Full wwPDB EM Validation Report

May 12, 2024 – 09:48 am BST

PDB ID	:	6RUI
EMDB ID	:	EMD-10006
Title	:	RNA Polymerase I Pre-initiation complex DNA opening intermediate 2
Authors	:	Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on	:	2019-05-28
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

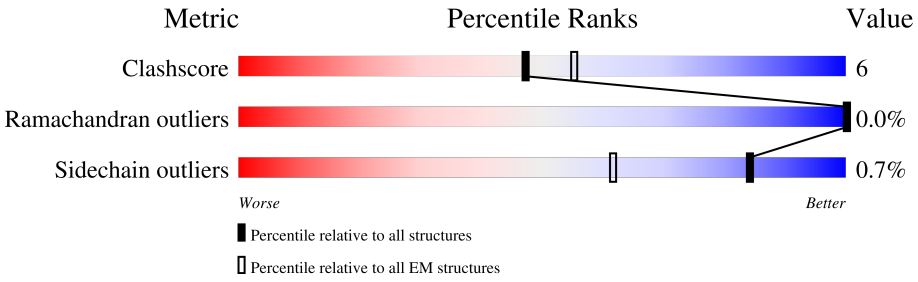
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	T	70	50% 46% 23% 31%
2	U	70	53% 44% 21% 34%
3	I	125	35% 82% 18%
4	N	233	35% 52% 8% 40%
5	M	415	13% 23% 74%
6	A	1664	5% 77% 11% 12%
7	B	1203	83% 15%
8	C	335	80% 10% 9%

Continued on next page...

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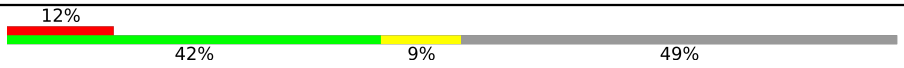
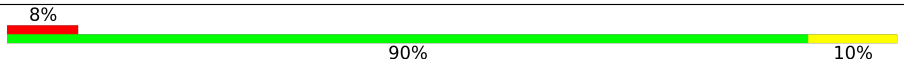
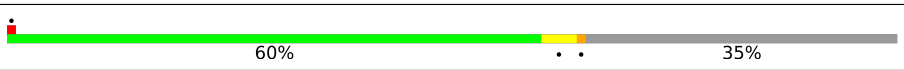
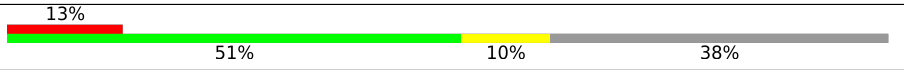
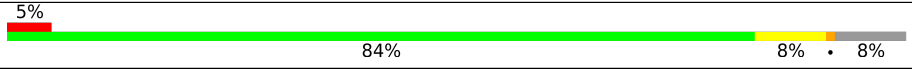
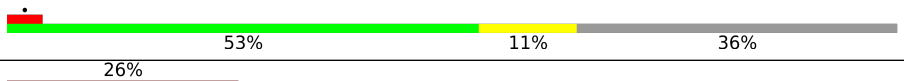
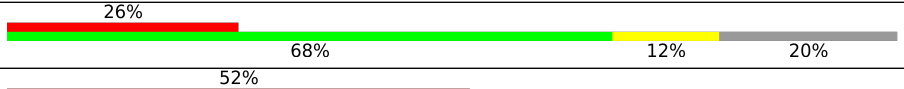
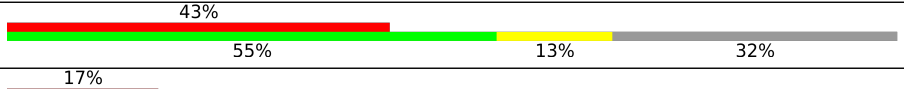
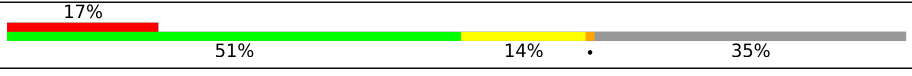
Mol	Chain	Length	Quality of chain
9	D	137	
10	E	215	
11	F	155	
12	G	326	
13	H	146	
14	J	70	
15	K	142	
16	L	70	
17	O	627	
18	Q	514	
19	S	894	
20	R	507	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51525 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 DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	T	48	958	462	153	295	48	0	0

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	U	46	965	457	197	266	45	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA12.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	139	1103	706	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	108	856	543	142	171	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1465	11565	7306	2011	2186	62	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	1180	Total	C	N	O	S	0	0
			9365	5920	1641	1754	50		

- Molecule 8 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	70	Total	C	N	O	S	0	0
			551	340	100	109	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	202	Total	C	N	O	S	0	0
			1600	1026	276	293	5		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	134	Total	C	N	O	S	0	0
			1072	676	181	211	4		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	103	Total	C	N	O	S	0	0
			810	506	132	167	5		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	504	Total	C	N	O	S	0	0
			4139	2663	666	788	22		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	477	Total	C	N	O	S	0	0
			3936	2529	675	712	20		

- Molecule 19 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	610	Total	C	N	O	S	0	0
			4963	3160	842	950	11		

- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	330	Total	C	N	O	S	0	0
			2771	1791	489	480	11		

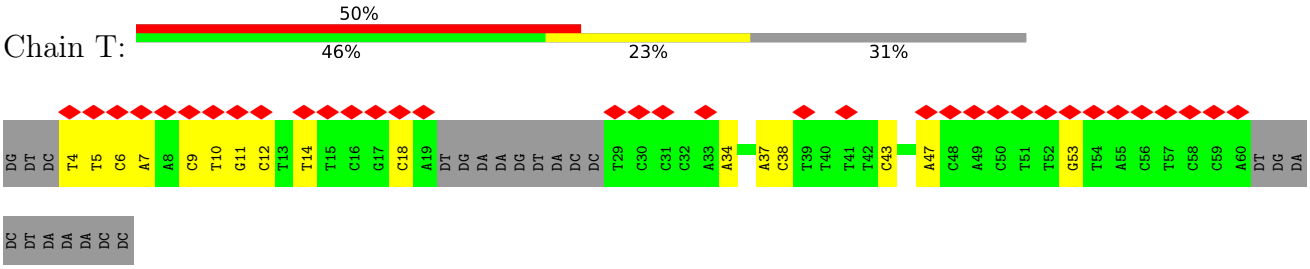
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
21	Q	1	1	1	0

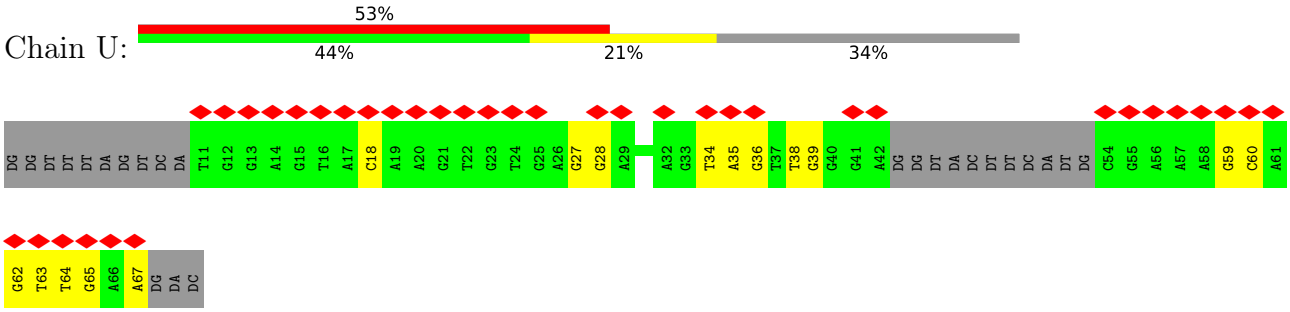
3 Residue-property plots (i)

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.

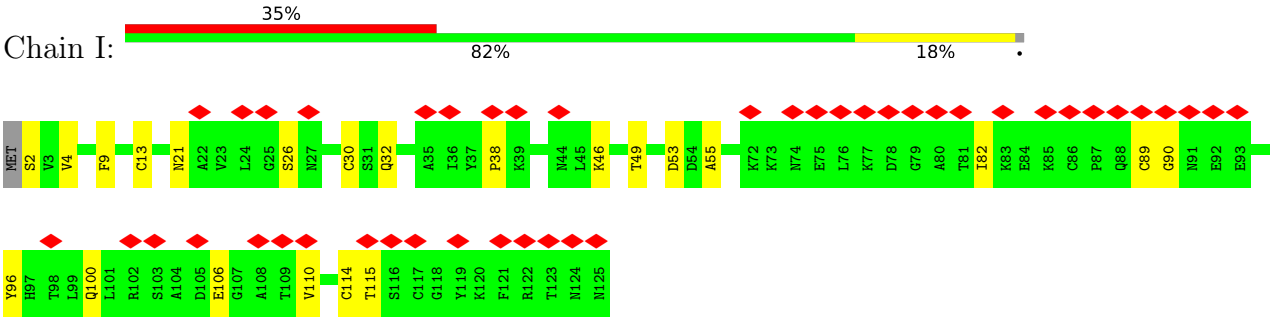
• Molecule 1: Template strand



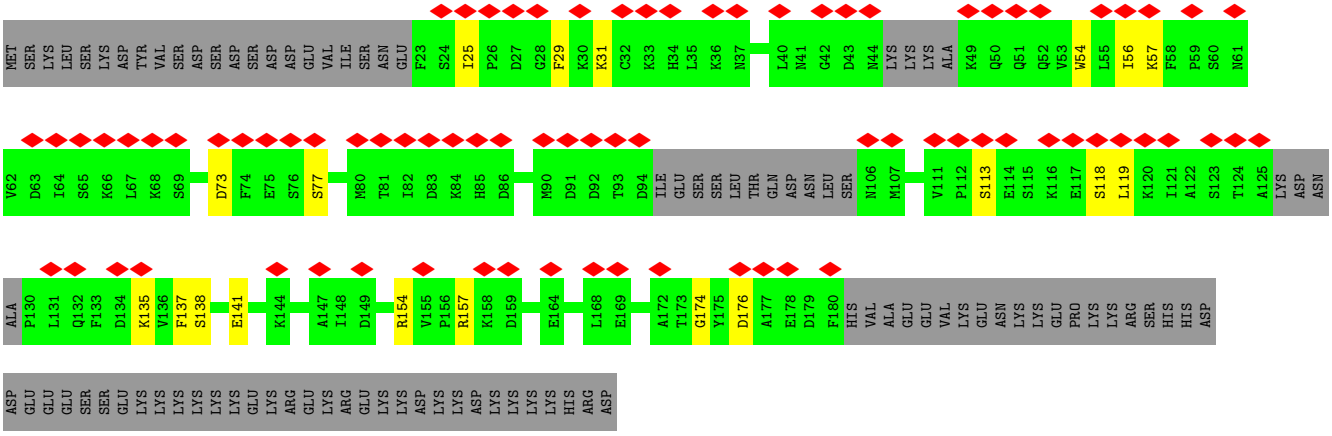
• Molecule 2: Nontemplate strand



• Molecule 3: DNA-directed RNA polymerase I subunit RPA12

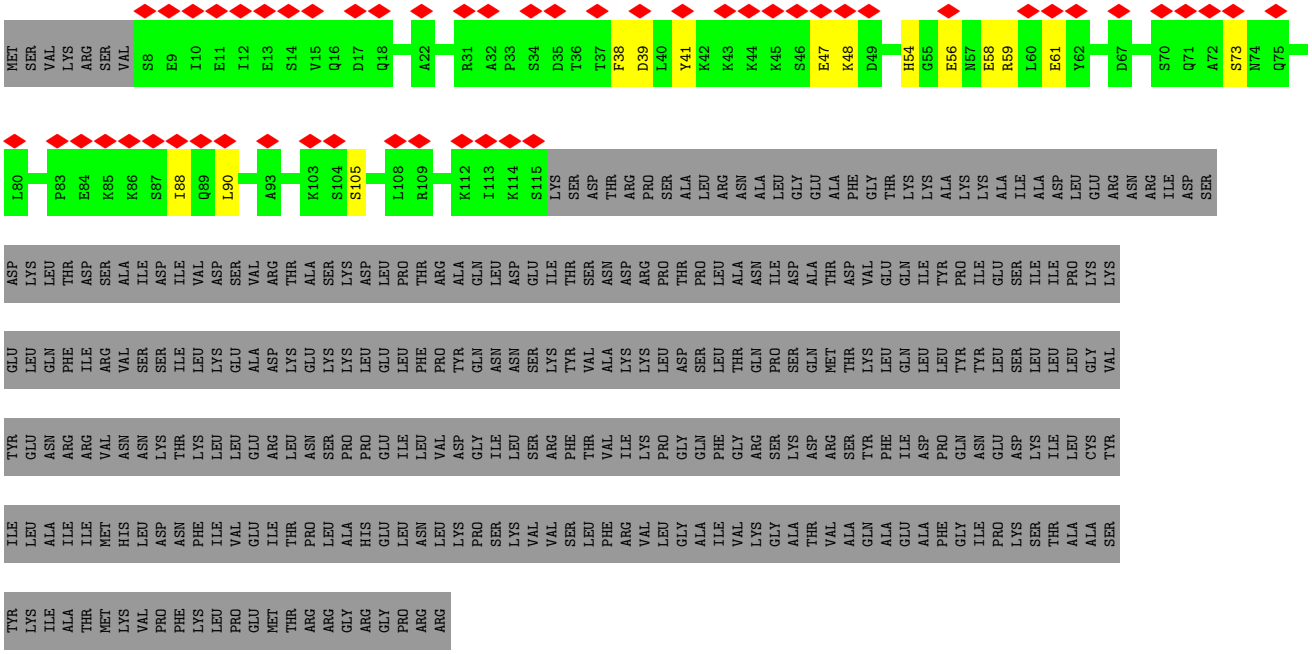


• Molecule 4: DNA-directed RNA polymerase I subunit RPA34



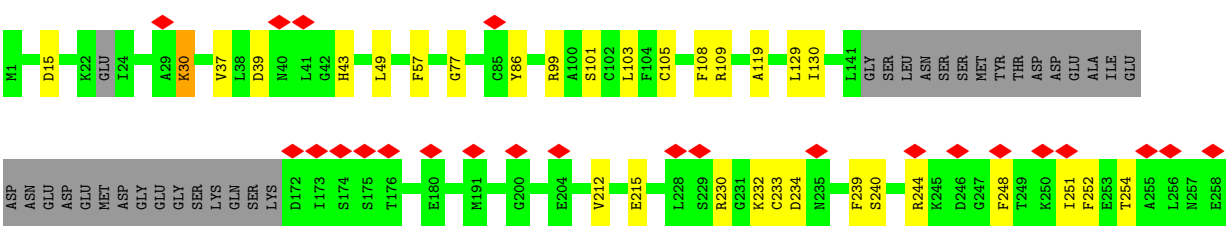
• Molecule 5: DNA-directed RNA polymerase I subunit RPA49

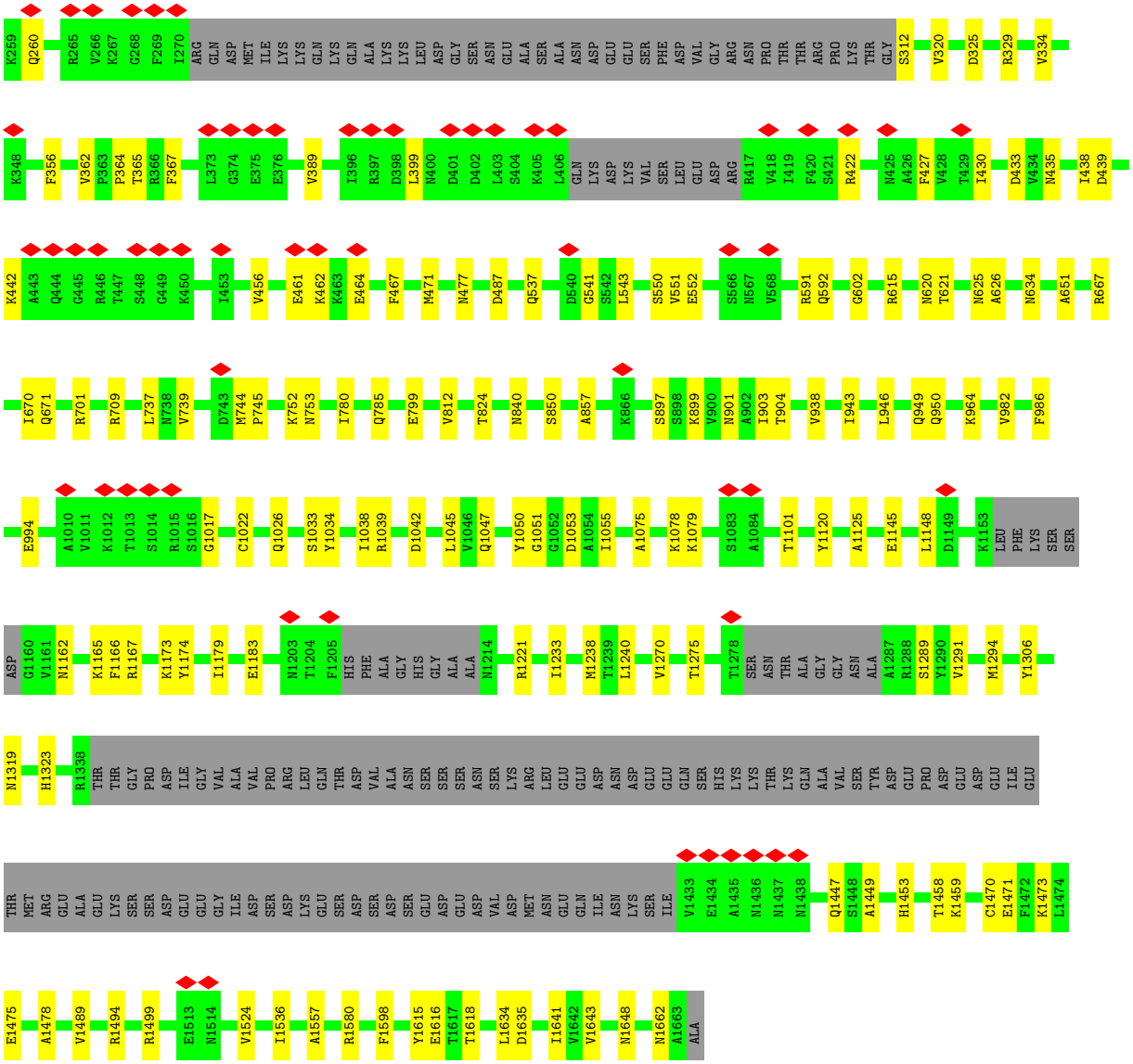
Chain M:



• Molecule 6: DNA-directed RNA polymerase I subunit RPA190

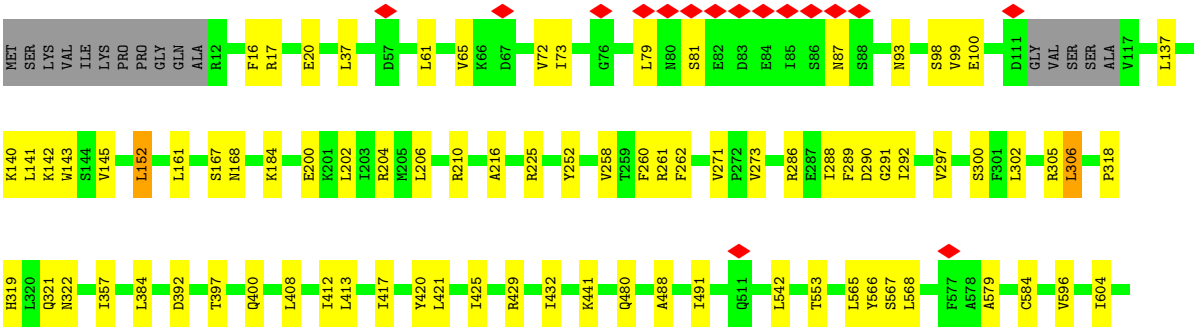
Chain A:

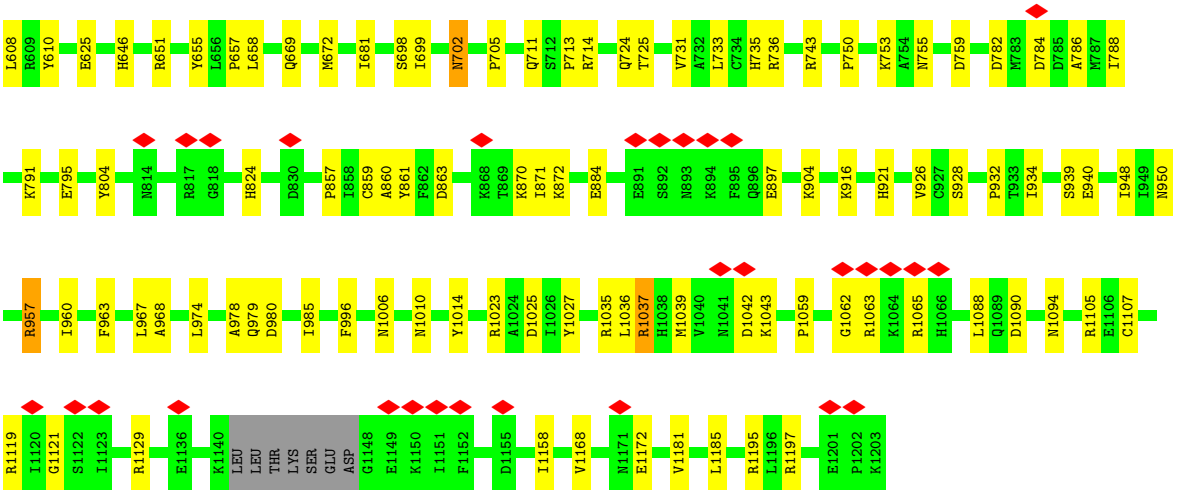




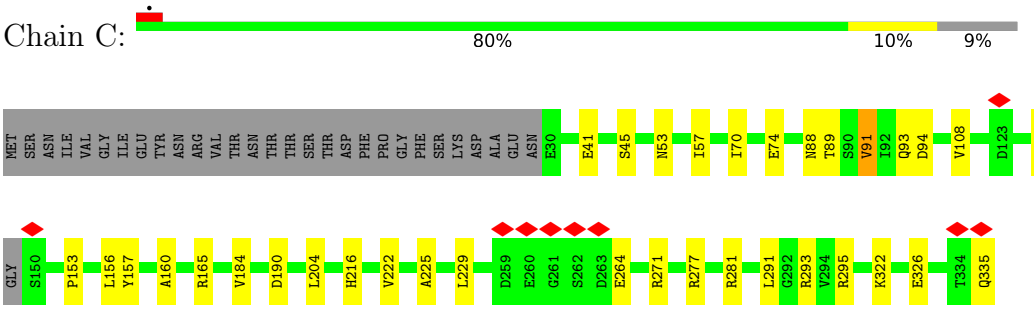
• Molecule 7: DNA-directed RNA polymerase I subunit RPA135

Chain B:

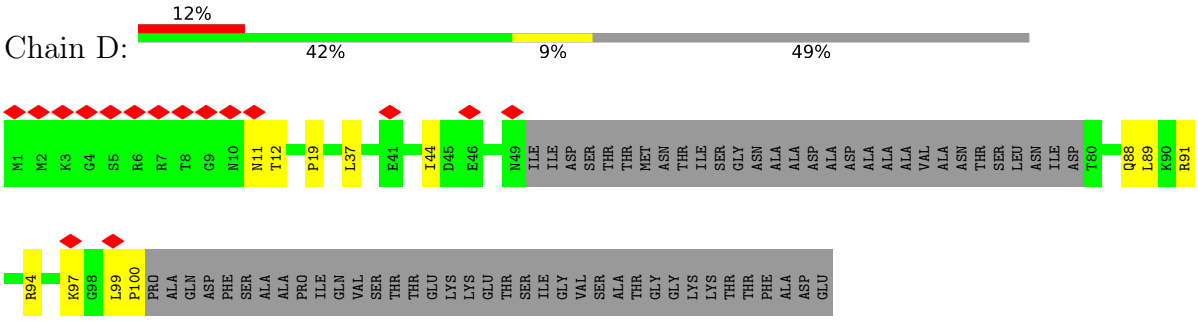




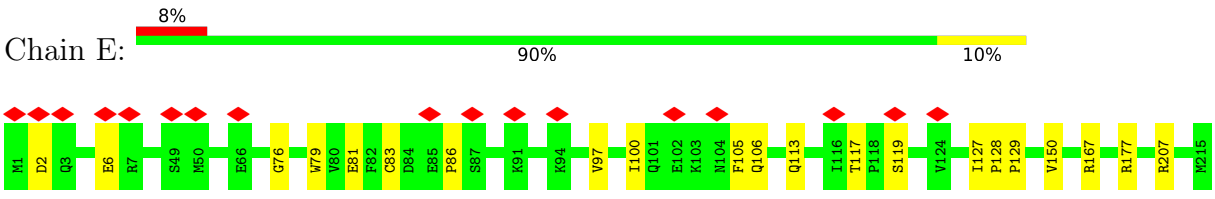
• Molecule 8: DNA-directed RNA polymerases I and III subunit RPAC1



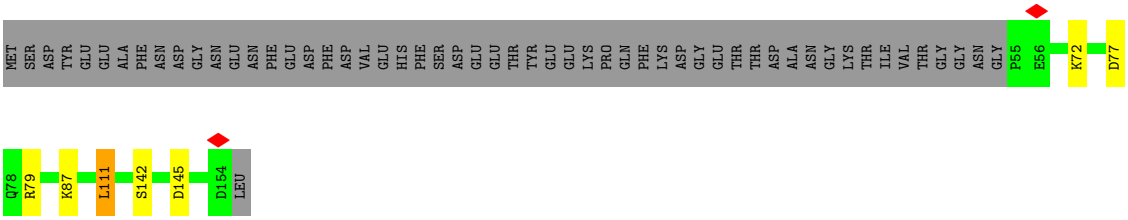
• Molecule 9: DNA-directed RNA polymerase I subunit RPA14



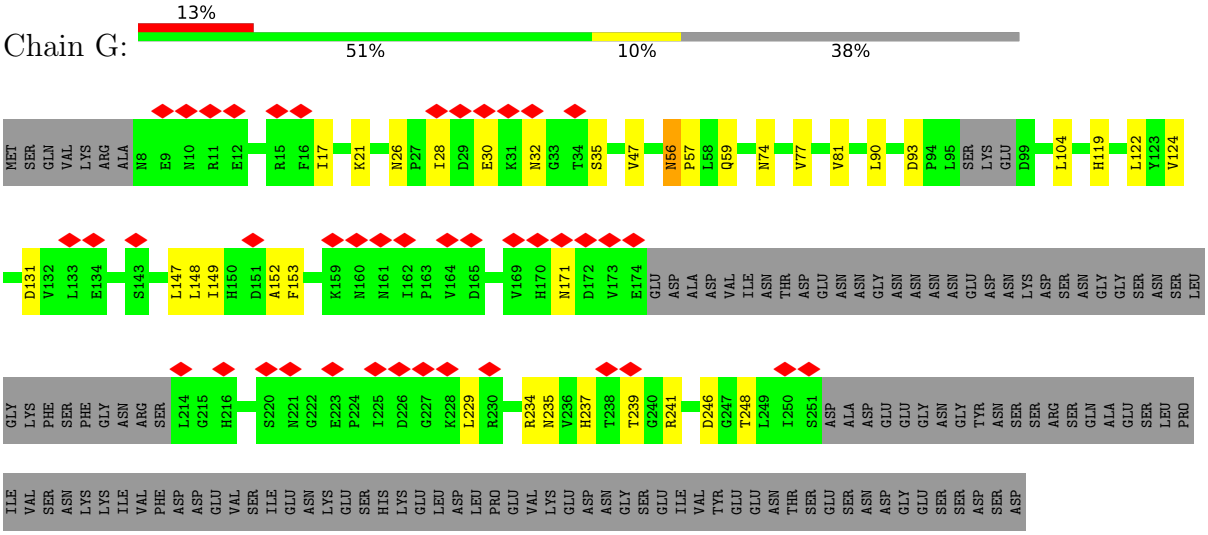
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC1



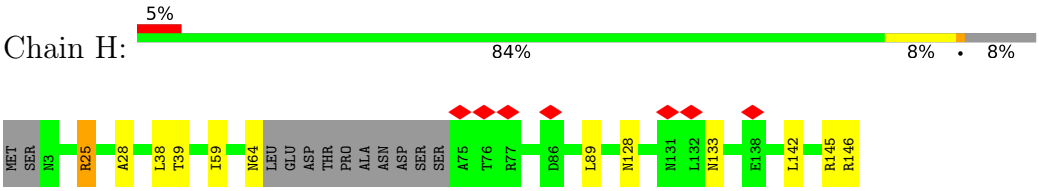
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC2



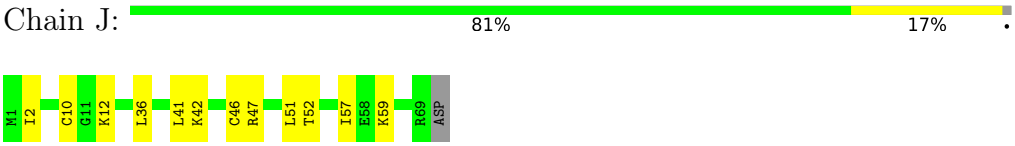
• Molecule 12: DNA-directed RNA polymerase I subunit RPA43



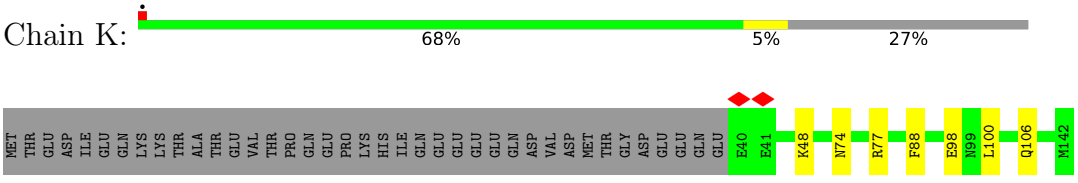
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC3



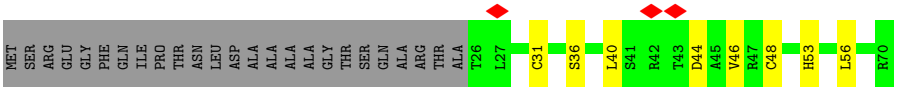
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 15: DNA-directed RNA polymerases I and III subunit RPAC2

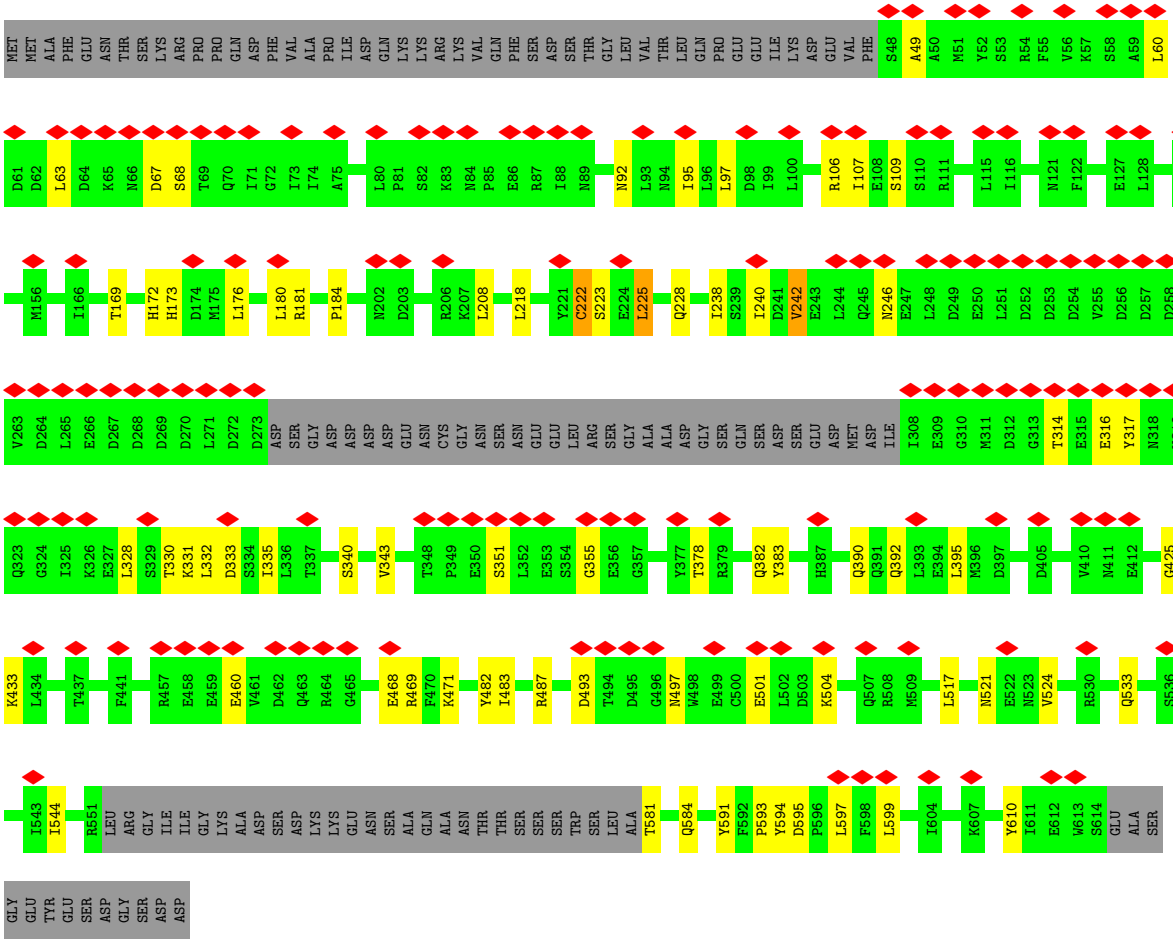


• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4



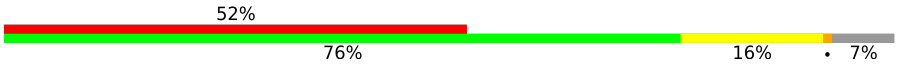
• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN3

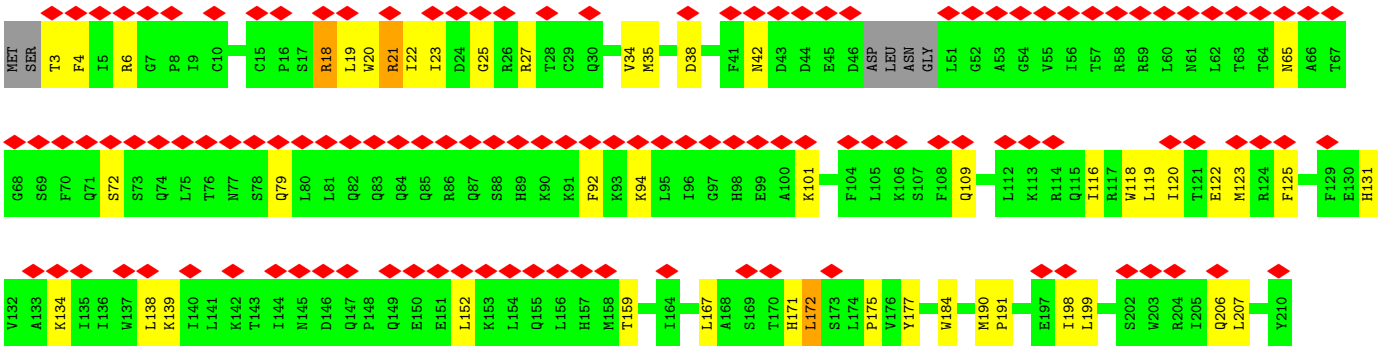
Chain O:

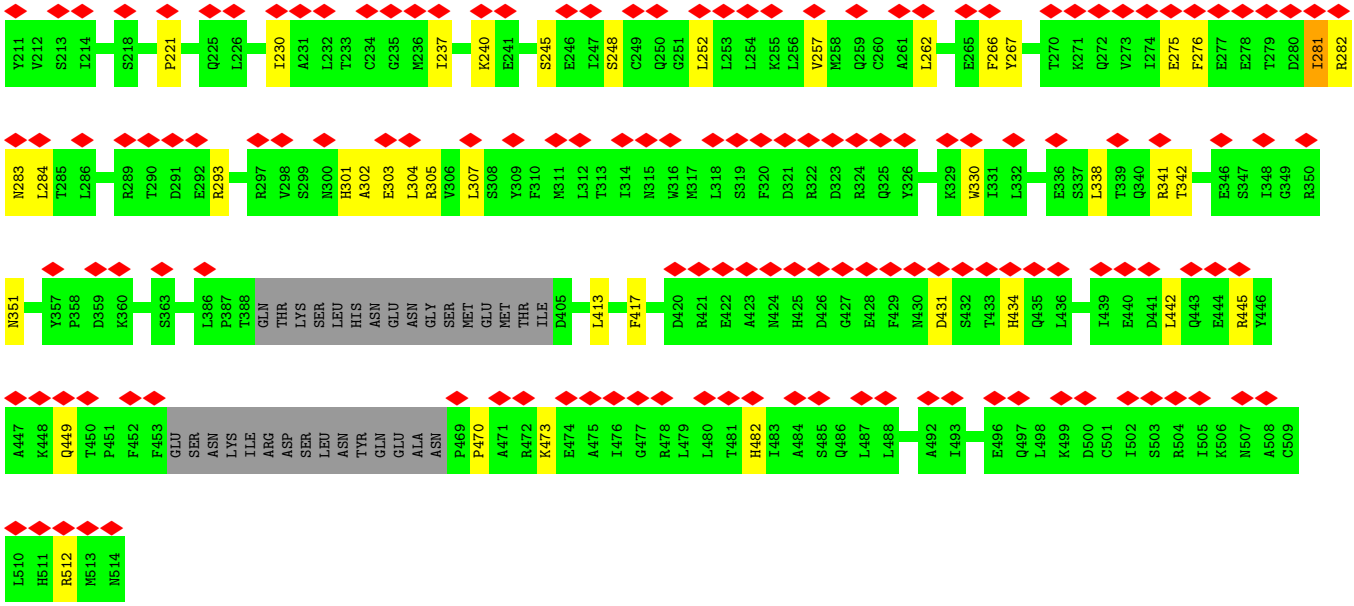


• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN7

Chain Q:

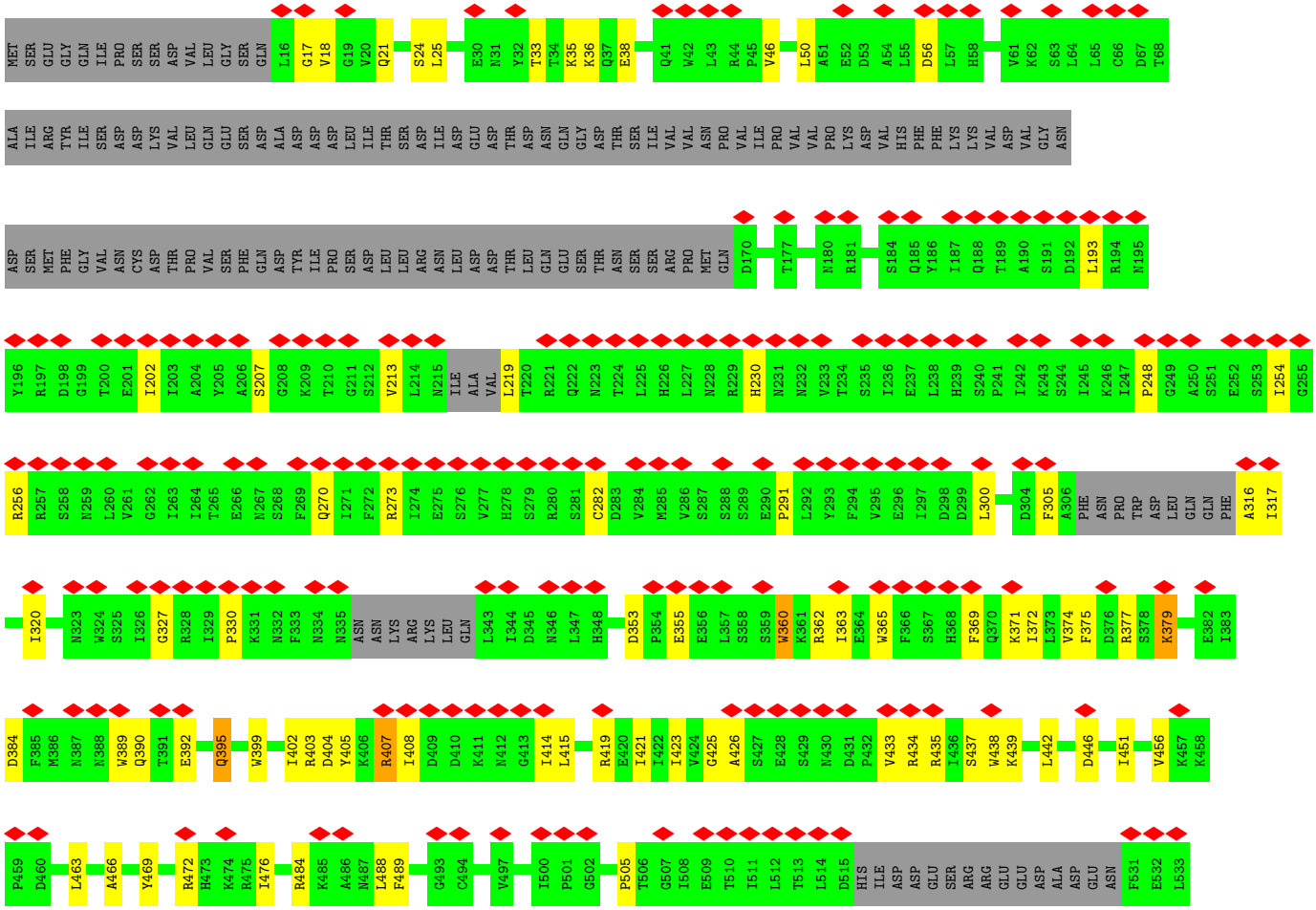


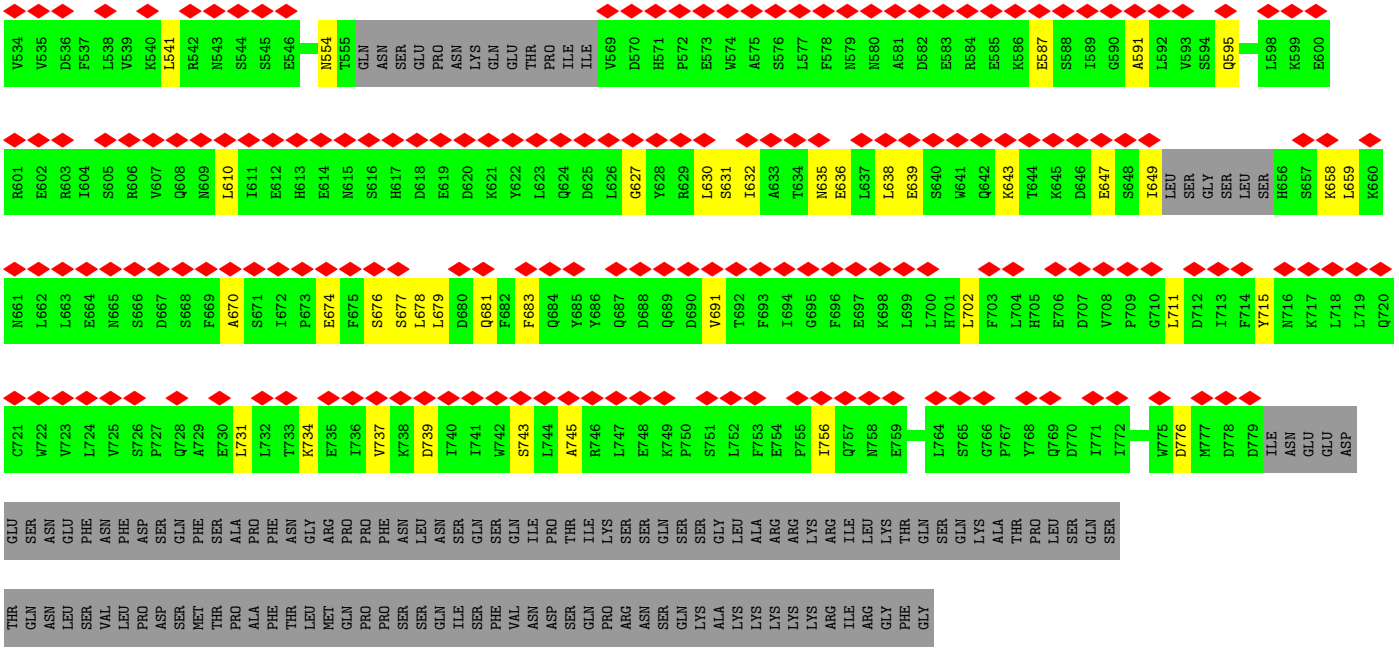




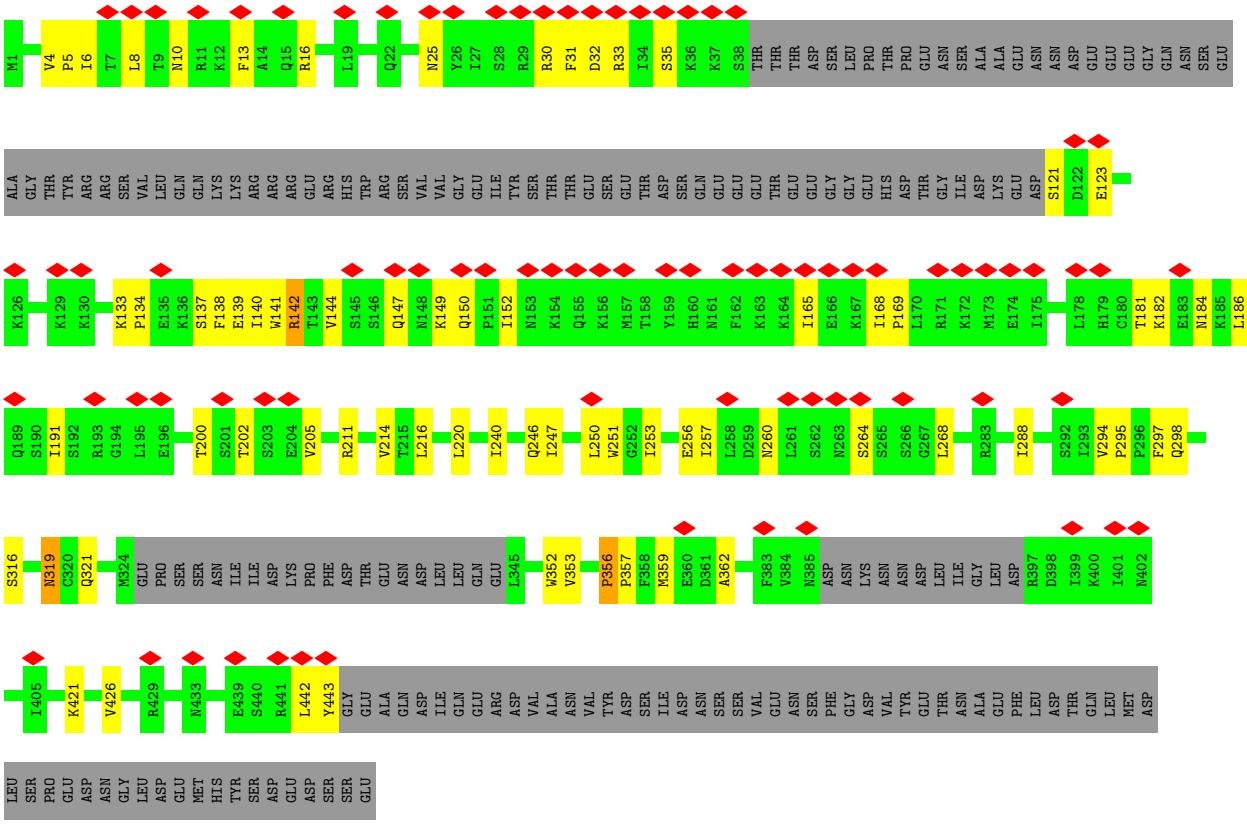
• Molecule 19: RNA polymerase I-specific transcription initiation factor RRN6

Chain S:





• Molecule 20: RNA polymerase I-specific transcription initiation factor RRN11



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42727	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 ($e^-/Å^2$)	1.1075	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.317	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	395.19998, 395.19998, 395.19998	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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

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	T	0.64	0/1065	0.98	0/1633
2	U	0.54	0/1089	0.85	0/1682
3	I	0.39	0/955	0.61	0/1288
4	N	0.34	0/1124	0.58	0/1512
5	M	0.37	0/872	0.63	0/1170
6	A	0.54	0/11776	0.61	0/15906
7	B	0.61	0/9572	0.66	0/12941
8	C	0.57	0/2469	0.64	0/3347
9	D	0.38	0/557	0.61	0/750
10	E	0.47	0/1795	0.56	0/2416
11	F	0.55	0/838	0.59	0/1129
12	G	0.43	0/1637	0.59	0/2226
13	H	0.58	0/1090	0.66	0/1476
14	J	0.71	0/578	0.75	0/775
15	K	0.57	0/821	0.63	0/1108
16	L	0.51	0/361	0.77	0/478
17	O	0.38	0/4226	0.59	0/5717
18	Q	0.36	0/4028	0.61	0/5441
19	S	0.35	0/5065	0.64	0/6859
20	R	0.43	0/2836	0.64	0/3817
All	All	0.50	0/52754	0.64	0/71671

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	T	958	0	547	34	0
2	U	965	0	518	27	0
3	I	942	0	937	21	0
4	N	1103	0	1106	15	0
5	M	856	0	855	10	0
6	A	11565	0	11657	115	0
7	B	9365	0	9232	152	0
8	C	2418	0	2401	25	0
9	D	551	0	558	11	0
10	E	1759	0	1788	15	0
11	F	823	0	841	4	0
12	G	1600	0	1600	21	0
13	H	1072	0	1042	7	0
14	J	569	0	589	11	0
15	K	810	0	801	4	0
16	L	359	0	385	4	0
17	O	4139	0	4061	53	0
18	Q	3936	0	3918	72	0
19	S	4963	0	4890	91	0
20	R	2771	0	2844	59	0
21	Q	1	0	0	0	0
All	All	51525	0	50570	644	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 6.

All (644) 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)
3:I:13:CYS:SG	3:I:32:GLN:HB2	1.68	1.33
7:B:860:ALA:CB	7:B:871:ILE:HG22	1.70	1.20
6:A:986:PHE:HB3	7:B:960:ILE:HD12	1.21	1.11
3:I:13:CYS:SG	3:I:32:GLN:CB	2.38	1.09
18:Q:101:LYS:HD2	18:Q:152:LEU:HD21	1.35	1.07
7:B:860:ALA:HB2	7:B:871:ILE:HG22	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:860:ALA:CA	7:B:871:ILE:HG22	1.85	1.05
14:J:41:LEU:HD22	14:J:46:CYS:SG	1.97	1.04
20:R:352:TRP:O	20:R:356:PRO:HD3	1.61	1.01
18:Q:171:HIS:CD2	18:Q:172:LEU:CD1	2.51	0.93
1:T:11:DG:H1	2:U:59:DG:N2	1.64	0.93
7:B:860:ALA:HA	7:B:871:ILE:HG22	1.50	0.93
7:B:857:PRO:HB3	7:B:871:ILE:HD13	1.50	0.93
6:A:986:PHE:CB	7:B:960:ILE:HD12	1.99	0.92
7:B:860:ALA:HB2	7:B:871:ILE:CG2	2.02	0.90
7:B:967:LEU:HD13	7:B:996:PHE:HB2	1.54	0.88
18:Q:171:HIS:CD2	18:Q:172:LEU:HD13	2.09	0.87
7:B:860:ALA:CB	7:B:871:ILE:CG2	2.52	0.87
18:Q:171:HIS:HD2	18:Q:172:LEU:HD13	1.39	0.87
7:B:861:TYR:CE2	7:B:870:LYS:HE3	2.10	0.87
18:Q:101:LYS:CD	18:Q:152:LEU:HD21	2.05	0.86
7:B:861:TYR:HE2	7:B:870:LYS:HE3	1.44	0.82
7:B:884:GLU:OE1	7:B:904:LYS:HD2	1.79	0.81
9:D:11:ASN:O	9:D:12:THR:HG22	1.80	0.81
16:L:48:CYS:SG	16:L:53:HIS:HB3	2.21	0.81
18:Q:19:LEU:HD22	18:Q:35:MET:SD	2.21	0.80
18:Q:171:HIS:HD2	18:Q:172:LEU:CD1	1.91	0.80
7:B:860:ALA:HA	7:B:871:ILE:HA	1.64	0.80
19:S:408:ILE:HD11	19:S:415:LEU:HB2	1.64	0.79
18:Q:338:LEU:HD23	18:Q:482:HIS:NE2	1.99	0.78
7:B:871:ILE:HD12	7:B:871:ILE:O	1.84	0.77
18:Q:338:LEU:CD2	18:Q:482:HIS:NE2	2.48	0.77
6:A:477:ASN:OD1	7:B:1059:PRO:HG3	1.84	0.76
6:A:467:PHE:CD1	6:A:471:MET:SD	2.79	0.76
18:Q:338:LEU:HB3	18:Q:482:HIS:NE2	2.02	0.75
1:T:37:DA:H2	2:U:34:DT:H3	1.35	0.75
18:Q:338:LEU:HD22	18:Q:482:HIS:CD2	2.23	0.74
1:T:11:DG:H1	2:U:59:DG:H22	1.36	0.74
14:J:41:LEU:CD2	14:J:46:CYS:SG	2.74	0.73
20:R:442:LEU:O	20:R:443:TYR:CD2	2.41	0.73
6:A:30:LYS:HZ1	7:B:1129:ARG:NH2	1.86	0.73
6:A:30:LYS:NZ	7:B:1129:ARG:NH2	2.37	0.72
1:T:43:DC:H42	2:U:28:DG:H1	1.37	0.72
13:H:145:ARG:HG2	13:H:146:ARG:HG3	1.71	0.72
18:Q:25:GLY:HA2	18:Q:38:ASP:HB3	1.70	0.71
17:O:180:LEU:CD2	17:O:222:CYS:SG	2.79	0.70
19:S:438:TRP:HD1	19:S:489:PHE:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:467:PHE:HD1	6:A:471:MET:SD	2.15	0.70
17:O:225:LEU:HD23	17:O:228:GLN:HB3	1.74	0.70
7:B:1119:ARG:HG3	7:B:1121:GLY:H	1.55	0.69
6:A:986:PHE:HB3	7:B:960:ILE:CD1	2.11	0.69
2:U:27:DG:C6	2:U:28:DG:C6	2.80	0.68
18:Q:275:GLU:HA	18:Q:281:ILE:HD12	1.75	0.68
1:T:9:DC:H1'	1:T:10:DT:H5'	1.75	0.68
1:T:11:DG:N1	2:U:59:DG:N2	2.41	0.68
20:R:353:VAL:O	20:R:356:PRO:HD2	1.94	0.67
18:Q:302:ALA:HA	18:Q:305:ARG:HE	1.60	0.67
1:T:12:DC:OP1	6:A:1616:GLU:HB2	1.94	0.67
1:T:47:DA:N1	18:Q:293:ARG:NH1	2.42	0.67
1:T:5:DT:O2	2:U:65:DG:N2	2.28	0.67
3:I:4:VAL:HG11	7:B:289:PHE:HZ	1.60	0.66
20:R:352:TRP:O	20:R:356:PRO:CD	2.41	0.66
19:S:377:ARG:NH2	19:S:403:ARG:HA	2.11	0.66
6:A:15:ASP:HB2	7:B:1197:ARG:HB3	1.77	0.66
18:Q:101:LYS:HD2	18:Q:152:LEU:CD2	2.19	0.66
4:N:119:LEU:HB3	5:M:38:PHE:H	1.61	0.65
16:L:31:CYS:SG	16:L:36:SER:OG	2.54	0.65
7:B:143:TRP:HB3	7:B:152:LEU:HB2	1.78	0.65
14:J:12:LYS:HD3	14:J:46:CYS:SG	2.37	0.65
8:C:335:GLN:OE1	15:K:48:LYS:NZ	2.29	0.64
18:Q:21:ARG:HA	18:Q:27:ARG:HA	1.77	0.64
19:S:403:ARG:HH21	19:S:419:ARG:HD3	1.63	0.64
7:B:65:VAL:HG12	7:B:417:ILE:CD1	2.28	0.64
7:B:860:ALA:HA	7:B:871:ILE:CG2	2.25	0.63
10:E:100:ILE:HG23	10:E:105:PHE:HB2	1.80	0.63
20:R:294:VAL:HG12	20:R:298:GLN:HE21	1.64	0.63
20:R:319:ASN:O	20:R:319:ASN:ND2	2.32	0.62
6:A:467:PHE:CE1	6:A:471:MET:SD	2.92	0.62
17:O:430:ARG:NH1	17:O:610:TYR:OH	2.32	0.62
6:A:670:ILE:HG12	6:A:671:GLN:HG3	1.80	0.62
4:N:119:LEU:HD13	5:M:38:PHE:HB2	1.80	0.62
4:N:157:ARG:NH2	7:B:985:ILE:O	2.33	0.62
7:B:292:ILE:HB	7:B:306:LEU:HD11	1.82	0.62
17:O:431:ALA:O	17:O:487:ARG:NH2	2.33	0.62
3:I:13:CYS:SG	3:I:32:GLN:CG	2.87	0.62
7:B:861:TYR:N	7:B:870:LYS:O	2.29	0.62
7:B:714:ARG:HE	7:B:957:ARG:CG	2.12	0.62
19:S:399:TRP:CD1	20:R:294:VAL:HG23	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:407:ARG:HA	19:S:414:ILE:HG23	1.82	0.61
12:G:17:ILE:HG22	12:G:21:LYS:HE3	1.83	0.61
6:A:964:LYS:NZ	7:B:672:MET:O	2.34	0.60
7:B:857:PRO:CB	7:B:871:ILE:HD13	2.30	0.60
14:J:10:CYS:SG	14:J:46:CYS:HB2	2.41	0.60
8:C:165:ARG:NH1	8:C:190:ASP:OD1	2.34	0.60
17:O:521:ASN:HB3	17:O:524:VAL:HG12	1.84	0.60
18:Q:257:VAL:HG22	18:Q:262:LEU:HD11	1.83	0.60
1:T:4:DT:O2	2:U:67:DA:H2	1.85	0.60
17:O:218:LEU:O	17:O:222:CYS:HB2	2.02	0.60
18:Q:22:ILE:HG23	18:Q:23:ILE:HG13	1.83	0.59
6:A:461:GLU:HG2	6:A:1618:THR:HB	1.83	0.59
7:B:731:VAL:HG21	14:J:59:LYS:HG2	1.84	0.59
20:R:5:PRO:HB2	20:R:246:GLN:H	1.67	0.59
20:R:442:LEU:O	20:R:443:TYR:CG	2.55	0.59
5:M:56:GLU:HG2	5:M:61:GLU:HG3	1.85	0.59
6:A:671:GLN:NE2	7:B:784:ASP:OD1	2.36	0.59
12:G:56:ASN:OD1	12:G:59:GLN:NE2	2.36	0.59
12:G:237:HIS:HB3	12:G:239:THR:HG23	1.85	0.59
7:B:1025:ASP:OD2	8:C:277:ARG:NH1	2.36	0.59
10:E:2:ASP:HB3	10:E:6:GLU:HB2	1.85	0.58
10:E:83:CYS:O	10:E:113:GLN:NE2	2.36	0.58
19:S:300:LEU:HA	19:S:320:ILE:HA	1.85	0.58
1:T:53:DG:H22	2:U:18:DC:H42	1.52	0.58
6:A:389:VAL:HG22	6:A:433:ASP:HB3	1.85	0.58
19:S:659:LEU:HB3	19:S:745:ALA:HB1	1.86	0.58
17:O:169:THR:HB	17:O:172:HIS:HB2	1.86	0.58
17:O:218:LEU:O	17:O:222:CYS:CB	2.51	0.58
6:A:943:ILE:HG12	7:B:960:ILE:HD11	1.84	0.58
7:B:916:LYS:HG2	7:B:926:VAL:HG12	1.86	0.58
1:T:43:DC:N4	2:U:28:DG:H1	2.02	0.58
6:A:435:ASN:ND2	6:A:442:LYS:O	2.37	0.57
3:I:100:GLN:NE2	3:I:106:GLU:O	2.37	0.57
4:N:57:LYS:HB2	4:N:138:SER:HA	1.86	0.57
7:B:967:LEU:HD12	7:B:968:ALA:N	2.20	0.57
6:A:487:ASP:HB2	6:A:615:ARG:HG2	1.86	0.57
9:D:88:GLN:NE2	17:O:184:PRO:O	2.37	0.57
6:A:744:MET:HG2	6:A:1078:LYS:HD2	1.85	0.57
13:H:64:ASN:H	13:H:89:LEU:HB2	1.67	0.57
4:N:31:LYS:HA	5:M:41:TYR:HA	1.86	0.57
6:A:986:PHE:CB	7:B:960:ILE:CD1	2.79	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:281:ILE:HG22	18:Q:282:ARG:HE	1.69	0.57
19:S:273:ARG:NH2	19:S:330:PRO:O	2.36	0.57
18:Q:19:LEU:CD2	18:Q:35:MET:SD	2.91	0.57
3:I:2:SER:N	3:I:9:PHE:O	2.37	0.57
20:R:4:VAL:HG11	20:R:214:VAL:HG22	1.87	0.57
2:U:63:DT:H1'	2:U:64:DT:H5'	1.87	0.57
7:B:408:LEU:O	7:B:412:ILE:HG22	2.05	0.57
16:L:40:LEU:HD12	16:L:44:ASP:HB3	1.86	0.57
17:O:180:LEU:HD21	17:O:222:CYS:SG	2.45	0.57
7:B:204:ARG:HH21	7:B:542:LEU:HD13	1.70	0.56
7:B:863:ASP:OD2	7:B:870:LYS:HE2	2.06	0.56
17:O:382:GLN:NE2	17:O:593:PRO:O	2.37	0.56
1:T:5:DT:H1'	2:U:65:DG:N2	2.21	0.56
7:B:714:ARG:HE	7:B:957:ARG:HG3	1.69	0.56
6:A:1458:THR:OG1	6:A:1475:GLU:OE1	2.21	0.56
13:H:59:ILE:HG12	13:H:142:LEU:HD12	1.88	0.56
12:G:149:ILE:HB	12:G:153:PHE:HB2	1.87	0.56
20:R:353:VAL:C	20:R:356:PRO:HD2	2.26	0.56
1:T:37:DA:C2	2:U:34:DT:N3	2.63	0.56
5:M:88:ILE:HD12	5:M:90:LEU:HD21	1.86	0.56
6:A:982:VAL:HG22	6:A:994:GLU:HB2	1.88	0.56
15:K:98:GLU:HG3	15:K:100:LEU:HD12	1.87	0.56
18:Q:257:VAL:HG21	18:Q:267:TYR:HB2	1.88	0.56
19:S:451:ILE:HD11	19:S:466:ALA:HB1	1.87	0.56
7:B:1006:ASN:HD22	7:B:1010:ASN:HB2	1.71	0.56
17:O:240:ILE:HG22	17:O:332:LEU:HD13	1.87	0.56
18:Q:330:TRP:HE1	18:Q:449:GLN:HB2	1.70	0.56
5:M:47:GLU:HG2	5:M:48:LYS:HG2	1.88	0.55
8:C:157:TYR:HB2	8:C:160:ALA:HB2	1.88	0.55
19:S:36:LYS:HG2	19:S:38:GLU:H	1.71	0.55
7:B:553:THR:O	7:B:646:HIS:ND1	2.35	0.55
1:T:4:DT:O2	2:U:67:DA:C2	2.59	0.55
7:B:200:GLU:OE2	7:B:736:ARG:NH2	2.39	0.55
17:O:208:LEU:HB3	17:O:335:ILE:HD11	1.89	0.55
17:O:392:GLN:HB2	17:O:395:LEU:HD13	1.88	0.55
6:A:752:LYS:O	6:A:785:GLN:NE2	2.39	0.55
6:A:857:ALA:HB2	6:A:899:LYS:HD2	1.87	0.55
7:B:967:LEU:CD1	7:B:996:PHE:HB2	2.32	0.55
20:R:133:LYS:NZ	20:R:288:ILE:O	2.40	0.55
10:E:97:VAL:HG13	10:E:127:ILE:HD11	1.89	0.55
3:I:21:ASN:HB3	6:A:1478:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:56:ILE:HG22	4:N:137:PHE:HB2	1.89	0.55
17:O:180:LEU:HD23	17:O:222:CYS:SG	2.46	0.55
18:Q:118:TRP:NE1	18:Q:122:GLU:OE1	2.32	0.55
7:B:260:PHE:HB2	7:B:273:VAL:HG22	1.87	0.55
7:B:804:TYR:OH	8:C:93:GLN:NE2	2.39	0.55
7:B:17:ARG:HB3	7:B:20:GLU:HB3	1.89	0.55
4:N:176:ASP:OD1	14:J:42:LYS:NZ	2.40	0.54
6:A:1051:GLY:HA3	6:A:1580:ARG:HG2	1.88	0.54
6:A:591:ARG:NH1	6:A:625:ASN:O	2.40	0.54
4:N:154:ARG:NH1	7:B:681:ILE:O	2.41	0.54
6:A:709:ARG:NH1	6:A:737:LEU:O	2.40	0.54
18:Q:338:LEU:CD2	18:Q:482:HIS:CD2	2.91	0.54
19:S:36:LYS:NZ	20:R:321:GLN:OE1	2.41	0.54
19:S:423:ILE:HD13	20:R:141:TRP:HZ2	1.71	0.54
7:B:782:ASP:O	7:B:950:ASN:ND2	2.41	0.54
1:T:37:DA:H2	2:U:34:DT:N3	2.02	0.54
6:A:1634:LEU:HD13	6:A:1643:VAL:HG11	1.90	0.54
9:D:12:THR:HG23	9:D:12:THR:O	2.06	0.54
3:I:13:CYS:SG	3:I:32:GLN:HG3	2.48	0.54
7:B:37:LEU:HD12	7:B:759:ASP:HB3	1.90	0.54
6:A:99:ARG:O	6:A:109:ARG:NH2	2.41	0.54
6:A:232:LYS:HA	6:A:239:PHE:HB3	1.90	0.54
7:B:584:CYS:HB3	7:B:596:VAL:HG23	1.90	0.54
6:A:230:ARG:NH2	6:A:234:ASP:OD2	2.41	0.53
7:B:861:TYR:O	7:B:870:LYS:N	2.35	0.53
19:S:25:LEU:HD23	19:S:437:SER:HA	1.90	0.53
6:A:1101:THR:HG22	6:A:1120:TYR:HB3	1.91	0.53
6:A:1145:GLU:OE2	6:A:1167:ARG:NH1	2.41	0.53
8:C:322:LYS:NZ	8:C:326:GLU:OE2	2.40	0.53
1:T:4:DT:H2"	1:T:5:DT:C5	2.43	0.53
1:T:6:DC:OP2	1:T:6:DC:H6	1.91	0.53
7:B:65:VAL:HG12	7:B:417:ILE:HD12	1.90	0.53
19:S:362:ARG:NH2	19:S:405:TYR:O	2.40	0.53
6:A:438:ILE:HA	6:A:456:VAL:HG22	1.90	0.53
6:A:1306:TYR:O	6:A:1499:ARG:NH2	2.42	0.53
18:Q:431:ASP:OD2	18:Q:434:HIS:ND1	2.40	0.53
4:N:174:GLY:HA3	8:C:53:ASN:HD22	1.74	0.53
13:H:128:ASN:N	13:H:128:ASN:OD1	2.40	0.53
18:Q:6:ARG:HD2	18:Q:18:ARG:HB3	1.89	0.53
19:S:202:ILE:HA	19:S:219:LEU:HD12	1.90	0.53
18:Q:27:ARG:HD3	18:Q:35:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:357:PRO:O	20:R:359:MET:HG3	2.09	0.53
6:A:621:THR:OG1	6:A:626:ALA:O	2.27	0.53
8:C:70:ILE:HG23	8:C:74:GLU:HB2	1.89	0.53
18:Q:167:LEU:HD21	18:Q:230:ILE:HG23	1.91	0.53
6:A:1635:ASP:O	6:A:1648:ASN:ND2	2.42	0.53
17:O:49:ALA:HB1	17:O:95:ILE:HD11	1.89	0.53
18:Q:283:ASN:OD1	19:S:658:LYS:NZ	2.39	0.53
19:S:395:GLN:HG3	20:R:142:ARG:HH12	1.73	0.53
6:A:477:ASN:OD1	7:B:1059:PRO:CG	2.54	0.52
7:B:884:GLU:OE1	7:B:904:LYS:CD	2.56	0.52
7:B:289:PHE:HD1	7:B:306:LEU:HD22	1.75	0.52
18:Q:109:GLN:NE2	19:S:776:ASP:OD1	2.42	0.52
7:B:491:ILE:HD12	7:B:1037:ARG:HG2	1.92	0.52
7:B:1014:TYR:OH	8:C:293:ARG:NH1	2.38	0.52
18:Q:65:ASN:HB2	18:Q:72:SER:HB2	1.90	0.52
6:A:248:PHE:HD2	6:A:442:LYS:HG3	1.75	0.52
6:A:745:PRO:HG2	6:A:1075:ALA:HB2	1.92	0.52
7:B:861:TYR:CE2	7:B:870:LYS:HB2	2.45	0.52
17:O:517:LEU:HD11	17:O:540:CYS:HB2	1.91	0.52
19:S:230:HIS:HB2	19:S:282:CYS:HB2	1.90	0.52
7:B:1105:ARG:NH1	7:B:1172:GLU:OE1	2.43	0.52
7:B:568:LEU:HD23	7:B:604:ILE:HG12	1.92	0.52
8:C:293:ARG:HB2	8:C:295:ARG:HE	1.75	0.52
7:B:750:PRO:HG2	7:B:753:LYS:HB3	1.91	0.52
17:O:176:LEU:HD21	17:O:218:LEU:HD13	1.91	0.52
19:S:472:ARG:NH2	20:R:200:THR:OG1	2.43	0.52
19:S:587:GLU:O	19:S:591:ALA:N	2.43	0.52
7:B:206:LEU:HD21	7:B:480:GLN:HE22	1.76	0.51
7:B:1035:ARG:NH2	7:B:1039:MET:SD	2.83	0.51
13:H:25:ARG:HE	13:H:39:THR:HG23	1.75	0.51
19:S:426:ALA:N	19:S:435:ARG:O	2.43	0.51
19:S:484:ARG:HD2	19:S:488:LEU:HD23	1.93	0.51
20:R:181:THR:OG1	20:R:184:ASN:OD1	2.28	0.51
17:O:92:ASN:HA	17:O:95:ILE:HD12	1.92	0.51
19:S:399:TRP:CH2	20:R:295:PRO:HG2	2.45	0.51
1:T:43:DC:N3	2:U:28:DG:N2	2.44	0.51
6:A:325:ASP:O	6:A:329:ARG:NH1	2.43	0.51
1:T:34:DA:N6	2:U:36:DG:H1	2.09	0.51
7:B:73:ILE:HG12	7:B:425:ILE:HG23	1.93	0.51
17:O:225:LEU:CD2	17:O:228:GLN:HB3	2.39	0.51
17:O:340:SER:HA	17:O:343:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:72:LYS:HB3	11:F:142:SER:HA	1.91	0.51
19:S:36:LYS:HE3	19:S:38:GLU:HB2	1.92	0.51
19:S:353:ASP:OD1	19:S:355:GLU:HG2	2.11	0.51
12:G:26:ASN:ND2	12:G:131:ASP:OD2	2.38	0.51
19:S:591:ALA:O	19:S:595:GLN:N	2.43	0.51
7:B:1065:ARG:HH21	18:Q:42:ASN:HB3	1.76	0.51
17:O:597:LEU:HG	17:O:599:LEU:H	1.75	0.51
7:B:98:SER:HB3	7:B:142:LYS:HB3	1.93	0.51
20:R:8:LEU:HD21	20:R:202:THR:HG22	1.92	0.51
7:B:100:GLU:OE2	7:B:140:LYS:NZ	2.42	0.51
6:A:552:GLU:O	17:O:246:ASN:ND2	2.44	0.50
6:A:739:VAL:HG11	6:A:812:VAL:HG21	1.93	0.50
12:G:241:ARG:NH2	17:O:152:GLN:OE1	2.44	0.50
19:S:715:TYR:HD1	19:S:737:VAL:HG21	1.76	0.50
1:T:37:DA:C2	1:T:38:DC:N3	2.80	0.50
7:B:714:ARG:HH21	7:B:957:ARG:HG3	1.75	0.50
8:C:91:VAL:HG11	14:J:57:ILE:HD12	1.94	0.50
19:S:632:ILE:HA	19:S:635:ASN:HB2	1.93	0.50
6:A:799:GLU:OE2	6:A:1173:LYS:NZ	2.36	0.50
6:A:1270:VAL:HG11	6:A:1489:VAL:HG11	1.93	0.50
17:O:314:THR:HG22	18:Q:6:ARG:H	1.75	0.50
18:Q:25:GLY:CA	18:Q:38:ASP:HB3	2.39	0.50
18:Q:276:PHE:O	18:Q:512:ARG:NH1	2.44	0.50
19:S:639:GLU:O	19:S:643:LYS:NZ	2.38	0.50
7:B:974:LEU:O	14:J:47:ARG:NH2	2.45	0.50
7:B:1090:ASP:HA	7:B:1094:ASN:HB2	1.92	0.50
19:S:21:GLN:OE1	19:S:24:SER:OG	2.23	0.50
20:R:32:ASP:HA	20:R:35:SER:HB3	1.93	0.50
10:E:100:ILE:HA	10:E:105:PHE:HD2	1.75	0.50
18:Q:101:LYS:CD	18:Q:152:LEU:CD2	2.84	0.50
8:C:222:VAL:HG21	8:C:225:ALA:HB2	1.93	0.50
1:T:4:DT:H2"	1:T:5:DT:H72	1.94	0.49
6:A:1238:MET:HE3	6:A:1524:VAL:HA	1.93	0.49
7:B:202:LEU:HD23	7:B:488:ALA:HB2	1.94	0.49
19:S:390:GLN:N	20:R:150:GLN:O	2.45	0.49
1:T:11:DG:H1	2:U:59:DG:H21	1.53	0.49
19:S:676:SER:HB3	19:S:711:LEU:HD22	1.93	0.49
18:Q:119:LEU:O	18:Q:125:PHE:HB2	2.12	0.49
8:C:229:LEU:HB3	8:C:293:ARG:HH11	1.78	0.49
12:G:234:ARG:HB2	12:G:248:THR:HG23	1.93	0.49
19:S:395:GLN:HB3	20:R:140:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:86:PRO:HA	10:E:113:GLN:HB2	1.95	0.49
20:R:216:LEU:O	20:R:220:LEU:N	2.45	0.49
7:B:216:ALA:HB1	7:B:384:LEU:HD22	1.94	0.49
5:M:39:ASP:N	5:M:54:HIS:O	2.46	0.49
18:Q:171:HIS:CD2	18:Q:172:LEU:HD12	2.44	0.49
5:M:105:SER:O	7:B:322:ASN:ND2	2.46	0.49
7:B:184:LYS:HD2	7:B:735:HIS:CD2	2.48	0.49
8:C:41:GLU:HB2	8:C:57:ILE:HB	1.95	0.49
8:C:136:LEU:HB3	8:C:204:LEU:HG	1.95	0.49
19:S:390:GLN:HB2	20:R:152:ILE:HG13	1.95	0.49
6:A:439:ASP:HB2	6:A:442:LYS:HB2	1.94	0.49
6:A:1042:ASP:OD1	6:A:1042:ASP:N	2.45	0.49
6:A:592:GLN:OE1	6:A:634:ASN:ND2	2.46	0.48
8:C:88:ASN:ND2	8:C:94:ASP:OD1	2.45	0.48
19:S:18:VAL:HG23	20:R:426:VAL:HA	1.94	0.48
19:S:270:GLN:HG2	19:S:291:PRO:HB3	1.95	0.48
6:A:103:LEU:N	6:A:240:SER:OG	2.39	0.48
6:A:799:GLU:O	6:A:1079:LYS:NZ	2.37	0.48
18:Q:139:LYS:HE3	18:Q:237:ILE:HD12	1.94	0.48
20:R:147:GLN:HA	20:R:147:GLN:OE1	2.13	0.48
1:T:5:DT:H2"	1:T:6:DC:C5	2.49	0.48
11:F:111:LEU:HD12	11:F:111:LEU:O	2.12	0.48
19:S:371:LYS:HG2	19:S:384:ASP:HB2	1.95	0.48
17:O:316:GLU:HG3	17:O:317:TYR:H	1.79	0.48
1:T:14:DT:H5"	6:A:1017:GLY:HA3	1.96	0.48
2:U:59:DG:H1'	2:U:60:DC:H5'	1.95	0.48
6:A:1449:ALA:O	6:A:1453:HIS:ND1	2.39	0.48
7:B:79:LEU:HB3	7:B:81:SER:HB3	1.96	0.48
9:D:44:ILE:HD11	9:D:89:LEU:HB3	1.95	0.48
18:Q:4:PHE:HE1	18:Q:20:TRP:HB2	1.78	0.48
19:S:360:TRP:HD1	19:S:377:ARG:HG2	1.79	0.48
6:A:1275:THR:HG23	6:A:1289:SER:HB2	1.95	0.48
17:O:383:TYR:OH	17:O:595:ASP:O	2.32	0.48
7:B:65:VAL:HG12	7:B:417:ILE:HD11	1.96	0.48
7:B:565:LEU:HD21	7:B:608:LEU:HD11	1.94	0.48
17:O:328:LEU:HG	17:O:331:LYS:HD2	1.95	0.48
19:S:638:LEU:HD21	19:S:691:VAL:HB	1.94	0.48
20:R:247:ILE:HA	20:R:250:LEU:HD12	1.95	0.48
20:R:31:PHE:HA	20:R:165:ILE:HD11	1.95	0.48
3:I:13:CYS:HB3	3:I:30:CYS:SG	2.54	0.48
3:I:89:CYS:SG	3:I:90:GLY:N	2.85	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:543:LEU:HB2	18:Q:34:VAL:HG21	1.96	0.48
15:K:74:ASN:OD1	15:K:77:ARG:NH2	2.47	0.48
6:A:1179:ILE:HD11	6:A:1183:GLU:HG2	1.95	0.47
18:Q:240:LYS:NZ	18:Q:245:SER:OG	2.42	0.47
19:S:254:ILE:HG23	19:S:256:ARG:H	1.79	0.47
19:S:360:TRP:CD1	19:S:377:ARG:HG2	2.48	0.47
7:B:288:ILE:O	7:B:292:ILE:HG13	2.14	0.47
17:O:97:LEU:HD22	17:O:135:LYS:HG2	1.96	0.47
19:S:679:LEU:O	19:S:683:PHE:N	2.45	0.47
6:A:620:ASN:OD1	6:A:667:ARG:NH2	2.47	0.47
6:A:850:SER:HB3	6:A:903:ILE:HG21	1.97	0.47
7:B:319:HIS:HA	7:B:321:GLN:HE22	1.80	0.47
7:B:755:ASN:ND2	7:B:980:ASP:OD2	2.48	0.47
20:R:16:ARG:HB3	20:R:184:ASN:HD22	1.79	0.47
6:A:753:ASN:ND2	6:A:780:ILE:O	2.36	0.47
7:B:960:ILE:HG22	7:B:960:ILE:O	2.14	0.47
20:R:251:TRP:NE1	20:R:297:PHE:O	2.43	0.47
12:G:147:LEU:HD21	12:G:229:LEU:HB3	1.97	0.47
19:S:438:TRP:CD1	19:S:489:PHE:HB2	2.44	0.47
1:T:6:DC:N3	2:U:64:DT:O2	2.48	0.47
7:B:824:HIS:ND1	7:B:897:GLU:OE2	2.48	0.47
7:B:491:ILE:HD11	7:B:724:GLN:HA	1.96	0.47
12:G:81:VAL:HA	12:G:124:VAL:HG12	1.97	0.47
19:S:248:PRO:HB3	19:S:305:PHE:HB2	1.97	0.47
19:S:610:LEU:HD23	19:S:670:ALA:HB2	1.96	0.47
20:R:268:LEU:HD11	20:R:316:SER:HB3	1.96	0.47
3:I:26:SER:OG	3:I:38:PRO:O	2.30	0.47
7:B:429:ARG:HA	7:B:432:ILE:HG12	1.97	0.47
7:B:860:ALA:HA	7:B:871:ILE:CA	2.42	0.47
10:E:76:GLY:N	10:E:106:GLN:OE1	2.44	0.47
17:O:430:ARG:NH1	17:O:594:TYR:O	2.48	0.47
18:Q:175:PRO:HG2	19:S:702:LEU:HD12	1.97	0.47
18:Q:284:LEU:HB3	18:Q:302:ALA:HB1	1.97	0.47
20:R:25:ASN:ND2	20:R:123:GLU:OE1	2.48	0.47
7:B:99:VAL:HG23	7:B:421:LEU:HD21	1.96	0.46
9:D:11:ASN:O	9:D:12:THR:CG2	2.59	0.46
12:G:74:ASN:HB3	12:G:77:VAL:HG22	1.97	0.46
17:O:351:SER:HA	17:O:355:GLY:H	1.81	0.46
20:R:442:LEU:C	20:R:443:TYR:CD2	2.88	0.46
2:U:65:DG:O5'	2:U:65:DG:H8	1.98	0.46
6:A:1022:CYS:SG	6:A:1615:TYR:OH	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:94:ARG:NH2	9:D:99:LEU:O	2.48	0.46
18:Q:252:LEU:HD11	18:Q:303:GLU:HG3	1.95	0.46
18:Q:413:LEU:HD21	20:R:240:ILE:HD12	1.97	0.46
18:Q:442:LEU:HA	18:Q:445:ARG:HB2	1.96	0.46
6:A:462:LYS:HD2	6:A:464:GLU:HG2	1.96	0.46
6:A:1125:ALA:O	10:E:167:ARG:NH2	2.42	0.46
6:A:1291:VAL:HG13	6:A:1473:LYS:HG2	1.97	0.46
3:I:55:ALA:O	6:A:1494:ARG:NH1	2.48	0.46
6:A:77:GLY:O	6:A:362:VAL:N	2.40	0.46
20:R:30:ARG:HD2	20:R:33:ARG:HD3	1.98	0.46
10:E:117:THR:HG22	10:E:119:SER:H	1.81	0.46
17:O:225:LEU:HD22	17:O:225:LEU:O	2.16	0.46
19:S:316:ALA:HB3	19:S:327:GLY:HA3	1.96	0.46
19:S:362:ARG:HB3	19:S:375:PHE:HB2	1.98	0.46
20:R:134:PRO:HG3	20:R:140:ILE:HB	1.98	0.46
7:B:859:CYS:O	7:B:872:LYS:N	2.48	0.46
6:A:244:ARG:HB3	6:A:252:PHE:HB2	1.97	0.46
12:G:77:VAL:HG21	12:G:124:VAL:HG11	1.98	0.46
19:S:317:ILE:HG21	19:S:365:TRP:HE1	1.79	0.46
20:R:362:ALA:HB2	20:R:421:LYS:HB2	1.97	0.46
19:S:389:TRP:HD1	20:R:149:LYS:HD2	1.80	0.46
7:B:252:TYR:OH	7:B:305:ARG:NE	2.41	0.46
18:Q:177:TYR:OH	18:Q:248:SER:O	2.32	0.46
18:Q:338:LEU:CB	18:Q:482:HIS:NE2	2.75	0.46
19:S:446:ASP:OD1	19:S:472:ARG:NH2	2.47	0.46
20:R:168:ILE:HG23	20:R:169:PRO:HD3	1.97	0.46
20:R:188:PHE:HA	20:R:191:ILE:HG12	1.98	0.46
20:R:205:VAL:HG12	20:R:211:ARG:HH21	1.81	0.46
6:A:215:GLU:OE2	10:E:177:ARG:NH2	2.45	0.45
19:S:469:TYR:HB3	19:S:476:ILE:HD12	1.97	0.45
7:B:1042:ASP:OD1	7:B:1043:LYS:NZ	2.45	0.45
19:S:647:GLU:HG3	19:S:649:ILE:HG22	1.98	0.45
7:B:861:TYR:HE1	7:B:872:LYS:HG2	1.81	0.45
14:J:36:LEU:HD11	14:J:51:LEU:HD13	1.98	0.45
19:S:363:ILE:HG22	19:S:374:VAL:HG22	1.98	0.45
7:B:979:GLN:HG2	7:B:996:PHE:CE1	2.51	0.45
9:D:94:ARG:HH12	9:D:100:PRO:HA	1.81	0.45
19:S:425:GLY:HA2	19:S:437:SER:H	1.81	0.45
17:O:316:GLU:OE1	18:Q:3:THR:N	2.50	0.45
17:O:482:TYR:HD1	17:O:524:VAL:HG21	1.82	0.45
19:S:360:TRP:CD1	19:S:360:TRP:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:114:CYS:SG	3:I:115:THR:N	2.89	0.45
6:A:251:ILE:HD13	6:A:320:VAL:HG21	1.98	0.45
7:B:725:THR:HA	7:B:1036:LEU:HA	1.98	0.45
17:O:378:THR:O	17:O:591:TYR:OH	2.32	0.45
18:Q:159:THR:HG22	18:Q:221:PRO:HG3	1.98	0.45
12:G:148:LEU:HD23	12:G:148:LEU:HA	1.84	0.45
17:O:581:THR:N	17:O:584:GLN:OE1	2.49	0.45
4:N:141:GLU:OE1	7:B:567:SER:OG	2.32	0.45
6:A:37:VAL:HG12	6:A:49:LEU:HB2	1.98	0.45
6:A:101:SER:HA	6:A:108:PHE:HA	1.98	0.45
6:A:105:CYS:HB3	6:A:233:CYS:SG	2.56	0.45
6:A:239:PHE:HZ	6:A:260:GLN:HB3	1.82	0.45
12:G:30:GLU:HG2	12:G:32:ASN:HB2	1.97	0.45
19:S:377:ARG:HD3	19:S:402:ILE:O	2.17	0.45
6:A:904:THR:HG23	6:A:946:LEU:HD11	1.98	0.45
17:O:173:HIS:HE1	17:O:218:LEU:HA	1.81	0.45
20:R:220:LEU:HD21	20:R:253:ILE:HD11	1.99	0.45
1:T:5:DT:C6	1:T:5:DT:O5'	2.70	0.44
7:B:258:VAL:HG12	7:B:273:VAL:HG21	2.00	0.44
7:B:963:PHE:O	7:B:1027:TYR:OH	2.34	0.44
7:B:1181:VAL:O	7:B:1185:LEU:N	2.48	0.44
20:R:121:SER:OG	20:R:123:GLU:OE2	2.33	0.44
6:A:1162:ASN:HB2	6:A:1165:LYS:HG2	1.99	0.44
6:A:1662:ASN:HB3	12:G:57:PRO:HD2	1.99	0.44
8:C:277:ARG:HG2	8:C:291:LEU:HD22	1.99	0.44
13:H:28:ALA:HB3	13:H:38:LEU:HB3	1.99	0.44
16:L:46:VAL:HG13	16:L:56:LEU:HD22	1.99	0.44
19:S:505:PRO:HA	19:S:541:LEU:HA	1.99	0.44
6:A:550:SER:OG	6:A:551:VAL:N	2.50	0.44
7:B:318:PRO:O	7:B:321:GLN:NE2	2.50	0.44
9:D:37:LEU:HD11	9:D:97:LYS:HD3	1.99	0.44
17:O:533:GLN:HG3	17:O:539:TYR:HE1	1.82	0.44
8:C:91:VAL:HG11	14:J:57:ILE:CD1	2.47	0.44
12:G:77:VAL:HG11	12:G:122:LEU:HD12	1.99	0.44
1:T:37:DA:H2	2:U:34:DT:C2	2.35	0.44
3:I:49:THR:HG22	7:B:300:SER:HB3	1.99	0.44
7:B:714:ARG:HE	7:B:957:ARG:HG2	1.83	0.44
15:K:88:PHE:HB3	15:K:106:GLN:HB2	2.00	0.44
17:O:425:GLY:HA2	17:O:483:ILE:HD11	1.99	0.44
19:S:392:GLU:HG2	20:R:142:ARG:HH11	1.83	0.44
7:B:788:ILE:HB	7:B:948:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:28:ILE:HA	12:G:35:SER:HA	2.00	0.44
17:O:390:GLN:HE21	17:O:433:LYS:H	1.65	0.44
20:R:182:LYS:O	20:R:186:LEU:N	2.44	0.44
6:A:57:PHE:HB2	6:A:365:THR:HG21	2.00	0.44
12:G:93:ASP:HB2	12:G:104:LEU:HD11	1.99	0.44
7:B:711:GLN:HG2	7:B:713:PRO:HD2	1.99	0.43
17:O:460:GLU:O	17:O:469:ARG:NH2	2.51	0.43
18:Q:134:LYS:O	18:Q:138:LEU:N	2.45	0.43
20:R:257:ILE:O	20:R:264:SER:OG	2.26	0.43
7:B:861:TYR:HE2	7:B:870:LYS:CE	2.24	0.43
19:S:423:ILE:HG12	19:S:439:LYS:HD3	1.98	0.43
6:A:30:LYS:HZ1	7:B:1129:ARG:HH21	1.64	0.43
6:A:1038:ILE:HD11	6:A:1050:TYR:HB2	1.99	0.43
10:E:79:TRP:NE1	10:E:81:GLU:OE1	2.49	0.43
17:O:238:ILE:O	17:O:242:VAL:HB	2.18	0.43
18:Q:118:TRP:CE3	18:Q:190:MET:HB3	2.53	0.43
18:Q:123:MET:CE	18:Q:184:TRP:HZ2	2.31	0.43
19:S:365:TRP:CD1	19:S:372:ILE:HG22	2.53	0.43
3:I:4:VAL:HG13	7:B:297:VAL:HG13	2.00	0.43
3:I:110:VAL:HG11	6:A:938:VAL:HG21	2.01	0.43
6:A:86:TYR:HA	6:A:356:PHE:HA	2.00	0.43
6:A:537:GLN:HE21	6:A:541:GLY:HA2	1.82	0.43
8:C:264:GLU:H	8:C:264:GLU:HG2	1.47	0.43
18:Q:131:HIS:HD2	19:S:756:ILE:HD11	1.82	0.43
19:S:677:SER:O	19:S:681:GLN:N	2.41	0.43
1:T:6:DC:OP2	1:T:6:DC:C6	2.70	0.43
4:N:73:ASP:OD2	4:N:77:SER:OG	2.32	0.43
7:B:651:ARG:HH21	7:B:669:GLN:HE21	1.66	0.43
7:B:782:ASP:HB3	7:B:788:ILE:HG12	2.01	0.43
19:S:365:TRP:O	19:S:407:ARG:NH2	2.52	0.43
9:D:91:ARG:HH22	17:O:181:ARG:HG3	1.82	0.43
18:Q:92:PHE:HD1	18:Q:206:GLN:HB3	1.82	0.43
19:S:21:GLN:HB3	19:S:24:SER:H	1.83	0.43
7:B:967:LEU:HD12	7:B:967:LEU:C	2.39	0.43
8:C:295:ARG:HA	8:C:295:ARG:HD3	1.86	0.43
12:G:152:ALA:HA	17:O:184:PRO:HG2	2.01	0.43
18:Q:304:LEU:HA	18:Q:307:LEU:HD12	2.00	0.43
19:S:392:GLU:HG2	20:R:142:ARG:NH1	2.34	0.43
19:S:434:ARG:HD2	19:S:434:ARG:HA	1.83	0.43
3:I:13:CYS:SG	3:I:32:GLN:HB3	2.49	0.43
18:Q:262:LEU:HD13	18:Q:266:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:674:GLU:O	19:S:678:LEU:N	2.50	0.43
20:R:10:ASN:HD22	20:R:13:PHE:HE2	1.67	0.43
6:A:254:THR:HA	6:A:312:SER:HA	2.00	0.43
6:A:1038:ILE:HB	6:A:1047:GLN:HB2	2.01	0.43
7:B:260:PHE:HB3	7:B:271:VAL:HG23	1.99	0.43
17:O:501:GLU:HB3	17:O:504:LYS:HB3	2.01	0.43
3:I:4:VAL:HG11	7:B:289:PHE:CZ	2.47	0.43
6:A:1026:GLN:HG3	6:A:1598:PHE:HD1	1.84	0.43
17:O:67:ASP:OD1	17:O:68:SER:N	2.52	0.43
17:O:493:ASP:OD1	17:O:497:ASN:N	2.45	0.43
19:S:392:GLU:OE2	19:S:395:GLN:CG	2.67	0.43
1:T:7:DA:N1	2:U:63:DT:O2	2.51	0.42
6:A:543:LEU:HB2	18:Q:34:VAL:CG2	2.49	0.42
7:B:655:TYR:CE2	7:B:657:PRO:HG2	2.54	0.42
10:E:127:ILE:HG22	10:E:129:PRO:HD2	2.00	0.42
4:N:25:ILE:HD12	4:N:29:PHE:HD2	1.84	0.42
6:A:39:ASP:OD1	6:A:43:HIS:N	2.52	0.42
7:B:291:GLY:O	7:B:579:ALA:CB	2.67	0.42
7:B:1062:GLY:HA3	7:B:1065:ARG:HB2	2.01	0.42
18:Q:338:LEU:HD22	18:Q:482:HIS:NE2	2.25	0.42
4:N:174:GLY:HA3	8:C:53:ASN:ND2	2.33	0.42
6:A:1120:TYR:O	10:E:207:ARG:NH2	2.50	0.42
7:B:286:ARG:HD2	7:B:286:ARG:HA	1.75	0.42
12:G:90:LEU:HD11	12:G:119:HIS:CE1	2.54	0.42
7:B:16:PHE:CD1	7:B:978:ALA:HB2	2.54	0.42
18:Q:342:THR:HG21	18:Q:445:ARG:NH2	2.34	0.42
1:T:4:DT:C2	2:U:67:DA:H2	2.37	0.42
6:A:399:LEU:HD11	6:A:422:ARG:HB3	2.02	0.42
14:J:2:ILE:H	14:J:2:ILE:HG12	1.52	0.42
18:Q:342:THR:HG21	18:Q:445:ARG:HH21	1.85	0.42
19:S:389:TRP:CD1	20:R:149:LYS:HD2	2.54	0.42
7:B:216:ALA:O	7:B:392:ASP:N	2.46	0.42
7:B:786:ALA:HB1	7:B:928:SER:HB2	2.01	0.42
7:B:934:ILE:H	7:B:934:ILE:HG13	1.45	0.42
12:G:235:ASN:HB3	12:G:246:ASP:HB3	2.01	0.42
17:O:63:LEU:HD21	17:O:109:SER:HB3	2.01	0.42
18:Q:94:LYS:NZ	18:Q:207:LEU:O	2.52	0.42
19:S:395:GLN:HB3	20:R:140:ILE:CG2	2.49	0.42
6:A:119:ALA:HB2	6:A:334:VAL:HG23	2.02	0.42
6:A:1039:ARG:HG2	6:A:1045:LEU:HA	2.02	0.42
7:B:93:ASN:OD1	7:B:93:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:286:ARG:O	7:B:290:ASP:N	2.39	0.42
7:B:1107:CYS:O	7:B:1195:ARG:NH2	2.53	0.42
18:Q:301:HIS:HB2	18:Q:304:LEU:HB3	2.01	0.42
19:S:392:GLU:O	20:R:142:ARG:HD2	2.19	0.42
6:A:1470:CYS:SG	6:A:1471:GLU:N	2.92	0.42
6:A:1557:ALA:HB2	10:E:150:VAL:HG22	2.01	0.42
8:C:108:VAL:HG22	8:C:184:VAL:HG22	2.02	0.42
9:D:19:PRO:HB3	12:G:47:VAL:HG12	2.01	0.42
19:S:353:ASP:HB2	19:S:379:LYS:NZ	2.34	0.42
19:S:627:GLY:HA2	19:S:630:LEU:HB2	2.02	0.42
7:B:137:LEU:HB2	7:B:161:LEU:HD23	2.02	0.42
7:B:141:LEU:HD11	7:B:420:TYR:HE2	1.83	0.42
7:B:859:CYS:O	7:B:871:ILE:HA	2.19	0.42
17:O:517:LEU:HD13	17:O:544:ILE:HG13	2.02	0.42
2:U:38:DT:H2'	2:U:39:DG:C8	2.55	0.42
6:A:364:PRO:HD2	6:A:367:PHE:HD2	1.84	0.42
6:A:897:SER:O	6:A:901:ASN:ND2	2.53	0.42
6:A:1033:SER:OG	6:A:1034:TYR:N	2.53	0.42
6:A:1053:ASP:OD2	6:A:1580:ARG:NH2	2.50	0.42
7:B:859:CYS:SG	7:B:872:LYS:HG3	2.59	0.42
6:A:427:PHE:HA	6:A:430:ILE:HG22	2.02	0.41
7:B:262:PHE:CD2	7:B:357:ILE:HD13	2.55	0.41
7:B:795:GLU:HB3	8:C:216:HIS:CE1	2.55	0.41
6:A:1148:LEU:HD21	6:A:1166:PHE:HD2	1.85	0.41
6:A:1270:VAL:HG22	6:A:1294:MET:HG2	2.03	0.41
7:B:791:LYS:HB3	7:B:932:PRO:HA	2.03	0.41
8:C:45:SER:HB2	8:C:271:ARG:HH12	1.85	0.41
13:H:133:ASN:OD1	13:H:133:ASN:N	2.48	0.41
19:S:731:LEU:HA	19:S:734:LYS:HB2	2.01	0.41
7:B:698:SER:O	7:B:702:ASN:HB2	2.21	0.41
17:O:60:LEU:HD11	17:O:107:ILE:HD11	2.02	0.41
18:Q:116:ILE:O	18:Q:120:ILE:N	2.41	0.41
18:Q:190:MET:HA	18:Q:191:PRO:HD3	1.91	0.41
19:S:17:GLY:HA3	19:S:35:LYS:NZ	2.35	0.41
19:S:632:ILE:O	19:S:636:GLU:N	2.53	0.41
20:R:256:GLU:O	20:R:260:ASN:HB2	2.20	0.41
7:B:167:SER:OG	7:B:168:ASN:N	2.54	0.41
7:B:698:SER:OG	7:B:699:ILE:N	2.53	0.41
17:O:468:GLU:O	17:O:471:LYS:NZ	2.49	0.41
7:B:939:SER:OG	7:B:940:GLU:N	2.53	0.41
19:S:739:ASP:O	19:S:743:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:113:SER:H	4:N:118:SER:HA	1.84	0.41
7:B:61:LEU:HD22	7:B:413:LEU:HD22	2.02	0.41
7:B:210:ARG:NH1	7:B:625:GLU:OE2	2.54	0.41
7:B:1158:ILE:HG12	7:B:1168:VAL:HG22	2.03	0.41
10:E:128:PRO:HG2	10:E:129:PRO:HD3	2.01	0.41
19:S:33:THR:HG21	19:S:50:LEU:H	1.84	0.41
19:S:207:SER:N	19:S:213:VAL:O	2.53	0.41
19:S:369:PHE:CD2	19:S:371:LYS:HE3	2.56	0.41
3:I:46:LYS:HG2	6:A:1275:THR:HB	2.01	0.41
7:B:705:PRO:HG2	7:B:921:HIS:CE1	2.55	0.41
18:Q:198:ILE:HG13	18:Q:199:LEU:HD22	2.03	0.41
19:S:56:ASP:N	19:S:56:ASP:OD1	2.52	0.41
20:R:137:SER:OG	20:R:139:GLU:O	2.32	0.41
3:I:82:ILE:HG12	3:I:96:TYR:CE1	2.56	0.41
4:N:54:TRP:CD1	4:N:135:LYS:HB2	2.56	0.41
6:A:949:GLN:NE2	6:A:950:GLN:O	2.53	0.41
7:B:145:VAL:HG11	7:B:441:LYS:HG2	2.03	0.41
7:B:857:PRO:HB3	7:B:871:ILE:CD1	2.37	0.41
7:B:863:ASP:CG	7:B:870:LYS:HE2	2.41	0.41
1:T:7:DA:N6	2:U:62:DG:O6	2.53	0.41
5:M:58:GLU:HG3	5:M:59:ARG:HG3	2.03	0.41
6:A:130:ILE:HD11	6:A:212:VAL:HG22	2.03	0.41
6:A:602:GLY:N	6:A:651:ALA:O	2.53	0.41
7:B:714:ARG:HD3	7:B:714:ARG:HA	1.82	0.41
19:S:404:ASP:OD2	19:S:451:ILE:N	2.50	0.41
19:S:421:ILE:HD12	20:R:138:PHE:HE2	1.86	0.41
19:S:433:VAL:HG23	19:S:434:ARG:H	1.86	0.41
20:R:202:THR:O	20:R:211:ARG:NH2	2.54	0.41
1:T:18:DC:OP1	7:B:1063:ARG:NH1	2.54	0.41
5:M:73:SER:HB2	7:B:566:TYR:HD2	1.85	0.41
6:A:1447:GLN:HE21	6:A:1459:LYS:HA	1.86	0.41
18:Q:123:MET:CE	18:Q:184:TRP:CZ2	3.03	0.41
20:R:216:LEU:HD23	20:R:216:LEU:HA	1.87	0.41
6:A:824:THR:HG23	7:B:1023:ARG:HB2	2.04	0.40
6:A:1459:LYS:HB2	6:A:1473:LYS:HB2	2.03	0.40
17:O:330:THR:HA	17:O:333:ASP:HB2	2.02	0.40
2:U:34:DT:C2	2:U:35:DA:N7	2.89	0.40
3:I:53:ASP:OD1	3:I:53:ASP:N	2.47	0.40
6:A:1053:ASP:OD1	6:A:1053:ASP:N	2.52	0.40
6:A:1055:ILE:HD11	6:A:1174:TYR:CE1	2.56	0.40
7:B:225:ARG:HH22	7:B:261:ARG:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:456:VAL:HB	19:S:463:LEU:HB2	2.03	0.40
6:A:1240:LEU:HB3	6:A:1536:ILE:HD12	2.04	0.40
6:A:1641:ILE:HD11	7:B:1088:LEU:HD21	2.02	0.40
7:B:291:GLY:O	7:B:579:ALA:HB2	2.21	0.40
7:B:397:THR:HA	7:B:400:GLN:HG2	2.04	0.40
8:C:153:PRO:HA	8:C:156:LEU:HB3	2.02	0.40
18:Q:341:ARG:NH2	18:Q:351:ASN:OD1	2.53	0.40
6:A:1221:ARG:HH12	6:A:1233:ILE:HG12	1.87	0.40
11:F:77:ASP:OD1	11:F:77:ASP:N	2.54	0.40
17:O:60:LEU:O	17:O:106:ARG:NH1	2.44	0.40
19:S:36:LYS:HG3	19:S:46:VAL:HG23	2.04	0.40
19:S:193:LEU:HD21	19:S:256:ARG:HE	1.86	0.40
19:S:627:GLY:O	19:S:631:SER:N	2.51	0.40
1:T:4:DT:H2"	1:T:5:DT:C7	2.51	0.40
6:A:1319:ASN:O	6:A:1323:HIS:ND1	2.52	0.40
7:B:610:TYR:HE1	7:B:658:LEU:HD11	1.87	0.40
7:B:733:LEU:CD1	7:B:743:ARG:HD2	2.51	0.40
7:B:884:GLU:OE1	7:B:904:LYS:CE	2.70	0.40
9:D:11:ASN:C	9:D:12:THR:HG22	2.39	0.40
11:F:79:ARG:NH1	11:F:145:ASP:O	2.55	0.40
18:Q:417:PHE:CZ	20:R:257:ILE:HD11	2.57	0.40
18:Q:470:PRO:HA	18:Q:473:LYS:HG2	2.04	0.40
20:R:6:ILE:HB	20:R:8:LEU:HD23	2.04	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	
3	I	122/125 (98%)	103 (84%)	19 (16%)	0	100	100
4	N	131/233 (56%)	119 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	106/415 (26%)	93 (88%)	13 (12%)	0	100	100
6	A	1449/1664 (87%)	1366 (94%)	83 (6%)	0	100	100
7	B	1174/1203 (98%)	1106 (94%)	68 (6%)	0	100	100
8	C	300/335 (90%)	287 (96%)	13 (4%)	0	100	100
9	D	66/137 (48%)	63 (96%)	3 (4%)	0	100	100
10	E	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
11	F	98/155 (63%)	93 (95%)	4 (4%)	1 (1%)	15	37
12	G	196/326 (60%)	185 (94%)	11 (6%)	0	100	100
13	H	130/146 (89%)	121 (93%)	9 (7%)	0	100	100
14	J	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
15	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
16	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
17	O	498/627 (79%)	465 (93%)	33 (7%)	0	100	100
18	Q	469/514 (91%)	414 (88%)	54 (12%)	1 (0%)	47	73
19	S	594/894 (66%)	524 (88%)	70 (12%)	0	100	100
20	R	322/507 (64%)	290 (90%)	31 (10%)	1 (0%)	41	66
All	All	6079/7778 (78%)	5632 (93%)	444 (7%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Q	281	ILE
11	F	87	LYS
20	R	356	PRO

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	
3	I	109/110 (99%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	128/220 (58%)	128 (100%)	0	100	100
5	M	98/371 (26%)	98 (100%)	0	100	100
6	A	1293/1465 (88%)	1289 (100%)	4 (0%)	92	98
7	B	1029/1053 (98%)	1021 (99%)	8 (1%)	81	93
8	C	269/296 (91%)	266 (99%)	3 (1%)	73	90
9	D	65/116 (56%)	65 (100%)	0	100	100
10	E	197/197 (100%)	197 (100%)	0	100	100
11	F	90/137 (66%)	89 (99%)	1 (1%)	73	90
12	G	180/291 (62%)	178 (99%)	2 (1%)	73	90
13	H	116/128 (91%)	115 (99%)	1 (1%)	78	92
14	J	64/65 (98%)	63 (98%)	1 (2%)	62	85
15	K	93/130 (72%)	93 (100%)	0	100	100
16	L	40/57 (70%)	40 (100%)	0	100	100
17	O	466/576 (81%)	462 (99%)	4 (1%)	78	92
18	Q	436/476 (92%)	432 (99%)	4 (1%)	78	92
19	S	563/828 (68%)	557 (99%)	6 (1%)	73	90
20	R	313/474 (66%)	310 (99%)	3 (1%)	76	91
All	All	5549/6990 (79%)	5512 (99%)	37 (1%)	84	94

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	30	LYS
6	A	129	LEU
6	A	701	ARG
6	A	840	ASN
7	B	72	VAL
7	B	87	ASN
7	B	152	LEU
7	B	302	LEU
7	B	306	LEU
7	B	702	ASN
7	B	957	ARG
7	B	1037	ARG
8	C	89	THR
8	C	91	VAL

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Mol	Chain	Res	Type
8	C	281	ARG
11	F	111	LEU
12	G	56	ASN
12	G	171	ASN
13	H	25	ARG
14	J	52	THR
17	O	222	CYS
17	O	223	SER
17	O	225	LEU
17	O	242	VAL
18	Q	18	ARG
18	Q	21	ARG
18	Q	79	GLN
18	Q	172	LEU
19	S	360	TRP
19	S	379	LYS
19	S	395	GLN
19	S	407	ARG
19	S	442	LEU
19	S	554	ASN
20	R	142	ARG
20	R	144	VAL
20	R	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	171	HIS
19	S	395	GLN
20	R	319	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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.

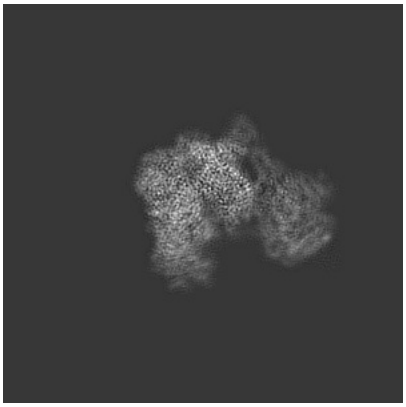
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10006. These allow visual inspection of the internal detail of the map and identification of artifacts.

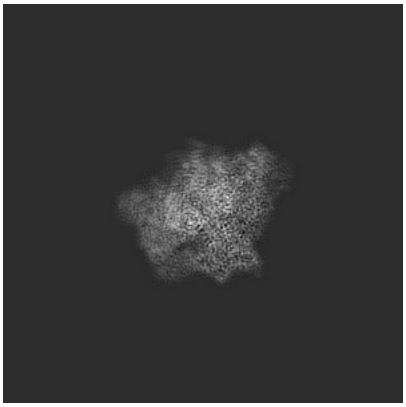
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

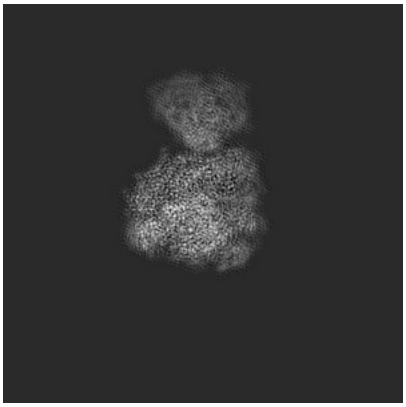
6.1.1 Primary map



X



Y

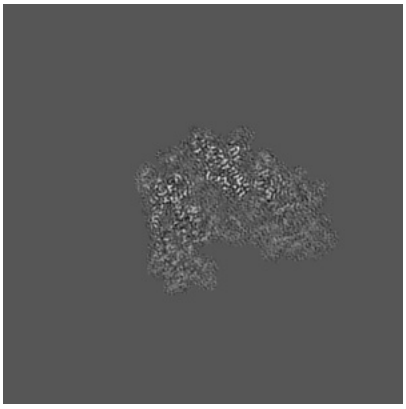


Z

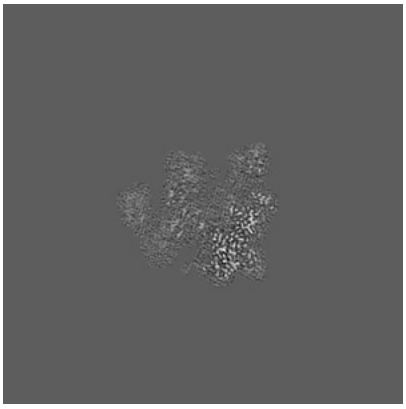
The images above show the map projected in three orthogonal directions.

6.2 Central slices

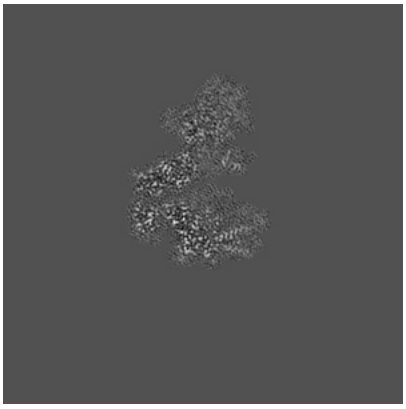
6.2.1 Primary map



X Index: 190



Y Index: 190

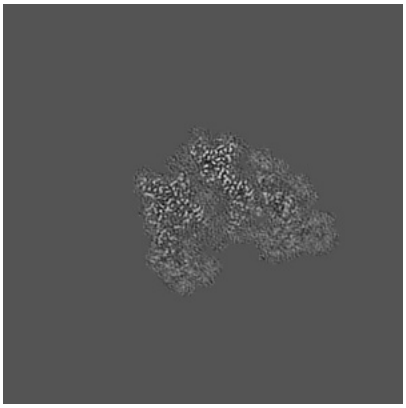


Z Index: 190

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

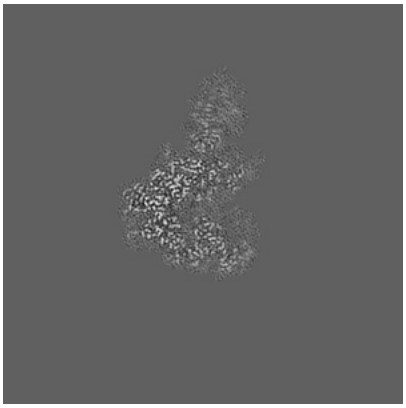
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 182

Y Index: 165

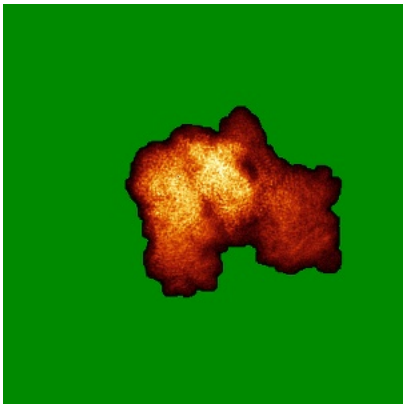


Z Index: 210

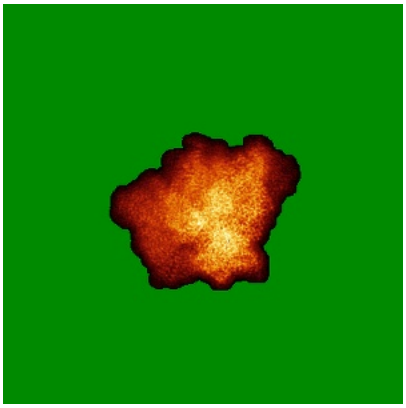
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

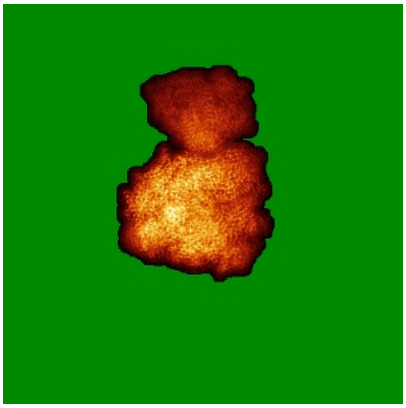
6.4.1 Primary map



X



Y



Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

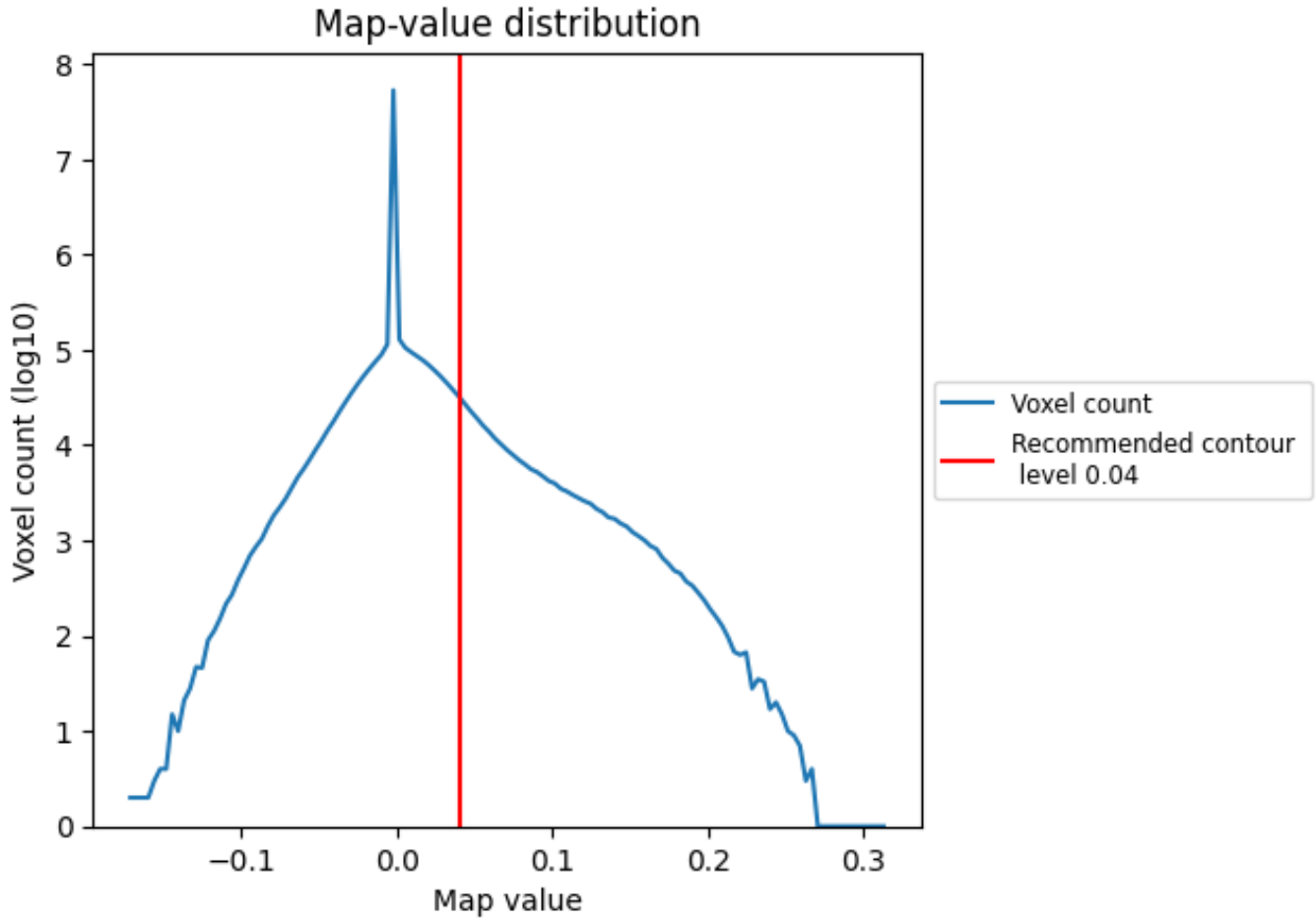
6.6 Mask visualisation (i)

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

7 Map analysis

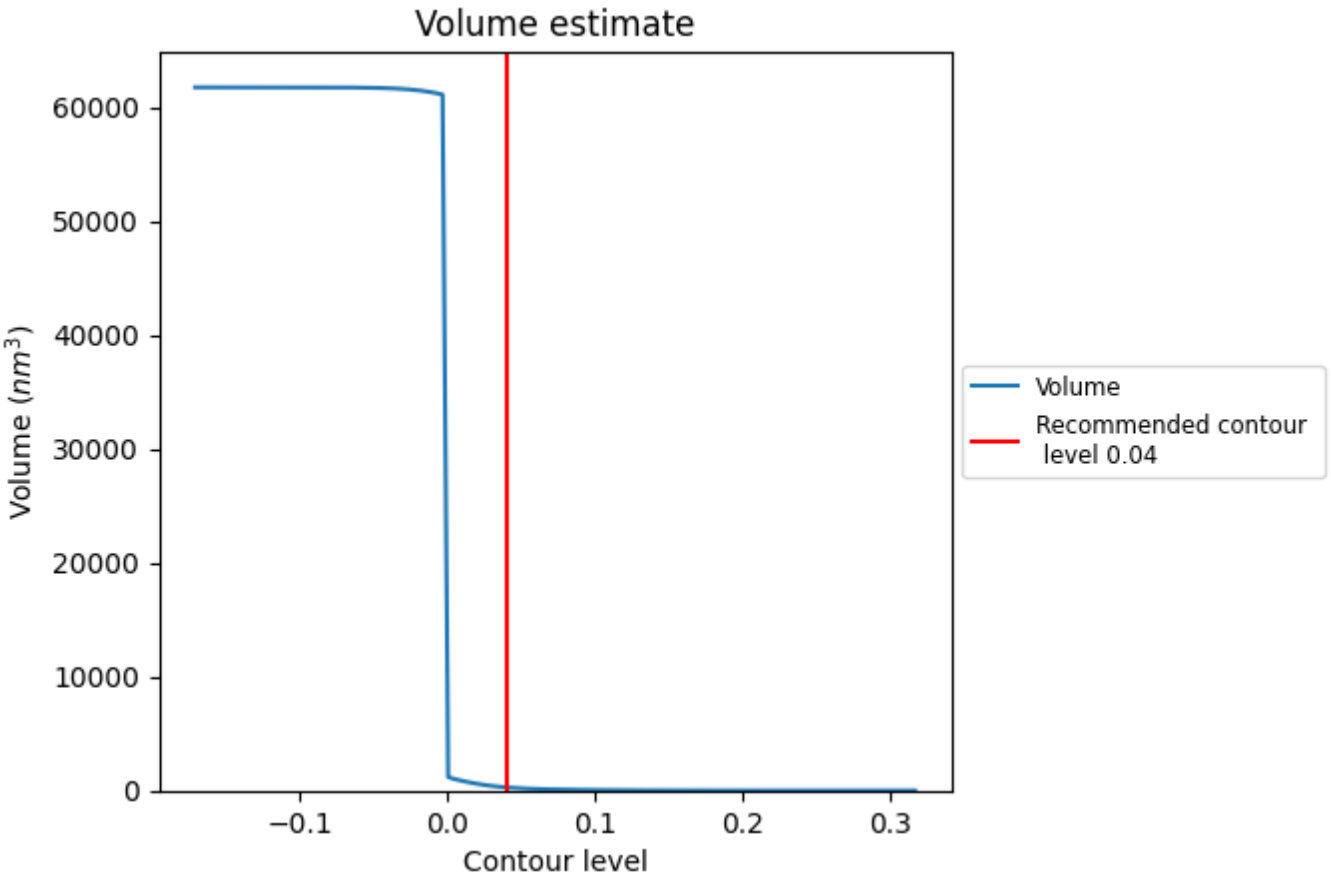
This section contains the results of statistical analysis of the map.

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.

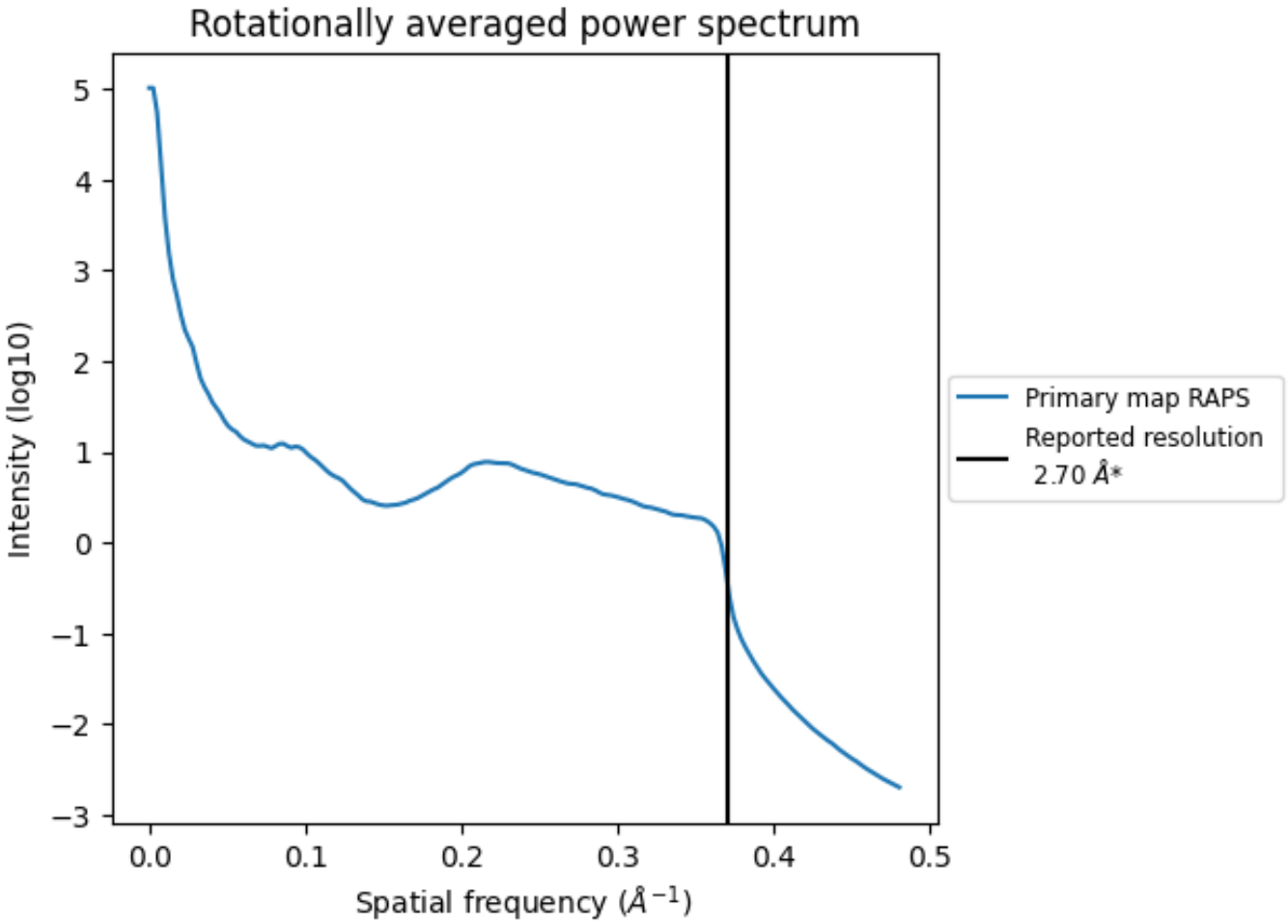
7.2 Volume estimate



The volume at the recommended contour level is 275 nm^3; this corresponds to an approximate mass of 249 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 0.370 Å^{-1}

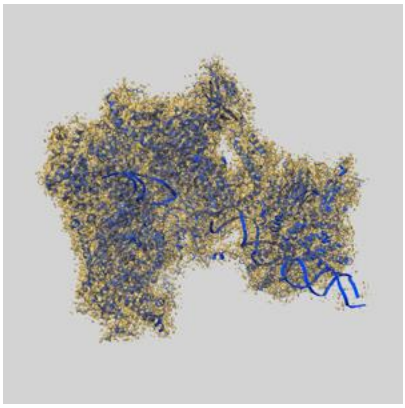
8 Fourier-Shell correlation (i)

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

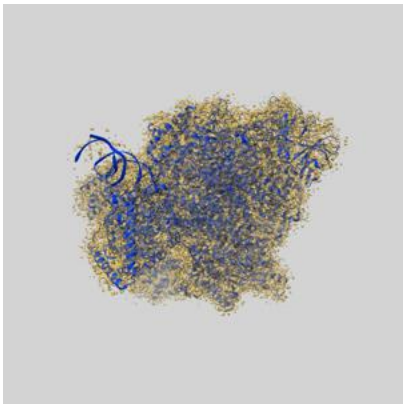
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10006 and PDB model 6RUI. Per-residue inclusion information can be found in section 3 on page 8.

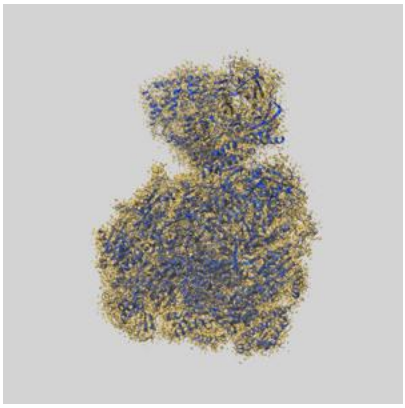
9.1 Map-model overlay



X



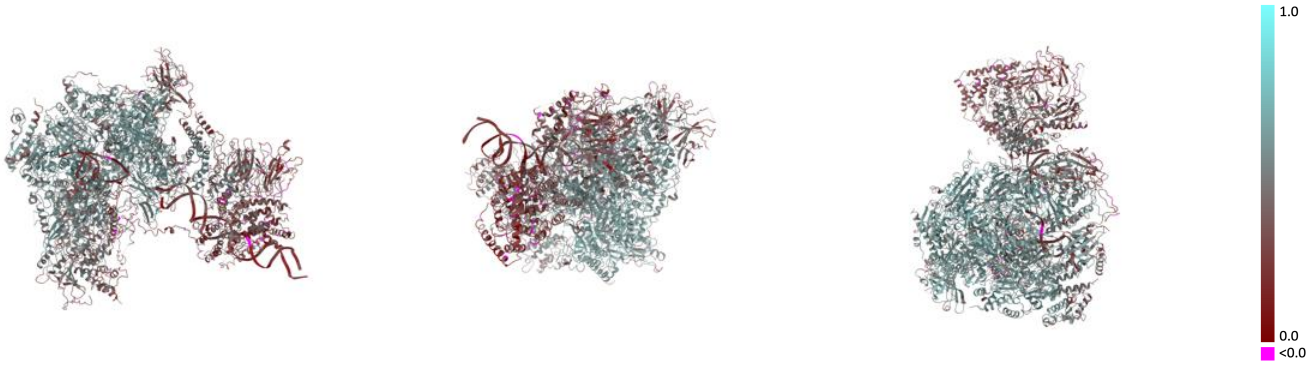
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

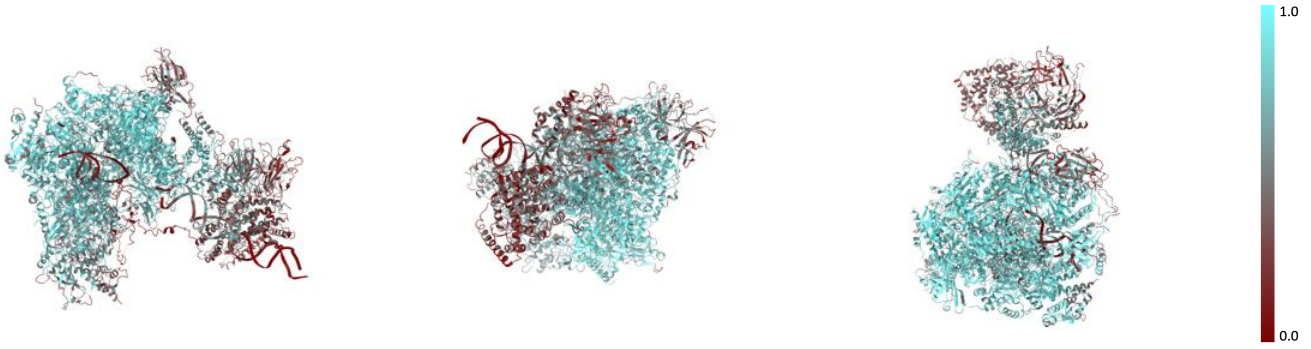
9.2 Q-score mapped to coordinate model (i)



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.

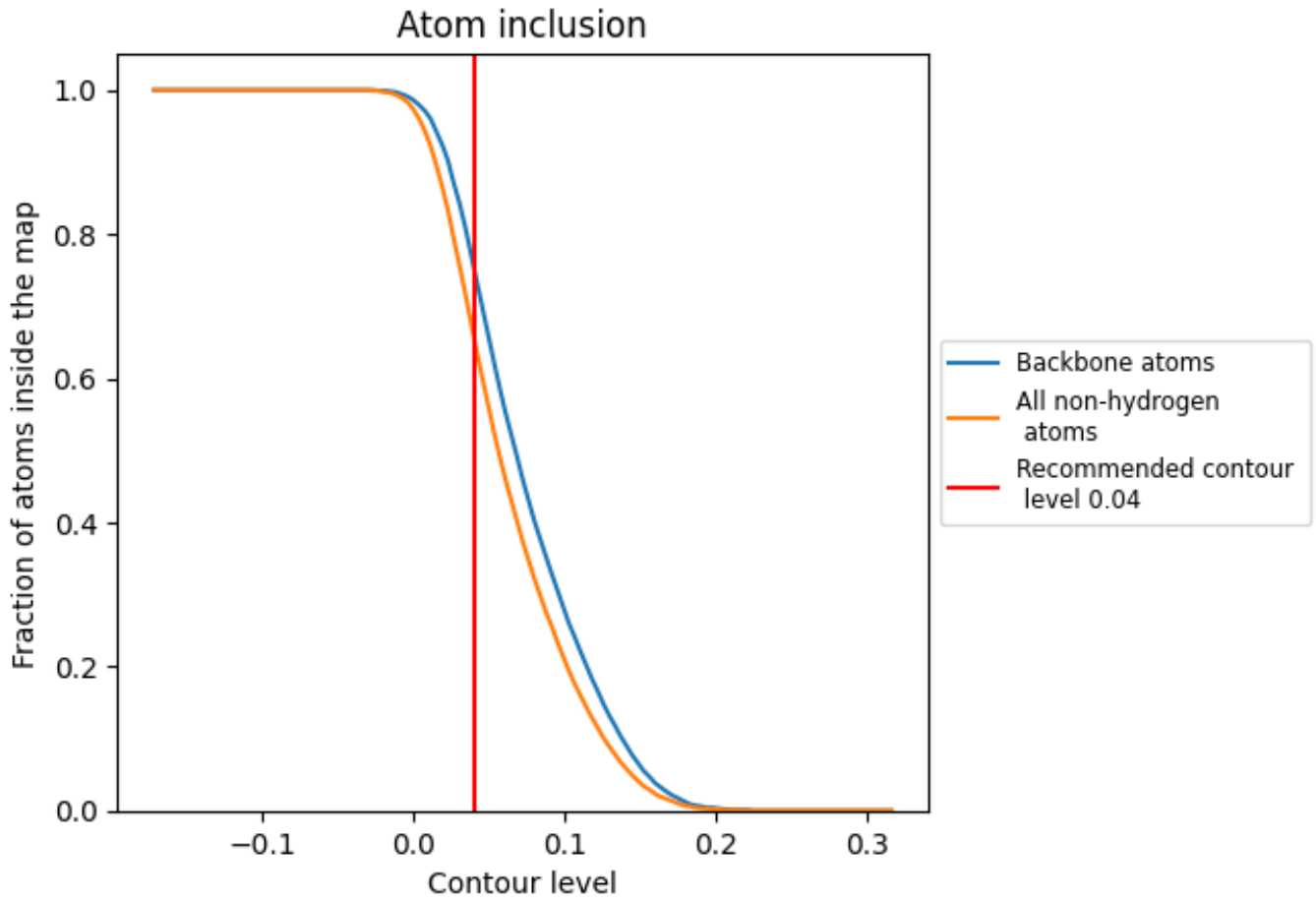
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 66% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.4630
A	0.8150	0.5450
B	0.8560	0.5700
C	0.8580	0.5710
D	0.5840	0.4270
E	0.7830	0.5280
F	0.8660	0.5880
G	0.6540	0.4550
H	0.8240	0.5500
I	0.5150	0.3850
J	0.9180	0.6120
K	0.8610	0.5820
L	0.8010	0.5330
M	0.3950	0.3650
N	0.3750	0.3680
O	0.5240	0.3870
Q	0.3740	0.3030
R	0.5910	0.4070
S	0.3510	0.2910
T	0.2300	0.2240
U	0.2250	0.2190