



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:27 PM UTC

PDB ID : 7AP8 / pdb_00007ap8
EMDB ID : EMD-11850
Title : Atomic structure of the poxvirus initially transcribing complex in conformation 2
Authors : Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on : 2020-10-16
Resolution : 3.15 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:

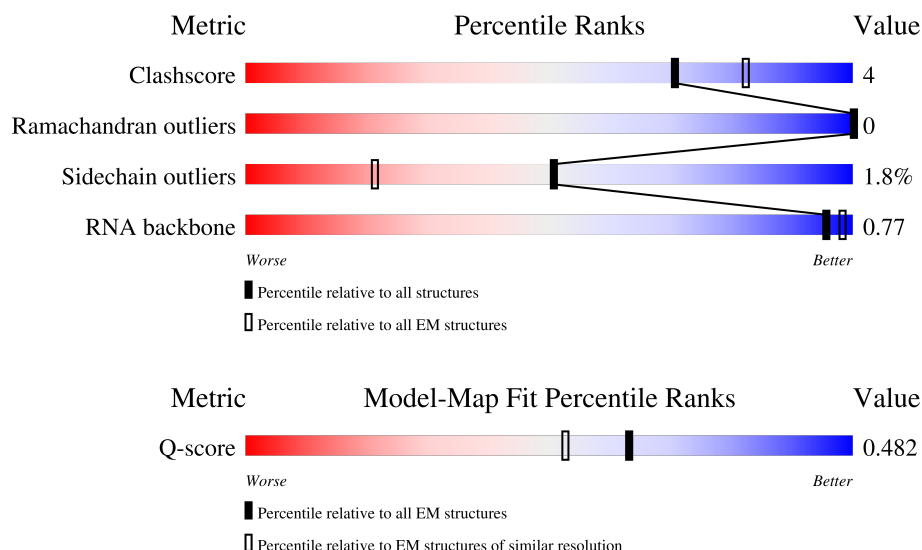
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.15 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14486 (2.65 - 3.65)

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	1286	
2	B	1164	
3	C	305	

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Mol	Chain	Length	Quality of chain
4	E	185	88% 12%
5	F	164	57% 5% 37%
6	G	161	5% 84% 11% 5%
7	I	795	12% 52% 6% 42%
8	J	63	78% 16%
9	N	60	27% 73%
10	P	5	80% 20%
11	S	259	5% 37% 8% 55%
12	T	60	27% 8% 65%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 62909 atoms, of which 31397 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1268	Total	C	H	N	O	S	0	0
			20500	6556	10312	1679	1908	45		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1129	Total	C	H	N	O	S	0	0
			18237	5794	9146	1554	1695	48		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	conflict	UNP Q49PH2

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	304	Total	C	H	N	O	S	0	0
			4954	1608	2470	399	464	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	184	Total	C	H	N	O	S	0	0
			3043	966	1548	248	276	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	103	Total	C	H	N	O	S	0	0
			1723	545	874	148	153	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	153	Total	C	H	N	O	S	0	0
			2373	753	1181	198	235	6		

- Molecule 7 is a protein called Protein H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	464	Total	C	H	N	O	S	0	0
			7808	2552	3905	627	710	14		

- Molecule 8 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	61	Total	C	H	N	O	S	0	0
			1020	310	530	88	88	4		

- Molecule 9 is a DNA chain called Synthetic promoter DNA oligomer, non-template strand.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	N	16	Total	C	H	N	O	P	0	0
			507	155	180	61	95	16		

- Molecule 10 is a RNA chain called RNA (5'-R(P*AP*UP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	5	Total	C	H	N	O	P	0	0
			163	49	55	22	32	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	116	Total	C	H	N	O	S	0	0
			1909	608	957	154	186	4		

- Molecule 12 is a DNA chain called Synthetic promoter DNA oligomer, template strand.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	T	21	Total	C	H	N	O	P	0	0
			667	206	239	76	126	20		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

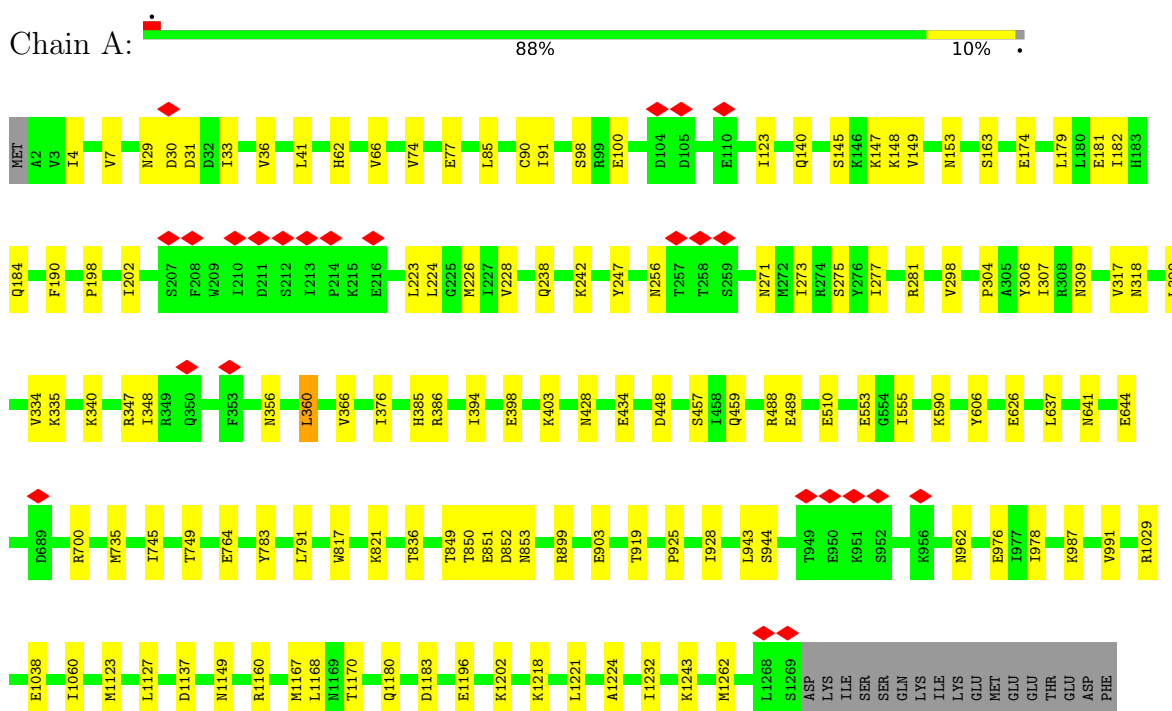
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

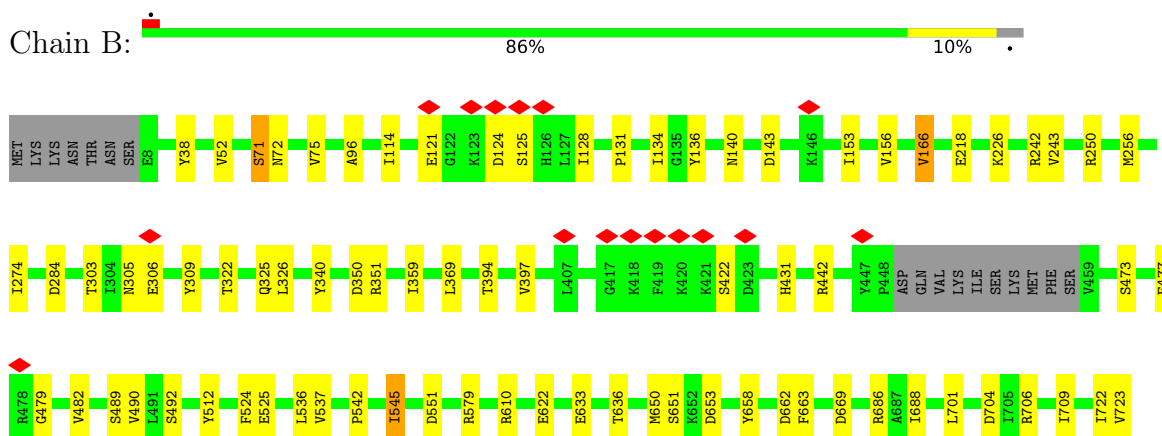
3 Residue-property plots [i](#)

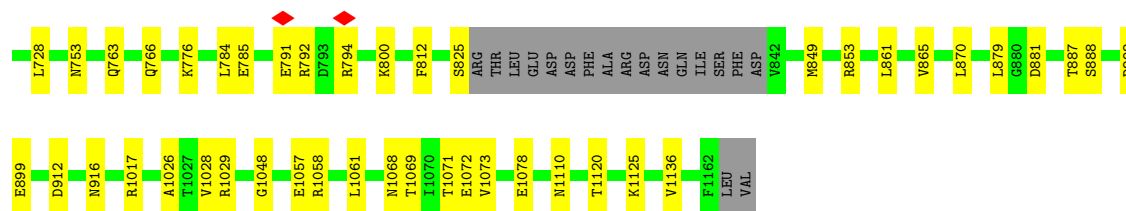
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 147 kDa polypeptide



- Molecule 2: DNA-directed RNA polymerase

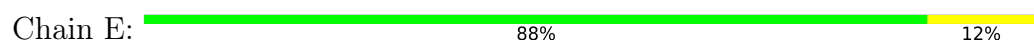




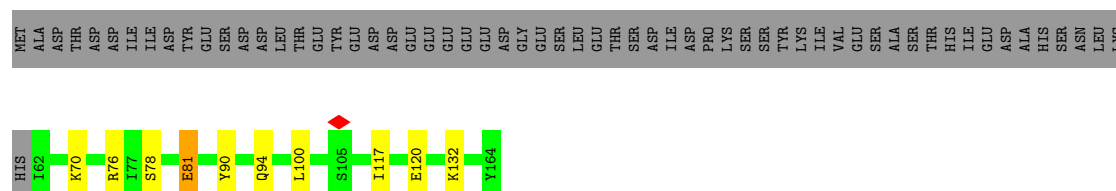
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit



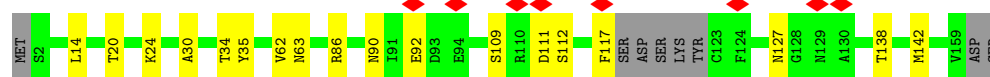
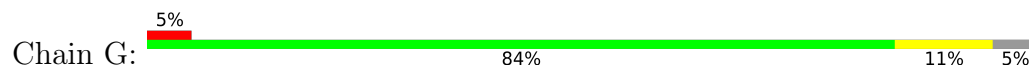
- Molecule 4: DNA-directed RNA polymerase subunit



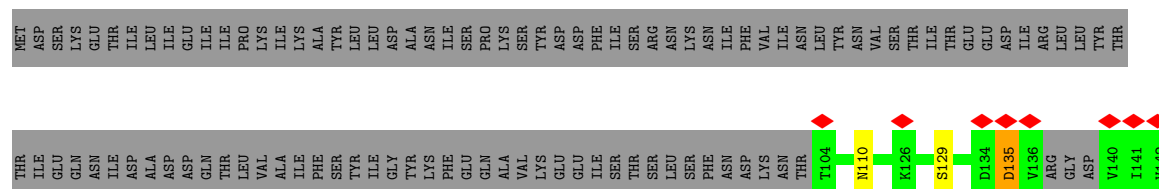
- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit



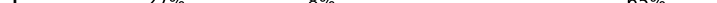
- Molecule 6: DNA-directed RNA polymerase 18 kDa subunit

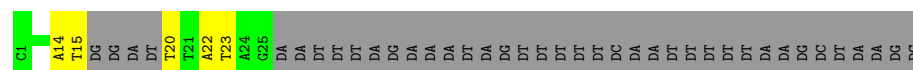


- Molecule 7: Protein H4



- Molecule 12: Synthetic promoter DNA oligomer, template strand

Chain T:  27% 8% 65%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73035	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 ($e^-/\text{\AA}^2$)	78.90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.026	Depositor
Map size ($\text{\AA}$)	340.32, 340.32, 340.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/10394	0.32	0/14052
2	B	0.16	0/9281	0.33	0/12537
3	C	0.16	0/2540	0.31	0/3440
4	E	0.16	0/1522	0.32	0/2069
5	F	0.18	0/863	0.32	0/1158
6	G	0.14	0/1209	0.30	0/1639
7	I	0.14	0/4000	0.32	0/5411
8	J	0.19	0/494	0.35	0/663
9	N	0.29	0/366	0.53	0/562
10	P	0.08	0/121	0.17	0/186
11	S	0.14	0/967	0.34	0/1294
12	T	0.24	0/478	0.51	0/734
All	All	0.16	0/32235	0.33	0/43745

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10188	10312	10312	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9091	9146	9146	75	0
3	C	2484	2470	2470	20	0
4	E	1495	1548	1548	13	0
5	F	849	874	874	7	0
6	G	1192	1181	1181	10	0
7	I	3903	3905	3905	33	0
8	J	490	530	530	6	0
9	N	327	180	180	0	0
10	P	108	55	55	1	0
11	S	952	957	957	11	0
12	T	428	239	241	4	0
13	A	1	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	I	1	0	0	0	0
All	All	31512	31397	31399	220	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 4.

All (220) 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:134:ILE:HD12	2:B:156:VAL:HG23	1.62	0.79
1:A:145:SER:OG	1:A:148:LYS:O	2.02	0.77
7:I:735:ASN:ND2	7:I:747:VAL:O	2.18	0.76
2:B:242:ARG:O	7:I:738:ARG:NH2	2.20	0.75
7:I:316:LYS:O	7:I:317:ARG:NH2	2.21	0.73
6:G:112:SER:O	6:G:127:ASN:ND2	2.21	0.72
1:A:1196:GLU:OE2	1:A:1202:LYS:N	2.22	0.71
2:B:38:TYR:OH	2:B:131:PRO:O	2.08	0.71
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.23	0.71
4:E:91:GLY:O	4:E:150:LYS:NZ	2.25	0.70
2:B:800:LYS:NZ	2:B:812:PHE:O	2.24	0.70
2:B:542:PRO:HA	2:B:545:ILE:HD13	1.73	0.70
1:A:764:GLU:OE1	2:B:1058:ARG:NH2	2.25	0.70
1:A:98:SER:OG	1:A:100:GLU:OE1	2.08	0.69
1:A:590:LYS:NZ	1:A:644:GLU:OE2	2.25	0.69
1:A:309:ASN:O	1:A:335:LYS:NZ	2.26	0.69
2:B:309:TYR:OH	7:I:725:GLU:OE2	2.11	0.69
2:B:477:GLU:N	2:B:477:GLU:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HD12	3:C:182:VAL:HG12	1.73	0.69
2:B:704:ASP:OD1	8:J:53:ASN:ND2	2.25	0.69
1:A:1060:ILE:O	11:S:130:LYS:NZ	2.26	0.69
3:C:132:ARG:NH1	7:I:591:ASP:O	2.27	0.68
6:G:109:SER:OG	6:G:111:ASP:OD1	2.10	0.68
1:A:919:THR:O	5:F:76:ARG:NH2	2.26	0.67
1:A:398:GLU:O	1:A:403:LYS:NZ	2.28	0.67
2:B:610:ARG:NH2	2:B:622:GLU:OE1	2.28	0.66
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.77	0.66
1:A:488:ARG:NH1	3:C:239:GLU:OE1	2.29	0.66
3:C:50:GLU:OE1	3:C:50:GLU:N	2.30	0.65
1:A:163:SER:OG	7:I:183:ARG:NH2	2.29	0.65
3:C:39:ILE:HG13	3:C:173:VAL:HG21	1.79	0.64
11:S:64:GLU:OE1	11:S:65:GLU:N	2.31	0.64
1:A:851:GLU:OE1	1:A:899:ARG:NE	2.31	0.64
1:A:100:GLU:OE1	1:A:100:GLU:N	2.31	0.63
2:B:250:ARG:NE	2:B:525:GLU:OE2	2.30	0.63
8:J:17:GLU:OE1	8:J:17:GLU:N	2.32	0.63
2:B:71:SER:OG	2:B:72:ASN:N	2.31	0.62
2:B:218:GLU:N	2:B:218:GLU:OE1	2.32	0.61
3:C:164:GLU:N	3:C:164:GLU:OE1	2.34	0.61
1:A:66:VAL:HG11	1:A:228:VAL:HG22	1.82	0.60
1:A:174:GLU:N	1:A:174:GLU:OE1	2.34	0.60
7:I:160:GLU:N	7:I:160:GLU:OE1	2.35	0.60
1:A:1262:MET:O	6:G:24:LYS:NZ	2.35	0.60
6:G:30:ALA:O	6:G:34:THR:HG22	2.02	0.60
8:J:18:ARG:NH2	8:J:47:GLN:OE1	2.35	0.60
2:B:121:GLU:N	2:B:121:GLU:OE1	2.34	0.59
2:B:763:GLN:OE1	2:B:763:GLN:N	2.34	0.59
2:B:524:PHE:CZ	7:I:749:VAL:HG11	2.36	0.59
1:A:340:LYS:NZ	2:B:1078:GLU:OE2	2.36	0.59
1:A:1180:GLN:N	1:A:1180:GLN:OE1	2.34	0.59
1:A:223:LEU:HD13	1:A:247:TYR:HA	1.85	0.58
3:C:173:VAL:O	3:C:177:ILE:N	2.37	0.58
7:I:689:LYS:NZ	7:I:723:ASP:OD2	2.34	0.58
1:A:334:VAL:HG13	1:A:366:VAL:HG13	1.84	0.58
2:B:812:PHE:CD1	3:C:176:ILE:HD13	2.39	0.58
1:A:386:ARG:NH1	1:A:448:ASP:OD1	2.36	0.58
3:C:226:ASN:HB3	3:C:257:MET:HE1	1.84	0.58
1:A:1160:ARG:NH1	1:A:1183:ASP:OD1	2.37	0.57
1:A:553:GLU:N	1:A:553:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ARG:NH2	7:I:593:GLU:O	2.37	0.57
3:C:25:GLY:HA3	3:C:223:LEU:HD21	1.87	0.57
6:G:92:GLU:N	6:G:92:GLU:OE1	2.38	0.57
1:A:356:ASN:O	7:I:320:ARG:NH2	2.38	0.57
2:B:512:TYR:OH	2:B:551:ASP:OD2	2.21	0.56
1:A:817:TRP:O	1:A:821:LYS:N	2.38	0.56
2:B:218:GLU:HB2	2:B:274:ILE:HD11	1.87	0.56
11:S:94:ILE:HG22	11:S:95:ALA:H	1.70	0.56
2:B:776:LYS:NZ	12:T:23:DT:OP1	2.38	0.56
4:E:1:MET:SD	4:E:46:THR:OG1	2.64	0.56
3:C:119:GLU:OE2	3:C:119:GLU:N	2.38	0.56
7:I:354:ILE:HG23	7:I:361:ALA:HB1	1.87	0.55
5:F:78:SER:N	5:F:81:GLU:OE2	2.40	0.55
1:A:123:ILE:CD1	1:A:179:LEU:HD21	2.36	0.55
7:I:695:ASN:OD1	7:I:794:ASN:ND2	2.39	0.55
1:A:637:LEU:O	1:A:641:ASN:ND2	2.39	0.55
1:A:36:VAL:HG21	1:A:224:LEU:HB3	1.89	0.54
1:A:347:ARG:NH2	1:A:348:ILE:O	2.39	0.54
2:B:490:VAL:HG13	2:B:669:ASP:O	2.07	0.54
3:C:15:GLU:N	3:C:15:GLU:OE1	2.39	0.54
2:B:1110:ASN:ND2	7:I:110:ASN:OD1	2.39	0.54
1:A:149:VAL:HG21	1:A:242:LYS:HB2	1.90	0.54
2:B:156:VAL:HG12	2:B:166:VAL:HG13	1.89	0.54
10:P:1:A:H61	12:T:22:DA:H61	1.56	0.54
2:B:791:GLU:O	2:B:794:ARG:NH2	2.39	0.53
6:G:34:THR:HG23	6:G:35:TYR:CD2	2.43	0.53
7:I:715:MET:O	7:I:757:ARG:NH2	2.37	0.53
1:A:317:VAL:HG11	1:A:360:LEU:HB2	1.90	0.53
1:A:903:GLU:N	1:A:903:GLU:OE1	2.42	0.53
2:B:579:ARG:NE	2:B:633:GLU:OE2	2.41	0.53
1:A:1167:MET:O	1:A:1170:THR:OG1	2.28	0.52
2:B:479:GLY:O	2:B:482:VAL:HG23	2.08	0.52
1:A:735:MET:HE1	2:B:688:ILE:HG13	1.91	0.52
4:E:129:GLN:O	5:F:70:LYS:NZ	2.42	0.52
7:I:363:CYS:SG	7:I:364:ARG:N	2.83	0.51
1:A:140:GLN:OE1	1:A:153:ASN:ND2	2.43	0.51
3:C:107:ASP:OD1	3:C:108:THR:N	2.43	0.51
2:B:303:THR:OG1	2:B:305:ASN:O	2.23	0.51
2:B:136:TYR:CD1	2:B:153:ILE:HG22	2.46	0.51
7:I:598:GLU:C	7:I:599:LEU:HD22	2.36	0.50
1:A:489:GLU:OE1	1:A:489:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASP:OD1	2:B:351:ARG:N	2.44	0.50
6:G:62:VAL:HG12	6:G:63:ASN:H	1.75	0.50
8:J:29:LYS:O	8:J:33:VAL:HG23	2.12	0.50
1:A:428:ASN:ND2	2:B:1072:GLU:OE2	2.44	0.50
1:A:318:ASN:ND2	5:F:94:GLN:OE1	2.45	0.50
7:I:660:VAL:HG12	7:I:661:HIS:H	1.77	0.50
2:B:489:SER:HG	2:B:492:SER:HG	1.59	0.49
2:B:898:ASP:OD1	2:B:899:GLU:N	2.45	0.49
1:A:74:VAL:HG22	1:A:190:PHE:CE2	2.47	0.49
1:A:943:LEU:O	1:A:944:SER:OG	2.21	0.49
1:A:1038:GLU:OE1	11:S:119:ARG:NH1	2.45	0.49
7:I:167:ASN:ND2	7:I:170:ASN:OD1	2.43	0.49
1:A:181:GLU:OE1	1:A:181:GLU:N	2.46	0.49
1:A:29:ASN:ND2	1:A:33:ILE:O	2.44	0.49
2:B:662:ASP:OD1	2:B:663:PHE:N	2.45	0.49
1:A:4:ILE:O	1:A:1243:LYS:NZ	2.37	0.49
1:A:849:THR:OG1	1:A:850:THR:N	2.45	0.49
1:A:273:ILE:HA	1:A:277:ILE:HD12	1.93	0.49
2:B:709:ILE:HG23	2:B:870:LEU:HB2	1.94	0.48
2:B:766:GLN:O	3:C:58:HIS:NE2	2.45	0.48
1:A:735:MET:HE2	2:B:473:SER:HA	1.95	0.48
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.44	0.48
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	1.96	0.48
4:E:11:LYS:NZ	4:E:103:ASP:OD2	2.40	0.48
4:E:77:ASP:OD1	4:E:78:TYR:N	2.47	0.48
4:E:117:ASP:OD1	4:E:118:THR:N	2.47	0.48
2:B:861:LEU:CD2	2:B:865:VAL:HG22	2.44	0.48
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.13	0.48
1:A:376:ILE:HB	1:A:394:ILE:HD11	1.96	0.48
1:A:30:ASP:OD1	1:A:31:ASP:N	2.46	0.47
2:B:75:VAL:HG12	2:B:96:ALA:HB2	1.96	0.47
2:B:256:MET:HE1	2:B:340:TYR:HB2	1.96	0.47
2:B:686:ARG:NH2	2:B:888:SER:O	2.45	0.47
2:B:912:ASP:OD2	8:J:9:THR:OG1	2.31	0.47
3:C:39:ILE:CG1	3:C:173:VAL:HG21	2.44	0.47
5:F:100:LEU:N	5:F:120:GLU:OE2	2.46	0.47
7:I:738:ARG:NH1	7:I:746:ASP:O	2.48	0.47
11:S:60:LYS:O	11:S:63:ILE:HG23	2.15	0.47
2:B:96:ALA:HB3	2:B:128:ILE:HB	1.95	0.47
2:B:651:SER:OG	2:B:653:ASP:OD1	2.25	0.47
7:I:211:TYR:CD1	7:I:230:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:709:PHE:O	7:I:734:TYR:OH	2.30	0.47
2:B:442:ARG:NH1	2:B:489:SER:O	2.49	0.46
8:J:39:CYS:SG	8:J:40:CYS:N	2.88	0.46
2:B:785:GLU:N	2:B:785:GLU:OE1	2.48	0.46
11:S:40:LEU:HD13	11:S:128:ILE:HD11	1.96	0.46
2:B:306:GLU:HG2	7:I:693:ILE:HG21	1.98	0.46
2:B:753:ASN:O	2:B:916:ASN:ND2	2.47	0.46
1:A:36:VAL:HG21	1:A:224:LEU:CB	2.46	0.45
1:A:783:TYR:OH	4:E:177:ASP:OD2	2.12	0.45
7:I:699:TYR:OH	7:I:714:PRO:O	2.16	0.45
1:A:987:LYS:NZ	1:A:1137:ASP:OD2	2.49	0.45
11:S:117:PHE:CE2	11:S:121:LEU:HD11	2.51	0.45
1:A:852:ASP:OD1	1:A:853:ASN:N	2.50	0.45
2:B:325:GLN:NE2	7:I:747:VAL:O	2.50	0.45
1:A:329:LEU:HD22	1:A:334:VAL:HG21	1.98	0.45
1:A:700:ARG:NH2	2:B:636:THR:O	2.45	0.45
1:A:991:VAL:CG1	1:A:1123:MET:HE1	2.48	0.44
1:A:745:ILE:O	1:A:749:THR:OG1	2.31	0.44
2:B:1069:THR:O	2:B:1073:VAL:HG23	2.17	0.44
1:A:1218:LYS:HD3	1:A:1221:LEU:HD12	1.99	0.44
5:F:76:ARG:O	5:F:132:LYS:NZ	2.51	0.44
1:A:976:GLU:OE2	1:A:1149:ASN:ND2	2.50	0.44
2:B:849:MET:SD	2:B:1026:ALA:HB3	2.58	0.44
1:A:41:LEU:O	1:A:62:HIS:N	2.46	0.44
2:B:853:ARG:NH1	3:C:50:GLU:OE2	2.50	0.44
4:E:168:ASN:ND2	4:E:171:THR:OG1	2.50	0.44
1:A:281:ARG:NH2	12:T:20:DT:OP1	2.49	0.43
1:A:1029:ARG:NH2	11:S:144:TYR:OH	2.45	0.43
1:A:510:GLU:OE1	1:A:510:GLU:N	2.51	0.43
2:B:722:ILE:HD12	2:B:723:VAL:N	2.34	0.43
2:B:322:THR:CG2	2:B:326:LEU:HD12	2.48	0.43
2:B:650:MET:HE1	2:B:658:TYR:CE2	2.53	0.43
2:B:722:ILE:HD12	2:B:723:VAL:HG23	2.00	0.43
11:S:94:ILE:HG22	11:S:95:ALA:N	2.32	0.43
1:A:317:VAL:HG12	1:A:317:VAL:O	2.19	0.43
2:B:887:THR:O	2:B:888:SER:OG	2.29	0.43
6:G:142:MET:HE2	6:G:142:MET:HA	2.00	0.43
4:E:170:VAL:HG23	4:E:171:THR:HG23	2.00	0.43
2:B:792:ARG:NH2	2:B:825:SER:O	2.52	0.43
3:C:40:VAL:HG23	3:C:53:LEU:HD21	2.01	0.43
7:I:129:SER:HB3	7:I:164:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:326:CYS:SG	7:I:327:GLU:N	2.92	0.43
1:A:304:PRO:HD2	1:A:307:ILE:HD12	2.01	0.43
7:I:772:VAL:HG21	7:I:777:TRP:CG	2.55	0.42
2:B:536:LEU:HD23	2:B:537:VAL:N	2.34	0.42
1:A:7:VAL:CG2	1:A:1232:ILE:HD11	2.50	0.42
1:A:123:ILE:HD12	1:A:179:LEU:HD21	1.99	0.42
1:A:978:ILE:N	1:A:978:ILE:HD12	2.35	0.42
1:A:1168:LEU:HD23	4:E:169:MET:HE1	2.02	0.42
2:B:71:SER:OG	2:B:72:ASN:OD1	2.37	0.42
2:B:722:ILE:CD1	2:B:723:VAL:HG23	2.49	0.42
6:G:90:ASN:ND2	6:G:92:GLU:OE2	2.48	0.42
1:A:85:LEU:HD22	1:A:182:ILE:HD11	2.01	0.42
1:A:434:GLU:OE2	2:B:1068:ASN:ND2	2.45	0.42
2:B:124:ASP:O	2:B:125:SER:OG	2.30	0.42
7:I:135:ASP:N	7:I:135:ASP:OD1	2.53	0.42
7:I:369:ASN:O	7:I:369:ASN:ND2	2.51	0.42
1:A:7:VAL:HG23	1:A:1232:ILE:HD11	2.00	0.42
11:S:127:CYS:O	11:S:131:GLY:N	2.47	0.42
11:S:99:GLU:OE1	11:S:99:GLU:N	2.48	0.42
7:I:710:ARG:NE	7:I:761:GLU:OE2	2.49	0.41
12:T:14:DA:H2'	12:T:15:DT:H71	2.03	0.41
2:B:706:ARG:NH2	3:C:45:SER:O	2.53	0.41
2:B:140:ASN:OD1	2:B:143:ASP:N	2.49	0.41
4:E:116:LEU:HD21	4:E:163:ARG:HB2	2.01	0.41
2:B:1057:GLU:OE1	2:B:1057:GLU:N	2.46	0.41
4:E:26:VAL:HG22	4:E:114:VAL:CG2	2.50	0.41
6:G:86:ARG:NH1	6:G:138:THR:OG1	2.54	0.41
4:E:129:GLN:HG2	4:E:136:THR:HG22	2.03	0.41
7:I:713:ASP:N	7:I:713:ASP:OD1	2.53	0.41
7:I:713:ASP:OD2	7:I:757:ARG:NH1	2.54	0.41
2:B:1120:THR:O	2:B:1125:LYS:NZ	2.54	0.41
2:B:242:ARG:NH2	2:B:284:ASP:OD1	2.53	0.41
5:F:90:TYR:HA	5:F:117:ILE:HD11	2.03	0.41
1:A:606:TYR:OH	1:A:626:GLU:OE2	2.35	0.40
1:A:198:PRO:HB2	1:A:202:ILE:HD11	2.04	0.40
1:A:271:ASN:O	1:A:275:SER:OG	2.35	0.40
3:C:52:TRP:HH2	3:C:94:ILE:HD12	1.86	0.40
1:A:925:PRO:HB2	1:A:928:ILE:HG22	2.03	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	1266/1286 (98%)	1202 (95%)	64 (5%)	0	100	100
2	B	1123/1164 (96%)	1072 (96%)	51 (4%)	0	100	100
3	C	302/305 (99%)	280 (93%)	22 (7%)	0	100	100
4	E	182/185 (98%)	171 (94%)	11 (6%)	0	100	100
5	F	101/164 (62%)	96 (95%)	5 (5%)	0	100	100
6	G	149/161 (92%)	142 (95%)	7 (5%)	0	100	100
7	I	456/795 (57%)	434 (95%)	22 (5%)	0	100	100
8	J	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
11	S	114/259 (44%)	98 (86%)	16 (14%)	0	100	100
All	All	3752/4382 (86%)	3550 (95%)	202 (5%)	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	1139/1157 (98%)	1121 (98%)	18 (2%)	55	71
2	B	1030/1064 (97%)	1012 (98%)	18 (2%)	53	70
3	C	286/287 (100%)	282 (99%)	4 (1%)	59	73
4	E	174/175 (99%)	173 (99%)	1 (1%)	78	81
5	F	94/151 (62%)	93 (99%)	1 (1%)	65	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	G	136/144 (94%)	133 (98%)	3 (2%)	45 67
7	I	440/755 (58%)	433 (98%)	7 (2%)	55 71
8	J	60/62 (97%)	55 (92%)	5 (8%)	10 34
11	S	107/240 (45%)	103 (96%)	4 (4%)	30 58
All	All	3466/4035 (86%)	3405 (98%)	61 (2%)	51 70

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	90	CYS
1	A	91	ILE
1	A	147	LYS
1	A	184	GLN
1	A	226	MET
1	A	238	GLN
1	A	256	ASN
1	A	298	VAL
1	A	360	LEU
1	A	385	HIS
1	A	457	SER
1	A	459	GLN
1	A	555	ILE
1	A	791	LEU
1	A	836	THR
1	A	962	ASN
1	A	1127	LEU
2	B	52	VAL
2	B	71	SER
2	B	114	ILE
2	B	166	VAL
2	B	226	LYS
2	B	243	VAL
2	B	359	ILE
2	B	369	LEU
2	B	394	THR
2	B	397	VAL
2	B	422	SER
2	B	545	ILE
2	B	728	LEU
2	B	784	LEU

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Mol	Chain	Res	Type
2	B	879	LEU
2	B	1028	VAL
2	B	1061	LEU
2	B	1071	THR
3	C	18	LEU
3	C	50	GLU
3	C	211	CYS
3	C	289	LYS
4	E	72	THR
5	F	81	GLU
6	G	14	LEU
6	G	20	THR
6	G	117	PHE
7	I	135	ASP
7	I	168	MET
7	I	220	LEU
7	I	235	VAL
7	I	300	LYS
7	I	302	LYS
7	I	317	ARG
8	J	3	PHE
8	J	10	CYS
8	J	17	GLU
8	J	21	LEU
8	J	39	CYS
11	S	77	GLU
11	S	98	LEU
11	S	110	THR
11	S	122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	459	GLN
1	A	830	GLN
1	A	1149	ASN
2	B	305	ASN
2	B	388	ASN
2	B	389	HIS
6	G	129	ASN
6	G	133	ASN

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Mol	Chain	Res	Type
7	I	178	ASN
11	S	62	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 ⓘ

There are no chain breaks in this entry.

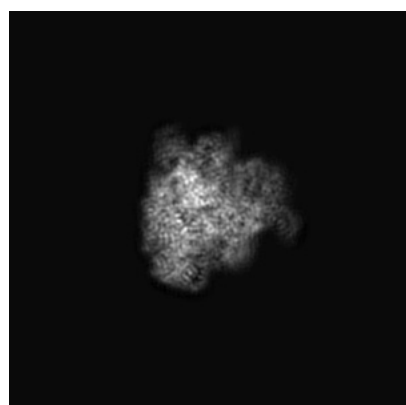
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11850. These allow visual inspection of the internal detail of the map and identification of artifacts.

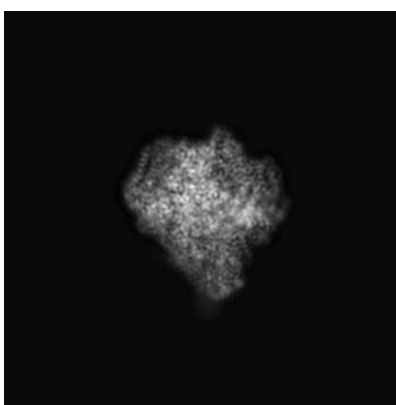
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

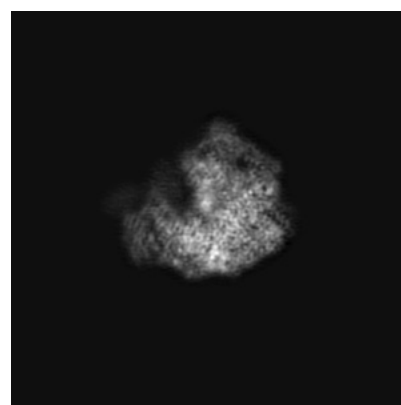
6.1.1 Primary map



X



Y

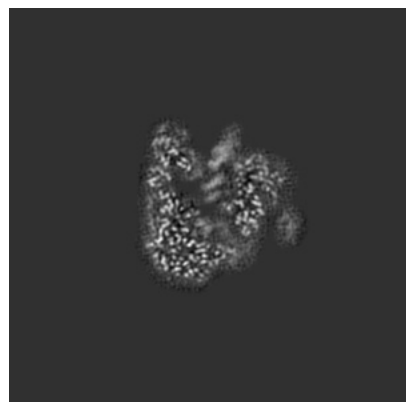


Z

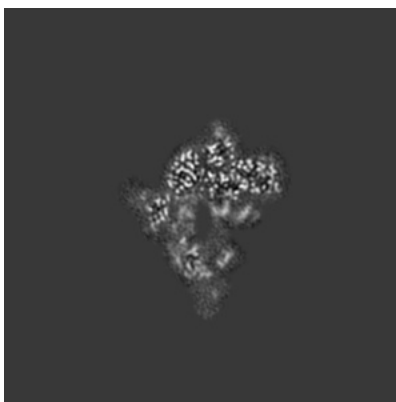
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

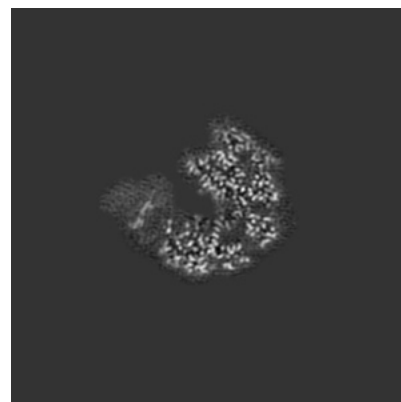
6.2.1 Primary map



X Index: 160



Y Index: 160

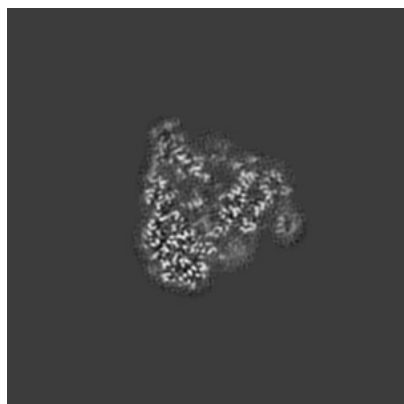


Z Index: 160

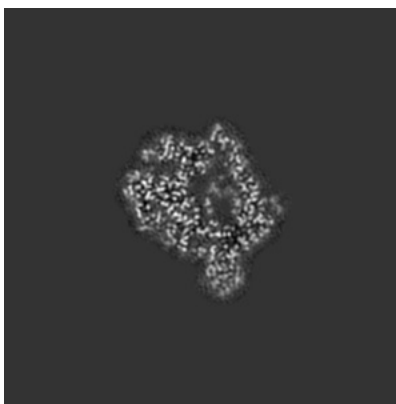
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

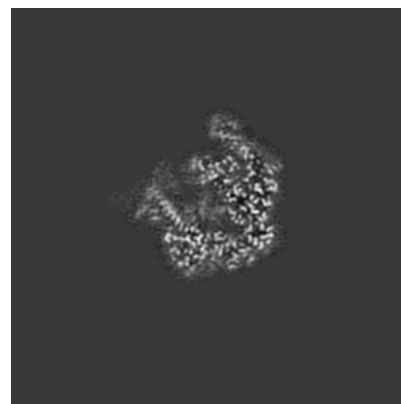
6.3.1 Primary map



X Index: 167



Y Index: 140

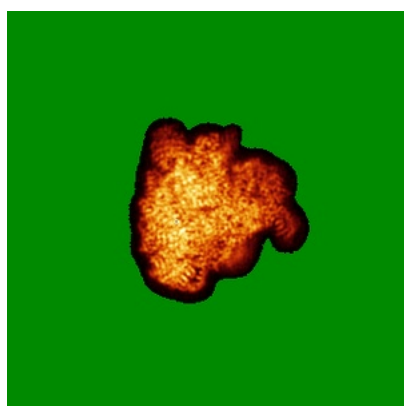


Z Index: 151

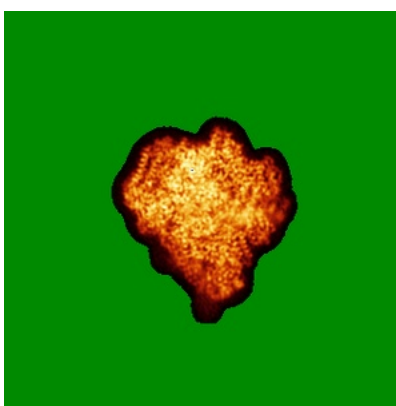
The images above show the largest variance slices of the map in three orthogonal directions.

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

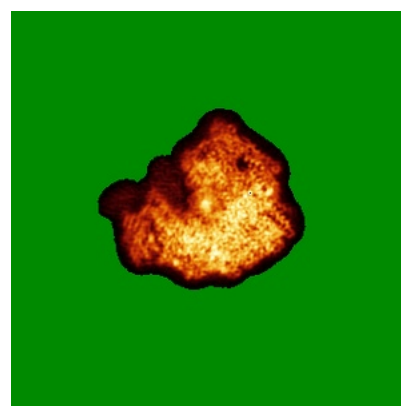
6.4.1 Primary map



X



Y



Z

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 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

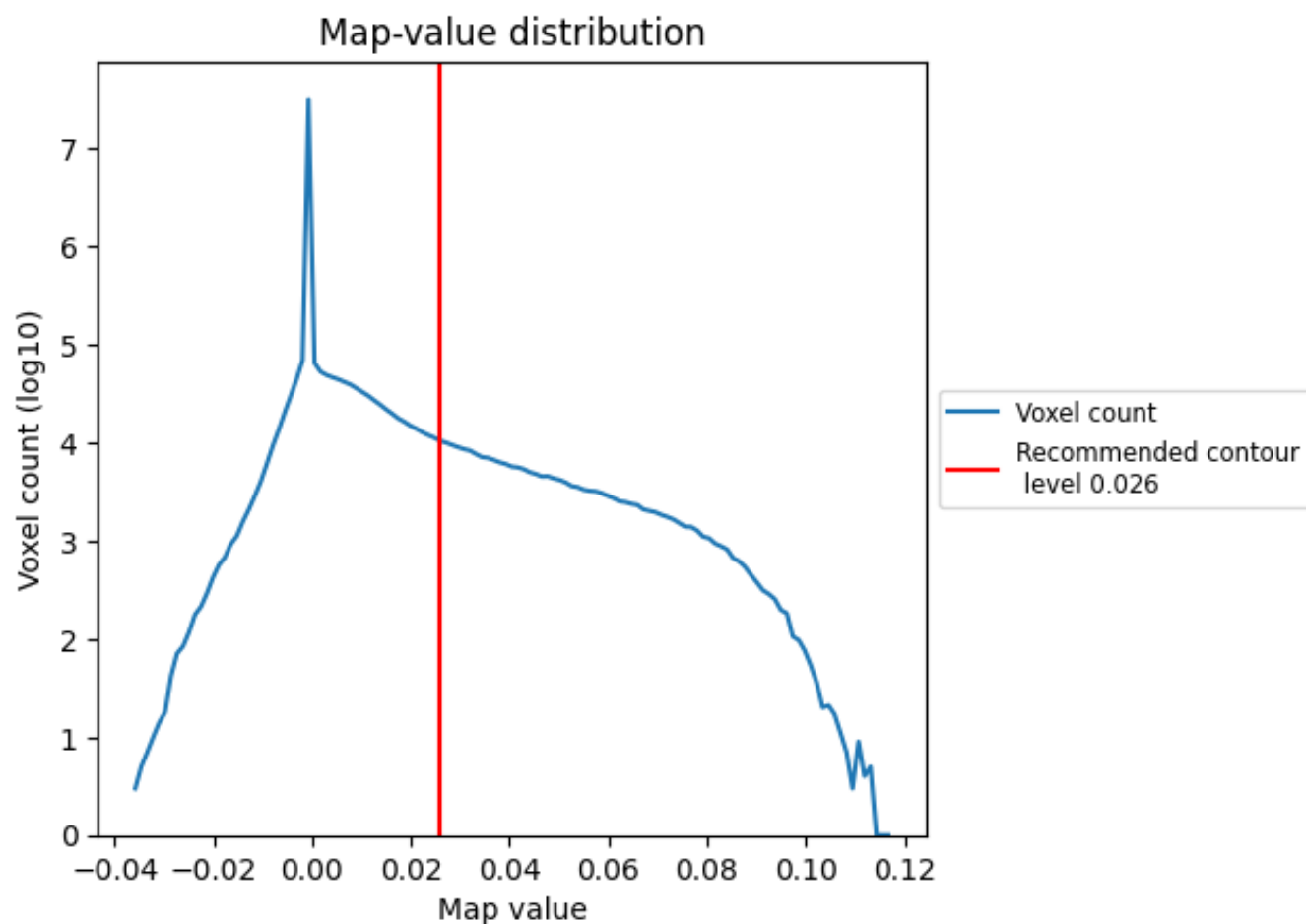
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

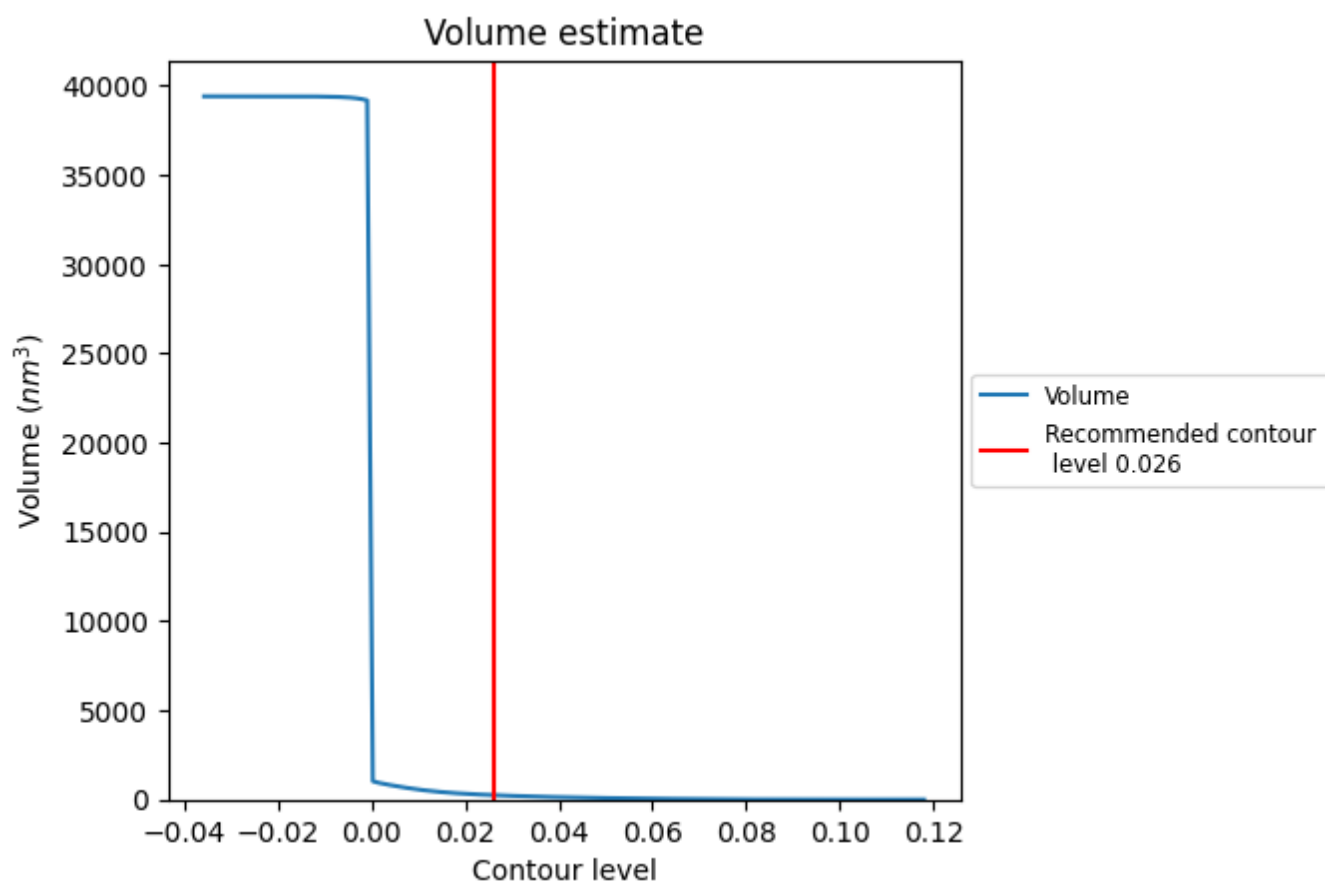
This section contains the results of statistical analysis of the map.

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.

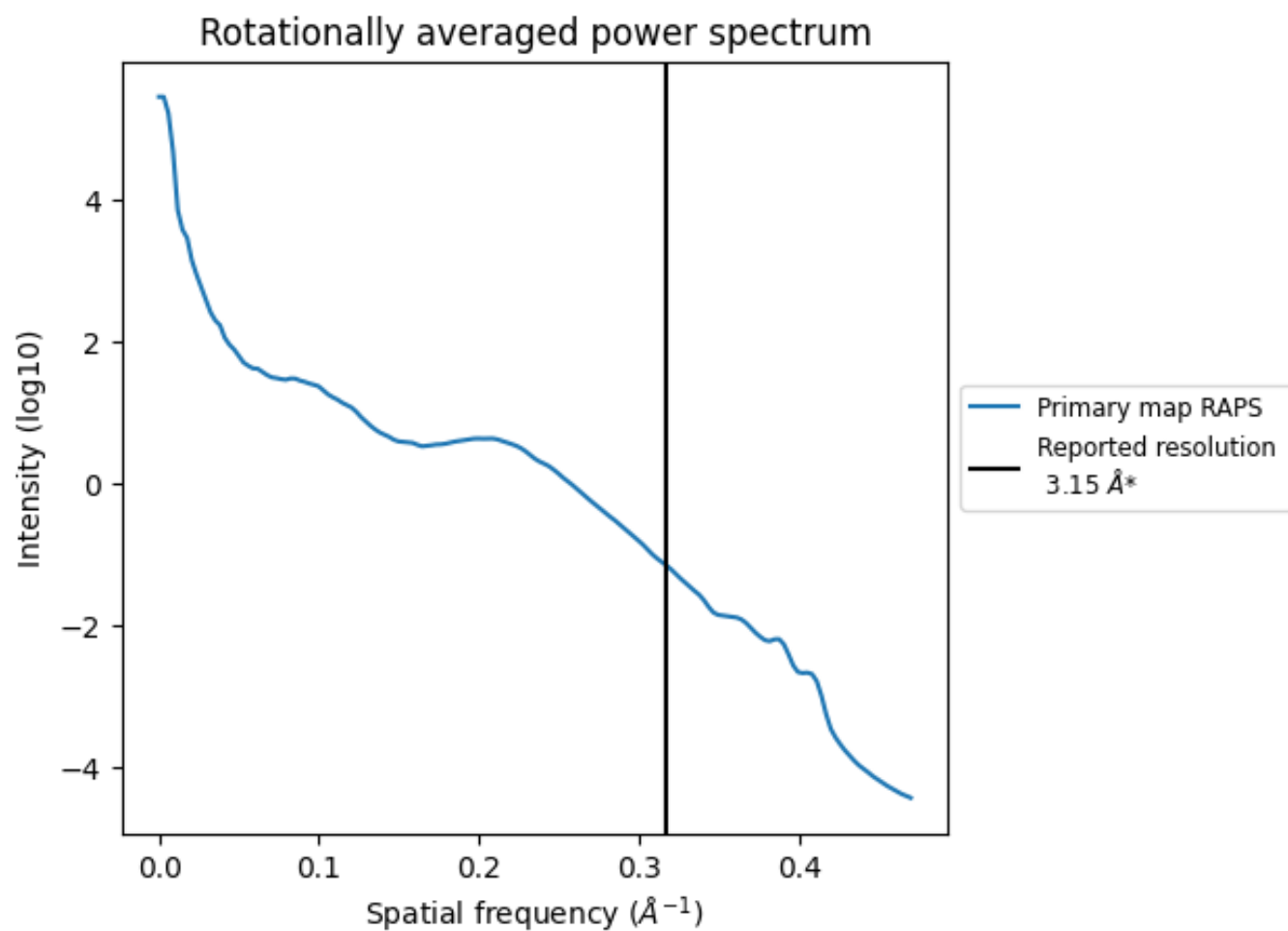
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 223 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 0.317 Å⁻¹

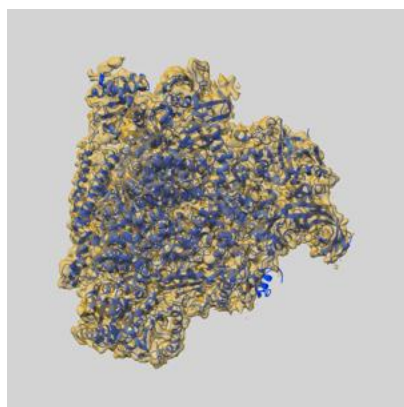
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

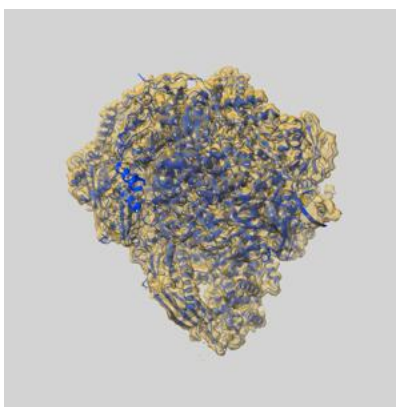
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11850 and PDB model 7AP8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

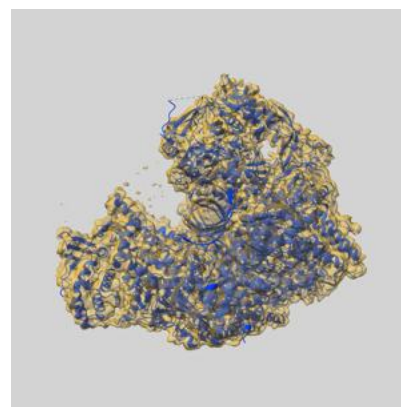
9.1 Map-model overlay [i](#)



X



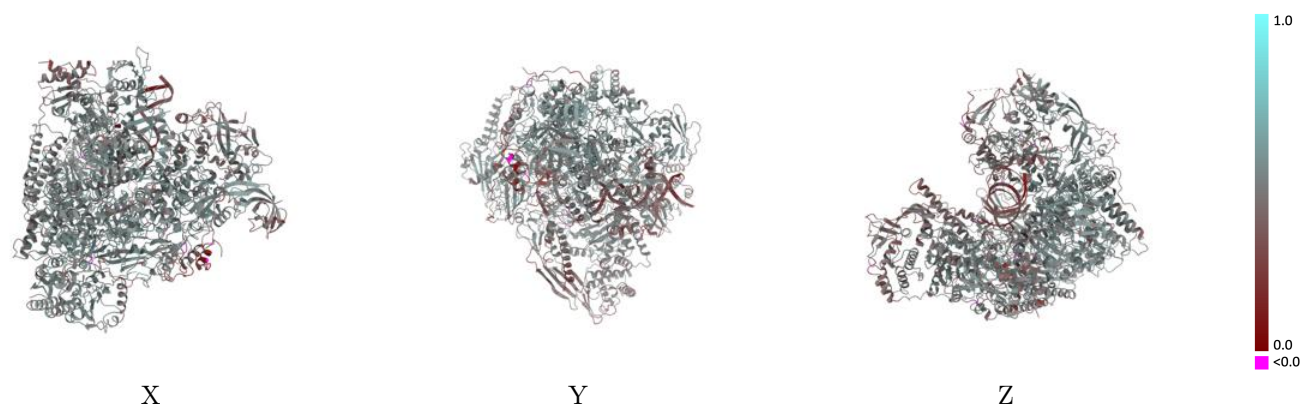
Y



Z

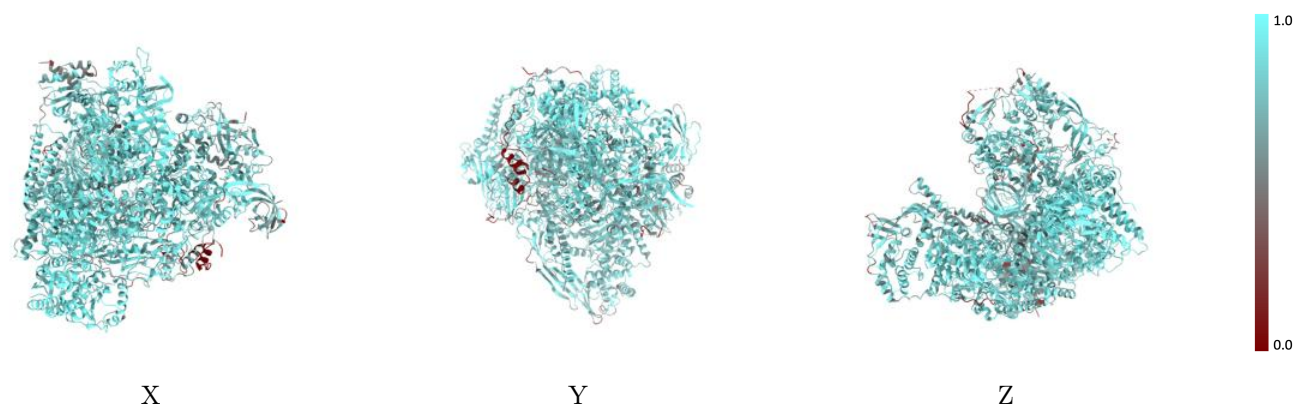
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



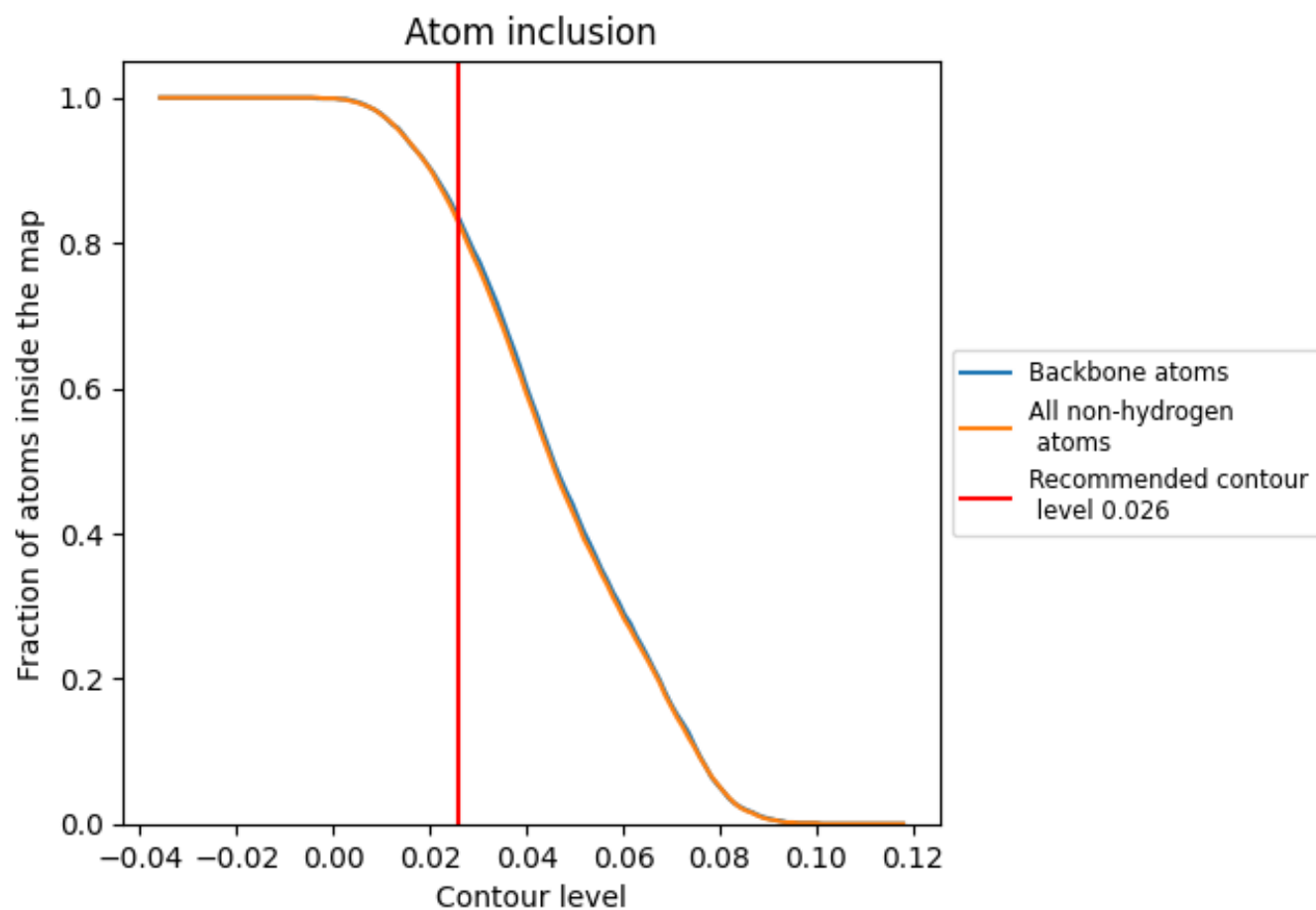
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.4820
A	 0.8580	 0.5010
B	 0.8700	 0.4980
C	 0.8970	 0.5100
E	 0.8980	 0.5210
F	 0.9020	 0.5220
G	 0.7690	 0.4810
I	 0.6440	 0.4060
J	 0.9000	 0.5180
N	 0.7370	 0.2290
P	 0.7680	 0.4060
S	 0.6790	 0.4190
T	 0.8880	 0.3160

