



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:47 AM UTC

PDB ID : 8S51 / pdb_00008s51
EMDB ID : EMD-19718
Title : RNA polymerase II core initially transcribing complex with an ordered RNA of 8 nt
Authors : Zhan, Y.; Grabbe, F.; Oberbeckmann, E.; Dienemann, C.; Cramer, P.
Deposited on : 2024-02-22
Resolution : 3.10 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

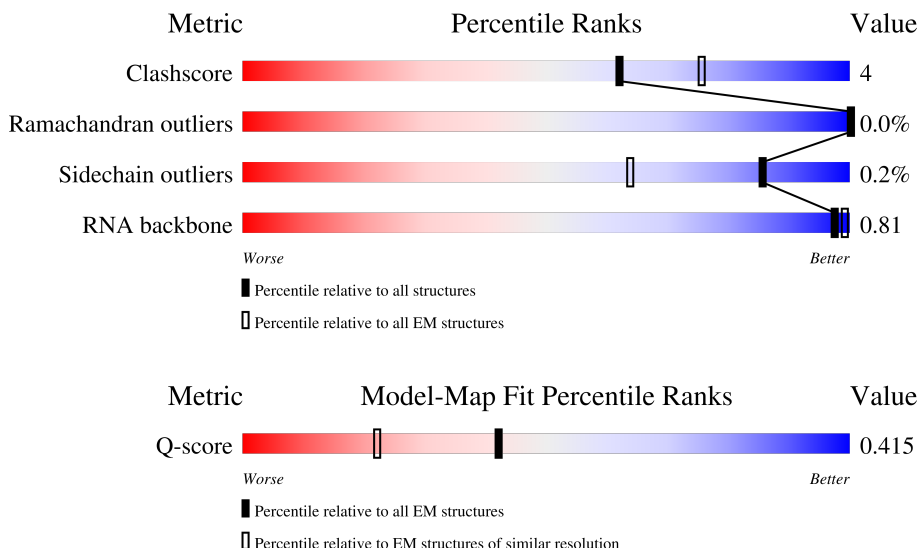
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1970	
2	B	1300	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	139	
15	O	339	
16	P	8	
17	Q	517	
18	R	249	
19	T	139	
20	U	376	
21	V	109	
22	W	439	
23	X	291	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 44796 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	1421	Total	C	N	O	S	0	0
			11257	7083	2013	2089	72		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1121	Total	C	N	O	S	0	0
			8971	5675	1574	1658	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	292	Total	C	N	O	S	0	0
			2252	1403	402	429	18		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	53	Total	C	N	O	P	0	0
			1113	521	226	313	53		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	8	Total	C	N	O	P	0	0
			169	76	32	53	8		

- Molecule 17 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 18 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	63	Total	C	N	O	P	0	0
			1270	604	218	385	63		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 22 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 23 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Zn	0
			2	2	
24	B	1	Total	Zn	0
			1	1	

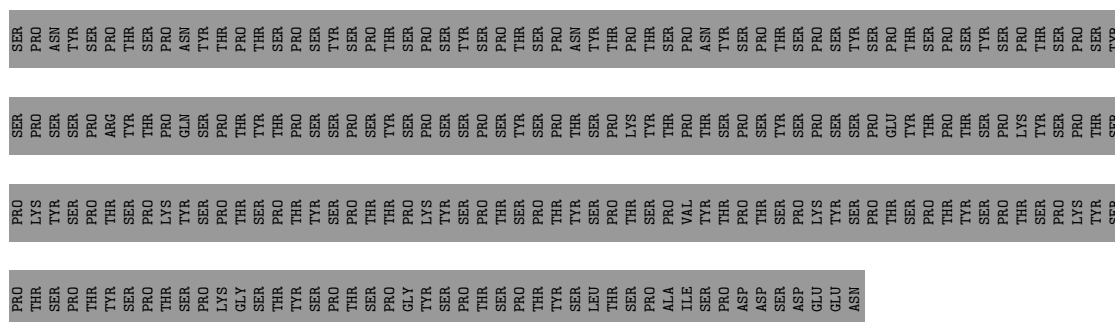
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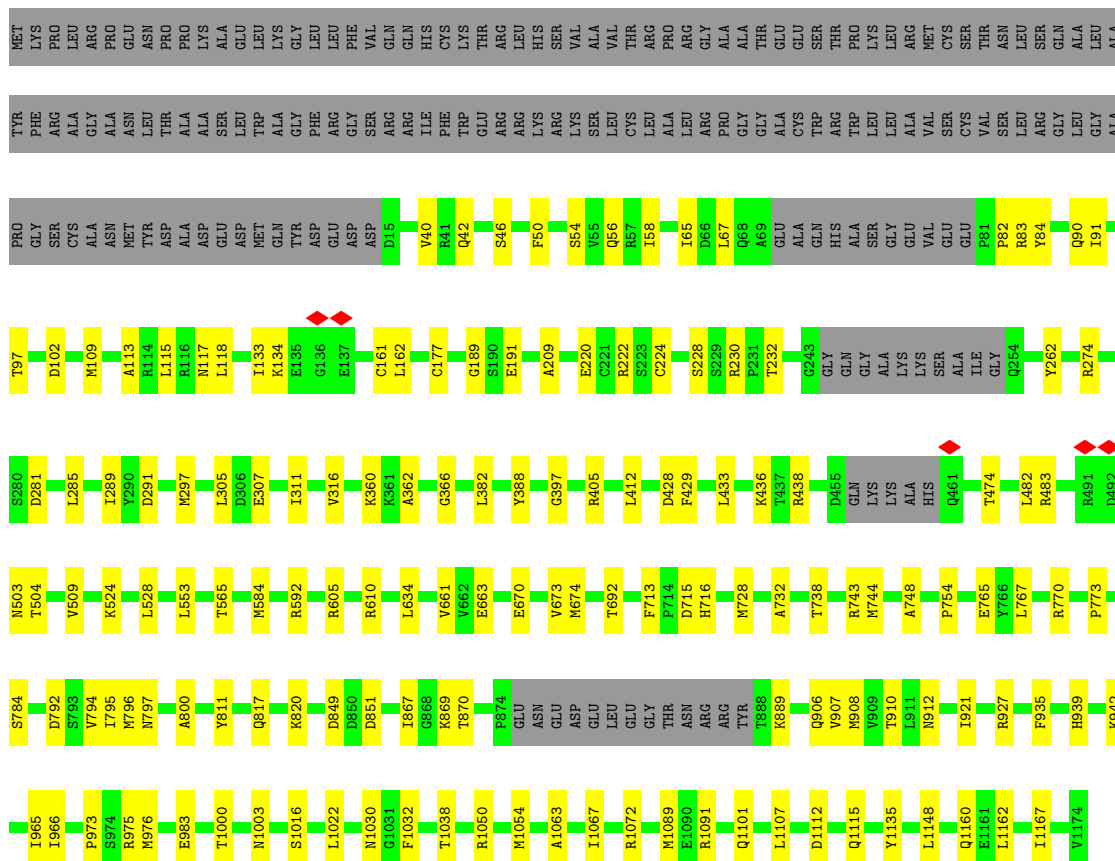
Mol	Chain	Residues	Atoms		AltConf
24	C	1	Total 1	Zn 1	0
24	I	2	Total 2	Zn 2	0
24	J	1	Total 1	Zn 1	0
24	L	1	Total 1	Zn 1	0
24	M	1	Total 1	Zn 1	0
24	W	1	Total 1	Zn 1	0

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

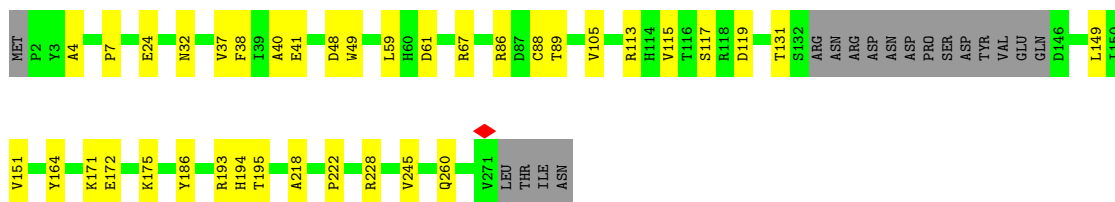
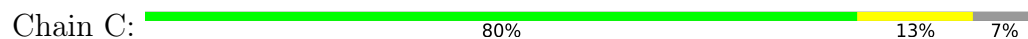
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 1	Mg 1	0



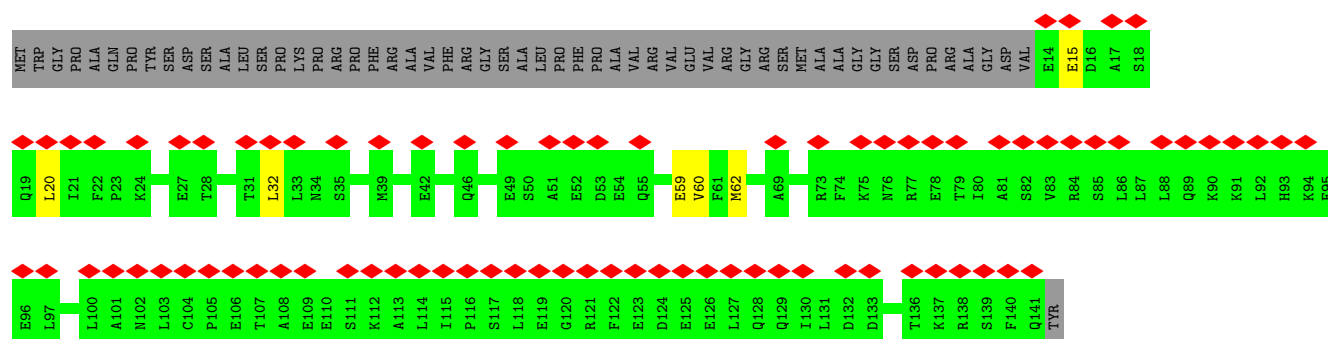
- Molecule 2: DNA-directed RNA polymerase subunit beta



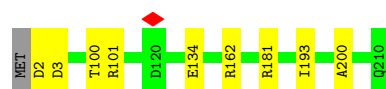
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



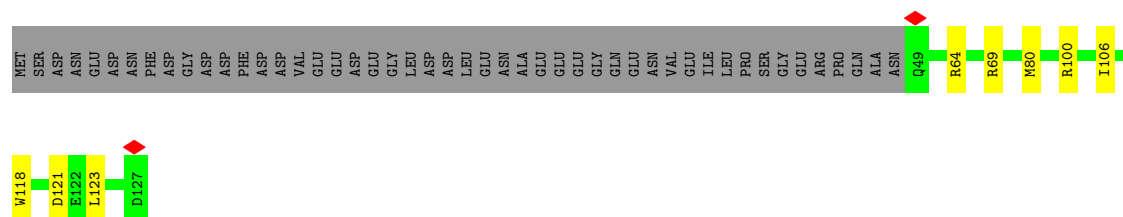
- Molecule 4: RNA polymerase II subunit D



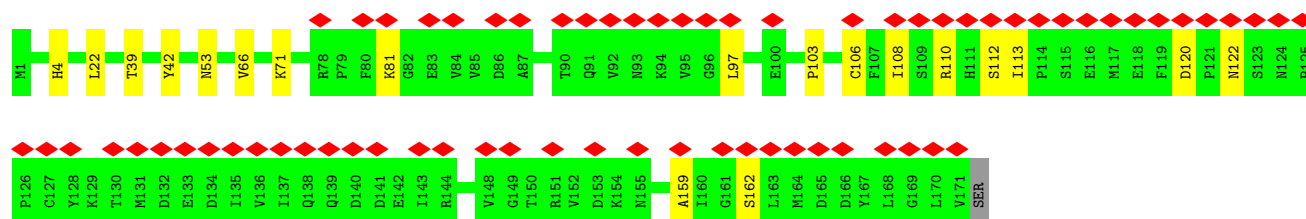
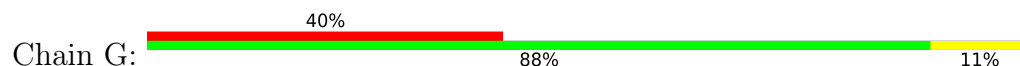
- Molecule 5: DNA-directed RNA polymerase II subunit E



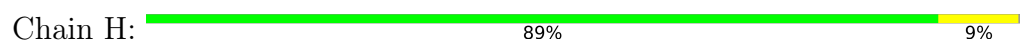
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

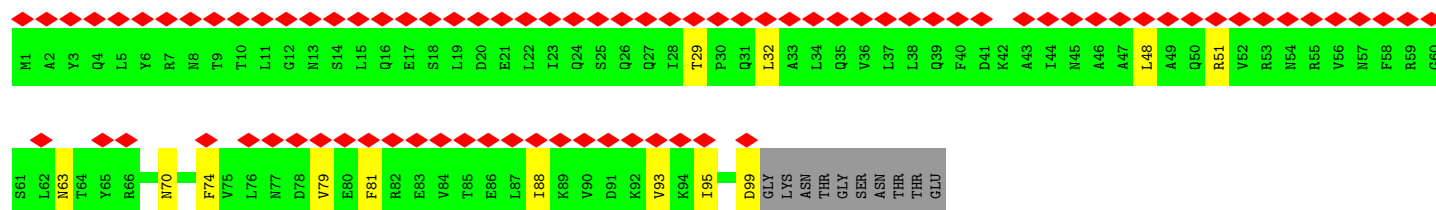
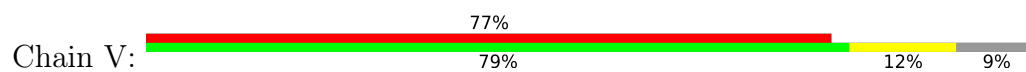


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

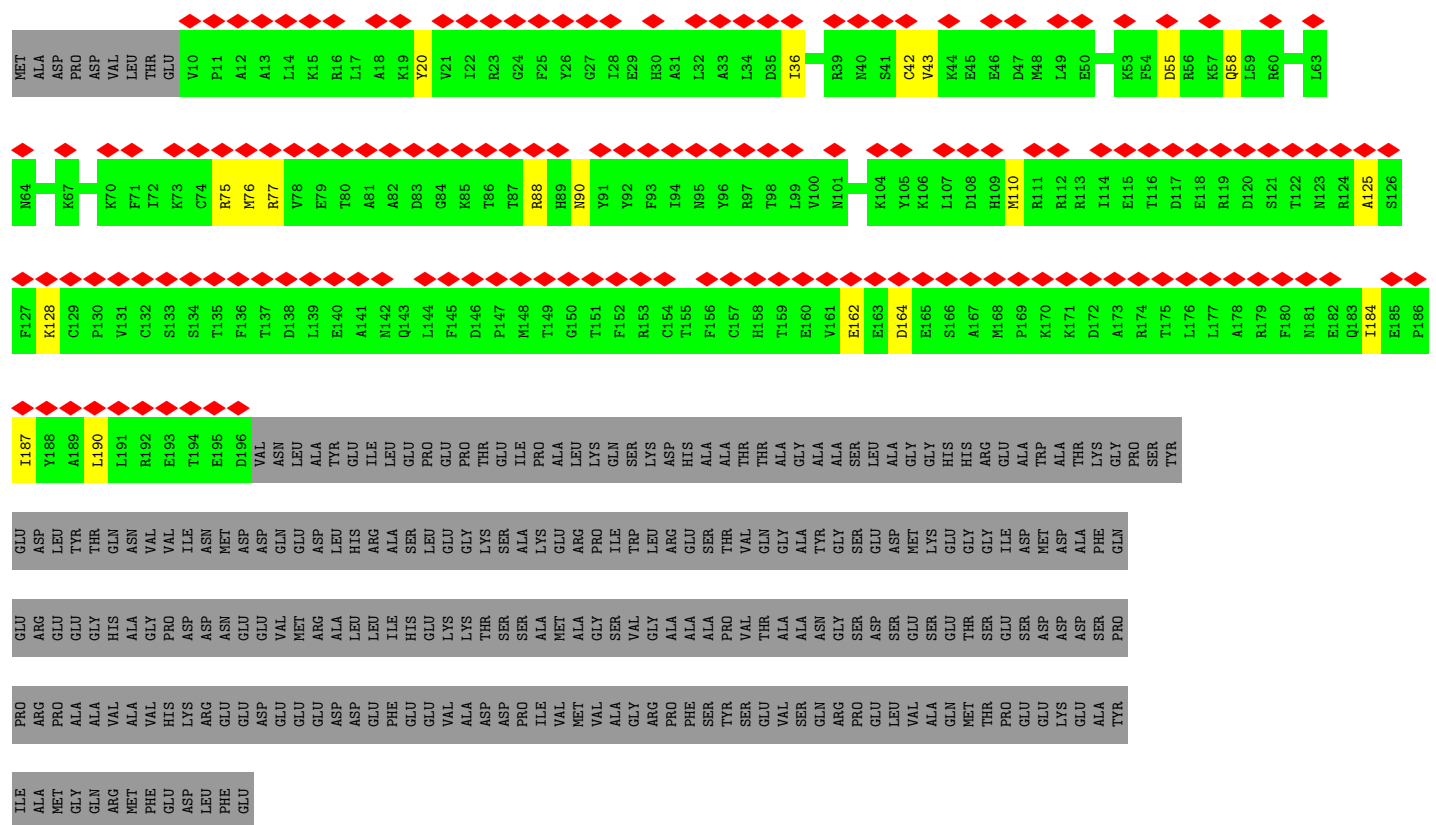


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

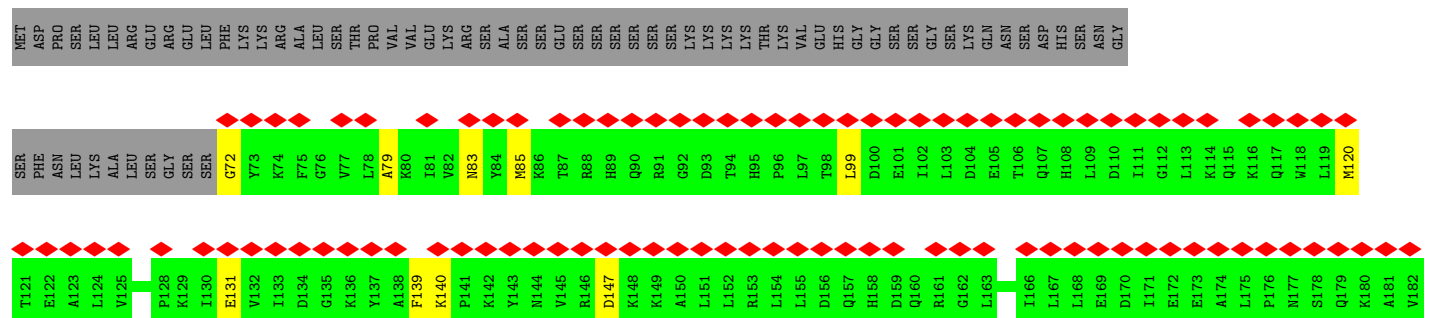




• Molecule 22: General transcription factor IIE subunit 1



• Molecule 23: Transcription initiation factor IIE subunit beta



SER	SER	MET	GLN	GLU	SER	GLY	PRO	PRO	LYS	LYS	VAL	ALA	ALA	PRO	ILE	GLN	ARG	ARG	LYS	LYS	PRO	ALA	ALA	SER	SER	GLN	LYS	LYS	ARG	ARG	PHE	LYS	LYS	THR	HIS	HIS	GLU	GLY	VAL	LEU	LYS	ASP	TYR	ASP	ILE	THR	SER	SER	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87097	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	54.772	Depositor
Minimum map value	-35.910	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.29	Depositor
Map size ($\text{\AA}$)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	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	0.36	0/11462	0.44	0/15473
2	B	0.39	0/9149	0.45	0/12349
3	C	0.39	0/2102	0.39	0/2857
4	D	0.15	0/1064	0.35	0/1428
5	E	0.32	0/1752	0.48	0/2366
6	F	0.34	0/646	0.39	0/871
7	G	0.17	0/1382	0.33	0/1874
8	H	0.31	0/1207	0.39	0/1628
9	I	0.25	0/949	0.45	0/1284
10	J	0.44	0/516	0.40	0/696
11	K	0.37	0/939	0.35	0/1271
12	L	0.29	0/378	0.41	0/500
13	M	0.36	0/2286	0.59	0/3084
14	N	0.59	0/1254	0.83	0/1937
15	O	0.33	0/1448	0.58	0/1948
16	P	0.72	0/188	0.81	0/290
17	Q	0.14	0/1167	0.36	0/1576
18	R	0.25	0/1817	0.49	0/2445
19	T	0.55	0/1416	0.87	0/2176
20	U	0.16	0/945	0.41	0/1274
21	V	0.11	0/816	0.32	0/1105
22	W	0.13	0/1560	0.35	0/2097
23	X	0.12	0/1427	0.32	0/1916
All	All	0.35	0/45870	0.48	0/62445

There are no bond length outliers.

There are no bond angle outliers.

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	11257	0	11394	119	0
2	B	8971	0	8999	107	0
3	C	2059	0	2007	25	0
4	D	1050	0	1033	4	0
5	E	1721	0	1737	6	0
6	F	636	0	665	7	0
7	G	1351	0	1358	12	0
8	H	1186	0	1147	10	0
9	I	928	0	859	11	0
10	J	507	0	523	4	0
11	K	920	0	942	12	0
12	L	373	0	378	13	0
13	M	2252	0	2269	18	0
14	N	1113	0	592	12	0
15	O	1422	0	1514	14	0
16	P	169	0	89	3	0
17	Q	1138	0	1103	17	0
18	R	1788	0	1819	10	0
19	T	1270	0	710	16	0
20	U	930	0	888	8	0
21	V	806	0	818	8	0
22	W	1535	0	1540	12	0
23	X	1403	0	1428	7	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	W	1	0	0	0	0
25	A	1	0	0	0	0
All	All	44796	0	43812	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (380) 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:74:CYS:SG	1:A:84:HIS:CE1	2.73	0.82
14:N:24:DG:H2'	14:N:25:DG:C8	2.16	0.81
1:A:74:CYS:SG	1:A:84:HIS:HE1	2.03	0.78
1:A:11:SER:N	2:B:1135:TYR:HH	1.83	0.77
1:A:367:ILE:HD13	1:A:501:MET:HE2	1.70	0.72
1:A:801:GLY:H	2:B:503:ASN:HD22	1.36	0.72
2:B:428:ASP:OD1	2:B:429:PHE:N	2.24	0.68
2:B:565:THR:HG22	2:B:610:ARG:HB3	1.77	0.67
19:T:84:DT:H2''	19:T:85:DT:H5'	1.76	0.67
19:T:52:DG:H2''	19:T:53:DT:H5'	1.77	0.66
14:N:24:DG:H2'	14:N:25:DG:H8	1.61	0.65
15:O:187:ALA:HB3	15:O:190:ALA:HB2	1.78	0.64
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.79	0.64
3:C:86:ARG:HD2	11:K:11:LEU:HD21	1.80	0.63
19:T:49:DG:H2'	19:T:50:DG:C8	2.33	0.63
1:A:65:ILE:HD13	1:A:258:LEU:HD12	1.81	0.62
1:A:642:LYS:HG2	1:A:773:GLY:HA3	1.82	0.62
2:B:610:ARG:HH11	9:I:69:ILE:HD12	1.64	0.62
13:M:127:ARG:HD2	13:M:183:VAL:HG13	1.81	0.62
13:M:165:TYR:OH	13:M:169:ARG:NH2	2.33	0.62
10:J:1:MET:HA	10:J:55:LEU:HB2	1.82	0.61
2:B:102:ASP:HA	13:M:173:VAL:HG21	1.83	0.61
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.67	0.60
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.35	0.60
4:D:32:LEU:HD11	7:G:4:HIS:HB2	1.83	0.60
1:A:458:PHE:HE2	1:A:501:MET:HE3	1.66	0.59
1:A:1030:SER:HB2	5:E:162:ARG:HE	1.67	0.59
21:V:74:PHE:HB2	21:V:95:ILE:HB	1.83	0.59
3:C:37:VAL:HG22	3:C:41:GLU:HG3	1.84	0.59
1:A:322:LEU:HD13	1:A:325:LEU:HD12	1.83	0.59
15:O:293:TYR:HB3	15:O:302:LEU:HB2	1.85	0.58
2:B:584:MET:HE3	2:B:605:ARG:HB2	1.86	0.58
2:B:360:LYS:HG2	2:B:553:LEU:HD23	1.86	0.58
1:A:67:ARG:NH2	13:M:32:MET:SD	2.77	0.58
9:I:71:ASP:OD1	9:I:74:GLN:NE2	2.36	0.58
16:P:8:G:H1	19:T:46:DC:H42	1.51	0.58
22:W:184:ILE:HD12	22:W:187:ILE:HD13	1.86	0.57
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.86	0.57
21:V:29:THR:HG23	21:V:32:LEU:H	1.70	0.57
22:W:75:ARG:HE	22:W:77:ARG:HH12	1.50	0.57
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:O	1:A:182:GLY:HA3	2.04	0.57
2:B:307:GLU:OE2	17:Q:167:ARG:NH2	2.38	0.57
23:X:131:GLU:HB3	23:X:140:LYS:HE3	1.86	0.57
1:A:454:ASP:OD1	1:A:512:ARG:NH2	2.37	0.56
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.38	0.56
6:F:118:TRP:HB3	6:F:123:LEU:HD11	1.87	0.56
1:A:1480:CYS:HA	6:F:80:MET:HE1	1.86	0.56
1:A:799:PRO:O	2:B:503:ASN:ND2	2.39	0.56
2:B:161:CYS:SG	2:B:162:LEU:N	2.78	0.56
3:C:67:ARG:NH2	3:C:149:LEU:O	2.35	0.56
1:A:67:ARG:HH12	13:M:45:VAL:HG23	1.71	0.56
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.88	0.56
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.88	0.56
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.88	0.56
1:A:1207:ILE:HA	1:A:1263:ASN:HA	1.87	0.55
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.37	0.55
2:B:817:GLN:OE1	2:B:912:ASN:ND2	2.40	0.55
17:Q:166:ARG:HE	17:Q:170:VAL:HG23	1.70	0.55
1:A:65:ILE:HD11	1:A:263:ALA:H	1.69	0.55
1:A:583:ARG:NH1	3:C:222:PRO:O	2.40	0.55
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.39	0.55
15:O:205:ARG:HH21	20:U:376:TRP:HE1	1.55	0.55
17:Q:15:VAL:O	17:Q:135:PHE:N	2.39	0.55
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.89	0.55
1:A:1200:PRO:HG2	1:A:1203:ASP:HB2	1.88	0.55
1:A:434:LYS:HE2	1:A:436:SER:HB3	1.89	0.54
1:A:82:PRO:O	2:B:1160:GLN:NE2	2.40	0.54
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.89	0.54
1:A:485:ASN:OD1	1:A:673:GLN:NE2	2.41	0.54
17:Q:13:GLU:HG2	18:R:42:LYS:HZ1	1.72	0.54
17:Q:153:ARG:HB2	17:Q:180:ARG:HE	1.72	0.54
2:B:910:THR:HG22	12:L:43:ILE:HA	1.88	0.54
15:O:258:MET:SD	15:O:258:MET:N	2.81	0.54
1:A:1458:ILE:HG21	2:B:1091:ARG:HD2	1.89	0.54
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.39	0.54
17:Q:43:ASN:OD1	17:Q:103:ASN:ND2	2.41	0.54
15:O:267:PRO:HB2	15:O:337:LYS:HD2	1.90	0.54
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.89	0.54
1:A:552:ASP:HB3	8:H:22:PHE:HB3	1.88	0.53
1:A:95:PHE:HB2	1:A:311:GLN:HE22	1.73	0.53
11:K:7:PHE:HB2	11:K:11:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:187:SER:OG	18:R:162:ASN:ND2	2.41	0.53
14:N:61:DT:H2''	14:N:62:DT:H5'	1.90	0.53
1:A:410:ASN:HD22	1:A:430:ARG:HD3	1.74	0.53
22:W:42:CYS:SG	22:W:75:ARG:NH2	2.81	0.53
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.91	0.53
6:F:100:ARG:NH2	6:F:121:ASP:O	2.42	0.53
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.53
23:X:79:ALA:O	23:X:83:ASN:ND2	2.41	0.53
13:M:263:GLN:OE1	13:M:268:LYS:NZ	2.35	0.53
1:A:1157:ILE:HD13	1:A:1160:ARG:HH21	1.73	0.52
22:W:125:ALA:O	22:W:128:LYS:NZ	2.42	0.52
2:B:1050:ARG:NH2	2:B:1054:MET:SD	2.82	0.52
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.91	0.52
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.92	0.52
2:B:1089:MET:HG3	19:T:47:DT:H4'	1.91	0.52
1:A:202:TRP:HD1	1:A:212:LYS:HA	1.75	0.52
2:B:230:ARG:NH2	2:B:262:TYR:OH	2.43	0.52
19:T:52:DG:H2''	19:T:53:DT:C5'	2.39	0.52
1:A:1475:LEU:HD22	7:G:66:VAL:HG21	1.92	0.52
2:B:509:VAL:HG11	2:B:524:LYS:HD2	1.91	0.52
7:G:97:LEU:HB2	7:G:108:ILE:HD12	1.92	0.52
14:N:25:DG:H2'	14:N:26:DG:H8	1.74	0.52
15:O:188:ARG:NH2	21:V:63:ASN:O	2.43	0.52
13:M:174:PRO:HG2	13:M:214:PHE:HE1	1.75	0.51
17:Q:35:ASP:OD1	17:Q:108:ARG:NH2	2.43	0.51
1:A:432:HIS:HE1	1:A:437:ASP:HB2	1.75	0.51
2:B:228:SER:O	2:B:405:ARG:NH1	2.43	0.51
14:N:25:DG:H2'	14:N:26:DG:C8	2.45	0.51
1:A:904:GLN:NE2	1:A:981:CYS:O	2.44	0.51
1:A:1486:ILE:HB	1:A:1487:PRO:HD3	1.92	0.51
1:A:923:ASP:N	1:A:923:ASP:OD1	2.44	0.51
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.44	0.51
18:R:88:VAL:HG22	18:R:113:ARG:HG3	1.92	0.51
20:U:342:ILE:HG12	20:U:351:PHE:HD1	1.76	0.51
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.44	0.51
3:C:172:GLU:OE2	12:L:58:ARG:NH2	2.42	0.51
1:A:274:ASP:OD1	1:A:275:ASP:N	2.43	0.50
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.92	0.50
2:B:797:ASN:OD1	2:B:800:ALA:N	2.43	0.50
15:O:268:ILE:HD13	15:O:332:LEU:HD22	1.93	0.50
21:V:79:VAL:HG21	21:V:93:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.44	0.50
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.42	0.50
1:A:871:VAL:HB	1:A:1088:GLY:HA3	1.94	0.50
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.44	0.50
1:A:48:GLU:HB2	1:A:53:LYS:HB2	1.94	0.50
7:G:53:ASN:O	7:G:71:LYS:NZ	2.45	0.50
2:B:1000:THR:HB	2:B:1003:ASN:HB2	1.93	0.50
9:I:69:ILE:HG22	9:I:71:ASP:H	1.75	0.50
1:A:1262:MET:HE1	1:A:1264:SER:HB2	1.94	0.49
3:C:4:ALA:HB2	11:K:93:ASP:HB3	1.94	0.49
3:C:193:ARG:NH2	3:C:218:ALA:O	2.42	0.49
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.93	0.49
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.94	0.49
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.94	0.49
7:G:120:ASP:OD1	7:G:122:ASN:ND2	2.45	0.49
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.44	0.49
12:L:35:ARG:NH1	12:L:36:CYS:O	2.45	0.49
1:A:637:MET:HB3	8:H:122:LEU:HD21	1.94	0.49
8:H:18:GLU:N	8:H:18:GLU:OE1	2.46	0.49
1:A:388:MET:HA	2:B:1063:ALA:HB2	1.93	0.49
2:B:592:ARG:NE	2:B:663:GLU:OE2	2.38	0.49
1:A:373:LEU:O	1:A:485:ASN:ND2	2.45	0.49
2:B:274:ARG:HG2	2:B:279:VAL:HA	1.95	0.49
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.49
19:T:50:DG:O5'	19:T:50:DG:H8	1.95	0.49
2:B:867:ILE:HG22	2:B:869:LYS:HB2	1.95	0.48
17:Q:13:GLU:HG2	18:R:42:LYS:NZ	2.28	0.48
19:T:51:DT:H2'	19:T:52:DG:O4'	2.12	0.48
2:B:433:LEU:O	13:M:127:ARG:NH2	2.46	0.48
21:V:81:PHE:HB2	21:V:88:ILE:HB	1.95	0.48
1:A:1279:MET:HA	17:Q:172:ASN:HD21	1.78	0.48
3:C:113:ARG:NH2	3:C:119:ASP:OD2	2.47	0.48
10:J:30:THR:HG23	10:J:33:ASP:H	1.77	0.48
1:A:487:SER:OG	1:A:673:GLN:NE2	2.46	0.48
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.47	0.48
3:C:7:PRO:O	11:K:104:ARG:NH1	2.46	0.48
3:C:88:CYS:SG	3:C:89:THR:N	2.86	0.48
23:X:99:LEU:HD22	23:X:120:MET:HE3	1.95	0.48
2:B:281:ASP:HB2	9:I:22:ASN:HA	1.96	0.48
1:A:413:TYR:OH	1:A:450:MET:O	2.26	0.48
1:A:921:ARG:NH1	1:A:953:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:HIS:HB3	2:B:784:SER:HB3	1.94	0.48
20:U:15:ARG:HA	20:U:18:ILE:HD12	1.95	0.48
1:A:46:THR:OG1	1:A:273:GLN:NE2	2.47	0.47
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.96	0.47
1:A:461:GLN:HG2	19:T:48:DG:H1'	1.95	0.47
22:W:20:TYR:HD2	22:W:190:LEU:HD11	1.79	0.47
22:W:55:ASP:H	22:W:58:GLN:HE21	1.62	0.47
8:H:74:GLU:N	8:H:74:GLU:OE1	2.47	0.47
2:B:177:CYS:SG	2:B:738:THR:OG1	2.58	0.47
15:O:206:GLU:OE1	15:O:236:LYS:NZ	2.48	0.47
2:B:56:GLN:HE22	2:B:90:GLN:HA	1.79	0.47
15:O:180:LEU:HD12	15:O:200:VAL:HG23	1.96	0.47
1:A:262:PRO:HG2	13:M:66:ARG:HH22	1.80	0.47
1:A:909:LEU:HD13	1:A:966:LEU:HB3	1.97	0.47
2:B:209:ALA:HB2	2:B:382:LEU:HD22	1.97	0.47
10:J:14:VAL:HG21	10:J:48:MET:HG2	1.96	0.47
11:K:29:ASN:HD22	11:K:79:PRO:HA	1.79	0.47
12:L:28:ILE:HG23	12:L:32:ASP:HB3	1.95	0.47
20:U:19:GLU:O	20:U:23:ASN:ND2	2.46	0.47
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.31	0.47
7:G:39:THR:HG23	7:G:42:TYR:H	1.79	0.47
1:A:583:ARG:HE	1:A:585:LEU:HD11	1.78	0.46
9:I:106:ASP:OD1	9:I:107:ALA:N	2.48	0.46
23:X:85:MET:HE1	23:X:139:PHE:HD1	1.79	0.46
2:B:291:ASP:OD1	2:B:291:ASP:N	2.48	0.46
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.96	0.46
4:D:15:GLU:O	7:G:81:LYS:NZ	2.40	0.46
17:Q:18:VAL:HG22	17:Q:137:ALA:HB3	1.97	0.46
3:C:48:ASP:HA	3:C:175:LYS:HZ1	1.80	0.46
16:P:8:G:N2	19:T:46:DC:N3	2.43	0.46
21:V:70:ASN:HD21	21:V:99:ASP:HB3	1.81	0.46
1:A:827:TYR:O	2:B:716:HIS:ND1	2.48	0.46
2:B:50:PHE:HA	2:B:54:SER:HB2	1.98	0.46
17:Q:22:THR:HG22	17:Q:24:LYS:H	1.81	0.46
1:A:869:GLU:OE2	1:A:1455:SER:OG	2.33	0.46
2:B:744:MET:SD	2:B:906:GLN:NE2	2.87	0.46
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.98	0.46
17:Q:43:ASN:H	17:Q:103:ASN:HD21	1.62	0.46
2:B:713:PHE:HB3	2:B:716:HIS:CD2	2.51	0.46
2:B:820:LYS:HD3	13:M:137:ARG:HH21	1.81	0.46
14:N:2:DA:H1'	14:N:3:DA:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:357:ILE:HB	21:V:48:LEU:HD21	1.97	0.46
13:M:293:TYR:HE2	13:M:315:GLN:HA	1.81	0.46
1:A:78:MET:O	2:B:1072:ARG:NH2	2.49	0.45
2:B:83:ARG:HB3	2:B:133:ILE:HB	1.98	0.45
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.49	0.45
1:A:1249:ASP:N	1:A:1249:ASP:OD1	2.46	0.45
2:B:674:MET:HE2	9:I:77:THR:HA	1.98	0.45
15:O:281:SER:HB3	15:O:293:TYR:HD1	1.82	0.45
9:I:65:LEU:HD21	9:I:124:THR:HB	1.99	0.45
20:U:20:ASP:OD2	21:V:51:ARG:NH2	2.49	0.45
1:A:320:ASN:ND2	1:A:336:LEU:O	2.34	0.45
15:O:239:ARG:HD2	20:U:314:LEU:HB3	1.98	0.45
23:X:147:ASP:OD1	23:X:147:ASP:N	2.49	0.45
1:A:62:GLN:HA	1:A:84:HIS:HB2	1.97	0.45
1:A:958:ARG:HH22	1:A:1014:LYS:HE3	1.82	0.45
2:B:927:ARG:HG3	2:B:1054:MET:HE1	1.99	0.45
3:C:186:TYR:OH	3:C:194:HIS:ND1	2.43	0.45
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.98	0.45
14:N:66:DC:H2''	14:N:67:DA:O4'	2.17	0.45
1:A:681:LEU:O	2:B:1030:ASN:ND2	2.49	0.45
1:A:1481:LYS:HZ3	7:G:22:LEU:H	1.64	0.45
2:B:362:ALA:O	2:B:366:GLY:N	2.46	0.45
17:Q:24:LYS:HD2	18:R:97:THR:HG21	1.99	0.45
1:A:491:PRO:HG3	1:A:535:MET:HE2	1.98	0.45
9:I:22:ASN:ND2	9:I:41:ASN:OD1	2.50	0.45
14:N:17:DA:C2'	14:N:18:DG:H5''	2.46	0.44
1:A:1364:GLU:HA	1:A:1367:THR:HG22	2.00	0.44
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.38	0.44
2:B:40:VAL:HG11	2:B:482:LEU:HD13	1.99	0.44
16:P:2:C:H2'	16:P:3:A:C8	2.52	0.44
19:T:51:DT:H5''	19:T:51:DT:H6	1.82	0.44
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.99	0.44
4:D:59:GLU:HA	4:D:62:MET:HG2	1.99	0.44
8:H:32:SER:HB3	8:H:37:MET:H	1.83	0.44
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.46	0.44
1:A:749:ARG:HD3	1:A:789:GLY:HA3	1.99	0.44
1:A:793:VAL:HG23	1:A:845:GLU:HG3	1.99	0.44
2:B:65:ILE:HD11	2:B:412:LEU:HD22	2.00	0.44
18:R:179:ASP:OD1	18:R:179:ASP:N	2.44	0.44
2:B:82:PRO:HB3	2:B:134:LYS:HD3	2.00	0.44
2:B:795:ILE:HB	2:B:966:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:THR:OG1	5:E:101:ARG:N	2.51	0.44
1:A:18:ILE:N	1:A:1462:GLN:OE1	2.48	0.44
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.44	0.44
1:A:1049:LEU:HD22	1:A:1054:MET:HE2	1.99	0.44
3:C:24:GLU:OE1	3:C:228:ARG:NH2	2.50	0.44
9:I:82:GLU:OE1	9:I:82:GLU:N	2.48	0.43
15:O:192:TYR:HB2	15:O:200:VAL:HG22	2.00	0.43
15:O:204:ILE:HG13	15:O:207:PRO:HD2	2.00	0.43
2:B:1038:THR:HA	3:C:195:THR:HA	2.00	0.43
7:G:106:CYS:HB2	7:G:159:ALA:HB3	2.00	0.43
19:T:54:DG:H2''	19:T:55:DA:C8	2.54	0.43
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.81	0.43
2:B:436:LYS:HD3	2:B:438:ARG:HB3	1.99	0.43
2:B:474:THR:OG1	2:B:732:ALA:O	2.30	0.43
2:B:634:LEU:HB3	2:B:661:VAL:HG12	2.00	0.43
2:B:46:SER:HB3	2:B:397:GLY:H	1.83	0.43
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	2.00	0.43
19:T:47:DT:H2'	19:T:48:DG:O4'	2.19	0.43
22:W:110:MET:HE1	23:X:223:VAL:HG21	2.00	0.43
1:A:183:GLY:O	1:A:184:CYS:SG	2.77	0.43
1:A:983:LEU:HB3	1:A:1048:THR:HG21	2.01	0.43
2:B:849:ASP:OD2	12:L:46:LYS:NZ	2.49	0.43
3:C:59:LEU:HD22	3:C:151:VAL:HG23	2.00	0.43
7:G:112:SER:HB2	7:G:162:SER:HA	2.00	0.43
1:A:769:MET:HE3	2:B:973:PRO:HG3	2.01	0.43
22:W:162:GLU:HG2	22:W:164:ASP:H	1.84	0.43
17:Q:109:LYS:HG3	17:Q:149:LEU:HB2	2.01	0.43
6:F:69:ARG:HD2	6:F:69:ARG:HA	1.82	0.43
9:I:82:GLU:HG3	9:I:93:GLU:HB3	2.01	0.43
1:A:11:SER:N	2:B:1135:TYR:OH	2.47	0.42
1:A:321:GLU:HB2	1:A:341:GLN:HE22	1.84	0.42
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.86	0.42
1:A:628:VAL:HA	1:A:638:GLY:HA3	2.02	0.42
1:A:902:GLU:OE1	1:A:982:ASN:ND2	2.52	0.42
2:B:191:GLU:OE2	2:B:743:ARG:NH1	2.41	0.42
2:B:870:THR:HB	2:B:889:LYS:HD3	2.02	0.42
12:L:18:ILE:HG13	12:L:47:LYS:HG2	2.01	0.42
1:A:901:VAL:HA	1:A:980:PRO:HA	2.02	0.42
1:A:1221:MET:HE3	1:A:1221:MET:HB3	1.90	0.42
2:B:56:GLN:HE22	2:B:91:ILE:H	1.67	0.42
9:I:60:HIS:HE1	9:I:105:GLU:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:ILE:HG21	11:K:84:GLN:HE21	1.84	0.42
18:R:192:GLU:HB3	23:X:72:GLY:HA3	2.02	0.42
1:A:853:LYS:HE2	1:A:1100:THR:HA	2.01	0.42
17:Q:36:LYS:HA	17:Q:36:LYS:HD2	1.81	0.42
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.02	0.42
2:B:388:TYR:H	2:B:504:THR:HG21	1.85	0.42
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.85	0.42
2:B:715:ASP:OD1	2:B:715:ASP:N	2.53	0.42
2:B:796:MET:HE1	2:B:935:PHE:CE1	2.55	0.42
7:G:110:ARG:HD2	7:G:113:ILE:HD12	2.02	0.42
8:H:90:TYR:HB3	8:H:145:MET:HB2	2.02	0.42
14:N:17:DA:H2'	14:N:18:DG:H5''	2.02	0.42
1:A:90:LEU:HD22	1:A:310:LEU:HD21	2.01	0.42
1:A:155:GLU:C	1:A:182:GLY:HA3	2.44	0.42
2:B:1016:SER:HB2	2:B:1022:LEU:HB3	2.02	0.42
8:H:36:LYS:HA	8:H:36:LYS:HD2	1.78	0.42
19:T:46:DC:H2'	19:T:47:DT:H71	2.02	0.42
1:A:370:ASP:HB2	1:A:483:ARG:HB3	2.02	0.41
1:A:1139:LEU:HG	1:A:1359:SER:HB3	2.02	0.41
1:A:432:HIS:CE1	1:A:437:ASP:HB2	2.53	0.41
1:A:485:ASN:OD1	1:A:486:LEU:N	2.53	0.41
2:B:1091:ARG:HG3	2:B:1107:LEU:HD11	2.03	0.41
3:C:67:ARG:NH1	10:J:3:ILE:O	2.50	0.41
8:H:28:LEU:N	8:H:41:LEU:O	2.50	0.41
1:A:841:MET:HE1	2:B:503:ASN:HA	2.01	0.41
2:B:42:GLN:HE22	2:B:483:ARG:HG2	1.86	0.41
12:L:25:GLU:N	12:L:25:GLU:OE1	2.53	0.41
1:A:1104:LEU:HG	1:A:1122:PRO:HD3	2.01	0.41
1:A:1199:MET:HE2	1:A:1199:MET:HB3	1.84	0.41
2:B:670:GLU:HA	2:B:673:VAL:HG12	2.02	0.41
5:E:2:ASP:OD1	5:E:3:ASP:N	2.53	0.41
13:M:289:TYR:HA	13:M:292:ILE:HG22	2.02	0.41
18:R:12:ALA:HB2	18:R:106:LEU:HD22	2.01	0.41
18:R:56:PHE:N	18:R:81:HIS:O	2.48	0.41
1:A:111:CYS:HA	1:A:188:GLN:HE22	1.86	0.41
1:A:467:MET:HG2	1:A:534:VAL:HG11	2.03	0.41
1:A:1118:THR:HG21	1:A:1135:LYS:HB3	2.03	0.41
6:F:106:ILE:N	6:F:118:TRP:O	2.49	0.41
17:Q:111:LYS:HG3	17:Q:149:LEU:HD11	2.02	0.41
22:W:36:ILE:HG22	22:W:43:VAL:HG21	2.02	0.41
1:A:275:ASP:HB3	1:A:336:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ILE:HD13	1:A:676:ILE:HA	1.89	0.41
1:A:681:LEU:HD23	1:A:681:LEU:HA	1.89	0.41
1:A:1285:LEU:HA	1:A:1288:ILE:HG22	2.03	0.41
1:A:1315:ASP:HA	1:A:1318:LYS:HB3	2.02	0.41
2:B:113:ALA:HA	2:B:118:LEU:HB2	2.01	0.41
2:B:115:LEU:HD22	2:B:908:MET:HE2	2.03	0.41
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.53	0.41
1:A:567:LEU:HD12	1:A:567:LEU:HA	1.89	0.41
1:A:567:LEU:HB3	1:A:570:TRP:HB2	2.01	0.41
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.94	0.41
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	2.03	0.41
2:B:67:LEU:HD12	2:B:84:TYR:HB2	2.02	0.41
2:B:528:LEU:HD21	2:B:767:LEU:HD21	2.01	0.41
13:M:94:ASP:N	13:M:98:ASN:O	2.48	0.41
13:M:125:ALA:HB1	13:M:130:LEU:HB2	2.03	0.41
14:N:2:DA:H2''	14:N:3:DA:H5'	2.02	0.41
2:B:97:THR:HG21	18:R:148:VAL:HB	2.02	0.41
2:B:117:ASN:HA	2:B:189:GLY:HA3	2.03	0.41
2:B:220:GLU:OE2	2:B:222:ARG:NH1	2.48	0.41
2:B:849:ASP:HB3	12:L:15:MET:HE1	2.02	0.41
3:C:117:SER:OG	3:C:131:THR:OG1	2.38	0.41
12:L:35:ARG:NH1	12:L:40:GLY:HA2	2.36	0.41
2:B:54:SER:O	2:B:58:ILE:HG12	2.21	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
14:N:76:DC:H1'	19:T:24:DG:H22	1.85	0.41
15:O:295:MET:HE3	15:O:298:PRO:HG2	2.02	0.41
22:W:55:ASP:HB2	22:W:58:GLN:HG2	2.02	0.41
1:A:875:TYR:HA	1:A:1083:PRO:HB3	2.03	0.40
2:B:1067:ILE:HD11	13:M:46:ILE:HG12	2.03	0.40
12:L:34:ILE:HG23	12:L:44:MET:HG2	2.03	0.40
13:M:212:GLY:HA2	13:M:215:MET:HG2	2.02	0.40
2:B:109:MET:HE3	2:B:109:MET:HA	2.04	0.40
2:B:796:MET:HE3	2:B:796:MET:HB2	1.83	0.40
22:W:76:MET:SD	22:W:88:ARG:NE	2.93	0.40
22:W:88:ARG:NH1	22:W:90:ASN:OD1	2.53	0.40
1:A:780:ASN:ND2	2:B:976:MET:SD	2.95	0.40
2:B:692:THR:O	2:B:692:THR:OG1	2.39	0.40
3:C:260:GLN:HB2	11:K:91:ILE:HG21	2.02	0.40
8:H:32:SER:OG	8:H:33:GLU:N	2.53	0.40
12:L:46:LYS:HE2	12:L:46:LYS:HB3	1.98	0.40
17:Q:17:ARG:N	17:Q:135:PHE:O	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:HIS:NE2	1:A:769:MET:SD	2.85	0.40
2:B:56:GLN:NE2	2:B:91:ILE:H	2.19	0.40
2:B:224:CYS:HB3	2:B:232:THR:HG22	2.03	0.40
2:B:285:LEU:HD11	2:B:305:LEU:HD11	2.04	0.40
2:B:405:ARG:HD3	2:B:405:ARG:HA	1.87	0.40
2:B:728:MET:SD	2:B:942:LYS:HE2	2.62	0.40
11:K:51:LEU:HD23	11:K:51:LEU:HA	1.82	0.40
14:N:23:DT:H2'	14:N:24:DG:C8	2.57	0.40
20:U:29:PHE:HE2	20:U:39:LEU:HD13	1.86	0.40
2:B:289:ILE:HD12	2:B:297:MET:HB3	2.04	0.40
2:B:1089:MET:CG	19:T:47:DT:H4'	2.51	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	1411/1970 (72%)	1355 (96%)	56 (4%)	0	100	100
2	B	1111/1300 (86%)	1062 (96%)	49 (4%)	0	100	100
3	C	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
4	D	126/184 (68%)	124 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
10	J	62/67 (92%)	62 (100%)	0	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
13	M	288/316 (91%)	280 (97%)	8 (3%)	0	100	100
15	O	177/339 (52%)	171 (97%)	6 (3%)	0	100	100
17	Q	134/517 (26%)	128 (96%)	6 (4%)	0	100	100
18	R	218/249 (88%)	212 (97%)	5 (2%)	1 (0%)	24	57
20	U	109/376 (29%)	106 (97%)	2 (2%)	1 (1%)	14	44
21	V	97/109 (89%)	96 (99%)	1 (1%)	0	100	100
22	W	185/439 (42%)	182 (98%)	3 (2%)	0	100	100
23	X	169/291 (58%)	162 (96%)	7 (4%)	0	100	100
All	All	5206/7391 (70%)	5021 (96%)	183 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	U	346	LYS
18	R	231	ASN

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	1252/1749 (72%)	1249 (100%)	3 (0%)	87	89
2	B	985/1127 (87%)	985 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/160 (74%)	117 (99%)	1 (1%)	73	81
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	247/268 (92%)	246 (100%)	1 (0%)	84	86
15	O	154/293 (53%)	151 (98%)	3 (2%)	50	73
17	Q	121/448 (27%)	121 (100%)	0	100	100
18	R	196/218 (90%)	196 (100%)	0	100	100
20	U	105/324 (32%)	105 (100%)	0	100	100
21	V	90/98 (92%)	90 (100%)	0	100	100
22	W	169/373 (45%)	169 (100%)	0	100	100
23	X	154/261 (59%)	154 (100%)	0	100	100
All	All	4667/6487 (72%)	4659 (100%)	8 (0%)	85	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	ASP
1	A	500	GLU
1	A	1433	GLU
4	D	20	LEU
13	M	245	VAL
15	O	169	VAL
15	O	203	ARG
15	O	219	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	136	GLN
1	A	143	HIS
1	A	188	GLN
1	A	273	GLN
1	A	341	GLN
1	A	562	ASN
1	A	599	HIS
1	A	601	ASN

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Mol	Chain	Res	Type
1	A	673	GLN
1	A	742	ASN
1	A	780	ASN
1	A	790	GLN
1	A	791	GLN
1	A	913	ASN
1	A	1105	ASN
1	A	1190	GLN
1	A	1194	ASN
1	A	1410	HIS
1	A	1417	HIS
2	B	56	GLN
2	B	254	GLN
2	B	312	GLN
2	B	537	GLN
2	B	593	GLN
2	B	631	GLN
2	B	642	GLN
2	B	683	GLN
2	B	717	ASN
2	B	755	GLN
2	B	1049	GLN
2	B	1068	GLN
2	B	1117	HIS
2	B	1129	ASN
3	C	108	ASN
3	C	111	GLN
3	C	114	HIS
3	C	177	ASN
3	C	232	ASN
3	C	260	GLN
4	D	19	GLN
4	D	102	ASN
5	E	92	GLN
5	E	107	GLN
7	G	4	HIS
7	G	122	ASN
8	H	29	HIS
8	H	87	GLN
9	I	22	ASN
9	I	45	GLN
9	I	74	GLN

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Mol	Chain	Res	Type
11	K	29	ASN
11	K	89	ASN
11	K	113	GLN
13	M	271	GLN
15	O	257	ASN
15	O	277	HIS
15	O	278	GLN
17	Q	103	ASN
17	Q	129	GLN
17	Q	152	HIS
17	Q	172	ASN
18	R	29	GLN
18	R	30	GLN
18	R	64	ASN
18	R	81	HIS
18	R	91	GLN
18	R	112	GLN
18	R	123	ASN
18	R	162	ASN
18	R	194	HIS
18	R	195	GLN
18	R	208	GLN
18	R	229	HIS
20	U	48	ASN
20	U	326	GLN
21	V	39	GLN
22	W	58	GLN
22	W	89	HIS
22	W	95	ASN
22	W	101	ASN
23	X	188	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	7/8 (87%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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.

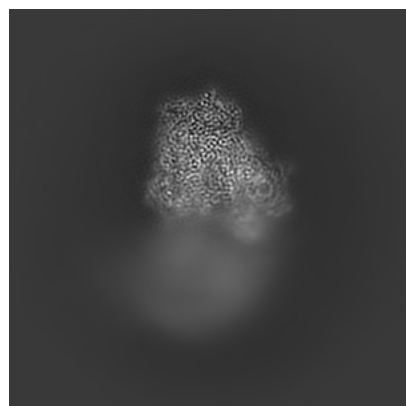
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19718. These allow visual inspection of the internal detail of the map and identification of artifacts.

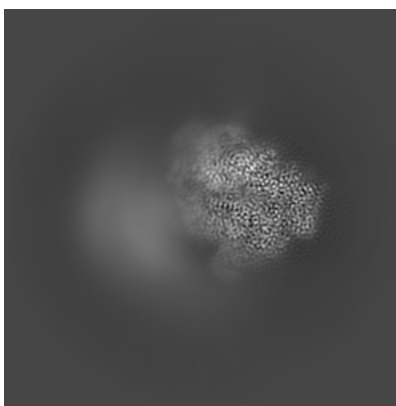
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

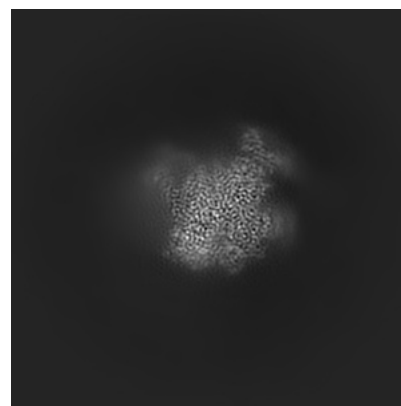
6.1.1 Primary map



X

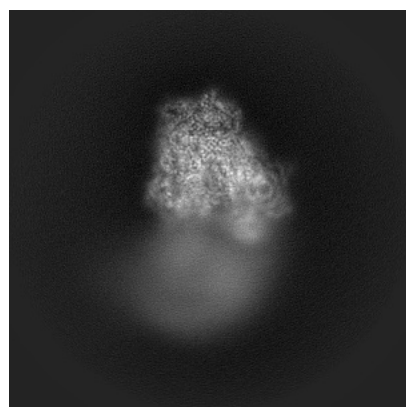


Y

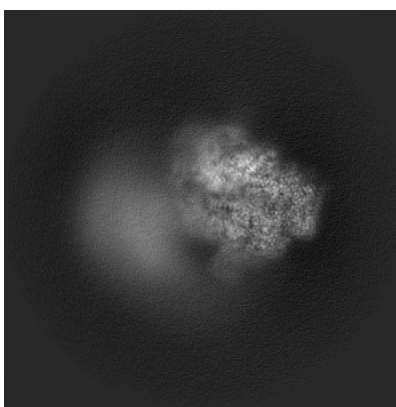


Z

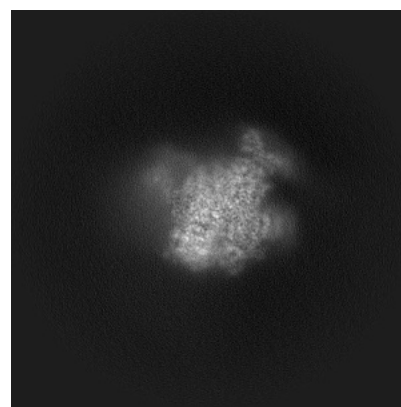
6.1.2 Raw map



X



Y



Z

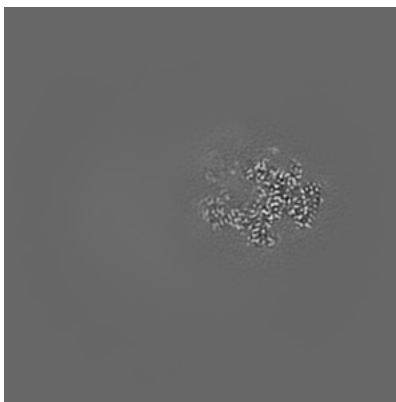
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

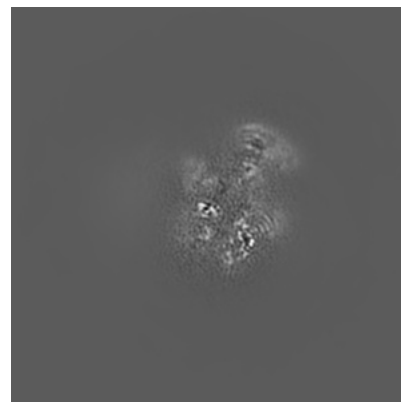
6.2.1 Primary map



X Index: 200

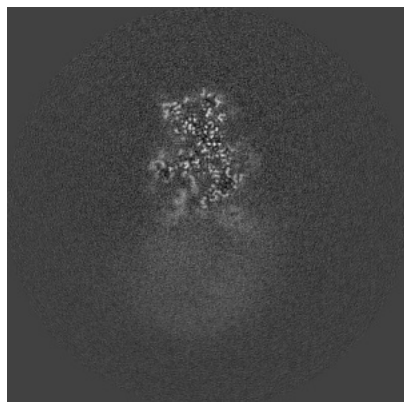


Y Index: 200

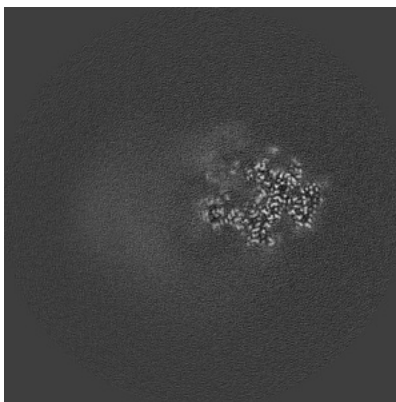


Z Index: 200

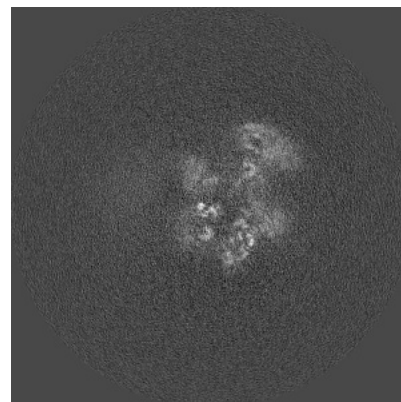
6.2.2 Raw map



X Index: 200



Y Index: 200

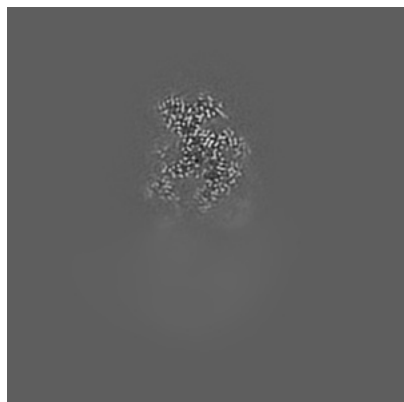


Z Index: 200

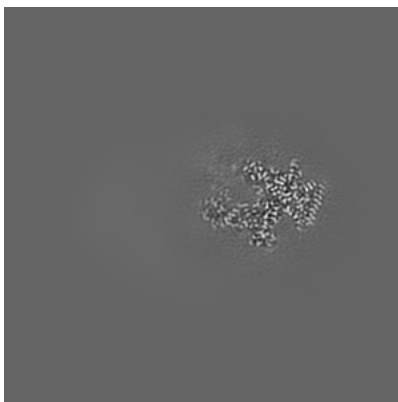
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

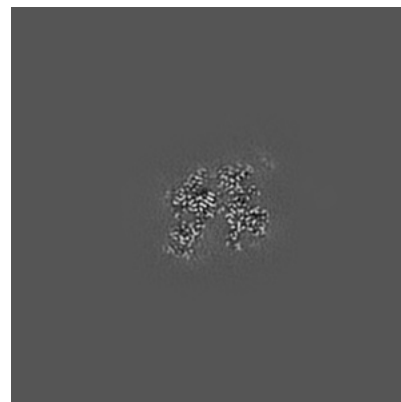
6.3.1 Primary map



X Index: 189

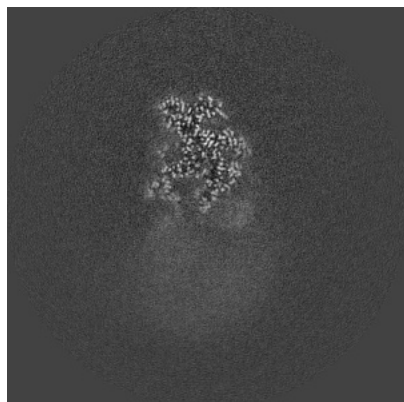


Y Index: 202

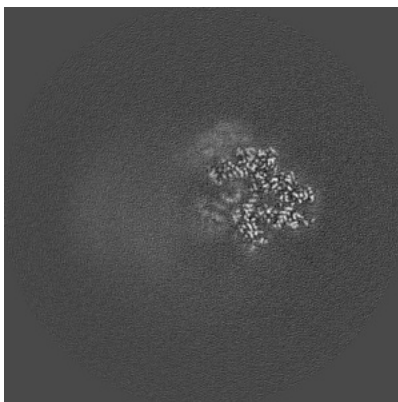


Z Index: 262

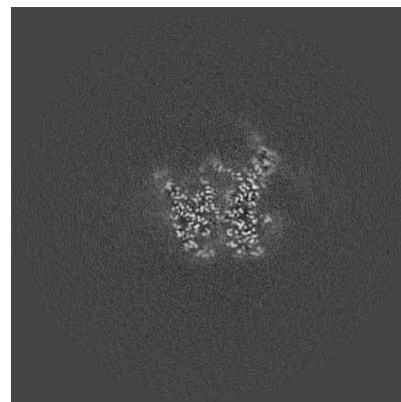
6.3.2 Raw map



X Index: 189



Y Index: 190

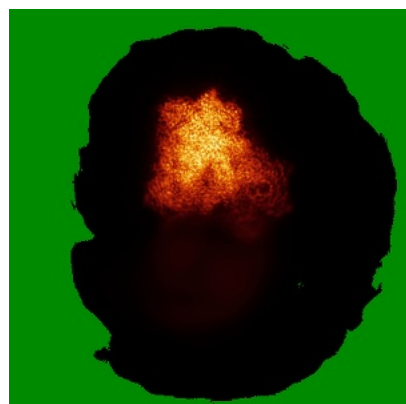


Z Index: 250

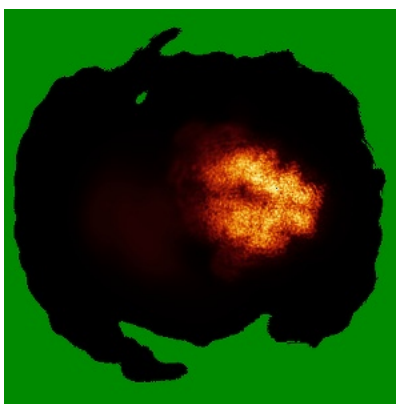
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

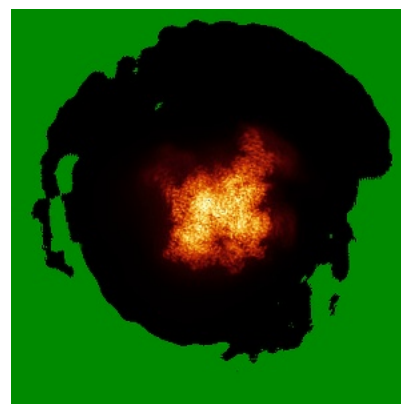
6.4.1 Primary map



X

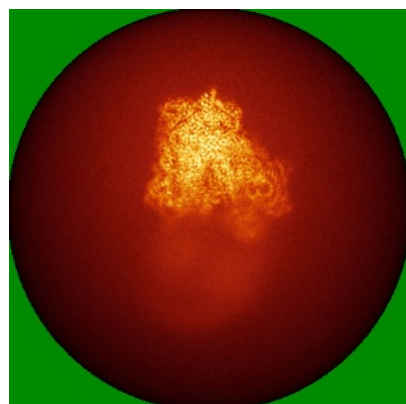


Y

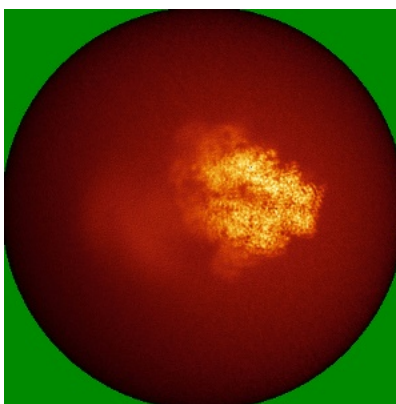


Z

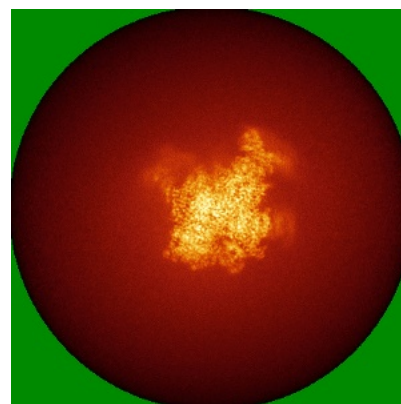
6.4.2 Raw map



X



Y

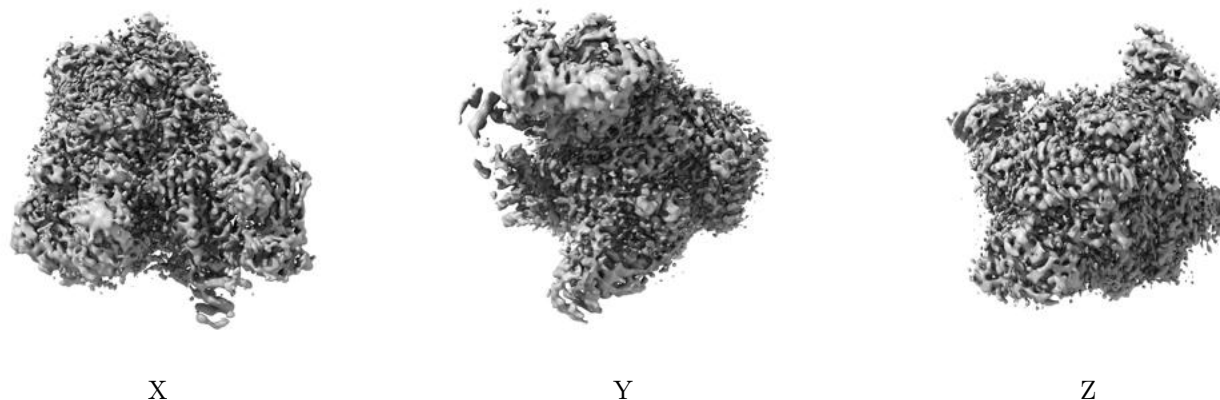


Z

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.

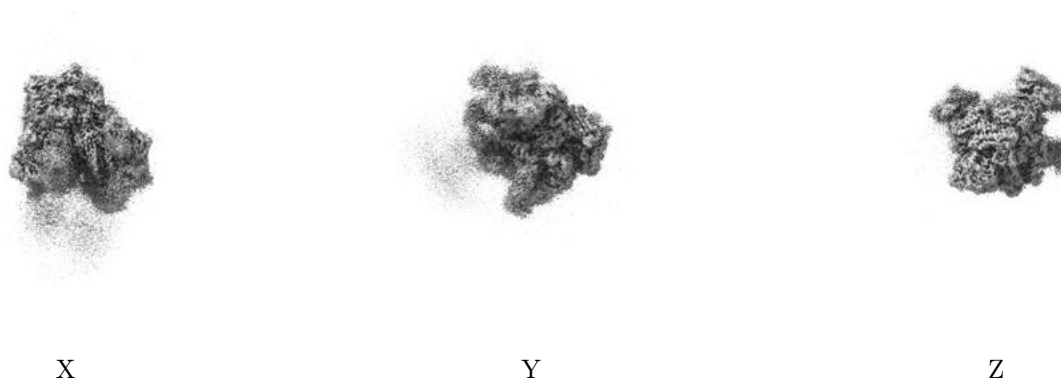
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.29. 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.

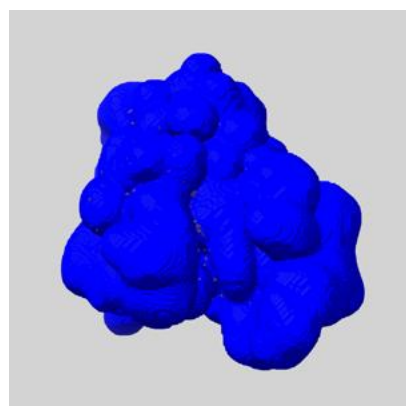
6.6 Mask visualisation [i](#)

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

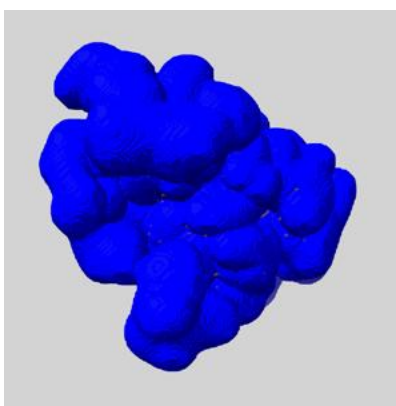
A mask typically either:

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

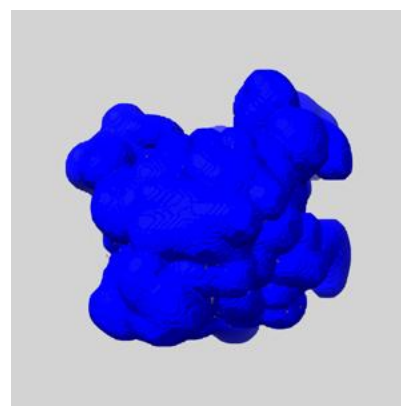
6.6.1 emd_19718_msk_1.map [i](#)



X



Y

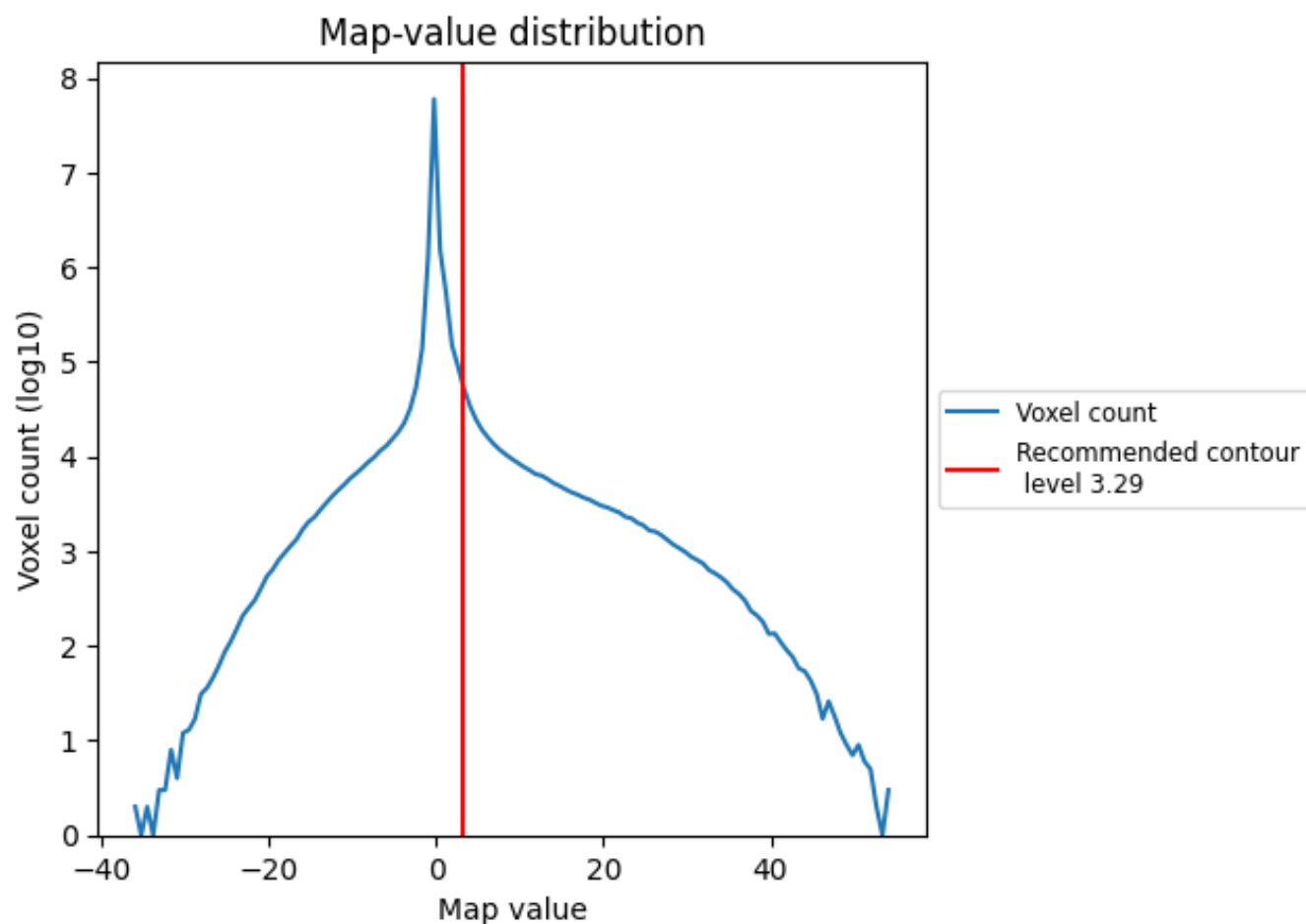


Z

7 Map analysis [i](#)

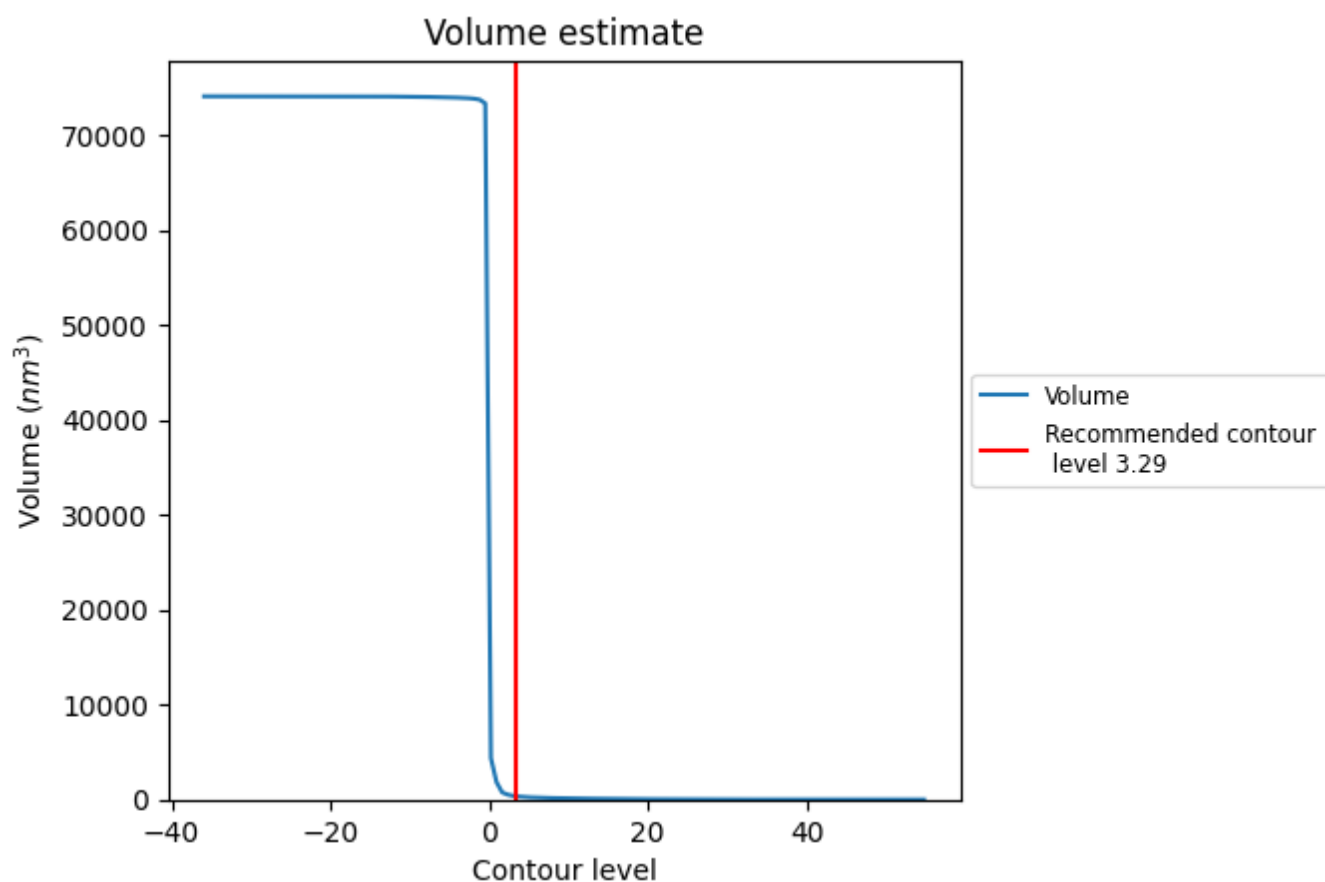
This section contains the results of statistical analysis of the map.

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.

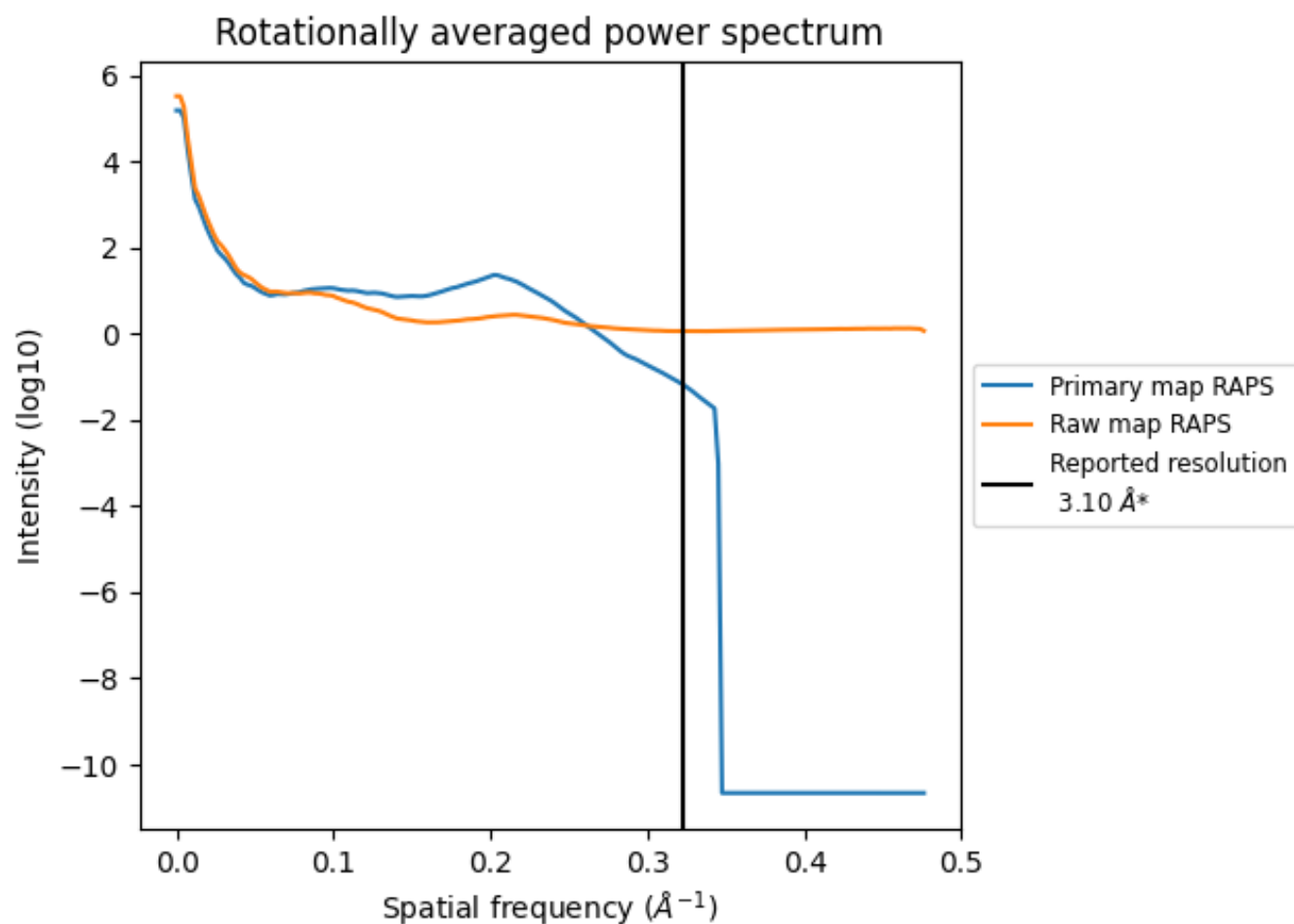
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 328 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 ⓘ

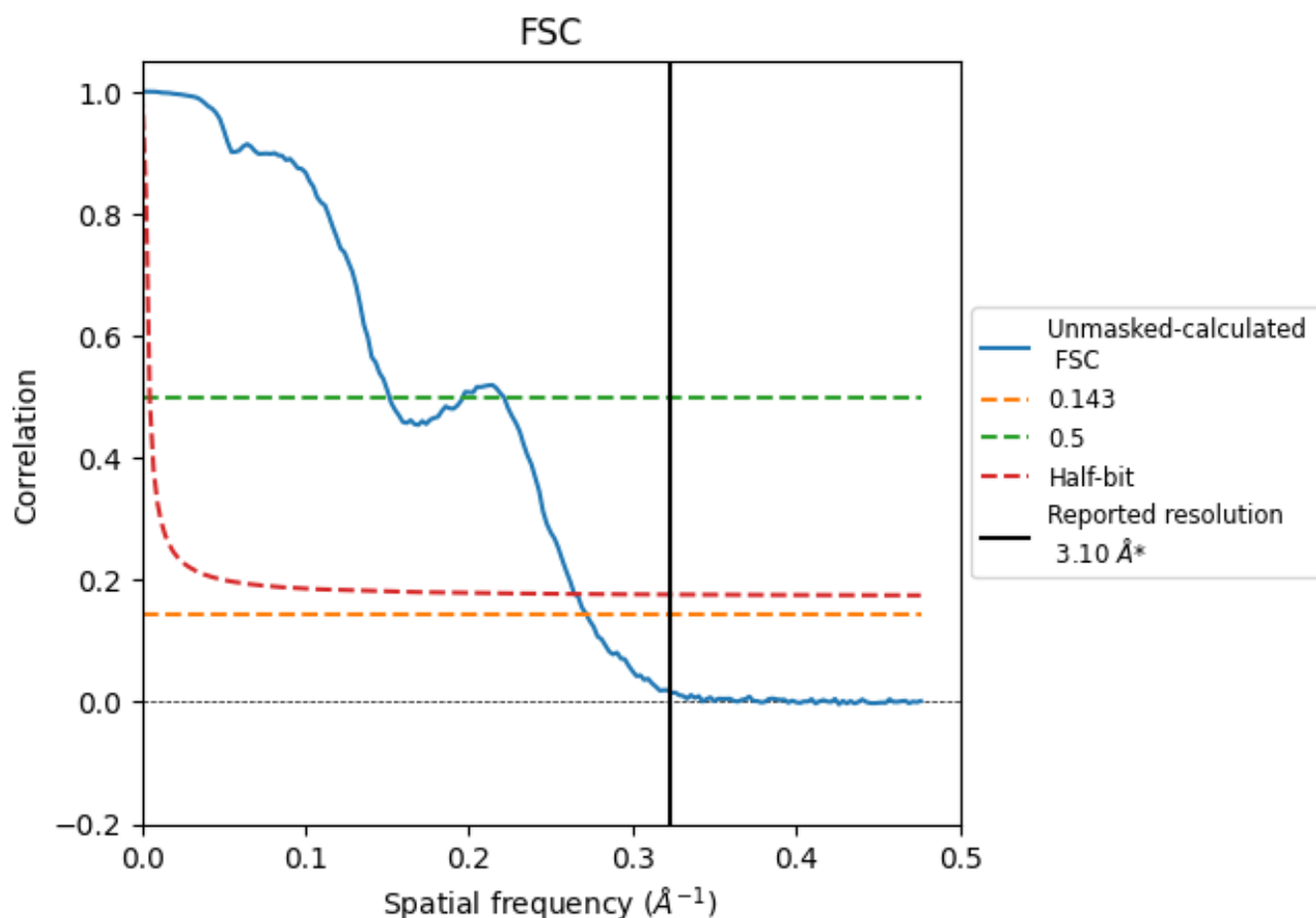


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

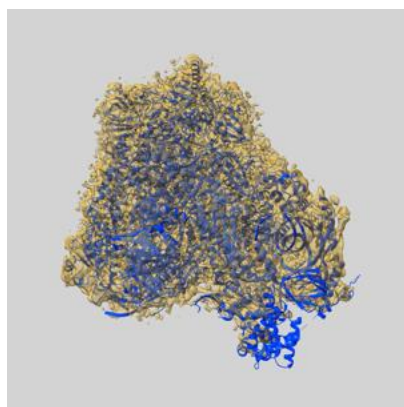
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	6.61	3.78

*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 3.68 differs from the reported value 3.1 by more than 10 %

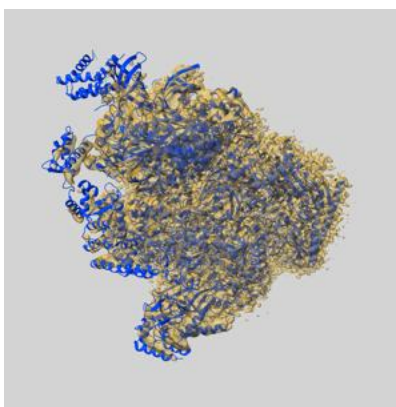
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19718 and PDB model 8S51. Per-residue inclusion information can be found in section [3](#) on page [9](#).

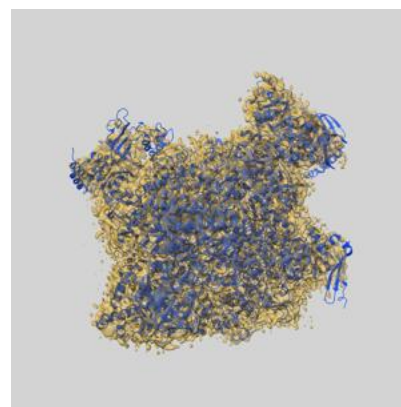
9.1 Map-model overlay [i](#)



X



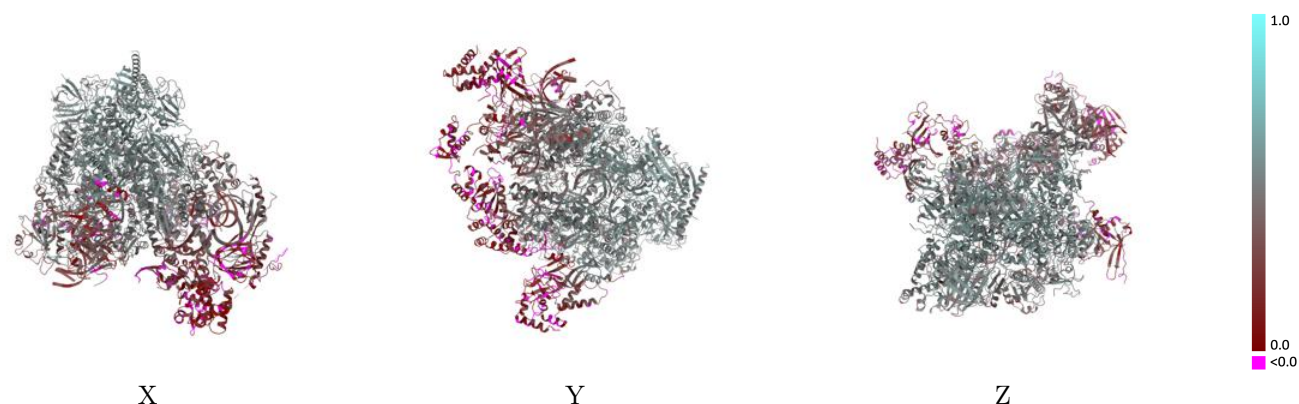
Y



Z

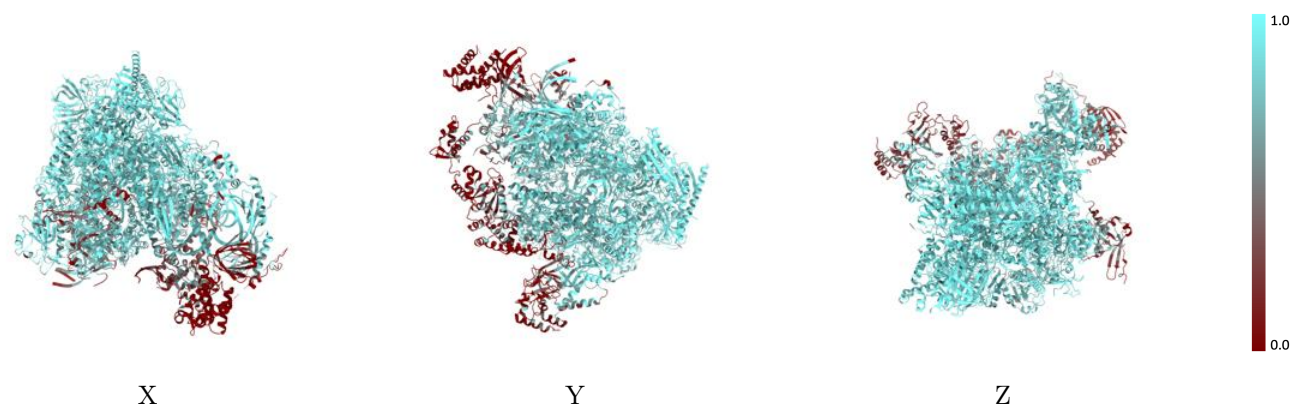
The images above show the 3D surface view of the map at the recommended contour level 3.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



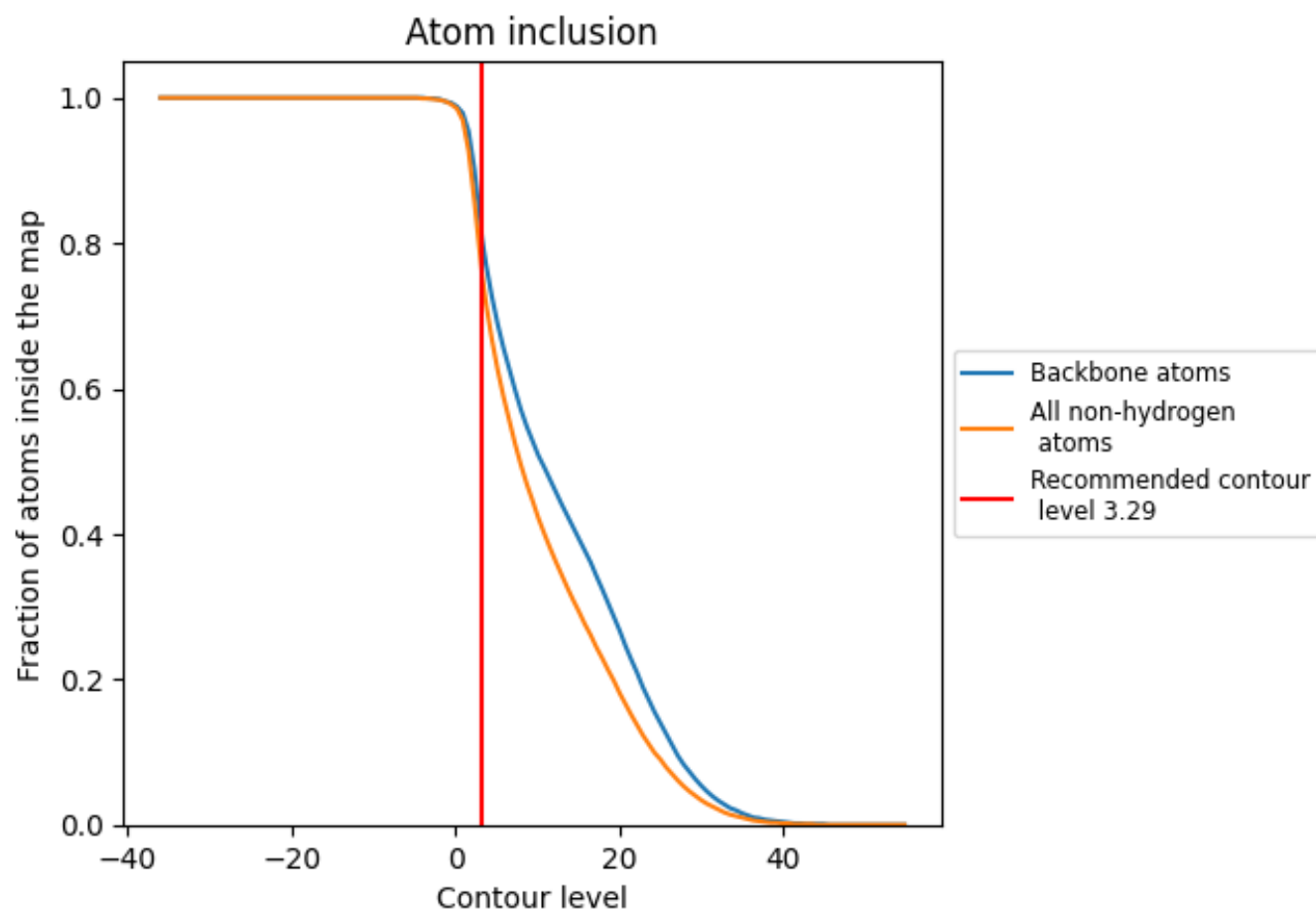
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.4150
A	 0.8850	 0.4940
B	 0.9020	 0.5130
C	 0.9180	 0.5270
D	 0.3260	 0.1510
E	 0.8730	 0.4750
F	 0.9090	 0.5200
G	 0.5410	 0.2610
H	 0.8960	 0.5010
I	 0.8380	 0.4420
J	 0.9390	 0.5390
K	 0.9060	 0.5190
L	 0.8910	 0.4960
M	 0.8350	 0.4530
N	 0.7920	 0.2980
O	 0.7770	 0.3410
P	 0.8520	 0.4580
Q	 0.5870	 0.2850
R	 0.4960	 0.2520
T	 0.8090	 0.3550
U	 0.1260	 0.1130
V	 0.1370	 0.1430
W	 0.2030	 0.1280
X	 0.1250	 0.1230

