



Full wwPDB EM Validation Report ⓘ

Jul 21, 2024 – 08:54 PM EDT

PDB ID : 9BCU
EMDB ID : EMD-44439
Title : Cryo-EM structure of Thermococcus kodakarensis FttA-dependent transcription pre-termination complex containing 52 nt RNA
Authors : You, L.; Ebright, R.H.
Deposited on : 2024-04-09
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

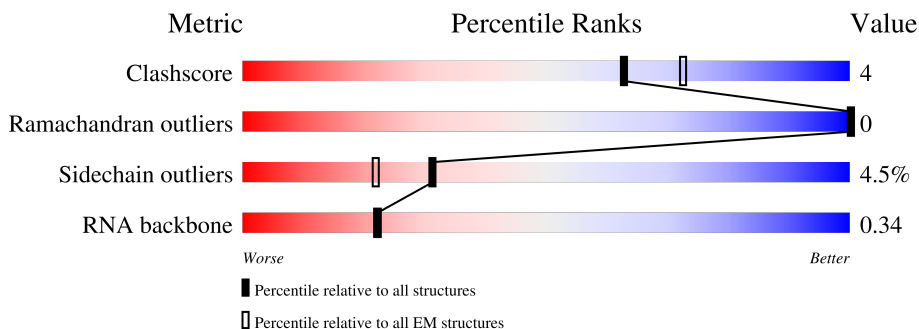
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 Å.

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



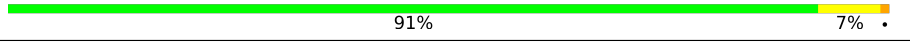
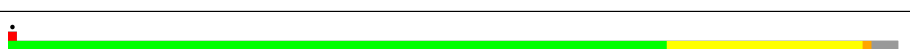






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	
2	B	1123	
3	C	391	
4	D	261	
5	E	190	
6	F	122	
7	H	82	

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Mol	Chain	Length	Quality of chain
8	K	60	 85% 7% 7%
9	L	94	 91% 7%
10	N	65	 85% 14%
11	P	49	 88% 8%
12	G	152	 74% 22%
13	I	73	 63% 25% 11%
14	J	648	 84% 15%
14	M	648	 83% 16%
15	5	36	 36% 19% 44%
16	6	36	 42% 36% 22%
17	7	52	 27% 21% 31% 44%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 39765 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 A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	900	Total	C	N	O	S	0	0
			7182	4536	1277	1330	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1103	Total	C	N	O	S	0	0
			8808	5565	1575	1632	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	378	Total	C	N	O	S	0	0
			2958	1868	512	568	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	256	Total	C	N	O	S	0	0
			2053	1322	339	388	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	183	Total	C	N	O	S	0	0
			1476	946	252	269	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	120	Total	C	N	O	S	0	0
			1003	643	167	189	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	H	77	636	412	106	118	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	56	433	284	75	73	1	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	94	776	493	134	147	2	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	65	530	340	89	95	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	48	373	233	74	62	4	0	0

- Molecule 12 is a protein called Transcription elongation factor Spt5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	G	147	1142	739	190	213	0	0

- Molecule 13 is a protein called Transcription elongation factor Spt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	65	511	319	95	93	4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-5	HIS	-	expression tag	UNP Q5JIY5
I	-4	HIS	-	expression tag	UNP Q5JIY5
I	-3	HIS	-	expression tag	UNP Q5JIY5
I	-2	HIS	-	expression tag	UNP Q5JIY5
I	-1	HIS	-	expression tag	UNP Q5JIY5
I	0	HIS	-	expression tag	UNP Q5JIY5

- Molecule 14 is a protein called Transcription termination factor FttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	645	Total	C	N	O	S	0	0
			5144	3284	903	941	16		
14	M	648	Total	C	N	O	S	0	0
			5155	3292	906	942	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	255	ALA	HIS	conflict	UNP Q5JH24
J	591	ALA	HIS	conflict	UNP Q5JH24
M	255	ALA	HIS	conflict	UNP Q5JH24
M	591	ALA	HIS	conflict	UNP Q5JH24

- Molecule 15 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	20	Total	C	N	O	P	0	0
			410	196	74	120	20		

- Molecule 16 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	28	Total	C	N	O	P	0	0
			575	273	102	172	28		

- Molecule 17 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7	29	Total	C	N	O	P	0	0
			591	265	75	222	29		

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

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

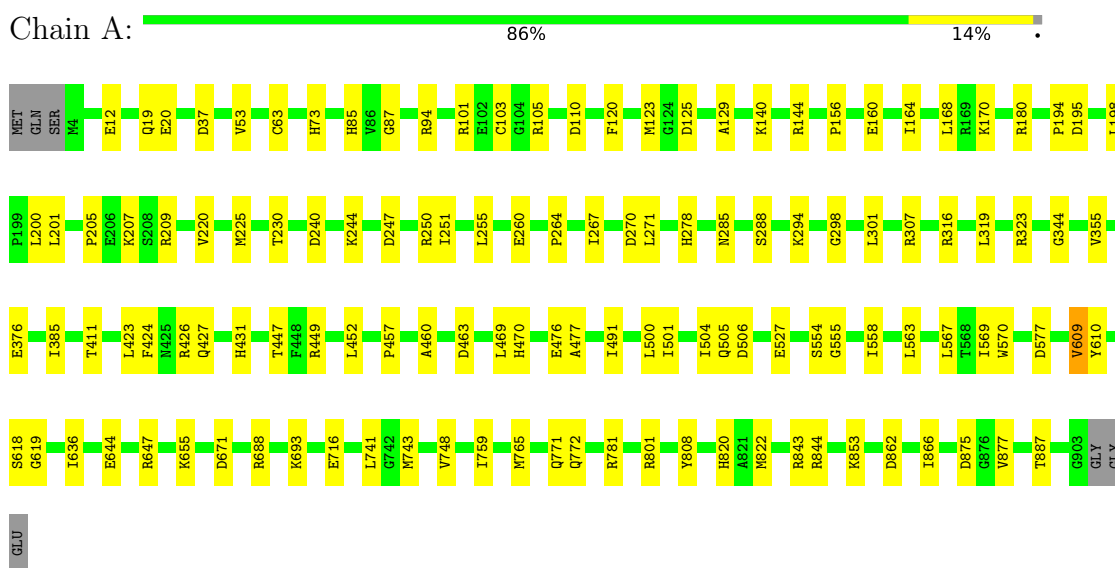
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
19	A	2	Total Zn 2 2	0
19	B	1	Total Zn 1 1	0
19	N	1	Total Zn 1 1	0
19	P	1	Total Zn 1 1	0
19	I	1	Total Zn 1 1	0
19	J	1	Total Zn 1 1	0
19	M	1	Total Zn 1 1	0

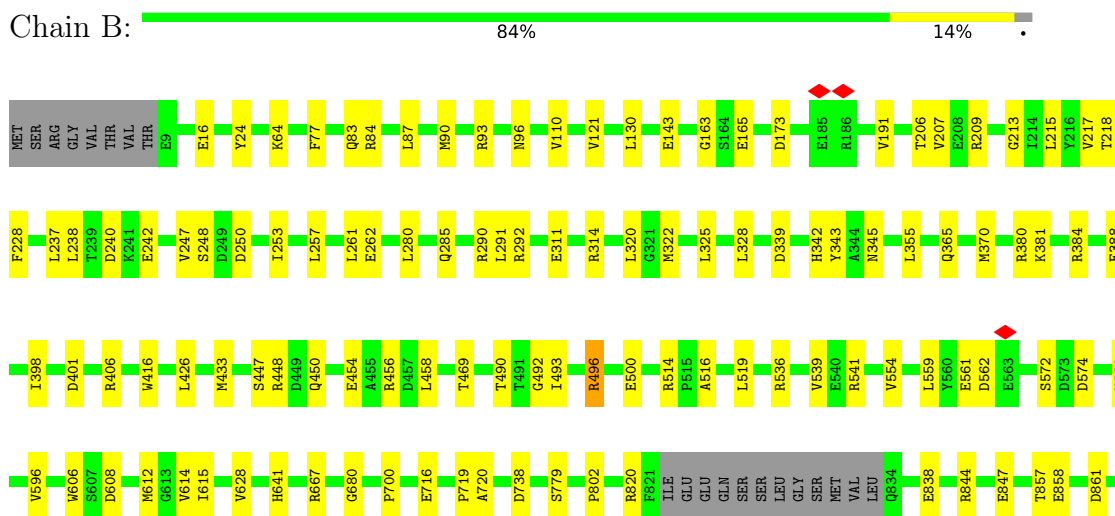
3 Residue-property plots

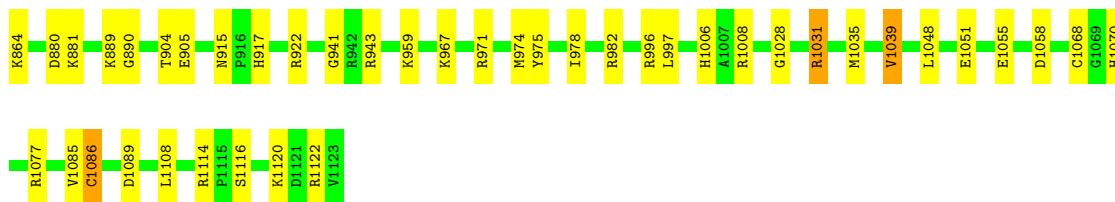
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

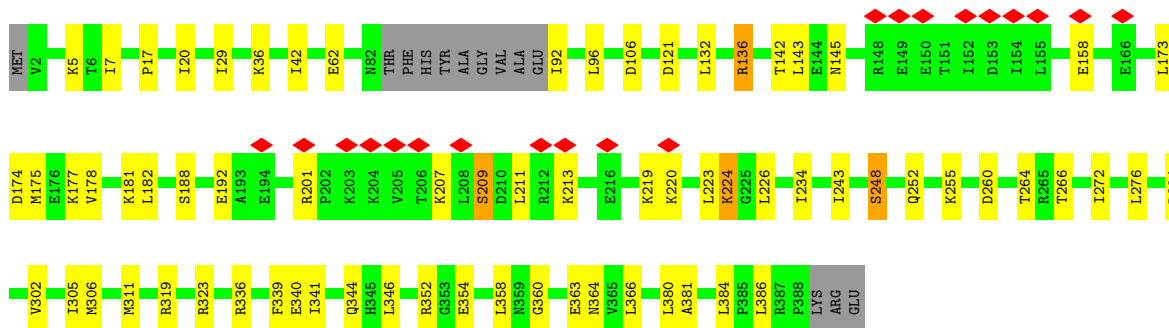
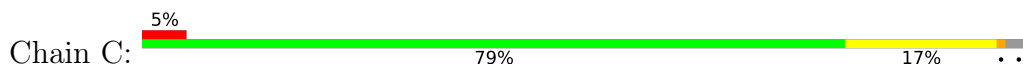


- Molecule 2: DNA-directed RNA polymerase subunit B

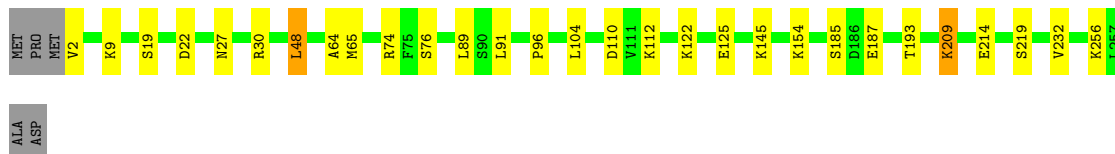
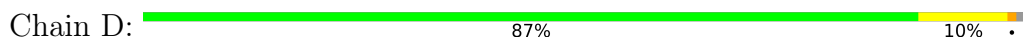




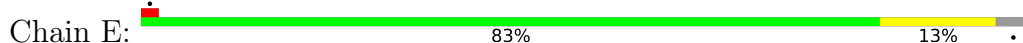
• Molecule 3: DNA-directed RNA polymerase subunit A"



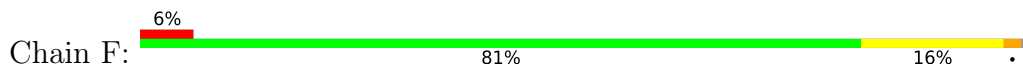
• Molecule 4: DNA-directed RNA polymerase subunit D



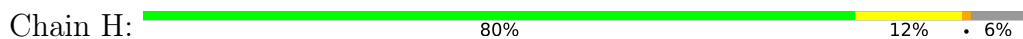
• Molecule 5: DNA-directed RNA polymerase subunit E



• Molecule 6: DNA-directed RNA polymerase subunit F

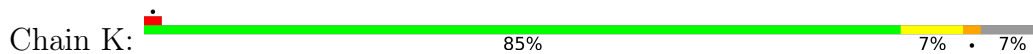


• Molecule 7: DNA-directed RNA polymerase subunit H

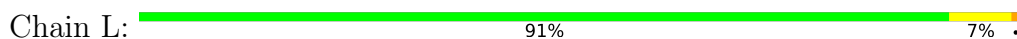




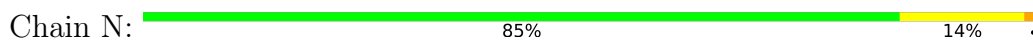
• Molecule 8: DNA-directed RNA polymerase subunit K



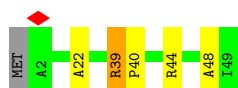
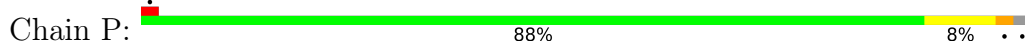
• Molecule 9: DNA-directed RNA polymerase subunit L



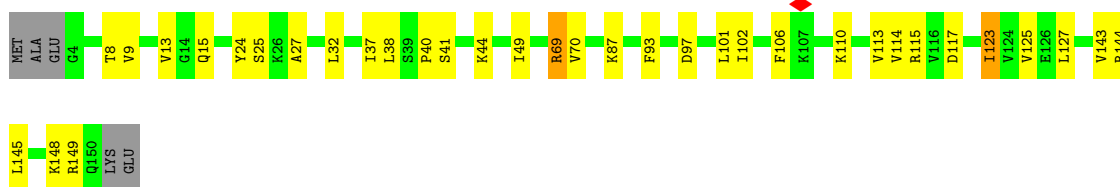
• Molecule 10: DNA-directed RNA polymerase subunit N



• Molecule 11: DNA-directed RNA polymerase subunit P



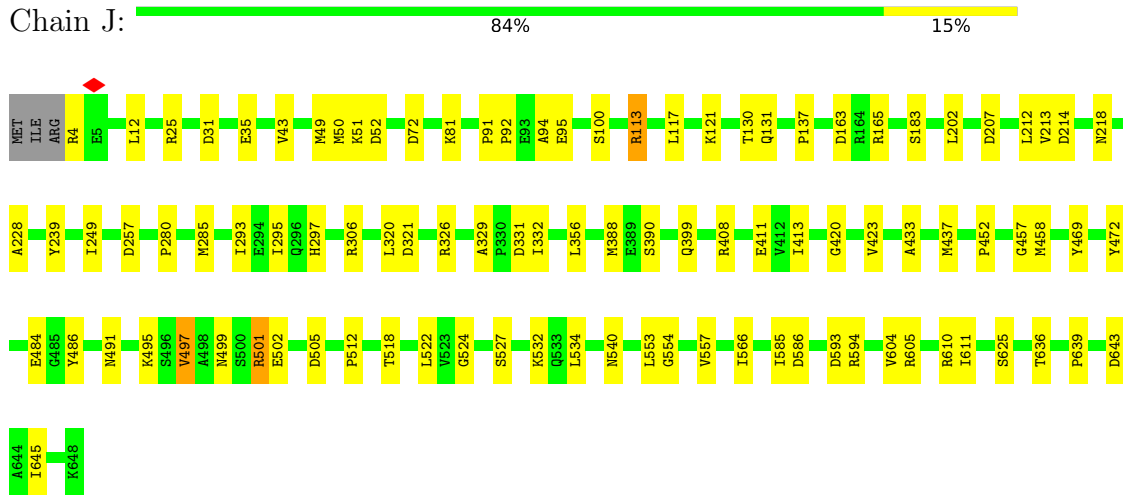
• Molecule 12: Transcription elongation factor Spt5



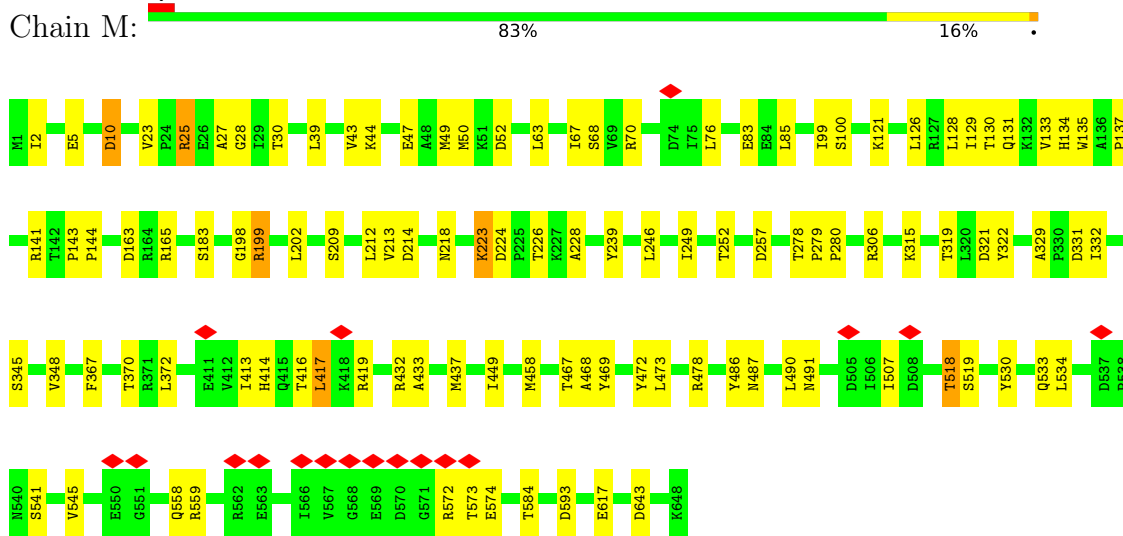
• Molecule 13: Transcription elongation factor Spt4



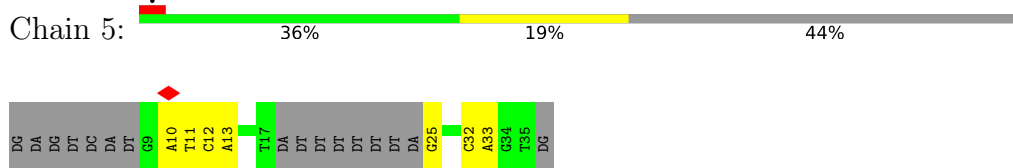
• Molecule 14: Transcription termination factor FttA



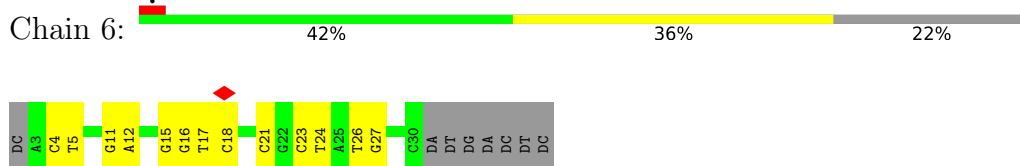
• Molecule 14: Transcription termination factor FttA



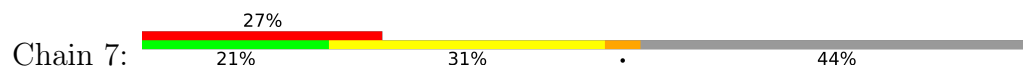
• Molecule 15: non-template strand DNA



• Molecule 16: template strand DNA



• Molecule 17: RNA (29-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137835	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.33	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.606	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	329.96002, 329.96002, 329.96002	wwPDB
Map dimensions	452, 452, 452	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.73, 0.73, 0.73	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	0.24	0/7325	0.48	0/9887
2	B	0.24	0/8985	0.50	0/12140
3	C	0.25	0/2994	0.51	0/4042
4	D	0.24	0/2098	0.47	0/2841
5	E	0.25	0/1502	0.50	0/2023
6	F	0.24	0/1023	0.51	0/1376
7	H	0.25	0/650	0.46	0/877
8	K	0.24	0/441	0.47	0/598
9	L	0.23	0/791	0.46	0/1066
10	N	0.24	0/539	0.47	0/723
11	P	0.23	0/378	0.58	0/507
12	G	0.24	0/1164	0.49	1/1577 (0.1%)
13	I	0.22	0/520	0.54	0/703
14	J	0.25	0/5253	0.50	1/7115 (0.0%)
14	M	0.25	0/5264	0.51	1/7132 (0.0%)
15	5	0.47	0/458	0.91	0/702
16	6	0.49	0/643	0.89	0/991
17	7	0.14	0/651	0.72	0/1004
All	All	0.25	0/40679	0.52	3/55304 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	52	ASP	CB-CG-OD1	6.21	123.89	118.30
14	M	128	LEU	CA-CB-CG	5.08	126.98	115.30
12	G	15	GLN	CA-CB-CG	5.03	124.46	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7182	0	7246	63	0
2	B	8808	0	8864	85	0
3	C	2958	0	3077	38	0
4	D	2053	0	2063	16	0
5	E	1476	0	1512	12	0
6	F	1003	0	1007	11	0
7	H	636	0	646	6	0
8	K	433	0	466	5	0
9	L	776	0	770	5	0
10	N	530	0	540	7	0
11	P	373	0	392	4	0
12	G	1142	0	1192	17	0
13	I	511	0	502	11	0
14	J	5144	0	5246	42	0
14	M	5155	0	5253	60	0
15	5	410	0	228	6	0
16	6	575	0	317	12	0
17	7	591	0	300	9	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	M	1	0	0	0	0
19	N	1	0	0	0	0
19	P	1	0	0	0	0
All	All	39765	0	39621	351	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 (351) 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)
1:A:63:CYS:SG	1:A:73:HIS:CE1	2.65	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:278:THR:HG22	14:M:280:PRO:HD2	1.62	0.80
5:E:114:MET:O	5:E:166:ARG:NH1	2.24	0.71
1:A:452:LEU:HB3	1:A:504:ILE:HD11	1.72	0.70
1:A:319:LEU:HB3	3:C:366:LEU:HD22	1.74	0.70
3:C:158:GLU:HA	3:C:211:LEU:HD21	1.75	0.69
14:J:239:TYR:HB2	14:M:239:TYR:HB2	1.75	0.66
2:B:700:PRO:HB2	2:B:719:PRO:HG2	1.77	0.65
1:A:877:VAL:HG21	1:A:887:THR:HG23	1.78	0.65
1:A:85:HIS:HD2	1:A:87:GLY:H	1.43	0.65
12:G:102:ILE:HD11	12:G:144:ARG:HE	1.63	0.64
1:A:344:GLY:HA3	1:A:449:ARG:HB2	1.81	0.62
2:B:802:PRO:HB2	11:P:39:ARG:HG3	1.81	0.62
2:B:121:VAL:HG21	2:B:398:ILE:HD13	1.81	0.62
1:A:385:ILE:HB	1:A:411:THR:HB	1.82	0.62
2:B:16:GLU:HG2	2:B:596:VAL:HG11	1.82	0.61
1:A:423:LEU:HB2	1:A:470:HIS:HB2	1.83	0.60
2:B:881:LYS:HD3	2:B:997:LEU:HD12	1.84	0.60
1:A:323:ARG:NH2	16:6:17:DT:OP1	2.34	0.60
1:A:207:LYS:O	2:B:1114:ARG:NH2	2.35	0.60
1:A:160:GLU:HB3	1:A:164:ILE:HB	1.83	0.60
1:A:12:GLU:HB2	2:B:1116:SER:HB2	1.84	0.59
2:B:1031:ARG:HG2	16:6:16:DG:H5''	1.84	0.59
2:B:539:VAL:HG21	2:B:559:LEU:HB2	1.85	0.59
2:B:450:GLN:HE22	15:5:25:DG:H21	1.50	0.58
3:C:358:LEU:HA	3:C:363:GLU:HG3	1.85	0.58
14:M:370:THR:HG22	14:M:372:LEU:H	1.69	0.58
14:J:486:TYR:OH	14:J:491:ASN:ND2	2.36	0.58
3:C:207:LYS:HD2	3:C:209:SER:HB3	1.86	0.57
1:A:426:ARG:HD2	1:A:460:ALA:HB2	1.86	0.57
14:J:295:ILE:HD11	17:7:-21:U:H2'	1.86	0.57
15:5:10:DA:H2''	15:5:11:DT:H5''	1.85	0.57
1:A:527:GLU:OE1	9:L:33:HIS:NE2	2.33	0.57
4:D:27:ASN:OD1	4:D:30:ARG:NH1	2.38	0.57
3:C:226:LEU:HD22	3:C:252:GLN:HB3	1.87	0.56
1:A:316:ARG:NH2	16:6:15:DG:OP1	2.38	0.56
2:B:380:ARG:HE	2:B:381:LYS:HD2	1.71	0.56
3:C:302:VAL:HA	3:C:305:ILE:HD12	1.88	0.56
1:A:822:MET:HG3	2:B:458:LEU:HD23	1.88	0.56
2:B:516:ALA:HB3	2:B:519:LEU:HG	1.88	0.56
14:J:130:THR:HB	14:J:137:PRO:HD3	1.88	0.56
14:M:433:ALA:O	14:M:437:MET:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:LEU:HD13	16:6:21:DC:H5''	1.88	0.56
2:B:1077:ARG:HD3	14:J:297:HIS:CE1	2.41	0.55
14:J:497:VAL:HG23	14:J:502:GLU:HB3	1.88	0.55
12:G:9:VAL:HG22	12:G:70:VAL:HG22	1.87	0.55
1:A:20:GLU:OE1	2:B:1114:ARG:NH1	2.39	0.55
2:B:614:VAL:HG12	2:B:615:ILE:HG13	1.87	0.55
14:M:47:GLU:OE2	14:M:134:HIS:NE2	2.39	0.55
14:M:144:PRO:HD2	14:M:467:THR:HB	1.89	0.55
3:C:344:GLN:NE2	16:6:11:DG:OP1	2.39	0.55
12:G:93:PHE:HE1	12:G:145:LEU:HB2	1.71	0.55
1:A:105:ARG:HD2	1:A:194:PRO:HG3	1.88	0.55
2:B:339:ASP:HB3	2:B:342:HIS:HB2	1.88	0.55
10:N:16:ASP:OD1	10:N:16:ASP:N	2.40	0.55
14:M:487:ASN:HB3	14:M:490:LEU:HB2	1.89	0.55
16:6:17:DT:H2'	16:6:18:DC:H6	1.71	0.54
4:D:96:PRO:HG3	4:D:125:GLU:HG2	1.89	0.54
2:B:738:ASP:OD1	2:B:922:ARG:NH2	2.40	0.54
14:J:35:GLU:OE2	14:J:165:ARG:NH1	2.41	0.54
14:J:413:ILE:HG12	14:J:423:VAL:HG11	1.90	0.54
2:B:206:THR:HB	2:B:218:THR:HB	1.90	0.54
13:I:5:ARG:HH22	13:I:17:ASP:HA	1.72	0.54
14:J:408:ARG:HD2	14:J:585:ILE:HG12	1.90	0.54
2:B:450:GLN:NE2	15:5:25:DG:H21	2.06	0.53
2:B:285:GLN:O	2:B:290:ARG:NH1	2.41	0.53
4:D:64:ALA:HB1	4:D:145:LYS:HD3	1.91	0.53
3:C:272:ILE:HG23	3:C:276:LEU:HD12	1.91	0.53
14:M:419:ARG:NH2	14:M:541:SER:OG	2.40	0.53
1:A:771:GLN:NE2	1:A:772:GLN:O	2.41	0.53
2:B:339:ASP:O	2:B:345:ASN:ND2	2.41	0.53
1:A:555:GLY:HA2	1:A:558:ILE:HD12	1.91	0.53
14:J:532:LYS:HE2	14:J:566:ILE:HD13	1.90	0.53
12:G:97:ASP:HB3	12:G:149:ARG:H	1.74	0.53
1:A:195:ASP:OD1	1:A:209:ARG:NH1	2.43	0.52
1:A:765:MET:HA	1:A:808:TYR:HB2	1.92	0.52
9:L:9:GLU:HB2	9:L:12:LEU:HB3	1.92	0.52
2:B:628:VAL:HG22	2:B:641:HIS:HB2	1.91	0.52
3:C:381:ALA:HB2	8:K:54:ILE:HD11	1.91	0.52
3:C:311:MET:O	3:C:319:ARG:NH2	2.43	0.52
14:M:279:PRO:HG3	14:M:319:THR:HB	1.92	0.52
2:B:253:ILE:HG23	2:B:328:LEU:HD12	1.92	0.51
3:C:62:GLU:OE2	8:K:6:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:THR:H	3:C:145:ASN:HD21	1.58	0.51
2:B:880:ASP:OD2	2:B:996:ARG:NH2	2.44	0.51
14:M:83:GLU:HG3	14:M:99:ILE:HD12	1.91	0.51
1:A:463:ASP:HA	2:B:890:GLY:HA2	1.92	0.51
2:B:864:LYS:NZ	11:P:22:ALA:O	2.42	0.51
1:A:323:ARG:HA	2:B:1031:ARG:HA	1.91	0.51
1:A:644:GLU:OE2	1:A:647:ARG:NH1	2.44	0.51
2:B:228:PHE:HE1	2:B:320:LEU:HB3	1.76	0.51
2:B:209:ARG:HB2	2:B:215:LEU:HD23	1.92	0.50
9:L:8:ARG:NH1	9:L:68:GLU:OE2	2.44	0.50
3:C:302:VAL:O	3:C:306:MET:HG3	2.11	0.50
14:M:63:LEU:HD12	14:M:67:ILE:HD11	1.93	0.50
2:B:889:LYS:NZ	17:7:-1:C:OP1	2.33	0.50
13:I:40:VAL:O	13:I:49:ARG:NH2	2.39	0.50
2:B:719:PRO:HG3	10:N:53:VAL:HG11	1.93	0.50
1:A:781:ARG:NH1	2:B:454:GLU:O	2.44	0.50
1:A:862:ASP:OD1	1:A:866:ILE:N	2.44	0.50
14:M:473:LEU:O	14:M:478:ARG:NH1	2.45	0.50
1:A:505:GLN:HB2	2:B:917:HIS:CD2	2.48	0.49
14:J:94:ALA:HB2	14:J:117:LEU:HB2	1.94	0.49
1:A:569:ILE:HD12	1:A:636:ILE:HG13	1.95	0.49
14:J:420:GLY:HA2	14:J:512:PRO:HG3	1.94	0.49
2:B:492:GLY:N	2:B:574:ASP:OD1	2.45	0.49
1:A:255:LEU:HA	1:A:271:LEU:HD13	1.93	0.49
14:J:611:ILE:HB	14:J:636:THR:HG22	1.95	0.49
17:7:-8:C:H2'	17:7:-7:G:C8	2.47	0.49
2:B:248:SER:HB2	2:B:325:LEU:HD13	1.94	0.49
3:C:17:PRO:HD2	3:C:20:ILE:HD12	1.94	0.49
6:F:18:LYS:HD2	6:F:49:GLU:HA	1.94	0.49
14:M:530:TYR:O	14:M:534:LEU:HB2	2.13	0.49
1:A:427:GLN:HB3	16:6:15:DG:H21	1.78	0.49
14:M:25:ARG:HH21	14:M:28:GLY:HA2	1.77	0.49
1:A:94:ARG:NH1	1:A:201:LEU:O	2.44	0.48
2:B:905:GLU:OE2	2:B:982:ARG:NH2	2.45	0.48
14:M:10:ASP:N	14:M:10:ASP:OD1	2.46	0.48
14:M:432:ARG:HD3	14:M:545:VAL:HG23	1.95	0.48
14:J:202:LEU:HB3	14:J:213:VAL:HB	1.94	0.48
1:A:230:THR:OG1	2:B:820:ARG:NH2	2.46	0.48
3:C:136:ARG:O	3:C:224:LYS:NZ	2.38	0.48
3:C:260:ASP:O	3:C:264:THR:OG1	2.29	0.48
1:A:264:PRO:HD2	1:A:267:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:GLU:OE1	2:B:943:ARG:NH2	2.45	0.48
6:F:92:ILE:HA	6:F:95:ILE:HG12	1.96	0.48
3:C:276:LEU:HA	7:H:9:ILE:HD11	1.95	0.48
1:A:477:ALA:HB1	2:B:1048:LEU:HD13	1.94	0.48
14:J:553:LEU:O	14:J:557:VAL:HG23	2.14	0.47
14:M:27:ALA:HB1	14:M:49:MET:HG2	1.96	0.47
1:A:123:MET:HE3	1:A:129:ALA:HB1	1.95	0.47
1:A:491:ILE:HA	1:A:501:ILE:HG13	1.96	0.47
2:B:590:LYS:HB3	2:B:614:VAL:HG22	1.96	0.47
12:G:87:LYS:HE2	12:G:87:LYS:HB2	1.66	0.47
2:B:365:GLN:OE1	2:B:406:ARG:NH1	2.42	0.47
2:B:1006:HIS:NE2	2:B:1028:GLY:O	2.43	0.47
5:E:7:VAL:HG11	6:F:2:ILE:HG22	1.97	0.47
1:A:247:ASP:OD1	1:A:250:ARG:NH2	2.47	0.47
2:B:802:PRO:HD2	11:P:40:PRO:HD3	1.97	0.47
14:J:218:ASN:HB3	14:J:228:ALA:HA	1.96	0.47
14:M:432:ARG:NH1	14:M:545:VAL:O	2.48	0.47
16:6:11:DG:H2"	16:6:12:DA:C8	2.50	0.47
1:A:156:PRO:HG2	1:A:168:LEU:HB2	1.95	0.47
2:B:1035:MET:O	2:B:1039:VAL:HG12	2.14	0.47
2:B:450:GLN:HE22	15:5:25:DG:N2	2.13	0.47
1:A:609:VAL:HA	1:A:619:GLY:HA3	1.96	0.46
3:C:252:GLN:OE1	3:C:255:LYS:NZ	2.45	0.46
5:E:15:PRO:HG2	8:K:22:MET:HG3	1.98	0.46
3:C:336:ARG:NH2	3:C:354:GLU:OE1	2.49	0.46
12:G:37:ILE:HG12	12:G:49:ILE:HG12	1.98	0.46
1:A:198:LEU:HD12	1:A:205:PRO:HA	1.95	0.46
6:F:61:GLU:O	6:F:65:LYS:HG3	2.16	0.46
6:F:110:GLU:O	6:F:114:VAL:HG12	2.16	0.46
14:M:133:VAL:HG13	14:M:135:TRP:HB2	1.97	0.46
14:M:558:GLN:NE2	14:M:584:THR:OG1	2.49	0.46
2:B:143:GLU:OE2	2:B:143:GLU:N	2.36	0.46
3:C:323:ARG:NH1	3:C:340:GLU:OE1	2.40	0.46
14:J:522:LEU:HD12	14:J:554:GLY:HA2	1.97	0.46
1:A:270:ASP:OD1	12:G:69:ARG:NH2	2.49	0.46
6:F:104:THR:OG1	6:F:107:GLU:OE1	2.34	0.46
7:H:30:LEU:HD11	7:H:37:ILE:HD13	1.98	0.46
5:E:180:LYS:HE2	6:F:90:LEU:HB3	1.97	0.46
7:H:20:ILE:HG13	7:H:53:LEU:HD13	1.97	0.46
12:G:101:LEU:HD22	12:G:106:PHE:HB2	1.97	0.46
3:C:384:LEU:HD23	5:E:22:PRO:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:586:ASP:OD2	14:J:586:ASP:N	2.43	0.45
14:M:52:ASP:N	14:M:52:ASP:OD1	2.46	0.45
14:M:486:TYR:OH	14:M:491:ASN:OD1	2.34	0.45
17:7:-5:C:H2'	17:7:-4:G:H8	1.81	0.45
2:B:93:ARG:NH1	2:B:165:GLU:OE2	2.48	0.45
5:E:6:LYS:HG2	6:F:7:LEU:HD12	1.98	0.45
14:M:321:ASP:OD1	14:M:472:TYR:OH	2.32	0.45
1:A:240:ASP:HB3	1:A:301:LEU:HB3	1.97	0.45
1:A:476:GLU:OE2	8:K:11:ARG:NH2	2.48	0.45
3:C:234:ILE:HG12	3:C:243:ILE:HG12	1.99	0.45
6:F:62:LEU:HD21	6:F:115:ILE:HG22	1.98	0.45
14:J:452:PRO:HB3	14:J:495:LYS:HE2	1.98	0.45
14:J:639:PRO:HG3	14:J:645:ILE:HD11	1.98	0.45
13:I:26:ASP:OD1	13:I:26:ASP:N	2.40	0.45
14:M:212:LEU:HB2	14:M:246:LEU:HD11	1.98	0.45
2:B:64:LYS:HG2	2:B:110:VAL:HB	1.99	0.45
2:B:978:ILE:O	4:D:27:ASN:ND2	2.49	0.45
4:D:64:ALA:HB2	11:P:48:ALA:HB1	1.99	0.45
14:M:518:THR:OG1	14:M:519:SER:N	2.49	0.45
2:B:905:GLU:HG2	2:B:975:TYR:HE1	1.82	0.45
3:C:380:LEU:HD11	8:K:11:ARG:HG3	1.98	0.45
1:A:20:GLU:OE2	2:B:1070:HIS:NE2	2.40	0.45
1:A:285:ASN:ND2	1:A:301:LEU:O	2.36	0.45
5:E:48:ILE:HD13	5:E:74:VAL:HG13	1.99	0.45
13:I:5:ARG:HH21	13:I:27:LEU:HD12	1.82	0.45
2:B:77:PHE:HB2	2:B:87:LEU:HD22	1.98	0.45
2:B:1089:ASP:OD1	2:B:1089:ASP:N	2.50	0.45
14:J:501:ARG:NH2	14:J:505:ASP:OD2	2.37	0.44
4:D:154:LYS:HB2	4:D:154:LYS:HE2	1.82	0.44
14:M:121:LYS:HA	14:M:121:LYS:HD3	1.83	0.44
2:B:967:LYS:HD2	2:B:967:LYS:HA	1.76	0.44
14:J:433:ALA:O	14:J:437:MET:HG3	2.17	0.44
14:M:141:ARG:NH2	17:7:-36:U:O2	2.51	0.44
1:A:140:LYS:HE3	1:A:140:LYS:HB2	1.73	0.44
1:A:844:ARG:NH1	3:C:106:ASP:OD1	2.51	0.44
2:B:247:VAL:HB	2:B:257:LEU:HD11	1.99	0.44
4:D:2:VAL:HG11	9:L:85:VAL:HG22	2.00	0.44
10:N:56:ILE:O	10:N:60:MET:HG3	2.18	0.44
13:I:32:PHE:HD2	13:I:65:ARG:HD3	1.82	0.44
14:M:280:PRO:HG3	14:M:469:TYR:CG	2.52	0.44
14:M:322:TYR:OH	14:M:345:SER:O	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ASP:OD1	2:B:971:ARG:NH1	2.49	0.44
2:B:1058:ASP:OD1	2:B:1058:ASP:N	2.51	0.44
3:C:248:SER:HG	3:C:266:THR:HG1	1.63	0.44
14:M:165:ARG:HD3	14:M:165:ARG:HA	1.84	0.44
14:M:212:LEU:HB3	14:M:249:ILE:HG12	1.98	0.44
14:M:223:LYS:H	14:M:223:LYS:HE2	1.81	0.44
1:A:808:TYR:OH	1:A:820:HIS:NE2	2.47	0.44
3:C:178:VAL:O	3:C:182:LEU:HD12	2.17	0.44
1:A:875:ASP:HB3	7:H:70:ALA:HB2	1.99	0.44
2:B:536:ARG:NH2	2:B:561:GLU:OE2	2.50	0.44
2:B:680:GLY:HA3	2:B:720:ALA:HA	2.00	0.44
14:J:43:VAL:HG11	14:J:49:MET:HG3	2.00	0.44
14:M:143:PRO:HB3	14:M:468:ALA:HB2	1.98	0.44
3:C:340:GLU:HG2	16:6:12:DA:H5"	2.00	0.43
5:E:118:VAL:HG21	5:E:127:PHE:HB3	1.99	0.43
12:G:113:VAL:HG22	12:G:123:ILE:HD11	1.99	0.43
14:J:524:GLY:HA3	17:7:-21:U:C2	2.53	0.43
14:M:209:SER:OG	14:M:331:ASP:OD1	2.34	0.43
2:B:915:ASN:OD1	2:B:917:HIS:ND1	2.40	0.43
4:D:154:LYS:NZ	4:D:193:THR:O	2.49	0.43
10:N:57:ASP:HA	10:N:60:MET:HE2	2.00	0.43
13:I:35:VAL:O	13:I:62:TYR:N	2.47	0.43
2:B:844:ARG:HB2	2:B:847:GLU:HG3	1.99	0.43
12:G:117:ASP:HB3	14:M:2:ILE:HG13	2.00	0.43
2:B:24:TYR:HB2	2:B:606:TRP:CE3	2.53	0.43
4:D:122:LYS:HE3	4:D:122:LYS:HB3	1.73	0.43
14:M:413:ILE:HA	14:M:416:THR:HG22	2.01	0.43
3:C:5:LYS:HA	3:C:5:LYS:HD3	1.85	0.43
1:A:225:MET:O	1:A:307:ARG:NH2	2.45	0.43
13:I:49:ARG:NH1	13:I:56:ALA:O	2.52	0.43
14:J:165:ARG:HA	14:J:165:ARG:HD3	1.81	0.43
2:B:96:ASN:HA	2:B:163:GLY:HA3	2.01	0.43
3:C:7:ILE:HG12	3:C:42:ILE:HD13	2.01	0.43
12:G:114:VAL:HG12	12:G:115:ARG:HG3	1.99	0.43
14:J:457:GLY:HA3	14:J:518:THR:HG21	2.01	0.43
14:M:47:GLU:HA	14:M:131:GLN:HE21	1.83	0.43
2:B:667:ARG:HA	2:B:667:ARG:HD3	1.83	0.43
2:B:904:THR:HG22	2:B:974:MET:HG2	2.01	0.43
14:J:280:PRO:HG3	14:J:469:TYR:CG	2.54	0.43
14:J:329:ALA:HB3	14:J:332:ILE:HB	2.00	0.43
14:M:331:ASP:OD1	14:M:331:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:413:ILE:O	14:M:417:LEU:HB2	2.18	0.43
2:B:496:ARG:NE	2:B:500:GLU:OE2	2.51	0.42
3:C:181:LYS:NZ	3:C:223:LEU:O	2.40	0.42
4:D:209:LYS:HD2	4:D:209:LYS:H	1.84	0.42
14:J:212:LEU:HB3	14:J:249:ILE:HG12	2.01	0.42
14:M:224:ASP:OD2	14:M:226:THR:OG1	2.37	0.42
14:M:329:ALA:HB3	14:M:332:ILE:HB	2.01	0.42
2:B:448:ARG:O	2:B:456:ARG:NH2	2.52	0.42
14:J:399:GLN:N	14:J:593:ASP:OD2	2.52	0.42
1:A:741:LEU:HB3	1:A:748:VAL:HG21	2.01	0.42
14:M:39:LEU:HD23	14:M:67:ILE:HG12	1.99	0.42
3:C:143:LEU:HB3	3:C:219:LYS:HA	2.01	0.42
1:A:844:ARG:HG3	3:C:339:PHE:HZ	1.85	0.42
14:J:331:ASP:OD1	14:J:331:ASP:N	2.51	0.42
14:M:43:VAL:HG11	14:M:49:MET:HG3	2.00	0.42
16:6:23:DC:H2'	16:6:24:DT:C6	2.54	0.42
17:7:-5:C:H2'	17:7:-4:G:C8	2.55	0.42
1:A:447:THR:HG23	1:A:449:ARG:HD2	2.01	0.42
14:M:126:LEU:O	14:M:129:ILE:HG13	2.20	0.42
2:B:1108:LEU:HD21	3:C:346:LEU:HD13	2.01	0.42
6:F:9:GLU:O	6:F:10:HIS:ND1	2.53	0.42
13:I:31:TRP:HZ3	13:I:34:LEU:HB2	1.84	0.42
12:G:27:ALA:HA	12:G:32:LEU:HB2	2.01	0.42
13:I:47:LYS:HA	13:I:47:LYS:HD2	1.83	0.42
14:M:218:ASN:HB3	14:M:228:ALA:HA	2.02	0.42
1:A:570:TRP:HB3	1:A:610:TYR:HD1	1.84	0.42
2:B:857:THR:OG1	2:B:858:GLU:N	2.52	0.42
14:J:321:ASP:OD1	14:J:472:TYR:OH	2.35	0.42
14:M:199:ARG:HB3	14:M:218:ASN:HB2	2.02	0.42
2:B:1068:CYS:SG	2:B:1086:CYS:HB3	2.59	0.42
2:B:1120:LYS:HB3	2:B:1120:LYS:HE3	1.88	0.42
14:M:572:ARG:NH2	14:M:573:THR:O	2.52	0.42
1:A:251:ILE:HG13	1:A:278:HIS:CD2	2.55	0.41
14:J:320:LEU:HD11	14:J:326:ARG:HG3	2.02	0.41
14:M:85:LEU:HD23	14:M:85:LEU:HA	1.90	0.41
14:M:126:LEU:HG	14:M:137:PRO:HG2	2.01	0.41
14:M:198:GLY:HA2	14:M:257:ASP:HB2	2.02	0.41
9:L:93:ILE:HD13	9:L:93:ILE:HA	1.87	0.41
12:G:13:VAL:HG13	12:G:44:LYS:HB3	2.01	0.41
14:J:207:ASP:OD1	14:J:207:ASP:N	2.51	0.41
14:M:202:LEU:HB3	14:M:213:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ARG:HE	2:B:213:GLY:HA2	1.84	0.41
7:H:37:ILE:HD12	7:H:37:ILE:HA	1.94	0.41
14:J:91:PRO:HA	14:J:92:PRO:HD3	1.96	0.41
14:J:257:ASP:OD1	17:7:-23:U:O2'	2.37	0.41
14:M:130:THR:HA	14:M:133:VAL:HG12	2.02	0.41
2:B:608:ASP:O	2:B:612:MET:HG3	2.21	0.41
2:B:959:LYS:HE2	2:B:959:LYS:HB2	1.87	0.41
1:A:294:LYS:HZ2	1:A:298:GLY:HA2	1.84	0.41
3:C:173:LEU:HA	3:C:177:LYS:HZ3	1.85	0.41
4:D:9:LYS:HE3	4:D:9:LYS:HB2	1.89	0.41
12:G:24:TYR:HB2	13:I:36:ILE:HG21	2.03	0.41
14:M:593:ASP:OD1	14:M:593:ASP:N	2.51	0.41
1:A:563:LEU:HB3	1:A:567:LEU:HD23	2.02	0.41
2:B:207:VAL:HG22	2:B:217:VAL:HG22	2.02	0.41
2:B:941:GLY:HA2	10:N:50:LEU:HD11	2.02	0.41
3:C:29:ILE:HD13	3:C:29:ILE:HA	1.89	0.41
4:D:65:MET:O	10:N:6:ARG:NH1	2.54	0.41
7:H:6:GLU:OE1	7:H:7:PHE:N	2.53	0.41
12:G:41:SER:HB3	13:I:33:ASP:H	1.86	0.41
1:A:801:ARG:HA	1:A:801:ARG:HD3	1.91	0.41
5:E:45:VAL:HA	5:E:76:VAL:HG12	2.01	0.41
14:M:76:LEU:HD23	14:M:76:LEU:HA	1.95	0.41
15:5:12:DC:H2''	15:5:13:DA:C8	2.56	0.41
16:6:26:DT:H2''	16:6:27:DG:C8	2.55	0.41
2:B:490:THR:HB	2:B:554:VAL:HG13	2.02	0.41
12:G:113:VAL:HA	12:G:125:VAL:HG12	2.02	0.41
14:J:50:MET:HG2	14:J:131:GLN:HE21	1.86	0.41
14:M:50:MET:HE2	14:M:131:GLN:HG3	2.03	0.41
1:A:457:PRO:HG3	1:A:500:LEU:HG	2.03	0.41
2:B:280:LEU:HD23	2:B:280:LEU:HA	1.89	0.41
5:E:174:GLU:H	5:E:174:GLU:CD	2.24	0.41
5:E:180:LYS:HA	5:E:180:LYS:HD3	1.88	0.41
6:F:61:GLU:HA	6:F:64:GLU:HG3	2.01	0.41
12:G:38:LEU:HG	12:G:40:PRO:HD3	2.03	0.41
14:J:604:VAL:O	14:J:605:ARG:NE	2.54	0.41
14:M:507:ILE:HG21	14:M:533:GLN:HG2	2.03	0.41
17:7:-7:G:H2'	17:7:-6:C:C6	2.56	0.41
1:A:716:GLU:H	1:A:716:GLU:HG3	1.70	0.41
4:D:48:LEU:HD13	4:D:48:LEU:HA	1.88	0.41
14:M:130:THR:HB	14:M:137:PRO:HG3	2.03	0.41
2:B:237:LEU:HD22	2:B:242:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ASP:HB3	2:B:253:ILE:HD12	2.03	0.40
14:J:95:GLU:HB2	14:J:113:ARG:HG3	2.02	0.40
14:J:213:VAL:HG12	14:J:214:ASP:OD2	2.21	0.40
14:J:534:LEU:HB3	14:J:540:ASN:HD22	1.86	0.40
14:M:469:TYR:HB3	14:M:472:TYR:HD2	1.85	0.40
1:A:170:LYS:HA	1:A:170:LYS:HD3	1.79	0.40
2:B:493:ILE:HD11	2:B:572:SER:HB2	2.04	0.40
3:C:360:GLY:O	3:C:364:ASN:ND2	2.43	0.40
3:C:384:LEU:O	3:C:386:LEU:N	2.54	0.40
4:D:91:LEU:HB2	4:D:104:LEU:HD23	2.02	0.40
2:B:240:ASP:HB3	2:B:261:LEU:HD13	2.02	0.40
5:E:91:GLU:HB3	5:E:98:PHE:HB2	2.04	0.40
15:5:32:DC:H2''	15:5:33:DA:C8	2.56	0.40
3:C:192:GLU:OE1	3:C:201:ARG:NH1	2.55	0.40
4:D:74:ARG:NH1	4:D:110:ASP:OD2	2.47	0.40
4:D:187:GLU:OE1	4:D:187:GLU:N	2.54	0.40
10:N:7:CYS:HB2	10:N:14:LEU:HD11	2.02	0.40
14:J:12:LEU:HD23	14:J:12:LEU:HA	1.96	0.40
2:B:1051:GLU:HA	2:B:1055:GLU:HB2	2.04	0.40
14:M:163:ASP:OD2	14:M:315:LYS:NZ	2.55	0.40
14:M:252:THR:HG22	14:M:348:VAL:HG23	2.04	0.40
16:6:4:DC:H2''	16:6:5:DT:H5'	2.04	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	898/906 (99%)	880 (98%)	18 (2%)	0	100	100
2	B	1099/1123 (98%)	1083 (98%)	16 (2%)	0	100	100
3	C	374/391 (96%)	365 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	254/261 (97%)	251 (99%)	3 (1%)	0	100	100
5	E	181/190 (95%)	179 (99%)	2 (1%)	0	100	100
6	F	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
7	H	75/82 (92%)	75 (100%)	0	0	100	100
8	K	54/60 (90%)	52 (96%)	2 (4%)	0	100	100
9	L	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
10	N	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
11	P	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
12	G	145/152 (95%)	143 (99%)	2 (1%)	0	100	100
13	I	63/73 (86%)	60 (95%)	3 (5%)	0	100	100
14	J	643/648 (99%)	629 (98%)	14 (2%)	0	100	100
14	M	646/648 (100%)	625 (97%)	21 (3%)	0	100	100
All	All	4751/4864 (98%)	4655 (98%)	96 (2%)	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	774/779 (99%)	742 (96%)	32 (4%)	30	39
2	B	950/969 (98%)	914 (96%)	36 (4%)	33	42
3	C	324/334 (97%)	307 (95%)	17 (5%)	23	28
4	D	226/230 (98%)	214 (95%)	12 (5%)	22	27
5	E	160/167 (96%)	151 (94%)	9 (6%)	21	25
6	F	105/107 (98%)	100 (95%)	5 (5%)	25	32
7	H	69/72 (96%)	65 (94%)	4 (6%)	20	23
8	K	45/49 (92%)	43 (96%)	2 (4%)	28	35
9	L	81/81 (100%)	79 (98%)	2 (2%)	47	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	N	59/59 (100%)	57 (97%)	2 (3%)	37	47
11	P	38/40 (95%)	36 (95%)	2 (5%)	22	27
12	G	127/131 (97%)	119 (94%)	8 (6%)	18	20
13	I	55/65 (85%)	51 (93%)	4 (7%)	14	15
14	J	562/565 (100%)	534 (95%)	28 (5%)	24	30
14	M	561/565 (99%)	536 (96%)	25 (4%)	27	34
All	All	4136/4213 (98%)	3948 (96%)	188 (4%)	31	34

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	37	ASP
1	A	53	VAL
1	A	101	ARG
1	A	103	CYS
1	A	110	ASP
1	A	120	PHE
1	A	125	ASP
1	A	144	ARG
1	A	180	ARG
1	A	200	LEU
1	A	220	VAL
1	A	244	LYS
1	A	260	GLU
1	A	288	SER
1	A	355	VAL
1	A	376	GLU
1	A	424	PHE
1	A	431	HIS
1	A	469	LEU
1	A	506	ASP
1	A	554	SER
1	A	577	ASP
1	A	609	VAL
1	A	618	SER
1	A	655	LYS
1	A	688	ARG
1	A	693	LYS
1	A	743	MET

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Mol	Chain	Res	Type
1	A	759	ILE
1	A	843	ARG
1	A	853	LYS
2	B	83	GLN
2	B	84	ARG
2	B	90	MET
2	B	130	LEU
2	B	173	ASP
2	B	191	VAL
2	B	238	LEU
2	B	262	GLU
2	B	291	LEU
2	B	292	ARG
2	B	311	GLU
2	B	314	ARG
2	B	322	MET
2	B	343	TYR
2	B	355	LEU
2	B	370	MET
2	B	384	ARG
2	B	388	GLU
2	B	401	ASP
2	B	416	TRP
2	B	433	MET
2	B	447	SER
2	B	469	THR
2	B	496	ARG
2	B	514	ARG
2	B	541	ARG
2	B	562	ASP
2	B	779	SER
2	B	838	GLU
2	B	861	ASP
2	B	1008	ARG
2	B	1031	ARG
2	B	1039	VAL
2	B	1085	VAL
2	B	1086	CYS
2	B	1122	ARG
3	C	36	LYS
3	C	92	ILE
3	C	96	LEU

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Mol	Chain	Res	Type
3	C	121	ASP
3	C	132	LEU
3	C	136	ARG
3	C	174	ASP
3	C	175	MET
3	C	188	SER
3	C	209	SER
3	C	213	LYS
3	C	220	LYS
3	C	224	LYS
3	C	248	SER
3	C	294	ARG
3	C	341	ILE
3	C	352	ARG
4	D	19	SER
4	D	22	ASP
4	D	48	LEU
4	D	76	SER
4	D	89	LEU
4	D	112	LYS
4	D	185	SER
4	D	209	LYS
4	D	214	GLU
4	D	219	SER
4	D	232	VAL
4	D	256	LYS
5	E	5	LEU
5	E	16	ARG
5	E	41	ASP
5	E	49	LEU
5	E	80	ARG
5	E	124	ASN
5	E	133	ASN
5	E	153	SER
5	E	163	MET
6	F	61	GLU
6	F	62	LEU
6	F	102	MET
6	F	113	LYS
6	F	119	ARG
7	H	6	GLU
7	H	34	ARG

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Mol	Chain	Res	Type
7	H	56	LYS
7	H	67	SER
8	K	6	ARG
8	K	46	LYS
9	L	9	GLU
9	L	77	LYS
10	N	47	ARG
10	N	53	VAL
11	P	39	ARG
11	P	44	ARG
12	G	8	THR
12	G	25	SER
12	G	69	ARG
12	G	110	LYS
12	G	123	ILE
12	G	127	LEU
12	G	143	VAL
12	G	148	LYS
13	I	24	SER
13	I	42	SER
13	I	43	ARG
13	I	65	ARG
14	J	4	ARG
14	J	25	ARG
14	J	31	ASP
14	J	51	LYS
14	J	72	ASP
14	J	81	LYS
14	J	100	SER
14	J	113	ARG
14	J	121	LYS
14	J	163	ASP
14	J	183	SER
14	J	285	MET
14	J	293	ILE
14	J	306	ARG
14	J	356	LEU
14	J	388	MET
14	J	390	SER
14	J	411	GLU
14	J	458	MET
14	J	484	GLU

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Mol	Chain	Res	Type
14	J	497	VAL
14	J	499	ASN
14	J	501	ARG
14	J	527	SER
14	J	594	ARG
14	J	610	ARG
14	J	625	SER
14	J	643	ASP
14	M	5	GLU
14	M	10	ASP
14	M	23	VAL
14	M	25	ARG
14	M	30	THR
14	M	44	LYS
14	M	68	SER
14	M	70	ARG
14	M	100	SER
14	M	183	SER
14	M	199	ARG
14	M	214	ASP
14	M	223	LYS
14	M	306	ARG
14	M	367	PHE
14	M	414	HIS
14	M	417	LEU
14	M	449	ILE
14	M	458	MET
14	M	518	THR
14	M	539	LYS
14	M	559	ARG
14	M	574	GLU
14	M	617	GLU
14	M	643	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	815	GLN
2	B	450	GLN
2	B	783	GLN
5	E	124	ASN

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Mol	Chain	Res	Type
5	E	126	GLN
12	G	150	GLN
14	J	21	GLN
14	J	131	GLN
14	J	158	GLN
14	J	253	HIS
14	M	131	GLN
14	M	158	GLN
14	M	349	HIS
14	M	399	GLN
14	M	480	GLN
14	M	558	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	7	27/52 (51%)	11 (40%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	7	-34	U
17	7	-28	U
17	7	-26	U
17	7	-25	U
17	7	-24	U
17	7	-23	U
17	7	-22	U
17	7	-21	U
17	7	-20	U
17	7	-11	U
17	7	-10	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

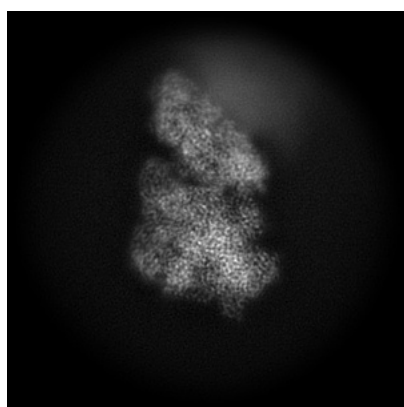
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44439. These allow visual inspection of the internal detail of the map and identification of artifacts.

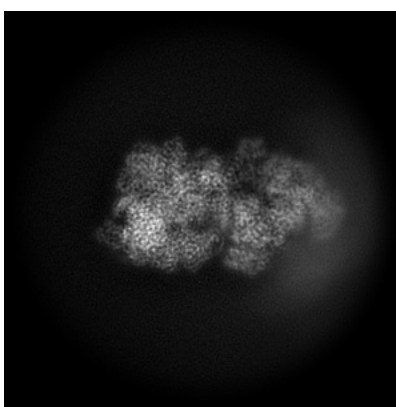
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

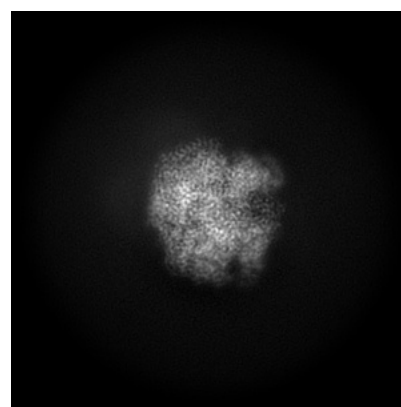
6.1.1 Primary map



X



Y

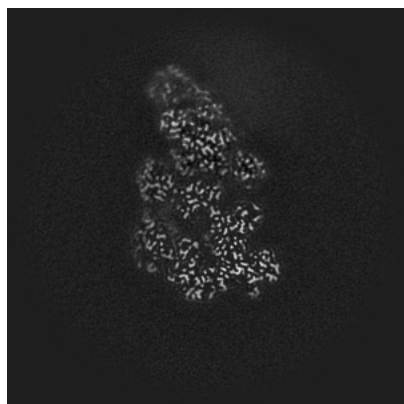


Z

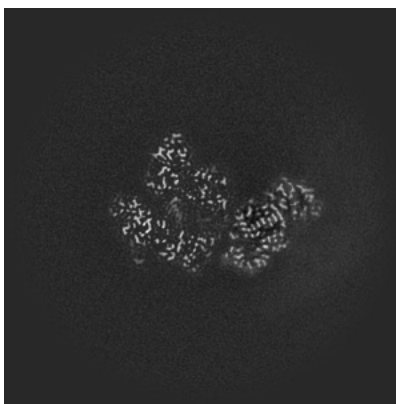
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

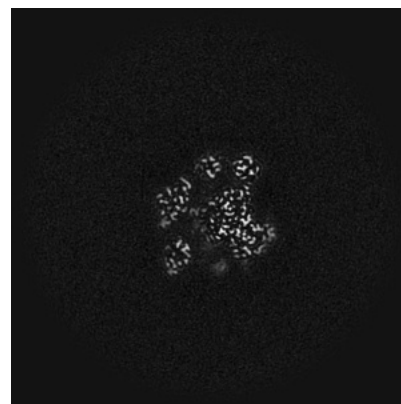
6.2.1 Primary map



X Index: 226



Y Index: 226

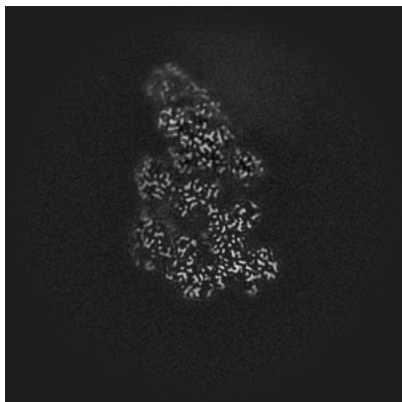


Z Index: 226

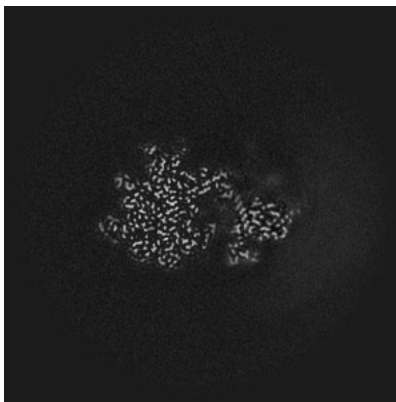
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

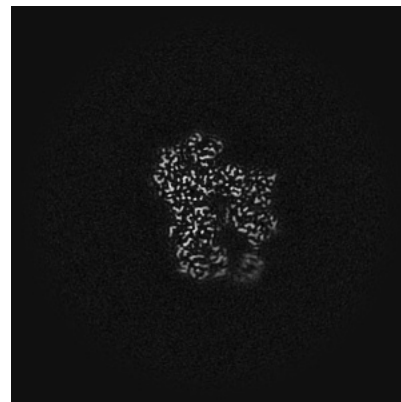
6.3.1 Primary map



X Index: 226



Y Index: 243

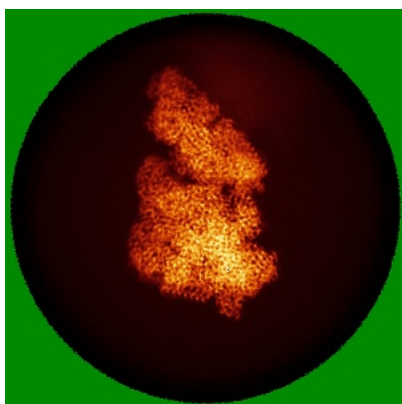


Z Index: 169

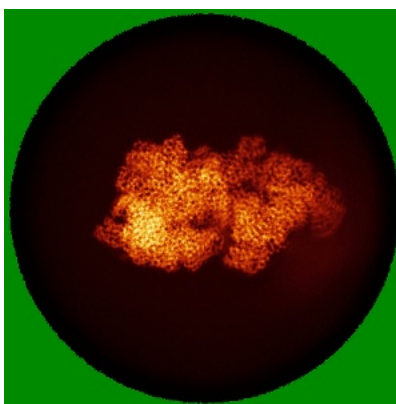
The images above show the largest variance slices of the map in three orthogonal directions.

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

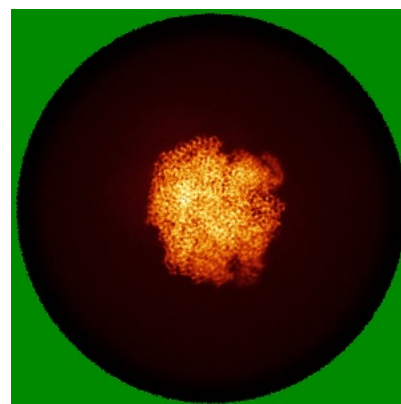
6.4.1 Primary map



X



Y



Z

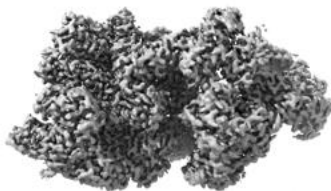
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

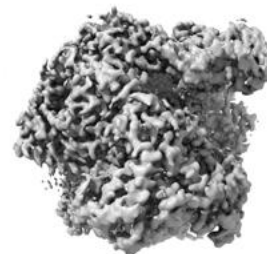
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

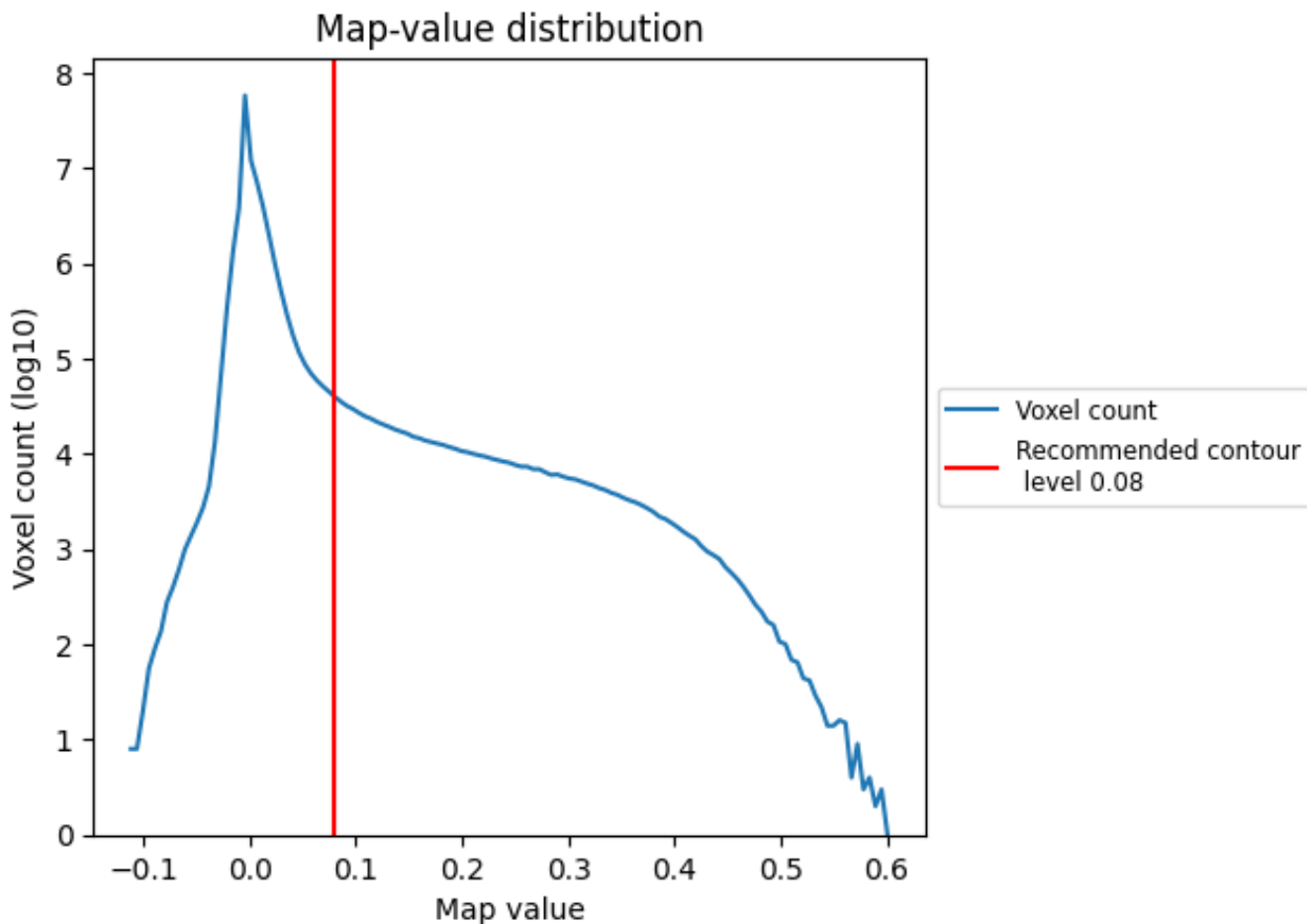
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

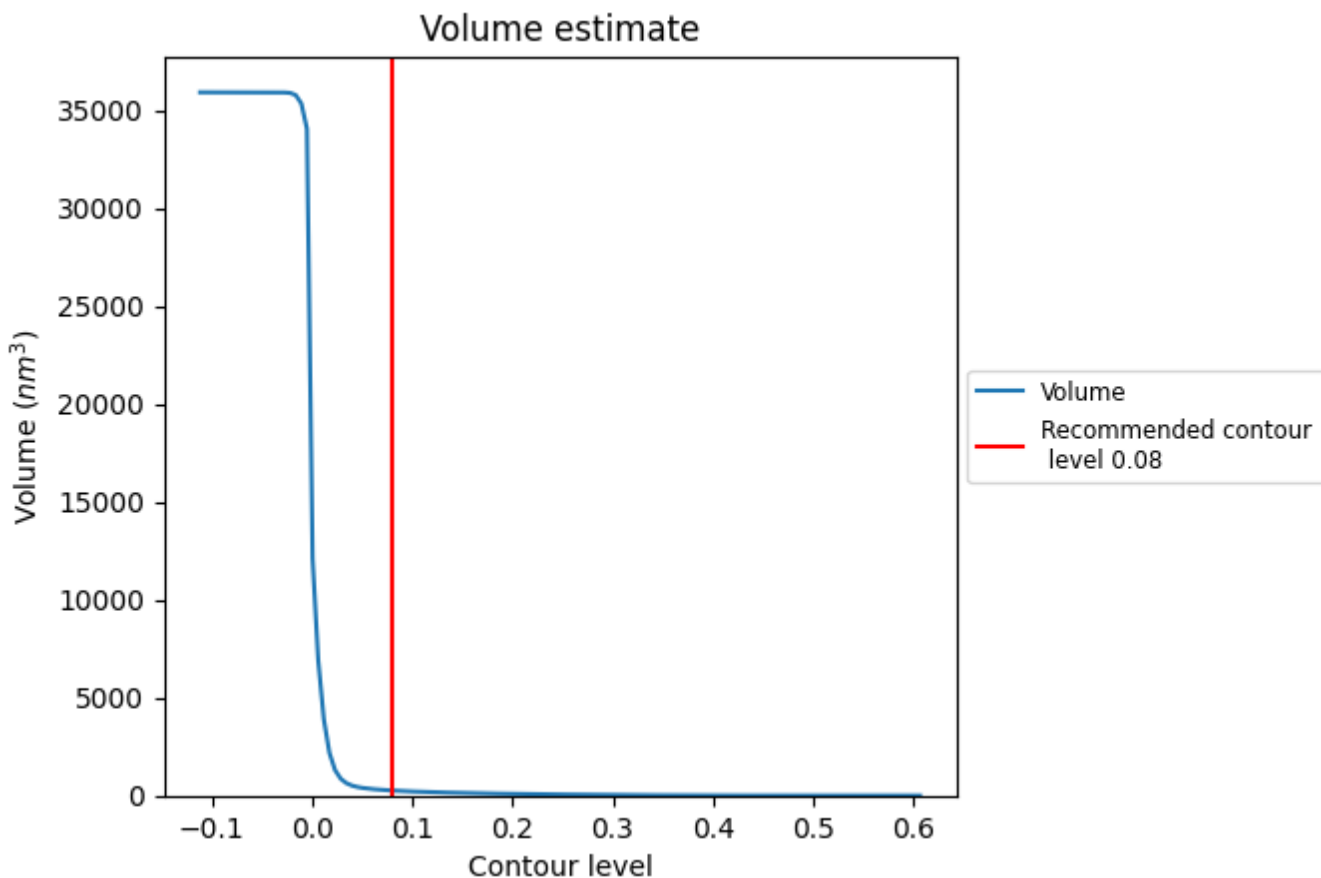
This section contains the results of statistical analysis of the map.

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.

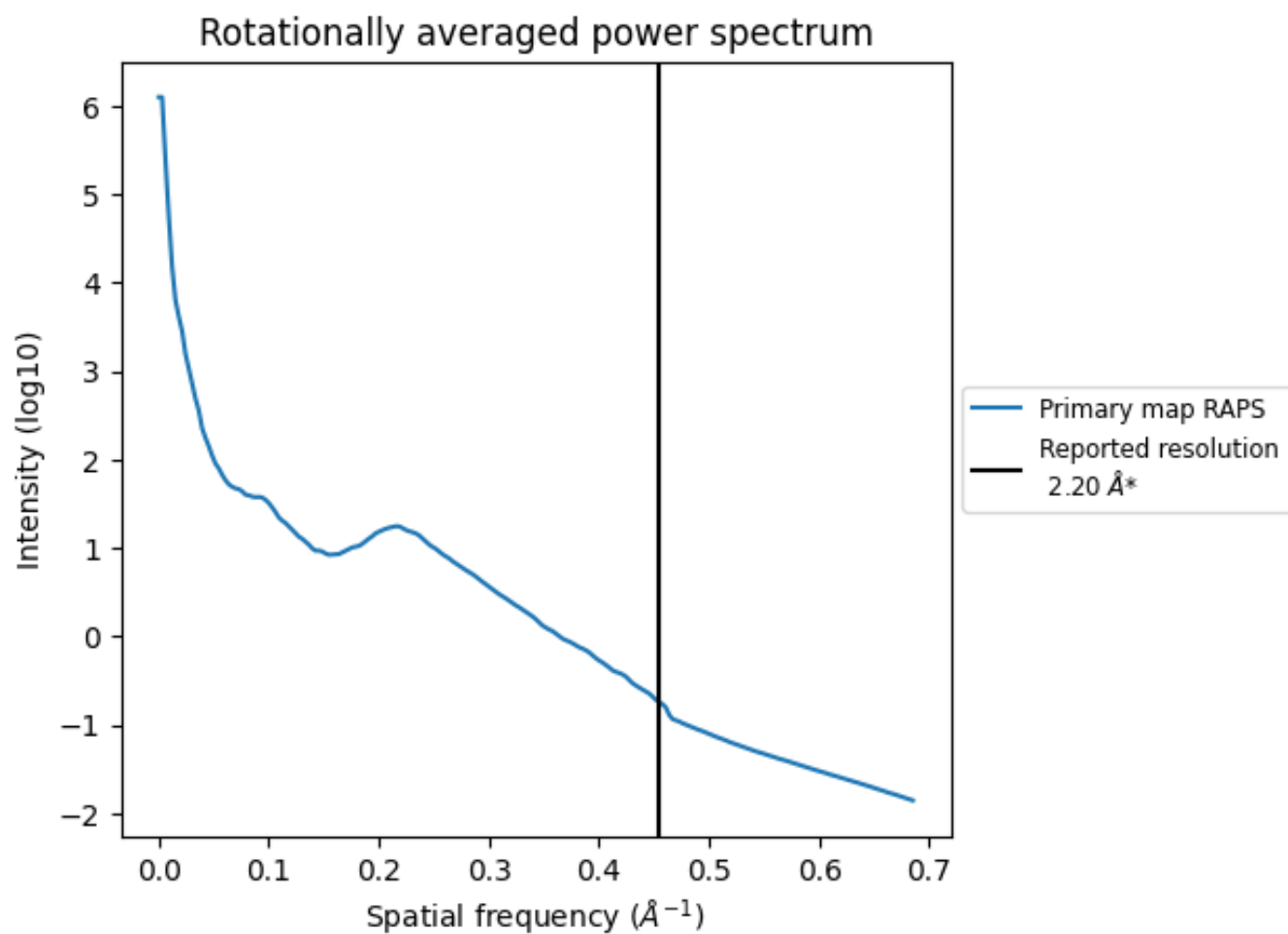
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm^3 ; this corresponds to an approximate mass of 232 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

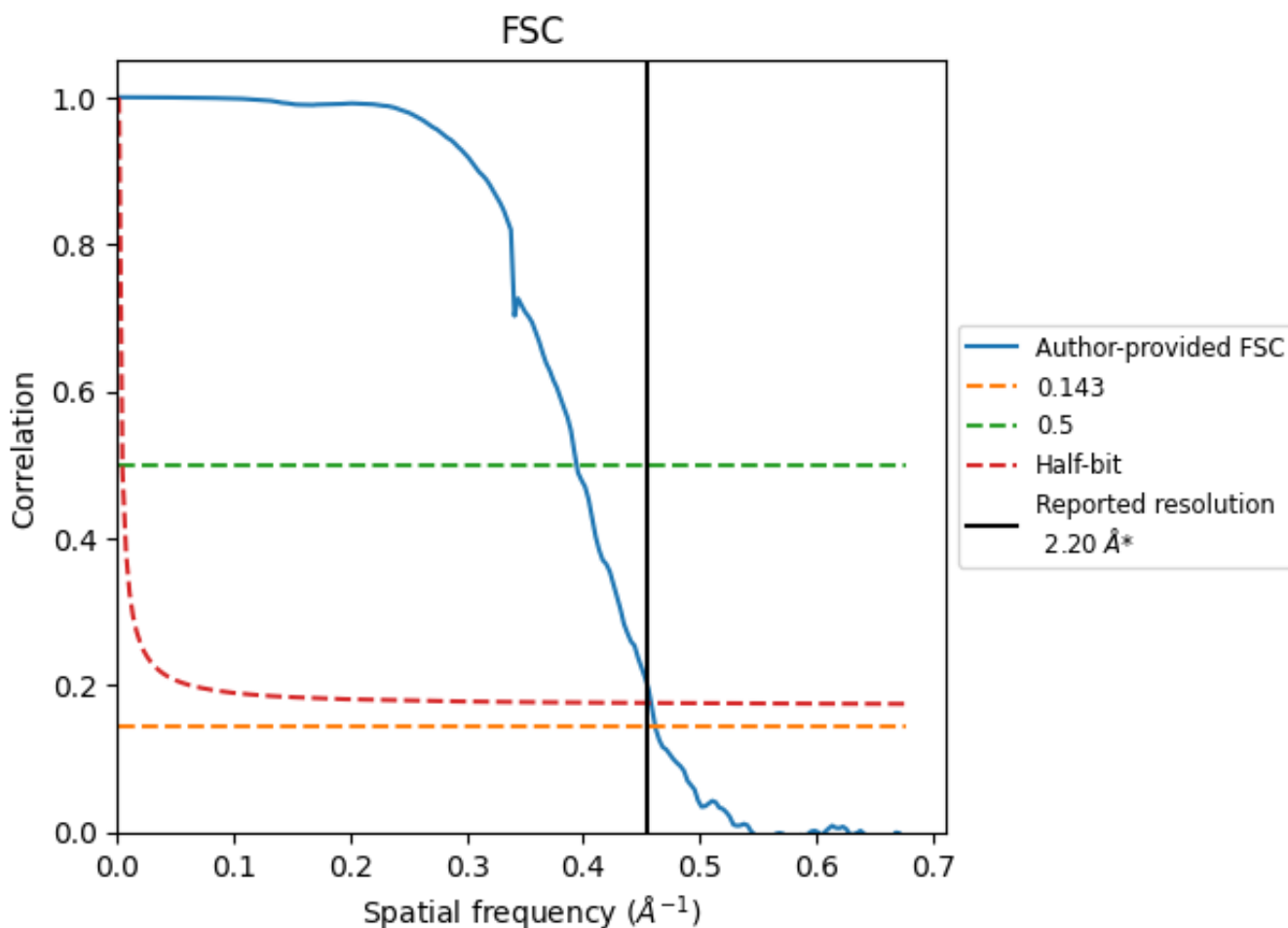


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

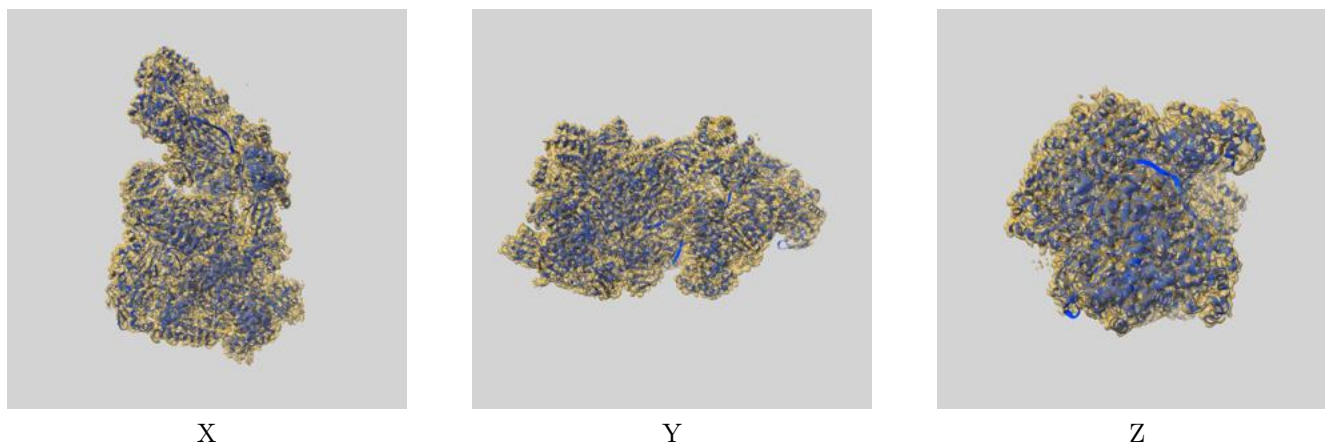
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.17	2.54	2.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

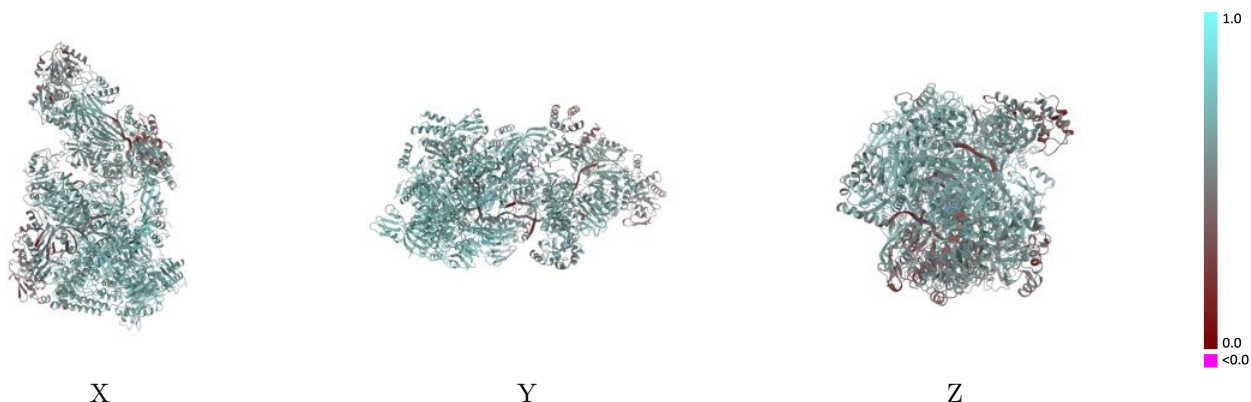
This section contains information regarding the fit between EMDB map EMD-44439 and PDB model 9BCU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



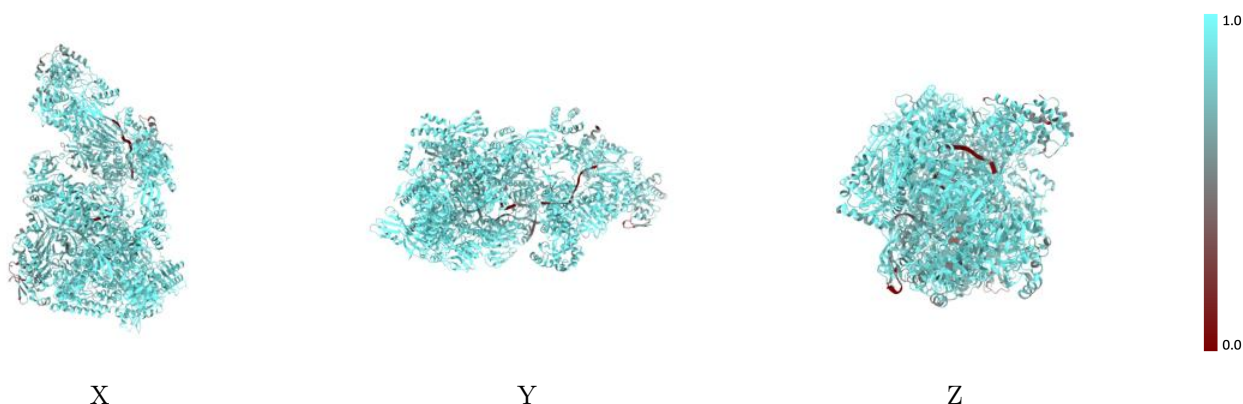
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



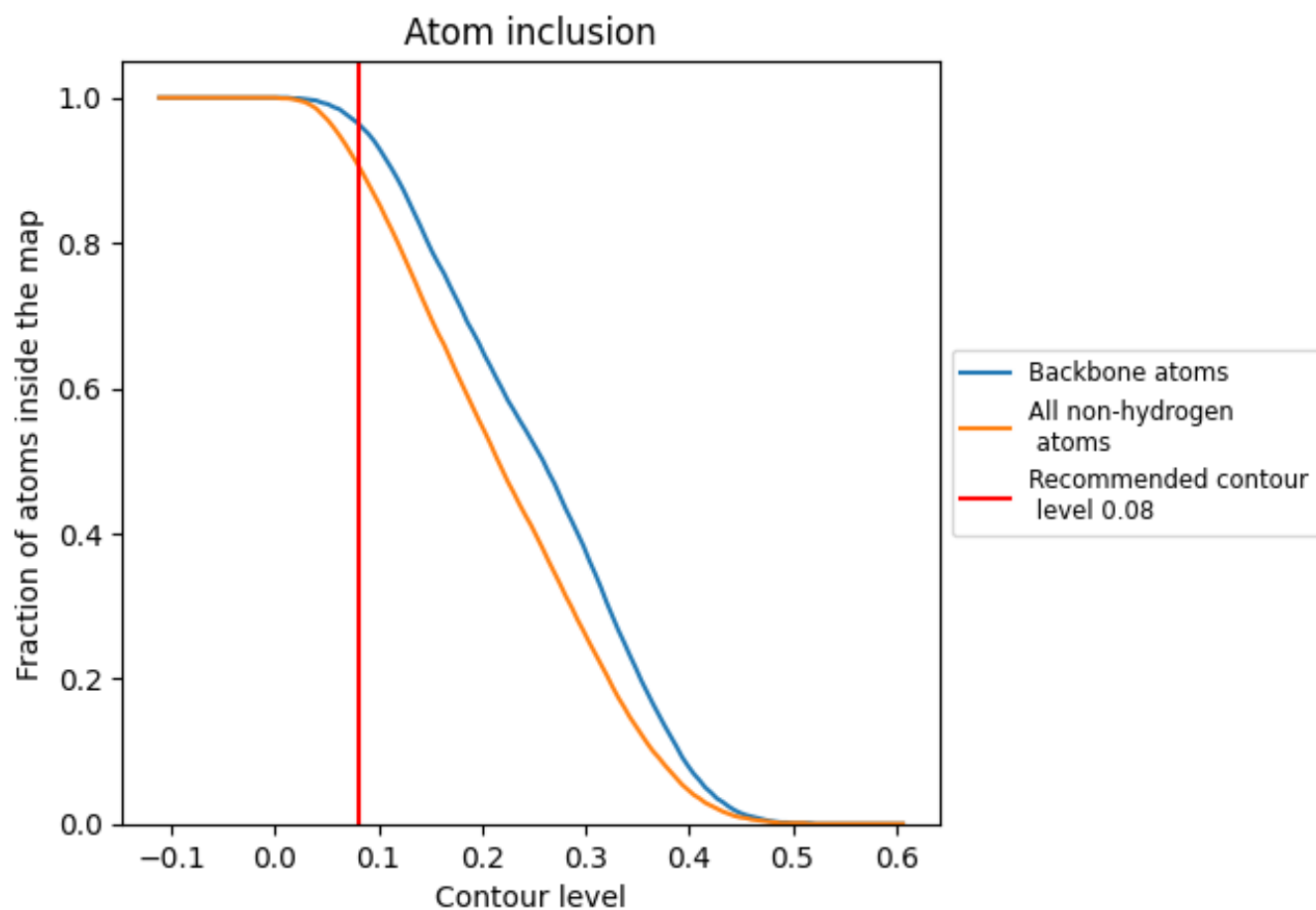
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.6130
5	 0.6980	 0.3790
6	 0.7360	 0.3980
7	 0.4770	 0.4620
A	 0.9520	 0.6650
B	 0.9470	 0.6570
C	 0.8670	 0.5880
D	 0.9680	 0.6700
E	 0.8650	 0.5720
F	 0.8230	 0.4700
G	 0.8510	 0.5740
H	 0.9450	 0.6620
I	 0.8100	 0.4880
J	 0.9350	 0.6150
K	 0.9500	 0.6650
L	 0.9670	 0.6760
M	 0.8630	 0.5460
N	 0.9730	 0.6760
P	 0.9360	 0.6310

