



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 01:31 AM EDT

PDB ID : 36RP / pdb_000036rp
EMDB ID : EMD-77810
Title : Cryo-EM structure of Sulfolobus acidocaldarius RNA polymerase without stalk
(no Rpo4/Rpo7)
Authors : Fordjour, G.N.R.; Armache, J.-P.; Murakami, K.S.
Deposited on : 2026-06-29
Resolution : 8.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

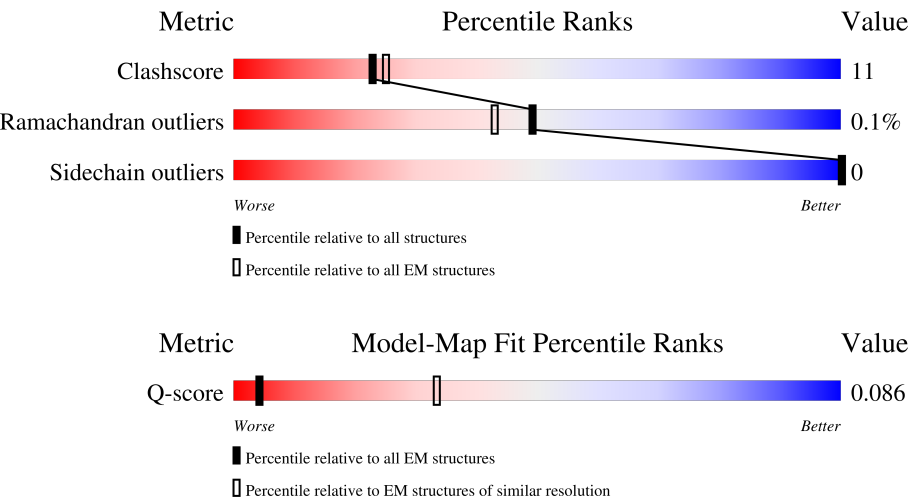
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 8.90 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.



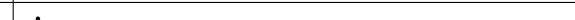
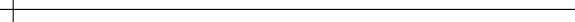
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	258 (8.40 - 9.40)

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	880	
2	B	1126	
3	C	393	
4	G	124	

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Mol	Chain	Length	Quality of chain
5	H	84	 70%23%7%
6	K	89	 71%26%.
7	L	90	 64%36%
8	N	66	 77%23%
9	Y	105	 32%10%58%
10	D	264	 66%33%.
11	P	48	 54%44%.

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25012 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 DNA-directed RNA polymerase subunit Rpo1N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	874	Total	C	N	O	S	0	0
			6982	4443	1230	1279	30		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit Rpo2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1109	Total	C	N	O	S	0	0
			8725	5531	1533	1628	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ILE	VAL	conflict	UNP P11513

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	377	Total	C	N	O	S	0	0
			2954	1856	508	577	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	122	Total	C	N	O	S	0	0
			991	637	155	190	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP Q4JAY4
G	2	LYS	-	expression tag	UNP Q4JAY4
G	3	GLU	-	expression tag	UNP Q4JAY4

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	78	Total	C	N	O	0	0
			617	399	104	114		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	86	Total	C	N	O	S	0
			690	441	120	127	2	0

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo11.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	90	Total	C	N	O	S	0
			707	459	112	134	2	0

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo10.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	66	Total	C	N	O	S	0
			534	339	97	91	7	0

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo13.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	44	Total	C	N	O	S	0
			357	226	57	72	2	0

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit Rpo3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	D	261	Total	C	N	O	S	0
			2066	1318	342	392	14	0

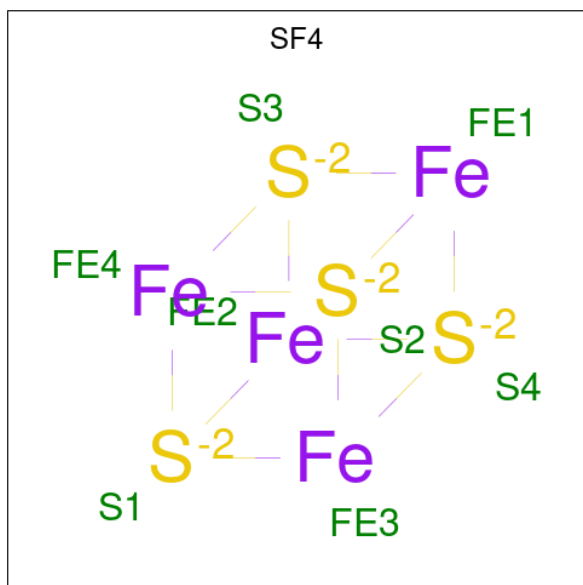
- Molecule 11 is a protein called DNA-directed RNA polymerase subunit Rpo12.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	47	Total	C	N	O	S	0
			376	241	67	63	5	0

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total 2	Zn 2	0
12	B	1	Total 1	Zn 1	0
12	N	1	Total 1	Zn 1	0
12	P	1	Total 1	Zn 1	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

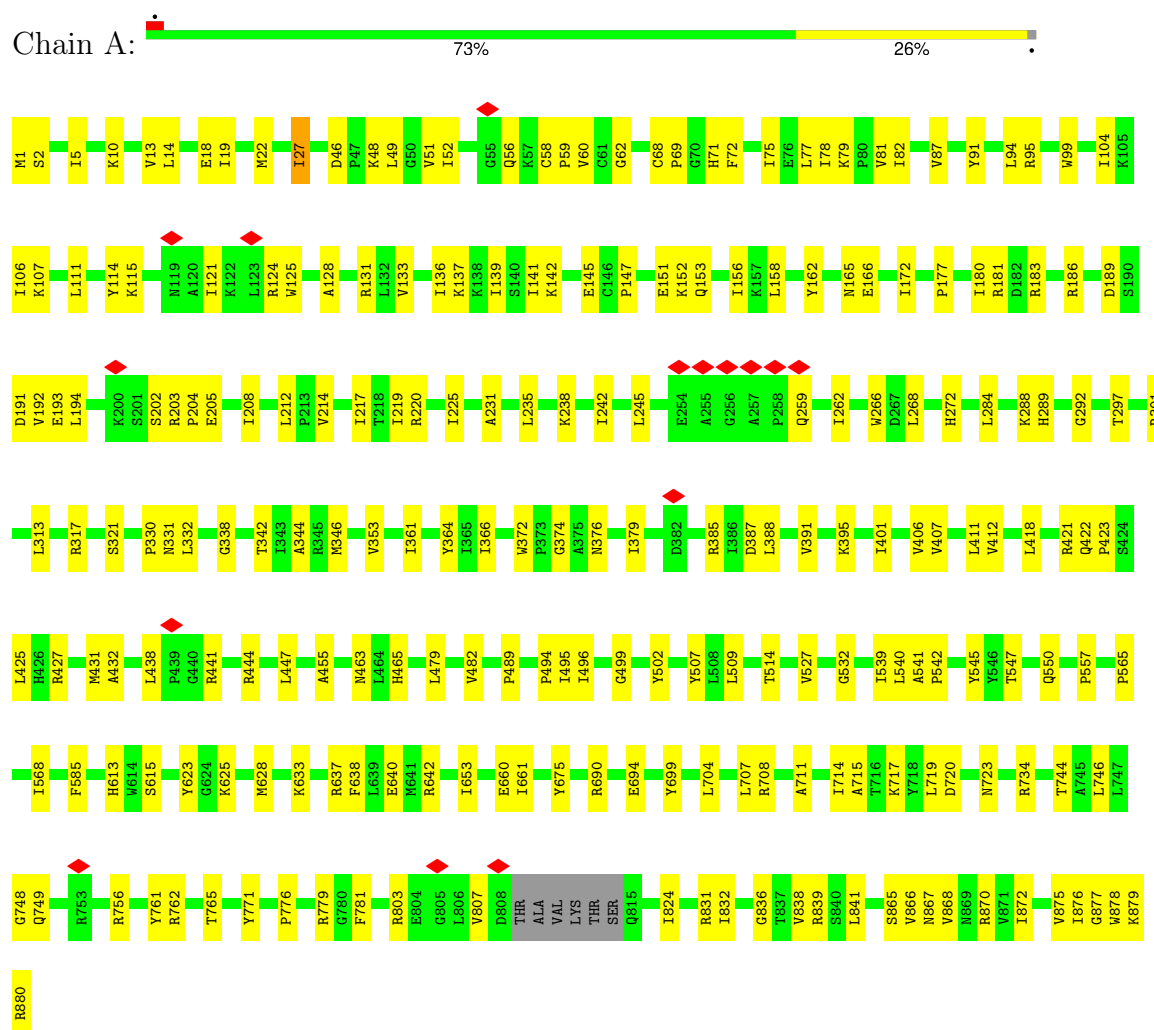


Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 8	Fe 4	S 4	0

3 Residue-property plots

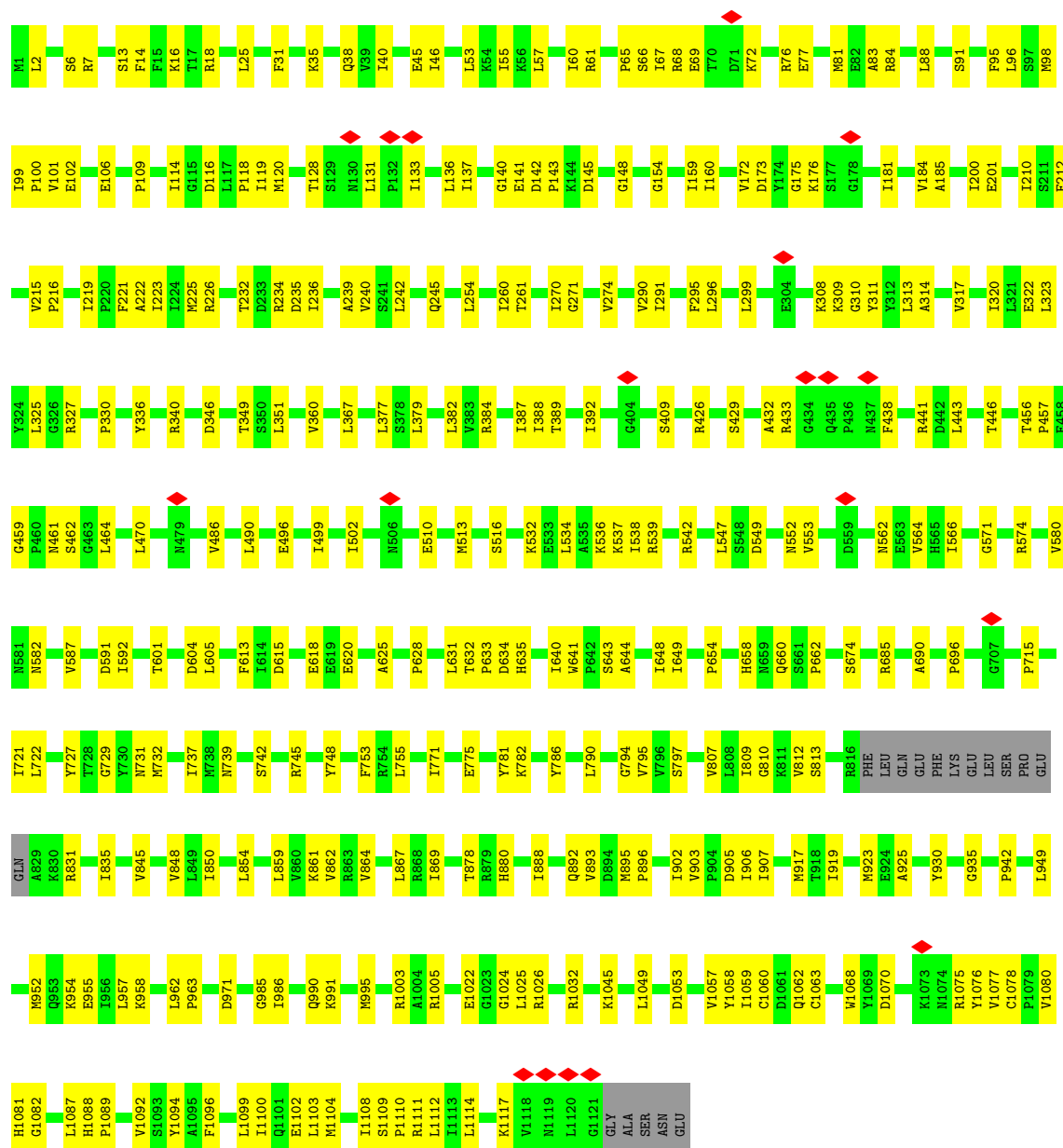
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase subunit Rpo1N

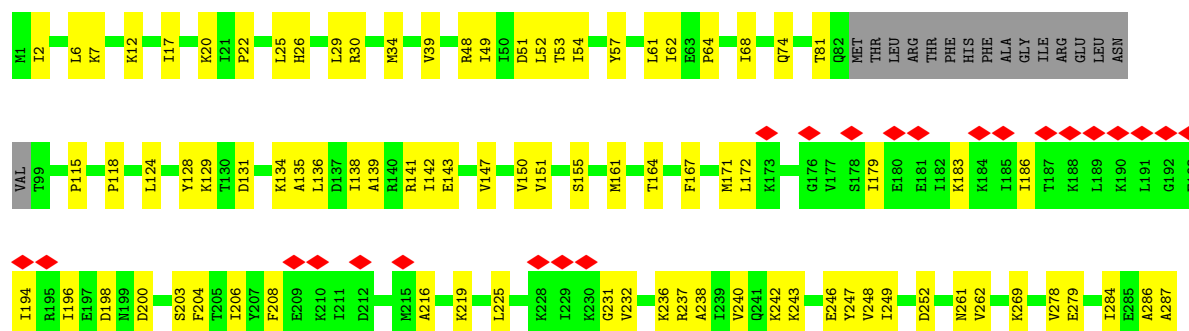


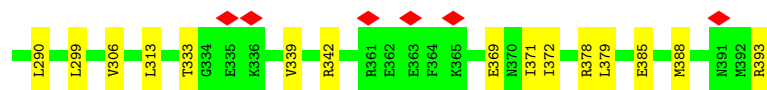
• Molecule 2: DNA-directed RNA polymerase subunit Rpo2



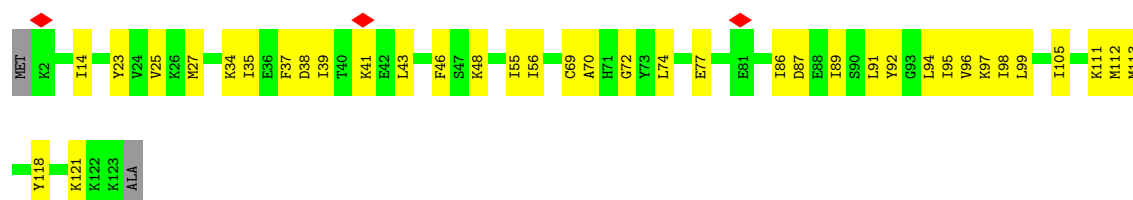


• Molecule 3: DNA-directed RNA polymerase subunit Rpo1C





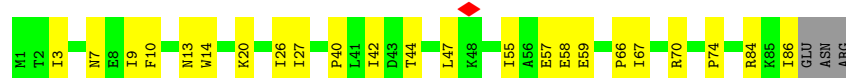
- Molecule 4: DNA-directed RNA polymerase subunit Rpo8



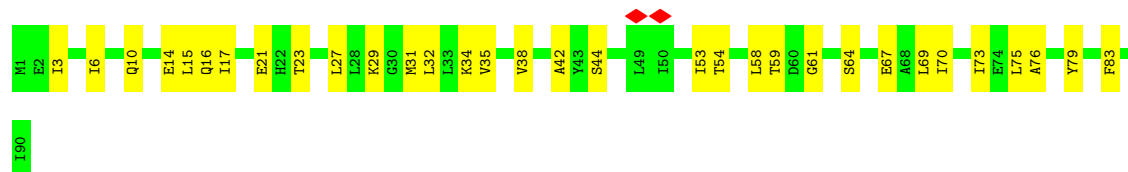
- Molecule 5: DNA-directed RNA polymerase subunit Rpo5



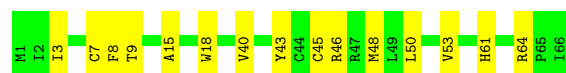
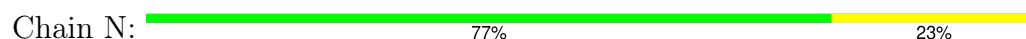
- Molecule 6: DNA-directed RNA polymerase subunit Rpo6



- Molecule 7: DNA-directed RNA polymerase subunit Rpo11

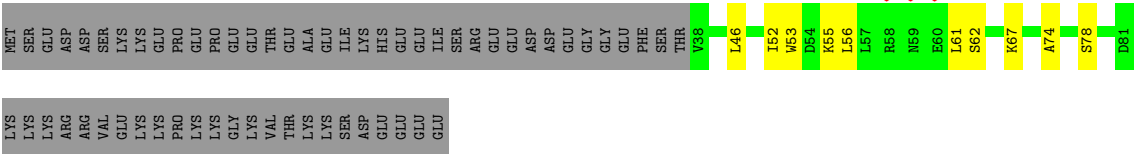


- Molecule 8: DNA-directed RNA polymerase subunit Rpo10

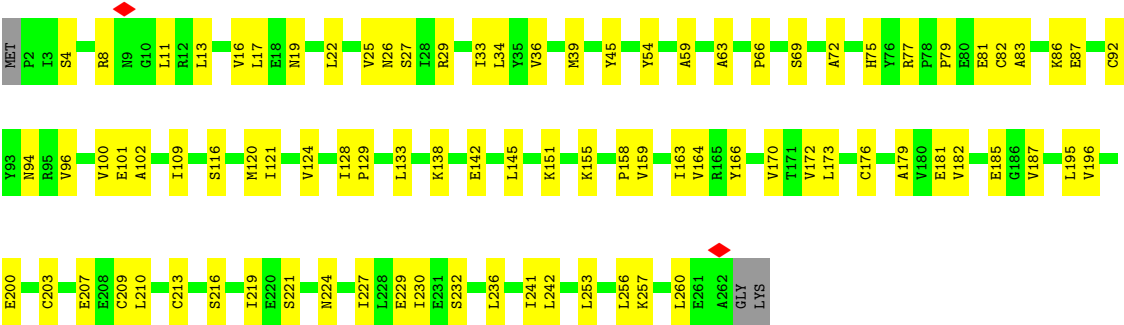


- Molecule 9: DNA-directed RNA polymerase subunit Rpo13

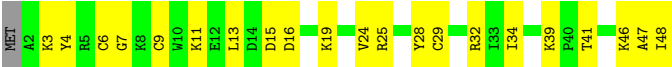




● Molecule 10: DNA-directed RNA polymerase subunit Rpo3



● Molecule 11: DNA-directed RNA polymerase subunit Rpo12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.944, 0.944, 0.944	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN

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	0.22	0/7131	0.50	0/9640
2	B	0.21	0/8885	0.47	0/12016
3	C	0.20	0/2979	0.53	0/4007
4	G	0.25	0/1006	0.60	0/1342
5	H	0.22	0/630	0.56	0/851
6	K	0.21	0/697	0.48	0/938
7	L	0.22	0/716	0.43	0/964
8	N	0.24	0/545	0.49	0/735
9	Y	0.25	0/360	0.51	0/482
10	D	0.23	0/2100	0.51	0/2839
11	P	0.25	0/382	0.60	1/510 (0.2%)
All	All	0.22	0/25431	0.50	1/34324 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
9	Y	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	24	VAL	N-CA-C	-6.07	105.44	111.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	ALA	Peptide
1	A	68	CYS	Peptide
9	Y	62	SER	Peptide

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	6982	0	7063	163	0
2	B	8725	0	8862	221	0
3	C	2954	0	3053	76	0
4	G	991	0	996	28	0
5	H	617	0	644	19	0
6	K	690	0	745	20	0
7	L	707	0	751	25	0
8	N	534	0	545	14	0
9	Y	357	0	360	9	0
10	D	2066	0	2117	62	0
11	P	376	0	398	17	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
13	D	8	0	0	0	0
All	All	25012	0	25534	566	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (566) 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)
11:P:9:CYS:HB3	11:P:29:CYS:SG	2.03	0.98
11:P:6:CYS:HB3	11:P:9:CYS:SG	2.12	0.90
8:N:8:PHE:H	8:N:48:MET:HE1	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:GLN:HE21	2:B:1081:HIS:CG	1.98	0.80
4:G:89:ILE:HB	4:G:96:VAL:HB	1.68	0.76
2:B:1062:GLN:NE2	2:B:1081:HIS:ND1	2.34	0.75
2:B:116:ASP:H	2:B:389:THR:HG22	1.53	0.72
2:B:31:PHE:HA	2:B:35:LYS:HB2	1.71	0.72
2:B:142:ASP:HB3	2:B:145:ASP:HB2	1.72	0.71
2:B:775:GLU:HB3	2:B:812:VAL:HG12	1.72	0.71
11:P:4:TYR:HB2	11:P:15:ASP:HB2	1.72	0.71
10:D:45:TYR:HB2	10:D:142:GLU:HB3	1.72	0.70
1:A:720:ASP:HB3	1:A:723:ASN:HD22	1.57	0.69
2:B:1076:TYR:HB3	2:B:1087:LEU:HB3	1.73	0.69
1:A:421:ARG:HG3	1:A:423:PRO:HD2	1.74	0.69
10:D:209:CYS:HB2	10:D:219:ILE:HD11	1.75	0.68
4:G:86:ILE:HG23	4:G:97:LYS:HG3	1.74	0.68
2:B:1032:ARG:HD2	3:C:371:ILE:HG21	1.74	0.68
2:B:648:ILE:HG23	2:B:649:ILE:HG13	1.76	0.68
2:B:351:LEU:HD21	2:B:392:ILE:HA	1.74	0.67
2:B:696:PRO:HB2	2:B:715:PRO:HG2	1.74	0.67
3:C:388:MET:HB3	6:K:67:ILE:HG12	1.76	0.67
1:A:165:ASN:HB2	1:A:172:ILE:HB	1.75	0.67
1:A:542:PRO:HD3	4:G:69:CYS:H	1.57	0.67
2:B:957:LEU:HD13	2:B:963:PRO:HD3	1.77	0.67
1:A:82:ILE:HG23	1:A:177:PRO:HB3	1.75	0.66
7:L:31:MET:HG3	7:L:76:ALA:HB2	1.77	0.66
10:D:4:SER:HB2	10:D:16:VAL:HB	1.76	0.66
2:B:216:PRO:HD2	2:B:274:VAL:HA	1.78	0.66
1:A:379:ILE:HB	1:A:406:VAL:HB	1.76	0.66
5:H:25:LEU:HB2	9:Y:67:LYS:HE3	1.77	0.66
1:A:427:ARG:HD3	1:A:489:PRO:HG2	1.77	0.65
2:B:46:ILE:HB	2:B:55:ILE:HB	1.77	0.65
3:C:284:ILE:HG23	3:C:286:ALA:H	1.61	0.65
2:B:727:TYR:H	2:B:731:ASN:HD21	1.45	0.64
4:G:37:PHE:HB3	4:G:96:VAL:HG13	1.77	0.64
3:C:284:ILE:HD13	5:H:45:ILE:HD12	1.79	0.64
3:C:216:ALA:H	3:C:219:LYS:HE2	1.63	0.64
1:A:418:LEU:HD23	1:A:432:ALA:HB2	1.79	0.64
4:G:27:MET:HB3	4:G:35:ILE:HB	1.79	0.64
10:D:36:VAL:HB	10:D:158:PRO:HG3	1.80	0.64
1:A:330:PRO:HB3	1:A:447:LEU:HD22	1.80	0.63
7:L:73:ILE:HG21	10:D:257:LYS:HB2	1.80	0.63
1:A:289:HIS:HB3	1:A:292:GLY:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:THR:H	2:B:604:ASP:HB2	1.63	0.63
1:A:14:LEU:HD11	1:A:19:ILE:HD11	1.79	0.62
1:A:342:THR:HB	1:A:441:ARG:HH22	1.65	0.62
1:A:418:LEU:HB2	1:A:465:HIS:HB2	1.81	0.62
1:A:539:ILE:HB	1:A:545:TYR:HB2	1.79	0.62
2:B:755:LEU:HD11	2:B:861:LYS:HB3	1.82	0.62
1:A:346:MET:HA	1:A:376:ASN:HD21	1.65	0.62
6:K:84:ARG:HD3	6:K:86:ILE:HD13	1.82	0.62
6:K:27:ILE:HD13	6:K:57:GLU:HG2	1.82	0.62
1:A:832:ILE:HG13	3:C:62:ILE:HG21	1.82	0.61
2:B:114:ILE:HG22	2:B:388:ILE:HG13	1.82	0.61
3:C:61:LEU:HD22	6:K:13:ASN:HD22	1.65	0.61
3:C:393:ARG:HG2	6:K:84:ARG:HH22	1.65	0.61
1:A:1:MET:HE3	1:A:2:SER:H	1.64	0.61
7:L:73:ILE:HG23	10:D:253:LEU:HB3	1.83	0.61
1:A:838:VAL:HG11	3:C:313:LEU:HD11	1.83	0.61
1:A:866:VAL:HG22	3:C:25:LEU:HD11	1.82	0.61
2:B:1060:CYS:SG	2:B:1078:CYS:CB	2.83	0.61
1:A:317:ARG:HG2	2:B:1026:ARG:HG2	1.83	0.61
1:A:875:VAL:HG12	1:A:876:ILE:HG23	1.83	0.61
10:D:170:VAL:H	10:D:200:GLU:HG3	1.66	0.61
1:A:121:ILE:HD12	1:A:124:ARG:HB3	1.83	0.60
3:C:147:VAL:HB	3:C:225:LEU:HA	1.82	0.60
2:B:1075:ARG:HG2	2:B:1077:VAL:HB	1.84	0.60
1:A:62:GLY:H	2:B:1070:ASP:HB2	1.66	0.60
1:A:708:ARG:HD3	1:A:748:GLY:HA3	1.82	0.60
2:B:172:VAL:HB	2:B:323:LEU:HD22	1.83	0.60
4:G:55:ILE:HG21	4:G:121:LYS:HE3	1.83	0.60
2:B:878:THR:HG23	2:B:880:HIS:H	1.65	0.60
10:D:173:LEU:HB2	10:D:216:SER:HA	1.82	0.60
4:G:77:GLU:HB2	4:G:105:ILE:HD12	1.82	0.60
8:N:15:ALA:HB1	10:D:129:PRO:HD2	1.84	0.60
2:B:553:VAL:HG23	2:B:566:ILE:HG12	1.83	0.59
2:B:690:ALA:HB3	2:B:753:PHE:HB2	1.84	0.59
3:C:242:LYS:HA	3:C:247:TYR:HA	1.85	0.59
1:A:719:LEU:HD11	1:A:744:THR:HG21	1.84	0.59
2:B:923:MET:HG2	2:B:949:LEU:HD13	1.83	0.59
1:A:361:ILE:HD12	1:A:407:VAL:HG11	1.84	0.59
2:B:296:LEU:HB2	2:B:309:LYS:HG2	1.85	0.59
1:A:145:GLU:HB3	1:A:152:LYS:HD2	1.84	0.59
2:B:1060:CYS:SG	2:B:1078:CYS:HB2	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:ILE:HD11	2:B:426:ARG:HB3	1.83	0.59
2:B:739:ASN:HB3	2:B:742:SER:HB3	1.83	0.59
7:L:3:ILE:HD12	7:L:15:LEU:HD11	1.84	0.59
9:Y:55:LYS:HG3	9:Y:61:LEU:HB2	1.85	0.59
1:A:124:ARG:HG3	1:A:125:TRP:HD1	1.66	0.58
4:G:56:ILE:HG22	4:G:118:TYR:HA	1.85	0.58
1:A:5:ILE:HG23	2:B:1117:LYS:HG2	1.83	0.58
2:B:470:LEU:HD12	2:B:644:ALA:HA	1.85	0.58
3:C:139:ALA:O	3:C:143:GLU:HB2	2.02	0.58
5:H:11:ILE:HB	5:H:14:HIS:HB2	1.84	0.58
4:G:34:LYS:HB2	4:G:99:LEU:HB2	1.85	0.58
2:B:240:VAL:HA	2:B:314:ALA:HB1	1.85	0.58
6:K:47:LEU:HG	6:K:55:ILE:HG12	1.85	0.58
1:A:183:ARG:HA	1:A:186:ARG:HH21	1.68	0.58
1:A:245:LEU:HD11	1:A:268:LEU:HD23	1.86	0.58
2:B:99:ILE:HG12	2:B:109:PRO:HB3	1.84	0.58
1:A:839:ARG:HD2	6:K:74:PRO:HG3	1.85	0.58
1:A:868:VAL:HG11	3:C:29:LEU:HA	1.85	0.57
2:B:69:GLU:HB3	2:B:76:ARG:HH21	1.69	0.57
2:B:1057:VAL:HG12	2:B:1092:VAL:HG11	1.86	0.57
7:L:44:SER:HB2	7:L:54:THR:HB	1.85	0.57
3:C:278:VAL:HG12	3:C:290:LEU:HD23	1.86	0.57
7:L:32:LEU:HD11	7:L:69:LEU:HD13	1.87	0.57
10:D:11:LEU:HD22	10:D:232:SER:HB3	1.87	0.57
2:B:782:LYS:HB3	2:B:786:TYR:HD2	1.70	0.57
10:D:19:ASN:HA	10:D:224:ASN:HB3	1.87	0.56
10:D:207:GLU:HG2	10:D:210:LEU:HD12	1.87	0.56
10:D:77:ARG:HD3	10:D:92:CYS:HB2	1.87	0.56
10:D:163:ILE:HB	10:D:229:GLU:HB2	1.87	0.56
1:A:421:ARG:HD3	1:A:455:ALA:HB2	1.88	0.56
7:L:16:GLN:HB2	7:L:54:THR:HG23	1.86	0.56
7:L:17:ILE:HD12	7:L:53:ILE:HD11	1.87	0.56
1:A:107:LYS:HA	1:A:147:PRO:HG3	1.86	0.56
4:G:14:ILE:HG12	4:G:25:VAL:HG13	1.87	0.56
2:B:68:ARG:HD3	2:B:72:LYS:HD2	1.87	0.56
10:D:59:ALA:HB1	11:P:47:ALA:HA	1.88	0.56
1:A:690:ARG:HB3	1:A:694:GLU:HG3	1.87	0.56
2:B:101:VAL:HG22	2:B:106:GLU:HA	1.88	0.56
5:H:28:ALA:HB1	5:H:62:ILE:HD12	1.87	0.56
7:L:6:ILE:HB	7:L:14:GLU:HB3	1.88	0.56
1:A:94:LEU:HD11	1:A:180:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:94:ASN:HB3	10:D:145:LEU:HB2	1.87	0.56
2:B:457:PRO:HG2	2:B:461:ASN:HB3	1.87	0.56
2:B:643:SER:HB2	2:B:942:PRO:HG2	1.88	0.56
1:A:353:VAL:HG22	1:A:361:ILE:HG21	1.88	0.55
7:L:31:MET:HE1	7:L:79:TYR:HD2	1.71	0.55
3:C:151:VAL:HA	3:C:167:PHE:HA	1.88	0.55
10:D:172:VAL:HG11	10:D:196:VAL:HA	1.88	0.55
3:C:143:GLU:HG3	3:C:238:ALA:H	1.71	0.55
1:A:95:ARG:HG2	1:A:156:ILE:HB	1.88	0.55
1:A:807:VAL:HA	2:B:459:GLY:HA2	1.87	0.55
1:A:831:ARG:HH22	3:C:378:ARG:HH21	1.55	0.55
3:C:333:THR:HG22	3:C:342:ARG:HD3	1.89	0.55
1:A:749:GLN:HA	1:A:781:PHE:HA	1.87	0.55
2:B:215:VAL:HG22	2:B:274:VAL:HB	1.89	0.55
3:C:124:LEU:HD23	3:C:128:TYR:HB3	1.90	0.54
8:N:40:VAL:HG13	8:N:45:CYS:HB2	1.88	0.54
1:A:225:ILE:HG12	1:A:231:ALA:HB2	1.89	0.54
10:D:77:ARG:HB3	10:D:81:GLU:HG3	1.89	0.54
2:B:384:ARG:HH21	2:B:387:ILE:HD11	1.72	0.54
1:A:22:MET:HG2	1:A:72:PHE:HB3	1.90	0.54
2:B:215:VAL:HG23	2:B:290:VAL:HG11	1.90	0.54
1:A:104:ILE:HG12	1:A:191:ASP:HB3	1.89	0.54
1:A:219:ILE:HD11	1:A:301:ARG:HH12	1.73	0.54
2:B:67:ILE:HD12	2:B:854:LEU:HD13	1.89	0.54
2:B:239:ALA:HA	2:B:499:ILE:HD11	1.90	0.53
4:G:38:ASP:HB2	4:G:94:LEU:HB3	1.89	0.53
6:K:40:PRO:HG2	6:K:44:THR:HB	1.89	0.53
2:B:57:LEU:HD22	2:B:96:LEU:HD21	1.90	0.53
1:A:78:ILE:HG13	1:A:79:LYS:HG2	1.90	0.53
2:B:100:PRO:HB3	2:B:379:LEU:HG	1.91	0.53
1:A:91:TYR:CZ	1:A:95:ARG:HD3	2.44	0.53
1:A:69:PRO:HG2	2:B:1068:TRP:HE3	1.73	0.53
1:A:75:ILE:HD12	1:A:212:LEU:HD22	1.91	0.53
2:B:66:SER:HB3	2:B:77:GLU:HG3	1.91	0.53
2:B:336:TYR:H	2:B:446:THR:HG21	1.74	0.53
2:B:632:THR:HG22	2:B:634:ASP:H	1.74	0.53
7:L:38:VAL:HG22	7:L:59:THR:HG22	1.91	0.53
1:A:69:PRO:HD2	2:B:1068:TRP:HB3	1.90	0.52
1:A:332:LEU:HD21	1:A:438:LEU:HD11	1.90	0.52
2:B:55:ILE:HG21	2:B:98:MET:HE3	1.91	0.52
2:B:6:SER:HB2	2:B:592:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:25:LEU:HA	5:H:28:ALA:HB3	1.91	0.52
1:A:27:ILE:HG13	1:A:214:VAL:HG21	1.92	0.52
3:C:124:LEU:HD11	3:C:249:ILE:HG13	1.91	0.52
1:A:344:ALA:HA	1:A:411:LEU:HB2	1.90	0.52
2:B:580:VAL:HG11	2:B:631:LEU:HD22	1.91	0.52
2:B:539:ARG:HH21	2:B:618:GLU:HG3	1.75	0.52
2:B:574:ARG:HH11	2:B:613:PHE:HB3	1.74	0.52
1:A:338:GLY:HA3	1:A:444:ARG:HB2	1.92	0.52
1:A:540:LEU:H	4:G:70:ALA:HA	1.74	0.52
10:D:34:LEU:HD13	10:D:151:LYS:HD3	1.91	0.52
3:C:172:LEU:HD21	3:C:179:ILE:HD11	1.92	0.52
1:A:479:LEU:HD23	6:K:20:LYS:HE2	1.92	0.52
2:B:295:PHE:HZ	2:B:313:LEU:HB2	1.74	0.52
2:B:628:PRO:HA	2:B:631:LEU:HG	1.91	0.52
3:C:183:LYS:HZ2	3:C:198:ASP:HB3	1.75	0.52
2:B:35:LYS:HA	2:B:38:GLN:HB3	1.90	0.52
2:B:574:ARG:HD3	2:B:613:PHE:HB3	1.92	0.52
2:B:587:VAL:HG22	2:B:605:LEU:HD22	1.92	0.52
8:N:40:VAL:HG12	8:N:46:ARG:HG3	1.91	0.52
10:D:63:ALA:HB2	11:P:47:ALA:HB1	1.91	0.52
1:A:761:TYR:HB3	2:B:620:GLU:HG2	1.91	0.52
1:A:366:ILE:HG12	1:A:395:LYS:HA	1.91	0.51
4:G:95:ILE:HG22	4:G:97:LYS:H	1.75	0.51
1:A:192:VAL:HG21	1:A:204:PRO:HD3	1.91	0.51
10:D:159:VAL:HA	10:D:232:SER:HA	1.93	0.51
2:B:486:VAL:HG21	2:B:547:LEU:HD13	1.92	0.51
2:B:534:LEU:HD23	2:B:564:VAL:HG11	1.92	0.51
2:B:795:VAL:HG11	2:B:850:ILE:HD11	1.92	0.51
1:A:547:THR:HG23	1:A:550:GLN:H	1.74	0.51
2:B:45:GLU:HA	2:B:57:LEU:HG	1.93	0.51
2:B:212:PHE:HE2	2:B:291:ILE:HG12	1.76	0.51
3:C:26:HIS:CE1	3:C:30:ARG:HH21	2.29	0.51
1:A:156:ILE:HG12	1:A:166:GLU:HG2	1.93	0.51
2:B:438:PHE:HA	2:B:441:ARG:HB2	1.93	0.51
11:P:4:TYR:HB3	11:P:34:ILE:HB	1.93	0.51
1:A:139:ILE:HA	1:A:142:LYS:HB2	1.93	0.51
2:B:786:TYR:HB3	2:B:807:VAL:HG23	1.93	0.51
2:B:790:LEU:HD23	2:B:794:GLY:HA2	1.93	0.51
10:D:230:ILE:HG13	10:D:242:LEU:HD21	1.91	0.51
8:N:64:ARG:HD3	10:D:54:TYR:HE1	1.76	0.50
2:B:1078:CYS:HB3	2:B:1082:GLY:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:ARG:H	2:B:464:LEU:HD13	1.76	0.50
2:B:83:ALA:HA	2:B:88:LEU:HB2	1.92	0.50
1:A:625:LYS:HA	1:A:628:MET:HE2	1.92	0.50
2:B:185:ALA:HB3	2:B:200:ILE:HB	1.93	0.50
2:B:739:ASN:HB2	2:B:905:ASP:HA	1.93	0.50
2:B:859:LEU:HD21	2:B:861:LYS:HE3	1.93	0.50
7:L:83:PHE:HE1	10:D:17:LEU:HD21	1.77	0.50
1:A:13:VAL:HG22	1:A:202:SER:HA	1.93	0.50
2:B:813:SER:HB2	2:B:831:ARG:HB3	1.92	0.50
3:C:129:LYS:HE3	3:C:246:GLU:HG3	1.94	0.50
1:A:189:ASP:O	1:A:193:GLU:HB2	2.12	0.50
1:A:259:GLN:HA	1:A:262:ILE:HG12	1.94	0.50
2:B:790:LEU:HD21	2:B:810:GLY:HA3	1.93	0.50
1:A:807:VAL:HG21	2:B:438:PHE:HE1	1.77	0.49
2:B:542:ARG:HG3	2:B:549:ASP:HA	1.93	0.49
4:G:14:ILE:HG23	4:G:25:VAL:HG22	1.93	0.49
2:B:486:VAL:HG11	2:B:547:LEU:HD22	1.93	0.49
2:B:1053:ASP:HB2	2:B:1094:TYR:HB3	1.94	0.49
5:H:29:TYR:HB2	9:Y:56:LEU:HD21	1.94	0.49
10:D:72:ALA:HB2	10:D:121:ILE:HD11	1.94	0.49
1:A:133:VAL:HA	1:A:136:ILE:HD12	1.94	0.49
1:A:431:MET:HG3	1:A:482:VAL:HG22	1.94	0.49
2:B:232:THR:HG22	2:B:234:ARG:H	1.76	0.49
1:A:60:VAL:HG12	2:B:1068:TRP:HE1	1.77	0.49
1:A:372:TRP:HZ2	1:A:412:VAL:HA	1.77	0.49
2:B:67:ILE:HD13	2:B:88:LEU:HD13	1.94	0.49
10:D:34:LEU:HB3	10:D:151:LYS:HB2	1.94	0.49
1:A:106:ILE:HB	1:A:111:LEU:HD12	1.94	0.49
1:A:704:LEU:HD11	1:A:776:PRO:HB3	1.94	0.49
2:B:902:ILE:HG23	8:N:9:THR:HG21	1.95	0.49
2:B:1060:CYS:HB2	2:B:1063:CYS:SG	2.51	0.49
1:A:447:LEU:HD21	2:B:732:MET:HG3	1.94	0.49
2:B:322:GLU:HG2	2:B:327:ARG:HD2	1.94	0.49
7:L:21:GLU:HG2	7:L:23:THR:H	1.77	0.49
2:B:591:ASP:HB3	2:B:605:LEU:HD21	1.94	0.49
10:D:63:ALA:HB1	10:D:155:LYS:HE2	1.95	0.49
10:D:77:ARG:HB2	10:D:82:CYS:HB2	1.94	0.49
2:B:367:LEU:HA	2:B:382:LEU:HD22	1.95	0.49
2:B:176:LYS:HD2	2:B:181:ILE:HD12	1.95	0.48
2:B:895:MET:HE3	2:B:903:VAL:HB	1.94	0.48
2:B:958:LYS:HE3	10:D:181:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:HIS:HE1	3:C:30:ARG:HH21	1.60	0.48
6:K:66:PRO:HB3	6:K:84:ARG:HE	1.78	0.48
7:L:10:GLN:HG3	7:L:61:GLY:HA2	1.94	0.48
1:A:565:PRO:HA	1:A:585:PHE:HA	1.94	0.48
2:B:46:ILE:HG12	2:B:360:VAL:HG13	1.95	0.48
2:B:641:TRP:HB3	2:B:644:ALA:HB2	1.95	0.48
2:B:748:TYR:HB3	2:B:991:LYS:HD2	1.95	0.48
2:B:896:PRO:HB3	2:B:971:ASP:HA	1.94	0.48
10:D:179:ALA:HA	10:D:182:VAL:HG22	1.95	0.48
2:B:133:ILE:HG23	2:B:143:PRO:HB3	1.95	0.48
2:B:721:ILE:H	2:B:905:ASP:HB2	1.77	0.48
2:B:1062:GLN:HE21	2:B:1081:HIS:CE1	2.30	0.48
1:A:52:ILE:HG23	1:A:217:ILE:HG22	1.95	0.48
1:A:867:ASN:HB3	1:A:870:ARG:HB3	1.95	0.48
2:B:137:ILE:HG23	8:N:61:HIS:HB3	1.95	0.48
2:B:242:LEU:HB2	2:B:513:MET:HE3	1.95	0.48
2:B:270:ILE:HD13	2:B:291:ILE:HD11	1.95	0.48
3:C:138:ILE:HD13	3:C:141:ARG:HH12	1.78	0.48
1:A:638:PHE:O	1:A:642:ARG:HB2	2.14	0.48
1:A:872:ILE:HG12	3:C:49:ILE:HD13	1.95	0.48
2:B:1003:ARG:HG2	2:B:1024:GLY:HA2	1.95	0.48
2:B:1103:LEU:HD13	2:B:1108:ILE:HD11	1.96	0.48
2:B:225:MET:HG2	2:B:236:ILE:HG23	1.96	0.48
10:D:36:VAL:HG21	10:D:241:ILE:HG23	1.95	0.48
1:A:18:GLU:HG3	2:B:1080:VAL:HB	1.96	0.48
1:A:714:ILE:HA	1:A:717:LYS:HE2	1.96	0.48
3:C:333:THR:HA	3:C:342:ARG:HH11	1.78	0.48
2:B:737:ILE:HB	2:B:907:ILE:HB	1.94	0.48
4:G:39:ILE:HA	4:G:43:LEU:HD12	1.96	0.48
7:L:83:PHE:HE2	10:D:242:LEU:HB3	1.77	0.48
1:A:824:ILE:HG23	3:C:74:GLN:HG2	1.95	0.48
2:B:892:GLN:HA	2:B:895:MET:HE2	1.95	0.48
6:K:26:ILE:HG23	6:K:67:ILE:HD12	1.95	0.48
10:D:102:ALA:HB2	10:D:133:LEU:HB3	1.95	0.48
10:D:166:TYR:HB3	10:D:221:SER:HB2	1.96	0.48
11:P:7:GLY:HA2	11:P:11:LYS:HA	1.96	0.48
2:B:1062:GLN:NE2	2:B:1081:HIS:CE1	2.81	0.47
1:A:94:LEU:HD21	1:A:180:ILE:HA	1.96	0.47
10:D:96:VAL:HG22	10:D:116:SER:HA	1.95	0.47
3:C:385:GLU:HB3	6:K:70:ARG:HB2	1.95	0.47
1:A:660:GLU:HB3	1:A:714:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:PRO:HG3	8:N:53:VAL:HG11	1.96	0.47
10:D:79:PRO:HA	10:D:83:ALA:H	1.80	0.47
1:A:331:ASN:HA	1:A:633:LYS:HE3	1.97	0.47
2:B:13:SER:HA	2:B:16:LYS:HG2	1.96	0.47
2:B:1059:ILE:HB	2:B:1114:LEU:HD11	1.96	0.47
5:H:63:ILE:HB	5:H:79:ARG:HB3	1.96	0.47
1:A:807:VAL:HG12	2:B:462:SER:HB3	1.97	0.47
1:A:87:VAL:HG22	1:A:158:LEU:HD11	1.97	0.47
1:A:539:ILE:HD13	4:G:43:LEU:HD11	1.96	0.47
1:A:879:LYS:HA	4:G:112:MET:HG2	1.96	0.47
2:B:957:LEU:HD22	2:B:963:PRO:HB3	1.95	0.47
2:B:1045:LYS:O	2:B:1049:LEU:HB3	2.13	0.47
3:C:29:LEU:HD22	3:C:53:THR:HG21	1.97	0.47
3:C:200:ASP:HB3	3:C:203:SER:HB3	1.97	0.47
1:A:841:LEU:HD21	3:C:379:LEU:HB3	1.96	0.47
2:B:175:GLY:HA3	2:B:184:VAL:HG12	1.95	0.47
3:C:179:ILE:HG23	3:C:204:PHE:HD2	1.78	0.47
1:A:5:ILE:HG12	2:B:1117:LYS:HA	1.96	0.47
1:A:181:ARG:HH11	1:A:208:ILE:HB	1.79	0.47
2:B:848:VAL:HG22	2:B:862:VAL:HG22	1.96	0.47
3:C:7:LYS:HG3	3:C:34:MET:HE1	1.97	0.47
3:C:278:VAL:HB	3:C:287:ALA:HB3	1.97	0.47
2:B:299:LEU:HD22	2:B:308:LYS:HZ2	1.79	0.47
2:B:128:THR:HG23	2:B:131:LEU:HD12	1.97	0.46
2:B:893:VAL:HG12	10:D:33:ILE:HD12	1.97	0.46
3:C:186:ILE:HG22	3:C:194:ILE:HG21	1.97	0.46
1:A:756:ARG:HB3	1:A:779:ARG:HB3	1.97	0.46
2:B:271:GLY:HA2	2:B:274:VAL:HG12	1.97	0.46
9:Y:52:ILE:HA	9:Y:55:LYS:HE3	1.97	0.46
10:D:22:LEU:HA	10:D:25:VAL:HG12	1.98	0.46
1:A:75:ILE:HB	1:A:212:LEU:HB3	1.97	0.46
1:A:425:LEU:HD22	3:C:81:THR:HG21	1.97	0.46
1:A:507:TYR:HE1	1:A:568:ILE:HD13	1.80	0.46
1:A:761:TYR:HE1	2:B:446:THR:HG23	1.81	0.46
3:C:2:ILE:HA	3:C:6:LEU:HD23	1.98	0.46
1:A:242:ILE:HD13	1:A:272:HIS:HB3	1.97	0.46
3:C:194:ILE:HG23	3:C:208:PHE:HE1	1.80	0.46
2:B:102:GLU:HB2	2:B:377:LEU:HD23	1.97	0.46
2:B:310:GLY:O	2:B:314:ALA:HB2	2.16	0.46
2:B:340:ARG:HB3	2:B:571:GLY:HA3	1.98	0.46
2:B:930:TYR:HE1	2:B:955:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:SER:HB2	1:A:623:TYR:HE2	1.80	0.46
3:C:141:ARG:HD2	3:C:262:VAL:HG23	1.98	0.46
8:N:43:TYR:HA	8:N:46:ARG:HB2	1.97	0.46
1:A:532:GLY:HA2	7:L:58:LEU:HD13	1.98	0.46
2:B:432:ALA:HB1	2:B:464:LEU:HB3	1.98	0.46
7:L:34:LYS:HD2	7:L:75:LEU:HD23	1.98	0.46
1:A:353:VAL:HG11	1:A:401:ILE:HD12	1.98	0.46
2:B:809:ILE:HB	2:B:835:ILE:HB	1.98	0.46
10:D:29:ARG:HD2	10:D:164:VAL:HG23	1.98	0.46
2:B:346:ASP:HA	2:B:349:THR:HG22	1.98	0.46
2:B:935:GLY:HA2	8:N:50:LEU:HD11	1.98	0.46
5:H:19:LYS:HE2	5:H:66:THR:HB	1.98	0.46
7:L:67:GLU:HA	7:L:70:ILE:HD12	1.98	0.46
1:A:330:PRO:HG3	2:B:729:GLY:HA3	1.97	0.46
2:B:660:GLN:HB2	2:B:917:MET:HB3	1.98	0.46
10:D:66:PRO:HG2	10:D:124:VAL:HB	1.98	0.46
2:B:46:ILE:HG13	2:B:57:LEU:HD21	1.98	0.45
3:C:136:LEU:HD22	3:C:240:VAL:HG21	1.97	0.45
10:D:179:ALA:HB3	10:D:195:LEU:HD11	1.98	0.45
2:B:317:VAL:HA	2:B:320:ILE:HG22	1.98	0.45
3:C:64:PRO:HG3	6:K:10:PHE:CE1	2.50	0.45
9:Y:52:ILE:HA	9:Y:55:LYS:HG2	1.97	0.45
10:D:39:MET:HB2	10:D:69:SER:HB3	1.98	0.45
1:A:162:TYR:HE1	1:A:284:LEU:HD21	1.81	0.45
10:D:39:MET:H	10:D:69:SER:HB3	1.81	0.45
1:A:675:TYR:CD2	1:A:699:TYR:HB3	2.51	0.45
3:C:61:LEU:HB3	6:K:14:TRP:HE1	1.82	0.45
4:G:14:ILE:HD11	4:G:46:PHE:HB2	1.98	0.45
1:A:104:ILE:HG22	1:A:106:ILE:HG13	1.99	0.45
1:A:114:TYR:HE2	1:A:139:ILE:HD11	1.81	0.45
1:A:364:TYR:HA	1:A:374:GLY:HA2	1.97	0.45
1:A:836:GLY:HA3	6:K:7:ASN:ND2	2.31	0.45
2:B:245:GLN:HE22	2:B:325:LEU:HD11	1.82	0.45
2:B:7:ARG:HB3	2:B:640:ILE:O	2.17	0.45
1:A:151:GLU:HB3	1:A:153:GLN:NE2	2.32	0.45
1:A:807:VAL:HB	2:B:441:ARG:HH21	1.81	0.45
2:B:136:LEU:HD22	2:B:141:GLU:HG2	1.98	0.45
7:L:29:LYS:HD2	7:L:42:ALA:HA	1.99	0.45
10:D:101:GLU:HG2	10:D:138:LYS:HA	1.98	0.45
1:A:880:ARG:HG3	3:C:39:VAL:HG21	1.99	0.45
2:B:660:GLN:HG2	2:B:662:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:ILE:HG12	2:B:888:ILE:HG22	1.99	0.45
3:C:17:ILE:HG23	3:C:20:LYS:HB2	1.99	0.45
3:C:141:ARG:HG2	3:C:231:GLY:HA2	1.99	0.45
6:K:42:ILE:HG23	6:K:59:GLU:HG2	1.99	0.45
1:A:219:ILE:HG23	1:A:220:ARG:HG3	1.98	0.45
1:A:235:LEU:HA	1:A:297:THR:HG22	1.98	0.45
3:C:143:GLU:HG3	3:C:237:ARG:HA	1.99	0.45
10:D:109:ILE:HD11	10:D:133:LEU:HD12	1.98	0.45
2:B:1058:TYR:CE2	2:B:1089:PRO:HG3	2.52	0.44
10:D:179:ALA:HB2	10:D:213:CYS:SG	2.57	0.44
10:D:185:GLU:HB2	10:D:187:VAL:HG23	1.99	0.44
11:P:3:LYS:HA	11:P:16:ASP:HA	1.99	0.44
1:A:494:PRO:HD3	1:A:613:HIS:HB2	1.99	0.44
1:A:653:ILE:HG21	1:A:715:ALA:HB1	1.98	0.44
1:A:865:SER:HB2	3:C:25:LEU:HD13	1.98	0.44
2:B:552:ASN:HD22	2:B:615:ASP:H	1.64	0.44
3:C:232:VAL:HG22	3:C:261:ASN:HB2	1.99	0.44
2:B:159:ILE:HG12	2:B:409:SER:HB3	1.98	0.44
2:B:775:GLU:HG2	2:B:781:TYR:CE1	2.51	0.44
10:D:26:ASN:HA	10:D:29:ARG:HG2	1.99	0.44
2:B:25:LEU:HD23	2:B:120:MET:HE1	1.99	0.44
10:D:187:VAL:HG21	10:D:203:CYS:HB2	2.00	0.44
11:P:19:LYS:HA	11:P:19:LYS:HD2	1.78	0.44
11:P:25:ARG:HG2	11:P:32:ARG:HD2	1.99	0.44
2:B:850:ILE:HG13	11:P:4:TYR:HE1	1.82	0.44
7:L:69:LEU:HG	10:D:260:LEU:HD11	1.99	0.44
1:A:661:ILE:HD12	1:A:711:ALA:HB1	1.98	0.44
2:B:98:MET:HE2	2:B:379:LEU:HD13	2.00	0.44
3:C:155:SER:HB2	3:C:164:THR:HB	1.99	0.44
2:B:223:ILE:HD11	2:B:260:ILE:HD13	1.99	0.44
1:A:499:GLY:H	1:A:502:TYR:HD2	1.66	0.44
3:C:279:GLU:HA	5:H:11:ILE:HD11	2.00	0.44
11:P:13:LEU:HB3	11:P:28:TYR:HD2	1.83	0.44
1:A:22:MET:HE1	2:B:1068:TRP:HH2	1.83	0.44
1:A:115:LYS:HG3	1:A:194:LEU:HD22	1.99	0.44
2:B:61:ARG:HE	2:B:95:PHE:HB2	1.83	0.44
1:A:181:ARG:HB2	1:A:208:ILE:HG21	1.99	0.43
1:A:203:ARG:HB3	1:A:205:GLU:HG2	2.00	0.43
2:B:91:SER:HA	2:B:118:PRO:HA	2.00	0.43
2:B:222:ALA:HB2	2:B:254:LEU:HA	2.01	0.43
2:B:1112:LEU:HG	2:B:1114:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:74:ALA:O	9:Y:78:SER:HB3	2.18	0.43
2:B:674:SER:HB2	2:B:990:GLN:HB3	2.00	0.43
2:B:721:ILE:HD13	2:B:986:ILE:HG12	2.01	0.43
2:B:991:LYS:HE2	2:B:995:MET:HE1	2.01	0.43
3:C:243:LYS:HE3	3:C:248:VAL:HG21	2.01	0.43
2:B:429:SER:HB2	2:B:432:ALA:HB2	2.00	0.43
2:B:1092:VAL:HG23	2:B:1096:PHE:HD2	1.82	0.43
3:C:286:ALA:O	5:H:17:VAL:HA	2.18	0.43
10:D:100:VAL:HG11	10:D:109:ILE:HG23	2.00	0.43
1:A:495:ILE:HG23	1:A:496:ILE:HG13	2.00	0.43
4:G:105:ILE:HG23	4:G:111:LYS:HA	2.01	0.43
5:H:19:LYS:HB2	5:H:66:THR:HB	2.01	0.43
1:A:509:LEU:HD12	1:A:514:THR:HG21	2.00	0.43
2:B:81:MET:HE1	2:B:685:ARG:HB3	2.00	0.43
2:B:952:MET:HE3	2:B:952:MET:HB3	1.89	0.43
4:G:23:TYR:HE1	4:G:41:LYS:HD3	1.84	0.43
8:N:3:ILE:HG12	8:N:18:TRP:HB2	2.01	0.43
2:B:232:THR:HB	2:B:235:ASP:HB2	2.01	0.43
2:B:516:SER:HA	2:B:562:ASN:HB3	1.99	0.43
3:C:57:TYR:HE2	6:K:9:ILE:HG21	1.83	0.43
4:G:74:LEU:HA	4:G:89:ILE:HA	2.01	0.43
1:A:313:LEU:HD22	3:C:372:ILE:HG23	2.01	0.43
1:A:385:ARG:NH2	2:B:1005:ARG:HH12	2.17	0.43
6:K:47:LEU:HD11	6:K:58:GLU:HB2	2.01	0.43
11:P:46:LYS:HG3	11:P:48:ILE:H	1.82	0.43
1:A:527:VAL:HG11	1:A:637:ARG:HD3	2.00	0.43
2:B:722:LEU:HA	2:B:906:ILE:HG13	2.01	0.43
2:B:845:VAL:HG12	2:B:864:VAL:HG22	2.00	0.43
3:C:269:LYS:HD2	3:C:269:LYS:HA	1.91	0.43
2:B:658:HIS:CG	2:B:923:MET:HE1	2.54	0.42
3:C:150:VAL:HA	3:C:171:MET:SD	2.59	0.42
3:C:161:MET:HG3	3:C:208:PHE:HB2	2.01	0.42
1:A:72:PHE:CE1	2:B:1104:MET:HG3	2.55	0.42
1:A:128:ALA:HA	1:A:131:ARG:HG2	2.01	0.42
1:A:707:LEU:HG	1:A:746:LEU:HD21	2.01	0.42
1:A:878:TRP:HE3	4:G:113:MET:HG3	1.84	0.42
2:B:490:LEU:HD13	2:B:537:LYS:HE2	2.00	0.42
5:H:9:ILE:HG22	5:H:11:ILE:HG23	2.01	0.42
5:H:83:THR:HG23	9:Y:46:LEU:HD13	2.02	0.42
1:A:137:LYS:O	1:A:141:ILE:HG12	2.19	0.42
1:A:708:ARG:HA	1:A:746:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:HB3	1:A:771:TYR:HE1	1.84	0.42
2:B:84:ARG:HA	2:B:154:GLY:HA2	2.00	0.42
2:B:962:LEU:HD23	2:B:962:LEU:HA	1.90	0.42
3:C:124:LEU:HD21	3:C:135:ALA:HA	2.01	0.42
11:P:3:LYS:HB3	11:P:3:LYS:HE3	1.78	0.42
11:P:4:TYR:CG	11:P:34:ILE:HD12	2.54	0.42
1:A:238:LYS:HA	1:A:238:LYS:HD2	1.86	0.42
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.89	0.42
2:B:510:GLU:HA	2:B:513:MET:HB2	2.01	0.42
4:G:87:ASP:HB2	4:G:98:ILE:HB	2.01	0.42
1:A:288:LYS:HE3	1:A:288:LYS:HB3	1.93	0.42
2:B:654:PRO:HG2	2:B:880:HIS:CE1	2.54	0.42
3:C:147:VAL:HA	3:C:150:VAL:HB	2.01	0.42
1:A:422:GLN:HG3	1:A:463:ASN:HD21	1.85	0.42
2:B:538:ILE:HG23	2:B:547:LEU:HD23	2.01	0.42
7:L:17:ILE:HD13	10:D:256:LEU:HD11	2.02	0.42
2:B:219:ILE:HG21	2:B:270:ILE:HG12	2.02	0.42
2:B:242:LEU:HD22	2:B:502:ILE:HD12	2.02	0.42
2:B:771:ILE:H	2:B:812:VAL:HG22	1.84	0.42
2:B:925:ALA:HB1	2:B:985:GLY:HA3	2.00	0.42
4:G:72:GLY:HA3	4:G:91:LEU:HA	2.01	0.42
10:D:236:LEU:HB2	10:D:241:ILE:HD11	2.01	0.42
1:A:637:ARG:HA	1:A:640:GLU:HG2	2.02	0.42
2:B:14:PHE:CE1	2:B:18:ARG:HD2	2.54	0.42
2:B:210:ILE:HD11	2:B:221:PHE:HD1	1.85	0.42
2:B:456:THR:HB	2:B:462:SER:HA	2.01	0.42
10:D:8:ARG:HG3	10:D:13:LEU:HD13	2.01	0.42
10:D:176:CYS:HB2	10:D:216:SER:HB2	2.01	0.42
1:A:99:TRP:CD1	1:A:99:TRP:H	2.38	0.42
3:C:339:VAL:HG22	3:C:342:ARG:HH21	1.84	0.42
5:H:38:LYS:HG3	5:H:40:GLU:H	1.84	0.42
1:A:547:THR:HG21	4:G:92:TYR:HB2	2.01	0.41
2:B:40:ILE:HG13	2:B:60:ILE:HB	2.02	0.41
2:B:532:LYS:HD2	2:B:536:LYS:NZ	2.35	0.41
2:B:625:ALA:HB2	2:B:635:HIS:CG	2.55	0.41
2:B:739:ASN:CG	2:B:895:MET:HE1	2.45	0.41
2:B:954:LYS:O	2:B:958:LYS:HG2	2.20	0.41
2:B:1058:TYR:HB3	2:B:1087:LEU:HG	2.01	0.41
3:C:142:ILE:HD11	3:C:249:ILE:HG21	2.02	0.41
1:A:60:VAL:HB	1:A:71:HIS:CE1	2.55	0.41
1:A:81:VAL:HG12	1:A:266:TRP:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TYR:HB3	1:A:136:ILE:HD11	2.02	0.41
2:B:120:MET:HE2	2:B:148:GLY:HA2	2.02	0.41
2:B:658:HIS:HB3	2:B:919:ILE:HB	2.02	0.41
3:C:131:ASP:HB2	3:C:134:LYS:HB2	2.01	0.41
10:D:69:SER:HB2	10:D:72:ALA:HB3	2.02	0.41
1:A:832:ILE:HG12	3:C:68:ILE:HB	2.02	0.41
2:B:1099:LEU:HA	2:B:1102:GLU:HG2	2.03	0.41
3:C:12:LYS:HE3	3:C:12:LYS:HB3	1.91	0.41
3:C:115:PRO:HD2	3:C:118:PRO:HB3	2.01	0.41
4:G:14:ILE:HB	4:G:48:LYS:HD3	2.02	0.41
5:H:78:TYR:CE2	6:K:3:ILE:HG22	2.55	0.41
1:A:877:GLY:HA2	1:A:880:ARG:HB2	2.01	0.41
2:B:226:ARG:HH11	2:B:261:THR:HA	1.84	0.41
2:B:311:TYR:HE2	2:B:496:GLU:HG2	1.85	0.41
7:L:73:ILE:HA	10:D:253:LEU:HD22	2.01	0.41
2:B:2:LEU:HB2	2:B:628:PRO:HG2	2.01	0.41
2:B:1003:ARG:HB2	2:B:1022:GLU:O	2.21	0.41
3:C:51:ASP:HA	3:C:54:ILE:HD12	2.02	0.41
5:H:78:TYR:HE2	6:K:3:ILE:HG22	1.86	0.41
1:A:124:ARG:HG3	1:A:125:TRP:H	1.85	0.41
2:B:1100:ILE:HG13	2:B:1110:PRO:HB2	2.02	0.41
5:H:23:LEU:HD12	5:H:62:ILE:HG22	2.01	0.41
8:N:15:ALA:HB3	10:D:128:ILE:HG23	2.02	0.41
1:A:51:VAL:HG21	1:A:56:GLN:HB3	2.01	0.41
1:A:77:LEU:HD11	1:A:212:LEU:HD12	2.02	0.41
7:L:27:LEU:HB2	10:D:27:SER:OG	2.21	0.41
10:D:227:ILE:HG22	10:D:229:GLU:HG2	2.03	0.41
2:B:184:VAL:HG23	2:B:201:GLU:HG2	2.03	0.41
2:B:582:ASN:HA	2:B:633:PRO:HA	2.02	0.41
1:A:48:LYS:HG2	1:A:59:PRO:HG2	2.02	0.41
1:A:49:LEU:HB3	1:A:217:ILE:HG12	2.02	0.41
1:A:321:SER:HB2	2:B:1025:LEU:HD12	2.02	0.41
1:A:557:PRO:HD3	1:A:623:TYR:CZ	2.55	0.41
1:A:803:ARG:HH12	2:B:456:THR:HG21	1.85	0.41
2:B:53:LEU:HD11	2:B:367:LEU:HD11	2.03	0.41
2:B:215:VAL:HG11	2:B:219:ILE:HD11	2.03	0.41
3:C:236:LYS:HB2	3:C:252:ASP:HB3	2.02	0.41
3:C:299:LEU:HD13	3:C:306:VAL:HB	2.03	0.41
4:G:35:ILE:HG13	4:G:98:ILE:HG12	2.02	0.41
7:L:10:GLN:O	7:L:64:SER:HA	2.21	0.41
7:L:31:MET:O	7:L:35:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:86:LYS:O	10:D:87:GLU:HG3	2.20	0.41
11:P:39:LYS:HG2	11:P:41:THR:HG23	2.03	0.41
2:B:173:ASP:HA	2:B:330:PRO:HB3	2.03	0.41
2:B:867:LEU:HG	2:B:869:ILE:HG13	2.03	0.41
10:D:75:HIS:ND1	10:D:120:MET:HE3	2.36	0.41
1:A:1:MET:HA	2:B:1088:HIS:CE1	2.56	0.40
1:A:10:LYS:HD3	2:B:1111:ARG:HD3	2.03	0.40
1:A:46:ASP:HB3	1:A:49:LEU:HD13	2.03	0.40
1:A:51:VAL:HB	1:A:58:CYS:HB3	2.02	0.40
2:B:65:PRO:HD3	2:B:119:ILE:HD12	2.03	0.40
2:B:797:SER:HB3	11:P:39:LYS:HE2	2.03	0.40
3:C:22:PRO:HD3	3:C:57:TYR:CZ	2.56	0.40
3:C:48:ARG:O	3:C:52:LEU:HB2	2.21	0.40
2:B:532:LYS:HD2	2:B:536:LYS:HZ3	1.86	0.40
4:G:94:LEU:H	4:G:94:LEU:HG	1.70	0.40
1:A:238:LYS:O	1:A:242:ILE:HG12	2.21	0.40
1:A:387:ASP:O	1:A:391:VAL:HG23	2.21	0.40
1:A:734:ARG:HA	1:A:734:ARG:HD3	1.83	0.40
3:C:196:ILE:HD12	3:C:206:ILE:HA	2.04	0.40
5:H:58:LYS:HD2	9:Y:74:ALA:HB1	2.02	0.40
1:A:14:LEU:HA	2:B:1109:SER:HB3	2.03	0.40
2:B:81:MET:HB2	2:B:140:GLY:O	2.21	0.40
2:B:219:ILE:HD13	2:B:270:ILE:HG12	2.04	0.40
2:B:742:SER:OG	8:N:8:PHE:HB3	2.22	0.40
5:H:25:LEU:HD22	9:Y:53:TRP:HZ2	1.86	0.40
2:B:443:LEU:HD12	2:B:443:LEU:HA	1.90	0.40
2:B:538:ILE:HB	2:B:553:VAL:HG11	2.04	0.40
2:B:745:ARG:HD3	8:N:7:CYS:O	2.21	0.40
3:C:198:ASP:HA	3:C:204:PHE:HA	2.03	0.40
3:C:369:GLU:H	3:C:369:GLU:HG2	1.73	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	870/880 (99%)	810 (93%)	58 (7%)	2 (0%)	43	78
2	B	1105/1126 (98%)	1027 (93%)	78 (7%)	0	100	100
3	C	373/393 (95%)	346 (93%)	27 (7%)	0	100	100
4	G	120/124 (97%)	98 (82%)	22 (18%)	0	100	100
5	H	76/84 (90%)	70 (92%)	6 (8%)	0	100	100
6	K	84/89 (94%)	79 (94%)	5 (6%)	0	100	100
7	L	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
8	N	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
9	Y	42/105 (40%)	41 (98%)	1 (2%)	0	100	100
10	D	259/264 (98%)	226 (87%)	33 (13%)	0	100	100
11	P	45/48 (94%)	41 (91%)	4 (9%)	0	100	100
All	All	3126/3269 (96%)	2884 (92%)	240 (8%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	THR
1	A	27	ILE

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	762/768 (99%)	762 (100%)	0	100	100
2	B	948/972 (98%)	948 (100%)	0	100	100
3	C	327/348 (94%)	327 (100%)	0	100	100
4	G	113/115 (98%)	113 (100%)	0	100	100
5	H	68/75 (91%)	68 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	78/81 (96%)	78 (100%)	0	100	100
7	L	78/78 (100%)	78 (100%)	0	100	100
8	N	60/60 (100%)	60 (100%)	0	100	100
9	Y	40/98 (41%)	40 (100%)	0	100	100
10	D	237/239 (99%)	237 (100%)	0	100	100
11	P	41/43 (95%)	41 (100%)	0	100	100
All	All	2752/2877 (96%)	2752 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	A	483	HIS
1	A	862	HIS
2	B	23	GLN
2	B	24	HIS
2	B	43	GLN
2	B	168	ASN
2	B	338	ASN
2	B	366	GLN
2	B	437	ASN
2	B	697	GLN
2	B	719	ASN
2	B	953	GLN
2	B	990	GLN
2	B	1051	ASN
2	B	1062	GLN
3	C	391	ASN
4	G	6	GLN
4	G	80	GLN
4	G	106	ASN
6	K	13	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	SF4	D	1001	10	0,12,12	-	-	-		

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	SF4	D	1001	10	-	-	0/6/5/5

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

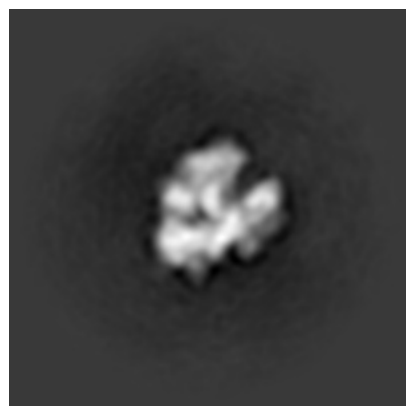
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77810. These allow visual inspection of the internal detail of the map and identification of artifacts.

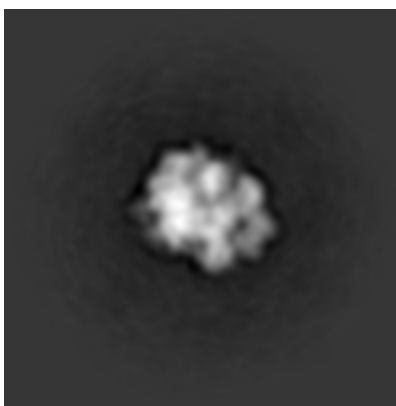
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

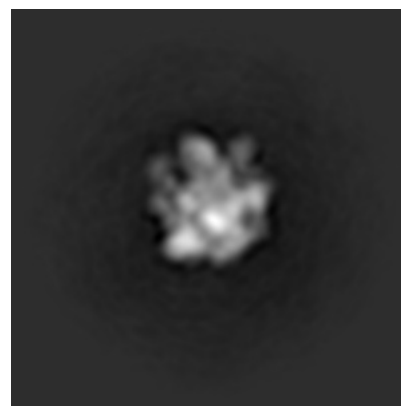
6.1.1 Primary map



X

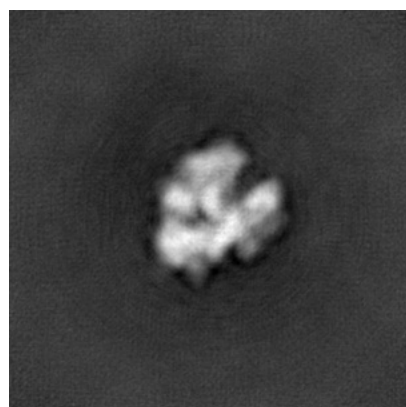


Y

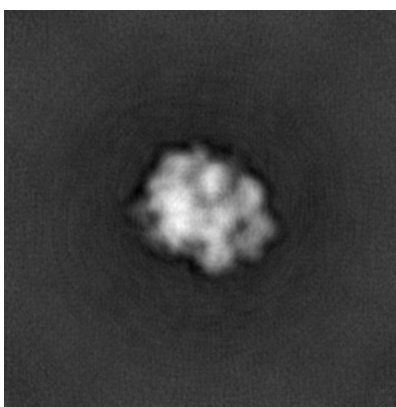


Z

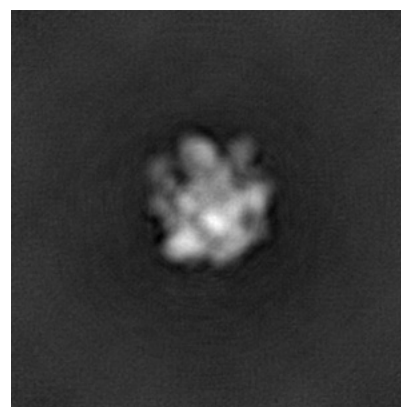
6.1.2 Raw map



X



Y

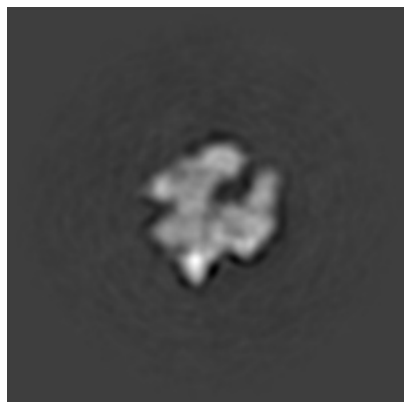


Z

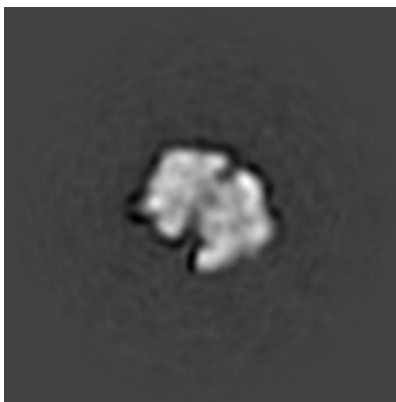
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

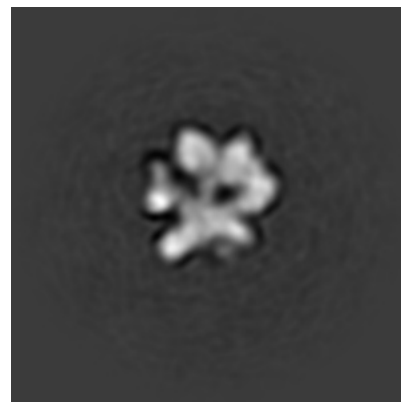
6.2.1 Primary map



X Index: 200

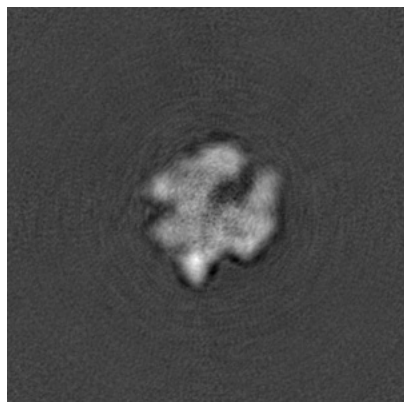


Y Index: 200

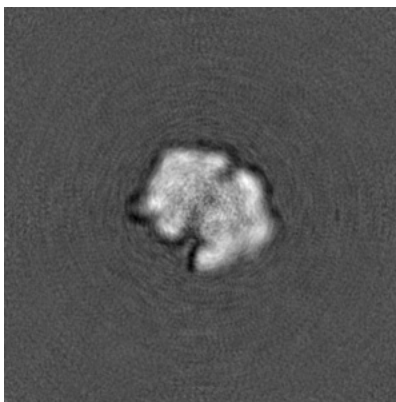


Z Index: 200

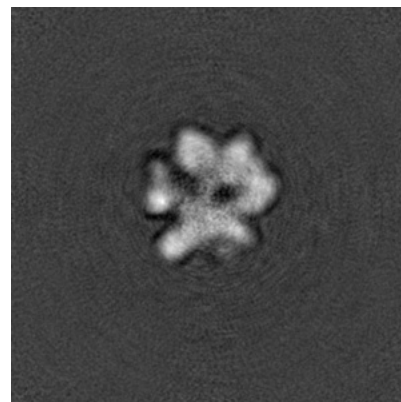
6.2.2 Raw map



X Index: 200



Y Index: 200

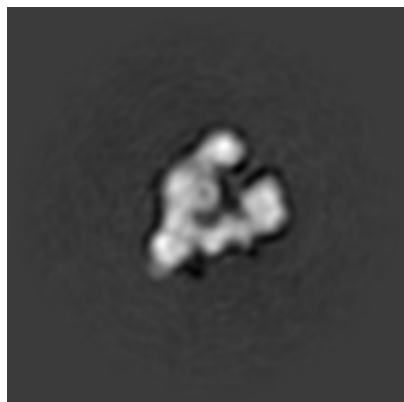


Z Index: 200

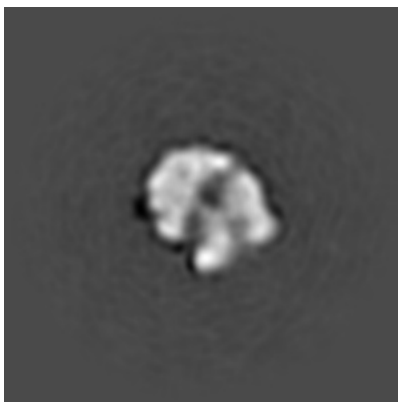
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

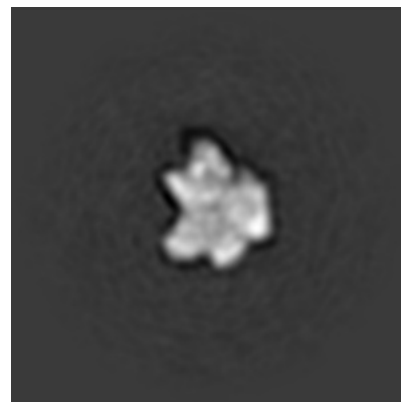
6.3.1 Primary map



X Index: 180

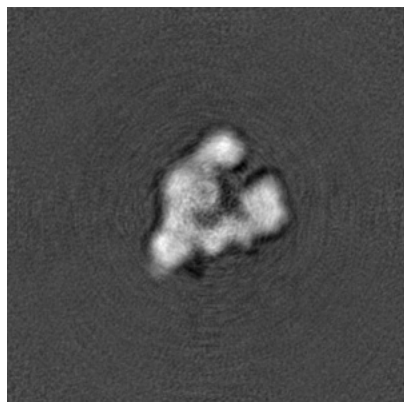


Y Index: 206

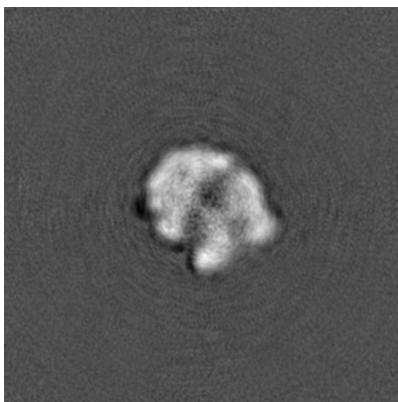


Z Index: 172

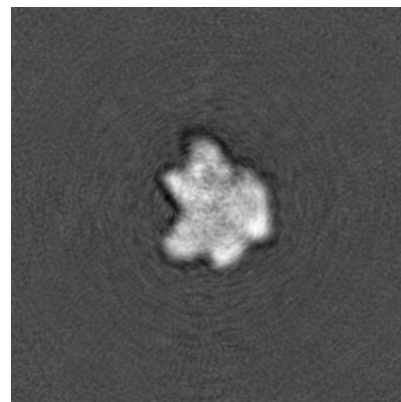
6.3.2 Raw map



X Index: 180



Y Index: 206

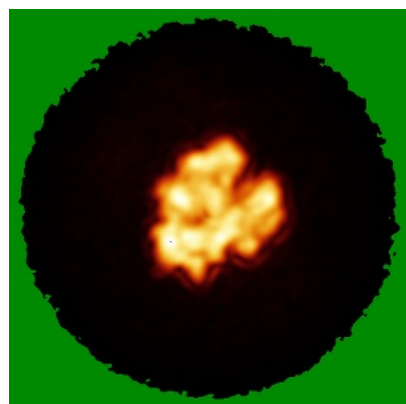


Z Index: 173

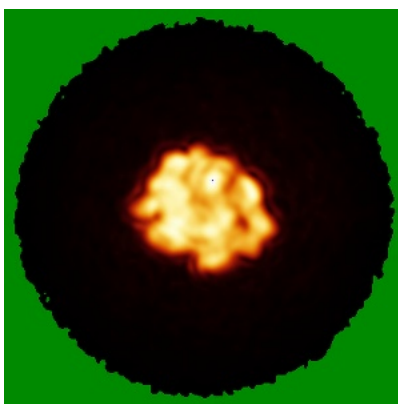
The images above show the largest variance slices of the map in three orthogonal directions.

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

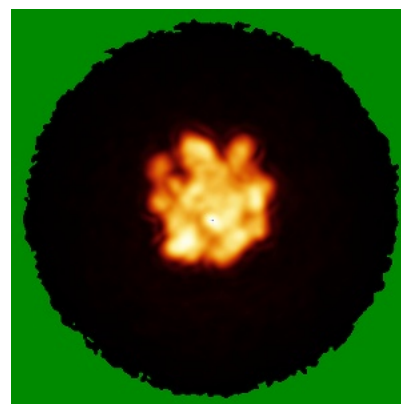
6.4.1 Primary map



X



Y

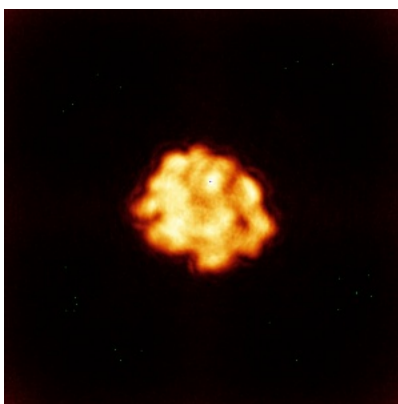


Z

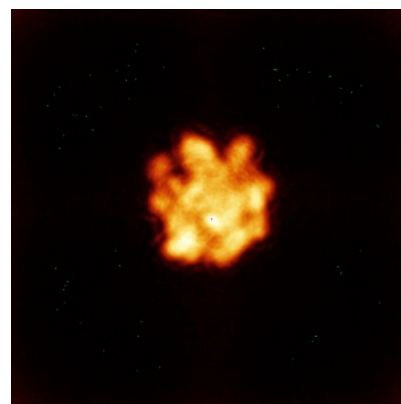
6.4.2 Raw map



X



Y

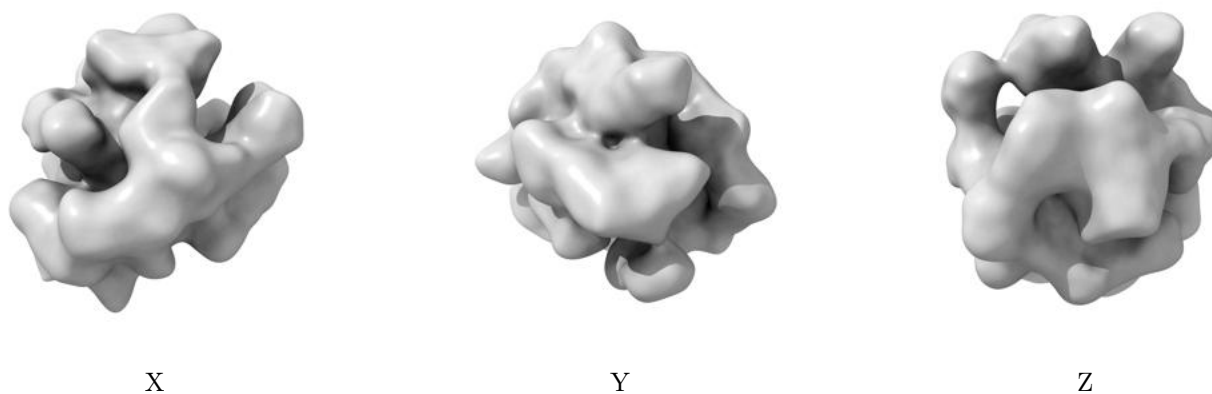


Z

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 0.11. 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.

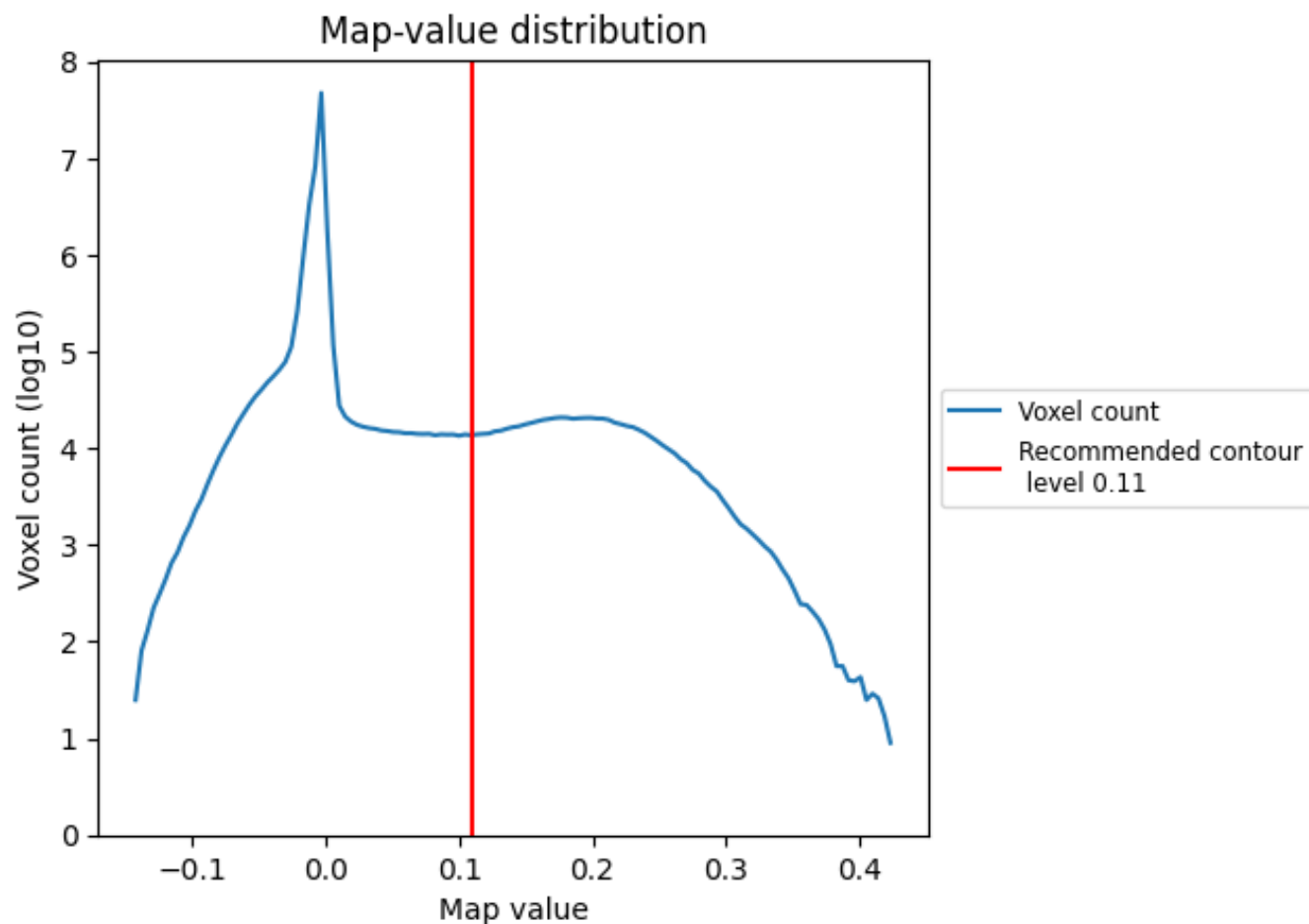
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

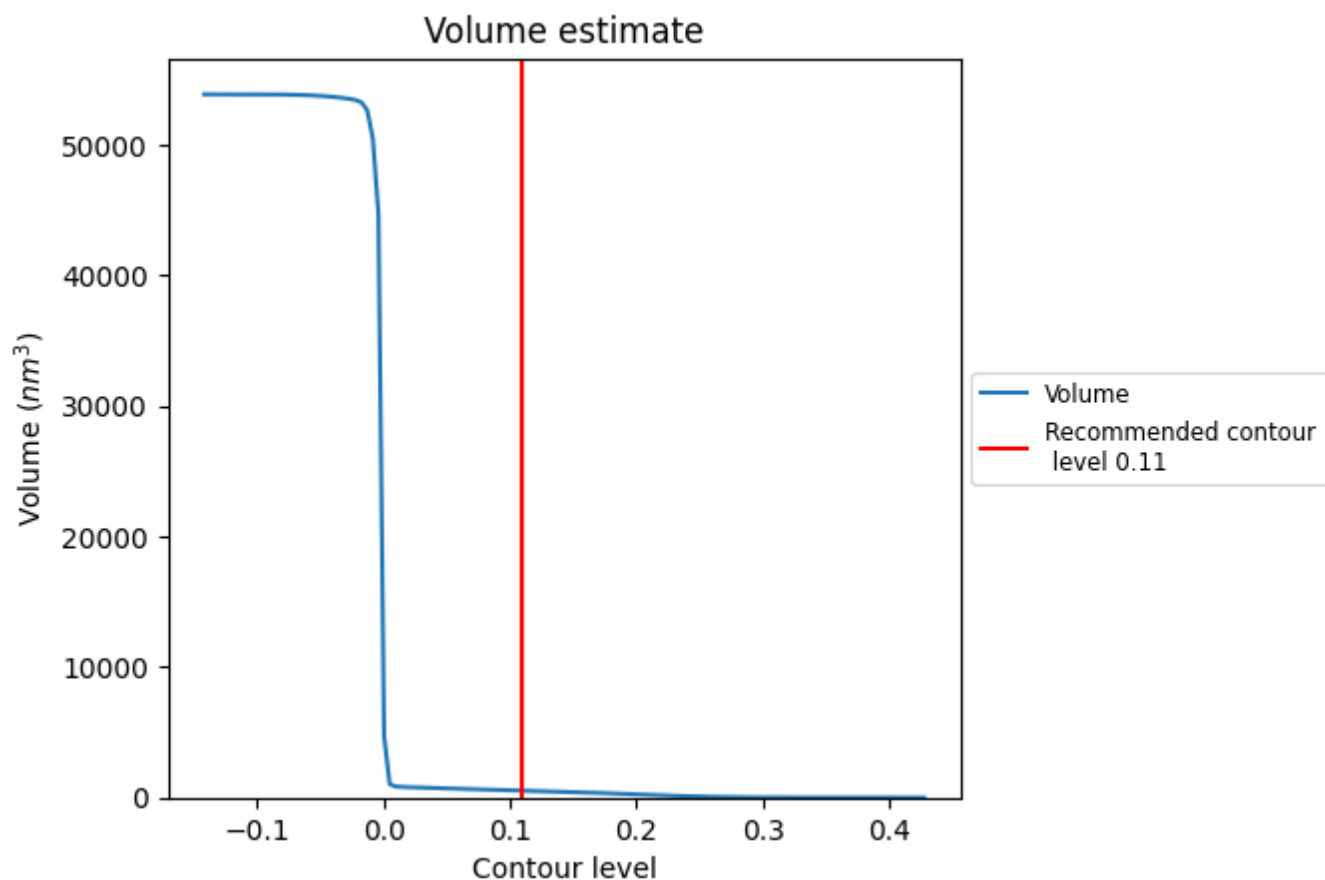
This section contains the results of statistical analysis of the map.

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.

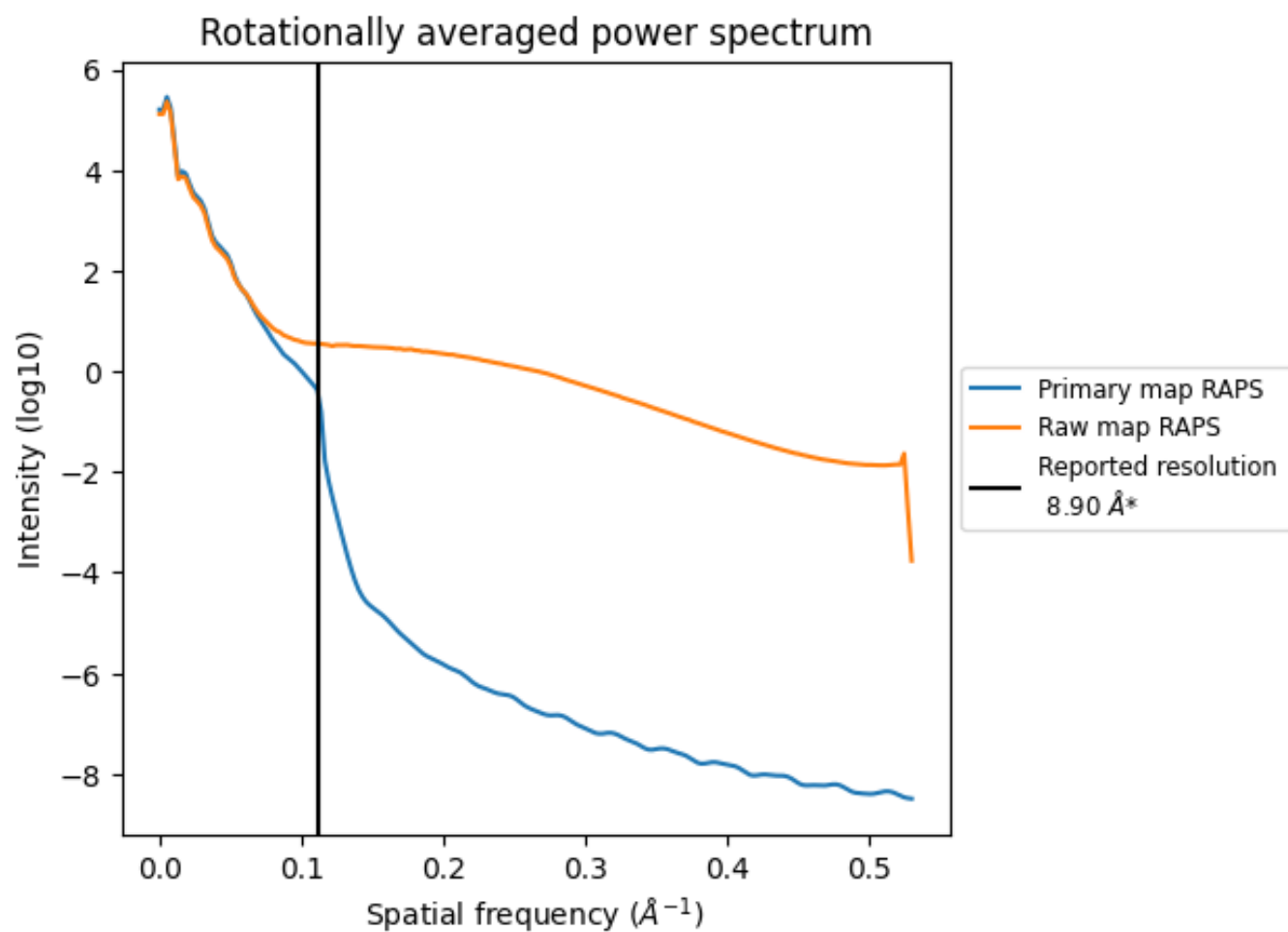
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 542 nm³; this corresponds to an approximate mass of 490 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 ⓘ

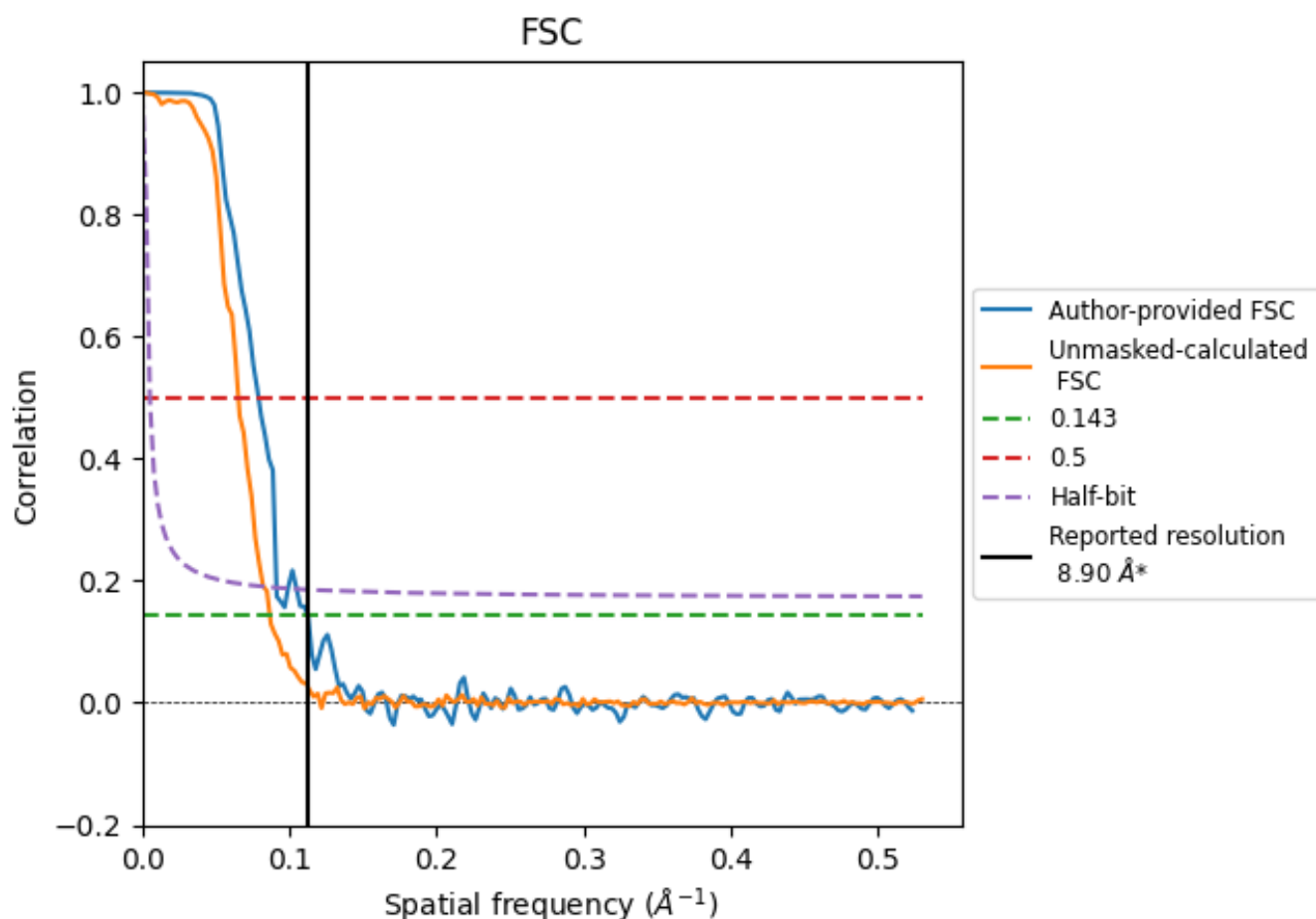


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

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 0.112 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

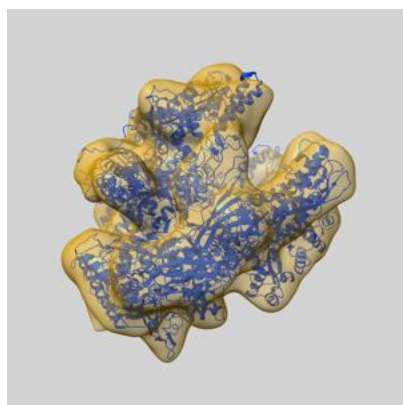
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.88	12.66	10.96
Unmasked-calculated*	11.53	15.31	12.14

*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 11.53 differs from the reported value 8.9 by more than 10 %

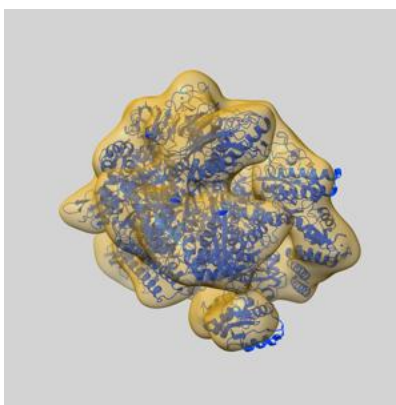
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77810 and PDB model 36RP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

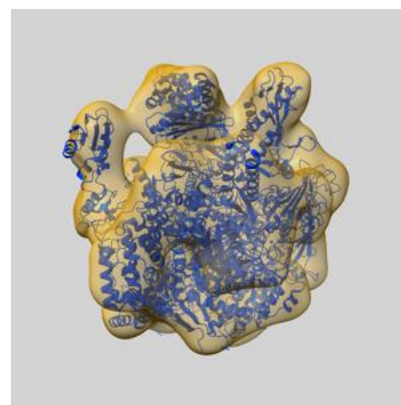
9.1 Map-model overlay [i](#)



X



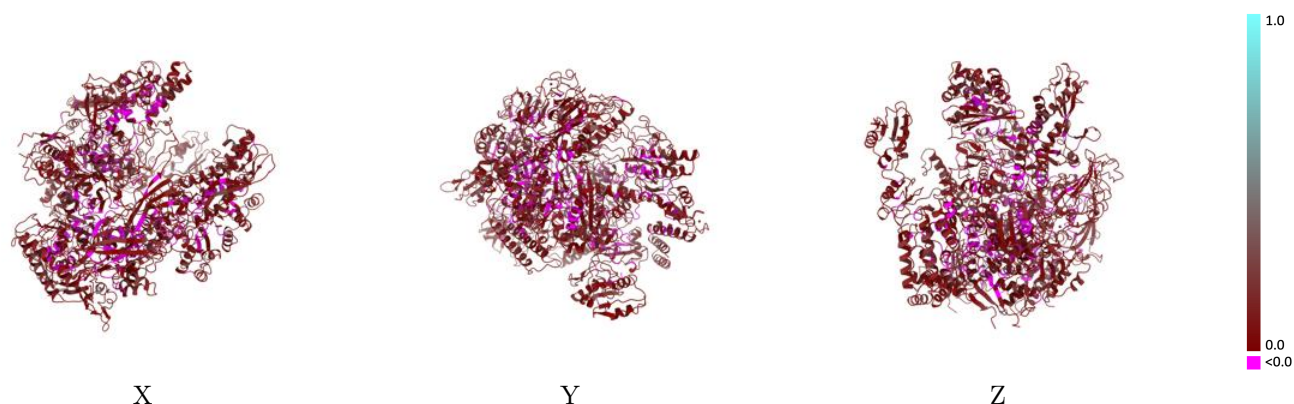
Y



Z

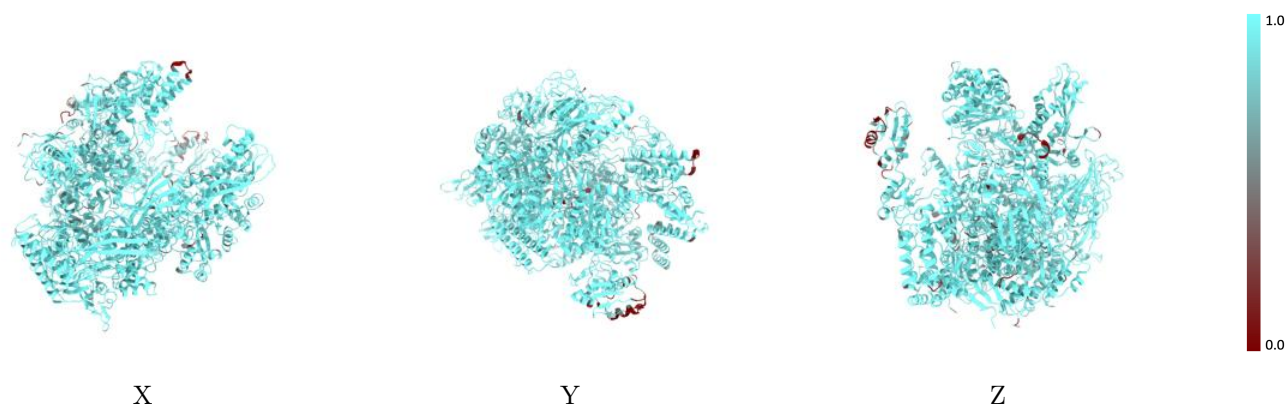
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



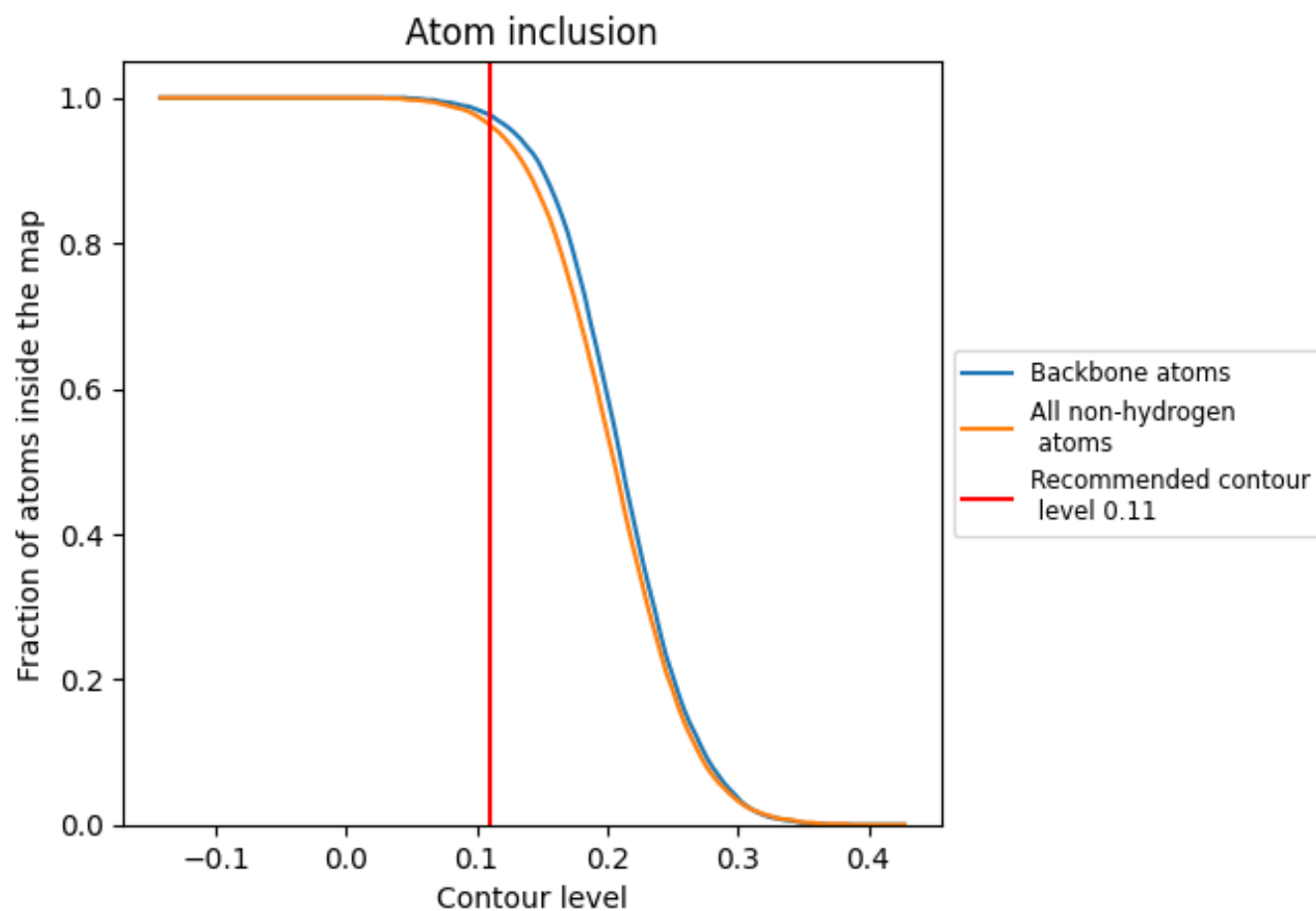
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.0860
A	 0.9710	 0.0850
B	 0.9680	 0.0800
C	 0.9030	 0.0830
D	 0.9880	 0.0910
G	 0.9780	 0.0960
H	 0.9650	 0.0720
K	 0.9750	 0.1000
L	 0.9700	 0.1050
N	 0.9900	 0.1070
P	 1.0000	 0.1030
Y	 0.8970	 0.1400

