Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 03:32 pm GMT

PDB ID	:	7AOZ
EMDB ID	:	EMD-11848
Title	:	Atomic structure of the poxvirus transcription initiation complex in conformation 1
Authors	:	Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on	:	2020-10-15
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

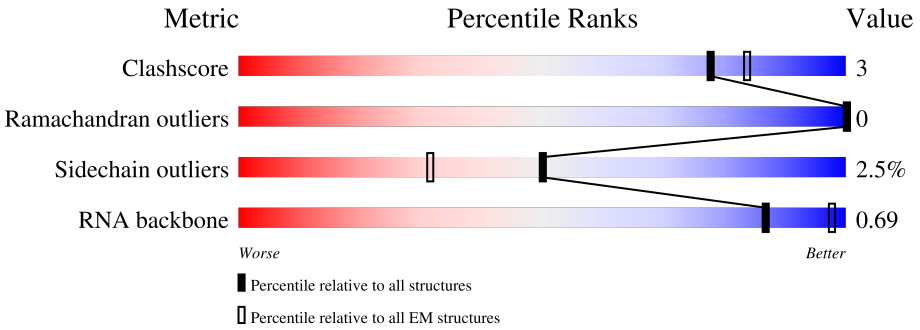
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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 <=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	89% 9% •
2	B	1164	87% 10% •
3	C	305	90% 9% •
4	E	185	87% 12% •
5	F	164	59% • • 37%
6	G	161	85% 10% 5%
7	I	795	• 52% 6% • 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	63	76% 17%
9	N	60	25% 73%
10	P	5	60% 40%
11	S	259	39% 5% 55%
12	T	60	32% 65%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 31512 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1268	10188	6556	1679	1908	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1129	9091	5794	1554	1695	48	0	0

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
			Total	C	N	O	S		
3	C	304	2484	1608	399	464	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	184	1495	966	248	276	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	103	849	545	148	153	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	153	1192	753	198	235	6	0	0

- Molecule 7 is a protein called Protein H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	464	3903	2552	627	710	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	61	490	310	88	88	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	N	16	327	155	61	95	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	P	5	108	49	22	32	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	116	952	608	154	186	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	T	21	428	206	76	126	20	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

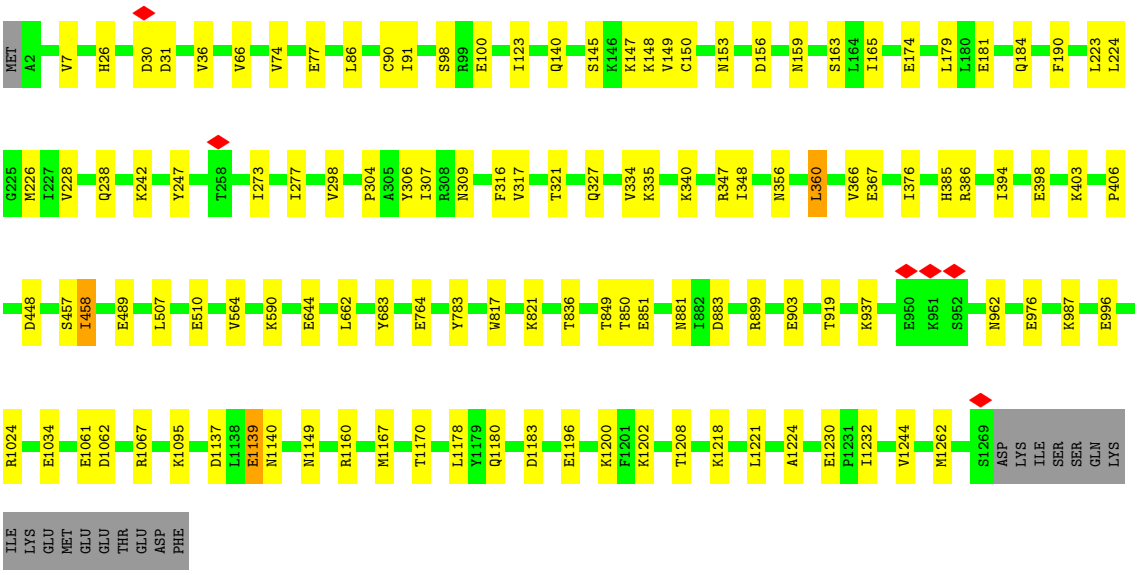
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
14	A	2	2	2	0
			Total	Zn	
14	B	1	1	1	0
			Total	Zn	
14	I	1	1	1	0

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.

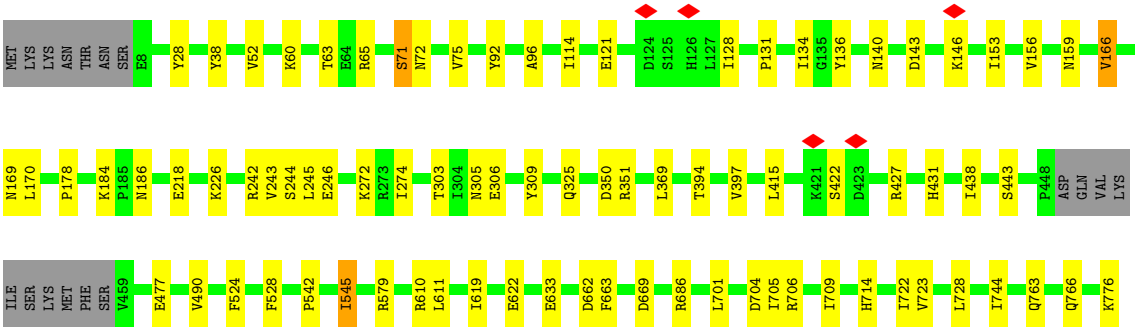
• Molecule 1: DNA-directed RNA polymerase 147 kDa polypeptide

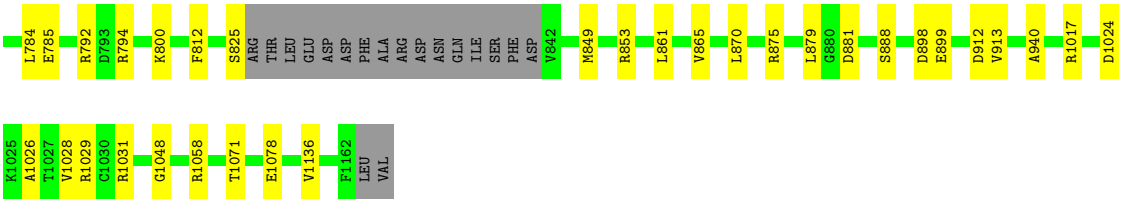
Chain A:



• Molecule 2: DNA-directed RNA polymerase

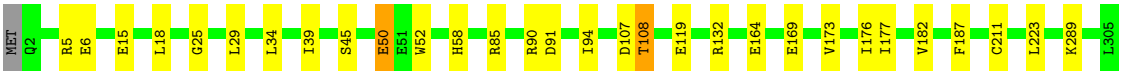
Chain B:





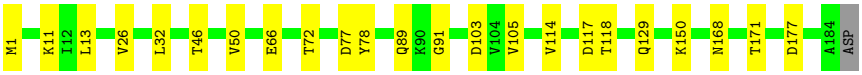
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit

Chain C:



- Molecule 4: DNA-directed RNA polymerase subunit

Chain E:



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

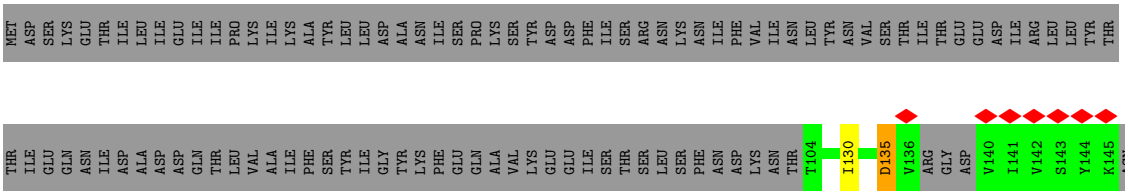
Chain F:

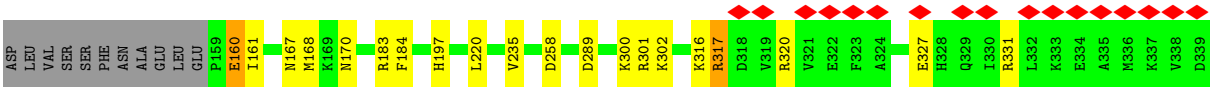
- Molecule 6: DNA-directed RNA polymerase 18 kDa subunit

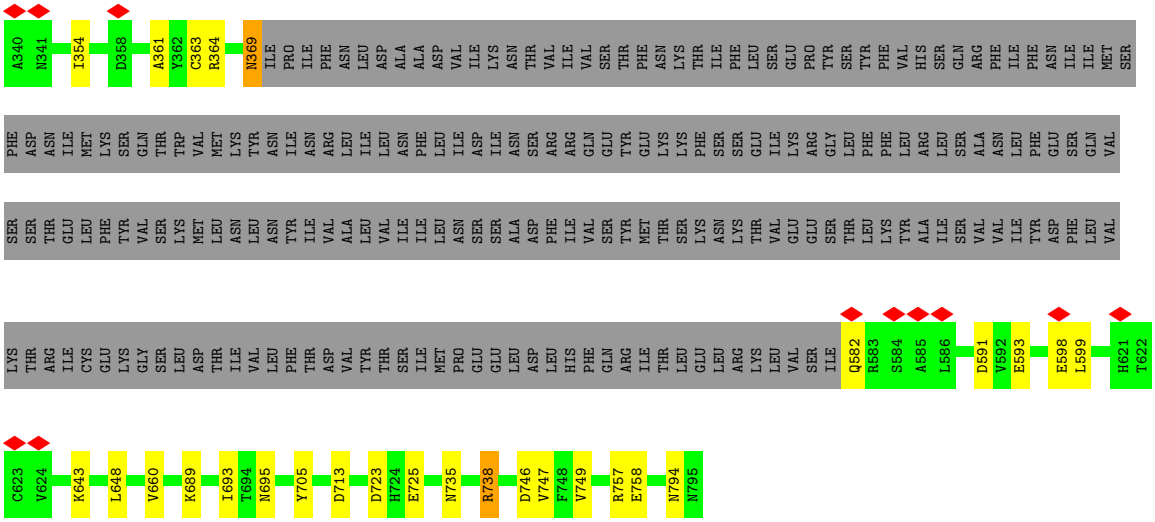
Chain G:

- Molecule 7: Protein H4

Chain I:

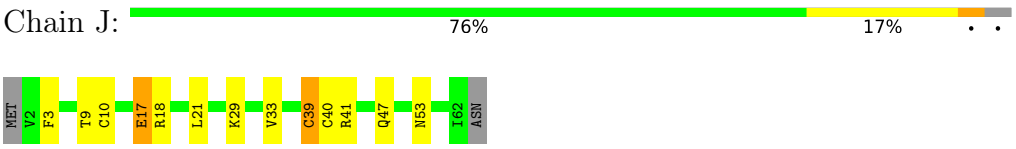






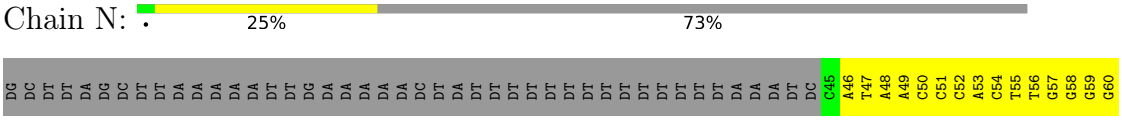
• Molecule 8: DNA-directed RNA polymerase 7 kDa subunit

Chain J:



• Molecule 9: Synthetic promoter DNA oligomer, non-template strand

Chain N:

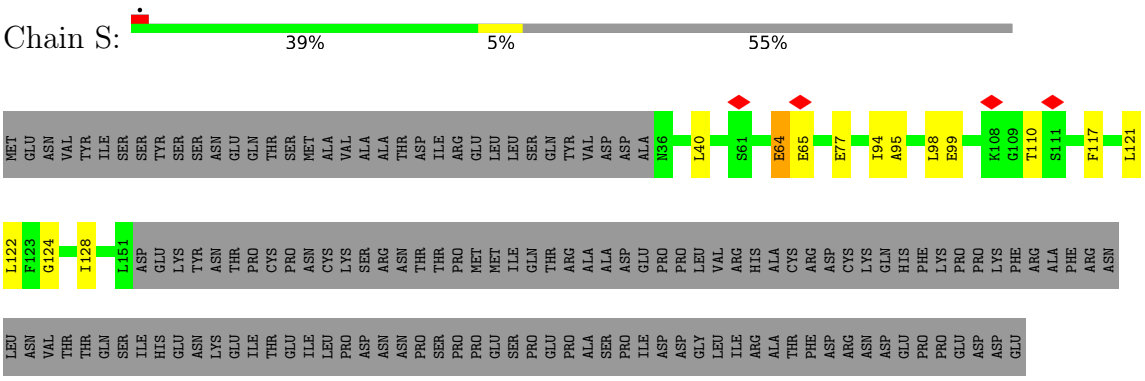


• Molecule 10: RNA (5'-R(P*AP*UP*AP*AP*A)-3')

Chain P:

• Molecule 11: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S:



• Molecule 12: Synthetic promoter DNA oligomer, template strand

Chain T: 32% 65%

C1
T15
DG
DG
DA
DT
T20
T21
A22
T23
A24
G25
DA
DA
DT
DT
DT
DA
DG
DA
DA
DA
DT
DA
DG
DT
DT
DT
DT
DC
DA
DA
DT
DT
DT
DT
DA
DA
DG
DC
DT
DA
DA
DG
DC

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133467	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 ($e^-/Å^2$)	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	0.190	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0163	Depositor
Map size (Å)	340.32, 340.32, 340.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 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	0.29	0/10394	0.50	0/14052
2	B	0.29	0/9281	0.51	0/12537
3	C	0.28	0/2540	0.49	0/3440
4	E	0.28	0/1522	0.52	0/2069
5	F	0.27	0/863	0.49	0/1158
6	G	0.27	0/1209	0.52	0/1639
7	I	0.28	0/4000	0.50	0/5411
8	J	0.27	0/494	0.53	0/663
9	N	1.58	14/366 (3.8%)	1.05	1/562 (0.2%)
10	P	0.20	0/121	0.68	0/186
11	S	0.28	0/967	0.52	0/1294
12	T	0.63	0/478	1.01	0/734
All	All	0.34	14/32235 (0.0%)	0.53	1/43745 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
7	I	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	55	DT	C3'-O3'	6.16	1.51	1.44
9	N	53	DA	C3'-O3'	6.12	1.51	1.44
9	N	54	DC	C3'-O3'	5.96	1.51	1.44
9	N	57	DG	C3'-O3'	5.91	1.51	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	48	DA	C3'-O3'	5.89	1.51	1.44
9	N	56	DT	C3'-O3'	5.82	1.51	1.44
9	N	58	DG	C3'-O3'	5.81	1.51	1.44
9	N	50	DC	C3'-O3'	5.64	1.51	1.44
9	N	52	DC	C3'-O3'	5.62	1.51	1.44
9	N	47	DT	C3'-O3'	5.61	1.51	1.44
9	N	49	DA	C3'-O3'	5.43	1.51	1.44
9	N	51	DC	C3'-O3'	5.39	1.50	1.44
9	N	59	DG	C3'-O3'	5.38	1.50	1.44
9	N	46	DA	C3'-O3'	5.29	1.50	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	60	DG	O4'-C1'-N9	-5.17	104.38	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	458	ILE	Peptide
7	I	660	VAL	Peptide

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	0	10312	63	0
2	B	9091	0	9146	62	0
3	C	2484	0	2470	20	0
4	E	1495	0	1548	12	0
5	F	849	0	874	5	0
6	G	1192	0	1181	8	0
7	I	3903	0	3905	25	0
8	J	490	0	530	7	0
9	N	327	0	180	0	0
10	P	108	0	55	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	S	952	0	957	6	0
12	T	428	0	241	2	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	0	31399	183	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 3.

All (183) 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	1.61	0.81
7:I:735:ASN:ND2	7:I:747:VAL:O	2.21	0.74
3:C:34:LEU:HD12	3:C:182:VAL:HG12	1.68	0.73
2:B:242:ARG:O	7:I:738:ARG:NH2	2.22	0.72
6:G:112:SER:O	6:G:127:ASN:ND2	2.22	0.72
1:A:98:SER:OG	1:A:100:GLU:OE1	2.08	0.71
7:I:316:LYS:O	7:I:317:ARG:NH2	2.24	0.71
3:C:132:ARG:NH1	7:I:591:ASP:O	2.24	0.70
2:B:38:TYR:OH	2:B:131:PRO:O	2.10	0.70
1:A:590:LYS:NZ	1:A:644:GLU:OE2	2.25	0.70
2:B:303:THR:OG1	2:B:305:ASN:O	2.10	0.69
2:B:542:PRO:HA	2:B:545:ILE:HD13	1.73	0.69
2:B:309:TYR:OH	7:I:725:GLU:OE2	2.10	0.69
1:A:398:GLU:O	1:A:403:LYS:NZ	2.25	0.68
1:A:145:SER:OG	1:A:148:LYS:O	2.09	0.68
1:A:764:GLU:OE1	2:B:1058:ARG:NH2	2.26	0.68
10:P:1:A:H61	12:T:22:DA:H61	1.42	0.67
2:B:427:ARG:NH1	10:P:3:A:OP1	2.28	0.66
1:A:783:TYR:OH	4:E:177:ASP:OD2	2.09	0.66
1:A:851:GLU:OE1	1:A:899:ARG:NE	2.29	0.65
1:A:1196:GLU:OE2	1:A:1202:LYS:N	2.30	0.65
1:A:163:SER:OG	7:I:183:ARG:NH2	2.30	0.64
1:A:1262:MET:O	6:G:24:LYS:NZ	2.30	0.64
3:C:132:ARG:NH2	7:I:593:GLU:O	2.31	0.63
2:B:704:ASP:OD1	8:J:53:ASN:ND2	2.31	0.63
1:A:1024:ARG:NH1	1:A:1034:GLU:OE1	2.31	0.63
2:B:477:GLU:OE1	2:B:477:GLU:N	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:327:GLU:OE2	7:I:331:ARG:NH2	2.32	0.63
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.32	0.62
1:A:66:VAL:HG11	1:A:228:VAL:HG22	1.81	0.61
2:B:610:ARG:NH2	2:B:622:GLU:OE1	2.33	0.61
6:G:30:ALA:O	6:G:34:THR:HG22	2.01	0.61
3:C:39:ILE:HG13	3:C:173:VAL:HG21	1.83	0.60
1:A:919:THR:O	5:F:76:ARG:NH2	2.35	0.60
2:B:579:ARG:NE	2:B:633:GLU:OE2	2.35	0.59
4:E:1:MET:SD	4:E:46:THR:OG1	2.61	0.59
8:J:18:ARG:NH2	8:J:47:GLN:OE1	2.36	0.58
1:A:223:LEU:HD13	1:A:247:TYR:HA	1.87	0.57
2:B:722:ILE:HD12	2:B:723:VAL:HG23	1.86	0.57
1:A:317:VAL:HG11	1:A:360:LEU:HB2	1.86	0.57
11:S:64:GLU:OE1	11:S:65:GLU:N	2.37	0.57
1:A:817:TRP:O	1:A:821:LYS:N	2.38	0.57
2:B:71:SER:OG	2:B:72:ASN:N	2.37	0.57
2:B:96:ALA:HB3	2:B:128:ILE:HB	1.87	0.56
1:A:100:GLU:OE1	1:A:100:GLU:N	2.39	0.56
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.88	0.56
2:B:912:ASP:OD2	8:J:9:THR:OG1	2.24	0.56
1:A:1139:GLU:OE1	1:A:1140:ASN:ND2	2.38	0.56
1:A:309:ASN:O	1:A:335:LYS:NZ	2.39	0.56
7:I:354:ILE:HG23	7:I:361:ALA:HB1	1.86	0.56
1:A:340:LYS:NZ	2:B:1078:GLU:OE2	2.39	0.56
2:B:121:GLU:OE1	2:B:121:GLU:N	2.39	0.56
1:A:334:VAL:HG13	1:A:366:VAL:HG13	1.88	0.55
1:A:356:ASN:O	7:I:320:ARG:NH2	2.39	0.55
11:S:94:ILE:HG22	11:S:95:ALA:H	1.71	0.55
1:A:123:ILE:CD1	1:A:179:LEU:HD21	2.36	0.55
3:C:164:GLU:OE1	3:C:164:GLU:N	2.39	0.55
1:A:36:VAL:HG21	1:A:224:LEU:HB3	1.89	0.55
7:I:689:LYS:NZ	7:I:723:ASP:OD2	2.36	0.55
1:A:347:ARG:NH2	1:A:348:ILE:O	2.39	0.55
1:A:386:ARG:NH1	1:A:448:ASP:OD1	2.40	0.54
3:C:173:VAL:O	3:C:177:ILE:N	2.41	0.54
2:B:812:PHE:CD1	3:C:176:ILE:HD13	2.44	0.53
3:C:25:GLY:HA3	3:C:223:LEU:HD21	1.91	0.53
4:E:129:GLN:O	5:F:70:LYS:NZ	2.41	0.53
2:B:792:ARG:NH2	2:B:825:SER:O	2.41	0.53
2:B:800:LYS:NZ	2:B:812:PHE:O	2.42	0.53
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:LYS:NZ	1:A:1137:ASP:OD2	2.42	0.53
1:A:174:GLU:N	1:A:174:GLU:OE1	2.43	0.52
2:B:776:LYS:NZ	12:T:23:DT:OP1	2.41	0.52
11:S:99:GLU:N	11:S:99:GLU:OE1	2.42	0.52
3:C:119:GLU:N	3:C:119:GLU:OE2	2.43	0.52
6:G:62:VAL:HG12	6:G:63:ASN:H	1.75	0.52
2:B:524:PHE:CZ	7:I:749:VAL:HG11	2.44	0.52
7:I:713:ASP:OD2	7:I:757:ARG:NH1	2.43	0.52
2:B:218:GLU:HB2	2:B:274:ILE:HD11	1.93	0.51
2:B:763:GLN:OE1	2:B:763:GLN:N	2.44	0.51
1:A:150:CYS:SG	1:A:159:ASN:ND2	2.83	0.51
2:B:709:ILE:HG23	2:B:870:LEU:HB2	1.93	0.51
6:G:34:THR:HG23	6:G:35:TYR:CD2	2.46	0.51
7:I:363:CYS:SG	7:I:364:ARG:N	2.83	0.51
2:B:875:ARG:NH1	2:B:1024:ASP:OD1	2.44	0.51
1:A:976:GLU:OE2	1:A:1149:ASN:ND2	2.44	0.50
1:A:903:GLU:OE1	1:A:903:GLU:N	2.44	0.50
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	1.93	0.50
2:B:490:VAL:HG13	2:B:669:ASP:O	2.11	0.50
6:G:109:SER:OG	6:G:111:ASP:OD1	2.25	0.50
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.11	0.50
1:A:1218:LYS:HD3	1:A:1221:LEU:HD12	1.92	0.49
1:A:367:GLU:OE2	2:B:1031:ARG:NH2	2.45	0.49
2:B:246:GLU:OE2	2:B:272:LYS:NZ	2.25	0.49
2:B:706:ARG:NH2	3:C:45:SER:O	2.44	0.49
8:J:29:LYS:O	8:J:33:VAL:HG23	2.12	0.49
5:F:76:ARG:O	5:F:132:LYS:NZ	2.46	0.48
1:A:489:GLU:N	1:A:489:GLU:OE1	2.47	0.48
1:A:1208:THR:OG1	1:A:1230:GLU:OE2	2.32	0.48
4:E:32:LEU:HD13	4:E:105:VAL:HG11	1.95	0.48
4:E:77:ASP:OD1	4:E:78:TYR:N	2.46	0.48
4:E:91:GLY:O	4:E:150:LYS:NZ	2.44	0.48
1:A:273:ILE:HA	1:A:277:ILE:HD12	1.95	0.48
3:C:15:GLU:OE1	3:C:15:GLU:N	2.45	0.48
1:A:140:GLN:OE1	1:A:153:ASN:ND2	2.47	0.47
7:I:695:ASN:OD1	7:I:794:ASN:ND2	2.47	0.47
11:S:117:PHE:CE2	11:S:121:LEU:HD11	2.49	0.47
1:A:881:ASN:ND2	1:A:883:ASP:OD2	2.46	0.47
1:A:149:VAL:HG21	1:A:242:LYS:HB2	1.96	0.47
2:B:159:ASN:HB3	2:B:415:LEU:HD23	1.97	0.47
2:B:350:ASP:OD1	2:B:351:ARG:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:78:SER:N	5:F:81:GLU:OE2	2.44	0.47
2:B:849:MET:SD	2:B:1026:ALA:HB3	2.55	0.47
1:A:406:PRO:HB3	1:A:458:ILE:HD11	1.97	0.46
4:E:26:VAL:HG22	4:E:114:VAL:CG2	2.46	0.46
1:A:181:GLU:OE1	1:A:181:GLU:N	2.49	0.46
1:A:1034:GLU:OE2	1:A:1034:GLU:N	2.46	0.46
2:B:156:VAL:HG12	2:B:166:VAL:HG13	1.97	0.46
1:A:376:ILE:HB	1:A:394:ILE:HD11	1.98	0.45
2:B:898:ASP:OD1	2:B:899:GLU:N	2.50	0.45
2:B:940:ALA:O	8:J:41:ARG:NH2	2.48	0.45
7:I:598:GLU:C	7:I:599:LEU:HD22	2.37	0.45
1:A:316:PHE:O	1:A:321:THR:OG1	2.30	0.45
2:B:75:VAL:HG12	2:B:96:ALA:HB2	1.98	0.45
3:C:107:ASP:OD1	3:C:108:THR:N	2.49	0.45
1:A:1061:GLU:OE2	1:A:1067:ARG:NE	2.50	0.45
2:B:92:TYR:OH	2:B:140:ASN:ND2	2.49	0.45
11:S:40:LEU:HD13	11:S:128:ILE:HD11	1.98	0.44
2:B:306:GLU:HG2	7:I:693:ILE:HG21	1.99	0.44
2:B:662:ASP:OD1	2:B:663:PHE:N	2.50	0.44
2:B:785:GLU:N	2:B:785:GLU:OE1	2.50	0.44
3:C:39:ILE:CG1	3:C:173:VAL:HG21	2.46	0.44
2:B:60:LYS:O	2:B:63:THR:OG1	2.12	0.44
7:I:160:GLU:N	7:I:160:GLU:OE1	2.50	0.44
2:B:686:ARG:NH2	2:B:888:SER:O	2.47	0.44
1:A:1160:ARG:NH1	1:A:1183:ASP:OD1	2.51	0.44
8:J:39:CYS:SG	8:J:40:CYS:N	2.90	0.44
4:E:117:ASP:OD1	4:E:118:THR:N	2.50	0.44
1:A:74:VAL:HG22	1:A:190:PHE:CE2	2.53	0.43
4:E:11:LYS:NZ	4:E:103:ASP:OD2	2.48	0.43
7:I:135:ASP:N	7:I:135:ASP:OD1	2.51	0.43
3:C:50:GLU:N	3:C:50:GLU:OE1	2.51	0.43
2:B:853:ARG:NH1	3:C:50:GLU:OE2	2.52	0.43
1:A:1180:GLN:N	1:A:1180:GLN:OE1	2.51	0.43
4:E:168:ASN:ND2	4:E:171:THR:OG1	2.51	0.43
2:B:528:PHE:HB2	2:B:545:ILE:HD11	2.00	0.43
7:I:167:ASN:ND2	7:I:170:ASN:OD1	2.48	0.43
1:A:30:ASP:OD1	1:A:31:ASP:N	2.48	0.43
11:S:40:LEU:HD11	11:S:124:GLY:HA3	2.00	0.43
2:B:169:ASN:ND2	2:B:443:SER:O	2.49	0.42
2:B:766:GLN:O	3:C:58:HIS:NE2	2.51	0.42
3:C:85:ARG:NH2	3:C:91:ASP:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:66:GLU:OE2	4:E:89:GLN:NE2	2.47	0.42
1:A:36:VAL:HG21	1:A:224:LEU:CB	2.48	0.42
1:A:1244:VAL:HG22	2:B:1071:THR:HG21	2.00	0.42
1:A:86:LEU:HD21	1:A:165:ILE:HG23	2.01	0.42
3:C:169:GLU:O	3:C:173:VAL:HG22	2.19	0.42
7:I:738:ARG:NH1	7:I:746:ASP:O	2.53	0.42
7:I:648:LEU:HD11	7:I:705:TYR:CE1	2.55	0.42
1:A:849:THR:OG1	1:A:850:THR:N	2.52	0.42
1:A:996:GLU:O	1:A:1095:LYS:NZ	2.52	0.42
2:B:28:TYR:OH	2:B:438:ILE:HD11	2.20	0.42
3:C:5:ARG:NH1	8:J:17:GLU:OE2	2.53	0.42
1:A:304:PRO:HD2	1:A:307:ILE:HD12	2.02	0.41
1:A:937:LYS:HG2	1:A:1178:LEU:HD11	2.02	0.41
1:A:1167:MET:O	1:A:1170:THR:OG1	2.39	0.41
2:B:744:ILE:HG22	2:B:913:VAL:HB	2.02	0.41
2:B:705:ILE:HD12	2:B:714:HIS:CG	2.55	0.41
2:B:861:LEU:CD2	2:B:865:VAL:HG22	2.50	0.41
3:C:52:TRP:HH2	3:C:94:ILE:HD12	1.84	0.41
1:A:317:VAL:HG12	1:A:317:VAL:O	2.20	0.41
2:B:722:ILE:HD12	2:B:723:VAL:N	2.35	0.41
1:A:850:THR:O	1:A:850:THR:OG1	2.36	0.41
7:I:130:ILE:HD12	7:I:161:ILE:HG23	2.02	0.41
7:I:289:ASP:N	7:I:289:ASP:OD1	2.53	0.41
7:I:369:ASN:O	7:I:369:ASN:ND2	2.51	0.41
2:B:244:SER:OG	2:B:245:LEU:N	2.54	0.40
2:B:611:LEU:CD1	2:B:619:ILE:HD11	2.50	0.40
4:E:13:LEU:O	4:E:50:VAL:HG21	2.22	0.40
5:F:100:LEU:N	5:F:120:GLU:OE2	2.49	0.40
6:G:93:ASP:OD1	6:G:94:GLU:N	2.51	0.40
1:A:7:VAL:HG23	1:A:1232:ILE:HD11	2.03	0.40
1:A:507:LEU:HD11	1:A:564:VAL:HG21	2.04	0.40
2:B:136:TYR:CD1	2:B:153:ILE:HG22	2.57	0.40
6:G:132:ASP:OD1	6:G:133:ASN:N	2.54	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	1266/1286 (98%)	1201 (95%)	65 (5%)	0	100	100
2	B	1123/1164 (96%)	1067 (95%)	56 (5%)	0	100	100
3	C	302/305 (99%)	279 (92%)	23 (8%)	0	100	100
4	E	182/185 (98%)	169 (93%)	13 (7%)	0	100	100
5	F	101/164 (62%)	97 (96%)	4 (4%)	0	100	100
6	G	149/161 (92%)	140 (94%)	9 (6%)	0	100	100
7	I	456/795 (57%)	428 (94%)	28 (6%)	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%)	3534 (94%)	218 (6%)	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	1139/1157 (98%)	1117 (98%)	22 (2%)	57	81
2	B	1030/1064 (97%)	1006 (98%)	24 (2%)	50	78
3	C	286/287 (100%)	277 (97%)	9 (3%)	40	71
4	E	174/175 (99%)	173 (99%)	1 (1%)	86	95
5	F	94/151 (62%)	93 (99%)	1 (1%)	73	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	136/144 (94%)	134 (98%)	2 (2%)	65	86
7	I	440/755 (58%)	423 (96%)	17 (4%)	32	63
8	J	60/62 (97%)	55 (92%)	5 (8%)	11	29
11	S	107/240 (45%)	102 (95%)	5 (5%)	26	56
All	All	3466/4035 (86%)	3380 (98%)	86 (2%)	50	76

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	77	GLU
1	A	90	CYS
1	A	91	ILE
1	A	147	LYS
1	A	156	ASP
1	A	184	GLN
1	A	226	MET
1	A	238	GLN
1	A	298	VAL
1	A	327	GLN
1	A	360	LEU
1	A	385	HIS
1	A	457	SER
1	A	510	GLU
1	A	662	LEU
1	A	683	TYR
1	A	836	THR
1	A	962	ASN
1	A	1062	ASP
1	A	1139	GLU
1	A	1200	LYS
2	B	52	VAL
2	B	65	ARG
2	B	71	SER
2	B	114	ILE
2	B	143	ASP
2	B	146	LYS
2	B	166	VAL
2	B	170	LEU
2	B	178	PRO
2	B	184	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	186	ASN
2	B	226	LYS
2	B	243	VAL
2	B	325	GLN
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
2	B	794	ARG
2	B	879	LEU
2	B	1028	VAL
3	C	6	GLU
3	C	18	LEU
3	C	29	LEU
3	C	50	GLU
3	C	90	ARG
3	C	108	THR
3	C	187	PHE
3	C	211	CYS
3	C	289	LYS
4	E	72	THR
5	F	81	GLU
6	G	20	THR
6	G	117	PHE
7	I	135	ASP
7	I	160	GLU
7	I	168	MET
7	I	184	PHE
7	I	197	HIS
7	I	220	LEU
7	I	235	VAL
7	I	258	ASP
7	I	300	LYS
7	I	301	ARG
7	I	302	LYS
7	I	317	ARG
7	I	369	ASN
7	I	582	GLN
7	I	643	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	I	738	ARG
7	I	758	GLU
8	J	3	PHE
8	J	10	CYS
8	J	17	GLU
8	J	21	LEU
8	J	39	CYS
11	S	64	GLU
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	65	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

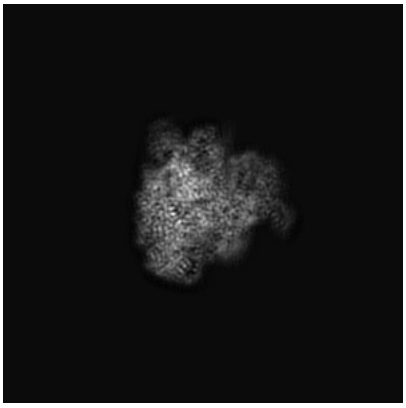
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11848. These allow visual inspection of the internal detail of the map and identification of artifacts.

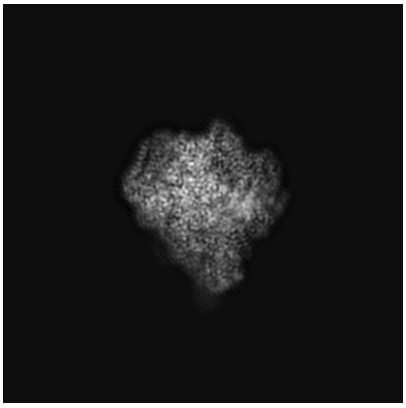
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

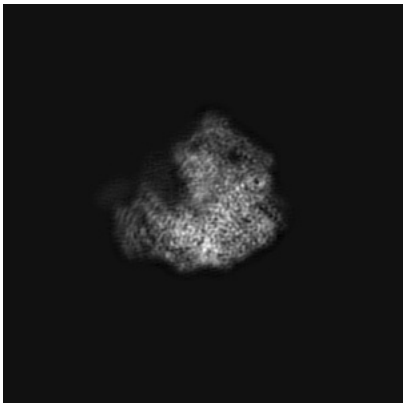
6.1.1 Primary map



X



Y

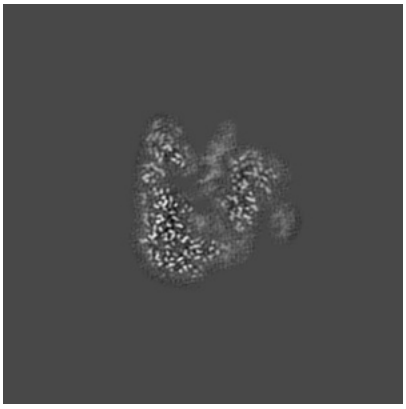


Z

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

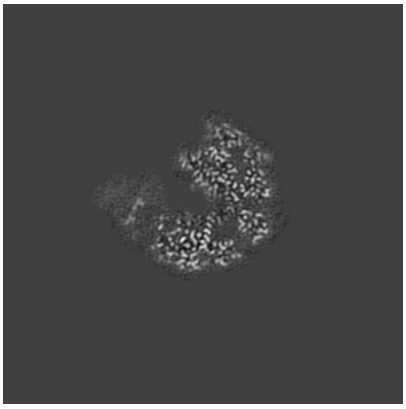
6.2 Central slices (i)

6.2.1 Primary map



X Index: 160

Y Index: 160

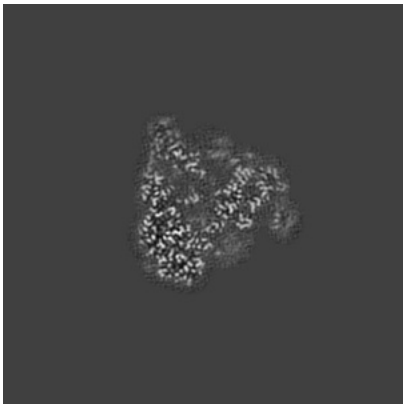


Z Index: 160

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

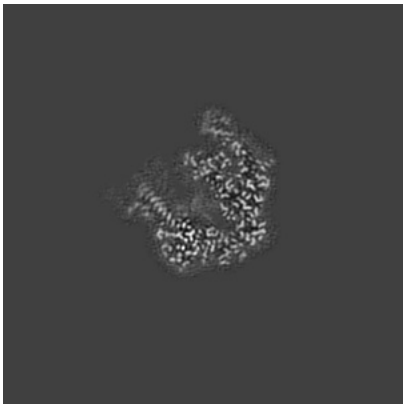
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 167

Y Index: 135

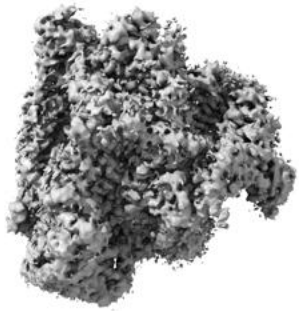


Z Index: 151

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

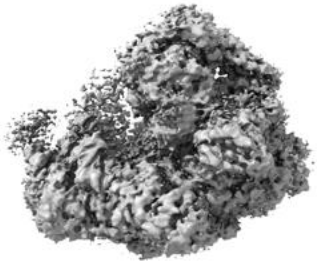
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0163. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

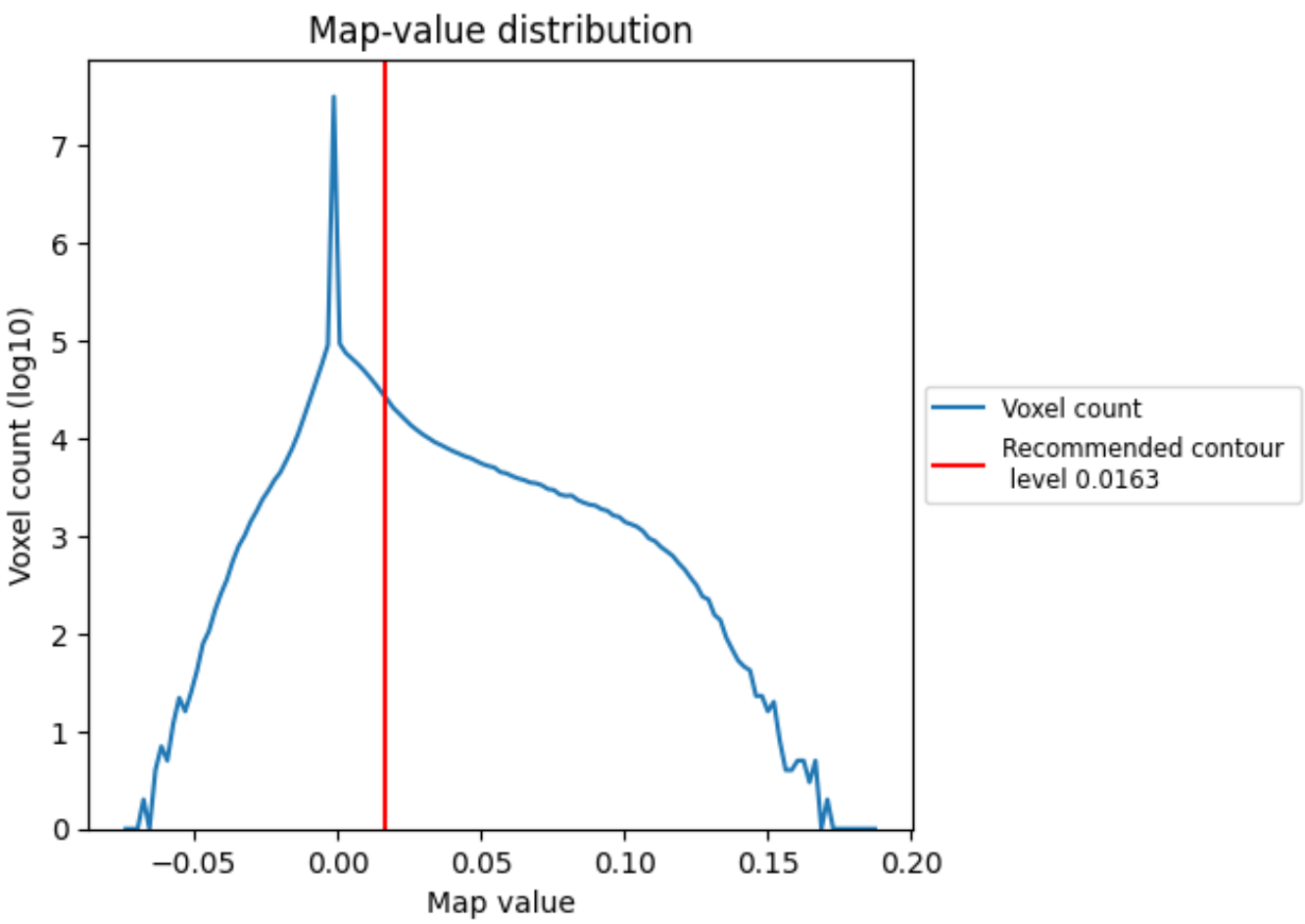
6.5 Mask visualisation (i)

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

7 Map analysis (i)

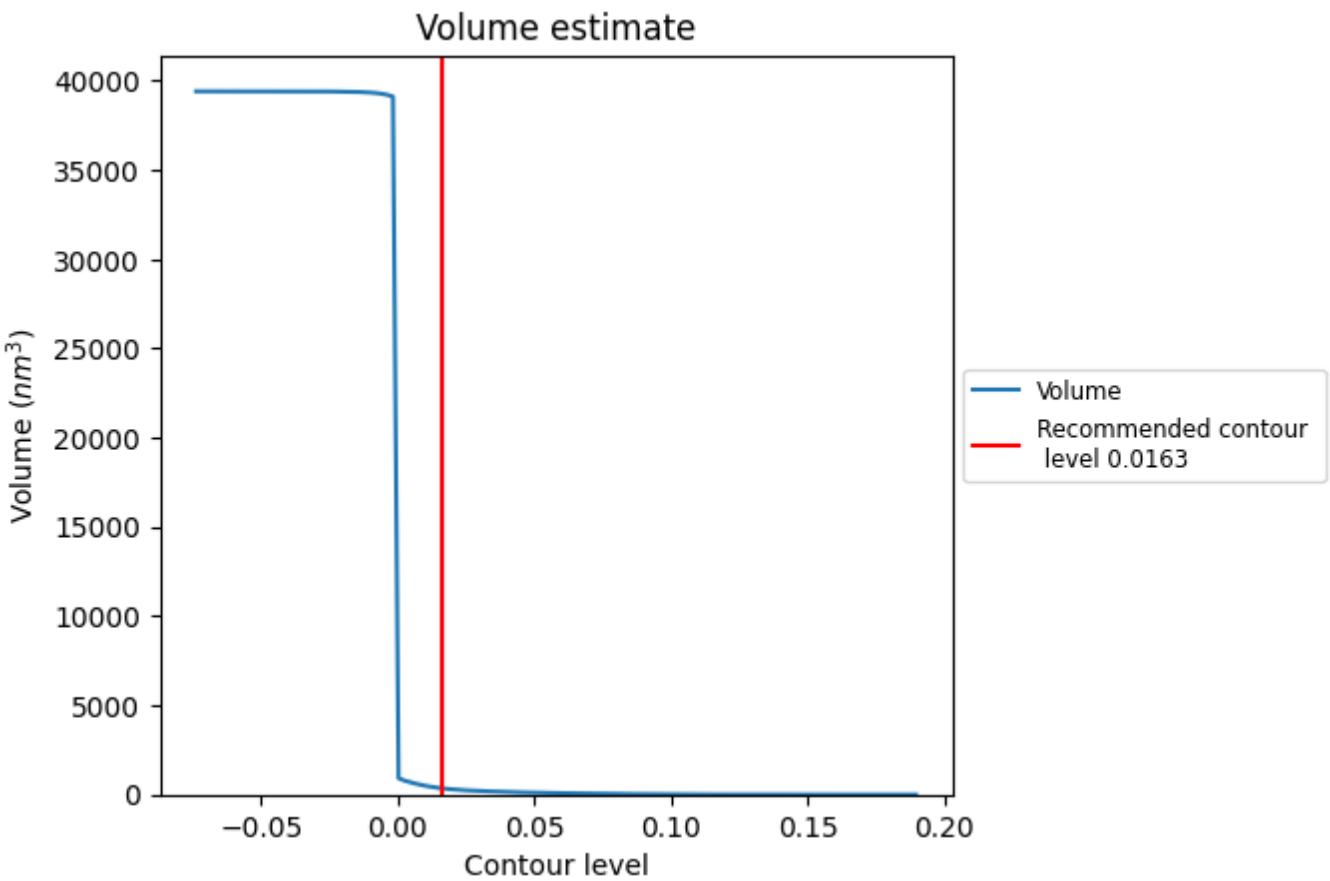
This section contains the results of statistical analysis of the map.

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.

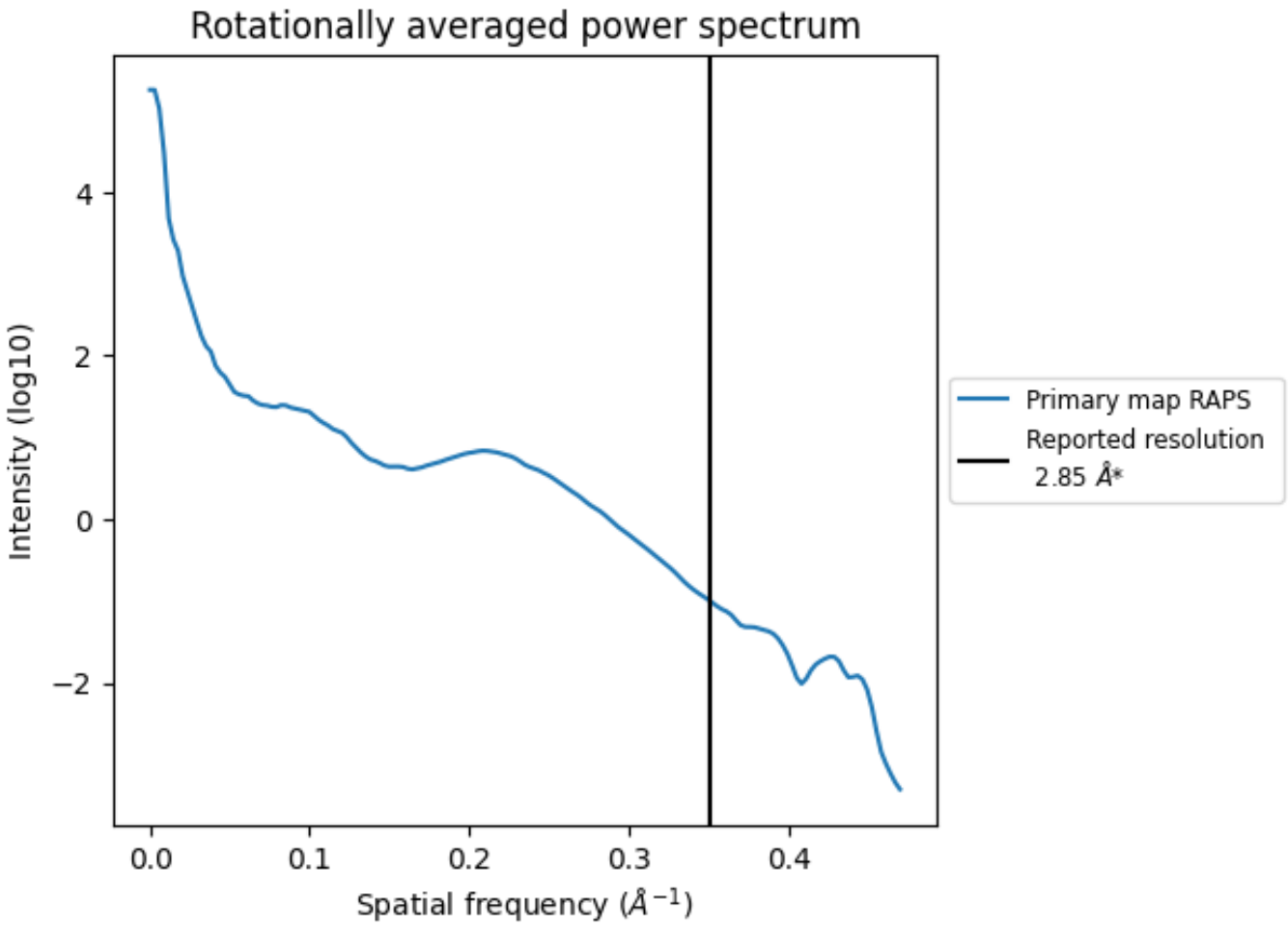
7.2 Volume estimate (i)



The volume at the recommended contour level is 347 nm^3; this corresponds to an approximate mass of 313 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 0.351 Å^{-1}

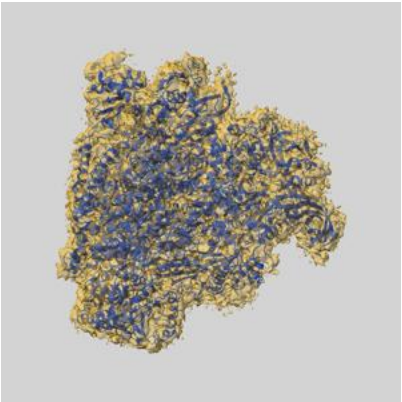
8 Fourier-Shell correlation (i)

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

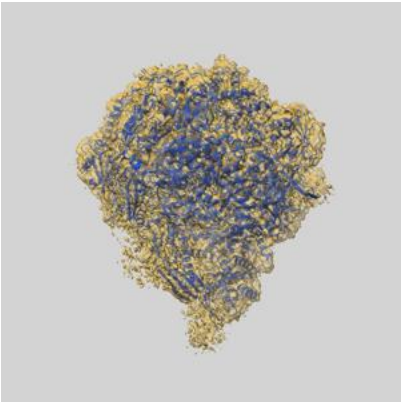
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11848 and PDB model 7AOZ. Per-residue inclusion information can be found in section 3 on page 7.

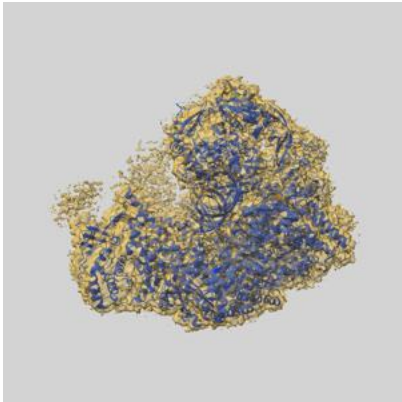
9.1 Map-model overlay (i)



X



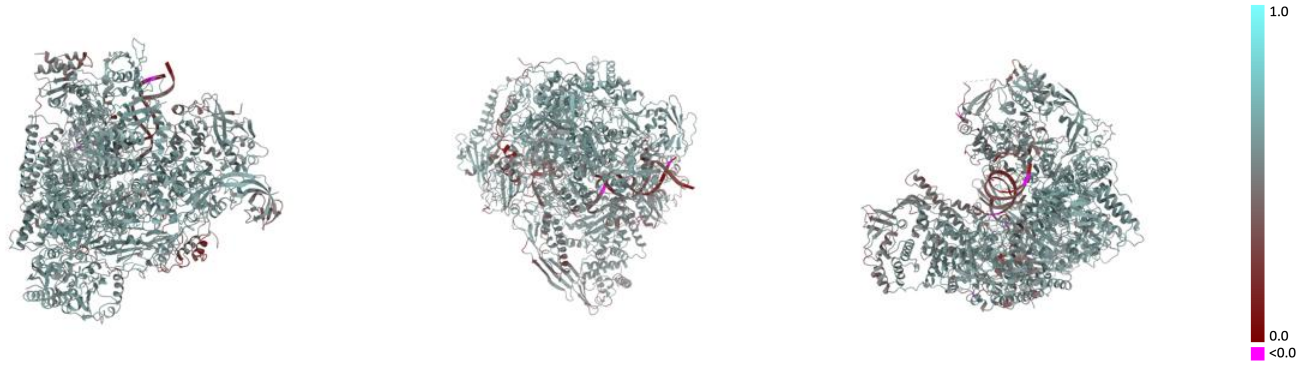
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0163 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.

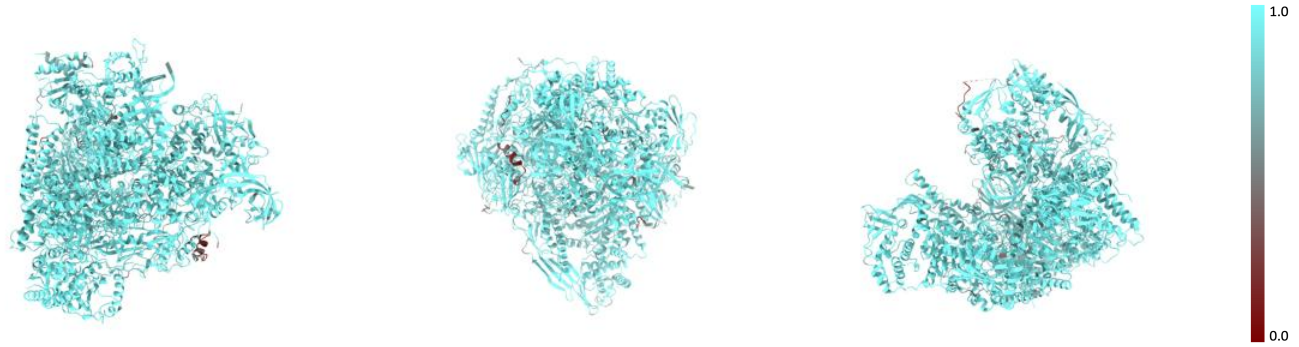
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

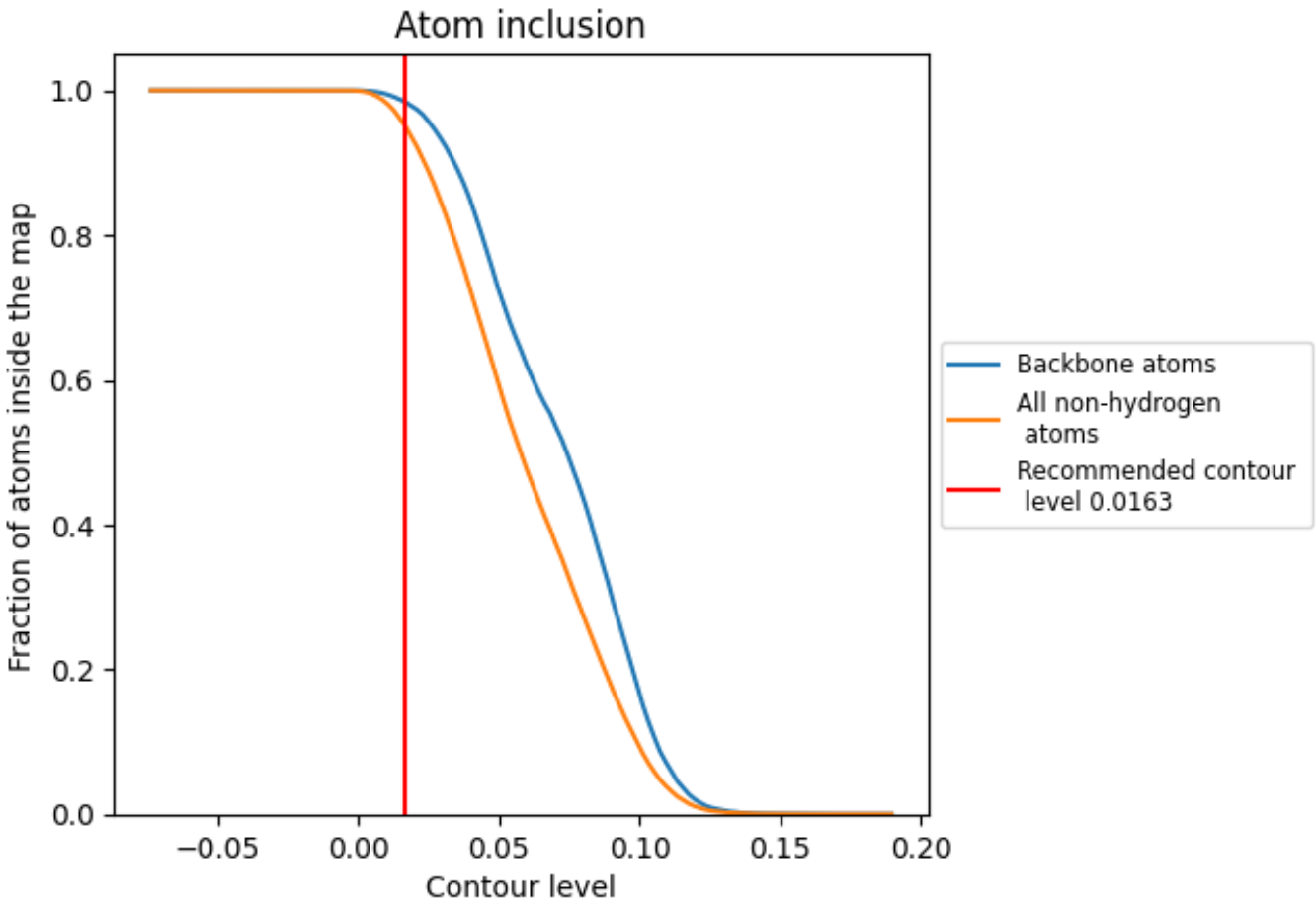
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0163).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0163) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9525	0.5450
A	0.9650	0.5640
B	0.9713	0.5690
C	0.9784	0.5690
E	0.9782	0.5740
F	0.9807	0.5900
G	0.9540	0.5370
I	0.8748	0.4820
J	0.9896	0.5770
N	0.8410	0.1770
P	0.9167	0.3950
S	0.8686	0.4690
T	0.9065	0.3170