Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 05:07 am GMT

PDB ID	:	6RUO
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:

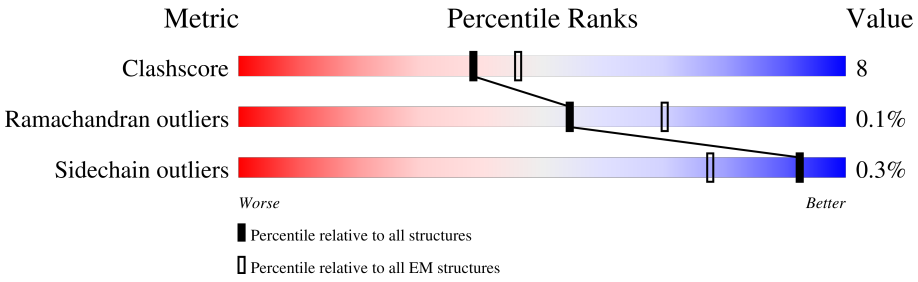
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 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)
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	Q	514	55% 67% 17% • 16%
2	M	415	19% 21% 5% 74%
3	A	1664	33% 70% 18% 12%
4	B	1203	38% 77% 21% •
5	C	335	30% 76% 15% 9%
6	D	137	27% 45% 7% 49%
7	E	215	37% 79% 21%
8	F	155	19% 57% 8% 35%

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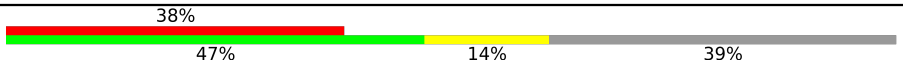
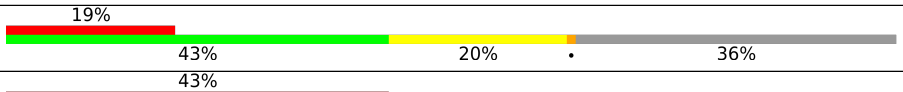
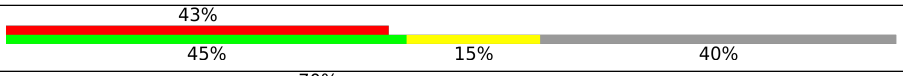
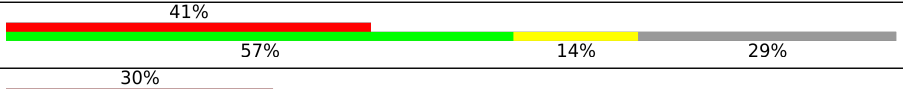
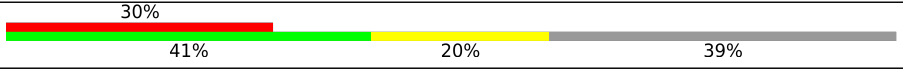
Mol	Chain	Length	Quality of chain
9	G	326	
10	H	146	
11	I	125	
12	J	70	
13	K	142	
14	L	70	
15	N	233	
16	O	627	
17	S	894	
18	R	507	
19	T	70	
20	U	70	

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
			Total	C	N	O	S		
1	Q	430	3572	2306	602	644	20	0	0

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

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

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

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

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

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

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

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

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

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

- 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 (three-letter code: ZN) (formula: Zn).

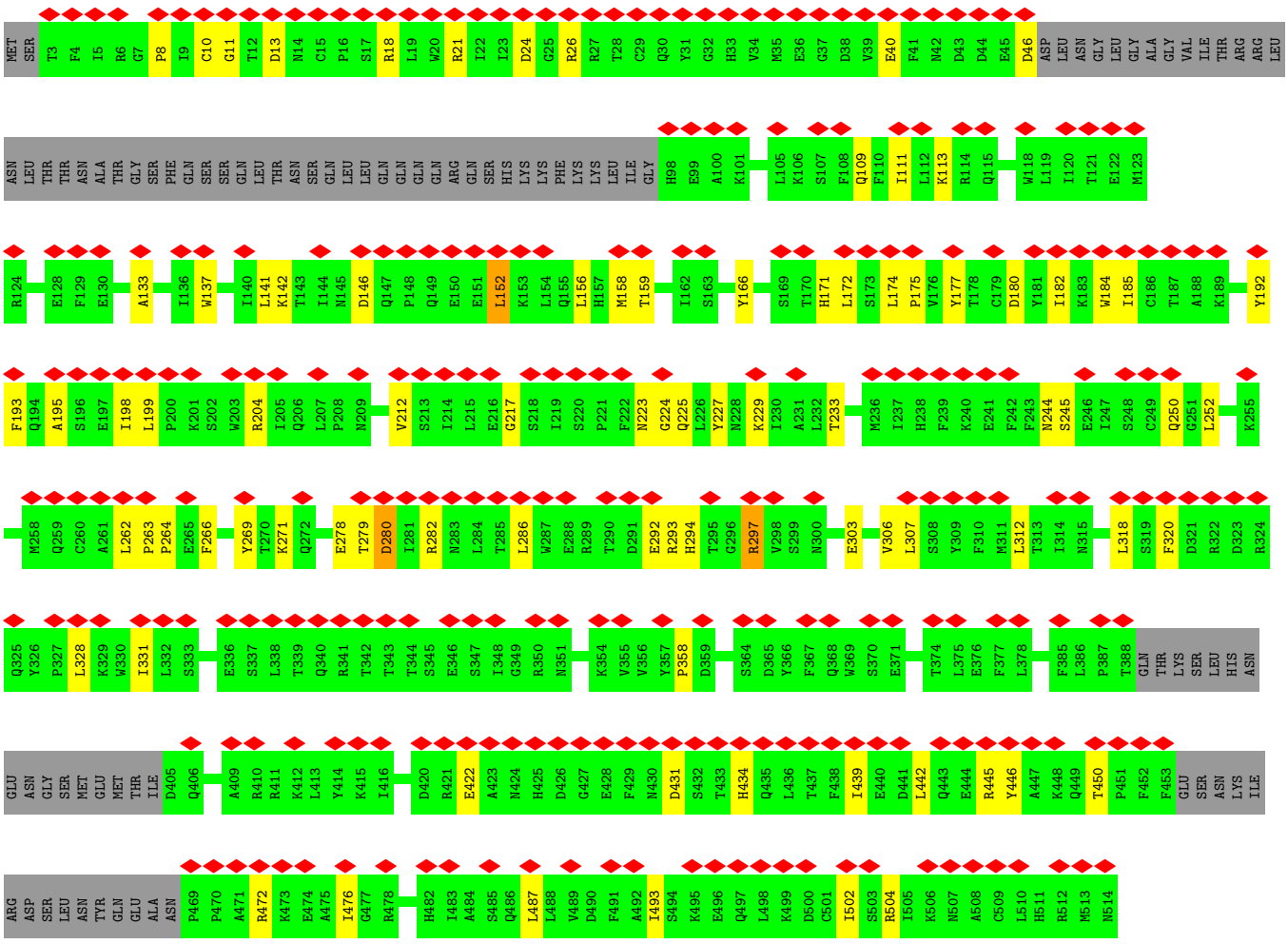
Mol	Chain	Residues	Atoms	AltConf
21	Q	1	Total Zn 1 1	0
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

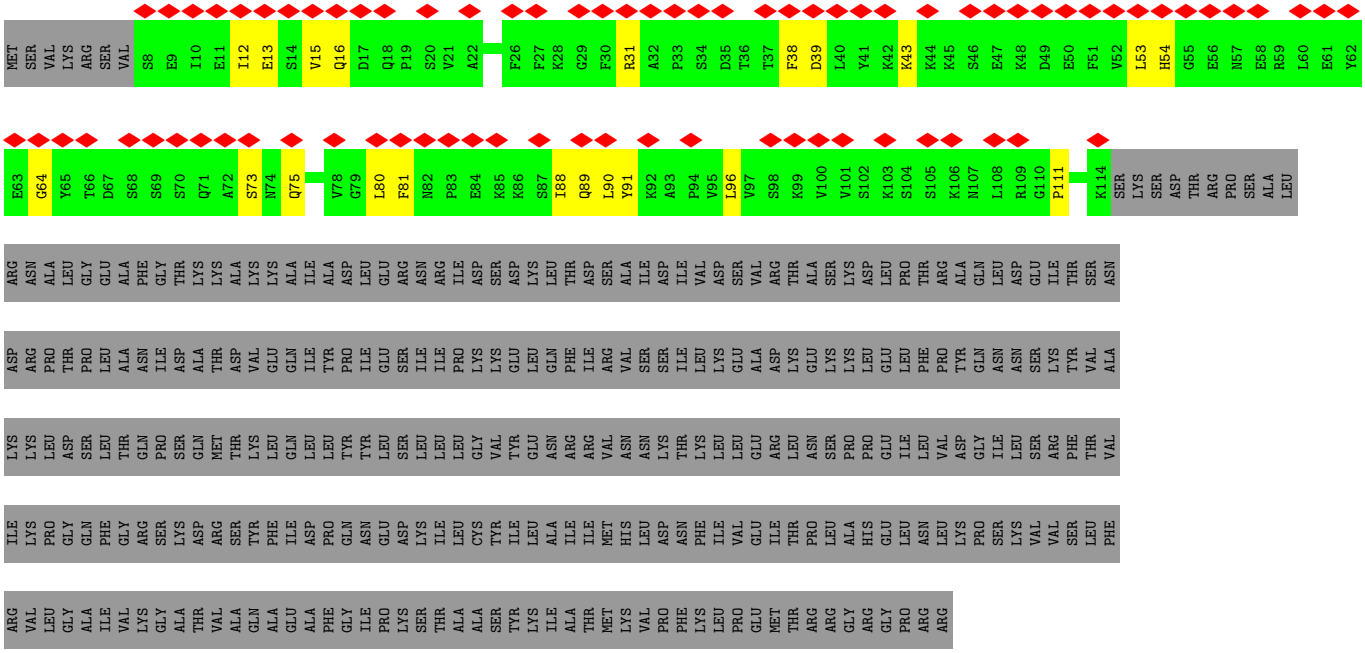
• Molecule 1: RNA polymerase I-specific transcription initiation factor RRN7

Chain Q:



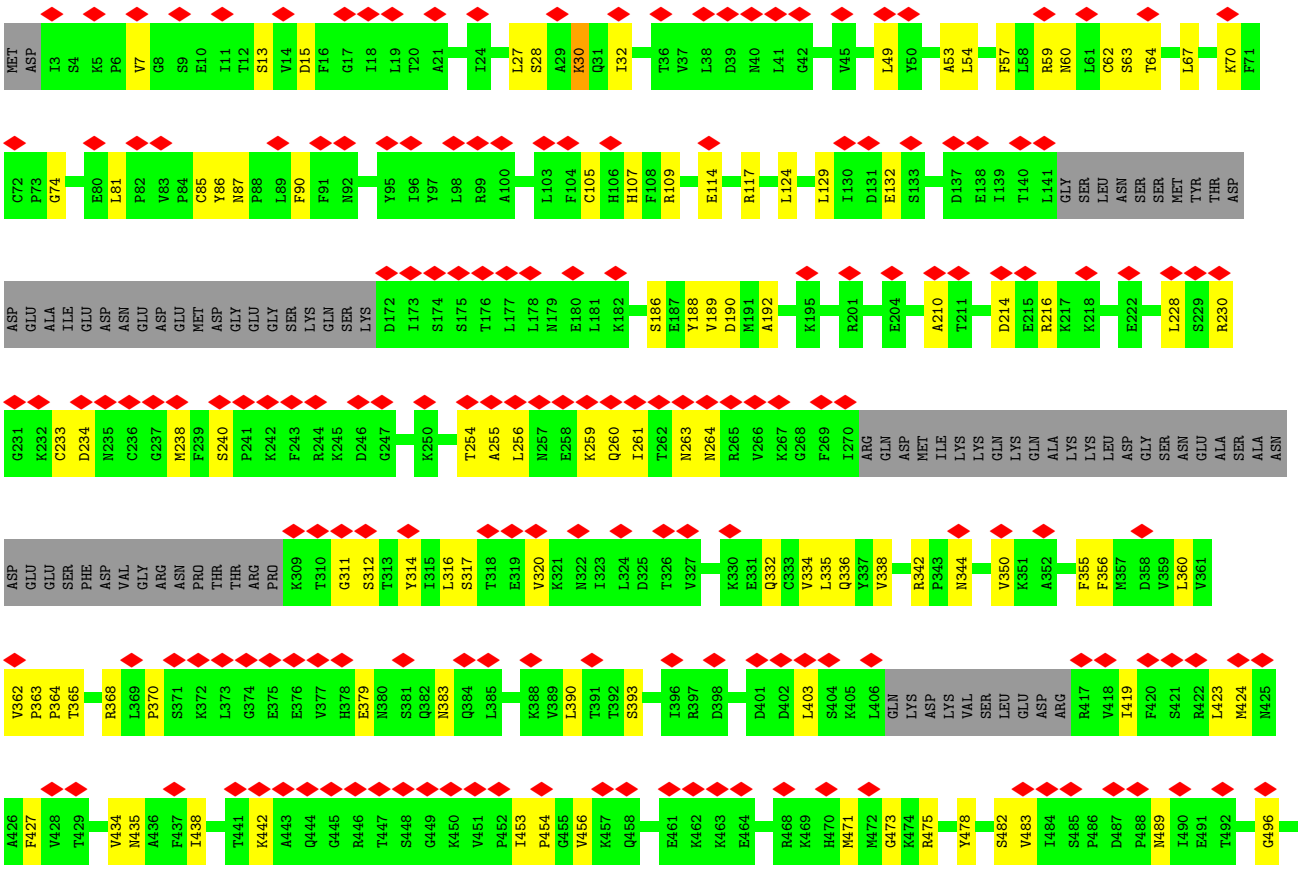
• Molecule 2: DNA-directed RNA polymerase I subunit RPA49

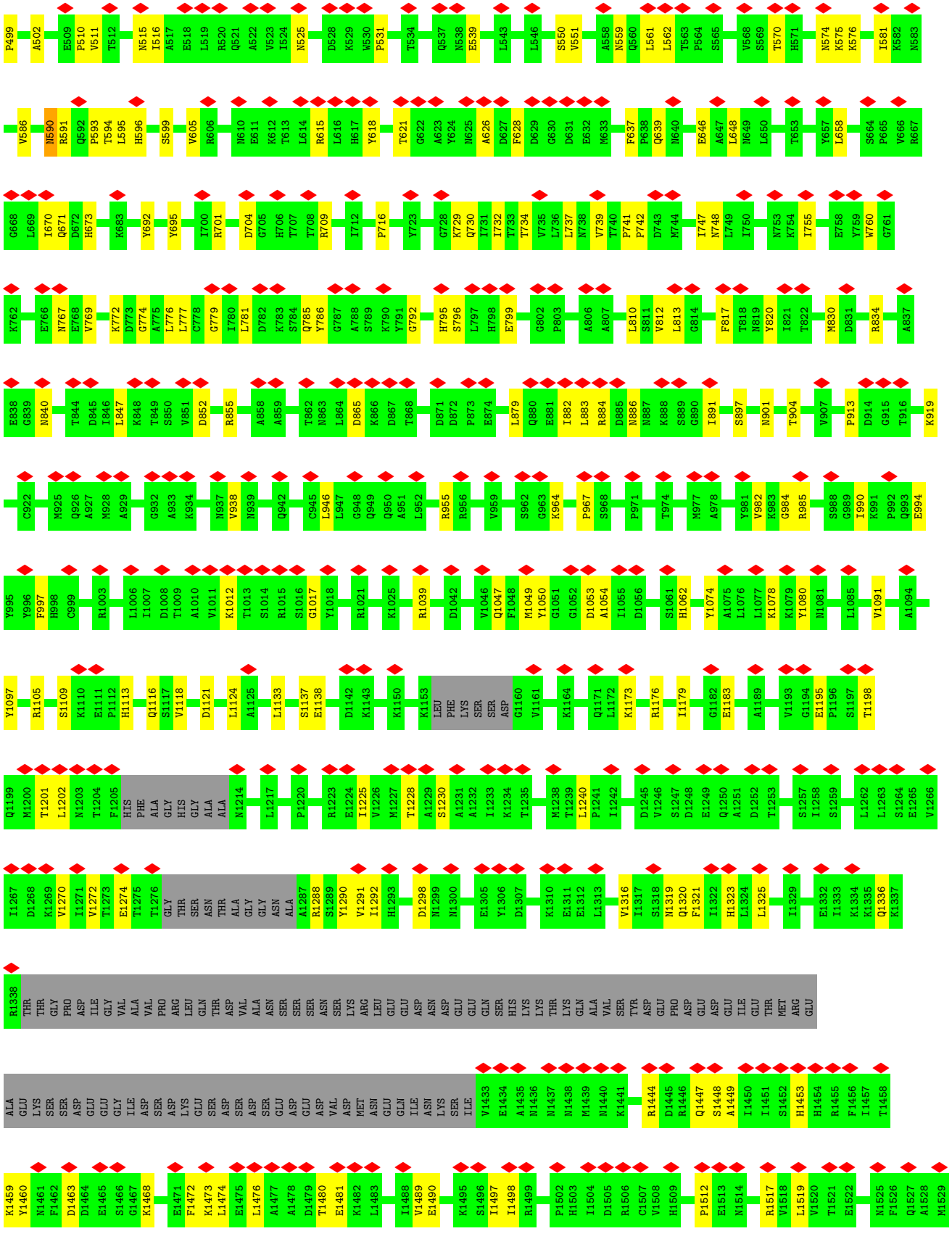
Chain M:

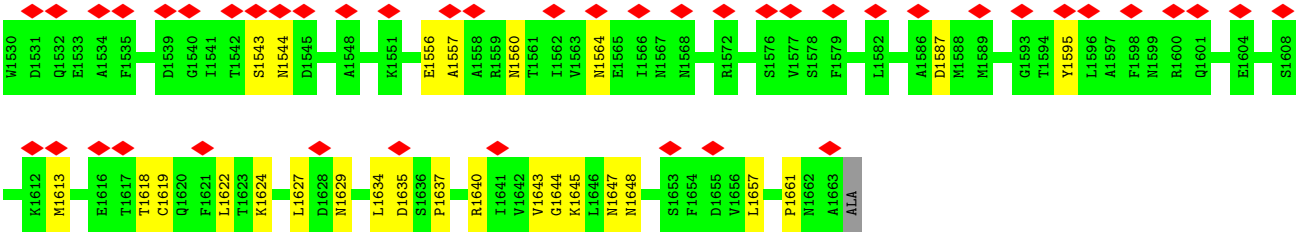


• Molecule 3: DNA-directed RNA polymerase I subunit RPA190

Chain A:

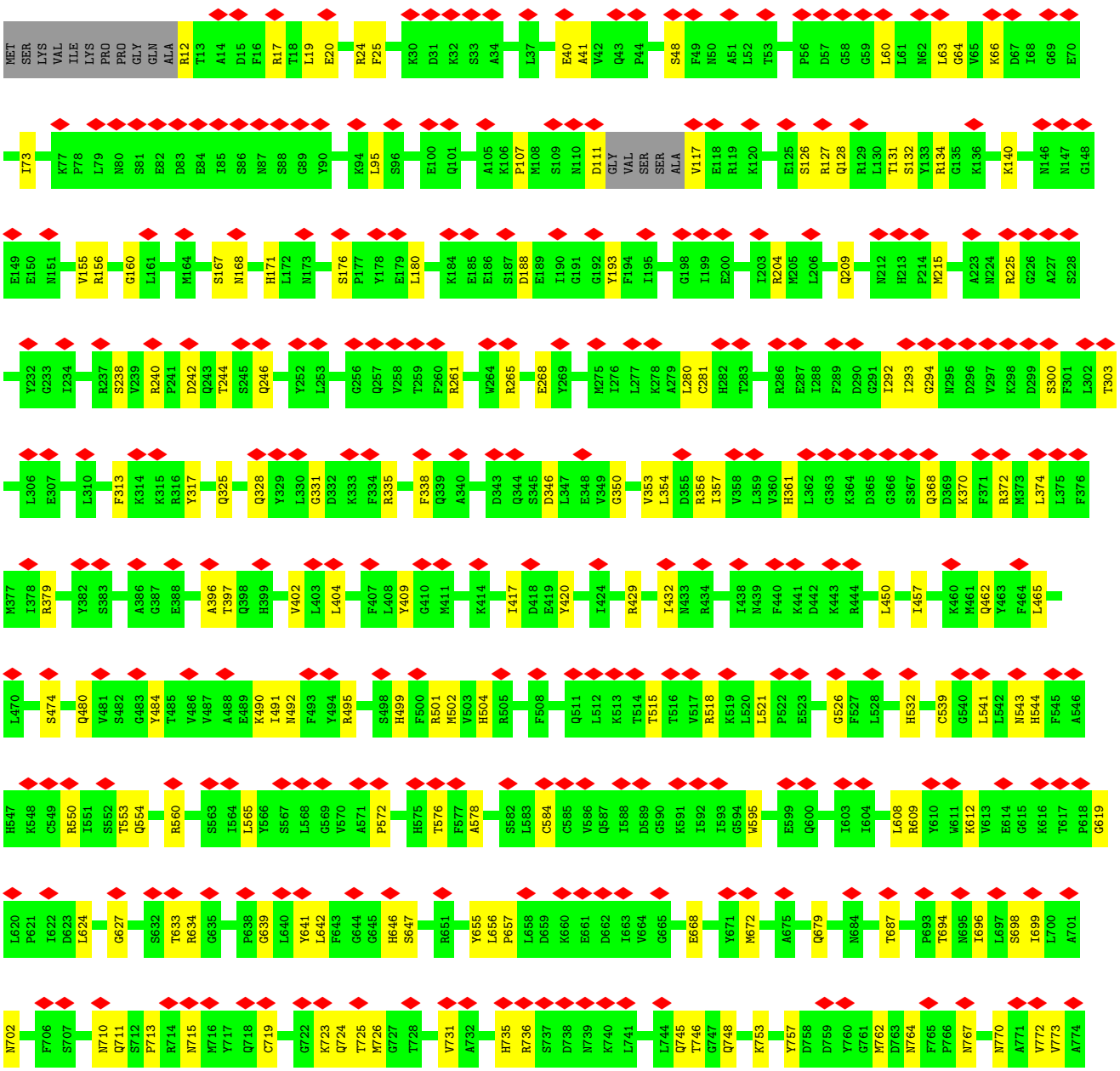


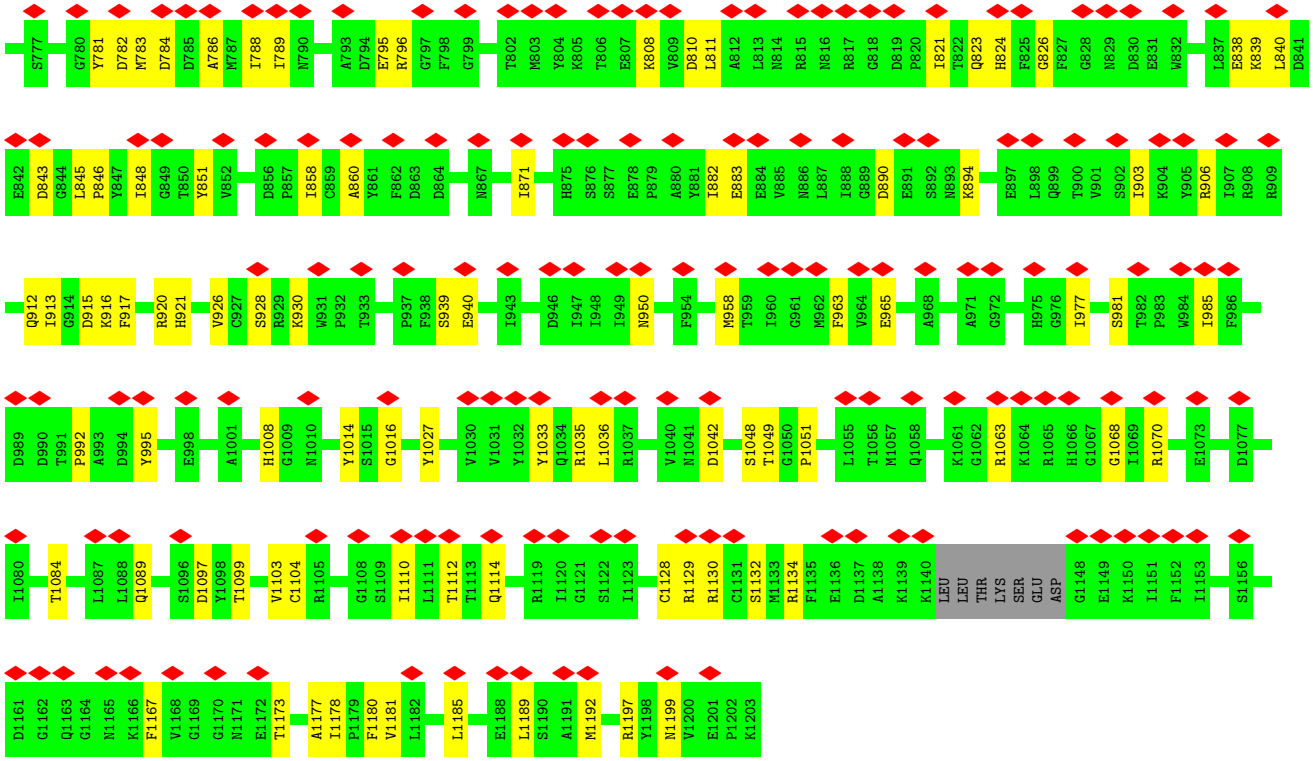

P499 A502 E509 P510 V511 T512 N515 I516 K517 E518 L519 R520 Q521 A522 V523 I524 N525 D528 K529 W530 P531 T534 Q537 N538 E539 L543 L546 S550 V551 A558 N559 Q560 L561 L562 T563 P564 S565 V568 S569 T570 H571 N574 K575 K576 I581 K582 N583
V586 N590 R591 Q592 P593 T594 L595 H596 S599 V605 R606 W610 E611 K612 T613 L614 R615 L616 H617 Y618 T621 G622 A623 Y624 N625 A626 D627 F628 D629 G630 D631 E632 M633 F637 P638 Q639 N640 E646 A647 L648 N649 L650 T653 Y657 L658 S664 P665 V666 R667
G668 L669 I670 Q671 D672 H673 K683 Y692 Y695 I700 R701 D704 G705 H706 T707 T708 R709 I712 P716 Y723 G728 K729 Q730 I731 I732 T733 T734 V735 L736 L737 N738 V739 T740 P741 P742 D743 M744 I747 N748 L749 I750 N753 K754 I755 E758 Y759 W760 G761
K762 E766 N767 E768 V769 K772 D773 G774 A775 L776 L777 C778 G779 I780 L781 D782 K783 S784 Q785 Y786 G787 A788 S789 K790 Y791 G792 H795 S796 L797 H798 E799 G802 P803 A806 A807 L810 S811 V812 L813 G814 F817 T818 N819 Y820 I821 T822 M830 D831 R834 A837
E838 G839 N840 T844 D845 I846 L847 K848 T849 S850 V851 D852 R855 A858 A859 T862 N863 L864 D865 K866 D867 T868 D871 D872 P873 E874 L879 Q880 E881 I882 L883 R884 D885 N886 N887 K888 S889 G890 I891 S897 N901 T904 V907 P913 D914 G915 T916 K919
C922 N925 Q926 A927 N928 A929 G932 A933 K934 N937 V938 N939 Q942 C945 L946 L947 G948 Q949 Q950 A951 L952 R955 R956 V959 S962 G963 K964 P967 S968 P971 T974 M977 A978 Y981 V982 K983 G984 R985 S988 G989 I990 K991 P992 Q993 E994
Y995 Y996 F997 H998 C999 R1003 L1006 I1007 D1008 T1009 A1010 V1011 K1012 T1013 S1014 R1015 S1016 G1017 Y1018 R1021 K1025 R1039 D1042 V1046 Q1047 F1048 M1049 Y1050 G1051 G1052 D1053 A1054 I1055 D1056 S1061 H1062 Y1074 A1075 L1076 L1077 K1078 K1079 Y1080 N1081 L1085 V1091 A1094
Y1097 R1105 S1109 K1110 E1111 P1112 H1113 Q1116 S1117 V1118 D1121 L1124 A1125 L1133 S1137 E1138 D1142 K1143 K1150 K1153 LEU PHE LYS SER SER ASP G1160 V1161 K1164 Q1171 L1172 K1173 R1176 I1179 G1182 E1183 A1189 V1193 G1194 E1195 P1196 S1197 T1198
Q1199 M1200 T1201 L1202 N1203 T1204 F1205 HIS PHE ALA GLY HIS GLY ALA ALA N1214 L1217 P1220 R1223 E1224 I1225 V1226 M1227 T1228 A1229 S1230 A1231 A1232 I1233 K1234 T1235 M1238 T1239 L1240 P1241 I1242 D1245 V1246 S1247 D1248 E1249 Q1250 A1251 D1252 T1253 S1257 I1258 S1259 L1262 L1263 S1264 E1265 V1266
I1267 D1268 K1269 V1270 I1271 V1272 T1273 E1274 T1275 T1276 GLY THR SER ASN THR ALA GLY GLY ASN ALA A1287 R1288 S1289 Y1290 V1291 I1292 H1293 D1298 N1299 N1300 E1305 Y1306 D1307 K1310 E1311 E1312 L1313 V1316 I1317 S1318 N1319 Q1320 F1321 I1322 H1323 L1324 L1325 I1329 E1332 I1333 K1334 K1335 Q1336 K1337
R1338 THR THR GLY PRO ASP ILE GLY VAL ALA VAL PRO ARG LEU GLN THR ASP VAL ALA ASN SER SER SER ASN SER LYS ARG LEU GLU GLU ASP ASN ASP GLU GLU GLN SER HIS LYS LYS THR LYS GLN ALA VAL SER TYR ASP GLU PRO ASP GLU ASP GLU ILE GLU THR MET ARG GLU
ALA GLU LYS SER SER ASP GLU GLU GLY ILE ASP SER ASP LYS GLU SER ASP SER ASP SER GLU ASP GLU ASP VAL ASP MET ASN GLU GLU GLN ILE ASN LYS SER ILE V1433 E1434 A1435 N1436 N1437 N1438 M1439 N1440 K1441 R1444 D1445 R1446 Q1447 S1448 A1449 I1450 I1451 S1452 H1453 H1454 R1455 F1456 I1457 T1458
K1459 Y1460 N1461 F1462 D1463 D1464 E1465 S1466 G1467 K1468 E1471 F1472 K1473 L1474 E1475 L1476 A1477 A1478 D1479 T1480 E1481 K1482 L1483 I1488 V1489 E1490 K1495 S1496 I1497 I1498 R1499 P1502 H1503 I1504 D1505 R1506 C1507 V1508 H1509 P1512 E1513 N1514 R1517 V1518 L1519 V1520 T1521 E1522 N1525 F1526 Q1527 A1528 M1529



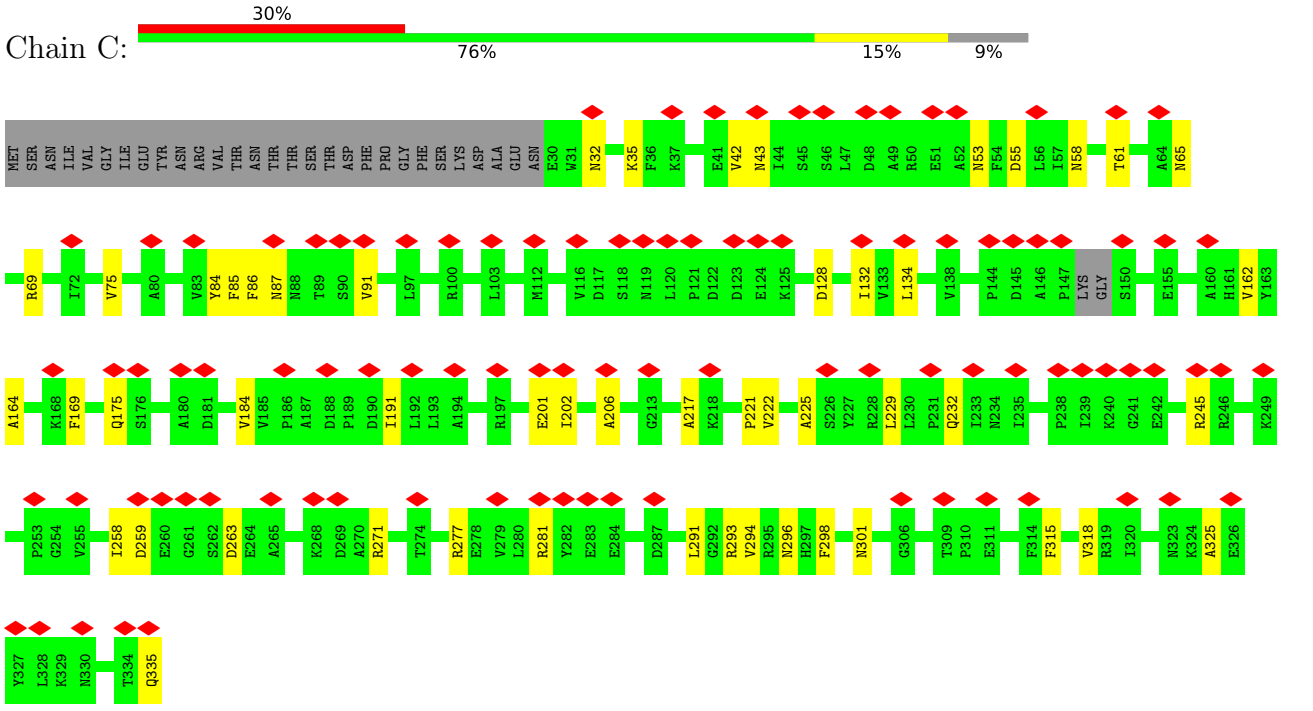
• Molecule 4: DNA-directed RNA polymerase I subunit RPA135

Chain B:

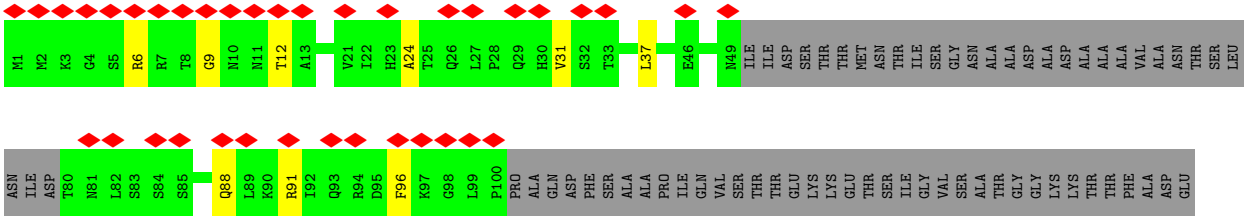




• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC1

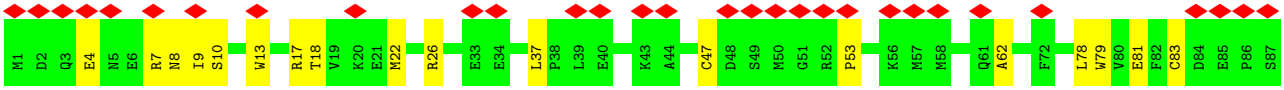


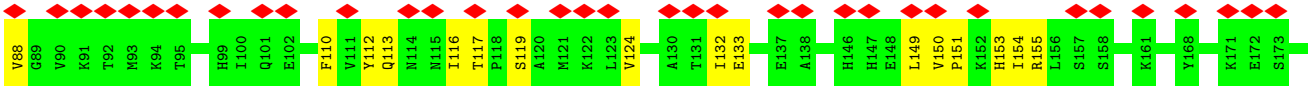
• Molecule 6: DNA-directed RNA polymerase I subunit RPA14

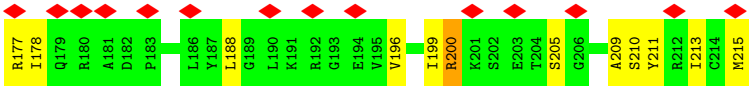


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

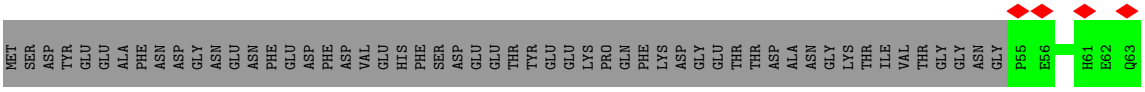


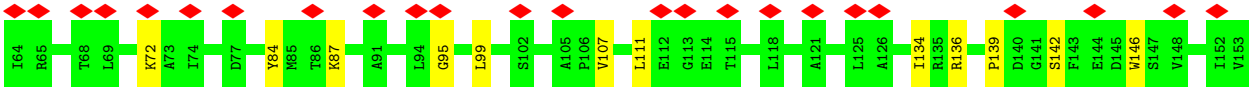




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

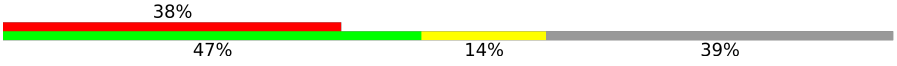
Chain F:

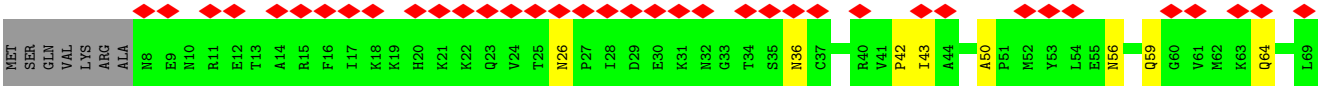


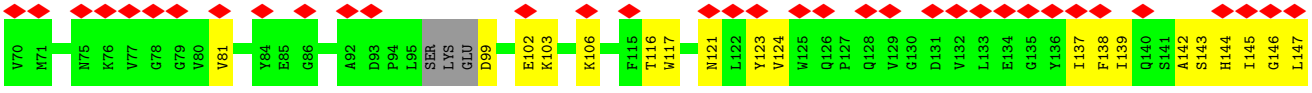


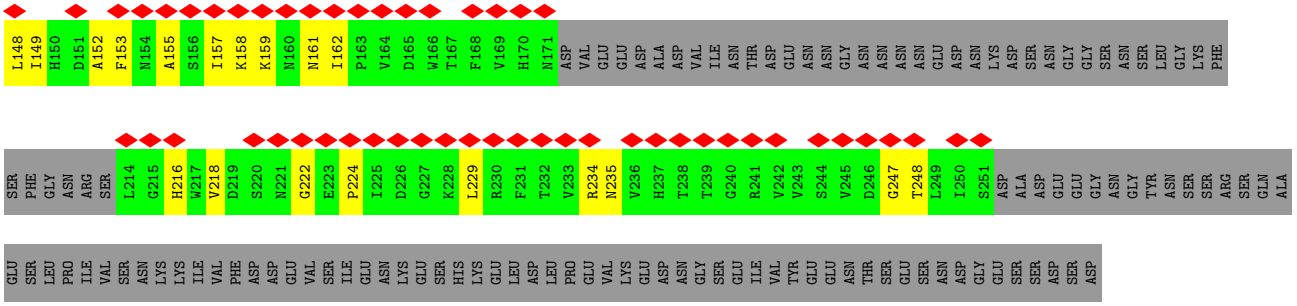
• Molecule 9: DNA-directed RNA polymerase I subunit RPA43

Chain G:



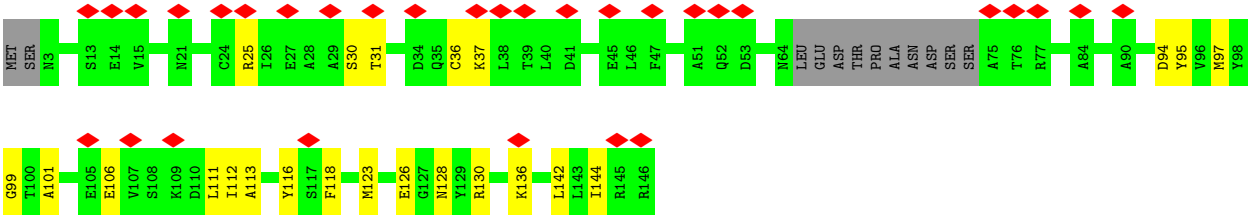






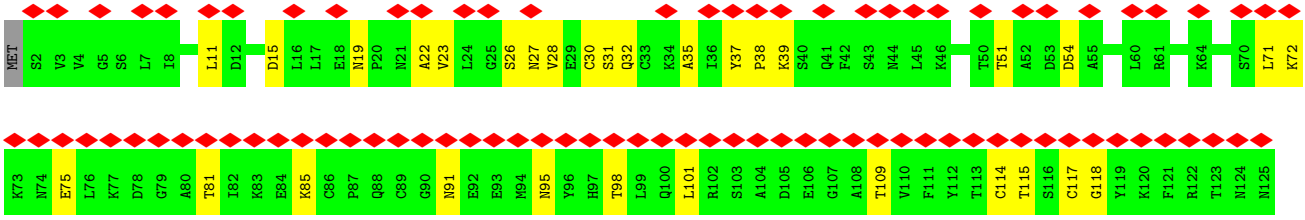
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



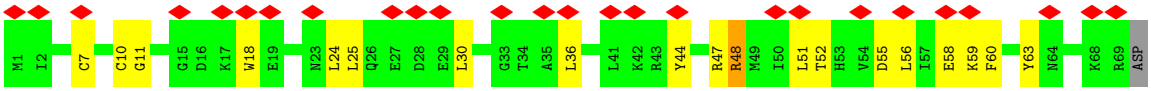
• Molecule 11: DNA-directed RNA polymerase I subunit RPA12

Chain I:



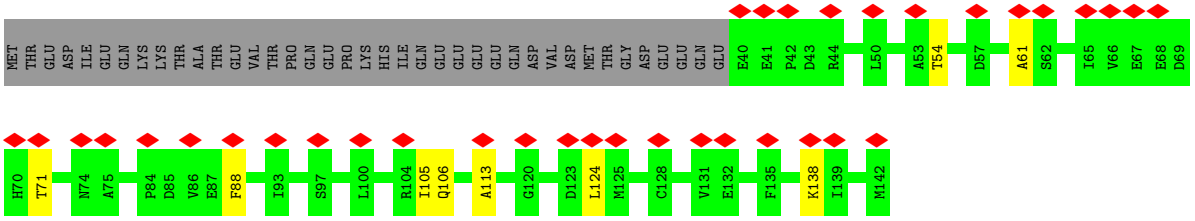
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



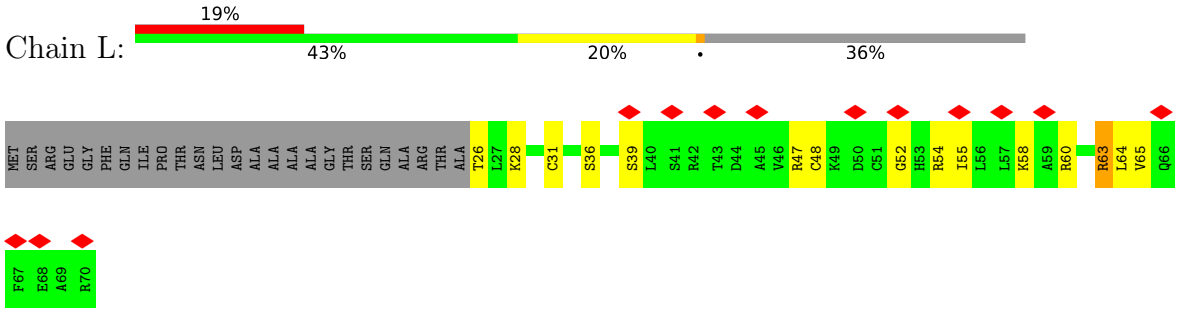
• Molecule 13: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



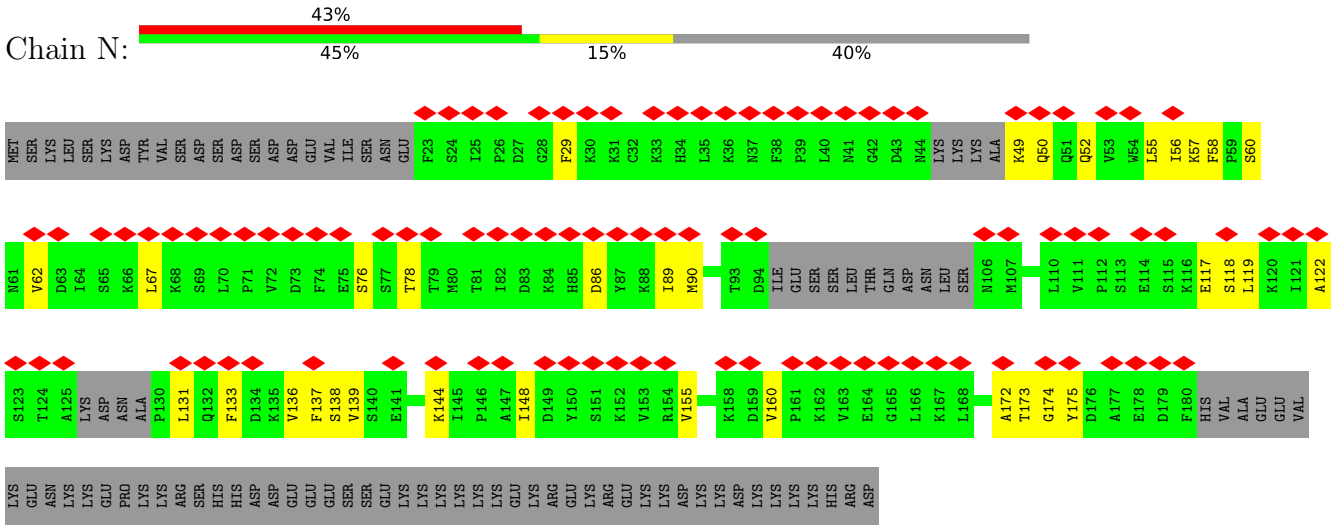
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



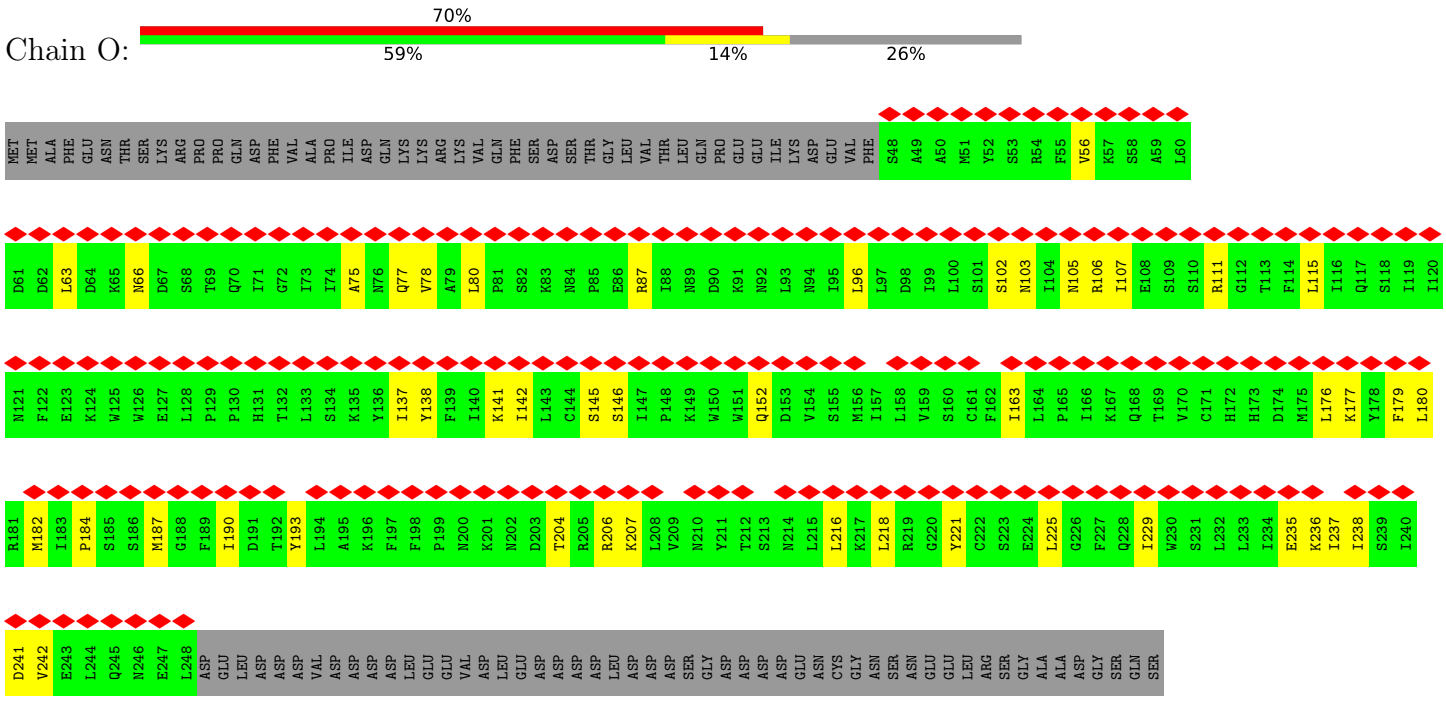
• Molecule 15: DNA-directed RNA polymerase I subunit RPA34

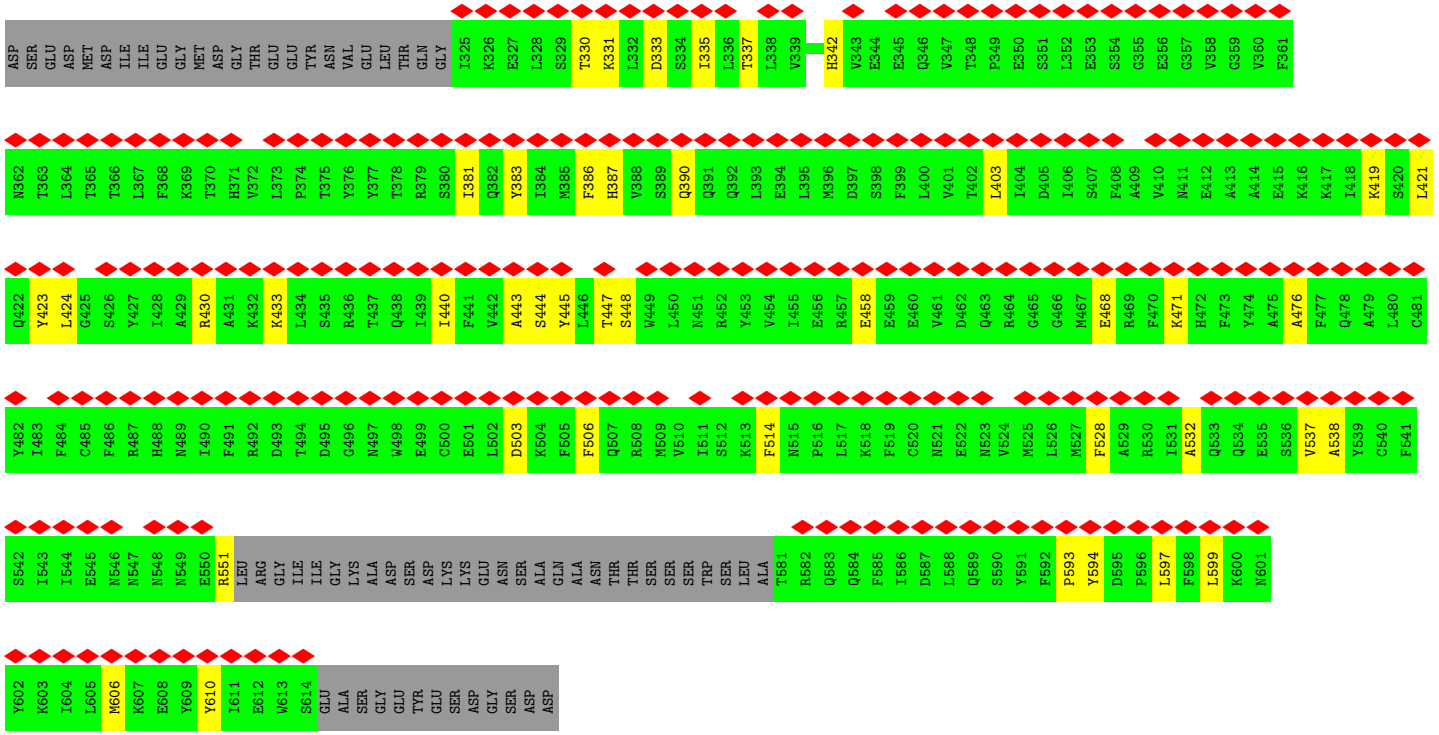
Chain N:



• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN3

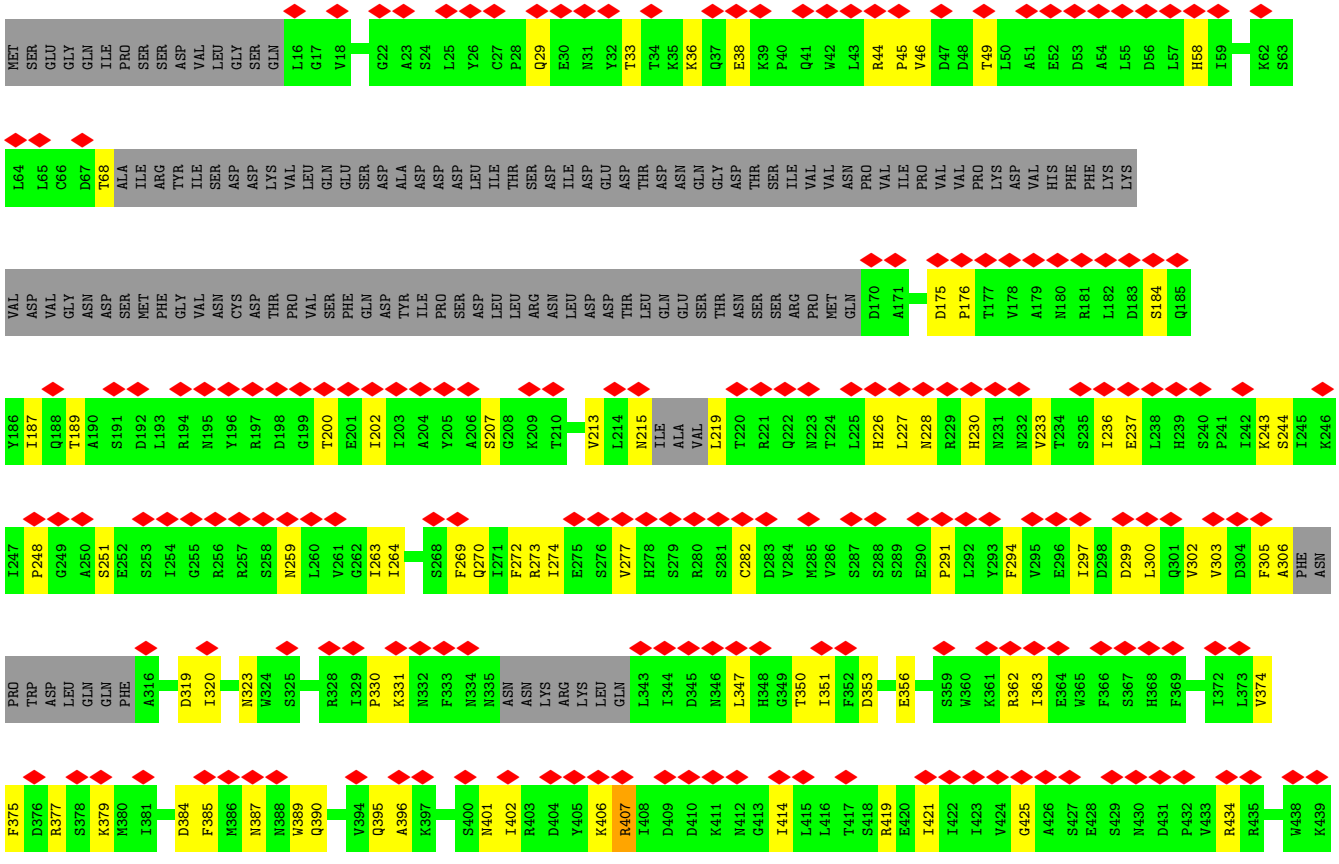
Chain O:

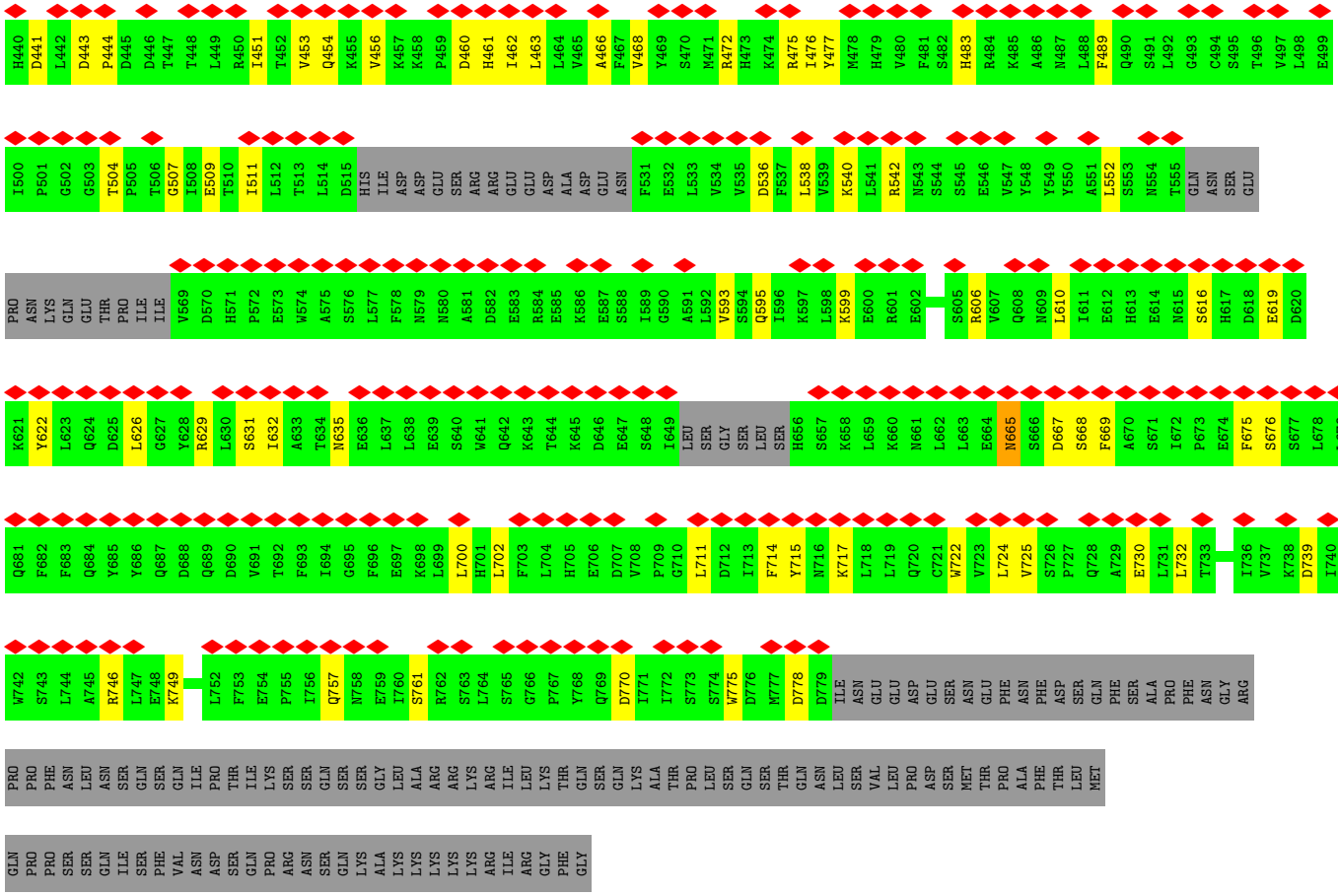




• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN6

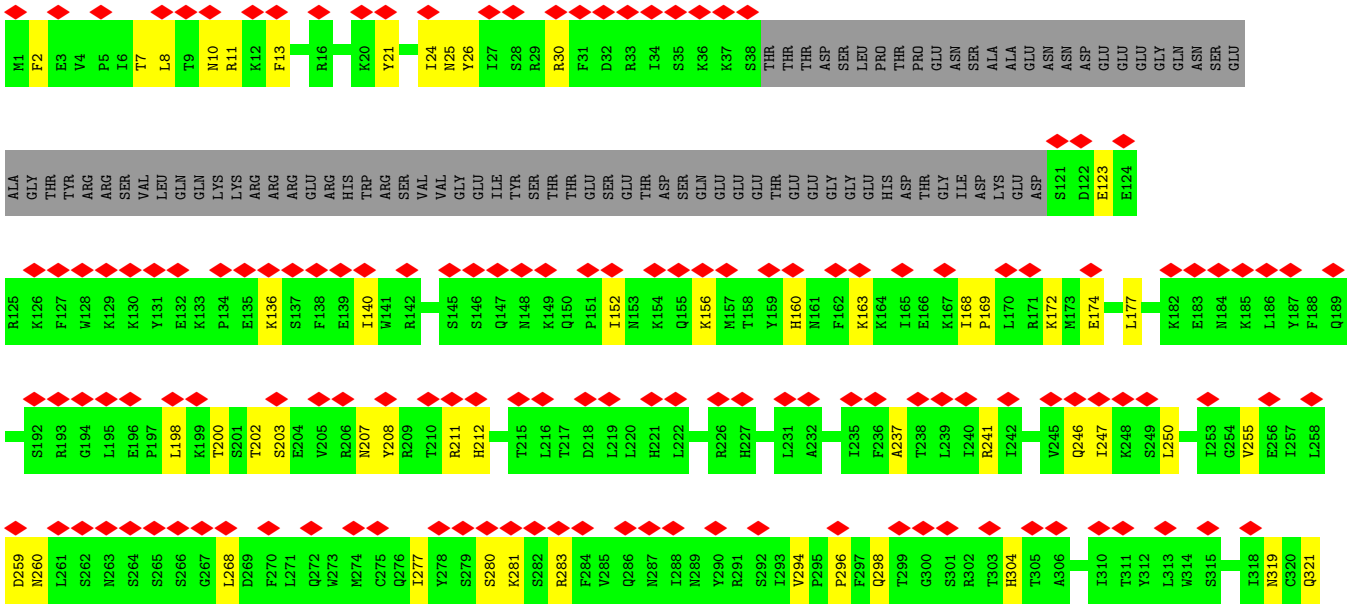
Chain S:

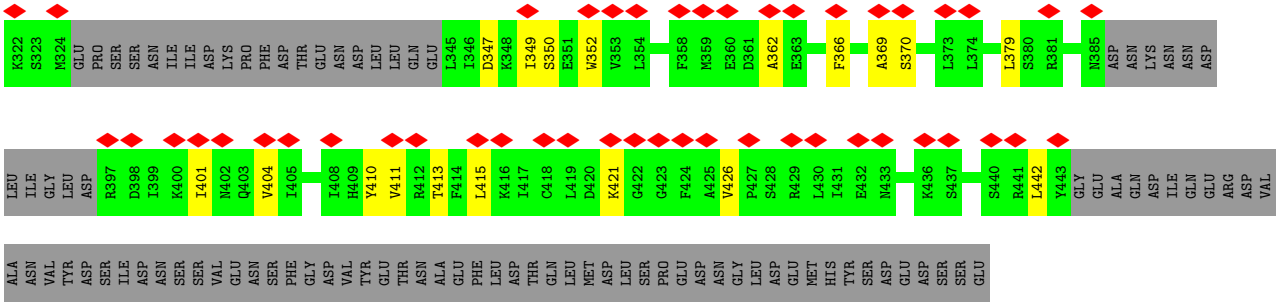




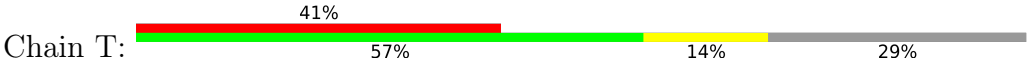
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11

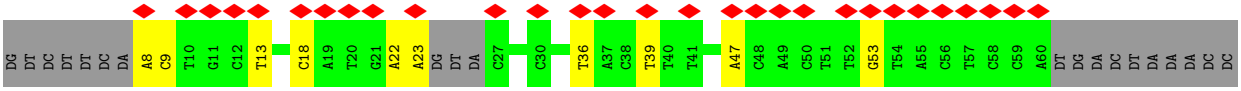
Chain R:



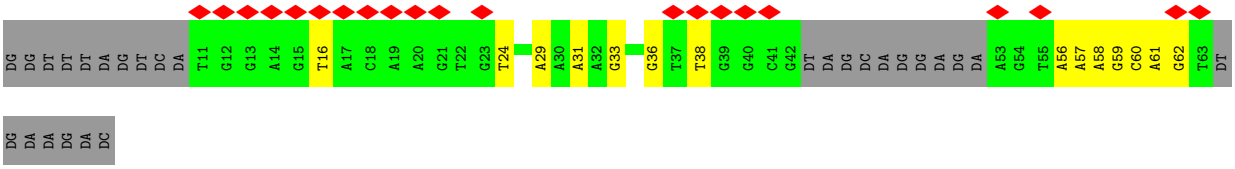


• Molecule 19: Template strand





• Molecule 20: Nontemplate strand



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Q	0.33	0/3661	0.60	0/4950
2	M	0.37	0/866	0.59	0/1162
3	A	0.41	0/11778	0.60	0/15908
4	B	0.44	0/9578	0.62	0/12948
5	C	0.43	0/2469	0.61	0/3347
6	D	0.32	0/557	0.58	0/750
7	E	0.39	0/1795	0.55	0/2416
8	F	0.39	0/838	0.58	0/1129
9	G	0.34	0/1613	0.57	0/2193
10	H	0.45	0/1090	0.67	0/1476
11	I	0.34	0/955	0.62	0/1288
12	J	0.50	0/578	0.63	0/775
13	K	0.42	0/821	0.64	0/1108
14	L	0.42	0/361	0.73	0/478
15	N	0.32	0/1124	0.58	0/1512
16	O	0.29	0/3893	0.54	0/5263
17	S	0.33	0/5065	0.63	0/6859
18	R	0.35	0/2836	0.59	0/3817
19	T	0.70	0/1113	1.04	0/1707
20	U	0.62	0/1016	0.91	0/1569
All	All	0.40	0/52007	0.62	0/70655

There are no bond length outliers.

There are no bond angle outliers.

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	Q	3572	0	3541	66	0
2	M	850	0	850	17	0
3	A	11567	0	11655	201	0
4	B	9371	0	9242	185	0
5	C	2418	0	2401	40	0
6	D	551	0	558	12	0
7	E	1759	0	1788	27	0
8	F	823	0	841	6	0
9	G	1576	0	1581	34	0
10	H	1072	0	1042	14	0
11	I	942	0	932	20	0
12	J	569	0	586	17	0
13	K	810	0	801	6	0
14	L	359	0	381	16	0
15	N	1103	0	1106	27	0
16	O	3807	0	3801	62	0
17	S	4963	0	4890	93	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
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	778	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 (778) 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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:646:GLU:OE1	4:B:1084:THR:OG1	2.22	0.57
3:A:1074:TYR:O	3:A:1078:LYS:NZ	2.37	0.57
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
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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
4:B:490:LYS:HZ3	4:B:736:ARG:HH12	1.57	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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:A:1080:TYR:OH	3:A:1173:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:S:36:LYS:NZ	18:R:321:GLN:OE1	2.34	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:845:LEU:HB2	14:L:58:LYS:HZ2	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:1097:ASP:N	4:B:1097:ASP:OD1	2.47	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
1:Q:446:TYR:HH	17:S:722:TRP:HE1	1.63	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
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
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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
15:N:76:SER:OG	15:N:90:MET:SD	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:334:VAL:HG13	3:A:335:LEU:HG	2.00	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:GLN:HA	3:A:263:ASN:HD22	1.84	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:37:LYS:NZ	10:H:126:GLU:OE1	2.44	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
10:H:95:TYR:OH	10:H:97:MET:SD	2.67	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
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:609:ARG:HH22	4:B:668:GLU:CD	2.23	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
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
4:B:1014:TYR:HH	5:C:293:ARG:HH12	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1099:THR:HG21	4:B:1180:PHE:HB2	2.00	0.42
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
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:471:MET:HE2	4:B:1181:VAL:HG12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:R:410:TYR:O	18:R:413:THR:OG1	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:S:476:ILE:HD12	17:S:476:ILE:HA	1.94	0.40
4:B:1129:ARG:O	4:B:1132:SER:OG	2.31	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
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%)	47 81
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%)	51 84
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%)	15 54
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%)	54 84

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 (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
1	Q	396/476 (83%)	393 (99%)	3 (1%)	81 91
2	M	97/371 (26%)	97 (100%)	0	100 100
3	A	1293/1465 (88%)	1291 (100%)	2 (0%)	93 98
4	B	1030/1053 (98%)	1030 (100%)	0	100 100
5	C	269/296 (91%)	268 (100%)	1 (0%)	91 96
6	D	65/116 (56%)	65 (100%)	0	100 100
7	E	197/197 (100%)	195 (99%)	2 (1%)	76 88
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%)	115 (99%)	1 (1%)	78 90
11	I	109/110 (99%)	109 (100%)	0	100 100
12	J	64/65 (98%)	62 (97%)	2 (3%)	40 70
13	K	93/130 (72%)	93 (100%)	0	100 100
14	L	40/57 (70%)	39 (98%)	1 (2%)	47 75
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%)	559 (99%)	4 (1%)	84 93
18	R	313/474 (66%)	312 (100%)	1 (0%)	92 97
All	All	5467/6990 (78%)	5450 (100%)	17 (0%)	92 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	18	ARG
1	Q	152	LEU
1	Q	297	ARG
3	A	30	LYS
3	A	590	ASN
5	C	281	ARG

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Mol	Chain	Res	Type
7	E	17	ARG
7	E	200	ARG
10	H	25	ARG
12	J	48	ARG
12	J	59	LYS
14	L	63	ARG
17	S	379	LYS
17	S	407	ARG
17	S	475	ARG
17	S	665	ASN
18	R	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	33	HIS
1	Q	294	HIS
1	Q	435	GLN
2	M	89	GLN
3	A	263	ASN
3	A	264	ASN
3	A	322	ASN
3	A	332	GLN
3	A	620	ASN
3	A	706	HIS
3	A	748	ASN
3	A	901	ASN
3	A	1036	ASN
3	A	1072	ASN
3	A	1314	GLN
3	A	1320	GLN
3	A	1447	GLN
3	A	1487	ASN
3	A	1560	ASN
3	A	1564	ASN
3	A	1620	GLN
4	B	62	ASN
4	B	248	ASN
4	B	361	HIS
4	B	368	GLN
4	B	427	GLN
4	B	462	GLN

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Mol	Chain	Res	Type
4	B	532	HIS
4	B	575	HIS
4	B	673	ASN
4	B	702	ASN
4	B	735	HIS
4	B	767	ASN
4	B	923	GLN
4	B	1008	HIS
4	B	1114	GLN
5	C	53	ASN
5	C	130	ASN
5	C	301	ASN
9	G	56	ASN
9	G	59	GLN
9	G	64	GLN
9	G	121	ASN
11	I	95	ASN
13	K	106	GLN
16	O	66	ASN
16	O	94	ASN
16	O	152	GLN
16	O	391	GLN
17	S	185	GLN
17	S	401	ASN
17	S	461	HIS
17	S	483	HIS
18	R	184	ASN
18	R	207	ASN
18	R	221	HIS
18	R	246	GLN
18	R	304	HIS
18	R	407	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

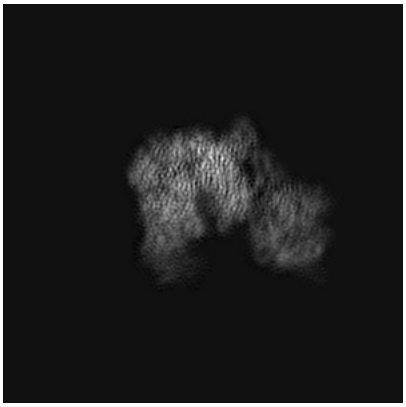
6 Map visualisation

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.

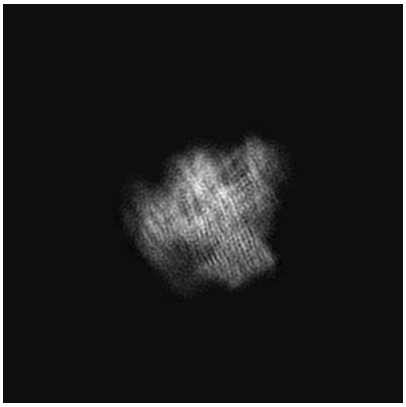
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

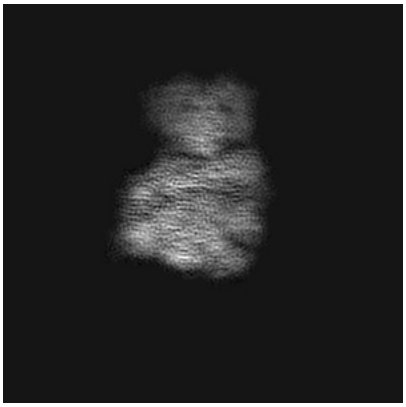
6.1.1 Primary map



X



Y

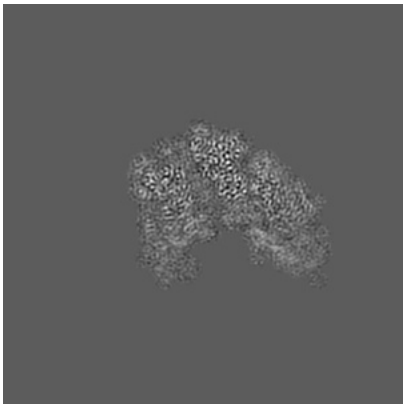


Z

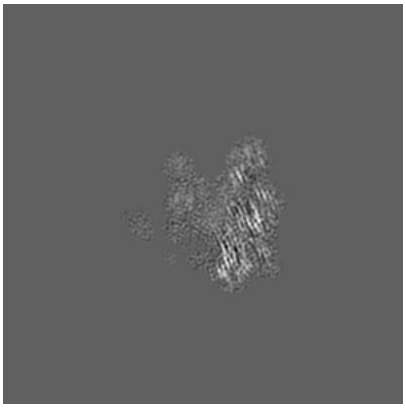
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 144



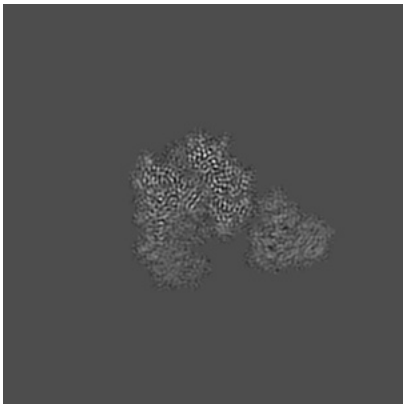
Y Index: 144

Z Index: 144

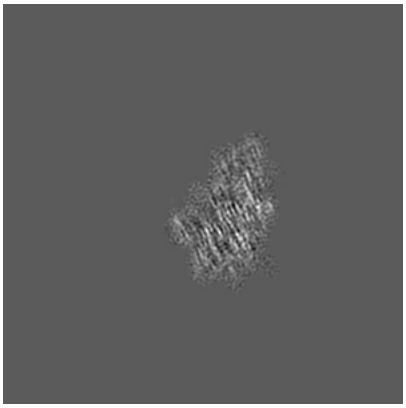
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

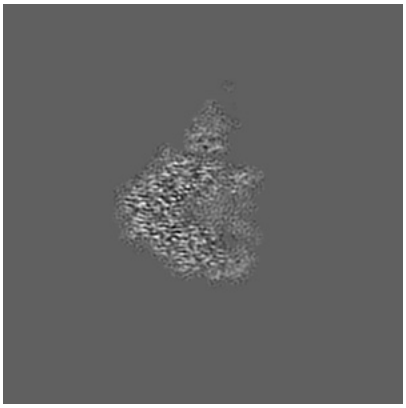
6.3.1 Primary map



X Index: 127



Y Index: 157



Z Index: 161

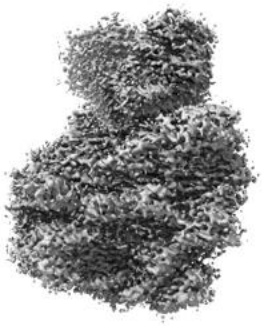
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal 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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

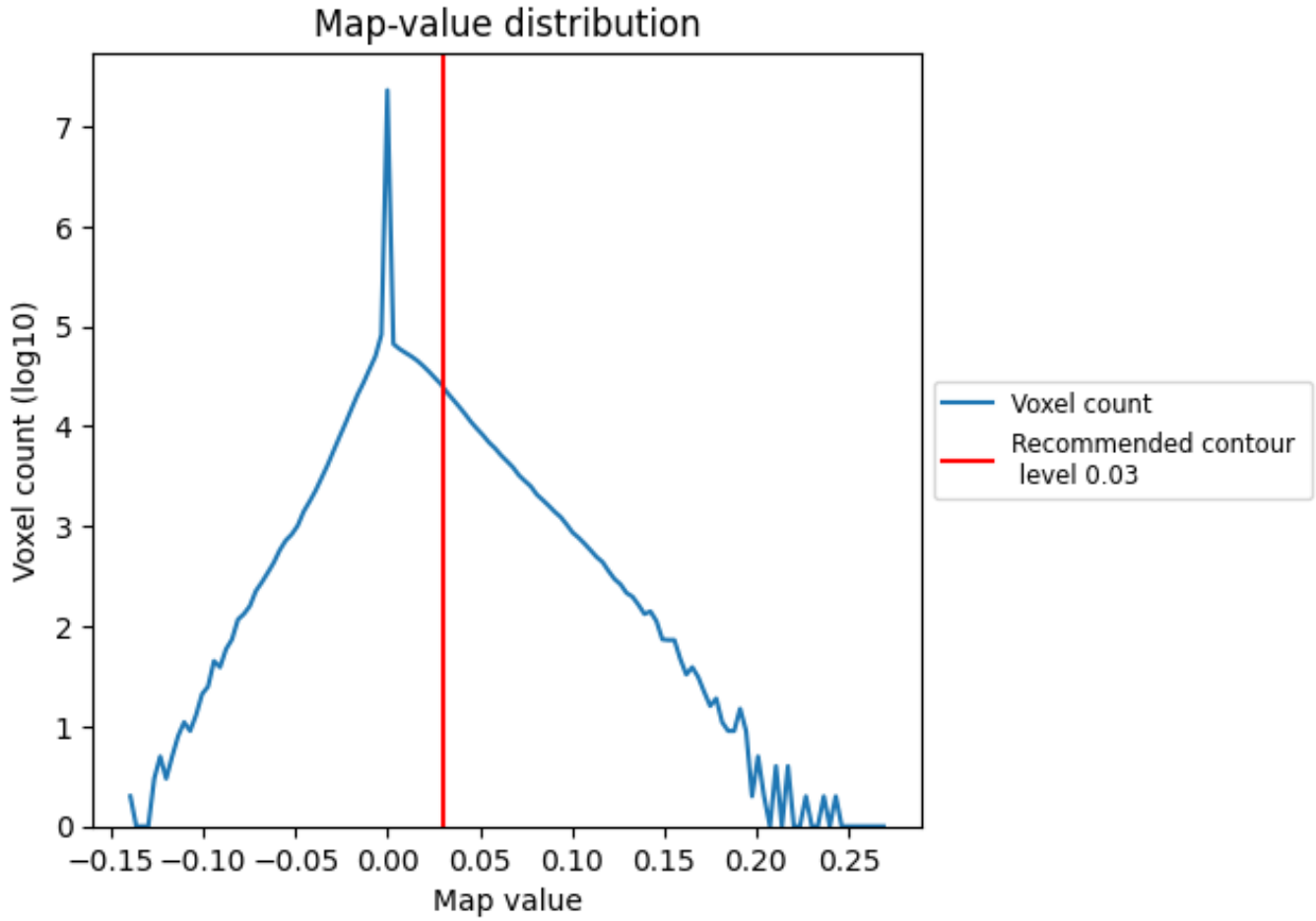
6.5 Mask visualisation (i)

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

7 Map analysis

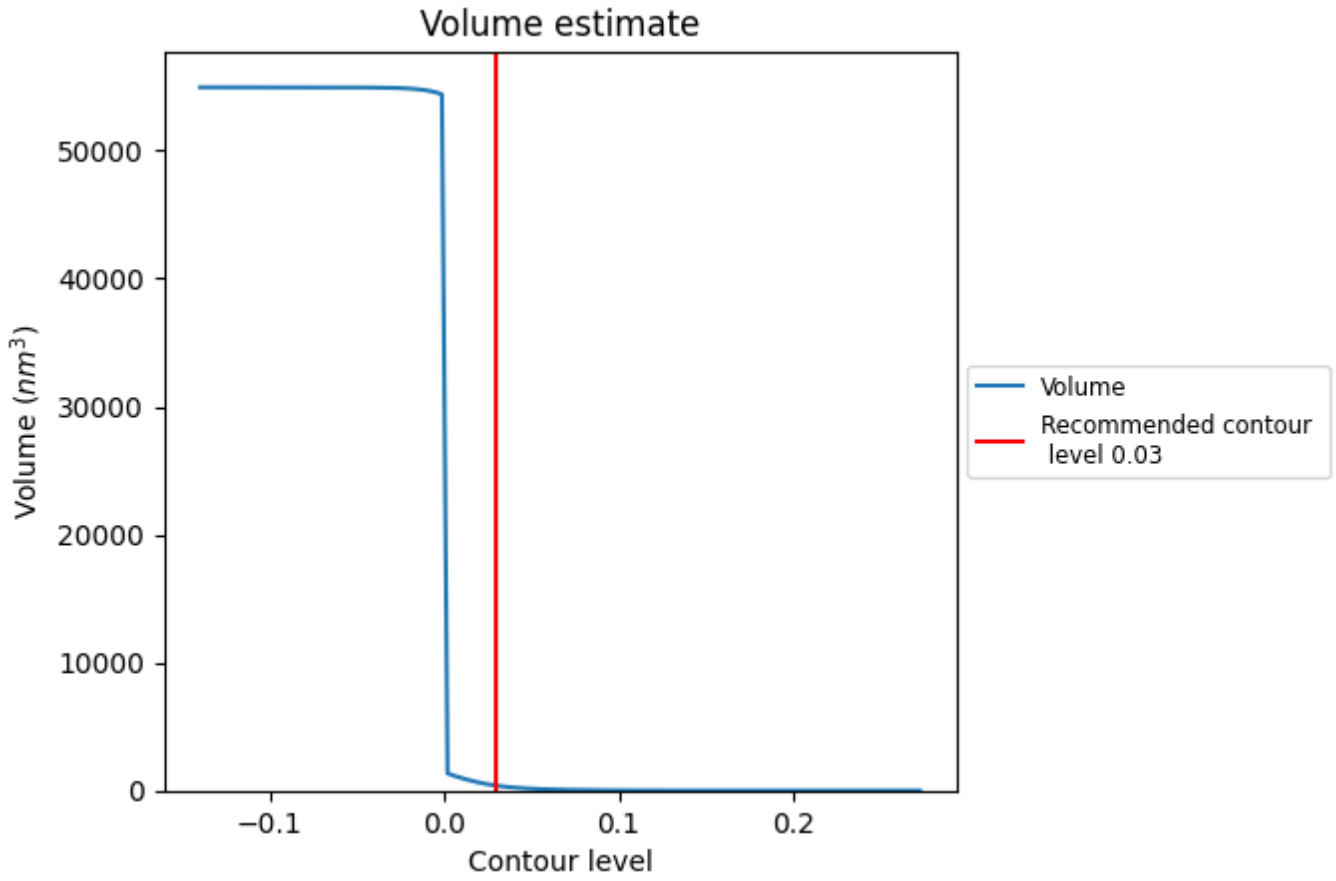
This section contains the results of statistical analysis of the map.

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.

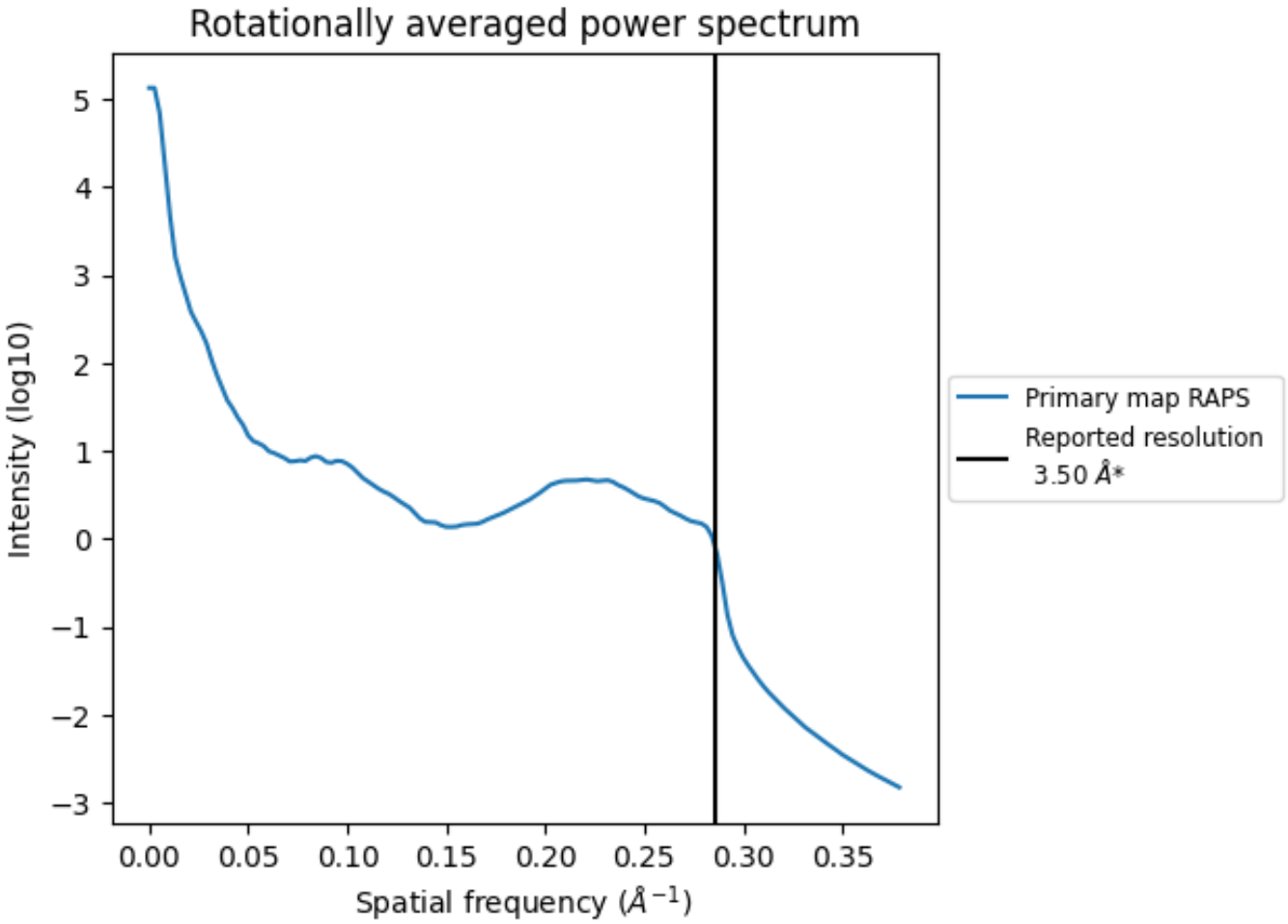
7.2 Volume estimate



The volume at the recommended contour level is 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 (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

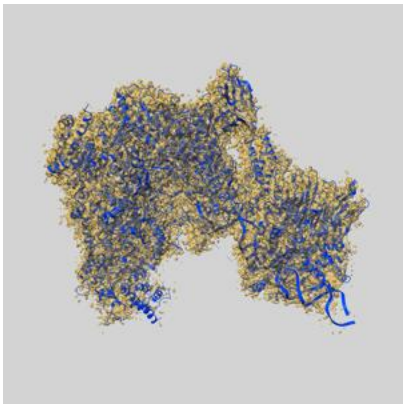
8 Fourier-Shell correlation (i)

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

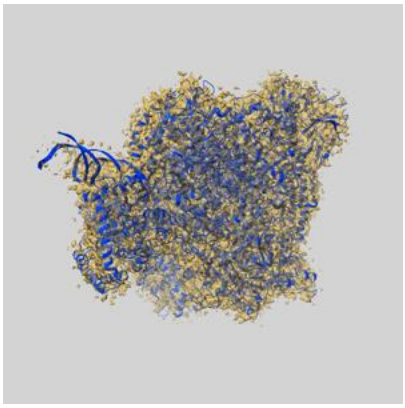
9 Map-model fit

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

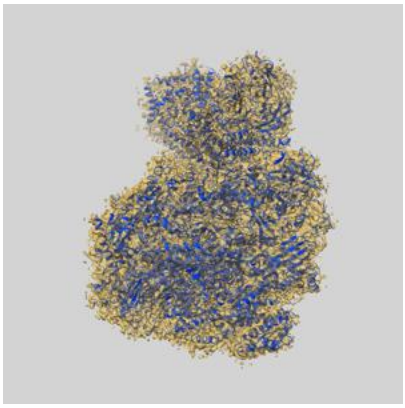
9.1 Map-model overlay



X



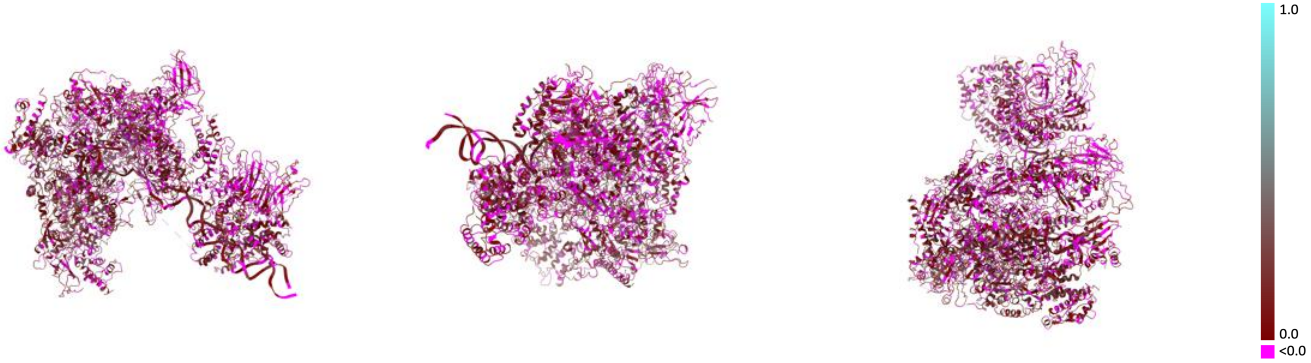
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

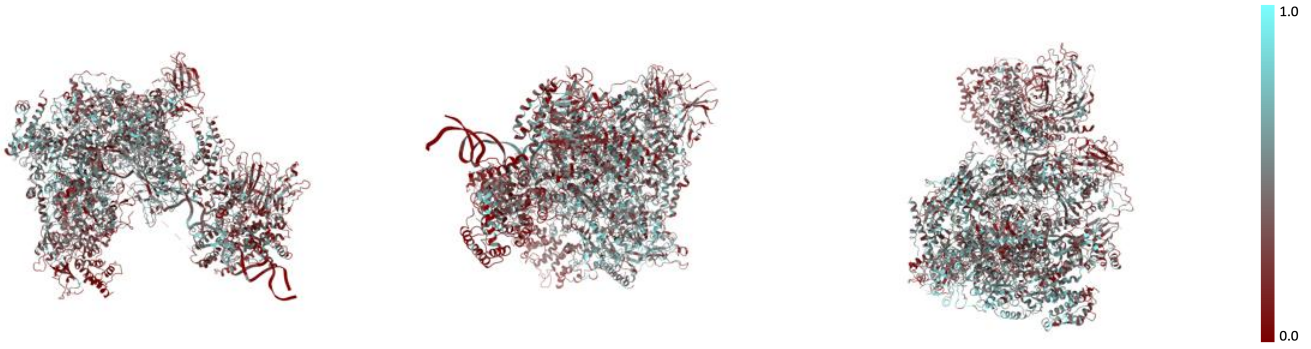
9.2 Q-score mapped to coordinate model (i)



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.

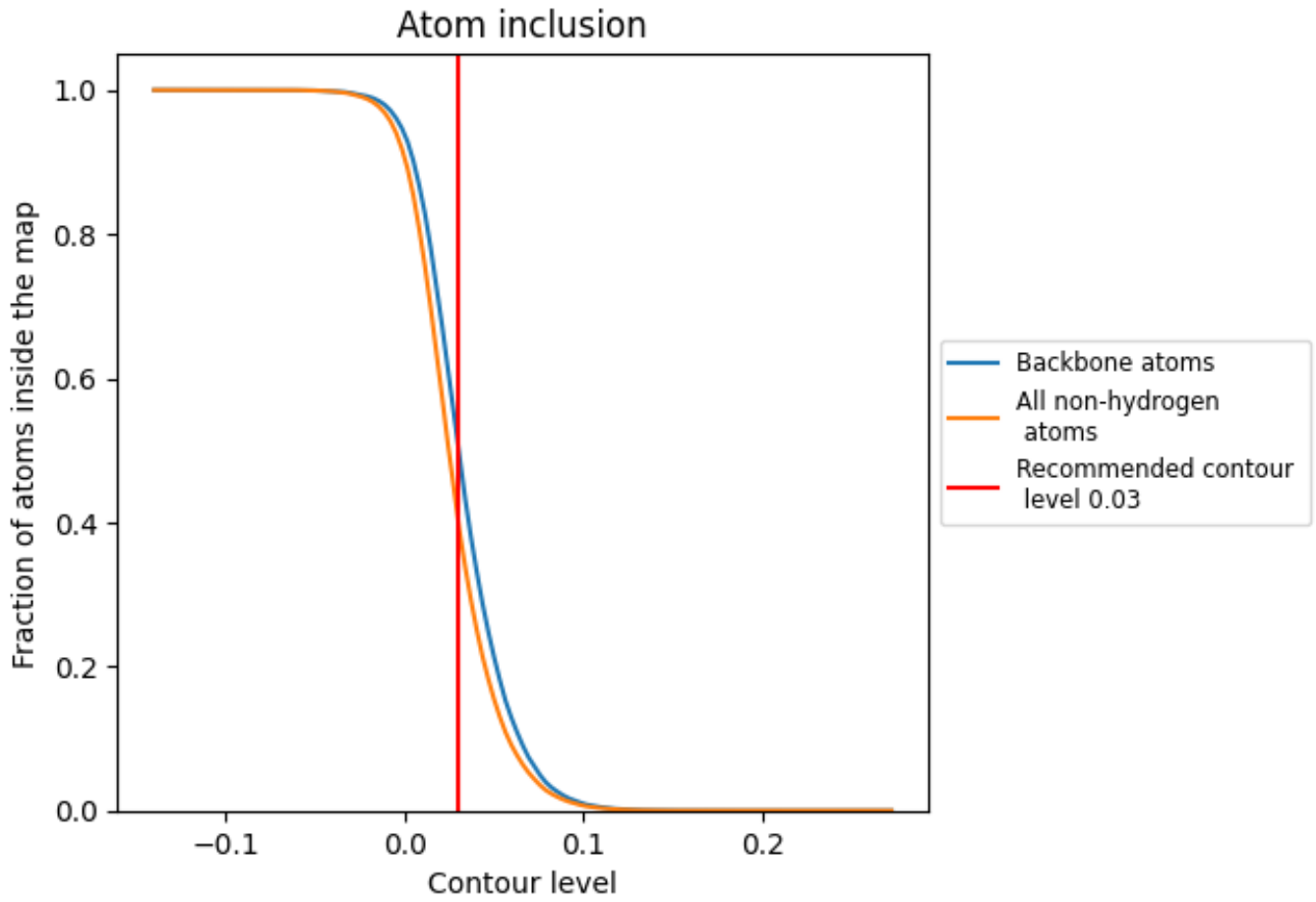
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 41% 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	0.4051	0.0890
A	0.4958	0.1120
B	0.4785	0.0900
C	0.5223	0.1060
D	0.3407	0.1150
E	0.5035	0.1180
F	0.5331	0.1540
G	0.3320	0.1270
H	0.5766	0.1550
I	0.2794	0.0640
J	0.4873	0.0340
K	0.5156	0.1200
L	0.5303	0.0910
M	0.2849	-0.0050
N	0.2858	0.0230
O	0.1236	0.0980
Q	0.3146	0.0740
R	0.3711	0.0490
S	0.2872	0.0380
T	0.3430	0.0830
U	0.3862	0.1040