



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 8K60 / pdb_00008k60
EMDB ID : EMD-36914
Title : Cryo-EM structure of Streptomyces coelicolor transcription initiation complex with the global transcription factor AfsR
Authors : Lin, W.; Shi, J.
Deposited on : 2023-07-24
Resolution : 3.40 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:

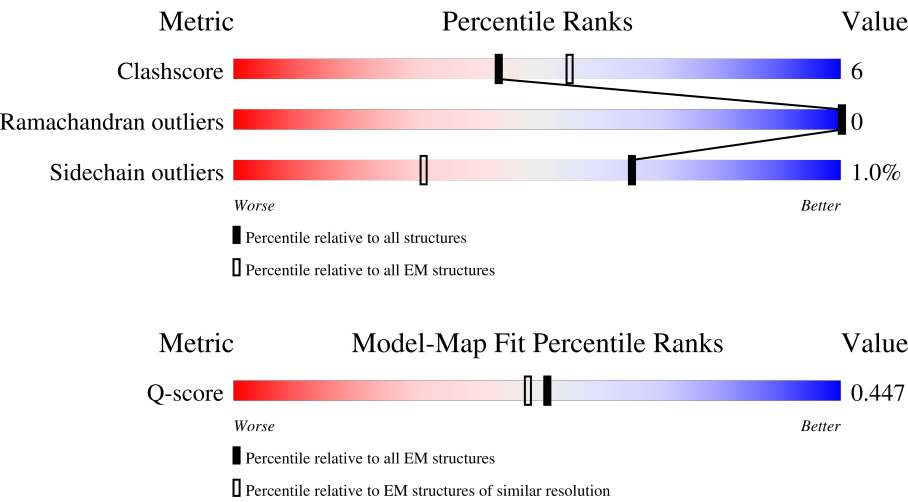
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	340	
1	B	340	
1	K	340	
2	C	1161	

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Mol	Chain	Length	Quality of chain
3	D	1299	7%84%12%.
4	E	90	11%78%8%14%
5	F	511	.53%8%38%
6	G	59	10%56%39%5%
7	H	59	20%69%27%.
8	I	993	.22%.75%
8	J	993	10%21%5%75%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 31659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1742	1102	302	334	4		
1	B	233	Total	C	N	O	S	0	0
			1785	1125	308	347	5		
1	K	57	Total	C	N	O	S	0	0
			438	274	77	85	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1116	Total	C	N	O	S	0	0
			8692	5450	1513	1698	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1259	Total	C	N	O	S	0	0
			9812	6137	1778	1856	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	77	Total	C	N	O	0	0
			594	379	98	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	315	Total	C	N	O	S	0	0
			2465	1546	437	475	7		

- Molecule 6 is a DNA chain called Non-template strand DNA for AfsS promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	56	Total	C	N	O	P	0	0
			1148	546	204	342	56		

- Molecule 7 is a DNA chain called Template strand DNA for AfsS promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	57	Total	C	N	O	P	0	0
			1180	557	232	334	57		

- Molecule 8 is a protein called Regulatory protein AfsR.

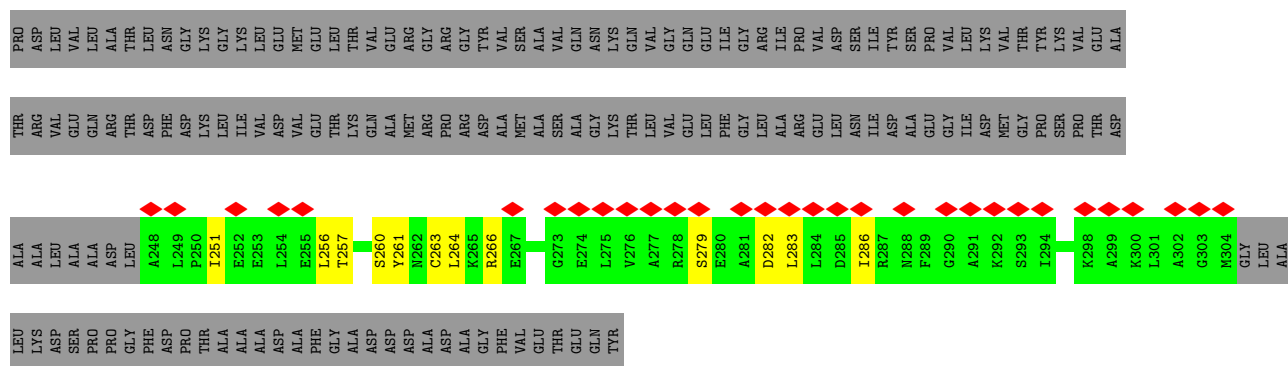
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	250	Total	C	N	O	S	0	0
			1904	1184	359	357	4		
8	J	249	Total	C	N	O	S	0	0
			1896	1178	358	356	4		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

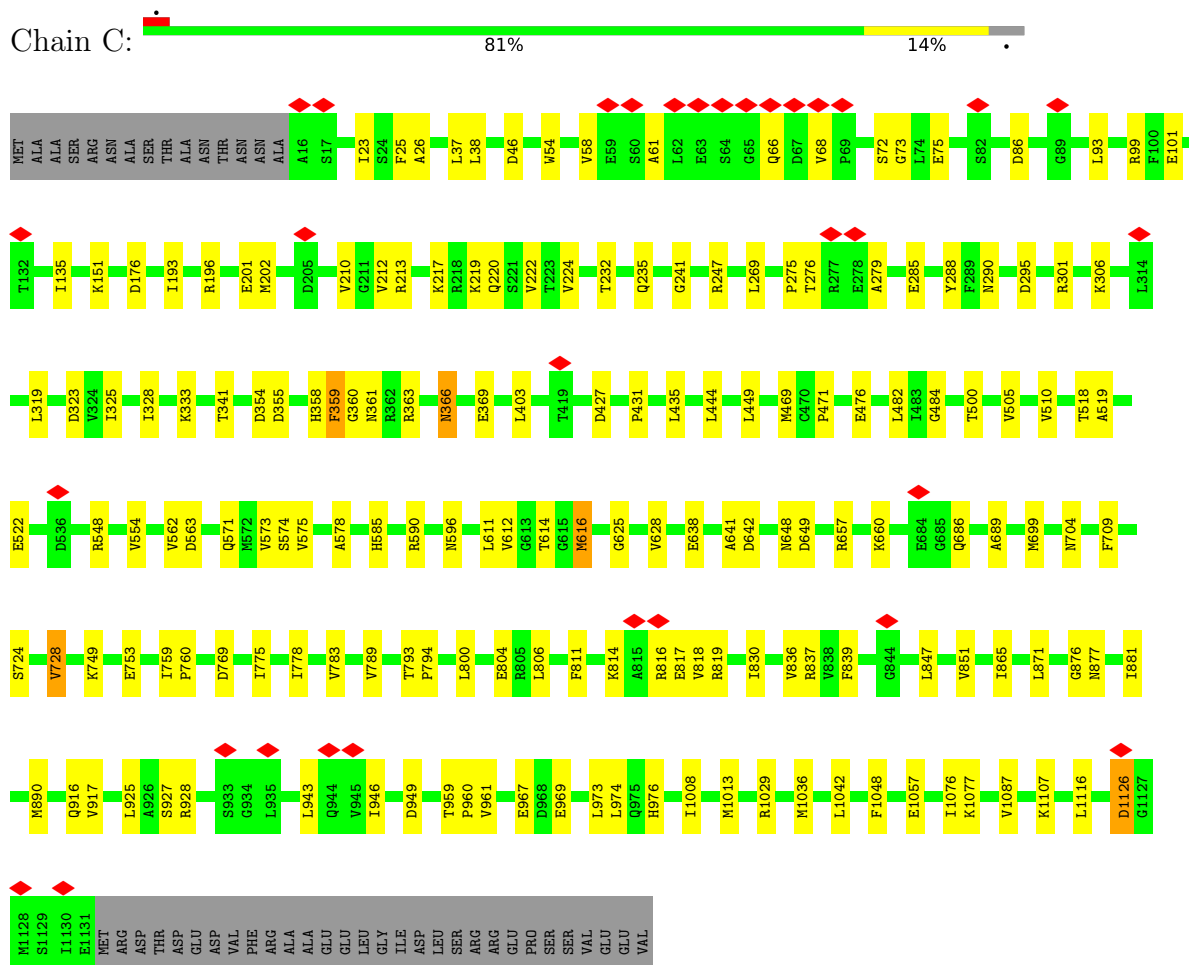
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

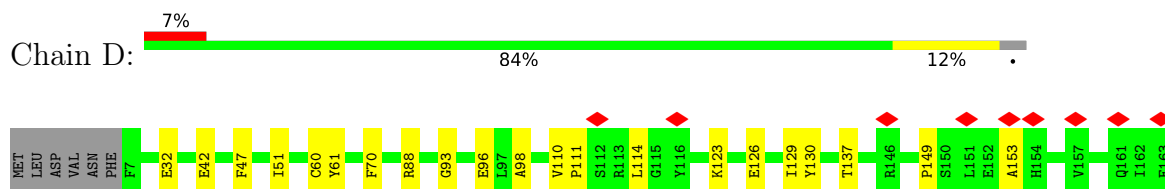
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

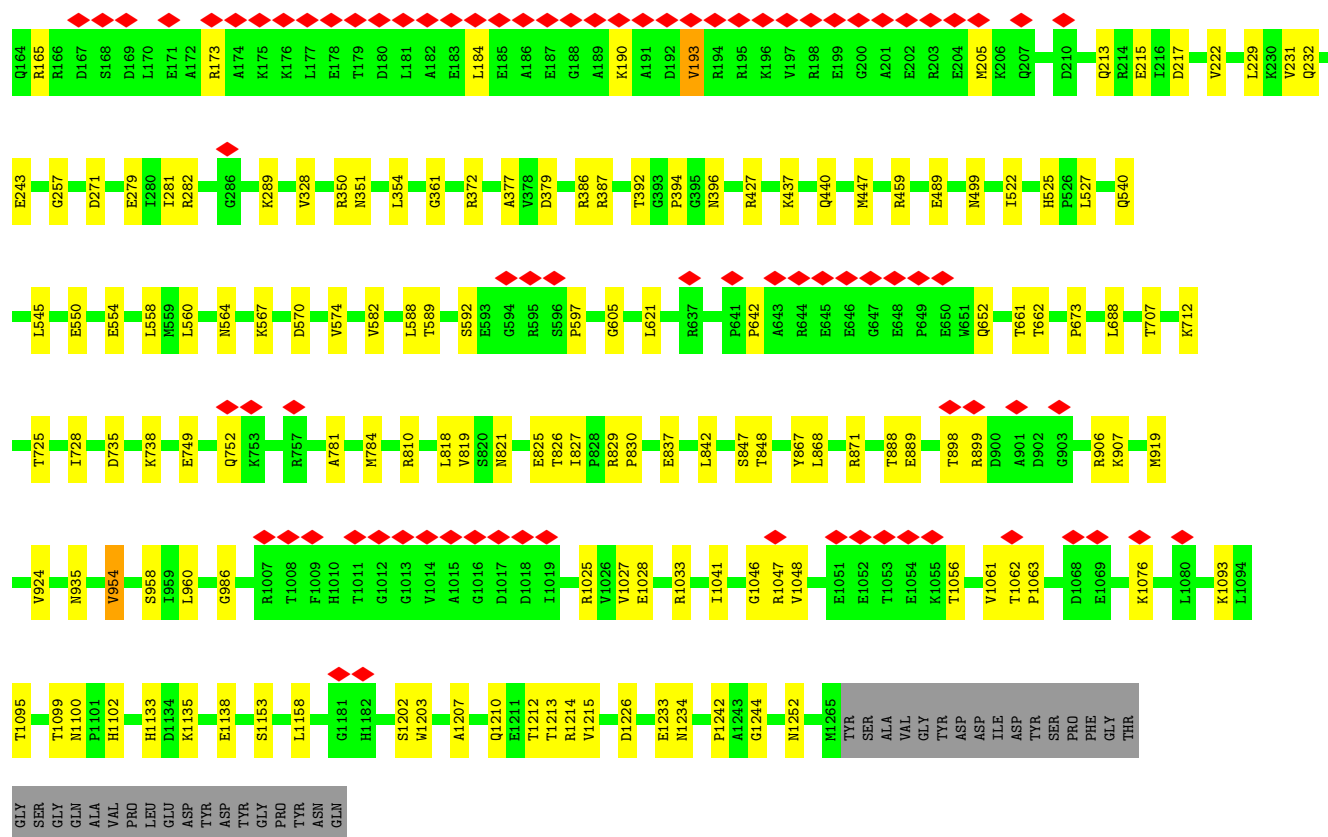


• Molecule 2: DNA-directed RNA polymerase subunit beta



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





- Molecule 8: Regulatory protein AfsR



LYS	GLY	ARG	ALA	GLU	GLY	ASP	THR	MET	L263	V199	E116	MET
LEU	LEU	ALA	PRO	ASP	GLY	ASP	ALA	ALA	Q264	S200	G117	ASP
PHE	ARG	LEU	GLU	THR	ALA	GLY	SER	VAL	D265	E201	A118	GLY
HIS	THR	ARG	ALA	TRP	ALA	ALA	ALA	ALA	D266	L202	L119	PRO
GLN	VAL	VAL	GLY	THR	ALA	HIS	LEU	LEU	P267	T203	D120	ARG
ALA	LEU	CYS	ALA	VAL	VAL	LEU	PRO	ALA	A268	A204	A122	VAL
SER	SER	VAL	SER	SER	SER	VAL	ASP	GLY	L269	L205	R123	ARG
ASP	ASP	GLN	VAL	VAL	VAL	ASP	SER	ILE	A270	T206	R123	PRO
PHE	LEU	SER	ARG	ASP	ALA	VAL	GLU	GLY	A271	A207	D126	GLN
LEU	VAL	LEU	LEU	VAL	ALA	VAL	GLY	VAL	LEU	A208	L127	ARG
ALA	THR	GLY	ASP	LYS	MET	ARG	ARG	GLY	SER	H209	G127	PRO
ASN	GLY	GLY	PHE	ALA	PRO	ALA	THR	ALA	ALA	P210	A130	PHE
ARG	ILE	ARG	GLY	ASP	GLY	LEU	THR	THR	ALA	L211	A131	PRO
ALA	GLY	ARG	LEU	THR	GLY	TYR	TYR	THR	ALA	R212	E132	ALA
HIS	GLY	HIS	ALA	ARG	ALA	ARG	VAL	VAL	GLY	E213	K133	GLU
GLU	ALA	ALA	THR	ARG	LEU	SER	SER	VAL	THR	R214	A134	GLU
ALA	ALA	ALA	ALA	VAL	ALA	VAL	VAL	HIS	ALA	L215	R135	GLU
GLY	GLU	GLY	LEU	ASP	PHE	LEU	LEU	VAL	THR	R216	G138	GLU
LEU	LEU	LEU	GLY	GLY	THR	LYS	THR	HIS	THR	E217	A137	SER
SER	ARG	ALA	VAL	GLN	ILE	ILE	ARG	ALA	LEU	L218	G138	GLU
ASN	LEU	LEU	ILE	ALA	ASP	VAL	VAL	ALA	ARG	L219	D139	SER
LEU	ALA	GLY	GLY	GLY	ALA	GLY	LEU	ALA	ALA	A222	H142	GLY
LEU	ALA	GLY	GLY	GLY	GLY	GLY	VAL	ALA	GLN	L223	A143	GLY
MET	MET	ALA	VAL	PHE	GLY	THR	LEU	PHE	LEU	R224	R144	GLY
ASN	ASN	ASP	GLY	GLY	VAL	VAL	ASP	ASP	PRO	E225	L147	GLY
VAL	VAL	SER	LEU	LEU	ARG	ALA	ALA	ASP	GLY	S226	R148	GLY
ALA	ALA	ALA	GLY	GLY	GLY	GLN	ALA	VAL	THR	R227	R149	GLY
ALA	VAL	ALA	GLY	ASP	GLY	ARG	ALA	VAL	ASP	R228	G161	GLY
GLU	GLU	GLY	LEU	LEU	LEU	ALA	ALA	ASP	PHE	Q229	D152	GLY
GLU	GLU	HIS	PRO	PRO	TYR	ALA	GLN	LEU	THR	A230	G161	GLY
ALA	VAL	ALA	THR	THR	PHE	GLY	VAL	GLY	GLY	E231	E157	GLY
ASP	TRP	ASP	GLY	GLY	HIS	ASP	PRO	ALA	ALA	A232	V158	GLY
ILE	ILE	VAL	PRO	GLY	ASP	VAL	VAL	GLY	ALA	L233	L159	GLY
ALA	ALA	ALA	GLY	GLY	LEU	GLY	LEU	ALA	PHE	Y236	A160	GLY
ASN	ASN	ALA	GLY	PRO	VAL	ALA	PRO	ARG	ARG	G162	V162	GLY
GLN	GLN	ALA	LEU	ALA	ALA	CYS	GLY	PRO	GLY	T239	Q168	GLY
GLY	ARG	ALA	THR	THR	THR	PHE	THR	ALA	SER	R240	Q168	GLY
LEU	LEU	GLY	THR	THR	ALA	LEU	GLY	PRO	SER	R241	R171	GLY
ALA	VAL	VAL	GLY	GLY	ALA	PRO	CYS	THR	VAL	L242	L181	GLY
TYR	TYR	CYS	SER	SER	CYS	ALA	ALA	VAL	SER	L243	L181	GLY
LEU	LEU	GLY	LEU	LEU	ALA	ILE	LEU	LEU	LEU	A244	R185	GLY
GLU	GLU	ALA	ALA	ALA	GLY	LEU	VAL	GLY	ALA	D245	L186	GLY
ARG	ARG	GLN	LEU	LEU	ILE	ILE	THR	SER	SER	E246	D187	GLY
THR	THR	ARG	ASP	ALA	ALA	ALA	ARG	LEU	GLY	L247	D187	GLY
MET	MET	TYR	THR	THR	GLY	SER	VAL	ARG	SER	G248	M183	GLY
ARG	ARG	ALA	TYR	THR	ASP	ARG	ALA	ALA	LEU	P251	D189	GLY
LEU	LEU	GLY	THR	GLU	GLY	PRO	MET	LEU	SER	R252	L190	GLY
					ASN	ASP	GLY	SER	ARG	P253	D191	GLY
						ASP	PRO	ARG	VAL	G254	Q192	ARG
										L255	G193	
										Q256	C194	
										E257	H195	
										L258	A196	
										Q259	E197	
										Q260	A198	
										R261		
										T262		

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/1768	0.70	1/2400 (0.0%)
1	B	0.33	0/1811	0.68	0/2459
1	K	0.25	0/441	0.64	0/591
2	C	0.42	0/8848	0.67	0/11982
3	D	0.41	0/9963	0.71	0/13446
4	E	0.42	0/604	0.72	0/822
5	F	0.31	0/2500	0.67	0/3377
6	G	0.35	0/1285	0.53	0/1982
7	H	0.39	0/1328	0.54	0/2049
8	I	0.29	0/1931	0.65	0/2620
8	J	0.24	0/1923	0.65	0/2609
All	All	0.38	0/32402	0.67	1/44337 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLU	N-CA-C	5.70	122.41	109.81

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	1742	0	1796	21	0
1	B	1785	0	1821	17	0
1	K	438	0	452	6	0
2	C	8692	0	8632	110	0
3	D	9812	0	9951	95	0
4	E	594	0	595	5	0
5	F	2465	0	2487	33	0
6	G	1148	0	633	61	0
7	H	1180	0	637	36	0
8	I	1904	0	1933	22	0
8	J	1896	0	1922	29	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	31659	0	30859	392	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 6.

All (392) 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)
6:G:6:DT:C6	6:G:7:DT:H72	1.80	1.14
6:G:8:DC:H2''	6:G:9:DA:H5'	1.22	1.08
6:G:6:DT:C5	6:G:7:DT:H72	1.94	1.02
6:G:8:DC:H2''	6:G:9:DA:C5'	2.00	0.91
7:H:47:DC:C6	7:H:48:DT:H71	2.07	0.89
6:G:8:DC:C2'	6:G:9:DA:H5'	2.01	0.88
7:H:49:DG:C2	7:H:50:DA:C4	2.64	0.86
6:G:9:DA:H2'	6:G:10:DG:C8	2.15	0.81
6:G:8:DC:C2	6:G:9:DA:N7	2.49	0.80
6:G:39:DG:H2'	6:G:40:DG:C8	2.18	0.78
6:G:9:DA:H4'	6:G:10:DG:OP1	1.82	0.78
3:D:427:ARG:HD2	3:D:540:GLN:HB3	1.67	0.76
7:H:47:DC:C6	7:H:48:DT:C7	2.68	0.76
7:H:47:DC:C2	7:H:48:DT:C6	2.73	0.76
6:G:6:DT:C6	6:G:7:DT:C7	2.68	0.74
2:C:877:ASN:HD21	2:C:1013:MET:HE1	1.53	0.74
6:G:9:DA:H2''	6:G:10:DG:O5'	1.88	0.74
2:C:232:THR:H	2:C:235:GLN:HE21	1.35	0.72
3:D:190:LYS:HG2	3:D:193:VAL:HG13	1.72	0.71
6:G:14:DT:H2''	6:G:15:DC:C6	2.25	0.71
7:H:35:DG:C2	7:H:36:DA:C5	2.80	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:49:DG:C4	7:H:50:DA:C8	2.81	0.69
7:H:47:DC:C5	7:H:48:DT:H73	2.28	0.69
6:G:16:DG:N2	7:H:41:DC:O2	2.26	0.69
2:C:814:LYS:HD2	2:C:816:ARG:HE	1.58	0.68
7:H:47:DC:C5	7:H:48:DT:C7	2.77	0.68
6:G:7:DT:C2	6:G:8:DC:C4	2.84	0.66
7:H:35:DG:N3	7:H:36:DA:C8	2.64	0.65
3:D:173:ARG:HB3	3:D:205:MET:HE3	1.80	0.64
3:D:361:GLY:HA3	5:F:272:ARG:HH22	1.64	0.63
6:G:14:DT:H2''	6:G:15:DC:H6	1.63	0.63
6:G:6:DT:C5	6:G:7:DT:C7	2.79	0.62
2:C:814:LYS:HG2	8:I:170:GLN:HE22	1.64	0.61
6:G:9:DA:C2	6:G:10:DG:C2	2.88	0.61
5:F:488:GLN:NE2	8:J:71:ASP:OD1	2.34	0.61
2:C:196:ARG:HD3	2:C:295:ASP:HB3	1.82	0.61
2:C:628:VAL:HB	2:C:689:ALA:HB3	1.83	0.60
2:C:1057:GLU:OE1	3:D:499:ASN:ND2	2.34	0.60
3:D:165:ARG:NH2	3:D:215:GLU:OE2	2.35	0.60
3:D:126:GLU:OE1	3:D:387:ARG:NH1	2.34	0.60
8:I:94:ARG:HH22	8:I:104:SER:HB2	1.67	0.60
2:C:366:ASN:OD1	2:C:366:ASN:N	2.35	0.60
8:J:135:ARG:HH11	8:J:188:MET:HE1	1.67	0.59
3:D:827:ILE:HG22	3:D:829:ARG:H	1.66	0.59
3:D:821:ASN:HD22	3:D:825:GLU:HB3	1.67	0.59
5:F:303:LEU:HD21	5:F:342:MET:SD	2.43	0.59
6:G:40:DG:C6	6:G:41:DA:C6	2.91	0.58
1:A:129:ASN:ND2	2:C:638:GLU:OE2	2.36	0.58
6:G:39:DG:H2''	6:G:40:DG:OP1	2.04	0.58
2:C:431:PRO:HB2	2:C:699:MET:HE1	1.85	0.58
6:G:9:DA:C2'	6:G:10:DG:C8	2.86	0.58
3:D:279:GLU:HG2	3:D:282:ARG:HH12	1.67	0.58
3:D:642:PRO:O	3:D:652:GLN:NE2	2.36	0.58
3:D:818:LEU:HD23	3:D:830:PRO:HB3	1.85	0.58
1:A:165:ASP:N	1:A:165:ASP:OD1	2.37	0.58
2:C:99:ARG:NH1	2:C:101:GLU:OE2	2.36	0.58
8:I:216:ARG:NH1	8:I:239:THR:OG1	2.37	0.57
8:J:205:LEU:HB3	8:J:215:LEU:HD13	1.86	0.57
2:C:288:TYR:HB3	2:C:319:LEU:HD21	1.87	0.57
2:C:151:LYS:HE2	2:C:625:GLY:HA3	1.87	0.57
2:C:176:ASP:OD1	2:C:176:ASP:N	2.37	0.57
3:D:567:LYS:HG3	3:D:574:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:40:DG:C6	6:G:41:DA:N6	2.73	0.57
7:H:35:DG:N3	7:H:36:DA:N7	2.53	0.57
6:G:9:DA:N6	7:H:49:DG:O6	2.38	0.56
3:D:437:LYS:H	3:D:440:GLN:HE21	1.52	0.56
6:G:6:DT:C7	6:G:7:DT:H72	2.35	0.56
8:I:65:THR:HG23	8:I:68:GLU:H	1.70	0.56
2:C:93:LEU:HD21	2:C:403:LEU:HD11	1.87	0.56
1:A:83:LEU:HA	1:A:120:ASN:HD21	1.71	0.56
7:H:49:DG:C2	7:H:50:DA:N9	2.73	0.56
1:K:283:LEU:HA	1:K:286:ILE:HD12	1.88	0.56
1:B:182:ARG:HH11	1:B:185:GLN:H	1.54	0.56
8:J:262:ILE:HD13	8:J:269:LEU:HD13	1.88	0.56
6:G:40:DG:C4	6:G:41:DA:N7	2.74	0.55
3:D:784:MET:HE1	3:D:810:ARG:HA	1.88	0.55
1:A:203:ARG:HH22	1:A:205:ARG:HD2	1.72	0.55
5:F:501:SER:OG	5:F:502:ARG:N	2.40	0.55
2:C:325:ILE:HA	2:C:328:ILE:HD12	1.89	0.55
5:F:413:ASP:OD1	7:H:17:DG:N2	2.39	0.55
2:C:574:SER:OG	2:C:575:VAL:N	2.40	0.55
6:G:39:DG:H2'	6:G:40:DG:N9	2.21	0.55
7:H:35:DG:C2	7:H:36:DA:N7	2.75	0.55
3:D:867:TYR:OH	3:D:1210:GLN:NE2	2.40	0.55
5:F:356:VAL:O	5:F:360:ASN:ND2	2.39	0.55
5:F:338:ILE:O	5:F:342:MET:HG2	2.07	0.54
6:G:7:DT:H2''	6:G:8:DC:C6	2.41	0.54
3:D:130:TYR:O	3:D:372:ARG:NH1	2.40	0.54
8:I:169:THR:OG1	8:I:170:GLN:NE2	2.39	0.54
2:C:72:SER:OG	2:C:73:GLY:N	2.38	0.54
2:C:201:GLU:HB2	2:C:213:ARG:HB2	1.90	0.54
3:D:554:GLU:HG3	4:E:30:VAL:HG21	1.88	0.54
7:H:49:DG:N3	7:H:50:DA:N9	2.56	0.54
8:J:130:ALA:HA	8:J:133:LYS:HD3	1.88	0.54
1:A:29:GLY:O	1:B:40:ARG:NH1	2.40	0.54
8:J:120:ASP:OD1	8:J:120:ASP:N	2.40	0.54
3:D:459:ARG:NH1	3:D:489:GLU:OE2	2.36	0.54
7:H:49:DG:H2''	7:H:50:DA:H8	1.73	0.54
2:C:877:ASN:ND2	2:C:916:GLN:OE1	2.41	0.54
6:G:40:DG:H2''	6:G:41:DA:H8	1.71	0.54
6:G:8:DC:N3	6:G:9:DA:N7	2.56	0.54
8:J:225:ARG:NH2	8:J:271:GLU:O	2.41	0.54
2:C:444:LEU:HD21	2:C:482:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:570:ASP:OD1	3:D:570:ASP:N	2.39	0.54
2:C:522:GLU:OE2	2:C:548:ARG:NH2	2.41	0.54
2:C:943:LEU:HD21	2:C:969:GLU:HG2	1.90	0.54
3:D:47:PHE:O	3:D:88:ARG:NH2	2.41	0.54
3:D:281:ILE:O	3:D:289:LYS:NZ	2.41	0.54
5:F:243:GLY:HA2	5:F:267:ILE:HG22	1.90	0.54
2:C:783:VAL:HA	2:C:830:ILE:HD12	1.90	0.53
2:C:793:THR:HG22	2:C:819:ARG:H	1.73	0.53
8:I:144:ARG:NE	8:I:189:ASP:OD1	2.41	0.53
3:D:213:GLN:NE2	3:D:217:ASP:OD1	2.40	0.53
8:J:144:ARG:HH12	8:J:189:ASP:HA	1.71	0.53
1:A:52:THR:HB	1:A:152:ASN:HD21	1.72	0.53
6:G:23:DT:H3	7:H:34:DA:H61	1.56	0.53
8:I:144:ARG:NH1	8:I:192:GLN:OE1	2.41	0.53
7:H:49:DG:N3	7:H:50:DA:C8	2.77	0.53
3:D:129:ILE:HA	3:D:257:GLY:HA2	1.91	0.53
2:C:554:VAL:HG13	3:D:842:LEU:HD13	1.91	0.52
2:C:817:GLU:OE1	8:I:62:ARG:NH2	2.42	0.52
3:D:1093:LYS:NZ	3:D:1095:THR:O	2.39	0.52
3:D:1202:SER:OG	3:D:1233:GLU:OE1	2.22	0.52
8:I:210:PRO:HG2	8:I:211:LEU:HD12	1.89	0.52
2:C:648:ASN:ND2	2:C:649:ASP:OD1	2.42	0.52
6:G:8:DC:C2	6:G:9:DA:C8	2.97	0.52
3:D:447:MET:HE1	3:D:522:ILE:HD11	1.92	0.52
6:G:5:DG:H2''	6:G:6:DT:H5''	1.92	0.52
3:D:111:PRO:HA	3:D:114:LEU:HG	1.91	0.52
3:D:427:ARG:HH22	7:H:14:DC:H2''	1.75	0.52
1:B:33:THR:OG1	1:B:34:LEU:N	2.43	0.52
1:B:98:ARG:HH11	1:B:135:GLU:HB3	1.75	0.52
2:C:275:PRO:HD2	5:F:203:GLN:HG2	1.90	0.52
2:C:611:LEU:HB2	2:C:704:ASN:HD22	1.75	0.52
2:C:301:ARG:NH1	2:C:323:ASP:OD2	2.36	0.52
2:C:871:LEU:HD22	2:C:881:ILE:HD11	1.91	0.52
1:K:263:CYS:HA	1:K:266:ARG:HH11	1.75	0.52
6:G:25:DC:H2''	6:G:26:DC:C6	2.44	0.51
5:F:450:LEU:HD11	5:F:497:LEU:HD21	1.92	0.51
2:C:427:ASP:OD1	2:C:427:ASP:N	2.43	0.51
3:D:32:GLU:OE2	5:F:350:ARG:NE	2.41	0.51
3:D:271:ASP:OD1	3:D:271:ASP:N	2.42	0.51
6:G:9:DA:H2''	6:G:10:DG:O4'	2.10	0.51
1:A:150:VAL:HA	1:A:153:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:389:THR:OG1	5:F:391:GLU:OE2	2.26	0.51
2:C:800:LEU:HD22	2:C:804:GLU:HG2	1.93	0.51
2:C:1036:MET:HB3	5:F:424:ASP:HB3	1.92	0.51
3:D:821:ASN:ND2	3:D:825:GLU:OE1	2.44	0.51
2:C:943:LEU:HA	2:C:946:ILE:HD12	1.92	0.51
8:I:120:ASP:N	8:I:120:ASP:OD1	2.44	0.51
3:D:560:LEU:O	3:D:564:ASN:ND2	2.44	0.51
5:F:198:ASP:OD1	5:F:198:ASP:N	2.44	0.51
6:G:39:DG:H2''	6:G:40:DG:O4'	2.11	0.51
1:B:54:ILE:HD12	1:B:80:ILE:HG21	1.93	0.50
7:H:49:DG:C6	7:H:50:DA:C6	2.98	0.50
7:H:35:DG:C4	7:H:36:DA:N7	2.80	0.50
2:C:196:ARG:O	6:G:43:DC:N4	2.45	0.50
1:B:97:LEU:HD13	1:B:110:ILE:HA	1.94	0.50
5:F:282:ASN:HD22	6:G:37:DT:H3	1.60	0.50
2:C:949:ASP:OD1	2:C:949:ASP:N	2.41	0.49
8:I:162:VAL:O	8:I:171:ARG:NH2	2.45	0.49
5:F:285:LEU:O	5:F:288:SER:OG	2.27	0.49
2:C:61:ALA:O	2:C:66:GLN:N	2.45	0.49
3:D:51:ILE:HD11	3:D:93:GLY:HA3	1.94	0.49
2:C:1036:MET:HE1	3:D:328:VAL:HG21	1.95	0.49
6:G:40:DG:C2'	6:G:41:DA:H8	2.24	0.49
5:F:269:GLU:OE2	5:F:273:ARG:NH1	2.45	0.49
1:B:182:ARG:HA	1:B:187:THR:HA	1.93	0.49
2:C:469:MET:HE3	2:C:484:GLY:HA3	1.94	0.49
2:C:563:ASP:N	2:C:563:ASP:OD1	2.44	0.49
2:C:1126:ASP:OD1	2:C:1126:ASP:N	2.35	0.49
2:C:760:PRO:HG3	2:C:818:VAL:HG23	1.95	0.49
3:D:32:GLU:HB3	3:D:42:GLU:HG3	1.94	0.49
8:J:168:GLN:OE1	8:J:171:ARG:NH1	2.45	0.49
2:C:709:PHE:HE2	2:C:917:VAL:HG22	1.78	0.48
3:D:735:ASP:OD2	3:D:735:ASP:N	2.45	0.48
2:C:778:ILE:HD11	2:C:836:VAL:HG12	1.95	0.48
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.95	0.48
2:C:724:SER:HB2	2:C:890:MET:HG3	1.96	0.48
3:D:231:VAL:HG23	3:D:232:GLN:HG3	1.95	0.48
6:G:8:DC:H5''	8:J:81:GLN:HG3	1.96	0.48
1:A:6:ARG:NH1	1:B:217:GLU:OE1	2.46	0.48
3:D:592:SER:HB2	3:D:597:PRO:HB3	1.96	0.48
3:D:958:SER:OG	3:D:1138:GLU:OE1	2.31	0.48
8:J:88:THR:HG22	8:J:92:ARG:HE	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:VAL:HG13	2:C:222:VAL:HG22	1.94	0.48
3:D:386:ARG:HH12	3:D:1213:THR:HG21	1.77	0.48
3:D:738:LYS:NZ	3:D:837:GLU:OE1	2.46	0.48
3:D:661:THR:OG1	3:D:662:THR:N	2.47	0.47
8:I:260:GLN:HA	8:I:263:LEU:HD12	1.95	0.47
2:C:355:ASP:O	2:C:361:ASN:ND2	2.47	0.47
2:C:927:SER:OG	2:C:928:ARG:NH1	2.40	0.47
3:D:906:ARG:NH1	3:D:907:LYS:O	2.47	0.47
7:H:49:DG:C6	7:H:50:DA:C5	3.02	0.47
7:H:49:DG:N1	7:H:50:DA:C4	2.81	0.47
6:G:40:DG:H2''	6:G:41:DA:O5'	2.14	0.47
8:J:243:LEU:O	8:J:248:GLY:N	2.48	0.47
2:C:806:LEU:HD22	5:F:443:LEU:HD11	1.96	0.47
4:E:65:GLU:OE1	4:E:73:ARG:NH2	2.48	0.47
2:C:518:THR:OG1	2:C:519:ALA:N	2.44	0.47
2:C:642:ASP:OD2	2:C:657:ARG:NH2	2.38	0.47
2:C:814:LYS:HB2	8:I:173:ARG:HD2	1.97	0.47
8:J:251:PRO:HB2	8:J:256:GLN:HE21	1.79	0.47
3:D:110:VAL:HG21	3:D:1214:ARG:HD3	1.96	0.47
3:D:898:THR:OG1	3:D:899:ARG:N	2.48	0.47
3:D:1252:ASN:HB3	4:E:85:ILE:HD11	1.97	0.47
7:H:47:DC:C2	7:H:48:DT:C5	3.03	0.47
6:G:39:DG:C2'	6:G:40:DG:C8	2.95	0.47
1:B:97:LEU:HD22	1:B:110:ILE:HD12	1.97	0.47
2:C:354:ASP:OD1	2:C:354:ASP:N	2.47	0.47
2:C:728:VAL:HG12	2:C:865:ILE:HG23	1.96	0.47
3:D:749:GLU:OE1	3:D:752:GLN:NE2	2.48	0.47
2:C:86:ASP:N	2:C:86:ASP:OD1	2.45	0.47
3:D:673:PRO:HD3	3:D:707:THR:HG21	1.96	0.47
2:C:476:GLU:OE2	2:C:596:ASN:ND2	2.47	0.46
1:A:93:VAL:HG11	1:A:116:VAL:HG21	1.96	0.46
2:C:505:VAL:HG22	2:C:510:VAL:HG22	1.98	0.46
2:C:775:ILE:HG23	2:C:789:VAL:HG12	1.97	0.46
3:D:527:LEU:HD21	3:D:712:LYS:HB2	1.97	0.46
3:D:868:LEU:HD13	3:D:1027:VAL:HG22	1.97	0.46
6:G:8:DC:C5'	8:J:81:GLN:HG3	2.45	0.46
3:D:919:MET:HE2	3:D:935:ASN:HA	1.96	0.46
2:C:202:MET:HG2	2:C:212:VAL:HG12	1.98	0.46
2:C:1008:ILE:HA	3:D:725:THR:HG21	1.96	0.46
8:I:141:CYS:SG	8:I:142:HIS:N	2.88	0.46
2:C:500:THR:OG1	2:C:571:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HG	1:B:159:ILE:HG12	1.97	0.46
3:D:1033:ARG:NH1	6:G:49:DC:O3'	2.49	0.46
7:H:35:DG:OP2	8:I:87:ARG:NH2	2.47	0.46
2:C:25:PHE:HD2	2:C:959:THR:HG22	1.81	0.46
2:C:1077:LYS:NZ	3:D:545:LEU:O	2.30	0.46
6:G:15:DC:H2''	6:G:16:DG:H5''	1.98	0.46
7:H:49:DG:C5	7:H:50:DA:C5	3.04	0.46
2:C:811:PHE:HE1	5:F:503:SER:HB2	1.80	0.46
2:C:847:LEU:HB3	2:C:851:VAL:HG23	1.97	0.46
2:C:363:ARG:NH1	2:C:369:GLU:OE1	2.34	0.45
7:H:42:DG:H2''	7:H:43:DA:C8	2.50	0.45
8:I:37:ARG:NH2	8:I:96:VAL:O	2.49	0.45
1:A:76:LEU:HD21	1:A:126:ALA:HB2	1.98	0.45
2:C:435:LEU:HD23	2:C:575:VAL:HG11	1.98	0.45
8:J:158:VAL:HG23	8:J:171:ARG:HG3	1.97	0.45
3:D:525:HIS:CE1	3:D:527:LEU:HD23	2.51	0.45
3:D:554:GLU:HG2	3:D:558:LEU:HD12	1.97	0.45
3:D:589:THR:O	3:D:589:THR:OG1	2.29	0.45
2:C:359:PHE:HD1	2:C:359:PHE:HA	1.67	0.45
3:D:1025:ARG:NH1	3:D:1028:GLU:OE2	2.50	0.45
5:F:429:VAL:HG13	5:F:432:ASP:HB2	1.97	0.45
1:B:78:LEU:HD22	3:D:605:GLY:HA2	1.99	0.45
2:C:471:PRO:HB2	3:D:848:THR:HG21	1.99	0.45
7:H:49:DG:C4	7:H:50:DA:N7	2.85	0.45
2:C:276:THR:HB	2:C:279:ALA:HB3	1.97	0.45
3:D:123:LYS:HB2	3:D:123:LYS:HE2	1.77	0.45
5:F:301:LEU:HD12	5:F:304:ILE:HD12	1.97	0.45
5:F:410:LEU:HD23	5:F:410:LEU:HA	1.77	0.45
3:D:1056:THR:HA	3:D:1076:LYS:HG2	1.97	0.45
2:C:26:ALA:HB2	2:C:960:PRO:HG3	1.98	0.44
3:D:781:ALA:HB2	3:D:810:ARG:HD3	1.99	0.44
1:B:87:SER:HB2	1:B:116:VAL:HG22	2.00	0.44
3:D:96:GLU:O	3:D:351:ASN:ND2	2.49	0.44
3:D:1153:SER:OG	3:D:1158:LEU:O	2.28	0.44
4:E:16:ILE:HG22	4:E:20:LEU:HD23	1.99	0.44
2:C:46:ASP:HB3	2:C:54:TRP:HB2	2.00	0.44
3:D:394:PRO:HB2	3:D:396:ASN:HD22	1.82	0.44
3:D:1203:TRP:CD1	3:D:1226:ASP:HB2	2.52	0.44
7:H:17:DG:H2'	7:H:18:DG:H21	1.82	0.44
2:C:37:LEU:HD12	2:C:37:LEU:HA	1.84	0.44
8:J:26:ARG:HB3	8:J:36:TRP:HE3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:ASN:OD1	2:C:704:ASN:N	2.48	0.44
3:D:350:ARG:HH11	3:D:377:ALA:HB2	1.82	0.44
3:D:1047:ARG:O	3:D:1062:THR:N	2.45	0.44
5:F:303:LEU:CD2	5:F:342:MET:SD	3.06	0.44
6:G:25:DC:H5''	6:G:25:DC:H6	1.82	0.44
3:D:229:LEU:HD23	3:D:229:LEU:HA	1.84	0.44
3:D:550:GLU:OE1	4:E:38:ARG:NH2	2.51	0.44
6:G:8:DC:O2	6:G:9:DA:C8	2.71	0.44
6:G:8:DC:O5'	8:J:81:GLN:HG3	2.18	0.44
8:I:228:ARG:HB3	8:I:231:GLU:HB2	2.00	0.44
8:J:162:VAL:O	8:J:171:ARG:NH2	2.50	0.44
1:A:90:ASP:OD1	1:A:90:ASP:N	2.50	0.44
5:F:501:SER:HB2	8:I:249:VAL:HG21	2.00	0.44
3:D:1041:ILE:HD11	3:D:1099:THR:HG23	1.99	0.44
8:J:87:ARG:HA	8:J:87:ARG:HD3	1.84	0.43
8:J:157:GLU:HG3	8:J:160:ALA:HB2	2.00	0.43
2:C:973:LEU:HA	2:C:976:HIS:NE2	2.33	0.43
6:G:9:DA:H2	6:G:10:DG:C2	2.36	0.43
8:I:30:LEU:HA	8:I:158:VAL:HG12	2.00	0.43
2:C:61:ALA:HB1	2:C:66:GLN:HB3	1.99	0.43
2:C:217:LYS:NZ	2:C:269:LEU:O	2.35	0.43
3:D:60:CYS:SG	3:D:61:TYR:N	2.92	0.43
3:D:1048:VAL:HA	3:D:1061:VAL:HA	2.00	0.43
1:A:15:ASP:OD2	1:A:16:GLU:N	2.51	0.43
1:B:3:ILE:HD11	1:B:233:ASP:H	1.83	0.43
2:C:58:VAL:HA	2:C:68:VAL:HG11	2.00	0.43
2:C:649:ASP:OD1	2:C:649:ASP:N	2.48	0.43
3:D:184:LEU:HD23	3:D:184:LEU:HA	1.80	0.43
1:A:64:THR:OG1	1:A:65:THR:N	2.51	0.43
2:C:769:ASP:OD1	2:C:769:ASP:N	2.39	0.43
5:F:239:ARG:HE	5:F:274:ALA:HB2	1.84	0.43
2:C:590:ARG:NH2	2:C:876:GLY:O	2.52	0.43
2:C:641:ALA:O	2:C:660:LYS:NZ	2.51	0.43
3:D:1133:HIS:ND1	3:D:1135:LYS:HG3	2.33	0.43
8:I:63:THR:HA	8:I:110:ALA:HB2	2.01	0.43
2:C:23:ILE:H	2:C:23:ILE:HG13	1.62	0.43
5:F:241:GLU:HA	5:F:244:LEU:HB2	2.00	0.43
8:J:32:PRO:O	8:J:34:ARG:NE	2.51	0.43
1:A:122:ASP:OD1	1:A:122:ASP:N	2.50	0.43
2:C:449:LEU:HD13	6:G:45:DG:H1	1.83	0.43
8:J:94:ARG:HA	8:J:94:ARG:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1153:SER:OG	3:D:1153:SER:O	2.36	0.43
1:B:186:ARG:HB2	1:B:189:PHE:HE1	1.83	0.43
2:C:38:LEU:HD23	2:C:38:LEU:HA	1.89	0.43
2:C:210:VAL:HG22	2:C:222:VAL:HG21	2.01	0.43
2:C:925:LEU:HD21	2:C:974:LEU:HA	2.01	0.43
2:C:358:HIS:CD2	2:C:360:GLY:H	2.37	0.42
5:F:196:ASP:OD2	5:F:196:ASP:N	2.51	0.42
2:C:72:SER:N	2:C:75:GLU:OE2	2.53	0.42
3:D:919:MET:HE2	3:D:919:MET:HB2	1.81	0.42
6:G:11:DC:H2''	6:G:12:DG:H5''	2.01	0.42
1:B:55:ARG:HH12	1:B:57:ASP:HA	1.85	0.42
3:D:149:PRO:O	3:D:153:ALA:N	2.49	0.42
6:G:7:DT:H2''	6:G:8:DC:C5	2.54	0.42
8:J:97:LEU:HD12	8:J:101:VAL:HG11	2.01	0.42
2:C:575:VAL:HG13	2:C:616:MET:HE1	2.01	0.42
8:J:216:ARG:HH22	8:J:242:LEU:HD22	1.85	0.42
3:D:1046:GLY:HA3	3:D:1063:PRO:HA	2.01	0.42
8:J:206:THR:HG22	8:J:215:LEU:HB2	2.00	0.42
2:C:590:ARG:HA	2:C:590:ARG:HD2	1.89	0.42
2:C:573:VAL:HG21	2:C:961:VAL:HG11	2.02	0.42
6:G:12:DG:O6	7:H:44:DA:N6	2.52	0.42
6:G:16:DG:N3	7:H:42:DG:N2	2.67	0.42
1:K:256:LEU:HD21	1:K:261:TYR:HB2	2.02	0.42
3:D:588:LEU:HD12	3:D:621:LEU:HD21	2.00	0.42
3:D:888:THR:OG1	3:D:889:GLU:N	2.52	0.42
5:F:282:ASN:ND2	6:G:37:DT:H3	2.18	0.42
5:F:499:HIS:HD2	8:I:211:LEU:HB3	1.85	0.42
6:G:40:DG:C2'	6:G:41:DA:C8	3.02	0.42
2:C:301:ARG:HA	2:C:301:ARG:HD2	1.73	0.42
5:F:394:ILE:HD13	5:F:394:ILE:HA	1.90	0.42
6:G:50:DG:H2''	6:G:51:DG:C8	2.55	0.42
8:J:30:LEU:HD12	8:J:120:ASP:HB2	2.02	0.42
1:K:251:ILE:HG12	1:K:264:LEU:HD12	2.00	0.42
1:K:279:SER:N	1:K:282:ASP:OD2	2.46	0.42
2:C:333:LYS:HD3	2:C:341:THR:HG21	2.02	0.41
3:D:924:VAL:HG11	3:D:954:VAL:HG13	2.02	0.41
8:J:236:TYR:CG	8:J:259:GLN:HG3	2.54	0.41
1:A:28:PRO:HD3	1:A:189:PHE:HD1	1.85	0.41
2:C:285:GLU:O	2:C:290:ASN:N	2.53	0.41
2:C:749:LYS:HE3	2:C:749:LYS:HB3	1.85	0.41
6:G:6:DT:H73	6:G:7:DT:H72	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:257:THR:HG23	1:K:260:SER:H	1.85	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.90	0.41
3:D:728:ILE:HD12	3:D:728:ILE:HA	1.91	0.41
3:D:1207:ALA:HA	3:D:1215:VAL:HG21	2.02	0.41
1:A:47:PRO:HB3	1:B:1:MET:HE1	2.01	0.41
5:F:492:LYS:O	5:F:495:SER:OG	2.33	0.41
6:G:39:DG:H4'	6:G:40:DG:OP2	2.20	0.41
6:G:40:DG:H2''	6:G:41:DA:C8	2.51	0.41
8:I:135:ARG:HD3	8:I:188:MET:HE2	2.02	0.41
1:B:98:ARG:NH2	1:B:137:GLU:OE1	2.53	0.41
3:D:582:VAL:HG22	3:D:688:LEU:HD23	2.03	0.41
5:F:458:VAL:HG21	5:F:493:THR:HG21	2.01	0.41
1:A:60:LEU:HD12	1:A:159:ILE:HG22	2.03	0.41
3:D:1100:ASN:HD21	3:D:1102:HIS:HB2	1.86	0.41
1:A:45:SER:O	1:A:45:SER:OG	2.33	0.41
1:A:53:SER:OG	1:A:54:ILE:N	2.53	0.41
2:C:753:GLU:HG3	2:C:794:PRO:HD3	2.03	0.41
2:C:1107:LYS:HA	2:C:1107:LYS:HD3	1.86	0.41
3:D:222:VAL:HG11	3:D:243:GLU:HG2	2.02	0.41
7:H:47:DC:C4	7:H:48:DT:C5	3.08	0.41
2:C:306:LYS:HB3	2:C:306:LYS:HE3	1.87	0.41
2:C:759:ILE:H	2:C:759:ILE:HG13	1.72	0.41
2:C:814:LYS:HE3	2:C:816:ARG:HH21	1.86	0.41
2:C:1029:ARG:NH1	2:C:1048:PHE:O	2.54	0.41
7:H:35:DG:C2	7:H:36:DA:C8	3.08	0.41
8:J:239:THR:HG21	8:J:255:LEU:HD21	2.02	0.41
3:D:819:VAL:HG21	3:D:847:SER:HA	2.03	0.41
5:F:216:LYS:HG2	6:G:39:DG:O6	2.21	0.41
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.34	0.40
3:D:1234:ASN:HD22	3:D:1242:PRO:HD3	1.86	0.40
2:C:837:ARG:HH21	2:C:839:PHE:HE1	1.69	0.40
3:D:986:GLY:O	3:D:1244:GLY:N	2.54	0.40
6:G:8:DC:C3'	6:G:9:DA:H5'	2.50	0.40
7:H:49:DG:H2''	7:H:50:DA:C8	2.56	0.40
1:A:97:LEU:HD23	1:A:136:MET:SD	2.61	0.40
2:C:241:GLY:O	2:C:247:ARG:NH1	2.54	0.40
8:J:225:ARG:NE	8:J:269:LEU:O	2.51	0.40
2:C:219:LYS:HD3	2:C:220:GLN:H	1.86	0.40
2:C:578:ALA:O	2:C:614:THR:HG21	2.20	0.40
7:H:22:DA:H2''	7:H:23:DT:N3	2.37	0.40
2:C:585:HIS:NE2	2:C:967:GLU:OE2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:ILE:HG23	2:C:1087:VAL:HG21	2.04	0.40
6:G:40:DG:O6	6:G:41:DA:N6	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/340 (66%)	218 (97%)	6 (3%)	0	100	100
1	B	231/340 (68%)	228 (99%)	3 (1%)	0	100	100
1	K	55/340 (16%)	55 (100%)	0	0	100	100
2	C	1114/1161 (96%)	1080 (97%)	34 (3%)	0	100	100
3	D	1257/1299 (97%)	1221 (97%)	36 (3%)	0	100	100
4	E	75/90 (83%)	74 (99%)	1 (1%)	0	100	100
5	F	313/511 (61%)	307 (98%)	6 (2%)	0	100	100
8	I	248/993 (25%)	245 (99%)	3 (1%)	0	100	100
8	J	247/993 (25%)	243 (98%)	4 (2%)	0	100	100
All	All	3764/6067 (62%)	3671 (98%)	93 (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	194/279 (70%)	193 (100%)	1 (0%)	81	81
1	B	197/279 (71%)	193 (98%)	4 (2%)	48	65
1	K	47/279 (17%)	47 (100%)	0	100	100
2	C	942/979 (96%)	929 (99%)	13 (1%)	59	70
3	D	1047/1087 (96%)	1038 (99%)	9 (1%)	70	76
4	E	63/74 (85%)	63 (100%)	0	100	100
5	F	261/413 (63%)	258 (99%)	3 (1%)	65	74
8	I	187/722 (26%)	187 (100%)	0	100	100
8	J	186/722 (26%)	184 (99%)	2 (1%)	65	74
All	All	3124/4834 (65%)	3092 (99%)	32 (1%)	65	75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	10	THR
1	B	11	GLU
1	B	13	VAL
1	B	106	THR
2	C	135	ILE
2	C	193	ILE
2	C	224	VAL
2	C	359	PHE
2	C	366	ASN
2	C	562	VAL
2	C	612	VAL
2	C	616	MET
2	C	686	GLN
2	C	728	VAL
2	C	1042	LEU
2	C	1116	LEU
2	C	1126	ASP
3	D	70	PHE
3	D	137	THR
3	D	193	VAL
3	D	392	THR
3	D	826	THR
3	D	871	ARG
3	D	954	VAL
3	D	960	LEU

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Mol	Chain	Res	Type
3	D	1212	THR
5	F	428	VAL
5	F	429	VAL
5	F	443	LEU
8	J	121	LEU
8	J	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	89	HIS
1	A	100	GLN
1	A	152	ASN
1	A	226	ASN
1	B	79	ASN
1	B	82	GLN
1	B	226	ASN
2	C	157	ASN
2	C	235	GLN
2	C	358	HIS
2	C	428	GLN
2	C	571	GLN
2	C	600	GLN
2	C	648	ASN
2	C	741	HIS
2	C	852	ASN
2	C	941	GLN
2	C	975	GLN
3	D	341	ASN
3	D	396	ASN
3	D	440	GLN
3	D	499	ASN
3	D	510	GLN
3	D	544	HIS
3	D	564	ASN
3	D	669	ASN
3	D	752	GLN
3	D	799	ASN
3	D	821	ASN
3	D	1102	HIS
3	D	1114	GLN

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Mol	Chain	Res	Type
3	D	1210	GLN
5	F	221	GLN
5	F	232	GLN
5	F	282	ASN
5	F	371	GLN
5	F	442	GLN
8	I	48	GLN
8	I	170	GLN
8	J	49	GLN
8	J	81	GLN
8	J	170	GLN
8	J	256	GLN
1	K	262	ASN
1	K	270	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 3 ligands modelled in this entry, 3 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.

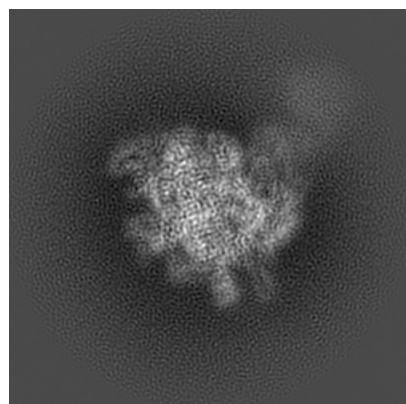
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36914. These allow visual inspection of the internal detail of the map and identification of artifacts.

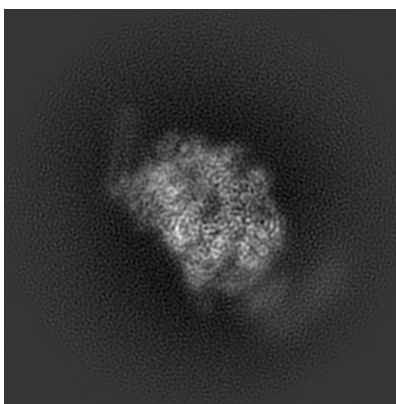
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

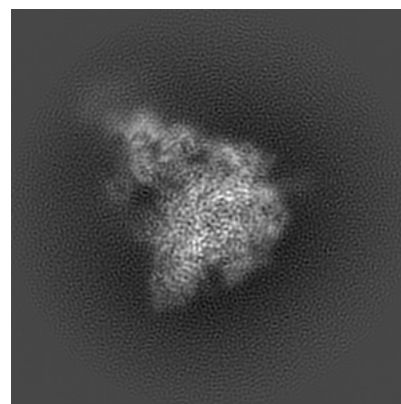
6.1.1 Primary map



X

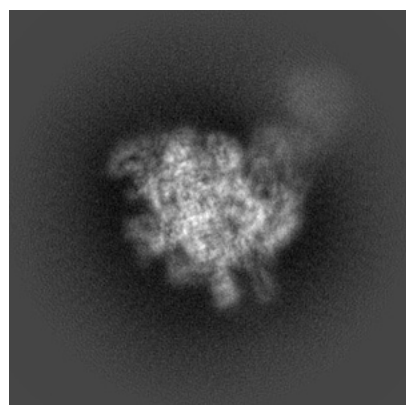


Y

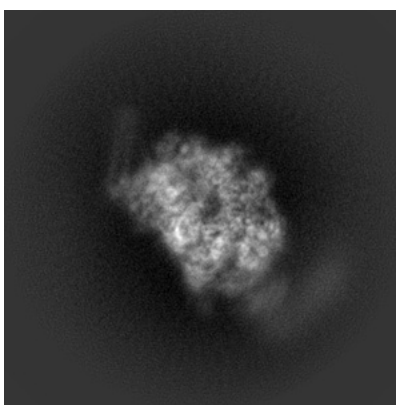


Z

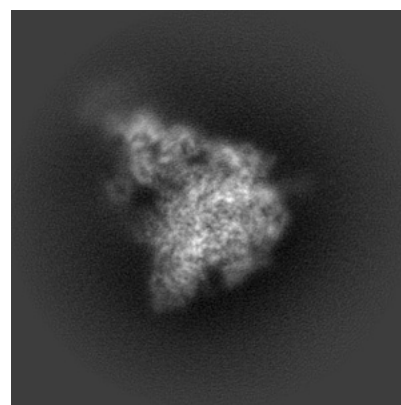
6.1.2 Raw map



X



Y

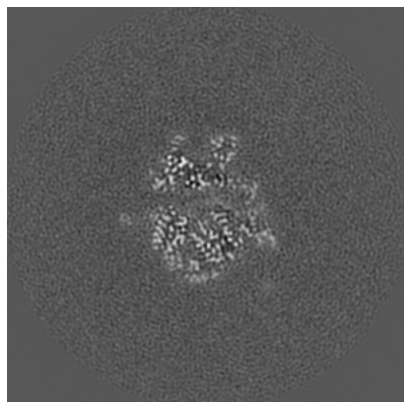


Z

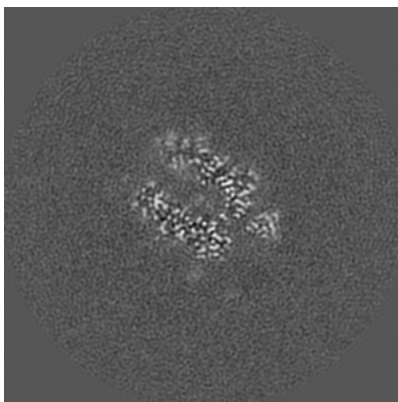
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

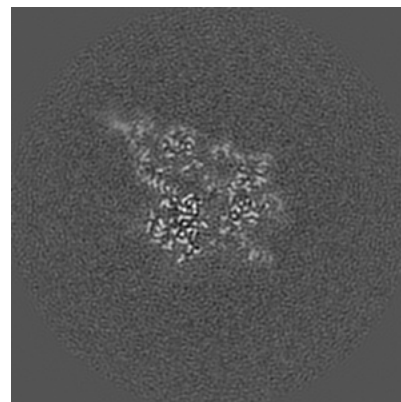
6.2.1 Primary map



X Index: 140

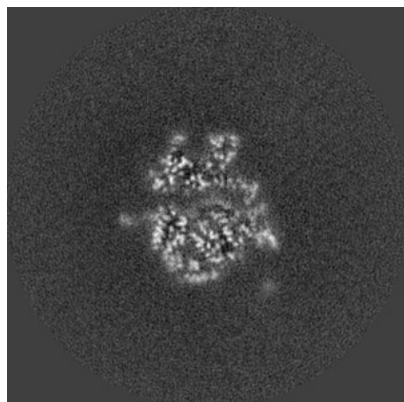


Y Index: 140

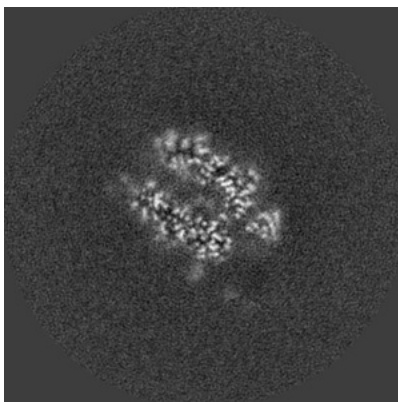


Z Index: 140

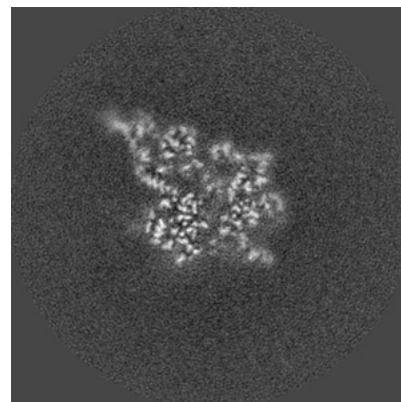
6.2.2 Raw map



X Index: 140



Y Index: 140

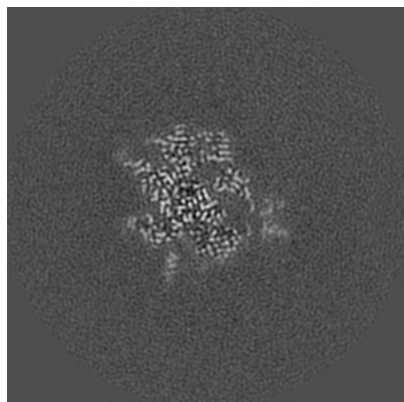


Z Index: 140

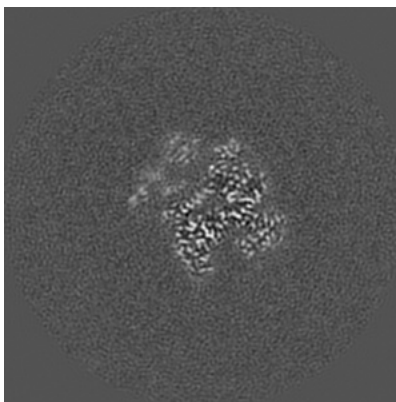
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

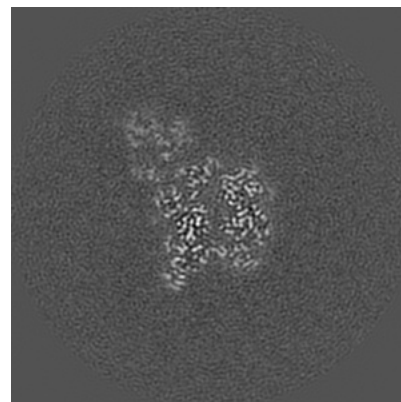
6.3.1 Primary map



X Index: 128

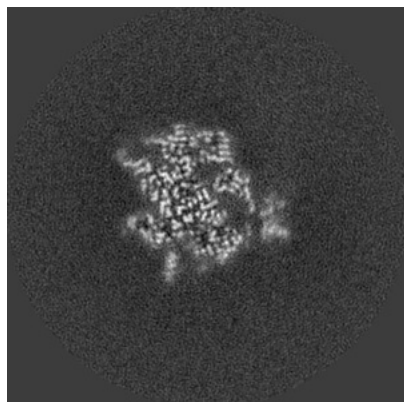


Y Index: 124

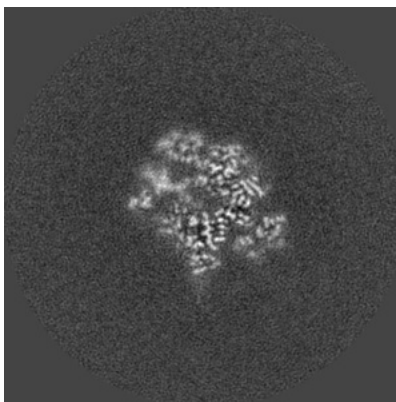


Z Index: 151

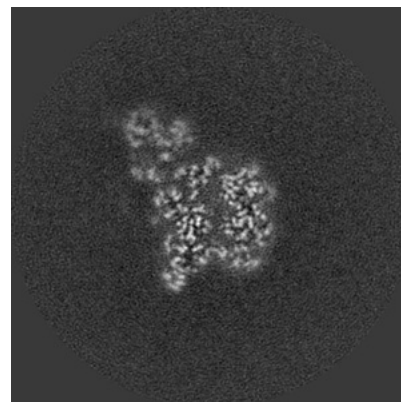
6.3.2 Raw map



X Index: 128



Y Index: 128

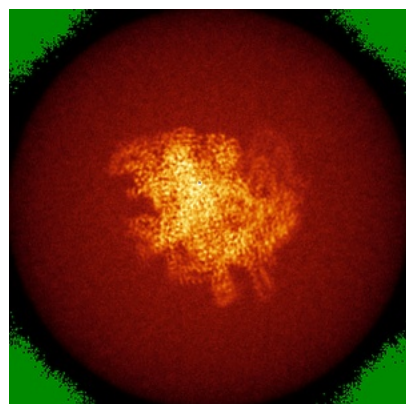


Z Index: 151

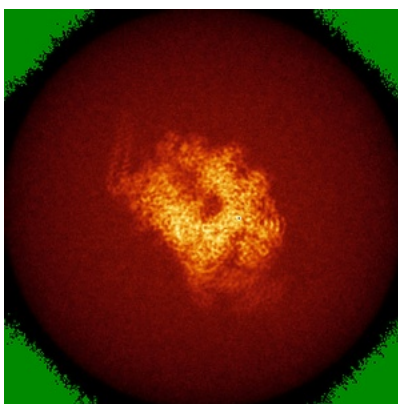
The images above show the largest variance slices of the map in three orthogonal directions.

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

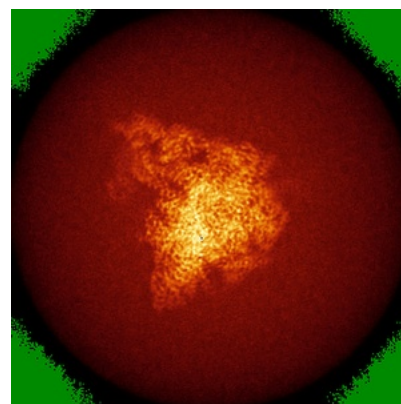
6.4.1 Primary map



X

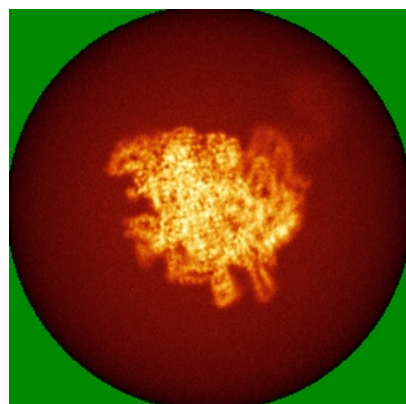


Y

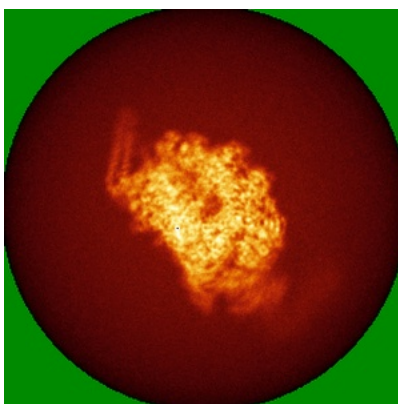


Z

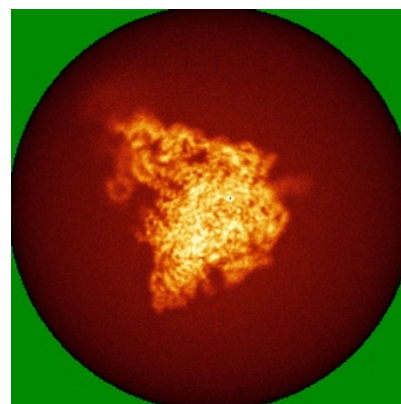
6.4.2 Raw map



X



Y

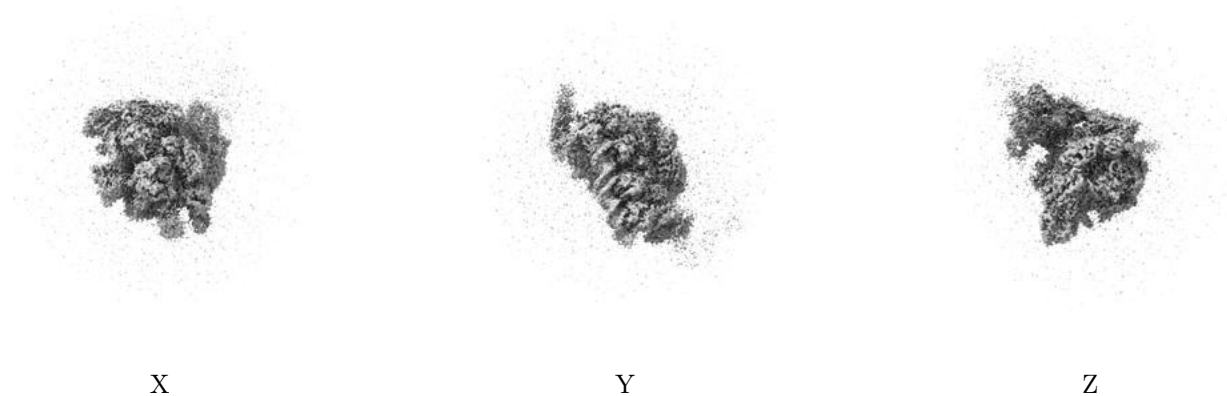


Z

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

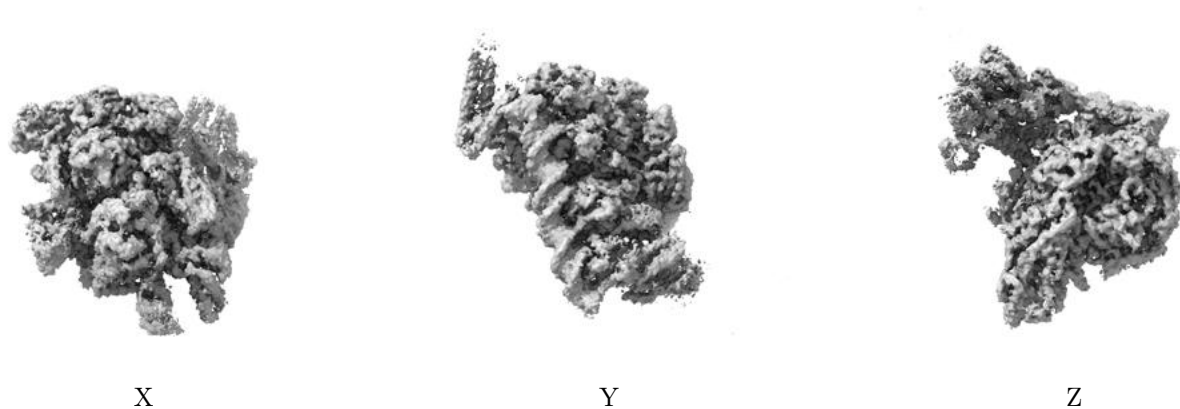
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

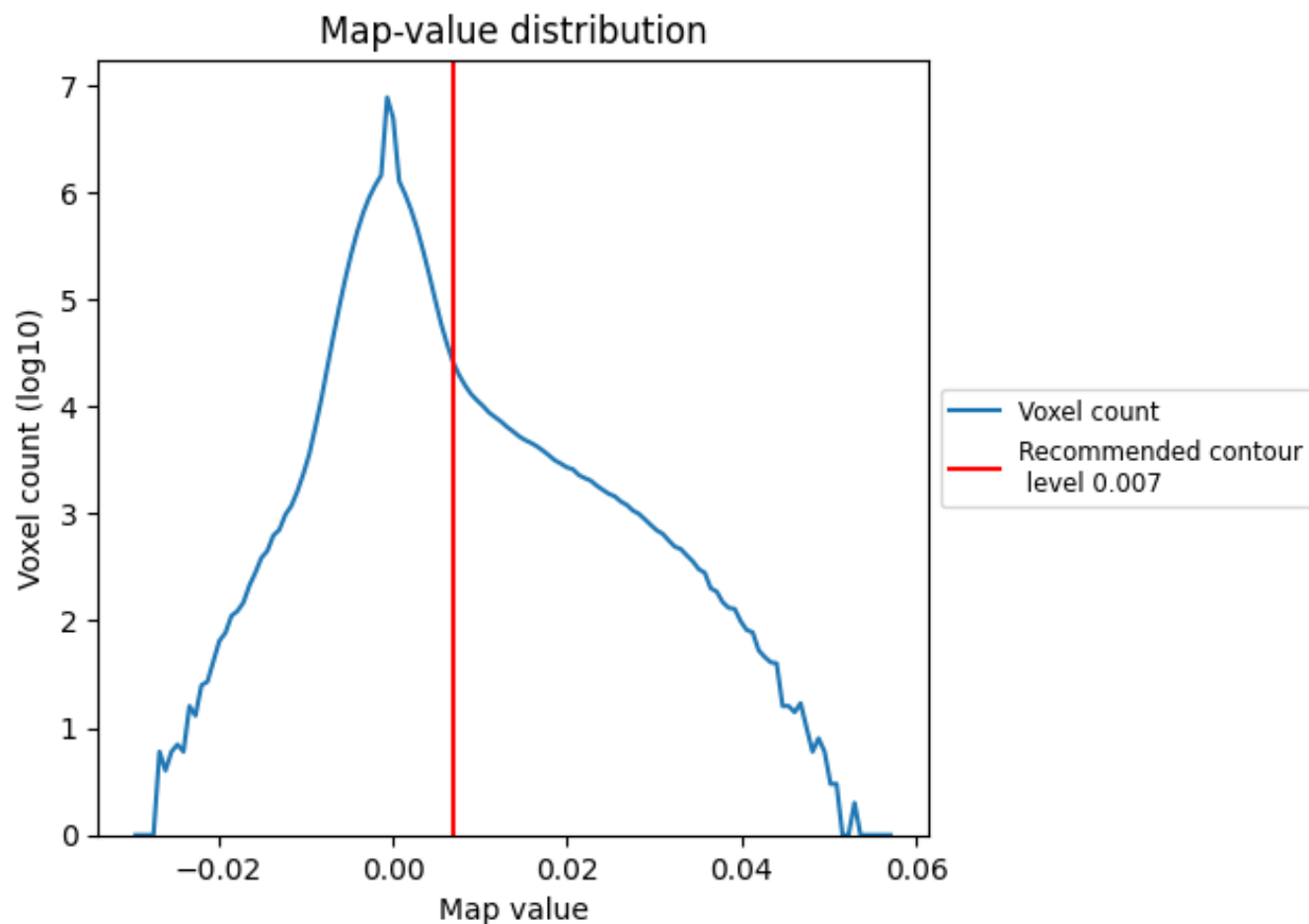
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

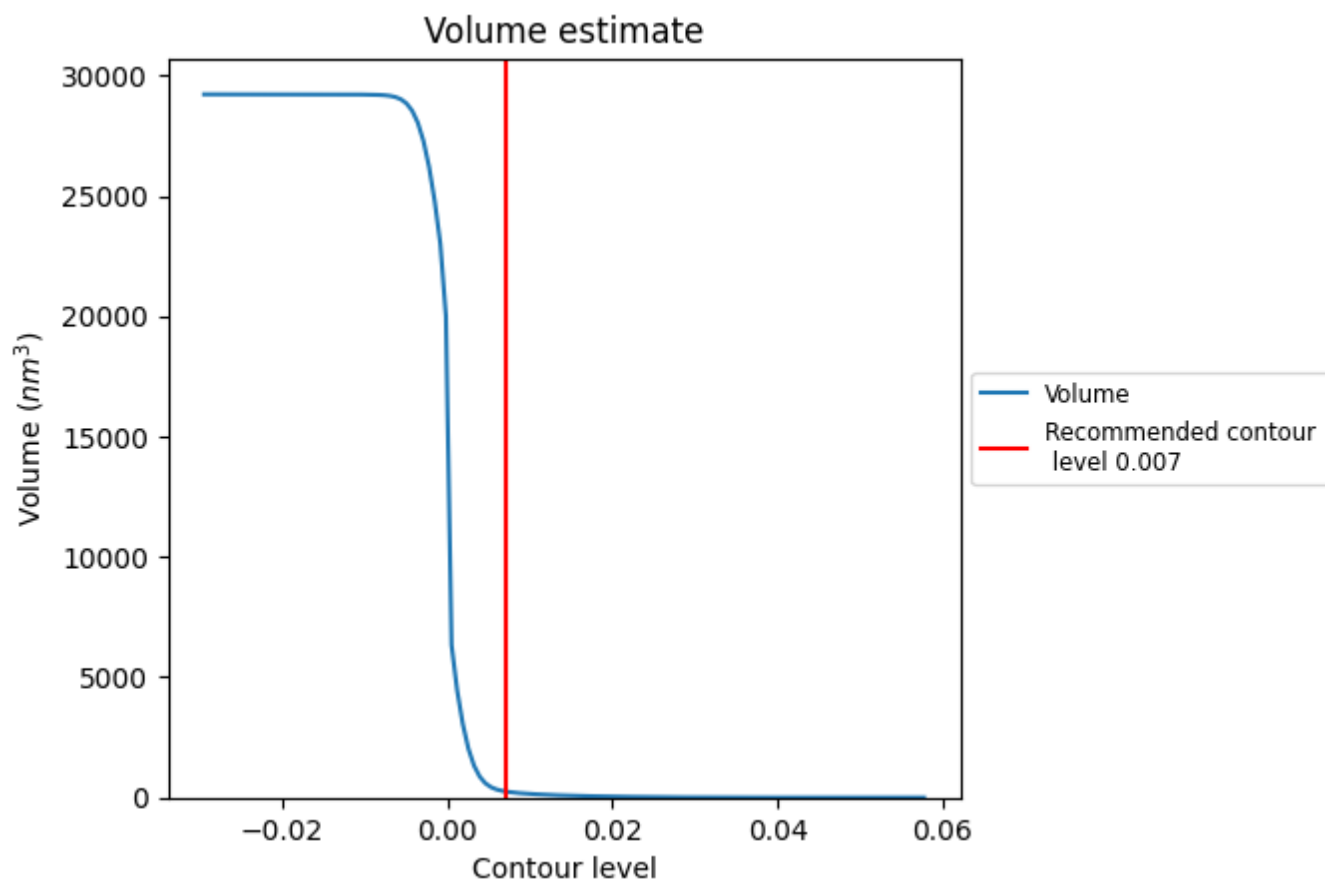
This section contains the results of statistical analysis of the map.

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.

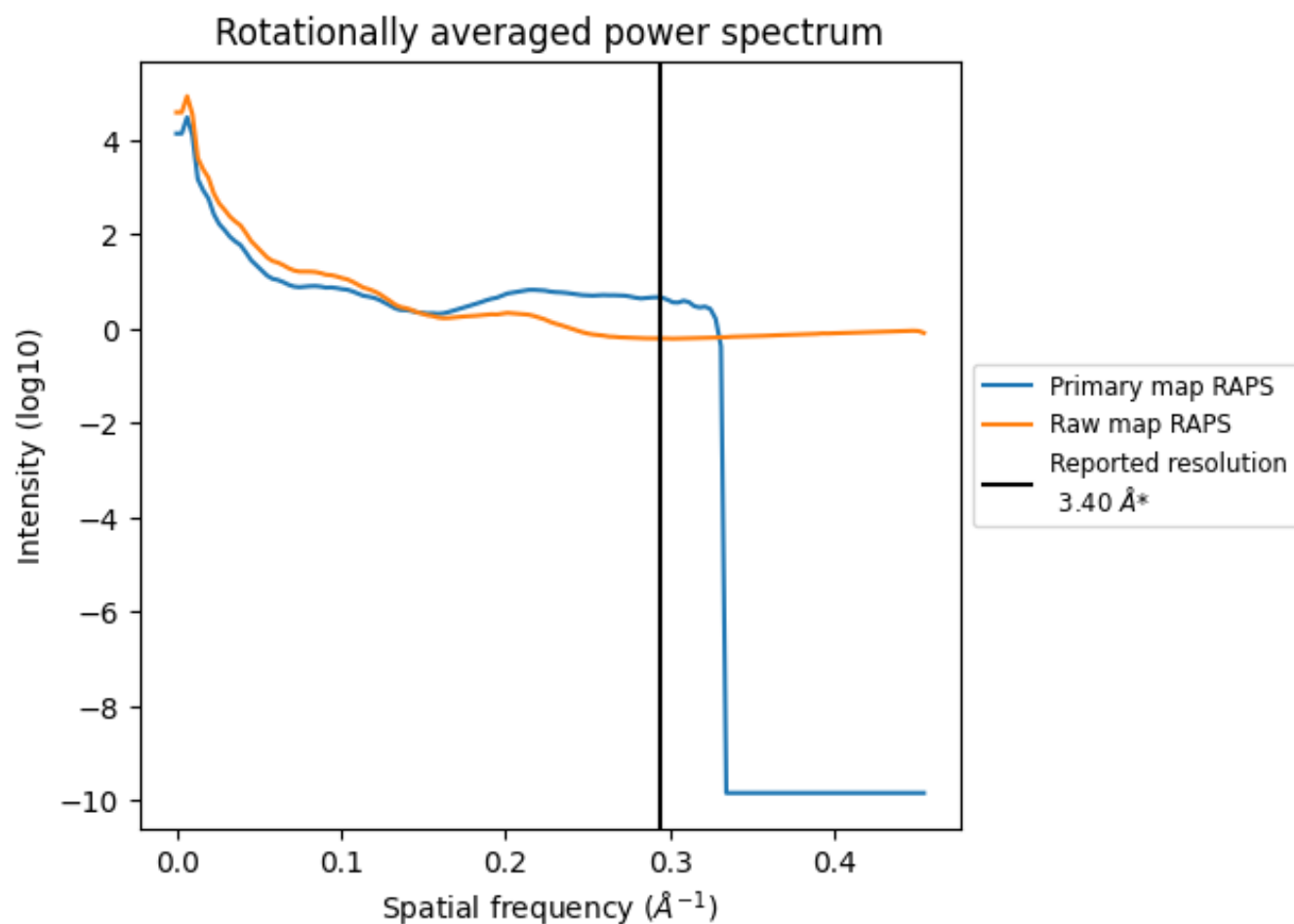
7.2 Volume estimate [i](#)



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 ⓘ

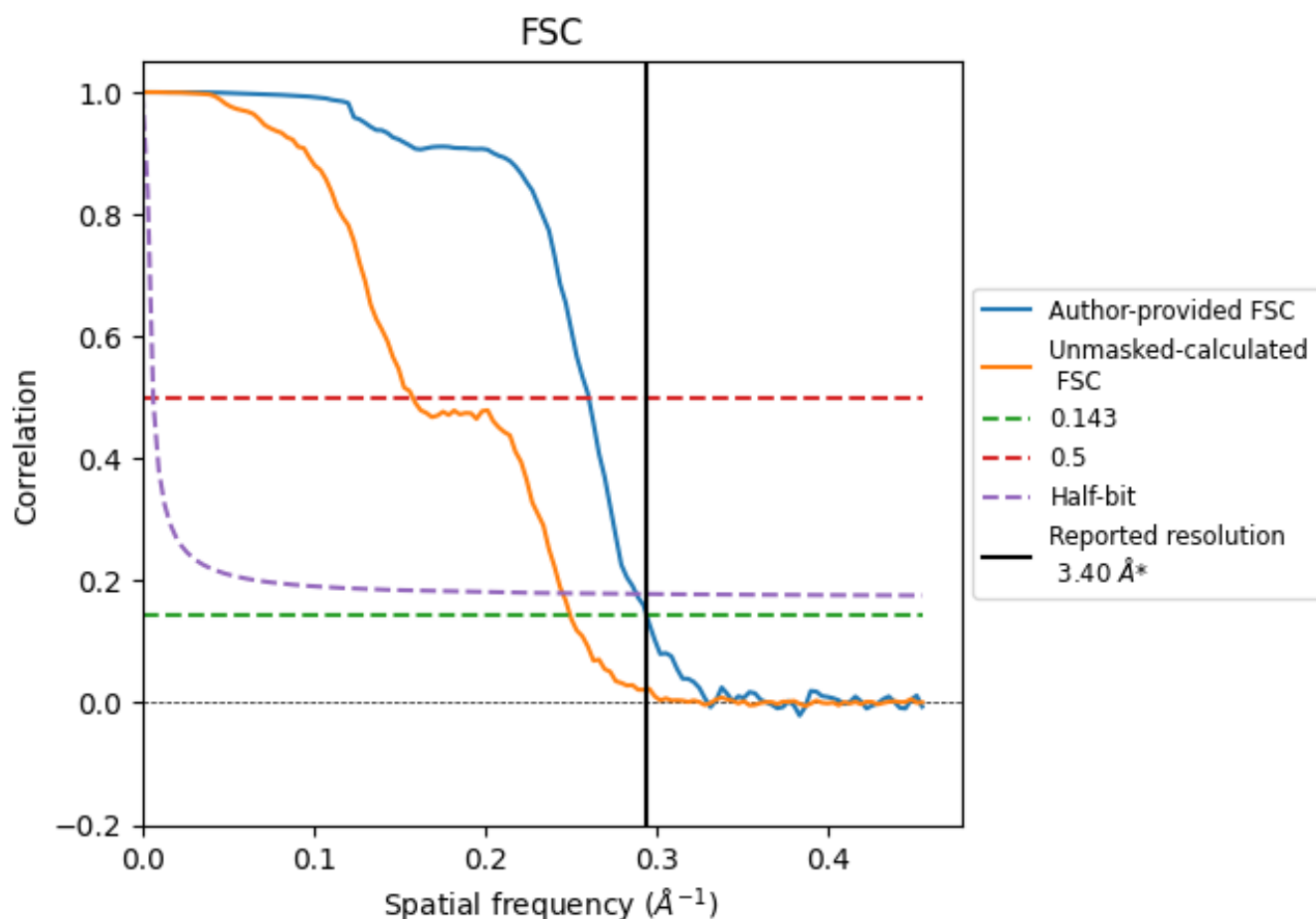


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

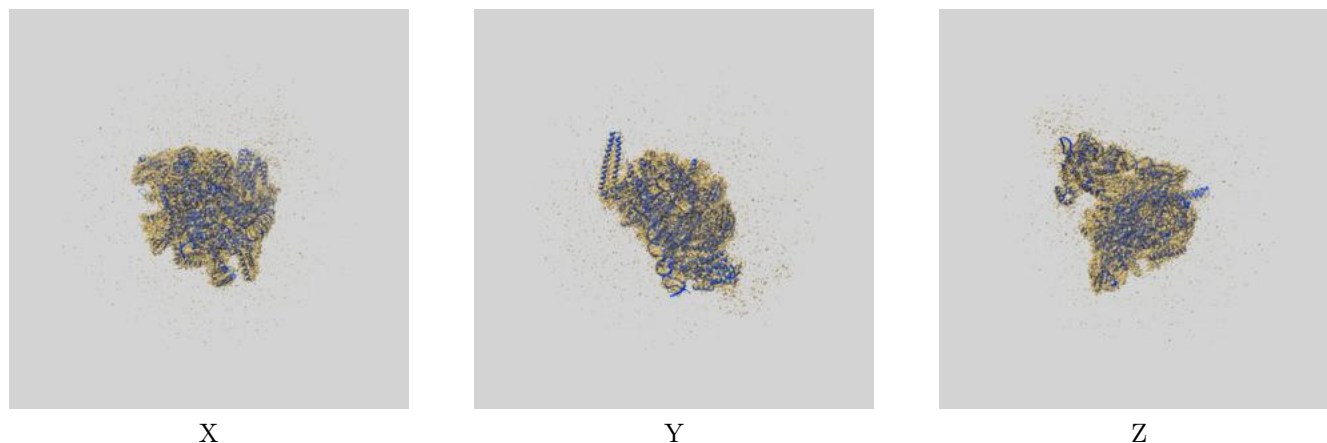
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.84	3.47
Unmasked-calculated*	4.01	6.35	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

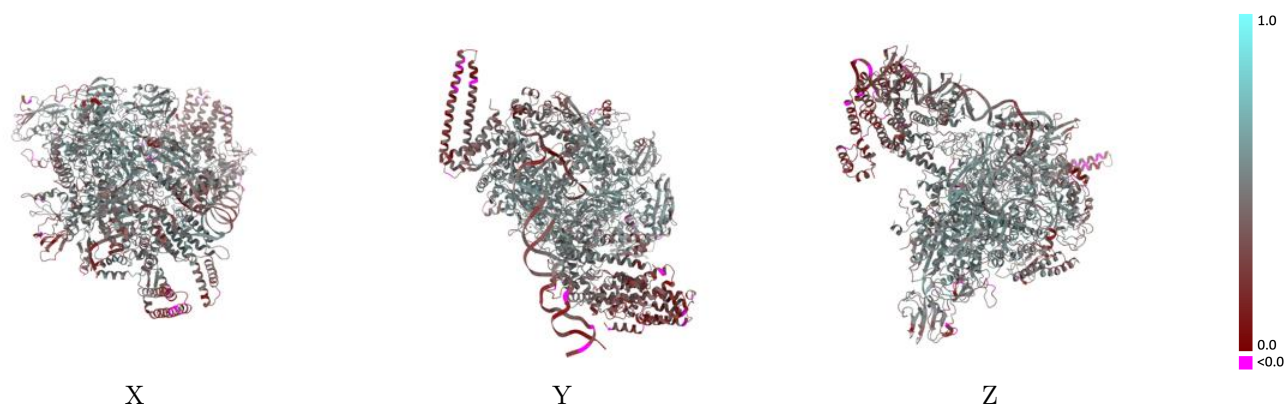
This section contains information regarding the fit between EMDB map EMD-36914 and PDB model 8K60. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



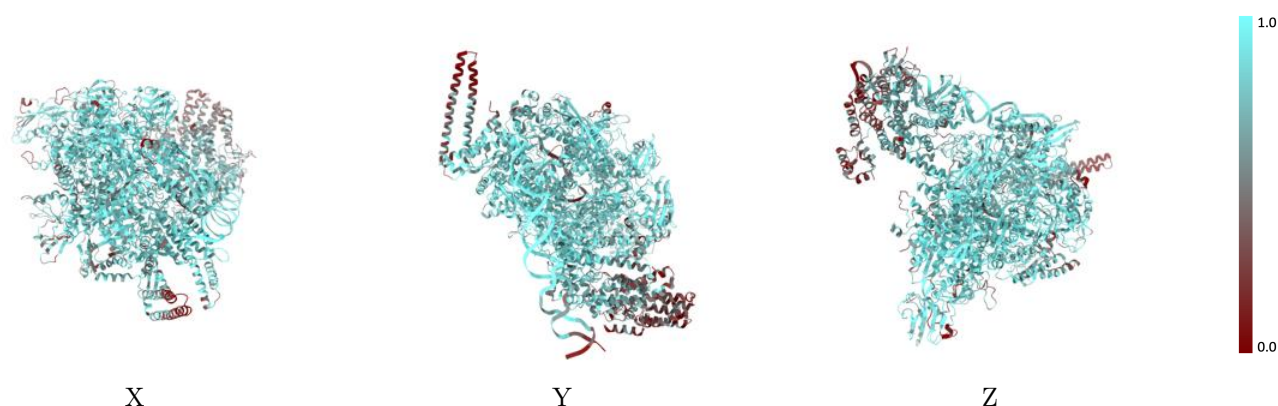
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



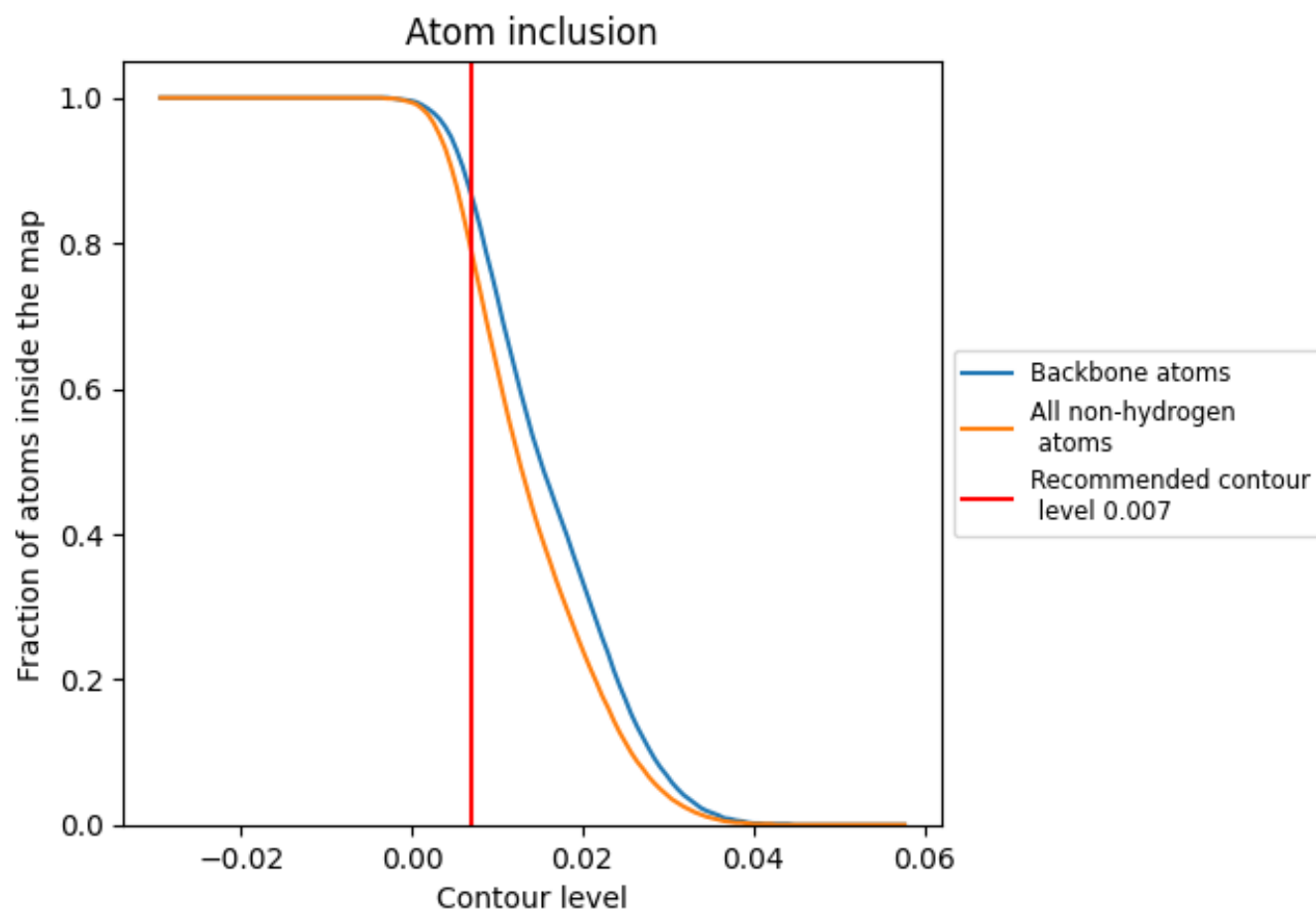
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.4470
A	0.8120	0.4780
B	0.7750	0.4560
C	0.8510	0.4900
D	0.8120	0.4680
E	0.7960	0.4700
F	0.7930	0.4410
G	0.8120	0.3690
H	0.6880	0.3010
I	0.7510	0.4200
J	0.5180	0.3180
K	0.4030	0.2510

1.0

0.0

<0.0