



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 6RIE / pdb_00006rie
EMDB ID : EMD-4890
Title : Structure of Vaccinia Virus DNA-dependent RNA polymerase co-transcriptional capping complex
Authors : Hillen, H.S.; Bartuli, J.; Grimm, C.; Dienemann, C.; Bedenk, K.; Szalar, A.; Fischer, U.; Cramer, P.
Deposited on : 2019-04-23
Resolution : 3.10 Å (reported)
Based on initial model : 4CKB

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:

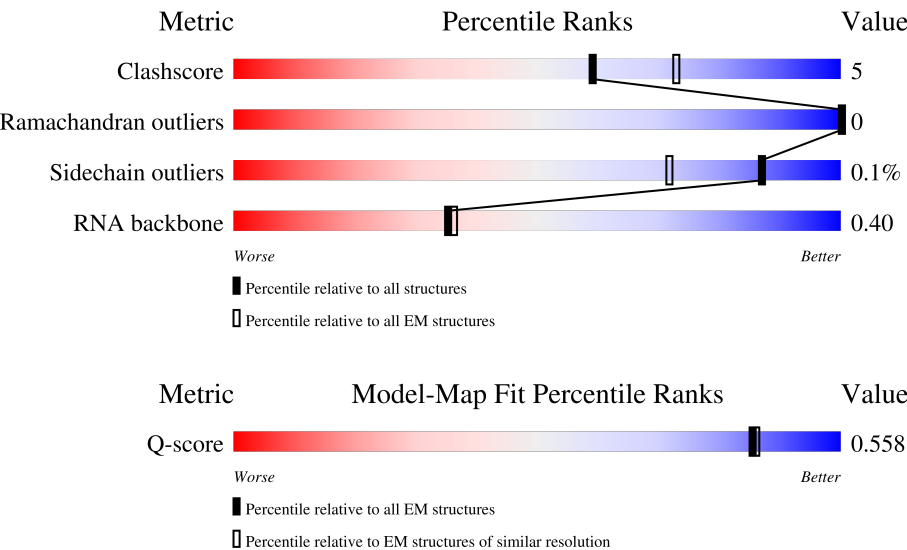
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



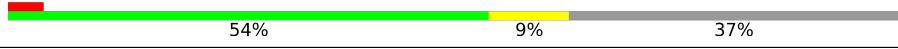
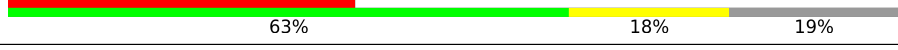
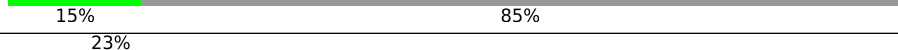
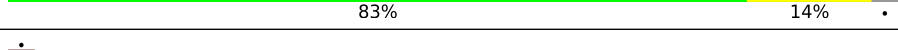
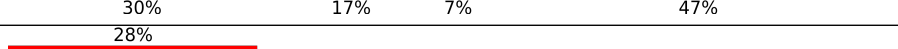
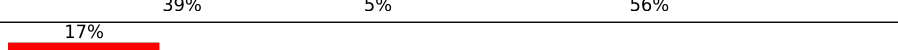
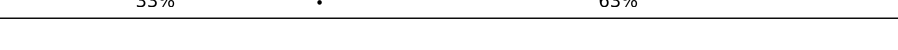
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1286	10% 89% 11%
2	B	1164	8% 84% 13% .

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Mol	Chain	Length	Quality of chain
3	C	305	
4	E	185	
5	F	164	
6	G	161	
7	J	63	
8	L	287	
9	N	48	
10	O	844	
11	P	30	
12	S	259	
13	T	48	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 36583 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-dependent RNA polymerase subunit rpo147.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0
			10330	6643	1700	1941	46		

- Molecule 2 is a protein called DNA-dependent RNA polymerase subunit rpo132.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1129	Total	C	N	O	S	0	0
			9089	5794	1551	1696	48		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	303	Total	C	N	O	S	0	0
			2475	1603	397	462	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	184	Total	C	N	O	S	0	0
			1495	966	248	276	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			849	545	148	153	3		

- Molecule 6 is a protein called DNA-dependent RNA polymerase subunit rpo18.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	131	Total	C	N	O	S	0	0
			1024	652	167	200	5		

- Molecule 7 is a protein called DNA-dependent RNA polymerase subunit rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	61	Total	C	N	O	S	0	0
			490	310	88	88	4		

- Molecule 8 is a protein called Small subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	287	Total	C	N	O	S	0	0
			2345	1508	391	433	13		

- Molecule 9 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	7	Total	C	N	O	P	0	0
			143	68	25	43	7		

- Molecule 10 is a protein called Large subunit of mRNA capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	822	Total	C	N	O	S	0	0
			6661	4293	1094	1255	19		

- Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	16	Total	C	N	O	P	0	0
			350	154	63	116	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	113	Total	C	N	O	S	0	0
			929	593	152	180	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	18	Total	C	N	O	P	0	0
			370	175	74	103	18		

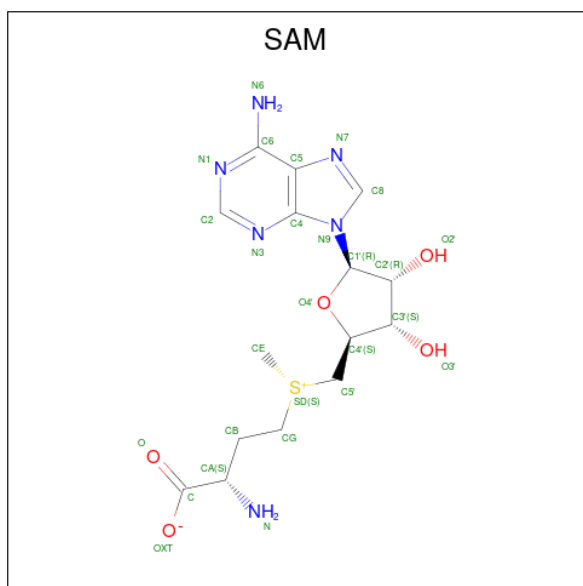
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 16 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).

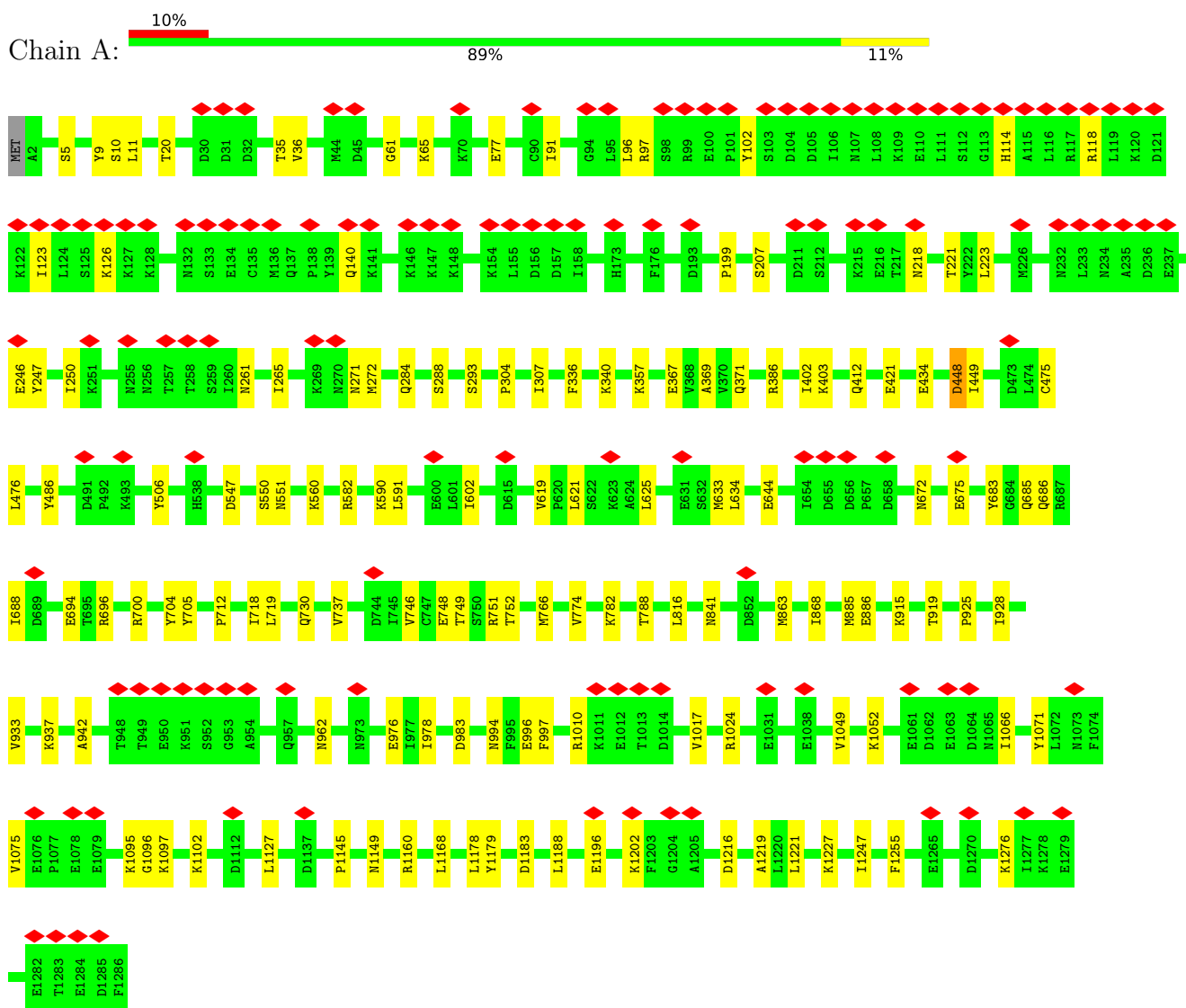


Mol	Chain	Residues	Atoms					AltConf
16	O	1	Total	C	N	O	S	0
			27	15	6	5	1	

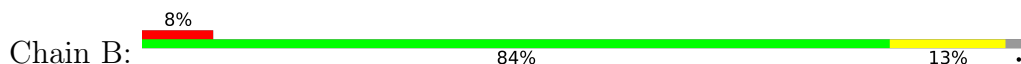
3 Residue-property plots

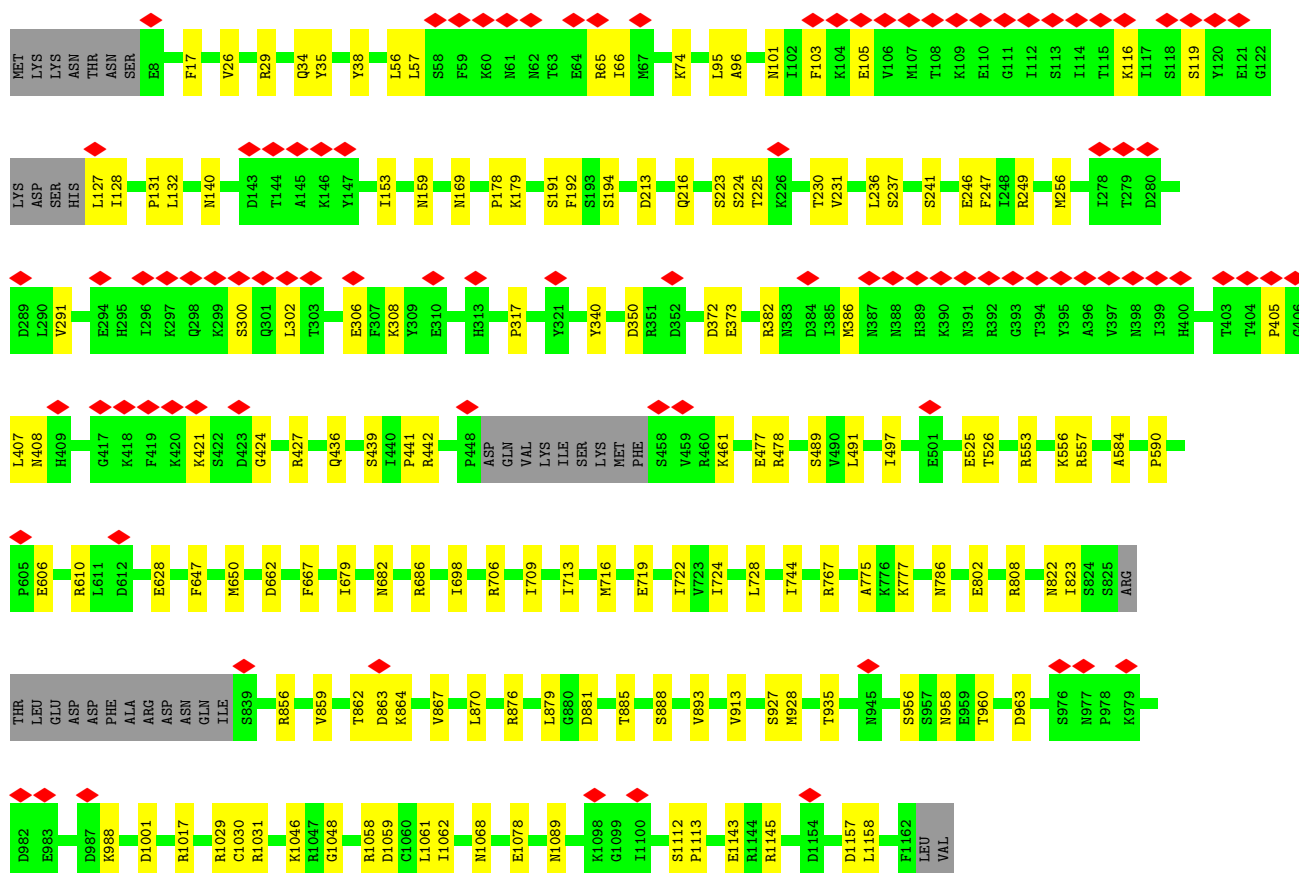
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent RNA polymerase subunit rpo147

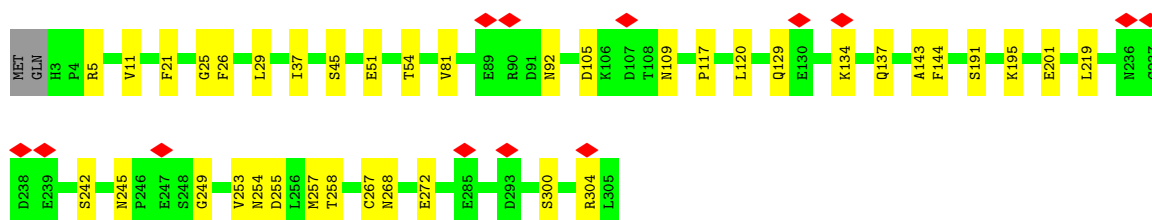
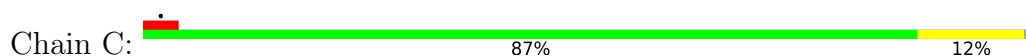


- Molecule 2: DNA-dependent RNA polymerase subunit rpo132

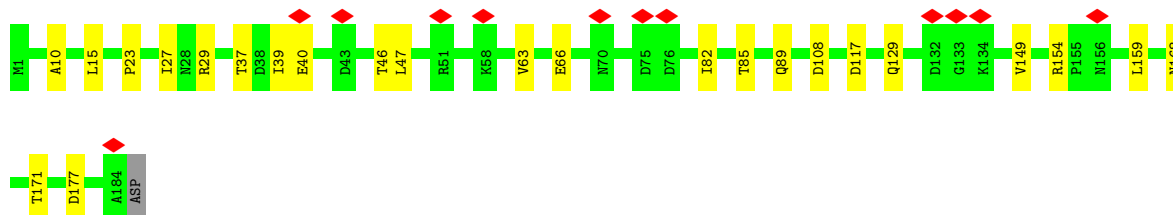
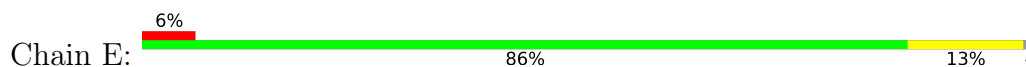




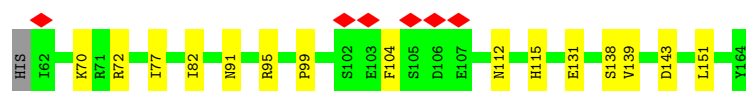
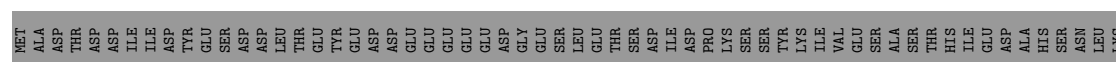
- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit



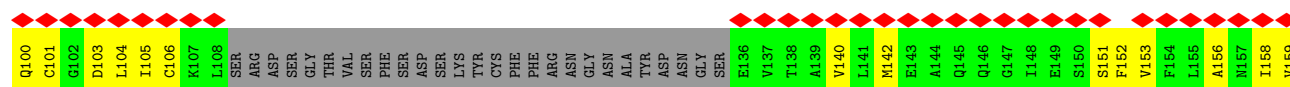
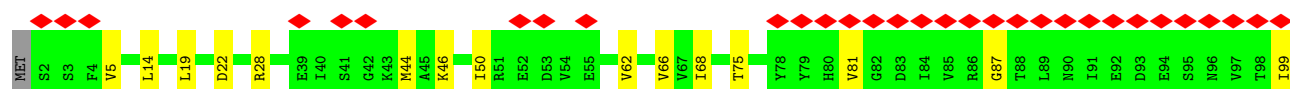
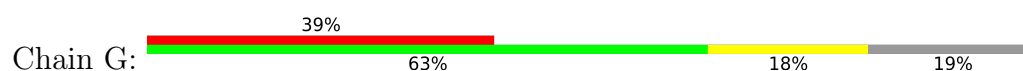
- Molecule 4: DNA-directed RNA polymerase subunit



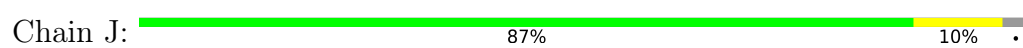
- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit



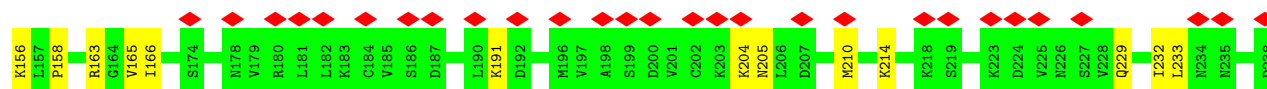
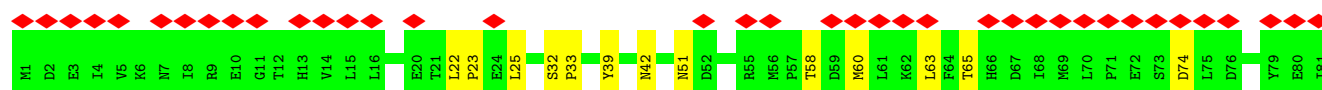
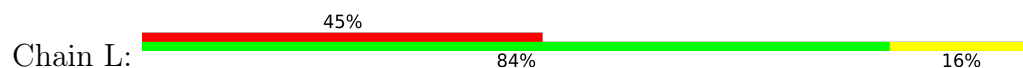
• Molecule 6: DNA-dependent RNA polymerase subunit rpo18



• Molecule 7: DNA-dependent RNA polymerase subunit rpo7



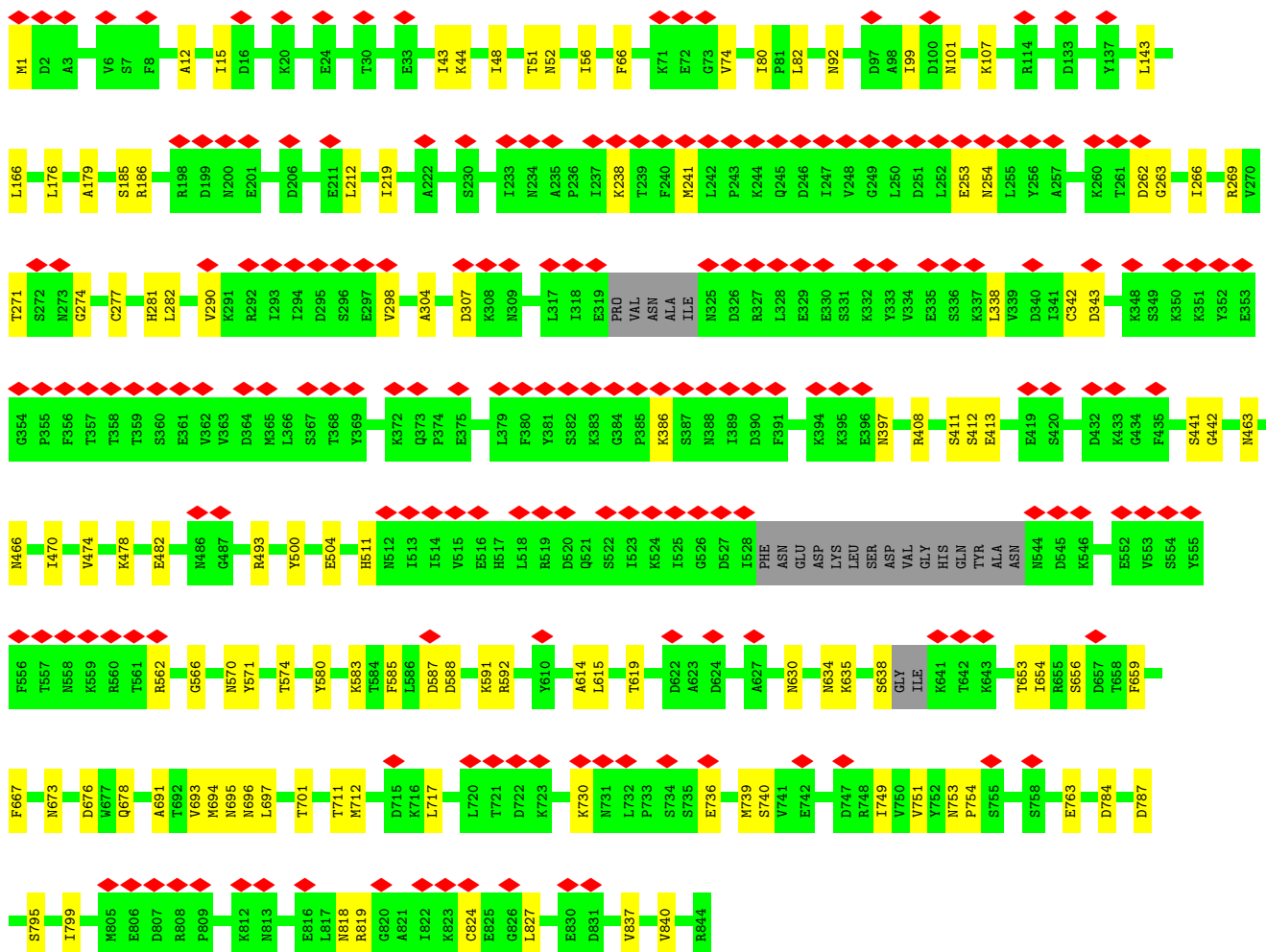
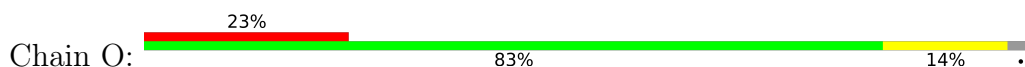
• Molecule 8: Small subunit of mRNA capping enzyme



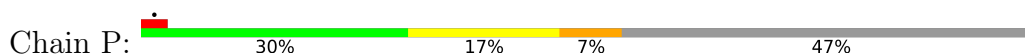
• Molecule 9: Non-template DNA strand



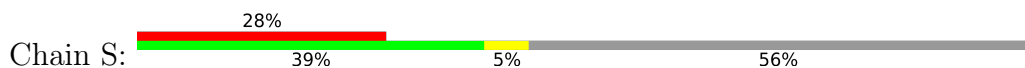
- Molecule 10: Large subunit of mRNA capping enzyme

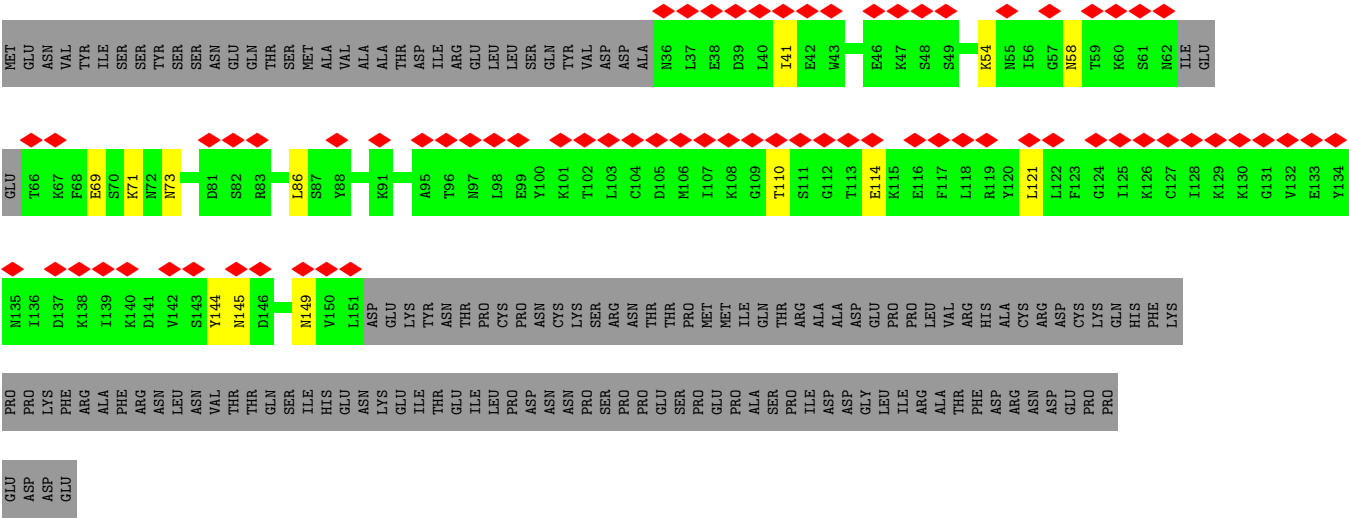


- Molecule 11: RNA

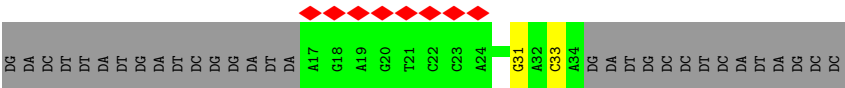


- Molecule 12: DNA-directed RNA polymerase 30 kDa polypeptide





● Molecule 13: Template strand DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77706	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 ($e^-/\text{\AA}^2$)	1.02	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	356.99997, 356.99997, 356.99997	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: GDP, SAM, 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	0.24	0/10537	0.46	0/14241
2	B	0.25	0/9278	0.45	0/12532
3	C	0.24	0/2531	0.44	0/3428
4	E	0.23	0/1522	0.41	0/2069
5	F	0.25	0/863	0.41	0/1158
6	G	0.22	0/1037	0.52	2/1408 (0.1%)
7	J	0.27	0/494	0.42	0/663
8	L	0.19	0/2392	0.40	0/3229
9	N	0.18	0/159	0.36	0/243
10	O	0.22	0/6796	0.47	2/9188 (0.0%)
11	P	0.22	0/359	0.48	0/555
12	S	0.16	0/943	0.41	0/1260
13	T	0.29	0/416	0.42	0/639
All	All	0.23	0/37327	0.45	4/50613 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
10	O	307	ASP	CA-C-N	6.75	134.43	121.54
10	O	307	ASP	C-N-CA	6.75	134.43	121.54
6	G	62	VAL	CA-C-N	5.87	132.74	121.54
6	G	62	VAL	C-N-CA	5.87	132.74	121.54

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	10330	0	10448	90	0
2	B	9089	0	9139	98	0
3	C	2475	0	2462	23	0
4	E	1495	0	1548	14	0
5	F	849	0	874	12	0
6	G	1024	0	1038	15	0
7	J	490	0	528	5	0
8	L	2345	0	2388	28	0
9	N	143	0	80	0	0
10	O	6661	0	6739	71	0
11	P	350	0	172	4	0
12	S	929	0	937	10	0
13	T	370	0	201	2	0
14	A	1	0	0	0	0
14	O	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
16	O	27	0	22	0	0
All	All	36583	0	36576	333	0

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

All (333) 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:357:LYS:HG3	10:O:412:SER:HB3	1.73	0.70
2:B:478:ARG:NH1	11:P:30:G:N7	2.46	0.64
1:A:336:PHE:HB2	1:A:367:GLU:HB2	1.79	0.64
2:B:405:PRO:HB2	2:B:407:LEU:HG	1.80	0.63
1:A:5:SER:HB3	2:B:1143:GLU:HB2	1.83	0.61
2:B:553:ARG:HA	2:B:556:LYS:HG2	1.82	0.61
8:L:114:ARG:HH21	8:L:127:ASN:HB2	1.63	0.60
2:B:436:GLN:HA	2:B:439:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:32:SER:HB2	8:L:229:GLN:HB2	1.84	0.60
2:B:128:ILE:HA	2:B:408:ASN:HD21	1.67	0.60
2:B:256:MET:HE1	2:B:340:TYR:HB2	1.84	0.59
2:B:373:GLU:HB3	2:B:407:LEU:HD22	1.84	0.59
2:B:525:GLU:HG2	2:B:526:THR:HG23	1.85	0.59
1:A:475:CYS:SG	1:A:476:LEU:N	2.77	0.58
4:E:10:ALA:HB1	4:E:37:THR:HG21	1.86	0.58
2:B:17:PHE:O	2:B:29:ARG:NH2	2.37	0.58
2:B:775:ALA:HB1	2:B:870:LEU:HD11	1.86	0.58
1:A:412:GLN:NE2	1:A:421:GLU:OE2	2.37	0.57
10:O:676:ASP:OD1	10:O:678:GLN:NE2	2.38	0.57
1:A:1097:LYS:HA	12:S:58:ASN:HB3	1.86	0.57
1:A:293:SER:HB2	1:A:403:LYS:HB3	1.87	0.57
4:E:40:GLU:HG2	4:E:47:LEU:HB2	1.87	0.57
10:O:185:SER:O	10:O:478:LYS:NZ	2.37	0.57
1:A:20:THR:O	1:A:65:LYS:NZ	2.38	0.57
10:O:482:GLU:HB2	10:O:493:ARG:HD3	1.87	0.56
1:A:97:ARG:HB2	1:A:123:ILE:HG23	1.85	0.56
2:B:26:VAL:HG21	2:B:29:ARG:HH11	1.70	0.56
10:O:736:GLU:HG3	10:O:754:PRO:HB2	1.87	0.56
1:A:1196:GLU:HG3	1:A:1202:LYS:HE2	1.86	0.56
2:B:65:ARG:NH2	2:B:105:GLU:OE2	2.39	0.56
2:B:442:ARG:NH2	2:B:489:SER:O	2.39	0.56
2:B:958:ASN:ND2	2:B:960:THR:O	2.38	0.56
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.39	0.56
8:L:136:LEU:HD13	8:L:165:VAL:HG22	1.85	0.56
1:A:994:ASN:HD21	12:S:54:LYS:H	1.53	0.56
10:O:186:ARG:NH1	10:O:500:TYR:O	2.39	0.56
10:O:739:MET:SD	10:O:753:ASN:ND2	2.79	0.56
10:O:298:VAL:HG11	10:O:338:LEU:HD11	1.88	0.55
1:A:978:ILE:HD12	1:A:1127:LEU:HB2	1.87	0.55
5:F:112:ASN:OD1	5:F:115:HIS:ND1	2.39	0.55
1:A:284:GLN:NE2	2:B:1030:CYS:SG	2.79	0.55
10:O:580:TYR:O	10:O:592:ARG:NH1	2.40	0.55
2:B:491:LEU:HD13	2:B:590:PRO:HG2	1.88	0.55
8:L:58:THR:HG21	8:L:113:GLU:HA	1.88	0.55
8:L:104:SER:HB3	8:L:158:PRO:HA	1.89	0.55
10:O:463:ASN:HA	10:O:466:ASN:HD21	1.72	0.55
8:L:258:TYR:OH	8:L:281:ARG:NH2	2.40	0.54
2:B:101:ASN:HD22	2:B:119:SER:HB3	1.72	0.54
2:B:1157:ASP:O	5:F:72:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:5:VAL:HG22	6:G:75:THR:HG23	1.88	0.54
1:A:1024:ARG:HH21	1:A:1066:ILE:HD11	1.73	0.54
1:A:223:LEU:HD13	1:A:247:TYR:HA	1.90	0.54
3:C:129:GLN:H	3:C:137:GLN:HE22	1.55	0.54
4:E:129:GLN:O	5:F:70:LYS:NZ	2.40	0.54
8:L:121:ASN:HD21	10:O:583:LYS:HE3	1.72	0.54
6:G:104:LEU:HD13	6:G:152:PHE:HB2	1.90	0.54
1:A:218:ASN:ND2	1:A:221:THR:OG1	2.41	0.53
1:A:602:ILE:HG23	1:A:633:MET:HE3	1.89	0.53
1:A:340:LYS:NZ	2:B:1078:GLU:OE2	2.40	0.53
1:A:304:PRO:HD2	1:A:307:ILE:HD12	1.90	0.53
10:O:824:CYS:HB2	10:O:827:LEU:HD12	1.91	0.53
4:E:66:GLU:HB2	4:E:85:THR:HA	1.91	0.53
10:O:241:MET:SD	10:O:397:ASN:ND2	2.82	0.53
2:B:1058:ARG:NH2	2:B:1059:ASP:OD1	2.41	0.53
10:O:784:ASP:HB3	10:O:840:VAL:HB	1.90	0.53
1:A:357:LYS:NZ	10:O:82:LEU:O	2.41	0.53
8:L:33:PRO:HB2	8:L:163:ARG:HD3	1.90	0.53
10:O:619:THR:HG21	10:O:659:PHE:HE1	1.74	0.52
10:O:408:ARG:HB2	10:O:411:SER:HB2	1.92	0.52
10:O:179:ALA:O	10:O:478:LYS:NZ	2.33	0.52
10:O:691:ALA:O	10:O:695:ASN:ND2	2.41	0.52
12:S:145:ASN:O	12:S:149:ASN:ND2	2.42	0.52
2:B:477:GLU:HG2	2:B:478:ARG:HG3	1.91	0.52
2:B:686:ARG:NH2	2:B:888:SER:O	2.38	0.52
4:E:66:GLU:OE2	4:E:89:GLN:NE2	2.43	0.52
2:B:876:ARG:HH11	3:C:54:THR:HG23	1.74	0.52
10:O:591:LYS:HB2	10:O:614:ALA:HB2	1.92	0.52
2:B:491:LEU:HG	2:B:667:PHE:HB3	1.92	0.52
1:A:288:SER:HB3	1:A:402:ILE:HG13	1.92	0.51
2:B:95:LEU:HB3	2:B:127:LEU:HD12	1.92	0.51
10:O:441:SER:OG	10:O:442:GLY:N	2.43	0.51
4:E:168:ASN:ND2	4:E:171:THR:OG1	2.43	0.51
10:O:99:ILE:HG22	10:O:101:ASN:H	1.75	0.51
1:A:582:ARG:NH2	2:B:963:ASP:OD1	2.43	0.51
1:A:868:ILE:HG21	1:A:886:GLU:HB2	1.91	0.51
1:A:1247:ILE:HD13	2:B:1062:ILE:HG23	1.93	0.51
8:L:111:LYS:NZ	8:L:128:LEU:O	2.43	0.51
1:A:91:ILE:HG21	1:A:140:GLN:HE22	1.76	0.51
10:O:281:HIS:HD2	10:O:470:ILE:HD11	1.75	0.50
2:B:478:ARG:NH2	11:P:30:G:O6	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:LYS:HG2	1:A:1178:LEU:HD11	1.92	0.50
1:A:271:ASN:OD1	1:A:271:ASN:N	2.44	0.50
10:O:654:ILE:O	10:O:696:ASN:ND2	2.44	0.50
2:B:194:SER:HB3	2:B:317:PRO:HD2	1.94	0.50
2:B:767:ARG:O	7:J:4:GLN:NE2	2.43	0.50
10:O:1:MET:HG2	10:O:269:ARG:HB2	1.92	0.50
2:B:557:ARG:NH2	2:B:628:GLU:OE1	2.43	0.49
6:G:44:MET:HE1	6:G:151:SER:HA	1.94	0.49
8:L:140:VAL:HG13	8:L:155:ILE:HG21	1.93	0.49
10:O:615:LEU:HD11	10:O:667:PHE:HE1	1.76	0.49
2:B:237:SER:O	2:B:241:SER:OG	2.30	0.49
2:B:724:ILE:HG22	2:B:728:LEU:HD23	1.94	0.49
10:O:52:ASN:ND2	10:O:219:ILE:O	2.44	0.49
10:O:711:THR:OG1	10:O:712:MET:N	2.45	0.49
2:B:606:GLU:O	2:B:610:ARG:HB2	2.12	0.49
2:B:1158:LEU:HD12	5:F:143:ASP:HB2	1.94	0.49
2:B:709:ILE:HG23	2:B:870:LEU:HB2	1.92	0.49
2:B:722:ILE:HD11	2:B:935:THR:HG23	1.95	0.49
1:A:9:TYR:O	1:A:1227:LYS:HA	2.13	0.49
1:A:207:SER:O	11:P:20:A:O2'	2.29	0.49
1:A:602:ILE:HG12	1:A:633:MET:HG2	1.95	0.49
8:L:273:SER:O	8:L:276:ASN:ND2	2.43	0.49
1:A:751:ARG:NH1	1:A:962:ASN:OD1	2.46	0.48
10:O:263:GLY:HA3	10:O:304:ALA:O	2.13	0.48
10:O:740:SER:O	10:O:751:VAL:HA	2.12	0.48
2:B:424:GLY:O	2:B:427:ARG:NH1	2.45	0.48
2:B:34:GLN:NE2	2:B:441:PRO:O	2.46	0.48
2:B:679:ILE:N	2:B:956:SER:O	2.43	0.48
2:B:1001:ASP:OD2	3:C:191:SER:OG	2.31	0.48
8:L:130:ILE:HG21	8:L:260:HIS:HE1	1.78	0.48
2:B:744:ILE:HG22	2:B:913:VAL:HB	1.95	0.48
6:G:28:ARG:HG2	6:G:50:ILE:HD12	1.95	0.48
8:L:204:LYS:NZ	8:L:205:ASN:OD1	2.44	0.48
2:B:300:SER:HB2	2:B:302:LEU:HD23	1.95	0.48
1:A:547:ASP:OD1	1:A:841:ASN:ND2	2.44	0.48
2:B:291:VAL:HG11	2:B:308:LYS:HG3	1.95	0.48
3:C:245:ASN:O	3:C:249:GLY:N	2.45	0.48
8:L:108:LYS:O	8:L:191:LYS:NZ	2.43	0.48
6:G:19:LEU:HD11	6:G:66:VAL:HG21	1.96	0.48
2:B:96:ALA:HB3	2:B:128:ILE:HG23	1.96	0.48
2:B:706:ARG:NH2	3:C:45:SER:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NE	1:A:448:ASP:OD2	2.43	0.47
2:B:213:ASP:HB3	2:B:216:GLN:HG2	1.96	0.47
1:A:997:PHE:O	1:A:1102:LYS:NZ	2.48	0.47
10:O:262:ASP:OD2	10:O:262:ASP:N	2.39	0.47
1:A:77:GLU:HG3	1:A:1221:LEU:HD22	1.95	0.47
6:G:105:ILE:HB	6:G:153:VAL:HG22	1.95	0.47
1:A:1049:VAL:HG12	12:S:86:LEU:HB3	1.95	0.47
2:B:38:TYR:OH	2:B:131:PRO:O	2.27	0.47
10:O:253:GLU:OE1	10:O:254:ASN:ND2	2.47	0.47
1:A:774:VAL:HB	1:A:782:LYS:HB2	1.97	0.47
1:A:976:GLU:OE1	1:A:1149:ASN:ND2	2.47	0.47
1:A:996:GLU:O	1:A:1095:LYS:NZ	2.48	0.47
2:B:372:ASP:OD2	2:B:421:LYS:NZ	2.48	0.47
3:C:191:SER:OG	3:C:191:SER:O	2.31	0.47
3:C:255:ASP:HB3	3:C:258:THR:HG22	1.97	0.47
10:O:92:ASN:HD22	10:O:143:LEU:HD22	1.79	0.47
1:A:1096:GLY:O	12:S:58:ASN:ND2	2.47	0.47
2:B:246:GLU:OE2	2:B:249:ARG:NH1	2.45	0.47
10:O:799:ILE:O	10:O:819:ARG:NH1	2.48	0.47
1:A:223:LEU:HD22	1:A:246:GLU:HG2	1.97	0.47
2:B:719:GLU:HG2	7:J:47:GLN:HG2	1.96	0.47
6:G:46:LYS:NZ	6:G:103:ASP:OD2	2.40	0.47
6:G:99:ILE:HB	6:G:106:CYS:HB2	1.97	0.47
2:B:179:LYS:HE3	2:B:191:SER:HB2	1.96	0.46
1:A:788:THR:HG22	1:A:885:MET:HE2	1.97	0.46
1:A:1160:ARG:NH1	1:A:1183:ASP:OD1	2.38	0.46
2:B:132:LEU:HD21	2:B:140:ASN:HD22	1.80	0.46
2:B:716:MET:HE3	3:C:51:GLU:HA	1.98	0.46
1:A:10:SER:OG	1:A:11:LEU:N	2.47	0.46
2:B:862:THR:HG23	2:B:864:LYS:H	1.79	0.46
1:A:685:GLN:NE2	1:A:686:GLN:O	2.46	0.46
1:A:357:LYS:HA	10:O:413:GLU:HG2	1.97	0.46
10:O:238:LYS:HB3	10:O:238:LYS:HE3	1.81	0.46
2:B:879:LEU:HD23	2:B:893:VAL:HG12	1.98	0.46
1:A:719:LEU:H	1:A:730:GLN:HE21	1.64	0.46
5:F:77:ILE:HD11	5:F:82:ILE:HB	1.98	0.46
8:L:51:ASN:HD22	10:O:585:PHE:HE1	1.62	0.46
1:A:265:ILE:HB	1:A:272:MET:HB2	1.98	0.46
6:G:158:ILE:HG22	6:G:159:VAL:HG13	1.98	0.46
10:O:66:PHE:HE2	10:O:80:ILE:HG13	1.80	0.46
2:B:859:VAL:HG13	2:B:867:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:65:THR:HG22	8:L:263:LEU:HD11	1.98	0.45
8:L:74:ASP:OD2	8:L:156:LYS:NZ	2.42	0.45
10:O:787:ASP:HA	10:O:837:VAL:HA	1.98	0.45
6:G:101:CYS:O	6:G:104:LEU:HB2	2.16	0.45
8:L:100:VAL:HG12	8:L:154:ILE:HB	1.99	0.45
1:A:35:THR:OG1	1:A:36:VAL:N	2.49	0.45
1:A:619:VAL:O	12:S:144:TYR:OH	2.31	0.45
2:B:822:ASN:N	2:B:822:ASN:OD1	2.49	0.45
4:E:10:ALA:HB2	4:E:39:ILE:HD11	1.97	0.45
10:O:630:ASN:O	10:O:634:ASN:ND2	2.47	0.45
2:B:1145:ARG:NH2	5:F:131:GLU:OE2	2.48	0.45
1:A:694:GLU:OE2	1:A:696:ARG:NH2	2.49	0.45
4:E:117:ASP:OD1	4:E:117:ASP:N	2.42	0.45
1:A:357:LYS:HE3	1:A:357:LYS:HB2	1.72	0.45
1:A:367:GLU:OE1	2:B:1031:ARG:NH2	2.49	0.45
1:A:590:LYS:NZ	1:A:644:GLU:OE1	2.43	0.45
2:B:497:ILE:HG22	2:B:584:ALA:HB2	1.99	0.45
8:L:128:LEU:HD13	8:L:130:ILE:HD12	1.99	0.45
8:L:232:ILE:HG23	8:L:233:LEU:HG	1.99	0.45
2:B:682:ASN:HD21	2:B:927:SER:H	1.65	0.45
5:F:99:PRO:HG2	5:F:104:PHE:HE1	1.82	0.45
2:B:34:GLN:HE22	2:B:169:ASN:HD21	1.65	0.44
3:C:25:GLY:O	3:C:29:LEU:HB2	2.17	0.44
3:C:242:SER:HB2	3:C:254:ASN:H	1.83	0.44
5:F:91:ASN:OD1	5:F:95:ARG:NH1	2.49	0.44
1:A:915:LYS:O	1:A:919:THR:OG1	2.30	0.44
6:G:22:ASP:OD1	6:G:22:ASP:N	2.46	0.44
10:O:386:LYS:HE3	10:O:386:LYS:HB2	1.85	0.44
10:O:717:LEU:HD13	10:O:749:ILE:HD13	1.98	0.44
1:A:61:GLY:HA3	1:A:199:PRO:HB3	2.00	0.44
1:A:96:LEU:H	1:A:102:TYR:HE2	1.65	0.44
1:A:983:ASP:OD1	1:A:983:ASP:N	2.50	0.44
2:B:698:ILE:HD12	2:B:713:ILE:HB	2.00	0.44
2:B:709:ILE:HG22	2:B:777:LYS:HG3	1.99	0.44
6:G:87:GLY:CA	6:G:100:GLN:O	2.65	0.44
8:L:22:LEU:HD12	8:L:23:PRO:HD2	2.00	0.44
8:L:60:MET:HA	8:L:63:LEU:HG	1.99	0.44
1:A:634:LEU:HD11	1:A:712:PRO:HB3	2.00	0.44
10:O:342:CYS:SG	10:O:343:ASP:N	2.90	0.44
2:B:786:ASN:ND2	2:B:823:ILE:O	2.42	0.44
4:E:46:THR:HB	4:E:63:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:281:ARG:HA	8:L:284:LYS:HG2	1.99	0.44
10:O:570:ASN:O	10:O:574:THR:OG1	2.31	0.44
1:A:748:GLU:O	1:A:752:THR:OG1	2.28	0.44
6:G:81:VAL:HG13	6:G:142:MET:HA	1.99	0.44
10:O:266:ILE:HD11	10:O:277:CYS:HB3	2.00	0.44
2:B:647:PHE:HA	2:B:650:MET:HE2	1.99	0.44
1:A:486:TYR:O	1:A:506:TYR:OH	2.27	0.44
2:B:159:ASN:ND2	13:T:33:DC:OP1	2.50	0.44
3:C:134:LYS:HA	3:C:134:LYS:HD3	1.78	0.44
1:A:766:MET:HE2	1:A:1188:LEU:HD13	2.00	0.43
10:O:566:GLY:O	10:O:570:ASN:HB2	2.18	0.43
1:A:1010:ARG:HG3	1:A:1017:VAL:HB	2.00	0.43
1:A:1255:PHE:HE1	5:F:131:GLU:HB2	1.84	0.43
2:B:35:TYR:OH	2:B:153:ILE:O	2.28	0.43
2:B:885:THR:HG21	2:B:928:MET:HE3	2.00	0.43
10:O:48:ILE:HG21	10:O:282:LEU:HD22	2.00	0.43
10:O:587:ASP:OD1	10:O:587:ASP:N	2.48	0.43
2:B:231:VAL:HG11	2:B:236:LEU:HD13	2.01	0.43
4:E:23:PRO:HB3	4:E:154:ARG:HG3	2.00	0.43
1:A:250:ILE:H	1:A:261:ASN:HD22	1.67	0.43
2:B:57:LEU:HD11	2:B:386:MET:HG3	2.01	0.43
3:C:5:ARG:NH2	3:C:201:GLU:OE2	2.51	0.43
3:C:105:ASP:O	3:C:109:ASN:N	2.52	0.43
10:O:12:ALA:HA	10:O:15:ILE:HG22	2.00	0.43
10:O:107:LYS:NZ	11:P:1:GDP:O2A	2.48	0.43
10:O:271:THR:OG1	10:O:274:GLY:O	2.36	0.43
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.52	0.43
8:L:22:LEU:HD21	8:L:25:LEU:HD11	2.00	0.43
10:O:588:ASP:O	10:O:592:ARG:NH2	2.52	0.43
10:O:749:ILE:HG23	10:O:763:GLU:HG3	2.01	0.43
2:B:856:ARG:NH1	7:J:56:VAL:O	2.38	0.42
3:C:21:PHE:HE1	3:C:257:MET:HG3	1.84	0.42
10:O:653:THR:O	10:O:656:SER:OG	2.36	0.42
10:O:730:LYS:HG3	10:O:827:LEU:HD11	2.01	0.42
1:A:369:ALA:O	1:A:371:GLN:NE2	2.53	0.42
1:A:1168:LEU:HD22	1:A:1179:TYR:HD1	1.83	0.42
3:C:267:CYS:SG	3:C:268:ASN:N	2.93	0.42
6:G:14:LEU:HD13	6:G:68:ILE:HD12	2.01	0.42
10:O:571:TYR:HB2	10:O:818:ASN:HD21	1.84	0.42
3:C:26:PHE:HD1	3:C:219:LEU:HD22	1.84	0.42
10:O:697:LEU:O	10:O:701:THR:OG1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.92	0.42
2:B:224:SER:OG	2:B:225:THR:N	2.52	0.42
1:A:688:ILE:HD11	1:A:737:VAL:HA	2.01	0.42
1:A:704:TYR:OH	2:B:662:ASP:OD2	2.35	0.42
2:B:728:LEU:HD12	2:B:728:LEU:HA	1.86	0.42
2:B:863:ASP:OD1	2:B:863:ASP:N	2.53	0.42
3:C:253:VAL:O	3:C:272:GLU:N	2.52	0.42
4:E:15:LEU:HD22	4:E:27:ILE:HG23	2.01	0.42
4:E:149:VAL:HG13	4:E:159:LEU:HD23	2.02	0.42
1:A:434:GLU:OE1	2:B:1068:ASN:ND2	2.41	0.42
1:A:1052:LYS:HE3	1:A:1075:VAL:HA	2.01	0.42
1:A:114:HIS:HD2	1:A:118:ARG:HH11	1.67	0.42
2:B:56:LEU:HD21	2:B:382:ARG:HA	2.02	0.42
2:B:302:LEU:HD12	2:B:306:GLU:HG3	2.02	0.42
2:B:350:ASP:OD1	2:B:350:ASP:N	2.41	0.42
5:F:138:SER:OG	5:F:139:VAL:N	2.53	0.42
2:B:103:PHE:HB3	2:B:116:LYS:HA	2.02	0.42
2:B:223:SER:HB3	2:B:230:THR:HG23	2.01	0.42
4:E:63:VAL:HA	4:E:82:ILE:O	2.20	0.42
1:A:683:TYR:HB3	1:A:718:ILE:HB	2.01	0.41
6:G:140:VAL:O	6:G:156:ALA:HA	2.20	0.41
8:L:210:MET:HE3	8:L:214:LYS:HE3	2.02	0.41
10:O:511:HIS:NE2	10:O:638:SER:O	2.53	0.41
1:A:925:PRO:HB2	1:A:928:ILE:HG22	2.03	0.41
3:C:81:VAL:HG12	3:C:143:ALA:HB3	2.02	0.41
7:J:42:LEU:HD23	7:J:42:LEU:HA	1.88	0.41
3:C:37:ILE:HB	3:C:144:PHE:HB2	2.02	0.41
1:A:560:LYS:HB3	1:A:560:LYS:HE2	1.78	0.41
12:S:71:LYS:HE2	12:S:71:LYS:HB3	1.81	0.41
2:B:57:LEU:HB2	2:B:66:ILE:HD12	2.03	0.41
2:B:74:LYS:O	2:B:96:ALA:HA	2.20	0.41
2:B:1078:GLU:OE2	5:F:95:ARG:NH2	2.54	0.41
10:O:43:ILE:HG22	10:O:44:LYS:HG2	2.03	0.41
10:O:592:ARG:HA	10:O:673:ASN:HD22	1.86	0.41
3:C:11:VAL:HG11	3:C:195:LYS:HE2	2.03	0.41
10:O:166:LEU:HD22	10:O:176:LEU:HA	2.03	0.41
1:A:621:LEU:HD22	1:A:625:LEU:HD23	2.02	0.41
1:A:748:GLU:HB3	1:A:942:ALA:HB1	2.02	0.41
1:A:863:MET:HE2	1:A:863:MET:HB3	2.00	0.41
4:E:29:ARG:NH1	4:E:108:ASP:OD1	2.43	0.41
10:O:693:VAL:HG12	10:O:694:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HA	1:A:126:LYS:HD3	1.82	0.41
1:A:1017:VAL:HG22	1:A:1071:TYR:HD1	1.84	0.41
2:B:802:GLU:HG3	2:B:808:ARG:HB3	2.03	0.41
2:B:988:LYS:HD2	2:B:988:LYS:HA	1.83	0.41
2:B:247:PHE:CZ	2:B:525:GLU:HB2	2.56	0.41
2:B:1046:LYS:NZ	13:T:31:DG:OP2	2.42	0.41
2:B:1089:ASN:HB2	2:B:1113:PRO:HB3	2.03	0.41
7:J:32:LEU:HD22	7:J:41:ARG:HG2	2.03	0.41
10:O:15:ILE:HD11	10:O:212:LEU:HB3	2.02	0.41
10:O:51:THR:HG23	10:O:474:VAL:HG23	2.02	0.41
12:S:110:THR:HG21	12:S:114:GLU:HB2	2.03	0.41
1:A:700:ARG:NH1	1:A:705:TYR:O	2.44	0.41
1:A:746:VAL:O	1:A:749:THR:OG1	2.32	0.41
1:A:1216:ASP:HB3	1:A:1219:ALA:HB2	2.02	0.41
2:B:461:LYS:HD3	2:B:461:LYS:HA	1.95	0.41
5:F:151:LEU:HD23	5:F:151:LEU:HA	1.89	0.41
8:L:39:TYR:HD2	8:L:166:ILE:HD12	1.85	0.41
1:A:449:ILE:HG13	1:A:933:VAL:HG21	2.03	0.40
1:A:1276:LYS:NZ	10:O:56:ILE:O	2.53	0.40
2:B:1061:LEU:HA	2:B:1061:LEU:HD23	1.89	0.40
3:C:92:ASN:ND2	3:C:129:GLN:O	2.54	0.40
10:O:635:LYS:HB3	10:O:635:LYS:HE2	1.90	0.40
1:A:550:SER:OG	1:A:551:ASN:N	2.54	0.40
2:B:178:PRO:HB3	2:B:192:PHE:HB3	2.03	0.40
8:L:42:ASN:ND2	10:O:795:SER:OG	2.54	0.40
10:O:263:GLY:CA	10:O:304:ALA:O	2.70	0.40
10:O:274:GLY:HA2	10:O:290:VAL:HG13	2.03	0.40
1:A:978:ILE:HG12	1:A:1145:PRO:HA	2.03	0.40
3:C:300:SER:O	3:C:304:ARG:NE	2.50	0.40
10:O:562:ARG:HG2	10:O:566:GLY:HA3	2.03	0.40
1:A:816:LEU:HD21	1:A:886:GLU:HB3	2.03	0.40
2:B:1112:SER:HA	2:B:1113:PRO:HD3	1.90	0.40
12:S:69:GLU:O	12:S:73:ASN:N	2.52	0.40
1:A:672:ASN:OD1	1:A:675:GLU:HG2	2.21	0.40
3:C:117:PRO:HG2	3:C:120:LEU:HG	2.04	0.40
8:L:130:ILE:HD13	8:L:260:HIS:CE1	2.57	0.40
10:O:186:ARG:NH2	10:O:504:GLU:O	2.55	0.40
12:S:41:ILE:HD13	12:S:121:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1283/1286 (100%)	1229 (96%)	54 (4%)	0	100	100
2	B	1121/1164 (96%)	1077 (96%)	44 (4%)	0	100	100
3	C	301/305 (99%)	289 (96%)	12 (4%)	0	100	100
4	E	182/185 (98%)	176 (97%)	6 (3%)	0	100	100
5	F	101/164 (62%)	100 (99%)	1 (1%)	0	100	100
6	G	127/161 (79%)	118 (93%)	9 (7%)	0	100	100
7	J	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
8	L	285/287 (99%)	268 (94%)	17 (6%)	0	100	100
10	O	814/844 (96%)	779 (96%)	35 (4%)	0	100	100
12	S	109/259 (42%)	102 (94%)	7 (6%)	0	100	100
All	All	4382/4718 (93%)	4196 (96%)	186 (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	1156/1157 (100%)	1155 (100%)	1 (0%)	88	90
2	B	1030/1064 (97%)	1030 (100%)	0	100	100
3	C	285/287 (99%)	285 (100%)	0	100	100
4	E	174/175 (99%)	173 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	94/151 (62%)	94 (100%)	0	100	100
6	G	118/144 (82%)	118 (100%)	0	100	100
7	J	60/62 (97%)	60 (100%)	0	100	100
8	L	272/272 (100%)	272 (100%)	0	100	100
10	O	756/774 (98%)	755 (100%)	1 (0%)	88	90
12	S	105/240 (44%)	105 (100%)	0	100	100
All	All	4050/4326 (94%)	4047 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	ASP
4	E	177	ASP
10	O	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	114	HIS
1	A	140	GLN
1	A	184	GLN
1	A	218	ASN
1	A	299	ASN
1	A	332	ASN
1	A	339	ASN
1	A	412	GLN
1	A	435	GLN
1	A	459	GLN
1	A	548	HIS
1	A	720	ASN
1	A	881	ASN
1	A	894	ASN
1	A	941	GLN
1	A	947	HIS
1	A	957	GLN
1	A	994	ASN
1	A	1140	ASN
1	A	1217	ASN

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Mol	Chain	Res	Type
1	A	1239	HIS
2	B	32	HIS
2	B	61	ASN
2	B	101	ASN
2	B	169	ASN
2	B	265	ASN
2	B	305	ASN
2	B	376	ASN
2	B	391	ASN
2	B	408	ASN
2	B	429	HIS
2	B	431	HIS
2	B	487	GLN
2	B	496	ASN
2	B	541	ASN
2	B	576	ASN
2	B	620	GLN
2	B	682	ASN
2	B	693	GLN
2	B	740	GLN
2	B	766	GLN
2	B	778	HIS
2	B	789	ASN
2	B	858	GLN
2	B	967	GLN
2	B	977	ASN
2	B	1023	GLN
2	B	1040	GLN
3	C	129	GLN
3	C	137	GLN
3	C	230	HIS
4	E	129	GLN
4	E	168	ASN
5	F	119	GLN
6	G	7	ASN
6	G	29	ASN
6	G	80	HIS
6	G	100	GLN
7	J	16	HIS
7	J	37	ASN
7	J	47	GLN
7	J	51	GLN

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Mol	Chain	Res	Type
7	J	53	ASN
8	L	13	HIS
8	L	42	ASN
8	L	51	ASN
8	L	122	HIS
8	L	234	ASN
8	L	260	HIS
8	L	276	ASN
8	L	278	HIS
8	L	279	GLN
10	O	35	ASN
10	O	70	ASN
10	O	86	HIS
10	O	254	ASN
10	O	397	ASN
10	O	455	ASN
10	O	466	ASN
10	O	521	GLN
10	O	550	ASN
10	O	818	ASN
12	S	36	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	P	15/30 (50%)	4 (26%)	1 (6%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	P	20	A
11	P	21	A
11	P	22	U
11	P	24	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	P	19	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	GDP	P	1	11	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GDP	P	1	11	-	5/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	1	GDP	C5-C4	3.06	1.47	1.38
11	P	1	GDP	C6-N1	-2.44	1.34	1.38
11	P	1	GDP	C5-N7	-2.08	1.34	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	1	GDP	C5-C4-N3	-5.99	118.86	128.39
11	P	1	GDP	C2-N3-C4	4.99	120.89	112.30
11	P	1	GDP	N9-C4-N3	4.48	134.92	125.95
11	P	1	GDP	C6-C5-N7	3.23	136.18	130.29
11	P	1	GDP	C4-C5-N7	-2.49	106.73	110.67
11	P	1	GDP	O6-C6-C5	-2.14	120.88	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	P	1	GDP	C5'-O5'-PA-O3A
11	P	1	GDP	C5'-O5'-PA-O1A
11	P	1	GDP	C5'-O5'-PA-O2A
11	P	1	GDP	PB-O3A-PA-O2A
11	P	1	GDP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	1	GDP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
16	SAM	O	901	-	27,29,29	1.07	4 (14%)	34,42,42	2.16	9 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SAM	O	901	-	-	9/17/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	901	SAM	C2-N3	2.49	1.38	1.33
16	O	901	SAM	C2-N1	2.28	1.38	1.33
16	O	901	SAM	OXT-C	-2.25	1.23	1.30
16	O	901	SAM	C5-N7	-2.22	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	901	SAM	C5-C4-N3	-5.53	119.10	126.72
16	O	901	SAM	N3-C2-N1	-5.52	120.23	128.58
16	O	901	SAM	N3-C4-N9	3.85	133.72	127.17
16	O	901	SAM	C2-N3-C4	3.82	121.16	111.83
16	O	901	SAM	C5-N7-C8	3.61	109.12	103.45
16	O	901	SAM	N9-C8-N7	-3.60	108.83	113.94
16	O	901	SAM	OXT-C-O	-2.64	118.09	124.08
16	O	901	SAM	C4-C5-N7	-2.53	107.69	110.58
16	O	901	SAM	C6-C5-C4	2.25	120.24	117.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

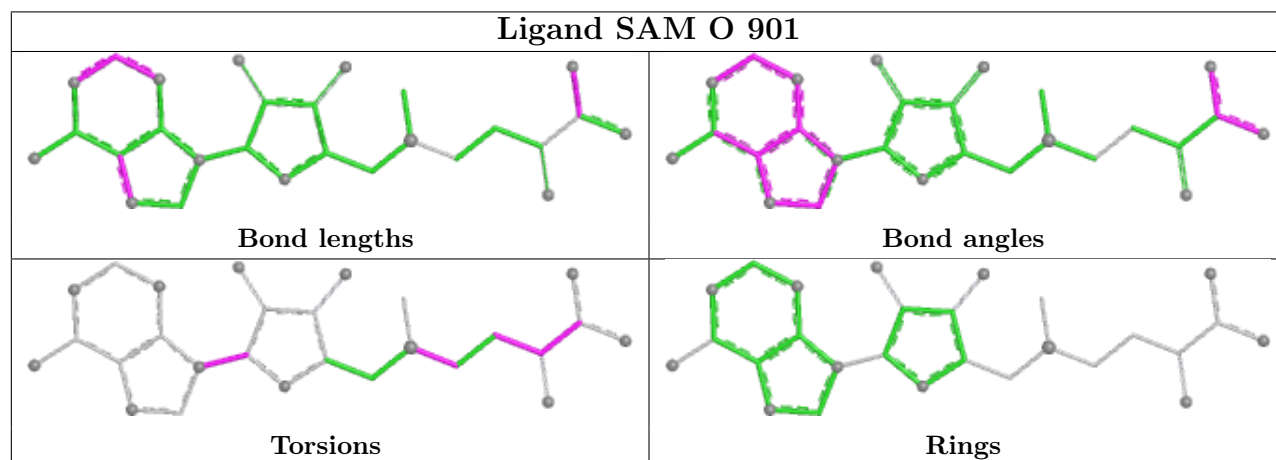
Mol	Chain	Res	Type	Atoms
16	O	901	SAM	O-C-CA-N
16	O	901	SAM	N-CA-CB-CG
16	O	901	SAM	C-CA-CB-CG
16	O	901	SAM	CB-CG-SD-CE
16	O	901	SAM	OXT-C-CA-N
16	O	901	SAM	O-C-CA-CB
16	O	901	SAM	OXT-C-CA-CB
16	O	901	SAM	CB-CG-SD-C5'
16	O	901	SAM	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

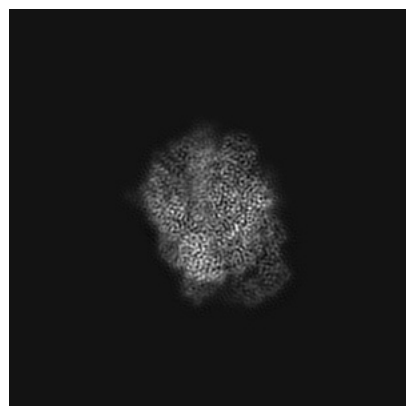
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4890. These allow visual inspection of the internal detail of the map and identification of artifacts.

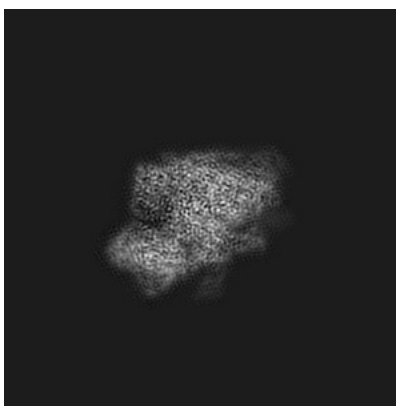
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

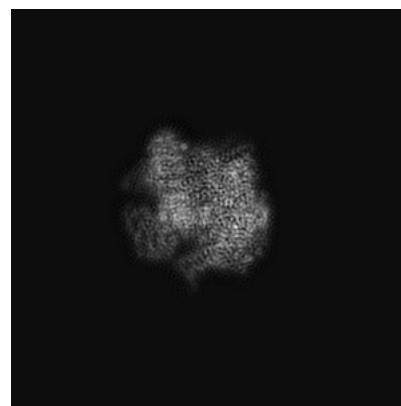
6.1.1 Primary map



X

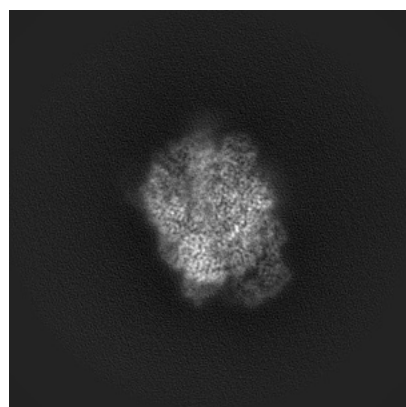


Y

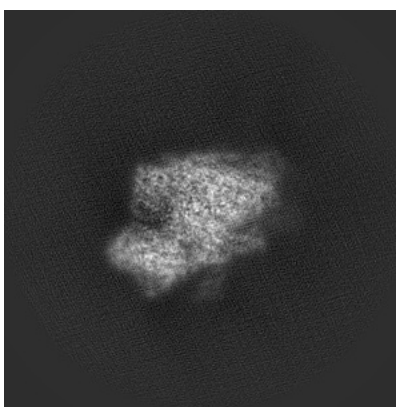


Z

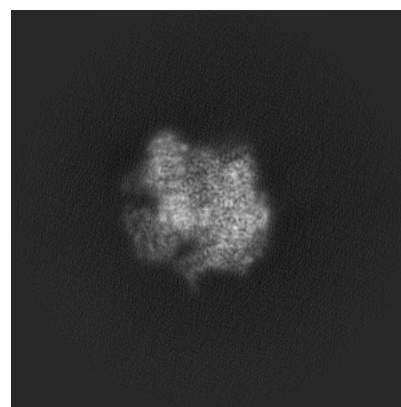
6.1.2 Raw map



X



Y

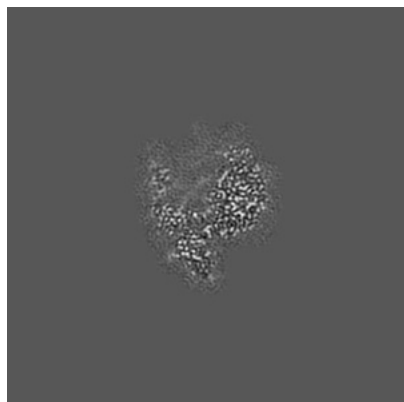


Z

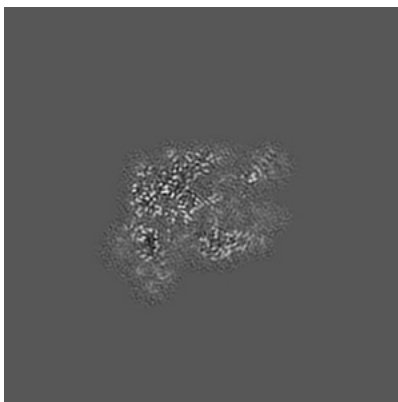
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

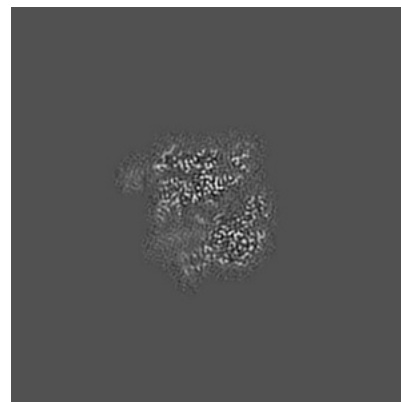
6.2.1 Primary map



X Index: 170

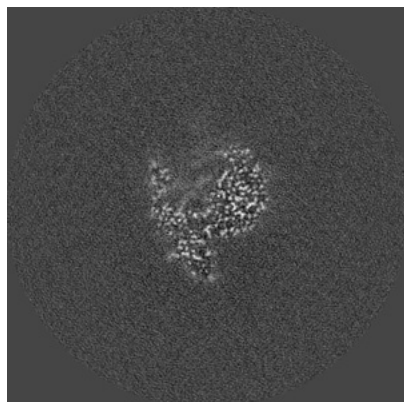


Y Index: 170

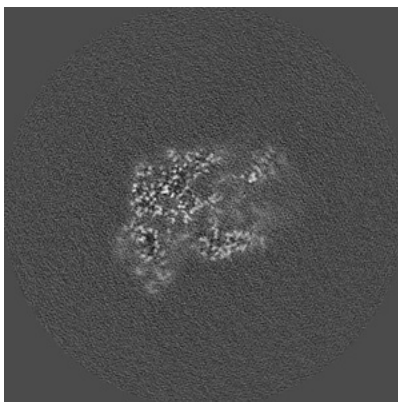


Z Index: 170

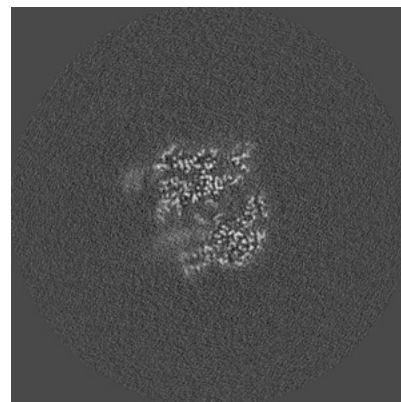
6.2.2 Raw map



X Index: 170



Y Index: 170

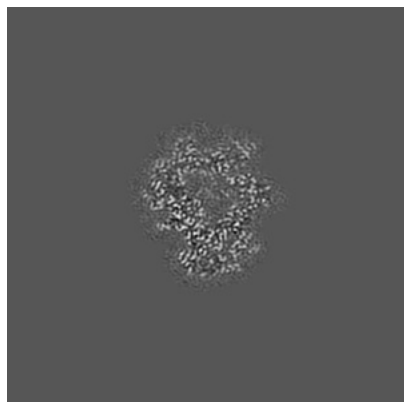


Z Index: 170

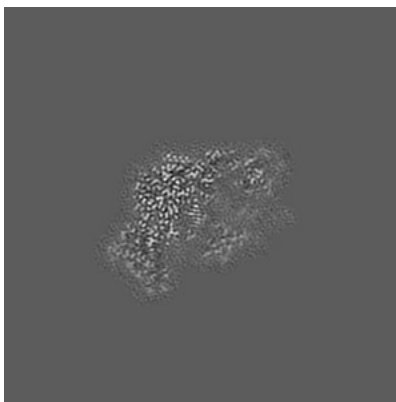
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

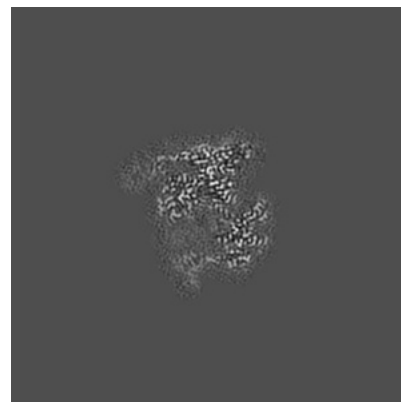
6.3.1 Primary map



X Index: 191

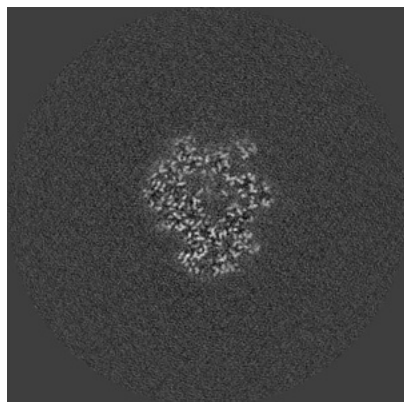


Y Index: 159

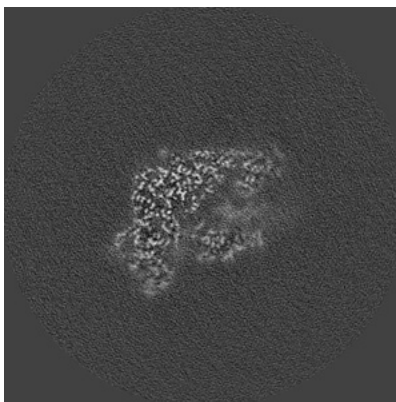


Z Index: 177

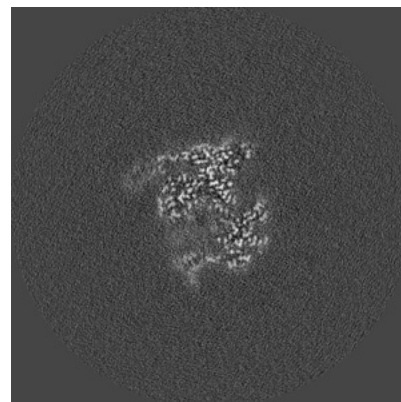
6.3.2 Raw map



X Index: 192



Y Index: 164

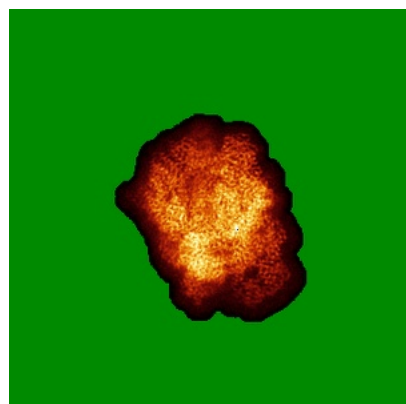


Z Index: 177

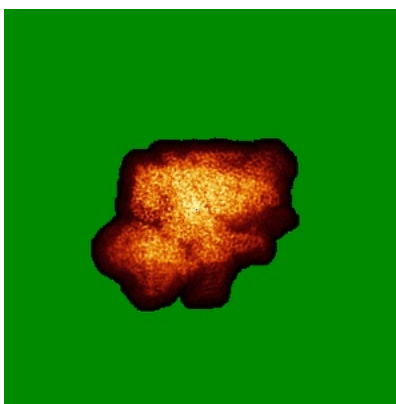
The images above show the largest variance slices of the map in three orthogonal directions.

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

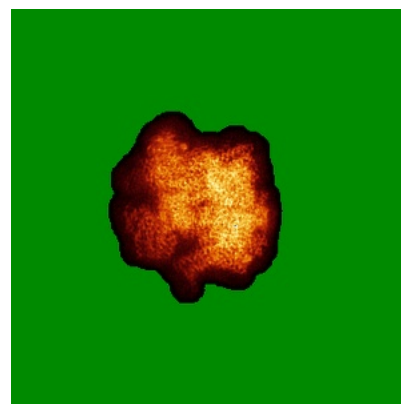
6.4.1 Primary map



X

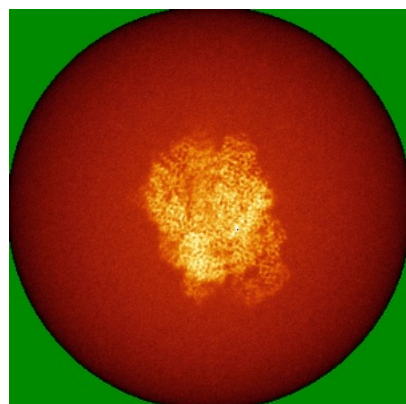


Y

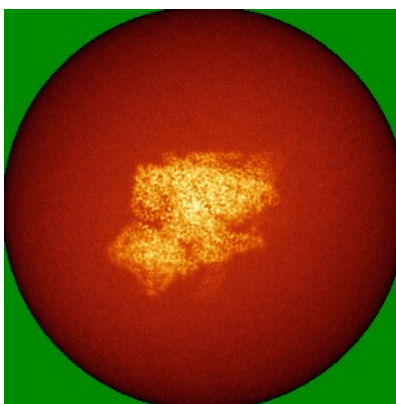


Z

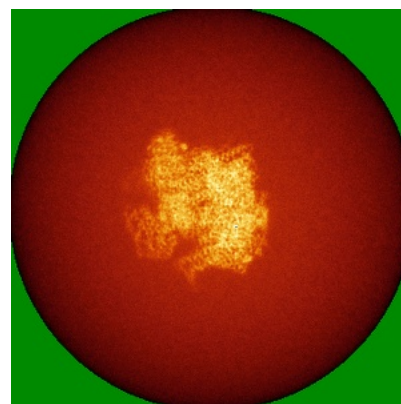
6.4.2 Raw map



X



Y

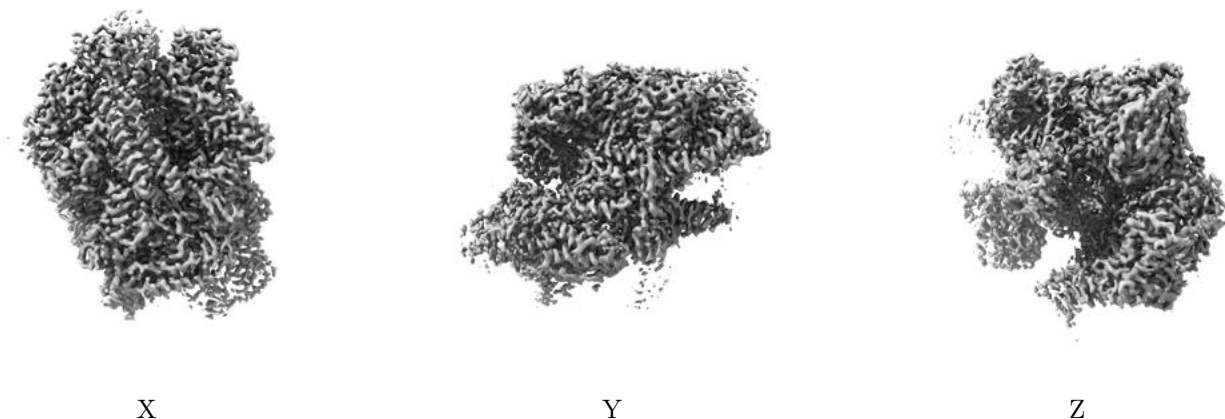


Z

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

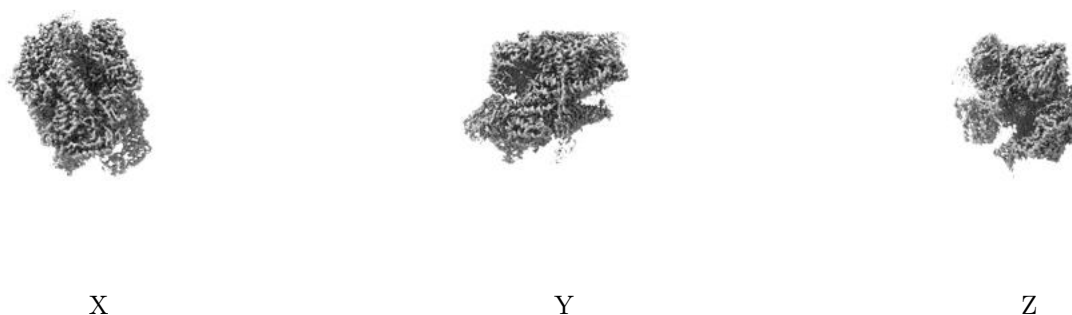
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

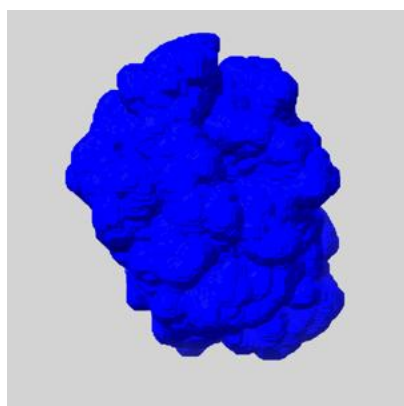
6.6 Mask visualisation [i](#)

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

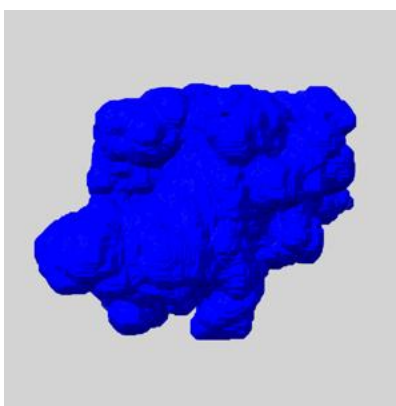
A mask typically either:

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

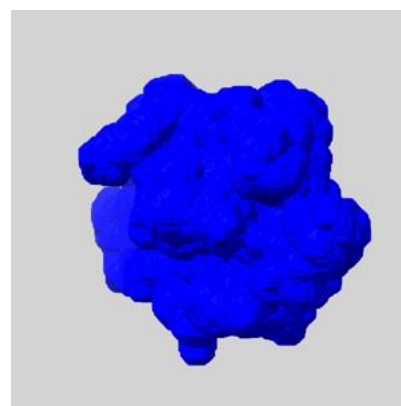
6.6.1 emd_4890_msk_1.map [i](#)



X



Y

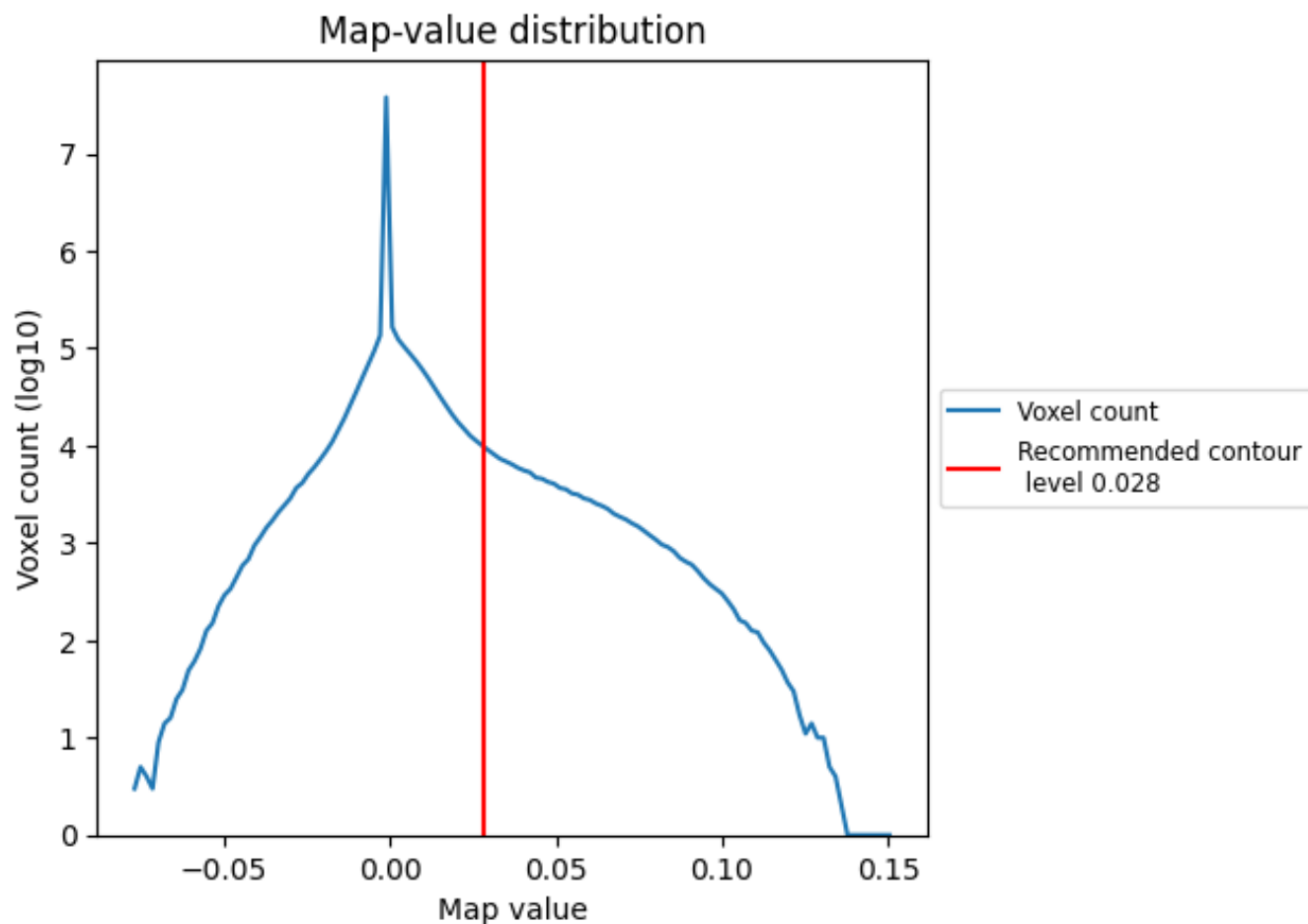


Z

7 Map analysis [i](#)

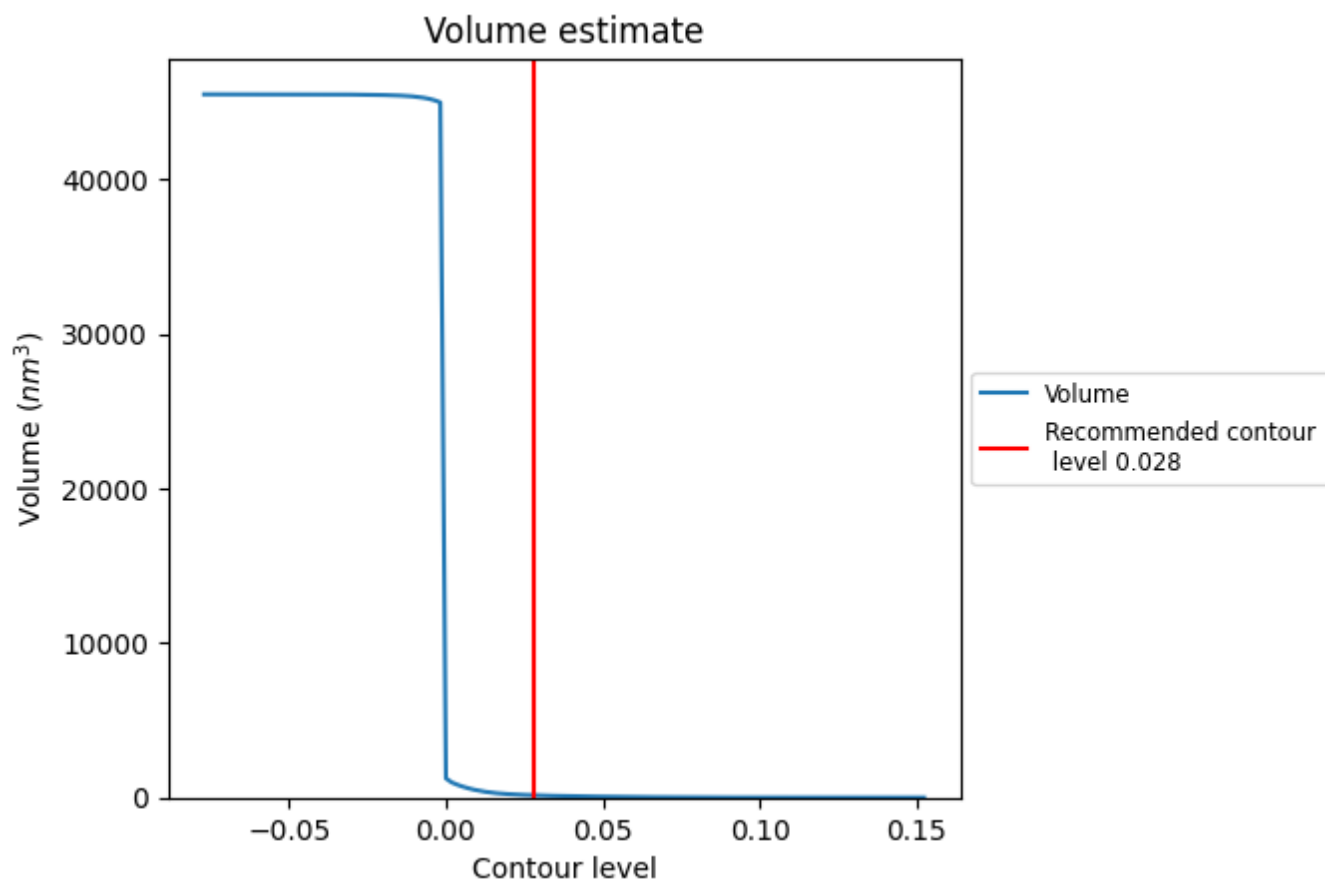
This section contains the results of statistical analysis of the map.

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.

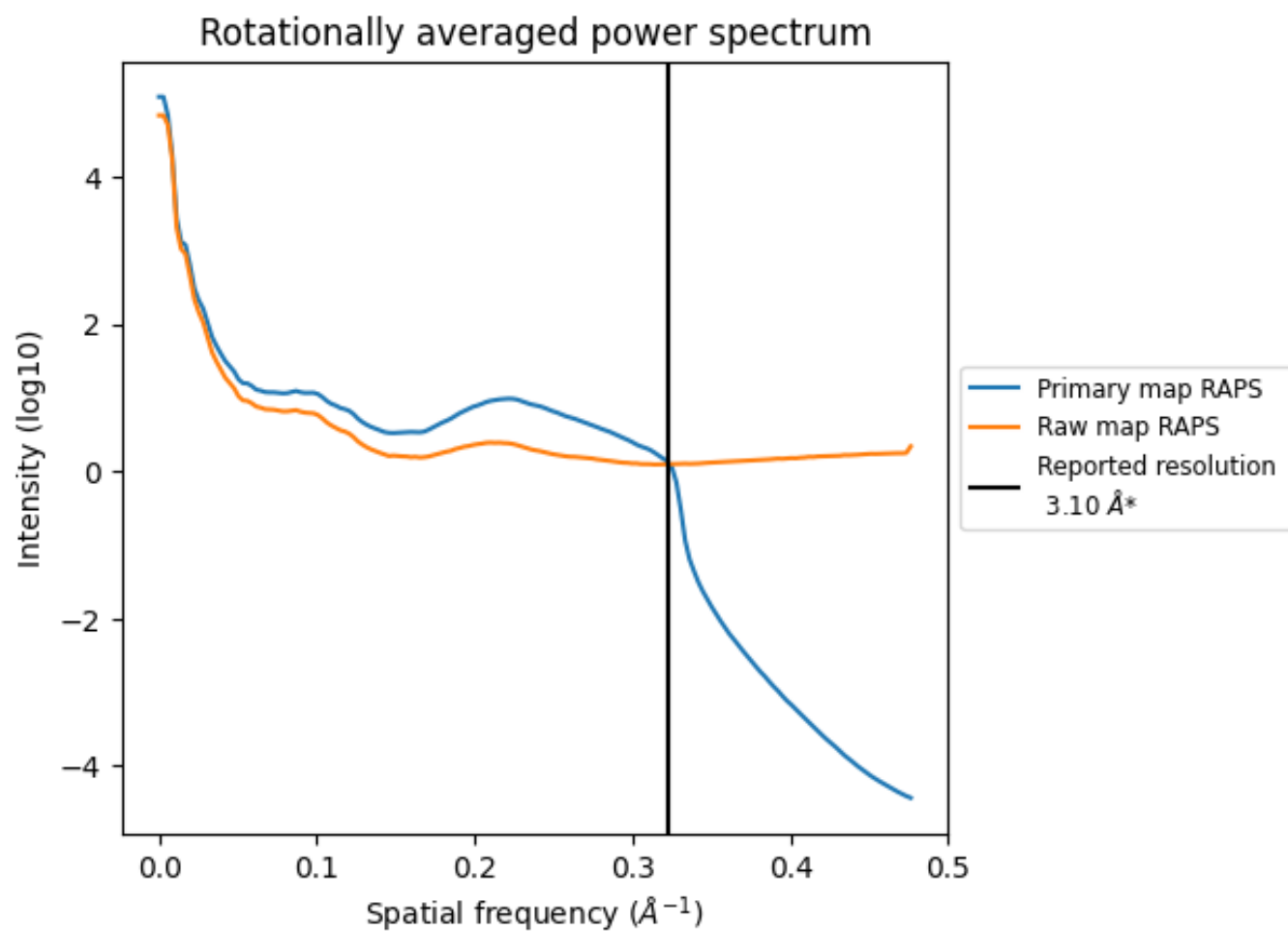
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

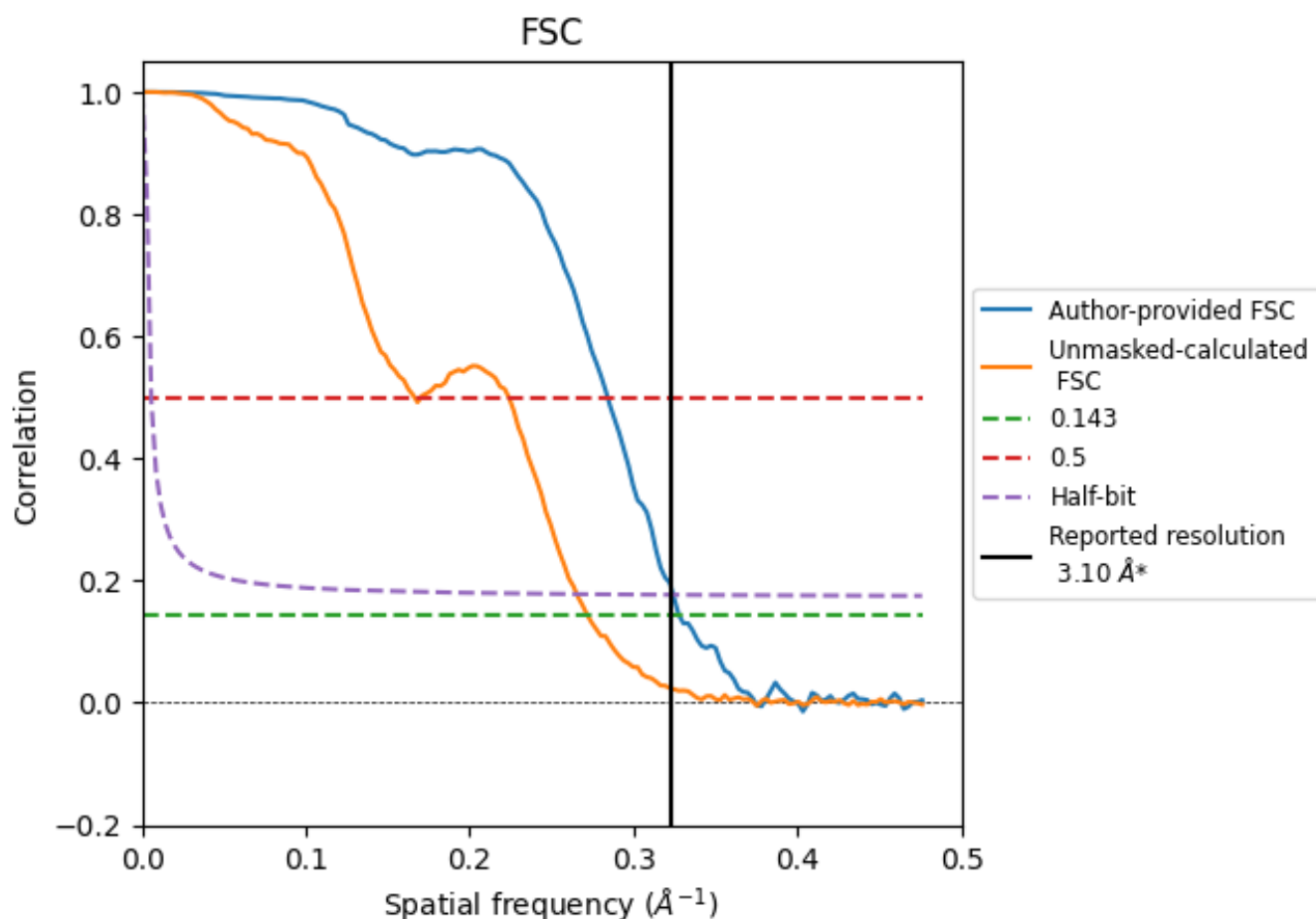


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

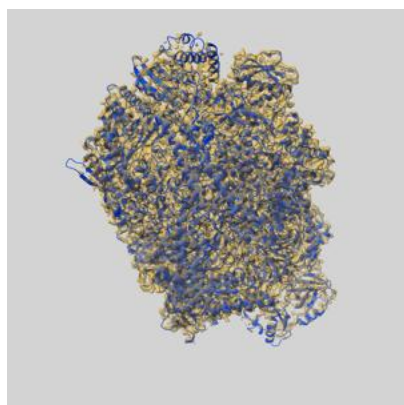
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.52	3.08
Unmasked-calculated*	3.68	6.02	3.77

*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 %

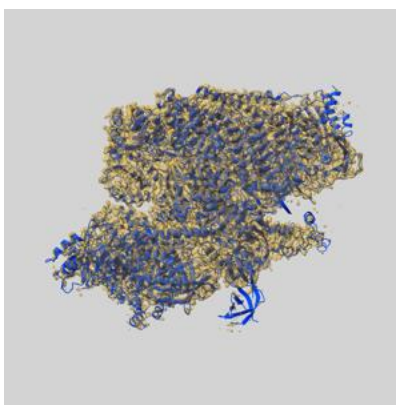
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4890 and PDB model 6RIE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

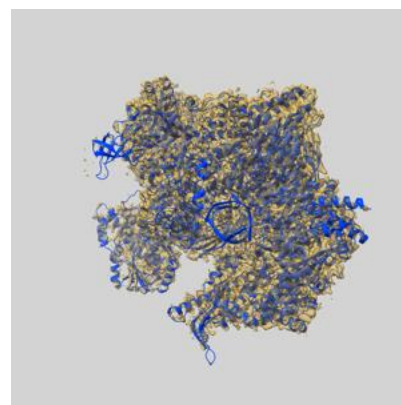
9.1 Map-model overlay [i](#)



X



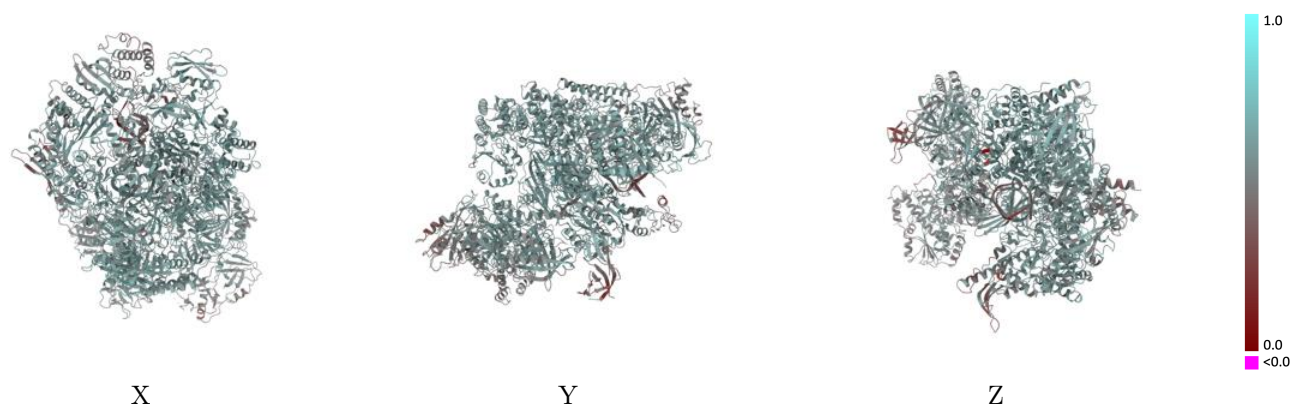
Y



Z

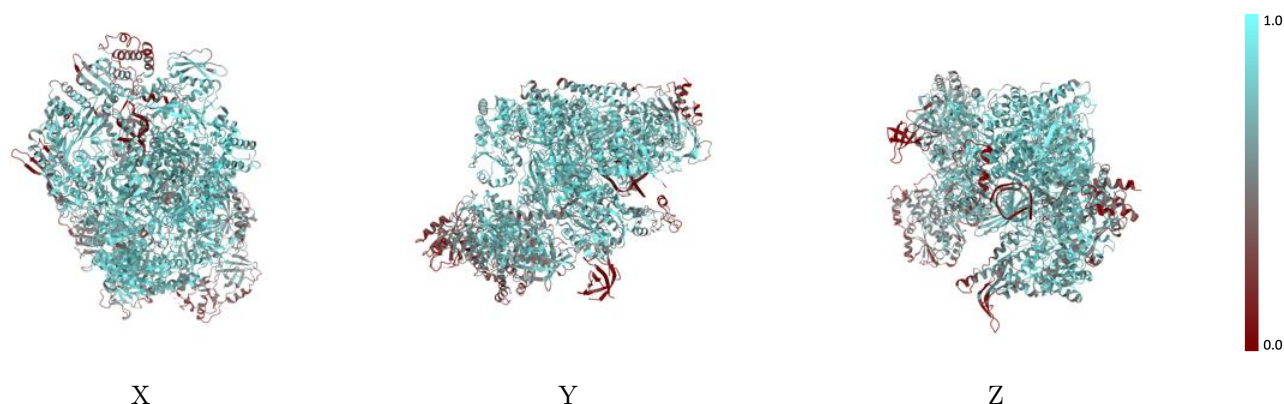
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



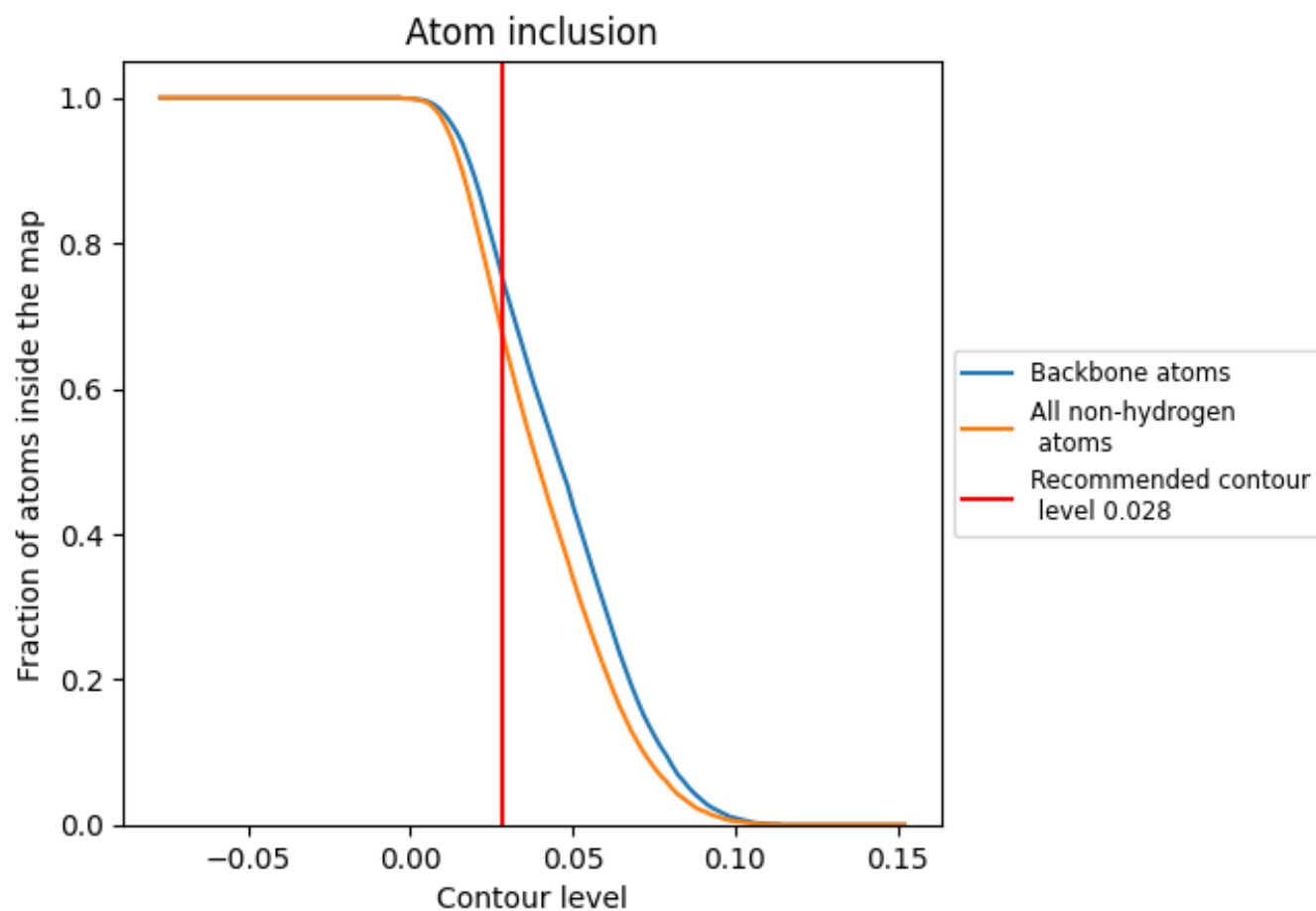
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.5580
A	0.7330	0.5720
B	0.7530	0.5740
C	0.7870	0.5870
E	0.7650	0.5850
F	0.8190	0.6030
G	0.4360	0.4920
J	0.8380	0.6000
L	0.4490	0.5000
N	0.0700	0.3530
O	0.6030	0.5400
P	0.7200	0.5360
S	0.3720	0.4980
T	0.5080	0.4670

1.0

0.0

<0.0