



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:16 AM UTC

PDB ID : 9BCU / pdb_00009bcu
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:

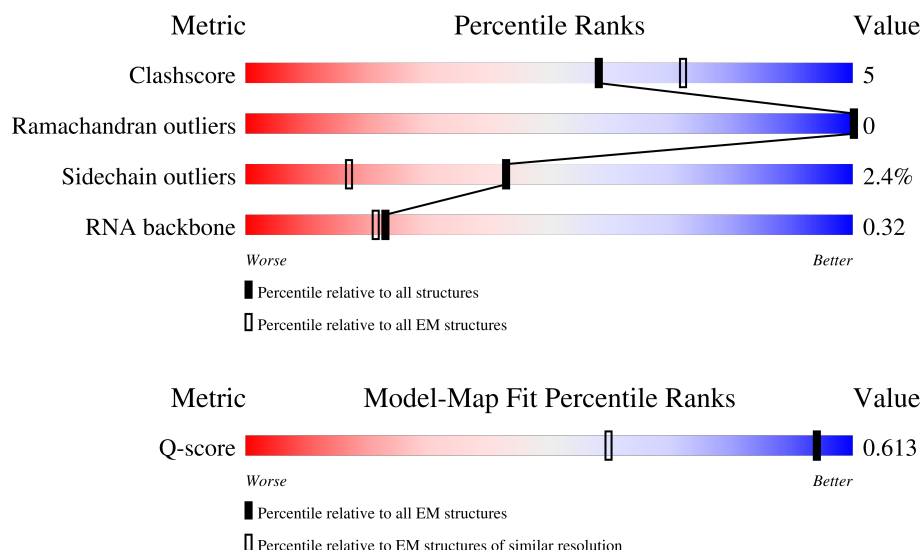
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



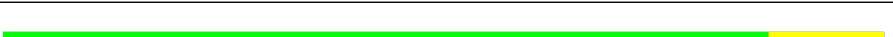
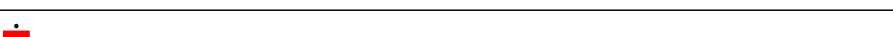
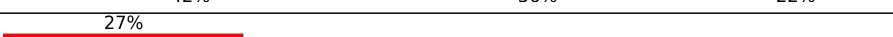
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	

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Mol	Chain	Length	Quality of chain
4	D	261	
5	E	190	
6	F	122	
7	H	82	
8	K	60	
9	L	94	
10	N	65	
11	P	49	
12	G	152	
13	I	73	
14	J	648	
14	M	648	
15	5	36	
16	6	36	
17	7	52	

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
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
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
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
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
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
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
7	H	77	Total	C	N	O	0	0
			636	412	106	118		

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

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

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

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

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

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

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

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

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

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

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

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

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 (CCD ID: MG) (formula: Mg).

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

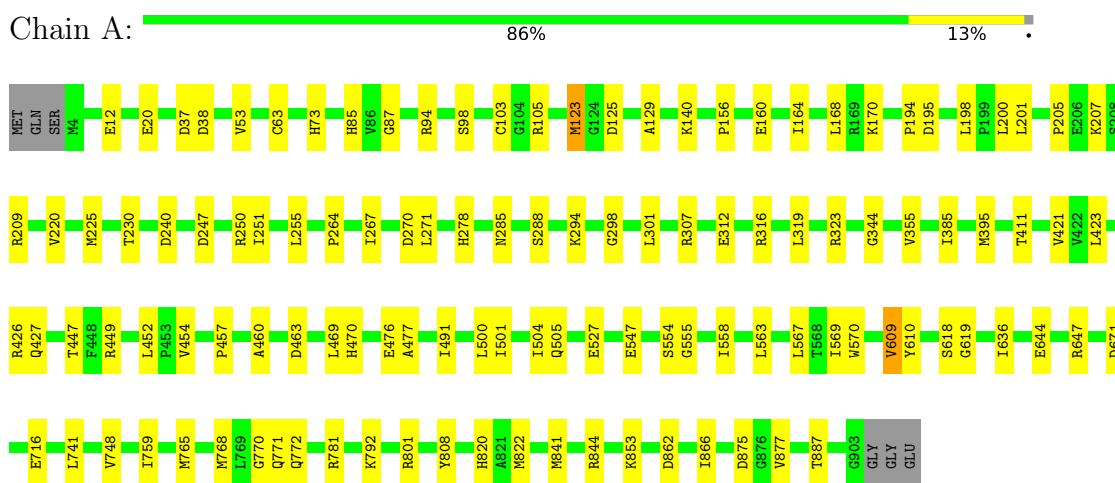
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

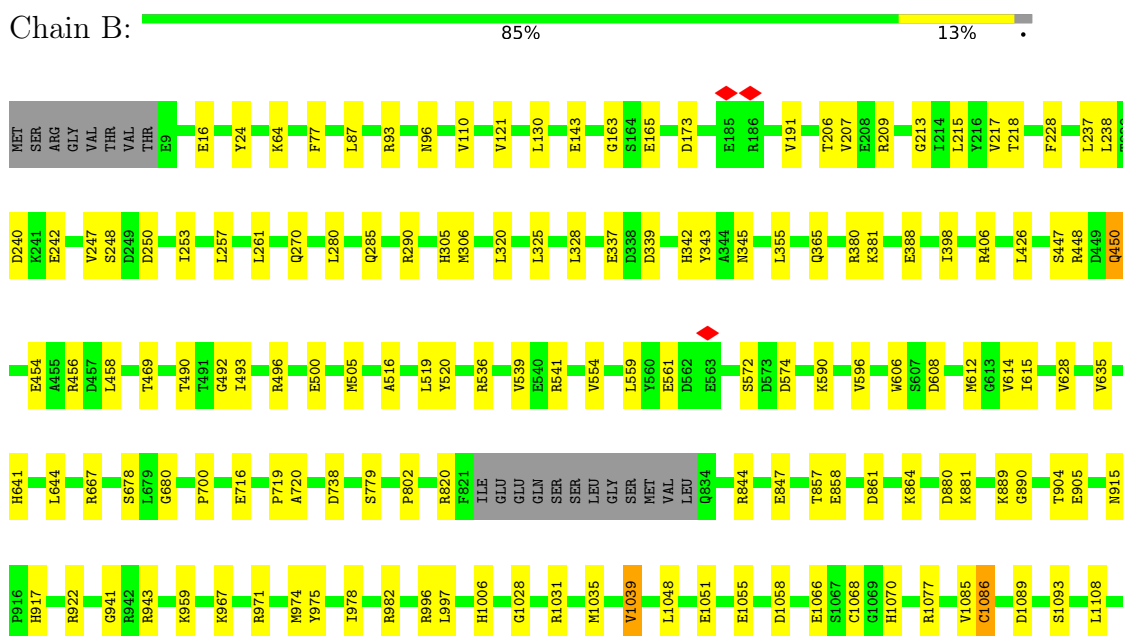
3 Residue-property plots

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'

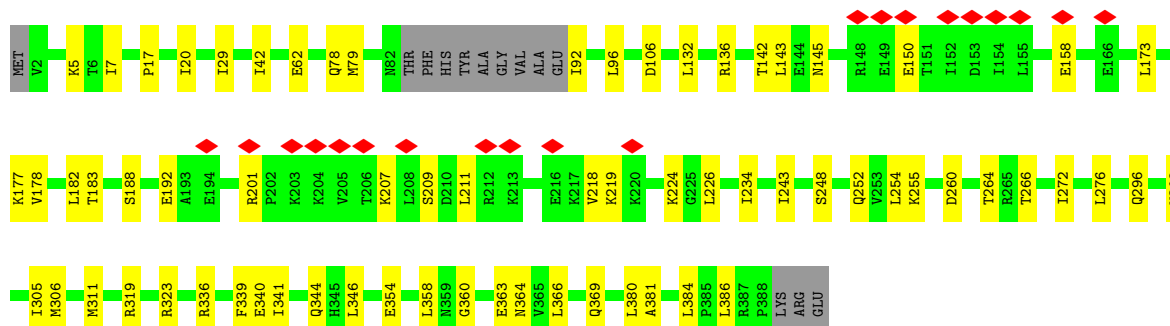
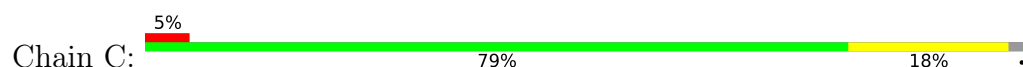


• Molecule 2: DNA-directed RNA polymerase subunit B

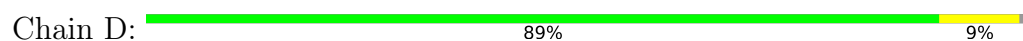




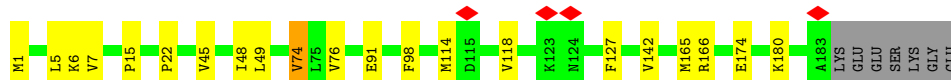
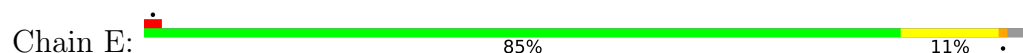
- Molecule 3: DNA-directed RNA polymerase subunit A"



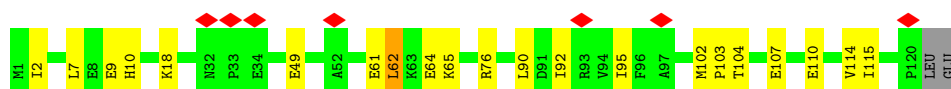
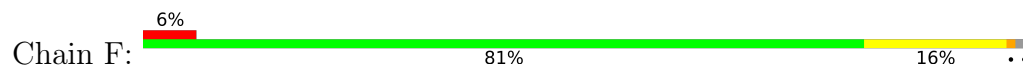
- Molecule 4: DNA-directed RNA polymerase subunit D



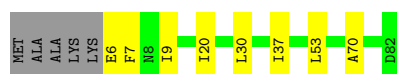
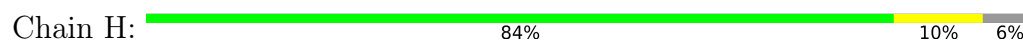
- Molecule 5: DNA-directed RNA polymerase subunit E



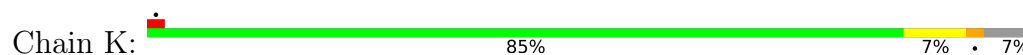
- Molecule 6: DNA-directed RNA polymerase subunit F



- Molecule 7: DNA-directed RNA polymerase subunit H



- Molecule 8: DNA-directed RNA polymerase subunit K





- Molecule 9: DNA-directed RNA polymerase subunit L

Chain L: 91% 7% .



- Molecule 10: DNA-directed RNA polymerase subunit N

Chain N: 86% 12% .



- Molecule 11: DNA-directed RNA polymerase subunit P

Chain P: 88% 10% .



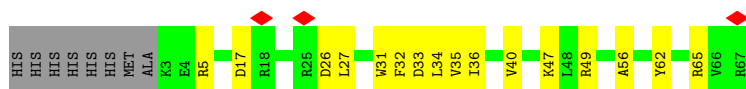
- Molecule 12: Transcription elongation factor Spt5

Chain G: 75% 21% . .



- Molecule 13: Transcription elongation factor Spt4

Chain I: 67% 22% 11%

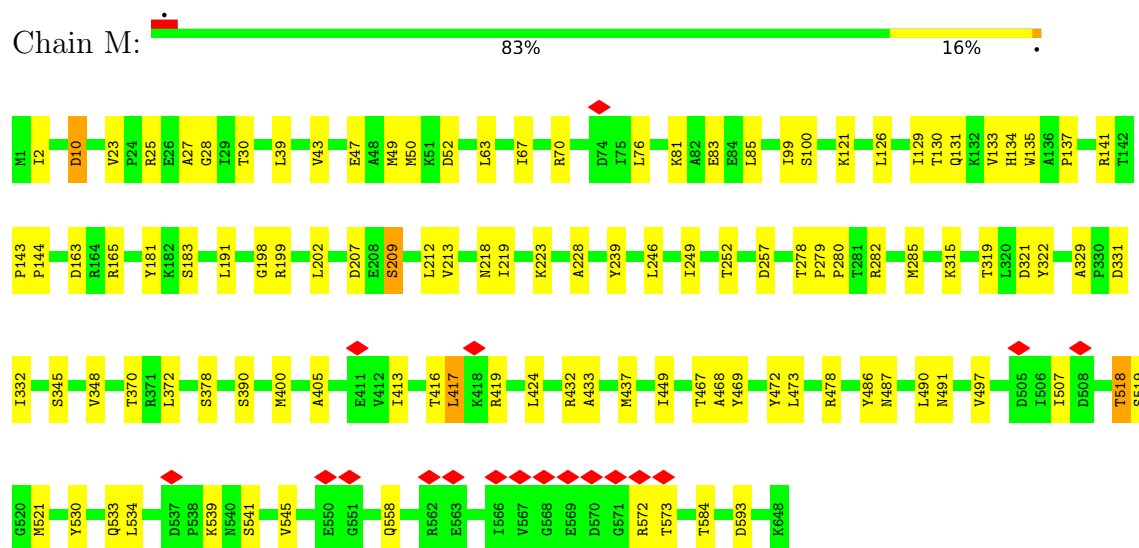


- Molecule 14: Transcription termination factor FttA

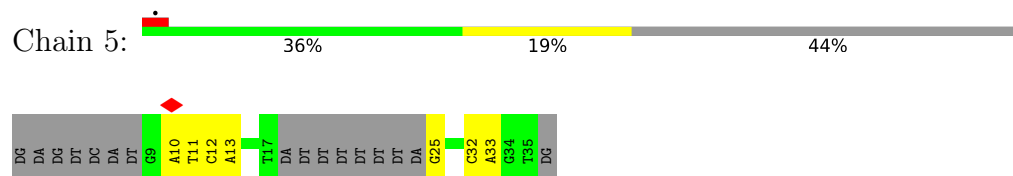
Chain J: 86% 13%



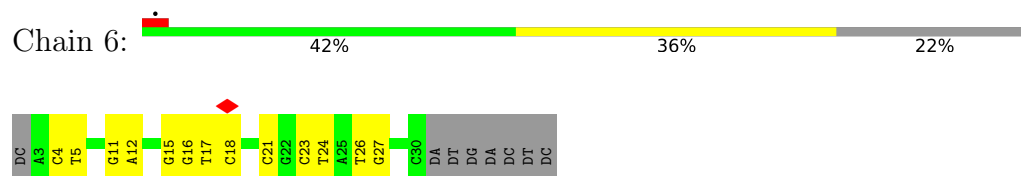
- Molecule 14: Transcription termination factor FttA



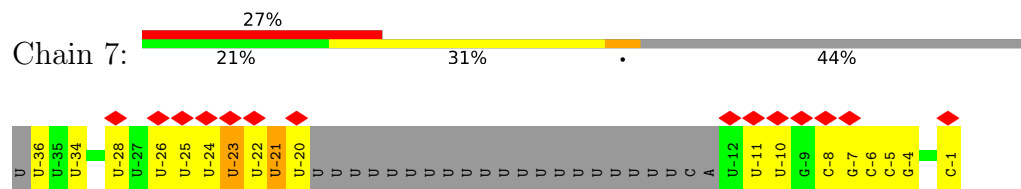
- Molecule 15: non-template strand DNA



- 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 ($\text{\AA}$)	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 ($\text{\AA}$)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/7325	0.22	0/9887
2	B	0.09	0/8985	0.23	0/12140
3	C	0.12	0/2994	0.31	0/4042
4	D	0.08	0/2098	0.22	0/2841
5	E	0.10	0/1502	0.29	0/2023
6	F	0.12	0/1023	0.32	0/1376
7	H	0.09	0/650	0.23	0/877
8	K	0.08	0/441	0.22	0/598
9	L	0.07	0/791	0.18	0/1066
10	N	0.08	0/539	0.22	0/723
11	P	0.06	0/378	0.22	0/507
12	G	0.09	0/1164	0.28	1/1577 (0.1%)
13	I	0.08	0/520	0.22	0/703
14	J	0.10	0/5253	0.25	0/7115
14	M	0.11	0/5264	0.30	0/7132
15	5	0.14	0/458	0.32	0/702
16	6	0.16	0/643	0.33	0/991
17	7	0.07	0/651	0.14	0/1004
All	All	0.10	0/40679	0.26	1/55304 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	15	GLN	CA-CB-CG	5.18	124.46	114.10

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	66	0
2	B	8808	0	8864	89	0
3	C	2958	0	3077	38	0
4	D	2053	0	2063	16	0
5	E	1476	0	1512	14	0
6	F	1003	0	1007	14	0
7	H	636	0	646	6	0
8	K	433	0	466	5	0
9	L	776	0	770	6	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	45	0
14	M	5155	0	5253	65	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	371	0

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

All (371) 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
14:M:282:ARG:HA	14:M:285:MET:HE2	1.88	0.56
3:C:226:LEU:HD22	3:C:252:GLN:HB3	1.87	0.56
2:B:505:MET:HE2	2:B:541:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:426:LEU:HD13	16:6:21:DC:H5''	1.88	0.56
14:M:50:MET:HE1	14:M:130:THR:HG23	1.87	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
14:J:282:ARG:HA	14:J:285:MET:HE2	1.87	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
5:E:142:VAL:HB	5:E:165:MET:HE1	1.90	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:123:MET:HE3	1:A:129:ALA:HB1	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:79:MET:HE2	3:C:296:GLN:HG3	1.93	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
6:F:102:MET:HE3	6:F:103:PRO:HD2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:N:57:ASP:HA	10:N:60:MET:HE2	1.95	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:491:ILE:HA	1:A:501:ILE:HG13	1.96	0.47
14:M:539:LYS:O	14:M:539:LYS:NZ	2.35	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
14:J:322:TYR:OH	14:J:345:SER:O	2.30	0.47
2:B:305:HIS:NE2	2:B:306:MET:HE3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:395:MET:HE2	1:A:395:MET:HB3	1.78	0.45
3:C:384:LEU:HD23	5:E:22:PRO:HB3	1.97	0.45
5:E:174:GLU:CD	5:E:174:GLU:H	2.24	0.45
14:J:586:ASP:OD2	14:J:586:ASP:N	2.43	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:52:ASP:N	14:M:52:ASP:OD1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
14:M:521:MET:HE2	14:M:521:MET:HA	1.99	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
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
13:I:35:VAL:O	13:I:62:TYR:N	2.47	0.43
1:A:841:MET:HE2	1:A:841:MET:HB3	1.87	0.43
2:B:844:ARG:HB2	2:B:847:GLU:HG3	1.99	0.43
3:C:248:SER:HG	3:C:266:THR:HG1	1.62	0.43
12:G:117:ASP:HB3	14:M:2:ILE:HG13	2.00	0.43
2:B:520:TYR:OH	2:B:561:GLU:OE1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:L:1:MET:HE3	9:L:1:MET:HB2	1.77	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
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
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: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
2:B:1066:GLU:OE2	2:B:1093:SER:OG	2.30	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:181:TYR:OH	14:M:207:ASP:OD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:M:209:SER:OG	14:M:331:ASP:OD1	2.34	0.41
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:J:261:MET:HE3	14:J:264:TYR:CG	2.56	0.41
14:M:130:THR:HA	14:M:133:VAL:HG12	2.02	0.41
14:M:400:MET:HE2	14:M:405:ALA:HA	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
4:D:9:LYS:HE3	4:D:9:LYS:HB2	1.89	0.41
6:F:102:MET:HE3	6:F:102:MET:HA	2.03	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:1:MET:HE3	6:F:76:ARG:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:294:LYS:HZ2	1:A:298:GLY:HA2	1.83	0.41
1:A:457:PRO:HG3	1:A:500:LEU:HG	2.03	0.41
1:A:768:MET:HE3	1:A:770:GLY:HA2	2.02	0.41
2:B:280:LEU:HD23	2:B:280:LEU:HA	1.89	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
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
14:M:81:LYS:HZ2	14:M:85:LEU:HG	1.85	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
3:C:173:LEU:HA	3:C:177:LYS:HZ3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:4:DC:H2''	16:6:5:DT:H5'	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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 ⓘ

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%)	752 (97%)	22 (3%)	38	52
2	B	950/969 (98%)	929 (98%)	21 (2%)	45	61
3	C	324/334 (97%)	313 (97%)	11 (3%)	32	44
4	D	226/230 (98%)	220 (97%)	6 (3%)	39	53
5	E	160/167 (96%)	157 (98%)	3 (2%)	50	66
6	F	105/107 (98%)	104 (99%)	1 (1%)	68	81
7	H	69/72 (96%)	69 (100%)	0	100	100
8	K	45/49 (92%)	43 (96%)	2 (4%)	25	34
9	L	81/81 (100%)	80 (99%)	1 (1%)	63	78
10	N	59/59 (100%)	58 (98%)	1 (2%)	53	69
11	P	38/40 (95%)	37 (97%)	1 (3%)	40	55
12	G	127/131 (97%)	122 (96%)	5 (4%)	28	39
13	I	55/65 (85%)	55 (100%)	0	100	100
14	J	562/565 (100%)	551 (98%)	11 (2%)	48	64
14	M	561/565 (99%)	545 (97%)	16 (3%)	37	51
All	All	4136/4213 (98%)	4035 (98%)	101 (2%)	43	58

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	38	ASP
1	A	53	VAL
1	A	98	SER
1	A	103	CYS
1	A	123	MET
1	A	125	ASP
1	A	200	LEU
1	A	220	VAL
1	A	288	SER

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	355	VAL
1	A	421	VAL
1	A	454	VAL
1	A	469	LEU
1	A	547	GLU
1	A	554	SER
1	A	609	VAL
1	A	618	SER
1	A	759	ILE
1	A	792	LYS
1	A	853	LYS
2	B	130	LEU
2	B	173	ASP
2	B	191	VAL
2	B	238	LEU
2	B	270	GLN
2	B	337	GLU
2	B	343	TYR
2	B	355	LEU
2	B	388	GLU
2	B	447	SER
2	B	450	GLN
2	B	469	THR
2	B	635	VAL
2	B	644	LEU
2	B	678	SER
2	B	779	SER
2	B	861	ASP
2	B	1039	VAL
2	B	1085	VAL
2	B	1086	CYS
2	B	1112	VAL
3	C	78	GLN
3	C	92	ILE
3	C	96	LEU
3	C	132	LEU
3	C	150	GLU
3	C	183	THR
3	C	188	SER
3	C	218	VAL
3	C	254	LEU

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Mol	Chain	Res	Type
3	C	341	ILE
3	C	369	GLN
4	D	19	SER
4	D	48	LEU
4	D	76	SER
4	D	185	SER
4	D	219	SER
4	D	232	VAL
5	E	5	LEU
5	E	49	LEU
5	E	74	VAL
6	F	62	LEU
8	K	22	MET
8	K	32	GLU
9	L	9	GLU
10	N	53	VAL
11	P	44	ARG
12	G	8	THR
12	G	57	VAL
12	G	123	ILE
12	G	127	LEU
12	G	143	VAL
14	J	107	GLU
14	J	108	VAL
14	J	183	SER
14	J	217	VAL
14	J	293	ILE
14	J	308	LYS
14	J	356	LEU
14	J	390	SER
14	J	497	VAL
14	J	499	ASN
14	J	527	SER
14	M	10	ASP
14	M	23	VAL
14	M	30	THR
14	M	70	ARG
14	M	100	SER
14	M	183	SER
14	M	191	LEU
14	M	209	SER
14	M	219	ILE

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Mol	Chain	Res	Type
14	M	378	SER
14	M	390	SER
14	M	417	LEU
14	M	424	LEU
14	M	449	ILE
14	M	497	VAL
14	M	518	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	295	HIS
1	A	538	ASN
1	A	612	GLN
1	A	772	GLN
1	A	815	GLN
1	A	850	GLN
2	B	78	GLN
2	B	116	GLN
2	B	270	GLN
2	B	373	GLN
2	B	450	GLN
2	B	771	GLN
2	B	783	GLN
3	C	268	ASN
4	D	117	ASN
4	D	227	ASN
5	E	82	GLN
5	E	124	ASN
5	E	126	GLN
5	E	133	ASN
5	E	162	ASN
6	F	58	GLN
12	G	150	GLN
14	J	21	GLN
14	J	45	ASN
14	J	158	GLN
14	J	253	HIS
14	J	556	GLN
14	J	629	HIS
14	M	45	ASN

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Mol	Chain	Res	Type
14	M	131	GLN
14	M	158	GLN
14	M	174	ASN
14	M	290	GLN
14	M	337	HIS
14	M	338	ASN
14	M	399	GLN
14	M	548	GLN
14	M	558	GLN
14	M	583	HIS

5.3.3 RNA ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

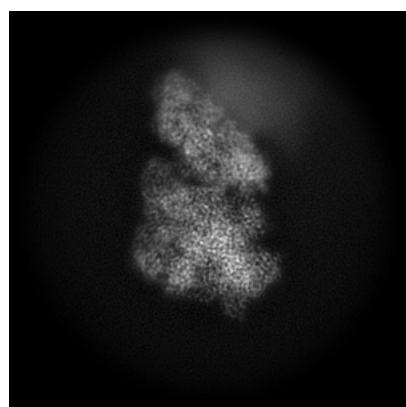
6 Map visualisation [i](#)

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

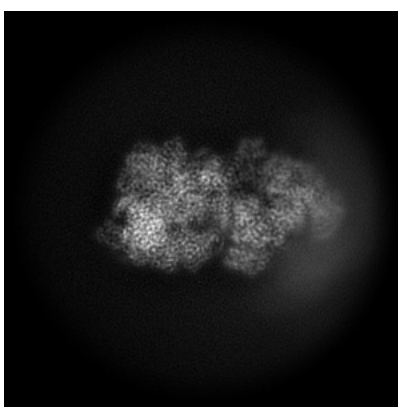
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

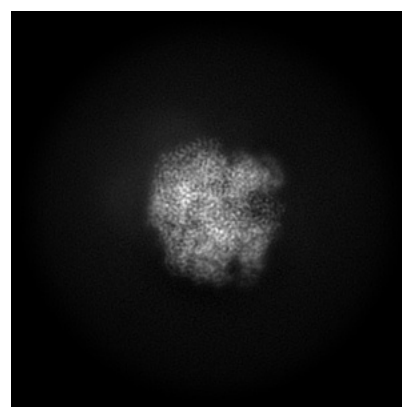
6.1.1 Primary map



X



Y

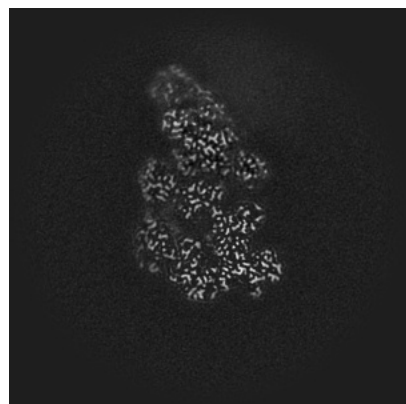


Z

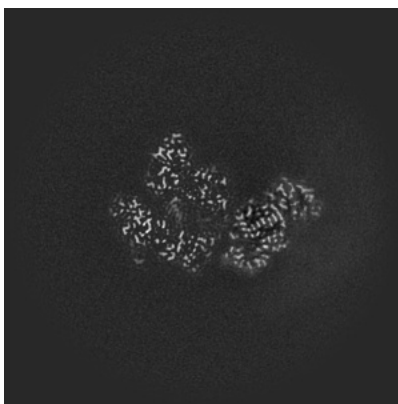
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

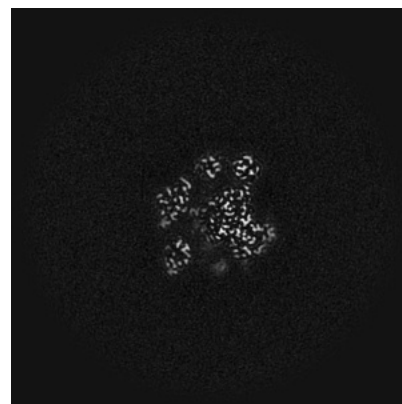
6.2.1 Primary map



X Index: 226



Y Index: 226

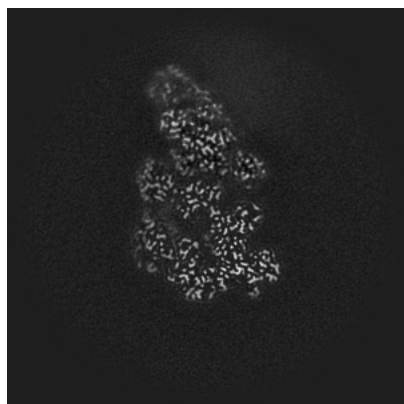


Z Index: 226

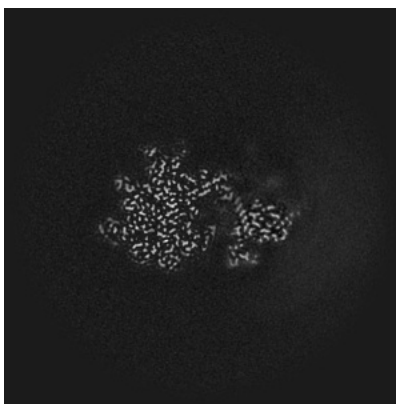
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

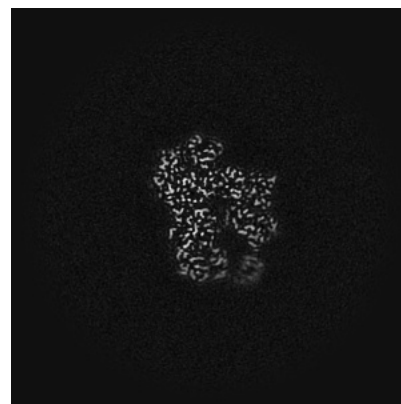
6.3.1 Primary map



X Index: 226



Y Index: 243

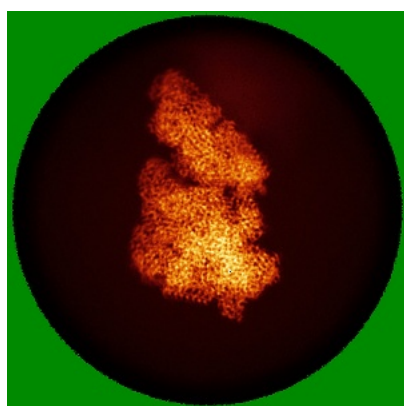


Z Index: 169

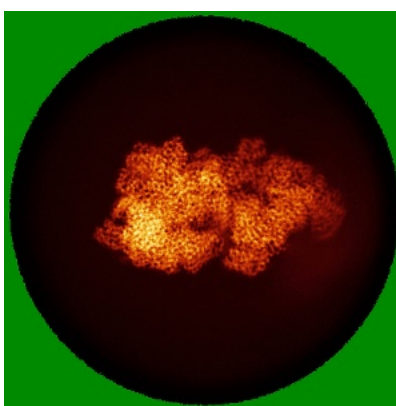
The images above show the largest variance slices of the map in three orthogonal directions.

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

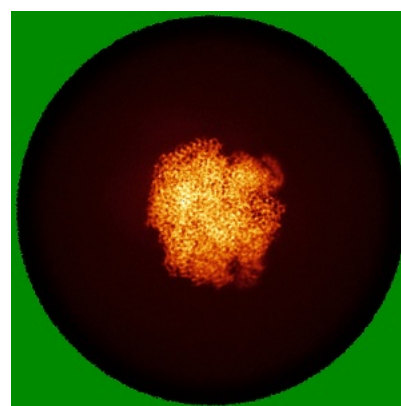
6.4.1 Primary map



X



Y



Z

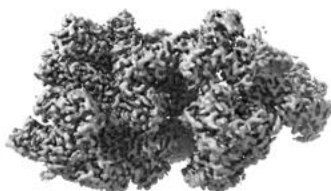
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

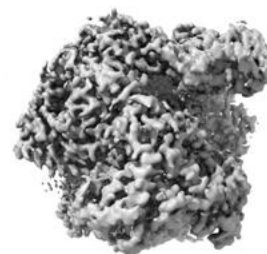
6.5.1 Primary map



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.

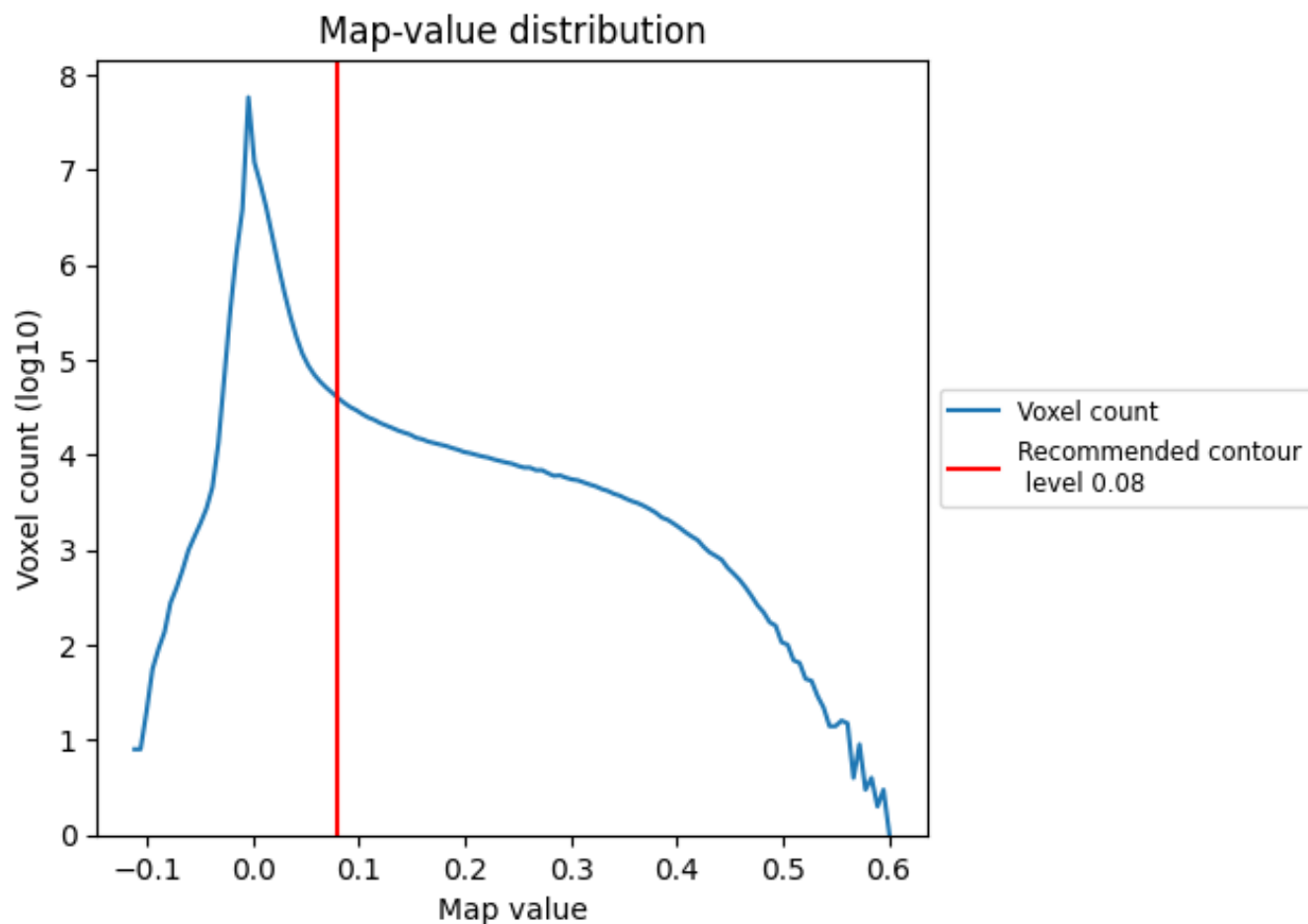
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

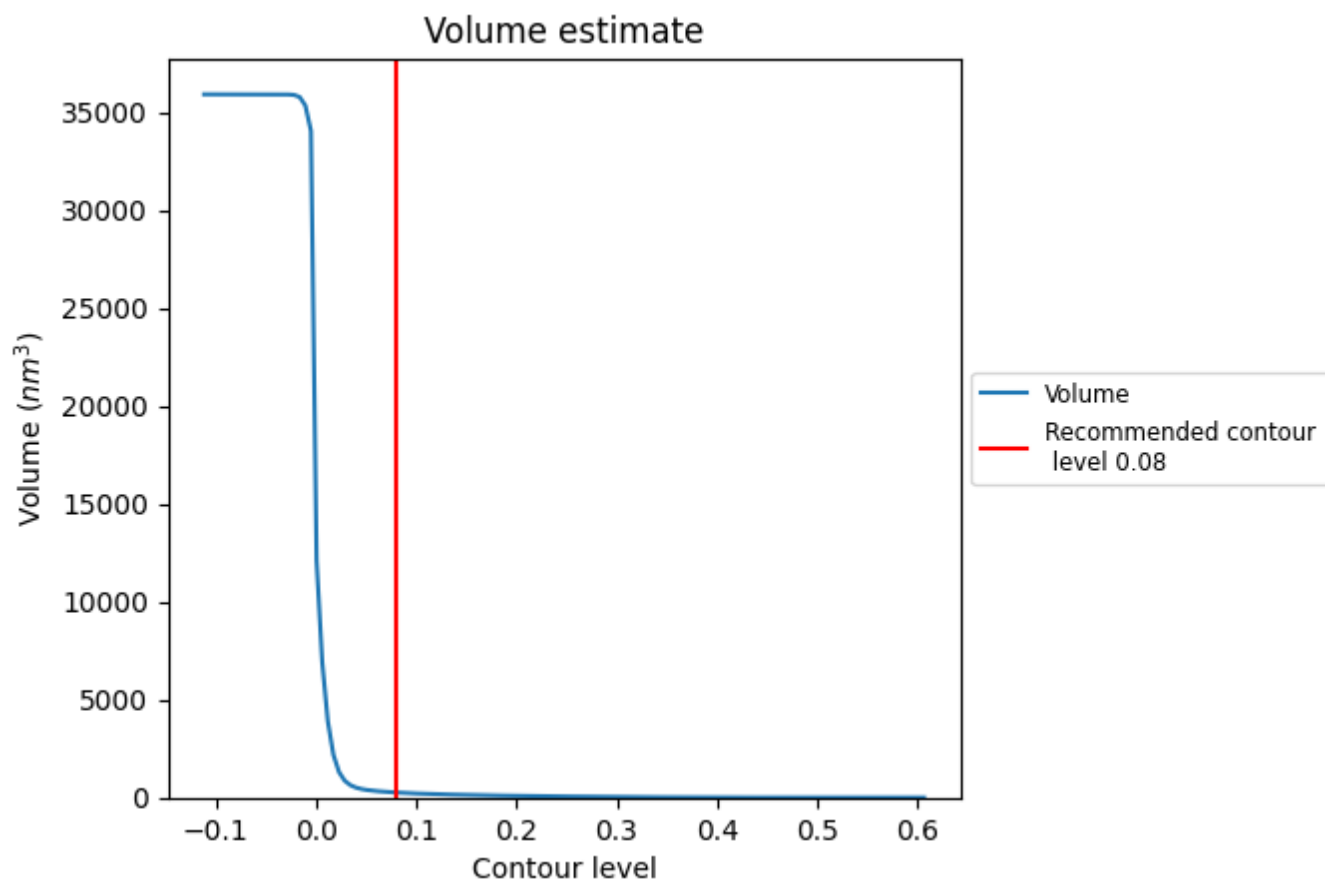
This section contains the results of statistical analysis of the map.

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.

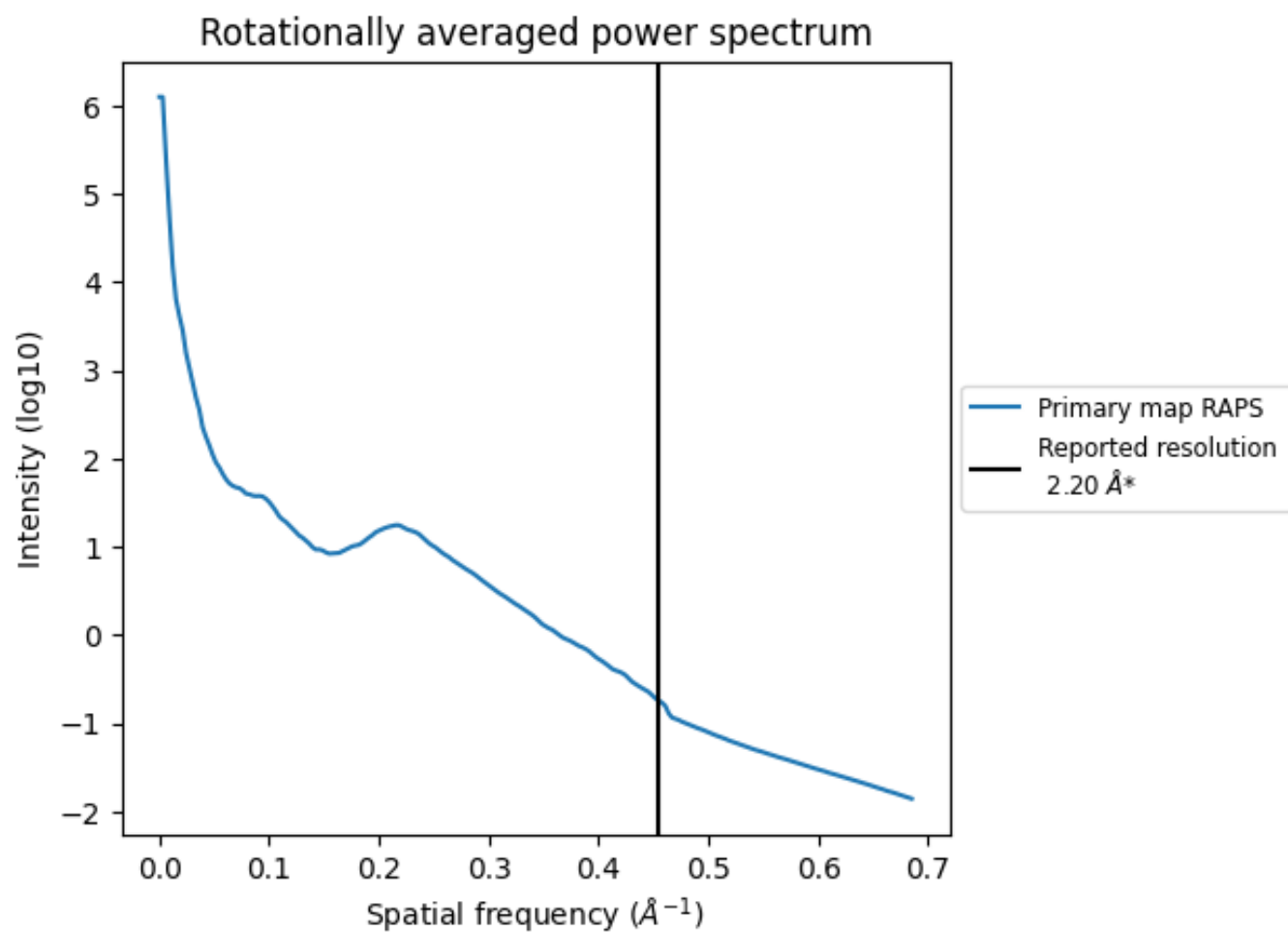
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; 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 ⓘ

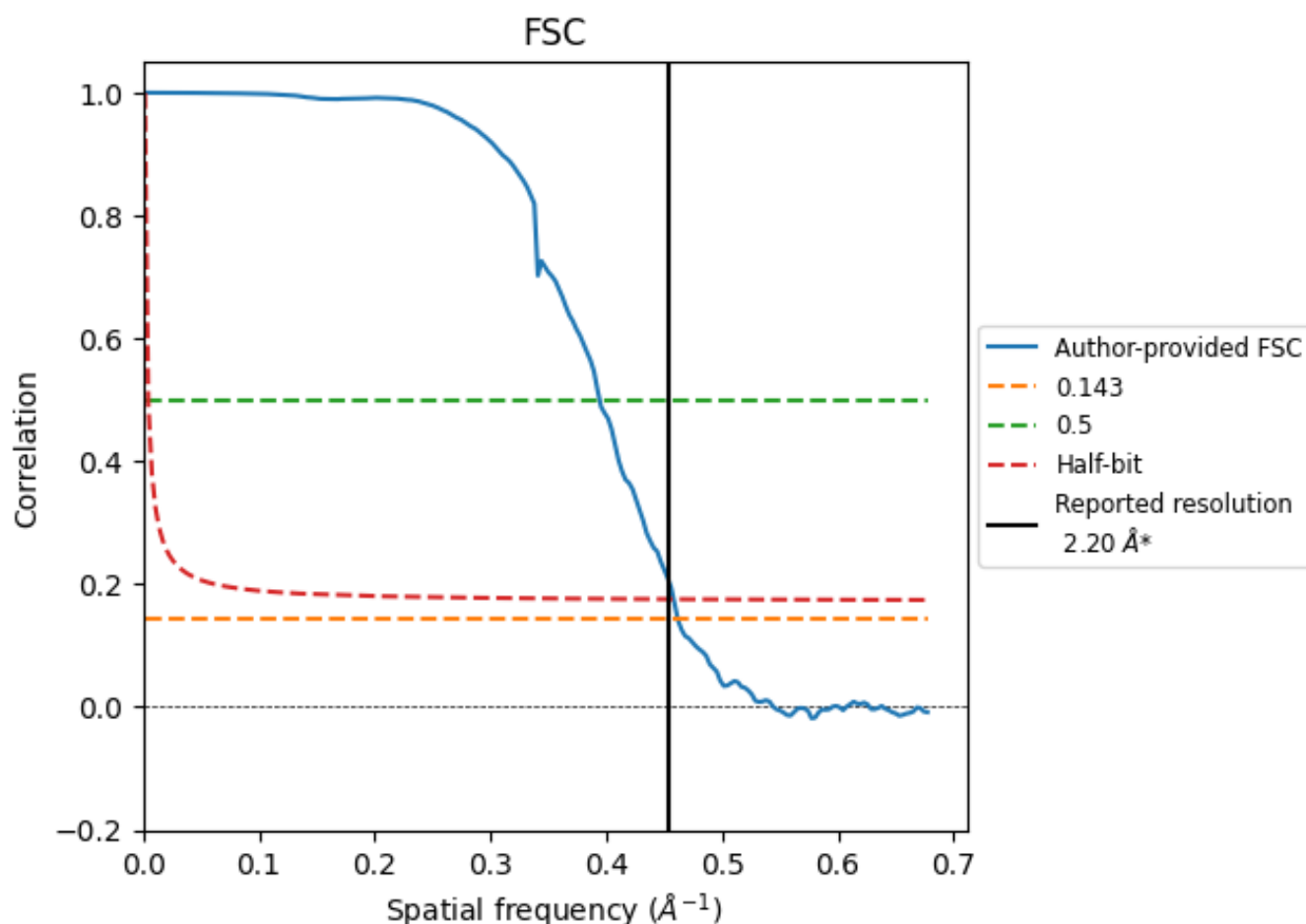


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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.

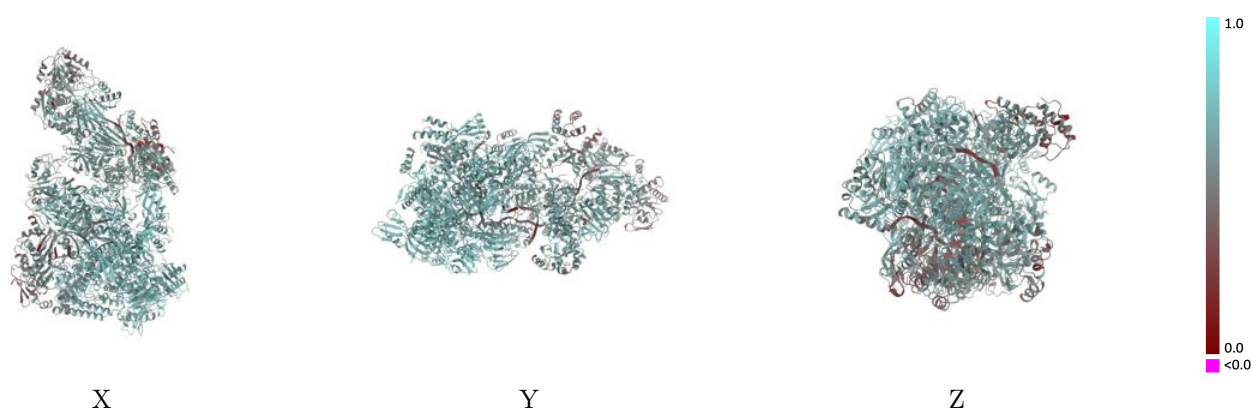
9 Map-model fit [i](#)

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](#)

This section was not generated.

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

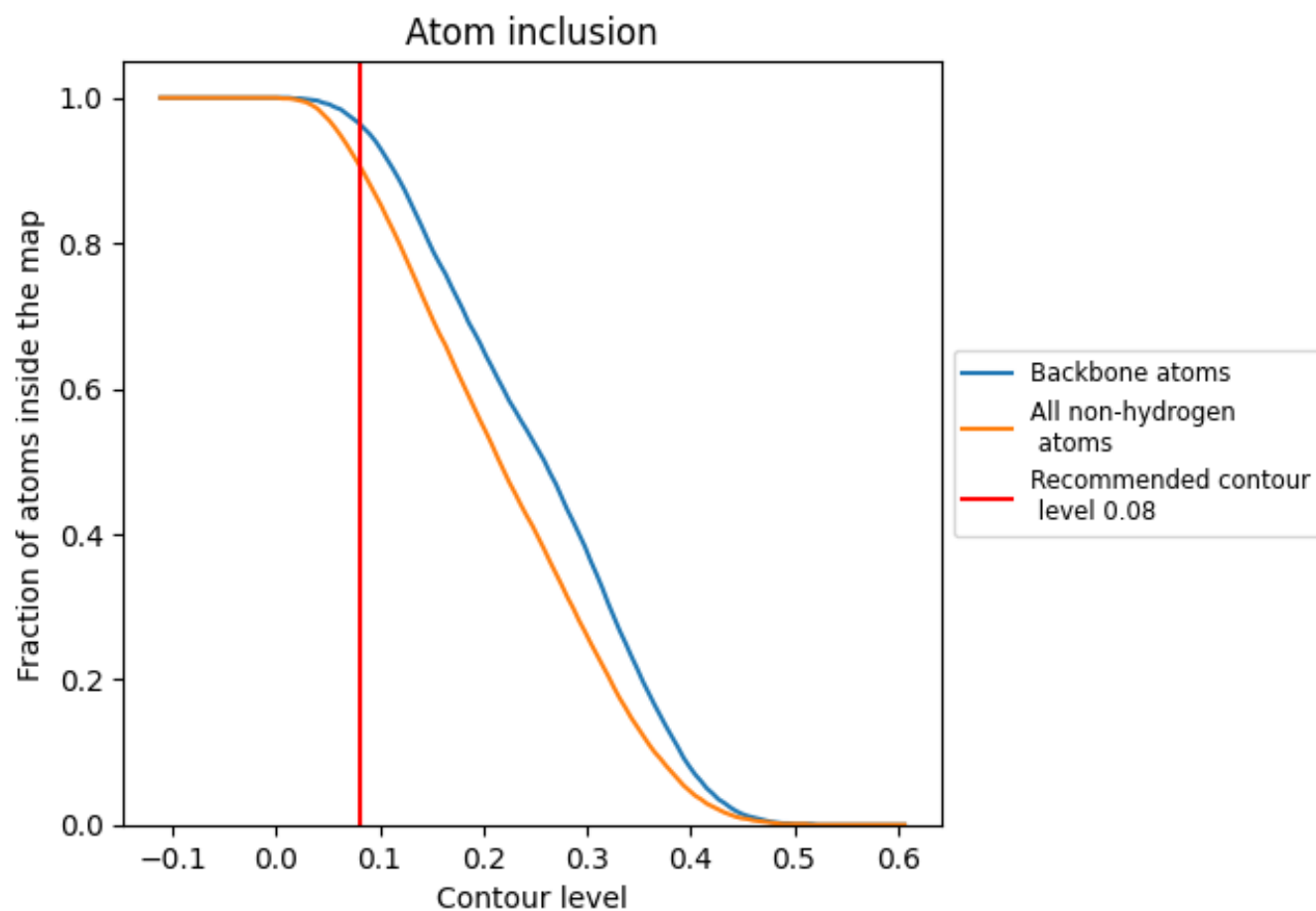


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



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

