



Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 01:34 am BST

PDB ID : 7OL0
EMDB ID : EMD-12974
Title : Structure of active transcription elongation complex Pol II-DSIF (SPT5-KOW5)
Authors : Chen, Y.; Vos, S.M.; Dienemann, C.; Ninov, M.; Urlaub, H.; Cramer, P.
Deposited on : 2021-05-18
Resolution : 3.00 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

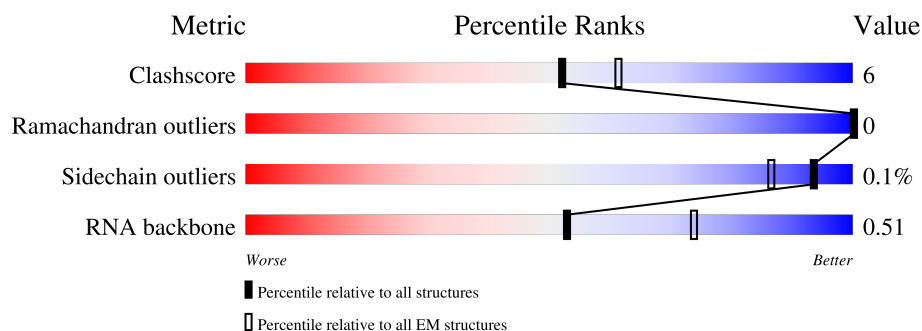
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	1970	
2	B	1251	
3	C	275	
4	D	184	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	<div><div></div><div>82%17%</div><div></div></div>
9	I	125	<div><div></div><div>7%75%18%7%</div><div></div></div>
10	J	67	<div><div></div><div>79%19%</div><div></div></div>
11	K	117	<div><div></div><div>93%5%</div><div></div></div>
12	L	58	<div><div></div><div>59%17%24%</div><div></div></div>
13	Z	1087	<div><div></div><div>95%</div><div></div></div>
14	P	47	<div><div></div><div>6%17%6%72%</div><div></div></div>
15	N	48	<div><div></div><div>27%42%15%44%</div><div></div></div>
16	T	48	<div><div></div><div>33%60%21%19%</div><div></div></div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32892 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1407	Total	C	N	O	S	0	0
			11149	7018	1998	2062	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9047	5721	1592	1670	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2068	1298	356	408	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	118	Total	C	N	O	S	0	0
			967	608	167	188	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

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 II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1347	872	218	249	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	116	Total	C	N	O	S	0	0
			926	574	162	179	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	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

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 RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 13 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	51	Total	C	N	O	S	0	0
			393	241	72	79	1		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	13	Total	C	N	O	P	0	0
			279	125	54	87	13		

- Molecule 15 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	27	Total	C	N	O	P	0	0
			549	264	96	162	27		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	39	Total	C	N	O	P	0	0
			808	385	149	235	39		

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

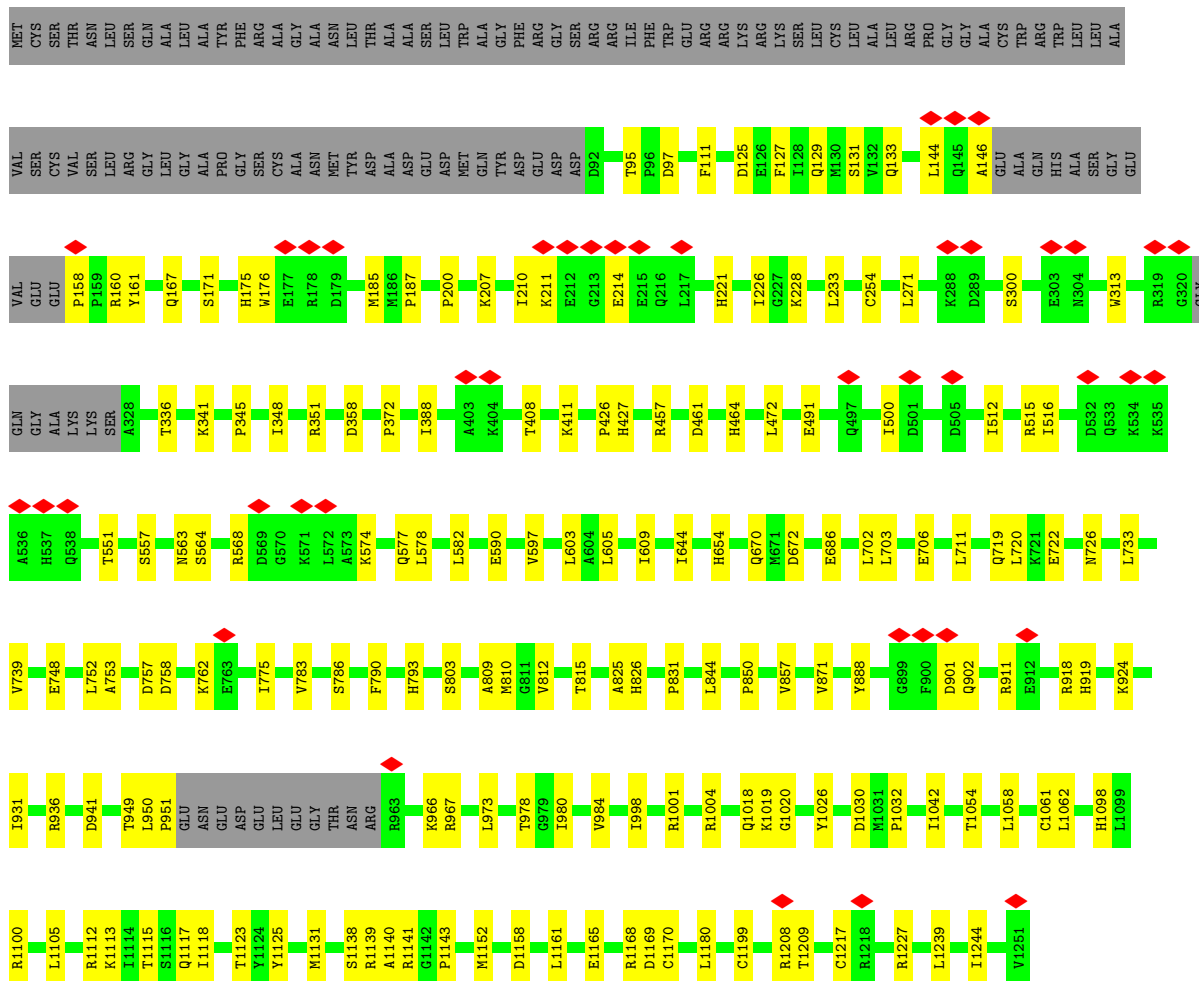
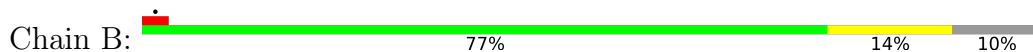
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).


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

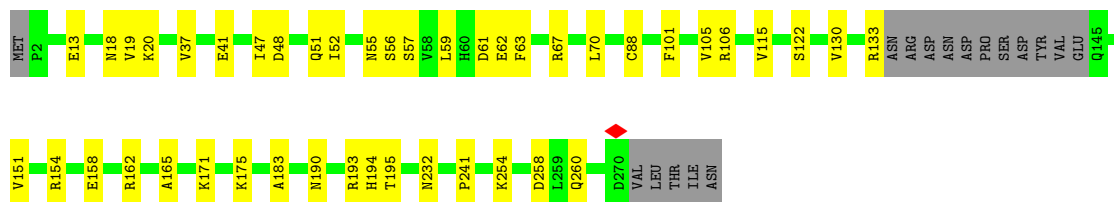


- Molecule 2: DNA-directed RNA polymerase subunit beta



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

Chain C:  78% 16% 6%



• Molecule 4: RNA polymerase II subunit D

Chain D:  59% 50% 14% 36%



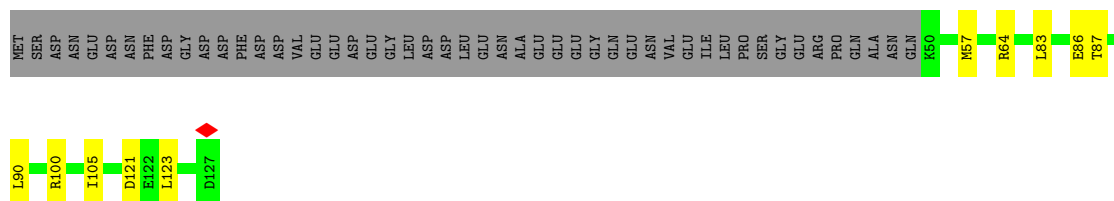
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  87% 12%




• Molecule 6: DNA-directed RNA polymerase II subunit F

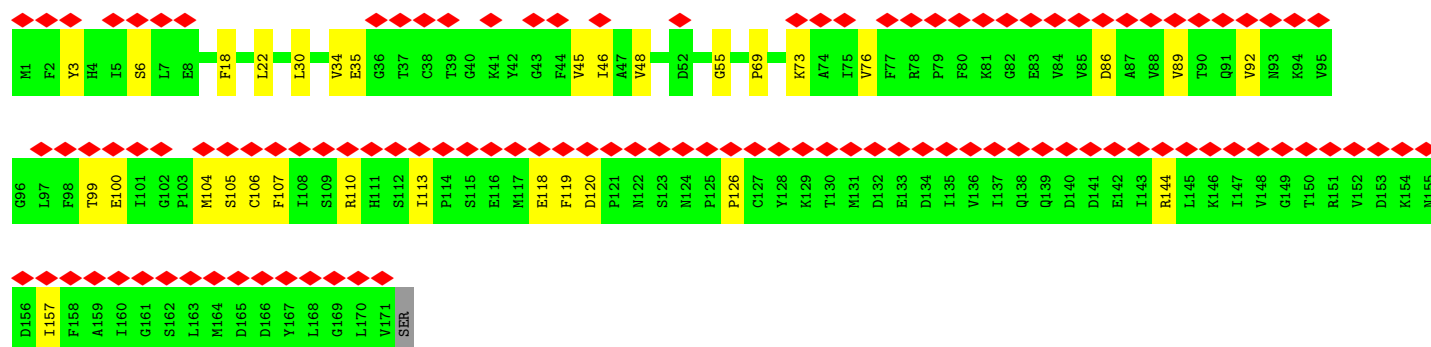
Chain F:  54% 8% 39%



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

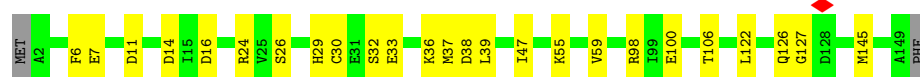
Chain G:  65% 81% 18%





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

Chain H: 82% 17% .



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

Chain I: 7% 75% 18% 7% .



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

Chain J: 79% 19% .



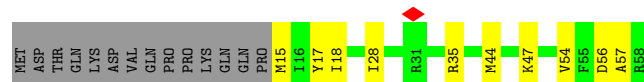
- Molecule 11: RNA_pol_L_2 domain-containing protein

Chain K: 93% 5% .



- Molecule 12: RNA polymerase II subunit K

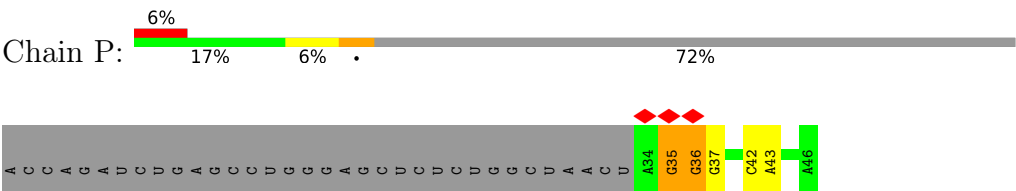
Chain L: 59% 17% 24% .



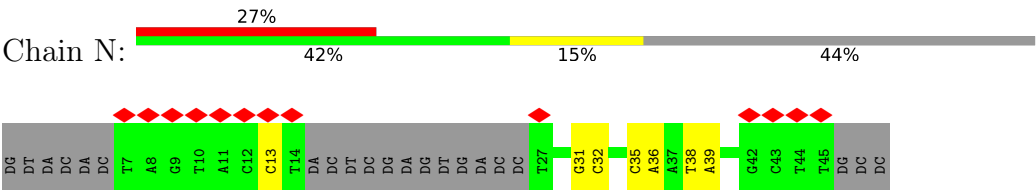
- Molecule 13: Transcription elongation factor SPT5

[illegible]

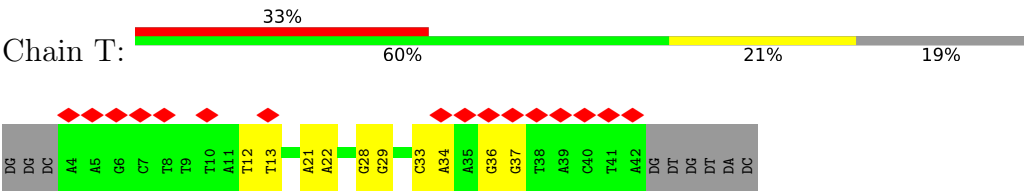
- Molecule 14: RNA



● Molecule 15: Non-template DNA



● Molecule 16: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.21	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.43	0/11350	0.55	2/15314 (0.0%)
2	B	0.50	0/9227	0.57	1/12454 (0.0%)
3	C	0.53	0/2111	0.52	0/2868
4	D	0.26	0/979	0.54	0/1312
5	E	0.41	0/1752	0.52	0/2366
6	F	0.50	0/636	0.57	0/859
7	G	0.35	0/1378	0.55	0/1870
8	H	0.51	0/1207	0.57	0/1628
9	I	0.46	0/948	0.57	0/1286
10	J	0.56	0/533	0.55	0/719
11	K	0.48	0/939	0.57	0/1271
12	L	0.49	0/378	0.64	0/500
13	Z	0.29	0/396	0.52	0/536
14	P	0.49	0/312	0.84	0/484
15	N	0.57	0/613	0.94	0/940
16	T	0.71	0/907	0.94	0/1400
All	All	0.47	0/33666	0.58	3/45807 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	LEU	CA-CB-CG	-6.32	100.77	115.30
1	A	883	ILE	CG1-CB-CG2	-5.11	100.16	111.40
2	B	973	LEU	CA-CB-CG	5.03	126.88	115.30

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	11149	0	11300	144	0
2	B	9047	0	9080	114	0
3	C	2068	0	2015	32	0
4	D	967	0	973	20	0
5	E	1721	0	1737	17	0
6	F	626	0	657	8	0
7	G	1347	0	1347	21	0
8	H	1186	0	1147	19	0
9	I	926	0	845	14	0
10	J	524	0	540	9	0
11	K	920	0	942	4	0
12	L	373	0	378	7	0
13	Z	393	0	400	10	0
14	P	279	0	142	3	0
15	N	549	0	308	4	0
16	T	808	0	442	7	0
17	A	1	0	0	0	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	32892	0	32253	372	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 6.

All (372) 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)
5:E:168:ASN:HA	5:E:172:ARG:HH21	1.29	0.95
2:B:300:SER:HG	2:B:427:HIS:HD1	1.22	0.86
1:A:1192:TRP:HB2	1:A:1248:ASN:HD22	1.48	0.79
1:A:1247:PHE:O	1:A:1248:ASN:OD1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:68:ILE:O	9:I:122:ARG:NH1	2.23	0.71
2:B:345:PRO:HG2	2:B:348:ILE:HD12	1.72	0.70
1:A:67:ARG:HE	14:P:36:G:H21	1.40	0.69
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.74	0.69
4:D:133:LYS:O	4:D:163:ARG:NH2	2.27	0.68
1:A:902:GLU:OE2	1:A:985:ARG:NH2	2.27	0.68
1:A:18:ILE:HD13	1:A:1460:LEU:HD23	1.76	0.68
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.76	0.67
8:H:32:SER:HB3	8:H:37:MET:H	1.60	0.67
2:B:1239:LEU:HD22	2:B:1244:ILE:HD12	1.77	0.67
2:B:1001:ARG:NH1	3:C:62:GLU:OE1	2.28	0.67
4:D:150:ALA:HB2	4:D:170:GLN:HB2	1.77	0.66
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.78	0.66
1:A:928:ARG:NH1	8:H:106:THR:O	2.29	0.66
2:B:160:ARG:HB2	2:B:210:ILE:HB	1.77	0.66
2:B:825:ALA:HB3	2:B:888:TYR:HB2	1.76	0.65
2:B:719:GLN:HG3	2:B:726:ASN:HD21	1.62	0.65
2:B:464:HIS:NE2	2:B:748:GLU:OE1	2.27	0.65
2:B:722:GLU:O	2:B:726:ASN:HB3	1.97	0.65
6:F:100:ARG:NH2	6:F:121:ASP:O	2.30	0.65
1:A:733:LEU:HD23	9:I:107:ALA:HA	1.79	0.65
2:B:936:ARG:NH2	13:Z:739:THR:O	2.29	0.64
7:G:100:GLU:HA	7:G:105:SER:HA	1.78	0.64
2:B:563:ASN:OD1	2:B:568:ARG:NH2	2.31	0.63
2:B:810:MET:HE2	2:B:826:HIS:HB3	1.82	0.62
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.82	0.62
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.82	0.62
2:B:1143:PRO:HB2	2:B:1152:MET:HG3	1.82	0.62
8:H:33:GLU:O	8:H:36:LYS:NZ	2.32	0.61
2:B:1004:ARG:NH1	2:B:1131:MET:SD	2.71	0.61
1:A:862:ARG:NH1	2:B:1165:GLU:OE1	2.33	0.61
9:I:65:LEU:HA	9:I:68:ILE:HD12	1.82	0.61
10:J:46:ARG:O	10:J:50:LEU:HB2	2.01	0.61
4:D:147:PRO:O	4:D:177:GLN:NE2	2.34	0.60
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.83	0.60
1:A:728:THR:H	1:A:736:THR:HG21	1.66	0.60
3:C:51:GLN:OE1	3:C:162:ARG:NH2	2.34	0.59
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.83	0.59
16:T:12:DT:H2"	16:T:13:DT:H5"	1.84	0.59
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.36	0.59
2:B:144:LEU:HB2	2:B:161:TYR:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:LEU:HA	4:D:163:ARG:HH22	1.66	0.59
7:G:18:PHE:HA	7:G:22:LEU:HD13	1.85	0.59
7:G:89:VAL:HG12	7:G:99:THR:HG22	1.84	0.58
6:F:57:MET:HG3	6:F:123:LEU:HD13	1.85	0.58
2:B:226:ILE:HG22	2:B:512:ILE:HG21	1.85	0.58
1:A:1207:ILE:N	1:A:1262:MET:SD	2.78	0.57
2:B:351:ARG:NH2	2:B:358:ASP:OD1	2.37	0.57
8:H:33:GLU:OE2	8:H:55:LYS:NZ	2.37	0.57
4:D:86:ARG:NH1	7:G:35:GLU:OE2	2.36	0.57
1:A:467:MET:HG3	1:A:524:MET:HB3	1.86	0.57
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.36	0.56
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.86	0.56
2:B:1098:HIS:CE1	2:B:1100:ARG:HB2	2.40	0.56
8:H:98:ARG:HE	8:H:100:GLU:HG3	1.70	0.56
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.88	0.56
2:B:936:ARG:HG2	2:B:980:ILE:HD13	1.87	0.56
3:C:56:SER:HB2	3:C:158:GLU:H	1.71	0.56
3:C:19:VAL:HG12	3:C:241:PRO:HB2	1.88	0.56
9:I:15:ARG:HB3	9:I:24:LEU:HD12	1.88	0.56
1:A:65:ILE:O	1:A:271:ARG:NH1	2.39	0.56
1:A:129:ILE:HA	1:A:132:LYS:HG2	1.87	0.56
7:G:92:VAL:HB	7:G:126:PRO:HB2	1.88	0.56
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.38	0.55
3:C:190:ASN:O	3:C:193:ARG:NH1	2.39	0.55
1:A:26:LEU:HB3	1:A:31:LEU:HD21	1.88	0.55
3:C:106:ARG:HG3	3:C:158:GLU:HB3	1.87	0.55
1:A:860:ILE:HD11	1:A:1125:LYS:HB2	1.88	0.55
1:A:330:GLN:OE1	1:A:334:ARG:NH1	2.39	0.55
4:D:71:ALA:HB1	7:G:3:TYR:CE1	2.42	0.55
5:E:168:ASN:CA	5:E:172:ARG:HH21	2.13	0.55
2:B:1018:GLN:NE2	2:B:1054:THR:OG1	2.38	0.55
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.39	0.54
2:B:786:SER:HB2	2:B:844:LEU:HD11	1.89	0.54
2:B:1112:ARG:NH1	2:B:1113:LYS:O	2.41	0.54
1:A:397:PHE:HB3	6:F:87:THR:HG23	1.90	0.54
2:B:127:PHE:HA	2:B:131:SER:HB2	1.89	0.54
2:B:144:LEU:HB3	2:B:500:ILE:HD13	1.90	0.54
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.90	0.54
2:B:757:ASP:O	2:B:762:LYS:NZ	2.41	0.54
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.89	0.54
7:G:106:CYS:SG	7:G:107:PHE:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.90	0.54
15:N:38:DT:H2"	15:N:39:DA:H5'	1.90	0.54
10:J:35:LEU:HD11	10:J:50:LEU:HD13	1.90	0.53
2:B:171:SER:HB3	2:B:200:PRO:HD2	1.90	0.53
3:C:13:GLU:OE1	3:C:18:ASN:ND2	2.40	0.53
13:Z:735:GLU:HA	13:Z:742:THR:HA	1.90	0.53
2:B:254:CYS:SG	2:B:815:THR:OG1	2.60	0.53
2:B:176:TRP:HZ3	2:B:228:LYS:HD3	1.74	0.53
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.90	0.53
5:E:82:VAL:HB	5:E:110:MET:HG2	1.90	0.53
2:B:457:ARG:NH2	2:B:686:GLU:HG2	2.24	0.53
8:H:14:ASP:HB3	8:H:29:HIS:HB2	1.91	0.53
9:I:20:CYS:HB3	9:I:42:CYS:SG	2.49	0.53
1:A:329:MET:HA	1:A:335:PRO:HA	1.91	0.52
1:A:1143:LEU:HB2	1:A:1148:ALA:HB2	1.91	0.52
1:A:1190:GLN:NE2	1:A:1194:ASN:OD1	2.41	0.52
9:I:28:GLU:O	9:I:30:LYS:NZ	2.43	0.52
12:L:15:MET:N	12:L:28:ILE:O	2.42	0.52
1:A:1474:LEU:HB2	6:F:105:ILE:HB	1.91	0.52
2:B:515:ARG:HH22	16:T:36:DG:H4'	1.74	0.52
1:A:360:ASP:OD1	2:B:1139:ARG:NE	2.33	0.52
12:L:18:ILE:HD11	12:L:47:LYS:HE2	1.92	0.52
2:B:590:GLU:HG3	2:B:803:SER:HB3	1.89	0.52
1:A:706:ILE:HG21	1:A:824:GLU:HG2	1.91	0.52
1:A:1052:ARG:HE	1:A:1056:GLU:HG3	1.74	0.52
2:B:850:PRO:HG3	10:J:53:VAL:HG21	1.92	0.52
4:D:177:GLN:HA	4:D:180:ARG:HD3	1.90	0.52
1:A:1281:ASP:O	1:A:1285:LEU:HB2	2.10	0.52
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.91	0.51
3:C:130:VAL:HG13	3:C:133:ARG:HH21	1.74	0.51
2:B:871:VAL:HG13	2:B:1042:ILE:HG23	1.91	0.51
2:B:1061:CYS:SG	2:B:1123:THR:OG1	2.50	0.51
2:B:702:LEU:HD13	2:B:752:LEU:HD21	1.92	0.51
2:B:978:THR:HG21	13:Z:740:CYS:HB2	1.92	0.51
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.74	0.51
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.92	0.51
7:G:104:MET:HG3	7:G:157:ILE:HG23	1.92	0.51
2:B:187:PRO:HB3	2:B:233:LEU:HD11	1.92	0.51
4:D:102:VAL:HA	4:D:105:LYS:HB2	1.92	0.51
1:A:15:LEU:HD11	2:B:1227:ARG:HG3	1.94	0.50
1:A:447:GLU:OE2	2:B:1141:ARG:NH2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:984:VAL:HG13	2:B:998:ILE:HG12	1.92	0.50
5:E:55:ARG:NE	5:E:107:GLN:OE1	2.44	0.50
2:B:722:GLU:O	2:B:726:ASN:CB	2.58	0.50
8:H:30:CYS:HB2	8:H:39:LEU:HB3	1.94	0.50
2:B:703:LEU:HD23	2:B:739:VAL:HG12	1.94	0.50
3:C:171:LYS:HE2	11:K:9:SER:HB3	1.93	0.50
1:A:513:ALA:HB2	6:F:90:LEU:HD11	1.94	0.50
1:A:1028:PRO:HA	1:A:1031:ARG:HG2	1.94	0.50
4:D:131:GLN:N	4:D:131:GLN:OE1	2.45	0.50
1:A:1168:LYS:HB3	1:A:1224:ARG:HH12	1.77	0.49
2:B:160:ARG:N	2:B:210:ILE:O	2.43	0.49
2:B:408:THR:HB	2:B:411:LYS:HB2	1.93	0.49
2:B:457:ARG:HH21	2:B:686:GLU:HG2	1.76	0.49
1:A:497:ASP:HB2	2:B:1019:LYS:HG3	1.94	0.49
1:A:740:GLN:HG2	1:A:743:ARG:HH12	1.77	0.49
2:B:931:ILE:HG22	2:B:998:ILE:HD13	1.93	0.49
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.45	0.49
2:B:578:LEU:HD12	2:B:582:LEU:HD12	1.94	0.49
4:D:84:GLU:O	4:D:88:GLN:N	2.44	0.49
1:A:936:GLU:HG3	1:A:940:LYS:HE2	1.95	0.49
3:C:55:ASN:ND2	3:C:61:ASP:OD1	2.38	0.49
2:B:133:GLN:HE22	2:B:167:GLN:HA	1.78	0.49
1:A:71:CYS:SG	1:A:72:GLN:N	2.86	0.48
1:A:267:GLN:O	2:B:967:ARG:NH2	2.46	0.48
1:A:467:MET:HG2	1:A:534:VAL:HG21	1.95	0.48
1:A:1118:THR:HG23	1:A:1123:ARG:HD3	1.95	0.48
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.95	0.48
1:A:756:ALA:HB2	1:A:786:ALA:HB2	1.95	0.48
1:A:1243:LEU:HD13	1:A:1259:ILE:HG23	1.95	0.48
2:B:372:PRO:HB3	9:I:13:GLY:HA2	1.94	0.48
2:B:949:THR:HA	2:B:966:LYS:HB3	1.94	0.48
10:J:1:MET:HA	10:J:55:LEU:HB2	1.96	0.48
1:A:90:LEU:HD22	1:A:310:LEU:HD11	1.96	0.48
2:B:857:VAL:HG21	2:B:1125:TYR:CE1	2.48	0.48
2:B:1117:GLN:NE2	3:C:195:THR:OG1	2.41	0.48
2:B:1199:CYS:HB3	2:B:1217:CYS:SG	2.53	0.48
8:H:16:ASP:OD2	8:H:26:SER:OG	2.26	0.48
3:C:13:GLU:HB3	3:C:20:LYS:HB3	1.94	0.48
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.96	0.48
3:C:175:LYS:NZ	12:L:57:ALA:O	2.43	0.48
7:G:89:VAL:HA	7:G:99:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:31:DG:H2'	15:N:32:DC:C6	2.48	0.48
2:B:557:SER:OG	2:B:590:GLU:OE2	2.26	0.47
7:G:86:ASP:HB3	7:G:144:ARG:HG3	1.95	0.47
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.96	0.47
2:B:783:VAL:HG13	2:B:844:LEU:HD22	1.95	0.47
2:B:790:PHE:HB3	2:B:793:HIS:CD2	2.49	0.47
8:H:38:ASP:HB3	8:H:126:GLN:HG3	1.95	0.47
2:B:924:LYS:NZ	2:B:941:ASP:OD2	2.47	0.47
2:B:111:PHE:HZ	2:B:605:LEU:HB3	1.80	0.47
1:A:413:TYR:O	1:A:415:GLY:N	2.48	0.47
2:B:175:HIS:HB2	2:B:185:MET:HB2	1.96	0.47
2:B:603:LEU:HD21	2:B:609:ILE:HD11	1.97	0.47
1:A:373:LEU:O	1:A:485:ASN:ND2	2.48	0.47
4:D:84:GLU:HA	4:D:87:LYS:HB3	1.97	0.47
7:G:6:SER:HB3	7:G:73:LYS:HD3	1.97	0.47
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.96	0.47
1:A:97:VAL:HA	1:A:100:LEU:HG	1.97	0.47
2:B:351:ARG:NH1	2:B:388:ILE:O	2.48	0.47
2:B:1139:ARG:NH1	2:B:1158:ASP:O	2.48	0.47
2:B:901:ASP:OD1	2:B:902:GLN:N	2.47	0.47
3:C:88:CYS:O	13:Z:718:LYS:NZ	2.48	0.47
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.95	0.46
1:A:1357:THR:O	5:E:142:HIS:NE2	2.42	0.46
12:L:35:ARG:HE	12:L:35:ARG:HB2	1.39	0.46
1:A:637:MET:HB3	8:H:122:LEU:HD21	1.96	0.46
2:B:313:TRP:HB2	2:B:336:THR:HB	1.98	0.46
2:B:706:GLU:HB2	2:B:711:LEU:HD21	1.98	0.46
2:B:1208:ARG:HG3	2:B:1209:THR:HG23	1.96	0.46
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	1.97	0.46
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.81	0.46
2:B:146:ALA:HA	2:B:158:PRO:HG2	1.98	0.46
2:B:551:THR:OG1	2:B:809:ALA:O	2.28	0.46
2:B:670:GLN:NE2	2:B:672:ASP:OD2	2.40	0.46
4:D:102:VAL:HG22	4:D:105:LYS:HD3	1.97	0.46
7:G:45:VAL:HA	7:G:76:VAL:HG22	1.97	0.46
16:T:36:DG:H2'	16:T:37:DG:C8	2.51	0.46
1:A:93:PRO:HB3	1:A:251:THR:HG22	1.96	0.46
1:A:118:LEU:O	1:A:151:LYS:NZ	2.48	0.46
1:A:847:LEU:HB3	2:B:597:VAL:HG21	1.97	0.46
5:E:52:ARG:HD2	5:E:52:ARG:HA	1.83	0.46
1:A:1210:TRP:CE2	1:A:1282:ASP:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:LYS:HB2	2:B:214:GLU:HB2	1.98	0.46
2:B:461:ASP:HB3	2:B:464:HIS:HB2	1.98	0.46
1:A:808:PRO:HG2	2:B:752:LEU:HD12	1.96	0.46
1:A:931:ARG:HG2	1:A:939:VAL:HG11	1.97	0.46
1:A:274:ASP:OD1	1:A:275:ASP:N	2.48	0.45
1:A:192:ARG:HH12	1:A:213:LYS:HE3	1.81	0.45
1:A:689:ILE:HG21	2:B:1062:LEU:HD22	1.97	0.45
3:C:254:LYS:NZ	3:C:258:ASP:OD2	2.38	0.45
1:A:394:VAL:HG22	1:A:402:LEU:HD12	1.97	0.45
1:A:693:ILE:HG12	1:A:828:LEU:HD21	1.98	0.45
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.49	0.45
9:I:58:ILE:HG22	9:I:59:THR:HG23	1.99	0.45
13:Z:724:VAL:HG22	13:Z:734:VAL:HG22	1.98	0.45
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.81	0.45
2:B:564:SER:O	2:B:568:ARG:NH1	2.42	0.45
4:D:73:THR:HG23	4:D:136:LYS:HB3	1.98	0.45
2:B:125:ASP:O	2:B:129:GLN:HB2	2.16	0.45
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.99	0.45
6:F:83:LEU:HB2	6:F:86:GLU:HB2	1.99	0.45
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.98	0.45
1:A:416:ALA:HA	1:A:448:ARG:HA	1.97	0.45
1:A:1347:LEU:HB3	5:E:137:ILE:HG21	1.99	0.45
2:B:1032:PRO:HB2	2:B:1105:LEU:HD13	1.99	0.45
4:D:75:LEU:HD13	4:D:140:ALA:HA	1.98	0.45
1:A:321:GLU:HG3	1:A:341:GLN:HE21	1.81	0.45
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.61	0.45
11:K:81:TYR:OH	11:K:89:ASN:ND2	2.39	0.44
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.53	0.44
5:E:102:ALA:HB3	5:E:127:LEU:HD23	2.00	0.44
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	2.00	0.44
1:A:723:ASN:ND2	9:I:125:GLU:OE2	2.50	0.44
1:A:1054:MET:HE3	1:A:1060:LEU:HB2	1.99	0.44
2:B:703:LEU:HG	2:B:775:ILE:HG12	2.00	0.44
2:B:918:ARG:O	14:P:35:G:N1	2.51	0.44
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.00	0.44
1:A:465:HIS:HB3	1:A:1097:GLU:HG2	1.99	0.44
1:A:497:ASP:HA	2:B:1020:GLY:HA2	1.98	0.44
16:T:28:DG:H2'	16:T:29:DG:C8	2.53	0.44
2:B:936:ARG:HG3	13:Z:737:HIS:CD2	2.52	0.44
7:G:120:ASP:N	7:G:120:ASP:OD1	2.51	0.44
14:P:42:C:H2'	14:P:43:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:13:DC:O2	16:T:37:DG:N1	2.50	0.44
1:A:362:SER:HB2	2:B:1161:LEU:HD12	1.99	0.44
2:B:1113:LYS:HB2	3:C:194:HIS:HB3	1.99	0.44
4:D:167:GLU:OE2	4:D:171:GLN:NE2	2.40	0.44
1:A:1172:ASN:HB3	1:A:1215:GLU:HB3	2.00	0.44
1:A:1217:ASP:O	1:A:1221:MET:HG2	2.17	0.44
3:C:55:ASN:OD1	3:C:57:SER:OG	2.32	0.44
1:A:544:ALA:O	1:A:548:PHE:HB2	2.18	0.44
1:A:1458:ILE:HD13	2:B:1168:ARG:HD2	1.99	0.44
8:H:145:MET:HE2	8:H:145:MET:HB3	1.75	0.44
9:I:54:TYR:CE2	9:I:56:ASN:HB2	2.53	0.44
1:A:495:ASP:OD1	1:A:495:ASP:N	2.51	0.43
1:A:511:THR:HA	1:A:514:GLU:HG2	1.99	0.43
2:B:644:ILE:HD11	2:B:654:HIS:HB2	1.99	0.43
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.43	0.43
4:D:106:THR:HG21	7:G:46:ILE:HD12	2.00	0.43
1:A:1221:MET:HG3	1:A:1255:LEU:HD13	2.00	0.43
1:A:1282:ASP:O	1:A:1286:ARG:HG3	2.17	0.43
3:C:47:ILE:HA	3:C:165:ALA:HA	1.99	0.43
4:D:86:ARG:HH12	7:G:48:VAL:H	1.65	0.43
5:E:139:ILE:HD13	5:E:178:PRO:HB2	1.99	0.43
1:A:260:VAL:O	1:A:342:ARG:NH2	2.45	0.43
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.99	0.43
5:E:61:LEU:HD11	5:E:99:ILE:HD13	2.00	0.43
2:B:1026:TYR:HB3	2:B:1030:ASP:HB2	2.00	0.43
7:G:30:LEU:O	7:G:34:VAL:HG12	2.19	0.43
2:B:341:LYS:HD3	2:B:341:LYS:HA	1.74	0.43
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.53	0.43
1:A:823:VAL:HA	1:A:835:GLU:HG2	2.01	0.43
2:B:720:LEU:HD11	2:B:733:LEU:HD22	2.00	0.43
7:G:110:ARG:HA	7:G:113:ILE:HD12	2.01	0.43
5:E:100:THR:HA	5:E:125:TYR:CD1	2.54	0.43
13:Z:728:THR:HG22	13:Z:729:GLU:H	1.84	0.43
1:A:384:ILE:HG12	2:B:1138:SER:HB3	2.01	0.43
7:G:55:GLY:HA3	7:G:69:PRO:HG2	2.00	0.43
8:H:6:PHE:HZ	8:H:37:MET:HG3	1.83	0.43
1:A:1312:PRO:O	1:A:1332:GLN:NE2	2.52	0.43
2:B:146:ALA:H	2:B:158:PRO:HB2	1.84	0.43
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.00	0.43
3:C:52:ILE:HD12	3:C:61:ASP:HB3	1.99	0.43
1:A:1231:ILE:O	1:A:1235:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:PHE:CZ	8:H:37:MET:HG3	2.54	0.42
16:T:33:DC:H2''	16:T:34:DA:C4	2.54	0.42
1:A:93:PRO:HD2	1:A:219:GLU:HG2	2.01	0.42
1:A:689:ILE:HD13	2:B:1058:LEU:HB2	2.01	0.42
5:E:54:ARG:HB3	5:E:57:ASP:HB2	1.99	0.42
1:A:402:LEU:HD13	1:A:446:VAL:HB	2.01	0.42
1:A:458:PHE:CE2	1:A:484:LEU:HD21	2.54	0.42
2:B:1115:THR:HA	3:C:195:THR:HA	2.01	0.42
3:C:67:ARG:NH1	10:J:3:ILE:O	2.42	0.42
1:A:618:TYR:HB3	1:A:621:ILE:O	2.19	0.42
1:A:732:THR:HG23	1:A:734:ARG:H	1.84	0.42
2:B:95:THR:OG1	2:B:97:ASP:OD1	2.33	0.42
2:B:472:LEU:HD21	2:B:609:ILE:HD12	2.01	0.42
4:D:127:SER:OG	4:D:128:LEU:N	2.53	0.42
1:A:734:ARG:HA	1:A:734:ARG:NE	2.35	0.42
1:A:322:LEU:O	1:A:327:ARG:NH2	2.47	0.42
1:A:279:LYS:HE2	1:A:336:LEU:HD12	2.01	0.42
1:A:603:ILE:HG12	1:A:629:VAL:HG22	2.01	0.42
1:A:734:ARG:HG3	9:I:105:GLU:HA	2.01	0.42
1:A:1319:LYS:HD3	1:A:1331:LEU:HD11	2.00	0.42
2:B:812:VAL:HG23	2:B:831:PRO:HG3	2.01	0.42
7:G:104:MET:SD	7:G:104:MET:N	2.92	0.42
1:A:120:ASP:HB3	1:A:123:ASN:HB2	2.02	0.42
1:A:865:ILE:HG21	2:B:1169:ASP:CG	2.40	0.42
9:I:73:SER:O	9:I:80:ARG:NH2	2.53	0.42
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.46	0.42
12:L:54:VAL:HG21	13:Z:721:ILE:HG13	2.02	0.42
13:Z:712:ILE:HD12	13:Z:720:TYR:HB2	2.01	0.42
1:A:1471:PHE:O	6:F:64:ARG:NH2	2.53	0.41
2:B:574:LYS:HA	2:B:577:GLN:HG2	2.02	0.41
1:A:466:LYS:HA	2:B:1170:CYS:SG	2.60	0.41
1:A:1192:TRP:HB2	1:A:1248:ASN:ND2	2.26	0.41
1:A:126:ILE:O	1:A:130:LEU:HG	2.20	0.41
16:T:21:DA:H2'	16:T:22:DA:C8	2.55	0.41
1:A:420:ILE:HB	1:A:445:LYS:HB2	2.03	0.41
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.52	0.41
15:N:35:DC:H2'	15:N:36:DA:C8	2.56	0.41
1:A:1427:LEU:HB2	1:A:1456:GLU:HG2	2.03	0.41
2:B:911:ARG:HH22	2:B:919:HIS:HA	1.85	0.41
4:D:129:LEU:HD22	4:D:134:LEU:HD11	2.02	0.41
5:E:12:LYS:HD2	5:E:12:LYS:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:GLY:HA3	5:E:52:ARG:HB3	2.01	0.41
1:A:485:ASN:OD1	1:A:673:GLN:NE2	2.49	0.41
2:B:207:LYS:HE2	2:B:221:HIS:CE1	2.56	0.41
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.79	0.41
2:B:950:LEU:HD12	2:B:951:PRO:HD2	2.01	0.41
12:L:56:ASP:H	13:Z:738:SER:HB3	1.84	0.41
1:A:102:LYS:NZ	1:A:1441:GLU:OE1	2.41	0.41
1:A:134:LYS:HE2	1:A:134:LYS:HB2	1.83	0.41
1:A:360:ASP:HB3	2:B:1140:ALA:O	2.21	0.41
1:A:890:ARG:HD3	1:A:890:ARG:HA	1.80	0.41
1:A:1317:LYS:NZ	1:A:1337:GLU:OE2	2.41	0.41
2:B:1168:ARG:NH2	2:B:1169:ASP:OD1	2.54	0.41
4:D:73:THR:HG22	7:G:3:TYR:HD1	1.85	0.41
1:A:48:GLU:N	1:A:51:ARG:O	2.54	0.41
1:A:467:MET:HE3	1:A:534:VAL:HG11	2.02	0.41
2:B:300:SER:HB3	2:B:426:PRO:HD2	2.03	0.41
2:B:753:ALA:HB1	2:B:758:ASP:HB2	2.03	0.41
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.03	0.41
1:A:1144:LEU:HG	1:A:1353:ASP:HA	2.03	0.40
1:A:1184:THR:HG23	1:A:1187:ALA:H	1.86	0.40
1:A:1458:ILE:HD11	2:B:1180:LEU:HD21	2.02	0.40
8:H:37:MET:SD	8:H:127:GLY:HA3	2.61	0.40
11:K:31:CYS:SG	11:K:84:GLN:NE2	2.95	0.40
1:A:642:LYS:HB3	1:A:642:LYS:HE3	1.82	0.40
2:B:1105:LEU:HG	2:B:1118:ILE:HB	2.02	0.40
3:C:59:LEU:HD13	3:C:63:PHE:CD2	2.57	0.40
1:A:369:PRO:HB3	1:A:486:LEU:HD21	2.04	0.40
1:A:546:ARG:HD3	1:A:772:SER:HB3	2.03	0.40
10:J:18:TRP:HE3	10:J:49:LEU:HD22	1.87	0.40
1:A:256:PRO:HG2	1:A:261:ARG:HD3	2.04	0.40
2:B:491:GLU:HG3	2:B:516:ILE:HD11	2.03	0.40
3:C:70:LEU:HD22	10:J:6:ARG:HG3	2.04	0.40
5:E:151:MET:HE1	5:E:206:TYR:HD1	1.85	0.40
7:G:118:GLU:HG2	7:G:119:PHE:N	2.37	0.40
1:A:276:LEU:HD21	1:A:339:LEU:HD21	2.04	0.40
1:A:552:ASP:O	8:H:24:ARG:NH2	2.50	0.40
1:A:758:LYS:HD3	1:A:758:LYS:HA	1.85	0.40
1:A:1394:ASN:HB3	1:A:1397:HIS:CD2	2.57	0.40
5:E:47:LYS:HE3	5:E:47:LYS:HB3	1.82	0.40
8:H:11:ASP:N	8:H:11:ASP:OD1	2.55	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	1393/1970 (71%)	1357 (97%)	36 (3%)	0	100	100
2	B	1123/1251 (90%)	1094 (97%)	29 (3%)	0	100	100
3	C	254/275 (92%)	250 (98%)	4 (2%)	0	100	100
4	D	114/184 (62%)	105 (92%)	9 (8%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	76/127 (60%)	74 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	114/125 (91%)	107 (94%)	7 (6%)	0	100	100
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
13	Z	49/1087 (4%)	49 (100%)	0	0	100	100
All	All	3864/5793 (67%)	3749 (97%)	115 (3%)	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	1239/1749 (71%)	1236 (100%)	3 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	991/1084 (91%)	991 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	101/112 (90%)	101 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	Z	45/940 (5%)	45 (100%)	0	100	100
All	All	3458/5101 (68%)	3455 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	538	VAL
1	A	1375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	1248	ASN
2	B	726	ASN
2	B	1102	ASN
11	K	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/47 (25%)	3 (25%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	G
14	P	36	G
14	P	37	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.

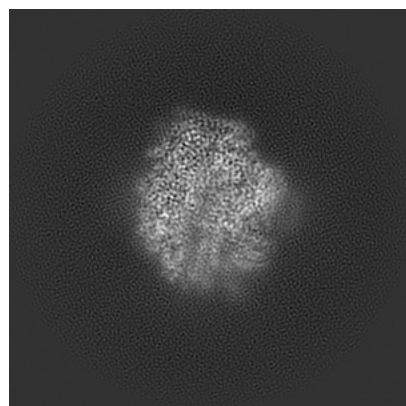
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12974. These allow visual inspection of the internal detail of the map and identification of artifacts.

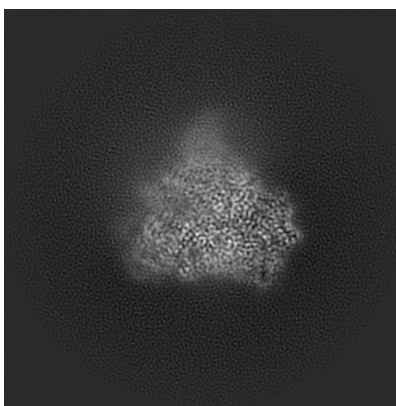
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

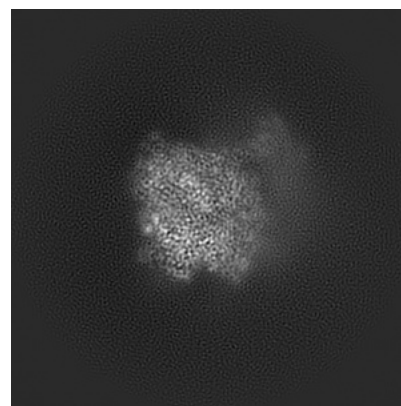
6.1.1 Primary map



X

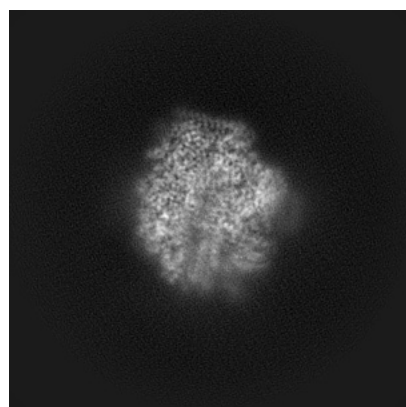


Y

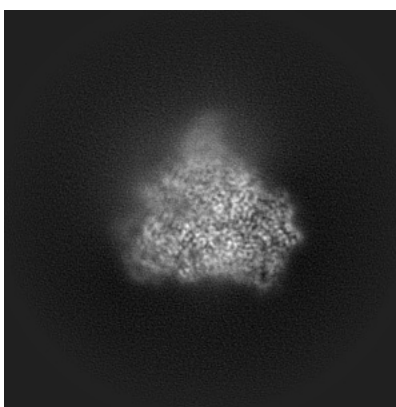


Z

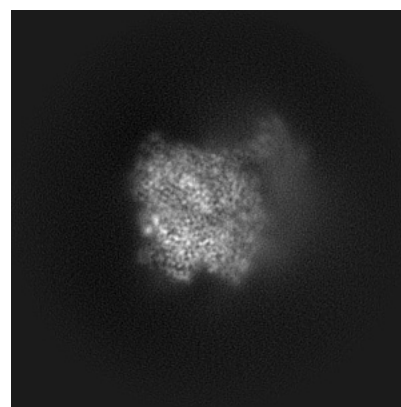
6.1.2 Raw map



X



Y

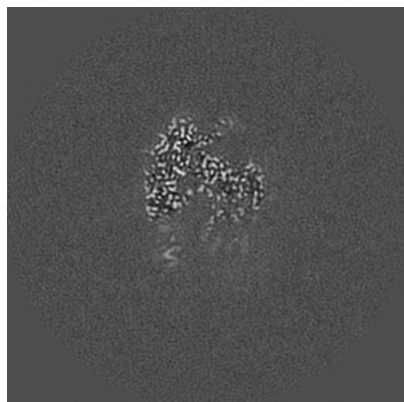


Z

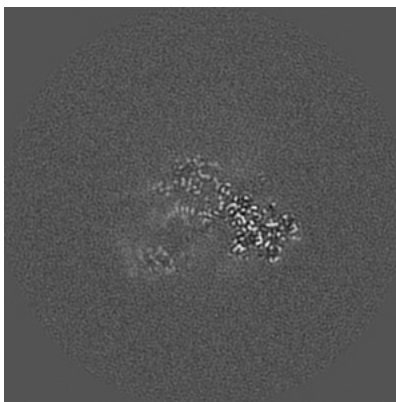
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

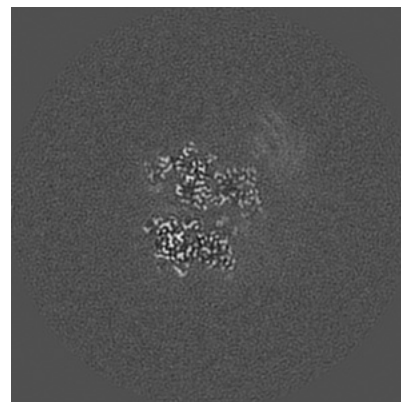
6.2.1 Primary map



X Index: 150

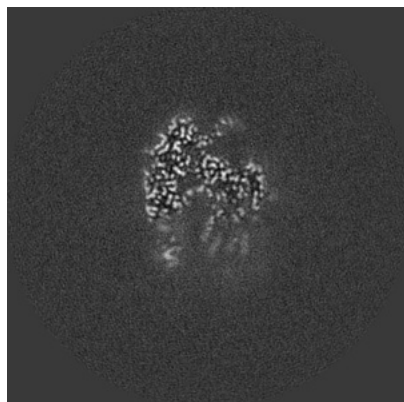


Y Index: 150

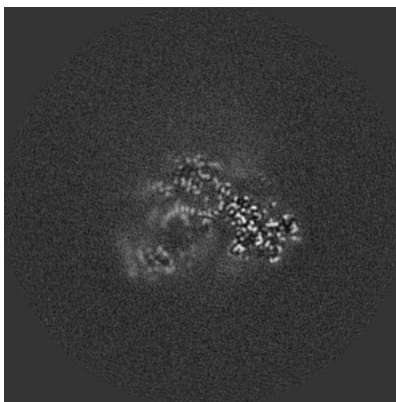


Z Index: 150

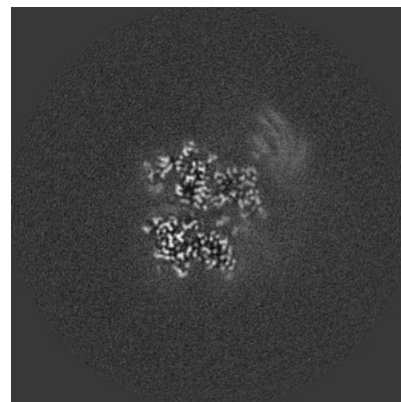
6.2.2 Raw map



X Index: 150



Y Index: 150

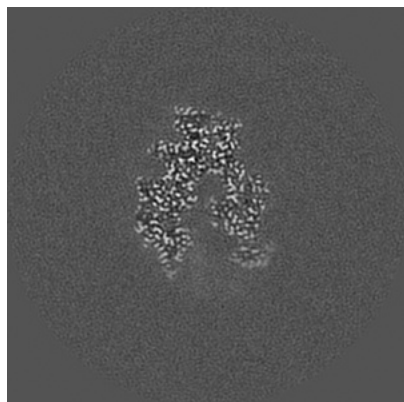


Z Index: 150

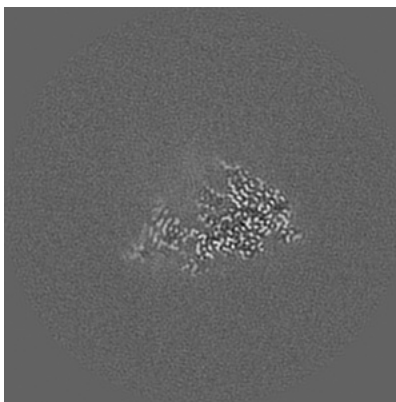
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

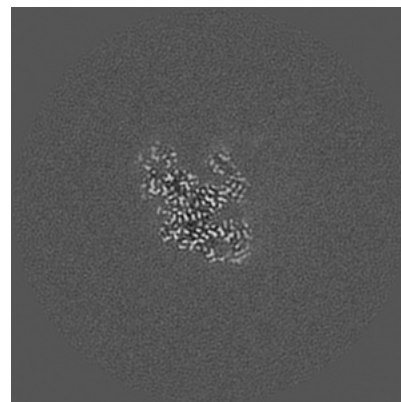
6.3.1 Primary map



X Index: 129

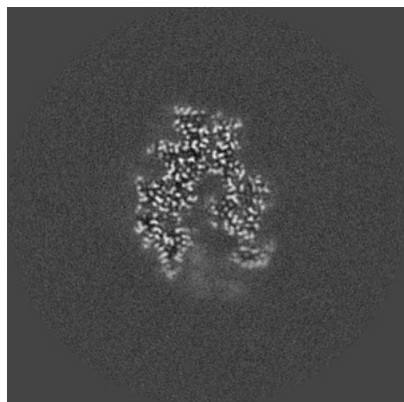


Y Index: 129

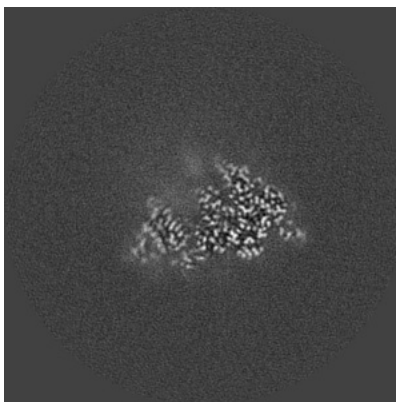


Z Index: 181

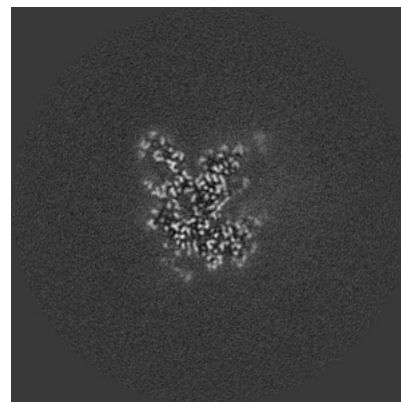
6.3.2 Raw map



X Index: 129



Y Index: 127

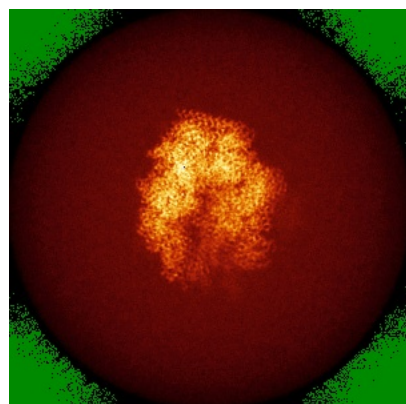


Z Index: 173

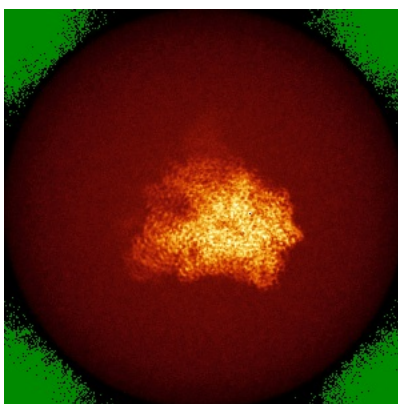
The images above show the largest variance slices of the map in three orthogonal directions.

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

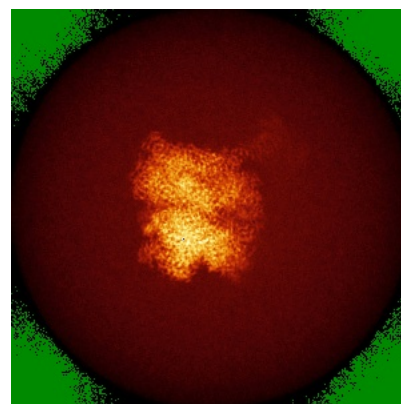
6.4.1 Primary map



X

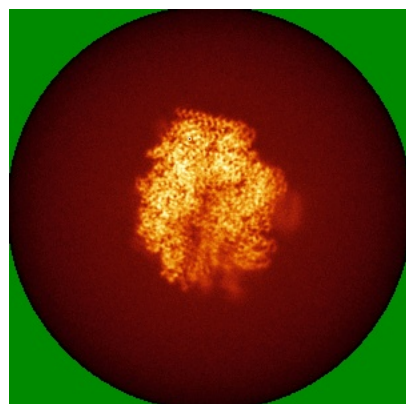


Y

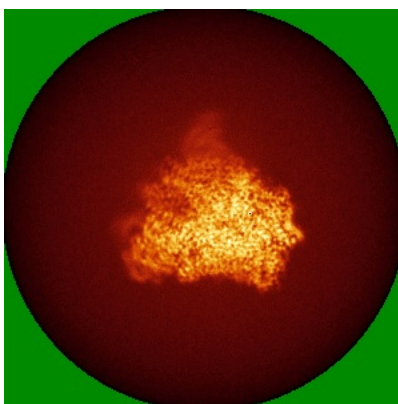


Z

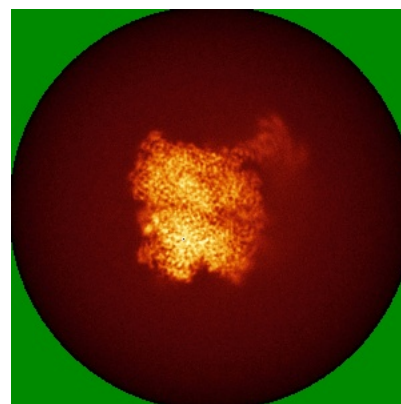
6.4.2 Raw map



X



Y

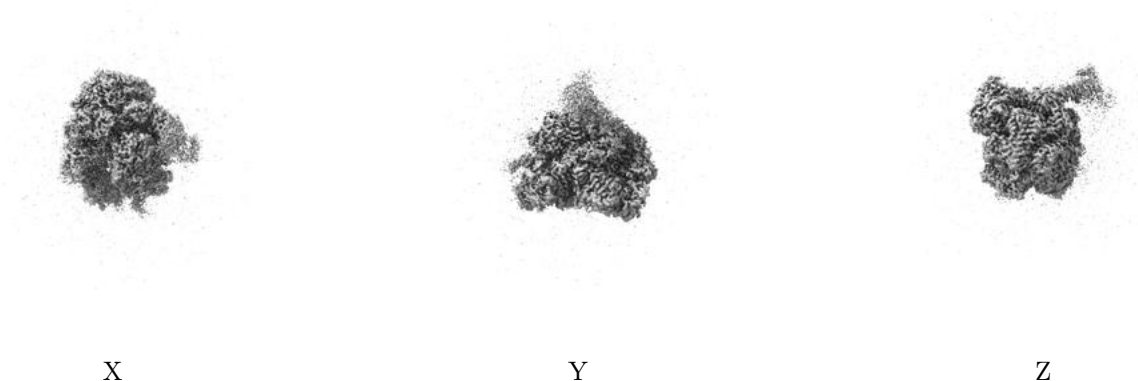


Z

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

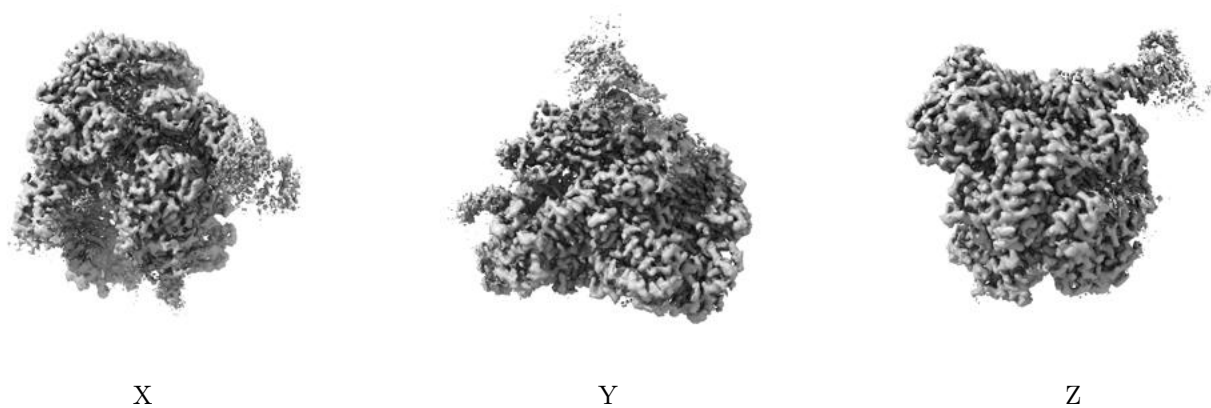
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

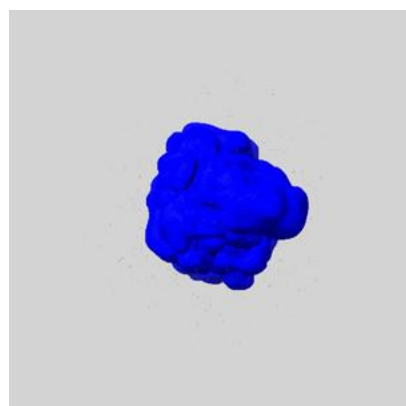
6.6 Mask visualisation [i](#)

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

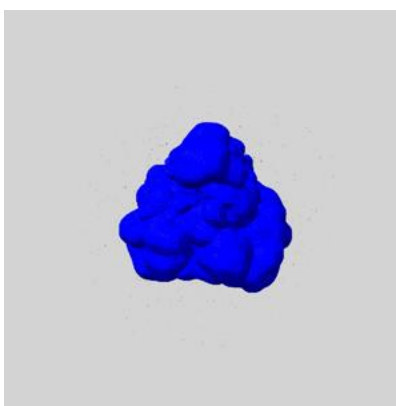
A mask typically either:

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

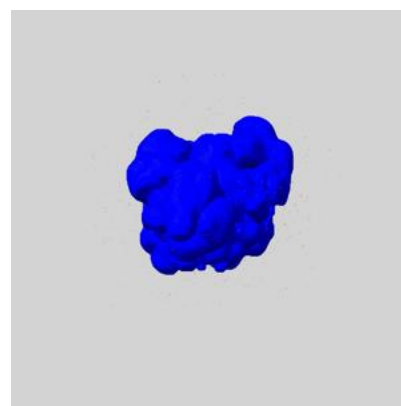
6.6.1 emd_12974_msk_1.map [i](#)



X



Y

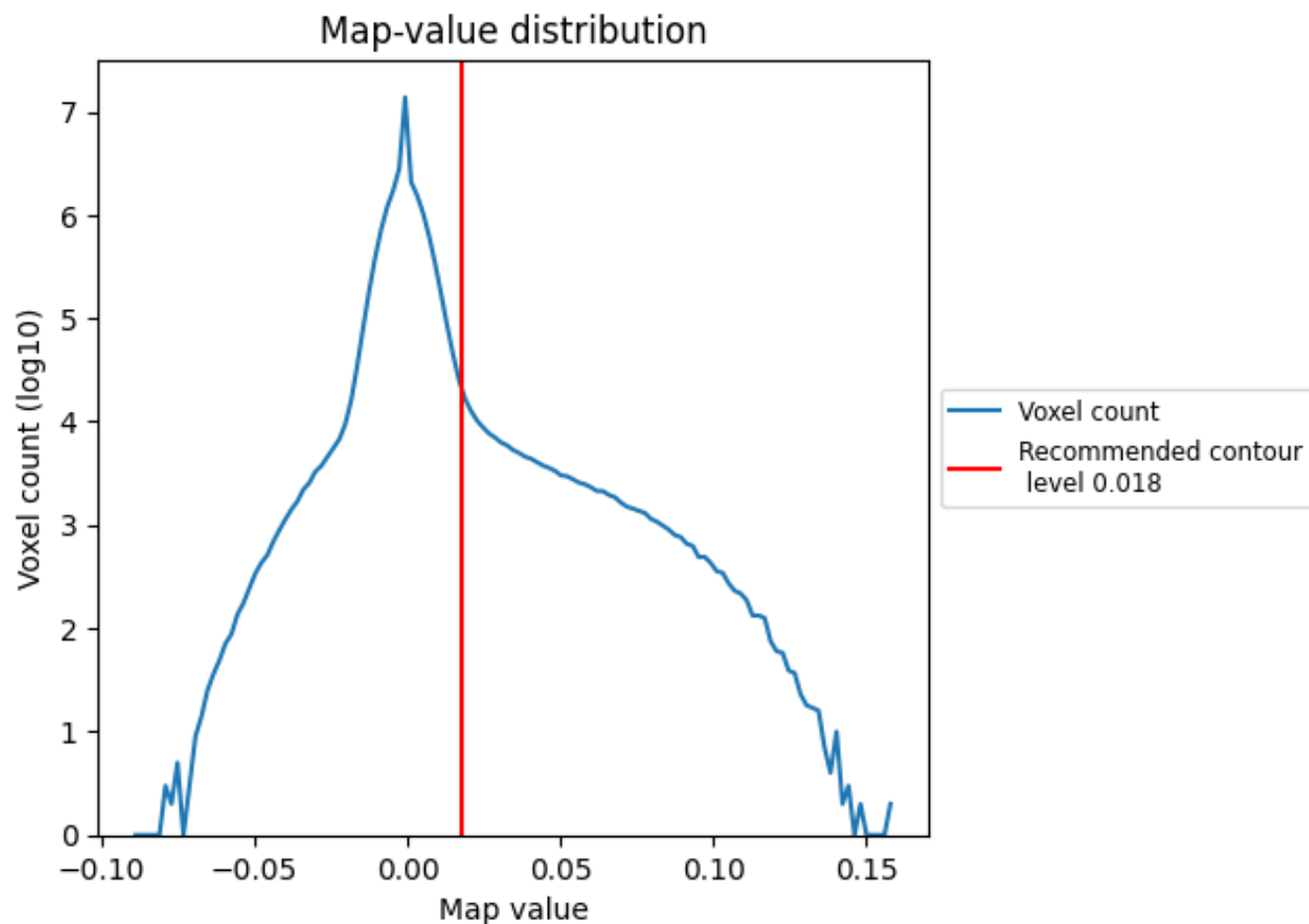


Z

7 Map analysis [i](#)

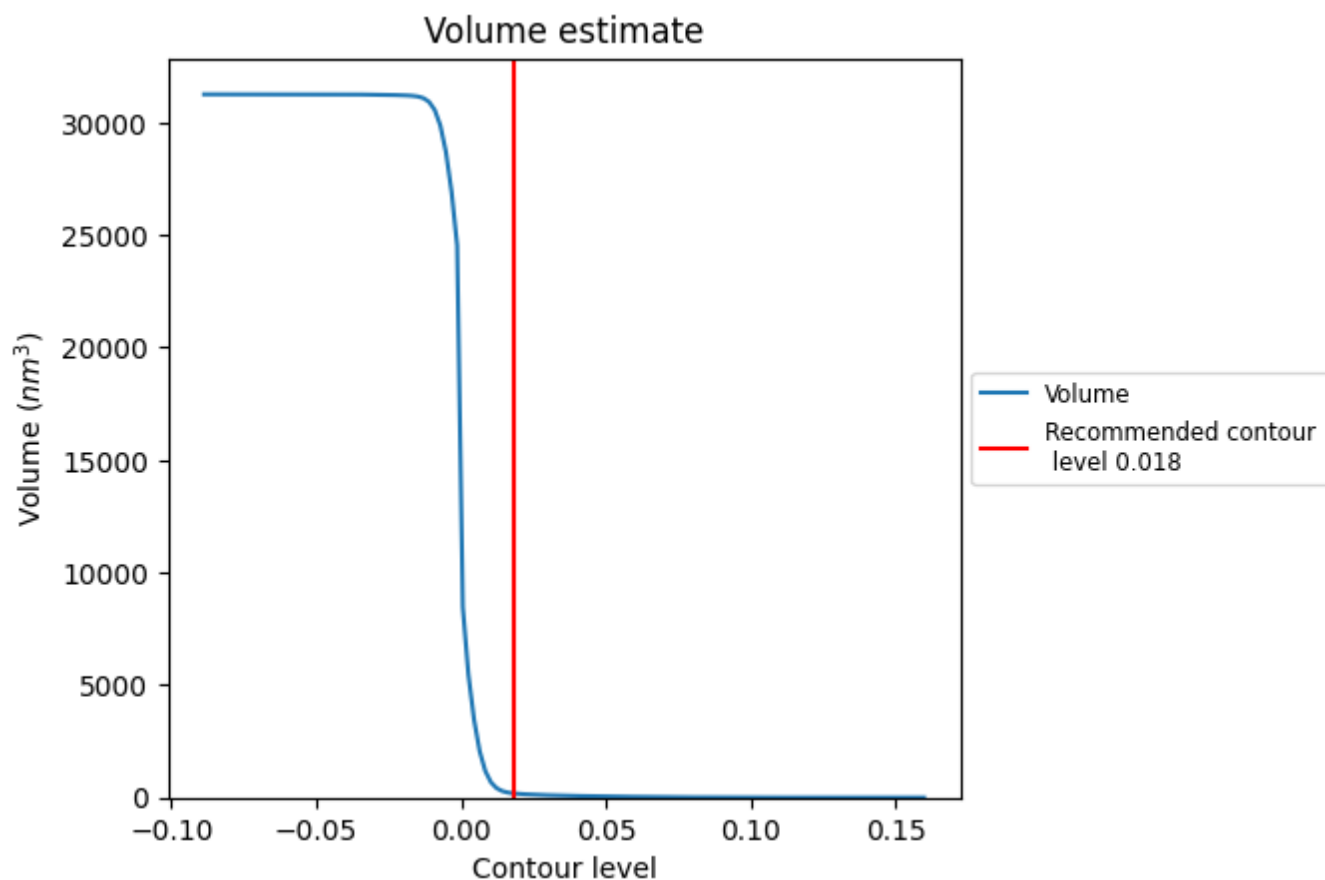
This section contains the results of statistical analysis of the map.

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.

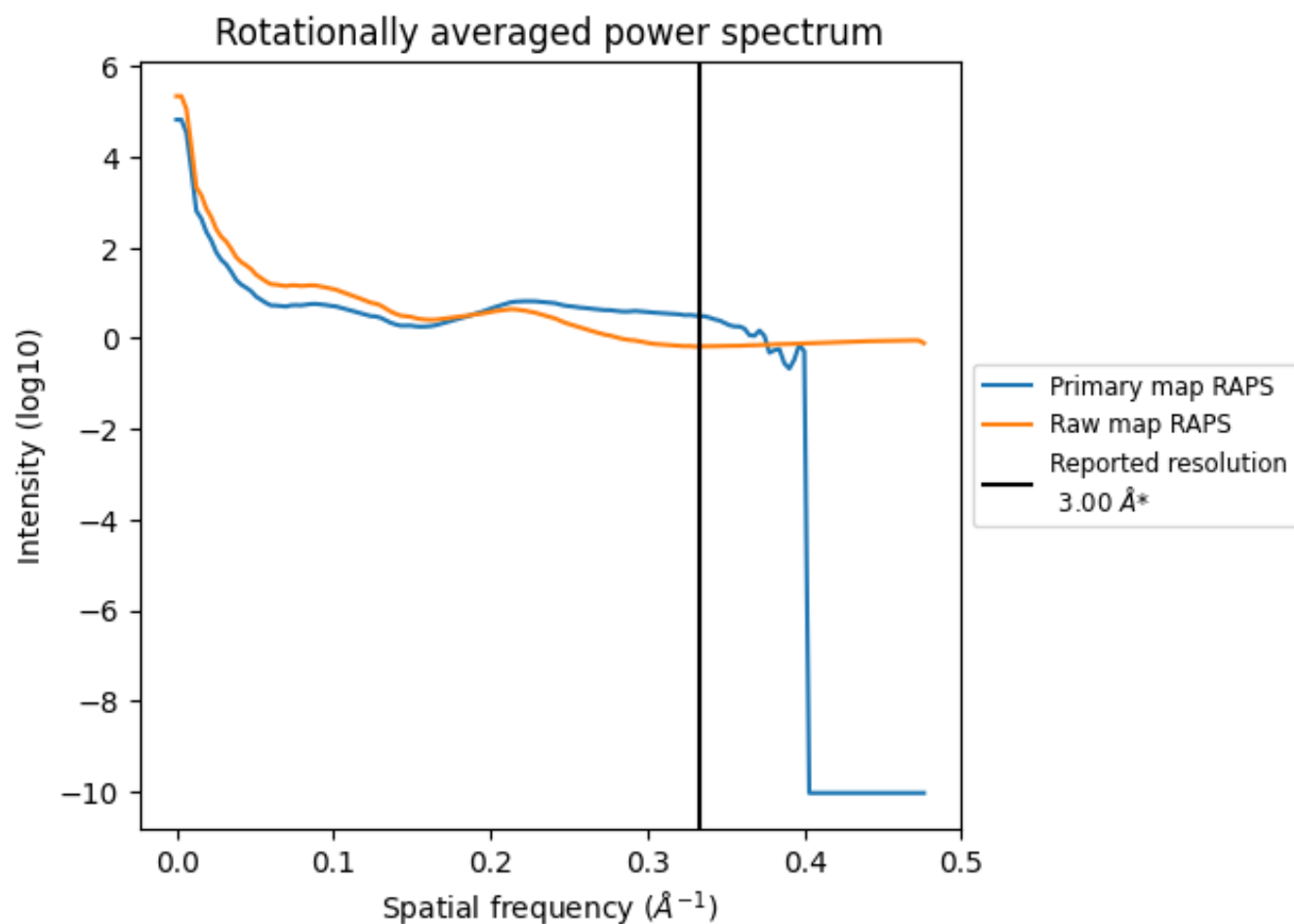
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 169 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 ⓘ

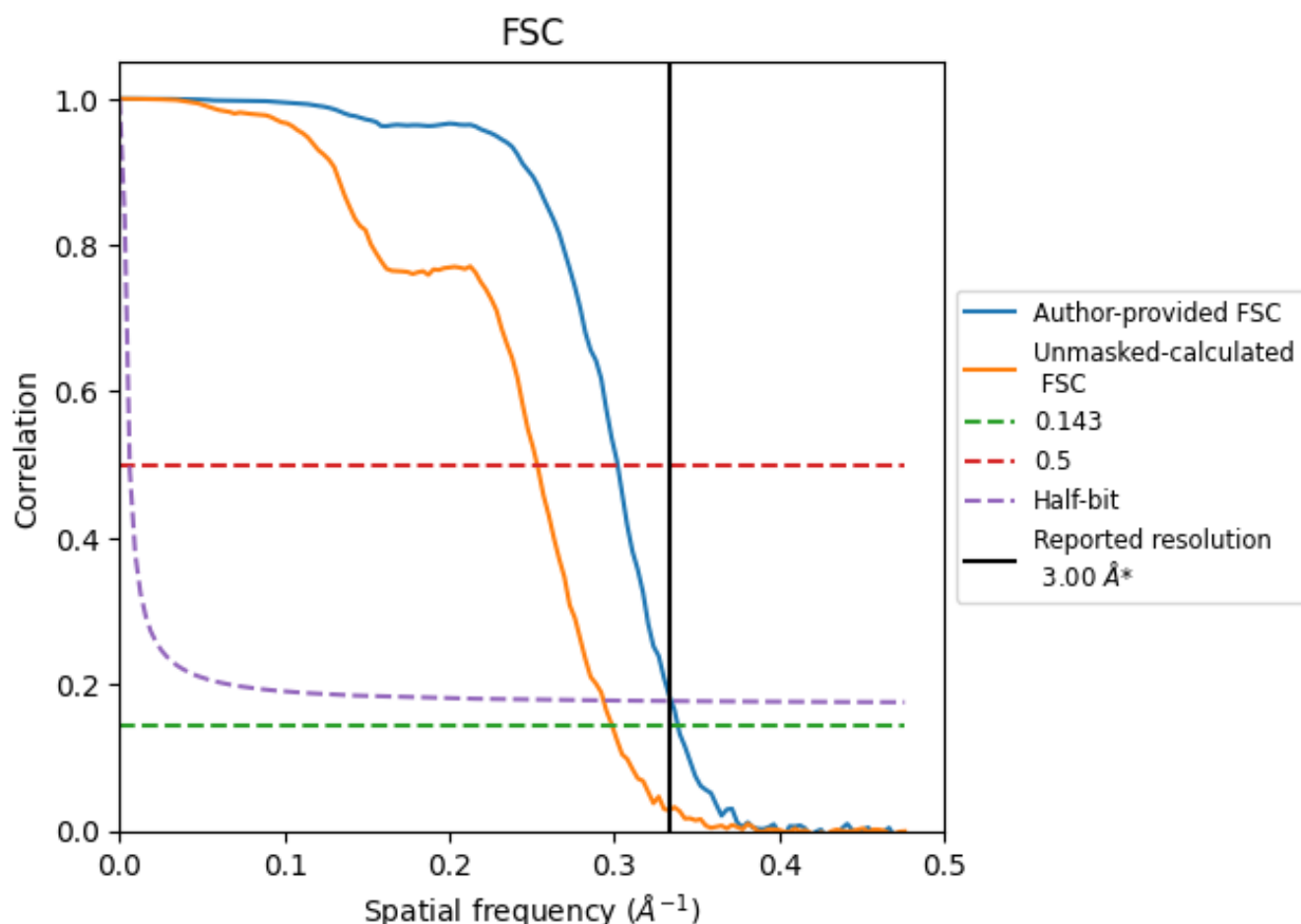


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

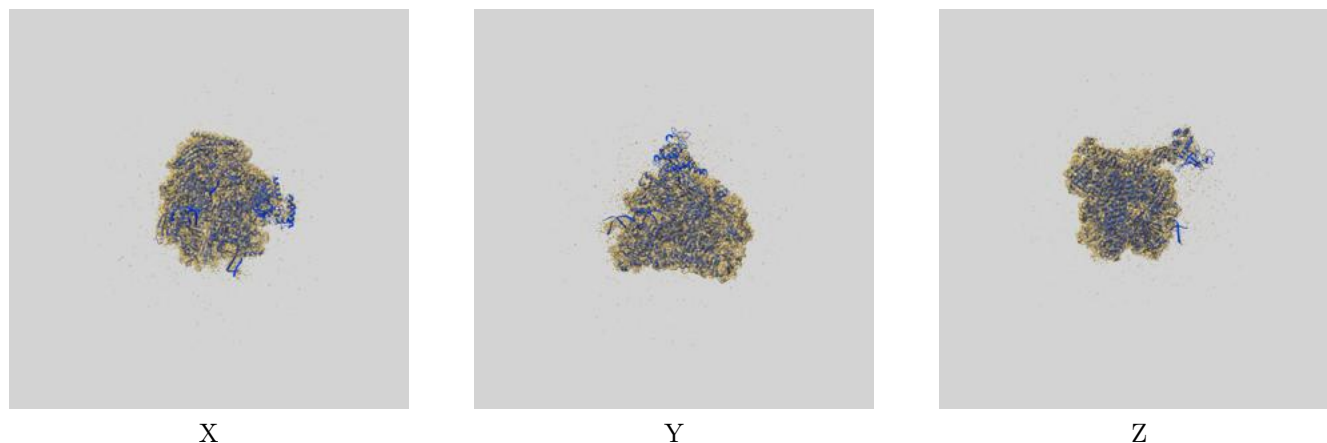
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.31	2.99
Unmasked-calculated*	3.35	3.95	3.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

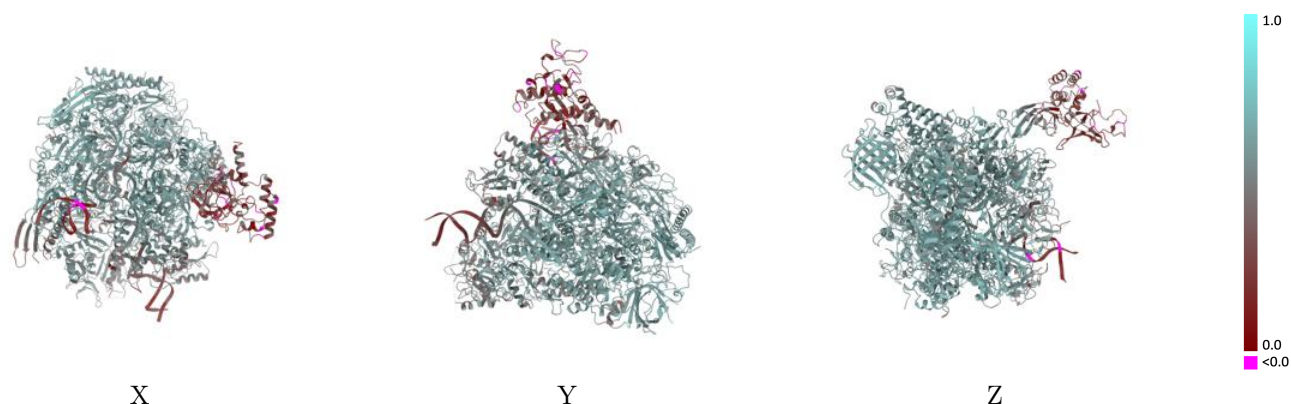
This section contains information regarding the fit between EMDB map EMD-12974 and PDB model 7OL0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



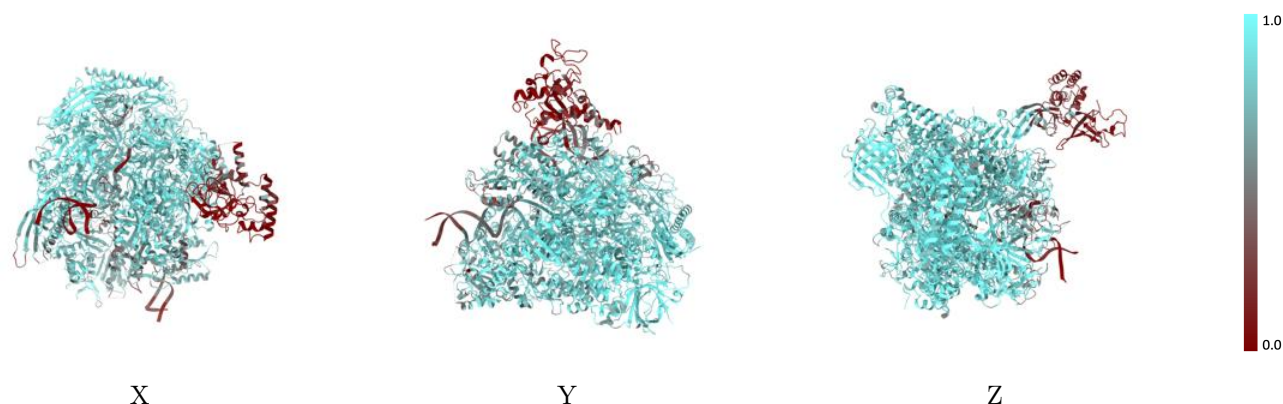
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



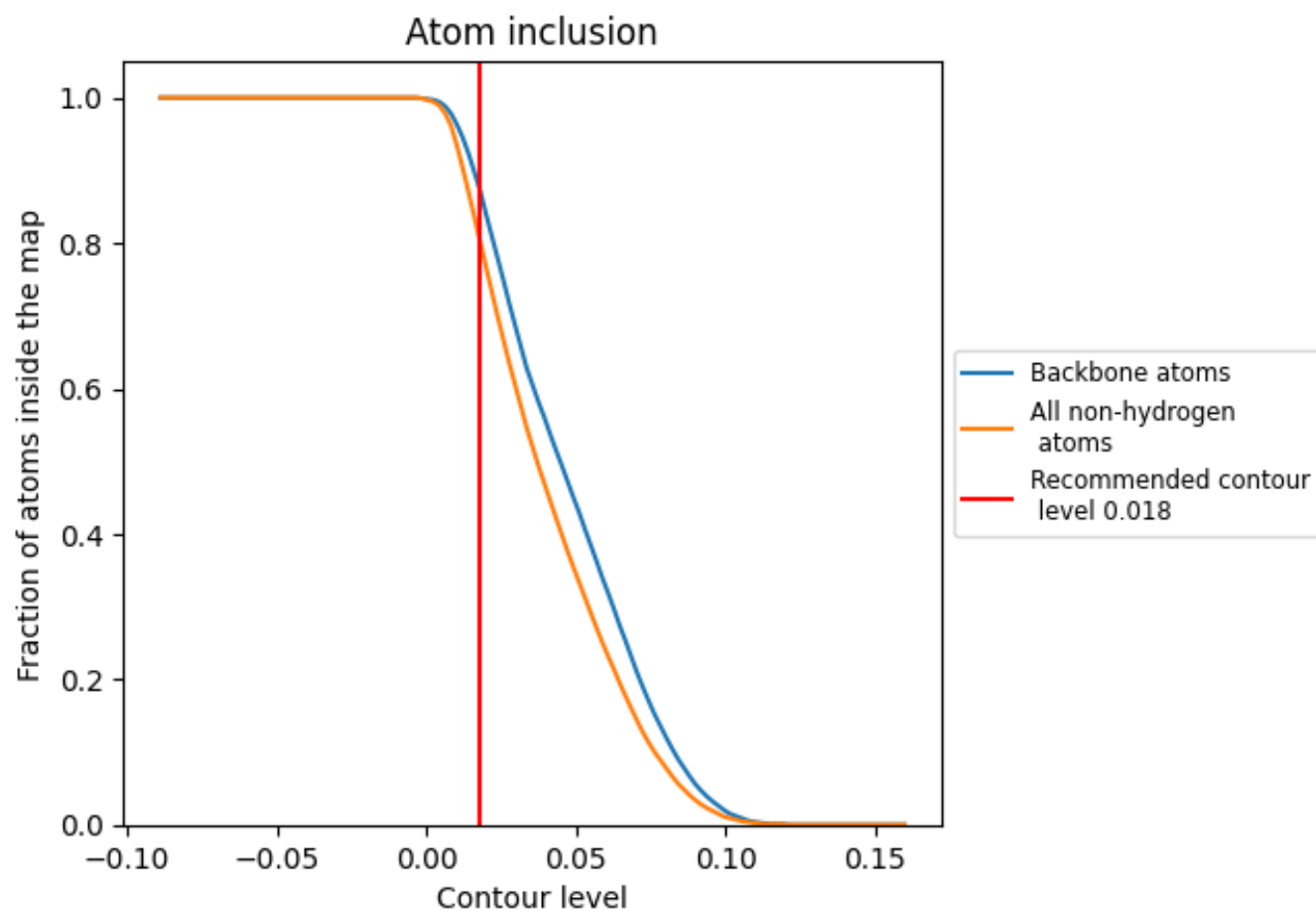
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.5580
A	 0.8460	 0.5810
B	 0.8820	 0.5920
C	 0.9220	 0.6180
D	 0.1410	 0.2850
E	 0.8310	 0.5600
F	 0.8980	 0.6140
G	 0.3240	 0.3390
H	 0.8920	 0.6000
I	 0.7990	 0.5360
J	 0.9510	 0.6300
K	 0.9100	 0.6080
L	 0.8380	 0.5700
N	 0.3860	 0.2950
P	 0.7130	 0.5400
T	 0.5250	 0.3740
Z	 0.5380	 0.5540

