Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 11:20 PM EST

PDB ID	:	7KIF
EMDB ID	:	EMD-22886
Title	:	Mycobacterium tuberculosis WT RNAP transcription open promoter complex with WhiB7 transcription factor
Authors	:	Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2020-10-23
Resolution	:	2.94 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:

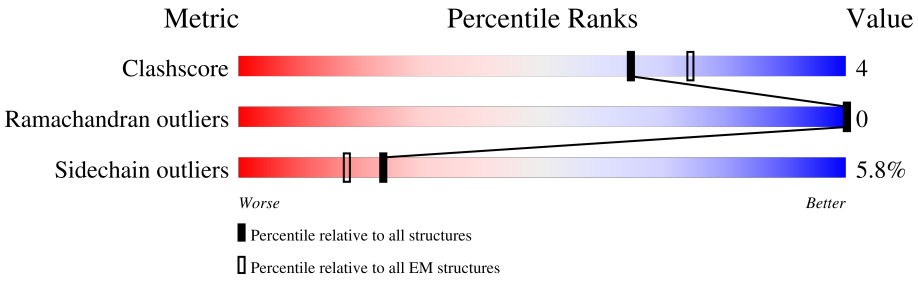
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.94 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

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	347	54% 10% 35%
1	B	347	57% 10% 32%
2	C	1172	79% 15% 5%
3	D	1318	85% 10%
4	E	110	61% 13% 25%
5	F	528	52% 9% 39%
6	J	111	5% 78% 20%
7	M	162	81% 17%

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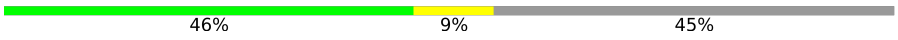
Mol	Chain	Length	Quality of chain
8	O	100	
9	P	100	
10	Z	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SF4	Z	101	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 30322 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8606	5392	1511	1664	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	322	Total	C	N	O	S	0	0
			2548	1588	461	490	9		

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	109	Total	C	N	O	S	0	0
			880	543	166	168	3		

- Molecule 7 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 8 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	63	Total	C	N	O	P	0	0
			1282	611	229	380	62		

- Molecule 9 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	55	Total	C	N	O	P	0	0
			1129	534	216	324	55		

- Molecule 10 is a protein called Probable transcriptional regulator WhiB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	76	Total	C	N	O	S	0	0
			581	369	110	98	4		

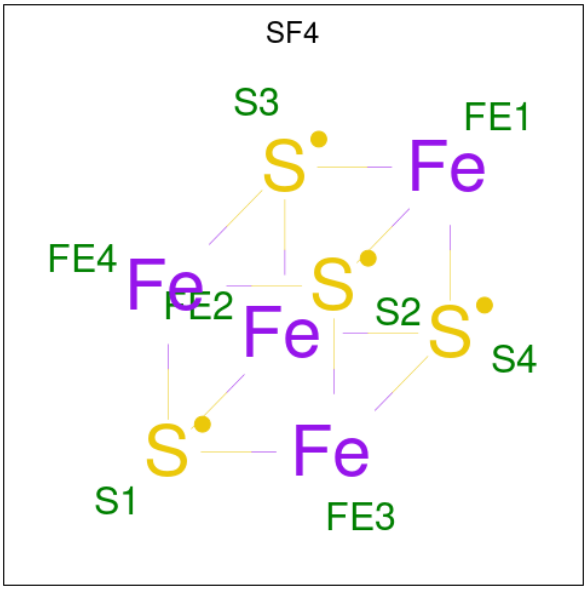
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
12	D	1	Total Mg 1 1	0

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



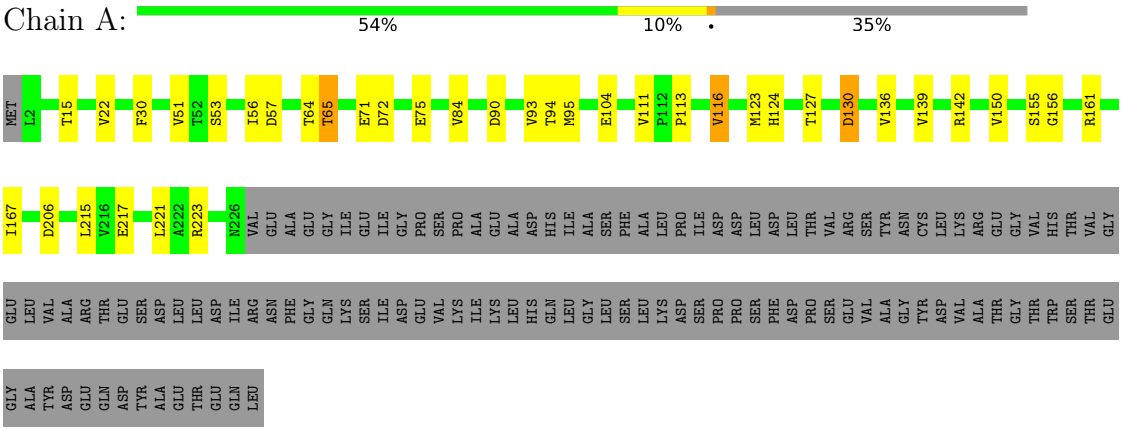
Mol	Chain	Residues	Atoms	AltConf
13	Z	1	Total Fe S 8 4 4	0

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.

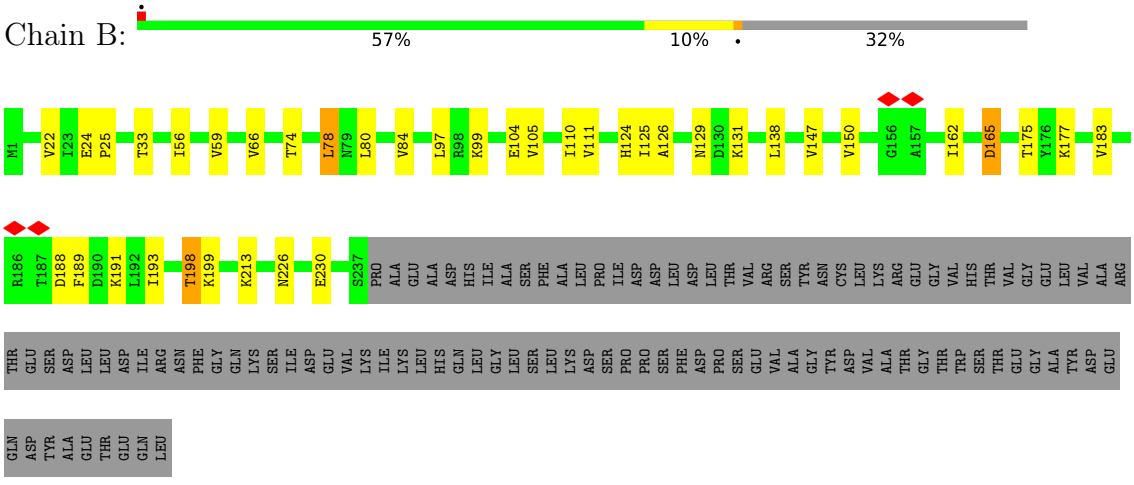
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



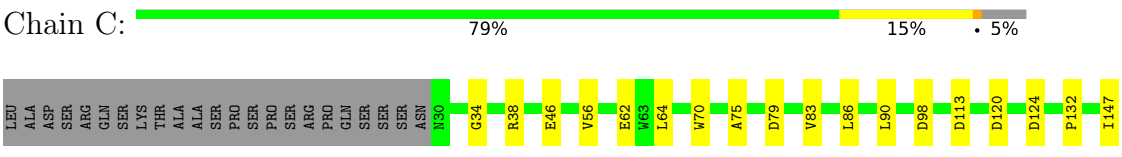
• Molecule 1: DNA-directed RNA polymerase subunit alpha

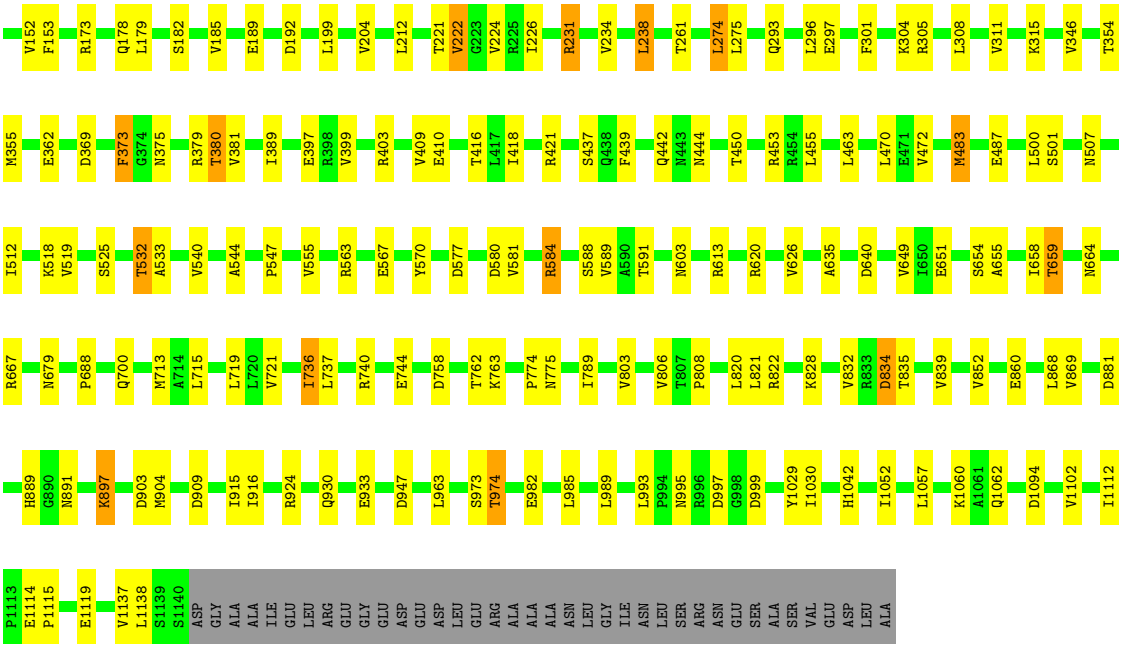
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

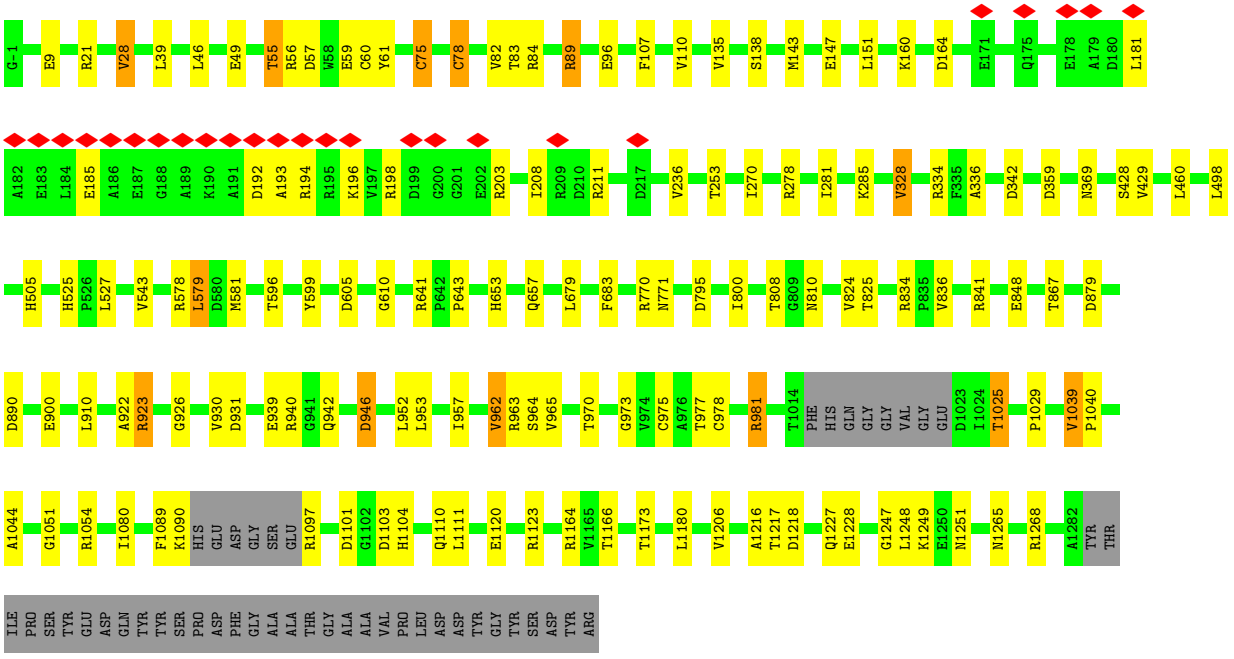
Chain C:





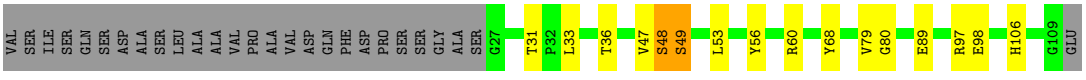
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



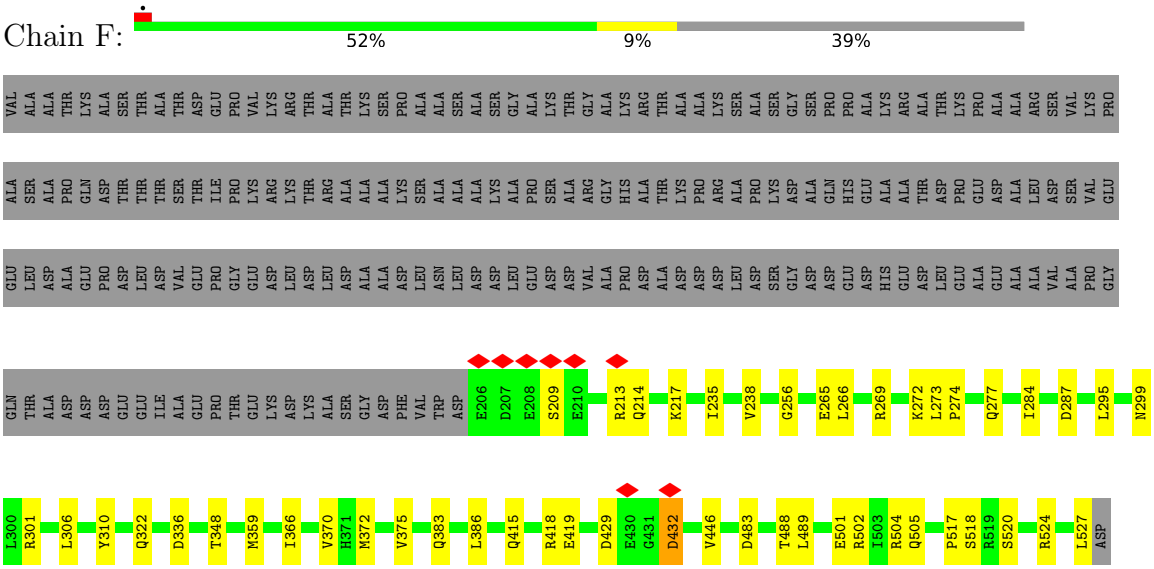
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



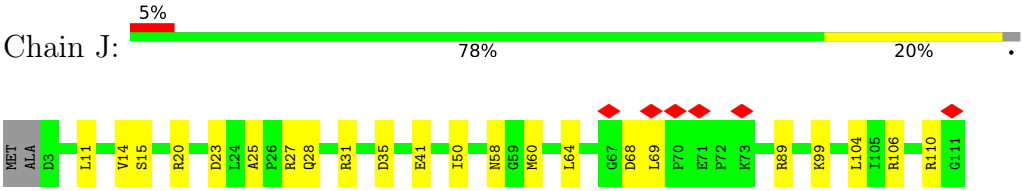
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



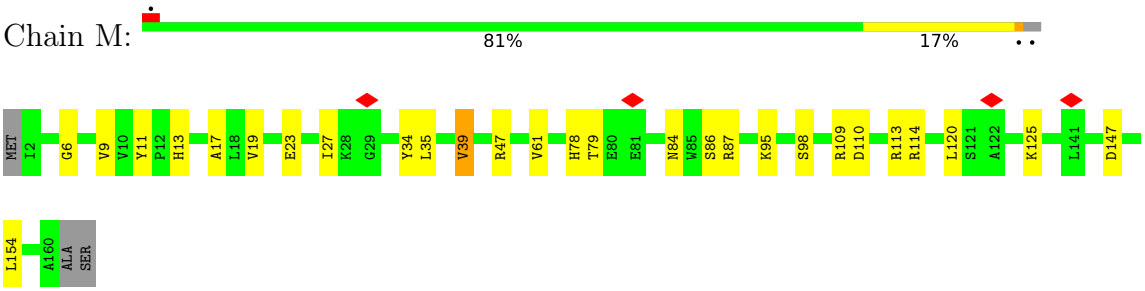
• Molecule 6: RNA polymerase-binding protein RbpA

Chain J:



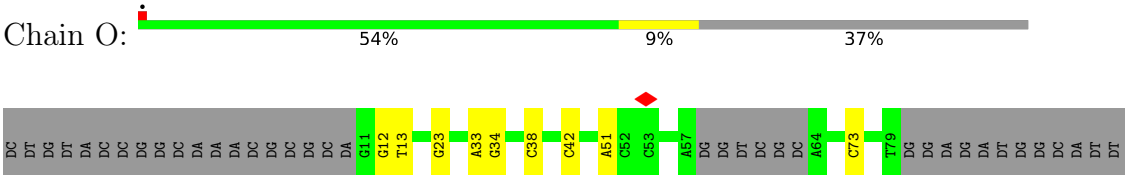
• Molecule 7: RNA polymerase-binding transcription factor CarD

Chain M:



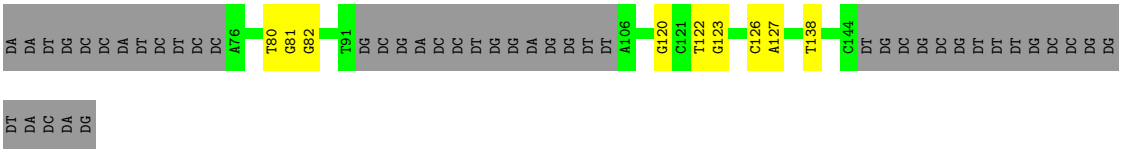
• Molecule 8: DNA (63-MER)

Chain O:

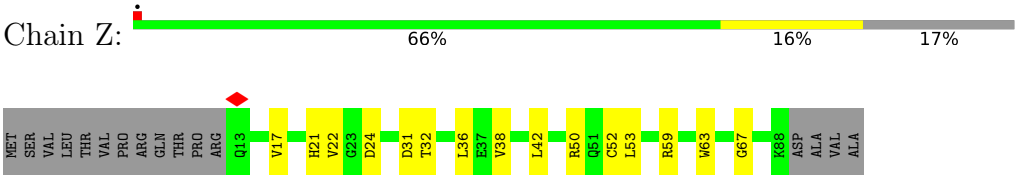


• Molecule 9: DNA (55-MER)

Chain P:



• Molecule 10: Probable transcriptional regulator WhiB7



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87743	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 ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	44.350	Depositor
Minimum map value	-19.151	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.008	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SF4, 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	0.44	0/1742	0.53	0/2370
1	B	0.40	0/1792	0.57	1/2442 (0.0%)
2	C	0.47	0/8765	0.54	0/11885
3	D	0.45	1/10078 (0.0%)	0.55	2/13624 (0.0%)
4	E	0.43	0/662	0.55	0/901
5	F	0.33	0/2579	0.48	0/3477
6	J	0.32	0/896	0.51	0/1210
7	M	0.29	0/1257	0.55	0/1700
8	O	0.71	0/1434	1.07	2/2208 (0.1%)
9	P	0.72	0/1267	1.01	2/1950 (0.1%)
10	Z	0.36	0/598	0.57	0/815
All	All	0.46	1/31070 (0.0%)	0.61	7/42582 (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
3	D	0	1
5	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	78	CYS	CB-SG	-7.75	1.69	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	579	LEU	CA-CB-CG	6.88	131.12	115.30
8	O	38	DC	O4'-C1'-N1	5.59	111.91	108.00
9	P	138	DT	O4'-C1'-N1	5.55	111.88	108.00
1	B	78	LEU	CA-CB-CG	5.25	127.38	115.30
3	D	460	LEU	CA-CB-CG	5.18	127.21	115.30
9	P	120	DG	O4'-C1'-N9	5.07	111.55	108.00
8	O	42	DC	P-O3'-C3'	5.04	125.75	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	579	LEU	Mainchain
5	F	273	LEU	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	1716	0	1756	17	0
1	B	1765	0	1794	17	0
2	C	8606	0	8544	88	0
3	D	9914	0	9986	69	0
4	E	649	0	645	7	0
5	F	2548	0	2569	27	0
6	J	880	0	852	13	0
7	M	1241	0	1259	14	0
8	O	1282	0	712	6	0
9	P	1129	0	616	6	0
10	Z	581	0	574	7	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
13	Z	8	0	0	3	0
All	All	30322	0	29307	247	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 (247) 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)
3:D:60:CYS:SG	3:D:61:TYR:N	2.65	0.70
3:D:147:GLU:O	3:D:151:LEU:HB2	1.94	0.68
3:D:181:LEU:O	3:D:185:GLU:HB2	1.93	0.68
6:J:28:GLN:HE22	6:J:50:ILE:HD11	1.59	0.67
2:C:75:ALA:HA	2:C:79:ASP:HB3	1.78	0.64
5:F:274:PRO:HB2	5:F:277:GLN:HB2	1.83	0.61
5:F:432:ASP:OD1	5:F:432:ASP:N	2.35	0.60
2:C:563:ARG:HB2	2:C:567:GLU:HG3	1.83	0.60
2:C:1057:LEU:HD23	2:C:1062:GLN:HG2	1.82	0.60
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.67	0.59
2:C:453:ARG:NH2	2:C:501:SER:O	2.35	0.59
3:D:181:LEU:HA	3:D:198:ARG:HH21	1.67	0.59
6:J:20:ARG:NH1	6:J:23:ASP:O	2.35	0.59
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.85	0.58
5:F:209:SER:O	5:F:213:ARG:HB2	2.04	0.58
6:J:31:ARG:HG2	6:J:41:GLU:HG2	1.85	0.57
3:D:952:LEU:HD22	3:D:957:ILE:HD11	1.85	0.57
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.38	0.57
2:C:532:THR:OG1	2:C:533:ALA:N	2.37	0.57
1:A:53:SER:OG	1:A:161:ARG:NH2	2.38	0.57
2:C:173:ARG:NH1	2:C:437:SER:O	2.38	0.57
3:D:56:ARG:HB2	3:D:59:GLU:HB3	1.87	0.57
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.70	0.56
5:F:504:ARG:NH2	9:P:127:DA:OP2	2.39	0.56
3:D:39:LEU:HB3	6:J:11:LEU:HD13	1.87	0.56
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.36	0.56
9:P:126:DC:H2"	9:P:127:DA:H2'	1.87	0.56
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.39	0.56
2:C:1119:GLU:OE2	3:D:89:ARG:NH1	2.39	0.56
3:D:75:CYS:HB3	3:D:78:CYS:SG	2.46	0.55
2:C:995:ASN:N	2:C:995:ASN:OD1	2.39	0.55
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.38	0.55
1:A:223:ARG:HH21	1:B:213:LYS:HB2	1.69	0.55
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.39	0.55
5:F:295:LEU:O	5:F:299:ASN:ND2	2.39	0.55
5:F:518:SER:HA	10:Z:21:HIS:HB3	1.89	0.55
1:A:139:VAL:HG21	1:A:161:ARG:HH22	1.71	0.55
2:C:380:THR:OG1	2:C:381:VAL:N	2.36	0.55
1:A:75:GLU:OE2	2:C:620:ARG:NH1	2.40	0.55
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.40	0.55
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:109:ARG:NH1	7:M:110:ASP:OD1	2.40	0.55
3:D:931:ASP:OD1	3:D:931:ASP:N	2.39	0.54
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.40	0.54
3:D:1025:THR:HG21	3:D:1029:PRO:HB2	1.90	0.54
2:C:222:VAL:HG22	2:C:261:THR:HG21	1.90	0.54
3:D:143:MET:SD	3:D:143:MET:N	2.81	0.54
3:D:1054:ARG:NH2	3:D:1101:ASP:OD1	2.41	0.54
1:A:206:ASP:OD1	1:B:226:ASN:ND2	2.41	0.54
3:D:1089:PHE:O	3:D:1097:ARG:N	2.41	0.54
2:C:588:SER:OG	2:C:589:VAL:N	2.40	0.53
5:F:502:ARG:HD3	8:O:23:DG:H2'	1.89	0.53
2:C:221:THR:OG1	2:C:231:ARG:NH2	2.42	0.53
1:B:97:LEU:HB3	1:B:110:ILE:HG22	1.90	0.53
3:D:194:ARG:O	3:D:198:ARG:NH1	2.42	0.53
2:C:455:LEU:HD21	2:C:500:LEU:HG	1.90	0.53
5:F:235:ILE:O	5:F:301:ARG:NH1	2.42	0.53
2:C:654:SER:OG	2:C:655:ALA:N	2.42	0.52
2:C:721:VAL:HG23	2:C:915:ILE:HG13	1.91	0.52
2:C:891:ASN:OD1	2:C:891:ASN:N	2.43	0.52
5:F:277:GLN:OE1	6:J:106:ARG:NH1	2.42	0.52
2:C:762:THR:OG1	2:C:763:LYS:N	2.42	0.52
3:D:334:ARG:NH1	5:F:419:GLU:O	2.43	0.52
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.35	0.52
3:D:160:LYS:NZ	3:D:164:ASP:OD1	2.43	0.52
3:D:1090:LYS:HD3	3:D:1097:ARG:HE	1.74	0.51
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.91	0.51
3:D:926:GLY:O	3:D:940:ARG:NH2	2.42	0.51
2:C:737:LEU:HD23	2:C:915:ILE:HG22	1.92	0.51
3:D:83:THR:OG1	3:D:84:ARG:N	2.43	0.51
3:D:1180:LEU:HD22	3:D:1206:VAL:HG11	1.93	0.51
5:F:483:ASP:N	5:F:483:ASP:OD1	2.44	0.51
2:C:444:ASN:N	2:C:444:ASN:OD1	2.43	0.51
7:M:87:ARG:NH2	8:O:51:DA:OP2	2.43	0.51
2:C:719:LEU:HD12	2:C:1030:ILE:HD11	1.92	0.51
2:C:487:GLU:OE2	2:C:613:ARG:NH1	2.42	0.51
2:C:1042:HIS:HB3	2:C:1060:LYS:HG3	1.92	0.51
1:A:94:THR:HG22	1:A:139:VAL:HG22	1.93	0.51
3:D:922:ALA:HB1	3:D:981:ARG:HG2	1.93	0.51
5:F:524:ARG:O	5:F:524:ARG:NH2	2.43	0.51
3:D:138:SER:HG	3:D:253:THR:HG1	1.56	0.50
7:M:78:HIS:O	7:M:109:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:278:ARG:HA	3:D:281:ILE:HG12	1.92	0.50
10:Z:31:ASP:OD1	10:Z:31:ASP:N	2.43	0.50
2:C:304:LYS:HD3	2:C:305:ARG:HG2	1.92	0.50
4:E:48:SER:OG	4:E:49:SER:N	2.45	0.50
2:C:46:GLU:OE2	2:C:584:ARG:NH2	2.45	0.50
2:C:822:ARG:NH1	2:C:828:LYS:O	2.45	0.50
2:C:577:ASP:OD1	2:C:577:ASP:N	2.45	0.50
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	1.94	0.50
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.94	0.50
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.45	0.49
7:M:147:ASP:OD1	7:M:147:ASP:N	2.45	0.49
1:B:25:PRO:HB2	1:B:189:PHE:HD2	1.77	0.49
2:C:659:THR:O	2:C:659:THR:OG1	2.30	0.49
2:C:120:ASP:OD1	2:C:120:ASP:N	2.44	0.49
2:C:947:ASP:OD1	2:C:947:ASP:N	2.43	0.49
3:D:946:ASP:OD1	3:D:946:ASP:N	2.32	0.49
3:D:143:MET:O	3:D:147:GLU:HB2	2.13	0.49
10:Z:52:CYS:HB3	13:Z:101:SF4:S4	2.53	0.49
2:C:182:SER:OG	2:C:315:LYS:NZ	2.46	0.49
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.95	0.49
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.95	0.48
2:C:758:ASP:HB3	2:C:868:LEU:HD12	1.94	0.48
4:E:60:ARG:NH2	4:E:98:GLU:OE2	2.46	0.48
3:D:49:GLU:OE2	3:D:55:THR:OG1	2.31	0.48
5:F:266:LEU:HD13	5:F:272:LYS:HE3	1.96	0.48
7:M:23:GLU:N	7:M:34:TYR:O	2.46	0.48
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.46	0.48
2:C:1138:LEU:HB2	3:D:9:GLU:HB2	1.95	0.48
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.95	0.48
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.37	0.48
3:D:975:CYS:SG	3:D:978:CYS:HB2	2.54	0.48
1:A:155:SER:OG	1:A:156:GLY:N	2.45	0.48
2:C:178:GLN:OE1	2:C:379:ARG:NH2	2.47	0.48
2:C:410:GLU:O	7:M:13:HIS:NE2	2.47	0.48
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.46	0.48
1:A:104:GLU:OE2	1:A:124:HIS:ND1	2.44	0.47
1:B:124:HIS:NE2	1:B:126:ALA:O	2.47	0.47
7:M:79:THR:OG1	7:M:113:ARG:NH1	2.47	0.47
3:D:342:ASP:N	3:D:342:ASP:OD1	2.47	0.47
3:D:1120:GLU:OE2	3:D:1123:ARG:NH2	2.39	0.47
1:A:57:ASP:OD1	1:A:57:ASP:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASP:OD1	2:C:881:ASP:N	2.43	0.47
2:C:835:THR:O	2:C:835:THR:OG1	2.32	0.47
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.97	0.47
2:C:518:LYS:O	2:C:525:SER:OG	2.30	0.47
3:D:939:GLU:OE2	3:D:942:GLN:NE2	2.48	0.47
6:J:25:ALA:O	6:J:27:ARG:NH2	2.47	0.47
2:C:974:THR:O	2:C:974:THR:OG1	2.33	0.46
7:M:114:ARG:HB3	7:M:120:LEU:HD11	1.97	0.46
1:A:130:ASP:OD1	1:A:130:ASP:N	2.48	0.46
5:F:238:VAL:O	5:F:301:ARG:NH2	2.46	0.46
1:B:22:VAL:HG12	1:B:193:ILE:HG23	1.98	0.46
5:F:310:TYR:HB3	5:F:359:MET:HE1	1.98	0.46
1:B:198:THR:OG1	1:B:199:LYS:O	2.27	0.46
3:D:1227:GLN:HG2	3:D:1228:GLU:HG3	1.97	0.46
3:D:605:ASP:OD1	3:D:605:ASP:N	2.49	0.46
1:B:99:LYS:NZ	1:B:104:GLU:O	2.43	0.46
5:F:256:GLY:HA2	5:F:284:ILE:HG22	1.96	0.46
2:C:274:LEU:HD11	2:C:293:GLN:HA	1.98	0.45
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.48	0.45
5:F:502:ARG:NE	8:O:23:DG:OP2	2.38	0.45
5:F:415:GLN:OE1	5:F:418:ARG:NH1	2.44	0.45
6:J:68:ASP:OD1	6:J:68:ASP:N	2.50	0.45
1:A:64:THR:OG1	1:A:65:THR:N	2.49	0.45
2:C:821:LEU:HD23	5:F:527:LEU:HB2	1.98	0.45
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.42	0.45
1:B:165:ASP:OD1	1:B:165:ASP:N	2.49	0.45
2:C:98:ASP:OD1	2:C:98:ASP:N	2.47	0.45
2:C:1102:VAL:HG23	2:C:1112:ILE:HG23	1.97	0.45
10:Z:52:CYS:CB	13:Z:101:SF4:S4	3.05	0.45
5:F:214:GLN:HA	5:F:217:LYS:HZ3	1.82	0.45
2:C:373:PHE:HE2	2:C:512:ILE:HD12	1.81	0.45
3:D:57:ASP:HB2	6:J:15:SER:H	1.81	0.45
1:A:93:VAL:HG21	1:A:116:VAL:HG11	1.99	0.45
2:C:775:ASN:N	2:C:775:ASN:OD1	2.50	0.45
3:D:328:VAL:HG13	3:D:336:ALA:HB3	1.99	0.45
10:Z:67:GLY:N	13:Z:101:SF4:S2	2.86	0.45
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.99	0.44
2:C:354:THR:OG1	2:C:362:GLU:OE1	2.31	0.44
3:D:21:ARG:NH2	3:D:96:GLU:OE2	2.46	0.44
1:B:129:ASN:N	1:B:129:ASN:OD1	2.51	0.44
3:D:910:LEU:HD13	3:D:910:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.99	0.44
2:C:924:ARG:HD3	3:D:808:THR:HB	1.99	0.44
3:D:1044:ALA:HB3	3:D:1110:GLN:HE21	1.81	0.44
9:P:80:DT:H2"	9:P:81:DG:H5"	1.98	0.44
2:C:224:VAL:HB	2:C:234:VAL:HG22	2.00	0.44
2:C:664:ASN:OD1	2:C:664:ASN:N	2.51	0.44
1:B:80:LEU:HD22	1:B:138:LEU:HD21	2.00	0.44
2:C:403:ARG:NH1	2:C:416:THR:O	2.45	0.44
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.99	0.44
6:J:58:ASN:HB2	6:J:60:MET:HG2	1.99	0.44
2:C:547:PRO:HB2	2:C:555:VAL:HB	2.00	0.43
1:A:90:ASP:OD1	1:A:90:ASP:N	2.36	0.43
1:B:177:LYS:HE3	1:B:177:LYS:HB2	1.87	0.43
2:C:985:LEU:HD23	2:C:985:LEU:HA	1.85	0.43
3:D:193:ALA:HA	3:D:196:LYS:HG2	2.00	0.43
3:D:208:ILE:HG12	3:D:211:ARG:HH22	1.82	0.43
9:P:81:DG:H2'	9:P:82:DG:C8	2.54	0.43
2:C:651:GLU:OE1	2:C:667:ARG:NH1	2.51	0.43
3:D:836:VAL:HG13	3:D:848:GLU:HB3	2.01	0.43
7:M:95:LYS:O	7:M:98:SER:OG	2.36	0.43
2:C:238:LEU:HD13	2:C:238:LEU:HA	1.91	0.43
3:D:369:ASN:OD1	5:F:322:GLN:NE2	2.51	0.43
1:A:72:ASP:OD1	1:A:72:ASP:N	2.46	0.42
2:C:421:ARG:NH2	5:F:383:GLN:OE1	2.52	0.42
2:C:736:ILE:HG13	2:C:916:ILE:HB	2.01	0.42
2:C:897:LYS:HE2	2:C:897:LYS:HB2	1.94	0.42
2:C:1052:ILE:O	3:D:89:ARG:NH2	2.53	0.42
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.91	0.42
5:F:517:PRO:HA	5:F:520:SER:HB3	2.00	0.42
3:D:834:ARG:HD2	3:D:834:ARG:HA	1.87	0.42
7:M:125:LYS:HE2	7:M:125:LYS:HB3	1.90	0.42
2:C:62:GLU:HG3	2:C:70:TRP:HB2	2.01	0.42
2:C:179:LEU:HD11	2:C:483:MET:HE3	2.00	0.42
1:B:59:VAL:HG21	1:B:66:VAL:HG22	2.02	0.42
2:C:774:PRO:HD2	2:C:834:ASP:HB2	2.02	0.42
3:D:970:THR:OG1	3:D:973:GLY:O	2.37	0.42
3:D:1051:GLY:O	3:D:1104:HIS:ND1	2.52	0.42
8:O:73:DC:N4	9:P:81:DG:O6	2.53	0.42
3:D:923:ARG:HD3	3:D:962:VAL:HG11	2.01	0.42
6:J:110:ARG:HD3	6:J:110:ARG:HA	1.91	0.42
2:C:544:ALA:HB2	2:C:580:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:270:ILE:H	3:D:270:ILE:HG12	1.60	0.41
3:D:810:ASN:OD1	3:D:810:ASN:N	2.53	0.41
2:C:369:ASP:O	2:C:375:ASN:ND2	2.44	0.41
2:C:903:ASP:OD1	2:C:903:ASP:N	2.48	0.41
8:O:12:DG:H2"	8:O:13:DT:H71	2.02	0.41
4:E:60:ARG:HH22	4:E:80:GLY:HA3	1.86	0.41
2:C:86:LEU:HD21	2:C:389:ILE:HD13	2.01	0.41
6:J:35:ASP:OD1	6:J:35:ASP:N	2.40	0.41
7:M:84:ASN:OD1	7:M:86:SER:OG	2.32	0.41
2:C:963:LEU:HD23	2:C:963:LEU:HA	1.90	0.41
3:D:599:TYR:HA	3:D:610:GLY:HA3	2.02	0.41
5:F:501:GLU:HA	5:F:504:ARG:HG2	2.03	0.41
2:C:79:ASP:OD1	2:C:79:ASP:N	2.54	0.41
6:J:23:ASP:OD2	6:J:23:ASP:N	2.52	0.41
5:F:372:MET:HA	5:F:375:VAL:HG22	2.03	0.41
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.86	0.41
2:C:789:ILE:HG23	2:C:803:VAL:HG22	2.03	0.41
3:D:203:ARG:HA	3:D:203:ARG:HD2	1.90	0.41
3:D:498:LEU:HG	3:D:543:VAL:HG22	2.03	0.41
8:O:33:DA:H2"	8:O:34:DG:H8	1.85	0.41
1:A:95:MET:HB3	1:A:113:PRO:HD3	2.03	0.41
2:C:34:GLY:HA3	2:C:700:GLN:HG3	2.03	0.41
2:C:152:VAL:HG21	2:C:418:ILE:HD12	2.04	0.41
2:C:715:LEU:N	2:C:1029:TYR:OH	2.54	0.40
4:E:36:THR:O	4:E:36:THR:OG1	2.35	0.40
4:E:68:TYR:HD1	4:E:68:TYR:HA	1.79	0.40
2:C:192:ASP:HB2	2:C:199:LEU:HD11	2.03	0.40
3:D:964:SER:OG	3:D:965:VAL:N	2.53	0.40
1:B:183:VAL:HG12	1:B:188:ASP:HA	2.04	0.40
3:D:28:VAL:HG21	3:D:46:LEU:HD23	2.03	0.40
2:C:297:GLU:HA	2:C:301:PHE:HD2	1.86	0.40
2:C:789:ILE:H	2:C:789:ILE:HG13	1.41	0.40
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.93	0.40
3:D:1103:ASP:OD1	3:D:1104:HIS:N	2.54	0.40
7:M:6:GLY:H	7:M:19:VAL:HG23	1.87	0.40
7:M:23:GLU:OE1	7:M:47:ARG:NH1	2.48	0.40
10:Z:38:VAL:O	10:Z:42:LEU:HB2	2.22	0.40
10:Z:50:ARG:HD3	10:Z:50:ARG:HA	1.90	0.40
2:C:113:ASP:HB2	2:C:132:PRO:HD2	2.04	0.40
3:D:192:ASP:O	3:D:196:LYS:N	2.55	0.40
7:M:17:ALA:HB2	7:M:39:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:122:DT:H2'	9:P:123:DG:C8	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	223/347 (64%)	204 (92%)	19 (8%)	0	100	100
1	B	235/347 (68%)	211 (90%)	24 (10%)	0	100	100
2	C	1109/1172 (95%)	1023 (92%)	86 (8%)	0	100	100
3	D	1264/1318 (96%)	1192 (94%)	72 (6%)	0	100	100
4	E	81/110 (74%)	77 (95%)	4 (5%)	0	100	100
5	F	320/528 (61%)	304 (95%)	16 (5%)	0	100	100
6	J	107/111 (96%)	97 (91%)	10 (9%)	0	100	100
7	M	157/162 (97%)	146 (93%)	11 (7%)	0	100	100
10	Z	74/92 (80%)	64 (86%)	10 (14%)	0	100	100
All	All	3570/4187 (85%)	3318 (93%)	252 (7%)	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	194/297 (65%)	176 (91%)	18 (9%)	9 25
1	B	195/297 (66%)	181 (93%)	14 (7%)	14 37
2	C	937/993 (94%)	875 (93%)	62 (7%)	16 42
3	D	1048/1095 (96%)	1006 (96%)	42 (4%)	31 62
4	E	69/90 (77%)	62 (90%)	7 (10%)	7 22
5	F	268/427 (63%)	256 (96%)	12 (4%)	27 58
6	J	92/97 (95%)	87 (95%)	5 (5%)	22 51
7	M	129/131 (98%)	122 (95%)	7 (5%)	22 51
10	Z	60/76 (79%)	52 (87%)	8 (13%)	4 11
All	All	2992/3503 (85%)	2817 (94%)	175 (6%)	24 48

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	22	VAL
1	A	30	PHE
1	A	51	VAL
1	A	56	ILE
1	A	65	THR
1	A	84	VAL
1	A	111	VAL
1	A	116	VAL
1	A	123	MET
1	A	127	THR
1	A	130	ASP
1	A	136	VAL
1	A	150	VAL
1	A	167	ILE
1	A	215	LEU
1	A	217	GLU
1	A	221	LEU
1	B	33	THR
1	B	56	ILE
1	B	74	THR
1	B	78	LEU
1	B	84	VAL
1	B	111	VAL
1	B	125	ILE
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	147	VAL
1	B	150	VAL
1	B	162	ILE
1	B	165	ASP
1	B	175	THR
1	B	198	THR
2	C	56	VAL
2	C	64	LEU
2	C	83	VAL
2	C	90	LEU
2	C	124	ASP
2	C	147	ILE
2	C	185	VAL
2	C	189	GLU
2	C	204	VAL
2	C	212	LEU
2	C	222	VAL
2	C	226	ILE
2	C	231	ARG
2	C	238	LEU
2	C	274	LEU
2	C	275	LEU
2	C	296	LEU
2	C	308	LEU
2	C	311	VAL
2	C	346	VAL
2	C	355	MET
2	C	373	PHE
2	C	380	THR
2	C	397	GLU
2	C	399	VAL
2	C	409	VAL
2	C	439	PHE
2	C	450	THR
2	C	463	LEU
2	C	470	LEU
2	C	472	VAL
2	C	483	MET
2	C	507	ASN
2	C	519	VAL
2	C	532	THR
2	C	540	VAL

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Mol	Chain	Res	Type
2	C	570	TYR
2	C	581	VAL
2	C	584	ARG
2	C	591	THR
2	C	603	ASN
2	C	626	VAL
2	C	640	ASP
2	C	649	VAL
2	C	659	THR
2	C	736	ILE
2	C	806	VAL
2	C	820	LEU
2	C	834	ASP
2	C	839	VAL
2	C	852	VAL
2	C	860	GLU
2	C	869	VAL
2	C	897	LYS
2	C	904	MET
2	C	909	ASP
2	C	974	THR
2	C	989	LEU
2	C	993	LEU
2	C	997	ASP
2	C	999	ASP
2	C	1137	VAL
3	D	28	VAL
3	D	55	THR
3	D	75	CYS
3	D	82	VAL
3	D	89	ARG
3	D	107	PHE
3	D	110	VAL
3	D	135	VAL
3	D	236	VAL
3	D	285	LYS
3	D	328	VAL
3	D	359	ASP
3	D	428	SER
3	D	429	VAL
3	D	505	HIS
3	D	578	ARG

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Mol	Chain	Res	Type
3	D	581	MET
3	D	596	THR
3	D	653	HIS
3	D	679	LEU
3	D	795	ASP
3	D	800	ILE
3	D	824	VAL
3	D	825	THR
3	D	867	THR
3	D	890	ASP
3	D	900	GLU
3	D	923	ARG
3	D	930	VAL
3	D	946	ASP
3	D	953	LEU
3	D	962	VAL
3	D	963	ARG
3	D	977	THR
3	D	981	ARG
3	D	1025	THR
3	D	1039	VAL
3	D	1080	ILE
3	D	1111	LEU
3	D	1166	THR
3	D	1173	THR
3	D	1248	LEU
4	E	31	THR
4	E	33	LEU
4	E	48	SER
4	E	49	SER
4	E	56	TYR
4	E	79	VAL
4	E	106	HIS
5	F	265	GLU
5	F	269	ARG
5	F	287	ASP
5	F	366	ILE
5	F	370	VAL
5	F	386	LEU
5	F	429	ASP
5	F	432	ASP
5	F	446	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	488	THR
5	F	489	LEU
5	F	505	GLN
6	J	14	VAL
6	J	64	LEU
6	J	69	LEU
6	J	99	LYS
6	J	104	LEU
7	M	9	VAL
7	M	11	TYR
7	M	27	ILE
7	M	35	LEU
7	M	39	VAL
7	M	61	VAL
7	M	154	LEU
10	Z	17	VAL
10	Z	22	VAL
10	Z	24	ASP
10	Z	32	THR
10	Z	36	LEU
10	Z	53	LEU
10	Z	59	ARG
10	Z	63	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	369	ASN
5	F	322	GLN
6	J	28	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	SF4	Z	101	10	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	Z	101	10	-	-	0/6/5/5

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.

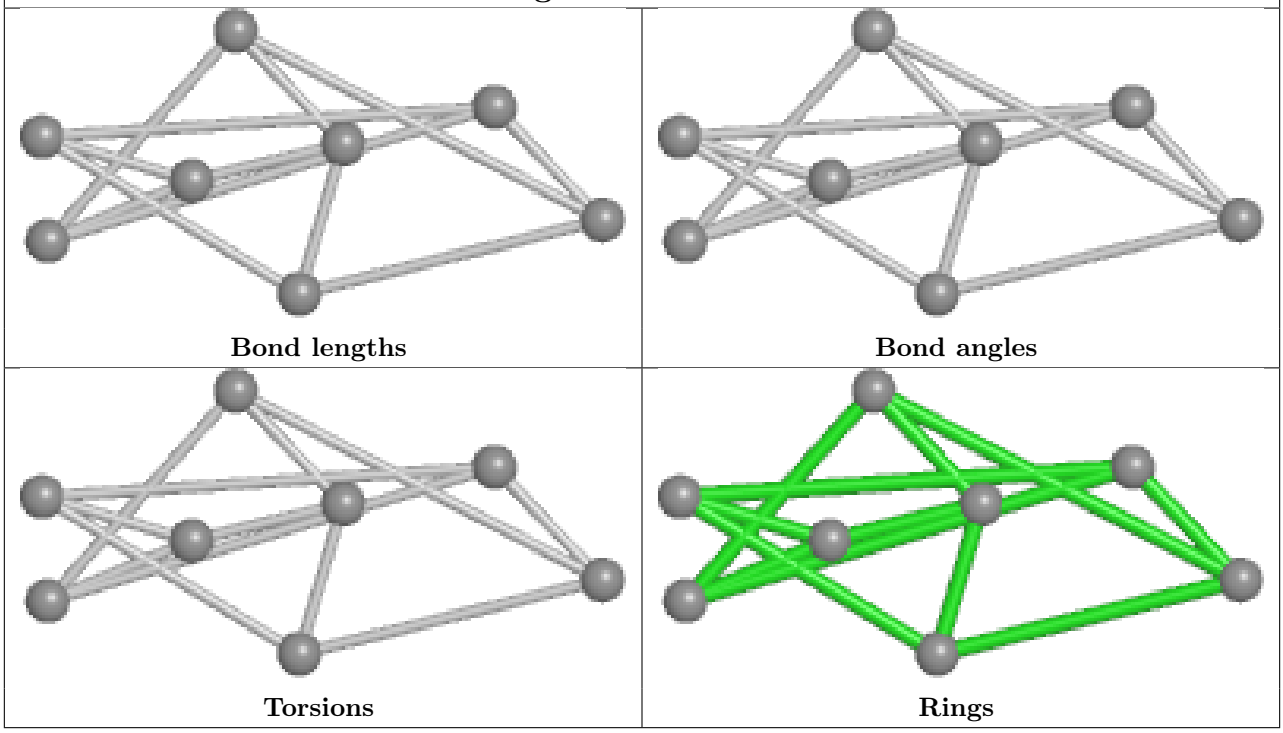
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	101	SF4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SF4 Z 101



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.

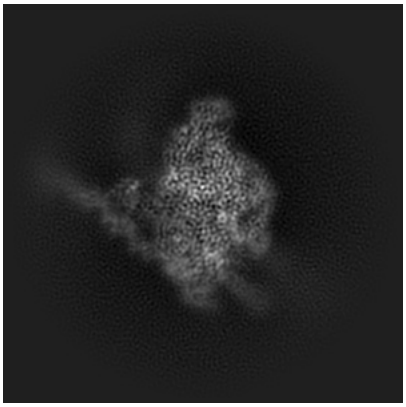
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22886. These allow visual inspection of the internal detail of the map and identification of artifacts.

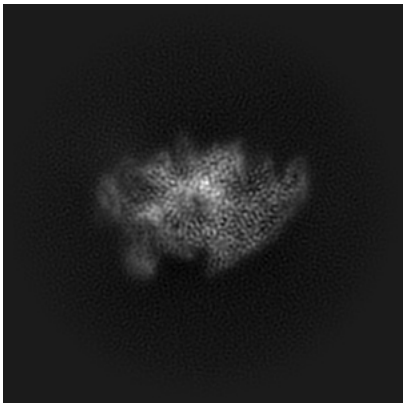
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

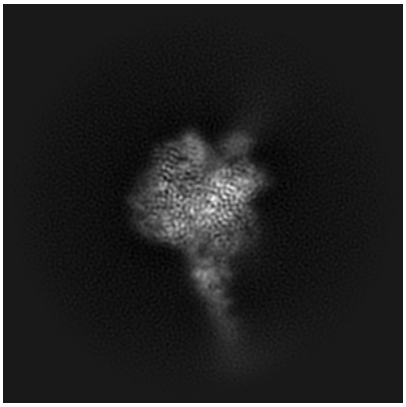
6.1.1 Primary map



X



Y

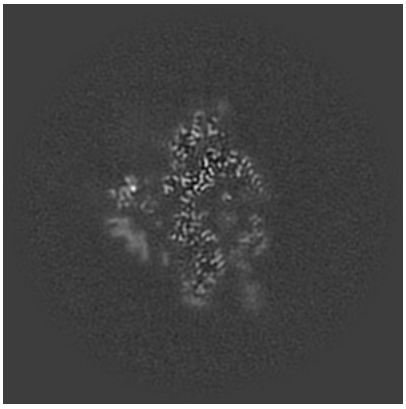


Z

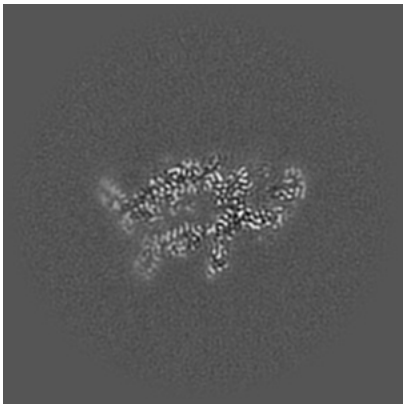
The images above show the map projected in three orthogonal directions.

6.2 Central slices

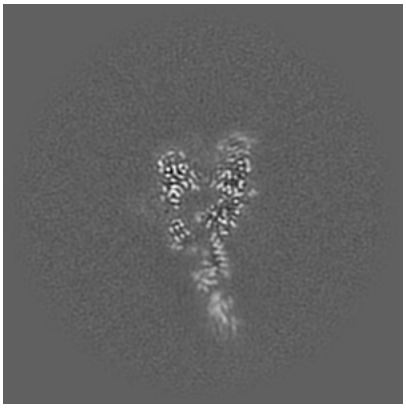
6.2.1 Primary map



X Index: 150



Y Index: 150

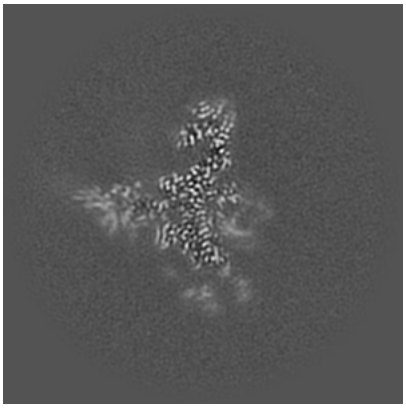


Z Index: 150

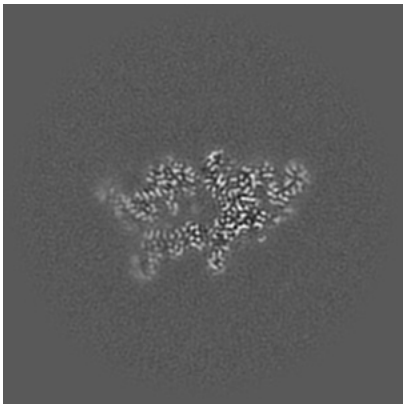
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

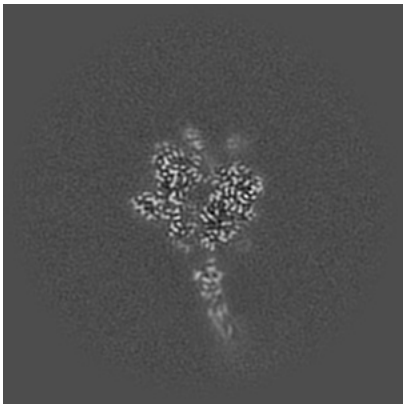
6.3.1 Primary map



X Index: 160



Y Index: 154



Z Index: 158

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

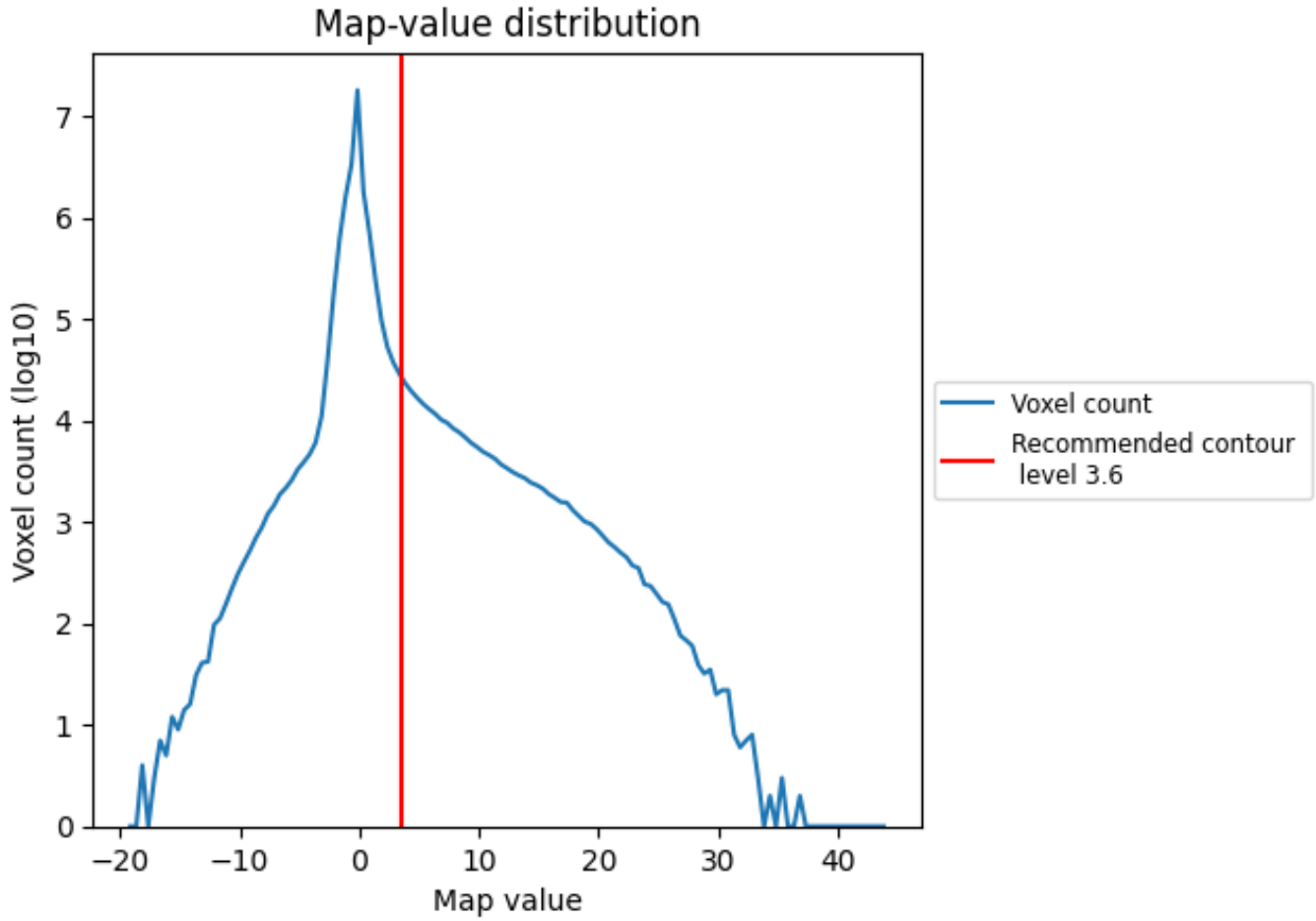
6.5 Mask visualisation (i)

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

7 Map analysis

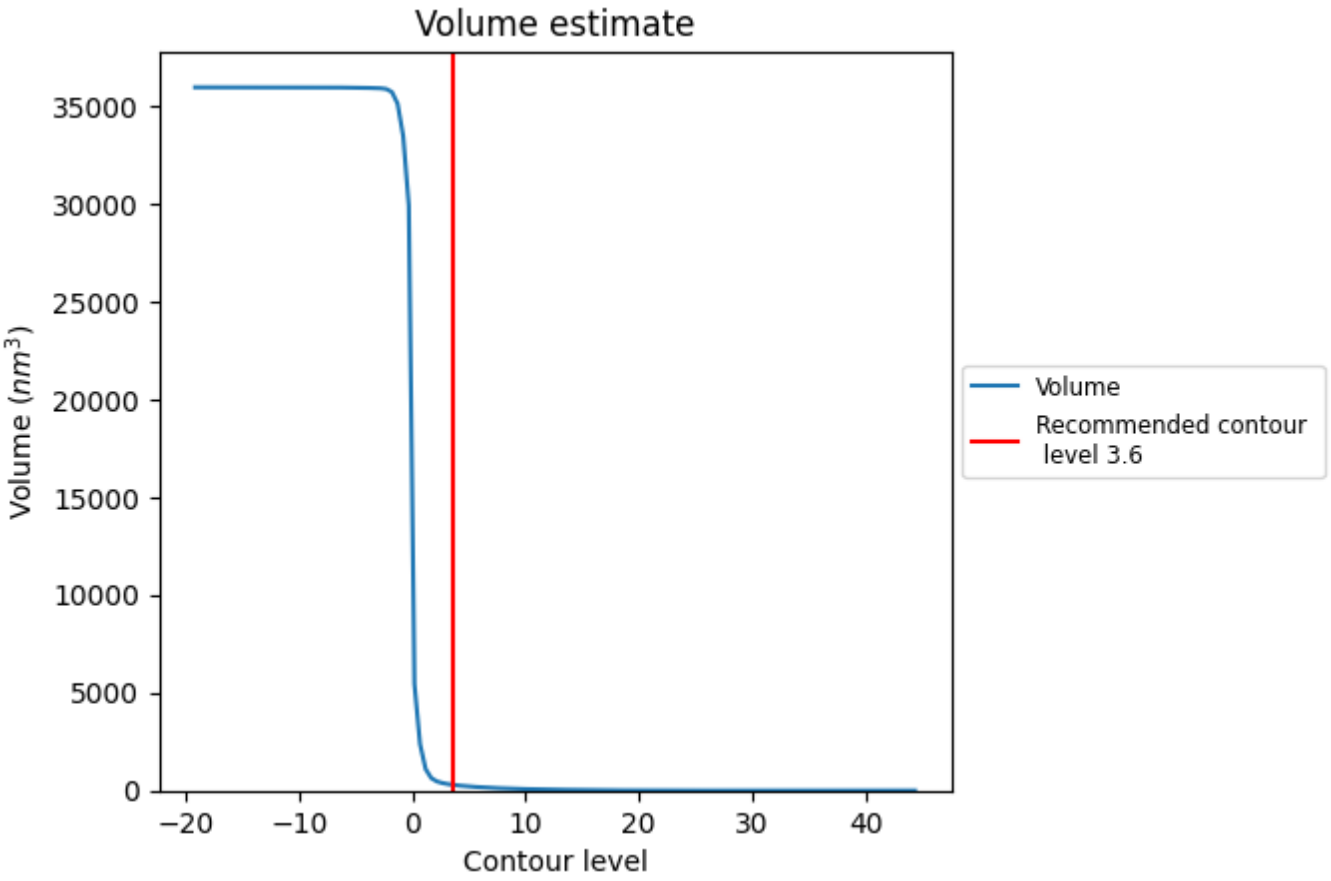
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

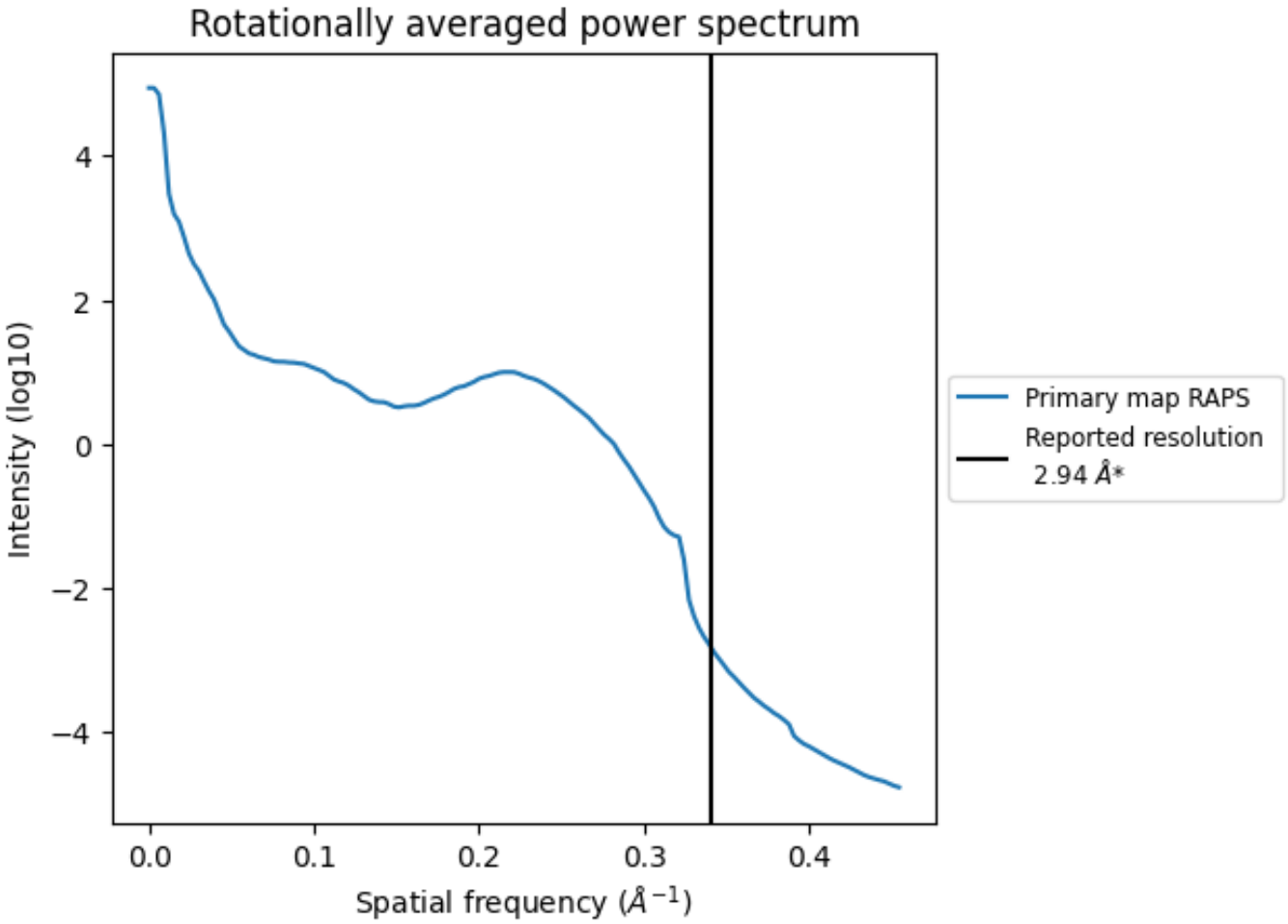
7.2 Volume estimate



The volume at the recommended contour level is 292 nm^3; this corresponds to an approximate mass of 264 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 0.340 Å^{-1}

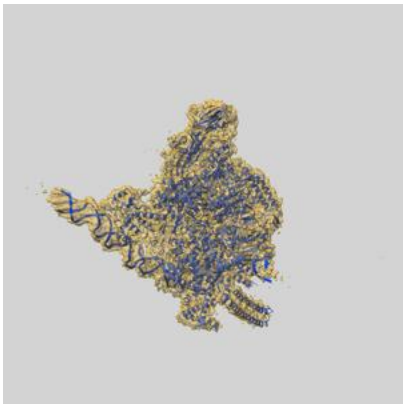
8 Fourier-Shell correlation

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

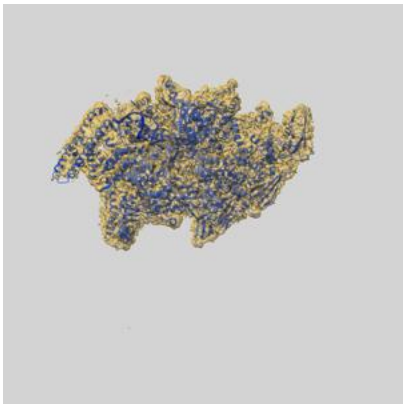
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22886 and PDB model 7KIF. Per-residue inclusion information can be found in section 3 on page 7.

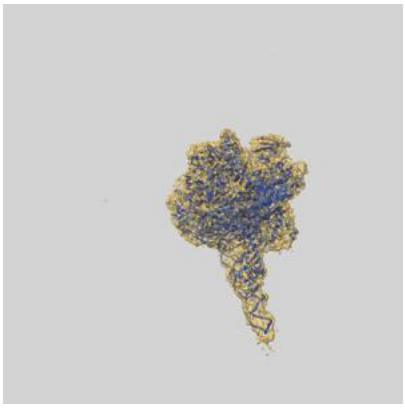
9.1 Map-model overlay



X



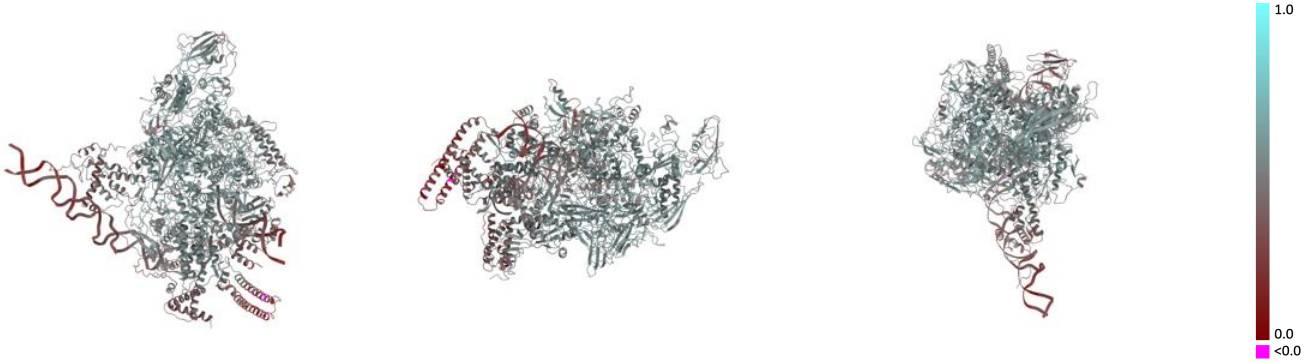
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6 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.

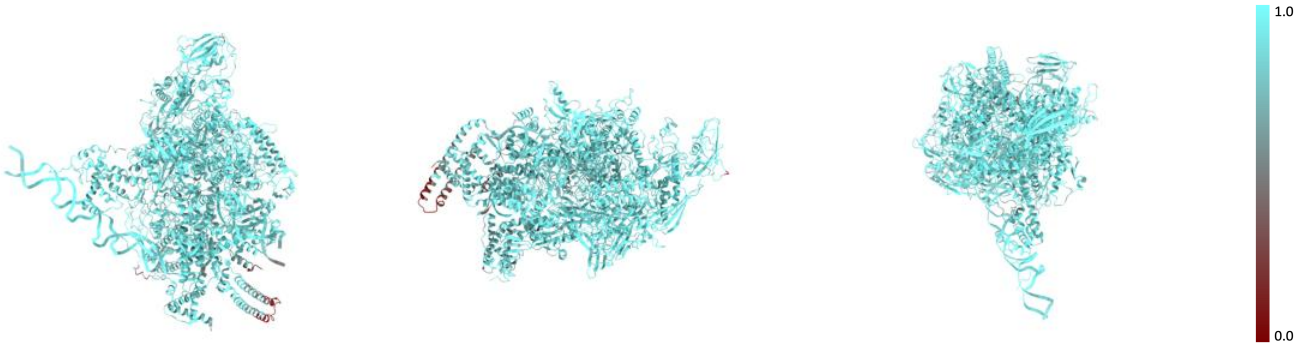
9.2 Q-score mapped to coordinate model (i)



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.

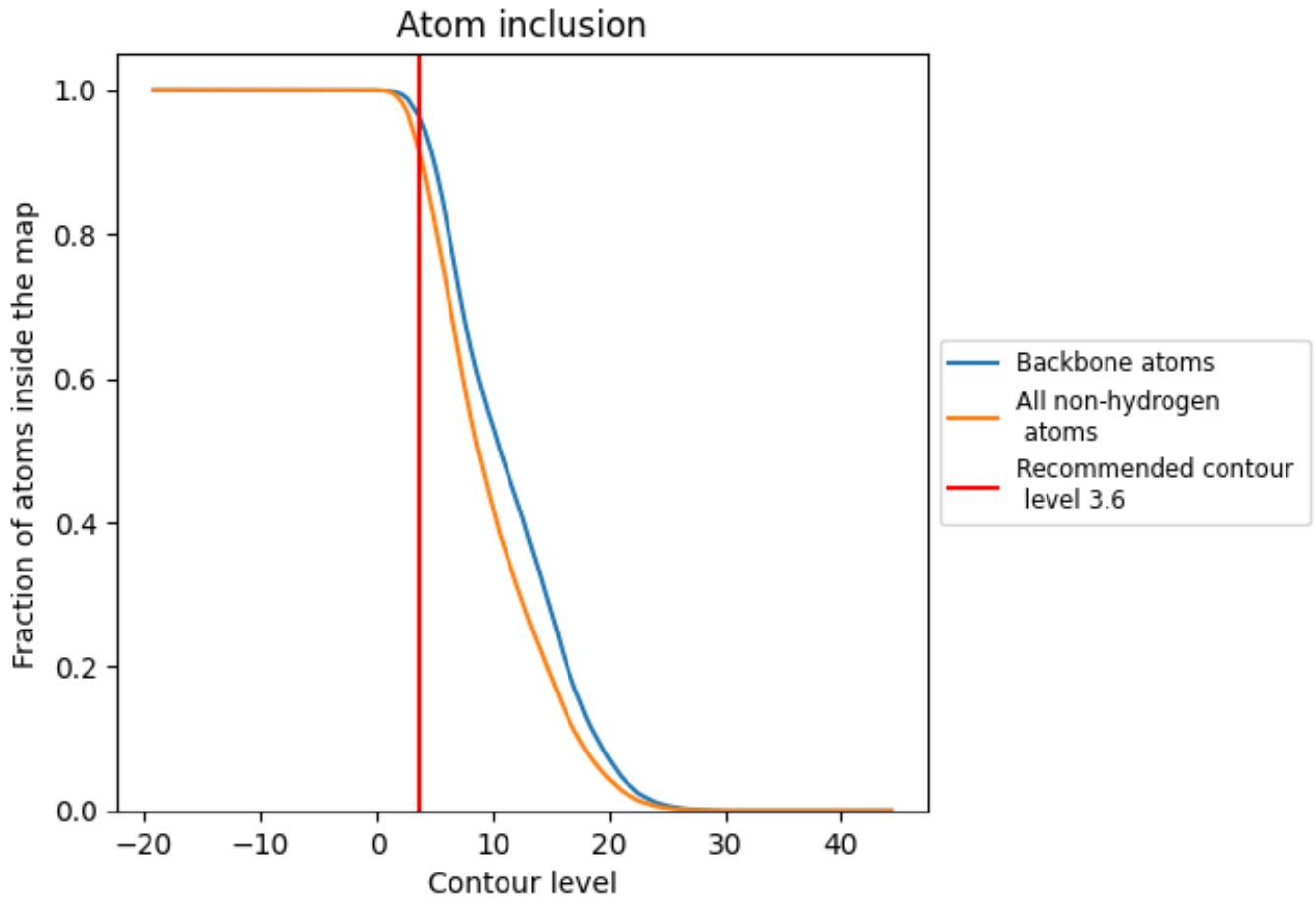
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.6).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.4900
A	0.9507	0.5400
B	0.9309	0.5090
C	0.9392	0.5300
D	0.9221	0.5140
E	0.9323	0.5270
F	0.8865	0.4560
J	0.8582	0.4450
M	0.8307	0.3790
O	0.9119	0.3370
P	0.9291	0.3080
Z	0.9441	0.4060