



Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 07:17 am BST

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.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

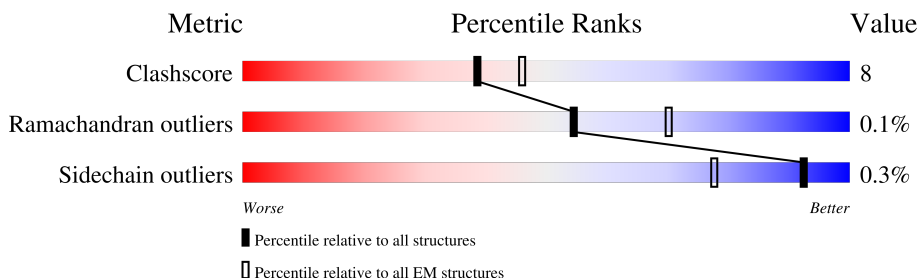
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



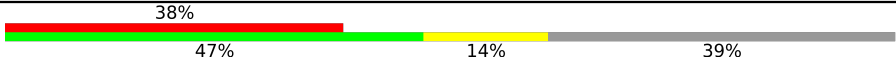
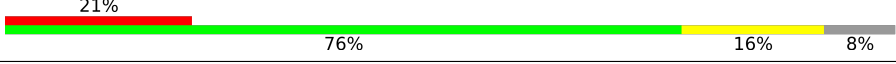
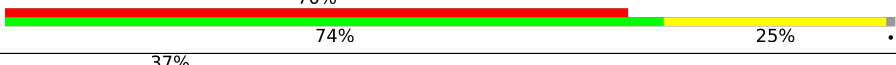


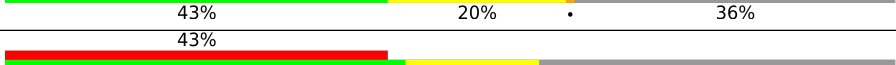


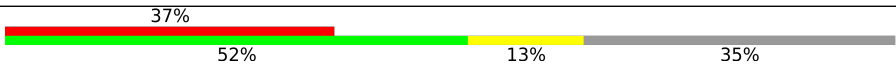
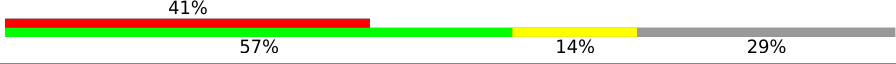
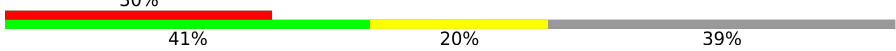

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	514	
2	M	415	
3	A	1664	
4	B	1203	
5	C	335	
6	D	137	
7	E	215	
8	F	155	

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 19 is a DNA chain called Template strand.

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

- Molecule 20 is a DNA chain called Nontemplate strand.

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

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

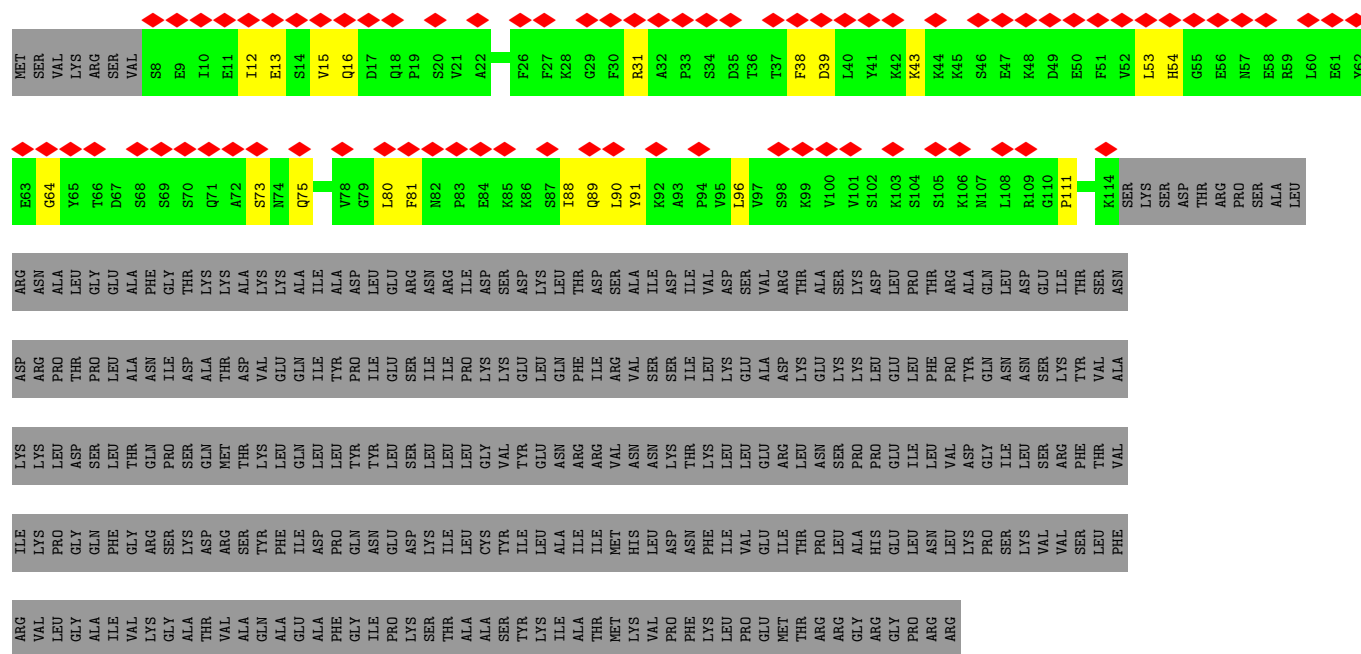
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

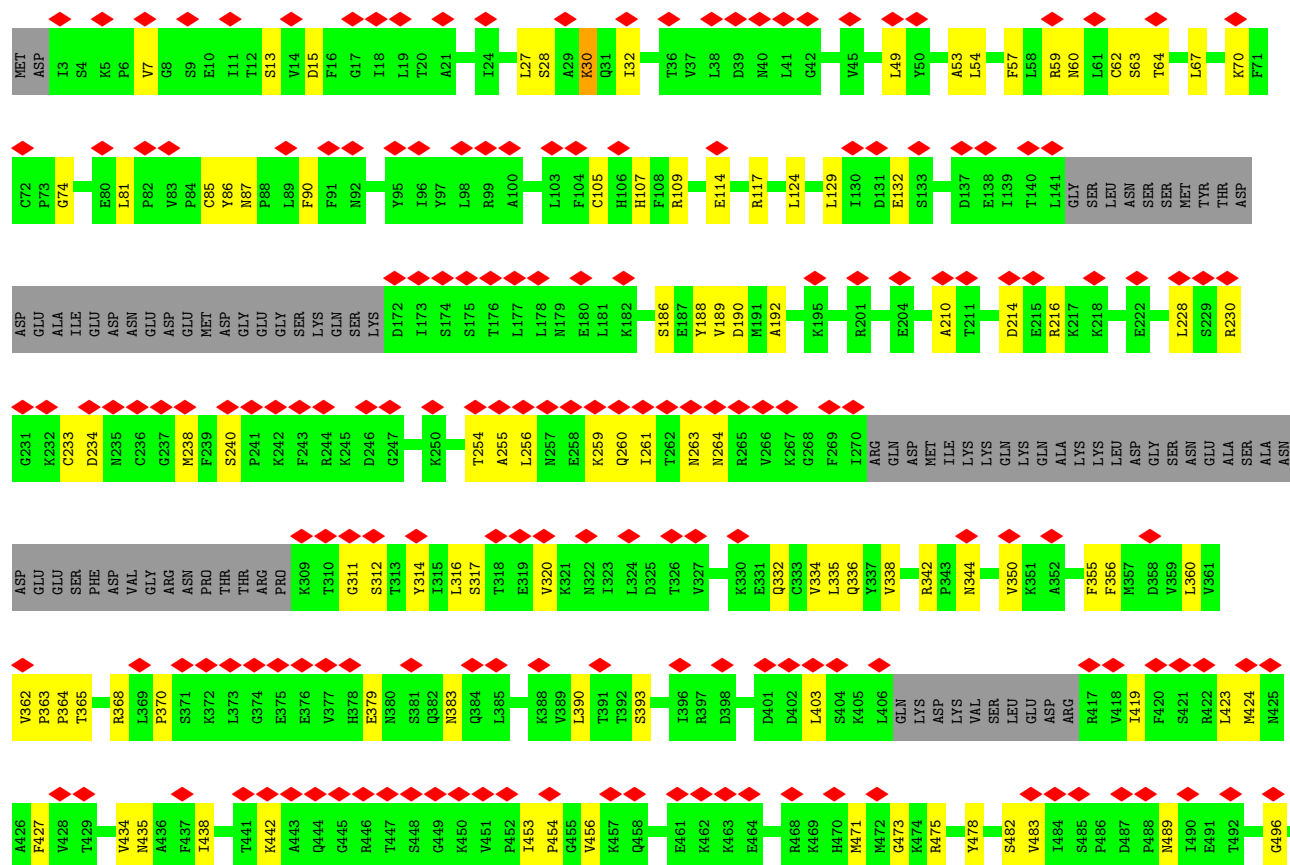


• Molecule 2: DNA-directed RNA polymerase I subunit RPA49

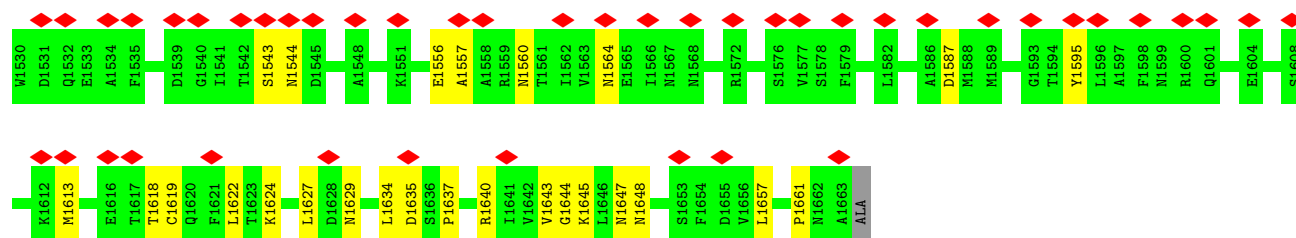




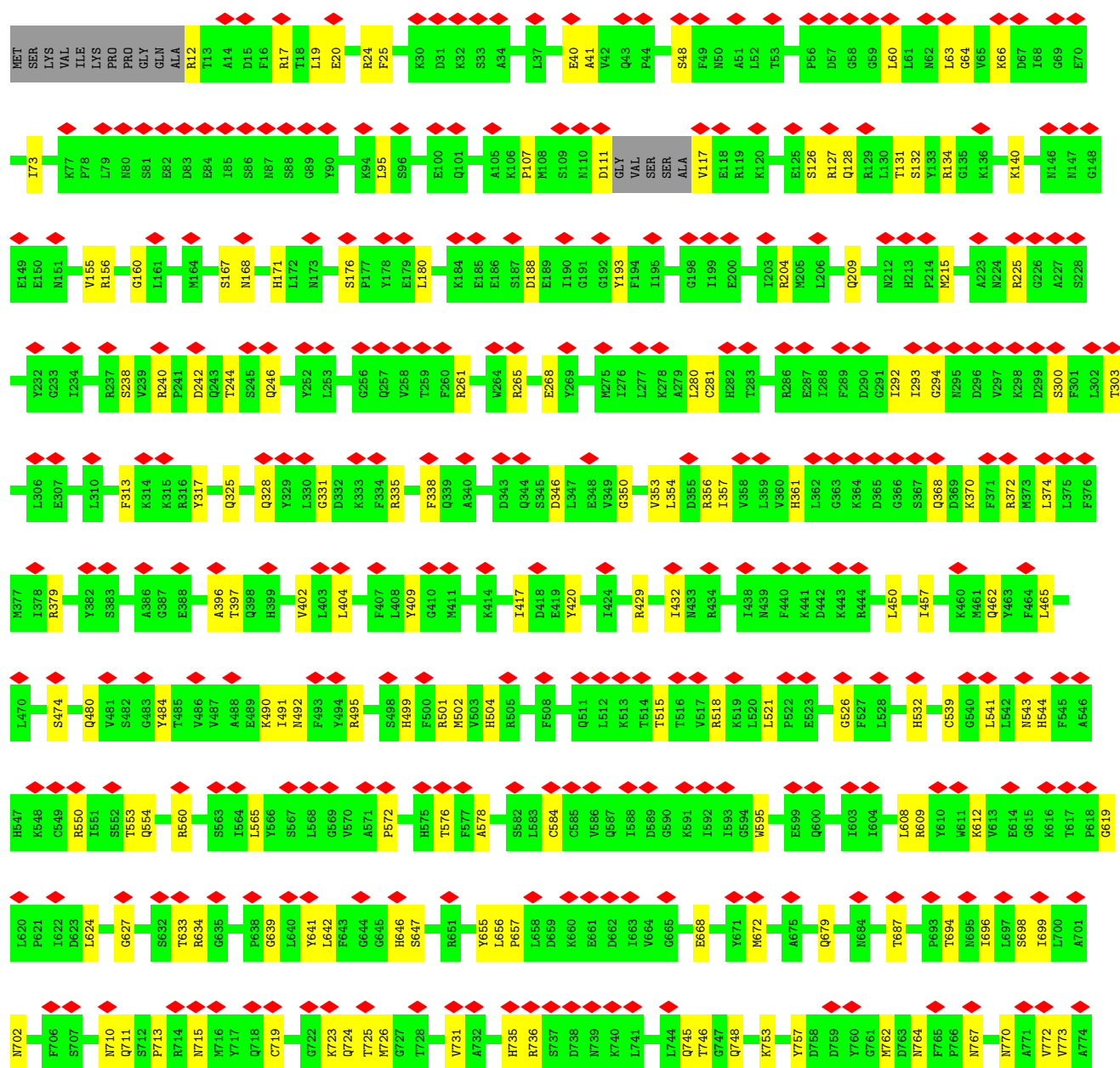
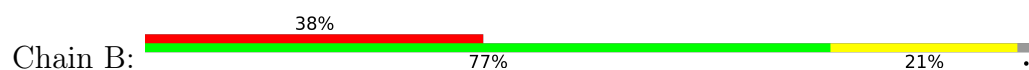
• Molecule 3: DNA-directed RNA polymerase I subunit RPA190

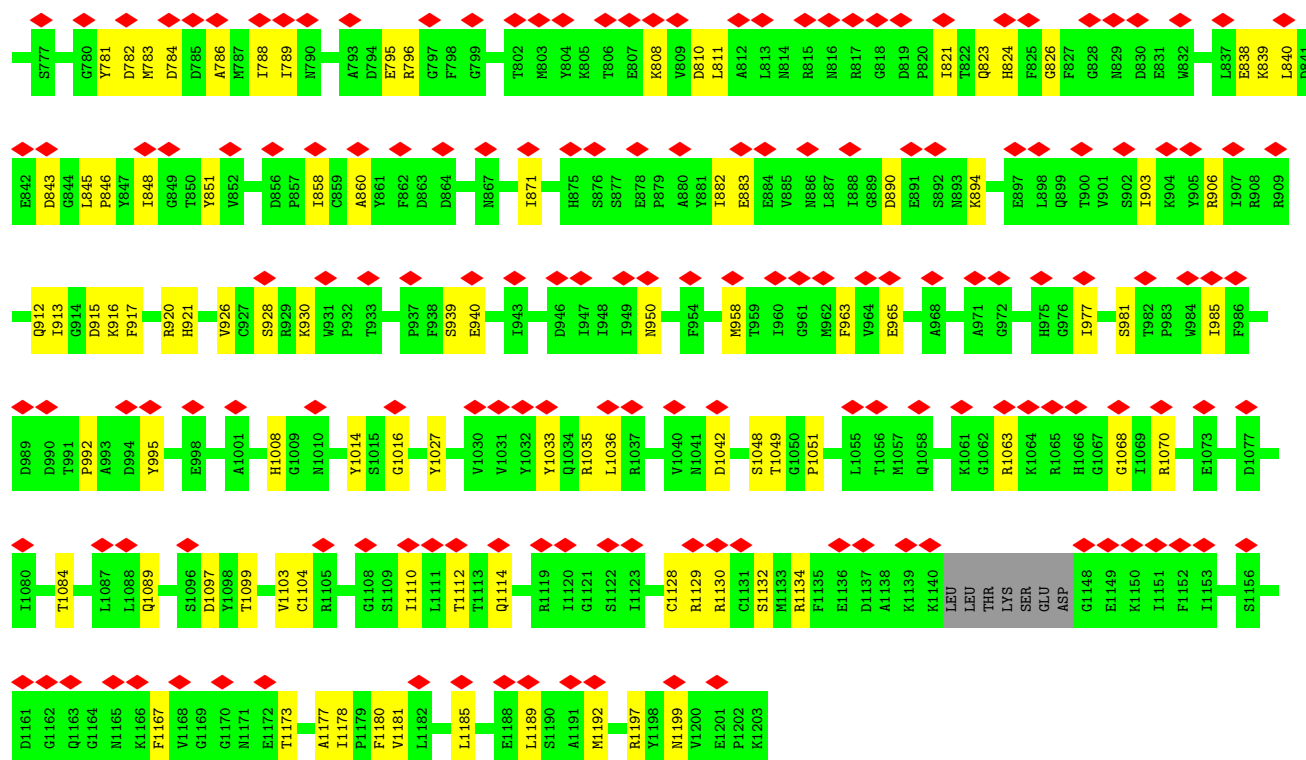


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V586	N590	R591	Q592	P593	T594	L595	H596	S599	V605	R606	N610	E611	K612	T613	L614	R615	L616	H617	Y618	T621	G622	A623	Y624	N625	A626	D627	F628	D629	G630	D631	E632	M633	F637	P638	Q639	N640	E646	A647	L648	N649	L650	T653	Y657	L658	S664	P665	V666	R667									
G668	L669	I670	Q671	H673	K683	Y692	Y695	I700	R701	D704	G705	H706	T707	T708	R709	I712	P716	Y723	G728	K729	Q730	N731	I732	I733	D734	V735	L736	L737	N738	V739	T740	P741	P742	D743	N744	I747	N748	L749	I750	N753	K754	I755	E758	Y759	W760	G761											
K762	E766	N767	E768	V769	K772	D773	G774	L775	L776	L777	C778	G779	I780	L781	D782	K783	S784	T785	Y786	G787	A788	S789	K790	Y791	G792	H795	S796	L797	H798	E799	G802	P803	A805	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	M925	Q926	A927	M928	A929	G932	A933	A934	K937	V938	N939	Q942	C945	L946	L947	Q948	Q949	Q950	A951	L952	R955	A956	V959	S962	G963	K964	P967	S968	P971	T974	M977	A978	Y981	V982	K983	G984	R985	S986	G989	I990	K991	P992	Q993	E994													
Y995	Y996	F997	H998	C999	R1003	L1006	I1007	D1008	T1009	A1010	V1011	K1012	T1013	S1014	S1015	S1016	G1017	Y1018	R1021	K1025	R1039	D1042	V1046	Q1047	F1048	M1049	Y1050	G1051	D1052	L1053	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	LEJ	PHE	LYS	SER	SER	ASP	G1160	V1161	K1164	Q1171	L1172	K1173	R1176	I1179	G1182	E1183	A1189	V1193	G1194	P1196	S1197	T1198																
Q1199	M1200	T1201	L1202	N1203	T1204	F1205	HIS	PHE	ALA	GLY	GLY	HIS	GLY	ALA	N1214	L1217	P1220	R1223	E1224	I1225	V1226	M1227	T1228	K1229	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	GLN	ASN	THR	ALA	ALA	R1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337						
R1338	THR	THR	GLY	SER	PRO	ASP	ILE	GLY	VAL	ALA	VAL	PRO	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D1298	M1299	N1300	E1305	Y1306	D1307	K1310	E1311	E1312	L1313	V1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	L1324	L1325	I1329	E1332	I1333	K1334	K1335	Q1336	K1337
ALA	GLU	LYS	SER	SER	PRO	ASP	GLU	GLY	ILE	ASP	VAL	ASP	ARG	GLY	THR	GLN	ASN	THR	ALA	ALA	GLY	ASN	ALA	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	D12																										

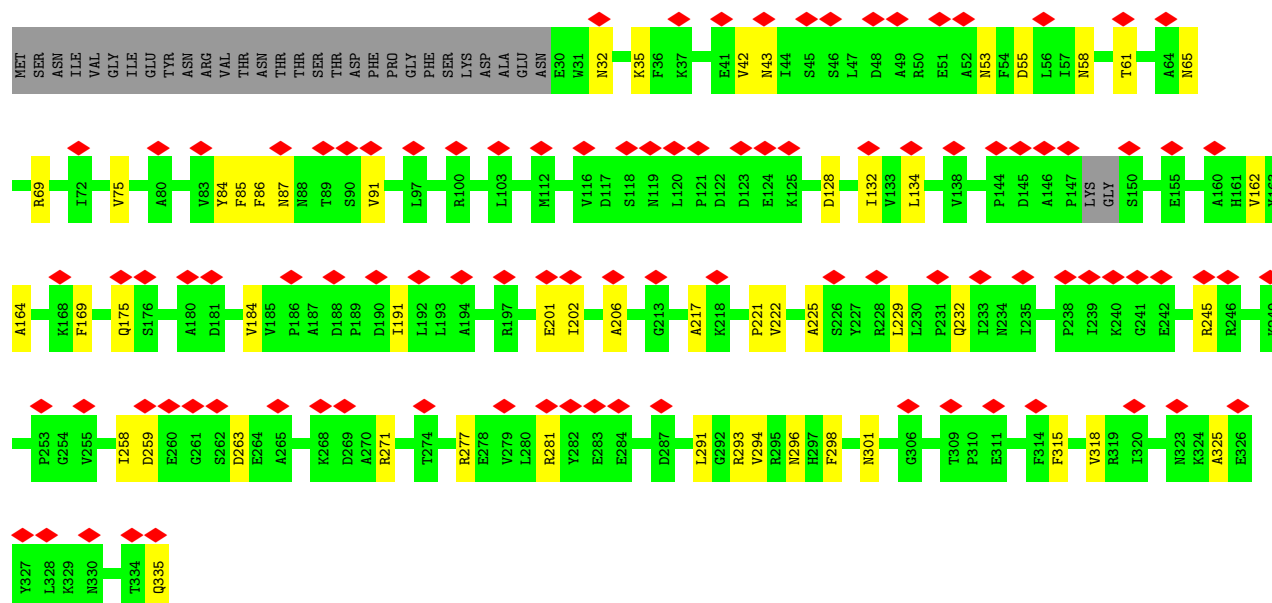
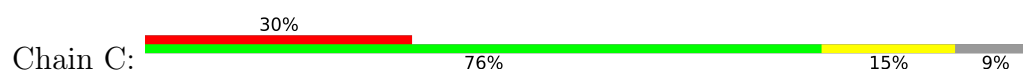


• Molecule 4: DNA-directed RNA polymerase I subunit RPA135

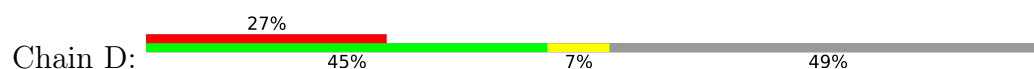


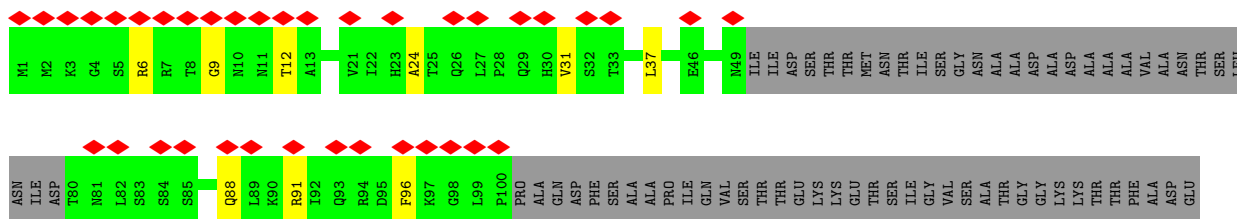


• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC1

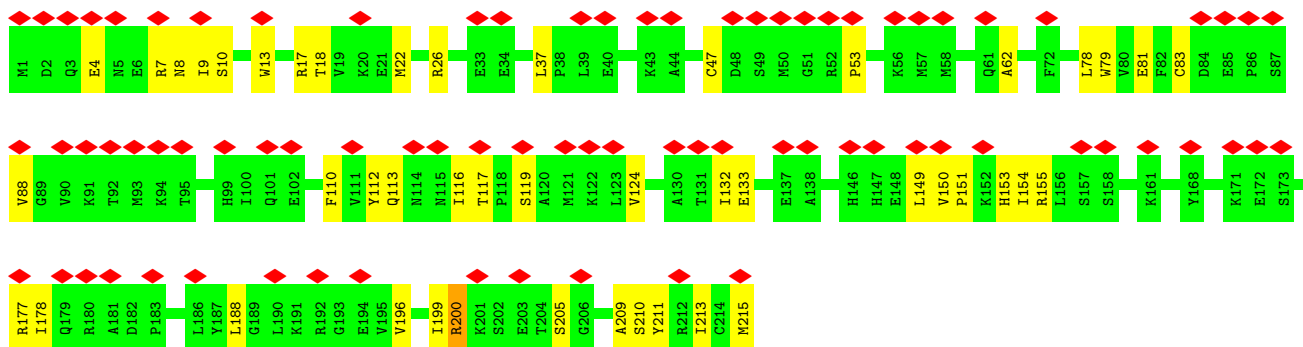
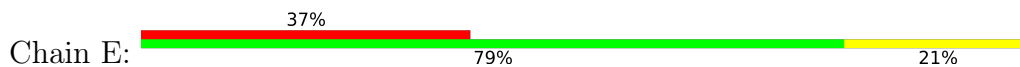


• Molecule 6: DNA-directed RNA polymerase I subunit RPA14

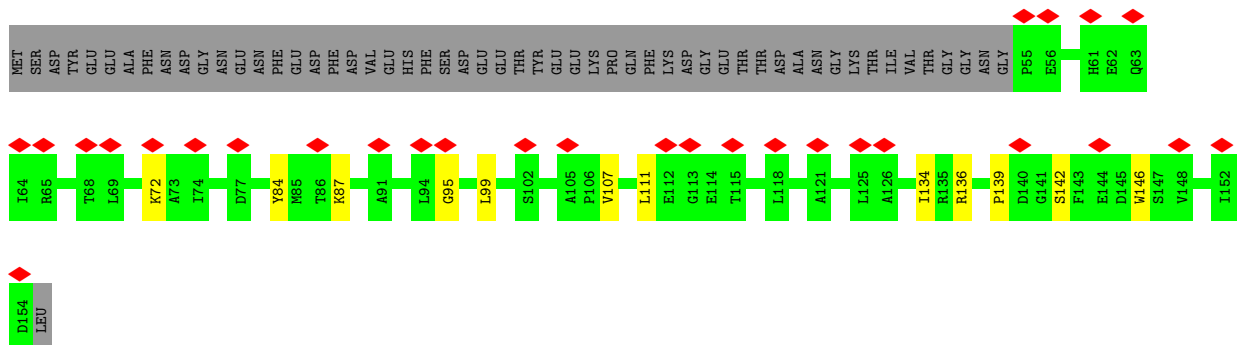




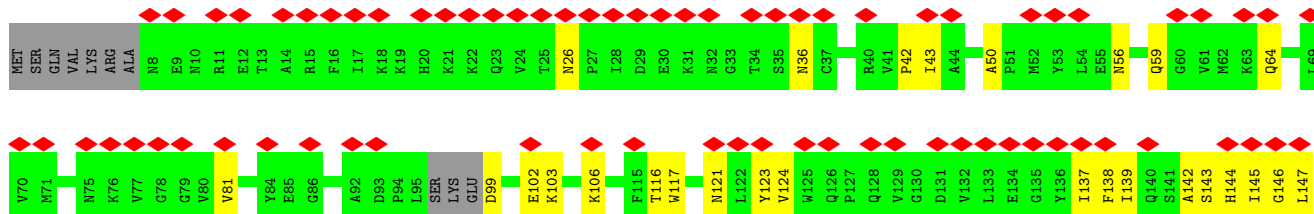
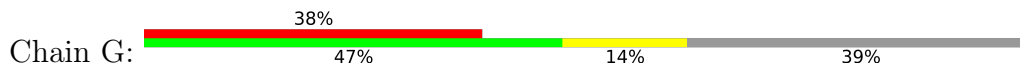
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

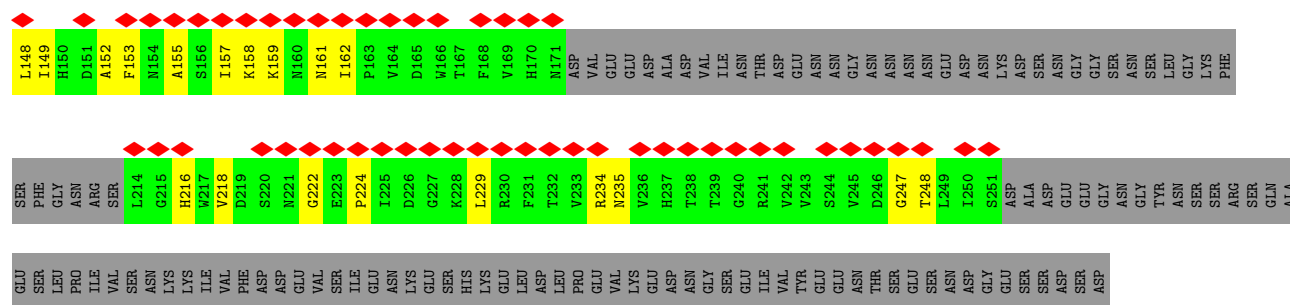


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

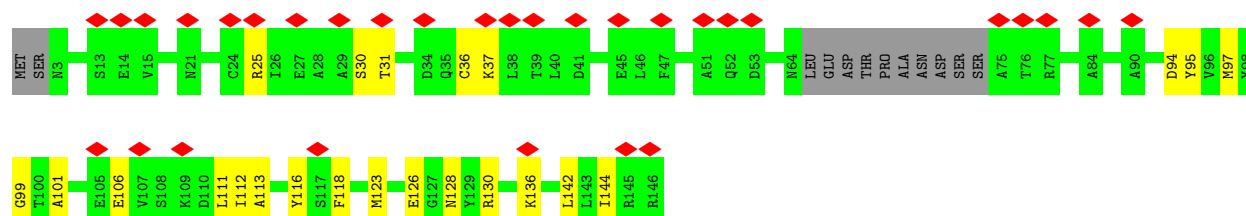
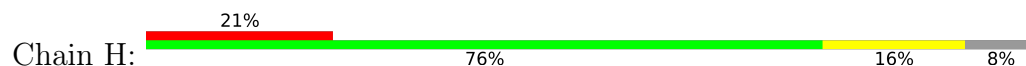


• Molecule 9: DNA-directed RNA polymerase I subunit RPA43

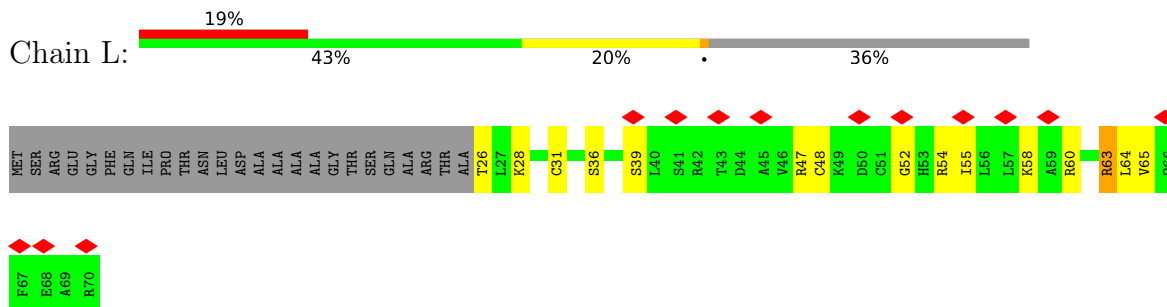




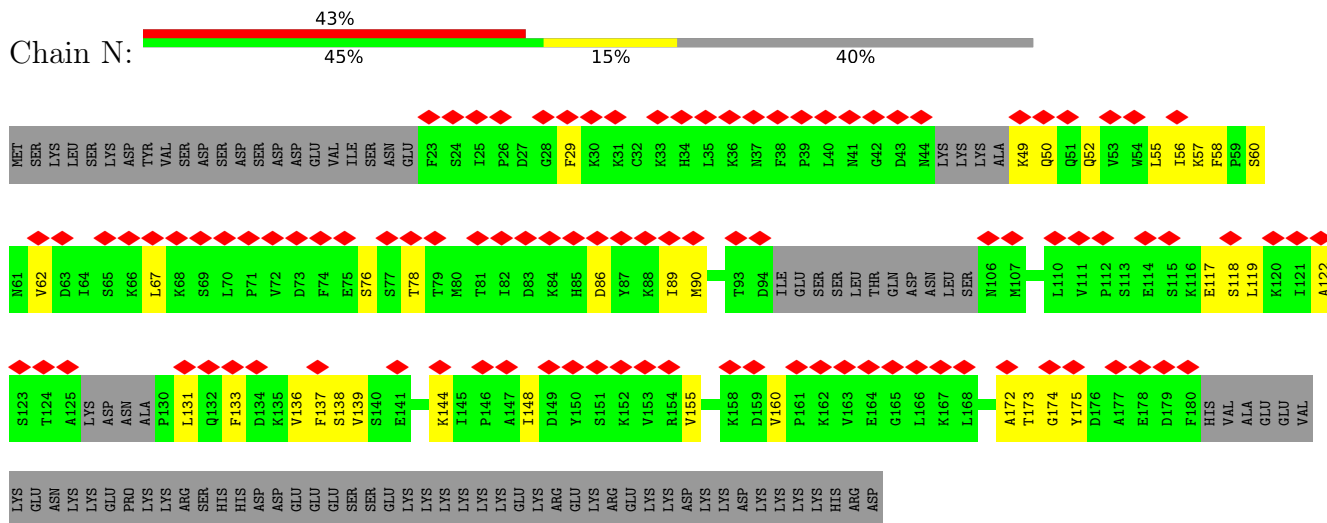
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



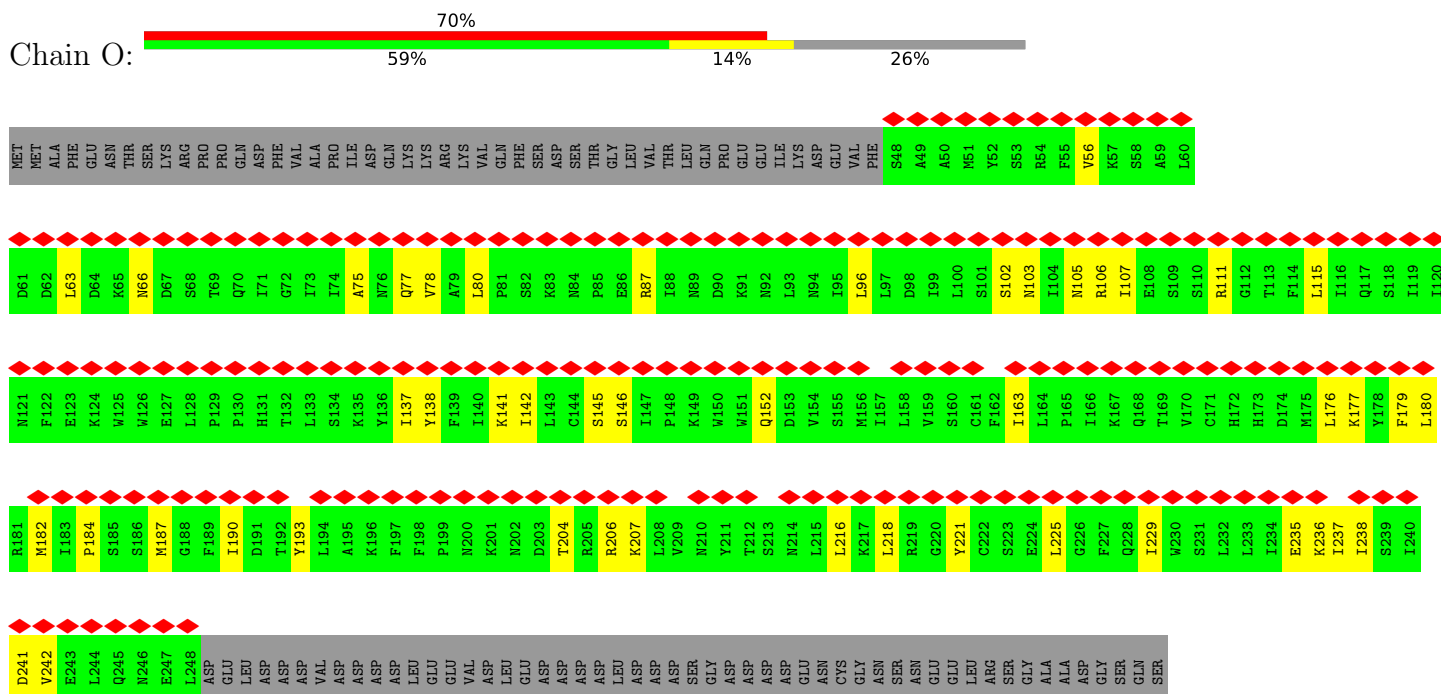
- Chain L:

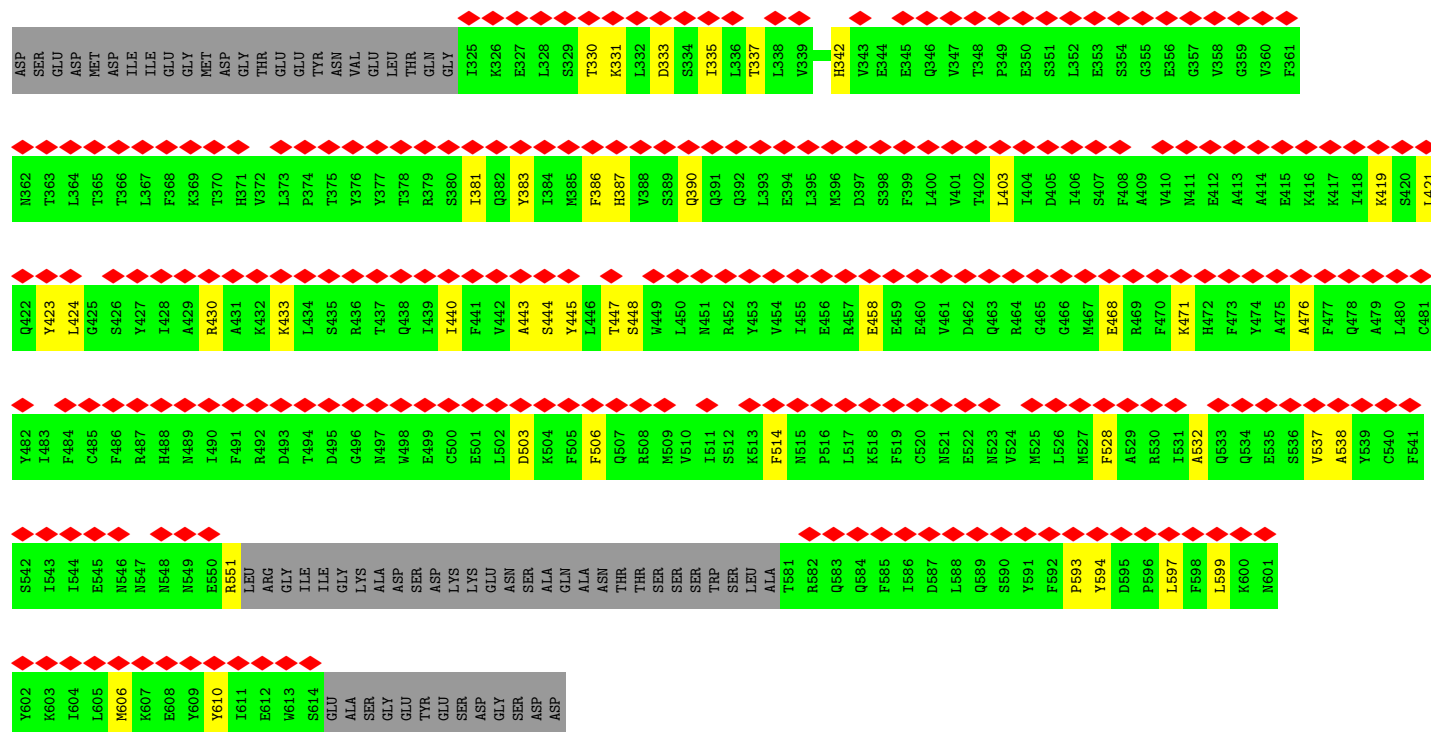


- Chain N:

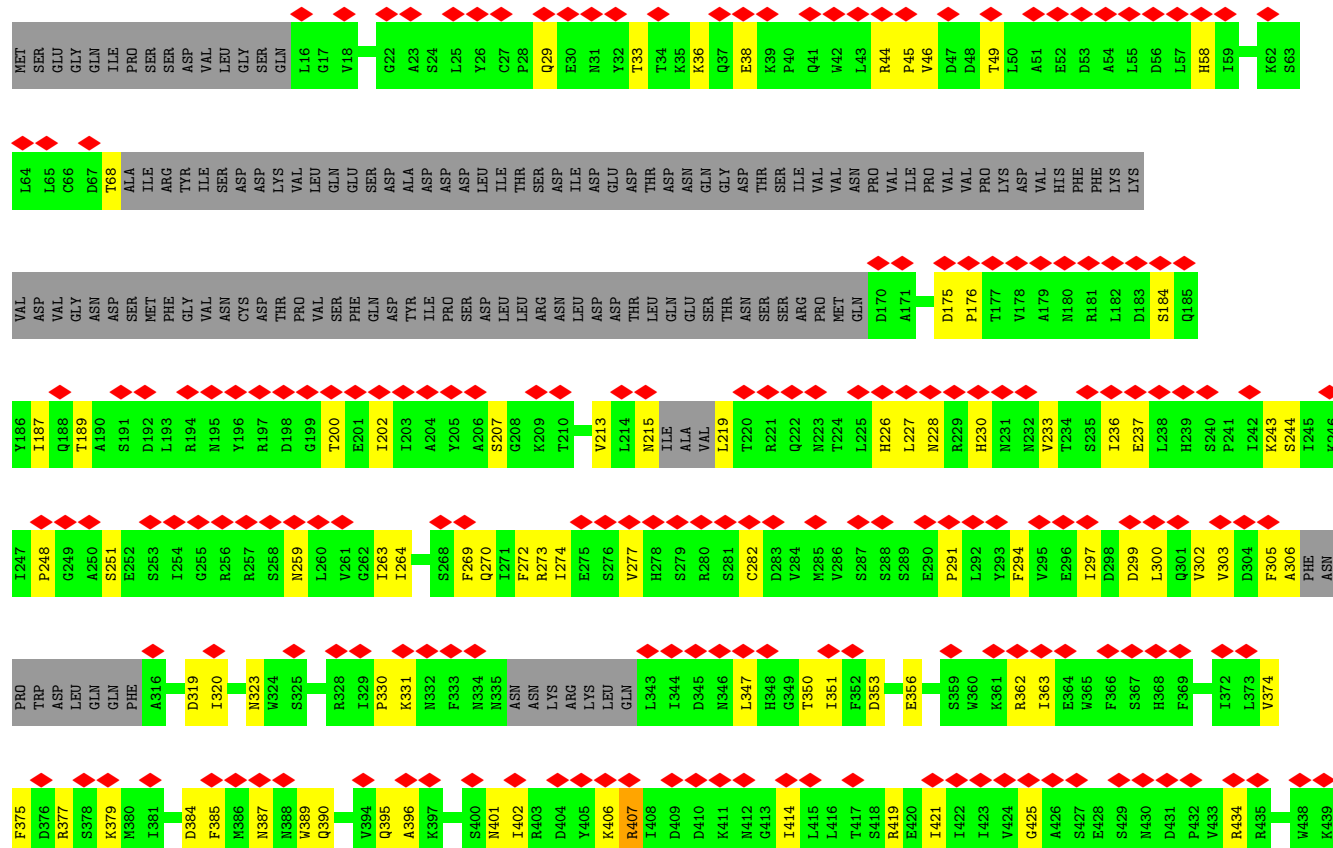


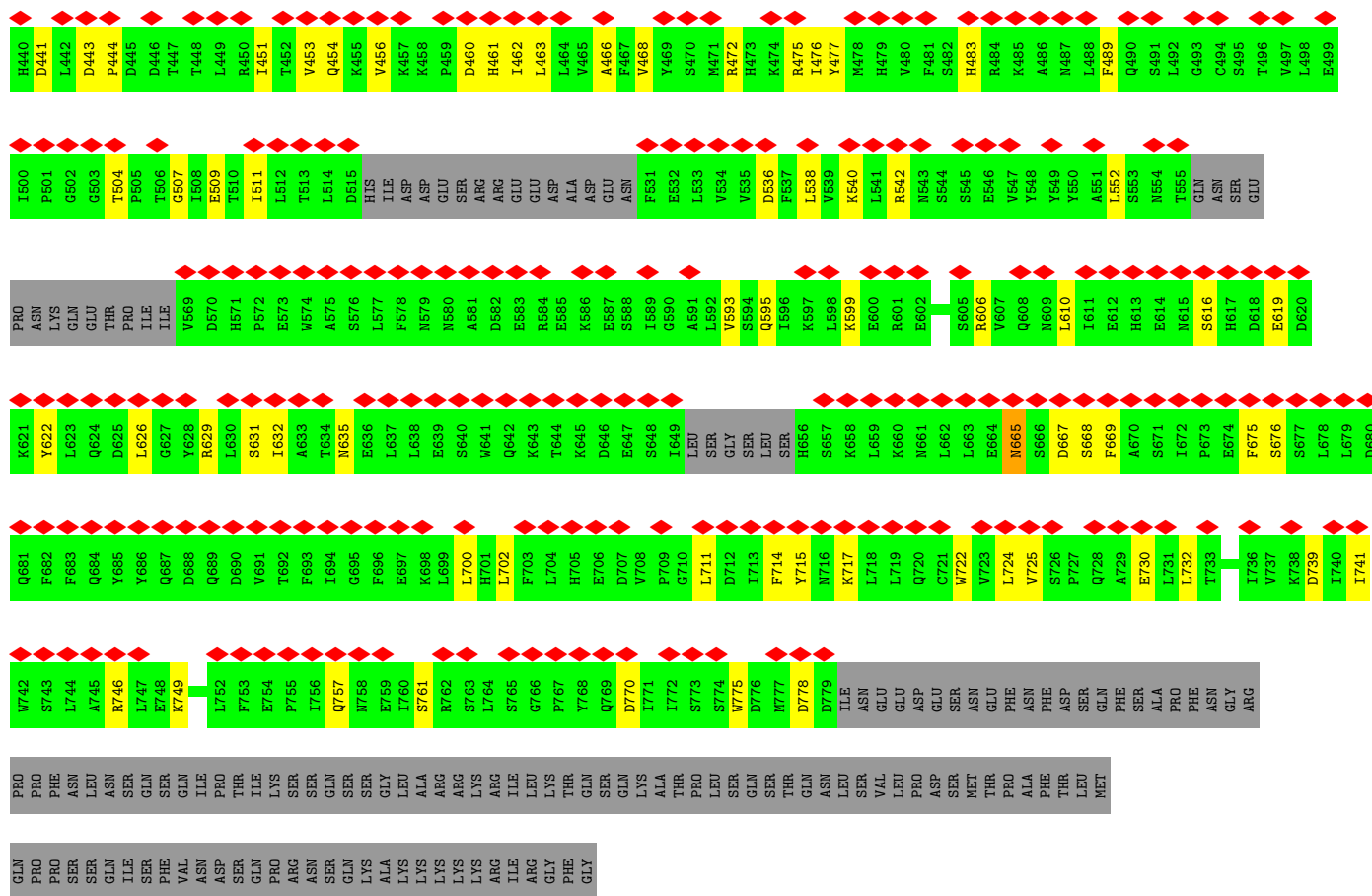
- Chain 0:



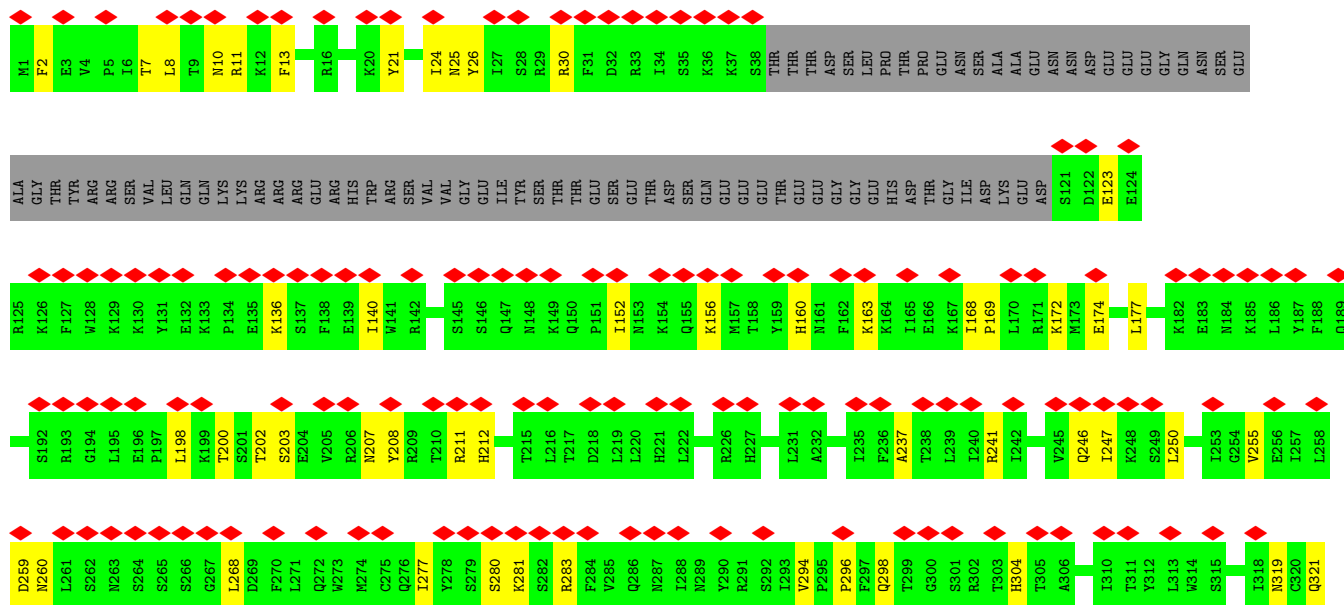


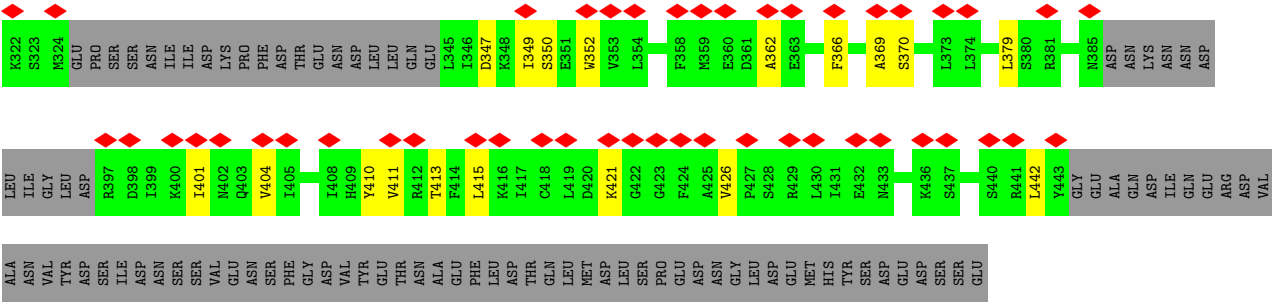
• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN6



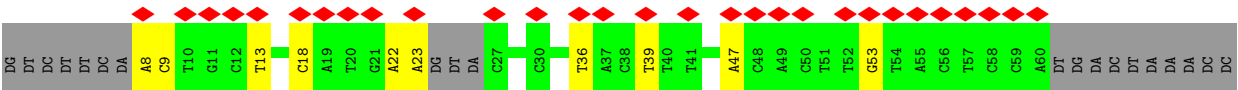
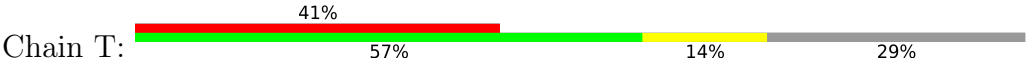


● Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11

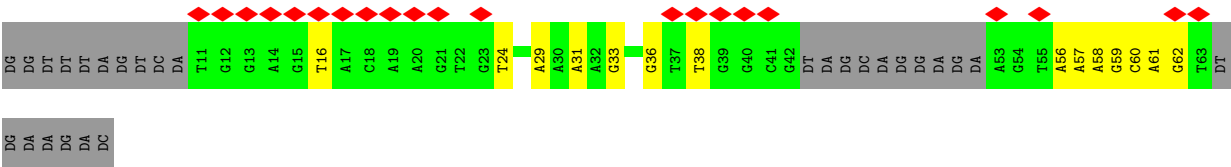




● Molecule 19: Template strand



● Molecule 20: Nontemplate strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.57175	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.272	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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 ⓘ

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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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.

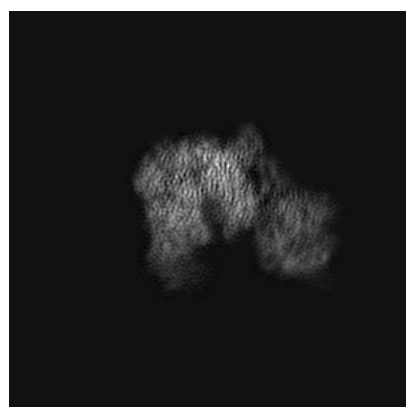
6 Map visualisation [i](#)

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

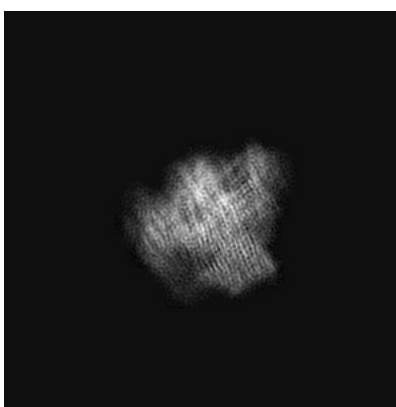
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

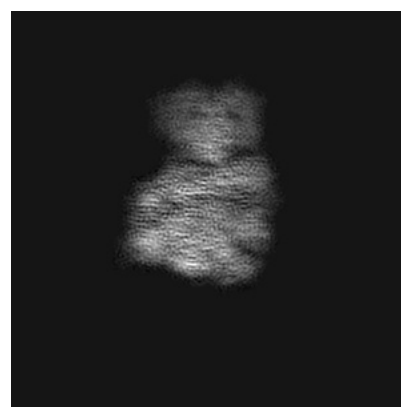
6.1.1 Primary map



X



Y

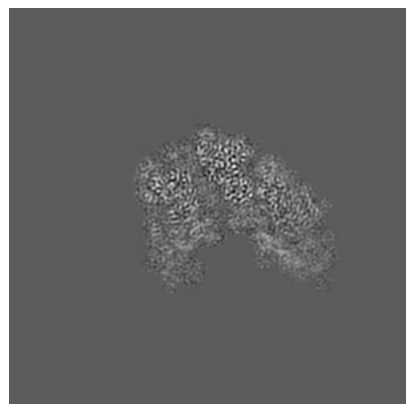


Z

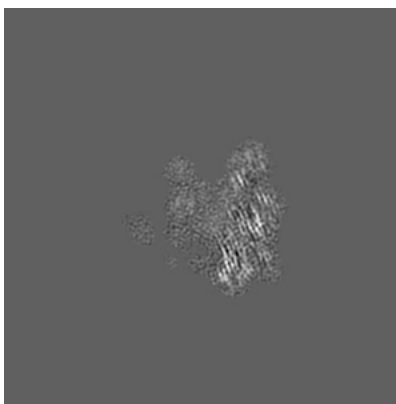
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

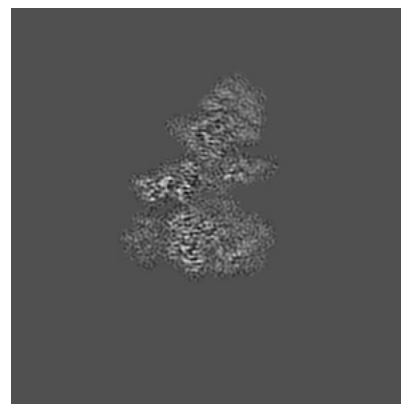
6.2.1 Primary map



X Index: 144



Y Index: 144

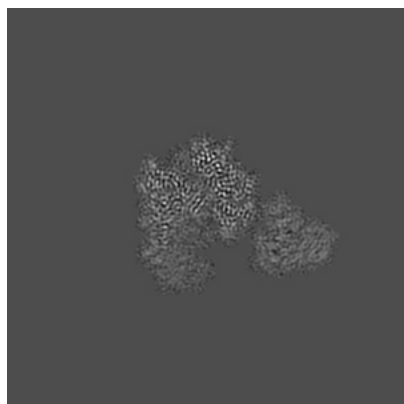


Z Index: 144

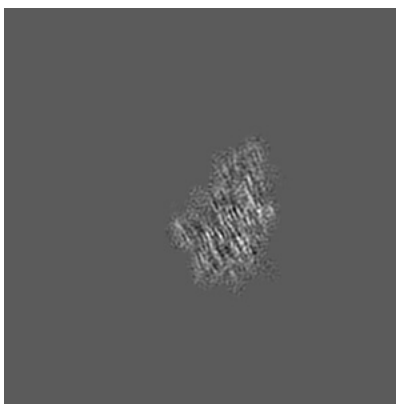
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

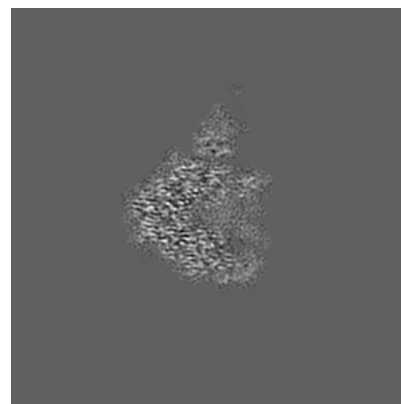
6.3.1 Primary map



X Index: 127



Y Index: 157

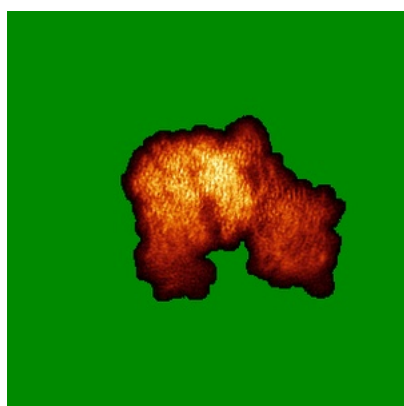


Z Index: 161

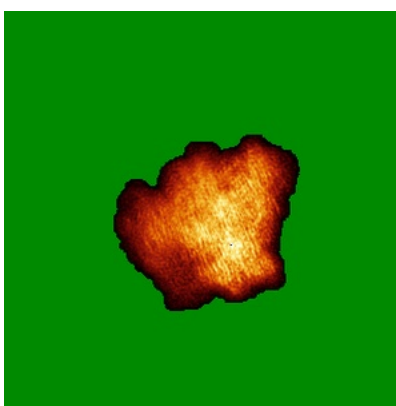
The images above show the largest variance slices of the map in three orthogonal directions.

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

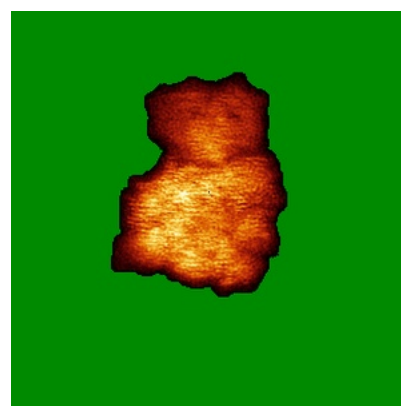
6.4.1 Primary map



X



Y



Z

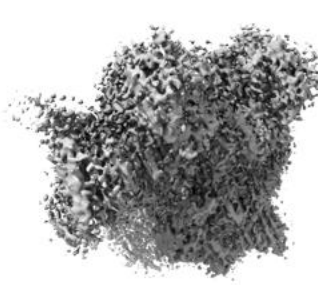
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

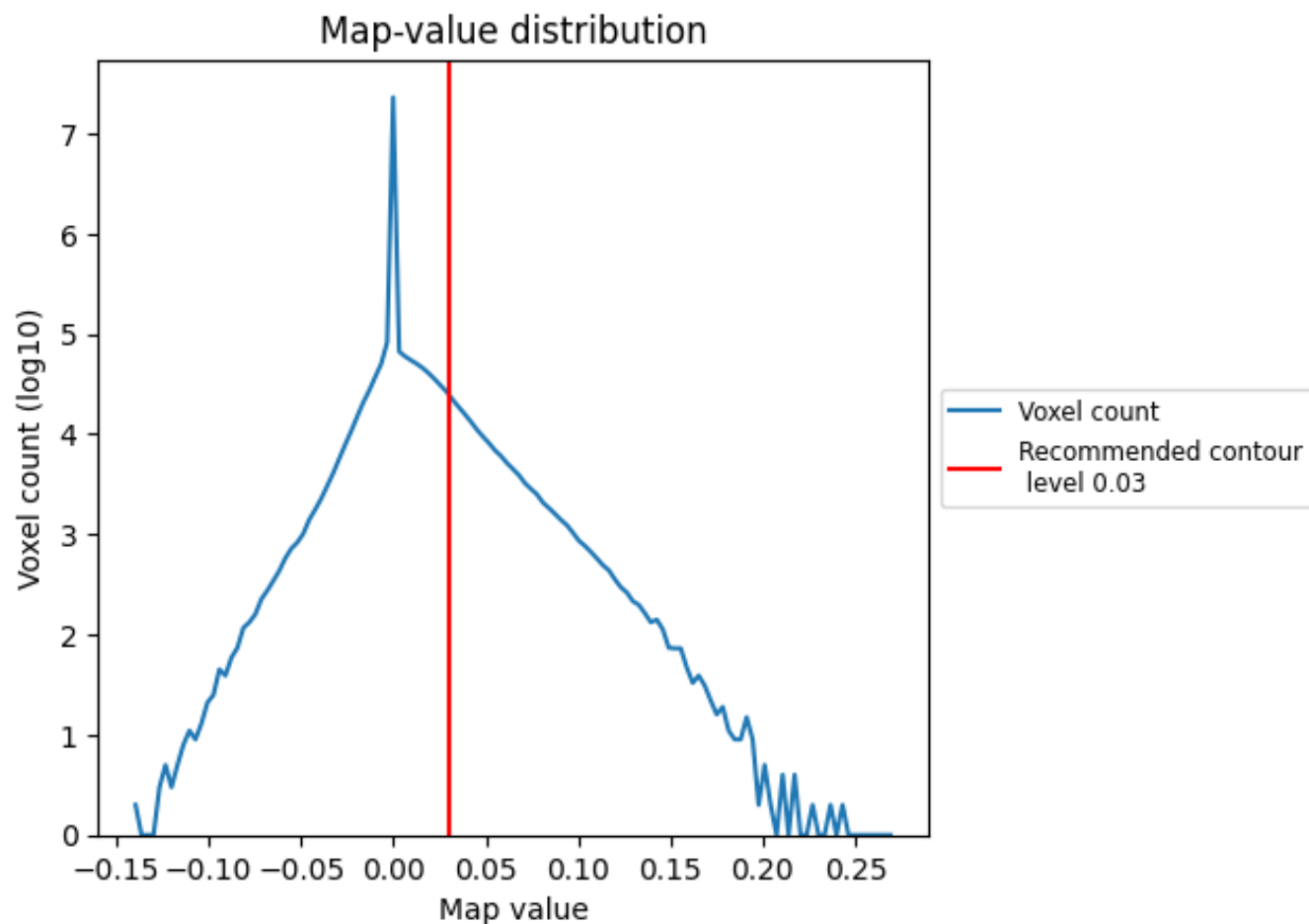
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

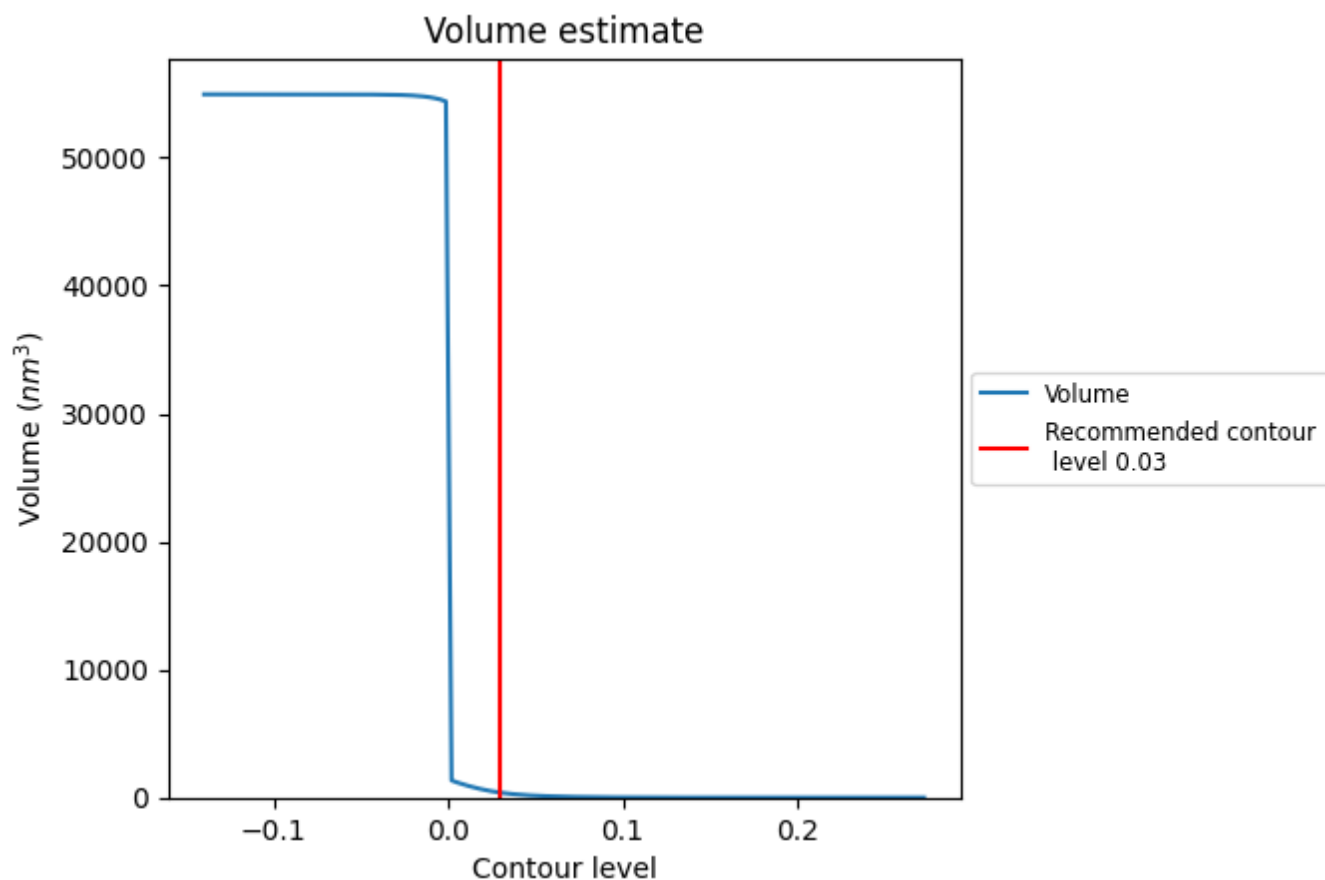
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

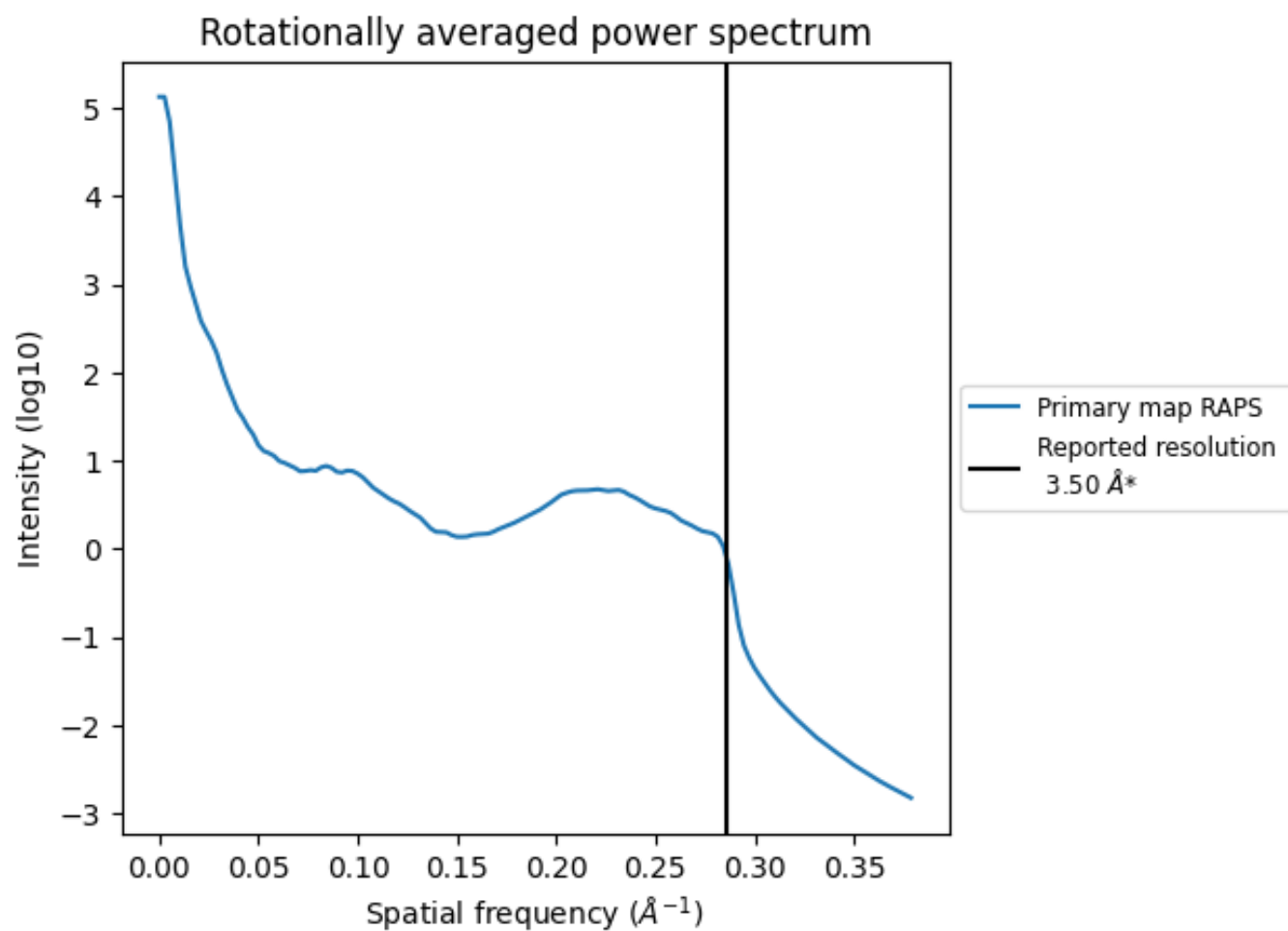
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

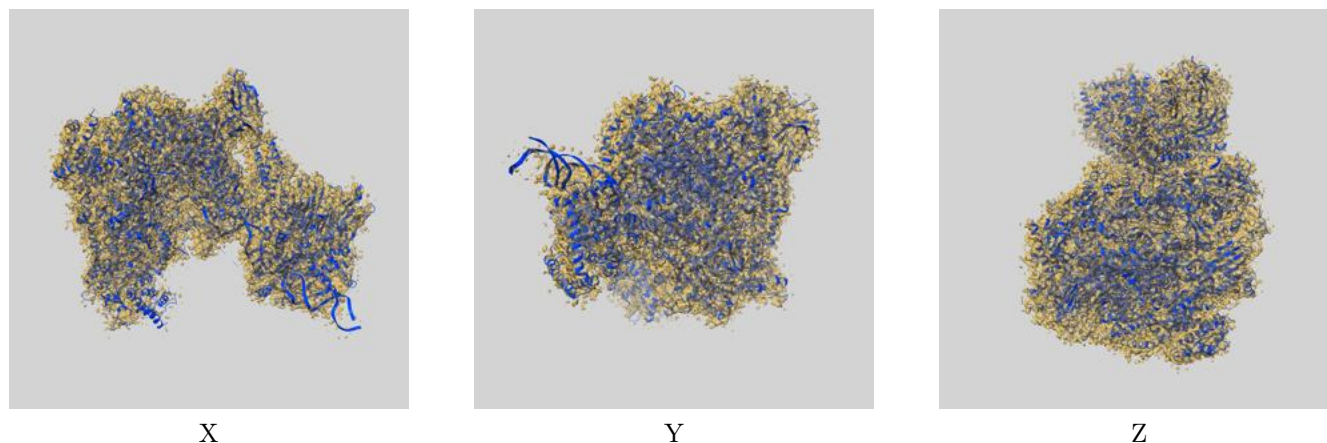
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

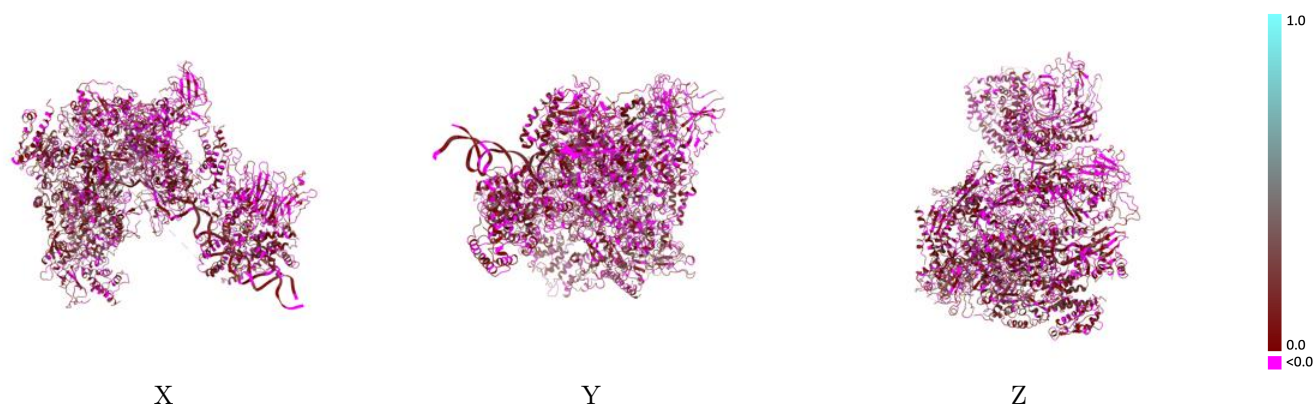
This section contains information regarding the fit between EMDB map EMD-10007 and PDB model 6RUO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



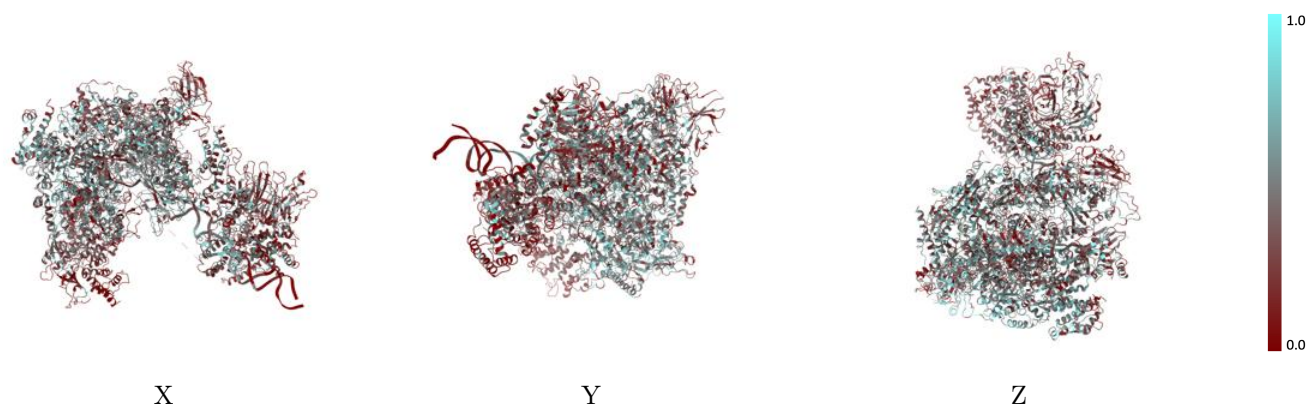
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



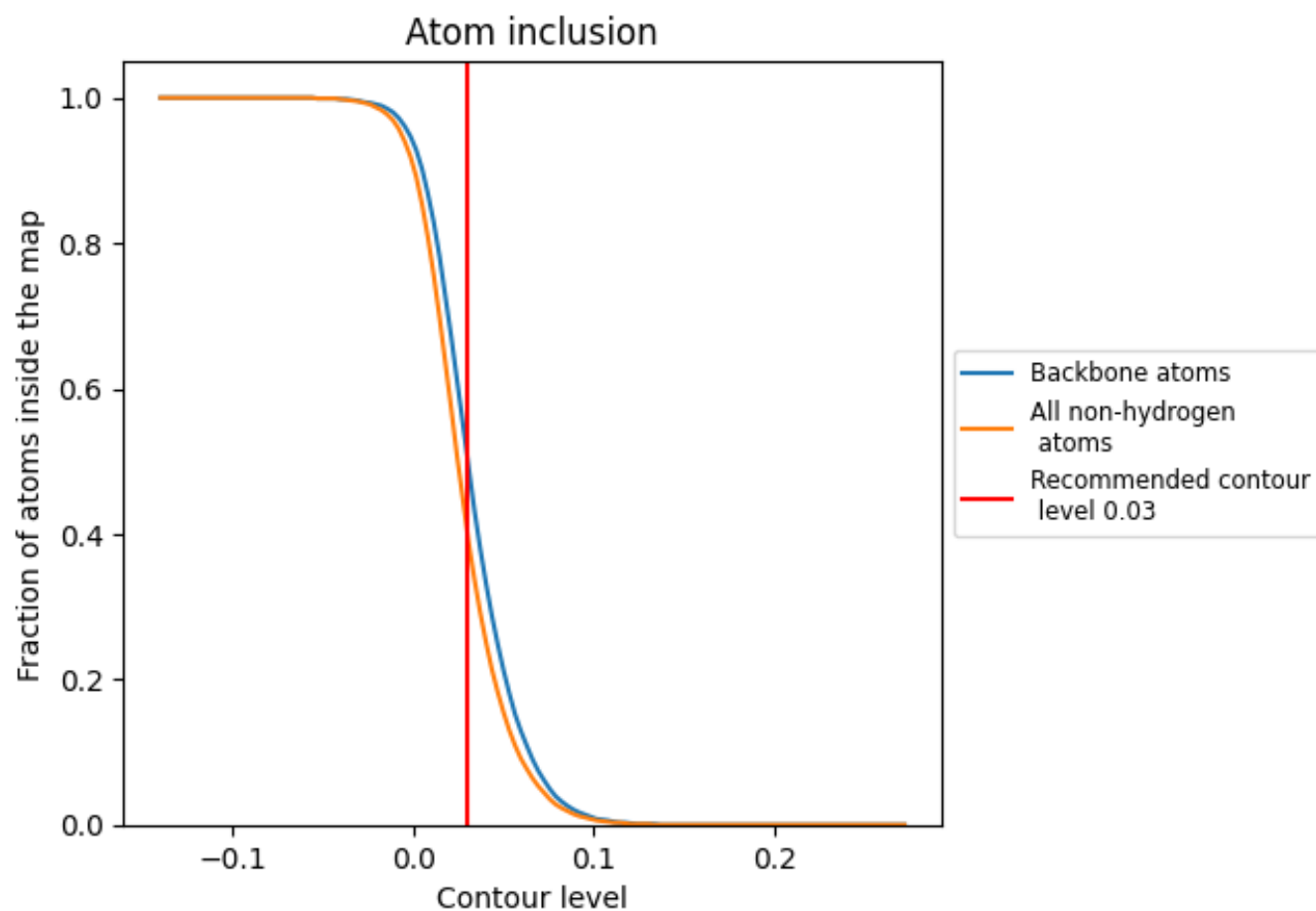
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

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

