



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 8P0K / pdb_00008p0k
EMDB ID : EMD-17335
Title : Cryo EM map and model of the vaccinia RNA polymerase intermediate pre-initiation open promoter complex, module 2 of capping enzyme mobile
Authors : Grimm, C.; Jungwirth, S.; Fischer, U.
Deposited on : 2023-05-10
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

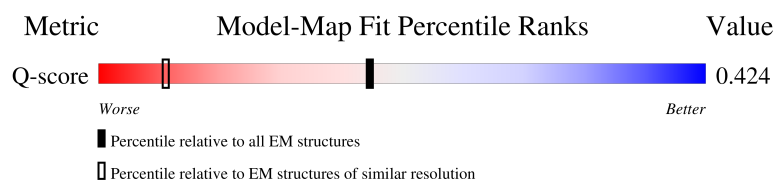
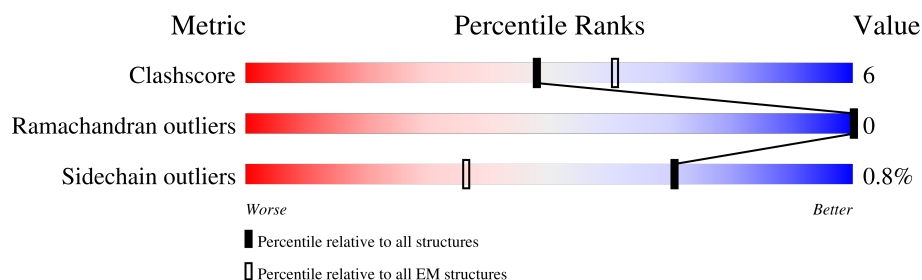
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8968 (2.14 - 3.14)

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	1286	
2	B	1164	
3	C	305	
4	E	185	

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Mol	Chain	Length	Quality of chain
5	F	164	
6	G	161	
7	H	382	
8	I	288	
9	J	63	
10	N	70	
11	O	844	
12	S	259	
13	T	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 76143 atoms, of which 37892 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1277	Total	C	H	N	O	S	0	0
			20617	6593	10357	1690	1931	46		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P20504
A	489	GLU	LYS	variant	UNP P20504
A	1015	LYS	ARG	variant	UNP P20504

- Molecule 2 is a protein called DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1155	Total	C	H	N	O	S	2	0
			18659	5934	9340	1595	1741	49		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	variant	UNP P68694
B	343	PHE	TYR	variant	UNP P68694

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	304	Total	C	H	N	O	S	0	0
			4947	1608	2463	399	464	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ASN	ASP	variant	UNP P21087

- Molecule 4 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	184	Total	C	H	N	O	S	0	0
			3041	966	1546	248	276	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	104	Total	C	H	N	O	S	0	0
			1736	551	877	151	154	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	153	Total	C	H	N	O	S	0	0
			2370	753	1178	198	235	6		

- Molecule 7 is a protein called Intermediate transcription factor 3 large subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	382	Total	C	H	N	O	S	0	0
			6298	2004	3164	522	590	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	58	PRO	HIS	variant	UNP P20998

- Molecule 8 is a protein called Intermediate transcription factor 3 small subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	276	Total	C	H	N	O	S	0	0
			4563	1469	2293	370	424	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	247	LYS	GLU	variant	UNP P20986

- Molecule 9 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	61	Total	C	H	N	O	S	0	0
			1017	310	527	88	88	4		

- Molecule 10 is a DNA chain called Non-template DNA oligomer.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	N	39	Total	C	H	N	O	P	0	0
			1236	383	442	142	230	39		

- Molecule 11 is a protein called mRNA-capping enzyme catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	525	Total	C	H	N	O	S	0	0
			8577	2741	4335	695	796	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	8	PHE	SER	variant	UNP P20979
O	202	THR	LYS	variant	UNP P20979

- Molecule 12 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	S	116	Total	C	H	N	O	S	0	0
			1916	609	961	155	187	4		

- Molecule 13 is a DNA chain called Template DNA oligomer.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	T	36	Total	C	H	N	O	P	0	0
			1161	360	409	141	215	36		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

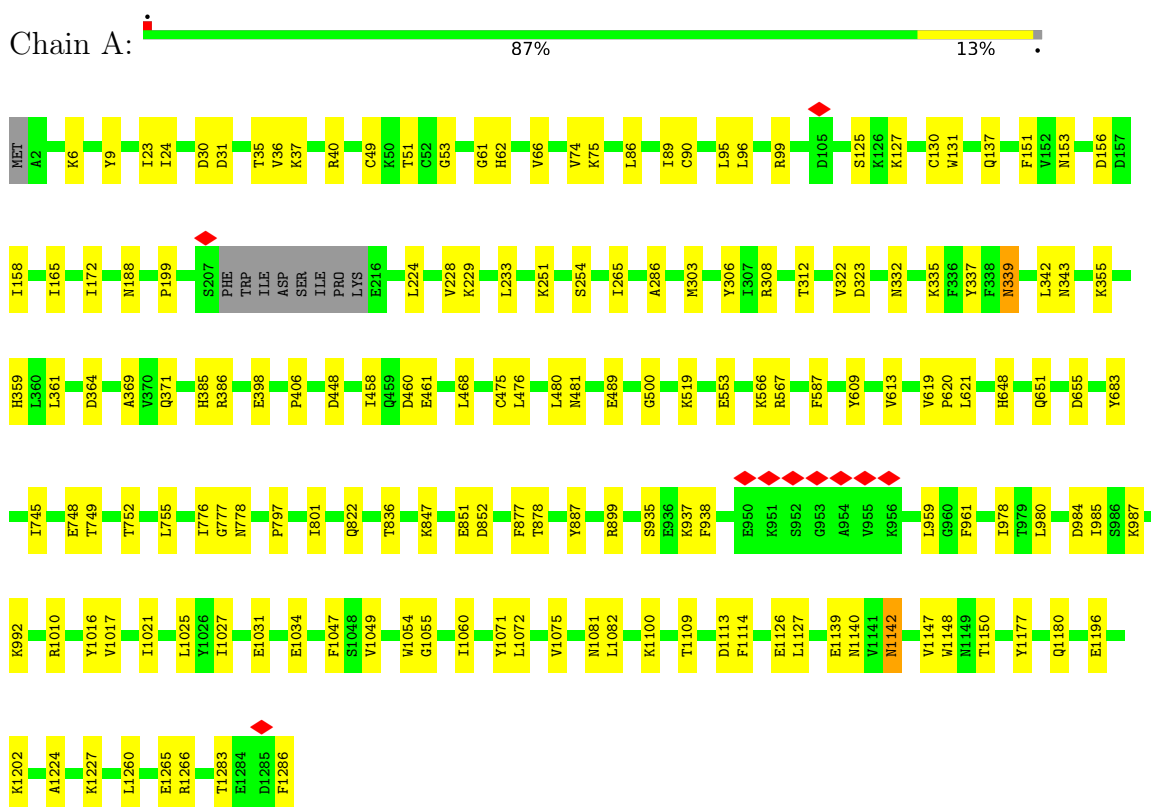
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

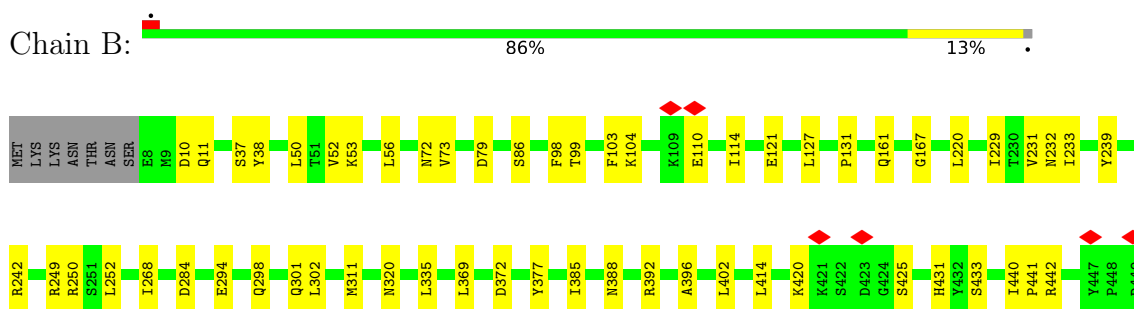
3 Residue-property plots [i](#)

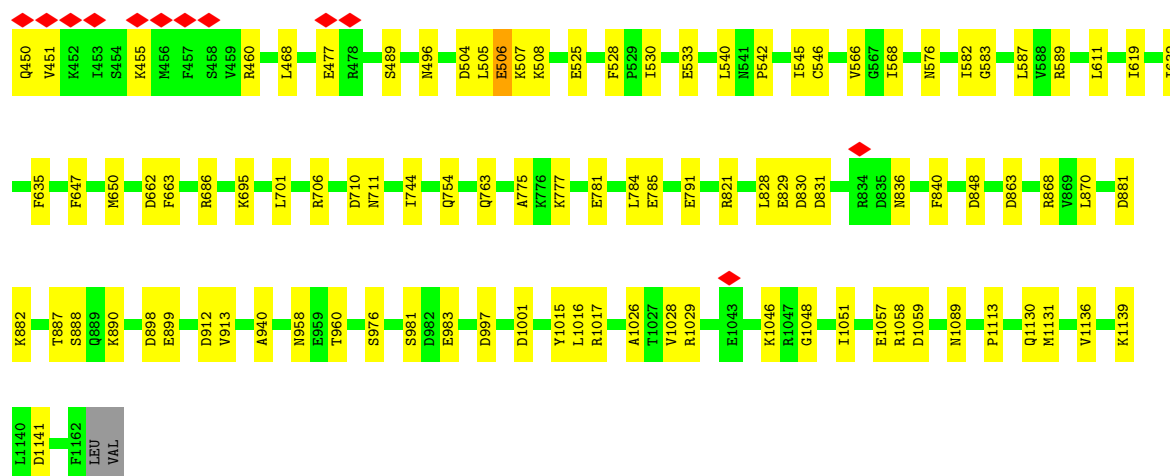
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 147 kDa polypeptide

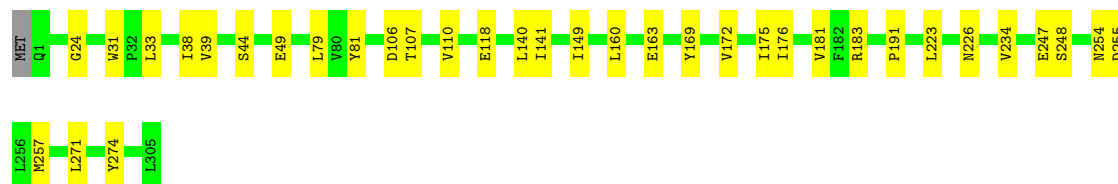
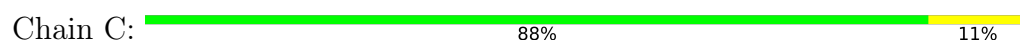


- Molecule 2: DNA-directed RNA polymerase 133 kDa polypeptide

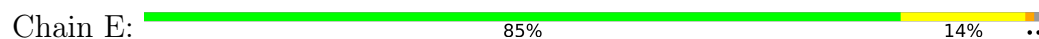




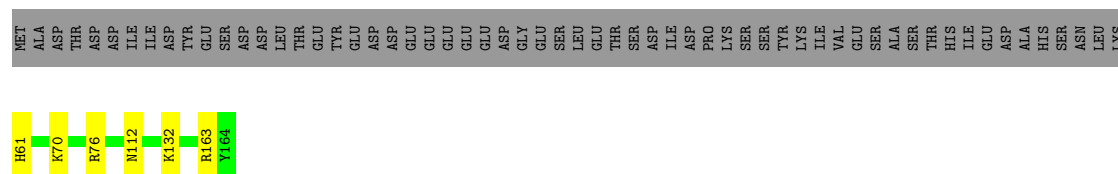
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit



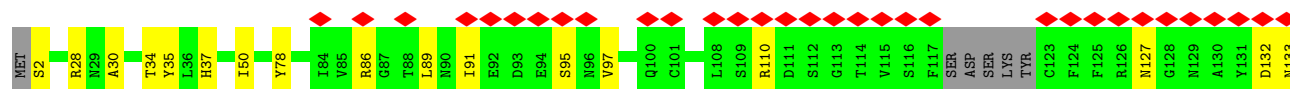
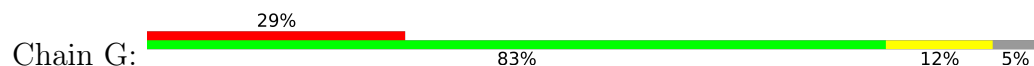
- Molecule 4: DNA-directed RNA polymerase 22 kDa subunit

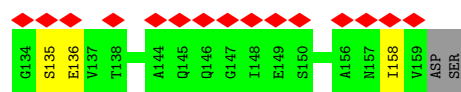


- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

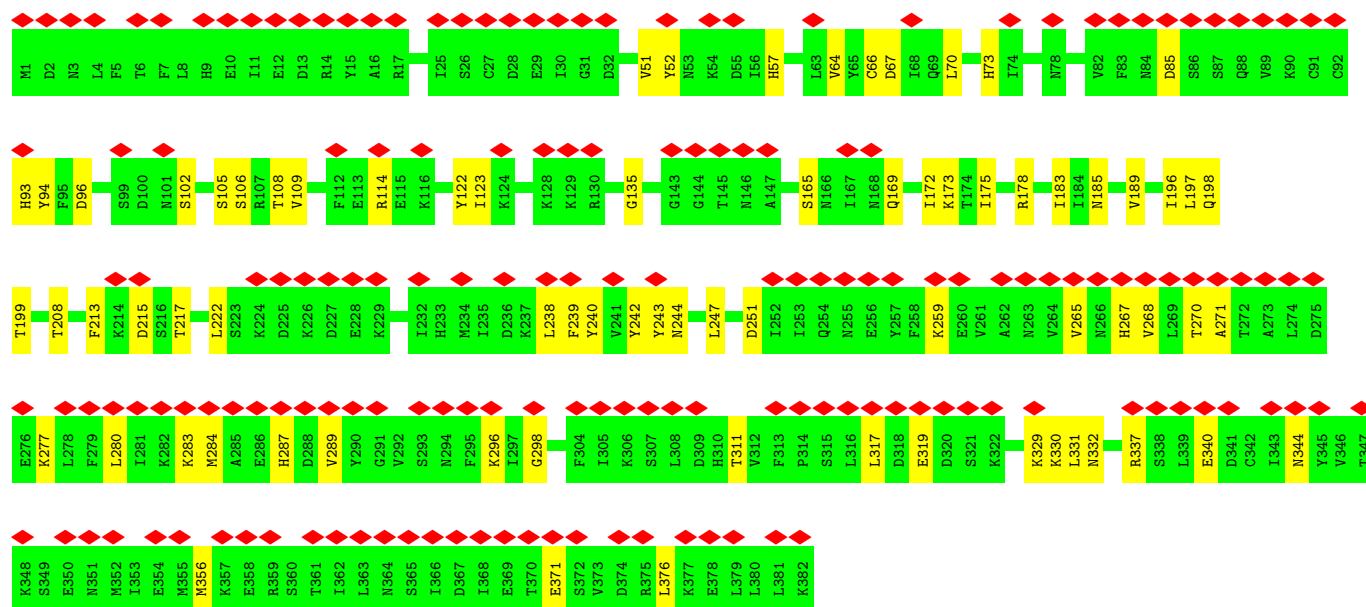
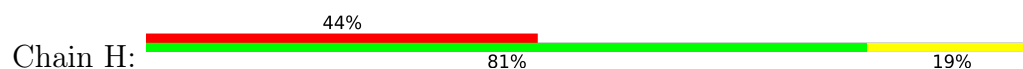


- Molecule 6: DNA-directed RNA polymerase 18 kDa subunit



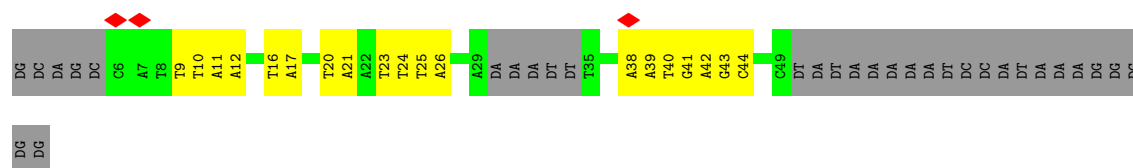


• Molecule 7: Intermediate transcription factor 3 large subunit



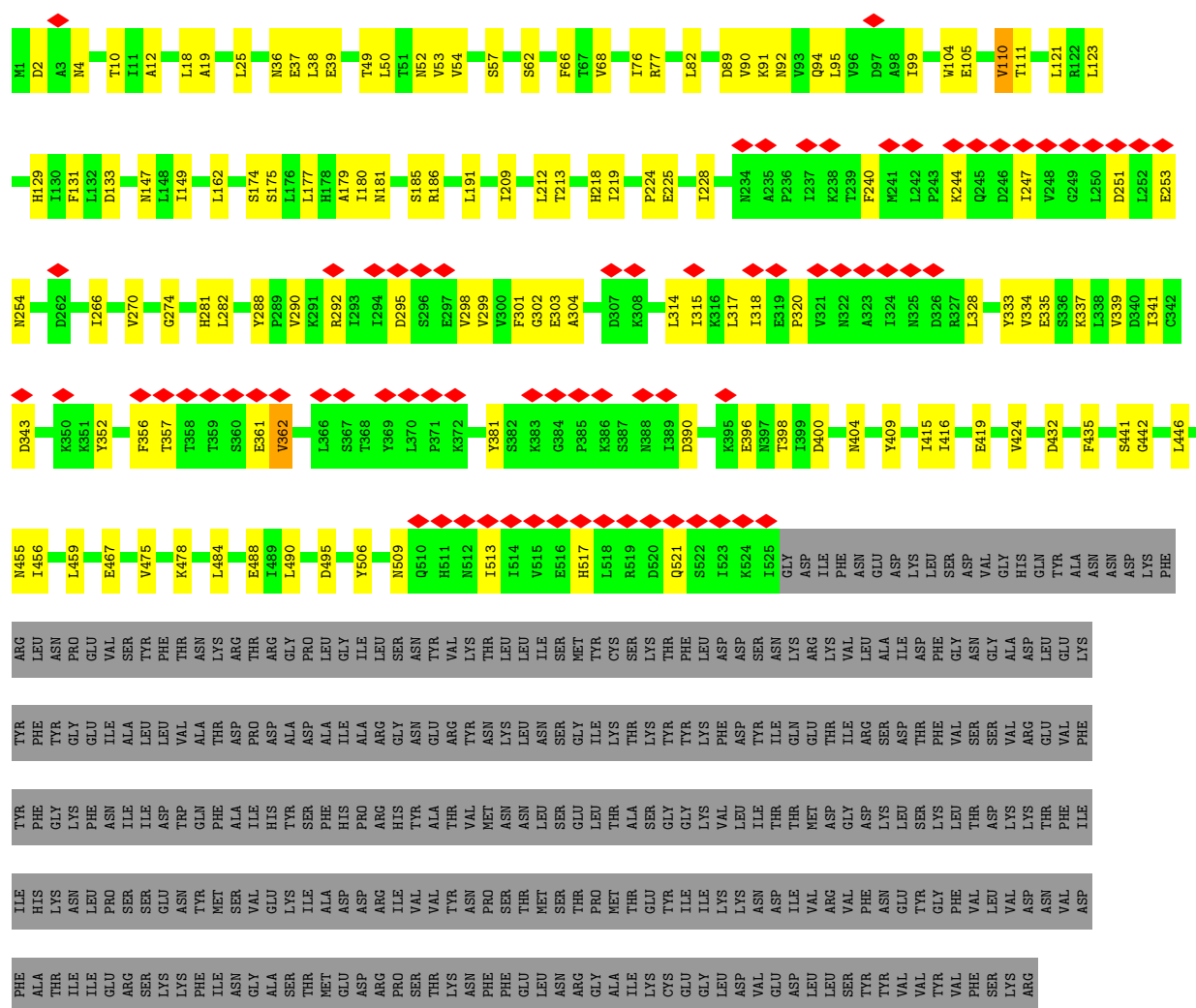
- Molecule 10: Non-template DNA oligomer

Chain N: 



- Molecule 11: mRNA-capping enzyme catalytic subunit

Chain O: 

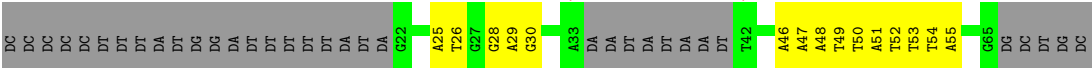
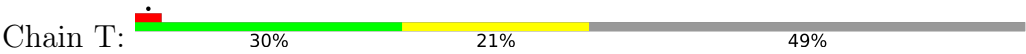


- Molecule 12: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S: 



● Molecule 13: Template DNA oligomer



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1052532	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.854	Depositor
Minimum map value	-0.364	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	408.38403, 408.38403, 408.38403	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/10462	0.36	0/14135
2	B	0.30	0/9525	0.37	0/12866
3	C	0.34	0/2540	0.38	0/3440
4	E	0.33	0/1522	0.36	0/2069
5	F	0.35	0/874	0.38	0/1173
6	G	0.24	0/1209	0.34	0/1639
7	H	0.14	0/3189	0.29	0/4288
8	I	0.15	0/2315	0.31	0/3123
9	J	0.33	0/494	0.37	0/663
10	N	0.22	0/889	0.47	0/1365
11	O	0.20	0/4328	0.26	0/5863
12	S	0.21	0/970	0.34	0/1298
13	T	0.24	0/845	0.45	0/1303
All	All	0.28	0/39162	0.35	0/53225

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 [i](#)

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	10260	10357	10377	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9319	9340	9359	102	0
3	C	2484	2463	2473	26	0
4	E	1495	1546	1548	19	0
5	F	859	877	881	3	0
6	G	1192	1178	1181	12	0
7	H	3134	3164	3176	51	0
8	I	2270	2293	2299	32	0
9	J	490	527	528	6	0
10	N	794	442	444	20	0
11	O	4242	4335	4345	85	0
12	S	955	961	961	14	0
13	T	752	409	411	24	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	J	1	0	0	0	0
All	All	38251	37892	37983	450	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 (450) 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)
2:B:239:TYR:O	2:B:242:ARG:NH1	1.93	1.01
1:A:745:ILE:O	1:A:749:THR:OG1	1.95	0.85
11:O:52:ASN:ND2	11:O:219:ILE:O	2.12	0.83
11:O:181:ASN:O	11:O:404:ASN:ND2	2.12	0.82
11:O:77:ARG:NH1	11:O:105:GLU:OE2	2.13	0.82
11:O:253:GLU:OE1	11:O:253:GLU:N	2.14	0.81
1:A:303:MET:O	1:A:308:ARG:NH1	2.15	0.79
6:G:86:ARG:NH1	6:G:136:GLU:OE1	2.17	0.78
11:O:89:ASP:O	11:O:174:SER:OG	2.02	0.77
7:H:283:LYS:O	7:H:287:HIS:ND1	2.17	0.77
11:O:292:ARG:NH2	11:O:337:LYS:O	2.18	0.76
1:A:937:LYS:NZ	1:A:1177:TYR:OH	2.19	0.74
3:C:33:LEU:HD12	3:C:181:VAL:HG12	1.70	0.74
1:A:822:GLN:NE2	4:E:167:ASN:OD1	2.20	0.73
2:B:301:GLN:N	2:B:301:GLN:OE1	2.21	0.73
11:O:49:THR:HG21	11:O:191:LEU:HD22	1.69	0.73
2:B:887:THR:O	2:B:888:SER:OG	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:ARG:NH2	2:B:1059:ASP:OD1	2.22	0.73
11:O:301:PHE:HB2	11:O:318:ILE:HD11	1.70	0.72
2:B:242:ARG:NH2	2:B:284:ASP:OD2	2.23	0.72
8:I:69:GLU:OE2	8:I:166:ARG:NH2	2.23	0.72
7:H:96:ASP:OD1	7:H:178:ARG:NH2	2.23	0.72
8:I:231:VAL:O	8:I:235:ASP:N	2.23	0.71
11:O:251:ASP:OD1	11:O:381:TYR:OH	2.09	0.70
7:H:215:ASP:OD2	7:H:217:THR:OG1	2.08	0.70
1:A:461:GLU:OE2	1:A:566:LYS:NZ	2.24	0.70
7:H:267:HIS:O	7:H:270:THR:OG1	2.09	0.70
8:I:155:GLU:N	8:I:155:GLU:OE1	2.23	0.70
11:O:53:VAL:O	11:O:57:SER:N	2.26	0.69
2:B:830:ASP:OD1	2:B:831:ASP:N	2.26	0.69
2:B:958:ASN:ND2	2:B:960:THR:O	2.25	0.69
1:A:153:ASN:ND2	1:A:156:ASP:OD1	2.26	0.69
11:O:180:ILE:O	11:O:478:LYS:NZ	2.25	0.68
11:O:400:ASP:N	11:O:509:ASN:OD1	2.24	0.68
11:O:357:THR:N	11:O:361:GLU:OE2	2.27	0.68
1:A:553:GLU:N	1:A:553:GLU:OE1	2.27	0.68
1:A:851:GLU:OE1	1:A:899:ARG:NE	2.27	0.68
7:H:135:GLY:N	10:N:24:DT:OP1	2.27	0.67
7:H:298:GLY:O	7:H:337:ARG:NE	2.28	0.67
8:I:15:GLU:O	11:O:409:TYR:N	2.27	0.67
2:B:294:GLU:OE2	2:B:298:GLN:NE2	2.27	0.66
3:C:247:GLU:O	3:C:248:SER:OG	2.12	0.66
1:A:1075:VAL:O	1:A:1081:ASN:ND2	2.28	0.66
2:B:121:GLU:N	2:B:121:GLU:OE1	2.28	0.66
1:A:1196:GLU:OE2	1:A:1202:LYS:N	2.29	0.66
2:B:940:ALA:O	2:B:976:SER:OG	2.13	0.65
7:H:51:VAL:O	7:H:57:HIS:NE2	2.27	0.65
2:B:711:ASN:OD1	2:B:777:LYS:N	2.28	0.65
2:B:763:GLN:OE1	2:B:763:GLN:N	2.30	0.64
6:G:30:ALA:O	6:G:34:THR:HG22	1.97	0.64
1:A:619:VAL:HG21	1:A:1025:LEU:HD12	1.79	0.64
7:H:85:ASP:O	7:H:114:ARG:NH1	2.31	0.64
3:C:163:GLU:OE1	3:C:163:GLU:N	2.30	0.63
8:I:127:LYS:O	8:I:130:LYS:NZ	2.31	0.63
4:E:129:GLN:O	5:F:70:LYS:NZ	2.32	0.63
1:A:1100:LYS:NZ	12:S:65:GLU:O	2.32	0.63
12:S:99:GLU:OE1	12:S:99:GLU:N	2.31	0.62
9:J:17:GLU:OE1	9:J:17:GLU:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:196:ILE:O	7:H:199:THR:OG1	2.17	0.62
8:I:130:LYS:NZ	8:I:133:SER:OG	2.23	0.62
11:O:317:LEU:HD13	11:O:334:VAL:HG21	1.82	0.62
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.81	0.62
7:H:340:GLU:OE2	7:H:344:ASN:ND2	2.33	0.62
6:G:95:SER:OG	6:G:110:ARG:NH1	2.33	0.61
1:A:75:LYS:NZ	1:A:188:ASN:O	2.34	0.61
2:B:848:ASP:OD1	2:B:1046:LYS:NZ	2.34	0.60
6:G:127:ASN:O	6:G:127:ASN:ND2	2.34	0.60
3:C:172:VAL:O	3:C:176:ILE:N	2.33	0.60
11:O:90:VAL:HG11	11:O:95:LEU:HD21	1.83	0.60
1:A:801:ILE:O	1:A:887:TYR:OH	2.04	0.60
1:A:1060:ILE:O	12:S:130:LYS:NZ	2.34	0.60
2:B:455:LYS:O	2:B:460:ARG:NH1	2.35	0.59
2:B:781:GLU:OE1	2:B:781:GLU:N	2.35	0.59
6:G:28:ARG:HG2	6:G:50:ILE:HD12	1.83	0.59
7:H:371:GLU:HB3	7:H:376:LEU:HD21	1.84	0.59
2:B:533:GLU:OE2	2:B:583:GLY:N	2.34	0.59
7:H:108:THR:OG1	7:H:185:ASN:O	2.20	0.59
7:H:268:VAL:HG22	7:H:280:LEU:HB3	1.84	0.59
8:I:167:ASP:OD1	8:I:168:GLU:N	2.33	0.59
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	1.85	0.59
2:B:706:ARG:NH1	3:C:44:SER:O	2.36	0.59
2:B:533:GLU:OE2	2:B:582:ILE:N	2.30	0.58
2:B:829:GLU:OE2	2:B:836:ASN:ND2	2.37	0.58
7:H:268:VAL:HG21	7:H:284:MET:SD	2.43	0.58
11:O:179:ALA:O	11:O:185:SER:OG	2.12	0.58
11:O:419:GLU:OE1	11:O:419:GLU:N	2.34	0.58
7:H:329:LYS:NZ	8:I:201:ASP:OD2	2.30	0.58
1:A:369:ALA:O	1:A:371:GLN:NE2	2.37	0.57
6:G:89:LEU:N	6:G:135:SER:O	2.28	0.57
2:B:377:TYR:OH	2:B:402:LEU:O	2.22	0.57
11:O:398:THR:HG22	11:O:484:LEU:HD23	1.85	0.57
11:O:12:ALA:N	11:O:224:PRO:O	2.36	0.57
1:A:1283:THR:HG21	11:O:218:HIS:ND1	2.20	0.57
2:B:686:ARG:NH2	2:B:888:SER:O	2.38	0.57
4:E:115:ARG:NH2	4:E:152:LEU:O	2.37	0.57
7:H:93:HIS:O	7:H:178:ARG:NH1	2.37	0.57
3:C:106:ASP:OD1	3:C:107:THR:N	2.38	0.56
11:O:62:SER:HB2	11:O:82:LEU:HD12	1.87	0.56
13:T:52:DT:H72	13:T:53:DT:H73	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:GLU:OE1	3:C:49:GLU:N	2.36	0.56
8:I:196:ILE:HD13	8:I:286:TYR:CZ	2.41	0.56
5:F:112:ASN:ND2	5:F:163:ARG:O	2.39	0.56
11:O:396:GLU:OE1	11:O:521:GLN:NE2	2.38	0.56
2:B:898:ASP:OD1	2:B:899:GLU:N	2.40	0.56
7:H:330:LYS:O	7:H:332:ASN:ND2	2.39	0.56
11:O:225:GLU:OE1	11:O:225:GLU:N	2.28	0.55
1:A:984:ASP:OD1	1:A:985:ILE:N	2.39	0.55
1:A:987:LYS:NZ	1:A:1139:GLU:O	2.38	0.55
3:C:172:VAL:O	3:C:175:ILE:N	2.39	0.55
1:A:86:LEU:HD21	1:A:165:ILE:HG23	1.89	0.55
6:G:34:THR:HG23	6:G:35:TYR:CD2	2.42	0.55
2:B:388:ASN:ND2	2:B:396:ALA:O	2.39	0.55
3:C:31:TRP:O	3:C:183:ARG:N	2.40	0.55
4:E:77:ASP:OD1	4:E:78:TYR:N	2.40	0.55
7:H:271:ALA:O	7:H:277:LYS:NZ	2.34	0.55
1:A:130:CYS:N	1:A:137:GLN:O	2.39	0.54
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.39	0.54
11:O:62:SER:OG	11:O:455:ASN:O	2.17	0.54
11:O:299:VAL:HG12	11:O:318:ILE:HD12	1.89	0.54
4:E:91:GLY:O	4:E:150:LYS:NZ	2.40	0.54
11:O:314:LEU:HD12	11:O:314:LEU:H	1.71	0.54
1:A:66:VAL:HG11	1:A:228:VAL:HG22	1.89	0.54
1:A:978:ILE:N	1:A:978:ILE:HD12	2.23	0.54
8:I:91:ILE:HD12	8:I:91:ILE:H	1.72	0.54
10:N:9:DT:H2'	10:N:10:DT:H72	1.90	0.54
1:A:1142:ASN:ND2	4:E:107:SER:O	2.41	0.53
2:B:587:LEU:HD12	2:B:632:ILE:HD12	1.89	0.53
6:G:2:SER:O	6:G:78:TYR:N	2.36	0.53
6:G:132:ASP:OD1	6:G:133:ASN:N	2.41	0.53
11:O:441:SER:OG	11:O:442:GLY:N	2.41	0.53
11:O:400:ASP:O	11:O:509:ASN:N	2.39	0.53
2:B:372:ASP:OD2	2:B:420:LYS:NZ	2.39	0.53
11:O:244:LYS:O	11:O:247:ILE:HG22	2.08	0.53
13:T:48:DA:H2'	13:T:49:DT:H72	1.90	0.53
11:O:76:ILE:HD12	11:O:76:ILE:N	2.23	0.53
11:O:149:ILE:HD12	11:O:149:ILE:N	2.24	0.53
1:A:1054:TRP:NE1	12:S:90:ASN:O	2.42	0.53
2:B:229:ILE:HG23	2:B:311:MET:SD	2.49	0.53
11:O:38:LEU:HD11	11:O:121:LEU:HD11	1.90	0.53
1:A:460:ASP:N	1:A:460:ASP:OD1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:ASN:O	4:E:3:GLN:HB3	2.10	0.52
2:B:505:LEU:HD21	2:B:566:VAL:HG22	1.92	0.52
11:O:177:LEU:O	11:O:181:ASN:ND2	2.43	0.52
9:J:18:ARG:NH2	9:J:47:GLN:OE1	2.39	0.52
1:A:398:GLU:OE1	1:A:398:GLU:N	2.35	0.52
3:C:33:LEU:HD12	3:C:181:VAL:CG1	2.38	0.52
1:A:475:CYS:SG	1:A:476:LEU:N	2.82	0.52
1:A:61:GLY:HA3	1:A:199:PRO:HB3	1.92	0.52
2:B:72:ASN:ND2	2:B:72:ASN:O	2.42	0.52
2:B:110:GLU:OE1	2:B:110:GLU:N	2.41	0.52
2:B:369:LEU:HD12	2:B:414:LEU:HD22	1.91	0.52
2:B:468:LEU:HD23	2:B:635:PHE:CZ	2.45	0.52
7:H:94:TYR:CG	7:H:123:ILE:HG21	2.45	0.52
1:A:30:ASP:OD1	1:A:31:ASP:N	2.43	0.52
1:A:49:CYS:O	1:A:53:GLY:N	2.41	0.51
7:H:105:SER:O	7:H:109:VAL:HG23	2.10	0.51
1:A:359:HIS:HB3	1:A:361:LEU:HD13	1.93	0.51
1:A:1055:GLY:HA3	12:S:94:ILE:HB	1.92	0.51
1:A:1180:GLN:N	1:A:1180:GLN:OE1	2.41	0.51
3:C:169:TYR:HA	3:C:172:VAL:HG22	1.91	0.51
7:H:66:CYS:O	7:H:198:GLN:N	2.43	0.51
1:A:1286:PHE:O	11:O:288:TYR:OH	2.28	0.51
2:B:38:TYR:OH	2:B:131:PRO:O	2.25	0.51
10:N:41:DG:H1'	13:T:29:DA:N6	2.25	0.51
11:O:2:ASP:OD2	11:O:4:ASN:ND2	2.43	0.51
13:T:50:DT:H2''	13:T:51:DA:N7	2.26	0.50
1:A:90:CYS:N	1:A:95:LEU:O	2.37	0.50
1:A:1126:GLU:O	1:A:1127:LEU:HD12	2.11	0.50
3:C:81:TYR:CE1	3:C:160:LEU:HD21	2.46	0.50
1:A:481:ASN:O	1:A:567:ARG:NH2	2.36	0.50
1:A:1265:GLU:OE1	1:A:1266:ARG:N	2.44	0.50
2:B:52:VAL:HG23	2:B:53:LYS:H	1.76	0.50
10:N:42:DA:C8	13:T:29:DA:C6	3.00	0.50
1:A:224:LEU:O	1:A:228:VAL:HG23	2.12	0.50
3:C:79:LEU:C	3:C:79:LEU:HD23	2.37	0.50
11:O:274:GLY:HA2	11:O:290:VAL:HG23	1.93	0.49
1:A:755:LEU:HD23	1:A:961:PHE:CE1	2.47	0.49
4:E:1:MET:N	4:E:65:ASN:OD1	2.43	0.49
11:O:270:VAL:HG12	11:O:298:VAL:O	2.12	0.49
1:A:265:ILE:HD13	2:B:1130:GLN:HG2	1.93	0.49
8:I:114:ILE:O	8:I:118:PHE:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:239:PHE:HD1	7:H:265:VAL:HG13	1.78	0.49
11:O:301:PHE:CB	11:O:318:ILE:HD11	2.39	0.49
1:A:386:ARG:NH2	1:A:448:ASP:OD1	2.45	0.49
11:O:186:ARG:NH2	11:O:506:TYR:O	2.43	0.49
12:S:142:VAL:HG23	12:S:144:TYR:CE2	2.47	0.49
2:B:997:ASP:O	2:B:1001:ASP:N	2.44	0.49
3:C:149:ILE:HD12	3:C:149:ILE:N	2.28	0.49
1:A:1060:ILE:N	1:A:1060:ILE:HD12	2.28	0.49
3:C:24:GLY:HA3	3:C:223:LEU:HD21	1.94	0.49
9:J:9:THR:O	9:J:10:CYS:SG	2.71	0.49
10:N:21:DA:C2	13:T:51:DA:C2	3.00	0.49
2:B:1089:ASN:HB2	2:B:1113:PRO:HB3	1.93	0.49
7:H:238:LEU:HD21	7:H:242:TYR:CZ	2.47	0.49
2:B:388:ASN:O	2:B:392:ARG:N	2.41	0.49
2:B:662:ASP:OD1	2:B:663:PHE:N	2.45	0.48
11:O:89:ASP:OD1	11:O:89:ASP:N	2.44	0.48
11:O:290:VAL:HG13	11:O:341:ILE:HG12	1.95	0.48
1:A:776:ILE:HG23	1:A:777:GLY:H	1.79	0.48
1:A:778:ASN:OD1	4:E:138:ARG:NH2	2.45	0.48
1:A:992:LYS:NZ	1:A:1031:GLU:OE1	2.42	0.48
11:O:18:LEU:HD23	11:O:121:LEU:HD13	1.94	0.48
2:B:450:GLN:HG2	10:N:38:DA:H2''	1.95	0.48
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.47	0.48
10:N:11:DA:H2'	10:N:12:DA:C8	2.48	0.48
2:B:785:GLU:OE2	8:I:56:ARG:NH2	2.38	0.48
2:B:863:ASP:OD1	2:B:863:ASP:N	2.47	0.48
4:E:5:ASN:HB2	4:E:100:LEU:HB3	1.95	0.48
6:G:158:ILE:HD12	6:G:158:ILE:H	1.79	0.48
7:H:196:ILE:HD11	13:T:54:DT:N3	2.29	0.48
2:B:10:ASP:OD1	2:B:11:GLN:N	2.47	0.48
7:H:240:TYR:O	7:H:244:ASN:ND2	2.38	0.48
11:O:147:ASN:ND2	11:O:456:ILE:O	2.47	0.48
8:I:88:LYS:HD3	13:T:49:DT:O4'	2.13	0.48
11:O:66:PHE:CD1	11:O:99:ILE:HD11	2.49	0.48
2:B:477:GLU:N	2:B:477:GLU:OE1	2.47	0.47
2:B:710:ASP:OD1	2:B:711:ASN:N	2.46	0.47
2:B:784:LEU:HD13	2:B:784:LEU:O	2.14	0.47
13:T:47:DA:H1'	13:T:48:DA:OP2	2.14	0.47
13:T:48:DA:O4'	13:T:48:DA:OP2	2.32	0.47
7:H:208:THR:HG23	7:H:222:LEU:HA	1.95	0.47
11:O:298:VAL:HG13	11:O:317:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:328:LEU:HD13	11:O:352:TYR:CE2	2.49	0.47
4:E:117:ASP:OD1	4:E:118:THR:N	2.46	0.47
11:O:335:GLU:O	11:O:339:VAL:HG13	2.15	0.47
1:A:1286:PHE:CE2	11:O:282:LEU:HD11	2.49	0.47
2:B:506:GLU:OE1	2:B:507:LYS:N	2.47	0.47
12:S:142:VAL:HG23	12:S:144:TYR:CZ	2.49	0.47
2:B:50:LEU:HD12	2:B:73:VAL:HG11	1.96	0.47
3:C:110:VAL:HG23	3:C:110:VAL:O	2.14	0.47
2:B:99:THR:HG23	2:B:121:GLU:HG3	1.95	0.47
2:B:161:GLN:N	2:B:161:GLN:OE1	2.48	0.47
3:C:38:ILE:HG13	3:C:172:VAL:HG21	1.96	0.47
8:I:231:VAL:HG13	8:I:236:SER:O	2.15	0.47
11:O:91:LYS:N	11:O:94:GLN:OE1	2.34	0.47
2:B:1051:ILE:N	2:B:1051:ILE:HD12	2.30	0.47
7:H:268:VAL:HA	7:H:280:LEU:HD13	1.97	0.47
1:A:852:ASP:OD1	1:A:852:ASP:N	2.48	0.46
11:O:10:THR:HG21	11:O:225:GLU:O	2.15	0.46
1:A:613:VAL:HG13	1:A:620:PRO:HG3	1.97	0.46
1:A:877:PHE:O	1:A:878:THR:OG1	2.28	0.46
7:H:376:LEU:HD22	8:I:195:LEU:CD1	2.46	0.46
2:B:775:ALA:HB1	2:B:870:LEU:HD11	1.98	0.46
8:I:92:ILE:C	8:I:92:ILE:HD12	2.41	0.46
10:N:43:DG:H2"	10:N:44:DC:C6	2.50	0.46
11:O:110:VAL:HG23	11:O:111:THR:HG22	1.98	0.46
1:A:23:ILE:N	1:A:23:ILE:HD12	2.31	0.46
2:B:86:SER:O	2:B:868:ARG:NH2	2.49	0.46
11:O:432:ASP:N	11:O:435:PHE:O	2.45	0.46
1:A:619:VAL:CG2	1:A:1025:LEU:HD12	2.44	0.46
1:A:1021:ILE:N	1:A:1021:ILE:HD12	2.31	0.46
3:C:254:ASN:HA	3:C:271:LEU:O	2.15	0.46
1:A:265:ILE:HD11	2:B:1131:MET:HE3	1.98	0.46
11:O:37:GLU:O	11:O:123:LEU:HD12	2.16	0.46
12:S:117:PHE:CE2	12:S:121:LEU:HD11	2.51	0.46
1:A:587:PHE:CZ	1:A:648:HIS:HB2	2.50	0.46
7:H:319:GLU:OE1	7:H:319:GLU:N	2.42	0.46
10:N:26:DA:C2	13:T:46:DA:C2	3.04	0.46
11:O:92:ASN:ND2	11:O:175:SER:OG	2.47	0.46
11:O:266:ILE:HG21	11:O:304:ALA:HB2	1.98	0.46
13:T:51:DA:C4	13:T:52:DT:C4	3.04	0.46
7:H:52:TYR:N	7:H:251:ASP:OD2	2.49	0.46
1:A:40:ARG:O	1:A:51:THR:OG1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG22	1:A:96:LEU:HD23	1.98	0.46
1:A:156:ASP:OD1	1:A:156:ASP:N	2.49	0.46
1:A:312:THR:HG22	1:A:335:LYS:HD2	1.97	0.46
2:B:252:LEU:HD11	2:B:335:LEU:HD23	1.98	0.46
1:A:24:ILE:HD12	1:A:35:THR:O	2.15	0.45
11:O:356:PHE:CG	11:O:362:VAL:HG12	2.51	0.45
11:O:513:ILE:O	11:O:517:HIS:ND1	2.35	0.45
4:E:1:MET:SD	4:E:46:THR:OG1	2.75	0.45
8:I:126:SER:HB2	13:T:51:DA:OP2	2.17	0.45
11:O:343:ASP:OD1	11:O:343:ASP:N	2.50	0.45
1:A:74:VAL:HG21	1:A:151:PHE:HE2	1.81	0.45
6:G:91:ILE:HG12	6:G:97:VAL:HG13	1.99	0.45
1:A:460:ASP:OD1	2:B:754:GLN:NE2	2.46	0.45
1:A:1140:ASN:HA	4:E:106:ILE:HD12	1.98	0.45
2:B:542:PRO:HA	2:B:545:ILE:HD13	1.97	0.45
10:N:23:DT:H2'	10:N:24:DT:H72	1.99	0.45
1:A:337:TYR:OH	1:A:364:ASP:OD2	2.30	0.45
1:A:609:TYR:HH	1:A:621:LEU:H	1.64	0.45
1:A:748:GLU:O	1:A:752:THR:HG23	2.17	0.45
3:C:234:VAL:HG12	3:C:234:VAL:O	2.16	0.45
2:B:647:PHE:HA	2:B:650:MET:HE2	1.98	0.45
7:H:238:LEU:C	7:H:238:LEU:HD23	2.42	0.45
11:O:459:LEU:N	11:O:475:VAL:O	2.46	0.45
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.17	0.45
1:A:797:PRO:HA	1:A:836:THR:O	2.16	0.45
8:I:197:ASN:O	8:I:201:ASP:N	2.49	0.45
9:J:2:VAL:HG12	9:J:2:VAL:O	2.17	0.45
11:O:162:LEU:N	11:O:162:LEU:HD12	2.31	0.45
8:I:8:LEU:HD23	11:O:175:SER:HB2	1.98	0.45
2:B:1057:GLU:OE1	2:B:1057:GLU:N	2.46	0.45
8:I:55:LEU:HD22	8:I:77:VAL:HG21	1.99	0.45
7:H:376:LEU:HB3	8:I:195:LEU:HD11	1.98	0.44
12:S:109:GLY:O	12:S:110:THR:OG1	2.31	0.44
13:T:48:DA:C2'	13:T:49:DT:H72	2.46	0.44
1:A:24:ILE:HB	1:A:66:VAL:HG12	1.97	0.44
1:A:406:PRO:HB3	1:A:458:ILE:HD11	1.99	0.44
2:B:37:SER:OG	2:B:496:ASN:ND2	2.45	0.44
2:B:1001:ASP:O	3:C:191:PRO:O	2.35	0.44
4:E:18:GLU:OE2	4:E:21:ARG:NH2	2.45	0.44
11:O:317:LEU:HD11	11:O:320:PRO:HG3	1.99	0.44
1:A:36:VAL:HG21	1:A:224:LEU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD2	1:A:158:ILE:HD12	2.17	0.44
1:A:1017:VAL:HG22	1:A:1071:TYR:HD1	1.82	0.44
8:I:231:VAL:HG22	8:I:236:SER:C	2.42	0.44
1:A:229:LYS:O	1:A:233:LEU:HD13	2.18	0.44
11:O:424:VAL:HG23	11:O:446:LEU:HD11	2.00	0.44
11:O:467:GLU:OE1	11:O:467:GLU:N	2.36	0.44
2:B:611:LEU:CD1	2:B:619:ILE:HD11	2.47	0.44
11:O:50:LEU:O	11:O:54:VAL:HG23	2.17	0.44
7:H:317:LEU:HD11	7:H:356:MET:CE	2.47	0.44
7:H:284:MET:HE3	7:H:289:VAL:HG11	1.99	0.44
8:I:185:SER:OG	8:I:246:SER:O	2.35	0.44
11:O:68:VAL:HG21	11:O:131:PHE:HE2	1.82	0.44
2:B:545:ILE:HG22	2:B:546:CYS:N	2.33	0.44
7:H:243:TYR:CE2	7:H:247:LEU:HD11	2.53	0.44
1:A:1010:ARG:NH2	1:A:1017:VAL:HG11	2.33	0.44
2:B:530:ILE:HD11	2:B:540:LEU:HB2	2.00	0.43
7:H:70:LEU:HD11	7:H:189:VAL:HG13	2.00	0.43
10:N:16:DT:H2''	10:N:17:DA:N7	2.32	0.43
11:O:39:GLU:O	11:O:121:LEU:HD12	2.18	0.43
2:B:98:PHE:CE1	2:B:127:LEU:HD23	2.52	0.43
8:I:165:ILE:HA	8:I:259:LEU:HB3	2.00	0.43
1:A:89:ILE:HG21	1:A:172:ILE:HD11	2.00	0.43
2:B:52:VAL:HG23	2:B:53:LYS:N	2.32	0.43
2:B:231:VAL:HG22	2:B:232:ASN:N	2.34	0.43
3:C:141:ILE:HD12	3:C:160:LEU:HD11	2.00	0.43
12:S:69:GLU:O	12:S:70:SER:HB3	2.18	0.43
7:H:102:SER:O	7:H:106:SER:N	2.43	0.43
10:N:40:DT:H2''	10:N:41:DG:O4'	2.18	0.43
11:O:240:PHE:N	11:O:390:ASP:O	2.49	0.43
2:B:433:SER:OG	2:B:695:LYS:O	2.24	0.43
2:B:440:ILE:HB	2:B:441:PRO:HD3	2.00	0.43
1:A:339:ASN:O	1:A:343:ASN:N	2.52	0.43
2:B:79:ASP:OD1	2:B:79:ASP:N	2.51	0.43
2:B:505:LEU:HD23	2:B:582:ILE:HB	2.01	0.43
4:E:83:ILE:N	4:E:83:ILE:HD12	2.34	0.43
7:H:213:PHE:CZ	10:N:17:DA:H1'	2.54	0.43
1:A:938:PHE:CD1	1:A:938:PHE:C	2.97	0.43
7:H:67:ASP:HA	7:H:198:GLN:H	1.84	0.43
1:A:1147:VAL:HG13	1:A:1148:TRP:N	2.33	0.43
7:H:122:TYR:CD2	13:T:53:DT:H4'	2.54	0.43
2:B:442:ARG:NH2	2:B:489:SER:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:PHE:CE2	2:B:576:ASN:HA	2.54	0.42
4:E:44:LEU:HD12	4:E:44:LEU:N	2.34	0.42
4:E:166:ARG:O	4:E:173:VAL:O	2.37	0.42
11:O:416:ILE:N	11:O:416:ILE:HD12	2.33	0.42
13:T:25:DA:H2'	13:T:26:DT:H71	2.01	0.42
1:A:1049:VAL:O	1:A:1049:VAL:HG22	2.18	0.42
2:B:504:ASP:OD2	2:B:508:LYS:NZ	2.50	0.42
1:A:9:TYR:O	1:A:1227:LYS:HA	2.19	0.42
1:A:609:TYR:HB2	12:S:147:TYR:HB3	2.01	0.42
1:A:1113:ASP:OD1	1:A:1114:PHE:N	2.44	0.42
2:B:489:SER:OG	2:B:589:ARG:NH1	2.51	0.42
3:C:226:ASN:HB3	3:C:257:MET:HE1	2.01	0.42
9:J:7:CYS:SG	9:J:9:THR:O	2.77	0.42
2:B:56:LEU:HD23	2:B:385:ILE:HD12	2.01	0.42
10:N:43:DG:O6	13:T:28:DG:N3	2.53	0.42
13:T:49:DT:H2''	13:T:50:DT:C6	2.55	0.42
13:T:51:DA:H1'	13:T:52:DT:C5	2.55	0.42
1:A:489:GLU:OE1	1:A:489:GLU:N	2.52	0.42
2:B:451:VAL:HG11	10:N:39:DA:N6	2.34	0.42
4:E:72:THR:HG23	4:E:72:THR:O	2.20	0.42
11:O:298:VAL:CG1	11:O:317:LEU:HD11	2.50	0.42
1:A:265:ILE:HD11	2:B:1131:MET:CE	2.49	0.42
1:A:776:ILE:HG23	1:A:777:GLY:N	2.35	0.42
2:B:912:ASP:OD1	9:J:9:THR:HB	2.20	0.42
3:C:118:GLU:OE1	3:C:118:GLU:N	2.43	0.42
7:H:122:TYR:HA	13:T:54:DT:OP1	2.20	0.42
8:I:88:LYS:O	10:N:25:DT:OP1	2.38	0.42
10:N:9:DT:C2'	10:N:10:DT:H72	2.49	0.42
11:O:484:LEU:HD12	11:O:488:GLU:OE2	2.19	0.42
1:A:322:VAL:HG13	1:A:323:ASP:N	2.35	0.42
1:A:468:LEU:O	1:A:500:GLY:HA3	2.19	0.42
1:A:980:LEU:N	1:A:980:LEU:HD12	2.35	0.42
8:I:222:ILE:HG21	8:I:275:ILE:HD13	2.00	0.42
2:B:220:LEU:HG	2:B:233:ILE:HG22	2.01	0.42
11:O:209:ILE:O	11:O:213:THR:HG23	2.19	0.42
13:T:29:DA:C6	13:T:30:DG:C2	3.08	0.42
6:G:37:HIS:O	6:G:37:HIS:ND1	2.52	0.41
7:H:169:GLN:HB2	7:H:172:ILE:HD12	2.02	0.41
11:O:292:ARG:NH1	11:O:339:VAL:O	2.53	0.41
11:O:495:ASP:OD1	11:O:495:ASP:N	2.52	0.41
1:A:286:ALA:CB	2:B:1028:VAL:HG12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:TRP:O	1:A:1055:GLY:C	2.63	0.41
7:H:64:VAL:HG13	7:H:73:HIS:CE1	2.55	0.41
11:O:36:ASN:HB3	11:O:123:LEU:HD11	2.01	0.41
11:O:254:ASN:O	11:O:381:TYR:HA	2.20	0.41
2:B:1015:TYR:C	2:B:1016:LEU:HD12	2.45	0.41
2:B:1139:LYS:NZ	2:B:1141:ASP:OD2	2.53	0.41
7:H:331:LEU:HD23	7:H:331:LEU:C	2.46	0.41
10:N:20:DT:H2"	10:N:21:DA:C8	2.55	0.41
1:A:286:ALA:HB2	2:B:1028:VAL:HG12	2.03	0.41
1:A:1140:ASN:HA	4:E:106:ILE:CD1	2.51	0.41
2:B:840:PHE:CD2	8:I:21:ILE:HG12	2.55	0.41
7:H:311:THR:HG23	8:I:198:LEU:O	2.20	0.41
11:O:19:ALA:HB2	11:O:212:LEU:HD12	2.02	0.41
1:A:1109:THR:HG23	1:A:1109:THR:O	2.21	0.41
2:B:103:PHE:CD2	2:B:114:ILE:HG23	2.55	0.41
2:B:249:ARG:NH1	2:B:268:ILE:HG21	2.35	0.41
5:F:76:ARG:O	5:F:132:LYS:NZ	2.54	0.41
7:H:331:LEU:HD23	7:H:332:ASN:N	2.36	0.41
8:I:154:PHE:CD1	8:I:190:THR:HG21	2.56	0.41
11:O:266:ILE:HG22	11:O:302:GLY:O	2.20	0.41
13:T:54:DT:H2"	13:T:55:DA:C8	2.55	0.41
2:B:250:ARG:NE	2:B:525:GLU:OE2	2.45	0.41
2:B:568:ILE:O	2:B:568:ILE:HG23	2.21	0.41
2:B:744:ILE:HA	2:B:913:VAL:O	2.21	0.41
2:B:882:LYS:HD3	2:B:890:LYS:HD2	2.03	0.41
3:C:39:VAL:HA	3:C:140:LEU:HD23	2.03	0.41
7:H:197:LEU:HD13	13:T:53:DT:O2	2.21	0.41
1:A:49:CYS:SG	1:A:62:HIS:CD2	3.13	0.41
1:A:125:SER:O	1:A:127:LYS:NZ	2.46	0.41
10:N:42:DA:C5	10:N:43:DG:C5	3.08	0.41
1:A:251:LYS:HA	1:A:254:SER:O	2.21	0.41
1:A:1047:PHE:O	12:S:85:LYS:HA	2.20	0.41
1:A:1147:VAL:O	1:A:1150:THR:HG22	2.21	0.41
11:O:10:THR:HG22	11:O:228:ILE:HG12	2.02	0.41
2:B:302:LEU:N	2:B:302:LEU:HD12	2.36	0.41
2:B:784:LEU:HD13	2:B:784:LEU:C	2.46	0.41
11:O:303:GLU:HG2	11:O:315:ILE:HD12	2.03	0.41
11:O:328:LEU:HD13	11:O:352:TYR:CZ	2.56	0.41
11:O:415:ILE:C	11:O:416:ILE:HD12	2.46	0.41
12:S:117:PHE:CZ	12:S:121:LEU:HD11	2.56	0.41
1:A:6:LYS:HB3	2:B:1141:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLN:NE2	1:A:655:ASP:OD2	2.54	0.40
7:H:122:TYR:HD2	13:T:53:DT:H4'	1.86	0.40
11:O:484:LEU:HG	11:O:490:LEU:HD11	2.04	0.40
12:S:102:THR:O	12:S:102:THR:HG22	2.21	0.40
1:A:99:ARG:HB3	1:A:131:TRP:CE3	2.56	0.40
2:B:167:GLY:HA2	2:B:425:SER:O	2.20	0.40
2:B:791:GLU:CD	2:B:821:ARG:HE	2.29	0.40
2:B:828:LEU:N	2:B:836:ASN:O	2.51	0.40
2:B:981:SER:C	2:B:983:GLU:H	2.29	0.40
3:C:31:TRP:HB3	3:C:183:ARG:HG3	2.02	0.40
8:I:91:ILE:HD12	8:I:91:ILE:N	2.37	0.40
11:O:104:TRP:N	11:O:129:HIS:O	2.54	0.40
1:A:935:SER:HA	1:A:938:PHE:CE2	2.57	0.40
1:A:1016:TYR:CE2	1:A:1082:LEU:HD22	2.56	0.40
8:I:51:ARG:NH1	8:I:80:VAL:O	2.55	0.40
1:A:36:VAL:HG13	1:A:37:LYS:HG3	2.04	0.40
1:A:1027:ILE:HD13	1:A:1034:GLU:HG3	2.02	0.40
7:H:165:SER:OG	7:H:173:LYS:NZ	2.42	0.40
1:A:480:LEU:HD13	3:C:274:TYR:O	2.22	0.40
7:H:109:VAL:HG22	7:H:183:ILE:HD12	2.03	0.40
7:H:175:ILE:N	7:H:175:ILE:HD12	2.36	0.40
8:I:69:GLU:HA	8:I:173:ILE:HD11	2.04	0.40
10:N:43:DG:H2''	10:N:44:DC:N1	2.36	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	1273/1286 (99%)	1231 (97%)	42 (3%)	0	100	100
2	B	1155/1164 (99%)	1113 (96%)	42 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	302/305 (99%)	287 (95%)	15 (5%)	0	100	100
4	E	182/185 (98%)	172 (94%)	10 (6%)	0	100	100
5	F	102/164 (62%)	99 (97%)	3 (3%)	0	100	100
6	G	149/161 (92%)	140 (94%)	9 (6%)	0	100	100
7	H	380/382 (100%)	372 (98%)	8 (2%)	0	100	100
8	I	272/288 (94%)	261 (96%)	11 (4%)	0	100	100
9	J	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
11	O	523/844 (62%)	500 (96%)	23 (4%)	0	100	100
12	S	114/259 (44%)	109 (96%)	5 (4%)	0	100	100
All	All	4511/5101 (88%)	4339 (96%)	172 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1148/1157 (99%)	1136 (99%)	12 (1%)	68	80
2	B	1057/1064 (99%)	1054 (100%)	3 (0%)	86	93
3	C	286/287 (100%)	285 (100%)	1 (0%)	86	93
4	E	174/175 (99%)	173 (99%)	1 (1%)	78	87
5	F	95/151 (63%)	94 (99%)	1 (1%)	65	79
6	G	136/144 (94%)	136 (100%)	0	100	100
7	H	363/363 (100%)	361 (99%)	2 (1%)	78	87
8	I	257/268 (96%)	254 (99%)	3 (1%)	63	78
9	J	60/62 (97%)	59 (98%)	1 (2%)	53	72
11	O	487/774 (63%)	480 (99%)	7 (1%)	59	75
12	S	108/240 (45%)	107 (99%)	1 (1%)	70	82
All	All	4171/4685 (89%)	4139 (99%)	32 (1%)	70	84

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

Mol	Chain	Res	Type
1	A	332	ASN
1	A	339	ASN
1	A	342	LEU
1	A	355	LYS
1	A	385	HIS
1	A	519	LYS
1	A	683	TYR
1	A	847	LYS
1	A	959	LEU
1	A	1072	LEU
1	A	1142	ASN
1	A	1260	LEU
2	B	104	LYS
2	B	320	ASN
2	B	506	GLU
3	C	255	ASP
4	E	106	ILE
5	F	61	HIS
7	H	259	LYS
7	H	296	LYS
8	I	128	LYS
8	I	227	LYS
8	I	231	VAL
9	J	9	THR
11	O	25	LEU
11	O	110	VAL
11	O	133	ASP
11	O	281	HIS
11	O	295	ASP
11	O	333	TYR
11	O	362	VAL
12	S	136	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	589	ASN
1	A	830	GLN
1	A	1275	GLN
2	B	389	HIS

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Mol	Chain	Res	Type
2	B	496	ASN
2	B	779	GLN
2	B	1068	ASN
3	C	228	HIS
4	E	2	ASN
5	F	150	HIS
6	G	80	HIS
6	G	96	ASN
6	G	127	ASN
7	H	23	HIS
7	H	69	GLN
7	H	93	HIS
7	H	185	ASN
7	H	263	ASN
8	I	44	HIS
8	I	123	ASN
8	I	125	HIS
8	I	218	ASN
8	I	229	GLN
8	I	257	ASN
11	O	21	ASN
12	S	62	ASN
12	S	73	ASN
12	S	97	ASN

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 5 ligands modelled in this entry, 5 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.

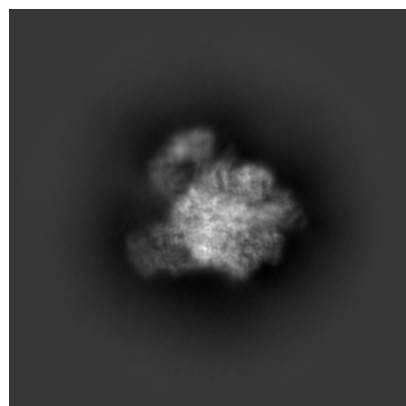
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17335. These allow visual inspection of the internal detail of the map and identification of artifacts.

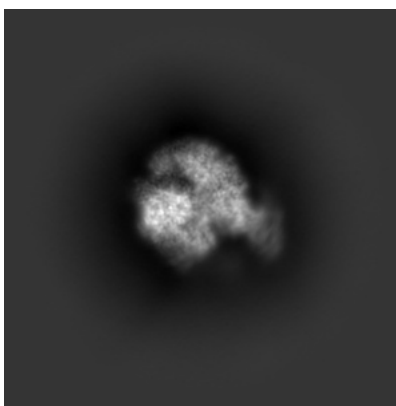
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

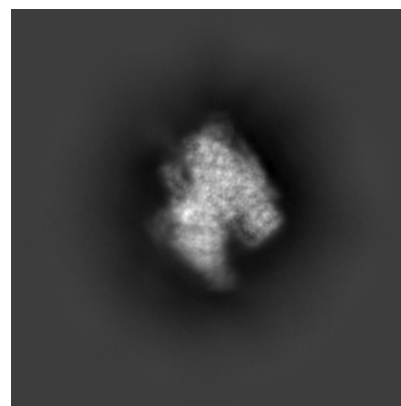
6.1.1 Primary map



X

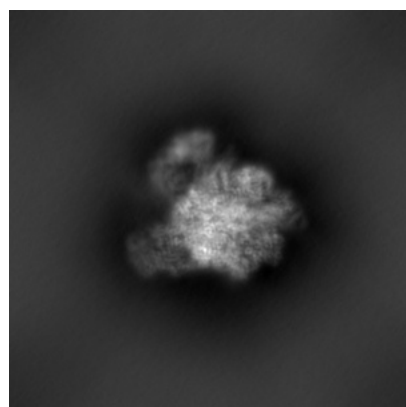


Y

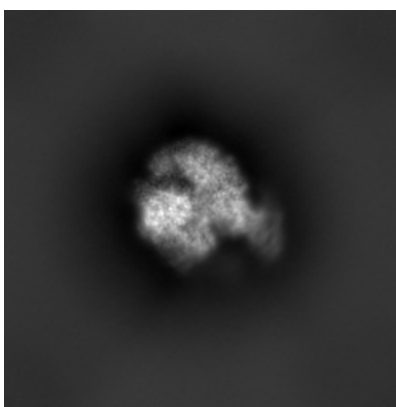


Z

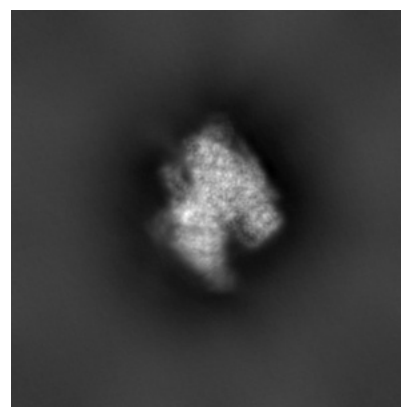
6.1.2 Raw map



X



Y

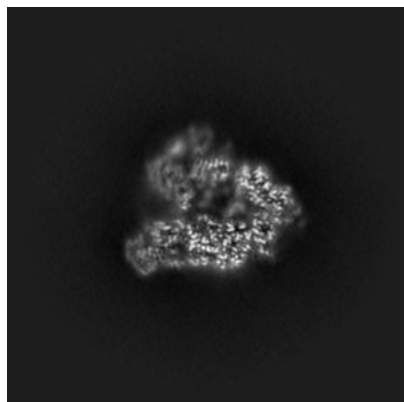


Z

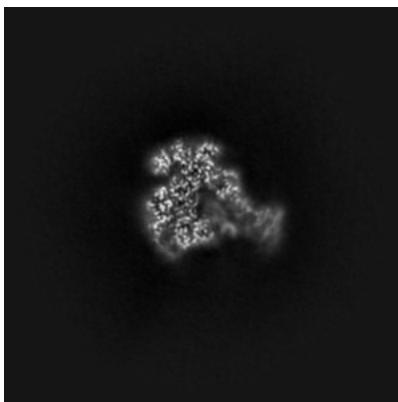
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

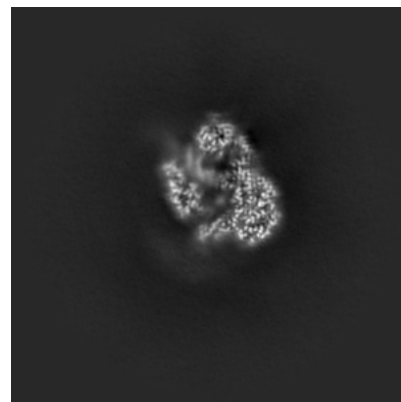
6.2.1 Primary map



X Index: 192

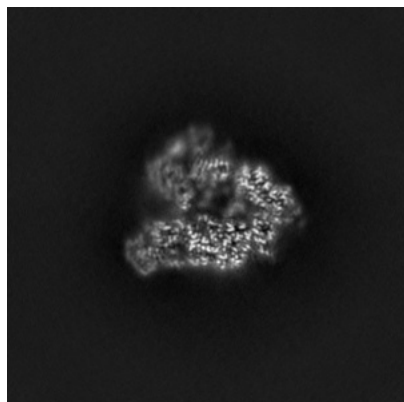


Y Index: 192

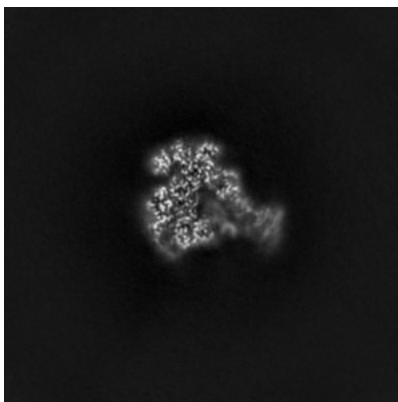


Z Index: 192

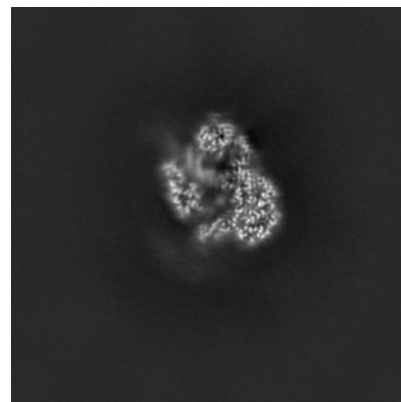
6.2.2 Raw map



X Index: 192



Y Index: 192

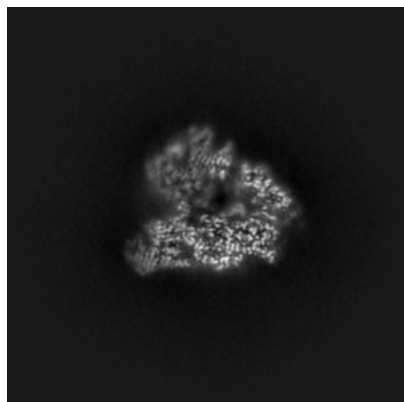


Z Index: 192

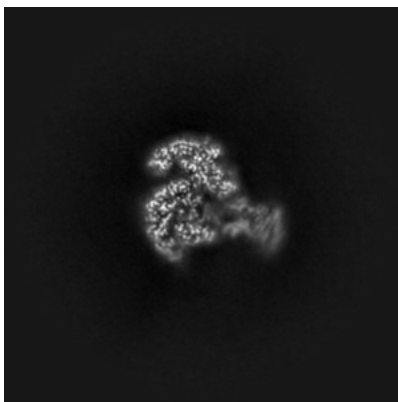
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

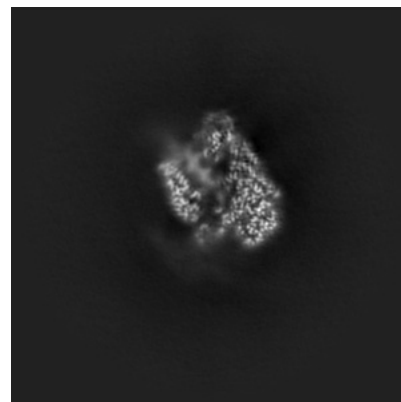
6.3.1 Primary map



X Index: 188

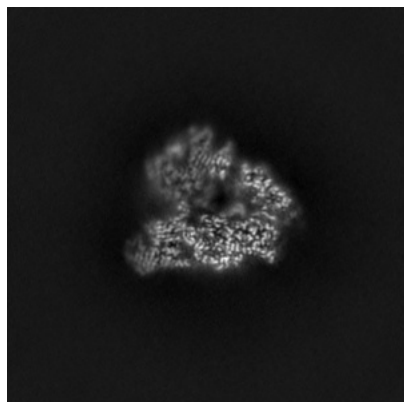


Y Index: 188

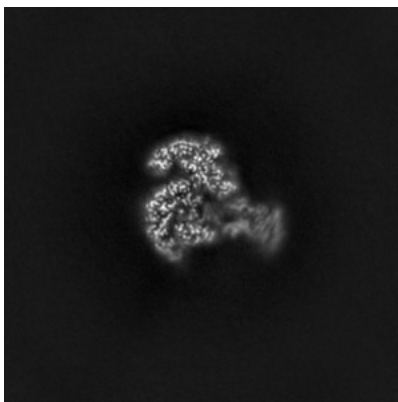


Z Index: 187

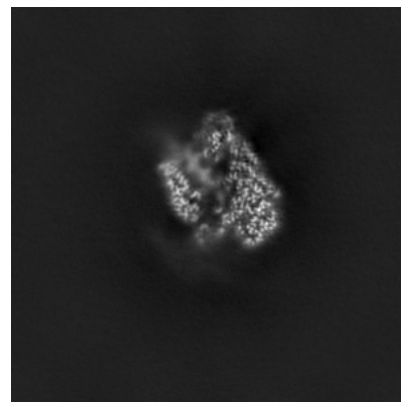
6.3.2 Raw map



X Index: 188



Y Index: 188

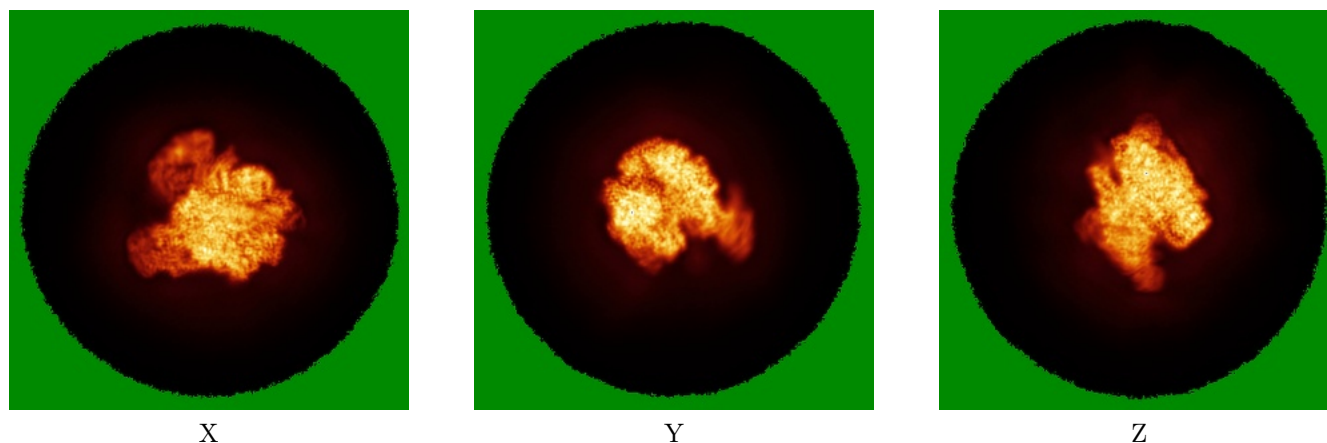


Z Index: 187

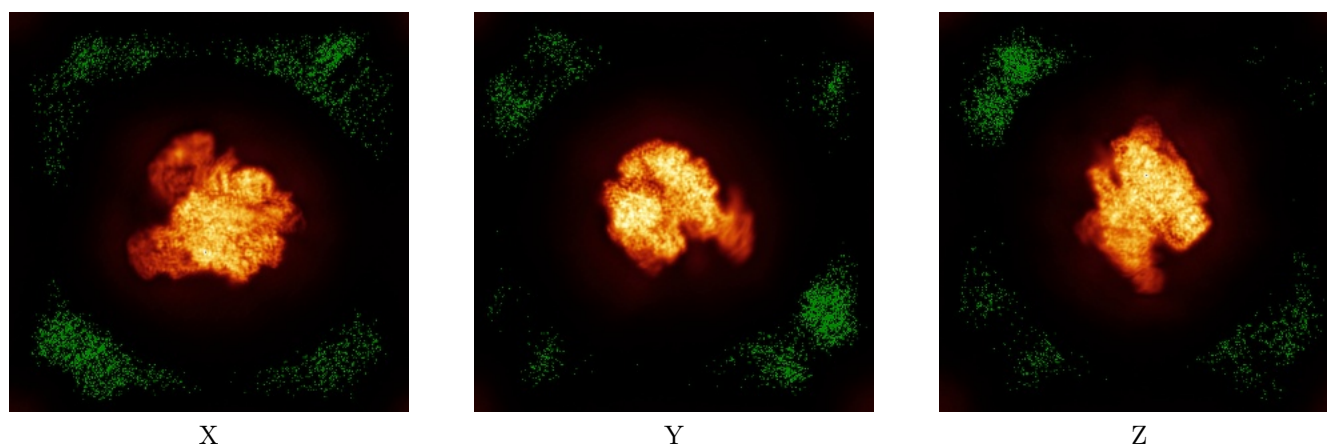
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

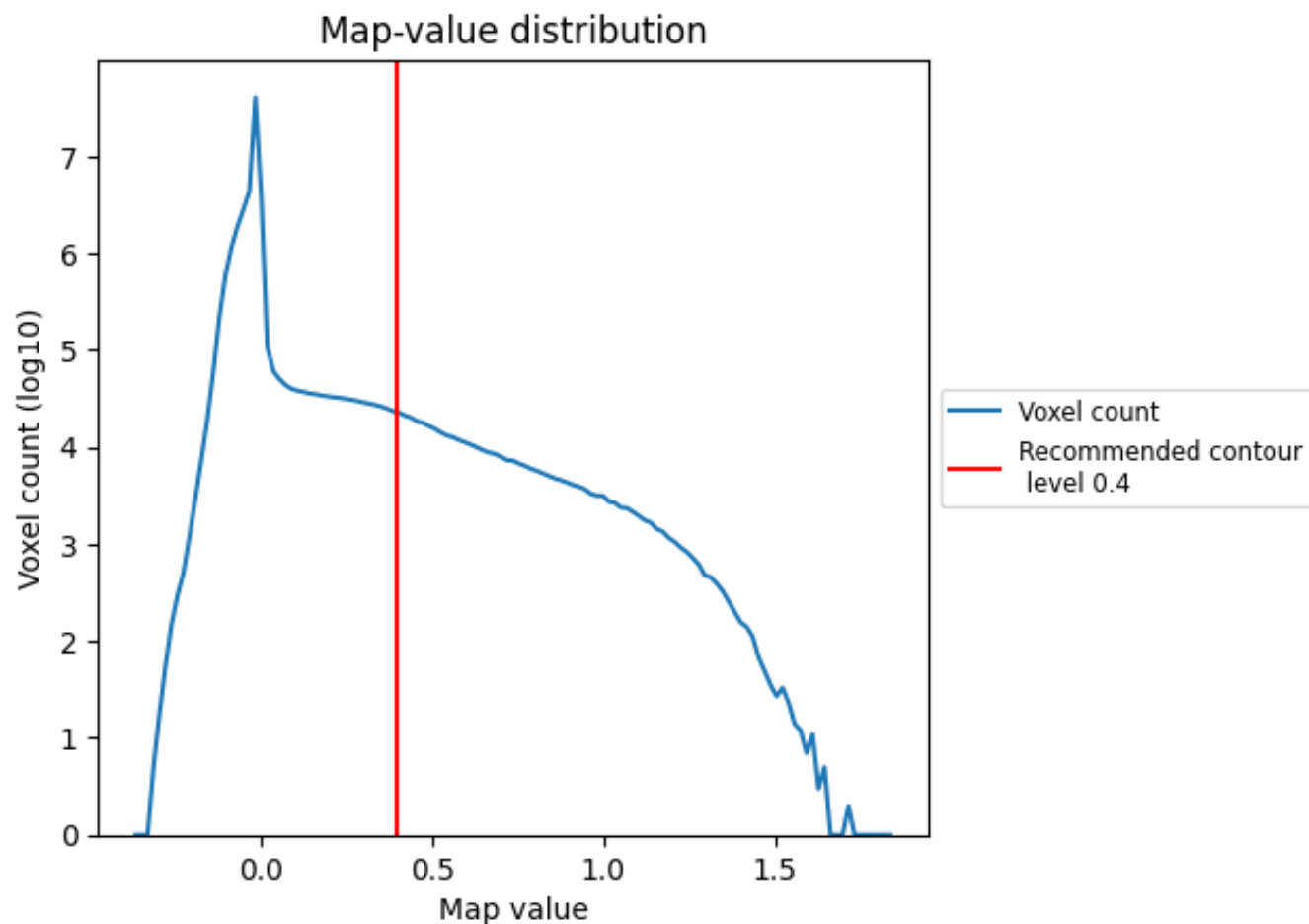
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

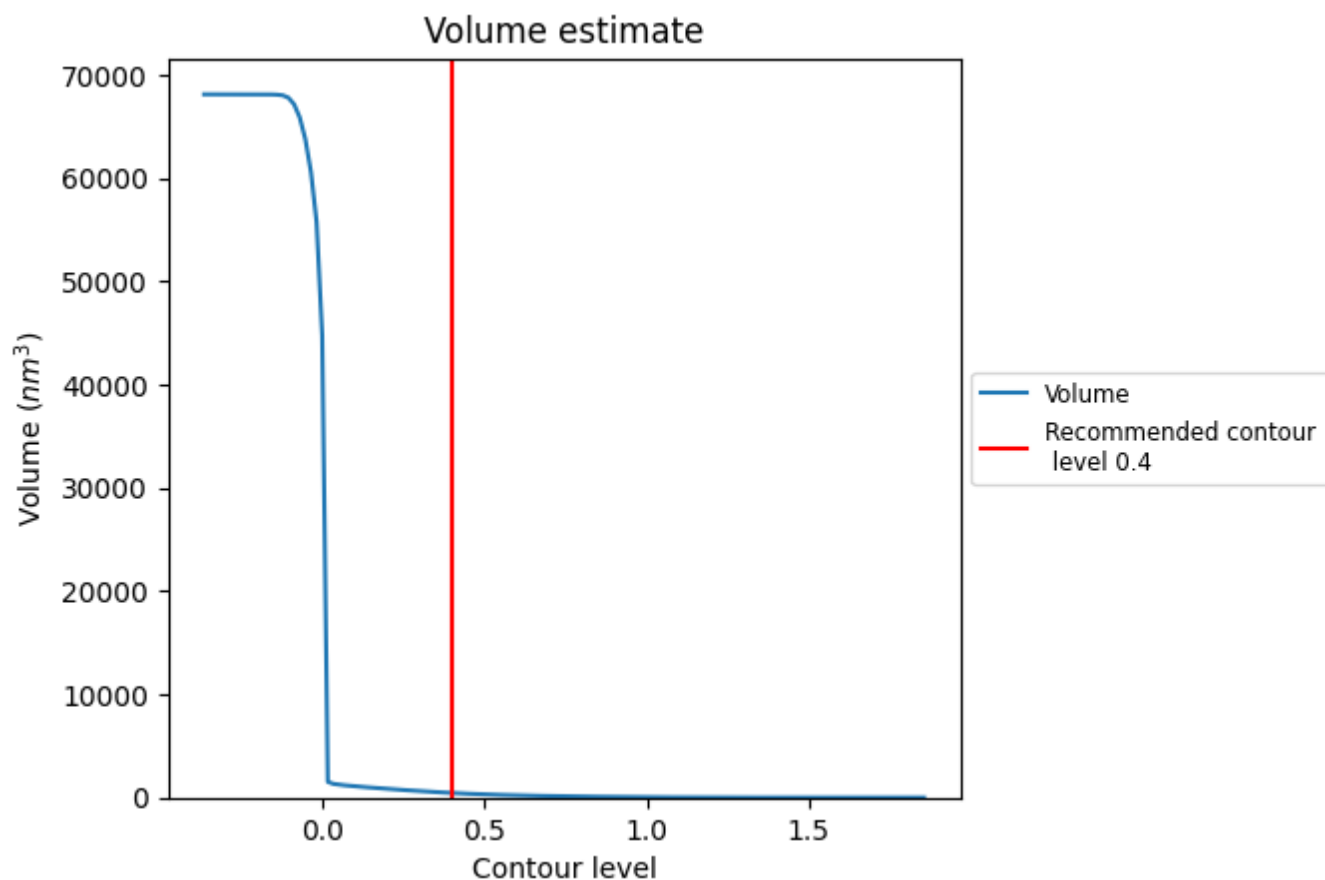
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

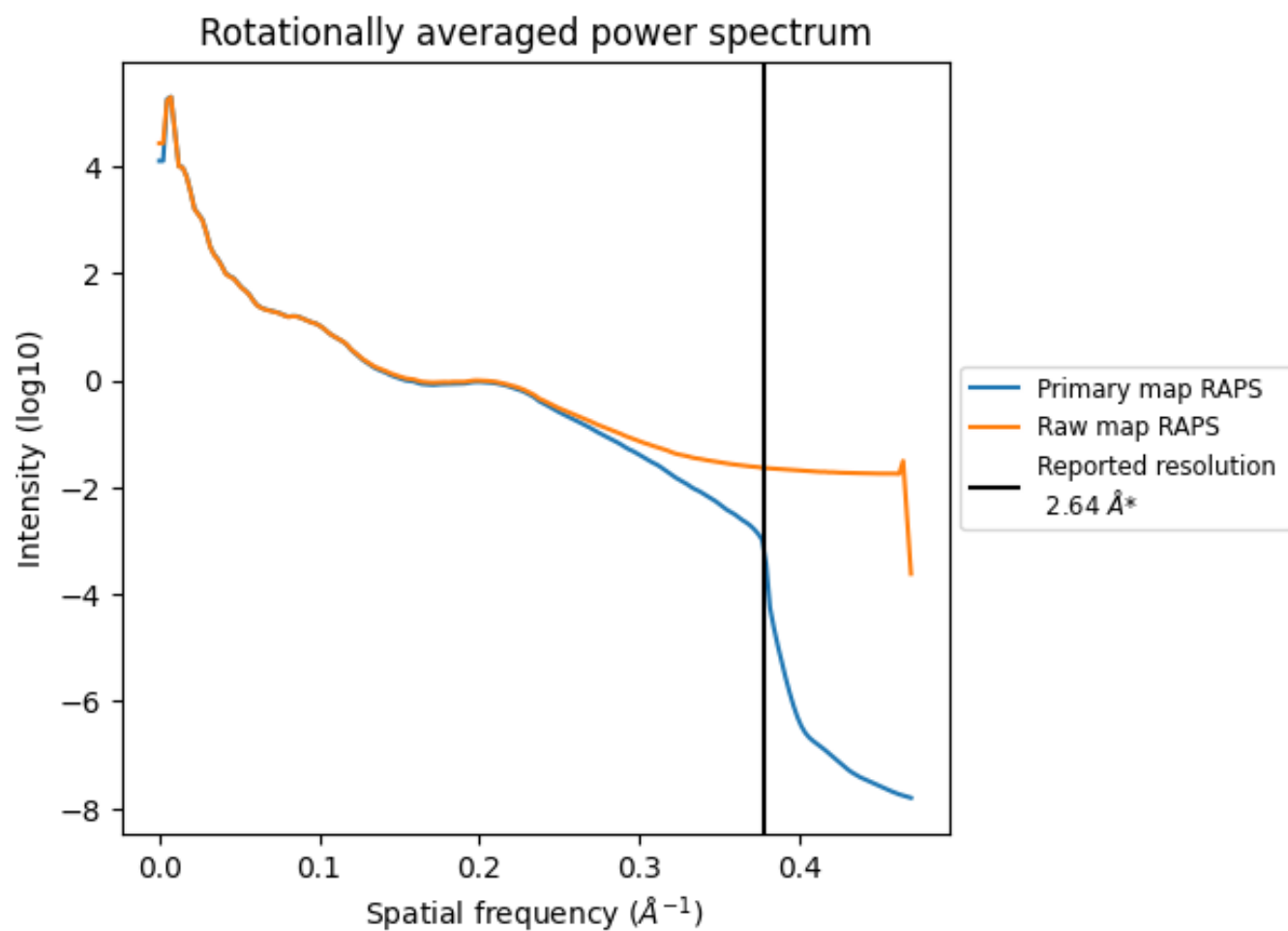
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 444 nm^3 ; this corresponds to an approximate mass of 401 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 ⓘ

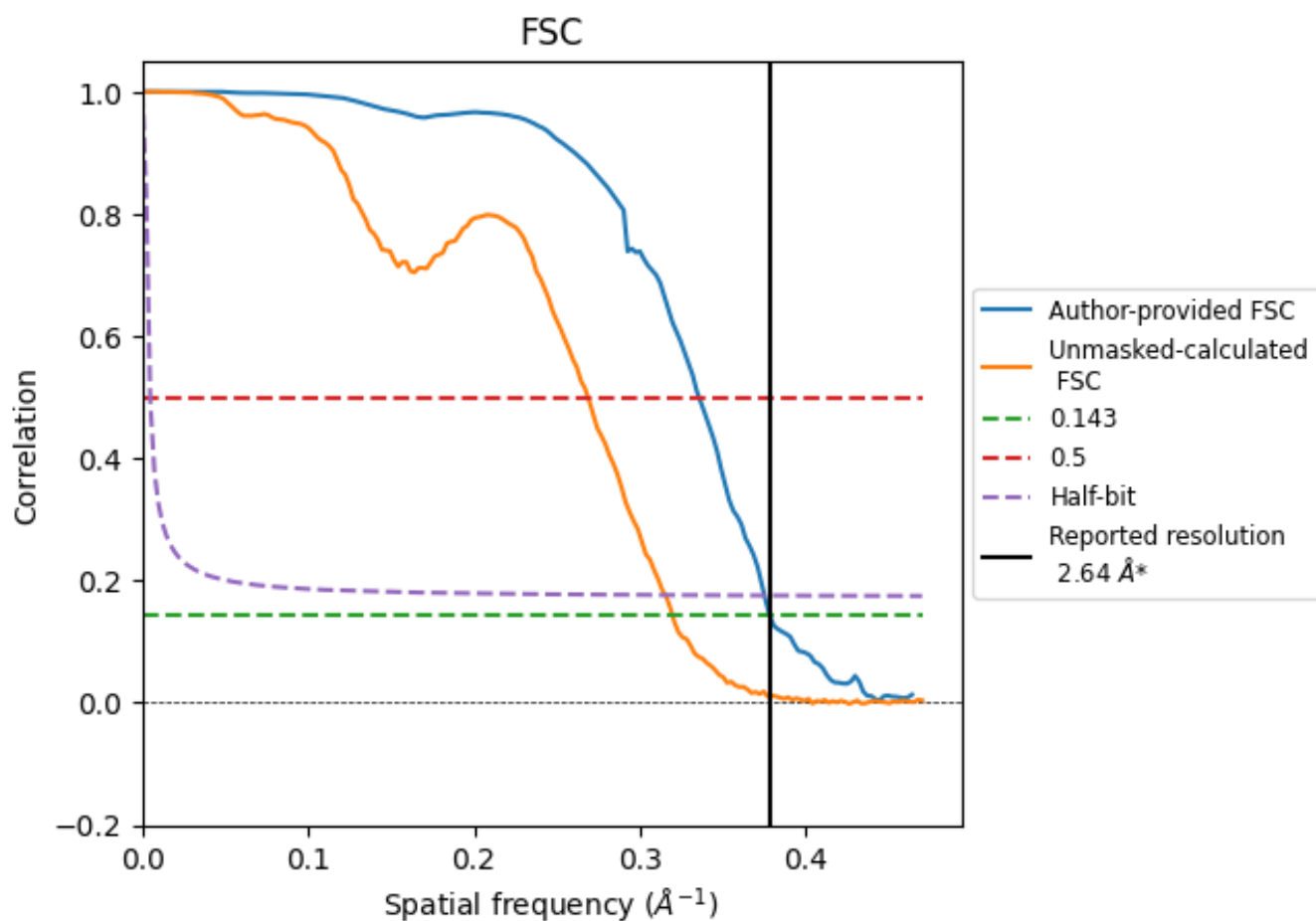


*Reported resolution corresponds to spatial frequency of $0.379 \text{ \AA}^{-1}$

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 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

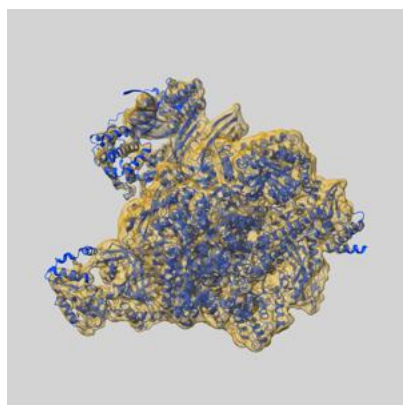
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	2.98	2.67
Unmasked-calculated*	3.13	3.72	3.17

*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 3.13 differs from the reported value 2.64 by more than 10 %

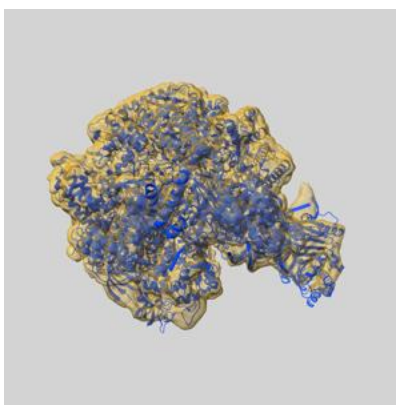
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17335 and PDB model 8P0K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

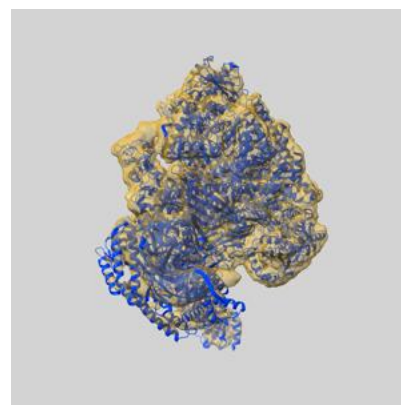
9.1 Map-model overlay [i](#)



X



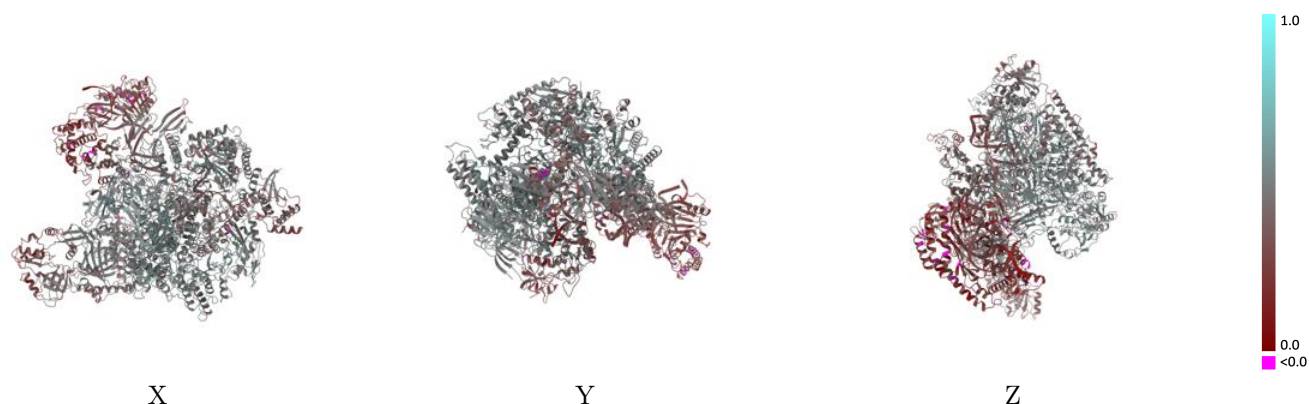
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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](#)

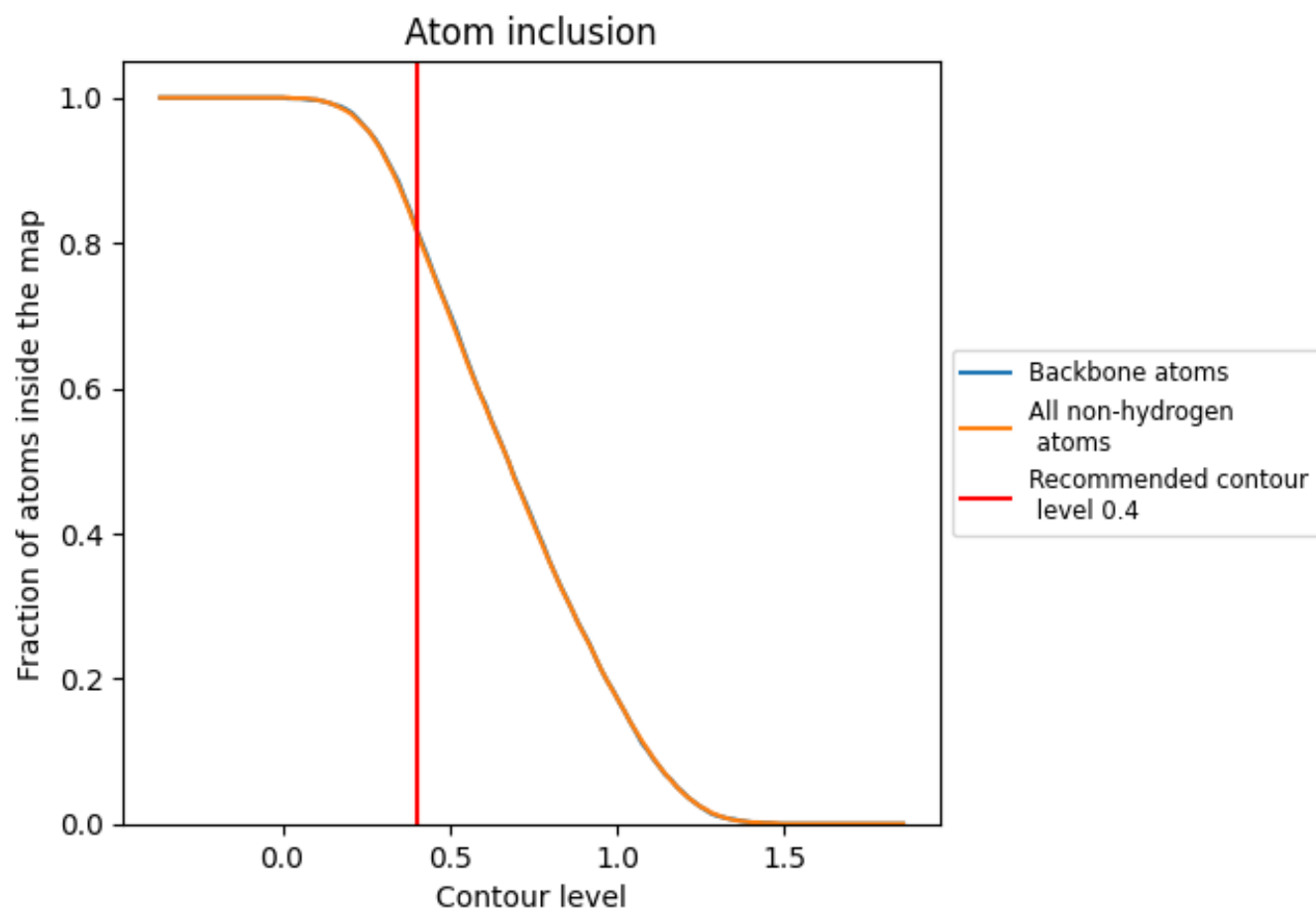


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4240
A	0.9220	0.4730
B	0.9370	0.4780
C	0.9680	0.4950
E	0.9590	0.5080
F	0.9760	0.5140
G	0.6490	0.3680
H	0.4640	0.2320
I	0.4400	0.2610
J	0.9900	0.5110
N	0.7920	0.2580
O	0.7370	0.3980
S	0.5550	0.3920
T	0.8250	0.2640

1.0

0.0

<0.0