



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:38 PM UTC

PDB ID : 9CL6 / pdb_00009cl6
EMDB ID : EMD-45663
Title : Ammonia monooxygenase in native membranes
Authors : Tucci, F.J.; Rosenzweig, A.C.
Deposited on : 2024-07-10
Resolution : 2.77 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:

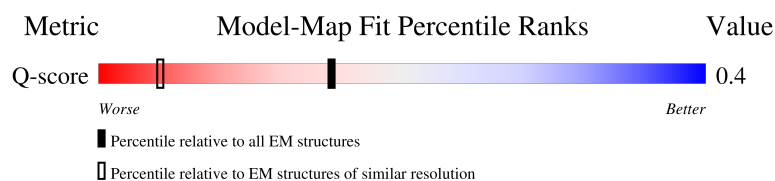
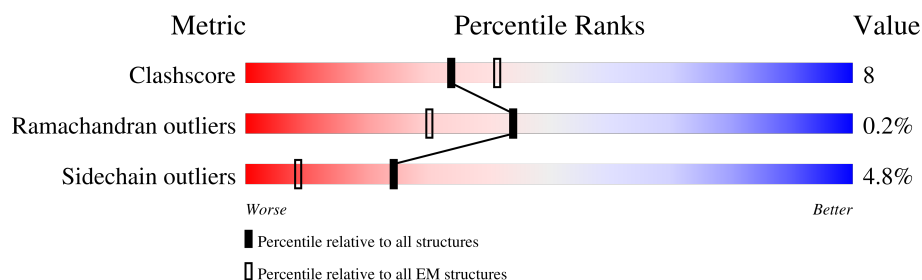
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.77 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	10695 (2.27 - 3.27)

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	C	254	
1	G	254	
1	J	254	
2	A	383	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	383	81%17%
2	H	383	6% 81%17%
3	B	274	8% 78%19%
3	F	274	6% 78%20%
3	I	274	5% 77%21%
4	Da	39	56% 51%38%8%
4	Db	39	36% 51%36%10%
4	Dc	39	41% 54%33%10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23928 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 Ammonia monooxygenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	254	Total	C	N	O	S	0	0
			2119	1421	333	348	17		
1	J	254	Total	C	N	O	S	0	0
			2119	1421	333	348	17		
1	G	254	Total	C	N	O	S	0	0
			2119	1421	333	348	17		

- Molecule 2 is a protein called Ammonia monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	383	Total	C	N	O	S	0	0
			3039	1963	522	542	12		
2	H	383	Total	C	N	O	S	0	0
			3039	1963	522	542	12		
2	E	383	Total	C	N	O	S	0	0
			3039	1963	522	542	12		

- Molecule 3 is a protein called Ammonia monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	274	Total	C	N	O	S	0	0
			2252	1517	357	362	16		
3	I	274	Total	C	N	O	S	0	0
			2252	1517	357	362	16		
3	F	274	Total	C	N	O	S	0	0
			2252	1517	357	362	16		

- Molecule 4 is a protein called ammonia monooxygenase supernumerary helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Da	39	Total	C	N	O	0	0
			290	190	48	52		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Db	39	Total	C	N	O	0	0
			290	190	48	52		
4	Dc	39	Total	C	N	O	0	0
			290	190	48	52		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Cu	0
			1	1	
5	A	1	Total	Cu	0
			1	1	
5	J	1	Total	Cu	0
			1	1	
5	G	1	Total	Cu	0
			1	1	
5	H	1	Total	Cu	0
			1	1	
5	E	1	Total	Cu	0
			1	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	C	53	Total	O	0
			53	53	
6	A	139	Total	O	0
			139	139	
6	B	74	Total	O	0
			74	74	
6	Da	7	Total	O	0
			7	7	
6	Db	7	Total	O	0
			7	7	
6	Dc	7	Total	O	0
			7	7	
6	I	76	Total	O	0
			76	76	
6	F	75	Total	O	0
			75	75	
6	J	53	Total	O	0
			53	53	

Continued on next page...

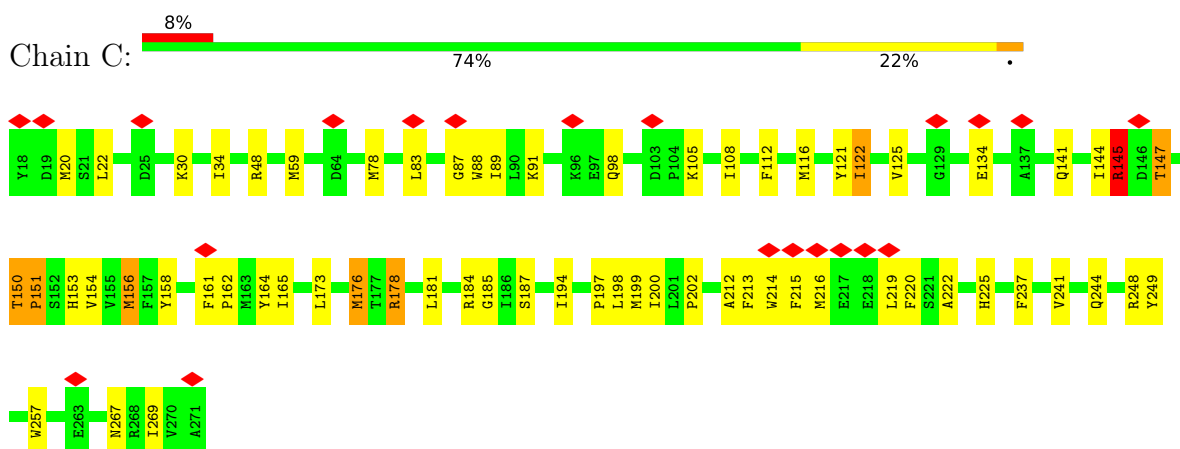
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
6	G	53	Total 53	O 53	0
6	H	139	Total 139	O 139	0
6	E	139	Total 139	O 139	0

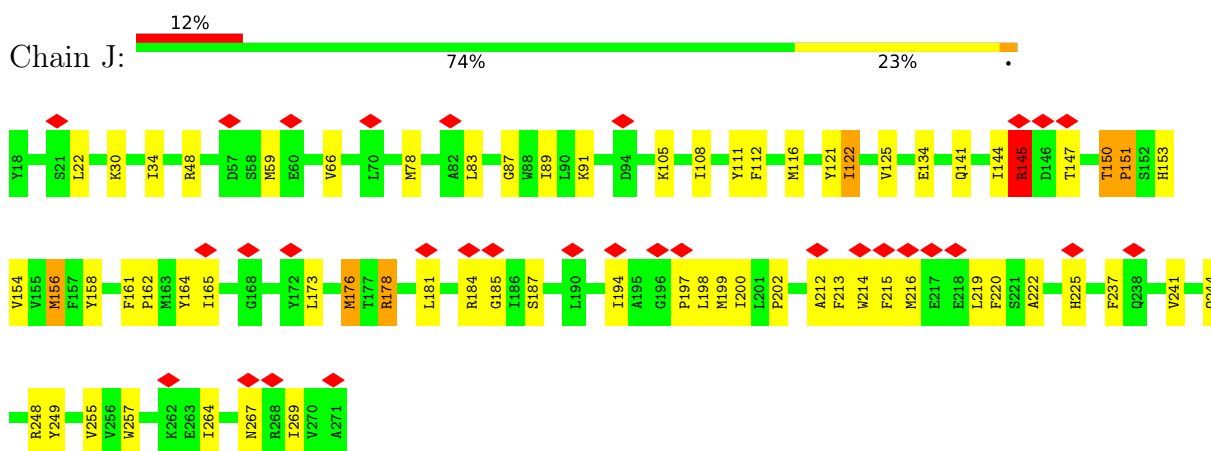
3 Residue-property plots

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.

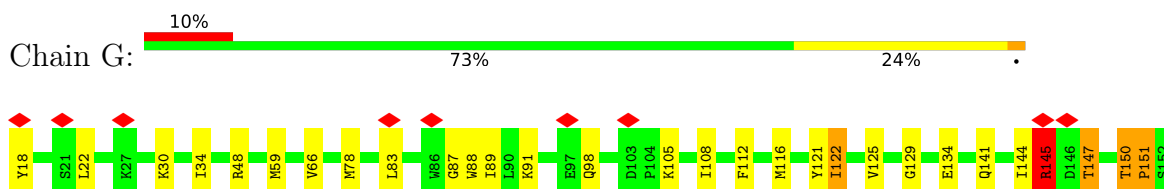
- Molecule 1: Ammonia monooxygenase subunit C

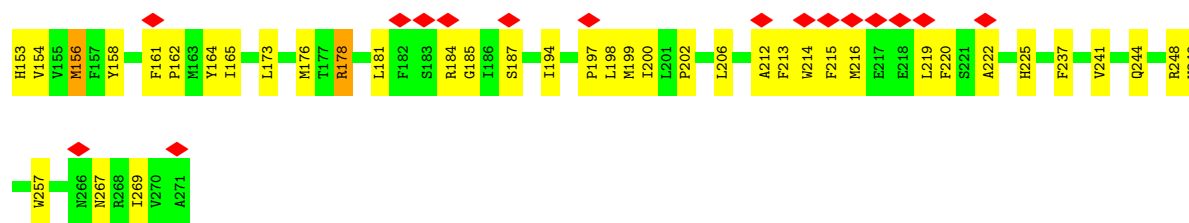


- Molecule 1: Ammonia monooxygenase subunit C

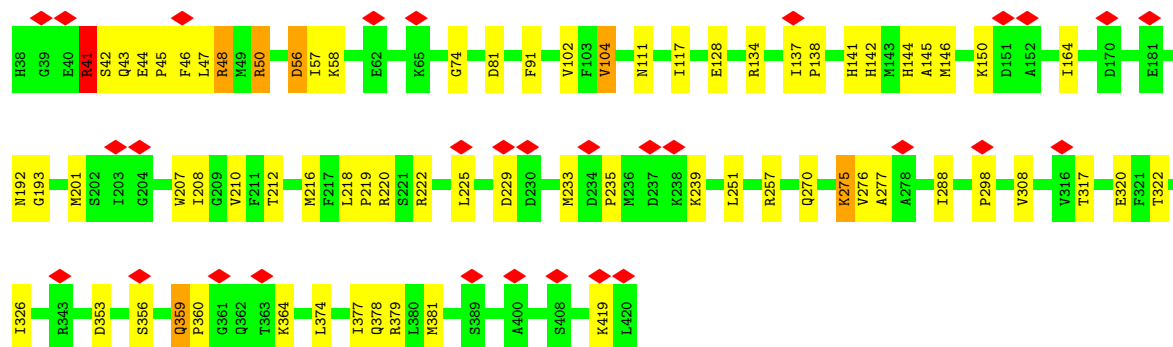
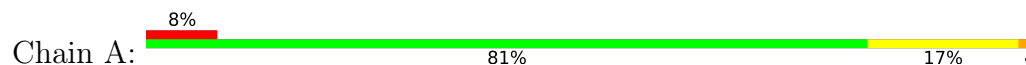


- Molecule 1: Ammonia monooxygenase subunit C

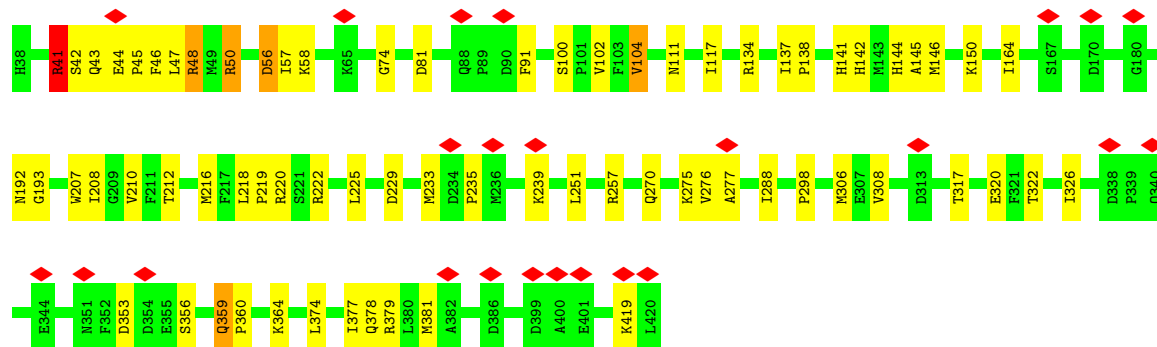
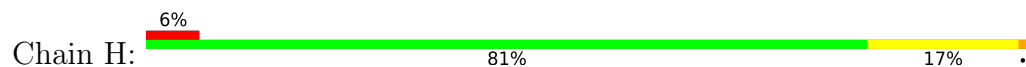




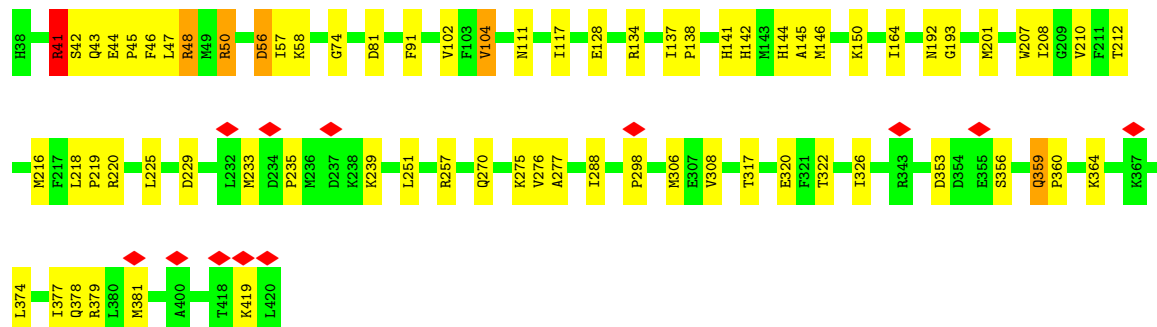
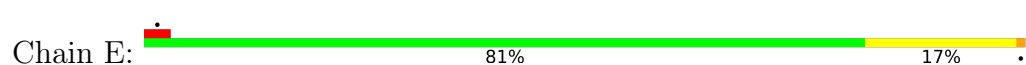
• Molecule 2: Ammonia monooxygenase beta subunit



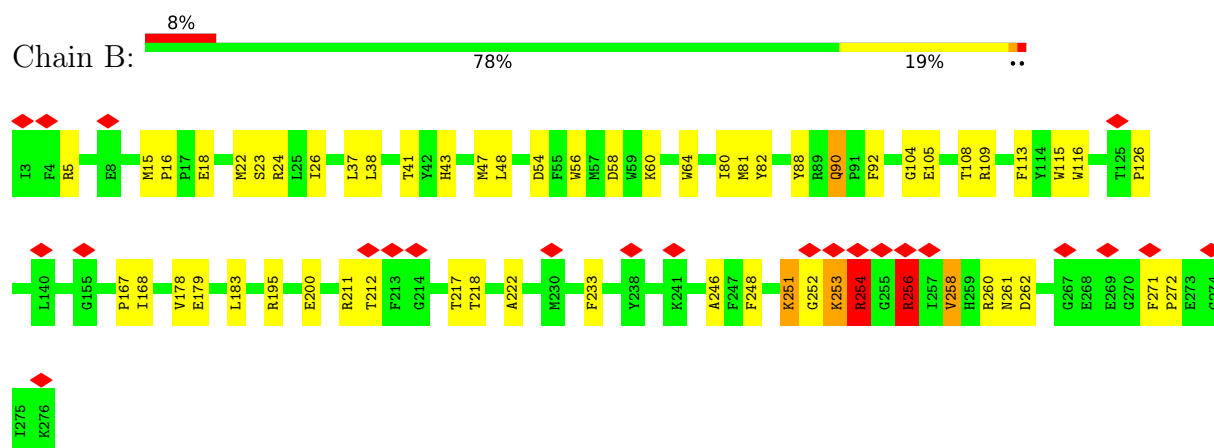
• Molecule 2: Ammonia monooxygenase beta subunit



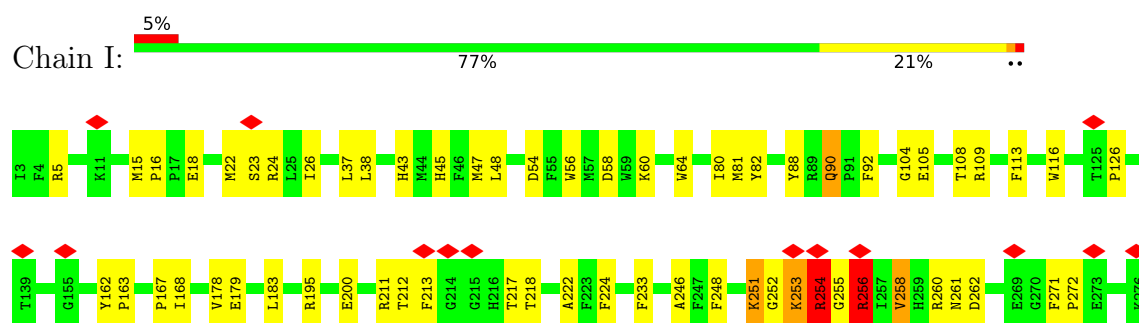
• Molecule 2: Ammonia monooxygenase beta subunit



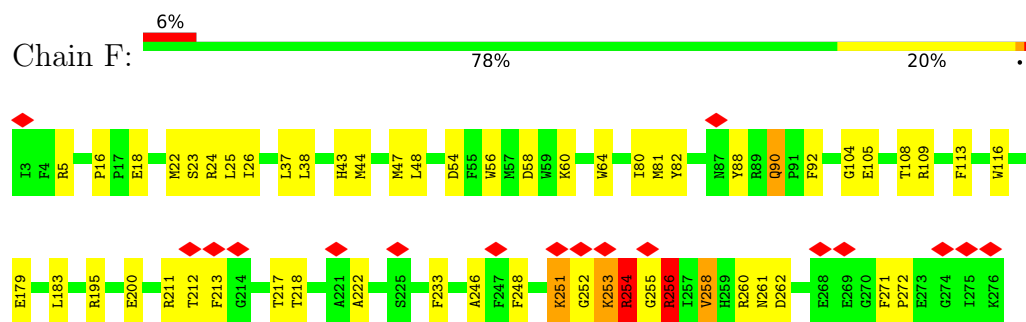
- Molecule 3: Ammonia monooxygenase alpha subunit



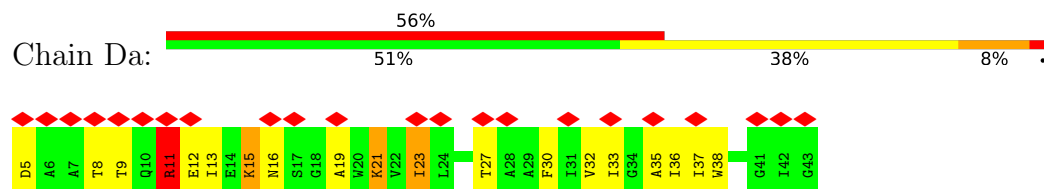
- Molecule 3: Ammonia monooxygenase alpha subunit



- Molecule 3: Ammonia monooxygenase alpha subunit

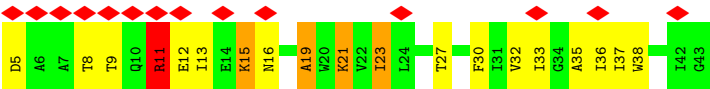


- Molecule 4: ammonia monooxygenase supernumerary helix

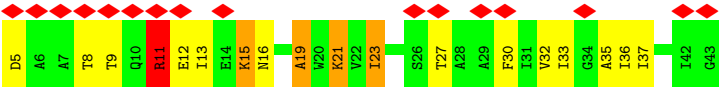


- Molecule 4: ammonia monooxygenase supernumerary helix





• Molecule 4: ammonia monooxygenase supernumerary helix



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79436	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.387	Depositor
Minimum map value	-4.704	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.193	Depositor
Recommended contour level	0.775	Depositor
Map size ($\text{\AA}$)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	C	0.53	0/2200	0.66	0/2997
1	G	0.53	0/2200	0.66	0/2997
1	J	0.53	0/2200	0.66	0/2997
2	A	0.43	2/3130 (0.1%)	0.54	3/4266 (0.1%)
2	E	0.43	2/3130 (0.1%)	0.54	3/4266 (0.1%)
2	H	0.43	2/3130 (0.1%)	0.53	3/4266 (0.1%)
3	B	0.28	0/2341	0.54	2/3199 (0.1%)
3	F	0.28	0/2341	0.54	2/3199 (0.1%)
3	I	0.28	0/2341	0.54	2/3199 (0.1%)
4	Da	1.11	1/295 (0.3%)	1.54	4/400 (1.0%)
4	Db	1.10	1/295 (0.3%)	1.54	4/400 (1.0%)
4	Dc	1.11	1/295 (0.3%)	1.54	4/400 (1.0%)
All	All	0.47	9/23898 (0.0%)	0.64	27/32586 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	G	0	3
1	J	0	3
2	A	0	2
2	E	0	2
2	H	0	2
3	B	0	2
3	F	0	2
3	I	0	2
4	Da	0	1
4	Db	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	Dc	0	1
All	All	0	24

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	58	LYS	C-O	-7.20	1.15	1.24
2	A	58	LYS	C-O	-7.16	1.15	1.24
2	E	58	LYS	C-O	-7.15	1.15	1.24
2	H	145	ALA	C-O	-7.13	1.15	1.24
2	A	145	ALA	C-O	-7.12	1.15	1.24
2	E	145	ALA	C-O	-7.12	1.15	1.24
4	Dc	19	ALA	CA-CB	-6.08	1.43	1.53
4	Db	19	ALA	CA-CB	-6.08	1.43	1.53
4	Da	19	ALA	CA-CB	-6.07	1.43	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Db	23	ILE	N-CA-C	-8.68	104.35	111.81
4	Da	23	ILE	N-CA-C	-8.65	104.37	111.81
4	Dc	23	ILE	N-CA-C	-8.61	104.41	111.81
2	A	144	HIS	CA-CB-CG	6.96	120.76	113.80
2	H	144	HIS	CA-CB-CG	6.96	120.76	113.80
2	E	144	HIS	CA-CB-CG	6.96	120.76	113.80
4	Da	16	ASN	CB-CA-C	-6.03	101.38	110.90
4	Dc	16	ASN	CB-CA-C	-6.01	101.40	110.90
4	Db	16	ASN	CB-CA-C	-6.01	101.40	110.90
2	E	142	HIS	CA-CB-CG	5.88	119.67	113.80
2	A	142	HIS	CA-CB-CG	5.84	119.64	113.80
2	H	142	HIS	CA-CB-CG	5.84	119.64	113.80
4	Da	12	GLU	CB-CG-CD	5.72	122.33	112.60
4	Dc	12	GLU	CB-CG-CD	5.70	122.28	112.60
4	Db	12	GLU	CB-CG-CD	5.69	122.27	112.60
3	F	258	VAL	N-CA-CB	-5.67	102.14	111.44
3	B	258	VAL	N-CA-CB	-5.65	102.17	111.44
3	I	258	VAL	N-CA-CB	-5.63	102.20	111.44
4	Db	30	PHE	CA-CB-CG	5.47	119.28	113.80
4	Dc	30	PHE	CA-CB-CG	5.46	119.26	113.80
4	Da	30	PHE	CA-CB-CG	5.43	119.23	113.80
3	F	252	GLY	CA-C-O	-5.19	116.39	121.06
3	I	252	GLY	CA-C-O	-5.17	116.41	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	252	GLY	CA-C-O	-5.14	116.43	121.06
2	E	141	HIS	CA-CB-CG	5.12	118.92	113.80
2	H	141	HIS	CA-CB-CG	5.11	118.91	113.80
2	A	141	HIS	CA-CB-CG	5.10	118.90	113.80

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	41	ARG	Sidechain
2	A	50	ARG	Sidechain
3	B	254	ARG	Sidechain
3	B	256	ARG	Sidechain
1	C	145	ARG	Sidechain
1	C	178	ARG	Sidechain
1	C	184	ARG	Sidechain
4	Da	11	ARG	Sidechain
4	Db	11	ARG	Sidechain
4	Dc	11	ARG	Sidechain
2	E	41	ARG	Sidechain
2	E	50	ARG	Sidechain
3	F	254	ARG	Sidechain
3	F	256	ARG	Sidechain
1	G	145	ARG	Sidechain
1	G	178	ARG	Sidechain
1	G	184	ARG	Sidechain
2	H	41	ARG	Sidechain
2	H	50	ARG	Sidechain
3	I	254	ARG	Sidechain
3	I	256	ARG	Sidechain
1	J	145	ARG	Sidechain
1	J	178	ARG	Sidechain
1	J	184	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	C	2119	0	2052	52	0
1	G	2119	0	2052	55	0
1	J	2119	0	2052	51	0
2	A	3039	0	3000	43	0
2	E	3039	0	3000	41	0
2	H	3039	0	3000	41	0
3	B	2252	0	2211	52	0
3	F	2252	0	2211	53	0
3	I	2252	0	2211	55	0
4	Da	290	0	297	7	0
4	Db	290	0	297	10	0
4	Dc	290	0	297	7	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
6	A	139	0	0	3	0
6	B	74	0	0	3	0
6	C	53	0	0	0	0
6	Da	7	0	0	0	0
6	Db	7	0	0	0	0
6	Dc	7	0	0	0	0
6	E	139	0	0	3	0
6	F	75	0	0	3	0
6	G	53	0	0	0	0
6	H	139	0	0	3	0
6	I	76	0	0	3	0
6	J	53	0	0	0	0
All	All	23928	0	22680	374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (374) 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)
3:I:248:PHE:HB3	1:J:185:GLY:HA3	1.67	0.76
1:C:257:TRP:HB3	3:B:16:PRO:HG2	1.69	0.74
3:F:16:PRO:HG2	1:G:257:TRP:HB3	1.69	0.74
1:G:154:VAL:HA	1:G:158:TYR:HD2	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLY:HA3	3:B:248:PHE:HB3	1.70	0.73
3:F:248:PHE:HB3	1:G:185:GLY:HA3	1.71	0.72
1:J:154:VAL:HA	1:J:158:TYR:HD2	1.54	0.72
1:C:154:VAL:HA	1:C:158:TYR:HD2	1.54	0.71
3:F:246:ALA:HB1	1:G:244:GLN:HG3	1.72	0.70
3:I:16:PRO:HG2	1:J:257:TRP:HB3	1.74	0.70
3:I:246:ALA:HB1	1:J:244:GLN:HG3	1.73	0.68
2:A:41:ARG:HG2	2:A:378:GLN:HA	1.75	0.68
3:I:183:LEU:HA	2:H:270:GLN:HG3	1.76	0.68
1:C:257:TRP:NE1	3:B:18:GLU:OE1	2.22	0.68
1:C:244:GLN:HG3	3:B:246:ALA:HB1	1.76	0.67
2:H:41:ARG:HG2	2:H:378:GLN:HA	1.76	0.67
3:I:18:GLU:OE1	1:J:257:TRP:NE1	2.24	0.67
2:E:41:ARG:HG2	2:E:378:GLN:HA	1.76	0.66
2:H:326:ILE:HG23	2:H:374:LEU:HD23	1.78	0.66
3:I:64:TRP:HE1	1:G:214:TRP:HZ2	1.42	0.65
2:A:270:GLN:HG3	3:B:183:LEU:HA	1.79	0.65
2:A:326:ILE:HG23	2:A:374:LEU:HD23	1.78	0.65
3:F:183:LEU:HA	2:E:270:GLN:HG3	1.79	0.65
2:E:326:ILE:HG23	2:E:374:LEU:HD23	1.78	0.64
3:F:18:GLU:OE1	1:G:257:TRP:NE1	2.28	0.64
3:I:217:THR:HG23	1:G:213:PHE:HZ	1.62	0.63
1:J:181:LEU:HD11	1:J:269:ILE:HG13	1.82	0.62
1:C:181:LEU:HD11	1:C:269:ILE:HG13	1.82	0.62
1:G:165:ILE:HG12	1:G:198:LEU:HA	1.82	0.61
1:C:165:ILE:HG12	1:C:198:LEU:HA	1.82	0.61
1:G:181:LEU:HD11	1:G:269:ILE:HG13	1.82	0.61
2:E:138:PRO:HA	2:E:164:ILE:HB	1.83	0.60
1:J:165:ILE:HG12	1:J:198:LEU:HA	1.82	0.60
2:A:138:PRO:HA	2:A:164:ILE:HB	1.83	0.60
2:H:138:PRO:HA	2:H:164:ILE:HB	1.83	0.59
3:I:212:THR:OG1	1:G:212:ALA:O	2.20	0.59
2:H:91:PHE:HB2	2:H:150:LYS:HB2	1.85	0.59
1:C:222:ALA:HB3	1:C:225:HIS:HD2	1.68	0.59
1:J:222:ALA:HB3	1:J:225:HIS:HD2	1.68	0.58
1:J:267:ASN:HD22	1:J:267:ASN:C	2.10	0.58
2:H:104:VAL:HG23	2:H:134:ARG:HB3	1.85	0.58
2:E:91:PHE:HB2	2:E:150:LYS:HB2	1.85	0.58
2:A:104:VAL:HG23	2:A:134:ARG:HB3	1.85	0.58
1:G:222:ALA:HB3	1:G:225:HIS:HD2	1.68	0.58
1:C:213:PHE:HZ	3:F:217:THR:HG23	1.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:GLN:HG3	2:E:360:PRO:HD2	1.86	0.57
2:A:91:PHE:HB2	2:A:150:LYS:HB2	1.85	0.57
2:A:359:GLN:HG3	2:A:360:PRO:HD2	1.86	0.57
1:C:267:ASN:C	1:C:267:ASN:HD22	2.10	0.57
2:A:320:GLU:OE2	2:A:322:THR:OG1	2.23	0.57
3:B:64:TRP:HE1	1:J:214:TRP:HZ2	1.53	0.57
2:H:320:GLU:OE2	2:H:322:THR:OG1	2.23	0.57
2:E:104:VAL:HG23	2:E:134:ARG:HB3	1.85	0.57
1:C:214:TRP:HZ2	3:F:64:TRP:HE1	1.50	0.57
2:H:359:GLN:HG3	2:H:360:PRO:HD2	1.86	0.56
2:E:320:GLU:OE2	2:E:322:THR:OG1	2.23	0.56
3:I:60:LYS:NZ	3:I:126:PRO:O	2.38	0.56
1:C:225:HIS:HB3	3:B:48:LEU:HD22	1.87	0.56
3:I:48:LEU:HD22	1:J:225:HIS:HB3	1.88	0.56
3:F:60:LYS:NZ	3:F:126:PRO:O	2.38	0.56
3:F:261:ASN:ND2	6:F:307:HOH:O	2.39	0.56
1:C:212:ALA:O	3:F:212:THR:OG1	2.22	0.56
3:B:60:LYS:NZ	3:B:126:PRO:O	2.38	0.55
1:J:153:HIS:HA	1:J:156:MET:HE3	1.89	0.55
1:C:153:HIS:HA	1:C:156:MET:HE3	1.89	0.55
3:B:261:ASN:ND2	6:B:307:HOH:O	2.39	0.55
1:G:153:HIS:HA	1:G:156:MET:HE3	1.89	0.55
3:I:261:ASN:ND2	6:I:307:HOH:O	2.39	0.54
2:E:102:VAL:HA	2:E:137:ILE:HD12	1.91	0.53
3:B:217:THR:HG23	1:J:213:PHE:HZ	1.73	0.53
1:C:134:GLU:HG2	3:B:113:PHE:HE1	1.74	0.53
1:G:161:PHE:HB2	1:G:162:PRO:HD3	1.91	0.53
2:H:102:VAL:HA	2:H:137:ILE:HD12	1.91	0.53
2:A:102:VAL:HA	2:A:137:ILE:HD12	1.91	0.53
3:I:56:TRP:HZ2	1:J:141:GLN:HG2	1.74	0.53
1:J:161:PHE:HB2	1:J:162:PRO:HD3	1.91	0.53
3:I:217:THR:HG23	1:G:213:PHE:CZ	2.43	0.52
2:H:353:ASP:OD1	2:H:353:ASP:N	2.43	0.52
1:C:161:PHE:HB2	1:C:162:PRO:HD3	1.91	0.52
3:B:212:THR:OG1	1:J:212:ALA:O	2.28	0.51
4:Db:19:ALA:HB2	1:G:88:TRP:CZ2	2.46	0.51
2:A:257:ARG:NH2	6:A:625:HOH:O	2.44	0.51
3:F:104:GLY:O	3:F:108:THR:HG23	2.11	0.51
3:B:43:HIS:HE1	3:B:105:GLU:HA	1.76	0.51
3:I:43:HIS:HE1	3:I:105:GLU:HA	1.76	0.51
3:F:43:HIS:HE1	3:F:105:GLU:HA	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:257:ARG:NH2	6:H:625:HOH:O	2.44	0.51
3:B:104:GLY:O	3:B:108:THR:HG23	2.11	0.51
1:G:267:ASN:C	1:G:267:ASN:HD22	2.10	0.50
2:A:220:ARG:NH2	6:A:626:HOH:O	2.44	0.50
3:I:81:MET:HE1	3:I:233:PHE:HE2	1.77	0.50
1:G:89:ILE:HG21	1:G:173:LEU:HB3	1.94	0.50
1:C:141:GLN:HG2	3:B:56:TRP:HZ2	1.77	0.50
4:Dc:35:ALA:C	4:Dc:37:ILE:N	2.70	0.50
3:I:54:ASP:O	3:I:109:ARG:NH2	2.45	0.50
3:I:104:GLY:O	3:I:108:THR:HG23	2.11	0.50
3:F:105:GLU:O	3:F:109:ARG:HG2	2.12	0.50
1:C:89:ILE:HG21	1:C:173:LEU:HB3	1.94	0.49
4:Db:11:ARG:O	4:Db:15:LYS:HG2	2.12	0.49
2:H:298:PRO:HG2	2:H:419:LYS:H	1.77	0.49
2:E:257:ARG:NH2	6:E:625:HOH:O	2.44	0.49
3:B:81:MET:HE1	3:B:233:PHE:HE2	1.77	0.49
1:G:150:THR:O	1:G:151:PRO:C	2.55	0.49
2:H:220:ARG:NH2	6:H:626:HOH:O	2.44	0.49
2:E:298:PRO:HG2	2:E:419:LYS:H	1.77	0.49
4:Da:11:ARG:O	4:Da:15:LYS:HG2	2.12	0.49
3:I:47:MET:HE2	1:J:220:PHE:HE2	1.77	0.49
2:A:298:PRO:HG2	2:A:419:LYS:H	1.77	0.49
3:B:54:ASP:O	3:B:109:ARG:NH2	2.45	0.49
3:F:54:ASP:O	3:F:109:ARG:NH2	2.45	0.49
2:H:50:ARG:HB3	2:H:81:ASP:O	2.12	0.49
2:A:50:ARG:HB3	2:A:81:ASP:O	2.12	0.49
1:J:89:ILE:HG21	1:J:173:LEU:HB3	1.94	0.49
3:B:254:ARG:HD2	2:E:225:LEU:HD22	1.93	0.49
2:E:50:ARG:HB3	2:E:81:ASP:O	2.12	0.49
3:B:105:GLU:O	3:B:109:ARG:HG2	2.12	0.49
4:Dc:11:ARG:O	4:Dc:15:LYS:HG2	2.12	0.49
3:I:105:GLU:O	3:I:109:ARG:HG2	2.12	0.48
1:J:150:THR:O	1:J:151:PRO:C	2.55	0.48
2:E:220:ARG:NH2	6:E:626:HOH:O	2.44	0.48
2:H:111:ASN:HB2	2:H:276:VAL:HG21	1.95	0.48
2:E:353:ASP:OD1	2:E:353:ASP:N	2.43	0.48
3:F:81:MET:HE1	3:F:233:PHE:HE2	1.77	0.48
2:E:379:ARG:NH1	6:E:628:HOH:O	2.47	0.48
1:G:30:LYS:O	1:G:34:ILE:HG12	2.14	0.48
3:I:56:TRP:CZ2	1:J:141:GLN:HG2	2.48	0.48
3:F:48:LEU:HD22	1:G:225:HIS:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:LYS:O	1:J:34:ILE:HG12	2.14	0.48
1:G:121:TYR:O	1:G:125:VAL:HG23	2.14	0.48
2:A:192:ASN:ND2	3:B:167:PRO:O	2.37	0.48
3:B:43:HIS:O	3:B:47:MET:HG2	2.14	0.48
3:F:43:HIS:O	3:F:47:MET:HG2	2.14	0.48
1:J:121:TYR:O	1:J:125:VAL:HG23	2.14	0.48
1:C:30:LYS:O	1:C:34:ILE:HG12	2.14	0.47
3:I:43:HIS:O	3:I:47:MET:HG2	2.14	0.47
1:C:150:THR:O	1:C:151:PRO:C	2.55	0.47
3:I:108:THR:HB	1:J:134:GLU:HB3	1.96	0.47
1:C:108:ILE:HG23	1:C:249:TYR:HE1	1.79	0.47
3:F:56:TRP:HZ2	1:G:141:GLN:HG2	1.79	0.47
3:I:113:PHE:HE1	1:J:134:GLU:HG2	1.79	0.47
1:G:161:PHE:HA	1:G:164:TYR:CE2	2.50	0.47
2:H:379:ARG:NH1	6:H:628:HOH:O	2.47	0.47
1:C:121:TYR:O	1:C:125:VAL:HG23	2.14	0.47
1:J:108:ILE:HG23	1:J:249:TYR:HE1	1.79	0.47
1:C:88:TRP:CZ2	4:Dc:19:ALA:HB2	2.50	0.47
2:A:193:GLY:HA2	3:B:168:ILE:HG23	1.97	0.47
2:A:111:ASN:HB2	2:A:276:VAL:HG21	1.95	0.47
2:A:353:ASP:OD1	2:A:353:ASP:N	2.43	0.47
1:J:22:LEU:HB3	1:J:105:LYS:HD3	1.96	0.47
2:E:111:ASN:HB2	2:E:276:VAL:HG21	1.95	0.47
1:C:134:GLU:HB3	3:B:108:THR:HB	1.96	0.47
1:C:269:ILE:HD11	3:B:262:ASP:HB2	1.95	0.47
3:F:113:PHE:HE1	1:G:134:GLU:HG2	1.79	0.47
3:F:116:TRP:CD1	1:G:48:ARG:HG3	2.49	0.47
1:J:161:PHE:HA	1:J:164:TYR:CE2	2.50	0.47
1:C:141:GLN:HG2	3:B:56:TRP:CZ2	2.50	0.47
1:C:220:PHE:HE2	3:B:47:MET:HE2	1.79	0.47
1:C:237:PHE:O	1:C:241:VAL:HG23	2.15	0.47
1:C:59:MET:HB2	2:A:41:ARG:HH12	1.80	0.46
1:C:161:PHE:HA	1:C:164:TYR:CE2	2.50	0.46
3:B:38:LEU:HD21	3:B:80:ILE:HG13	1.96	0.46
1:J:78:MET:HG2	1:J:162:PRO:HB2	1.98	0.46
1:J:144:ILE:HB	1:J:145:ARG:HH11	1.81	0.46
3:I:38:LEU:HD21	3:I:80:ILE:HG13	1.96	0.46
1:C:213:PHE:CZ	3:F:217:THR:HG23	2.49	0.46
4:Da:33:ILE:O	4:Da:37:ILE:HG13	2.15	0.46
4:Db:33:ILE:O	4:Db:37:ILE:HG13	2.15	0.46
4:Dc:33:ILE:O	4:Dc:37:ILE:HG13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:262:ASP:HB2	1:J:269:ILE:HD11	1.96	0.46
1:C:78:MET:HG2	1:C:162:PRO:HB2	1.98	0.46
3:F:38:LEU:HD21	3:F:80:ILE:HG13	1.96	0.46
1:G:237:PHE:O	1:G:241:VAL:HG23	2.15	0.46
1:G:144:ILE:HB	1:G:145:ARG:HH11	1.81	0.46
2:A:379:ARG:NH1	6:A:628:HOH:O	2.47	0.46
1:G:22:LEU:HB3	1:G:105:LYS:HD3	1.97	0.46
2:A:44:GLU:HB2	2:A:47:LEU:HD12	1.98	0.46
3:I:167:PRO:O	2:H:192:ASN:ND2	2.42	0.46
1:G:108:ILE:HG23	1:G:249:TYR:HE1	1.79	0.46
2:H:288:ILE:HG12	2:H:308:VAL:HG12	1.98	0.46
2:E:44:GLU:HB2	2:E:47:LEU:HD12	1.98	0.46
1:C:267:ASN:C	1:C:267:ASN:ND2	2.74	0.46
4:Db:35:ALA:C	4:Db:37:ILE:N	2.70	0.46
3:I:251:LYS:HB3	3:I:251:LYS:HE2	1.66	0.46
3:F:37:LEU:HD13	1:G:122:ILE:HG12	1.97	0.46
2:H:44:GLU:HB2	2:H:47:LEU:HD12	1.98	0.46
1:C:144:ILE:HB	1:C:145:ARG:HH11	1.81	0.46
3:B:254:ARG:HG2	3:B:256:ARG:HG2	1.98	0.46
1:J:237:PHE:O	1:J:241:VAL:HG23	2.15	0.45
2:E:216:MET:HA	2:E:220:ARG:HD2	1.98	0.45
1:C:22:LEU:HB3	1:C:105:LYS:HD3	1.96	0.45
2:A:374:LEU:HA	2:A:377:ILE:HD12	1.98	0.45
3:I:82:TYR:CD1	3:I:82:TYR:C	2.95	0.45
3:F:167:PRO:O	2:E:192:ASN:ND2	2.39	0.45
1:J:267:ASN:C	1:J:267:ASN:ND2	2.74	0.45
4:Da:21:LYS:HB3	4:Da:21:LYS:HE3	1.62	0.45
3:F:195:ARG:NH2	6:F:314:HOH:O	2.50	0.45
2:A:216:MET:HA	2:A:220:ARG:HD2	1.98	0.45
4:Da:35:ALA:C	4:Da:37:ILE:N	2.70	0.45
3:I:23:SER:OG	2:H:218:LEU:HB3	2.16	0.45
3:F:254:ARG:HD2	2:H:225:LEU:HD22	1.98	0.45
1:J:176:MET:HE2	1:J:176:MET:HB2	1.58	0.45
1:J:87:GLY:O	1:J:91:LYS:HB3	2.17	0.45
2:E:374:LEU:HA	2:E:377:ILE:HD12	1.98	0.45
4:Db:11:ARG:NH1	1:G:98:GLN:HG2	2.31	0.45
1:G:78:MET:HG2	1:G:162:PRO:HB2	1.98	0.45
1:C:87:GLY:O	1:C:91:LYS:HB3	2.17	0.45
3:B:82:TYR:CD1	3:B:82:TYR:C	2.95	0.45
3:I:47:MET:HE2	1:J:220:PHE:CE2	2.52	0.45
1:G:87:GLY:O	1:G:91:LYS:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:ILE:HG13	2:A:378:GLN:HG3	1.99	0.45
3:I:254:ARG:HG2	3:I:256:ARG:HG2	1.98	0.45
2:H:326:ILE:HG13	2:H:378:GLN:HG3	1.99	0.45
2:A:218:LEU:HB3	3:B:23:SER:OG	2.17	0.44
1:J:59:MET:HB2	2:H:41:ARG:HH12	1.82	0.44
4:Dc:21:LYS:HE3	4:Dc:21:LYS:HB3	1.62	0.44
3:F:82:TYR:CD1	3:F:82:TYR:C	2.95	0.44
2:A:225:LEU:HD22	3:I:254:ARG:HD2	1.99	0.44
3:F:88:TYR:O	2:E:220:ARG:NH1	2.48	0.44
1:G:173:LEU:HD23	1:G:173:LEU:HA	1.78	0.44
3:I:22:MET:HE3	3:I:26:ILE:HD11	2.00	0.44
3:F:22:MET:HE3	3:F:26:ILE:HD11	2.00	0.44
3:F:168:ILE:HG23	2:E:193:GLY:HA2	1.98	0.44
3:F:262:ASP:HB2	1:G:269:ILE:HD11	1.99	0.44
3:I:195:ARG:NH2	6:I:314:HOH:O	2.50	0.44
2:H:374:LEU:HA	2:H:377:ILE:HD12	1.98	0.44
2:E:326:ILE:HG13	2:E:378:GLN:HG3	1.99	0.44
1:C:176:MET:HE2	1:C:176:MET:HB2	1.58	0.44
2:A:288:ILE:HG12	2:A:308:VAL:HG12	1.98	0.44
3:B:24:ARG:HD2	3:B:24:ARG:HA	1.80	0.44
1:C:48:ARG:HG3	3:B:116:TRP:CD1	2.53	0.44
3:I:218:THR:O	3:I:222:ALA:N	2.51	0.44
3:F:254:ARG:HG2	3:F:256:ARG:HG2	1.98	0.44
3:B:22:MET:HE3	3:B:26:ILE:HD11	2.00	0.44
2:H:216:MET:HA	2:H:220:ARG:HD2	1.98	0.44
2:E:288:ILE:HG12	2:E:308:VAL:HG12	1.98	0.44
2:E:306:MET:HE2	2:E:306:MET:HB3	1.89	0.44
3:B:195:ARG:NH2	6:B:314:HOH:O	2.50	0.43
3:I:213:PHE:CZ	1:G:147:THR:HA	2.53	0.43
1:C:197:PRO:O	1:C:200:ILE:HB	2.18	0.43
2:A:235:PRO:O	2:A:239:LYS:HG3	2.18	0.43
1:J:197:PRO:O	1:J:200:ILE:HB	2.18	0.43
1:G:267:ASN:C	1:G:267:ASN:ND2	2.74	0.43
2:A:201:MET:HB2	2:A:201:MET:HE2	1.83	0.43
3:B:253:LYS:HA	3:B:253:LYS:HD3	1.93	0.43
1:G:197:PRO:O	1:G:200:ILE:HB	2.18	0.43
1:C:48:ARG:HD3	3:B:115:TRP:CZ3	2.54	0.43
3:I:200:GLU:OE1	2:H:117:ILE:HG23	2.19	0.43
3:B:22:MET:HE3	3:B:26:ILE:CD1	2.49	0.43
4:Db:21:LYS:HB3	4:Db:21:LYS:HE3	1.62	0.43
3:I:116:TRP:CD1	1:J:48:ARG:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:HD2	1:C:248:ARG:HA	1.87	0.43
1:C:267:ASN:ND2	1:C:267:ASN:O	2.40	0.43
4:Da:38:TRP:CZ3	1:J:66:VAL:HA	2.53	0.43
3:I:24:ARG:HD2	3:I:24:ARG:HA	1.80	0.43
3:I:168:ILE:HG23	2:H:193:GLY:HA2	2.01	0.43
1:G:216:MET:HE1	1:G:219:LEU:HD12	2.01	0.43
4:Da:38:TRP:HZ3	1:J:66:VAL:HA	1.84	0.43
4:Db:11:ARG:HH12	1:G:98:GLN:HG2	1.84	0.43
2:H:235:PRO:O	2:H:239:LYS:HG3	2.19	0.43
3:I:251:LYS:HA	3:I:256:ARG:O	2.19	0.43
3:F:24:ARG:HD2	3:F:24:ARG:HA	1.80	0.43
3:F:58:ASP:OD1	3:F:58:ASP:N	2.38	0.43
3:I:178:VAL:HG12	3:I:179:GLU:HG2	2.01	0.42
3:F:23:SER:OG	2:E:218:LEU:HB3	2.18	0.42
2:E:235:PRO:O	2:E:239:LYS:HG3	2.19	0.42
3:I:37:LEU:HD13	1:J:122:ILE:HG12	2.00	0.42
3:F:251:LYS:HA	3:F:256:ARG:O	2.19	0.42
2:E:43:GLN:HB2	2:E:48:ARG:HD3	2.01	0.42
1:G:121:TYR:OH	1:G:194:ILE:HA	2.19	0.42
2:H:43:GLN:HB2	2:H:48:ARG:HD3	2.01	0.42
2:H:306:MET:HE2	2:H:306:MET:HB3	1.89	0.42
2:E:229:ASP:O	2:E:233:MET:HG2	2.19	0.42
1:C:98:GLN:HG2	4:Dc:11:ARG:NH1	2.35	0.42
1:C:122:ILE:HG12	3:B:37:LEU:HD13	2.02	0.42
3:I:90:GLN:HB3	3:I:92:PHE:CE2	2.54	0.42
1:J:248:ARG:HA	1:J:248:ARG:HD2	1.87	0.42
2:E:111:ASN:N	2:E:128:GLU:O	2.32	0.42
2:E:218:LEU:HB3	2:E:219:PRO:HD3	2.01	0.42
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.78	0.42
2:A:275:LYS:HB2	2:A:275:LYS:HE3	1.94	0.42
3:B:218:THR:O	3:B:222:ALA:N	2.51	0.42
3:B:251:LYS:HA	3:B:256:ARG:O	2.19	0.42
3:F:22:MET:HE3	3:F:26:ILE:CD1	2.49	0.42
2:H:218:LEU:HB3	2:H:219:PRO:HD3	2.01	0.42
1:C:112:PHE:O	1:C:116:MET:HG3	2.20	0.42
1:C:121:TYR:OH	1:C:194:ILE:HA	2.19	0.42
2:A:229:ASP:O	2:A:233:MET:HG2	2.19	0.42
2:A:356:SER:OG	2:A:364:LYS:NZ	2.53	0.42
3:B:178:VAL:HG12	3:B:179:GLU:HG2	2.01	0.42
3:F:218:THR:O	3:F:222:ALA:N	2.51	0.42
1:J:216:MET:HE1	1:J:219:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:ILE:O	2:E:212:THR:HG23	2.20	0.42
2:E:356:SER:OG	2:E:364:LYS:NZ	2.53	0.42
2:A:208:ILE:O	2:A:212:THR:HG23	2.19	0.42
3:F:90:GLN:HB3	3:F:92:PHE:CE2	2.54	0.42
1:J:112:PHE:O	1:J:116:MET:HG3	2.20	0.42
1:J:181:LEU:HA	1:J:181:LEU:HD12	1.84	0.42
2:H:356:SER:OG	2:H:364:LYS:NZ	2.53	0.42
2:E:56:ASP:O	2:E:74:GLY:HA2	2.20	0.42
3:B:90:GLN:HB3	3:B:92:PHE:CE2	2.54	0.42
1:G:59:MET:HB2	2:E:41:ARG:HH12	1.84	0.42
2:H:56:ASP:O	2:H:74:GLY:HA2	2.20	0.42
3:I:58:ASP:OD1	3:I:58:ASP:N	2.38	0.42
3:F:25:LEU:HD23	3:F:25:LEU:HA	1.90	0.42
3:F:200:GLU:OE1	2:E:117:ILE:HG23	2.19	0.42
1:J:121:TYR:OH	1:J:194:ILE:HA	2.19	0.42
2:H:100:SER:O	2:H:102:VAL:N	2.50	0.42
2:H:208:ILE:O	2:H:212:THR:HG23	2.20	0.42
2:E:111:ASN:ND2	2:E:277:ALA:O	2.53	0.42
3:B:258:VAL:HG22	3:B:260:ARG:HH12	1.85	0.42
3:I:271:PHE:HB3	3:I:272:PRO:HD3	2.02	0.42
2:A:111:ASN:ND2	2:A:277:ALA:O	2.53	0.41
2:A:220:ARG:NH1	3:B:88:TYR:O	2.47	0.41
3:B:37:LEU:O	3:B:41:THR:OG1	2.33	0.41
3:B:253:LYS:HB2	6:B:301:HOH:O	2.20	0.41
4:Db:35:ALA:O	4:Db:36:ILE:C	2.63	0.41
3:I:22:MET:HE3	3:I:26:ILE:CD1	2.49	0.41
3:F:47:MET:HE2	1:G:220:PHE:HE2	1.84	0.41
1:C:220:PHE:CE2	3:B:47:MET:HE2	2.55	0.41
3:F:56:TRP:CZ2	1:G:141:GLN:HG2	2.54	0.41
3:F:271:PHE:HB3	3:F:272:PRO:HD3	2.02	0.41
2:H:207:TRP:O	2:H:210:VAL:HG12	2.20	0.41
3:F:178:VAL:HG12	3:F:179:GLU:HG2	2.01	0.41
1:G:248:ARG:HA	1:G:248:ARG:HD2	1.87	0.41
1:C:216:MET:HE1	1:C:219:LEU:HD12	2.01	0.41
2:A:207:TRP:O	2:A:210:VAL:HG12	2.20	0.41
1:C:147:THR:HA	3:F:213:PHE:CZ	2.56	0.41
2:A:117:ILE:HG23	3:B:200:GLU:OE1	2.21	0.41
2:A:212:THR:O	2:A:212:THR:OG1	2.34	0.41
3:B:58:ASP:OD1	3:B:58:ASP:N	2.38	0.41
3:F:18:GLU:HG3	1:G:18:TYR:CG	2.56	0.41
2:H:45:PRO:O	2:H:46:PHE:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:MET:HB2	2:E:201:MET:HE2	1.83	0.41
3:B:258:VAL:CG2	3:B:260:ARG:HH12	2.34	0.41
3:I:258:VAL:CG2	3:I:260:ARG:HH12	2.34	0.41
3:I:258:VAL:HG22	3:I:260:ARG:HH12	1.85	0.41
2:H:229:ASP:O	2:H:233:MET:HG2	2.19	0.41
2:E:207:TRP:O	2:E:210:VAL:HG12	2.20	0.41
3:I:253:LYS:HB2	6:I:301:HOH:O	2.20	0.41
1:G:181:LEU:HD12	1:G:181:LEU:HA	1.84	0.41
1:G:181:LEU:HD22	1:G:248:ARG:HD3	2.03	0.41
1:C:20:MET:HE2	1:C:20:MET:HB2	1.87	0.41
2:A:43:GLN:HB2	2:A:48:ARG:HD3	2.01	0.41
1:G:112:PHE:O	1:G:116:MET:HG3	2.20	0.41
2:H:111:ASN:ND2	2:H:277:ALA:O	2.53	0.41
2:A:56:ASP:O	2:A:74:GLY:HA2	2.20	0.41
4:Da:35:ALA:O	4:Da:36:ILE:C	2.63	0.41
3:I:224:PHE:CE1	1:G:206:LEU:HD13	2.56	0.41
3:F:258:VAL:CG2	3:F:260:ARG:HH12	2.34	0.41
1:J:181:LEU:HD22	1:J:248:ARG:HD3	2.03	0.41
1:C:199:MET:C	1:C:202:PRO:HD2	2.46	0.41
3:I:88:TYR:O	2:H:220:ARG:NH1	2.50	0.41
2:E:45:PRO:O	2:E:46:PHE:C	2.64	0.41
3:B:271:PHE:HB3	3:B:272:PRO:HD3	2.02	0.40
4:Db:38:TRP:HZ3	1:G:66:VAL:HA	1.86	0.40
3:I:253:LYS:C	3:I:255:GLY:N	2.79	0.40
3:F:258:VAL:HG22	3:F:260:ARG:HH12	1.85	0.40
2:A:218:LEU:HB3	2:A:219:PRO:HD3	2.01	0.40
3:F:108:THR:HB	1:G:134:GLU:HB3	2.03	0.40
3:F:253:LYS:C	3:F:255:GLY:N	2.79	0.40
1:J:111:TYR:CZ	1:J:248:ARG:HG2	2.57	0.40
2:A:45:PRO:O	2:A:46:PHE:C	2.64	0.40
4:Db:38:TRP:CZ3	1:G:66:VAL:HA	2.57	0.40
3:F:253:LYS:HB2	6:F:301:HOH:O	2.20	0.40
1:J:173:LEU:HA	1:J:173:LEU:HD23	1.78	0.40
1:J:199:MET:C	1:J:202:PRO:HD2	2.46	0.40
2:A:222:ARG:HD3	3:B:15:MET:HE2	2.03	0.40
3:I:15:MET:HE2	2:H:222:ARG:HD3	2.03	0.40
3:F:44:MET:HG3	1:G:129:GLY:O	2.21	0.40
2:A:111:ASN:N	2:A:128:GLU:O	2.32	0.40
4:Dc:35:ALA:O	4:Dc:36:ILE:C	2.63	0.40
3:I:162:TYR:HB3	3:I:163:PRO:HD3	2.04	0.40
1:J:255:VAL:HG23	1:J:264:ILE:HD11	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:MET:C	1:G:202:PRO:HD2	2.46	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	C	252/254 (99%)	227 (90%)	24 (10%)	1 (0%)	30	57
1	G	252/254 (99%)	227 (90%)	24 (10%)	1 (0%)	30	57
1	J	252/254 (99%)	227 (90%)	24 (10%)	1 (0%)	30	57
2	A	381/383 (100%)	368 (97%)	13 (3%)	0	100	100
2	E	381/383 (100%)	367 (96%)	14 (4%)	0	100	100
2	H	381/383 (100%)	368 (97%)	13 (3%)	0	100	100
3	B	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	30	57
3	F	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	30	57
3	I	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	30	57
4	Da	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
4	Db	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
4	Dc	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
All	All	2826/2850 (99%)	2657 (94%)	163 (6%)	6 (0%)	44	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	5	ARG
3	I	5	ARG
3	F	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	187	SER
1	J	187	SER
1	G	187	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	220/220 (100%)	210 (96%)	10 (4%)	24	55
1	G	220/220 (100%)	210 (96%)	10 (4%)	24	55
1	J	220/220 (100%)	210 (96%)	10 (4%)	24	55
2	A	323/323 (100%)	311 (96%)	12 (4%)	30	62
2	E	323/323 (100%)	311 (96%)	12 (4%)	30	62
2	H	323/323 (100%)	311 (96%)	12 (4%)	30	62
3	B	233/233 (100%)	227 (97%)	6 (3%)	40	72
3	F	233/233 (100%)	227 (97%)	6 (3%)	40	72
3	I	233/233 (100%)	226 (97%)	7 (3%)	36	69
4	Da	28/28 (100%)	18 (64%)	10 (36%)	0	0
4	Db	28/28 (100%)	18 (64%)	10 (36%)	0	0
4	Dc	28/28 (100%)	18 (64%)	10 (36%)	0	0
All	All	2412/2412 (100%)	2297 (95%)	115 (5%)	24	53

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	LEU
1	C	122	ILE
1	C	145	ARG
1	C	147	THR
1	C	150	THR
1	C	151	PRO
1	C	156	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	176	MET
1	C	178	ARG
1	C	215	PHE
2	A	41	ARG
2	A	42	SER
2	A	48	ARG
2	A	56	ASP
2	A	57	ILE
2	A	104	VAL
2	A	146	MET
2	A	251	LEU
2	A	275	LYS
2	A	317	THR
2	A	359	GLN
2	A	381	MET
3	B	90	GLN
3	B	211	ARG
3	B	251	LYS
3	B	253	LYS
3	B	254	ARG
3	B	256	ARG
4	Da	5	ASP
4	Da	8	THR
4	Da	9	THR
4	Da	11	ARG
4	Da	13	ILE
4	Da	15	LYS
4	Da	21	LYS
4	Da	23	ILE
4	Da	27	THR
4	Da	32	VAL
4	Db	5	ASP
4	Db	8	THR
4	Db	9	THR
4	Db	11	ARG
4	Db	13	ILE
4	Db	15	LYS
4	Db	21	LYS
4	Db	23	ILE
4	Db	27	THR
4	Db	32	VAL
4	Dc	5	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Dc	8	THR
4	Dc	9	THR
4	Dc	11	ARG
4	Dc	13	ILE
4	Dc	15	LYS
4	Dc	21	LYS
4	Dc	23	ILE
4	Dc	27	THR
4	Dc	32	VAL
3	I	45	HIS
3	I	90	GLN
3	I	211	ARG
3	I	251	LYS
3	I	253	LYS
3	I	254	ARG
3	I	256	ARG
3	F	90	GLN
3	F	211	ARG
3	F	251	LYS
3	F	253	LYS
3	F	254	ARG
3	F	256	ARG
1	J	83	LEU
1	J	122	ILE
1	J	145	ARG
1	J	147	THR
1	J	150	THR
1	J	151	PRO
1	J	156	MET
1	J	176	MET
1	J	178	ARG
1	J	215	PHE
1	G	83	LEU
1	G	122	ILE
1	G	145	ARG
1	G	147	THR
1	G	150	THR
1	G	151	PRO
1	G	156	MET
1	G	176	MET
1	G	178	ARG
1	G	215	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	41	ARG
2	H	42	SER
2	H	48	ARG
2	H	56	ASP
2	H	57	ILE
2	H	104	VAL
2	H	146	MET
2	H	251	LEU
2	H	275	LYS
2	H	317	THR
2	H	359	GLN
2	H	381	MET
2	E	41	ARG
2	E	42	SER
2	E	48	ARG
2	E	56	ASP
2	E	57	ILE
2	E	104	VAL
2	E	146	MET
2	E	251	LEU
2	E	275	LYS
2	E	317	THR
2	E	359	GLN
2	E	381	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	GLN
1	C	101	ASN
1	C	135	GLN
1	C	207	ASN
1	C	211	HIS
1	C	225	HIS
2	A	38	HIS
2	A	88	GLN
2	A	173	ASN
2	A	263	HIS
2	A	311	ASN
3	B	43	HIS
3	B	122	ASN
3	I	122	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	261	ASN
3	F	43	HIS
3	F	122	ASN
3	F	261	ASN
1	J	47	GLN
1	J	101	ASN
1	J	135	GLN
1	J	207	ASN
1	J	211	HIS
1	J	225	HIS
1	G	47	GLN
1	G	101	ASN
1	G	135	GLN
1	G	207	ASN
1	G	211	HIS
1	G	225	HIS
2	H	38	HIS
2	H	88	GLN
2	H	173	ASN
2	H	263	HIS
2	H	311	ASN
2	E	38	HIS
2	E	88	GLN
2	E	173	ASN
2	E	263	HIS
2	E	311	ASN

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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

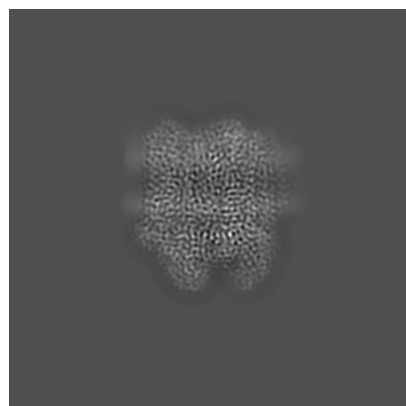
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45663. These allow visual inspection of the internal detail of the map and identification of artifacts.

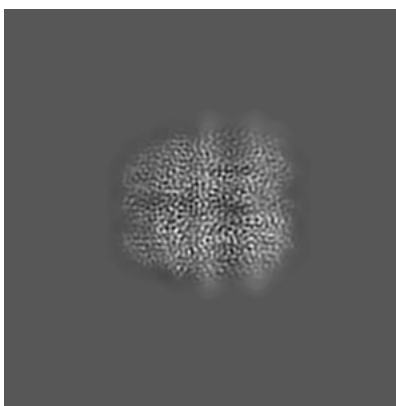
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

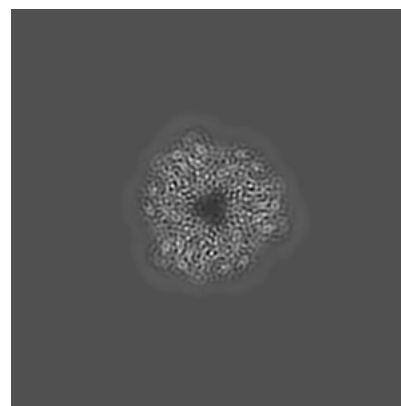
6.1.1 Primary map



X

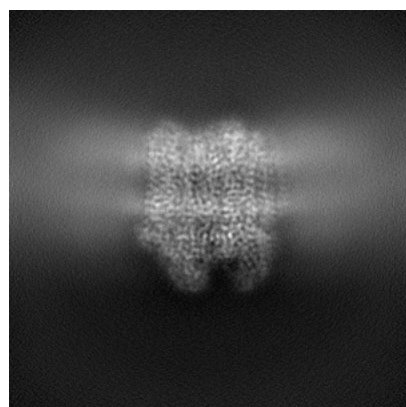


Y

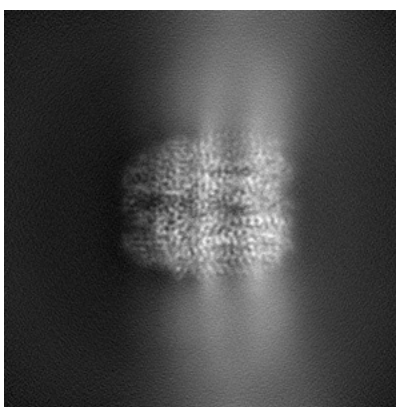


Z

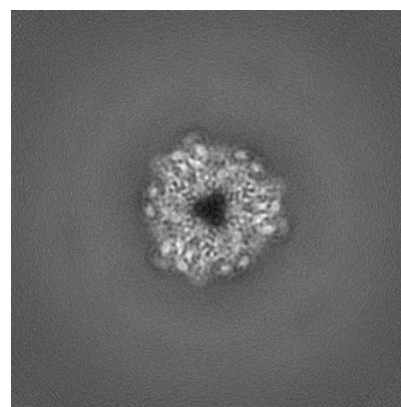
6.1.2 Raw map



X



Y

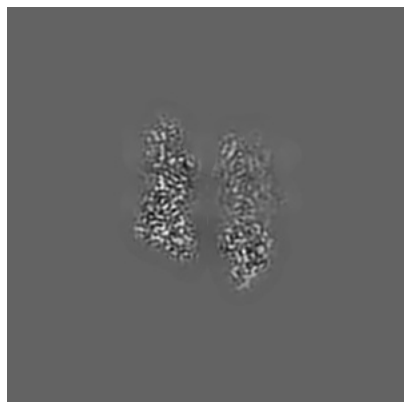


Z

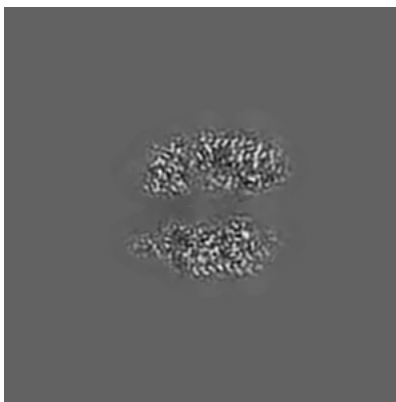
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

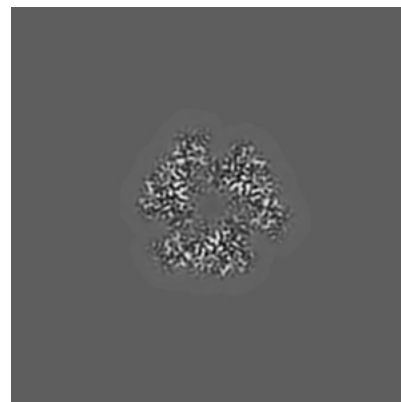
6.2.1 Primary map



X Index: 160

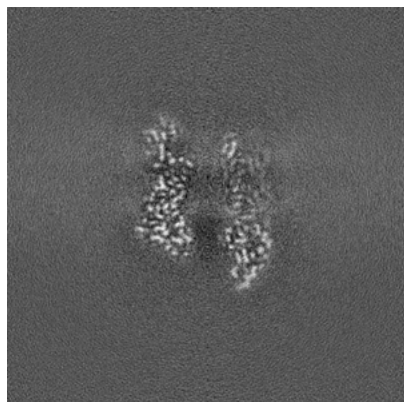


Y Index: 160

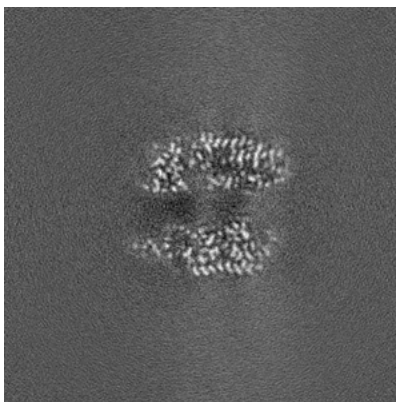


Z Index: 160

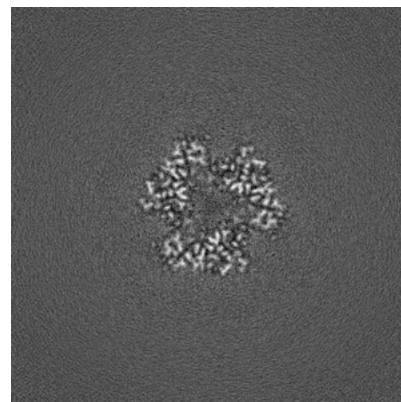
6.2.2 Raw map



X Index: 160



Y Index: 160

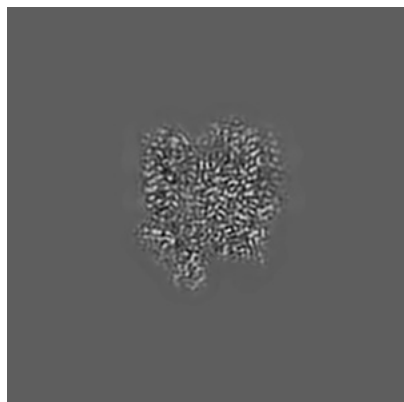


Z Index: 160

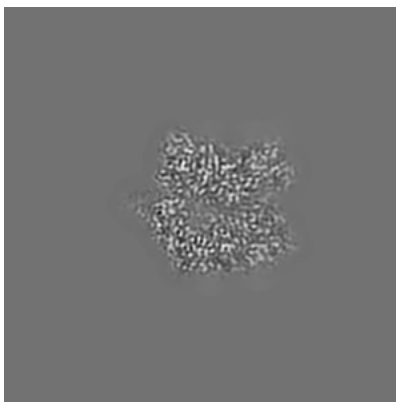
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

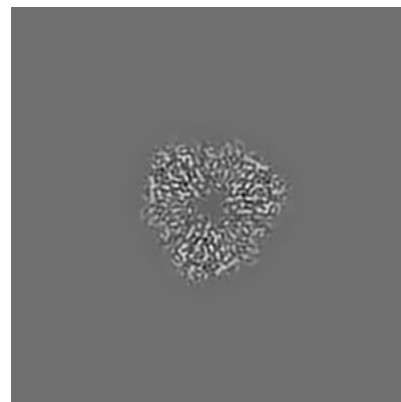
6.3.1 Primary map



X Index: 138

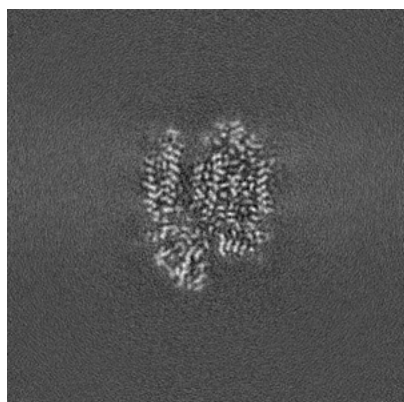


Y Index: 178

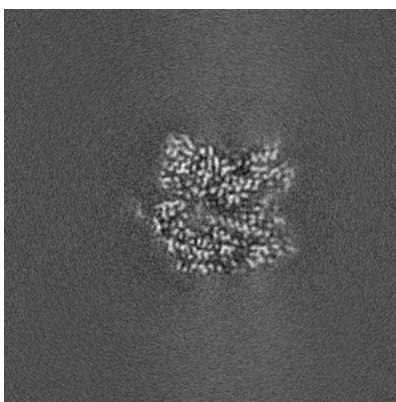


Z Index: 139

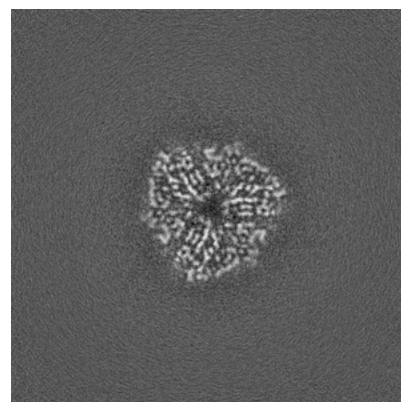
6.3.2 Raw map



X Index: 134



Y Index: 178

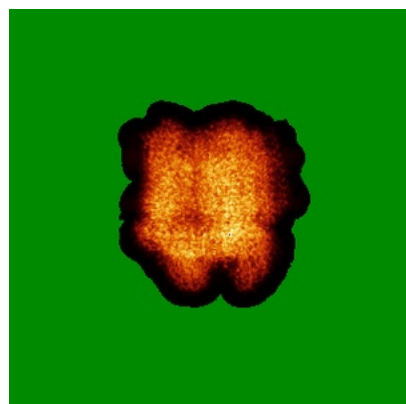


Z Index: 138

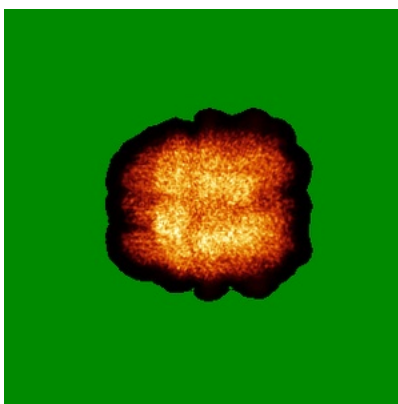
The images above show the largest variance slices of the map in three orthogonal directions.

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

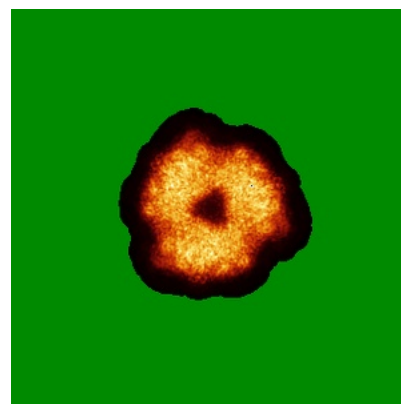
6.4.1 Primary map



X

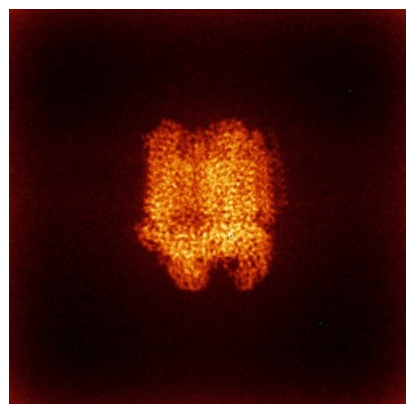


Y

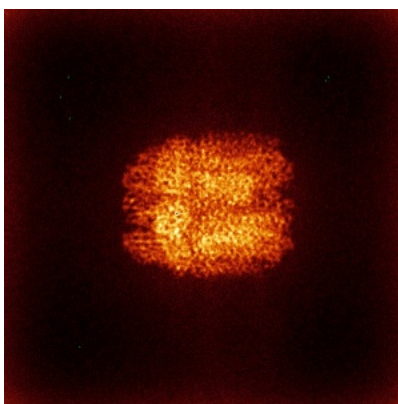


Z

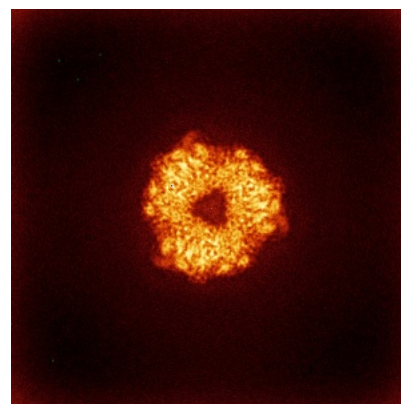
6.4.2 Raw map



X



Y

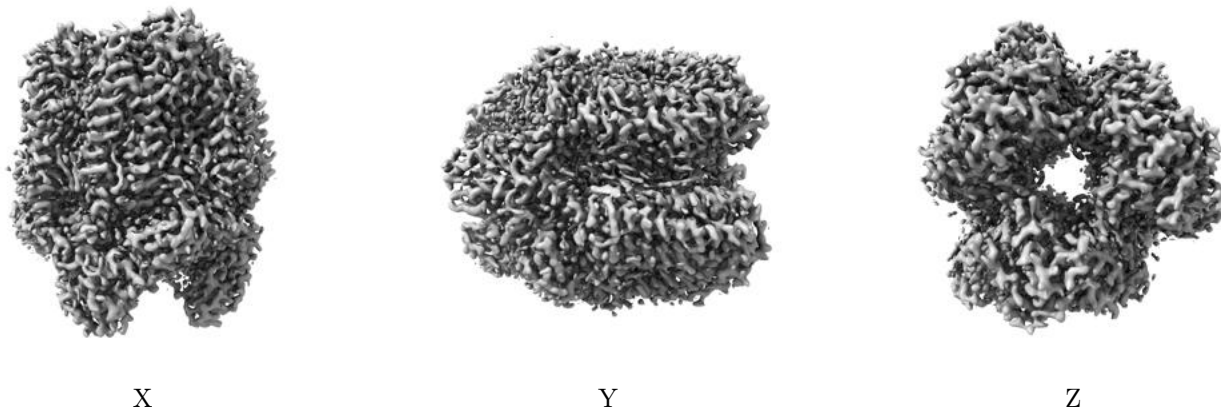


Z

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

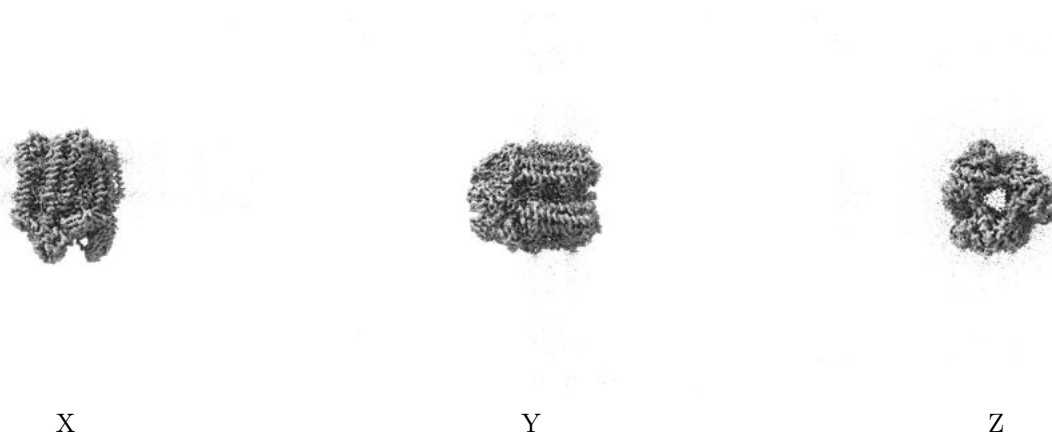
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.775. 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.

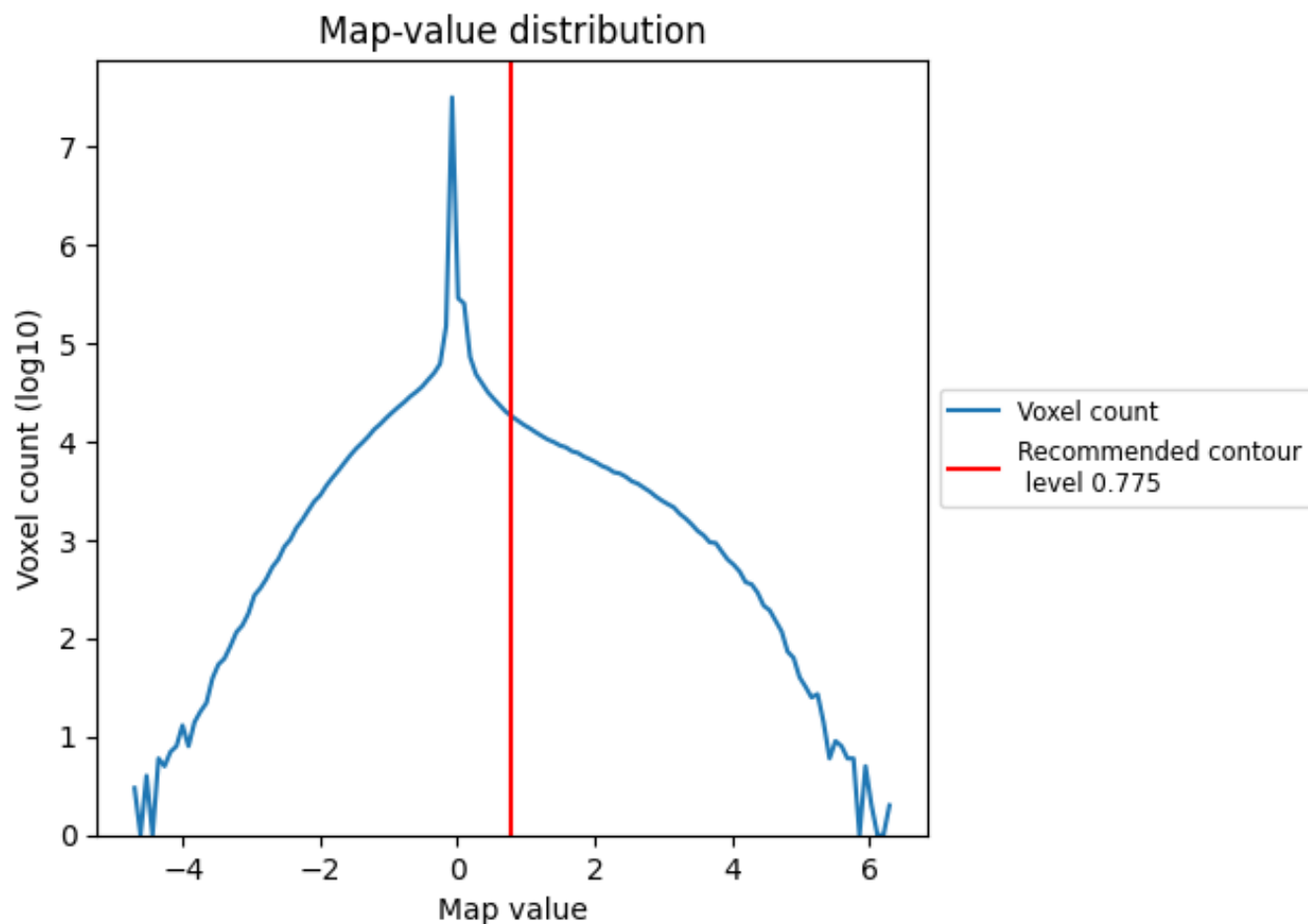
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

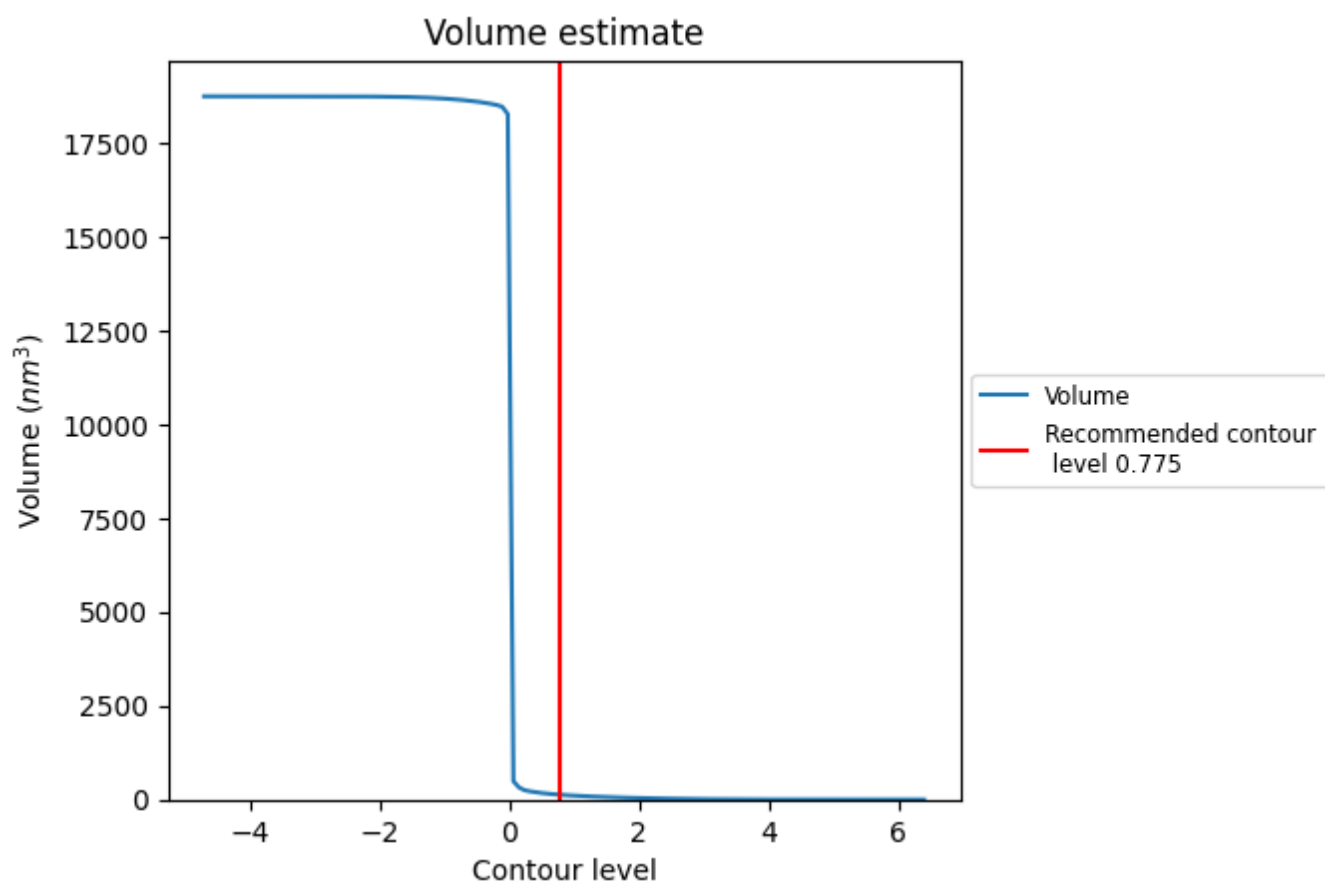
This section contains the results of statistical analysis of the map.

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.

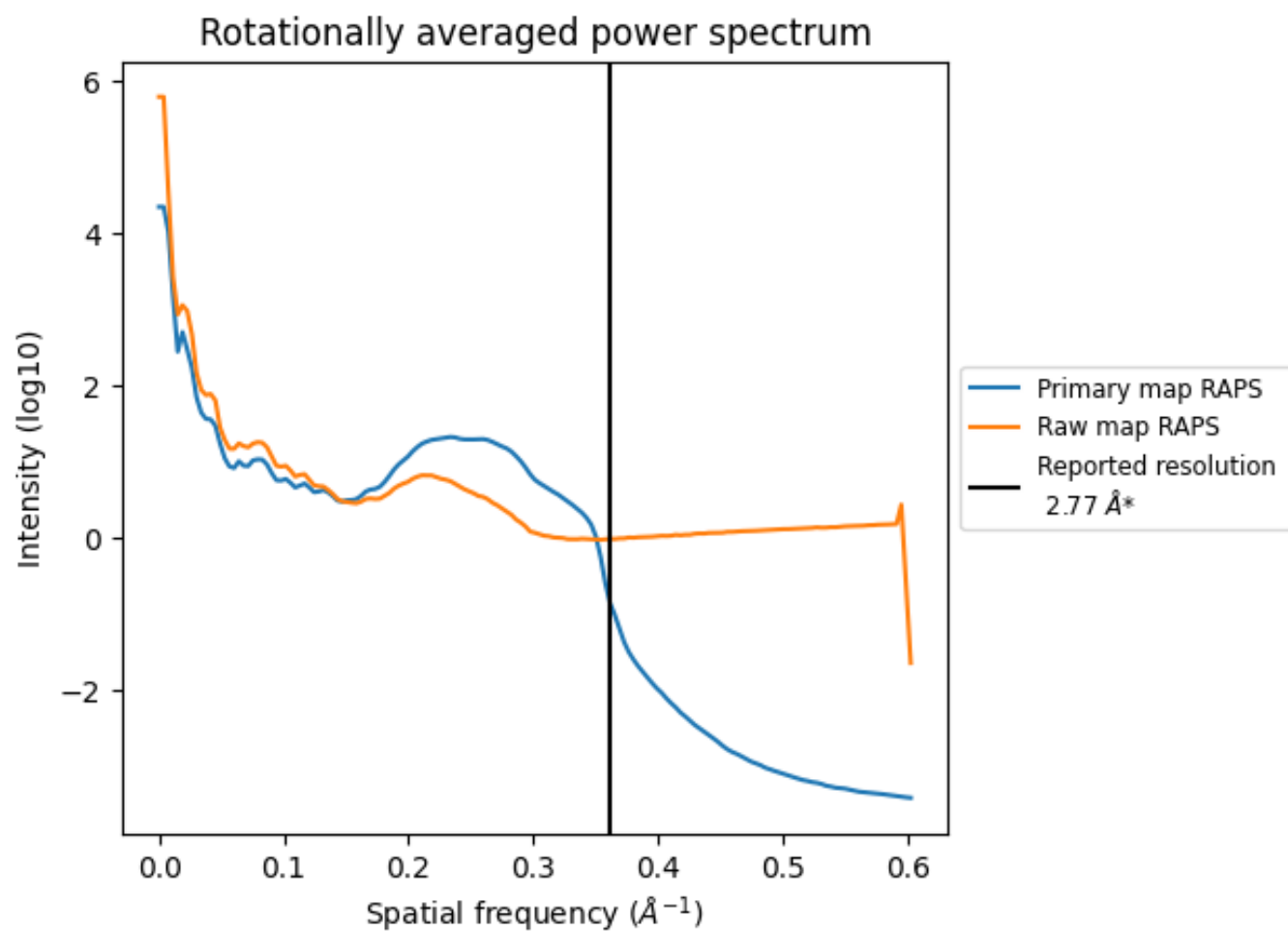
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 117 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 ⓘ

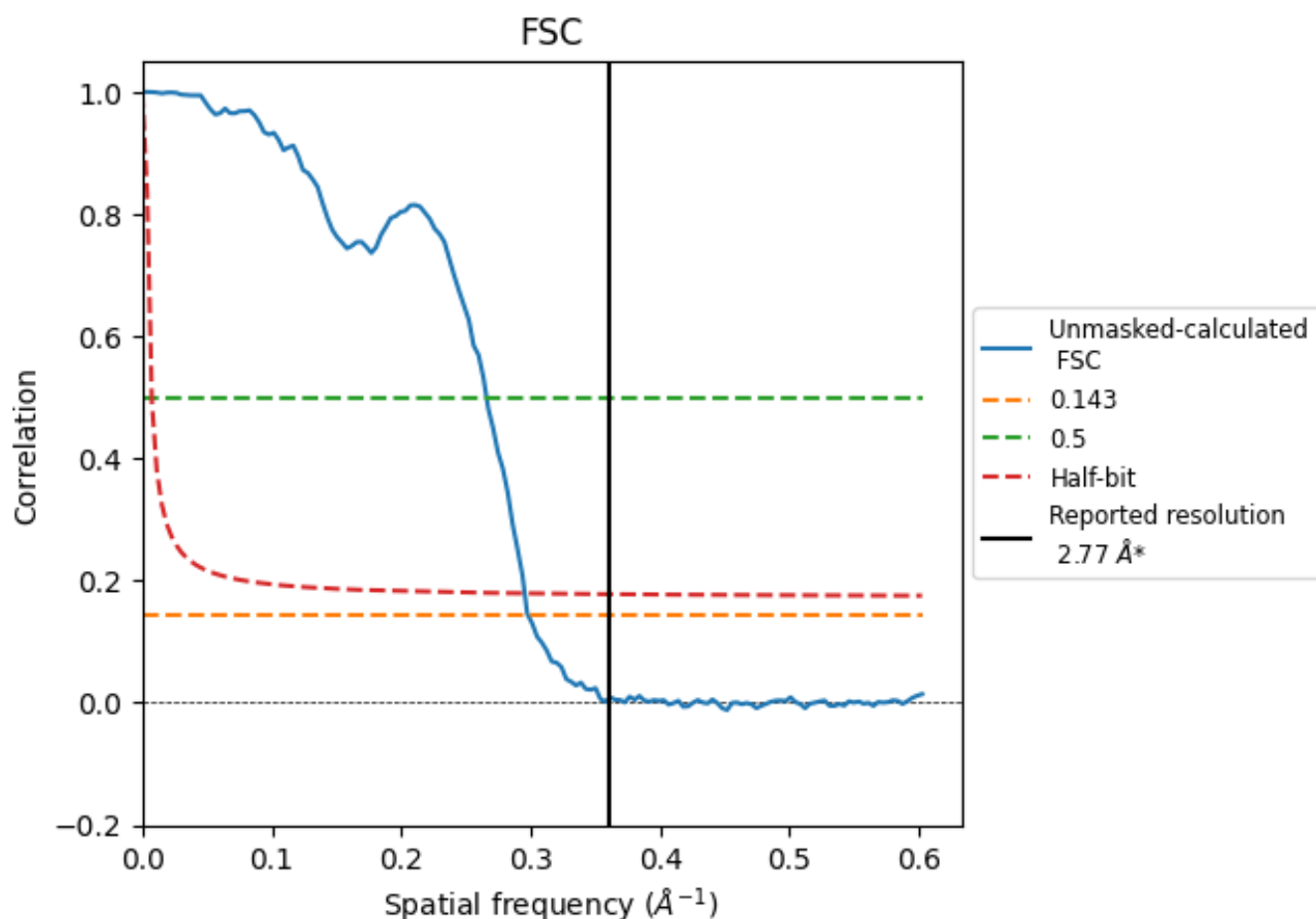


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

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 $0.361 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

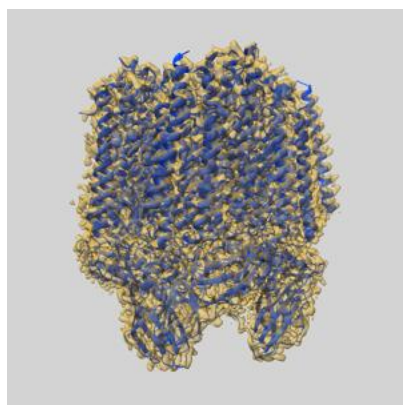
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.35	3.76	3.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.77 by more than 10 %

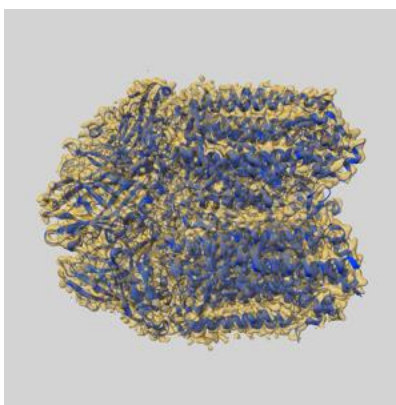
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45663 and PDB model 9CL6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

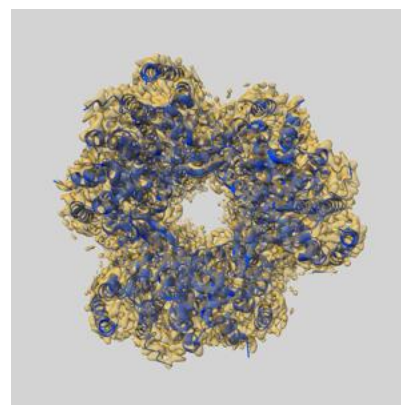
9.1 Map-model overlay [i](#)



X



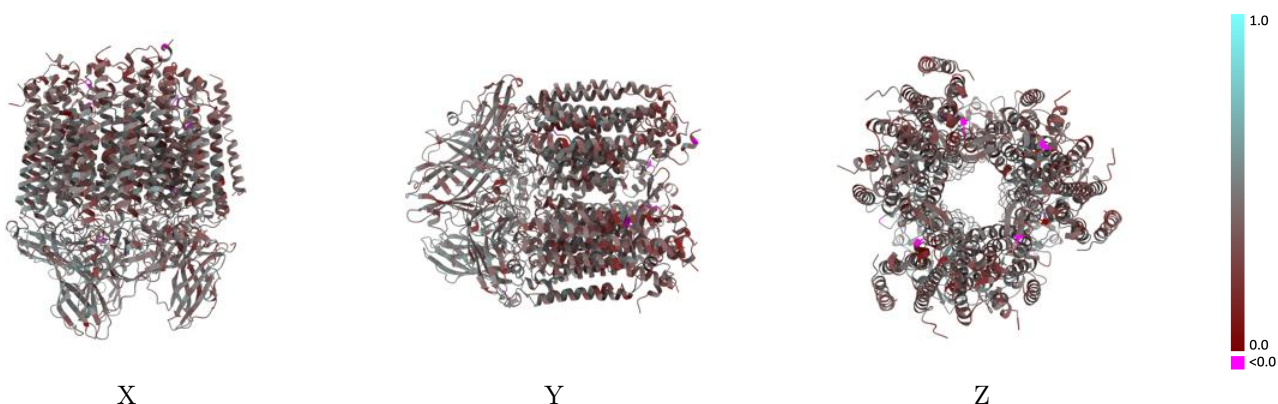
Y



Z

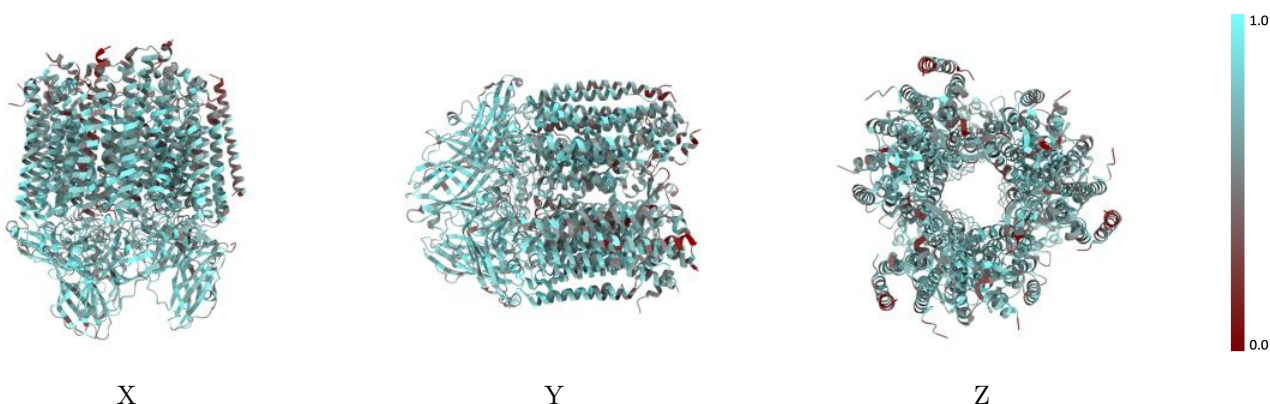
The images above show the 3D surface view of the map at the recommended contour level 0.775 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



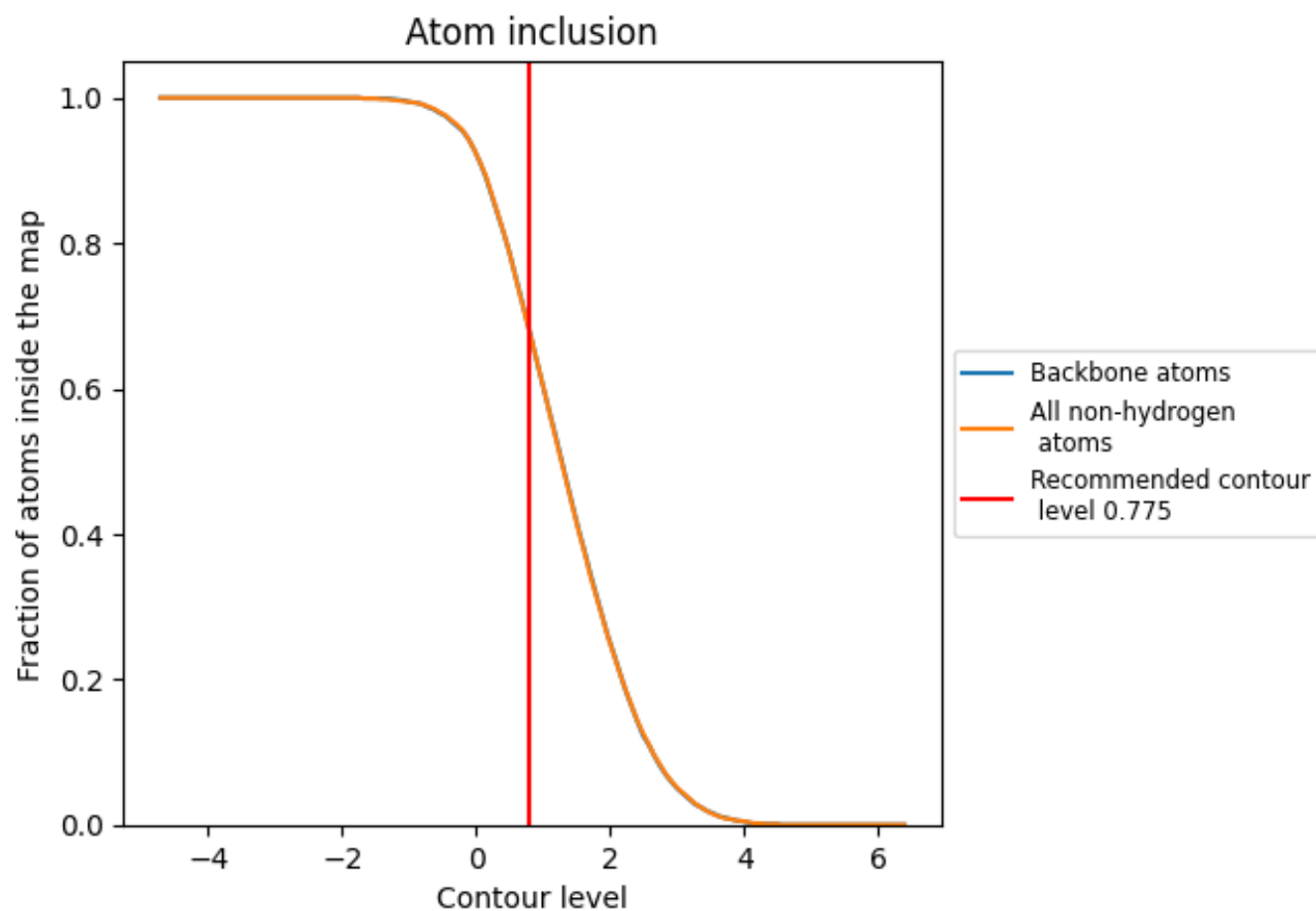
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.775).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.775) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4000
A	0.6990	0.4030
B	0.6910	0.3860
C	0.6530	0.3780
Da	0.4020	0.3330
Db	0.4890	0.3900
Dc	0.4300	0.3430
E	0.7530	0.4640
F	0.7280	0.3970
G	0.6840	0.3950
H	0.7150	0.4150
I	0.7230	0.4040
J	0.6250	0.3400

1.0

0.0

<0.0