



Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 04:47 pm BST

PDB ID : 9G27 / pdb_00009g27
EMDB ID : EMD-50966
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site, pre-translocation state
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 2.80 Å(reported)
Based on initial model : 6hko

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

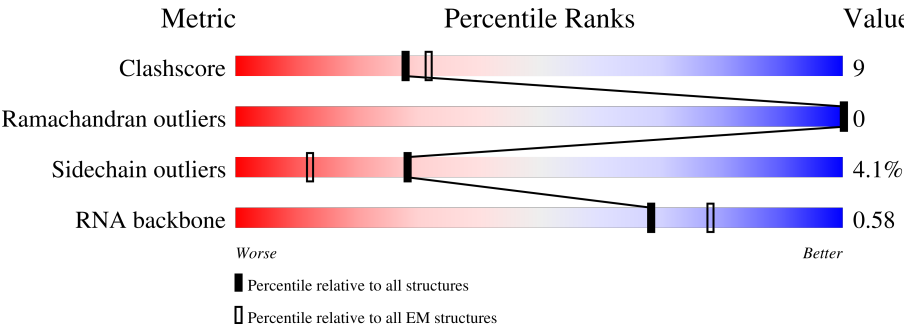
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1664	<div> <div>6%</div> <div>64%</div> <div>22%</div> <div>•</div> <div>13%</div> </div>
2	B	1203	<div> <div>•</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
3	C	335	<div> <div>•</div> <div>70%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>
4	D	137	<div> <div>10%</div> <div>•</div> <div>87%</div> </div>
5	E	215	<div> <div>14%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>
6	F	155	<div> <div>•</div> <div>50%</div> <div>15%</div> <div>35%</div> </div>
7	G	326	<div> <div>5%</div> <div>20%</div> <div>7%</div> <div>73%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	R	13	
14	S	38	
15	T	38	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31262 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1451	Total	C	N	O	S	0	0
			11462	7240	1993	2168	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1159	Total	C	N	O	S	0	0
			9214	5828	1619	1716	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2415	1535	414	458	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	18	Total	C	N	O	0	0
			133	84	23	26		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			827	524	145	155	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	88	Total	C	N	O	S	0	0
			700	462	111	123	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	93	Total	C	N	O	S	0	0
			707	442	119	140	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			766	481	124	156	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

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

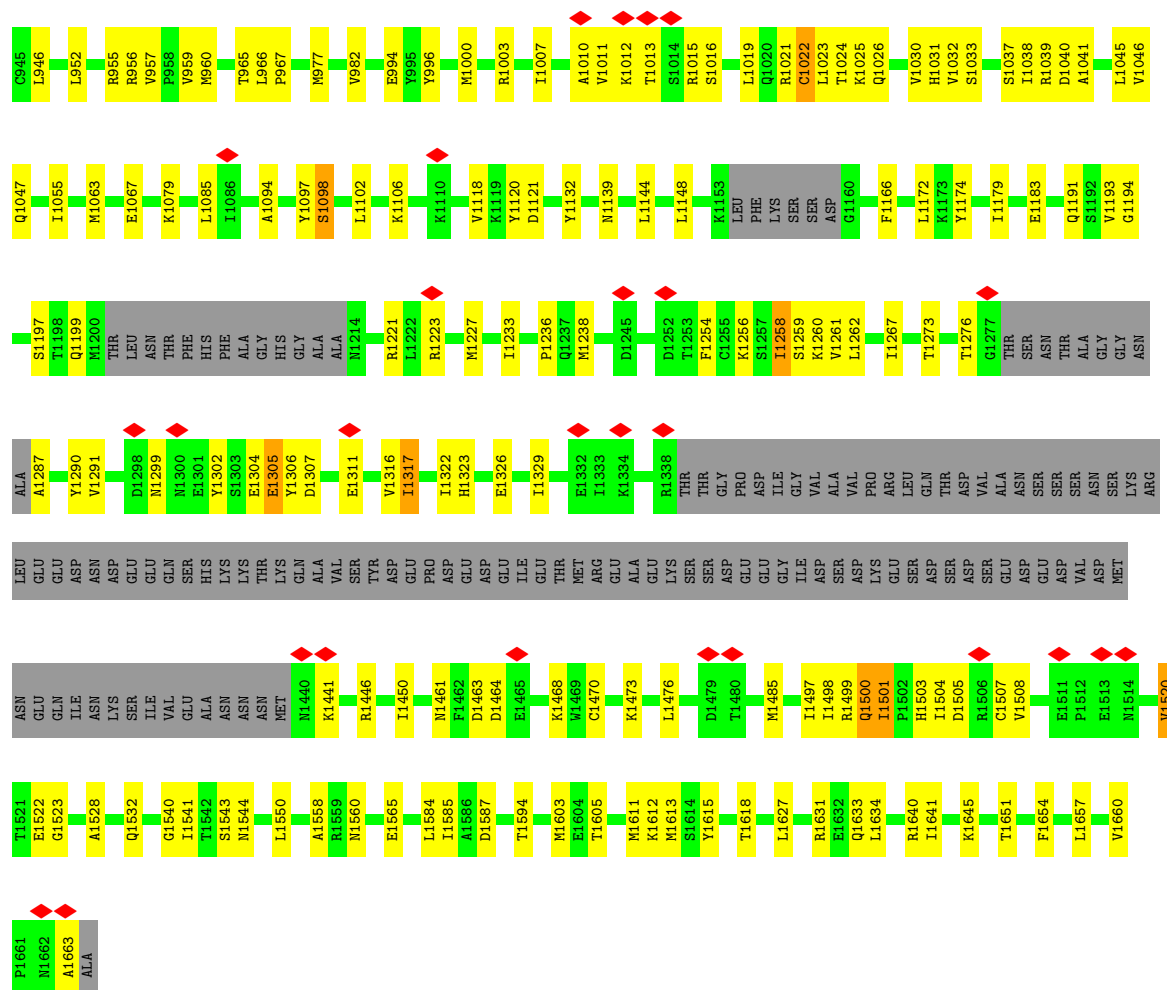
Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	23	Total	C	N	O	P	0	0
			468	224	79	142	23		

- Molecule 15 is a DNA chain called Template DNA.

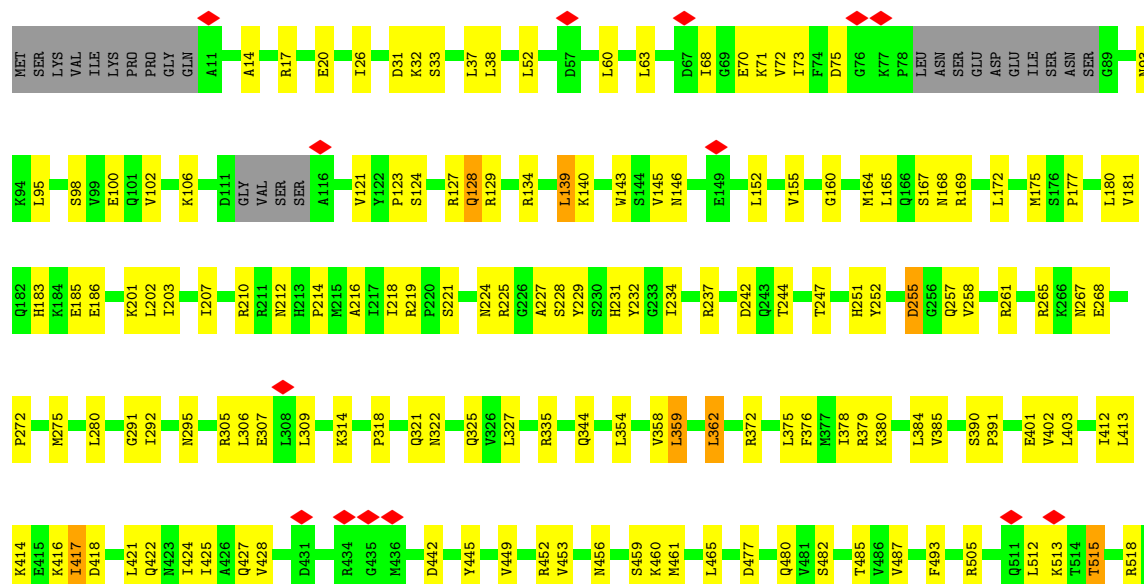
Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	32	Total	C	N	O	P	0	0
			643	307	112	192	32		

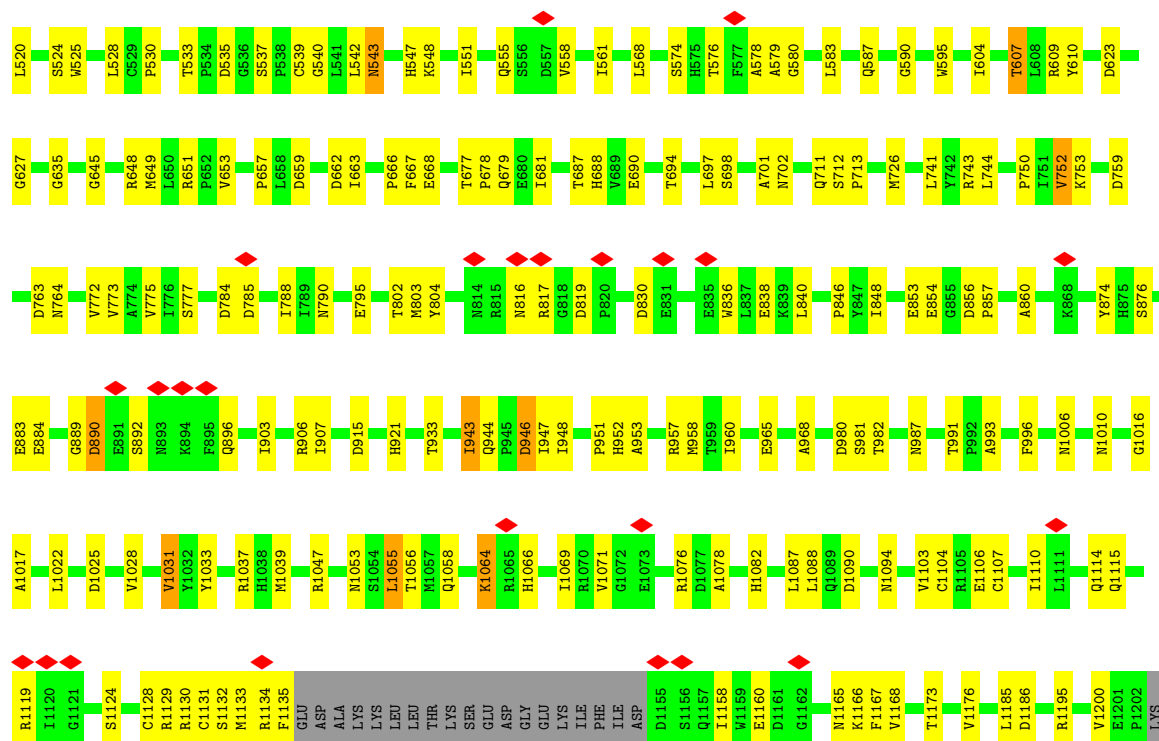
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	1	Total	Zn	0
			1	1	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	



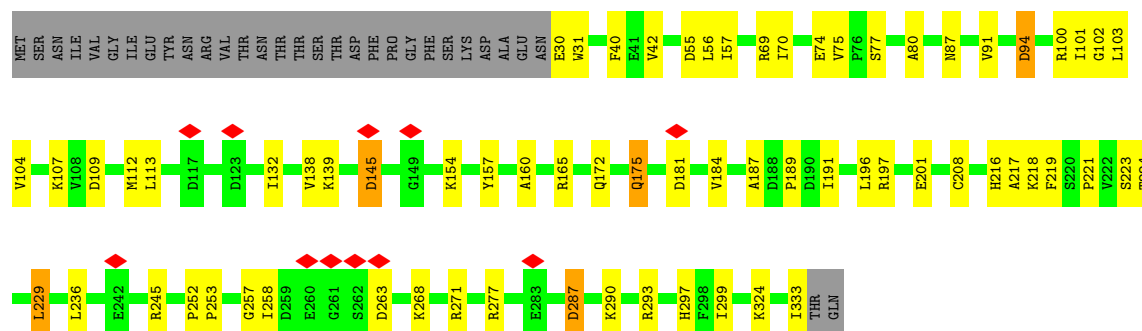
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135





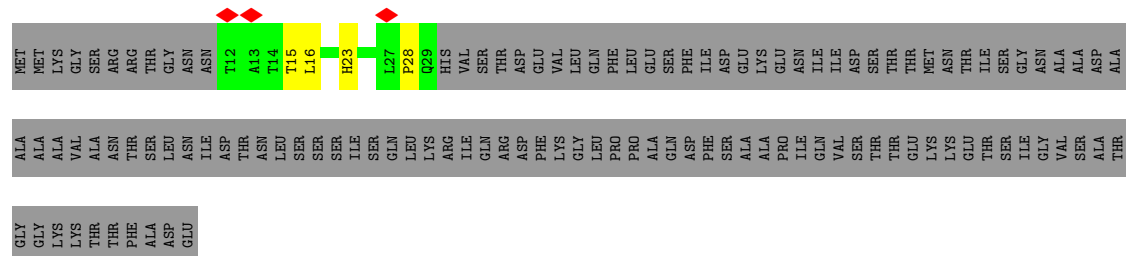
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 70% 19% 9%

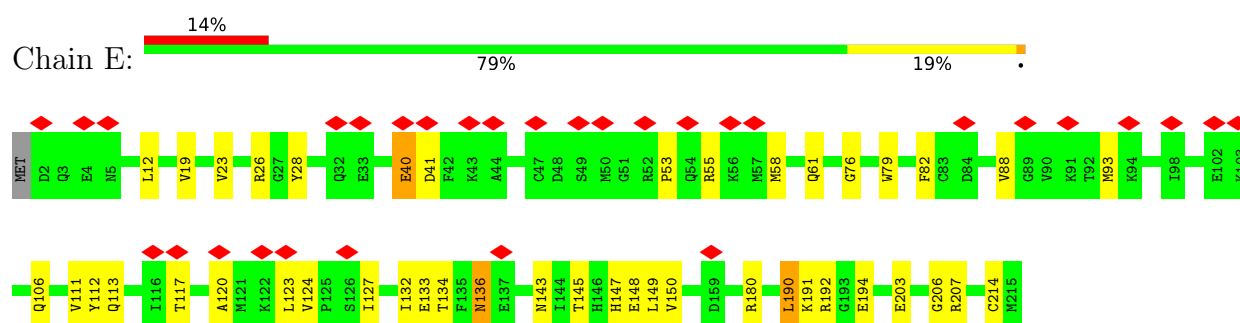


• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

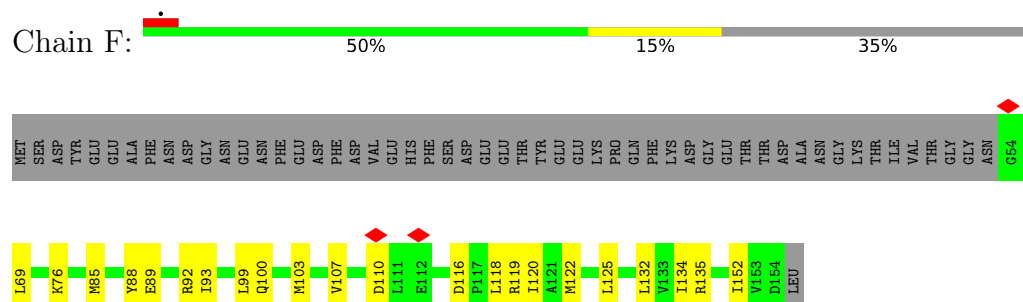
Chain D: 10% 87%



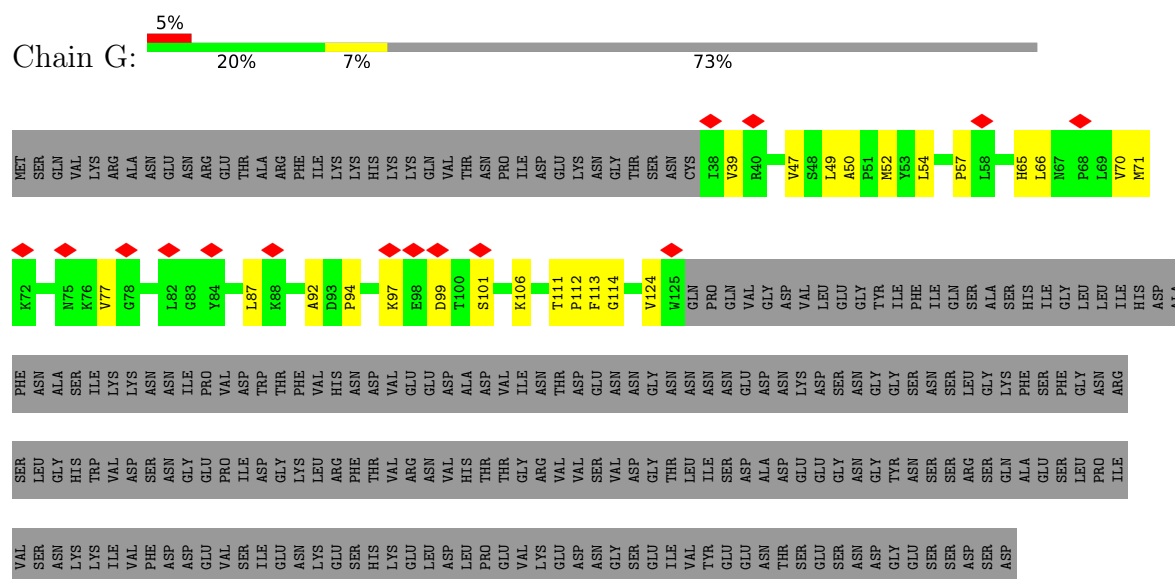
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



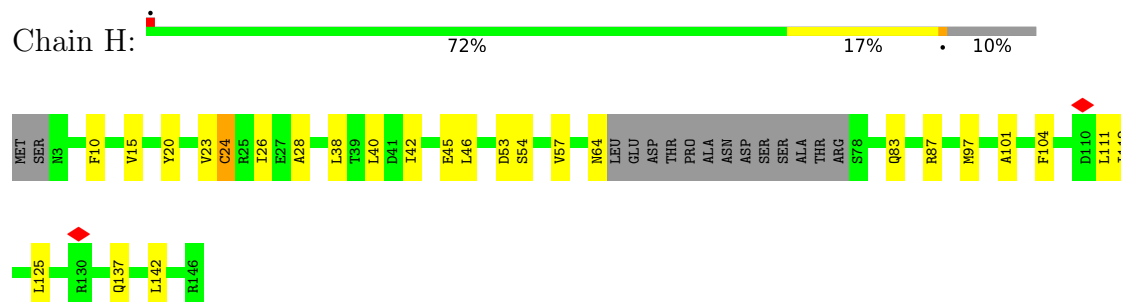
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



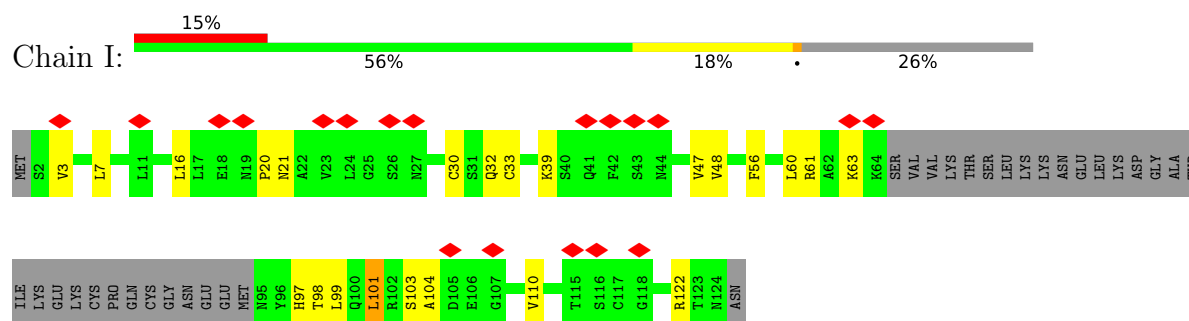
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43



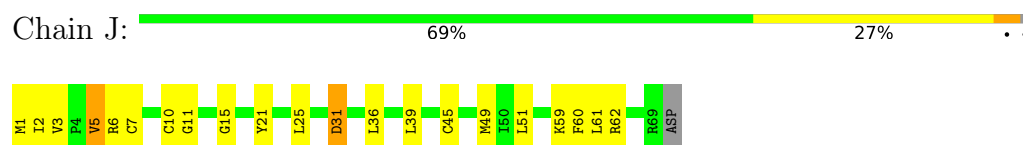
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



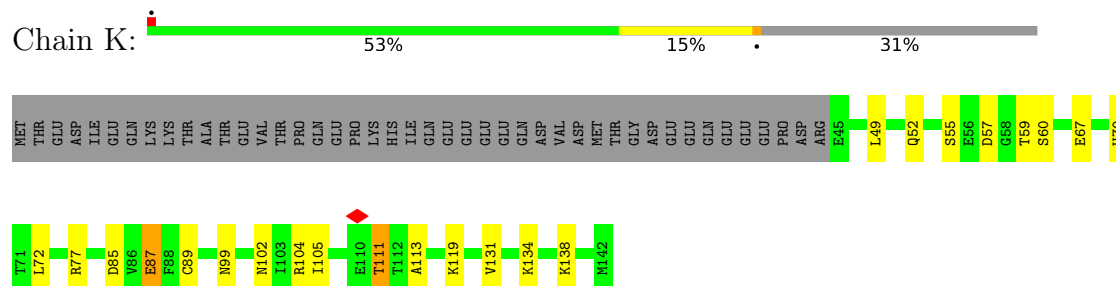
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



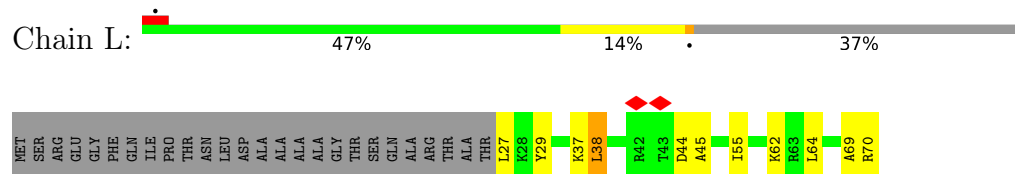
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



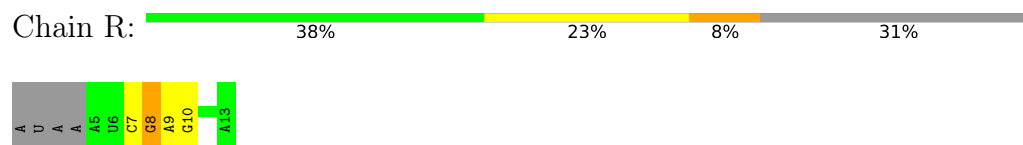
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



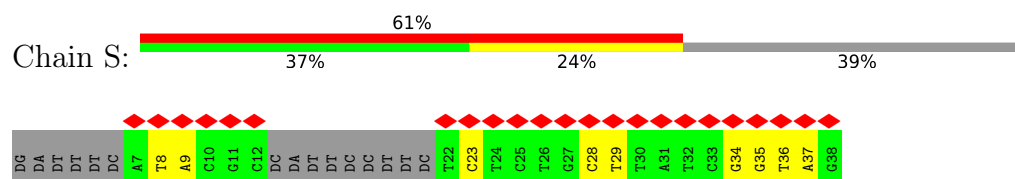
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



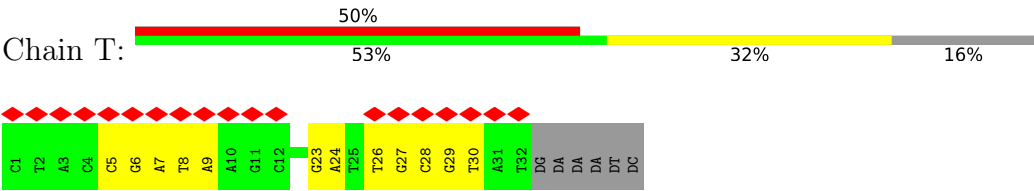
- Molecule 13: RNA



- Molecule 14: Non-template DNA



● Molecule 15: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.569	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0759	Depositor
Map size (\AA)	323.0, 323.0, 323.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.646, 0.646, 0.646	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: ZN, 3DR

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	0.14	0/11670	0.30	0/15758
2	B	0.15	0/9419	0.30	0/12733
3	C	0.14	0/2467	0.26	0/3344
4	D	0.09	0/135	0.31	0/188
5	E	0.11	0/1787	0.27	0/2406
6	F	0.13	0/842	0.27	0/1135
7	G	0.11	0/719	0.25	0/981
8	H	0.12	0/1070	0.25	0/1449
9	I	0.10	0/718	0.29	0/971
10	J	0.16	0/578	0.27	0/775
11	K	0.12	0/776	0.27	0/1047
12	L	0.14	0/354	0.30	0/468
13	R	0.12	0/221	0.26	0/343
14	S	0.17	0/521	0.35	0/799
15	T	0.21	0/706	0.41	0/1084
All	All	0.14	0/31983	0.29	0/43481

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	11462	0	11548	257	0
2	B	9214	0	9104	211	0
3	C	2415	0	2403	48	0
4	D	133	0	138	3	0
5	E	1751	0	1776	27	0
6	F	827	0	843	16	0
7	G	700	0	720	17	0
8	H	1052	0	1021	13	0
9	I	707	0	688	17	0
10	J	569	0	585	16	0
11	K	766	0	765	17	0
12	L	352	0	374	9	0
13	R	197	0	99	2	0
14	S	468	0	263	6	0
15	T	643	0	359	7	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	31262	0	30686	582	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 9.

All (582) 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:836:TRP:HB2	2:B:857:PRO:HG3	1.59	0.84
2:B:172:LEU:HD21	2:B:185:GLU:HG3	1.69	0.74
2:B:607:THR:OG1	9:I:101:LEU:O	2.04	0.73
1:A:641:GLU:HB2	6:F:99:LEU:HD12	1.69	0.73
2:B:321:GLN:O	9:I:32:GLN:NE2	2.22	0.72
2:B:623:ASP:O	2:B:648:ARG:NH2	2.21	0.72
2:B:1103:VAL:HG22	2:B:1110:ILE:HG22	1.71	0.71
1:A:826:PHE:HB3	2:B:777:SER:HB3	1.74	0.70
2:B:314:LYS:NZ	9:I:16:LEU:O	2.24	0.70
1:A:1221:ARG:NH2	1:A:1565:GLU:OE2	2.26	0.69
3:C:139:LYS:HG3	3:C:201:GLU:HB3	1.73	0.68
2:B:677:THR:HG22	2:B:679:GLN:H	1.59	0.68
2:B:70:GLU:HB3	2:B:98:SER:HB3	1.76	0.68
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.27	0.68
2:B:214:PRO:O	2:B:380:LYS:NZ	2.26	0.68
1:A:336:GLN:HE21	1:A:350:VAL:HG12	1.60	0.67
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	1.76	0.67
1:A:461:GLU:HG3	1:A:462:LYS:HG3	1.75	0.67
1:A:498:PRO:HB3	1:A:611:GLU:HA	1.77	0.66
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.75	0.66
1:A:1446:ARG:NH2	1:A:1464:ASP:OD2	2.28	0.66
1:A:1030:VAL:HG11	1:A:1584:LEU:HD11	1.78	0.66
7:G:111:THR:HG22	7:G:113:PHE:H	1.59	0.66
3:C:104:VAL:HG23	3:C:191:ILE:HD12	1.79	0.65
2:B:255:ASP:OD1	2:B:255:ASP:N	2.28	0.65
2:B:128:GLN:HB3	12:L:55:ILE:HD13	1.78	0.65
2:B:678:PRO:HA	2:B:681:ILE:HD13	1.78	0.65
1:A:1055:ILE:HD13	1:A:1063:MET:HE1	1.78	0.65
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.78	0.65
2:B:412:ILE:HG22	2:B:461:MET:HE1	1.79	0.64
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.80	0.64
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.79	0.64
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.79	0.64
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.80	0.64
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.78	0.64
2:B:140:LYS:HB3	2:B:155:VAL:HG12	1.79	0.64
7:G:77:VAL:HG11	7:G:124:VAL:HG21	1.79	0.64
1:A:1094:ALA:O	1:A:1098:SER:OG	2.15	0.63
2:B:480:GLN:NE2	2:B:482:SER:O	2.31	0.63
1:A:838:GLU:HA	1:A:841:LYS:HE3	1.80	0.63
2:B:890:ASP:OD1	2:B:890:ASP:N	2.31	0.63
2:B:892:SER:OG	2:B:896:GLN:NE2	2.29	0.63
1:A:1223:ARG:HA	1:A:1227:MET:HB2	1.80	0.63
11:K:60:SER:OG	11:K:104:ARG:NH2	2.32	0.63
1:A:15:ASP:N	1:A:15:ASP:OD1	2.32	0.63
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.81	0.63
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.16	0.63
2:B:698:SER:O	2:B:702:ASN:ND2	2.32	0.63
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.81	0.63
2:B:752:VAL:HG12	2:B:981:SER:HB3	1.79	0.63
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.32	0.63
2:B:134:ARG:HD3	2:B:160:GLY:HA3	1.79	0.63
3:C:196:LEU:O	3:C:197:ARG:NH1	2.28	0.62
2:B:318:PRO:O	2:B:321:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:LYS:H	6:F:76:LYS:HD2	1.63	0.62
1:A:1179:ILE:HD11	1:A:1183:GLU:HG2	1.80	0.62
2:B:218:ILE:HD13	2:B:391:PRO:HG3	1.81	0.62
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.81	0.62
1:A:19:LEU:HD11	2:B:1130:ARG:HH12	1.64	0.62
2:B:1076:ARG:HG3	2:B:1088:LEU:HD11	1.80	0.62
1:A:668:GLY:HA3	1:A:787:GLY:HA2	1.80	0.61
1:A:1120:TYR:O	5:E:207:ARG:NH2	2.33	0.61
2:B:225:ARG:NH1	2:B:268:GLU:OE1	2.33	0.61
1:A:1238:MET:HA	1:A:1543:SER:HA	1.83	0.61
2:B:741:LEU:HB2	2:B:804:TYR:HB2	1.83	0.61
8:H:64:ASN:O	8:H:87:ARG:NH2	2.34	0.61
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.19	0.61
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.83	0.61
2:B:651:ARG:NH2	2:B:690:GLU:OE1	2.34	0.61
6:F:99:LEU:HD23	7:G:112:PRO:HD3	1.83	0.61
1:A:904:THR:HG23	1:A:946:LEU:HD21	1.83	0.60
1:A:344:ASN:OD1	1:A:344:ASN:N	2.32	0.60
2:B:71:LYS:HD2	2:B:421:LEU:HB3	1.82	0.60
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.83	0.60
2:B:201:LYS:NZ	2:B:465:LEU:O	2.32	0.60
2:B:518:ARG:NH1	2:B:539:CYS:O	2.35	0.60
3:C:324:LYS:HD3	11:K:72:LEU:HB2	1.83	0.60
10:J:31:ASP:OD1	10:J:31:ASP:N	2.30	0.60
1:A:1021:ARG:HA	1:A:1024:THR:HG22	1.82	0.60
2:B:26:ILE:O	10:J:62:ARG:NH1	2.35	0.60
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.84	0.60
9:I:98:THR:HG22	9:I:110:VAL:HG22	1.84	0.60
1:A:439:ASP:OD1	1:A:440:SER:N	2.35	0.59
2:B:610:TYR:OH	9:I:122:ARG:NH1	2.34	0.59
2:B:816:ASN:OD1	2:B:817:ARG:NH1	2.35	0.59
5:E:136:ASN:OD1	5:E:136:ASN:N	2.35	0.59
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.84	0.59
1:A:799:GLU:O	1:A:1079:LYS:NZ	2.36	0.59
1:A:339:PHE:HD2	1:A:350:VAL:HG21	1.67	0.59
1:A:467:PHE:HA	1:A:471:MET:HE3	1.85	0.59
8:H:104:PHE:HD2	8:H:112:ILE:HD11	1.68	0.59
2:B:272:PRO:HD2	2:B:275:MET:HE2	1.83	0.59
5:E:26:ARG:NH1	5:E:133:GLU:OE1	2.35	0.59
1:A:943:ILE:HD13	2:B:960:ILE:HD11	1.84	0.59
2:B:307:GLU:HB2	9:I:7:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.84	0.58
2:B:933:THR:OG1	2:B:944:GLN:OE1	2.21	0.58
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.85	0.58
2:B:764:ASN:OD1	10:J:59:LYS:NZ	2.35	0.58
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.35	0.58
1:A:825:ALA:HB3	2:B:1022:LEU:HD13	1.86	0.58
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.85	0.58
1:A:1322:ILE:O	1:A:1326:GLU:HG2	2.03	0.58
2:B:543:ASN:OD1	2:B:543:ASN:N	2.34	0.58
3:C:287:ASP:N	3:C:287:ASP:OD1	2.36	0.58
1:A:1191:GLN:HE22	2:B:1078:ALA:HA	1.69	0.58
2:B:991:THR:HG22	2:B:993:ALA:H	1.68	0.57
2:B:558:VAL:HG23	2:B:561:ILE:HD12	1.86	0.57
1:A:91:PHE:HE2	1:A:245:LYS:HE2	1.69	0.57
3:C:57:ILE:HG23	3:C:297:HIS:HD2	1.68	0.57
2:B:38:LEU:HD11	2:B:493:PHE:HZ	1.70	0.57
2:B:14:ALA:HB2	2:B:980:ASP:HB3	1.85	0.57
1:A:415:ASP:OD1	1:A:415:ASP:N	2.31	0.57
2:B:416:LYS:HE2	2:B:460:LYS:HB3	1.87	0.57
1:A:1501:ILE:HD11	1:A:1528:ALA:HB1	1.86	0.57
1:A:490:ILE:HD11	1:A:606:ARG:HB3	1.85	0.57
1:A:886:ASN:OD1	1:A:955:ARG:NH2	2.38	0.57
1:A:511:VAL:HG12	1:A:519:LEU:HD23	1.86	0.57
1:A:132:GLU:HG2	1:A:192:ALA:HB1	1.86	0.56
2:B:376:PHE:HA	2:B:379:ARG:HD3	1.87	0.56
1:A:519:LEU:HD12	1:A:579:ARG:HH11	1.71	0.56
2:B:772:VAL:HG11	2:B:943:ILE:HD11	1.86	0.56
1:A:518:GLU:OE1	1:A:582:LYS:NZ	2.37	0.56
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.21	0.56
6:F:57:ASP:OD1	6:F:60:GLN:NE2	2.37	0.56
1:A:1038:ILE:HG12	1:A:1047:GLN:HB2	1.86	0.56
1:A:1085:LEU:HD23	1:A:1172:LEU:HD11	1.86	0.56
2:B:456:ASN:HB3	2:B:459:SER:HB3	1.88	0.56
1:A:15:ASP:HB3	1:A:1631:ARG:HB2	1.88	0.56
1:A:627:ASP:OD1	1:A:628:PHE:N	2.36	0.56
1:A:399:LEU:HD11	1:A:422:ARG:HG2	1.87	0.56
2:B:252:TYR:OH	2:B:305:ARG:NE	2.29	0.56
2:B:280:LEU:HA	2:B:354:LEU:HD21	1.88	0.56
1:A:952:LEU:HD12	1:A:957:VAL:HA	1.88	0.55
1:A:18:ILE:HG21	1:A:354:SER:HB3	1.87	0.55
2:B:37:LEU:HD12	2:B:759:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.40	0.55
14:S:34:DG:H2'	14:S:35:DG:C8	2.41	0.55
1:A:381:SER:HB3	1:A:453:ILE:HG23	1.88	0.55
1:A:831:ASP:N	1:A:831:ASP:OD1	2.39	0.55
5:E:112:TYR:HE2	5:E:134:THR:HB	1.71	0.55
1:A:590:ASN:OD1	1:A:592:GLN:NE2	2.40	0.55
2:B:255:ASP:OD2	2:B:257:GLN:NE2	2.39	0.55
7:G:50:ALA:HB1	7:G:52:MET:HE3	1.89	0.55
1:A:498:PRO:HB2	1:A:500:VAL:HG12	1.88	0.55
2:B:75:ASP:OD1	2:B:75:ASP:N	2.36	0.55
1:A:439:ASP:OD1	1:A:458:GLN:NE2	2.34	0.55
11:K:67:GLU:HG2	11:K:99:ASN:HD22	1.71	0.55
1:A:821:ILE:HD11	1:A:826:PHE:HB2	1.88	0.55
5:E:190:LEU:HD23	5:E:214:CYS:HB2	1.89	0.55
1:A:665:PRO:HD2	1:A:790:LYS:HG2	1.89	0.55
1:A:693:GLN:NE2	11:K:87:GLU:O	2.31	0.54
2:B:379:ARG:HE	2:B:579:ALA:HB1	1.72	0.54
1:A:236:CYS:O	1:A:238:MET:N	2.39	0.54
1:A:568:VAL:O	1:A:571:HIS:ND1	2.26	0.54
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.89	0.54
2:B:212:ASN:HB3	2:B:590:GLY:HA3	1.87	0.54
2:B:1107:CYS:O	2:B:1195:ARG:NH2	2.39	0.54
3:C:245:ARG:HH22	3:C:258:ILE:HG21	1.72	0.54
1:A:589:MET:HE1	1:A:614:LEU:HD13	1.89	0.54
2:B:943:ILE:HD12	10:J:45:CYS:HB3	1.88	0.54
1:A:759:TYR:HE1	1:A:913:PRO:HG3	1.72	0.54
2:B:1114:GLN:OE1	2:B:1129:ARG:NH1	2.34	0.54
3:C:42:VAL:O	11:K:138:LYS:NZ	2.31	0.54
3:C:100:ARG:NH1	10:J:3:VAL:O	2.35	0.54
1:A:734:THR:O	1:A:738:ASN:ND2	2.36	0.54
1:A:88:PRO:O	1:A:442:LYS:NZ	2.41	0.54
2:B:219:ARG:HH12	14:S:23:DC:H1'	1.73	0.54
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.90	0.54
2:B:172:LEU:HG	2:B:175:MET:HE2	1.90	0.53
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.89	0.53
1:A:86:TYR:N	1:A:431:GLN:OE1	2.41	0.53
2:B:207:ILE:HG22	2:B:505:ARG:HA	1.90	0.53
1:A:365:THR:HA	1:A:368:ARG:HG2	1.89	0.53
2:B:203:ILE:HG12	2:B:485:THR:HG22	1.90	0.53
2:B:662:ASP:OD1	2:B:663:ILE:N	2.42	0.53
7:G:97:LYS:HE2	7:G:99:ASP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:VAL:HG12	2:B:449:VAL:HG21	1.91	0.53
2:B:687:THR:HG22	9:I:97:HIS:CE1	2.44	0.53
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.90	0.53
1:A:701:ARG:HD2	11:K:102:ASN:HD22	1.73	0.53
3:C:245:ARG:NH2	3:C:263:ASP:OD1	2.41	0.53
1:A:722:PRO:HD2	8:H:46:LEU:HD23	1.92	0.52
1:A:1307:ASP:O	1:A:1499:ARG:NH1	2.39	0.52
7:G:70:VAL:HG12	7:G:71:MET:HG2	1.90	0.52
1:A:928:MET:HE1	2:B:951:PRO:HB2	1.92	0.52
1:A:701:ARG:NE	1:A:704:ASP:OD2	2.42	0.52
2:B:1119:ARG:NE	2:B:1160:GLU:OE2	2.42	0.52
1:A:24:ILE:HA	1:A:27:LEU:HG	1.92	0.52
1:A:827:THR:OG1	2:B:775:VAL:O	2.17	0.52
1:A:1033:SER:OG	1:A:1037:SER:O	2.22	0.52
2:B:1104:CYS:HA	2:B:1173:THR:HG22	1.91	0.52
3:C:109:ASP:HB3	3:C:112:MET:HE2	1.91	0.52
13:R:7:C:O2'	13:R:8:G:H8	1.93	0.52
1:A:36:THR:HG23	1:A:45:VAL:HG11	1.92	0.52
1:A:1254:PHE:HE1	1:A:1532:GLN:HG2	1.75	0.52
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.91	0.52
1:A:339:PHE:O	1:A:340:HIS:ND1	2.43	0.52
1:A:1613:MET:HB2	1:A:1618:THR:HG23	1.91	0.52
2:B:292:ILE:HD13	2:B:378:ILE:HG21	1.92	0.52
1:A:760:TRP:HZ2	1:A:780:ILE:HD13	1.74	0.52
1:A:1183:GLU:OE1	6:F:88:TYR:OH	2.24	0.52
2:B:123:PRO:HB3	2:B:165:LEU:HD11	1.90	0.52
1:A:499:PRO:HD2	1:A:611:GLU:HG2	1.92	0.51
5:E:55:ARG:NH1	5:E:113:GLN:OE1	2.43	0.51
2:B:63:LEU:HB3	2:B:242:ASP:HB3	1.93	0.51
2:B:1107:CYS:SG	2:B:1131:CYS:HB3	2.49	0.51
2:B:627:GLY:HA2	2:B:668:GLU:HB3	1.92	0.51
3:C:107:LYS:HG3	3:C:187:ALA:HA	1.92	0.51
15:T:8:DT:H2''	15:T:9:DA:C8	2.45	0.51
1:A:6:PRO:HB3	7:G:111:THR:HG21	1.92	0.51
2:B:379:ARG:HE	2:B:580:GLY:H	1.58	0.51
2:B:830:ASP:OD1	2:B:830:ASP:N	2.41	0.51
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.31	0.51
15:T:29:DG:H4'	15:T:30:DT:OP1	2.11	0.51
1:A:707:THR:HG22	1:A:709:ARG:H	1.76	0.51
3:C:30:GLU:HG2	3:C:31:TRP:H	1.76	0.51
2:B:795:GLU:OE1	3:C:217:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ARG:HB3	2:B:20:GLU:HG2	1.92	0.51
2:B:854:GLU:OE2	2:B:876:SER:N	2.44	0.51
3:C:333:ILE:HD11	11:K:49:LEU:HB2	1.94	0.50
6:F:85:MET:HE1	6:F:125:LEU:HD11	1.94	0.50
1:A:10:GLU:OE2	1:A:1645:LYS:NZ	2.45	0.50
1:A:141:LEU:HD21	1:A:177:LEU:HB3	1.93	0.50
2:B:379:ARG:HH21	2:B:580:GLY:N	2.08	0.50
1:A:982:VAL:HG22	1:A:994:GLU:HB3	1.92	0.50
1:A:1148:LEU:HD21	1:A:1166:PHE:HD2	1.76	0.50
2:B:819:ASP:OD1	2:B:819:ASP:N	2.42	0.50
3:C:132:ILE:HG21	3:C:184:VAL:HG11	1.94	0.50
15:T:7:DA:H2"	15:T:8:DT:H71	1.94	0.50
2:B:102:VAL:HG22	2:B:139:LEU:HD22	1.93	0.50
2:B:987:ASN:OD1	2:B:987:ASN:N	2.44	0.50
1:A:1260:LYS:HD2	1:A:1505:ASP:HA	1.92	0.50
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.94	0.50
2:B:71:LYS:HZ3	2:B:422:GLN:HG3	1.77	0.50
1:A:6:PRO:HD2	4:D:16:LEU:HD11	1.94	0.49
1:A:657:TYR:CE2	1:A:665:PRO:HB3	2.47	0.49
1:A:1223:ARG:HG2	1:A:1227:MET:SD	2.51	0.49
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.94	0.49
1:A:659:THR:HG23	1:A:666:VAL:HB	1.94	0.49
1:A:703:GLU:O	11:K:52:GLN:NE2	2.44	0.49
2:B:1064:LYS:H	2:B:1064:LYS:HZ3	1.60	0.49
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.78	0.49
2:B:335:ARG:NH2	2:B:344:GLN:O	2.25	0.49
1:A:14:VAL:HG12	1:A:1634:LEU:HD21	1.95	0.49
1:A:925:MET:HE2	1:A:943:ILE:HD12	1.94	0.49
10:J:5:VAL:HA	10:J:15:GLY:HA3	1.94	0.49
2:B:232:TYR:CG	2:B:385:VAL:HG12	2.48	0.49
2:B:840:LEU:HD13	2:B:860:ALA:HB2	1.95	0.49
2:B:164:MET:O	2:B:167:SER:OG	2.21	0.49
2:B:31:ASP:OD1	2:B:32:LYS:N	2.45	0.49
3:C:197:ARG:HG2	10:J:61:LEU:HD22	1.95	0.49
10:J:10:CYS:SG	10:J:11:GLY:N	2.86	0.49
1:A:1003:ARG:HE	2:B:520:LEU:HD12	1.78	0.48
2:B:1055:LEU:HD12	2:B:1056:THR:H	1.78	0.48
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.95	0.48
10:J:7:CYS:HA	10:J:49:MET:HE2	1.94	0.48
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.94	0.48
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:SER:HB3	1:A:1507:CYS:H	1.78	0.48
3:C:236:LEU:HD11	3:C:290:LYS:HG2	1.95	0.48
1:A:131:ASP:OD1	1:A:131:ASP:N	2.45	0.48
1:A:846:ILE:O	1:A:849:THR:OG1	2.30	0.48
2:B:73:ILE:HG22	2:B:95:LEU:HB3	1.95	0.48
14:S:28:DC:H2'	14:S:29:DT:H71	1.95	0.48
1:A:19:LEU:HD13	2:B:1195:ARG:HB2	1.94	0.48
1:A:360:LEU:HD11	1:A:434:VAL:HG22	1.95	0.48
1:A:537:GLN:HB3	1:A:576:LYS:HB2	1.96	0.48
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.95	0.48
1:A:857:ALA:HB2	1:A:899:LYS:HD3	1.95	0.48
1:A:934:LYS:HG3	2:B:952:HIS:HB3	1.96	0.48
1:A:551:VAL:HG13	1:A:554:ARG:HH12	1.78	0.48
2:B:100:GLU:OE1	2:B:100:GLU:N	2.45	0.48
3:C:101:ILE:O	3:C:104:VAL:HG12	2.14	0.48
12:L:44:ASP:OD1	12:L:45:ALA:N	2.47	0.48
1:A:684:ASP:HB2	8:H:20:TYR:HD1	1.78	0.48
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.96	0.48
5:E:180:ARG:HD3	5:E:192:ARG:HG3	1.95	0.48
1:A:1038:ILE:HD12	1:A:1584:LEU:HD13	1.96	0.48
1:A:1663:ALA:HB2	7:G:101:SER:HA	1.95	0.48
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.47	0.48
1:A:1102:LEU:HD11	1:A:1106:LYS:HE3	1.96	0.48
1:A:967:PRO:HG2	2:B:525:TRP:CD1	2.50	0.47
2:B:803:MET:HB3	2:B:907:ILE:HB	1.95	0.47
2:B:915:ASP:HB3	2:B:1039:MET:HA	1.96	0.47
1:A:85:CYS:HA	1:A:431:GLN:HE22	1.78	0.47
2:B:649:MET:HE3	2:B:666:PRO:HG2	1.96	0.47
1:A:1097:TYR:OH	1:A:1121:ASP:OD1	2.26	0.47
5:E:143:ASN:OD1	5:E:145:THR:OG1	2.28	0.47
1:A:1193:VAL:HG21	1:A:1585:ILE:HD11	1.96	0.47
5:E:191:LYS:O	5:E:194:GLU:HG2	2.14	0.47
1:A:106:HIS:HB2	1:A:330:LYS:HD2	1.95	0.47
1:A:700:ILE:HD13	1:A:738:ASN:HB2	1.97	0.47
1:A:1305:GLU:OE2	9:I:63:LYS:NZ	2.43	0.47
2:B:127:ARG:HH12	2:B:185:GLU:CD	2.23	0.47
2:B:207:ILE:HG21	2:B:505:ARG:HD2	1.97	0.47
1:A:507:TYR:HD1	1:A:509:GLU:HG2	1.80	0.47
1:A:752:LYS:O	1:A:785:GLN:NE2	2.48	0.47
1:A:1139:ASN:OD1	5:E:206:GLY:N	2.48	0.47
2:B:1128:CYS:O	2:B:1132:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ILE:HB	3:C:208:CYS:SG	2.54	0.47
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.50	0.47
9:I:56:PHE:HB2	9:I:61:ARG:HH22	1.79	0.47
5:E:53:PRO:O	5:E:55:ARG:HG3	2.14	0.47
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.96	0.47
1:A:596:HIS:CE1	1:A:598:ALA:HB3	2.50	0.47
2:B:1160:GLU:HA	2:B:1166:LYS:HA	1.96	0.47
3:C:77:SER:OG	3:C:219:PHE:O	2.26	0.47
1:A:368:ARG:NH2	1:A:386:LEU:HD12	2.30	0.47
2:B:657:PRO:C	2:B:659:ASP:H	2.22	0.47
2:B:515:THR:HG23	2:B:518:ARG:HD2	1.97	0.46
2:B:1134:ARG:HH22	2:B:1165:ASN:ND2	2.13	0.46
1:A:98:LEU:HD13	1:A:320:VAL:HG23	1.97	0.46
1:A:699:CYS:HB3	1:A:816:LEU:HB2	1.96	0.46
1:A:1329:ILE:HG12	1:A:1485:MET:HE1	1.97	0.46
1:A:1007:ILE:HG21	2:B:515:THR:HG21	1.96	0.46
2:B:413:LEU:O	2:B:417:ILE:HG23	2.15	0.46
1:A:32:ILE:HD11	1:A:54:LEU:HD11	1.97	0.46
1:A:81:LEU:HD21	1:A:434:VAL:HG21	1.98	0.46
1:A:856:GLU:O	1:A:860:GLU:HG2	2.14	0.46
1:A:484:ILE:HD13	1:A:633:MET:HE3	1.97	0.46
1:A:597:LYS:HD2	2:B:1082:HIS:ND1	2.31	0.46
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.51	0.46
1:A:1463:ASP:HB3	1:A:1468:LYS:H	1.80	0.46
11:K:67:GLU:N	11:K:99:ASN:O	2.49	0.46
1:A:1194:GLY:O	1:A:1197:SER:OG	2.18	0.46
2:B:533:THR:HG21	2:B:540:GLY:H	1.80	0.46
3:C:87:ASN:HB2	12:L:62:LYS:HD2	1.97	0.46
3:C:257:GLY:HA3	3:C:268:LYS:HD2	1.98	0.46
2:B:402:VAL:HG11	2:B:551:ILE:HD13	1.98	0.46
2:B:292:ILE:O	2:B:379:ARG:HG2	2.15	0.46
5:E:40:GLU:OE1	5:E:41:ASP:N	2.49	0.46
1:A:608:LEU:HD12	1:A:615:ARG:HD3	1.98	0.46
1:A:1003:ARG:HH11	2:B:540:GLY:HA2	1.81	0.46
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.50	0.46
2:B:1064:LYS:H	2:B:1064:LYS:NZ	2.14	0.46
15:T:5:DC:H2"	15:T:6:DG:H8	1.81	0.46
2:B:221:SER:HA	2:B:224:ASN:HB3	1.99	0.45
2:B:1135:PHE:HB2	2:B:1167:PHE:HA	1.98	0.45
1:A:1302:TYR:HA	9:I:60:LEU:HD11	1.98	0.45
2:B:251:HIS:NE2	2:B:261:ARG:HD3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:VAL:HG21	2:B:1031:VAL:HG22	1.98	0.45
2:B:968:ALA:HB2	2:B:996:PHE:CE2	2.51	0.45
1:A:13:SER:HB3	1:A:1633:GLN:HA	1.98	0.45
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.43	0.45
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.98	0.45
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.98	0.45
1:A:141:LEU:HB2	1:A:181:LEU:HD22	1.98	0.45
1:A:1019:LEU:HD13	1:A:1227:MET:HG3	1.98	0.45
2:B:687:THR:OG1	2:B:688:HIS:ND1	2.41	0.45
1:A:93:GLN:HG3	1:A:1627:LEU:HD11	1.98	0.45
1:A:1262:LEU:HD23	1:A:1497:ILE:HG22	1.98	0.45
2:B:533:THR:CG2	2:B:540:GLY:H	2.30	0.45
1:A:94:LEU:HG	1:A:355:PHE:CD2	2.52	0.45
1:A:261:ILE:O	1:A:265:ARG:N	2.48	0.45
1:A:416:ARG:O	1:A:419:ILE:HG22	2.17	0.45
2:B:71:LYS:NZ	2:B:418:ASP:OD1	2.29	0.45
3:C:102:GLY:HA3	12:L:69:ALA:HB1	1.98	0.45
5:E:55:ARG:HB3	5:E:82:PHE:HB3	1.99	0.45
1:A:747:ILE:HG13	1:A:797:LEU:HD23	1.98	0.45
1:A:1039:ARG:NH2	1:A:1045:LEU:HD12	2.30	0.45
3:C:94:ASP:N	3:C:94:ASP:OD1	2.48	0.45
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.98	0.45
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.51	0.45
15:T:28:DC:H2''	15:T:29:DG:O5'	2.17	0.45
1:A:510:PRO:HA	1:A:576:LYS:HA	1.97	0.45
2:B:75:ASP:OD1	2:B:93:ASN:N	2.49	0.45
2:B:578:ALA:HB1	2:B:583:LEU:HD12	1.99	0.45
1:A:96:ILE:HG23	1:A:228:LEU:HD21	1.99	0.44
1:A:54:LEU:HB2	1:A:365:THR:HG23	1.99	0.44
2:B:555:GLN:HA	2:B:645:GLY:HA2	1.98	0.44
2:B:568:LEU:HD13	2:B:604:ILE:HG23	1.99	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.17	0.44
7:G:47:VAL:HB	7:G:65:HIS:NE2	2.32	0.44
1:A:937:ASN:O	1:A:941:SER:OG	2.28	0.44
1:A:1003:ARG:NH1	2:B:540:GLY:HA2	2.33	0.44
1:A:1540:GLY:HA2	5:E:148:GLU:OE1	2.17	0.44
2:B:425:ILE:HD13	2:B:425:ILE:HA	1.88	0.44
3:C:197:ARG:HD3	3:C:197:ARG:HA	1.83	0.44
1:A:1118:VAL:C	1:A:1120:TYR:H	2.25	0.44
2:B:33:SER:HA	2:B:177:PRO:HG3	1.99	0.44
2:B:322:ASN:OD1	2:B:325:GLN:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:GLU:H	2:B:1106:GLU:CD	2.26	0.44
11:K:55:SER:OG	11:K:57:ASP:OD1	2.29	0.44
2:B:785:ASP:CG	2:B:957:ARG:HH22	2.24	0.44
1:A:755:ILE:HD12	1:A:780:ILE:HD11	2.00	0.44
1:A:943:ILE:HD11	2:B:958:MET:HG2	2.00	0.44
3:C:100:ARG:NH2	10:J:2:ILE:HG23	2.32	0.44
2:B:1158:ILE:HD13	2:B:1168:VAL:HB	2.00	0.44
1:A:213:ASN:ND2	1:A:1605:THR:HA	2.32	0.44
3:C:40:PHE:CZ	11:K:131:VAL:HG23	2.52	0.44
3:C:165:ARG:HB3	3:C:189:PRO:HB2	1.99	0.44
5:E:40:GLU:H	5:E:40:GLU:HG3	1.56	0.44
1:A:718:THR:HB	1:A:730:GLN:NE2	2.33	0.43
2:B:237:ARG:NH2	2:B:401:GLU:OE2	2.51	0.43
14:S:8:DT:H2"	14:S:9:DA:N7	2.33	0.43
1:A:94:LEU:HG	1:A:355:PHE:HD2	1.83	0.43
2:B:265:ARG:O	2:B:267:ASN:N	2.47	0.43
8:H:15:VAL:HG13	8:H:24:CYS:SG	2.58	0.43
1:A:403:LEU:HD12	1:A:419:ILE:HG23	1.99	0.43
1:A:1015:ARG:HH12	2:B:513:LYS:NZ	2.16	0.43
2:B:528:LEU:HD13	2:B:543:ASN:ND2	2.33	0.43
5:E:58:MET:HE2	5:E:58:MET:HB3	1.88	0.43
1:A:977:MET:SD	1:A:977:MET:N	2.78	0.43
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.53	0.43
2:B:846:PRO:HG3	2:B:903:ILE:HD13	2.00	0.43
7:G:66:LEU:HD11	7:G:87:LEU:HD13	2.01	0.43
2:B:816:ASN:H	2:B:819:ASP:CG	2.26	0.43
6:F:119:ARG:HA	6:F:122:MET:HE3	1.99	0.43
6:F:135:ARG:NH2	7:G:92:ALA:O	2.43	0.43
1:A:368:ARG:HH22	1:A:382:GLN:HB3	1.83	0.43
2:B:788:ILE:HB	2:B:948:ILE:HB	2.00	0.43
2:B:874:TYR:CZ	2:B:876:SER:HB2	2.53	0.43
3:C:103:LEU:O	10:J:6:ARG:NH1	2.52	0.43
1:A:918:LYS:O	1:A:923:ASN:ND2	2.38	0.43
2:B:1016:GLY:O	3:C:69:ARG:NH1	2.51	0.43
3:C:75:VAL:HB	3:C:221:PRO:HG3	2.00	0.43
7:G:49:LEU:N	7:G:114:GLY:O	2.49	0.43
1:A:1067:GLU:OE1	1:A:1067:GLU:N	2.42	0.43
2:B:1053:ASN:N	2:B:1058:GLN:O	2.47	0.43
12:L:27:LEU:HD13	12:L:37:LYS:HB2	2.01	0.43
1:A:1148:LEU:HD21	1:A:1166:PHE:CD2	2.53	0.43
1:A:1503:HIS:O	1:A:1523:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:ASP:HB3	2:B:445:TYR:HB3	2.01	0.43
2:B:697:LEU:HB3	2:B:701:ALA:HB3	2.01	0.43
3:C:172:GLN:H	3:C:175:GLN:HG2	1.83	0.43
8:H:97:MET:HE3	8:H:142:LEU:HD23	2.00	0.43
1:A:581:ILE:HG12	1:A:605:VAL:HG11	2.00	0.43
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.99	0.43
1:A:1011:VAL:HG13	1:A:1015:ARG:HH21	1.84	0.43
2:B:416:LYS:HG3	2:B:461:MET:HE2	2.00	0.43
2:B:609:ARG:NH2	2:B:668:GLU:OE1	2.46	0.43
2:B:953:ALA:O	2:B:957:ARG:HG2	2.19	0.43
3:C:154:LYS:HE3	3:C:154:LYS:HB2	1.84	0.43
3:C:229:LEU:HB3	3:C:293:ARG:HB3	2.00	0.43
1:A:389:VAL:HG22	1:A:433:ASP:HB3	2.01	0.42
1:A:671:GLN:NE2	1:A:934:LYS:HD3	2.33	0.42
1:A:257:ASN:HB2	1:A:260:GLN:HG3	2.01	0.42
1:A:1505:ASP:HB2	1:A:1522:GLU:HB2	2.01	0.42
2:B:219:ARG:NH2	2:B:221:SER:HB3	2.34	0.42
2:B:390:SER:N	2:B:635:GLY:O	2.52	0.42
1:A:1276:THR:O	9:I:21:ASN:ND2	2.46	0.42
3:C:70:ILE:HG23	3:C:74:GLU:HB2	2.01	0.42
6:F:110:ASP:OD1	6:F:110:ASP:N	2.47	0.42
1:A:619:ALA:HA	1:A:668:GLY:O	2.19	0.42
1:A:1039:ARG:HA	1:A:1046:VAL:HG23	2.01	0.42
1:A:407:GLN:NE2	1:A:416:ARG:HE	2.17	0.42
1:A:1025:LYS:HD2	1:A:1611:MET:HG2	2.01	0.42
1:A:1290:TYR:CD1	1:A:1485:MET:HG2	2.55	0.42
2:B:258:VAL:H	2:B:309:LEU:HD13	1.83	0.42
2:B:743:ARG:NH2	10:J:1:MET:SD	2.93	0.42
3:C:216:HIS:HB2	12:L:70:ARG:NH1	2.34	0.42
1:A:610:ASN:HB2	1:A:615:ARG:NH2	2.35	0.42
2:B:129:ARG:NH1	2:B:889:GLY:O	2.49	0.42
2:B:372:ARG:NH2	2:B:574:SER:HA	2.35	0.42
3:C:181:ASP:OD1	3:C:181:ASP:N	2.51	0.42
9:I:20:PRO:HB3	9:I:39:LYS:HZ1	1.84	0.42
1:A:482:SER:HB2	1:A:501:PHE:HZ	1.84	0.42
1:A:845:ASP:HA	1:A:848:LYS:HE2	2.01	0.42
1:A:1446:ARG:O	1:A:1450:ILE:HG12	2.20	0.42
2:B:726:MET:O	2:B:744:LEU:HB2	2.19	0.42
6:F:118:LEU:HG	6:F:122:MET:HE2	2.02	0.42
1:A:6:PRO:O	4:D:15:THR:OG1	2.29	0.42
1:A:628:PHE:HD2	2:B:784:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:THR:O	1:A:908:VAL:HG12	2.19	0.42
1:A:1256:LYS:NZ	1:A:1304:GLU:O	2.52	0.42
1:A:1634:LEU:O	1:A:1640:ARG:HD3	2.20	0.42
3:C:218:LYS:NZ	12:L:69:ALA:O	2.48	0.42
1:A:697:TYR:CZ	11:K:104:ARG:HB2	2.55	0.42
2:B:175:MET:SD	2:B:183:HIS:ND1	2.92	0.42
2:B:1037:ARG:HA	2:B:1039:MET:HE2	2.02	0.42
5:E:117:THR:OG1	14:S:37:DA:OP1	2.38	0.42
11:K:89:CYS:HA	11:K:104:ARG:O	2.20	0.42
11:K:105:ILE:HB	11:K:113:ALA:HB1	2.02	0.42
1:A:916:THR:HG23	1:A:944:MET:HE1	2.02	0.42
1:A:917:MET:HE3	1:A:917:MET:HB3	1.94	0.42
1:A:1026:GLN:HG2	1:A:1603:MET:HE2	2.02	0.42
1:A:1258:ILE:HD13	1:A:1258:ILE:HA	1.89	0.42
2:B:52:LEU:HA	2:B:60:LEU:HB2	2.00	0.42
2:B:712:SER:OG	2:B:713:PRO:HD3	2.19	0.42
1:A:440:SER:H	1:A:458:GLN:HE22	1.68	0.41
1:A:838:GLU:O	1:A:841:LYS:HG2	2.20	0.41
1:A:996:TYR:CE1	2:B:530:PRO:HG3	2.54	0.41
1:A:1012:LYS:HE2	1:A:1012:LYS:HB2	1.95	0.41
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.55	0.41
2:B:853:GLU:N	2:B:856:ASP:OD2	2.33	0.41
3:C:55:ASP:OD1	3:C:271:ARG:NH1	2.53	0.41
9:I:103:SER:OG	9:I:104:ALA:N	2.54	0.41
1:A:120:CYS:HB3	1:A:189:VAL:HG21	2.02	0.41
1:A:413:LEU:O	1:A:417:ARG:N	2.42	0.41
1:A:1287:ALA:N	1:A:1476:LEU:O	2.54	0.41
2:B:210:ARG:NH2	2:B:667:PHE:HB2	2.36	0.41
2:B:547:HIS:CD2	2:B:548:LYS:HG2	2.55	0.41
2:B:653:VAL:HG13	2:B:688:HIS:HD2	1.86	0.41
14:S:35:DG:H2'	14:S:36:DT:C6	2.56	0.41
1:A:9:SER:HB3	2:B:1200:VAL:HG13	2.02	0.41
1:A:261:ILE:HA	1:A:264:ASN:HB2	2.02	0.41
1:A:326:THR:HG22	1:A:329:ARG:HH12	1.84	0.41
1:A:498:PRO:HG3	1:A:613:THR:O	2.21	0.41
1:A:1316:VAL:HG11	1:A:1498:ILE:HA	2.02	0.41
2:B:68:ILE:HD11	2:B:414:LYS:HG3	2.01	0.41
2:B:140:LYS:HA	2:B:155:VAL:HA	2.02	0.41
2:B:424:ILE:HG22	2:B:453:VAL:HG21	2.02	0.41
2:B:1115:GLN:OE1	2:B:1124:SER:OG	2.29	0.41
9:I:30:CYS:HB3	9:I:33:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:SER:OG	1:A:928:MET:HE3	2.20	0.41
1:A:1010:ALA:O	1:A:1013:THR:HG22	2.20	0.41
1:A:1441:LYS:HE2	1:A:1441:LYS:HB2	1.92	0.41
5:E:127:ILE:HD11	5:E:132:ILE:HD11	2.01	0.41
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.55	0.41
13:R:9:A:H2'	13:R:10:G:O4'	2.20	0.41
1:A:485:SER:O	1:A:615:ARG:HA	2.21	0.41
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	2.02	0.41
1:A:1317:ILE:HG21	1:A:1470:CYS:SG	2.61	0.41
2:B:1017:ALA:HB1	11:K:70:HIS:CE1	2.56	0.41
3:C:271:ARG:HH12	3:C:299:ILE:HG23	1.85	0.41
11:K:134:LYS:HE3	11:K:134:LYS:HB2	1.88	0.41
15:T:23:DG:C4	15:T:24:DA:C8	3.08	0.41
1:A:261:ILE:HA	1:A:264:ASN:HD22	1.85	0.41
1:A:1016:SER:OG	1:A:1016:SER:O	2.37	0.41
3:C:157:TYR:HB2	3:C:160:ALA:HB2	2.01	0.41
15:T:26:DT:H2''	15:T:27:DG:C8	2.56	0.41
1:A:43:HIS:CG	1:A:44:PRO:HD2	2.56	0.41
1:A:316:LEU:HB2	1:A:319:GLU:HG3	2.01	0.41
1:A:363:PRO:O	1:A:368:ARG:HD2	2.21	0.41
1:A:942:GLN:HA	1:A:946:LEU:O	2.21	0.41
1:A:1267:ILE:O	9:I:61:ARG:NH2	2.53	0.41
1:A:1306:TYR:O	1:A:1499:ARG:NH2	2.26	0.41
2:B:129:ARG:HG3	12:L:55:ILE:HD11	2.02	0.41
2:B:177:PRO:O	2:B:181:VAL:HG13	2.20	0.41
3:C:145:ASP:OD1	3:C:145:ASP:N	2.53	0.41
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.03	0.41
1:A:1233:ILE:HD11	1:A:1236:PRO:HA	2.03	0.41
1:A:1641:ILE:HD12	1:A:1641:ILE:HA	1.92	0.41
2:B:68:ILE:HD12	2:B:417:ILE:HD11	2.01	0.41
2:B:225:ARG:HB3	2:B:229:TYR:HD2	1.85	0.41
2:B:413:LEU:HD23	2:B:461:MET:HE3	2.03	0.41
2:B:848:ILE:HD12	2:B:884:GLU:HA	2.03	0.41
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.54	0.41
4:D:28:PRO:HB2	7:G:39:VAL:HG11	2.03	0.41
8:H:40:LEU:HD11	8:H:97:MET:HE1	2.02	0.41
10:J:21:TYR:HB2	10:J:39:LEU:HD11	2.02	0.41
2:B:247:THR:OG1	2:B:477:ASP:OD2	2.38	0.41
3:C:70:ILE:HA	3:C:74:GLU:HB2	2.03	0.41
6:F:89:GLU:CD	6:F:134:ILE:HG21	2.46	0.41
6:F:100:GLN:HE22	6:F:132:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:LEU:HD23	8:H:111:LEU:HA	1.92	0.41
12:L:29:TYR:HB2	12:L:38:LEU:HD12	2.02	0.41
1:A:1311:GLU:CD	1:A:1311:GLU:H	2.28	0.40
1:A:1497:ILE:HD13	1:A:1500:GLN:HG2	2.04	0.40
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.03	0.40
6:F:69:LEU:HG	7:G:94:PRO:HG3	2.03	0.40
8:H:53:ASP:OD1	8:H:54:SER:N	2.40	0.40
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.57	0.40
2:B:227:ALA:O	2:B:228:SER:OG	2.32	0.40
2:B:359:LEU:HB3	2:B:362:LEU:HD23	2.02	0.40
1:A:230:ARG:HD3	1:A:230:ARG:HA	1.80	0.40
1:A:604:LYS:HE3	1:A:604:LYS:HB3	1.88	0.40
1:A:880:GLN:O	1:A:884:ARG:HG2	2.22	0.40
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.92	0.40
1:A:1221:ARG:NH2	1:A:1544:ASN:HB3	2.37	0.40
2:B:307:GLU:HA	9:I:7:LEU:HD21	2.02	0.40
2:B:576:THR:HG21	2:B:595:TRP:HD1	1.85	0.40
2:B:1133:MET:O	2:B:1167:PHE:HB2	2.22	0.40
1:A:734:THR:HG22	1:A:738:ASN:ND2	2.37	0.40
1:A:893:ASP:HA	1:A:956:ARG:HD2	2.03	0.40
1:A:1000:MET:HG2	2:B:520:LEU:HB3	2.03	0.40
1:A:1550:LEU:HB2	1:A:1558:ALA:HB2	2.02	0.40
2:B:106:LYS:HE2	2:B:168:ASN:O	2.21	0.40
2:B:180:LEU:HB3	2:B:186:GLU:O	2.22	0.40
2:B:753:LYS:O	2:B:980:ASP:HA	2.20	0.40
3:C:252:PRO:HA	3:C:253:PRO:HD3	1.98	0.40
6:F:116:ASP:O	6:F:120:ILE:HG13	2.21	0.40
8:H:101:ALA:HB3	8:H:137:GLN:HA	2.04	0.40
1:A:781:LEU:HB3	1:A:786:TYR:CE1	2.56	0.40
1:A:1022:CYS:SG	1:A:1023:LEU:N	2.94	0.40
1:A:1508:VAL:HG12	1:A:1520:VAL:HG23	2.03	0.40
2:B:169:ARG:HD3	2:B:169:ARG:HA	1.80	0.40
2:B:1006:ASN:HD21	2:B:1010:ASN:HB2	1.87	0.40
5:E:61:GLN:HB2	5:E:79:TRP:CZ3	2.57	0.40
5:E:123:LEU:HD23	5:E:123:LEU:H	1.86	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	1433/1664 (86%)	1378 (96%)	55 (4%)	0	100	100
2	B	1151/1203 (96%)	1104 (96%)	47 (4%)	0	100	100
3	C	302/335 (90%)	294 (97%)	8 (3%)	0	100	100
4	D	16/137 (12%)	14 (88%)	2 (12%)	0	100	100
5	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
6	F	99/155 (64%)	96 (97%)	3 (3%)	0	100	100
7	G	86/326 (26%)	84 (98%)	2 (2%)	0	100	100
8	H	127/146 (87%)	123 (97%)	4 (3%)	0	100	100
9	I	89/125 (71%)	82 (92%)	7 (8%)	0	100	100
10	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
11	K	96/142 (68%)	91 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	40 (95%)	2 (5%)	0	100	100
All	All	3720/4588 (81%)	3574 (96%)	146 (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	1282/1465 (88%)	1237 (96%)	45 (4%)	31	65
2	B	1013/1053 (96%)	966 (95%)	47 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	268/296 (90%)	258 (96%)	10 (4%)	29	63
4	D	16/116 (14%)	15 (94%)	1 (6%)	15	42
5	E	196/197 (100%)	188 (96%)	8 (4%)	26	59
6	F	90/137 (66%)	86 (96%)	4 (4%)	24	56
7	G	79/291 (27%)	78 (99%)	1 (1%)	65	88
8	H	115/128 (90%)	109 (95%)	6 (5%)	19	50
9	I	81/110 (74%)	77 (95%)	4 (5%)	21	52
10	J	64/65 (98%)	62 (97%)	2 (3%)	35	69
11	K	88/130 (68%)	83 (94%)	5 (6%)	17	46
12	L	39/57 (68%)	37 (95%)	2 (5%)	20	51
All	All	3331/4045 (82%)	3196 (96%)	135 (4%)	28	59

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	15	ASP
1	A	36	THR
1	A	199	ASP
1	A	212	VAL
1	A	344	ASN
1	A	345	LEU
1	A	350	VAL
1	A	399	LEU
1	A	411	VAL
1	A	415	ASP
1	A	453	ILE
1	A	497	VAL
1	A	506	THR
1	A	512	THR
1	A	544	VAL
1	A	581	ILE
1	A	587	VAL
1	A	642	ASN
1	A	646	GLU
1	A	653	THR
1	A	690	GLU
1	A	743	ASP

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Mol	Chain	Res	Type
1	A	747	ILE
1	A	770	LEU
1	A	917	MET
1	A	959	VAL
1	A	960	MET
1	A	965	THR
1	A	1022	CYS
1	A	1031	HIS
1	A	1098	SER
1	A	1144	LEU
1	A	1199	GLN
1	A	1258	ILE
1	A	1261	VAL
1	A	1305	GLU
1	A	1317	ILE
1	A	1323	HIS
1	A	1461	ASN
1	A	1500	GLN
1	A	1501	ILE
1	A	1520	VAL
1	A	1594	THR
1	A	1651	THR
2	B	72	VAL
2	B	121	VAL
2	B	124	SER
2	B	128	GLN
2	B	139	LEU
2	B	145	VAL
2	B	146	ASN
2	B	202	LEU
2	B	231	HIS
2	B	234	ILE
2	B	244	THR
2	B	255	ASP
2	B	295	ASN
2	B	306	LEU
2	B	327	LEU
2	B	358	VAL
2	B	359	LEU
2	B	362	LEU
2	B	403	LEU
2	B	417	ILE

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Mol	Chain	Res	Type
2	B	487	VAL
2	B	512	LEU
2	B	515	THR
2	B	535	ASP
2	B	537	SER
2	B	542	LEU
2	B	543	ASN
2	B	587	GLN
2	B	607	THR
2	B	752	VAL
2	B	763	ASP
2	B	802	THR
2	B	838	GLU
2	B	890	ASP
2	B	943	ILE
2	B	946	ASP
2	B	982	THR
2	B	1028	VAL
2	B	1031	VAL
2	B	1033	TYR
2	B	1055	LEU
2	B	1064	LYS
2	B	1071	VAL
2	B	1087	LEU
2	B	1176	VAL
2	B	1185	LEU
2	B	1186	ASP
3	C	56	LEU
3	C	94	ASP
3	C	113	LEU
3	C	138	VAL
3	C	145	ASP
3	C	175	GLN
3	C	223	SER
3	C	224	THR
3	C	229	LEU
3	C	287	ASP
4	D	23	HIS
5	E	12	LEU
5	E	40	GLU
5	E	88	VAL
5	E	111	VAL

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Mol	Chain	Res	Type
5	E	124	VAL
5	E	136	ASN
5	E	190	LEU
5	E	203	GLU
6	F	93	ILE
6	F	103	MET
6	F	107	VAL
6	F	152	ILE
7	G	54	LEU
8	H	23	VAL
8	H	24	CYS
8	H	42	ILE
8	H	45	GLU
8	H	57	VAL
8	H	83	GLN
9	I	3	VAL
9	I	47	VAL
9	I	99	LEU
9	I	101	LEU
10	J	5	VAL
10	J	31	ASP
11	K	59	THR
11	K	77	ARG
11	K	87	GLU
11	K	111	THR
11	K	119	LYS
12	L	38	LEU
12	L	64	LEU

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	336	GLN
1	A	407	GLN
1	A	432	ASN
1	A	493	ASN
1	A	583	ASN
1	A	649	ASN
1	A	671	GLN
1	A	950	GLN
1	A	1108	HIS
1	A	1191	GLN

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Mol	Chain	Res	Type
1	A	1199	GLN
1	A	1319	ASN
1	A	1323	HIS
1	A	1560	ASN
2	B	146	ASN
2	B	151	ASN
2	B	254	ASN
2	B	267	ASN
2	B	454	ASN
2	B	480	GLN
2	B	636	GLN
2	B	814	ASN
2	B	1010	ASN
3	C	159	ASN
3	C	301	ASN
9	I	32	GLN
9	I	95	ASN
9	I	97	HIS
11	K	102	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/13 (61%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	8	G

There are no RNA pucker outliers to report.

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	$\# Z > 2$
15	3DR	T	17	15	8,11,12	0.56	0	9,14,17	0.52	0

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
15	3DR	T	17	15	-	0/3/15/16	0/1/1/1

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.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

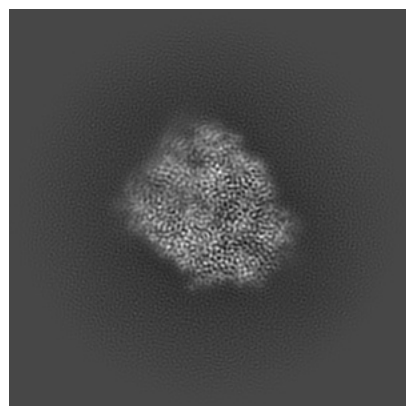
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50966. These allow visual inspection of the internal detail of the map and identification of artifacts.

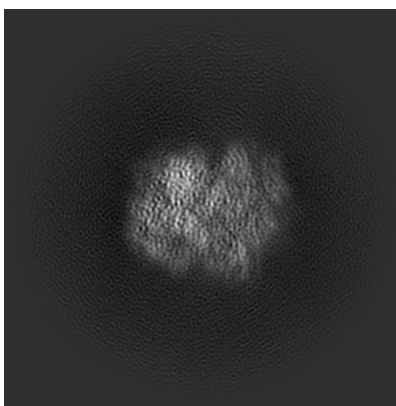
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

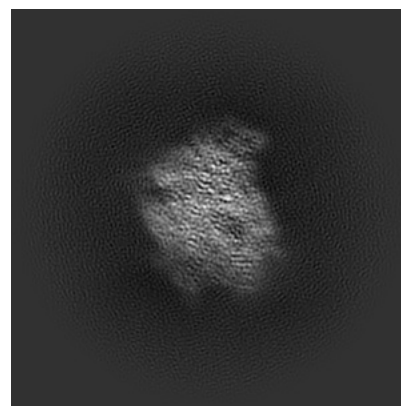
6.1.1 Primary map



X

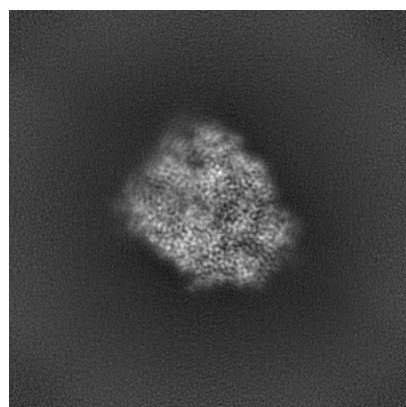


Y

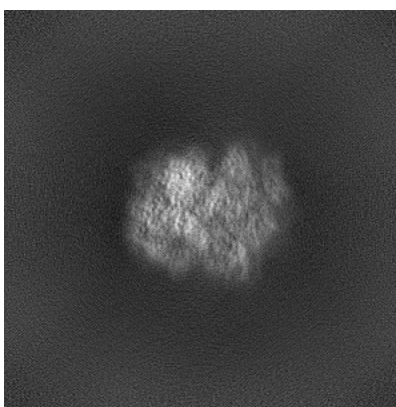


Z

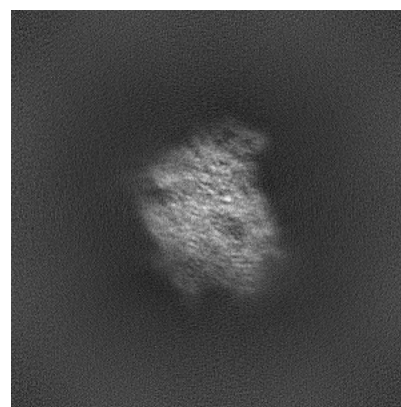
6.1.2 Raw map



X



Y

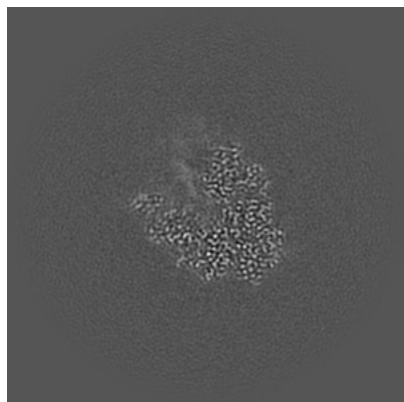


Z

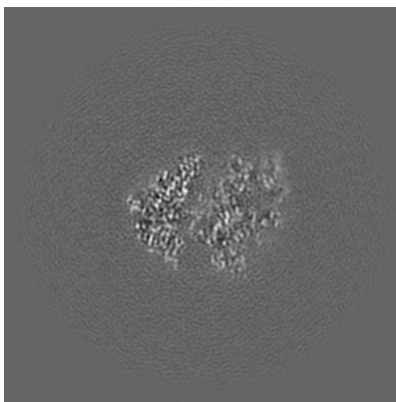
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

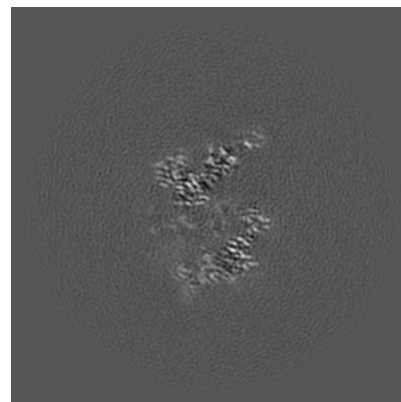
6.2.1 Primary map



X Index: 250

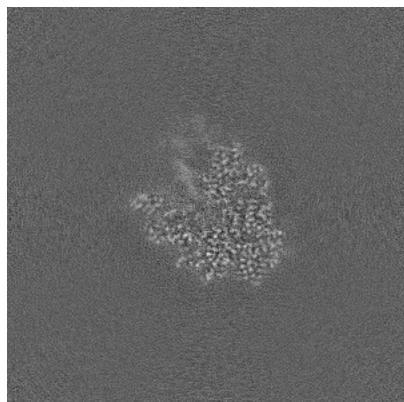


Y Index: 250

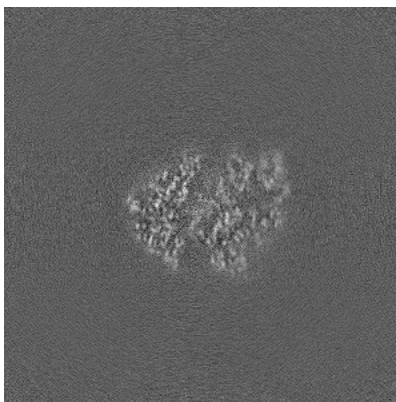


Z Index: 250

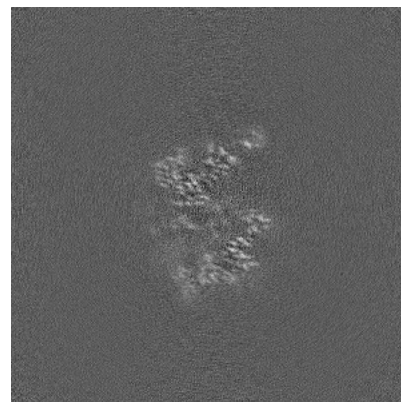
6.2.2 Raw map



X Index: 250



Y Index: 250

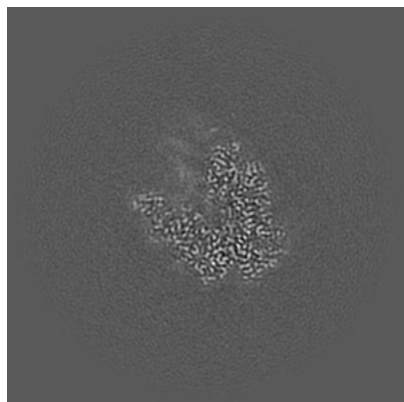


Z Index: 250

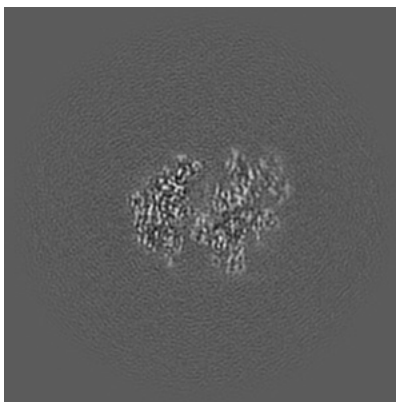
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

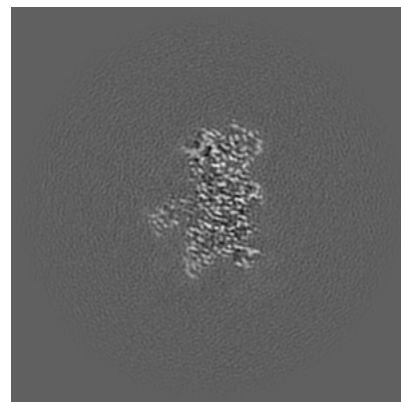
6.3.1 Primary map



X Index: 253

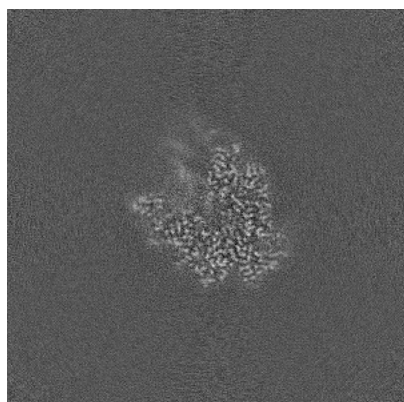


Y Index: 254

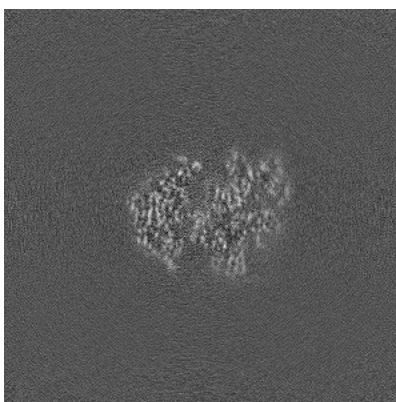


Z Index: 217

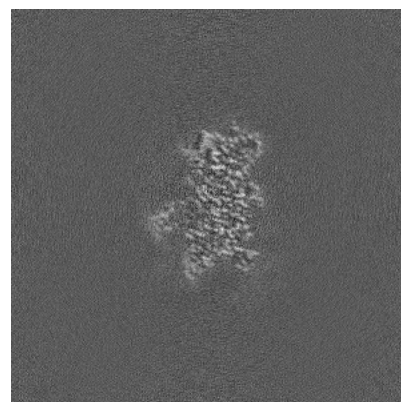
6.3.2 Raw map



X Index: 253



Y Index: 253

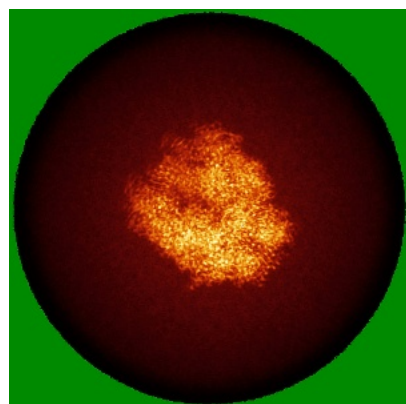


Z Index: 218

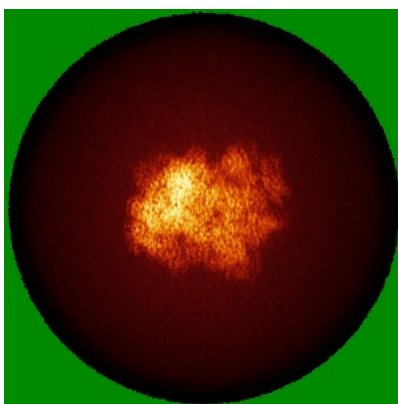
The images above show the largest variance slices of the map in three orthogonal directions.

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

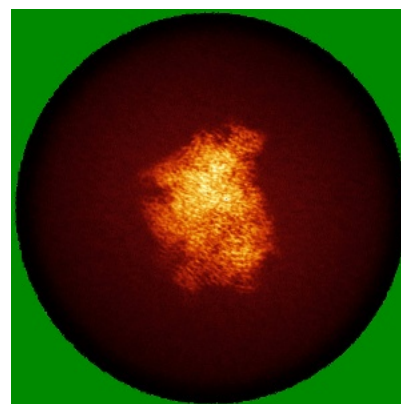
6.4.1 Primary map



X

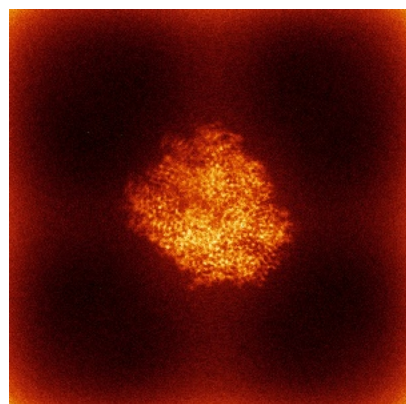


Y

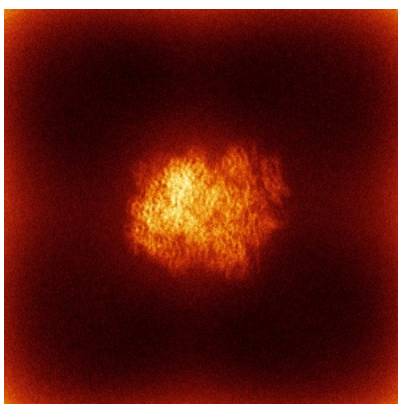


Z

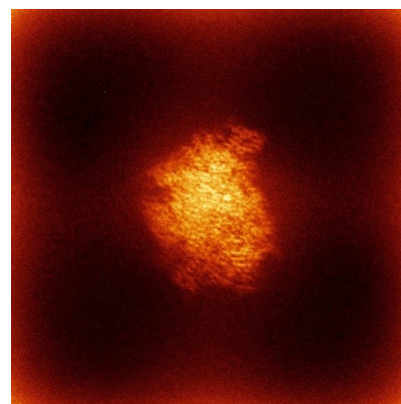
6.4.2 Raw map



X



Y

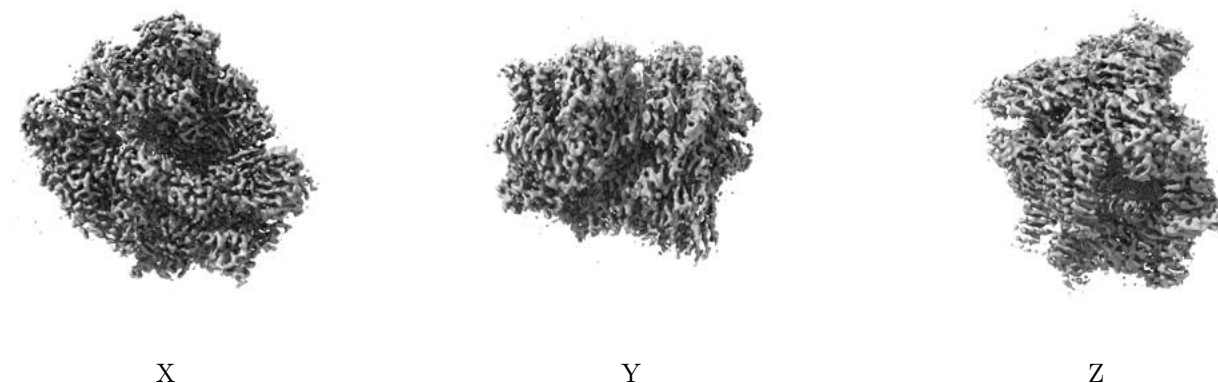


Z

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.

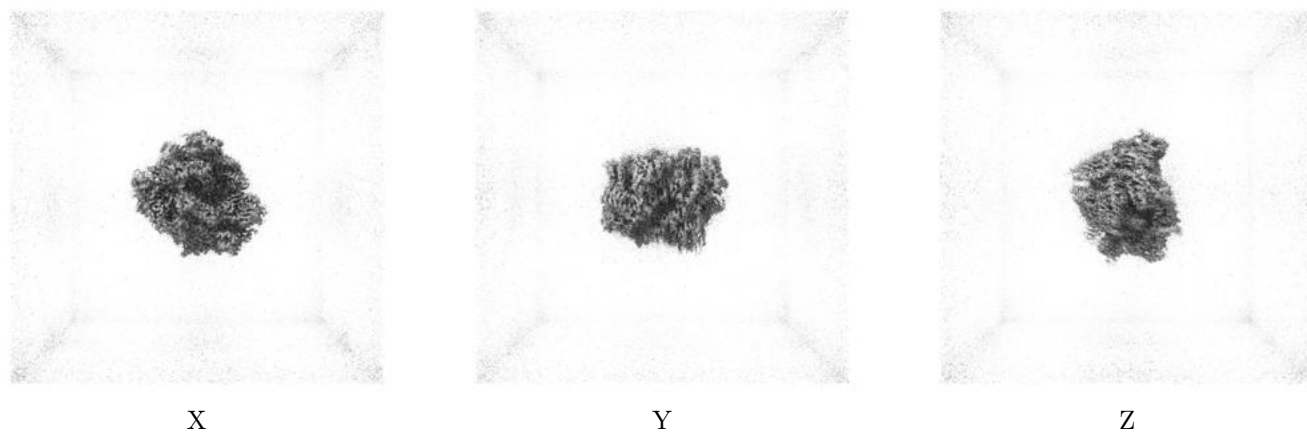
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0759. 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.

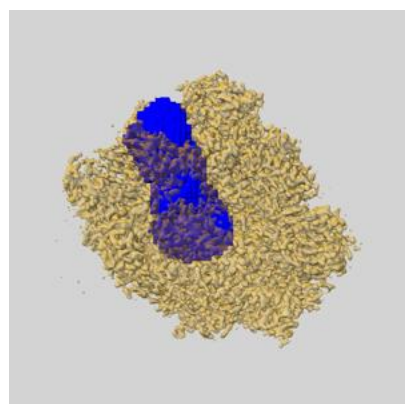
6.6 Mask visualisation [i](#)

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

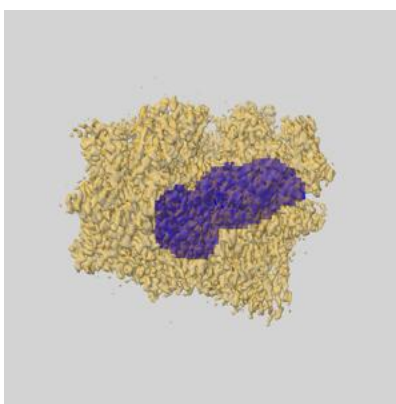
A mask typically either:

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

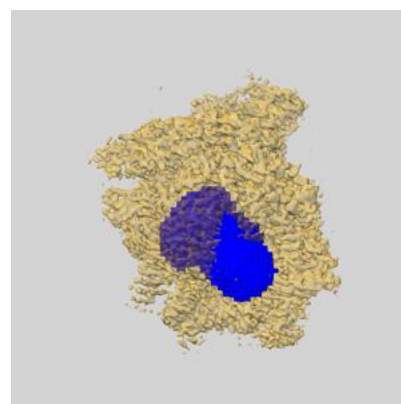
6.6.1 emd_50966_msk_2.map [i](#)



X

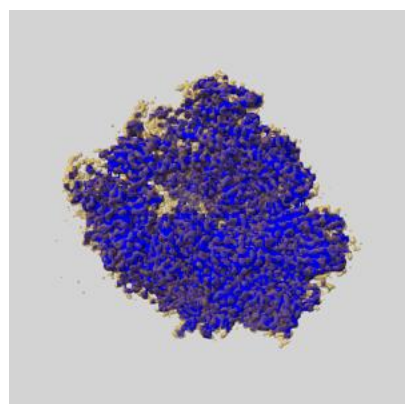


Y

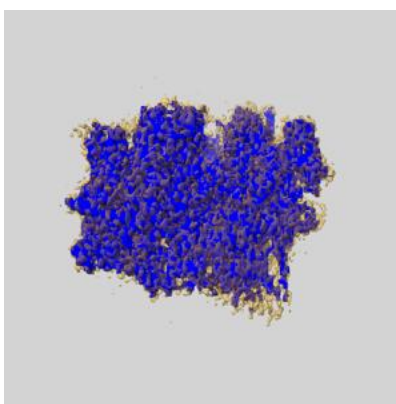


Z

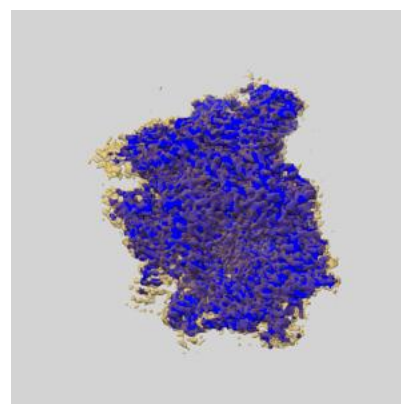
6.6.2 emd_50966_msk_1.map [i](#)



X



Y

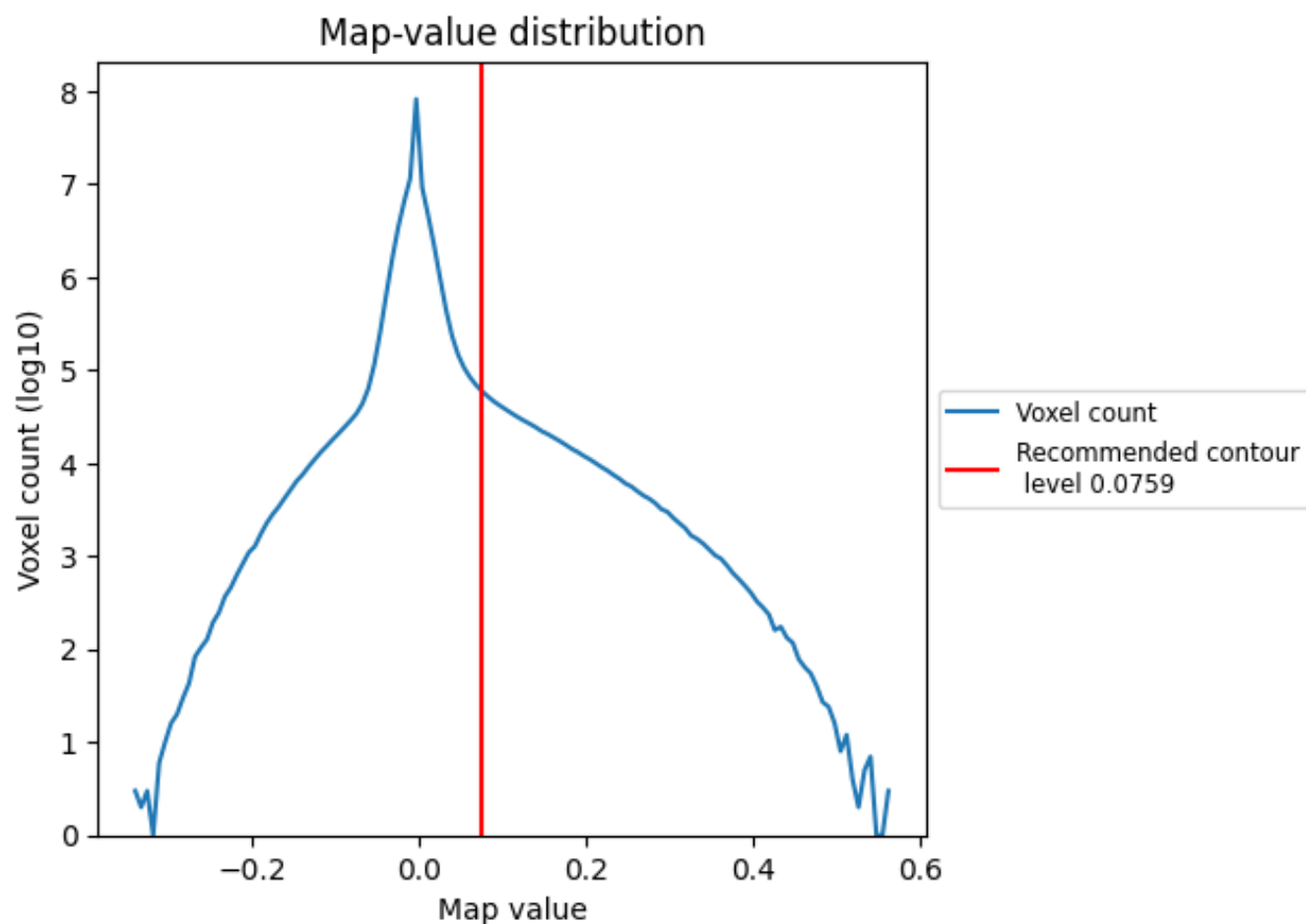


Z

7 Map analysis [i](#)

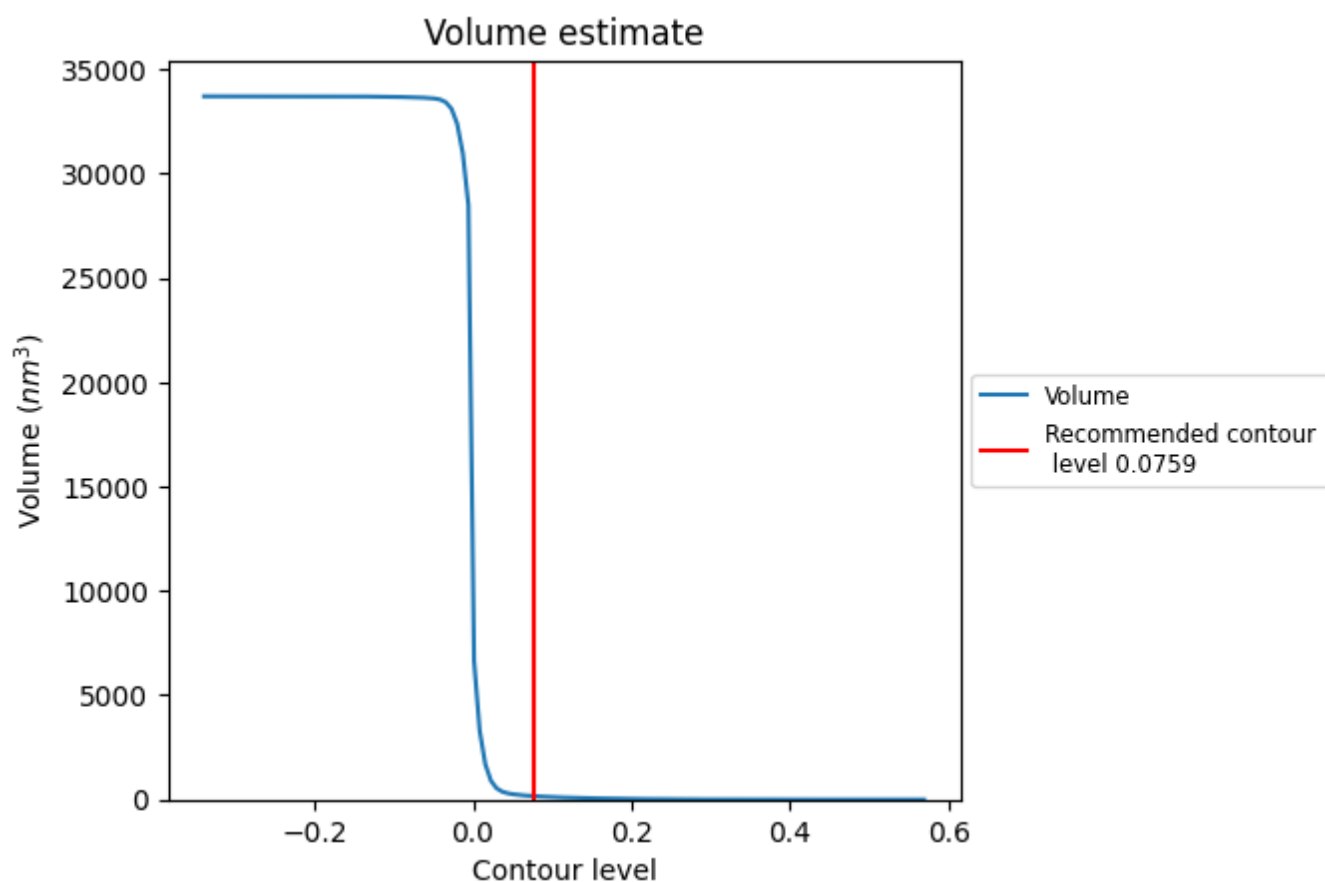
This section contains the results of statistical analysis of the map.

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.

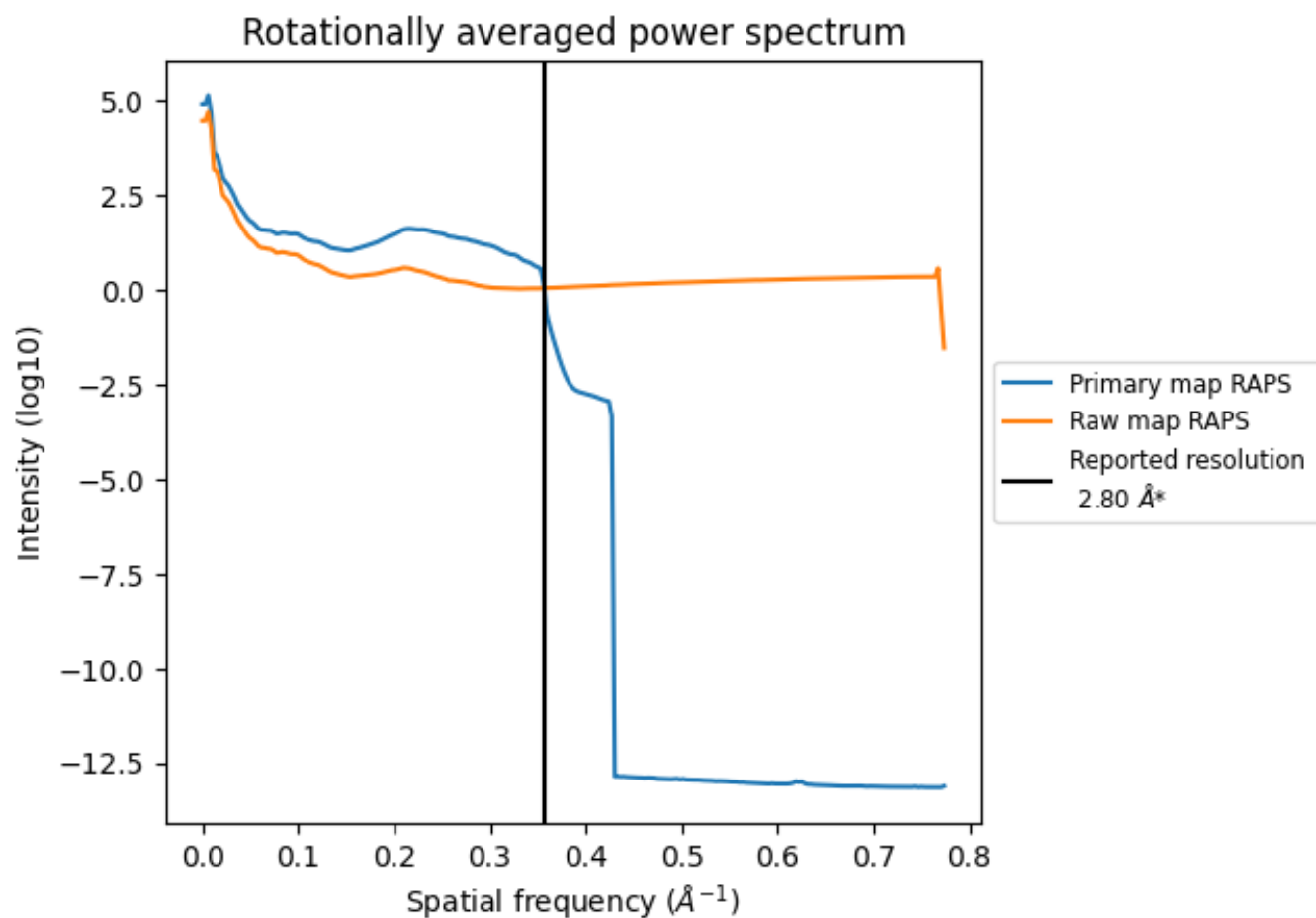
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

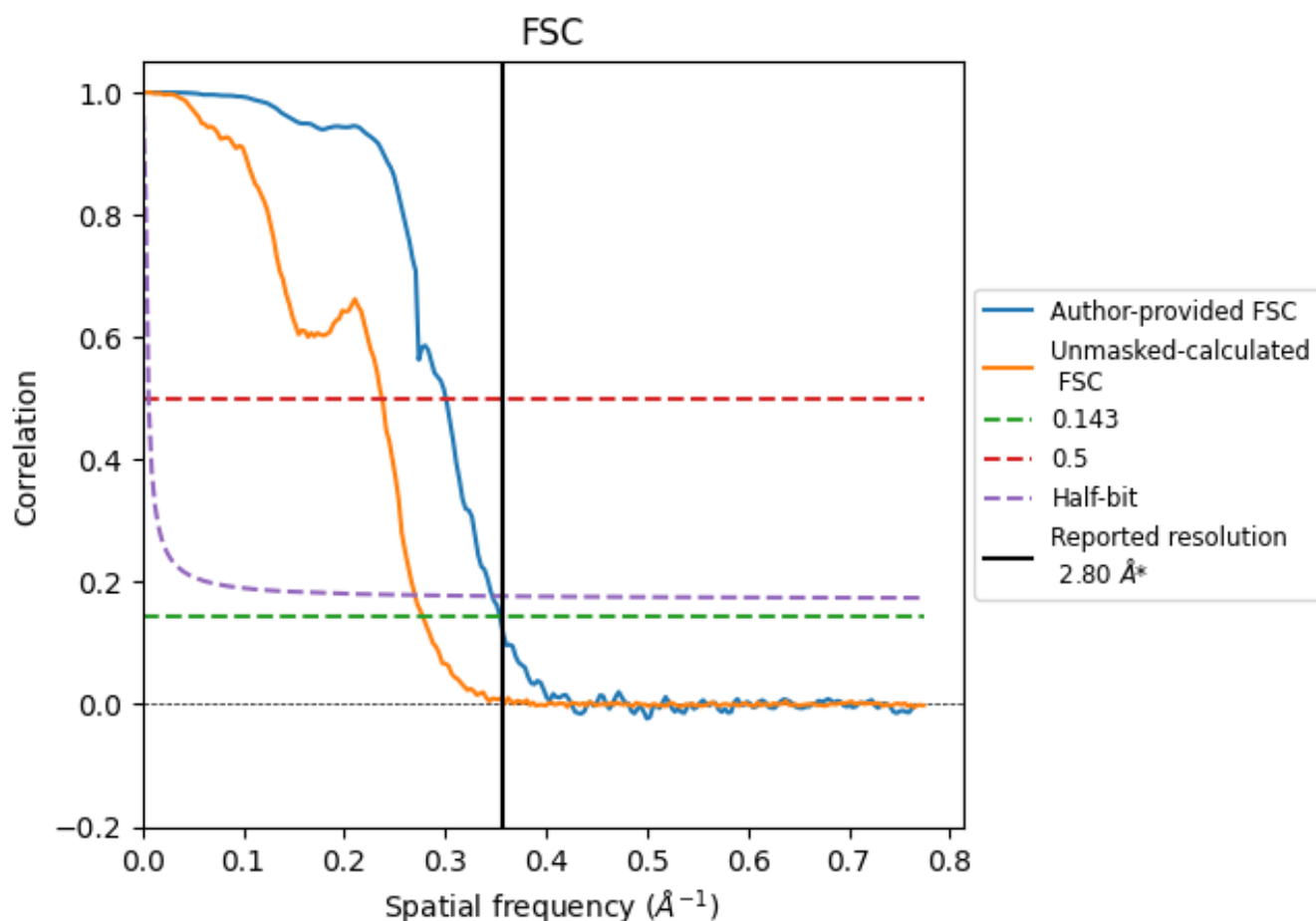


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

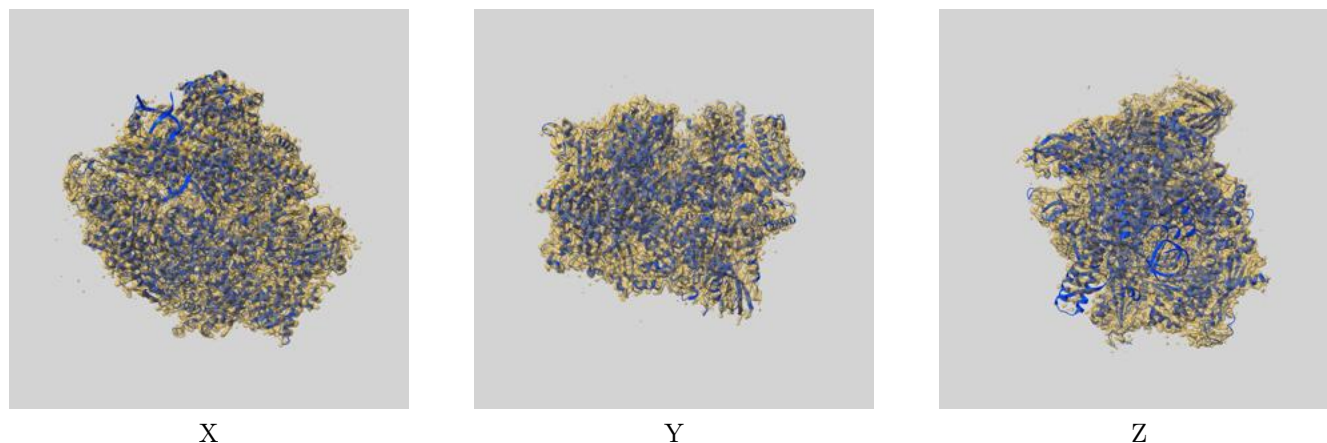
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.33	2.88
Unmasked-calculated*	3.60	4.21	3.70

*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 3.60 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

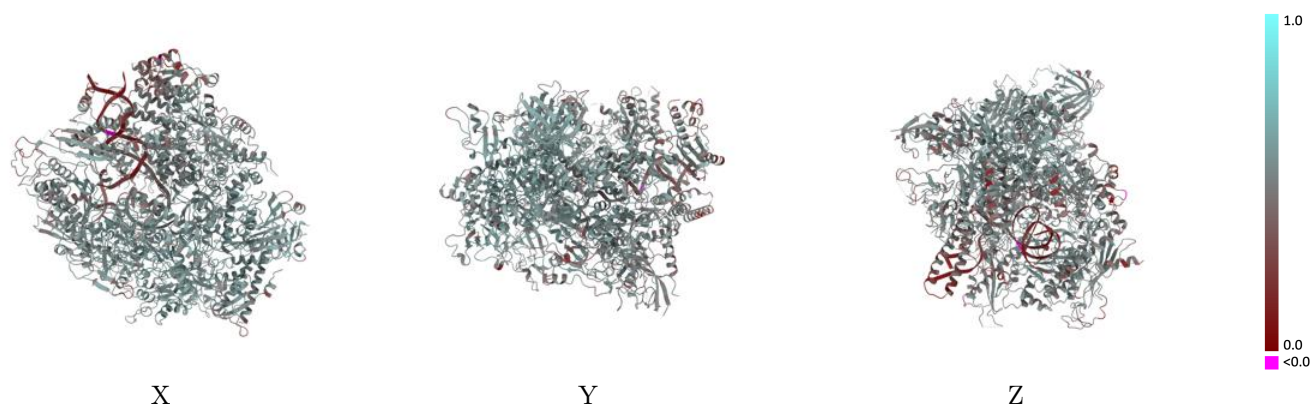
This section contains information regarding the fit between EMDB map EMD-50966 and PDB model 9G27. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



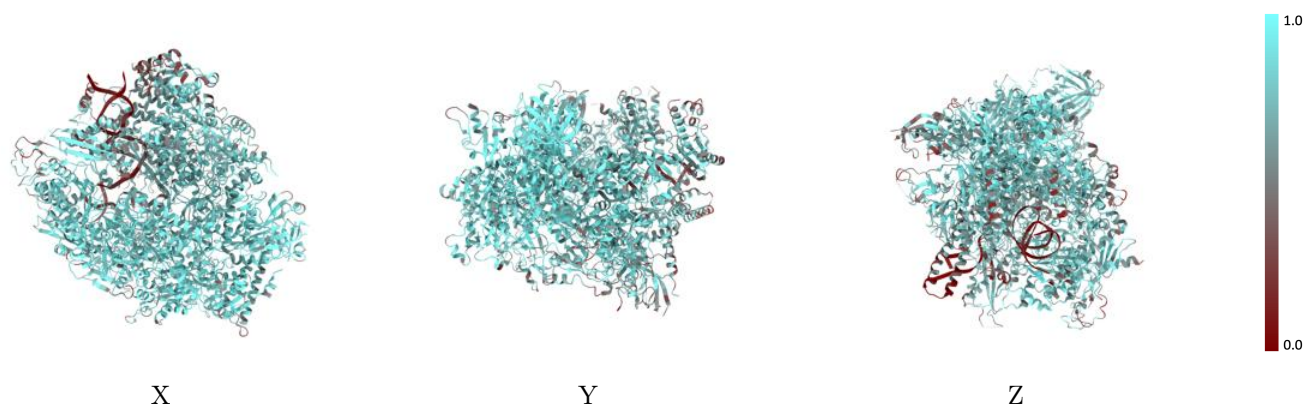
The images above show the 3D surface view of the map at the recommended contour level 0.0759 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



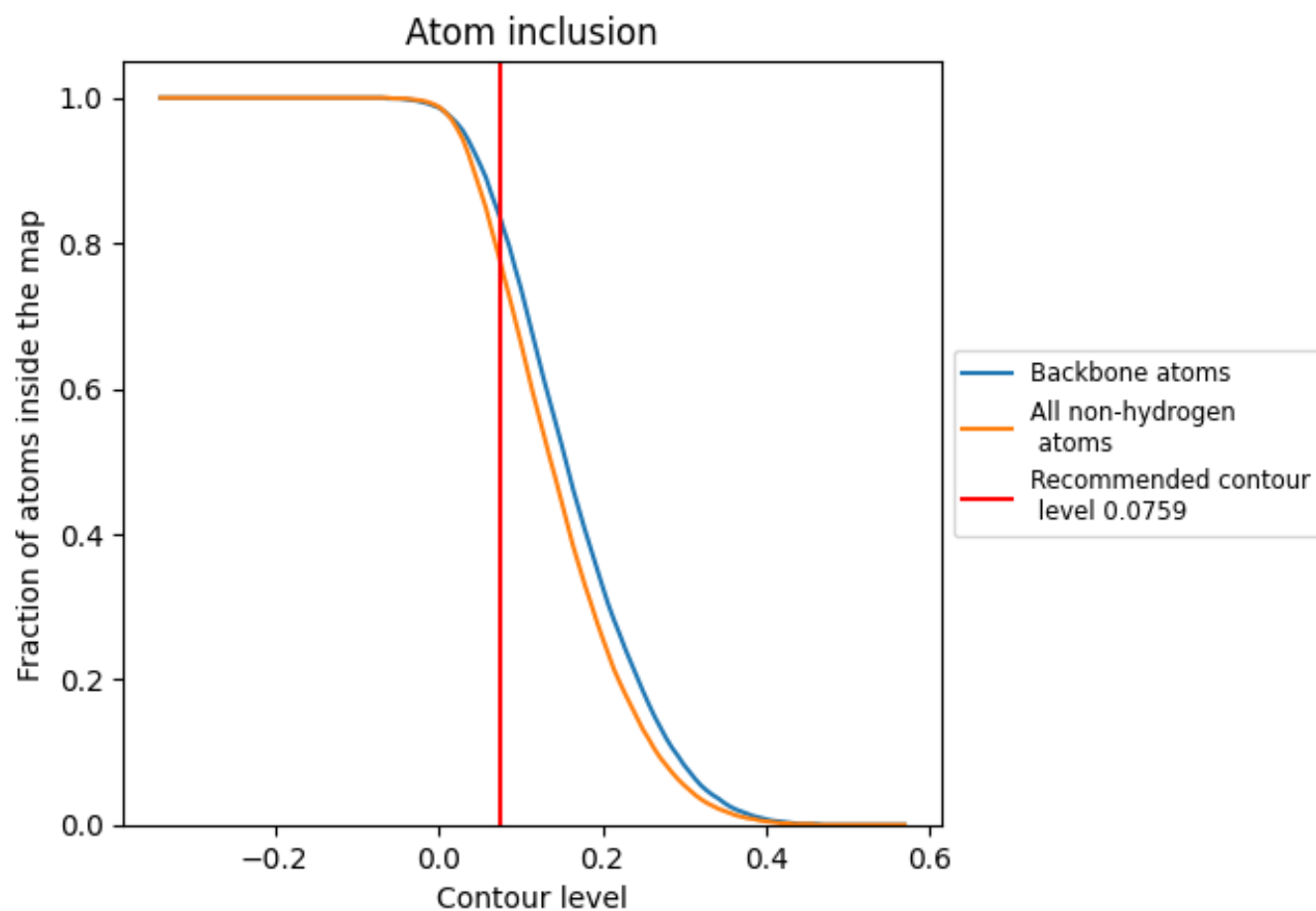
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0759).

































9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.0759) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5150
A	 0.7740	 0.5150
B	 0.8390	 0.5430
C	 0.8330	 0.5500
D	 0.6390	 0.4910
E	 0.6930	 0.4750
F	 0.7690	 0.5300
G	 0.6410	 0.4820
H	 0.8370	 0.5540
I	 0.6160	 0.4600
J	 0.9040	 0.5770
K	 0.8370	 0.5510
L	 0.8090	 0.5410
R	 0.8020	 0.4520
S	 0.1000	 0.1490
T	 0.3510	 0.2780

