



Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 04:37 PM EDT

PDB ID : 9YCZ / pdb_00009ycz
EMDB ID : EMD-72792
Title : RNA polymerase II on Super pause sequence in the sidetracked state
Authors : Vazquez Nunez, R.; Vos, S.M.
Deposited on : 2025-09-20
Resolution : 2.90 Å(reported)
Based on initial model : 8A40

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:

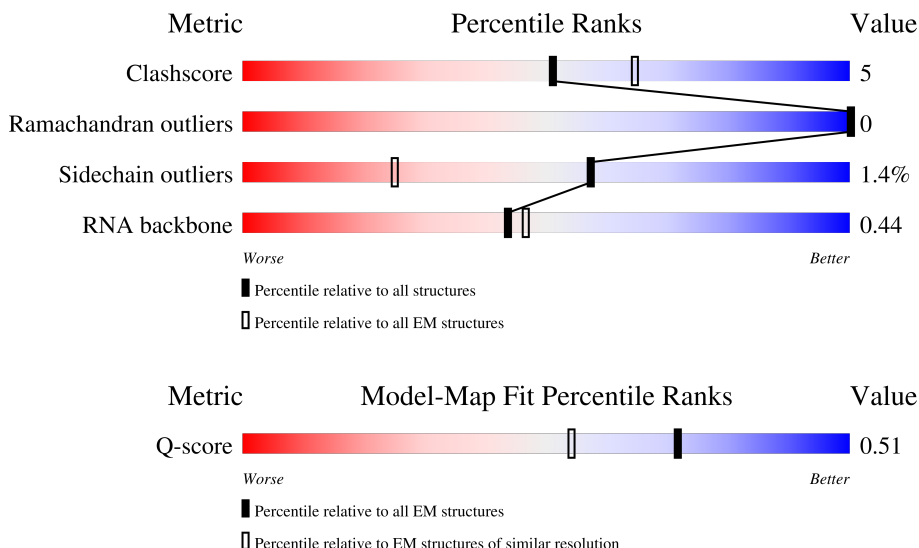
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.90 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1475	
2	B	1161	
3	C	267	

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Mol	Chain	Length	Quality of chain
4	D	128	
5	E	209	
6	F	78	
7	G	171	
8	H	148	
9	I	114	
10	J	67	
11	K	115	
12	L	44	
13	N	38	
14	P	16	
15	T	37	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31947 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1379	Total	C	N	O	S	0	0
			10950	6896	1960	2024	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1092	Total	C	N	O	S	0	0
			8739	5539	1526	1610	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	254	Total	C	N	O	S	0	0
			2038	1282	348	402	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	32	GLY	GLU	conflict	UNP A0A4X1VTX4
E	46	GLY	ASP	conflict	UNP A0A4X1VTX4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	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	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	108	Total	C	N	O	S	0	0
			877	542	158	166	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	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
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	27	Total	C	N	O	P	0	0
			549	262	98	162	27		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	16	Total	C	N	O	P	0	0
			340	151	56	117	16		

- Molecule 15 is a DNA chain called Template DNA strand.

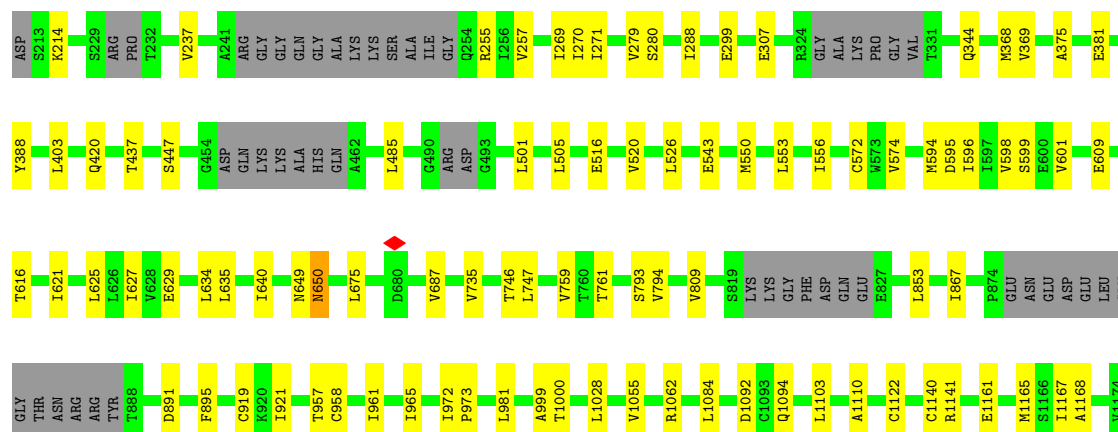
Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	37	Total	C	N	O	P	0	0
			758	359	139	223	37		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	C	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

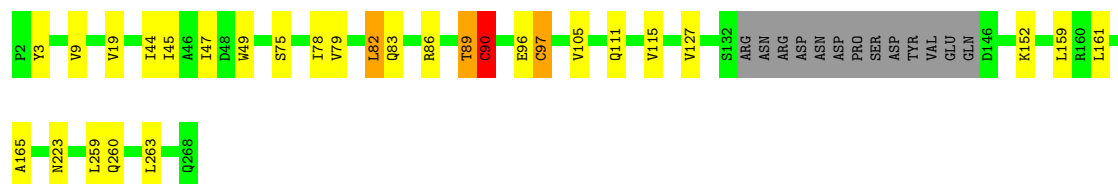
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	



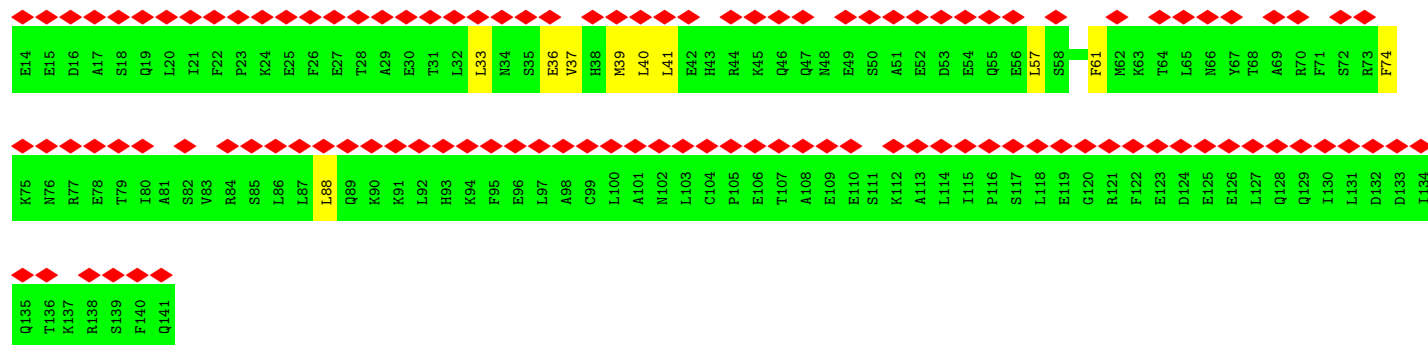
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 84% 9% 5%



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 88% 92% 8%



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 85% 14% 1%

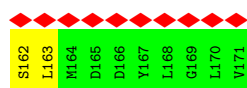
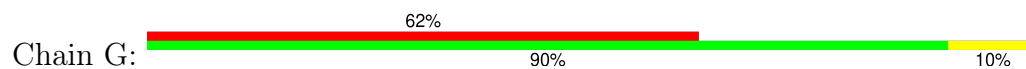


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

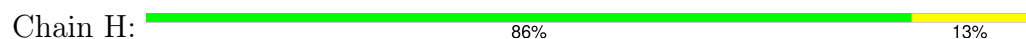
Chain F: 96% 0% 0%



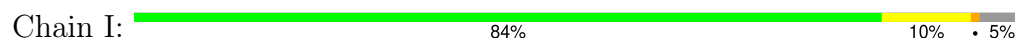
- Molecule 7: DNA-directed RNA polymerase subunit



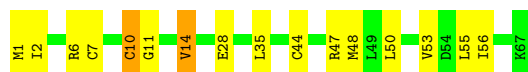
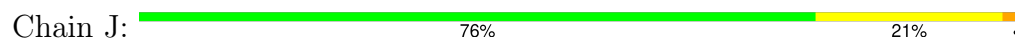
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



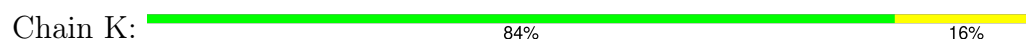
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



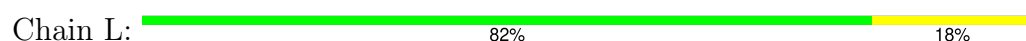
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

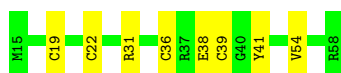


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

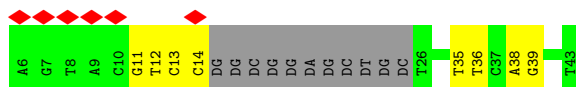


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

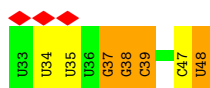




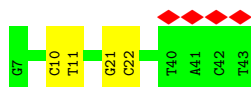
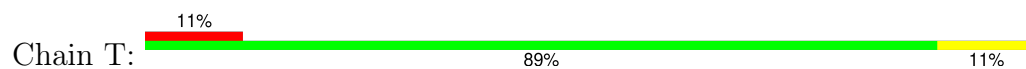
- Molecule 13: Non-template DNA strand



- Molecule 14: RNA



- Molecule 15: Template DNA strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	250	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.264	Depositor
Minimum map value	-0.143	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0289	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0/11143	0.37	3/15033 (0.0%)
2	B	0.21	0/8907	0.27	0/12021
3	C	0.25	0/2081	0.53	5/2828 (0.2%)
4	D	0.08	0/1019	0.23	0/1374
5	E	0.18	0/1742	0.28	0/2353
6	F	0.19	0/636	0.26	0/859
7	G	0.11	0/1365	0.24	0/1853
8	H	0.19	0/1207	0.26	0/1628
9	I	0.15	0/895	0.31	0/1208
10	J	0.36	0/542	0.62	2/730 (0.3%)
11	K	0.22	0/939	0.29	0/1271
12	L	0.23	0/377	0.39	0/500
13	N	0.18	0/613	0.38	0/940
14	P	0.22	0/378	0.26	0/587
15	T	0.27	0/849	0.42	0/1308
All	All	0.21	0/32693	0.34	10/44493 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	CYS	CB-CA-C	-18.17	70.57	110.19
1	A	74	CYS	N-CA-CB	-12.54	91.53	110.60
3	C	97	CYS	CB-CA-C	8.50	127.33	110.42
1	A	154	CYS	CB-CA-C	-7.73	97.71	110.85
3	C	89	THR	CA-C-N	-6.55	108.74	121.06
3	C	89	THR	C-N-CA	-6.55	108.74	121.06
10	J	10	CYS	N-CA-CB	-5.79	101.48	110.39
3	C	90	CYS	N-CA-CB	5.50	117.92	110.38
10	J	14	VAL	N-CA-C	-5.23	106.33	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	CYS	N-CA-CB	5.10	117.70	110.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10950	0	11086	152	0
2	B	8739	0	8767	81	0
3	C	2038	0	1990	26	0
4	D	1005	0	964	7	0
5	E	1711	0	1733	23	0
6	F	626	0	657	2	0
7	G	1334	0	1333	13	0
8	H	1186	0	1147	17	0
9	I	877	0	818	9	0
10	J	533	0	553	14	0
11	K	920	0	942	15	0
12	L	372	0	379	6	0
13	N	549	0	306	5	0
14	P	340	0	171	4	0
15	T	758	0	416	3	0
16	A	2	0	0	1	0
16	B	1	0	0	0	0
16	C	1	0	0	1	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31947	0	31262	346	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 5.

All (346) 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)
1:A:71:CYS:HB2	1:A:74:CYS:SG	1.26	1.67
1:A:71:CYS:CB	1:A:74:CYS:SG	2.02	1.45
1:A:114:CYS:SG	1:A:184:CYS:HB3	1.78	1.21
1:A:64:VAL:HG23	1:A:71:CYS:SG	1.96	1.05
1:A:114:CYS:SG	1:A:184:CYS:CB	2.49	1.00
2:B:1122:CYS:SG	2:B:1140:CYS:SG	2.64	0.96
1:A:1189:ASP:HB2	1:A:1192:TRP:HE1	1.31	0.94
1:A:71:CYS:HB3	1:A:74:CYS:SG	2.07	0.94
1:A:74:CYS:SG	1:A:81:CYS:SG	2.68	0.92
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.13	0.89
1:A:64:VAL:CG2	1:A:71:CYS:SG	2.61	0.88
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.61	0.81
1:A:114:CYS:SG	1:A:184:CYS:SG	2.80	0.80
1:A:126:ILE:HD12	1:A:126:ILE:O	1.84	0.76
8:H:59:VAL:HG12	8:H:59:VAL:O	1.86	0.76
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.67	0.75
10:J:7:CYS:CB	10:J:10:CYS:SG	2.73	0.74
1:A:629:VAL:HG12	1:A:629:VAL:O	1.87	0.74
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.53	0.73
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	1.89	0.72
1:A:74:CYS:SG	16:A:2001:ZN:ZN	1.79	0.71
12:L:22:CYS:SG	12:L:39:CYS:SG	2.88	0.71
3:C:78:ILE:HG21	3:C:127:VAL:CG2	2.22	0.70
3:C:90:CYS:SG	16:C:301:ZN:ZN	1.79	0.69
1:A:111:CYS:SG	1:A:184:CYS:SG	2.87	0.68
2:B:572:CYS:O	2:B:574:VAL:HG13	1.93	0.67
2:B:601:VAL:HG22	2:B:616:THR:HG22	1.77	0.67
3:C:9:VAL:HG11	11:K:105:PHE:CD1	2.30	0.67
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.76	0.66
11:K:42:LEU:O	11:K:46:ILE:HD12	1.95	0.66
5:E:61:LEU:HD13	5:E:73:PHE:CE1	2.32	0.65
1:A:1118:THR:H	1:A:1136:THR:HG21	1.62	0.65
2:B:594:MET:HE3	2:B:594:MET:HA	1.79	0.65
6:F:83:LEU:HD12	6:F:83:LEU:O	1.96	0.64
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.79	0.64
2:B:550:MET:HE1	2:B:574:VAL:HG23	1.79	0.64
1:A:316:THR:HG21	1:A:328:ALA:CB	2.27	0.64
1:A:74:CYS:HB3	1:A:84:HIS:CE1	2.32	0.64
2:B:526:LEU:CD2	2:B:621:ILE:HD11	2.28	0.63
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.34	0.63
1:A:852:VAL:HG13	1:A:853:LYS:HG2	1.79	0.63
2:B:1141:ARG:HD2	2:B:1141:ARG:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:GLU:O	3:C:97:CYS:HB3	2.00	0.62
7:G:89:VAL:HA	7:G:99:THR:HG22	1.81	0.62
2:B:403:LEU:HD11	2:B:447:SER:OG	2.00	0.61
5:E:94:MET:HG2	5:E:99:ILE:HD11	1.81	0.61
1:A:480:SER:O	1:A:481:THR:HG23	1.99	0.61
2:B:526:LEU:HD21	2:B:621:ILE:HD11	1.81	0.61
1:A:1189:ASP:HB2	1:A:1192:TRP:NE1	2.08	0.61
4:D:39:MET:SD	4:D:40:LEU:HD23	2.40	0.60
5:E:86:THR:HG22	5:E:90:TYR:CE2	2.37	0.60
1:A:1218:ARG:HH11	1:A:1255:LEU:HB2	1.66	0.59
2:B:972:ILE:HG21	2:B:981:LEU:HD11	1.84	0.59
3:C:111:GLN:N	3:C:111:GLN:OE1	2.35	0.59
1:A:706:ILE:HD11	1:A:787:VAL:CG2	2.33	0.59
2:B:550:MET:O	2:B:550:MET:HG3	2.01	0.59
2:B:126:VAL:HG12	2:B:149:ILE:HG21	1.84	0.59
1:A:470:MET:CE	1:A:521:VAL:HG13	2.33	0.58
2:B:501:LEU:CD1	2:B:505:LEU:HD12	2.31	0.58
5:E:52:ARG:HD3	5:E:52:ARG:N	2.17	0.58
5:E:60:VAL:HG22	5:E:74:VAL:HG22	1.86	0.58
7:G:162:SER:O	7:G:163:LEU:HD23	2.04	0.58
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.43	0.58
1:A:1304:ILE:HG22	1:A:1304:ILE:O	2.03	0.58
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.44	0.57
1:A:316:THR:HG21	1:A:328:ALA:HB3	1.85	0.57
3:C:49:TRP:CE2	12:L:54:VAL:HG21	2.40	0.57
7:G:145:LEU:HD12	7:G:145:LEU:O	2.04	0.57
3:C:82:LEU:HD22	3:C:97:CYS:HA	1.87	0.56
1:A:480:SER:O	2:B:1055:VAL:HG21	2.05	0.56
3:C:83:GLN:O	3:C:97:CYS:HB2	2.06	0.56
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.41	0.56
1:A:868:MET:HE1	1:A:1401:LEU:HA	1.86	0.56
1:A:1182:GLN:HA	1:A:1186:VAL:HG13	1.86	0.56
1:A:847:LEU:HB3	2:B:520:VAL:HG21	1.88	0.55
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.87	0.55
5:E:84:ILE:HD11	5:E:113:SER:OG	2.06	0.55
1:A:955:GLU:OE2	1:A:1010:VAL:HG22	2.06	0.55
1:A:321:GLU:N	1:A:321:GLU:OE1	2.39	0.55
1:A:687:ILE:HD11	1:A:766:PHE:CE2	2.42	0.55
1:A:999:ARG:NH2	8:H:112:LEU:HD21	2.21	0.55
1:A:64:VAL:HG22	1:A:71:CYS:SG	2.47	0.55
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:LEU:HD12	1:A:1212:LEU:N	2.23	0.54
3:C:82:LEU:CD2	3:C:97:CYS:HA	2.37	0.54
10:J:28:GLU:HA	10:J:28:GLU:OE2	2.08	0.54
5:E:167:GLU:H	5:E:167:GLU:CD	2.15	0.54
1:A:981:CYS:HB3	1:A:986:MET:HE1	1.89	0.54
2:B:957:THR:HG22	2:B:958:CYS:H	1.71	0.54
1:A:184:CYS:SG	1:A:186:ARG:HB2	2.48	0.54
8:H:59:VAL:O	8:H:59:VAL:CG1	2.56	0.54
1:A:629:VAL:O	1:A:629:VAL:CG1	2.55	0.54
4:D:36:GLU:O	4:D:40:LEU:HG	2.08	0.54
3:C:86:ARG:HD2	11:K:11:LEU:HD11	1.90	0.53
5:E:61:LEU:HD13	5:E:73:PHE:HE1	1.73	0.53
1:A:937:ASP:OD2	1:A:937:ASP:C	2.52	0.53
2:B:91:ILE:HD12	2:B:91:ILE:O	2.08	0.53
4:D:57:LEU:HD13	4:D:61:PHE:CD2	2.43	0.53
1:A:486:LEU:O	1:A:489:THR:HG22	2.09	0.53
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.90	0.53
2:B:147:THR:O	2:B:149:ILE:HG23	2.09	0.53
7:G:76:VAL:HG22	7:G:77:PHE:H	1.73	0.53
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.07	0.53
7:G:10:GLU:HG2	7:G:67:LEU:HD11	1.91	0.52
10:J:1:MET:O	10:J:56:ILE:HG23	2.09	0.52
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.39	0.52
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.44	0.52
11:K:99:SER:O	11:K:103:GLU:HG3	2.09	0.52
1:A:74:CYS:HB3	1:A:84:HIS:NE2	2.24	0.52
1:A:1378:LEU:HD21	1:A:1405:MET:SD	2.50	0.52
1:A:316:THR:HG21	1:A:328:ALA:HB2	1.92	0.51
1:A:471:GLY:O	1:A:521:VAL:HG23	2.10	0.51
11:K:97:GLU:OE2	11:K:97:GLU:C	2.53	0.51
1:A:600:ILE:HG23	1:A:655:ILE:CG2	2.41	0.51
1:A:848:ILE:O	1:A:852:VAL:HG12	2.11	0.51
5:E:120:ASP:OD1	5:E:120:ASP:C	2.54	0.51
2:B:156:LEU:HD22	2:B:184:TYR:CE2	2.46	0.51
2:B:598:VAL:HG12	2:B:601:VAL:HG23	1.93	0.51
3:C:49:TRP:NE1	12:L:54:VAL:HG21	2.26	0.50
7:G:145:LEU:HD12	7:G:145:LEU:C	2.36	0.50
3:C:152:LYS:HE3	10:J:56:ILE:HD11	1.92	0.50
6:F:112:ASP:OD1	6:F:112:ASP:C	2.54	0.50
7:G:92:VAL:HG21	7:G:126:PRO:O	2.11	0.50
1:A:494:ALA:HB2	1:A:501:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:CD1	11:K:19:ILE:HD11	2.41	0.50
1:A:549:THR:HG22	1:A:549:THR:O	2.11	0.50
7:G:28:GLN:C	7:G:28:GLN:OE1	2.55	0.50
3:C:78:ILE:HG21	3:C:127:VAL:HG23	1.93	0.50
10:J:10:CYS:SG	10:J:11:GLY:N	2.85	0.50
1:A:1211:LEU:HD12	1:A:1211:LEU:C	2.37	0.50
1:A:909:LEU:HD21	1:A:973:GLY:HA2	1.93	0.49
7:G:5:ILE:HD13	7:G:7:LEU:HG	1.94	0.49
5:E:185:ILE:CG2	5:E:209:VAL:HG21	2.42	0.49
9:I:82:GLU:OE2	9:I:82:GLU:HA	2.12	0.49
10:J:35:LEU:HD11	10:J:50:LEU:HD13	1.92	0.49
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.77	0.49
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.93	0.49
1:A:503:LEU:HD23	1:A:503:LEU:O	2.12	0.49
1:A:1099:ALA:O	1:A:1100:THR:C	2.54	0.49
4:D:36:GLU:HA	4:D:39:MET:HE3	1.95	0.49
1:A:1100:THR:HG23	14:P:48:U:C2	2.48	0.49
1:A:709:ALA:HB2	1:A:748:ALA:HB2	1.94	0.49
2:B:598:VAL:CG1	2:B:601:VAL:HG23	2.43	0.49
2:B:609:GLU:HA	2:B:609:GLU:OE1	2.12	0.49
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.94	0.49
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.95	0.49
1:A:360:ASP:O	1:A:361:PHE:C	2.55	0.49
1:A:470:MET:HE3	1:A:521:VAL:HG13	1.94	0.49
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.95	0.48
1:A:934:LEU:HD21	1:A:1006:PRO:HD3	1.94	0.48
1:A:936:GLU:N	1:A:936:GLU:OE1	2.45	0.48
2:B:17:ILE:HG22	2:B:18:THR:N	2.27	0.48
5:E:130:PHE:O	5:E:131:LEU:C	2.56	0.48
8:H:60:ILE:CD1	8:H:123:MET:HE1	2.43	0.48
10:J:10:CYS:HB3	10:J:44:CYS:SG	2.54	0.48
10:J:14:VAL:HG21	10:J:48:MET:HG2	1.96	0.48
5:E:61:LEU:HD12	5:E:62:VAL:N	2.27	0.48
1:A:24:GLY:O	2:B:1168:ALA:HB3	2.13	0.48
2:B:381:GLU:OE2	2:B:381:GLU:N	2.47	0.48
1:A:364:ARG:HB2	2:B:1084:LEU:HD21	1.95	0.48
1:A:419:ILE:O	1:A:420:ILE:C	2.56	0.48
1:A:1382:LEU:HB3	1:A:1398:LEU:HD22	1.95	0.48
7:G:76:VAL:HG22	7:G:77:PHE:N	2.28	0.48
1:A:367:ILE:HD13	1:A:501:MET:HE3	1.94	0.48
2:B:735:VAL:HG11	10:J:55:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:ARG:HA	12:L:31:ARG:NE	2.29	0.48
1:A:74:CYS:SG	1:A:84:HIS:NE2	2.87	0.48
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.95	0.47
1:A:464:LEU:HD11	1:A:1100:THR:HG21	1.96	0.47
2:B:288:ILE:HD12	2:B:369:VAL:HG11	1.96	0.47
2:B:598:VAL:HG22	2:B:599:SER:N	2.30	0.47
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.78	0.47
8:H:40:ILE:O	8:H:123:MET:HA	2.14	0.47
1:A:419:ILE:O	1:A:419:ILE:HG22	2.14	0.47
1:A:1133:LYS:O	1:A:1133:LYS:HG2	2.14	0.47
1:A:629:VAL:O	1:A:630:VAL:C	2.56	0.47
1:A:1227:THR:HG22	1:A:1229:GLU:H	1.79	0.47
2:B:155:MET:O	2:B:158:SER:OG	2.33	0.47
8:H:43:VAL:HG23	8:H:90:TYR:CE1	2.49	0.47
4:D:74:PHE:CD1	4:D:74:PHE:N	2.81	0.47
1:A:343:LEU:HD12	1:A:1436:VAL:HG22	1.96	0.47
14:P:37:G:H2'	14:P:38:G:C8	2.50	0.47
1:A:362:SER:N	1:A:388:MET:HE1	2.29	0.46
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.50	0.46
1:A:63:GLY:C	1:A:71:CYS:SG	2.98	0.46
2:B:746:THR:O	2:B:747:LEU:HD23	2.15	0.46
14:P:38:G:O2'	14:P:39:C:P	2.73	0.46
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.96	0.46
2:B:279:VAL:HG23	2:B:280:SER:N	2.31	0.46
9:I:53:ILE:HD12	9:I:53:ILE:N	2.30	0.46
2:B:66:ASP:O	2:B:67:LEU:HD22	2.15	0.46
1:A:26:LEU:HG	2:B:1168:ALA:HB2	1.97	0.46
1:A:687:ILE:HD13	2:B:972:ILE:HB	1.98	0.46
5:E:84:ILE:HD12	5:E:84:ILE:H	1.81	0.46
1:A:1259:ILE:HG22	1:A:1260:ARG:N	2.31	0.46
1:A:497:ASP:OD1	1:A:497:ASP:C	2.59	0.46
12:L:38:GLU:OE1	12:L:38:GLU:N	2.49	0.46
15:T:10:DC:H4'	15:T:11:DT:OP1	2.16	0.45
1:A:427:ILE:O	1:A:427:ILE:HG22	2.16	0.45
1:A:518:LEU:O	1:A:524:MET:HE3	2.17	0.45
1:A:865:ILE:CG2	2:B:1092:ASP:OD2	2.62	0.45
8:H:96:VAL:HG12	8:H:139:SER:O	2.16	0.45
1:A:57:LEU:HD11	1:A:281:ALA:HA	1.98	0.45
3:C:44:ILE:HA	3:C:79:VAL:HG21	1.97	0.45
1:A:117:LEU:HD22	1:A:119:VAL:HG12	1.98	0.45
1:A:343:LEU:CD1	1:A:1436:VAL:HG22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:VAL:HG22	2:B:1084:LEU:O	2.16	0.45
3:C:47:ILE:HA	3:C:165:ALA:HA	1.98	0.45
10:J:47:ARG:CZ	10:J:48:MET:HE1	2.47	0.45
3:C:45:ILE:HD11	3:C:82:LEU:HD12	1.99	0.45
4:D:37:VAL:O	4:D:41:LEU:HG	2.16	0.45
5:E:115:LYS:HA	5:E:118:LEU:HD12	1.99	0.45
1:A:343:LEU:HA	1:A:349:ARG:H	1.82	0.45
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.98	0.45
1:A:828:LEU:HD13	1:A:828:LEU:O	2.17	0.45
9:I:29:ASP:C	9:I:29:ASP:OD1	2.60	0.45
2:B:598:VAL:HG22	2:B:599:SER:H	1.81	0.45
2:B:649:ASN:O	2:B:650:ASN:OD1	2.35	0.45
1:A:470:MET:HE1	1:A:521:VAL:HG13	1.99	0.44
3:C:3:TYR:HA	11:K:93:ASP:OD1	2.16	0.44
9:I:53:ILE:N	9:I:53:ILE:CD1	2.80	0.44
1:A:112:PHE:CD1	1:A:112:PHE:C	2.95	0.44
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.44
2:B:126:VAL:HG12	2:B:149:ILE:CG2	2.47	0.44
1:A:709:ALA:CB	1:A:748:ALA:HB2	2.48	0.44
1:A:971:PRO:C	1:A:972:THR:HG23	2.42	0.44
1:A:1220:HIS:HA	1:A:1223:ASP:HB3	1.99	0.44
2:B:1140:CYS:O	2:B:1141:ARG:HB3	2.17	0.44
9:I:31:GLU:N	9:I:31:GLU:OE1	2.51	0.44
13:N:35:DT:H2'	13:N:36:DT:H72	1.98	0.44
1:A:565:MET:SD	11:K:60:GLY:C	3.01	0.44
1:A:910:LYS:N	1:A:911:PRO:HD2	2.32	0.44
9:I:65:LEU:HD12	9:I:65:LEU:H	1.80	0.44
1:A:484:LEU:HD11	1:A:496:PHE:CE1	2.53	0.44
1:A:484:LEU:HD12	1:A:484:LEU:O	2.18	0.44
1:A:865:ILE:HD13	2:B:1092:ASP:OD2	2.18	0.44
2:B:759:VAL:HG12	2:B:999:ALA:HB2	2.00	0.44
5:E:148:HIS:CD2	5:E:179:VAL:HG11	2.53	0.44
8:H:84:ARG:HD3	8:H:84:ARG:N	2.33	0.44
1:A:1228:MET:N	1:A:1228:MET:HE3	2.33	0.43
4:D:88:LEU:C	4:D:88:LEU:HD12	2.43	0.43
1:A:600:ILE:HG23	1:A:655:ILE:HG22	2.00	0.43
2:B:972:ILE:N	2:B:973:PRO:CD	2.81	0.43
2:B:972:ILE:N	2:B:973:PRO:HD2	2.32	0.43
13:N:13:DC:H2''	13:N:14:DC:C6	2.54	0.43
14:P:38:G:H2'	14:P:39:C:C6	2.54	0.43
1:A:1165:THR:HG22	1:A:1166:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:LEU:HD21	2:B:526:LEU:HG	2.01	0.43
5:E:71:GLN:HB2	5:E:99:ILE:HG22	2.00	0.43
7:G:5:ILE:C	7:G:5:ILE:HD12	2.43	0.43
8:H:91:VAL:HG22	8:H:144:LEU:HD23	2.00	0.43
1:A:369:PRO:HD3	2:B:793:SER:OG	2.18	0.43
1:A:786:ALA:O	1:A:787:VAL:HG23	2.18	0.43
3:C:45:ILE:HB	3:C:75:SER:HB3	2.00	0.43
13:N:35:DT:C2'	13:N:36:DT:H72	2.48	0.43
1:A:872:MET:HE1	1:A:1465:PRO:O	2.19	0.43
1:A:1004:LEU:HD21	1:A:1009:VAL:CG2	2.47	0.43
8:H:59:VAL:O	8:H:60:ILE:C	2.60	0.43
1:A:153:ILE:HD11	1:A:185:GLY:C	2.43	0.43
1:A:1016:LEU:HD21	1:A:1072:ILE:HG21	2.00	0.43
8:H:37:MET:HE1	8:H:131:ASN:HB2	2.00	0.43
1:A:154:CYS:HB2	1:A:184:CYS:SG	2.59	0.43
2:B:269:ILE:HD12	2:B:270:ILE:N	2.34	0.43
10:J:6:ARG:HG2	10:J:11:GLY:O	2.19	0.43
1:A:1304:ILE:O	1:A:1305:SER:C	2.62	0.42
2:B:1094:GLN:HB2	2:B:1103:LEU:HD13	2.01	0.42
13:N:38:DA:C2	13:N:39:DG:C6	3.07	0.42
1:A:543:THR:HG22	1:A:543:THR:O	2.19	0.42
1:A:1171:ALA:HB2	1:A:1217:ASP:HB2	2.01	0.42
1:A:1219:LYS:HE3	1:A:1219:LYS:HB3	1.44	0.42
2:B:595:ASP:O	2:B:596:ILE:C	2.61	0.42
2:B:635:LEU:HD21	2:B:640:ILE:HD11	2.02	0.42
11:K:45:ILE:HG23	11:K:46:ILE:N	2.35	0.42
1:A:1136:THR:HG23	1:A:1136:THR:O	2.19	0.42
1:A:1481:LYS:O	1:A:1482:TYR:C	2.62	0.42
1:A:384:ILE:O	1:A:388:MET:HG2	2.20	0.42
1:A:1095:LEU:HD13	1:A:1401:LEU:HD22	2.00	0.42
1:A:1257:LEU:O	1:A:1257:LEU:HG	2.20	0.42
2:B:104:ALA:HB3	2:B:105:PRO:HD3	2.01	0.42
2:B:271:ILE:N	2:B:271:ILE:HD13	2.34	0.42
2:B:891:ASP:CG	2:B:891:ASP:O	2.62	0.42
1:A:537:ILE:HG12	1:A:672:ILE:HG21	2.01	0.42
1:A:1121:VAL:N	1:A:1122:PRO:HD2	2.35	0.42
1:A:1170:THR:HG23	1:A:1214:VAL:HG23	2.00	0.42
2:B:961:ILE:O	2:B:961:ILE:HG22	2.20	0.42
1:A:419:ILE:HD11	1:A:429:LEU:HD11	2.02	0.42
3:C:19:VAL:O	3:C:19:VAL:HG13	2.19	0.42
7:G:54:ILE:HD12	7:G:70:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.54	0.42
2:B:368:MET:HE3	2:B:368:MET:HB2	1.94	0.42
5:E:72:MET:SD	5:E:103:LEU:HD13	2.60	0.42
5:E:106:VAL:HG12	5:E:107:GLN:N	2.35	0.42
1:A:98:GLY:CA	1:A:1440:MET:HE3	2.50	0.41
9:I:54:TYR:C	9:I:54:TYR:CD2	2.98	0.41
1:A:760:LEU:HD11	1:A:781:ILE:HG21	2.02	0.41
2:B:687:VAL:HG13	2:B:687:VAL:O	2.20	0.41
9:I:95:VAL:HG13	9:I:115:THR:CG2	2.50	0.41
10:J:53:VAL:O	10:J:53:VAL:HG13	2.19	0.41
2:B:853:LEU:HD13	2:B:919:CYS:SG	2.61	0.41
1:A:600:ILE:HG23	1:A:655:ILE:HG21	2.02	0.41
3:C:89:THR:O	3:C:90:CYS:C	2.59	0.41
3:C:263:LEU:HD22	11:K:87:PHE:HD2	1.85	0.41
8:H:59:VAL:HG21	8:H:88:PHE:CE2	2.55	0.41
11:K:100:LEU:HD11	11:K:104:ARG:HE	1.85	0.41
2:B:145:GLN:O	2:B:146:LYS:C	2.64	0.41
8:H:15:ILE:CD1	8:H:28:LEU:HD23	2.51	0.41
15:T:10:DC:C6	15:T:11:DT:H72	2.55	0.41
1:A:534:VAL:HG13	1:A:535:MET:HG3	2.02	0.41
1:A:939:VAL:HG12	1:A:943:LEU:HD12	2.02	0.41
2:B:895:PHE:N	2:B:895:PHE:CD2	2.88	0.41
2:B:1161:GLU:O	2:B:1165:MET:HG3	2.20	0.41
9:I:27:LYS:NZ	9:I:36:LEU:HB3	2.36	0.41
2:B:761:THR:HG23	2:B:1000:THR:HA	2.03	0.41
13:N:11:DG:C8	13:N:12:DT:H72	2.56	0.41
1:A:74:CYS:CB	1:A:84:HIS:NE2	2.84	0.41
1:A:722:ASN:O	1:A:723:ASN:C	2.63	0.41
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.45	0.41
1:A:873:VAL:HG22	1:A:879:VAL:HG22	2.02	0.41
1:A:1296:MET:HE2	1:A:1296:MET:HA	2.03	0.41
2:B:553:LEU:O	2:B:556:ILE:HG22	2.20	0.41
2:B:629:GLU:HG3	2:B:634:LEU:HD11	2.01	0.41
8:H:70:LEU:HD23	8:H:70:LEU:H	1.85	0.41
8:H:100:GLU:O	8:H:112:LEU:HD23	2.20	0.41
1:A:361:PHE:HA	2:B:1062:ARG:O	2.21	0.41
1:A:1102:MET:HE3	1:A:1120:GLY:HA2	2.03	0.41
2:B:237:VAL:O	2:B:237:VAL:HG12	2.20	0.41
2:B:255:ARG:HE	2:B:307:GLU:HG3	1.86	0.41
3:C:159:LEU:HD11	3:C:161:LEU:HD23	2.02	0.41
5:E:47:LYS:O	5:E:51:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:VAL:HG11	5:E:109:GLY:C	2.46	0.41
8:H:59:VAL:HG21	8:H:88:PHE:CZ	2.56	0.41
1:A:982:ASN:C	1:A:986:MET:HE3	2.46	0.40
8:H:60:ILE:HD13	8:H:123:MET:HE1	2.03	0.40
1:A:319:ASP:OD2	1:A:322:LEU:HD23	2.22	0.40
1:A:743:ARG:HG3	1:A:743:ARG:HH11	1.86	0.40
1:A:74:CYS:CB	1:A:81:CYS:SG	3.09	0.40
1:A:360:ASP:HB2	2:B:1110:ALA:O	2.21	0.40
2:B:81:PRO:N	2:B:82:PRO:CD	2.84	0.40
2:B:867:ILE:HG13	2:B:921:ILE:HD12	2.03	0.40
1:A:65:ILE:H	1:A:65:ILE:HD12	1.87	0.40
1:A:1050:CYS:O	1:A:1051:SER:C	2.64	0.40
2:B:543:GLU:OE1	2:B:543:GLU:HA	2.20	0.40
5:E:110:MET:SD	5:E:118:LEU:HD11	2.62	0.40
15:T:21:DG:H2"	15:T:22:DC:C5	2.57	0.40
1:A:502:ASN:ND2	2:B:1084:LEU:HD23	2.37	0.40
5:E:103:LEU:O	5:E:104:ILE:C	2.63	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	1353/1475 (92%)	1253 (93%)	100 (7%)	0	100	100
2	B	1068/1161 (92%)	988 (92%)	80 (8%)	0	100	100
3	C	250/267 (94%)	231 (92%)	19 (8%)	0	100	100
4	D	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
5	E	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
6	F	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
7	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	146/148 (99%)	127 (87%)	19 (13%)	0	100	100
9	I	102/114 (90%)	92 (90%)	10 (10%)	0	100	100
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
12	L	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
All	All	3717/3977 (94%)	3452 (93%)	265 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1298 (94%)	1199 (98%)	19 (2%)	55	83
2	B	962/1015 (95%)	950 (99%)	12 (1%)	63	86
3	C	231/244 (95%)	228 (99%)	3 (1%)	61	86
4	D	106/118 (90%)	105 (99%)	1 (1%)	70	90
5	E	189/189 (100%)	186 (98%)	3 (2%)	55	83
6	F	68/68 (100%)	67 (98%)	1 (2%)	57	84
7	G	147/152 (97%)	147 (100%)	0	100	100
8	H	129/129 (100%)	127 (98%)	2 (2%)	55	83
9	I	97/103 (94%)	94 (97%)	3 (3%)	35	69
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/104 (100%)	103 (99%)	1 (1%)	68	89
12	L	41/41 (100%)	40 (98%)	1 (2%)	43	75
All	All	3348/3517 (95%)	3302 (99%)	46 (1%)	57	85

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	MET
1	A	113	PHE
1	A	238	MET
1	A	423	ASN
1	A	484	LEU
1	A	769	MET
1	A	883	ILE
1	A	1007	ILE
1	A	1150	ASP
1	A	1188	GLU
1	A	1189	ASP
1	A	1190	GLN
1	A	1191	GLU
1	A	1215	GLU
1	A	1216	LEU
1	A	1218	ARG
1	A	1219	LYS
1	A	1221	MET
1	A	1441	GLU
2	B	132	VAL
2	B	214	LYS
2	B	257	VAL
2	B	299	GLU
2	B	344	GLN
2	B	388	TYR
2	B	420	GLN
2	B	516	GLU
2	B	627	ILE
2	B	650	ASN
2	B	809	VAL
2	B	1028	LEU
3	C	82	LEU
3	C	90	CYS
3	C	223	ASN
4	D	33	LEU
5	E	60	VAL
5	E	74	VAL
5	E	86	THR
6	F	90	LEU
8	H	106	THR
8	H	123	MET
9	I	42	CYS
9	I	58	ILE

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Mol	Chain	Res	Type
9	I	95	VAL
11	K	81	TYR
12	L	41	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	313	HIS
1	A	387	ASN
1	A	504	HIS
1	A	723	ASN
1	A	783	GLN
1	A	885	GLN
1	A	905	ASN
1	A	1101	GLN
1	A	1190	GLN
2	B	582	GLN
2	B	650	ASN
2	B	986	GLN
4	D	34	ASN
4	D	38	HIS
5	E	169	GLN
7	G	111	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	15/16 (93%)	6 (40%)	1 (6%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	34	U
14	P	35	U
14	P	37	G
14	P	39	C
14	P	47	C
14	P	48	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	38	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

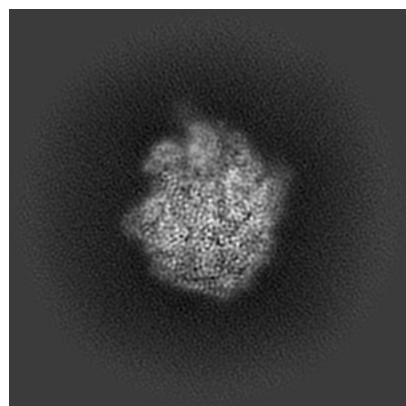
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72792. These allow visual inspection of the internal detail of the map and identification of artifacts.

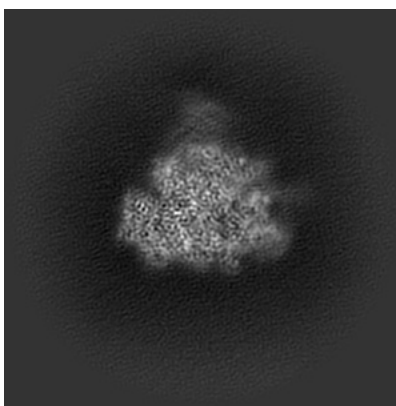
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

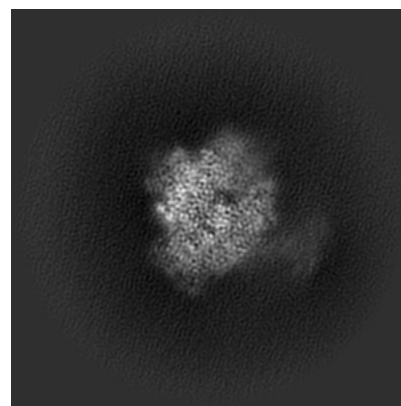
6.1.1 Primary map



X

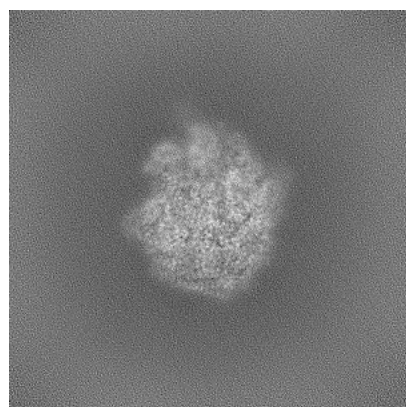


Y

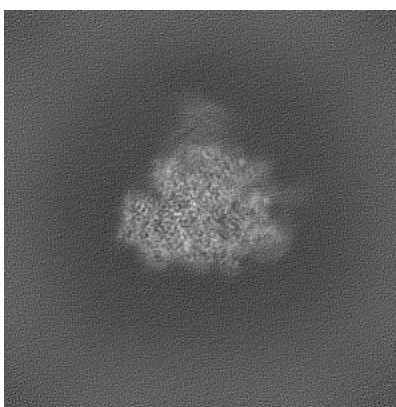


Z

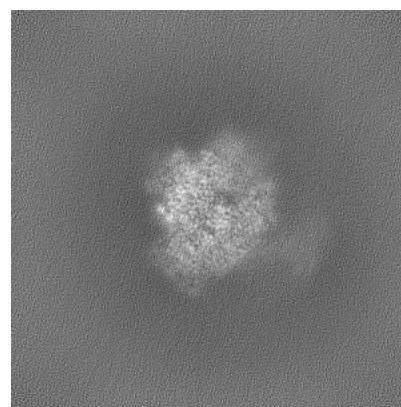
6.1.2 Raw map



X



Y

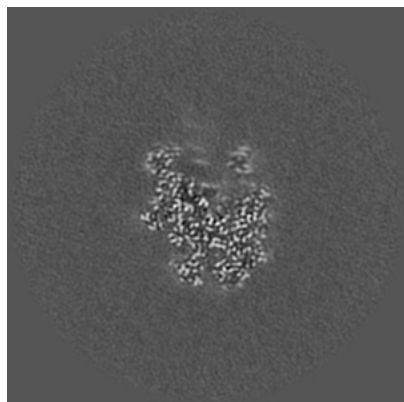


Z

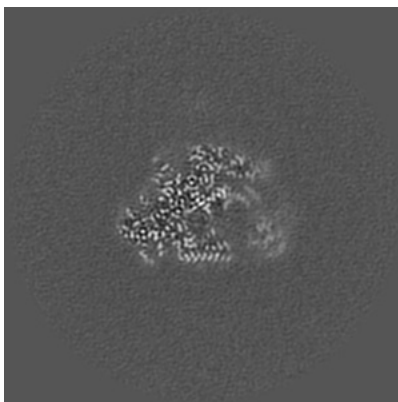
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

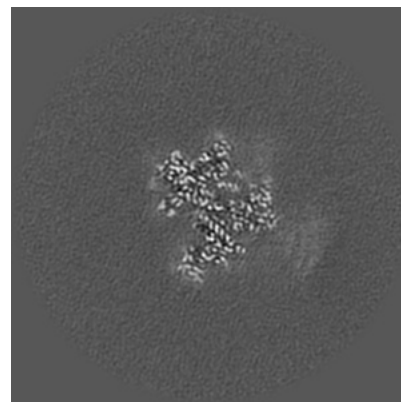
6.2.1 Primary map



X Index: 200

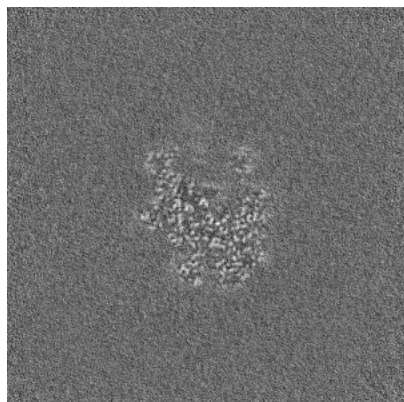


Y Index: 200

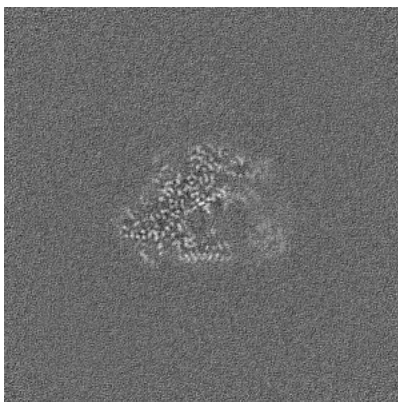


Z Index: 200

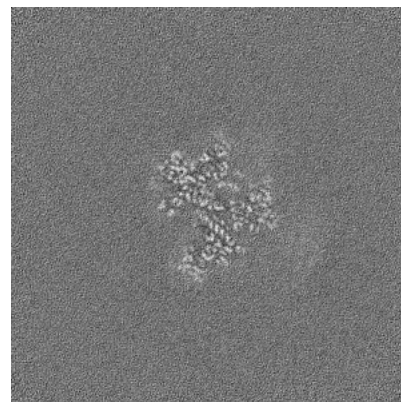
6.2.2 Raw map



X Index: 200



Y Index: 200

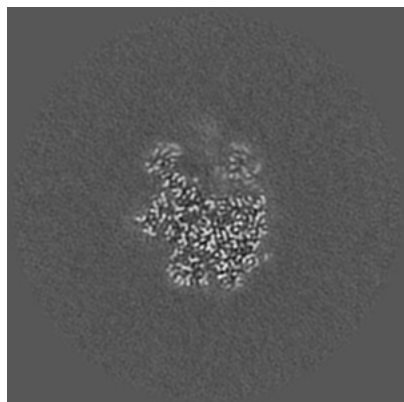


Z Index: 200

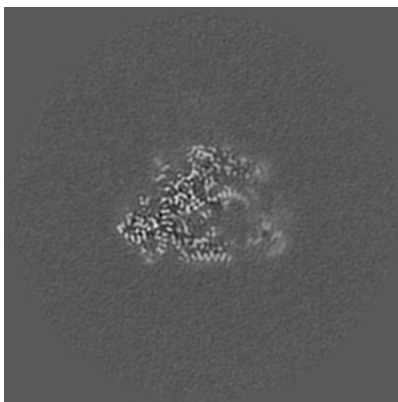
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

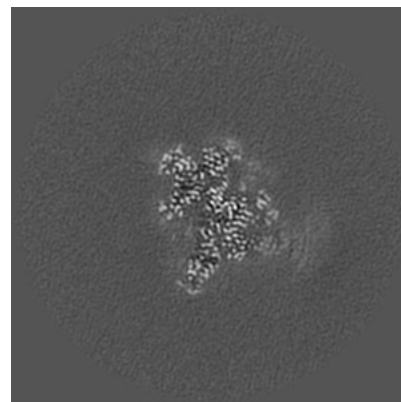
6.3.1 Primary map



X Index: 195

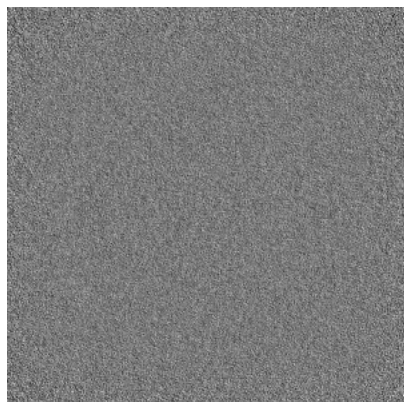


Y Index: 202

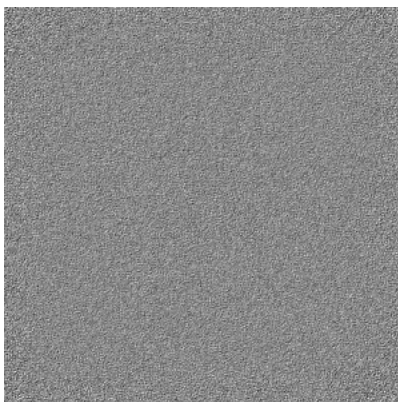


Z Index: 187

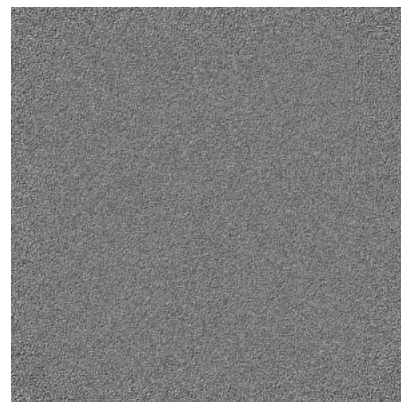
6.3.2 Raw map



X Index: 0



Y Index: 0

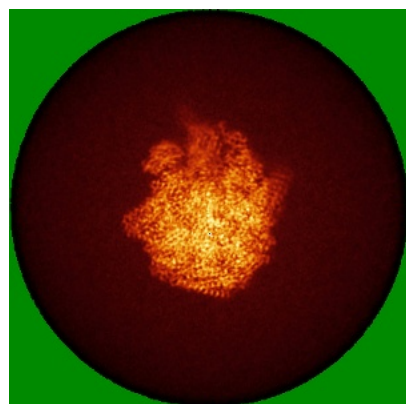


Z Index: 0

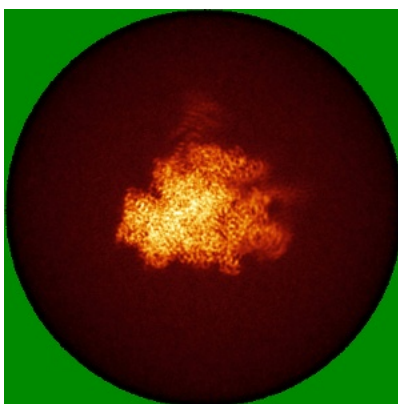
The images above show the largest variance slices of the map in three orthogonal directions.

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

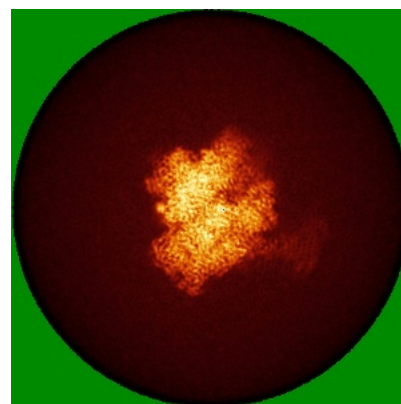
6.4.1 Primary map



X

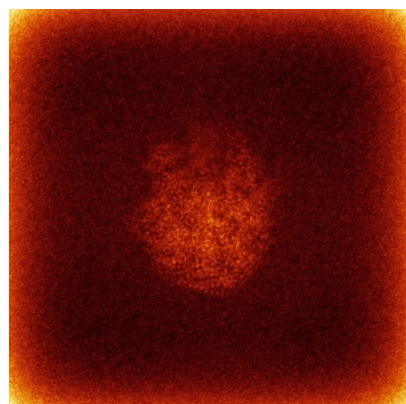


Y

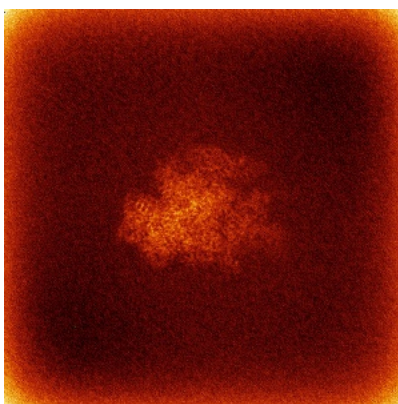


Z

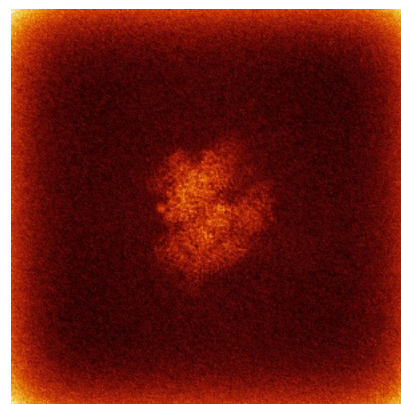
6.4.2 Raw map



X



Y

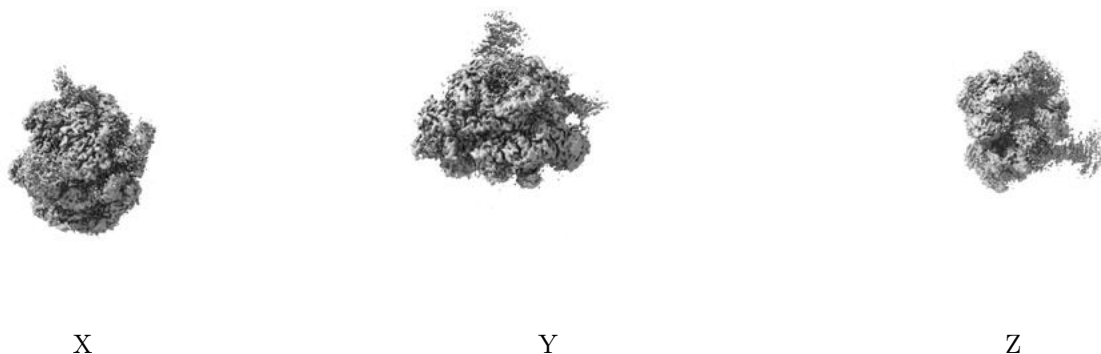


Z

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.

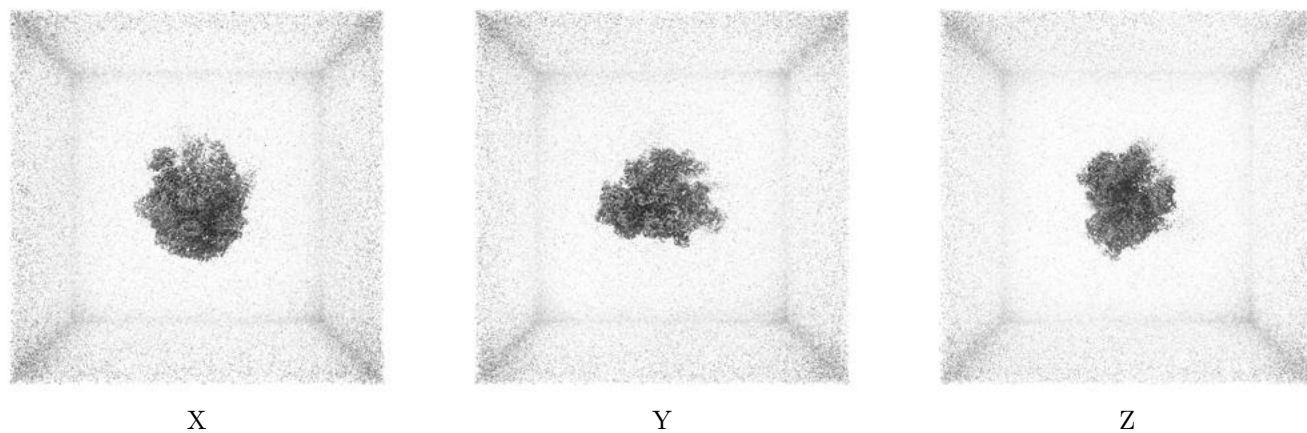
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0289. 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.

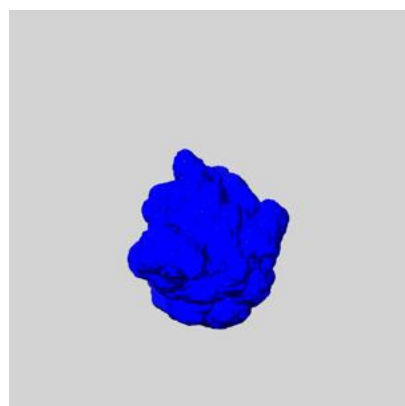
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

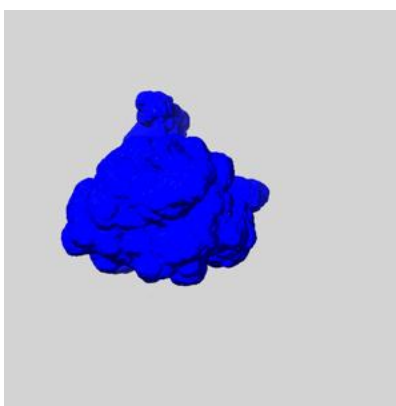
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

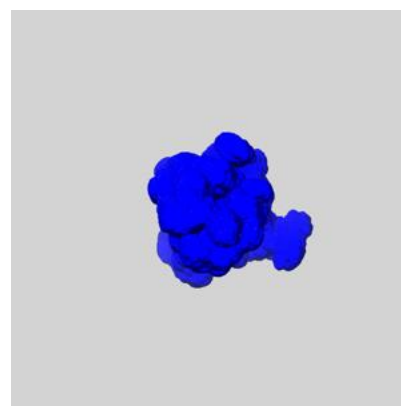
6.6.1 emd_72792_msk_1.map [i](#)



X



Y

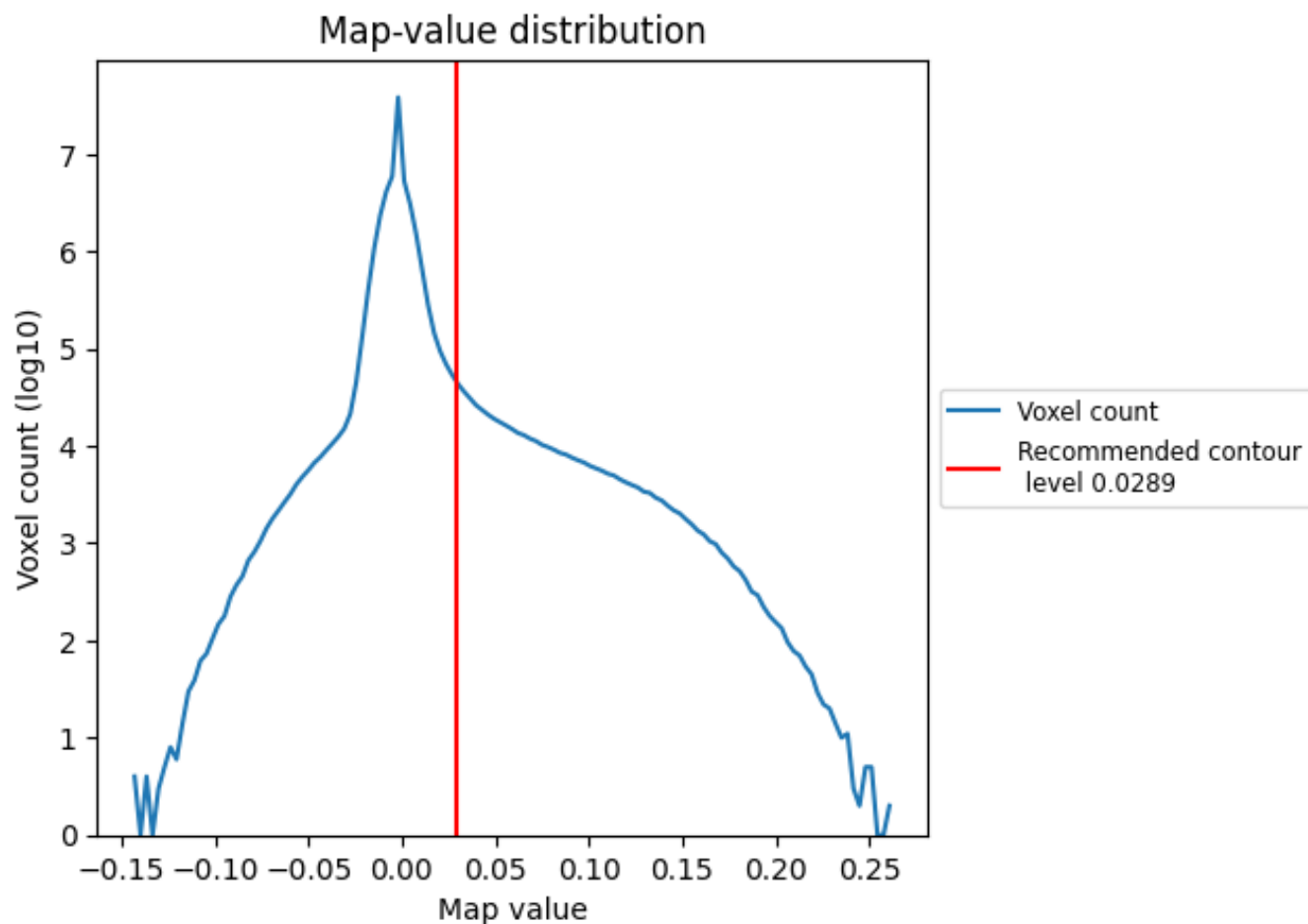


Z

7 Map analysis [i](#)

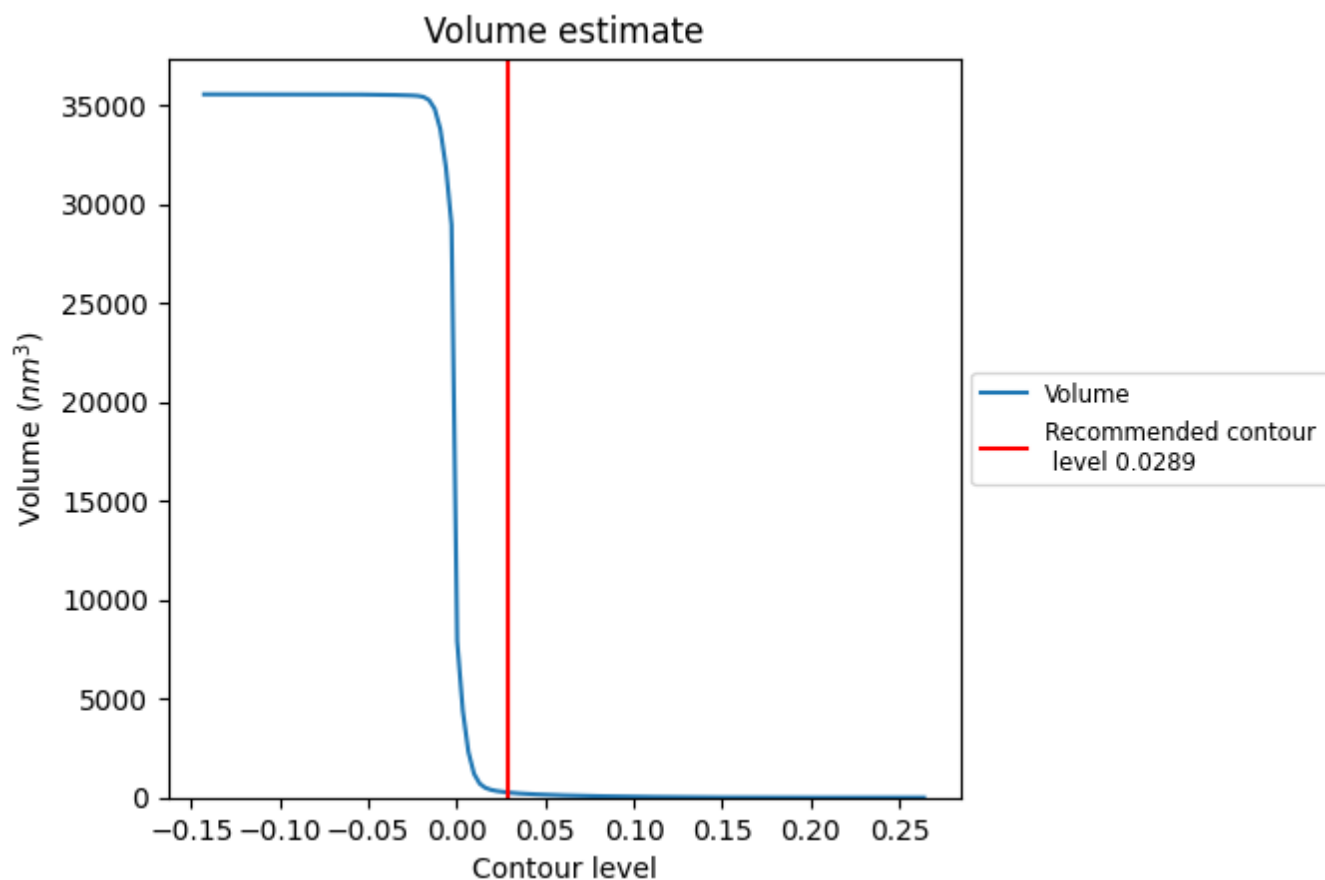
This section contains the results of statistical analysis of the map.

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.

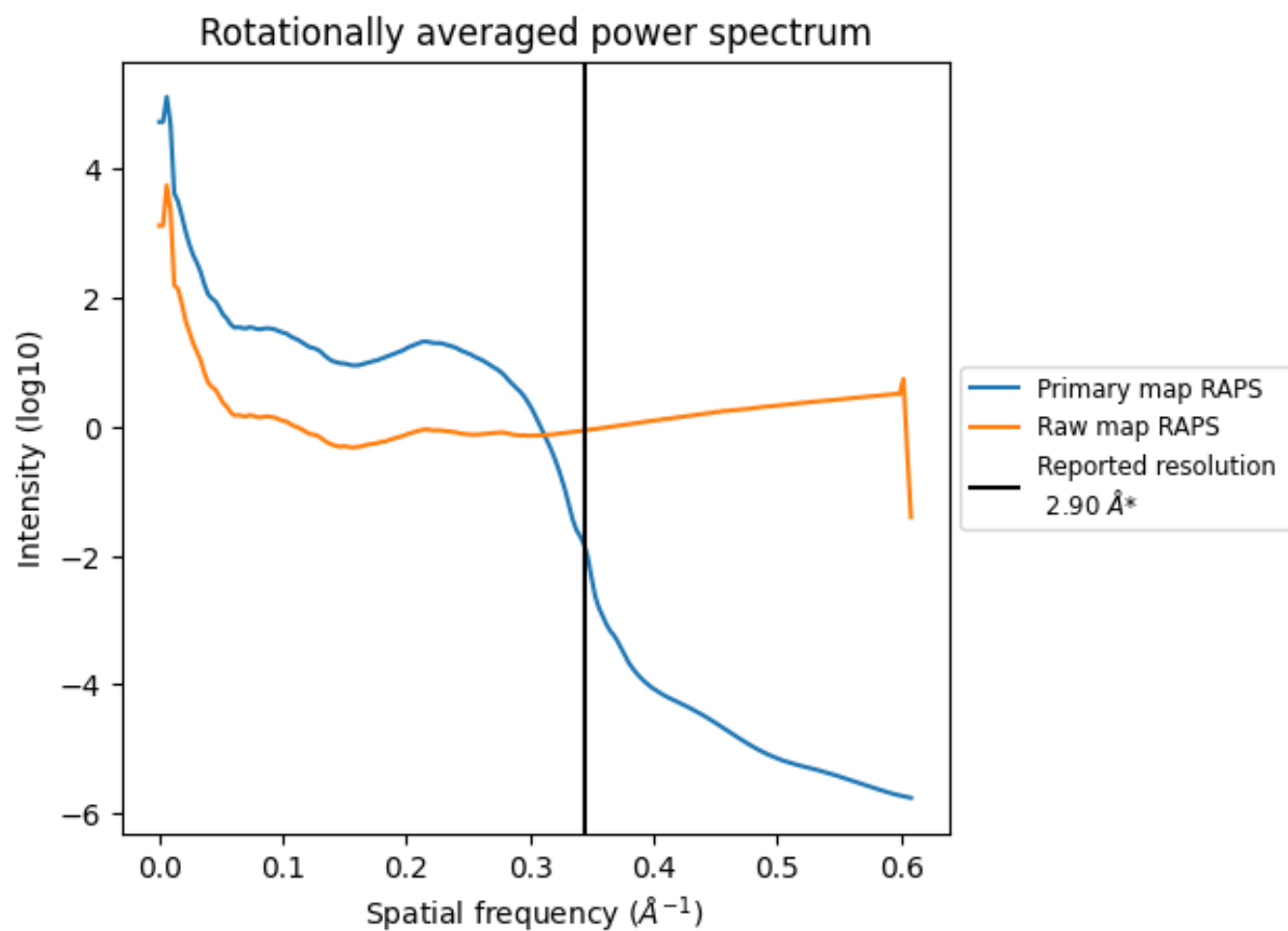
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 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 ⓘ

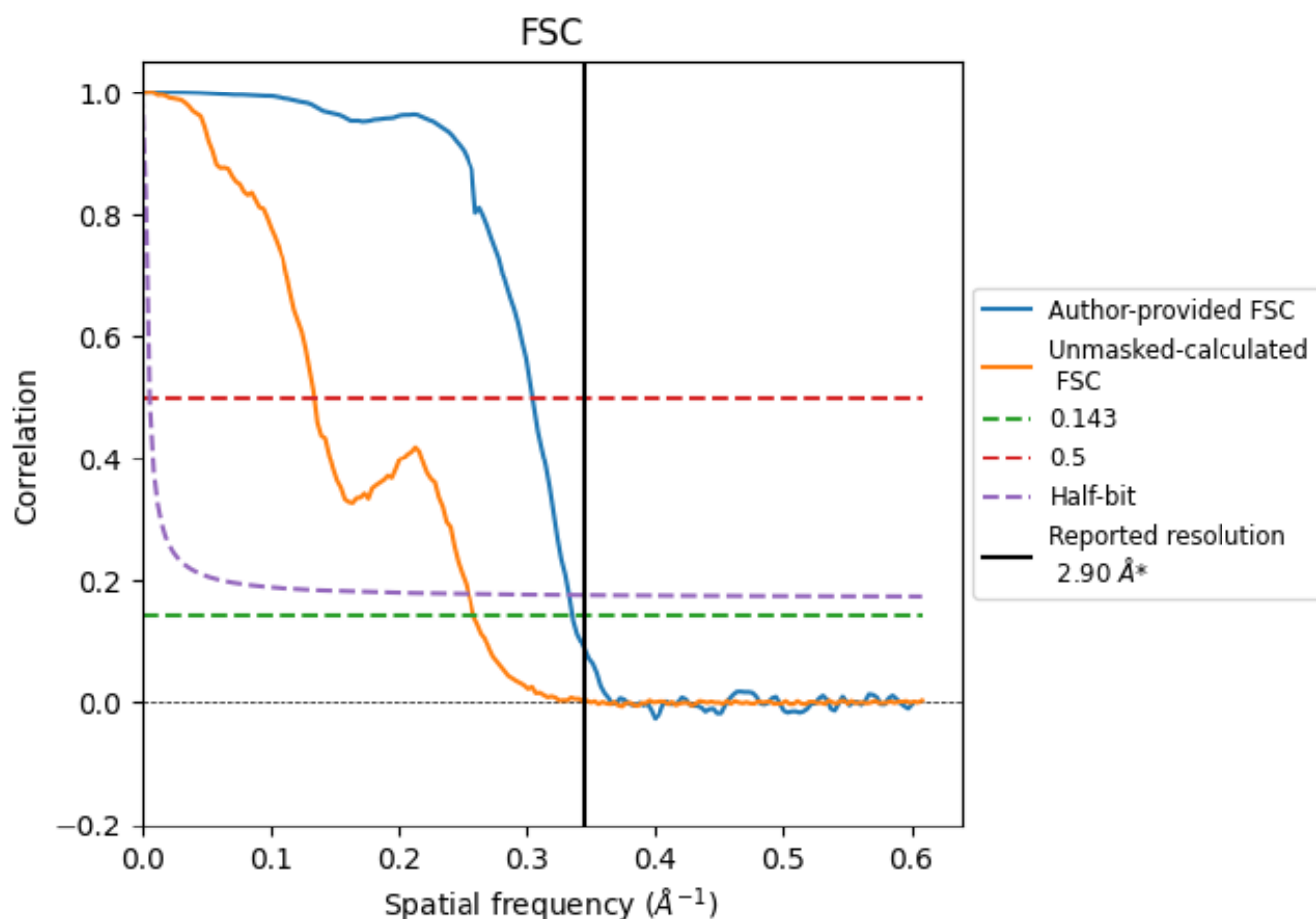


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

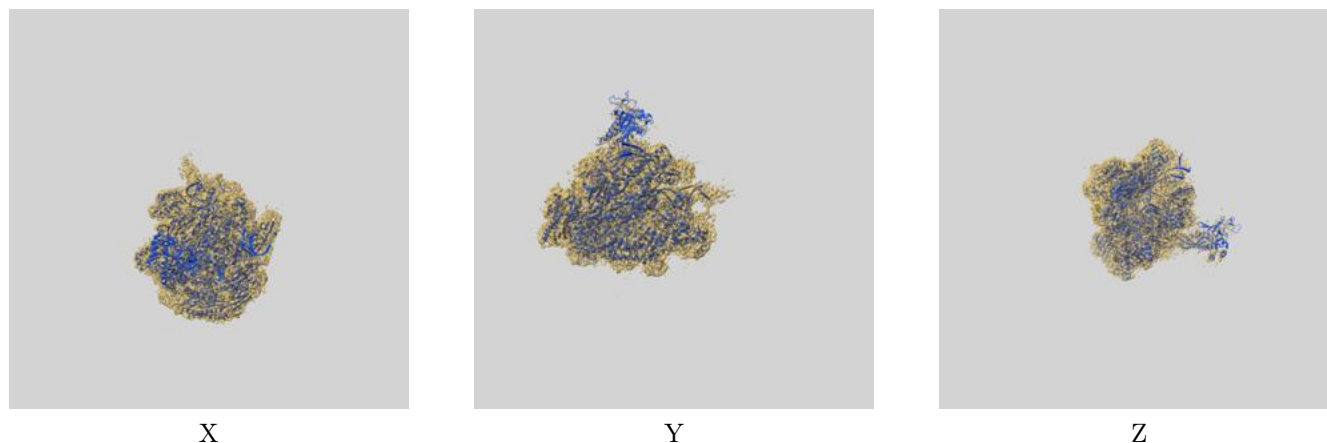
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.98	3.29	3.00
Unmasked-calculated*	3.87	7.43	3.93

*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 3.87 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

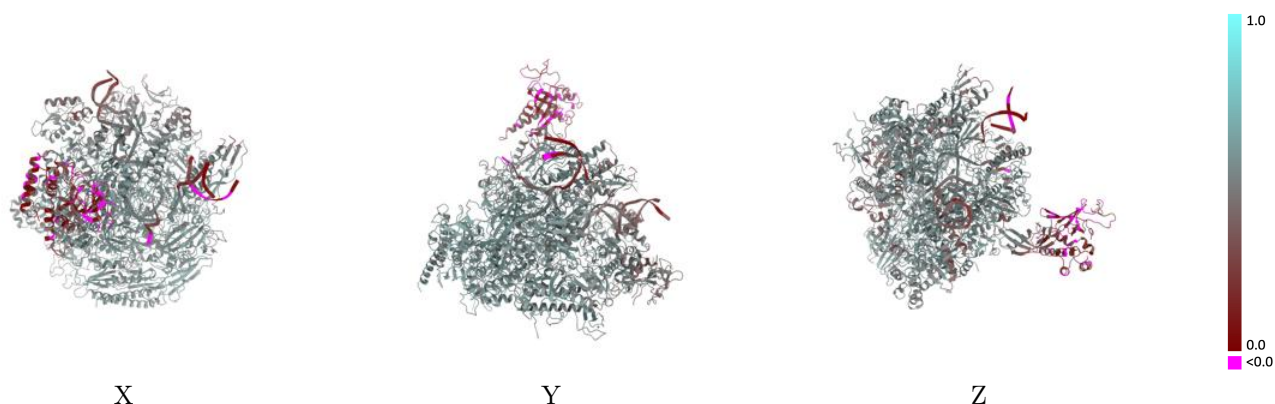
This section contains information regarding the fit between EMDB map EMD-72792 and PDB model 9YCZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



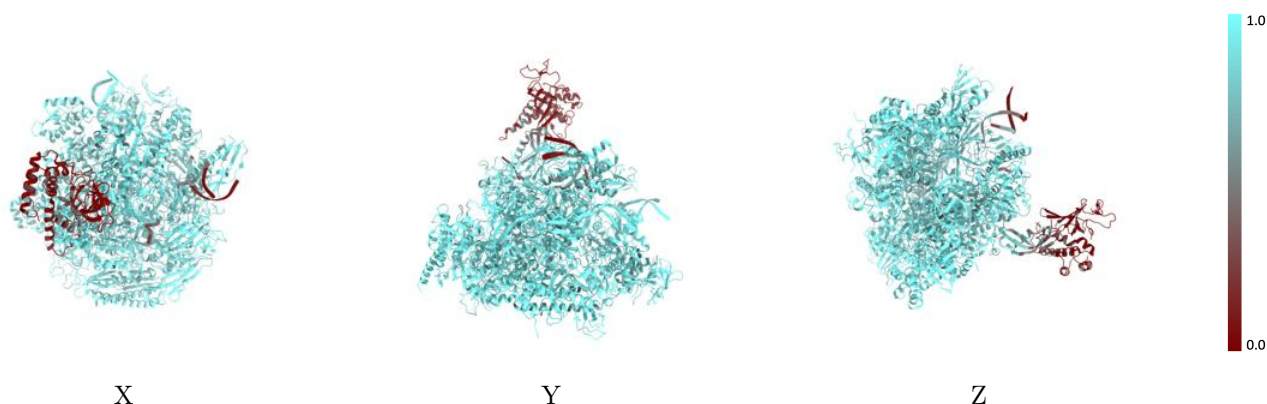
The images above show the 3D surface view of the map at the recommended contour level 0.0289 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



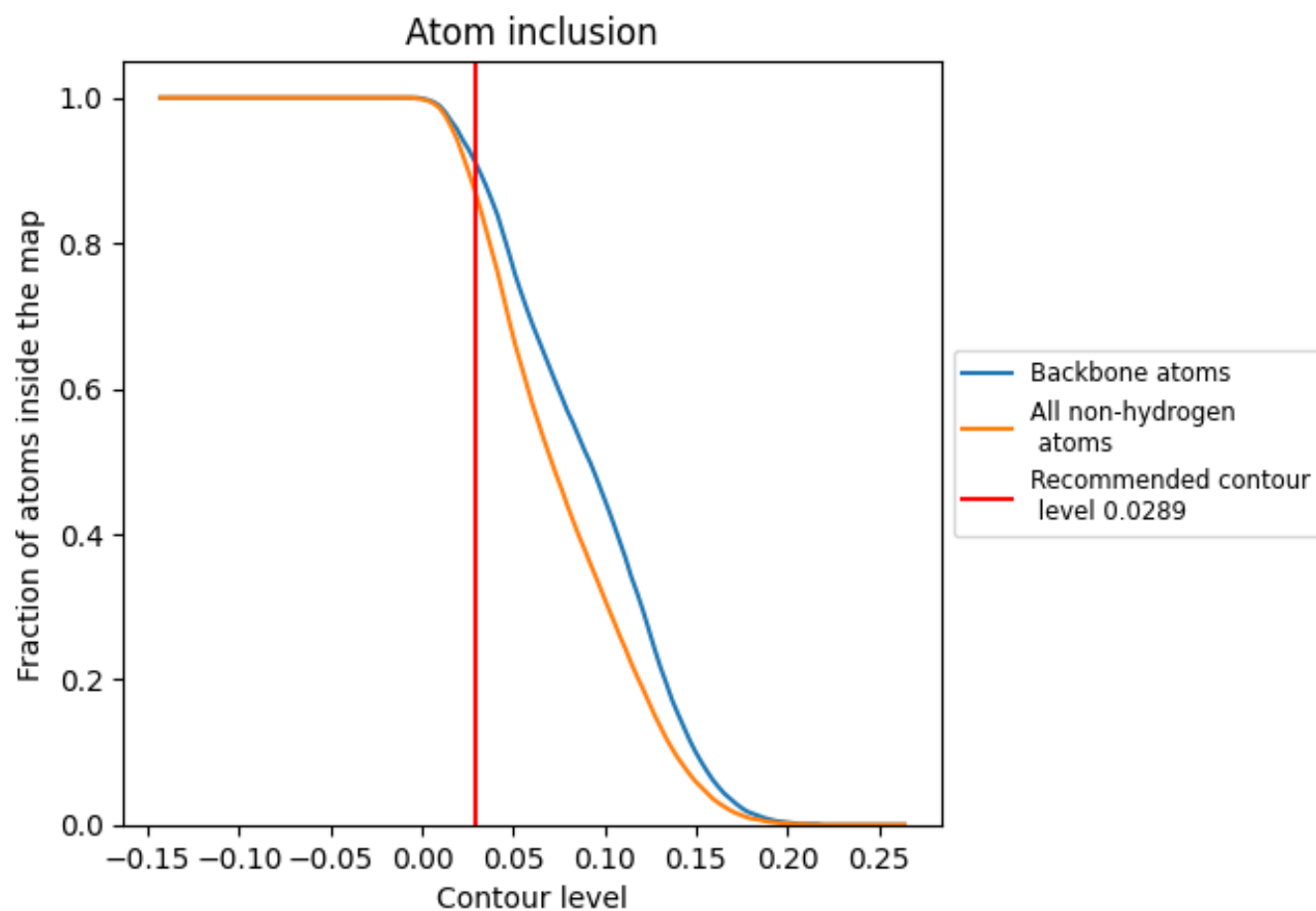
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0289).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.0289) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.5100
A	0.9200	0.5390
B	0.9320	0.5460
C	0.9520	0.5610
D	0.1510	0.1910
E	0.9270	0.5130
F	0.9460	0.5580
G	0.3490	0.2770
H	0.9340	0.5480
I	0.9370	0.4880
J	0.9500	0.5660
K	0.9470	0.5600
L	0.9380	0.5300
N	0.7010	0.2890
P	0.8120	0.4420
T	0.8050	0.3630

1.0
0.0
<0.0