



Full wwPDB EM Validation Report ⓘ

Jan 16, 2024 – 10:30 AM EST

PDB ID : 8TVV
EMDB ID : EMD-41652
Title : Cryo-EM structure of backtracked Pol II
Authors : Sarsam, R.D.; Lahiri, I.; Leschziner, A.E.
Deposited on : 2023-08-18
Resolution : 3.70 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:

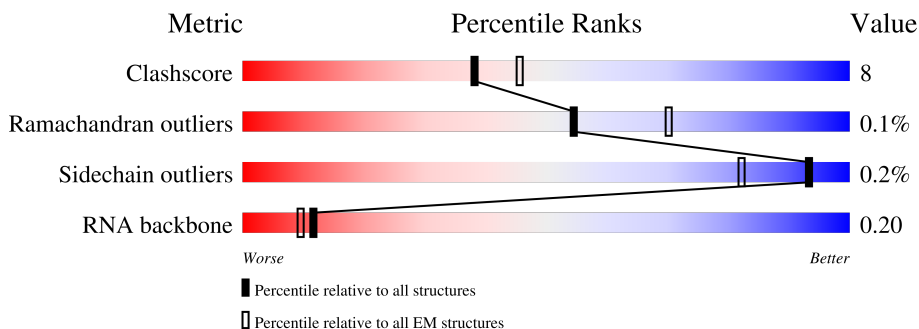
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	64% (green), 15% (yellow), 21% (grey)
2	B	1224	72% (green), 13% (yellow), 15% (grey)
3	C	318	69% (green), 14% (yellow), 16% (grey)
4	D	221	60% (green), 5% (yellow), 36% (grey)
5	E	215	79% (green), 21% (yellow)
6	F	155	44% (green), 8% (yellow), 48% (grey); 10% (red) above bar
7	G	171	84% (green), 16% (yellow); 10% (red) above bar

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Mol	Chain	Length	Quality of chain
8	H	146	 75% 16% 9%
9	I	122	 6% 67% 27% . .
10	J	70	 71% 21% 7%
11	K	120	 70% 17% 13%
12	L	70	 50% 16% 34%
13	N	47	 11% 21% . 66%
14	T	47	 21% 36% . 40%
15	R	17	 18% 35% 35% 29%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 58341 atoms, of which 28238 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
			Total	C	H	N	O	S		
1	A	1366	21323	6731	10649	1878	2004	61	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1041	15603	5065	7581	1417	1490	50	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	266	4148	1317	2053	348	417	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	D	142	1581	582	636	175	188	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	215	3548	1116	1788	310	322	12	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	81	1330	419	673	111	124	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	171	1762	690	664	197	207	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	133	2090	668	1030	174	213	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	117	1666	550	770	164	173	9	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	65	1074	339	542	93	94	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	104	1673	534	839	142	157	1	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	46	752	224	388	72	64	4	0	0

- Molecule 13 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
13	N	16	517	158	177	76	90	16	0	0

- Molecule 14 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
14	T	28	871	266	317	85	175	28	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
15	R	12	394	117	131	53	81	12	0	0

- Molecule 16 is ZINC ION (three-letter code: 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	

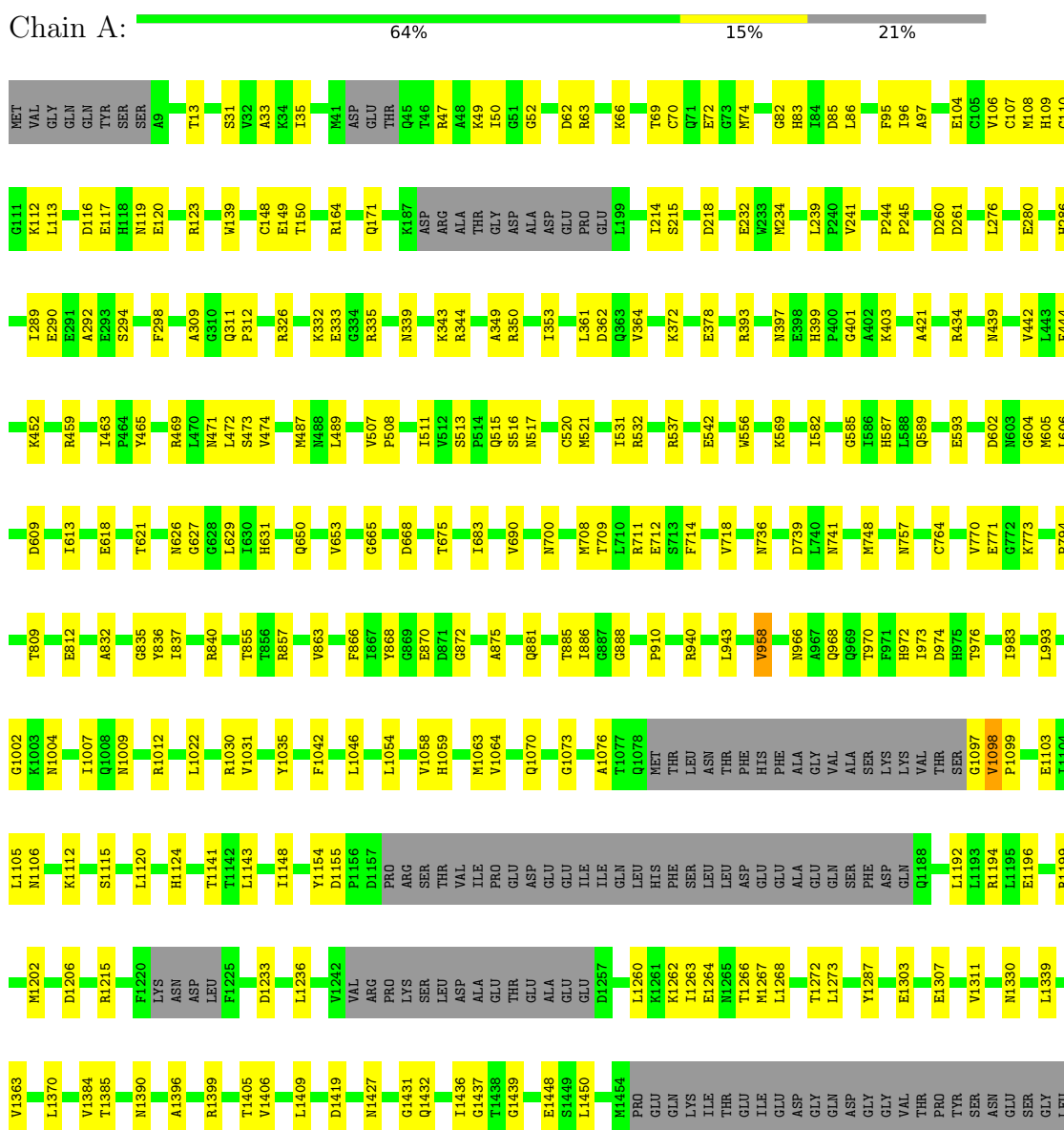
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

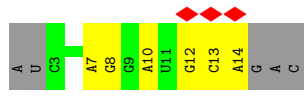
3 Residue-property plots

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 15: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.186	Depositor
Minimum map value	-1.622	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.599	Depositor
Map size (\AA)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.27	0/10862	0.49	1/14683 (0.0%)
2	B	0.28	0/8168	0.51	4/11029 (0.0%)
3	C	0.29	0/2133	0.44	0/2891
4	D	0.25	0/949	0.57	1/1289 (0.1%)
5	E	0.28	0/1796	0.50	0/2416
6	F	0.30	0/669	0.50	0/903
7	G	0.31	0/1112	0.68	5/1513 (0.3%)
8	H	0.31	0/1076	0.50	0/1455
9	I	0.26	0/911	0.55	0/1231
10	J	0.33	0/541	0.52	0/727
11	K	0.30	0/850	0.48	0/1148
12	L	0.26	0/366	0.57	0/485
13	N	0.82	1/385 (0.3%)	0.91	0/594
14	T	0.72	1/614 (0.2%)	0.87	1/941 (0.1%)
15	R	0.47	0/295	0.64	0/459
All	All	0.31	2/30727 (0.0%)	0.53	12/41764 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	7	DG	C1'-N9	-5.37	1.39	1.47
13	N	42	DA	C1'-N9	-5.16	1.40	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	PRO	N-CA-CB	6.52	111.12	103.30
4	D	196	PRO	N-CA-CB	6.52	111.12	103.30
1	A	910	PRO	N-CA-CB	6.51	111.11	103.30
7	G	105	PRO	N-CA-CB	6.50	111.10	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	81	PRO	N-CA-CB	6.50	111.10	103.30
2	B	877	PRO	N-CA-CB	6.50	111.10	103.30
7	G	128	PRO	N-CA-CB	6.50	111.09	103.30
2	B	114	PRO	N-CA-CB	6.49	111.09	103.30
2	B	171	PRO	N-CA-CB	6.49	111.09	103.30
7	G	116	PRO	N-CA-CB	6.49	111.09	103.30
7	G	127	PRO	N-CA-CB	6.49	111.09	103.30
14	T	22	DC	C1'-O4'-C4'	-5.56	104.54	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	10674	10649	10700	191	0
2	B	8022	7581	7762	112	0
3	C	2095	2053	2051	31	0
4	D	945	636	776	6	0
5	E	1760	1788	1788	31	0
6	F	657	673	673	10	0
7	G	1098	664	858	17	0
8	H	1060	1030	1030	17	0
9	I	896	770	805	26	0
10	J	532	542	542	11	0
11	K	834	839	839	16	0
12	L	364	388	388	10	0
13	N	340	177	177	15	0
14	T	554	317	318	40	0
15	R	263	131	132	6	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	1	0	0	0	0
All	All	30103	28238	28839	466	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 (466) 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:776:GLN:NE2	15:R:10:A:OP1	1.79	1.15
14:T:5:DC:H2''	14:T:6:DT:H72	1.48	0.93
1:A:832:ALA:O	14:T:18:DC:OP2	1.91	0.88
1:A:556:TRP:O	11:K:26:LYS:NZ	2.10	0.85
14:T:5:DC:H2''	14:T:6:DT:C5	2.15	0.82
1:A:1262:LYS:O	1:A:1266:THR:OG1	1.97	0.82
1:A:675:THR:OG1	1:A:736:ASN:OD1	1.97	0.82
1:A:700:ASN:OD1	9:I:96:SER:OG	1.97	0.82
14:T:5:DC:H2''	14:T:6:DT:C7	2.09	0.81
2:B:822:ASN:O	10:J:48:ARG:NH1	2.13	0.81
2:B:1033:LYS:NZ	2:B:1070:GLU:OE2	2.14	0.80
1:A:364:VAL:HG21	1:A:444:PHE:CZ	2.16	0.79
2:B:769:TYR:OH	15:R:13:C:N4	2.15	0.79
2:B:526:GLU:OE2	2:B:752:ALA:N	2.15	0.78
1:A:832:ALA:C	14:T:18:DC:OP2	2.22	0.78
1:A:770:VAL:HG22	1:A:771:GLU:OE1	1.83	0.77
1:A:1115:SER:OG	1:A:1330:ASN:OD1	2.02	0.77
2:B:523:CYS:SG	2:B:750:GLY:N	2.58	0.77
3:C:14:SER:OG	3:C:16:ASP:OD1	2.01	0.76
1:A:712:GLU:N	1:A:712:GLU:OE1	2.18	0.76
1:A:344:ARG:NE	2:B:1120:GLU:OE2	2.19	0.76
7:G:1:MET:N	7:G:80:LYS:O	2.19	0.75
1:A:148:CYS:SG	1:A:171:GLN:NE2	2.59	0.75
5:E:157:SER:N	5:E:160:GLU:OE2	2.20	0.75
2:B:986:GLN:OE1	2:B:1020:ARG:NH1	2.21	0.74
1:A:855:THR:OG1	1:A:857:ARG:NH1	2.20	0.74
2:B:394:ASP:OD2	2:B:395:GLN:N	2.21	0.73
1:A:832:ALA:HB1	14:T:18:DC:OP2	1.88	0.73
1:A:587:HIS:O	1:A:589:GLN:NE2	2.22	0.73
1:A:149:GLU:N	1:A:149:GLU:OE1	2.20	0.72
1:A:606:LEU:HD13	8:H:102:TYR:OH	1.88	0.72
4:D:205:ASP:OD2	4:D:206:GLU:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASN:OD1	3:C:141:GLY:N	2.21	0.72
1:A:709:THR:OG1	9:I:93:LYS:NZ	2.22	0.71
1:A:870:GLU:OE1	5:E:202:SER:OG	2.02	0.71
2:B:786:ASN:OD1	2:B:787:VAL:N	2.24	0.70
1:A:372:LYS:O	1:A:403:LYS:NZ	2.24	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.69
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.72	0.69
1:A:885:THR:O	1:A:940:ARG:NH1	2.26	0.69
1:A:966:ASN:O	1:A:970:THR:OG1	2.07	0.69
5:E:66:GLU:N	5:E:66:GLU:OE1	2.27	0.68
1:A:465:TYR:CD1	2:B:976:ILE:HD12	2.29	0.68
9:I:19:ASP:N	9:I:24:ARG:O	2.26	0.68
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.27	0.68
1:A:116:ASP:OD2	1:A:164:ARG:NE	2.27	0.67
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.76	0.67
13:N:42:DA:C2	14:T:7:DG:C2	2.83	0.67
1:A:393:ARG:NH1	1:A:421:ALA:O	2.27	0.67
1:A:1307:GLU:OE1	1:A:1307:GLU:N	2.28	0.67
2:B:233:PRO:O	2:B:260:GLY:N	2.28	0.67
5:E:13:TRP:NE1	5:E:37:LEU:O	2.29	0.66
2:B:604:ARG:NH2	2:B:692:TYR:O	2.27	0.66
2:B:259:TYR:O	2:B:266:ALA:N	2.27	0.66
1:A:350:ARG:NE	14:T:21:DC:H4'	2.11	0.66
12:L:27:LEU:HD11	12:L:37:LYS:NZ	2.10	0.66
1:A:332:LYS:NZ	1:A:333:GLU:OE2	2.29	0.65
10:J:9:SER:OG	10:J:45:CYS:SG	2.53	0.65
13:N:42:DA:C2	14:T:7:DG:N1	2.65	0.65
1:A:1396:ALA:N	1:A:1419:ASP:OD1	2.30	0.65
1:A:1448:GLU:OE1	7:G:58:ARG:NH1	2.30	0.65
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.30	0.64
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.28	0.64
3:C:108:GLU:N	3:C:108:GLU:OE1	2.29	0.64
1:A:372:LYS:NZ	1:A:397:ASN:O	2.23	0.64
2:B:562:GLY:O	2:B:590:HIS:ND1	2.30	0.64
2:B:620:ARG:NE	9:I:89:GLN:OE1	2.31	0.64
2:B:712:PRO:O	2:B:716:ASN:N	2.29	0.64
11:K:29:ASN:ND2	11:K:77:THR:OG1	2.30	0.64
4:D:40:HIS:O	7:G:73:LYS:NZ	2.21	0.64
1:A:286:HIS:NE2	1:A:290:GLU:OE2	2.31	0.64
13:N:42:DA:N1	14:T:7:DG:C6	2.66	0.64
1:A:668:ASP:O	1:A:741:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:169:ARG:NE	6:F:140:ASP:OD2	2.31	0.64
1:A:832:ALA:CA	14:T:18:DC:OP2	2.46	0.64
2:B:748:ILE:HG23	2:B:749:LEU:HD22	1.79	0.64
1:A:35:ILE:HD13	1:A:241:VAL:HG21	1.80	0.63
1:A:832:ALA:O	14:T:18:DC:P	2.56	0.63
2:B:227:LYS:NZ	2:B:235:SER:OG	2.31	0.63
9:I:68:LEU:HD12	9:I:69:PRO:HD2	1.79	0.63
14:T:5:DC:C2'	14:T:6:DT:H72	2.26	0.63
2:B:776:GLN:NE2	15:R:10:A:P	2.70	0.63
9:I:103:CYS:O	9:I:107:SER:N	2.29	0.63
2:B:298:LEU:O	2:B:302:CYS:N	2.30	0.62
1:A:232:GLU:OE1	1:A:232:GLU:N	2.32	0.62
14:T:12:DT:H2'	14:T:13:DT:H72	1.81	0.62
3:C:66:ARG:NH2	3:C:143:LEU:O	2.31	0.61
5:E:54:GLN:O	5:E:56:LYS:N	2.33	0.61
2:B:397:ASP:OD2	2:B:515:HIS:NE2	2.32	0.61
5:E:61:GLN:NE2	5:E:62:ALA:O	2.33	0.61
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.83	0.61
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.31	0.61
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.34	0.60
7:G:28:THR:O	7:G:32:GLU:OE1	2.19	0.60
8:H:33:GLN:OE1	8:H:35:GLN:NE2	2.34	0.60
9:I:70:ARG:HD3	9:I:84:VAL:HG12	1.83	0.60
2:B:183:GLU:N	2:B:183:GLU:OE1	2.33	0.60
2:B:221:ASN:N	2:B:241:ARG:O	2.35	0.60
1:A:626:ASN:O	1:A:631:HIS:ND1	2.33	0.60
1:A:1215:ARG:NE	1:A:1272:THR:O	2.29	0.60
8:H:94:ASP:OD2	8:H:146:ARG:N	2.32	0.60
1:A:66:LYS:O	1:A:69:THR:N	2.35	0.59
1:A:66:LYS:O	1:A:70:CYS:N	2.33	0.59
1:A:835:GLY:HA3	14:T:18:DC:H4'	1.83	0.59
2:B:487:THR:HG21	2:B:777:ALA:O	2.02	0.59
3:C:75:MET:O	3:C:246:ARG:NH2	2.35	0.59
1:A:113:LEU:O	1:A:164:ARG:NH1	2.35	0.59
1:A:362:ASP:O	1:A:459:ARG:N	2.35	0.59
11:K:45:LEU:HD21	11:K:94:ILE:HD12	1.83	0.59
13:N:47:DG:C2	14:T:2:DG:C2	2.91	0.59
5:E:21:GLU:OE2	5:E:146:HIS:NE2	2.36	0.59
1:A:86:LEU:HD11	1:A:239:LEU:HD23	1.84	0.59
13:N:40:DG:H2''	13:N:41:DC:C6	2.38	0.59
1:A:683:ILE:HD11	1:A:764:CYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.35	0.58
2:B:498:THR:OG1	2:B:537:LYS:O	2.15	0.58
14:T:3:DC:C2'	14:T:4:DT:H72	2.33	0.58
1:A:613:ILE:HG21	8:H:102:TYR:CE1	2.38	0.58
3:C:92:CYS:SG	3:C:94:LYS:NZ	2.76	0.58
2:B:570:VAL:HG12	2:B:573:GLN:OE1	2.04	0.58
1:A:72:GLU:N	1:A:72:GLU:OE1	2.37	0.57
1:A:832:ALA:CB	14:T:18:DC:OP2	2.52	0.57
1:A:1405:THR:O	1:A:1409:LEU:HD23	2.04	0.57
2:B:223:VAL:HG11	2:B:384:ARG:NH2	2.19	0.57
3:C:16:ASP:OD1	3:C:17:ASN:N	2.38	0.57
10:J:23:ASN:O	10:J:27:GLU:N	2.37	0.57
1:A:1436:ILE:O	1:A:1439:GLY:N	2.35	0.57
13:N:40:DG:H2''	13:N:41:DC:C5	2.40	0.57
14:T:8:DC:H2'	14:T:9:DT:H71	1.87	0.56
14:T:12:DT:H2'	14:T:13:DT:C7	2.35	0.56
2:B:219:ALA:HB3	2:B:222:ILE:HD13	1.86	0.56
2:B:238:ALA:HB2	2:B:385:LEU:HD21	1.87	0.56
2:B:1053:GLU:N	2:B:1053:GLU:OE1	2.35	0.56
9:I:24:ARG:NH2	9:I:37:GLU:OE2	2.38	0.56
9:I:85:PHE:CD1	9:I:99:LEU:HD23	2.39	0.56
3:C:5:GLY:O	3:C:24:ASN:ND2	2.37	0.56
1:A:294:SER:O	1:A:298:PHE:N	2.36	0.56
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.87	0.56
5:E:32:GLN:O	5:E:36:GLU:N	2.35	0.56
14:T:3:DC:C6	14:T:4:DT:H72	2.41	0.56
1:A:361:LEU:HD21	1:A:473:SER:OG	2.06	0.55
1:A:1148:ILE:N	1:A:1196:GLU:O	2.39	0.55
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.36	0.55
2:B:128:LEU:N	2:B:168:GLY:O	2.36	0.55
2:B:452:THR:O	2:B:456:GLY:N	2.38	0.55
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.35	0.55
1:A:1004:ASN:OD1	5:E:167:ARG:NE	2.40	0.55
1:A:83:HIS:NE2	1:A:85:ASP:OD1	2.35	0.55
1:A:1059:HIS:HB3	6:F:86:THR:HG23	1.89	0.55
1:A:309:ALA:HB1	14:T:14:DC:OP2	2.08	0.55
1:A:757:ASN:ND2	2:B:1018:PRO:O	2.40	0.54
1:A:863:VAL:HG23	5:E:170:LEU:HD11	1.90	0.54
1:A:968:GLN:HA	1:A:973:ILE:HD12	1.89	0.54
2:B:301:ILE:O	2:B:383:ASN:ND2	2.37	0.54
9:I:7:CYS:O	9:I:11:ASN:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:ASP:HB2	9:I:26:LEU:HD23	1.90	0.54
1:A:966:ASN:O	1:A:970:THR:N	2.41	0.54
5:E:116:ILE:HG23	5:E:121:MET:HE1	1.90	0.54
2:B:624:LEU:HD23	2:B:625:LYS:N	2.23	0.54
2:B:223:VAL:HG11	2:B:384:ARG:HH22	1.73	0.54
2:B:547:VAL:N	2:B:612:GLU:OE2	2.37	0.54
2:B:578:THR:HG23	2:B:622:LYS:C	2.29	0.53
9:I:101:PHE:N	9:I:110:PHE:O	2.41	0.53
1:A:472:LEU:HD22	2:B:835:GLN:HG3	1.90	0.53
2:B:1223:ASP:O	2:B:1224:PHE:HB3	2.08	0.53
1:A:50:ILE:HG22	1:A:52:GLY:H	1.73	0.53
1:A:1427:ASN:O	1:A:1431:GLY:N	2.40	0.53
8:H:27:GLU:OE2	8:H:28:ALA:N	2.41	0.53
2:B:280:ILE:CG2	2:B:284:ILE:HD11	2.39	0.53
7:G:65:ASP:OD2	7:G:65:ASP:N	2.41	0.53
1:A:771:GLU:O	1:A:773:LYS:NZ	2.35	0.53
11:K:49:GLU:OE1	11:K:94:ILE:HG12	2.09	0.53
2:B:816:GLU:OE2	10:J:59:LYS:NZ	2.39	0.53
11:K:53:ASP:OD1	11:K:54:ARG:N	2.42	0.53
12:L:31:CYS:SG	12:L:36:SER:OG	2.67	0.53
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.39	0.53
8:H:26:ILE:HG13	8:H:42:ILE:HD12	1.89	0.53
1:A:665:GLY:N	1:A:668:ASP:OD2	2.38	0.53
2:B:745:PRO:O	2:B:748:ILE:HG22	2.09	0.52
7:G:39:THR:O	7:G:43:GLY:N	2.42	0.52
10:J:19:GLU:OE1	10:J:19:GLU:N	2.35	0.52
5:E:112:TYR:CE2	5:E:134:THR:HB	2.44	0.52
5:E:100:ILE:O	5:E:104:ASN:N	2.43	0.52
5:E:68:SER:O	5:E:72:PHE:N	2.36	0.52
5:E:138:ALA:O	5:E:141:VAL:HG22	2.10	0.52
1:A:31:SER:OG	1:A:33:ALA:O	2.27	0.51
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.43	0.51
2:B:836:GLU:OE1	2:B:836:GLU:HA	2.09	0.51
2:B:1010:LEU:HD23	2:B:1011:ILE:N	2.26	0.51
13:N:47:DG:N2	14:T:2:DG:C4	2.79	0.51
1:A:335:ARG:NE	1:A:339:ASN:OD1	2.41	0.51
3:C:48:SER:OG	12:L:66:GLN:OE1	2.20	0.51
1:A:353:ILE:HG21	1:A:487:MET:CE	2.40	0.51
1:A:711:ARG:NH2	9:I:95:THR:OG1	2.36	0.51
1:A:837:ILE:HD12	1:A:840:ARG:HE	1.75	0.51
2:B:272:THR:OG1	2:B:279:ASP:OD1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLU:N	1:A:593:GLU:OE1	2.37	0.51
1:A:517:ASN:ND2	1:A:875:ALA:O	2.44	0.51
2:B:958:GLN:OE1	2:B:958:GLN:N	2.37	0.51
13:N:42:DA:H2''	13:N:43:DG:C8	2.45	0.51
1:A:604:GLY:O	1:A:605:MET:CE	2.59	0.51
13:N:42:DA:C2	14:T:7:DG:C6	2.99	0.51
1:A:74:MET:O	2:B:1116:ARG:NH2	2.40	0.50
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.46	0.50
12:L:60:ARG:HE	12:L:61:THR:H	1.59	0.50
9:I:8:ARG:NH1	9:I:32:CYS:SG	2.79	0.50
10:J:32:GLU:OE1	10:J:32:GLU:N	2.43	0.50
1:A:108:MET:O	1:A:109:HIS:HB2	2.11	0.50
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.93	0.50
3:C:169:LYS:NZ	12:L:69:ALA:O	2.38	0.50
5:E:157:SER:OG	5:E:160:GLU:OE1	2.29	0.50
5:E:170:LEU:HD23	5:E:171:LYS:O	2.12	0.50
1:A:117:GLU:O	1:A:123:ARG:NH1	2.45	0.50
1:A:881:GLN:NE2	1:A:958:VAL:O	2.45	0.50
7:G:39:THR:HG23	7:G:42:PHE:H	1.76	0.50
1:A:1063:MET:HG2	2:B:1139:ILE:HG22	1.92	0.50
1:A:13:THR:OG1	1:A:1432:GLN:OE1	2.26	0.50
1:A:474:VAL:HG22	1:A:474:VAL:O	2.11	0.50
3:C:167:HIS:NE2	12:L:70:ARG:O	2.39	0.50
14:T:18:DC:H2'	14:T:19:DA:C8	2.46	0.50
1:A:1054:LEU:HD13	6:F:84:TYR:HE2	1.77	0.50
8:H:16:ASP:OD1	8:H:18:GLY:N	2.43	0.50
5:E:175:LEU:HD12	5:E:213:ILE:HD11	1.94	0.50
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.12	0.49
1:A:1202:MET:O	1:A:1206:ASP:N	2.45	0.49
2:B:87:LYS:N	2:B:137:TYR:O	2.45	0.49
11:K:49:GLU:OE2	11:K:93:SER:HB3	2.11	0.49
2:B:1156:ASP:O	2:B:1198:TYR:N	2.44	0.49
14:T:12:DT:C6	14:T:13:DT:H72	2.47	0.49
1:A:1141:THR:O	1:A:1273:LEU:N	2.44	0.49
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.94	0.49
2:B:576:ASP:OD1	2:B:622:LYS:NZ	2.44	0.49
14:T:23:DT:H3	15:R:7:A:H61	1.61	0.49
11:K:45:LEU:HD21	11:K:94:ILE:CD1	2.43	0.49
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.40	0.49
8:H:145:ARG:O	8:H:146:ARG:HB2	2.12	0.49
13:N:42:DA:N3	14:T:7:DG:C2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:VAL:HG21	2:B:318:VAL:HA	1.95	0.49
12:L:27:LEU:HD11	12:L:37:LYS:CE	2.43	0.49
9:I:63:GLY:O	9:I:70:ARG:NH2	2.46	0.48
1:A:399:HIS:O	1:A:401:GLY:N	2.44	0.48
1:A:886:ILE:HD11	1:A:943:LEU:HD23	1.94	0.48
11:K:49:GLU:OE2	11:K:90:ALA:HA	2.13	0.48
1:A:626:ASN:OD1	1:A:627:GLY:N	2.47	0.48
1:A:983:ILE:HD12	1:A:983:ILE:H	1.78	0.48
14:T:6:DT:H73	14:T:6:DT:OP2	2.14	0.48
2:B:791:THR:HG22	2:B:858:SER:O	2.14	0.48
6:F:149:GLU:N	6:F:149:GLU:OE1	2.40	0.48
1:A:739:ASP:OD1	8:H:19:ARG:NH2	2.46	0.48
2:B:310:MET:CG	2:B:386:LEU:HD13	2.44	0.48
1:A:585:GLY:N	1:A:609:ASP:OD1	2.43	0.48
2:B:280:ILE:HG23	2:B:284:ILE:HD11	1.94	0.48
13:N:47:DG:N1	14:T:2:DG:C6	2.82	0.48
1:A:107:CYS:N	1:A:112:LYS:O	2.44	0.48
1:A:364:VAL:HG21	1:A:444:PHE:HZ	1.76	0.48
14:T:3:DC:H2'	14:T:4:DT:H72	1.96	0.48
2:B:60:GLN:OE1	2:B:95:ILE:N	2.47	0.48
2:B:1120:GLU:N	2:B:1120:GLU:OE1	2.47	0.48
9:I:75:CYS:O	9:I:79:HIS:N	2.42	0.48
5:E:96:PHE:CE2	5:E:100:ILE:HD11	2.49	0.48
1:A:582:ILE:HD12	1:A:629:LEU:HD21	1.95	0.47
1:A:1106:ASN:OD1	1:A:1385:THR:HG21	2.14	0.47
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.95	0.47
8:H:11:GLN:NE2	8:H:52:GLN:O	2.46	0.47
9:I:87:GLN:NE2	9:I:88:SER:O	2.46	0.47
2:B:174:LEU:HD12	2:B:202:TYR:CZ	2.49	0.47
15:R:14:A:O5'	15:R:14:A:H8	1.97	0.47
1:A:62:ASP:OD1	1:A:63:ARG:N	2.47	0.47
1:A:1263:ILE:O	1:A:1267:MET:HE1	2.14	0.47
2:B:835:GLN:O	2:B:1013:ASN:ND2	2.47	0.47
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.96	0.47
11:K:113:THR:O	11:K:117:ASP:N	2.42	0.47
1:A:1103:GLU:OE2	1:A:1112:LYS:N	2.37	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.50	0.47
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.43	0.47
5:E:28:TYR:CE1	5:E:78:LEU:HD11	2.50	0.47
1:A:150:THR:O	1:A:164:ARG:N	2.47	0.47
1:A:809:THR:OG1	1:A:812:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:O	2:B:288:ALA:N	2.44	0.47
2:B:711:GLU:O	2:B:715:ALA:N	2.38	0.47
3:C:89:GLU:O	3:C:91:HIS:N	2.47	0.47
3:C:265:MET:HG2	11:K:21:ILE:HD12	1.97	0.47
5:E:112:TYR:CE1	5:E:116:ILE:HB	2.50	0.47
1:A:260:ASP:OD1	1:A:261:ASP:N	2.47	0.47
1:A:276:LEU:HD12	1:A:292:ALA:HB3	1.96	0.47
1:A:605:MET:HG3	1:A:621:THR:OG1	2.15	0.47
1:A:1390:ASN:OD1	1:A:1399:ARG:HG3	2.15	0.47
2:B:500:THR:OG1	2:B:535:LEU:O	2.21	0.46
7:G:57:GLN:O	7:G:58:ARG:HB2	2.14	0.46
3:C:58:LEU:HD21	10:J:57:ILE:HD13	1.96	0.46
1:A:613:ILE:HG21	8:H:102:TYR:CD1	2.50	0.46
1:A:690:VAL:HG11	1:A:794:PRO:HG3	1.96	0.46
1:A:1097:GLY:O	1:A:1098:VAL:HB	2.15	0.46
11:K:113:THR:HG22	11:K:117:ASP:OD1	2.15	0.46
14:T:3:DC:H2''	14:T:4:DT:C7	2.44	0.46
1:A:1105:LEU:HD12	1:A:1384:VAL:HG21	1.97	0.46
1:A:508:PRO:O	1:A:511:ILE:HG12	2.15	0.46
4:D:72:ARG:NH2	7:G:24:GLN:OE1	2.47	0.46
11:K:24:ASP:OD1	11:K:25:THR:N	2.47	0.46
1:A:339:ASN:ND2	2:B:1117:GLN:OE1	2.46	0.46
1:A:1199:ARG:CZ	1:A:1236:LEU:HD21	2.46	0.46
2:B:950:ASP:OD1	2:B:969:ARG:NH1	2.41	0.46
3:C:86:CYS:SG	3:C:94:LYS:NZ	2.83	0.46
3:C:163:ILE:HG22	3:C:165:LYS:H	1.81	0.46
12:L:68:GLU:O	12:L:68:GLU:HG2	2.15	0.46
3:C:148:ARG:NE	10:J:61:LEU:O	2.43	0.46
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.48	0.46
1:A:542:GLU:OE2	1:A:569:LYS:NZ	2.37	0.46
1:A:832:ALA:O	14:T:18:DC:O5'	2.34	0.46
1:A:511:ILE:HD13	1:A:521:MET:HE2	1.97	0.46
2:B:310:MET:HG3	2:B:386:LEU:HD13	1.98	0.46
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.44	0.46
2:B:554:ILE:HD12	2:B:554:ILE:H	1.81	0.45
2:B:757:PRO:HG3	2:B:983:ARG:HE	1.80	0.45
1:A:532:ARG:NH2	1:A:748:MET:SD	2.89	0.45
1:A:1339:LEU:HD13	5:E:144:ILE:HG23	1.99	0.45
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.81	0.45
4:D:165:GLN:O	4:D:169:SER:OG	2.20	0.45
1:A:507:VAL:N	1:A:508:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLN:CD	1:A:516:SER:HG	2.10	0.45
1:A:836:TYR:HB2	14:T:17:DC:O3'	2.16	0.45
2:B:1169:MET:SD	2:B:1169:MET:N	2.89	0.45
7:G:49:LEU:N	7:G:75:ARG:O	2.48	0.45
1:A:335:ARG:NH2	1:A:339:ASN:OD1	2.48	0.45
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.16	0.45
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.99	0.45
1:A:472:LEU:HD22	2:B:835:GLN:CG	2.47	0.45
1:A:1054:LEU:HD13	6:F:84:TYR:CE2	2.51	0.45
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	1.98	0.45
6:F:85:MET:SD	6:F:89:GLU:HG3	2.56	0.45
1:A:215:SER:OG	1:A:218:ASP:OD2	2.31	0.45
1:A:613:ILE:HG23	8:H:117:SER:HB2	1.99	0.45
1:A:1268:LEU:N	1:A:1268:LEU:HD12	2.32	0.45
2:B:1122:ARG:HB3	14:T:23:DT:OP2	2.16	0.45
9:I:17:ARG:N	9:I:26:LEU:O	2.49	0.45
2:B:1026:LEU:HD12	2:B:1026:LEU:H	1.81	0.45
3:C:58:LEU:HD11	10:J:2:ILE:HD13	1.98	0.45
1:A:311:GLN:N	1:A:312:PRO:CD	2.80	0.44
5:E:50:MET:O	5:E:50:MET:SD	2.75	0.44
1:A:349:ALA:CB	2:B:1105:ALA:HB2	2.46	0.44
1:A:708:MET:SD	1:A:712:GLU:HB2	2.57	0.44
2:B:261:ARG:O	2:B:266:ALA:HB3	2.17	0.44
2:B:832:GLY:O	2:B:835:GLN:HG2	2.17	0.44
11:K:93:SER:OG	11:K:97:LYS:NZ	2.50	0.44
1:A:604:GLY:O	1:A:605:MET:HG2	2.17	0.44
1:A:1215:ARG:NH2	1:A:1272:THR:O	2.51	0.44
3:C:61:GLU:OE1	3:C:61:GLU:N	2.37	0.44
3:C:136:ASP:OD2	3:C:139:GLY:N	2.51	0.44
1:A:1260:LEU:O	1:A:1264:GLU:N	2.46	0.44
9:I:74:GLU:OE1	9:I:74:GLU:N	2.49	0.44
14:T:3:DC:C2'	14:T:4:DT:C7	2.96	0.44
14:T:14:DC:H2''	14:T:15:DT:H5'	1.99	0.44
2:B:386:LEU:O	2:B:390:LEU:N	2.36	0.44
9:I:24:ARG:NH2	9:I:38:ALA:O	2.50	0.44
15:R:7:A:H2'	15:R:8:G:C8	2.52	0.44
1:A:513:SER:HB2	1:A:520:CYS:SG	2.58	0.44
1:A:1311:VAL:HG13	1:A:1311:VAL:O	2.18	0.44
2:B:1084:GLN:OE1	3:C:192:TRP:N	2.43	0.44
4:D:41:GLN:NE2	7:G:6:ASP:OD2	2.39	0.44
7:G:64:THR:OG1	7:G:65:ASP:OD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:ASP:OD1	2:B:199:MET:N	2.51	0.44
3:C:44:LEU:HD21	3:C:97:VAL:HG11	1.99	0.44
1:A:537:ARG:NH2	1:A:602:ASP:OD1	2.51	0.43
1:A:531:ILE:CG1	1:A:653:VAL:HG21	2.48	0.43
1:A:1287:TYR:O	1:A:1303:GLU:N	2.51	0.43
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.00	0.43
1:A:452:LYS:N	1:A:1070:GLN:OE1	2.51	0.43
3:C:39:ALA:HB3	3:C:40:GLU:OE1	2.18	0.43
1:A:1097:GLY:O	1:A:1099:PRO:HD2	2.18	0.43
1:A:280:GLU:HA	1:A:289:ILE:HD11	2.00	0.43
2:B:211:VAL:HG22	2:B:212:LEU:N	2.34	0.43
1:A:47:ARG:O	1:A:49:LYS:NZ	2.47	0.43
1:A:1155:ASP:HB2	1:A:1192:LEU:HD11	2.01	0.43
3:C:39:ALA:O	3:C:164:ALA:HB3	2.19	0.43
6:F:96:THR:O	6:F:100:GLN:HG2	2.19	0.43
1:A:439:ASN:OD1	1:A:459:ARG:NH1	2.49	0.43
12:L:27:LEU:HD11	12:L:37:LYS:HE2	2.00	0.43
1:A:35:ILE:HD13	1:A:241:VAL:CG2	2.47	0.42
1:A:244:PRO:N	1:A:245:PRO:CD	2.82	0.42
1:A:866:PHE:N	5:E:208:TYR:OH	2.51	0.42
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.19	0.42
2:B:60:GLN:NE2	2:B:93:GLY:O	2.45	0.42
2:B:381:MET:O	2:B:385:LEU:HD23	2.19	0.42
6:F:77:ASP:OD2	6:F:77:ASP:N	2.51	0.42
2:B:1193:GLN:O	2:B:1194:ILE:HD13	2.18	0.42
7:G:30:LEU:HD22	7:G:72:VAL:CG1	2.47	0.42
11:K:57:LEU:HD21	11:K:78:THR:HG22	2.01	0.42
1:A:106:VAL:HG21	1:A:214:ILE:HD11	2.01	0.42
1:A:618:GLU:N	1:A:618:GLU:OE1	2.53	0.42
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.20	0.42
2:B:356:LEU:O	2:B:374:LYS:NZ	2.44	0.42
2:B:1070:GLU:N	2:B:1070:GLU:OE1	2.52	0.42
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.20	0.42
8:H:32:THR:O	8:H:33:GLN:NE2	2.52	0.42
2:B:423:LYS:NZ	2:B:452:THR:HG21	2.34	0.42
13:N:44:DA:H2"	13:N:45:DG:C8	2.54	0.42
1:A:613:ILE:HG23	8:H:117:SER:CB	2.49	0.42
2:B:444:MET:SD	2:B:444:MET:N	2.90	0.42
3:C:33:LEU:O	3:C:36:VAL:HG12	2.20	0.42
2:B:786:ASN:OD1	2:B:787:VAL:HG23	2.19	0.42
2:B:227:LYS:HD2	2:B:236:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ILE:HD11	2:B:691:GLU:HG3	2.02	0.42
1:A:872:GLY:O	1:A:1058:VAL:HG12	2.20	0.42
2:B:387:LEU:O	2:B:391:ASP:N	2.53	0.42
11:K:21:ILE:HA	11:K:33:ILE:HG22	2.01	0.42
1:A:31:SER:CB	1:A:83:HIS:HB2	2.49	0.41
1:A:95:PHE:HB3	1:A:234:MET:HE2	2.01	0.41
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.55	0.41
1:A:1143:LEU:HD22	1:A:1267:MET:HB3	2.02	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.55	0.41
6:F:128:LYS:O	6:F:129:LYS:HE2	2.20	0.41
9:I:18:GLU:HA	9:I:25:LEU:HD23	2.01	0.41
1:A:107:CYS:CB	1:A:110:CYS:HB3	2.51	0.41
14:T:12:DT:C2'	14:T:13:DT:H72	2.47	0.41
1:A:1405:THR:OG1	1:A:1406:VAL:N	2.53	0.41
2:B:956:THR:HG22	12:L:46:VAL:HG21	2.02	0.41
8:H:39:THR:O	8:H:123:MET:HA	2.20	0.41
1:A:119:ASN:OD1	1:A:120:GLU:N	2.54	0.41
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.45	0.41
1:A:531:ILE:HG12	1:A:653:VAL:HG21	2.02	0.41
1:A:106:VAL:HG12	1:A:107:CYS:N	2.35	0.41
5:E:116:ILE:HG13	5:E:120:ALA:HB3	2.01	0.41
2:B:1122:ARG:HB3	14:T:23:DT:P	2.60	0.41
9:I:24:ARG:NH1	9:I:25:LEU:O	2.53	0.41
9:I:43:VAL:HG13	9:I:44:TYR:CD1	2.56	0.41
1:A:364:VAL:HG23	1:A:469:ARG:O	2.20	0.41
5:E:9:ILE:HG21	5:E:43:LYS:HG2	2.03	0.41
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.02	0.41
8:H:102:TYR:N	8:H:115:TYR:O	2.49	0.41
9:I:26:LEU:O	9:I:26:LEU:HD12	2.21	0.41
1:A:35:ILE:HD11	1:A:82:GLY:HA3	2.02	0.41
1:A:353:ILE:HG21	1:A:487:MET:HE2	2.02	0.41
1:A:471:ASN:ND2	1:A:650:GLN:OE1	2.38	0.41
1:A:972:HIS:O	1:A:972:HIS:ND1	2.54	0.41
1:A:1002:GLY:H	1:A:1007:ILE:HG21	1.86	0.41
1:A:1154:TYR:HB2	9:I:25:LEU:HD11	2.03	0.41
2:B:235:SER:N	2:B:258:LEU:O	2.50	0.41
2:B:254:LEU:HD23	2:B:255:GLN:N	2.36	0.41
2:B:370:PHE:O	2:B:374:LYS:N	2.49	0.41
2:B:615:MET:N	2:B:615:MET:SD	2.94	0.41
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.21	0.41
2:B:983:ARG:NH1	2:B:1091:TYR:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:TYR:CZ	5:E:78:LEU:HD11	2.55	0.41
5:E:196:VAL:O	5:E:211:TYR:HA	2.21	0.41
7:G:37:SER:HB2	7:G:45:ILE:HD12	2.03	0.41
9:I:26:LEU:HD13	9:I:35:VAL:HG13	2.03	0.41
14:T:6:DT:C7	14:T:6:DT:OP2	2.69	0.41
1:A:463:ILE:HD13	1:A:469:ARG:HG3	2.03	0.41
2:B:546:SER:OG	2:B:632:ARG:N	2.42	0.41
2:B:639:ILE:HD12	2:B:689:LEU:C	2.41	0.41
2:B:1122:ARG:NH1	2:B:1122:ARG:HG2	2.36	0.41
4:D:50:LEU:HG	4:D:55:ALA:HB2	2.03	0.41
1:A:515:GLN:NE2	1:A:1363:VAL:HG12	2.37	0.40
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	2.02	0.40
2:B:612:GLU:O	2:B:632:ARG:NH2	2.49	0.40
1:A:974:ASP:OD1	1:A:976:THR:OG1	2.23	0.40
13:N:35:DA:H2''	13:N:36:DA:C8	2.56	0.40
1:A:96:ILE:HG23	1:A:97:ALA:N	2.36	0.40
6:F:131:PRO:O	6:F:132:LEU:HD23	2.21	0.40
7:G:27:LYS:NZ	7:G:52:ASP:OD1	2.45	0.40
10:J:64:ASN:N	10:J:65:PRO:CD	2.85	0.40
1:A:1436:ILE:O	1:A:1437:GLY:C	2.60	0.40
11:K:42:LEU:HD23	11:K:42:LEU:H	1.87	0.40
13:N:33:DA:H2''	13:N:34:DG:C8	2.57	0.40
1:A:714:PHE:O	1:A:718:VAL:HG23	2.21	0.40
13:N:44:DA:H2''	13:N:45:DG:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1352/1733 (78%)	1296 (96%)	54 (4%)	2 (0%)	51 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1019/1224 (83%)	969 (95%)	50 (5%)	0	100	100
3	C	264/318 (83%)	259 (98%)	5 (2%)	0	100	100
4	D	138/221 (62%)	137 (99%)	1 (1%)	0	100	100
5	E	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
6	F	79/155 (51%)	74 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	158 (94%)	11 (6%)	0	100	100
8	H	127/146 (87%)	117 (92%)	10 (8%)	0	100	100
9	I	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
11	K	102/120 (85%)	100 (98%)	2 (2%)	0	100	100
12	L	44/70 (63%)	41 (93%)	3 (7%)	0	100	100
All	All	3685/4565 (81%)	3533 (96%)	150 (4%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1098	VAL
1	A	958	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1167/1520 (77%)	1166 (100%)	1 (0%)	93	98
2	B	822/1061 (78%)	821 (100%)	1 (0%)	93	98
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	68/200 (34%)	68 (100%)	0	100	100
5	E	197/197 (100%)	196 (100%)	1 (0%)	88	94
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	72/152 (47%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	117/128 (91%)	116 (99%)	1 (1%)	78	88
9	I	93/116 (80%)	91 (98%)	2 (2%)	52	72
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	89/102 (87%)	89 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3031/4009 (76%)	3025 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1194	ARG
2	B	444	MET
5	E	7	ARG
8	H	87	ARG
9	I	8	ARG
9	I	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	HIS
1	A	760	GLN
1	A	851	HIS
2	B	587	HIS
4	D	40	HIS
11	K	29	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	11/17 (64%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	12	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

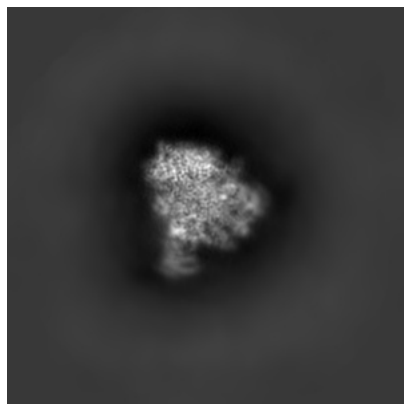
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41652. These allow visual inspection of the internal detail of the map and identification of artifacts.

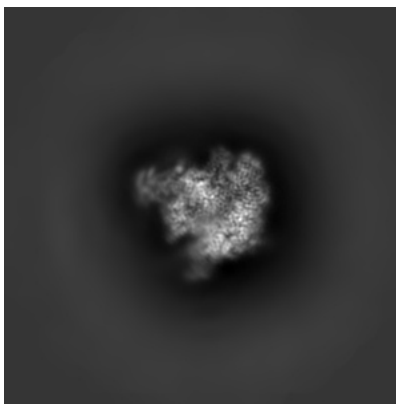
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

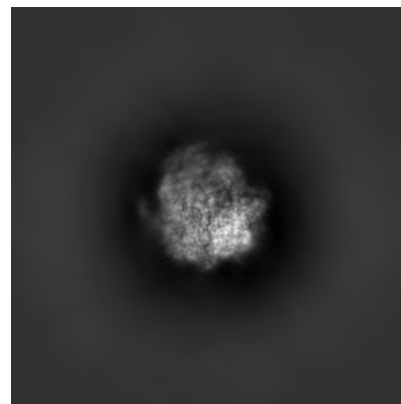
6.1.1 Primary map



X

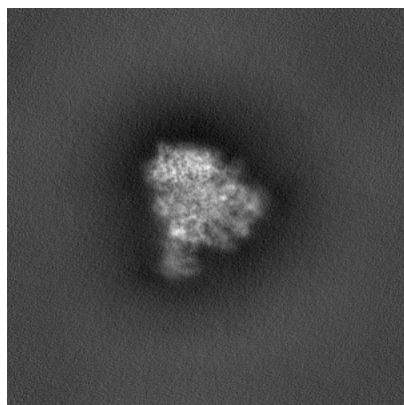


Y

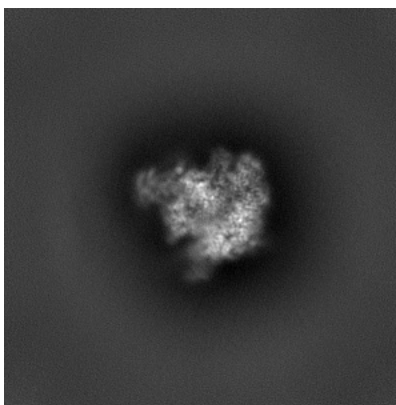


Z

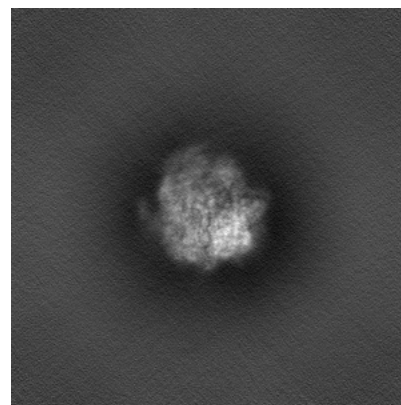
6.1.2 Raw map



X



Y

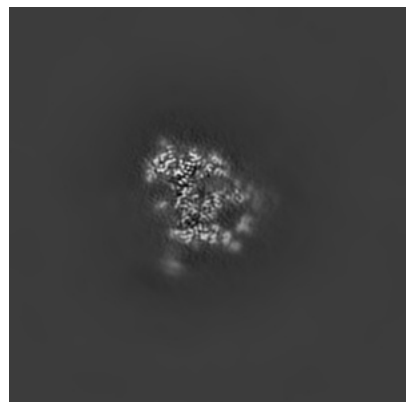


Z

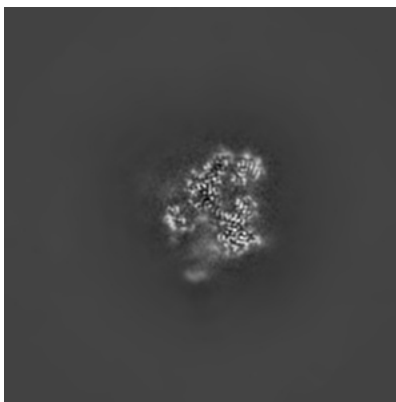
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

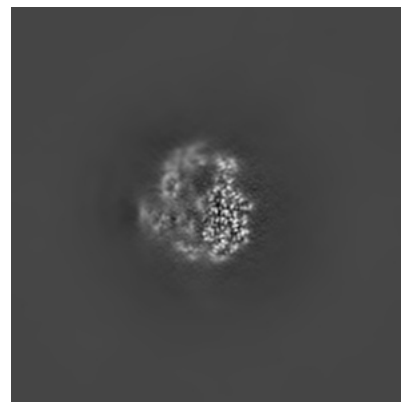
6.2.1 Primary map



X Index: 192

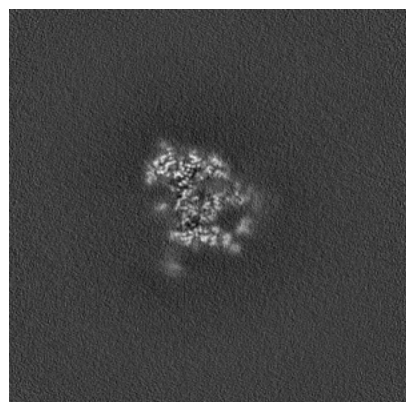


Y Index: 192

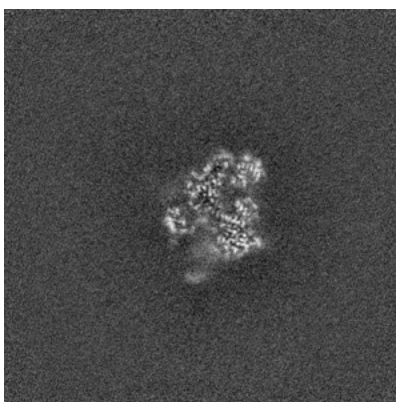


Z Index: 192

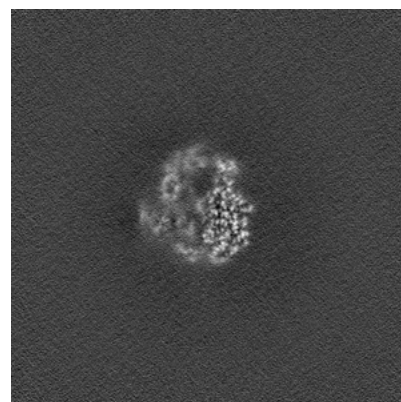
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

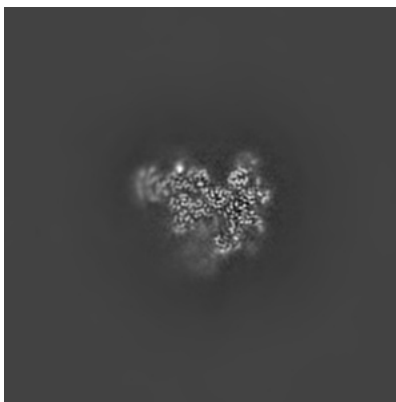
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

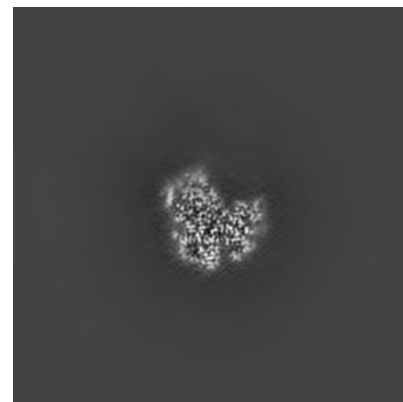
6.3.1 Primary map



X Index: 215

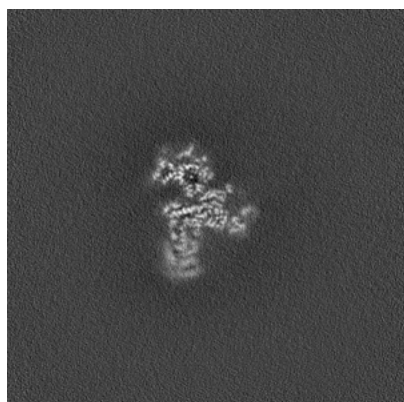


Y Index: 167

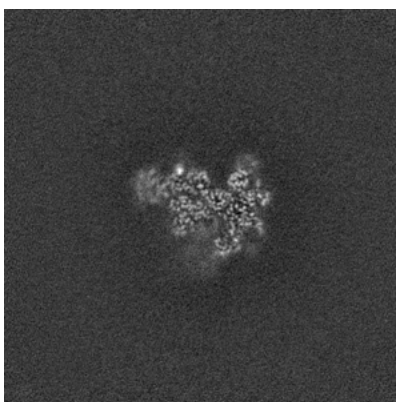


Z Index: 226

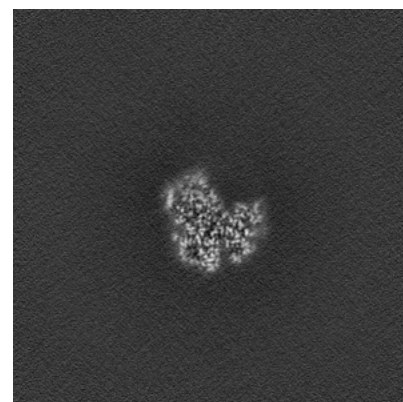
6.3.2 Raw map



X Index: 215



Y Index: 167

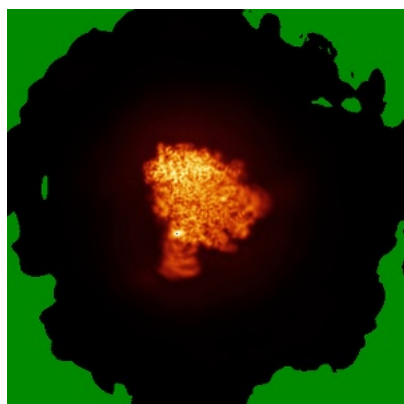


Z Index: 226

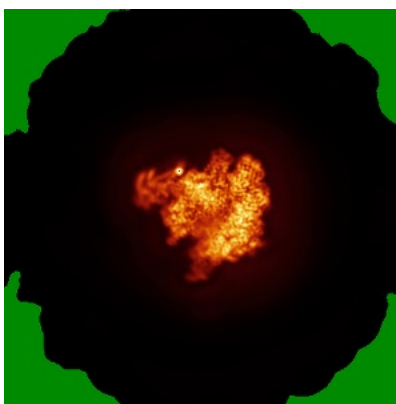
The images above show the largest variance slices of the map in three orthogonal directions.

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

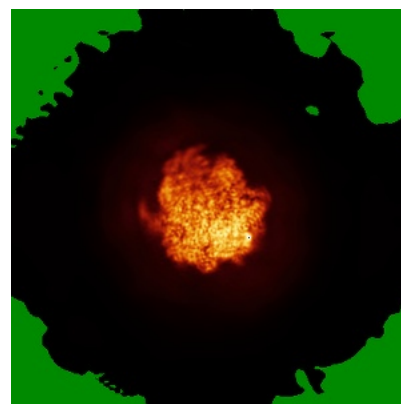
6.4.1 Primary map



X

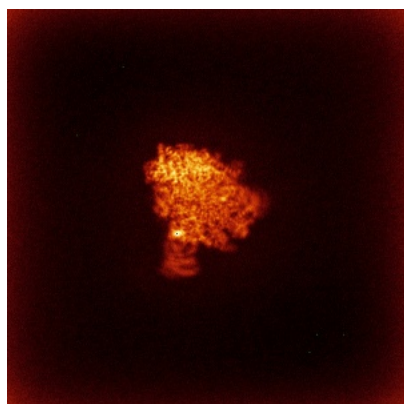


Y

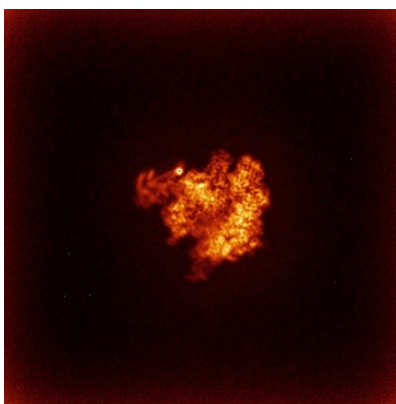


Z

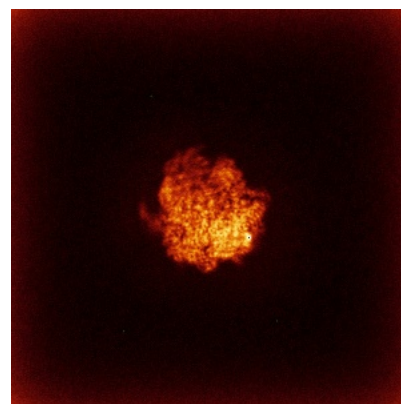
6.4.2 Raw map



X



Y

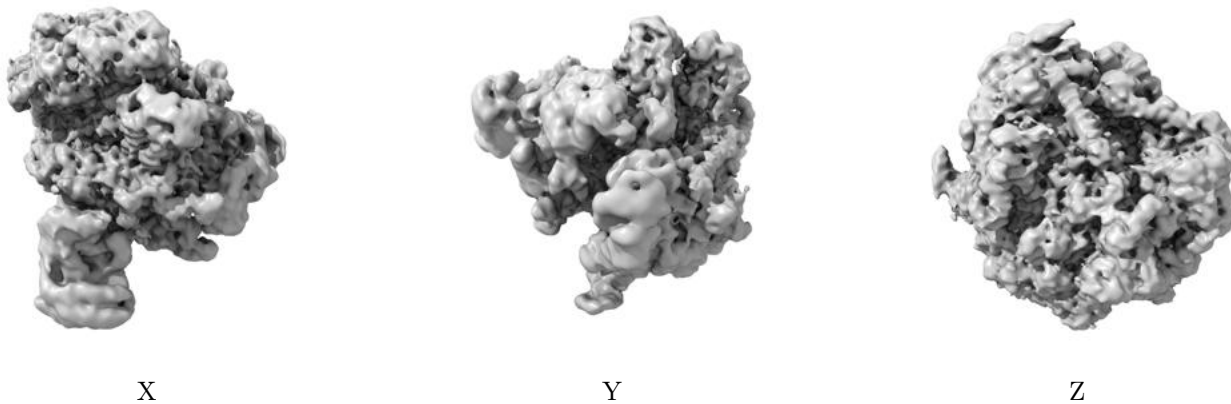


Z

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.

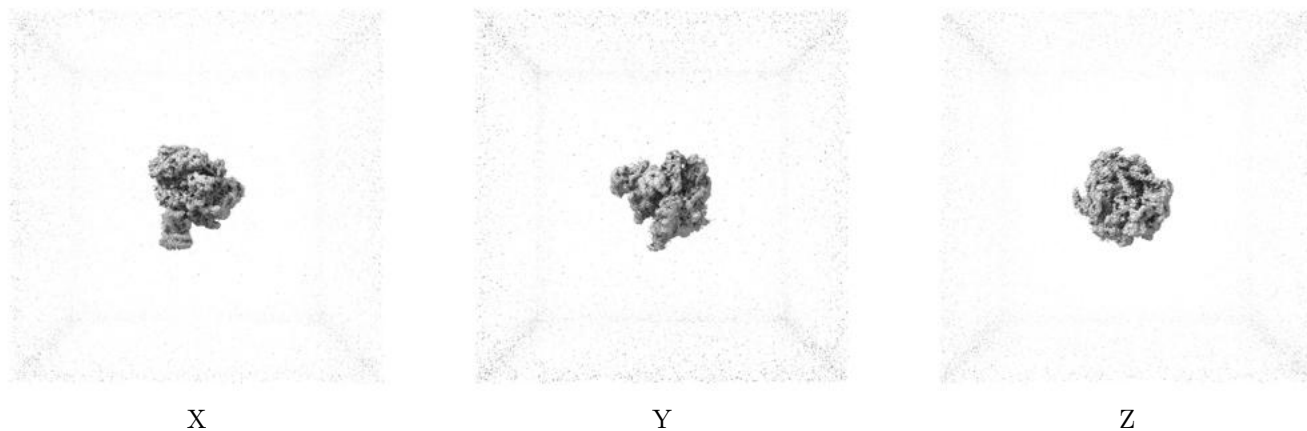
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.599. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

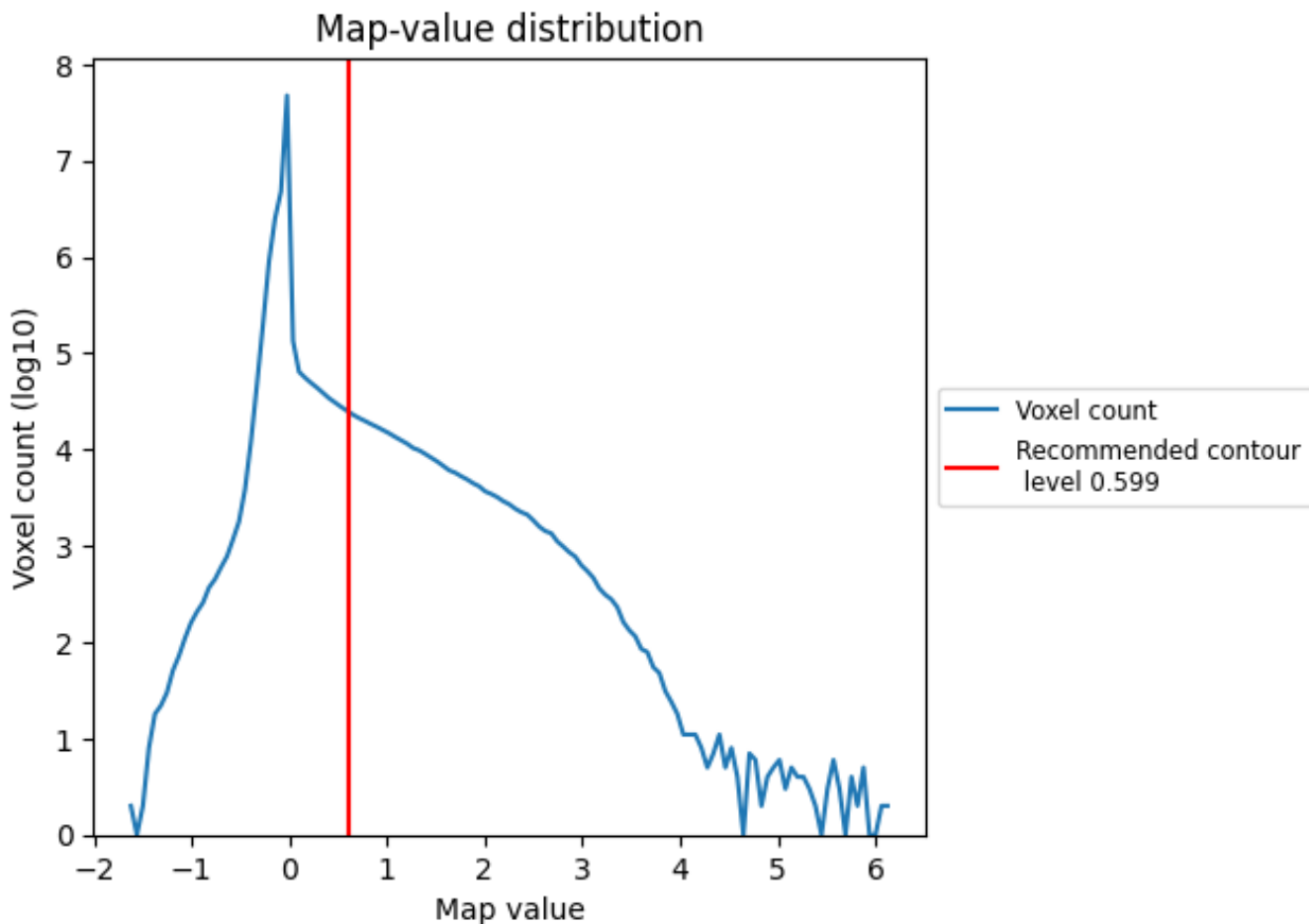
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

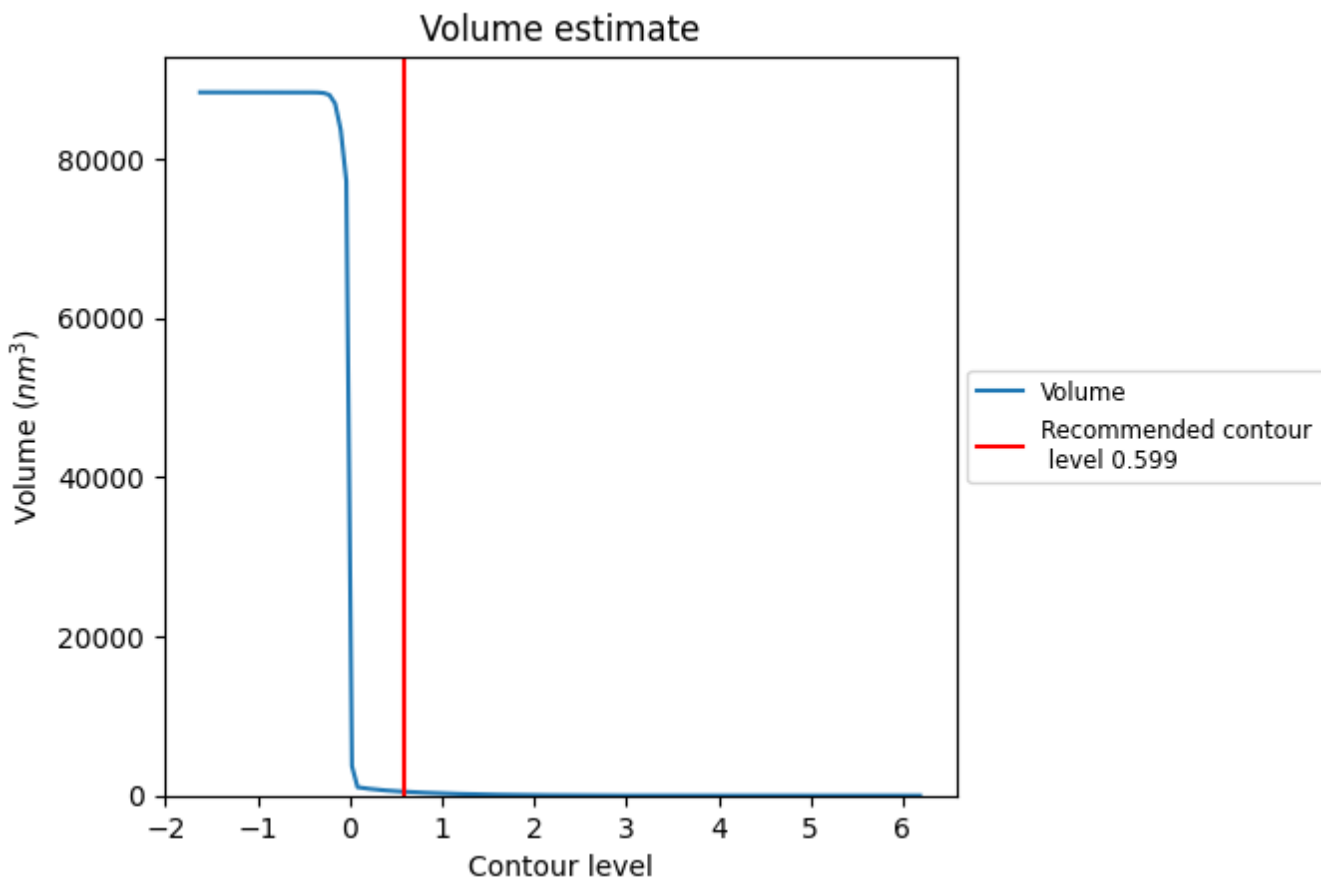
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

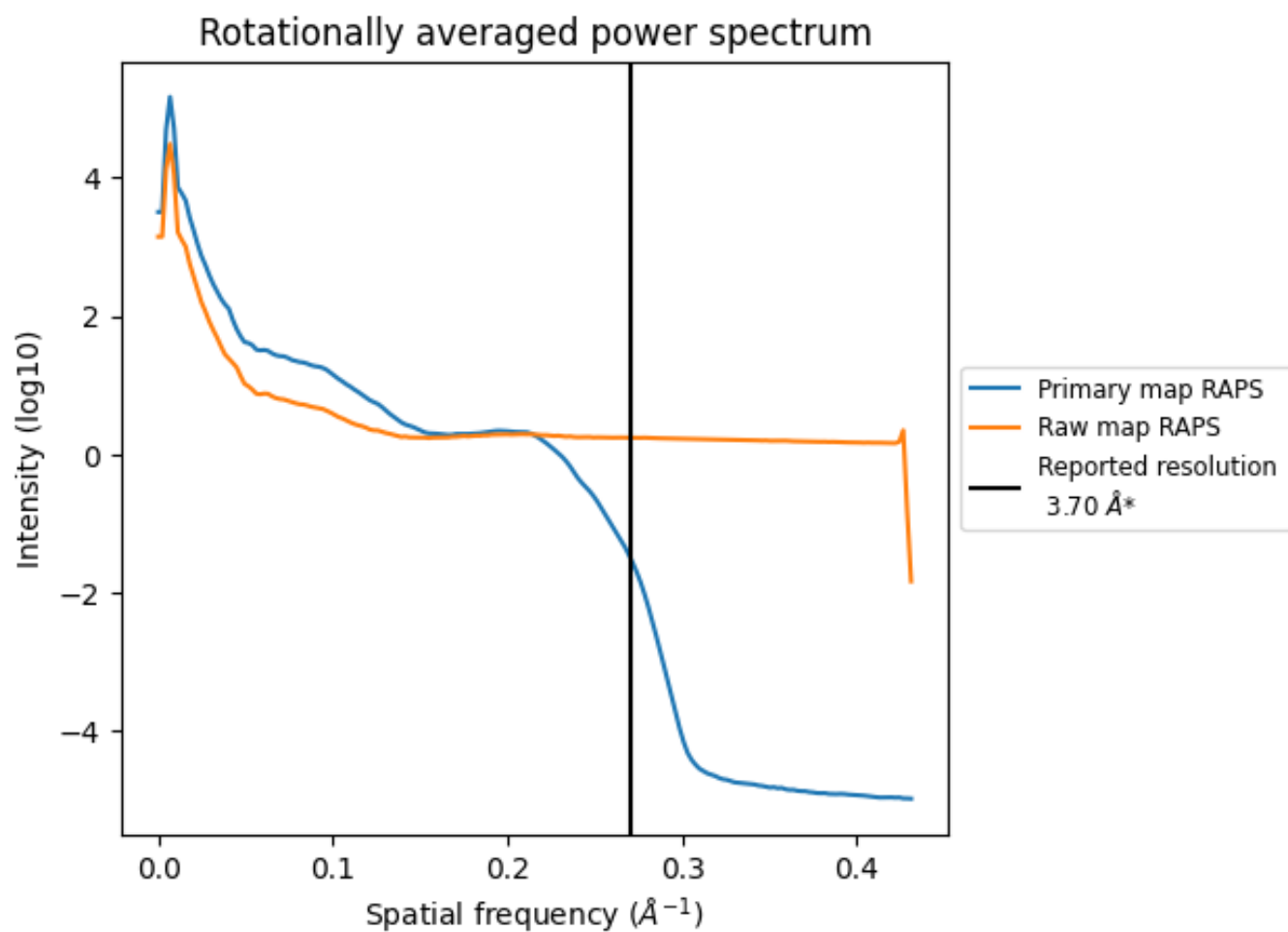
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 482 nm^3 ; this corresponds to an approximate mass of 435 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 i

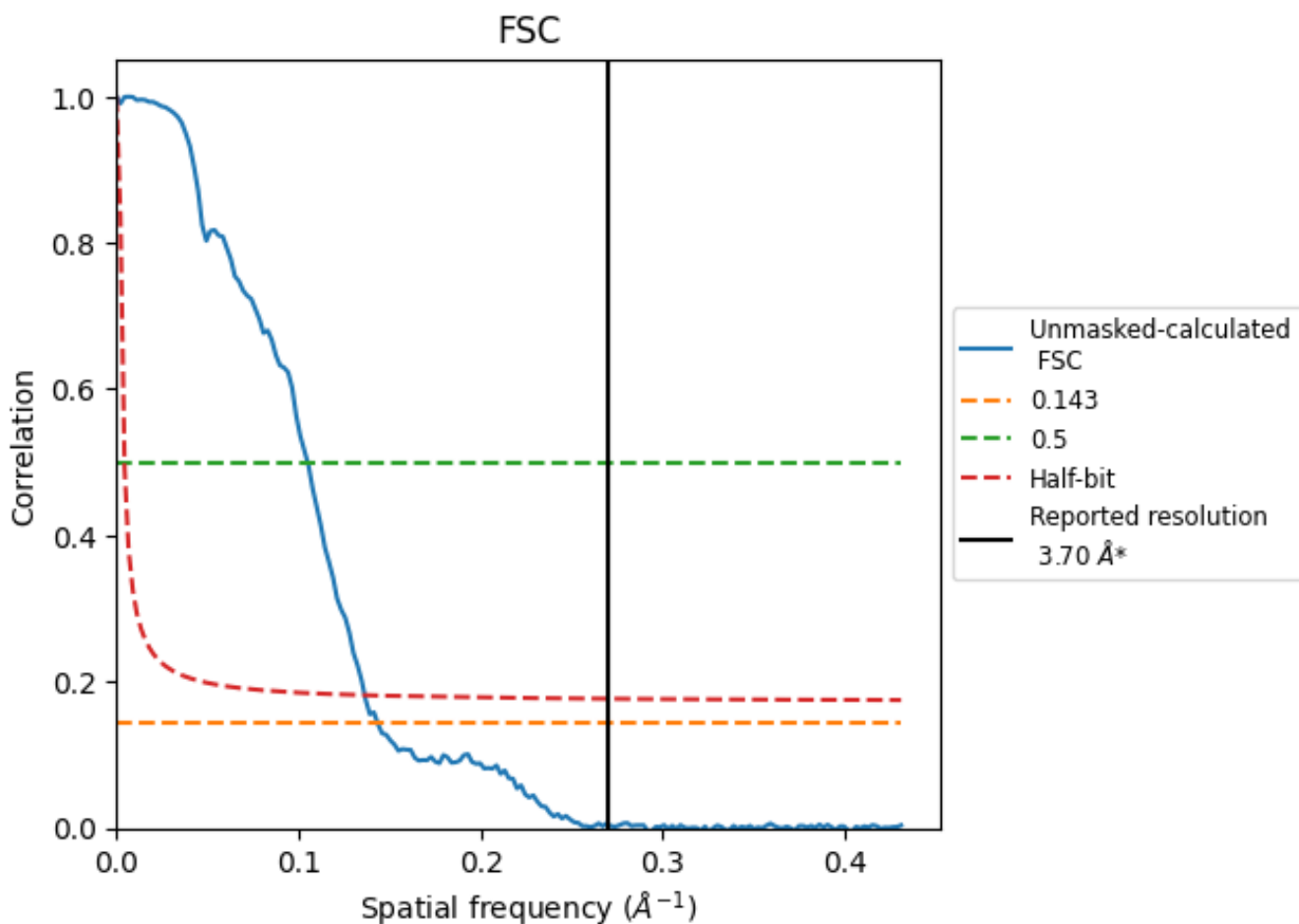


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

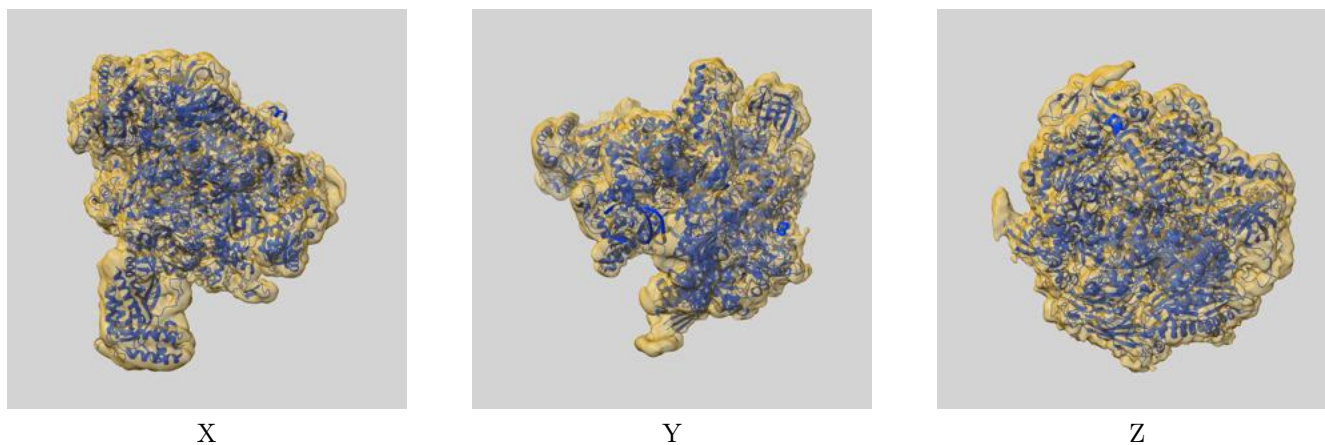
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.97	9.52	7.33

*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 6.97 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

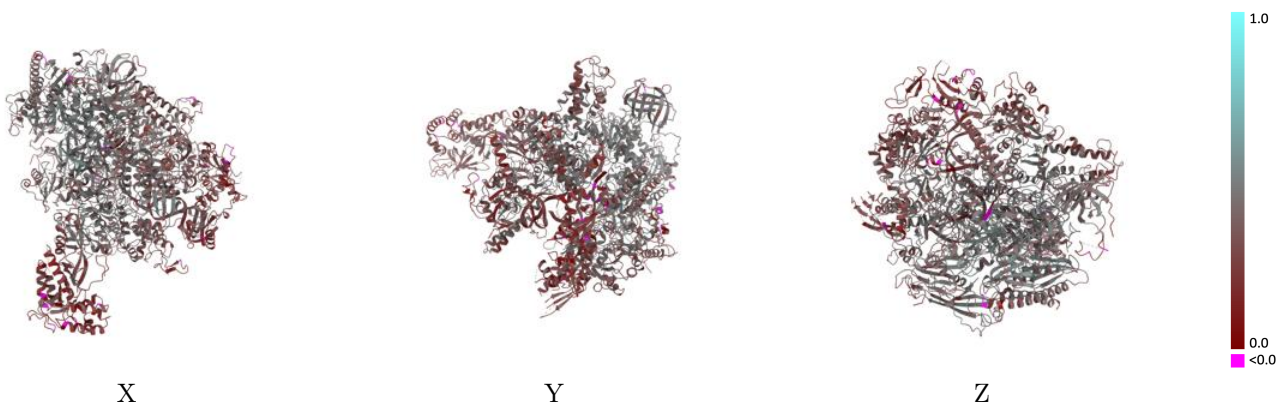
This section contains information regarding the fit between EMDB map EMD-41652 and PDB model 8TVV. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



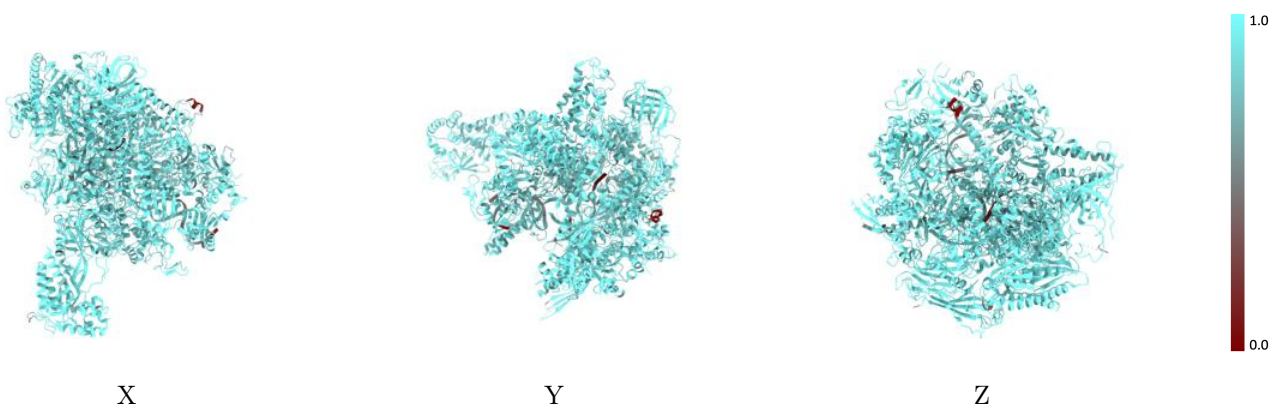
The images above show the 3D surface view of the map at the recommended contour level 0.599 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



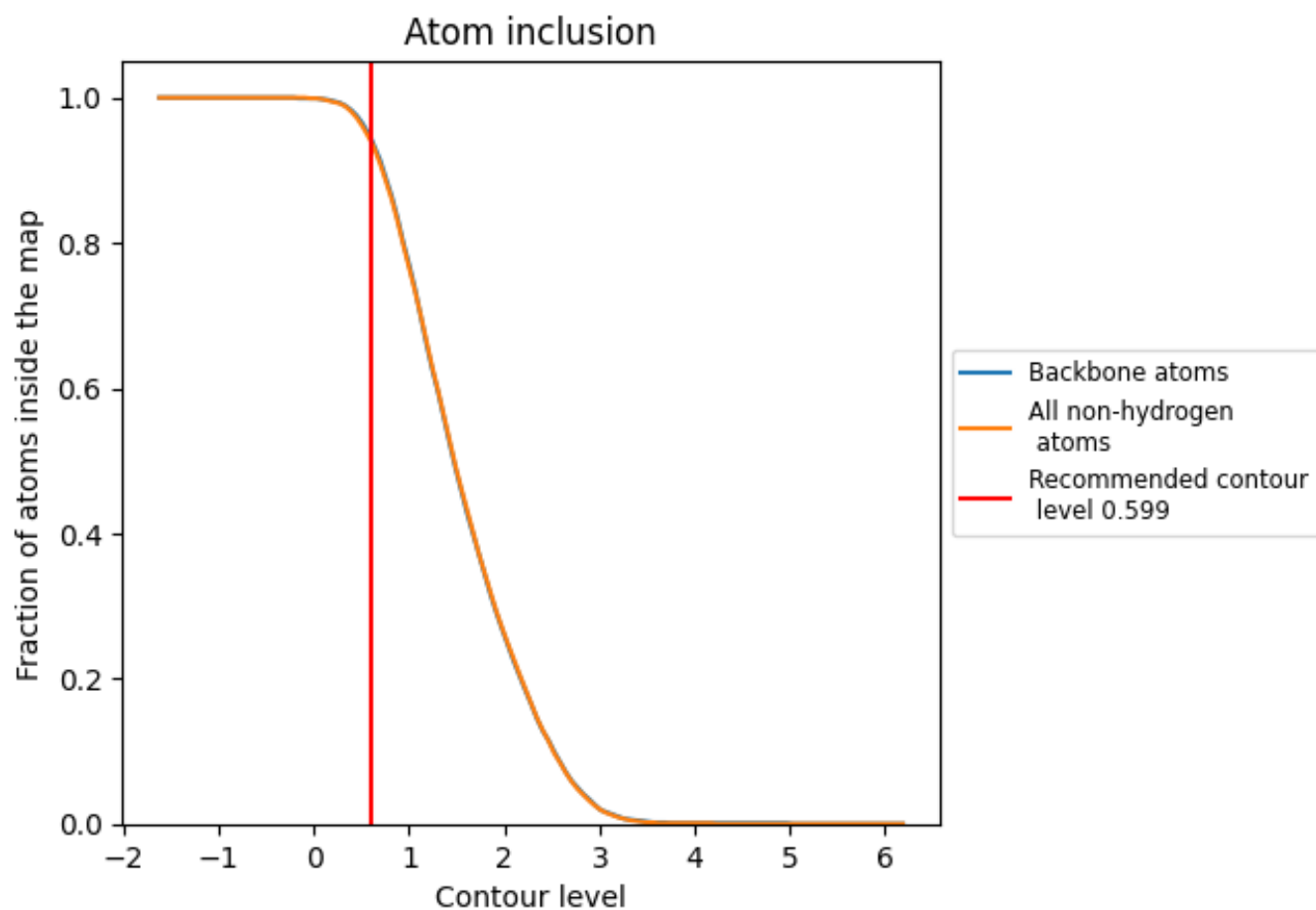
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.599).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.599) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.3700
A	 0.9310	 0.3870
B	 0.9530	 0.3900
C	 0.9740	 0.4360
D	 0.9650	 0.2080
E	 0.9650	 0.3330
F	 0.9610	 0.4160
G	 0.9560	 0.2910
H	 0.9700	 0.3800
I	 0.9290	 0.2630
J	 0.9880	 0.4370
K	 0.9580	 0.4110
L	 0.9740	 0.3370
N	 0.7090	 0.2150
R	 0.6730	 0.1980
T	 0.7310	 0.2460

