



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:53 PM UTC

PDB ID : 6RWE / pdb_00006rwe
EMDB ID : EMD-10038
Title : RNA Polymerase I Open Complex conformation 2
Authors : Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on : 2019-06-04
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

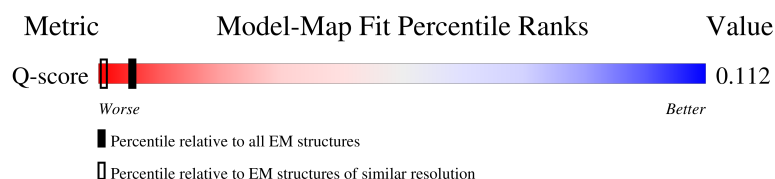
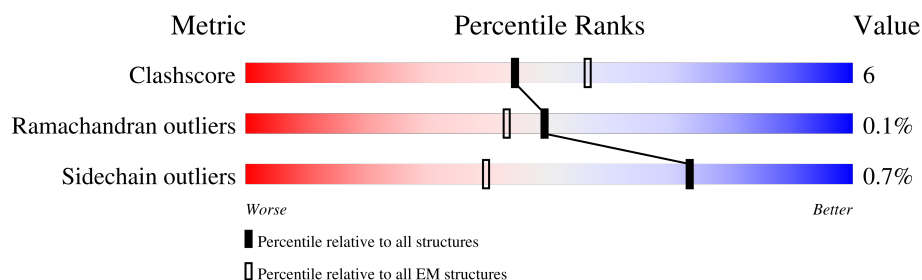
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	T	70	
2	U	70	
3	M	415	
4	A	1664	

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Mol	Chain	Length	Quality of chain
5	B	1203	
6	C	335	
7	D	137	
8	E	215	
9	F	155	
10	G	326	
11	H	146	
12	I	125	
13	J	70	
14	K	142	
15	L	70	
16	N	233	
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 53719 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	50	Total	C	N	O	P	0	0
			1000	481	164	305	50		

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	45	Total	C	N	O	P	0	0
			944	447	192	261	44		

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	392	Total	C	N	O	S	0	0
			3100	1978	525	593	4		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1464	Total	C	N	O	S	0	0
			11558	7303	2011	2183	61		

- Molecule 5 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1180	Total	C	N	O	S	0	0
			9371	5923	1644	1754	50		

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	199	Total	C	N	O	S	0	0
			1576	1012	273	286	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA12.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA34.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	499	Total	C	N	O	S	0	0
			4086	2636	661	767	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		

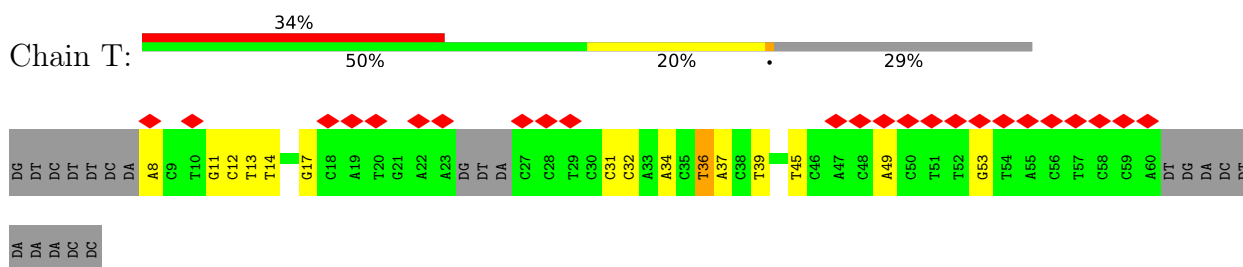
- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

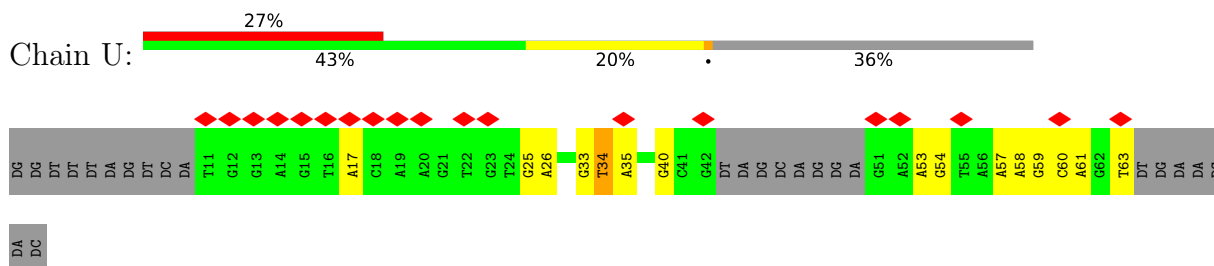
3 Residue-property plots [i](#)

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.

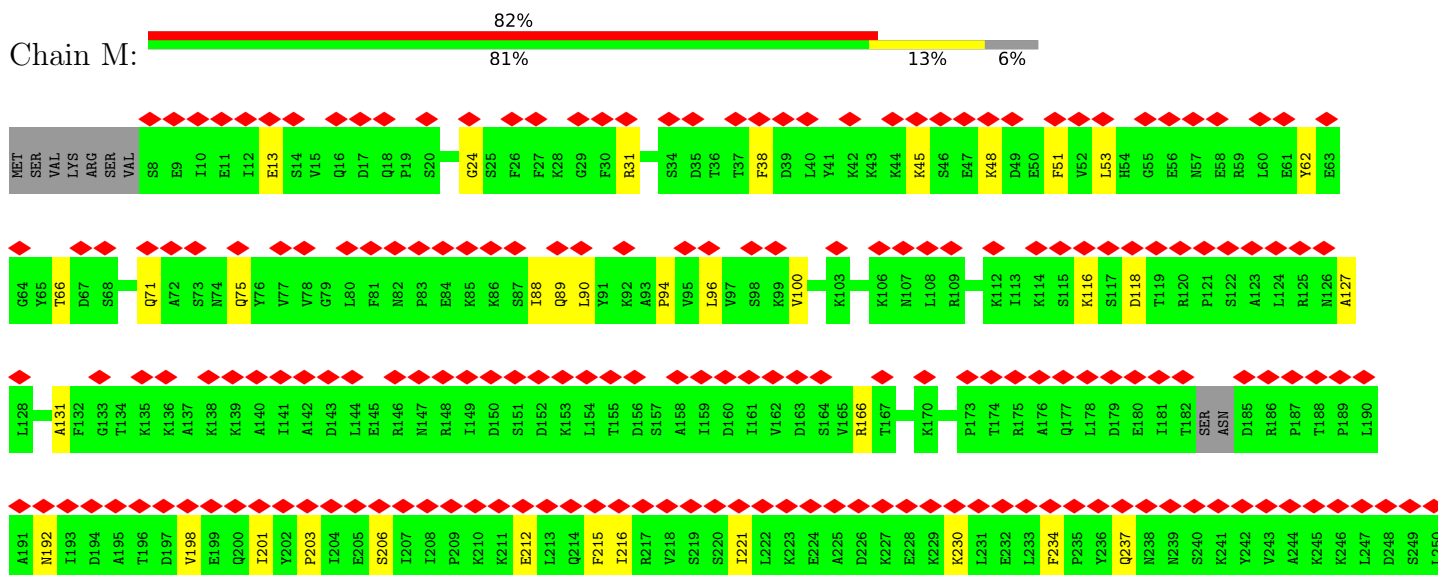
- Molecule 1: Template strand

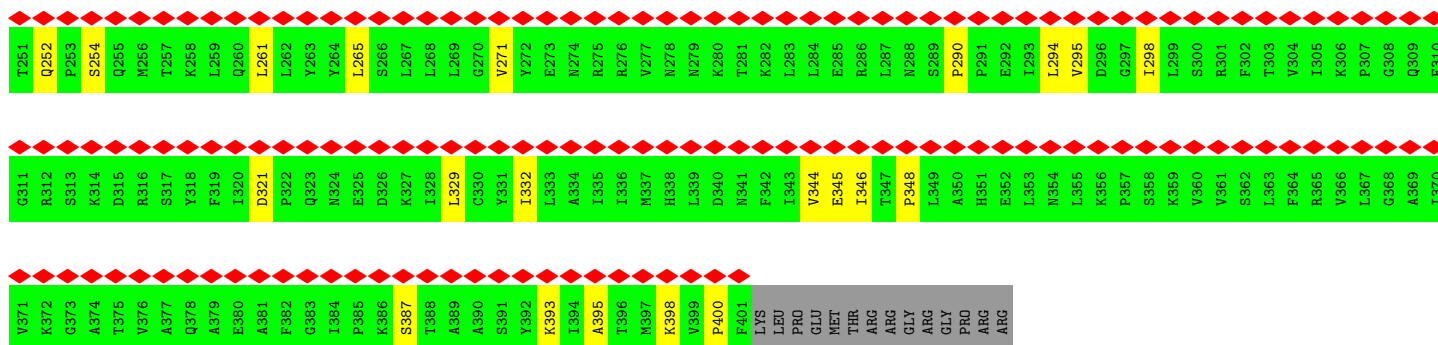


- Molecule 2: Nontemplate strand

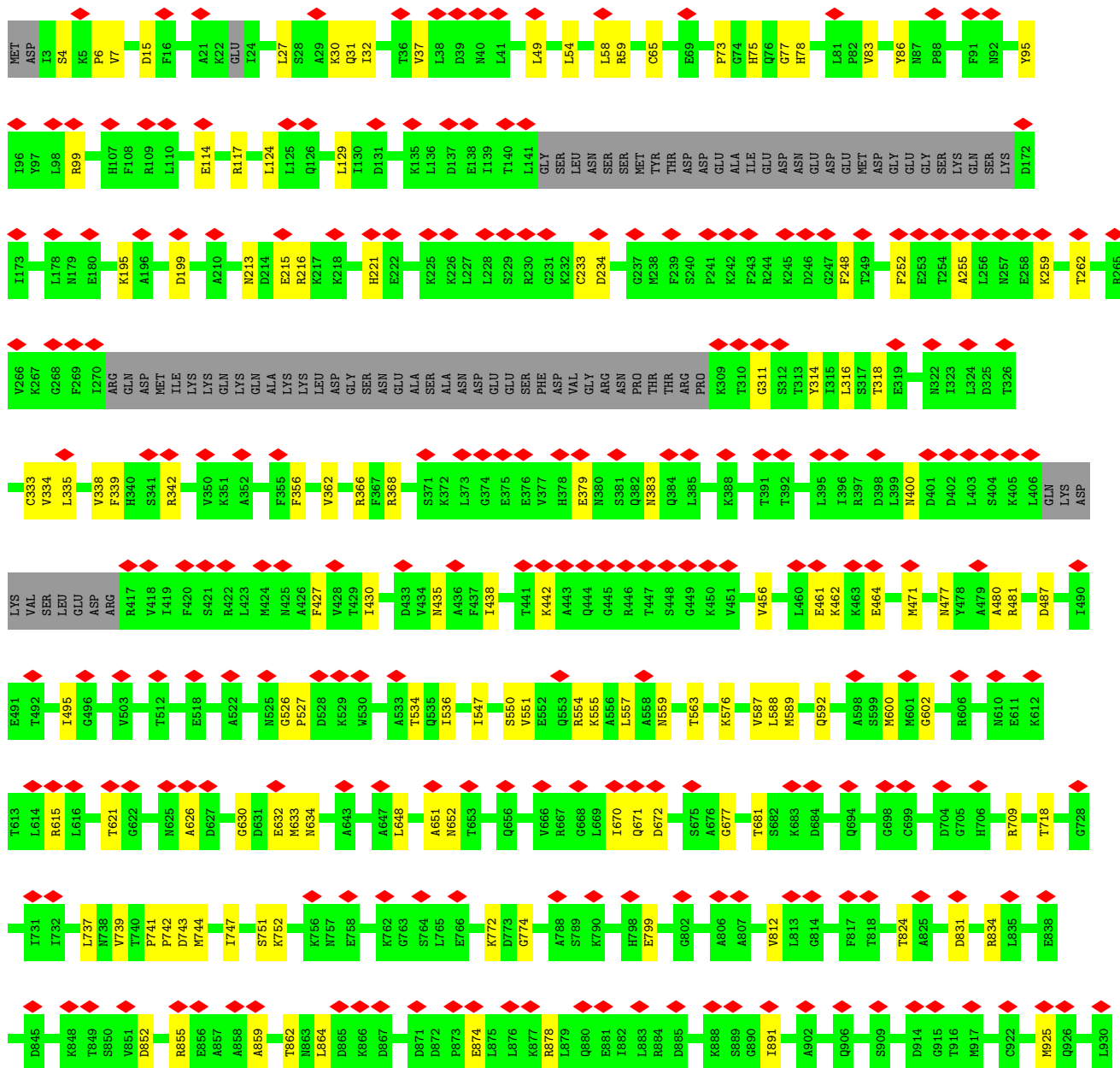
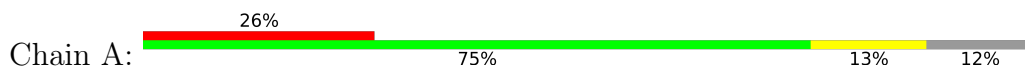


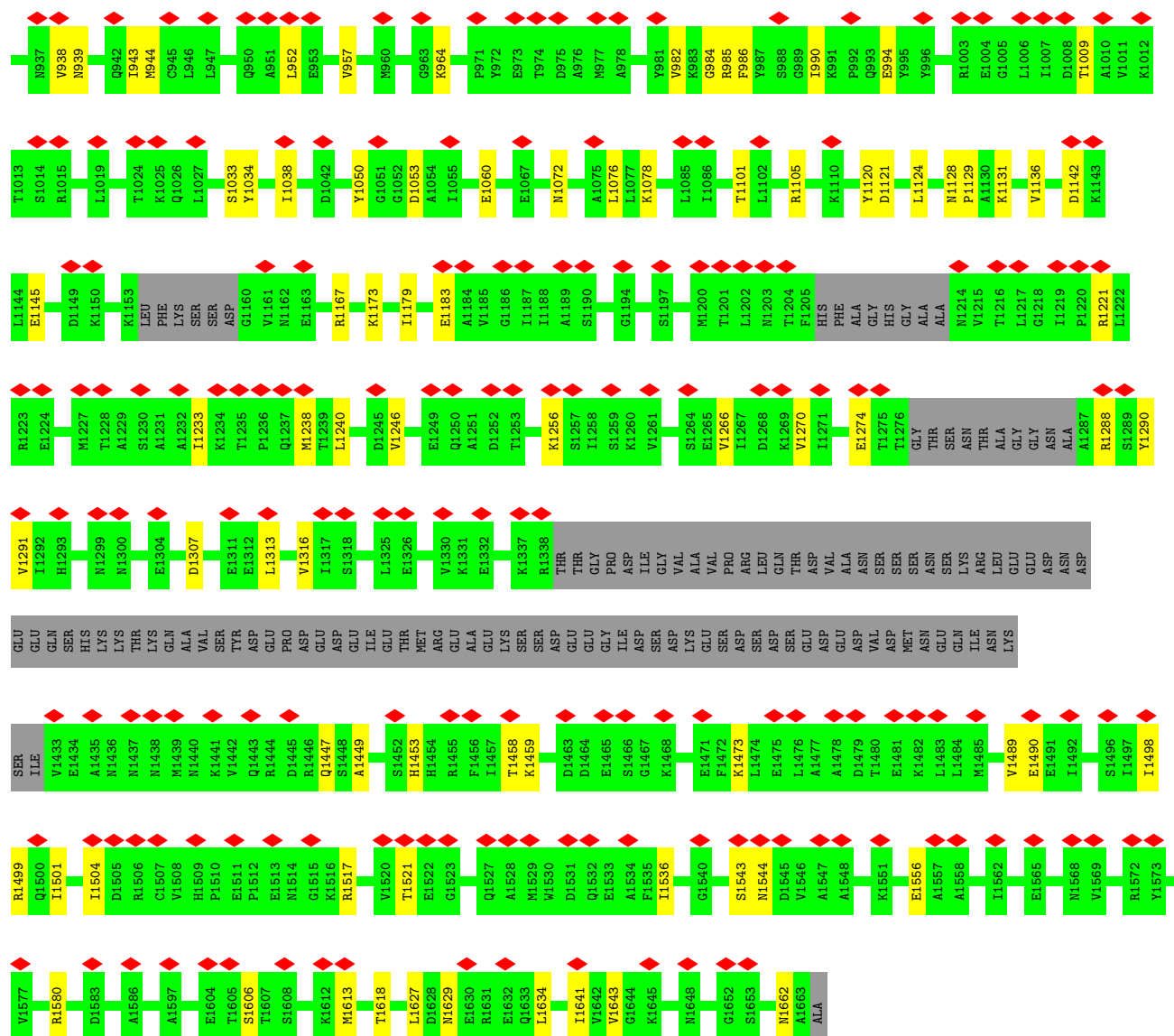
- Molecule 3: DNA-directed RNA polymerase I subunit RPA49



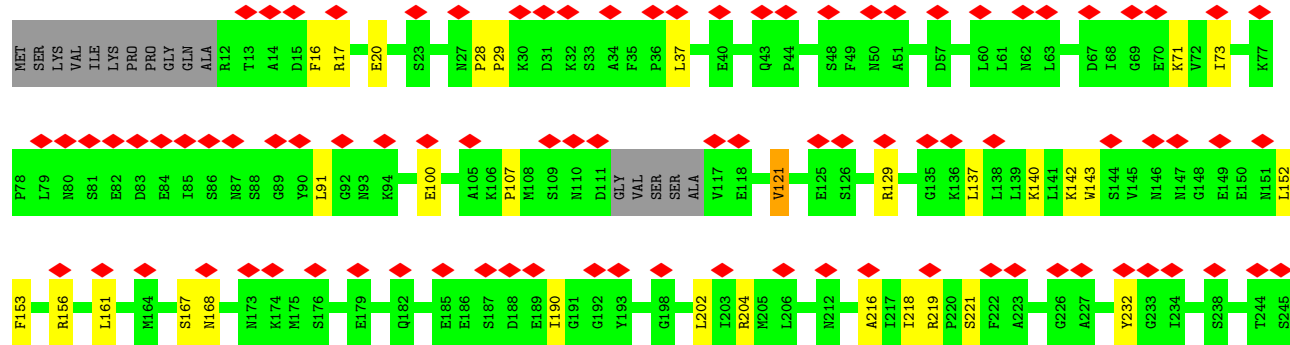
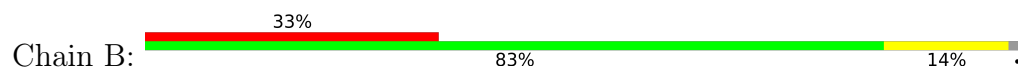


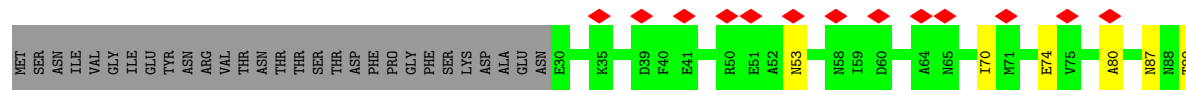
• Molecule 4: DNA-directed RNA polymerase I subunit RPA190

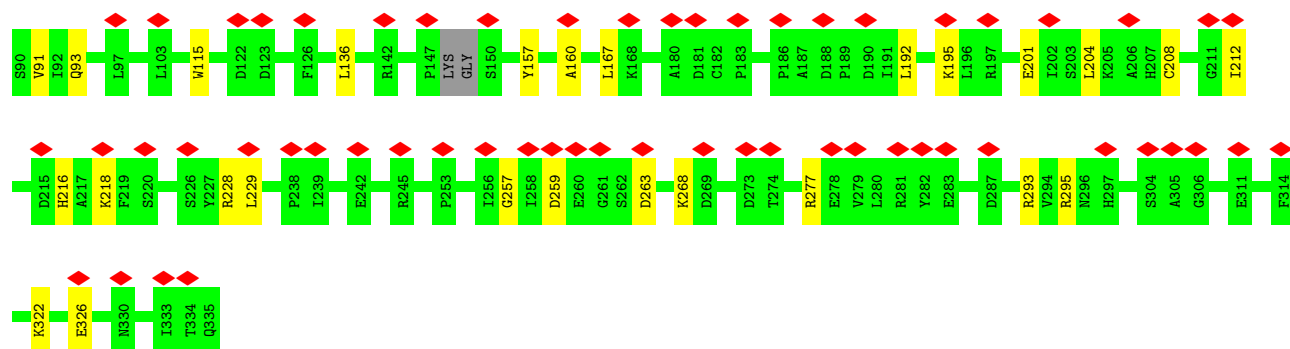




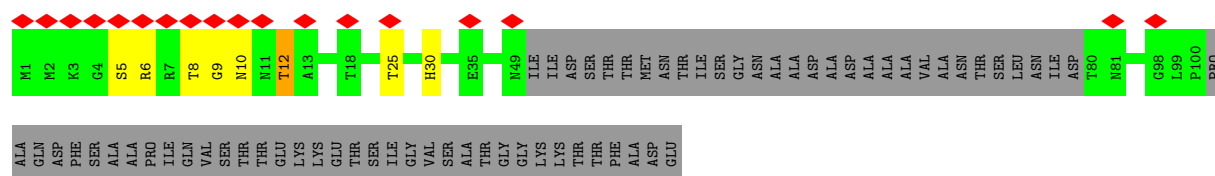
• Molecule 5: DNA-directed RNA polymerase I subunit RPA135



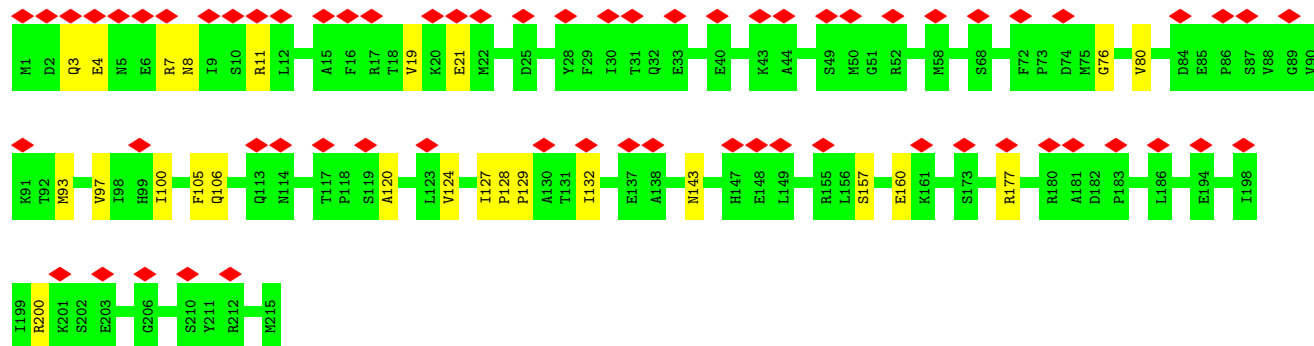
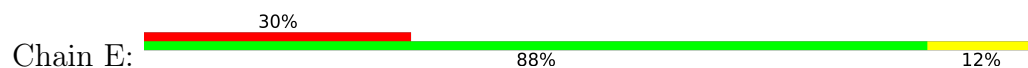




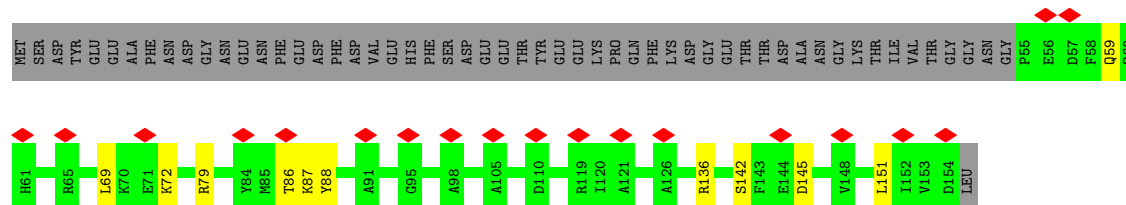
• Molecule 7: DNA-directed RNA polymerase I subunit RPA14



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

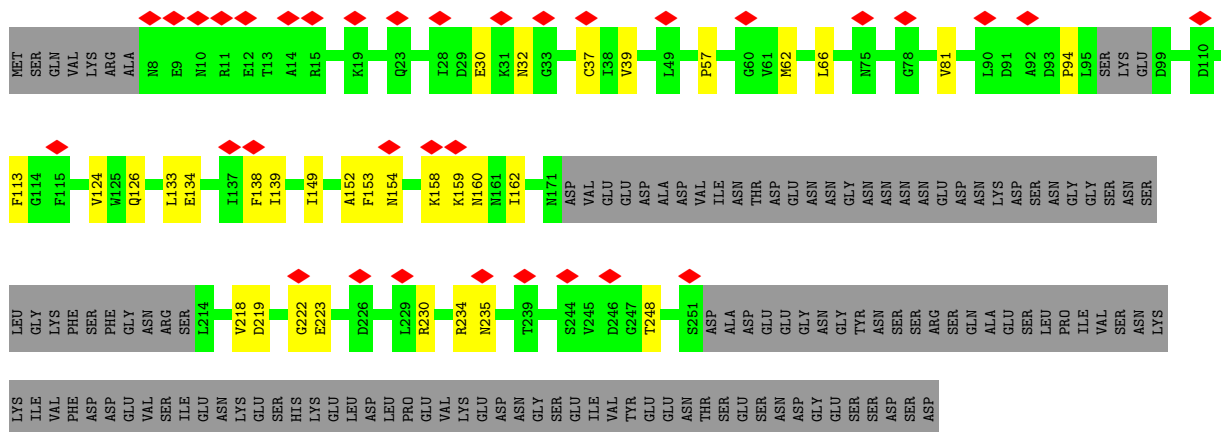


• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

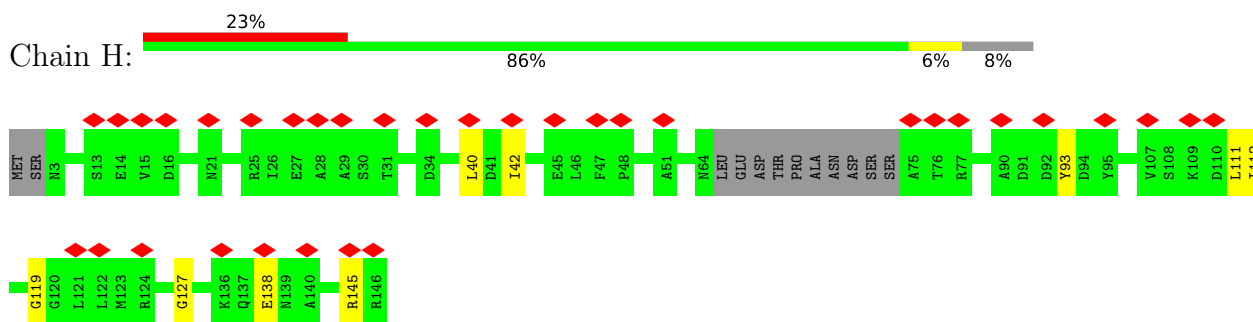


• Molecule 10: DNA-directed RNA polymerase I subunit RPA43

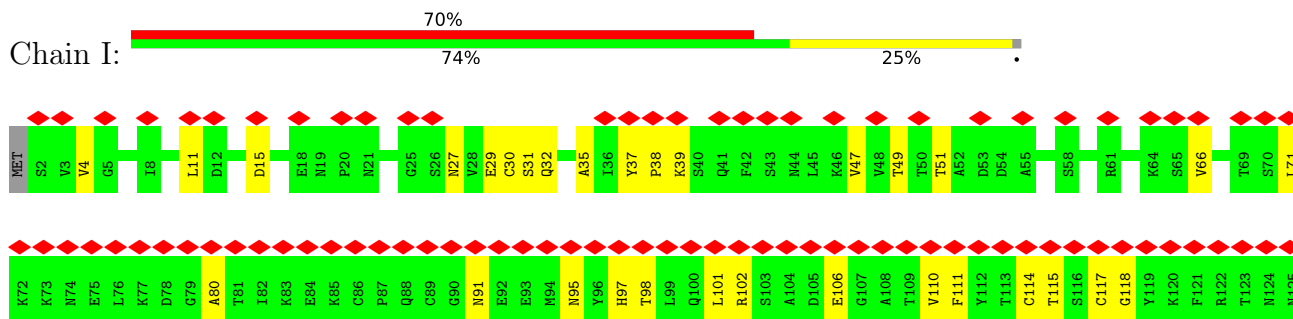




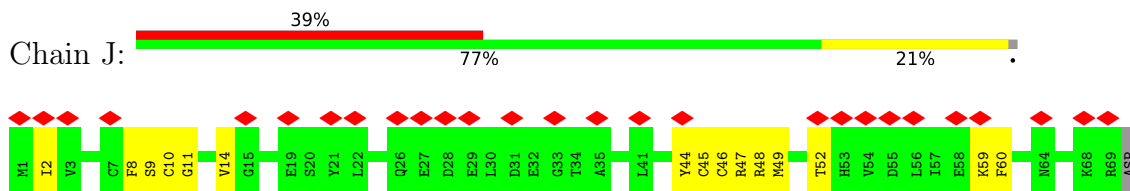
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3



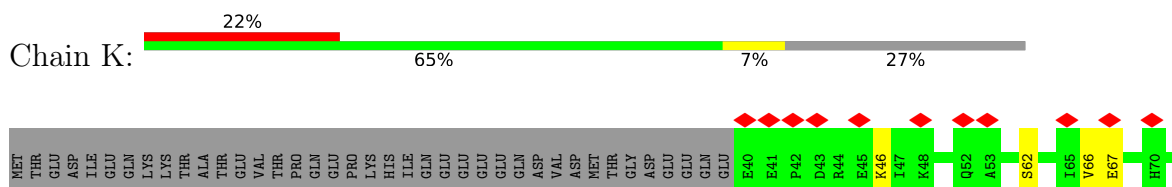
- Molecule 12: DNA-directed RNA polymerase I subunit RPA12

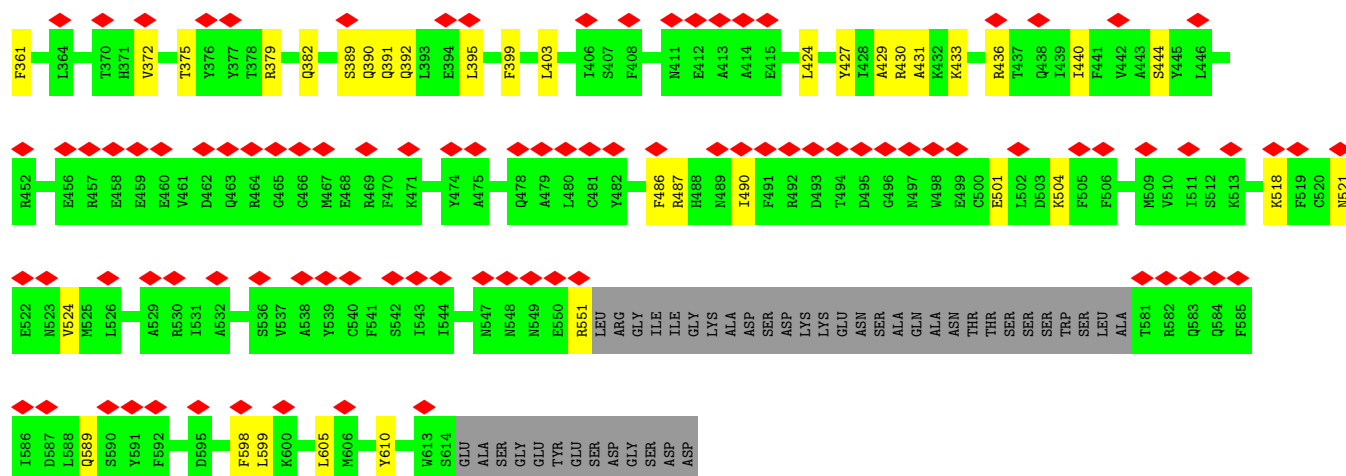


- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

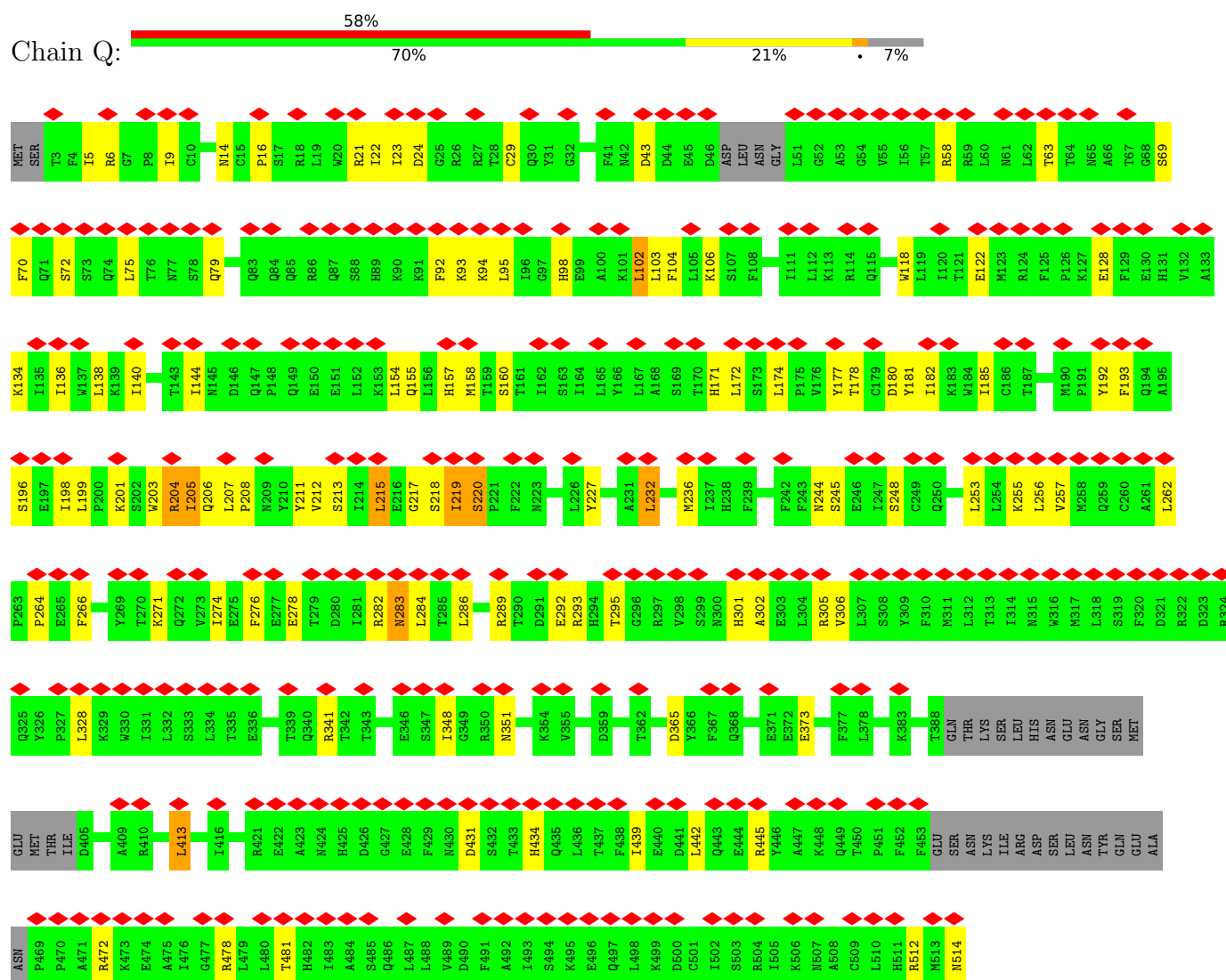


- Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2





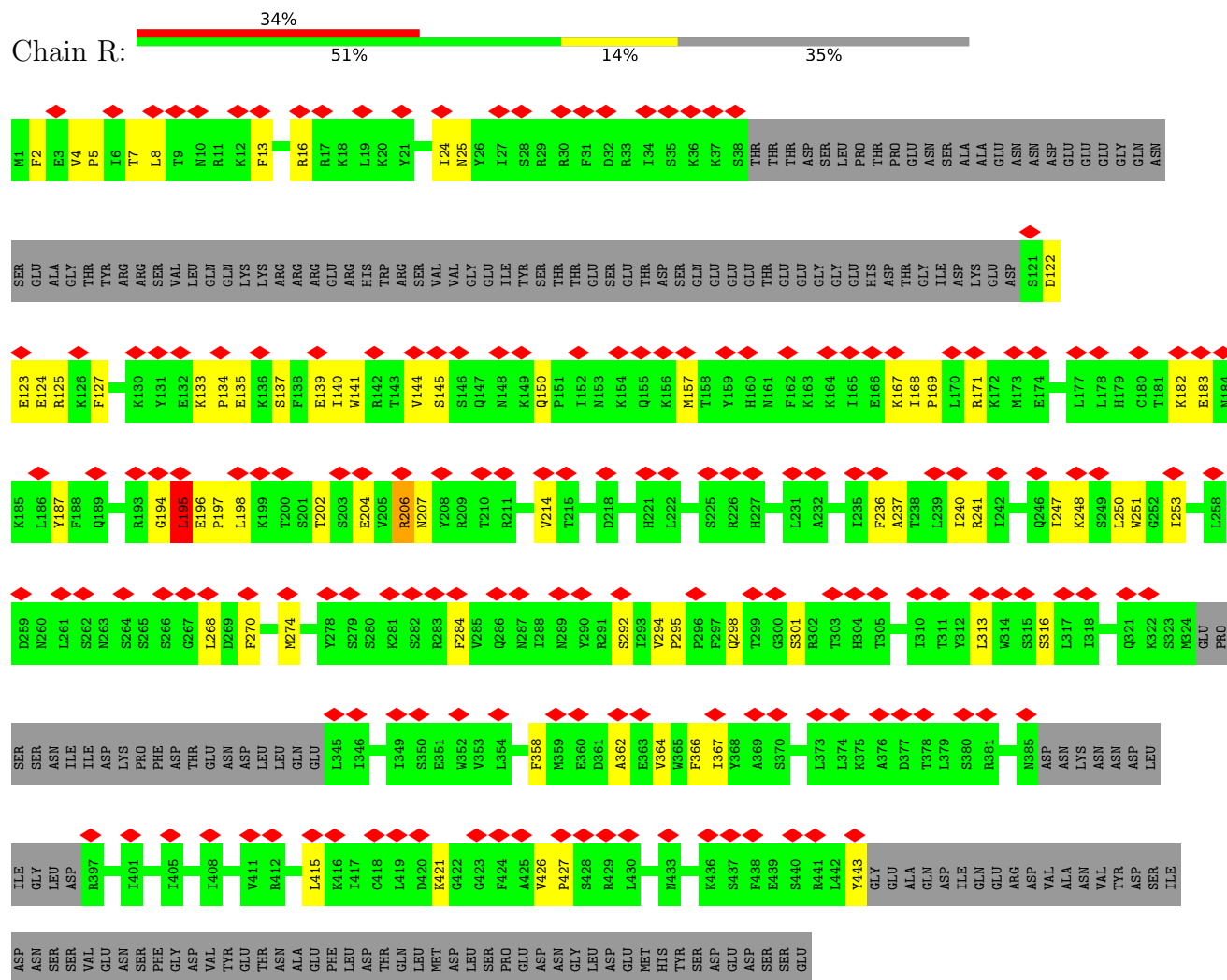
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN7



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59963	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 ($e^-/\text{\AA}^2$)	1.57175	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	0.453	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.32	0/1113	0.74	3/1707 (0.2%)
2	U	0.28	0/1065	0.56	1/1645 (0.1%)
3	M	0.22	0/3152	0.50	0/4252
4	A	0.44	0/11769	0.57	0/15896
5	B	0.48	0/9578	0.61	0/12948
6	C	0.46	0/2469	0.56	0/3347
7	D	0.34	0/557	0.51	0/750
8	E	0.35	0/1795	0.48	0/2416
9	F	0.44	0/838	0.56	0/1129
10	G	0.33	0/1613	0.52	0/2193
11	H	0.42	0/1090	0.52	0/1476
12	I	0.24	0/955	0.49	0/1288
13	J	0.55	0/578	0.71	1/775 (0.1%)
14	K	0.46	0/821	0.53	0/1108
15	L	0.46	0/361	0.67	0/478
16	N	0.28	0/1124	0.52	0/1512
17	O	0.25	0/4173	0.52	0/5645
18	Q	0.39	0/4028	0.77	6/5441 (0.1%)
19	S	0.29	0/5065	0.62	2/6859 (0.0%)
20	R	0.39	0/2836	0.70	1/3817 (0.0%)
All	All	0.39	0/54980	0.60	14/74682 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	49	DA	O3'-P-O5'	7.70	115.55	104.00
13	J	14	VAL	N-CA-C	-6.01	107.64	113.53
20	R	295	PRO	N-CA-C	5.77	117.74	110.70
18	Q	292	GLU	O-C-N	-5.63	116.25	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	292	GLU	CA-C-N	5.48	132.22	122.31
18	Q	292	GLU	C-N-CA	5.48	132.22	122.31
1	T	34	DA	C2'-C3'-O3'	-5.45	103.33	111.50
18	Q	155	GLN	O-C-N	5.25	129.22	122.93
18	Q	220	SER	CA-C-N	5.18	125.43	119.83
18	Q	220	SER	C-N-CA	5.18	125.43	119.83
2	U	34	DT	C2'-C3'-O3'	-5.18	103.73	111.50
19	S	377	ARG	N-CA-C	-5.17	106.82	112.72
19	S	31	ASN	N-CA-C	-5.11	99.92	110.80
1	T	36	DT	C2'-C3'-O3'	-5.04	103.94	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1000	0	568	22	0
2	U	944	0	507	31	0
3	M	3100	0	3207	34	0
4	A	11558	0	11648	140	0
5	B	9371	0	9239	118	0
6	C	2418	0	2401	21	0
7	D	551	0	558	6	0
8	E	1759	0	1788	15	0
9	F	823	0	841	7	0
10	G	1576	0	1581	24	0
11	H	1072	0	1042	6	0
12	I	942	0	931	20	0
13	J	569	0	586	8	0
14	K	810	0	801	5	0
15	L	359	0	381	4	0
16	N	1103	0	1106	13	0
17	O	4086	0	4024	46	0
18	Q	3936	0	3918	111	0
19	S	4963	0	4890	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	2771	0	2844	52	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
21	Q	1	0	0	0	0
All	All	53719	0	52861	665	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 (665) 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)
19:S:31:ASN:OD1	19:S:32:TYR:N	1.97	0.96
18:Q:92:PHE:CD1	18:Q:205:ILE:HG21	2.02	0.95
18:Q:218:SER:HB3	20:R:207:ASN:OD1	1.70	0.92
18:Q:92:PHE:CD1	18:Q:205:ILE:CG2	2.57	0.88
19:S:450:ARG:HH11	19:S:450:ARG:HG2	1.40	0.87
18:Q:193:PHE:HD1	18:Q:217:GLY:O	1.59	0.85
18:Q:104:PHE:CD1	18:Q:211:TYR:CD1	2.65	0.85
20:R:122:ASP:CB	20:R:125:ARG:HD3	2.09	0.83
19:S:360:TRP:CG	19:S:377:ARG:HH21	1.96	0.81
19:S:31:ASN:CG	19:S:32:TYR:H	1.88	0.81
18:Q:193:PHE:CD1	18:Q:217:GLY:O	2.33	0.80
18:Q:104:PHE:CD1	18:Q:211:TYR:HD1	2.00	0.80
18:Q:144:ILE:HD12	18:Q:154:LEU:HB2	1.64	0.79
20:R:204:GLU:N	20:R:204:GLU:OE1	2.16	0.79
19:S:292:LEU:HD12	19:S:292:LEU:O	1.84	0.78
1:T:17:DG:H1	2:U:53:DA:H2	1.33	0.76
7:D:9:GLY:HA2	7:D:12:THR:HG23	1.70	0.74
18:Q:196:SER:OG	18:Q:215:LEU:HB3	1.86	0.74
20:R:122:ASP:HB3	20:R:125:ARG:HD3	1.68	0.74
18:Q:219:ILE:HG12	18:Q:219:ILE:O	1.87	0.73
19:S:377:ARG:HG3	19:S:402:ILE:O	1.90	0.72
20:R:125:ARG:NH1	20:R:125:ARG:HG2	2.04	0.71
18:Q:196:SER:O	18:Q:204:ARG:HD2	1.89	0.71
20:R:125:ARG:HG2	20:R:125:ARG:HH11	1.55	0.71
18:Q:289:ARG:NH1	18:Q:295:THR:HA	2.04	0.71
4:A:15:ASP:HB2	5:B:1197:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:670:ILE:HG12	4:A:671:GLN:HG3	1.74	0.70
19:S:268:SER:HB3	19:S:293:TYR:CE1	2.26	0.70
20:R:122:ASP:HB2	20:R:125:ARG:HD3	1.72	0.70
18:Q:92:PHE:HB3	18:Q:205:ILE:HD12	1.74	0.70
4:A:964:LYS:NZ	5:B:672:MET:O	2.25	0.70
4:A:477:ASN:OD1	5:B:1047:ARG:NH1	2.25	0.69
19:S:360:TRP:CD2	19:S:377:ARG:NH2	2.60	0.69
18:Q:282:ARG:HG3	18:Q:283:ASN:N	2.09	0.67
3:M:66:THR:HB	3:M:71:GLN:HG3	1.77	0.67
19:S:360:TRP:CG	19:S:377:ARG:NH2	2.63	0.66
18:Q:136:ILE:O	18:Q:140:ILE:HG12	1.95	0.66
20:R:167:LYS:HG2	20:R:171:ARG:HE	1.60	0.66
18:Q:22:ILE:HG23	18:Q:23:ILE:HG13	1.78	0.66
18:Q:92:PHE:CB	18:Q:205:ILE:HD12	2.26	0.66
2:U:59:DG:OP1	4:A:221:HIS:HE1	1.79	0.65
18:Q:232:LEU:CD2	18:Q:289:ARG:HH21	2.08	0.65
18:Q:282:ARG:HG3	18:Q:283:ASN:H	1.61	0.65
18:Q:232:LEU:HD23	18:Q:289:ARG:HH21	1.61	0.64
18:Q:278:GLU:HA	18:Q:278:GLU:OE1	1.96	0.64
19:S:360:TRP:CB	19:S:377:ARG:HH21	2.10	0.64
6:C:70:ILE:HG23	6:C:74:GLU:HB2	1.81	0.64
18:Q:193:PHE:HZ	18:Q:220:SER:HB3	1.63	0.63
4:A:1101:THR:HG22	4:A:1120:TYR:HB3	1.80	0.63
4:A:233:CYS:SG	4:A:234:ASP:N	2.72	0.63
4:A:65:CYS:SG	4:A:75:HIS:NE2	2.64	0.62
19:S:270:GLN:CG	19:S:291:PRO:HB3	2.29	0.62
17:O:430:ARG:NH1	17:O:610:TYR:OH	2.32	0.62
3:M:38:PHE:HB2	16:N:119:LEU:HB2	1.80	0.62
20:R:124:GLU:O	20:R:127:PHE:HB3	2.00	0.62
19:S:317:ILE:HG13	19:S:327:GLY:H	1.64	0.62
4:A:27:LEU:HB3	5:B:1130:ARG:HB3	1.81	0.61
18:Q:93:LYS:HB3	18:Q:95:LEU:HD22	1.82	0.61
18:Q:481:THR:HG21	19:S:570:ASP:HA	1.82	0.61
4:A:982:VAL:HG22	4:A:994:GLU:HB2	1.81	0.61
8:E:97:VAL:HG13	8:E:127:ILE:HD11	1.82	0.61
19:S:451:ILE:HD11	19:S:466:ALA:HB1	1.81	0.61
12:I:27:ASN:HA	12:I:38:PRO:HA	1.81	0.61
5:B:726:MET:SD	5:B:1035:ARG:NH1	2.74	0.61
20:R:122:ASP:O	20:R:123:GLU:HB2	2.01	0.61
18:Q:154:LEU:HD23	18:Q:154:LEU:O	2.01	0.61
19:S:63:SER:HB3	19:S:549:TYR:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:206:ARG:HG3	20:R:206:ARG:O	2.01	0.61
5:B:143:TRP:HB3	5:B:152:LEU:HB2	1.83	0.60
18:Q:293:ARG:O	18:Q:293:ARG:HG3	2.01	0.60
4:A:709:ARG:NH1	4:A:737:LEU:O	2.33	0.60
12:I:30:CYS:SG	12:I:31:SER:N	2.74	0.60
19:S:395:GLN:HB3	20:R:140:ILE:HG23	1.82	0.60
3:M:344:VAL:HB	3:M:395:ALA:HB3	1.84	0.60
18:Q:276:PHE:O	18:Q:512:ARG:NH1	2.34	0.60
18:Q:103:LEU:HD12	18:Q:103:LEU:O	2.02	0.59
10:G:159:LYS:HA	10:G:162:ILE:HD12	1.85	0.59
18:Q:14:ASN:ND2	18:Q:29:CYS:SG	2.76	0.59
18:Q:274:ILE:O	18:Q:278:GLU:HB2	2.03	0.59
4:A:1145:GLU:OE2	4:A:1167:ARG:NH1	2.34	0.59
12:I:97:HIS:HB3	12:I:111:PHE:HB2	1.85	0.59
20:R:194:GLY:O	20:R:195:LEU:O	2.20	0.59
3:M:127:ALA:HA	3:M:131:ALA:HB3	1.84	0.59
6:C:229:LEU:HB2	6:C:293:ARG:HH11	1.68	0.59
18:Q:102:LEU:HD21	19:S:769:GLN:OE1	2.03	0.58
18:Q:104:PHE:HD1	18:Q:211:TYR:CD1	2.19	0.58
4:A:824:THR:HG23	5:B:1023:ARG:HB2	1.84	0.58
17:O:501:GLU:HB3	17:O:504:LYS:HB3	1.85	0.58
3:M:53:LEU:HB2	3:M:96:LEU:HD13	1.85	0.58
5:B:565:LEU:HD21	5:B:608:LEU:HD11	1.85	0.58
19:S:401:ASN:H	19:S:419:ARG:HG2	1.66	0.58
4:A:86:TYR:HA	4:A:356:PHE:HA	1.86	0.57
17:O:431:ALA:O	17:O:487:ARG:NH2	2.36	0.57
2:U:54:DG:H1'	5:B:513:LYS:NZ	2.19	0.57
3:M:234:PHE:O	3:M:237:GLN:NE2	2.37	0.57
5:B:71:LYS:NZ	5:B:418:ASP:OD1	2.37	0.57
9:F:136:ARG:HH12	9:F:151:LEU:HD21	1.70	0.57
3:M:13:GLU:HB2	3:M:89:GLN:HB3	1.87	0.57
4:A:114:GLU:OE2	4:A:117:ARG:NH2	2.38	0.57
10:G:138:PHE:HB3	17:O:182:MET:HE3	1.86	0.57
18:Q:278:GLU:OE2	18:Q:284:LEU:CD2	2.52	0.57
3:M:398:LYS:HG2	3:M:400:PRO:HD2	1.87	0.57
6:C:53:ASN:HD22	16:N:174:GLY:HA3	1.70	0.57
19:S:270:GLN:HG2	19:S:291:PRO:HB3	1.86	0.57
18:Q:271:LYS:NZ	19:S:739:ASP:OD2	2.36	0.57
4:A:592:GLN:OE1	4:A:634:ASN:ND2	2.38	0.56
6:C:192:LEU:HD21	6:C:195:LYS:HE3	1.87	0.56
2:U:54:DG:H8	2:U:54:DG:H5''	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1459:LYS:HD2	4:A:1473:LYS:HD3	1.87	0.56
4:A:32:ILE:HD11	4:A:54:LEU:HD11	1.88	0.56
17:O:518:LYS:HD2	17:O:551:ARG:HB2	1.87	0.56
19:S:25:LEU:HD23	19:S:437:SER:HA	1.88	0.56
2:U:25:DG:N2	18:Q:293:ARG:NH2	2.53	0.56
19:S:433:VAL:HG21	20:R:145:SER:HB3	1.88	0.56
19:S:454:GLN:NE2	19:S:511:ILE:O	2.39	0.56
18:Q:103:LEU:HD11	18:Q:203:TRP:HB3	1.88	0.56
18:Q:118:TRP:NE1	18:Q:122:GLU:OE1	2.38	0.56
19:S:292:LEU:HD12	19:S:292:LEU:C	2.31	0.56
20:R:237:ALA:O	20:R:241:ARG:NH2	2.39	0.55
17:O:92:ASN:HA	17:O:95:ILE:HD12	1.87	0.55
19:S:31:ASN:OD1	19:S:32:TYR:O	2.24	0.55
4:A:1288:ARG:NH2	4:A:1290:TYR:OH	2.40	0.55
4:A:462:LYS:HD2	4:A:464:GLU:HG2	1.88	0.55
4:A:1053:ASP:OD2	4:A:1580:ARG:NH2	2.38	0.55
10:G:139:ILE:HG12	17:O:182:MET:HE1	1.89	0.55
20:R:294:VAL:H	20:R:298:GLN:HE21	1.54	0.55
5:B:1014:TYR:OH	6:C:293:ARG:NH1	2.36	0.55
2:U:26:DA:H8	3:M:387:SER:HG	1.47	0.55
19:S:290:GLU:OE2	19:S:290:GLU:HA	2.07	0.55
19:S:362:ARG:HB3	19:S:375:PHE:HB2	1.87	0.55
18:Q:92:PHE:CD1	18:Q:205:ILE:HG23	2.41	0.54
6:C:257:GLY:HA3	6:C:268:LYS:HE2	1.89	0.54
18:Q:204:ARG:NH1	18:Q:212:VAL:HG21	2.23	0.54
2:U:54:DG:H1'	5:B:513:LYS:HZ1	1.72	0.54
16:N:56:ILE:HG22	16:N:137:PHE:HB2	1.90	0.54
19:S:407:ARG:HH11	19:S:411:LYS:HG2	1.71	0.54
4:A:1449:ALA:O	4:A:1453:HIS:ND1	2.37	0.54
18:Q:182:ILE:HD12	18:Q:185:ILE:HD11	1.89	0.54
19:S:215:ASN:HB2	19:S:233:VAL:HB	1.90	0.54
2:U:26:DA:C8	3:M:387:SER:OG	2.61	0.54
4:A:438:ILE:HA	4:A:456:VAL:HG22	1.90	0.54
17:O:337:THR:HG23	17:O:605:LEU:HD11	1.89	0.54
19:S:423:ILE:HD13	20:R:141:TRP:HZ2	1.72	0.54
19:S:450:ARG:HH11	19:S:450:ARG:CG	2.12	0.54
19:S:174:TRP:CD1	20:R:198:LEU:HD13	2.43	0.54
4:A:1179:ILE:HD11	4:A:1183:GLU:HG2	1.90	0.53
5:B:894:LYS:HG2	15:L:54:ARG:HH22	1.72	0.53
4:A:4:SER:OG	4:A:576:LYS:NZ	2.39	0.53
4:A:874:GLU:OE2	4:A:878:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:167:SER:OG	5:B:168:ASN:N	2.41	0.53
19:S:300:LEU:HA	19:S:320:ILE:HA	1.90	0.53
4:A:747:ILE:HG22	4:A:774:GLY:HA2	1.90	0.53
18:Q:302:ALA:HA	18:Q:305:ARG:HE	1.72	0.53
4:A:435:ASN:ND2	4:A:442:LYS:O	2.42	0.53
10:G:158:LYS:NZ	17:O:108:GLU:OE1	2.40	0.53
20:R:8:LEU:HD21	20:R:202:THR:HG22	1.90	0.53
5:B:37:LEU:HD12	5:B:759:ASP:HB3	1.91	0.53
18:Q:351:ASN:ND2	18:Q:373:GLU:OE2	2.41	0.53
17:O:109:SER:O	17:O:113:THR:OG1	2.27	0.53
20:R:4:VAL:HG11	20:R:214:VAL:HG22	1.89	0.53
5:B:429:ARG:HA	5:B:432:ILE:HG12	1.91	0.53
6:C:87:ASN:ND2	6:C:201:GLU:OE2	2.40	0.53
1:T:8:DA:O5'	1:T:8:DA:H8	1.92	0.52
4:A:1274:GLU:OE2	4:A:1288:ARG:NH2	2.42	0.52
5:B:1014:TYR:HE2	6:C:228:ARG:HA	1.75	0.52
18:Q:177:TYR:OH	18:Q:248:SER:O	2.27	0.52
1:T:11:DG:H2''	1:T:12:DC:H5'	1.91	0.52
5:B:412:ILE:HG23	5:B:461:MET:HE1	1.89	0.52
18:Q:21:ARG:NH1	18:Q:24:ASP:OD1	2.41	0.52
20:R:313:LEU:HB3	20:R:367:ILE:HD13	1.90	0.52
1:T:37:DA:C2	2:U:35:DA:C2	2.98	0.52
5:B:534:PRO:HG3	5:B:542:LEU:HD23	1.92	0.52
17:O:71:ILE:HG23	17:O:115:LEU:HD23	1.91	0.52
12:I:80:ALA:O	12:I:95:ASN:ND2	2.40	0.52
4:A:1124:LEU:HD22	4:A:1129:PRO:HG3	1.92	0.52
4:A:1291:VAL:HG22	4:A:1473:LYS:HG2	1.91	0.52
8:E:4:GLU:O	8:E:8:ASN:ND2	2.41	0.52
5:B:91:LEU:HD21	5:B:342:PRO:HB2	1.90	0.52
5:B:142:LYS:HG3	5:B:153:PHE:HE1	1.74	0.52
10:G:149:ILE:HB	10:G:153:PHE:HB2	1.92	0.52
18:Q:103:LEU:HD13	18:Q:106:LYS:HE3	1.91	0.52
19:S:243:LYS:NZ	19:S:299:ASP:OD2	2.43	0.52
19:S:269:PHE:HB3	19:S:292:LEU:HG	1.92	0.52
4:A:248:PHE:HD2	4:A:442:LYS:HG3	1.74	0.52
4:A:536:ILE:HG12	4:A:557:LEU:HD21	1.91	0.52
14:K:74:ASN:OD1	14:K:77:ARG:NH2	2.43	0.52
4:A:7:VAL:HG21	5:B:1177:ALA:HB2	1.91	0.52
4:A:772:LYS:NZ	11:H:138:GLU:OE2	2.43	0.52
4:A:939:ASN:HD22	5:B:958:MET:HE3	1.75	0.52
6:C:157:TYR:HB2	6:C:160:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1662:ASN:HB3	10:G:57:PRO:HD2	1.92	0.52
13:J:45:CYS:SG	13:J:46:CYS:N	2.83	0.52
18:Q:295:THR:O	18:Q:295:THR:OG1	2.27	0.52
19:S:355:GLU:HB2	20:R:24:ILE:HG23	1.91	0.52
19:S:476:ILE:HG22	19:S:497:VAL:H	1.74	0.52
5:B:1105:ARG:NH2	5:B:1172:GLU:OE1	2.43	0.52
20:R:5:PRO:HB3	20:R:248:LYS:HB2	1.92	0.52
3:M:212:GLU:HA	3:M:215:PHE:HD2	1.75	0.51
5:B:1090:ASP:HA	5:B:1094:ASN:HB2	1.91	0.51
4:A:878:ARG:NH1	12:I:66:VAL:O	2.44	0.51
4:A:259:LYS:O	4:A:262:THR:OG1	2.27	0.51
18:Q:94:LYS:NZ	18:Q:207:LEU:O	2.33	0.51
3:M:345:GLU:HG2	3:M:348:PRO:HD2	1.92	0.51
19:S:175:ASP:OD1	20:R:195:LEU:CD2	2.58	0.51
19:S:360:TRP:CD1	19:S:360:TRP:C	2.88	0.51
4:A:944:MET:O	4:A:985:ARG:NH1	2.44	0.51
5:B:100:GLU:OE2	5:B:140:LYS:NZ	2.44	0.51
14:K:67:GLU:HA	14:K:99:ASN:HB3	1.92	0.51
18:Q:198:ILE:HG13	18:Q:199:LEU:HG	1.91	0.51
18:Q:9:ILE:HG22	18:Q:16:PRO:HA	1.93	0.51
3:M:88:ILE:HD12	3:M:90:LEU:HD21	1.91	0.51
5:B:202:LEU:HD23	5:B:488:ALA:HB2	1.92	0.51
13:J:10:CYS:SG	13:J:11:GLY:N	2.83	0.51
18:Q:514:ASN:ND2	19:S:585:GLU:OE2	2.44	0.51
19:S:184:SER:N	19:S:509:GLU:OE2	2.43	0.51
1:T:17:DG:N2	2:U:54:DG:N2	2.59	0.51
2:U:60:DC:H2"	2:U:61:DA:C8	2.46	0.51
4:A:1221:ARG:HH12	4:A:1233:ILE:HG12	1.75	0.51
17:O:205:ARG:HG2	17:O:331:LYS:HG2	1.91	0.51
17:O:390:GLN:HE21	17:O:433:LYS:H	1.59	0.51
14:K:62:SER:OG	14:K:104:ARG:NH1	2.40	0.50
17:O:200:ASN:ND2	17:O:202:ASN:OD1	2.44	0.50
5:B:785:ASP:OD1	5:B:957:ARG:NH2	2.43	0.50
18:Q:154:LEU:HD23	18:Q:154:LEU:N	2.26	0.50
19:S:269:PHE:HZ	19:S:303:VAL:HG21	1.76	0.50
5:B:1021:GLU:OE2	6:C:295:ARG:NH2	2.44	0.50
6:C:80:ALA:HA	6:C:208:CYS:HA	1.94	0.50
1:T:39:DT:N3	2:U:33:DG:N2	2.60	0.50
4:A:1105:ARG:NH2	4:A:1142:ASP:OD1	2.45	0.50
10:G:62:MET:HA	10:G:66:LEU:HB2	1.94	0.50
19:S:244:SER:HB3	19:S:264:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:504:THR:O	19:S:542:ARG:N	2.42	0.50
5:B:300:SER:HB3	12:I:49:THR:HG22	1.93	0.50
5:B:417:ILE:HG22	5:B:457:ILE:HD13	1.92	0.50
12:I:15:ASP:OD2	12:I:32:GLN:NE2	2.44	0.50
19:S:380:MET:HE2	19:S:394:VAL:HG23	1.94	0.50
1:T:39:DT:C2	2:U:33:DG:N2	2.79	0.50
18:Q:171:HIS:ND1	18:Q:244:ASN:OD1	2.44	0.50
4:A:648:LEU:O	4:A:652:ASN:ND2	2.44	0.50
17:O:201:LYS:HG3	17:O:240:ILE:HG13	1.93	0.50
9:F:72:LYS:HB3	9:F:142:SER:HA	1.94	0.50
17:O:200:ASN:ND2	18:Q:14:ASN:O	2.45	0.50
17:O:392:GLN:HB2	17:O:395:LEU:HD13	1.93	0.50
18:Q:178:THR:HA	18:Q:181:TYR:HB2	1.94	0.50
4:A:30:LYS:NZ	5:B:1129:ARG:CZ	2.74	0.50
5:B:341:SER:OG	5:B:343:ASP:OD1	2.28	0.50
5:B:898:LEU:HB3	15:L:46:VAL:HG21	1.94	0.50
8:E:100:ILE:HG23	8:E:105:PHE:HB2	1.93	0.50
13:J:8:PHE:H	13:J:49:MET:HE1	1.75	0.50
17:O:379:ARG:HA	17:O:382:GLN:HE22	1.76	0.50
19:S:189:THR:HA	19:S:259:ASN:HD22	1.76	0.50
19:S:323:ASN:HA	19:S:350:THR:HA	1.92	0.50
2:U:57:DA:H2'	2:U:58:DA:C8	2.46	0.49
4:A:58:LEU:HD22	18:Q:70:PHE:HD1	1.75	0.49
18:Q:92:PHE:CE1	18:Q:205:ILE:HG21	2.45	0.49
19:S:407:ARG:HA	19:S:414:ILE:HG23	1.94	0.49
4:A:799:GLU:OE2	4:A:1173:LYS:NZ	2.35	0.49
4:A:1246:VAL:O	4:A:1517:ARG:NH2	2.41	0.49
5:B:335:ARG:NH2	5:B:341:SER:O	2.45	0.49
5:B:402:VAL:O	5:B:647:SER:OG	2.25	0.49
4:A:952:LEU:HD12	4:A:957:VAL:HA	1.93	0.49
19:S:438:TRP:CD1	19:S:489:PHE:HB2	2.46	0.49
18:Q:439:ILE:HG22	19:S:704:LEU:HD22	1.93	0.49
6:C:53:ASN:ND2	16:N:173:THR:O	2.45	0.49
18:Q:262:LEU:HD13	18:Q:266:PHE:HB2	1.94	0.49
19:S:421:ILE:HA	19:S:441:ASP:HA	1.93	0.49
4:A:938:VAL:HG11	12:I:98:THR:HG21	1.95	0.49
19:S:31:ASN:O	19:S:32:TYR:CG	2.66	0.49
4:A:1447:GLN:HE21	4:A:1459:LYS:HA	1.77	0.49
5:B:129:ARG:HB2	15:L:55:ILE:HD11	1.95	0.49
5:B:568:LEU:HD23	5:B:604:ILE:HG12	1.94	0.49
18:Q:203:TRP:CD1	18:Q:203:TRP:N	2.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:26:TYR:HB3	19:S:28:PRO:HD3	1.94	0.49
4:A:83:VAL:HG11	4:A:427:PHE:HE1	1.77	0.49
4:A:1038:ILE:HD11	4:A:1050:TYR:HB2	1.95	0.49
18:Q:104:PHE:CE1	18:Q:211:TYR:HD1	2.29	0.49
5:B:204:ARG:HH21	5:B:486:VAL:HG11	1.78	0.48
12:I:98:THR:HG22	12:I:110:VAL:HG22	1.95	0.48
17:O:440:ILE:O	17:O:444:SER:N	2.41	0.48
2:U:26:DA:H8	3:M:387:SER:OG	1.95	0.48
3:M:192:ASN:HB3	3:M:201:ILE:HA	1.94	0.48
4:A:480:ALA:HB2	5:B:1046:VAL:HG23	1.94	0.48
5:B:1025:ASP:OD2	6:C:277:ARG:NH1	2.46	0.48
18:Q:75:LEU:HD22	18:Q:79:GLN:HG3	1.95	0.48
19:S:746:ARG:HH22	19:S:749:LYS:HD2	1.77	0.48
3:M:271:VAL:HG21	3:M:298:ILE:HG21	1.95	0.48
4:A:1307:ASP:HB3	4:A:1499:ARG:HH12	1.78	0.48
5:B:807:GLU:OE1	5:B:905:TYR:OH	2.26	0.48
19:S:322:GLY:O	19:S:350:THR:OG1	2.26	0.48
19:S:444:PRO:HA	20:R:2:PHE:HA	1.94	0.48
1:T:37:DA:C2	2:U:34:DT:N3	2.81	0.48
4:A:602:GLY:N	4:A:651:ALA:O	2.46	0.48
4:A:739:VAL:HG11	4:A:812:VAL:HG21	1.95	0.48
4:A:1053:ASP:OD1	4:A:1053:ASP:N	2.45	0.48
11:H:93:TYR:HE1	11:H:145:ARG:HH11	1.62	0.48
20:R:13:PHE:HA	20:R:16:ARG:HG2	1.96	0.48
4:A:621:THR:OG1	4:A:626:ALA:O	2.31	0.48
5:B:247:THR:OG1	5:B:477:ASP:OD1	2.28	0.48
5:B:698:SER:OG	5:B:699:ILE:N	2.46	0.48
4:A:1033:SER:OG	4:A:1034:TYR:N	2.45	0.48
17:O:63:LEU:HD22	17:O:106:ARG:HA	1.96	0.48
18:Q:264:PRO:HD3	19:S:722:TRP:CD1	2.49	0.48
4:A:718:THR:HG21	11:H:119:GLY:HA3	1.96	0.48
4:A:891:ILE:HD12	12:I:71:LEU:HG	1.96	0.48
5:B:219:ARG:HG2	5:B:221:SER:H	1.79	0.48
5:B:883:GLU:OE1	5:B:906:ARG:NH1	2.37	0.48
19:S:450:ARG:CG	19:S:450:ARG:NH1	2.73	0.48
20:R:187:TYR:HE1	20:R:197:PRO:HB3	1.79	0.48
3:M:216:ILE:HD11	3:M:294:LEU:HD11	1.95	0.48
4:A:30:LYS:NZ	5:B:1129:ARG:NH2	2.60	0.48
5:B:258:VAL:HG12	5:B:273:VAL:HG21	1.95	0.48
4:A:339:PHE:HE1	4:A:1627:LEU:HD22	1.79	0.48
4:A:342:ARG:NH1	4:A:1629:ASN:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:786:ALA:HB1	5:B:928:SER:HB2	1.96	0.48
7:D:25:THR:OG1	9:F:59:GLN:OE1	2.32	0.48
5:B:1061:LYS:O	5:B:1065:ARG:NH1	2.47	0.48
10:G:152:ALA:HA	17:O:184:PRO:HG2	1.96	0.48
19:S:21:GLN:OE1	19:S:24:SER:OG	2.28	0.48
5:B:963:PHE:O	5:B:1027:TYR:OH	2.31	0.47
5:B:1006:ASN:HD22	5:B:1010:ASN:HB2	1.79	0.47
17:O:219:ARG:HH22	17:O:360:VAL:HG22	1.78	0.47
18:Q:192:TYR:C	18:Q:192:TYR:CD2	2.92	0.47
19:S:505:PRO:HA	19:S:541:LEU:HA	1.94	0.47
4:A:943:ILE:HG12	5:B:960:ILE:HD11	1.95	0.47
5:B:291:GLY:HA3	5:B:375:LEU:HD13	1.95	0.47
5:B:750:PRO:HG2	5:B:753:LYS:HB3	1.96	0.47
5:B:1065:ARG:NH2	18:Q:43:ASP:O	2.47	0.47
18:Q:193:PHE:CZ	18:Q:220:SER:HB3	2.48	0.47
20:R:122:ASP:CB	20:R:125:ARG:CD	2.87	0.47
20:R:247:ILE:HA	20:R:250:LEU:HD12	1.96	0.47
16:N:117:GLU:HG2	16:N:118:SER:H	1.79	0.47
18:Q:232:LEU:CD2	18:Q:232:LEU:N	2.76	0.47
4:A:195:LYS:NZ	4:A:199:ASP:OD2	2.47	0.47
6:C:136:LEU:HB3	6:C:204:LEU:HG	1.97	0.47
7:D:6:ARG:O	7:D:10:ASN:N	2.47	0.47
3:M:203:PRO:HG2	3:M:206:SER:HB3	1.97	0.47
4:A:939:ASN:HA	5:B:958:MET:HE2	1.95	0.47
4:A:1270:VAL:HG11	4:A:1489:VAL:HG11	1.97	0.47
5:B:296:ASP:HB3	5:B:299:ASP:HB2	1.96	0.47
17:O:403:LEU:HD22	17:O:424:LEU:HD13	1.97	0.47
18:Q:144:ILE:HD12	18:Q:154:LEU:CB	2.41	0.47
18:Q:154:LEU:N	18:Q:154:LEU:CD2	2.78	0.47
18:Q:284:LEU:HD13	18:Q:306:VAL:HG22	1.97	0.47
19:S:360:TRP:CE3	19:S:377:ARG:NH2	2.80	0.47
19:S:511:ILE:HD11	19:S:538:LEU:HD23	1.95	0.47
4:A:589:MET:HG3	4:A:633:MET:HE2	1.97	0.47
5:B:815:ARG:NH2	5:B:899:GLN:OE1	2.47	0.47
5:B:1091:ARG:HA	5:B:1091:ARG:HD3	1.61	0.47
5:B:934:ILE:H	5:B:934:ILE:HG13	1.54	0.46
12:I:91:ASN:ND2	12:I:115:THR:OG1	2.48	0.46
3:M:290:PRO:HB2	3:M:295:VAL:HG21	1.96	0.46
3:M:116:LYS:HE3	3:M:118:ASP:HB3	1.97	0.46
4:A:834:ARG:HH21	5:B:993:ALA:HB1	1.80	0.46
5:B:921:HIS:NE2	5:B:965:GLU:OE1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:450:ARG:HG2	19:S:450:ARG:NH1	2.17	0.46
19:S:406:LYS:HD3	19:S:453:VAL:H	1.80	0.46
20:R:137:SER:OG	20:R:139:GLU:O	2.31	0.46
4:A:551:VAL:HG12	4:A:554:ARG:HH21	1.80	0.46
17:O:314:THR:HG22	18:Q:5:ILE:HG22	1.96	0.46
5:B:492:ASN:ND2	5:B:725:THR:OG1	2.49	0.46
13:J:9:SER:HB2	13:J:45:CYS:HB2	1.97	0.46
4:A:316:LEU:HD23	4:A:318:THR:H	1.81	0.46
5:B:286:ARG:HH12	12:I:4:VAL:HG21	1.80	0.46
17:O:97:LEU:HD22	17:O:135:LYS:HG2	1.96	0.46
18:Q:439:ILE:HD12	19:S:717:LYS:HE2	1.97	0.46
19:S:270:GLN:HG3	19:S:291:PRO:HB3	1.98	0.46
4:A:73:PRO:O	4:A:366:ARG:NH2	2.49	0.46
4:A:1634:LEU:HD13	4:A:1643:VAL:HG11	1.98	0.46
8:E:3:GLN:HB2	8:E:7:ARG:HH12	1.80	0.46
19:S:18:VAL:HG21	20:R:366:PHE:CZ	2.51	0.46
19:S:507:GLY:O	19:S:540:LYS:N	2.48	0.46
19:S:583:GLU:HA	19:S:586:LYS:HB2	1.97	0.46
12:I:37:TYR:HD1	12:I:39:LYS:HE2	1.80	0.46
18:Q:92:PHE:HB3	18:Q:205:ILE:HG23	1.97	0.46
19:S:532:GLU:HA	19:S:554:ASN:HB3	1.97	0.46
1:T:17:DG:N1	2:U:53:DA:H2	2.09	0.46
5:B:190:ILE:HD13	5:B:496:PHE:HE2	1.80	0.46
6:C:216:HIS:HD2	6:C:218:LYS:H	1.64	0.46
10:G:133:LEU:HD13	10:G:149:ILE:HD13	1.98	0.46
4:A:481:ARG:HH21	4:A:632:GLU:HB2	1.81	0.45
8:E:93:MET:HG3	8:E:120:ALA:HB1	1.98	0.45
3:M:31:ARG:HG3	12:I:11:LEU:HB3	1.98	0.45
3:M:261:LEU:O	3:M:265:LEU:N	2.48	0.45
4:A:216:ARG:NH2	4:A:338:VAL:O	2.49	0.45
5:B:906:ARG:HD2	6:C:93:GLN:HG2	1.98	0.45
4:A:124:LEU:HD22	4:A:129:LEU:HD11	1.99	0.45
4:A:215:GLU:OE2	8:E:177:ARG:NH2	2.40	0.45
4:A:1641:ILE:HD11	5:B:1088:LEU:HD21	1.97	0.45
10:G:134:GLU:OE2	10:G:230:ARG:NE	2.46	0.45
18:Q:245:SER:HB2	18:Q:286:LEU:HB3	1.98	0.45
20:R:415:LEU:HD11	20:R:426:VAL:HG21	1.98	0.45
3:M:221:ILE:HG23	3:M:230:LYS:HG3	1.99	0.45
4:A:77:GLY:O	4:A:362:VAL:N	2.40	0.45
5:B:1103:VAL:HG22	5:B:1110:ILE:HG12	1.98	0.45
10:G:234:ARG:HB2	10:G:248:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:360:TRP:CD1	19:S:360:TRP:O	2.70	0.45
2:U:61:DA:O5'	2:U:61:DA:H8	1.99	0.45
4:A:982:VAL:HG12	4:A:984:GLY:H	1.81	0.45
4:A:1556:GLU:OE1	8:E:200:ARG:NH1	2.50	0.45
5:B:532:HIS:ND1	5:B:719:CYS:HB3	2.31	0.45
6:C:136:LEU:HB2	6:C:167:LEU:HD23	1.99	0.45
18:Q:98:HIS:O	18:Q:98:HIS:CG	2.70	0.45
2:U:59:DG:OP1	4:A:221:HIS:CE1	2.66	0.45
4:A:925:MET:HE1	5:B:955:PRO:HA	1.97	0.45
6:C:115:TRP:HH2	6:C:212:ILE:HG23	1.82	0.45
4:A:1121:ASP:OD1	4:A:1121:ASP:N	2.49	0.45
5:B:1119:ARG:NH2	5:B:1160:GLU:OE2	2.49	0.45
7:D:30:HIS:HA	10:G:39:VAL:HG23	1.99	0.45
12:I:29:GLU:HA	12:I:35:ALA:HB3	1.99	0.45
17:O:97:LEU:HD11	17:O:136:TYR:HA	1.97	0.45
17:O:429:ALA:HB1	17:O:486:PHE:HD2	1.81	0.45
19:S:353:ASP:OD2	19:S:356:GLU:N	2.49	0.45
19:S:600:GLU:O	19:S:604:ILE:N	2.45	0.45
3:M:51:PHE:CD2	3:M:94:PRO:HG3	2.52	0.45
4:A:495:ILE:HG12	4:A:589:MET:HE3	1.99	0.45
4:A:555:LYS:O	4:A:559:ASN:ND2	2.49	0.45
4:A:588:LEU:HD13	4:A:600:MET:HE2	1.98	0.45
18:Q:442:LEU:HD23	18:Q:445:ARG:HD2	1.98	0.45
19:S:360:TRP:CB	19:S:377:ARG:NH2	2.79	0.45
1:T:12:DC:H2''	1:T:13:DT:H5''	1.99	0.45
4:A:1240:LEU:HB3	4:A:1536:ILE:HD12	1.98	0.45
5:B:584:CYS:HB3	5:B:596:VAL:HG23	1.99	0.45
5:B:731:VAL:HG21	13:J:59:LYS:HG2	1.99	0.45
16:N:78:THR:OG1	16:N:89:ILE:O	2.31	0.45
20:R:358:PHE:HB2	20:R:364:VAL:HG21	1.99	0.45
20:R:5:PRO:HA	20:R:248:LYS:HD2	1.98	0.45
20:R:7:THR:HG23	20:R:292:SER:HB3	1.98	0.45
20:R:135:GLU:OE2	20:R:301:SER:OG	2.34	0.45
1:T:11:DG:OP2	1:T:11:DG:C8	2.70	0.44
4:A:461:GLU:HG2	4:A:1618:THR:HB	2.00	0.44
5:B:216:ALA:HB2	5:B:380:LYS:HD3	1.99	0.44
10:G:134:GLU:HG2	10:G:230:ARG:HA	1.99	0.44
16:N:89:ILE:HG13	16:N:139:VAL:HG22	1.98	0.44
4:A:255:ALA:HB2	4:A:311:GLY:HA2	2.00	0.44
19:S:768:TYR:HA	19:S:771:ILE:HG12	1.98	0.44
20:R:251:TRP:HA	20:R:270:PHE:HE2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:852:ASP:OD1	4:A:855:ARG:NH2	2.51	0.44
4:A:1128:ASN:HB3	4:A:1131:LYS:HB3	1.99	0.44
4:A:1490:GLU:OE2	12:I:51:THR:OG1	2.33	0.44
8:E:21:GLU:OE1	8:E:143:ASN:ND2	2.43	0.44
10:G:219:ASP:OD1	10:G:223:GLU:N	2.43	0.44
18:Q:158:MET:HB3	18:Q:192:TYR:CE1	2.52	0.44
18:Q:282:ARG:HA	18:Q:282:ARG:NE	2.32	0.44
4:A:672:ASP:HB3	5:B:783:MET:HE1	1.98	0.44
12:I:114:CYS:SG	12:I:115:THR:N	2.90	0.44
4:A:527:PRO:HB3	4:A:534:THR:HA	1.98	0.44
5:B:935:ASP:OD1	5:B:935:ASP:N	2.41	0.44
9:F:69:LEU:HD23	10:G:94:PRO:HG3	1.98	0.44
19:S:261:VAL:HG13	19:S:272:PHE:HB2	1.98	0.44
3:M:75:GLN:HG3	16:N:58:PHE:HB2	2.00	0.44
4:A:1238:MET:HB3	4:A:1521:THR:HB	2.00	0.44
17:O:311:MET:HB3	18:Q:6:ARG:HG2	1.99	0.44
17:O:361:PHE:HZ	17:O:399:PHE:HB2	1.82	0.44
19:S:68:THR:HG23	19:S:207:SER:HB3	1.98	0.44
5:B:647:SER:OG	5:B:647:SER:O	2.34	0.44
5:B:664:VAL:HG21	5:B:672:MET:HE1	2.00	0.44
10:G:218:VAL:HG13	10:G:222:GLY:HA2	1.98	0.44
17:O:194:LEU:HD21	17:O:218:LEU:HD23	2.00	0.44
4:A:550:SER:OG	4:A:551:VAL:N	2.51	0.44
5:B:204:ARG:NH1	5:B:502:MET:SD	2.91	0.44
18:Q:219:ILE:HG22	20:R:206:ARG:O	2.18	0.44
3:M:252:GLN:HG3	3:M:254:SER:H	1.83	0.44
3:M:346:ILE:HD13	3:M:393:LYS:HB2	2.00	0.44
4:A:37:VAL:HG12	4:A:49:LEU:HB2	2.00	0.44
5:B:107:PRO:HB2	5:B:121:VAL:HG13	1.99	0.44
5:B:543:ASN:OD1	5:B:543:ASN:N	2.51	0.44
5:B:893:ASN:N	5:B:893:ASN:HD22	2.15	0.44
11:H:40:LEU:HG	11:H:42:ILE:HG23	2.00	0.44
19:S:264:ILE:HG23	19:S:300:LEU:HD21	2.00	0.44
19:S:319:ASP:HB2	19:S:363:ILE:HG12	1.99	0.44
19:S:699:LEU:HD22	19:S:744:LEU:HD21	1.98	0.44
4:A:30:LYS:HZ1	5:B:1129:ARG:CZ	2.31	0.43
10:G:234:ARG:HG2	10:G:235:ASN:H	1.82	0.43
18:Q:278:GLU:OE2	18:Q:284:LEU:HD23	2.18	0.43
19:S:390:GLN:N	20:R:150:GLN:O	2.51	0.43
3:M:24:GLY:N	16:N:108:THR:O	2.51	0.43
3:M:321:ASP:OD1	3:M:321:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:32:ILE:HD12	4:A:362:VAL:HG21	1.99	0.43
4:A:335:LEU:HD23	4:A:335:LEU:HA	1.87	0.43
4:A:741:PRO:HA	4:A:742:PRO:HD3	1.86	0.43
4:A:831:ASP:N	4:A:831:ASP:OD1	2.50	0.43
4:A:1256:LYS:O	4:A:1499:ARG:NH2	2.51	0.43
18:Q:208:PRO:HD2	18:Q:211:TYR:HB2	2.00	0.43
19:S:248:PRO:HB3	19:S:305:PHE:HB2	1.99	0.43
19:S:657:SER:HA	19:S:748:GLU:HB2	2.00	0.43
4:A:213:ASN:ND2	4:A:1606:SER:O	2.52	0.43
6:C:259:ASP:HB3	6:C:263:ASP:HB3	2.00	0.43
7:D:6:ARG:HD2	17:O:196:LYS:HE3	2.00	0.43
18:Q:180:ASP:OD1	18:Q:255:LYS:NZ	2.51	0.43
19:S:421:ILE:HG13	19:S:441:ASP:HA	1.99	0.43
1:T:36:DT:H3	2:U:35:DA:N6	2.17	0.43
4:A:471:MET:HE1	5:B:1185:LEU:HD22	1.99	0.43
4:A:526:GLY:HA3	4:A:554:ARG:NH1	2.33	0.43
5:B:28:PRO:HA	5:B:29:PRO:HD3	1.93	0.43
5:B:547:HIS:CE1	5:B:548:LYS:HE3	2.53	0.43
10:G:149:ILE:N	10:G:153:PHE:O	2.49	0.43
4:A:487:ASP:HB2	4:A:615:ARG:HG2	2.00	0.43
5:B:714:ARG:HD3	5:B:714:ARG:HA	1.77	0.43
17:O:119:ILE:O	17:O:136:TYR:OH	2.30	0.43
1:T:45:DT:O4	2:U:26:DA:N1	2.50	0.43
2:U:59:DG:H2'	2:U:59:DG:O5'	2.18	0.43
4:A:368:ARG:HH11	4:A:383:ASN:HD21	1.66	0.43
4:A:563:THR:HG22	17:O:375:THR:HG22	2.00	0.43
8:E:76:GLY:N	8:E:106:GLN:OE1	2.51	0.43
18:Q:103:LEU:HG	18:Q:207:LEU:HD13	2.00	0.43
18:Q:207:LEU:HD12	18:Q:207:LEU:HA	1.81	0.43
18:Q:413:LEU:HD21	20:R:240:ILE:HD12	2.00	0.43
1:T:36:DT:C2	2:U:35:DA:N1	2.86	0.43
4:A:743:ASP:OD1	4:A:743:ASP:N	2.52	0.43
5:B:156:ARG:HH12	5:B:446:MET:HE2	1.84	0.43
5:B:823:GLN:HA	5:B:863:ASP:HA	2.01	0.43
18:Q:154:LEU:CD2	18:Q:154:LEU:H	2.32	0.43
19:S:362:ARG:NH1	19:S:363:ILE:O	2.52	0.43
4:A:677:GLY:O	4:A:681:THR:OG1	2.25	0.43
4:A:855:ARG:O	4:A:859:ALA:N	2.45	0.43
4:A:1613:MET:HB3	4:A:1618:THR:HG23	2.00	0.43
5:B:17:ARG:HB3	5:B:20:GLU:HB3	2.00	0.43
5:B:218:ILE:HG23	5:B:391:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:8:ASN:OD1	8:E:11:ARG:NH2	2.51	0.43
12:I:102:ARG:HB2	12:I:106:GLU:HB3	1.99	0.43
14:K:46:LYS:HA	14:K:66:VAL:HG22	1.99	0.43
17:O:113:THR:HA	17:O:116:ILE:HD12	1.99	0.43
18:Q:193:PHE:HZ	18:Q:220:SER:CB	2.30	0.43
19:S:665:ASN:ND2	19:S:668:SER:OG	2.50	0.43
20:R:135:GLU:HG3	20:R:284:PHE:CD2	2.54	0.43
5:B:232:TYR:CD2	5:B:385:VAL:HG12	2.53	0.43
17:O:340:SER:HA	17:O:343:VAL:HG12	2.01	0.43
4:A:58:LEU:HD23	18:Q:69:SER:HA	2.01	0.43
4:A:1543:SER:OG	4:A:1544:ASN:N	2.51	0.43
18:Q:282:ARG:HG3	18:Q:283:ASN:OD1	2.19	0.43
18:Q:282:ARG:HA	18:Q:282:ARG:HE	1.83	0.43
18:Q:431:ASP:OD2	18:Q:434:HIS:ND1	2.52	0.43
19:S:31:ASN:O	19:S:32:TYR:CD1	2.72	0.43
19:S:221:ARG:NH2	19:S:549:TYR:OH	2.52	0.43
20:R:362:ALA:HB2	20:R:421:LYS:HB2	2.01	0.43
5:B:657:PRO:HD3	16:N:148:ILE:HG12	2.00	0.42
10:G:37:CYS:O	10:G:126:GLN:N	2.44	0.42
3:M:198:VAL:HA	3:M:201:ILE:HG12	2.01	0.42
17:O:436:ARG:HG2	17:O:490:ILE:HG23	2.01	0.42
17:O:521:ASN:HB2	17:O:589:GLN:HB3	2.01	0.42
18:Q:253:LEU:O	18:Q:257:VAL:N	2.49	0.42
2:U:53:DA:H5'	5:B:512:LEU:HD22	2.02	0.42
6:C:91:VAL:HG11	13:J:60:PHE:HB3	2.00	0.42
7:D:5:SER:O	7:D:8:THR:OG1	2.32	0.42
15:L:41:SER:OG	15:L:44:ASP:OD2	2.30	0.42
16:N:92:ASP:OD1	16:N:92:ASP:N	2.51	0.42
18:Q:172:LEU:HD23	18:Q:174:LEU:HD11	2.01	0.42
18:Q:205:ILE:HD13	18:Q:205:ILE:O	2.20	0.42
4:A:59:ARG:HG3	18:Q:69:SER:HB3	2.01	0.42
12:I:117:CYS:SG	12:I:118:GLY:N	2.92	0.42
14:K:88:PHE:HB3	14:K:106:GLN:HB2	2.02	0.42
19:S:264:ILE:HG12	19:S:300:LEU:HD11	2.02	0.42
19:S:408:ILE:HD11	19:S:415:LEU:HB2	2.00	0.42
20:R:125:ARG:HH11	20:R:125:ARG:CG	2.23	0.42
20:R:268:LEU:HD11	20:R:316:SER:HB3	2.01	0.42
9:F:86:THR:O	9:F:88:TYR:N	2.48	0.42
10:G:160:ASN:H	17:O:105:ASN:HD21	1.68	0.42
20:R:122:ASP:HB2	20:R:125:ARG:CD	2.45	0.42
6:C:322:LYS:NZ	6:C:326:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:44:TYR:HA	13:J:47:ARG:HB3	2.02	0.42
17:O:389:SER:O	17:O:427:TYR:OH	2.37	0.42
18:Q:244:ASN:OD1	18:Q:244:ASN:N	2.52	0.42
3:M:166:ARG:NH2	4:A:400:ASN:O	2.52	0.42
5:B:979:GLN:HG2	5:B:996:PHE:HE1	1.85	0.42
5:B:1042:ASP:HA	5:B:1063:ARG:HH12	1.83	0.42
11:H:111:LEU:HD23	11:H:111:LEU:HA	1.92	0.42
17:O:150:TRP:O	17:O:154:VAL:N	2.49	0.42
18:Q:253:LEU:HA	18:Q:256:LEU:HB2	2.02	0.42
1:T:53:DG:N2	2:U:17:DA:N1	2.68	0.42
4:A:333:CYS:SG	4:A:334:VAL:N	2.93	0.42
4:A:427:PHE:HA	4:A:430:ILE:HG22	2.01	0.42
11:H:112:ILE:N	11:H:127:GLY:O	2.53	0.42
4:A:751:SER:OG	4:A:752:LYS:N	2.52	0.42
4:A:1009:THR:OG1	12:I:101:LEU:O	2.32	0.42
5:B:553:THR:O	5:B:646:HIS:ND1	2.35	0.42
5:B:655:TYR:CE2	5:B:657:PRO:HG2	2.55	0.42
8:E:19:VAL:HG11	8:E:80:VAL:HG11	2.01	0.42
8:E:124:VAL:HG13	8:E:132:ILE:HB	2.02	0.42
10:G:30:GLU:HG2	10:G:32:ASN:HB2	2.02	0.42
19:S:302:VAL:HG11	19:S:362:ARG:HD2	2.01	0.42
1:T:14:DT:H6	1:T:14:DT:H2'	1.72	0.41
16:N:123:SER:HA	16:N:131:LEU:HB2	2.02	0.41
18:Q:227:TYR:HB3	18:Q:301:HIS:CD2	2.54	0.41
19:S:187:ILE:HD11	19:S:259:ASN:HA	2.02	0.41
20:R:168:ILE:HG23	20:R:169:PRO:HD3	2.02	0.41
18:Q:157:HIS:O	18:Q:160:SER:N	2.36	0.41
20:R:25:ASN:ND2	20:R:123:GLU:OE1	2.53	0.41
1:T:31:DC:H42	2:U:40:DG:H1	1.67	0.41
4:A:630:GLY:HA3	5:B:916:LYS:HE2	2.02	0.41
4:A:1501:ILE:HG23	4:A:1504:ILE:HB	2.01	0.41
5:B:137:LEU:HD22	5:B:161:LEU:HD23	2.02	0.41
5:B:617:THR:HG22	5:B:619:GLY:H	1.84	0.41
1:T:32:DC:O2	5:B:817:ARG:NH1	2.53	0.41
3:M:45:LYS:NZ	3:M:48:LYS:O	2.53	0.41
4:A:6:PRO:HG3	10:G:113:PHE:CD2	2.55	0.41
4:A:1266:VAL:HG21	4:A:1313:LEU:HD21	2.02	0.41
5:B:318:PRO:O	5:B:321:GLN:NE2	2.53	0.41
17:O:332:LEU:HD23	17:O:599:LEU:HD11	2.01	0.41
19:S:269:PHE:CZ	19:S:303:VAL:HG21	2.55	0.41
4:A:1072:ASN:O	4:A:1076:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:567:SER:OG	16:N:141:GLU:OE1	2.37	0.41
5:B:708:ASP:OD1	5:B:708:ASP:N	2.54	0.41
5:B:789:ILE:HG22	5:B:930:LYS:HA	2.02	0.41
13:J:48:ARG:HH12	13:J:49:MET:HE3	1.86	0.41
4:A:1291:VAL:HG22	4:A:1473:LYS:HE3	2.01	0.41
5:B:939:SER:OG	5:B:940:GLU:N	2.53	0.41
17:O:251:LEU:HA	17:O:598:PHE:HE1	1.85	0.41
18:Q:128:GLU:HB3	19:S:749:LYS:HE3	2.01	0.41
18:Q:134:LYS:O	18:Q:138:LEU:N	2.48	0.41
19:S:269:PHE:HD2	19:S:292:LEU:HD21	1.85	0.41
19:S:403:ARG:HE	19:S:419:ARG:HB3	1.86	0.41
20:R:236:PHE:CD1	20:R:253:ILE:HD11	2.56	0.41
1:T:8:DA:H2	2:U:63:DT:H3	1.69	0.41
1:T:36:DT:H3	2:U:35:DA:H61	1.69	0.41
3:M:329:LEU:HD23	3:M:332:ILE:HD12	2.02	0.41
4:A:31:GLN:HG2	4:A:78:HIS:CE1	2.56	0.41
5:B:1022:LEU:HD23	5:B:1026:ILE:HD11	2.03	0.41
18:Q:215:LEU:HD12	18:Q:215:LEU:HA	1.76	0.41
18:Q:341:ARG:NH1	18:Q:365:ASP:OD2	2.54	0.41
19:S:18:VAL:HG23	20:R:427:PRO:HD2	2.03	0.41
2:U:58:DA:H8	2:U:58:DA:O5'	2.04	0.41
4:A:95:TYR:CZ	4:A:99:ARG:HD2	2.56	0.41
4:A:862:THR:HG23	4:A:864:LEU:H	1.86	0.41
5:B:16:PHE:CD1	5:B:978:ALA:HB2	2.56	0.41
10:G:81:VAL:HA	10:G:124:VAL:HG12	2.02	0.41
10:G:154:ASN:ND2	17:O:182:MET:O	2.47	0.41
17:O:128:LEU:HD13	17:O:132:THR:HG22	2.03	0.41
20:R:124:GLU:O	20:R:127:PHE:N	2.53	0.41
20:R:251:TRP:HB3	20:R:274:MET:HE2	2.03	0.41
5:B:547:HIS:ND1	5:B:548:LYS:HG2	2.36	0.41
5:B:979:GLN:HG2	5:B:996:PHE:CE1	2.56	0.41
4:A:547:ILE:HB	18:Q:22:ILE:HD11	2.03	0.40
5:B:782:ASP:O	5:B:950:ASN:ND2	2.54	0.40
17:O:347:VAL:HG11	17:O:391:GLN:HG3	2.03	0.40
19:S:277:VAL:HG12	19:S:284:VAL:HA	2.02	0.40
1:T:17:DG:O6	2:U:53:DA:N1	2.54	0.40
4:A:744:MET:HG2	4:A:1078:LYS:HD2	2.03	0.40
4:A:1060:GLU:OE2	4:A:1580:ARG:NH1	2.54	0.40
5:B:625:GLU:HG2	5:B:643:PHE:HB2	2.03	0.40
8:E:128:PRO:HG2	8:E:129:PRO:HD3	2.03	0.40
8:E:157:SER:OG	8:E:160:GLU:OE1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:328:LEU:HD13	18:Q:472:ARG:HA	2.02	0.40
3:M:62:TYR:HB3	3:M:100:VAL:HA	2.02	0.40
4:A:252:PHE:HE1	4:A:314:TYR:HD1	1.69	0.40
4:A:379:GLU:OE1	18:Q:58:ARG:NE	2.52	0.40
5:B:156:ARG:CZ	5:B:450:LEU:HD22	2.52	0.40
5:B:1082:HIS:HB2	5:B:1084:THR:HG22	2.03	0.40
5:B:1133:MET:O	5:B:1168:VAL:N	2.39	0.40
18:Q:63:THR:HG21	18:Q:72:SER:HB3	2.03	0.40
18:Q:198:ILE:O	18:Q:201:LYS:NZ	2.45	0.40
19:S:366:PHE:HB2	19:S:373:LEU:HG	2.03	0.40
1:T:17:DG:C2	2:U:54:DG:N2	2.90	0.40
9:F:79:ARG:NH1	9:F:145:ASP:O	2.54	0.40
18:Q:348:ILE:HA	18:Q:351:ASN:HD22	1.86	0.40
18:Q:478:ARG:HD3	19:S:570:ASP:HB2	2.04	0.40
19:S:317:ILE:HG21	19:S:365:TRP:HE1	1.87	0.40
20:R:133:LYS:HA	20:R:134:PRO:HD3	1.90	0.40
4:A:986:PHE:HB3	5:B:960:ILE:HD12	2.02	0.40
4:A:990:ILE:HB	4:A:994:GLU:HG3	2.04	0.40
4:A:1316:VAL:HG21	4:A:1498:ILE:HG23	2.04	0.40
8:E:100:ILE:HA	8:E:105:PHE:HD2	1.85	0.40
9:F:86:THR:C	9:F:88:TYR:H	2.29	0.40
17:O:521:ASN:HB3	17:O:524:VAL:HG12	2.03	0.40
18:Q:102:LEU:HA	18:Q:102:LEU:HD12	1.89	0.40
19:S:672:ILE:O	19:S:676:SER:N	2.53	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	M	388/415 (94%)	356 (92%)	32 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1448/1664 (87%)	1368 (94%)	79 (6%)	1 (0%)	48	80
5	B	1174/1203 (98%)	1103 (94%)	71 (6%)	0	100	100
6	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
7	D	66/137 (48%)	62 (94%)	4 (6%)	0	100	100
8	E	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
9	F	98/155 (63%)	93 (95%)	4 (4%)	1 (1%)	12	45
10	G	193/326 (59%)	182 (94%)	11 (6%)	0	100	100
11	H	130/146 (89%)	117 (90%)	13 (10%)	0	100	100
12	I	122/125 (98%)	108 (88%)	14 (12%)	0	100	100
13	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
14	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
15	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
16	N	131/233 (56%)	114 (87%)	16 (12%)	1 (1%)	16	50
17	O	493/627 (79%)	453 (92%)	40 (8%)	0	100	100
18	Q	469/514 (91%)	415 (88%)	53 (11%)	1 (0%)	43	76
19	S	594/894 (66%)	517 (87%)	77 (13%)	0	100	100
20	R	322/507 (64%)	289 (90%)	32 (10%)	1 (0%)	36	70
All	All	6352/7778 (82%)	5874 (92%)	473 (7%)	5 (0%)	49	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	R	195	LEU
18	Q	283	ASN
4	A	1458	THR
9	F	87	LYS
16	N	118	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	350/371 (94%)	350 (100%)	0	100	100
4	A	1292/1465 (88%)	1290 (100%)	2 (0%)	87	92
5	B	1030/1053 (98%)	1022 (99%)	8 (1%)	73	86
6	C	269/296 (91%)	268 (100%)	1 (0%)	84	90
7	D	65/116 (56%)	64 (98%)	1 (2%)	57	80
8	E	197/197 (100%)	197 (100%)	0	100	100
9	F	90/137 (66%)	90 (100%)	0	100	100
10	G	177/291 (61%)	177 (100%)	0	100	100
11	H	116/128 (91%)	116 (100%)	0	100	100
12	I	109/110 (99%)	108 (99%)	1 (1%)	70	85
13	J	64/65 (98%)	62 (97%)	2 (3%)	35	68
14	K	93/130 (72%)	93 (100%)	0	100	100
15	L	40/57 (70%)	40 (100%)	0	100	100
16	N	128/220 (58%)	128 (100%)	0	100	100
17	O	457/576 (79%)	453 (99%)	4 (1%)	70	85
18	Q	436/476 (92%)	426 (98%)	10 (2%)	44	74
19	S	563/828 (68%)	558 (99%)	5 (1%)	70	85
20	R	313/474 (66%)	305 (97%)	8 (3%)	40	72
All	All	5789/6990 (83%)	5747 (99%)	42 (1%)	73	86

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	587	VAL
4	A	1136	VAL
5	B	73	ILE
5	B	121	VAL
5	B	471	VAL
5	B	561	ILE
5	B	893	ASN
5	B	898	LEU
5	B	934	ILE
5	B	1151	ILE
6	C	89	THR
7	D	12	THR
12	I	47	VAL
13	J	2	ILE

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Mol	Chain	Res	Type
13	J	52	THR
17	O	163	ILE
17	O	201	LYS
17	O	234	ILE
17	O	372	VAL
18	Q	102	LEU
18	Q	204	ARG
18	Q	205	ILE
18	Q	206	GLN
18	Q	213	SER
18	Q	215	LEU
18	Q	219	ILE
18	Q	232	LEU
18	Q	236	MET
18	Q	413	LEU
19	S	49	THR
19	S	360	TRP
19	S	363	ILE
19	S	377	ARG
19	S	744	LEU
20	R	144	VAL
20	R	157	MET
20	R	182	LYS
20	R	183	GLU
20	R	195	LEU
20	R	196	GLU
20	R	206	ARG
20	R	443	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	338	HIS
4	A	78	HIS
4	A	116	HIS
4	A	221	HIS
4	A	322	ASN
4	A	332	GLN
4	A	559	ASN
4	A	753	ASN
4	A	785	GLN
4	A	798	HIS

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Mol	Chain	Res	Type
4	A	1447	GLN
4	A	1620	GLN
5	B	128	GLN
5	B	168	ASN
5	B	248	ASN
5	B	575	HIS
5	B	695	ASN
5	B	710	ASN
5	B	764	ASN
5	B	893	ASN
5	B	896	GLN
5	B	912	GLN
5	B	1066	HIS
5	B	1171	ASN
7	D	30	HIS
8	E	61	GLN
8	E	174	GLN
10	G	65	HIS
12	I	32	GLN
13	J	26	GLN
13	J	53	HIS
14	K	64	GLN
14	K	102	ASN
16	N	44	ASN
17	O	121	ASN
17	O	323	GLN
18	Q	109	GLN
18	Q	145	ASN
18	Q	149	GLN
18	Q	301	HIS
18	Q	430	ASN
18	Q	482	HIS
19	S	215	ASN
19	S	230	HIS
19	S	270	GLN
19	S	454	GLN
19	S	595	GLN
19	S	665	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

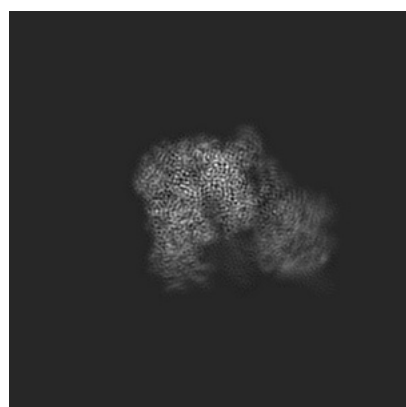
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10038. These allow visual inspection of the internal detail of the map and identification of artifacts.

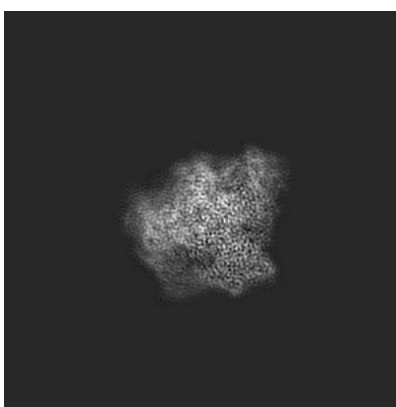
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

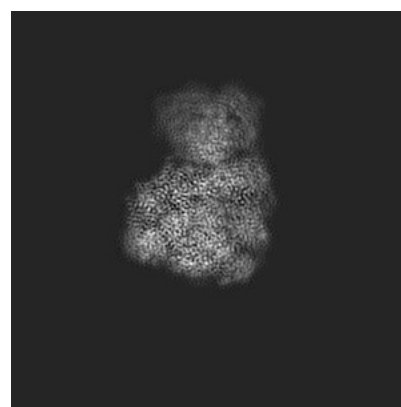
6.1.1 Primary map



X



Y

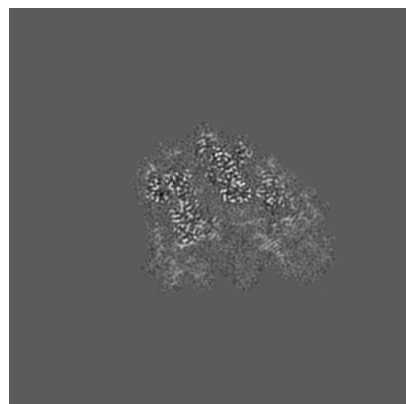


Z

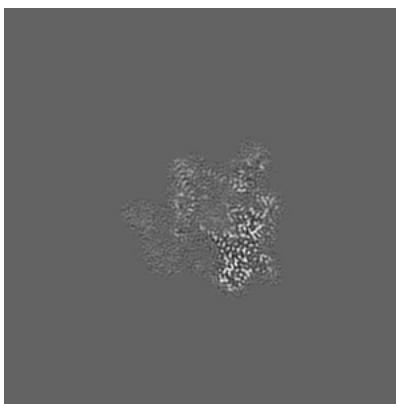
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144



Y Index: 144

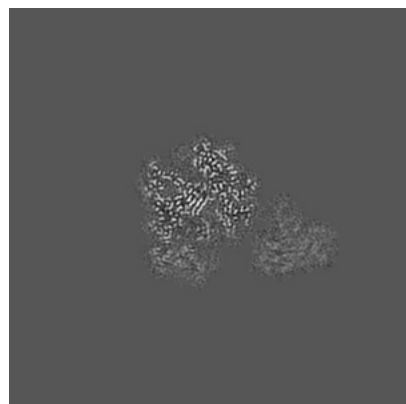


Z Index: 144

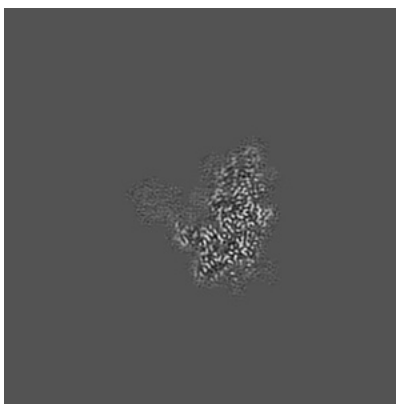
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

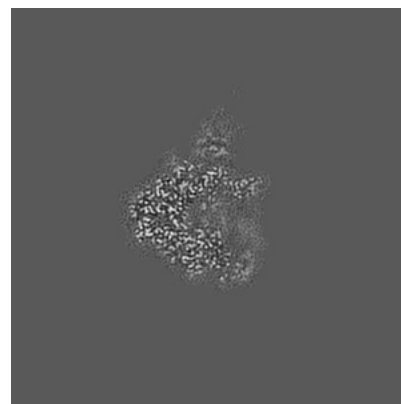
6.3.1 Primary map



X Index: 125



Y Index: 156

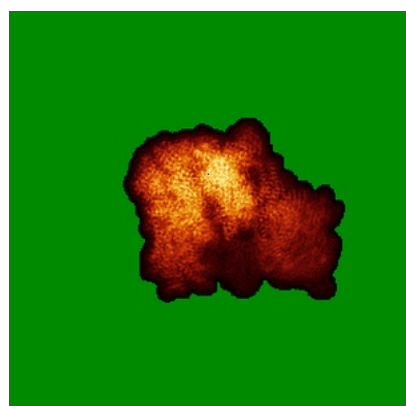


Z Index: 161

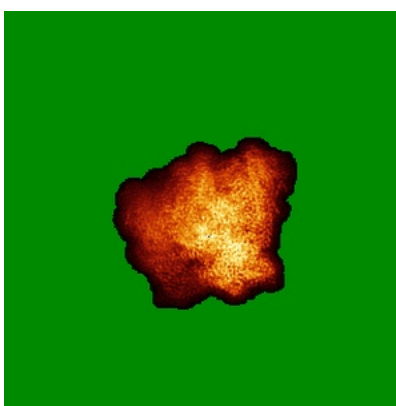
The images above show the largest variance slices of the map in three orthogonal directions.

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

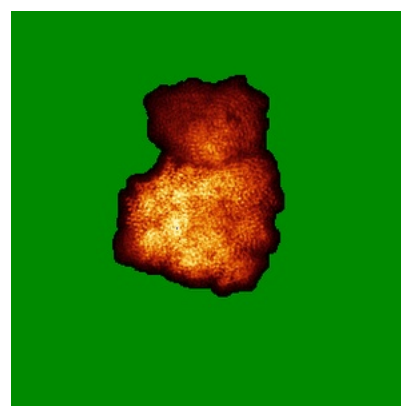
6.4.1 Primary map



X



Y

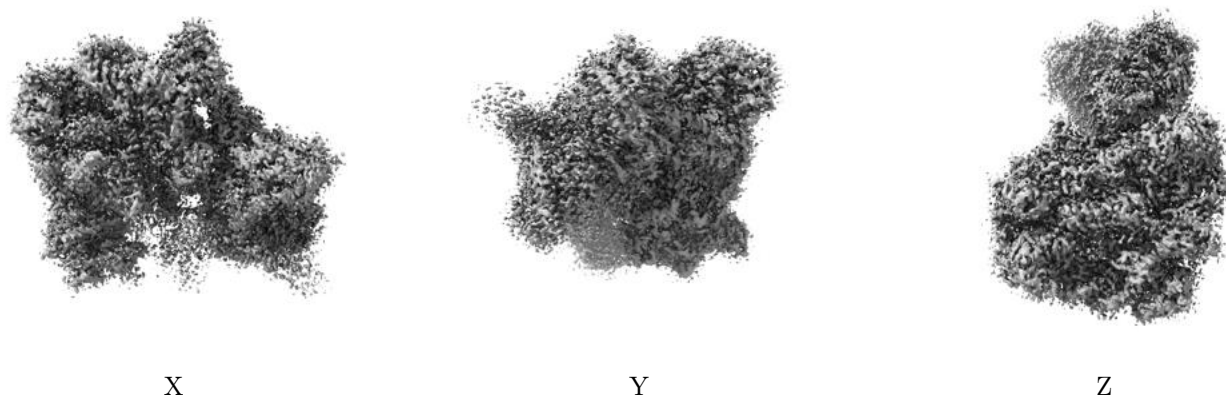


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

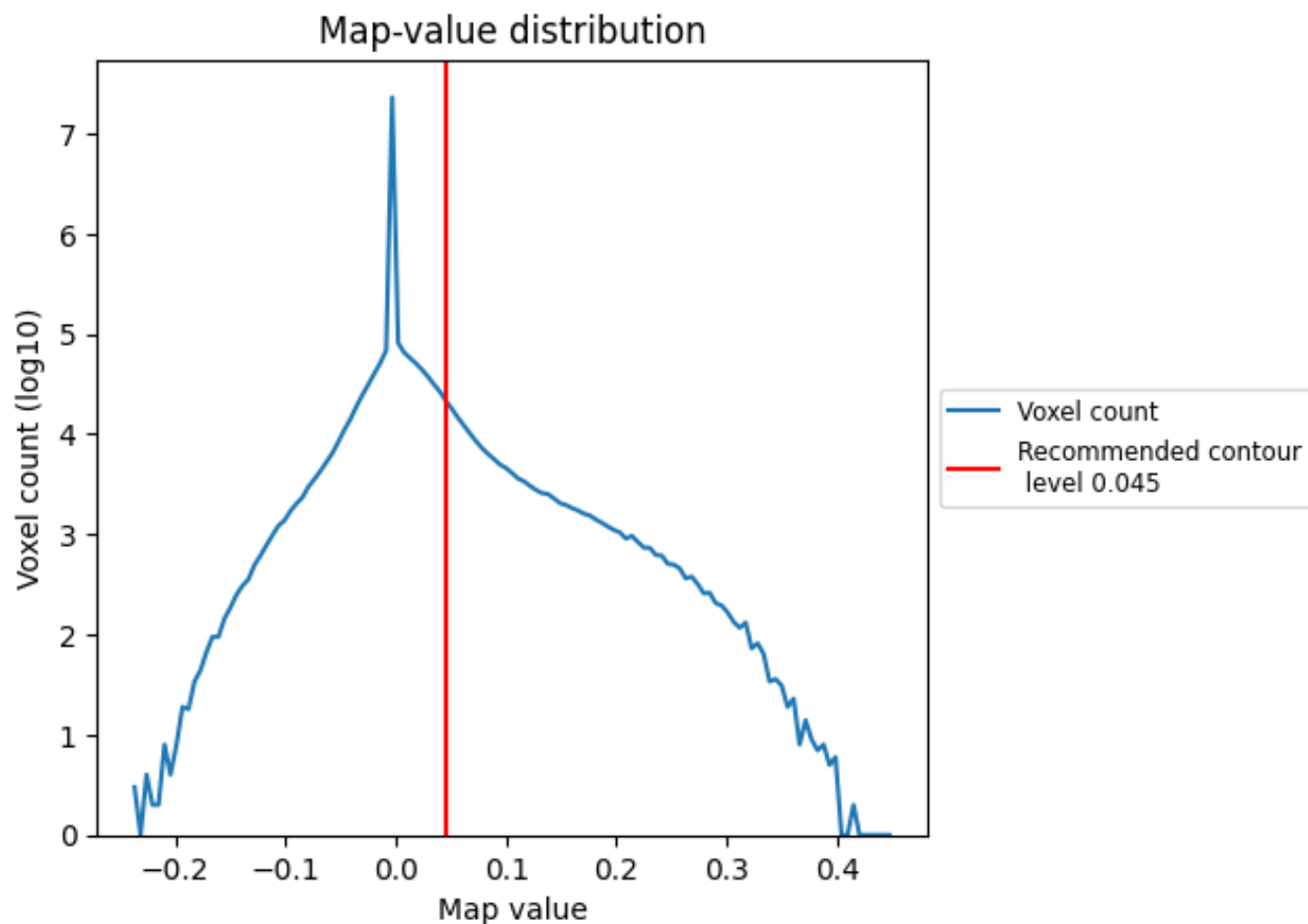
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

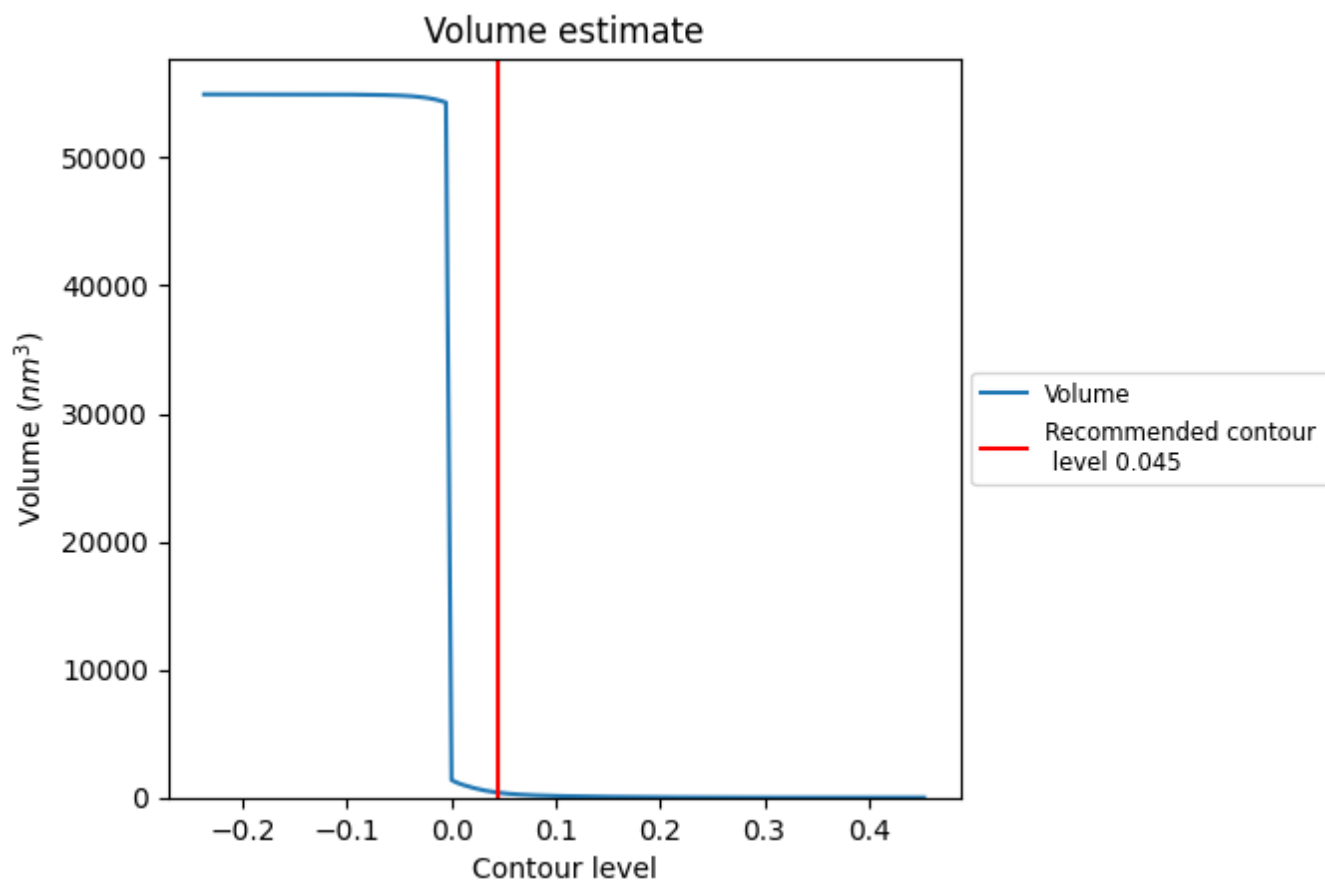
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

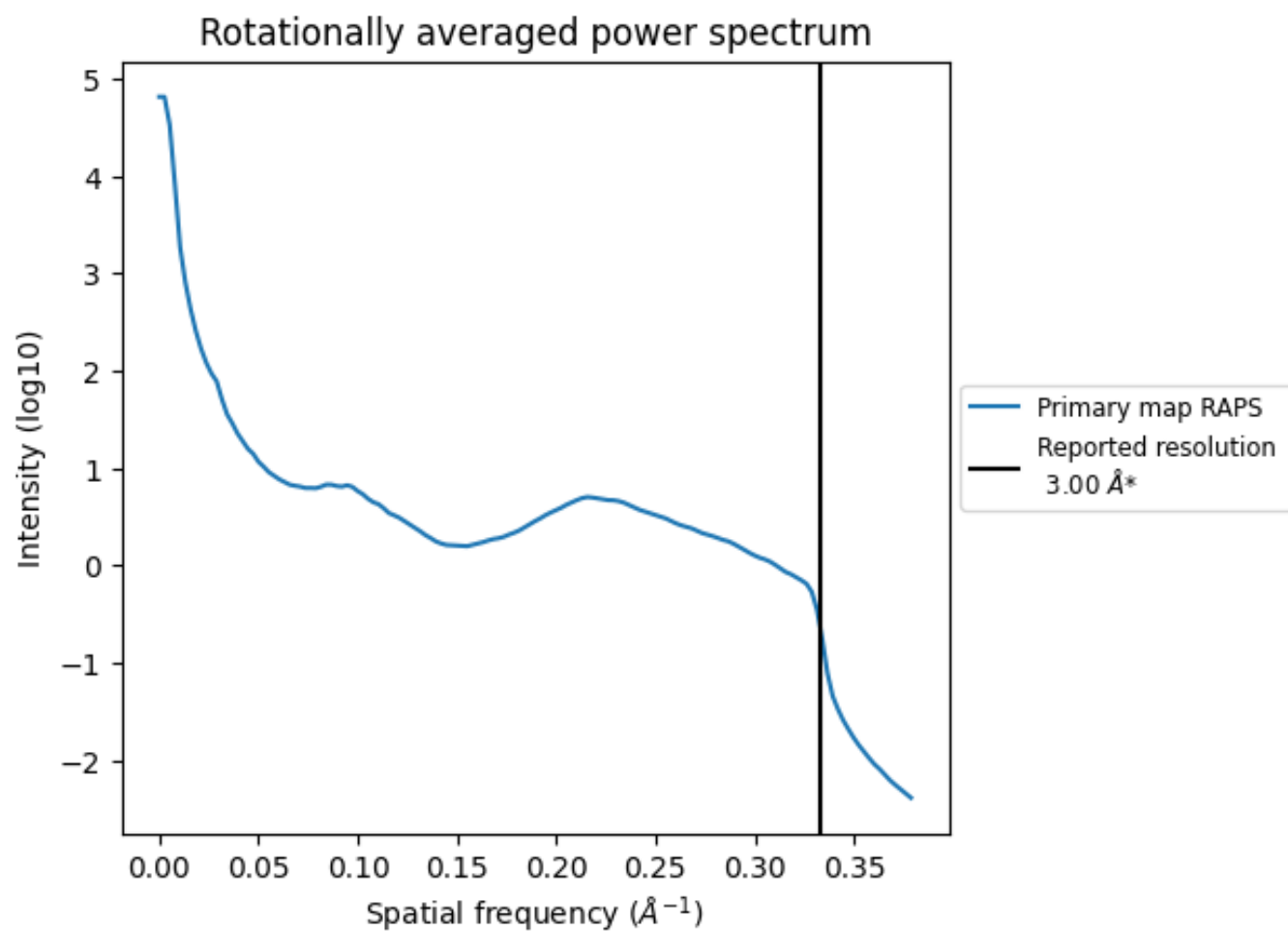
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385 nm³; this corresponds to an approximate mass of 348 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

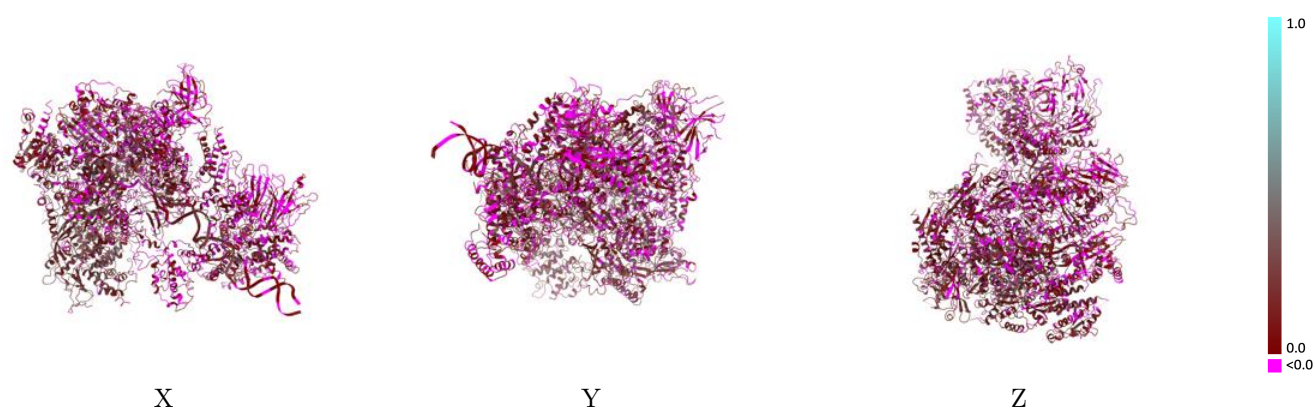
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10038 and PDB model 6RWE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

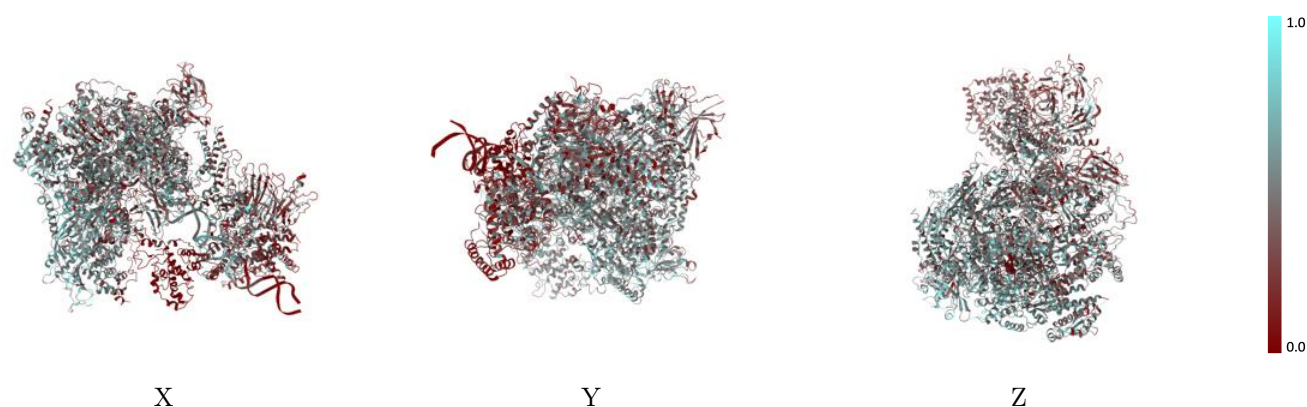
This section was not generated.

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



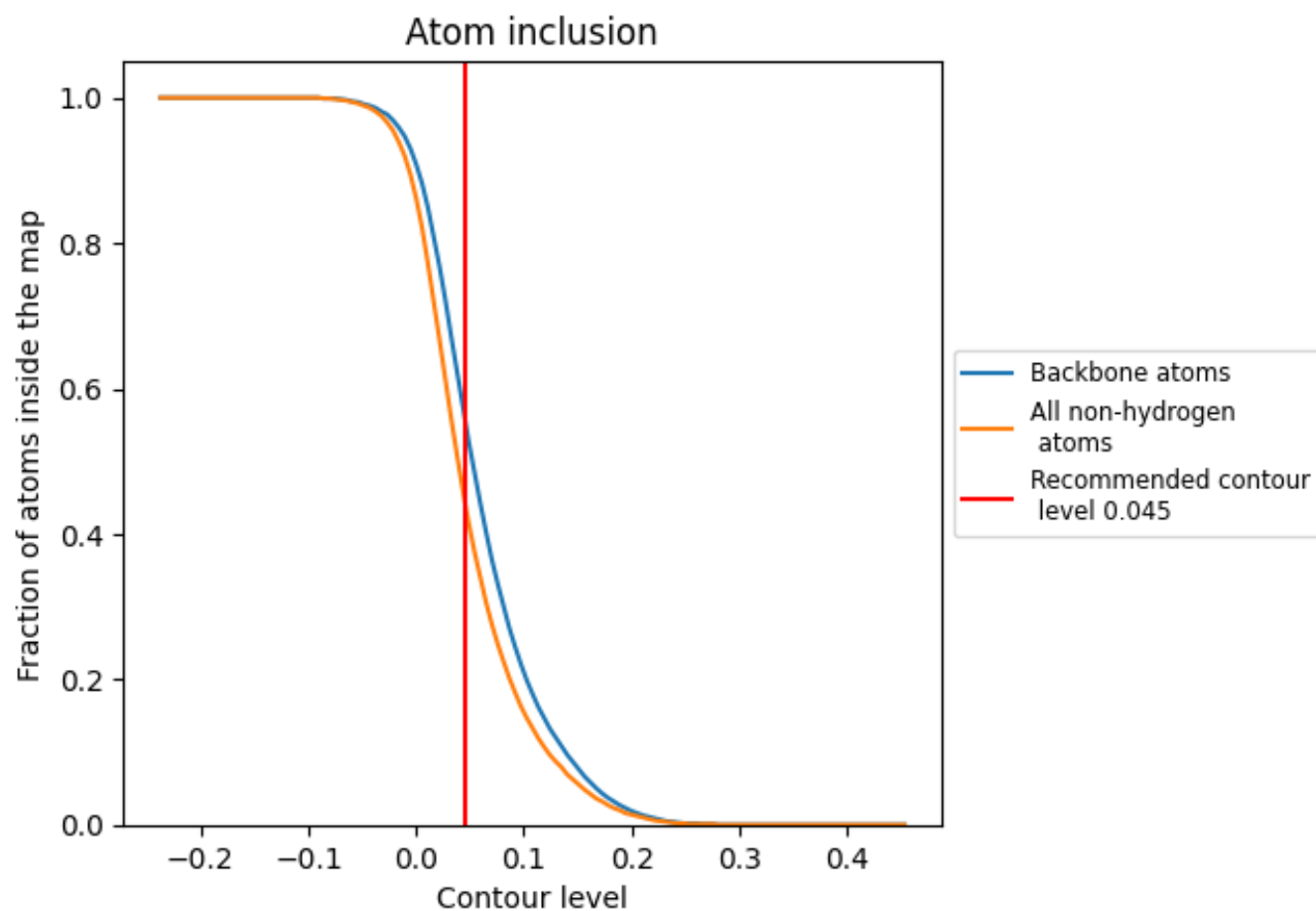
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 45% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4460	 0.1120
A	 0.5290	 0.1360
B	 0.4990	 0.1040
C	 0.5530	 0.1420
D	 0.5410	 0.2240
E	 0.5220	 0.1210
F	 0.6160	 0.2060
G	 0.5840	 0.2200
H	 0.5670	 0.1660
I	 0.2730	 0.0640
J	 0.4750	 0.0500
K	 0.5470	 0.1750
L	 0.5270	 0.1000
M	 0.1440	 0.0350
N	 0.3520	 0.0390
O	 0.4410	 0.1800
Q	 0.3400	 0.0880
R	 0.4280	 0.0650
S	 0.3020	 0.0370
T	 0.3920	 0.1100
U	 0.4020	 0.1240

