



Full wwPDB EM Validation Report ⓘ

Jul 18, 2024 – 04:27 PM JST

PDB ID : 8XMD
EMDB ID : EMD-38472
Title : Pre-translocated Pol IV transcription elongation complex
Authors : Huang, K.; Fang, C.L.; Zhang, Y.
Deposited on : 2023-12-27
Resolution : 3.40 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:

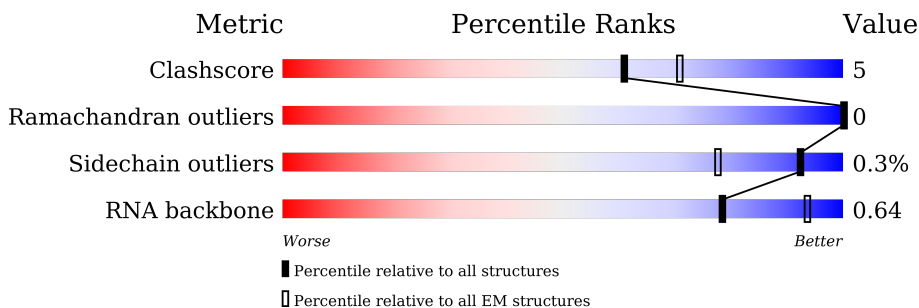
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.40 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.




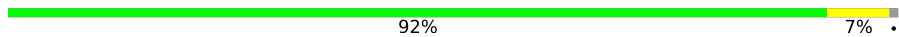




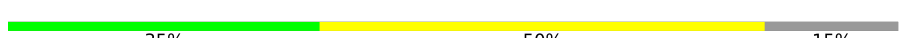


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1498	68% (green), 9% (yellow), 23% (grey)
2	B	1172	80% (green), 10% (yellow), 9% (grey)
3	C	319	80% (green), 9% (yellow), 11% (grey)
4	D	205	7% (red), 47% (green), 8% (yellow), 45% (grey)
5	E	205	88% (green), 9% (yellow), 5% (grey)
6	F	144	49% (green), 47% (grey)
7	G	174	94% (green), 5% (yellow), 1% (grey)

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Mol	Chain	Length	Quality of chain
8	H	146	 71% 15% 14%
9	I	114	 92% 7%
10	J	71	 70% 15% 13%
11	K	116	 73% 8% 19%
12	L	51	 67% 16% 18%
13	M	1133	 82% 11% 7%
14	N	20	 35% 50% 15%
15	O	16	 44% 12% 12% 31%
16	Q	35	 46% 34% 20%

2 Entry composition i

There are 18 unique types of molecules in this entry. The entry contains 35276 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 IV subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1159	8588	5456	1488	1589	55	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1454	GLY	-	expression tag	UNP Q9LQ02
A	1455	SER	-	expression tag	UNP Q9LQ02
A	1456	GLY	-	expression tag	UNP Q9LQ02
A	1457	SER	-	expression tag	UNP Q9LQ02
A	1458	GLY	-	expression tag	UNP Q9LQ02
A	1459	SER	-	expression tag	UNP Q9LQ02
A	1460	ASP	-	expression tag	UNP Q9LQ02
A	1461	TYR	-	expression tag	UNP Q9LQ02
A	1462	LYS	-	expression tag	UNP Q9LQ02
A	1463	ASP	-	expression tag	UNP Q9LQ02
A	1464	HIS	-	expression tag	UNP Q9LQ02
A	1465	ASP	-	expression tag	UNP Q9LQ02
A	1466	GLY	-	expression tag	UNP Q9LQ02
A	1467	ASP	-	expression tag	UNP Q9LQ02
A	1468	TYR	-	expression tag	UNP Q9LQ02
A	1469	LYS	-	expression tag	UNP Q9LQ02
A	1470	ASP	-	expression tag	UNP Q9LQ02
A	1471	HIS	-	expression tag	UNP Q9LQ02
A	1472	ASP	-	expression tag	UNP Q9LQ02
A	1473	ILE	-	expression tag	UNP Q9LQ02
A	1474	ASP	-	expression tag	UNP Q9LQ02
A	1475	TYR	-	expression tag	UNP Q9LQ02
A	1476	LYS	-	expression tag	UNP Q9LQ02
A	1477	ASP	-	expression tag	UNP Q9LQ02
A	1478	ASP	-	expression tag	UNP Q9LQ02
A	1479	ASP	-	expression tag	UNP Q9LQ02
A	1480	ASP	-	expression tag	UNP Q9LQ02
A	1481	LYS	-	expression tag	UNP Q9LQ02

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1482	GLU	-	expression tag	UNP Q9LQ02
A	1483	ASN	-	expression tag	UNP Q9LQ02
A	1484	LEU	-	expression tag	UNP Q9LQ02
A	1485	TYR	-	expression tag	UNP Q9LQ02
A	1486	PHE	-	expression tag	UNP Q9LQ02
A	1487	GLN	-	expression tag	UNP Q9LQ02
A	1488	GLY	-	expression tag	UNP Q9LQ02
A	1489	HIS	-	expression tag	UNP Q9LQ02
A	1490	HIS	-	expression tag	UNP Q9LQ02
A	1491	HIS	-	expression tag	UNP Q9LQ02
A	1492	HIS	-	expression tag	UNP Q9LQ02
A	1493	HIS	-	expression tag	UNP Q9LQ02
A	1494	HIS	-	expression tag	UNP Q9LQ02
A	1495	HIS	-	expression tag	UNP Q9LQ02
A	1496	HIS	-	expression tag	UNP Q9LQ02
A	1497	HIS	-	expression tag	UNP Q9LQ02
A	1498	HIS	-	expression tag	UNP Q9LQ02

- Molecule 2 is a protein called DNA-directed RNA polymerases IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1061	8056	5134	1458	1417	47	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases II, IV and V subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	283	2111	1346	364	387	14	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases IV and V subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	113	866	548	139	173	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases II and IV subunit 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	198	1505	973	269	254	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases II, IV and V subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	76	568	363	101	101	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	174	1096	707	185	200	4	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases II, IV and V subunit 8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	126	953	627	156	163	7	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases II, IV and V subunit 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	113	830	511	156	151	12	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	62	476	310	84	76	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases II, IV and V subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	94	715	458	131	125	1	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	42	312	192	59	57	4	0	0

- Molecule 13 is a protein called RNA-dependent RNA polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	1052	8035	5132	1378	1474	51	0	0

- Molecule 14 is a DNA chain called Nontemplate_DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	17	348	168	60	104	16	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	O	11	246	109	52	74	11	0	0

- Molecule 16 is a DNA chain called Template_DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	Q	28	561	269	97	167	28	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	3	Total	Zn	0
			3	3	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

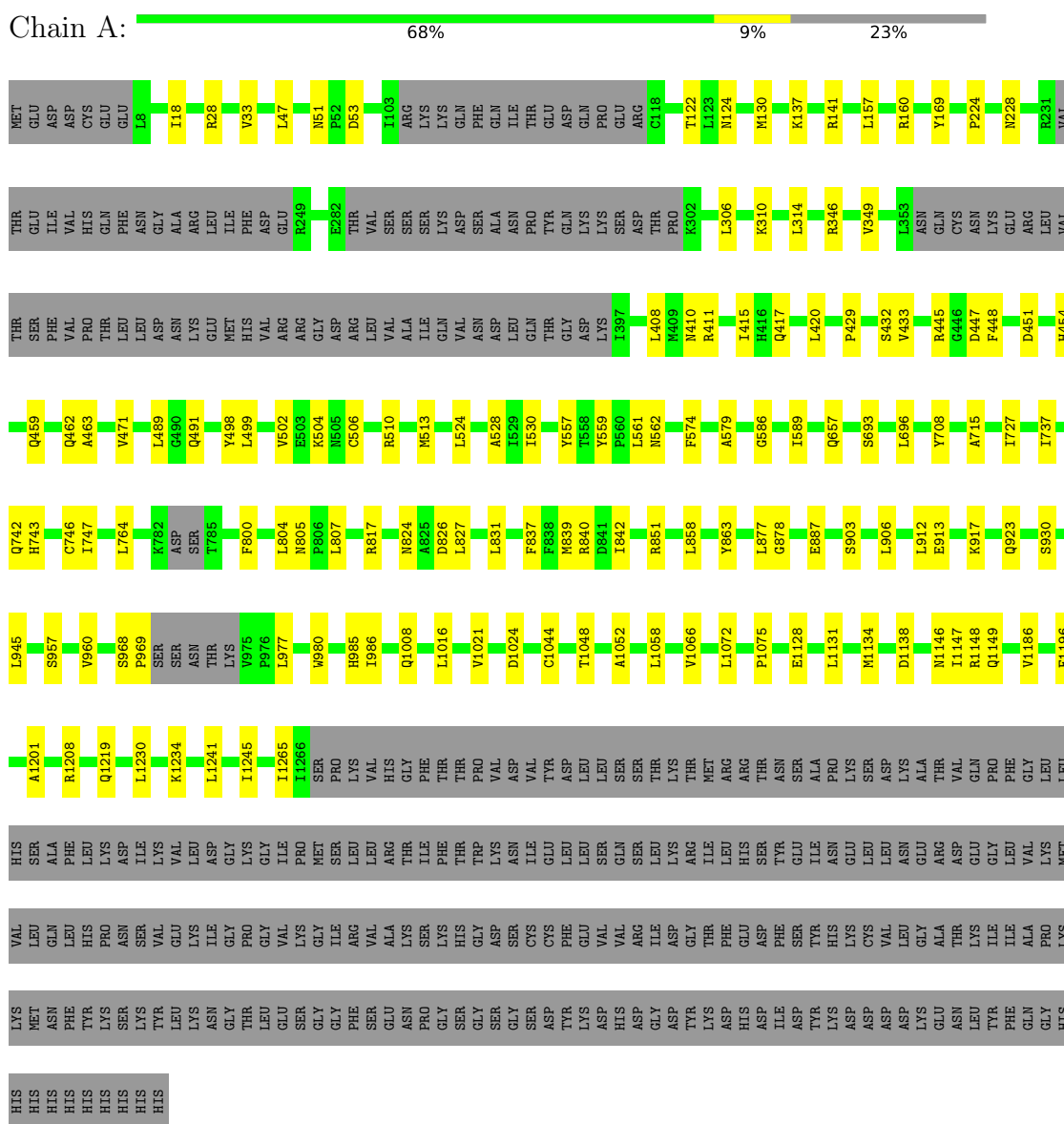
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots [i](#)

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.

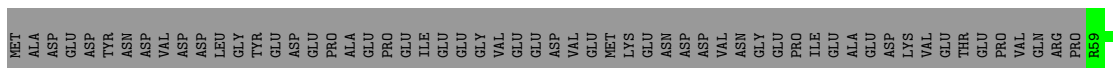
- Molecule 1: DNA-directed RNA polymerase IV subunit 1



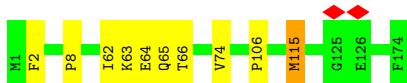
- Molecule 2: DNA-directed RNA polymerases IV and V subunit 2



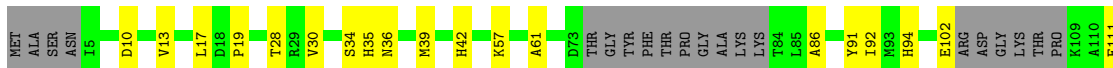
- Molecule 6: DNA-directed RNA polymerases II, IV and V subunit 6A



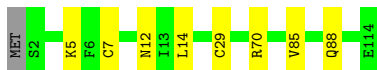
- Molecule 7: DNA-directed RNA polymerase IV subunit 7



- Molecule 8: DNA-directed RNA polymerases II, IV and V subunit 8B



- Molecule 9: DNA-directed RNA polymerases II, IV and V subunit 9A

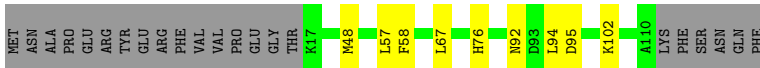


- Molecule 10: DNA-directed RNA polymerases II, IV and V subunit 10



- Molecule 11: DNA-directed RNA polymerases II, IV and V subunit 11





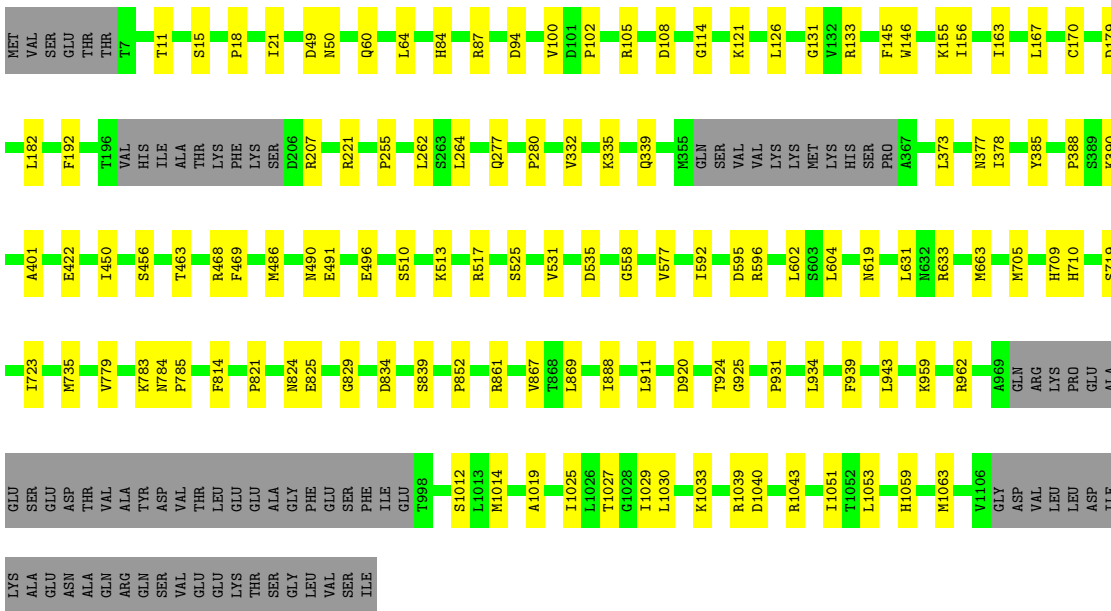
- Molecule 12: DNA-directed RNA polymerases II, IV and V subunit 12

Chain L: 67% 16% 18%



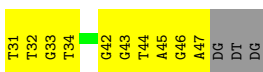
- Molecule 13: RNA-dependent RNA polymerase 2

Chain M: 82% 11% 7%



- Molecule 14: Nontemplate_DNA

Chain N: 35% 50% 15%



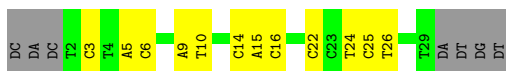
- Molecule 15: RNA

Chain O: 44% 12% 12% 31%



- Molecule 16: Template_DNA

Chain Q: 46% 34% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.971	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.0626	Depositor
Map size (\AA)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	0.24	0/8752	0.44	0/11894
2	B	0.24	0/8224	0.46	0/11124
3	C	0.24	0/2141	0.48	0/2902
4	D	0.24	0/878	0.42	0/1187
5	E	0.23	0/1529	0.46	0/2073
6	F	0.24	0/578	0.47	0/783
7	G	0.24	0/1112	0.43	0/1528
8	H	0.25	0/968	0.46	0/1301
9	I	0.24	0/847	0.50	0/1150
10	J	0.23	0/483	0.50	0/654
11	K	0.23	0/729	0.43	0/992
12	L	0.23	0/315	0.49	0/423
13	M	0.24	0/8203	0.45	0/11114
14	N	0.49	0/389	1.00	0/600
15	O	0.26	0/277	0.89	0/432
16	Q	0.52	0/626	0.89	0/960
All	All	0.25	0/36051	0.48	0/49117

There are no bond length outliers.

There are no bond angle outliers.

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	8588	0	8247	89	0
2	B	8056	0	7801	85	0
3	C	2111	0	2119	19	0
4	D	866	0	880	11	0
5	E	1505	0	1474	13	0
6	F	568	0	542	3	0
7	G	1096	0	896	9	0
8	H	953	0	933	13	0
9	I	830	0	727	7	0
10	J	476	0	485	9	0
11	K	715	0	681	8	0
12	L	312	0	278	4	0
13	M	8035	0	7719	66	0
14	N	348	0	196	9	0
15	O	246	0	121	5	0
16	Q	561	0	316	8	0
17	A	3	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	35276	0	33415	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (313) 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:49:ILE:HD13	2:B:490:LEU:HD13	1.72	0.72
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.73	0.70
13:M:182:LEU:HD11	13:M:264:LEU:HD11	1.73	0.69
2:B:49:ILE:HD11	2:B:204:GLN:HB2	1.76	0.68
2:B:771:ASN:HD21	10:J:51:THR:HG21	1.60	0.67
1:A:742:GLN:HE21	2:B:955:GLN:HE22	1.40	0.67
13:M:1025:ILE:HG13	13:M:1051:ILE:HD11	1.77	0.67
1:A:417:GLN:O	2:B:1086:HIS:NE2	2.27	0.66
12:L:29:CYS:SG	12:L:32:CYS:HB3	2.35	0.66
4:D:136:TYR:HE2	4:D:203:LYS:H	1.43	0.65
13:M:155:LYS:HB3	13:M:192:PHE:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:963:ALA:HB1	2:B:1033:GLY:HA3	1.79	0.64
14:N:33:DG:H2''	14:N:34:DT:H5''	1.78	0.64
1:A:528:ALA:HA	8:H:94:HIS:HB3	1.80	0.64
1:A:47:LEU:O	1:A:228:ASN:ND2	2.31	0.63
16:Q:14:DC:H2''	16:Q:15:DA:H5''	1.79	0.63
1:A:411:ARG:NH2	15:O:10:A:O2'	2.32	0.62
2:B:797:ARG:HD2	10:J:8:PHE:HA	1.82	0.62
8:H:42:HIS:HB2	8:H:122:LEU:HB3	1.81	0.62
5:E:17:LEU:HD21	5:E:69:ILE:HD13	1.82	0.62
7:G:115:MET:SD	7:G:115:MET:N	2.70	0.62
13:M:221:ARG:NH1	13:M:422:GLU:OE2	2.33	0.62
1:A:903:SER:HB3	1:A:906:LEU:HD23	1.82	0.61
1:A:923:GLN:OE1	1:A:1149:GLN:NE2	2.33	0.61
4:D:91:CYS:N	7:G:2:PHE:O	2.33	0.61
12:L:12:CYS:SG	12:L:13:GLY:N	2.70	0.61
13:M:469:PHE:HB3	13:M:486:MET:HB3	1.82	0.61
1:A:429:PRO:HD2	11:K:67:LEU:HD13	1.81	0.61
13:M:558:GLY:HA3	13:M:592:ILE:HG22	1.82	0.61
1:A:433:VAL:HG11	2:B:910:LEU:HD23	1.81	0.61
14:N:45:DA:H2''	14:N:46:DG:C8	2.35	0.61
4:D:177:ILE:HG13	4:D:179:SER:H	1.65	0.60
3:C:297:ARG:NH1	11:K:92:ASN:OD1	2.34	0.60
1:A:504:LYS:NZ	1:A:574:PHE:O	2.27	0.60
2:B:917:MET:SD	2:B:1038:GLN:NE2	2.75	0.60
13:M:821:PRO:HG2	13:M:824:ASN:HB2	1.83	0.60
13:M:64:LEU:HG	13:M:100:VAL:HG21	1.84	0.59
1:A:708:TYR:HH	1:A:746:CYS:HG	1.50	0.59
3:C:158:ARG:HE	10:J:60:LEU:HB3	1.67	0.59
2:B:1136:CYS:SG	2:B:1137:VAL:N	2.75	0.59
1:A:1008:GLN:NE2	1:A:1075:PRO:O	2.35	0.59
2:B:577:ASN:HD21	2:B:622:THR:H	1.50	0.59
1:A:410:ASN:HD22	1:A:454:HIS:HE1	1.49	0.59
13:M:735:MET:HG2	13:M:814:PHE:HB2	1.84	0.59
16:Q:9:DA:H2'	16:Q:10:DT:H71	1.84	0.59
1:A:1128:GLU:OE1	5:E:9:ARG:NH1	2.31	0.59
10:J:3:ILE:HG13	10:J:18:TRP:HB2	1.84	0.58
13:M:1027:THR:HG23	13:M:1029:ILE:H	1.68	0.58
1:A:804:LEU:HB2	2:B:708:ASN:HB2	1.85	0.58
1:A:130:MET:SD	1:A:169:TYR:OH	2.55	0.58
13:M:133:ARG:HB3	13:M:146:TRP:HB2	1.84	0.58
1:A:499:LEU:HD21	1:A:727:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:LYS:HG3	9:I:14:LEU:HD12	1.86	0.58
2:B:599:ARG:NH1	2:B:635:GLU:OE1	2.37	0.58
2:B:795:LEU:HD22	2:B:908:PRO:HG2	1.85	0.58
1:A:122:THR:HG22	1:A:124:ASN:H	1.68	0.57
3:C:297:ARG:NH2	11:K:95:ASP:OD2	2.37	0.57
13:M:339:GLN:NE2	13:M:1012:SER:OG	2.37	0.57
1:A:445:ARG:NH1	1:A:887:GLU:OE2	2.37	0.57
3:C:62:LEU:HD12	3:C:155:VAL:HG12	1.86	0.57
1:A:506:CYS:SG	2:B:1027:ARG:NH2	2.77	0.57
2:B:354:LEU:O	2:B:368:LYS:NZ	2.38	0.57
2:B:921:LYS:NZ	15:O:10:A:OP1	2.32	0.57
4:D:125:ARG:HG3	7:G:106:PRO:HG2	1.87	0.57
1:A:657:GLN:OE1	9:I:70:ARG:NH2	2.38	0.57
2:B:226:LYS:HD3	2:B:577:ASN:HB3	1.86	0.57
8:H:10:ASP:OD2	8:H:34:SER:OG	2.23	0.57
3:C:25:GLU:HG2	3:C:267:ILE:HG12	1.87	0.56
14:N:42:DG:H2''	14:N:43:DG:H5'	1.87	0.56
1:A:137:LYS:HA	1:A:141:ARG:HA	1.86	0.56
2:B:238:SER:OG	2:B:240:ARG:NH1	2.37	0.56
8:H:13:VAL:HG22	8:H:57:LYS:HG2	1.87	0.56
1:A:510:ARG:NH2	11:K:57:LEU:O	2.39	0.56
1:A:513:MET:HG3	1:A:524:LEU:HD11	1.87	0.56
2:B:365:LEU:HD12	2:B:368:LYS:HD2	1.87	0.56
6:F:108:ARG:NH2	6:F:129:ASP:O	2.31	0.56
13:M:388:PRO:HB3	13:M:450:ILE:HD12	1.87	0.55
13:M:1039:ARG:NH1	13:M:1040:ASP:OD2	2.39	0.55
1:A:817:ARG:NH2	2:B:519:PHE:O	2.38	0.55
1:A:764:LEU:HA	1:A:807:LEU:HD23	1.89	0.55
13:M:633:ARG:NH2	13:M:719:SER:O	2.40	0.55
1:A:1265:ILE:HG12	7:G:62:ILE:HD11	1.88	0.55
13:M:108:ASP:HA	13:M:131:GLY:HA2	1.89	0.55
1:A:824:ASN:HA	1:A:827:LEU:HD13	1.89	0.55
1:A:945:LEU:HD13	9:I:88:GLN:HG3	1.89	0.54
14:N:46:DG:H1	16:Q:3:DC:H42	1.55	0.54
1:A:957:SER:HB3	1:A:1072:LEU:HB3	1.90	0.54
1:A:346:ARG:O	2:B:1052:ASN:ND2	2.41	0.54
13:M:861:ARG:NH1	13:M:925:GLY:O	2.40	0.54
13:M:1030:LEU:O	13:M:1033:LYS:NZ	2.35	0.54
3:C:25:GLU:OE1	3:C:27:ARG:NH2	2.41	0.54
3:C:52:LEU:HD23	3:C:168:ILE:HD11	1.89	0.54
8:H:19:PRO:HG2	8:H:28:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:525:SER:HB3	13:M:619:ASN:HB2	1.89	0.54
2:B:918:HIS:NE2	2:B:962:GLU:OE1	2.37	0.54
15:O:9:U:H2'	15:O:10:A:H8	1.73	0.54
3:C:226:VAL:HG23	3:C:227:THR:HG23	1.90	0.54
1:A:462:GLN:NE2	7:G:64:GLU:OE1	2.37	0.54
2:B:859:ILE:HG13	2:B:874:LYS:HG2	1.89	0.54
13:M:145:PHE:HB2	13:M:156:ILE:HB	1.90	0.54
2:B:516:ARG:NH1	2:B:667:GLU:OE1	2.41	0.53
1:A:530:ILE:HB	8:H:92:ILE:HB	1.91	0.53
7:G:8:PRO:HB3	7:G:74:VAL:HG22	1.91	0.53
14:N:31:DT:H2''	14:N:32:DT:H5''	1.91	0.52
4:D:177:ILE:HD12	4:D:178:PRO:HD2	1.91	0.52
8:H:61:ALA:HB3	8:H:142:LEU:HB2	1.89	0.52
8:H:102:GLU:HA	8:H:111:GLU:HG2	1.90	0.52
9:I:14:LEU:HD23	9:I:29:CYS:HB3	1.91	0.52
1:A:157:LEU:HD23	1:A:160:ARG:HH12	1.74	0.52
2:B:714:ARG:HG3	2:B:956:THR:HG22	1.92	0.52
13:M:332:VAL:HA	13:M:335:LYS:HE3	1.90	0.52
1:A:977:LEU:HD11	1:A:1048:THR:HB	1.92	0.52
12:L:28:GLN:HE21	12:L:33:GLY:HA2	1.73	0.52
13:M:510:SER:HB3	13:M:513:LYS:HB2	1.91	0.52
13:M:121:LYS:HE3	13:M:262:LEU:HG	1.93	0.52
13:M:163:ILE:HD11	13:M:255:PRO:HD2	1.92	0.52
13:M:463:THR:HG22	13:M:468:ARG:HG3	1.91	0.52
15:O:9:U:H2'	15:O:10:A:C8	2.45	0.52
2:B:518:CYS:HG	2:B:521:SER:HG	1.55	0.51
1:A:985:HIS:CD2	1:A:1044:CYS:SG	3.03	0.51
2:B:749:GLN:NE2	2:B:771:ASN:OD1	2.43	0.51
1:A:1201:ALA:HB1	1:A:1219:GLN:HE22	1.75	0.51
3:C:191:GLU:OE1	3:C:265:SER:OG	2.28	0.51
5:E:13:ILE:HD12	5:E:130:MET:HB2	1.91	0.51
13:M:373:LEU:HA	13:M:377:ASN:HA	1.93	0.51
2:B:990:THR:HB	2:B:993:SER:HB2	1.93	0.51
11:K:58:PHE:HB3	11:K:76:HIS:HB2	1.91	0.51
2:B:774:VAL:HG22	2:B:944:ILE:HB	1.92	0.51
5:E:21:LEU:HD11	5:E:69:ILE:HD11	1.91	0.51
2:B:845:ASP:OD2	12:L:10:TYR:OH	2.24	0.50
13:M:535:ASP:OD1	13:M:535:ASP:N	2.43	0.50
13:M:18:PRO:HB2	13:M:21:ILE:HG23	1.92	0.50
1:A:51:ASN:HD21	1:A:53:ASP:HB2	1.76	0.50
1:A:1016:LEU:HD23	1:A:1066:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:VAL:HA	1:A:986:ILE:HG12	1.92	0.50
3:C:209:LYS:NZ	3:C:228:ARG:O	2.44	0.50
13:M:490:ASN:OD1	13:M:491:GLU:N	2.44	0.50
13:M:888:ILE:HG23	13:M:911:LEU:HD12	1.93	0.50
1:A:1146:ASN:OD1	1:A:1147:ILE:N	2.45	0.49
10:J:30:THR:HG23	10:J:33:ASP:H	1.76	0.49
4:D:178:PRO:HA	4:D:181:LYS:HD3	1.94	0.49
1:A:913:GLU:O	1:A:917:LYS:NZ	2.42	0.49
2:B:718:GLN:NE2	2:B:916:SER:O	2.45	0.49
1:A:831:LEU:HD11	1:A:912:LEU:HD12	1.93	0.49
1:A:851:ARG:HG2	1:A:858:LEU:HD23	1.95	0.49
2:B:707:ALA:HB3	2:B:991:PRO:HB3	1.95	0.49
13:M:663:MET:HB3	13:M:710:HIS:CE1	2.48	0.49
13:M:779:VAL:HG13	13:M:839:SER:H	1.77	0.49
2:B:1101:ASP:N	2:B:1101:ASP:OD1	2.46	0.49
5:E:5:GLU:HA	5:E:8:LYS:HE2	1.93	0.49
1:A:415:ILE:HD11	1:A:445:ARG:HG3	1.95	0.49
2:B:586:ASP:OD1	2:B:586:ASP:N	2.46	0.49
8:H:86:ALA:HA	8:H:92:ILE:HD11	1.94	0.48
2:B:291:ASP:OD2	9:I:12:ASN:ND2	2.42	0.48
2:B:692:ASP:OD2	2:B:694:SER:OG	2.31	0.48
16:Q:15:DA:H2''	16:Q:16:DC:H5''	1.94	0.48
2:B:617:GLU:OE2	2:B:619:ARG:NH2	2.41	0.48
2:B:628:LEU:HD13	2:B:661:LEU:HB3	1.94	0.48
13:M:867:VAL:HG12	13:M:869:LEU:H	1.78	0.48
2:B:790:MET:HG2	2:B:944:ILE:HG12	1.96	0.48
3:C:87:SER:HB2	3:C:170:ARG:HD3	1.96	0.48
13:M:114:GLY:HA2	13:M:126:LEU:HD13	1.95	0.48
13:M:631:LEU:HB2	13:M:723:ILE:HB	1.96	0.48
2:B:629:ARG:NH2	2:B:667:GLU:OE2	2.47	0.48
1:A:805:ASN:HD21	2:B:674:TRP:HZ3	1.61	0.48
2:B:75:LEU:HA	2:B:94:THR:HG22	1.94	0.48
5:E:146:LEU:HD21	5:E:187:LYS:HB2	1.95	0.47
8:H:91:TYR:HB3	8:H:143:MET:HB2	1.95	0.47
13:M:18:PRO:HD2	13:M:21:ILE:HD13	1.96	0.47
6:F:73:ILE:HD11	6:F:114:ILE:HD11	1.97	0.47
16:Q:25:DC:H2'	16:Q:26:DT:H71	1.95	0.47
4:D:149:LEU:HD13	4:D:154:ILE:HG23	1.96	0.47
1:A:310:LYS:HA	1:A:314:LEU:HB2	1.95	0.47
9:I:70:ARG:HG2	9:I:85:VAL:HG22	1.97	0.47
13:M:783:LYS:NZ	13:M:829:GLY:HA3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ARG:NH2	2:B:662:ILE:O	2.47	0.47
1:A:562:ASN:HD21	1:A:579:ALA:HB3	1.80	0.47
13:M:102:PRO:HA	13:M:105:ARG:HD2	1.97	0.47
1:A:411:ARG:HH21	1:A:451:ASP:CG	2.18	0.46
1:A:28:ARG:HE	1:A:224:PRO:HD3	1.80	0.46
1:A:306:LEU:HG	1:A:310:LYS:HE3	1.97	0.46
1:A:858:LEU:HD11	5:E:160:VAL:HG11	1.96	0.46
13:M:280:PRO:HG3	13:M:390:LYS:HB2	1.96	0.46
2:B:95:VAL:HG12	2:B:138:VAL:HG12	1.97	0.46
3:C:99:CYS:SG	3:C:100:GLU:N	2.88	0.46
5:E:21:LEU:HD22	5:E:26:TYR:HD2	1.81	0.46
1:A:432:SER:O	2:B:1044:SER:OG	2.33	0.46
1:A:1021:VAL:HG21	1:A:1052:ALA:HB2	1.98	0.46
14:N:43:DG:H2'	14:N:44:DT:C6	2.51	0.46
13:M:920:ASP:OD2	13:M:924:THR:OG1	2.30	0.46
1:A:693:SER:HB2	1:A:696:LEU:HB2	1.98	0.46
2:B:210:ILE:HG13	2:B:456:PHE:HB3	1.98	0.46
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.98	0.46
1:A:980:TRP:NE1	1:A:1058:LEU:O	2.49	0.45
2:B:797:ARG:NH1	10:J:8:PHE:O	2.49	0.45
1:A:349:VAL:HA	1:A:459:GLN:HE22	1.81	0.45
2:B:612:ASP:OD1	2:B:612:ASP:N	2.50	0.45
14:N:43:DG:H4'	14:N:44:DT:OP1	2.17	0.45
2:B:359:PHE:HD2	2:B:368:LYS:HB2	1.80	0.45
7:G:63:LYS:HD3	7:G:65:GLN:HE22	1.82	0.45
1:A:33:VAL:HA	2:B:1134:ARG:HH11	1.82	0.45
2:B:783:ASN:HA	2:B:787:SER:HB3	1.97	0.45
3:C:286:ILE:HG21	11:K:102:LYS:HB2	1.99	0.45
4:D:168:GLU:N	4:D:168:GLU:OE1	2.50	0.45
2:B:535:SER:OG	2:B:695:PHE:O	2.34	0.44
13:M:531:VAL:HG11	13:M:602:LEU:HD12	1.98	0.44
5:E:95:PHE:HA	5:E:120:PHE:HD1	1.82	0.44
13:M:50:ASN:O	13:M:207:ARG:NH2	2.50	0.44
1:A:1148:ARG:NH1	1:A:1196:PHE:O	2.50	0.44
13:M:931:PRO:HG2	13:M:934:LEU:HB2	1.99	0.44
8:H:34:SER:HB3	8:H:39:MET:H	1.83	0.44
13:M:167:LEU:HB2	13:M:182:LEU:HB2	1.99	0.44
1:A:448:PHE:H	2:B:785:GLU:HB3	1.82	0.44
2:B:1109:ARG:NH1	2:B:1169:THR:OG1	2.51	0.44
5:E:9:ARG:O	5:E:13:ILE:HG12	2.17	0.44
1:A:491:GLN:NE2	2:B:785:GLU:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:ASP:OD1	1:A:1024:ASP:N	2.49	0.44
2:B:510:HIS:CG	2:B:511:PRO:HD2	2.53	0.44
13:M:939:PHE:HB3	13:M:943:LEU:HD12	1.99	0.44
13:M:959:LYS:HD2	13:M:962:ARG:HH21	1.83	0.44
2:B:722:HIS:CG	2:B:915:SER:HG	2.35	0.44
2:B:920:GLN:OE1	2:B:954:ARG:NH1	2.40	0.44
1:A:18:ILE:HD12	1:A:1241:LEU:HD21	1.99	0.44
1:A:51:ASN:ND2	1:A:53:ASP:HB2	2.32	0.44
1:A:826:ASP:OD1	1:A:826:ASP:N	2.51	0.44
2:B:969:ILE:HD11	2:B:987:ARG:HA	2.01	0.43
1:A:447:ASP:OD1	1:A:447:ASP:N	2.50	0.43
1:A:800:PHE:HE1	1:A:804:LEU:HD11	1.84	0.43
2:B:78:PRO:HD3	2:B:430:LEU:HD23	2.01	0.43
2:B:548:VAL:HG21	2:B:622:THR:HG21	1.99	0.43
13:M:49:ASP:N	13:M:49:ASP:OD1	2.51	0.43
13:M:1014:MET:O	13:M:1019:ALA:N	2.51	0.43
1:A:498:TYR:CZ	1:A:502:VAL:HG21	2.54	0.43
2:B:1097:PHE:CZ	2:B:1146:TYR:HB3	2.54	0.43
13:M:496:GLU:OE1	13:M:496:GLU:N	2.41	0.43
3:C:40:VAL:HG21	3:C:289:LEU:HD13	2.01	0.43
14:N:32:DT:H2"	14:N:33:DG:H8	1.84	0.43
1:A:742:GLN:HG2	1:A:747:ILE:HA	2.00	0.43
2:B:51:HIS:CD2	2:B:52:GLN:HG3	2.54	0.43
13:M:1059:HIS:O	13:M:1063:MET:HG2	2.19	0.43
2:B:632:LEU:O	2:B:689:CYS:N	2.49	0.43
2:B:940:ILE:HD11	10:J:42:ARG:HB3	2.01	0.43
4:D:143:ARG:O	4:D:147:GLU:HG3	2.19	0.43
5:E:17:LEU:HD21	5:E:69:ILE:HG21	2.01	0.43
13:M:513:LYS:O	13:M:517:ARG:HG2	2.18	0.43
1:A:557:TYR:OH	1:A:586:GLY:O	2.29	0.42
2:B:722:HIS:CE1	2:B:915:SER:HG	2.36	0.42
13:M:834:ASP:OD1	13:M:834:ASP:N	2.52	0.42
1:A:33:VAL:HA	2:B:1134:ARG:NH1	2.34	0.42
2:B:73:GLU:HA	2:B:419:ARG:HH22	1.82	0.42
2:B:203:ASP:OD1	2:B:203:ASP:N	2.52	0.42
2:B:523:PRO:HA	2:B:720:GLN:HG2	2.01	0.42
2:B:773:ILE:HD13	2:B:1034:PRO:HB3	2.00	0.42
13:M:825:GLU:HG2	13:M:852:PRO:HG3	2.01	0.42
13:M:595:ASP:OD1	13:M:596:ARG:N	2.52	0.42
13:M:783:LYS:HZ1	13:M:829:GLY:HA3	1.83	0.42
3:C:73:LEU:HB3	10:J:6:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:674:TRP:HB3	2:B:693:LEU:HD21	2.01	0.42
16:Q:5:DA:H2'	16:Q:6:DC:C6	2.55	0.42
1:A:840:ARG:NH1	2:B:1080:ARG:HH12	2.17	0.42
7:G:63:LYS:HE2	7:G:63:LYS:HB3	1.90	0.42
16:Q:24:DT:H2'	16:Q:25:DC:C6	2.55	0.42
1:A:930:SER:HA	1:A:1138:ASP:HB2	2.02	0.41
1:A:454:HIS:O	1:A:454:HIS:ND1	2.49	0.41
1:A:489:LEU:HG	1:A:589:ILE:HD11	2.01	0.41
5:E:22:ARG:HG3	5:E:33:LEU:HD11	2.01	0.41
13:M:377:ASN:HB3	13:M:401:ALA:HB3	2.02	0.41
13:M:784:ASN:HB2	13:M:785:PRO:HD3	2.01	0.41
1:A:463:ALA:HB1	2:B:1091:ASN:ND2	2.34	0.41
2:B:518:CYS:SG	2:B:521:SER:OG	2.69	0.41
14:N:46:DG:H2''	14:N:47:DA:C8	2.55	0.41
1:A:715:ALA:HB3	1:A:737:ILE:HD11	2.01	0.41
2:B:706:PHE:HB3	2:B:709:HIS:HB2	2.02	0.41
3:C:32:SER:HB3	11:K:48:MET:HG3	2.02	0.41
13:M:385:TYR:HE2	13:M:1043:ARG:HH22	1.69	0.41
1:A:408:LEU:HD11	1:A:420:LEU:HB3	2.02	0.41
1:A:1230:LEU:HG	1:A:1234:LYS:HE3	2.02	0.41
2:B:220:GLN:HE22	2:B:496:GLN:HE21	1.69	0.41
13:M:277:GLN:HE22	13:M:456:SER:HB3	1.85	0.41
3:C:99:CYS:HB3	3:C:103:SER:H	1.86	0.41
13:M:11:THR:HG22	13:M:60:GLN:HB2	2.03	0.41
13:M:705:MET:O	13:M:709:HIS:ND1	2.35	0.41
1:A:743:HIS:NE2	2:B:955:GLN:HG3	2.36	0.41
1:A:863:TYR:CE1	1:A:877:LEU:HD13	2.56	0.41
2:B:633:VAL:HG22	2:B:635:GLU:H	1.85	0.41
2:B:913:LYS:HE3	2:B:1040:LEU:HD12	2.01	0.41
4:D:147:GLU:N	4:D:148:PRO:HD2	2.36	0.41
5:E:166:PRO:HB2	5:E:202:ARG:HD2	2.01	0.41
1:A:840:ARG:HH11	1:A:1245:ILE:HB	1.86	0.41
2:B:671:ASN:ND2	2:B:685:ILE:O	2.54	0.41
8:H:35:HIS:O	8:H:36:ASN:ND2	2.54	0.41
1:A:410:ASN:HD22	1:A:454:HIS:CE1	2.36	0.40
4:D:160:CYS:O	4:D:164:ASN:ND2	2.31	0.40
1:A:842:ILE:HB	1:A:878:GLY:HA3	2.03	0.40
1:A:1131:LEU:HA	1:A:1134:MET:HG2	2.02	0.40
2:B:278:PRO:HD2	2:B:281:LEU:HD12	2.02	0.40
2:B:1074:LYS:N	16:Q:22:DC:OP1	2.44	0.40
8:H:17:LEU:HD22	8:H:30:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:TYR:CE2	1:A:561:LEU:HB3	2.57	0.40
1:A:1208:ARG:HA	1:A:1208:ARG:HD3	1.91	0.40
11:K:94:LEU:HD12	11:K:94:LEU:HA	1.95	0.40
13:M:11:THR:HG21	13:M:94:ASP:HA	2.03	0.40
13:M:170:CYS:HA	13:M:179:ASP:H	1.86	0.40
13:M:378:ILE:HD12	13:M:1053:LEU:HD21	2.03	0.40
1:A:839:MET:SD	1:A:1186:VAL:HG22	2.61	0.40
1:A:968:SER:OG	1:A:969:PRO:HD3	2.22	0.40
2:B:916:SER:HB3	2:B:920:GLN:HB2	2.02	0.40
3:C:104:VAL:HG21	3:C:132:VAL:HG21	2.02	0.40
3:C:176:ASP:OD1	3:C:176:ASP:N	2.53	0.40
13:M:15:SER:HB2	13:M:87:ARG:HB2	2.04	0.40
15:O:3:G:H2'	15:O:4:A:C8	2.56	0.40
6:F:83:MET:HE3	7:G:66:THR:HA	2.03	0.40
13:M:18:PRO:HG3	13:M:84:HIS:CD2	2.57	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	1145/1498 (76%)	1117 (98%)	28 (2%)	0	100	100
2	B	1041/1172 (89%)	1022 (98%)	19 (2%)	0	100	100
3	C	279/319 (88%)	271 (97%)	8 (3%)	0	100	100
4	D	111/205 (54%)	104 (94%)	7 (6%)	0	100	100
5	E	194/205 (95%)	191 (98%)	3 (2%)	0	100	100
6	F	74/144 (51%)	73 (99%)	1 (1%)	0	100	100
7	G	172/174 (99%)	165 (96%)	7 (4%)	0	100	100
8	H	120/146 (82%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	111/114 (97%)	109 (98%)	2 (2%)	0	100	100
10	J	60/71 (84%)	56 (93%)	4 (7%)	0	100	100
11	K	92/116 (79%)	91 (99%)	1 (1%)	0	100	100
12	L	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
13	M	1044/1133 (92%)	1014 (97%)	30 (3%)	0	100	100
All	All	4483/5348 (84%)	4368 (97%)	115 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	883/1332 (66%)	881 (100%)	2 (0%)	93	98
2	B	816/1029 (79%)	815 (100%)	1 (0%)	93	98
3	C	221/280 (79%)	221 (100%)	0	100	100
4	D	100/181 (55%)	99 (99%)	1 (1%)	76	88
5	E	145/191 (76%)	145 (100%)	0	100	100
6	F	53/128 (41%)	53 (100%)	0	100	100
7	G	74/151 (49%)	73 (99%)	1 (1%)	67	83
8	H	91/127 (72%)	91 (100%)	0	100	100
9	I	81/104 (78%)	81 (100%)	0	100	100
10	J	48/66 (73%)	46 (96%)	2 (4%)	30	59
11	K	68/105 (65%)	68 (100%)	0	100	100
12	L	28/45 (62%)	27 (96%)	1 (4%)	35	63
13	M	817/1005 (81%)	815 (100%)	2 (0%)	93	98
All	All	3425/4744 (72%)	3415 (100%)	10 (0%)	92	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	VAL
1	A	837	PHE
2	B	184	LEU
4	D	98	PHE
7	G	115	MET
10	J	8	PHE
10	J	10	CYS
12	L	15	CYS
13	M	577	VAL
13	M	604	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	410	ASN
1	A	459	GLN
1	A	491	GLN
1	A	562	ASN
1	A	634	GLN
1	A	652	GLN
1	A	742	GLN
1	A	1182	HIS
1	A	1219	GLN
1	A	1227	GLN
2	B	220	GLN
2	B	222	GLN
2	B	316	HIS
2	B	417	HIS
2	B	477	ASN
2	B	543	GLN
2	B	577	ASN
2	B	600	GLN
2	B	642	GLN
2	B	652	HIS
2	B	711	HIS
2	B	749	GLN
2	B	779	HIS
2	B	804	GLN
2	B	1003	GLN
2	B	1091	ASN
3	C	280	GLN
5	E	126	GLN

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Mol	Chain	Res	Type
8	H	36	ASN
8	H	124	GLN
9	I	80	GLN
11	K	51	HIS
11	K	89	GLN
11	K	104	GLN
12	L	17	GLN
12	L	28	GLN
12	L	47	GLN
13	M	84	HIS
13	M	298	GLN
13	M	339	GLN
13	M	873	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	O	10/16 (62%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	O	3	G
15	O	4	A

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 10 ligands modelled in this entry, 10 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.

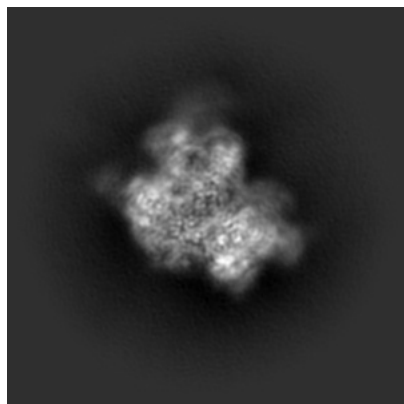
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38472. These allow visual inspection of the internal detail of the map and identification of artifacts.

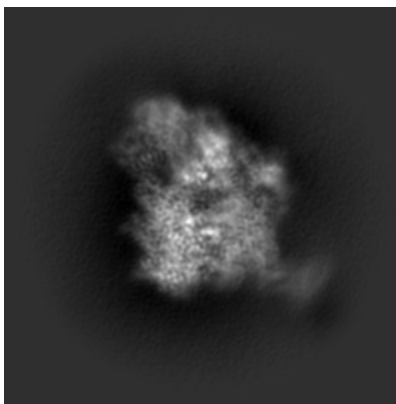
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

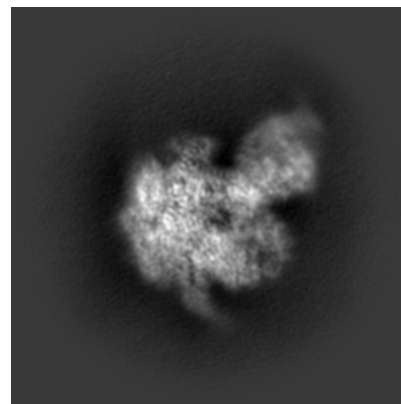
6.1.1 Primary map



X

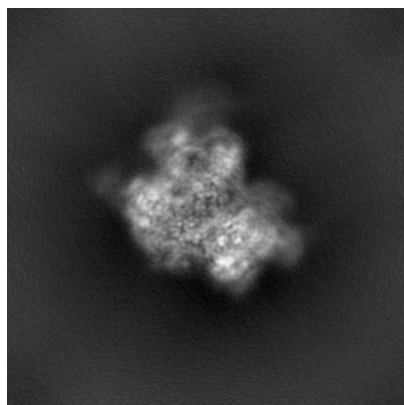


Y

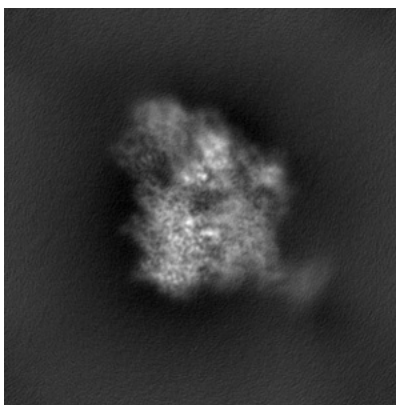


Z

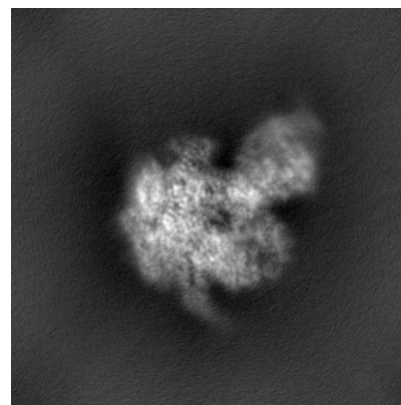
6.1.2 Raw map



X



Y

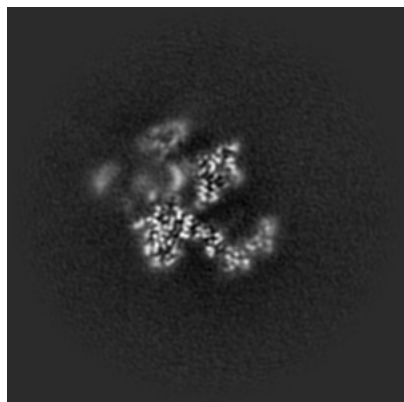


Z

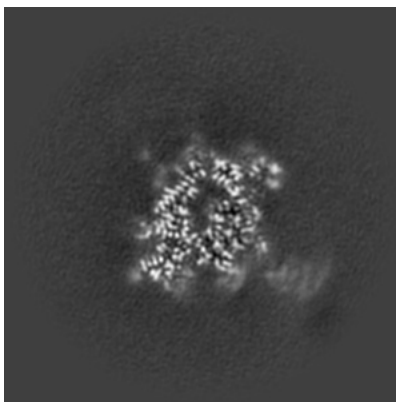
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

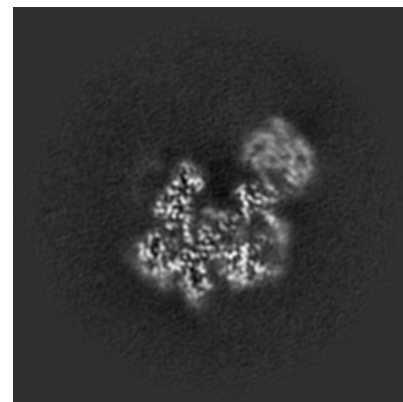
6.2.1 Primary map



X Index: 144

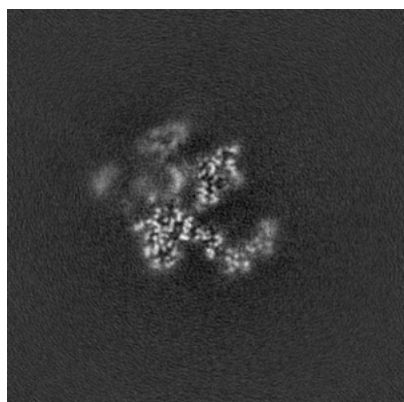


Y Index: 144

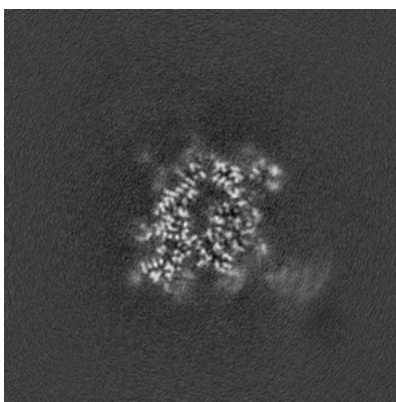


Z Index: 144

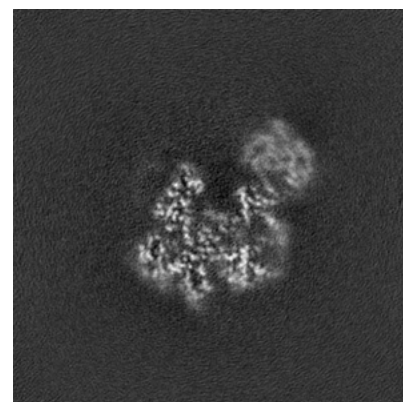
6.2.2 Raw map



X Index: 144



Y Index: 144

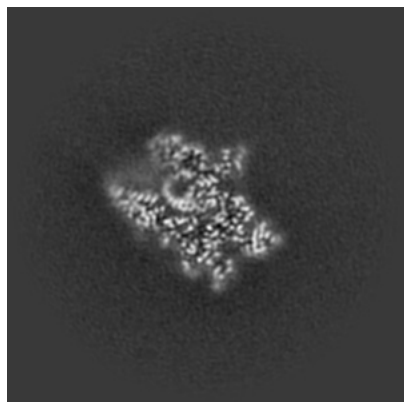


Z Index: 144

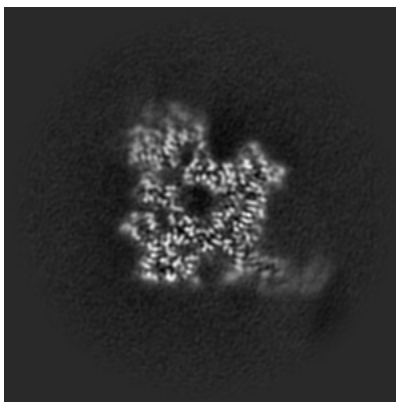
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

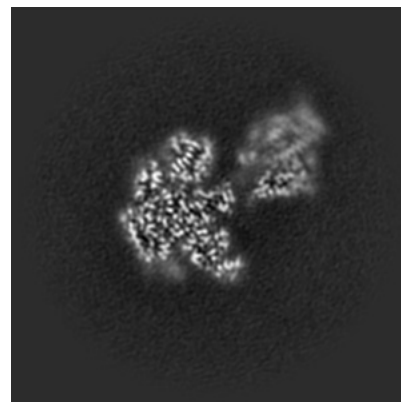
6.3.1 Primary map



X Index: 125

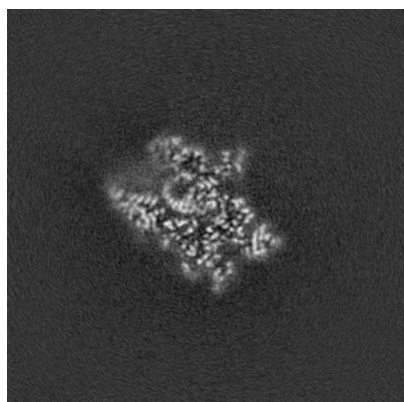


Y Index: 154

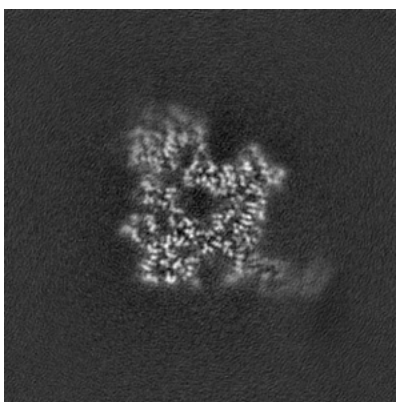


Z Index: 120

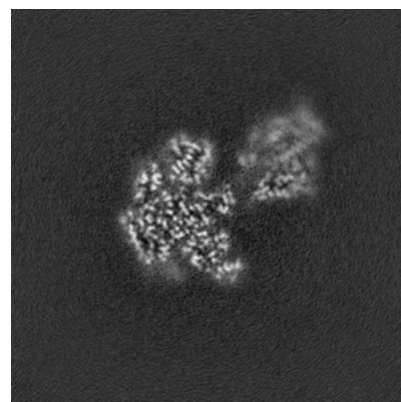
6.3.2 Raw map



X Index: 125



Y Index: 154

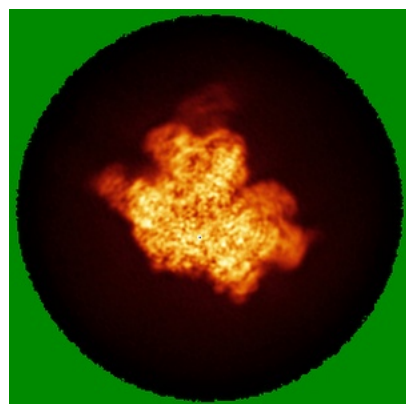


Z Index: 120

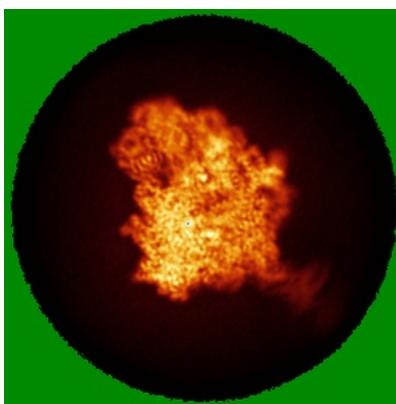
The images above show the largest variance slices of the map in three orthogonal directions.

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

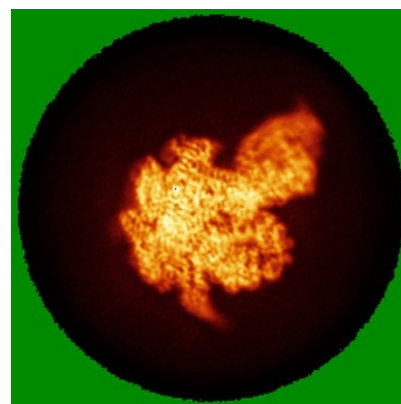
6.4.1 Primary map



X

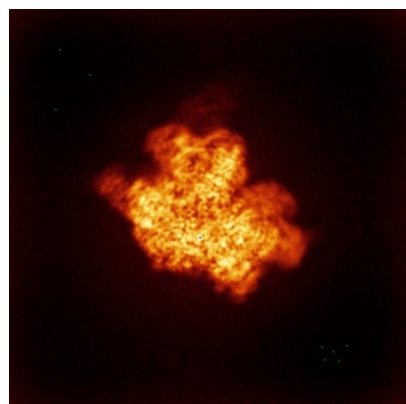


Y

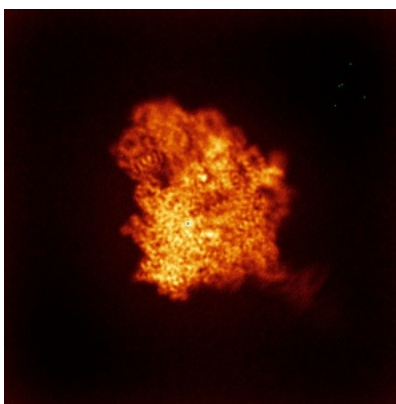


Z

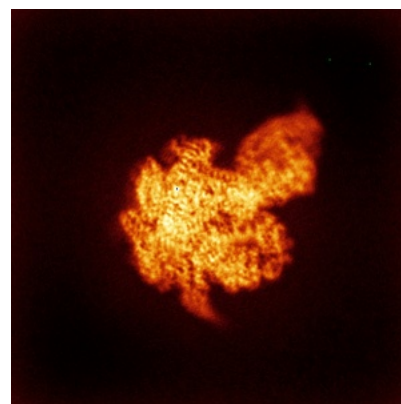
6.4.2 Raw map



X



Y

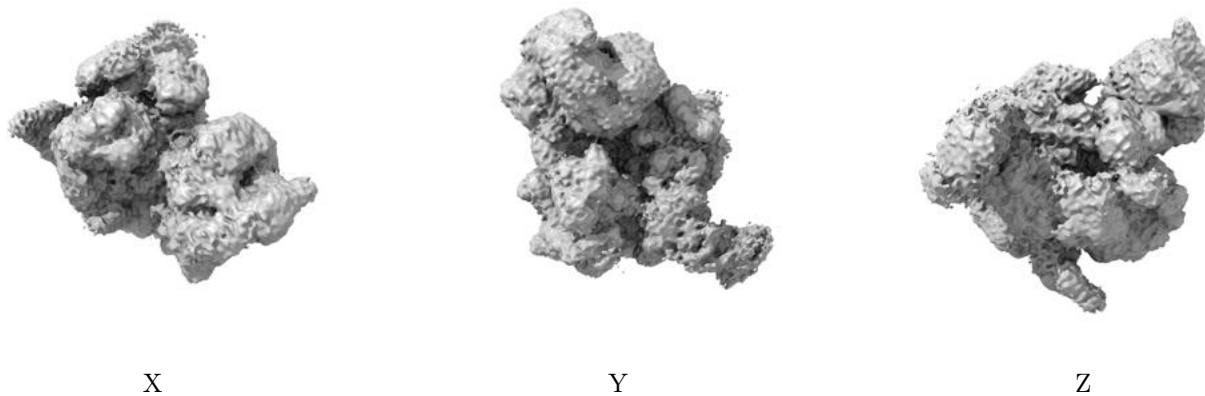


Z

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.

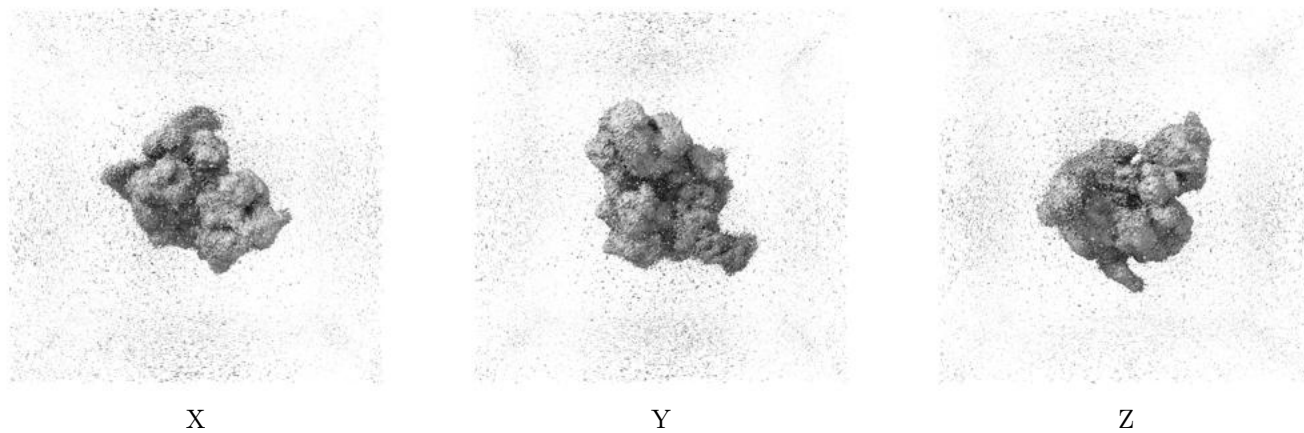
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0626. 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.

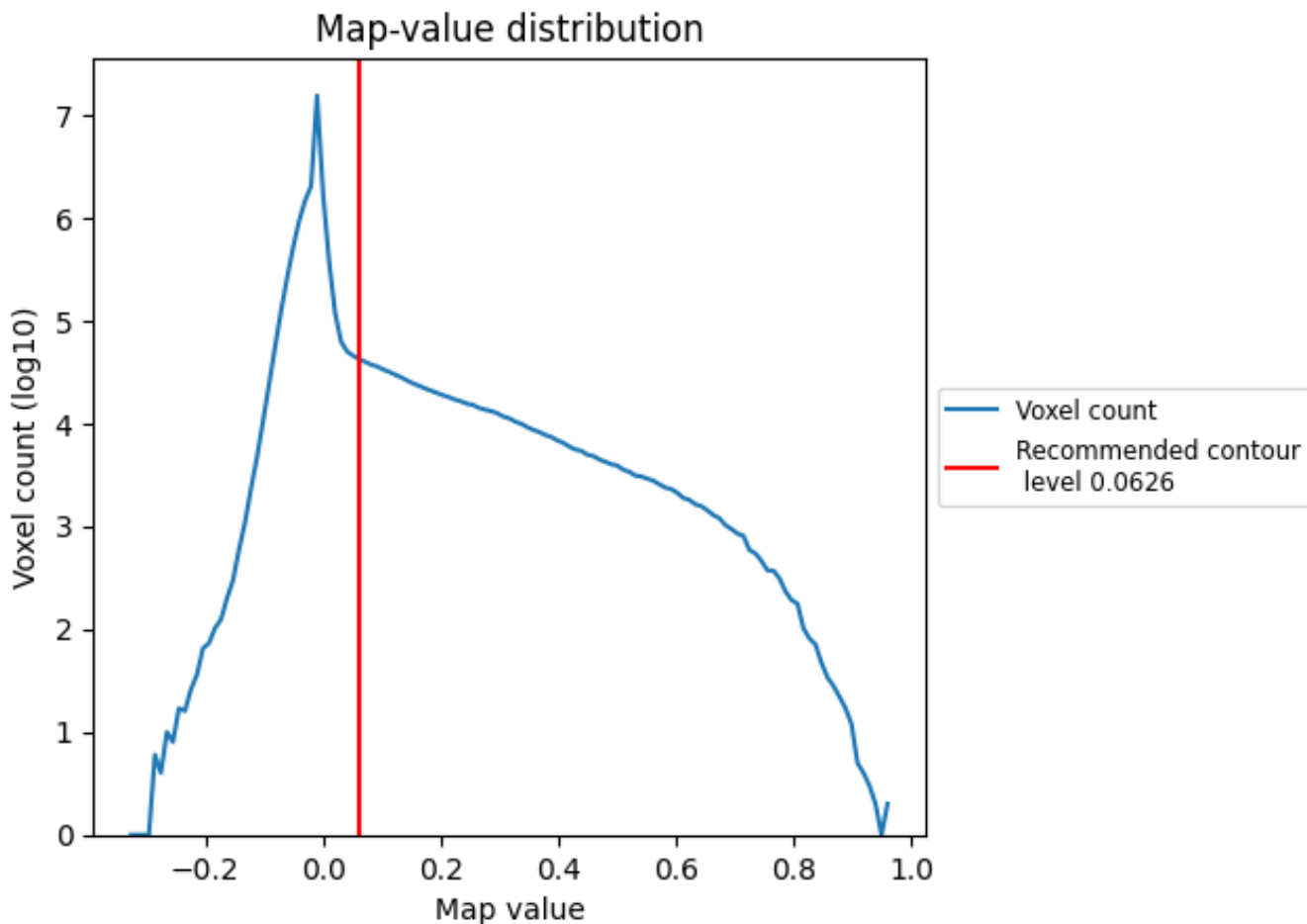
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

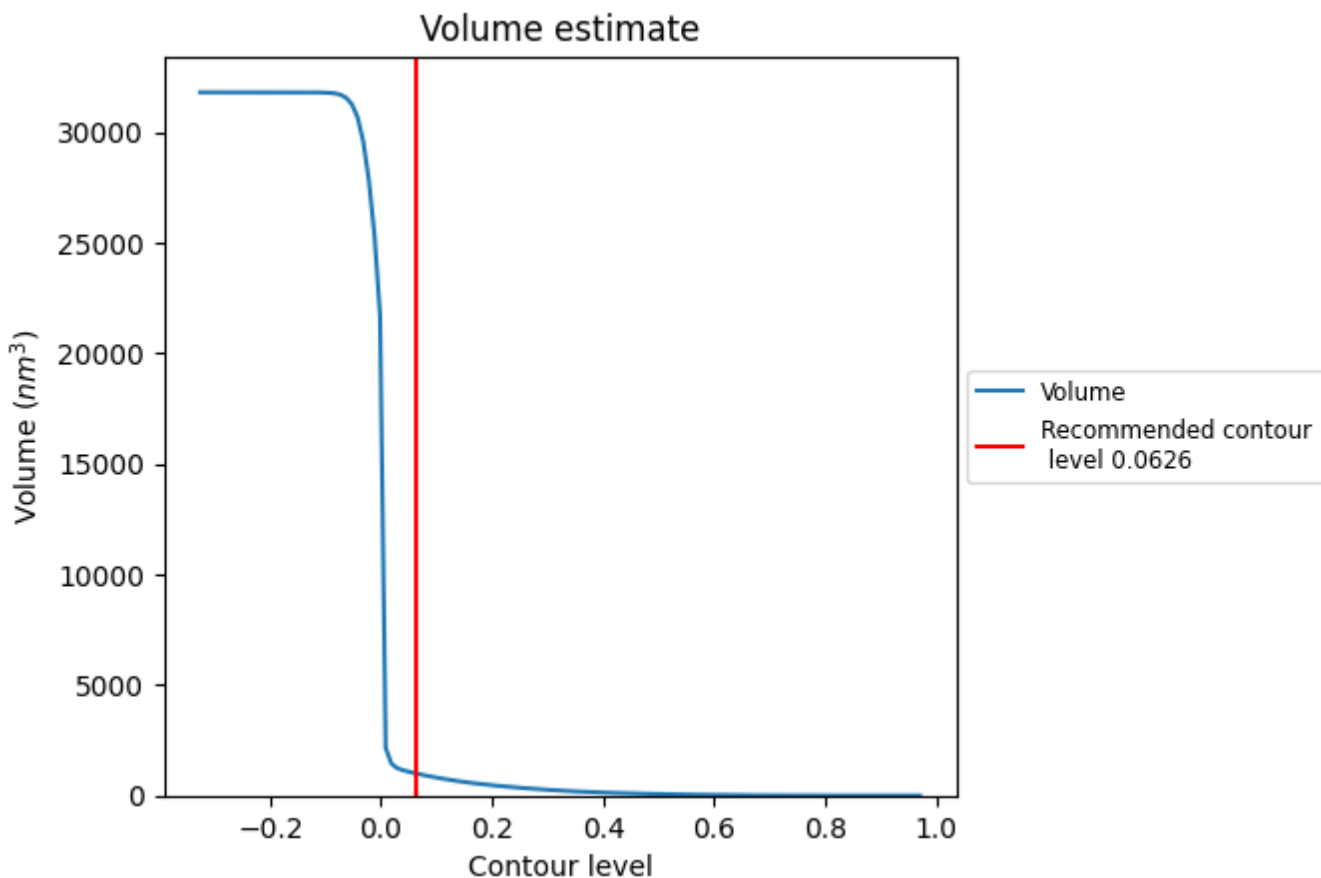
This section contains the results of statistical analysis of the map.

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.

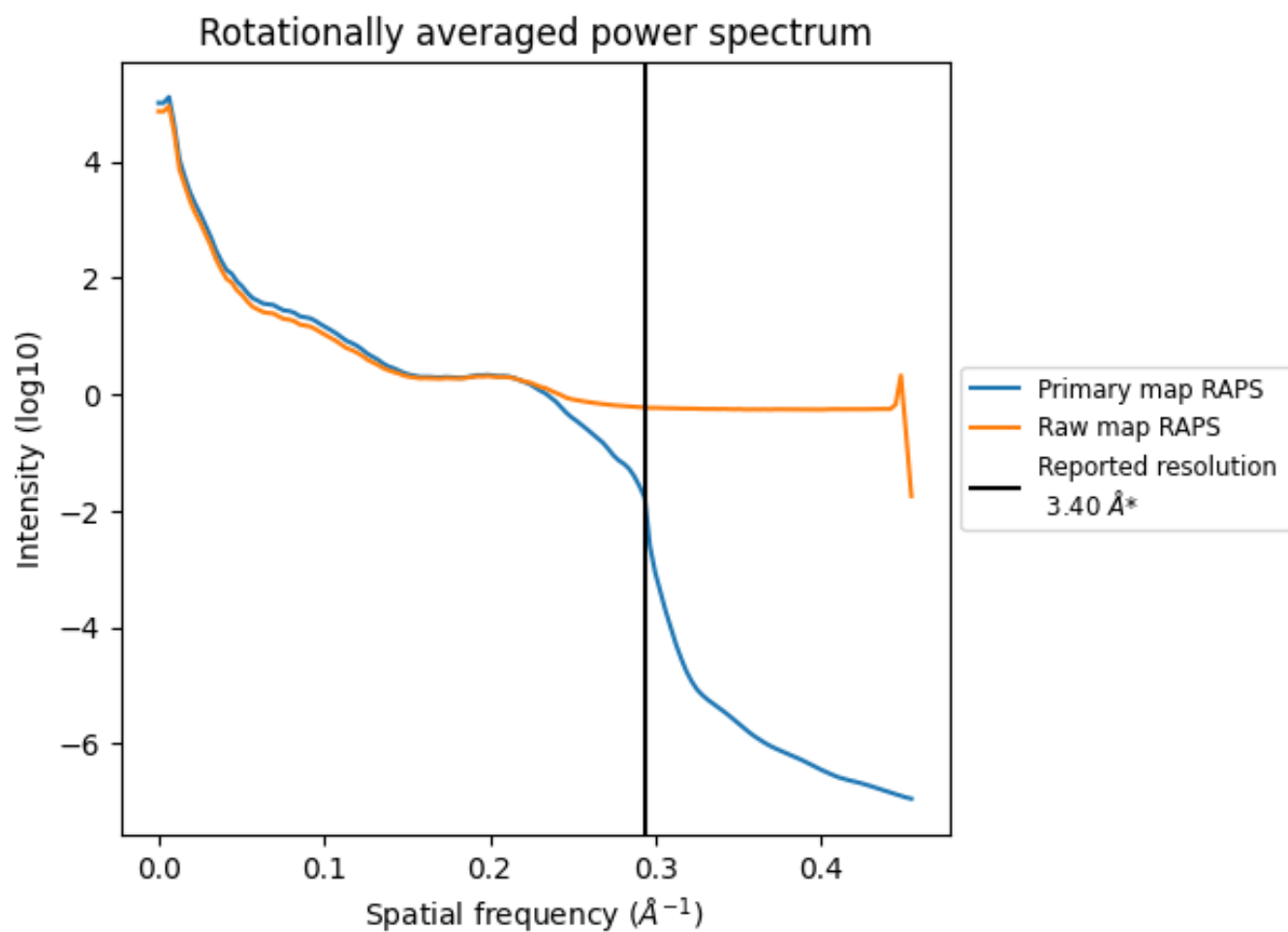
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1001 nm^3 ; this corresponds to an approximate mass of 905 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

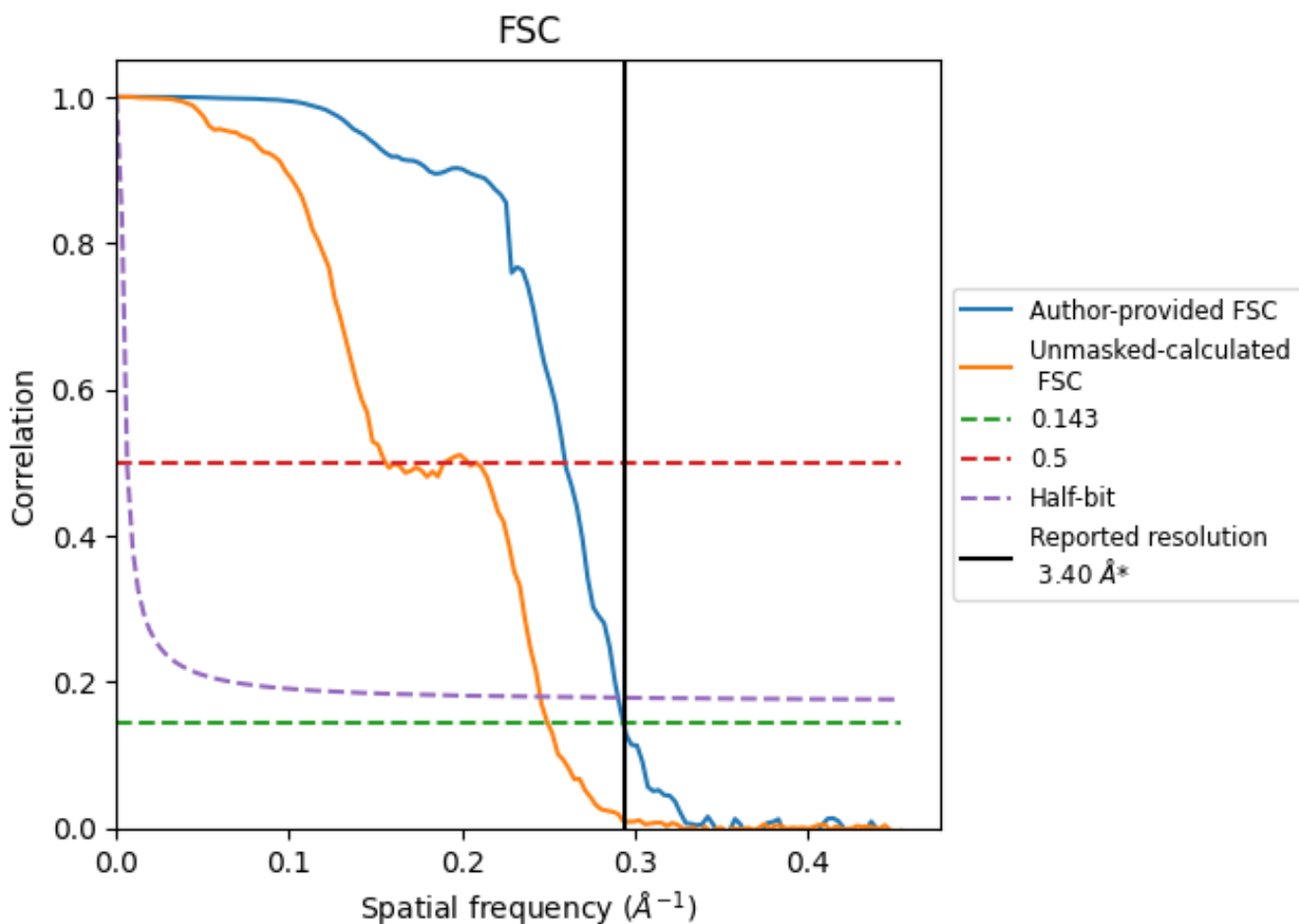


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

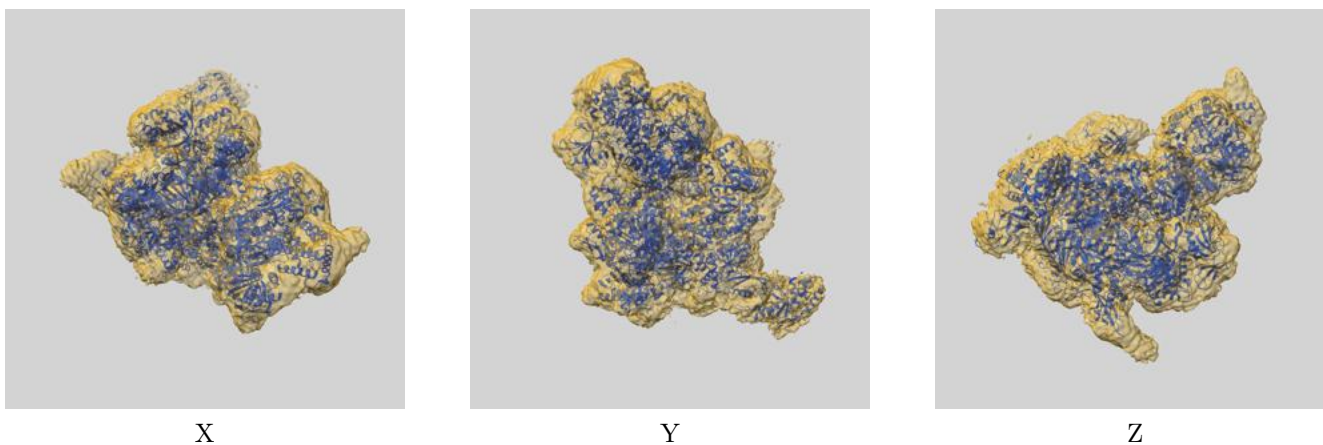
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.85	3.44
Unmasked-calculated*	4.00	6.42	4.07

*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 4.00 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

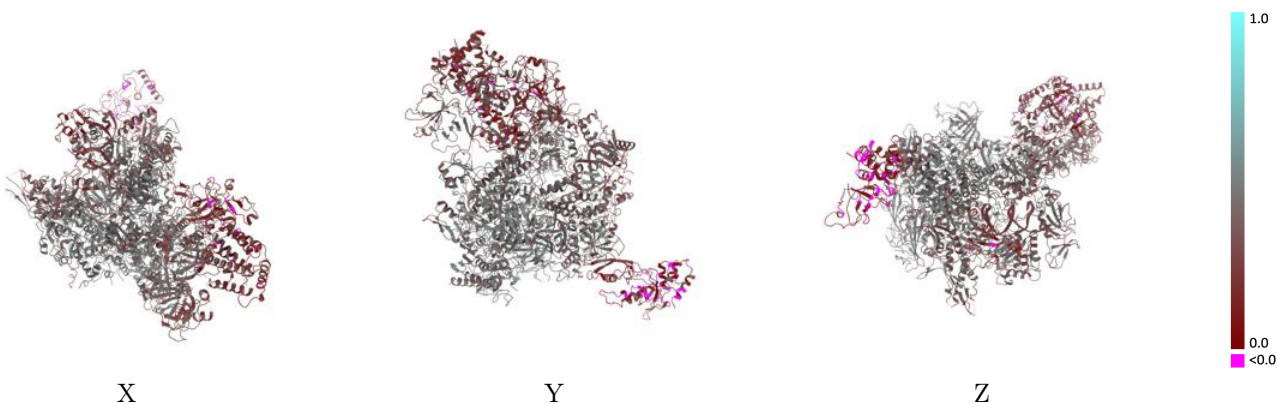
This section contains information regarding the fit between EMDB map EMD-38472 and PDB model 8XMD. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



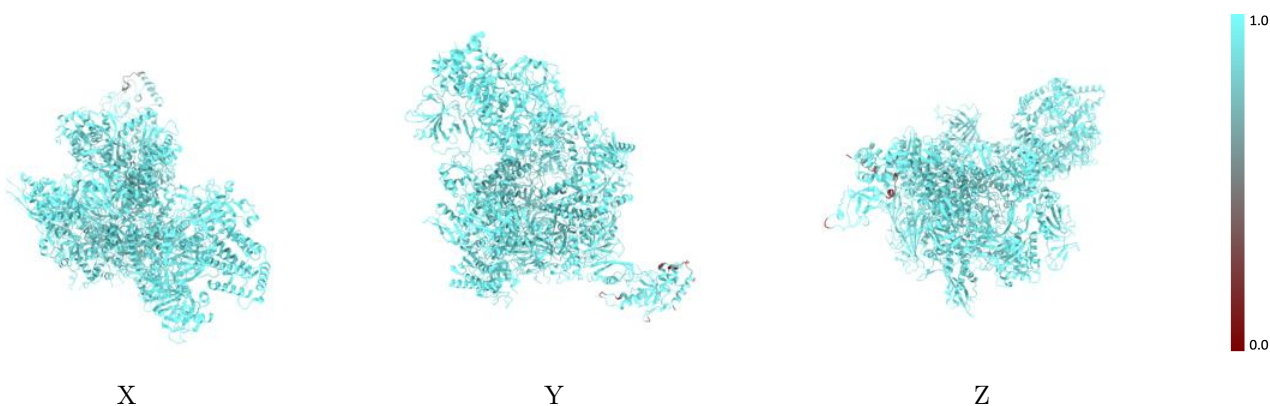
The images above show the 3D surface view of the map at the recommended contour level 0.0626 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



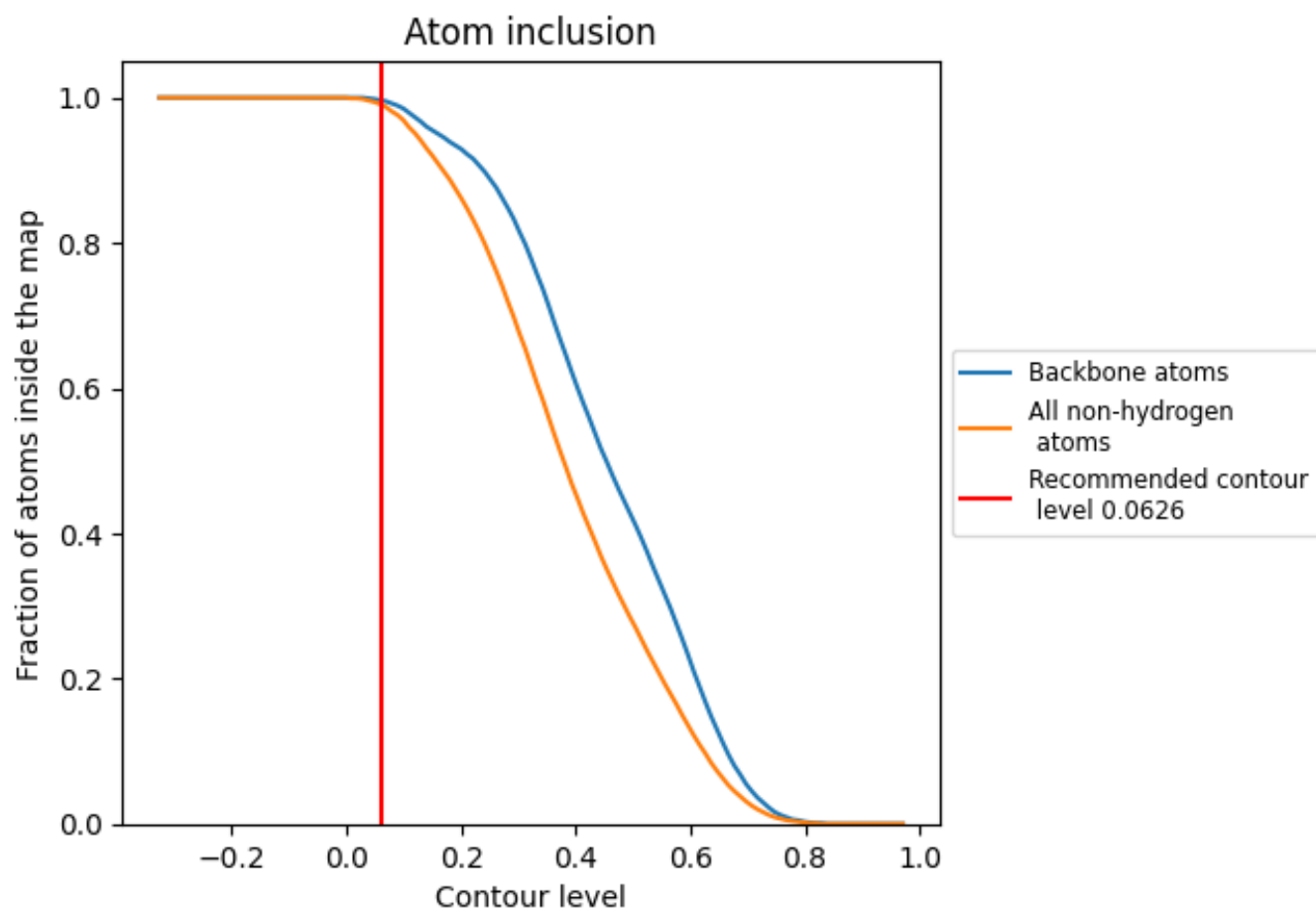
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0626).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0626) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9900	 0.3830
A	 0.9920	 0.4120
B	 0.9970	 0.4470
C	 1.0000	 0.4450
D	 0.8100	 0.0680
E	 0.9990	 0.4060
F	 1.0000	 0.4220
G	 0.9690	 0.1630
H	 0.9980	 0.4410
I	 0.9950	 0.3990
J	 1.0000	 0.4510
K	 0.9970	 0.4580
L	 1.0000	 0.4310
M	 0.9950	 0.3150
N	 0.9940	 0.2620
O	 0.9920	 0.3750
Q	 1.0000	 0.3250

