



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:34 PM UTC

PDB ID : 6RUO / pdb_00006ruo
EMDB ID : EMD-10007
Title : RNA Polymerase I Open Complex conformation 1
Authors : Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on : 2019-05-28
Resolution : 3.50 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:

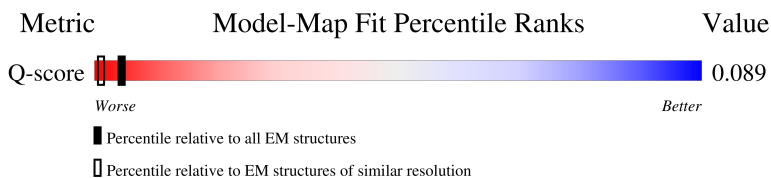
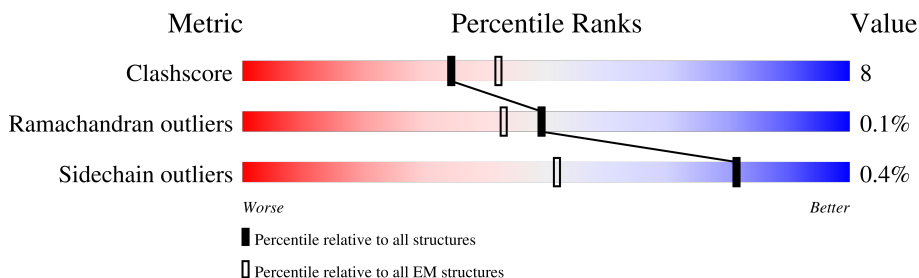
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.50 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	13950 (3.00 - 4.00)

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	Q	514	55% 66% 17% 16%
2	M	415	19% 20% 5% 74%
3	A	1664	33% 69% 19% 12%
4	B	1203	38% 76% 22% .

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Mol	Chain	Length	Quality of chain
5	C	335	
6	D	137	
7	E	215	
8	F	155	
9	G	326	
10	H	146	
11	I	125	
12	J	70	
13	K	142	
14	L	70	
15	N	233	
16	O	627	
17	S	894	
18	R	507	
19	T	70	
20	U	70	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 50792 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	430	Total	C	N	O	S	0	0
			3572	2306	602	644	20		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA49.

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

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1465	Total	C	N	O	S	0	0
			11567	7308	2012	2186	61		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA135.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA43.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA12.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA34.

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

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	462	Total	C	N	O	S	0	0
			3807	2471	622	693	21		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

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

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

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

- Molecule 19 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	50	Total	C	N	O	P	0	0
			1000	481	164	305	50		

- Molecule 20 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	43	Total	C	N	O	P	0	0
			901	427	182	250	42		

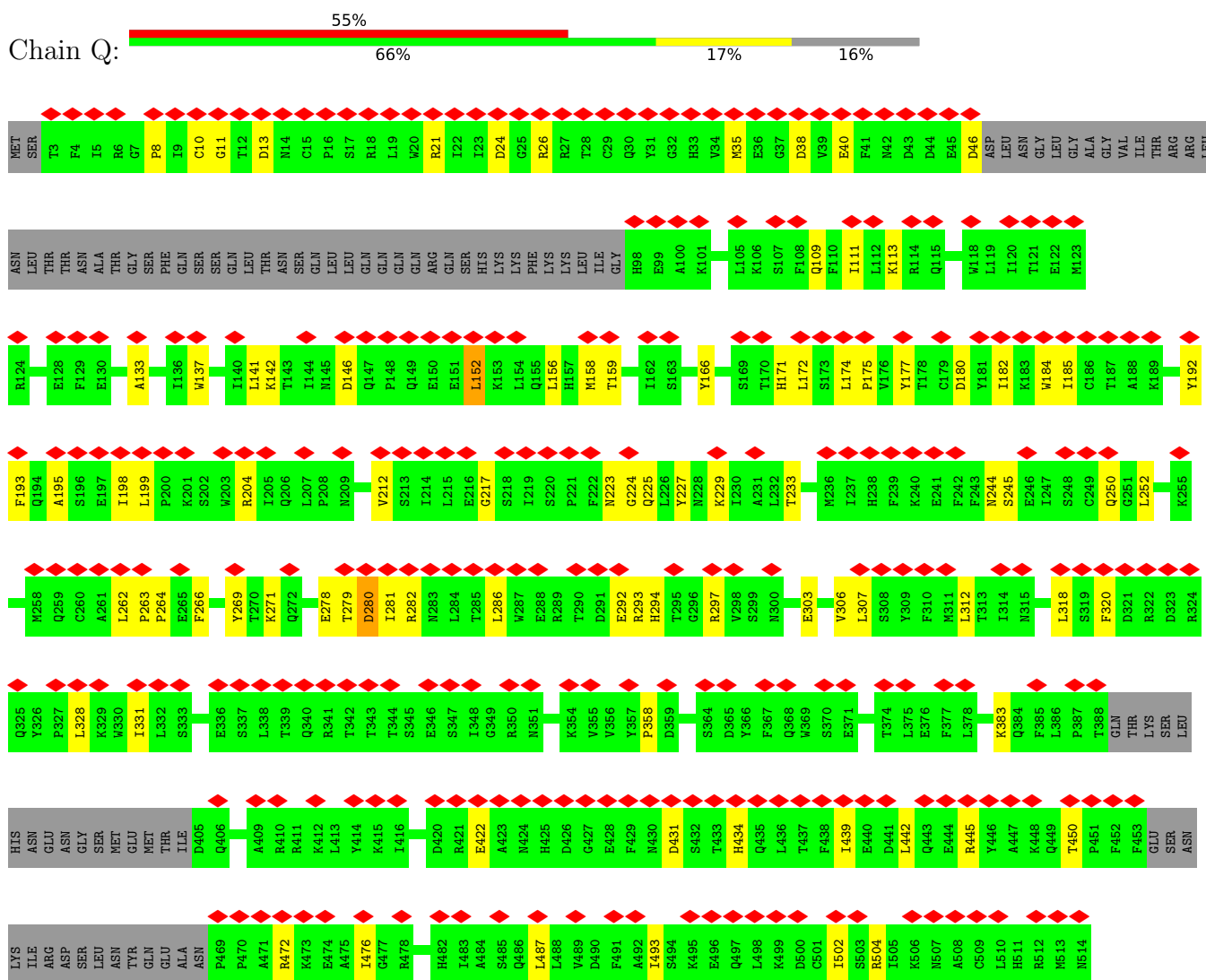
- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

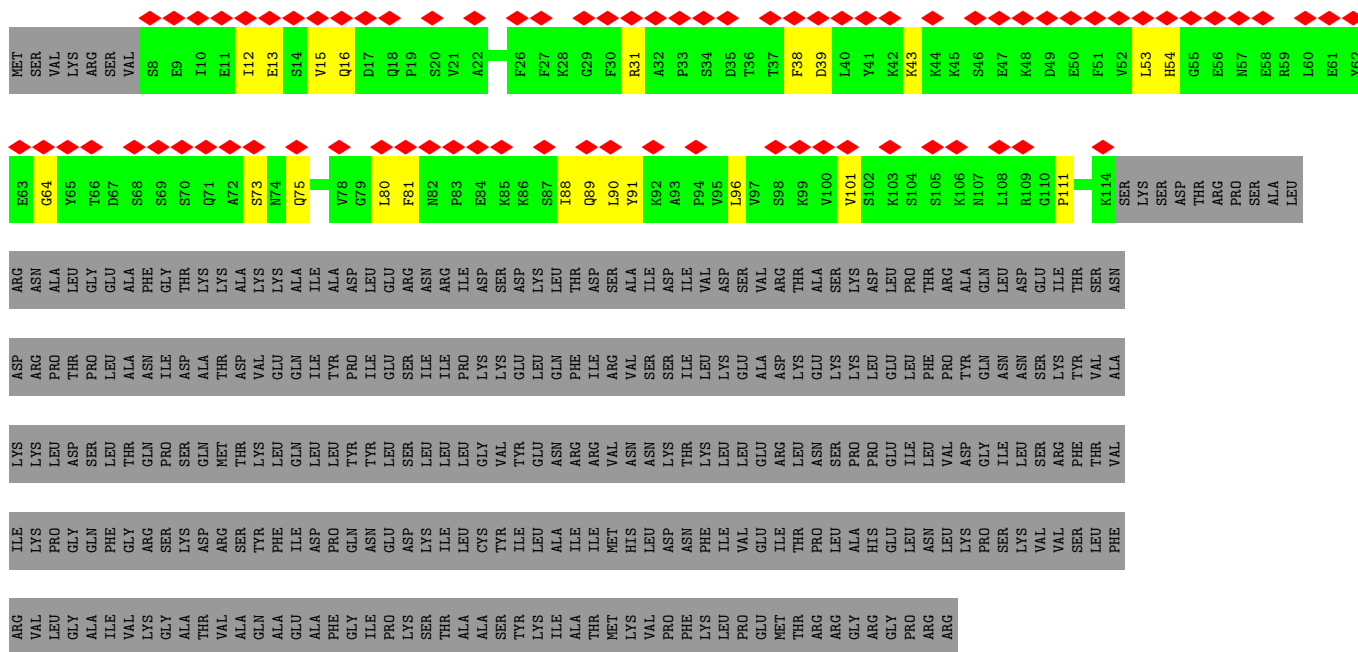
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA polymerase I-specific transcription initiation factor RRN7

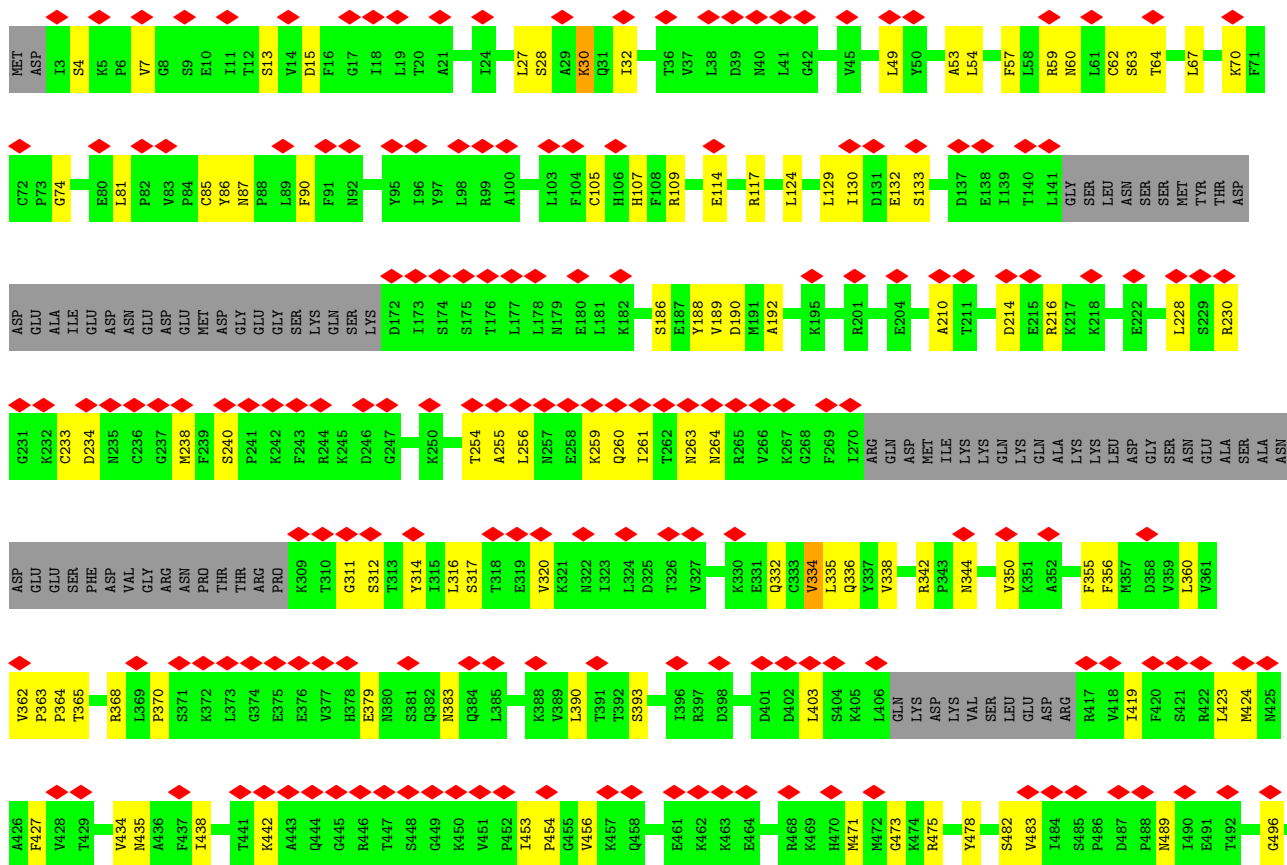


- Molecule 2: DNA-directed RNA polymerase I subunit RPA49

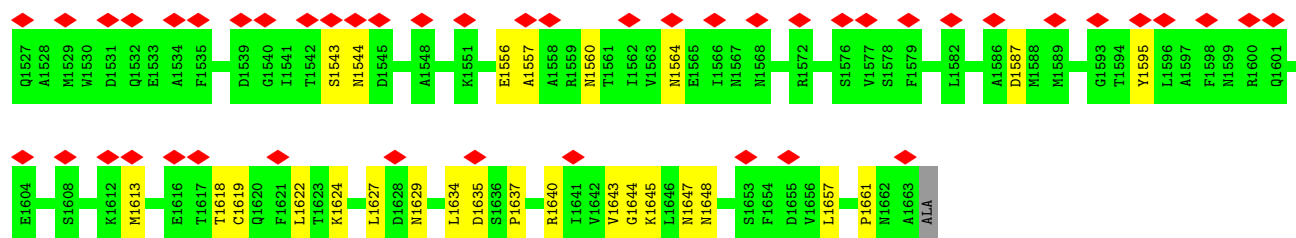




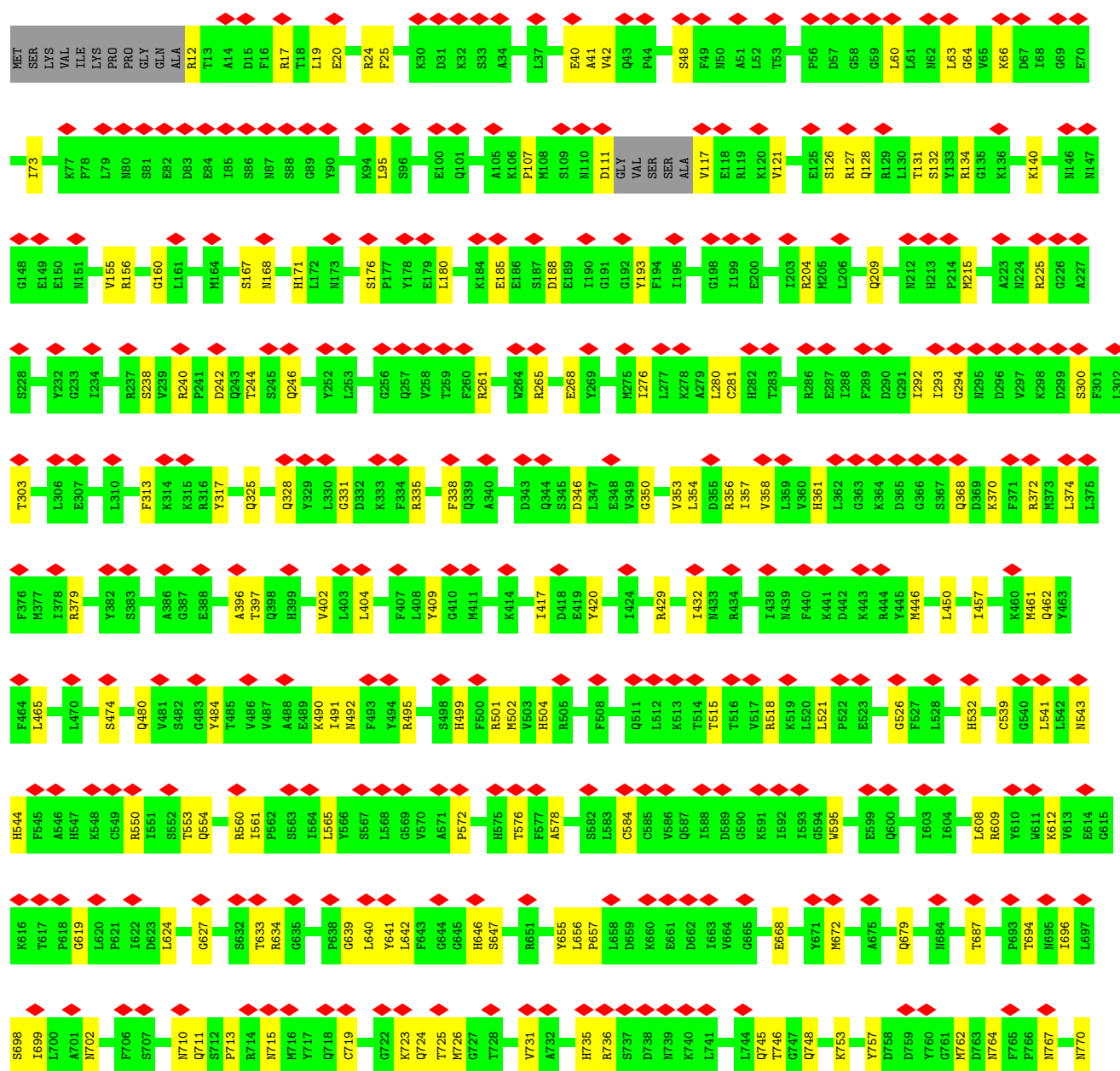
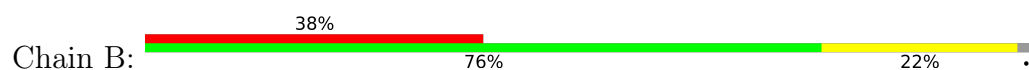
• Molecule 3: DNA-directed RNA polymerase I subunit RPA190

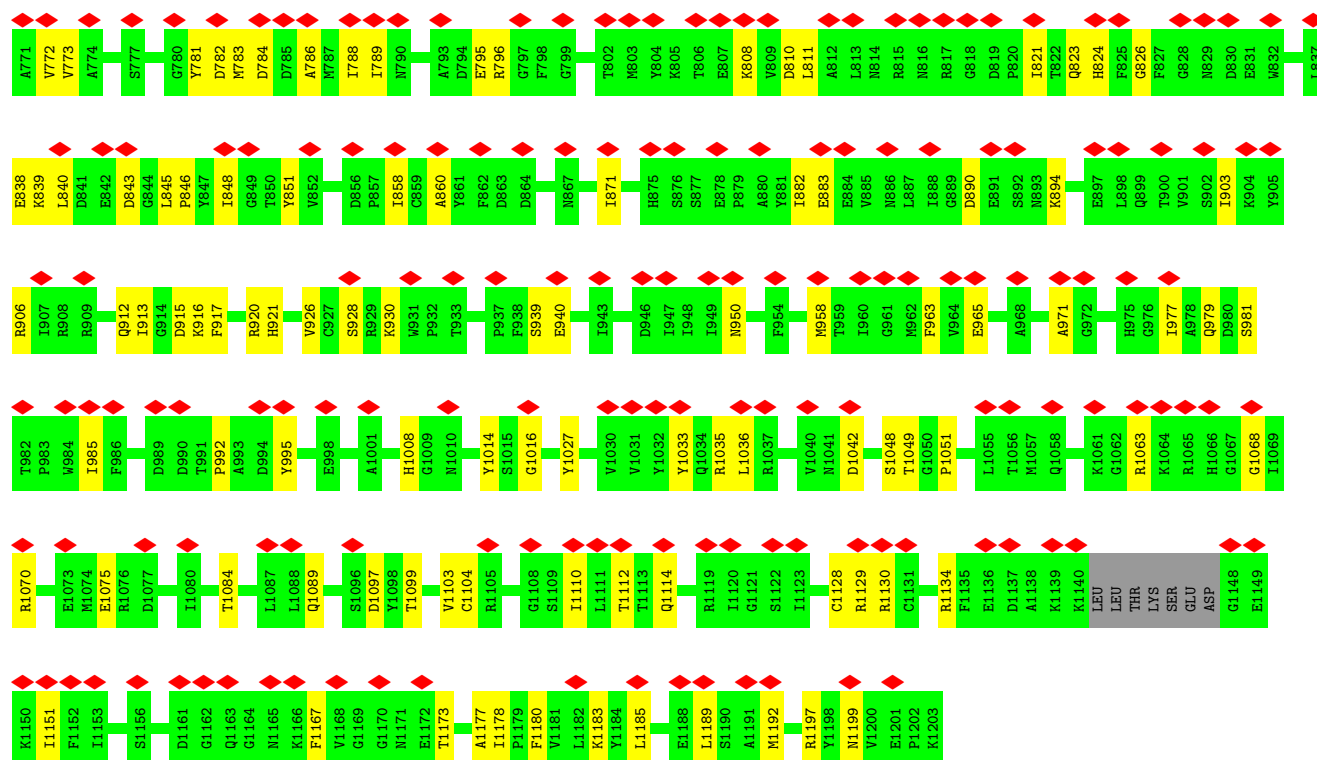




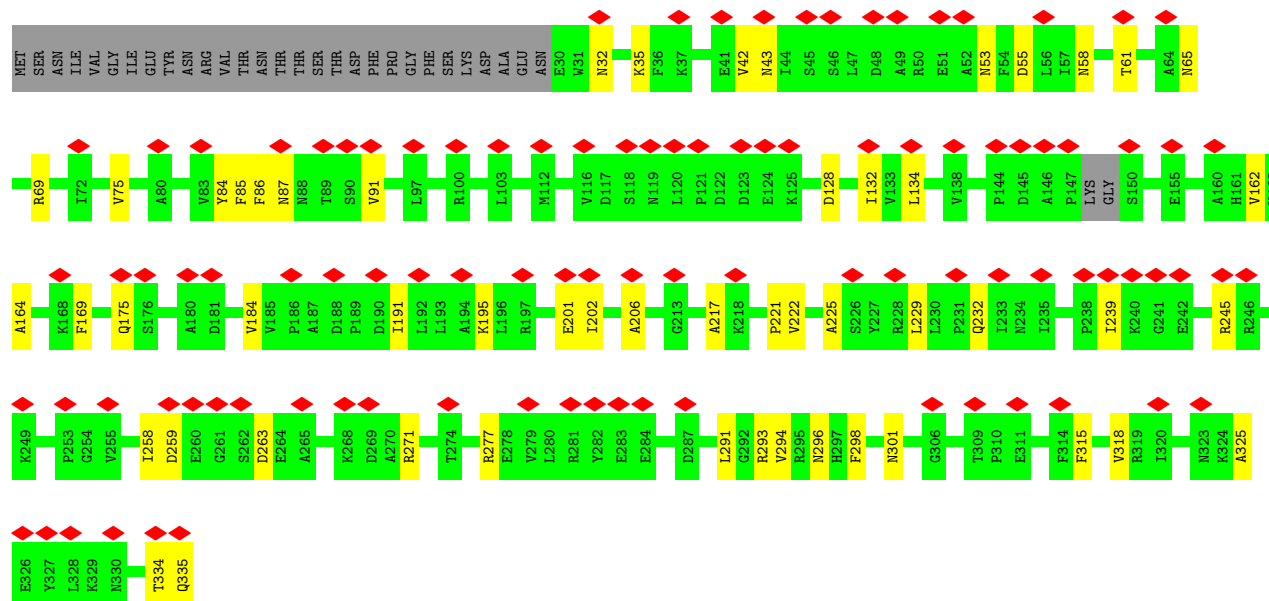
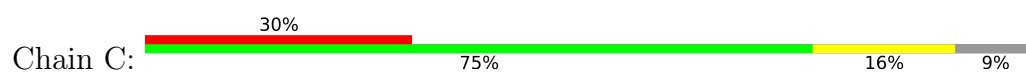


• Molecule 4: DNA-directed RNA polymerase I subunit RPA135

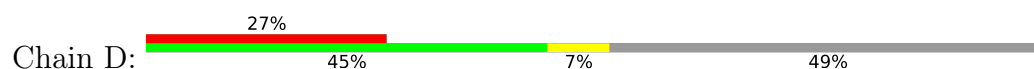




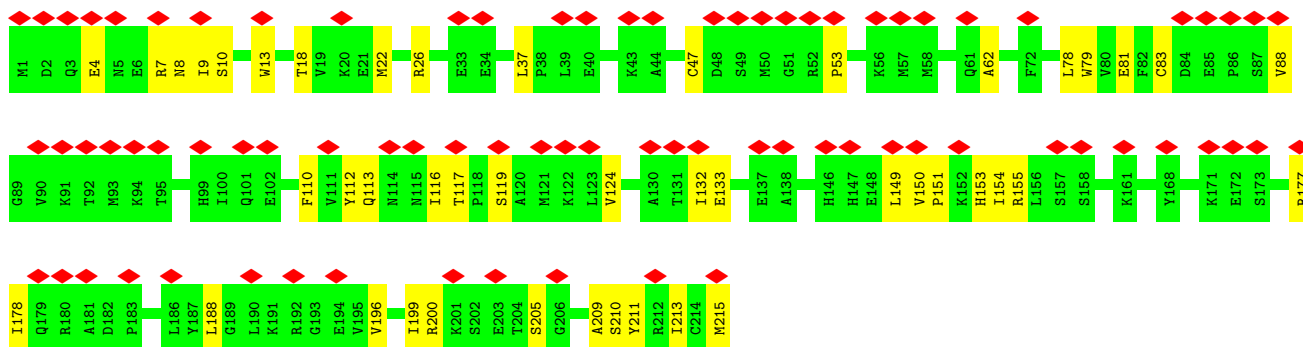
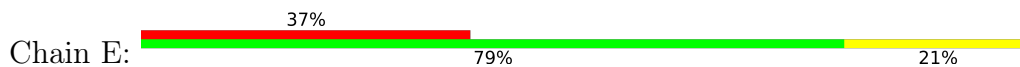
• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC1



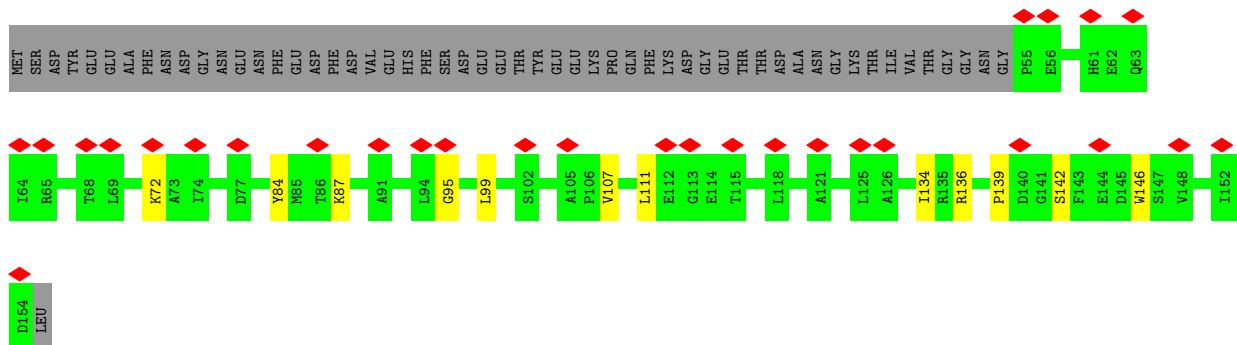
• Molecule 6: DNA-directed RNA polymerase I subunit RPA14



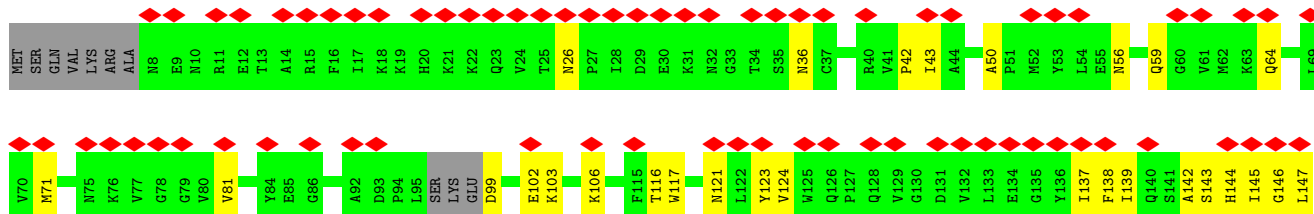
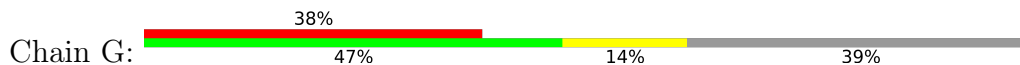
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

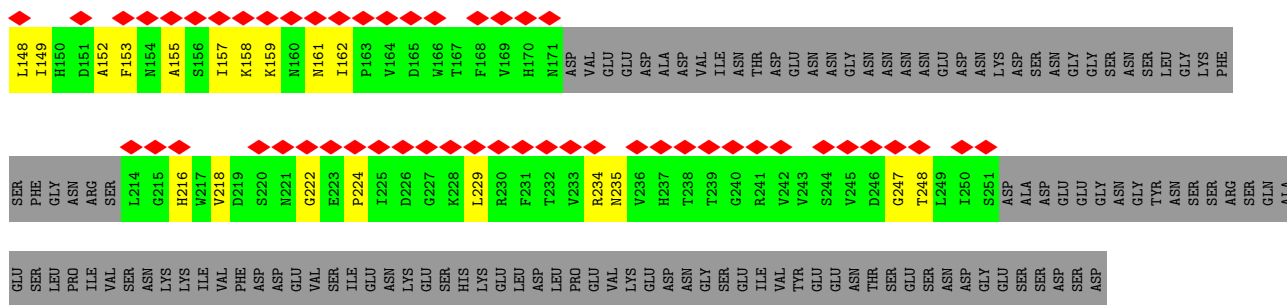


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

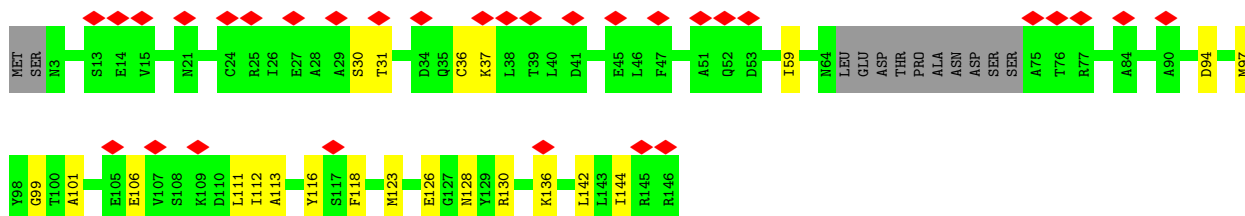
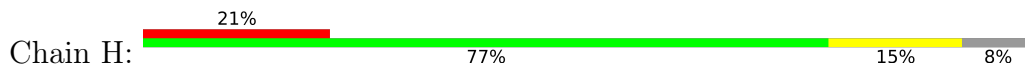


- Molecule 9: DNA-directed RNA polymerase I subunit RPA43

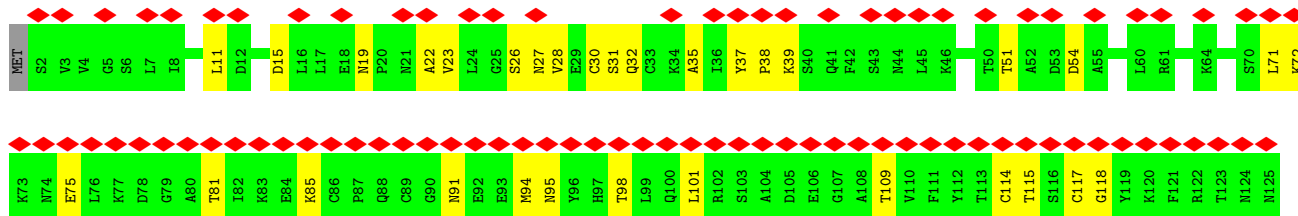




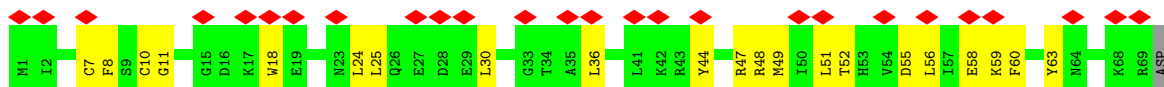
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



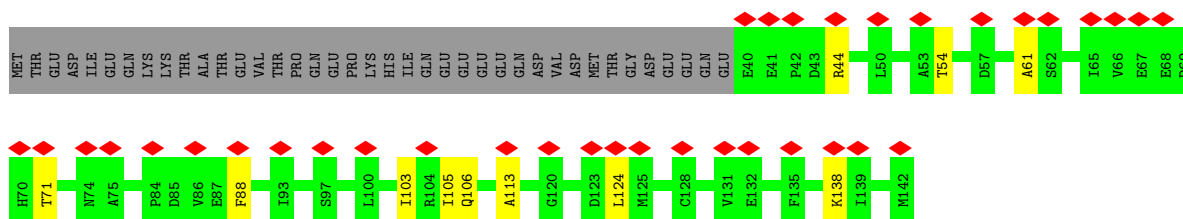
- Molecule 11: DNA-directed RNA polymerase I subunit RPA12

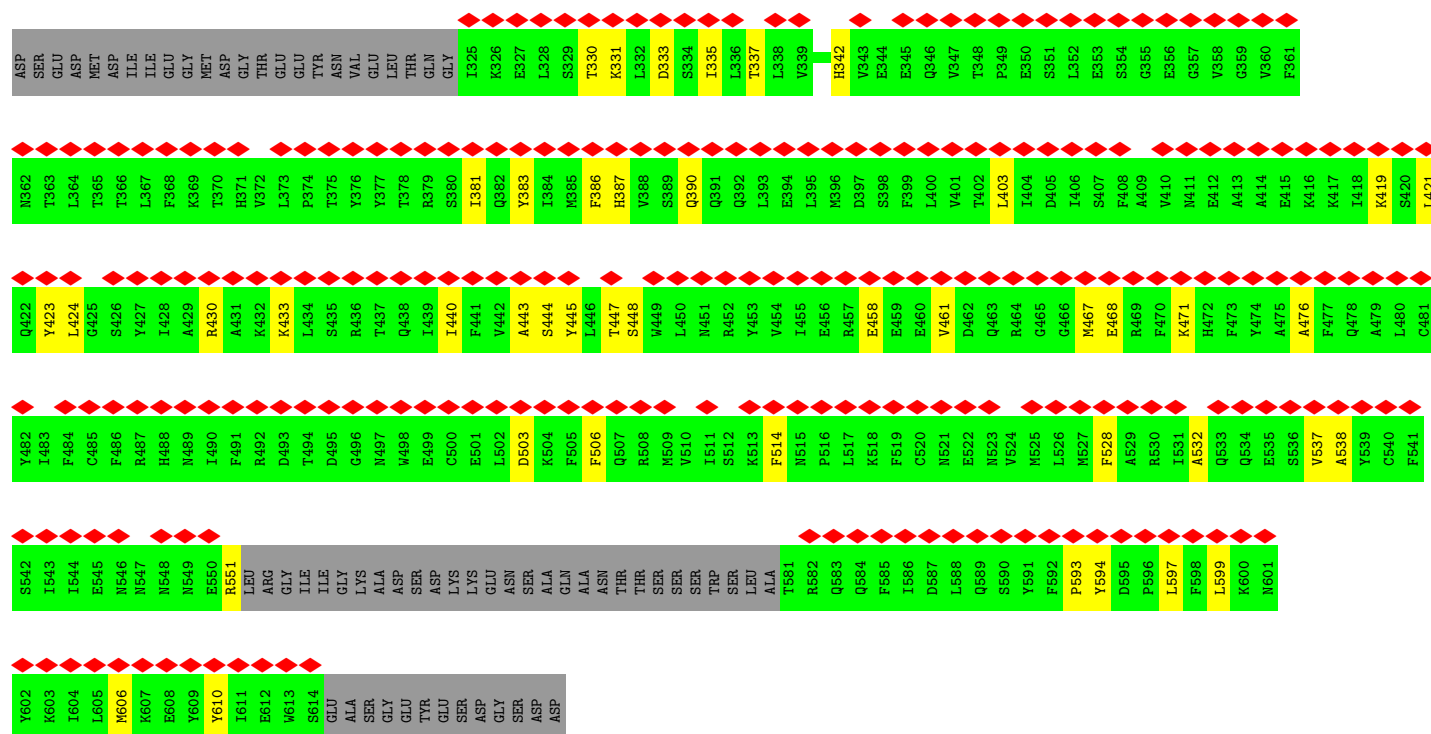


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

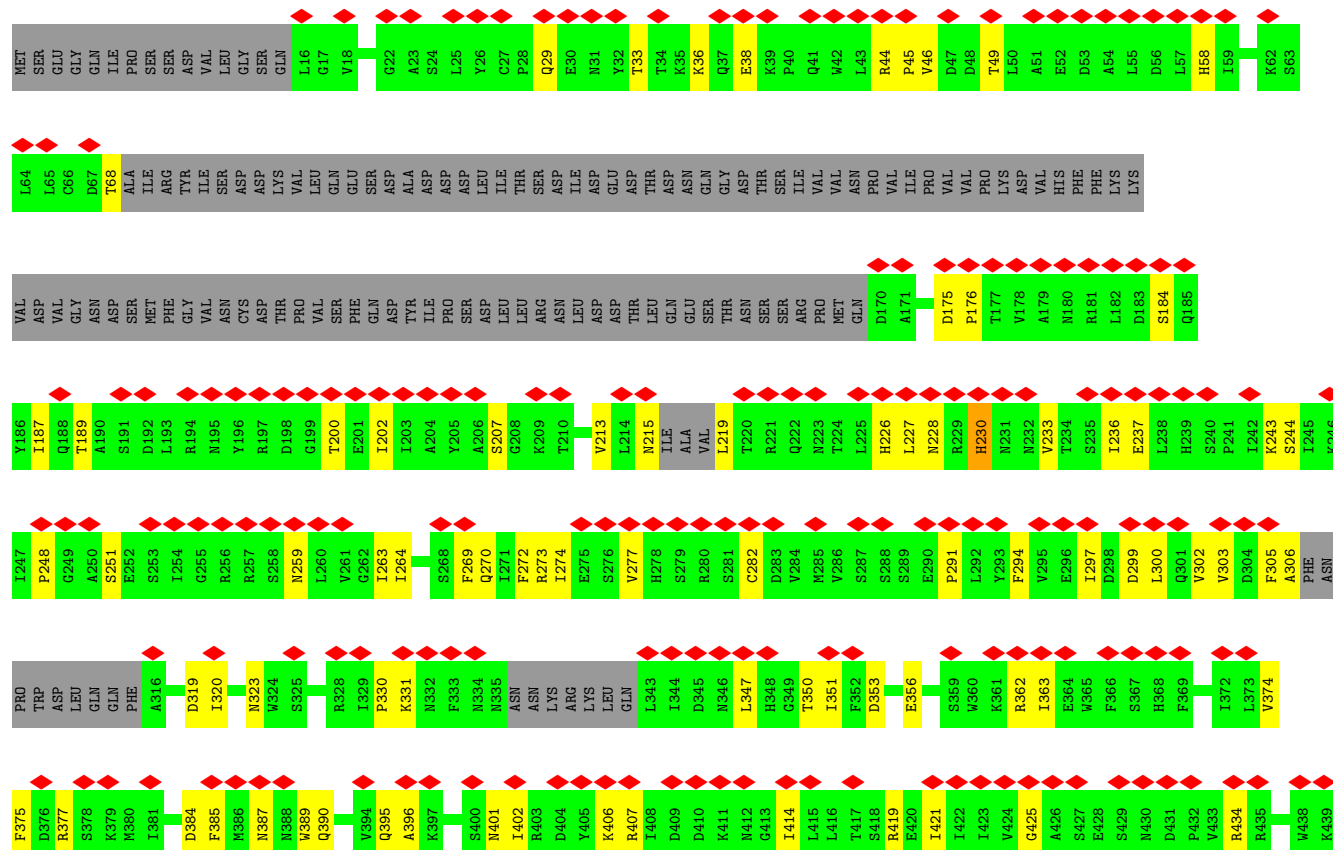


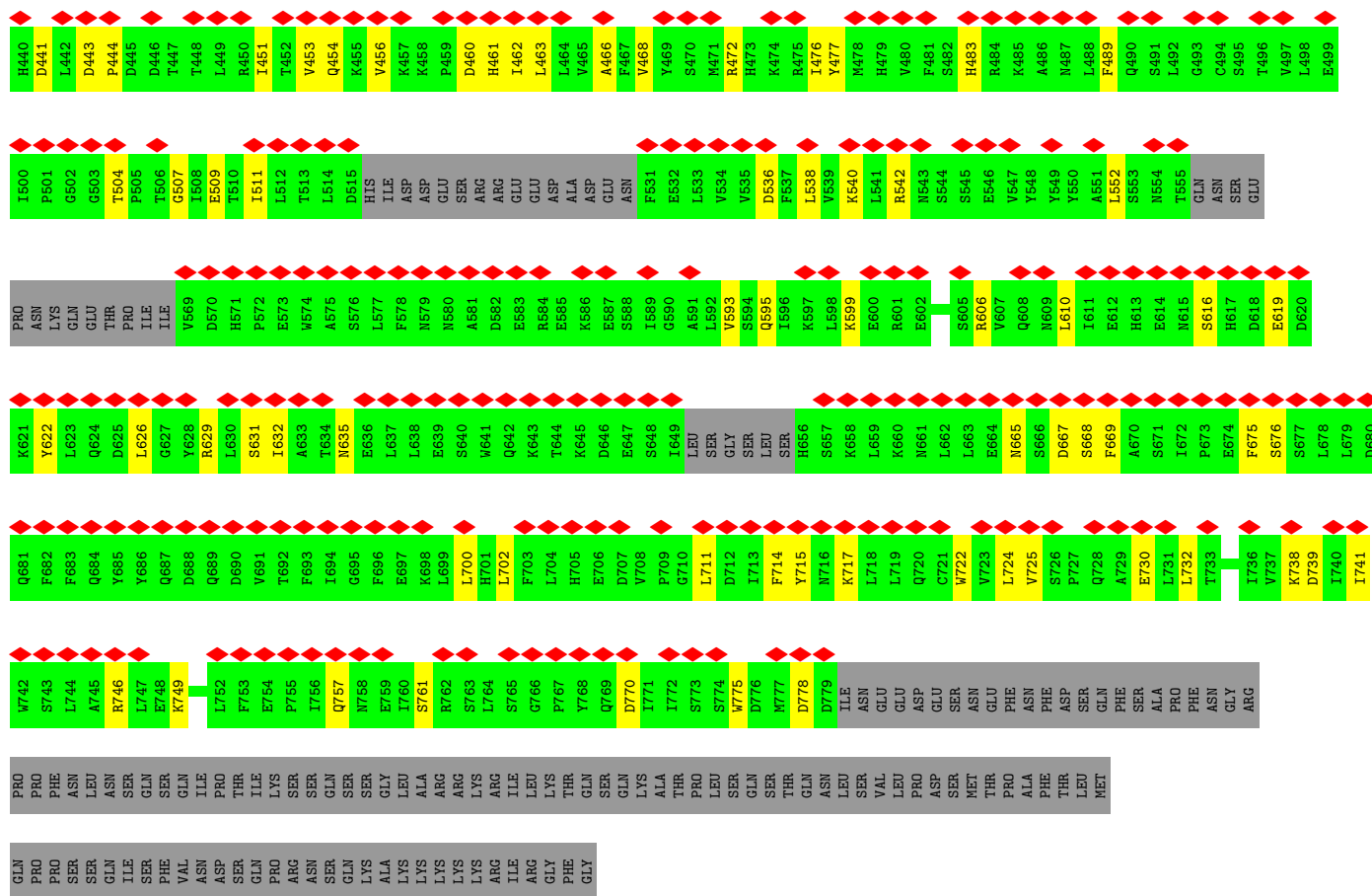
- Molecule 13: DNA-directed RNA polymerases I and III subunit RPAC2



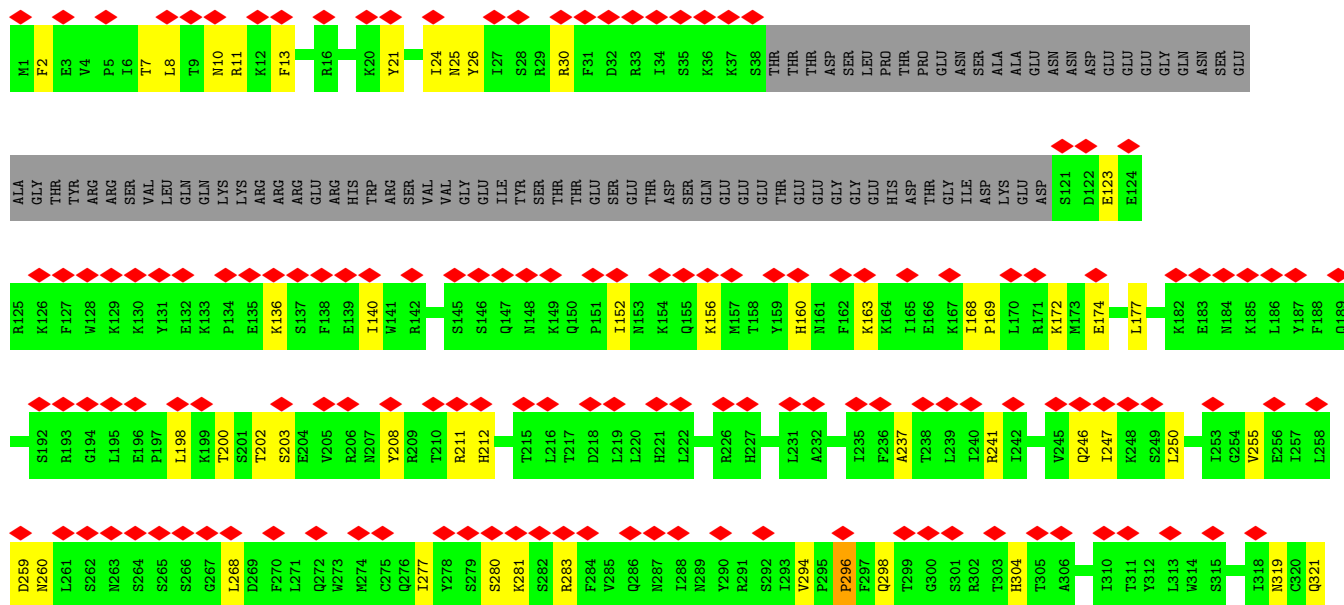


• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN6





● Molecule 18: 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	75851	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	0.272	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	Q	0.28	0/3661	0.64	1/4950 (0.0%)
2	M	0.29	0/866	0.59	0/1162
3	A	0.35	1/11778 (0.0%)	0.61	1/15908 (0.0%)
4	B	0.39	0/9578	0.64	2/12948 (0.0%)
5	C	0.38	0/2469	0.62	0/3347
6	D	0.26	0/557	0.62	0/750
7	E	0.32	0/1795	0.54	0/2416
8	F	0.33	0/838	0.60	0/1129
9	G	0.27	0/1613	0.54	0/2193
10	H	0.35	0/1090	0.63	0/1476
11	I	0.25	0/955	0.57	0/1288
12	J	0.45	0/578	0.69	0/775
13	K	0.40	0/821	0.63	0/1108
14	L	0.37	0/361	0.71	0/478
15	N	0.26	0/1124	0.57	0/1512
16	O	0.21	0/3893	0.56	3/5263 (0.1%)
17	S	0.27	0/5065	0.61	2/6859 (0.0%)
18	R	0.29	0/2836	0.63	0/3817
19	T	0.33	0/1113	0.61	0/1707
20	U	0.27	0/1016	0.43	0/1569
All	All	0.33	1/52007 (0.0%)	0.61	9/70655 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	659	THR	C-N	-5.86	1.28	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	237	ILE	N-CA-C	-10.31	102.65	112.96
16	O	236	LYS	CA-C-N	7.05	129.80	121.84
16	O	236	LYS	C-N-CA	7.05	129.80	121.84
17	S	230	HIS	CA-C-N	5.77	130.59	122.46
17	S	230	HIS	C-N-CA	5.77	130.59	122.46
1	Q	281	ILE	N-CA-C	5.53	116.92	110.62
3	A	1329	ILE	N-CA-C	-5.37	107.55	111.90
4	B	42	VAL	CA-C-N	5.20	126.59	120.09
4	B	42	VAL	C-N-CA	5.20	126.59	120.09

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	Q	3572	0	3541	66	0
2	M	850	0	850	17	0
3	A	11567	0	11655	207	0
4	B	9371	0	9242	189	0
5	C	2418	0	2401	41	0
6	D	551	0	558	14	0
7	E	1759	0	1788	27	0
8	F	823	0	841	6	0
9	G	1576	0	1581	35	0
10	H	1072	0	1042	15	0
11	I	942	0	932	21	0
12	J	569	0	586	20	0
13	K	810	0	801	7	0
14	L	359	0	381	16	0
15	N	1103	0	1106	26	0
16	O	3807	0	3801	63	0
17	S	4963	0	4890	94	0
18	R	2771	0	2844	46	0
19	T	1000	0	568	11	0
20	U	901	0	485	15	0
21	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	50792	0	49893	796	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 8.

All (796) 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)
4:B:731:VAL:HG11	12:J:56:LEU:CD2	1.74	1.18
16:O:237:ILE:HG21	16:O:381:ILE:CD1	1.74	1.17
4:B:731:VAL:CG1	12:J:56:LEU:HD21	1.75	1.15
16:O:237:ILE:CG2	16:O:381:ILE:HD13	1.78	1.13
3:A:30:LYS:HE3	4:B:1129:ARG:HH22	0.98	1.13
1:Q:152:LEU:HD23	1:Q:152:LEU:H	1.20	1.01
3:A:30:LYS:HE3	4:B:1129:ARG:NH2	1.75	1.01
6:D:12:THR:HG22	6:D:12:THR:O	1.76	0.84
16:O:237:ILE:HG21	16:O:381:ILE:HD13	0.87	0.82
4:B:731:VAL:HG11	12:J:56:LEU:HD21	0.86	0.74
1:Q:152:LEU:H	1:Q:152:LEU:CD2	1.98	0.74
18:R:294:VAL:HG22	18:R:296:PRO:HD2	1.70	0.74
3:A:27:LEU:HB3	4:B:1130:ARG:HB3	1.72	0.72
12:J:56:LEU:HD23	12:J:56:LEU:O	1.90	0.71
1:Q:152:LEU:HD23	1:Q:152:LEU:N	2.02	0.71
17:S:270:GLN:HG2	17:S:291:PRO:HB3	1.74	0.69
3:A:30:LYS:CE	4:B:1129:ARG:HH22	1.92	0.69
4:B:731:VAL:CG1	12:J:56:LEU:CD2	2.52	0.69
3:A:1291:VAL:HG22	3:A:1473:LYS:HG2	1.75	0.68
3:A:673:HIS:HD2	3:A:817:PHE:HB2	1.59	0.68
1:Q:177:TYR:H	1:Q:180:ASP:HB2	1.58	0.67
3:A:74:GLY:HA3	3:A:364:PRO:HB3	1.77	0.67
17:S:700:LEU:HD21	17:S:714:PHE:CG	2.29	0.67
1:Q:193:PHE:HA	1:Q:217:GLY:HA3	1.77	0.66
17:S:323:ASN:HD22	18:R:156:LYS:HB2	1.59	0.66
5:C:58:ASN:HA	5:C:296:ASN:HB3	1.77	0.66
13:K:88:PHE:HB3	13:K:106:GLN:HB2	1.78	0.65
3:A:342:ARG:NH1	3:A:1629:ASN:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:964:LYS:NZ	4:B:672:MET:O	2.29	0.64
3:A:1118:VAL:HG21	7:E:154:ILE:HG12	1.79	0.64
8:F:72:LYS:HB3	8:F:142:SER:HA	1.78	0.64
2:M:13:GLU:HB2	2:M:89:GLN:HB3	1.80	0.64
4:B:1016:GLY:O	5:C:69:ARG:NH2	2.31	0.64
4:B:111:ASP:OD2	14:L:54:ARG:NH2	2.31	0.63
3:A:1240:LEU:HB2	3:A:1519:LEU:HB2	1.81	0.63
3:A:884:ARG:NH2	4:B:633:THR:O	2.32	0.62
1:Q:245:SER:HB2	1:Q:286:LEU:HB3	1.81	0.62
5:C:134:LEU:HB2	5:C:206:ALA:HB3	1.80	0.62
17:S:384:ASP:HB3	17:S:389:TRP:HB3	1.81	0.62
17:S:401:ASN:H	17:S:419:ARG:HG2	1.65	0.62
4:B:368:GLN:O	4:B:372:ARG:NH1	2.32	0.62
3:A:438:ILE:HA	3:A:456:VAL:HG22	1.80	0.62
4:B:711:GLN:HG2	4:B:713:PRO:HD2	1.82	0.62
17:S:444:PRO:HA	18:R:2:PHE:HA	1.80	0.62
18:R:208:TYR:O	18:R:212:HIS:ND1	2.30	0.62
3:A:510:PRO:O	3:A:515:ASN:ND2	2.32	0.61
4:B:1014:TYR:OH	5:C:293:ARG:NH1	2.32	0.61
1:Q:328:LEU:HD13	1:Q:472:ARG:HG3	1.83	0.61
2:M:81:PHE:HB3	15:N:52:GLN:HB2	1.82	0.61
17:S:243:LYS:NZ	17:S:299:ASP:OD2	2.33	0.61
17:S:273:ARG:NH2	17:S:330:PRO:O	2.33	0.61
7:E:153:HIS:HB3	7:E:188:LEU:HD11	1.81	0.61
17:S:362:ARG:HB3	17:S:375:PHE:HB2	1.82	0.61
1:Q:279:THR:O	1:Q:280:ASP:O	2.19	0.61
3:A:1661:PRO:HA	9:G:102:GLU:HG2	1.83	0.60
6:D:9:GLY:HA2	6:D:12:THR:OG1	2.01	0.60
3:A:1017:GLY:HA3	19:T:18:DC:H4'	1.81	0.60
16:O:331:LYS:HA	16:O:335:ILE:HD12	1.83	0.60
4:B:940:GLU:OE2	5:C:293:ARG:NH2	2.34	0.60
1:Q:10:CYS:SG	1:Q:11:GLY:N	2.73	0.60
3:A:86:TYR:HA	3:A:356:PHE:HA	1.83	0.60
18:R:283:ARG:HH11	20:U:38:DT:H5'	1.65	0.60
4:B:281:CYS:SG	4:B:368:GLN:NE2	2.75	0.60
3:A:471:MET:HE1	4:B:1185:LEU:HD22	1.83	0.60
2:M:15:VAL:HG22	2:M:90:LEU:HD12	1.84	0.60
9:G:50:ALA:HB2	9:G:64:GLN:HE22	1.66	0.60
16:O:235:GLU:HG3	16:O:236:LYS:HG3	1.83	0.60
1:Q:223:ASN:HA	1:Q:493:ILE:HA	1.82	0.59
4:B:657:PRO:HD3	15:N:148:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:218:VAL:HG13	9:G:222:GLY:HA2	1.83	0.59
2:M:80:LEU:HD23	2:M:89:GLN:HE21	1.66	0.59
3:A:747:ILE:HG22	3:A:774:GLY:HA2	1.84	0.59
4:B:167:SER:OG	4:B:168:ASN:N	2.34	0.59
9:G:147:LEU:HB2	9:G:155:ALA:HB3	1.84	0.59
16:O:430:ARG:NH1	16:O:610:TYR:OH	2.35	0.59
17:S:676:SER:HB3	17:S:711:LEU:HD22	1.84	0.59
4:B:916:LYS:HG2	4:B:926:VAL:HG12	1.84	0.59
4:B:409:TYR:HE1	4:B:465:LEU:HD11	1.68	0.59
17:S:36:LYS:NZ	18:R:321:GLN:OE1	2.34	0.59
4:B:490:LYS:HZ3	4:B:736:ARG:HH12	1.48	0.59
16:O:423:TYR:HA	16:O:593:PRO:HG2	1.84	0.59
19:T:39:DT:O4	20:U:31:DA:N6	2.35	0.59
18:R:7:THR:OG1	18:R:246:GLN:NE2	2.36	0.59
1:Q:171:HIS:ND1	1:Q:244:ASN:OD1	2.35	0.59
3:A:496:GLY:HA3	3:A:615:ARG:HB2	1.85	0.59
16:O:225:LEU:HD23	16:O:229:ILE:HD11	1.85	0.59
1:Q:271:LYS:NZ	17:S:739:ASP:OD2	2.35	0.59
1:Q:293:ARG:NH1	20:U:24:DT:O4	2.32	0.59
5:C:86:PHE:O	14:L:60:ARG:NH2	2.35	0.59
17:S:351:ILE:HG21	17:S:374:VAL:HG11	1.84	0.59
15:N:172:ALA:HB3	15:N:175:TYR:HB2	1.84	0.58
4:B:40:GLU:OE1	4:B:550:ARG:NH2	2.35	0.58
3:A:255:ALA:HB2	3:A:311:GLY:HA2	1.84	0.58
3:A:886:ASN:OD1	3:A:955:ARG:NH2	2.36	0.58
5:C:87:ASN:ND2	5:C:201:GLU:OE2	2.36	0.58
3:A:581:ILE:HD11	3:A:605:VAL:HG21	1.84	0.58
5:C:53:ASN:ND2	15:N:173:THR:O	2.37	0.58
5:C:301:ASN:HD22	15:N:173:THR:HB	1.68	0.58
3:A:475:ARG:NH1	4:B:1068:GLY:O	2.36	0.58
3:A:709:ARG:NH1	3:A:737:LEU:O	2.34	0.58
3:A:1091:VAL:HG13	3:A:1133:LEU:HD23	1.85	0.58
9:G:143:SER:O	16:O:105:ASN:ND2	2.36	0.58
9:G:144:HIS:HA	9:G:158:LYS:HA	1.85	0.58
9:G:152:ALA:HA	16:O:184:PRO:HG2	1.85	0.58
1:Q:10:CYS:SG	3:A:70:LYS:NZ	2.77	0.58
4:B:292:ILE:O	4:B:379:ARG:NH1	2.36	0.58
4:B:838:GLU:O	14:L:63:ARG:NH2	2.36	0.58
1:Q:141:LEU:HD21	17:S:770:ASP:HB3	1.86	0.57
3:A:1074:TYR:O	3:A:1078:LYS:NZ	2.37	0.57
11:I:94:MET:HE2	11:I:114:CYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:700:LEU:HD21	17:S:714:PHE:CD1	2.39	0.57
3:A:594:THR:HG23	3:A:599:SER:HB2	1.85	0.57
4:B:518:ARG:NH1	4:B:539:CYS:O	2.36	0.57
3:A:32:ILE:HD12	3:A:362:VAL:HG21	1.86	0.57
4:B:156:ARG:HH12	4:B:446:MET:HE2	1.68	0.57
11:I:114:CYS:SG	11:I:115:THR:N	2.77	0.57
17:S:472:ARG:NH2	18:R:198:LEU:O	2.38	0.57
11:I:91:ASN:ND2	11:I:114:CYS:SG	2.75	0.57
12:J:8:PHE:H	12:J:49:MET:HE1	1.70	0.57
4:B:188:ASP:OD2	4:B:764:ASN:ND2	2.38	0.57
5:C:245:ARG:HE	5:C:258:ILE:HD11	1.69	0.57
6:D:88:GLN:NE2	16:O:184:PRO:O	2.37	0.57
9:G:149:ILE:HB	9:G:153:PHE:HB2	1.86	0.57
17:S:406:LYS:HD3	17:S:453:VAL:H	1.69	0.57
18:R:255:VAL:HG22	18:R:259:ASP:HB2	1.85	0.57
3:A:938:VAL:HG11	11:I:98:THR:HG21	1.85	0.57
17:S:202:ILE:HA	17:S:219:LEU:HD13	1.87	0.57
4:B:132:SER:OG	4:B:462:GLN:NE2	2.38	0.57
5:C:222:VAL:HG21	5:C:225:ALA:HB2	1.86	0.57
16:O:430:ARG:NH1	16:O:594:TYR:O	2.37	0.57
19:T:39:DT:O2	20:U:33:DG:N2	2.38	0.57
4:B:107:PRO:O	4:B:171:HIS:NE2	2.36	0.57
4:B:890:ASP:O	14:L:54:ARG:NH1	2.37	0.57
6:D:12:THR:O	6:D:12:THR:CG2	2.49	0.56
9:G:81:VAL:HA	9:G:124:VAL:HG12	1.85	0.56
4:B:354:LEU:O	4:B:370:LYS:NZ	2.38	0.56
3:A:840:ASN:HD21	3:A:985:ARG:HH22	1.52	0.56
1:Q:182:ILE:HD12	1:Q:185:ILE:HD11	1.88	0.56
3:A:1556:GLU:O	3:A:1560:ASN:ND2	2.39	0.56
4:B:1128:CYS:SG	4:B:1129:ARG:N	2.79	0.56
17:S:396:ALA:O	17:S:401:ASN:ND2	2.39	0.56
9:G:161:ASN:ND2	9:G:247:GLY:O	2.38	0.56
3:A:57:PHE:HB2	3:A:365:THR:HG21	1.86	0.56
4:B:710:ASN:HB2	4:B:715:ASN:HD21	1.71	0.56
4:B:939:SER:OG	4:B:940:GLU:N	2.39	0.56
11:I:81:THR:OG1	11:I:95:ASN:ND2	2.39	0.56
18:R:237:ALA:O	18:R:241:ARG:NH2	2.39	0.56
2:M:53:LEU:HB2	2:M:96:LEU:HD13	1.87	0.56
4:B:860:ALA:HA	4:B:871:ILE:HG22	1.88	0.56
11:I:23:VAL:HG11	11:I:28:VAL:HG12	1.88	0.56
16:O:421:LEU:HD13	16:O:476:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:292:GLU:HG3	1:Q:294:HIS:HD2	1.71	0.56
4:B:748:GLN:OE1	4:B:770:ASN:ND2	2.37	0.56
6:D:9:GLY:O	6:D:12:THR:OG1	2.24	0.56
3:A:15:ASP:HB2	4:B:1197:ARG:HB3	1.88	0.55
9:G:159:LYS:HA	9:G:162:ILE:HB	1.88	0.55
14:L:28:LYS:HG2	14:L:39:SER:HB2	1.88	0.55
3:A:628:PHE:H	4:B:784:ASP:HB3	1.71	0.55
4:B:839:LYS:NZ	4:B:851:TYR:O	2.38	0.55
3:A:1124:LEU:HD11	3:A:1137:SER:HA	1.88	0.55
18:R:200:THR:HG22	18:R:202:THR:H	1.70	0.55
10:H:59:ILE:HD11	10:H:123:MET:HE1	1.87	0.55
17:S:462:ILE:HD12	17:S:483:HIS:HD2	1.71	0.55
1:Q:266:PHE:HA	1:Q:269:TYR:HB2	1.88	0.55
3:A:913:PRO:O	3:A:919:LYS:NZ	2.35	0.55
3:A:1049:MET:HB3	3:A:1054:ALA:HB2	1.89	0.55
4:B:292:ILE:HG23	4:B:379:ARG:HD3	1.89	0.55
4:B:294:GLY:HA3	4:B:578:ALA:HA	1.89	0.55
4:B:565:LEU:HD21	4:B:608:LEU:HD11	1.89	0.55
16:O:532:ALA:HB1	16:O:538:ALA:H	1.72	0.55
1:Q:21:ARG:NH1	1:Q:24:ASP:OD1	2.40	0.55
1:Q:26:ARG:NH2	4:B:1049:THR:OG1	2.40	0.55
3:A:109:ARG:HH21	3:A:240:SER:H	1.53	0.55
4:B:338:PHE:HZ	4:B:357:ILE:HD11	1.72	0.55
5:C:335:GLN:O	16:O:551:ARG:NH1	2.39	0.55
18:R:294:VAL:HG12	18:R:298:GLN:HE21	1.72	0.55
3:A:646:GLU:OE1	4:B:1084:THR:OG1	2.22	0.54
3:A:692:TYR:OH	3:A:734:THR:OG1	2.25	0.54
16:O:387:HIS:ND1	16:O:606:MET:SD	2.80	0.54
3:A:216:ARG:NH2	3:A:338:VAL:O	2.41	0.54
3:A:1657:LEU:HG	9:G:106:LYS:HA	1.90	0.54
4:B:719:CYS:O	4:B:723:LYS:NZ	2.38	0.54
3:A:586:VAL:HG21	3:A:648:LEU:HG	1.88	0.54
4:B:402:VAL:O	4:B:647:SER:OG	2.25	0.54
5:C:75:VAL:HB	5:C:221:PRO:HG3	1.88	0.54
4:B:811:LEU:HD13	4:B:823:GLN:HG3	1.88	0.54
1:Q:8:PRO:HB3	3:A:59:ARG:HD2	1.88	0.54
16:O:80:LEU:O	16:O:87:ARG:NH1	2.40	0.54
17:S:395:GLN:HB3	18:R:140:ILE:HG23	1.90	0.54
1:Q:13:ASP:OD2	6:D:6:ARG:NE	2.38	0.54
3:A:188:TYR:O	3:A:192:ALA:N	2.38	0.54
4:B:515:THR:HG22	4:B:518:ARG:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:42:VAL:O	13:K:138:LYS:NZ	2.39	0.54
10:H:113:ALA:HA	10:H:126:GLU:HA	1.89	0.54
12:J:10:CYS:SG	12:J:11:GLY:N	2.81	0.54
3:A:596:HIS:HB3	3:A:1195:GLU:HG3	1.89	0.54
2:M:111:PRO:HA	4:B:328:GLN:HE22	1.73	0.54
17:S:29:GLN:NE2	17:S:443:ASP:OD2	2.40	0.54
17:S:757:GLN:O	17:S:761:SER:OG	2.25	0.54
3:A:1179:ILE:HD11	3:A:1183:GLU:HG2	1.89	0.53
8:F:84:TYR:O	8:F:136:ARG:NH2	2.39	0.53
17:S:456:VAL:HB	17:S:463:LEU:HB2	1.90	0.53
3:A:852:ASP:OD1	3:A:855:ARG:NH2	2.41	0.53
3:A:897:SER:O	3:A:901:ASN:ND2	2.41	0.53
3:A:1447:GLN:HE21	3:A:1459:LYS:HA	1.74	0.53
4:B:48:SER:HB2	4:B:404:LEU:HD13	1.89	0.53
5:C:229:LEU:O	5:C:293:ARG:NH1	2.41	0.53
17:S:58:HIS:HB3	17:S:552:LEU:HD22	1.91	0.53
18:R:349:ILE:HA	18:R:352:TRP:HB2	1.90	0.53
3:A:1543:SER:OG	3:A:1544:ASN:N	2.41	0.53
1:Q:40:GLU:HG2	4:B:1051:PRO:HB3	1.89	0.53
9:G:143:SER:OG	16:O:103:ASN:ND2	2.41	0.53
3:A:233:CYS:SG	3:A:234:ASP:N	2.82	0.53
3:A:670:ILE:HG12	3:A:671:GLN:HG3	1.91	0.53
4:B:985:ILE:HG22	15:N:160:VAL:HG22	1.89	0.53
7:E:88:VAL:HB	7:E:116:ILE:HA	1.91	0.53
17:S:184:SER:N	17:S:509:GLU:OE2	2.42	0.53
17:S:215:ASN:HB2	17:S:233:VAL:HB	1.90	0.53
3:A:49:LEU:HD23	3:A:383:ASN:HD22	1.74	0.53
5:C:128:ASP:O	5:C:175:GLN:NE2	2.41	0.53
17:S:300:LEU:HA	17:S:320:ILE:HA	1.90	0.53
3:A:1270:VAL:HG11	3:A:1489:VAL:HG11	1.91	0.53
3:A:1560:ASN:O	3:A:1564:ASN:ND2	2.41	0.53
4:B:63:LEU:HA	4:B:66:LYS:HE3	1.89	0.53
14:L:36:SER:OG	14:L:48:CYS:SG	2.67	0.53
17:S:294:PHE:HB3	17:S:297:ILE:HA	1.91	0.53
18:R:200:THR:HB	18:R:203:SER:HB2	1.91	0.53
3:A:701:ARG:NE	3:A:704:ASP:OD2	2.40	0.53
3:A:1557:ALA:HB2	7:E:150:VAL:HG22	1.91	0.53
4:B:265:ARG:HD3	4:B:474:SER:HA	1.91	0.53
1:Q:293:ARG:NH2	19:T:47:DA:N1	2.56	0.53
11:I:35:ALA:HB1	11:I:37:TYR:HD2	1.74	0.53
16:O:503:ASP:HA	16:O:537:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:45:PRO:O	18:R:321:GLN:NE2	2.41	0.53
18:R:10:ASN:HB2	18:R:13:PHE:HD2	1.74	0.53
1:Q:46:ASP:OD2	19:T:23:DA:N6	2.39	0.52
3:A:32:ILE:HD11	3:A:54:LEU:HD11	1.91	0.52
1:Q:439:ILE:HD12	17:S:717:LYS:HE2	1.91	0.52
3:A:105:CYS:O	3:A:107:HIS:ND1	2.42	0.52
3:A:370:PRO:HB3	3:A:379:GLU:HA	1.90	0.52
17:S:595:GLN:OE1	17:S:599:LYS:NZ	2.41	0.52
1:Q:13:ASP:HB2	6:D:6:ARG:HH11	1.74	0.52
1:Q:142:LYS:O	1:Q:146:ASP:N	2.41	0.52
4:B:17:ARG:HB3	4:B:20:GLU:HB3	1.92	0.52
4:B:883:GLU:OE1	4:B:906:ARG:NH1	2.42	0.52
17:S:302:VAL:HG21	17:S:362:ARG:HA	1.91	0.52
3:A:637:PHE:O	3:A:639:GLN:NE2	2.39	0.52
4:B:627:GLY:N	4:B:641:TYR:O	2.41	0.52
10:H:106:GLU:HA	10:H:112:ILE:HA	1.91	0.52
15:N:56:ILE:HG22	15:N:137:PHE:HB2	1.91	0.52
16:O:461:VAL:HG22	16:O:467:MET:HE1	1.91	0.52
17:S:213:VAL:HG12	17:S:237:GLU:HA	1.91	0.52
17:S:746:ARG:HH22	17:S:749:LYS:HD2	1.74	0.52
1:Q:442:LEU:HD23	1:Q:445:ARG:HD2	1.91	0.52
3:A:561:LEU:HA	3:A:575:LYS:HD2	1.92	0.52
3:A:1490:GLU:OE2	11:I:51:THR:OG1	2.26	0.52
4:B:126:SER:OG	4:B:131:THR:O	2.28	0.52
4:B:1042:ASP:O	4:B:1063:ARG:NH1	2.43	0.52
1:Q:172:LEU:HD23	1:Q:174:LEU:HD11	1.91	0.52
3:A:510:PRO:HG3	3:A:576:LYS:HE3	1.91	0.52
18:R:136:LYS:HD2	18:R:304:HIS:HD2	1.74	0.52
4:B:25:PHE:HB3	12:J:58:GLU:HB2	1.91	0.52
4:B:396:ALA:HA	4:B:521:LEU:HD13	1.91	0.52
18:R:401:ILE:HA	18:R:442:LEU:HD11	1.91	0.52
3:A:1319:ASN:O	3:A:1323:HIS:ND1	2.43	0.52
4:B:20:GLU:HG2	4:B:24:ARG:HH12	1.74	0.52
13:K:105:ILE:HB	13:K:113:ALA:HB1	1.92	0.52
16:O:383:TYR:HA	16:O:386:PHE:HB3	1.92	0.52
2:M:13:GLU:N	2:M:88:ILE:O	2.40	0.51
16:O:468:GLU:O	16:O:471:LYS:NZ	2.39	0.51
3:A:511:VAL:O	3:A:574:ASN:ND2	2.43	0.51
3:A:1113:HIS:HA	3:A:1116:GLN:HG2	1.92	0.51
4:B:12:ARG:HE	4:B:977:ILE:HG22	1.76	0.51
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:117:GLU:HG2	15:N:118:SER:H	1.75	0.51
1:Q:422:GLU:OE2	18:R:260:ASN:ND2	2.43	0.51
3:A:130:ILE:O	3:A:133:SER:OG	2.26	0.51
3:A:1619:CYS:HA	3:A:1622:LEU:HB3	1.90	0.51
11:I:72:LYS:HB2	11:I:75:GLU:HB2	1.91	0.51
1:Q:109:GLN:O	1:Q:113:LYS:N	2.42	0.51
4:B:261:ARG:NH2	4:B:268:GLU:OE2	2.42	0.51
4:B:679:GLN:NE2	15:N:155:VAL:O	2.44	0.51
16:O:78:VAL:O	16:O:87:ARG:NH2	2.44	0.51
4:B:921:HIS:NE2	4:B:965:GLU:OE1	2.33	0.51
9:G:146:GLY:HA3	16:O:145:SER:HB3	1.92	0.51
4:B:492:ASN:HD22	4:B:767:ASN:HD21	1.58	0.51
10:H:30:SER:OG	10:H:31:THR:N	2.44	0.51
3:A:256:LEU:HD23	3:A:261:ILE:HG13	1.91	0.51
3:A:1644:GLY:O	4:B:1089:GLN:NE2	2.43	0.51
4:B:624:LEU:HD21	4:B:642:LEU:HD23	1.93	0.51
4:B:913:ILE:HD11	4:B:930:LYS:H	1.76	0.51
4:B:920:ARG:NH2	4:B:965:GLU:OE2	2.38	0.51
6:D:88:GLN:HB3	9:G:71:MET:HE2	1.92	0.51
7:E:4:GLU:O	7:E:8:ASN:ND2	2.44	0.51
9:G:26:ASN:ND2	9:G:36:ASN:O	2.38	0.51
16:O:216:LEU:O	16:O:342:HIS:NE2	2.44	0.51
3:A:904:THR:HA	3:A:946:LEU:HD11	1.94	0.50
16:O:333:ASP:O	16:O:337:THR:OG1	2.24	0.50
19:T:53:DG:N1	20:U:16:DT:O4	2.37	0.50
1:Q:312:LEU:HD11	1:Q:502:ILE:HG23	1.94	0.50
2:M:39:ASP:N	2:M:54:HIS:O	2.44	0.50
3:A:49:LEU:O	3:A:368:ARG:NH1	2.42	0.50
5:C:43:ASN:HB2	5:C:55:ASP:HB2	1.93	0.50
10:H:126:GLU:O	10:H:130:ARG:NH1	2.45	0.50
16:O:443:ALA:O	16:O:447:THR:OG1	2.26	0.50
16:O:597:LEU:HG	16:O:599:LEU:H	1.75	0.50
3:A:1640:ARG:O	3:A:1645:LYS:N	2.45	0.50
4:B:185:GLU:O	12:J:63:TYR:OH	2.26	0.50
16:O:141:LYS:HG2	16:O:179:PHE:HZ	1.76	0.50
4:B:240:ARG:NH2	4:B:356:ARG:O	2.44	0.50
3:A:1444:ARG:O	3:A:1448:SER:N	2.42	0.50
5:C:53:ASN:HD22	15:N:174:GLY:HA3	1.77	0.50
17:S:68:THR:HG23	17:S:207:SER:HB3	1.94	0.50
1:Q:175:PRO:HG2	17:S:702:LEU:HB2	1.93	0.50
3:A:1039:ARG:HD2	8:F:139:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1050:TYR:HB3	3:A:1054:ALA:HA	1.93	0.50
3:A:1556:GLU:OE1	7:E:200:ARG:NH1	2.44	0.50
10:H:37:LYS:NZ	10:H:126:GLU:OE1	2.44	0.50
2:M:38:PHE:HB2	15:N:119:LEU:HB2	1.93	0.50
9:G:137:ILE:HD11	9:G:229:LEU:HD22	1.92	0.50
9:G:145:ILE:N	9:G:157:ILE:O	2.40	0.50
1:Q:250:GLN:HE22	1:Q:282:ARG:HH12	1.60	0.50
4:B:60:LEU:O	4:B:64:GLY:N	2.44	0.50
4:B:1112:THR:HB	4:B:1129:ARG:HB2	1.94	0.50
3:A:228:LEU:HD21	20:U:60:DC:OP1	2.12	0.50
4:B:576:THR:HG21	4:B:595:TRP:HB2	1.94	0.50
3:A:499:PRO:HA	3:A:502:ALA:HB3	1.94	0.49
3:A:781:LEU:HA	3:A:785:GLN:HG3	1.93	0.49
3:A:525:ASN:ND2	3:A:531:PRO:O	2.40	0.49
3:A:1634:LEU:HD13	3:A:1643:VAL:HG11	1.94	0.49
3:A:1635:ASP:O	3:A:1648:ASN:ND2	2.41	0.49
17:S:775:TRP:CD1	17:S:778:ASP:HB3	2.48	0.49
3:A:772:LYS:HB3	3:A:777:LEU:HD12	1.94	0.49
3:A:1560:ASN:ND2	7:E:149:LEU:O	2.46	0.49
12:J:44:TYR:HA	12:J:47:ARG:HB3	1.94	0.49
18:R:136:LYS:HD2	18:R:304:HIS:CD2	2.48	0.49
1:Q:198:ILE:HG13	1:Q:199:LEU:HD22	1.94	0.49
4:B:543:ASN:OD1	4:B:543:ASN:N	2.44	0.49
9:G:149:ILE:HD11	9:G:155:ALA:HB2	1.95	0.49
17:S:606:ARG:NH1	17:S:667:ASP:OD2	2.39	0.49
3:A:114:GLU:OE2	3:A:117:ARG:NH2	2.45	0.49
3:A:186:SER:HA	3:A:189:VAL:HB	1.94	0.49
4:B:789:ILE:HD13	4:B:917:PHE:HE2	1.77	0.49
9:G:159:LYS:H	16:O:105:ASN:HD21	1.60	0.49
1:Q:229:LYS:O	1:Q:233:THR:N	2.46	0.49
3:A:57:PHE:O	3:A:60:ASN:ND2	2.45	0.49
4:B:491:ILE:HD12	4:B:724:GLN:HA	1.94	0.49
1:Q:133:ALA:O	1:Q:137:TRP:N	2.45	0.49
3:A:403:LEU:HD13	3:A:423:LEU:HD22	1.95	0.49
3:A:879:LEU:HD23	3:A:882:ILE:HD12	1.94	0.49
3:A:1197:SER:HA	3:A:1200:MET:HE3	1.94	0.49
4:B:526:GLY:HA2	4:B:696:ILE:HA	1.95	0.49
4:B:796:ARG:NH1	12:J:7:CYS:O	2.46	0.49
10:H:94:ASP:N	10:H:144:ILE:O	2.45	0.49
12:J:36:LEU:HD11	12:J:51:LEU:HB2	1.94	0.49
18:R:347:ASP:HA	18:R:350:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:252:LEU:HD11	1:Q:303:GLU:HG3	1.94	0.49
3:A:403:LEU:HD12	3:A:419:ILE:HG13	1.95	0.49
3:A:834:ARG:HH12	4:B:1008:HIS:HD2	1.61	0.49
3:A:1298:ASP:HA	3:A:1468:LYS:HE2	1.95	0.48
5:C:195:LYS:NZ	12:J:58:GLU:OE2	2.35	0.48
13:K:54:THR:HG23	13:K:61:ALA:HA	1.94	0.48
3:A:336:GLN:OE1	3:A:344:ASN:ND2	2.46	0.48
3:A:473:GLY:O	4:B:1070:ARG:NH1	2.45	0.48
3:A:1080:TYR:OH	3:A:1173:LYS:NZ	2.38	0.48
5:C:65:ASN:O	5:C:69:ARG:N	2.46	0.48
16:O:176:LEU:HD13	16:O:218:LEU:HD11	1.94	0.48
17:S:425:GLY:HA3	17:S:434:ARG:HH11	1.77	0.48
1:Q:431:ASP:OD2	1:Q:434:HIS:ND1	2.44	0.48
3:A:559:ASN:HB2	16:O:242:VAL:HG21	1.96	0.48
4:B:417:ILE:HA	4:B:420:TYR:HB3	1.95	0.48
4:B:492:ASN:HD22	4:B:767:ASN:ND2	2.11	0.48
18:R:160:HIS:HA	18:R:163:LYS:HE3	1.96	0.48
1:Q:318:LEU:HD23	1:Q:476:ILE:HD12	1.96	0.48
3:A:210:ALA:O	3:A:214:ASP:N	2.45	0.48
3:A:238:MET:HA	3:A:264:ASN:HD22	1.79	0.48
3:A:539:GLU:HB3	3:A:570:THR:HB	1.95	0.48
3:A:1321:PHE:O	3:A:1325:LEU:N	2.45	0.48
5:C:169:PHE:HB2	5:C:184:VAL:HB	1.95	0.48
8:F:107:VAL:HG11	8:F:111:LEU:HD23	1.95	0.48
9:G:234:ARG:H	9:G:247:GLY:HA2	1.79	0.48
3:A:769:VAL:HA	3:A:779:GLY:HA3	1.95	0.48
3:A:1097:TYR:OH	3:A:1121:ASP:OD1	2.30	0.48
4:B:612:LYS:HD2	4:B:624:LEU:HB3	1.95	0.48
11:I:37:TYR:HD1	11:I:39:LYS:HE2	1.79	0.48
17:S:451:ILE:HD11	17:S:466:ALA:HB1	1.95	0.48
2:M:75:GLN:HG3	15:N:58:PHE:HB2	1.96	0.48
4:B:300:SER:HA	4:B:303:THR:HG22	1.96	0.48
5:C:91:VAL:HG11	12:J:60:PHE:HB3	1.96	0.48
6:D:24:ALA:HA	9:G:43:ILE:HA	1.95	0.48
17:S:631:SER:O	17:S:635:ASN:ND2	2.47	0.48
1:Q:297:ARG:O	1:Q:504:ARG:NH2	2.46	0.48
3:A:799:GLU:HG2	3:A:1062:HIS:HB2	1.96	0.48
6:D:31:VAL:HG11	9:G:123:TYR:HE1	1.78	0.48
16:O:440:ILE:O	16:O:444:SER:N	2.47	0.48
18:R:8:LEU:HD21	18:R:202:THR:HG22	1.96	0.48
3:A:482:SER:OG	3:A:483:VAL:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:142:ALA:HB3	16:O:102:SER:HB2	1.96	0.48
16:O:137:ILE:O	16:O:141:LYS:N	2.35	0.48
16:O:152:GLN:NE2	16:O:193:TYR:OH	2.46	0.48
9:G:147:LEU:N	9:G:155:ALA:O	2.44	0.47
16:O:187:MET:HA	16:O:190:ILE:HD12	1.96	0.47
17:S:483:HIS:HA	17:S:489:PHE:HB3	1.95	0.47
18:R:25:ASN:ND2	18:R:123:GLU:OE1	2.46	0.47
3:A:435:ASN:ND2	3:A:442:LYS:O	2.41	0.47
5:C:277:ARG:HG2	5:C:291:LEU:HD22	1.96	0.47
16:O:138:TYR:HA	16:O:141:LYS:HD3	1.95	0.47
3:A:109:ARG:NH2	3:A:240:SER:O	2.47	0.47
7:E:7:ARG:HA	7:E:10:SER:HB3	1.96	0.47
16:O:383:TYR:HE2	16:O:597:LEU:HD22	1.80	0.47
18:R:369:ALA:HB1	18:R:411:VAL:HG13	1.96	0.47
4:B:346:ASP:O	4:B:350:GLY:N	2.44	0.47
17:S:454:GLN:NE2	17:S:511:ILE:O	2.48	0.47
19:T:36:DT:O2	20:U:36:DG:N2	2.47	0.47
3:A:755:ILE:HG21	3:A:760:TRP:HE1	1.78	0.47
3:A:1512:PRO:HB3	3:A:1517:ARG:HA	1.97	0.47
3:A:1635:ASP:OD1	3:A:1635:ASP:N	2.47	0.47
4:B:1103:VAL:HG22	4:B:1110:ILE:HG12	1.95	0.47
7:E:117:THR:HG22	7:E:119:SER:H	1.78	0.47
17:S:347:LEU:HD13	17:S:385:PHE:HB2	1.96	0.47
1:Q:204:ARG:HE	1:Q:212:VAL:HG21	1.79	0.47
1:Q:264:PRO:HD3	17:S:722:TRP:CD1	2.49	0.47
2:M:31:ARG:HG3	11:I:11:LEU:HB3	1.97	0.47
3:A:595:LEU:HD13	3:A:1198:THR:HG21	1.97	0.47
3:A:1613:MET:HB3	3:A:1618:THR:HG23	1.97	0.47
7:E:83:CYS:O	7:E:113:GLN:NE2	2.48	0.47
17:S:629:ARG:HA	17:S:632:ILE:HD12	1.96	0.47
3:A:62:CYS:SG	3:A:63:SER:N	2.88	0.47
3:A:1012:LYS:HA	3:A:1201:THR:HG21	1.97	0.47
4:B:609:ARG:HH22	4:B:668:GLU:CD	2.23	0.47
5:C:334:THR:OG1	13:K:44:ARG:O	2.31	0.47
18:R:280:SER:OG	18:R:281:LYS:N	2.47	0.47
1:Q:307:LEU:HB3	1:Q:487:LEU:HD21	1.96	0.47
2:M:16:GLN:HB3	2:M:91:TYR:HA	1.96	0.47
3:A:1272:VAL:HG22	3:A:1292:ILE:HA	1.96	0.47
4:B:107:PRO:HG2	4:B:171:HIS:CD2	2.49	0.47
4:B:313:PHE:O	4:B:317:TYR:N	2.42	0.47
5:C:61:THR:HG22	5:C:298:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:315:PHE:HA	5:C:318:VAL:HG12	1.97	0.47
15:N:86:ASP:OD2	15:N:144:LYS:NZ	2.48	0.47
17:S:472:ARG:HD3	18:R:198:LEU:HG	1.97	0.47
3:A:739:VAL:HG11	3:A:812:VAL:HG21	1.96	0.47
3:A:792:GLY:O	3:A:796:SER:N	2.48	0.47
3:A:1225:ILE:O	3:A:1595:TYR:OH	2.28	0.47
4:B:584:CYS:HB2	4:B:639:GLY:HA2	1.95	0.47
16:O:176:LEU:HG	16:O:180:LEU:HD13	1.97	0.47
18:R:415:LEU:HD11	18:R:426:VAL:HG21	1.96	0.47
3:A:621:THR:OG1	3:A:626:ALA:O	2.33	0.46
4:B:826:GLY:N	4:B:860:ALA:O	2.45	0.46
4:B:1104:CYS:HA	4:B:1173:THR:HG22	1.97	0.46
4:B:1185:LEU:O	4:B:1189:LEU:N	2.42	0.46
17:S:226:HIS:ND1	17:S:227:LEU:O	2.38	0.46
17:S:244:SER:HB3	17:S:264:ILE:HB	1.96	0.46
1:Q:166:TYR:HE1	1:Q:177:TYR:HA	1.81	0.46
3:A:28:SER:HA	4:B:1129:ARG:HH21	1.80	0.46
3:A:438:ILE:O	3:A:456:VAL:N	2.49	0.46
4:B:698:SER:OG	4:B:699:ILE:N	2.47	0.46
4:B:753:LYS:O	4:B:981:SER:N	2.43	0.46
3:A:64:THR:O	4:B:1114:GLN:NE2	2.48	0.46
4:B:711:GLN:HB2	4:B:958:MET:HB2	1.97	0.46
4:B:845:LEU:HB2	14:L:58:LYS:HZ2	1.81	0.46
15:N:55:LEU:HB3	15:N:136:VAL:HG22	1.96	0.46
17:S:319:ASP:HB2	17:S:363:ILE:HG12	1.98	0.46
17:S:468:VAL:HG23	17:S:477:TYR:HB3	1.97	0.46
17:S:610:LEU:HD11	17:S:668:SER:HA	1.97	0.46
3:A:332:GLN:HE22	3:A:350:VAL:H	1.63	0.46
7:E:13:TRP:NE1	7:E:37:LEU:O	2.35	0.46
9:G:161:ASN:HB3	9:G:248:THR:HA	1.98	0.46
17:S:406:LYS:NZ	17:S:453:VAL:O	2.41	0.46
17:S:665:ASN:OD1	17:S:668:SER:OG	2.32	0.46
1:Q:195:ALA:HA	1:Q:199:LEU:HD23	1.97	0.46
3:A:732:ILE:HG21	3:A:781:LEU:HD11	1.96	0.46
3:A:1463:ASP:OD2	3:A:1468:LYS:N	2.48	0.46
8:F:95:GLY:O	8:F:99:LEU:N	2.49	0.46
9:G:234:ARG:HG2	9:G:235:ASN:H	1.81	0.46
11:I:15:ASP:OD2	11:I:32:GLN:NE2	2.48	0.46
11:I:101:LEU:HD13	11:I:109:THR:HB	1.98	0.46
4:B:687:THR:HG22	15:N:148:ILE:HD11	1.98	0.46
7:E:47:CYS:HA	7:E:53:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:748:ASN:HD22	3:A:772:LYS:HA	1.81	0.46
17:S:507:GLY:O	17:S:540:LYS:N	2.48	0.46
20:U:61:DA:O5'	20:U:61:DA:H8	1.99	0.46
3:A:186:SER:O	3:A:190:ASP:N	2.45	0.46
3:A:363:PRO:O	3:A:368:ARG:NE	2.48	0.46
3:A:1047:GLN:NE2	3:A:1587:ASP:OD2	2.45	0.46
4:B:783:MET:SD	4:B:950:ASN:ND2	2.88	0.46
15:N:49:LYS:HG3	15:N:50:GLN:HG3	1.96	0.46
16:O:163:ILE:HG23	16:O:207:LYS:HA	1.98	0.46
3:A:27:LEU:O	4:B:1129:ARG:NE	2.49	0.46
3:A:767:ASN:HD21	11:I:85:LYS:HE3	1.81	0.46
4:B:725:THR:HA	4:B:1036:LEU:HA	1.98	0.46
3:A:673:HIS:CD2	3:A:817:PHE:HB2	2.47	0.45
3:A:1274:GLU:OE2	3:A:1288:ARG:NH2	2.36	0.45
3:A:390:LEU:HA	3:A:393:SER:HB3	1.99	0.45
4:B:117:VAL:HB	18:R:277:ILE:HG22	1.98	0.45
4:B:353:VAL:HG13	4:B:357:ILE:HD12	1.97	0.45
5:C:164:ALA:HB3	5:C:191:ILE:HB	1.99	0.45
9:G:148:LEU:HD11	16:O:182:MET:HG3	1.97	0.45
15:N:122:ALA:HB1	15:N:131:LEU:HD13	1.98	0.45
3:A:317:SER:HA	3:A:320:VAL:HB	1.97	0.45
1:Q:35:MET:HE3	1:Q:38:ASP:HB2	1.98	0.45
3:A:62:CYS:N	3:A:67:LEU:O	2.39	0.45
4:B:495:ARG:HH11	4:B:723:LYS:HD3	1.81	0.45
16:O:330:THR:HA	16:O:333:ASP:HB2	1.97	0.45
17:S:230:HIS:HB2	17:S:282:CYS:HB2	1.97	0.45
1:Q:262:LEU:HD13	1:Q:266:PHE:HB2	1.97	0.45
3:A:964:LYS:HZ1	3:A:967:PRO:HA	1.81	0.45
3:A:990:ILE:HB	3:A:994:GLU:HG3	1.99	0.45
4:B:1099:THR:OG1	4:B:1178:ILE:O	2.32	0.45
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.99	0.45
10:H:118:PHE:CE1	10:H:142:LEU:HB2	2.51	0.45
17:S:353:ASP:HB3	17:S:356:GLU:HB2	1.98	0.45
1:Q:263:PRO:HG3	17:S:725:VAL:HB	1.99	0.45
3:A:87:ASN:ND2	4:B:1192:MET:O	2.50	0.45
3:A:810:LEU:HD23	3:A:813:LEU:HD12	1.98	0.45
3:A:1637:PRO:HB3	3:A:1647:ASN:HD21	1.82	0.45
4:B:73:ILE:HD11	4:B:95:LEU:HD13	1.99	0.45
4:B:429:ARG:HA	4:B:432:ILE:HG12	1.98	0.45
4:B:894:LYS:HG2	14:L:54:ARG:HH22	1.82	0.45
15:N:57:LYS:HB2	15:N:138:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:715:TYR:OH	17:S:730:GLU:OE2	2.35	0.45
18:R:136:LYS:HA	18:R:304:HIS:HD2	1.81	0.45
4:B:417:ILE:HG22	4:B:457:ILE:HD13	1.99	0.45
3:A:1476:LEU:HD23	3:A:1480:THR:HG21	1.99	0.45
12:J:18:TRP:NE1	12:J:55:ASP:OD2	2.46	0.45
4:B:204:ARG:NH1	4:B:502:MET:SD	2.90	0.45
4:B:848:ILE:HD11	14:L:60:ARG:HB3	1.99	0.45
17:S:251:SER:OG	17:S:306:ALA:O	2.31	0.45
17:S:390:GLN:HB2	18:R:152:ILE:HG13	1.99	0.45
18:R:347:ASP:OD1	18:R:347:ASP:N	2.49	0.45
3:A:847:LEU:HD21	3:A:946:LEU:HD22	1.99	0.44
3:A:1080:TYR:HD1	3:A:1176:ARG:HG3	1.81	0.44
4:B:795:GLU:OE1	5:C:217:ALA:N	2.49	0.44
4:B:840:LEU:HA	4:B:846:PRO:HA	1.99	0.44
5:C:325:ALA:HB2	13:K:124:LEU:HD22	1.99	0.44
9:G:138:PHE:HD2	9:G:139:ILE:HG12	1.82	0.44
17:S:511:ILE:HD11	17:S:538:LEU:HD23	1.98	0.44
18:R:268:LEU:HD22	18:R:319:ASN:HD22	1.82	0.44
3:A:64:THR:HG22	4:B:1114:GLN:HE22	1.82	0.44
3:A:817:PHE:HA	3:A:820:TYR:HB3	1.99	0.44
4:B:127:ARG:NH2	4:B:193:TYR:OH	2.49	0.44
4:B:912:GLN:N	4:B:915:ASP:OD2	2.50	0.44
15:N:78:THR:HG21	15:N:89:ILE:HB	1.99	0.44
16:O:63:LEU:HB2	16:O:106:ARG:HA	1.99	0.44
18:R:168:ILE:HG23	18:R:169:PRO:HD3	1.98	0.44
3:A:1121:ASP:OD1	3:A:1121:ASP:N	2.48	0.44
4:B:504:HIS:ND1	4:B:541:LEU:O	2.50	0.44
4:B:608:LEU:O	4:B:612:LYS:N	2.47	0.44
9:G:56:ASN:ND2	9:G:59:GLN:OE1	2.51	0.44
3:A:1105:ARG:O	3:A:1109:SER:OG	2.31	0.44
7:E:79:TRP:NE1	7:E:81:GLU:OE1	2.43	0.44
8:F:134:ILE:N	8:F:146:TRP:O	2.44	0.44
4:B:209:GLN:NE2	4:B:215:MET:SD	2.91	0.44
4:B:634:ARG:NH2	11:I:54:ASP:OD2	2.50	0.44
4:B:882:ILE:HG12	4:B:903:ILE:HD11	1.99	0.44
4:B:1014:TYR:OH	5:C:229:LEU:N	2.50	0.44
18:R:410:TYR:O	18:R:413:THR:OG1	2.35	0.44
3:A:334:VAL:HG13	3:A:335:LEU:HG	2.00	0.44
3:A:658:LEU:HD21	3:A:795:HIS:HE2	1.82	0.44
6:D:91:ARG:HH11	16:O:184:PRO:HG3	1.81	0.44
10:H:128:ASN:OD1	10:H:128:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:331:ILE:HG21	1:Q:476:ILE:HD13	1.99	0.44
12:J:24:LEU:HB3	12:J:30:LEU:HD12	1.99	0.44
18:R:247:ILE:HA	18:R:250:LEU:HD12	1.99	0.44
3:A:4:SER:OG	3:A:576:LYS:NZ	2.35	0.44
3:A:53:ALA:HA	3:A:63:SER:HB2	2.00	0.44
3:A:618:TYR:HB3	3:A:670:ILE:HG22	2.00	0.44
4:B:140:LYS:HB3	4:B:155:VAL:HG22	2.00	0.44
4:B:572:PRO:O	4:B:576:THR:OG1	2.28	0.44
4:B:858:ILE:HD12	4:B:858:ILE:HA	1.92	0.44
7:E:177:ARG:HE	7:E:215:MET:HB2	1.83	0.44
17:S:44:ARG:O	17:S:46:VAL:N	2.51	0.44
3:A:254:THR:HA	3:A:312:SER:HA	2.00	0.44
4:B:156:ARG:CZ	4:B:450:LEU:HD22	2.47	0.44
4:B:553:THR:O	4:B:646:HIS:ND1	2.31	0.44
4:B:821:ILE:HG12	4:B:824:HIS:CE1	2.53	0.43
15:N:89:ILE:HG13	15:N:139:VAL:HG22	2.00	0.43
18:R:169:PRO:HA	18:R:172:LYS:HE2	1.98	0.43
3:A:590:ASN:ND2	3:A:591:ARG:O	2.51	0.43
17:S:228:ASN:HD22	17:S:282:CYS:HB3	1.83	0.43
1:Q:252:LEU:HD22	1:Q:306:VAL:HG11	2.01	0.43
3:A:1320:GLN:HE22	3:A:1497:ILE:HG13	1.83	0.43
4:B:1134:ARG:HA	4:B:1167:PHE:HA	1.99	0.43
5:C:85:PHE:HB2	14:L:65:VAL:HG23	1.99	0.43
9:G:149:ILE:N	9:G:153:PHE:O	2.44	0.43
16:O:56:VAL:HG11	16:O:96:LEU:HD13	2.00	0.43
16:O:216:LEU:HB3	16:O:342:HIS:CG	2.52	0.43
16:O:506:PHE:HB3	16:O:528:PHE:HZ	1.83	0.43
17:S:189:THR:HA	17:S:259:ASN:HD22	1.83	0.43
17:S:384:ASP:OD2	17:S:387:ASN:N	2.44	0.43
18:R:174:GLU:HA	18:R:177:LEU:HD12	2.00	0.43
3:A:260:GLN:HA	3:A:263:ASN:HD22	1.84	0.43
4:B:1097:ASP:N	4:B:1097:ASP:OD1	2.47	0.43
18:R:26:TYR:O	18:R:30:ARG:N	2.41	0.43
3:A:109:ARG:NH1	3:A:230:ARG:O	2.51	0.43
3:A:489:ASN:OD1	4:B:781:TYR:OH	2.31	0.43
4:B:225:ARG:CZ	4:B:261:ARG:HH22	2.31	0.43
4:B:808:LYS:HE2	4:B:810:ASP:HB2	2.00	0.43
6:D:37:LEU:HD13	6:D:96:PHE:HB2	1.99	0.43
7:E:199:ILE:HA	7:E:209:ALA:HA	2.01	0.43
16:O:238:ILE:HA	16:O:241:ASP:HB3	2.00	0.43
17:S:33:THR:HB	17:S:49:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:259:ASN:O	17:S:274:ILE:N	2.51	0.43
18:R:21:TYR:HA	18:R:24:ILE:HD12	2.00	0.43
2:M:73:SER:HA	15:N:60:SER:HB2	2.00	0.43
3:A:314:TYR:HE2	3:A:316:LEU:HD12	1.83	0.43
9:G:216:HIS:HB3	9:G:224:PRO:HB3	2.00	0.43
17:S:669:PHE:O	17:S:738:LYS:NZ	2.43	0.43
3:A:695:TYR:HE1	3:A:820:TYR:HA	1.84	0.43
3:A:865:ASP:OD1	3:A:865:ASP:N	2.51	0.43
4:B:554:GLN:HA	4:B:646:HIS:CE1	2.53	0.43
5:C:55:ASP:OD2	5:C:271:ARG:NH1	2.51	0.43
5:C:164:ALA:N	5:C:191:ILE:O	2.47	0.43
20:U:60:DC:H2''	20:U:61:DA:C8	2.54	0.43
1:Q:182:ILE:HA	1:Q:185:ILE:HG12	2.01	0.43
3:A:81:LEU:HD11	3:A:360:LEU:HG	2.01	0.43
3:A:1316:VAL:HG21	3:A:1498:ILE:HA	2.01	0.43
4:B:128:GLN:HB2	14:L:55:ILE:HD13	2.01	0.43
4:B:238:SER:HA	4:B:361:HIS:HD2	1.84	0.43
4:B:1110:ILE:HD13	4:B:1178:ILE:HD13	1.99	0.43
11:I:30:CYS:SG	11:I:31:SER:N	2.91	0.43
16:O:66:ASN:HD22	16:O:111:ARG:HH22	1.66	0.43
1:Q:111:ILE:HD13	1:Q:195:ALA:HB1	2.01	0.43
3:A:129:LEU:HD13	3:A:132:GLU:HB2	2.00	0.43
4:B:238:SER:O	4:B:246:GLN:N	2.51	0.43
16:O:204:THR:HG23	16:O:206:ARG:H	1.84	0.43
17:S:36:LYS:HG2	17:S:38:GLU:H	1.83	0.43
17:S:236:ILE:HG21	17:S:272:PHE:HE2	1.84	0.43
3:A:7:VAL:HG21	4:B:1177:ALA:HB2	2.01	0.43
4:B:134:ARG:HB3	4:B:160:GLY:HA3	2.00	0.43
4:B:963:PHE:O	4:B:1027:TYR:OH	2.28	0.43
16:O:177:LYS:HD3	16:O:221:TYR:HB3	2.00	0.43
2:M:12:ILE:HD11	15:N:67:LEU:HD12	2.01	0.42
7:E:18:THR:O	7:E:22:MET:N	2.51	0.42
19:T:9:DC:H6	19:T:9:DC:H2'	1.70	0.42
2:M:53:LEU:N	2:M:64:GLY:O	2.52	0.42
3:A:716:PRO:O	3:A:730:GLN:NE2	2.42	0.42
3:A:781:LEU:HB3	3:A:786:TYR:HE1	1.84	0.42
3:A:1105:ARG:HH12	3:A:1138:GLU:HB3	1.84	0.42
4:B:242:ASP:OD1	4:B:244:THR:OG1	2.34	0.42
14:L:31:CYS:HB3	14:L:36:SER:H	1.83	0.42
16:O:419:LYS:O	16:O:423:TYR:N	2.47	0.42
20:U:59:DG:H2''	20:U:60:DC:H5'	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1449:ALA:O	3:A:1453:HIS:ND1	2.45	0.42
5:C:69:ARG:HG2	13:K:71:THR:HA	2.00	0.42
5:C:84:TYR:HB3	14:L:64:LEU:HD11	2.02	0.42
19:T:8:DA:O5'	19:T:8:DA:H8	2.01	0.42
1:Q:250:GLN:HE22	1:Q:282:ARG:NH1	2.16	0.42
5:C:162:VAL:HG21	5:C:202:ILE:HD12	2.00	0.42
10:H:111:LEU:HD23	10:H:111:LEU:HA	1.92	0.42
11:I:19:ASN:HB3	11:I:22:ALA:HB3	2.01	0.42
17:S:675:PHE:HE2	17:S:741:ILE:HG21	1.84	0.42
1:Q:264:PRO:HG2	17:S:732:LEU:HD13	2.01	0.42
3:A:259:LYS:O	3:A:263:ASN:ND2	2.53	0.42
3:A:982:VAL:HG22	3:A:994:GLU:HB2	2.00	0.42
4:B:325:GLN:HA	4:B:328:GLN:HB2	2.02	0.42
4:B:532:HIS:HD2	4:B:544:HIS:CG	2.37	0.42
10:H:36:CYS:HB2	10:H:130:ARG:HH12	1.84	0.42
11:I:27:ASN:HA	11:I:38:PRO:HA	2.02	0.42
4:B:292:ILE:HG22	4:B:293:ILE:HG12	2.01	0.42
4:B:757:TYR:CE1	4:B:762:MET:HB2	2.54	0.42
4:B:782:ASP:OD1	4:B:782:ASP:N	2.49	0.42
4:B:1178:ILE:HD11	4:B:1183:LYS:HZ1	1.84	0.42
16:O:403:LEU:HD22	16:O:424:LEU:HD13	2.00	0.42
17:S:504:THR:O	17:S:542:ARG:N	2.36	0.42
3:A:424:MET:HA	3:A:427:PHE:HD2	1.85	0.42
4:B:992:PRO:HA	4:B:995:TYR:HB3	2.02	0.42
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.53	0.42
3:A:13:SER:HG	4:B:1199:ASN:HD22	1.63	0.42
3:A:550:SER:OG	3:A:551:VAL:N	2.52	0.42
4:B:368:GLN:HB3	4:B:372:ARG:HH12	1.84	0.42
4:B:560:ARG:HG2	4:B:619:GLY:HA3	2.01	0.42
4:B:655:TYR:CE2	4:B:657:PRO:HG2	2.55	0.42
4:B:773:VAL:HG21	4:B:1033:TYR:HE2	1.85	0.42
3:A:830:MET:SD	4:B:963:PHE:HB3	2.60	0.42
4:B:461:MET:HE3	4:B:461:MET:HB3	1.94	0.42
7:E:210:SER:OG	7:E:211:TYR:N	2.53	0.42
15:N:119:LEU:HD23	15:N:119:LEU:HA	1.94	0.42
17:S:248:PRO:HG3	17:S:305:PHE:HD2	1.85	0.42
17:S:263:ILE:HD11	17:S:270:GLN:HB2	2.02	0.42
17:S:622:TYR:O	17:S:626:LEU:N	2.52	0.42
4:B:786:ALA:HB1	4:B:928:SER:HB2	2.02	0.42
4:B:971:ALA:C	4:B:979:GLN:HE22	2.28	0.42
4:B:1099:THR:HG21	4:B:1180:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:232:GLN:HB2	5:C:294:VAL:HG23	2.01	0.42
16:O:77:GLN:HA	16:O:80:LEU:HD13	2.02	0.42
17:S:421:ILE:HA	17:S:441:ASP:HA	2.02	0.42
3:A:847:LEU:HD23	3:A:847:LEU:HA	1.90	0.41
3:A:879:LEU:O	3:A:883:LEU:N	2.50	0.41
4:B:782:ASP:HB3	4:B:788:ILE:HG12	2.01	0.41
5:C:132:ILE:HG21	5:C:184:VAL:HG21	2.00	0.41
14:L:47:ARG:HH21	14:L:52:GLY:HA3	1.85	0.41
16:O:142:ILE:O	16:O:146:SER:N	2.53	0.41
18:R:362:ALA:HB2	18:R:421:LYS:HB2	2.00	0.41
20:U:56:DA:H2'	20:U:57:DA:C4	2.55	0.41
1:Q:224:GLY:HA2	1:Q:227:TYR:HD2	1.84	0.41
2:M:43:LYS:HB2	15:N:29:PHE:HE1	1.85	0.41
3:A:90:PHE:HB3	3:A:355:PHE:HD1	1.85	0.41
3:A:478:TYR:HA	4:B:1048:SER:HA	2.02	0.41
3:A:1053:ASP:HB3	7:E:205:SER:HB3	2.02	0.41
3:A:1202:LEU:H	3:A:1202:LEU:HG	1.72	0.41
3:A:1290:TYR:HB2	3:A:1474:LEU:HB2	2.02	0.41
4:B:821:ILE:HG12	4:B:824:HIS:HE1	1.85	0.41
6:D:9:GLY:C	6:D:12:THR:OG1	2.63	0.41
7:E:150:VAL:HA	7:E:151:PRO:HD3	1.90	0.41
16:O:445:TYR:HA	16:O:448:SER:HB3	2.02	0.41
1:Q:158:MET:HB3	1:Q:192:TYR:CE1	2.56	0.41
3:A:741:PRO:HA	3:A:742:PRO:HD3	1.83	0.41
4:B:41:ALA:HA	4:B:501:ARG:HH21	1.85	0.41
10:H:99:GLY:HA3	10:H:118:PHE:HA	2.02	0.41
3:A:1228:THR:OG1	3:A:1230:SER:OG	2.32	0.41
4:B:176:SER:O	4:B:180:LEU:N	2.52	0.41
4:B:480:GLN:O	4:B:484:TYR:OH	2.29	0.41
4:B:735:HIS:HE1	12:J:63:TYR:HB3	1.85	0.41
5:C:32:ASN:HB3	5:C:35:LYS:HG3	2.03	0.41
17:S:200:THR:HG21	17:S:277:VAL:HG21	2.03	0.41
17:S:323:ASN:HA	17:S:350:THR:HA	2.03	0.41
4:B:770:ASN:HD21	12:J:52:THR:HG21	1.85	0.41
4:B:843:ASP:OD1	4:B:843:ASP:N	2.48	0.41
16:O:237:ILE:HD13	16:O:381:ILE:CD1	2.50	0.41
18:R:366:PHE:O	18:R:370:SER:N	2.53	0.41
2:M:75:GLN:NE2	15:N:62:VAL:O	2.54	0.41
3:A:1336:GLN:NE2	3:A:1481:GLU:OE2	2.53	0.41
3:A:1460:TYR:HD1	3:A:1472:PHE:HB3	1.85	0.41
4:B:694:THR:HB	4:B:702:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:9:GLY:CA	6:D:12:THR:OG1	2.68	0.41
17:S:273:ARG:HH12	17:S:331:LYS:HA	1.84	0.41
19:T:22:DA:H2"	19:T:23:DA:H8	1.86	0.41
1:Q:358:PRO:HB3	18:R:211:ARG:HH11	1.86	0.41
3:A:516:ILE:HG12	3:A:562:LEU:HD11	2.02	0.41
4:B:495:ARG:HG3	4:B:499:HIS:HE1	1.85	0.41
7:E:124:VAL:HA	7:E:132:ILE:HD12	2.02	0.41
17:S:619:GLU:HB2	17:S:669:PHE:HD1	1.86	0.41
18:R:379:LEU:HB3	18:R:404:VAL:HG22	2.02	0.41
3:A:28:SER:OG	3:A:30:LYS:HG2	2.21	0.41
3:A:994:GLU:HA	3:A:997:PHE:HD2	1.86	0.41
4:B:726:MET:SD	4:B:1035:ARG:NH1	2.94	0.41
11:I:26:SER:OG	11:I:38:PRO:O	2.36	0.41
16:O:390:GLN:HG2	16:O:433:LYS:HB3	2.02	0.41
17:S:269:PHE:HZ	17:S:303:VAL:HG21	1.85	0.41
19:T:13:DT:O4	20:U:56:DA:N6	2.54	0.41
1:Q:8:PRO:HB3	3:A:59:ARG:HH11	1.86	0.41
1:Q:159:THR:HG21	1:Q:225:GLN:HG2	2.03	0.41
3:A:124:LEU:HD22	3:A:129:LEU:HD11	2.03	0.41
3:A:891:ILE:HD12	11:I:71:LEU:HG	2.02	0.41
5:C:259:ASP:HB3	5:C:263:ASP:HB3	2.02	0.41
7:E:9:ILE:HD11	7:E:53:PRO:HD3	2.03	0.41
9:G:42:PRO:HB3	9:G:121:ASN:HD22	1.86	0.41
17:S:175:ASP:HA	17:S:176:PRO:HD3	1.91	0.41
17:S:407:ARG:HA	17:S:414:ILE:HG23	2.03	0.41
17:S:460:ASP:HB2	17:S:461:HIS:HD2	1.86	0.41
17:S:536:ASP:OD1	17:S:536:ASP:N	2.53	0.41
20:U:61:DA:H2'	20:U:62:DG:C8	2.56	0.41
1:Q:278:GLU:HG3	1:Q:280:ASP:O	2.21	0.41
3:A:658:LEU:HD21	3:A:795:HIS:NE2	2.36	0.41
3:A:982:VAL:HG12	3:A:984:GLY:H	1.86	0.41
4:B:331:GLY:O	4:B:335:ARG:N	2.54	0.41
7:E:110:PHE:HE2	7:E:112:TYR:HB3	1.86	0.41
14:L:26:THR:O	14:L:28:LYS:NZ	2.46	0.41
17:S:616:SER:HB3	17:S:619:GLU:HG2	2.03	0.41
18:R:11:ARG:HH22	20:U:29:DA:H62	1.69	0.41
1:Q:156:LEU:HD23	1:Q:156:LEU:HA	1.91	0.40
4:B:772:VAL:HG23	12:J:48:ARG:HH21	1.85	0.40
7:E:178:ILE:N	7:E:213:ILE:O	2.48	0.40
10:H:101:ALA:HB3	10:H:136:LYS:HA	2.03	0.40
16:O:458:GLU:HA	16:O:514:PHE:HZ	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:476:ILE:HD12	17:S:476:ILE:HA	1.94	0.40
3:A:600:MET:HE1	4:B:1075:GLU:HA	2.03	0.40
3:A:736:LEU:O	3:A:740:THR:OG1	2.36	0.40
16:O:137:ILE:HG22	16:O:141:LYS:HG3	2.02	0.40
17:S:377:ARG:O	17:S:402:ILE:N	2.44	0.40
1:Q:180:ASP:O	1:Q:184:TRP:HD1	2.04	0.40
3:A:85:CYS:HB3	3:A:434:VAL:HG11	2.02	0.40
3:A:453:ILE:HA	3:A:454:PRO:HD3	1.83	0.40
3:A:591:ARG:HG3	3:A:593:PRO:HD2	2.03	0.40
4:B:19:LEU:HD11	12:J:25:LEU:HB3	2.02	0.40
4:B:280:LEU:HD23	4:B:354:LEU:HD23	2.03	0.40
4:B:374:LEU:HD23	4:B:374:LEU:HA	1.94	0.40
4:B:656:LEU:HD23	4:B:656:LEU:HA	1.91	0.40
4:B:745:GLN:HG3	4:B:746:THR:HG23	2.04	0.40
7:E:155:ARG:HA	7:E:196:VAL:HA	2.03	0.40
10:H:116:TYR:HB2	10:H:123:MET:HB3	2.04	0.40
11:I:117:CYS:SG	11:I:118:GLY:N	2.94	0.40
1:Q:320:PHE:HD2	17:S:593:VAL:HG21	1.86	0.40
16:O:75:ALA:HA	16:O:78:VAL:HG12	2.02	0.40
17:S:187:ILE:O	17:S:200:THR:OG1	2.31	0.40
1:Q:450:THR:HB	17:S:724:LEU:HD21	2.04	0.40
3:A:729:LYS:HA	3:A:776:LEU:HD23	2.03	0.40
3:A:1624:LYS:HA	3:A:1627:LEU:HD12	2.04	0.40
5:C:85:PHE:N	14:L:65:VAL:O	2.55	0.40
9:G:99:ASP:N	9:G:103:LYS:HZ1	2.19	0.40
9:G:116:THR:OG1	9:G:117:TRP:N	2.54	0.40
10:H:97:MET:HE3	10:H:142:LEU:HD13	2.03	0.40
15:N:55:LEU:HB2	15:N:133:PHE:CD1	2.57	0.40
16:O:107:ILE:HG21	16:O:115:LEU:HD11	2.03	0.40
20:U:58:DA:H2"	20:U:59:DG:N7	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	422/514 (82%)	379 (90%)	42 (10%)	1 (0%)	43	74
2	M	105/415 (25%)	93 (89%)	12 (11%)	0	100	100
3	A	1449/1664 (87%)	1326 (92%)	123 (8%)	0	100	100
4	B	1174/1203 (98%)	1045 (89%)	128 (11%)	1 (0%)	48	79
5	C	300/335 (90%)	264 (88%)	36 (12%)	0	100	100
6	D	66/137 (48%)	64 (97%)	2 (3%)	0	100	100
7	E	213/215 (99%)	198 (93%)	15 (7%)	0	100	100
8	F	98/155 (63%)	89 (91%)	8 (8%)	1 (1%)	12	44
9	G	193/326 (59%)	170 (88%)	23 (12%)	0	100	100
10	H	130/146 (89%)	120 (92%)	10 (8%)	0	100	100
11	I	122/125 (98%)	103 (84%)	19 (16%)	0	100	100
12	J	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
13	K	101/142 (71%)	88 (87%)	13 (13%)	0	100	100
14	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
15	N	131/233 (56%)	107 (82%)	24 (18%)	0	100	100
16	O	456/627 (73%)	411 (90%)	45 (10%)	0	100	100
17	S	594/894 (66%)	513 (86%)	81 (14%)	0	100	100
18	R	322/507 (64%)	290 (90%)	32 (10%)	0	100	100
All	All	5986/7778 (77%)	5353 (89%)	630 (10%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	280	ASP
8	F	87	LYS
4	B	397	THR

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	
1	Q	396/476 (83%)	394 (100%)	2 (0%)	81	80
2	M	97/371 (26%)	96 (99%)	1 (1%)	68	75
3	A	1293/1465 (88%)	1285 (99%)	8 (1%)	78	79
4	B	1030/1053 (98%)	1024 (99%)	6 (1%)	78	79
5	C	269/296 (91%)	268 (100%)	1 (0%)	84	81
6	D	65/116 (56%)	65 (100%)	0	100	100
7	E	197/197 (100%)	197 (100%)	0	100	100
8	F	90/137 (66%)	90 (100%)	0	100	100
9	G	177/291 (61%)	177 (100%)	0	100	100
10	H	116/128 (91%)	116 (100%)	0	100	100
11	I	109/110 (99%)	109 (100%)	0	100	100
12	J	64/65 (98%)	63 (98%)	1 (2%)	55	70
13	K	93/130 (72%)	92 (99%)	1 (1%)	65	74
14	L	40/57 (70%)	40 (100%)	0	100	100
15	N	128/220 (58%)	128 (100%)	0	100	100
16	O	427/576 (74%)	427 (100%)	0	100	100
17	S	563/828 (68%)	563 (100%)	0	100	100
18	R	313/474 (66%)	311 (99%)	2 (1%)	78	79
All	All	5467/6990 (78%)	5445 (100%)	22 (0%)	81	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	152	LEU
1	Q	383	LYS
2	M	101	VAL
3	A	30	LYS
3	A	334	VAL
3	A	780	ILE
3	A	959	VAL
3	A	1086	ILE
3	A	1202	LEU
3	A	1233	ILE
3	A	1497	ILE
4	B	121	VAL

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Mol	Chain	Res	Type
4	B	276	ILE
4	B	358	VAL
4	B	561	ILE
4	B	640	LEU
4	B	1151	ILE
5	C	239	ILE
12	J	59	LYS
13	K	103	ILE
18	R	296	PRO
18	R	401	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	33	HIS
1	Q	109	GLN
1	Q	272	GLN
1	Q	294	HIS
1	Q	300	ASN
1	Q	301	HIS
1	Q	435	GLN
1	Q	507	ASN
2	M	89	GLN
3	A	43	HIS
3	A	263	ASN
3	A	264	ASN
3	A	332	GLN
3	A	378	HIS
3	A	458	GLN
3	A	636	HIS
3	A	649	ASN
3	A	706	HIS
3	A	748	ASN
3	A	819	ASN
3	A	840	ASN
3	A	880	GLN
3	A	937	ASN
3	A	949	GLN
3	A	1036	ASN
3	A	1062	HIS
3	A	1072	ASN
3	A	1108	HIS

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Mol	Chain	Res	Type
3	A	1162	ASN
3	A	1314	GLN
3	A	1320	GLN
3	A	1447	GLN
3	A	1487	ASN
3	A	1532	GLN
3	A	1560	ASN
3	A	1581	HIS
3	A	1620	GLN
3	A	1633	GLN
4	B	248	ASN
4	B	282	HIS
4	B	351	GLN
4	B	361	HIS
4	B	368	GLN
4	B	427	GLN
4	B	462	GLN
4	B	532	HIS
4	B	544	HIS
4	B	575	HIS
4	B	673	ASN
4	B	702	ASN
4	B	718	GLN
4	B	735	HIS
4	B	767	ASN
4	B	823	GLN
4	B	899	GLN
4	B	1008	HIS
4	B	1114	GLN
4	B	1115	GLN
5	C	53	ASN
5	C	130	ASN
5	C	172	GLN
5	C	301	ASN
6	D	23	HIS
7	E	54	GLN
9	G	56	ASN
9	G	59	GLN
9	G	64	GLN
9	G	121	ASN
9	G	170	HIS
9	G	216	HIS

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Mol	Chain	Res	Type
11	I	32	GLN
11	I	95	ASN
12	J	53	HIS
13	K	106	GLN
14	L	53	HIS
16	O	66	ASN
16	O	94	ASN
16	O	152	GLN
16	O	547	ASN
17	S	37	GLN
17	S	185	GLN
17	S	270	GLN
17	S	461	HIS
17	S	483	HIS
17	S	705	HIS
17	S	728	GLN
17	S	769	GLN
18	R	184	ASN
18	R	207	ASN
18	R	246	GLN
18	R	304	HIS
18	R	319	ASN
18	R	407	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

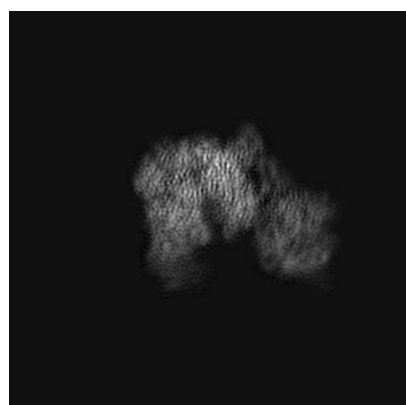
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10007. These allow visual inspection of the internal detail of the map and identification of artifacts.

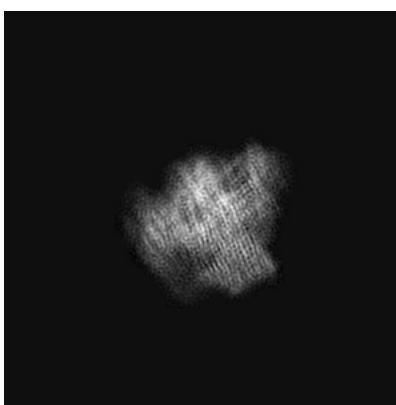
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

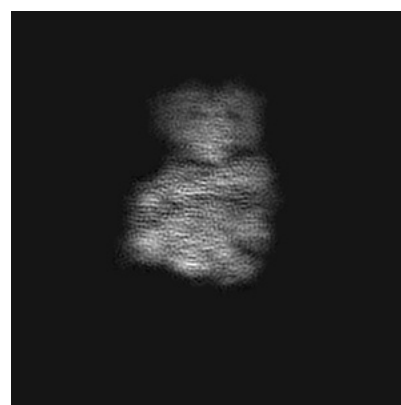
6.1.1 Primary map



X



Y

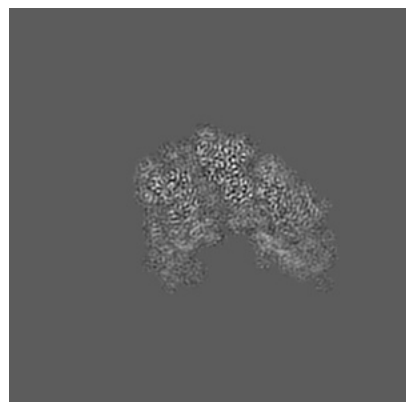


Z

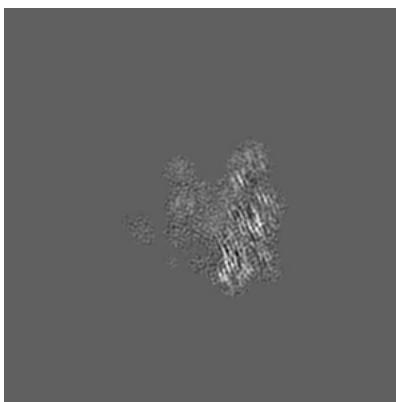
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

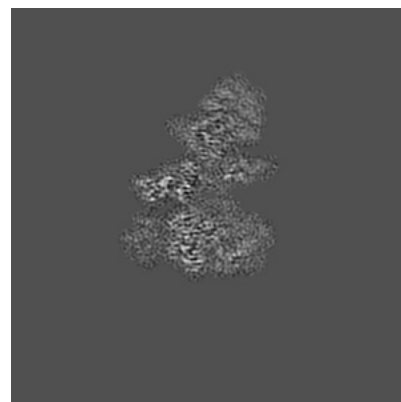
6.2.1 Primary map



X Index: 144



Y Index: 144



Z Index: 144

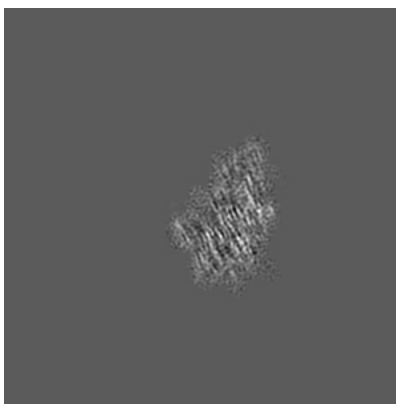
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

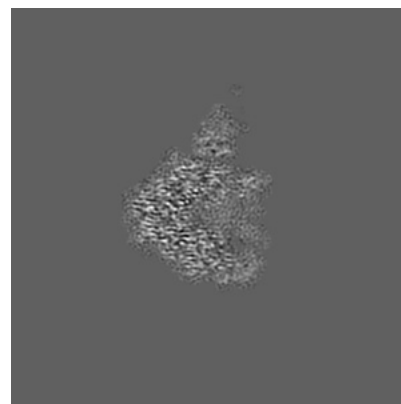
6.3.1 Primary map



X Index: 127



Y Index: 157

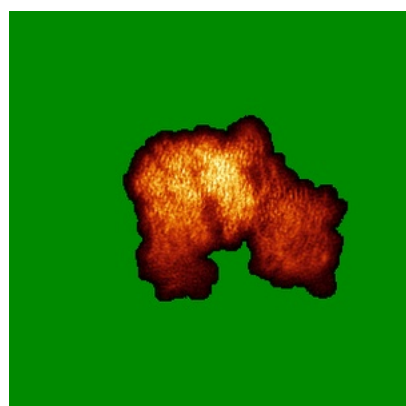


Z Index: 161

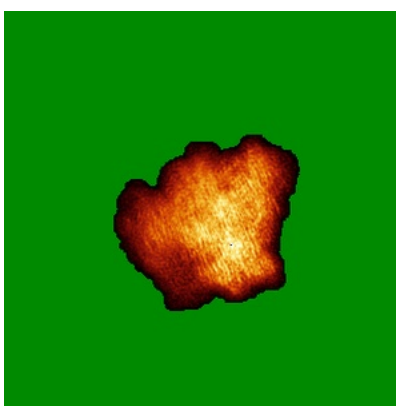
The images above show the largest variance slices of the map in three orthogonal directions.

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

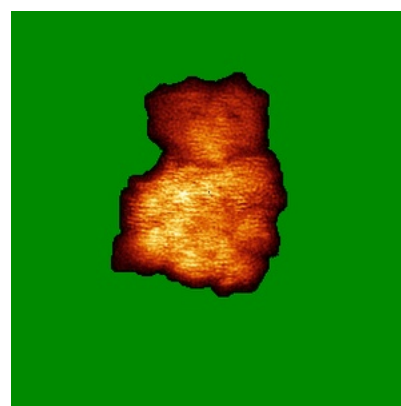
6.4.1 Primary map



X



Y



Z

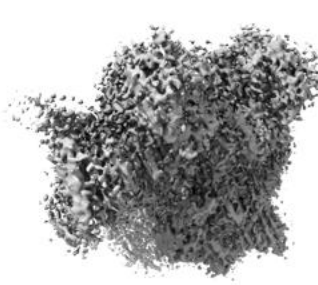
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

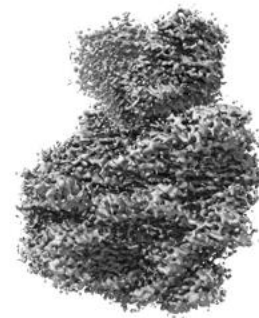
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

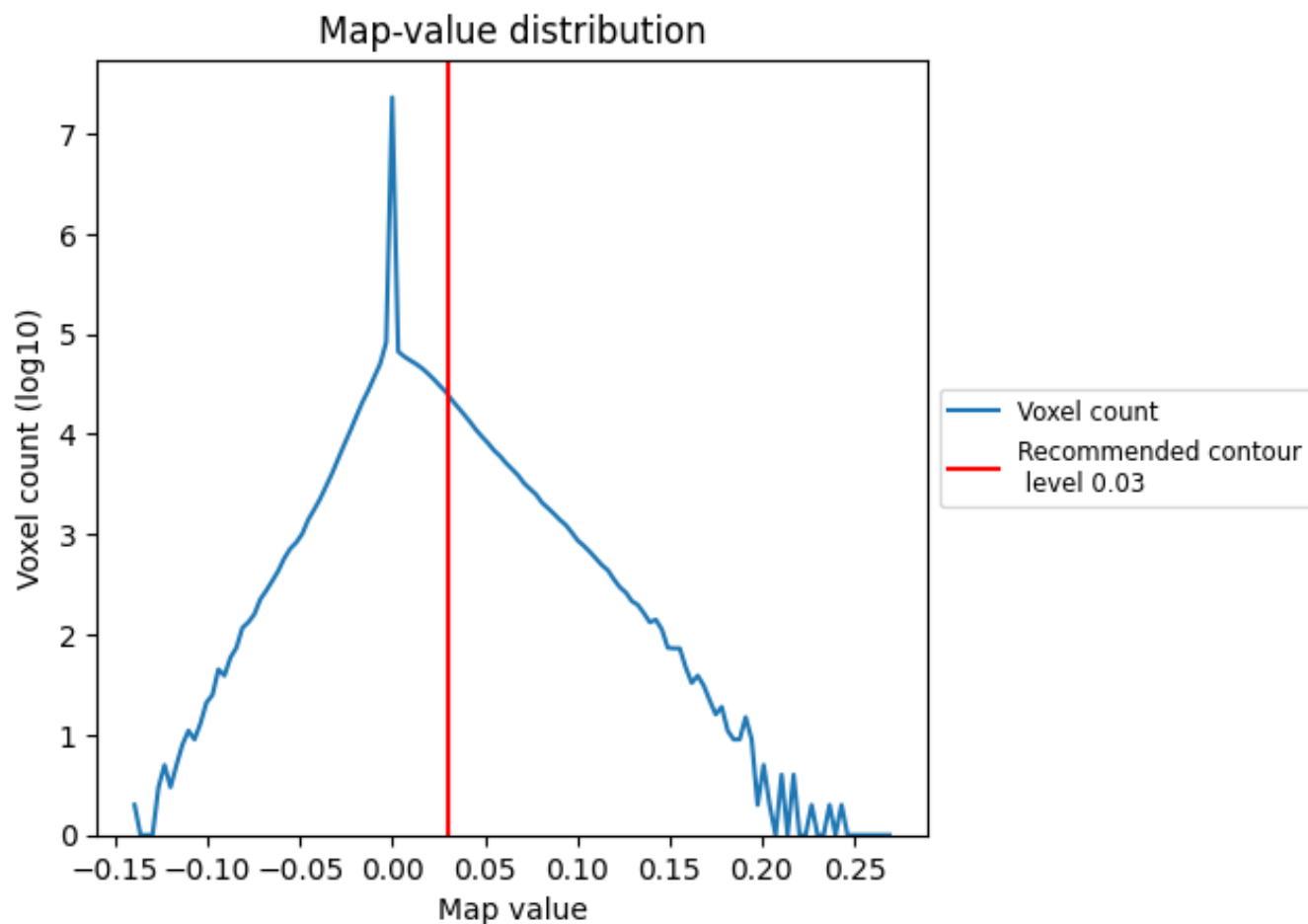
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

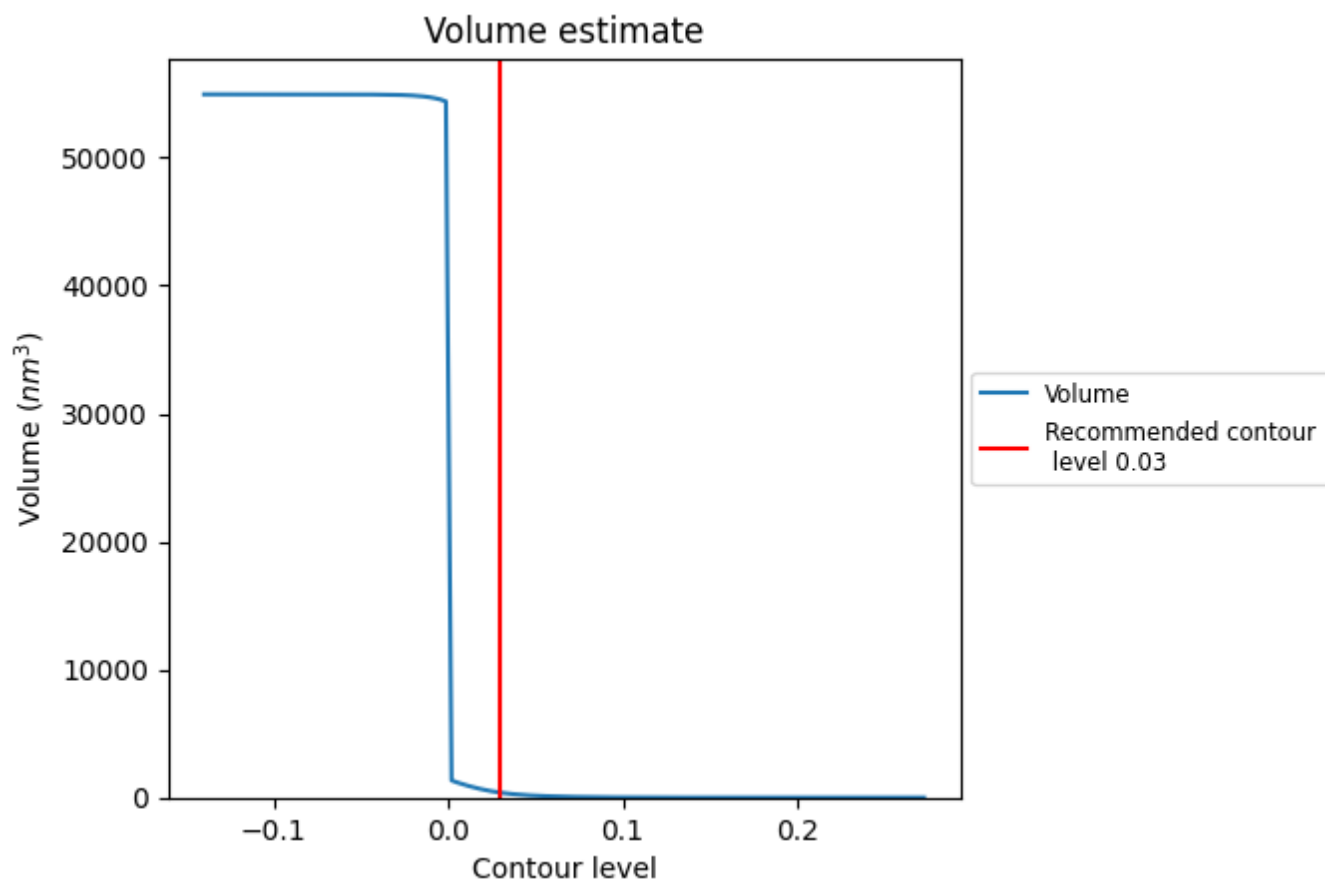
This section contains the results of statistical analysis of the map.

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.

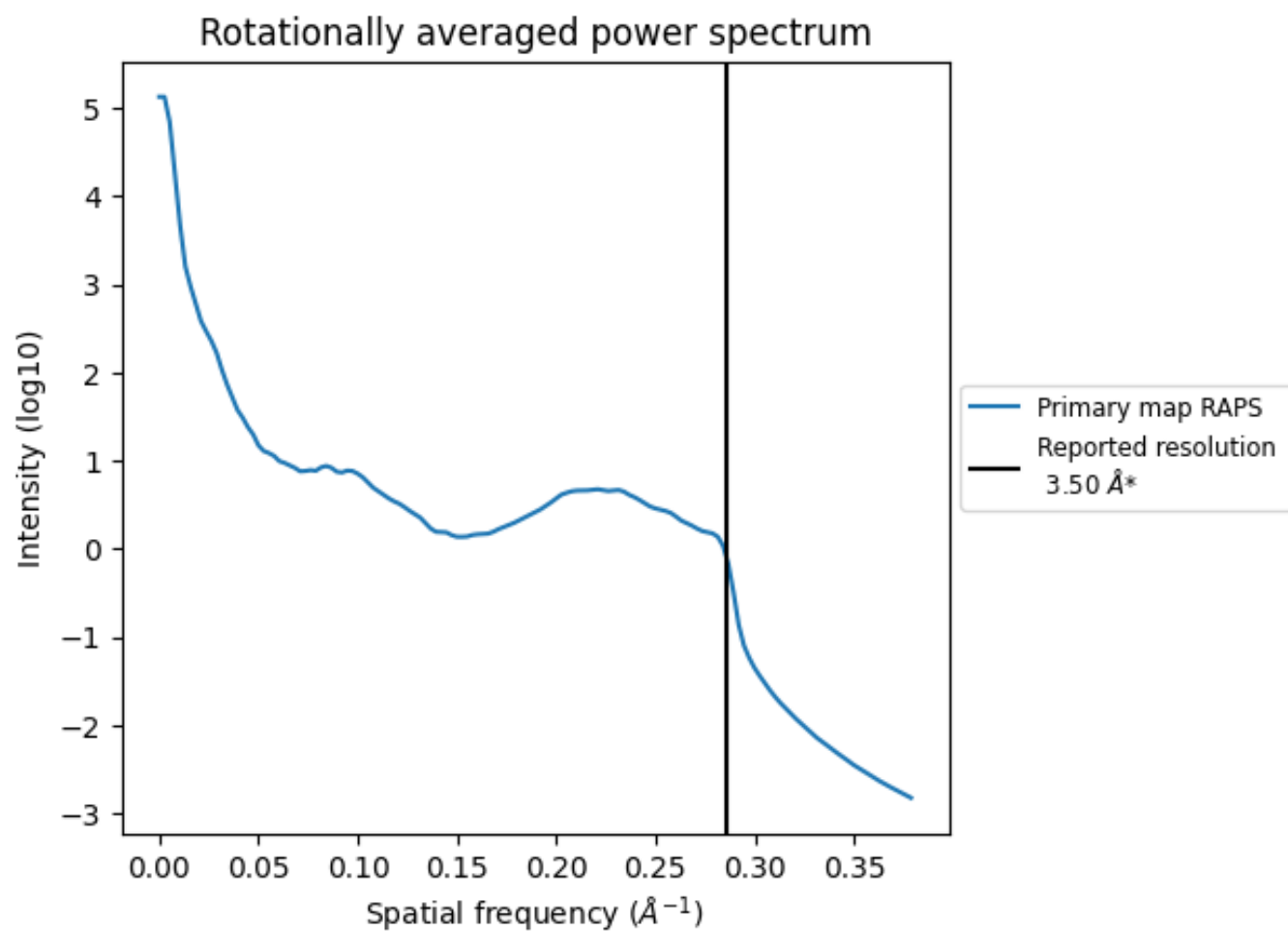
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm^3 ; this corresponds to an approximate mass of 347 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 0.286 Å⁻¹

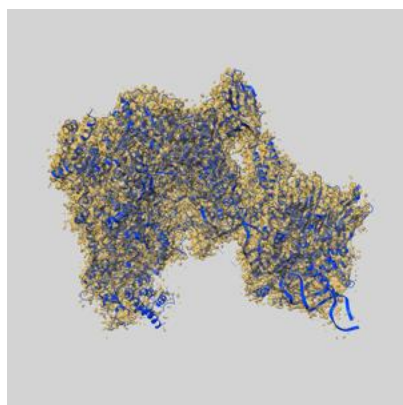
8 Fourier-Shell correlation

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

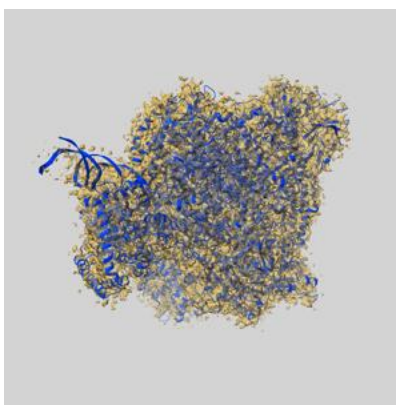
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10007 and PDB model 6RUO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

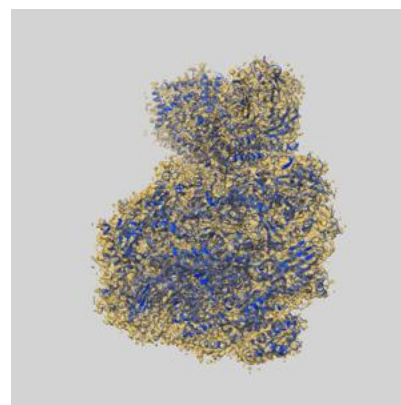
9.1 Map-model overlay [i](#)



X



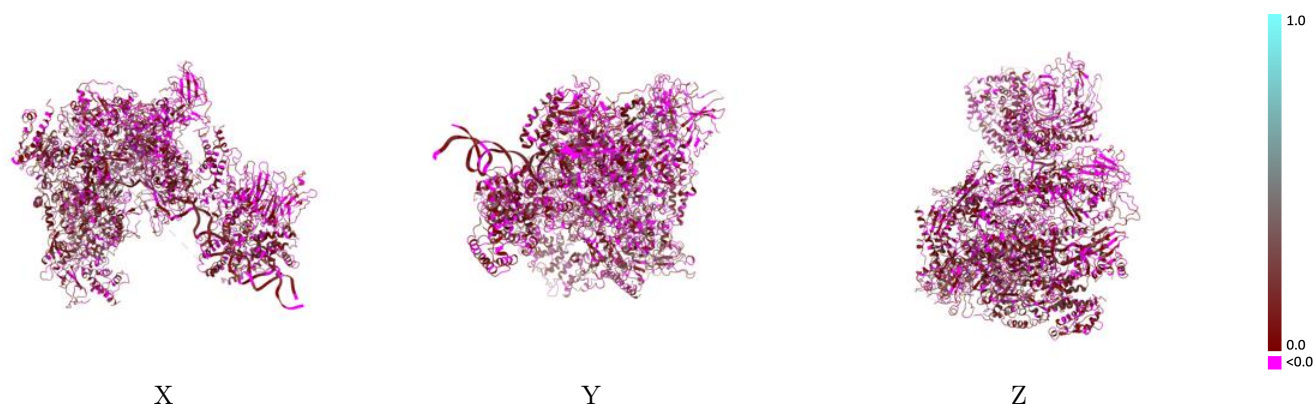
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

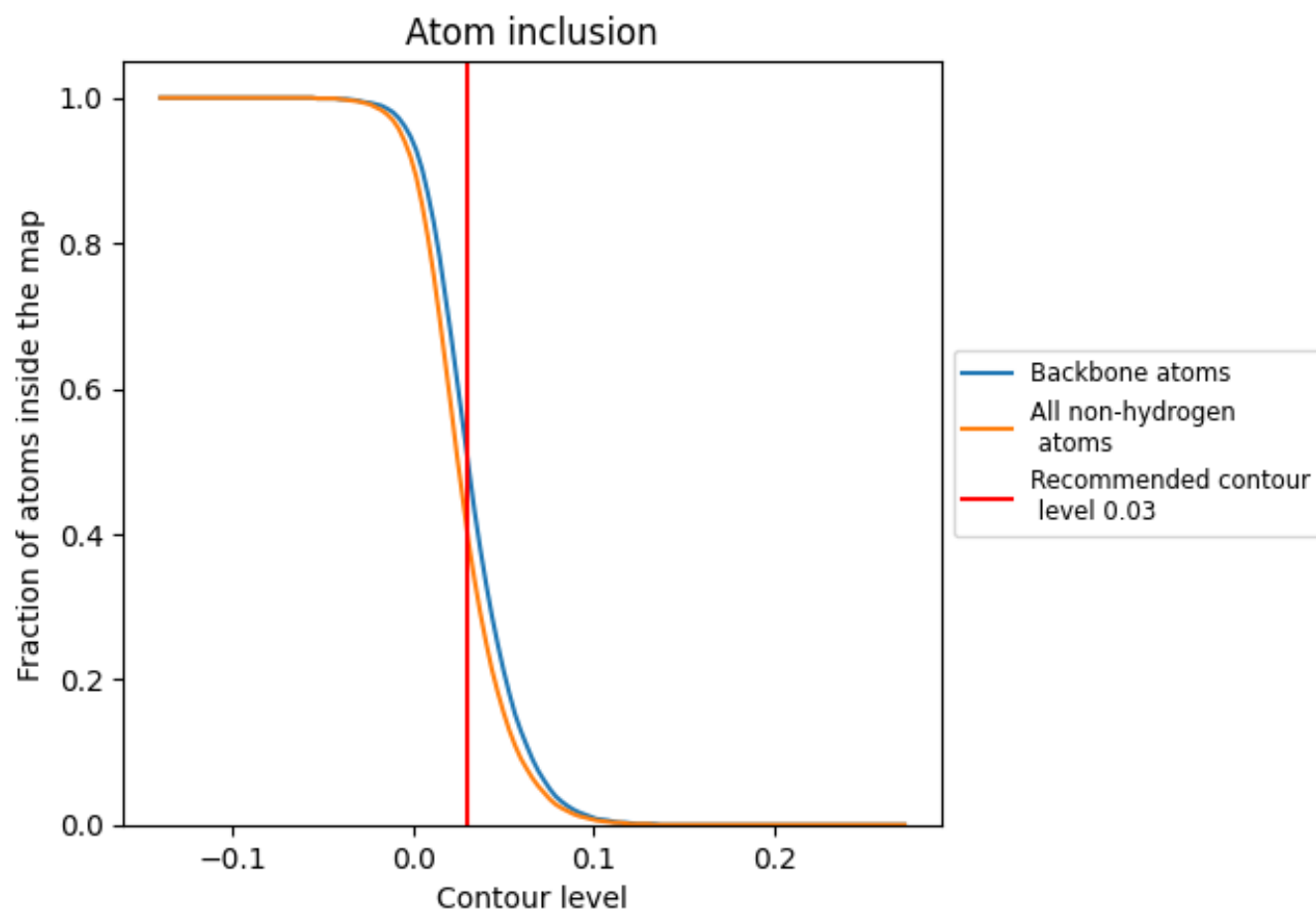


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 40% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4050	 0.0890
A	 0.4960	 0.1120
B	 0.4780	 0.0900
C	 0.5220	 0.1060
D	 0.3410	 0.1150
E	 0.5030	 0.1180
F	 0.5330	 0.1540
G	 0.3320	 0.1270
H	 0.5770	 0.1550
I	 0.2790	 0.0650
J	 0.4870	 0.0340
K	 0.5160	 0.1200
L	 0.5300	 0.0910
M	 0.2850	 -0.0050
N	 0.2860	 0.0230
O	 0.1240	 0.0980
Q	 0.3150	 0.0740
R	 0.3710	 0.0490
S	 0.2870	 0.0380
T	 0.3430	 0.0830
U	 0.3860	 0.1040

