



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 01:09 PM EDT

PDB ID : 9ZPK / pdb_00009zpk
EMDB ID : EMD-74528
Title : Cryo-EM structure of the complete *Saccharomyces cerevisiae* RNA polymerase II in closed clamp conformation
Authors : Fordjour, G.N.R.; Murakami, K.; Armache, J.-P.; Murakami, K.S.
Deposited on : 2025-12-16
Resolution : 3.31 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:

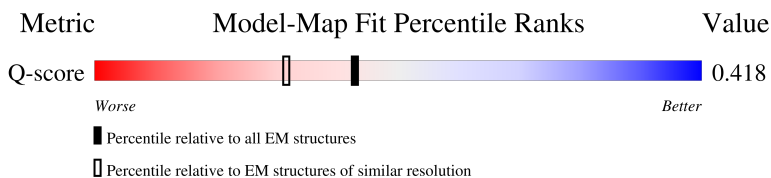
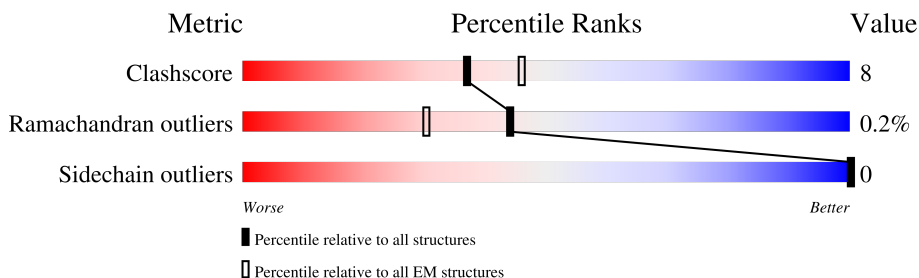
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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	1733	
2	B	1224	
3	C	318	
4	D	221	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	84%16%
6	F	155	44%12%44%
7	G	171	16%73%27%
8	H	146	70%23%7%
9	I	122	83%11%7%
10	J	70	67%27%6%
11	K	120	6%74%22%.
12	L	70	53%10%37%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 31439 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0
			11189	7046	1955	2126	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1160	Total	C	N	O	S	0	0
			9197	5805	1614	1723	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	685	184	215	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total	Zn	0
			2	2	
13	B	1	Total	Zn	0
			1	1	

Continued on next page...

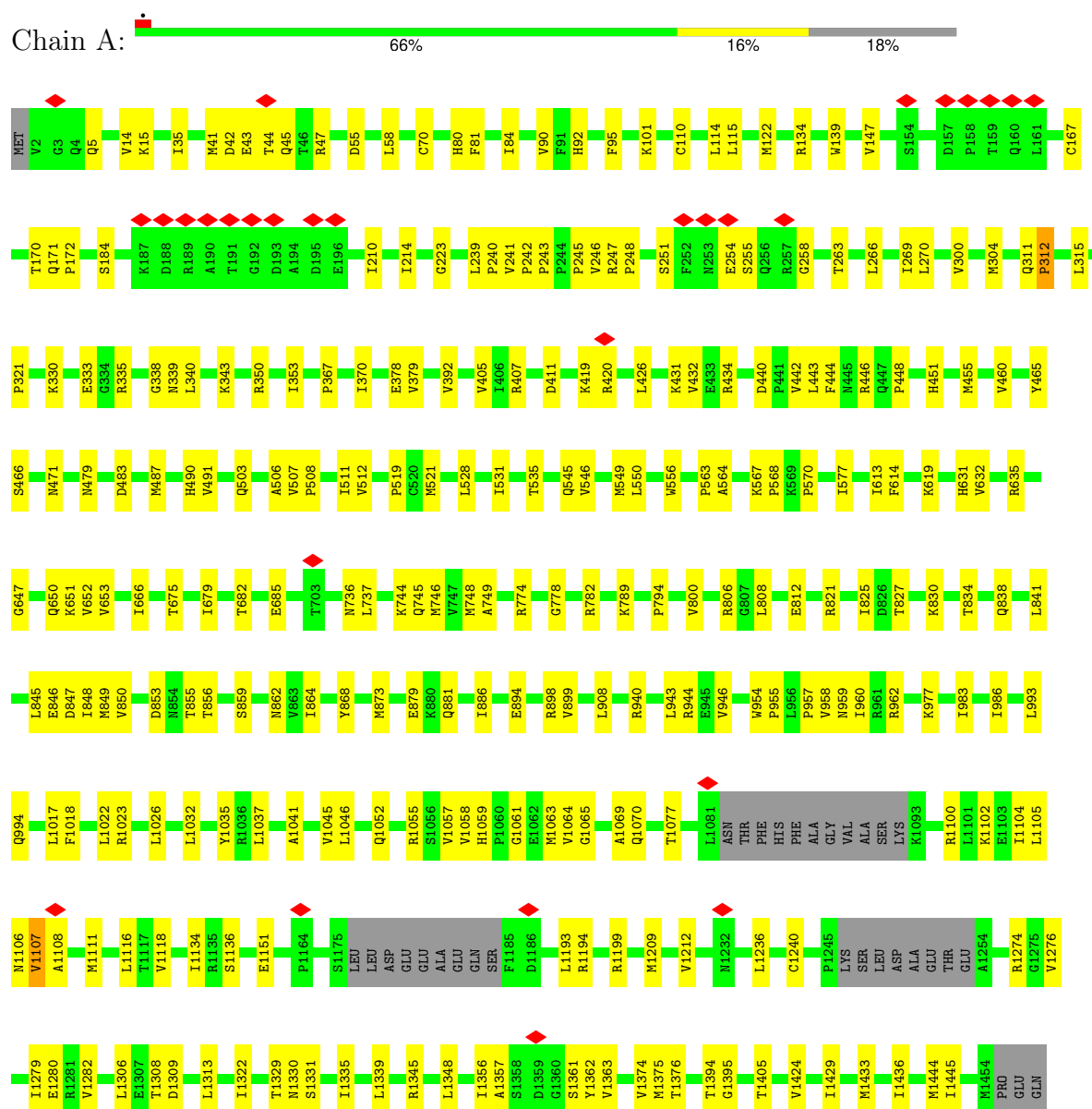
Continued from previous page...

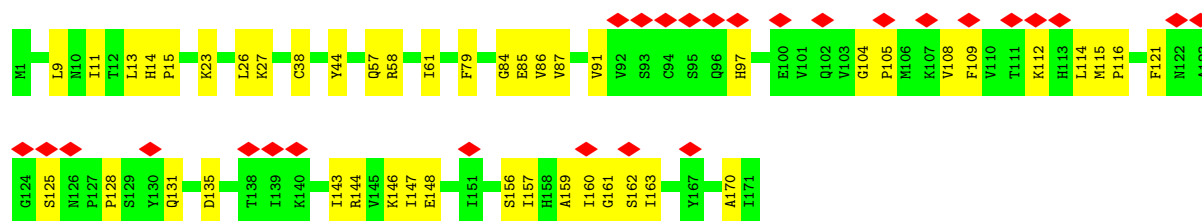
Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total 1	Zn 1	0
13	I	2	Total 2	Zn 2	0
13	J	1	Total 1	Zn 1	0
13	L	1	Total 1	Zn 1	0

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 II subunit RPB1

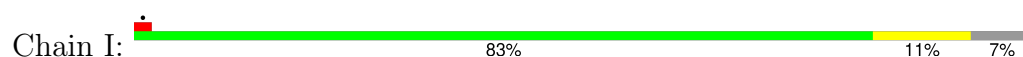




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



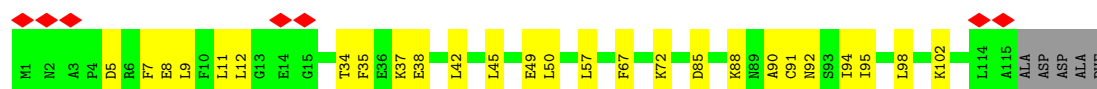
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



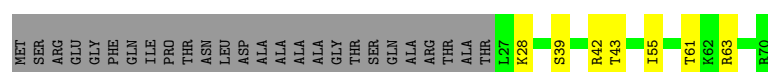
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208045	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)	-800	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.907	Depositor
Minimum map value	-1.617	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 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	0.16	0/11390	0.41	2/15408 (0.0%)
2	B	0.18	0/9371	0.45	5/12636 (0.0%)
3	C	0.15	0/2124	0.36	0/2879
4	D	0.15	0/1339	0.43	0/1793
5	E	0.14	0/1788	0.35	0/2406
6	F	0.19	0/717	0.45	0/967
7	G	0.12	0/1367	0.38	1/1844 (0.1%)
8	H	0.14	0/1107	0.41	0/1498
9	I	0.11	0/945	0.30	0/1273
10	J	0.19	0/549	0.45	0/738
11	K	0.15	0/942	0.35	0/1272
12	L	0.14	0/354	0.47	0/468
All	All	0.16	0/31993	0.41	8/43182 (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
2	B	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	918	ILE	CA-C-N	5.85	132.24	121.70
2	B	918	ILE	C-N-CA	5.85	132.24	121.70
1	A	1107	VAL	CA-C-N	5.70	131.97	121.70
1	A	1107	VAL	C-N-CA	5.70	131.97	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	GLY	CA-C-N	5.47	131.26	121.15
2	B	144	GLY	C-N-CA	5.47	131.26	121.15
7	G	57	GLN	CB-CA-C	-5.09	110.69	116.54
2	B	75	ALA	N-CA-C	-5.04	106.98	114.64

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	74	LEU	Peptide
2	B	79	THR	Peptide
2	B	82	ASP	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	11189	0	11224	186	0
2	B	9197	0	9180	158	0
3	C	2086	0	2045	32	0
4	D	1331	0	1345	21	0
5	E	1752	0	1776	22	0
6	F	705	0	731	15	0
7	G	1339	0	1357	29	0
8	H	1089	0	1063	31	0
9	I	927	0	880	8	0
10	J	540	0	553	15	0
11	K	924	0	934	17	0
12	L	352	0	374	4	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	31439	0	31462	480	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 (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.02	0.98
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.60	0.82
2:B:102:VAL:HG12	2:B:112:LEU:HD21	1.63	0.80
8:H:57:VAL:HG12	8:H:144:ILE:HG22	1.65	0.79
8:H:93:TYR:HB3	8:H:145:ARG:HH21	1.47	0.79
2:B:997:GLU:HB2	3:C:35:ARG:HG2	1.66	0.78
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.67	0.77
1:A:848:ILE:HG23	1:A:1065:GLY:HA3	1.65	0.76
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.24	0.76
2:B:64:CYS:HA	2:B:67:SER:HB3	1.69	0.74
1:A:330:LYS:HA	1:A:1405:THR:HG21	1.68	0.74
1:A:1280:GLU:HB2	1:A:1309:ASP:HB3	1.70	0.73
1:A:567:LYS:HG2	8:H:95:TYR:HA	1.70	0.73
1:A:841:LEU:HD11	1:A:1105:LEU:HD23	1.71	0.72
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.70	0.72
2:B:44:VAL:HG11	2:B:200:GLY:HA2	1.72	0.72
5:E:175:LEU:HD22	5:E:213:ILE:HG13	1.72	0.71
1:A:782:ARG:HB3	1:A:789:LYS:HA	1.73	0.70
1:A:567:LYS:HG3	1:A:568:PRO:HD3	1.74	0.70
7:G:108:VAL:HG13	7:G:161:GLY:H	1.55	0.70
2:B:839:MET:HG3	2:B:1010:LEU:HD12	1.73	0.70
1:A:1329:THR:HG22	1:A:1331:SER:H	1.57	0.70
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.31	0.69
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.32	0.69
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.72	0.69
5:E:43:LYS:O	5:E:47:CYS:HB2	1.91	0.69
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.75	0.69
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.76	0.68
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.75	0.68
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.76	0.68
3:C:41:ILE:HD12	3:C:42:PRO:HD2	1.74	0.68
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.58	0.67
2:B:90:ILE:HG13	2:B:432:MET:HE1	1.75	0.67
2:B:175:ARG:HH22	2:B:199:MET:HA	1.60	0.67
11:K:38:GLU:HG2	11:K:42:LEU:HD12	1.77	0.66
1:A:367:PRO:HG2	1:A:370:ILE:HD13	1.76	0.66
1:A:443:LEU:HB2	1:A:490:HIS:HB2	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:THR:HG23	2:B:465:ASN:H	1.60	0.66
2:B:766:ARG:HE	2:B:1020:ARG:HD3	1.61	0.66
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.78	0.66
2:B:551:PRO:HB3	2:B:628:THR:HG21	1.77	0.65
1:A:881:GLN:HE22	1:A:960:ILE:HG12	1.61	0.65
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.78	0.65
1:A:862:ASN:HD22	5:E:174:GLN:HA	1.61	0.65
2:B:313:MET:HG3	2:B:390:LEU:HD21	1.79	0.65
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.79	0.65
2:B:509:ALA:HB2	2:B:515:HIS:HD2	1.61	0.65
5:E:80:VAL:HG12	5:E:109:ILE:HB	1.77	0.65
2:B:706:GLN:HB3	2:B:709:ASP:HB3	1.79	0.65
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.80	0.64
12:L:28:LYS:HB2	12:L:39:SER:HA	1.79	0.63
1:A:1151:GLU:HB2	1:A:1194:ARG:HB3	1.81	0.63
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.81	0.63
8:H:56:THR:HB	8:H:145:ARG:HB2	1.81	0.63
4:D:164:ILE:HA	4:D:167:LEU:HB3	1.81	0.63
7:G:105:PRO:HB3	7:G:156:SER:HB2	1.79	0.62
6:F:133:VAL:HG21	7:G:58:ARG:HE	1.63	0.62
11:K:91:CYS:HA	11:K:94:ILE:HD12	1.81	0.62
1:A:251:SER:H	1:A:258:GLY:HA3	1.64	0.62
1:A:737:LEU:HB3	1:A:744:LYS:HD2	1.80	0.62
2:B:848:ARG:HH22	2:B:996:ARG:HH21	1.47	0.62
4:D:179:GLN:HG2	7:G:85:GLU:HG2	1.82	0.62
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.65	0.61
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.81	0.61
1:A:407:ARG:HE	1:A:411:ASP:HB2	1.63	0.61
1:A:340:LEU:HD21	1:A:1429:ILE:HG23	1.81	0.61
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.66	0.60
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.82	0.60
2:B:1135:ARG:HG2	2:B:1147:LEU:HD11	1.82	0.60
1:A:531:ILE:O	1:A:535:THR:HG22	2.02	0.60
2:B:448:ILE:HD12	2:B:451:LYS:HD3	1.83	0.60
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.83	0.60
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.82	0.60
10:J:24:LEU:O	10:J:28:ASP:HB2	2.02	0.60
2:B:446:LEU:HA	2:B:449:ASN:HB2	1.84	0.59
3:C:50:GLU:HB2	3:C:156:THR:HB	1.85	0.59
4:D:35:LEU:HD12	4:D:36:LYS:HG2	1.83	0.59
3:C:39:ALA:HB1	3:C:165:LYS:HG3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:LEU:HB3	8:H:145:ARG:NH2	2.18	0.59
1:A:879:GLU:HG3	1:A:959:ASN:HB2	1.82	0.59
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.83	0.59
3:C:175:ALA:HB3	3:C:233:GLU:HB3	1.84	0.59
1:A:782:ARG:HD2	1:A:789:LYS:HB3	1.85	0.59
2:B:401:PHE:H	2:B:517:THR:HG21	1.68	0.59
1:A:774:ARG:HH22	1:A:794:PRO:HA	1.68	0.59
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.68	0.59
2:B:911:ILE:HG21	2:B:966:VAL:HG21	1.84	0.59
10:J:36:LEU:HD22	10:J:47:ARG:HG3	1.85	0.58
4:D:198:LEU:HD13	4:D:204:ASP:HB3	1.85	0.58
1:A:114:LEU:HD11	1:A:171:GLN:HE22	1.68	0.58
1:A:440:ASP:H	1:A:460:VAL:HG12	1.68	0.58
1:A:808:LEU:HB2	2:B:760:ASP:HB2	1.85	0.58
2:B:301:ILE:HD11	2:B:382:ILE:HB	1.85	0.58
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.86	0.58
3:C:37:MET:HE1	3:C:243:VAL:HG23	1.84	0.57
1:A:1136:SER:HB2	1:A:1274:ARG:HH22	1.68	0.57
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.86	0.57
2:B:844:SER:HB3	2:B:848:ARG:HH21	1.68	0.57
8:H:130:ARG:HB2	8:H:133:ASN:HB2	1.84	0.57
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.68	0.57
1:A:647:GLY:O	1:A:651:LYS:HB2	2.03	0.57
9:I:42:LEU:HD21	9:I:45:ARG:HG2	1.86	0.57
2:B:621:GLU:HB3	2:B:623:GLU:HG2	1.85	0.57
1:A:35:ILE:HD13	1:A:241:VAL:HG21	1.86	0.57
1:A:650:GLN:HA	1:A:653:VAL:HG12	1.86	0.57
3:C:142:VAL:HG23	10:J:15:GLY:HA3	1.87	0.57
1:A:392:VAL:HG11	1:A:426:LEU:HD11	1.87	0.57
1:A:834:THR:HG21	1:A:1077:THR:HB	1.86	0.56
2:B:298:LEU:HA	2:B:301:ILE:HG22	1.88	0.56
5:E:195:VAL:HG22	5:E:213:ILE:HG12	1.88	0.56
8:H:93:TYR:HB3	8:H:145:ARG:NH2	2.19	0.56
2:B:618:ASP:HB3	2:B:623:GLU:HB2	1.88	0.56
2:B:684:LEU:HD22	2:B:689:LEU:HD12	1.88	0.56
8:H:37:LYS:H	8:H:126:GLU:HB2	1.71	0.56
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.71	0.55
2:B:863:GLU:HB2	2:B:961:LEU:HB3	1.88	0.55
4:D:56:ARG:HD3	4:D:148:LEU:HG	1.86	0.55
11:K:34:THR:HG22	11:K:72:LYS:HG2	1.88	0.55
1:A:1134:ILE:HG21	1:A:1322:ILE:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.70	0.55
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.89	0.55
12:L:42:ARG:HG2	12:L:43:THR:HG23	1.89	0.55
1:A:511:ILE:HD13	1:A:521:MET:HG3	1.89	0.55
1:A:886:ILE:HD13	1:A:943:LEU:HB3	1.88	0.55
2:B:826:ALA:HB3	2:B:1011:ILE:HD13	1.88	0.55
2:B:1215:ARG:HH21	4:D:15:LEU:HD13	1.71	0.55
1:A:210:ILE:O	1:A:214:ILE:HD12	2.07	0.54
7:G:13:LEU:HD11	7:G:26:LEU:HG	1.89	0.54
8:H:143:LEU:HB3	8:H:145:ARG:HH22	1.71	0.54
2:B:428:ILE:HA	2:B:445:LYS:HD3	1.88	0.54
7:G:147:ILE:HD11	7:G:159:ALA:HB3	1.88	0.54
1:A:14:VAL:HG21	2:B:1216:LEU:HD23	1.90	0.54
1:A:1209:MET:HA	1:A:1212:VAL:HG22	1.89	0.54
1:A:451:HIS:HA	1:A:1070:GLN:HG2	1.90	0.54
1:A:247:ARG:HD2	1:A:263:THR:HB	1.91	0.54
2:B:1024:ALA:HA	2:B:1027:ILE:HG22	1.89	0.54
2:B:128:LEU:HD22	2:B:170:LEU:HD22	1.89	0.53
2:B:580:VAL:HG22	2:B:624:LEU:HD23	1.89	0.53
1:A:1445:ILE:HB	7:G:61:ILE:HD11	1.90	0.53
1:A:853:ASP:HB3	1:A:855:THR:HG22	1.91	0.53
1:A:940:ARG:HE	1:A:944:ARG:HE	1.57	0.53
3:C:248:ILE:HG21	11:K:102:LYS:HB3	1.91	0.53
1:A:353:ILE:HD13	1:A:487:MET:HE1	1.90	0.53
5:E:110:PHE:HB3	5:E:134:THR:HG22	1.91	0.53
12:L:61:THR:HG22	12:L:63:ARG:H	1.74	0.53
8:H:95:TYR:H	8:H:145:ARG:NH1	2.06	0.52
1:A:115:LEU:HB3	1:A:122:MET:HE3	1.91	0.52
1:A:737:LEU:HD23	1:A:744:LYS:HB2	1.91	0.52
2:B:240:ILE:HB	2:B:381:MET:HE2	1.90	0.52
1:A:993:LEU:HG	1:A:1046:LEU:HB3	1.91	0.52
8:H:129:TYR:CE2	8:H:130:ARG:HD2	2.45	0.52
5:E:88:VAL:HB	5:E:116:ILE:HG23	1.92	0.52
1:A:1357:ALA:HA	1:A:1361:SER:HB3	1.92	0.52
1:A:254:GLU:HG2	1:A:255:SER:H	1.74	0.52
1:A:15:LYS:HB3	2:B:1220:ARG:HH11	1.75	0.52
1:A:147:VAL:HA	1:A:170:THR:HA	1.91	0.52
1:A:42:ASP:HB3	1:A:45:GLN:HB2	1.92	0.52
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.92	0.52
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.92	0.52
1:A:849:MET:HB3	1:A:1063:MET:SD	2.50	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:MET:HE1	1:A:1057:VAL:HG22	1.91	0.52
1:A:304:MET:HB3	2:B:1210:MET:HE1	1.91	0.51
1:A:350:ARG:HB2	2:B:1128:LEU:HD21	1.92	0.51
2:B:72:GLU:HA	2:B:88:TYR:H	1.75	0.51
2:B:82:ASP:OD2	2:B:143:PRO:HD2	2.10	0.51
2:B:137:TYR:CE2	2:B:139:ALA:HB2	2.44	0.51
2:B:996:ARG:HH22	10:J:9:SER:C	2.17	0.51
7:G:114:LEU:HD13	7:G:163:ILE:H	1.74	0.51
2:B:605:ARG:HH21	2:B:639:ILE:HD11	1.75	0.51
2:B:454:THR:HG22	2:B:458:LYS:HE2	1.93	0.51
1:A:1444:MET:HB2	6:F:133:VAL:HG23	1.92	0.51
8:H:93:TYR:HB3	8:H:145:ARG:HE	1.74	0.51
1:A:675:THR:HG21	1:A:736:ASN:HB2	1.93	0.51
1:A:563:PRO:HG3	1:A:570:PRO:HB3	1.92	0.51
1:A:666:ILE:HG13	2:B:1026:LEU:HB3	1.93	0.51
4:D:194:LEU:HG	4:D:195:ILE:H	1.76	0.51
2:B:802:PRO:HG2	2:B:805:THR:HB	1.91	0.50
1:A:315:LEU:HA	1:A:321:PRO:HA	1.93	0.50
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.94	0.50
1:A:379:VAL:HG12	1:A:431:LYS:HG2	1.93	0.50
1:A:1055:ARG:HG3	6:F:155:LEU:HD11	1.94	0.50
1:A:378:GLU:HG3	1:A:434:ARG:HE	1.75	0.50
4:D:163:VAL:HG22	4:D:217:LEU:HB2	1.93	0.50
9:I:18:GLU:HA	9:I:25:LEU:HA	1.92	0.50
1:A:994:GLN:HE22	1:A:1023:ARG:HH21	1.60	0.50
1:A:367:PRO:HB3	1:A:466:SER:HA	1.93	0.50
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.93	0.50
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.93	0.50
1:A:81:PHE:HE1	1:A:243:PRO:HD3	1.76	0.50
1:A:507:VAL:HG23	1:A:508:PRO:HD3	1.92	0.50
1:A:1348:LEU:HD13	1:A:1375:MET:HE2	1.94	0.50
1:A:1356:ILE:HG21	1:A:1363:VAL:HG22	1.93	0.50
1:A:444:PHE:O	1:A:455:MET:HA	2.12	0.49
1:A:821:ARG:HH11	2:B:514:LEU:HD13	1.77	0.49
2:B:448:ILE:HA	2:B:451:LYS:HG2	1.93	0.49
2:B:230:ALA:HA	2:B:261:ARG:HH12	1.77	0.49
5:E:94:LYS:HA	5:E:97:VAL:HG12	1.93	0.49
4:D:122:GLU:O	4:D:126:ILE:HG12	2.13	0.49
2:B:1207:LEU:HD22	2:B:1214:PRO:HG3	1.95	0.49
8:H:40:LEU:HD11	8:H:142:LEU:HD21	1.93	0.49
2:B:492:LEU:HB3	2:B:751:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	1.95	0.49
1:A:41:MET:HE2	1:A:47:ARG:HE	1.78	0.49
1:A:838:GLN:HE22	1:A:1070:GLN:HG3	1.77	0.49
1:A:1329:THR:HB	1:A:1335:ILE:HD11	1.94	0.49
5:E:91:LYS:HD3	5:E:94:LYS:HD3	1.95	0.49
11:K:92:ASN:O	11:K:95:ILE:HG22	2.13	0.49
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.93	0.49
2:B:878:GLN:HB2	2:B:881:ASN:HB2	1.95	0.49
2:B:848:ARG:HH22	2:B:996:ARG:NH2	2.11	0.48
2:B:944:THR:HG21	2:B:1122:ARG:HH12	1.77	0.48
1:A:442:VAL:HG23	1:A:491:VAL:HA	1.95	0.48
2:B:574:SER:HB3	2:B:577:ALA:HB2	1.96	0.48
2:B:1208:MET:HE3	2:B:1214:PRO:HG2	1.95	0.48
4:D:143:ASN:HD21	7:G:104:GLY:HA2	1.79	0.48
1:A:110:CYS:CB	1:A:167:CYS:SG	2.96	0.48
1:A:446:ARG:HH12	1:A:479:ASN:HB3	1.78	0.48
1:A:745:GLN:O	1:A:749:ALA:HB2	2.14	0.48
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.94	0.48
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.95	0.48
10:J:5:VAL:HA	10:J:14:VAL:O	2.14	0.48
3:C:44:LEU:HD22	3:C:129:ILE:HG23	1.95	0.48
11:K:85:ASP:HA	11:K:88:LYS:HG2	1.96	0.48
1:A:1282:VAL:HG12	1:A:1308:THR:HA	1.96	0.48
2:B:806:THR:HB	2:B:1044:ALA:HB3	1.96	0.48
3:C:165:LYS:HZ1	11:K:9:LEU:HD13	1.79	0.48
2:B:201:GLY:H	2:B:495:LEU:HD11	1.79	0.47
2:B:274:PRO:HA	2:B:275:TYR:HA	1.53	0.47
4:D:190:GLU:HB2	4:D:194:LEU:H	1.78	0.47
6:F:70:LYS:O	6:F:71:GLU:HG3	2.14	0.47
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.95	0.47
1:A:567:LYS:HB3	8:H:96:VAL:H	1.79	0.47
2:B:120:ARG:HB3	2:B:122:LEU:HD23	1.97	0.47
1:A:847:ASP:HB2	1:A:859:SER:HB2	1.96	0.47
3:C:174:ALA:HB1	10:J:11:GLY:HA3	1.96	0.47
7:G:109:PHE:HD2	7:G:160:ILE:HG12	1.79	0.47
1:A:1116:LEU:HB3	1:A:1329:THR:HG23	1.95	0.47
2:B:930:ALA:HA	2:B:931:TYR:C	2.39	0.47
1:A:465:TYR:HB2	11:K:67:PHE:HE2	1.79	0.47
1:A:682:THR:O	1:A:685:GLU:HG3	2.15	0.47
1:A:1059:HIS:HE1	6:F:155:LEU:HD13	1.79	0.47
2:B:75:ALA:HB2	2:B:83:ASN:HD22	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:ARG:HH12	2:B:996:ARG:HH21	1.61	0.47
11:K:5:ASP:HB2	11:K:8:GLU:HG3	1.95	0.47
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.78	0.47
1:A:958:VAL:HG11	1:A:1052:GLN:HB3	1.97	0.47
2:B:238:ALA:HB1	2:B:381:MET:HE3	1.97	0.47
2:B:316:PRO:HA	2:B:319:GLU:HG2	1.97	0.47
2:B:348:ARG:HG2	2:B:351:TYR:H	1.79	0.47
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.96	0.47
8:H:8:ASP:HB3	8:H:10:PHE:HE1	1.79	0.47
1:A:44:THR:N	1:A:45:GLN:HA	2.30	0.47
1:A:528:LEU:HD21	1:A:619:LYS:HB3	1.96	0.47
1:A:546:VAL:HG23	1:A:577:ILE:HD12	1.97	0.47
2:B:445:LYS:HG3	2:B:446:LEU:HG	1.97	0.47
1:A:848:ILE:HD11	1:A:856:THR:HG22	1.96	0.47
9:I:17:ARG:HG2	9:I:18:GLU:H	1.79	0.47
11:K:49:GLU:OE2	11:K:90:ALA:HB1	2.15	0.47
10:J:9:SER:OG	10:J:45:CYS:HB2	2.14	0.47
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.80	0.46
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.81	0.46
8:H:99:GLY:HA3	8:H:118:PHE:CD1	2.47	0.46
1:A:940:ARG:HE	1:A:944:ARG:HH21	1.63	0.46
4:D:192:LYS:HA	4:D:207:LEU:HD23	1.97	0.46
5:E:40:GLU:HA	5:E:43:LYS:HG2	1.97	0.46
1:A:1199:ARG:HD2	1:A:1236:LEU:HD11	1.97	0.46
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.75	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.97	0.46
1:A:1331:SER:O	1:A:1335:ILE:HD12	2.16	0.46
1:A:1433:MET:HB2	2:B:1148:LYS:HD3	1.97	0.46
2:B:83:ASN:O	2:B:142:VAL:HG12	2.15	0.46
2:B:173:MET:HE3	2:B:173:MET:HB3	1.76	0.46
2:B:1194:ILE:HG22	2:B:1196:ILE:HG23	1.98	0.46
7:G:38:CYS:HB3	7:G:157:ILE:HG12	1.98	0.46
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.31	0.46
2:B:848:ARG:HH22	2:B:996:ARG:HE	1.64	0.46
9:I:25:LEU:HG	9:I:38:ALA:HB3	1.97	0.46
10:J:10:CYS:HB3	10:J:45:CYS:SG	2.56	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.46
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.51	0.46
7:G:91:VAL:HG21	7:G:143:ILE:HD12	1.97	0.46
1:A:881:GLN:NE2	1:A:960:ILE:H	2.14	0.46
1:A:1345:ARG:HD2	1:A:1376:THR:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LEU:HD11	12:L:55:ILE:HD12	1.97	0.46
7:G:131:GLN:H	7:G:135:ASP:HB3	1.81	0.46
2:B:952:VAL:HG13	2:B:966:VAL:HG12	1.98	0.46
3:C:251:LEU:HD22	11:K:98:LEU:HD21	1.98	0.46
11:K:50:LEU:HD13	11:K:90:ALA:HB2	1.98	0.46
1:A:43:GLU:HG2	1:A:44:THR:H	1.80	0.45
1:A:101:LYS:HG2	1:A:139:TRP:CE2	2.51	0.45
1:A:448:PRO:HB2	2:B:1133:MET:HE1	1.97	0.45
2:B:209:GLU:CD	2:B:788:ARG:HH22	2.23	0.45
2:B:848:ARG:NH2	2:B:996:ARG:HE	2.14	0.45
6:F:98:ALA:O	6:F:102:SER:HB2	2.16	0.45
8:H:129:TYR:CZ	8:H:130:ARG:HD2	2.52	0.45
1:A:254:GLU:HG2	1:A:255:SER:N	2.31	0.45
2:B:834:ASN:HB3	2:B:840:ILE:HD12	1.99	0.45
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	1.98	0.45
2:B:780:VAL:HG12	2:B:795:ILE:HG23	1.98	0.45
2:B:916:THR:HB	2:B:935:ARG:HB3	1.99	0.45
3:C:240:VAL:HA	3:C:243:VAL:HG22	1.99	0.45
1:A:43:GLU:HG2	1:A:44:THR:N	2.31	0.45
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.98	0.45
1:A:266:LEU:HA	1:A:269:ILE:HG22	1.98	0.45
1:A:503:GLN:HG2	6:F:90:ARG:HH12	1.81	0.45
1:A:675:THR:O	1:A:679:ILE:HG12	2.17	0.45
2:B:116:GLU:O	2:B:120:ARG:HB2	2.16	0.45
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.97	0.45
2:B:802:PRO:HB3	2:B:983:ARG:HH12	1.81	0.45
9:I:63:GLY:HA3	9:I:104:LEU:HD21	1.99	0.45
3:C:41:ILE:HD13	3:C:246:ARG:HB3	1.97	0.45
4:D:67:ARG:HB2	4:D:129:LEU:HD11	1.99	0.45
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.98	0.45
1:A:827:THR:HA	1:A:830:LYS:HG2	1.99	0.45
2:B:803:LEU:HD22	10:J:52:THR:HG21	1.99	0.45
1:A:894:GLU:O	1:A:898:ARG:HB3	2.17	0.44
7:G:121:PHE:HA	7:G:131:GLN:HE21	1.81	0.44
1:A:1107:VAL:HA	1:A:1108:ALA:HB3	1.99	0.44
2:B:530:GLY:O	2:B:531:GLN:HG3	2.16	0.44
5:E:95:THR:HA	5:E:98:ILE:HG12	1.99	0.44
6:F:103:MET:HE1	7:G:15:PRO:HD2	1.99	0.44
1:A:631:HIS:O	1:A:635:ARG:HG2	2.17	0.44
1:A:1100:ARG:O	1:A:1104:ILE:HD12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:ILE:HG13	4:D:145:MET:HE2	1.97	0.44
5:E:55:ARG:HD2	5:E:84:ASP:HA	1.99	0.44
1:A:806:ARG:HD3	2:B:728:ARG:HA	1.99	0.44
1:A:983:ILE:HD13	1:A:986:ILE:HD11	1.99	0.44
2:B:521:LEU:HD12	2:B:635:ARG:HD3	1.98	0.44
2:B:827:ILE:HA	2:B:1012:ILE:HG23	1.99	0.44
5:E:165:LEU:HD13	5:E:170:LEU:HB2	1.98	0.44
8:H:6:PHE:O	8:H:58:THR:HA	2.17	0.44
1:A:248:PRO:HG3	2:B:1114:LEU:HB2	1.99	0.44
2:B:438:GLU:HA	2:B:439:ALA:HA	1.64	0.44
3:C:103:ALA:HB3	3:C:153:LEU:HB3	1.99	0.44
1:A:343:LYS:HG3	2:B:1151:LEU:HD12	1.99	0.44
7:G:115:MET:HE3	7:G:116:PRO:HD2	2.00	0.44
1:A:850:VAL:HG23	1:A:1061:GLY:H	1.83	0.44
1:A:957:PRO:HG2	1:A:1018:PHE:CD1	2.53	0.44
2:B:1099:VAL:O	2:B:1103:ILE:HG12	2.18	0.44
7:G:85:GLU:HG3	7:G:86:VAL:H	1.83	0.44
8:H:115:TYR:HE1	8:H:124:ARG:HD3	1.83	0.44
1:A:1111:MET:HE1	1:A:1330:ASN:HB3	1.99	0.43
4:D:182:SER:HB3	7:G:87:VAL:HG12	1.99	0.43
7:G:146:LYS:H	7:G:163:ILE:HG22	1.82	0.43
2:B:341:LEU:HD23	2:B:344:LYS:HG3	1.99	0.43
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.99	0.43
5:E:165:LEU:HD11	5:E:172:GLU:H	1.82	0.43
1:A:5:GLN:HG3	2:B:1175:LEU:HG	2.01	0.43
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.43
4:D:54:GLU:HB2	4:D:164:ILE:HD13	1.99	0.43
5:E:65:THR:O	5:E:69:ILE:HD12	2.19	0.43
1:A:744:LYS:O	1:A:748:MET:HG2	2.18	0.43
1:A:1041:ALA:O	1:A:1045:VAL:HG13	2.19	0.43
2:B:848:ARG:NH2	2:B:996:ARG:HH21	2.14	0.43
6:F:86:THR:HG23	6:F:89:GLU:H	1.82	0.43
1:A:243:PRO:O	1:A:246:VAL:HG12	2.18	0.43
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.99	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
4:D:71:LYS:HA	4:D:74:GLN:HB2	2.00	0.43
2:B:130:VAL:HB	2:B:167:ILE:HG13	1.99	0.43
1:A:550:LEU:HD12	1:A:556:TRP:NE1	2.34	0.43
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.19	0.43
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.54	0.43
3:C:8:VAL:HG12	3:C:22:LEU:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:LEU:HD13	7:G:162:SER:HA	2.00	0.43
11:K:45:LEU:O	11:K:49:GLU:HG3	2.18	0.43
1:A:846:GLU:HB3	1:A:1424:VAL:HG11	2.00	0.43
1:A:983:ILE:HD11	1:A:1032:LEU:HD11	1.99	0.43
1:A:1017:LEU:HD23	1:A:1017:LEU:HA	1.82	0.43
2:B:100:PRO:HG3	2:B:124:TYR:CZ	2.54	0.43
6:F:112:GLU:HG2	6:F:123:LYS:HZ2	1.83	0.43
2:B:1205:GLN:HA	2:B:1208:MET:SD	2.59	0.43
2:B:877:PRO:HB3	2:B:882:THR:HG21	2.01	0.43
1:A:134:ARG:HH21	1:A:223:GLY:HA2	1.84	0.42
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.67	0.42
1:A:405:VAL:HG22	1:A:432:VAL:HG22	2.01	0.42
1:A:746:MET:HE3	2:B:1018:PRO:HG2	2.00	0.42
1:A:899:VAL:HG21	1:A:908:LEU:HD23	2.00	0.42
1:A:1059:HIS:CE1	6:F:155:LEU:HD13	2.54	0.42
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.01	0.42
2:B:744:HIS:HB3	2:B:747:MET:HG2	2.01	0.42
3:C:242:GLN:O	3:C:246:ARG:HB2	2.19	0.42
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.72	0.42
1:A:419:LYS:HG3	1:A:420:ARG:HG2	2.01	0.42
2:B:47:GLN:HE22	2:B:173:MET:HG3	1.84	0.42
2:B:898:LEU:HD11	2:B:964:VAL:HG11	2.01	0.42
5:E:93:MET:HE2	5:E:93:MET:HB2	1.97	0.42
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.59	0.42
1:A:172:PRO:HB2	1:A:184:SER:H	1.85	0.42
1:A:490:HIS:HB3	2:B:1150:ARG:HH12	1.85	0.42
1:A:1100:ARG:HH22	1:A:1111:MET:HE3	1.84	0.42
2:B:824:ILE:HA	2:B:1089:PRO:HA	2.01	0.42
3:C:34:ARG:HG2	3:C:176:ILE:HD13	2.00	0.42
1:A:90:VAL:HG21	1:A:300:VAL:HG11	2.01	0.42
1:A:958:VAL:HG21	1:A:1052:GLN:HB3	2.01	0.42
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.54	0.42
5:E:110:PHE:HE1	5:E:112:TYR:HB3	1.84	0.42
2:B:582:VAL:HB	2:B:587:HIS:CE1	2.54	0.42
1:A:55:ASP:HA	1:A:58:LEU:HD23	2.02	0.42
2:B:383:ASN:O	2:B:387:LEU:HD23	2.20	0.42
1:A:613:ILE:HG22	1:A:614:PHE:HD2	1.85	0.42
5:E:179:GLN:HG3	5:E:181:ALA:H	1.85	0.42
8:H:4:THR:HA	8:H:60:ALA:HA	2.02	0.42
1:A:549:MET:HB3	1:A:652:VAL:HG23	2.01	0.42
3:C:142:VAL:HG21	10:J:5:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:HD2	3:C:148:ARG:O	2.20	0.42
4:D:150:ASN:HA	4:D:155:ARG:HG3	2.01	0.42
1:A:564:ALA:O	8:H:97:MET:HG2	2.20	0.42
2:B:82:ASP:O	2:B:83:ASN:HB2	2.19	0.42
2:B:408:LEU:HD23	2:B:545:ILE:HG21	2.02	0.42
4:D:184:ALA:HB3	7:G:144:ARG:HD2	2.01	0.42
9:I:65:ASP:HB3	9:I:68:LEU:HD23	2.01	0.42
2:B:147:LEU:O	2:B:148:LYS:HG3	2.20	0.41
2:B:284:ILE:HG12	2:B:324:ILE:HD12	2.01	0.41
2:B:755:ILE:HA	2:B:809:MET:SD	2.60	0.41
3:C:41:ILE:CD1	3:C:246:ARG:HB3	2.50	0.41
8:H:58:THR:HG23	8:H:143:LEU:HD12	2.01	0.41
8:H:135:LEU:HB3	8:H:137:GLN:HG2	2.02	0.41
1:A:943:LEU:HA	1:A:946:VAL:HG12	2.02	0.41
1:A:1361:SER:HA	1:A:1362:TYR:HA	1.65	0.41
5:E:154:ILE:HG23	5:E:197:LYS:HB3	2.02	0.41
7:G:44:TYR:CZ	7:G:79:PHE:HB3	2.55	0.41
8:H:145:ARG:HD3	8:H:145:ARG:HA	1.78	0.41
1:A:545:GLN:O	1:A:549:MET:HG2	2.20	0.41
1:A:825:ILE:HD13	2:B:533:CYS:HB2	2.02	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.01	0.41
3:C:69:LEU:HG	10:J:6:ARG:HD2	2.02	0.41
5:E:91:LYS:HD3	5:E:91:LYS:HA	1.87	0.41
8:H:39:THR:HB	8:H:124:ARG:HB3	2.02	0.41
1:A:70:CYS:HB3	2:B:1172:ILE:HD11	2.03	0.41
1:A:80:HIS:O	1:A:243:PRO:HB3	2.20	0.41
1:A:977:LYS:HA	1:A:977:LYS:HD3	1.76	0.41
3:C:102:GLN:HE22	3:C:154:LYS:HE2	1.85	0.41
4:D:154:PHE:H	4:D:160:VAL:HG21	1.86	0.41
7:G:9:LEU:HD23	7:G:11:ILE:HD11	2.03	0.41
7:G:14:HIS:HA	7:G:15:PRO:HD3	1.94	0.41
7:G:97:HIS:HB2	7:G:112:LYS:HD2	2.03	0.41
7:G:97:HIS:HA	7:G:125:SER:HA	2.01	0.41
7:G:128:PRO:HG2	7:G:170:ALA:HB3	2.02	0.41
8:H:81:PRO:HD2	11:K:57:LEU:HD22	2.03	0.41
1:A:239:LEU:HD12	1:A:240:PRO:HD2	2.02	0.41
6:F:109:VAL:HG21	6:F:124:GLU:HA	2.03	0.41
1:A:1313:LEU:HD11	1:A:1329:THR:HG21	2.03	0.41
2:B:834:ASN:HD22	2:B:1011:ILE:HG22	1.85	0.41
2:B:344:LYS:HA	2:B:344:LYS:HD3	1.92	0.41
2:B:976:ILE:HD12	2:B:992:ILE:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:GLN:HA	5:E:35:VAL:HG22	2.02	0.41
7:G:23:LYS:HE3	7:G:27:LYS:HE3	2.01	0.41
1:A:632:VAL:HG13	1:A:962:ARG:HD3	2.03	0.41
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.57	0.41
2:B:1203:LEU:O	2:B:1207:LEU:HB2	2.21	0.41
3:C:258:ILE:HG12	11:K:35:PHE:HE2	1.86	0.41
2:B:58:THR:O	2:B:62:ILE:HG12	2.21	0.40
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.03	0.40
7:G:84:GLY:H	7:G:148:GLU:HG3	1.85	0.40
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.03	0.40
2:B:708:GLU:HA	2:B:711:GLU:HG2	2.02	0.40
2:B:1072:MET:HE1	2:B:1087:PHE:CD1	2.56	0.40
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.40
1:A:825:ILE:HD11	2:B:512:ARG:HD3	2.02	0.40
1:A:1276:VAL:HB	1:A:1279:ILE:HD12	2.04	0.40
2:B:67:SER:HA	2:B:92:PHE:HD2	1.87	0.40
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.57	0.40
3:C:183:TRP:CE2	3:C:207:CYS:HB2	2.57	0.40
4:D:16:LYS:HB2	4:D:16:LYS:HE3	1.83	0.40
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.36	0.40
1:A:549:MET:HB2	1:A:577:ILE:HD11	2.02	0.40
1:A:666:ILE:HG21	2:B:1052:VAL:HG21	2.02	0.40
1:A:1022:LEU:HD12	1:A:1026:LEU:HD23	2.03	0.40
2:B:551:PRO:O	2:B:554:ILE:HG12	2.20	0.40
2:B:867:GLY:HA3	2:B:868:MET:C	2.47	0.40
2:B:1139:ILE:HD13	2:B:1139:ILE:HA	1.87	0.40
8:H:38:LEU:HD21	8:H:40:LEU:HB2	2.04	0.40
8:H:103:LYS:HB3	8:H:115:TYR:HB2	2.03	0.40
8:H:135:LEU:HG	8:H:136:LYS:H	1.86	0.40
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.35	0.40
2:B:1010:LEU:HD11	2:B:1092:TYR:CE2	2.57	0.40
2:B:1152:MET:SD	2:B:1157:ALA:HA	2.62	0.40
8:H:146:ARG:HA	8:H:146:ARG:HD2	1.85	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	1417/1733 (82%)	1296 (92%)	120 (8%)	1 (0%)	48	76
2	B	1142/1224 (93%)	1031 (90%)	106 (9%)	5 (0%)	30	60
3	C	263/318 (83%)	243 (92%)	20 (8%)	0	100	100
4	D	164/221 (74%)	139 (85%)	24 (15%)	1 (1%)	21	52
5	E	212/215 (99%)	197 (93%)	15 (7%)	0	100	100
6	F	85/155 (55%)	76 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	150 (89%)	19 (11%)	0	100	100
8	H	132/146 (90%)	121 (92%)	11 (8%)	0	100	100
9	I	112/122 (92%)	106 (95%)	6 (5%)	0	100	100
10	J	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
11	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
12	L	42/70 (60%)	29 (69%)	13 (31%)	0	100	100
All	All	3915/4565 (86%)	3557 (91%)	351 (9%)	7 (0%)	44	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	PRO
2	B	78	THR
2	B	82	ASP
4	D	162	ALA
2	B	80	GLU
2	B	143	PRO
2	B	472	ALA

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	1240/1520 (82%)	1240 (100%)	0	100	100
2	B	999/1061 (94%)	999 (100%)	0	100	100
3	C	233/274 (85%)	233 (100%)	0	100	100
4	D	146/200 (73%)	146 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	108/116 (93%)	108 (100%)	0	100	100
10	J	61/65 (94%)	61 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3469/4009 (86%)	3469 (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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	313	GLN
1	A	471	ASN
1	A	587	HIS
1	A	603	ASN
1	A	742	ASN
1	A	745	GLN
1	A	760	GLN
1	A	838	GLN
1	A	862	ASN
1	A	881	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	906	HIS
1	A	1059	HIS
1	A	1232	ASN
1	A	1278	ASN
2	B	76	GLN
2	B	278	GLN
2	B	366	GLN
2	B	415	GLN
2	B	1112	GLN
3	C	102	GLN
3	C	242	GLN
5	E	5	ASN
5	E	101	GLN
5	E	106	GLN
5	E	179	GLN
8	H	137	GLN
10	J	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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.

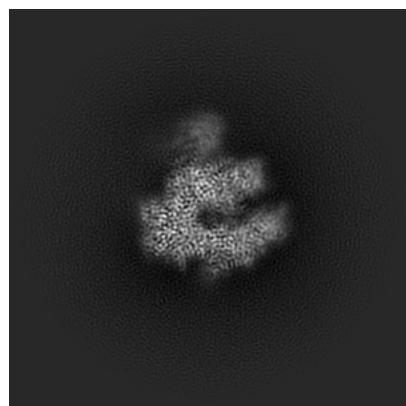
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74528. These allow visual inspection of the internal detail of the map and identification of artifacts.

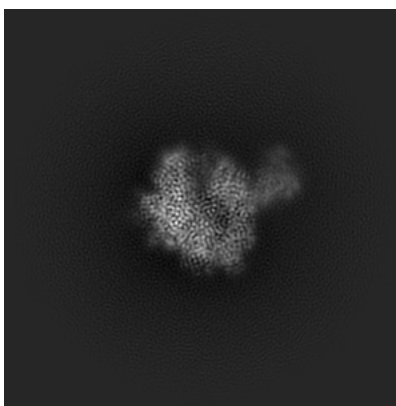
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

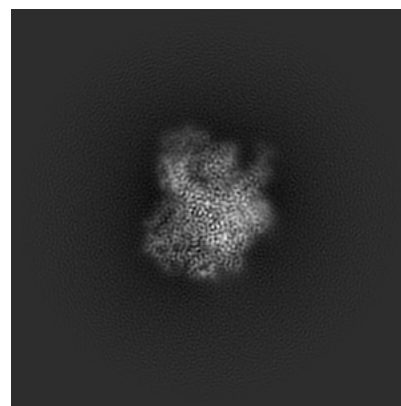
6.1.1 Primary map



X

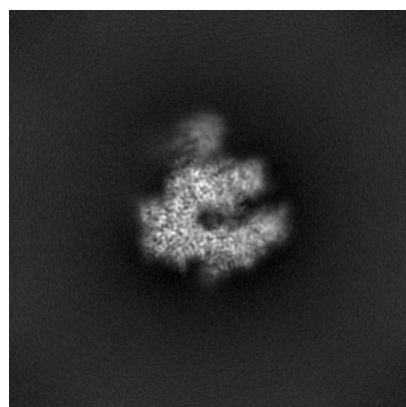


Y

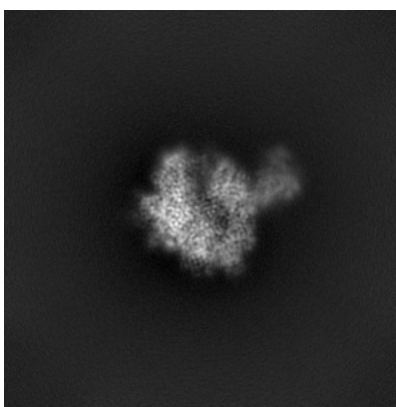


Z

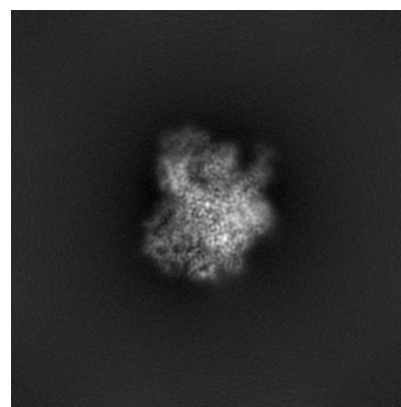
6.1.2 Raw map



X



Y

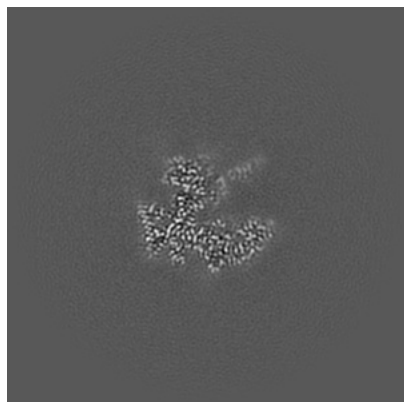


Z

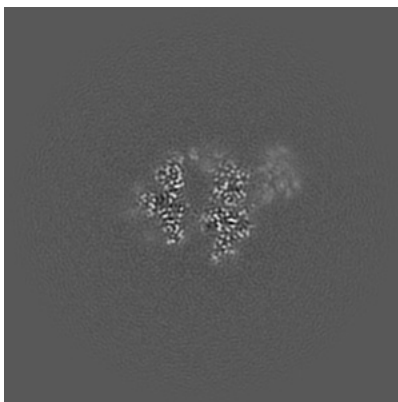
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

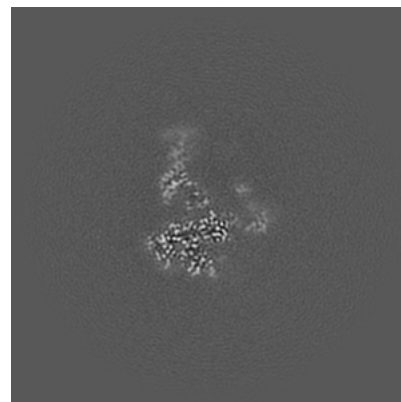
6.2.1 Primary map



X Index: 200

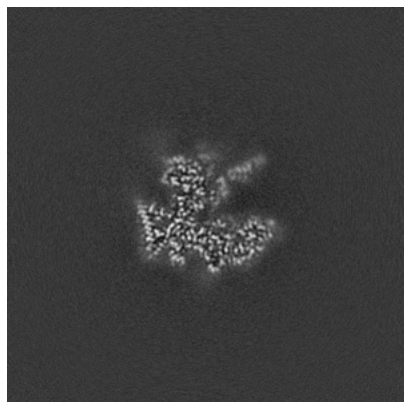


Y Index: 200

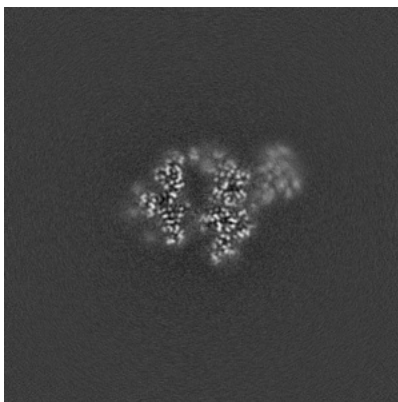


Z Index: 200

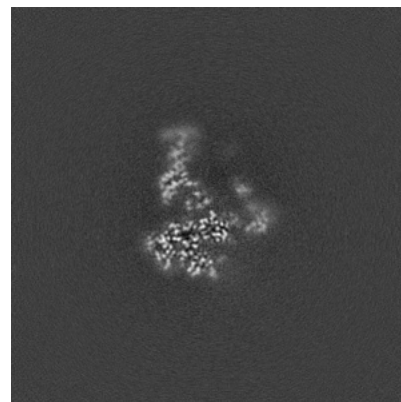
6.2.2 Raw map



X Index: 200



Y Index: 200

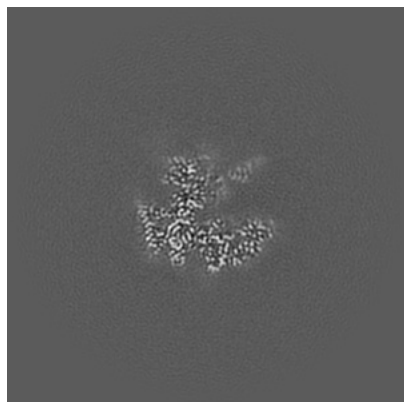


Z Index: 200

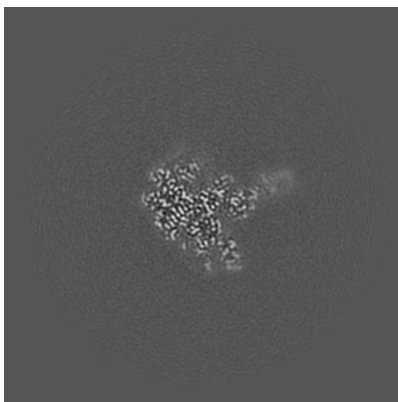
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

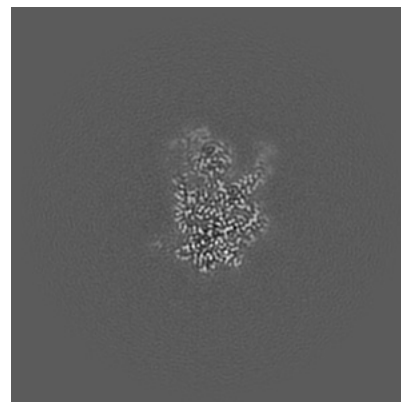
6.3.1 Primary map



X Index: 201

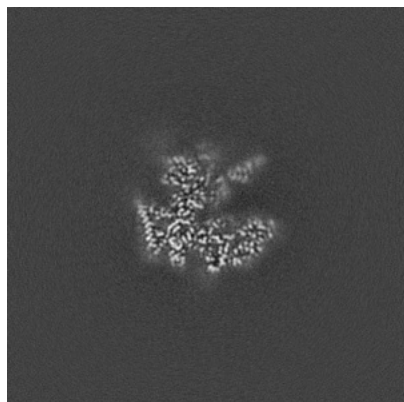


Y Index: 173

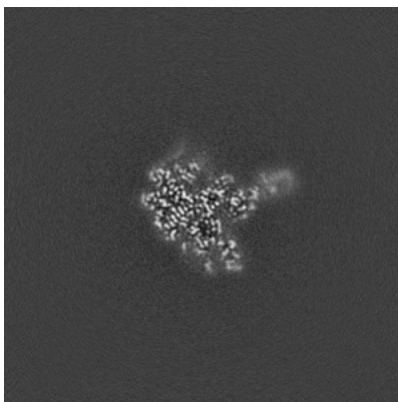


Z Index: 175

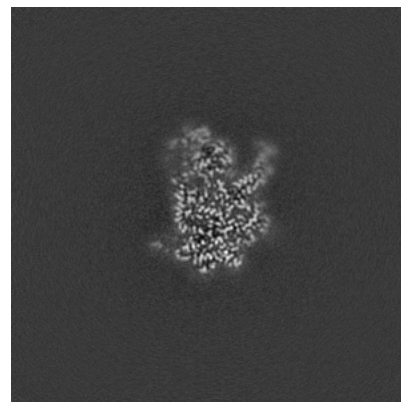
6.3.2 Raw map



X Index: 201



Y Index: 173

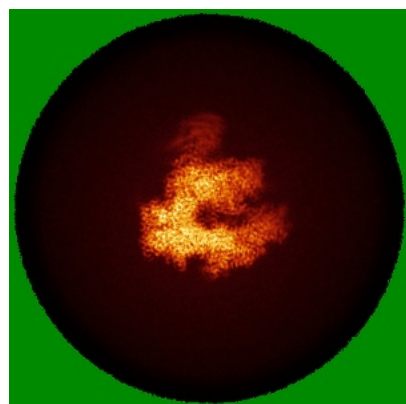


Z Index: 175

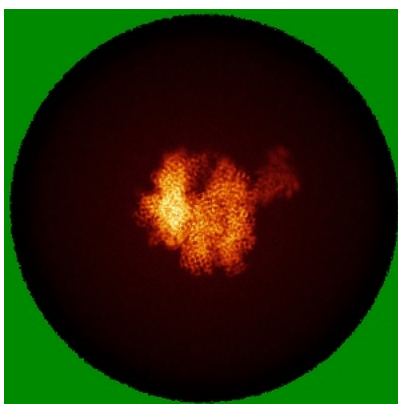
The images above show the largest variance slices of the map in three orthogonal directions.

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

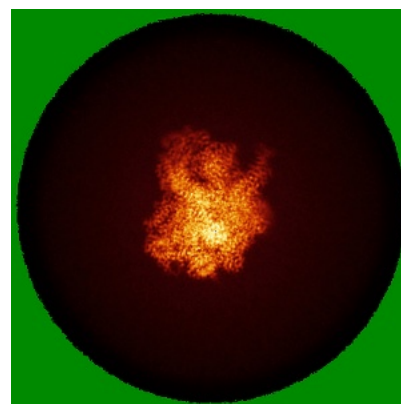
6.4.1 Primary map



X

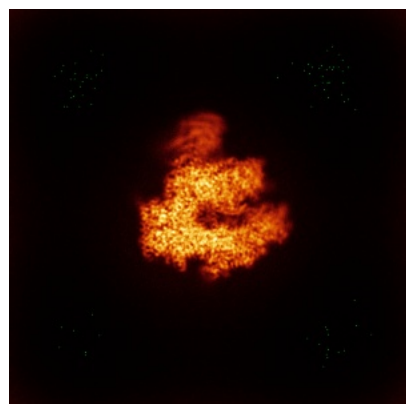


Y

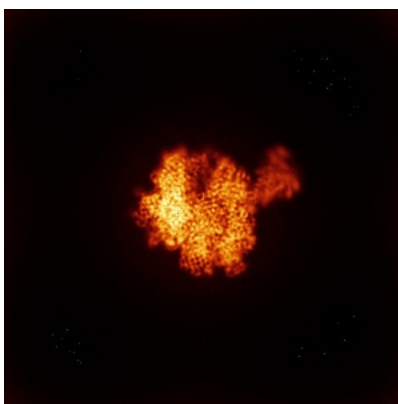


Z

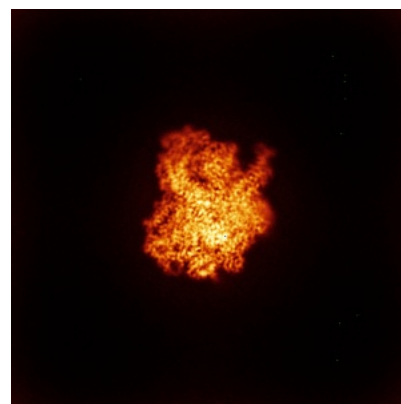
6.4.2 Raw map



X



Y



Z

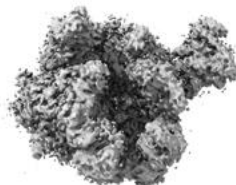
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

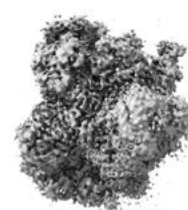
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



X



Y



Z

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.

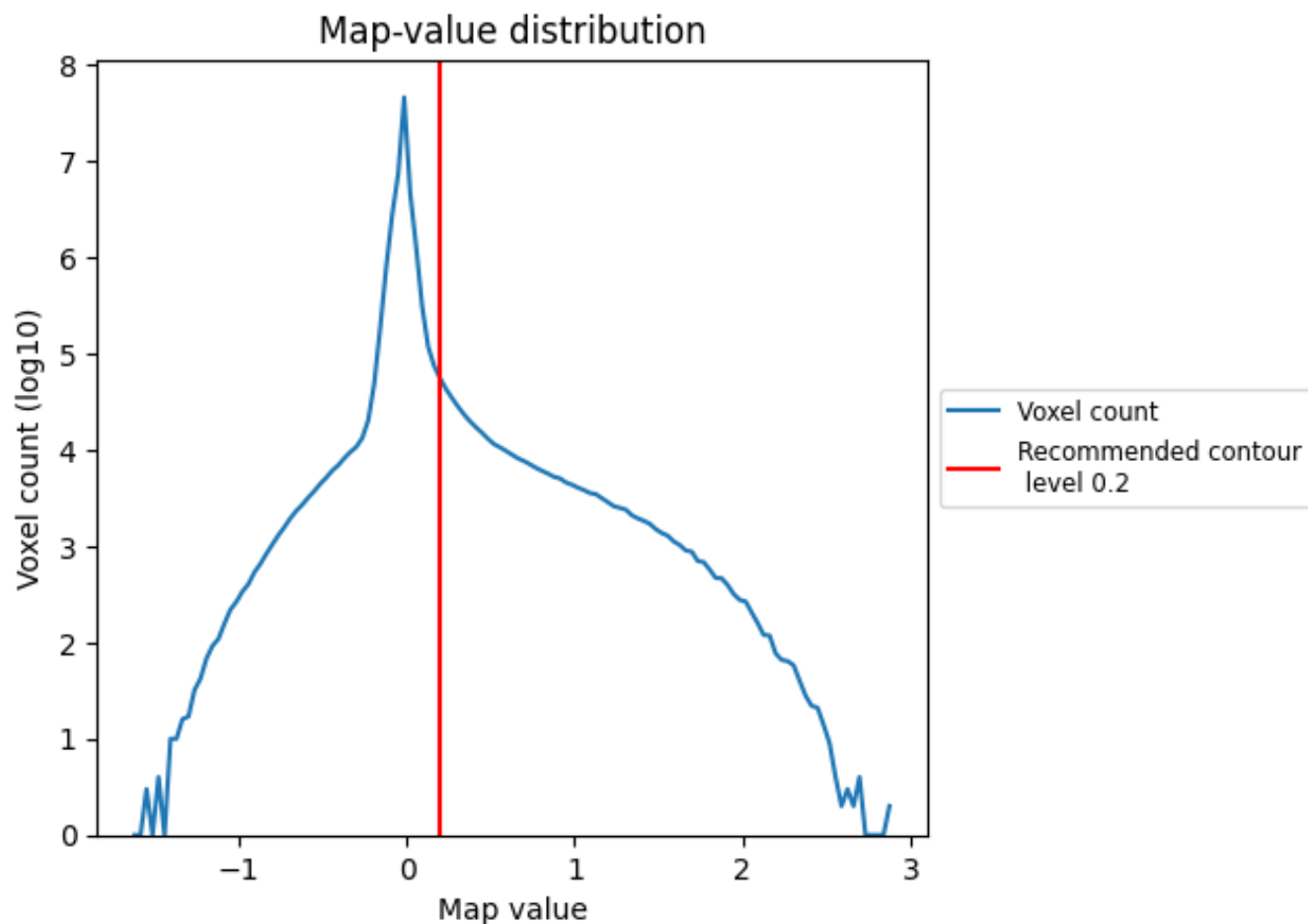
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

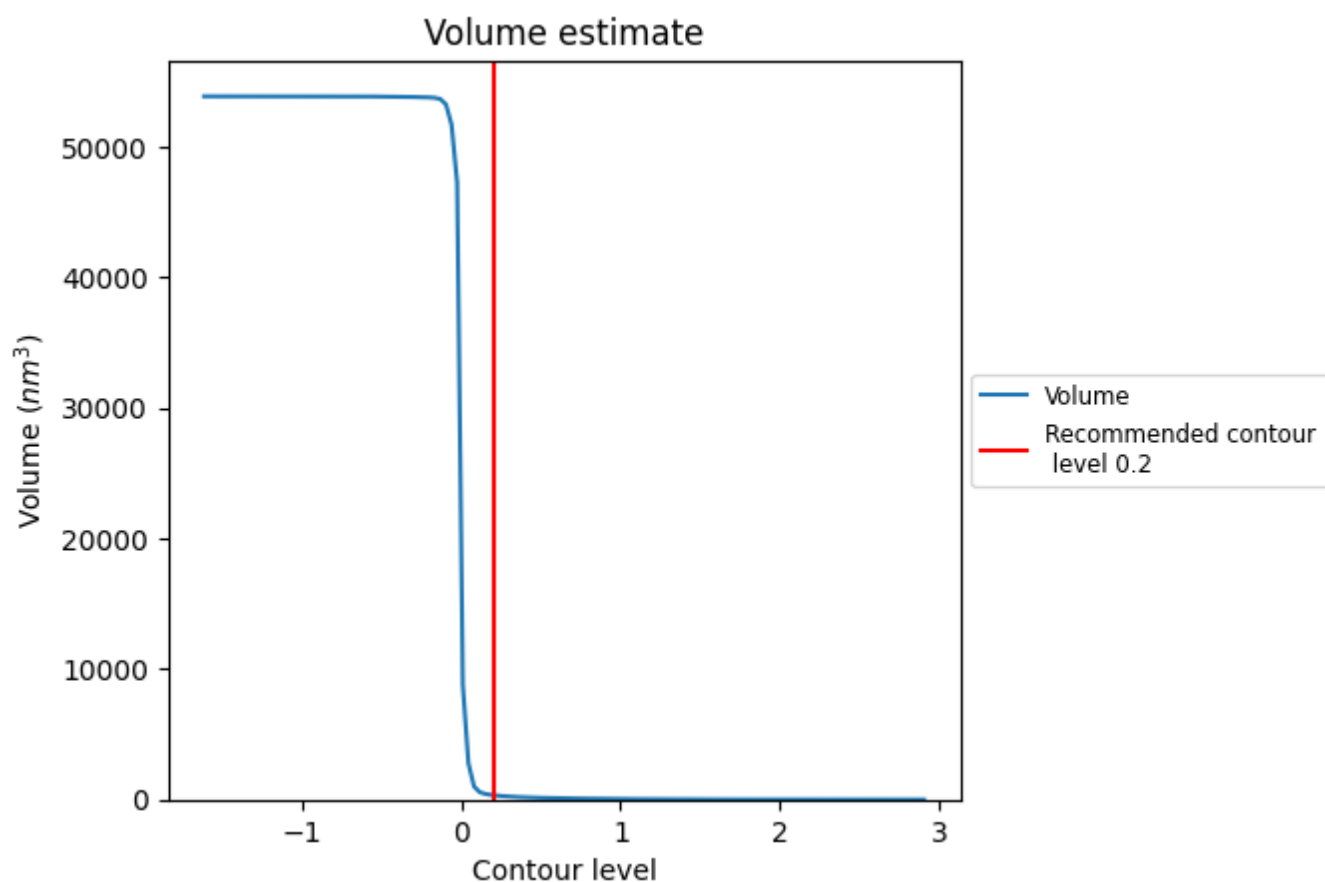
This section contains the results of statistical analysis of the map.

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.

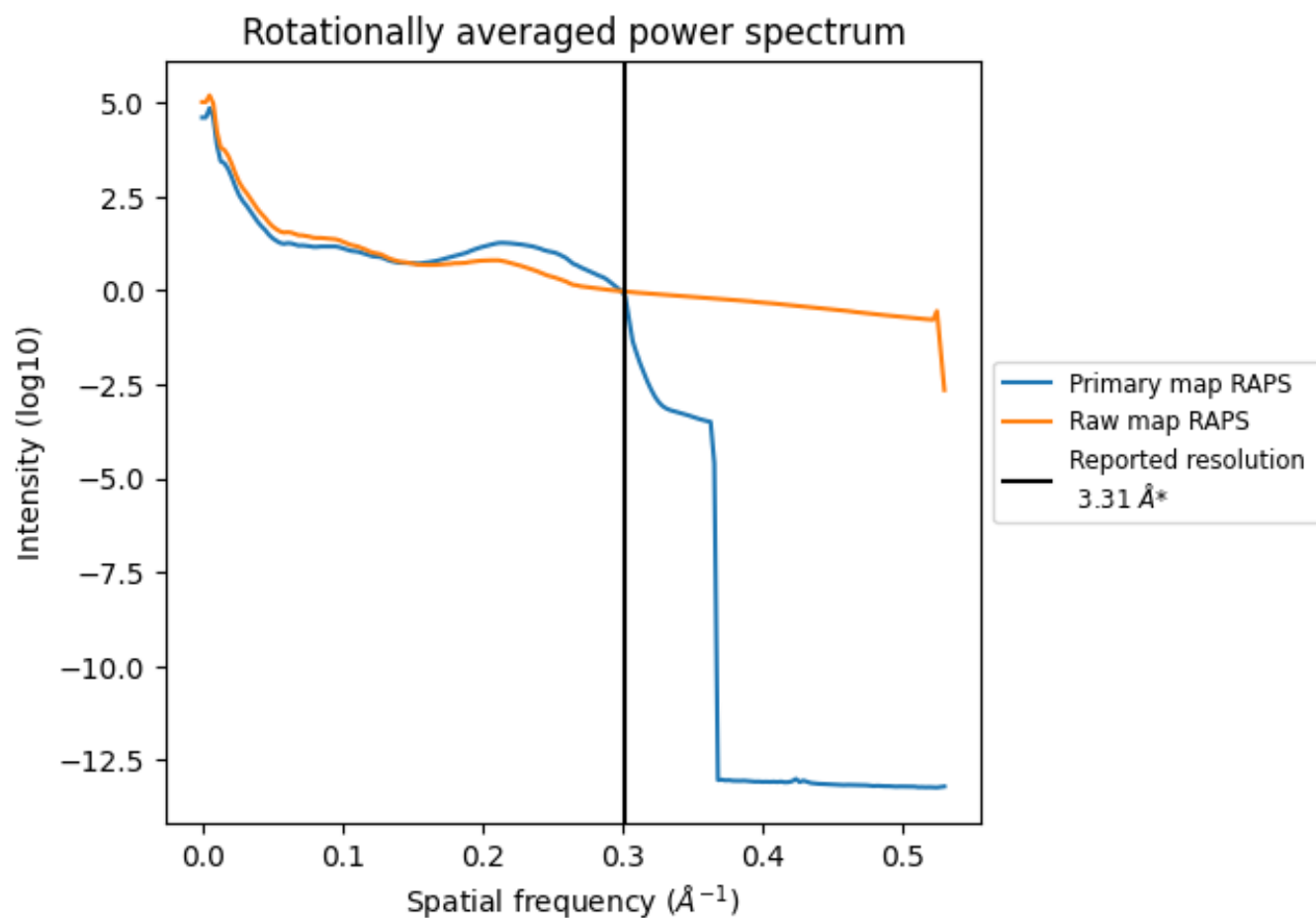
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm^3 ; this corresponds to an approximate mass of 305 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 ⓘ

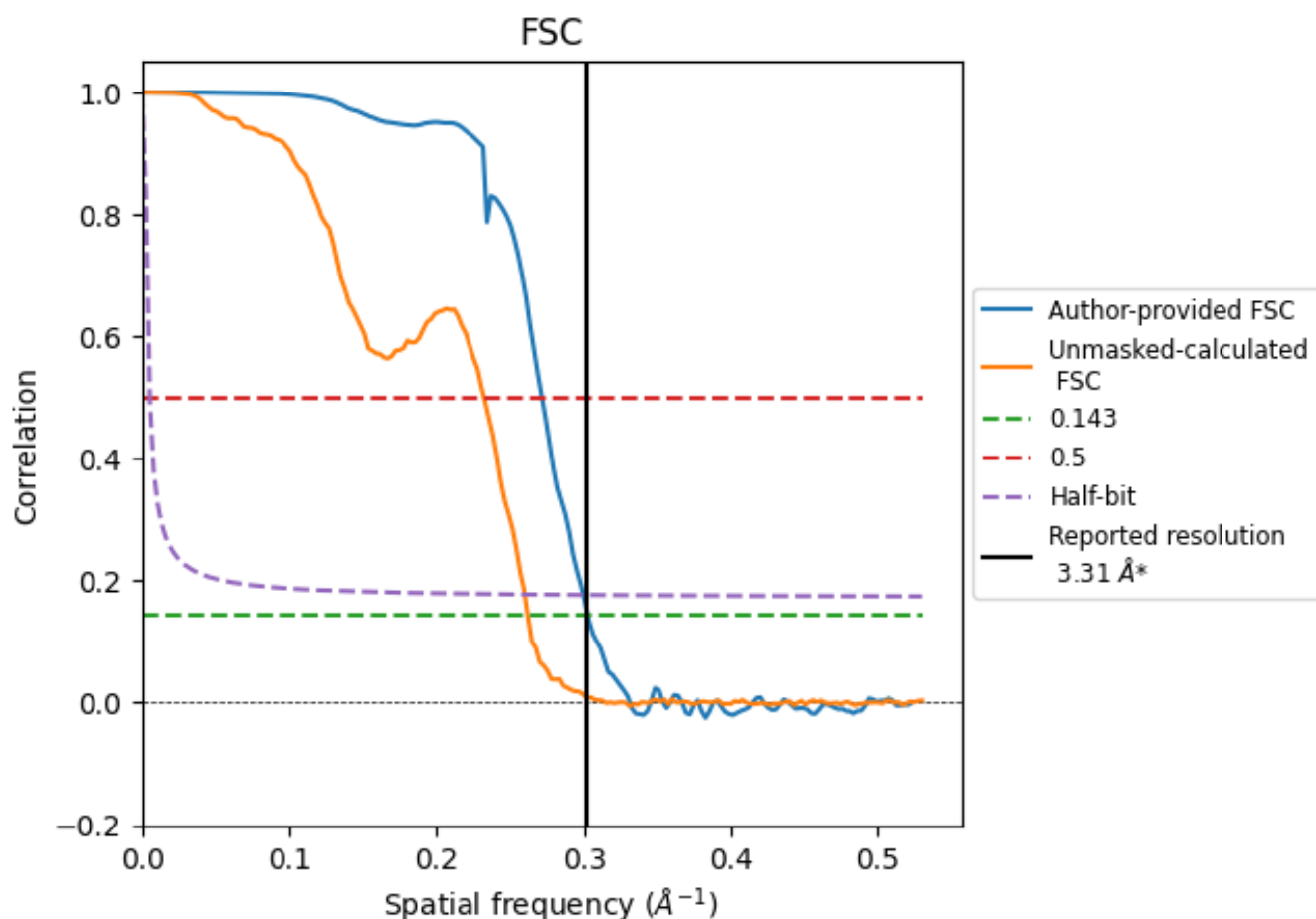


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

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 0.302 Å⁻¹

8.2 Resolution estimates [i](#)

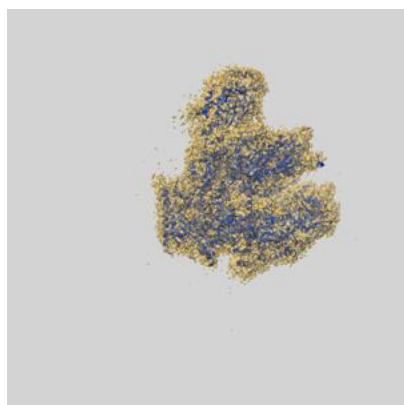
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.68	3.34
Unmasked-calculated*	3.82	4.31	3.85

*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 3.82 differs from the reported value 3.31 by more than 10 %

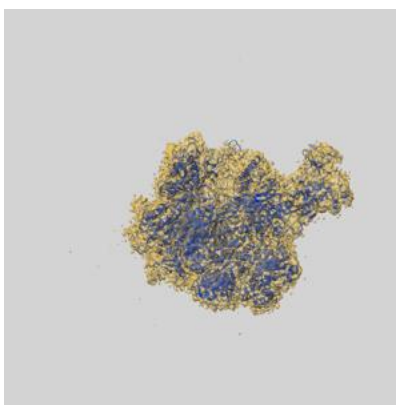
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74528 and PDB model 9ZPK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

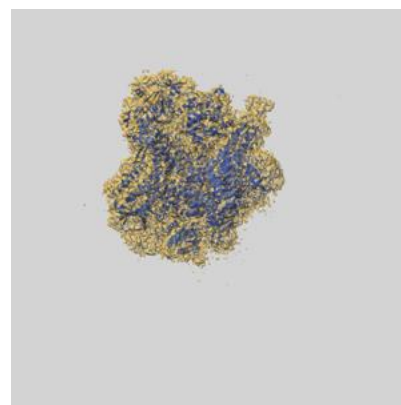
9.1 Map-model overlay [i](#)



X



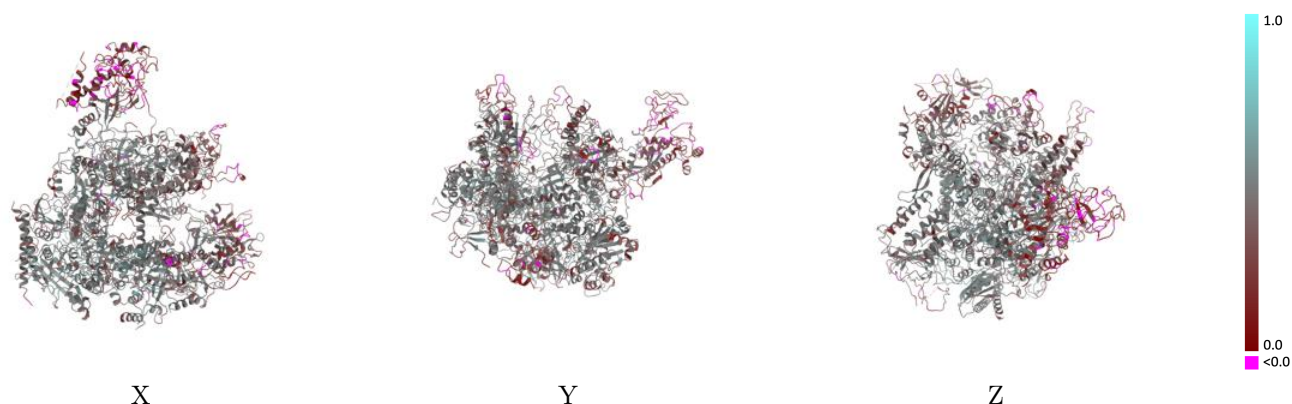
Y



Z

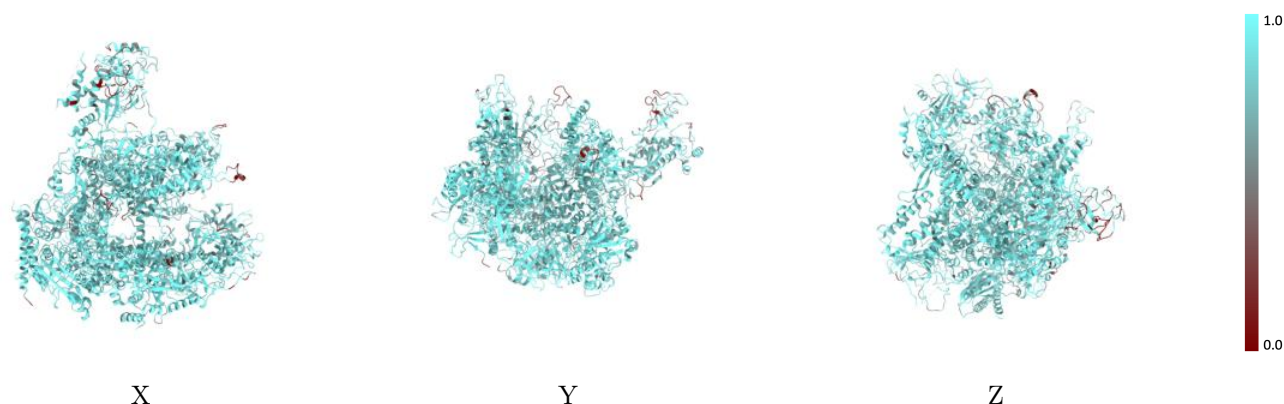
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



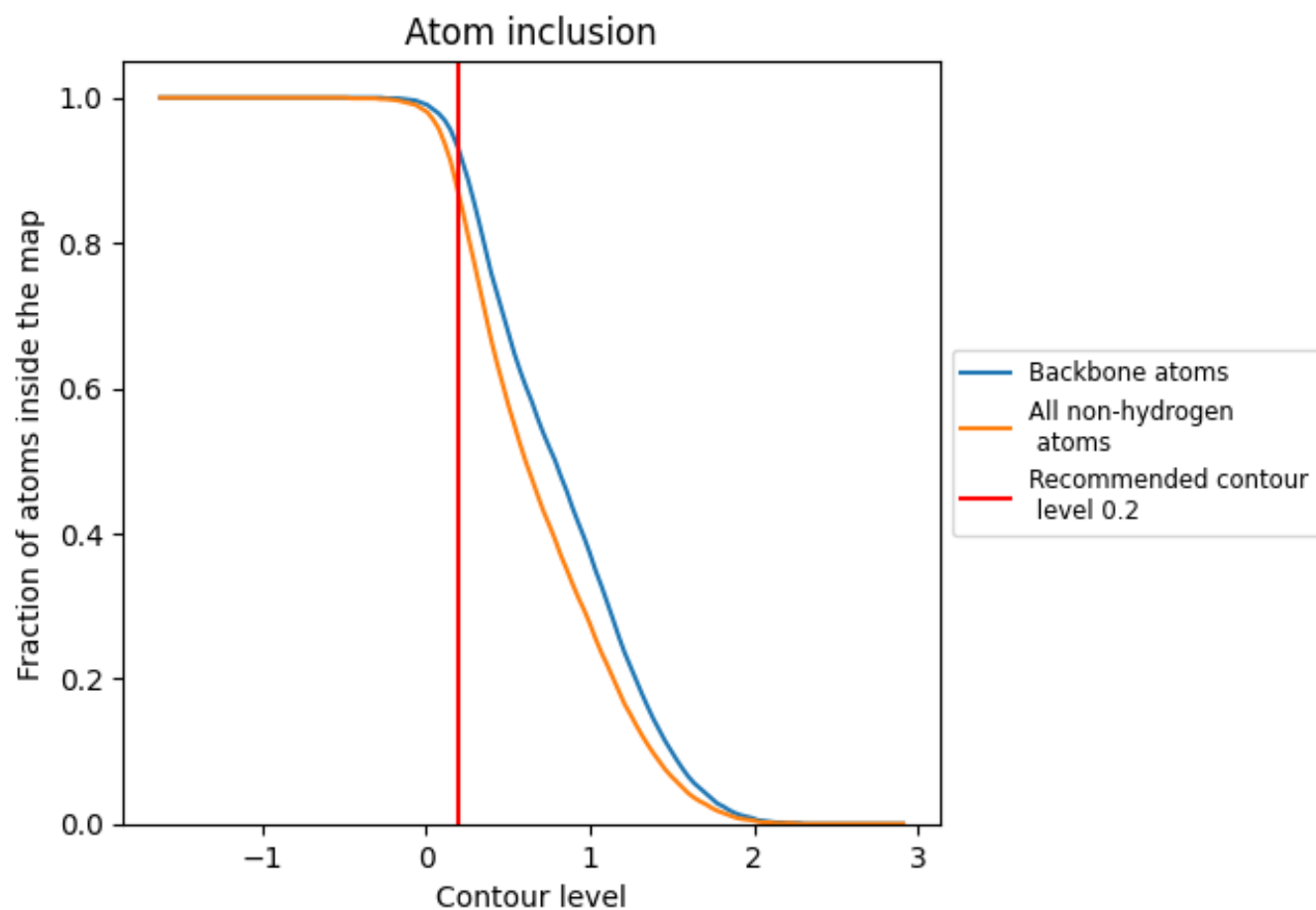
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.4180
A	 0.8700	 0.4250
B	 0.8810	 0.4400
C	 0.9120	 0.4820
D	 0.7650	 0.1970
E	 0.8960	 0.4270
F	 0.8790	 0.4570
G	 0.7540	 0.2890
H	 0.8660	 0.4100
I	 0.8760	 0.3840
J	 0.9240	 0.4910
K	 0.8530	 0.4410
L	 0.8680	 0.3800

