Full wwPDB EM Validation Report ⓘ

May 19, 2024 – 03:59 am BST

PDB ID	:	6RRD
EMDB ID	:	EMD-4987
Title	:	RNA Polymerase I Pre-initiation complex DNA opening intermediate 1
Authors	:	Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on	:	2019-05-17
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

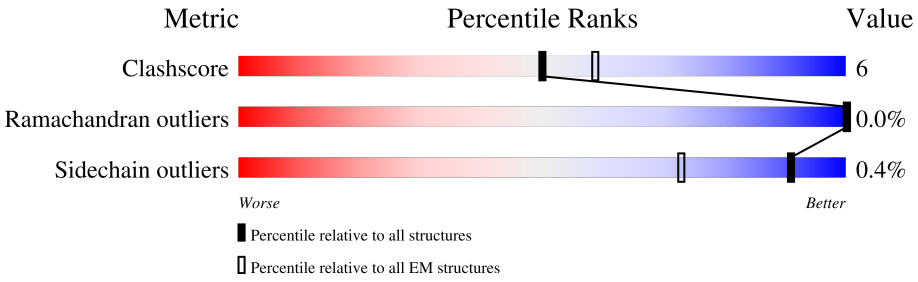
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	43% 53% 17% · 27%
2	U	70	40% 59% 10% 31%
3	Q	514	58% 73% 19% · 7%
4	S	894	41% 52% 16% 32%
5	R	507	18% 56% 9% 35%
6	I	125	26% 80% 19% ·
7	N	233	12% 52% 7% · 40%
8	M	415	5% 20% 6% 74%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	A	1664	77% 11% 12%
10	B	1203	85% 13%
11	C	335	81% 10% 9%
12	D	137	11% 42% 9% 49%
13	E	215	89% 11%
14	F	155	59% 5% 35%
15	G	326	5% 50% 12% 38%
16	H	146	81% 11% 8%
17	J	70	84% 13%
18	K	142	66% 6% 27%
19	L	70	57% 7% 36%
20	O	627	20% 67% 13% 20%

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 51631 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
1	T	51	Total	C	N	O	P	0	0
			1019	491	163	314	51		

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	48	Total	C	N	O	P	0	0
			1010	478	206	279	47		

- Molecule 3 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

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

- Molecule 4 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

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

- Molecule 5 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA12.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA34.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA49.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA190.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA135.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA43.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

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

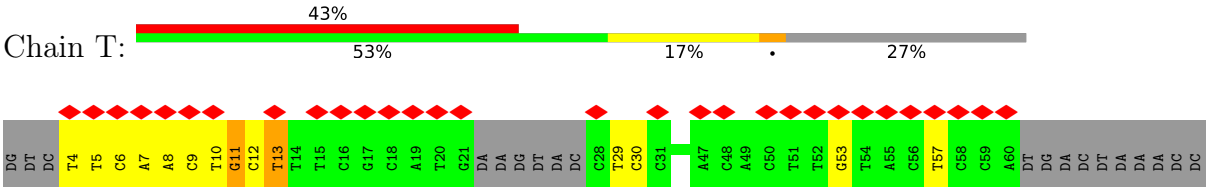
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

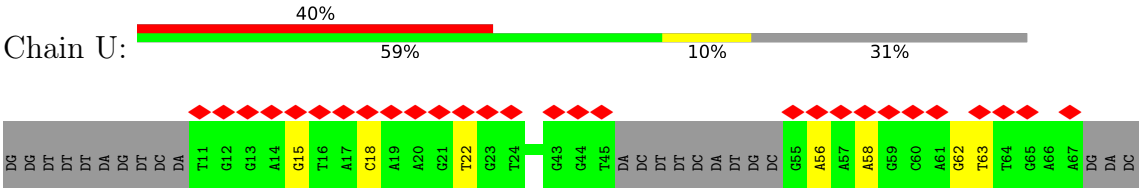
3 Residue-property plots (i)

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.

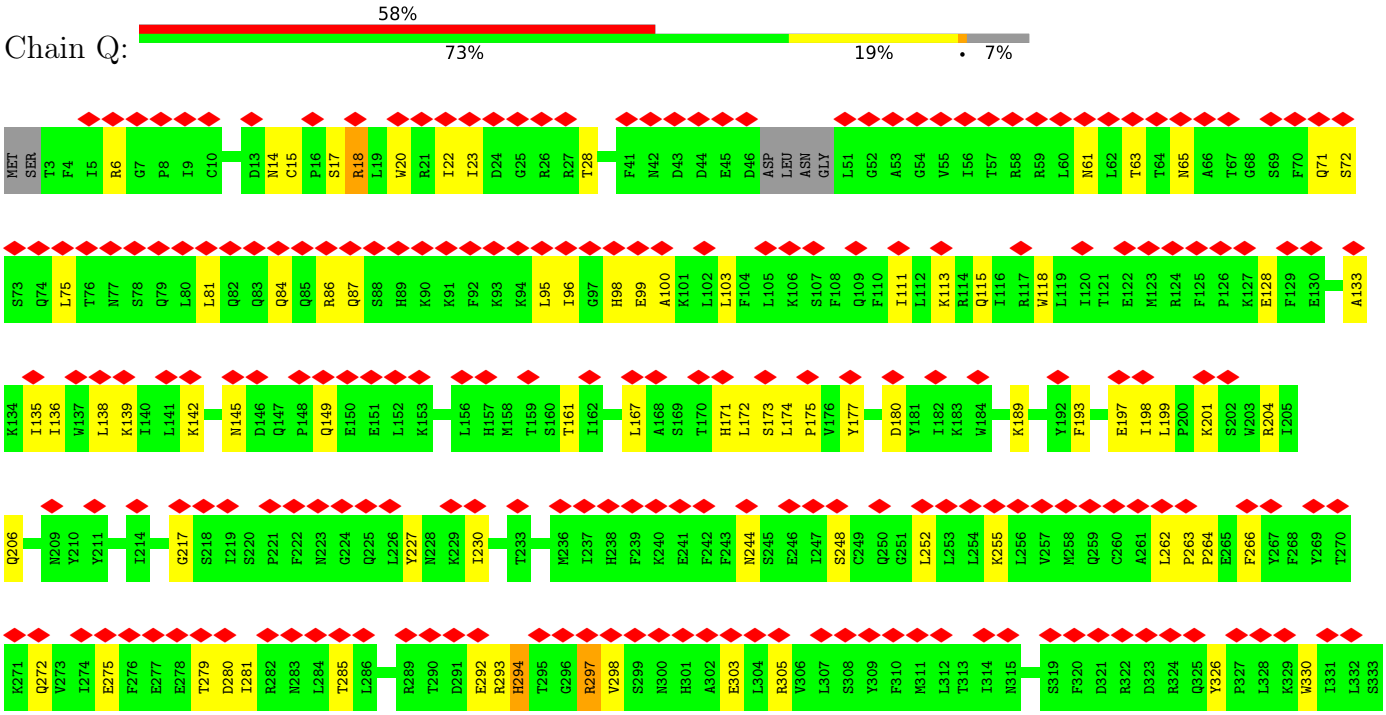
• Molecule 1: Template strand

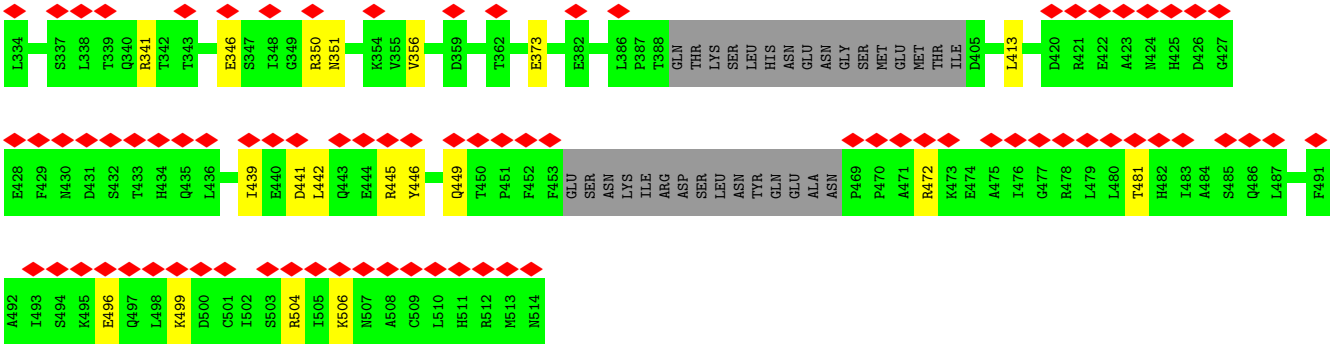


• Molecule 2: Nontemplate strand



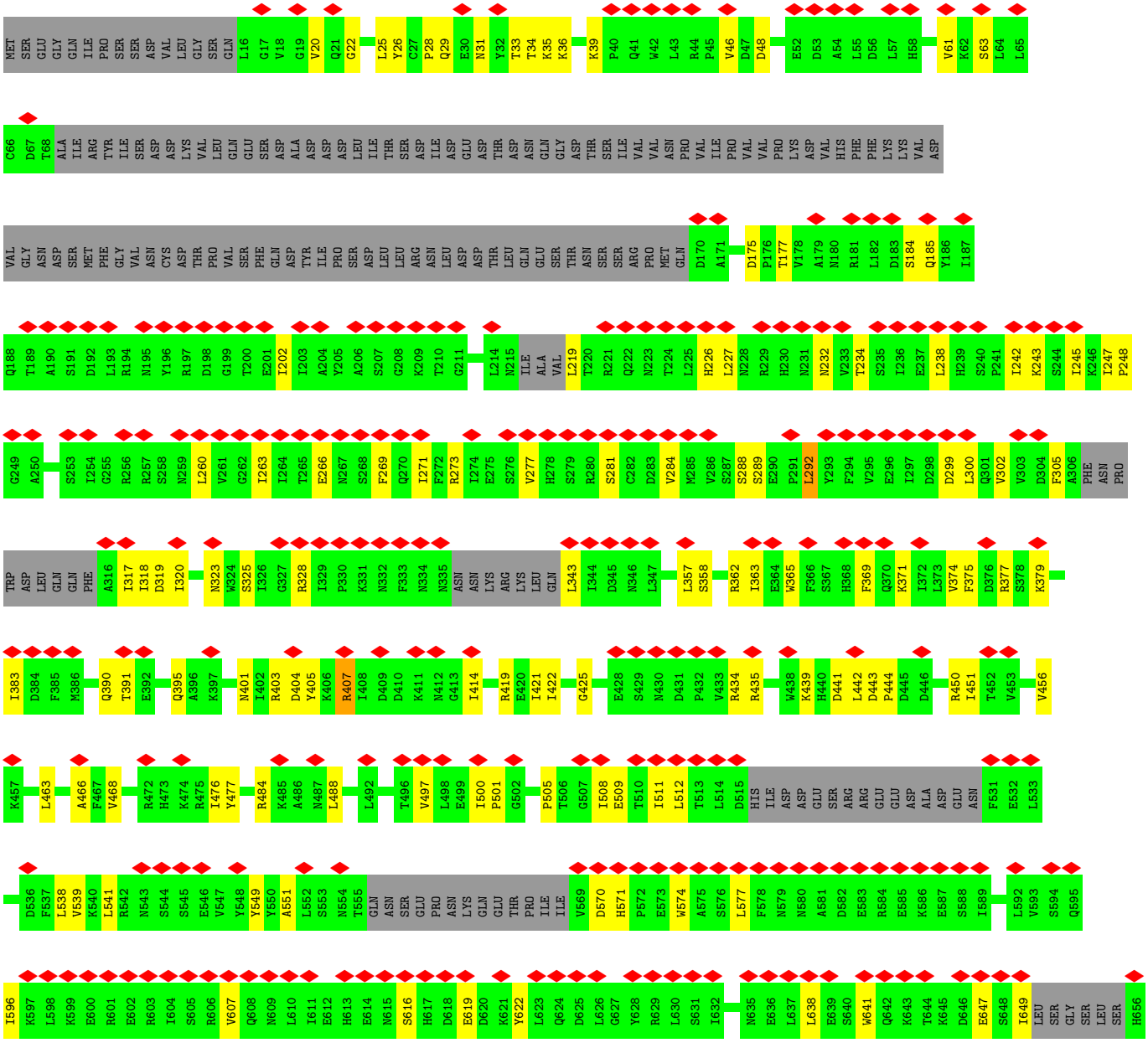
• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN7

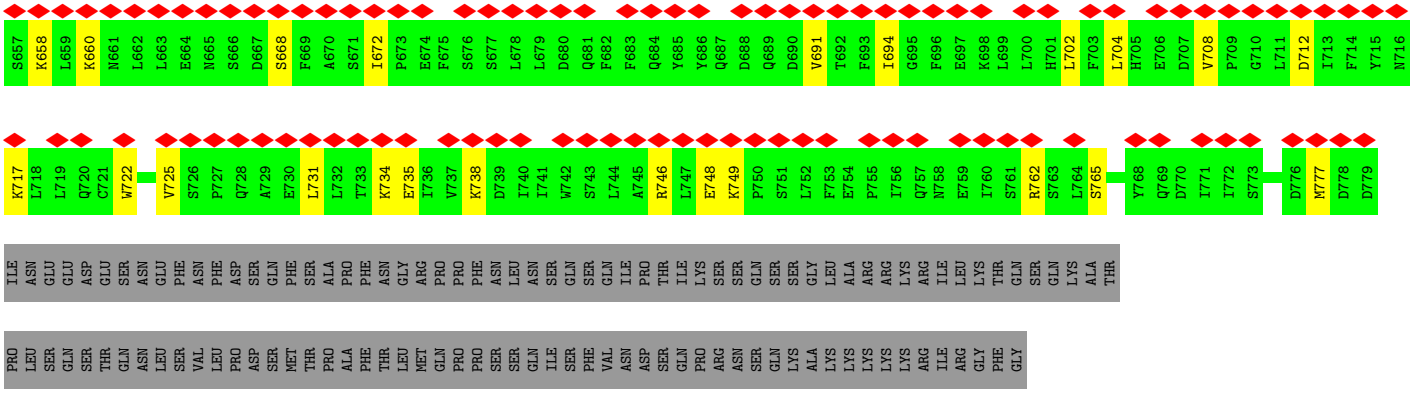




• Molecule 4: RNA polymerase I-specific transcription initiation factor RRN6

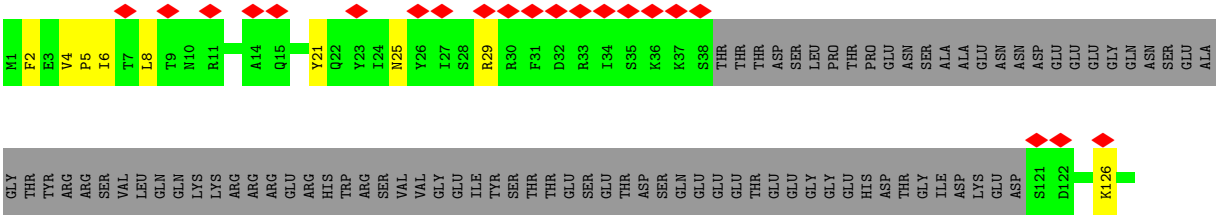
Chain S:





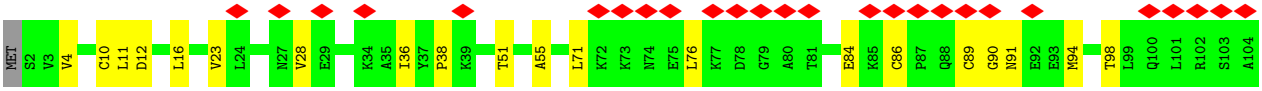
• Molecule 5: RNA polymerase I-specific transcription initiation factor RRN11

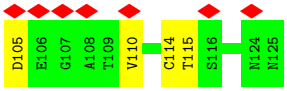
Chain R:



• Molecule 6: DNA-directed RNA polymerase I subunit RPA12

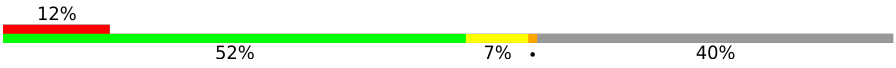
Chain I:

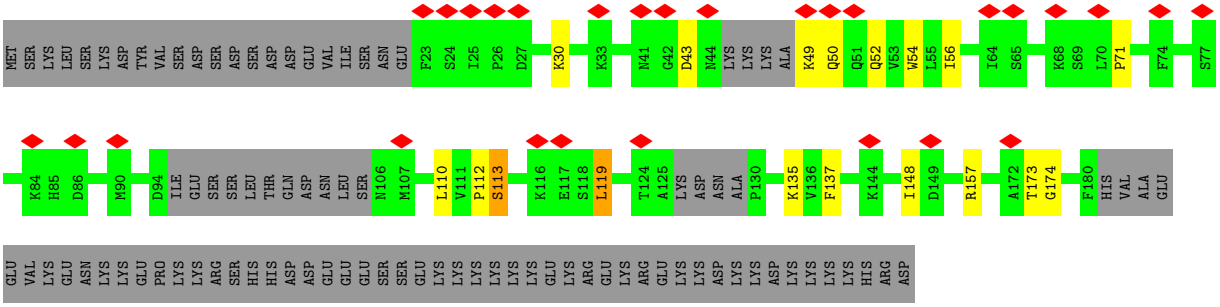




• Molecule 7: DNA-directed RNA polymerase I subunit RPA34

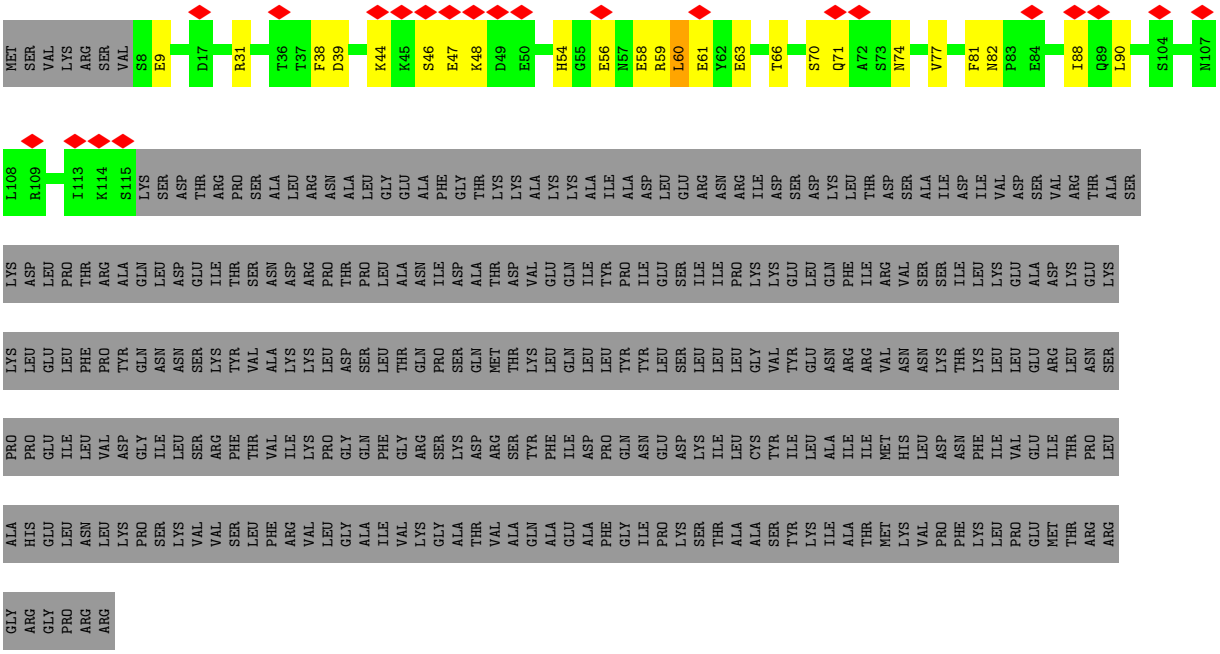
Chain N:





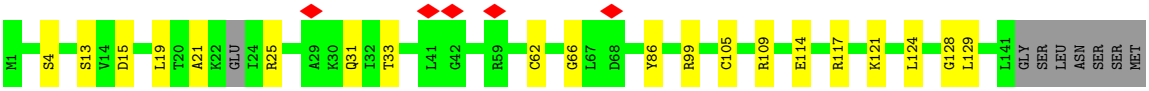
• Molecule 8: DNA-directed RNA polymerase I subunit RPA49

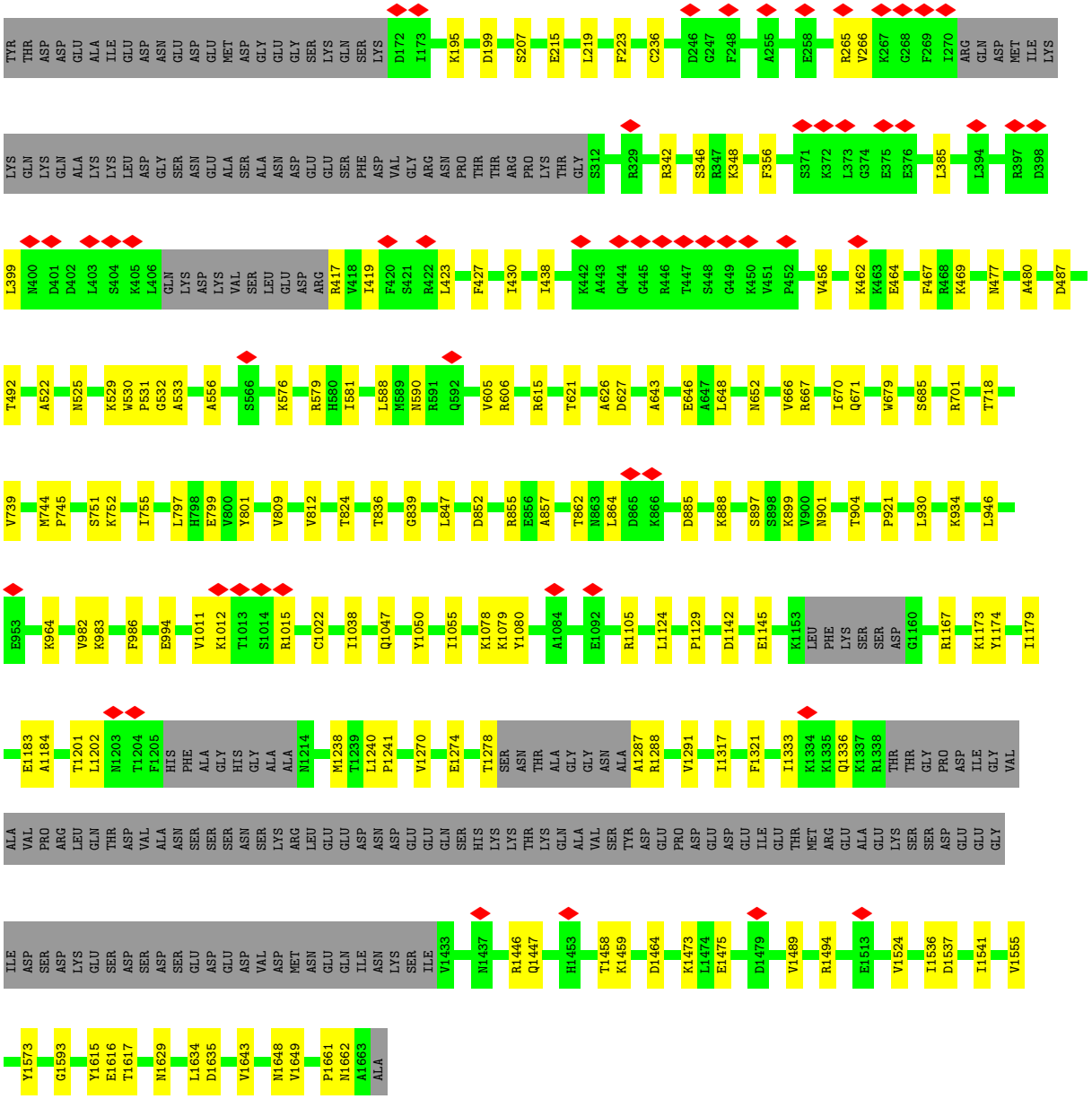
Chain M:



• Molecule 9: DNA-directed RNA polymerase I subunit RPA190

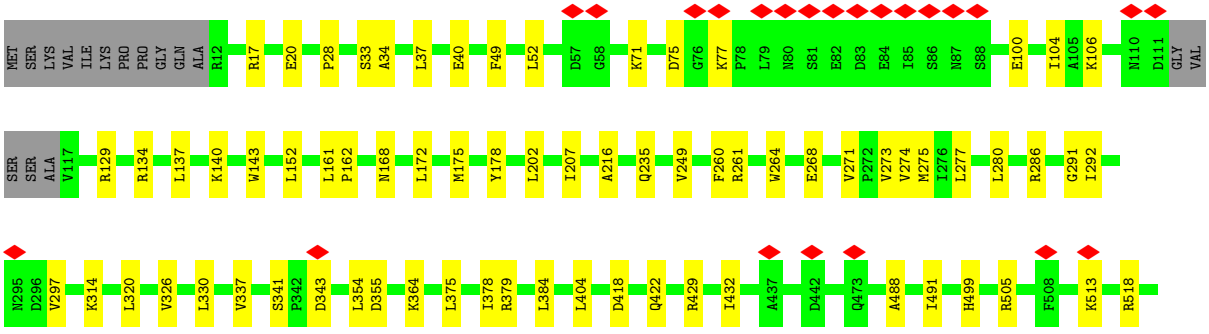
Chain A:

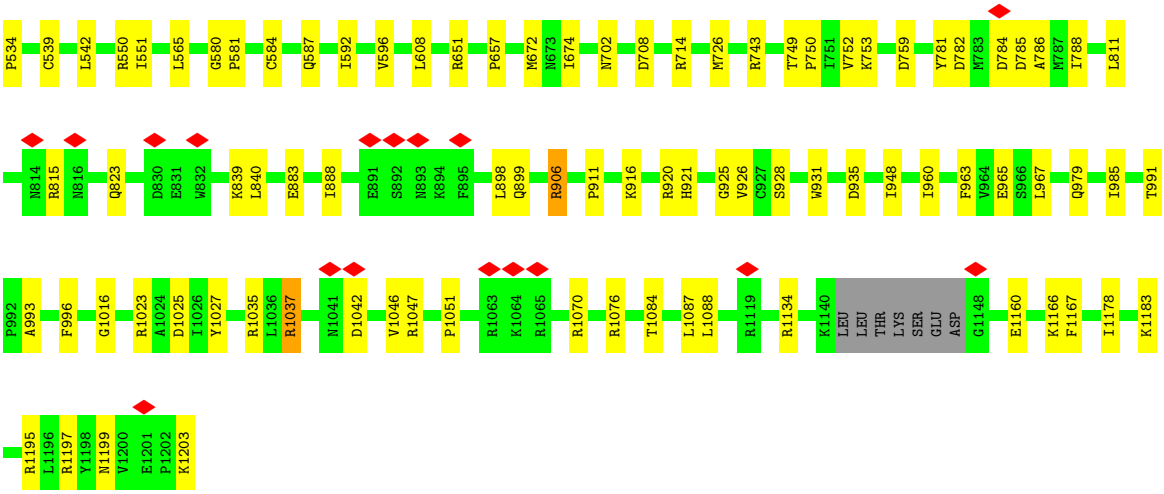




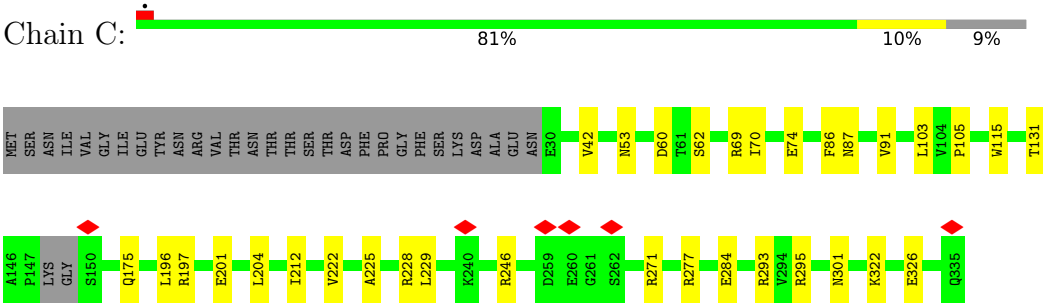
• Molecule 10: DNA-directed RNA polymerase I subunit RPA135

Chain B:

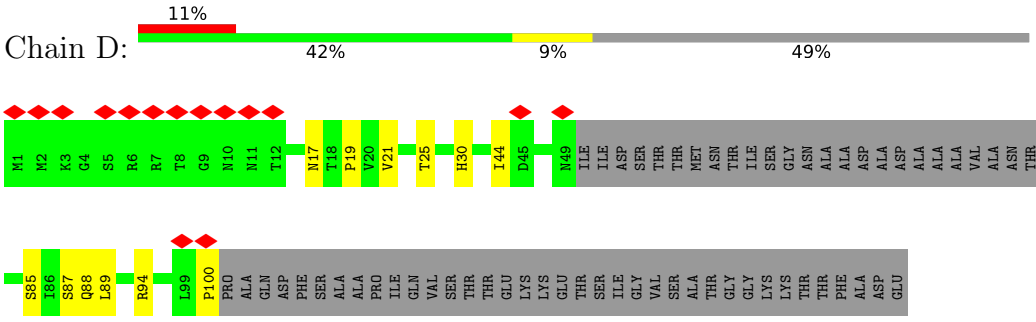




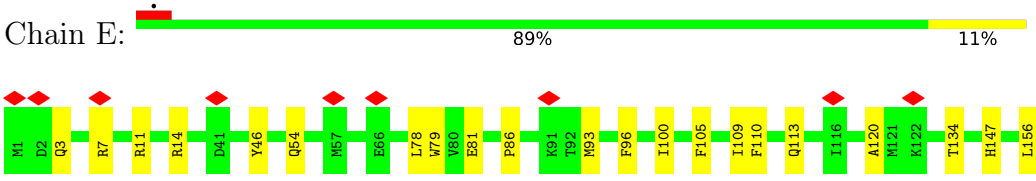
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC1



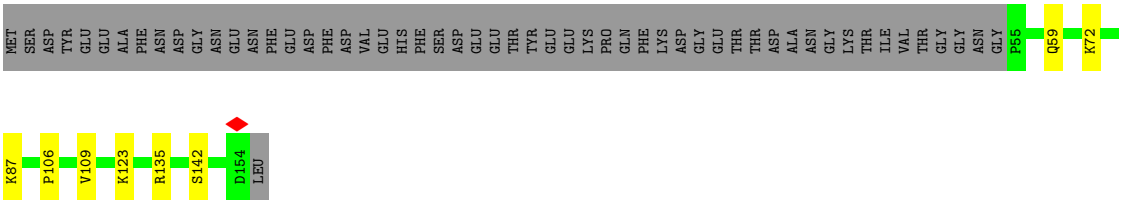
• Molecule 12: DNA-directed RNA polymerase I subunit RPA14



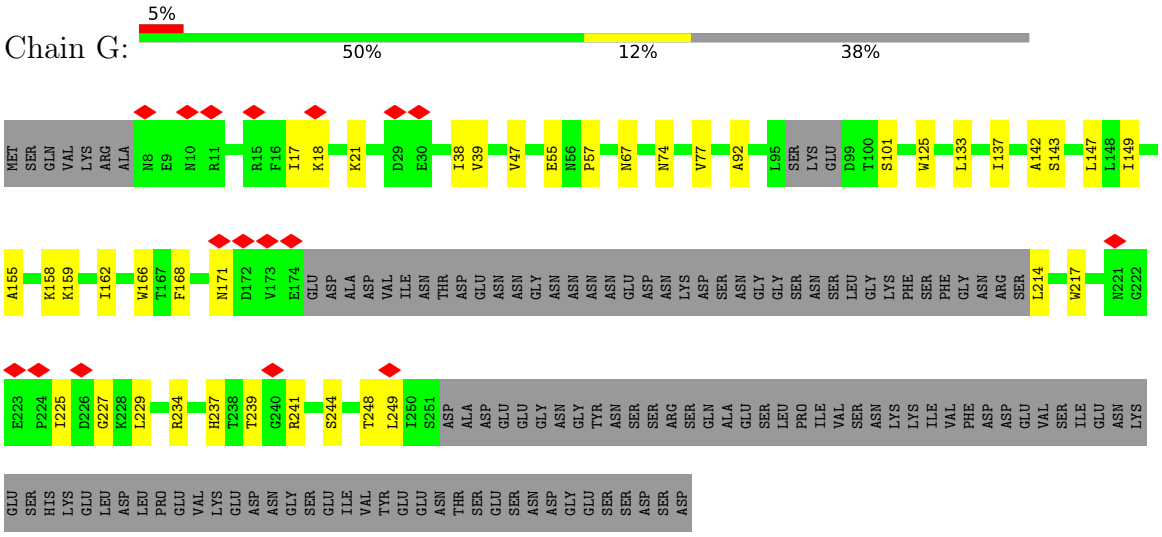
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



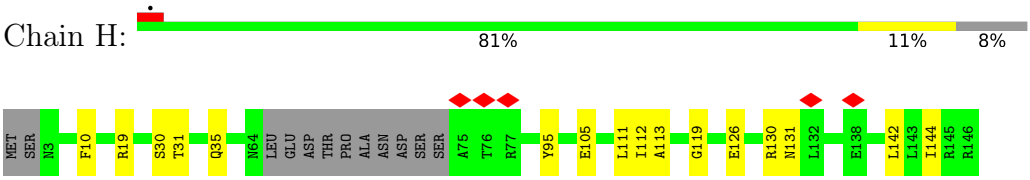
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2



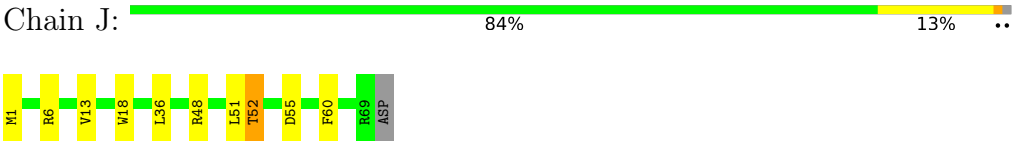
• Molecule 15: DNA-directed RNA polymerase I subunit RPA43



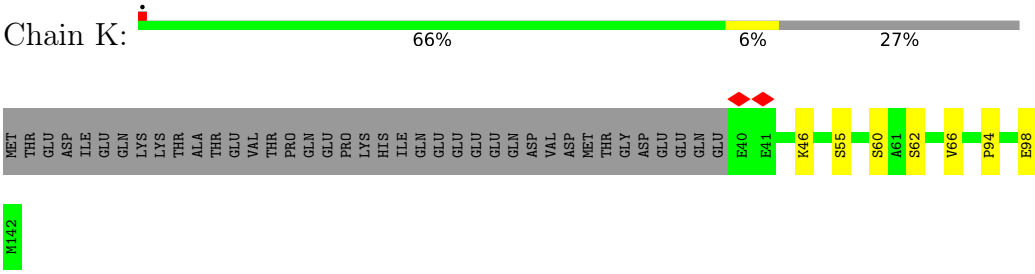
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

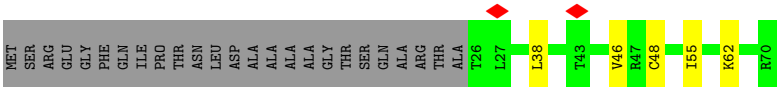


• Molecule 18: DNA-directed RNA polymerases I and III subunit RPAC2



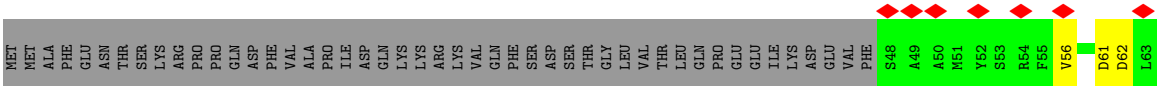
• Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC4

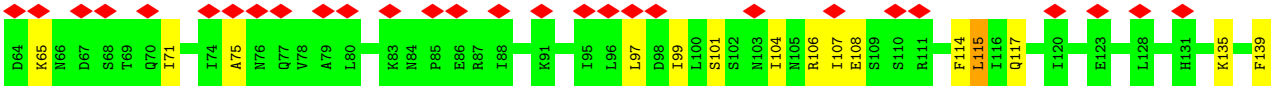
Chain L:

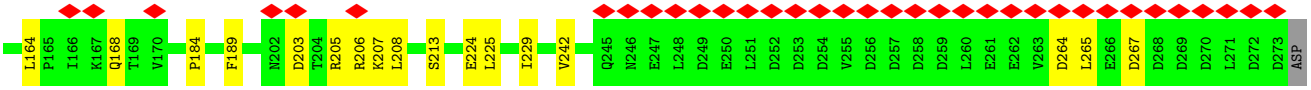


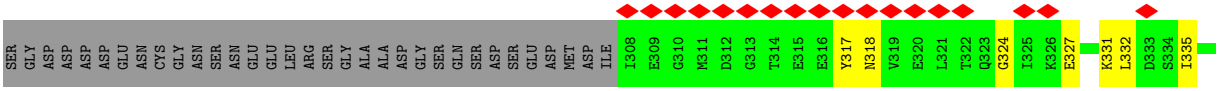
• Molecule 20: RNA polymerase I-specific transcription initiation factor RRN3

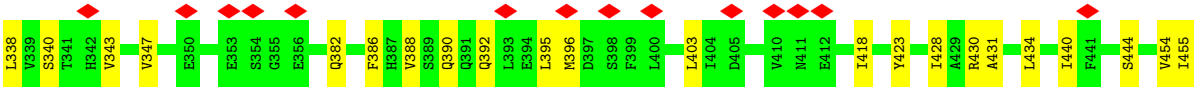
Chain O:

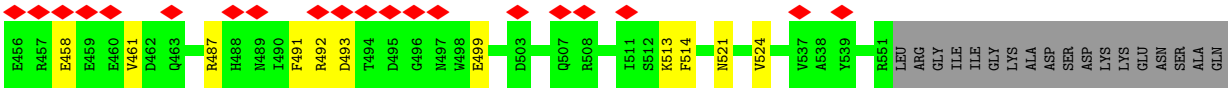


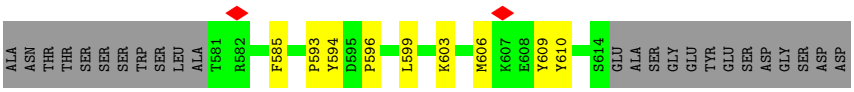












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24848	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 ($e^-/Å^2$)	1.054	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	0.265	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	395.58002, 395.58002, 395.58002	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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	0.69	1/1133 (0.1%)	1.10	1/1738 (0.1%)
2	U	0.59	0/1140	1.01	0/1762
3	Q	0.33	0/4028	0.64	0/5441
4	S	0.32	0/5065	0.62	0/6859
5	R	0.36	0/2836	0.62	0/3817
6	I	0.35	0/955	0.61	0/1288
7	N	0.32	0/1124	0.63	0/1512
8	M	0.35	0/872	0.62	0/1170
9	A	0.43	0/11776	0.60	0/15906
10	B	0.47	0/9572	0.64	0/12941
11	C	0.44	0/2469	0.62	0/3347
12	D	0.32	0/557	0.58	0/750
13	E	0.38	0/1795	0.54	0/2416
14	F	0.47	0/838	0.58	0/1129
15	G	0.37	0/1637	0.58	0/2226
16	H	0.45	0/1090	0.65	0/1476
17	J	0.51	0/578	0.70	0/775
18	K	0.43	0/821	0.62	0/1108
19	L	0.42	0/361	0.72	0/478
20	O	0.34	0/4226	0.59	0/5717
All	All	0.42	1/52873 (0.0%)	0.64	1/71856 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	11	DG	O3'-P	6.26	1.68	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	13	DT	C2'-C3'-O3'	-5.14	95.63	112.60

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	1019	0	581	23	0
2	U	1010	0	541	15	0
3	Q	3936	0	3920	67	0
4	S	4963	0	4890	109	0
5	R	2771	0	2844	38	0
6	I	942	0	937	18	0
7	N	1103	0	1106	17	0
8	M	856	0	855	17	0
9	A	11565	0	11657	130	0
10	B	9365	0	9232	111	0
11	C	2418	0	2401	24	0
12	D	551	0	558	10	0
13	E	1759	0	1788	14	0
14	F	823	0	841	5	0
15	G	1600	0	1600	28	0
16	H	1072	0	1042	9	0
17	J	569	0	589	8	0
18	K	810	0	801	6	0
19	L	359	0	385	4	0
20	O	4139	0	4061	55	0
21	Q	1	0	0	0	0
All	All	51631	0	50629	599	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 (599) 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)
9:A:1012:LYS:HD2	9:A:1201:THR:CG2	1.68	1.23
9:A:1012:LYS:CD	9:A:1201:THR:HG21	1.69	1.22
2:U:22:DT:H72	3:Q:294:HIS:CD2	1.78	1.19
2:U:22:DT:H72	3:Q:294:HIS:NE2	1.68	1.08
4:S:269:PHE:HD2	4:S:292:LEU:HD21	1.13	1.06
10:B:291:GLY:HA3	10:B:375:LEU:HD13	1.33	1.04
4:S:269:PHE:CD2	4:S:292:LEU:HD21	1.96	1.01
2:U:22:DT:C7	3:Q:294:HIS:CD2	2.44	0.99
1:T:53:DG:N2	2:U:18:DC:H42	1.62	0.97
2:U:58:DA:OP1	10:B:513:LYS:HD3	1.66	0.96
9:A:1012:LYS:CD	9:A:1201:THR:CG2	2.34	0.95
4:S:26:TYR:CE1	4:S:439:LYS:HD2	2.05	0.91
9:A:1012:LYS:HD2	9:A:1201:THR:HG21	0.91	0.91
5:R:138:PHE:CE2	5:R:297:PHE:CE2	2.63	0.86
1:T:12:DC:H4'	9:A:1617:THR:CG2	2.08	0.83
20:O:225:LEU:O	20:O:229:ILE:HG12	1.79	0.83
2:U:22:DT:C7	3:Q:294:HIS:NE2	2.41	0.82
4:S:26:TYR:HE1	4:S:439:LYS:HD2	1.45	0.81
5:R:345:LEU:O	5:R:345:LEU:HD23	1.83	0.79
9:A:31:GLN:HE21	9:A:33:THR:CG2	1.98	0.77
1:T:4:DT:H2"	1:T:5:DT:H5'	1.64	0.77
1:T:13:DT:H5"	9:A:1616:GLU:HB2	1.70	0.74
4:S:390:GLN:HB2	5:R:152:ILE:HG13	1.70	0.73
20:O:71:ILE:HG23	20:O:115:LEU:HD23	1.71	0.73
5:R:138:PHE:CZ	5:R:297:PHE:CD2	2.76	0.73
7:N:112:PRO:O	7:N:113:SER:O	2.07	0.71
1:T:12:DC:H4'	9:A:1617:THR:HG22	1.73	0.70
5:R:8:LEU:HD12	5:R:8:LEU:O	1.91	0.70
5:R:345:LEU:HG	5:R:348:LYS:HD2	1.74	0.69
1:T:7:DA:H2"	1:T:8:DA:H5'	1.74	0.69
9:A:1022:CYS:HG	9:A:1615:TYR:HH	1.39	0.69
10:B:967:LEU:CD1	10:B:996:PHE:HB2	2.22	0.69
6:I:12:ASP:HB3	8:M:60:LEU:HD21	1.75	0.68
4:S:269:PHE:O	4:S:292:LEU:CD2	2.41	0.67
9:A:1012:LYS:CD	9:A:1201:THR:HG23	2.23	0.67
1:T:53:DG:H21	2:U:18:DC:H42	1.41	0.67
4:S:185:GLN:HB3	4:S:247:ILE:HD11	1.75	0.67
4:S:647:GLU:HB3	4:S:649:ILE:HG22	1.74	0.67
3:Q:96:ILE:CG2	3:Q:99:GLU:O	2.42	0.66
10:B:104:ILE:HG12	10:B:161:LEU:HD21	1.77	0.66
1:T:12:DC:H5"	9:A:1617:THR:HG22	1.78	0.66
9:A:921:PRO:HG2	16:H:19:ARG:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1016:GLY:O	11:C:69:ARG:NH2	2.29	0.66
4:S:323:ASN:HD22	5:R:156:LYS:HB2	1.61	0.66
9:A:417:ARG:HG3	9:A:419:ILE:H	1.61	0.66
20:O:430:ARG:NH1	20:O:610:TYR:OH	2.30	0.66
4:S:362:ARG:HB3	4:S:375:PHE:HB2	1.77	0.65
10:B:726:MET:SD	10:B:1035:ARG:NH1	2.70	0.65
16:H:112:ILE:HD12	16:H:131:ASN:HD22	1.62	0.64
20:O:115:LEU:HD13	20:O:115:LEU:O	1.96	0.64
5:R:138:PHE:HE2	5:R:297:PHE:CE2	2.15	0.64
6:I:36:ILE:HG22	6:I:38:PRO:HD3	1.80	0.64
10:B:137:LEU:HD13	10:B:161:LEU:HD23	1.79	0.63
4:S:383:ILE:HG12	4:S:390:GLN:HG3	1.79	0.63
10:B:100:GLU:OE2	10:B:140:LYS:NZ	2.32	0.63
20:O:458:GLU:HG2	20:O:514:PHE:HE2	1.64	0.63
9:A:824:THR:HG23	10:B:1023:ARG:HB2	1.81	0.63
1:T:12:DC:C4'	9:A:1617:THR:HG22	2.28	0.63
9:A:1012:LYS:HD3	9:A:1201:THR:HG23	1.79	0.63
4:S:484:ARG:HB2	4:S:488:LEU:HB3	1.81	0.62
7:N:43:ASP:HB2	7:N:50:GLN:HG3	1.80	0.62
9:A:477:ASN:OD1	10:B:1047:ARG:NH1	2.32	0.62
20:O:431:ALA:O	20:O:487:ARG:NH2	2.32	0.62
9:A:31:GLN:HE21	9:A:33:THR:HG23	1.64	0.62
20:O:454:VAL:HG13	20:O:455:ILE:HG13	1.82	0.61
4:S:269:PHE:HD2	4:S:292:LEU:CD2	2.01	0.61
11:C:87:ASN:ND2	11:C:201:GLU:OE2	2.32	0.61
9:A:964:LYS:NZ	10:B:672:MET:O	2.33	0.61
10:B:106:LYS:NZ	10:B:168:ASN:O	2.34	0.61
9:A:1012:LYS:HD3	9:A:1201:THR:CG2	2.29	0.60
10:B:202:LEU:HD23	10:B:488:ALA:HB2	1.83	0.60
4:S:302:VAL:HG11	4:S:362:ARG:HD2	1.82	0.60
9:A:21:ALA:O	9:A:25:ARG:NH1	2.34	0.60
20:O:521:ASN:HB3	20:O:524:VAL:HG12	1.83	0.60
4:S:468:VAL:HG22	4:S:477:TYR:HB3	1.83	0.60
4:S:29:GLN:NE2	4:S:443:ASP:OD2	2.35	0.60
3:Q:22:ILE:HG12	3:Q:23:ILE:HG13	1.84	0.60
3:Q:341:ARG:NH2	3:Q:351:ASN:OD1	2.34	0.60
10:B:1047:ARG:NH2	10:B:1051:PRO:O	2.35	0.60
3:Q:252:LEU:HD11	3:Q:303:GLU:HG3	1.84	0.60
9:A:1012:LYS:HG2	9:A:1012:LYS:O	2.01	0.60
7:N:157:ARG:NH2	10:B:985:ILE:O	2.34	0.59
12:D:88:GLN:NE2	20:O:184:PRO:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:606:ARG:NH2	18:K:98:GLU:OE2	2.35	0.59
6:I:84:GLU:HB3	6:I:94:MET:HB3	1.85	0.59
10:B:967:LEU:C	10:B:967:LEU:HD12	2.23	0.59
9:A:799:GLU:OE2	9:A:1173:LYS:NZ	2.33	0.59
10:B:75:ASP:HB3	10:B:77:LYS:H	1.67	0.59
11:C:86:PHE:HB3	19:L:62:LYS:HG3	1.85	0.58
6:I:86:CYS:SG	6:I:91:ASN:N	2.76	0.58
6:I:114:CYS:SG	6:I:115:THR:N	2.77	0.58
20:O:264:ASP:HB3	20:O:267:ASP:HB2	1.85	0.58
3:Q:15:CYS:SG	3:Q:17:SER:OG	2.59	0.58
3:Q:279:THR:O	3:Q:280:ASP:HB2	2.04	0.58
4:S:26:TYR:CD1	4:S:439:LYS:HD2	2.38	0.58
9:A:105:CYS:HB2	9:A:236:CYS:HB2	1.85	0.58
10:B:161:LEU:O	10:B:161:LEU:HD12	2.03	0.58
10:B:534:PRO:HG3	10:B:542:LEU:HD23	1.86	0.58
3:Q:145:ASN:ND2	4:S:765:SER:O	2.37	0.57
11:C:228:ARG:NH2	11:C:271:ARG:O	2.36	0.57
10:B:17:ARG:HB3	10:B:20:GLU:HB3	1.86	0.57
4:S:358:SER:HA	5:R:194:GLY:HA2	1.86	0.57
3:Q:356:VAL:HA	5:R:211:ARG:HG2	1.84	0.57
9:A:342:ARG:NH1	9:A:1629:ASN:O	2.38	0.57
10:B:291:GLY:HA3	10:B:375:LEU:CD1	2.23	0.57
4:S:357:LEU:H	4:S:377:ARG:HH21	1.52	0.57
9:A:15:ASP:HB2	10:B:1197:ARG:HB3	1.87	0.57
9:A:836:THR:HG23	9:A:839:GLY:H	1.69	0.57
10:B:71:LYS:NZ	10:B:418:ASP:OD1	2.35	0.57
3:Q:198:ILE:O	3:Q:201:LYS:NZ	2.38	0.57
9:A:982:VAL:HG22	9:A:994:GLU:HB2	1.86	0.57
10:B:137:LEU:HD13	10:B:161:LEU:CD2	2.33	0.57
20:O:206:ARG:NH2	20:O:265:LEU:O	2.38	0.57
4:S:226:HIS:ND1	4:S:227:LEU:O	2.35	0.57
9:A:1012:LYS:CG	9:A:1201:THR:HG21	2.33	0.56
15:G:38:ILE:HG13	15:G:125:TRP:HD1	1.69	0.56
4:S:35:LYS:HB3	4:S:48:ASP:HA	1.86	0.56
4:S:641:TRP:HH2	4:S:748:GLU:HB3	1.69	0.56
9:A:897:SER:O	9:A:901:ASN:ND2	2.38	0.56
9:A:1145:GLU:OE2	9:A:1167:ARG:NH1	2.31	0.56
10:B:260:PHE:HB3	10:B:271:VAL:HG23	1.87	0.56
20:O:213:SER:HB2	20:O:338:LEU:HD21	1.86	0.56
4:S:292:LEU:HD23	4:S:292:LEU:O	2.04	0.56
5:R:294:VAL:H	5:R:298:GLN:HE21	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:565:LEU:HD21	10:B:608:LEU:HD11	1.88	0.56
4:S:243:LYS:HD2	4:S:266:GLU:HG2	1.88	0.56
4:S:571:HIS:HB2	4:S:574:TRP:HD1	1.70	0.56
11:C:222:VAL:HG21	11:C:225:ALA:HB2	1.87	0.56
2:U:22:DT:C7	3:Q:294:HIS:HD2	2.10	0.55
4:S:269:PHE:HB3	4:S:292:LEU:HD21	1.88	0.55
7:N:56:ILE:HG22	7:N:137:PHE:HB2	1.88	0.55
9:A:847:LEU:HD21	9:A:946:LEU:HD22	1.88	0.55
9:A:857:ALA:HB2	9:A:899:LYS:HD2	1.87	0.55
10:B:743:ARG:NH2	17:J:1:MET:SD	2.79	0.55
14:F:135:ARG:NH2	15:G:92:ALA:O	2.31	0.55
6:I:12:ASP:HB3	8:M:60:LEU:CD2	2.35	0.55
9:A:934:LYS:NZ	10:B:784:ASP:OD1	2.33	0.55
9:A:1022:CYS:SG	9:A:1615:TYR:OH	2.59	0.55
10:B:1203:LYS:HG2	12:D:21:VAL:HG11	1.88	0.55
13:E:93:MET:HG3	13:E:120:ALA:HB1	1.89	0.55
4:S:484:ARG:HD2	4:S:488:LEU:HD23	1.89	0.55
13:E:46:TYR:O	13:E:54:GLN:NE2	2.39	0.55
15:G:158:LYS:NZ	20:O:108:GLU:OE1	2.39	0.55
4:S:658:LYS:HG3	4:S:660:LYS:H	1.72	0.55
9:A:646:GLU:OE1	10:B:1084:THR:OG1	2.22	0.55
3:Q:285:THR:O	3:Q:305:ARG:NH1	2.39	0.55
3:Q:326:TYR:O	3:Q:472:ARG:NH2	2.38	0.55
4:S:184:SER:N	4:S:509:GLU:OE2	2.40	0.55
4:S:300:LEU:HA	4:S:320:ILE:HA	1.89	0.55
3:Q:506:LYS:NZ	4:S:577:LEU:O	2.40	0.55
2:U:22:DT:H73	3:Q:294:HIS:CD2	2.41	0.55
10:B:1178:ILE:HD11	10:B:1183:LYS:HZ1	1.72	0.55
1:T:10:DT:H2"	1:T:11:DG:H5'	1.89	0.55
9:A:1278:THR:O	9:A:1287:ALA:N	2.40	0.55
5:R:412:ARG:NH2	5:R:439:GLU:OE2	2.40	0.54
4:S:28:PRO:HG2	4:S:31:ASN:HB3	1.89	0.54
6:I:91:ASN:ND2	6:I:114:CYS:SG	2.70	0.54
9:A:1270:VAL:HG11	9:A:1489:VAL:HG11	1.89	0.54
5:R:255:VAL:HG22	5:R:259:ASP:HB2	1.89	0.54
1:T:11:DG:H2"	1:T:12:DC:H5'	1.88	0.54
1:T:12:DC:C5'	9:A:1617:THR:HG22	2.37	0.54
9:A:99:ARG:O	9:A:109:ARG:NH2	2.40	0.54
5:R:247:ILE:HA	5:R:250:LEU:HD12	1.88	0.54
9:A:438:ILE:HA	9:A:456:VAL:HG22	1.90	0.54
4:S:234:THR:OG1	4:S:284:VAL:O	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:147:LEU:HB2	15:G:155:ALA:HB3	1.90	0.54
20:O:97:LEU:HD22	20:O:135:LYS:HG2	1.89	0.54
9:A:718:THR:HG21	16:H:119:GLY:HA3	1.90	0.54
5:R:313:LEU:HB3	5:R:367:ILE:HD13	1.88	0.54
10:B:963:PHE:O	10:B:1027:TYR:OH	2.26	0.54
20:O:440:ILE:O	20:O:444:SER:N	2.39	0.54
4:S:269:PHE:HB3	4:S:292:LEU:CD2	2.38	0.54
10:B:292:ILE:O	10:B:379:ARG:NH1	2.35	0.54
4:S:508:ILE:HG12	4:S:539:VAL:HG12	1.90	0.53
10:B:815:ARG:NH1	10:B:899:GLN:OE1	2.42	0.53
10:B:967:LEU:HD13	10:B:996:PHE:HB2	1.89	0.53
12:D:87:SER:HB2	20:O:224:GLU:HG2	1.89	0.53
3:Q:413:LEU:HD21	5:R:240:ILE:HD12	1.90	0.53
9:A:4:SER:OG	9:A:576:LYS:NZ	2.35	0.53
13:E:100:ILE:HG23	13:E:105:PHE:HB2	1.90	0.53
16:H:35:GLN:HB3	16:H:111:LEU:HD21	1.89	0.53
4:S:395:GLN:HB3	5:R:140:ILE:HG23	1.91	0.53
9:A:862:THR:HG23	9:A:864:LEU:H	1.73	0.53
3:Q:481:THR:HG21	4:S:570:ASP:HA	1.91	0.53
4:S:456:VAL:HB	4:S:463:LEU:HB2	1.89	0.53
9:A:1012:LYS:HG3	9:A:1201:THR:OG1	2.09	0.53
10:B:320:LEU:HD13	10:B:326:VAL:HG23	1.91	0.53
10:B:404:LEU:HD21	10:B:551:ILE:HG21	1.90	0.53
10:B:883:GLU:OE1	10:B:906:ARG:NH1	2.38	0.53
9:A:128:GLY:HA3	9:A:207:SER:HB3	1.91	0.53
20:O:491:PHE:HD1	20:O:499:GLU:HB2	1.73	0.53
9:A:666:VAL:HG23	9:A:667:ARG:HG3	1.91	0.53
8:M:66:THR:HB	8:M:71:GLN:HG3	1.90	0.53
5:R:138:PHE:CE2	5:R:297:PHE:CD2	2.97	0.53
20:O:75:ALA:HB2	20:O:115:LEU:HD22	1.91	0.53
7:N:49:LYS:O	8:M:82:ASN:ND2	2.42	0.52
1:T:29:DT:H5”	1:T:30:DC:H5’	1.91	0.52
4:S:28:PRO:HG3	5:R:297:PHE:HE1	1.74	0.52
6:I:89:CYS:SG	6:I:90:GLY:N	2.83	0.52
10:B:921:HIS:NE2	10:B:965:GLU:OE1	2.38	0.52
3:Q:441:ASP:O	3:Q:445:ARG:N	2.42	0.52
11:C:246:ARG:NH1	11:C:284:GLU:OE1	2.37	0.52
9:A:215:GLU:OE2	13:E:177:ARG:NH2	2.43	0.52
4:S:36:LYS:HG3	4:S:46:VAL:HG23	1.91	0.52
17:J:48:ARG:HA	17:J:51:LEU:HB3	1.91	0.52
8:M:56:GLU:HG2	8:M:61:GLU:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:202:ILE:HA	4:S:219:LEU:HD13	1.92	0.52
9:A:1635:ASP:O	9:A:1648:ASN:ND2	2.33	0.52
3:Q:100:ALA:HA	3:Q:103:LEU:HB3	1.92	0.52
3:Q:292:GLU:HG3	3:Q:294:HIS:HB2	1.92	0.52
4:S:704:LEU:HD12	4:S:708:VAL:HG22	1.92	0.52
9:A:745:PRO:O	9:A:801:TYR:OH	2.26	0.52
20:O:347:VAL:HG11	20:O:388:VAL:HG13	1.92	0.52
15:G:137:ILE:HB	15:G:227:GLY:HA2	1.92	0.51
3:Q:175:PRO:HG2	4:S:702:LEU:HD12	1.91	0.51
4:S:232:ASN:ND2	4:S:281:SER:O	2.42	0.51
10:B:143:TRP:HB3	10:B:152:LEU:HB2	1.92	0.51
10:B:584:CYS:HB3	10:B:596:VAL:HG23	1.93	0.51
10:B:261:ARG:NH2	10:B:268:GLU:OE2	2.43	0.51
11:C:322:LYS:NZ	11:C:326:GLU:OE2	2.42	0.51
18:K:62:SER:OG	18:K:104:ARG:NH1	2.39	0.51
9:A:1179:ILE:HD11	9:A:1183:GLU:HG2	1.92	0.51
4:S:377:ARG:O	4:S:401:ASN:ND2	2.40	0.51
4:S:511:ILE:HD11	4:S:538:LEU:HD23	1.92	0.51
10:B:839:LYS:HB2	10:B:840:LEU:HD12	1.93	0.51
3:Q:180:ASP:OD1	3:Q:255:LYS:NZ	2.43	0.51
3:Q:496:GLU:HA	3:Q:499:LYS:HB2	1.92	0.51
4:S:672:ILE:HG12	4:S:734:LYS:HE3	1.93	0.51
10:B:341:SER:OG	10:B:343:ASP:OD1	2.25	0.51
13:E:79:TRP:NE1	13:E:81:GLU:OE1	2.43	0.51
3:Q:177:TYR:OH	3:Q:248:SER:O	2.29	0.51
8:M:88:ILE:HD12	8:M:90:LEU:HD21	1.93	0.51
11:C:136:LEU:HB3	11:C:204:LEU:HG	1.93	0.51
3:Q:227:TYR:HA	3:Q:230:ILE:HD12	1.92	0.51
5:R:138:PHE:CE2	5:R:297:PHE:HE2	2.21	0.51
10:B:708:ASP:OD1	10:B:708:ASP:N	2.43	0.51
11:C:229:LEU:HD21	11:C:295:ARG:HD3	1.91	0.51
3:Q:262:LEU:HD13	3:Q:266:PHE:HB2	1.93	0.50
4:S:369:PHE:HD2	4:S:371:LYS:HE3	1.76	0.50
4:S:421:ILE:HA	4:S:441:ASP:HA	1.92	0.50
9:A:1080:TYR:OH	9:A:1173:LYS:NZ	2.44	0.50
10:B:1084:THR:HG21	10:B:1087:LEU:HD12	1.93	0.50
20:O:164:LEU:HD13	20:O:168:GLN:HG2	1.92	0.50
4:S:245:ILE:HA	4:S:263:ILE:HG22	1.94	0.50
7:N:52:GLN:N	8:M:81:PHE:O	2.42	0.50
7:N:56:ILE:HG13	8:M:77:VAL:HB	1.93	0.50
10:B:379:ARG:HE	10:B:581:PRO:HD3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:264:PRO:HD3	4:S:722:TRP:CD1	2.47	0.50
9:A:114:GLU:OE2	9:A:117:ARG:NH2	2.45	0.50
9:A:1184:ALA:HB2	9:A:1649:VAL:HG11	1.94	0.50
11:C:196:LEU:O	11:C:197:ARG:NH1	2.44	0.50
10:B:355:ASP:HB3	10:B:364:LYS:HE2	1.93	0.50
13:E:110:PHE:HB3	13:E:134:THR:HG22	1.93	0.50
20:O:392:GLN:HB2	20:O:395:LEU:HB2	1.92	0.50
10:B:788:ILE:HB	10:B:948:ILE:HB	1.94	0.50
20:O:382:GLN:NE2	20:O:593:PRO:O	2.42	0.50
6:I:10:CYS:SG	6:I:11:LEU:N	2.85	0.50
6:I:55:ALA:O	9:A:1494:ARG:NH1	2.38	0.50
4:S:63:SER:HB3	4:S:549:TYR:HB3	1.92	0.49
9:A:1274:GLU:OE2	9:A:1288:ARG:NH2	2.34	0.49
4:S:323:ASN:ND2	5:R:157:MET:O	2.45	0.49
12:D:44:ILE:HD11	12:D:89:LEU:HB3	1.92	0.49
20:O:340:SER:HA	20:O:343:VAL:HG12	1.94	0.49
6:I:11:LEU:HB2	8:M:31:ARG:HD3	1.94	0.49
9:A:1661:PRO:O	15:G:101:SER:OG	2.29	0.49
10:B:518:ARG:NH1	10:B:539:CYS:O	2.46	0.49
15:G:74:ASN:HB3	15:G:77:VAL:HG22	1.94	0.49
4:S:444:PRO:HA	5:R:2:PHE:HA	1.93	0.49
9:A:701:ARG:HH12	18:K:94:PRO:HA	1.76	0.49
1:T:5:DT:P	1:T:5:DT:H3'	2.52	0.49
9:A:648:LEU:O	9:A:652:ASN:ND2	2.46	0.49
9:A:744:MET:HG2	9:A:1078:LYS:HD2	1.94	0.49
3:Q:128:GLU:HB3	4:S:749:LYS:HE3	1.94	0.49
4:S:243:LYS:NZ	4:S:299:ASP:OD2	2.45	0.49
1:T:5:DT:H3'	1:T:5:DT:OP2	2.13	0.49
2:U:62:DG:H2"	2:U:63:DT:H5'	1.94	0.49
5:R:251:TRP:HA	5:R:270:PHE:HE2	1.78	0.49
4:S:22:GLY:HA2	4:S:435:ARG:HH12	1.78	0.49
4:S:425:GLY:O	4:S:434:ARG:NH1	2.45	0.49
4:S:476:ILE:HG22	4:S:497:VAL:H	1.78	0.49
3:Q:263:PRO:HG3	4:S:725:VAL:HB	1.95	0.48
20:O:114:PHE:HA	20:O:117:GLN:HB2	1.94	0.48
4:S:269:PHE:CD2	4:S:292:LEU:CD2	2.85	0.48
7:N:30:LYS:HB2	8:M:44:LYS:HE2	1.95	0.48
10:B:782:ASP:N	10:B:782:ASP:OD1	2.45	0.48
11:C:70:ILE:HG23	11:C:74:GLU:HB2	1.96	0.48
20:O:208:LEU:HB3	20:O:335:ILE:HD11	1.95	0.48
20:O:423:TYR:HA	20:O:593:PRO:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:57:DT:O2	2:U:15:DG:N2	2.46	0.48
9:A:487:ASP:HB2	9:A:615:ARG:HG2	1.96	0.48
20:O:461:VAL:HG11	20:O:513:LYS:HB3	1.95	0.48
20:O:56:VAL:HG23	20:O:99:ILE:HG13	1.95	0.48
3:Q:272:GLN:HG3	4:S:596:ILE:HD13	1.96	0.48
3:Q:298:VAL:HG22	3:Q:504:ARG:HH22	1.79	0.48
4:S:319:ASP:HB2	4:S:363:ILE:HG12	1.95	0.48
9:A:847:LEU:HD22	9:A:983:LYS:HG2	1.94	0.48
9:A:1446:ARG:NH1	9:A:1464:ASP:OD2	2.47	0.48
10:B:264:TRP:HD1	10:B:337:VAL:HG22	1.79	0.48
4:S:175:ASP:OD2	4:S:177:THR:OG1	2.26	0.48
5:R:4:VAL:HG11	5:R:214:VAL:HG22	1.94	0.48
5:R:362:ALA:HB2	5:R:421:LYS:HB2	1.96	0.48
9:A:462:LYS:HD2	9:A:464:GLU:HG2	1.95	0.48
3:Q:111:ILE:HG12	3:Q:199:LEU:HG	1.95	0.48
12:D:19:PRO:HB3	15:G:47:VAL:HG12	1.96	0.48
4:S:269:PHE:O	4:S:292:LEU:HD22	2.13	0.47
10:B:40:GLU:OE1	10:B:550:ARG:NH2	2.47	0.47
3:Q:135:ILE:HA	3:Q:138:LEU:HB2	1.96	0.47
9:A:621:THR:HG21	9:A:670:ILE:HD12	1.96	0.47
9:A:1241:PRO:HD2	9:A:1541:ILE:HG22	1.95	0.47
7:N:174:GLY:HA3	11:C:53:ASN:HD22	1.78	0.47
9:A:1011:VAL:HG13	9:A:1015:ARG:HH21	1.78	0.47
9:A:1038:ILE:HD11	9:A:1050:TYR:HB2	1.97	0.47
4:S:25:LEU:O	4:S:439:LYS:HE3	2.15	0.47
13:E:11:ARG:HG2	13:E:14:ARG:HH21	1.78	0.47
9:A:581:ILE:HD11	9:A:605:VAL:HG21	1.95	0.47
4:S:269:PHE:O	4:S:292:LEU:HD23	2.13	0.47
4:S:288:SER:OG	4:S:289:SER:O	2.33	0.47
3:Q:341:ARG:NH2	3:Q:373:GLU:OE2	2.48	0.47
4:S:61:VAL:HB	4:S:551:ALA:HB3	1.97	0.47
4:S:403:ARG:HH21	4:S:419:ARG:HD2	1.80	0.47
4:S:505:PRO:HA	4:S:541:LEU:HA	1.96	0.47
9:A:31:GLN:O	9:A:31:GLN:HG3	2.15	0.47
9:A:1038:ILE:HB	9:A:1047:GLN:HB2	1.95	0.47
12:D:25:THR:OG1	14:F:59:GLN:OE1	2.32	0.47
15:G:171:ASN:HD22	15:G:214:LEU:HD22	1.80	0.47
20:O:603:LYS:HA	20:O:606:MET:HB2	1.97	0.47
9:A:1458:THR:OG1	9:A:1475:GLU:OE1	2.22	0.47
10:B:207:ILE:HB	10:B:505:ARG:HA	1.97	0.47
20:O:430:ARG:HH12	20:O:596:PRO:HD3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:58:DA:OP1	10:B:513:LYS:CD	2.51	0.47
3:Q:86:ARG:NH1	3:Q:87:GLN:OE1	2.47	0.47
6:I:4:VAL:HG13	10:B:297:VAL:HG13	1.97	0.47
9:A:533:ALA:HA	9:A:579:ARG:HA	1.97	0.47
17:J:36:LEU:HD11	17:J:51:LEU:HD13	1.97	0.47
20:O:97:LEU:HD21	20:O:139:PHE:HB2	1.96	0.47
9:A:1240:LEU:HB3	9:A:1536:ILE:HD12	1.97	0.46
10:B:71:LYS:HZ3	10:B:422:GLN:HG3	1.81	0.46
10:B:275:MET:HG2	10:B:330:LEU:HD12	1.96	0.46
10:B:749:THR:HG23	17:J:52:THR:HG22	1.98	0.46
15:G:143:SER:HB3	20:O:104:ILE:HG22	1.97	0.46
20:O:440:ILE:HD13	20:O:499:GLU:HG3	1.97	0.46
7:N:174:GLY:HA3	11:C:53:ASN:ND2	2.30	0.46
10:B:1025:ASP:OD2	11:C:277:ARG:NH1	2.48	0.46
11:C:105:PRO:HG3	17:J:13:VAL:HG21	1.97	0.46
15:G:217:TRP:HB3	15:G:225:ILE:HG12	1.97	0.46
1:T:7:DA:H2'	1:T:8:DA:C8	2.50	0.46
9:A:1291:VAL:HG22	9:A:1473:LYS:HG2	1.97	0.46
3:Q:171:HIS:ND1	3:Q:244:ASN:OD1	2.39	0.46
5:R:5:PRO:HD2	5:R:217:THR:HG21	1.97	0.46
9:A:525:ASN:ND2	9:A:531:PRO:O	2.47	0.46
10:B:935:ASP:N	10:B:935:ASP:OD1	2.48	0.46
4:S:328:ARG:O	4:S:343:LEU:N	2.48	0.46
7:N:110:LEU:HB3	7:N:119:LEU:HD21	1.97	0.46
9:A:219:LEU:O	9:A:223:PHE:N	2.41	0.46
3:Q:330:TRP:NE1	3:Q:449:GLN:OE1	2.44	0.46
9:A:427:PHE:HA	9:A:430:ILE:HG22	1.97	0.46
10:B:429:ARG:HA	10:B:432:ILE:HG12	1.97	0.46
13:E:100:ILE:HA	13:E:105:PHE:HD2	1.80	0.46
3:Q:6:ARG:HH11	3:Q:18:ARG:HB3	1.81	0.46
3:Q:442:LEU:HA	3:Q:445:ARG:HB2	1.97	0.46
9:A:62:CYS:SG	9:A:66:GLY:N	2.89	0.46
3:Q:20:TRP:N	3:Q:28:THR:O	2.48	0.46
3:Q:115:GLN:OE1	3:Q:161:THR:OG1	2.28	0.46
4:S:260:LEU:HA	4:S:273:ARG:HA	1.98	0.46
4:S:404:ASP:HB2	4:S:450:ARG:HA	1.98	0.46
20:O:431:ALA:HB1	20:O:434:LEU:HD13	1.98	0.46
9:A:1105:ARG:NH2	9:A:1142:ASP:OD1	2.49	0.45
10:B:161:LEU:HD12	10:B:162:PRO:O	2.15	0.45
10:B:216:ALA:HB1	10:B:384:LEU:HD22	1.98	0.45
15:G:17:ILE:O	15:G:21:LYS:N	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:203:ASP:HB3	20:O:207:LYS:HD2	1.97	0.45
3:Q:61:ASN:HD21	3:Q:75:LEU:HD11	1.79	0.45
3:Q:113:LYS:HE3	4:S:777:MET:H	1.80	0.45
3:Q:193:PHE:HA	3:Q:217:GLY:HA3	1.97	0.45
10:B:672:MET:HE2	10:B:674:ILE:HD11	1.98	0.45
4:S:318:ILE:HD11	4:S:325:SER:HB2	1.98	0.45
9:A:19:LEU:HG	10:B:1195:ARG:HB2	1.97	0.45
10:B:782:ASP:HA	10:B:786:ALA:HB3	1.97	0.45
10:B:916:LYS:HG2	10:B:926:VAL:HG12	1.97	0.45
8:M:54:HIS:HA	8:M:63:GLU:HA	1.98	0.45
3:Q:446:TYR:HD1	4:S:725:VAL:HG11	1.81	0.45
10:B:129:ARG:HB2	19:L:55:ILE:HD11	1.98	0.45
10:B:752:VAL:O	10:B:920:ARG:NH2	2.37	0.45
11:C:293:ARG:HB2	11:C:295:ARG:HE	1.82	0.45
1:T:10:DT:H2"	1:T:11:DG:C5'	2.47	0.45
3:Q:172:LEU:HD23	3:Q:174:LEU:HD11	1.99	0.45
9:A:1238:MET:HE3	9:A:1524:VAL:HA	1.98	0.45
10:B:134:ARG:HA	10:B:162:PRO:HA	1.99	0.45
10:B:273:VAL:HG11	10:B:378:ILE:HD11	1.98	0.45
18:K:46:LYS:HA	18:K:66:VAL:HG22	1.99	0.45
20:O:332:LEU:HG	20:O:599:LEU:HD21	1.98	0.45
4:S:33:THR:OG1	4:S:34:THR:N	2.48	0.45
9:A:469:LYS:HA	10:B:1070:ARG:HH22	1.81	0.45
9:A:480:ALA:HB2	10:B:1046:VAL:HG23	1.98	0.45
10:B:235:GLN:HG3	10:B:249:VAL:HG22	1.99	0.45
10:B:1076:ARG:HG3	10:B:1088:LEU:HD11	1.99	0.45
20:O:418:ILE:HG12	20:O:585:PHE:HE1	1.82	0.45
3:Q:96:ILE:HG22	3:Q:99:GLU:O	2.17	0.45
4:S:735:GLU:HA	4:S:738:LYS:HE3	1.99	0.45
9:A:346:SER:OG	9:A:348:LYS:NZ	2.39	0.45
9:A:385:LEU:HD23	9:A:385:LEU:HA	1.87	0.45
19:L:38:LEU:HD11	19:L:48:CYS:HA	1.99	0.45
3:Q:297:ARG:H	3:Q:297:ARG:HD2	1.82	0.45
6:I:71:LEU:HD13	6:I:76:LEU:HD13	1.99	0.45
7:N:173:THR:HB	11:C:301:ASN:HB2	1.98	0.44
9:A:1634:LEU:HD13	9:A:1643:VAL:HG11	1.99	0.44
15:G:237:HIS:HB2	15:G:244:SER:HB3	1.99	0.44
7:N:119:LEU:HB3	8:M:38:PHE:HB2	1.99	0.44
8:M:39:ASP:N	8:M:54:HIS:O	2.49	0.44
10:B:491:ILE:HD12	10:B:1037:ARG:HG2	2.00	0.44
10:B:1134:ARG:HA	10:B:1167:PHE:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1160:GLU:HG2	10:B:1166:LYS:HG2	1.98	0.44
20:O:205:ARG:HA	20:O:331:LYS:HE2	2.00	0.44
1:T:9:DC:H6	1:T:9:DC:H2'	1.70	0.44
2:U:62:DG:H2"	2:U:63:DT:C5'	2.47	0.44
4:S:363:ILE:HG22	4:S:374:VAL:HG22	2.00	0.44
4:S:500:ILE:HA	4:S:501:PRO:HD3	1.81	0.44
9:A:739:VAL:HG11	9:A:812:VAL:HG21	1.99	0.44
13:E:86:PRO:HA	13:E:113:GLN:HB2	2.00	0.44
1:T:6:DC:H6	1:T:6:DC:O5'	2.00	0.44
3:Q:142:LYS:HB2	4:S:762:ARG:HD2	1.99	0.44
5:R:21:TYR:O	5:R:25:ASN:ND2	2.50	0.44
6:I:23:VAL:HG11	6:I:28:VAL:HG12	1.97	0.44
9:A:13:SER:OG	10:B:1199:ASN:ND2	2.40	0.44
10:B:28:PRO:HB2	10:B:178:TYR:HA	1.99	0.44
15:G:143:SER:OG	20:O:101:SER:O	2.32	0.44
20:O:428:ILE:O	20:O:487:ARG:NE	2.50	0.44
2:U:56:DA:C8	2:U:56:DA:OP2	2.70	0.44
10:B:587:GLN:HG2	10:B:592:ILE:HA	1.99	0.44
4:S:365:TRP:O	4:S:407:ARG:NH2	2.50	0.44
10:B:202:LEU:HD21	10:B:499:HIS:HB3	1.99	0.44
10:B:1042:ASP:OD1	10:B:1042:ASP:N	2.50	0.44
20:O:492:ARG:HG2	20:O:493:ASP:O	2.18	0.44
9:A:751:SER:OG	9:A:752:LYS:N	2.51	0.44
10:B:750:PRO:HG2	10:B:753:LYS:HB3	2.00	0.44
12:D:82:LEU:HD12	12:D:85:SER:HB2	2.00	0.44
11:C:131:THR:O	11:C:175:GLN:NE2	2.47	0.44
4:S:185:GLN:HE21	4:S:512:LEU:HD22	1.83	0.43
4:S:451:ILE:HD11	4:S:466:ALA:HB1	2.00	0.43
9:A:86:TYR:HA	9:A:356:PHE:HA	2.00	0.43
10:B:911:PRO:HA	10:B:1035:ARG:HH21	1.82	0.43
11:C:103:LEU:HD22	17:J:6:ARG:HD2	1.99	0.43
3:Q:98:HIS:NE2	3:Q:149:GLN:O	2.40	0.43
4:S:277:VAL:HG12	4:S:284:VAL:HA	2.00	0.43
4:S:357:LEU:H	4:S:377:ARG:NH2	2.16	0.43
10:B:991:THR:HG22	10:B:993:ALA:H	1.83	0.43
4:S:238:LEU:HD22	4:S:242:ILE:HD11	2.01	0.43
9:A:885:ASP:OD2	9:A:888:LYS:NZ	2.41	0.43
16:H:105:GLU:O	16:H:113:ALA:N	2.45	0.43
4:S:622:TYR:CZ	4:S:668:SER:HB2	2.53	0.43
8:M:70:SER:O	8:M:74:ASN:N	2.44	0.43
9:A:1124:LEU:HD22	9:A:1129:PRO:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:786:ALA:HB1	10:B:928:SER:HB2	1.99	0.43
3:Q:81:LEU:HA	3:Q:84:GLN:HG2	1.99	0.43
7:N:71:PRO:HA	8:M:9:GLU:HA	2.00	0.43
18:K:55:SER:HB2	18:K:60:SER:HB2	1.99	0.43
3:Q:275:GLU:HA	3:Q:281:ILE:HG23	2.00	0.43
6:I:51:THR:HG22	9:A:1270:VAL:H	1.84	0.43
6:I:98:THR:HG22	6:I:110:VAL:HG22	2.00	0.43
14:F:109:VAL:HG21	14:F:123:LYS:HG2	2.01	0.43
5:R:210:THR:HA	5:R:213:ILE:HD12	2.00	0.43
9:A:643:ALA:HB1	10:B:1087:LEU:HD23	2.00	0.43
13:E:79:TRP:HD1	13:E:96:PHE:HE1	1.67	0.43
8:M:47:GLU:HG2	8:M:48:LYS:HG2	2.00	0.43
16:H:126:GLU:O	16:H:130:ARG:NH1	2.52	0.43
17:J:18:TRP:NE1	17:J:55:ASP:OD2	2.50	0.43
3:Q:172:LEU:HD11	4:S:694:ILE:HG21	2.01	0.43
3:Q:173:SER:HB3	4:S:746:ARG:HB2	2.00	0.43
4:S:269:PHE:CZ	4:S:271:ILE:HD11	2.54	0.43
13:E:3:GLN:O	13:E:7:ARG:NH1	2.48	0.43
15:G:166:TRP:HZ3	15:G:249:LEU:HD13	1.84	0.43
3:Q:197:GLU:HA	3:Q:204:ARG:HH22	1.83	0.43
4:S:317:ILE:HG22	4:S:363:ILE:HD13	2.00	0.43
10:B:37:LEU:HD12	10:B:759:ASP:HB3	2.01	0.43
10:B:274:VAL:HA	10:B:277:LEU:HB2	2.01	0.43
20:O:71:ILE:HD12	20:O:115:LEU:HD23	1.99	0.43
20:O:386:PHE:HE2	20:O:609:TYR:HB3	1.84	0.43
20:O:390:GLN:HA	20:O:396:MET:HE3	2.01	0.43
4:S:407:ARG:HA	4:S:414:ILE:HG23	2.01	0.42
5:R:361:ASP:OD1	5:R:361:ASP:N	2.48	0.42
9:A:522:ALA:HA	9:A:532:GLY:HA2	2.01	0.42
1:T:12:DC:H4'	9:A:1617:THR:HG21	1.97	0.42
4:S:219:LEU:N	4:S:226:HIS:O	2.52	0.42
5:R:188:PHE:O	5:R:192:SER:N	2.52	0.42
15:G:133:LEU:HD13	15:G:149:ILE:HD13	2.01	0.42
13:E:156:LEU:HB3	13:E:160:GLU:HG2	2.00	0.42
1:T:13:DT:H5"	9:A:1616:GLU:CB	2.45	0.42
5:R:29:ARG:HH11	5:R:126:LYS:HD2	1.83	0.42
9:A:525:ASN:HB3	9:A:529:LYS:HB2	2.00	0.42
9:A:670:ILE:HG12	9:A:671:GLN:HG3	2.00	0.42
9:A:799:GLU:O	9:A:1079:LYS:NZ	2.37	0.42
9:A:1447:GLN:HE21	9:A:1459:LYS:HA	1.84	0.42
9:A:1662:ASN:HB3	15:G:57:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:115:TRP:HH2	11:C:212:ILE:HG23	1.85	0.42
15:G:18:LYS:HD3	15:G:21:LYS:HD2	2.01	0.42
16:H:10:PHE:HA	16:H:30:SER:HA	2.01	0.42
7:N:148:ILE:HG12	10:B:657:PRO:HD3	2.00	0.42
3:Q:103:LEU:HD21	3:Q:206:GLN:HG3	2.02	0.42
6:I:16:LEU:O	10:B:314:LYS:NZ	2.52	0.42
9:A:904:THR:HG23	9:A:946:LEU:HD11	2.01	0.42
15:G:162:ILE:HG12	15:G:249:LEU:HD12	2.01	0.42
15:G:237:HIS:HB3	15:G:239:THR:HG23	2.01	0.42
4:S:638:LEU:HD21	4:S:691:VAL:HB	2.01	0.42
9:A:1055:ILE:HD11	9:A:1174:TYR:CE1	2.55	0.42
10:B:931:TRP:NE1	10:B:935:ASP:O	2.38	0.42
20:O:386:PHE:HZ	20:O:431:ALA:HA	1.84	0.42
1:T:6:DC:O5'	1:T:6:DC:C6	2.73	0.42
3:Q:135:ILE:HG22	3:Q:139:LYS:HE2	2.01	0.42
4:S:20:VAL:HA	4:S:25:LEU:HD13	2.01	0.42
14:F:106:PRO:HG3	15:G:55:GLU:HB2	2.02	0.42
20:O:324:GLY:HA3	20:O:327:GLU:HB2	2.02	0.42
7:N:112:PRO:C	7:N:113:SER:O	2.58	0.42
9:A:1459:LYS:HB2	9:A:1473:LYS:HB2	2.02	0.42
9:A:1541:ILE:O	13:E:147:HIS:NE2	2.45	0.42
4:S:607:VAL:HG11	4:S:731:LEU:HD13	2.02	0.42
5:R:6:ILE:HD13	5:R:210:THR:HB	2.02	0.42
5:R:310:ILE:HA	5:R:313:LEU:HD12	2.02	0.42
9:A:556:ALA:HB1	20:O:242:VAL:HG13	2.02	0.42
10:B:33:SER:OG	10:B:34:ALA:O	2.33	0.42
10:B:898:LEU:HB3	19:L:46:VAL:HG21	2.02	0.42
11:C:91:VAL:HG11	17:J:60:PHE:HB3	2.01	0.42
15:G:234:ARG:HB2	15:G:248:THR:HG23	2.02	0.42
3:Q:63:THR:HB	3:Q:72:SER:HB3	2.01	0.41
15:G:241:ARG:HE	20:O:189:PHE:HB3	1.85	0.41
4:S:39:LYS:HE2	5:R:430:LEU:HD21	2.01	0.41
9:A:852:ASP:OD1	9:A:855:ARG:NH2	2.53	0.41
4:S:391:THR:HG21	5:R:144:VAL:HG23	2.03	0.41
9:A:621:THR:OG1	9:A:626:ALA:O	2.36	0.41
9:A:755:ILE:HG12	9:A:930:LEU:HB3	2.02	0.41
10:B:161:LEU:HD12	10:B:161:LEU:C	2.41	0.41
10:B:811:LEU:O	10:B:823:GLN:NE2	2.48	0.41
12:D:30:HIS:HA	15:G:39:VAL:HG23	2.02	0.41
12:D:82:LEU:HD22	15:G:67:ASN:CG	2.40	0.41
9:A:492:THR:HB	9:A:667:ARG:HH22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1202:LEU:HG	9:A:1573:TYR:HE1	1.84	0.41
11:C:197:ARG:HD3	11:C:197:ARG:HA	1.94	0.41
16:H:95:TYR:HD2	16:H:144:ILE:HD13	1.85	0.41
5:R:167:LYS:HE3	5:R:171:ARG:HE	1.85	0.41
9:A:195:LYS:NZ	9:A:199:ASP:OD2	2.51	0.41
14:F:72:LYS:HB3	14:F:142:SER:HA	2.02	0.41
15:G:142:ALA:HB2	15:G:168:PHE:CD2	2.56	0.41
20:O:332:LEU:HD23	20:O:599:LEU:HD11	2.03	0.41
3:Q:167:LEU:HA	3:Q:167:LEU:HD23	1.83	0.41
3:Q:346:GLU:O	3:Q:350:ARG:N	2.49	0.41
4:S:616:SER:HB3	4:S:619:GLU:HG2	2.02	0.41
5:R:8:LEU:HD12	5:R:8:LEU:C	2.40	0.41
10:B:49:PHE:HA	10:B:52:LEU:HD13	2.03	0.41
10:B:137:LEU:HB2	10:B:161:LEU:HD23	2.02	0.41
20:O:430:ARG:HH11	20:O:610:TYR:HH	1.66	0.41
3:Q:118:TRP:CH2	3:Q:189:LYS:HB3	2.55	0.41
4:S:362:ARG:NH2	4:S:405:TYR:O	2.53	0.41
6:I:105:ASP:HA	10:B:714:ARG:HH12	1.85	0.41
9:A:124:LEU:HD22	9:A:129:LEU:HD11	2.02	0.41
10:B:286:ARG:HA	10:B:286:ARG:HD2	1.84	0.41
13:E:78:LEU:HD11	13:E:109:ILE:HG13	2.02	0.41
9:A:399:LEU:HD22	9:A:423:LEU:HD13	2.03	0.41
11:C:60:ASP:OD2	11:C:62:SER:OG	2.30	0.41
20:O:423:TYR:HH	20:O:594:TYR:HH	1.61	0.41
4:S:451:ILE:HD12	4:S:468:VAL:HG12	2.01	0.41
7:N:54:TRP:NE1	7:N:135:LYS:HB2	2.36	0.41
9:A:588:LEU:HD11	10:B:1087:LEU:HD22	2.02	0.41
9:A:627:ASP:OD1	9:A:627:ASP:N	2.54	0.41
10:B:172:LEU:HA	10:B:175:MET:SD	2.61	0.41
10:B:280:LEU:HD23	10:B:354:LEU:HD23	2.03	0.41
10:B:379:ARG:NE	10:B:580:GLY:HA2	2.36	0.41
10:B:979:GLN:HG2	10:B:996:PHE:HE1	1.86	0.41
11:C:42:VAL:HG11	18:K:135:PHE:HD1	1.86	0.41
20:O:62:ASP:HA	20:O:65:LYS:HB2	2.03	0.41
20:O:104:ILE:HD12	20:O:107:ILE:HD13	2.03	0.41
4:S:434:ARG:HA	4:S:434:ARG:HD2	1.89	0.41
9:A:265:ARG:HG3	9:A:266:VAL:HG13	2.02	0.41
9:A:530:TRP:O	9:A:532:GLY:N	2.54	0.41
9:A:679:TRP:O	9:A:685:SER:OG	2.35	0.41
10:B:781:TYR:HB2	10:B:788:ILE:HD11	2.03	0.41
10:B:785:ASP:O	10:B:925:GLY:HA3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:30:SER:OG	16:H:31:THR:N	2.54	0.41
20:O:61:ASP:OD1	20:O:106:ARG:NH2	2.54	0.41
20:O:317:TYR:HB3	20:O:318:ASN:H	1.68	0.41
5:R:255:VAL:HA	5:R:258:LEU:HB2	2.02	0.40
8:M:58:GLU:HG3	8:M:59:ARG:HG3	2.02	0.40
9:A:797:LEU:HD13	9:A:809:VAL:HG21	2.02	0.40
9:A:1241:PRO:HG2	9:A:1537:ASP:HB3	2.03	0.40
9:A:1317:ILE:HA	9:A:1321:PHE:HB3	2.02	0.40
12:D:94:ARG:HH12	12:D:100:PRO:N	2.19	0.40
15:G:159:LYS:HA	15:G:162:ILE:HD12	2.02	0.40
4:S:422:ILE:HD11	4:S:442:LEU:HD13	2.03	0.40
3:Q:439:ILE:HD12	4:S:717:LYS:HE2	2.03	0.40
9:A:986:PHE:HB3	10:B:960:ILE:HD12	2.03	0.40
9:A:1555:VAL:HG21	9:A:1593:GLY:HA2	2.02	0.40
10:B:129:ARG:HD3	10:B:888:ILE:HG23	2.03	0.40
2:U:63:DT:OP2	2:U:63:DT:C7	2.70	0.40
3:Q:65:ASN:HB3	3:Q:71:GLN:HE21	1.85	0.40
3:Q:133:ALA:HA	3:Q:136:ILE:HD12	2.03	0.40
9:A:1011:VAL:O	9:A:1015:ARG:NE	2.36	0.40
15:G:137:ILE:HD11	15:G:229:LEU:HD22	2.03	0.40
4:S:248:PRO:HB3	4:S:305:PHE:HB2	2.04	0.40
4:S:712:ASP:N	4:S:712:ASP:OD1	2.53	0.40
9:A:121:LYS:HE2	9:A:219:LEU:HD11	2.04	0.40
9:A:1333:ILE:HA	9:A:1336:GLN:HB3	2.03	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	Q	469/514 (91%)	409 (87%)	60 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	594/894 (66%)	509 (86%)	85 (14%)	0	100	100
5	R	322/507 (64%)	286 (89%)	36 (11%)	0	100	100
6	I	122/125 (98%)	103 (84%)	19 (16%)	0	100	100
7	N	131/233 (56%)	118 (90%)	12 (9%)	1 (1%)	19	54
8	M	106/415 (26%)	94 (89%)	11 (10%)	1 (1%)	17	52
9	A	1449/1664 (87%)	1362 (94%)	87 (6%)	0	100	100
10	B	1174/1203 (98%)	1096 (93%)	78 (7%)	0	100	100
11	C	300/335 (90%)	284 (95%)	16 (5%)	0	100	100
12	D	66/137 (48%)	60 (91%)	6 (9%)	0	100	100
13	E	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
14	F	98/155 (63%)	94 (96%)	3 (3%)	1 (1%)	15	49
15	G	196/326 (60%)	179 (91%)	17 (9%)	0	100	100
16	H	130/146 (89%)	125 (96%)	5 (4%)	0	100	100
17	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
18	K	101/142 (71%)	94 (93%)	7 (7%)	0	100	100
19	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
20	O	498/627 (79%)	464 (93%)	34 (7%)	0	100	100
All	All	6079/7778 (78%)	5582 (92%)	494 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	113	SER
14	F	87	LYS
8	M	46	SER

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	Q	436/476 (92%)	430 (99%)	6 (1%)	67 86
4	S	563/828 (68%)	560 (100%)	3 (0%)	88 94
5	R	313/474 (66%)	312 (100%)	1 (0%)	92 96
6	I	109/110 (99%)	109 (100%)	0	100 100
7	N	128/220 (58%)	127 (99%)	1 (1%)	81 92
8	M	98/371 (26%)	97 (99%)	1 (1%)	76 90
9	A	1293/1465 (88%)	1291 (100%)	2 (0%)	93 97
10	B	1029/1053 (98%)	1025 (100%)	4 (0%)	91 96
11	C	269/296 (91%)	269 (100%)	0	100 100
12	D	65/116 (56%)	64 (98%)	1 (2%)	65 85
13	E	197/197 (100%)	197 (100%)	0	100 100
14	F	90/137 (66%)	90 (100%)	0	100 100
15	G	180/291 (62%)	180 (100%)	0	100 100
16	H	116/128 (91%)	115 (99%)	1 (1%)	78 91
17	J	64/65 (98%)	63 (98%)	1 (2%)	62 84
18	K	93/130 (72%)	93 (100%)	0	100 100
19	L	40/57 (70%)	40 (100%)	0	100 100
20	O	466/576 (81%)	464 (100%)	2 (0%)	91 96
All	All	5549/6990 (79%)	5526 (100%)	23 (0%)	91 96

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	18	ARG
3	Q	95	LEU
3	Q	293	ARG
3	Q	294	HIS
3	Q	297	ARG
4	S	292	LEU
4	S	379	LYS
4	S	407	ARG
5	R	207	ASN
7	N	119	LEU
8	M	60	LEU
9	A	467	PHE
9	A	590	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	651	ARG
10	B	702	ASN
10	B	906	ARG
10	B	1037	ARG
12	D	17	ASN
16	H	142	LEU
17	J	52	THR
20	O	115	LEU
20	O	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	A	221	HIS

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.

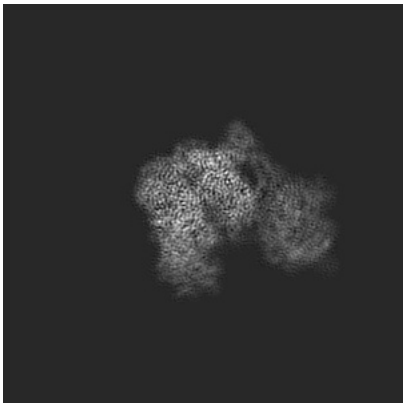
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4987. These allow visual inspection of the internal detail of the map and identification of artifacts.

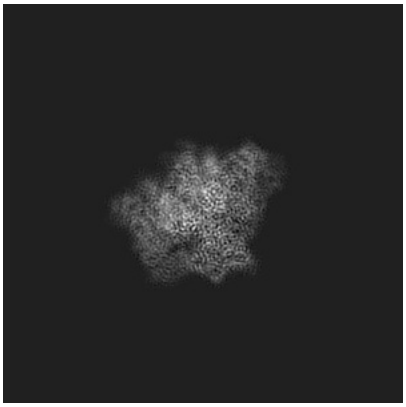
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

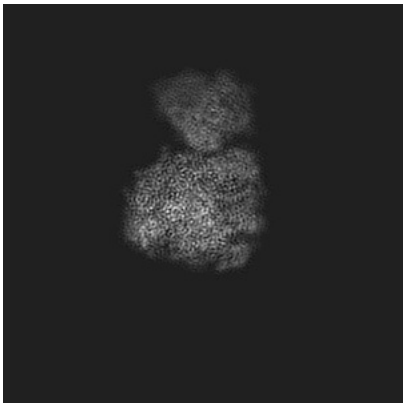
6.1.1 Primary map



X



Y

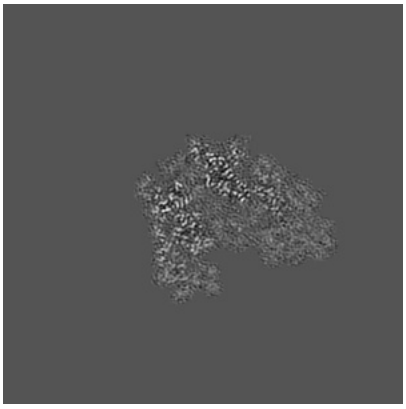


Z

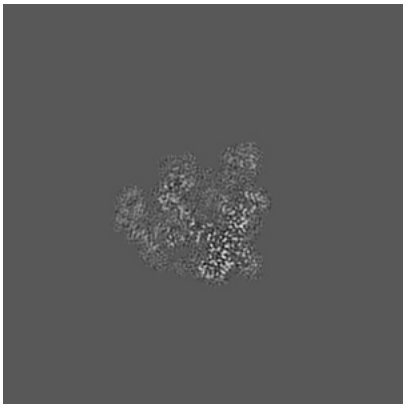
The images above show the map projected in three orthogonal directions.

6.2 Central slices

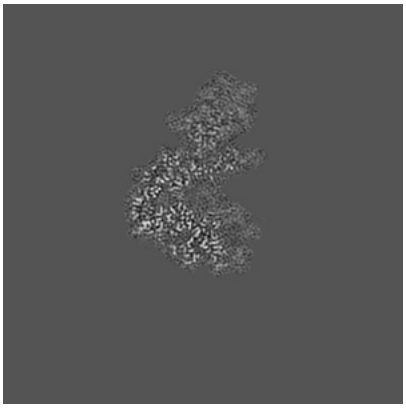
6.2.1 Primary map



X Index: 190



Y Index: 190

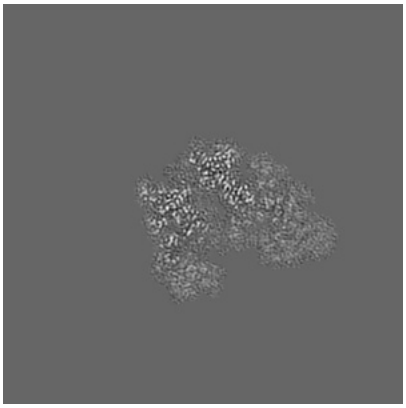


Z Index: 190

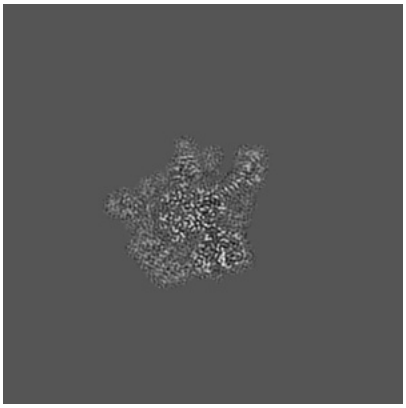
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 183



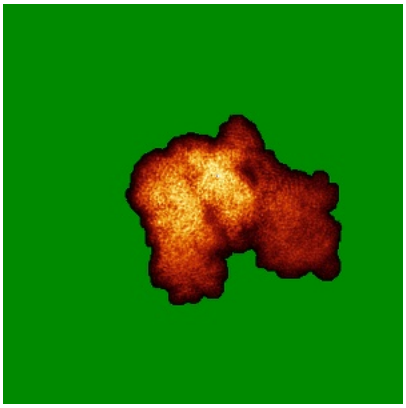
Y Index: 167

Z Index: 195

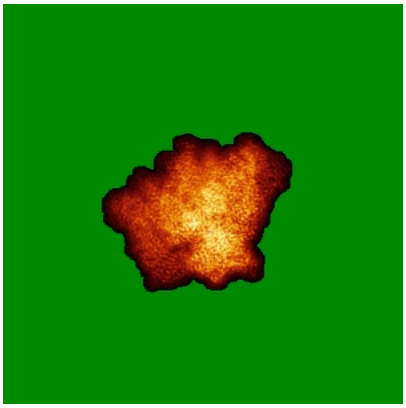
The images above show the largest variance slices of the map in three orthogonal directions.

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

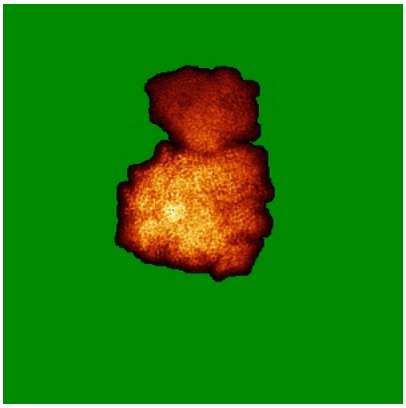
6.4.1 Primary map



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

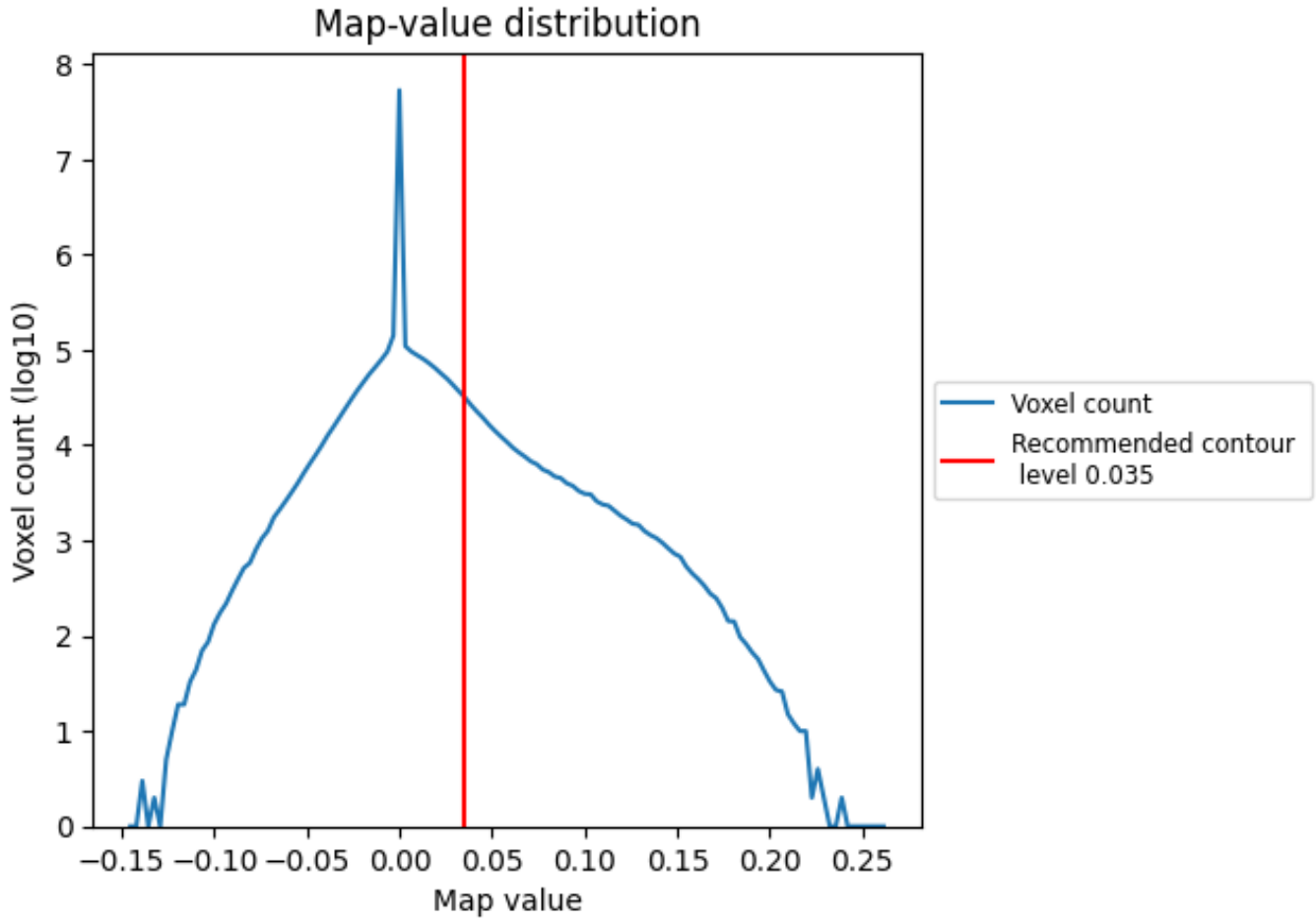
6.6 Mask visualisation (i)

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

7 Map analysis

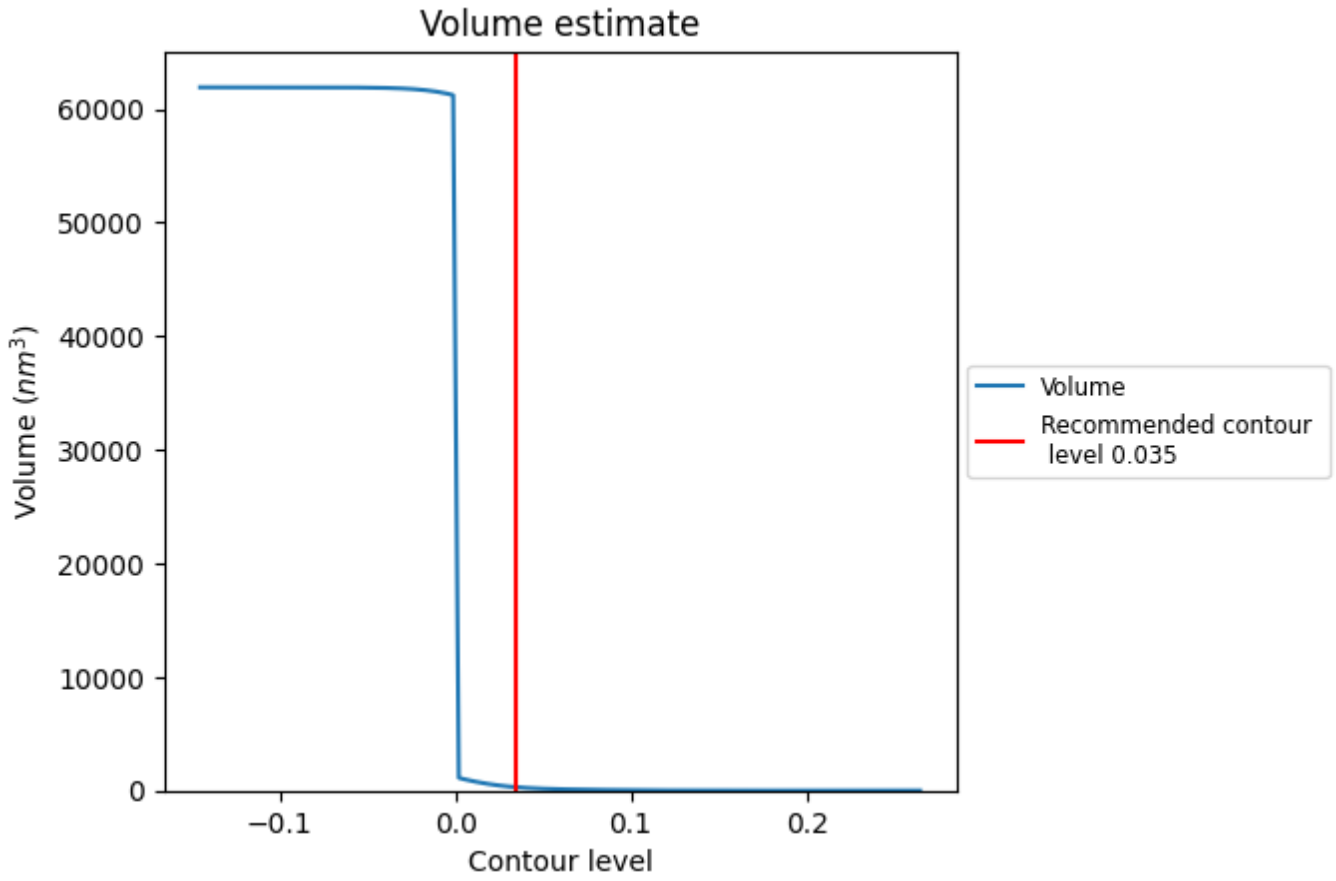
This section contains the results of statistical analysis of the map.

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.

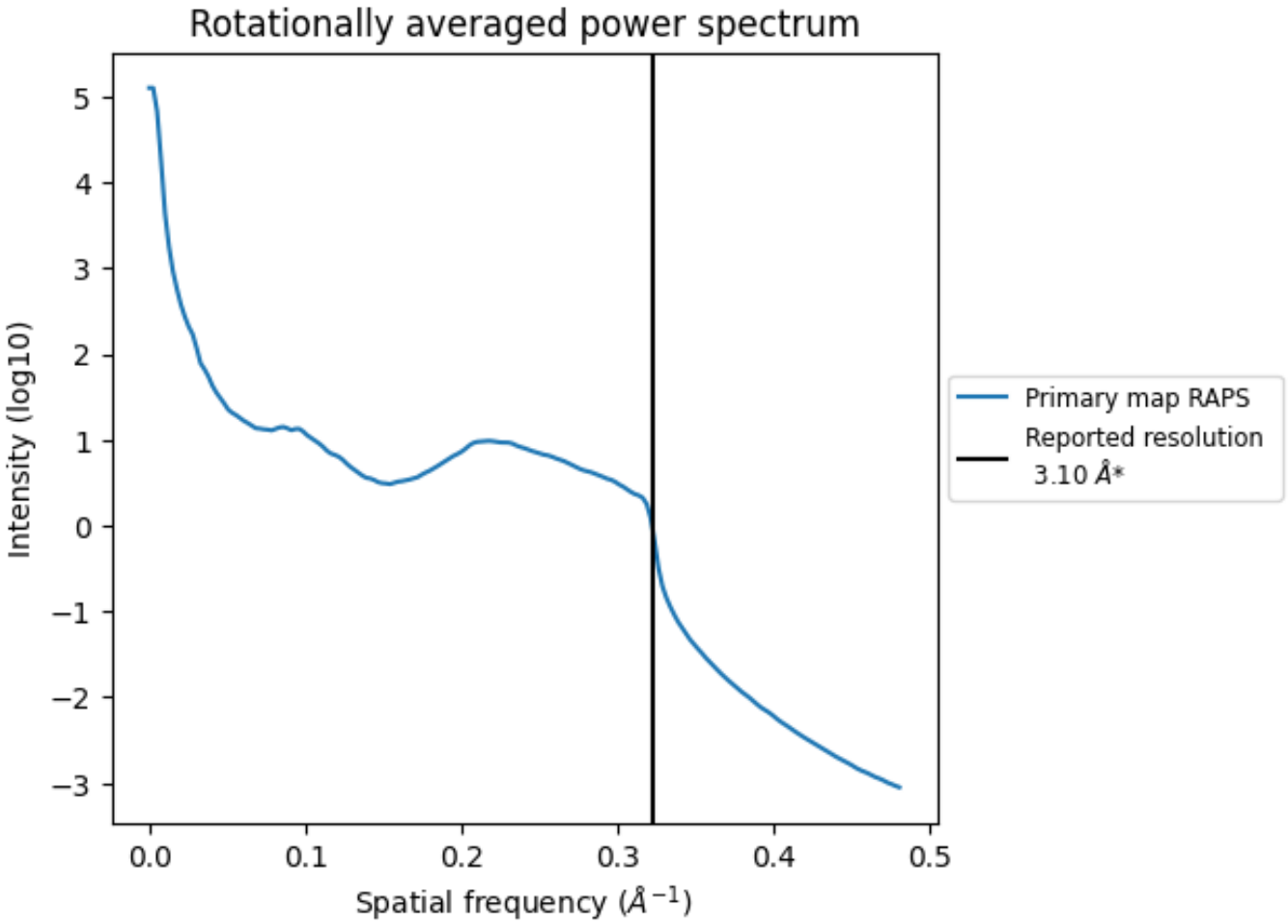
7.2 Volume estimate



The volume at the recommended contour level is 293 nm^3; this corresponds to an approximate mass of 265 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 0.323 Å^{-1}

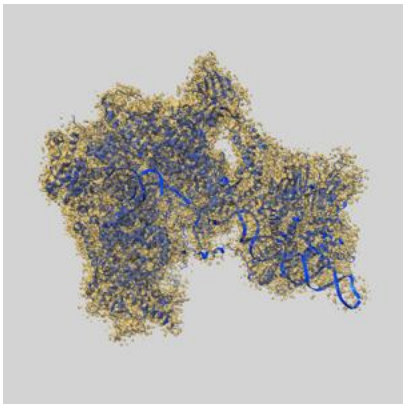
8 Fourier-Shell correlation

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

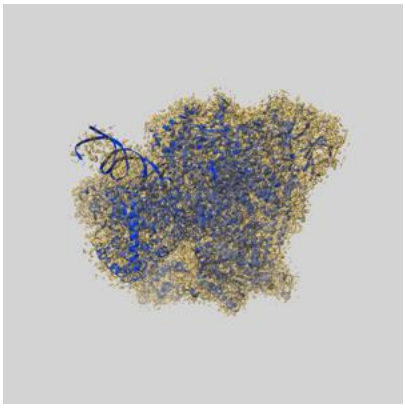
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4987 and PDB model 6RRD. Per-residue inclusion information can be found in section 3 on page 8.

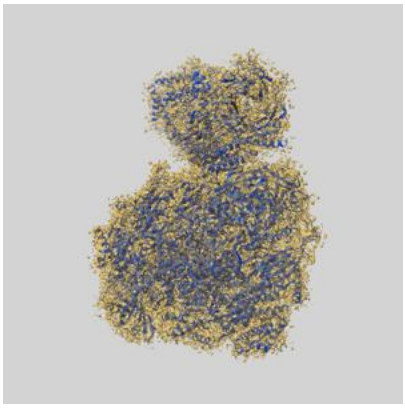
9.1 Map-model overlay



X



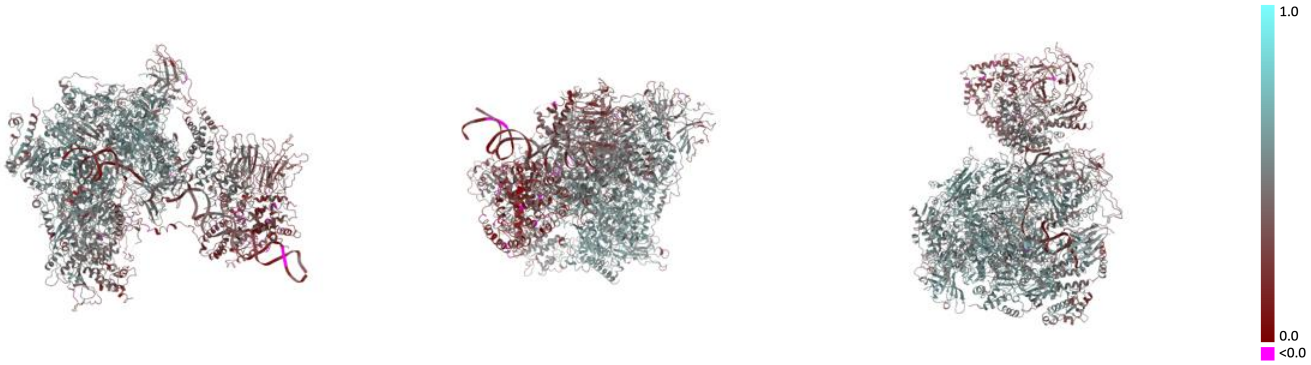
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

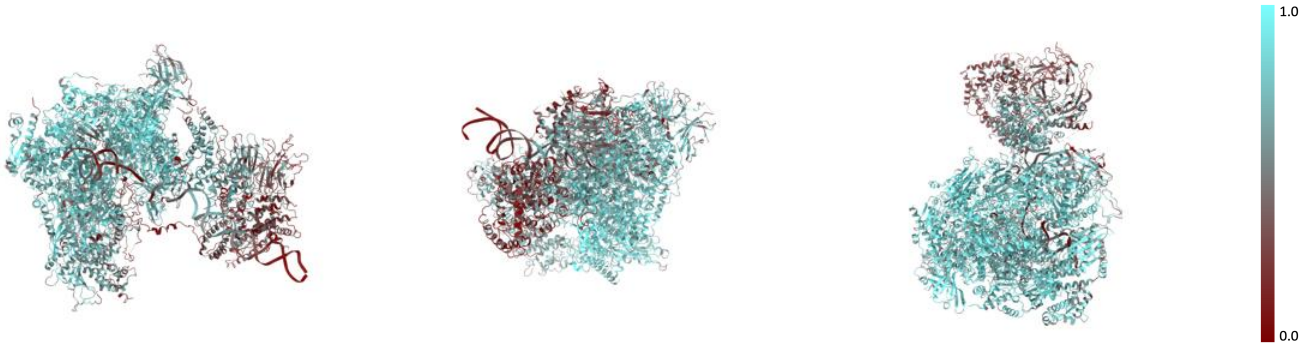
9.2 Q-score mapped to coordinate model (i)



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.

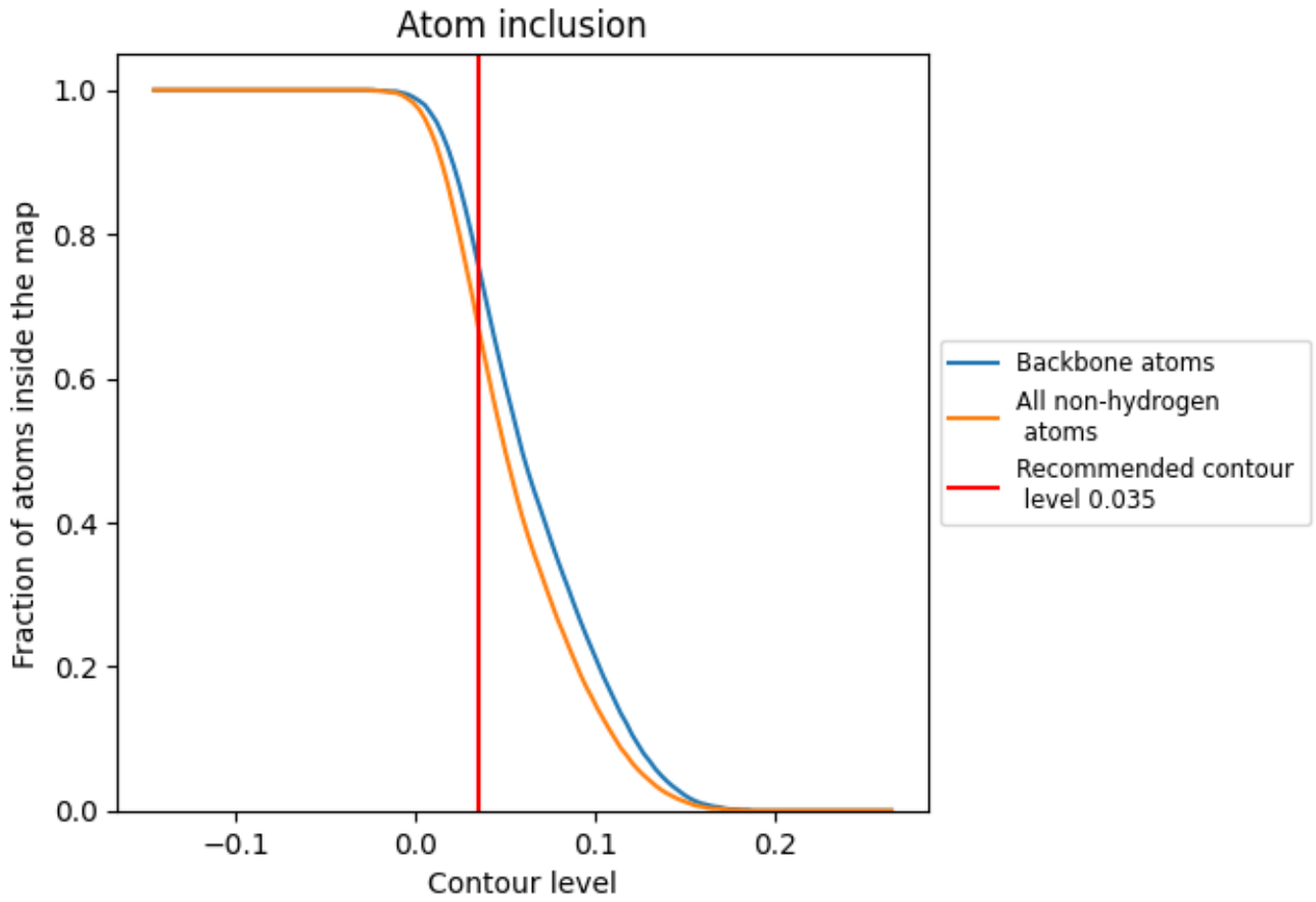
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.4520
A	0.8070	0.5240
B	0.8310	0.5400
C	0.8430	0.5400
D	0.6430	0.4530
E	0.7610	0.5020
F	0.8410	0.5580
G	0.7320	0.4710
H	0.8390	0.5360
I	0.5460	0.4220
J	0.8970	0.5740
K	0.8330	0.5480
L	0.7860	0.5130
M	0.5780	0.3950
N	0.5950	0.4110
O	0.5700	0.3850
Q	0.3580	0.2890
R	0.5700	0.4050
S	0.3660	0.2970
T	0.3260	0.2570
U	0.3740	0.2740