Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:56 am GMT

PDB ID	:	6H68
EMDB ID	:	EMD-0147
Title	:	Yeast RNA polymerase I elongation complex stalled by cyclobutane pyrimidine dimer (CPD) with fully-ordered A49
Authors	:	Sanz-Murillo, M.; Xu, J.; Gil-Carton, D.; Wang, D.; Fernandez-Tornero, C.
Deposited on	:	2018-07-26
Resolution	:	4.60 Å(reported)
Based on initial models	:	5M3F, 4C3I

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:

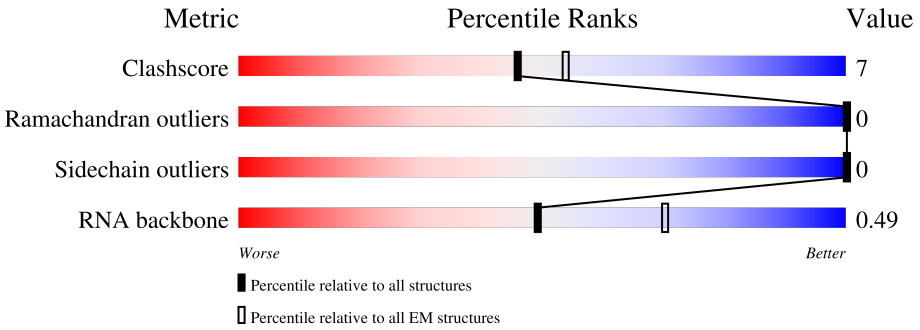
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	24% 73% 15% 11%
2	B	1203	23% 79% 18% .
3	C	335	21% 77% 15% 9%
4	D	137	36% 34% 9% 57%
5	E	215	27% 86% 14%
6	F	155	14% 54% 10% 35%
7	G	326	46% 48% 13% 38%

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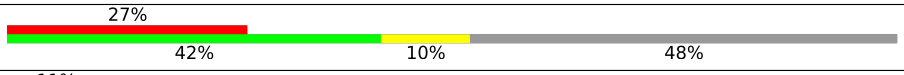
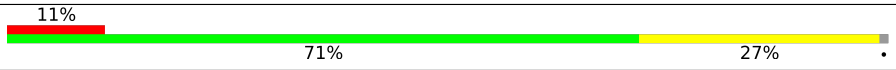
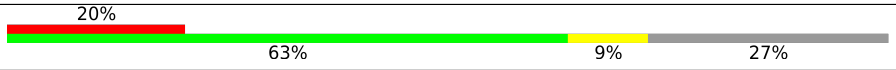
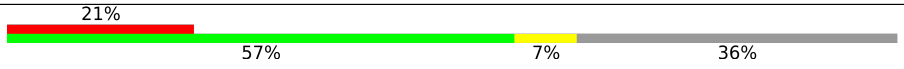
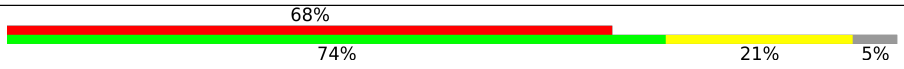
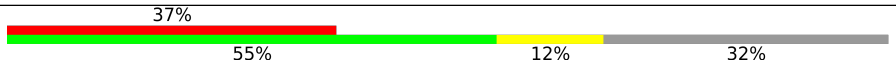
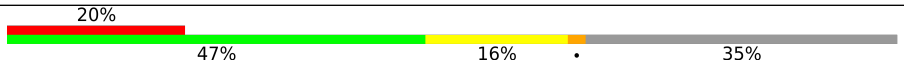
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	10	
16	T	51	
17	U	52	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 37103 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
			Total	C	N	O	S		
1	A	1473	11637	7352	2023	2200	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1175	9327	5900	1633	1743	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	306	2431	1544	417	462	8	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	201	Total	C	N	O	S	0	0
			1592	1022	275	290	5		

- 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
			1059	670	177	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	103	Total	C	N	O	S	0	0
			810	506	132	167	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	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	396	Total	C	N	O	S	0	0
			3131	1997	531	599	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1254	799	205	246	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	33	Total	C	N	O	P	0	0
			685	329	109	213	34		

- Molecule 17 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	24	Total	C	N	O	P	0	0
			496	234	99	139	24		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

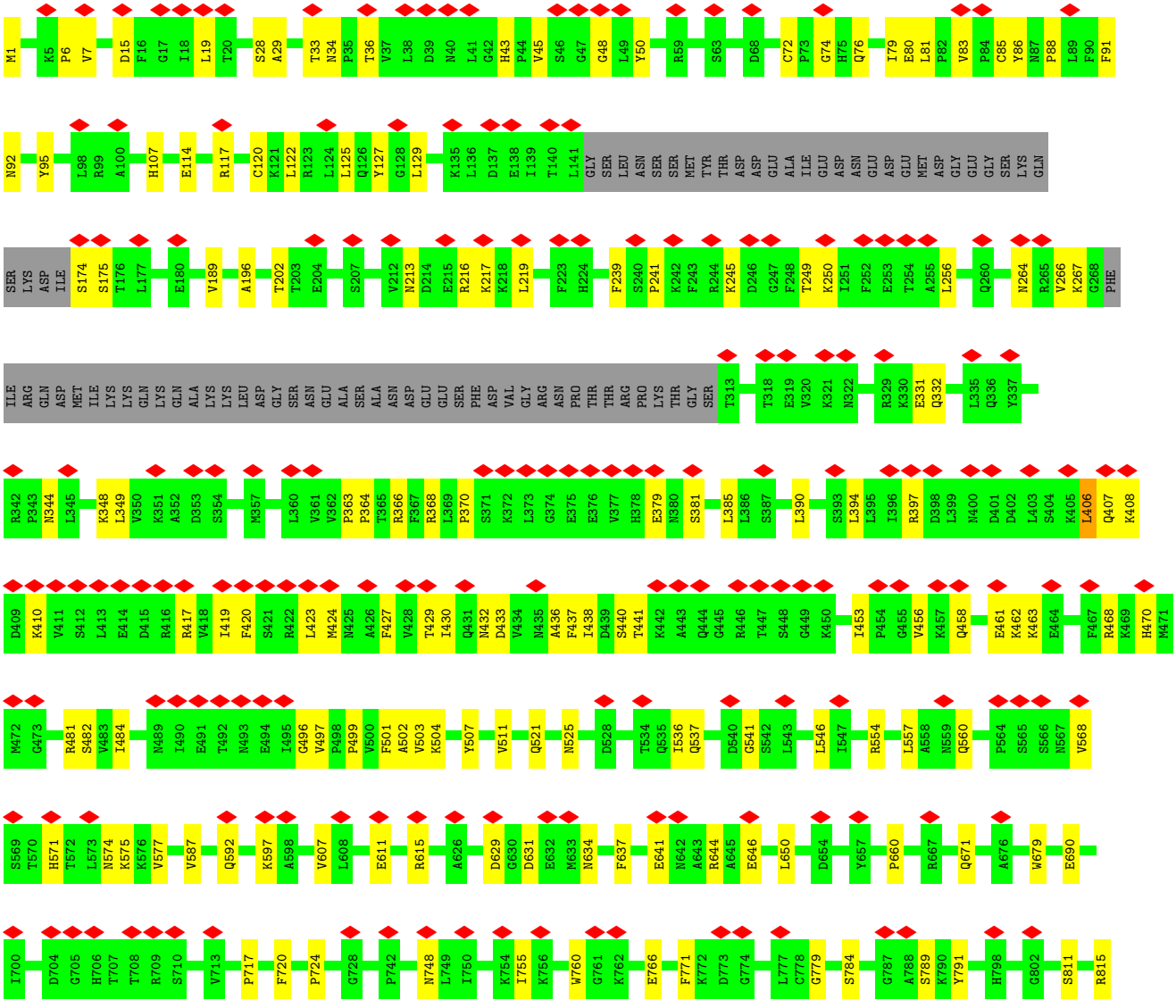
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

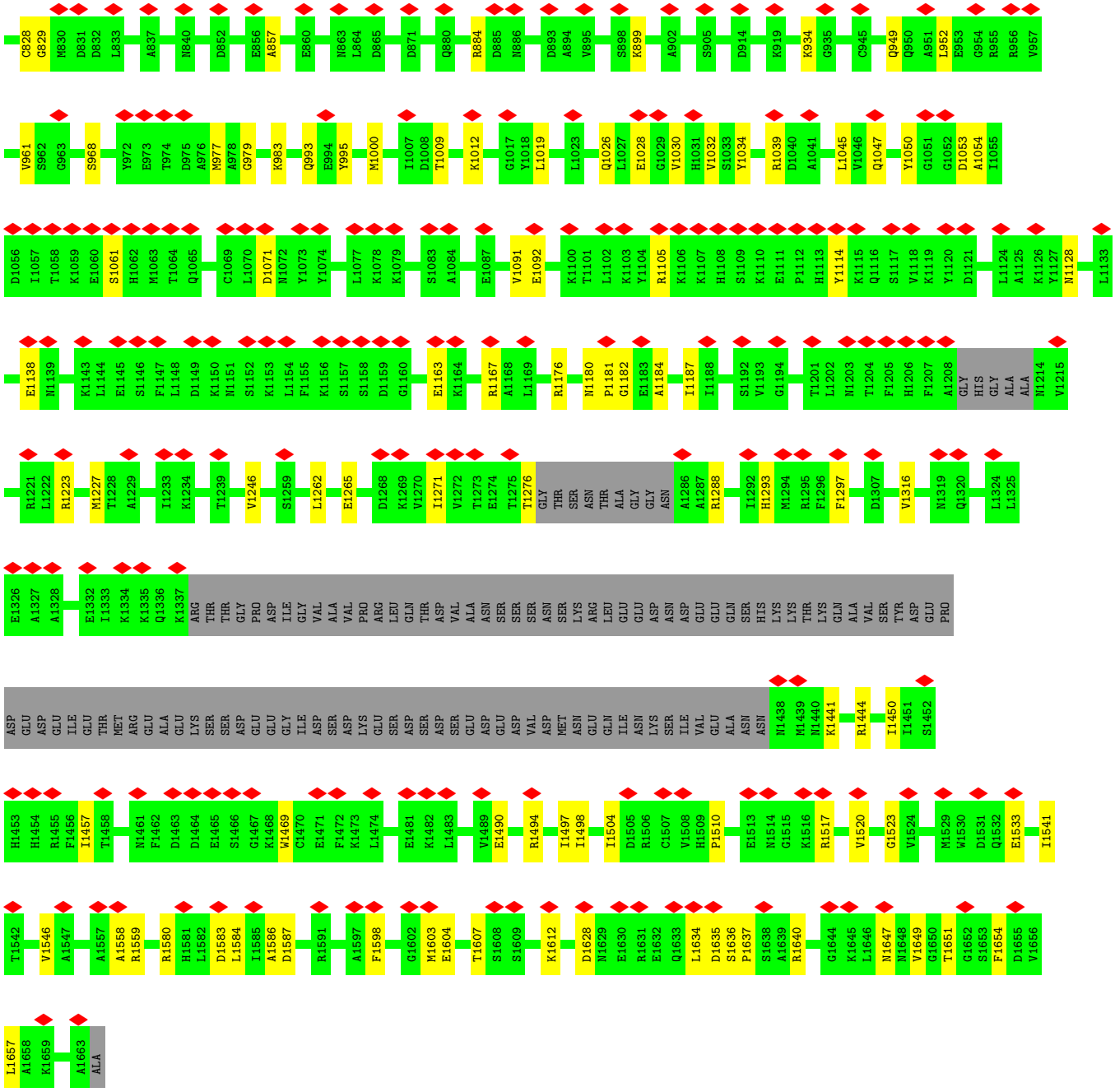
3 Residue-property plots (i)

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

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

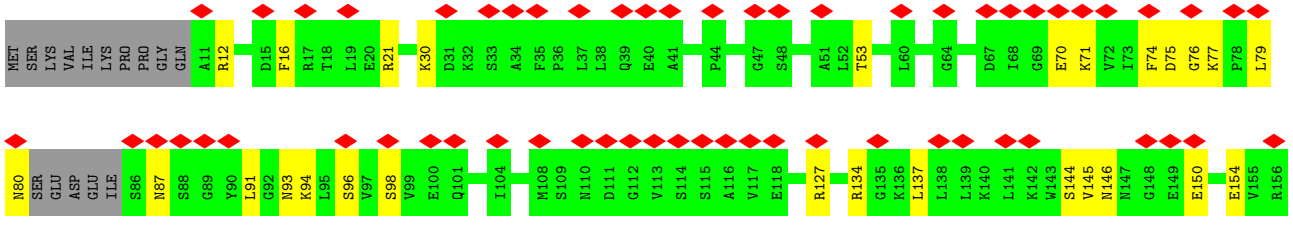
Chain A:

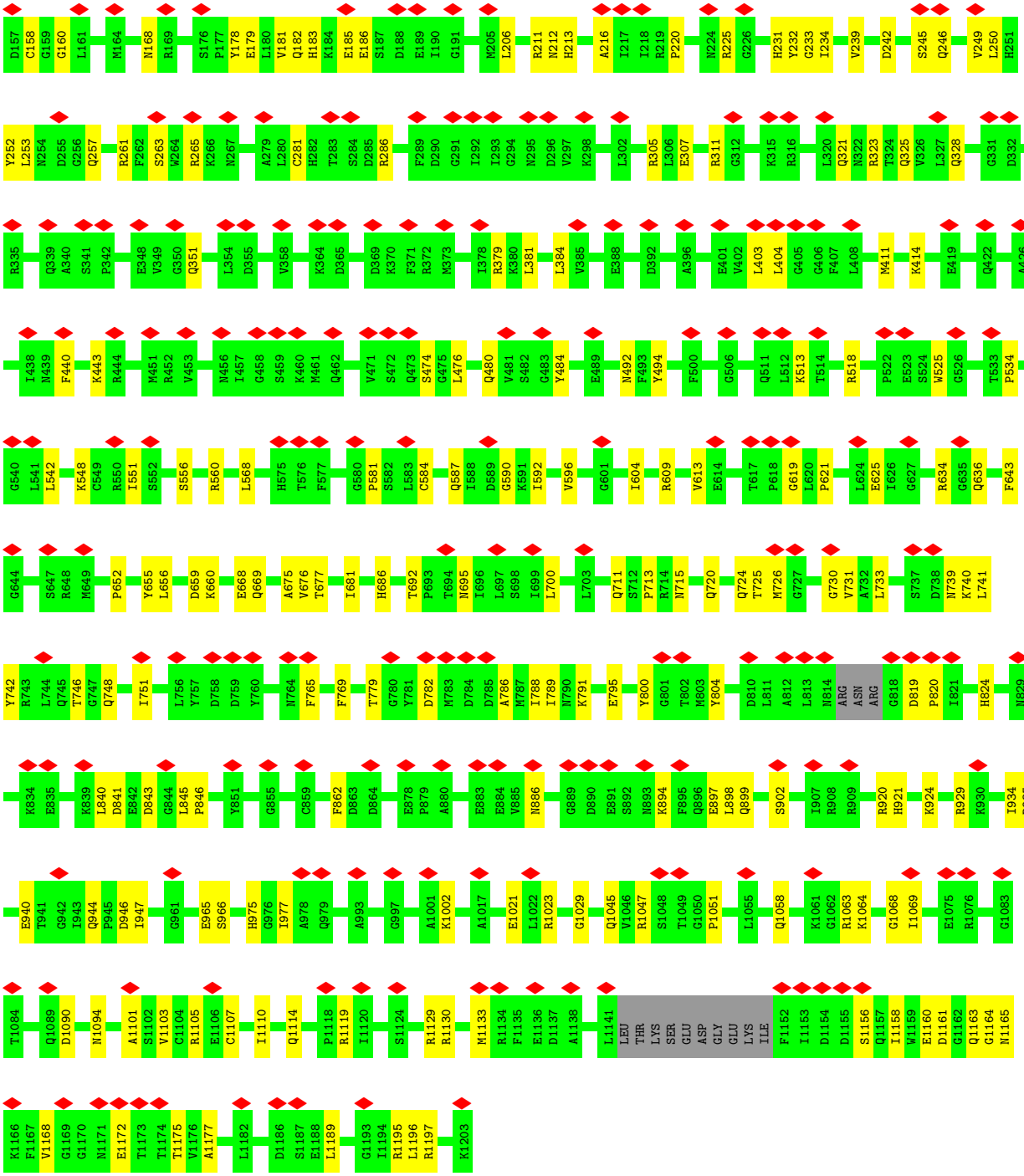




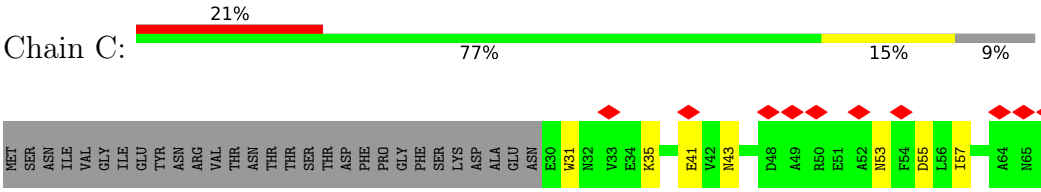
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

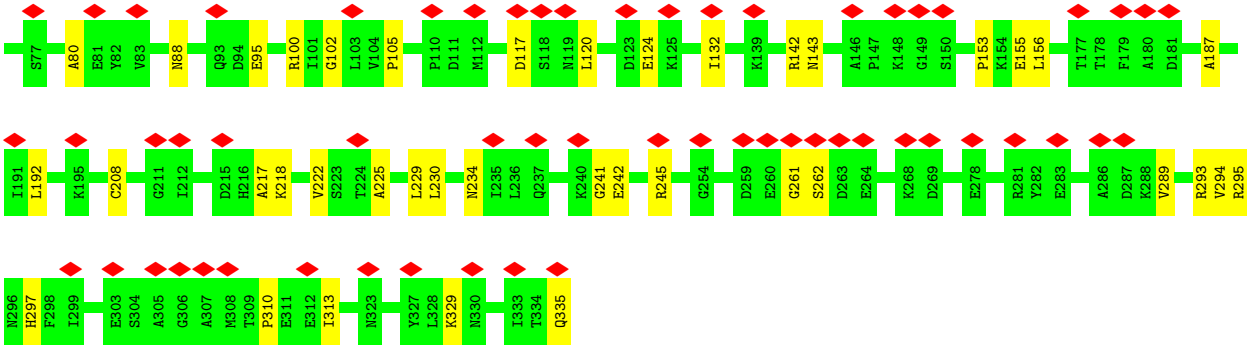
Chain B:



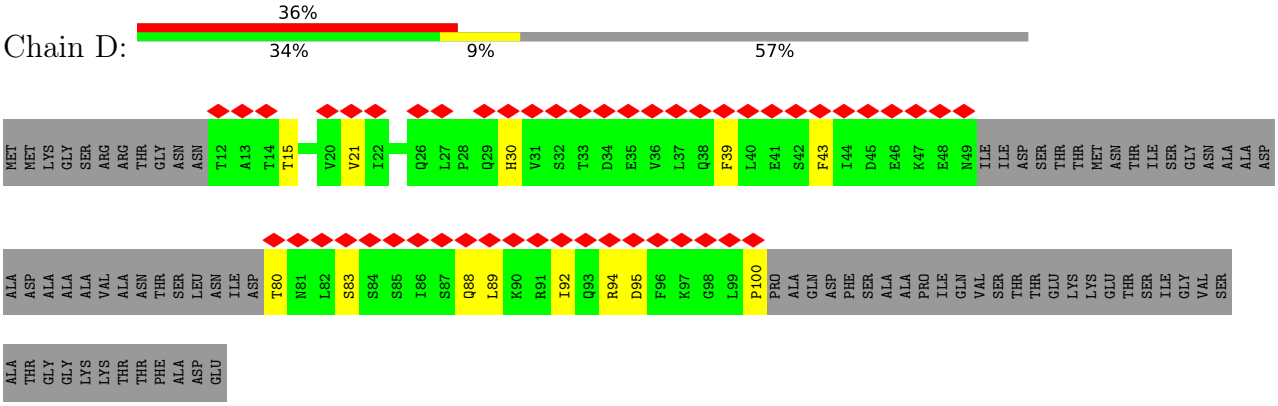


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

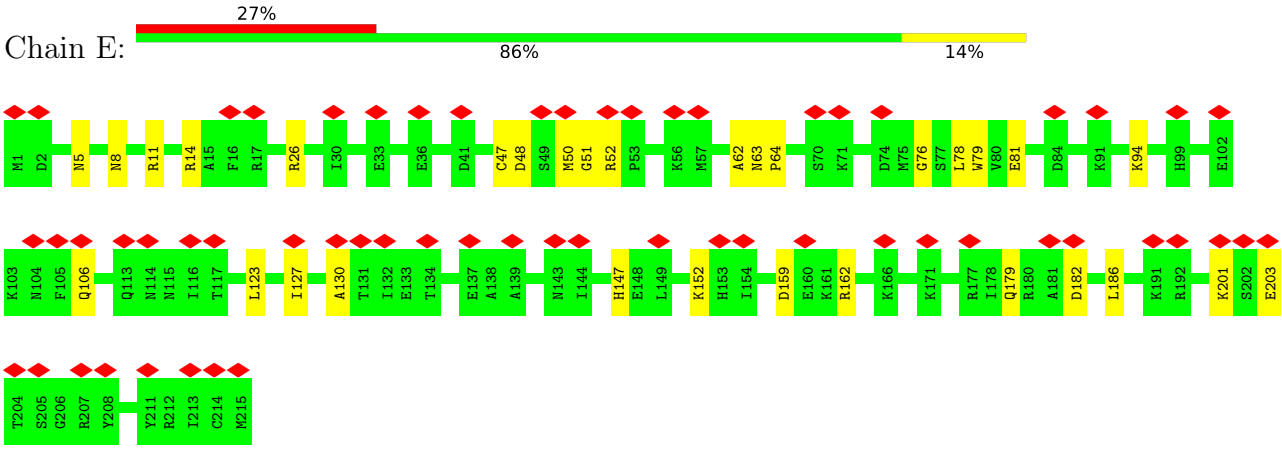




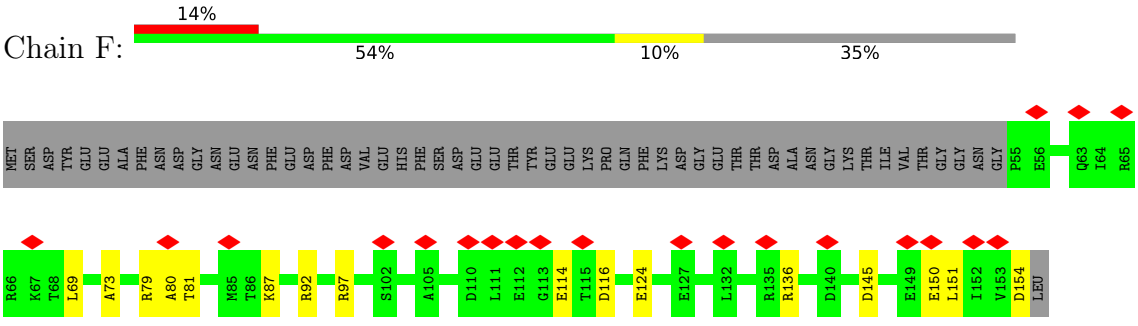
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14



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

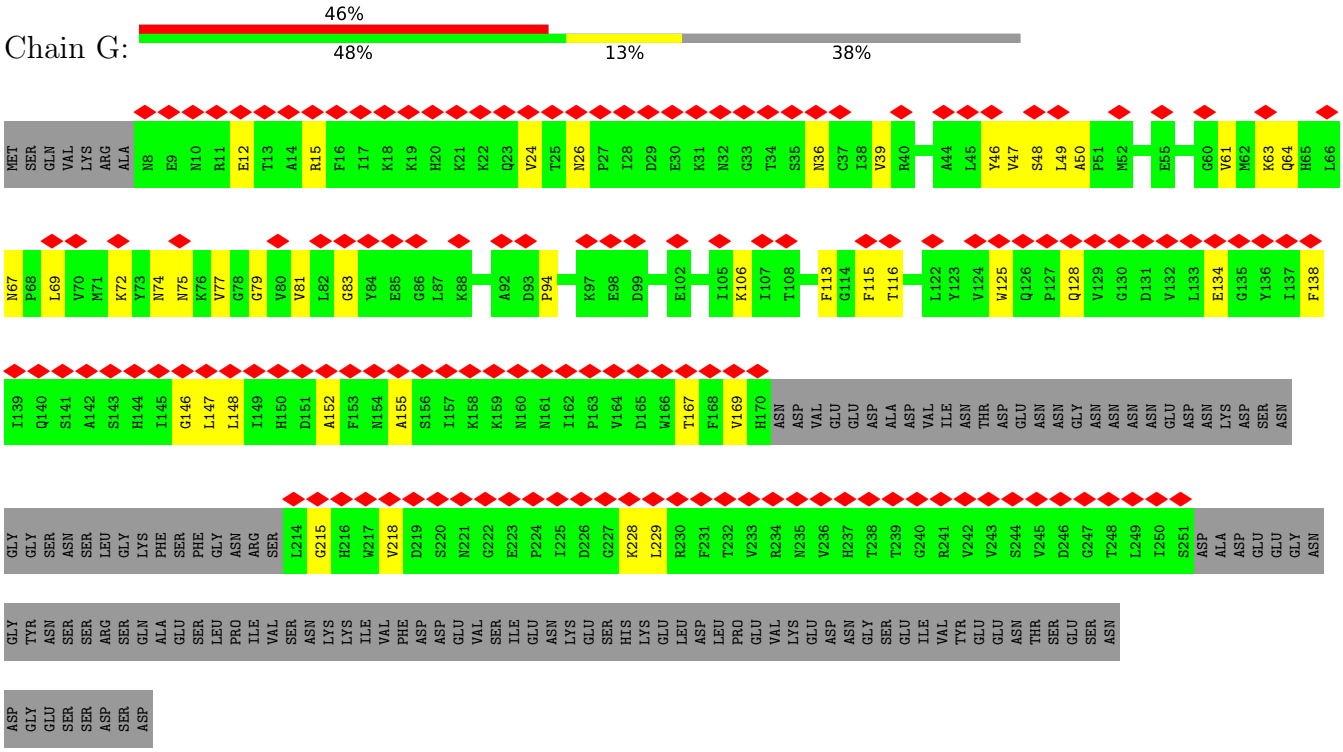


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



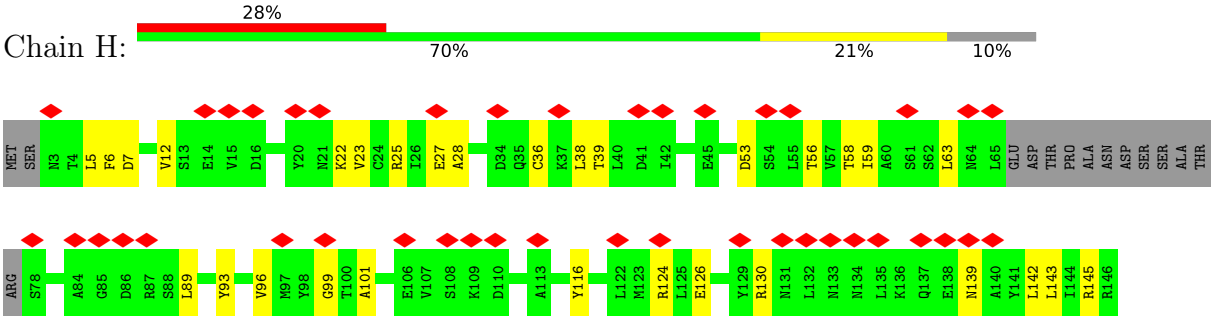
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G:



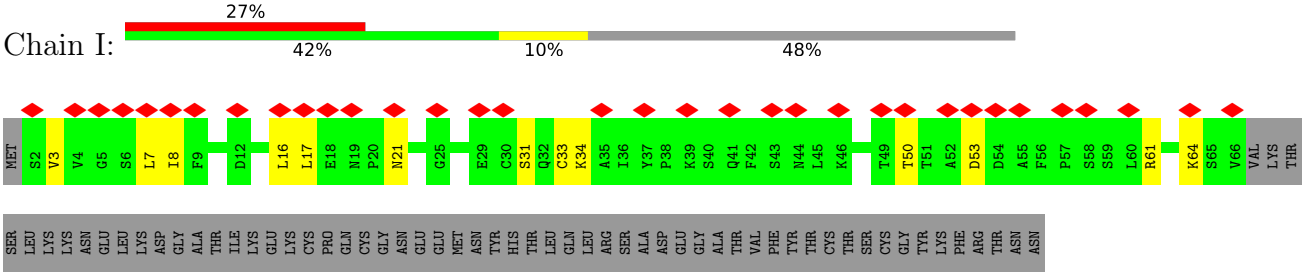
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



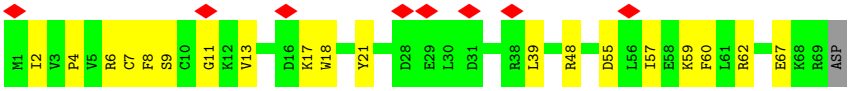
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:



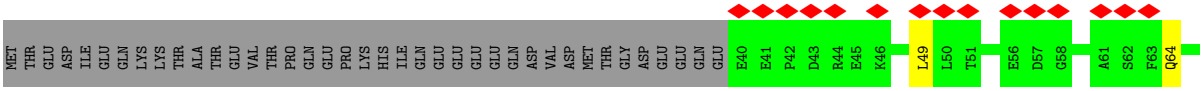
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

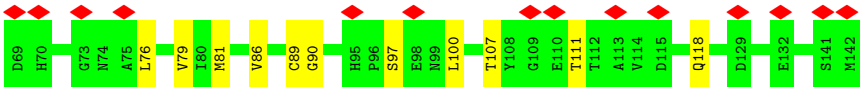
Chain J:



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

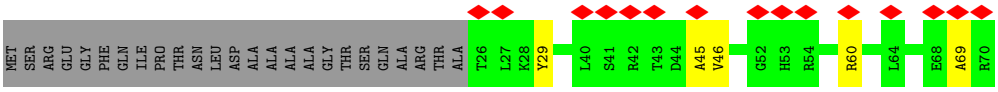
Chain K:





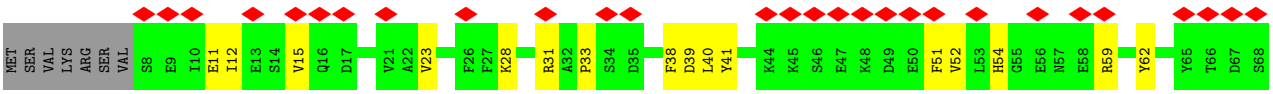
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

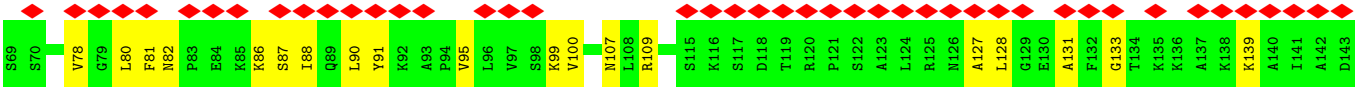
Chain L:

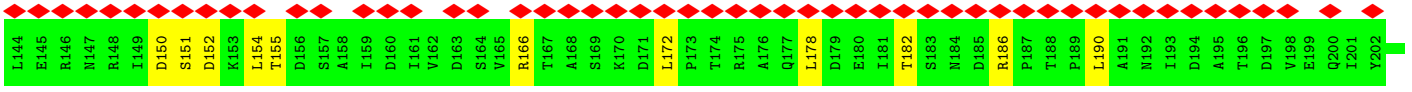


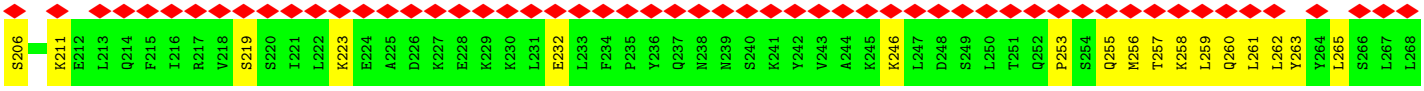
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

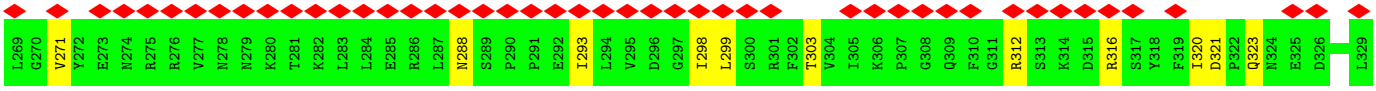
Chain M:

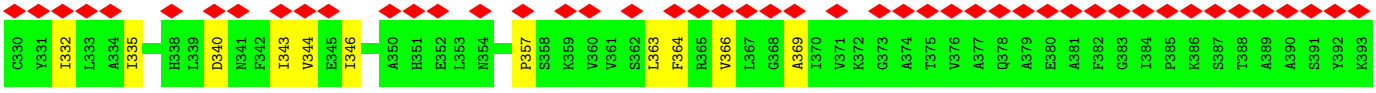


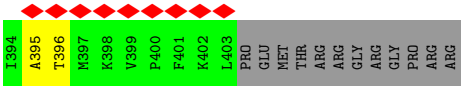




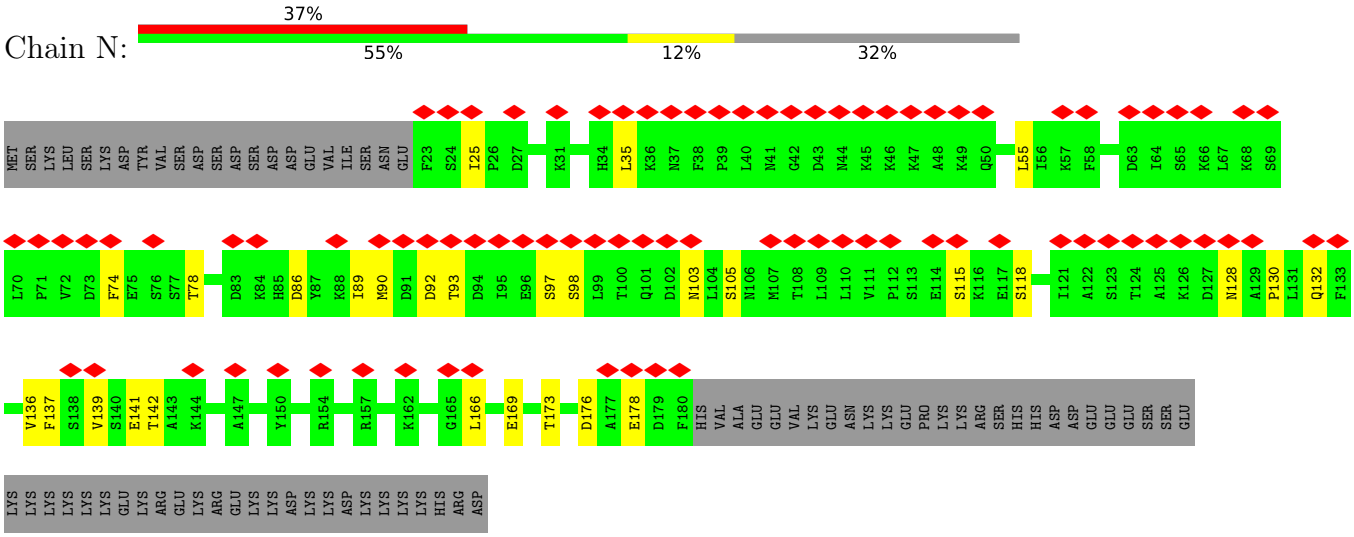




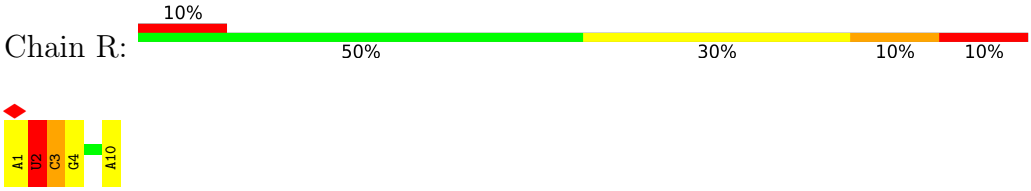




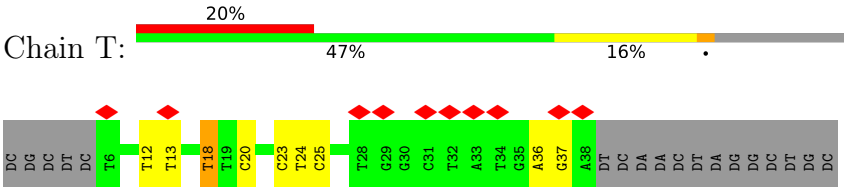
• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



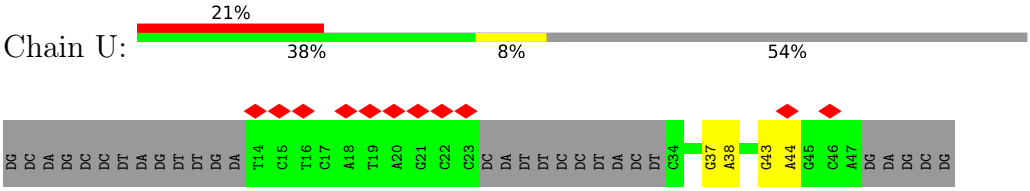
• Molecule 15: RNA



• Molecule 16: Template DNA



• Molecule 17: Non-template DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	5.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0239	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, TTD

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	0.31	0/11852	0.52	1/16008 (0.0%)
2	B	0.32	0/9533	0.53	0/12886
3	C	0.30	0/2483	0.51	0/3366
4	D	0.27	0/473	0.49	0/641
5	E	0.30	0/1795	0.50	0/2416
6	F	0.30	0/838	0.50	0/1129
7	G	0.28	0/1630	0.52	0/2216
8	H	0.29	0/1077	0.54	0/1460
9	I	0.29	0/485	0.57	0/657
10	J	0.34	0/578	0.50	0/775
11	K	0.28	0/821	0.50	0/1108
12	L	0.32	0/360	0.53	0/478
13	M	0.28	0/3184	0.52	0/4296
14	N	0.30	0/1279	0.59	0/1724
15	R	0.55	0/247	1.25	2/384 (0.5%)
16	T	0.62	0/717	1.01	0/1100
17	U	0.62	0/557	0.93	0/855
All	All	0.32	0/37909	0.56	3/51499 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
14	N	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	LEU	CA-CB-CG	5.93	128.94	115.30
15	R	3	C	C5-C6-N1	5.78	123.89	121.00
15	R	2	U	N3-C4-O4	5.07	122.95	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	LYS	Peptide
2	B	819	ASP	Peptide
14	N	25	ILE	Peptide

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	11637	0	11722	160	0
2	B	9327	0	9217	154	0
3	C	2431	0	2418	35	0
4	D	467	0	468	10	0
5	E	1759	0	1788	17	0
6	F	823	0	841	13	0
7	G	1592	0	1600	26	0
8	H	1059	0	1032	18	0
9	I	479	0	482	11	0
10	J	569	0	587	16	0
11	K	810	0	801	9	0
12	L	358	0	382	5	0
13	M	3131	0	3243	64	0
14	N	1254	0	1266	20	0
15	R	220	0	110	3	0
16	T	685	0	388	10	0
17	U	496	0	269	2	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	37103	0	36614	486	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 7.

All (486) 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)
8:H:36:CYS:HA	8:H:126:GLU:O	1.68	0.92
14:N:86:ASP:HB2	14:N:142:THR:O	1.71	0.91
7:G:146:GLY:HA2	7:G:155:ALA:O	1.71	0.88
13:M:23:VAL:O	13:M:95:VAL:HA	1.81	0.81
2:B:80:ASN:H	2:B:87:ASN:HD21	1.36	0.73
7:G:79:GLY:HA3	7:G:125:TRP:O	1.89	0.73
1:A:406:LEU:HA	1:A:410:LYS:HD2	1.71	0.72
2:B:225:ARG:HH22	13:M:133:GLY:H	1.40	0.69
1:A:239:PHE:HB2	1:A:264:ASN:HD21	1.58	0.68
13:M:41:TYR:HB2	13:M:52:VAL:HB	1.76	0.67
10:J:18:TRP:O	10:J:21:TYR:HB3	1.95	0.67
1:A:1227:MET:HA	1:A:1598:PHE:HB2	1.75	0.67
2:B:134:ARG:HH11	2:B:160:GLY:HA3	1.60	0.66
3:C:41:GLU:HB2	3:C:57:ILE:HB	1.78	0.66
8:H:96:VAL:HA	8:H:142:LEU:O	1.96	0.66
2:B:625:GLU:HB3	2:B:643:PHE:HB2	1.78	0.65
1:A:249:THR:HG22	1:A:250:LYS:HG3	1.77	0.65
1:A:1163:GLU:O	1:A:1167:ARG:HB2	1.96	0.65
2:B:249:VAL:HB	2:B:261:ARG:HB2	1.80	0.64
2:B:1103:VAL:HG22	2:B:1110:ILE:HG22	1.80	0.64
3:C:230:LEU:HB3	3:C:294:VAL:HB	1.79	0.64
1:A:748:ASN:HA	1:A:771:PHE:O	1.98	0.63
2:B:1105:ARG:HH12	4:D:21:VAL:HB	1.64	0.63
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.81	0.63
1:A:1559:ARG:NH2	1:A:1583:ASP:OD1	2.32	0.63
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.80	0.62
2:B:840:LEU:HA	2:B:846:PRO:HA	1.80	0.62
2:B:782:ASP:HA	2:B:786:ALA:HB3	1.82	0.62
13:M:78:VAL:HB	13:M:91:TYR:HB2	1.82	0.62
13:M:258:LYS:O	13:M:261:LEU:HB3	1.99	0.61
2:B:934:ILE:HB	3:C:69:ARG:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ASN:ND2	2:B:725:THR:OG1	2.34	0.60
2:B:1156:SER:HB2	7:G:75:ASN:HD22	1.66	0.60
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.82	0.60
1:A:546:LEU:HD22	1:A:554:ARG:HG2	1.84	0.60
13:M:80:LEU:O	13:M:88:ILE:HA	2.01	0.60
2:B:1133:MET:HB2	2:B:1168:VAL:HB	1.83	0.60
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.84	0.60
2:B:1002:LYS:HG2	14:N:166:LEU:HD13	1.83	0.60
7:G:74:ASN:HB3	7:G:77:VAL:HG22	1.83	0.60
8:H:39:THR:HB	8:H:124:ARG:HB3	1.83	0.60
2:B:212:ASN:HB3	2:B:590:GLY:HA3	1.84	0.59
2:B:494:TYR:HB3	2:B:700:LEU:HD21	1.84	0.59
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.82	0.59
3:C:241:GLY:H	3:C:262:SER:HA	1.66	0.59
3:C:143:ASN:ND2	3:C:155:GLU:O	2.35	0.59
2:B:966:SER:HB3	2:B:1029:GLY:HA3	1.85	0.59
5:E:26:ARG:NH2	5:E:186:LEU:O	2.36	0.59
1:A:1637:PRO:HB3	1:A:1647:ASN:HD21	1.68	0.59
7:G:81:VAL:HG12	7:G:83:GLY:H	1.68	0.59
9:I:33:CYS:HB2	13:M:59:ARG:HE	1.68	0.58
1:A:266:VAL:HG23	1:A:267:LYS:HG3	1.84	0.58
1:A:977:MET:SD	1:A:983:LYS:NZ	2.76	0.58
4:D:39:PHE:O	4:D:43:PHE:HB2	2.04	0.58
2:B:1105:ARG:NH2	2:B:1172:GLU:OE1	2.36	0.58
8:H:63:LEU:HD22	8:H:89:LEU:HB3	1.85	0.58
1:A:461:GLU:HG3	1:A:462:LYS:HG3	1.84	0.58
1:A:720:PHE:HB2	8:H:96:VAL:HB	1.85	0.58
2:B:789:ILE:HG12	2:B:947:ILE:HG12	1.85	0.58
2:B:924:LYS:NZ	15:R:10:A:OP1	2.36	0.58
2:B:71:LYS:O	2:B:96:SER:HA	2.04	0.57
13:M:211:LYS:HG2	13:M:293:ILE:HD11	1.86	0.57
1:A:417:ARG:NH2	13:M:152:ASP:OD1	2.38	0.57
2:B:94:LYS:HB3	2:B:146:ASN:HA	1.87	0.57
2:B:886:ASN:HB2	2:B:902:SER:HB3	1.87	0.57
7:G:134:GLU:HB3	7:G:228:LYS:HB3	1.86	0.57
13:M:246:LYS:NZ	13:M:340:ASP:OD1	2.37	0.57
13:M:232:GLU:O	13:M:288:ASN:ND2	2.37	0.57
1:A:125:LEU:HD11	1:A:219:LEU:HD12	1.87	0.57
1:A:114:GLU:OE2	1:A:117:ARG:NH2	2.36	0.57
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.86	0.57
1:A:828:CYS:SG	1:A:829:GLY:N	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1635:ASP:HA	1:A:1640:ARG:HH21	1.69	0.56
5:E:8:ASN:OD1	5:E:11:ARG:NH2	2.37	0.56
9:I:53:ASP:OD1	9:I:61:ARG:NH1	2.37	0.56
2:B:181:VAL:HG11	10:J:62:ARG:HE	1.70	0.56
2:B:1047:ARG:NH2	2:B:1051:PRO:O	2.37	0.56
1:A:1019:LEU:HD13	1:A:1223:ARG:HG3	1.87	0.56
2:B:560:ARG:HD2	2:B:619:GLY:HA3	1.87	0.56
2:B:929:ARG:NH1	11:K:97:SER:OG	2.39	0.56
2:B:935:ASP:OD1	3:C:69:ARG:NH1	2.35	0.56
13:M:186:ARG:HD2	13:M:366:VAL:HG21	1.86	0.56
2:B:311:ARG:HD2	9:I:16:LEU:HD21	1.87	0.56
8:H:22:LYS:HG3	8:H:23:VAL:HG23	1.86	0.56
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.88	0.56
2:B:739:ASN:ND2	16:T:25:DC:OP1	2.39	0.56
1:A:43:HIS:ND1	13:M:323:GLN:OE1	2.38	0.56
1:A:1657:LEU:HG	7:G:106:LYS:HA	1.88	0.56
6:F:79:ARG:NH1	6:F:150:GLU:OE2	2.38	0.56
1:A:1271:ILE:HG12	9:I:50:THR:HG22	1.88	0.56
1:A:1634:LEU:O	1:A:1640:ARG:NH2	2.39	0.56
2:B:733:LEU:HD22	2:B:741:LEU:HD21	1.88	0.55
13:M:253:PRO:O	13:M:256:MET:HB2	2.07	0.55
2:B:946:ASP:OD1	10:J:9:SER:OG	2.24	0.55
1:A:217:LYS:NZ	1:A:1604:GLU:O	2.38	0.55
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.88	0.55
1:A:28:SER:O	2:B:1129:ARG:NH2	2.37	0.55
1:A:884:ARG:NH2	1:A:961:VAL:O	2.39	0.55
2:B:788:ILE:O	2:B:947:ILE:HA	2.07	0.55
2:B:492:ASN:ND2	2:B:725:THR:O	2.39	0.55
3:C:242:GLU:OE2	3:C:245:ARG:NH2	2.40	0.55
11:K:86:VAL:HA	11:K:107:THR:HG22	1.89	0.55
1:A:1450:ILE:HG22	1:A:1457:ILE:HG21	1.88	0.55
1:A:1163:GLU:O	1:A:1167:ARG:CB	2.55	0.54
1:A:420:PHE:O	1:A:423:LEU:HB3	2.07	0.54
2:B:127:ARG:NH1	2:B:185:GLU:OE2	2.40	0.54
13:M:271:VAL:HG21	13:M:298:ILE:HG21	1.90	0.54
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.41	0.54
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.88	0.54
7:G:134:GLU:HA	7:G:229:LEU:O	2.07	0.54
1:A:1091:VAL:HG23	1:A:1092:GLU:HG3	1.90	0.54
1:A:1128:ASN:ND2	6:F:80:ALA:O	2.41	0.54
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:HD3	13:M:172:LEU:HB3	1.89	0.54
7:G:26:ASN:ND2	7:G:36:ASN:O	2.41	0.54
13:M:190:LEU:HB3	13:M:206:SER:HB2	1.91	0.54
2:B:211:ARG:HD2	2:B:239:VAL:HG21	1.89	0.53
14:N:105:SER:HB2	14:N:132:GLN:HG2	1.90	0.53
4:D:94:ARG:HB3	4:D:100:PRO:HA	1.89	0.53
7:G:12:GLU:OE1	7:G:15:ARG:NH2	2.40	0.53
2:B:655:TYR:O	2:B:659:ASP:HA	2.08	0.53
3:C:153:PRO:HA	3:C:156:LEU:HB3	1.90	0.53
2:B:791:LYS:NZ	2:B:795:GLU:OE2	2.41	0.53
3:C:120:LEU:HD23	3:C:124:GLU:HB3	1.91	0.53
1:A:511:VAL:O	1:A:574:ASN:ND2	2.42	0.53
1:A:1504:ILE:HA	1:A:1523:GLY:HA3	1.90	0.53
2:B:76:GLY:H	2:B:91:LEU:HD21	1.73	0.53
7:G:69:LEU:HD12	7:G:72:LYS:HD3	1.90	0.53
8:H:5:LEU:O	8:H:130:ARG:NH2	2.42	0.53
8:H:12:VAL:HB	8:H:53:ASP:H	1.73	0.53
13:M:344:VAL:HB	13:M:395:ALA:HB3	1.91	0.53
2:B:145:VAL:HB	2:B:150:GLU:HB3	1.91	0.53
2:B:779:THR:HG21	2:B:788:ILE:HG13	1.91	0.53
5:E:201:LYS:NZ	5:E:203:GLU:OE2	2.42	0.53
1:A:597:LYS:HE3	1:A:660:PRO:HG3	1.91	0.53
2:B:1119:ARG:NH2	2:B:1158:ILE:O	2.42	0.53
1:A:766:GLU:HA	1:A:779:GLY:HA2	1.91	0.52
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.41	0.52
1:A:107:HIS:ND1	1:A:331:GLU:OE2	2.38	0.52
2:B:30:LYS:HG2	2:B:178:TYR:HB2	1.91	0.52
2:B:587:GLN:HG2	2:B:592:ILE:HA	1.90	0.52
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.91	0.52
2:B:1107:CYS:O	2:B:1130:ARG:NH2	2.42	0.52
7:G:24:VAL:O	7:G:128:GLN:NE2	2.41	0.52
2:B:568:LEU:HD23	14:N:141:GLU:HB3	1.90	0.52
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.91	0.52
2:B:1101:ALA:O	2:B:1175:THR:HA	2.10	0.52
1:A:1:MET:HB2	2:B:1094:ASN:HB3	1.92	0.52
1:A:34:ASN:HB3	1:A:48:GLY:HA2	1.91	0.52
1:A:521:GLN:HE21	1:A:525:ASN:HD21	1.58	0.52
2:B:720:GLN:O	2:B:724:GLN:NE2	2.39	0.52
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.92	0.52
3:C:53:ASN:ND2	14:N:173:THR:O	2.42	0.52
1:A:127:TYR:HD1	1:A:202:THR:HG21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.43	0.51
2:B:534:PRO:HG3	2:B:542:LEU:HD23	1.91	0.51
13:M:219:SER:O	13:M:223:LYS:HB2	2.10	0.51
1:A:995:TYR:OH	2:B:715:ASN:ND2	2.43	0.51
2:B:548:LYS:HB3	2:B:652:PRO:HD2	1.93	0.51
13:M:255:GLN:O	13:M:258:LYS:HB2	2.10	0.51
1:A:1028:GLU:OE2	1:A:1636:SER:OG	2.29	0.51
3:C:31:TRP:HD1	3:C:35:LYS:HD3	1.74	0.51
9:I:8:ILE:HG23	9:I:17:LEU:HD21	1.92	0.51
1:A:1640:ARG:HD2	1:A:1647:ASN:HA	1.92	0.51
2:B:656:LEU:HD21	2:B:681:ILE:HD13	1.92	0.51
2:B:53:THR:OG1	2:B:168:ASN:ND2	2.43	0.51
2:B:253:LEU:HD12	2:B:257:GLN:HB3	1.91	0.51
5:E:159:ASP:OD1	5:E:162:ARG:NH2	2.43	0.51
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.92	0.51
2:B:1195:ARG:HH12	2:B:1197:ARG:HD2	1.76	0.51
5:E:127:ILE:HD12	5:E:130:ALA:HB3	1.93	0.51
13:M:312:ARG:HE	13:M:316:ARG:HD2	1.76	0.51
13:M:312:ARG:HG3	13:M:316:ARG:HB2	1.93	0.51
14:N:78:THR:OG1	14:N:89:ILE:O	2.28	0.51
1:A:1316:VAL:HG11	1:A:1498:ILE:HG12	1.92	0.51
6:F:69:LEU:HG	7:G:94:PRO:HG3	1.92	0.51
1:A:432:ASN:O	1:A:436:ALA:N	2.44	0.50
1:A:1047:GLN:NE2	1:A:1583:ASP:OD2	2.44	0.50
7:G:167:THR:HB	7:G:218:VAL:HB	1.92	0.50
13:M:127:ALA:O	13:M:131:ALA:HB2	2.11	0.50
2:B:325:GLN:HE21	13:M:107:ASN:HB3	1.74	0.50
13:M:31:ARG:HG2	14:N:130:PRO:HD3	1.93	0.50
13:M:364:PHE:HB3	13:M:369:ALA:HB3	1.93	0.50
2:B:613:VAL:HG12	2:B:660:LYS:HE3	1.93	0.50
10:J:17:LYS:HD3	10:J:39:LEU:HB3	1.92	0.50
1:A:1533:GLU:OE1	5:E:14:ARG:NH1	2.44	0.50
2:B:96:SER:HB2	2:B:144:SER:HB2	1.92	0.50
13:M:343:ILE:HG23	13:M:396:THR:HG22	1.93	0.50
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.44	0.50
2:B:692:THR:O	2:B:695:ASN:ND2	2.44	0.50
2:B:824:HIS:O	2:B:862:PHE:N	2.43	0.50
6:F:114:GLU:HG3	6:F:116:ASP:H	1.77	0.50
2:B:746:THR:HG21	10:J:8:PHE:HZ	1.76	0.50
1:A:6:PRO:O	4:D:15:THR:OG1	2.30	0.50
2:B:1107:CYS:HB2	2:B:1130:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:TYR:HA	7:G:116:THR:O	2.11	0.50
7:G:47:VAL:O	7:G:115:PHE:HA	2.11	0.50
1:A:33:THR:HA	1:A:390:LEU:HD22	1.93	0.50
1:A:80:GLU:O	1:A:397:ARG:NH2	2.45	0.50
1:A:216:ARG:NH1	1:A:1628:ASP:OD1	2.41	0.50
1:A:470:HIS:ND1	2:B:1058:GLN:OE1	2.34	0.50
13:M:261:LEU:HG	13:M:335:ILE:HG23	1.94	0.50
1:A:1654:PHE:O	6:F:92:ARG:NH1	2.43	0.50
2:B:246:GLN:NE2	2:B:263:SER:O	2.43	0.50
5:E:48:ASP:OD1	5:E:52:ARG:N	2.40	0.50
8:H:96:VAL:HG22	8:H:143:LEU:HG	1.93	0.50
1:A:83:VAL:HG11	1:A:427:PHE:HE1	1.77	0.49
2:B:741:LEU:HB3	2:B:804:TYR:HB2	1.94	0.49
1:A:536:ILE:HD12	1:A:557:LEU:HD13	1.93	0.49
1:A:884:ARG:HB3	2:B:634:ARG:HD2	1.93	0.49
1:A:1009:THR:HA	1:A:1012:LYS:HE2	1.92	0.49
2:B:404:LEU:HD21	2:B:551:ILE:HG21	1.93	0.49
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.93	0.49
13:M:260:GLN:O	13:M:263:TYR:HB3	2.12	0.49
14:N:74:PHE:HB2	14:N:78:THR:HG22	1.95	0.49
1:A:497:VAL:HB	1:A:607:VAL:HA	1.94	0.49
2:B:74:PHE:HB3	2:B:91:LEU:HD22	1.94	0.49
2:B:898:LEU:HD13	12:L:46:VAL:HG21	1.95	0.49
10:J:6:ARG:HA	10:J:13:VAL:HA	1.94	0.49
2:B:800:TYR:OH	3:C:95:GLU:OE1	2.30	0.49
1:A:81:LEU:HD22	1:A:430:ILE:HD11	1.95	0.49
1:A:755:ILE:HG21	1:A:760:TRP:HE1	1.78	0.49
1:A:1105:ARG:NH2	1:A:1138:GLU:OE1	2.46	0.49
2:B:323:ARG:NH2	2:B:351:GLN:OE1	2.42	0.49
8:H:93:TYR:HD2	8:H:143:LEU:HB3	1.78	0.49
1:A:92:ASN:O	1:A:95:TYR:HB3	2.13	0.49
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	1.95	0.49
6:F:79:ARG:NH1	6:F:145:ASP:O	2.44	0.49
6:F:81:THR:OG1	6:F:136:ARG:NH1	2.45	0.49
13:M:303:THR:HG22	13:M:320:ILE:HG12	1.94	0.49
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.95	0.49
1:A:88:PRO:HA	1:A:91:PHE:HB2	1.94	0.48
13:M:150:ASP:HA	13:M:154:LEU:HD23	1.94	0.48
1:A:440:SER:H	1:A:458:GLN:HE22	1.61	0.48
1:A:537:GLN:HE21	1:A:541:GLY:HA2	1.78	0.48
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:12:ILE:HG12	13:M:88:ILE:HD11	1.95	0.48
14:N:92:ASP:N	14:N:136:VAL:O	2.46	0.48
1:A:213:ASN:HD22	1:A:1607:THR:HG22	1.79	0.48
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.41	0.48
5:E:47:CYS:HB3	5:E:51:GLY:HA2	1.94	0.48
1:A:611:GLU:OE2	1:A:615:ARG:NE	2.39	0.48
2:B:321:GLN:NE2	9:I:31:SER:O	2.45	0.48
13:M:62:TYR:HB3	13:M:100:VAL:HG22	1.94	0.48
13:M:151:SER:O	13:M:155:THR:N	2.45	0.48
1:A:748:ASN:HB2	1:A:1071:ASP:HB3	1.96	0.48
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.95	0.48
3:C:43:ASN:HB3	3:C:55:ASP:HB2	1.95	0.48
5:E:5:ASN:ND2	5:E:50:MET:O	2.43	0.48
1:A:241:PRO:HA	1:A:256:LEU:HD21	1.94	0.48
3:C:142:ARG:NH2	10:J:67:GLU:OE2	2.43	0.48
1:A:129:LEU:HD11	1:A:196:ALA:HB2	1.96	0.47
10:J:17:LYS:O	10:J:21:TYR:N	2.39	0.47
1:A:381:SER:HB3	1:A:453:ILE:HB	1.97	0.47
2:B:379:ARG:HH21	2:B:581:PRO:HD3	1.80	0.47
1:A:74:GLY:HA3	1:A:364:PRO:HB3	1.97	0.47
1:A:560:GLN:O	1:A:575:LYS:NZ	2.45	0.47
1:A:568:VAL:HA	1:A:571:HIS:HB3	1.95	0.47
1:A:592:GLN:OE1	1:A:634:ASN:ND2	2.48	0.47
1:A:1176:ARG:NH2	6:F:154:ASP:O	2.48	0.47
2:B:154:GLU:OE1	2:B:443:LYS:NZ	2.47	0.47
2:B:242:ASP:OD2	2:B:414:LYS:NZ	2.36	0.47
2:B:518:ARG:NH1	2:B:539:CYS:O	2.46	0.47
13:M:88:ILE:HD12	13:M:90:LEU:HD21	1.97	0.47
14:N:35:LEU:H	14:N:115:SER:HA	1.79	0.47
14:N:55:LEU:HB3	14:N:136:VAL:HG22	1.97	0.47
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.96	0.47
5:E:94:LYS:HD3	5:E:123:LEU:HD22	1.97	0.47
13:M:299:LEU:O	13:M:303:THR:OG1	2.28	0.47
14:N:93:THR:O	14:N:98:SER:OG	2.30	0.47
2:B:676:VAL:HG12	2:B:677:THR:HG23	1.97	0.47
2:B:1160:GLU:HB3	2:B:1164:GLY:HA2	1.96	0.47
17:U:37:DG:H2"	17:U:38:DA:H5"	1.96	0.47
1:A:1180:ASN:HD22	6:F:87:LYS:HE2	1.80	0.46
13:M:344:VAL:N	13:M:395:ALA:O	2.45	0.46
3:C:241:GLY:N	3:C:261:GLY:O	2.49	0.46
1:A:370:PRO:HB3	1:A:379:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:LYS:HD3	16:T:18:TTD:H71	1.97	0.46
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.97	0.46
7:G:138:PHE:HB2	7:G:148:LEU:HB2	1.96	0.46
11:K:76:LEU:HA	11:K:79:VAL:HG22	1.98	0.46
2:B:281:CYS:SG	13:M:99:LYS:NZ	2.75	0.46
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.98	0.46
3:C:88:ASN:O	12:L:60:ARG:NH1	2.48	0.46
3:C:218:LYS:NZ	12:L:69:ALA:O	2.42	0.46
13:M:33:PRO:HA	14:N:128:ASN:HD21	1.80	0.46
1:A:174:SER:OG	1:A:175:SER:N	2.45	0.46
13:M:265:LEU:HB2	13:M:335:ILE:HG21	1.98	0.46
1:A:481:ARG:HB2	2:B:1069:ILE:HG21	1.98	0.46
2:B:655:TYR:O	2:B:659:ASP:CA	2.63	0.46
6:F:73:ALA:HB2	7:G:94:PRO:HG2	1.97	0.46
1:A:72:CYS:O	1:A:366:ARG:NH1	2.49	0.46
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.98	0.46
1:A:470:HIS:HA	2:B:1058:GLN:HE22	1.81	0.46
1:A:857:ALA:HB2	1:A:899:LYS:HD3	1.98	0.46
13:M:321:ASP:OD1	13:M:321:ASP:N	2.49	0.46
3:C:229:LEU:HD13	3:C:295:ARG:HA	1.98	0.46
9:I:3:VAL:HB	9:I:8:ILE:HD12	1.98	0.46
7:G:63:LYS:HA	7:G:67:ASN:HB2	1.98	0.46
2:B:894:LYS:HD2	12:L:45:ALA:HB3	1.97	0.45
2:B:1064:LYS:NZ	16:T:24:DT:OP2	2.40	0.45
8:H:7:ASP:HB3	8:H:58:THR:HG23	1.97	0.45
8:H:7:ASP:OD1	8:H:7:ASP:N	2.49	0.45
2:B:179:GLU:O	2:B:183:HIS:N	2.46	0.45
3:C:100:ARG:HH12	10:J:4:PRO:HA	1.82	0.45
6:F:97:ARG:NH2	6:F:124:GLU:OE2	2.43	0.45
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.99	0.45
1:A:717:PRO:HG3	1:A:724:PRO:HB3	1.99	0.45
1:A:1114:TYR:HA	5:E:152:LYS:HD3	1.99	0.45
1:A:1276:THR:OG1	9:I:21:ASN:ND2	2.50	0.45
8:H:99:GLY:O	8:H:139:ASN:HA	2.17	0.45
13:M:257:THR:O	13:M:260:GLN:HB2	2.16	0.45
1:A:1490:GLU:HB3	1:A:1494:ARG:HH12	1.82	0.45
1:A:641:GLU:OE1	1:A:644:ARG:NH1	2.48	0.45
13:M:265:LEU:HD11	13:M:332:ILE:HG23	1.99	0.45
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.99	0.45
1:A:28:SER:OG	1:A:76:GLN:O	2.29	0.45
1:A:679:TRP:HB3	2:B:1023:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:SER:OG	1:A:993:GLN:NE2	2.50	0.45
2:B:525:TRP:O	2:B:669:GLN:NE2	2.50	0.45
13:M:40:LEU:HD11	13:M:51:PHE:HB3	1.99	0.45
1:A:50:TYR:OH	1:A:379:GLU:OE2	2.33	0.45
2:B:568:LEU:HD13	2:B:604:ILE:HG23	1.99	0.45
2:B:975:HIS:CD2	14:N:169:GLU:HG3	2.52	0.45
4:D:95:ASP:HA	4:D:100:PRO:HG3	1.98	0.45
1:A:85:CYS:SG	1:A:86:TYR:N	2.90	0.45
2:B:307:GLU:HB2	9:I:7:LEU:HD11	1.98	0.45
13:M:11:GLU:HG2	13:M:86:LYS:HE2	1.99	0.45
17:U:43:DG:H2"	17:U:44:DA:C8	2.52	0.45
1:A:332:GLN:HB2	1:A:349:LEU:HD11	1.98	0.44
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.99	0.44
2:B:239:VAL:HG12	2:B:245:SER:HB2	1.99	0.44
2:B:897:GLU:OE2	2:B:899:GLN:NE2	2.50	0.44
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.50	0.44
3:C:310:PRO:HA	3:C:313:ILE:HD12	1.99	0.44
5:E:76:GLY:N	5:E:106:GLN:OE1	2.41	0.44
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.39	0.44
1:A:507:TYR:OH	1:A:641:GLU:OE2	2.29	0.44
2:B:940:GLU:OE2	3:C:293:ARG:NH2	2.48	0.44
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.49	0.44
16:T:23:DC:H2'	16:T:24:DT:H71	1.99	0.44
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.29	0.44
3:C:329:LYS:HE2	11:K:118:GLN:HB3	1.97	0.44
13:M:39:ASP:HB2	13:M:54:HIS:HB3	2.00	0.44
15:R:2:U:H2'	15:R:3:C:C6	2.53	0.44
1:A:36:THR:HB	1:A:45:VAL:HG11	1.98	0.44
1:A:79:ILE:HG12	1:A:390:LEU:HD21	1.99	0.44
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.99	0.44
13:M:128:LEU:HD22	13:M:139:LYS:HD3	1.98	0.44
1:A:646:GLU:HG2	1:A:650:LEU:HD12	1.99	0.44
1:A:671:GLN:HG2	1:A:934:LYS:HG2	2.00	0.44
1:A:949:GLN:NE2	1:A:979:GLY:O	2.44	0.44
2:B:795:GLU:OE1	3:C:217:ALA:N	2.49	0.44
13:M:178:LEU:HD12	13:M:182:THR:HG21	2.00	0.44
15:R:3:C:H2'	15:R:4:G:C8	2.52	0.44
1:A:463:LYS:HA	1:A:468:ARG:HB2	1.99	0.44
1:A:690:GLU:HA	11:K:81:MET:HE2	2.00	0.44
1:A:791:TYR:OH	1:A:1061:SER:O	2.28	0.44
2:B:841:ASP:N	2:B:845:LEU:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.99	0.44
1:A:499:PRO:HA	1:A:502:ALA:HB3	1.99	0.44
2:B:655:TYR:O	2:B:659:ASP:N	2.51	0.44
2:B:1021:GLU:OE2	3:C:293:ARG:NH1	2.51	0.44
7:G:48:SER:HB2	7:G:113:PHE:HB3	2.00	0.44
1:A:811:SER:HB3	1:A:815:ARG:HH12	1.82	0.43
1:A:1026:GLN:HE22	1:A:1603:MET:HB2	1.83	0.43
1:A:1651:THR:HB	6:F:92:ARG:HD2	2.00	0.43
4:D:80:THR:HB	4:D:83:SER:HB2	2.00	0.43
13:M:178:LEU:O	13:M:182:THR:OG1	2.28	0.43
2:B:556:SER:HB3	2:B:621:PRO:HG3	2.00	0.43
2:B:1133:MET:N	2:B:1168:VAL:O	2.46	0.43
3:C:335:GLN:HG2	11:K:49:LEU:HD23	2.00	0.43
1:A:344:ASN:HD21	1:A:348:LYS:HB3	1.82	0.43
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	1.99	0.43
2:B:179:GLU:HA	2:B:182:GLN:HB2	2.00	0.43
2:B:286:ARG:HH21	13:M:28:LYS:HB2	1.84	0.43
16:T:12:DT:H2'	16:T:13:DT:C6	2.53	0.43
1:A:884:ARG:NE	2:B:634:ARG:O	2.41	0.43
2:B:740:LYS:NZ	16:T:24:DT:OP1	2.42	0.43
3:C:117:ASP:HB3	3:C:120:LEU:HD13	2.01	0.43
11:K:89:CYS:SG	11:K:90:GLY:N	2.92	0.43
1:A:629:ASP:HB2	2:B:924:LYS:HE3	2.01	0.43
1:A:1441:LYS:HA	1:A:1444:ARG:HB2	2.00	0.43
2:B:232:TYR:HD1	2:B:384:LEU:HG	1.84	0.43
4:D:89:LEU:HA	4:D:92:ILE:HD12	1.99	0.43
5:E:63:ASN:HA	5:E:64:PRO:HD3	1.91	0.43
1:A:28:SER:OG	1:A:29:ALA:N	2.51	0.43
1:A:587:VAL:HG12	1:A:637:PHE:HD1	1.82	0.43
4:D:80:THR:HG22	4:D:83:SER:H	1.84	0.43
8:H:101:ALA:HA	8:H:116:TYR:HA	2.00	0.43
13:M:38:PHE:H	14:N:118:SER:HB2	1.83	0.43
13:M:256:MET:O	13:M:259:LEU:HB3	2.19	0.43
16:T:18:TTD:H2"	16:T:18:TTD:H6	1.56	0.43
1:A:441:THR:HG23	1:A:458:GLN:HE21	1.84	0.43
1:A:1497:ILE:H	1:A:1497:ILE:HG13	1.73	0.43
11:K:64:GLN:HE21	11:K:100:LEU:HD13	1.83	0.43
13:M:346:ILE:HD11	13:M:395:ALA:HB2	2.00	0.43
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	2.00	0.42
10:J:8:PHE:HD2	10:J:48:ARG:HH12	1.66	0.42
1:A:503:VAL:HG23	1:A:504:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:SER:HA	1:A:789:SER:HB2	2.01	0.42
2:B:186:GLU:OE2	2:B:731:VAL:N	2.45	0.42
2:B:252:TYR:OH	2:B:305:ARG:NE	2.44	0.42
2:B:730:GLY:HA2	2:B:765:PHE:HE1	1.84	0.42
1:A:1034:TYR:HA	1:A:1181:PRO:HB3	2.01	0.42
1:A:1276:THR:HG22	1:A:1288:ARG:HG3	2.00	0.42
1:A:394:LEU:HD23	1:A:397:ARG:HD2	2.01	0.42
1:A:1297:PHE:HE1	9:I:64:LYS:HD2	1.85	0.42
7:G:147:LEU:HB2	7:G:155:ALA:HB3	2.01	0.42
1:A:122:LEU:HD23	1:A:125:LEU:HD12	2.01	0.42
2:B:77:LYS:HE3	2:B:79:LEU:HB2	2.02	0.42
2:B:233:GLY:HA2	2:B:250:LEU:O	2.20	0.42
1:A:429:THR:O	1:A:433:ASP:N	2.49	0.42
1:A:481:ARG:HD3	2:B:1045:GLN:HE21	1.83	0.42
1:A:1184:ALA:HB2	1:A:1649:VAL:HG11	2.01	0.42
1:A:1293:HIS:CE1	1:A:1469:TRP:HB2	2.54	0.42
1:A:91:PHE:HE2	1:A:245:LYS:HD2	1.83	0.42
1:A:363:PRO:O	1:A:368:ARG:NH1	2.51	0.42
1:A:592:GLN:HG2	16:T:20:DC:H2"	2.02	0.42
2:B:70:GLU:HG2	2:B:98:SER:HB3	2.02	0.42
7:G:50:ALA:HB3	7:G:64:GLN:HE22	1.85	0.42
1:A:1026:GLN:HG3	1:A:1598:PHE:CG	2.55	0.42
1:A:1262:LEU:HB2	1:A:1265:GLU:HG3	2.02	0.42
6:F:151:LEU:HD23	6:F:151:LEU:HA	1.92	0.42
13:M:15:VAL:HG22	13:M:90:LEU:HD12	2.02	0.42
13:M:81:PHE:HA	13:M:87:SER:O	2.20	0.42
2:B:411:MET:HE1	2:B:476:LEU:HB3	2.01	0.42
1:A:1559:ARG:HG3	1:A:1586:ALA:HB1	2.01	0.41
2:B:21:ARG:HH12	10:J:55:ASP:H	1.67	0.41
2:B:920:ARG:NH2	2:B:965:GLU:OE2	2.47	0.41
3:C:57:ILE:HG12	3:C:297:HIS:ND1	2.35	0.41
14:N:90:MET:O	14:N:137:PHE:HA	2.20	0.41
1:A:1030:VAL:HG11	1:A:1584:LEU:HD21	2.02	0.41
1:A:1032:VAL:HB	1:A:1182:GLY:H	1.84	0.41
1:A:1546:VAL:HG13	1:A:1558:ALA:HB1	2.01	0.41
2:B:1163:GLN:HE21	2:B:1165:ASN:HD22	1.68	0.41
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.85	0.41
2:B:675:ALA:HB2	2:B:686:HIS:CG	2.55	0.41
2:B:1161:ASP:OD2	2:B:1163:GLN:NE2	2.52	0.41
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.02	0.41
13:M:82:ASN:O	13:M:86:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:HE22	13:M:166:ARG:HE	1.67	0.41
2:B:220:PRO:HA	2:B:231:HIS:CE1	2.56	0.41
2:B:265:ARG:HH11	2:B:474:SER:HB3	1.85	0.41
3:C:70:ILE:HA	3:C:74:GLU:HB2	2.02	0.41
10:J:7:CYS:HB3	10:J:11:GLY:H	1.86	0.41
1:A:536:ILE:HG12	1:A:577:VAL:HG22	2.02	0.41
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	2.01	0.41
2:B:93:ASN:HB3	2:B:440:PHE:HE2	1.85	0.41
2:B:213:HIS:HE1	2:B:636:GLN:HE22	1.69	0.41
2:B:944:GLN:NE2	10:J:9:SER:O	2.53	0.41
2:B:1047:ARG:HH11	2:B:1068:GLY:H	1.69	0.41
14:N:176:ASP:HB3	14:N:178:GLU:HG3	2.01	0.41
2:B:480:GLN:O	2:B:484:TYR:OH	2.30	0.41
3:C:105:PRO:HG2	3:C:187:ALA:HB3	2.02	0.41
8:H:56:THR:HB	8:H:145:ARG:HB3	2.03	0.41
1:A:419:ILE:O	1:A:423:LEU:N	2.54	0.41
1:A:484:ILE:HG12	1:A:631:ASP:HB2	2.03	0.41
2:B:137:LEU:HB3	2:B:158:CYS:HB2	2.02	0.41
13:M:31:ARG:HH21	14:N:103:ASN:HD21	1.68	0.41
13:M:261:LEU:HD11	13:M:335:ILE:HG12	2.03	0.41
14:N:92:ASP:O	14:N:97:SER:OG	2.32	0.41
16:T:36:DA:H2"	16:T:37:DG:C8	2.56	0.41
1:A:424:MET:O	1:A:427:PHE:HB3	2.21	0.41
2:B:16:PHE:HZ	2:B:751:ILE:HG12	1.85	0.41
2:B:328:GLN:OE1	13:M:109:ARG:N	2.44	0.41
2:B:1114:GLN:HE22	2:B:1129:ARG:HH11	1.69	0.41
7:G:49:LEU:HD13	7:G:61:VAL:HG23	2.03	0.41
9:I:34:LYS:H	13:M:59:ARG:NE	2.18	0.41
2:B:75:ASP:OD1	2:B:75:ASP:N	2.54	0.41
2:B:206:LEU:HB2	2:B:403:LEU:HB3	2.03	0.41
3:C:192:LEU:HG	10:J:2:ILE:HD11	2.04	0.41
4:D:88:GLN:HE21	7:G:152:ALA:HA	1.85	0.41
1:A:1039:ARG:HA	1:A:1045:LEU:HA	2.02	0.40
2:B:12:ARG:HD2	2:B:977:ILE:HG23	2.03	0.40
2:B:1119:ARG:HD3	2:B:1160:GLU:HB2	2.03	0.40
3:C:234:ASN:O	3:C:289:VAL:HA	2.21	0.40
1:A:1028:GLU:HA	1:A:1187:ILE:HD11	2.03	0.40
2:B:820:PRO:HB2	13:M:357:PRO:HG2	2.02	0.40
13:M:186:ARG:HD3	13:M:363:LEU:HD23	2.02	0.40
1:A:482:SER:HB2	1:A:501:PHE:HE2	1.86	0.40
2:B:609:ARG:NH2	2:B:668:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:169:VAL:O	7:G:215:GLY:HA2	2.22	0.40
11:K:107:THR:OG1	11:K:111:THR:O	2.33	0.40
13:M:262:LEU:O	13:M:265:LEU:HB3	2.22	0.40
16:T:18:TTD:O5P	16:T:18:TTD:H1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	1461/1664 (88%)	1348 (92%)	113 (8%)	0	100	100
2	B	1167/1203 (97%)	1084 (93%)	83 (7%)	0	100	100
3	C	304/335 (91%)	287 (94%)	17 (6%)	0	100	100
4	D	55/137 (40%)	54 (98%)	1 (2%)	0	100	100
5	E	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
6	F	98/155 (63%)	91 (93%)	7 (7%)	0	100	100
7	G	197/326 (60%)	186 (94%)	11 (6%)	0	100	100
8	H	128/146 (88%)	118 (92%)	10 (8%)	0	100	100
9	I	63/125 (50%)	57 (90%)	6 (10%)	0	100	100
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	101/142 (71%)	98 (97%)	3 (3%)	0	100	100
12	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
13	M	394/415 (95%)	363 (92%)	31 (8%)	0	100	100
14	N	156/233 (67%)	135 (86%)	21 (14%)	0	100	100
All	All	4447/5236 (85%)	4123 (93%)	324 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	1301/1465 (89%)	1301 (100%)	0	100	100
2	B	1027/1053 (98%)	1027 (100%)	0	100	100
3	C	270/296 (91%)	270 (100%)	0	100	100
4	D	56/116 (48%)	56 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	179/291 (62%)	179 (100%)	0	100	100
8	H	116/128 (91%)	116 (100%)	0	100	100
9	I	57/110 (52%)	57 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	93/130 (72%)	93 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	354/371 (95%)	354 (100%)	0	100	100
14	N	146/220 (66%)	146 (100%)	0	100	100
All	All	3990/4636 (86%)	3990 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	213	ASN
1	A	221	HIS
1	A	340	HIS
1	A	344	ASN
1	A	407	GLN
1	A	521	GLN
1	A	525	ASN
1	A	642	ASN

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Mol	Chain	Res	Type
1	A	730	GLN
1	A	993	GLN
1	A	998	HIS
1	A	1026	GLN
1	A	1180	ASN
1	A	1319	ASN
1	A	1461	ASN
1	A	1629	ASN
2	B	87	ASN
2	B	168	ASN
2	B	213	HIS
2	B	575	HIS
2	B	683	ASN
2	B	715	ASN
2	B	745	GLN
2	B	1010	ASN
2	B	1094	ASN
2	B	1165	ASN
3	C	161	HIS
3	C	175	GLN
4	D	88	GLN
7	G	26	ASN
9	I	21	ASN
13	M	323	GLN
13	M	351	HIS
14	N	128	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	10/10 (100%)	1 (10%)	1 (10%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	2	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	R	1	A

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

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	$\#\|Z\| > 2$
16	TTD	T	18	16	42,45,46	3.21	18 (42%)	62,74,77	2.69	24 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	TTD	T	18	16	-	12/22/109/110	0/5/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	18	TTD	C2-N1	7.55	1.51	1.36
16	T	18	TTD	C5-C6	-7.40	1.46	1.55
16	T	18	TTD	C5T-C6T	-6.91	1.47	1.55
16	T	18	TTD	C2T-N3T	6.32	1.49	1.38
16	T	18	TTD	C2-N3	6.29	1.49	1.38
16	T	18	TTD	C2T-N1T	6.00	1.48	1.36
16	T	18	TTD	C2'-C3R	-5.81	1.39	1.52
16	T	18	TTD	C4T-N3T	5.40	1.45	1.37
16	T	18	TTD	C4-N3	4.95	1.45	1.37
16	T	18	TTD	C3'-C4'	-2.57	1.45	1.53
16	T	18	TTD	C6-N1	2.53	1.50	1.46
16	T	18	TTD	PB-O3R	2.44	1.66	1.60
16	T	18	TTD	O4-C4	-2.43	1.18	1.22
16	T	18	TTD	O2T-C2T	-2.37	1.18	1.23
16	T	18	TTD	O2-C2	-2.35	1.18	1.23
16	T	18	TTD	C6T-C6	2.20	1.63	1.56
16	T	18	TTD	O4T-C4T	-2.08	1.19	1.22
16	T	18	TTD	C2'-C1'	-2.07	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	18	TTD	O4R-C1R-N1T	10.05	120.55	108.65
16	T	18	TTD	O4'-C1'-N1	7.39	117.40	108.65
16	T	18	TTD	C4-N3-C2	-5.02	118.96	126.67
16	T	18	TTD	N3-C2-N1	4.67	121.54	116.69
16	T	18	TTD	C2'-C1'-N1	-4.45	109.58	115.59
16	T	18	TTD	C3R-C2'-C1'	4.33	111.20	102.91
16	T	18	TTD	O2-C2-N3	-4.29	113.50	121.50
16	T	18	TTD	C5T-C6T-N1T	4.07	121.31	115.61
16	T	18	TTD	C5-C4-N3	3.93	119.48	116.06
16	T	18	TTD	C4T-N3T-C2T	-3.89	120.69	126.67
16	T	18	TTD	C5T-C4T-N3T	3.77	119.34	116.06
16	T	18	TTD	N3T-C2T-N1T	3.52	120.35	116.69
16	T	18	TTD	C6-C5-C4	3.18	123.56	114.50
16	T	18	TTD	O4-C4-C5	-3.16	120.35	122.88
16	T	18	TTD	C5T-C6T-C6	-2.86	84.59	89.28
16	T	18	TTD	C4'-O4R-C1R	-2.61	103.15	109.45
16	T	18	TTD	O2T-C2T-N1T	-2.58	119.48	123.49
16	T	18	TTD	C5-C5T-C6T	2.41	91.38	88.38
16	T	18	TTD	C5M-C5T-C6T	-2.41	106.77	114.16
16	T	18	TTD	PB-O5R-C5R	-2.26	108.45	121.68
16	T	18	TTD	C5'-C4R-C3R	-2.19	109.53	114.53
16	T	18	TTD	C5-C5T-C4T	2.19	120.43	113.21
16	T	18	TTD	O4P-PB-O3R	2.18	115.40	106.78
16	T	18	TTD	O4T-C4T-N3T	-2.17	117.05	120.50

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	T	18	TTD	C2'-C3R-O3R-PB
16	T	18	TTD	O4'-C1'-N1-C2
16	T	18	TTD	O4'-C1'-N1-C6
16	T	18	TTD	O4R-C4'-C5R-O5R
16	T	18	TTD	O4'-C4R-C5'-O5'
16	T	18	TTD	C3'-C4'-C5R-O5R
16	T	18	TTD	C2R-C1R-N1T-C6T
16	T	18	TTD	C2R-C1R-N1T-C2T
16	T	18	TTD	O4R-C1R-N1T-C6T
16	T	18	TTD	O4R-C1R-N1T-C2T
16	T	18	TTD	C5R-O5R-PB-O3R
16	T	18	TTD	C4'-C5R-O5R-PB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	18	TTD	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

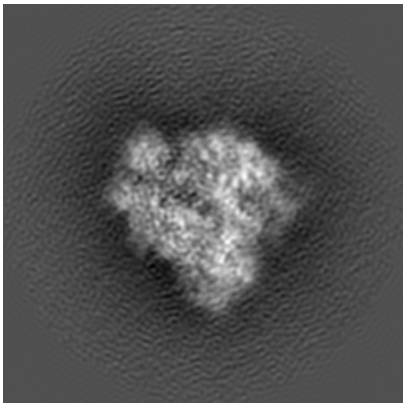
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0147. These allow visual inspection of the internal detail of the map and identification of artifacts.

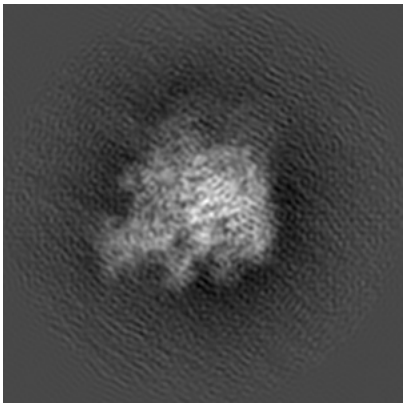
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

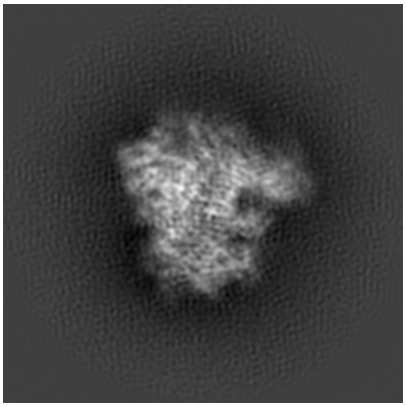
6.1.1 Primary map



X



Y

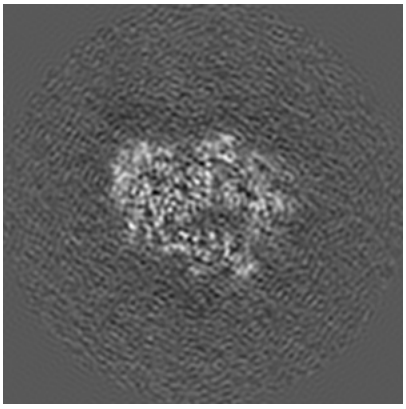


Z

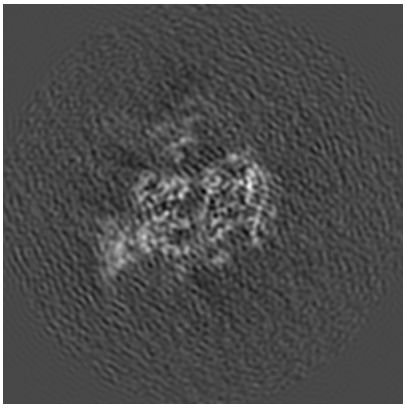
The images above show the map projected in three orthogonal directions.

6.2 Central slices

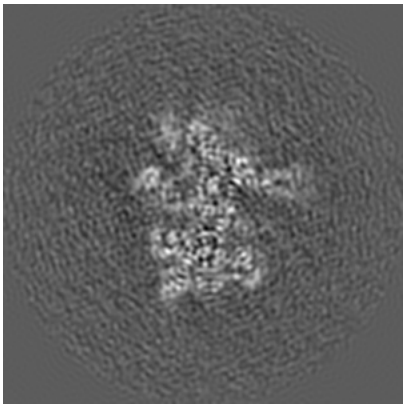
6.2.1 Primary map



X Index: 144



Y Index: 144

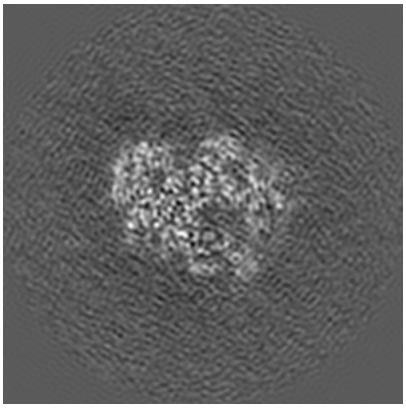


Z Index: 144

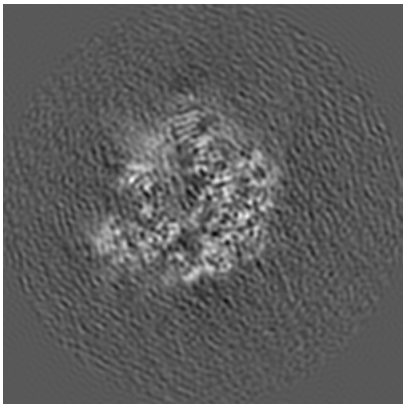
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

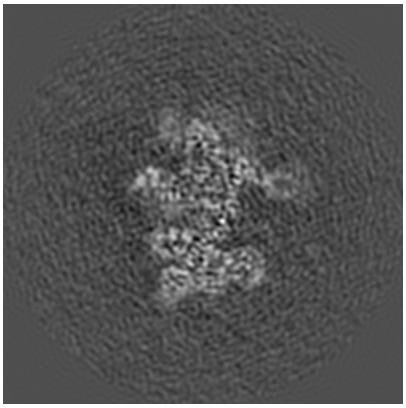
6.3.1 Primary map



X Index: 146



Y Index: 158



Z Index: 146

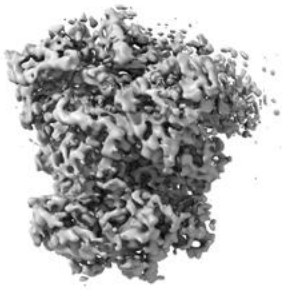
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

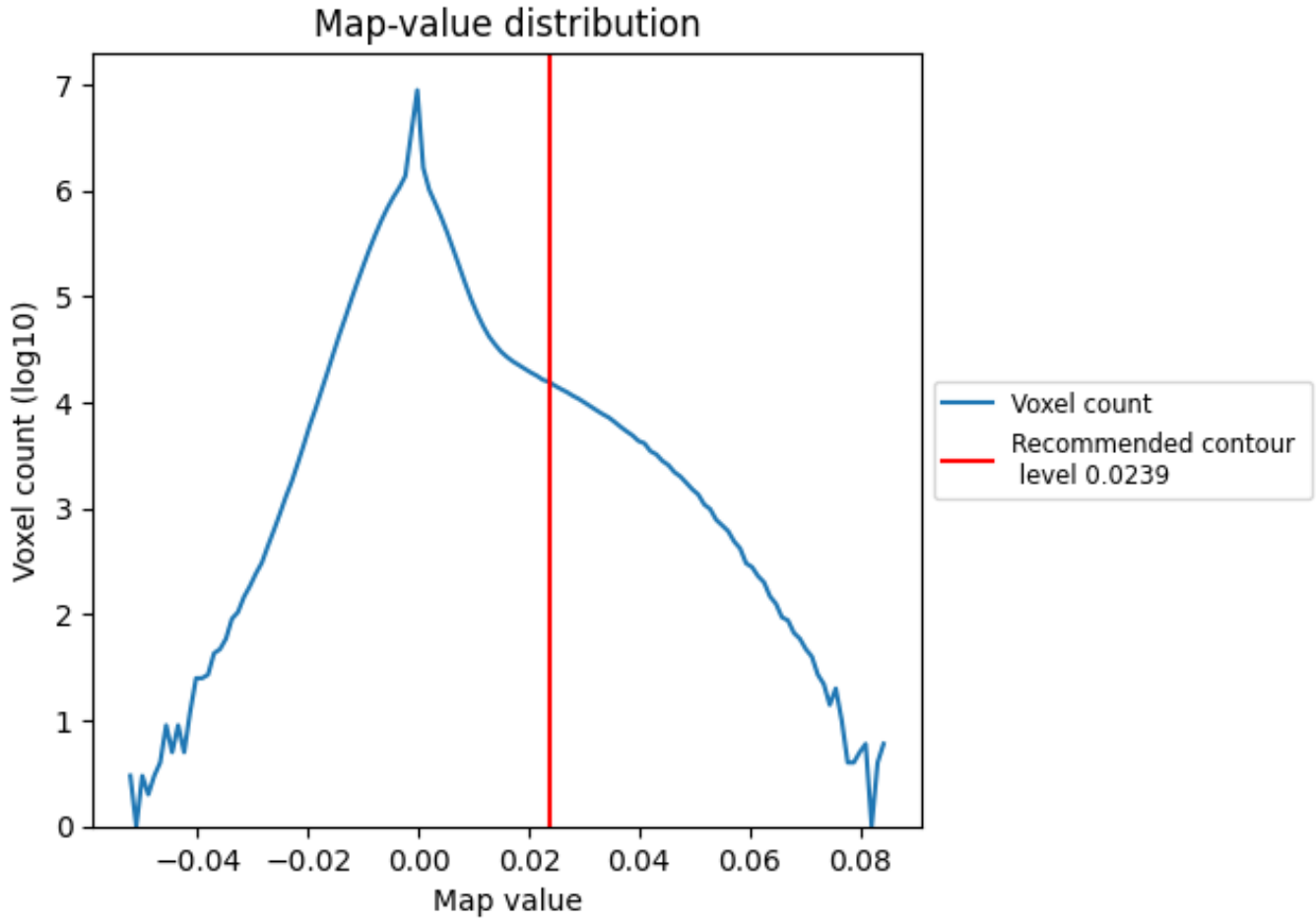
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

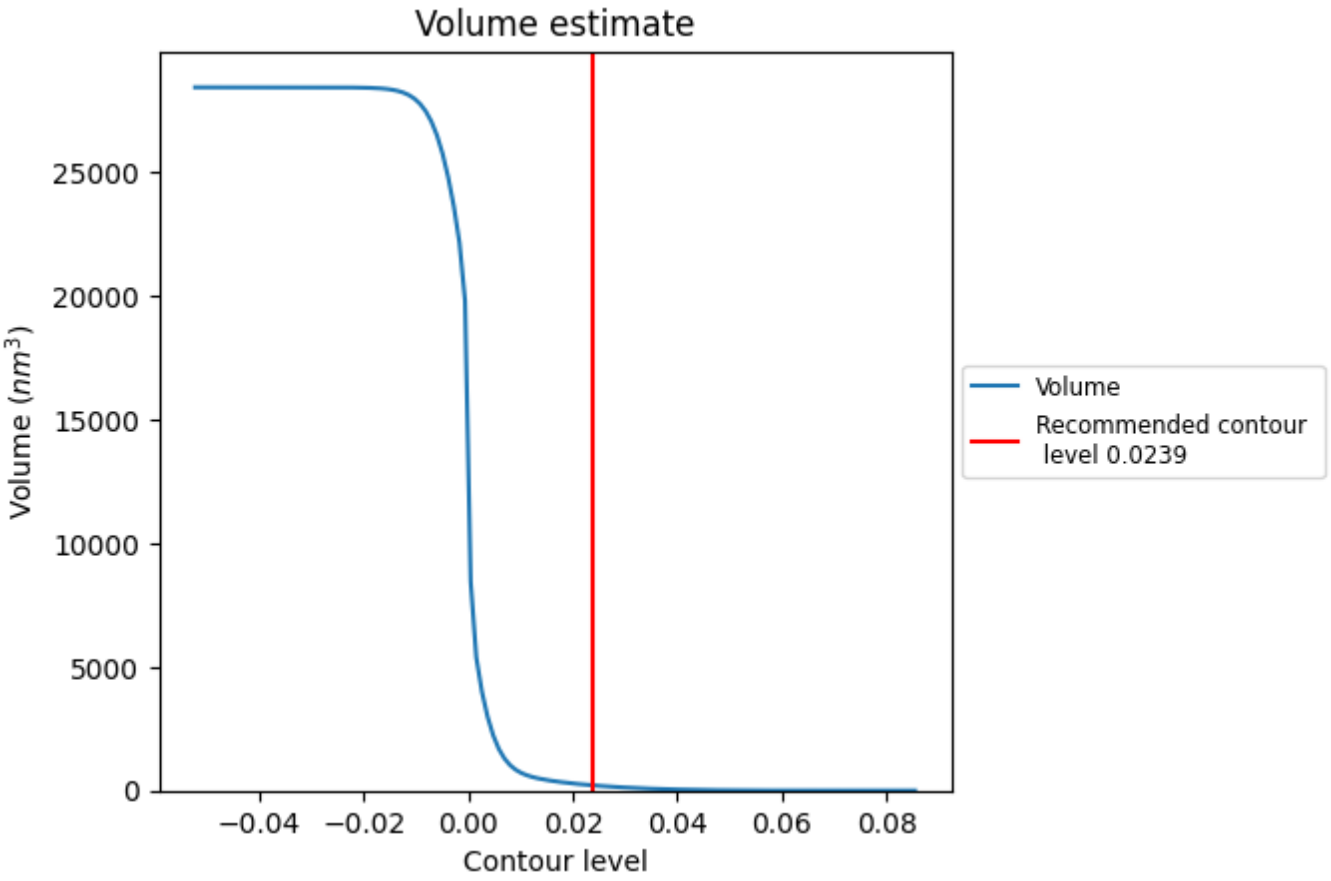
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

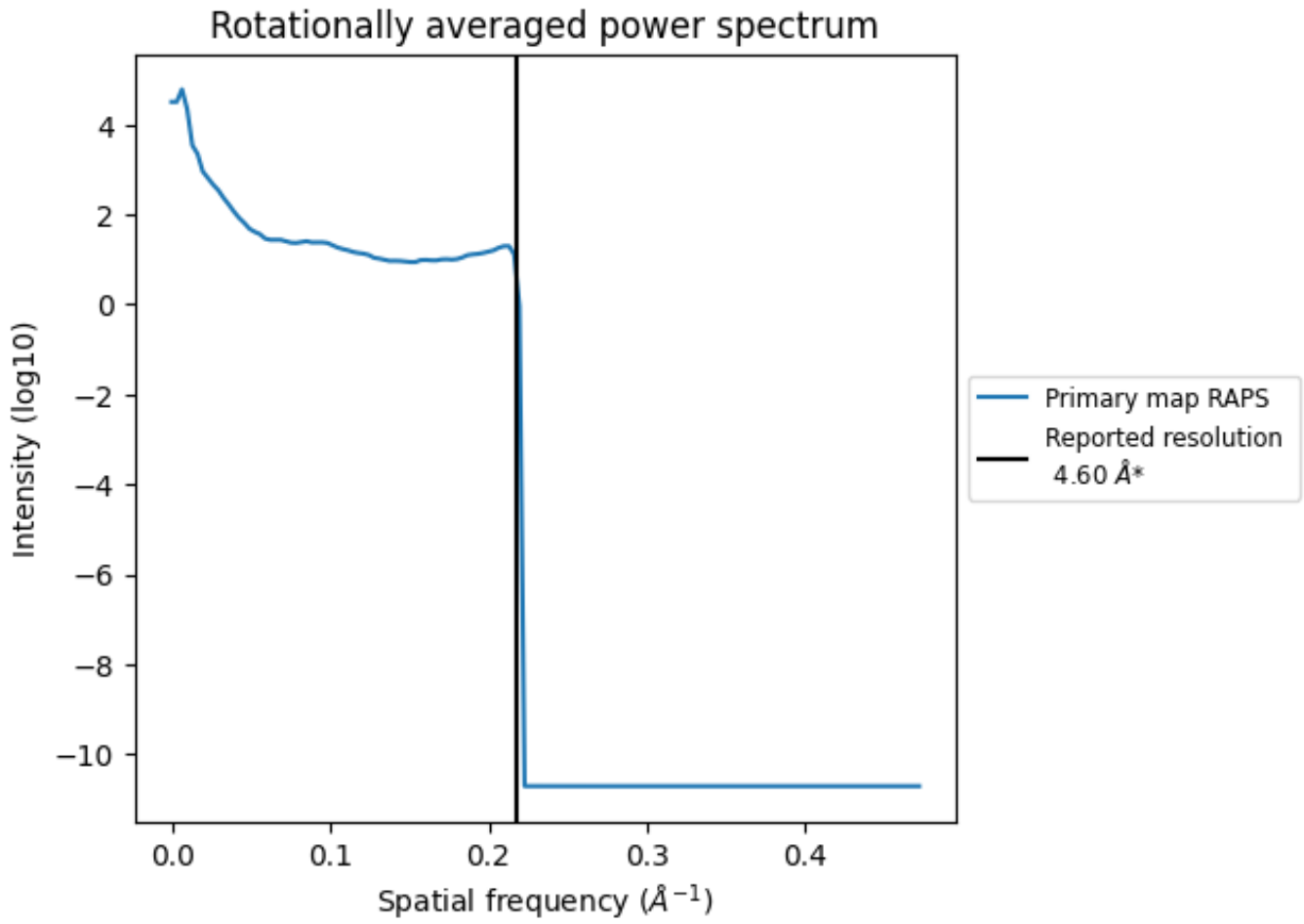
7.2 Volume estimate



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 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 (i)



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

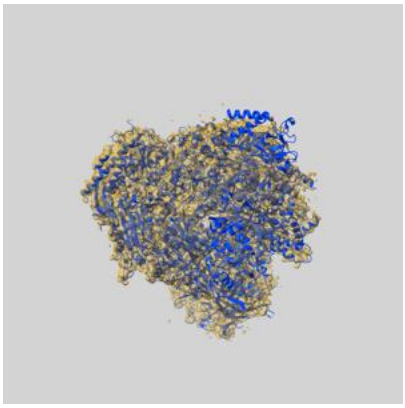
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

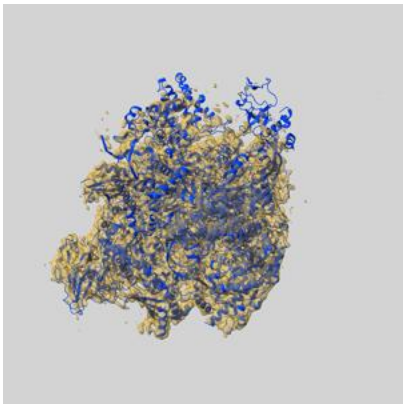
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0147 and PDB model 6H68. Per-residue inclusion information can be found in section 3 on page 7.

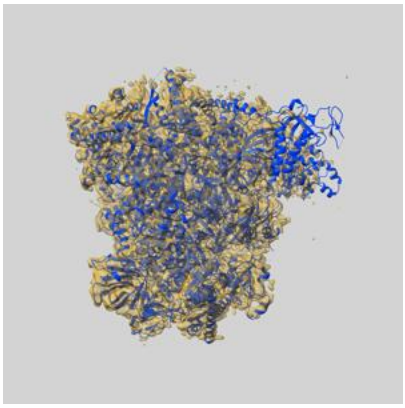
9.1 Map-model overlay



X



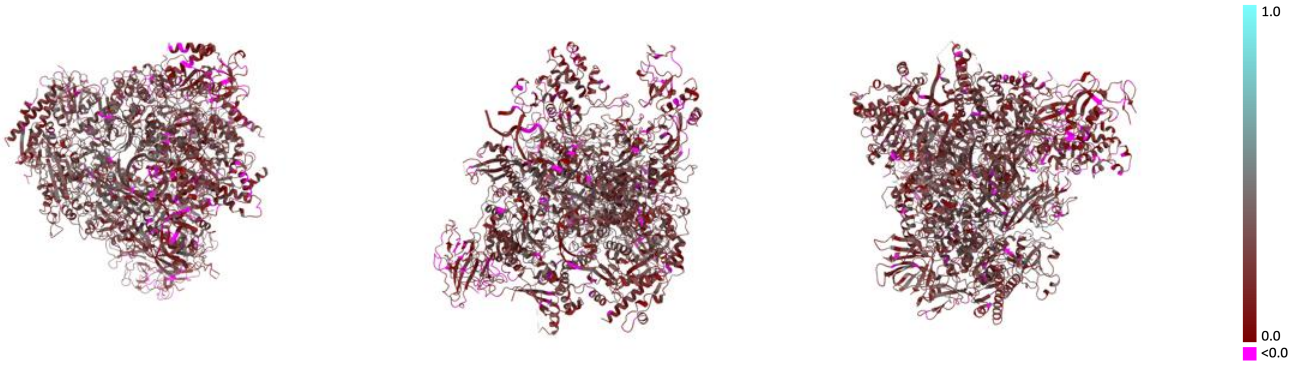
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0239 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.

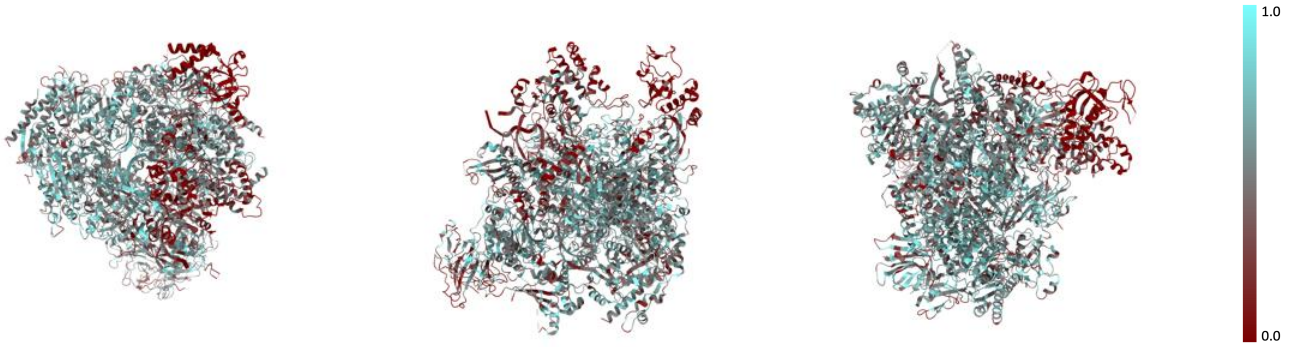
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

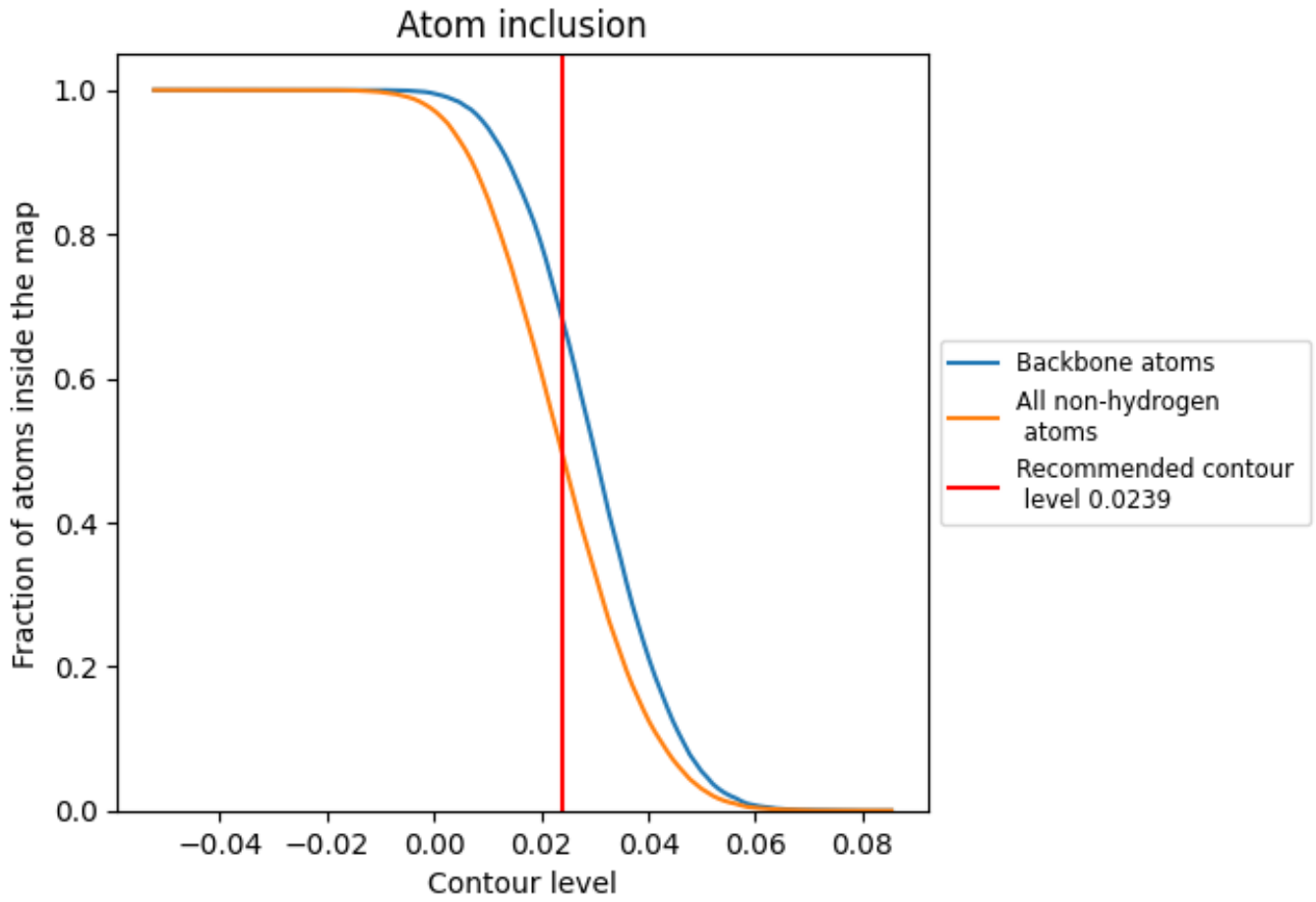
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0239).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 50% 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 (0.0239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4968	0.2470
A	0.5366	0.2640
B	0.5730	0.2840
C	0.5656	0.2740
D	0.1274	0.1340
E	0.5163	0.2290
F	0.5868	0.2410
G	0.2204	0.1630
H	0.5392	0.2440
I	0.3962	0.1910
J	0.6322	0.2930
K	0.5131	0.2450
L	0.5289	0.2950
M	0.2496	0.1650
N	0.3748	0.1770
R	0.7000	0.2960
T	0.5153	0.2030
U	0.3911	0.1650