Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 04:28 am GMT

PDB ID	:	6RQL
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:

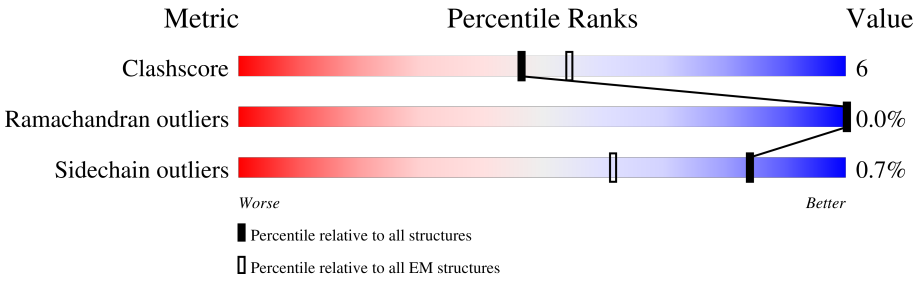
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	T	70	60% 53% 7% 40%
2	U	70	60% 56% · 40%
3	Q	514	86% 75% 17% · 7%
4	S	894	68% 53% 15% 32%
5	R	507	64% 53% 12% 35%
6	M	415	13% 21% 5% 74%
7	A	1664	9% 80% 12% 7%
8	B	1203	· 82% 16% ·

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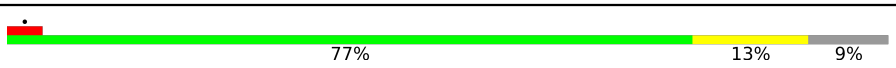
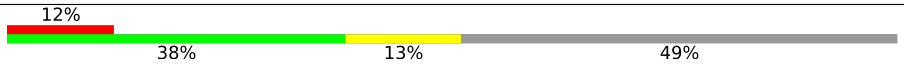
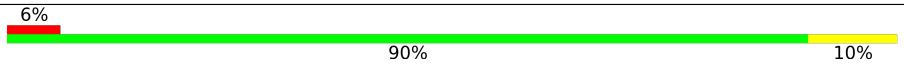
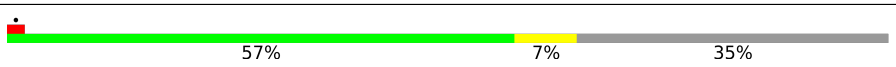
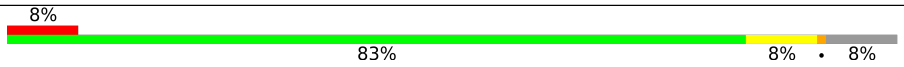
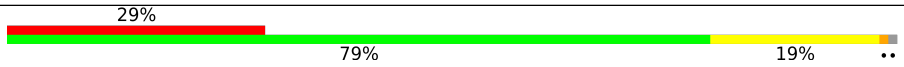
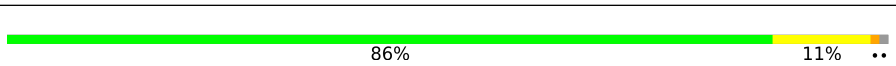
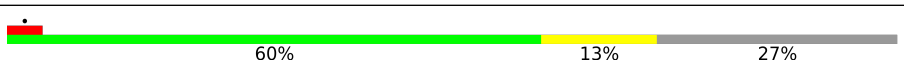
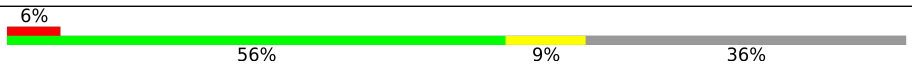
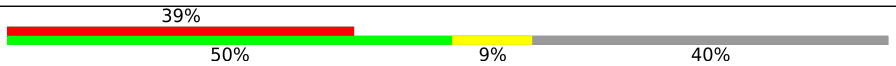
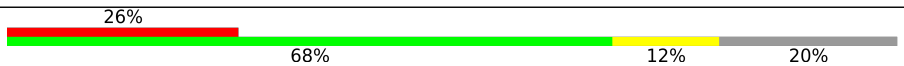
Mol	Chain	Length	Quality of chain
9	C	335	
10	D	137	
11	E	215	
12	F	155	
13	G	326	
14	H	146	
15	I	125	
16	J	70	
17	K	142	
18	L	70	
19	N	233	
20	O	627	

2 Entry composition (i)

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
			Total	C	N	O	P		
1	T	42	842	405	141	254	42	0	0

- Molecule 2 is a DNA chain called Nontemplate strand.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	476	3931	2526	674	711	20	0	0

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

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

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

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA49.

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

- 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.

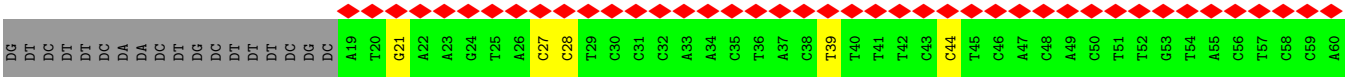
Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	499	Total	C	N	O	S	0	0
			4086	2636	661	767	22		

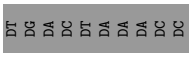
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Template strand

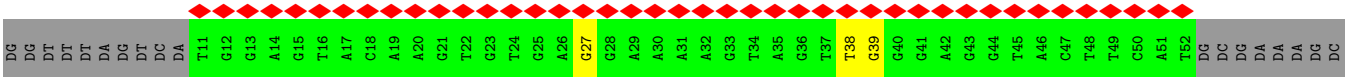
Chain T:

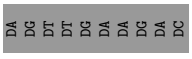




• Molecule 2: Nontemplate strand

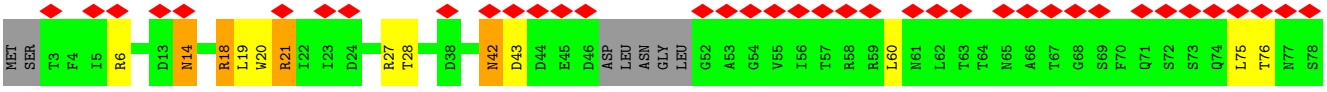
Chain U:

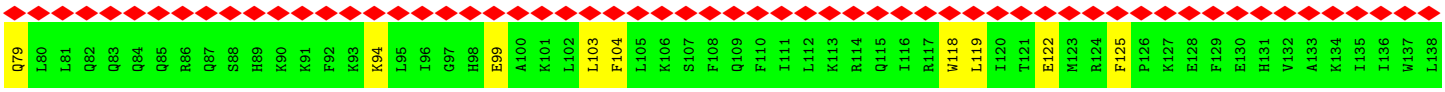


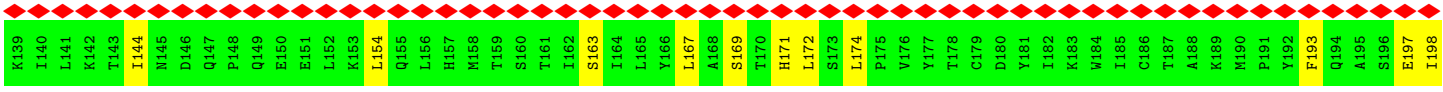


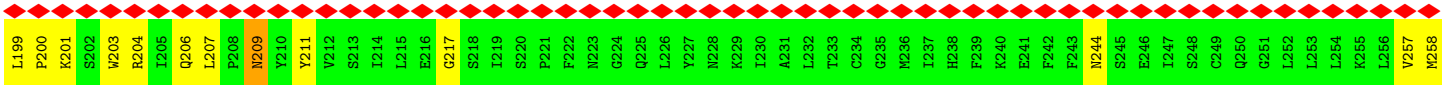
• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN7

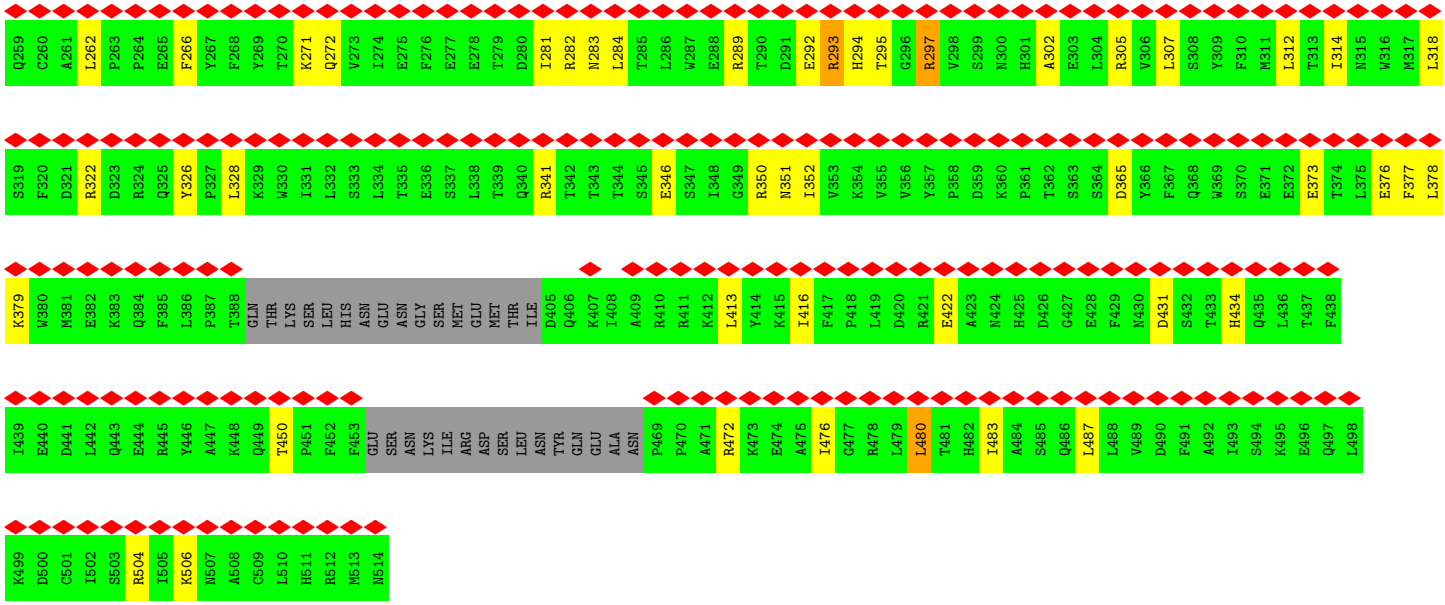
Chain Q:





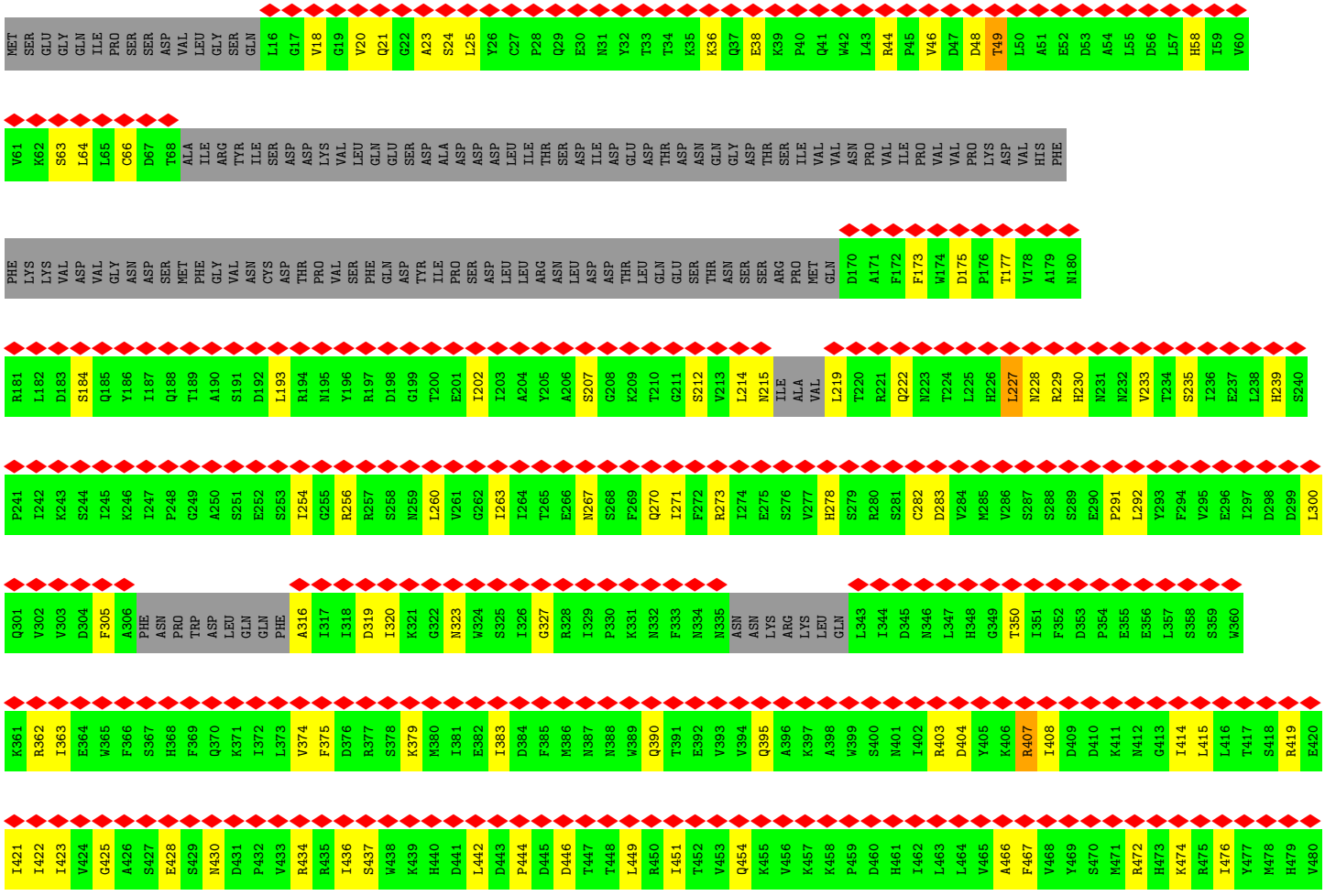


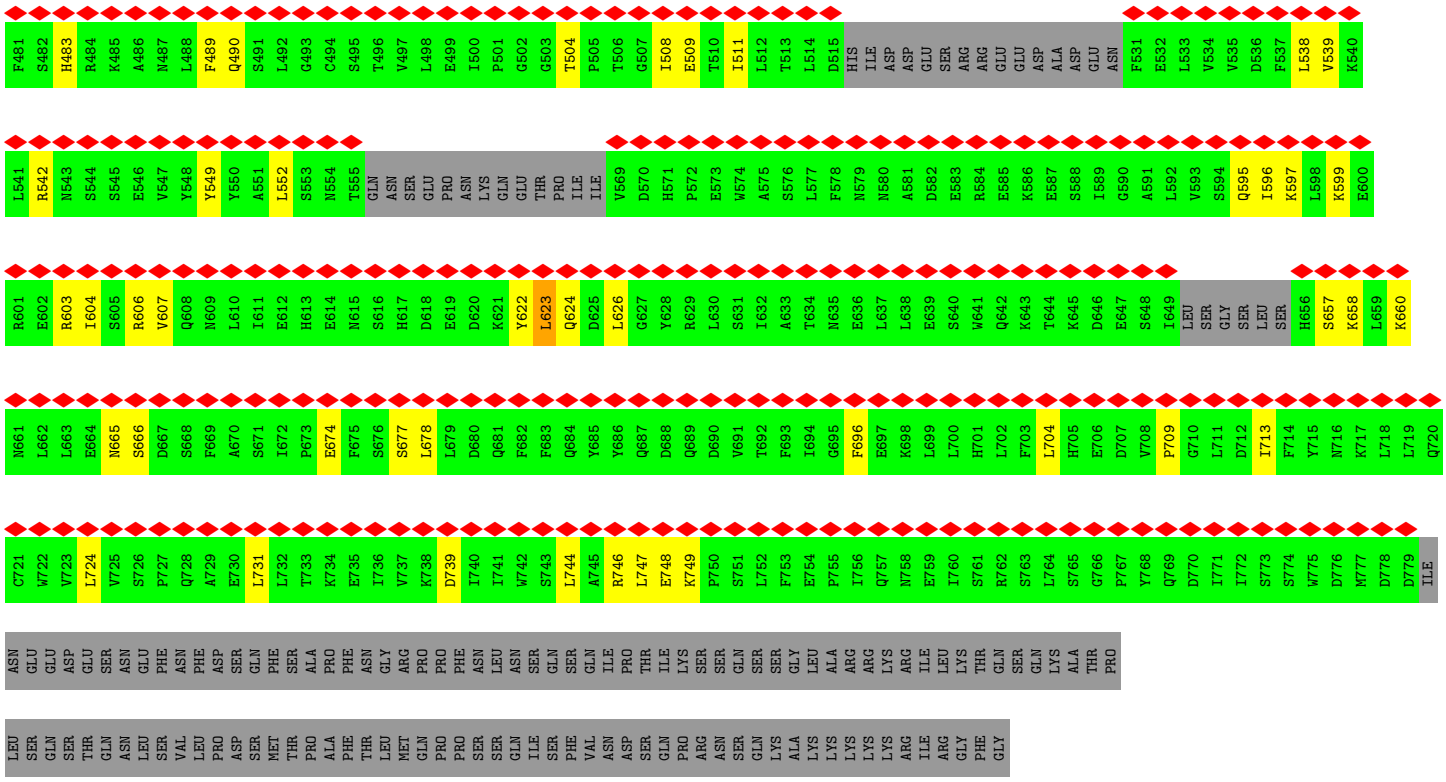




- Molecule 4: RNA polymerase I-specific transcription initiation factor RRN6

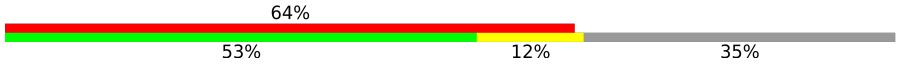
Chain S:

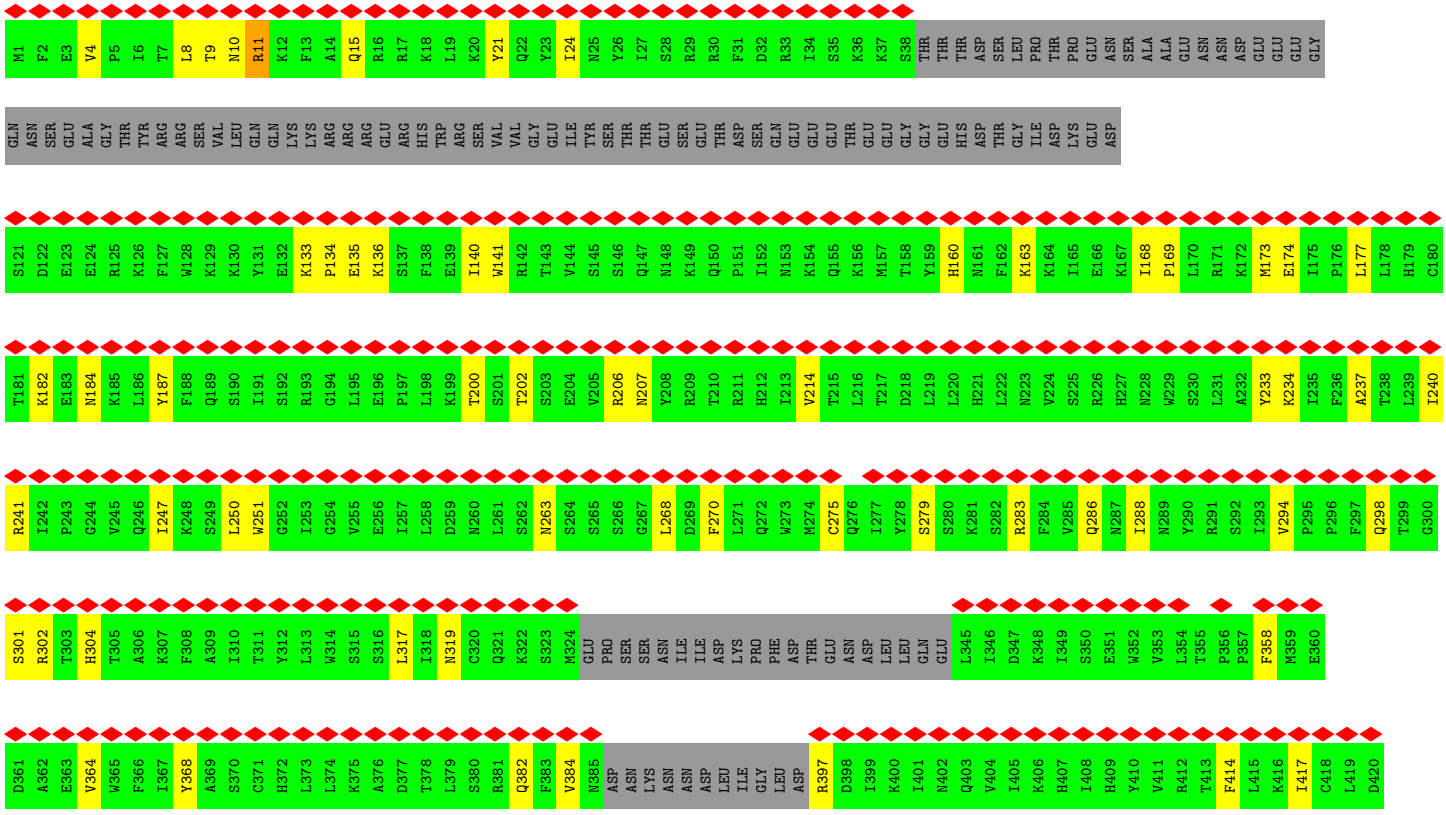


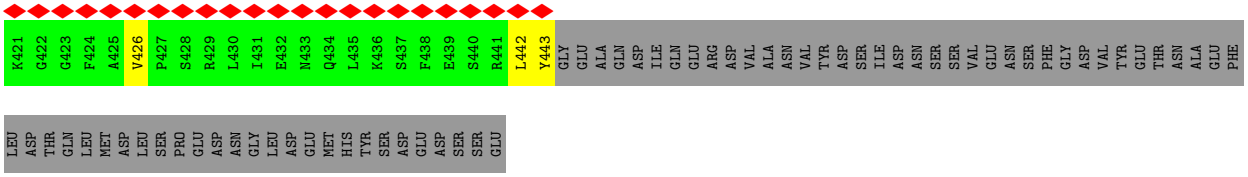


• Molecule 5: RNA polymerase I-specific transcription initiation factor RRN11

Chain R:

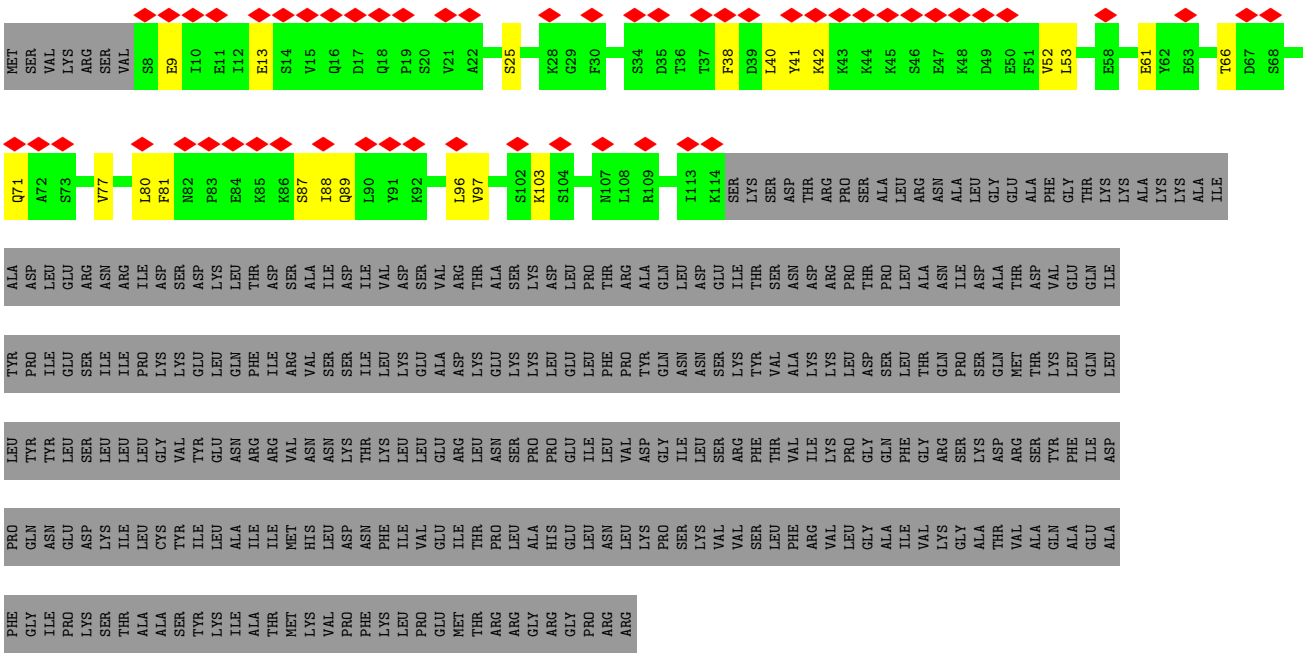






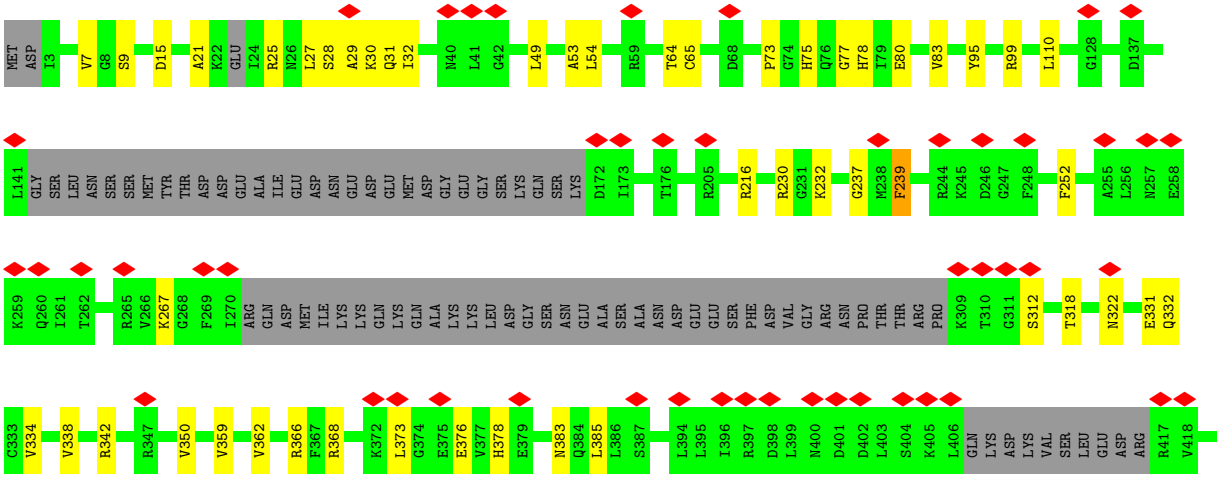
• Molecule 6: DNA-directed RNA polymerase I subunit RPA49

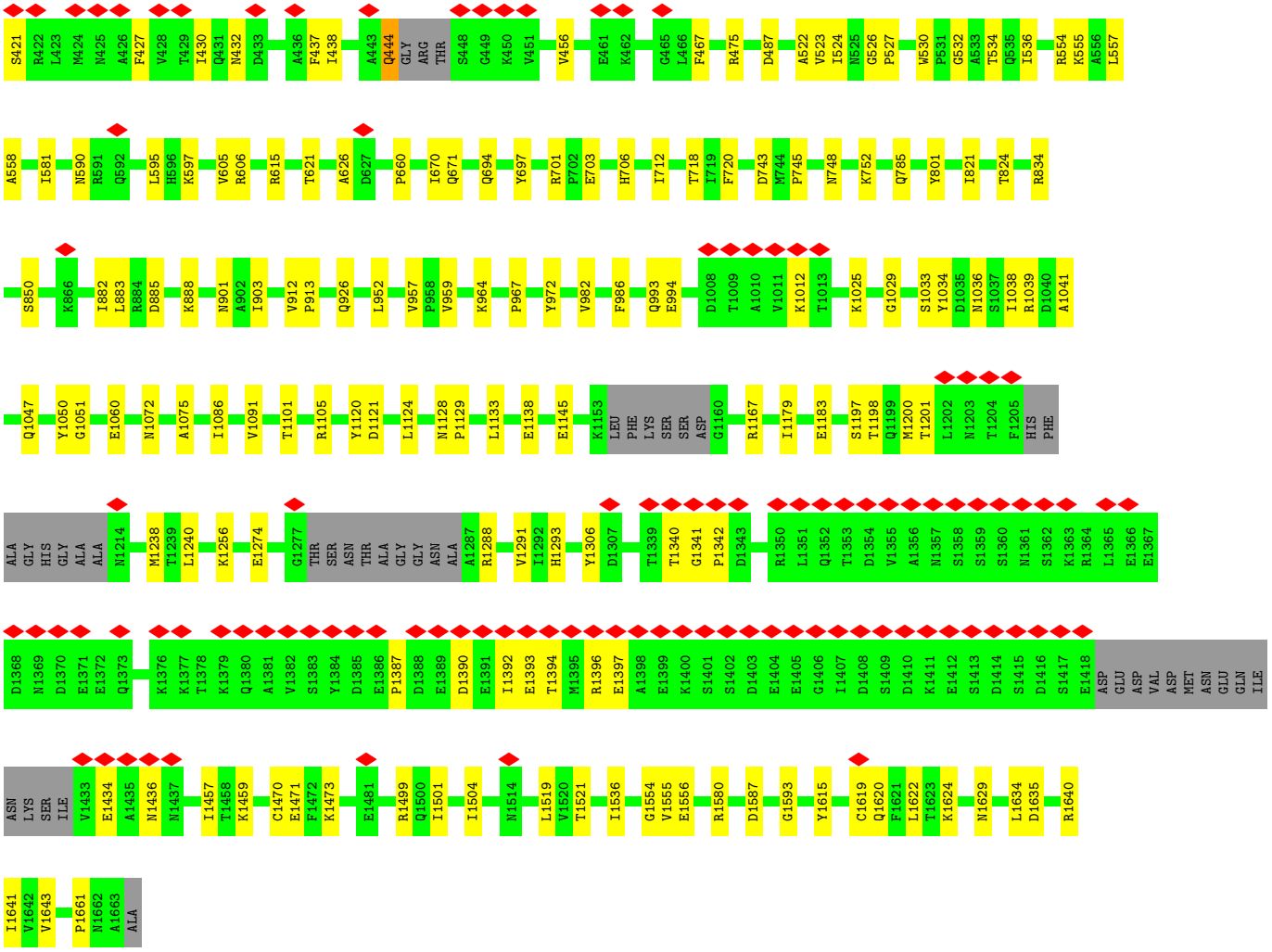
Chain M:



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

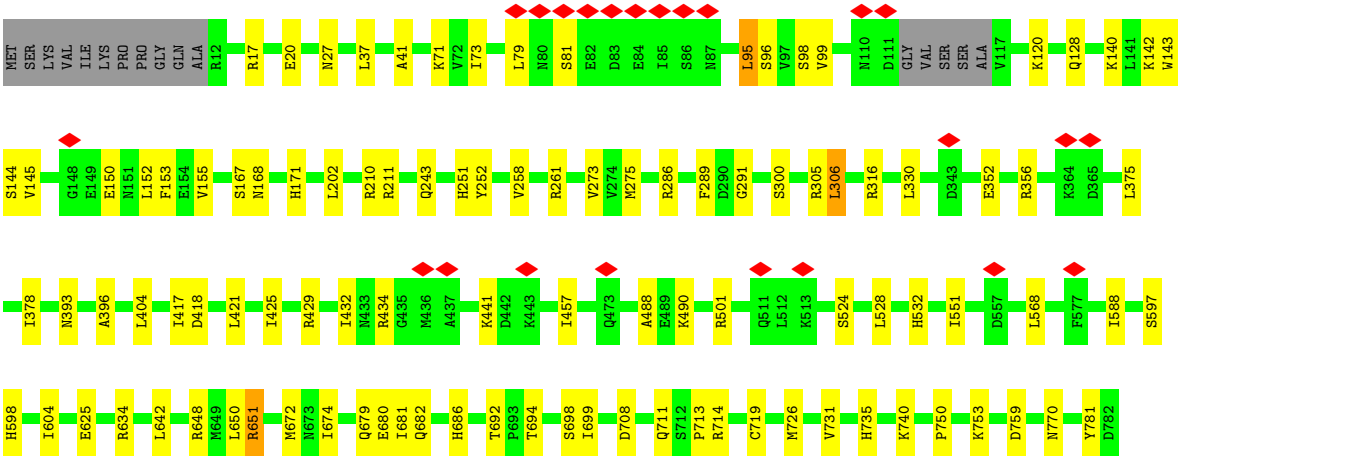
Chain A:

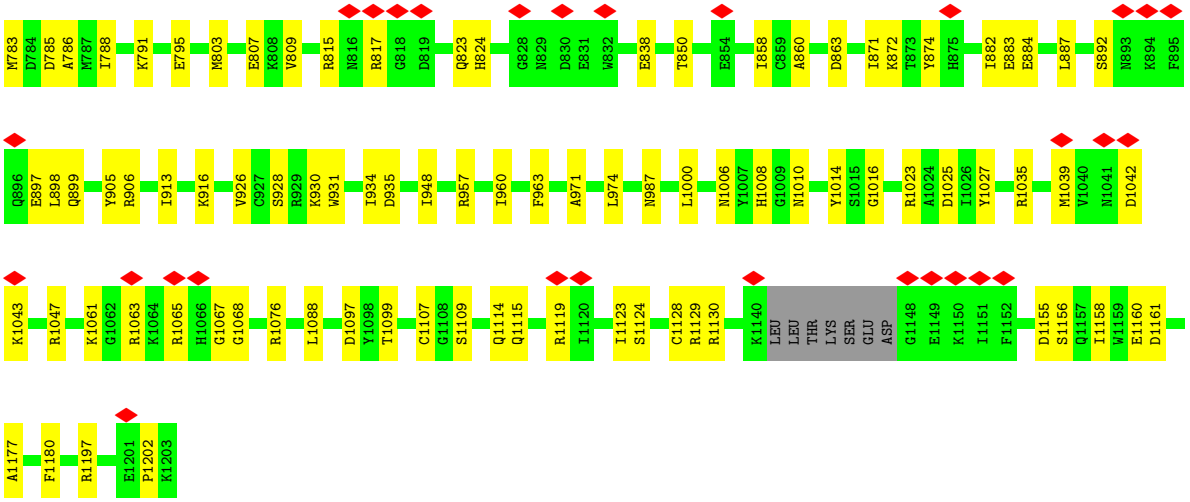




• Molecule 8: DNA-directed RNA polymerase I subunit RPA135

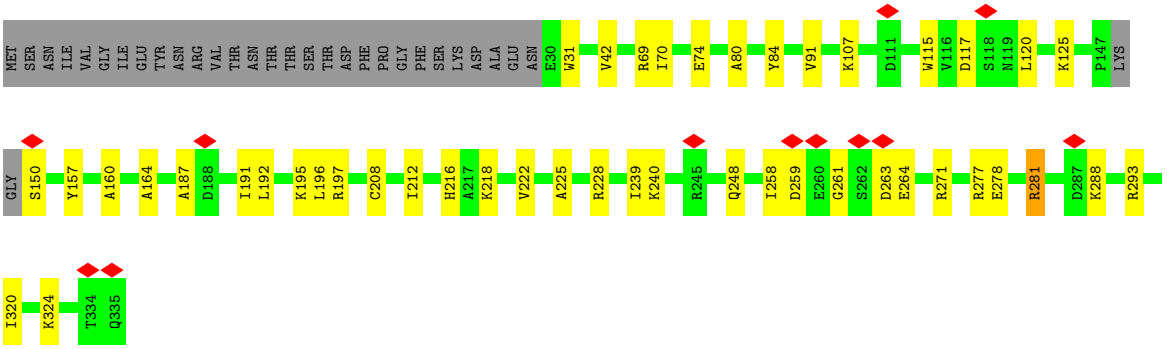
Chain B:





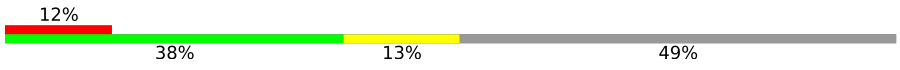
• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1

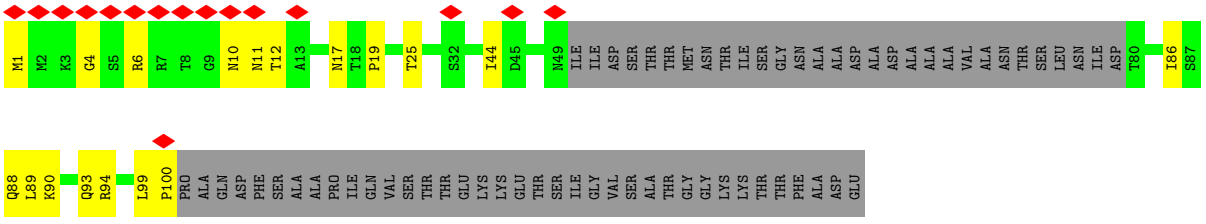
Chain C:



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

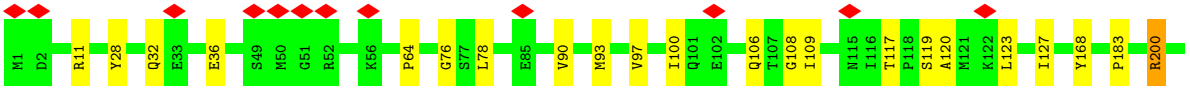
Chain D:





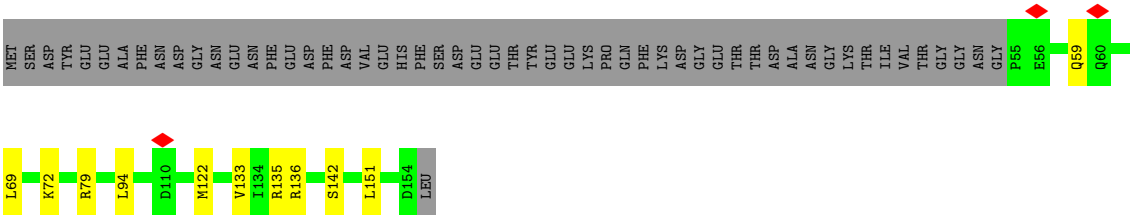
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



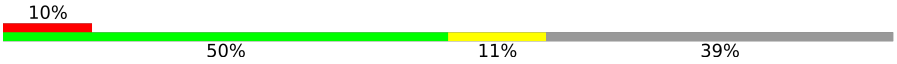
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

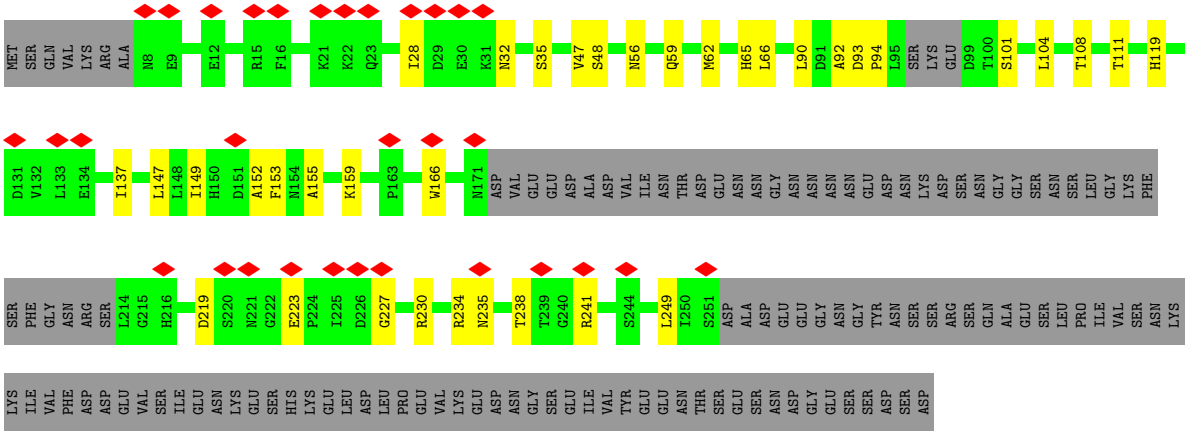
Chain F:



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

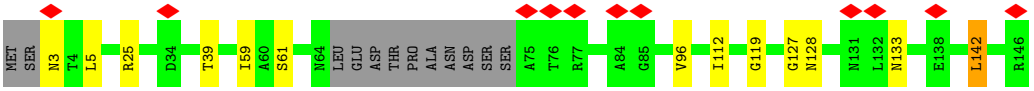
Chain G:





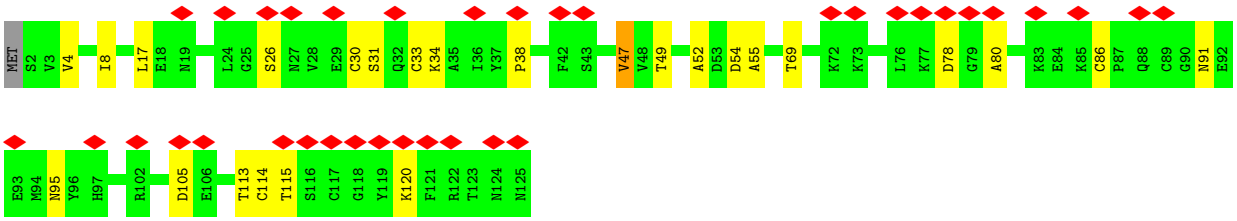
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



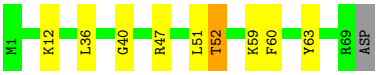
• Molecule 15: DNA-directed RNA polymerase I subunit RPA12

Chain I:



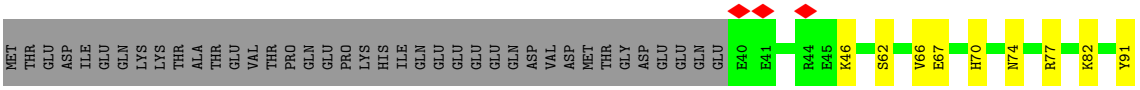
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

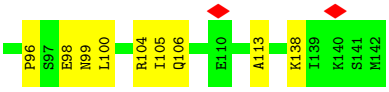
Chain J:



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

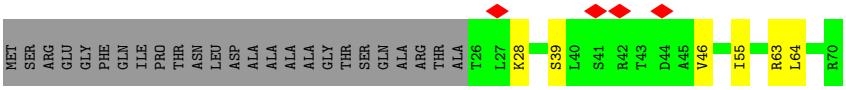
Chain K:





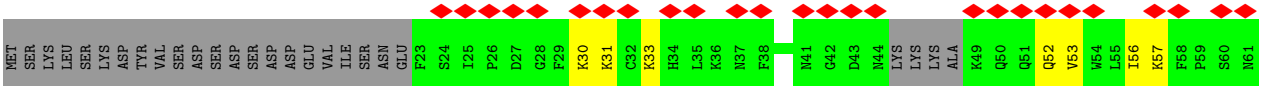
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC4

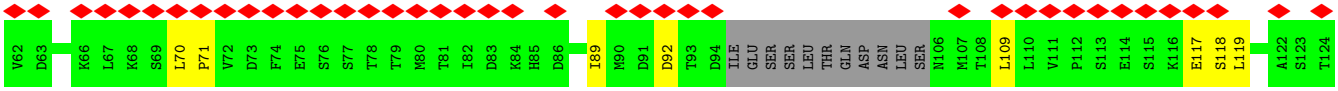
Chain L:

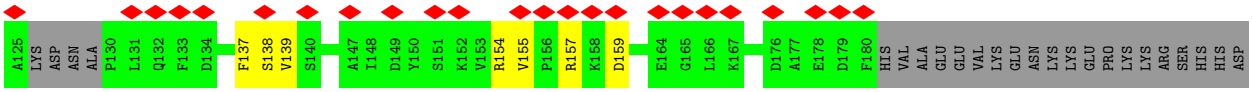


• Molecule 19: DNA-directed RNA polymerase I subunit RPA34

Chain N:

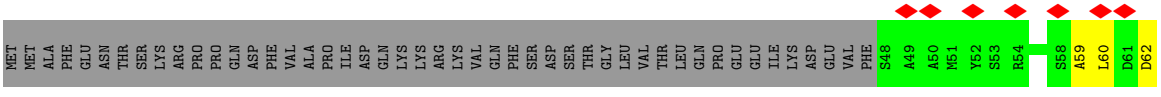


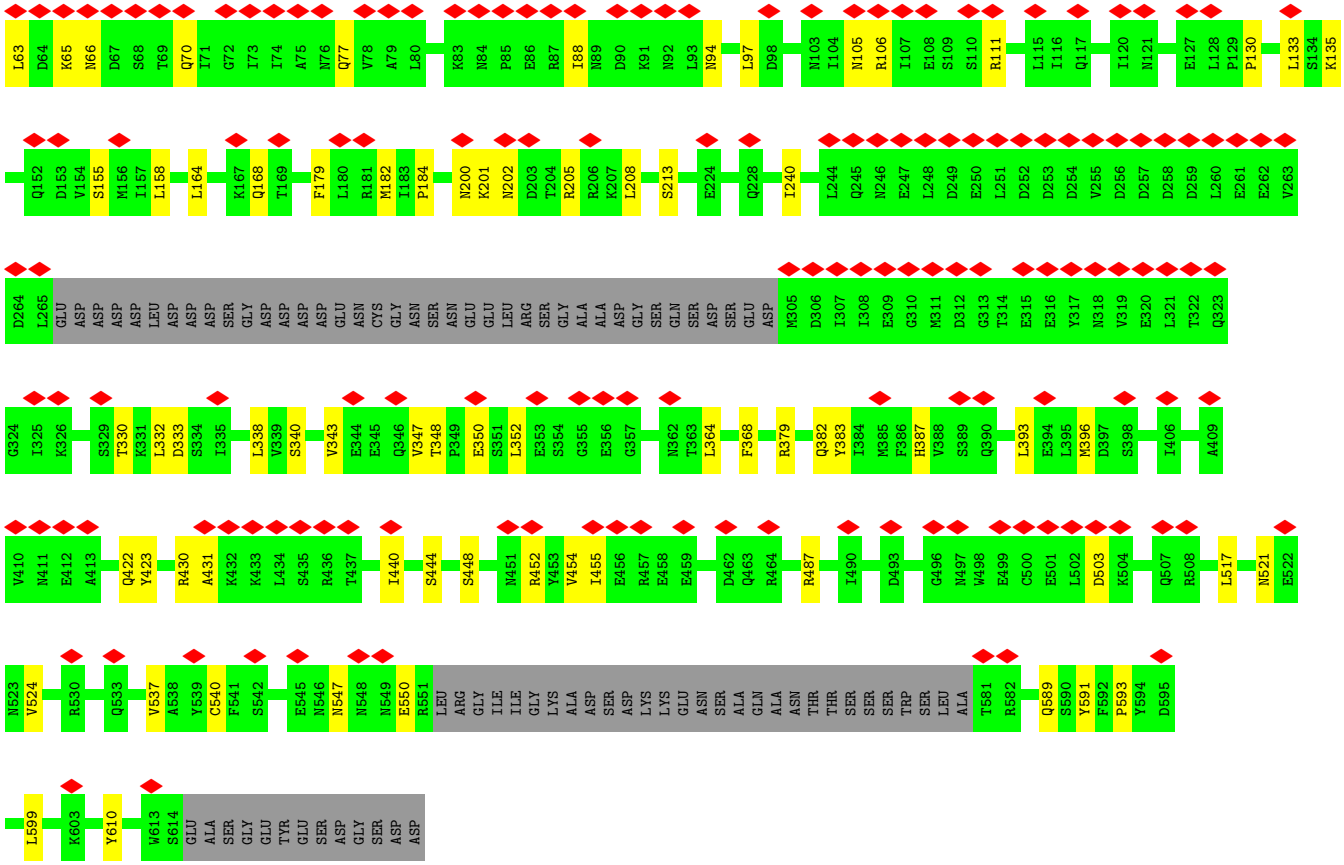




• Molecule 20: RNA polymerase I-specific transcription initiation factor RRN3

Chain O:




L63 D64 K65 N66 D67 S68 T69 Q70 I71 G72 I73 I74 A75 N76 Q77 V78 A79 L80 K83 N84 P85 E86 R87 I88 N89 D90 K91 N92 L93 N94 L97 D98 N103 I104 N105 R106 I107 E108 S109 S110 R111 L115 I116 Q117 I120 N121 E127 L128 P129 P130 L133 S134 K135
Q152 D153 V154 S155 M156 I157 L158 L164 K167 Q168 T169 F179 L180 R181 M182 I183 P184 N200 K201 N202 D203 T204 R205 R206 K207 L208 S213 E224 Q228 I240 L244 Q245 N246 E247 L248 D249 E250 L251 D252 D253 D254 V255 D256 D257 D258 D259 L260 E261 E262 V263
D264 L265 GLU ASP ASP ASP ASP LEU ASP ASP SER GLY ASP ASP ASP ASP GLU ASN CYS GLY ASN SER ASN GLU GLU LEU ARG SER GLY ALA ALA ASP GLY SER GLN SER ASP SER GLU ASP M305 D306 I307 I308 E309 G310 M311 D312 G313 T314 E315 E316 Y317 N318 V319 E320 L321 T322 Q323
G324 I325 K326 S329 T330 K331 L332 D333 S334 I335 L338 V339 S340 V343 E344 E345 Q346 V347 T348 P349 E350 S351 L352 E353 S354 G355 E356 G357 N362 T363 L364 F368 R379 Q382 Y383 I384 M385 F386 H387 V388 S389 Q390 L393 E394 L395 M396 D397 S398 I406 A409
V410 N411 E412 A413 Q422 Y423 R430 A431 K432 K433 L434 S435 R436 T437 I440 S444 S448 N451 R452 Y453 V454 I455 E456 R457 E458 E459 D462 Q463 R464 R487 I490 D493 G496 N497 W498 E499 C500 E501 L502 D503 K504 Q507 R508 L517 N521 E522
N523 V524 R530 Q533 V537 A538 Y539 C540 F541 S542 E545 N546 N547 N548 N549 E550 R551 LEU ARG GLY ILE ILE GLY LYS ALA ASP SER ASP LYS LYS GLU ASN SER ALA GLN ALA ASN THR THR SER SER SER TRP SER LEU ALA T581 R582 Q589 S590 Y591 F592 P593 Y594 D595
L599 K603 Y610 W613 S614 GLU ALA SER GLY GLU TYR GLU SER ASP GLY SER ASP ASP

4 Experimental information (i)

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 ($e^-/Å^2$)	1.1075	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.274	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

5.1 Standard geometry

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	0.75	0/939	1.05	0/1442
2	U	0.64	0/988	0.92	0/1528
3	Q	0.36	0/4023	0.64	1/5434 (0.0%)
4	S	0.35	0/5065	0.63	0/6859
5	R	0.41	0/2836	0.65	0/3817
6	M	0.35	0/866	0.61	0/1162
7	A	0.47	0/12165	0.60	1/16450 (0.0%)
8	B	0.53	0/9578	0.65	0/12948
9	C	0.48	0/2469	0.61	0/3347
10	D	0.35	0/557	0.59	0/750
11	E	0.41	0/1795	0.54	0/2416
12	F	0.52	0/838	0.60	0/1129
13	G	0.40	0/1613	0.59	0/2193
14	H	0.49	0/1090	0.61	0/1476
15	I	0.37	0/955	0.61	0/1288
16	J	0.58	0/578	0.71	0/775
17	K	0.48	0/821	0.61	0/1108
18	L	0.49	0/361	0.77	0/478
19	N	0.32	0/1124	0.58	0/1512
20	O	0.36	0/4173	0.57	0/5645
All	All	0.46	0/52834	0.64	2/71757 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	60	LEU	CA-CB-CG	5.55	128.07	115.30
7	A	1387	PRO	N-CA-CB	5.17	109.50	103.30

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	67	0
4	S	4963	0	4890	99	0
5	R	2771	0	2844	42	0
6	M	850	0	850	15	0
7	A	11953	0	11848	152	0
8	B	9371	0	9243	141	0
9	C	2418	0	2401	41	0
10	D	551	0	558	14	0
11	E	1759	0	1788	13	0
12	F	823	0	841	7	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	8	0
17	K	810	0	801	15	0
18	L	359	0	385	5	0
19	N	1103	0	1106	18	0
20	O	4086	0	4024	43	0
All	All	51626	0	50597	644	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (644) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
13:G:108:THR:HG1	13:G:111:THR:HG1	1.38	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:HD12	9:C:120:LEU:C	2.13	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
4:S:623:LEU:HD12	4:S:623:LEU:C	2.19	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
4:S:442:LEU:HD23	4:S:442:LEU:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:Q:293:ARG:O	3:Q:293:ARG:HG3	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	8:B:1097:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1042:ASP:O	8:B:1063:ARG:NH1	2.42	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
7:A:444:GLN:NE2	7:A:444:GLN:N	2.60	0.49
8:B:1014:TYR:HH	9:C:293:ARG:HH12	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
8:B:95:LEU:HD13	8:B:95:LEU:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
8:B:672:MET:HE1	8:B:674:ILE:HD11	1.94	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: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
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
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: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
4:S:230:HIS:ND1	4:S:282:CYS:SG	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
4:S:175:ASP:OD2	4:S:177:THR:OG1	2.26	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:H:128:ASN:N	14:H:128:ASN:OD1	2.48	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
8:B:770:ASN:HD22	16:J:52:THR:HG21	1.81	0.45
19:N:92:ASP:OD1	19:N:92:ASP:N	2.50	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
3:Q:289:ARG:HH12	3:Q:294:HIS:C	2.20	0.44
4:S:215:ASN:HB3	4:S:235:SER:HA	1.98	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
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
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
9:C:120:LEU:C	9:C:120:LEU:CD1	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
20:O:130:PRO:HA	20:O:133:LEU:HB3	1.99	0.44
4:S:623:LEU:C	4:S:623:LEU:CD1	2.85	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
4:S:442:LEU:CD2	4:S:442:LEU:C	2.86	0.43
5:R:233:TYR:CD2	5:R:233:TYR:C	2.91	0.43
3:Q:144:ILE:HD12	3:Q:154:LEU:HB2	2.00	0.43
8:B:95:LEU:CD1	8:B:95:LEU:C	2.86	0.43
8:B:1155:ASP:HA	8:B:1158:ILE:HD12	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
5:R:275:CYS:O	5:R:279:SER:OG	2.32	0.43
6:M:66:THR:HB	6:M:71:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:S:228:ASN:HD22	4:S:282:CYS:HB3	1.83	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:432:ASN:CG	7:A:444:GLN:OE1	2.55	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: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
4:S:696:PHE:HZ	4:S:747:LEU:HD11	1.85	0.42
7:A:444:GLN:N	7:A:444:GLN:CD	2.73	0.42
4:S:36:LYS:HG2	4:S:38:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:A:743:ASP:N	7:A:743:ASP:OD1	2.49	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: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
7:A:239:PHE:CD2	7:A:239:PHE:C	2.94	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
5:R:442:LEU:C	5:R:443:TYR:CD2	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:M:42:LYS:N	19:N:30:LYS:O	2.53	0.41
7:A:239:PHE:HD2	7:A:239:PHE:C	2.23	0.41
7:A:1661:PRO:O	13:G:101:SER:OG	2.33	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
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
20:O:393:LEU:HA	20:O:396:MET:HE3	2.03	0.41
3:Q:258:MET:HE3	4:S:704:LEU:HD23	2.02	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: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
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
4:S:230:HIS:CE1	4:S:282:CYS:HG	2.39	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
20:O:164:LEU:HB3	20:O:168:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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%)	47 78
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	436/476 (92%)	427 (98%)	9 (2%)	53	81
4	S	563/828 (68%)	555 (99%)	8 (1%)	67	89
5	R	313/474 (66%)	305 (97%)	8 (3%)	46	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%)	1293 (100%)	4 (0%)	92 98
8	B	1030/1053 (98%)	1026 (100%)	4 (0%)	91 97
9	C	269/296 (91%)	268 (100%)	1 (0%)	91 97
10	D	65/116 (56%)	65 (100%)	0	100 100
11	E	197/197 (100%)	195 (99%)	2 (1%)	76 92
12	F	90/137 (66%)	89 (99%)	1 (1%)	73 92
13	G	177/291 (61%)	177 (100%)	0	100 100
14	H	116/128 (91%)	115 (99%)	1 (1%)	78 93
15	I	109/110 (99%)	108 (99%)	1 (1%)	78 93
16	J	64/65 (98%)	63 (98%)	1 (2%)	62 86
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%)	457 (100%)	0	100 100
All	All	5541/6990 (79%)	5501 (99%)	40 (1%)	84 95

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	18	ARG
3	Q	21	ARG
3	Q	42	ASN
3	Q	79	GLN
3	Q	209	ASN
3	Q	293	ARG
3	Q	297	ARG
3	Q	480	LEU
4	S	49	THR
4	S	227	LEU
4	S	292	LEU
4	S	379	LYS
4	S	407	ARG
4	S	623	LEU
4	S	665	ASN
4	S	744	LEU

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Mol	Chain	Res	Type
5	R	11	ARG
5	R	182	LYS
5	R	206	ARG
5	R	207	ASN
5	R	283	ARG
5	R	288	ILE
5	R	317	LEU
5	R	368	TYR
7	A	239	PHE
7	A	444	GLN
7	A	467	PHE
7	A	590	ASN
8	B	95	LEU
8	B	306	LEU
8	B	651	ARG
8	B	783	MET
9	C	281	ARG
11	E	11	ARG
11	E	200	ARG
12	F	79	ARG
14	H	142	LEU
15	I	47	VAL
16	J	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	42	ASN
3	Q	149	GLN
3	Q	206	GLN
3	Q	228	ASN
3	Q	294	HIS
3	Q	482	HIS
4	S	222	GLN
4	S	267	ASN
4	S	440	HIS
4	S	461	HIS
4	S	483	HIS
4	S	487	ASN
5	R	207	ASN
5	R	263	ASN

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Mol	Chain	Res	Type
5	R	286	GLN
5	R	304	HIS
5	R	319	ASN
5	R	382	GLN
6	M	89	GLN
7	A	322	ASN
7	A	332	GLN
7	A	383	ASN
7	A	431	GLN
7	A	592	GLN
7	A	636	HIS
7	A	706	HIS
7	A	748	ASN
7	A	785	GLN
7	A	880	GLN
7	A	926	GLN
7	A	1062	HIS
7	A	1072	ASN
7	A	1436	ASN
7	A	1487	ASN
7	A	1620	GLN
7	A	1629	ASN
8	B	62	ASN
8	B	212	ASN
8	B	231	HIS
8	B	243	GLN
8	B	248	ASN
8	B	251	HIS
8	B	361	HIS
8	B	427	GLN
8	B	456	ASN
8	B	686	HIS
8	B	735	HIS
8	B	770	ASN
8	B	1008	HIS
8	B	1041	ASN
8	B	1115	GLN
9	C	248	GLN
9	C	297	HIS
11	E	32	GLN
11	E	147	HIS
13	G	65	HIS

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Mol	Chain	Res	Type
15	I	95	ASN
17	K	106	GLN
20	O	66	ASN
20	O	94	ASN
20	O	105	ASN
20	O	200	ASN
20	O	318	ASN
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 monosaccharides 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.

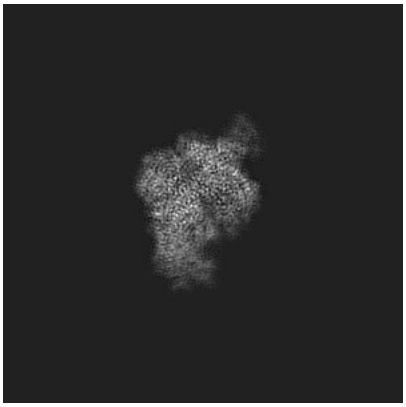
6 Map visualisation

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.

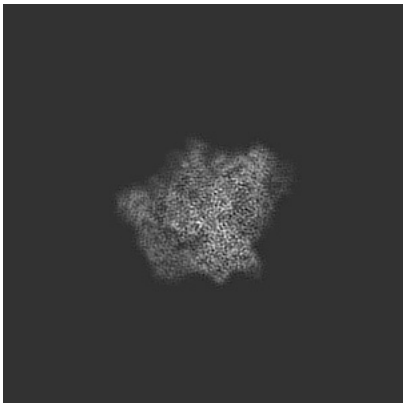
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

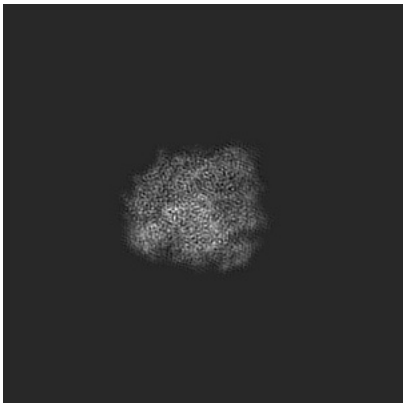
6.1.1 Primary map



X



Y

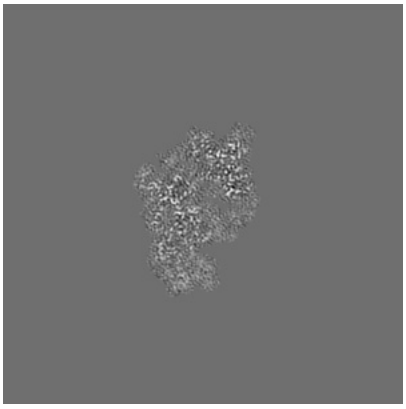


Z

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

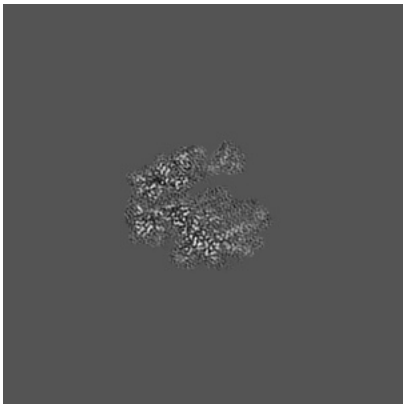
6.2 Central slices

6.2.1 Primary map



X Index: 190

Y Index: 190

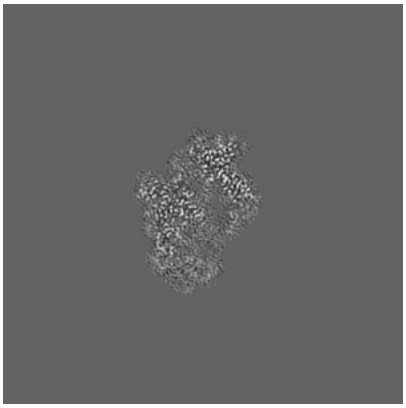


Z Index: 190

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

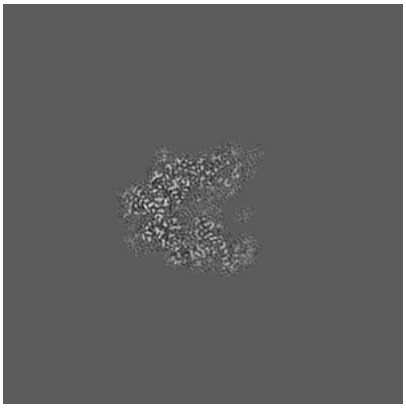
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 181

Y Index: 168

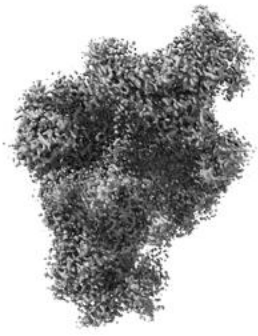


Z Index: 209

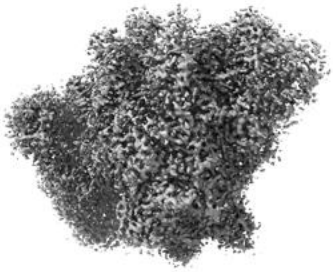
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

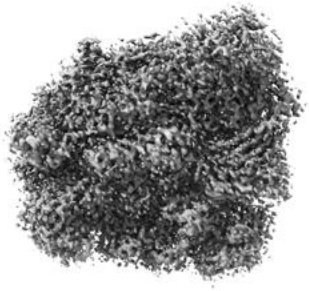
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

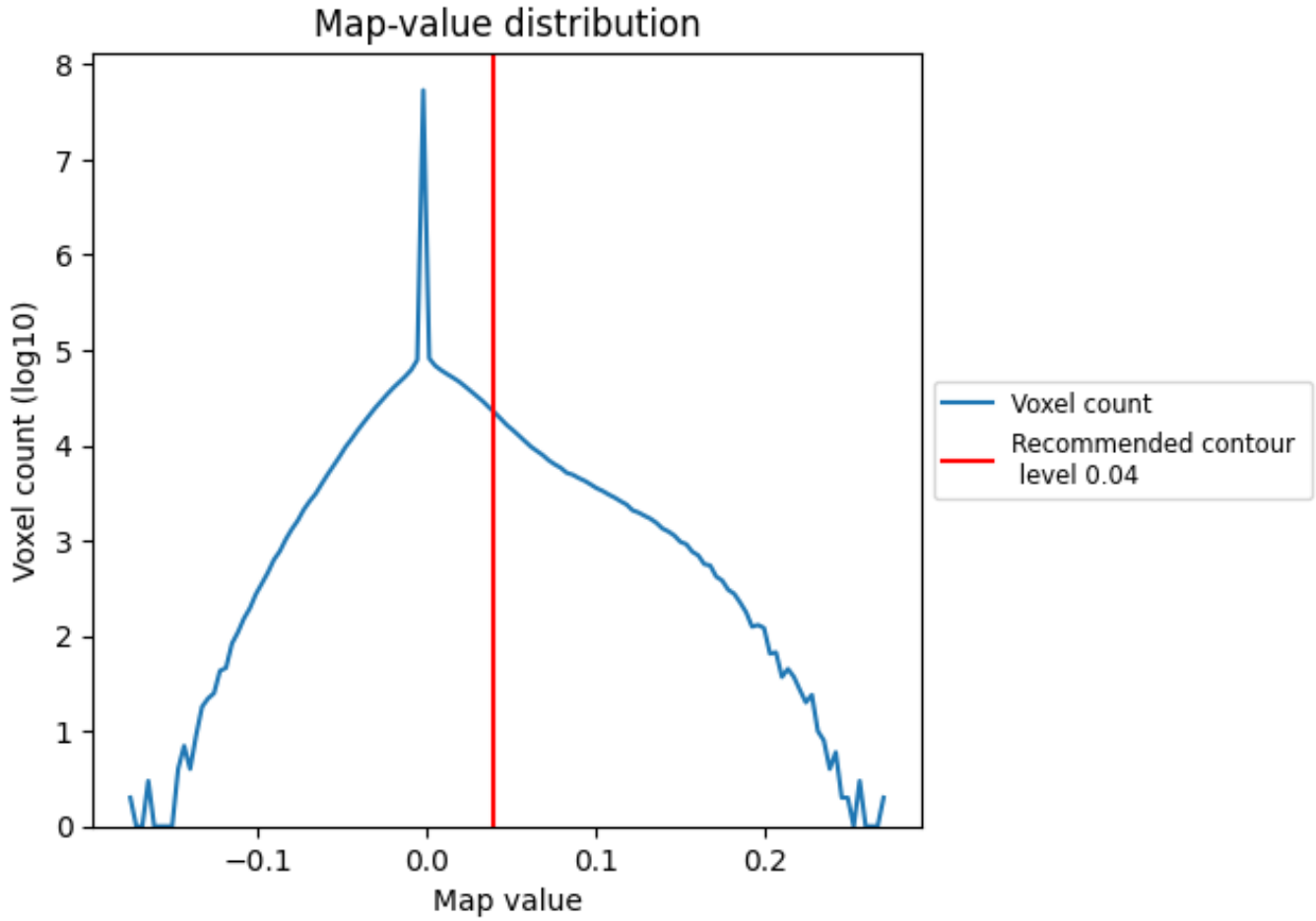
6.5 Mask visualisation (i)

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

7 Map analysis

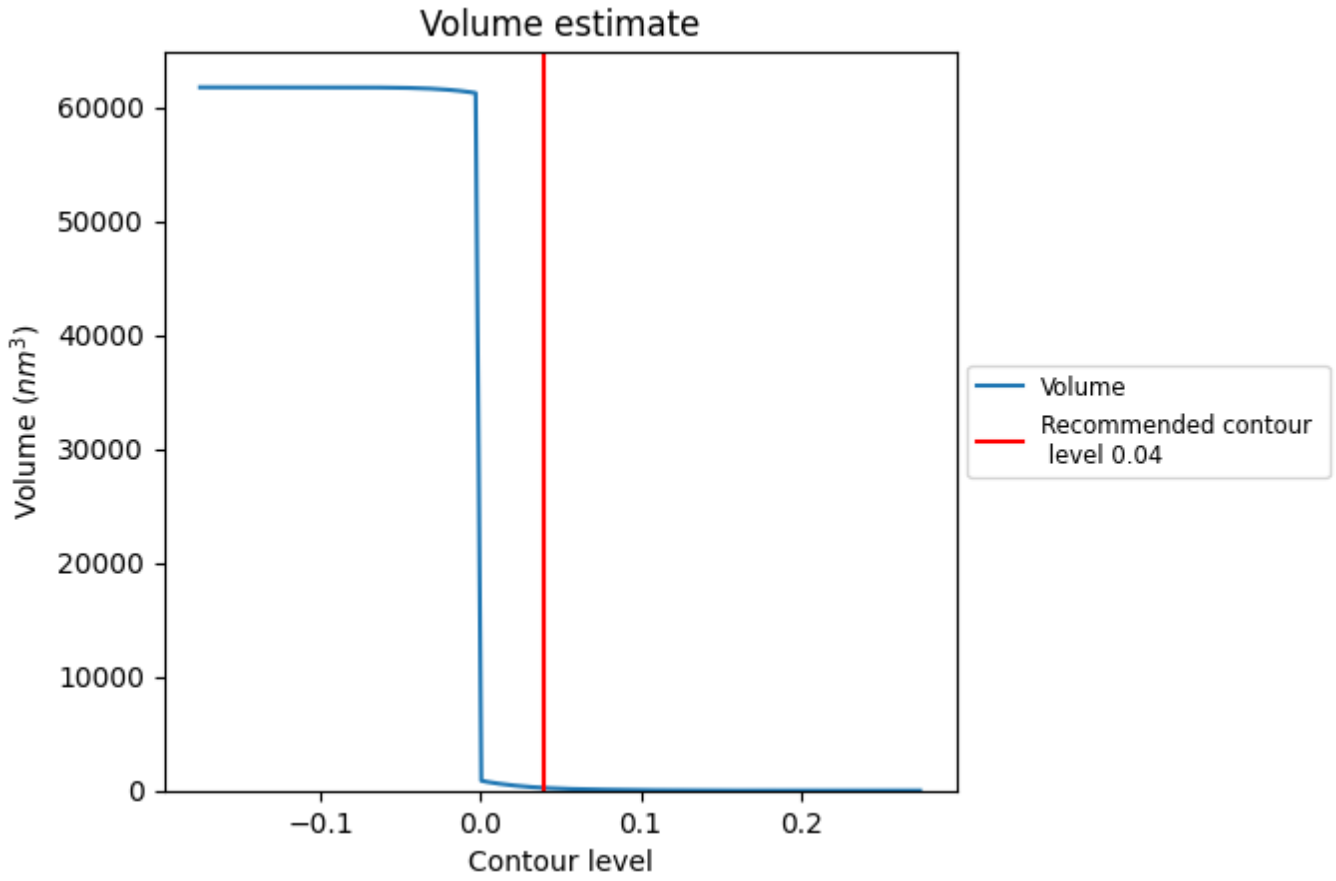
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

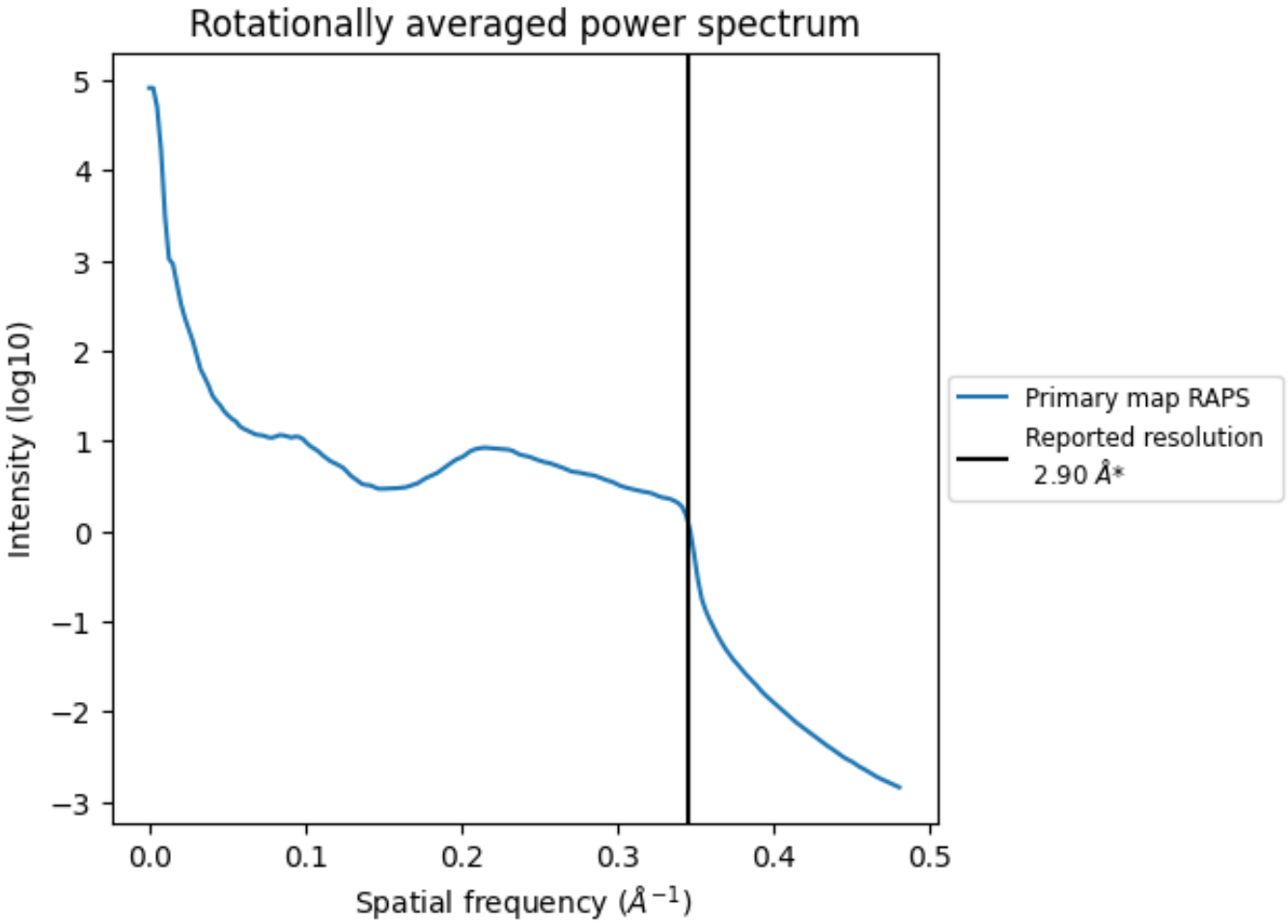
7.2 Volume estimate



The volume at the recommended contour level is 233 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

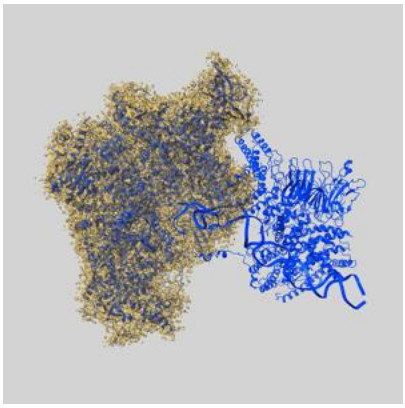
8 Fourier-Shell correlation (i)

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

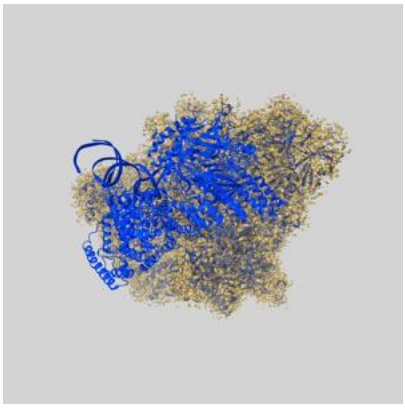
9 Map-model fit

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

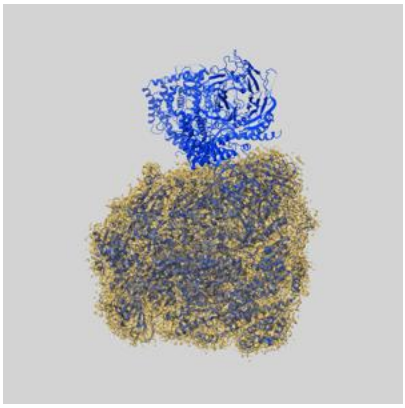
9.1 Map-model overlay



X



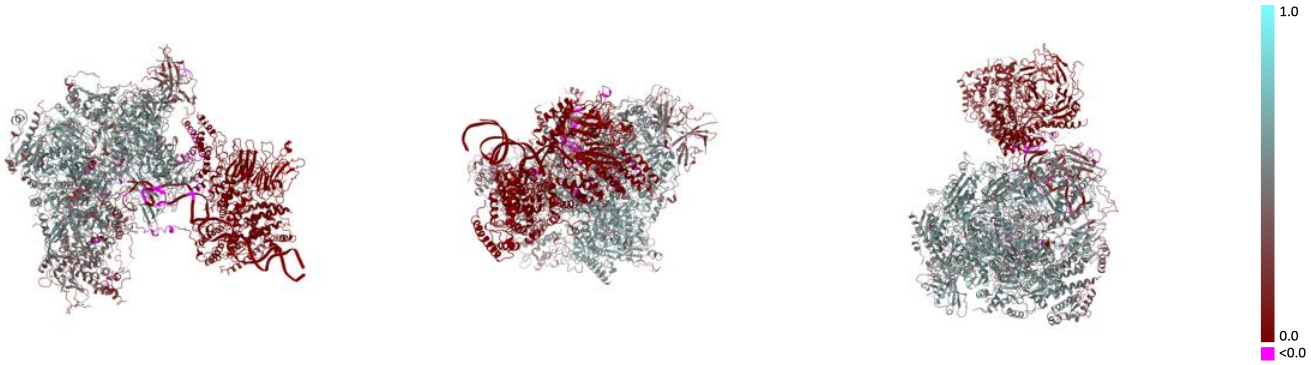
Y



Z

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

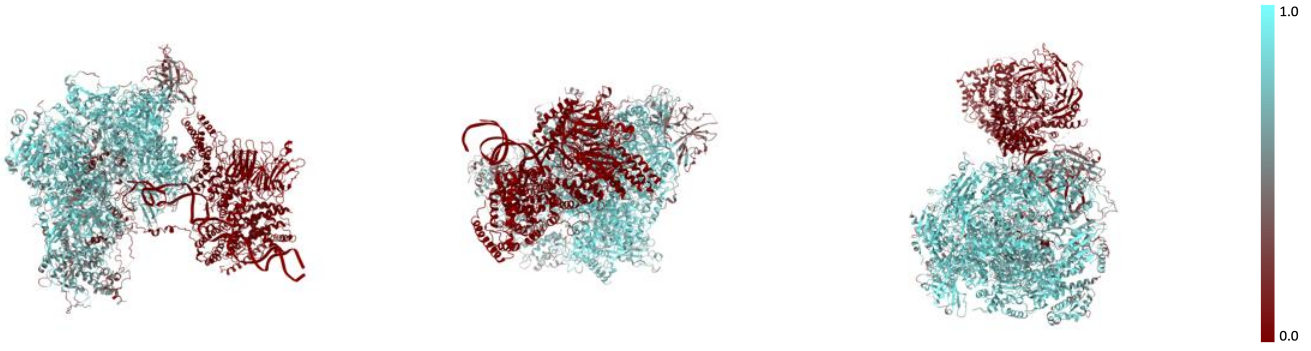
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

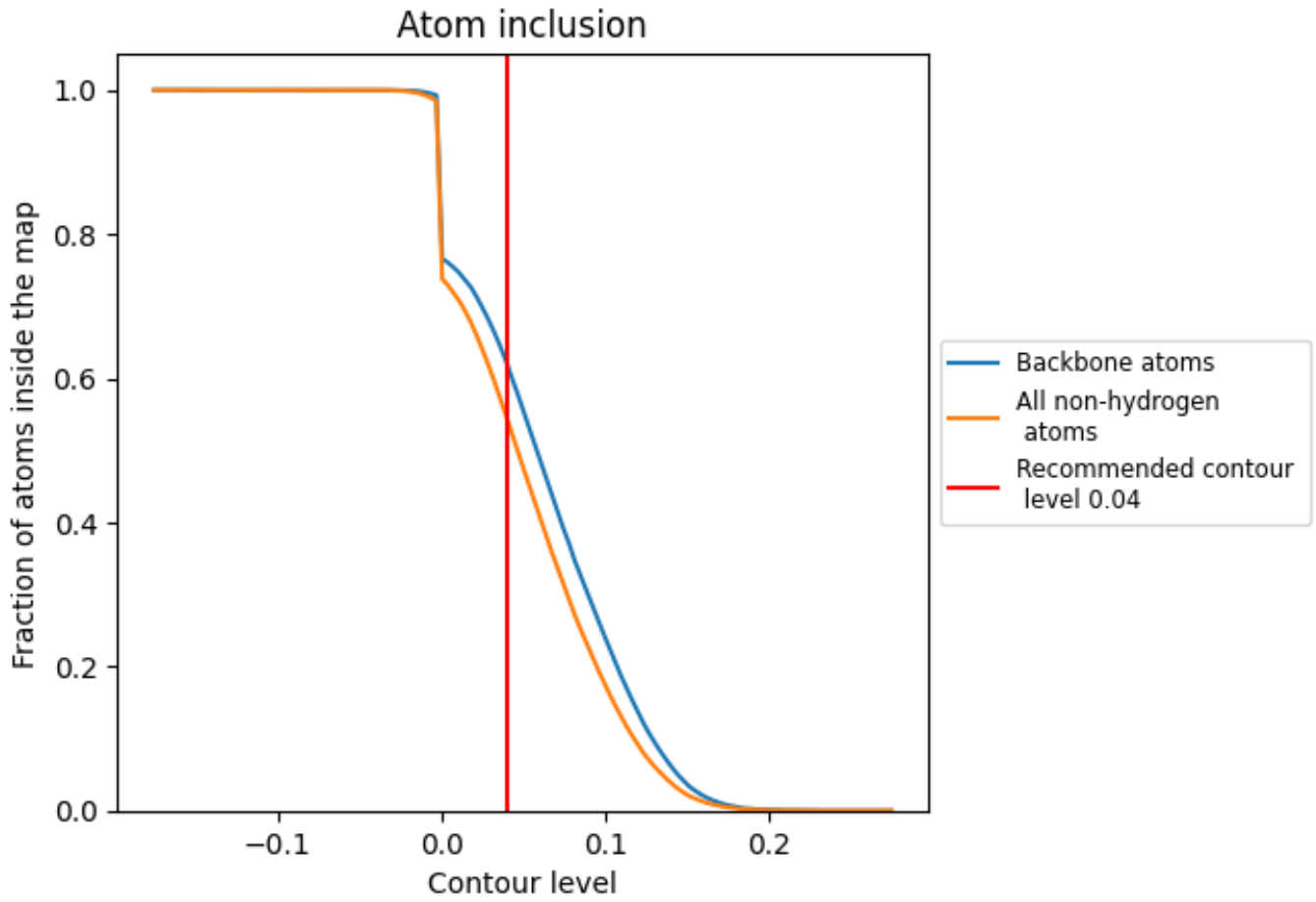
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 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	0.5443	0.3550
A	0.7696	0.5030
B	0.8188	0.5260
C	0.7957	0.5050
D	0.5893	0.3940
E	0.7564	0.4740
F	0.8190	0.5470
G	0.6686	0.4190
H	0.7720	0.4890
I	0.5494	0.3860
J	0.8947	0.5630
K	0.7953	0.5230
L	0.7775	0.4850
M	0.3957	0.3260
N	0.3498	0.3050
O	0.5298	0.3390
Q	0.0618	0.0400
R	0.0070	0.0080
S	0.0000	0.0000
T	0.0095	0.0080
U	0.0034	0.0100