



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:20 PM UTC

PDB ID : 6RQL / pdb_00006rql
EMDB ID : EMD-4984
Title : RNA Polymerase I Closed Conformation 2 (CC2)
Authors : Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on : 2019-05-16
Resolution : 2.90 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:

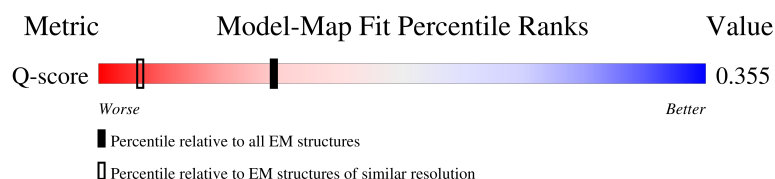
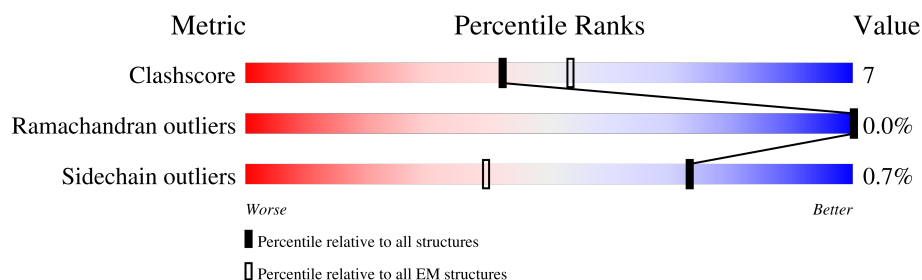
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.90 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	13054 (2.40 - 3.40)

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	Q	514	
4	S	894	

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Mol	Chain	Length	Quality of chain
5	R	507	
6	M	415	
7	A	1664	
8	B	1203	
9	C	335	
10	D	137	
11	E	215	
12	F	155	
13	G	326	
14	H	146	
15	I	125	
16	J	70	
17	K	142	
18	L	70	
19	N	233	
20	O	627	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51626 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	42	Total	C	N	O	P	0	0
			842	405	141	254	42		

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	42	Total	C	N	O	P	0	0
			877	417	171	248	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	476	Total	C	N	O	S	0	0
			3931	2526	674	711	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 RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	107	Total	C	N	O	0	0
			850	540	141	169		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1542	Total	C	N	O	S	0	0
			11953	7543	2086	2263	61		

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA135.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA43.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA12.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 19 is a protein called DNA-directed RNA polymerase I subunit RPA34.

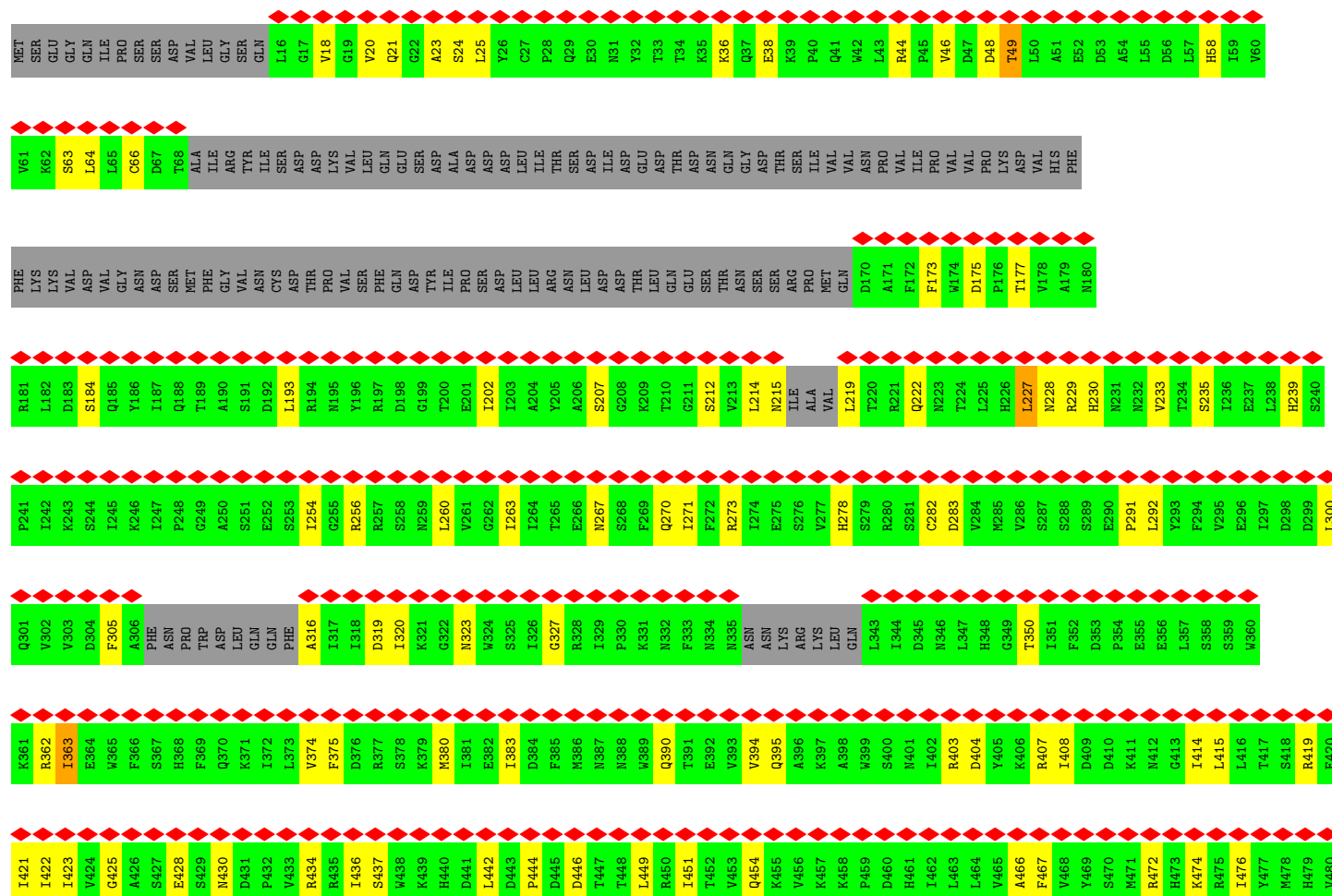
Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

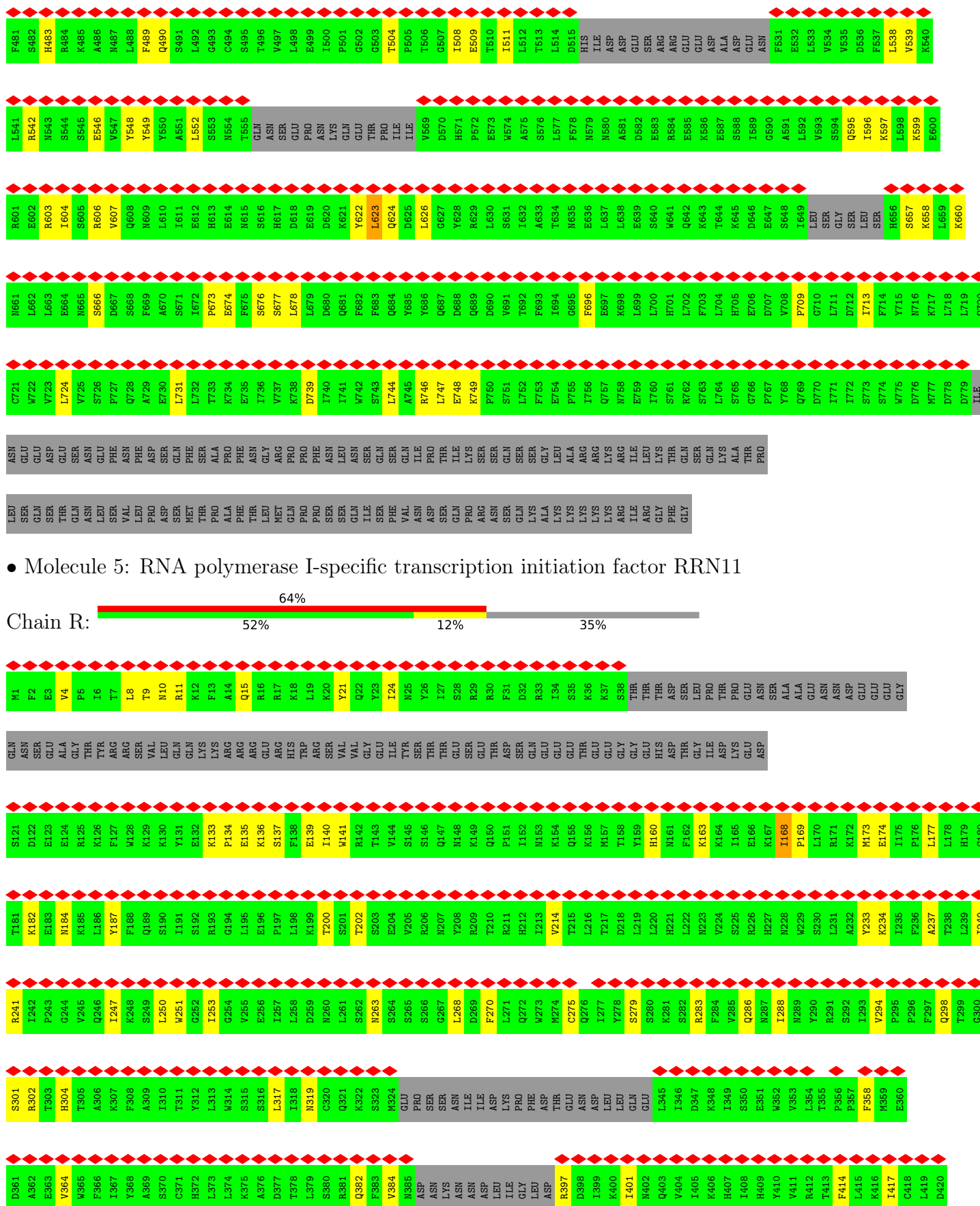
- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

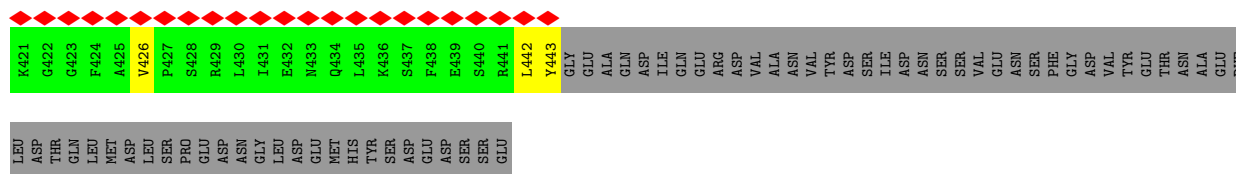
Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	499	Total	C	N	O	S	0	0
			4086	2636	661	767	22		



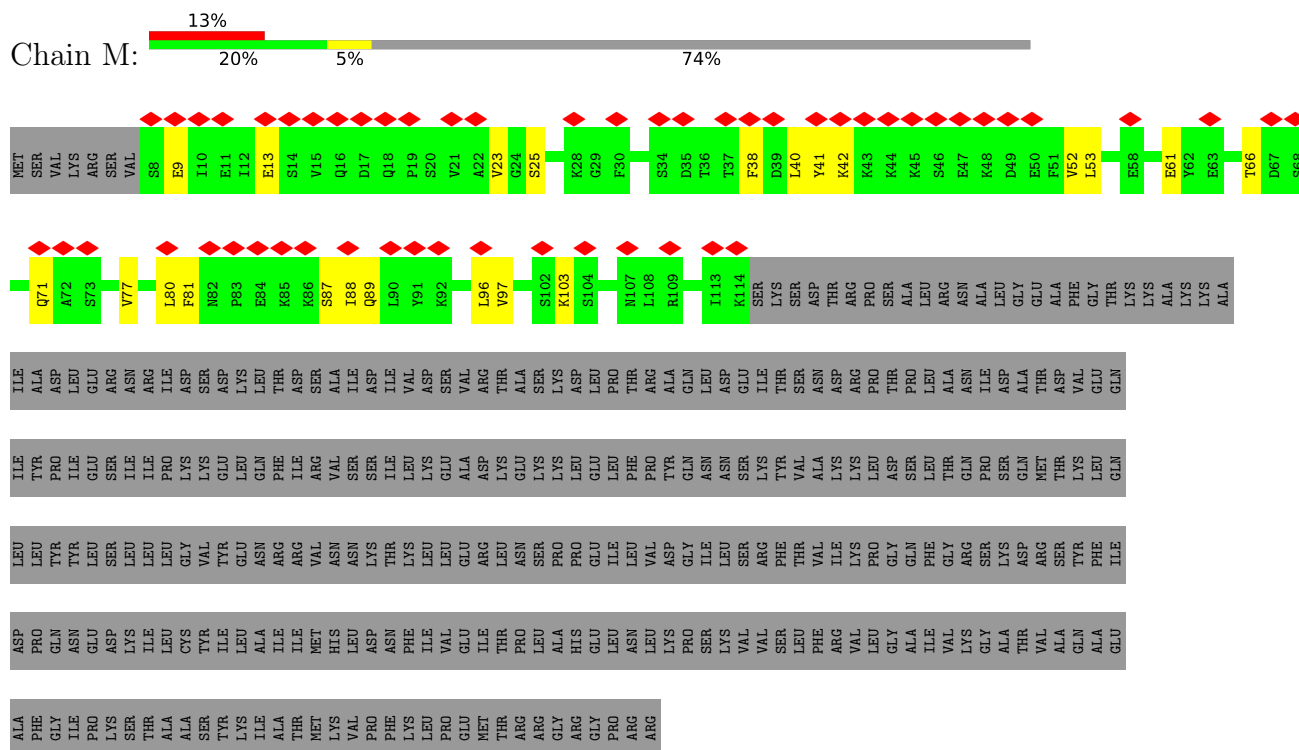
• Molecule 4: RNA polymerase I-specific transcription initiation factor RRN6



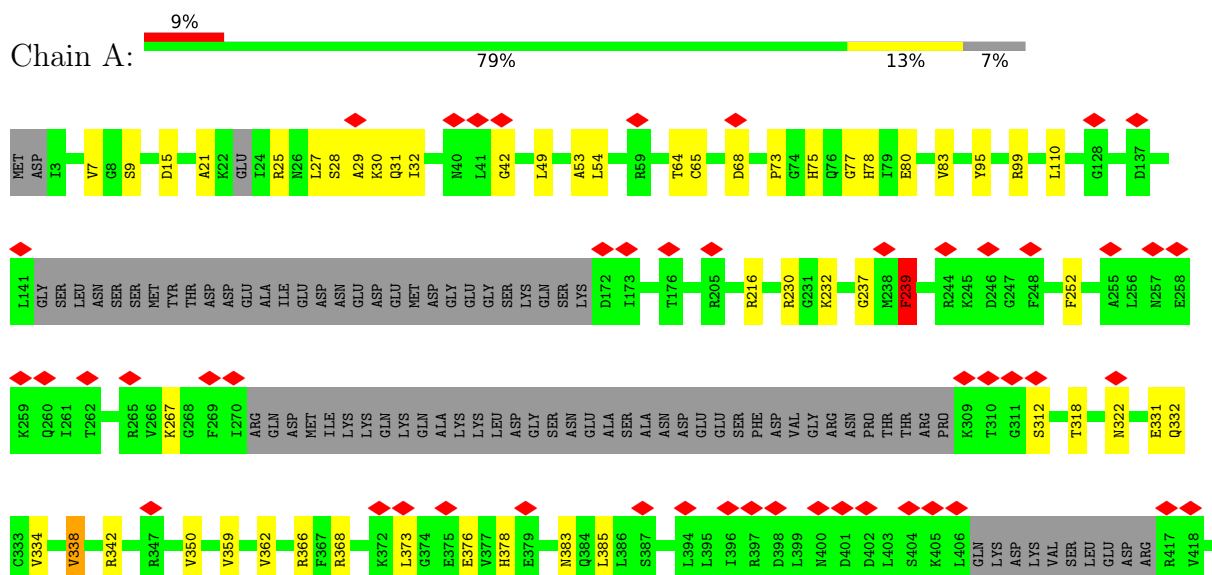


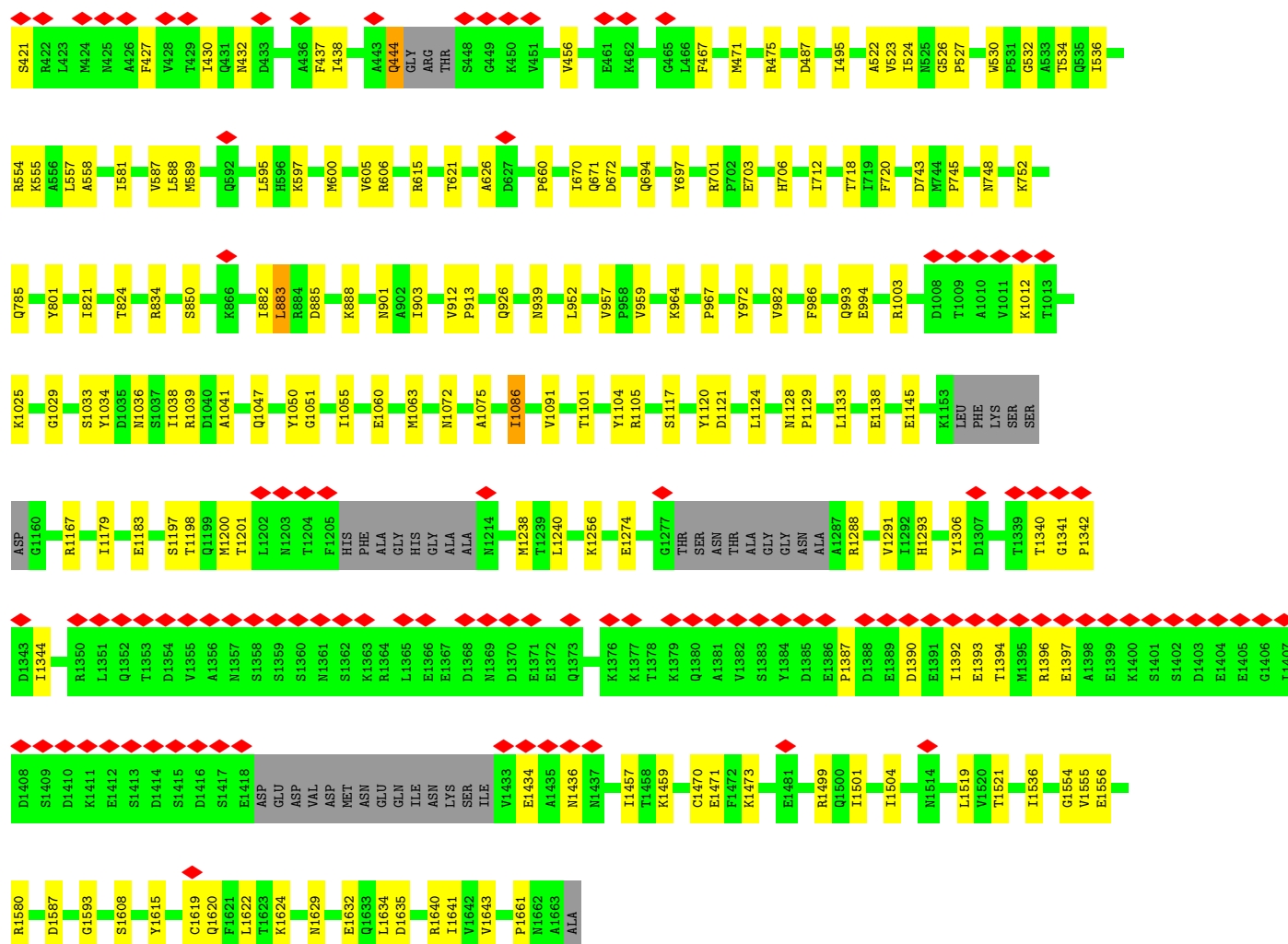


• Molecule 6: DNA-directed RNA polymerase I subunit RPA49



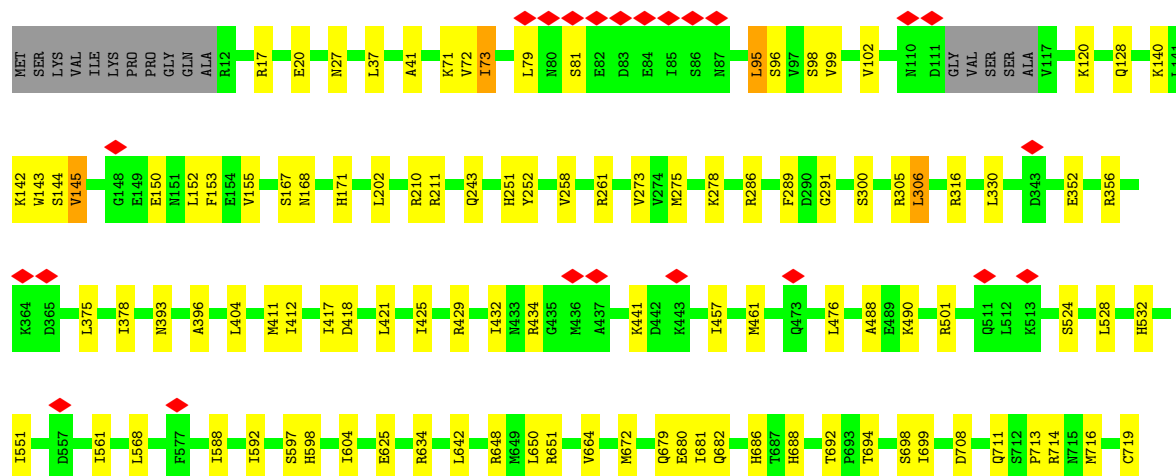
• Molecule 7: DNA-directed RNA polymerase I subunit RPA190

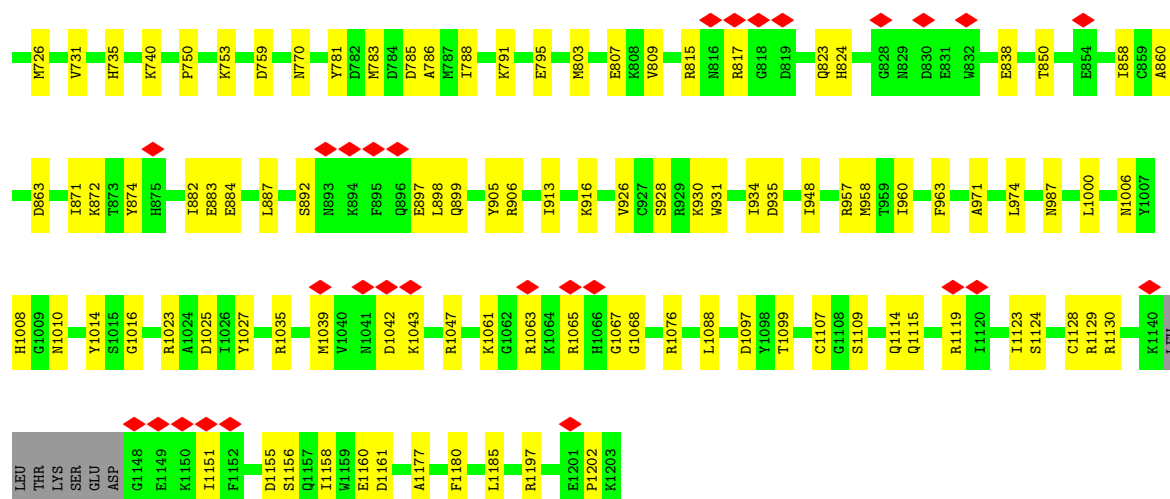




• Molecule 8: DNA-directed RNA polymerase I subunit RPA135

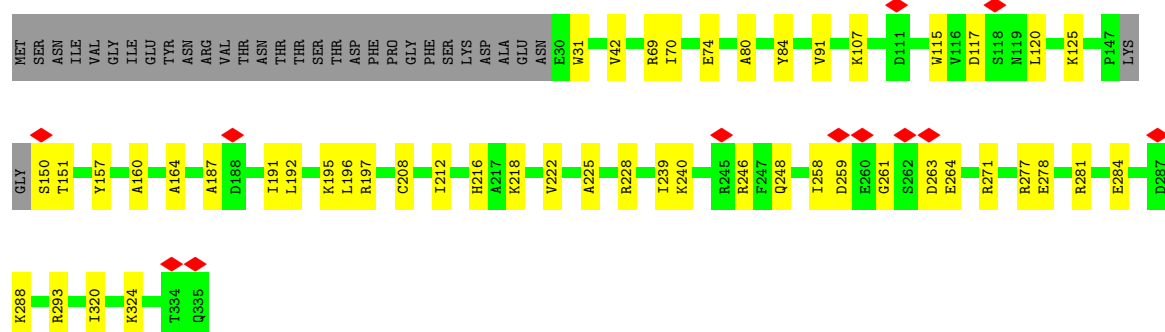
Chain B: 81% 17%





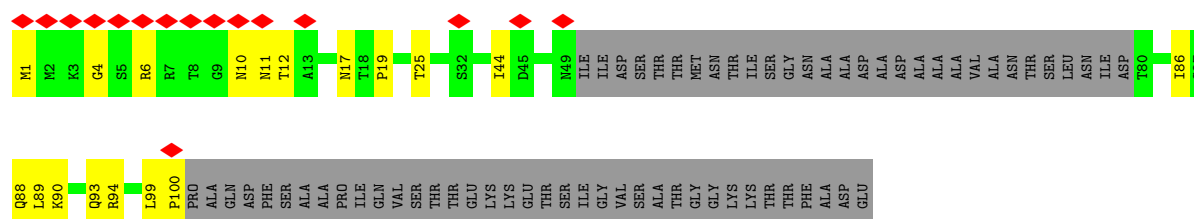
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 76% 15% 9%



- Molecule 10: DNA-directed RNA polymerase I subunit RPA14

Chain D: 12% 38% 13% 49%



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC1

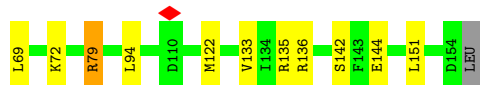
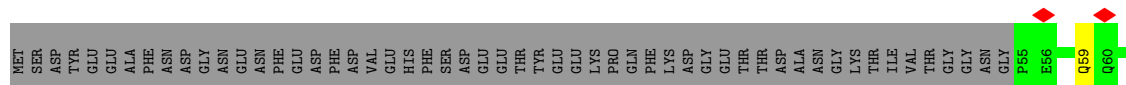
Chain E: 6% 89% 11%





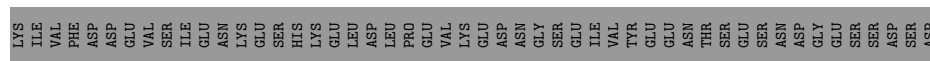
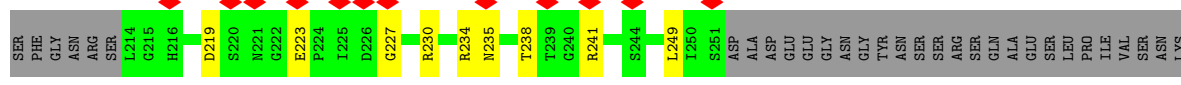
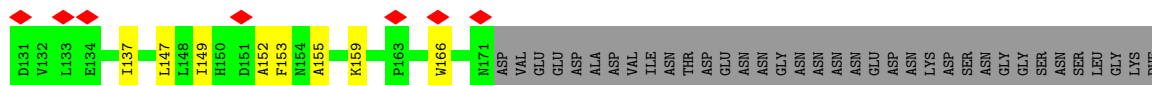
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 57% 7% 35%



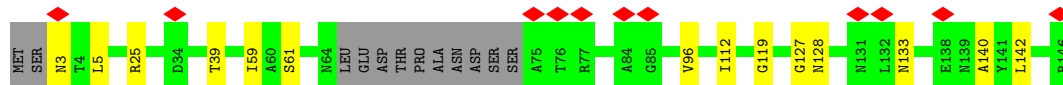
- Molecule 13: DNA-directed RNA polymerase I subunit RPA43

Chain G: 10% 50% 11% 39%



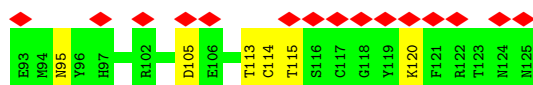
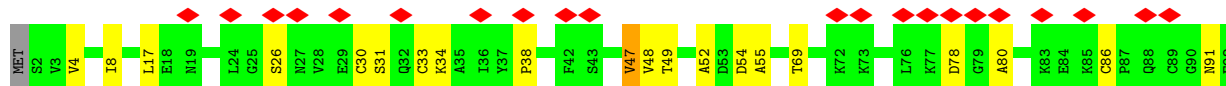
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 8% 82% 10% 8%



- Molecule 15: DNA-directed RNA polymerase I subunit RPA12

Chain I: 29% 78% 20% 2%



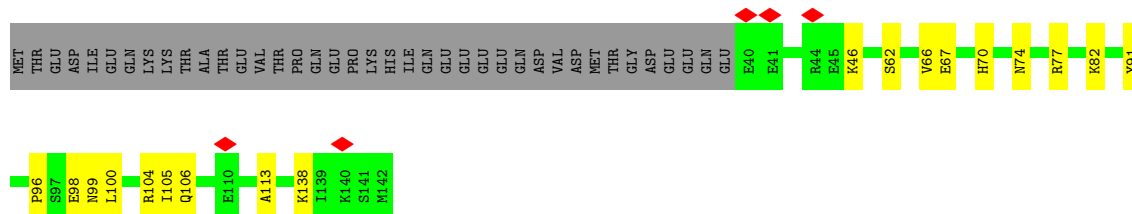
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



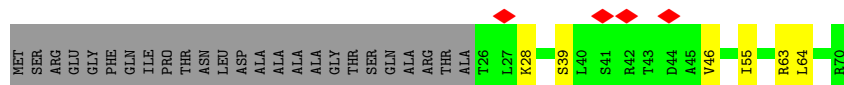
- Molecule 17: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 

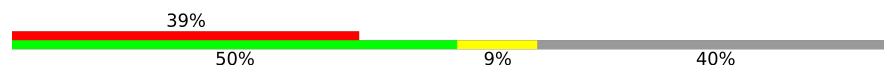


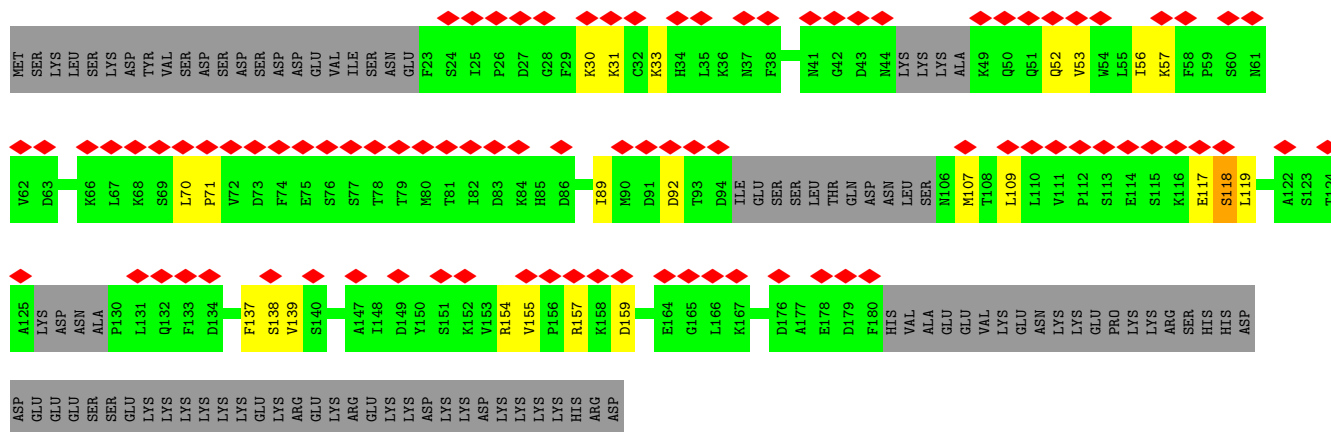
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



- Molecule 19: DNA-directed RNA polymerase I subunit RPA34

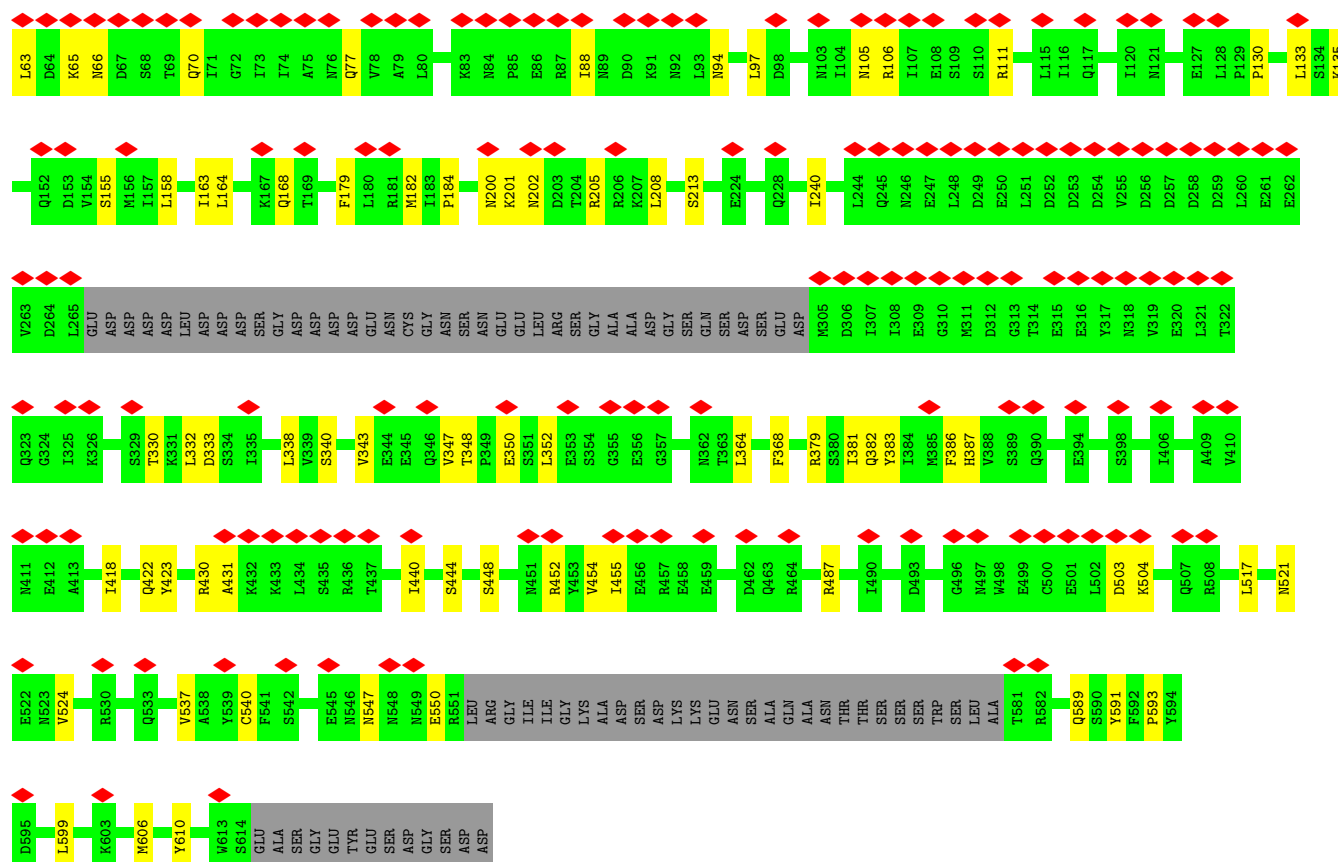
Chain N: 



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

Chain O: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24482	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 ($e^-/\text{\AA}^2$)	1.1075	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.274	Depositor
Minimum map value	-0.175	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	395.19998, 395.19998, 395.19998	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/939	0.54	0/1442
2	U	0.27	0/988	0.46	0/1528
3	Q	0.33	0/4023	0.73	0/5434
4	S	0.31	0/5065	0.67	0/6859
5	R	0.38	0/2836	0.71	0/3817
6	M	0.27	0/866	0.57	0/1162
7	A	0.43	0/12165	0.64	8/16450 (0.0%)
8	B	0.49	0/9578	0.68	0/12948
9	C	0.45	0/2469	0.63	2/3347 (0.1%)
10	D	0.31	0/557	0.57	0/750
11	E	0.38	1/1795 (0.1%)	0.55	0/2416
12	F	0.46	0/838	0.68	0/1129
13	G	0.34	0/1613	0.60	0/2193
14	H	0.44	1/1090 (0.1%)	0.54	0/1476
15	I	0.32	0/955	0.61	0/1288
16	J	0.54	0/578	0.70	0/775
17	K	0.46	0/821	0.65	0/1108
18	L	0.46	0/361	0.76	0/478
19	N	0.25	0/1124	0.61	2/1512 (0.1%)
20	O	0.29	0/4173	0.61	2/5645 (0.0%)
All	All	0.40	2/52834 (0.0%)	0.65	14/71757 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	140	ALA	CA-CB	-5.86	1.45	1.52
11	E	124	VAL	C-N	5.75	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	239	PHE	CA-C-N	8.87	134.16	120.68
7	A	239	PHE	C-N-CA	8.87	134.16	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	883	LEU	N-CA-C	-7.14	105.75	114.75
7	A	1387	PRO	N-CA-CB	6.48	109.50	103.41
7	A	338	VAL	N-CA-C	-5.93	106.71	111.81
7	A	68	ASP	CA-C-N	5.52	128.44	120.38
7	A	68	ASP	C-N-CA	5.52	128.44	120.38
20	O	381	ILE	N-CA-C	-5.35	108.63	113.71
9	C	151	THR	CA-C-N	5.28	128.38	120.83
9	C	151	THR	C-N-CA	5.28	128.38	120.83
20	O	504	LYS	N-CA-C	-5.10	108.08	114.56
19	N	118	SER	CA-C-N	5.09	131.26	121.54
19	N	118	SER	C-N-CA	5.09	131.26	121.54
7	A	42	GLY	N-CA-C	5.06	120.86	113.48

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	842	0	476	9	0
2	U	877	0	475	2	0
3	Q	3931	0	3918	68	0
4	S	4963	0	4890	100	0
5	R	2771	0	2844	43	0
6	M	850	0	850	16	0
7	A	11953	0	11848	162	0
8	B	9371	0	9243	148	0
9	C	2418	0	2401	42	0
10	D	551	0	558	14	0
11	E	1759	0	1788	14	0
12	F	823	0	841	8	0
13	G	1576	0	1581	24	0
14	H	1072	0	1042	8	0
15	I	942	0	937	17	0
16	J	569	0	589	10	0
17	K	810	0	801	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	359	0	385	5	0
19	N	1103	0	1106	19	0
20	O	4086	0	4024	43	0
All	All	51626	0	50597	667	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (667) 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)
7:A:232:LYS:HG2	7:A:239:PHE:CD1	1.59	1.36
4:S:442:LEU:HD21	4:S:444:PRO:CG	1.63	1.27
4:S:623:LEU:HD12	4:S:624:GLN:N	1.56	1.19
7:A:30:LYS:HD2	7:A:53:ALA:HB1	1.29	1.15
4:S:442:LEU:HD23	4:S:444:PRO:HD2	1.32	1.11
4:S:442:LEU:CD2	4:S:444:PRO:HG2	1.78	1.10
8:B:73:ILE:CD1	8:B:95:LEU:HD11	1.83	1.09
7:A:30:LYS:HD2	7:A:53:ALA:CB	1.89	1.03
7:A:232:LYS:CG	7:A:239:PHE:HD1	1.72	1.03
4:S:442:LEU:HD23	4:S:444:PRO:CD	1.90	1.01
9:C:120:LEU:HD11	9:C:125:LYS:HA	1.41	1.01
4:S:442:LEU:CD2	4:S:444:PRO:CD	2.39	1.00
7:A:432:ASN:ND2	7:A:444:GLN:OE1	1.99	0.96
4:S:442:LEU:CD2	4:S:444:PRO:CG	2.42	0.95
4:S:442:LEU:CD2	4:S:444:PRO:HD2	1.95	0.94
7:A:30:LYS:CD	7:A:53:ALA:HB1	1.98	0.92
7:A:232:LYS:HG2	7:A:239:PHE:HD1	0.79	0.91
1:T:39:DT:C7	5:R:11:ARG:NH2	2.34	0.91
4:S:623:LEU:HD12	4:S:624:GLN:H	1.36	0.89
9:C:120:LEU:HD11	9:C:125:LYS:CA	2.02	0.88
4:S:442:LEU:HD21	4:S:444:PRO:HG2	0.88	0.88
8:B:740:LYS:HE2	8:B:803:MET:SD	2.13	0.87
10:D:11:ASN:O	10:D:12:THR:HG22	1.74	0.87
7:A:373:LEU:CD2	7:A:378:HIS:NE2	2.42	0.83
8:B:934:ILE:HD12	9:C:69:ARG:HD2	1.60	0.82
8:B:807:GLU:OE1	8:B:905:TYR:OH	1.98	0.82
9:C:117:ASP:HB3	9:C:120:LEU:HD23	1.62	0.82
7:A:373:LEU:HD23	7:A:378:HIS:NE2	1.96	0.81
4:S:193:LEU:HD11	4:S:256:ARG:HH21	1.49	0.77
7:A:748:ASN:H	7:A:1072:ASN:HD21	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:73:ILE:HD11	8:B:95:LEU:HD11	1.67	0.76
9:C:120:LEU:O	9:C:120:LEU:HD12	1.85	0.76
10:D:12:THR:HG23	10:D:12:THR:O	1.85	0.76
1:T:39:DT:C5	5:R:11:ARG:NH2	2.55	0.75
8:B:73:ILE:CG1	8:B:95:LEU:HD11	2.17	0.75
7:A:672:ASP:HB3	8:B:783:MET:HE3	1.70	0.74
9:C:120:LEU:HD12	9:C:120:LEU:C	2.13	0.73
3:Q:262:LEU:HD13	3:Q:266:PHE:HB2	1.70	0.73
8:B:73:ILE:HD12	8:B:95:LEU:HD11	1.66	0.73
9:C:117:ASP:HB3	9:C:120:LEU:CD2	2.19	0.72
8:B:898:LEU:HB3	18:L:46:VAL:HG21	1.70	0.72
7:A:373:LEU:HD23	7:A:378:HIS:CD2	2.24	0.72
7:A:232:LYS:CG	7:A:239:PHE:CD1	2.55	0.71
3:Q:266:PHE:CE1	3:Q:314:ILE:HD12	2.27	0.70
8:B:73:ILE:CD1	8:B:95:LEU:CD1	2.68	0.70
1:T:39:DT:H73	5:R:11:ARG:NH2	2.07	0.70
9:C:120:LEU:HD11	9:C:125:LYS:CB	2.23	0.69
4:S:46:VAL:HG22	4:S:48:ASP:H	1.57	0.68
7:A:15:ASP:HB2	8:B:1197:ARG:HB3	1.76	0.68
8:B:73:ILE:HG13	8:B:95:LEU:HD11	1.75	0.68
4:S:66:CYS:HB3	4:S:227:LEU:HD13	1.78	0.66
7:A:373:LEU:HD21	7:A:378:HIS:NE2	2.09	0.66
7:A:701:ARG:H	7:A:706:HIS:HD2	1.44	0.66
7:A:670:ILE:HG12	7:A:671:GLN:HG3	1.78	0.66
4:S:623:LEU:HD12	4:S:623:LEU:C	2.19	0.66
7:A:606:ARG:NH2	17:K:98:GLU:OE2	2.29	0.66
4:S:623:LEU:HB2	4:S:678:LEU:HD12	1.78	0.65
4:S:442:LEU:HD23	4:S:442:LEU:C	2.20	0.65
4:S:442:LEU:HD21	4:S:444:PRO:CD	2.11	0.65
8:B:714:ARG:HH12	15:I:105:ASP:HA	1.62	0.65
7:A:232:LYS:HG2	7:A:239:PHE:CE1	2.29	0.65
6:M:53:LEU:HB2	6:M:96:LEU:HD13	1.80	0.64
6:M:80:LEU:HD23	6:M:89:GLN:HE21	1.63	0.64
8:B:785:ASP:OD2	8:B:957:ARG:NH2	2.31	0.64
15:I:113:THR:HG23	15:I:120:LYS:HE2	1.79	0.64
16:J:8:PHE:H	16:J:49:MET:HE1	1.63	0.63
8:B:73:ILE:HD12	8:B:95:LEU:CD1	2.27	0.63
20:O:431:ALA:O	20:O:487:ARG:NH2	2.31	0.63
8:B:95:LEU:HD12	8:B:95:LEU:H	1.64	0.63
7:A:964:LYS:NZ	8:B:672:MET:O	2.24	0.63
7:A:65:CYS:SG	7:A:75:HIS:NE2	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:79:LEU:HD22	8:B:81:SER:HB3	1.80	0.62
8:B:143:TRP:HB3	8:B:152:LEU:HB2	1.81	0.62
3:Q:292:GLU:HG3	3:Q:294:HIS:CD2	2.34	0.62
7:A:526:GLY:HA3	7:A:554:ARG:HH11	1.64	0.62
8:B:931:TRP:NE1	8:B:935:ASP:O	2.30	0.62
5:R:358:PHE:HB2	5:R:364:VAL:HG11	1.82	0.62
20:O:547:ASN:HA	20:O:550:GLU:HB3	1.82	0.62
4:S:362:ARG:HB3	4:S:375:PHE:HB2	1.81	0.62
3:Q:289:ARG:HH22	3:Q:295:THR:HG22	1.64	0.61
7:A:1459:LYS:HD3	7:A:1473:LYS:HD3	1.82	0.61
11:E:97:VAL:HG13	11:E:127:ILE:HD11	1.83	0.61
14:H:3:ASN:HB3	14:H:61:SER:HB3	1.83	0.61
9:C:120:LEU:CD1	9:C:125:LYS:HA	2.23	0.61
9:C:70:ILE:HG23	9:C:74:GLU:HB2	1.82	0.61
7:A:1179:ILE:HD11	7:A:1183:GLU:HG2	1.83	0.60
8:B:417:ILE:HG22	8:B:457:ILE:HD13	1.83	0.60
4:S:454:GLN:NE2	4:S:511:ILE:O	2.34	0.60
8:B:211:ARG:HH12	8:B:243:GLN:HE22	1.47	0.60
6:M:38:PHE:HB2	19:N:119:LEU:HB2	1.83	0.60
17:K:104:ARG:HE	17:K:106:GLN:HE21	1.48	0.60
3:Q:292:GLU:HG3	3:Q:294:HIS:CG	2.37	0.60
15:I:78:ASP:O	15:I:95:ASN:ND2	2.35	0.60
8:B:1014:TYR:OH	9:C:293:ARG:NH1	2.34	0.59
7:A:471:MET:HE1	8:B:1185:LEU:HD22	1.84	0.59
7:A:850:SER:HB3	7:A:903:ILE:HG21	1.82	0.59
15:I:114:CYS:SG	15:I:115:THR:N	2.75	0.59
7:A:1101:THR:HG22	7:A:1120:TYR:HB3	1.84	0.59
3:Q:289:ARG:NH1	3:Q:294:HIS:O	2.36	0.59
8:B:17:ARG:HB3	8:B:20:GLU:HB3	1.84	0.59
5:R:15:GLN:OE1	5:R:184:ASN:ND2	2.36	0.59
8:B:300:SER:HB3	15:I:49:THR:HG22	1.85	0.59
14:H:5:LEU:O	14:H:133:ASN:ND2	2.36	0.59
3:Q:272:GLN:HG3	4:S:596:ILE:HD13	1.85	0.58
9:C:278:GLU:OE2	9:C:281:ARG:NH1	2.36	0.58
7:A:536:ILE:HG12	7:A:557:LEU:HD21	1.86	0.58
20:O:340:SER:HA	20:O:343:VAL:HG12	1.85	0.58
3:Q:14:ASN:ND2	20:O:200:ASN:OD1	2.37	0.58
7:A:475:ARG:NH1	8:B:1068:GLY:O	2.35	0.58
20:O:66:ASN:HA	20:O:111:ARG:HH12	1.69	0.58
8:B:41:ALA:HA	8:B:501:ARG:HH21	1.69	0.57
9:C:248:GLN:HE21	9:C:258:ILE:HG23	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:179:PHE:HA	20:O:182:MET:HB3	1.86	0.57
3:Q:193:PHE:HA	3:Q:217:GLY:HA3	1.86	0.57
7:A:30:LYS:HD2	7:A:53:ALA:HB3	1.82	0.57
7:A:21:ALA:O	7:A:25:ARG:NH1	2.37	0.57
7:A:982:VAL:HG22	7:A:994:GLU:HB2	1.85	0.57
3:Q:171:HIS:ND1	3:Q:244:ASN:OD1	2.37	0.57
3:Q:271:LYS:NZ	4:S:739:ASP:OD2	2.37	0.57
8:B:568:LEU:HD23	8:B:604:ILE:HG12	1.86	0.57
13:G:149:ILE:HB	13:G:153:PHE:HB2	1.87	0.57
20:O:97:LEU:HD22	20:O:135:LYS:HG2	1.86	0.57
16:J:36:LEU:HB2	16:J:47:ARG:HH21	1.68	0.57
8:B:974:LEU:O	16:J:47:ARG:NH1	2.37	0.57
4:S:511:ILE:HD11	4:S:538:LEU:HD23	1.87	0.56
8:B:1016:GLY:O	9:C:69:ARG:NH2	2.38	0.56
8:B:1047:ARG:HH11	8:B:1067:GLY:HA3	1.70	0.56
4:S:222:GLN:HE21	4:S:229:ARG:HH22	1.51	0.56
8:B:251:HIS:HE1	8:B:261:ARG:HD3	1.71	0.56
4:S:603:ARG:HE	4:S:606:ARG:HH21	1.54	0.56
4:S:623:LEU:CD1	4:S:624:GLN:N	2.49	0.56
13:G:32:ASN:O	13:G:230:ARG:NH2	2.38	0.56
7:A:30:LYS:HE3	7:A:53:ALA:O	2.05	0.56
13:G:219:ASP:OD1	13:G:223:GLU:N	2.36	0.56
7:A:1274:GLU:OE2	7:A:1288:ARG:NH2	2.35	0.56
4:S:508:ILE:HG12	4:S:539:VAL:HG12	1.88	0.55
7:A:27:LEU:HB3	8:B:1130:ARG:HB3	1.88	0.55
7:A:1256:LYS:O	7:A:1499:ARG:NH2	2.38	0.55
8:B:681:ILE:O	19:N:154:ARG:NH1	2.39	0.55
8:B:817:ARG:HH12	8:B:892:SER:HB2	1.70	0.55
7:A:1556:GLU:OE1	11:E:200:ARG:NH1	2.39	0.55
17:K:98:GLU:HG3	17:K:100:LEU:HD12	1.88	0.55
17:K:74:ASN:OD1	17:K:77:ARG:NH2	2.40	0.55
5:R:160:HIS:HA	5:R:163:LYS:HE3	1.88	0.55
20:O:66:ASN:HD22	20:O:111:ARG:HH22	1.54	0.55
8:B:291:GLY:HA3	8:B:375:LEU:HD13	1.88	0.55
8:B:1119:ARG:NH2	8:B:1160:GLU:OE2	2.40	0.55
3:Q:203:TRP:HD1	3:Q:206:GLN:HE21	1.55	0.55
8:B:95:LEU:HD12	8:B:95:LEU:N	2.20	0.55
8:B:934:ILE:HD12	9:C:69:ARG:CD	2.35	0.55
9:C:42:VAL:O	17:K:138:LYS:NZ	2.38	0.55
5:R:8:LEU:HD21	5:R:202:THR:HG22	1.88	0.54
7:A:7:VAL:HG21	8:B:1177:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:368:ARG:HH11	7:A:383:ASN:HD21	1.55	0.54
5:R:442:LEU:O	5:R:443:TYR:CD2	2.60	0.54
20:O:503:ASP:HA	20:O:537:VAL:HG13	1.89	0.54
3:Q:118:TRP:NE1	3:Q:122:GLU:OE1	2.37	0.54
7:A:1036:ASN:ND2	7:A:1128:ASN:OD1	2.40	0.54
4:S:442:LEU:HD23	4:S:444:PRO:N	2.21	0.54
8:B:1097:ASP:OD1	8:B:1097:ASP:N	2.40	0.54
15:I:95:ASN:HB2	15:I:113:THR:HB	1.90	0.54
1:T:39:DT:H71	5:R:11:ARG:NH2	2.22	0.54
10:D:12:THR:O	10:D:17:ASN:ND2	2.38	0.54
3:Q:328:LEU:HD13	3:Q:472:ARG:HG3	1.89	0.54
4:S:278:HIS:HB2	4:S:283:ASP:H	1.73	0.54
8:B:1076:ARG:HG3	8:B:1088:LEU:HD11	1.90	0.54
9:C:157:TYR:HB2	9:C:160:ALA:HB2	1.90	0.54
13:G:152:ALA:HA	20:O:184:PRO:HG2	1.90	0.54
4:S:300:LEU:HA	4:S:320:ILE:HA	1.89	0.54
5:R:136:LYS:HD2	5:R:304:HIS:HD2	1.73	0.54
4:S:451:ILE:HD11	4:S:466:ALA:HB1	1.89	0.54
7:A:237:GLY:HA3	7:A:267:LYS:HG2	1.89	0.53
8:B:1042:ASP:OD1	8:B:1043:LYS:NZ	2.41	0.53
3:Q:94:LYS:NZ	3:Q:207:LEU:O	2.34	0.53
3:Q:341:ARG:NH2	3:Q:373:GLU:OE2	2.40	0.53
4:S:407:ARG:HA	4:S:414:ILE:HG23	1.89	0.53
4:S:423:ILE:HD13	5:R:141:TRP:HZ2	1.73	0.53
7:A:32:ILE:HD11	7:A:54:LEU:HD11	1.91	0.53
9:C:196:LEU:O	9:C:197:ARG:NH1	2.41	0.53
13:G:147:LEU:HB2	13:G:155:ALA:HB3	1.90	0.53
3:Q:341:ARG:NH2	3:Q:351:ASN:OD1	2.42	0.53
7:A:1340:THR:HG23	8:B:316:ARG:HD3	1.90	0.53
7:A:1434:GLU:OE1	7:A:1436:ASN:ND2	2.42	0.53
9:C:120:LEU:CD1	9:C:125:LYS:CA	2.83	0.53
20:O:422:GLN:NE2	20:O:591:TYR:O	2.40	0.53
1:T:44:DC:H42	2:U:27:DG:H1	1.57	0.53
8:B:27:ASN:OD1	9:C:150:SER:N	2.41	0.53
4:S:623:LEU:O	4:S:626:LEU:N	2.41	0.53
8:B:95:LEU:HD13	8:B:95:LEU:C	2.34	0.53
8:B:1042:ASP:O	8:B:1063:ARG:NH1	2.42	0.53
7:A:495:ILE:HG12	7:A:589:MET:HE3	1.89	0.53
8:B:883:GLU:HG3	8:B:884:GLU:HG3	1.91	0.53
8:B:731:VAL:HG21	16:J:59:LYS:HG2	1.91	0.53
12:F:136:ARG:HH12	12:F:151:LEU:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:169:SER:HA	3:Q:174:LEU:HD12	1.91	0.53
4:S:63:SER:HB3	4:S:549:TYR:HB3	1.90	0.53
5:R:294:VAL:H	5:R:298:GLN:HE21	1.56	0.53
8:B:71:LYS:NZ	8:B:418:ASP:OD1	2.41	0.53
3:Q:14:ASN:O	20:O:200:ASN:ND2	2.42	0.52
7:A:939:ASN:HD22	8:B:958:MET:HE3	1.74	0.52
3:Q:104:PHE:HE1	3:Q:211:TYR:O	1.92	0.52
4:S:18:VAL:HG23	5:R:426:VAL:HA	1.91	0.52
8:B:1039:MET:O	8:B:1043:LYS:NZ	2.42	0.52
20:O:521:ASN:HB3	20:O:524:VAL:HG12	1.92	0.52
11:E:28:TYR:HA	11:E:64:PRO:HA	1.92	0.52
9:C:91:VAL:HG11	16:J:60:PHE:HB3	1.91	0.52
3:Q:422:GLU:HG3	5:R:263:ASN:HD22	1.74	0.52
5:R:382:GLN:HE22	5:R:442:LEU:HA	1.74	0.52
8:B:698:SER:OG	8:B:699:ILE:N	2.42	0.52
8:B:786:ALA:HB1	8:B:928:SER:HB2	1.92	0.52
3:Q:266:PHE:CD1	3:Q:314:ILE:HD12	2.44	0.52
8:B:963:PHE:O	8:B:1027:TYR:OH	2.28	0.52
4:S:657:SER:HA	4:S:748:GLU:HB2	1.91	0.52
8:B:883:GLU:OE1	8:B:906:ARG:NH1	2.38	0.52
14:H:25:ARG:HE	14:H:39:THR:HG23	1.75	0.52
4:S:595:GLN:OE1	4:S:599:LYS:NZ	2.43	0.52
7:A:73:PRO:O	7:A:366:ARG:NH2	2.43	0.52
7:A:1291:VAL:HG22	7:A:1473:LYS:HG2	1.92	0.52
10:D:11:ASN:O	10:D:12:THR:CG2	2.54	0.52
1:T:39:DT:C7	5:R:11:ARG:HH22	2.15	0.51
3:Q:302:ALA:HA	3:Q:305:ARG:HE	1.75	0.51
7:A:1619:CYS:HA	7:A:1622:LEU:HB3	1.91	0.51
7:A:1635:ASP:HA	7:A:1640:ARG:HE	1.75	0.51
4:S:316:ALA:HB3	4:S:327:GLY:HA3	1.90	0.51
5:R:4:VAL:HG11	5:R:214:VAL:HG22	1.91	0.51
6:M:13:GLU:OE2	6:M:87:SER:OG	2.27	0.51
9:C:69:ARG:HH12	17:K:70:HIS:HB2	1.75	0.51
7:A:883:LEU:HD11	7:A:959:VAL:HG11	1.92	0.51
6:M:25:SER:HB3	6:M:97:VAL:HA	1.92	0.51
8:B:858:ILE:HD13	8:B:874:TYR:HB2	1.93	0.51
4:S:260:LEU:HA	4:S:273:ARG:HA	1.93	0.51
4:S:604:ILE:HD12	4:S:731:LEU:HD11	1.90	0.51
5:R:133:LYS:H	5:R:286:GLN:HE21	1.57	0.51
7:A:239:PHE:HD2	7:A:239:PHE:O	1.93	0.51
8:B:286:ARG:HH22	15:I:4:VAL:HG21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:80:ALA:HA	9:C:208:CYS:HA	1.92	0.51
9:C:228:ARG:NH2	9:C:271:ARG:O	2.40	0.51
7:A:1051:GLY:HA3	7:A:1580:ARG:HG2	1.92	0.51
7:A:1306:TYR:O	7:A:1499:ARG:NH2	2.44	0.51
20:O:213:SER:HB2	20:O:338:LEU:HD21	1.91	0.51
3:Q:352:ILE:CD1	3:Q:377:PHE:CE1	2.93	0.51
7:A:888:LYS:HE2	15:I:69:THR:HG22	1.93	0.51
7:A:1039:ARG:NH2	11:E:168:TYR:O	2.44	0.51
8:B:142:LYS:HG3	8:B:153:PHE:HE1	1.75	0.51
5:R:136:LYS:HD2	5:R:304:HIS:CD2	2.46	0.51
7:A:252:PHE:HB3	7:A:312:SER:HB2	1.92	0.51
15:I:26:SER:OG	15:I:38:PRO:O	2.29	0.51
20:O:423:TYR:HA	20:O:593:PRO:HG2	1.92	0.51
7:A:487:ASP:HB2	7:A:615:ARG:HG2	1.93	0.51
3:Q:284:LEU:HB3	3:Q:302:ALA:HB1	1.93	0.51
3:Q:431:ASP:OD2	3:Q:434:HIS:ND1	2.41	0.51
7:A:993:GLN:NE2	8:B:680:GLU:OE1	2.44	0.51
3:Q:378:LEU:HD13	5:R:234:LYS:HB3	1.91	0.50
4:S:607:VAL:HB	4:S:731:LEU:HD13	1.93	0.50
7:A:712:ILE:H	17:K:106:GLN:HE22	1.59	0.50
8:B:916:LYS:HG2	8:B:926:VAL:HG12	1.92	0.50
9:C:239:ILE:HG22	9:C:288:LYS:HD3	1.92	0.50
20:O:200:ASN:ND2	20:O:202:ASN:OD1	2.44	0.50
7:A:885:ASP:HB3	7:A:888:LYS:HB2	1.92	0.50
16:J:12:LYS:NZ	16:J:40:GLY:O	2.44	0.50
20:O:94:ASN:HD22	20:O:135:LYS:HD2	1.76	0.50
4:S:408:ILE:HD11	4:S:415:LEU:HB2	1.93	0.50
8:B:987:ASN:HD22	19:N:157:ARG:HE	1.60	0.50
8:B:1061:LYS:O	8:B:1065:ARG:NH1	2.40	0.50
3:Q:119:LEU:HB3	3:Q:125:PHE:HD2	1.76	0.50
8:B:99:VAL:HG23	8:B:421:LEU:HD21	1.94	0.50
4:S:709:PRO:HD2	4:S:713:ILE:HD11	1.93	0.50
7:A:216:ARG:NH2	7:A:338:VAL:O	2.44	0.50
7:A:1145:GLU:OE2	7:A:1167:ARG:NH1	2.43	0.50
8:B:1156:SER:HB3	13:G:238:THR:HG21	1.93	0.50
15:I:52:ALA:HB3	15:I:55:ALA:HB2	1.94	0.50
20:O:348:THR:HG23	20:O:350:GLU:HG2	1.94	0.50
3:Q:293:ARG:O	3:Q:293:ARG:HG3	2.05	0.50
4:S:404:ASP:OD2	4:S:451:ILE:N	2.44	0.50
7:A:824:THR:HG23	8:B:1023:ARG:HB2	1.94	0.50
7:A:964:LYS:HZ1	7:A:967:PRO:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:252:TYR:OH	8:B:305:ARG:NE	2.40	0.50
3:Q:198:ILE:HG13	3:Q:199:LEU:HD22	1.94	0.50
4:S:214:LEU:HD22	4:S:263:ILE:HD13	1.94	0.50
4:S:415:LEU:HD21	4:S:422:ILE:HG23	1.94	0.50
7:A:912:VAL:O	7:A:926:GLN:NE2	2.45	0.50
7:A:1341:GLY:HA3	8:B:316:ARG:HE	1.77	0.50
8:B:37:LEU:HD12	8:B:759:ASP:HB3	1.93	0.50
7:A:1003:ARG:HG3	8:B:716:MET:HE1	1.94	0.49
3:Q:200:PRO:HB3	3:Q:203:TRP:HB2	1.94	0.49
8:B:393:ASN:HB3	8:B:396:ALA:HB2	1.94	0.49
8:B:809:VAL:HG13	8:B:872:LYS:HE2	1.94	0.49
20:O:60:LEU:O	20:O:106:ARG:NH1	2.39	0.49
8:B:404:LEU:HD21	8:B:551:ILE:HG21	1.94	0.49
9:C:222:VAL:HG21	9:C:225:ALA:HB2	1.95	0.49
13:G:149:ILE:HD11	13:G:155:ALA:HB2	1.94	0.49
3:Q:289:ARG:HH12	3:Q:294:HIS:C	2.20	0.49
7:A:444:GLN:NE2	7:A:444:GLN:N	2.60	0.49
11:E:90:VAL:HA	11:E:120:ALA:HB2	1.93	0.49
4:S:173:PHE:HZ	5:R:187:TYR:HA	1.77	0.49
4:S:383:ILE:HG12	4:S:390:GLN:HG3	1.93	0.49
3:Q:346:GLU:OE2	3:Q:350:ARG:NH1	2.45	0.49
7:A:1293:HIS:ND1	7:A:1471:GLU:OE1	2.46	0.49
3:Q:322:ARG:HB3	4:S:597:LYS:HZ3	1.78	0.49
7:A:697:TYR:OH	7:A:703:GLU:OE2	2.23	0.49
7:A:834:ARG:HH12	8:B:1008:HIS:CD2	2.31	0.49
8:B:167:SER:OG	8:B:168:ASN:N	2.46	0.49
8:B:726:MET:SD	8:B:1035:ARG:NH1	2.85	0.49
10:D:25:THR:OG1	12:F:59:GLN:OE1	2.30	0.49
7:A:80:GLU:HA	7:A:359:VAL:HG12	1.95	0.49
8:B:95:LEU:CD1	8:B:95:LEU:C	2.86	0.49
8:B:95:LEU:HA	8:B:145:VAL:HA	1.94	0.49
8:B:1114:GLN:HE22	8:B:1161:ASP:HB3	1.78	0.49
4:S:21:GLN:OE1	4:S:24:SER:OG	2.26	0.49
4:S:49:THR:HG22	4:S:490:GLN:HA	1.94	0.49
8:B:1025:ASP:OD2	9:C:277:ARG:NH1	2.46	0.49
20:O:347:VAL:HG23	20:O:352:LEU:HD11	1.95	0.49
4:S:260:LEU:HB3	4:S:273:ARG:HG3	1.93	0.48
7:A:373:LEU:O	7:A:373:LEU:HG	2.13	0.48
7:A:752:LYS:O	7:A:785:GLN:NE2	2.47	0.48
7:A:1038:ILE:HD11	7:A:1050:TYR:HB2	1.95	0.48
8:B:823:GLN:HB3	8:B:863:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:28:ILE:HA	13:G:35:SER:HA	1.95	0.48
20:O:440:ILE:O	20:O:444:SER:N	2.44	0.48
4:S:25:LEU:HD23	4:S:437:SER:HA	1.94	0.48
7:A:332:GLN:HE22	7:A:350:VAL:H	1.61	0.48
8:B:971:ALA:HB2	8:B:1000:LEU:HD12	1.95	0.48
11:E:117:THR:HG22	11:E:119:SER:H	1.77	0.48
5:R:135:GLU:OE2	5:R:301:SER:OG	2.32	0.48
8:B:1107:CYS:SG	8:B:1109:SER:OG	2.60	0.48
10:D:19:PRO:HB3	13:G:47:VAL:HG12	1.95	0.48
4:S:483:HIS:HA	4:S:489:PHE:HB3	1.95	0.48
4:S:623:LEU:C	4:S:623:LEU:CD1	2.85	0.48
5:R:233:TYR:C	5:R:233:TYR:CD2	2.91	0.48
8:B:682:GLN:H	8:B:686:HIS:HD2	1.61	0.48
17:K:62:SER:OG	17:K:104:ARG:NH1	2.41	0.48
3:Q:6:ARG:HE	3:Q:18:ARG:HB3	1.78	0.48
4:S:425:GLY:HA3	4:S:434:ARG:HH11	1.78	0.48
18:L:28:LYS:HG2	18:L:39:SER:HB2	1.94	0.48
14:H:59:ILE:HG12	14:H:142:LEU:HD12	1.96	0.48
3:Q:307:LEU:HD22	3:Q:487:LEU:HD21	1.95	0.48
5:R:9:THR:O	5:R:10:ASN:OD1	2.30	0.48
10:D:44:ILE:HD11	10:D:89:LEU:HB3	1.96	0.48
13:G:90:LEU:HD11	13:G:119:HIS:CE1	2.48	0.48
20:O:430:ARG:NH1	20:O:610:TYR:OH	2.46	0.48
5:R:275:CYS:O	5:R:279:SER:OG	2.32	0.48
4:S:395:GLN:HB3	5:R:140:ILE:HG23	1.96	0.48
7:A:1238:MET:HB3	7:A:1521:THR:HB	1.96	0.48
8:B:202:LEU:HD23	8:B:488:ALA:HB2	1.95	0.48
8:B:289:PHE:HD1	8:B:306:LEU:HD22	1.77	0.48
5:R:21:TYR:HA	5:R:24:ILE:HB	1.94	0.48
8:B:412:ILE:HG23	8:B:461:MET:HE1	1.96	0.48
8:B:913:ILE:HG13	8:B:930:LYS:HE2	1.95	0.48
8:B:1006:ASN:HD22	8:B:1010:ASN:HB2	1.78	0.48
14:H:112:ILE:N	14:H:127:GLY:O	2.46	0.48
20:O:448:SER:O	20:O:452:ARG:N	2.47	0.48
4:S:421:ILE:HA	4:S:442:LEU:H	1.79	0.47
7:A:720:PHE:HB2	14:H:96:VAL:HB	1.96	0.47
12:F:94:LEU:HD13	12:F:122:MET:HG2	1.96	0.47
6:M:40:LEU:HD22	19:N:119:LEU:HD11	1.97	0.47
8:B:750:PRO:HG2	8:B:753:LYS:HB3	1.96	0.47
20:O:330:THR:HA	20:O:333:ASP:HB2	1.96	0.47
4:S:175:ASP:OD2	4:S:177:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:215:ASN:HB2	4:S:233:VAL:HB	1.96	0.47
8:B:95:LEU:HD13	8:B:95:LEU:O	2.14	0.47
7:A:432:ASN:CG	7:A:444:GLN:OE1	2.55	0.47
8:B:588:ILE:HG22	8:B:642:LEU:HB2	1.96	0.47
8:B:860:ALA:HA	8:B:871:ILE:HG22	1.96	0.47
4:S:442:LEU:CD2	4:S:442:LEU:C	2.86	0.47
5:R:442:LEU:O	5:R:443:TYR:CG	2.67	0.47
7:A:1124:LEU:HD22	7:A:1129:PRO:HG3	1.96	0.47
4:S:270:GLN:HG2	4:S:291:PRO:HB3	1.97	0.47
7:A:882:ILE:HG22	7:A:888:LYS:HB3	1.97	0.47
7:A:1555:VAL:HG21	7:A:1593:GLY:HA2	1.96	0.47
4:S:428:GLU:HG2	4:S:430:ASN:H	1.80	0.47
5:R:247:ILE:HA	5:R:250:LEU:HD12	1.96	0.47
6:M:41:TYR:HB2	6:M:52:VAL:HB	1.95	0.47
7:A:444:GLN:N	7:A:444:GLN:CD	2.73	0.47
7:A:1047:GLN:NE2	7:A:1587:ASP:OD2	2.45	0.47
17:K:46:LYS:HA	17:K:66:VAL:HG22	1.96	0.47
3:Q:312:LEU:HD21	3:Q:506:LYS:HB2	1.96	0.47
4:S:184:SER:N	4:S:509:GLU:OE2	2.45	0.47
7:A:1197:SER:HA	7:A:1200:MET:HG2	1.97	0.47
19:N:89:ILE:HG13	19:N:139:VAL:HG22	1.96	0.47
20:O:383:TYR:O	20:O:387:HIS:N	2.45	0.47
4:S:472:ARG:NH2	5:R:200:THR:OG1	2.48	0.46
7:A:883:LEU:HD22	7:A:972:TYR:HE1	1.81	0.46
8:B:708:ASP:OD1	8:B:708:ASP:N	2.46	0.46
3:Q:21:ARG:HA	3:Q:27:ARG:HA	1.96	0.46
4:S:20:VAL:HG12	4:S:25:LEU:HD13	1.96	0.46
7:A:1091:VAL:HG13	7:A:1133:LEU:HD23	1.98	0.46
8:B:98:SER:HB3	8:B:142:LYS:HB3	1.96	0.46
15:I:86:CYS:HB3	15:I:91:ASN:HB3	1.96	0.46
12:F:133:VAL:HG21	13:G:104:LEU:HD22	1.97	0.46
20:O:521:ASN:HB2	20:O:589:GLN:HB3	1.97	0.46
3:Q:297:ARG:O	3:Q:504:ARG:NH2	2.49	0.46
4:S:622:TYR:O	4:S:626:LEU:N	2.48	0.46
7:A:239:PHE:C	7:A:239:PHE:CD2	2.94	0.46
5:R:442:LEU:C	5:R:443:TYR:CD2	2.93	0.46
7:A:1641:ILE:HD11	8:B:1088:LEU:HD21	1.97	0.46
6:M:88:ILE:HD11	19:N:70:LEU:HD13	1.97	0.46
7:A:49:LEU:HD23	7:A:383:ASN:HD22	1.81	0.46
7:A:524:ILE:HG12	7:A:555:LYS:HG2	1.97	0.46
9:C:84:TYR:HB3	18:L:64:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:107:LYS:HE3	9:C:187:ALA:HA	1.98	0.46
10:D:86:ILE:HG22	10:D:90:LYS:HE3	1.98	0.46
11:E:97:VAL:HG21	11:E:123:LEU:HB3	1.97	0.46
1:T:28:DC:OP1	8:B:434:ARG:NH1	2.49	0.46
7:A:239:PHE:HD2	7:A:239:PHE:C	2.23	0.46
19:N:117:GLU:HG2	19:N:118:SER:H	1.81	0.46
5:R:237:ALA:O	5:R:241:ARG:NH2	2.41	0.46
7:A:318:THR:O	7:A:322:ASN:ND2	2.49	0.46
7:A:694:GLN:NE2	17:K:91:TYR:O	2.43	0.46
8:B:634:ARG:NH1	15:I:54:ASP:OD2	2.49	0.46
1:T:21:DG:OP1	7:A:421:SER:OG	2.34	0.46
8:B:824:HIS:ND1	8:B:897:GLU:OE1	2.40	0.46
15:I:30:CYS:SG	15:I:31:SER:N	2.89	0.46
7:A:342:ARG:NH1	7:A:1629:ASN:O	2.48	0.45
13:G:93:ASP:HB2	13:G:104:LEU:HD11	1.98	0.45
20:O:379:ARG:HA	20:O:382:GLN:HE22	1.81	0.45
5:R:169:PRO:O	5:R:173:MET:N	2.49	0.45
11:E:93:MET:HG3	11:E:120:ALA:HB1	1.98	0.45
4:S:58:HIS:HB3	4:S:552:LEU:HD22	1.99	0.45
7:A:718:THR:HG21	14:H:119:GLY:HA3	1.98	0.45
13:G:159:LYS:HB3	20:O:105:ASN:HD21	1.82	0.45
4:S:442:LEU:CD2	4:S:444:PRO:N	2.80	0.45
6:M:13:GLU:HB2	6:M:89:GLN:HB3	1.98	0.45
7:A:239:PHE:O	7:A:239:PHE:CD2	2.70	0.45
7:A:581:ILE:HD11	7:A:605:VAL:HG21	1.99	0.45
8:B:887:LEU:HD23	8:B:898:LEU:HD22	1.98	0.45
8:B:935:ASP:N	8:B:935:ASP:OD1	2.38	0.45
13:G:108:THR:OG1	13:G:111:THR:OG1	2.30	0.45
3:Q:450:THR:HB	4:S:724:LEU:HD21	1.98	0.45
4:S:504:THR:O	4:S:542:ARG:N	2.39	0.45
4:S:746:ARG:HH22	4:S:749:LYS:HD2	1.82	0.45
7:A:77:GLY:O	7:A:362:VAL:N	2.46	0.45
8:B:711:GLN:HG2	8:B:713:PRO:HD2	1.98	0.45
4:S:239:HIS:O	4:S:267:ASN:ND2	2.50	0.45
7:A:32:ILE:HD12	7:A:362:VAL:HG21	1.98	0.45
13:G:166:TRP:HZ3	13:G:249:LEU:HD13	1.81	0.45
3:Q:172:LEU:HD23	3:Q:174:LEU:HD11	1.99	0.45
3:Q:413:LEU:HD21	5:R:240:ILE:HD12	1.99	0.45
7:A:1240:LEU:HB2	7:A:1519:LEU:HB2	1.98	0.45
8:B:128:GLN:HB2	18:L:55:ILE:HD13	1.98	0.45
8:B:735:HIS:HE1	16:J:63:TYR:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:770:ASN:HD22	16:J:52:THR:HG21	1.81	0.45
3:Q:99:GLU:O	3:Q:103:LEU:N	2.47	0.45
4:S:202:ILE:HA	4:S:219:LEU:HD13	1.98	0.45
5:R:302:ARG:NH2	8:B:155:VAL:O	2.49	0.45
7:A:331:GLU:HB3	7:A:334:VAL:HG12	1.97	0.45
12:F:135:ARG:NH2	13:G:92:ALA:O	2.42	0.45
8:B:664:VAL:HG21	8:B:672:MET:HE1	1.99	0.45
4:S:215:ASN:HB3	4:S:235:SER:HA	1.98	0.44
4:S:230:HIS:ND1	4:S:282:CYS:SG	2.88	0.44
5:R:268:LEU:HD22	5:R:319:ASN:HD22	1.82	0.44
7:A:373:LEU:HD11	7:A:376:GLU:OE1	2.17	0.44
7:A:438:ILE:HA	7:A:456:VAL:HG22	1.98	0.44
8:B:838:GLU:O	18:L:63:ARG:NH2	2.50	0.44
9:C:192:LEU:HD21	9:C:195:LYS:HE3	1.99	0.44
9:C:216:HIS:HD2	9:C:218:LYS:H	1.65	0.44
4:S:674:GLU:O	4:S:677:SER:OG	2.30	0.44
7:A:1038:ILE:HB	7:A:1047:GLN:HB2	1.99	0.44
9:C:259:ASP:HB3	9:C:263:ASP:HB3	1.99	0.44
14:H:128:ASN:OD1	14:H:128:ASN:N	2.48	0.44
7:A:427:PHE:HA	7:A:430:ILE:HG22	2.00	0.44
7:A:1105:ARG:NH1	7:A:1138:GLU:HB3	2.33	0.44
19:N:57:LYS:HB2	19:N:138:SER:HA	1.98	0.44
19:N:157:ARG:HH12	19:N:159:ASP:HA	1.82	0.44
20:O:454:VAL:HG13	20:O:455:ILE:HG13	1.99	0.44
19:N:53:VAL:HG11	19:N:109:LEU:HD22	2.00	0.44
3:Q:163:SER:O	3:Q:167:LEU:N	2.42	0.44
3:Q:209:ASN:OD1	3:Q:209:ASN:N	2.37	0.44
3:Q:257:VAL:HG22	3:Q:262:LEU:HD11	1.99	0.44
3:Q:258:MET:HE2	3:Q:438:PHE:HE2	1.83	0.44
7:A:31:GLN:HB3	7:A:78:HIS:CE1	2.52	0.44
7:A:1390:ASP:O	7:A:1394:THR:N	2.43	0.44
12:F:72:LYS:HB3	12:F:142:SER:HA	2.00	0.44
5:R:251:TRP:HA	5:R:270:PHE:HE2	1.82	0.44
7:A:745:PRO:HG2	7:A:1075:ALA:HB2	2.00	0.44
8:B:1123:ILE:HD11	13:G:241:ARG:HH11	1.82	0.44
8:B:1128:CYS:SG	8:B:1129:ARG:N	2.91	0.44
10:D:1:MET:HG3	10:D:4:GLY:H	1.82	0.44
7:A:701:ARG:H	7:A:706:HIS:CD2	2.29	0.44
7:A:901:ASN:HB3	15:I:80:ALA:N	2.33	0.44
7:A:1029:GLY:HA3	7:A:1041:ALA:HB2	2.00	0.44
7:A:1501:ILE:HG23	7:A:1504:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1634:LEU:HD13	7:A:1643:VAL:HG11	2.00	0.44
10:D:94:ARG:HH12	10:D:100:PRO:HA	1.83	0.44
11:E:25:ASP:OD2	11:E:187:TYR:OH	2.28	0.44
20:O:130:PRO:HA	20:O:133:LEU:HB3	1.99	0.44
7:A:1086:ILE:H	7:A:1086:ILE:HG13	1.57	0.44
8:B:352:GLU:OE2	8:B:356:ARG:NH2	2.51	0.44
8:B:429:ARG:HA	8:B:432:ILE:HG12	1.99	0.44
8:B:1115:GLN:NE2	8:B:1124:SER:OG	2.49	0.44
3:Q:144:ILE:HD12	3:Q:154:LEU:HB2	2.00	0.43
8:B:1155:ASP:HA	8:B:1158:ILE:HD12	1.99	0.43
9:C:120:LEU:C	9:C:120:LEU:CD1	2.85	0.43
19:N:92:ASP:OD1	19:N:92:ASP:N	2.50	0.43
4:S:380:MET:HE2	4:S:394:VAL:HG23	1.99	0.43
6:M:9:GLU:HA	19:N:71:PRO:HA	2.00	0.43
9:C:31:TRP:HB3	17:K:82:LYS:HB3	1.99	0.43
4:S:23:ALA:HA	4:S:436:ILE:HD13	2.01	0.43
8:B:532:HIS:ND1	8:B:719:CYS:HB3	2.34	0.43
8:B:781:TYR:HE2	17:K:96:PRO:HG2	1.84	0.43
20:O:63:LEU:O	20:O:66:ASN:ND2	2.52	0.43
20:O:201:LYS:HG3	20:O:240:ILE:HG13	1.99	0.43
4:S:323:ASN:HA	4:S:350:THR:HA	2.01	0.43
6:M:77:VAL:HB	19:N:56:ILE:HG13	2.01	0.43
13:G:234:ARG:HG2	13:G:235:ASN:H	1.83	0.43
20:O:62:ASP:HA	20:O:65:LYS:HB2	2.00	0.43
4:S:44:ARG:O	4:S:46:VAL:N	2.51	0.43
7:A:1012:LYS:HG3	7:A:1201:THR:HG21	1.98	0.43
10:D:88:GLN:NE2	20:O:184:PRO:O	2.51	0.43
3:Q:42:ASN:HD22	3:Q:43:ASP:N	2.17	0.43
3:Q:198:ILE:O	3:Q:201:LYS:NZ	2.51	0.43
4:S:363:ILE:HG22	4:S:374:VAL:HG22	2.00	0.43
5:R:133:LYS:HA	5:R:134:PRO:HD3	1.90	0.43
6:M:66:THR:HB	6:M:71:GLN:HG3	2.00	0.43
7:A:1055:ILE:HD13	7:A:1063:MET:HE1	2.01	0.43
7:A:1470:CYS:SG	7:A:1471:GLU:N	2.92	0.43
8:B:850:THR:HB	8:B:882:ILE:HD13	2.01	0.43
16:J:36:LEU:HD11	16:J:51:LEU:HD12	2.00	0.43
20:O:517:LEU:HD11	20:O:540:CYS:HB2	2.01	0.43
3:Q:42:ASN:HD22	3:Q:43:ASP:H	1.66	0.43
3:Q:352:ILE:HD13	3:Q:377:PHE:CE1	2.54	0.43
7:A:83:VAL:HG11	7:A:427:PHE:HE1	1.83	0.43
7:A:1393:GLU:O	7:A:1397:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:311:MET:HE3	3:Q:487:LEU:HD22	2.00	0.43
4:S:228:ASN:HD22	4:S:282:CYS:HB3	1.83	0.43
4:S:673:PRO:O	4:S:676:SER:OG	2.30	0.43
7:A:64:THR:O	8:B:1114:GLN:NE2	2.52	0.43
7:A:1274:GLU:HB3	15:I:47:VAL:HG23	2.01	0.43
3:Q:20:TRP:N	3:Q:28:THR:O	2.52	0.43
7:A:595:LEU:HD13	7:A:1198:THR:HG21	2.01	0.43
7:A:1060:GLU:OE2	7:A:1580:ARG:NH1	2.44	0.43
7:A:1240:LEU:HB3	7:A:1536:ILE:HD12	2.01	0.43
8:B:651:ARG:HH11	8:B:651:ARG:HD3	1.72	0.43
13:G:48:SER:H	13:G:65:HIS:CE1	2.37	0.43
13:G:56:ASN:ND2	13:G:59:GLN:OE1	2.52	0.43
20:O:205:ARG:HA	20:O:208:LEU:HB2	2.01	0.43
3:Q:351:ASN:ND2	3:Q:373:GLU:OE2	2.49	0.42
4:S:474:LYS:HE3	4:S:474:LYS:HB2	1.87	0.42
7:A:444:GLN:NE2	7:A:444:GLN:CA	2.81	0.42
7:A:1457:ILE:HD13	7:A:1457:ILE:HA	1.84	0.42
20:O:77:GLN:HG2	20:O:88:ILE:HB	1.99	0.42
11:E:76:GLY:N	11:E:106:GLN:OE1	2.39	0.42
12:F:69:LEU:HD23	13:G:94:PRO:HG3	2.01	0.42
19:N:31:LYS:HG3	19:N:33:LYS:HE3	2.01	0.42
4:S:254:ILE:HG23	4:S:256:ARG:H	1.84	0.42
7:A:373:LEU:HG	7:A:376:GLU:HB2	2.01	0.42
7:A:1025:LYS:HG3	7:A:1615:TYR:HD1	1.84	0.42
7:A:1554:GLY:HA2	11:E:183:PRO:HD2	2.01	0.42
7:A:1608:SER:OG	7:A:1632:GLU:OE2	2.32	0.42
7:A:1620:GLN:HE21	7:A:1624:LYS:NZ	2.17	0.42
8:B:140:LYS:HB3	8:B:155:VAL:HG22	2.00	0.42
8:B:692:THR:HG22	8:B:694:THR:H	1.84	0.42
13:G:137:ILE:HB	13:G:227:GLY:HA2	2.00	0.42
8:B:815:ARG:NH2	8:B:899:GLN:OE1	2.52	0.42
17:K:67:GLU:HA	17:K:99:ASN:HB3	2.02	0.42
20:O:386:PHE:HD2	20:O:606:MET:HE1	1.83	0.42
4:S:696:PHE:HZ	4:S:747:LEU:HD11	1.85	0.42
4:S:36:LYS:HG2	4:S:38:GLU:H	1.85	0.42
15:I:33:CYS:SG	15:I:34:LYS:N	2.92	0.42
3:Q:413:LEU:HA	3:Q:416:ILE:HG22	2.02	0.42
5:R:174:GLU:HA	5:R:177:LEU:HD12	2.00	0.42
7:A:110:LEU:HD13	7:A:230:ARG:HH11	1.84	0.42
7:A:530:TRP:O	7:A:532:GLY:N	2.53	0.42
8:B:150:GLU:HG2	8:B:441:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:524:SER:HB3	8:B:528:LEU:HB2	2.02	0.42
10:D:89:LEU:O	10:D:93:GLN:N	2.44	0.42
15:I:8:ILE:HG23	15:I:17:LEU:HB2	2.01	0.42
4:S:36:LYS:HG3	4:S:46:VAL:HG23	2.02	0.42
5:R:414:PHE:HA	5:R:417:ILE:HG22	2.02	0.42
7:A:28:SER:O	7:A:78:HIS:ND1	2.51	0.42
8:B:258:VAL:HG12	8:B:273:VAL:HG21	2.00	0.42
7:A:95:TYR:CZ	7:A:99:ARG:HD2	2.55	0.42
7:A:743:ASP:N	7:A:743:ASP:OD1	2.49	0.42
7:A:1121:ASP:OD1	7:A:1121:ASP:N	2.50	0.42
8:B:96:SER:N	8:B:144:SER:O	2.48	0.42
20:O:332:LEU:HD23	20:O:599:LEU:HD11	2.02	0.42
7:A:9:SER:HA	8:B:1202:PRO:HG2	2.01	0.42
7:A:621:THR:OG1	7:A:626:ALA:O	2.37	0.42
7:A:745:PRO:O	7:A:801:TYR:OH	2.34	0.42
3:Q:341:ARG:NH1	3:Q:365:ASP:OD2	2.54	0.41
3:Q:480:LEU:HA	3:Q:483:ILE:HG22	2.01	0.41
6:M:81:PHE:HB3	19:N:52:GLN:HB2	2.02	0.41
8:B:273:VAL:HG11	8:B:378:ILE:HD11	2.02	0.41
3:Q:197:GLU:HA	3:Q:204:ARG:HH22	1.85	0.41
4:S:63:SER:OG	4:S:64:LEU:N	2.53	0.41
4:S:271:ILE:HD12	4:S:305:PHE:HZ	1.85	0.41
4:S:546:GLU:OE1	4:S:548:TYR:OH	2.28	0.41
8:B:210:ARG:NH1	8:B:625:GLU:OE2	2.53	0.41
8:B:714:ARG:HD3	8:B:714:ARG:HA	1.75	0.41
9:C:115:TRP:HH2	9:C:212:ILE:HG23	1.86	0.41
10:D:99:LEU:HD12	10:D:100:PRO:HD2	2.02	0.41
3:Q:326:TYR:O	3:Q:472:ARG:NH2	2.37	0.41
7:A:986:PHE:HB3	8:B:960:ILE:HD12	2.02	0.41
13:G:62:MET:HA	13:G:66:LEU:HD12	2.02	0.41
20:O:59:ALA:HB2	20:O:70:GLN:HB2	2.01	0.41
3:Q:376:GLU:HA	3:Q:379:LYS:HB2	2.02	0.41
7:A:952:LEU:HD12	7:A:957:VAL:HA	2.03	0.41
8:B:71:LYS:HB3	8:B:425:ILE:HG13	2.02	0.41
8:B:1014:TYR:HE2	9:C:228:ARG:HA	1.85	0.41
4:S:467:PHE:HB3	4:S:476:ILE:HD11	2.01	0.41
4:S:626:LEU:HD11	4:S:666:SER:HA	2.01	0.41
4:S:658:LYS:HG3	4:S:660:LYS:H	1.86	0.41
5:R:384:VAL:HG22	5:R:397:ARG:HD3	2.03	0.41
7:A:597:LYS:HE3	7:A:660:PRO:HG2	2.02	0.41
7:A:821:ILE:HD13	7:A:821:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:788:ILE:HB	8:B:948:ILE:HB	2.02	0.41
8:B:823:GLN:HA	8:B:863:ASP:HA	2.02	0.41
9:C:320:ILE:O	9:C:324:LYS:N	2.51	0.41
16:J:49:MET:HB2	16:J:49:MET:HE3	1.75	0.41
6:M:42:LYS:N	19:N:30:LYS:O	2.53	0.41
7:A:1661:PRO:O	13:G:101:SER:OG	2.33	0.41
8:B:672:MET:HE3	8:B:688:HIS:CE1	2.56	0.41
20:O:364:LEU:O	20:O:368:PHE:N	2.53	0.41
4:S:446:ASP:HB3	4:S:449:LEU:HG	2.03	0.41
7:A:522:ALA:HA	7:A:532:GLY:HA2	2.02	0.41
11:E:32:GLN:HE21	11:E:36:GLU:HG3	1.86	0.41
12:F:79:ARG:HB2	12:F:144:GLU:CD	2.46	0.41
5:R:137:SER:OG	5:R:139:GLU:O	2.35	0.41
6:M:23:VAL:HG11	19:N:107:MET:HE2	2.03	0.41
7:A:385:LEU:HD13	7:A:437:PHE:HA	2.03	0.41
9:C:264:GLU:H	9:C:264:GLU:HG2	1.66	0.41
3:Q:284:LEU:HA	3:Q:284:LEU:HD23	1.88	0.41
4:S:207:SER:O	4:S:212:SER:N	2.54	0.41
4:S:319:ASP:HB2	4:S:363:ILE:HG12	2.03	0.41
7:A:588:LEU:HD13	7:A:600:MET:HE2	2.02	0.41
7:A:912:VAL:HG23	7:A:913:PRO:HD3	2.02	0.41
7:A:1392:ILE:O	7:A:1396:ARG:N	2.52	0.41
8:B:597:SER:OG	8:B:598:HIS:N	2.54	0.41
8:B:679:GLN:NE2	19:N:155:VAL:O	2.52	0.41
8:B:1014:TYR:HH	9:C:293:ARG:HH12	1.65	0.41
17:K:104:ARG:HE	17:K:106:GLN:NE2	2.18	0.41
20:O:155:SER:HA	20:O:158:LEU:HB2	2.03	0.41
4:S:472:ARG:HH21	4:S:472:ARG:HD3	1.74	0.41
11:E:78:LEU:HD11	11:E:109:ILE:HG13	2.02	0.41
11:E:100:ILE:HD11	11:E:108:GLY:HA3	2.02	0.41
19:N:56:ILE:HG22	19:N:137:PHE:HB2	2.02	0.41
2:U:38:DT:H2'	2:U:39:DG:C8	2.56	0.40
3:Q:19:LEU:HD13	3:Q:27:ARG:HE	1.85	0.40
7:A:1063:MET:HE2	7:A:1063:MET:HB3	1.94	0.40
7:A:1341:GLY:HA2	7:A:1342:PRO:HD3	1.93	0.40
8:B:791:LYS:O	8:B:795:GLU:HG2	2.21	0.40
9:C:164:ALA:HB2	9:C:191:ILE:HB	2.03	0.40
9:C:246:ARG:HH12	9:C:284:GLU:CD	2.29	0.40
20:O:164:LEU:HB3	20:O:168:GLN:HG2	2.03	0.40
3:Q:75:LEU:HD13	3:Q:76:THR:HG23	2.03	0.40
4:S:403:ARG:HH21	4:S:419:ARG:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:168:ILE:HG23	5:R:169:PRO:HD3	2.04	0.40
7:A:373:LEU:O	7:A:373:LEU:CG	2.69	0.40
7:A:1033:SER:OG	7:A:1034:TYR:N	2.54	0.40
9:C:240:LYS:HB2	9:C:261:GLY:HA2	2.03	0.40
3:Q:318:LEU:HB3	3:Q:476:ILE:HD12	2.03	0.40
3:Q:352:ILE:CD1	3:Q:377:PHE:CD1	3.04	0.40
7:A:523:VAL:HB	7:A:558:ALA:HB2	2.03	0.40
7:A:1104:TYR:OH	7:A:1117:SER:OG	2.29	0.40
8:B:411:MET:HE2	8:B:476:LEU:HD23	2.02	0.40
8:B:648:ARG:NH1	8:B:650:LEU:HD21	2.36	0.40
10:D:6:ARG:O	10:D:10:ASN:N	2.54	0.40
17:K:105:ILE:HB	17:K:113:ALA:HB1	2.02	0.40
7:A:29:ALA:HA	7:A:78:HIS:HE1	1.86	0.40
1:T:27:DC:H5'	8:B:434:ARG:HD2	2.04	0.40
3:Q:103:LEU:HD21	3:Q:206:GLN:HG3	2.02	0.40
3:Q:282:ARG:HG3	3:Q:283:ASN:H	1.86	0.40
6:M:61:GLU:HB2	6:M:103:LYS:HD2	2.03	0.40
7:A:527:PRO:HB3	7:A:534:THR:HG22	2.02	0.40
8:B:120:LYS:HG3	8:B:171:HIS:CE1	2.57	0.40
8:B:275:MET:HG2	8:B:330:LEU:HD12	2.04	0.40
8:B:490:LYS:HD2	8:B:490:LYS:HA	1.90	0.40
8:B:1099:THR:HG21	8:B:1180:PHE:HD1	1.86	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	468/514 (91%)	409 (87%)	58 (12%)	1 (0%)	43	72
4	S	594/894 (66%)	509 (86%)	85 (14%)	0	100	100
5	R	322/507 (64%)	292 (91%)	30 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	M	105/415 (25%)	98 (93%)	7 (7%)	0	100	100
7	A	1524/1664 (92%)	1416 (93%)	108 (7%)	0	100	100
8	B	1174/1203 (98%)	1095 (93%)	79 (7%)	0	100	100
9	C	300/335 (90%)	283 (94%)	17 (6%)	0	100	100
10	D	66/137 (48%)	62 (94%)	4 (6%)	0	100	100
11	E	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
12	F	98/155 (63%)	93 (95%)	5 (5%)	0	100	100
13	G	193/326 (59%)	178 (92%)	15 (8%)	0	100	100
14	H	130/146 (89%)	118 (91%)	12 (9%)	0	100	100
15	I	122/125 (98%)	104 (85%)	18 (15%)	0	100	100
16	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
17	K	101/142 (71%)	95 (94%)	6 (6%)	0	100	100
18	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
19	N	131/233 (56%)	115 (88%)	16 (12%)	0	100	100
20	O	493/627 (79%)	453 (92%)	40 (8%)	0	100	100
All	All	6144/7778 (79%)	5633 (92%)	510 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	281	ILE

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	Q	436/476 (92%)	431 (99%)	5 (1%)	65	88
4	S	563/828 (68%)	557 (99%)	6 (1%)	65	88
5	R	313/474 (66%)	306 (98%)	7 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	97/371 (26%)	97 (100%)	0	100	100
7	A	1297/1465 (88%)	1291 (100%)	6 (0%)	81	93
8	B	1030/1053 (98%)	1020 (99%)	10 (1%)	68	89
9	C	269/296 (91%)	269 (100%)	0	100	100
10	D	65/116 (56%)	65 (100%)	0	100	100
11	E	197/197 (100%)	197 (100%)	0	100	100
12	F	90/137 (66%)	89 (99%)	1 (1%)	65	88
13	G	177/291 (61%)	177 (100%)	0	100	100
14	H	116/128 (91%)	116 (100%)	0	100	100
15	I	109/110 (99%)	107 (98%)	2 (2%)	51	80
16	J	64/65 (98%)	62 (97%)	2 (3%)	35	69
17	K	93/130 (72%)	93 (100%)	0	100	100
18	L	40/57 (70%)	40 (100%)	0	100	100
19	N	128/220 (58%)	128 (100%)	0	100	100
20	O	457/576 (79%)	455 (100%)	2 (0%)	84	94
All	All	5541/6990 (79%)	5500 (99%)	41 (1%)	73	92

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	209	ASN
3	Q	293	ARG
3	Q	294	HIS
3	Q	419	LEU
3	Q	480	LEU
4	S	49	THR
4	S	227	LEU
4	S	292	LEU
4	S	363	ILE
4	S	623	LEU
4	S	744	LEU
5	R	168	ILE
5	R	182	LYS
5	R	253	ILE
5	R	283	ARG
5	R	288	ILE
5	R	317	LEU

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Mol	Chain	Res	Type
5	R	401	ILE
7	A	239	PHE
7	A	444	GLN
7	A	467	PHE
7	A	587	VAL
7	A	1086	ILE
7	A	1344	ILE
8	B	72	VAL
8	B	73	ILE
8	B	95	LEU
8	B	102	VAL
8	B	145	VAL
8	B	278	LYS
8	B	306	LEU
8	B	561	ILE
8	B	592	ILE
8	B	1151	ILE
12	F	79	ARG
15	I	47	VAL
15	I	48	VAL
16	J	2	ILE
16	J	52	THR
20	O	163	ILE
20	O	418	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	42	ASN
3	Q	79	GLN
3	Q	84	GLN
3	Q	206	GLN
3	Q	228	ASN
3	Q	294	HIS
3	Q	482	HIS
3	Q	514	ASN
4	S	29	GLN
4	S	222	GLN
4	S	267	ASN
4	S	440	HIS
4	S	461	HIS

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Mol	Chain	Res	Type
4	S	483	HIS
4	S	656	HIS
5	R	15	GLN
5	R	179	HIS
5	R	184	ASN
5	R	207	ASN
5	R	212	HIS
5	R	263	ASN
5	R	298	GLN
5	R	304	HIS
5	R	319	ASN
5	R	382	GLN
6	M	18	GLN
6	M	89	GLN
7	A	116	HIS
7	A	322	ASN
7	A	332	GLN
7	A	340	HIS
7	A	383	ASN
7	A	489	ASN
7	A	592	GLN
7	A	649	ASN
7	A	706	HIS
7	A	748	ASN
7	A	785	GLN
7	A	819	ASN
7	A	880	GLN
7	A	926	GLN
7	A	949	GLN
7	A	1062	HIS
7	A	1072	ASN
7	A	1116	GLN
7	A	1319	ASN
7	A	1323	HIS
7	A	1527	GLN
7	A	1620	GLN
8	B	62	ASN
8	B	168	ASN
8	B	231	HIS
8	B	243	GLN
8	B	248	ASN
8	B	251	HIS

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Mol	Chain	Res	Type
8	B	321	GLN
8	B	361	HIS
8	B	427	GLN
8	B	433	ASN
8	B	456	ASN
8	B	504	HIS
8	B	532	HIS
8	B	686	HIS
8	B	695	ASN
8	B	735	HIS
8	B	770	ASN
8	B	814	ASN
8	B	952	HIS
8	B	1008	HIS
8	B	1041	ASN
8	B	1066	HIS
8	B	1114	GLN
8	B	1115	GLN
9	C	297	HIS
9	C	323	ASN
10	D	30	HIS
10	D	88	GLN
11	E	32	GLN
11	E	99	HIS
11	E	179	GLN
13	G	26	ASN
13	G	65	HIS
13	G	67	ASN
13	G	140	GLN
13	G	154	ASN
15	I	21	ASN
15	I	32	GLN
15	I	74	ASN
16	J	53	HIS
17	K	106	GLN
20	O	66	ASN
20	O	94	ASN
20	O	105	ASN
20	O	121	ASN
20	O	200	ASN
20	O	228	GLN
20	O	318	ASN

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Mol	Chain	Res	Type
20	O	346	GLN
20	O	371	HIS
20	O	438	GLN
20	O	533	GLN
20	O	547	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

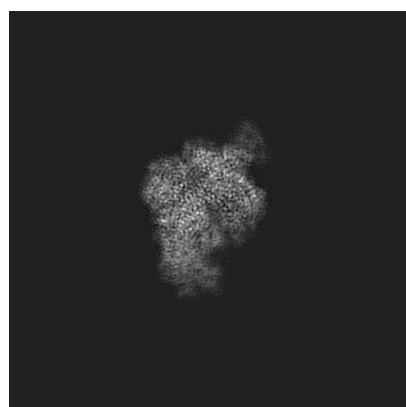
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4984. These allow visual inspection of the internal detail of the map and identification of artifacts.

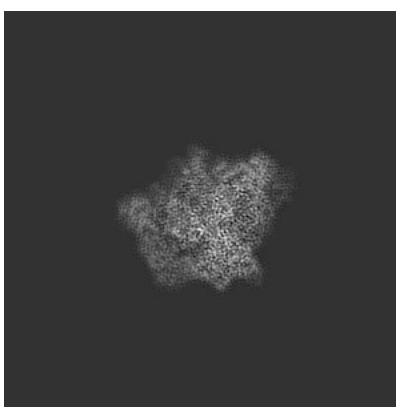
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

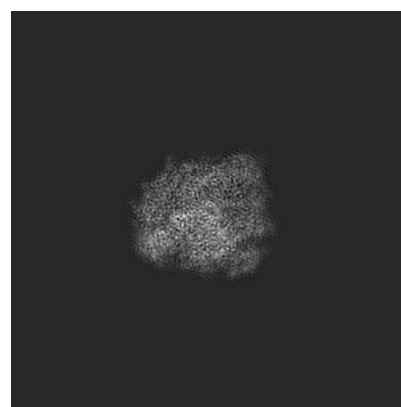
6.1.1 Primary map



X



Y

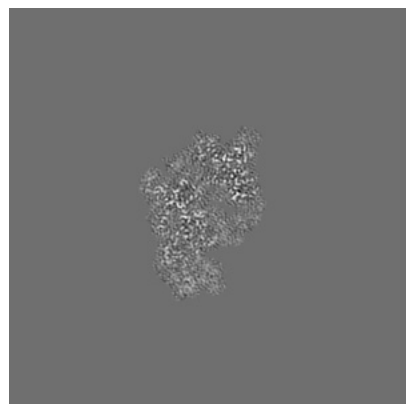


Z

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

6.2 Central slices [i](#)

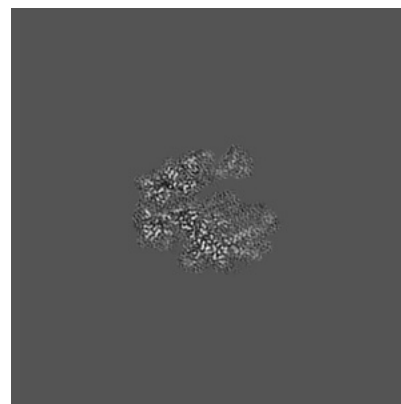
6.2.1 Primary map



X Index: 190



Y Index: 190

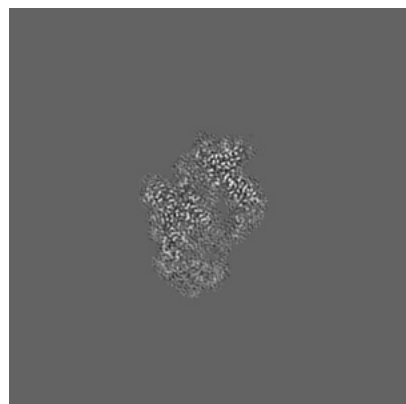


Z Index: 190

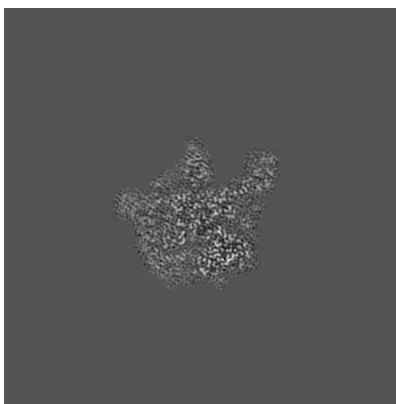
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

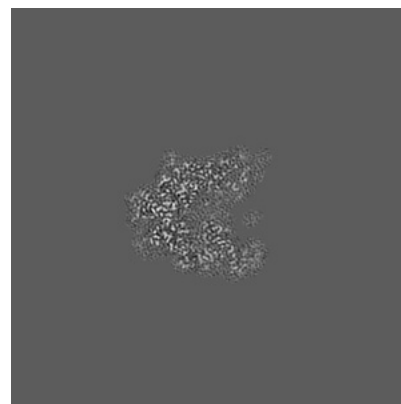
6.3.1 Primary map



X Index: 181



Y Index: 168

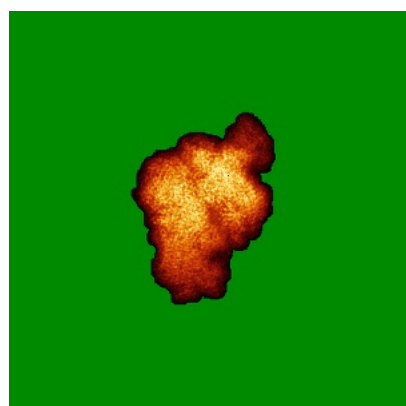


Z Index: 209

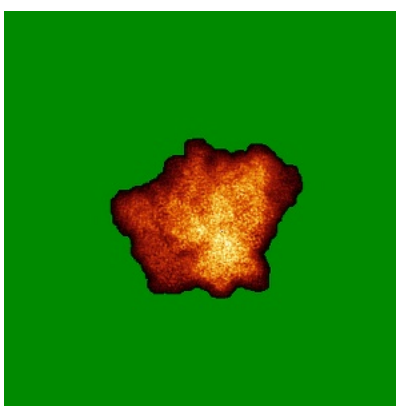
The images above show the largest variance slices of the map in three orthogonal directions.

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

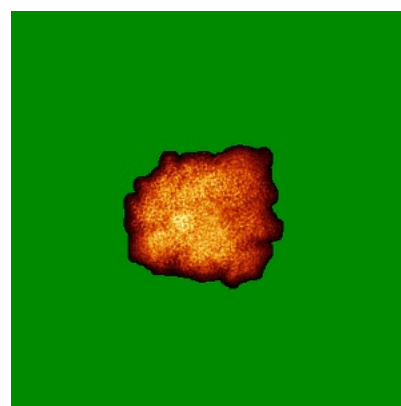
6.4.1 Primary map



X



Y

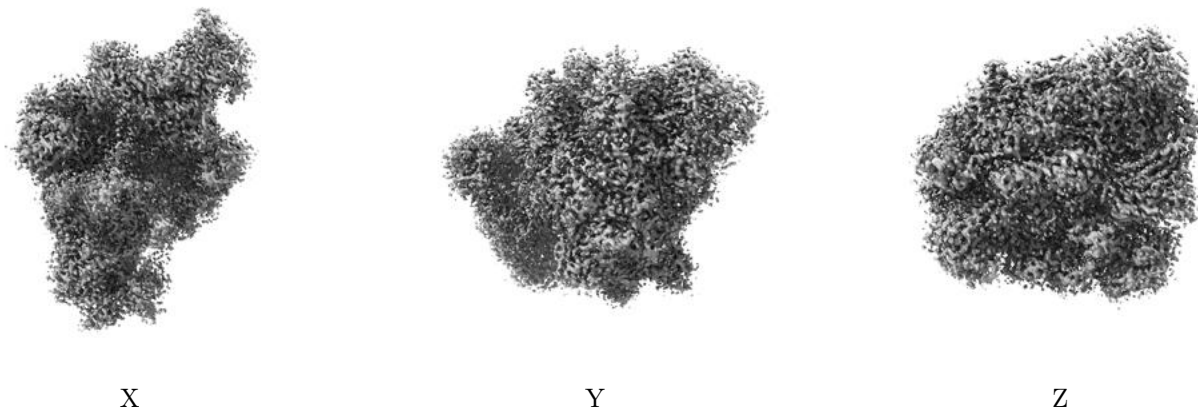


Z

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

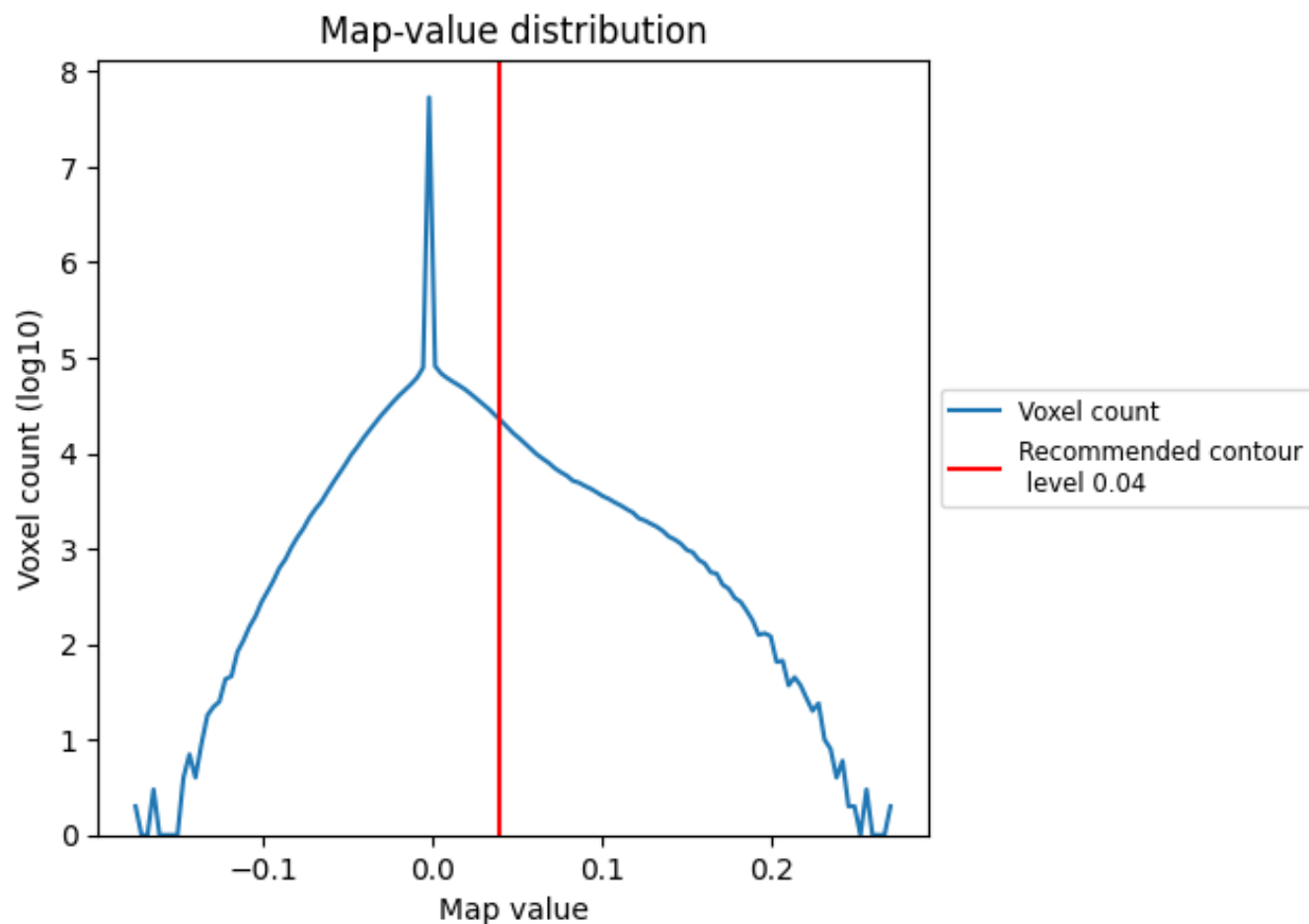
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

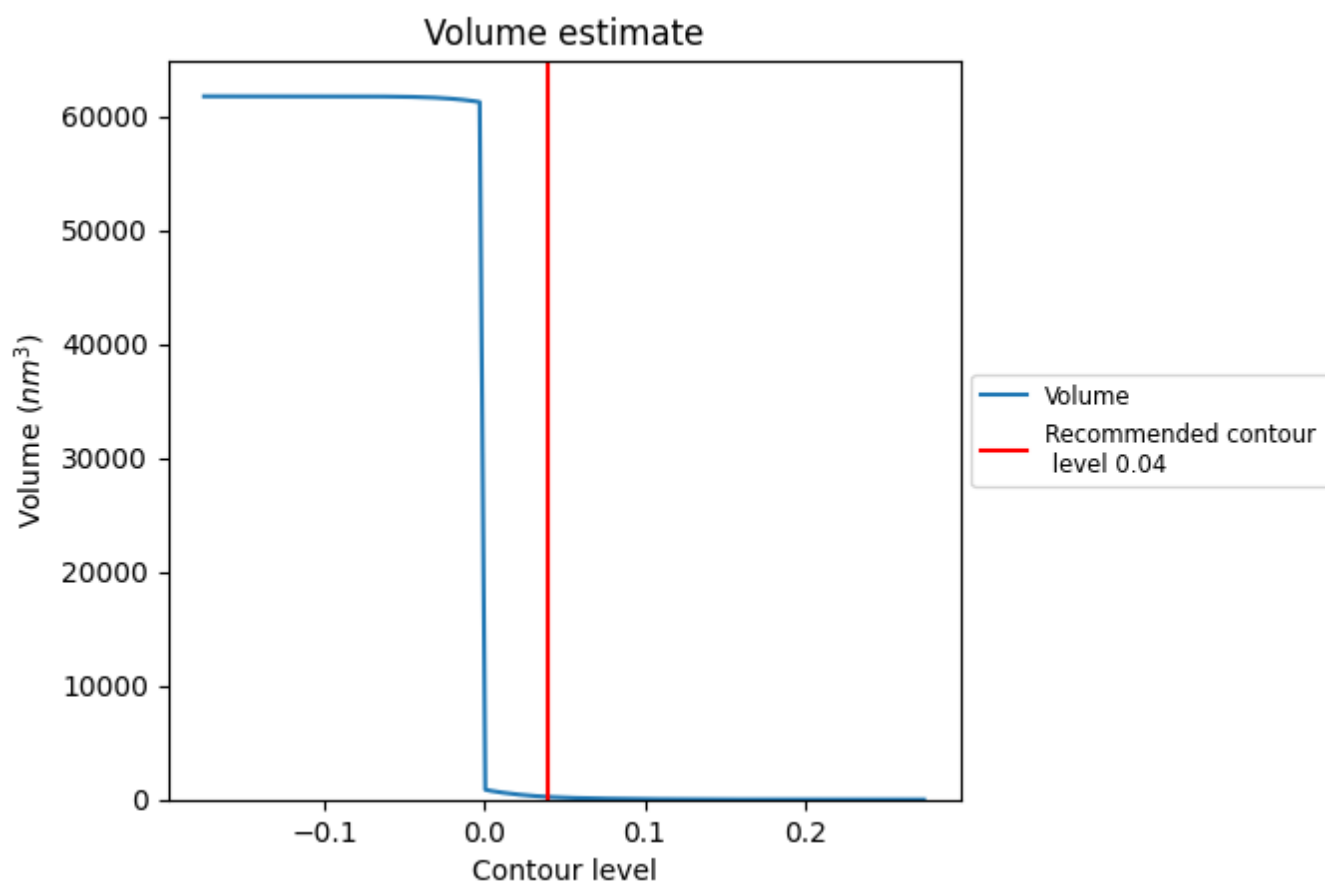
This section contains the results of statistical analysis of the map.

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.

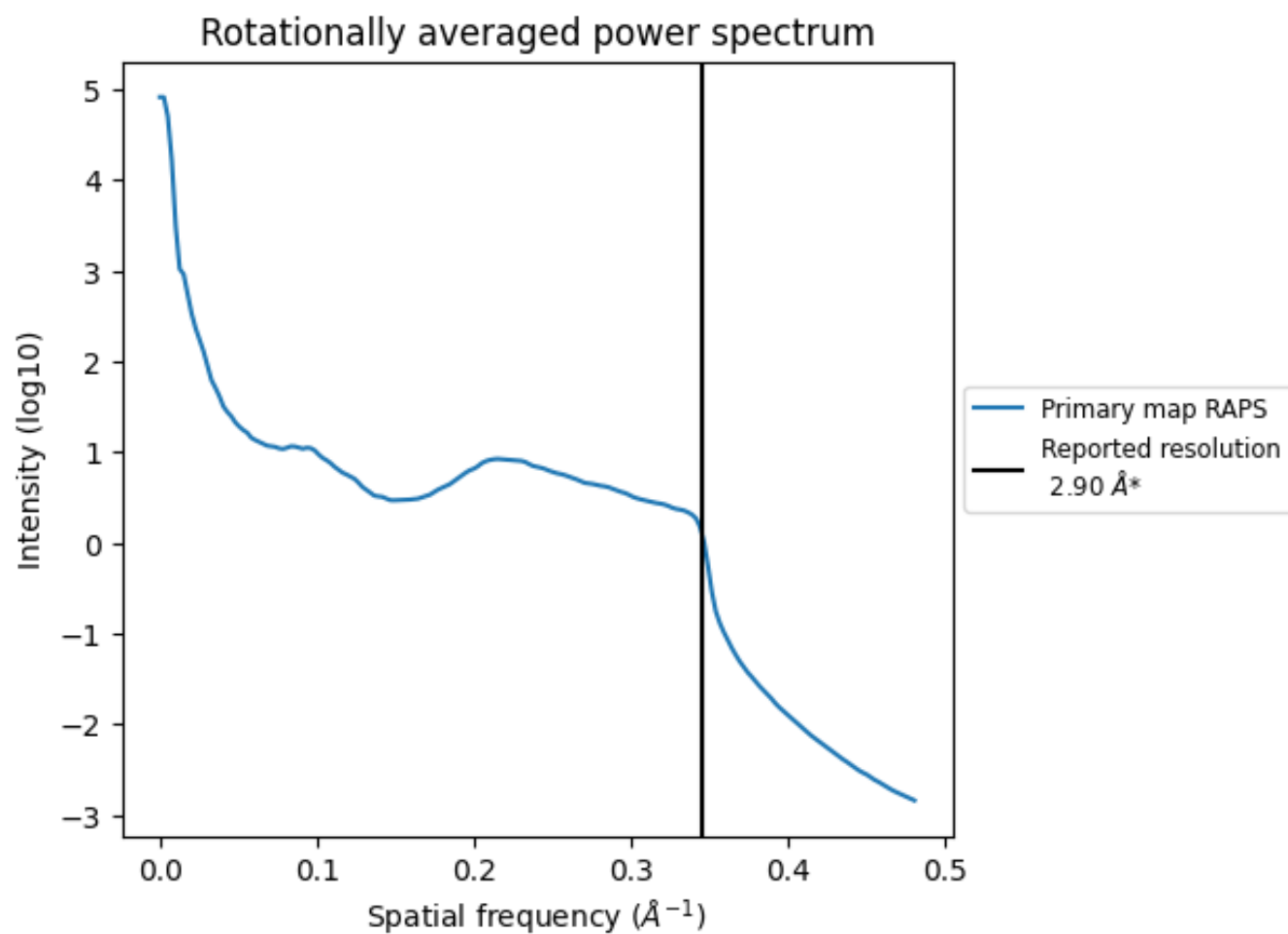
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 233 nm³; this corresponds to an approximate mass of 210 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 0.345 Å⁻¹

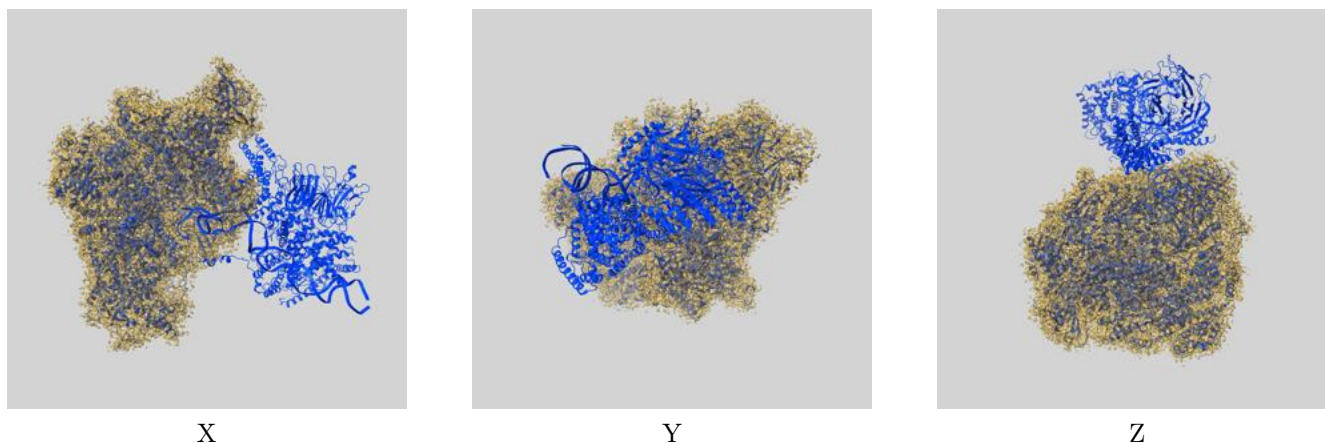
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

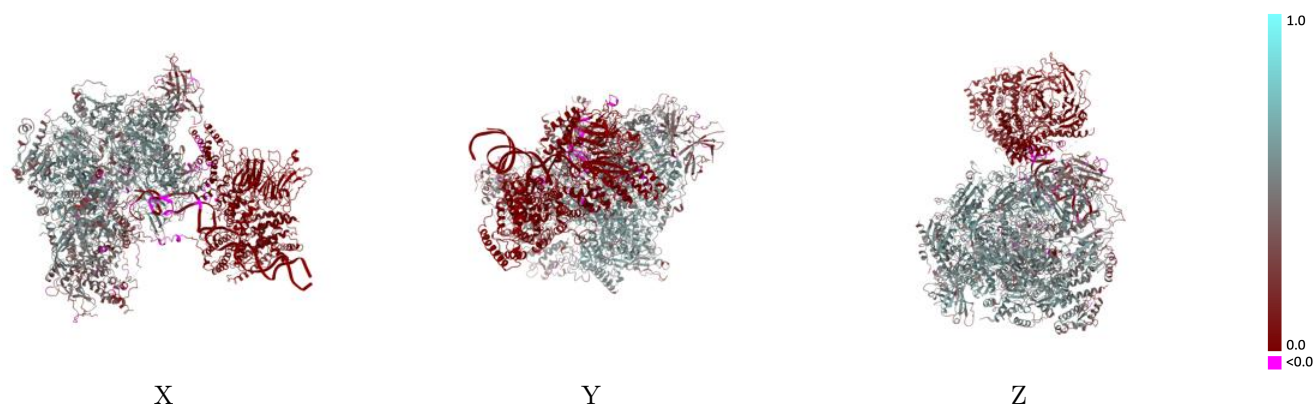
This section contains information regarding the fit between EMDB map EMD-4984 and PDB model 6RQL. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



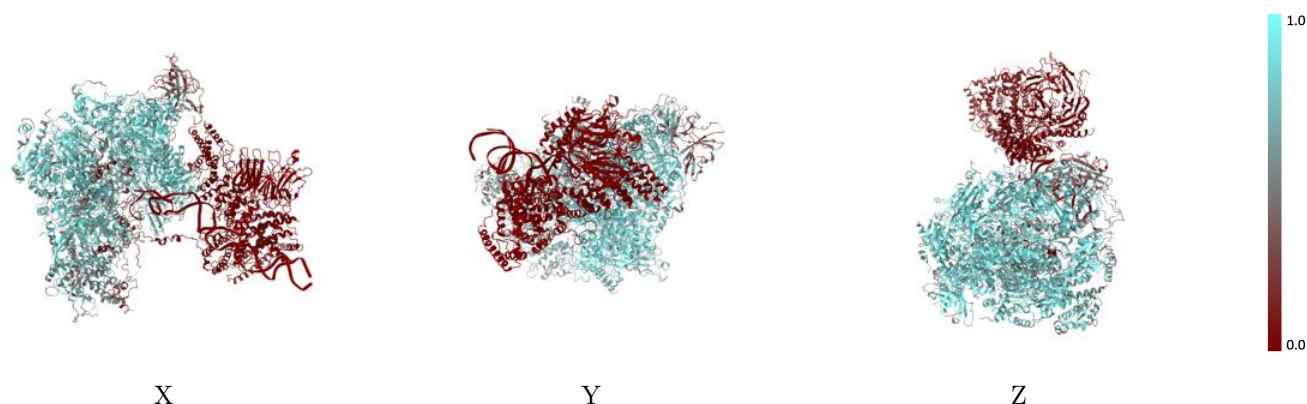
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



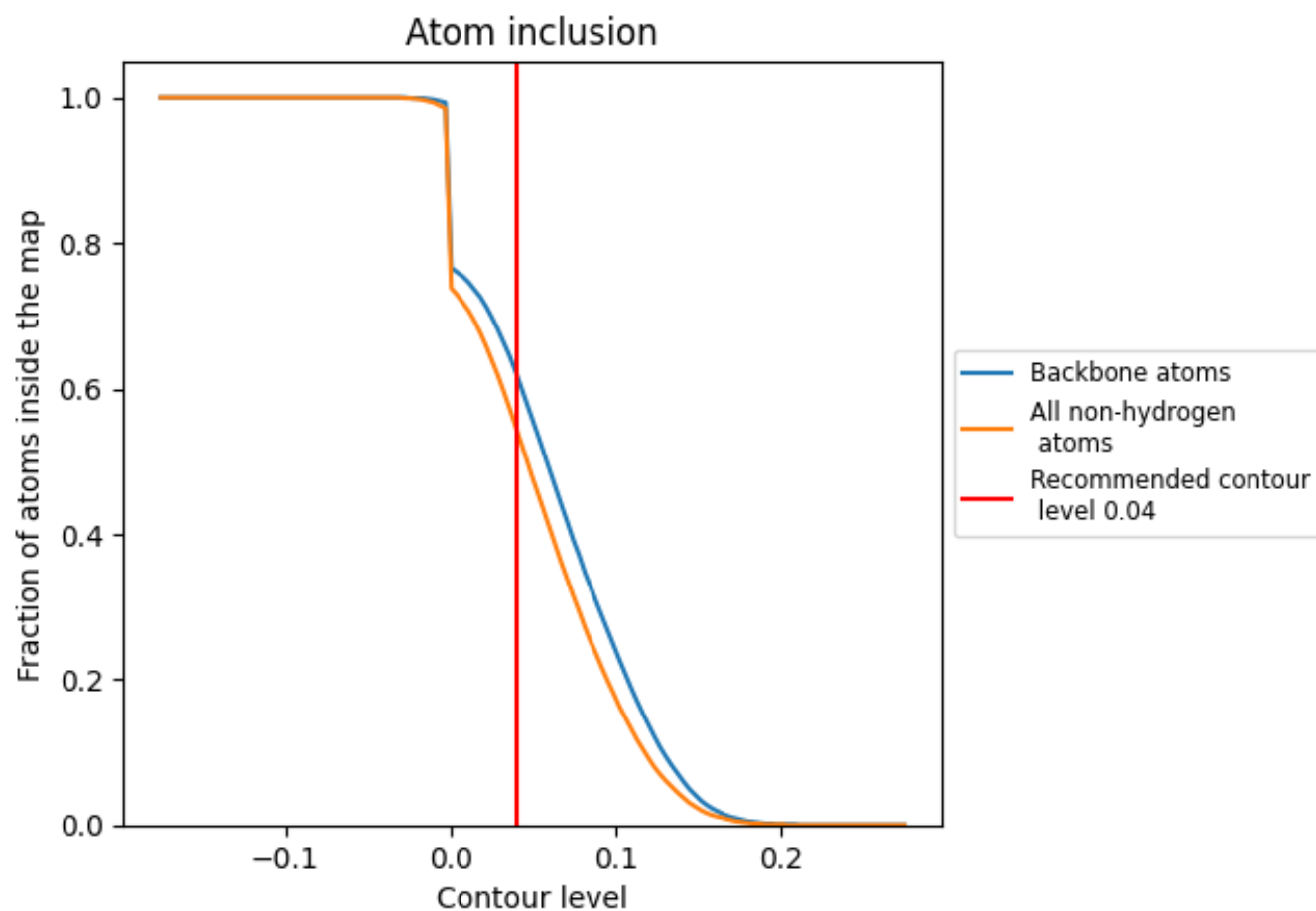
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5440	 0.3550
A	 0.7700	 0.5030
B	 0.8190	 0.5260
C	 0.7960	 0.5050
D	 0.5890	 0.3940
E	 0.7560	 0.4740
F	 0.8190	 0.5470
G	 0.6690	 0.4190
H	 0.7720	 0.4890
I	 0.5490	 0.3860
J	 0.8950	 0.5630
K	 0.7950	 0.5230
L	 0.7770	 0.4850
M	 0.3960	 0.3260
N	 0.3500	 0.3050
O	 0.5300	 0.3390
Q	 0.0620	 0.0400
R	 0.0070	 0.0080
S	 0.0000	 0.0000
T	 0.0090	 0.0070
U	 0.0030	 0.0100

