



Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 04:22 pm BST

PDB ID : 9G29 / pdb_00009g29
EMDB ID : EMD-50970
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site with the C-terminal of A12 in the funnel
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.30 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

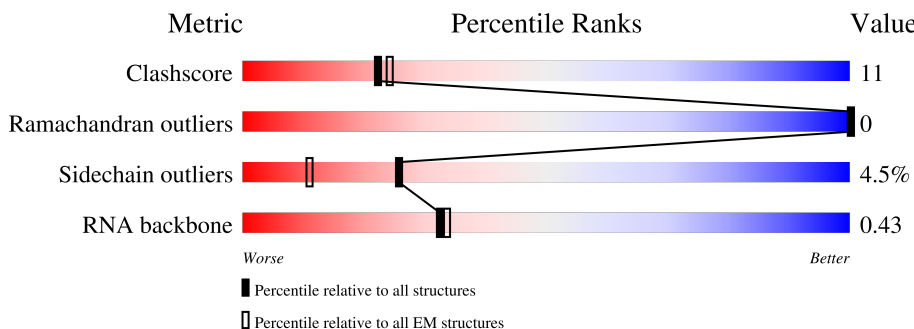
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1664	<div> <div>18%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>
2	B	1203	<div> <div>14%</div> <div>67%</div> <div>28%</div> <div>• •</div> </div>
3	C	335	<div> <div>14%</div> <div>68%</div> <div>22%</div> <div>•</div> <div>9%</div> </div>
4	D	137	<div> <div>7%</div> <div>9%</div> <div>•</div> <div>87%</div> </div>
5	E	215	<div> <div>35%</div> <div>68%</div> <div>28%</div> <div>•</div> </div>
6	F	155	<div> <div>9%</div> <div>46%</div> <div>17%</div> <div>•</div> <div>35%</div> </div>
7	G	326	<div> <div>13%</div> <div>18%</div> <div>9%</div> <div>72%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	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 33493 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	1464	Total	C	N	O	S	0	0
			11563	7301	2012	2188	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9232	5839	1622	1720	51		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	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	132	Total	C	N	O	S	0	0
			1060	670	177	209	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	124	Total	C	N	O	S	0	0
			942	584	160	189	9		

- 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	103	Total	C	N	O		0	0
			814	517	134	163			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	128	Total	C	N	O	S	0	0
			1018	656	169	189	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	24	Total	C	N	O	P	0	0
			487	233	82	148	24		

- Molecule 17 is a DNA chain called Template DNA.

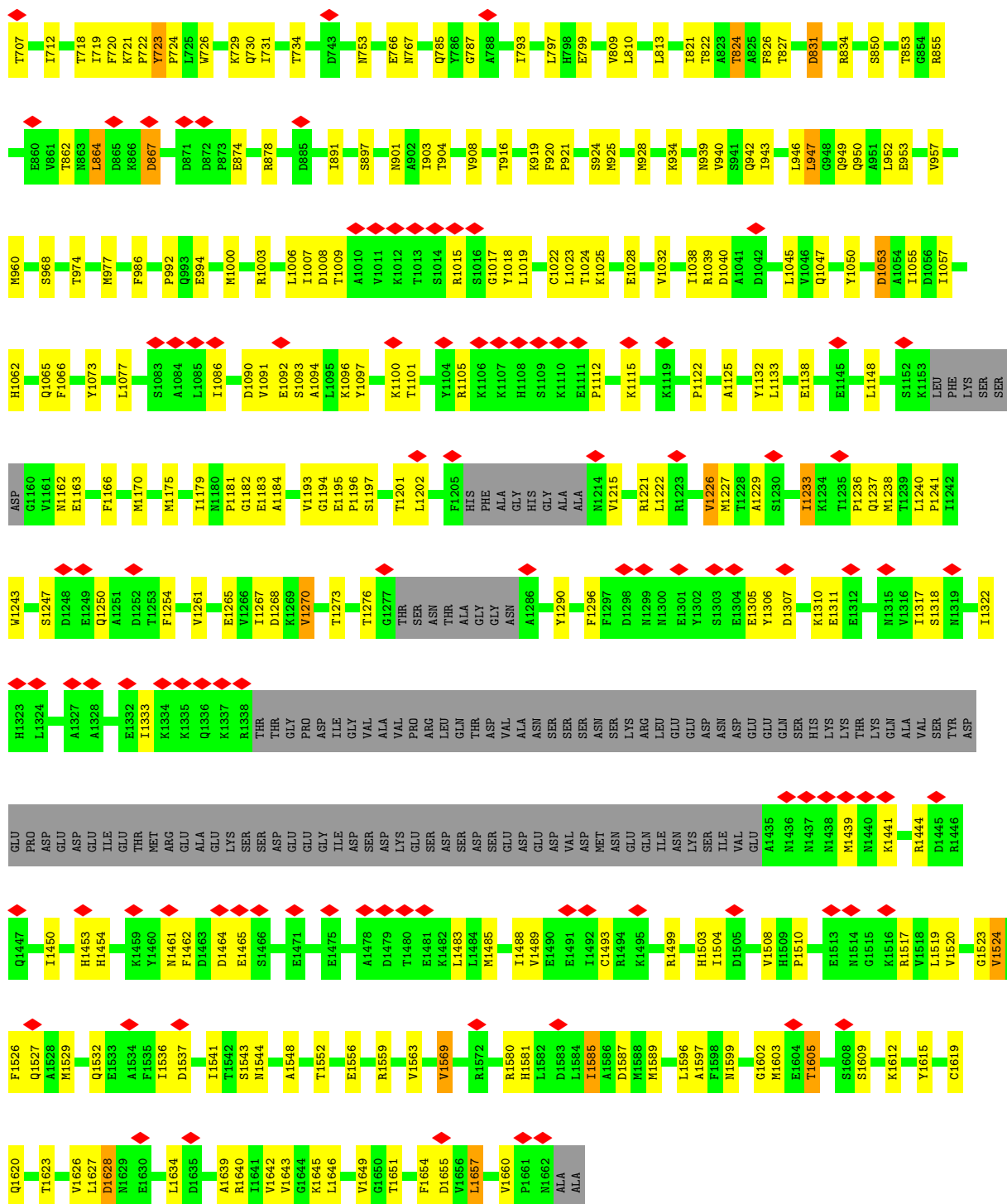
Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	32	Total	C	N	O	P	0	0
			643	307	112	192	32		

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

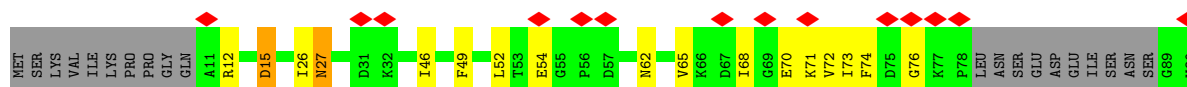
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

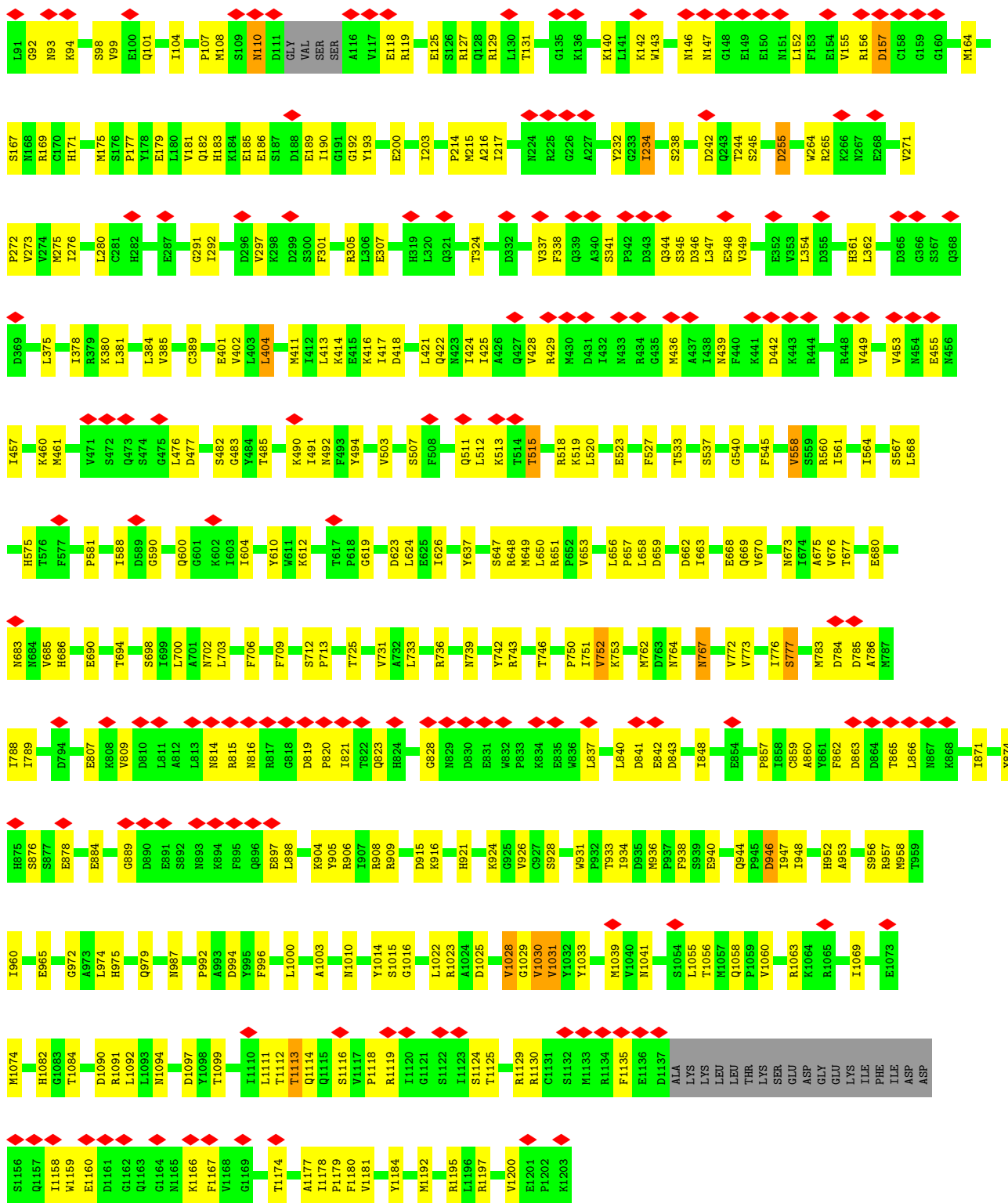
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



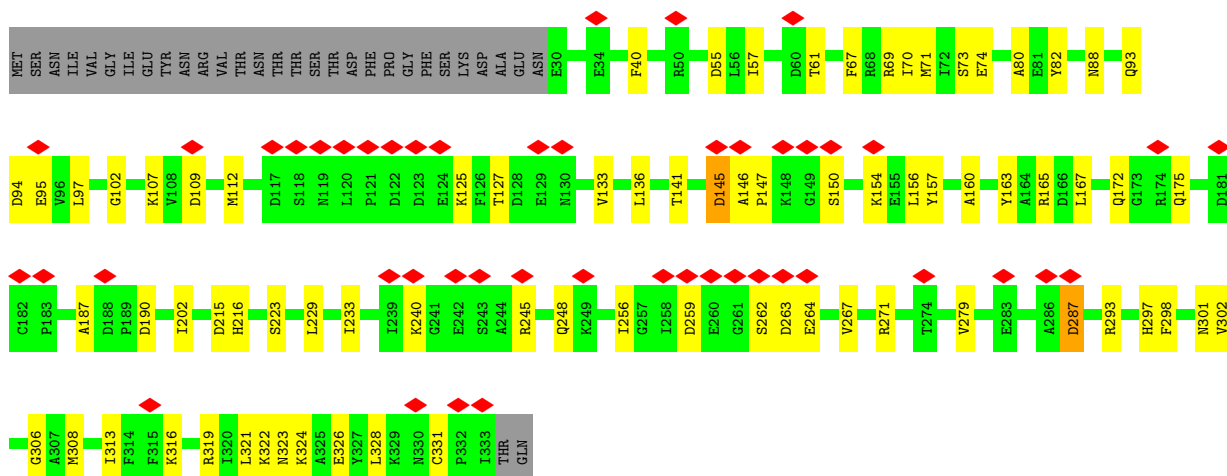
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



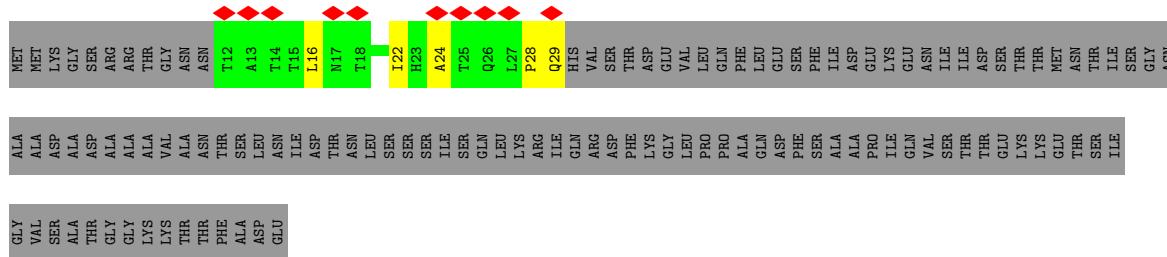


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

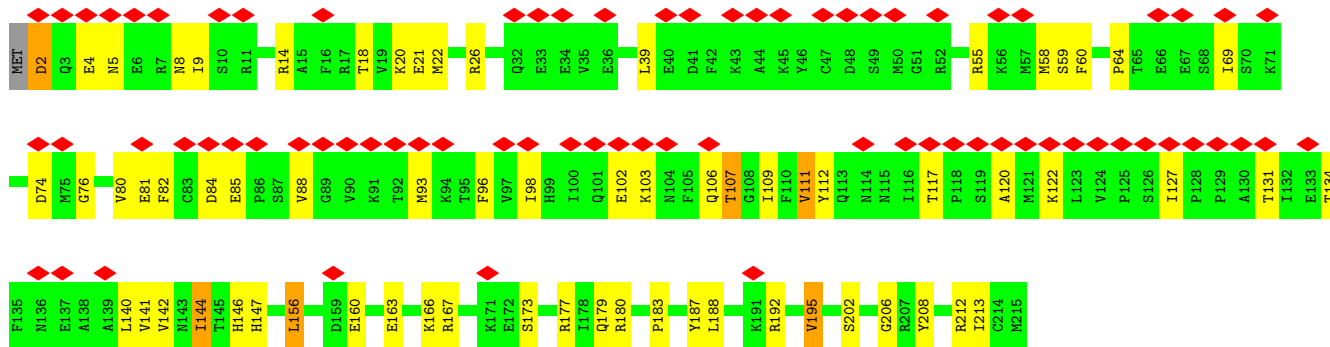




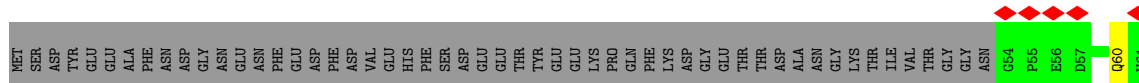
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

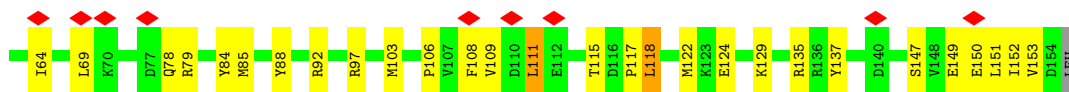


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

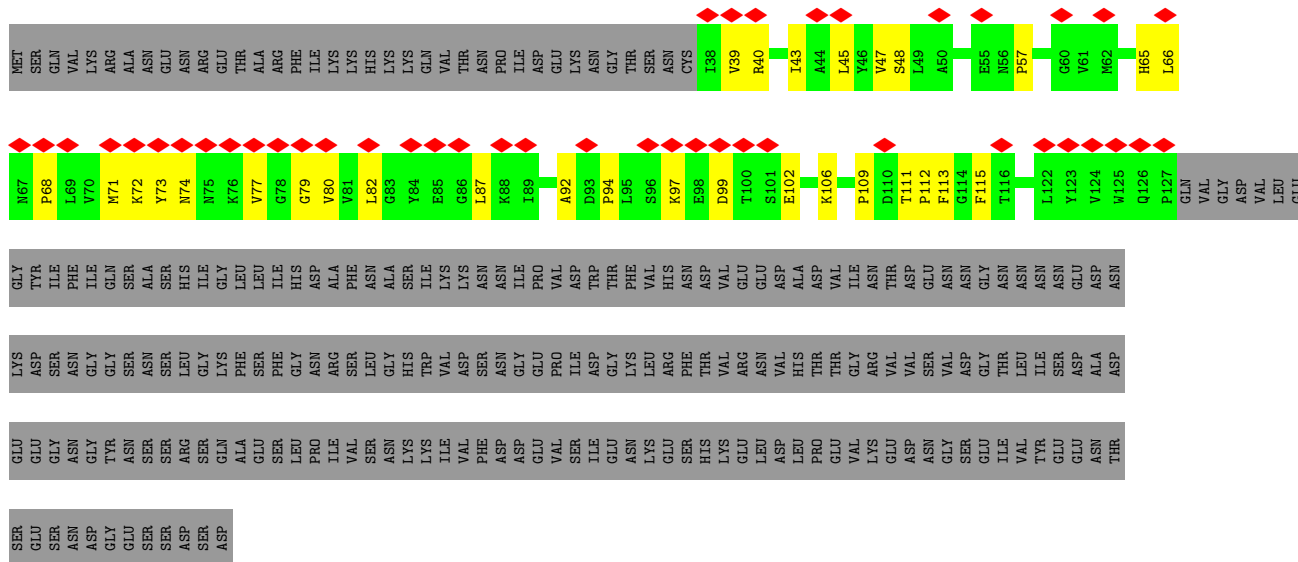


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

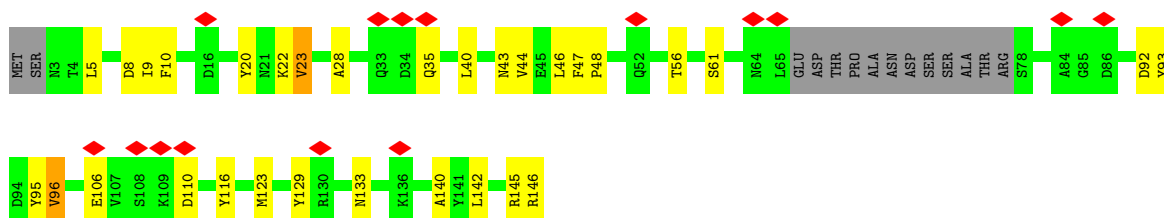




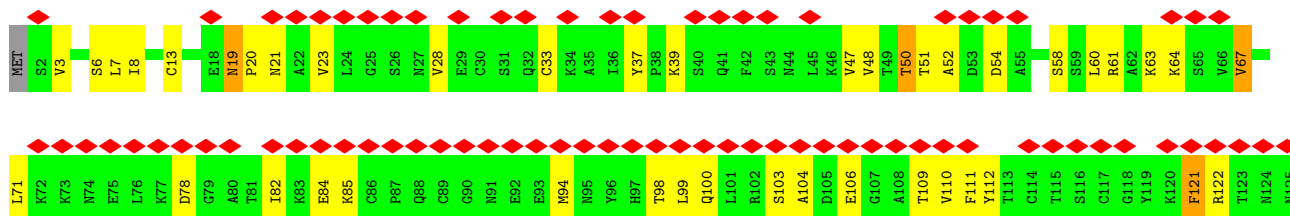
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43



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

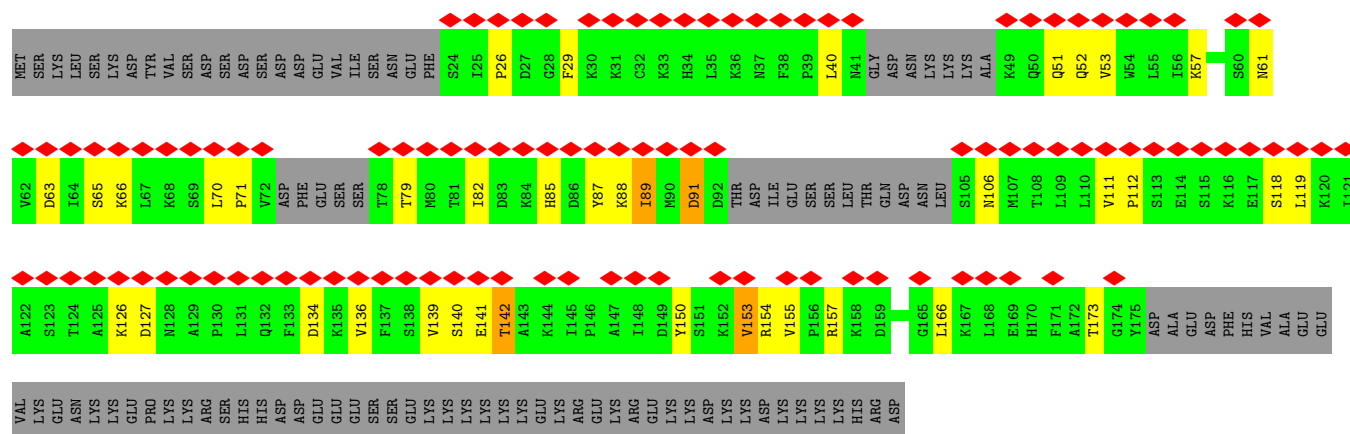


• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



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

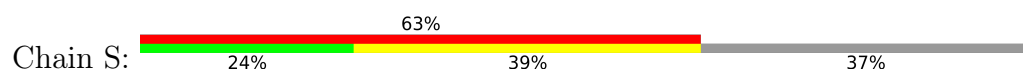




• Molecule 15: RNA



• Molecule 16: Non-template DNA



• Molecule 17: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137196	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	0.150	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0274	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	0.24	0/11773	0.35	0/15900
2	B	0.25	0/9437	0.35	0/12756
3	C	0.24	0/2467	0.31	0/3344
4	D	0.16	0/135	0.27	0/188
5	E	0.19	0/1787	0.32	0/2406
6	F	0.23	0/842	0.32	0/1135
7	G	0.18	0/736	0.31	0/1005
8	H	0.22	0/1078	0.30	0/1460
9	I	0.16	0/955	0.33	0/1288
10	J	0.29	0/578	0.35	0/775
11	K	0.23	0/776	0.31	0/1047
12	L	0.20	0/354	0.33	0/468
13	M	0.14	0/829	0.30	0/1114
14	N	0.15	0/1037	0.28	0/1394
15	R	0.18	0/221	0.28	0/343
16	S	0.20	0/542	0.38	0/831
17	T	0.24	0/706	0.41	0/1084
All	All	0.23	0/34253	0.34	0/46538

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	11563	0	11644	295	0
2	B	9232	0	9123	242	0
3	C	2415	0	2403	58	0
4	D	133	0	138	6	0
5	E	1751	0	1776	41	0
6	F	827	0	843	24	0
7	G	716	0	735	25	0
8	H	1060	0	1032	21	0
9	I	942	0	929	28	0
10	J	569	0	585	14	0
11	K	766	0	765	27	0
12	L	352	0	374	11	0
13	M	814	0	804	23	0
14	N	1018	0	1055	30	0
15	R	197	0	98	3	0
16	S	487	0	274	11	0
17	T	643	0	359	10	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
All	All	33493	0	32937	746	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 11.

All (746) 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:1010:ASN:HB3	2:B:1025:ASP:HB3	1.62	0.81
2:B:71:LYS:HD2	2:B:421:LEU:HB3	1.61	0.81
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.64	0.80
2:B:1135:PHE:HB2	2:B:1167:PHE:HA	1.64	0.79
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.65	0.79
1:A:216:ARG:NH2	1:A:340:HIS:O	2.18	0.77
1:A:380:ASN:HB3	1:A:383:ASN:HD22	1.48	0.77
5:E:144:ILE:HD13	5:E:183:PRO:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.68	0.76
2:B:214:PRO:O	2:B:380:LYS:NZ	2.20	0.74
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.52	0.74
9:I:98:THR:HG22	9:I:110:VAL:HG22	1.66	0.74
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.72	0.72
1:A:703:GLU:O	11:K:52:GLN:NE2	2.22	0.72
2:B:182:GLN:O	10:J:69:ARG:NH1	2.23	0.71
2:B:743:ARG:HH12	3:C:93:GLN:HE22	1.38	0.71
11:K:60:SER:OG	11:K:104:ARG:NH2	2.24	0.71
1:A:1003:ARG:HD2	2:B:520:LEU:HB2	1.73	0.71
17:T:2:DT:H2''	17:T:3:DA:C8	2.26	0.71
2:B:651:ARG:NH1	2:B:669:GLN:OE1	2.24	0.70
10:J:28:ASP:N	10:J:28:ASP:OD1	2.19	0.70
1:A:339:PHE:O	1:A:340:HIS:ND1	2.22	0.70
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.20	0.70
1:A:245:LYS:NZ	1:A:247:GLY:O	2.24	0.70
1:A:1122:PRO:HG3	5:E:208:TYR:HA	1.74	0.70
11:K:67:GLU:OE2	11:K:99:ASN:ND2	2.25	0.69
7:G:111:THR:HG22	7:G:113:PHE:H	1.56	0.69
8:H:92:ASP:HB3	8:H:145:ARG:HH21	1.57	0.69
2:B:878:GLU:OE1	2:B:909:ARG:NH2	2.26	0.69
1:A:1243:TRP:O	1:A:1517:ARG:NH2	2.25	0.69
2:B:129:ARG:NH2	2:B:889:GLY:O	2.26	0.69
2:B:933:THR:OG1	2:B:944:GLN:OE1	2.09	0.69
10:J:7:CYS:HA	10:J:49:MET:HE2	1.74	0.69
1:A:672:ASP:H	2:B:783:MET:HE3	1.56	0.69
1:A:32:ILE:HB	1:A:79:ILE:HG22	1.75	0.68
2:B:1195:ARG:HH22	2:B:1197:ARG:HH11	1.41	0.68
6:F:135:ARG:NH2	7:G:92:ALA:O	2.25	0.68
1:A:130:ILE:HD13	1:A:215:GLU:HG3	1.74	0.68
11:K:64:GLN:OE1	11:K:102:ASN:ND2	2.26	0.68
2:B:764:ASN:OD1	10:J:59:LYS:NZ	2.26	0.68
5:E:177:ARG:NH2	5:E:179:GLN:OE1	2.24	0.68
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.75	0.68
9:I:13:CYS:HB3	9:I:33:CYS:SG	2.34	0.67
1:A:597:LYS:HE2	1:A:660:PRO:HG3	1.77	0.67
1:A:1175:MET:SD	6:F:84:TYR:OH	2.52	0.67
2:B:677:THR:OG1	2:B:680:GLU:OE1	2.12	0.67
1:A:721:LYS:NZ	8:H:93:TYR:O	2.24	0.66
5:E:55:ARG:HD2	5:E:84:ASP:HA	1.78	0.66
16:S:10:DC:H2''	16:S:11:DG:C8	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.76	0.66
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.29	0.66
8:H:48:PRO:O	8:H:146:ARG:NH2	2.26	0.66
13:M:112:LYS:HG2	13:M:113:ILE:HG13	1.78	0.66
1:A:1105:ARG:NH1	1:A:1138:GLU:OE2	2.29	0.65
1:A:949:GLN:NE2	1:A:950:GLN:O	2.27	0.65
1:A:1439:MET:SD	1:A:1461:ASN:ND2	2.69	0.65
14:N:150:TYR:HA	14:N:153:VAL:HG12	1.78	0.65
3:C:229:LEU:HB2	3:C:293:ARG:HH11	1.62	0.65
1:A:238:MET:SD	1:A:264:ASN:ND2	2.70	0.65
2:B:54:GLU:OE2	2:B:169:ARG:NH2	2.29	0.64
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.13	0.64
2:B:1058:GLN:NE2	2:B:1097:ASP:OD2	2.26	0.64
2:B:15:ASP:OD1	2:B:15:ASP:N	2.30	0.64
2:B:215:MET:HE3	2:B:217:ILE:HD11	1.80	0.64
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.80	0.64
1:A:1097:TYR:HA	1:A:1100:LYS:HE2	1.80	0.64
2:B:651:ARG:NH2	2:B:690:GLU:OE2	2.31	0.64
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.80	0.64
1:A:637:PHE:O	1:A:639:GLN:NE2	2.29	0.64
2:B:785:ASP:OD1	2:B:957:ARG:NH2	2.31	0.64
1:A:671:GLN:NE2	2:B:784:ASP:OD1	2.31	0.64
1:A:1183:GLU:OE1	6:F:88:TYR:OH	2.14	0.64
2:B:518:ARG:NH2	2:B:537:SER:O	2.31	0.63
1:A:831:ASP:N	1:A:831:ASP:OD1	2.25	0.63
1:A:1125:ALA:O	5:E:167:ARG:NH2	2.32	0.63
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.79	0.63
13:M:61:GLU:OE2	13:M:106:LYS:NZ	2.31	0.63
1:A:456:VAL:HG12	2:B:1192:MET:HE3	1.80	0.63
1:A:485:SER:HG	1:A:613:THR:HG1	1.46	0.63
2:B:301:PHE:HZ	2:B:385:VAL:HG23	1.64	0.63
2:B:558:VAL:HG13	2:B:561:ILE:HD12	1.79	0.63
13:M:15:VAL:HG11	14:N:65:SER:HA	1.81	0.63
1:A:824:THR:OG1	2:B:1023:ARG:NH1	2.32	0.62
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.82	0.62
2:B:662:ASP:OD1	2:B:663:ILE:N	2.32	0.62
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.31	0.62
2:B:280:LEU:HA	2:B:354:LEU:HD21	1.81	0.62
2:B:1099:THR:HG21	2:B:1180:PHE:HD2	1.65	0.62
7:G:74:ASN:HB3	7:G:77:VAL:HG22	1.82	0.62
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:O	1:A:347:ARG:NH1	2.29	0.61
2:B:533:THR:HG21	2:B:540:GLY:H	1.63	0.61
1:A:1268:ASP:O	9:I:61:ARG:NH2	2.33	0.61
2:B:255:ASP:OD1	2:B:255:ASP:N	2.32	0.61
2:B:361:HIS:NE2	2:B:590:GLY:O	2.25	0.61
5:E:18:THR:HG21	5:E:140:LEU:O	1.99	0.61
11:K:57:ASP:OD1	11:K:57:ASP:N	2.33	0.61
1:A:1296:PHE:HZ	1:A:1317:ILE:HD11	1.64	0.61
9:I:109:THR:HG21	9:I:122:ARG:HE	1.64	0.61
1:A:573:LEU:HD11	4:D:16:LEU:HD22	1.82	0.61
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.65	0.61
1:A:718:THR:OG1	1:A:730:GLN:OE1	2.13	0.61
1:A:579:ARG:NH1	1:A:585:ASP:OD2	2.32	0.61
10:J:45:CYS:O	10:J:48:ARG:NH1	2.34	0.61
1:A:722:PRO:HD2	8:H:46:LEU:HD23	1.83	0.61
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.18	0.61
1:A:1485:MET:H	1:A:1488:ILE:HD13	1.66	0.61
2:B:897:GLU:HG2	12:L:43:THR:HA	1.83	0.60
1:A:54:LEU:HB2	1:A:365:THR:HG23	1.82	0.60
1:A:612:LYS:NZ	2:B:1041:ASN:OD1	2.33	0.60
2:B:71:LYS:HE2	2:B:422:GLN:HG2	1.83	0.60
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	1.82	0.60
2:B:568:LEU:HB3	2:B:604:ILE:HD12	1.84	0.60
1:A:1504:ILE:HD11	1:A:1529:MET:HE1	1.84	0.60
1:A:589:MET:HE3	1:A:633:MET:HE2	1.83	0.60
2:B:492:ASN:HD21	2:B:767:ASN:HD21	1.50	0.60
13:M:9:GLU:HA	14:N:71:PRO:HA	1.82	0.60
1:A:891:ILE:HD12	9:I:71:LEU:HB2	1.84	0.59
2:B:909:ARG:HG3	2:B:1039:MET:HE3	1.84	0.59
1:A:127:TYR:HB3	1:A:202:THR:HG21	1.84	0.59
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.84	0.59
3:C:107:LYS:HG3	3:C:187:ALA:HA	1.85	0.59
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.84	0.59
2:B:436:MET:SD	2:B:436:MET:N	2.75	0.59
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.84	0.59
1:A:23:GLU:OE1	2:B:1130:ARG:NH1	2.35	0.59
1:A:51:ASP:OD1	1:A:52:LEU:N	2.35	0.59
2:B:238:SER:OG	2:B:361:HIS:ND1	2.24	0.59
2:B:242:ASP:OD2	2:B:244:THR:OG1	2.21	0.59
2:B:1014:TYR:OH	3:C:293:ARG:NH1	2.35	0.59
3:C:248:GLN:HG3	3:C:256:ILE:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:PRO:HB3	2:B:871:ILE:HD12	1.84	0.59
2:B:1160:GLU:HG2	2:B:1166:LYS:HB3	1.83	0.59
2:B:673:ASN:ND2	2:B:685:VAL:O	2.30	0.59
1:A:1317:ILE:HD12	1:A:1462:PHE:HE2	1.67	0.59
2:B:492:ASN:HD21	2:B:767:ASN:ND2	2.01	0.59
8:H:8:ASP:OD1	8:H:9:ILE:N	2.35	0.59
13:M:59:ARG:O	13:M:103:LYS:N	2.36	0.59
1:A:1179:ILE:HD11	1:A:1183:GLU:HG2	1.86	0.58
1:A:1193:VAL:HG21	1:A:1585:ILE:HD12	1.85	0.58
1:A:412:SER:HA	1:A:416:ARG:HD3	1.85	0.58
1:A:492:THR:HG22	1:A:667:ARG:HH21	1.67	0.58
2:B:232:TYR:CG	2:B:385:VAL:HG12	2.38	0.58
2:B:1041:ASN:O	2:B:1063:ARG:NH2	2.35	0.58
14:N:88:LYS:HG3	14:N:142:THR:HB	1.84	0.58
1:A:1556:GLU:OE2	5:E:212:ARG:NE	2.33	0.58
2:B:27:ASN:O	2:B:27:ASN:ND2	2.36	0.58
1:A:753:ASN:OD1	1:A:767:ASN:ND2	2.35	0.58
2:B:428:VAL:HG12	2:B:449:VAL:HG21	1.84	0.58
2:B:623:ASP:HB3	2:B:648:ARG:HH22	1.69	0.58
3:C:319:ARG:O	3:C:323:ASN:ND2	2.35	0.58
14:N:63:ASP:OD2	14:N:65:SER:OG	2.22	0.58
15:R:6:U:H2'	15:R:7:C:C6	2.38	0.58
1:A:81:LEU:HD21	1:A:434:VAL:HG21	1.86	0.58
3:C:147:PRO:HG2	3:C:150:SER:HB2	1.85	0.58
14:N:85:HIS:NE2	14:N:141:GLU:OE2	2.37	0.58
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.86	0.57
1:A:86:TYR:N	1:A:431:GLN:OE1	2.34	0.57
2:B:725:THR:OG1	2:B:767:ASN:OD1	2.20	0.57
1:A:1148:LEU:HD21	1:A:1166:PHE:HD2	1.68	0.57
5:E:64:PRO:HB2	5:E:69:ILE:HG12	1.87	0.57
2:B:411:MET:HE3	2:B:476:LEU:HG	1.86	0.57
2:B:698:SER:O	2:B:702:ASN:HB2	2.05	0.57
3:C:163:TYR:OH	10:J:19:GLU:OE2	2.14	0.57
8:H:23:VAL:HA	8:H:43:ASN:HA	1.87	0.57
16:S:32:DT:H2''	16:S:33:DC:C5	2.39	0.57
1:A:399:LEU:HD22	1:A:423:LEU:HD13	1.87	0.57
2:B:101:GLN:HB3	2:B:140:LYS:HD3	1.86	0.57
2:B:324:THR:HG23	2:B:347:LEU:HD13	1.87	0.57
1:A:368:ARG:HB3	1:A:383:ASN:HD21	1.70	0.56
2:B:545:PHE:HE1	2:B:649:MET:HE3	1.69	0.56
1:A:1039:ARG:NH2	1:A:1045:LEU:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1548:ALA:O	1:A:1552:THR:HG22	2.05	0.56
2:B:76:GLY:H	2:B:92:GLY:HA3	1.70	0.56
1:A:1032:VAL:O	1:A:1182:GLY:N	2.36	0.56
3:C:71:MET:HE1	3:C:302:VAL:HG21	1.88	0.56
5:E:4:GLU:OE1	5:E:8:ASN:ND2	2.38	0.56
5:E:112:TYR:HE2	5:E:134:THR:HB	1.71	0.56
13:M:21:VAL:HB	13:M:93:ALA:HB2	1.86	0.56
14:N:88:LYS:NZ	14:N:141:GLU:O	2.34	0.56
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.88	0.56
1:A:654:ASP:OD1	1:A:654:ASP:N	2.37	0.56
8:H:56:THR:HB	8:H:145:ARG:HB3	1.88	0.56
1:A:464:GLU:HA	1:A:469:LYS:HD2	1.87	0.56
1:A:952:LEU:HD23	1:A:957:VAL:HA	1.88	0.56
2:B:70:GLU:HG2	2:B:98:SER:HB3	1.87	0.56
5:E:187:TYR:HD1	5:E:188:LEU:HD22	1.71	0.55
6:F:69:LEU:HG	7:G:94:PRO:HG3	1.87	0.55
1:A:389:VAL:HG22	1:A:433:ASP:HB3	1.88	0.55
2:B:709:PHE:CZ	2:B:992:PRO:HG3	2.42	0.55
6:F:97:ARG:NH2	6:F:106:PRO:O	2.38	0.55
14:N:91:ASP:N	14:N:91:ASP:OD1	2.38	0.55
1:A:1628:ASP:N	1:A:1628:ASP:OD1	2.39	0.55
3:C:287:ASP:N	3:C:287:ASP:OD1	2.39	0.55
5:E:59:SER:OG	5:E:80:VAL:O	2.20	0.55
9:I:19:ASN:OD1	9:I:19:ASN:N	2.37	0.55
1:A:704:ASP:HB2	1:A:706:HIS:CE1	2.41	0.55
1:A:942:GLN:HA	1:A:946:LEU:O	2.08	0.54
2:B:49:PHE:HA	2:B:52:LEU:HD23	1.90	0.54
2:B:751:ILE:HD12	2:B:1030:VAL:HG21	1.89	0.54
1:A:1238:MET:HE3	1:A:1524:VAL:HG23	1.90	0.54
1:A:202:THR:HG22	1:A:203:THR:H	1.73	0.54
2:B:656:LEU:HD22	14:N:153:VAL:HG21	1.90	0.54
3:C:40:PHE:HE2	11:K:131:VAL:HA	1.73	0.54
14:N:71:PRO:HD2	14:N:89:ILE:HD12	1.89	0.54
1:A:592:GLN:OE1	1:A:634:ASN:ND2	2.40	0.54
2:B:848:ILE:HD12	2:B:884:GLU:HA	1.89	0.54
17:T:8:DT:H2'	17:T:9:DA:C8	2.43	0.53
2:B:156:ARG:NH2	2:B:455:GLU:OE1	2.30	0.53
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.43	0.53
1:A:56:ALA:HB3	1:A:69:GLU:HA	1.91	0.53
1:A:703:GLU:HB3	11:K:52:GLN:HE21	1.73	0.53
15:R:5:A:H2'	15:R:6:U:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLN:OE1	1:A:592:GLN:N	2.42	0.53
13:M:13:GLU:HG2	13:M:87:SER:HB2	1.90	0.53
2:B:307:GLU:HB2	9:I:7:LEU:HD11	1.91	0.53
9:I:103:SER:HB3	9:I:106:GLU:HB2	1.92	0.52
1:A:549:MET:HE1	1:A:557:LEU:HD22	1.92	0.52
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.42	0.52
2:B:680:GLU:OE1	2:B:680:GLU:N	2.42	0.52
3:C:55:ASP:OD2	3:C:271:ARG:NH1	2.41	0.52
5:E:107:THR:HG22	5:E:131:THR:HB	1.91	0.52
1:A:1450:ILE:O	1:A:1454:HIS:ND1	2.36	0.52
3:C:248:GLN:NE2	3:C:256:ILE:O	2.42	0.52
7:G:102:GLU:N	7:G:102:GLU:OE1	2.42	0.52
10:J:1:MET:HG2	10:J:57:ILE:HB	1.91	0.52
2:B:773:VAL:HG21	2:B:1031:VAL:HG22	1.91	0.52
1:A:1222:LEU:HD21	1:A:1569:VAL:HG11	1.92	0.52
2:B:860:ALA:HA	2:B:871:ILE:HG22	1.90	0.52
9:I:20:PRO:HB3	9:I:39:LYS:HG2	1.92	0.52
2:B:272:PRO:HD2	2:B:275:MET:HE2	1.91	0.52
5:E:180:ARG:HH11	5:E:192:ARG:HG3	1.74	0.52
1:A:1270:VAL:HG21	1:A:1489:VAL:HG11	1.92	0.52
13:M:10:ILE:N	14:N:70:LEU:O	2.37	0.52
13:M:38:PHE:N	14:N:118:SER:OG	2.43	0.52
1:A:827:THR:HG22	2:B:776:ILE:HA	1.91	0.52
1:A:953:GLU:OE2	2:B:519:LYS:NZ	2.34	0.52
2:B:68:ILE:HD11	2:B:414:LYS:HG2	1.92	0.52
2:B:110:ASN:N	2:B:110:ASN:OD1	2.42	0.52
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.91	0.52
16:S:30:DT:H2"	16:S:31:DA:C8	2.44	0.52
1:A:474:LYS:HD2	2:B:1092:LEU:O	2.10	0.51
1:A:729:LYS:NZ	1:A:766:GLU:OE2	2.40	0.51
2:B:203:ILE:HG12	2:B:485:THR:HG22	1.92	0.51
13:M:70:SER:O	13:M:74:ASN:ND2	2.43	0.51
1:A:1221:ARG:NH2	1:A:1544:ASN:OD1	2.43	0.51
2:B:916:LYS:HG2	2:B:926:VAL:HG12	1.91	0.51
3:C:55:ASP:CG	3:C:271:ARG:HH12	2.18	0.51
1:A:203:THR:HG23	1:A:205:ARG:H	1.75	0.51
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.25	0.51
1:A:1238:MET:O	1:A:1520:VAL:HA	2.10	0.51
1:A:1318:SER:HB3	1:A:1450:ILE:HD11	1.92	0.51
2:B:694:THR:O	2:B:702:ASN:ND2	2.39	0.51
1:A:1039:ARG:HH21	1:A:1045:LEU:HD12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HD23	2:B:354:LEU:HD21	1.92	0.51
2:B:1119:ARG:NH2	2:B:1160:GLU:OE2	2.41	0.51
12:L:40:LEU:HD21	12:L:46:VAL:HG22	1.93	0.51
14:N:52:GLN:HB3	14:N:134:ASP:HB2	1.92	0.51
1:A:52:LEU:HB3	1:A:63:SER:HB3	1.91	0.51
2:B:558:VAL:HG11	2:B:588:ILE:HG21	1.92	0.51
2:B:1116:SER:HB2	2:B:1159:TRP:HB2	1.93	0.51
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.92	0.51
5:E:55:ARG:HA	5:E:58:MET:HG3	1.93	0.51
1:A:824:THR:OG1	1:A:824:THR:O	2.22	0.51
2:B:94:LYS:NZ	2:B:147:ASN:OD1	2.31	0.51
2:B:841:ASP:OD1	2:B:842:GLU:N	2.40	0.51
9:I:23:VAL:HG21	9:I:28:VAL:HG23	1.92	0.51
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.45	0.51
1:A:1657:LEU:HD21	6:F:135:ARG:HB2	1.92	0.51
1:A:110:LEU:HD23	1:A:115:VAL:HG23	1.93	0.51
2:B:575:HIS:NE2	13:M:76:TYR:OH	2.28	0.51
3:C:57:ILE:HD12	3:C:297:HIS:CD2	2.46	0.51
1:A:1000:MET:HG2	2:B:520:LEU:HD22	1.93	0.50
1:A:1254:PHE:HE1	1:A:1532:GLN:HG2	1.76	0.50
1:A:471:MET:HE3	1:A:1642:VAL:HG13	1.93	0.50
2:B:752:VAL:HG11	2:B:965:GLU:HG3	1.93	0.50
2:B:99:VAL:HG23	2:B:421:LEU:HD11	1.92	0.50
2:B:494:TYR:CE1	2:B:762:MET:HE2	2.46	0.50
2:B:683:ASN:HB2	14:N:154:ARG:HH22	1.76	0.50
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.93	0.50
3:C:240:LYS:NZ	3:C:264:GLU:OE2	2.40	0.50
1:A:483:VAL:HG22	1:A:632:GLU:HG2	1.92	0.50
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.93	0.50
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.44	0.50
2:B:175:MET:SD	2:B:183:HIS:ND1	2.80	0.50
2:B:816:ASN:N	2:B:819:ASP:OD1	2.43	0.50
1:A:372:LYS:HG3	1:A:377:VAL:HG22	1.93	0.49
1:A:697:TYR:CE1	1:A:702:PRO:HD2	2.47	0.49
1:A:1654:PHE:HZ	6:F:92:ARG:HB3	1.76	0.49
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.94	0.49
2:B:341:SER:HB2	2:B:344:GLN:HG3	1.94	0.49
2:B:527:PHE:HB3	2:B:649:MET:HE2	1.94	0.49
2:B:600:GLN:O	2:B:604:ILE:HG12	2.11	0.49
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.46	0.49
2:B:94:LYS:HD2	2:B:146:ASN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:623:ASP:HB3	2:B:648:ARG:NH2	2.27	0.49
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.95	0.49
2:B:772:VAL:N	2:B:946:ASP:OD1	2.45	0.49
1:A:1603:MET:HE2	1:A:1612:LYS:HG2	1.95	0.49
2:B:610:TYR:CE1	2:B:658:LEU:HD11	2.46	0.49
1:A:21:ALA:HA	1:A:24:ILE:HD12	1.94	0.49
1:A:99:ARG:HB3	1:A:228:LEU:HD11	1.94	0.49
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.93	0.49
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.94	0.49
1:A:1032:VAL:HG12	1:A:1181:PRO:HA	1.94	0.49
2:B:1082:HIS:HB3	2:B:1084:THR:HG23	1.95	0.49
1:A:1526:PHE:CD2	1:A:1552:THR:HG21	2.48	0.49
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.43	0.49
2:B:975:HIS:HE1	2:B:1003:ALA:HB2	1.76	0.49
1:A:631:ASP:OD1	1:A:631:ASP:N	2.45	0.49
2:B:119:ARG:HH12	2:B:125:GLU:CD	2.21	0.49
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.38	0.49
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.94	0.49
2:B:840:LEU:HD11	2:B:857:PRO:HB2	1.94	0.49
16:S:37:DA:H5'	16:S:37:DA:H8	1.76	0.49
1:A:316:LEU:HB3	1:A:319:GLU:HG3	1.94	0.49
2:B:234:ILE:HG13	2:B:381:LEU:HB2	1.94	0.49
2:B:380:LYS:HG3	2:B:637:TYR:CD2	2.48	0.49
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.47	0.49
11:K:87:GLU:OE2	11:K:106:GLN:NE2	2.46	0.49
1:A:1503:HIS:O	1:A:1523:GLY:HA3	2.13	0.49
2:B:157:ASP:OD1	2:B:157:ASP:N	2.38	0.49
9:I:100:GLN:NE2	9:I:106:GLU:O	2.42	0.49
2:B:140:LYS:HB3	2:B:155:VAL:HG12	1.95	0.48
2:B:175:MET:HB3	2:B:179:GLU:HB2	1.95	0.48
2:B:809:VAL:HG11	2:B:859:CYS:SG	2.52	0.48
3:C:216:HIS:HB2	12:L:70:ARG:NH1	2.28	0.48
1:A:37:VAL:HG23	1:A:38:LEU:H	1.78	0.48
1:A:701:ARG:NE	11:K:92:SER:OG	2.44	0.48
2:B:164:MET:O	2:B:167:SER:OG	2.17	0.48
1:A:498:PRO:HB3	1:A:611:GLU:O	2.12	0.48
15:R:4:A:H2'	15:R:5:A:C8	2.48	0.48
1:A:499:PRO:O	1:A:503:VAL:HG23	2.14	0.48
1:A:609:PRO:HG3	11:K:98:GLU:HG2	1.95	0.48
1:A:1007:ILE:HG21	2:B:515:THR:HG23	1.94	0.48
6:F:118:LEU:O	6:F:122:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	1.95	0.48
1:A:1657:LEU:HD12	7:G:106:LYS:HA	1.96	0.48
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.96	0.48
5:E:117:THR:HG23	5:E:120:ALA:H	1.78	0.48
13:M:80:LEU:HD21	14:N:40:LEU:HB3	1.95	0.48
4:D:22:ILE:HG12	7:G:45:LEU:HD11	1.96	0.48
5:E:202:SER:N	5:E:206:GLY:O	2.46	0.48
11:K:53:ALA:HB1	11:K:104:ARG:HH12	1.78	0.48
1:A:363:PRO:O	1:A:368:ARG:NH1	2.39	0.48
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	2.32	0.48
1:A:855:ARG:HA	1:A:974:THR:HB	1.96	0.48
14:N:82:ILE:HB	14:N:87:TYR:HE2	1.79	0.48
17:T:18:DC:H2'	17:T:19:DT:C6	2.49	0.48
1:A:862:THR:HA	9:I:67:VAL:HG13	1.96	0.48
1:A:1101:THR:O	1:A:1105:ARG:HG3	2.14	0.48
1:A:1306:TYR:O	1:A:1499:ARG:NH2	2.45	0.48
6:F:60:GLN:O	6:F:64:ILE:HG12	2.14	0.48
17:T:6:DG:H2''	17:T:7:DA:N7	2.29	0.48
2:B:512:LEU:HD12	2:B:513:LYS:H	1.79	0.48
2:B:940:GLU:CD	3:C:293:ARG:HH22	2.21	0.48
8:H:35:GLN:N	8:H:35:GLN:OE1	2.46	0.48
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.96	0.47
2:B:610:TYR:HE1	2:B:658:LEU:HD21	1.77	0.47
4:D:28:PRO:HB3	7:G:39:VAL:HG11	1.95	0.47
11:K:51:THR:HA	11:K:54:THR:HG22	1.96	0.47
1:A:94:LEU:HD11	1:A:324:LEU:HD13	1.96	0.47
1:A:692:TYR:OH	1:A:734:THR:OG1	2.19	0.47
2:B:439:ASN:HB3	2:B:442:ASP:HB2	1.96	0.47
1:A:1023:LEU:HD11	1:A:1226:VAL:HG11	1.96	0.47
1:A:1038:ILE:HG12	1:A:1047:GLN:HB2	1.96	0.47
1:A:1651:THR:OG1	6:F:92:ARG:HB2	2.14	0.47
1:A:608:LEU:HD12	1:A:615:ARG:HG3	1.95	0.47
1:A:1003:ARG:NH2	2:B:533:THR:OG1	2.46	0.47
1:A:1238:MET:HE1	1:A:1526:PHE:HA	1.96	0.47
1:A:1310:LYS:NZ	1:A:1464:ASP:O	2.42	0.47
1:A:1655:ASP:OD2	7:G:106:LYS:HE3	2.15	0.47
2:B:906:ARG:NH2	3:C:95:GLU:OE1	2.37	0.47
3:C:136:LEU:HB2	3:C:167:LEU:HD23	1.96	0.47
7:G:97:LYS:HE2	7:G:99:ASP:HB3	1.95	0.47
8:H:92:ASP:HB3	8:H:145:ARG:NH2	2.27	0.47
1:A:36:THR:HB	1:A:45:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.96	0.47
2:B:127:ARG:HH12	2:B:185:GLU:CD	2.23	0.47
2:B:733:LEU:O	2:B:904:LYS:NZ	2.47	0.47
5:E:22:MET:O	5:E:26:ARG:HG3	2.14	0.47
5:E:82:PHE:HA	5:E:111:VAL:HG22	1.97	0.47
2:B:301:PHE:CZ	2:B:385:VAL:HG23	2.49	0.47
3:C:67:PHE:O	3:C:71:MET:HG3	2.14	0.47
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.32	0.47
11:K:69:ASP:N	11:K:69:ASP:OD1	2.48	0.47
2:B:346:ASP:HA	2:B:349:VAL:HG12	1.97	0.47
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.96	0.47
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.96	0.47
8:H:110:ASP:HA	8:H:129:TYR:CD1	2.49	0.47
9:I:52:ALA:C	9:I:54:ASP:H	2.22	0.47
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.48	0.47
1:A:88:PRO:O	1:A:442:LYS:NZ	2.48	0.46
1:A:683:LYS:HB2	8:H:20:TYR:CE1	2.50	0.46
1:A:1240:LEU:HD13	1:A:1529:MET:HG2	1.97	0.46
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.33	0.46
2:B:1195:ARG:NH2	2:B:1197:ARG:HH11	2.09	0.46
5:E:20:LYS:HE3	5:E:60:PHE:CZ	2.49	0.46
1:A:646:GLU:OE2	2:B:1084:THR:HA	2.15	0.46
1:A:1091:VAL:HG23	1:A:1133:LEU:HB3	1.96	0.46
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.50	0.46
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.49	0.46
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.80	0.46
16:S:34:DG:H2''	16:S:35:DG:C8	2.50	0.46
1:A:411:VAL:HG12	1:A:414:GLU:H	1.80	0.46
1:A:412:SER:H	1:A:416:ARG:HB3	1.81	0.46
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.80	0.46
1:A:855:ARG:HH12	1:A:867:ASP:HA	1.81	0.46
1:A:1184:ALA:HB2	1:A:1649:VAL:HG11	1.97	0.46
16:S:27:DG:H2'	16:S:28:DC:C6	2.50	0.46
1:A:585:ASP:O	1:A:605:VAL:HG22	2.15	0.46
1:A:1090:ASP:OD2	1:A:1093:SER:OG	2.28	0.46
2:B:62:ASN:HA	2:B:65:VAL:HG22	1.97	0.46
3:C:107:LYS:NZ	3:C:306:GLY:O	2.47	0.46
1:A:491:GLU:C	1:A:493:ASN:H	2.23	0.46
2:B:623:ASP:O	2:B:648:ARG:NH1	2.47	0.46
2:B:743:ARG:HH12	3:C:93:GLN:NE2	2.09	0.46
9:I:3:VAL:HA	9:I:8:ILE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:TYR:HE1	8:H:46:LEU:HD11	1.81	0.46
2:B:129:ARG:HB2	2:B:131:THR:HG22	1.97	0.46
2:B:568:LEU:O	14:N:140:SER:HB3	2.16	0.46
2:B:626:ILE:N	2:B:668:GLU:OE1	2.49	0.46
3:C:133:VAL:HG21	3:C:172:GLN:NE2	2.30	0.46
5:E:141:VAL:HG23	5:E:142:VAL:HG23	1.98	0.46
14:N:26:PRO:HB2	14:N:29:PHE:CD1	2.51	0.46
2:B:650:LEU:HD22	2:B:663:ILE:HG22	1.98	0.46
1:A:864:LEU:HD12	1:A:864:LEU:HA	1.75	0.46
2:B:909:ARG:HA	2:B:909:ARG:HD3	1.71	0.46
3:C:259:ASP:HB3	3:C:262:SER:O	2.16	0.46
5:E:81:GLU:HB3	5:E:96:PHE:HE1	1.81	0.46
1:A:1307:ASP:HB3	1:A:1499:ARG:HH22	1.81	0.46
1:A:1333:ILE:HD11	1:A:1483:LEU:HD11	1.98	0.46
2:B:108:MET:HB3	2:B:118:GLU:HB2	1.98	0.46
12:L:30:ILE:HG23	12:L:35:SER:HA	1.98	0.46
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.50	0.45
2:B:245:SER:OG	2:B:477:ASP:OD2	2.25	0.45
2:B:564:ILE:HD11	2:B:619:GLY:HA3	1.97	0.45
2:B:1174:THR:HG21	2:B:1200:VAL:HG11	1.98	0.45
5:E:85:GLU:OE1	5:E:85:GLU:N	2.30	0.45
1:A:947:LEU:HD11	1:A:986:PHE:CZ	2.52	0.45
1:A:1605:THR:O	1:A:1605:THR:OG1	2.33	0.45
2:B:819:ASP:HB2	2:B:820:PRO:HD2	1.97	0.45
2:B:1099:THR:OG1	2:B:1178:ILE:O	2.23	0.45
1:A:11:ILE:HD12	1:A:1643:VAL:HG13	1.99	0.45
1:A:916:THR:O	1:A:919:LYS:NZ	2.47	0.45
1:A:1066:PHE:CD1	1:A:1170:MET:HE2	2.51	0.45
2:B:1179:PRO:HB2	2:B:1181:VAL:HG12	1.98	0.45
3:C:145:ASP:OD1	3:C:145:ASP:N	2.49	0.45
4:D:24:ALA:HA	7:G:43:ILE:HD13	1.99	0.45
5:E:14:ARG:O	5:E:18:THR:HG22	2.17	0.45
11:K:60:SER:OG	11:K:106:GLN:HG2	2.16	0.45
1:A:349:LEU:HD12	1:A:349:LEU:H	1.81	0.45
1:A:672:ASP:HB2	2:B:783:MET:HG2	1.96	0.45
1:A:960:MET:SD	2:B:523:GLU:HG3	2.56	0.45
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.51	0.45
2:B:1118:PRO:HB3	2:B:1124:SER:HB2	1.98	0.45
1:A:1233:ILE:HD13	1:A:1236:PRO:HA	1.97	0.45
2:B:1015:SER:HB2	2:B:1022:LEU:HD21	1.99	0.45
1:A:1050:TYR:CE2	1:A:1580:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:934:ILE:HD13	3:C:73:SER:OG	2.16	0.45
2:B:1028:VAL:HG12	2:B:1029:GLY:H	1.82	0.45
1:A:1112:PRO:HG2	1:A:1115:LYS:HB2	1.98	0.45
2:B:815:ARG:HD2	2:B:821:ILE:HA	1.99	0.45
9:I:103:SER:OG	9:I:104:ALA:N	2.50	0.45
1:A:1015:ARG:HH21	2:B:513:LYS:HD3	1.81	0.45
1:A:1237:GLN:O	1:A:1543:SER:OG	2.22	0.45
2:B:73:ILE:HG13	2:B:429:ARG:NH2	2.32	0.45
2:B:345:SER:HB3	2:B:348:GLU:HG2	1.99	0.45
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.99	0.45
8:H:133:ASN:OD1	8:H:133:ASN:N	2.50	0.45
12:L:61:THR:OG1	12:L:62:LYS:N	2.50	0.45
1:A:100:ALA:HB2	1:A:228:LEU:HA	1.99	0.45
1:A:627:ASP:OD1	1:A:627:ASP:N	2.44	0.45
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.46	0.45
2:B:424:ILE:HG22	2:B:453:VAL:HG21	1.99	0.45
3:C:245:ARG:NH1	3:C:263:ASP:OD2	2.48	0.45
9:I:50:THR:OG1	9:I:51:THR:N	2.48	0.45
1:A:509:GLU:HB3	1:A:519:LEU:HD21	1.99	0.45
2:B:107:PRO:O	2:B:171:HIS:HE1	2.00	0.45
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.52	0.45
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.24	0.44
2:B:292:ILE:HD13	2:B:378:ILE:HG21	1.99	0.44
2:B:936:MET:HE1	2:B:948:ILE:HG13	2.00	0.44
8:H:106:GLU:OE1	8:H:106:GLU:N	2.50	0.44
8:H:116:TYR:HE2	8:H:140:ALA:HB3	1.82	0.44
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.52	0.44
16:S:34:DG:C2	17:T:6:DG:C2	3.05	0.44
17:T:18:DC:H2'	17:T:19:DT:H6	1.82	0.44
3:C:308:MET:HB2	3:C:313:ILE:HD11	1.99	0.44
1:A:494:GLU:HG3	1:A:604:LYS:HB2	1.99	0.44
1:A:799:GLU:OE2	1:A:1062:HIS:HB2	2.17	0.44
1:A:1465:GLU:H	1:A:1465:GLU:CD	2.26	0.44
2:B:987:ASN:OD1	14:N:157:ARG:NH2	2.51	0.44
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.70	0.44
6:F:111:LEU:H	6:F:111:LEU:HD22	1.83	0.44
7:G:65:HIS:C	7:G:68:PRO:HD2	2.41	0.44
11:K:66:VAL:HG12	11:K:100:LEU:HD23	1.99	0.44
1:A:368:ARG:HB3	1:A:383:ASN:ND2	2.32	0.44
2:B:1000:LEU:HD23	2:B:1000:LEU:HA	1.77	0.44
9:I:6:SER:O	9:I:6:SER:OG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:VAL:O	1:A:571:HIS:ND1	2.39	0.44
1:A:1441:LYS:HA	1:A:1444:ARG:HB2	1.99	0.44
2:B:712:SER:OG	2:B:713:PRO:HD3	2.18	0.44
3:C:69:ARG:NE	11:K:71:THR:OG1	2.49	0.44
3:C:93:GLN:OE1	3:C:93:GLN:N	2.48	0.44
3:C:154:LYS:HE3	3:C:154:LYS:HB2	1.75	0.44
1:A:730:GLN:HE21	1:A:730:GLN:HB3	1.58	0.44
3:C:40:PHE:CE2	11:K:131:VAL:HA	2.51	0.44
16:S:36:DT:H2"	16:S:37:DA:C8	2.53	0.44
1:A:668:GLY:HA3	1:A:787:GLY:HA2	1.99	0.44
1:A:925:MET:HG3	1:A:940:VAL:HG22	1.99	0.44
2:B:972:GLY:N	2:B:979:GLN:HE22	2.14	0.44
1:A:1527:GLN:OE1	1:A:1527:GLN:N	2.50	0.44
1:A:1599:ASN:OD1	1:A:1602:GLY:N	2.48	0.44
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.91	0.44
2:B:823:GLN:HG3	2:B:863:ASP:HB3	1.99	0.44
2:B:908:ARG:HE	2:B:908:ARG:HB3	1.57	0.44
5:E:112:TYR:CE2	5:E:134:THR:HB	2.51	0.44
14:N:127:ASP:N	14:N:127:ASP:OD1	2.48	0.44
1:A:1241:PRO:HB2	1:A:1537:ASP:HB3	2.00	0.44
1:A:1508:VAL:O	1:A:1510:PRO:HD3	2.18	0.44
2:B:417:ILE:HG22	2:B:457:ILE:HD13	2.00	0.44
9:I:99:LEU:HD12	9:I:111:PHE:CE1	2.53	0.44
1:A:205:ARG:HG2	1:A:345:LEU:HD11	2.00	0.43
1:A:251:ILE:HG13	1:A:315:ILE:HD11	2.00	0.43
1:A:498:PRO:HD3	1:A:614:LEU:HD23	2.00	0.43
2:B:413:LEU:O	2:B:417:ILE:HG23	2.18	0.43
6:F:147:SER:OG	6:F:149:GLU:OE1	2.29	0.43
14:N:57:LYS:O	14:N:139:VAL:HB	2.18	0.43
17:T:4:DC:H2"	17:T:5:DC:H5"	2.00	0.43
1:A:1267:ILE:HD12	1:A:1493:CYS:SG	2.57	0.43
3:C:308:MET:HE1	3:C:316:LYS:HG3	2.00	0.43
5:E:195:VAL:HA	5:E:213:ILE:HA	1.99	0.43
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.51	0.43
1:A:97:TYR:HD1	1:A:97:TYR:HA	1.70	0.43
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.99	0.43
1:A:1450:ILE:HG23	1:A:1454:HIS:CE1	2.53	0.43
2:B:581:PRO:HG3	2:B:637:TYR:CE2	2.53	0.43
3:C:331:CYS:HB3	11:K:47:ILE:HG22	2.01	0.43
12:L:27:LEU:HB3	12:L:37:LYS:HB3	2.00	0.43
13:M:11:GLU:HB2	13:M:86:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:C	1:A:340:HIS:HD1	2.23	0.43
1:A:671:GLN:OE1	1:A:934:LYS:HE2	2.18	0.43
1:A:697:TYR:HB2	11:K:88:PHE:CE1	2.53	0.43
2:B:416:LYS:HD2	2:B:460:LYS:HD3	1.99	0.43
1:A:850:SER:O	1:A:850:SER:OG	2.31	0.43
1:A:1519:LEU:HD12	1:A:1536:ILE:HD11	2.01	0.43
2:B:938:PHE:CZ	2:B:1014:TYR:HB2	2.53	0.43
1:A:107:HIS:CE1	1:A:330:LYS:HB3	2.53	0.43
2:B:924:LYS:HB2	2:B:924:LYS:HE3	1.79	0.43
2:B:1016:GLY:O	3:C:69:ARG:NH1	2.51	0.43
3:C:55:ASP:HB3	3:C:57:ILE:HD11	2.01	0.43
3:C:82:TYR:OH	3:C:125:LYS:NZ	2.44	0.43
1:A:102:CYS:HB2	1:A:109:ARG:HG2	2.01	0.43
1:A:651:ALA:HB2	2:B:1084:THR:HG21	2.01	0.43
2:B:404:LEU:HA	2:B:404:LEU:HD13	1.61	0.43
2:B:612:LYS:HD3	2:B:624:LEU:HB3	2.01	0.43
9:I:112:TYR:N	9:I:121:PHE:O	2.52	0.43
1:A:27:LEU:HA	2:B:1129:ARG:O	2.19	0.43
1:A:100:ALA:HB2	1:A:228:LEU:HD13	2.00	0.43
2:B:706:PHE:HB3	2:B:709:PHE:CD1	2.53	0.43
3:C:322:LYS:NZ	3:C:326:GLU:OE1	2.45	0.43
7:G:48:SER:HB3	7:G:115:PHE:CE2	2.54	0.43
13:M:23:VAL:HB	13:M:95:VAL:HA	2.00	0.43
17:T:13:DA:H2''	17:T:14:DG:C8	2.54	0.43
1:A:375:GLU:OE2	2:B:814:ASN:ND2	2.52	0.43
1:A:387:SER:O	1:A:391:THR:HG23	2.19	0.43
1:A:419:ILE:HD12	1:A:419:ILE:HA	1.82	0.43
1:A:874:GLU:HG3	1:A:878:ARG:HE	1.84	0.43
1:A:939:ASN:ND2	2:B:956:SER:HA	2.33	0.43
1:A:943:ILE:HD13	2:B:960:ILE:HD11	2.01	0.43
2:B:482:SER:OG	2:B:483:GLY:N	2.52	0.43
3:C:301:ASN:ND2	14:N:173:THR:HB	2.34	0.43
8:H:5:LEU:HD11	8:H:61:SER:HB2	2.00	0.43
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.78	0.43
1:A:1609:SER:HA	1:A:1612:LYS:HE2	2.01	0.43
1:A:1655:ASP:CG	6:F:137:TYR:HE2	2.27	0.43
2:B:788:ILE:HB	2:B:948:ILE:HB	2.01	0.43
5:E:5:ASN:O	5:E:9:ILE:HG12	2.19	0.43
13:M:114:LYS:HD2	13:M:114:LYS:N	2.34	0.43
14:N:82:ILE:HB	14:N:87:TYR:CE2	2.54	0.43
16:S:24:DT:H2''	16:S:25:DC:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:TYR:OH	6:F:117:PRO:HG3	2.19	0.42
1:A:1634:LEU:HD23	1:A:1639:ALA:HB1	2.01	0.42
2:B:915:ASP:OD1	2:B:915:ASP:N	2.52	0.42
3:C:233:ILE:HB	3:C:267:VAL:HG21	2.00	0.42
13:M:39:ASP:N	13:M:54:HIS:O	2.44	0.42
13:M:79:GLY:HA2	13:M:89:GLN:O	2.18	0.42
16:S:26:DT:H2'	16:S:27:DG:O4'	2.19	0.42
1:A:660:PRO:O	1:A:1581:HIS:HE1	2.01	0.42
1:A:867:ASP:OD1	1:A:867:ASP:N	2.52	0.42
1:A:904:THR:O	1:A:908:VAL:HG23	2.19	0.42
1:A:1024:THR:O	1:A:1028:GLU:HB3	2.19	0.42
2:B:807:GLU:OE2	2:B:905:TYR:OH	2.36	0.42
2:B:1113:THR:OG1	2:B:1114:GLN:N	2.53	0.42
3:C:70:ILE:HD11	3:C:321:LEU:HD13	2.01	0.42
3:C:172:GLN:O	3:C:175:GLN:HG2	2.18	0.42
4:D:29:GLN:HG2	7:G:40:ARG:HH21	1.84	0.42
13:M:53:LEU:HB2	13:M:96:LEU:HD22	2.01	0.42
1:A:1073:TYR:CZ	1:A:1077:LEU:HD22	2.55	0.42
2:B:74:PHE:HA	2:B:93:ASN:O	2.19	0.42
1:A:618:TYR:HB3	1:A:670:ILE:HD11	2.00	0.42
1:A:697:TYR:HB2	11:K:88:PHE:CZ	2.54	0.42
1:A:1654:PHE:CZ	6:F:92:ARG:HD3	2.54	0.42
2:B:507:SER:O	2:B:511:GLN:HG2	2.20	0.42
2:B:581:PRO:HG3	2:B:637:TYR:CZ	2.54	0.42
7:G:45:LEU:HD12	7:G:45:LEU:HA	1.82	0.42
13:M:11:GLU:N	13:M:11:GLU:OE1	2.52	0.42
2:B:177:PRO:O	2:B:181:VAL:HG23	2.18	0.42
3:C:146:ALA:HB1	3:C:156:LEU:HD23	2.01	0.42
5:E:21:GLU:OE1	5:E:146:HIS:NE2	2.52	0.42
6:F:103:MET:HG3	7:G:112:PRO:HG3	2.02	0.42
7:G:72:LYS:O	7:G:80:VAL:HA	2.20	0.42
14:N:63:ASP:OD2	14:N:66:LYS:HG2	2.19	0.42
1:A:1317:ILE:O	1:A:1322:ILE:HG13	2.20	0.42
2:B:457:ILE:O	2:B:461:MET:HG2	2.20	0.42
2:B:656:LEU:HD23	2:B:656:LEU:HA	1.83	0.42
2:B:898:LEU:HB3	12:L:46:VAL:HG21	2.02	0.42
3:C:70:ILE:HG23	3:C:74:GLU:HB3	2.01	0.42
8:H:22:LYS:O	8:H:44:VAL:HG22	2.19	0.42
14:N:126:LYS:HA	14:N:126:LYS:HD2	1.80	0.42
1:A:334:VAL:O	1:A:338:VAL:HG23	2.20	0.42
1:A:627:ASP:OD2	1:A:629:ASP:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ILE:O	1:A:724:PRO:HA	2.20	0.42
2:B:271:VAL:HG11	2:B:276:ILE:HG13	2.01	0.42
13:M:59:ARG:HA	13:M:103:LYS:HB2	2.01	0.42
1:A:230:ARG:HA	1:A:230:ARG:HD3	1.74	0.42
1:A:492:THR:HG23	1:A:619:ALA:HB3	2.02	0.42
1:A:853:THR:HG21	1:A:903:ILE:HG13	2.01	0.42
1:A:1238:MET:HB3	1:A:1240:LEU:HD21	2.01	0.42
2:B:337:VAL:HG23	2:B:338:PHE:HD1	1.85	0.42
2:B:564:ILE:O	2:B:567:SER:OG	2.31	0.42
2:B:837:LEU:HD13	2:B:837:LEU:HA	1.87	0.42
1:A:634:ASN:OD1	2:B:1069:ILE:HD12	2.20	0.42
1:A:720:PHE:HB2	8:H:96:VAL:HG13	2.01	0.42
1:A:826:PHE:HB3	2:B:777:SER:HB2	2.02	0.42
1:A:1623:THR:HA	1:A:1626:VAL:HG12	2.02	0.42
3:C:324:LYS:HD3	11:K:72:LEU:HB2	2.01	0.42
7:G:73:TYR:CD1	7:G:79:GLY:HA2	2.55	0.42
9:I:84:GLU:HG3	9:I:85:LYS:N	2.35	0.42
11:K:89:CYS:HA	11:K:104:ARG:O	2.20	0.42
2:B:46:ILE:HD11	2:B:192:GLY:N	2.35	0.42
2:B:401:GLU:HB2	2:B:647:SER:O	2.20	0.42
5:E:81:GLU:HB3	5:E:96:PHE:CE1	2.54	0.42
5:E:156:LEU:HG	5:E:160:GLU:HG3	2.02	0.42
6:F:135:ARG:HH22	7:G:92:ALA:C	2.22	0.42
1:A:527:PRO:HG2	1:A:547:ILE:HA	2.02	0.41
1:A:1022:CYS:SG	1:A:1227:MET:HG2	2.60	0.41
1:A:1265:GLU:HA	9:I:58:SER:HB3	2.01	0.41
5:E:102:GLU:OE1	5:E:103:LYS:HG3	2.20	0.41
14:N:106:ASN:OD1	14:N:106:ASN:N	2.50	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.75	0.41
1:A:211:THR:OG1	5:E:173:SER:HB3	2.20	0.41
1:A:977:MET:HE3	1:A:994:GLU:HG3	2.02	0.41
1:A:1541:ILE:C	5:E:147:HIS:HE2	2.28	0.41
2:B:1111:LEU:H	2:B:1111:LEU:HD23	1.85	0.41
11:K:45:GLU:OE1	11:K:45:GLU:N	2.52	0.41
16:S:26:DT:H5''	16:S:26:DT:H6	1.85	0.41
17:T:4:DC:H4'	17:T:5:DC:OP1	2.19	0.41
1:A:1008:ASP:HB3	1:A:1202:LEU:HD12	2.02	0.41
1:A:1017:GLY:O	1:A:1018:TYR:HB3	2.19	0.41
1:A:1017:GLY:C	1:A:1019:LEU:H	2.29	0.41
1:A:1589:MET:O	1:A:1596:LEU:HB2	2.21	0.41
1:A:1646:LEU:HD22	7:G:109:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:LYS:HA	3:C:263:ASP:O	2.19	0.41
10:J:49:MET:HE3	10:J:49:MET:HB3	1.92	0.41
1:A:85:CYS:HB3	1:A:431:GLN:NE2	2.36	0.41
1:A:93:GLN:HG2	1:A:1627:LEU:HD13	2.02	0.41
2:B:490:LYS:HD2	2:B:490:LYS:HA	1.95	0.41
2:B:788:ILE:CG2	2:B:931:TRP:HB2	2.50	0.41
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.55	0.41
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.55	0.41
9:I:82:ILE:HG23	9:I:84:GLU:H	1.85	0.41
2:B:98:SER:O	2:B:142:LYS:N	2.54	0.41
2:B:200:GLU:OE2	2:B:736:ARG:NH2	2.53	0.41
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.73	0.41
6:F:109:VAL:HG13	6:F:124:GLU:HG2	2.03	0.41
9:I:82:ILE:HG22	9:I:94:MET:O	2.21	0.41
10:J:10:CYS:SG	10:J:11:GLY:N	2.93	0.41
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.40	0.41
2:B:26:ILE:O	10:J:62:ARG:NH1	2.54	0.41
6:F:108:PHE:HB2	6:F:129:LYS:HB3	2.03	0.41
7:G:66:LEU:HD11	7:G:87:LEU:HD13	2.01	0.41
17:T:4:DC:OP2	17:T:4:DC:H3'	2.20	0.41
1:A:897:SER:O	1:A:901:ASN:ND2	2.54	0.41
1:A:1194:GLY:O	1:A:1197:SER:OG	2.22	0.41
1:A:1559:ARG:NE	1:A:1587:ASP:OD1	2.53	0.41
2:B:843:ASP:HB3	12:L:28:LYS:HZ1	1.86	0.41
5:E:39:LEU:HD12	5:E:39:LEU:HA	1.87	0.41
9:I:28:VAL:HG12	9:I:37:TYR:HB2	2.02	0.41
1:A:470:HIS:ND1	2:B:1056:THR:HG21	2.36	0.41
1:A:799:GLU:CD	1:A:1062:HIS:HB2	2.46	0.41
1:A:1092:GLU:O	1:A:1096:LYS:HG3	2.20	0.41
1:A:591:ARG:HD2	1:A:626:ALA:HB2	2.03	0.41
1:A:726:TRP:HE3	1:A:726:TRP:H	1.69	0.41
1:A:947:LEU:HD11	1:A:986:PHE:CE2	2.56	0.41
1:A:986:PHE:CD2	2:B:958:MET:HE2	2.56	0.41
1:A:1006:LEU:O	1:A:1009:THR:HG22	2.21	0.41
1:A:1247:SER:HB2	1:A:1250:GLN:HG3	2.03	0.41
1:A:1465:GLU:OE1	1:A:1465:GLU:N	2.50	0.41
2:B:953:ALA:O	2:B:957:ARG:HD3	2.21	0.41
9:I:60:LEU:O	9:I:64:LYS:N	2.54	0.41
11:K:105:ILE:HB	11:K:113:ALA:HB1	2.02	0.41
14:N:66:LYS:HE2	14:N:66:LYS:HB3	1.88	0.41
14:N:112:PRO:HA	14:N:119:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD22	1:A:397:ARG:HE	1.86	0.41
1:A:1305:GLU:OE2	9:I:63:LYS:NZ	2.48	0.41
1:A:1640:ARG:HH11	1:A:1645:LYS:HE3	1.85	0.41
2:B:865:THR:HG22	2:B:866:LEU:HD22	2.03	0.41
5:E:93:MET:HE3	5:E:93:MET:HB3	1.93	0.41
7:G:102:GLU:H	7:G:102:GLU:CD	2.29	0.41
1:A:347:ARG:HA	1:A:347:ARG:HD2	1.92	0.40
1:A:924:SER:O	1:A:928:MET:HG2	2.21	0.40
1:A:942:GLN:OE1	2:B:958:MET:HE1	2.21	0.40
3:C:109:ASP:HB3	3:C:112:MET:HE3	2.03	0.40
14:N:61:ASN:O	14:N:87:TYR:OH	2.35	0.40
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	2.01	0.40
1:A:1162:ASN:OD1	1:A:1162:ASN:N	2.52	0.40
1:A:1276:THR:O	9:I:21:ASN:ND2	2.54	0.40
2:B:492:ASN:OD1	2:B:494:TYR:HB2	2.21	0.40
5:E:93:MET:HG3	5:E:120:ALA:HA	2.04	0.40
1:A:228:LEU:HA	1:A:228:LEU:HD13	1.91	0.40
1:A:514:TYR:HD2	6:F:115:THR:HA	1.86	0.40
1:A:672:ASP:HA	2:B:952:HIS:CE1	2.55	0.40
1:A:703:GLU:HG2	11:K:50:LEU:HD12	2.03	0.40
2:B:12:ARG:NH1	10:J:32:GLU:OE1	2.50	0.40
2:B:301:PHE:O	2:B:305:ARG:HG2	2.22	0.40
2:B:560:ARG:O	2:B:564:ILE:HG13	2.22	0.40
2:B:675:ALA:HB2	2:B:686:HIS:ND1	2.36	0.40
3:C:97:LEU:HD21	3:C:202:ILE:HD13	2.02	0.40
1:A:440:SER:OG	1:A:455:GLY:N	2.54	0.40
2:B:381:LEU:O	2:B:385:VAL:HG13	2.21	0.40
2:B:657:PRO:C	2:B:659:ASP:H	2.28	0.40
2:B:974:LEU:HD23	10:J:44:TYR:HB3	2.03	0.40
3:C:61:THR:HG22	3:C:298:PHE:CZ	2.56	0.40
3:C:216:HIS:HB2	12:L:70:ARG:HH12	1.87	0.40
4:D:22:ILE:HG12	7:G:45:LEU:CD1	2.52	0.40
5:E:2:ASP:N	5:E:2:ASP:OD1	2.53	0.40
5:E:163:GLU:HA	5:E:166:LYS:HE2	2.03	0.40
13:M:111:PRO:HG2	13:M:114:LYS:HE3	2.03	0.40
1:A:992:PRO:HB2	2:B:676:VAL:HG21	2.04	0.40
1:A:1053:ASP:OD1	1:A:1055:ILE:HG12	2.21	0.40
1:A:1115:LYS:HB2	1:A:1115:LYS:HE2	1.96	0.40
2:B:491:ILE:HG23	2:B:742:TYR:HD2	1.87	0.40
3:C:97:LEU:HD12	3:C:97:LEU:HA	1.87	0.40
11:K:49:LEU:HD11	11:K:61:ALA:HB1	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	1448/1664 (87%)	1361 (94%)	87 (6%)	0	100	100
2	B	1153/1203 (96%)	1074 (93%)	79 (7%)	0	100	100
3	C	302/335 (90%)	288 (95%)	14 (5%)	0	100	100
4	D	16/137 (12%)	15 (94%)	1 (6%)	0	100	100
5	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	F	99/155 (64%)	94 (95%)	5 (5%)	0	100	100
7	G	88/326 (27%)	80 (91%)	8 (9%)	0	100	100
8	H	128/146 (88%)	123 (96%)	5 (4%)	0	100	100
9	I	122/125 (98%)	109 (89%)	13 (11%)	0	100	100
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
12	L	42/70 (60%)	40 (95%)	2 (5%)	0	100	100
13	M	99/415 (24%)	93 (94%)	6 (6%)	0	100	100
14	N	120/233 (52%)	110 (92%)	10 (8%)	0	100	100
All	All	3992/5236 (76%)	3751 (94%)	241 (6%)	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	1293/1465 (88%)	1234 (95%)	59 (5%)	23	52
2	B	1015/1053 (96%)	973 (96%)	42 (4%)	26	54
3	C	268/296 (90%)	262 (98%)	6 (2%)	47	69
4	D	16/116 (14%)	16 (100%)	0	100	100
5	E	196/197 (100%)	185 (94%)	11 (6%)	17	45
6	F	90/137 (66%)	85 (94%)	5 (6%)	17	45
7	G	81/291 (28%)	79 (98%)	2 (2%)	42	67
8	H	116/128 (91%)	113 (97%)	3 (3%)	41	66
9	I	109/110 (99%)	103 (94%)	6 (6%)	18	45
10	J	64/65 (98%)	61 (95%)	3 (5%)	22	51
11	K	88/130 (68%)	84 (96%)	4 (4%)	23	52
12	L	39/57 (68%)	37 (95%)	2 (5%)	20	48
13	M	93/371 (25%)	87 (94%)	6 (6%)	14	40
14	N	119/220 (54%)	108 (91%)	11 (9%)	7	26
All	All	3587/4636 (77%)	3427 (96%)	160 (4%)	26	52

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	69	GLU
1	A	83	VAL
1	A	97	TYR
1	A	129	LEU
1	A	130	ILE
1	A	202	THR
1	A	238	MET
1	A	250	LYS
1	A	315	ILE
1	A	349	LEU
1	A	360	LEU
1	A	361	VAL
1	A	407	GLN
1	A	453	ILE
1	A	471	MET
1	A	485	SER
1	A	512	THR
1	A	557	LEU

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Mol	Chain	Res	Type
1	A	568	VAL
1	A	577	VAL
1	A	587	VAL
1	A	631	ASP
1	A	654	ASP
1	A	658	LEU
1	A	670	ILE
1	A	703	GLU
1	A	707	THR
1	A	723	TYR
1	A	731	ILE
1	A	813	LEU
1	A	822	THR
1	A	824	THR
1	A	831	ASP
1	A	864	LEU
1	A	867	ASP
1	A	947	LEU
1	A	968	SER
1	A	1040	ASP
1	A	1053	ASP
1	A	1057	ILE
1	A	1065	GLN
1	A	1086	ILE
1	A	1201	THR
1	A	1215	VAL
1	A	1226	VAL
1	A	1233	ILE
1	A	1261	VAL
1	A	1270	VAL
1	A	1290	TYR
1	A	1311	GLU
1	A	1453	HIS
1	A	1524	VAL
1	A	1563	VAL
1	A	1569	VAL
1	A	1585	ILE
1	A	1605	THR
1	A	1628	ASP
1	A	1657	LEU
2	B	15	ASP
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	72	VAL
2	B	104	ILE
2	B	110	ASN
2	B	157	ASP
2	B	190	ILE
2	B	234	ILE
2	B	255	ASP
2	B	273	VAL
2	B	297	VAL
2	B	362	LEU
2	B	389	CYS
2	B	402	VAL
2	B	404	LEU
2	B	418	ASP
2	B	425	ILE
2	B	503	VAL
2	B	515	THR
2	B	558	VAL
2	B	653	VAL
2	B	670	VAL
2	B	700	LEU
2	B	703	LEU
2	B	739	ASN
2	B	746	THR
2	B	752	VAL
2	B	767	ASN
2	B	777	SER
2	B	789	ILE
2	B	946	ASP
2	B	1028	VAL
2	B	1030	VAL
2	B	1031	VAL
2	B	1033	TYR
2	B	1055	LEU
2	B	1060	VAL
2	B	1074	MET
2	B	1112	THR
2	B	1113	THR
2	B	1125	THR
2	B	1158	ILE
3	C	127	THR
3	C	141	THR

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Mol	Chain	Res	Type
3	C	145	ASP
3	C	223	SER
3	C	279	VAL
3	C	287	ASP
5	E	2	ASP
5	E	74	ASP
5	E	88	VAL
5	E	98	ILE
5	E	107	THR
5	E	111	VAL
5	E	122	LYS
5	E	127	ILE
5	E	144	ILE
5	E	156	LEU
5	E	195	VAL
6	F	78	GLN
6	F	111	LEU
6	F	118	LEU
6	F	152	ILE
6	F	153	VAL
7	G	71	MET
7	G	82	LEU
8	H	23	VAL
8	H	96	VAL
8	H	142	LEU
9	I	19	ASN
9	I	47	VAL
9	I	50	THR
9	I	67	VAL
9	I	78	ASP
9	I	121	PHE
10	J	28	ASP
10	J	31	ASP
10	J	54	VAL
11	K	57	ASP
11	K	65	ILE
11	K	87	GLU
11	K	93	ILE
12	L	30	ILE
12	L	61	THR
13	M	20	SER
13	M	40	LEU

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Mol	Chain	Res	Type
13	M	77	VAL
13	M	88	ILE
13	M	89	GLN
13	M	101	VAL
14	N	51	GLN
14	N	53	VAL
14	N	79	THR
14	N	89	ILE
14	N	91	ASP
14	N	111	VAL
14	N	136	VAL
14	N	142	THR
14	N	153	VAL
14	N	155	VAL
14	N	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	322	ASN
1	A	336	GLN
1	A	383	ASN
1	A	384	GLN
1	A	553	GLN
1	A	656	GLN
1	A	785	GLN
1	A	901	ASN
1	A	926	GLN
1	A	949	GLN
1	A	1020	GLN
1	A	1081	ASN
1	A	1108	HIS
1	A	1443	GLN
2	B	209	GLN
2	B	235	GLN
2	B	254	ASN
2	B	427	GLN
2	B	492	ASN
2	B	499	HIS
2	B	899	GLN
2	B	975	HIS

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Mol	Chain	Res	Type
2	B	1066	HIS
3	C	232	GLN
3	C	234	ASN
6	F	59	GLN
8	H	11	GLN
9	I	21	ASN
11	K	52	GLN
11	K	102	ASN
13	M	57	ASN
14	N	51	GLN

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	0.57	0	9,14,17	0.47	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	-	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
17	T	17	3DR	O4'-C4'-C5'-O5'

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 8 ligands modelled in this entry, 8 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 ⓘ

There are no chain breaks in this entry.

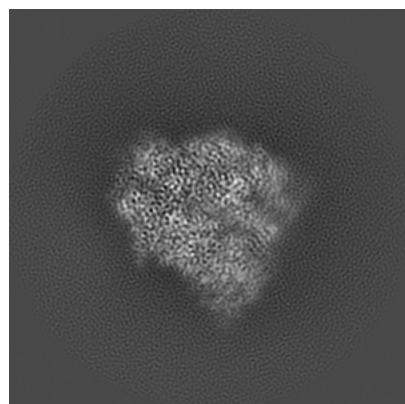
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50970. These allow visual inspection of the internal detail of the map and identification of artifacts.

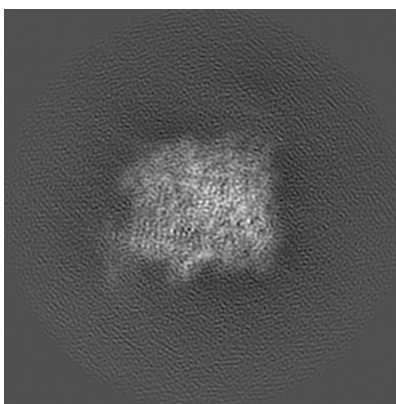
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

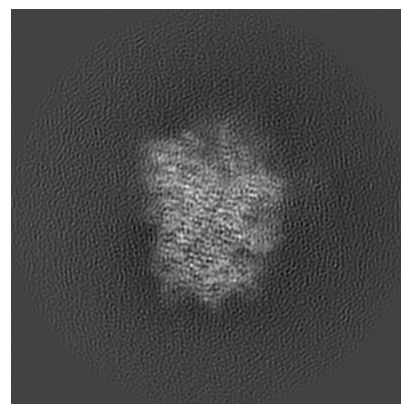
6.1.1 Primary map



X

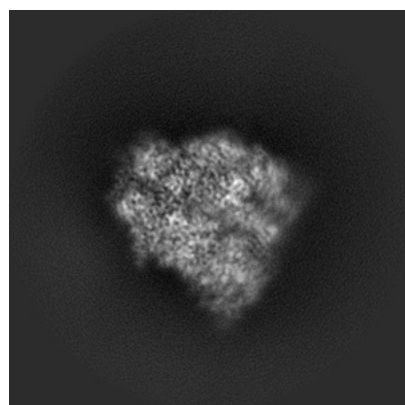


Y

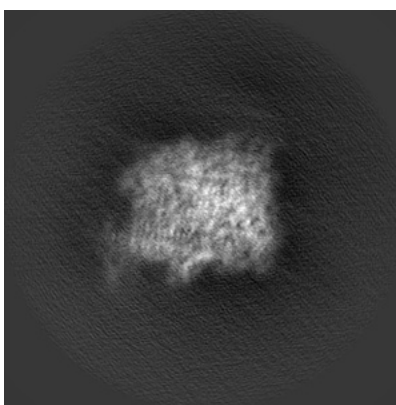


Z

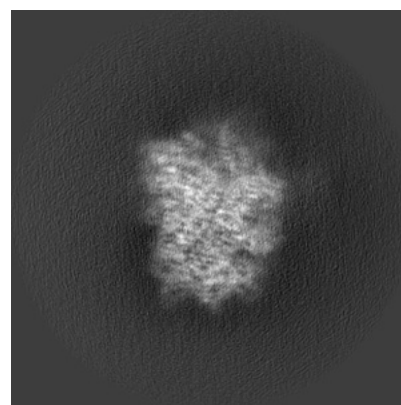
6.1.2 Raw map



X



Y

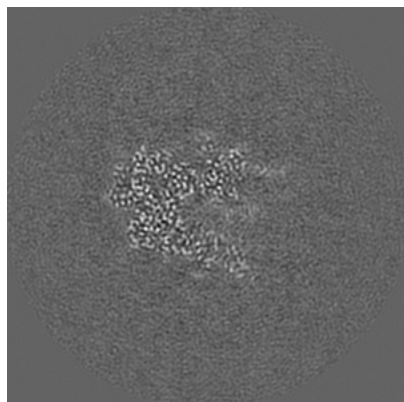


Z

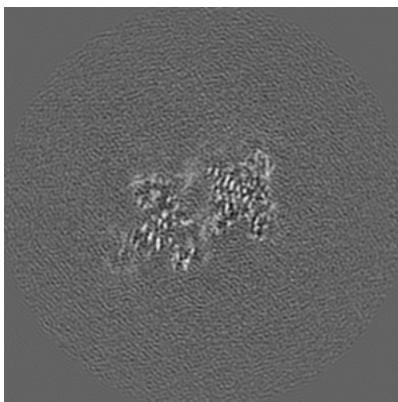
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

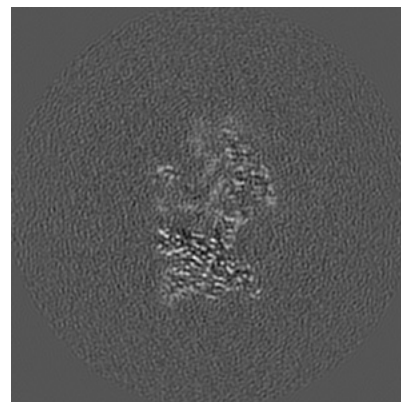
6.2.1 Primary map



X Index: 144

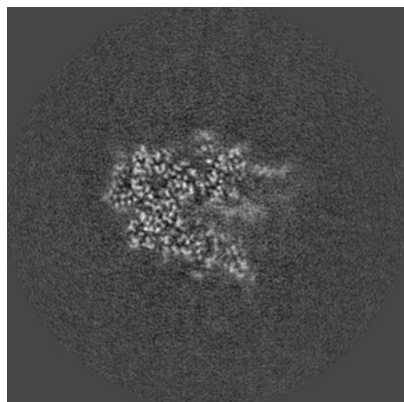


Y Index: 144

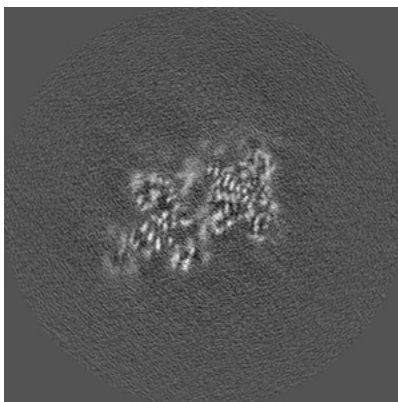


Z Index: 144

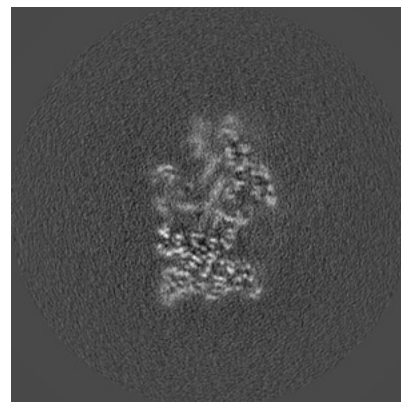
6.2.2 Raw map



X Index: 144



Y Index: 144

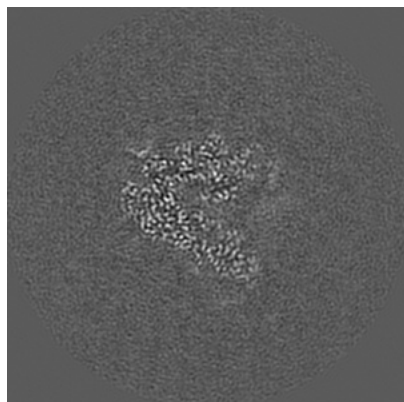


Z Index: 144

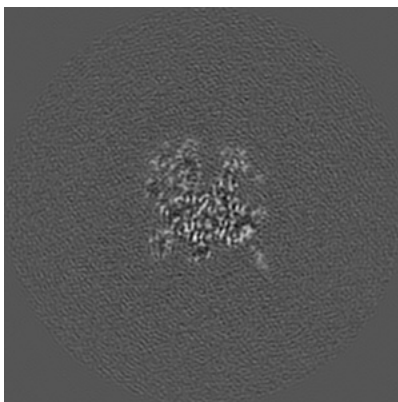
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

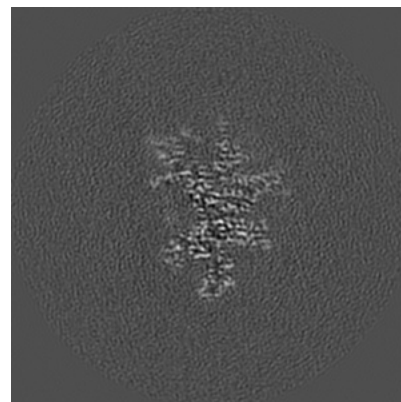
6.3.1 Primary map



X Index: 134

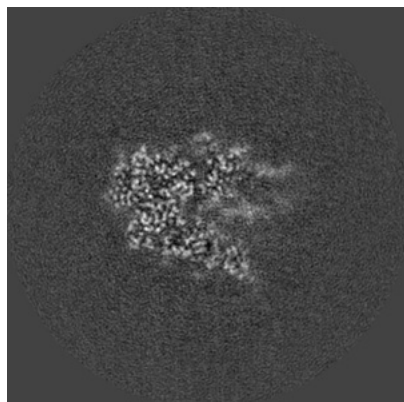


Y Index: 120

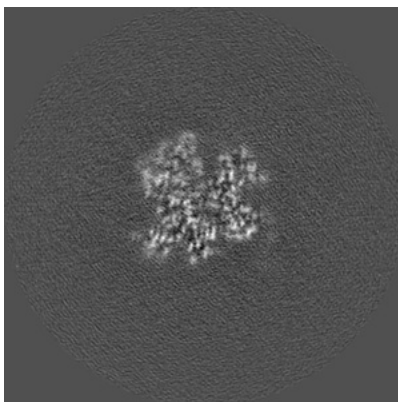


Z Index: 163

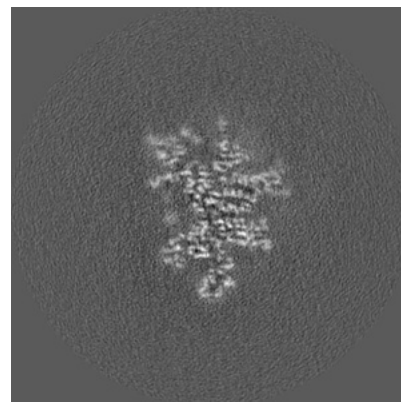
6.3.2 Raw map



X Index: 143



Y Index: 124

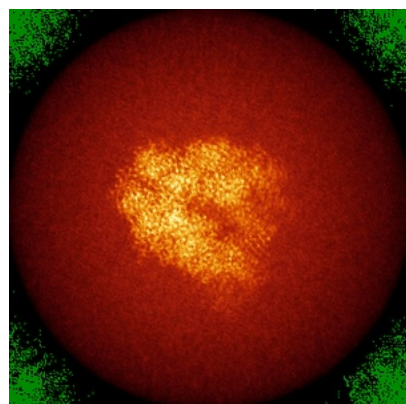


Z Index: 163

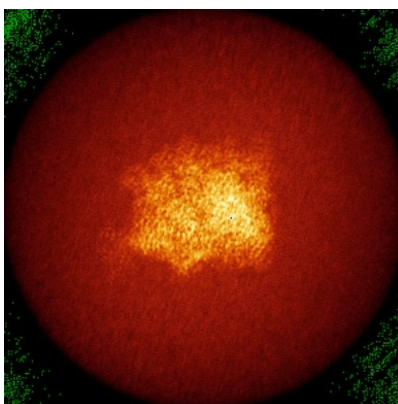
The images above show the largest variance slices of the map in three orthogonal directions.

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

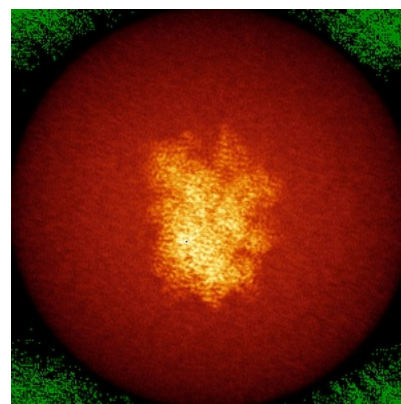
6.4.1 Primary map



X

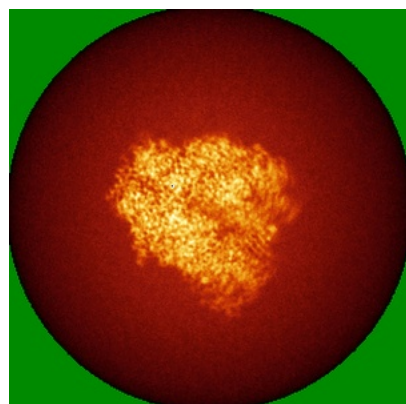


Y

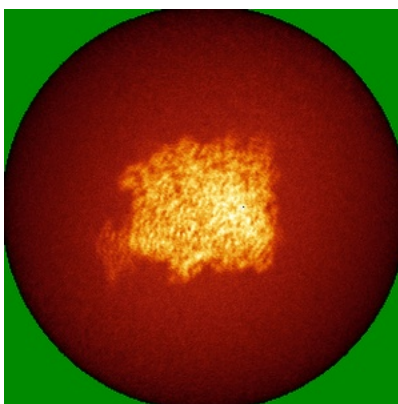


Z

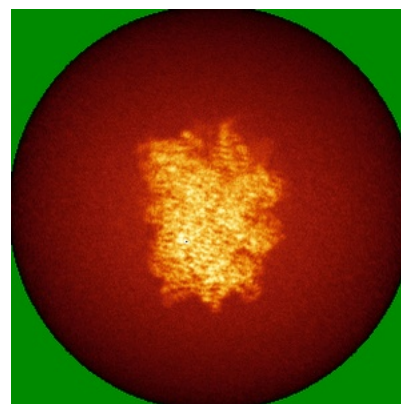
6.4.2 Raw map



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



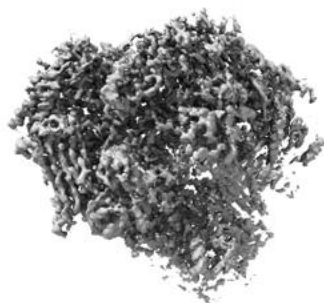
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

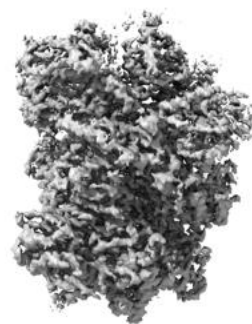
6.5.2 Raw map



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.

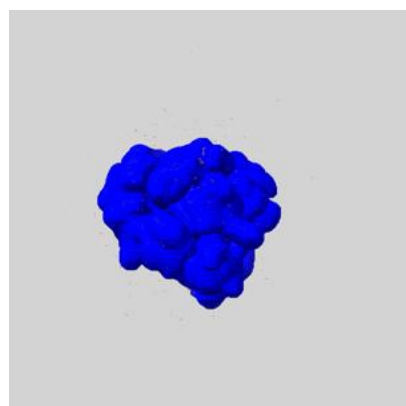
6.6 Mask visualisation [i](#)

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

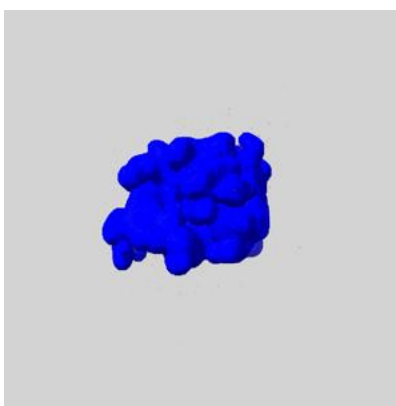
A mask typically either:

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

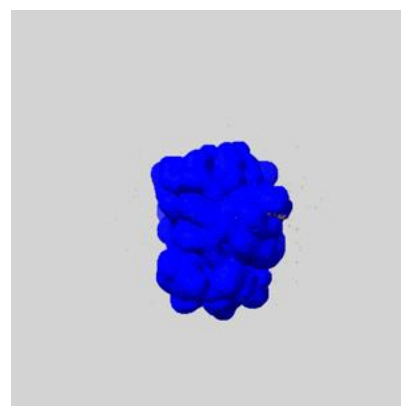
6.6.1 emd_50970_msk_1.map [i](#)



X

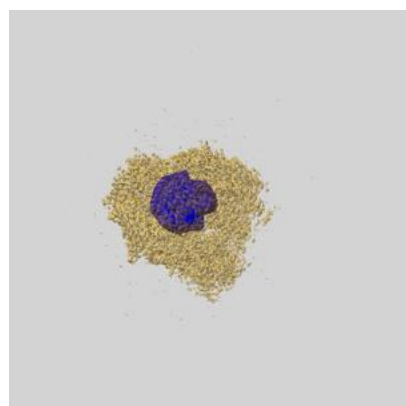


Y

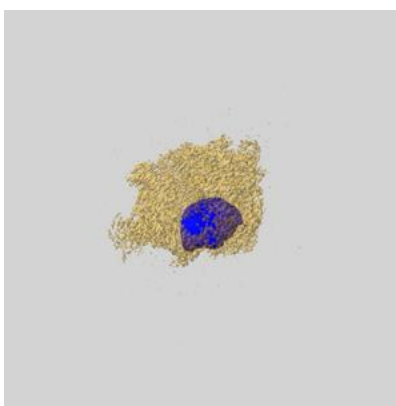


Z

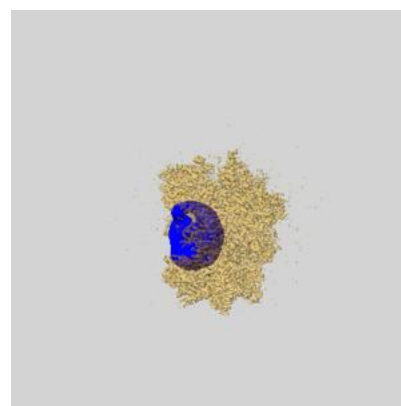
6.6.2 emd_50970_msk_2.map [i](#)



X



Y

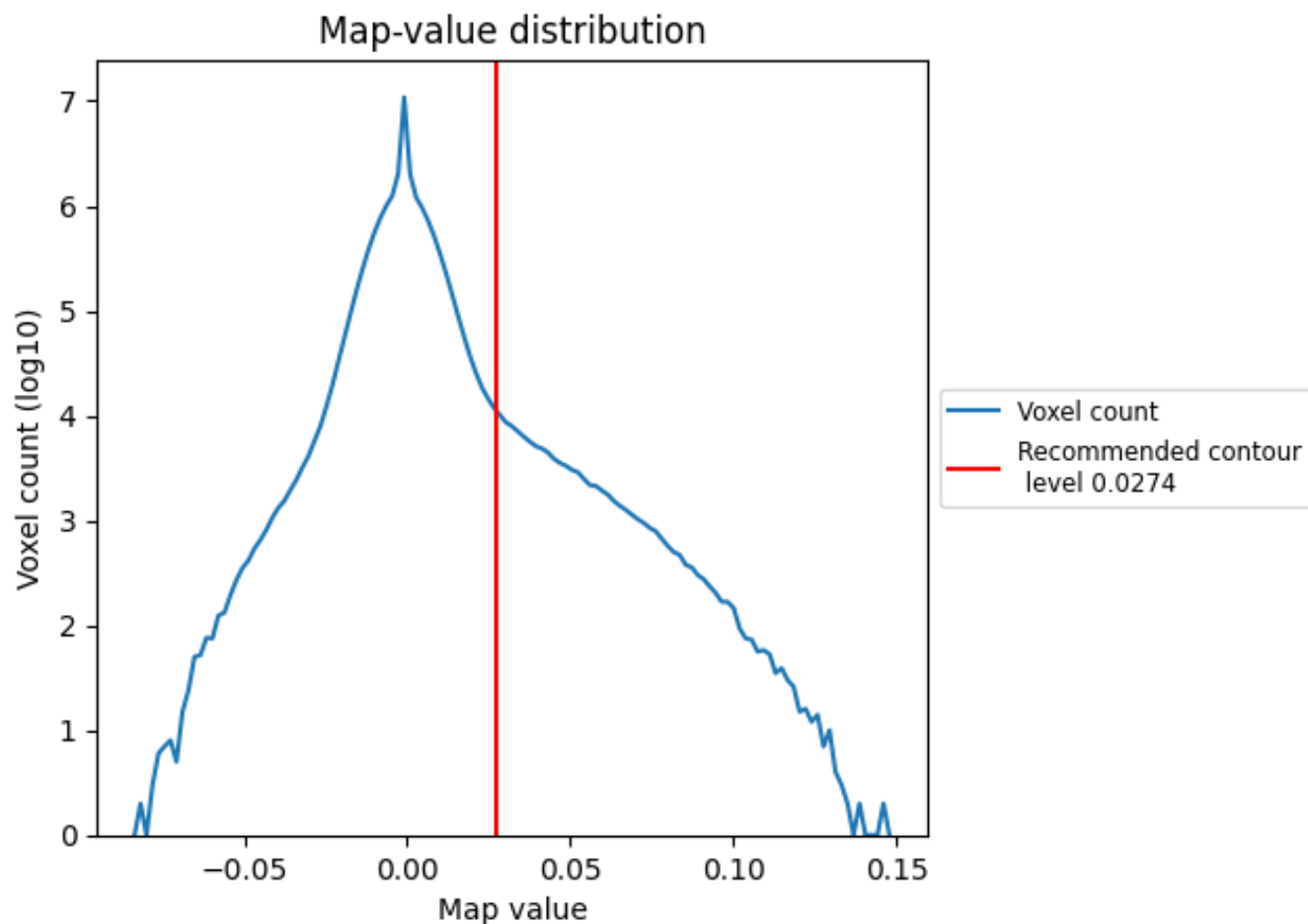


Z

7 Map analysis [i](#)

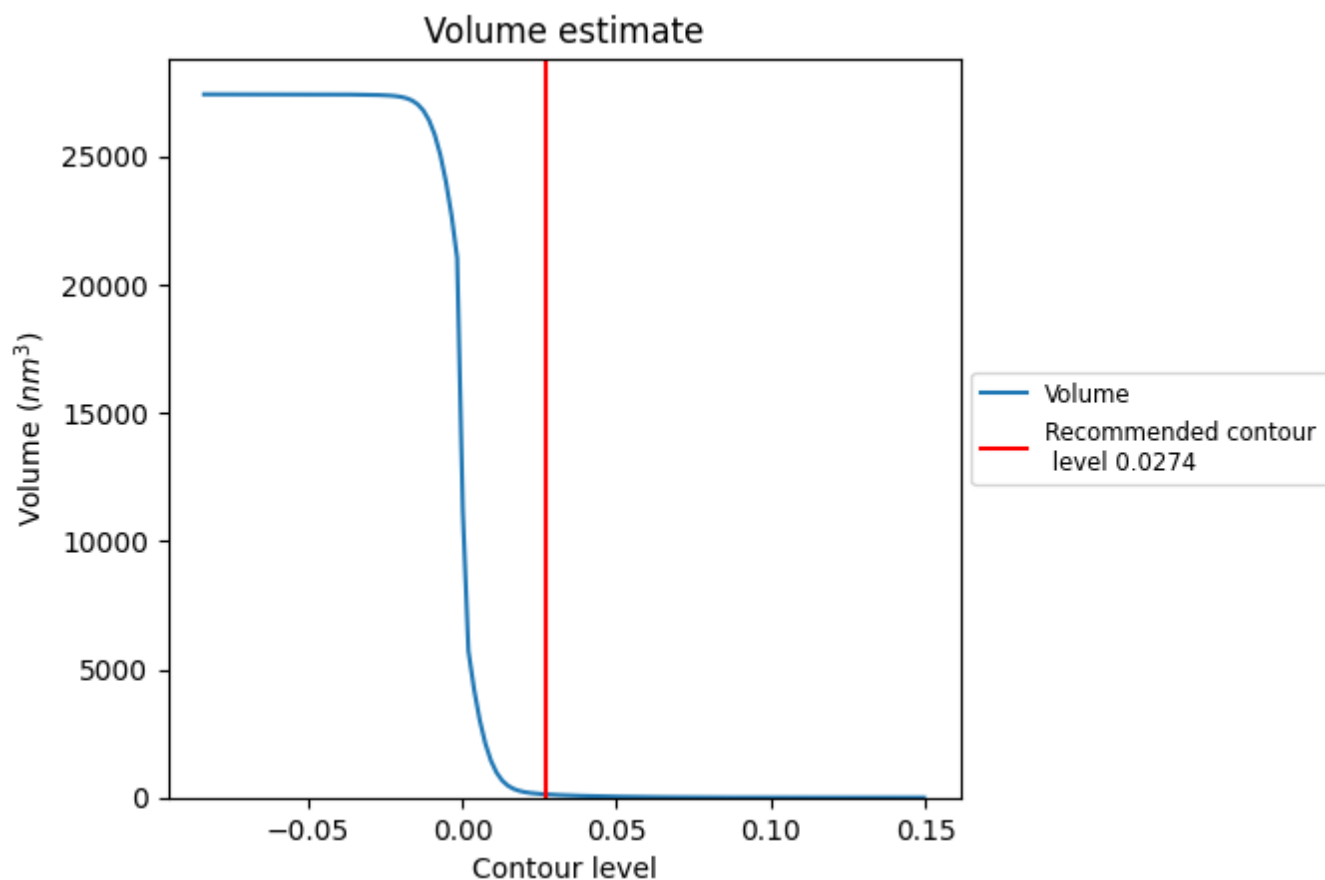
This section contains the results of statistical analysis of the map.

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.

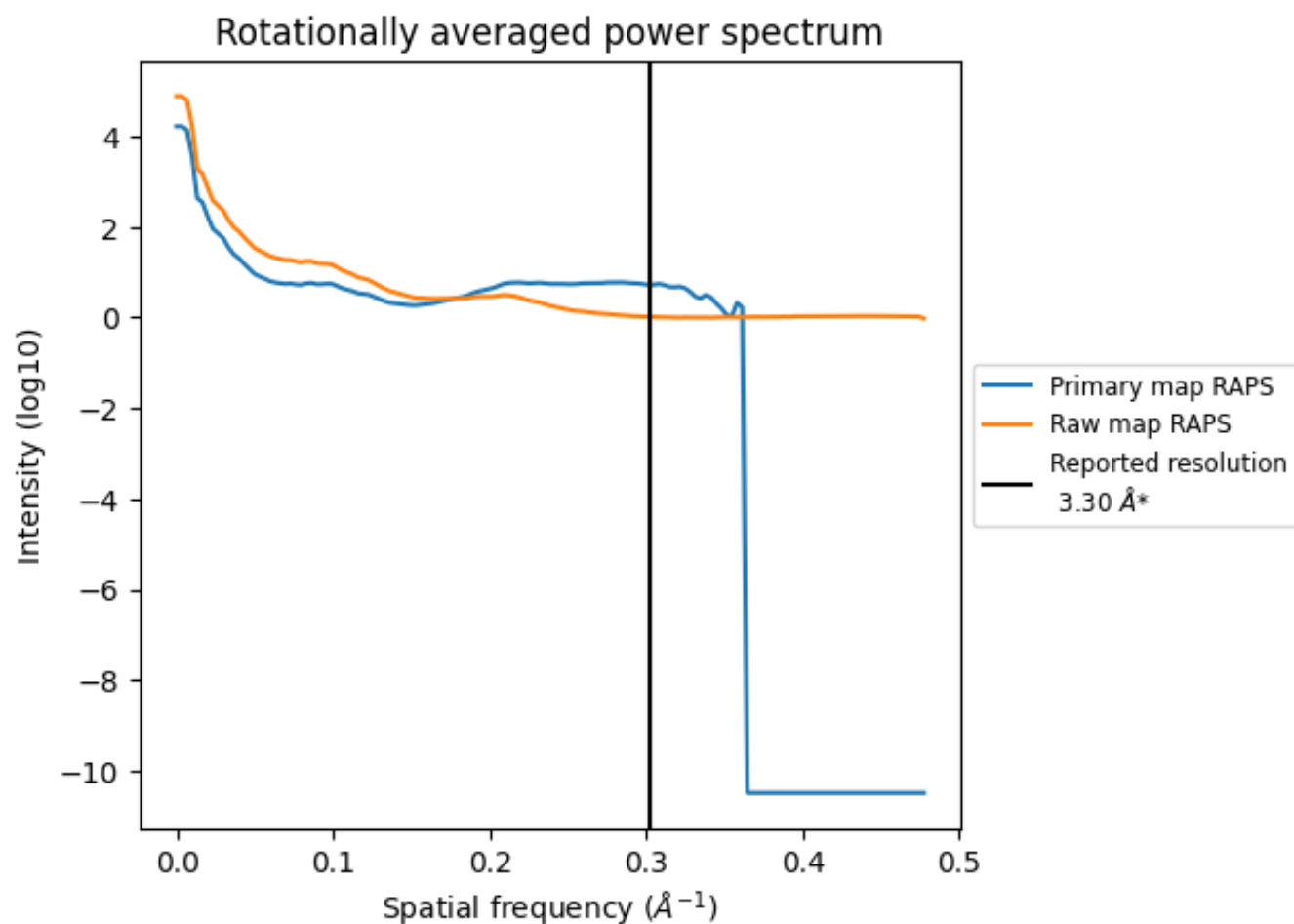
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 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 ⓘ

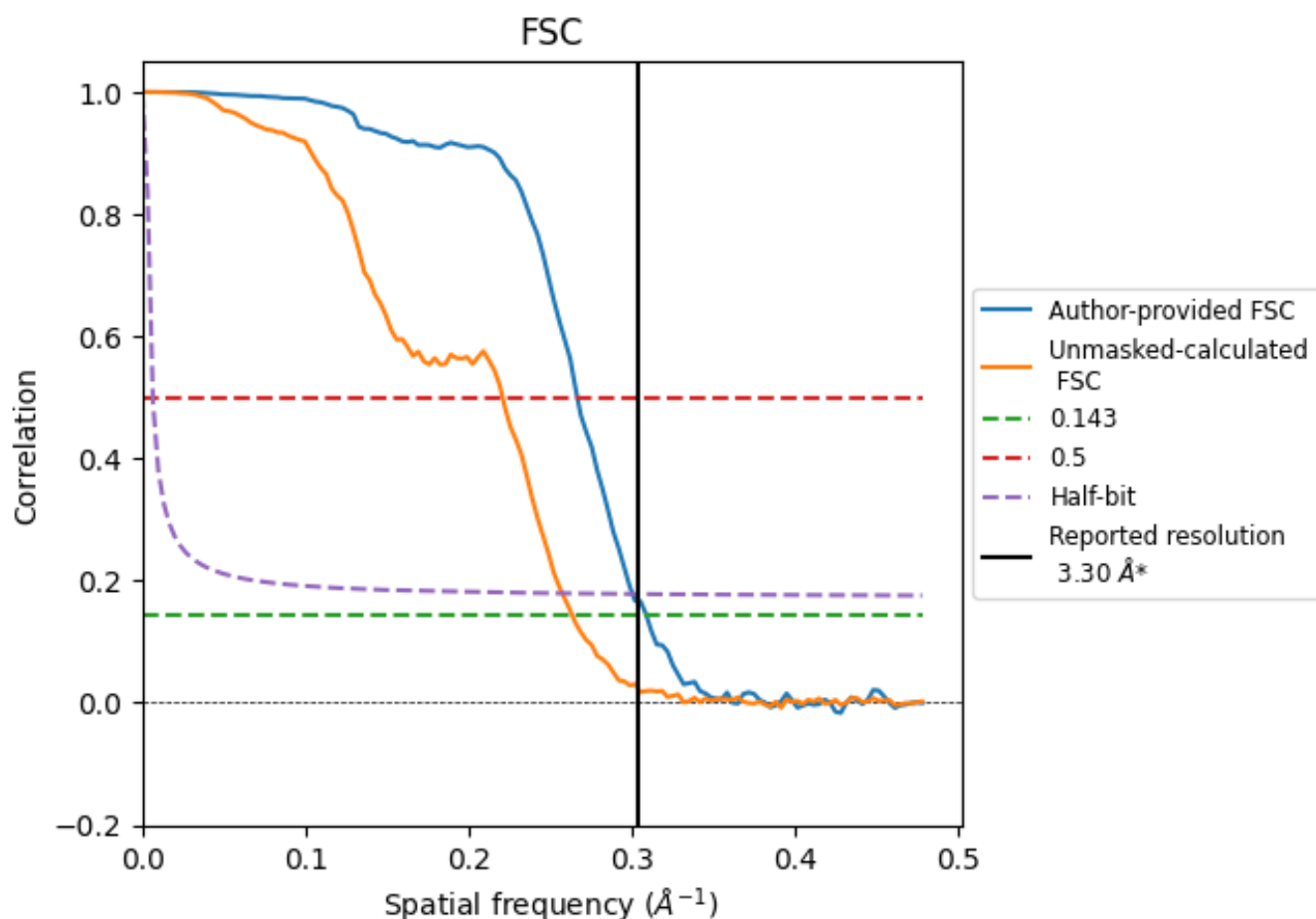


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

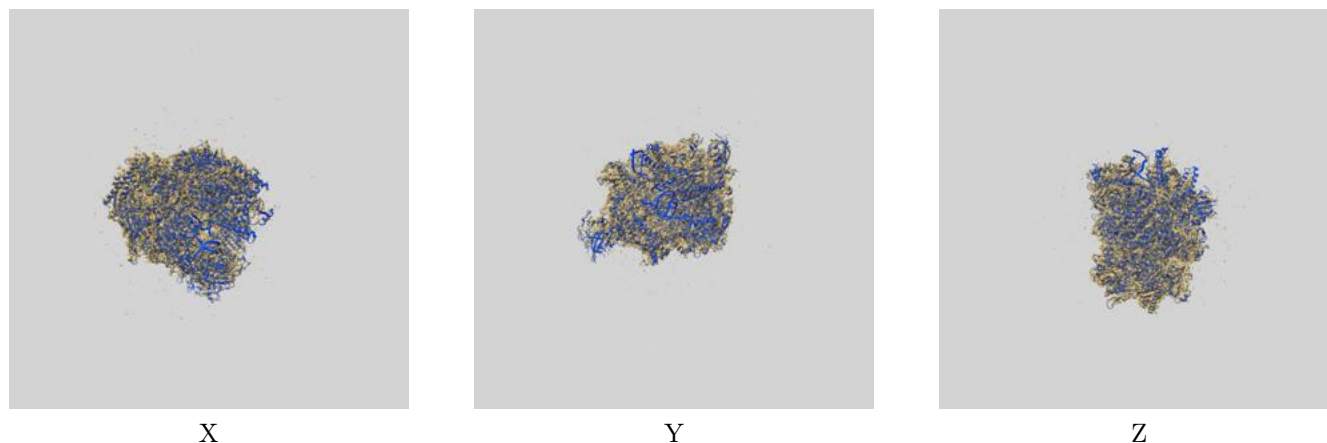
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.75	3.33
Unmasked-calculated*	3.80	4.53	3.89

*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 3.80 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

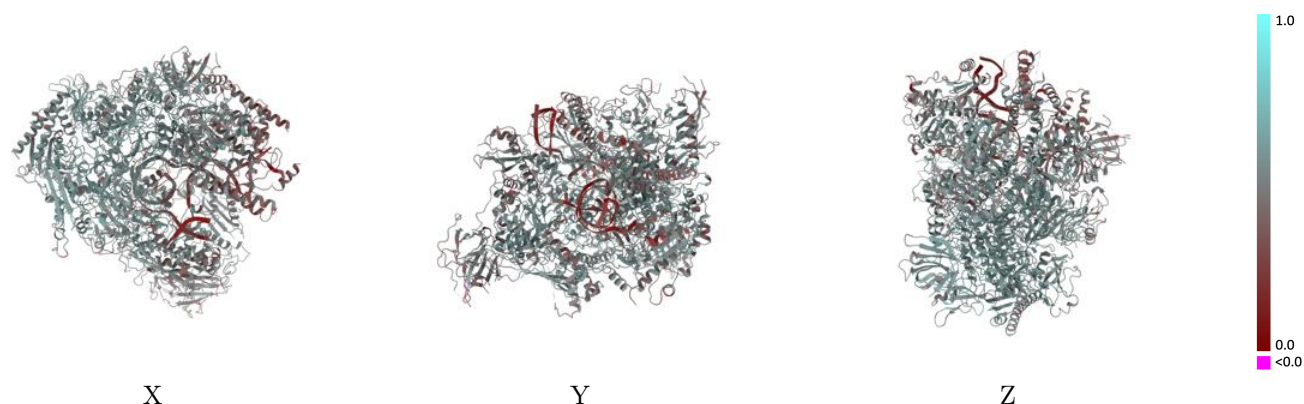
This section contains information regarding the fit between EMDB map EMD-50970 and PDB model 9G29. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



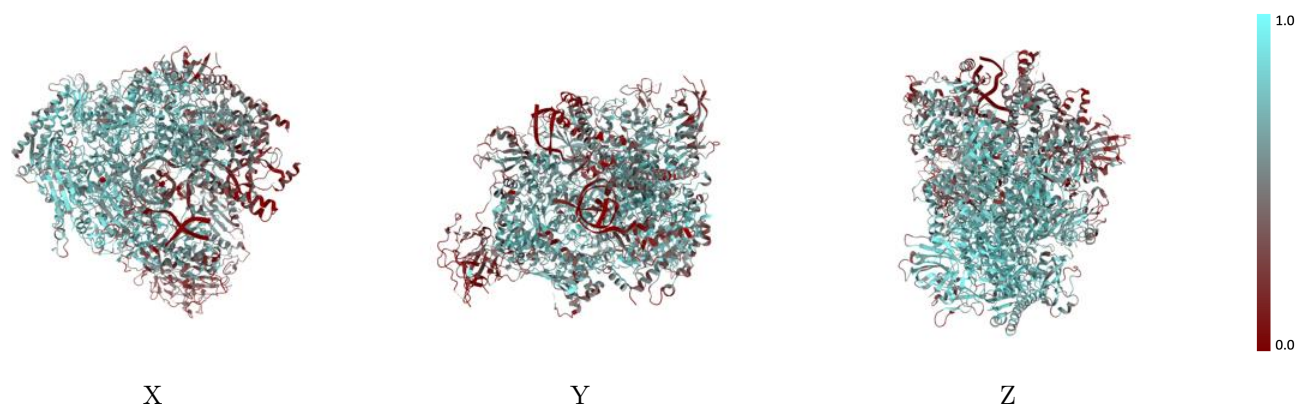
The images above show the 3D surface view of the map at the recommended contour level 0.0274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



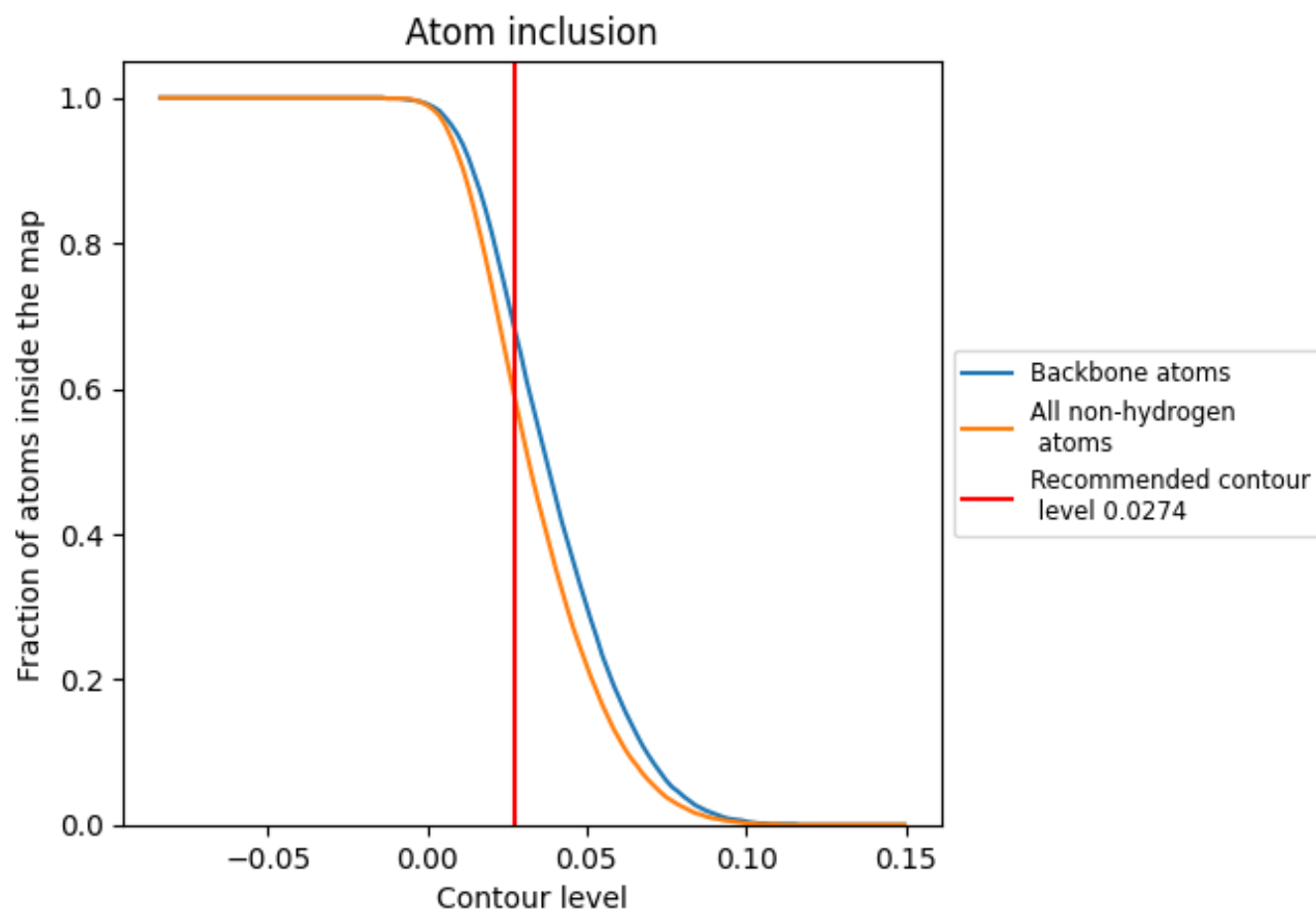
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0274).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 59% 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 (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.5070
A	 0.6290	 0.5170
B	 0.6710	 0.5330
C	 0.6660	 0.5390
D	 0.3910	 0.4880
E	 0.5140	 0.4740
F	 0.6460	 0.5200
G	 0.4360	 0.4870
H	 0.6930	 0.5540
I	 0.3140	 0.4370
J	 0.7950	 0.5850
K	 0.7090	 0.5440
L	 0.6060	 0.5150
M	 0.1940	 0.4420
N	 0.1840	 0.4380
R	 0.5280	 0.4740
S	 0.0820	 0.2040
T	 0.1990	 0.2900

