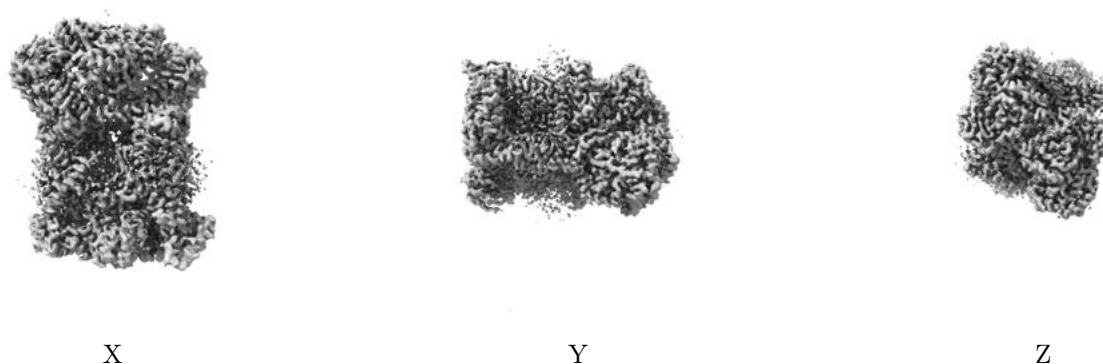


Z

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



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.

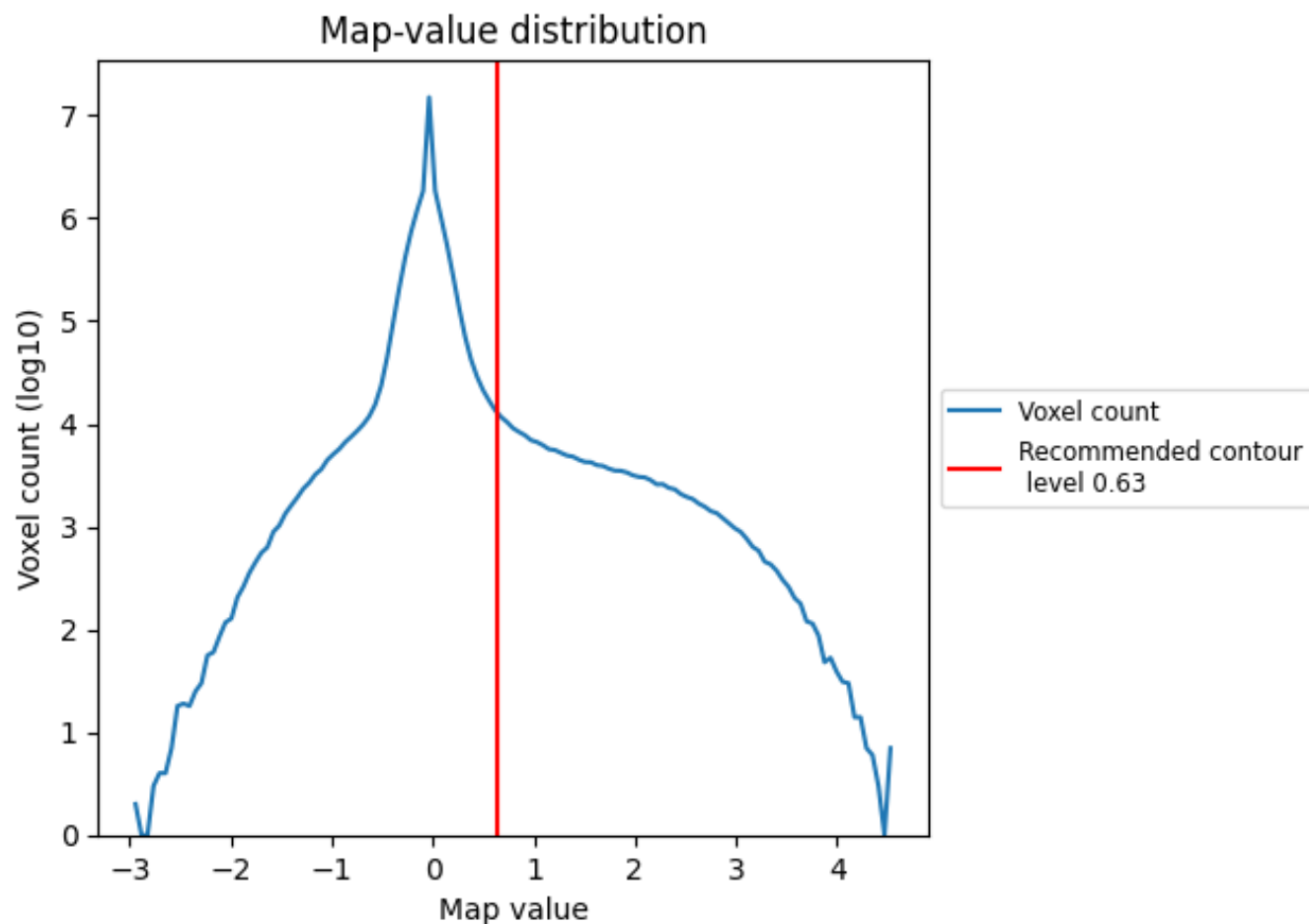
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

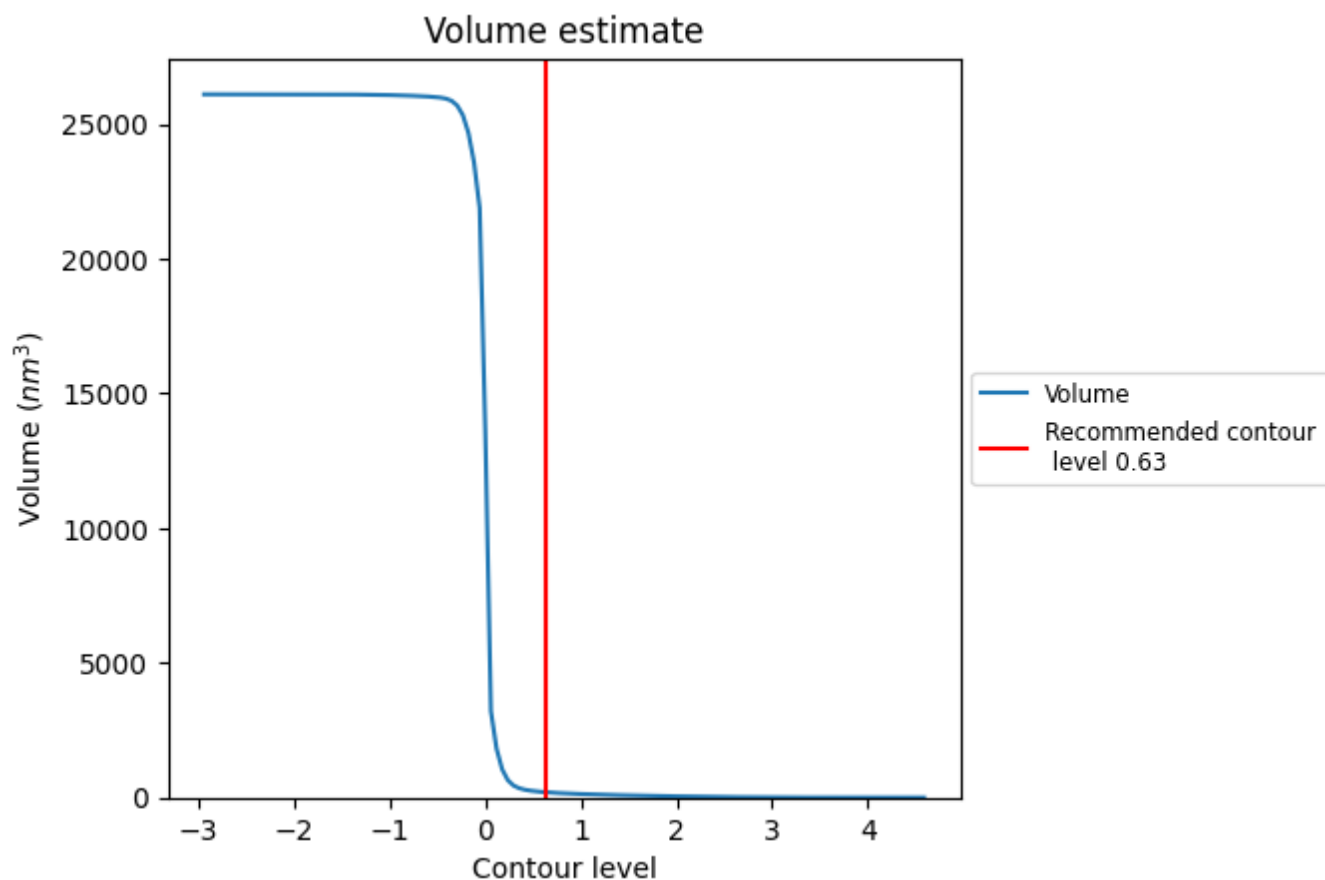
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

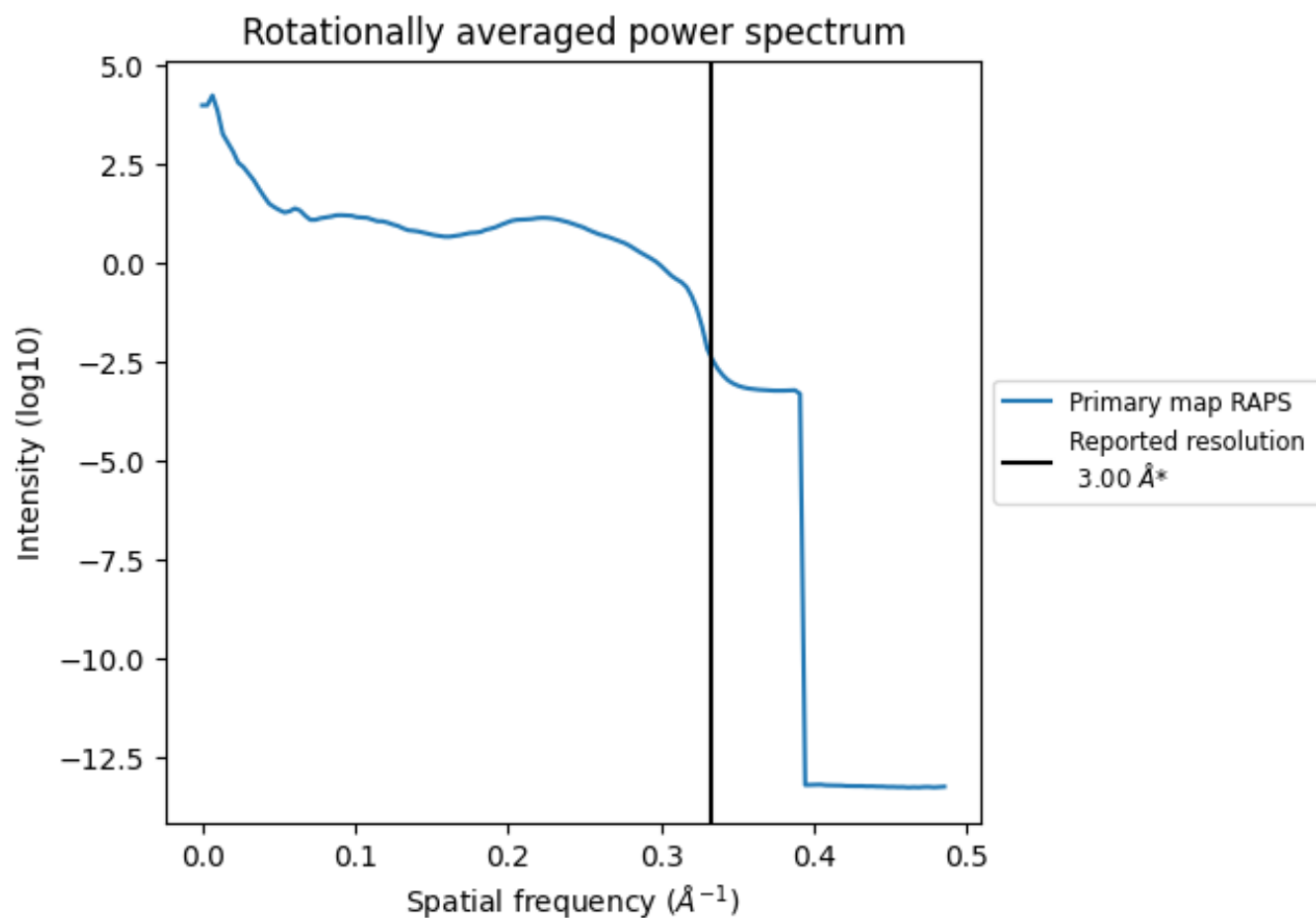
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm³; this corresponds to an approximate mass of 179 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 ⓘ

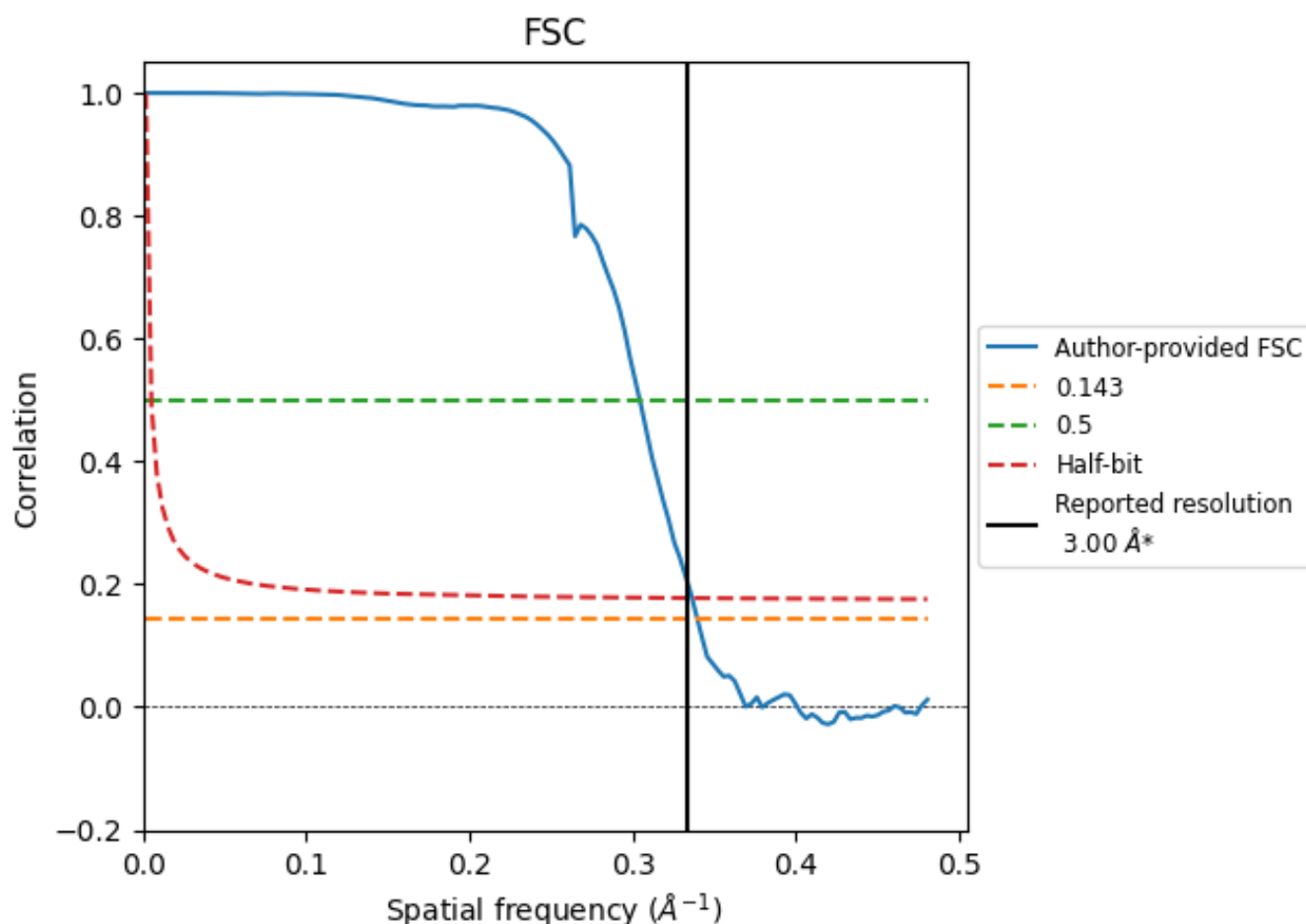


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

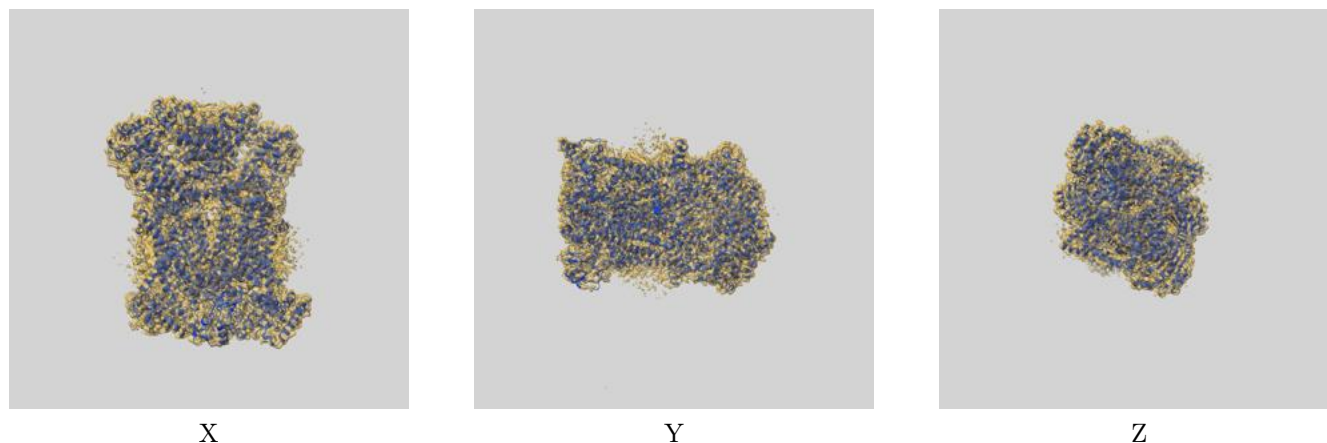
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.29	2.97
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

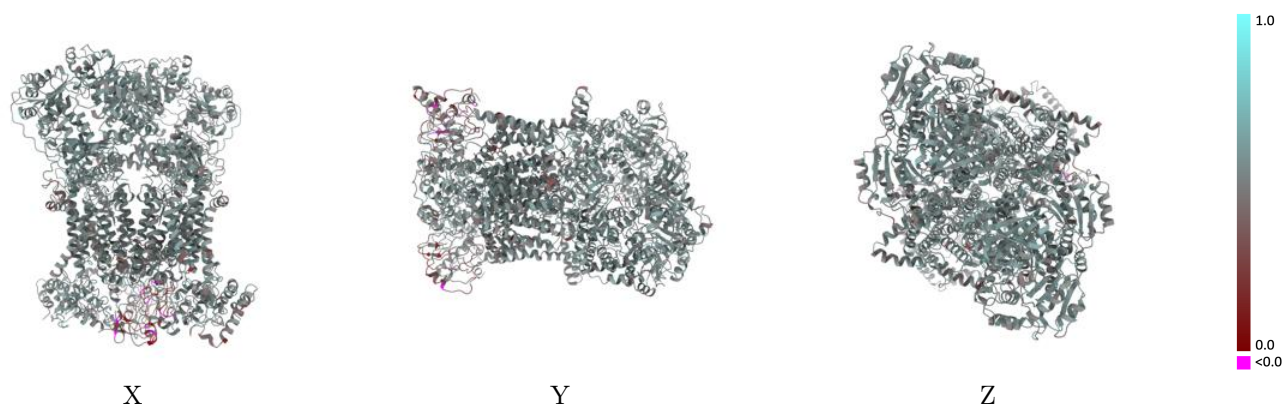
This section contains information regarding the fit between EMDB map EMD-24482 and PDB model 7RJA. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



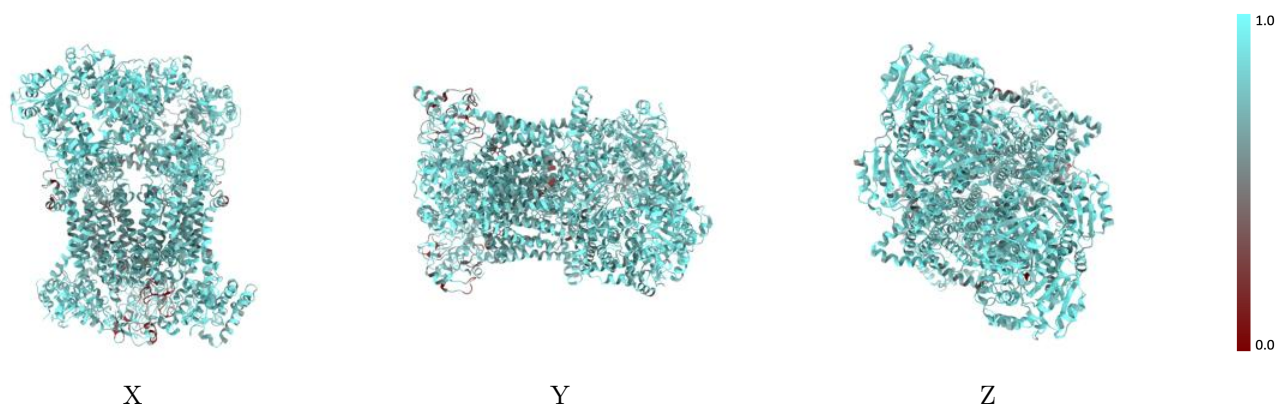
The images above show the 3D surface view of the map at the recommended contour level 0.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



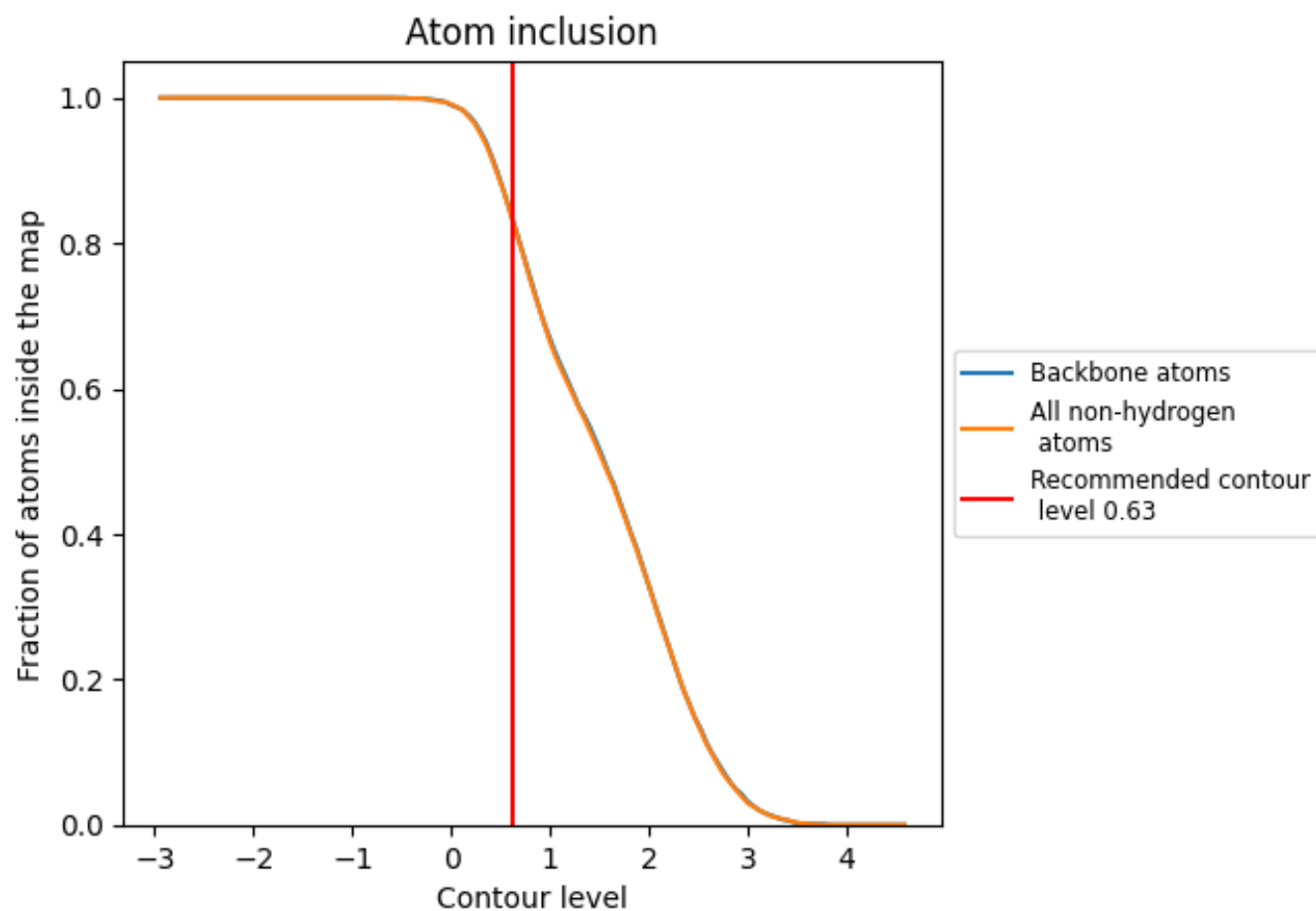
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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, 83% 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	 0.8280	 0.5230
A	 0.8620	 0.5410
B	 0.8560	 0.5350
C	 0.7020	 0.4340
D	 0.8690	 0.5370
F	 0.8110	 0.5100
G	 0.8510	 0.5380
H	 0.8220	 0.4910
I	 0.8410	 0.5160
J	 0.8590	 0.5380
K	 0.8360	 0.5400
L	 0.8530	 0.5330
M	 0.6310	 0.3950
N	 0.8570	 0.5270
P	 0.7940	 0.5120
Q	 0.8170	 0.5220
R	 0.7950	 0.4760
S	 0.8320	 0.5120
T	 0.8190	 0.5300

