



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 12:51 AM UTC

PDB ID : 9G1V / pdb_00009g1v
EMDB ID : EMD-50955
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

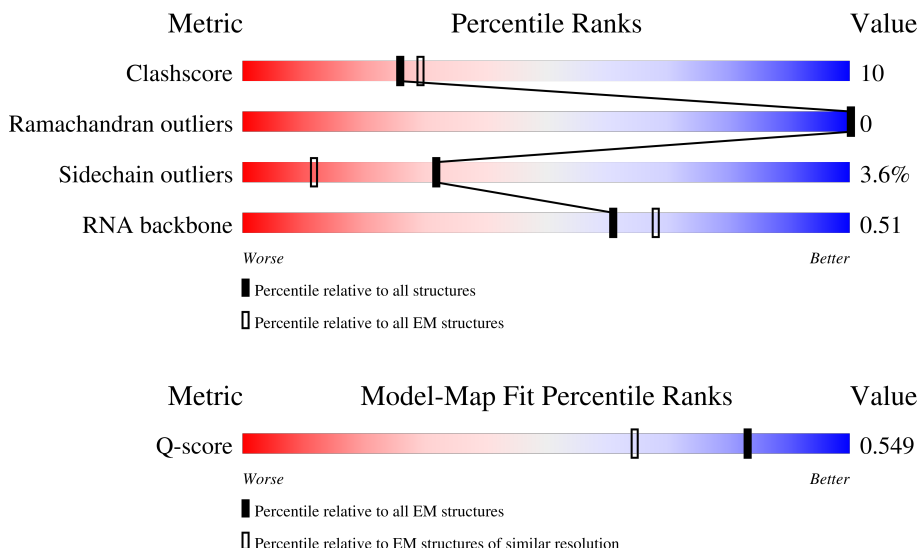
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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



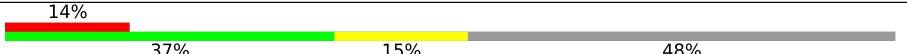
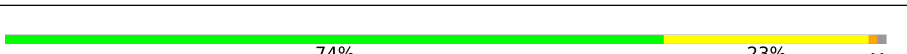
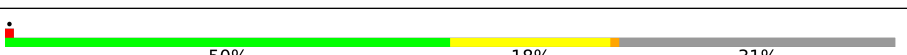
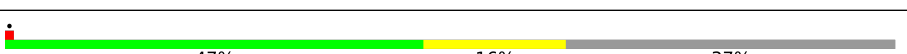
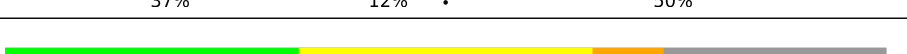
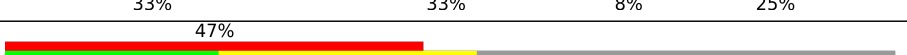
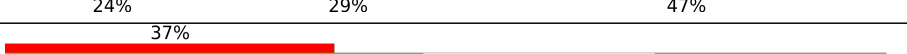
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	

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Mol	Chain	Length	Quality of chain
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	12	
16	S	38	
17	T	38	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 32718 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	1456	Total	C	N	O	S	0	0
			11500	7262	2003	2174	61		

- 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	5852	1626	1725	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	19	Total	C	N	O	0	0
			143	91	26	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	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	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

- 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 protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	100	Total	C	N	O		0	0
			791	503	131	157			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	117	Total	C	N	O	S	0	0
			933	603	153	173	4		

- Molecule 15 is a RNA chain called RNA.

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

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	20	Total	C	N	O	P	0	0
			402	193	65	124	20		

- Molecule 17 is a DNA chain called Template DNA.

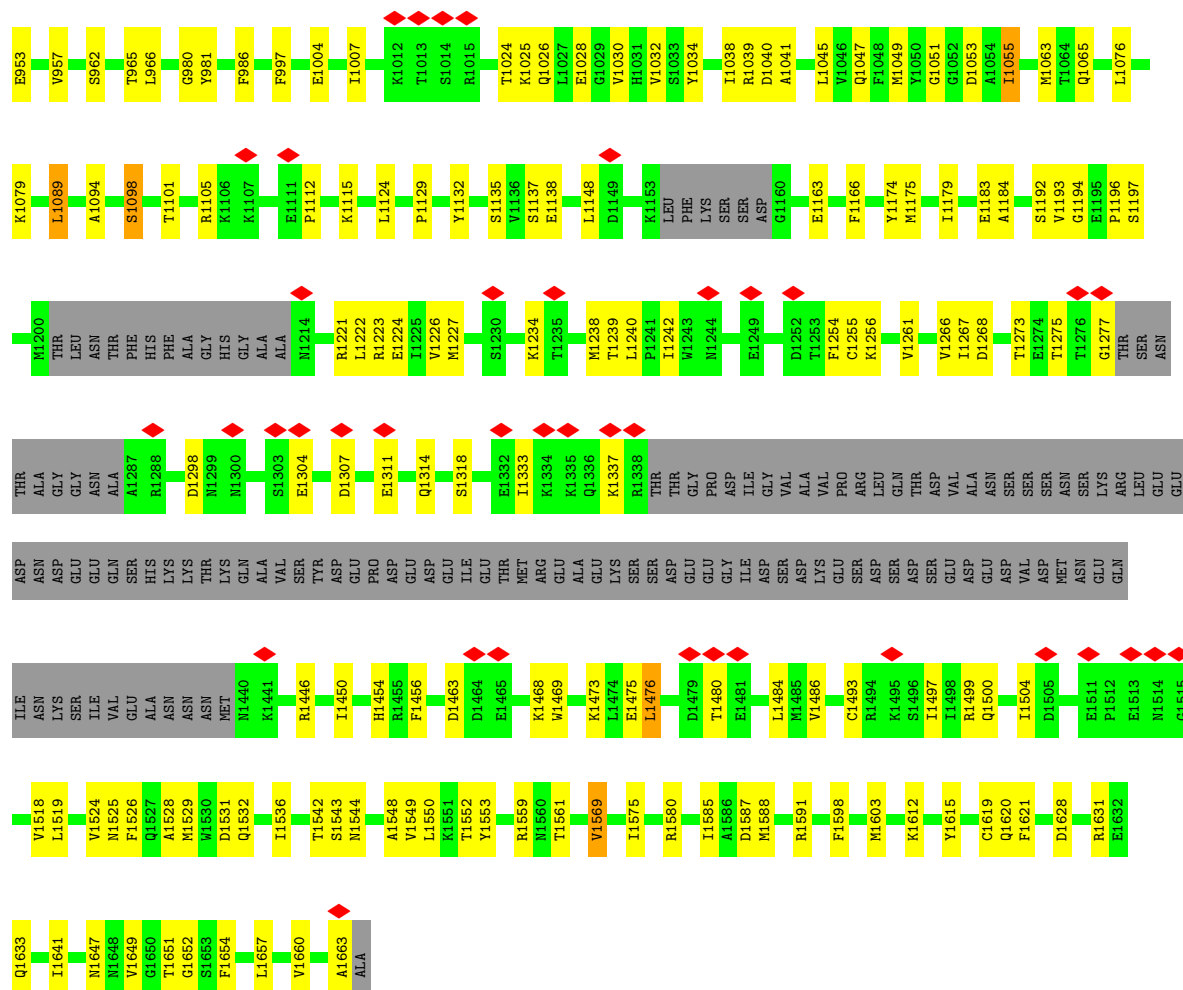
Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	28	Total	C	N	O	P	0	0
			564	269	99	168	28		

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

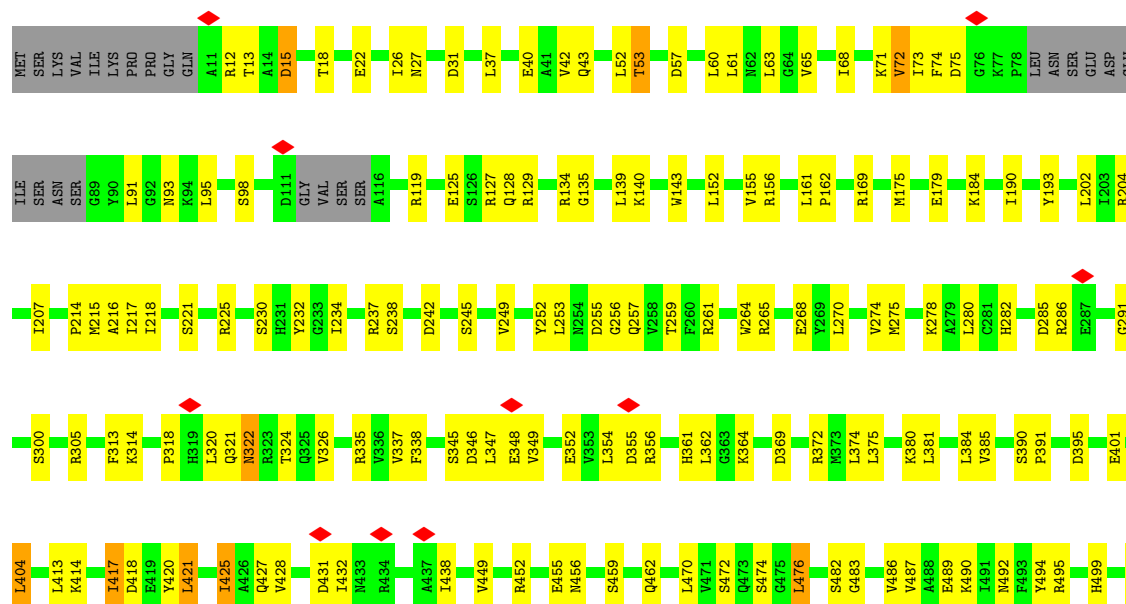
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

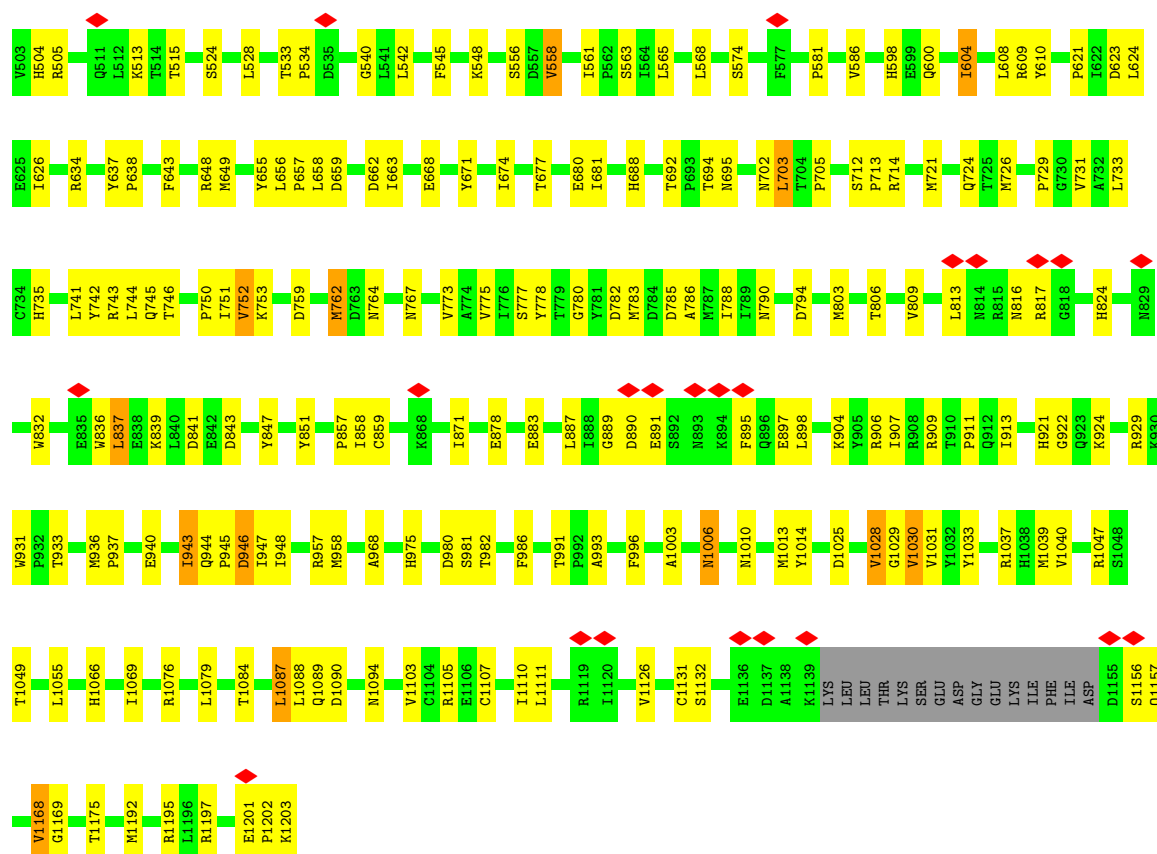
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



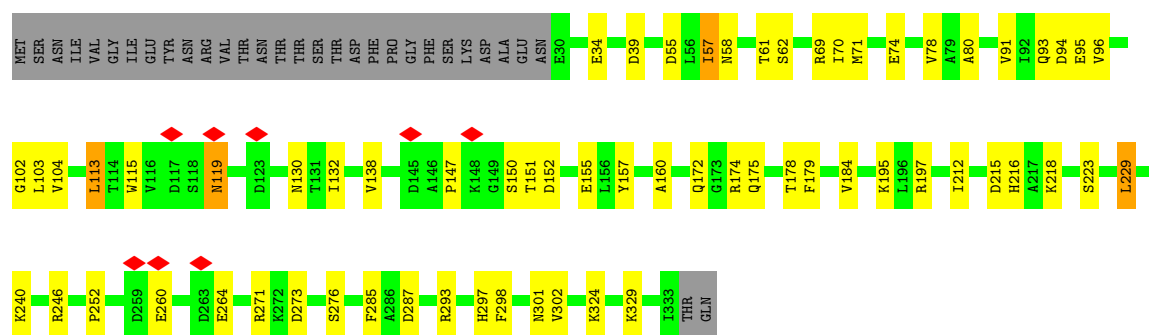
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135





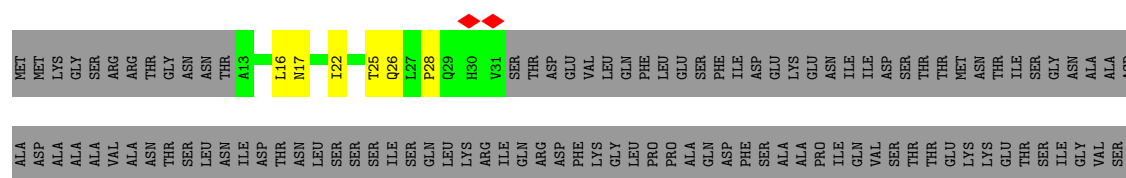
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

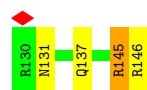
Chain C: 71% 18% 9%



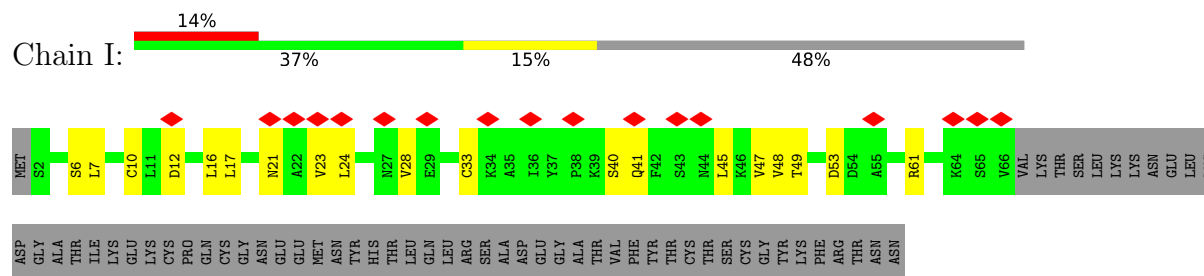
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

Chain D: 9% 86%

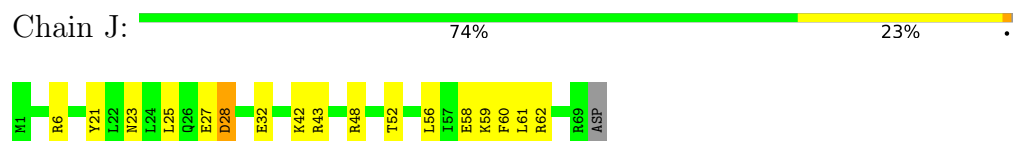




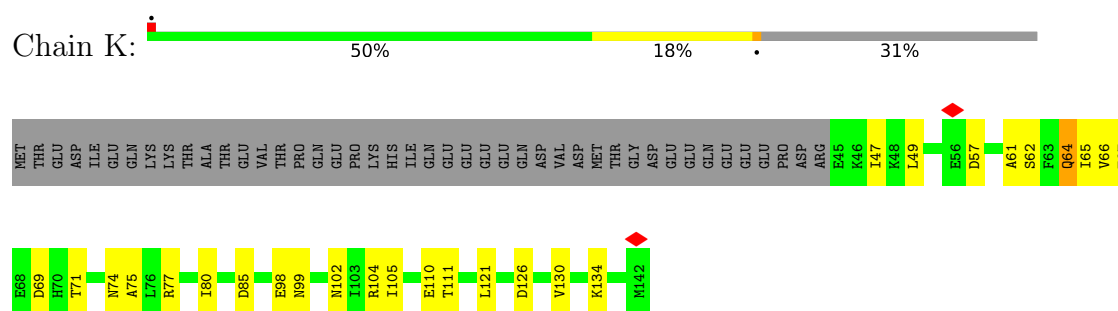
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



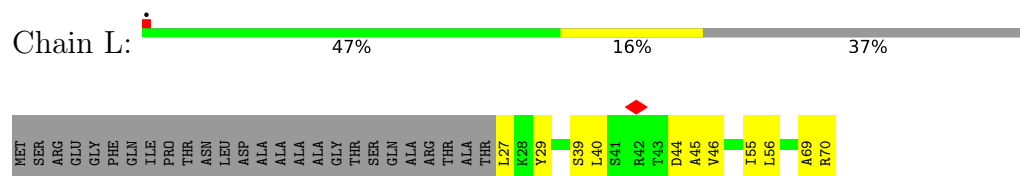
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



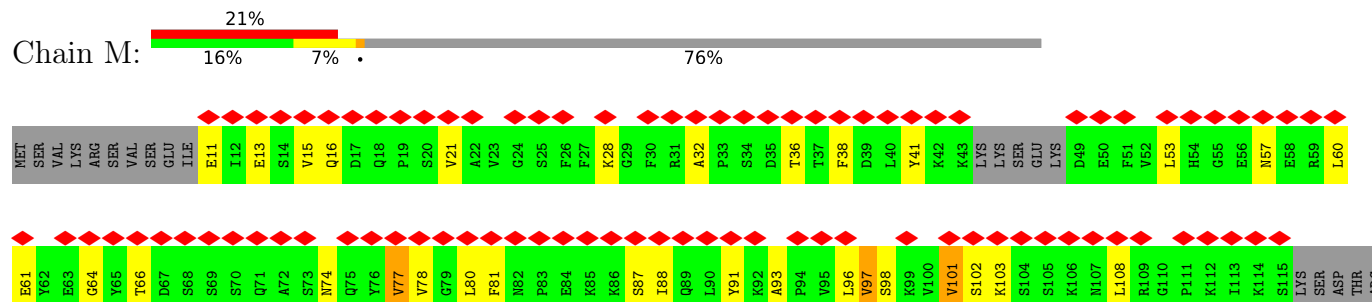
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



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



- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	834570	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	0.157	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0203	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3DR, MG

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	0.22	0/11709	0.33	0/15811
2	B	0.24	0/9459	0.33	0/12785
3	C	0.24	0/2467	0.29	0/3344
4	D	0.14	0/146	0.23	0/203
5	E	0.18	0/1787	0.29	0/2406
6	F	0.22	0/842	0.29	0/1135
7	G	0.18	0/736	0.30	0/1005
8	H	0.22	0/1070	0.30	0/1449
9	I	0.15	0/485	0.34	0/657
10	J	0.28	0/578	0.33	0/775
11	K	0.23	0/776	0.28	0/1047
12	L	0.23	0/354	0.32	0/468
13	M	0.11	0/806	0.29	0/1083
14	N	0.11	0/950	0.27	0/1276
15	R	0.23	0/221	0.31	0/343
16	S	0.18	0/446	0.40	0/682
17	T	0.25	0/618	0.37	0/949
All	All	0.22	0/33450	0.32	0/45418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11500	0	11589	249	0
2	B	9254	0	9145	238	0
3	C	2415	0	2403	46	0
4	D	143	0	147	6	0
5	E	1751	0	1776	35	0
6	F	827	0	843	14	0
7	G	716	0	735	25	0
8	H	1052	0	1021	14	0
9	I	479	0	481	10	0
10	J	569	0	585	14	0
11	K	766	0	765	20	0
12	L	352	0	374	11	0
13	M	791	0	782	27	0
14	N	933	0	960	24	0
15	R	197	0	98	5	0
16	S	402	0	229	10	0
17	T	564	0	314	7	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
All	All	32718	0	32247	660	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 10.

All (660) 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:1107:CYS:HB3	2:B:1131:CYS:SG	2.08	0.93
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.60	0.83
2:B:225:ARG:NH2	2:B:268:GLU:OE2	2.16	0.78
7:G:111:THR:HG22	7:G:113:PHE:H	1.50	0.76
1:A:239:PHE:HB2	1:A:264:ASN:HD21	1.51	0.76
8:H:92:ASP:O	8:H:145:ARG:NH1	2.19	0.75
9:I:12:ASP:HB3	13:M:60:LEU:HD11	1.70	0.73
1:A:606:ARG:NH2	11:K:98:GLU:OE2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:ASP:HB3	1:A:1499:ARG:HH12	1.53	0.72
1:A:700:ILE:O	1:A:706:HIS:ND1	2.22	0.72
1:A:1055:ILE:O	1:A:1580:ARG:NH1	2.23	0.71
11:K:74:ASN:OD1	11:K:77:ARG:NH2	2.24	0.71
17:T:8:DT:H2"	17:T:9:DA:C8	2.25	0.71
5:E:156:LEU:HG	5:E:160:GLU:HG3	1.73	0.71
8:H:93:TYR:HA	8:H:145:ARG:HG3	1.73	0.70
1:A:672:ASP:H	2:B:783:MET:HE3	1.56	0.70
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.72	0.70
1:A:6:PRO:HD2	4:D:16:LEU:HD11	1.73	0.70
1:A:782:ASP:OD1	1:A:783:LYS:N	2.23	0.69
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.74	0.69
1:A:1559:ARG:NE	1:A:1587:ASP:OD1	2.25	0.68
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.74	0.68
1:A:524:ILE:O	1:A:554:ARG:NH1	2.26	0.68
1:A:1254:PHE:HE1	1:A:1532:GLN:HG2	1.58	0.68
13:M:15:VAL:HG11	14:N:65:SER:HA	1.76	0.68
4:D:25:THR:HG22	4:D:26:GLN:HG3	1.74	0.68
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.73	0.68
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.76	0.68
1:A:671:GLN:NE2	2:B:783:MET:O	2.27	0.68
2:B:318:PRO:O	2:B:321:GLN:NE2	2.26	0.68
2:B:662:ASP:OD1	2:B:663:ILE:N	2.27	0.68
13:M:21:VAL:HG23	13:M:93:ALA:HB2	1.74	0.68
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.75	0.68
1:A:591:ARG:HB2	1:A:633:MET:HE2	1.76	0.68
1:A:734:THR:O	1:A:738:ASN:ND2	2.28	0.66
1:A:492:THR:HG22	1:A:667:ARG:HH21	1.59	0.66
1:A:709:ARG:NH1	1:A:737:LEU:O	2.28	0.66
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.78	0.65
1:A:1089:LEU:HD11	1:A:1175:MET:HE1	1.75	0.65
14:N:150:TYR:HB3	14:N:154:ARG:HD2	1.79	0.65
1:A:1179:ILE:HD11	1:A:1183:GLU:HG2	1.79	0.65
2:B:1014:TYR:HE2	3:C:229:LEU:HD22	1.61	0.65
9:I:53:ASP:OD1	9:I:61:ARG:NH1	2.29	0.65
2:B:502:MET:HE3	2:B:542:LEU:HD21	1.76	0.65
5:E:18:THR:HG21	5:E:140:LEU:O	1.96	0.65
1:A:608:LEU:HD12	1:A:615:ARG:HG3	1.79	0.65
1:A:1137:SER:OG	1:A:1174:TYR:OH	2.12	0.65
5:E:55:ARG:NH1	5:E:83:CYS:O	2.29	0.65
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HA	2:B:354:LEU:HD21	1.79	0.64
1:A:213:ASN:OD1	1:A:217:LYS:NZ	2.30	0.64
11:K:64:GLN:OE1	11:K:102:ASN:ND2	2.26	0.64
2:B:1195:ARG:HH22	2:B:1197:ARG:HH11	1.45	0.64
1:A:32:ILE:HB	1:A:79:ILE:HG22	1.79	0.63
2:B:743:ARG:HH12	3:C:93:GLN:HE22	1.44	0.63
2:B:140:LYS:HB3	2:B:155:VAL:HG12	1.81	0.63
2:B:933:THR:OG1	2:B:944:GLN:OE1	2.13	0.63
1:A:1549:VAL:HG11	1:A:1561:THR:HG21	1.80	0.63
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	1.80	0.62
1:A:1183:GLU:OE1	6:F:88:TYR:OH	2.13	0.62
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.80	0.62
2:B:1079:LEU:HD22	2:B:1087:LEU:HB3	1.81	0.62
1:A:6:PRO:HB3	7:G:111:THR:HG21	1.81	0.62
1:A:1275:THR:HG22	1:A:1277:GLY:H	1.65	0.62
13:M:61:GLU:HG3	13:M:103:LYS:HD3	1.82	0.62
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.16	0.62
1:A:1194:GLY:O	1:A:1197:SER:OG	2.13	0.62
1:A:824:THR:O	1:A:824:THR:OG1	2.17	0.61
1:A:94:LEU:HD11	1:A:324:LEU:HD13	1.80	0.61
2:B:836:TRP:HB2	2:B:857:PRO:HG3	1.82	0.61
2:B:221:SER:OG	16:S:23:DC:OP1	2.16	0.61
1:A:826:PHE:HB3	2:B:777:SER:HB3	1.80	0.61
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.17	0.61
1:A:1588:MET:O	1:A:1591:ARG:NH1	2.33	0.61
2:B:1006:ASN:OD1	2:B:1006:ASN:N	2.33	0.61
14:N:63:ASP:OD2	14:N:65:SER:OG	2.19	0.61
1:A:101:SER:HA	1:A:108:PHE:HA	1.82	0.61
1:A:549:MET:HE1	1:A:557:LEU:HD22	1.82	0.61
3:C:119:ASN:OD1	3:C:119:ASN:N	2.35	0.60
2:B:300:SER:HB3	9:I:49:THR:HG22	1.84	0.60
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.19	0.60
10:J:28:ASP:N	10:J:28:ASP:OD1	2.32	0.60
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.82	0.60
2:B:839:LYS:NZ	2:B:851:TYR:O	2.31	0.60
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.35	0.60
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.83	0.60
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	1.83	0.60
1:A:389:VAL:HG22	1:A:433:ASP:HB3	1.83	0.60
1:A:439:ASP:OD1	1:A:458:GLN:NE2	2.33	0.60
2:B:237:ARG:NH2	2:B:401:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:LEU:HD21	2:B:476:LEU:HD23	1.84	0.60
5:E:32:GLN:NE2	5:E:36:GLU:OE1	2.34	0.60
2:B:568:LEU:O	14:N:140:SER:OG	2.12	0.60
2:B:12:ARG:NH1	10:J:32:GLU:OE1	2.33	0.59
1:A:130:ILE:HD11	1:A:215:GLU:HG3	1.82	0.59
1:A:260:GLN:O	1:A:264:ASN:ND2	2.26	0.59
1:A:1641:ILE:HD13	2:B:1076:ARG:HD2	1.83	0.59
1:A:606:ARG:NH1	1:A:607:VAL:O	2.35	0.59
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.84	0.59
4:D:28:PRO:HB2	7:G:39:VAL:HG11	1.84	0.59
1:A:831:ASP:N	1:A:831:ASP:OD1	2.32	0.59
1:A:874:GLU:HG3	1:A:878:ARG:HE	1.67	0.59
3:C:329:LYS:HG3	11:K:121:LEU:HB3	1.85	0.59
5:E:55:ARG:HB3	5:E:82:PHE:HB2	1.85	0.59
2:B:764:ASN:OD1	10:J:59:LYS:NZ	2.33	0.59
8:H:48:PRO:O	8:H:146:ARG:NH2	2.35	0.58
2:B:15:ASP:OD1	2:B:15:ASP:N	2.36	0.58
2:B:259:THR:HG21	2:B:270:LEU:HD23	1.84	0.58
14:N:38:PHE:HD2	14:N:40:LEU:HD22	1.67	0.58
2:B:53:THR:OG1	2:B:169:ARG:NH2	2.37	0.58
3:C:132:ILE:HD13	3:C:184:VAL:HG21	1.85	0.58
1:A:456:VAL:HG12	2:B:1192:MET:HE3	1.86	0.58
7:G:74:ASN:HB3	7:G:77:VAL:HG22	1.86	0.58
10:J:23:ASN:ND2	10:J:27:GLU:OE2	2.37	0.58
1:A:518:GLU:OE2	1:A:584:ARG:NH1	2.34	0.57
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.37	0.57
3:C:70:ILE:HG23	3:C:74:GLU:HB3	1.86	0.57
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.37	0.57
1:A:121:LYS:HE2	1:A:219:LEU:HD11	1.86	0.57
9:I:6:SER:HA	9:I:45:LEU:HB3	1.87	0.57
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.87	0.57
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.37	0.57
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.86	0.57
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.87	0.57
2:B:943:ILE:HG22	10:J:43:ARG:HD2	1.86	0.57
8:H:23:VAL:HA	8:H:43:ASN:HA	1.87	0.57
1:A:877:LYS:O	1:A:881:GLU:HG2	2.05	0.56
2:B:545:PHE:HE1	2:B:649:MET:HE3	1.70	0.56
2:B:1006:ASN:HB3	3:C:276:SER:O	2.05	0.56
2:B:75:ASP:OD1	2:B:93:ASN:N	2.34	0.56
1:A:953:GLU:H	1:A:1004:GLU:CD	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:ALA:O	1:A:1098:SER:OG	2.23	0.56
2:B:134:ARG:NH1	2:B:462:GLN:OE1	2.38	0.56
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.23	0.56
1:A:94:LEU:HD13	1:A:355:PHE:CG	2.41	0.56
2:B:816:ASN:OD1	2:B:817:ARG:NH1	2.39	0.56
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.87	0.56
1:A:36:THR:HG23	1:A:45:VAL:HG11	1.88	0.56
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.88	0.56
1:A:641:GLU:HB2	6:F:99:LEU:HG	1.86	0.56
15:R:4:A:H2'	15:R:5:A:C8	2.41	0.56
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.39	0.56
2:B:214:PRO:O	2:B:380:LYS:NZ	2.28	0.55
2:B:355:ASP:HB3	2:B:364:LYS:HG3	1.88	0.55
1:A:1548:ALA:O	1:A:1552:THR:HG22	2.06	0.55
2:B:18:THR:O	2:B:22:GLU:HG2	2.06	0.55
2:B:533:THR:HG21	2:B:540:GLY:H	1.72	0.55
16:S:8:DT:H2''	16:S:9:DA:C5	2.42	0.55
1:A:1222:LEU:HD21	1:A:1569:VAL:HG11	1.88	0.55
2:B:420:TYR:HE1	2:B:455:GLU:HG2	1.72	0.55
14:N:150:TYR:O	14:N:154:ARG:HB2	2.06	0.55
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.37	0.55
1:A:703:GLU:OE2	11:K:62:SER:OG	2.23	0.55
2:B:337:VAL:HG23	2:B:338:PHE:HD1	1.72	0.55
17:T:6:DG:H2''	17:T:7:DA:N7	2.22	0.55
1:A:1239:THR:OG1	1:A:1542:THR:O	2.24	0.55
5:E:161:LYS:HE3	5:E:193:GLY:O	2.07	0.55
1:A:484:ILE:HD13	1:A:633:MET:HE3	1.89	0.54
2:B:264:TRP:CD1	2:B:265:ARG:HG3	2.42	0.54
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.73	0.54
1:A:1039:ARG:NH2	1:A:1045:LEU:HD12	2.22	0.54
5:E:5:ASN:O	5:E:9:ILE:HG12	2.07	0.54
12:L:40:LEU:HD21	12:L:46:VAL:HG22	1.88	0.54
1:A:722:PRO:HD2	8:H:46:LEU:HD23	1.88	0.54
1:A:1254:PHE:CE1	1:A:1532:GLN:HG2	2.41	0.54
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.90	0.54
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.89	0.54
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.88	0.54
1:A:203:THR:HG23	1:A:205:ARG:H	1.72	0.54
14:N:144:LYS:NZ	14:N:145:ILE:O	2.40	0.54
1:A:1603:MET:HE2	1:A:1612:LYS:HG2	1.89	0.54
2:B:832:TRP:HZ3	2:B:837:LEU:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:H	1:A:212:VAL:HG22	1.72	0.54
1:A:509:GLU:OE1	1:A:515:ASN:ND2	2.39	0.54
1:A:490:ILE:HD11	1:A:606:ARG:HG2	1.89	0.54
1:A:1148:LEU:HD21	1:A:1166:PHE:HD2	1.72	0.54
2:B:1103:VAL:HG22	2:B:1110:ILE:HD13	1.89	0.54
1:A:511:VAL:HG12	1:A:519:LEU:HD23	1.90	0.54
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.42	0.54
2:B:216:ALA:HA	2:B:234:ILE:HD13	1.89	0.54
2:B:314:LYS:NZ	9:I:16:LEU:O	2.38	0.53
2:B:98:SER:HA	2:B:421:LEU:HD21	1.88	0.53
2:B:27:ASN:O	2:B:27:ASN:ND2	2.41	0.53
2:B:324:THR:HG23	2:B:347:LEU:HD13	1.89	0.53
2:B:745:GLN:HG3	2:B:746:THR:HG23	1.89	0.53
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.88	0.53
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.90	0.53
2:B:898:LEU:HD23	2:B:898:LEU:H	1.73	0.53
13:M:57:ASN:ND2	13:M:60:LEU:HB2	2.23	0.53
2:B:129:ARG:NH1	2:B:889:GLY:O	2.26	0.53
2:B:432:ILE:HD11	2:B:438:ILE:HG12	1.90	0.53
3:C:216:HIS:HD2	3:C:218:LYS:H	1.56	0.53
6:F:85:MET:HE2	6:F:153:VAL:HG12	1.90	0.53
2:B:565:LEU:HD21	2:B:608:LEU:HD11	1.91	0.53
2:B:714:ARG:NH1	2:B:922:GLY:O	2.39	0.53
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.91	0.53
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.91	0.53
2:B:824:HIS:ND1	2:B:897:GLU:OE1	2.41	0.53
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.91	0.52
1:A:1055:ILE:HD12	1:A:1063:MET:HE1	1.92	0.52
2:B:278:LYS:NZ	2:B:285:ASP:OD1	2.38	0.52
2:B:898:LEU:HB3	12:L:46:VAL:HG21	1.91	0.52
2:B:558:VAL:HG23	2:B:561:ILE:HD12	1.90	0.52
1:A:904:THR:HG23	1:A:946:LEU:HD23	1.90	0.52
3:C:260:GLU:OE1	3:C:260:GLU:N	2.42	0.52
2:B:37:LEU:HD12	2:B:759:ASP:HB3	1.91	0.52
7:G:93:ASP:HB2	7:G:104:LEU:HD12	1.91	0.52
9:I:10:CYS:HB2	9:I:17:LEU:HD21	1.91	0.52
12:L:44:ASP:OD1	12:L:45:ALA:N	2.42	0.52
15:R:6:U:H2'	15:R:7:C:C6	2.44	0.52
1:A:952:LEU:HD23	1:A:957:VAL:HA	1.91	0.52
2:B:495:ARG:NH2	15:R:9:A:O3'	2.43	0.52
6:F:128:LYS:HE2	6:F:149:GLU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	1.92	0.52
1:A:730:GLN:O	1:A:734:THR:HG22	2.10	0.52
13:M:66:THR:HG22	13:M:96:LEU:HA	1.91	0.52
1:A:665:PRO:HD2	1:A:790:LYS:HG2	1.92	0.52
4:D:28:PRO:HB3	7:G:41:VAL:HG22	1.91	0.52
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.45	0.52
13:M:36:THR:HG22	13:M:57:ASN:HB3	1.92	0.52
1:A:1239:THR:OG1	1:A:1542:THR:OG1	2.26	0.52
6:F:79:ARG:NH1	6:F:145:ASP:O	2.43	0.52
11:K:80:ILE:HD13	11:K:105:ILE:HD11	1.92	0.52
1:A:942:GLN:HG2	1:A:947:LEU:HA	1.92	0.51
2:B:752:VAL:HG12	2:B:981:SER:HB3	1.92	0.51
2:B:803:MET:HE3	2:B:907:ILE:HD13	1.91	0.51
2:B:456:ASN:HB3	2:B:459:SER:HB3	1.91	0.51
1:A:94:LEU:HD22	1:A:355:PHE:HB3	1.92	0.51
1:A:1024:THR:O	1:A:1028:GLU:HB3	2.10	0.51
13:M:80:LEU:HD22	14:N:51:GLN:HB3	1.93	0.51
1:A:701:ARG:HG2	1:A:703:GLU:OE1	2.11	0.51
2:B:175:MET:HB3	2:B:179:GLU:HB2	1.92	0.51
1:A:1039:ARG:HB3	1:A:1045:LEU:HA	1.91	0.51
2:B:991:THR:HG22	2:B:993:ALA:H	1.74	0.51
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.93	0.51
1:A:1663:ALA:HB2	7:G:101:SER:HA	1.92	0.51
2:B:242:ASP:OD2	2:B:414:LYS:NZ	2.42	0.51
8:H:12:VAL:HG13	8:H:26:ILE:HG23	1.92	0.51
3:C:287:ASP:N	3:C:287:ASP:OD1	2.43	0.51
1:A:91:PHE:HE2	1:A:245:LYS:HE2	1.74	0.51
1:A:590:ASN:OD1	1:A:592:GLN:NE2	2.43	0.51
2:B:249:VAL:HG21	2:B:261:ARG:HH21	1.76	0.51
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.27	0.51
3:C:71:MET:HE1	3:C:302:VAL:HG21	1.93	0.51
1:A:126:GLN:NE2	1:A:340:HIS:O	2.42	0.51
1:A:1298:ASP:OD1	1:A:1468:LYS:NZ	2.29	0.50
2:B:788:ILE:HB	2:B:948:ILE:HB	1.93	0.50
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.45	0.50
1:A:1526:PHE:CD2	1:A:1552:THR:HG21	2.46	0.50
14:N:107:MET:HB3	14:N:133:PHE:HE2	1.75	0.50
1:A:661:THR:HA	1:A:1192:SER:HB2	1.93	0.50
2:B:215:MET:HE3	2:B:217:ILE:HD11	1.92	0.50
3:C:147:PRO:HG2	3:C:150:SER:HB2	1.94	0.50
15:R:4:A:H2'	15:R:5:A:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LEU:HA	2:B:60:LEU:HB2	1.92	0.50
16:S:8:DT:H2"	16:S:9:DA:N7	2.27	0.50
1:A:697:TYR:CE1	1:A:702:PRO:HD2	2.47	0.50
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.93	0.50
2:B:230:SER:OG	2:B:252:TYR:O	2.27	0.50
2:B:568:LEU:HB3	2:B:604:ILE:HD12	1.94	0.50
2:B:724:GLN:O	2:B:1037:ARG:HG2	2.12	0.50
3:C:69:ARG:NH2	11:K:69:ASP:OD2	2.42	0.50
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.94	0.50
1:A:363:PRO:O	1:A:368:ARG:NH1	2.41	0.50
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.93	0.50
2:B:61:LEU:HD22	2:B:413:LEU:HD23	1.94	0.50
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.94	0.50
10:J:48:ARG:O	10:J:52:THR:OG1	2.29	0.50
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.49
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.94	0.49
2:B:129:ARG:HG3	12:L:55:ILE:HD11	1.94	0.49
13:M:78:VAL:O	13:M:91:TYR:N	2.45	0.49
1:A:1543:SER:OG	1:A:1544:ASN:N	2.45	0.49
9:I:23:VAL:HG22	9:I:24:LEU:H	1.76	0.49
1:A:1476:LEU:HD12	1:A:1480:THR:HG21	1.94	0.49
2:B:1156:SER:OG	2:B:1157:GLN:OE1	2.30	0.49
3:C:57:ILE:HD12	3:C:297:HIS:CD2	2.47	0.49
1:A:84:PRO:O	1:A:317:SER:OG	2.28	0.49
1:A:953:GLU:N	1:A:1004:GLU:OE2	2.38	0.49
1:A:1531:ASP:HA	5:E:14:ARG:HH12	1.77	0.49
2:B:204:ARG:HD2	2:B:486:VAL:HG13	1.95	0.49
2:B:253:LEU:HD12	2:B:257:GLN:HG3	1.94	0.49
12:L:27:LEU:HD23	12:L:39:SER:HB2	1.94	0.49
1:A:1268:ASP:O	9:I:61:ARG:NH2	2.46	0.49
5:E:55:ARG:HA	5:E:58:MET:HG3	1.93	0.49
1:A:866:LYS:H	1:A:866:LYS:HD2	1.77	0.49
3:C:115:TRP:HH2	3:C:212:ILE:HG23	1.78	0.49
3:C:175:GLN:HB2	3:C:179:PHE:HD2	1.78	0.49
1:A:569:SER:OG	4:D:17:ASN:ND2	2.46	0.49
1:A:1450:ILE:HG23	1:A:1454:HIS:CE1	2.48	0.49
2:B:40:GLU:HA	2:B:43:GLN:HB2	1.94	0.49
7:G:42:PRO:HA	7:G:121:ASN:HA	1.95	0.49
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.95	0.49
1:A:32:ILE:HG21	1:A:49:LEU:HD23	1.94	0.48
1:A:1242:ILE:HD11	1:A:1519:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ARG:NH1	2:B:346:ASP:OD1	2.45	0.48
13:M:81:PHE:HA	13:M:88:ILE:HG13	1.95	0.48
2:B:71:LYS:HG2	2:B:425:ILE:HD12	1.95	0.48
2:B:395:ASP:HA	2:B:505:ARG:HH21	1.78	0.48
5:E:97:VAL:HG13	5:E:127:ILE:HG21	1.94	0.48
1:A:347:ARG:O	1:A:347:ARG:NH1	2.38	0.48
1:A:1240:LEU:HB3	1:A:1536:ILE:HD12	1.95	0.48
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.44	0.48
2:B:322:ASN:OD1	2:B:322:ASN:N	2.45	0.48
2:B:986:PHE:CD1	14:N:160:VAL:HG21	2.48	0.48
3:C:215:ASP:CG	12:L:70:ARG:HH22	2.21	0.48
1:A:100:ALA:HB1	1:A:227:LEU:HB3	1.95	0.48
1:A:712:ILE:HG13	11:K:104:ARG:NH1	2.29	0.48
1:A:1049:MET:HE2	1:A:1124:LEU:HB3	1.96	0.48
1:A:1193:VAL:HG21	1:A:1585:ILE:HD12	1.95	0.48
9:I:40:SER:O	9:I:41:GLN:HG2	2.12	0.48
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.95	0.48
11:K:126:ASP:O	11:K:130:VAL:HG13	2.13	0.48
1:A:95:TYR:O	1:A:99:ARG:HG2	2.14	0.48
2:B:489:GLU:HG2	2:B:499:HIS:NE2	2.29	0.48
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.96	0.48
1:A:250:LYS:HD3	1:A:314:TYR:HE1	1.78	0.48
1:A:498:PRO:HG3	1:A:613:THR:O	2.13	0.48
2:B:140:LYS:HA	2:B:155:VAL:HA	1.96	0.48
2:B:1105:ARG:HD3	2:B:1203:LYS:HA	1.96	0.48
1:A:646:GLU:OE1	2:B:1087:LEU:N	2.40	0.48
1:A:1267:ILE:HD12	1:A:1493:CYS:SG	2.54	0.48
2:B:255:ASP:OD1	2:B:256:GLY:N	2.47	0.48
2:B:390:SER:OG	2:B:634:ARG:O	2.32	0.48
3:C:78:VAL:HG21	3:C:113:LEU:HD21	1.95	0.48
1:A:396:ILE:HD11	1:A:427:PHE:CE1	2.48	0.48
1:A:864:LEU:HD23	1:A:868:THR:HG21	1.95	0.48
2:B:75:ASP:OD1	2:B:75:ASP:N	2.47	0.48
2:B:492:ASN:ND2	2:B:767:ASN:OD1	2.47	0.48
1:A:611:GLU:CD	2:B:913:ILE:HD12	2.40	0.47
2:B:598:HIS:HE1	2:B:638:PRO:HB2	1.79	0.47
1:A:515:ASN:HB3	1:A:519:LEU:HD22	1.95	0.47
2:B:42:VAL:HG11	2:B:190:ILE:HD12	1.97	0.47
6:F:106:PRO:HG2	7:G:55:GLU:HG2	1.96	0.47
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.49	0.47
1:A:1333:ILE:O	1:A:1337:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.96	0.47
2:B:782:ASP:HA	2:B:786:ALA:HB3	1.96	0.47
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.78	0.47
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.50	0.47
1:A:1138:GLU:OE2	5:E:207:ARG:NH1	2.46	0.47
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.48	0.47
16:S:10:DC:H2''	16:S:11:DG:C5	2.49	0.47
1:A:855:ARG:HH12	1:A:867:ASP:H	1.62	0.47
1:A:1129:PRO:HA	1:A:1135:SER:HB3	1.97	0.47
2:B:232:TYR:CG	2:B:385:VAL:HG12	2.50	0.47
3:C:172:GLN:O	3:C:175:GLN:HG2	2.15	0.47
11:K:47:ILE:HD12	11:K:65:ILE:HG12	1.96	0.47
11:K:57:ASP:OD1	11:K:57:ASP:N	2.47	0.47
1:A:1038:ILE:HG12	1:A:1047:GLN:HB2	1.97	0.47
2:B:221:SER:O	2:B:225:ARG:HG2	2.15	0.47
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.97	0.47
1:A:387:SER:O	1:A:391:THR:HG23	2.15	0.47
1:A:399:LEU:HD11	1:A:422:ARG:HB3	1.96	0.47
1:A:570:THR:HA	1:A:573:LEU:HD13	1.97	0.47
2:B:680:GLU:N	2:B:680:GLU:OE1	2.48	0.47
7:G:49:LEU:N	7:G:114:GLY:O	2.48	0.47
1:A:509:GLU:HB3	1:A:519:LEU:HD21	1.97	0.47
2:B:490:LYS:NZ	2:B:729:PRO:O	2.48	0.47
2:B:1201:GLU:HB2	2:B:1202:PRO:HD3	1.97	0.47
1:A:711:LYS:HA	11:K:104:ARG:HH22	1.81	0.46
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.50	0.46
3:C:113:LEU:HB2	3:C:130:ASN:HA	1.97	0.46
3:C:197:ARG:HG2	10:J:61:LEU:HD22	1.97	0.46
1:A:117:ARG:HB2	1:A:185:ARG:NH1	2.30	0.46
1:A:316:LEU:O	1:A:319:GLU:HG3	2.14	0.46
1:A:1256:LYS:NZ	1:A:1304:GLU:O	2.43	0.46
1:A:1473:LYS:NZ	1:A:1475:GLU:OE1	2.48	0.46
2:B:218:ILE:HD12	2:B:391:PRO:HG3	1.96	0.46
8:H:32:THR:OG1	8:H:33:GLN:N	2.48	0.46
3:C:55:ASP:OD1	3:C:271:ARG:NH1	2.48	0.46
5:E:201:LYS:HE3	5:E:201:LYS:HB3	1.77	0.46
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.78	0.46
17:T:18:DC:H2'	17:T:19:DT:C6	2.51	0.46
1:A:653:THR:HG1	1:A:667:ARG:NH1	2.13	0.46
2:B:657:PRO:C	2:B:659:ASP:H	2.24	0.46
2:B:705:PRO:HG2	2:B:921:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD12	1:A:230:ARG:HE	1.80	0.46
1:A:712:ILE:HG13	11:K:104:ARG:HH12	1.81	0.46
2:B:252:TYR:HH	2:B:305:ARG:HE	1.63	0.46
2:B:832:TRP:CZ3	2:B:837:LEU:HD21	2.51	0.46
1:A:613:THR:HG22	2:B:1040:VAL:HG21	1.98	0.46
1:A:827:THR:OG1	2:B:775:VAL:O	2.28	0.46
1:A:1076:LEU:O	1:A:1079:LYS:HG2	2.15	0.46
2:B:31:ASP:OD1	2:B:31:ASP:N	2.44	0.46
6:F:75:PRO:HA	7:G:95:LEU:HD13	1.98	0.46
11:K:67:GLU:N	11:K:99:ASN:O	2.44	0.46
3:C:61:THR:HG22	3:C:298:PHE:HZ	1.81	0.46
6:F:77:ASP:N	6:F:77:ASP:OD1	2.47	0.46
1:A:372:LYS:HG3	1:A:377:VAL:HG22	1.97	0.46
1:A:396:ILE:HB	1:A:426:ALA:HB1	1.98	0.46
1:A:657:TYR:CE2	1:A:665:PRO:HB3	2.51	0.46
2:B:726:MET:O	2:B:744:LEU:HB2	2.15	0.46
2:B:890:ASP:OD1	2:B:890:ASP:N	2.45	0.46
11:K:49:LEU:HD11	11:K:61:ALA:HB1	1.97	0.46
1:A:1314:GLN:OE1	1:A:1318:SER:OG	2.34	0.46
2:B:753:LYS:O	2:B:980:ASP:HA	2.16	0.46
15:R:5:A:H2'	15:R:6:U:C6	2.51	0.46
1:A:490:ILE:O	1:A:617:HIS:ND1	2.44	0.45
2:B:1028:VAL:HG12	2:B:1029:GLY:H	1.81	0.45
1:A:850:SER:HB2	1:A:903:ILE:HG21	1.98	0.45
7:G:91:ASP:OD1	7:G:93:ASP:N	2.30	0.45
1:A:381:SER:HB3	1:A:453:ILE:HG23	1.98	0.45
1:A:1221:ARG:NH1	1:A:1224:GLU:OE1	2.46	0.45
1:A:1223:ARG:HA	1:A:1227:MET:HB2	1.97	0.45
2:B:320:LEU:HB3	2:B:326:VAL:HG22	1.98	0.45
2:B:556:SER:HB3	2:B:621:PRO:HG3	1.97	0.45
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.98	0.45
14:N:26:PRO:HB2	14:N:29:PHE:CD1	2.52	0.45
1:A:475:ARG:NH1	17:T:20:DC:OP1	2.49	0.45
1:A:659:THR:HG23	1:A:666:VAL:HB	1.98	0.45
1:A:1497:ILE:HD12	1:A:1500:GLN:HB3	1.99	0.45
2:B:184:LYS:HB3	2:B:735:HIS:CD2	2.51	0.45
2:B:533:THR:CG2	2:B:540:GLY:H	2.29	0.45
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.98	0.45
1:A:740:THR:HG23	1:A:801:TYR:CE1	2.51	0.45
1:A:925:MET:HG3	1:A:940:VAL:HG22	1.98	0.45
2:B:581:PRO:HG3	2:B:637:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:LEU:HD11	2:B:681:ILE:HD13	1.99	0.45
1:A:81:LEU:HD21	1:A:434:VAL:HG21	1.99	0.45
2:B:1111:LEU:H	2:B:1111:LEU:HD23	1.82	0.45
5:E:180:ARG:HH11	5:E:192:ARG:HG3	1.82	0.45
6:F:118:LEU:O	6:F:122:MET:HG3	2.17	0.45
14:N:113:SER:HB2	14:N:120:LYS:HD2	1.99	0.45
1:A:406:LEU:HD22	1:A:411:VAL:HG21	1.98	0.45
1:A:1255:CYS:SG	1:A:1519:LEU:HD11	2.57	0.45
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.98	0.45
1:A:251:ILE:HG23	1:A:315:ILE:HG12	1.97	0.45
1:A:942:GLN:OE1	2:B:958:MET:HE1	2.16	0.45
2:B:929:ARG:HD3	2:B:931:TRP:CZ3	2.52	0.45
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.99	0.45
1:A:140:THR:HG22	1:A:185:ARG:HH21	1.82	0.44
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.52	0.44
2:B:655:TYR:HB2	2:B:662:ASP:HB2	1.99	0.44
1:A:913:PRO:HB3	1:A:926:GLN:OE1	2.17	0.44
2:B:404:LEU:HD13	2:B:404:LEU:HA	1.81	0.44
2:B:751:ILE:HD12	2:B:1030:VAL:HG21	1.98	0.44
1:A:1238:MET:SD	1:A:1524:VAL:HA	2.57	0.44
2:B:940:GLU:CD	3:C:293:ARG:HH22	2.25	0.44
8:H:106:GLU:OE1	8:H:106:GLU:N	2.50	0.44
7:G:56:ASN:OD1	7:G:56:ASN:N	2.51	0.44
16:S:24:DT:H2"	16:S:25:DC:H5"	1.98	0.44
1:A:77:GLY:C	1:A:362:VAL:HG22	2.42	0.44
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.87	0.44
1:A:1034:TYR:CE1	6:F:136:ARG:HD3	2.53	0.44
2:B:428:VAL:HG12	2:B:449:VAL:HG21	1.99	0.44
2:B:431:ASP:OD2	2:B:452:ARG:NH2	2.50	0.44
2:B:534:PRO:HG3	2:B:542:LEU:HD13	1.99	0.44
2:B:135:GLY:O	2:B:161:LEU:N	2.51	0.44
2:B:913:ILE:HD13	2:B:929:ARG:HA	1.99	0.44
3:C:102:GLY:HA3	12:L:69:ALA:HB1	1.99	0.44
1:A:818:THR:O	1:A:822:THR:HG23	2.18	0.44
1:A:1450:ILE:O	1:A:1454:HIS:ND1	2.45	0.44
5:E:82:PHE:HA	5:E:111:VAL:HG22	2.00	0.44
1:A:1112:PRO:HG2	1:A:1115:LYS:HB2	1.99	0.44
1:A:1504:ILE:HD11	1:A:1529:MET:HE1	1.98	0.44
2:B:261:ARG:HD2	2:B:268:GLU:OE2	2.18	0.44
2:B:494:TYR:CZ	2:B:703:LEU:HD23	2.53	0.44
2:B:733:LEU:HD22	2:B:741:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:GLU:OE1	5:E:85:GLU:N	2.34	0.44
8:H:101:ALA:HB3	8:H:137:GLN:HA	2.00	0.44
13:M:77:VAL:N	14:N:56:ILE:O	2.47	0.44
14:N:54:TRP:CD1	14:N:135:LYS:HB3	2.53	0.44
1:A:652:ASN:ND2	1:A:654:ASP:OD1	2.50	0.43
1:A:1184:ALA:HB2	1:A:1649:VAL:HG11	2.00	0.43
2:B:482:SER:OG	2:B:483:GLY:N	2.51	0.43
3:C:62:SER:OG	11:K:75:ALA:HA	2.17	0.43
5:E:163:GLU:HA	5:E:166:LYS:HE2	1.99	0.43
11:K:134:LYS:HE3	11:K:134:LYS:HB2	1.67	0.43
1:A:18:ILE:HG21	1:A:354:SER:HB2	2.00	0.43
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.85	0.43
2:B:73:ILE:HG12	2:B:74:PHE:H	1.84	0.43
5:E:61:GLN:HB2	5:E:79:TRP:CZ3	2.53	0.43
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.00	0.43
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.53	0.43
13:M:38:PHE:HB3	13:M:53:LEU:HD11	2.00	0.43
1:A:130:ILE:HG21	5:E:215:MET:HE2	1.99	0.43
2:B:13:THR:HG22	14:N:161:PRO:HG2	2.01	0.43
2:B:161:LEU:HD12	2:B:162:PRO:HD2	2.00	0.43
2:B:909:ARG:HD2	2:B:1039:MET:HG2	1.99	0.43
1:A:105:CYS:O	1:A:330:LYS:NZ	2.35	0.43
1:A:947:LEU:HD21	1:A:986:PHE:CZ	2.53	0.43
2:B:809:VAL:HG11	2:B:859:CYS:SG	2.58	0.43
1:A:629:ASP:OD2	2:B:924:LYS:NZ	2.51	0.43
1:A:1101:THR:O	1:A:1105:ARG:HG3	2.19	0.43
2:B:238:SER:OG	2:B:361:HIS:ND1	2.30	0.43
2:B:417:ILE:HG13	2:B:418:ASP:N	2.33	0.43
2:B:794:ASP:OD1	2:B:911:PRO:HG2	2.17	0.43
7:G:71:MET:HE1	7:G:82:LEU:HD13	2.00	0.43
1:A:612:LYS:HB3	1:A:612:LYS:HE2	1.84	0.43
2:B:345:SER:HB3	2:B:348:GLU:HG2	2.00	0.43
2:B:420:TYR:CE1	2:B:455:GLU:HG2	2.54	0.43
2:B:887:LEU:HB2	12:L:56:LEU:HB2	2.00	0.43
14:N:142:THR:OG1	14:N:143:ALA:N	2.51	0.43
16:S:32:DT:H2"	16:S:33:DC:C5	2.54	0.43
1:A:32:ILE:HG22	1:A:390:LEU:HD11	2.00	0.43
1:A:1026:GLN:HB2	1:A:1598:PHE:CE1	2.54	0.43
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.48	0.43
2:B:677:THR:OG1	2:B:680:GLU:OE1	2.36	0.43
1:A:1234:LYS:HD2	1:A:1234:LYS:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:LEU:HD21	2:B:762:MET:SD	2.59	0.43
2:B:891:GLU:H	2:B:891:GLU:CD	2.27	0.43
3:C:246:ARG:HG3	3:C:285:PHE:HZ	1.84	0.43
8:H:110:ASP:HA	8:H:129:TYR:CE1	2.54	0.43
1:A:102:CYS:SG	1:A:233:CYS:HB2	2.58	0.43
1:A:613:THR:O	1:A:615:ARG:NH1	2.51	0.43
1:A:821:ILE:HD12	1:A:821:ILE:HA	1.81	0.43
2:B:374:LEU:HD23	2:B:374:LEU:HA	1.93	0.43
5:E:79:TRP:HB2	5:E:105:PHE:CD2	2.54	0.43
13:M:16:GLN:HG3	13:M:91:TYR:CE1	2.53	0.43
1:A:1222:LEU:O	1:A:1226:VAL:HG12	2.19	0.43
2:B:119:ARG:HH22	2:B:125:GLU:CD	2.26	0.43
2:B:156:ARG:HH21	2:B:455:GLU:CD	2.26	0.43
2:B:1132:SER:HA	2:B:1169:GLY:HA3	2.01	0.43
5:E:14:ARG:O	5:E:18:THR:HG22	2.19	0.43
2:B:352:GLU:O	2:B:356:ARG:HB2	2.19	0.42
8:H:81:PRO:HA	8:H:82:PRO:HD3	1.95	0.42
16:S:10:DC:C4	16:S:11:DG:N2	2.87	0.42
1:A:124:LEU:HD13	1:A:132:GLU:HB3	2.01	0.42
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.93	0.42
2:B:275:MET:HG3	2:B:313:PHE:HE1	1.85	0.42
3:C:152:ASP:OD2	3:C:155:GLU:N	2.51	0.42
1:A:1055:ILE:H	1:A:1055:ILE:HG12	1.70	0.42
2:B:813:LEU:H	2:B:813:LEU:HD23	1.84	0.42
6:F:60:GLN:O	6:F:64:ILE:HG12	2.18	0.42
1:A:488:PRO:HG3	2:B:780:GLY:O	2.19	0.42
1:A:880:GLN:O	1:A:884:ARG:HG2	2.19	0.42
2:B:255:ASP:OD1	2:B:257:GLN:HG2	2.19	0.42
2:B:937:PRO:HB2	2:B:1013:MET:HE2	2.01	0.42
16:S:31:DA:H2"	16:S:32:DT:C6	2.55	0.42
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.20	0.42
1:A:1612:LYS:HD2	1:A:1621:PHE:CE1	2.54	0.42
2:B:623:ASP:HB3	2:B:648:ARG:HH22	1.84	0.42
2:B:1079:LEU:HD13	2:B:1088:LEU:HA	2.02	0.42
3:C:34:GLU:N	3:C:34:GLU:OE1	2.53	0.42
4:D:22:ILE:HG22	7:G:76:LYS:HG2	2.02	0.42
7:G:43:ILE:HD13	7:G:122:LEU:HD22	2.00	0.42
13:M:13:GLU:HG3	13:M:87:SER:HB3	2.02	0.42
1:A:20:THR:O	1:A:24:ILE:HG13	2.20	0.42
1:A:830:MET:O	1:A:834:ARG:HG3	2.20	0.42
2:B:369:ASP:OD1	2:B:372:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:THR:HG22	2:B:778:TYR:O	2.20	0.42
1:A:986:PHE:CD2	2:B:958:MET:HE2	2.54	0.42
2:B:91:LEU:HD12	2:B:91:LEU:H	1.84	0.42
2:B:837:LEU:HD13	2:B:837:LEU:HA	1.83	0.42
2:B:968:ALA:HB2	2:B:996:PHE:CE2	2.55	0.42
2:B:1157:GLN:O	2:B:1168:VAL:HA	2.20	0.42
5:E:202:SER:HB2	5:E:208:TYR:CE1	2.55	0.42
1:A:130:ILE:HG21	5:E:215:MET:SD	2.60	0.42
1:A:498:PRO:HB3	1:A:612:LYS:HA	2.02	0.42
1:A:811:SER:OG	1:A:815:ARG:NH1	2.53	0.42
2:B:68:ILE:HD12	2:B:417:ILE:HD11	2.01	0.42
2:B:207:ILE:HG22	2:B:504:HIS:O	2.20	0.42
2:B:232:TYR:CD2	2:B:385:VAL:HG12	2.55	0.42
2:B:909:ARG:HA	2:B:909:ARG:HD3	1.78	0.42
1:A:1484:LEU:HD13	1:A:1484:LEU:HA	1.89	0.42
2:B:624:LEU:HD12	2:B:643:PHE:O	2.20	0.42
2:B:836:TRP:CE3	2:B:871:ILE:HD13	2.55	0.42
16:S:11:DG:H21	17:T:29:DG:H1	1.68	0.42
17:T:6:DG:H2"	17:T:7:DA:C8	2.53	0.42
2:B:841:ASP:HA	2:B:847:TYR:CZ	2.55	0.41
2:B:975:HIS:HE1	2:B:1003:ALA:HB2	1.85	0.41
5:E:112:TYR:HE2	5:E:134:THR:HB	1.85	0.41
11:K:67:GLU:HA	11:K:99:ASN:HB2	2.02	0.41
1:A:94:LEU:HA	1:A:94:LEU:HD12	1.85	0.41
2:B:712:SER:OG	2:B:713:PRO:HD3	2.20	0.41
2:B:883:GLU:HB3	2:B:904:LYS:HB3	2.03	0.41
2:B:895:PHE:HB3	12:L:45:ALA:HB2	2.02	0.41
3:C:301:ASN:ND2	14:N:173:THR:HB	2.35	0.41
5:E:38:PRO:HD2	5:E:41:ASP:HB2	2.01	0.41
1:A:390:LEU:HA	1:A:390:LEU:HD23	1.82	0.41
1:A:730:GLN:HE21	1:A:730:GLN:HB3	1.57	0.41
2:B:72:VAL:HA	2:B:95:LEU:O	2.20	0.41
2:B:472:SER:HB2	2:B:474:SER:O	2.21	0.41
2:B:548:LYS:HG3	2:B:695:ASN:HB2	2.03	0.41
5:E:137:GLU:N	5:E:137:GLU:OE1	2.53	0.41
10:J:42:LYS:HE2	10:J:42:LYS:HB2	1.81	0.41
13:M:64:GLY:HA2	13:M:98:SER:HA	2.02	0.41
1:A:498:PRO:HB3	1:A:611:GLU:O	2.20	0.41
1:A:1007:ILE:HG21	2:B:515:THR:HG23	2.02	0.41
1:A:1446:ARG:O	1:A:1450:ILE:HG12	2.21	0.41
3:C:240:LYS:HG2	3:C:264:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:PRO:HG2	3:C:273:ASP:HA	2.03	0.41
5:E:83:CYS:SG	5:E:112:TYR:HA	2.60	0.41
5:E:163:GLU:HG3	5:E:166:LYS:HE2	2.02	0.41
7:G:73:TYR:CD1	7:G:79:GLY:HA2	2.55	0.41
7:G:79:GLY:HA3	7:G:126:GLN:HB3	2.01	0.41
8:H:110:ASP:HA	8:H:129:TYR:HE1	1.86	0.41
16:S:30:DT:H2''	16:S:31:DA:H8	1.85	0.41
1:A:486:PRO:HD3	1:A:628:PHE:CG	2.55	0.41
1:A:658:LEU:HD22	1:A:663:GLY:O	2.20	0.41
1:A:1463:ASP:OD2	1:A:1469:TRP:NE1	2.54	0.41
2:B:1084:THR:HB	2:B:1087:LEU:HB2	2.01	0.41
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.91	0.41
3:C:103:LEU:HD22	10:J:6:ARG:HD2	2.02	0.41
3:C:175:GLN:HB2	3:C:179:PHE:CD2	2.55	0.41
5:E:91:LYS:HD3	5:E:92:THR:HG23	2.01	0.41
1:A:413:LEU:HD22	1:A:416:ARG:HD2	2.02	0.41
2:B:26:ILE:O	10:J:62:ARG:NH1	2.53	0.41
2:B:913:ILE:CD1	2:B:929:ARG:HA	2.50	0.41
7:G:66:LEU:HB3	7:G:84:TYR:CE2	2.56	0.41
17:T:15:DA:H2'	17:T:16:DT:C6	2.55	0.41
1:A:861:VAL:HG21	1:A:892:LEU:HA	2.03	0.41
1:A:1552:THR:HG23	1:A:1553:TYR:CD2	2.56	0.41
2:B:57:ASP:HB3	2:B:63:LEU:HD21	2.02	0.41
2:B:878:GLU:OE1	2:B:909:ARG:NH2	2.50	0.41
13:M:80:LEU:HA	14:N:52:GLN:O	2.21	0.41
14:N:25:ILE:HD11	14:N:29:PHE:O	2.21	0.41
2:B:68:ILE:HD11	2:B:414:LYS:HG3	2.02	0.41
2:B:731:VAL:HG21	10:J:59:LYS:HG2	2.02	0.41
2:B:878:GLU:CD	2:B:909:ARG:HH21	2.28	0.41
1:A:721:LYS:HB2	8:H:96:VAL:HG12	2.02	0.41
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.89	0.41
1:A:1525:ASN:ND2	1:A:1528:ALA:HB2	2.36	0.41
2:B:282:HIS:CE1	13:M:101:VAL:HG13	2.56	0.41
2:B:565:LEU:HD13	2:B:586:VAL:HG11	2.03	0.41
2:B:785:ASP:CG	2:B:957:ARG:HH22	2.29	0.41
3:C:174:ARG:O	3:C:178:THR:HG23	2.21	0.41
6:F:119:ARG:HD3	6:F:119:ARG:HA	1.87	0.41
7:G:102:GLU:N	7:G:102:GLU:OE1	2.54	0.41
13:M:108:LEU:HD12	13:M:108:LEU:HA	1.94	0.41
2:B:286:ARG:NH2	13:M:28:LYS:HB3	2.35	0.41
2:B:610:TYR:CE2	2:B:658:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:HG23	5:E:120:ALA:H	1.86	0.41
13:M:28:LYS:HD2	14:N:104:LEU:C	2.46	0.41
13:M:32:ALA:HB3	14:N:121:ILE:HD12	2.03	0.41
2:B:61:LEU:O	2:B:65:VAL:HG13	2.22	0.40
2:B:413:LEU:O	2:B:417:ILE:HG23	2.22	0.40
2:B:609:ARG:HB2	2:B:626:ILE:HD11	2.03	0.40
13:M:11:GLU:OE1	13:M:11:GLU:N	2.53	0.40
14:N:144:LYS:HA	14:N:144:LYS:HD2	1.85	0.40
1:A:191:MET:HE2	1:A:191:MET:HB2	1.90	0.40
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.57	0.40
2:B:335:ARG:HA	2:B:335:ARG:HD2	1.88	0.40
2:B:346:ASP:HA	2:B:349:VAL:HG12	2.03	0.40
2:B:513:LYS:HD3	2:B:513:LYS:HA	1.78	0.40
2:B:600:GLN:O	2:B:604:ILE:HG12	2.21	0.40
2:B:714:ARG:HA	2:B:714:ARG:HD3	1.85	0.40
5:E:54:GLN:H	5:E:54:GLN:HG3	1.70	0.40
7:G:62:MET:HA	7:G:66:LEU:HB2	2.02	0.40
1:A:467:PHE:HA	1:A:471:MET:SD	2.61	0.40
1:A:1647:ASN:O	1:A:1652:GLY:HA3	2.21	0.40
2:B:381:LEU:O	2:B:385:VAL:HG13	2.22	0.40
2:B:565:LEU:HD23	2:B:565:LEU:HA	1.85	0.40
2:B:936:MET:HE2	2:B:945:PRO:O	2.21	0.40
3:C:69:ARG:HE	11:K:71:THR:HG1	1.60	0.40
3:C:94:ASP:OD1	3:C:94:ASP:N	2.54	0.40
3:C:95:GLU:HG2	3:C:96:VAL:N	2.37	0.40
5:E:6:GLU:OE1	5:E:43:LYS:NZ	2.54	0.40
5:E:122:LYS:O	5:E:126:SER:OG	2.38	0.40
1:A:949:GLN:HA	1:A:981:TYR:HA	2.03	0.40
1:A:1641:ILE:CD1	2:B:1076:ARG:HD2	2.50	0.40
1:A:1663:ALA:N	7:G:101:SER:O	2.54	0.40
2:B:237:ARG:HG2	2:B:245:SER:OG	2.22	0.40
1:A:962:SER:HB3	2:B:671:TYR:CE1	2.56	0.40
1:A:1631:ARG:O	1:A:1633:GLN:NE2	2.54	0.40
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.56	0.40
2:B:65:VAL:HG12	2:B:417:ILE:CD1	2.52	0.40
3:C:39:ASP:O	3:C:58:ASN:ND2	2.33	0.40
5:E:180:ARG:HD3	5:E:192:ARG:HG3	2.04	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	1440/1664 (86%)	1377 (96%)	63 (4%)	0	100	100
2	B	1156/1203 (96%)	1102 (95%)	54 (5%)	0	100	100
3	C	302/335 (90%)	288 (95%)	14 (5%)	0	100	100
4	D	17/137 (12%)	15 (88%)	2 (12%)	0	100	100
5	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
6	F	99/155 (64%)	95 (96%)	4 (4%)	0	100	100
7	G	88/326 (27%)	87 (99%)	1 (1%)	0	100	100
8	H	127/146 (87%)	119 (94%)	8 (6%)	0	100	100
9	I	63/125 (50%)	53 (84%)	10 (16%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	96/142 (68%)	92 (96%)	4 (4%)	0	100	100
12	L	42/70 (60%)	39 (93%)	3 (7%)	0	100	100
13	M	96/415 (23%)	91 (95%)	5 (5%)	0	100	100
14	N	107/233 (46%)	101 (94%)	6 (6%)	0	100	100
All	All	3912/5236 (75%)	3725 (95%)	187 (5%)	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	1285/1465 (88%)	1245 (97%)	40 (3%)	35	65
2	B	1017/1053 (97%)	976 (96%)	41 (4%)	28	56
3	C	268/296 (90%)	259 (97%)	9 (3%)	32	62
4	D	17/116 (15%)	17 (100%)	0	100	100
5	E	196/197 (100%)	190 (97%)	6 (3%)	35	65
6	F	90/137 (66%)	86 (96%)	4 (4%)	25	53
7	G	81/291 (28%)	77 (95%)	4 (5%)	22	49
8	H	115/128 (90%)	110 (96%)	5 (4%)	26	54
9	I	57/110 (52%)	52 (91%)	5 (9%)	9	23
10	J	64/65 (98%)	62 (97%)	2 (3%)	35	65
11	K	88/130 (68%)	85 (97%)	3 (3%)	32	62
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	90/371 (24%)	85 (94%)	5 (6%)	19	44
14	N	109/220 (50%)	106 (97%)	3 (3%)	38	68
All	All	3516/4636 (76%)	3389 (96%)	127 (4%)	32	60

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	129	LEU
1	A	212	VAL
1	A	315	ILE
1	A	382	GLN
1	A	394	LEU
1	A	395	LEU
1	A	396	ILE
1	A	432	ASN
1	A	460	LEU
1	A	516	ILE
1	A	519	LEU
1	A	557	LEU
1	A	587	VAL
1	A	632	GLU
1	A	656	GLN
1	A	670	ILE
1	A	703	GLU
1	A	731	ILE

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Mol	Chain	Res	Type
1	A	821	ILE
1	A	824	THR
1	A	831	ASP
1	A	864	LEU
1	A	965	THR
1	A	1030	VAL
1	A	1055	ILE
1	A	1065	GLN
1	A	1089	LEU
1	A	1098	SER
1	A	1261	VAL
1	A	1266	VAL
1	A	1311	GLU
1	A	1456	PHE
1	A	1476	LEU
1	A	1486	VAL
1	A	1518	VAL
1	A	1550	LEU
1	A	1569	VAL
1	A	1628	ASP
1	A	1651	THR
2	B	15	ASP
2	B	53	THR
2	B	72	VAL
2	B	128	GLN
2	B	139	LEU
2	B	202	LEU
2	B	274	VAL
2	B	322	ASN
2	B	362	LEU
2	B	404	LEU
2	B	417	ILE
2	B	421	LEU
2	B	425	ILE
2	B	476	LEU
2	B	487	VAL
2	B	558	VAL
2	B	563	SER
2	B	604	ILE
2	B	692	THR
2	B	703	LEU
2	B	721	MET

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Mol	Chain	Res	Type
2	B	752	VAL
2	B	762	MET
2	B	806	THR
2	B	837	LEU
2	B	858	ILE
2	B	943	ILE
2	B	946	ASP
2	B	982	THR
2	B	1006	ASN
2	B	1028	VAL
2	B	1030	VAL
2	B	1031	VAL
2	B	1033	TYR
2	B	1049	THR
2	B	1055	LEU
2	B	1087	LEU
2	B	1089	GLN
2	B	1126	VAL
2	B	1168	VAL
2	B	1175	THR
3	C	57	ILE
3	C	104	VAL
3	C	113	LEU
3	C	119	ASN
3	C	138	VAL
3	C	151	THR
3	C	223	SER
3	C	229	LEU
3	C	324	LYS
5	E	54	GLN
5	E	58	MET
5	E	112	TYR
5	E	124	VAL
5	E	190	LEU
5	E	196	VAL
6	F	71	GLU
6	F	77	ASP
6	F	115	THR
6	F	152	ILE
7	G	45	LEU
7	G	48	SER
7	G	122	LEU

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Mol	Chain	Res	Type
7	G	126	GLN
8	H	5	LEU
8	H	45	GLU
8	H	96	VAL
8	H	131	ASN
8	H	145	ARG
9	I	7	LEU
9	I	21	ASN
9	I	28	VAL
9	I	33	CYS
9	I	47	VAL
10	J	28	ASP
10	J	56	LEU
11	K	64	GLN
11	K	66	VAL
11	K	110	GLU
13	M	74	ASN
13	M	77	VAL
13	M	97	VAL
13	M	101	VAL
13	M	102	SER
14	N	25	ILE
14	N	51	GLN
14	N	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	264	ASN
1	A	425	ASN
1	A	432	ASN
1	A	489	ASN
1	A	560	GLN
1	A	671	GLN
1	A	1062	HIS
1	A	1151	ASN
1	A	1180	ASN
1	A	1300	ASN
1	A	1487	ASN
1	A	1532	GLN
1	A	1544	ASN

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Mol	Chain	Res	Type
1	A	1567	ASN
2	B	45	HIS
2	B	50	ASN
2	B	166	GLN
2	B	254	ASN
2	B	344	GLN
2	B	399	HIS
2	B	636	GLN
2	B	720	GLN
2	B	735	HIS
2	B	814	ASN
2	B	823	GLN
2	B	975	HIS
2	B	1010	ASN
2	B	1114	GLN
2	B	1171	ASN
3	C	161	HIS
3	C	207	HIS
3	C	301	ASN
4	D	23	HIS
5	E	63	ASN
5	E	115	ASN
7	G	126	GLN
8	H	137	GLN
13	M	75	GLN
13	M	82	ASN
13	M	89	GLN
14	N	85	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	8/12 (66%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	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	$\# Z > 2$
17	3DR	T	17	17	8,11,12	0.47	0	7,14,17	0.50	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
17	3DR	T	17	17	-	2/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	T	17	3DR	C3'-C4'-C5'-O5'
17	T	17	3DR	O4'-C4'-C5'-O5'

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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

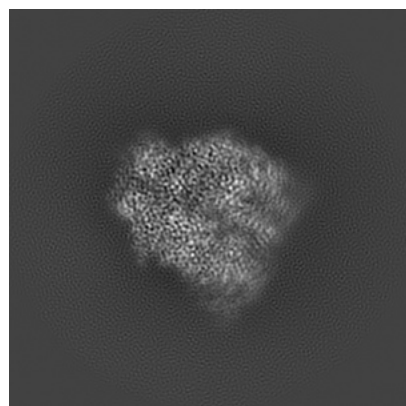
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50955. These allow visual inspection of the internal detail of the map and identification of artifacts.

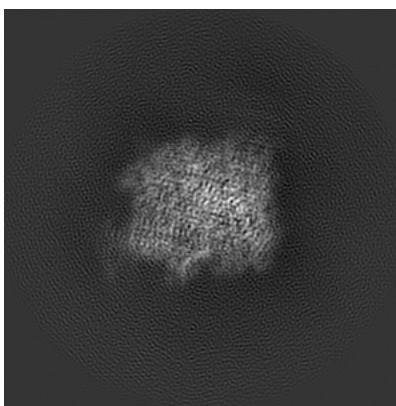
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

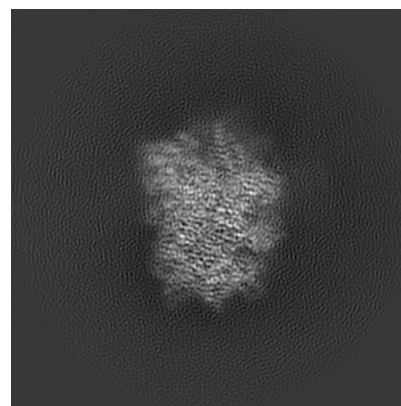
6.1.1 Primary map



X

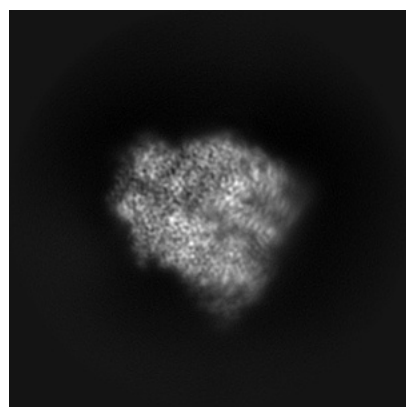


Y

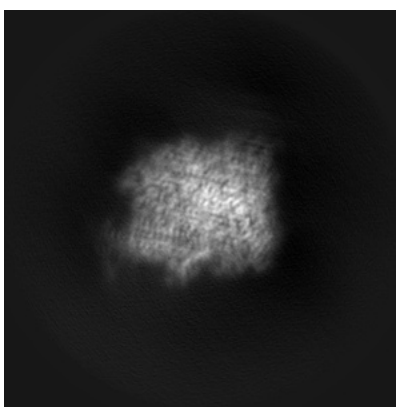


Z

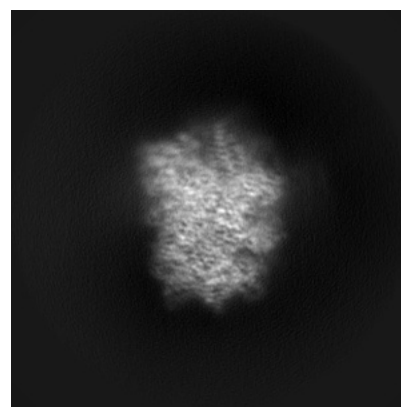
6.1.2 Raw map



X



Y

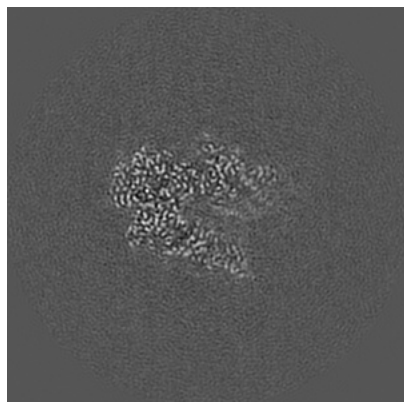


Z

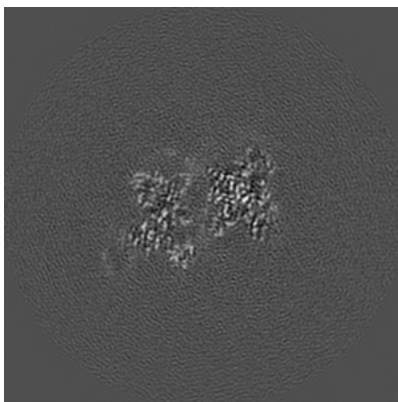
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

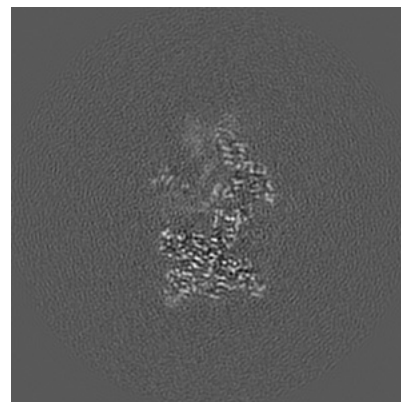
6.2.1 Primary map



X Index: 144

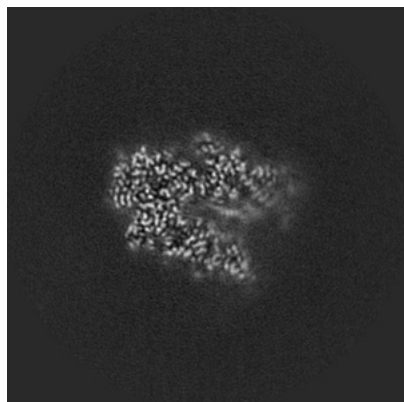


Y Index: 144

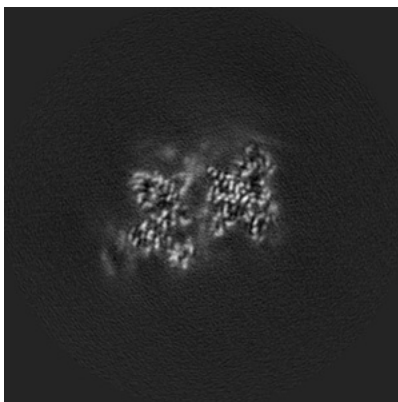


Z Index: 144

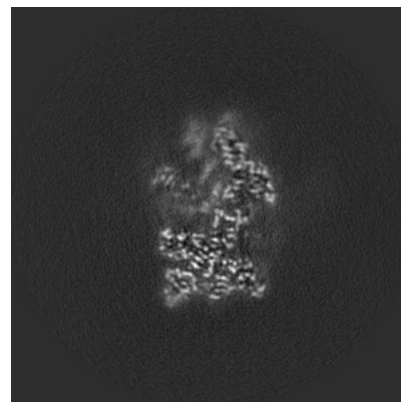
6.2.2 Raw map



X Index: 144



Y Index: 144

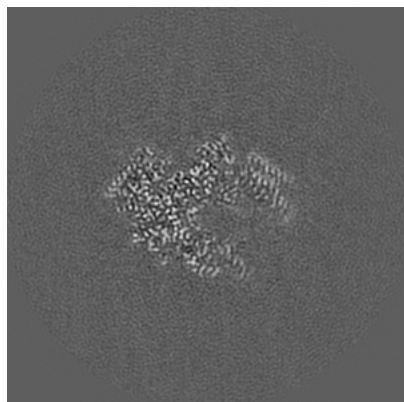


Z Index: 144

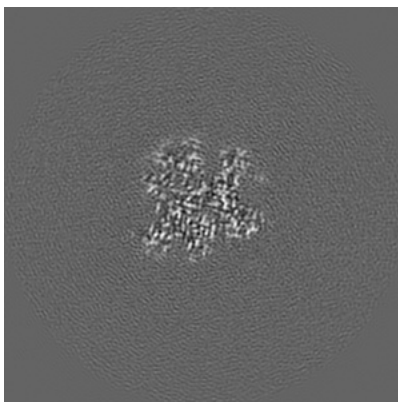
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

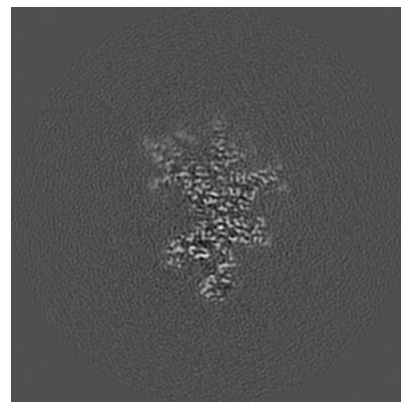
6.3.1 Primary map



X Index: 150

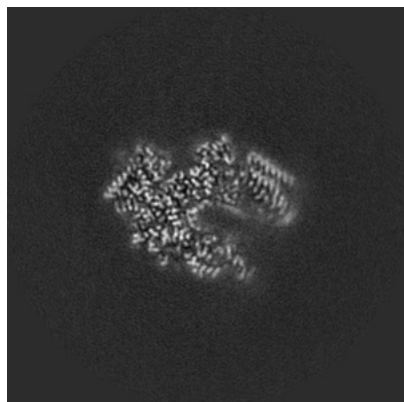


Y Index: 123

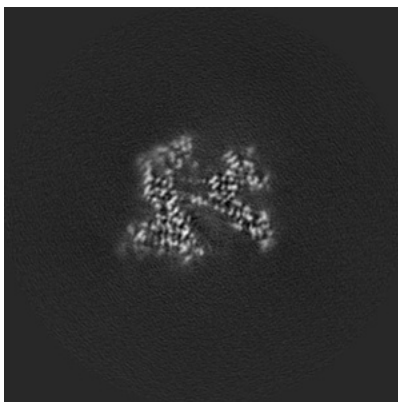


Z Index: 162

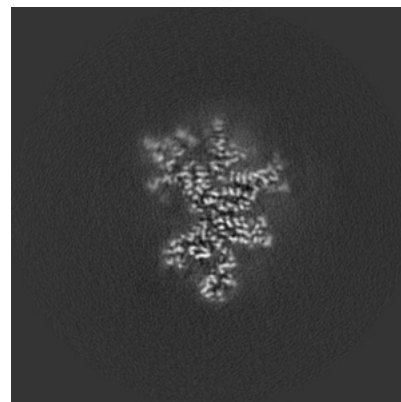
6.3.2 Raw map



X Index: 150



Y Index: 130

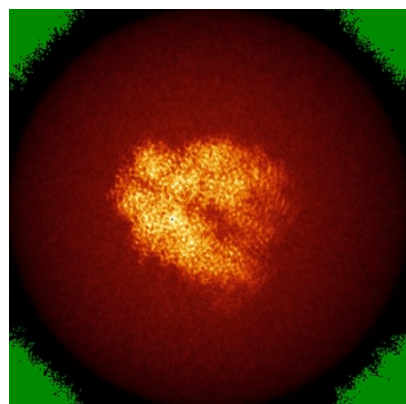


Z Index: 162

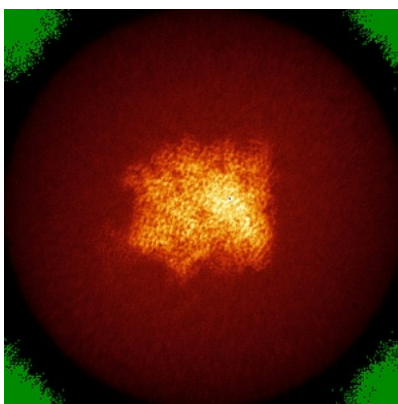
The images above show the largest variance slices of the map in three orthogonal directions.

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

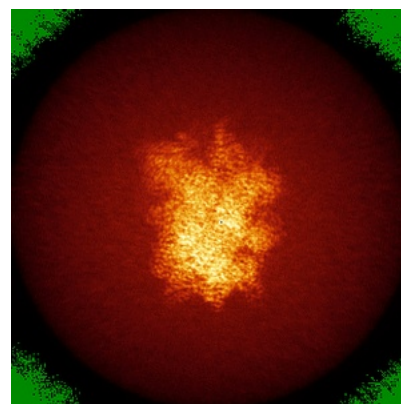
6.4.1 Primary map



X

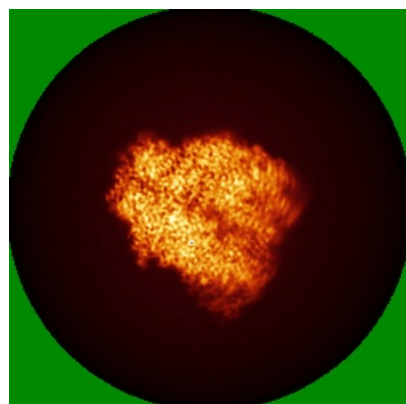


Y

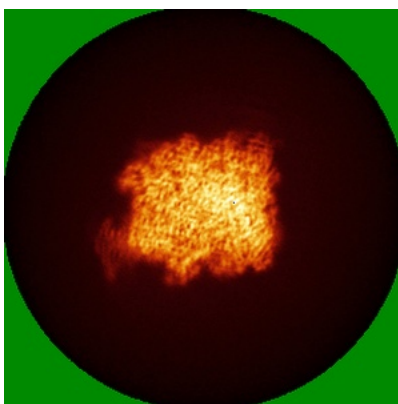


Z

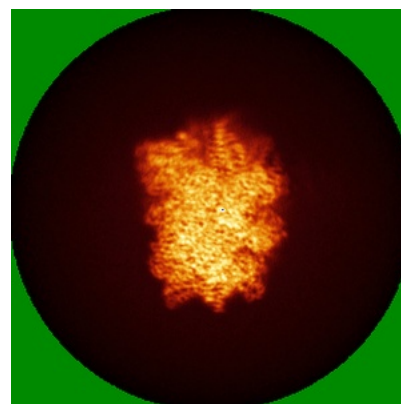
6.4.2 Raw map



X



Y

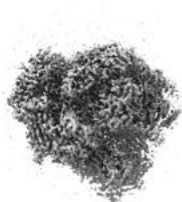


Z

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



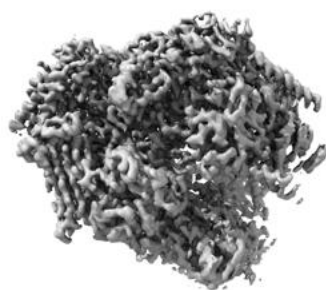
Y



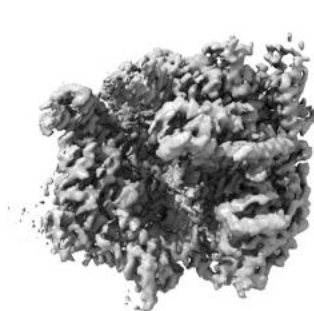
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

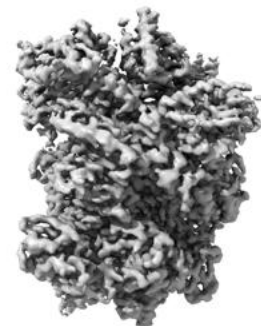
6.5.2 Raw map



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.

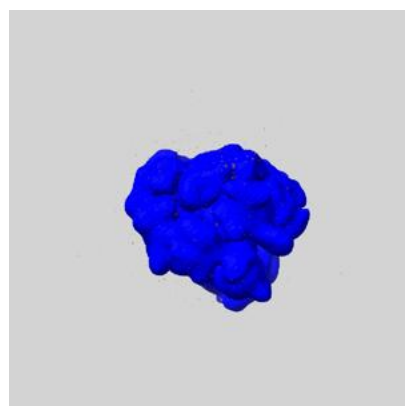
6.6 Mask visualisation [i](#)

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

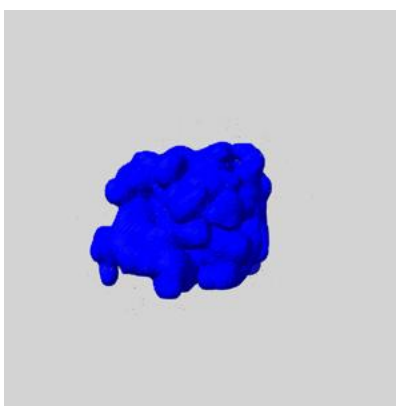
A mask typically either:

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

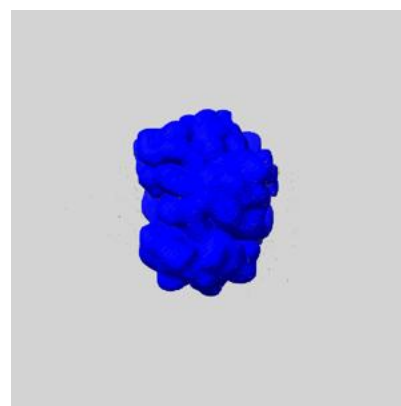
6.6.1 emd_50955_msk_1.map [i](#)



X



Y

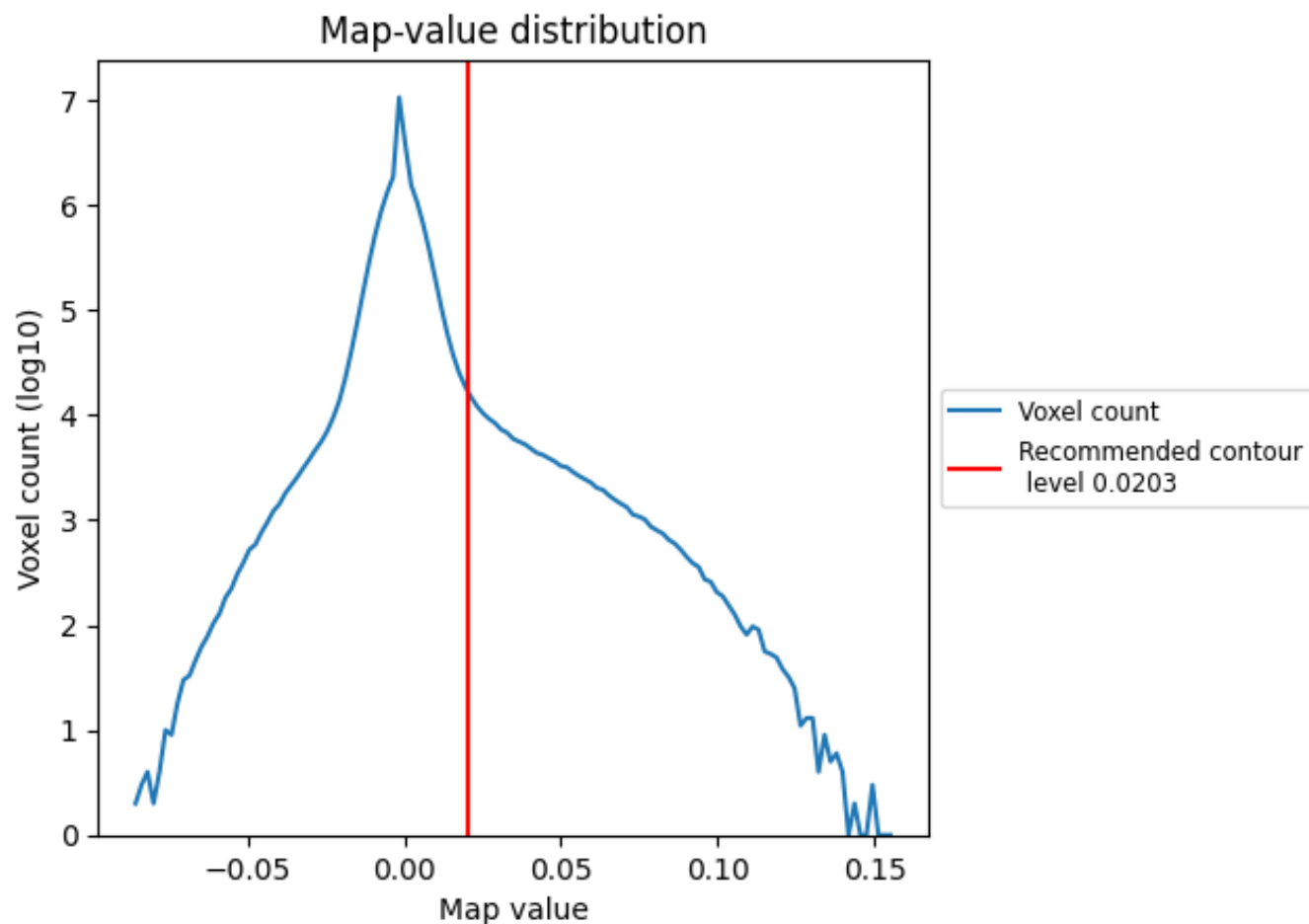


Z

7 Map analysis [i](#)

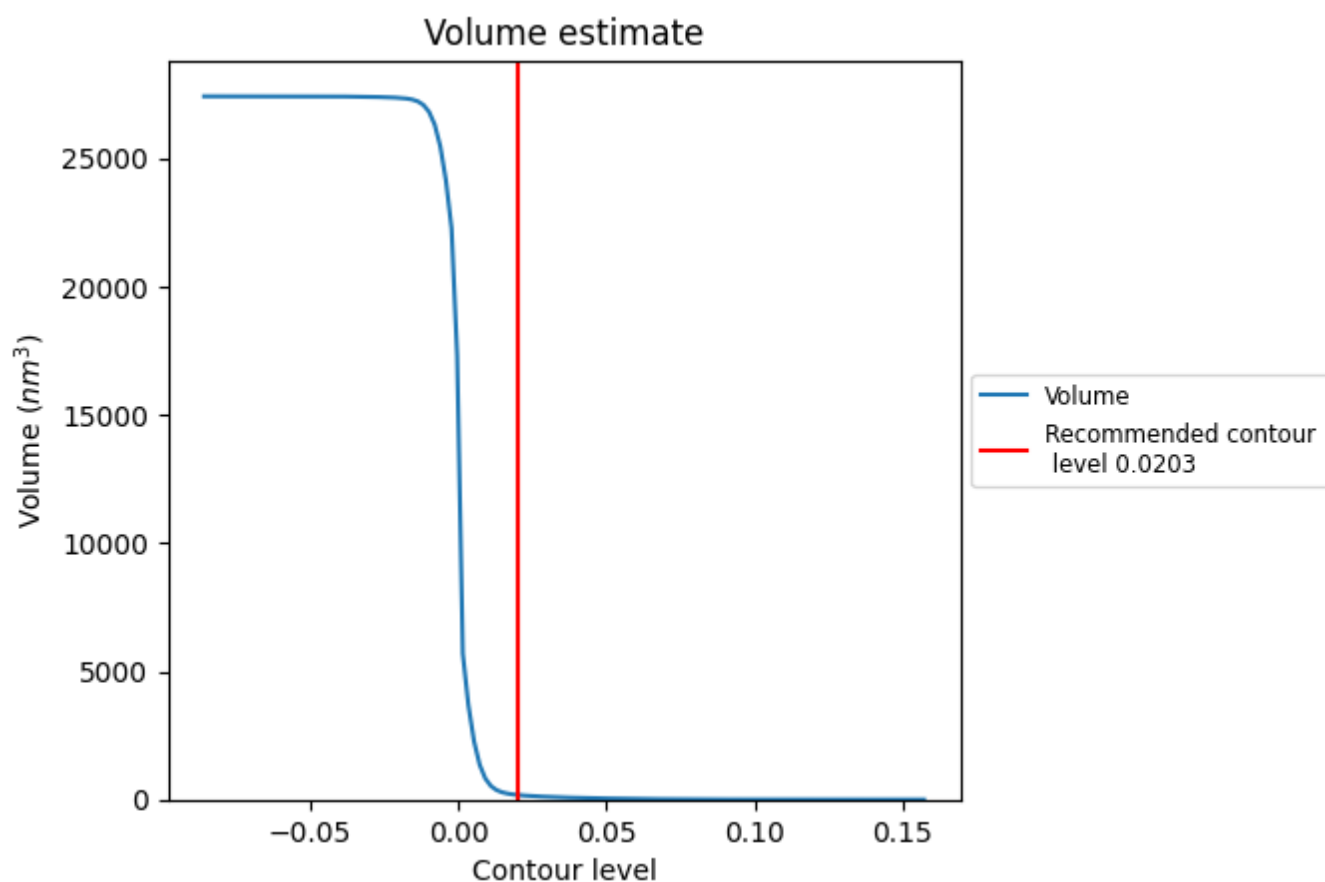
This section contains the results of statistical analysis of the map.

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.

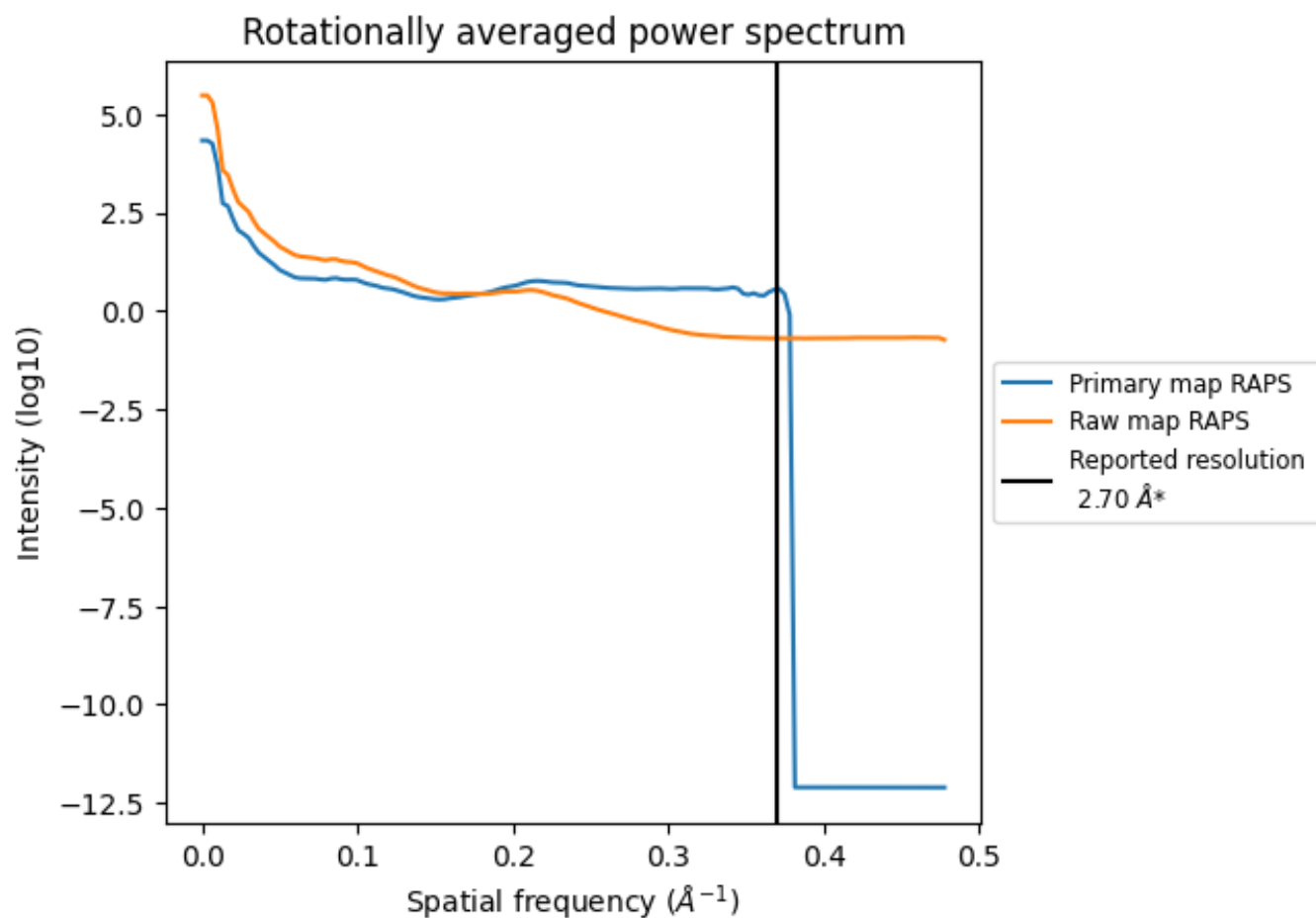
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

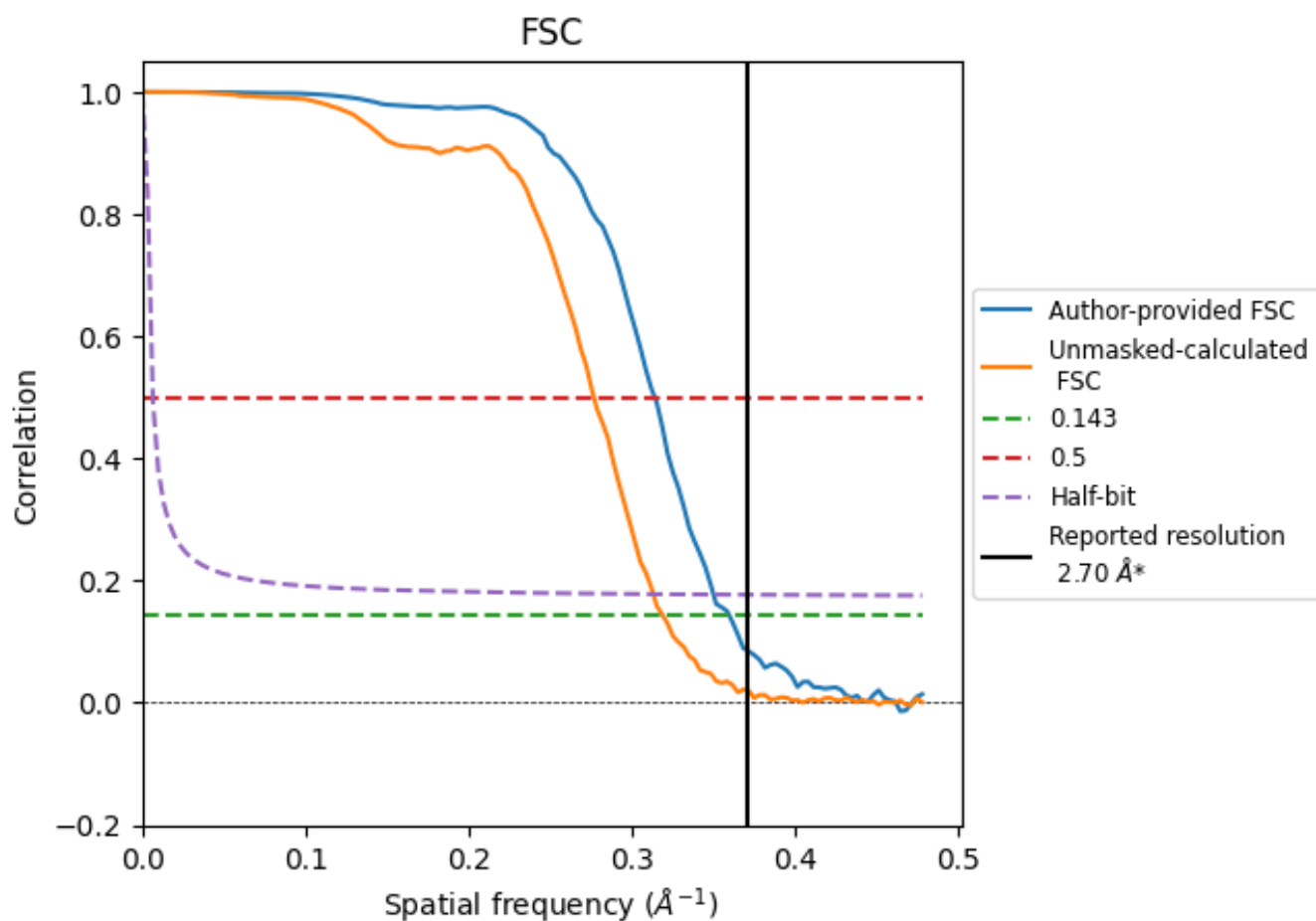


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

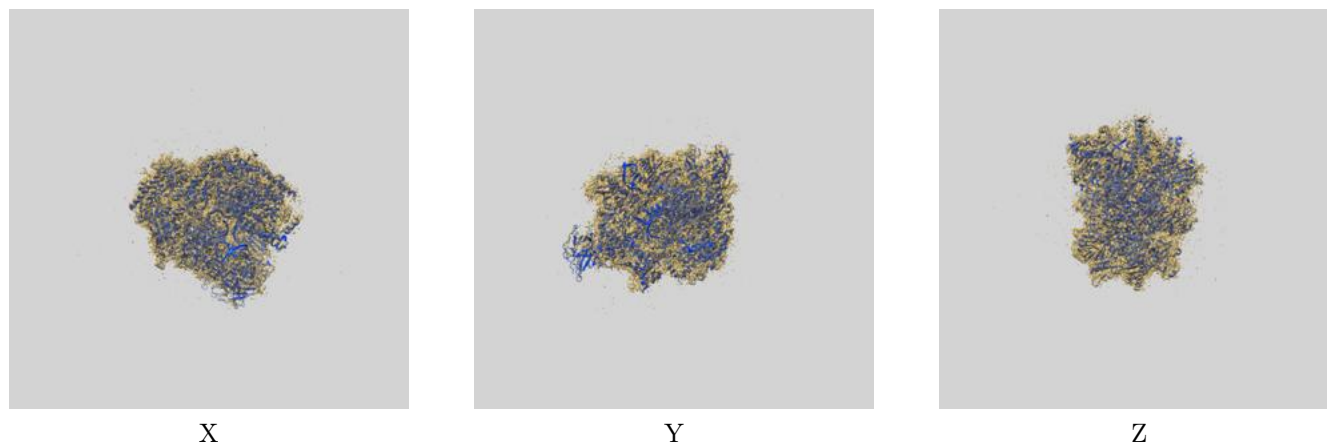
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.78	3.19	2.86
Unmasked-calculated*	3.14	3.62	3.19

*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 3.14 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

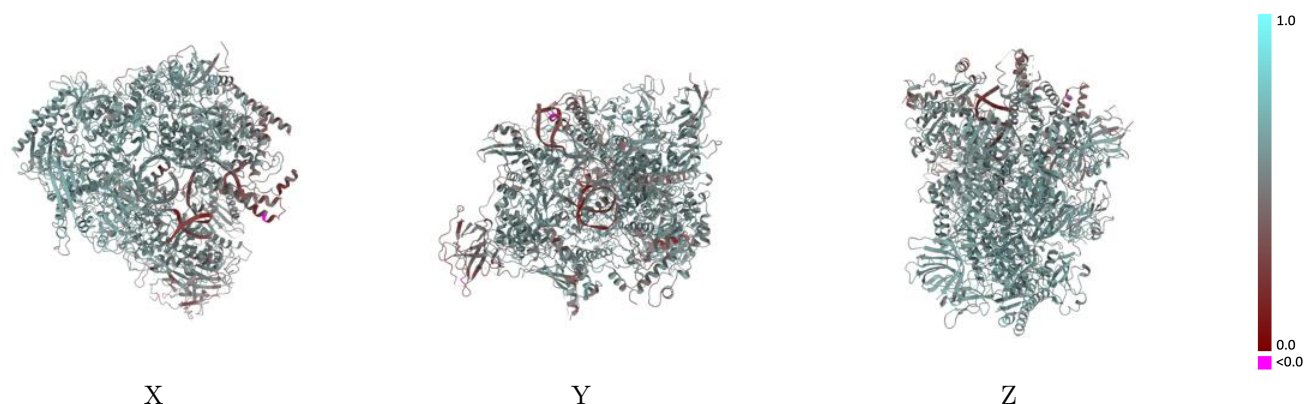
This section contains information regarding the fit between EMDB map EMD-50955 and PDB model 9G1V. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



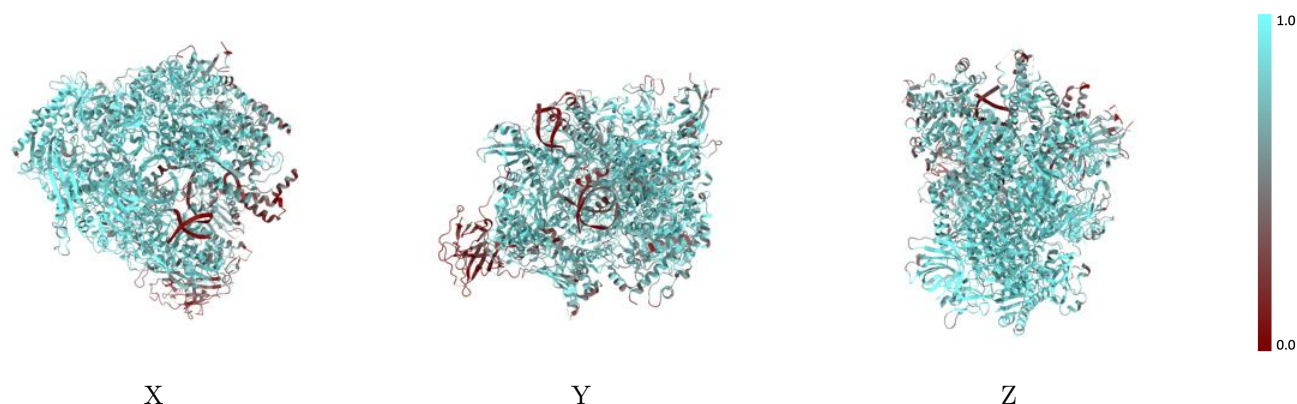
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



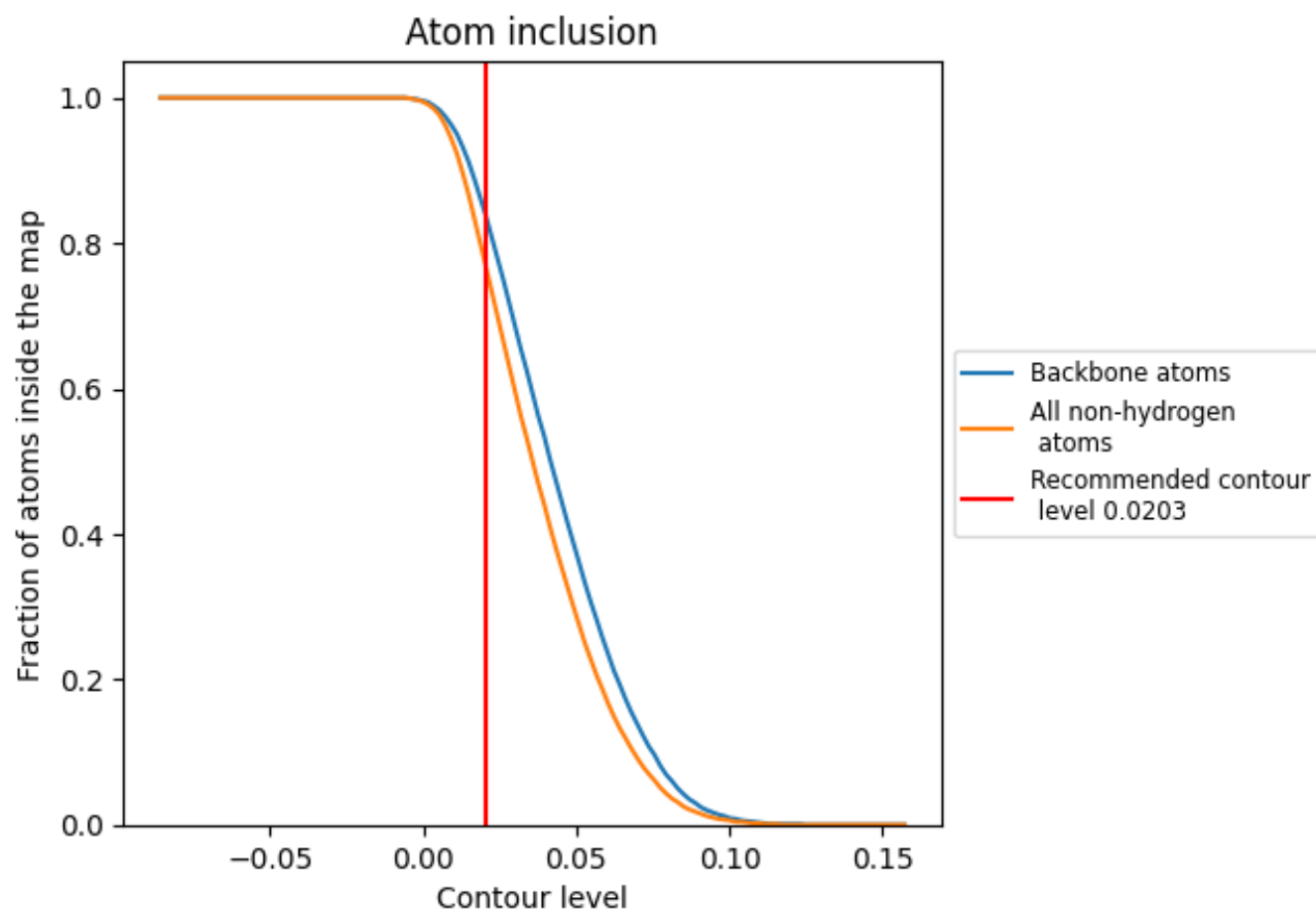
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5490
A	0.7930	0.5540
B	0.8580	0.5780
C	0.8620	0.5850
D	0.7060	0.5460
E	0.7230	0.5090
F	0.8520	0.5760
G	0.7090	0.5430
H	0.8490	0.5840
I	0.5660	0.4880
J	0.9200	0.6160
K	0.8740	0.5840
L	0.8500	0.5740
M	0.1870	0.4090
N	0.2260	0.4250
R	0.8880	0.5540
S	0.1990	0.2640
T	0.4680	0.3890

1.0

0.0

<0.0