



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:14 PM UTC

PDB ID : 6KF4 / pdb_00006kf4
EMDB ID : EMD-9961
Title : Cryo-EM structure of Thermococcus kodakarensis RNA polymerase
Authors : Jun, S.-H.; Hyun, J.; Jeong, H.; Cha, J.S.; Kim, H.; Bartlett, M.S.; Cho, H.-S.;
Murakami, K.S.
Deposited on : 2019-07-06
Resolution : 3.97 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

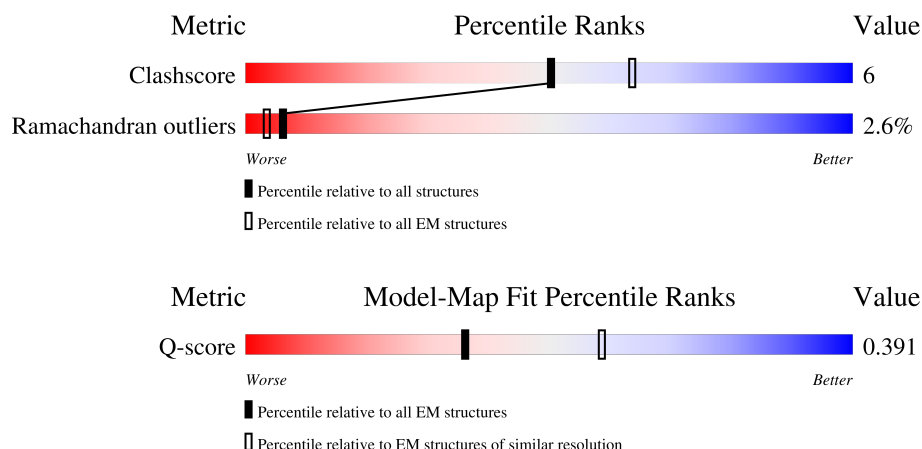
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	 13% 84% 14% ..
2	B	1123	 11% 79% 19% ..
3	C	391	 26% 75% 21% ..
4	D	259	 1% 87% 12% .
5	E	190	 25% 81% 14% 5%

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Mol	Chain	Length	Quality of chain
6	F	122	
7	H	82	
8	K	57	
9	L	94	
10	N	65	
11	P	49	
12	G	185	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27747 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	901	Total	C	N	O	S	0	0
			7189	4540	1278	1331	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8892	5616	1587	1652	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3037	1920	525	582	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	257	Total	C	N	O	S	0	0
			2058	1325	340	389	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	181	Total	C	N	O	S	0	0
			1465	939	250	267	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	122	Total	C	N	O	S	0	0
			1020	654	169	193	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	expression tag	UNP Q5JI52
F	116	ASP	-	expression tag	UNP Q5JI52
F	117	GLU	-	expression tag	UNP Q5JI52
F	118	TYR	-	expression tag	UNP Q5JI52
F	119	ARG	-	expression tag	UNP Q5JI52
F	120	PRO	-	expression tag	UNP Q5JI52
F	121	LEU	-	expression tag	UNP Q5JI52
F	122	GLU	-	expression tag	UNP Q5JI52

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	76	Total	C	N	O	0	0
			627	408	105	114		

- 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
			775	493	134	146	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
			529	340	89	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	42	Total	C	N	O	S	0	0
			329	206	65	54	4		

- Molecule 12 is a protein called Transcription factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	166	Total	C	N	O	S	0	0
			1386	881	228	267	10		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

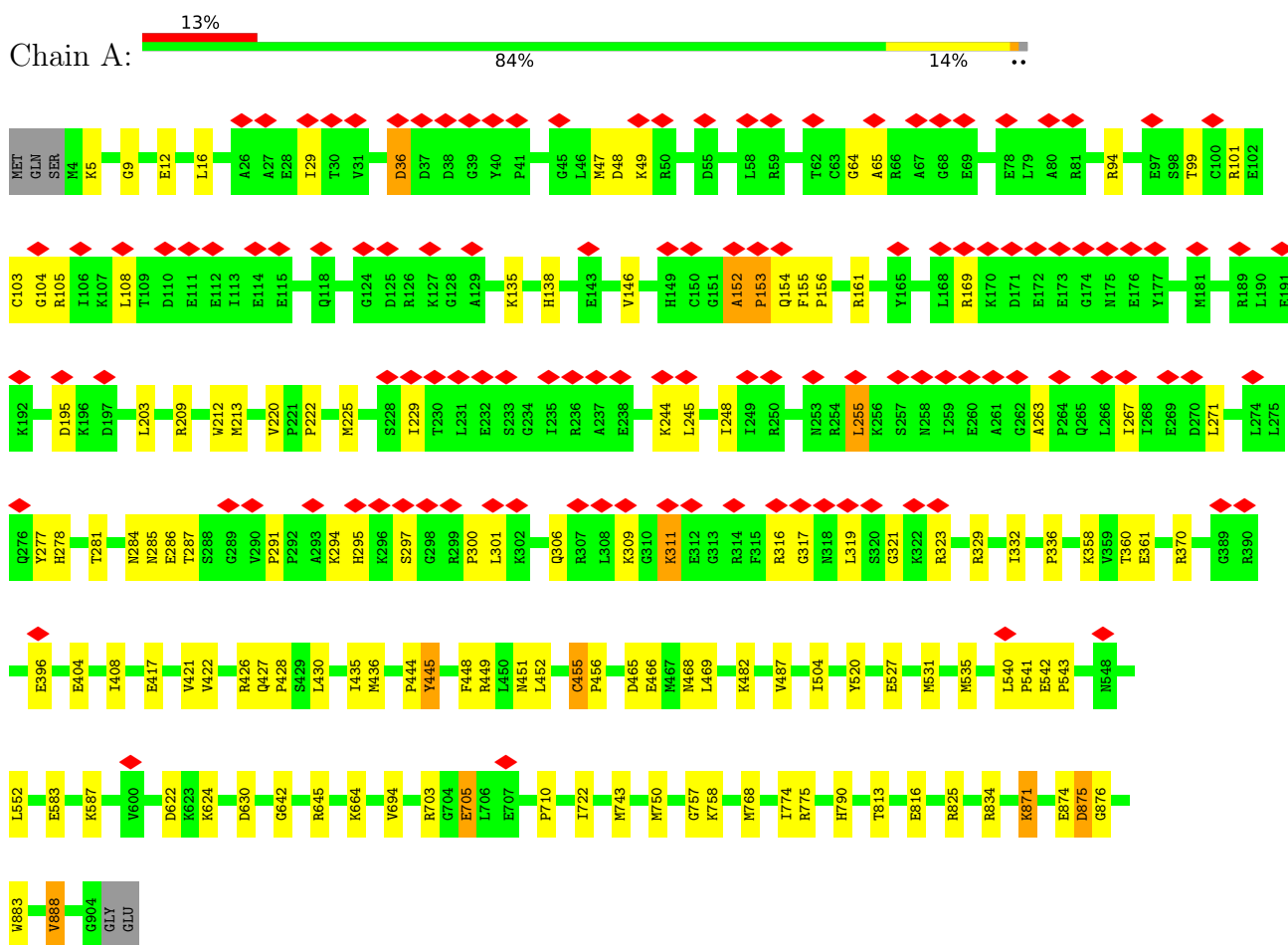
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	Zn	0
			2	2	
14	B	1	Total	Zn	0
			1	1	
14	N	1	Total	Zn	0
			1	1	
14	P	1	Total	Zn	0
			1	1	
14	G	1	Total	Zn	0
			1	1	

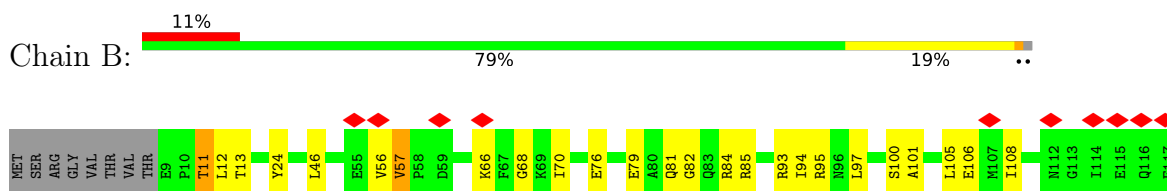
3 Residue-property plots

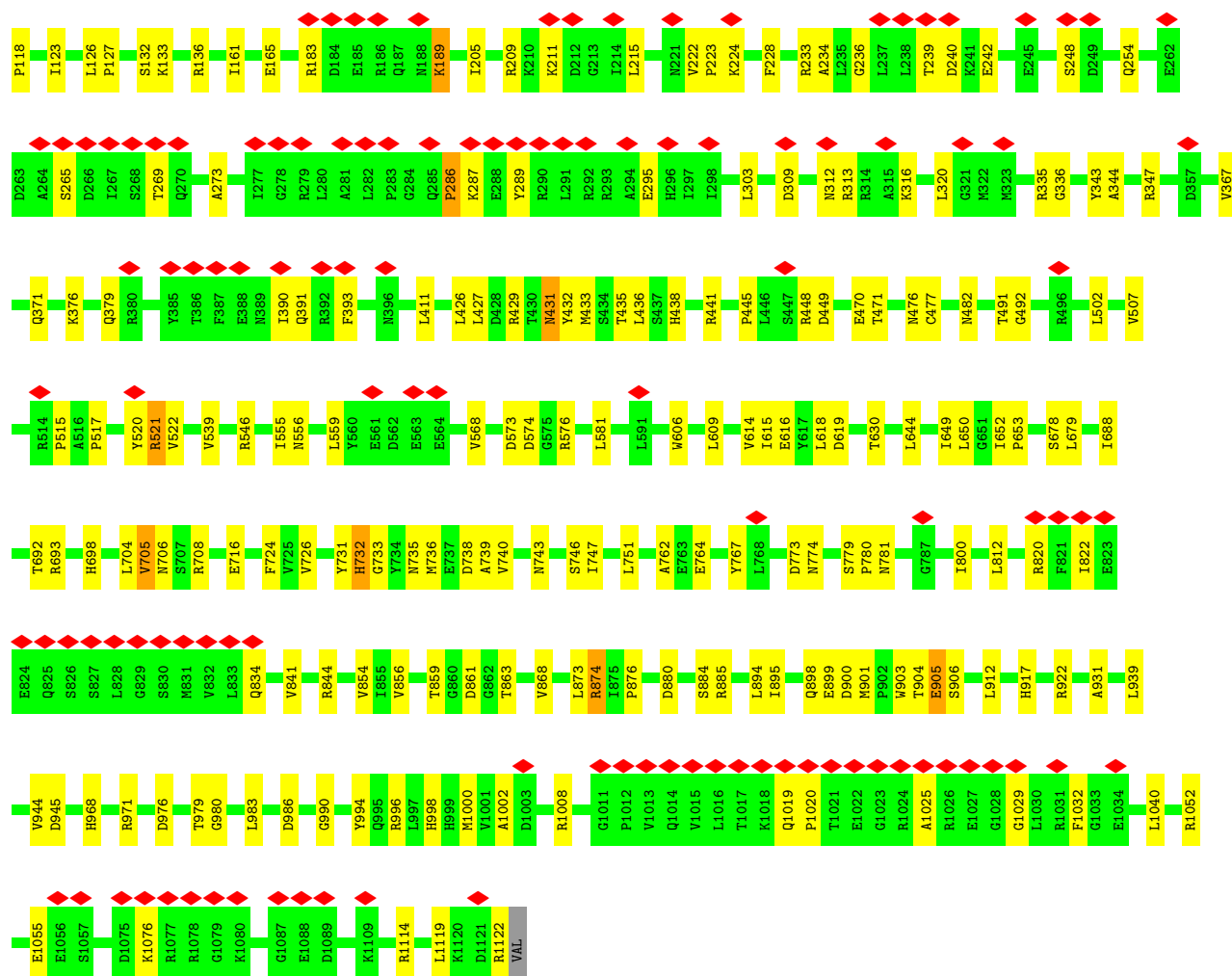
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

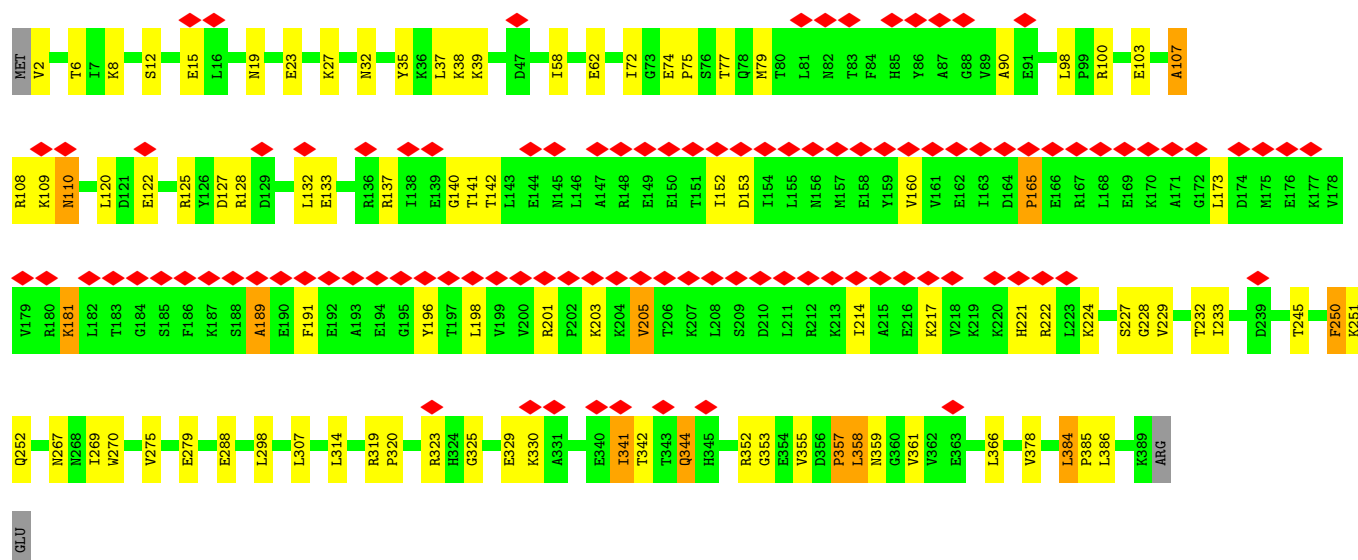
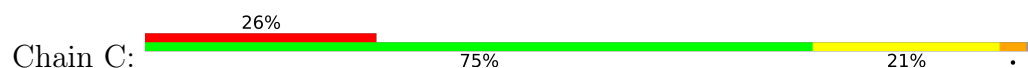


- Molecule 2: DNA-directed RNA polymerase subunit beta

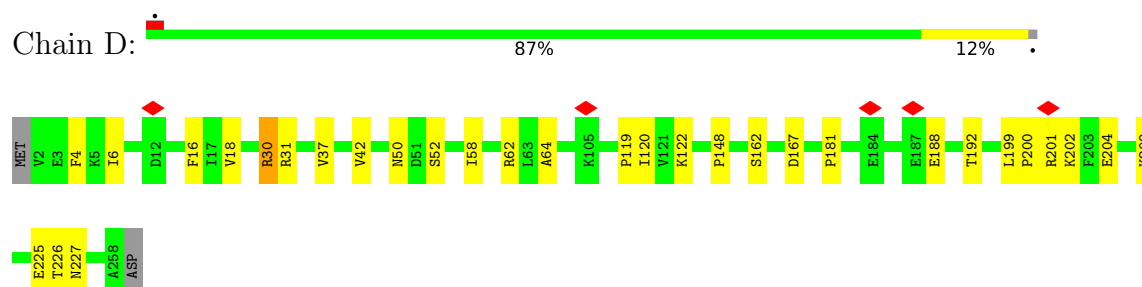




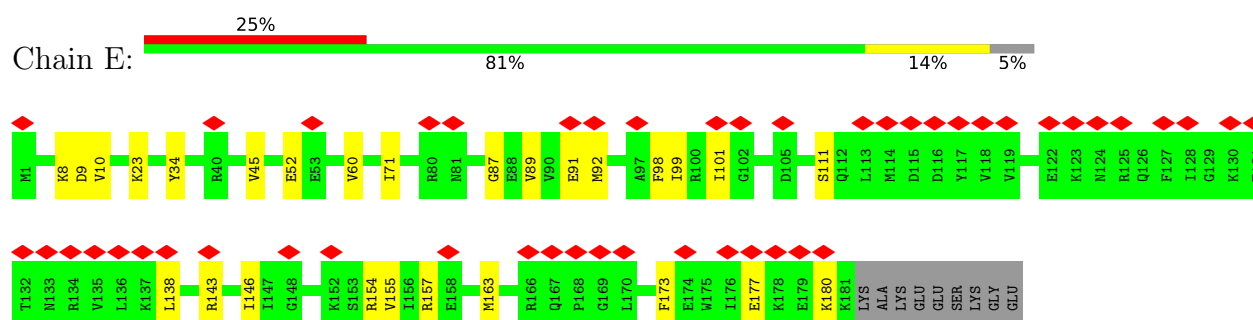
• Molecule 3: DNA-directed RNA polymerase subunit A''



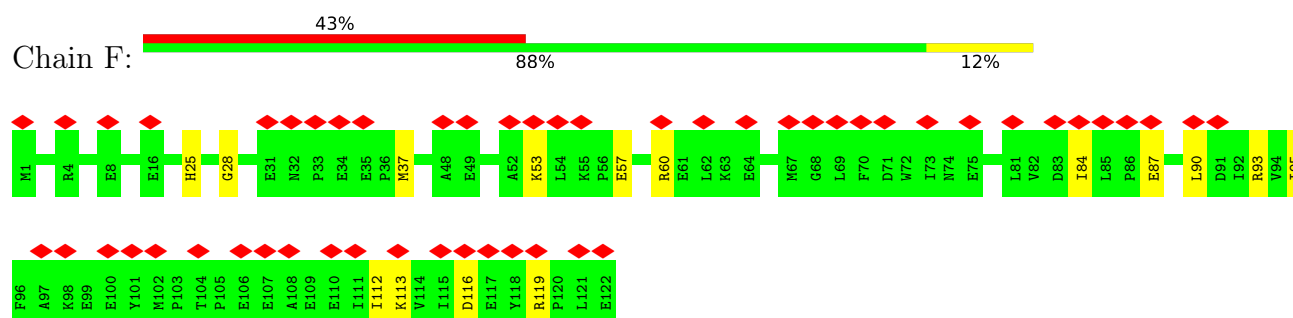
- Molecule 4: DNA-directed RNA polymerase subunit D



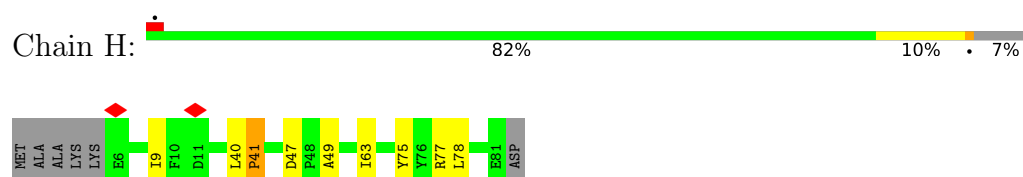
- Molecule 5: DNA-directed RNA polymerase, subunit E



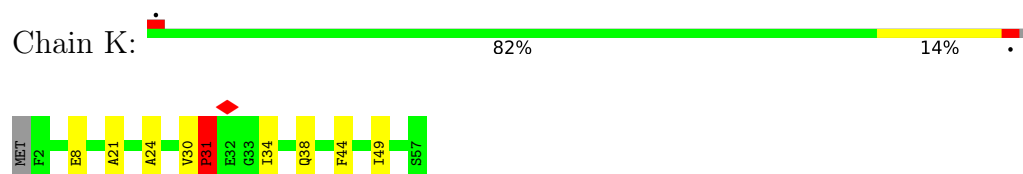
- Molecule 6: DNA-directed RNA polymerase, subunit F



- 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:  88% 12%



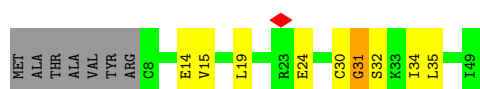
- Molecule 10: DNA-directed RNA polymerase subunit N

Chain N:  75% 22%



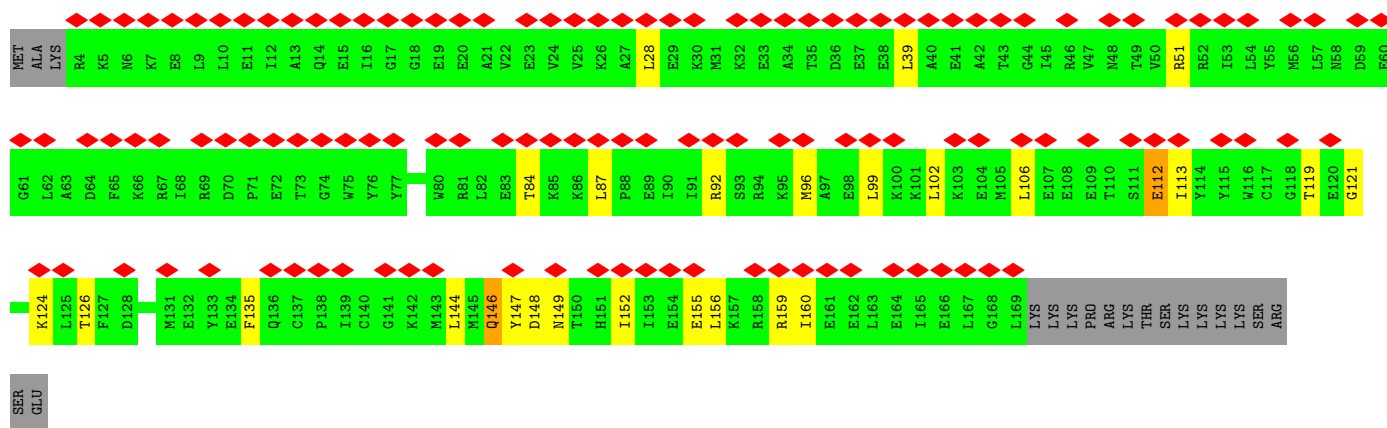
- Molecule 11: DNA-directed RNA polymerase subunit P

Chain P:  67% 16% 14%



- Molecule 12: Transcription factor E

Chain G:  67% 75% 14% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252508	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 ($e^-/\text{\AA}^2$)	35.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.816	Depositor
Minimum map value	-0.470	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	246.4, 246.4, 246.4	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	0.52	0/7332	0.99	22/9895 (0.2%)
2	B	0.54	0/9070	0.99	14/12256 (0.1%)
3	C	0.45	0/3077	1.09	10/4156 (0.2%)
4	D	0.53	0/2103	0.78	1/2848 (0.0%)
5	E	0.36	0/1491	0.73	0/2008
6	F	0.28	0/1040	0.75	2/1399 (0.1%)
7	H	0.49	0/641	1.00	1/866 (0.1%)
8	K	0.52	0/441	0.95	2/598 (0.3%)
9	L	0.48	0/790	0.87	0/1066
10	N	0.65	0/538	1.17	5/723 (0.7%)
11	P	0.49	0/333	1.22	1/445 (0.2%)
12	G	0.24	0/1409	0.62	0/1890
All	All	0.50	0/28265	0.96	58/38150 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	2
3	C	0	4
8	K	0	1
12	G	0	3
All	All	0	14

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	LEU	CA-C-N	9.14	144.10	121.80
2	B	12	LEU	C-N-CA	9.14	144.10	121.80
3	C	110	ASN	N-CA-C	8.32	128.21	109.81
3	C	35	TYR	N-CA-C	-7.16	103.19	113.21
1	A	444	PRO	CA-C-N	7.06	135.03	121.54
1	A	444	PRO	C-N-CA	7.06	135.03	121.54
7	H	41	PRO	N-CA-C	6.92	124.06	113.75
10	N	45	CYS	CA-CB-SG	6.81	130.06	114.40
3	C	250	PHE	N-CA-C	6.70	125.06	110.80
2	B	57	VAL	CA-C-N	6.67	143.01	127.00
2	B	57	VAL	C-N-CA	6.67	143.01	127.00
2	B	894	LEU	CA-CB-CG	6.30	138.34	116.30
6	F	28	GLY	CA-C-N	6.26	132.98	121.70
6	F	28	GLY	C-N-CA	6.26	132.98	121.70
2	B	57	VAL	C-N-CD	-6.23	106.89	120.60
1	A	101	ARG	CA-C-N	6.22	133.42	121.54
1	A	101	ARG	C-N-CA	6.22	133.42	121.54
3	C	109	LYS	CA-C-N	6.18	136.88	121.80
3	C	109	LYS	C-N-CA	6.18	136.88	121.80
3	C	357	PRO	CA-C-N	6.12	133.22	121.54
3	C	357	PRO	C-N-CA	6.12	133.22	121.54
1	A	444	PRO	N-CA-C	6.05	120.78	110.74
1	A	757	GLY	CA-C-N	5.86	132.73	121.54
1	A	757	GLY	C-N-CA	5.86	132.73	121.54
8	K	31	PRO	N-CA-C	5.85	124.53	112.47
11	P	24	GLU	N-CA-C	5.78	118.86	110.42
1	A	874	GLU	CA-CB-CG	5.72	125.55	114.10
8	K	30	VAL	N-CA-C	5.63	121.05	108.88
10	N	5	VAL	CA-C-N	5.60	132.24	121.54
10	N	5	VAL	C-N-CA	5.60	132.24	121.54
2	B	899	GLU	CA-CB-CG	-5.59	102.93	114.10
1	A	543	PRO	N-CA-C	5.54	126.49	112.10
1	A	883	TRP	N-CA-C	5.53	118.38	107.98
3	C	35	TYR	CA-C-N	5.43	131.92	121.54
3	C	35	TYR	C-N-CA	5.43	131.92	121.54
2	B	426	LEU	CA-CB-CG	5.42	135.26	116.30
1	A	888	VAL	N-CA-C	5.32	120.41	109.34
4	D	30	ARG	CB-CG-CD	-5.31	99.09	111.30
2	B	1076	LYS	CA-C-N	5.27	131.60	121.54
2	B	1076	LYS	C-N-CA	5.27	131.60	121.54
2	B	905	GLU	CA-C-N	5.24	131.56	121.54
2	B	905	GLU	C-N-CA	5.24	131.56	121.54
1	A	541	PRO	CA-C-N	5.23	134.56	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	PRO	C-N-CA	5.23	134.56	121.80
1	A	768	MET	CB-CG-SD	-5.22	97.03	112.70
1	A	705	GLU	CA-C-N	5.21	131.48	121.54
1	A	705	GLU	C-N-CA	5.21	131.48	121.54
1	A	267	ILE	CA-CB-CG1	5.19	119.23	110.40
1	A	874	GLU	CA-C-N	5.19	131.46	121.54
1	A	874	GLU	C-N-CA	5.19	131.46	121.54
10	N	6	ARG	N-CA-C	-5.16	99.81	110.80
1	A	255	LEU	CA-CB-CG	5.14	134.30	116.30
1	A	36	ASP	CA-C-N	5.14	130.95	121.70
1	A	36	ASP	C-N-CA	5.14	130.95	121.70
2	B	81	GLN	CA-CB-CG	5.13	124.35	114.10
3	C	384	LEU	N-CA-C	5.06	121.00	109.81
2	B	732	HIS	N-CA-C	5.04	121.54	110.80
10	N	45	CYS	CB-CA-C	-5.03	101.01	110.67

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	GLN	Peptide
1	A	455	CYS	Peptide
1	A	535	MET	Peptide
1	A	540	LEU	Peptide
2	B	11	THR	Peptide
2	B	704	LEU	Peptide
3	C	110	ASN	Peptide
3	C	173	LEU	Peptide
3	C	203	LYS	Peptide
3	C	342	THR	Peptide
12	G	112	GLU	Peptide
12	G	146	GLN	Peptide
12	G	147	TYR	Peptide
8	K	31	PRO	Peptide

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	7189	0	7262	77	0
2	B	8892	0	8950	127	0
3	C	3037	0	3151	53	0
4	D	2058	0	2068	25	0
5	E	1465	0	1503	15	0
6	F	1020	0	1024	9	0
7	H	627	0	642	5	0
8	K	433	0	466	5	0
9	L	775	0	770	6	0
10	N	529	0	542	14	0
11	P	329	0	355	5	0
12	G	1386	0	1384	15	0
13	A	1	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	G	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
All	All	27747	0	28117	313	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 (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:VAL:N	3:C:6:THR:HG1	1.74	0.85
2:B:66:LYS:HB3	2:B:108:ILE:HB	1.69	0.75
1:A:774:ILE:HG12	1:A:775:ARG:HD3	1.74	0.70
2:B:286:PRO:HB2	2:B:289:TYR:HB2	1.74	0.69
1:A:445:TYR:HB2	1:A:449:ARG:HH22	1.58	0.68
2:B:706:ASN:ND2	2:B:716:GLU:OE2	2.28	0.67
3:C:279:GLU:HG3	7:H:63:ILE:HD13	1.75	0.67
10:N:7:CYS:SG	10:N:8:PHE:N	2.69	0.65
1:A:213:MET:SD	3:C:352:ARG:NH1	2.66	0.65
3:C:232:THR:HG22	3:C:245:THR:HG22	1.79	0.65
2:B:576:ARG:NH1	2:B:619:ASP:OD2	2.31	0.64
1:A:12:GLU:HG2	3:C:355:VAL:HG12	1.80	0.64
1:A:203:LEU:HD21	3:C:352:ARG:HH21	1.62	0.63
3:C:100:ARG:NH2	3:C:288:GLU:OE2	2.31	0.63
1:A:311:LYS:O	1:A:316:ARG:NH2	2.31	0.63
2:B:95:ARG:HG3	2:B:97:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ILE:HD11	2:B:834:GLN:HB3	1.81	0.63
2:B:652:ILE:HG23	2:B:653:PRO:HD3	1.80	0.63
2:B:581:LEU:HD12	2:B:618:LEU:HD12	1.80	0.62
5:E:146:ILE:HA	5:E:163:MET:HG2	1.81	0.62
2:B:546:ARG:NH2	2:B:616:GLU:OE2	2.33	0.62
2:B:556:ASN:ND2	2:B:619:ASP:OD2	2.33	0.62
2:B:233:ARG:NH2	2:B:240:ASP:OD1	2.34	0.61
1:A:871:LYS:HB3	1:A:875:ASP:HB3	1.82	0.61
2:B:93:ARG:NH1	2:B:165:GLU:OE2	2.34	0.61
2:B:679:LEU:HD21	2:B:998:HIS:HB3	1.81	0.61
1:A:156:PRO:HG3	1:A:169:ARG:HG3	1.82	0.61
2:B:189:LYS:HE3	2:B:211:LYS:HG3	1.83	0.61
3:C:267:ASN:ND2	3:C:288:GLU:OE2	2.34	0.60
1:A:436:MET:HE2	1:A:487:VAL:HG22	1.83	0.60
2:B:884:SER:OG	2:B:885:ARG:N	2.34	0.60
5:E:91:GLU:HB3	5:E:98:PHE:HB2	1.83	0.60
1:A:426:ARG:NH2	1:A:465:ASP:OD2	2.34	0.60
4:D:62:ARG:NH2	10:N:2:ILE:O	2.35	0.60
6:F:25:HIS:ND1	6:F:37:MET:SD	2.74	0.60
1:A:103:CYS:SG	1:A:104:GLY:N	2.75	0.60
1:A:263:ALA:O	12:G:51:ARG:NH1	2.34	0.59
6:F:116:ASP:HA	6:F:119:ARG:HE	1.66	0.59
2:B:546:ARG:NH1	2:B:555:ILE:O	2.35	0.59
9:L:6:ILE:HG22	9:L:7:ARG:HG3	1.85	0.59
1:A:694:VAL:HG13	1:A:722:ILE:HD12	1.85	0.59
1:A:195:ASP:OD1	1:A:209:ARG:NH1	2.36	0.59
3:C:107:ALA:HB1	3:C:270:TRP:HZ2	1.68	0.59
5:E:177:GLU:HA	5:E:180:LYS:HD2	1.84	0.59
2:B:165:GLU:OE1	2:B:429:ARG:NH2	2.36	0.59
1:A:284:ASN:HB3	1:A:287:THR:HG23	1.85	0.58
2:B:573:ASP:OD1	2:B:576:ARG:NE	2.32	0.58
2:B:70:ILE:HG12	2:B:105:LEU:HD23	1.84	0.58
2:B:726:VAL:HG12	2:B:912:LEU:HB2	1.84	0.58
1:A:5:LYS:O	2:B:1122:ARG:NH1	2.36	0.58
1:A:317:GLY:O	2:B:1019:GLN:NE2	2.37	0.58
1:A:255:LEU:HG	1:A:271:LEU:HD11	1.84	0.58
2:B:427:LEU:HD23	2:B:429:ARG:HH21	1.68	0.58
7:H:41:PRO:HB2	7:H:77:ARG:HG2	1.86	0.58
1:A:520:TYR:HB3	1:A:552:LEU:HD13	1.85	0.57
2:B:874:ARG:HH12	2:B:1002:ALA:HB3	1.68	0.57
1:A:332:ILE:HG22	1:A:448:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:ARG:HH22	10:N:2:ILE:HB	1.69	0.57
1:A:531:MET:HE1	9:L:58:LYS:HD3	1.87	0.57
1:A:834:ARG:NH1	3:C:79:MET:O	2.36	0.57
2:B:85:ARG:NH1	11:P:31:GLY:O	2.33	0.57
4:D:37:VAL:HB	4:D:148:PRO:HG3	1.85	0.57
2:B:614:VAL:HG13	2:B:615:ILE:HG12	1.86	0.57
1:A:370:ARG:NE	1:A:417:GLU:OE2	2.37	0.57
1:A:323:ARG:NH1	2:B:1029:GLY:O	2.38	0.56
1:A:323:ARG:HB2	2:B:1020:PRO:HB2	1.88	0.56
3:C:122:GLU:HG2	3:C:125:ARG:HH12	1.71	0.56
3:C:181:LYS:NZ	3:C:189:ALA:O	2.39	0.56
2:B:108:ILE:HD13	2:B:118:PRO:HB3	1.88	0.56
5:E:23:LYS:NZ	5:E:52:GLU:O	2.39	0.56
6:F:53:LYS:NZ	6:F:84:ILE:O	2.39	0.56
2:B:239:THR:HB	2:B:242:GLU:HG2	1.88	0.56
1:A:321:GLY:O	2:B:1019:GLN:NE2	2.39	0.56
1:A:285:ASN:ND2	1:A:301:LEU:O	2.39	0.56
1:A:47:MET:O	1:A:49:LYS:N	2.39	0.56
1:A:360:THR:OG1	1:A:361:GLU:N	2.33	0.55
9:L:2:ARG:NH2	9:L:4:GLU:OE2	2.40	0.55
3:C:100:ARG:NH1	3:C:103:GLU:OE1	2.39	0.55
9:L:8:ARG:NH1	9:L:68:GLU:OE2	2.38	0.55
2:B:900:ASP:OD1	4:D:31:ARG:NH1	2.37	0.55
2:B:1008:ARG:HH22	2:B:1020:PRO:HB3	1.72	0.55
8:K:34:ILE:HG23	8:K:38:GLN:HB2	1.87	0.55
2:B:431:ASN:ND2	2:B:678:SER:OG	2.38	0.54
7:H:9:ILE:HD13	7:H:49:ALA:HA	1.88	0.54
2:B:800:ILE:HD11	2:B:812:LEU:HA	1.89	0.54
3:C:15:GLU:HG2	3:C:23:GLU:HG2	1.89	0.54
1:A:94:ARG:HG3	1:A:138:HIS:HD2	1.72	0.54
1:A:813:THR:OG1	1:A:816:GLU:OE1	2.26	0.54
4:D:62:ARG:NH1	4:D:120:ILE:O	2.40	0.54
4:D:50:ASN:HD22	4:D:52:SER:H	1.56	0.53
6:F:87:GLU:HA	6:F:119:ARG:HH12	1.72	0.53
12:G:119:THR:OG1	12:G:121:GLY:O	2.27	0.53
2:B:76:GLU:OE1	2:B:84:ARG:NH2	2.41	0.53
2:B:344:ALA:O	2:B:347:ARG:NH1	2.39	0.53
2:B:708:ARG:NH2	2:B:945:ASP:OD2	2.42	0.53
1:A:245:LEU:HD23	1:A:248:ILE:HD12	1.89	0.53
3:C:165:PRO:HB3	3:C:196:TYR:HB3	1.90	0.53
6:F:57:GLU:OE1	6:F:60:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:ASP:OD1	3:C:127:ASP:N	2.41	0.52
2:B:738:ASP:OD2	2:B:922:ARG:NH2	2.42	0.52
12:G:99:LEU:HD23	12:G:102:LEU:HD12	1.91	0.52
12:G:135:PHE:HA	12:G:144:LEU:HD12	1.91	0.52
3:C:325:GLY:O	3:C:329:GLU:N	2.42	0.52
2:B:449:ASP:OD1	2:B:449:ASP:N	2.41	0.52
2:B:100:SER:OG	2:B:101:ALA:N	2.39	0.52
2:B:448:ARG:NH1	2:B:476:ASN:OD1	2.42	0.52
5:E:143:ARG:HH21	5:E:173:PHE:HE1	1.58	0.52
1:A:329:ARG:NH1	1:A:466:GLU:OE1	2.43	0.52
2:B:347:ARG:NE	2:B:573:ASP:OD2	2.43	0.52
2:B:574:ASP:OD1	2:B:574:ASP:N	2.43	0.52
2:B:161:ILE:HD12	2:B:411:LEU:HD22	1.91	0.51
1:A:583:GLU:OE2	1:A:587:LYS:NZ	2.44	0.51
2:B:132:SER:OG	2:B:133:LYS:N	2.39	0.51
3:C:74:GLU:O	3:C:77:THR:OG1	2.27	0.51
3:C:378:VAL:HG21	8:K:8:GLU:HG2	1.93	0.51
10:N:8:PHE:HB2	10:N:47:ARG:HH22	1.75	0.51
1:A:309:LYS:NZ	3:C:344:GLN:OE1	2.44	0.51
5:E:92:MET:HG2	5:E:138:LEU:HD23	1.93	0.51
12:G:156:LEU:HD23	12:G:159:ARG:HD2	1.92	0.50
2:B:939:LEU:O	10:N:46:ARG:NH1	2.44	0.50
2:B:968:HIS:ND1	4:D:201:ARG:HD2	2.26	0.50
1:A:527:GLU:OE2	9:L:41:ALA:N	2.42	0.50
2:B:880:ASP:OD2	2:B:996:ARG:NH2	2.40	0.50
3:C:90:ALA:HA	3:C:233:ILE:HG21	1.92	0.50
2:B:688:ILE:HD11	10:N:62:TYR:HB3	1.94	0.50
2:B:556:ASN:OD1	2:B:556:ASN:N	2.43	0.50
1:A:750:MET:HE3	2:B:917:HIS:CD2	2.47	0.49
2:B:731:TYR:O	2:B:733:GLY:N	2.45	0.49
4:D:4:PHE:HE1	4:D:18:VAL:HG23	1.77	0.49
5:E:8:LYS:HG2	5:E:71:ILE:HG12	1.94	0.49
1:A:319:LEU:HD23	3:C:366:LEU:HD11	1.94	0.49
1:A:422:VAL:HG21	1:A:469:LEU:HD13	1.93	0.49
2:B:24:TYR:HB2	2:B:606:TRP:CE2	2.48	0.49
3:C:37:LEU:HD23	3:C:37:LEU:H	1.77	0.49
6:F:84:ILE:HG21	6:F:95:ILE:HD11	1.94	0.49
2:B:764:GLU:HG3	2:B:773:ASP:HB2	1.94	0.49
3:C:133:GLU:OE1	3:C:137:ARG:NH2	2.45	0.49
1:A:277:TYR:HE1	1:A:291:PRO:HD2	1.78	0.48
1:A:421:VAL:HG21	1:A:482:LYS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:PRO:HD2	10:N:15:ALA:HB1	1.94	0.48
2:B:904:THR:O	2:B:906:SER:N	2.43	0.48
8:K:49:ILE:H	8:K:49:ILE:HG13	1.40	0.48
1:A:622:ASP:OD1	1:A:622:ASP:N	2.44	0.48
3:C:152:ILE:HG12	3:C:153:ASP:H	1.78	0.48
4:D:122:LYS:HB3	10:N:60:MET:HE1	1.95	0.48
3:C:191:PHE:HB3	3:C:198:LEU:HB2	1.95	0.47
2:B:884:SER:HB2	2:B:994:TYR:CE1	2.49	0.47
10:N:5:VAL:HG22	10:N:15:ALA:HB2	1.96	0.47
1:A:630:ASP:N	1:A:630:ASP:OD1	2.46	0.47
12:G:28:LEU:HD13	12:G:39:LEU:HD11	1.96	0.47
12:G:148:ASP:OD2	12:G:149:ASN:ND2	2.47	0.47
2:B:295:GLU:HG2	2:B:313:ARG:HH22	1.79	0.47
2:B:502:LEU:HB3	2:B:507:VAL:HG21	1.97	0.47
12:G:106:LEU:HD11	12:G:160:ILE:HB	1.96	0.47
2:B:746:SER:HB3	2:B:751:LEU:HD12	1.97	0.47
4:D:201:ARG:HE	4:D:204:GLU:HG3	1.80	0.47
4:D:226:THR:OG1	4:D:227:ASN:N	2.35	0.47
1:A:875:ASP:N	1:A:875:ASP:OD1	2.47	0.47
2:B:705:VAL:HB	2:B:944:VAL:HB	1.96	0.47
2:B:856:VAL:HG13	11:P:35:LEU:HB2	1.97	0.47
3:C:251:LYS:HG2	3:C:252:GLN:HG2	1.98	0.46
5:E:111:SER:OG	12:G:146:GLN:OE1	2.33	0.46
4:D:162:SER:HA	4:D:188:GLU:HB3	1.97	0.46
12:G:112:GLU:HB3	12:G:113:ILE:H	1.57	0.46
1:A:244:LYS:HB2	1:A:244:LYS:HE2	1.71	0.46
2:B:433:MET:HE1	2:B:652:ILE:HG13	1.97	0.46
3:C:8:LYS:HD3	3:C:27:LYS:HZ3	1.81	0.46
3:C:142:THR:HA	3:C:222:ARG:HB3	1.98	0.46
3:C:330:LYS:H	3:C:330:LYS:HD2	1.81	0.46
2:B:68:GLY:HA3	2:B:106:GLU:HG3	1.98	0.46
3:C:201:ARG:HH22	3:C:214:ILE:HG21	1.81	0.46
6:F:90:LEU:HA	6:F:93:ARG:HE	1.80	0.46
2:B:335:ARG:HB3	2:B:336:GLY:H	1.60	0.45
2:B:376:LYS:HD2	2:B:379:GLN:HE22	1.81	0.45
2:B:903:TRP:NE1	4:D:30:ARG:HH12	2.14	0.45
2:B:903:TRP:CD1	4:D:30:ARG:HH22	2.33	0.45
1:A:875:ASP:HA	1:A:876:GLY:HA2	1.68	0.45
2:B:234:ALA:HB2	2:B:273:ALA:HB3	1.99	0.45
2:B:735:ASN:HA	2:B:739:ALA:HB3	1.97	0.45
3:C:107:ALA:HB2	3:C:320:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HD13	2:B:1040:LEU:HD21	1.99	0.45
2:B:649:ILE:HD13	2:B:649:ILE:HA	1.83	0.45
3:C:79:MET:HG2	3:C:98:LEU:HB2	1.98	0.45
2:B:1008:ARG:HH12	2:B:1020:PRO:HB3	1.81	0.45
3:C:141:THR:HG23	3:C:224:LYS:HB2	1.99	0.45
4:D:42:VAL:HB	4:D:64:ALA:HA	1.98	0.45
2:B:971:ARG:HB3	2:B:986:ASP:HB3	1.99	0.45
1:A:452:LEU:HB3	1:A:504:ILE:HD11	1.98	0.45
1:A:146:VAL:HA	1:A:152:ALA:HB2	1.99	0.44
1:A:222:PRO:HD2	1:A:225:MET:HE2	1.99	0.44
2:B:1122:ARG:HH21	5:E:60:VAL:HG11	1.82	0.44
3:C:72:ILE:HD12	3:C:72:ILE:HA	1.82	0.44
2:B:931:ALA:HB1	2:B:990:GLY:HA3	1.99	0.44
7:H:63:ILE:HG23	7:H:75:TYR:HB3	2.00	0.44
12:G:152:ILE:HA	12:G:155:GLU:HB3	1.99	0.44
2:B:46:LEU:HD23	2:B:46:LEU:HA	1.81	0.44
2:B:968:HIS:H	4:D:201:ARG:NH1	2.15	0.44
2:B:979:THR:OG1	2:B:980:GLY:N	2.48	0.44
2:B:903:TRP:HE1	4:D:30:ARG:HH12	1.65	0.44
1:A:451:ASN:HD22	1:A:452:LEU:H	1.65	0.44
2:B:491:THR:OG1	2:B:492:GLY:N	2.51	0.44
2:B:692:THR:HG22	2:B:693:ARG:HD3	2.00	0.44
2:B:976:ASP:HB2	2:B:983:LEU:HD21	1.99	0.44
3:C:120:LEU:O	3:C:125:ARG:NH2	2.51	0.44
12:G:124:LYS:HE2	12:G:149:ASN:HD21	1.82	0.44
3:C:319:ARG:HH21	3:C:329:GLU:HG3	1.81	0.44
2:B:522:VAL:HG22	2:B:568:VAL:HB	2.00	0.44
4:D:167:ASP:OD2	4:D:202:LYS:NZ	2.39	0.44
1:A:294:LYS:HG2	1:A:300:PRO:HA	2.00	0.43
2:B:762:ALA:HB2	2:B:841:VAL:HG21	2.00	0.43
3:C:227:SER:O	3:C:229:VAL:N	2.50	0.43
3:C:269:ILE:H	3:C:269:ILE:HG13	1.46	0.43
4:D:6:ILE:HD13	4:D:16:PHE:HB3	1.99	0.43
5:E:9:ASP:OD1	5:E:10:VAL:N	2.43	0.43
11:P:14:GLU:HB3	11:P:15:VAL:H	1.43	0.43
12:G:84:THR:HB	12:G:87:LEU:HD11	2.00	0.43
1:A:153:PRO:HD2	1:A:155:PHE:CE1	2.53	0.43
1:A:286:GLU:H	1:A:306:GLN:HE22	1.66	0.43
2:B:1000:MET:H	2:B:1000:MET:HG2	1.64	0.43
1:A:311:LYS:H	3:C:341:ILE:HG21	1.84	0.43
2:B:309:ASP:H	2:B:312:ASN:HD22	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:ILE:HD12	2:B:876:PRO:HG2	1.99	0.43
1:A:135:LYS:HA	1:A:138:HIS:HB3	2.01	0.43
2:B:94:ILE:HD13	11:P:34:ILE:HD11	2.00	0.43
3:C:75:PRO:HB3	3:C:298:LEU:HD13	2.00	0.43
3:C:250:PHE:HB3	3:C:275:VAL:HG21	2.01	0.43
12:G:92:ARG:O	12:G:96:MET:N	2.48	0.43
1:A:825:ARG:HH22	2:B:471:THR:HG21	1.84	0.43
2:B:698:HIS:CD2	4:D:58:ILE:HD11	2.53	0.43
2:B:859:THR:HG22	2:B:863:THR:H	1.82	0.43
2:B:126:LEU:HD12	2:B:127:PRO:HD2	2.00	0.43
1:A:16:LEU:HG	2:B:1114:ARG:HB3	2.01	0.43
2:B:650:LEU:H	2:B:650:LEU:HG	1.53	0.43
3:C:8:LYS:HD3	3:C:27:LYS:NZ	2.34	0.43
1:A:664:LYS:HA	1:A:664:LYS:HD3	1.85	0.43
2:B:573:ASP:OD1	2:B:573:ASP:N	2.50	0.43
2:B:724:PHE:CD2	2:B:994:TYR:HB2	2.53	0.43
2:B:1032:PHE:HE2	2:B:1052:ARG:HD2	1.83	0.43
2:B:740:VAL:HG22	2:B:912:LEU:HD22	2.00	0.43
2:B:779:SER:O	2:B:781:ASN:N	2.51	0.43
4:D:181:PRO:HG2	4:D:192:THR:HB	2.01	0.43
1:A:295:HIS:HB2	1:A:301:LEU:HD11	2.01	0.42
6:F:113:LYS:HD2	6:F:113:LYS:HA	1.90	0.42
1:A:99:THR:OG1	1:A:105:ARG:O	2.30	0.42
2:B:228:PHE:HE1	2:B:320:LEU:HD22	1.82	0.42
2:B:303:LEU:HB2	2:B:316:LYS:HD3	2.00	0.42
12:G:113:ILE:HG12	12:G:126:THR:HG22	2.01	0.42
7:H:40:LEU:HB2	7:H:78:LEU:HD13	2.00	0.42
1:A:29:ILE:HD13	1:A:220:VAL:HG21	2.01	0.42
2:B:470:GLU:HB3	2:B:482:ASN:HD22	1.84	0.42
1:A:645:ARG:HA	1:A:645:ARG:HD2	1.92	0.42
2:B:343:TYR:HD1	2:B:343:TYR:HA	1.71	0.42
3:C:358:LEU:HB3	3:C:359:ASN:H	1.55	0.42
1:A:9:GLY:H	2:B:1119:LEU:HA	1.85	0.42
2:B:609:LEU:HD22	2:B:614:VAL:HG11	2.01	0.42
3:C:386:LEU:HD12	3:C:386:LEU:HA	1.89	0.42
6:F:112:ILE:O	6:F:116:ASP:N	2.53	0.42
1:A:336:PRO:HB3	1:A:452:LEU:HD12	2.02	0.42
2:B:438:HIS:HD2	2:B:441:ARG:HE	1.68	0.42
1:A:790:HIS:HD2	2:B:630:THR:HG23	1.85	0.42
1:A:108:LEU:HD13	1:A:108:LEU:HA	1.85	0.41
4:D:50:ASN:ND2	4:D:52:SER:OG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:2:ILE:H	10:N:2:ILE:HG13	1.43	0.41
10:N:2:ILE:HG12	10:N:56:ILE:HG21	2.02	0.41
11:P:30:CYS:C	11:P:32:SER:H	2.28	0.41
2:B:390:ILE:HA	2:B:393:PHE:HB2	2.01	0.41
4:D:225:GLU:OE2	10:N:42:ARG:NH1	2.52	0.41
8:K:44:PHE:HD1	8:K:49:ILE:HG12	1.84	0.41
2:B:971:ARG:HD3	2:B:986:ASP:HB2	2.02	0.41
5:E:34:TYR:HB3	5:E:45:VAL:HG11	2.02	0.41
1:A:358:LYS:HG2	8:K:21:ALA:HB1	2.02	0.41
2:B:901:MET:HE3	2:B:901:MET:HB3	1.89	0.41
5:E:89:VAL:HG22	5:E:99:ILE:HG12	2.03	0.41
1:A:229:ILE:H	1:A:229:ILE:HG13	1.58	0.41
1:A:758:LYS:HD2	1:A:758:LYS:HA	1.87	0.41
3:C:19:ASN:O	3:C:23:GLU:HG3	2.21	0.41
10:N:3:VAL:HG11	10:N:18:TYR:CG	2.56	0.41
1:A:278:HIS:O	1:A:281:THR:OG1	2.37	0.41
1:A:743:MET:SD	1:A:743:MET:N	2.94	0.41
3:C:128:ARG:HH12	3:C:132:LEU:HD21	1.85	0.41
1:A:468:ASN:OD1	1:A:468:ASN:N	2.46	0.41
1:A:703:ARG:HG3	1:A:705:GLU:HG3	2.02	0.41
2:B:205:ILE:HD11	2:B:303:LEU:H	1.85	0.41
2:B:233:ARG:NH2	2:B:265:SER:OG	2.48	0.41
3:C:12:SER:HA	3:C:15:GLU:CD	2.46	0.41
3:C:58:ILE:HD11	3:C:62:GLU:HG2	2.03	0.41
2:B:248:SER:O	2:B:254:GLN:NE2	2.55	0.41
2:B:539:VAL:HG11	2:B:559:LEU:HD23	2.03	0.41
2:B:844:ARG:HH21	2:B:1025:ALA:HB2	1.86	0.41
3:C:307:LEU:HD22	3:C:307:LEU:HA	1.90	0.41
1:A:209:ARG:HB2	1:A:212:TRP:CD2	2.56	0.40
2:B:209:ARG:HA	2:B:215:LEU:HA	2.02	0.40
2:B:435:THR:OG1	2:B:436:LEU:N	2.54	0.40
2:B:767:TYR:CG	2:B:820:ARG:HD2	2.56	0.40
2:B:873:LEU:HD22	2:B:873:LEU:HA	1.89	0.40
3:C:205:VAL:H	3:C:205:VAL:HG23	1.66	0.40
5:E:87:GLY:HA3	5:E:101:ILE:HG22	2.02	0.40
2:B:736:MET:HE2	2:B:736:MET:HB3	1.83	0.40
2:B:854:VAL:HG13	2:B:868:VAL:HG22	2.03	0.40
2:B:895:ILE:HD13	2:B:895:ILE:HG21	1.89	0.40
3:C:2:VAL:N	3:C:6:THR:OG1	2.45	0.40
3:C:38:LYS:HG3	3:C:39:LYS:H	1.85	0.40
10:N:14:LEU:HA	10:N:14:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HE3	1:A:311:LYS:HB3	1.92	0.40
2:B:367:VAL:O	2:B:371:GLN:HG2	2.21	0.40
1:A:624:LYS:HA	1:A:624:LYS:HD3	1.80	0.40
2:B:123:ILE:HD13	2:B:123:ILE:HG21	1.84	0.40
2:B:743:ASN:HD21	2:B:898:GLN:HA	1.87	0.40
5:E:154:ARG:H	5:E:154:ARG:HG2	1.57	0.40
5:E:155:VAL:HG12	5:E:157:ARG:H	1.86	0.40
9:L:77:LYS:HE2	9:L:77:LYS:HB2	1.98	0.40
2:B:520:TYR:HB3	2:B:521:ARG:H	1.56	0.40
4:D:199:LEU:HD12	4:D:200:PRO:HD2	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	899/906 (99%)	735 (82%)	140 (16%)	24 (3%)	4	28
2	B	1112/1123 (99%)	920 (83%)	159 (14%)	33 (3%)	3	26
3	C	386/391 (99%)	294 (76%)	70 (18%)	22 (6%)	1	17
4	D	255/259 (98%)	243 (95%)	11 (4%)	1 (0%)	30	65
5	E	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
6	F	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
7	H	74/82 (90%)	63 (85%)	10 (14%)	1 (1%)	9	39
8	K	54/57 (95%)	44 (82%)	8 (15%)	2 (4%)	2	23
9	L	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	5	31
10	N	63/65 (97%)	50 (79%)	12 (19%)	1 (2%)	7	37
11	P	40/49 (82%)	22 (55%)	16 (40%)	2 (5%)	1	19
12	G	164/185 (89%)	153 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3438/3523 (98%)	2878 (84%)	472 (14%)	88 (3%)	6	29

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	445	TYR
1	A	642	GLY
1	A	888	VAL
2	B	287	LYS
2	B	431	ASN
2	B	432	TYR
2	B	477	CYS
2	B	732	HIS
2	B	905	GLU
3	C	181	LYS
3	C	357	PRO
7	H	47	ASP
1	A	153	PRO
2	B	56	VAL
2	B	82	GLY
2	B	136	ARG
2	B	183	ARG
2	B	521	ARG
2	B	705	VAL
2	B	1055	GLU
3	C	205	VAL
3	C	228	GLY
3	C	358	LEU
4	D	209	LYS
9	L	49	ILE
11	P	19	LEU
11	P	31	GLY
1	A	65	ALA
1	A	875	ASP
2	B	11	THR
2	B	286	PRO
2	B	391	GLN
2	B	874	ARG
3	C	107	ALA
3	C	108	ARG
3	C	165	PRO

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Mol	Chain	Res	Type
3	C	314	LEU
3	C	341	ILE
8	K	31	PRO
10	N	6	ARG
1	A	64	GLY
1	A	161	ARG
1	A	311	LYS
1	A	396	GLU
1	A	430	LEU
1	A	455	CYS
1	A	542	GLU
2	B	57	VAL
2	B	515	PRO
2	B	780	PRO
2	B	861	ASP
3	C	189	ALA
3	C	217	LYS
3	C	323	ARG
1	A	36	ASP
1	A	154	GLN
1	A	871	LYS
2	B	79	GLU
2	B	189	LYS
2	B	222	VAL
2	B	223	PRO
2	B	236	GLY
2	B	644	LEU
2	B	774	ASN
3	C	32	ASN
3	C	221	HIS
3	C	344	GLN
9	L	23	THR
1	A	152	ALA
1	A	297	SER
1	A	404	GLU
1	A	428	PRO
1	A	456	PRO
2	B	13	THR
2	B	269	THR
3	C	384	LEU
3	C	385	PRO
1	A	710	PRO

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Mol	Chain	Res	Type
2	B	224	LYS
2	B	445	PRO
3	C	140	GLY
3	C	160	VAL
3	C	353	GLY
3	C	361	VAL
1	A	408	ILE
8	K	24	ALA
2	B	517	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

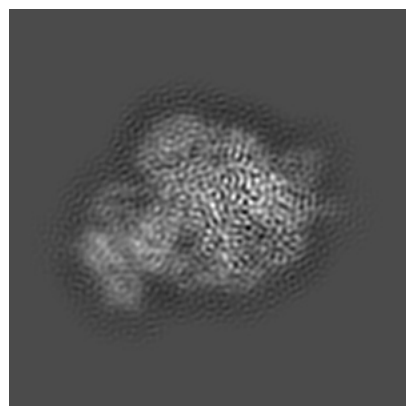
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9961. These allow visual inspection of the internal detail of the map and identification of artifacts.

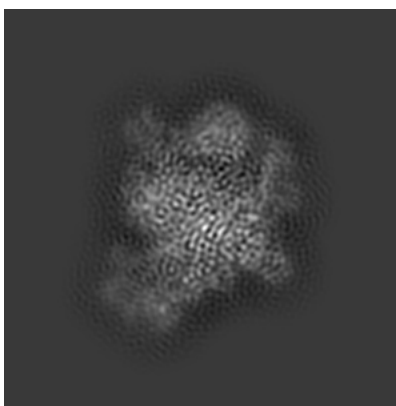
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

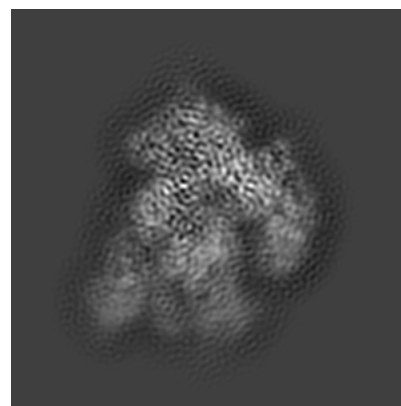
6.1.1 Primary map



X

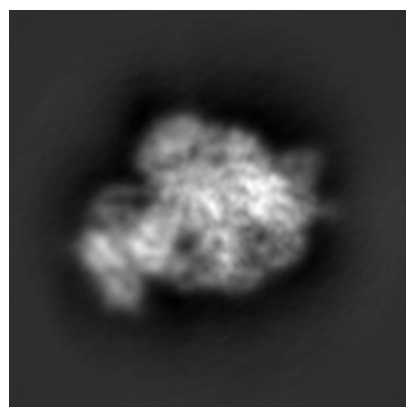


Y

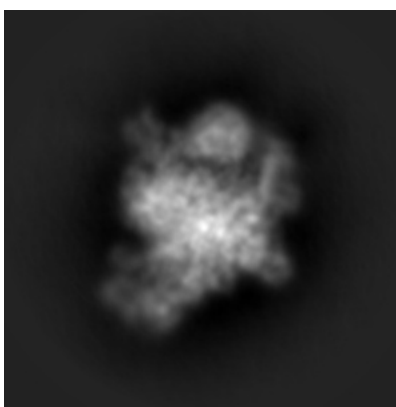


Z

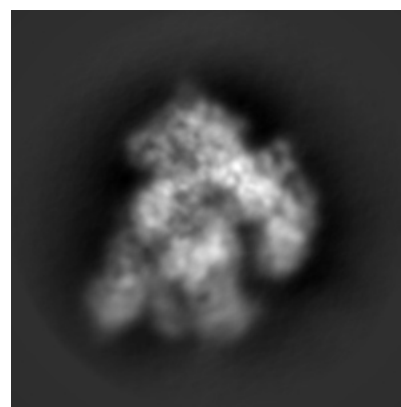
6.1.2 Raw map



X



Y

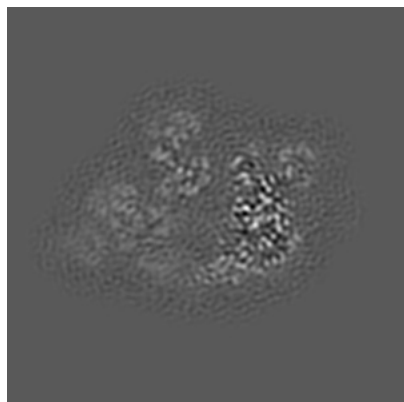


Z

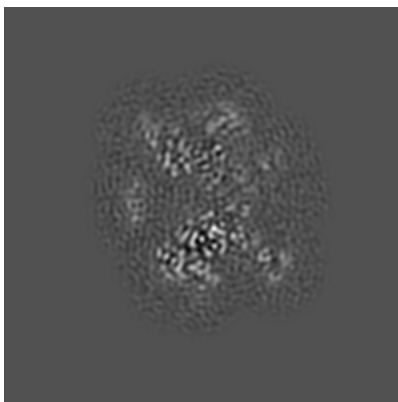
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

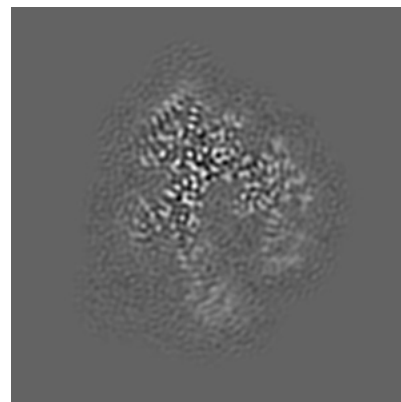
6.2.1 Primary map



X Index: 88

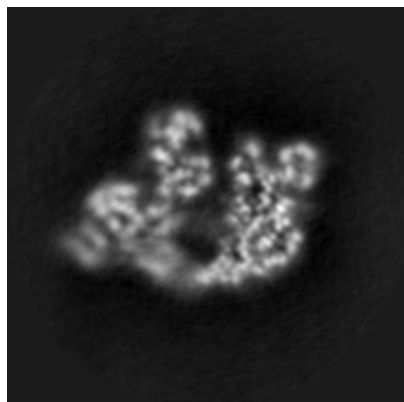


Y Index: 88

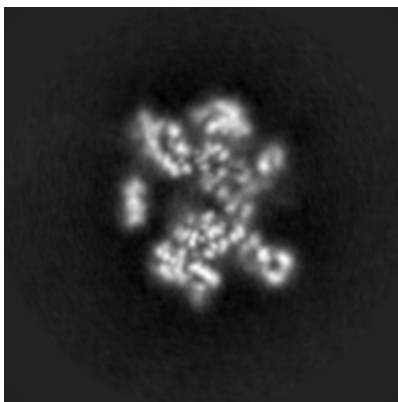


Z Index: 88

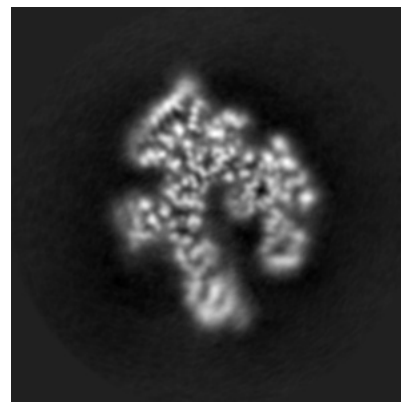
6.2.2 Raw map



X Index: 88



Y Index: 88

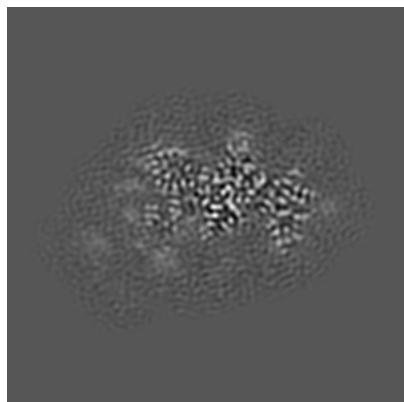


Z Index: 88

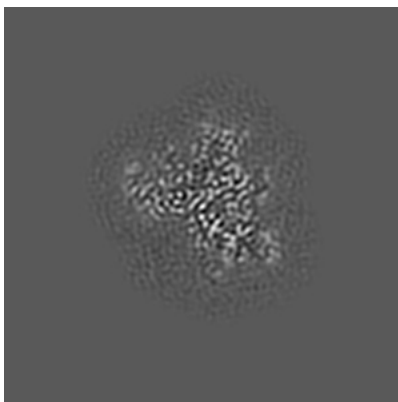
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

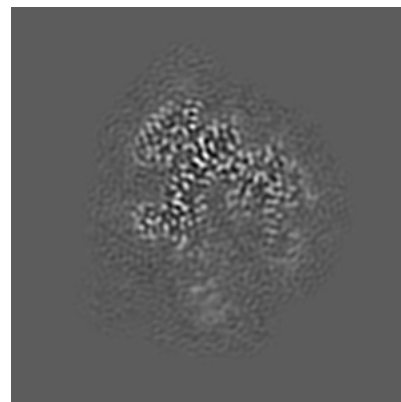
6.3.1 Primary map



X Index: 76

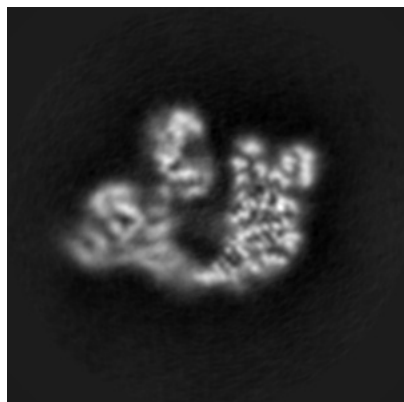


Y Index: 105

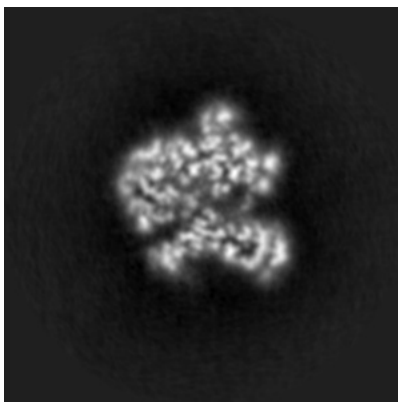


Z Index: 90

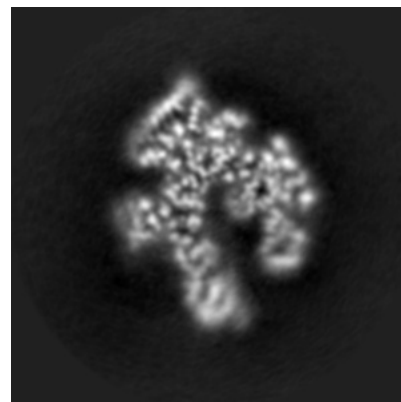
6.3.2 Raw map



X Index: 90



Y Index: 98

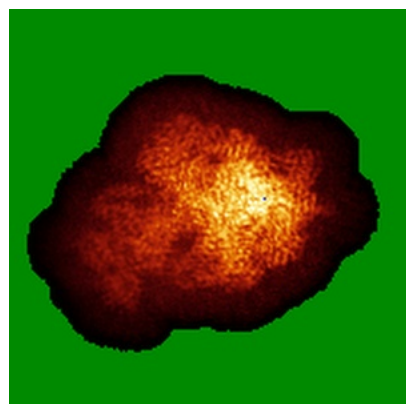


Z Index: 88

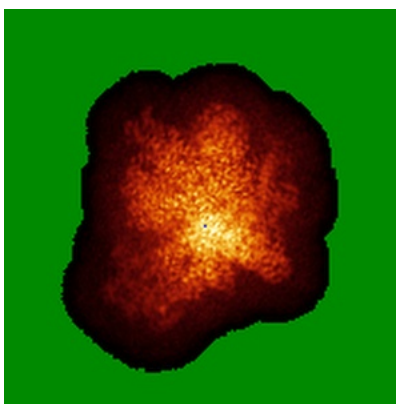
The images above show the largest variance slices of the map in three orthogonal directions.

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

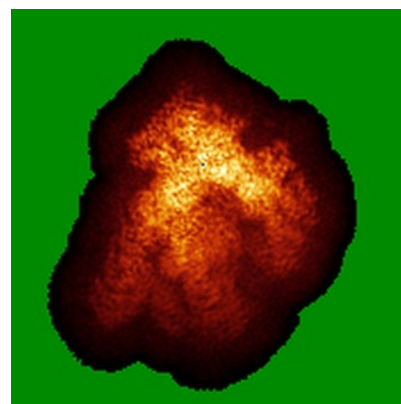
6.4.1 Primary map



X

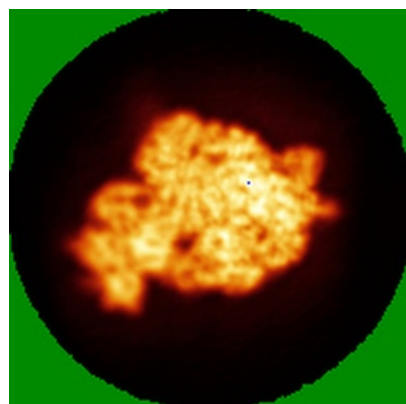


Y

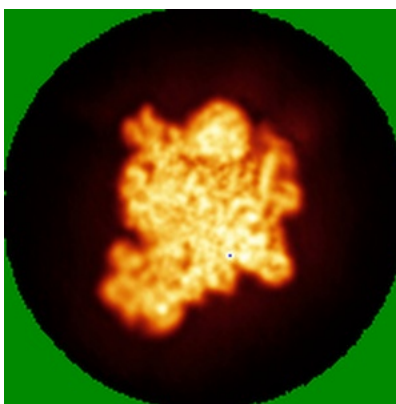


Z

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](#)

This section was not generated.

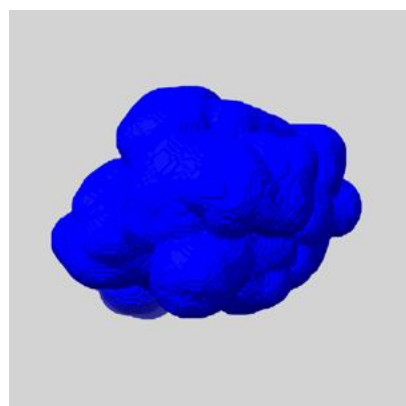
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

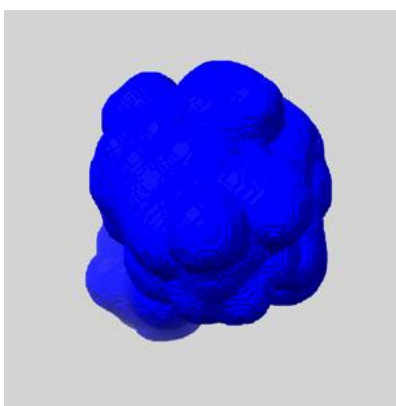
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

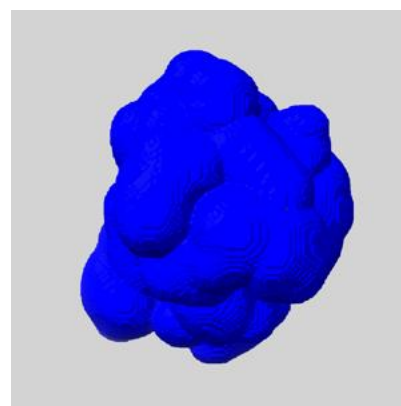
6.6.1 emd_9961_msk_1.map [i](#)



X



Y

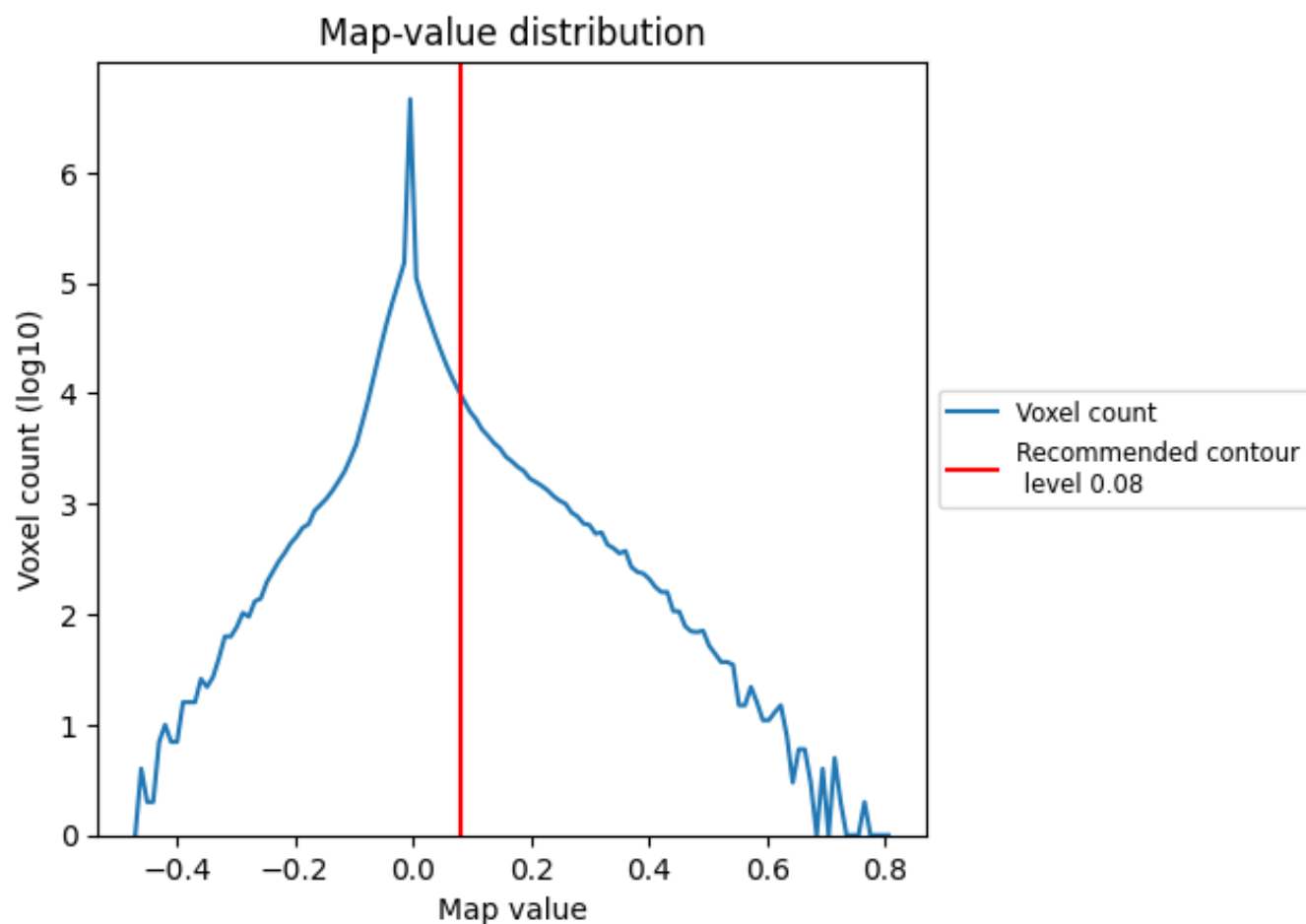


Z

7 Map analysis [i](#)

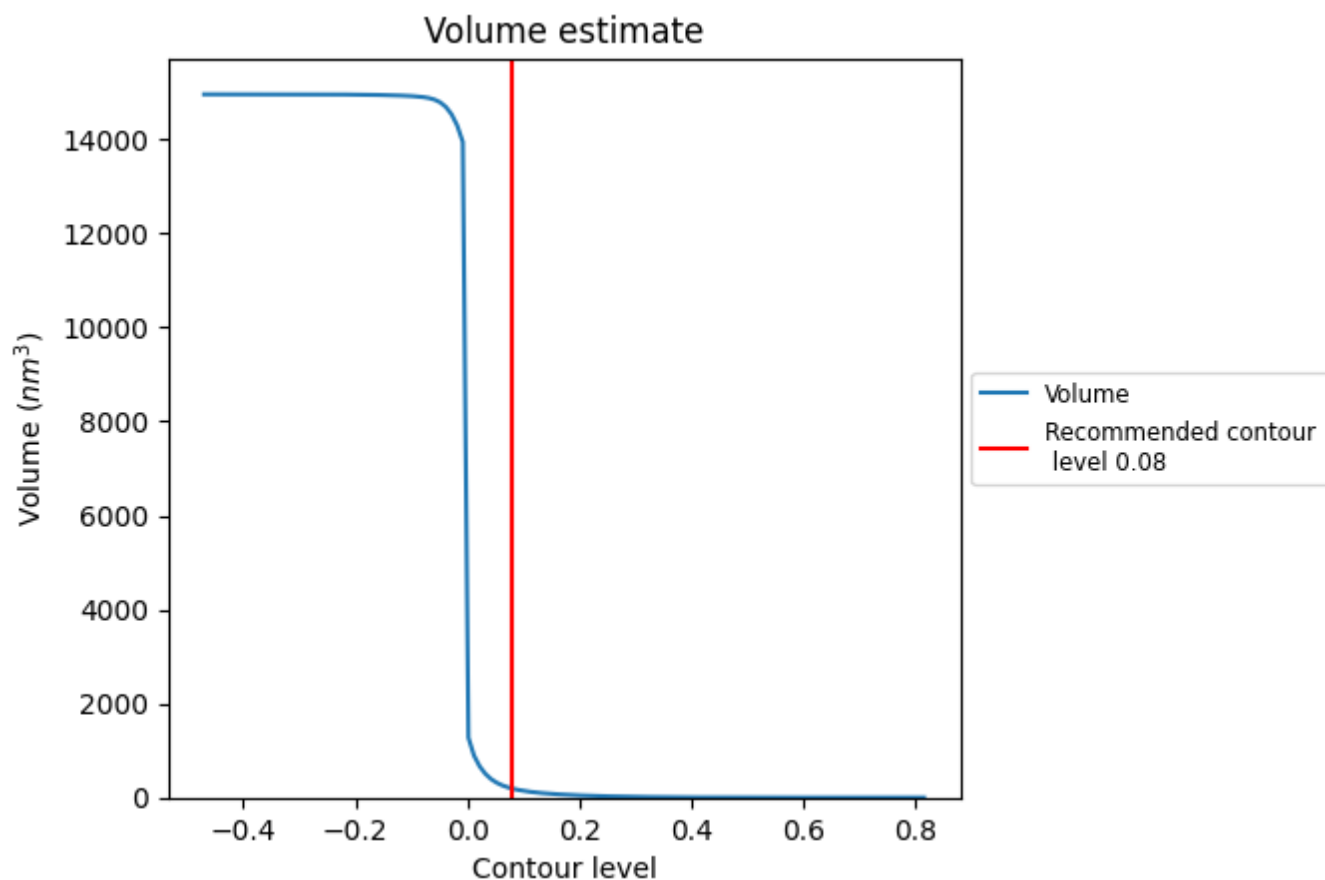
This section contains the results of statistical analysis of the map.

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.

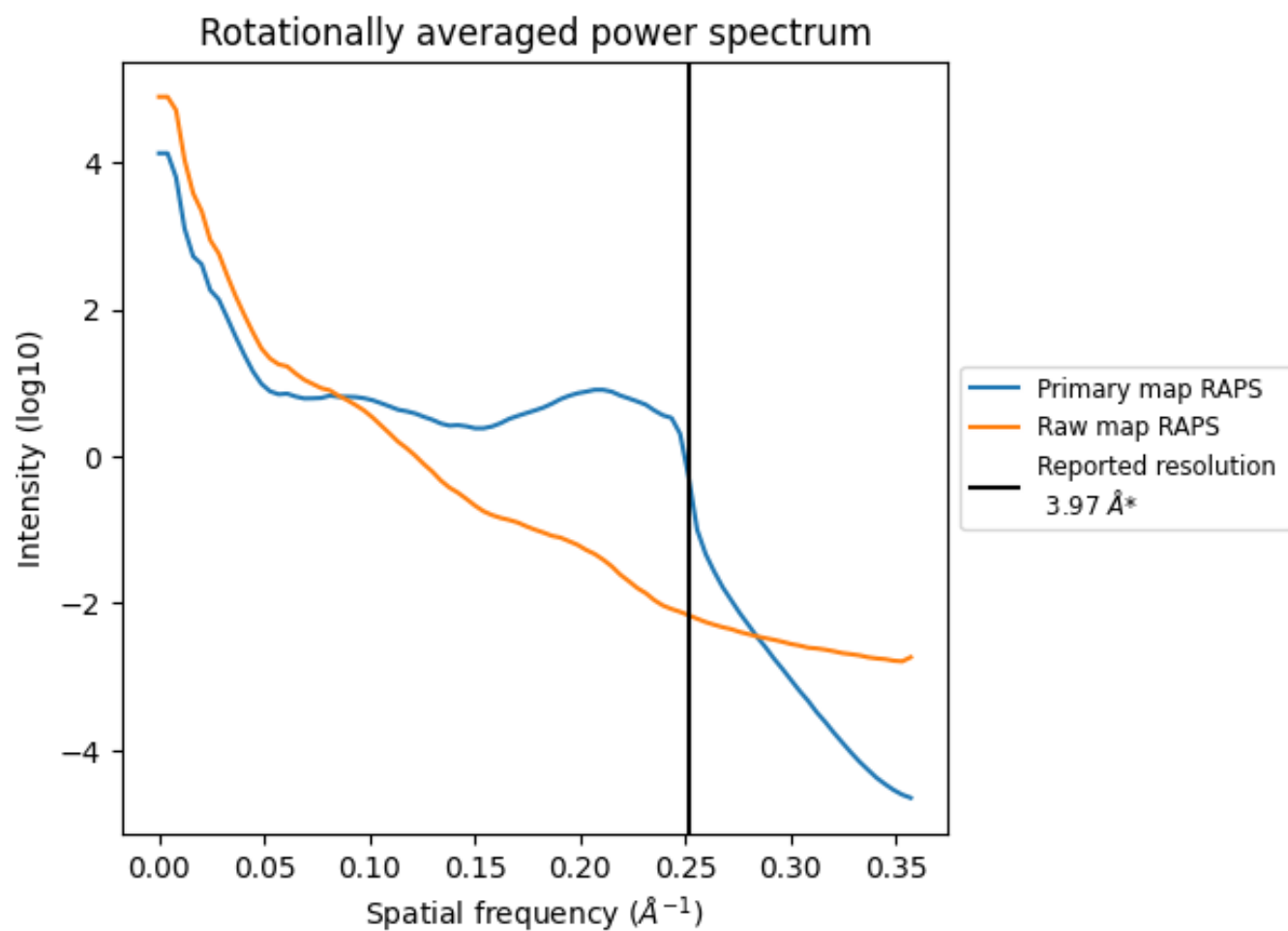
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 ⓘ

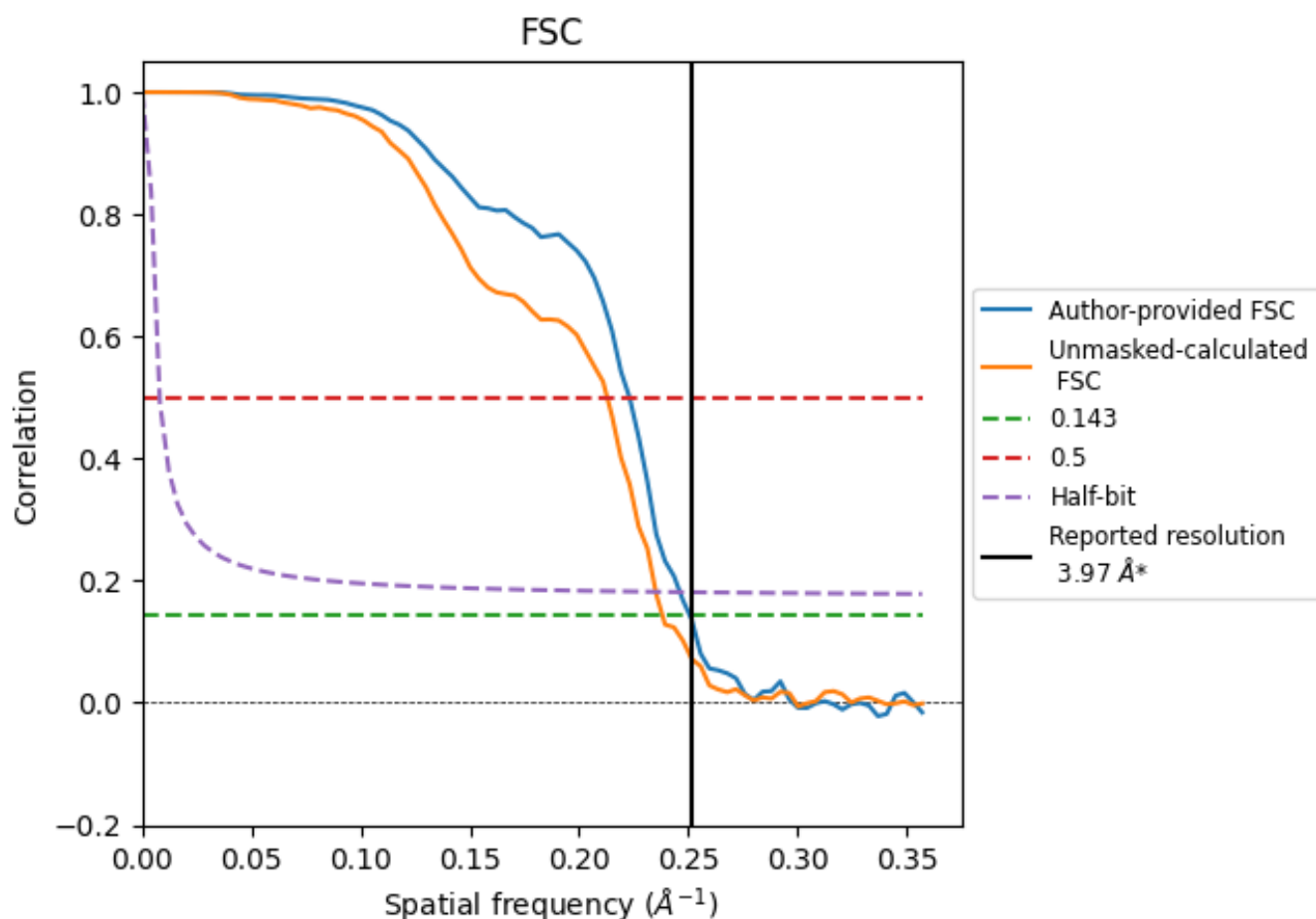


*Reported resolution corresponds to spatial frequency of 0.252 Å⁻¹

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 0.252 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

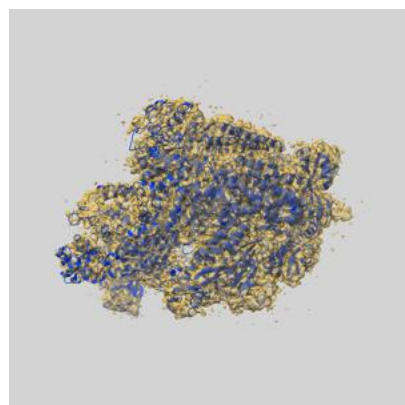
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.99	4.48	4.06
Unmasked-calculated*	4.20	4.70	4.25

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

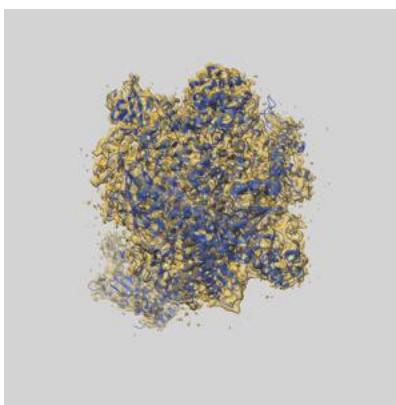
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9961 and PDB model 6KF4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

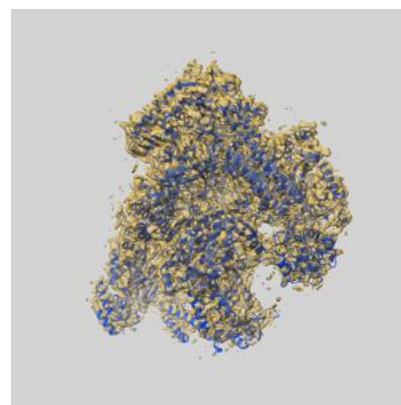
9.1 Map-model overlay [i](#)



X



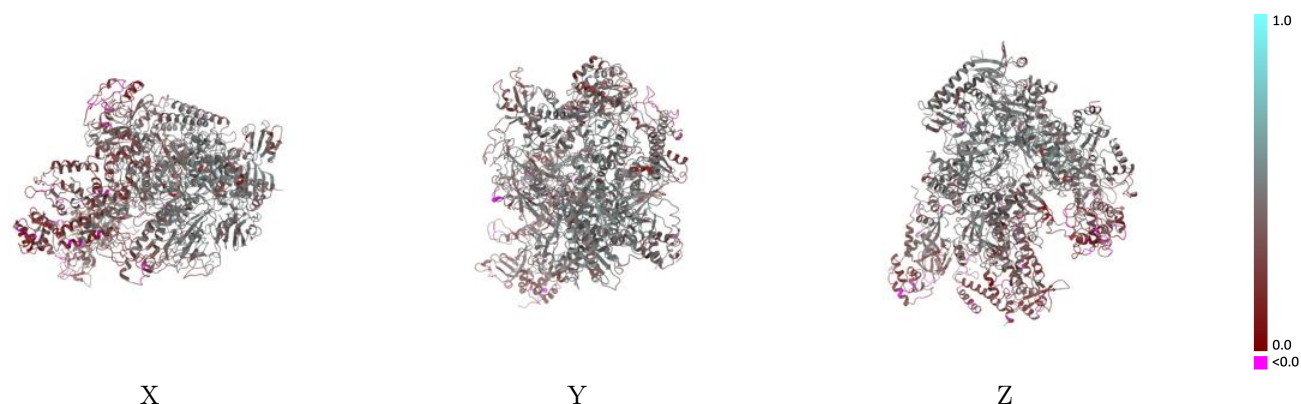
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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](#)

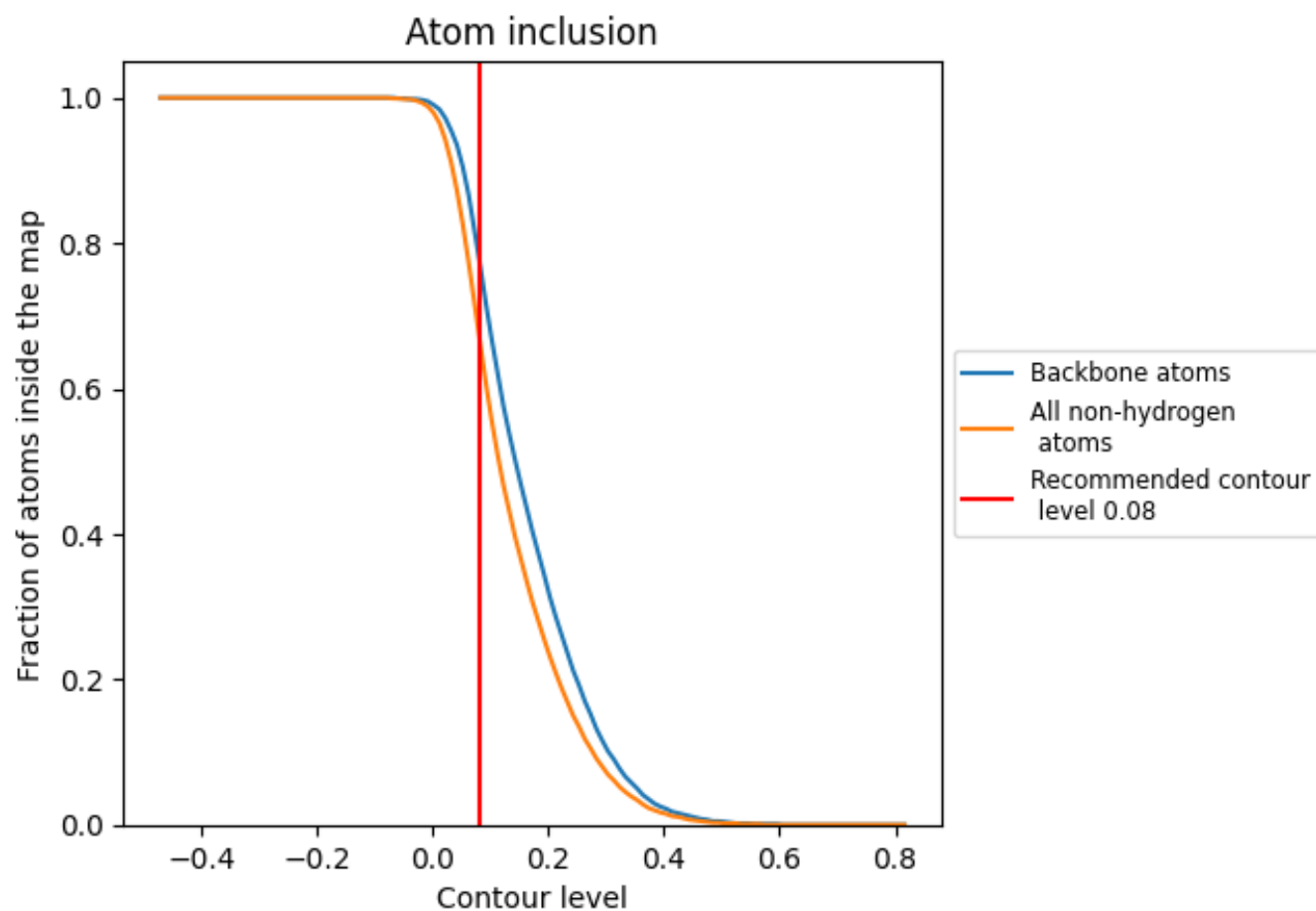


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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	0.6750	0.3910
A	0.7120	0.4030
B	0.7170	0.4180
C	0.5810	0.3480
D	0.8130	0.4490
E	0.5530	0.3220
F	0.4340	0.2360
G	0.2620	0.2180
H	0.7790	0.4350
K	0.7910	0.4580
L	0.8250	0.4670
N	0.8510	0.4750
P	0.8070	0.4220

1.0

0.0

<0.0