



Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 03:32 PM EDT

PDB ID : 9CG3 / pdb_00009cg3
EMDB ID : EMD-45567
Title : Human kidney respiratory complex III
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-06-28
Resolution : 2.96 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

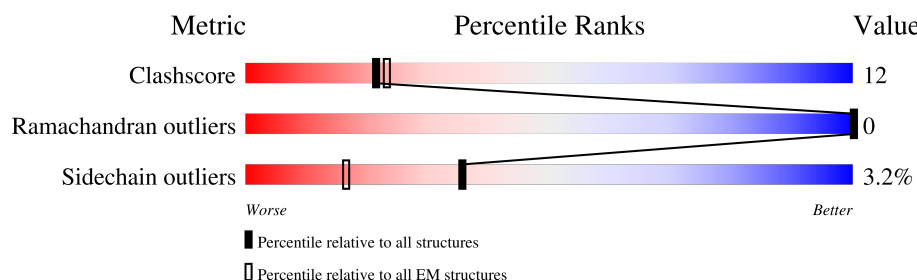
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	82	
1	N	82	
2	C	274	
2	P	274	
3	D	63	
3	Q	63	
4	E	91	
4	R	91	

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Mol	Chain	Length	Quality of chain
5	F	111	
5	S	111	
6	G	56	
6	T	56	
7	H	325	
7	U	325	
8	J	380	
8	V	380	
9	K	453	
9	W	453	
10	L	480	
10	Y	480	

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
11	FES	C	301	-	-	X	-
11	FES	P	301	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 31844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	79	Total	C	N	O	S	0	0
			659	428	121	109	1		
1	N	79	Total	C	N	O	S	0	0
			681	442	123	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	194	Total	C	N	O	S	0	0
			1506	952	261	286	7		
2	P	195	Total	C	N	O	S	0	0
			1515	957	263	288	7		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	54	Total	C	N	O	S	0	0
			446	293	76	76	1		
3	Q	55	Total	C	N	O	S	0	0
			451	296	77	77	1		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	68	Total	C	N	O	S	0	0
			541	328	101	107	5		
4	R	68	Total	C	N	O	S	0	0
			550	333	102	110	5		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	101	Total	C	N	O	S	0	0
			892	572	157	161	2		
5	S	104	Total	C	N	O	S	0	0
			909	581	160	166	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	51	Total	C	N	O		0	0
			425	287	72	66			
6	T	51	Total	C	N	O		0	0
			425	287	72	66			

- Molecule 7 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	239	Total	C	N	O	S	0	0
			1908	1222	326	345	15		
7	U	239	Total	C	N	O	S	0	0
			1908	1222	326	345	15		

- Molecule 8 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	378	Total	C	N	O	S	0	0
			3008	2017	467	508	16		
8	V	378	Total	C	N	O	S	0	0
			3008	2017	467	508	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	418	Total	C	N	O	S	0	0
			3148	1978	551	609	10		
9	W	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

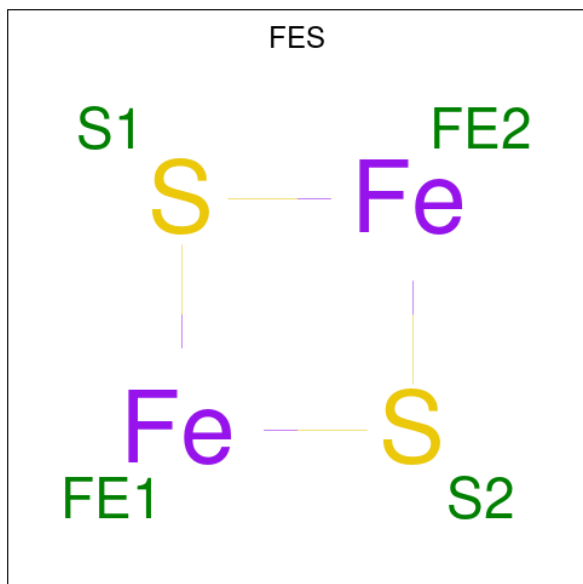
Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	411	Total	C	N	O	S	0	0
			3208	2017	563	609	19		

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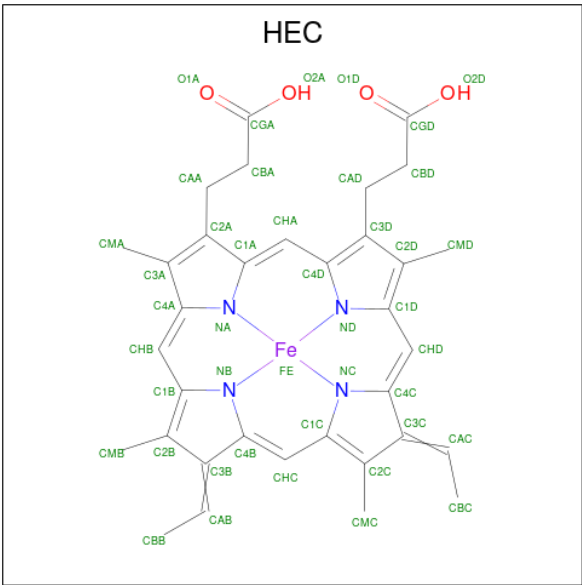
Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	414	Total	C	N	O	S	0	0
			3228	2028	567	614	19		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



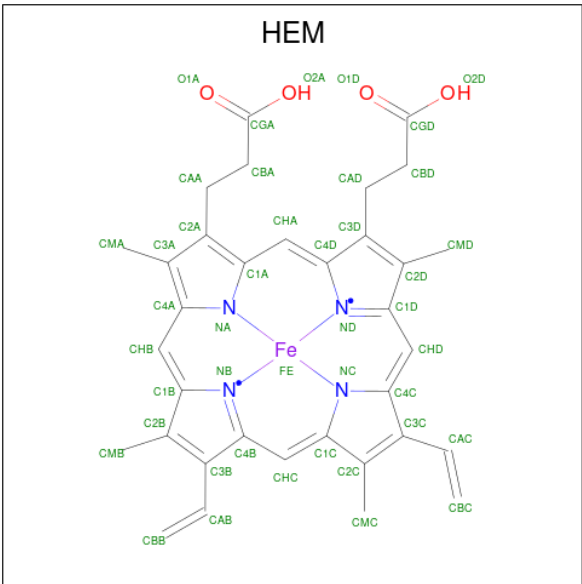
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	Fe	S	0
			4	2	2	
11	P	1	Total	Fe	S	0
			4	2	2	

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



Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
13	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
13	J	1	Total 43	C 34	Fe 1	N 4	O 4	0
13	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
13	V	1	Total 43	C 34	Fe 1	N 4	O 4	0

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.

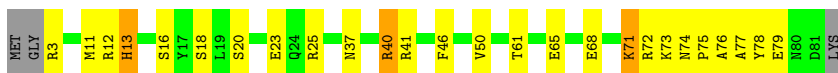
- Molecule 1: Cytochrome b-c1 complex subunit 8

Chain A: 



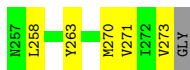
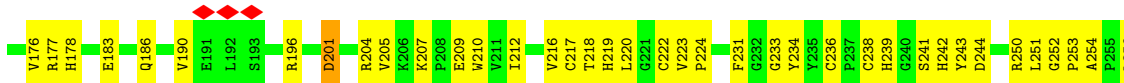
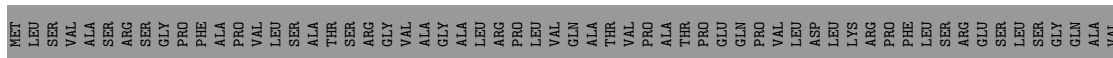
- Molecule 1: Cytochrome b-c1 complex subunit 8

Chain N: 



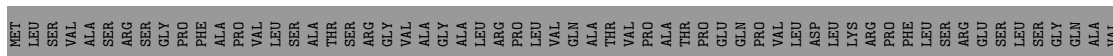
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C: 



- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P: 





- Molecule 3: Cytochrome b-c1 complex subunit 9

Chain D: 76% 10% 14%



- Molecule 3: Cytochrome b-c1 complex subunit 9

Chain Q: 67% 21% 13%



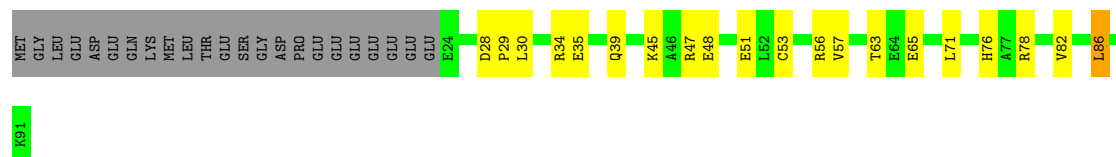
- Molecule 4: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain E: 49% 22% 25%



- Molecule 4: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain R: 53% 21% 25%



- Molecule 5: Cytochrome b-c1 complex subunit 7

Chain F: 65% 25% 9%




- Molecule 5: Cytochrome b-c1 complex subunit 7

Chain S: 




- Molecule 6: Cytochrome b-c1 complex subunit 10

Chain G: 



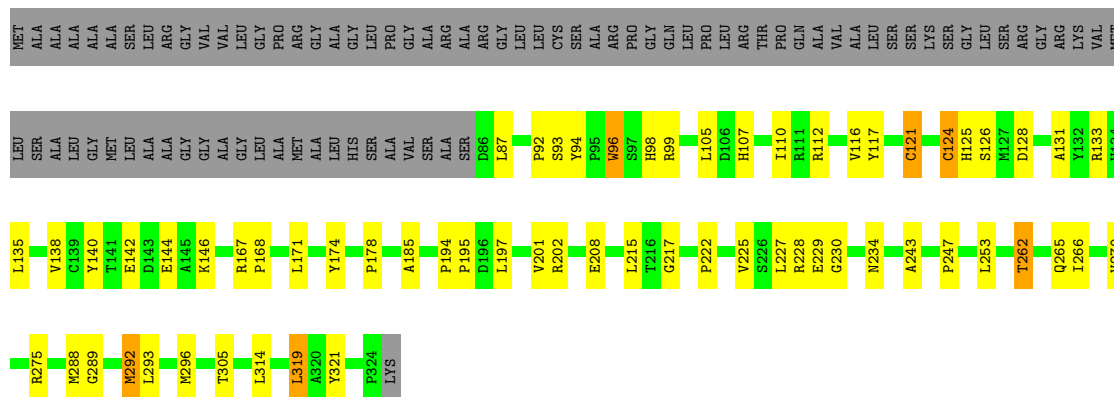
- Molecule 6: Cytochrome b-c1 complex subunit 10

Chain T: 



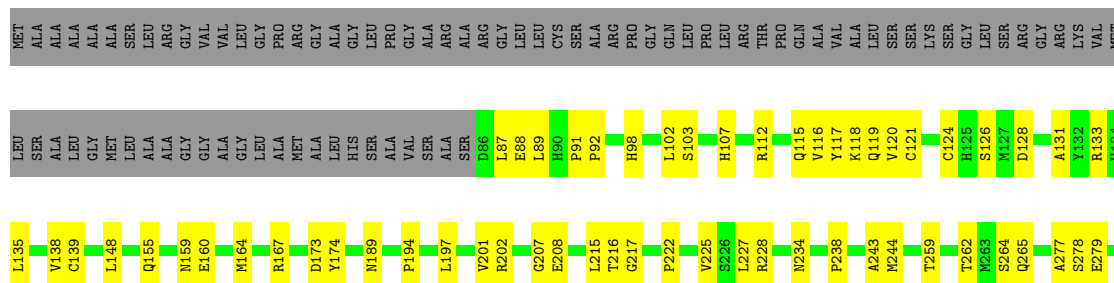
- Molecule 7: Cytochrome c1, heme protein, mitochondrial

Chain H: 



- Molecule 7: Cytochrome c1, heme protein, mitochondrial

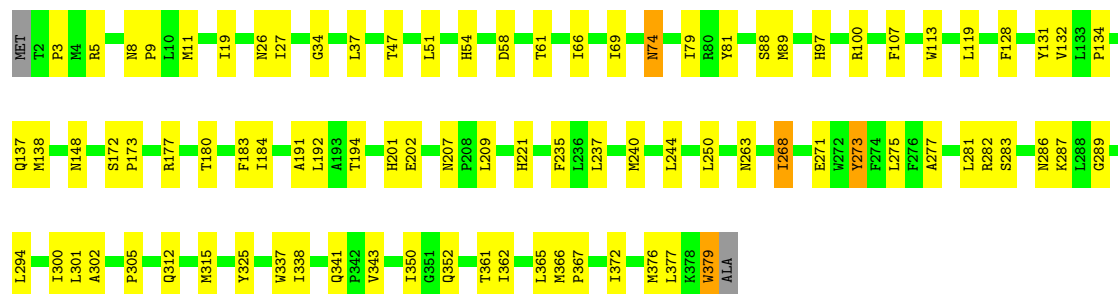
Chain U: 





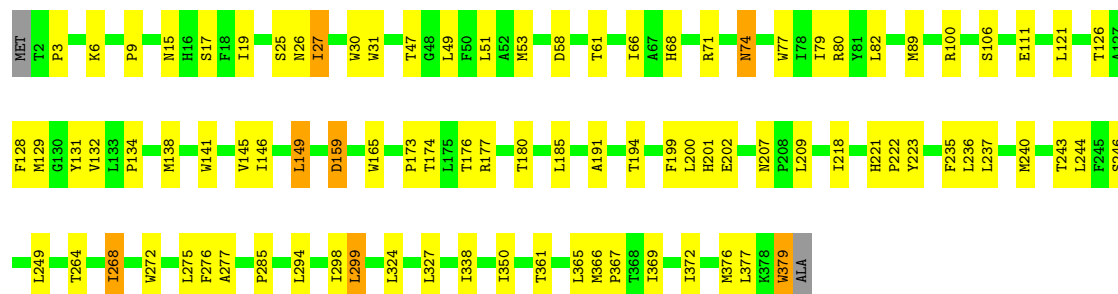
- Molecule 8: Cytochrome b

Chain J: 76% 22% ..



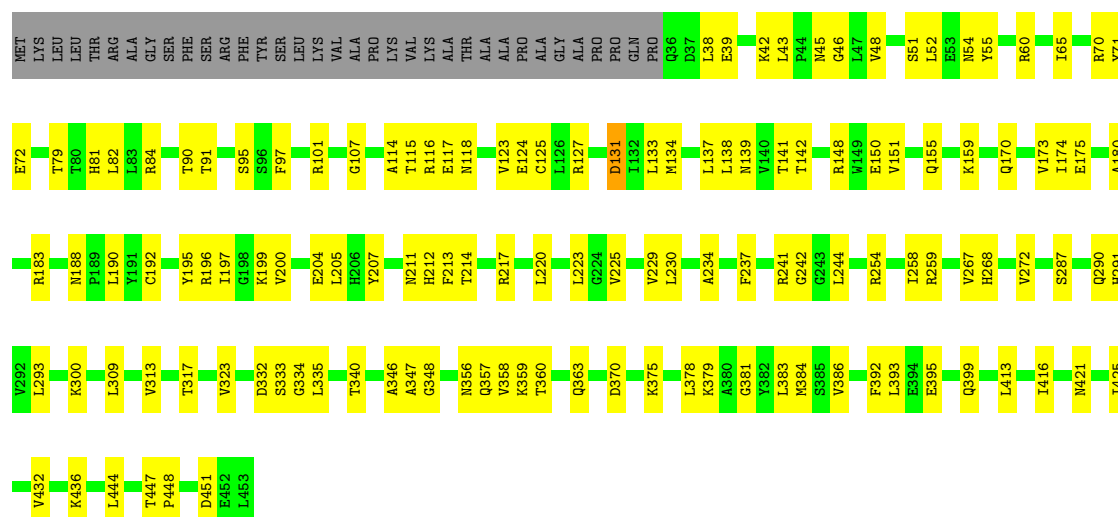
- Molecule 8: Cytochrome b

Chain V: 75% 22% ..



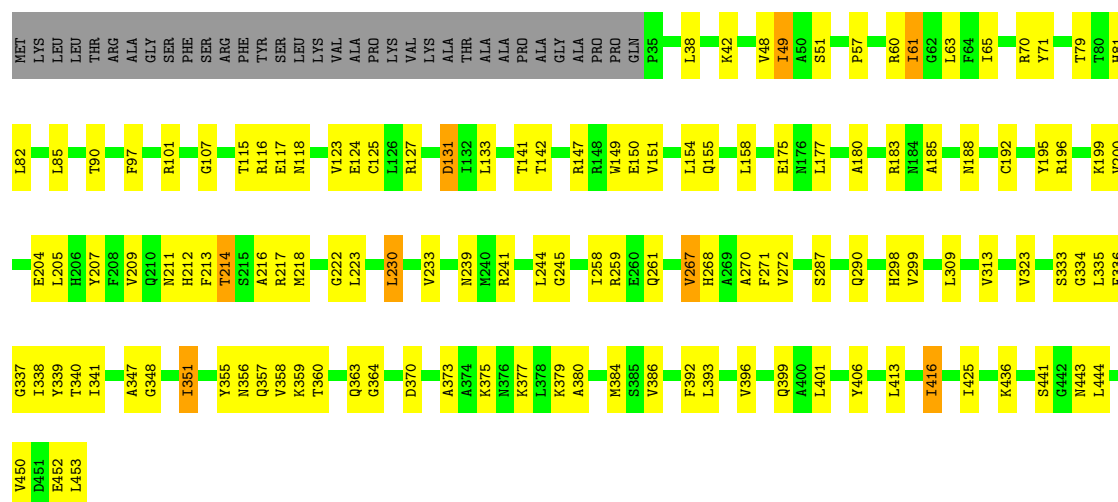
- Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain K: 63% 29% 8%



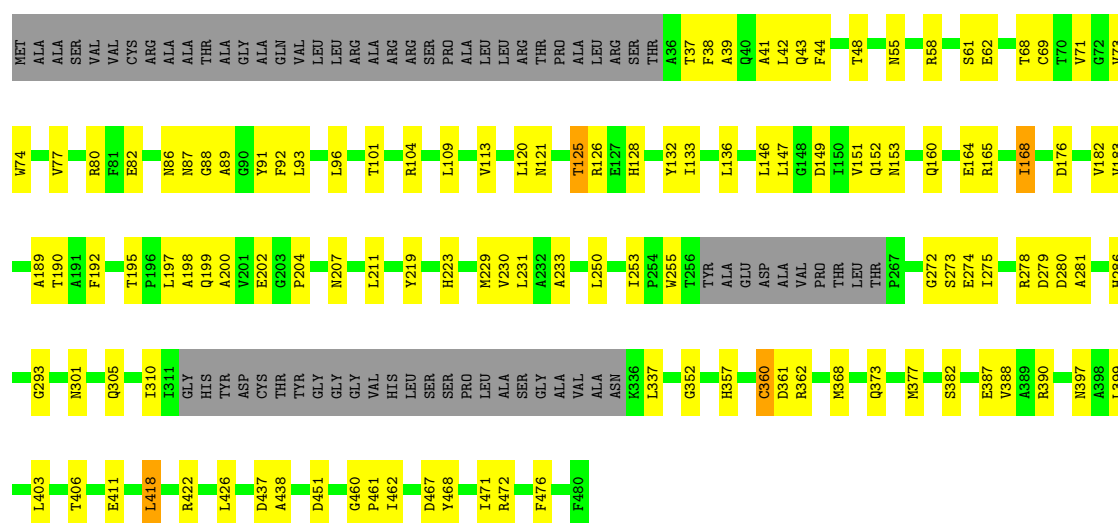
- Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain W: 



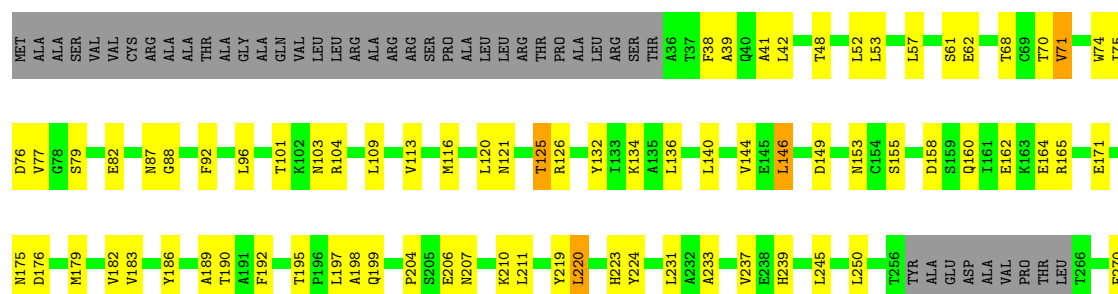
• Molecule 10: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L: 



• Molecule 10: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Y: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.940	Depositor
Minimum map value	-0.511	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 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	0.12	0/679	0.27	0/918
1	N	0.12	0/702	0.30	0/948
2	C	0.12	0/1539	0.31	0/2087
2	P	0.26	0/1548	0.37	0/2096
3	D	0.14	0/457	0.25	0/615
3	Q	0.13	0/462	0.24	0/622
4	E	0.14	0/548	0.30	0/738
4	R	0.14	0/557	0.27	0/747
5	F	0.10	0/913	0.24	0/1223
5	S	0.38	0/930	0.52	0/1246
6	G	0.13	0/442	0.32	0/608
6	T	0.10	0/442	0.32	0/608
7	H	0.33	0/1967	0.46	0/2672
7	U	0.12	0/1967	0.30	0/2672
8	J	0.28	0/3107	0.41	0/4254
8	V	0.28	0/3107	0.42	0/4254
9	K	0.12	0/3205	0.28	0/4346
9	W	0.22	0/3220	0.34	0/4365
10	L	0.13	0/3273	0.30	0/4433
10	Y	0.13	0/3293	0.30	0/4462
All	All	0.21	0/32358	0.35	0/43914

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
5	S	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	S	34	ARG	Sidechain

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	659	0	640	15	0
1	N	681	0	667	21	0
2	C	1506	0	1484	57	0
2	P	1515	0	1500	50	0
3	D	446	0	449	5	0
3	Q	451	0	454	10	0
4	E	541	0	497	14	0
4	R	550	0	514	13	0
5	F	892	0	881	21	0
5	S	909	0	896	22	0
6	G	425	0	422	5	0
6	T	425	0	422	5	0
7	H	1908	0	1856	49	0
7	U	1908	0	1856	47	0
8	J	3008	0	3065	58	0
8	V	3008	0	3065	65	0
9	K	3148	0	3111	83	0
9	W	3162	0	3139	82	0
10	L	3208	0	3146	84	0
10	Y	3228	0	3163	105	0
11	C	4	0	0	9	0
11	P	4	0	0	9	0
12	H	43	0	32	8	0
12	U	43	0	32	7	0
13	J	86	0	60	8	0
13	V	86	0	60	9	0
All	All	31844	0	31411	730	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (730) 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:C:236:CYS:SG	11:C:301:FES:FE2	1.19	1.34
2:C:217:CYS:SG	11:C:301:FES:FE2	1.52	1.00
2:C:236:CYS:SG	11:C:301:FES:S2	2.65	0.94
2:C:222:CYS:SG	11:C:301:FES:S2	2.69	0.91
7:H:146:LYS:HG2	7:H:171:LEU:HD11	1.57	0.87
2:C:238:CYS:HB2	11:C:301:FES:S2	2.17	0.84
2:C:162:GLY:HA2	2:C:178:HIS:HB3	1.60	0.82
13:V:401:HEM:HBC2	13:V:401:HEM:HHD	1.59	0.82
9:K:313:VAL:HG21	9:K:323:VAL:HG21	1.59	0.81
2:P:155:LYS:HG3	2:P:271:VAL:HG13	1.63	0.81
2:C:224:PRO:HB2	2:C:234:TYR:HB3	1.63	0.80
2:P:236:CYS:HG	11:P:301:FES:FE2	0.94	0.80
4:R:34:ARG:HG3	4:R:78:ARG:HD3	1.64	0.79
2:P:234:TYR:HB2	2:P:243:TYR:HB2	1.64	0.78
8:V:138:MET:HE1	8:V:268:ILE:HA	1.67	0.77
10:Y:338:CYS:SG	10:Y:339:GLN:N	2.56	0.77
9:W:313:VAL:HG21	9:W:323:VAL:HG21	1.65	0.75
4:R:71:LEU:HD22	7:U:222:PRO:HG3	1.69	0.75
7:H:195:PRO:HG2	12:H:401:HEC:HBA1	1.69	0.75
10:L:42:LEU:HD22	10:L:426:LEU:HB3	1.69	0.74
10:Y:278:ARG:O	10:Y:460:GLY:HA3	1.88	0.73
2:P:239:HIS:HB2	11:P:301:FES:S1	2.29	0.73
2:C:219:HIS:HB2	2:C:254:ALA:HA	1.70	0.73
9:K:125:CYS:HB3	9:K:133:LEU:HD22	1.72	0.72
2:C:204:ARG:NH2	2:C:258:LEU:O	2.22	0.72
2:P:217:CYS:HG	11:P:301:FES:FE2	1.02	0.72
2:P:236:CYS:SG	11:P:301:FES:FE2	1.80	0.72
10:Y:183:VAL:HG21	10:Y:286:HIS:HB3	1.70	0.72
3:Q:11:TYR:HA	3:Q:15:PHE:HB2	1.71	0.71
1:N:12:ARG:HG2	1:N:13:HIS:CE1	2.25	0.71
10:Y:113:VAL:HG21	10:Y:120:LEU:HD23	1.72	0.71
2:P:96:VAL:HG21	2:P:101:LYS:HD3	1.72	0.71
7:U:277:ALA:O	8:V:71:ARG:NH2	2.24	0.71
2:C:163:LYS:HE2	7:U:228:ARG:HH21	1.56	0.70
10:L:48:THR:HG22	10:L:62:GLU:HB2	1.74	0.70
8:V:82:LEU:HD23	8:V:243:THR:HG21	1.74	0.70
8:V:298:ILE:HG22	8:V:299:LEU:HD22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:131:ALA:HA	7:U:174:TYR:HA	1.73	0.69
2:P:216:VAL:HG13	2:P:221:GLY:HA2	1.75	0.69
10:Y:113:VAL:HG22	10:Y:146:LEU:HD21	1.74	0.69
9:W:384:MET:HE2	10:Y:134:LYS:HG3	1.75	0.68
10:L:87:ASN:HD22	10:L:204:PRO:HD3	1.58	0.68
8:J:286:ASN:HD22	8:J:289:GLY:H	1.41	0.67
7:H:247:PRO:HB3	12:H:401:HEC:HHC	1.75	0.67
7:H:131:ALA:HA	7:H:174:TYR:HA	1.76	0.67
9:K:195:TYR:O	9:K:199:LYS:NZ	2.27	0.67
1:N:68:GLU:HG2	1:N:72:ARG:HH21	1.59	0.67
2:P:217:CYS:SG	11:P:301:FES:FE2	1.86	0.67
9:K:259:ARG:NH2	9:K:447:THR:O	2.28	0.67
7:U:202:ARG:HH11	7:U:279:GLU:HG2	1.59	0.66
9:W:272:VAL:HG11	9:W:335:LEU:HB3	1.78	0.66
9:W:125:CYS:HB3	9:W:133:LEU:HD22	1.76	0.66
2:P:236:CYS:SG	11:P:301:FES:S1	2.94	0.66
10:Y:87:ASN:HD22	10:Y:204:PRO:HD3	1.60	0.66
9:K:134:MET:HE3	9:K:237:PHE:HE2	1.61	0.65
4:R:29:PRO:HD2	7:U:262:THR:HG21	1.77	0.65
12:U:401:HEC:HBC3	12:U:401:HEC:HHD	1.79	0.65
2:C:239:HIS:HB2	11:C:301:FES:S1	2.36	0.65
9:K:196:ARG:NH2	9:K:204:GLU:OE1	2.29	0.65
8:J:300:ILE:HG21	8:J:362:ILE:HD12	1.77	0.64
9:K:107:GLY:O	10:L:397:ASN:ND2	2.29	0.64
1:A:27:TYR:HE2	7:H:305:THR:HG22	1.61	0.64
8:J:277:ALA:HB1	8:J:294:LEU:HD13	1.80	0.64
10:Y:53:LEU:HD12	10:Y:57:LEU:HD23	1.80	0.64
7:H:247:PRO:CB	12:H:401:HEC:HHC	2.27	0.64
9:W:379:LYS:HE3	9:W:413:LEU:HG	1.80	0.64
13:J:401:HEM:HMC1	13:J:401:HEM:HBC2	1.79	0.64
10:L:388:VAL:HG21	10:L:438:ALA:HA	1.80	0.64
3:Q:16:ARG:NH1	10:Y:446:SER:OG	2.30	0.64
12:U:401:HEC:HBB3	12:U:401:HEC:HHC	1.79	0.64
9:W:107:GLY:O	10:Y:397:ASN:ND2	2.30	0.64
10:Y:42:LEU:HD22	10:Y:426:LEU:HB3	1.80	0.64
4:E:37:CYS:SG	4:E:78:ARG:HA	2.38	0.64
9:W:196:ARG:NH2	9:W:204:GLU:OE1	2.30	0.64
2:P:196:ARG:NH2	2:P:252:GLY:O	2.31	0.64
7:U:112:ARG:NH1	7:U:265:GLN:OE1	2.31	0.64
7:H:112:ARG:NH1	7:H:265:GLN:OE1	2.30	0.64
9:K:72:GLU:O	9:K:188:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:195:THR:HG22	10:Y:197:LEU:H	1.64	0.64
7:U:159:ASN:ND2	7:U:160:GLU:O	2.31	0.63
9:W:270:ALA:HB2	9:W:339:TYR:HD1	1.61	0.63
9:K:259:ARG:HG2	9:K:444:LEU:HD13	1.79	0.63
8:J:97:HIS:CE1	8:J:100:ARG:HH21	2.16	0.63
10:Y:451:ASP:OD1	10:Y:472:ARG:NH2	2.31	0.63
13:V:402:HEM:HMC2	13:V:402:HEM:HBC2	1.81	0.63
9:W:141:THR:HG23	9:W:142:THR:HG23	1.80	0.63
9:W:299:VAL:HG13	10:Y:120:LEU:HD11	1.81	0.63
7:U:88:GLU:HB3	7:U:238:PRO:HA	1.80	0.62
10:Y:144:VAL:HG11	10:Y:245:LEU:HB3	1.81	0.62
10:Y:304:LEU:HD13	10:Y:354:LEU:HD22	1.80	0.62
7:H:117:TYR:HA	7:H:121:CYS:SG	2.38	0.62
2:C:236:CYS:SG	11:C:301:FES:S1	2.96	0.62
9:K:267:VAL:HG11	9:K:347:ALA:HB2	1.80	0.62
5:F:70:ASN:HD22	8:J:26:ASN:HD22	1.46	0.62
5:S:52:PRO:HG2	5:S:55:LEU:HB2	1.82	0.62
10:L:55:ASN:HA	10:L:255:TRP:HD1	1.65	0.61
9:W:61:ILE:HG13	9:W:123:VAL:HG13	1.82	0.61
10:Y:39:ALA:HA	10:Y:42:LEU:HD12	1.82	0.61
10:L:195:THR:HG22	10:L:197:LEU:H	1.66	0.61
2:C:80:HIS:ND1	10:L:176:ASP:OD1	2.29	0.61
2:C:242:HIS:HD2	2:C:251:LEU:HD12	1.66	0.61
7:H:93:SER:HB2	7:H:99:ARG:HH12	1.66	0.61
2:C:241:SER:HA	2:C:252:GLY:HA3	1.82	0.61
8:V:47:THR:HG23	8:V:79:ILE:HG23	1.83	0.61
2:C:220:LEU:HD22	8:V:149:LEU:HA	1.83	0.60
13:J:402:HEM:HBC2	13:J:402:HEM:HMC2	1.82	0.60
9:W:38:LEU:HD11	9:W:406:TYR:CG	2.36	0.60
8:V:246:SER:HB3	8:V:249:LEU:HB2	1.82	0.60
10:L:451:ASP:OD1	10:L:472:ARG:NH2	2.34	0.60
4:R:76:HIS:HB2	7:U:89:LEU:HD11	1.83	0.60
10:Y:388:VAL:HG21	10:Y:438:ALA:HA	1.83	0.60
2:P:175:PHE:HZ	2:P:223:VAL:HG13	1.65	0.60
8:V:361:THR:HG22	8:V:365:LEU:HD12	1.82	0.60
9:K:272:VAL:HG21	9:K:335:LEU:HB3	1.84	0.59
10:Y:165:ARG:NH2	10:Y:211:LEU:O	2.35	0.59
9:W:212:HIS:O	9:W:217:ARG:NH1	2.35	0.59
10:L:360:CYS:HB3	10:L:368:MET:SD	2.42	0.59
1:A:3:ARG:HH12	8:J:201:HIS:CE1	2.20	0.59
2:C:130:LYS:HD3	6:G:34:TRP:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:MET:HE1	5:F:64:LYS:HD2	1.85	0.59
4:R:82:VAL:O	4:R:86:LEU:HB2	2.03	0.59
5:S:70:ASN:HD22	8:V:26:ASN:HD22	1.50	0.58
9:W:60:ARG:HG3	9:W:124:GLU:HG2	1.84	0.58
7:H:135:LEU:HA	7:H:138:VAL:HG12	1.83	0.58
9:K:159:LYS:HG2	9:K:197:ILE:HD13	1.85	0.58
10:L:77:VAL:HG21	10:L:223:HIS:HB3	1.85	0.58
10:L:82:GLU:HG2	10:L:219:TYR:HE2	1.69	0.58
8:J:282:ARG:HE	8:J:343:VAL:HG22	1.69	0.58
8:J:283:SER:O	8:J:352:GLN:NE2	2.36	0.58
7:U:289:GLY:HA2	8:V:244:LEU:HD23	1.86	0.58
9:K:137:LEU:O	9:K:141:THR:HG22	2.04	0.58
9:K:212:HIS:O	9:K:217:ARG:NH1	2.36	0.57
2:P:94:LEU:HG	1:N:25:ARG:HH22	1.68	0.57
8:V:15:ASN:HA	8:V:19:ILE:HB	1.85	0.57
5:F:34:ARG:NH2	5:F:92:GLU:OE2	2.37	0.57
10:L:93:LEU:HD23	10:L:96:LEU:HD11	1.86	0.57
2:C:219:HIS:O	11:C:301:FES:S2	2.62	0.57
7:U:215:LEU:HD11	12:U:401:HEC:HMB3	1.86	0.57
10:Y:301:ASN:O	10:Y:305:GLN:HG2	2.05	0.57
10:L:165:ARG:NH2	10:L:211:LEU:O	2.37	0.57
10:Y:286:HIS:CE1	10:Y:359:VAL:HG22	2.39	0.57
8:J:9:PRO:HG3	8:V:202:GLU:HG3	1.86	0.57
9:K:183:ARG:NH1	9:W:452:GLU:OE1	2.38	0.57
9:W:63:LEU:HD21	9:W:218:MET:HE3	1.87	0.57
9:W:375:LYS:NZ	9:W:416:ILE:O	2.35	0.57
1:N:37:ASN:OD1	1:N:40:ARG:NH1	2.38	0.57
1:A:18:SER:HB2	10:L:274:GLU:HG2	1.86	0.57
9:K:317:THR:HG21	9:K:346:ALA:HB1	1.87	0.56
9:K:379:LYS:HE3	9:K:413:LEU:HG	1.87	0.56
9:W:338:ILE:HD11	9:W:358:VAL:HG21	1.86	0.56
10:Y:360:CYS:HA	10:Y:368:MET:HE1	1.86	0.56
8:J:287:LYS:NZ	2:P:219:HIS:O	2.38	0.56
9:K:375:LYS:NZ	9:K:416:ILE:O	2.38	0.56
9:K:70:ARG:HD2	9:K:117:GLU:HG2	1.88	0.56
8:V:272:TRP:HA	8:V:275:LEU:HG	1.87	0.56
9:W:49:ILE:HD11	9:W:230:LEU:HB3	1.87	0.56
10:Y:61:SER:HA	10:Y:233:ALA:O	2.04	0.56
10:Y:71:VAL:HG13	10:Y:233:ALA:HB2	1.87	0.56
5:S:34:ARG:HG2	5:S:34:ARG:HH11	1.70	0.56
8:V:106:SER:OG	13:V:402:HEM:O2D	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:100:ARG:HH22	13:J:402:HEM:HBD2	1.70	0.56
10:L:280:ASP:O	10:L:362:ARG:NH2	2.38	0.56
13:V:402:HEM:HMB1	13:V:402:HEM:HBB2	1.87	0.56
10:Y:76:ASP:HB2	10:Y:418:LEU:HD12	1.88	0.56
10:Y:462:ILE:HG23	10:Y:465:LEU:HB3	1.87	0.56
10:L:109:LEU:HG	10:L:146:LEU:HD11	1.87	0.56
10:Y:82:GLU:O	10:Y:199:GLN:NE2	2.39	0.56
13:V:402:HEM:HBA1	13:V:402:HEM:HHA	1.88	0.56
13:J:401:HEM:HBB2	13:J:401:HEM:HMB2	1.87	0.56
10:L:39:ALA:O	10:L:43:GLN:HG2	2.05	0.56
10:L:279:ASP:H	10:L:460:GLY:HA3	1.69	0.56
9:K:451:ASP:OD2	9:W:183:ARG:NH2	2.39	0.55
9:K:60:ARG:HG3	9:K:124:GLU:HG2	1.89	0.55
9:K:173:VAL:HG21	9:K:268:HIS:HB2	1.88	0.55
7:U:121:CYS:SG	12:U:401:HEC:HBB2	2.45	0.55
10:Y:286:HIS:HE1	10:Y:359:VAL:HG22	1.71	0.55
4:E:29:PRO:HB3	4:E:89:ASN:HD22	1.72	0.55
9:K:115:THR:HG23	9:K:118:ASN:H	1.71	0.55
8:V:240:MET:O	8:V:244:LEU:HB2	2.06	0.55
10:L:183:VAL:HG21	10:L:286:HIS:HB3	1.87	0.55
10:L:301:ASN:O	10:L:305:GLN:HG2	2.06	0.55
10:L:82:GLU:O	10:L:199:GLN:NE2	2.40	0.55
5:S:28:ASN:HD22	5:S:82:THR:HB	1.72	0.55
8:V:74:ASN:OD1	8:V:74:ASN:N	2.29	0.55
2:C:172:LYS:HD3	2:C:216:VAL:HG21	1.89	0.55
7:H:247:PRO:HB3	12:H:401:HEC:CHC	2.37	0.55
10:L:160:GLN:HE21	10:L:164:GLU:HG2	1.71	0.55
10:L:190:THR:O	10:L:273:SER:OG	2.25	0.55
10:L:104:ARG:NH1	10:L:149:ASP:OD2	2.40	0.54
2:C:217:CYS:N	2:C:222:CYS:O	2.38	0.54
7:H:167:ARG:HG2	7:H:168:PRO:HD2	1.88	0.54
10:Y:77:VAL:HG21	10:Y:223:HIS:HB3	1.88	0.54
9:W:42:LYS:HG2	9:W:48:VAL:HG22	1.90	0.54
10:L:109:LEU:O	10:L:113:VAL:HG23	2.07	0.54
8:J:47:THR:HG23	8:J:79:ILE:HG23	1.90	0.54
8:J:361:THR:HG22	8:J:365:LEU:HD12	1.88	0.54
10:Y:109:LEU:O	10:Y:113:VAL:HG23	2.06	0.54
10:Y:415:ARG:O	10:Y:419:THR:HB	2.08	0.54
7:H:107:HIS:ND1	7:H:138:VAL:O	2.40	0.54
10:L:189:ALA:HA	10:L:198:ALA:HB1	1.89	0.54
8:J:107:PHE:HB2	8:J:305:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:160:GLN:NE2	10:Y:164:GLU:OE2	2.41	0.54
8:J:8:ASN:HD22	8:J:11:MET:H	1.55	0.54
8:J:172:SER:N	8:J:173:PRO:HD2	2.23	0.54
7:U:135:LEU:HA	7:U:138:VAL:HG12	1.89	0.54
9:W:115:THR:HG23	9:W:118:ASN:H	1.72	0.54
9:W:82:LEU:HD21	9:W:151:VAL:HG13	1.89	0.53
10:Y:192:PHE:HB2	10:Y:198:ALA:HB2	1.90	0.53
2:C:241:SER:OG	11:C:301:FES:S1	2.53	0.53
5:F:36:ASP:OD1	5:F:90:TYR:OH	2.20	0.53
9:W:396:VAL:HA	9:W:399:GLN:HE21	1.73	0.53
9:W:223:LEU:HD11	9:W:393:LEU:HB2	1.90	0.53
2:P:241:SER:OG	11:P:301:FES:S1	2.59	0.53
1:A:27:TYR:CE2	7:H:305:THR:HG22	2.43	0.53
10:L:80:ARG:HD3	10:L:197:LEU:HD13	1.91	0.53
7:U:155:GLN:HE21	7:U:164:MET:HG2	1.72	0.53
9:K:141:THR:HG23	9:K:142:THR:HG23	1.90	0.53
10:L:152:GLN:HE21	10:L:253:ILE:HG13	1.74	0.53
7:U:133:ARG:C	7:U:135:LEU:H	2.17	0.53
9:K:180:ALA:HB2	9:K:258:ILE:HG13	1.91	0.53
7:U:288:MET:HE2	8:V:77:TRP:CH2	2.44	0.53
7:U:324:PRO:HD3	1:N:13:HIS:CE1	2.44	0.53
10:Y:70:THR:OG1	10:Y:410:CYS:SG	2.66	0.53
2:P:236:CYS:SG	11:P:301:FES:S2	3.07	0.53
9:W:131:ASP:N	9:W:131:ASP:OD1	2.42	0.53
9:K:207:TYR:O	9:K:211:ASN:ND2	2.34	0.53
8:V:221:HIS:HB3	10:Y:470:ARG:NH1	2.24	0.52
9:K:175:GLU:OE2	9:K:190:LEU:N	2.40	0.52
10:L:280:ASP:HA	10:L:461:PRO:HB3	1.89	0.52
9:W:60:ARG:HG2	9:W:393:LEU:HD22	1.91	0.52
10:Y:274:GLU:HG2	1:N:18:SER:HB2	1.92	0.52
7:H:140:TYR:HB3	7:H:144:GLU:HG3	1.90	0.52
9:K:359:LYS:O	9:K:363:GLN:HG2	2.09	0.52
9:W:209:VAL:HG12	9:W:241:ARG:HH12	1.74	0.52
8:J:315:MET:HE1	8:J:325:TYR:HB2	1.90	0.52
9:W:370:ASP:N	9:W:370:ASP:OD1	2.43	0.52
8:J:5:ARG:HA	8:J:11:MET:HB3	1.90	0.52
8:V:165:TRP:O	8:V:174:THR:OG1	2.22	0.52
9:W:151:VAL:O	9:W:155:GLN:HG2	2.10	0.52
7:U:117:TYR:HA	7:U:121:CYS:SG	2.50	0.52
1:A:66:GLU:OE1	1:A:69:ARG:NH1	2.43	0.52
9:K:183:ARG:HE	9:K:254:ARG:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:386:VAL:HG13	9:W:392:PHE:HD1	1.75	0.52
1:A:61:THR:O	1:A:65:GLU:HG2	2.09	0.52
10:L:68:THR:HG22	10:L:136:LEU:HD12	1.91	0.52
5:S:38:ILE:HD12	8:V:379:TRP:HE1	1.75	0.51
1:N:61:THR:O	1:N:65:GLU:HG2	2.10	0.51
2:C:101:LYS:HG3	2:C:105:GLU:HB3	1.92	0.51
3:D:25:ILE:O	3:D:29:VAL:HG23	2.10	0.51
4:E:28:ASP:OD1	7:H:262:THR:OG1	2.28	0.51
5:F:36:ASP:OD2	5:F:62:ARG:NH1	2.42	0.51
7:H:217:GLY:O	7:H:234:ASN:ND2	2.44	0.51
9:W:180:ALA:HB2	9:W:258:ILE:HG13	1.93	0.51
5:F:107:GLU:HG3	5:F:111:LYS:HE2	1.92	0.51
7:H:133:ARG:C	7:H:135:LEU:H	2.17	0.51
7:H:125:HIS:HE1	7:H:195:PRO:HD2	1.75	0.51
9:K:82:LEU:HD21	9:K:151:VAL:HG13	1.92	0.51
10:L:120:LEU:HD13	10:L:133:ILE:HG12	1.92	0.51
7:U:98:HIS:NE2	7:U:208:GLU:OE2	2.38	0.51
8:J:128:PHE:O	8:J:132:VAL:HG23	2.10	0.51
8:J:287:LYS:HE2	2:P:255:PRO:HG3	1.93	0.51
8:J:372:ILE:O	8:J:376:MET:HG2	2.11	0.51
9:W:70:ARG:HB2	9:W:185:ALA:HB1	1.91	0.51
9:W:271:PHE:CE1	9:W:351:ILE:HG22	2.46	0.51
10:Y:190:THR:HB	10:Y:275:ILE:HG13	1.92	0.51
10:Y:411:GLU:OE1	10:Y:415:ARG:NH1	2.44	0.51
9:K:123:VAL:HG21	9:K:133:LEU:HB3	1.92	0.51
10:L:403:LEU:HD12	10:L:426:LEU:HD11	1.93	0.51
5:F:109:ALA:O	6:T:9:ARG:HD3	2.10	0.51
13:J:402:HEM:HBA1	13:J:402:HEM:HHA	1.92	0.51
10:L:310:ILE:HD11	10:L:388:VAL:HA	1.93	0.51
2:P:164:ASN:HD22	2:P:226:ALA:HB2	1.76	0.51
10:Y:68:THR:HG22	10:Y:136:LEU:HA	1.92	0.51
10:Y:87:ASN:HD21	10:Y:199:GLN:HB2	1.76	0.51
9:K:357:GLN:O	9:K:360:THR:OG1	2.23	0.51
7:H:228:ARG:HG3	7:H:230:GLY:H	1.76	0.50
8:J:26:ASN:HD21	8:J:207:ASN:HD22	1.59	0.50
8:J:131:TYR:O	8:J:134:PRO:HD2	2.11	0.50
5:S:69:LEU:HD11	5:S:76:LEU:HD13	1.92	0.50
7:U:189:ASN:HD22	7:U:194:PRO:HD3	1.75	0.50
1:A:74:ASN:HD22	1:A:74:ASN:H	1.58	0.50
5:F:69:LEU:HD11	5:F:76:LEU:HD13	1.93	0.50
10:L:231:LEU:HD22	10:L:250:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:202:ARG:NH2	8:J:81:TYR:OH	2.38	0.50
2:P:145:ASP:OD1	2:P:146:VAL:N	2.45	0.50
7:U:202:ARG:HG3	7:U:278:SER:HB3	1.94	0.50
7:U:262:THR:HG22	7:U:264:SER:H	1.75	0.50
8:V:128:PHE:O	8:V:132:VAL:HG23	2.11	0.50
8:V:146:ILE:O	8:V:149:LEU:HB3	2.12	0.50
8:V:277:ALA:HB1	8:V:294:LEU:HD13	1.92	0.50
2:C:85:VAL:HG22	10:L:275:ILE:HD11	1.92	0.50
10:Y:103:ASN:OD1	10:Y:153:ASN:ND2	2.44	0.50
5:F:13:TRP:CE2	5:F:17:ILE:HD11	2.46	0.50
9:K:60:ARG:HG2	9:K:393:LEU:HD22	1.93	0.50
9:W:359:LYS:O	9:W:363:GLN:HG2	2.12	0.50
8:J:137:GLN:NE2	8:J:263:ASN:O	2.45	0.50
9:K:370:ASP:N	9:K:370:ASP:OD1	2.44	0.50
5:S:34:ARG:NH2	5:S:92:GLU:OE2	2.44	0.50
9:W:216:ALA:HB3	9:W:244:LEU:H	1.77	0.50
9:W:272:VAL:HG22	9:W:337:GLY:HA3	1.93	0.50
7:H:142:GLU:O	7:H:146:LYS:HG3	2.11	0.50
8:J:119:LEU:HD11	8:J:192:LEU:HB3	1.94	0.50
10:Y:121:ASN:ND2	10:Y:132:TYR:OH	2.45	0.50
1:A:12:ARG:HB3	1:A:13:HIS:CE1	2.47	0.50
9:K:155:GLN:NE2	9:K:200:VAL:O	2.45	0.50
10:L:121:ASN:ND2	10:L:132:TYR:OH	2.45	0.50
10:Y:206:GLU:HG3	10:Y:210:LYS:HE3	1.93	0.50
10:Y:231:LEU:HD22	10:Y:250:LEU:HD12	1.93	0.50
2:C:123:VAL:HA	3:D:29:VAL:HG22	1.93	0.49
9:K:223:LEU:HG	9:K:393:LEU:HD13	1.93	0.49
10:Y:294:PRO:HG3	10:Y:448:TYR:CZ	2.47	0.49
10:Y:190:THR:O	10:Y:273:SER:OG	2.30	0.49
10:Y:383:ALA:H	10:Y:442:ARG:HD3	1.77	0.49
7:U:117:TYR:CD1	7:U:121:CYS:HB2	2.47	0.49
9:W:85:LEU:HD12	9:W:158:LEU:HD23	1.93	0.49
10:Y:42:LEU:HD11	10:Y:430:GLU:HG3	1.94	0.49
10:Y:373:GLN:O	10:Y:377:MET:HG2	2.11	0.49
10:L:101:THR:OG1	10:L:153:ASN:O	2.26	0.49
5:F:67:LEU:HD23	8:J:209:LEU:HD12	1.94	0.49
5:F:13:TRP:O	5:F:17:ILE:HG13	2.12	0.49
8:J:19:ILE:HG23	8:J:221:HIS:HB2	1.95	0.49
8:J:119:LEU:CD1	8:J:192:LEU:HB3	2.43	0.49
8:V:26:ASN:HD21	8:V:207:ASN:HD22	1.61	0.49
10:Y:104:ARG:NH1	10:Y:149:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:240:MET:O	8:J:244:LEU:HB2	2.12	0.49
10:L:89:ALA:HA	10:L:211:LEU:HD21	1.95	0.49
4:R:47:ARG:O	4:R:51:GLU:HG2	2.12	0.49
9:W:65:ILE:HG21	9:W:213:PHE:CD1	2.48	0.49
2:P:101:LYS:HE3	2:P:105:GLU:HG3	1.94	0.49
8:V:141:TRP:O	8:V:145:VAL:HG23	2.12	0.49
10:L:91:TYR:CE2	10:L:202:GLU:HG3	2.47	0.49
10:L:437:ASP:OD1	10:L:438:ALA:N	2.45	0.49
9:W:155:GLN:HE22	9:W:200:VAL:HB	1.77	0.49
9:K:127:ARG:HD2	10:L:41:ALA:HB2	1.94	0.48
10:Y:278:ARG:HH22	10:Y:463:GLU:CD	2.21	0.48
10:Y:310:ILE:HD11	10:Y:388:VAL:HA	1.94	0.48
8:J:366:MET:HB3	8:J:367:PRO:HD3	1.95	0.48
9:K:38:LEU:HG	9:K:52:LEU:HD13	1.94	0.48
3:Q:25:ILE:O	3:Q:29:VAL:HG23	2.13	0.48
5:S:29:LYS:HB3	5:S:75:ILE:HG13	1.95	0.48
5:F:17:ILE:HG22	8:J:376:MET:HE1	1.93	0.48
9:K:71:TYR:HB3	9:K:212:HIS:CE1	2.48	0.48
9:K:348:GLY:HA2	9:K:448:PRO:HD3	1.94	0.48
2:P:209:GLU:HG2	2:P:210:TRP:CD1	2.48	0.48
9:W:223:LEU:HG	9:W:393:LEU:HD13	1.94	0.48
2:C:158:ASP:OD1	2:C:159:ILE:N	2.36	0.48
7:U:201:VAL:O	7:U:207:GLY:HA2	2.14	0.48
8:V:201:HIS:HB3	1:N:3:ARG:HH22	1.78	0.48
9:W:333:SER:OG	9:W:334:GLY:N	2.47	0.48
8:V:3:PRO:HG2	8:V:6:LYS:HG2	1.96	0.48
10:Y:101:THR:OG1	10:Y:153:ASN:O	2.27	0.48
10:Y:171:GLU:OE2	10:Y:175:ASN:ND2	2.47	0.48
9:K:65:ILE:HG21	9:K:213:PHE:CD1	2.48	0.48
2:C:222:CYS:SG	8:V:145:VAL:HG22	2.53	0.48
2:C:234:TYR:HB2	2:C:243:TYR:HB2	1.94	0.48
9:K:333:SER:OG	9:K:334:GLY:N	2.46	0.48
7:U:112:ARG:O	7:U:116:VAL:HG23	2.14	0.48
7:H:215:LEU:HD11	12:H:401:HEC:HMB3	1.96	0.48
10:L:373:GLN:O	10:L:377:MET:HG2	2.13	0.48
2:P:233:GLY:HA3	2:P:244:ASP:C	2.38	0.48
7:H:289:GLY:HA2	8:J:244:LEU:HD23	1.96	0.48
9:K:131:ASP:N	9:K:131:ASP:OD1	2.46	0.48
2:C:138:SER:O	2:C:141:SER:OG	2.29	0.47
8:V:30:TRP:O	8:V:100:ARG:HD3	2.14	0.47
2:C:209:GLU:HG3	2:C:210:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:47:ARG:O	4:E:51:GLU:HG2	2.14	0.47
8:J:148:ASN:ND2	2:P:221:GLY:HA3	2.29	0.47
10:Y:337:LEU:O	10:Y:368:MET:HE2	2.13	0.47
9:K:421:ASN:O	9:K:425:ILE:HG12	2.14	0.47
9:K:386:VAL:HG13	9:K:392:PHE:HD1	1.79	0.47
10:L:48:THR:HA	10:L:61:SER:O	2.15	0.47
2:P:154:ILE:HA	2:P:272:ILE:HG22	1.97	0.47
2:P:181:GLN:HA	2:P:184:ILE:HD12	1.95	0.47
8:V:222:PRO:HG2	8:V:223:TYR:CD2	2.49	0.47
9:W:355:TYR:CE1	9:W:436:LYS:HE2	2.50	0.47
10:Y:270:PHE:CG	10:Y:292:GLU:HB2	2.49	0.47
1:A:13:HIS:N	10:L:278:ARG:O	2.48	0.47
8:V:25:SER:HB3	8:V:218:ILE:HG13	1.97	0.47
4:E:37:CYS:O	4:E:40:LEU:N	2.30	0.47
9:K:159:LYS:HG2	9:K:197:ILE:HG21	1.96	0.47
4:R:35:GLU:O	4:R:39:GLN:HG2	2.15	0.47
7:U:126:SER:OG	7:U:128:ASP:OD1	2.28	0.47
7:U:222:PRO:HD2	7:U:225:VAL:HG11	1.97	0.47
9:W:71:TYR:HB3	9:W:212:HIS:CE1	2.49	0.47
9:W:261:GLN:NE2	9:W:443:ASN:O	2.47	0.47
10:Y:403:LEU:HD23	10:Y:403:LEU:HA	1.74	0.47
10:Y:189:ALA:HA	10:Y:198:ALA:HB1	1.96	0.47
10:Y:416:SER:OG	10:Y:422:ARG:O	2.31	0.47
10:Y:437:ASP:OD1	10:Y:438:ALA:N	2.46	0.47
2:C:186:GLN:O	2:C:190:VAL:HG23	2.14	0.47
2:P:176:VAL:HG13	2:P:212:ILE:HG12	1.97	0.47
8:V:366:MET:HB3	8:V:367:PRO:HD3	1.98	0.46
9:W:177:LEU:HD21	9:W:272:VAL:HG21	1.97	0.46
5:F:29:LYS:HD3	5:F:75:ILE:HD13	1.96	0.46
8:J:177:ARG:HD3	8:V:53:MET:HB3	1.98	0.46
5:S:97:GLU:OE1	5:S:100:ARG:NH2	2.48	0.46
10:Y:92:PHE:O	10:Y:96:LEU:HG	2.15	0.46
10:Y:278:ARG:HH12	10:Y:463:GLU:HG3	1.80	0.46
5:F:34:ARG:HD2	8:J:377:LEU:HB3	1.98	0.46
7:H:116:VAL:HA	7:H:253:LEU:HD13	1.98	0.46
8:J:183:PHE:CZ	13:J:401:HEM:HBC1	2.50	0.46
10:L:71:VAL:HG13	10:L:233:ALA:HB2	1.98	0.46
10:L:293:GLY:N	10:L:352:GLY:O	2.45	0.46
2:P:199:GLN:CD	2:P:204:ARG:HE	2.24	0.46
9:W:357:GLN:O	9:W:360:THR:OG1	2.23	0.46
10:Y:101:THR:HA	10:Y:155:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:158:ASP:O	10:Y:162:GLU:HG2	2.16	0.46
9:K:84:ARG:HH11	9:K:114:ALA:HB3	1.80	0.46
9:K:323:VAL:HG13	9:K:340:THR:HG22	1.96	0.46
5:S:28:ASN:ND2	5:S:82:THR:O	2.48	0.46
7:H:201:VAL:HG11	7:H:275:ARG:HD2	1.98	0.46
9:K:195:TYR:CZ	9:K:196:ARG:HG2	2.51	0.46
10:L:96:LEU:HB3	10:L:164:GLU:HG3	1.98	0.46
10:L:377:MET:HE2	10:L:476:PHE:HA	1.98	0.46
7:U:217:GLY:O	7:U:234:ASN:ND2	2.49	0.46
10:L:92:PHE:O	10:L:96:LEU:HG	2.15	0.46
10:L:168:ILE:N	10:L:168:ILE:HD13	2.31	0.46
8:J:191:ALA:O	8:J:194:THR:OG1	2.24	0.46
7:U:296:MET:HG3	8:V:237:LEU:HD13	1.98	0.46
8:V:89:MET:HB3	8:V:235:PHE:HE1	1.81	0.46
9:W:323:VAL:HG22	9:W:340:THR:HG22	1.98	0.46
9:W:323:VAL:HG13	9:W:340:THR:HG22	1.98	0.46
4:E:45:LYS:O	4:E:48:GLU:HG2	2.15	0.45
10:L:86:ASN:HB2	10:L:89:ALA:HB2	1.98	0.45
10:L:113:VAL:HG22	10:L:146:LEU:HD21	1.97	0.45
2:P:131:ASN:O	2:P:135:GLN:HG2	2.15	0.45
7:U:243:ALA:HB3	12:U:401:HEC:HBD2	1.97	0.45
10:Y:296:TRP:HB3	10:Y:419:THR:HG23	1.97	0.45
8:J:74:ASN:N	8:J:74:ASN:OD1	2.49	0.45
10:L:387:GLU:OE2	10:L:390:ARG:NH2	2.46	0.45
10:Y:96:LEU:HB3	10:Y:164:GLU:HG3	1.99	0.45
10:Y:125:THR:HG22	10:Y:126:ARG:H	1.81	0.45
1:N:20:SER:HB3	1:N:23:GLU:HG2	1.98	0.45
4:R:28:ASP:OD1	4:R:28:ASP:N	2.41	0.45
4:R:53:CYS:HA	4:R:56:ARG:HH11	1.81	0.45
7:U:306:ILE:O	7:U:310:LYS:HG2	2.16	0.45
8:V:27:ILE:HG23	8:V:31:TRP:HB2	1.97	0.45
9:W:356:ASN:HA	9:W:359:LYS:HD3	1.99	0.45
5:F:38:ILE:HD12	8:J:379:TRP:HE1	1.81	0.45
9:K:241:ARG:HB3	9:K:242:GLY:H	1.53	0.45
8:J:138:MET:HE1	8:J:268:ILE:HA	1.98	0.45
10:L:151:VAL:HG11	10:L:229:MET:HE1	1.98	0.45
2:C:111:LYS:NZ	10:L:451:ASP:O	2.46	0.45
2:C:155:LYS:HB2	2:C:273:VAL:HB	1.99	0.45
2:C:159:ILE:HG23	2:C:210:TRP:CZ2	2.52	0.45
8:J:3:PRO:HB2	8:J:5:ARG:HG2	1.99	0.45
13:V:402:HEM:HHA	13:V:402:HEM:HBD1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:HB2	10:L:272:GLY:O	2.16	0.45
2:C:123:VAL:HG13	3:D:29:VAL:HA	1.98	0.45
5:F:71:LEU:HD21	7:H:314:LEU:HB3	1.99	0.45
7:H:105:LEU:HB3	7:H:110:ILE:HD11	1.98	0.45
7:H:126:SER:OG	7:H:128:ASP:OD1	2.33	0.45
7:H:171:LEU:HD12	7:H:171:LEU:H	1.82	0.45
7:U:167:ARG:NH1	7:U:173:ASP:OD2	2.37	0.45
7:U:244:MET:HB2	12:U:401:HEC:C1D	2.47	0.45
8:V:121:LEU:HD21	8:V:298:ILE:HG21	1.99	0.45
2:P:244:ASP:OD1	2:P:248:ARG:N	2.49	0.45
10:Y:74:TRP:CZ2	10:Y:411:GLU:HA	2.52	0.45
1:A:20:SER:HB3	1:A:23:GLU:HG2	1.98	0.45
9:W:287:SER:O	9:W:290:GLN:HG2	2.16	0.45
9:K:287:SER:O	9:K:290:GLN:HG2	2.17	0.45
10:L:87:ASN:HD21	10:L:199:GLN:HB2	1.82	0.45
10:L:192:PHE:HB2	10:L:198:ALA:HB2	1.99	0.45
5:S:34:ARG:HD2	8:V:377:LEU:HB3	1.99	0.45
9:K:90:THR:HG22	9:K:150:GLU:OE1	2.17	0.44
9:K:115:THR:OG1	9:K:116:ARG:N	2.49	0.44
2:P:151:LYS:H	2:P:170:ARG:HH21	1.65	0.44
3:Q:48:ASN:HD21	7:U:103:SER:HA	1.80	0.44
2:C:151:LYS:HA	2:C:170:ARG:HH21	1.81	0.44
6:G:39:ARG:HA	6:G:42:LEU:HB2	2.00	0.44
9:K:55:TYR:HA	9:K:127:ARG:HH21	1.82	0.44
7:U:115:GLN:O	7:U:119:GLN:HG2	2.17	0.44
9:W:195:TYR:CZ	9:W:196:ARG:HG2	2.52	0.44
8:J:89:MET:HB3	8:J:235:PHE:HE1	1.81	0.44
9:K:291:HIS:CD2	9:K:378:LEU:HG	2.53	0.44
9:K:356:ASN:HA	9:K:359:LYS:HD3	1.99	0.44
10:L:467:ASP:OD1	10:L:468:TYR:N	2.49	0.44
2:P:231:PHE:CE2	2:P:250:ARG:HB2	2.53	0.44
9:W:364:GLY:HA2	9:W:425:ILE:HD13	2.00	0.44
1:N:76:ALA:HA	1:N:79:GLU:HB3	2.00	0.44
9:K:244:LEU:HD23	9:K:244:LEU:HA	1.88	0.44
10:L:126:ARG:HH12	10:L:200:ALA:HA	1.83	0.44
9:W:57:PRO:HB2	10:Y:400:VAL:HG11	1.99	0.44
9:W:81:HIS:CD2	9:W:192:CYS:H	2.35	0.44
10:Y:140:LEU:HD22	10:Y:237:VAL:HG22	1.99	0.44
2:C:196:ARG:NH1	2:C:254:ALA:O	2.51	0.44
7:H:266:ILE:O	7:H:270:VAL:HG23	2.18	0.44
8:J:202:GLU:HG3	8:V:9:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:54:ASN:O	9:K:127:ARG:NH2	2.51	0.44
9:K:183:ARG:HB3	9:K:254:ARG:HD2	1.99	0.44
10:L:87:ASN:ND2	10:L:199:GLN:HB2	2.32	0.44
8:V:191:ALA:O	8:V:194:THR:OG1	2.29	0.44
1:A:16:SER:HA	7:H:319:LEU:HA	1.99	0.44
8:J:271:GLU:HG2	8:J:273:TYR:CZ	2.52	0.44
9:K:134:MET:HE1	9:K:220:LEU:HD11	1.98	0.44
10:L:58:ARG:HB2	10:L:230:VAL:HG22	1.99	0.44
10:L:160:GLN:NE2	10:L:164:GLU:OE2	2.50	0.44
4:R:57:VAL:HG13	4:R:63:THR:HG21	2.00	0.44
7:U:319:LEU:HA	1:N:16:SER:HA	2.00	0.44
9:K:214:THR:HG21	9:K:244:LEU:C	2.43	0.44
2:C:80:HIS:CD2	10:L:182:VAL:HG22	2.52	0.44
9:K:451:ASP:OD1	9:K:451:ASP:N	2.50	0.44
9:W:70:ARG:HD2	9:W:117:GLU:HG2	2.00	0.44
9:W:271:PHE:HE1	9:W:351:ILE:HG22	1.82	0.44
4:E:60:ARG:HH22	4:E:65:GLU:HB2	1.83	0.44
5:F:37:THR:HG22	8:J:312:GLN:HG2	1.99	0.44
7:H:185:ALA:HB1	7:H:194:PRO:HD2	2.00	0.44
10:L:460:GLY:HA2	10:L:462:ILE:N	2.33	0.44
2:P:262:THR:O	2:P:273:VAL:HG11	2.18	0.44
8:V:200:LEU:HD13	13:V:402:HEM:HAD2	1.98	0.44
7:H:296:MET:HG2	8:J:237:LEU:HG	1.99	0.43
8:J:173:PRO:O	8:J:177:ARG:HG2	2.18	0.43
10:L:125:THR:HG22	10:L:126:ARG:H	1.83	0.43
3:Q:34:ARG:NE	6:T:51:LYS:HB3	2.33	0.43
8:V:372:ILE:O	8:V:376:MET:HG2	2.18	0.43
9:W:271:PHE:CD2	9:W:453:LEU:HD21	2.53	0.43
8:J:51:LEU:HD13	13:J:401:HEM:HBD1	2.00	0.43
10:Y:278:ARG:HD3	1:N:11:MET:HB2	2.00	0.43
4:E:34:ARG:HG3	4:E:78:ARG:HD2	2.00	0.43
9:K:81:HIS:CD2	9:K:192:CYS:H	2.37	0.43
8:V:58:ASP:HB2	8:V:61:THR:OG1	2.18	0.43
8:V:361:THR:HA	8:V:365:LEU:HB2	2.00	0.43
10:Y:160:GLN:O	10:Y:164:GLU:HG2	2.18	0.43
10:Y:338:CYS:HA	10:Y:368:MET:HE2	2.00	0.43
2:C:218:THR:OG1	2:C:254:ALA:HB1	2.17	0.43
2:C:223:VAL:HB	8:V:264:THR:OG1	2.19	0.43
7:H:107:HIS:CE1	7:H:138:VAL:HG23	2.53	0.43
10:L:69:CYS:HA	10:L:406:THR:HG21	1.99	0.43
2:P:161:GLU:HG3	2:P:178:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:177:ARG:HB3	2:P:211:VAL:HG13	2.01	0.43
8:V:126:THR:HG21	13:V:401:HEM:HBB2	2.00	0.43
9:W:214:THR:HG21	9:W:245:GLY:H	1.82	0.43
9:W:267:VAL:HG11	9:W:347:ALA:HB2	1.98	0.43
10:Y:88:GLY:H	10:Y:207:ASN:ND2	2.15	0.43
2:C:201:ASP:O	2:C:205:VAL:HG22	2.19	0.43
9:K:293:LEU:HD21	9:K:358:VAL:HG22	2.01	0.43
9:W:90:THR:HG22	9:W:150:GLU:OE1	2.18	0.43
5:S:43:ASP:OD2	5:S:102:ARG:NH1	2.51	0.43
6:T:39:ARG:NH2	6:T:52:PHE:HB3	2.33	0.43
8:J:88:SER:HB3	8:J:250:LEU:HD23	2.01	0.43
9:K:91:THR:OG1	9:K:139:ASN:HB3	2.19	0.43
10:L:41:ALA:HA	10:L:44:PHE:HD2	1.83	0.43
3:Q:52:LEU:HD12	3:Q:54:LYS:HE3	1.99	0.43
7:H:228:ARG:HD2	7:H:229:GLU:H	1.83	0.43
9:K:381:GLY:HA2	9:K:384:MET:HE2	1.99	0.43
10:L:38:PHE:CE2	10:L:42:LEU:HD11	2.54	0.43
8:V:129:MET:HE1	8:V:185:LEU:HD12	2.00	0.43
8:V:377:LEU:HD23	8:V:377:LEU:HA	1.90	0.43
2:C:157:SER:O	2:C:270:MET:HA	2.19	0.43
9:K:45:ASN:OD1	9:K:46:GLY:N	2.52	0.43
9:K:51:SER:OG	9:K:225:VAL:O	2.36	0.43
9:K:97:PHE:O	9:K:101:ARG:HG2	2.19	0.43
9:K:395:GLU:OE2	9:K:399:GLN:NE2	2.49	0.43
2:P:186:GLN:O	2:P:190:VAL:HG23	2.19	0.43
10:Y:75:ILE:HG22	10:Y:77:VAL:HG23	2.01	0.43
2:C:155:LYS:HZ3	2:C:168:LYS:H	1.66	0.43
2:P:123:VAL:HA	3:Q:29:VAL:HG22	2.01	0.43
5:S:83:LYS:HB2	5:S:86:GLU:HB3	2.01	0.43
9:W:79:THR:HG23	9:W:205:LEU:HD23	2.01	0.43
9:W:116:ARG:NH1	9:W:188:ASN:O	2.51	0.43
9:W:272:VAL:HG13	9:W:336:PHE:C	2.44	0.43
10:Y:48:THR:HA	10:Y:61:SER:O	2.18	0.43
10:Y:82:GLU:HG2	10:Y:219:TYR:HE1	1.84	0.43
1:N:73:LYS:HG2	1:N:74:ASN:H	1.84	0.43
2:C:172:LYS:HE2	2:C:172:LYS:HB3	1.84	0.42
8:J:338:ILE:HD11	8:J:350:ILE:HG22	2.00	0.42
9:K:432:VAL:O	9:K:436:LYS:NZ	2.52	0.42
10:L:160:GLN:O	10:L:164:GLU:HG2	2.19	0.42
2:P:130:LYS:HD2	6:T:34:TRP:CE2	2.53	0.42
9:W:259:ARG:HH21	9:W:444:LEU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:387:GLU:OE2	10:Y:390:ARG:NH2	2.46	0.42
2:C:253:PRO:HA	8:V:285:PRO:O	2.18	0.42
4:E:35:GLU:O	4:E:39:GLN:HG2	2.19	0.42
9:K:309:LEU:HD23	9:K:323:VAL:HG12	2.01	0.42
2:P:217:CYS:HB3	2:P:222:CYS:H	1.82	0.42
8:V:173:PRO:HB2	8:V:177:ARG:NH1	2.34	0.42
8:V:276:PHE:CG	8:V:277:ALA:N	2.87	0.42
9:W:127:ARG:HD2	10:Y:41:ALA:HB2	2.01	0.42
10:Y:405:GLY:C	10:Y:408:PRO:HD2	2.45	0.42
2:C:160:PRO:HD2	2:C:210:TRP:CZ3	2.55	0.42
3:D:51:LYS:O	7:H:107:HIS:HD2	2.03	0.42
4:E:46:ALA:HB1	4:E:74:PHE:HA	2.01	0.42
10:L:128:HIS:ND1	10:L:418:LEU:HD23	2.34	0.42
4:E:60:ARG:NH2	4:E:63:THR:OG1	2.52	0.42
8:J:34:GLY:O	8:J:37:LEU:HB2	2.19	0.42
2:P:80:HIS:HB2	10:Y:182:VAL:HG22	2.00	0.42
5:S:75:ILE:HD11	5:S:81:TRP:CZ2	2.54	0.42
8:V:324:LEU:HD23	8:V:324:LEU:HA	1.87	0.42
10:Y:336:LYS:HG3	10:Y:337:LEU:HD22	2.01	0.42
9:K:60:ARG:HE	9:K:60:ARG:HB2	1.73	0.42
7:U:91:PRO:HA	7:U:92:PRO:HD3	1.87	0.42
10:Y:467:ASP:OD1	10:Y:468:TYR:N	2.49	0.42
2:C:183:GLU:HA	2:C:186:GLN:HG2	2.02	0.42
7:H:135:LEU:HA	7:H:138:VAL:CG1	2.49	0.42
8:J:180:THR:O	8:J:184:ILE:HG22	2.19	0.42
4:R:45:LYS:HA	4:R:48:GLU:HG2	2.00	0.42
6:T:9:ARG:HE	10:Y:384:THR:HG21	1.85	0.42
8:V:176:THR:O	8:V:180:THR:HG23	2.20	0.42
8:V:369:ILE:HD13	8:V:369:ILE:HA	1.94	0.42
9:W:401:LEU:HD23	9:W:401:LEU:HA	1.86	0.42
10:Y:113:VAL:HA	10:Y:116:MET:HE2	2.01	0.42
1:N:40:ARG:HG3	1:N:41:ARG:N	2.35	0.42
7:H:270:VAL:HG11	12:H:401:HEC:HBB3	2.00	0.42
10:L:88:GLY:H	10:L:207:ASN:ND2	2.18	0.42
2:P:123:VAL:HG13	3:Q:29:VAL:HA	2.02	0.42
2:P:241:SER:HA	2:P:252:GLY:HA3	2.00	0.42
7:U:124:CYS:SG	12:U:401:HEC:HBC2	2.60	0.42
6:G:13:LEU:HD11	10:L:382:SER:HB3	2.02	0.42
9:K:42:LYS:HG2	9:K:48:VAL:HG22	2.01	0.42
9:K:141:THR:HG23	9:K:142:THR:N	2.35	0.42
4:R:30:LEU:HD21	7:U:216:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:220:LEU:HD23	10:Y:224:TYR:CD2	2.54	0.42
4:E:82:VAL:O	4:E:86:LEU:HB2	2.19	0.42
5:F:43:ASP:OD2	5:F:102:ARG:NH1	2.52	0.42
7:H:292:MET:HG3	7:H:293:LEU:N	2.33	0.42
8:J:337:TRP:O	8:J:341:GLN:HG2	2.20	0.42
9:K:170:GLN:O	9:K:174:ILE:HG12	2.19	0.42
10:L:73:VAL:HG23	10:L:147:LEU:HD13	2.00	0.42
8:V:236:LEU:O	8:V:240:MET:HG2	2.20	0.42
9:W:97:PHE:O	9:W:101:ARG:HG2	2.20	0.42
9:W:268:HIS:CD2	9:W:441:SER:HB3	2.55	0.42
9:W:373:ALA:O	9:W:377:LYS:HG3	2.19	0.42
10:Y:121:ASN:HB3	10:Y:132:TYR:CE2	2.55	0.42
1:A:12:ARG:HH11	10:L:281:ALA:HB3	1.83	0.42
9:K:383:LEU:HD12	10:L:136:LEU:HD11	2.02	0.42
10:L:361:ASP:OD1	10:L:362:ARG:N	2.53	0.42
8:V:100:ARG:HH22	13:V:402:HEM:HBD2	1.85	0.42
9:W:51:SER:HA	9:W:222:GLY:O	2.19	0.42
2:C:231:PHE:CE2	2:C:250:ARG:HB2	2.55	0.41
2:P:242:HIS:HD2	2:P:251:LEU:HD22	1.85	0.41
5:S:44:VAL:O	5:S:48:ILE:HG12	2.19	0.41
9:W:57:PRO:O	9:W:127:ARG:HG3	2.19	0.41
9:W:348:GLY:O	9:W:351:ILE:HG13	2.20	0.41
2:C:217:CYS:N	2:C:224:PRO:HD3	2.35	0.41
9:K:43:LEU:HD11	9:K:234:ALA:HB1	2.01	0.41
9:K:300:LYS:HB2	10:L:121:ASN:HA	2.02	0.41
5:S:34:ARG:HD3	8:V:377:LEU:HD22	2.01	0.41
9:W:147:ARG:HD3	9:W:149:TRP:CZ2	2.55	0.41
7:H:98:HIS:NE2	7:H:208:GLU:OE2	2.44	0.41
8:J:54:HIS:HB2	8:J:69:ILE:HG12	2.02	0.41
9:W:298:HIS:HE1	9:W:377:LYS:HG2	1.84	0.41
10:Y:48:THR:HG22	10:Y:62:GLU:HB2	2.02	0.41
10:Y:179:MET:HE2	10:Y:286:HIS:HB2	2.03	0.41
7:H:288:MET:HE3	7:H:288:MET:HB3	1.82	0.41
8:J:58:ASP:HB2	8:J:61:THR:OG1	2.21	0.41
13:J:402:HEM:HMB1	13:J:402:HEM:HBB2	2.01	0.41
10:L:74:TRP:CZ2	10:L:411:GLU:HA	2.56	0.41
10:L:286:HIS:HD2	10:L:357:HIS:HE1	1.68	0.41
2:P:217:CYS:SG	2:P:243:TYR:OH	2.70	0.41
9:W:207:TYR:O	9:W:211:ASN:ND2	2.37	0.41
10:Y:87:ASN:ND2	10:Y:199:GLN:HB2	2.34	0.41
10:Y:278:ARG:O	10:Y:279:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:124:CYS:SG	12:H:401:HEC:HAC	2.60	0.41
7:H:222:PRO:O	7:H:225:VAL:HG12	2.21	0.41
9:K:148:ARG:HH22	5:S:52:PRO:HD3	1.85	0.41
2:P:201:ASP:O	2:P:205:VAL:HG22	2.20	0.41
10:Y:38:PHE:O	10:Y:42:LEU:HG	2.19	0.41
10:Y:338:CYS:HA	10:Y:368:MET:SD	2.60	0.41
1:N:74:ASN:N	1:N:75:PRO:HD3	2.34	0.41
2:C:157:SER:HB2	2:C:271:VAL:CG1	2.51	0.41
4:E:79:ASP:HB3	7:H:92:PRO:HG2	2.02	0.41
5:F:76:LEU:O	5:F:81:TRP:NE1	2.46	0.41
9:K:70:ARG:NH2	9:K:332:ASP:OD2	2.44	0.41
10:L:337:LEU:O	10:L:368:MET:HE2	2.20	0.41
2:P:222:CYS:SG	11:P:301:FES:S2	3.19	0.41
1:A:46:PHE:CE2	1:A:50:VAL:HG21	2.56	0.41
7:H:94:TYR:HB2	7:H:96:TRP:CZ3	2.55	0.41
4:R:65:GLU:HB2	1:N:78:TYR:CG	2.56	0.41
7:U:118:LYS:HD3	7:U:148:LEU:HD11	2.01	0.41
8:V:51:LEU:HD11	8:V:80:ARG:HA	2.01	0.41
8:V:111:GLU:HG2	8:V:199:PHE:CE1	2.55	0.41
2:C:205:VAL:HA	2:C:263:TYR:OH	2.20	0.41
6:G:9:ARG:NE	5:S:109:ALA:O	2.43	0.41
7:U:87:LEU:H	1:N:71:LYS:NZ	2.19	0.41
7:U:228:ARG:H	7:U:228:ARG:HD2	1.86	0.41
7:U:262:THR:HG22	7:U:264:SER:N	2.36	0.41
10:Y:293:GLY:N	10:Y:352:GLY:O	2.45	0.41
2:C:80:HIS:CG	10:L:182:VAL:HG22	2.56	0.41
2:C:164:ASN:HB2	2:C:177:ARG:HD3	2.02	0.41
2:C:233:GLY:HA3	2:C:244:ASP:C	2.46	0.41
5:F:44:VAL:O	5:F:48:ILE:HG12	2.21	0.41
5:F:61:PHE:CD1	7:H:321:TYR:HB2	2.55	0.41
3:Q:55:HIS:HA	3:Q:58:HIS:CD2	2.56	0.41
5:S:22:TYR:CD2	5:S:84:TYR:HB2	2.55	0.41
5:S:67:LEU:HD23	8:V:209:LEU:HD12	2.02	0.41
8:V:131:TYR:O	8:V:134:PRO:HD2	2.20	0.41
8:V:159:ASP:OD1	8:V:159:ASP:N	2.54	0.41
9:W:65:ILE:HG13	9:W:218:MET:HG2	2.03	0.41
10:Y:153:ASN:OD1	10:Y:153:ASN:N	2.53	0.41
10:Y:413:ILE:HG12	10:Y:423:ARG:HE	1.86	0.41
1:N:46:PHE:CE2	1:N:50:VAL:HG21	2.56	0.41
1:N:74:ASN:HB3	1:N:77:ALA:HB3	2.03	0.41
2:C:130:LYS:HD3	6:G:34:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40:LEU:HB2	4:E:43:CYS:SG	2.61	0.41
2:P:179:ARG:NH2	2:P:205:VAL:HG21	2.36	0.41
2:P:248:ARG:HA	2:P:257:ASN:HB3	2.02	0.41
5:S:12:LYS:HB3	5:S:12:LYS:HE3	1.77	0.41
8:V:49:LEU:O	8:V:53:MET:HG3	2.21	0.41
8:V:338:ILE:HD11	8:V:350:ILE:HG22	2.03	0.41
2:C:176:VAL:HG22	2:C:212:ILE:HG12	2.03	0.40
10:L:373:GLN:NE2	10:L:471:ILE:HG23	2.37	0.40
2:P:220:LEU:HD12	2:P:239:HIS:CE1	2.56	0.40
7:U:138:VAL:HG13	7:U:139:CYS:N	2.37	0.40
9:W:154:LEU:HA	9:W:154:LEU:HD23	1.84	0.40
10:Y:403:LEU:HD12	10:Y:426:LEU:HD11	2.03	0.40
10:Y:405:GLY:O	10:Y:409:VAL:HG22	2.20	0.40
2:C:155:LYS:NZ	2:C:168:LYS:HE3	2.36	0.40
9:K:79:THR:HG23	9:K:205:LEU:HD23	2.04	0.40
9:K:90:THR:OG1	9:K:95:SER:HA	2.21	0.40
3:Q:51:LYS:O	7:U:107:HIS:ND1	2.53	0.40
9:W:115:THR:OG1	9:W:116:ARG:N	2.54	0.40
9:W:195:TYR:O	9:W:199:LYS:HE2	2.21	0.40
9:W:380:ALA:HB2	10:Y:136:LEU:HD11	2.03	0.40
10:Y:79:SER:HA	10:Y:82:GLU:OE1	2.21	0.40
10:Y:361:ASP:OD1	10:Y:362:ARG:N	2.52	0.40
2:C:160:PRO:HD2	2:C:210:TRP:CH2	2.56	0.40
7:H:124:CYS:C	7:H:178:PRO:HG2	2.47	0.40
8:V:17:SER:HB2	8:V:201:HIS:HE1	1.86	0.40
7:H:243:ALA:HB3	12:H:401:HEC:HBD2	2.04	0.40
8:J:113:TRP:NE1	8:J:301:LEU:O	2.46	0.40
8:J:302:ALA:O	8:J:305:PRO:HD2	2.22	0.40
2:P:83:ILE:HG12	10:Y:186:TYR:HE1	1.85	0.40
2:P:207:LYS:NZ	2:P:268:ASP:HA	2.36	0.40
5:S:72:LYS:HE2	5:S:72:LYS:HB3	1.86	0.40
10:Y:61:SER:HB3	10:Y:239:HIS:HD2	1.87	0.40
3:D:17:ARG:NH1	3:D:19:SER:OG	2.54	0.40
7:U:313:VAL:HG23	1:N:18:SER:HB3	2.03	0.40
9:W:230:LEU:HA	9:W:233:VAL:HG22	2.02	0.40
10:Y:279:ASP:OD1	1:N:13:HIS:ND1	2.54	0.40
10:Y:363:MET:HE3	10:Y:363:MET:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
1	N	77/82 (94%)	73 (95%)	4 (5%)	0	100	100
2	C	192/274 (70%)	180 (94%)	12 (6%)	0	100	100
2	P	193/274 (70%)	178 (92%)	15 (8%)	0	100	100
3	D	52/63 (82%)	51 (98%)	1 (2%)	0	100	100
3	Q	53/63 (84%)	52 (98%)	1 (2%)	0	100	100
4	E	66/91 (72%)	62 (94%)	4 (6%)	0	100	100
4	R	66/91 (72%)	65 (98%)	1 (2%)	0	100	100
5	F	99/111 (89%)	99 (100%)	0	0	100	100
5	S	102/111 (92%)	100 (98%)	2 (2%)	0	100	100
6	G	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
6	T	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
7	H	237/325 (73%)	229 (97%)	8 (3%)	0	100	100
7	U	237/325 (73%)	229 (97%)	8 (3%)	0	100	100
8	J	376/380 (99%)	364 (97%)	12 (3%)	0	100	100
8	V	376/380 (99%)	366 (97%)	10 (3%)	0	100	100
9	K	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
9	W	417/453 (92%)	400 (96%)	17 (4%)	0	100	100
10	L	405/480 (84%)	392 (97%)	13 (3%)	0	100	100
10	Y	408/480 (85%)	396 (97%)	12 (3%)	0	100	100
All	All	3947/4630 (85%)	3811 (97%)	136 (3%)	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	68/75 (91%)	65 (96%)	3 (4%)	24	49
1	N	73/75 (97%)	70 (96%)	3 (4%)	26	51
2	C	164/229 (72%)	158 (96%)	6 (4%)	29	54
2	P	165/229 (72%)	159 (96%)	6 (4%)	30	55
3	D	47/53 (89%)	46 (98%)	1 (2%)	48	70
3	Q	47/53 (89%)	46 (98%)	1 (2%)	48	70
4	E	59/86 (69%)	55 (93%)	4 (7%)	13	32
4	R	61/86 (71%)	60 (98%)	1 (2%)	58	77
5	F	92/98 (94%)	88 (96%)	4 (4%)	25	49
5	S	94/98 (96%)	91 (97%)	3 (3%)	34	59
6	G	42/47 (89%)	41 (98%)	1 (2%)	44	68
6	T	42/47 (89%)	40 (95%)	2 (5%)	21	46
7	H	205/259 (79%)	196 (96%)	9 (4%)	24	49
7	U	205/259 (79%)	198 (97%)	7 (3%)	32	57
8	J	330/331 (100%)	322 (98%)	8 (2%)	44	68
8	V	330/331 (100%)	320 (97%)	10 (3%)	36	60
9	K	332/360 (92%)	327 (98%)	5 (2%)	60	78
9	W	335/360 (93%)	322 (96%)	13 (4%)	27	52
10	L	342/391 (88%)	335 (98%)	7 (2%)	50	72
10	Y	344/391 (88%)	330 (96%)	14 (4%)	26	51
All	All	3377/3858 (88%)	3269 (97%)	108 (3%)	36	59

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	40	ARG
1	A	74	ASN

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Mol	Chain	Res	Type
2	C	100	THR
2	C	153	GLU
2	C	168	LYS
2	C	201	ASP
2	C	207	LYS
2	C	256	LEU
3	D	47	ILE
4	E	30	LEU
4	E	43	CYS
4	E	65	GLU
4	E	86	LEU
5	F	14	LEU
5	F	15	ASP
5	F	65	ARG
5	F	71	LEU
6	G	18	VAL
7	H	87	LEU
7	H	96	TRP
7	H	121	CYS
7	H	124	CYS
7	H	197	LEU
7	H	227	LEU
7	H	262	THR
7	H	292	MET
7	H	319	LEU
8	J	27	ILE
8	J	66	ILE
8	J	74	ASN
8	J	268	ILE
8	J	273	TYR
8	J	275	LEU
8	J	281	LEU
8	J	379	TRP
9	K	39	GLU
9	K	131	ASP
9	K	138	LEU
9	K	229	VAL
9	K	230	LEU
10	L	37	THR
10	L	125	THR
10	L	168	ILE
10	L	360	CYS

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Mol	Chain	Res	Type
10	L	399	LEU
10	L	418	LEU
10	L	422	ARG
2	P	83	ILE
2	P	97	LEU
2	P	154	ILE
2	P	256	LEU
2	P	271	VAL
2	P	273	VAL
3	Q	23	LEU
4	R	86	LEU
5	S	12	LYS
5	S	36	ASP
5	S	71	LEU
6	T	13	LEU
6	T	18	VAL
7	U	102	LEU
7	U	120	VAL
7	U	197	LEU
7	U	227	LEU
7	U	259	THR
7	U	292	MET
7	U	313	VAL
8	V	27	ILE
8	V	66	ILE
8	V	68	HIS
8	V	74	ASN
8	V	149	LEU
8	V	159	ASP
8	V	268	ILE
8	V	299	LEU
8	V	327	LEU
8	V	379	TRP
9	W	49	ILE
9	W	61	ILE
9	W	131	ASP
9	W	175	GLU
9	W	214	THR
9	W	230	LEU
9	W	239	ASN
9	W	267	VAL
9	W	309	LEU

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Mol	Chain	Res	Type
9	W	341	ILE
9	W	351	ILE
9	W	416	ILE
9	W	450	VAL
10	Y	52	LEU
10	Y	71	VAL
10	Y	125	THR
10	Y	146	LEU
10	Y	176	ASP
10	Y	220	LEU
10	Y	271	THR
10	Y	279	ASP
10	Y	286	HIS
10	Y	359	VAL
10	Y	418	LEU
10	Y	419	THR
10	Y	424	ILE
10	Y	462	ILE
1	N	13	HIS
1	N	40	ARG
1	N	71	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	29	HIS
1	A	74	ASN
2	C	242	HIS
4	E	39	GLN
5	F	23	ASN
6	G	16	ASN
6	G	49	ASN
7	H	205	HIS
7	H	282	HIS
8	J	8	ASN
8	J	26	ASN
8	J	97	HIS
8	J	114	ASN
8	J	206	ASN
8	J	286	ASN
9	K	36	GLN

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Mol	Chain	Res	Type
9	K	81	HIS
9	K	178	HIS
9	K	206	HIS
9	K	291	HIS
9	K	308	HIS
9	K	310	HIS
9	K	319	GLN
9	K	327	ASN
9	K	357	GLN
9	K	363	GLN
10	L	40	GLN
10	L	43	GLN
10	L	63	GLN
10	L	87	ASN
10	L	121	ASN
10	L	152	GLN
10	L	153	ASN
10	L	188	HIS
10	L	239	HIS
10	L	249	HIS
10	L	357	HIS
10	L	452	GLN
2	P	164	ASN
2	P	178	HIS
3	Q	48	ASN
3	Q	58	HIS
4	R	39	GLN
5	S	23	ASN
5	S	28	ASN
5	S	54	ASN
6	T	16	ASN
6	T	49	ASN
7	U	155	GLN
7	U	159	ASN
7	U	189	ASN
7	U	234	ASN
7	U	282	HIS
7	U	309	HIS
8	V	26	ASN
8	V	54	HIS
8	V	114	ASN
8	V	137	GLN

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Mol	Chain	Res	Type
8	V	201	HIS
9	W	36	GLN
9	W	54	ASN
9	W	81	HIS
9	W	155	GLN
9	W	212	HIS
9	W	268	HIS
9	W	284	ASN
9	W	298	HIS
9	W	308	HIS
9	W	363	GLN
9	W	399	GLN
9	W	421	ASN
9	W	426	ASN
9	W	443	ASN
10	Y	43	GLN
10	Y	87	ASN
10	Y	128	HIS
10	Y	160	GLN
10	Y	223	HIS
10	Y	239	HIS
10	Y	249	HIS
10	Y	357	HIS
10	Y	402	HIS
10	Y	452	GLN
1	N	29	HIS

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

8 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	HEM	J	402	8	42,50,50	1.48	5 (11%)	46,82,82	1.34	7 (15%)
11	FES	P	301	2	0,4,4	-	-	-	-	-
11	FES	C	301	2	0,4,4	-	-	-	-	-
13	HEM	V	401	8	42,50,50	1.33	6 (14%)	46,82,82	1.80	9 (19%)
13	HEM	V	402	8	42,50,50	1.48	5 (11%)	46,82,82	1.32	8 (17%)
12	HEC	H	401	7	32,50,50	2.39	12 (37%)	30,82,82	2.07	5 (16%)
12	HEC	U	401	7	32,50,50	2.16	3 (9%)	30,82,82	1.96	5 (16%)
13	HEM	J	401	8	42,50,50	1.48	5 (11%)	46,82,82	1.32	7 (15%)

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	HEM	J	402	8	-	4/12/54/54	-
11	FES	P	301	2	-	-	0/1/1/1
11	FES	C	301	2	-	-	0/1/1/1
13	HEM	V	401	8	-	7/12/54/54	-
13	HEM	V	402	8	-	5/12/54/54	-
12	HEC	H	401	7	-	2/10/54/54	-
12	HEC	U	401	7	-	1/10/54/54	-
13	HEM	J	401	8	-	2/12/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	401	HEC	C2B-C3B	6.72	1.48	1.40
12	H	401	HEC	C3C-C2C	6.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	401	HEC	C2B-C3B	-6.21	1.33	1.40
12	U	401	HEC	C3C-C2C	-6.04	1.34	1.40
12	U	401	HEC	C3D-C2D	5.41	1.53	1.37
13	V	402	HEM	C3C-C2C	-4.14	1.34	1.40
13	J	402	HEM	C3C-C2C	-4.12	1.34	1.40
13	J	401	HEM	C3C-C2C	-4.09	1.34	1.40
12	H	401	HEC	C2A-C3A	3.51	1.48	1.37
13	J	401	HEM	C3C-CAC	3.44	1.55	1.47
13	J	402	HEM	C3C-CAC	3.43	1.55	1.47
13	V	402	HEM	C3C-CAC	3.42	1.55	1.47
12	H	401	HEC	C3D-C2D	3.39	1.47	1.37
13	V	401	HEM	C1B-NB	-3.29	1.34	1.40
12	H	401	HEC	C3C-C4C	3.25	1.49	1.43
13	V	401	HEM	C4D-ND	-3.20	1.34	1.40
13	J	402	HEM	CAB-C3B	3.07	1.55	1.47
13	J	401	HEM	CAB-C3B	3.07	1.55	1.47
13	V	402	HEM	CAB-C3B	3.06	1.55	1.47
12	H	401	HEC	C2A-C1A	2.84	1.48	1.42
12	H	401	HEC	C4D-CHA	2.77	1.48	1.41
12	H	401	HEC	C4B-C3B	2.74	1.48	1.43
12	H	401	HEC	C3A-C4A	2.72	1.48	1.42
12	H	401	HEC	C1D-CHD	2.69	1.48	1.41
13	J	402	HEM	C3C-C4C	2.60	1.45	1.41
13	J	401	HEM	C3C-C4C	2.55	1.45	1.41
12	H	401	HEC	C1B-CHB	2.53	1.48	1.41
13	V	402	HEM	C3C-C4C	2.51	1.45	1.41
12	H	401	HEC	C1C-CHC	2.42	1.47	1.41
13	V	401	HEM	FE-NB	2.40	2.11	1.98
13	V	401	HEM	C1D-ND	-2.31	1.34	1.38
13	V	401	HEM	CHB-C1B	2.22	1.40	1.34
13	V	401	HEM	C4B-NB	-2.10	1.34	1.38
13	J	401	HEM	CMB-C2B	2.07	1.55	1.50
13	V	402	HEM	CMB-C2B	2.04	1.55	1.50
13	J	402	HEM	CMB-C2B	2.04	1.54	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	401	HEC	C1D-C2D-C3D	-5.65	103.07	107.00
12	U	401	HEC	CBB-CAB-C3B	-5.32	115.05	127.49
12	U	401	HEC	CBC-CAC-C3C	-5.28	115.14	127.49
12	H	401	HEC	CMC-C2C-C3C	5.18	131.91	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V	401	HEM	CHC-C4B-NB	5.09	129.91	124.44
12	H	401	HEC	CMB-C2B-C3B	5.00	131.70	125.82
13	V	401	HEM	CHD-C1D-ND	4.45	129.22	124.44
12	U	401	HEC	CMC-C2C-C1C	-3.72	123.00	128.46
13	V	401	HEM	CHB-C1B-NB	3.45	128.65	124.37
13	V	401	HEM	CHA-C4D-ND	3.27	128.42	124.37
13	V	401	HEM	C1B-NB-C4B	3.22	109.02	105.21
12	H	401	HEC	CAA-CBA-CGA	-2.75	106.43	113.83
13	V	401	HEM	CHD-C1D-C2D	-2.69	120.78	125.03
13	V	402	HEM	C4B-CHC-C1C	2.57	125.95	122.56
13	V	402	HEM	C4A-C3A-C2A	2.55	108.77	107.00
13	J	402	HEM	C4A-C3A-C2A	2.51	108.74	107.00
13	J	402	HEM	C4D-ND-C1D	2.49	108.16	105.21
13	V	401	HEM	CBA-CAA-C2A	-2.44	108.44	112.54
13	V	401	HEM	C3B-C4B-NB	-2.44	107.72	109.47
13	V	402	HEM	C4D-ND-C1D	2.38	108.03	105.21
12	U	401	HEC	CMB-C2B-C1B	-2.36	124.99	128.46
13	J	402	HEM	CMC-C2C-C3C	2.33	129.34	124.68
13	J	401	HEM	C4C-CHD-C1D	2.32	125.61	122.56
13	J	402	HEM	CMA-C3A-C4A	-2.30	125.08	128.46
12	U	401	HEC	C1D-C2D-C3D	-2.25	105.43	107.00
13	J	402	HEM	C3D-C4D-ND	-2.25	107.71	110.17
13	J	401	HEM	C4D-ND-C1D	2.24	107.86	105.21
13	J	401	HEM	C3D-C4D-ND	-2.21	107.75	110.17
13	V	402	HEM	C1B-NB-C4B	2.18	107.79	105.21
13	V	402	HEM	CMC-C2C-C3C	2.18	129.04	124.68
13	J	402	HEM	C4B-CHC-C1C	2.18	125.43	122.56
13	V	402	HEM	CMA-C3A-C4A	-2.16	125.29	128.46
12	H	401	HEC	CMA-C3A-C2A	2.14	128.99	124.94
13	V	402	HEM	C3D-C4D-ND	-2.13	107.84	110.17
13	J	401	HEM	C4B-CHC-C1C	2.12	125.36	122.56
13	J	401	HEM	C3B-C2B-C1B	2.10	107.99	106.41
13	V	402	HEM	C3B-C2B-C1B	2.10	107.99	106.41
13	J	402	HEM	C1B-NB-C4B	2.08	107.67	105.21
13	J	401	HEM	C1B-NB-C4B	2.05	107.63	105.21
13	V	401	HEM	CHB-C1B-C2B	-2.02	121.21	126.94
13	J	401	HEM	C4A-C3A-C2A	2.00	108.39	107.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	J	402	HEM	C1A-C2A-CAA-CBA
13	J	402	HEM	C3A-C2A-CAA-CBA
13	V	401	HEM	C2B-C3B-CAB-CBB
13	V	402	HEM	C1A-C2A-CAA-CBA
13	V	402	HEM	C3A-C2A-CAA-CBA
13	V	402	HEM	C4D-C3D-CAD-CBD
13	V	401	HEM	C4B-C3B-CAB-CBB
13	J	401	HEM	C3D-CAD-CBD-CGD
13	V	402	HEM	C2D-C3D-CAD-CBD
13	J	402	HEM	C4D-C3D-CAD-CBD
13	V	401	HEM	CAA-CBA-CGA-O1A
13	V	401	HEM	CAD-CBD-CGD-O1D
13	J	402	HEM	C2D-C3D-CAD-CBD
13	V	401	HEM	CAA-CBA-CGA-O2A
13	V	401	HEM	CAD-CBD-CGD-O2D
12	H	401	HEC	CAA-CBA-CGA-O2A
13	V	401	HEM	C3D-CAD-CBD-CGD
12	H	401	HEC	CAA-CBA-CGA-O1A
13	V	402	HEM	CAD-CBD-CGD-O2D
12	U	401	HEC	C1A-C2A-CAA-CBA
13	J	401	HEM	CAA-CBA-CGA-O2A

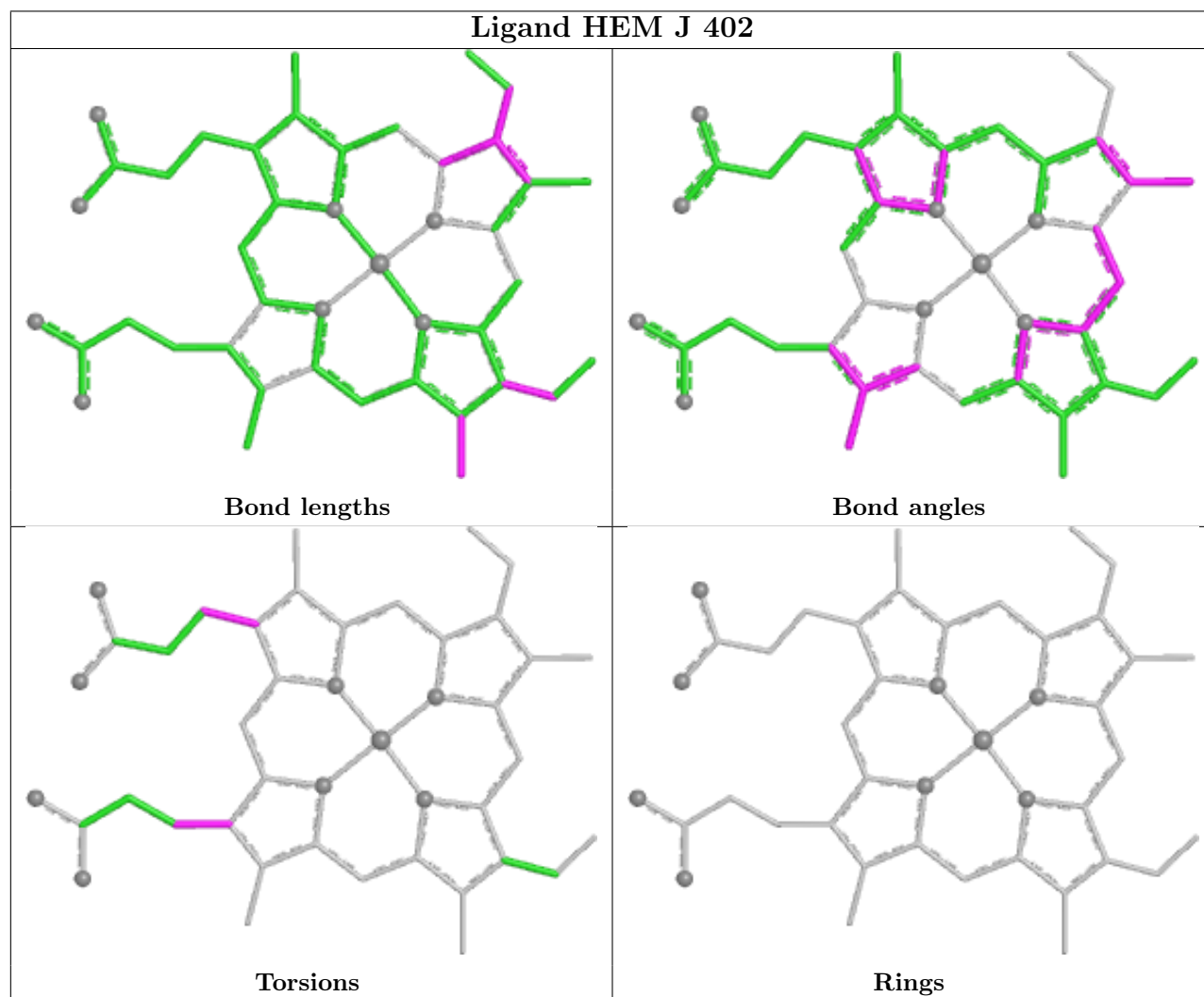
There are no ring outliers.

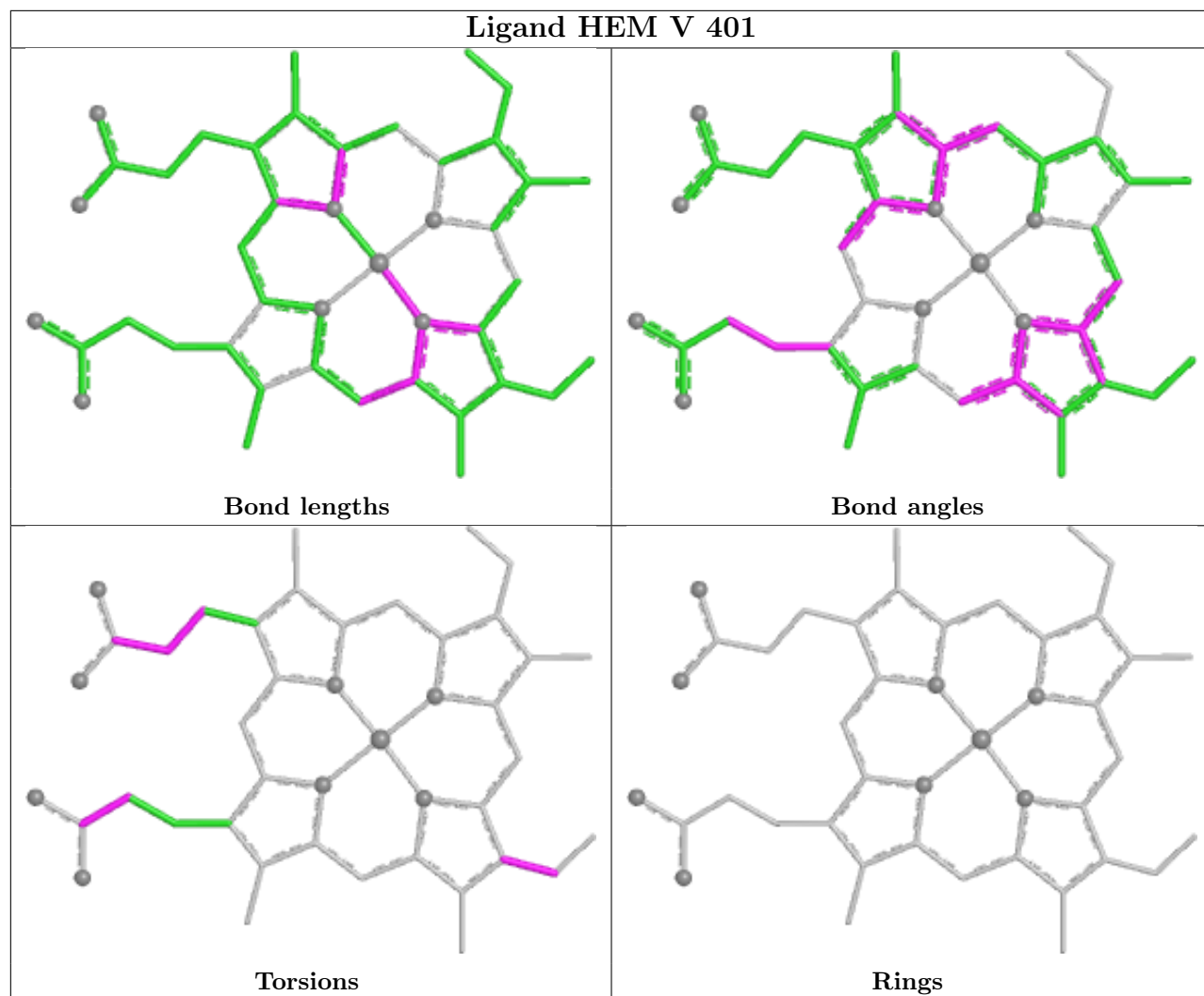
8 monomers are involved in 50 short contacts:

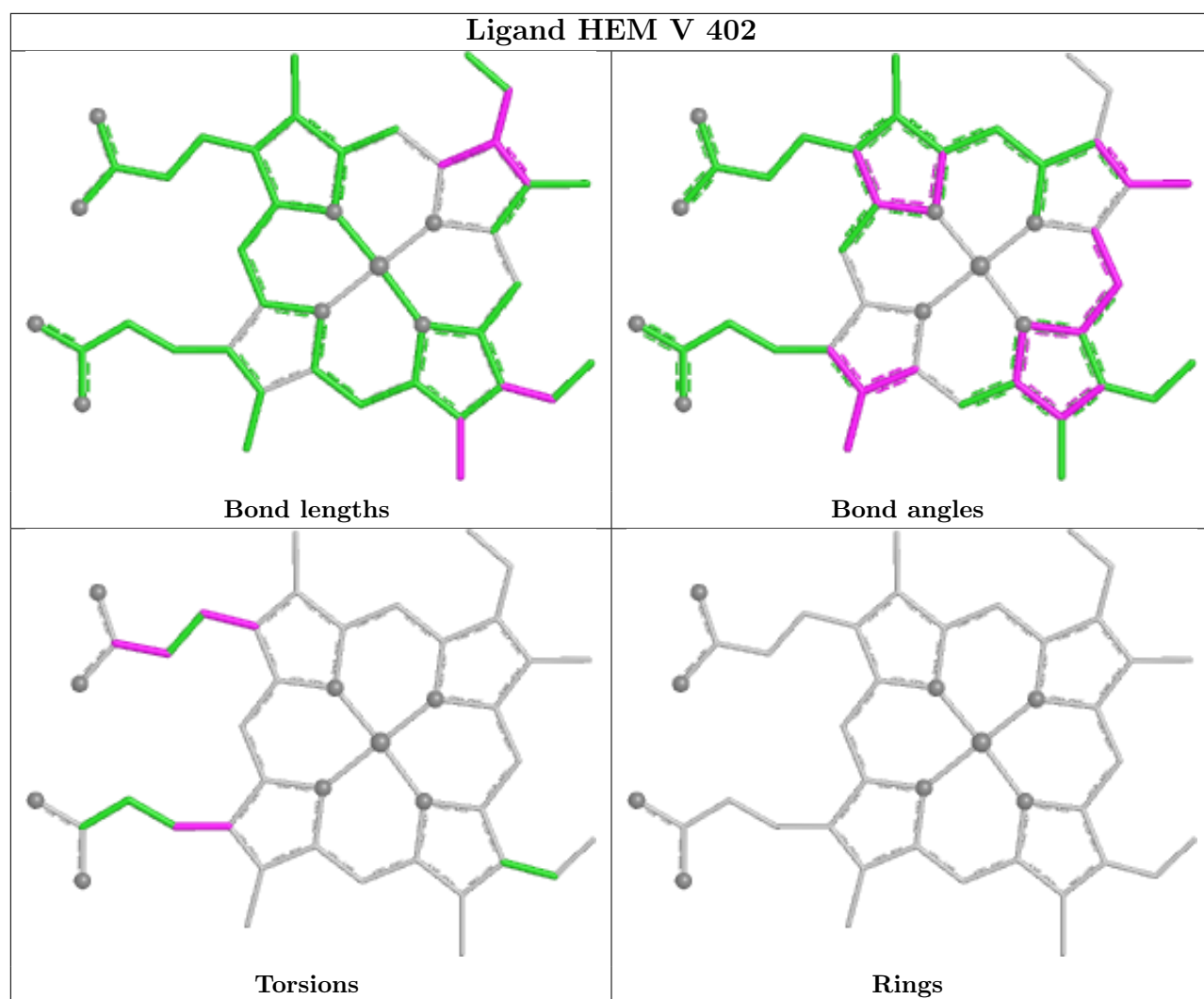
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	J	402	HEM	4	0
11	P	301	FES	9	0
11	C	301	FES	9	0
13	V	401	HEM	2	0
13	V	402	HEM	7	0
12	H	401	HEC	8	0
12	U	401	HEC	7	0
13	J	401	HEM	4	0

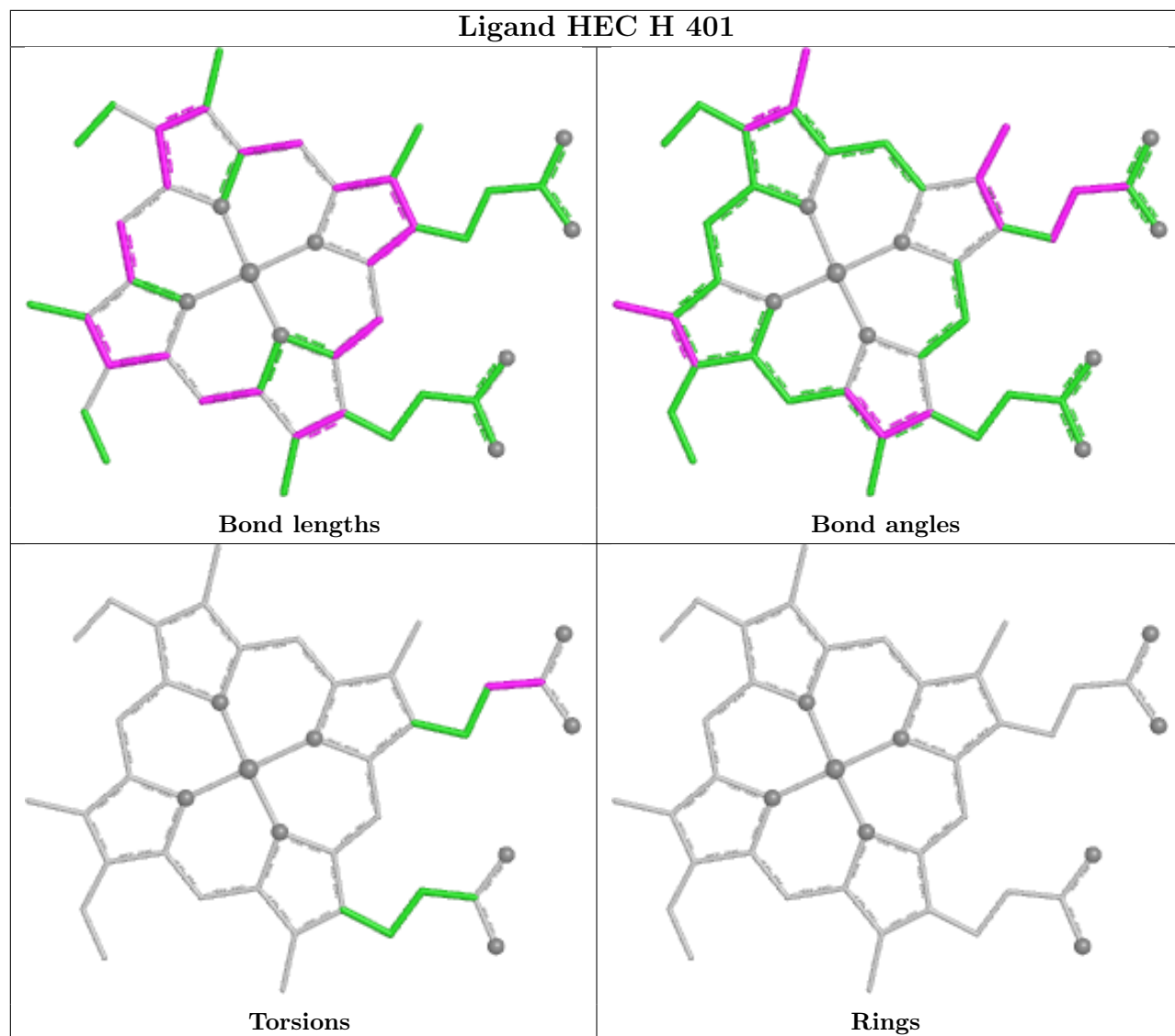
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

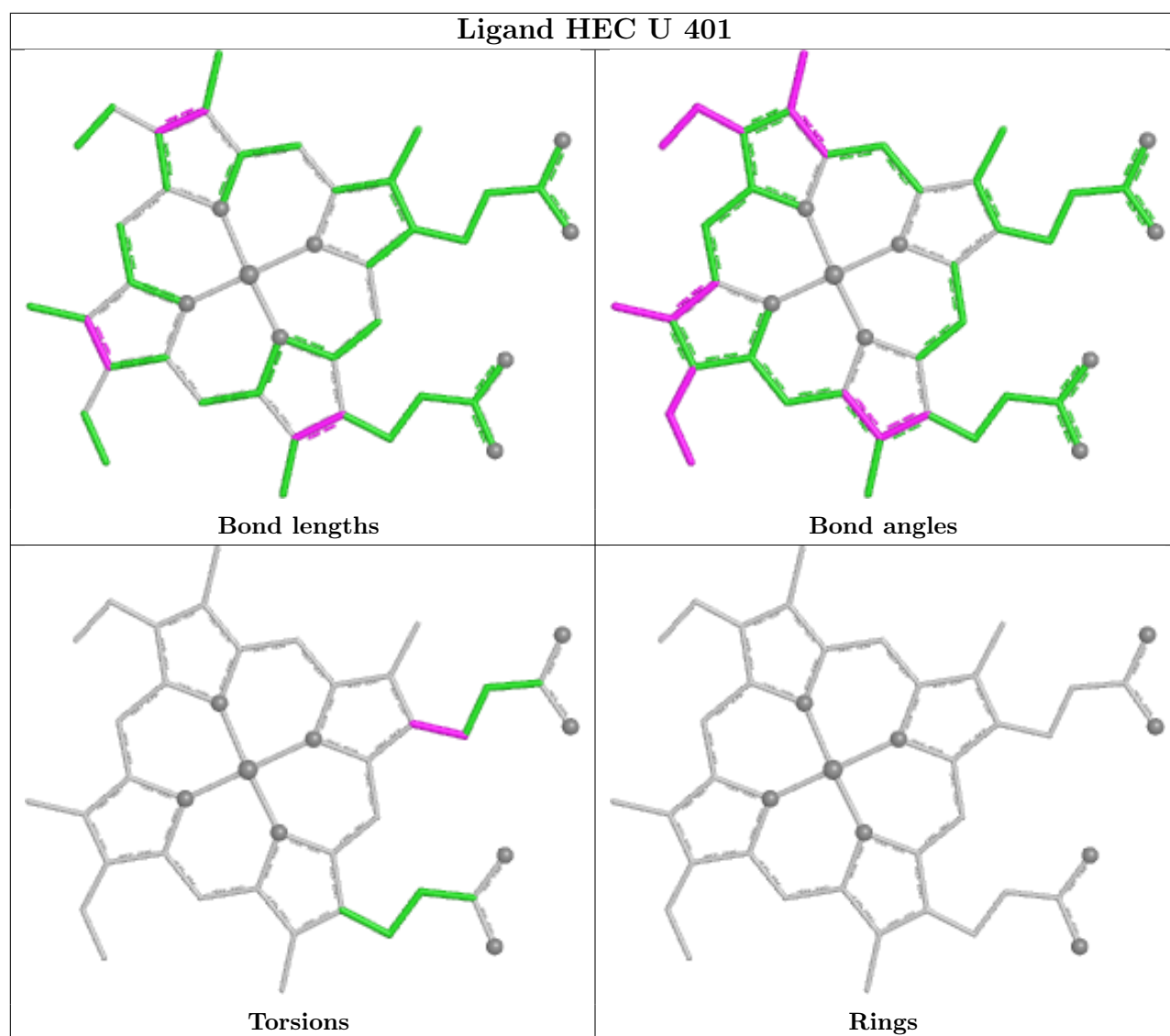
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

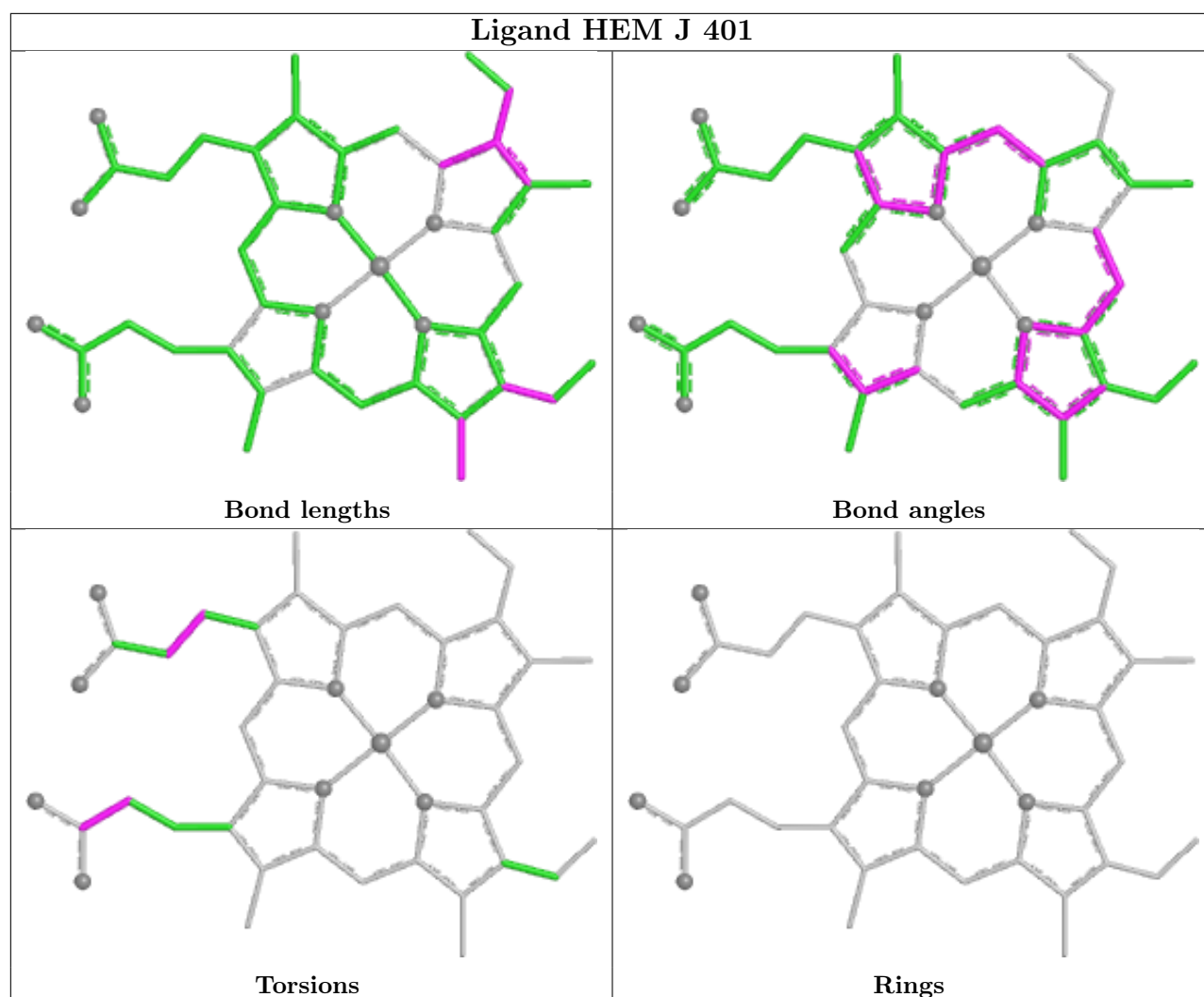












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

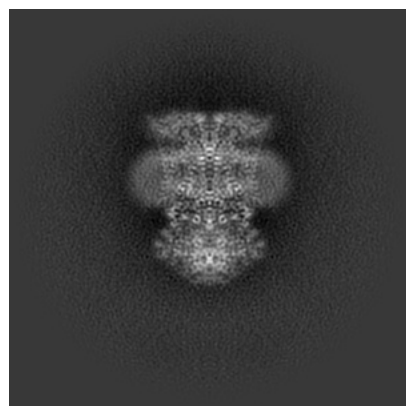
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45567. These allow visual inspection of the internal detail of the map and identification of artifacts.

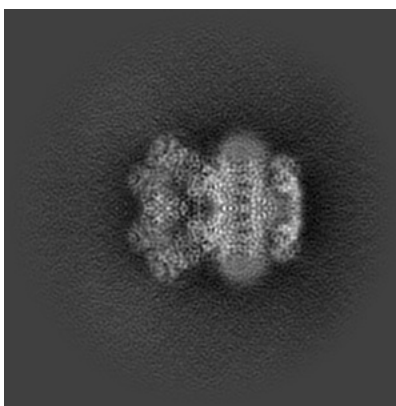
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

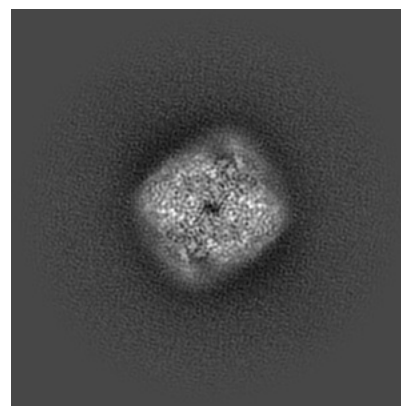
6.1.1 Primary map



X

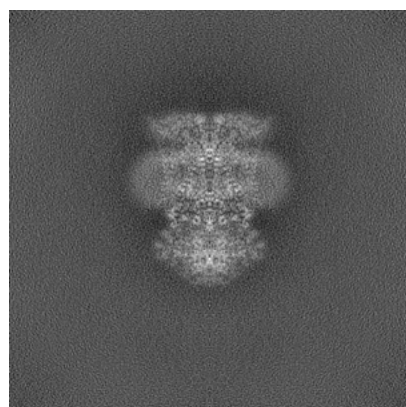


Y

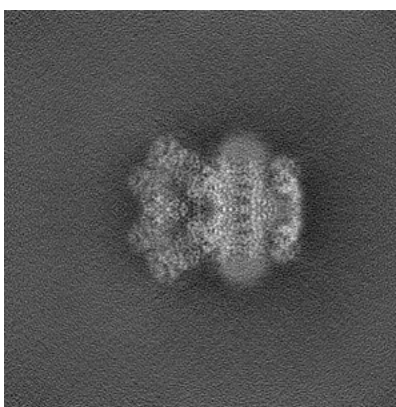


Z

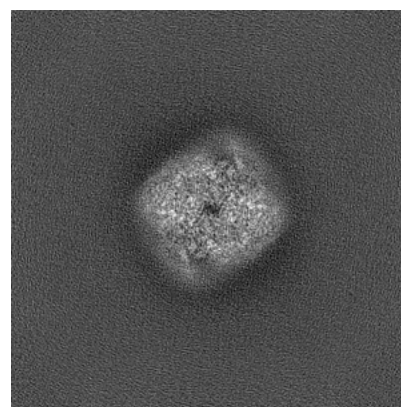
6.1.2 Raw map



X



Y

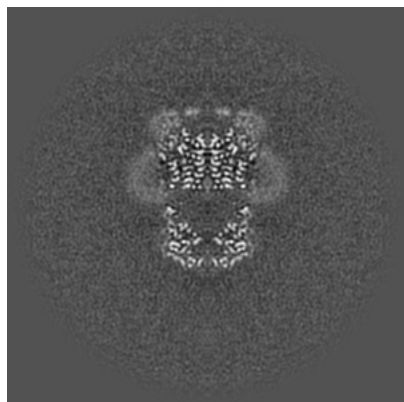


Z

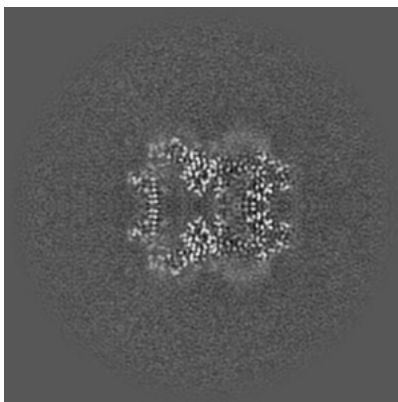
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

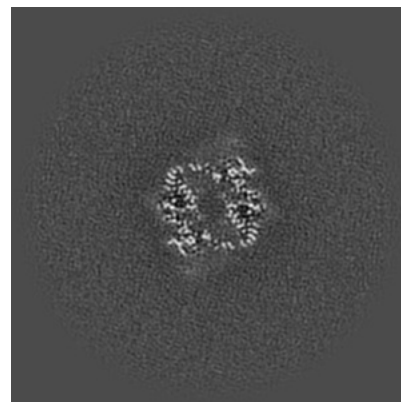
6.2.1 Primary map



X Index: 160

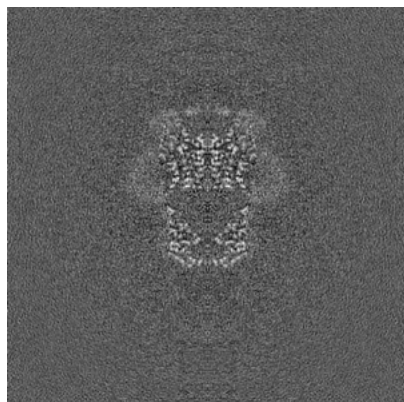


Y Index: 160

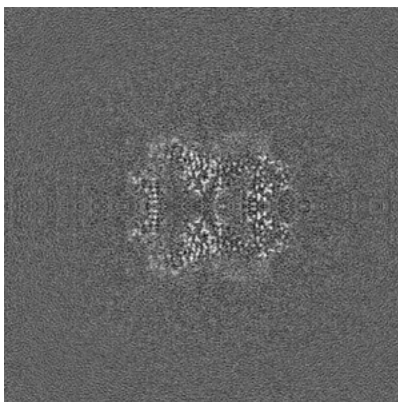


Z Index: 160

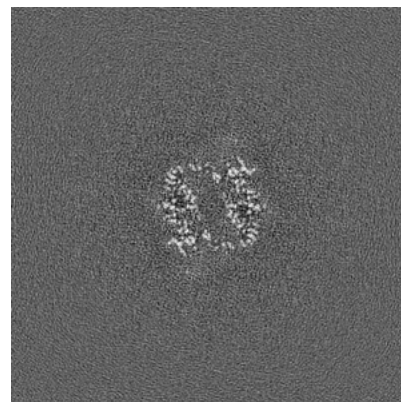
6.2.2 Raw map



X Index: 160



Y Index: 160

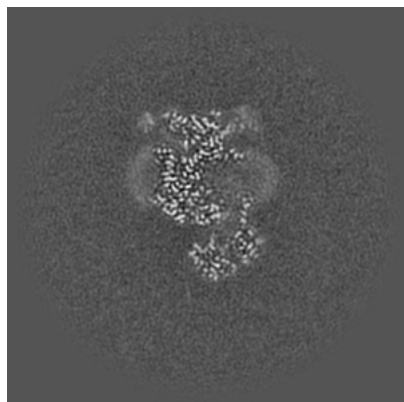


Z Index: 160

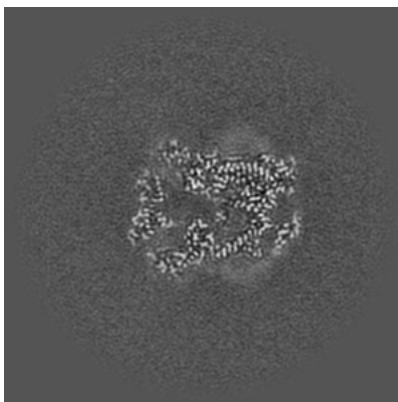
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

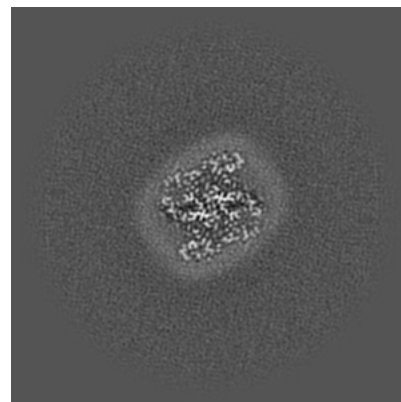
6.3.1 Primary map



X Index: 145

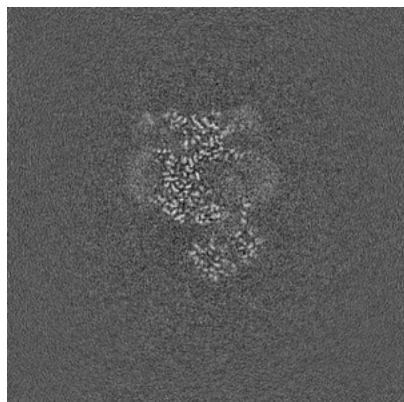


Y Index: 164

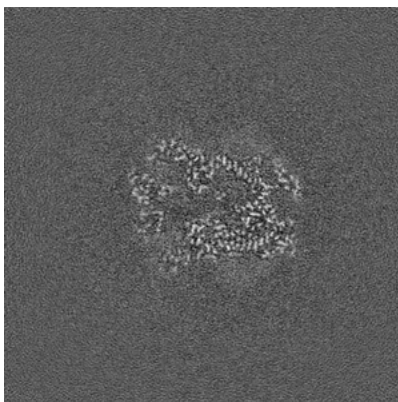


Z Index: 200

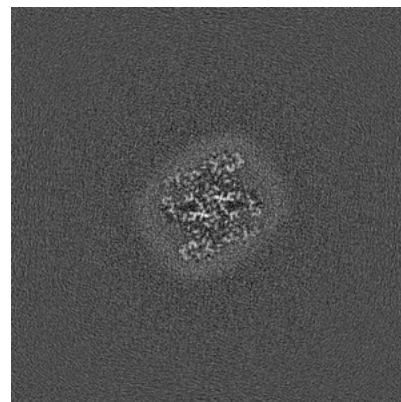
6.3.2 Raw map



X Index: 145



Y Index: 156

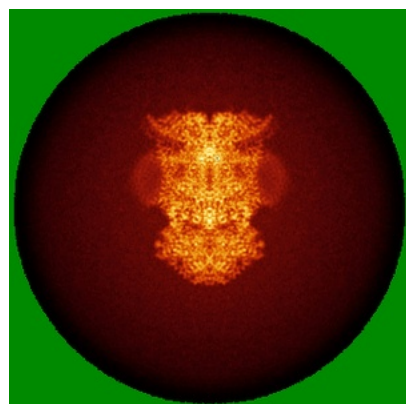


Z Index: 200

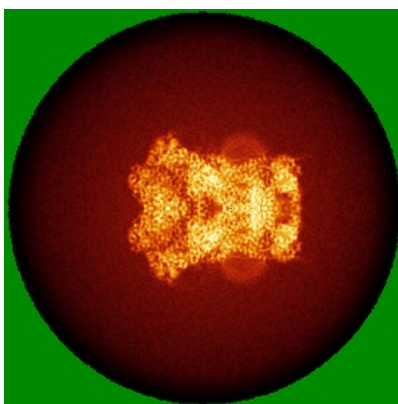
The images above show the largest variance slices of the map in three orthogonal directions.

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

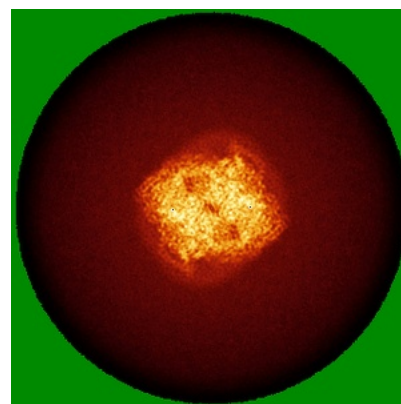
6.4.1 Primary map



X

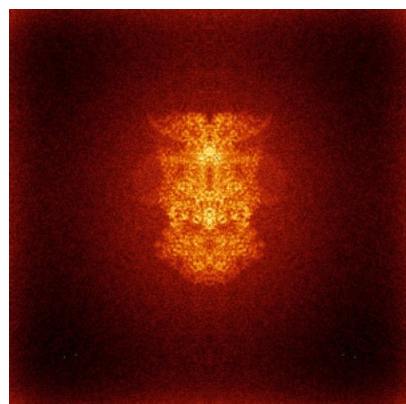


Y

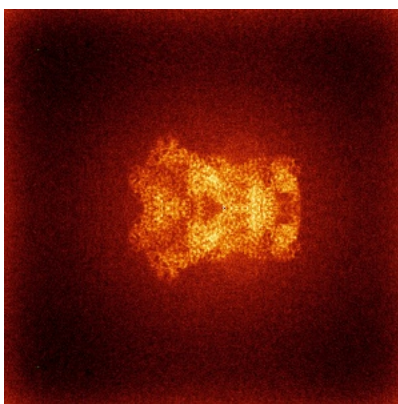


Z

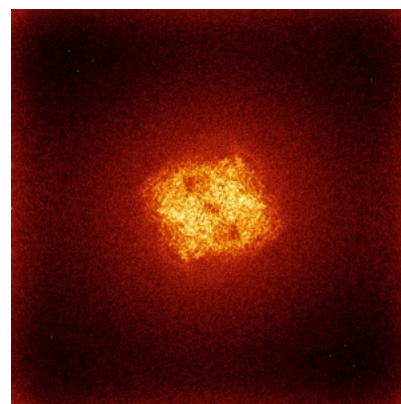
6.4.2 Raw map



X



Y

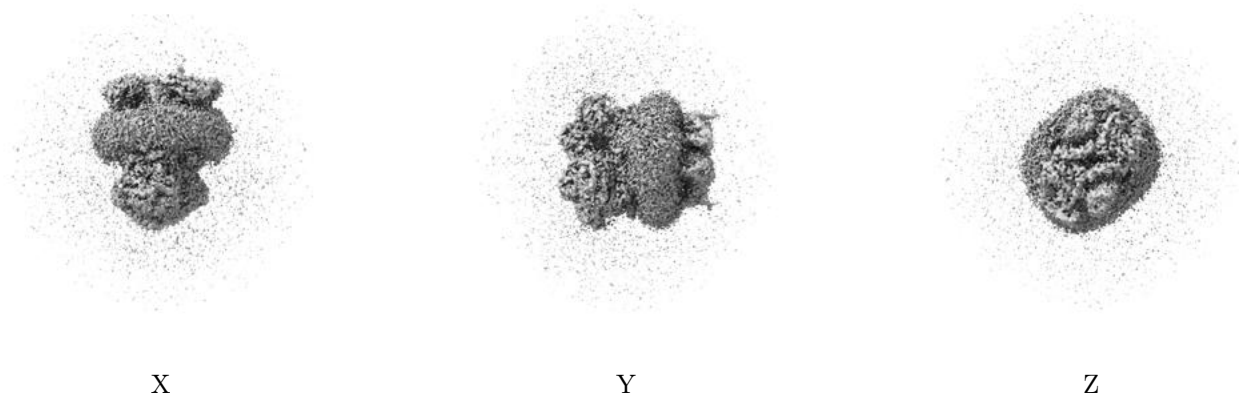


Z

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

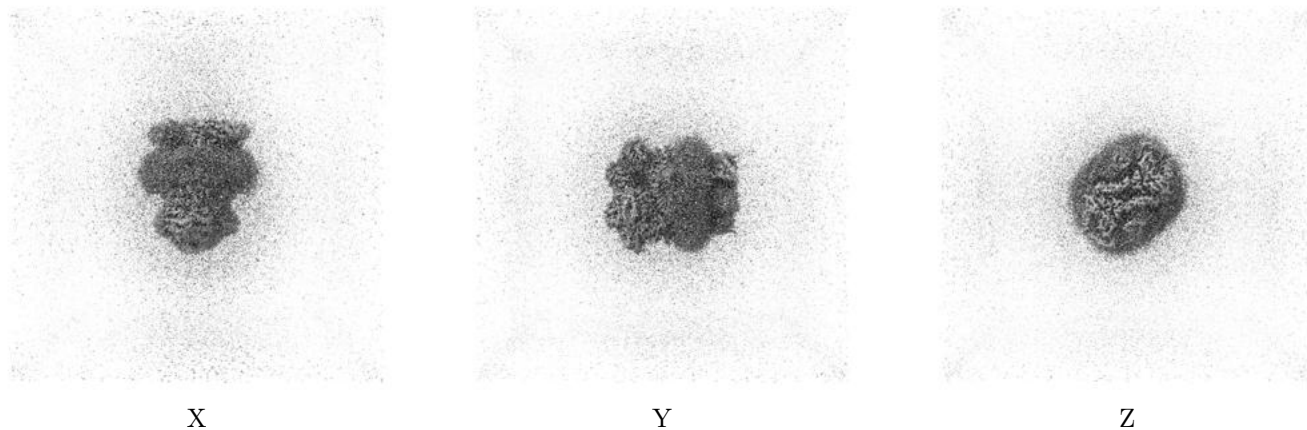
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

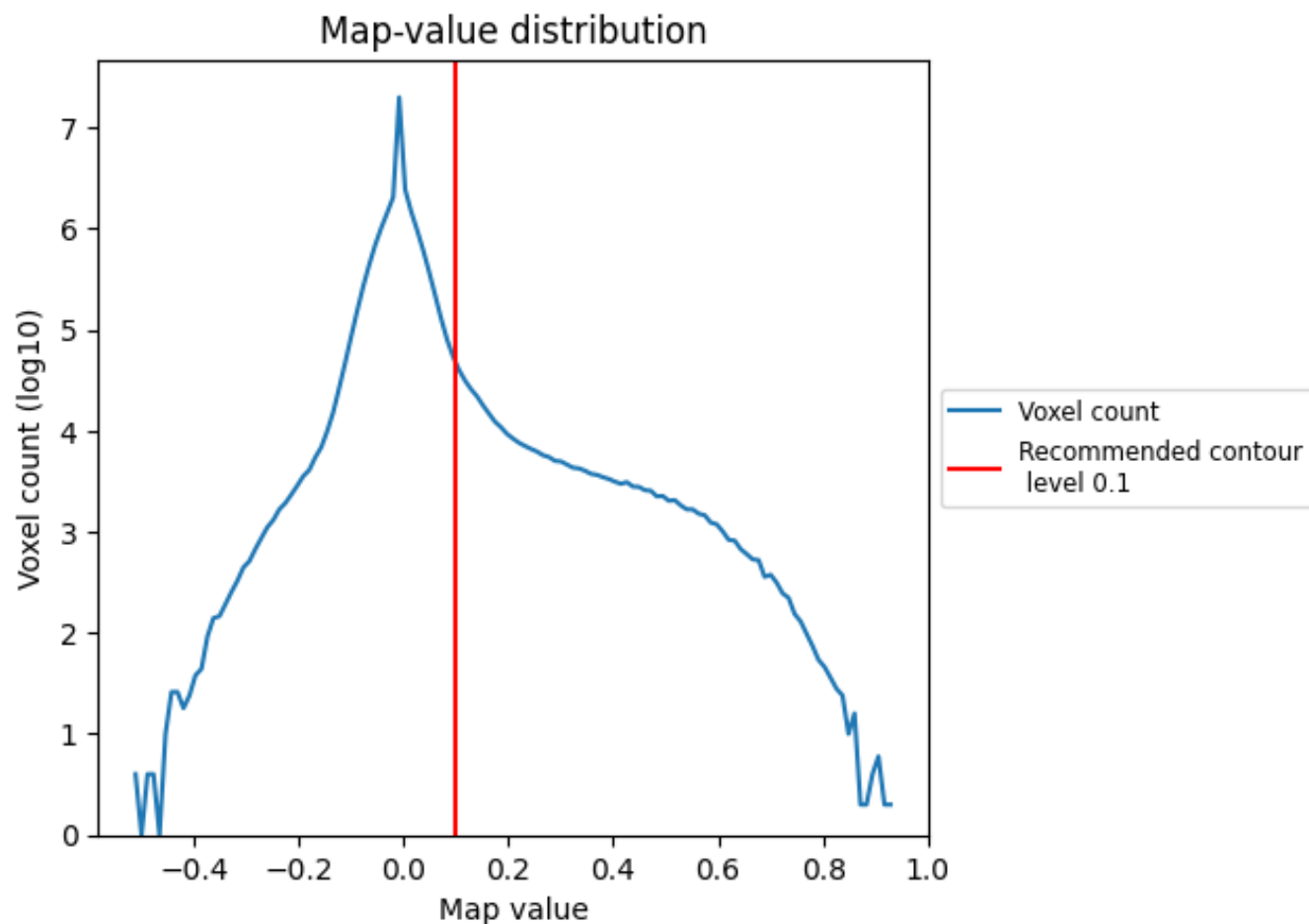
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

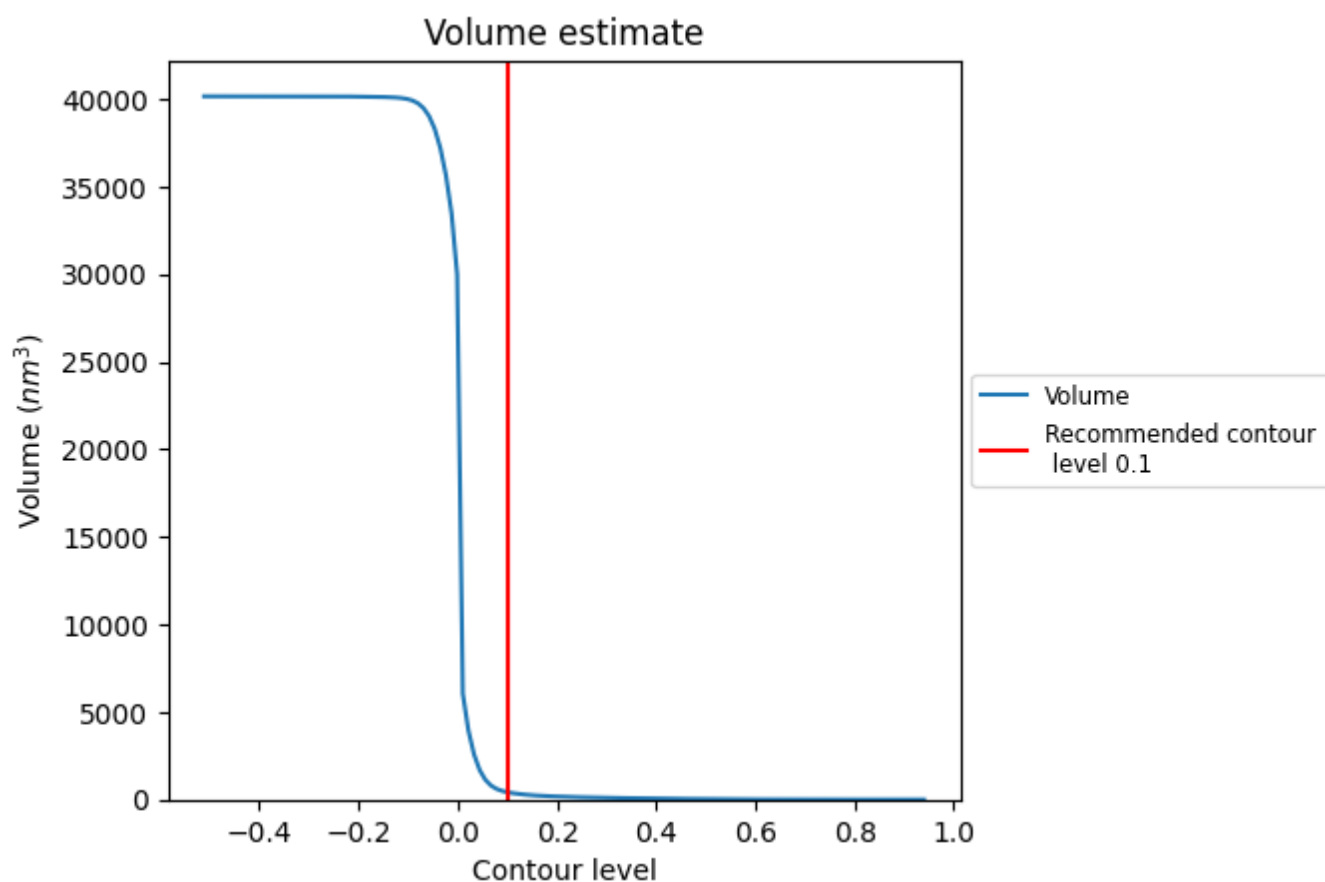
This section contains the results of statistical analysis of the map.

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.

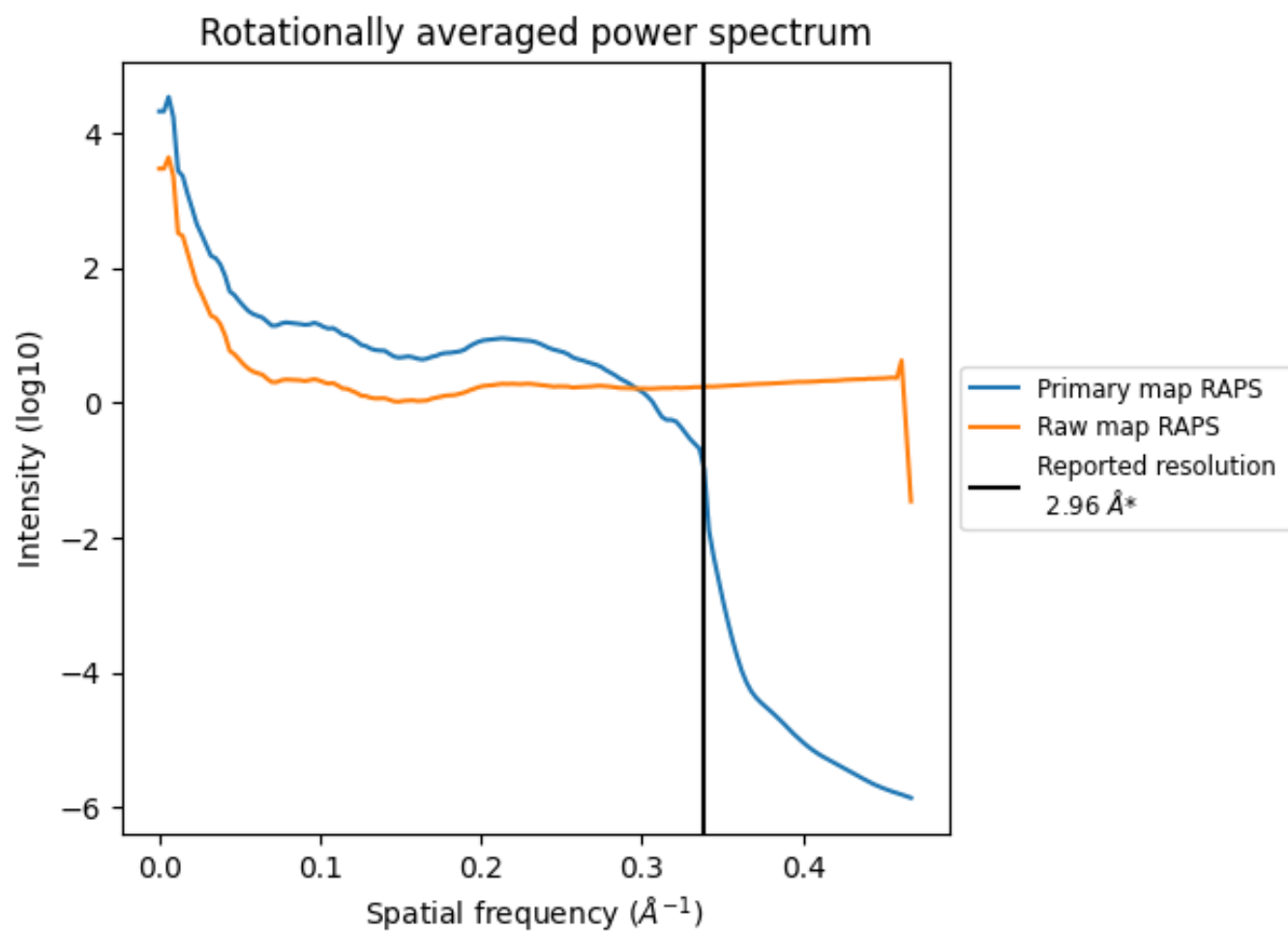
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm³; this corresponds to an approximate mass of 381 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 ⓘ

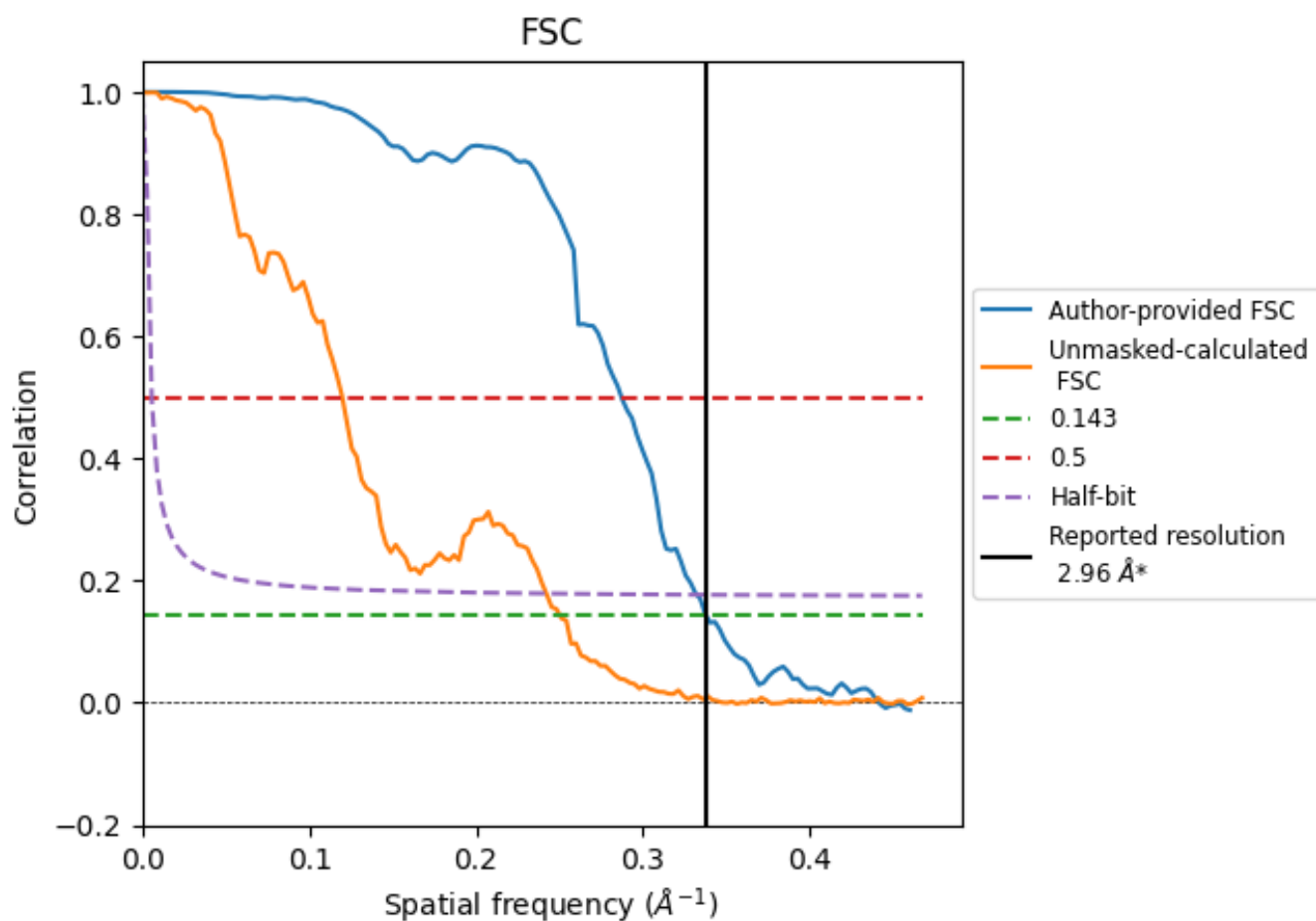


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

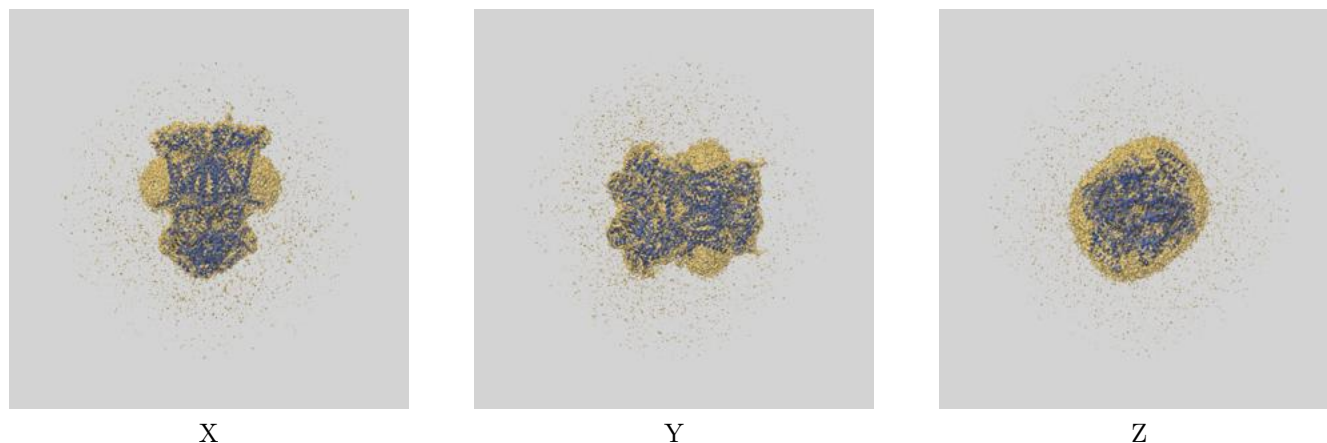
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.48	3.01
Unmasked-calculated*	4.00	8.34	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

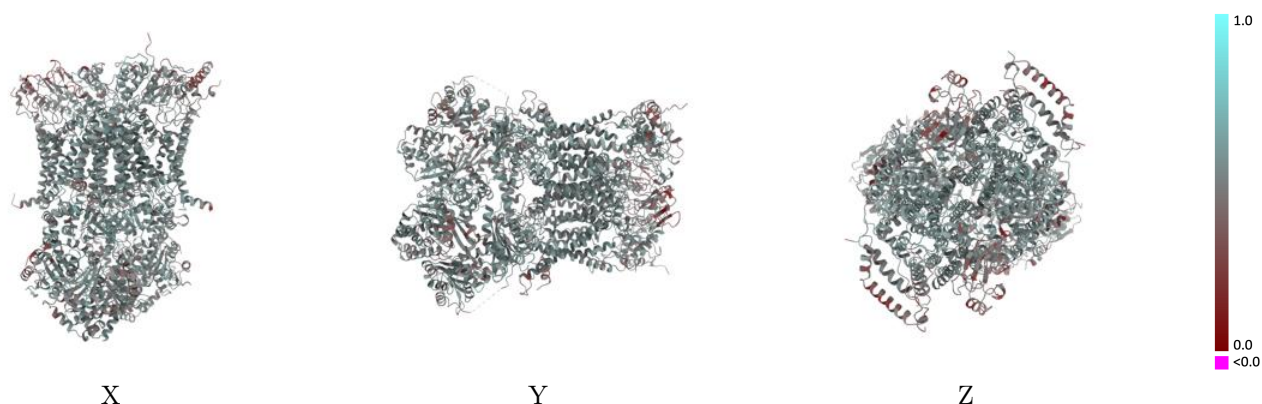
This section contains information regarding the fit between EMDB map EMD-45567 and PDB model 9CG3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



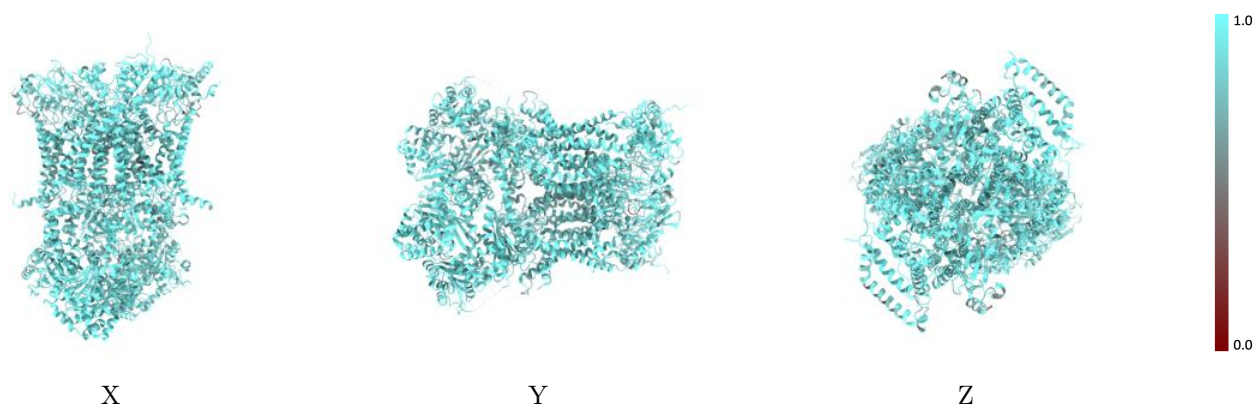
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



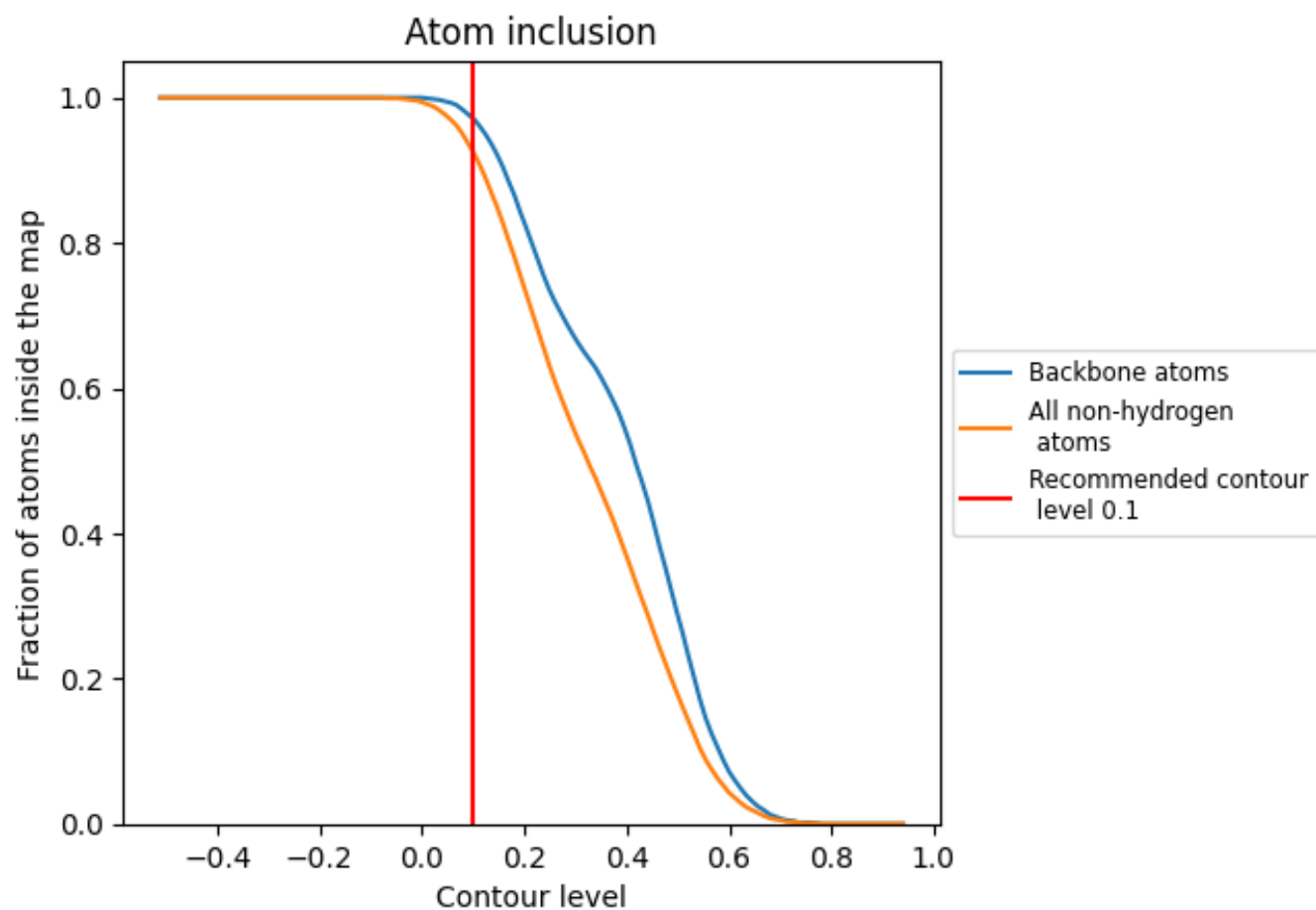
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.5150
A	 0.9350	 0.5230
C	 0.8400	 0.4420
D	 0.9270	 0.4920
E	 0.9130	 0.4430
F	 0.9210	 0.5380
G	 0.9410	 0.5200
H	 0.9540	 0.5340
J	 0.9350	 0.5460
K	 0.9400	 0.5170
L	 0.9310	 0.5170
N	 0.9020	 0.4970
P	 0.8540	 0.4480
Q	 0.9070	 0.4850
R	 0.8900	 0.4370
S	 0.9210	 0.5300
T	 0.9460	 0.5250
U	 0.9590	 0.5360
V	 0.9270	 0.5440
W	 0.9370	 0.5160
Y	 0.9290	 0.5160

