



Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 04:21 pm BST

PDB ID : 9G2B / pdb_00009g2b
EMDB ID : EMD-50971
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site, 12-subunit
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.20 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

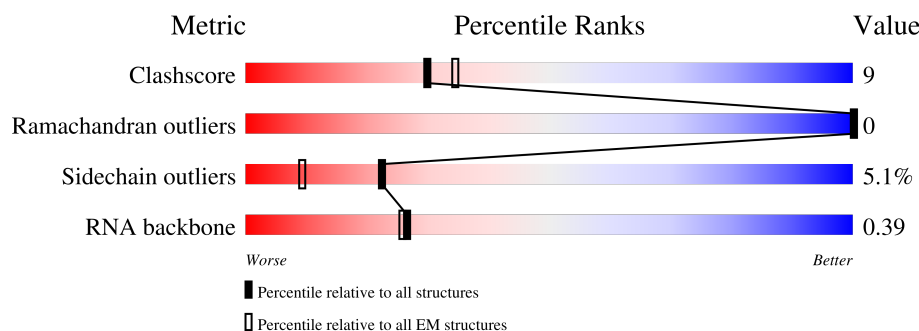
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	

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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	12	
14	S	38	
15	T	38	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31429 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	1461	Total	C	N	O	S	0	0
			11538	7284	2008	2184	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1164	Total	C	N	O	S	0	0
			9254	5851	1626	1726	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	212	Total	C	N	O	S	0	0
			1734	1102	306	315	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	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	90	Total	C	N	O	S	0	0
			716	472	114	126	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	95	Total	C	N	O	S	0	0
			720	450	121	143	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	11	Total	C	N	O	P	0	0
			239	107	47	74	11		

- 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	

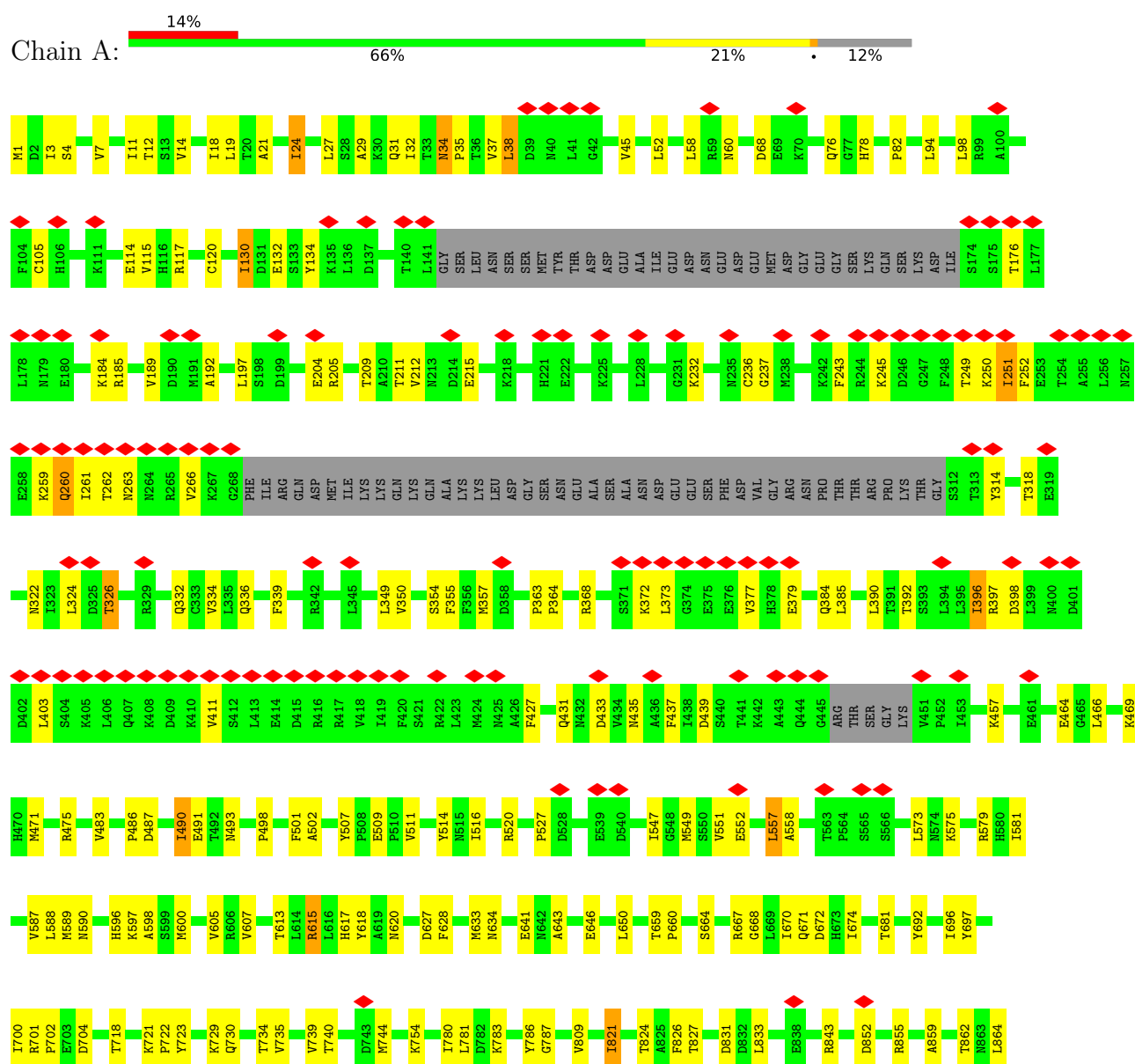
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

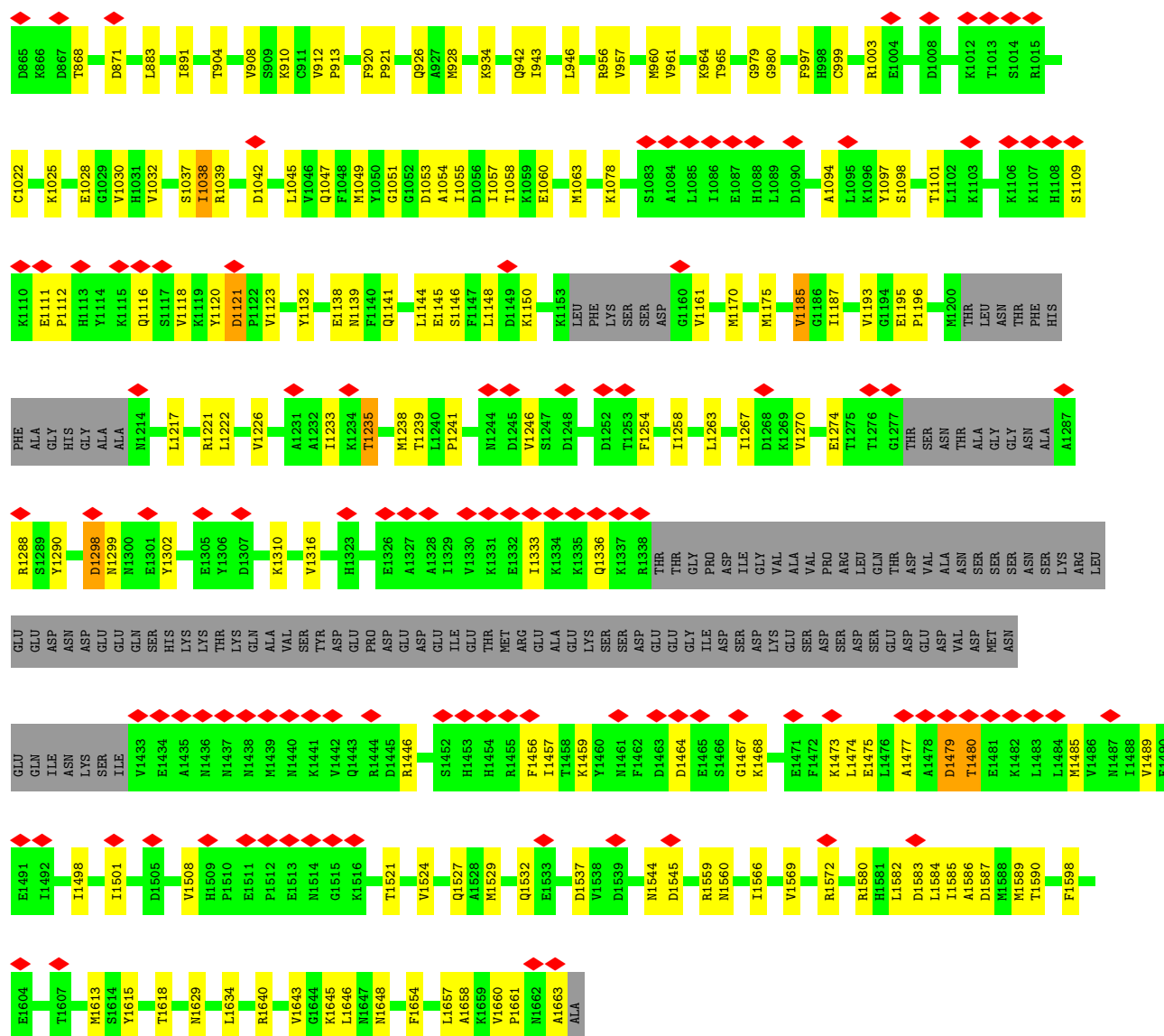
Mol	Chain	Residues	Atoms		AltConf
17	R	1	Total	Mg	0
			1	1	

3 Residue-property plots

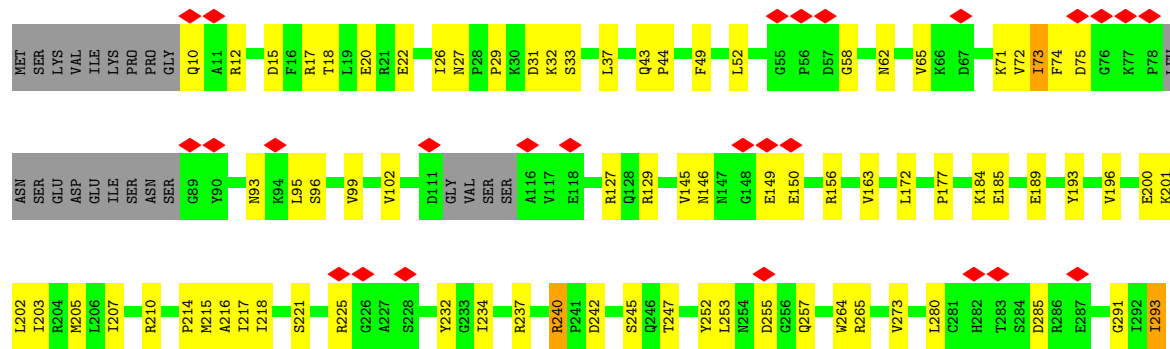
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

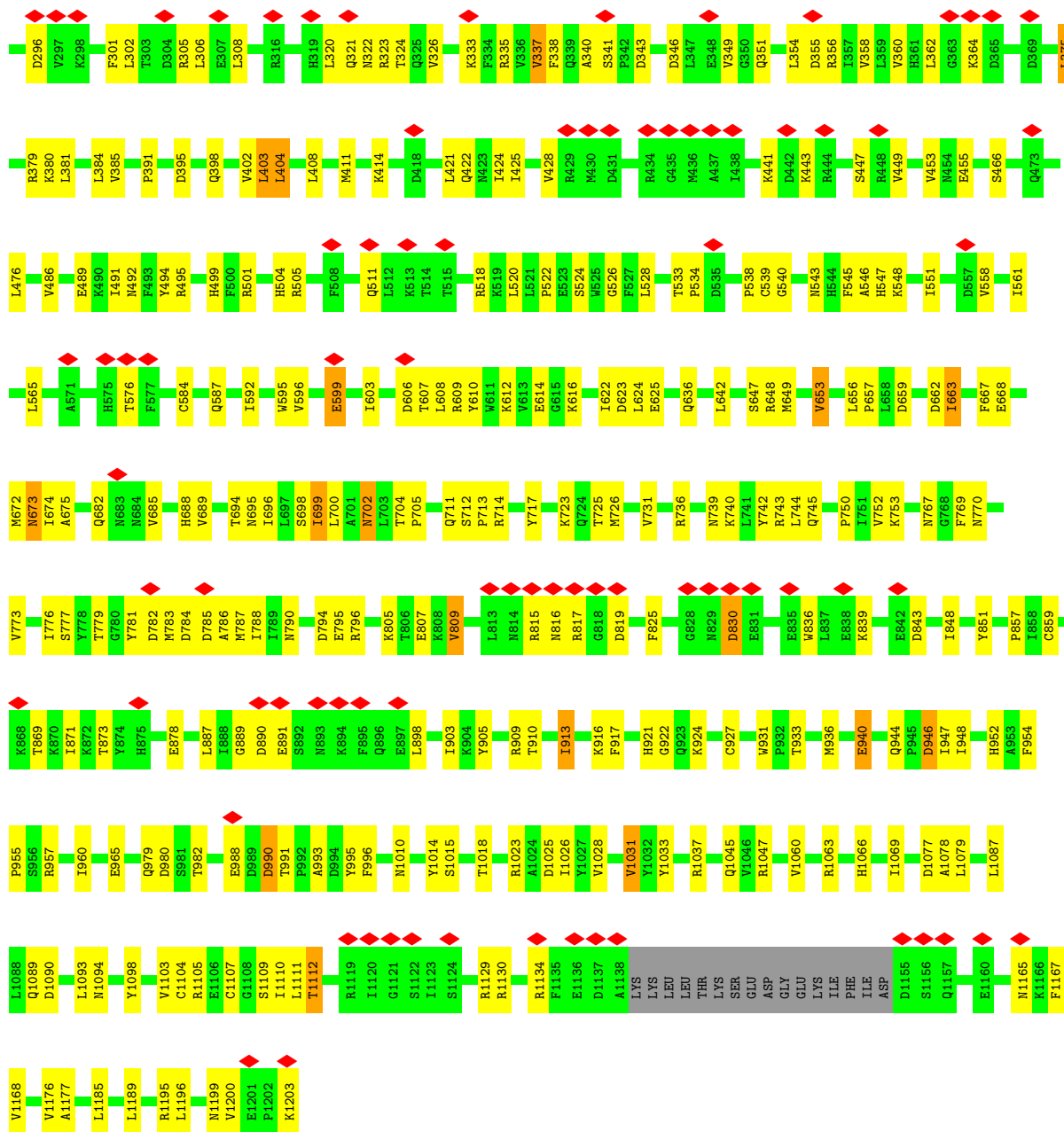
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190



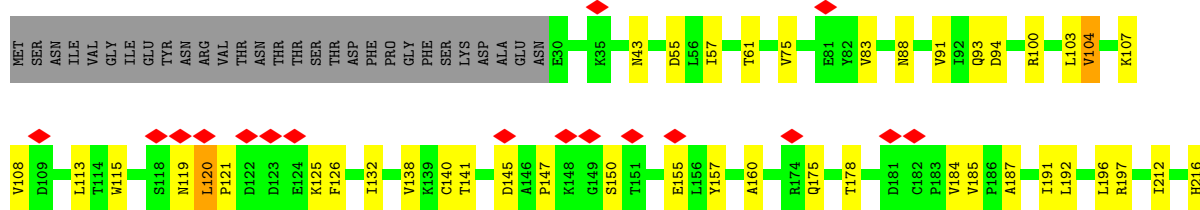
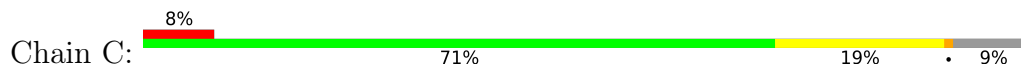


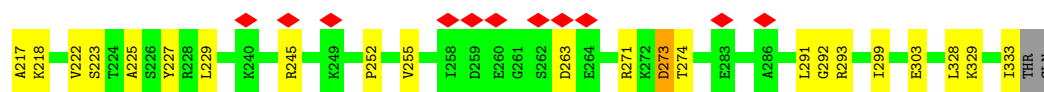
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



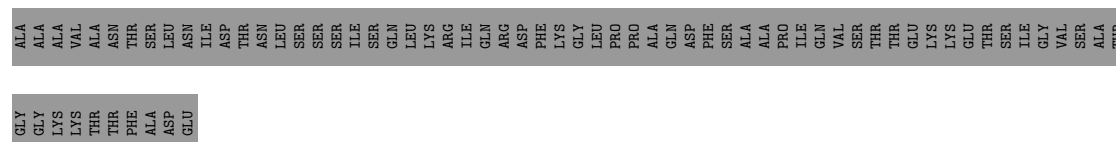
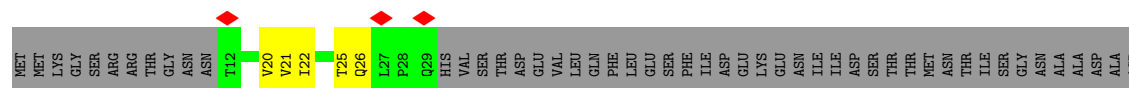


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

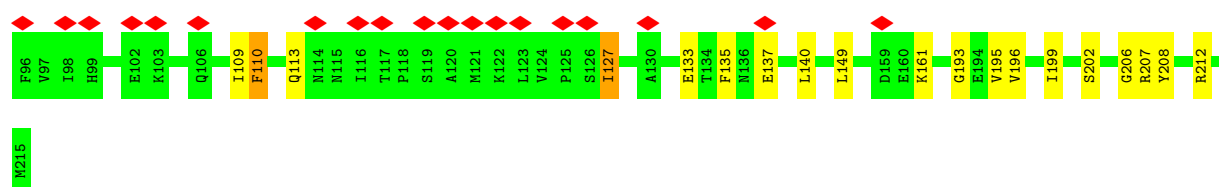
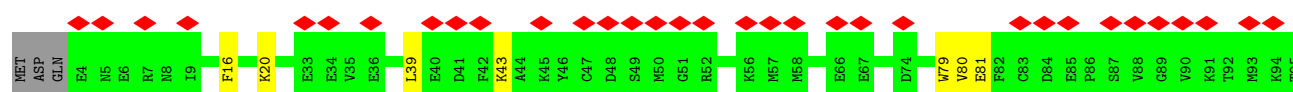
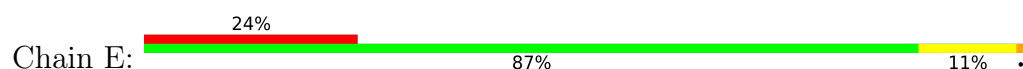




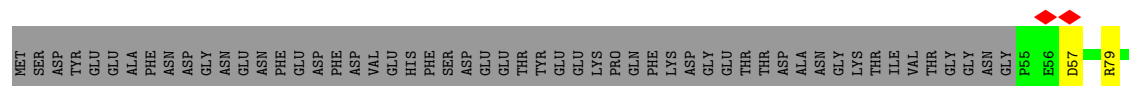
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14



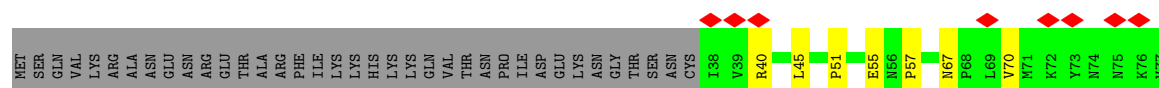
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

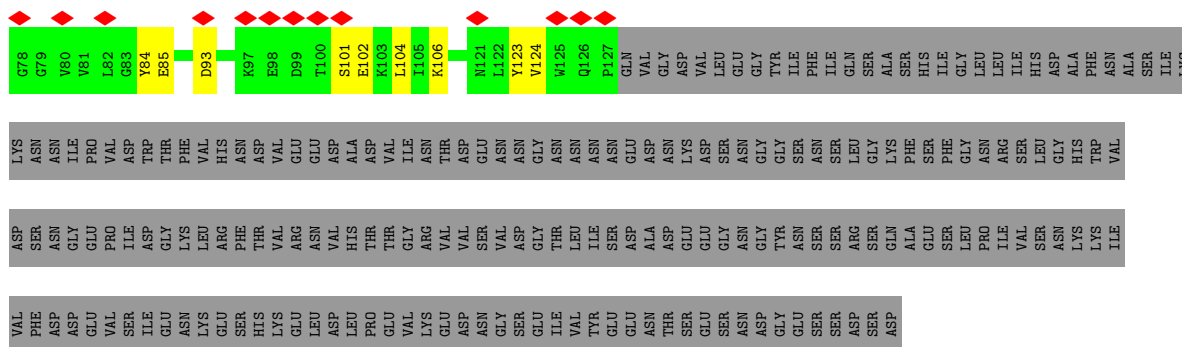


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

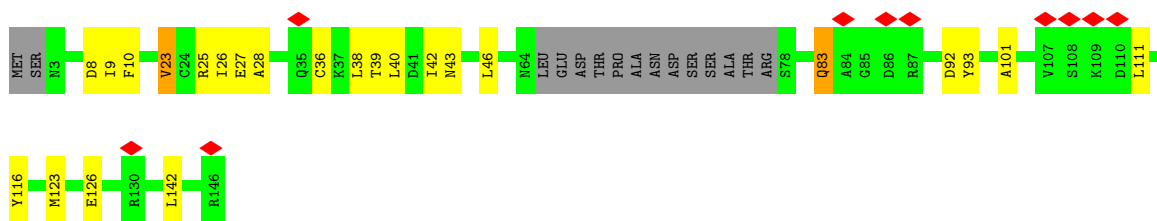


• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

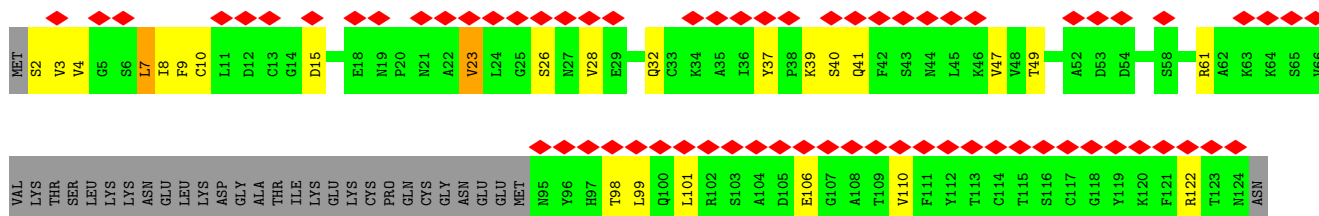




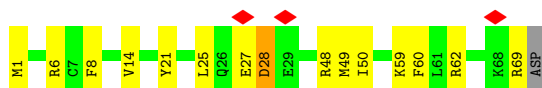
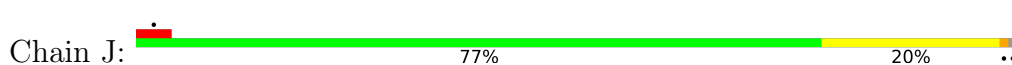
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



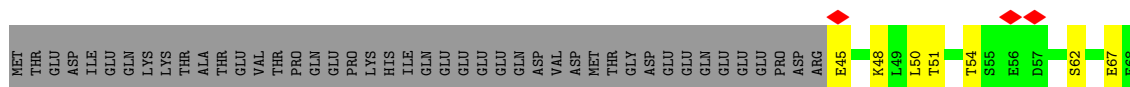
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



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

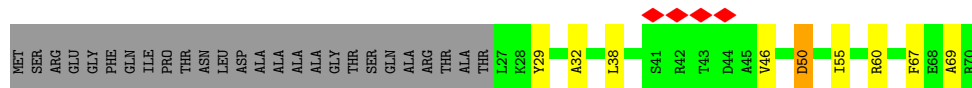


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

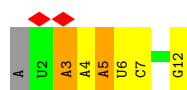




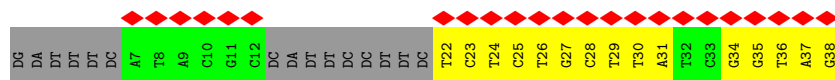
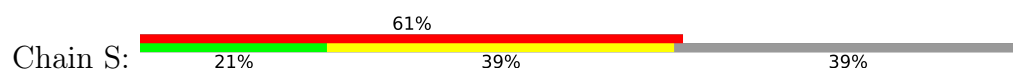
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



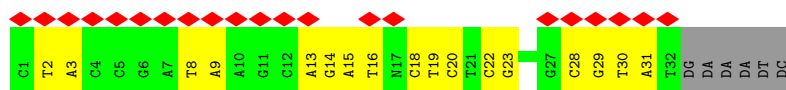
- Molecule 13: RNA



- 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	283214	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	0.144	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (\AA)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.047, 1.047, 1.047	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.12	0/11747	0.28	0/15864
2	B	0.14	0/9459	0.30	0/12786
3	C	0.12	0/2467	0.27	0/3344
4	D	0.10	0/135	0.24	0/188
5	E	0.11	0/1770	0.27	0/2383
6	F	0.11	0/838	0.25	0/1129
7	G	0.10	0/736	0.27	0/1005
8	H	0.12	0/1070	0.29	0/1449
9	I	0.08	0/731	0.31	0/989
10	J	0.13	0/578	0.26	0/775
11	K	0.14	0/776	0.31	0/1047
12	L	0.11	0/354	0.26	0/468
13	R	0.15	0/268	0.32	0/416
14	S	0.18	0/521	0.42	0/799
15	T	0.20	0/706	0.38	0/1084
All	All	0.13	0/32156	0.29	0/43726

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	11538	0	11619	225	0
2	B	9254	0	9140	227	0
3	C	2415	0	2403	40	0
4	D	133	0	138	2	0
5	E	1734	0	1764	19	0
6	F	823	0	841	15	0
7	G	716	0	735	11	0
8	H	1052	0	1021	14	0
9	I	720	0	702	14	0
10	J	569	0	585	13	0
11	K	766	0	765	13	0
12	L	352	0	374	9	0
13	R	239	0	119	6	0
14	S	468	0	263	15	0
15	T	643	0	359	13	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
17	R	1	0	0	0	0
All	All	31429	0	30828	554	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 (554) 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:584:CYS:HB3	2:B:596:VAL:O	1.64	0.97
1:A:105:CYS:HB3	1:A:236:CYS:SG	2.14	0.87
1:A:672:ASP:H	2:B:783:MET:HE3	1.47	0.78
2:B:674:ILE:HG22	2:B:688:HIS:HB2	1.64	0.78
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.65	0.78
14:S:34:DG:H2'	14:S:35:DG:C8	2.21	0.76
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.69	0.74
1:A:34:ASN:N	1:A:34:ASN:OD1	2.20	0.74
2:B:836:TRP:HB2	2:B:857:PRO:HG3	1.70	0.73
2:B:240:ARG:HH11	2:B:360:VAL:HG21	1.55	0.72
1:A:1559:ARG:NH2	1:A:1583:ASP:OD1	2.22	0.72
14:S:35:DG:H2'	14:S:36:DT:C6	2.25	0.71
14:S:28:DC:H2'	14:S:29:DT:H71	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.73	0.70
13:R:4:A:H2'	13:R:5:A:C8	2.25	0.70
2:B:146:ASN:HB2	2:B:149:GLU:HB2	1.72	0.70
2:B:185:GLU:HG3	2:B:189:GLU:HG3	1.73	0.70
1:A:597:LYS:HE2	1:A:660:PRO:HG3	1.74	0.69
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.74	0.69
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.39	0.69
2:B:779:THR:HG22	2:B:781:TYR:H	1.58	0.69
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.75	0.69
1:A:722:PRO:HD2	8:H:46:LEU:HD23	1.75	0.68
2:B:788:ILE:HB	2:B:948:ILE:HB	1.76	0.68
3:C:255:VAL:HG21	3:C:273:ASP:HB3	1.75	0.67
1:A:961:VAL:HG11	2:B:636:GLN:HB2	1.78	0.66
2:B:740:LYS:HE2	2:B:805:LYS:HE2	1.78	0.66
2:B:830:ASP:OD1	2:B:830:ASP:N	2.23	0.66
1:A:864:LEU:HB3	1:A:868:THR:HG21	1.77	0.66
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.60	0.66
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.76	0.66
1:A:826:PHE:HB3	2:B:777:SER:HB3	1.78	0.66
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	1.77	0.66
2:B:694:THR:O	2:B:702:ASN:ND2	2.28	0.66
1:A:1118:VAL:HG21	5:E:199:ILE:HG12	1.78	0.65
8:H:23:VAL:HA	8:H:43:ASN:HA	1.78	0.65
2:B:924:LYS:NZ	13:R:12:G:OP1	2.29	0.65
1:A:671:GLN:NE2	2:B:783:MET:O	2.29	0.65
1:A:1055:ILE:HD13	1:A:1063:MET:HE1	1.78	0.65
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.79	0.65
2:B:558:VAL:HG13	2:B:561:ILE:HD12	1.79	0.65
1:A:1270:VAL:HG11	1:A:1489:VAL:HG11	1.79	0.65
2:B:770:ASN:O	10:J:48:ARG:NH1	2.29	0.65
3:C:252:PRO:HG2	3:C:273:ASP:HA	1.79	0.65
10:J:8:PHE:H	10:J:49:MET:HE3	1.62	0.64
10:J:28:ASP:N	10:J:28:ASP:OD1	2.30	0.64
2:B:1014:TYR:OH	3:C:293:ARG:NH2	2.30	0.64
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.30	0.64
6:F:101:ILE:HD12	6:F:107:VAL:HG22	1.79	0.64
1:A:1479:ASP:N	1:A:1479:ASP:OD1	2.29	0.64
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.80	0.63
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.24	0.63
1:A:1097:TYR:HD2	1:A:1123:VAL:HG12	1.63	0.63
2:B:411:MET:HE2	2:B:476:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:NH1	1:A:558:ALA:O	2.32	0.63
1:A:668:GLY:HA3	1:A:787:GLY:HA2	1.80	0.63
1:A:681:THR:O	1:A:729:LYS:NZ	2.30	0.63
2:B:184:LYS:NZ	12:L:32:ALA:O	2.23	0.63
1:A:1121:ASP:OD1	1:A:1121:ASP:N	2.32	0.62
2:B:293:ILE:HD12	2:B:302:LEU:HB3	1.80	0.62
6:F:111:LEU:HD22	6:F:120:ILE:HD12	1.80	0.62
1:A:1217:LEU:HD21	1:A:1572:ARG:HG3	1.81	0.62
2:B:607:THR:OG1	9:I:101:LEU:O	2.11	0.62
14:S:26:DT:O2	15:T:14:DG:N2	2.33	0.61
1:A:237:GLY:O	1:A:263:ASN:ND2	2.31	0.61
3:C:120:LEU:HD13	3:C:121:PRO:HD2	1.82	0.61
14:S:36:DT:H2'	14:S:37:DA:C8	2.35	0.61
1:A:339:PHE:O	1:A:1629:ASN:ND2	2.33	0.61
6:F:79:ARG:NH1	6:F:145:ASP:O	2.33	0.61
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.82	0.61
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.81	0.61
1:A:130:ILE:HD12	1:A:215:GLU:HG3	1.83	0.61
1:A:1290:TYR:HB2	1:A:1474:LEU:HB3	1.83	0.61
3:C:91:VAL:HG21	10:J:60:PHE:HB3	1.81	0.61
1:A:1241:PRO:HB2	1:A:1537:ASP:HB3	1.83	0.60
2:B:214:PRO:O	2:B:380:LYS:NZ	2.25	0.60
2:B:129:ARG:NH1	2:B:889:GLY:O	2.30	0.60
1:A:744:MET:HE2	1:A:1078:LYS:HG2	1.83	0.60
1:A:29:ALA:HB2	2:B:1129:ARG:HH12	1.66	0.60
1:A:852:ASP:OD2	1:A:855:ARG:NH2	2.34	0.60
2:B:129:ARG:HH22	2:B:890:ASP:HA	1.66	0.59
2:B:940:GLU:OE2	3:C:293:ARG:NH2	2.35	0.59
3:C:175:GLN:HA	3:C:178:THR:HG22	1.84	0.59
1:A:859:ALA:HA	1:A:862:THR:HG22	1.85	0.59
6:F:106:PRO:HG3	7:G:55:GLU:HG2	1.83	0.59
2:B:991:THR:HG22	2:B:993:ALA:H	1.66	0.59
4:D:25:THR:HG22	4:D:26:GLN:HG3	1.83	0.59
1:A:701:ARG:NH1	1:A:704:ASP:OD2	2.36	0.59
1:A:1039:ARG:HB3	1:A:1045:LEU:HD12	1.83	0.59
2:B:1105:ARG:HD3	2:B:1203:LYS:HA	1.84	0.59
9:I:10:CYS:SG	9:I:37:TYR:OH	2.56	0.59
2:B:242:ASP:OD2	2:B:414:LYS:NZ	2.33	0.59
1:A:1333:ILE:HA	1:A:1336:GLN:HG2	1.84	0.59
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.29	0.59
15:T:30:DT:H2''	15:T:31:DA:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:27:DG:H2'	14:S:28:DC:C6	2.38	0.58
1:A:646:GLU:OE1	2:B:1087:LEU:N	2.35	0.58
1:A:960:MET:HE2	2:B:522:PRO:HB2	1.86	0.58
1:A:590:ASN:HB2	1:A:600:MET:HG3	1.84	0.58
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.84	0.58
2:B:203:ILE:HD11	2:B:408:LEU:HD23	1.86	0.57
2:B:990:ASP:OD1	2:B:990:ASP:N	2.37	0.57
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.68	0.57
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.37	0.57
1:A:1258:ILE:HG23	1:A:1501:ILE:HD12	1.87	0.57
2:B:26:ILE:O	10:J:62:ARG:NH1	2.37	0.57
2:B:72:VAL:HG12	2:B:96:SER:HA	1.87	0.57
3:C:150:SER:OG	3:C:155:GLU:OE1	2.23	0.57
2:B:215:MET:HE3	2:B:217:ILE:HD11	1.87	0.57
1:A:11:ILE:HG13	2:B:1176:VAL:HG11	1.86	0.57
1:A:862:THR:HG23	1:A:864:LEU:H	1.70	0.57
1:A:1477:ALA:O	1:A:1480:THR:OG1	2.22	0.57
1:A:76:GLN:HG2	1:A:364:PRO:HD3	1.87	0.57
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.38	0.57
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.38	0.56
2:B:225:ARG:HH22	14:S:22:DT:H4'	1.69	0.56
2:B:346:ASP:HA	2:B:349:VAL:HG12	1.87	0.56
2:B:807:GLU:OE2	2:B:905:TYR:OH	2.20	0.56
2:B:99:VAL:HG23	2:B:421:LEU:HD21	1.87	0.56
3:C:328:LEU:HD22	11:K:72:LEU:HD21	1.86	0.56
1:A:397:ARG:NH2	1:A:398:ASP:OD1	2.39	0.56
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.87	0.56
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.23	0.56
2:B:526:GLY:H	2:B:696:ILE:HG23	1.71	0.56
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.88	0.56
1:A:1193:VAL:HG21	1:A:1585:ILE:HD12	1.88	0.55
1:A:27:LEU:HD22	2:B:1130:ARG:HH21	1.71	0.55
1:A:943:ILE:HG23	2:B:960:ILE:HD11	1.88	0.55
1:A:1640:ARG:NH1	1:A:1648:ASN:OD1	2.39	0.55
3:C:103:LEU:HD22	10:J:6:ARG:HD2	1.89	0.55
1:A:464:GLU:HA	1:A:469:LYS:HD2	1.88	0.55
8:H:40:LEU:HG	8:H:42:ILE:HG23	1.88	0.55
14:S:34:DG:H2'	14:S:35:DG:H8	1.67	0.55
2:B:196:VAL:HG11	2:B:466:SER:HB3	1.88	0.55
14:S:35:DG:H2'	14:S:36:DT:H6	1.71	0.55
1:A:487:ASP:HB2	1:A:615:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:HG21	2:B:1026:ILE:HG23	1.87	0.55
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.47	0.54
2:B:547:HIS:CD2	2:B:695:ASN:HA	2.43	0.54
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.89	0.54
2:B:898:LEU:HB3	12:L:46:VAL:HG21	1.90	0.54
13:R:4:A:H2'	13:R:5:A:H8	1.71	0.54
2:B:547:HIS:HB2	2:B:699:ILE:HD13	1.90	0.54
7:G:85:GLU:OE1	7:G:123:TYR:OH	2.24	0.54
1:A:700:ILE:HD11	1:A:735:VAL:HG22	1.89	0.54
2:B:395:ASP:HA	2:B:505:ARG:HH12	1.73	0.54
1:A:263:ASN:HA	1:A:266:VAL:HG22	1.90	0.54
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.41	0.54
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.90	0.53
1:A:502:ALA:HA	1:A:581:ILE:HG22	1.89	0.53
3:C:119:ASN:OD1	3:C:119:ASN:N	2.42	0.53
15:T:18:DC:H2'	15:T:19:DT:C6	2.44	0.53
1:A:827:THR:HG22	2:B:776:ILE:HA	1.90	0.53
2:B:402:VAL:O	2:B:647:SER:HB2	2.09	0.53
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.73	0.53
2:B:443:LYS:NZ	2:B:447:SER:OG	2.37	0.53
3:C:245:ARG:NH2	3:C:263:ASP:OD2	2.42	0.53
11:K:45:GLU:OE1	11:K:45:GLU:N	2.42	0.53
1:A:332:GLN:OE1	1:A:336:GLN:NE2	2.41	0.52
2:B:58:GLY:O	2:B:62:ASN:ND2	2.41	0.52
3:C:216:HIS:HD2	3:C:218:LYS:H	1.55	0.52
1:A:1657:LEU:HB2	6:F:133:VAL:HB	1.90	0.52
1:A:471:MET:HE1	2:B:1185:LEU:HD22	1.91	0.52
2:B:428:VAL:HG12	2:B:449:VAL:HG21	1.90	0.52
2:B:878:GLU:OE1	2:B:909:ARG:NH2	2.31	0.52
15:T:8:DT:H2''	15:T:9:DA:C8	2.44	0.52
1:A:588:LEU:HD21	2:B:1079:LEU:HD21	1.92	0.52
5:E:202:SER:HB2	5:E:208:TYR:HE1	1.75	0.52
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.92	0.52
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.92	0.52
2:B:1103:VAL:HG22	2:B:1110:ILE:HD13	1.91	0.52
1:A:1038:ILE:HG12	1:A:1047:GLN:HB2	1.91	0.52
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.91	0.52
1:A:739:VAL:HG21	1:A:809:VAL:HG22	1.91	0.52
1:A:1613:MET:O	1:A:1618:THR:HG22	2.10	0.52
2:B:610:TYR:OH	9:I:122:ARG:NH1	2.43	0.52
1:A:1170:MET:HE2	1:A:1170:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASP:OD2	2:B:379:ARG:NH2	2.41	0.52
2:B:606:ASP:HB3	9:I:99:LEU:HD21	1.92	0.52
6:F:85:MET:HE2	6:F:153:VAL:HG12	1.90	0.52
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.91	0.51
2:B:216:ALA:HA	2:B:234:ILE:HD13	1.92	0.51
2:B:221:SER:HB2	14:S:23:DC:H1'	1.92	0.51
1:A:94:LEU:HD13	1:A:355:PHE:CG	2.46	0.51
1:A:114:GLU:HG3	1:A:117:ARG:HH21	1.76	0.51
2:B:337:VAL:HG13	2:B:338:PHE:HD1	1.75	0.51
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.93	0.51
2:B:625:GLU:HG3	2:B:668:GLU:HB2	1.93	0.51
4:D:20:VAL:HG12	4:D:21:VAL:HG23	1.91	0.51
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.92	0.51
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.93	0.51
1:A:589:MET:HE3	1:A:633:MET:HE2	1.93	0.51
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.40	0.51
1:A:260:GLN:N	1:A:260:GLN:HE21	2.08	0.51
1:A:1003:ARG:HD2	2:B:520:LEU:HB2	1.93	0.51
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	1.92	0.51
1:A:1138:GLU:OE2	5:E:207:ARG:NH1	2.44	0.51
2:B:398:GLN:HG3	2:B:667:PHE:HA	1.92	0.51
2:B:543:ASN:OD1	2:B:543:ASN:N	2.44	0.51
2:B:931:TRP:HD1	2:B:936:MET:HG2	1.76	0.51
2:B:1107:CYS:SG	2:B:1109:SER:OG	2.60	0.51
3:C:100:ARG:NH2	3:C:192:LEU:O	2.41	0.51
8:H:36:CYS:HA	8:H:126:GLU:O	2.11	0.51
1:A:831:ASP:OD1	1:A:831:ASP:N	2.40	0.51
1:A:843:ARG:NH2	2:B:988:GLU:OE2	2.38	0.51
1:A:1235:THR:O	1:A:1235:THR:OG1	2.21	0.50
2:B:662:ASP:OD1	2:B:663:ILE:N	2.44	0.50
1:A:1263:LEU:HG	1:A:1267:ILE:HD11	1.91	0.50
2:B:1112:THR:HG21	2:B:1130:ARG:HB2	1.92	0.50
1:A:372:LYS:HG3	1:A:377:VAL:HG22	1.92	0.50
1:A:613:THR:O	1:A:615:ARG:NH2	2.41	0.50
1:A:721:LYS:NZ	8:H:93:TYR:O	2.34	0.50
13:R:6:U:H2'	13:R:7:C:C6	2.47	0.50
2:B:75:ASP:OD2	2:B:93:ASN:ND2	2.44	0.50
2:B:533:THR:HG21	2:B:540:GLY:H	1.76	0.50
1:A:1037:SER:OG	1:A:1047:GLN:O	2.26	0.50
1:A:19:LEU:HD13	2:B:1195:ARG:HB2	1.94	0.50
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ARG:NH1	2:B:245:SER:OG	2.45	0.50
5:E:39:LEU:HG	5:E:43:LYS:HE3	1.94	0.49
1:A:1586:ALA:O	1:A:1590:THR:HG22	2.13	0.49
2:B:31:ASP:OD1	2:B:32:LYS:N	2.43	0.49
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.76	0.49
1:A:904:THR:HG23	1:A:946:LEU:HD11	1.94	0.49
2:B:73:ILE:HD13	2:B:428:VAL:HG23	1.94	0.49
9:I:3:VAL:HG22	9:I:8:ILE:HG22	1.94	0.49
1:A:1221:ARG:NH2	1:A:1544:ASN:OD1	2.45	0.49
2:B:816:ASN:O	2:B:817:ARG:HG2	2.12	0.49
5:E:161:LYS:HE3	5:E:193:GLY:O	2.12	0.49
1:A:35:PRO:HB3	1:A:390:LEU:HB2	1.94	0.49
1:A:1446:ARG:NH2	1:A:1464:ASP:OD2	2.44	0.49
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.48	0.49
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.43	0.49
13:R:5:A:H2'	13:R:6:U:C6	2.47	0.49
14:S:37:DA:H2''	14:S:38:DG:C8	2.48	0.49
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.95	0.49
2:B:745:GLN:O	10:J:1:MET:N	2.44	0.49
2:B:200:GLU:OE2	2:B:736:ARG:NH2	2.46	0.48
2:B:285:ASP:HB2	9:I:15:ASP:HA	1.95	0.48
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.48	0.48
2:B:291:GLY:HA3	2:B:375:LEU:HD23	1.94	0.48
9:I:26:SER:H	9:I:39:LYS:HD2	1.78	0.48
2:B:145:VAL:HG22	2:B:150:GLU:HB3	1.96	0.48
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.93	0.48
1:A:1298:ASP:HA	1:A:1468:LYS:HE2	1.95	0.48
10:J:14:VAL:HB	10:J:50:ILE:HD11	1.95	0.48
15:T:18:DC:H2'	15:T:19:DT:H6	1.78	0.48
2:B:492:ASN:ND2	2:B:725:THR:OG1	2.47	0.48
9:I:40:SER:O	9:I:41:GLN:HG2	2.14	0.48
1:A:115:VAL:HG13	1:A:334:VAL:HG11	1.95	0.48
1:A:134:TYR:OH	1:A:215:GLU:OE1	2.31	0.48
2:B:210:ARG:NH2	2:B:625:GLU:OE1	2.46	0.48
1:A:431:GLN:O	1:A:435:ASN:ND2	2.36	0.48
1:A:833:LEU:HD13	2:B:960:ILE:HD13	1.95	0.48
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.95	0.48
2:B:489:GLU:HB3	2:B:491:ILE:HG13	1.95	0.48
2:B:599:GLU:O	2:B:603:ILE:HG12	2.13	0.48
1:A:68:ASP:OD1	1:A:68:ASP:N	2.39	0.48
2:B:518:ARG:NH1	2:B:539:CYS:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:GLU:HG2	2:B:672:MET:HE2	1.96	0.48
5:E:202:SER:HB2	5:E:208:TYR:CE1	2.49	0.48
1:A:82:PRO:HB2	1:A:396:ILE:HD13	1.96	0.48
2:B:18:THR:O	2:B:22:GLU:HG2	2.13	0.48
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.95	0.48
2:B:739:ASN:HD21	15:T:23:DG:H5''	1.78	0.48
2:B:753:LYS:O	2:B:980:ASP:HA	2.14	0.48
1:A:1585:ILE:O	1:A:1589:MET:HG3	2.14	0.47
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.46	0.47
7:G:93:ASP:HB3	7:G:104:LEU:HD12	1.95	0.47
10:J:8:PHE:CD2	10:J:49:MET:HE1	2.49	0.47
2:B:603:ILE:O	2:B:607:THR:OG1	2.32	0.47
3:C:328:LEU:HD23	11:K:121:LEU:HD21	1.95	0.47
11:K:51:THR:HA	11:K:54:THR:HG22	1.95	0.47
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.79	0.47
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.96	0.47
2:B:673:ASN:ND2	2:B:685:VAL:O	2.46	0.47
1:A:392:THR:O	1:A:396:ILE:HG22	2.14	0.47
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.97	0.47
1:A:1060:GLU:HA	1:A:1063:MET:HG3	1.96	0.47
1:A:1042:ASP:OD1	1:A:1042:ASP:N	2.46	0.47
2:B:172:LEU:HD13	2:B:185:GLU:HG2	1.95	0.47
2:B:424:ILE:HG22	2:B:453:VAL:HG11	1.97	0.47
2:B:547:HIS:CE1	2:B:548:LYS:HE2	2.50	0.47
15:T:13:DA:H2''	15:T:14:DG:C8	2.50	0.47
1:A:1022:CYS:HG	1:A:1615:TYR:HH	1.55	0.47
11:K:50:LEU:HD12	11:K:62:SER:HB3	1.96	0.47
1:A:250:LYS:HG2	1:A:314:TYR:HE1	1.79	0.47
2:B:12:ARG:NH2	2:B:990:ASP:OD2	2.48	0.47
2:B:321:GLN:O	9:I:32:GLN:NE2	2.48	0.47
2:B:623:ASP:HB3	2:B:648:ARG:HH22	1.80	0.47
15:T:15:DA:H2''	15:T:16:DT:O4'	2.14	0.47
3:C:107:LYS:HE3	3:C:187:ALA:HA	1.96	0.47
3:C:229:LEU:HB3	3:C:293:ARG:HB3	1.96	0.47
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.97	0.47
2:B:545:PHE:HE1	2:B:649:MET:HE3	1.80	0.46
2:B:773:VAL:HG21	2:B:1031:VAL:HG22	1.96	0.46
2:B:145:VAL:HG21	2:B:441:LYS:HG2	1.97	0.46
3:C:125:LYS:HE3	3:C:126:PHE:CZ	2.50	0.46
1:A:1038:ILE:HD11	1:A:1584:LEU:HD13	1.96	0.46
2:B:156:ARG:NH2	2:B:455:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:PRO:O	2:B:717:TYR:HD1	1.98	0.46
3:C:223:SER:N	3:C:303:GLU:O	2.48	0.46
1:A:549:MET:HE1	1:A:557:LEU:HD22	1.97	0.46
2:B:205:MET:HA	2:B:403:LEU:O	2.15	0.46
2:B:491:ILE:HG21	2:B:1037:ARG:HD3	1.97	0.46
1:A:31:GLN:HB3	1:A:78:HIS:CE1	2.51	0.46
1:A:1274:GLU:OE2	1:A:1288:ARG:NH2	2.35	0.46
3:C:115:TRP:HH2	3:C:212:ILE:HG23	1.80	0.46
8:H:26:ILE:O	8:H:39:THR:HA	2.15	0.46
8:H:123:MET:HE2	8:H:142:LEU:HD13	1.97	0.46
1:A:942:GLN:HA	1:A:946:LEU:O	2.16	0.46
1:A:1139:ASN:OD1	5:E:206:GLY:N	2.47	0.46
1:A:52:LEU:HD11	1:A:60:ASN:HB3	1.98	0.46
2:B:830:ASP:OD2	2:B:869:THR:N	2.48	0.46
15:T:22:DC:H2'	15:T:23:DG:C8	2.51	0.46
1:A:643:ALA:HB1	2:B:1087:LEU:HD23	1.97	0.46
1:A:674:ILE:HD13	1:A:783:LYS:HB2	1.98	0.46
1:A:871:ASP:OD1	1:A:871:ASP:N	2.42	0.46
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.51	0.46
5:E:80:VAL:HG22	5:E:109:ILE:HD11	1.96	0.46
12:L:50:ASP:OD1	12:L:50:ASP:N	2.48	0.46
2:B:33:SER:HA	2:B:177:PRO:HG3	1.97	0.46
2:B:1015:SER:OG	2:B:1018:THR:OG1	2.27	0.46
1:A:259:LYS:O	1:A:262:THR:OG1	2.32	0.46
1:A:260:GLN:HE21	1:A:260:GLN:H	1.64	0.46
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.98	0.46
9:I:28:VAL:HB	9:I:37:TYR:HB2	1.98	0.45
2:B:656:LEU:HB3	2:B:657:PRO:HD3	1.98	0.45
1:A:1049:MET:HG3	1:A:1054:ALA:HB2	1.99	0.45
2:B:1134:ARG:HA	2:B:1167:PHE:HD1	1.80	0.45
1:A:37:VAL:HB	1:A:38:LEU:HD23	1.98	0.45
1:A:964:LYS:NZ	2:B:672:MET:O	2.44	0.45
2:B:17:ARG:HB3	2:B:20:GLU:HB3	1.97	0.45
2:B:333:LYS:HD3	2:B:333:LYS:HA	1.77	0.45
3:C:252:PRO:HD2	3:C:273:ASP:HB2	1.98	0.45
1:A:486:PRO:HD3	1:A:628:PHE:CG	2.52	0.45
2:B:15:ASP:OD1	2:B:15:ASP:N	2.49	0.45
2:B:301:PHE:O	2:B:305:ARG:HG2	2.16	0.45
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.98	0.45
7:G:67:ASN:OD1	7:G:84:TYR:OH	2.20	0.45
1:A:628:PHE:CD2	2:B:784:ASP:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:GLN:HB2	2:B:685:VAL:HG22	1.98	0.45
2:B:848:ILE:O	12:L:60:ARG:NH1	2.50	0.45
6:F:107:VAL:HG11	6:F:111:LEU:HD21	1.99	0.45
1:A:672:ASP:OD1	2:B:952:HIS:ND1	2.49	0.45
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.47	0.45
1:A:1559:ARG:NE	1:A:1587:ASP:OD1	2.40	0.45
1:A:204:GLU:HG2	1:A:205:ARG:HG3	1.98	0.45
1:A:1222:LEU:HD21	1:A:1569:VAL:HG11	1.99	0.45
1:A:466:LEU:HG	1:A:471:MET:HE3	1.98	0.45
1:A:1238:MET:HB3	1:A:1521:THR:OG1	2.17	0.45
1:A:1:MET:HE1	1:A:3:ILE:HG22	1.99	0.44
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.89	0.44
2:B:74:PHE:HA	2:B:93:ASN:O	2.16	0.44
2:B:232:TYR:CG	2:B:385:VAL:HG12	2.52	0.44
2:B:526:GLY:N	2:B:696:ILE:HG23	2.33	0.44
3:C:55:ASP:CG	3:C:271:ARG:HH12	2.24	0.44
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.98	0.44
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.52	0.44
1:A:1098:SER:OG	1:A:1141:GLN:OE1	2.35	0.44
1:A:1175:MET:HE2	1:A:1175:MET:HB3	1.83	0.44
2:B:726:MET:O	2:B:744:LEU:HB2	2.16	0.44
1:A:1456:PHE:HB2	1:A:1475:GLU:O	2.18	0.44
1:A:29:ALA:HA	2:B:1129:ARG:HH22	1.82	0.44
1:A:1590:THR:HG23	5:E:212:ARG:HH22	1.83	0.44
2:B:489:GLU:H	2:B:499:HIS:CE1	2.35	0.44
2:B:795:GLU:OE1	3:C:217:ALA:N	2.50	0.44
2:B:1077:ASP:OD1	2:B:1078:ALA:N	2.50	0.44
9:I:23:VAL:O	9:I:39:LYS:NZ	2.51	0.44
14:S:37:DA:H4'	14:S:38:DG:OP1	2.17	0.44
1:A:322:ASN:O	1:A:326:THR:OG1	2.35	0.44
1:A:511:VAL:HG12	1:A:575:LYS:O	2.17	0.44
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.52	0.44
2:B:587:GLN:HG2	2:B:592:ILE:HG13	1.98	0.44
3:C:140:CYS:HB2	3:C:196:LEU:HB3	1.99	0.44
14:S:25:DC:H5'	14:S:25:DC:C6	2.53	0.44
1:A:498:PRO:HD2	1:A:501:PHE:CD2	2.53	0.44
1:A:730:GLN:O	1:A:734:THR:HG22	2.18	0.44
1:A:1141:GLN:O	1:A:1145:GLU:HG2	2.17	0.44
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.52	0.44
2:B:809:VAL:HG21	2:B:859:CYS:SG	2.57	0.44
2:B:890:ASP:OD1	2:B:891:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ARG:NH2	8:H:27:GLU:OE2	2.51	0.44
1:A:507:TYR:OH	1:A:641:GLU:OE2	2.33	0.44
1:A:1663:ALA:HB2	7:G:101:SER:HA	2.00	0.44
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.53	0.44
5:E:161:LYS:HD2	5:E:195:VAL:HG23	2.00	0.44
1:A:641:GLU:HB2	6:F:99:LEU:HG	1.99	0.44
1:A:1028:GLU:HA	1:A:1187:ILE:HG12	1.98	0.44
15:T:2:DT:H2''	15:T:3:DA:C8	2.53	0.44
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.49	0.44
1:A:1226:VAL:HG13	1:A:1598:PHE:CD2	2.53	0.44
2:B:714:ARG:NH1	2:B:922:GLY:O	2.49	0.44
1:A:363:PRO:HG2	1:A:368:ARG:HD3	1.99	0.43
1:A:634:ASN:HB3	2:B:1069:ILE:HD12	2.00	0.43
1:A:1146:SER:O	1:A:1150:LYS:HG2	2.17	0.43
1:A:1524:VAL:HG21	1:A:1545:ASP:HB2	1.99	0.43
2:B:320:LEU:HB3	2:B:326:VAL:HG22	2.00	0.43
2:B:576:THR:HG21	2:B:595:TRP:CD1	2.53	0.43
2:B:954:PHE:N	2:B:955:PRO:HD2	2.33	0.43
9:I:2:SER:HB2	9:I:9:PHE:O	2.18	0.43
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.53	0.43
11:K:91:TYR:HA	11:K:102:ASN:O	2.18	0.43
1:A:490:ILE:O	1:A:617:HIS:ND1	2.52	0.43
1:A:396:ILE:HD11	1:A:427:PHE:HE1	1.83	0.43
1:A:491:GLU:C	1:A:493:ASN:H	2.25	0.43
1:A:1238:MET:HE3	1:A:1524:VAL:HA	2.00	0.43
1:A:1566:ILE:HG23	1:A:1582:LEU:HG	2.00	0.43
3:C:104:VAL:HG23	3:C:191:ILE:HD12	2.00	0.43
5:E:113:GLN:HA	5:E:137:GLU:HG2	2.01	0.43
1:A:94:LEU:HD11	1:A:324:LEU:HD13	1.99	0.43
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.54	0.43
1:A:1254:PHE:CE1	1:A:1532:GLN:HG2	2.53	0.43
1:A:1643:VAL:HG13	1:A:1645:LYS:HG3	2.00	0.43
2:B:27:ASN:O	2:B:27:ASN:ND2	2.52	0.43
2:B:913:ILE:HA	2:B:927:CYS:HB3	2.00	0.43
11:K:67:GLU:N	11:K:99:ASN:O	2.46	0.43
1:A:373:LEU:HB2	13:R:3:A:N7	2.34	0.43
1:A:486:PRO:HB3	1:A:628:PHE:CE2	2.54	0.43
15:T:22:DC:H2'	15:T:23:DG:H8	1.81	0.43
1:A:4:SER:HB2	1:A:573:LEU:HD22	2.01	0.43
1:A:184:LYS:HA	1:A:184:LYS:HD3	1.82	0.43
2:B:796:ARG:NH1	10:J:8:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ILE:HD13	3:C:184:VAL:HG21	2.01	0.43
1:A:514:TYR:OH	6:F:117:PRO:HG3	2.19	0.43
1:A:1057:ILE:H	1:A:1057:ILE:HD12	1.84	0.43
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	2.01	0.43
2:B:306:LEU:HD12	2:B:306:LEU:HA	1.80	0.43
2:B:653:VAL:HG22	2:B:689:VAL:O	2.19	0.43
1:A:1290:TYR:CE1	1:A:1485:MET:HG2	2.54	0.42
2:B:264:TRP:HH2	2:B:356:ARG:HD3	1.84	0.42
2:B:424:ILE:HG22	2:B:453:VAL:HG21	2.01	0.42
2:B:839:LYS:NZ	2:B:851:TYR:O	2.48	0.42
6:F:87:LYS:H	6:F:87:LYS:HG2	1.56	0.42
14:S:24:DT:H2"	14:S:25:DC:C5	2.54	0.42
1:A:32:ILE:HD12	1:A:390:LEU:HD11	2.00	0.42
1:A:1109:SER:HA	1:A:1116:GLN:NE2	2.34	0.42
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.01	0.42
1:A:21:ALA:HA	1:A:24:ILE:HD11	2.01	0.42
1:A:692:TYR:O	1:A:696:ILE:HG12	2.18	0.42
2:B:785:ASP:CG	2:B:957:ARG:HH22	2.27	0.42
2:B:815:ARG:HB2	2:B:819:ASP:OD1	2.19	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.49	0.42
1:A:1037:SER:OG	1:A:1045:LEU:HD11	2.20	0.42
2:B:612:LYS:HE3	2:B:622:ILE:O	2.19	0.42
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.54	0.42
1:A:1030:VAL:HG11	1:A:1584:LEU:HD11	2.01	0.42
1:A:1258:ILE:HD13	1:A:1529:MET:HE1	2.01	0.42
2:B:836:TRP:CD1	2:B:836:TRP:C	2.98	0.42
2:B:184:LYS:HE3	10:J:69:ARG:NH2	2.35	0.42
3:C:329:LYS:HZ1	11:K:122:LYS:HE2	1.85	0.42
7:G:40:ARG:HD3	7:G:123:TYR:HE1	1.84	0.42
11:K:81:MET:SD	11:K:89:CYS:HB3	2.59	0.42
1:A:52:LEU:HD13	1:A:52:LEU:HA	1.85	0.42
1:A:928:MET:SD	2:B:955:PRO:HG3	2.59	0.42
2:B:787:MET:SD	2:B:917:PHE:HB2	2.60	0.42
2:B:909:ARG:HA	2:B:909:ARG:HD3	1.82	0.42
3:C:147:PRO:HD2	3:C:155:GLU:HB3	2.01	0.42
1:A:117:ARG:HB2	1:A:185:ARG:NH1	2.35	0.42
1:A:1111:GLU:HB2	1:A:1112:PRO:HD2	2.01	0.42
2:B:565:LEU:HD23	2:B:565:LEU:HA	1.91	0.42
2:B:825:PHE:HD2	2:B:898:LEU:HG	1.85	0.42
3:C:216:HIS:CD2	3:C:218:LYS:H	2.36	0.42
6:F:103:MET:HB2	7:G:51:PRO:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HE3	1:A:245:LYS:HB3	1.86	0.42
1:A:1101:THR:HG22	1:A:1120:TYR:HB3	2.02	0.42
2:B:534:PRO:HG2	2:B:538:PRO:HB2	2.02	0.42
2:B:782:ASP:HA	2:B:786:ALA:HB3	2.01	0.42
3:C:197:ARG:HD3	3:C:197:ARG:HA	1.86	0.42
11:K:48:LYS:HE2	11:K:48:LYS:HB3	1.85	0.42
11:K:69:ASP:OD1	11:K:70:HIS:ND1	2.52	0.42
1:A:821:ILE:HD12	1:A:821:ILE:HA	1.84	0.42
1:A:833:LEU:HD22	1:A:943:ILE:HG21	2.01	0.42
2:B:698:SER:O	2:B:702:ASN:HB2	2.20	0.42
5:E:110:PHE:HD1	5:E:110:PHE:HA	1.69	0.42
9:I:4:VAL:O	9:I:7:LEU:HD12	2.20	0.42
9:I:98:THR:HG22	9:I:110:VAL:HG22	2.01	0.42
1:A:439:ASP:CG	1:A:457:LYS:HD3	2.45	0.41
2:B:10:GLN:HB2	2:B:995:TYR:OH	2.19	0.41
2:B:264:TRP:CH2	2:B:356:ARG:HD3	2.55	0.41
2:B:355:ASP:HB3	2:B:364:LYS:HE2	2.02	0.41
8:H:83:GLN:H	8:H:83:GLN:HG2	1.71	0.41
1:A:98:LEU:HA	1:A:324:LEU:HD21	2.03	0.41
2:B:43:GLN:N	2:B:44:PRO:HD2	2.34	0.41
2:B:74:PHE:CZ	2:B:343:ASP:HB2	2.55	0.41
2:B:280:LEU:HD23	2:B:354:LEU:HD13	2.02	0.41
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.93	0.41
8:H:111:LEU:HD23	8:H:111:LEU:HA	1.85	0.41
1:A:957:VAL:HG11	1:A:997:PHE:CE1	2.55	0.41
2:B:599:GLU:H	2:B:599:GLU:HG2	1.58	0.41
2:B:614:GLU:O	2:B:616:LYS:N	2.50	0.41
2:B:699:ILE:H	2:B:699:ILE:HG12	1.61	0.41
5:E:79:TRP:CD1	5:E:81:GLU:HG2	2.55	0.41
1:A:781:LEU:HB3	1:A:786:TYR:CE1	2.55	0.41
1:A:1254:PHE:HE1	1:A:1532:GLN:HG2	1.85	0.41
2:B:49:PHE:O	2:B:52:LEU:HG	2.20	0.41
2:B:218:ILE:HG13	2:B:391:PRO:HB3	2.03	0.41
3:C:227:TYR:HA	3:C:299:ILE:O	2.21	0.41
1:A:392:THR:OG1	1:A:433:ASP:OD2	2.36	0.41
1:A:1310:LYS:HG2	1:A:1467:GLY:HA3	2.02	0.41
2:B:29:PRO:O	2:B:177:PRO:HG2	2.21	0.41
2:B:495:ARG:HD3	2:B:723:LYS:HB3	2.02	0.41
2:B:624:LEU:HD21	2:B:642:LEU:HD23	2.02	0.41
2:B:705:PRO:HG2	2:B:921:HIS:CE1	2.54	0.41
2:B:1098:TYR:CE1	2:B:1177:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:GLY:O	3:C:293:ARG:HD2	2.21	0.41
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.56	0.41
2:B:494:TYR:HB3	2:B:700:LEU:HD21	2.01	0.41
3:C:43:ASN:HB3	3:C:55:ASP:HB2	2.01	0.41
1:A:588:LEU:HD23	1:A:600:MET:HE2	2.03	0.41
1:A:659:THR:HG22	1:A:664:SER:O	2.20	0.41
2:B:253:LEU:HD12	2:B:257:GLN:HE21	1.85	0.41
2:B:548:LYS:HA	2:B:548:LYS:HD3	1.85	0.41
2:B:887:LEU:HD11	12:L:29:TYR:CE1	2.56	0.41
6:F:123:LYS:HE3	6:F:123:LYS:HB2	1.84	0.41
1:A:132:GLU:HG2	1:A:192:ALA:HB1	2.03	0.41
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.85	0.41
2:B:322:ASN:OD1	2:B:322:ASN:N	2.54	0.41
2:B:492:ASN:H	2:B:495:ARG:HB3	1.85	0.41
1:A:379:GLU:OE2	1:A:384:GLN:HG2	2.20	0.41
1:A:999:CYS:HA	2:B:712:SER:OG	2.21	0.41
2:B:129:ARG:HG3	12:L:55:ILE:HD11	2.02	0.41
2:B:335:ARG:NH2	2:B:341:SER:O	2.54	0.41
2:B:657:PRO:C	2:B:659:ASP:H	2.29	0.41
3:C:218:LYS:NZ	12:L:69:ALA:O	2.35	0.41
5:E:127:ILE:H	5:E:127:ILE:HG13	1.77	0.41
6:F:97:ARG:O	6:F:101:ILE:HG12	2.21	0.41
1:A:904:THR:O	1:A:908:VAL:HG23	2.21	0.41
1:A:1634:LEU:O	1:A:1640:ARG:NH1	2.54	0.41
14:S:30:DT:H1'	14:S:31:DA:H5'	2.03	0.41
1:A:252:PHE:HE1	1:A:314:TYR:HD1	1.69	0.40
1:A:475:ARG:NH1	15:T:20:DC:OP1	2.54	0.40
1:A:1185:VAL:HG12	1:A:1584:LEU:HD22	2.03	0.40
2:B:335:ARG:HG3	2:B:340:ALA:HB3	2.03	0.40
15:T:28:DC:H2''	15:T:29:DG:O5'	2.21	0.40
1:A:209:THR:H	1:A:212:VAL:HG22	1.85	0.40
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.55	0.40
1:A:1661:PRO:HA	7:G:102:GLU:HG2	2.04	0.40
2:B:916:LYS:HE2	2:B:916:LYS:HB3	1.92	0.40
5:E:79:TRP:NE1	5:E:81:GLU:OE2	2.53	0.40
1:A:249:THR:HG23	1:A:431:GLN:HB3	2.02	0.40
1:A:1658:ALA:O	7:G:104:LEU:HA	2.22	0.40
2:B:72:VAL:HA	2:B:95:LEU:O	2.20	0.40
2:B:492:ASN:HD21	2:B:725:THR:H	1.68	0.40
2:B:584:CYS:CB	2:B:596:VAL:O	2.52	0.40
2:B:1196:LEU:HD23	2:B:1196:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:LYS:HG2	2:B:952:HIS:O	2.21	0.40
2:B:71:LYS:HE3	2:B:422:GLN:HG3	2.03	0.40
2:B:779:THR:HG23	2:B:931:TRP:CH2	2.57	0.40
11:K:89:CYS:HA	11:K:104:ARG:O	2.22	0.40
1:A:754:LYS:HD2	1:A:783:LYS:HB3	2.03	0.40
2:B:501:ARG:NH2	2:B:546:ALA:O	2.55	0.40
3:C:83:VAL:O	12:L:67:PHE:N	2.54	0.40
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.57	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	1445/1664 (87%)	1390 (96%)	55 (4%)	0	100	100
2	B	1156/1203 (96%)	1116 (96%)	40 (4%)	0	100	100
3	C	302/335 (90%)	297 (98%)	5 (2%)	0	100	100
4	D	16/137 (12%)	16 (100%)	0	0	100	100
5	E	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
6	F	98/155 (63%)	98 (100%)	0	0	100	100
7	G	88/326 (27%)	88 (100%)	0	0	100	100
8	H	127/146 (87%)	126 (99%)	1 (1%)	0	100	100
9	I	91/125 (73%)	84 (92%)	7 (8%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	96/142 (68%)	91 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	41 (98%)	1 (2%)	0	100	100
All	All	3738/4588 (82%)	3619 (97%)	119 (3%)	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	1290/1465 (88%)	1227 (95%)	63 (5%)	21	54
2	B	1017/1053 (97%)	953 (94%)	64 (6%)	15	46
3	C	268/296 (90%)	253 (94%)	15 (6%)	17	50
4	D	16/116 (14%)	15 (94%)	1 (6%)	15	46
5	E	194/197 (98%)	191 (98%)	3 (2%)	60	81
6	F	90/137 (66%)	87 (97%)	3 (3%)	33	64
7	G	81/291 (28%)	78 (96%)	3 (4%)	29	62
8	H	115/128 (90%)	111 (96%)	4 (4%)	31	63
9	I	83/110 (76%)	77 (93%)	6 (7%)	12	41
10	J	64/65 (98%)	62 (97%)	2 (3%)	35	66
11	K	88/130 (68%)	84 (96%)	4 (4%)	23	56
12	L	39/57 (68%)	37 (95%)	2 (5%)	20	53
All	All	3345/4045 (83%)	3175 (95%)	170 (5%)	22	53

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	12	THR
1	A	14	VAL
1	A	18	ILE
1	A	24	ILE
1	A	34	ASN
1	A	38	LEU
1	A	45	VAL
1	A	58	LEU
1	A	130	ILE
1	A	176	THR

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Mol	Chain	Res	Type
1	A	197	LEU
1	A	211	THR
1	A	232	LYS
1	A	251	ILE
1	A	260	GLN
1	A	261	ILE
1	A	318	THR
1	A	326	THR
1	A	349	LEU
1	A	350	VAL
1	A	354	SER
1	A	357	MET
1	A	396	ILE
1	A	403	LEU
1	A	411	VAL
1	A	483	VAL
1	A	490	ILE
1	A	516	ILE
1	A	551	VAL
1	A	552	GLU
1	A	557	LEU
1	A	587	VAL
1	A	607	VAL
1	A	615	ARG
1	A	627	ASP
1	A	650	LEU
1	A	723	TYR
1	A	740	THR
1	A	780	ILE
1	A	821	ILE
1	A	883	LEU
1	A	891	ILE
1	A	910	LYS
1	A	912	VAL
1	A	965	THR
1	A	1038	ILE
1	A	1058	THR
1	A	1121	ASP
1	A	1144	LEU
1	A	1148	LEU
1	A	1161	VAL
1	A	1185	VAL

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Mol	Chain	Res	Type
1	A	1233	ILE
1	A	1235	THR
1	A	1239	THR
1	A	1246	VAL
1	A	1298	ASP
1	A	1457	ILE
1	A	1479	ASP
1	A	1480	THR
1	A	1508	VAL
1	A	1527	GLN
2	B	37	LEU
2	B	65	VAL
2	B	73	ILE
2	B	102	VAL
2	B	163	VAL
2	B	201	LYS
2	B	202	LEU
2	B	207	ILE
2	B	240	ARG
2	B	247	THR
2	B	255	ASP
2	B	273	VAL
2	B	293	ILE
2	B	308	LEU
2	B	324	THR
2	B	337	VAL
2	B	358	VAL
2	B	362	LEU
2	B	375	LEU
2	B	403	LEU
2	B	404	LEU
2	B	425	ILE
2	B	486	VAL
2	B	504	HIS
2	B	511	GLN
2	B	599	GLU
2	B	608	LEU
2	B	653	VAL
2	B	663	ILE
2	B	673	ASN
2	B	699	ILE
2	B	702	ASN

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Mol	Chain	Res	Type
2	B	704	THR
2	B	743	ARG
2	B	752	VAL
2	B	767	ASN
2	B	769	PHE
2	B	794	ASP
2	B	809	VAL
2	B	830	ASP
2	B	871	ILE
2	B	873	THR
2	B	903	ILE
2	B	910	THR
2	B	913	ILE
2	B	933	THR
2	B	940	GLU
2	B	944	GLN
2	B	946	ASP
2	B	982	THR
2	B	990	ASP
2	B	1028	VAL
2	B	1031	VAL
2	B	1033	TYR
2	B	1060	VAL
2	B	1089	GLN
2	B	1093	LEU
2	B	1111	LEU
2	B	1112	THR
2	B	1165	ASN
2	B	1168	VAL
2	B	1189	LEU
2	B	1199	ASN
2	B	1200	VAL
3	C	57	ILE
3	C	61	THR
3	C	75	VAL
3	C	104	VAL
3	C	108	VAL
3	C	113	LEU
3	C	120	LEU
3	C	138	VAL
3	C	141	THR
3	C	145	ASP

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Mol	Chain	Res	Type
3	C	185	VAL
3	C	273	ASP
3	C	274	THR
3	C	291	LEU
3	C	333	ILE
4	D	22	ILE
5	E	110	PHE
5	E	127	ILE
5	E	196	VAL
6	F	57	ASP
6	F	111	LEU
6	F	152	ILE
7	G	45	LEU
7	G	70	VAL
7	G	124	VAL
8	H	23	VAL
8	H	38	LEU
8	H	83	GLN
8	H	92	ASP
9	I	7	LEU
9	I	23	VAL
9	I	47	VAL
9	I	49	THR
9	I	61	ARG
9	I	106	GLU
10	J	27	GLU
10	J	28	ASP
11	K	86	VAL
11	K	93	ILE
11	K	110	GLU
11	K	139	ILE
12	L	38	LEU
12	L	50	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	116	HIS
1	A	260	GLN
1	A	489	ASN
1	A	559	ASN

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Mol	Chain	Res	Type
1	A	671	GLN
1	A	730	GLN
1	A	926	GLN
1	A	1443	GLN
1	A	1509	HIS
1	A	1532	GLN
2	B	27	ASN
2	B	93	ASN
2	B	231	HIS
2	B	254	ASN
2	B	257	GLN
2	B	351	GLN
2	B	398	GLN
2	B	399	HIS
2	B	492	ASN
2	B	499	HIS
2	B	636	GLN
2	B	673	ASN
2	B	682	GLN
2	B	739	ASN
2	B	767	ASN
2	B	1114	GLN
3	C	58	ASN
3	C	137	ASN
3	C	216	HIS
3	C	323	ASN
4	D	29	GLN
5	E	146	HIS
5	E	179	GLN
7	G	121	ASN
12	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	10/12 (83%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	3	A

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Mol	Chain	Res	Type
13	R	5	A

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	0.64	0	9,14,17	0.58	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	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	17	3DR	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

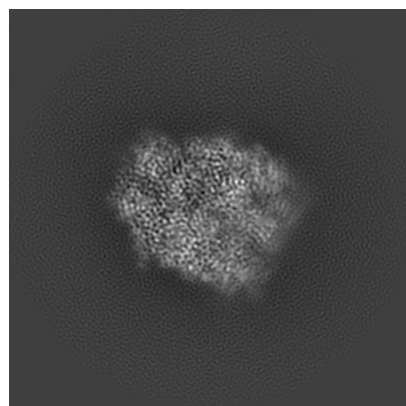
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50971. These allow visual inspection of the internal detail of the map and identification of artifacts.

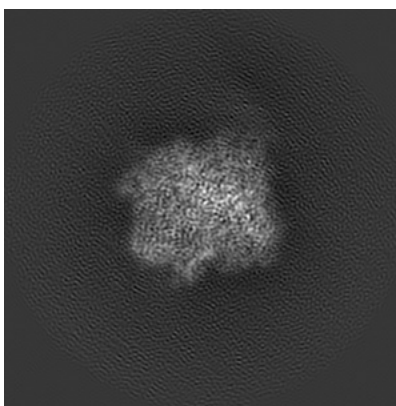
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

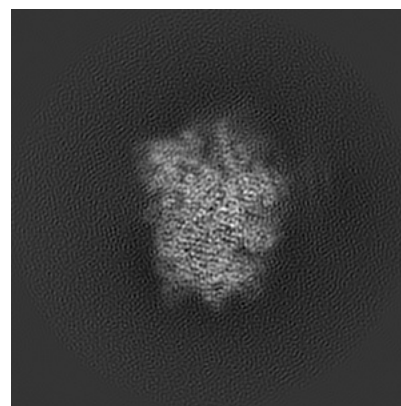
6.1.1 Primary map



X

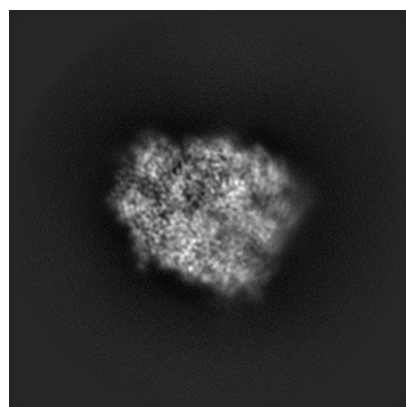


Y

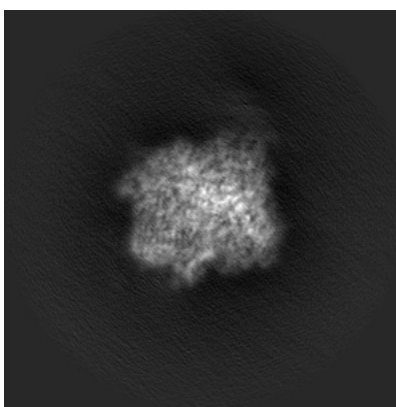


Z

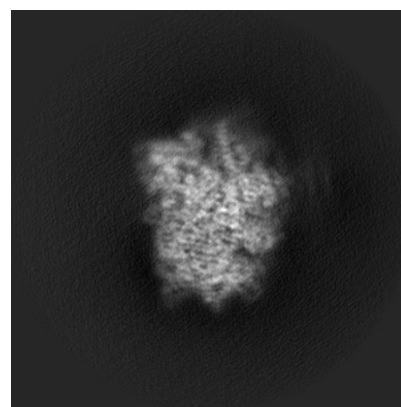
6.1.2 Raw map



X



Y

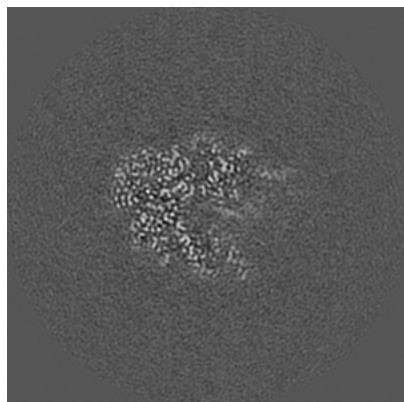


Z

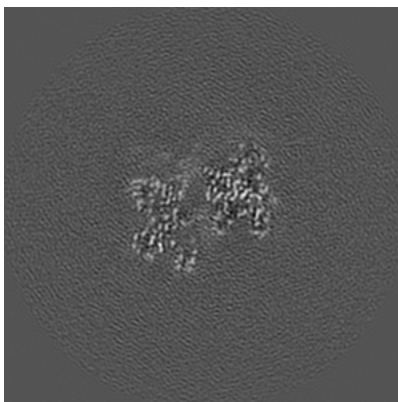
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

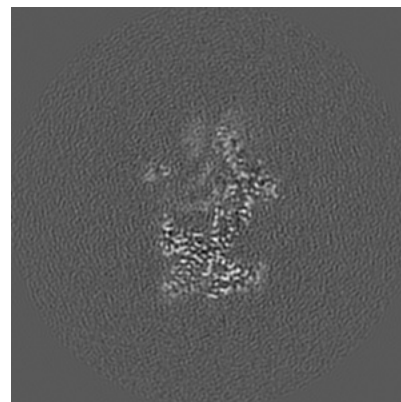
6.2.1 Primary map



X Index: 144

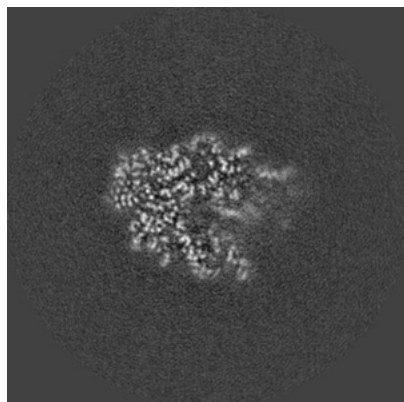


Y Index: 144

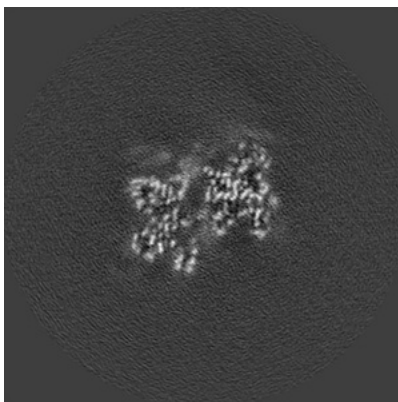


Z Index: 144

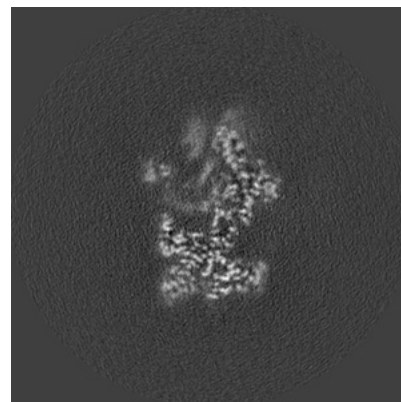
6.2.2 Raw map



X Index: 144



Y Index: 144

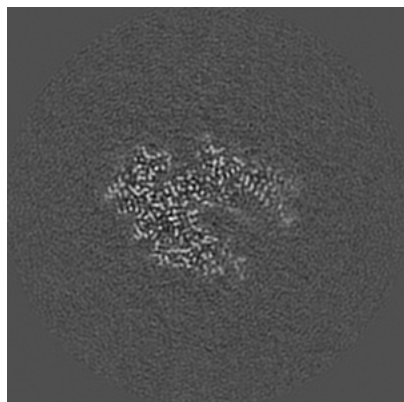


Z Index: 144

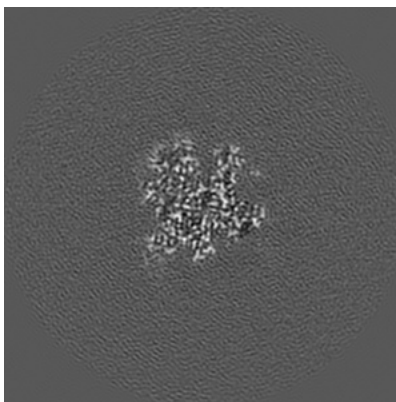
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

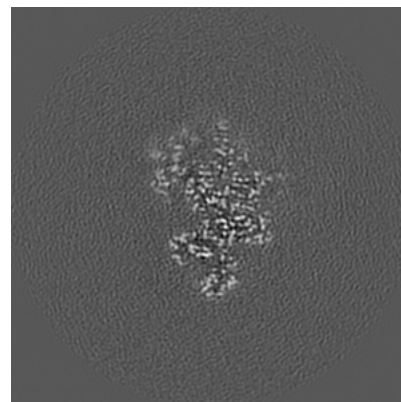
6.3.1 Primary map



X Index: 149

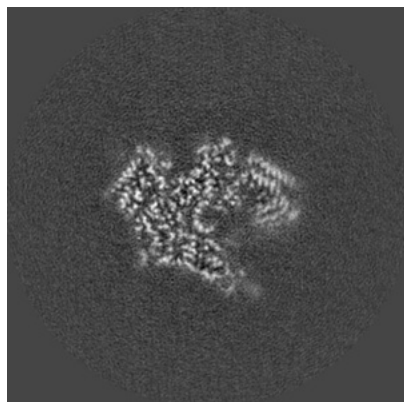


Y Index: 123

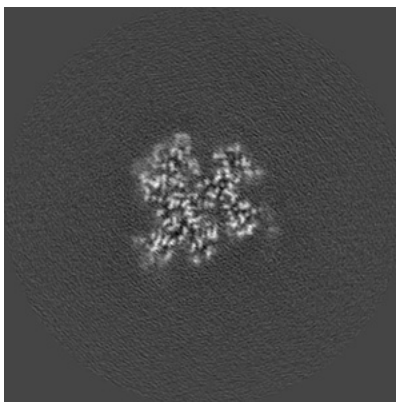


Z Index: 162

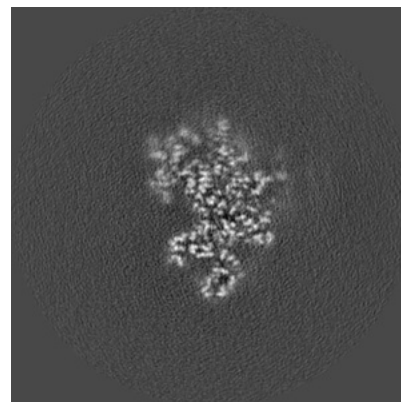
6.3.2 Raw map



X Index: 153



Y Index: 125

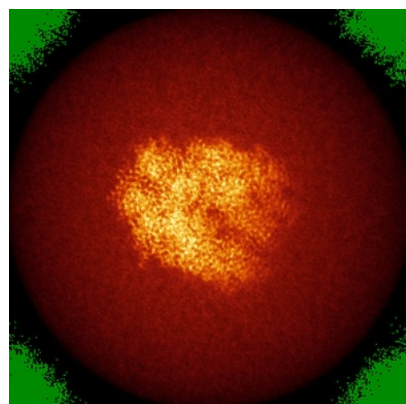


Z Index: 163

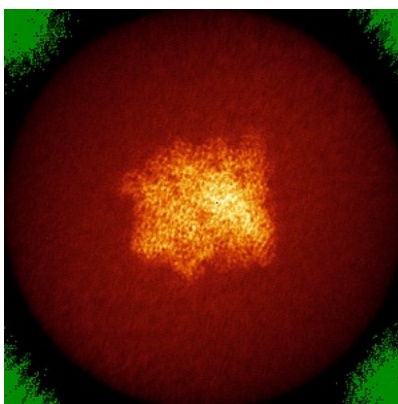
The images above show the largest variance slices of the map in three orthogonal directions.

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

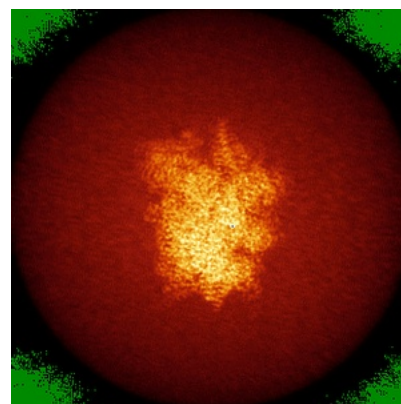
6.4.1 Primary map



X

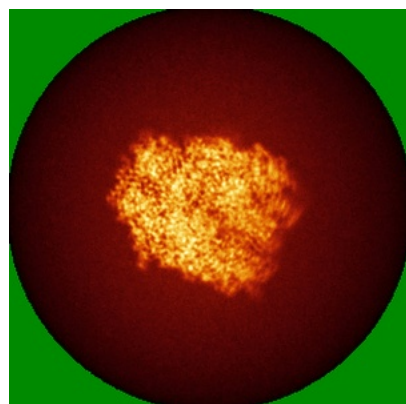


Y

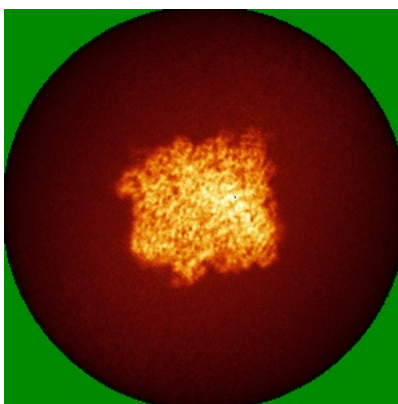


Z

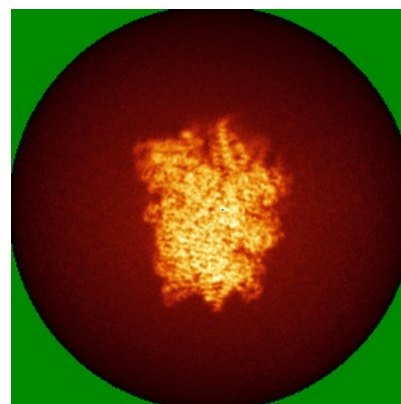
6.4.2 Raw map



X



Y



Z

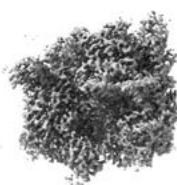
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



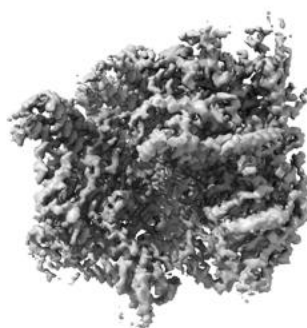
Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. 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



X



Y



Z

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.

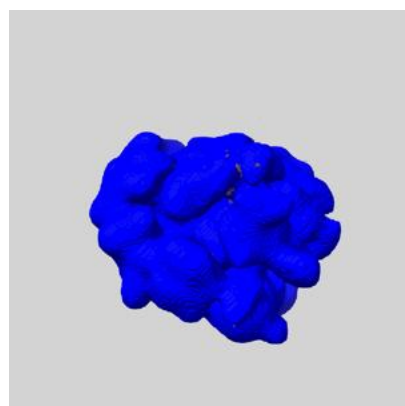
6.6 Mask visualisation [i](#)

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

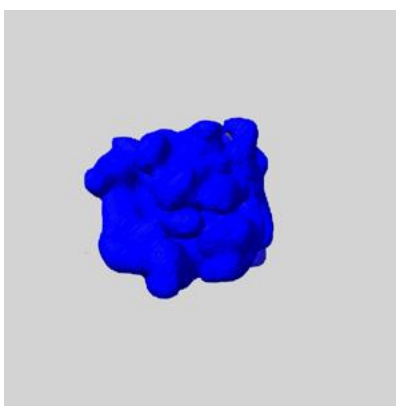
A mask typically either:

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

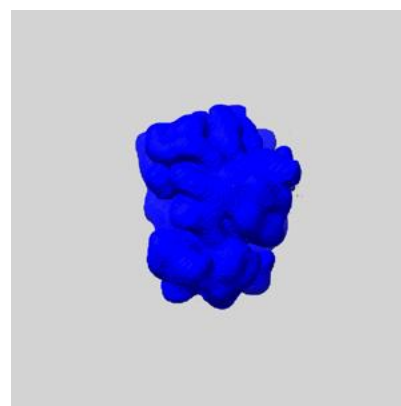
6.6.1 emd_50971_msk_1.map [i](#)



X



Y

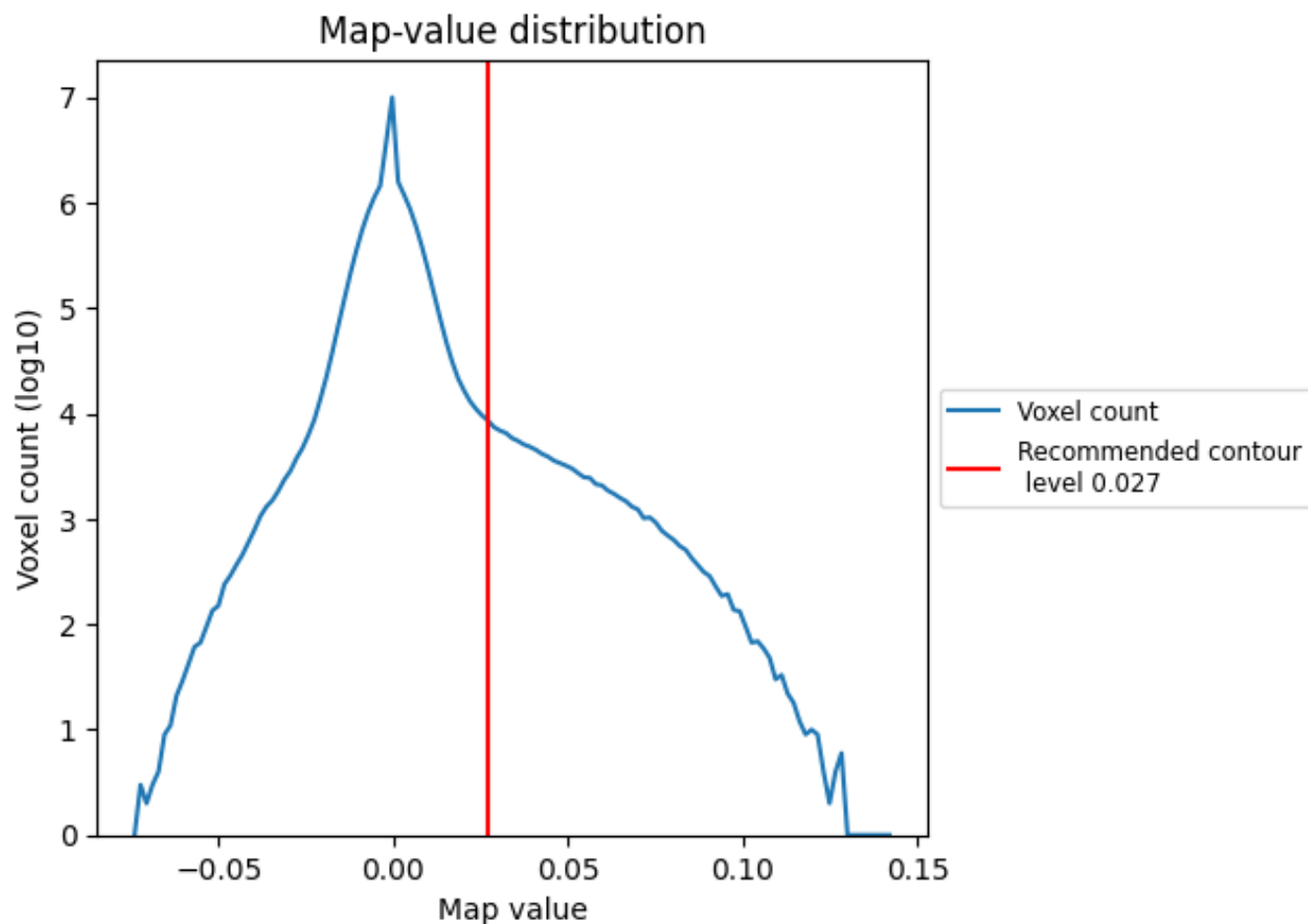


Z

7 Map analysis [i](#)

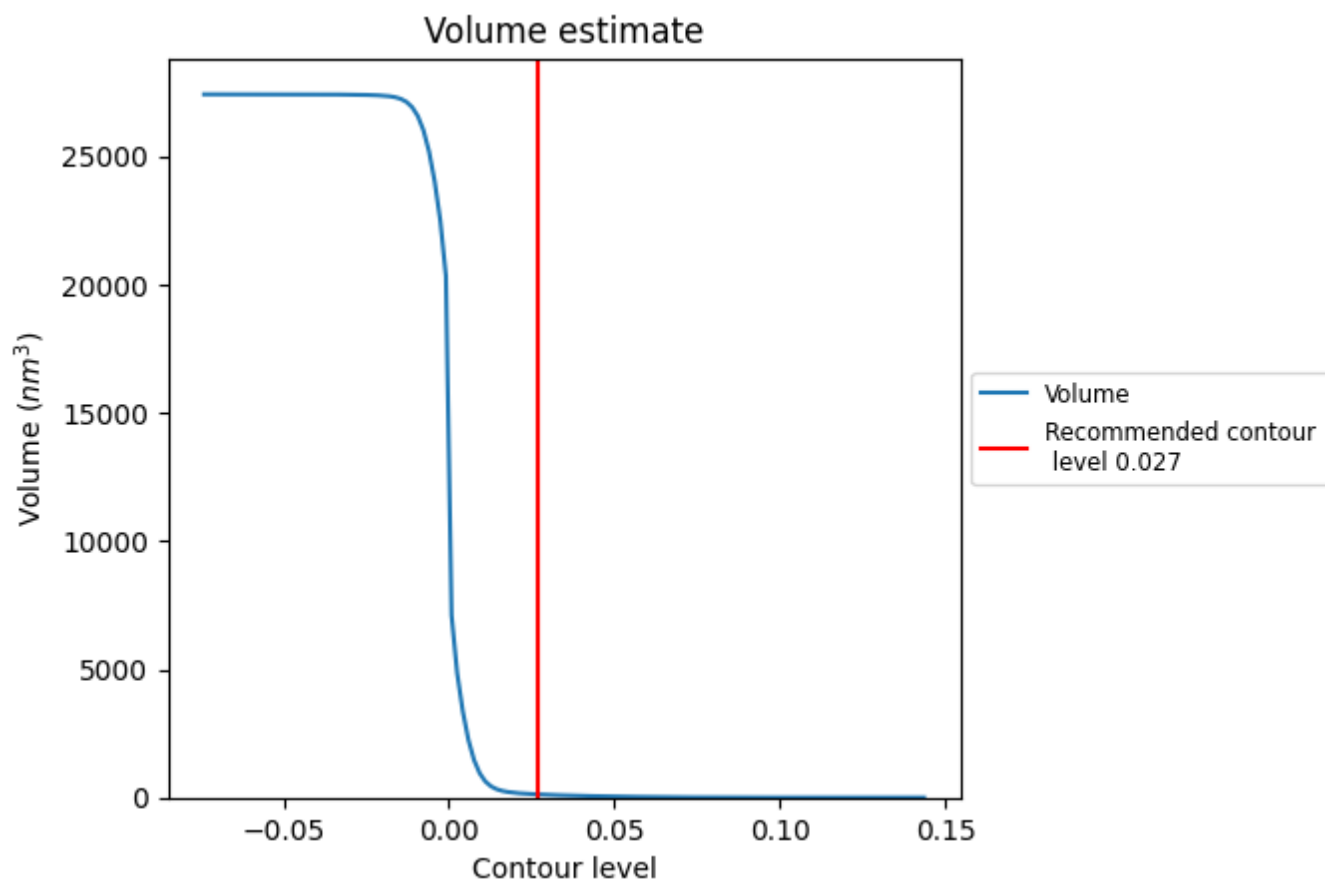
This section contains the results of statistical analysis of the map.

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.

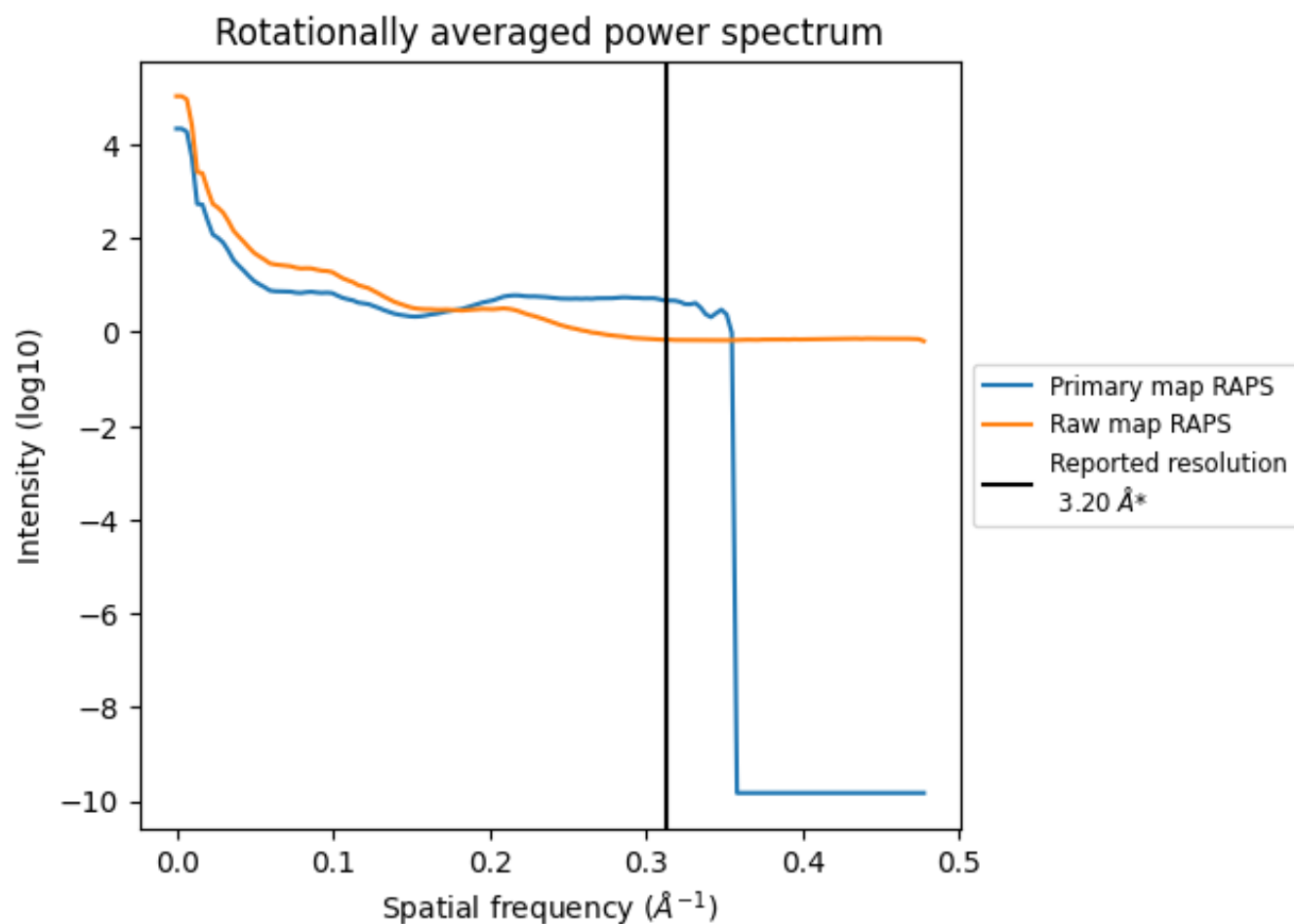
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm³; this corresponds to an approximate mass of 111 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 ⓘ

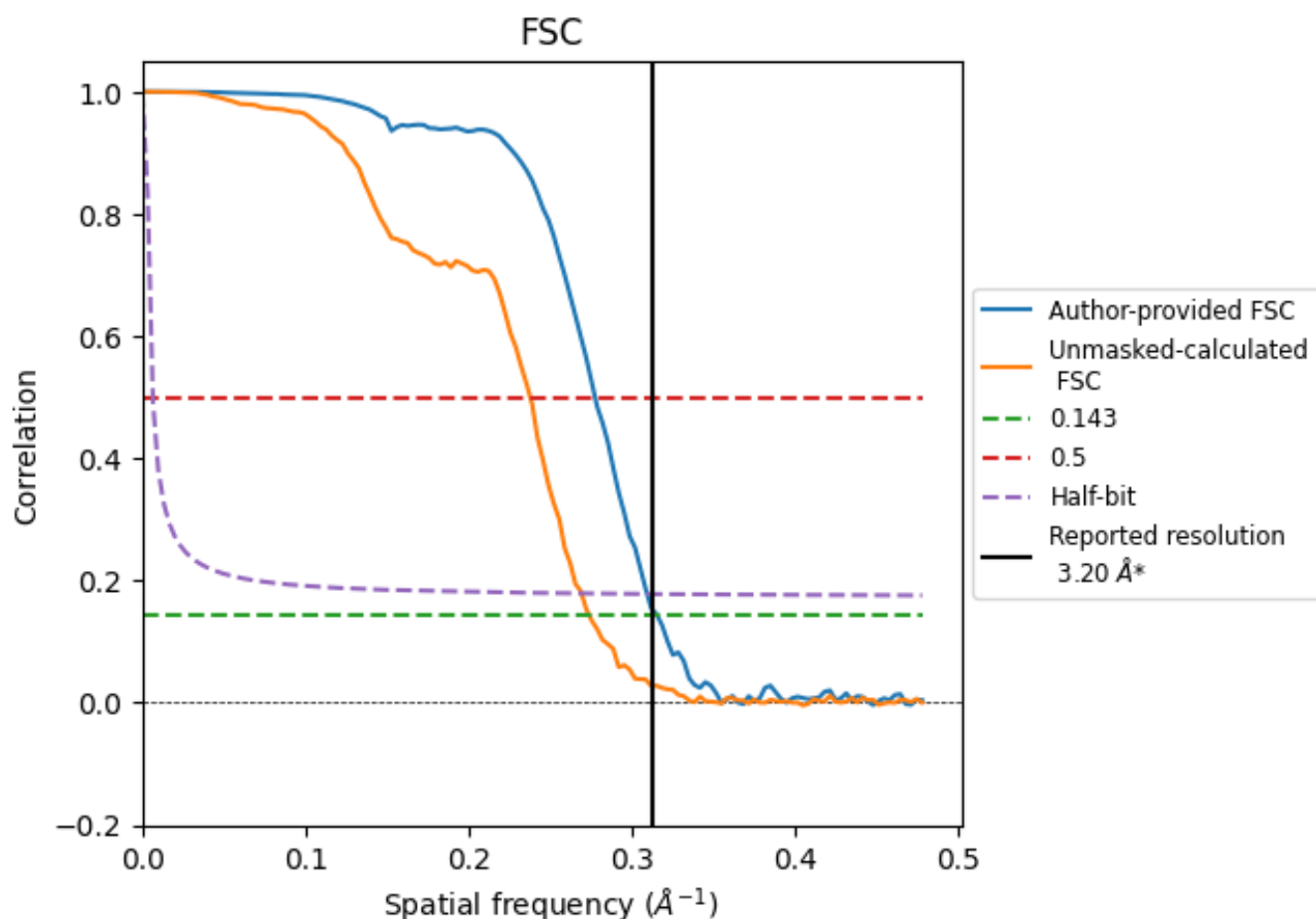


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

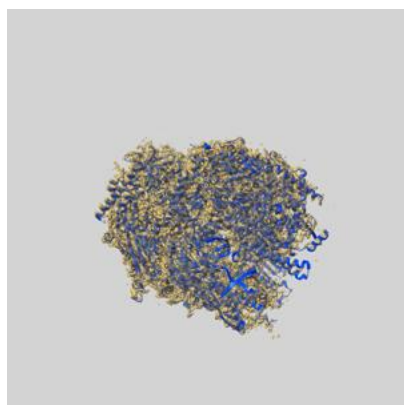
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.61	3.23
Unmasked-calculated*	3.65	4.21	3.72

*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 3.65 differs from the reported value 3.2 by more than 10 %

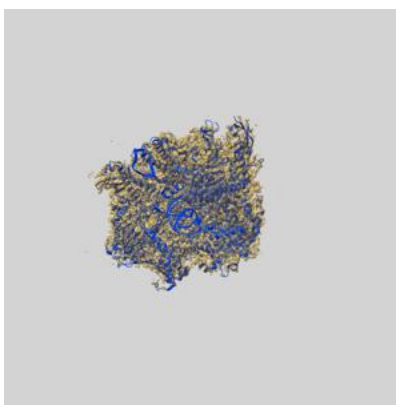
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50971 and PDB model 9G2B. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

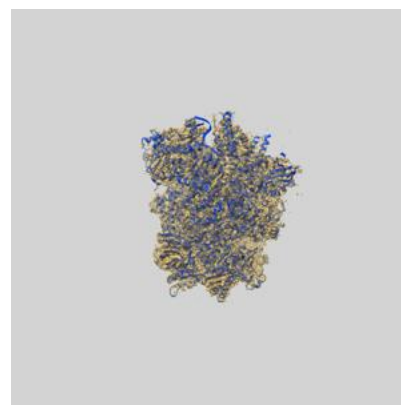
9.1 Map-model overlay [i](#)



X



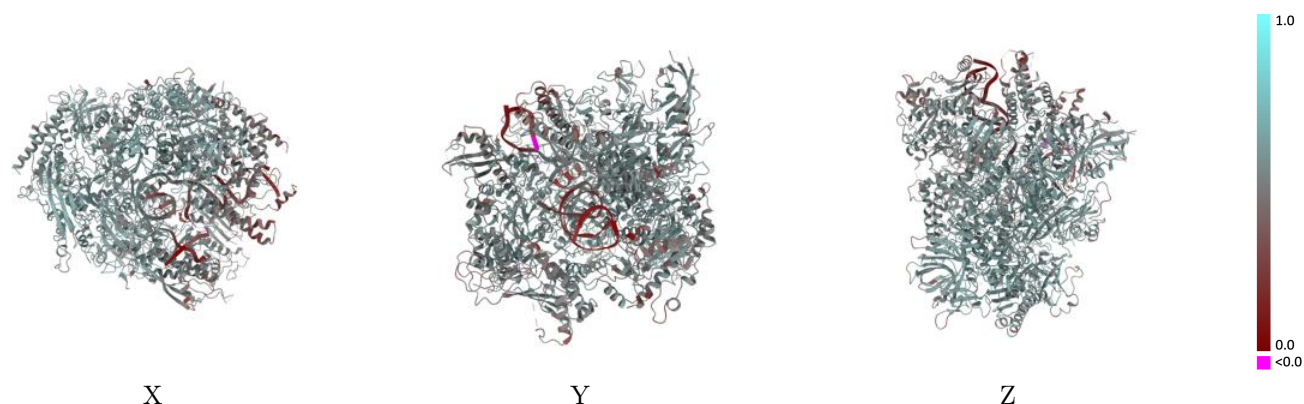
Y



Z

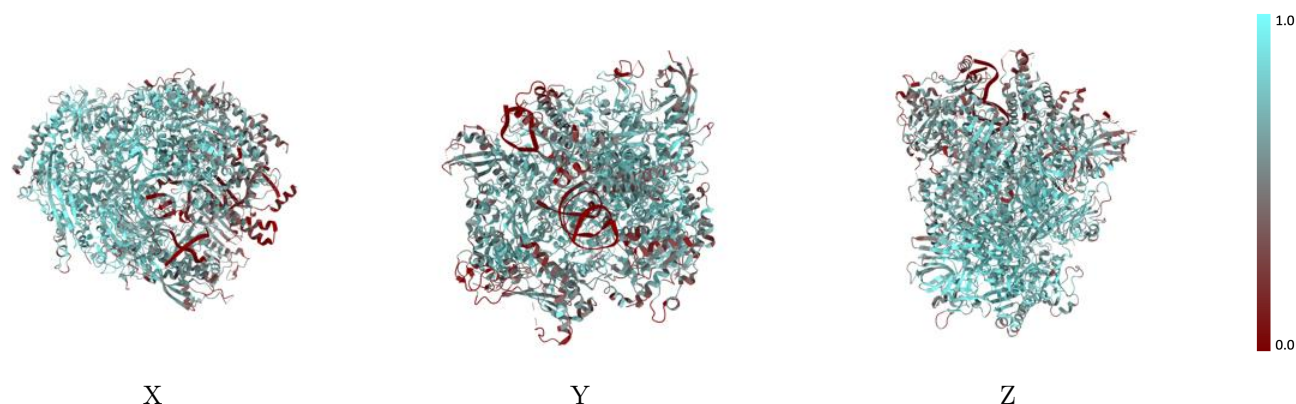
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



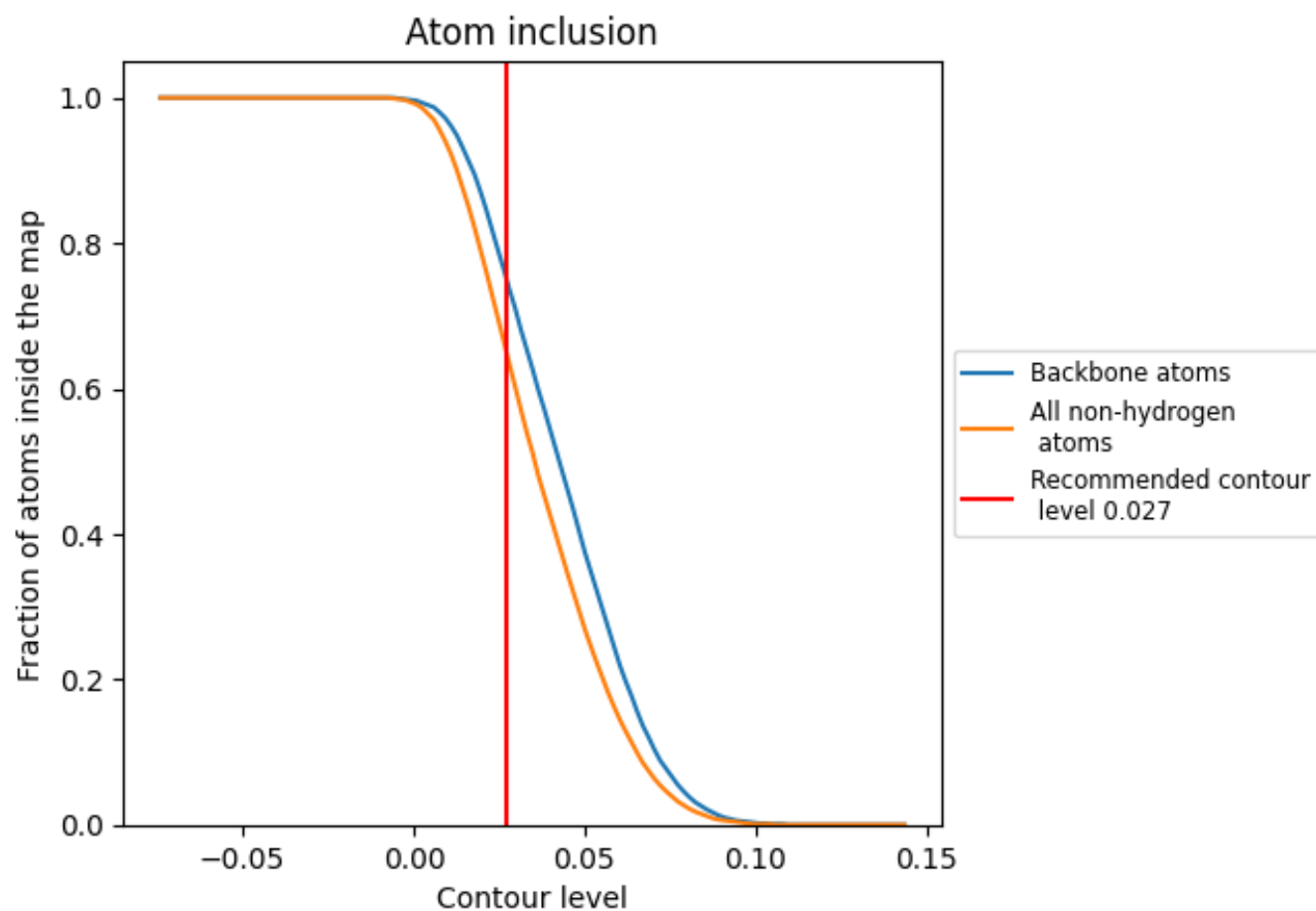
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 65% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6520	<div></div> 0.5280
A	<div></div> 0.6540	<div></div> 0.5320
B	<div></div> 0.7160	<div></div> 0.5510
C	<div></div> 0.7150	<div></div> 0.5510
D	<div></div> 0.5560	<div></div> 0.5450
E	<div></div> 0.5710	<div></div> 0.4970
F	<div></div> 0.7300	<div></div> 0.5570
G	<div></div> 0.5690	<div></div> 0.5330
H	<div></div> 0.7060	<div></div> 0.5480
I	<div></div> 0.2740	<div></div> 0.4560
J	<div></div> 0.7920	<div></div> 0.5770
K	<div></div> 0.7310	<div></div> 0.5520
L	<div></div> 0.6880	<div></div> 0.5440
R	<div></div> 0.6500	<div></div> 0.4940
S	<div></div> 0.0410	<div></div> 0.1870
T	<div></div> 0.2810	<div></div> 0.3060

1.0

0.0

<0.0