



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:30 PM UTC

PDB ID : 6EU1 / pdb_00006eu1
EMDB ID : EMD-3956
Title : RNA Polymerase III - open DNA complex (OC-POL3).
Authors : Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A.
Deposited on : 2017-10-27
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

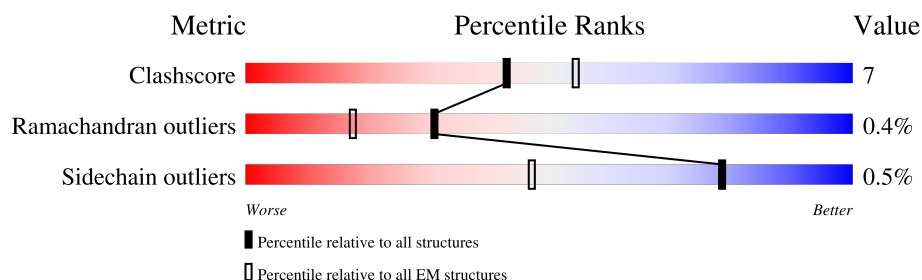
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A	1460	76% 82% 16% ..
2	B	1149	75% 78% 19% .
3	C	335	77% 83% 17%
4	D	161	66% 78% 8% 14%
5	E	215	77% 89% 10% .
6	F	155	41% 49% 5% 46%
7	G	212	77% 81% 18%
8	H	146	84% 88% 12%

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	70	
19	S	70	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 40547 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1433	Total	C	N	O	S	0	0
			11187	7046	1975	2108	58		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1070	679	180	205	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	211	Total	C	N	O	S	0	0
			1690	1093	275	316	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	44	Total	C	N	O	S	0	0
			341	216	53	66	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	104	Total	C	N	O	S	0	0
			815	509	133	168	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	1	0
			366	226	74	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	172	Total	C	N	O	S	0	0
			1402	893	240	268	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			864	547	156	158	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	551	Total	C	N	O	S	0	0
			4426	2815	760	832	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	151	Total	C	N	O	S	0	0
			1210	781	189	236	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	89	Total	C	N	O	S	0	0
			707	448	120	138	1		

- Molecule 18 is a DNA chain called Non-Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	19	Total	C	N	O	P	0	0
			386	184	68	115	19		

- Molecule 19 is a DNA chain called Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	24	Total	C	N	O	P	0	0
			493	234	93	142	24		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	I	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

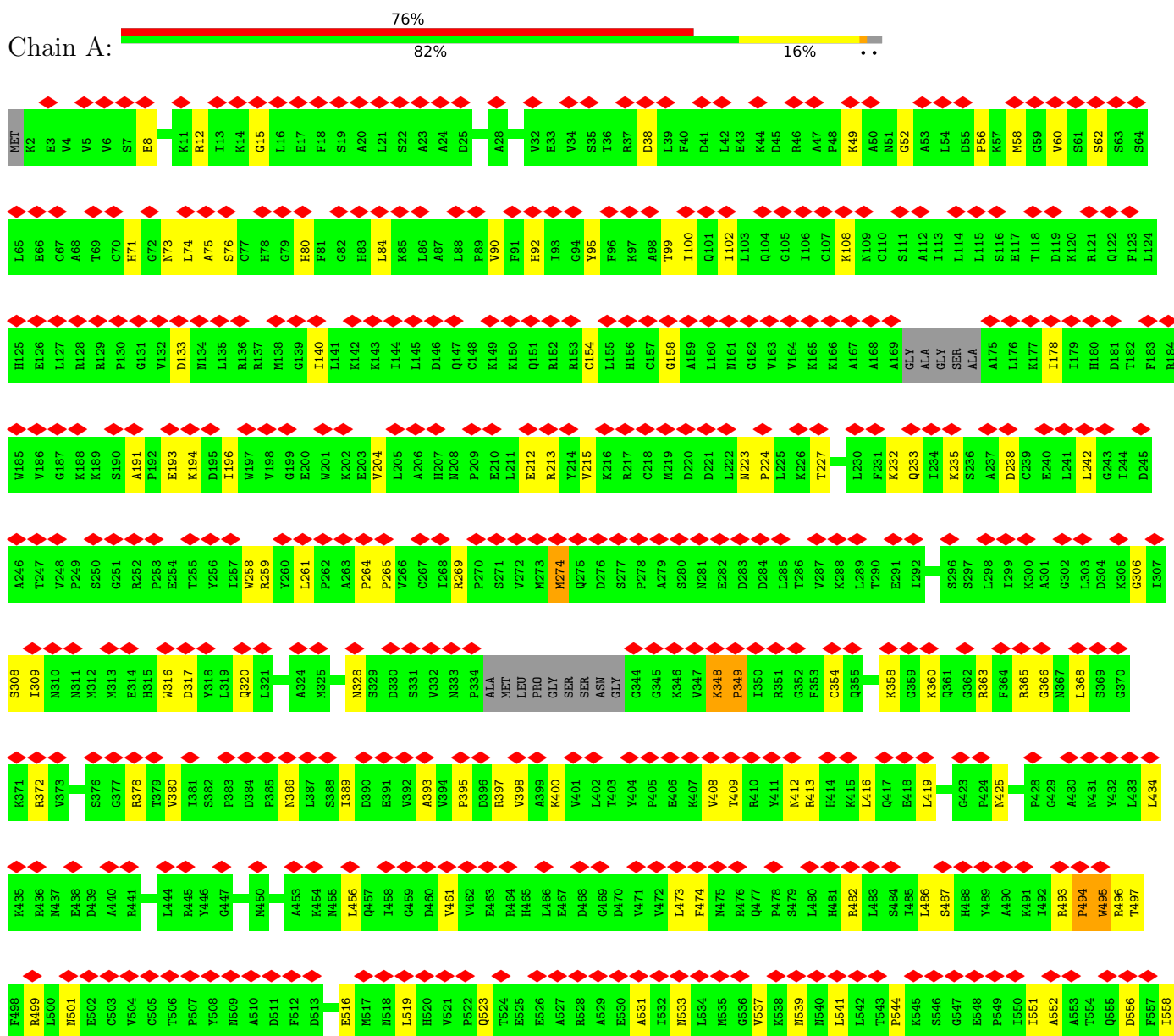
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0

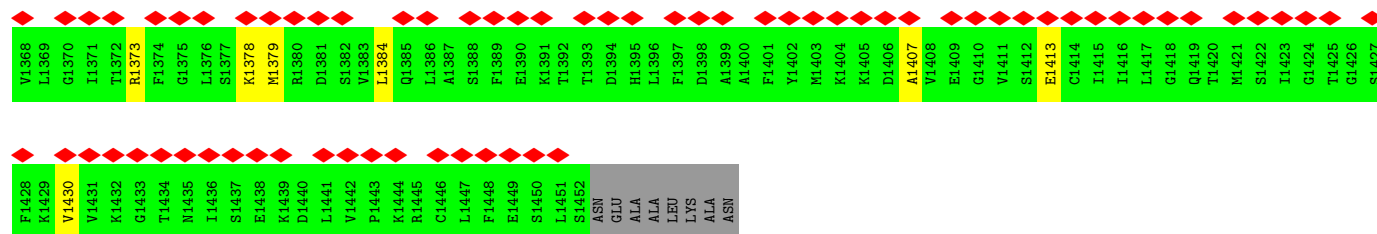
3 Residue-property plots

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.

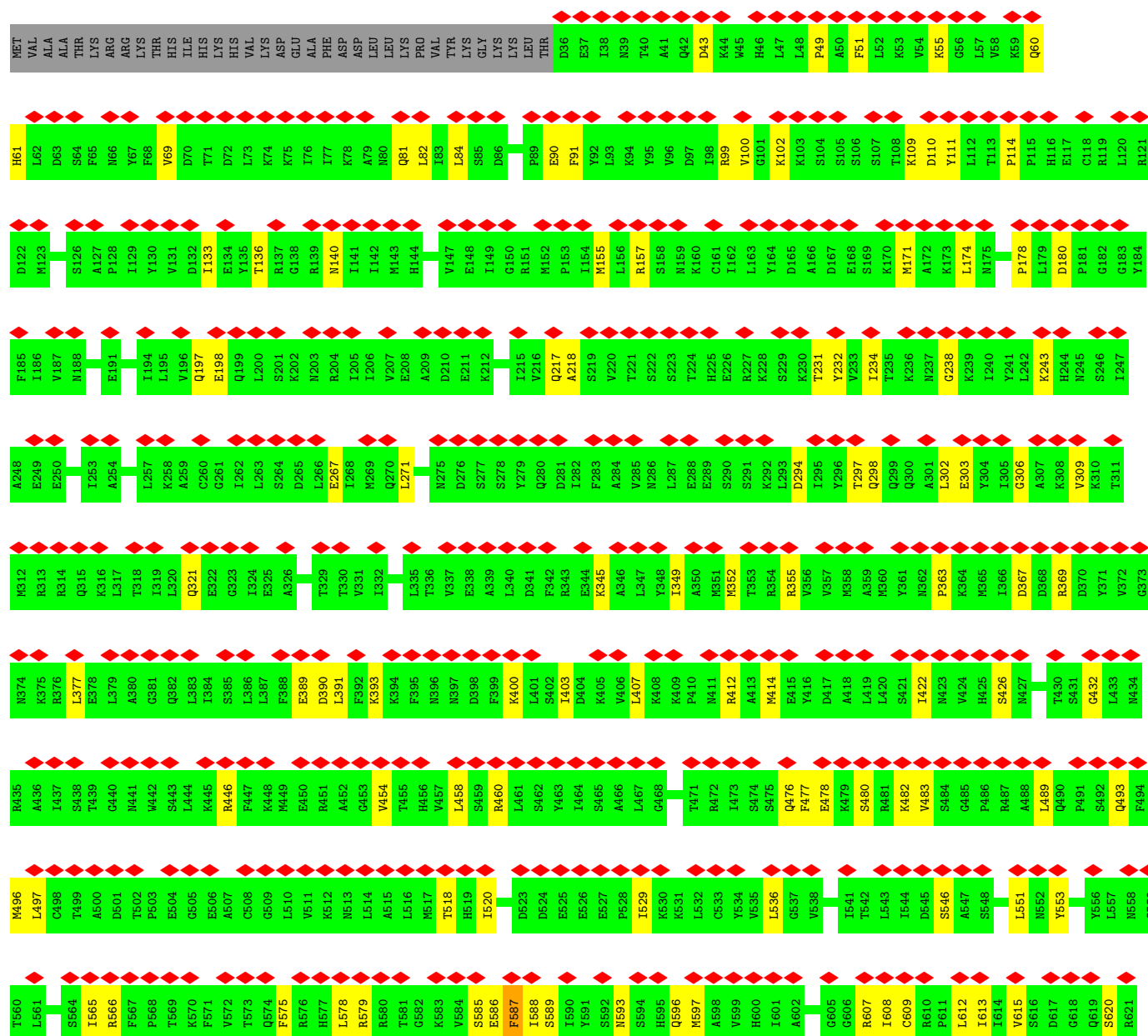
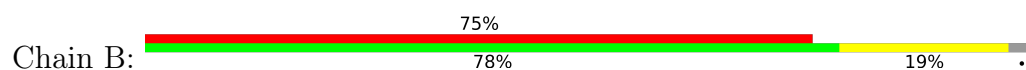
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

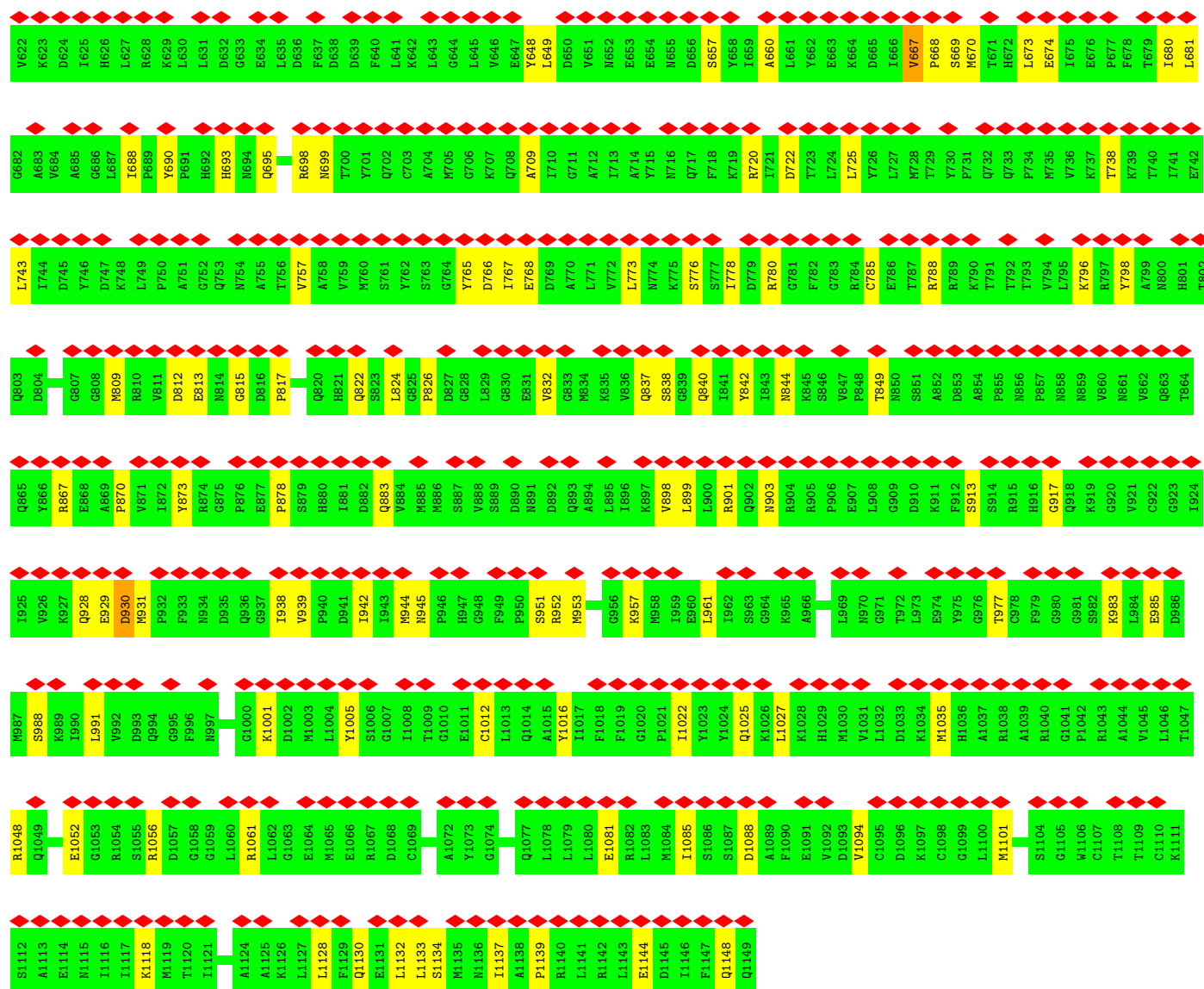


D1307	G1308	V1309	I1310	G1311	S1312	R1313	T1314	T1315	T1316	M1317	H1318	V1319	L1320	E1321	V1322	F1323	G1324	V1325	L1326	E1329	A1330	R1331	R1332	Y1333	S1334	I1335	R1336	R1337	E1338	M1339	M1340	Y1341	T1342	M1343	S1344	M1345	H1346	G1347	M1348	S1349	V1350	D1351	P1352	R1353	H1354	I1355	Q1356	L1357	L1358	G1359	D1360	V1361	M1362	T1363	Y1364	K1365	G1366	E1367		
S1247	A1248	K1249	E1250	P1251	S1252	E1253	N1254	D1255	V1256	F1257	Y1258	R1259	M1260	Q1261	Q1262	L1263	R1264	R1265	A1266	L1267	P1268	D1269	V1270	V1271	V1272	K1273	G1274	L1275	P1276	L1277	D1278	S1279	R1280	A1281	V1282	I1283	N1284	I1285	R1286	D1287	D1288	G1289	K1290	R1291	E1292	L1293	L1294	V1295	E1296	G1297	Y1298	G1299	L1300	R1301	D1302	V1303	M1304	G1305	T1306	
F1183	I1184	R1187	I1188	D1189	G1190	G1191	T1192	I1193	D1194	T1195	L1196	Q1197	L1198	E1199	L1200	T1201	I1202	E1203	D1204	I1205	A1206	T1210	R1211	A1212	S1213	K1214	L1215	K1216	I1217	Q1218	A1219	S1220	D1221	V1222	M1223	I1224	I1225	G1226	K1227	D1228	R1229	I1230	A1231	I1232	M1233	P1236	E1237	G1238	Y1239	K1240	A1241	K1242	S1243	I1244	S1245	T1246				
V1119	T1120	L1121	P1124	R1125	L1126	K1127	E1128	I1129	R1130	N1131	A1132	S1133	K1134	V1135	L1136	S1137	T1138	P1139	I1140	I1141	N1142	L1145	V1146	N1147	D1148	N1149	L1150	E1151	R1152	A1153	A1154	R1155	V1156	G1159	R1160	V1161	E1162	K1163	T1164	L1165	L1166	S1167	D1168	V1169	A1170	F1171	Y1172	D1175	V1176	Y1177	K1178	D1179	N1180	L1181	S1182					
L1059	Y1060	R1061	T1062	S1063	E1064	K1065	S1066	V1067	R1068	K1069	F1070	L1071	E1072	T1073	A1074	L1075	F1076	K1077	Y1078	K1080	A1081	R1082	L1083	E1084	P1085	G1086	A1088	T1087	I1089	G1090	A1091	I1092	G1093	A1094	Q1095	S1096	I1097	G1098	E1099	P1100	G1101	T1102	Q1103	M1104	T1105	L1106	K1107	T1108	F1109	H1110	PHE	ALA	GLY	VAL	A1115	S1116	M1117	N1118		
Q997	Y998	D999	A1000	E1001	R1002	D1003	F1004	Y1005	H1006	S1007	L1008	R1009	E1010	Y1011	I1012	N1013	G1014	K1015	A1016	T1017	A1018	L1019	A1020	N1021	L1022	R1023	K1024	S1025	R1026	G1027	M1028	L1029	G1030	L1031	L1032	E1033	P1034	P1035	A1036	K1037	E1038	L1039	Q1040	G1041	I1042	D1043	P1044	D1045	E1046	T1047	V1048	P1049	D1050	K991	A992	E993	Y994	V995	D996	
R937	S938	N939	D940	H941	A942	Y943	N944	T945	T946	F947	N948	N949	Q950	D951	K952	Q953	L954	L955	P956	Y957	A958	I959	M960	E961	T962	A963	N964	E965	L966	G968	P969	L970	E971	E972	R973	L974	N975	R976	Y977	D978	N979	S980	G981	C982	L983	N984	K985	R986	E987	D988	L989	N990	K991	A992	E993	Y994	V995	D996		
V873	D874	Q875	A876	V877	K878	T879	A880	E881	T882	M885	S886	R887	R888	L889	M890	K891	S892	L893	L896	S897	Q898	Q899	Y900	D901	S903	T903	Y904	R905	A908	I911	V912	Q913	F914	T915	Y916	G917	G918	D919	G920	L921	D922	P923	L924	E925	M926	E927	G928	N929	A930	Q931	P932	V933	N934	F935	N936					
V813	G814	Q815	Q816	I817	T818	S819	G820	N821	R822	V823	P824	D825	G826	F827	Q828	D829	R830	S831	L832	P833	H834	F835	P836	N838	S839	K840	T841	P842	Q843	S844	K845	G846	F847	V848	R849	N850	S851	F852	F853	S854	G855	L856	S857	P858	P859	E860	F861	L862	F863	H864	S865	L866	Q867	G868	R869	E870	G871	L872		
E749	L750	E751	T752	Q753	P754	G755	C756	N757	E758	T761	L762	E763	A764	K765	I766	G767	G768	L769	L770	S771	K772	V773	R774	E775	E776	V777	D778	T779	V780	I782	N783	E784	D786	N787	M788	N789	L792	I793	M794	A795	T796	S799	K800	T803	L804	N805	V806	S807	Q808	F809	E810	K811	L812	L813	H814	K815	P816	N817	H818	N819
S620	V623	I624	N625	L626	D627	A628	K629	M630	S631	V632	F633	V634	P635	P636	K637	S638	K639	S640	L641	P642	N643	E644	M645	S646	Q647	N648	D649	G650	F651	V652	I654	R655	G658	I659	L660	S661	C662	V663	M664	D665	K666	V668	L669	G670	D671	G672	K673	K674	H675	S676	P677	F678	Y679	T680	I681					
L682	R683	D684	E689	A690	N691	N692	A693	M694	R695	R696	M697	L700	C701	F704	L705	G706	N707	L708	P709	N710	E711	S712	S713	G714	I715	D716	A720	D721	D722	L723	K724	Q725	K726	K727	E728	E729	L730	V731	E732	I733	A734	Y735	H736	K737	C738	D739	E740	L741	H742	T743	L744	F745	N746	K747	G748					

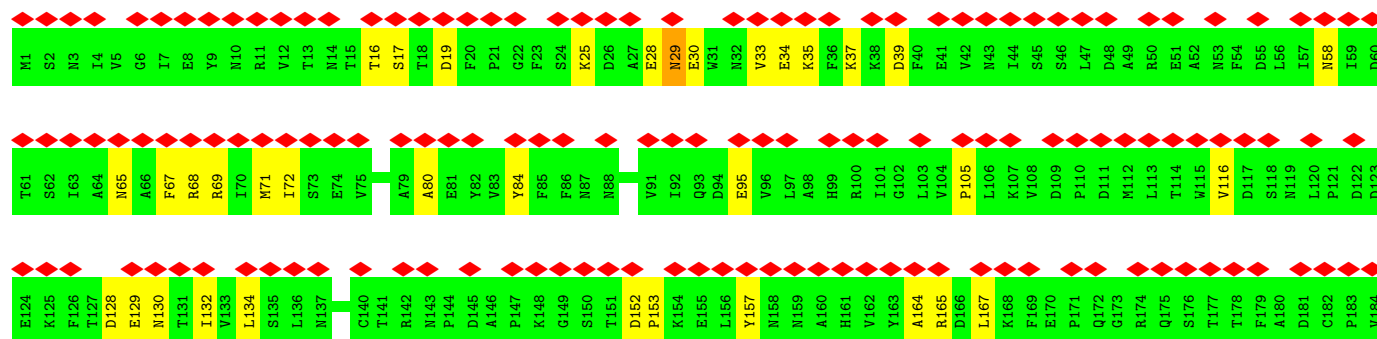
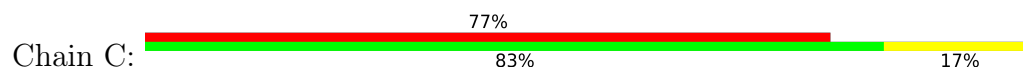


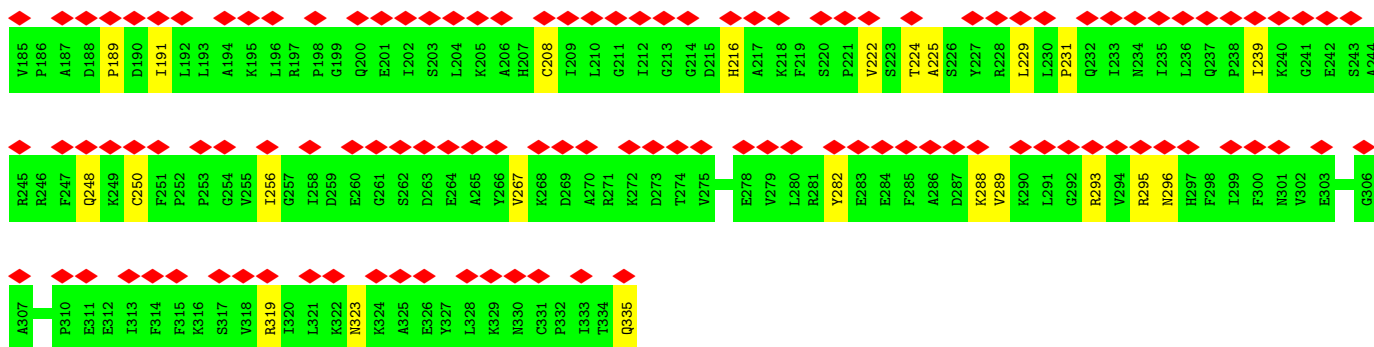
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



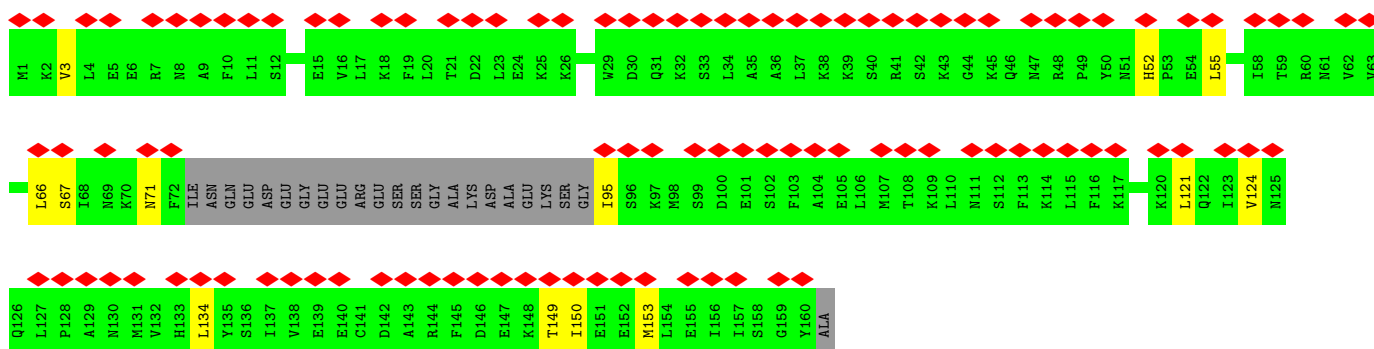
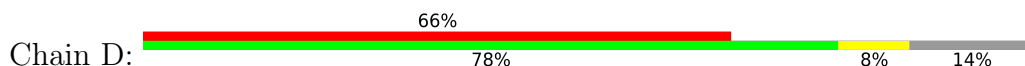


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

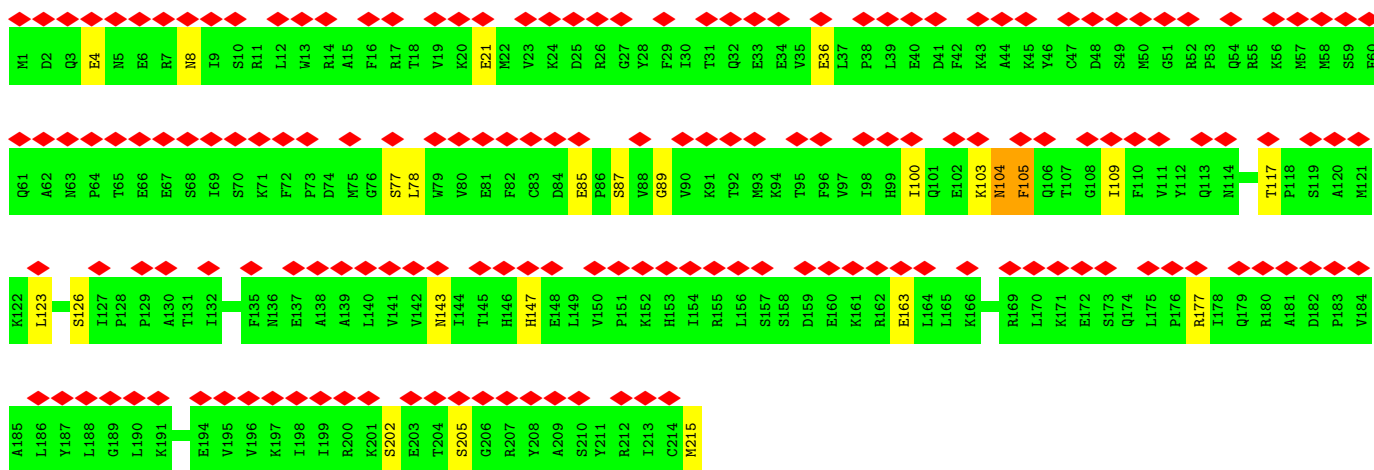
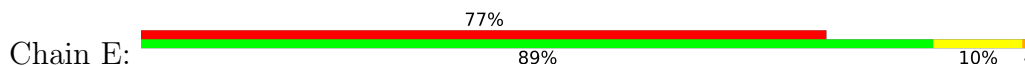




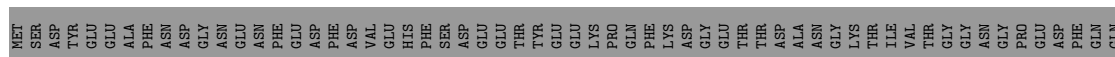
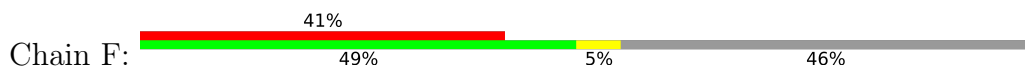
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

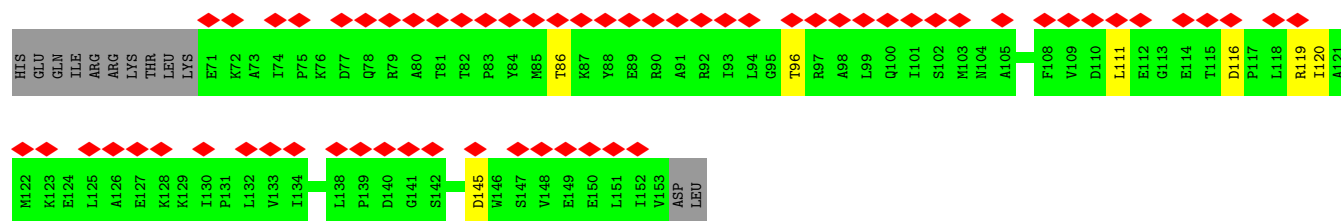


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

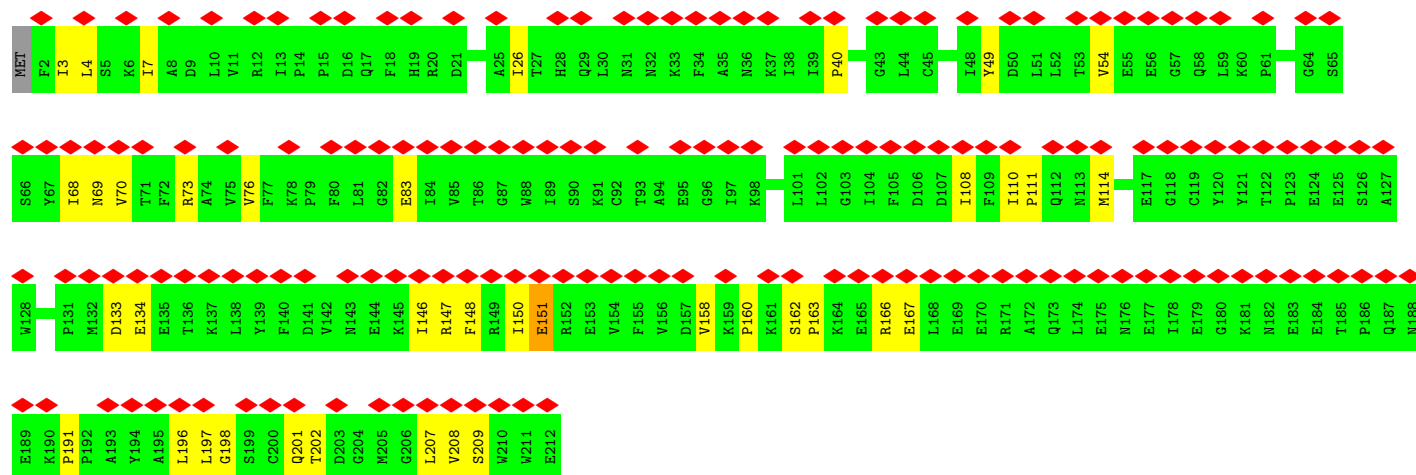
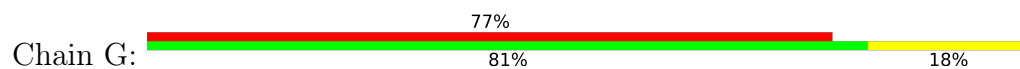


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

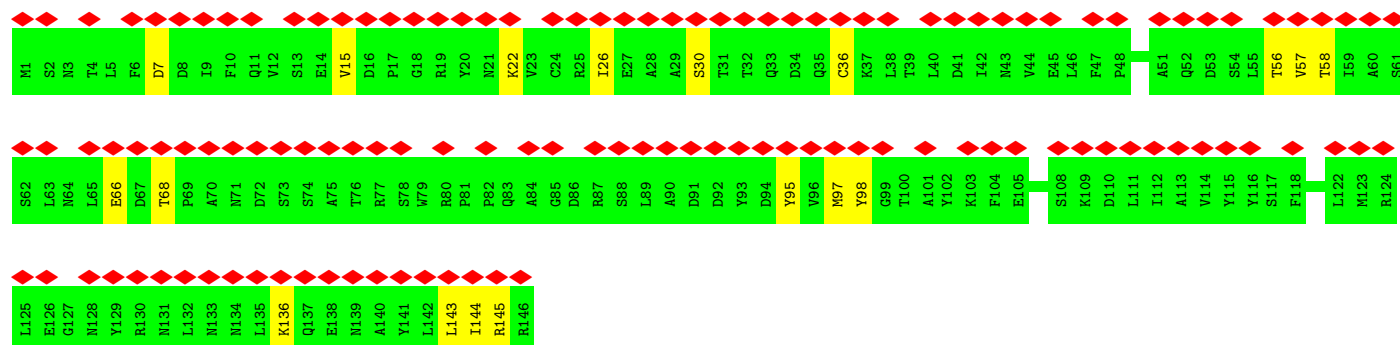
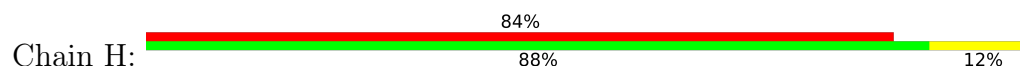




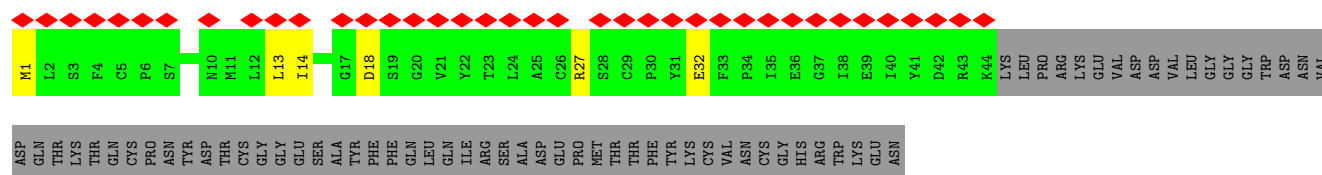
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



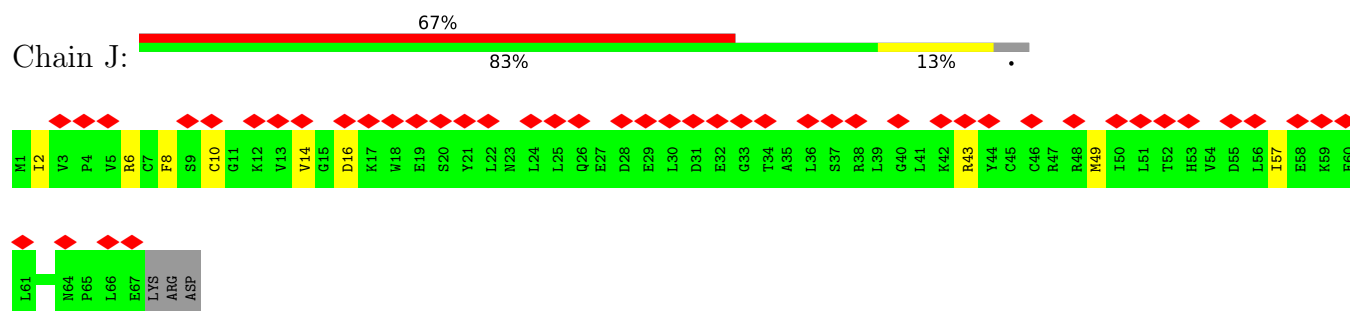
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



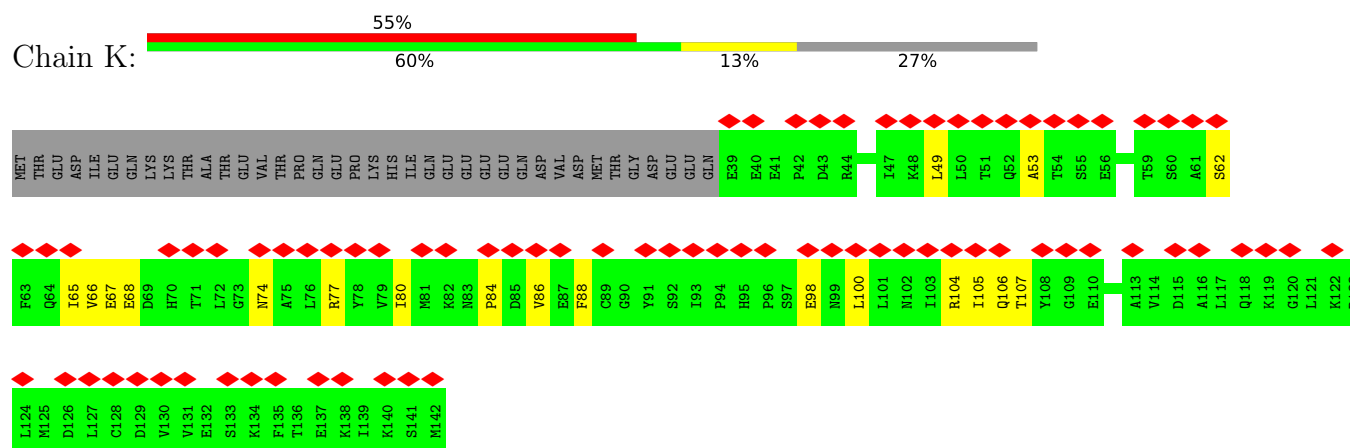
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10



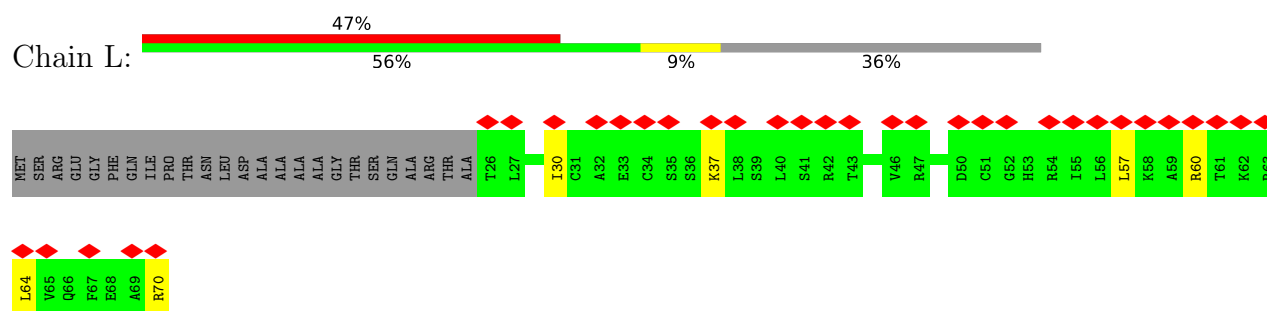
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

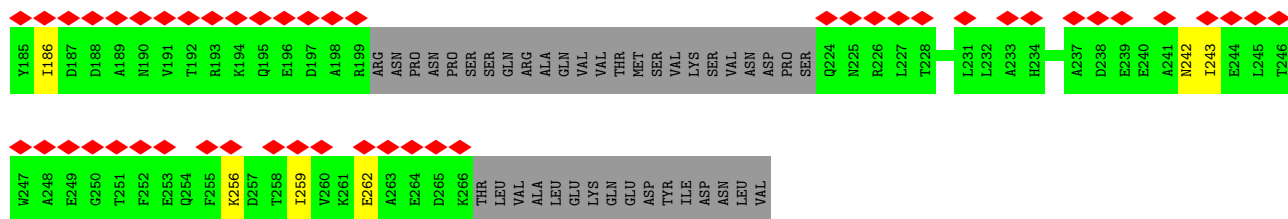


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

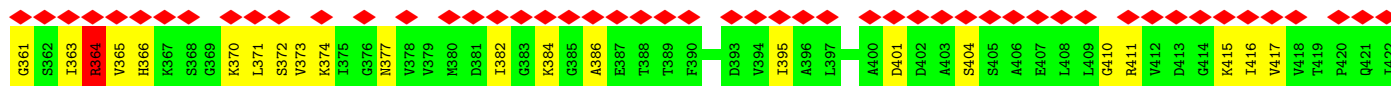
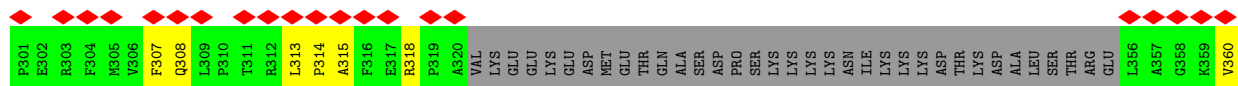
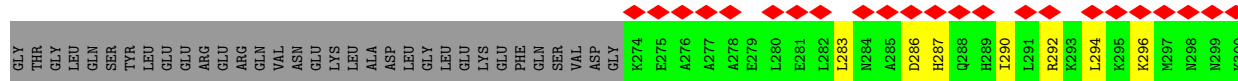
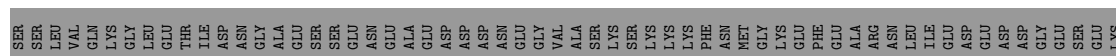
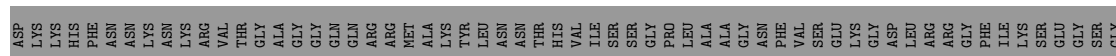
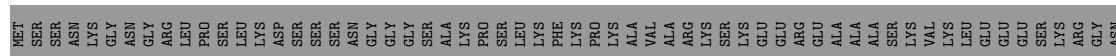


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

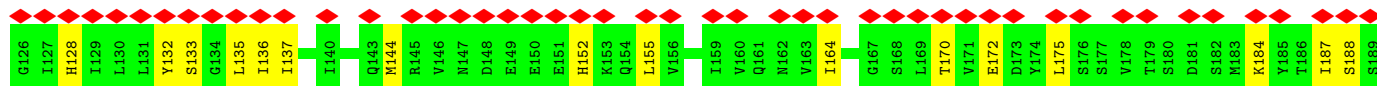
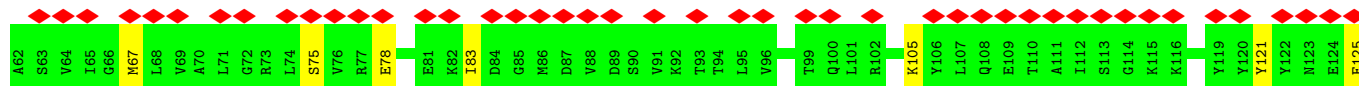
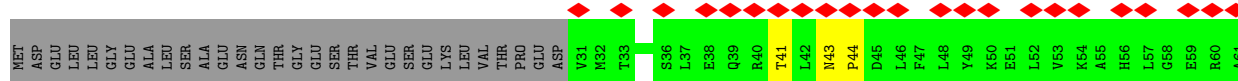


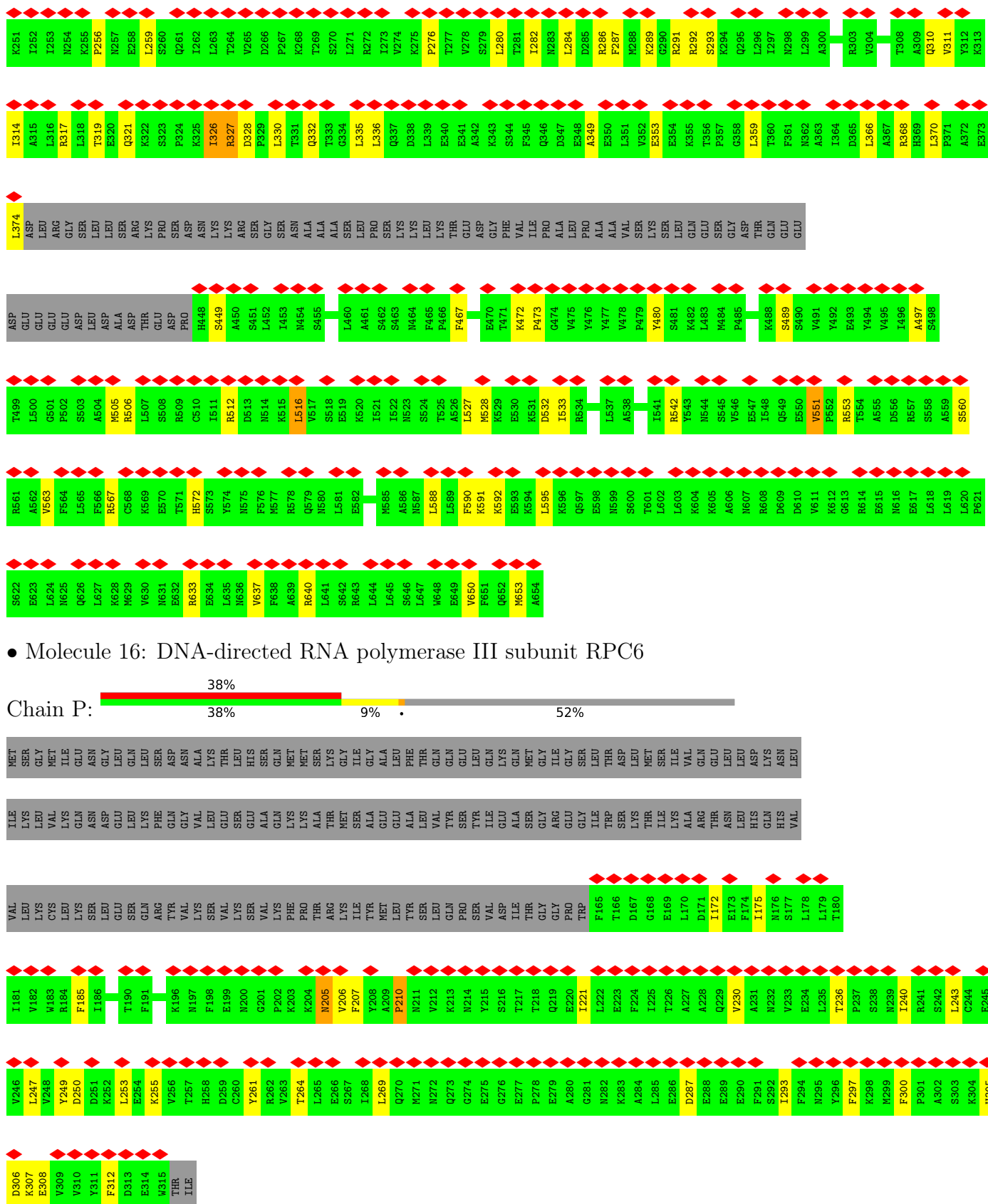


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4



• Molecule 15: DNA-directed RNA polymerase III subunit RPC3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100237	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 ($e^-/\text{\AA}^2$)	40	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	0.396	Depositor
Minimum map value	-0.249	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	323.4, 323.4, 323.4	wwPDB
Map dimensions	308, 308, 308	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.24	0/11385	0.65	9/15382 (0.1%)
2	B	0.23	0/8943	0.64	4/12068 (0.0%)
3	C	0.21	0/2711	0.62	0/3676
4	D	0.16	0/1088	0.46	0/1455
5	E	0.25	1/1795 (0.1%)	0.60	4/2416 (0.2%)
6	F	0.21	0/683	0.56	0/923
7	G	0.26	0/1732	0.70	4/2352 (0.2%)
8	H	0.20	0/1181	0.58	0/1602
9	I	0.21	0/348	0.55	0/470
10	J	0.26	0/558	0.74	1/750 (0.1%)
11	K	0.23	0/826	0.64	0/1115
12	L	0.22	0/371	0.65	0/492
13	M	0.27	0/1433	0.78	5/1936 (0.3%)
14	N	0.23	0/874	0.73	1/1175 (0.1%)
15	O	0.25	0/4493	0.65	0/6062
16	P	0.26	0/1239	0.76	2/1682 (0.1%)
17	Q	0.27	0/719	0.78	2/966 (0.2%)
18	R	0.18	0/431	0.39	0/662
19	S	0.21	0/553	0.40	0/851
All	All	0.24	1/41363 (0.0%)	0.65	32/56035 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
2	B	0	6
3	C	0	2
5	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
13	M	0	2
15	O	0	6
16	P	0	4
17	Q	0	1
All	All	0	32

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	36	GLU	CA-CB	5.64	1.61	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	LYS	CA-C-N	6.85	134.62	121.54
1	A	666	LYS	C-N-CA	6.85	134.62	121.54
1	A	274	MET	CA-C-N	6.75	132.28	122.36
1	A	274	MET	C-N-CA	6.75	132.28	122.36
1	A	349	PRO	N-CA-CB	6.65	110.24	103.25
16	P	240	ILE	N-CA-C	-6.44	106.45	112.83
1	A	348	LYS	CA-C-N	6.11	127.47	119.84
1	A	348	LYS	C-N-CA	6.11	127.47	119.84
16	P	230	VAL	N-CA-C	-5.95	106.61	111.91
10	J	14	VAL	N-CA-C	-5.93	108.08	113.71
17	Q	41	LEU	N-CA-C	5.88	122.80	109.81
14	N	410	GLY	N-CA-C	5.63	126.53	113.18
5	E	104	ASN	CA-C-N	5.62	132.28	121.54
5	E	104	ASN	C-N-CA	5.62	132.28	121.54
13	M	77	LYS	CA-C-N	-5.40	116.49	123.19
13	M	77	LYS	C-N-CA	-5.40	116.49	123.19
13	M	118	LEU	CA-CB-CG	5.37	135.11	116.30
13	M	242	ASN	CA-C-N	5.35	131.60	121.97
13	M	242	ASN	C-N-CA	5.35	131.60	121.97
2	B	43	ASP	CA-C-N	5.28	131.62	121.54
2	B	43	ASP	C-N-CA	5.28	131.62	121.54
5	E	103	LYS	CA-C-N	5.20	131.48	121.54
5	E	103	LYS	C-N-CA	5.20	131.48	121.54
17	Q	45	GLY	N-CA-C	5.20	122.94	112.34
7	G	40	PRO	CA-C-N	5.13	131.33	121.54
7	G	40	PRO	C-N-CA	5.13	131.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1243	SER	CA-C-N	5.02	131.01	121.97
1	A	1243	SER	C-N-CA	5.02	131.01	121.97
7	G	151	GLU	CA-C-N	5.02	131.13	121.54
7	G	151	GLU	C-N-CA	5.02	131.13	121.54
2	B	551	LEU	CA-C-N	5.01	131.12	121.54
2	B	551	LEU	C-N-CA	5.01	131.12	121.54

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	PRO	Peptide
1	A	1267	LEU	Peptide
1	A	233	GLN	Peptide
1	A	274	MET	Peptide
1	A	306	GLY	Peptide
1	A	494	PRO	Peptide
1	A	600	PRO	Peptide
1	A	667	SER	Peptide
2	B	109	LYS	Peptide
2	B	110	ASP	Peptide
2	B	363	PRO	Peptide
2	B	587	PHE	Peptide
2	B	813	GLU	Peptide
2	B	930	ASP	Peptide
3	C	128	ASP	Peptide
3	C	29	ASN	Peptide
5	E	105	PHE	Peptide
7	G	114	MET	Peptide
8	H	136	LYS	Peptide
13	M	116	SER	Peptide
13	M	174	GLU	Peptide
15	O	327	ARG	Peptide
15	O	328	ASP	Peptide
15	O	467	PHE	Peptide
15	O	472	LYS	Peptide
15	O	551	VAL	Peptide
15	O	560	SER	Peptide
16	P	205	ASN	Peptide
16	P	210	PRO	Peptide
16	P	236	THR	Peptide
16	P	255	LYS	Peptide

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Mol	Chain	Res	Type	Group
17	Q	41	LEU	Peptide

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	A	11187	0	11278	146	0
2	B	8788	0	8904	137	0
3	C	2655	0	2628	39	0
4	D	1070	0	1023	7	0
5	E	1759	0	1788	13	0
6	F	671	0	692	5	0
7	G	1690	0	1660	22	0
8	H	1161	0	1124	10	0
9	I	341	0	332	5	0
10	J	549	0	562	7	0
11	K	815	0	803	13	0
12	L	366	0	396	5	0
13	M	1402	0	1365	70	0
14	N	864	0	903	56	0
15	O	4426	0	4594	60	0
16	P	1210	0	1131	17	0
17	Q	707	0	724	6	0
18	R	386	0	215	0	0
19	S	493	0	270	5	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	1	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	40547	0	40392	531	0

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

All (531) 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)
13:M:74:PHE:CE2	14:N:294:LEU:HD21	1.26	1.62
13:M:75:PRO:HG3	13:M:166:MET:SD	1.39	1.61
13:M:74:PHE:CZ	14:N:294:LEU:HD21	1.53	1.40
13:M:74:PHE:CE2	14:N:294:LEU:CD2	2.16	1.27
13:M:76:LEU:HB3	14:N:361:GLY:HA2	1.28	1.15
13:M:72:GLU:O	14:N:364:ARG:HB3	1.45	1.14
13:M:75:PRO:CG	13:M:166:MET:SD	2.35	1.14
14:N:364:ARG:NH1	14:N:374:LYS:HG2	1.63	1.11
14:N:364:ARG:NH1	14:N:374:LYS:CG	2.14	1.11
13:M:74:PHE:CZ	14:N:294:LEU:CD2	2.37	1.07
13:M:75:PRO:CD	13:M:166:MET:HG2	1.87	1.03
14:N:364:ARG:HH11	14:N:374:LYS:HG3	1.23	1.03
14:N:364:ARG:HH11	14:N:374:LYS:CG	1.70	1.03
13:M:76:LEU:HD13	13:M:168:VAL:HG12	1.41	1.01
13:M:75:PRO:HG3	13:M:166:MET:CG	1.90	0.99
14:N:283:LEU:O	14:N:287:HIS:HB2	1.63	0.99
15:O:349:ALA:O	15:O:353:GLU:HB2	1.62	0.99
13:M:74:PHE:HE2	14:N:294:LEU:HD21	1.31	0.91
13:M:76:LEU:O	14:N:360:VAL:O	1.90	0.90
13:M:75:PRO:CG	13:M:166:MET:HG2	2.06	0.86
13:M:75:PRO:CG	13:M:166:MET:CG	2.54	0.85
13:M:72:GLU:O	14:N:364:ARG:CB	2.26	0.83
13:M:164:LYS:O	13:M:166:MET:N	2.12	0.82
13:M:74:PHE:HE2	14:N:294:LEU:CD2	1.85	0.81
13:M:76:LEU:HD23	14:N:363:ILE:HG23	1.64	0.80
13:M:76:LEU:HD23	14:N:363:ILE:CG2	2.14	0.76
2:B:403:ILE:O	2:B:407:LEU:HB2	1.85	0.76
13:M:75:PRO:HG2	13:M:167:GLN:N	2.01	0.76
13:M:76:LEU:HD13	13:M:168:VAL:CG1	2.14	0.76
13:M:77:LYS:HD3	13:M:262:GLU:HB2	1.68	0.73
14:N:371:LEU:HB3	14:N:384:LYS:HZ3	1.56	0.70
13:M:77:LYS:HD3	13:M:262:GLU:CG	2.22	0.69
13:M:164:LYS:C	13:M:166:MET:N	2.48	0.69
1:A:597:ILE:HG22	8:H:97:MET:HG2	1.75	0.69
1:A:556:ASP:HB2	2:B:767:ILE:HG12	1.74	0.69
2:B:612:LEU:HD12	2:B:649:LEU:HD12	1.75	0.68
13:M:74:PHE:CZ	14:N:294:LEU:CG	2.76	0.67
5:E:100:ILE:HG22	5:E:104:ASN:HD22	1.59	0.66
2:B:695:GLN:HG2	2:B:953:MET:HB2	1.78	0.66
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.78	0.65
13:M:75:PRO:HD2	13:M:166:MET:HG2	1.77	0.65
13:M:76:LEU:CD2	14:N:363:ILE:HG21	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ARG:HH11	2:B:720:ARG:HH22	1.45	0.64
13:M:76:LEU:HD22	14:N:363:ILE:HD13	1.78	0.64
13:M:154:GLU:HB2	13:M:175:ARG:HG3	1.79	0.64
15:O:330:LEU:HD23	15:O:332:GLN:H	1.63	0.64
14:N:364:ARG:HH12	14:N:374:LYS:HG2	1.55	0.64
13:M:77:LYS:HD3	13:M:262:GLU:CB	2.29	0.63
13:M:164:LYS:C	13:M:166:MET:H	2.06	0.63
16:P:253:LEU:HD12	16:P:261:TYR:HB3	1.81	0.63
13:M:77:LYS:HD3	13:M:262:GLU:CD	2.24	0.63
5:E:177:ARG:NH1	5:E:215:MET:SD	2.72	0.62
14:N:364:ARG:HD3	14:N:372:SER:OG	1.99	0.62
14:N:364:ARG:HH12	14:N:374:LYS:HE2	1.64	0.61
5:E:89:GLY:HA2	5:E:117:THR:HG21	1.82	0.61
1:A:567:LYS:NZ	1:A:649:ASP:OD1	2.34	0.61
14:N:364:ARG:NH1	14:N:374:LYS:CE	2.63	0.61
14:N:366:HIS:HB3	14:N:370:LYS:HB3	1.82	0.61
10:J:8:PHE:H	10:J:49:MET:HE1	1.65	0.60
2:B:114:PRO:HB3	2:B:174:LEU:HD12	1.83	0.60
1:A:599:LYS:HE2	3:C:25:LYS:HD2	1.82	0.60
13:M:164:LYS:O	13:M:165:ASP:C	2.45	0.60
14:N:363:ILE:HG22	14:N:373:VAL:HG23	1.84	0.60
1:A:58:MET:HA	1:A:80:HIS:HB2	1.83	0.60
2:B:722:ASP:HB2	2:B:725:LEU:HD22	1.84	0.60
1:A:473:LEU:HD13	1:A:487:SER:HB3	1.82	0.60
15:O:650:VAL:HA	15:O:653:MET:HE2	1.84	0.60
13:M:164:LYS:NZ	13:M:169:TYR:OH	2.35	0.59
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.82	0.59
15:O:310:GLN:HG2	15:O:374:LEU:HD13	1.83	0.59
1:A:568:ASP:HB2	8:H:22:LYS:HE3	1.84	0.59
3:C:16:THR:O	3:C:295:ARG:NH1	2.36	0.59
3:C:116:VAL:HA	3:C:130:ASN:HD21	1.66	0.59
10:J:10:CYS:SG	10:J:43:ARG:NH1	2.76	0.59
13:M:76:LEU:HB3	14:N:361:GLY:CA	2.18	0.59
13:M:77:LYS:CD	13:M:262:GLU:CD	2.75	0.59
2:B:1132:LEU:HD22	2:B:1137:ILE:HD11	1.84	0.59
2:B:1148:GLN:NE2	7:G:69:ASN:OD1	2.36	0.59
13:M:75:PRO:HD3	13:M:166:MET:HG2	1.80	0.59
13:M:76:LEU:CD2	14:N:363:ILE:CG2	2.80	0.59
14:N:364:ARG:N	14:N:364:ARG:HD2	2.17	0.59
15:O:592:LYS:HB2	15:O:637:VAL:HG11	1.83	0.59
2:B:837:GLN:HB3	2:B:878:PRO:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:75:PRO:HG2	13:M:167:GLN:CA	2.33	0.58
13:M:74:PHE:CZ	14:N:294:LEU:HD11	2.38	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.85	0.58
15:O:175:LEU:HD13	15:O:184:LYS:HE2	1.86	0.58
7:G:110:ILE:HD13	7:G:198:GLY:H	1.68	0.58
15:O:128:HIS:O	15:O:132:TYR:HB2	2.04	0.58
1:A:587:ILE:HG12	11:K:53:ALA:HB2	1.86	0.58
5:E:100:ILE:O	5:E:104:ASN:ND2	2.37	0.58
8:H:57:VAL:HA	8:H:144:ILE:HG22	1.86	0.58
1:A:49:LYS:HG2	1:A:56:PRO:HD3	1.85	0.57
1:A:1365:LYS:NZ	1:A:1379:MET:SD	2.76	0.57
2:B:298:GLN:HG2	2:B:302:LEU:HD13	1.86	0.57
2:B:377:LEU:HD11	2:B:520:ILE:HD13	1.86	0.57
1:A:1384:LEU:HB2	1:A:1413:GLU:HG2	1.86	0.57
2:B:667:VAL:HG13	2:B:669:SER:H	1.69	0.57
2:B:99:ARG:HG3	2:B:102:LYS:HB3	1.86	0.57
13:M:155:ASN:HB3	13:M:158:GLN:HE22	1.70	0.56
1:A:541:LEU:HD22	1:A:551:ILE:HD11	1.87	0.56
15:O:640:ARG:NH2	16:P:306:ASP:O	2.37	0.56
1:A:360:LYS:H	1:A:365:ARG:HG2	1.70	0.56
2:B:303:GLU:HG2	2:B:321:GLN:HG3	1.87	0.56
1:A:713:GLY:HA3	2:B:1001:LYS:HD2	1.86	0.56
13:M:158:GLN:HG2	13:M:173:ILE:HG21	1.87	0.56
1:A:808:GLN:HE21	1:A:813:VAL:HG13	1.70	0.56
2:B:883:GLN:HE22	12:L:57:LEU:HD22	1.70	0.56
2:B:197:GLN:HE21	2:B:454:VAL:HG23	1.70	0.56
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.87	0.56
1:A:533:ASN:O	1:A:539:ASN:ND2	2.38	0.56
15:O:489:SER:OG	15:O:512:ARG:NH1	2.39	0.56
4:D:67:SER:HB3	4:D:71:ASN:HD21	1.71	0.56
14:N:364:ARG:HH12	14:N:374:LYS:CE	2.18	0.56
1:A:71:HIS:ND1	7:G:167:GLU:OE1	2.39	0.56
15:O:286:ARG:HH21	15:O:321:GLN:HB3	1.70	0.55
16:P:243:LEU:O	16:P:247:LEU:HB2	2.06	0.55
2:B:480:SER:OG	2:B:483:VAL:O	2.24	0.55
2:B:593:ASN:ND2	2:B:596:GLN:OE1	2.40	0.55
6:F:116:ASP:OD2	6:F:119:ARG:NH1	2.39	0.55
2:B:607:ARG:NH1	2:B:609:CYS:SG	2.80	0.55
1:A:413:ARG:NH1	1:A:456:LEU:O	2.40	0.55
1:A:60:VAL:HG12	1:A:62:SER:H	1.72	0.55
11:K:66:VAL:HG22	11:K:67:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:ARG:NH2	1:A:1228:ASP:OD2	2.39	0.55
1:A:73:ASN:H	1:A:76:SER:HB3	1.72	0.54
1:A:976:ARG:NH1	1:A:989:LEU:O	2.40	0.54
14:N:313:LEU:HD12	14:N:377:ASN:HD22	1.73	0.54
3:C:34:GLU:HB2	3:C:37:LYS:HB3	1.90	0.54
12:L:30:ILE:HG13	12:L:37:LYS:HG2	1.90	0.54
2:B:773:LEU:HG	2:B:942:ILE:HG12	1.90	0.54
17:Q:98:GLU:H	17:Q:102:ASN:HD22	1.56	0.54
1:A:830:ARG:NH2	2:B:657:SER:O	2.40	0.54
2:B:812:ASP:HB3	2:B:815:GLY:HA3	1.90	0.54
1:A:400:LYS:NZ	1:A:425:ASN:O	2.41	0.54
2:B:944:MET:SD	2:B:957:LYS:NZ	2.70	0.54
2:B:660:ALA:HB2	2:B:670:MET:HG2	1.90	0.54
2:B:849:THR:HB	2:B:867:ARG:HB2	1.90	0.54
3:C:239:ILE:HD11	3:C:288:LYS:HE2	1.91	0.53
14:N:386:ALA:HB2	14:N:417:VAL:HG13	1.90	0.53
2:B:688:ILE:HD13	2:B:699:ASN:HD22	1.72	0.53
1:A:487:SER:OG	1:A:531:ALA:O	2.24	0.53
16:P:253:LEU:HB3	16:P:261:TYR:HD1	1.73	0.53
1:A:92:HIS:HB3	1:A:95:TYR:HB2	1.91	0.53
1:A:923:PRO:HA	1:A:926:MET:HE2	1.89	0.53
2:B:422:ILE:O	2:B:426:SER:N	2.40	0.53
7:G:4:LEU:HD21	7:G:73:ARG:HD3	1.90	0.53
11:K:65:ILE:HD13	11:K:68:GLU:HB2	1.90	0.53
1:A:1335:ILE:HD13	1:A:1362:MET:HE3	1.89	0.53
2:B:738:THR:HG23	2:B:977:THR:HA	1.89	0.53
2:B:776:SER:O	2:B:780:ARG:NH1	2.42	0.53
15:O:172:GLU:HB3	15:O:276:PRO:HB3	1.91	0.53
15:O:542:ARG:NH1	16:P:312:PHE:O	2.36	0.53
16:P:207:PHE:HB2	16:P:210:PRO:HB3	1.89	0.53
3:C:65:ASN:HD21	3:C:68:ARG:HH21	1.56	0.53
15:O:292:ARG:HD2	15:O:327:ARG:HH11	1.74	0.53
1:A:1430:VAL:HG11	6:F:96:THR:HG21	1.91	0.52
2:B:929:GLU:HB3	3:C:69:ARG:HG3	1.91	0.52
2:B:84:LEU:O	2:B:400:LYS:NZ	2.42	0.52
2:B:698:ARG:NH1	2:B:917:GLY:O	2.42	0.52
1:A:1160:ARG:NH1	1:A:1307:ASP:O	2.42	0.52
1:A:971:GLU:OE1	1:A:1009:ARG:NH2	2.43	0.52
1:A:1202:ILE:HD11	1:A:1224:ILE:HD13	1.92	0.52
1:A:386:ASN:ND2	2:B:765:TYR:OH	2.43	0.52
2:B:1005:TYR:OH	3:C:293:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ARG:HB3	3:C:189:PRO:HB3	1.92	0.52
1:A:805:ASN:HD21	2:B:951:SER:HA	1.75	0.52
1:A:380:VAL:O	1:A:497:THR:OG1	2.27	0.52
2:B:788:ARG:HD3	2:B:899:LEU:HD21	1.92	0.52
15:O:256:PRO:HA	15:O:259:LEU:HD22	1.91	0.52
13:M:137:GLU:HB3	13:M:186:ILE:HG13	1.92	0.52
15:O:292:ARG:HH22	15:O:326:ILE:HG22	1.74	0.52
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.91	0.51
15:O:240:GLN:NE2	15:O:244:ASN:OD1	2.44	0.51
2:B:983:LYS:HG3	2:B:985:GLU:H	1.75	0.51
1:A:8:GLU:OE1	2:B:1118:LYS:NZ	2.37	0.51
1:A:264:PRO:O	1:A:269:ARG:NH1	2.37	0.51
2:B:217:GLN:NE2	2:B:232:TYR:OH	2.42	0.51
1:A:552:ALA:HB3	1:A:671:ASP:HB3	1.93	0.51
2:B:546:SER:OG	13:M:89:GLN:NE2	2.43	0.51
2:B:609:CYS:HB3	2:B:648:TYR:HB3	1.92	0.51
1:A:154:CYS:SG	1:A:158:GLY:N	2.82	0.51
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.93	0.51
15:O:125:GLU:HB3	15:O:284:LEU:HD21	1.91	0.51
1:A:1325:VAL:HG23	1:A:1326:LEU:HG	1.92	0.51
2:B:579:ARG:NH1	2:B:588:ILE:O	2.44	0.51
3:C:231:PRO:HA	3:C:293:ARG:HA	1.93	0.51
8:H:30:SER:OG	8:H:36:CYS:SG	2.66	0.51
13:M:243:ILE:HG23	14:N:404:SER:HA	1.91	0.51
2:B:60:GLN:HG2	2:B:520:ILE:HD12	1.92	0.51
8:H:56:THR:HG21	8:H:145:ARG:HH21	1.75	0.51
3:C:153:PRO:HB3	3:C:157:TYR:HD2	1.76	0.50
3:C:319:ARG:HE	3:C:323:ASN:HD21	1.60	0.50
2:B:832:VAL:HB	12:L:60:ARG:HA	1.94	0.50
2:B:988:SER:HA	2:B:991:LEU:HD23	1.94	0.50
13:M:161:ALA:HB1	13:M:168:VAL:HG22	1.93	0.50
1:A:1012:ILE:HD11	1:A:1071:LEU:HD21	1.92	0.50
2:B:566:ARG:NH2	14:N:286:ASP:OD2	2.44	0.50
1:A:259:ARG:HH22	15:O:41:THR:HB	1.77	0.50
16:P:269:LEU:HG	16:P:293:ILE:HD12	1.93	0.50
1:A:74:LEU:O	2:B:1048:ARG:NH1	2.44	0.50
1:A:1283:ILE:HA	1:A:1293:LEU:HA	1.94	0.50
15:O:293:SER:OG	15:O:317:ARG:NH1	2.44	0.50
3:C:30:GLU:HG2	11:K:84:PRO:HD3	1.94	0.50
3:C:224:THR:HG21	10:J:43:ARG:HH12	1.77	0.50
2:B:403:ILE:HG22	2:B:407:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:ARG:NH1	3:C:95:GLU:OE1	2.44	0.49
2:B:389:GLU:HG2	2:B:393:LYS:HE2	1.94	0.49
2:B:767:ILE:HG22	2:B:768:GLU:HG3	1.94	0.49
9:I:13:LEU:HD21	9:I:27:ARG:H	1.78	0.49
2:B:234:ILE:HD11	2:B:238:GLY:HA2	1.95	0.49
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.95	0.49
2:B:297:THR:OG1	2:B:298:GLN:N	2.43	0.49
15:O:43:ASN:HD22	15:O:44:PRO:HD2	1.78	0.49
1:A:960:MET:HE1	1:A:1013:ASN:HA	1.92	0.49
3:C:35:LYS:NZ	3:C:39:ASP:OD2	2.46	0.49
4:D:66:LEU:O	4:D:95:ILE:N	2.46	0.49
15:O:136:ILE:HG21	15:O:282:ILE:HD11	1.93	0.49
1:A:416:LEU:HD13	1:A:419:LEU:HD22	1.94	0.49
2:B:613:ILE:HG23	2:B:673:LEU:HB3	1.94	0.49
1:A:95:TYR:O	1:A:99:THR:OG1	2.28	0.49
13:M:76:LEU:CD1	13:M:168:VAL:CG1	2.88	0.49
14:N:290:ILE:HD12	14:N:416:ILE:HD13	1.95	0.49
17:Q:48:THR:OG1	17:Q:51:GLU:OE1	2.31	0.49
1:A:1188:ILE:HD13	1:A:1230:ILE:HD13	1.95	0.49
13:M:74:PHE:HZ	14:N:294:LEU:CG	2.23	0.49
1:A:1178:LYS:HG3	1:A:1182:SER:HB2	1.95	0.48
2:B:198:GLU:HA	2:B:377:LEU:HA	1.95	0.48
2:B:529:ILE:HD11	2:B:575:PHE:HZ	1.76	0.48
2:B:612:LEU:HD22	2:B:674:GLU:HA	1.95	0.48
2:B:824:LEU:HD11	2:B:844:ASN:HB2	1.95	0.48
14:N:314:PRO:HB3	14:N:318:ARG:HG2	1.95	0.48
15:O:319:THR:HG22	15:O:359:LEU:HD21	1.95	0.48
1:A:75:ALA:HA	2:B:1048:ARG:HH12	1.78	0.48
1:A:397:ARG:HB3	2:B:1035:MET:HE1	1.94	0.48
2:B:157:ARG:NH1	2:B:180:ASP:O	2.46	0.48
2:B:938:ILE:HD11	10:J:43:ARG:HB2	1.94	0.48
1:A:564:ILE:O	1:A:569:SER:OG	2.30	0.48
15:O:528:MET:HB3	15:O:532:ASP:HB3	1.94	0.48
16:P:185:PHE:HE2	16:P:221:ILE:HD12	1.77	0.48
2:B:667:VAL:HG22	2:B:668:PRO:HD2	1.95	0.48
13:M:74:PHE:CE1	14:N:294:LEU:HD11	2.49	0.48
15:O:588:LEU:HG	15:O:637:VAL:HG13	1.94	0.48
1:A:360:LYS:NZ	19:S:20:DC:OP2	2.45	0.48
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.46	0.48
2:B:369:ARG:NH1	2:B:478:GLU:OE2	2.47	0.48
1:A:393:ALA:HB1	1:A:493:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.96	0.48
1:A:212:GLU:HG2	1:A:213:ARG:HG2	1.96	0.48
1:A:541:LEU:HD12	1:A:682:LEU:HD13	1.94	0.48
9:I:32:GLU:HB2	13:M:130:PHE:HB2	1.94	0.48
1:A:980:SER:HA	5:E:163:GLU:HG3	1.94	0.48
2:B:390:ASP:OD1	2:B:446:ARG:NH1	2.46	0.48
2:B:690:TYR:HB3	2:B:693:HIS:HD2	1.78	0.48
3:C:248:GLN:HA	3:C:256:ILE:HD11	1.95	0.48
13:M:78:ILE:HG12	13:M:170:LEU:HD22	1.95	0.48
16:P:287:ASP:OD2	17:Q:50:LYS:NZ	2.40	0.48
1:A:649:ASP:HB3	1:A:662:GLY:HA2	1.95	0.48
1:A:832:LEU:HD23	1:A:834:HIS:HD2	1.79	0.48
2:B:913:SER:HB3	2:B:1025:GLN:HB2	1.94	0.48
1:A:785:LEU:HD23	1:A:792:LEU:HD12	1.96	0.48
2:B:709:ALA:HA	2:B:1027:LEU:HA	1.95	0.48
15:O:335:LEU:HG	15:O:336:LEU:HD12	1.94	0.48
2:B:217:GLN:HE22	2:B:352:MET:HG2	1.79	0.47
15:O:591:LYS:NZ	16:P:305:HIS:O	2.40	0.47
1:A:597:ILE:HD11	1:A:603:LEU:HB2	1.95	0.47
2:B:355:ARG:NH2	2:B:367:ASP:OD2	2.46	0.47
13:M:79:SER:HB3	13:M:262:GLU:HB3	1.94	0.47
2:B:345:LYS:HZ2	2:B:349:ILE:HD11	1.80	0.47
7:G:151:GLU:N	7:G:197:LEU:O	2.44	0.47
9:I:18:ASP:OD2	13:M:133:LYS:NZ	2.47	0.47
1:A:1022:LEU:HD12	1:A:1056:VAL:HG23	1.97	0.47
2:B:267:GLU:O	2:B:271:LEU:N	2.45	0.47
13:M:74:PHE:HE2	14:N:294:LEU:HD23	1.75	0.47
13:M:74:PHE:HZ	14:N:294:LEU:HG	1.80	0.47
13:M:77:LYS:HD2	13:M:262:GLU:CD	2.39	0.47
1:A:389:ILE:HD13	1:A:694:MET:HE3	1.96	0.47
1:A:711:SER:OG	2:B:1016:TYR:O	2.31	0.47
1:A:881:GLU:HG3	2:B:482:LYS:HE2	1.95	0.47
11:K:80:ILE:HG21	11:K:105:ILE:HD12	1.95	0.47
15:O:133:SER:HA	15:O:136:ILE:HD12	1.97	0.47
15:O:135:LEU:HD13	15:O:291:ARG:HH11	1.79	0.47
1:A:600:PRO:HG3	8:H:95:TYR:HA	1.97	0.47
1:A:654:ILE:HG12	1:A:659:ILE:HG12	1.95	0.47
1:A:1224:ILE:HD11	1:A:1229:ARG:H	1.79	0.47
2:B:51:PHE:O	2:B:55:LYS:HB2	2.15	0.47
2:B:391:LEU:HD21	2:B:432:GLY:HA3	1.97	0.47
2:B:518:THR:HB	2:B:608:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:SER:HB2	5:E:105:PHE:HB3	1.97	0.47
1:A:598:MET:HE1	8:H:98:TYR:HB2	1.97	0.47
2:B:1094:VAL:HG12	2:B:1101:MET:HG2	1.97	0.47
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.96	0.47
3:C:164:ALA:HB2	3:C:191:ILE:HB	1.97	0.47
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.48	0.47
11:K:104:ARG:HE	11:K:106:GLN:HE21	1.61	0.47
15:O:497:ALA:HB2	15:O:505:MET:HB3	1.97	0.47
15:O:528:MET:HB2	15:O:533:ILE:HG13	1.97	0.47
1:A:12:ARG:NH1	2:B:1144:GLU:OE2	2.48	0.47
1:A:583:MET:HE3	1:A:696:ARG:HD3	1.97	0.47
2:B:1005:TYR:HA	2:B:1012:CYS:HA	1.97	0.47
15:O:311:VAL:HA	15:O:314:ILE:HG22	1.96	0.47
1:A:100:ILE:HD11	1:A:178:ILE:HD12	1.97	0.46
1:A:317:ASP:HA	1:A:320:GLN:HG2	1.97	0.46
3:C:17:SER:OG	3:C:19:ASP:OD1	2.33	0.46
2:B:496:MET:SD	2:B:496:MET:N	2.88	0.46
19:S:14:DC:H2"	19:S:15:DG:C8	2.50	0.46
1:A:366:GLY:HA2	2:B:1061:ARG:HH22	1.80	0.46
1:A:785:LEU:HG	1:A:789:ASN:HD21	1.80	0.46
1:A:1365:LYS:HE3	1:A:1378:LYS:HG2	1.96	0.46
2:B:294:ASP:OD1	2:B:294:ASP:N	2.49	0.46
2:B:809:MET:HG3	2:B:826:PRO:HA	1.97	0.46
7:G:158:VAL:HG21	7:G:191:PRO:HG2	1.98	0.46
13:M:77:LYS:HE2	13:M:262:GLU:O	2.14	0.46
16:P:307:LYS:HG3	16:P:308:GLU:H	1.80	0.46
2:B:61:HIS:HB3	2:B:155:MET:HE1	1.97	0.46
7:G:160:PRO:HG2	7:G:166:ARG:HH22	1.80	0.46
1:A:777:VAL:HA	1:A:780:VAL:HG22	1.98	0.46
13:M:107:ILE:HB	13:M:124:PRO:HD2	1.97	0.46
1:A:1034:PRO:O	1:A:1036:ALA:N	2.49	0.46
1:A:1322:VAL:HG13	1:A:1326:LEU:HD12	1.98	0.46
2:B:796:LYS:HE2	2:B:798:TYR:HE1	1.81	0.46
3:C:105:PRO:HG3	10:J:6:ARG:HH22	1.80	0.46
6:F:111:LEU:HD21	6:F:120:ILE:HG23	1.98	0.46
13:M:148:LEU:HA	13:M:182:PHE:H	1.81	0.46
1:A:378:ARG:HH21	1:A:516:GLU:HG3	1.79	0.46
2:B:412:ARG:HD2	2:B:414:MET:H	1.81	0.46
2:B:587:PHE:O	2:B:607:ARG:NH2	2.37	0.46
10:J:2:ILE:HG13	10:J:57:ILE:HG21	1.97	0.46
14:N:364:ARG:NE	14:N:372:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:CYS:O	1:A:358:LYS:N	2.48	0.46
16:P:172:ILE:HD12	16:P:175:ILE:HD13	1.97	0.46
1:A:102:ILE:HG23	1:A:242:LEU:HD13	1.98	0.46
1:A:625:ASN:HD21	1:A:941:HIS:HA	1.81	0.46
16:P:297:PHE:HB3	16:P:300:PHE:HE2	1.80	0.46
1:A:1311:GLY:O	5:E:147:HIS:ND1	2.42	0.45
2:B:49:PRO:HG3	2:B:743:LEU:HD11	1.98	0.45
3:C:67:PHE:O	3:C:71:MET:HB2	2.17	0.45
5:E:4:GLU:O	5:E:8:ASN:ND2	2.49	0.45
5:E:85:GLU:HG3	5:E:87:SER:H	1.80	0.45
1:A:232:LYS:HE3	15:O:44:PRO:HD3	1.98	0.45
13:M:74:PHE:CZ	14:N:294:LEU:CD1	2.99	0.45
1:A:1275:LEU:HB2	1:A:1278:ILE:HD12	1.97	0.45
2:B:476:GLN:HG3	2:B:477:PHE:H	1.81	0.45
15:O:75:SER:OG	15:O:78:GLU:OE1	2.34	0.45
15:O:289:LYS:HE3	15:O:326:ILE:HB	1.97	0.45
1:A:84:LEU:HD22	1:A:261:LEU:HD23	1.97	0.45
3:C:250:CYS:SG	3:C:282:TYR:OH	2.69	0.45
13:M:110:ALA:HB1	13:M:121:ILE:HA	1.99	0.45
1:A:368:LEU:HD11	2:B:1128:LEU:HD22	1.97	0.45
15:O:235:LEU:HD13	15:O:238:ARG:HD2	1.98	0.45
15:O:527:LEU:HD22	16:P:247:LEU:HD21	1.99	0.45
19:S:20:DC:H2''	19:S:21:DA:C8	2.52	0.45
1:A:235:LYS:HG3	1:A:238:ASP:HB2	1.99	0.45
1:A:360:LYS:HZ1	19:S:19:DA:H3'	1.82	0.45
7:G:3:ILE:HG13	7:G:76:VAL:HG13	1.99	0.45
2:B:377:LEU:HD11	2:B:520:ILE:HG21	1.99	0.45
3:C:33:VAL:HA	3:C:34:GLU:HA	1.62	0.45
7:G:26:ILE:HD11	7:G:68:ILE:HD13	1.99	0.45
14:N:363:ILE:HA	14:N:373:VAL:HA	1.98	0.45
1:A:523:GLN:N	2:B:1081:GLU:OE2	2.48	0.45
1:A:308:SER:OG	1:A:309:ILE:N	2.50	0.45
2:B:842:TYR:HE2	2:B:898:VAL:HG11	1.82	0.45
2:B:844:ASN:HA	2:B:870:PRO:HB3	1.98	0.45
7:G:110:ILE:HD12	7:G:111:PRO:HD2	1.99	0.45
13:M:90:TYR:HA	13:M:179:LEU:HD11	1.97	0.45
15:O:164:ILE:HG12	15:O:282:ILE:HD12	1.97	0.45
14:N:364:ARG:N	14:N:364:ARG:CD	2.77	0.45
15:O:551:VAL:HG22	15:O:563:VAL:HG13	1.97	0.45
15:O:506:ARG:O	16:P:249:TYR:OH	2.32	0.44
1:A:1257:PHE:HE2	9:I:14:ILE:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1052:GLU:O	2:B:1056:ARG:NH2	2.50	0.44
15:O:155:LEU:HD11	15:O:187:ILE:HG12	1.99	0.44
1:A:80:HIS:H	1:A:265:PRO:HB3	1.82	0.44
1:A:1181:LEU:HD13	1:A:1256:VAL:HG22	2.00	0.44
2:B:553:TYR:HA	2:B:597:MET:HB3	1.99	0.44
3:C:288:LYS:HG3	3:C:289:VAL:HG23	1.98	0.44
8:H:66:GLU:HG3	8:H:68:THR:HG23	2.00	0.44
14:N:373:VAL:HG13	14:N:382:ILE:HA	1.99	0.44
1:A:1141:ILE:N	1:A:1295:VAL:O	2.49	0.44
3:C:335:GLN:HG2	11:K:49:LEU:HB3	1.98	0.44
7:G:54:VAL:HG22	7:G:70:VAL:HG12	1.98	0.44
2:B:725:LEU:HD21	2:B:788:ARG:HD2	1.99	0.44
2:B:817:PRO:HG2	2:B:822:GLN:HA	2.00	0.44
7:G:133:ASP:HA	7:G:134:GLU:HA	1.77	0.44
7:G:147:ARG:H	7:G:201:GLN:HB2	1.83	0.44
13:M:256:LYS:HA	13:M:259:ILE:HG22	1.99	0.44
15:O:449:SER:OG	16:P:205:ASN:ND2	2.50	0.44
1:A:38:ASP:HA	1:A:52:GLY:HA2	1.98	0.44
1:A:495:TRP:O	1:A:499:ARG:NH2	2.51	0.44
14:N:395:ILE:HD12	14:N:411:ARG:H	1.82	0.44
1:A:474:PHE:HD1	1:A:519:LEU:HD12	1.83	0.44
1:A:1184:ILE:HG13	1:A:1260:MET:HE3	1.99	0.44
3:C:80:ALA:HA	3:C:208:CYS:HA	2.00	0.44
4:D:3:VAL:HG22	7:G:7:ILE:HD13	1.99	0.44
7:G:108:ILE:HD12	7:G:196:LEU:HB3	2.00	0.44
1:A:1201:THR:H	1:A:1204:ASP:HB2	1.83	0.43
5:E:202:SER:HB2	5:E:205:SER:HB3	2.00	0.43
11:K:74:ASN:HA	11:K:77:ARG:HG3	2.00	0.43
13:M:135:LYS:HA	13:M:136:ALA:HA	1.55	0.43
15:O:353:GLU:HG2	15:O:480:TYR:CZ	2.53	0.43
1:A:763:GLU:HA	1:A:766:ILE:HG22	2.00	0.43
1:A:800:LYS:HE3	2:B:951:SER:HB3	1.99	0.43
2:B:232:TYR:HA	2:B:243:LYS:HB3	2.00	0.43
2:B:837:GLN:H	2:B:840:GLN:HE21	1.67	0.43
2:B:69:VAL:HB	2:B:100:VAL:HG21	1.99	0.43
15:O:144:MET:HB3	15:O:152:HIS:CE1	2.53	0.43
16:P:250:ASP:OD1	16:P:250:ASP:N	2.51	0.43
1:A:365:ARG:NH1	1:A:887:ARG:HE	2.16	0.43
2:B:766:ASP:O	2:B:945:ASN:ND2	2.52	0.43
15:O:244:ASN:HA	15:O:247:THR:HG22	1.99	0.43
1:A:108:LYS:O	15:O:572:HIS:NE2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HA	2:B:1061:ARG:HA	2.00	0.43
1:A:644:GLU:HB3	1:A:651:PHE:HB3	1.99	0.43
2:B:615:VAL:HA	2:B:620:SER:HA	2.01	0.43
15:O:233:SER:OG	15:O:234:ASP:N	2.50	0.43
3:C:58:ASN:N	3:C:296:ASN:O	2.51	0.43
14:N:308:GLN:HE22	14:N:415:LYS:HG2	1.84	0.43
1:A:598:MET:HB3	1:A:599:LYS:H	1.73	0.43
2:B:81:GLN:HG2	2:B:82:LEU:HD22	2.01	0.43
2:B:680:ILE:HG23	2:B:681:LEU:HD12	2.00	0.43
7:G:202:THR:HA	7:G:209:SER:HB2	2.00	0.43
15:O:190:LEU:HA	15:O:193:GLN:HB2	2.00	0.43
1:A:486:LEU:HD23	1:A:537:VAL:HG22	2.00	0.43
1:A:1243:SER:O	1:A:1245:SER:N	2.52	0.43
1:A:1373:ARG:NH1	19:S:16:DC:O3'	2.51	0.43
2:B:489:LEU:HG	2:B:493:GLN:HE21	1.84	0.42
4:D:52:HIS:HB3	4:D:55:LEU:HB3	2.00	0.42
15:O:516:LEU:HB2	15:O:567:ARG:HE	1.82	0.42
1:A:1127:LYS:O	1:A:1131:ASN:HB2	2.19	0.42
2:B:785:CYS:O	2:B:903:ASN:ND2	2.52	0.42
2:B:838:SER:H	2:B:873:TYR:HD2	1.67	0.42
7:G:49:TYR:HB3	7:G:73:ARG:HG3	2.01	0.42
1:A:395:PRO:HB3	1:A:496:ARG:HA	2.01	0.42
2:B:913:SER:HB2	2:B:1027:LEU:HD21	2.01	0.42
9:I:1:MET:HE2	9:I:14:ILE:HD12	2.00	0.42
1:A:818:ILE:HD11	1:A:824:PRO:HD2	2.01	0.42
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.51	0.42
15:O:170:THR:HG23	17:Q:77:LEU:HD11	2.02	0.42
1:A:215:VAL:HG13	15:O:553:ARG:HG2	2.02	0.42
1:A:224:PRO:HA	1:A:227:THR:HG22	2.01	0.42
2:B:458:LEU:HD22	2:B:460:ARG:HE	1.83	0.42
2:B:565:ILE:H	2:B:565:ILE:HG13	1.72	0.42
2:B:589:SER:HB2	2:B:607:ARG:HH21	1.84	0.42
11:K:62:SER:OG	11:K:104:ARG:NH1	2.46	0.42
11:K:86:VAL:HA	11:K:107:THR:HA	2.01	0.42
11:K:98:GLU:HB3	11:K:100:LEU:HD13	2.01	0.42
13:M:103:GLU:HG2	13:M:104:HIS:CD2	2.55	0.42
13:M:148:LEU:HD13	13:M:179:LEU:HD13	2.02	0.42
2:B:171:MET:HG3	2:B:178:PRO:HB3	2.02	0.42
2:B:773:LEU:HD22	2:B:778:ILE:HD11	2.02	0.42
3:C:134:LEU:HD23	3:C:167:LEU:HB3	2.02	0.42
11:K:53:ALA:HB1	11:K:104:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:MET:HG3	15:O:83:ILE:HG22	2.02	0.42
15:O:137:ILE:HD11	17:Q:57:LYS:HG2	2.01	0.42
2:B:757:VAL:HG11	2:B:1022:ILE:HD12	2.02	0.42
4:D:121:LEU:HA	4:D:124:VAL:HG12	2.01	0.42
7:G:146:ILE:HG22	7:G:148:PHE:HD1	1.85	0.42
13:M:76:LEU:HD12	13:M:77:LYS:N	2.34	0.42
2:B:493:GLN:HB2	2:B:497:LEU:HB2	2.01	0.42
15:O:516:LEU:H	15:O:567:ARG:HG2	1.84	0.42
1:A:1084:GLU:HB3	6:F:86:THR:HG23	2.02	0.42
1:A:683:ARG:O	1:A:1077:LYS:NZ	2.52	0.42
1:A:1283:ILE:HG12	1:A:1293:LEU:HB3	2.01	0.42
2:B:536:LEU:HD21	2:B:578:LEU:HD11	2.02	0.42
2:B:928:GLN:HE22	3:C:72:ILE:HD13	1.85	0.42
1:A:766:ILE:HD11	1:A:842:PRO:HD3	2.02	0.41
1:A:1169:VAL:HG12	1:A:1188:ILE:HG23	2.02	0.41
1:A:223:ASN:HB2	1:A:316:TRP:HH2	1.85	0.41
1:A:666:LYS:HA	1:A:670:GLY:HA3	2.01	0.41
7:G:150:ILE:HB	7:G:196:LEU:HD11	2.02	0.41
8:H:7:ASP:HA	8:H:58:THR:HG22	2.02	0.41
14:N:401:ASP:OD1	14:N:401:ASP:N	2.53	0.41
1:A:90:VAL:HG13	1:A:258:TRP:HB2	2.02	0.41
1:A:627:ASP:OD1	1:A:627:ASP:N	2.53	0.41
2:B:961:LEU:HB2	2:B:1022:ILE:HD11	2.01	0.41
4:D:134:LEU:HD23	4:D:150:ILE:HG23	2.03	0.41
15:O:188:SER:HA	15:O:191:PHE:HD2	1.84	0.41
3:C:28:GLU:HA	3:C:29:ASN:HA	1.78	0.41
7:G:83:GLU:HB3	7:G:150:ILE:HD11	2.01	0.41
13:M:76:LEU:HD12	13:M:76:LEU:C	2.45	0.41
14:N:365:VAL:HG22	14:N:371:LEU:HD13	2.01	0.41
1:A:328:ASN:HA	1:A:354:CYS:HB2	2.02	0.41
3:C:229:LEU:HB2	3:C:293:ARG:HE	1.84	0.41
15:O:368:ARG:HG3	15:O:370:LEU:HD22	2.03	0.41
17:Q:108:TYR:HB3	17:Q:112:TYR:HE2	1.86	0.41
1:A:408:VAL:HA	1:A:412:ASN:HB2	2.03	0.41
1:A:984:VAL:HG13	1:A:988:ASP:HB3	2.02	0.41
2:B:1081:GLU:HA	2:B:1085:ILE:HB	2.03	0.41
3:C:132:ILE:HB	3:C:208:CYS:HB3	2.02	0.41
14:N:292:ARG:HH12	14:N:296:LYS:HE2	1.86	0.41
1:A:398:VAL:HG23	2:B:1035:MET:HE3	2.03	0.41
1:A:1163:LYS:HA	1:A:1163:LYS:HD2	1.89	0.41
3:C:152:ASP:HA	3:C:153:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD13	5:E:109:ILE:HD11	2.03	0.41
1:A:191:ALA:HB3	1:A:194:LYS:H	1.85	0.41
3:C:84:TYR:HD1	12:L:64:LEU:HD21	1.86	0.41
15:O:200:LEU:HD23	15:O:280:LEU:HD22	2.03	0.41
1:A:434:LEU:HB3	1:A:461:VAL:HB	2.02	0.41
1:A:570:PHE:HB3	1:A:603:LEU:HD23	2.02	0.41
1:A:921:LEU:HA	1:A:1082:ARG:HA	2.02	0.41
2:B:90:GLU:HG2	2:B:91:PHE:H	1.86	0.41
2:B:218:ALA:HB2	2:B:231:THR:HG23	2.03	0.41
2:B:1133:LEU:HD12	2:B:1139:PRO:HD2	2.01	0.41
5:E:123:LEU:HB3	5:E:126:SER:HB3	2.03	0.41
13:M:168:VAL:HG11	14:N:307:PHE:HE2	1.86	0.41
14:N:308:GLN:HE21	14:N:417:VAL:HG12	1.86	0.41
1:A:193:GLU:HA	1:A:196:ILE:HG22	2.03	0.41
2:B:585:SER:OG	2:B:586:GLU:N	2.53	0.41
15:O:136:ILE:HA	15:O:287:PHE:CZ	2.56	0.41
1:A:204:VAL:HG21	15:O:516:LEU:HD12	2.03	0.40
1:A:544:PRO:HA	1:A:924:LEU:HG	2.03	0.40
2:B:306:GLY:HA2	2:B:309:VAL:HG12	2.02	0.40
3:C:256:ILE:HG22	3:C:267:VAL:HG23	2.01	0.40
7:G:162:SER:HA	7:G:163:PRO:HD3	1.96	0.40
3:C:216:HIS:HD2	12:L:70:ARG:HG3	1.87	0.40
1:A:84:LEU:HB3	1:A:261:LEU:HB3	2.01	0.40
2:B:928:GLN:HG2	2:B:939:VAL:HG21	2.03	0.40
3:C:191:ILE:HG12	10:J:16:ASP:HB3	2.03	0.40
6:F:145:ASP:OD1	6:F:145:ASP:N	2.53	0.40
14:N:287:HIS:CE1	14:N:371:LEU:H	2.39	0.40
1:A:1241:ALA:HB3	1:A:1244:ILE:HD12	2.03	0.40
2:B:136:THR:HB	2:B:140:ASN:HA	2.03	0.40
2:B:698:ARG:CZ	2:B:952:ARG:HD2	2.52	0.40
2:B:1130:GLN:O	2:B:1134:SER:OG	2.37	0.40
4:D:149:THR:HG22	4:D:153:MET:HE2	2.02	0.40
14:N:315:ALA:HA	14:N:377:ASN:HB2	2.03	0.40
15:O:595:LEU:HD13	15:O:633:ARG:HH21	1.85	0.40
1:A:133:ASP:OD2	1:A:1365:LYS:NZ	2.48	0.40
1:A:363:ARG:O	1:A:368:LEU:N	2.50	0.40
2:B:883:GLN:HB3	2:B:899:LEU:HB3	2.03	0.40
7:G:207:LEU:HB3	7:G:208:VAL:H	1.74	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	A	1425/1460 (98%)	1204 (84%)	213 (15%)	8 (1%)	21	50
2	B	1112/1149 (97%)	926 (83%)	183 (16%)	3 (0%)	36	65
3	C	333/335 (99%)	285 (86%)	47 (14%)	1 (0%)	36	65
4	D	134/161 (83%)	121 (90%)	13 (10%)	0	100	100
5	E	213/215 (99%)	184 (86%)	29 (14%)	0	100	100
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	209/212 (99%)	156 (75%)	53 (25%)	0	100	100
8	H	144/146 (99%)	127 (88%)	17 (12%)	0	100	100
9	I	42/110 (38%)	37 (88%)	5 (12%)	0	100	100
10	J	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
11	K	102/142 (72%)	91 (89%)	11 (11%)	0	100	100
12	L	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
13	M	168/282 (60%)	116 (69%)	50 (30%)	2 (1%)	10	35
14	N	110/422 (26%)	88 (80%)	21 (19%)	1 (1%)	14	42
15	O	547/654 (84%)	464 (85%)	82 (15%)	1 (0%)	43	71
16	P	149/317 (47%)	109 (73%)	38 (26%)	2 (1%)	9	33
17	Q	87/251 (35%)	73 (84%)	14 (16%)	0	100	100
All	All	4965/6151 (81%)	4148 (84%)	799 (16%)	18 (0%)	31	59

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	LYS
1	A	349	PRO
1	A	1244	ILE
2	B	111	TYR
3	C	129	GLU

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Mol	Chain	Res	Type
13	M	165	ASP
1	A	495	TRP
13	M	166	MET
1	A	667	SER
2	B	930	ASP
14	N	364	ARG
15	O	473	PRO
1	A	601	TYR
1	A	494	PRO
1	A	666	LYS
2	B	931	MET
16	P	264	THR
16	P	206	VAL

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	A	1231/1257 (98%)	1226 (100%)	5 (0%)	84	83
2	B	975/1006 (97%)	973 (100%)	2 (0%)	87	85
3	C	296/296 (100%)	296 (100%)	0	100	100
4	D	113/145 (78%)	113 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	184/190 (97%)	184 (100%)	0	100	100
8	H	128/128 (100%)	127 (99%)	1 (1%)	73	77
9	I	40/98 (41%)	40 (100%)	0	100	100
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	93/130 (72%)	93 (100%)	0	100	100
12	L	41/57 (72%)	41 (100%)	0	100	100
13	M	148/249 (59%)	141 (95%)	7 (5%)	23	50
14	N	92/360 (26%)	91 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	505/593 (85%)	501 (99%)	4 (1%)	73	77
16	P	130/285 (46%)	130 (100%)	0	100	100
17	Q	81/212 (38%)	79 (98%)	2 (2%)	42	62
All	All	4389/5405 (81%)	4367 (100%)	22 (0%)	78	81

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

Mol	Chain	Res	Type
1	A	140	ILE
1	A	409	THR
1	A	501	ASN
1	A	558	ILE
1	A	848	VAL
2	B	133	ILE
2	B	667	VAL
8	H	143	LEU
13	M	71	ILE
13	M	72	GLU
13	M	73	GLU
13	M	76	LEU
13	M	77	LYS
13	M	166	MET
13	M	167	GLN
14	N	364	ARG
15	O	326	ILE
15	O	366	LEU
15	O	516	LEU
15	O	590	PHE
17	Q	59	ILE
17	Q	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	180	HIS
1	A	233	GLN
1	A	311	ASN
1	A	315	HIS
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	386	ASN
1	A	427	HIS
1	A	488	HIS
1	A	501	ASN
1	A	555	GLN
1	A	805	ASN
1	A	808	GLN
1	A	815	GLN
1	A	834	HIS
1	A	838	ASN
1	A	850	ASN
1	A	941	HIS
1	A	944	ASN
1	A	1040	GLN
1	A	1180	ASN
1	A	1261	GLN
1	A	1262	GLN
2	B	61	HIS
2	B	80	ASN
2	B	197	GLN
2	B	217	GLN
2	B	244	HIS
2	B	476	GLN
2	B	493	GLN
2	B	552	ASN
2	B	577	HIS
2	B	600	HIS
2	B	699	ASN
2	B	708	GLN
2	B	754	ASN
2	B	774	ASN
2	B	821	HIS
2	B	883	GLN
2	B	902	GLN
2	B	903	ASN
2	B	936	GLN
2	B	970	ASN
2	B	1049	GLN
2	B	1148	GLN
3	C	65	ASN
3	C	130	ASN
3	C	137	ASN

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Mol	Chain	Res	Type
3	C	172	GLN
3	C	323	ASN
4	D	61	ASN
4	D	71	ASN
4	D	125	ASN
5	E	8	ASN
5	E	54	GLN
5	E	104	ASN
5	E	114	ASN
5	E	136	ASN
5	E	146	HIS
7	G	17	GLN
7	G	28	HIS
7	G	69	ASN
7	G	176	ASN
8	H	3	ASN
8	H	33	GLN
8	H	35	GLN
8	H	83	GLN
8	H	134	ASN
8	H	139	ASN
10	J	23	ASN
11	K	102	ASN
11	K	106	GLN
13	M	89	GLN
13	M	117	HIS
13	M	141	ASN
13	M	146	GLN
13	M	155	ASN
14	N	289	HIS
14	N	377	ASN
14	N	421	GLN
15	O	43	ASN
15	O	154	GLN
15	O	193	GLN
15	O	222	HIS
15	O	225	ASN
15	O	240	GLN
15	O	310	GLN
15	O	456	HIS
15	O	469	ASN
15	O	631	ASN

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Mol	Chain	Res	Type
16	P	197	ASN
16	P	205	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

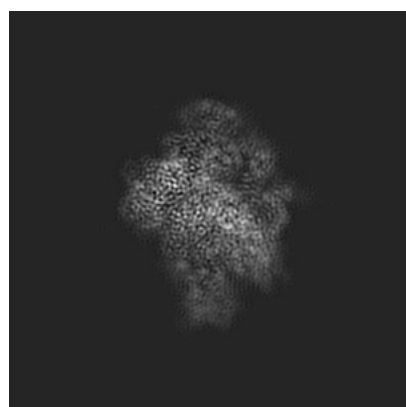
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3956. These allow visual inspection of the internal detail of the map and identification of artifacts.

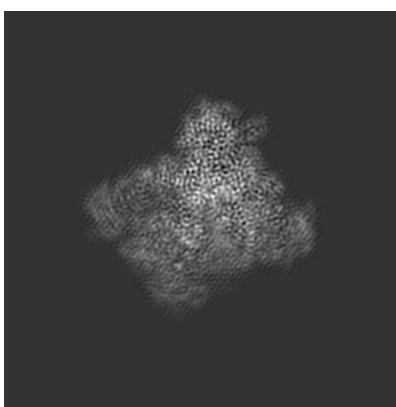
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

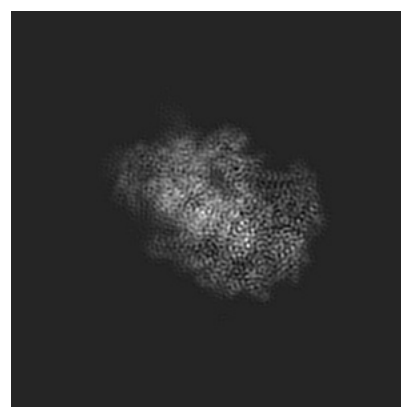
6.1.1 Primary map



X



Y

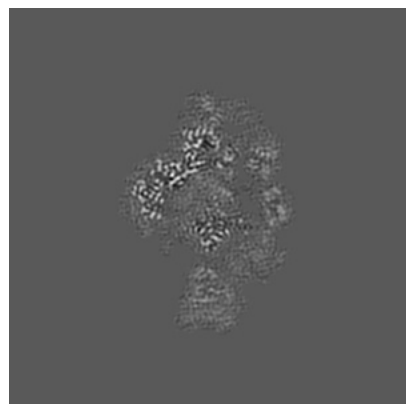


Z

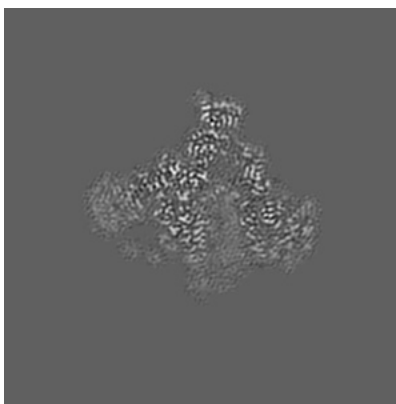
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

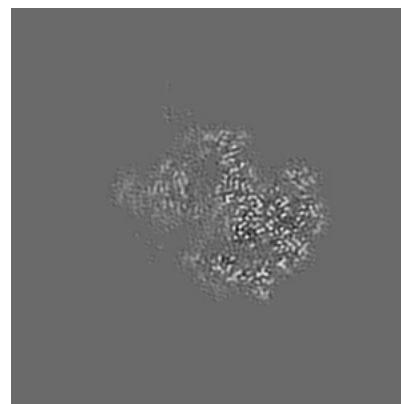
6.2.1 Primary map



X Index: 154



Y Index: 154

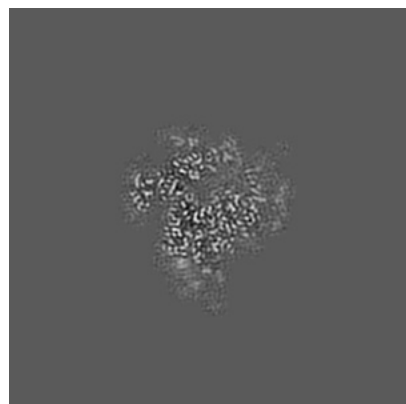


Z Index: 154

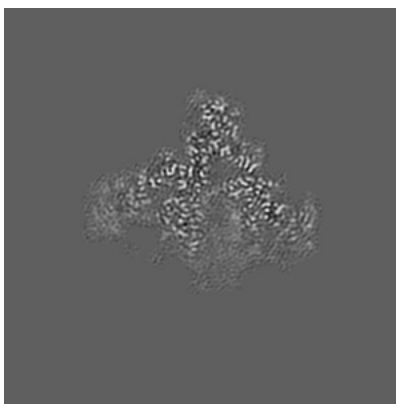
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

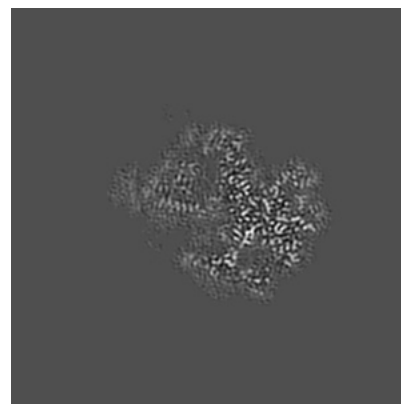
6.3.1 Primary map



X Index: 178



Y Index: 150

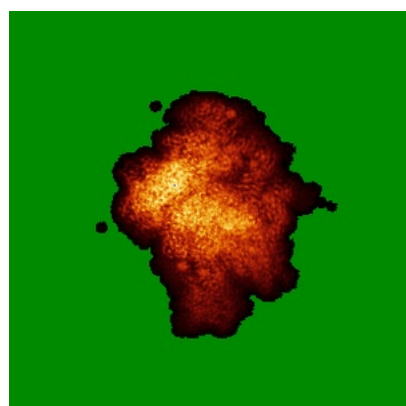


Z Index: 152

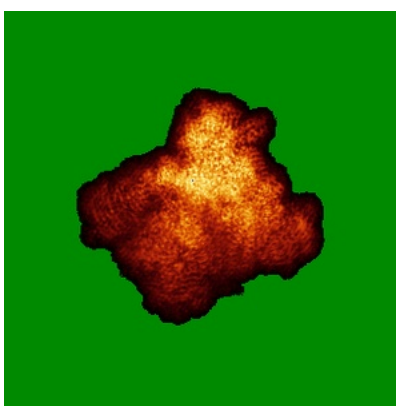
The images above show the largest variance slices of the map in three orthogonal directions.

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

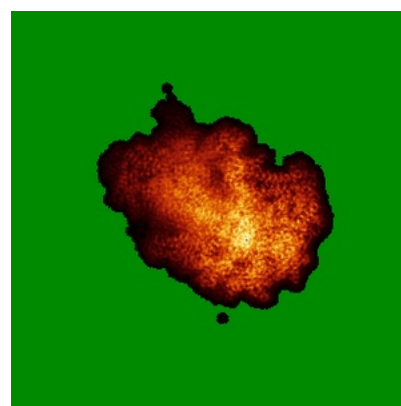
6.4.1 Primary map



X



Y

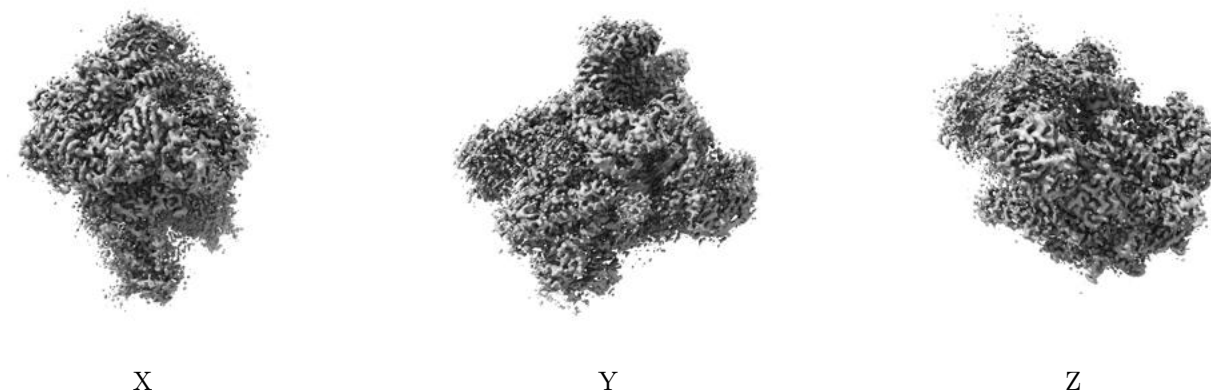


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

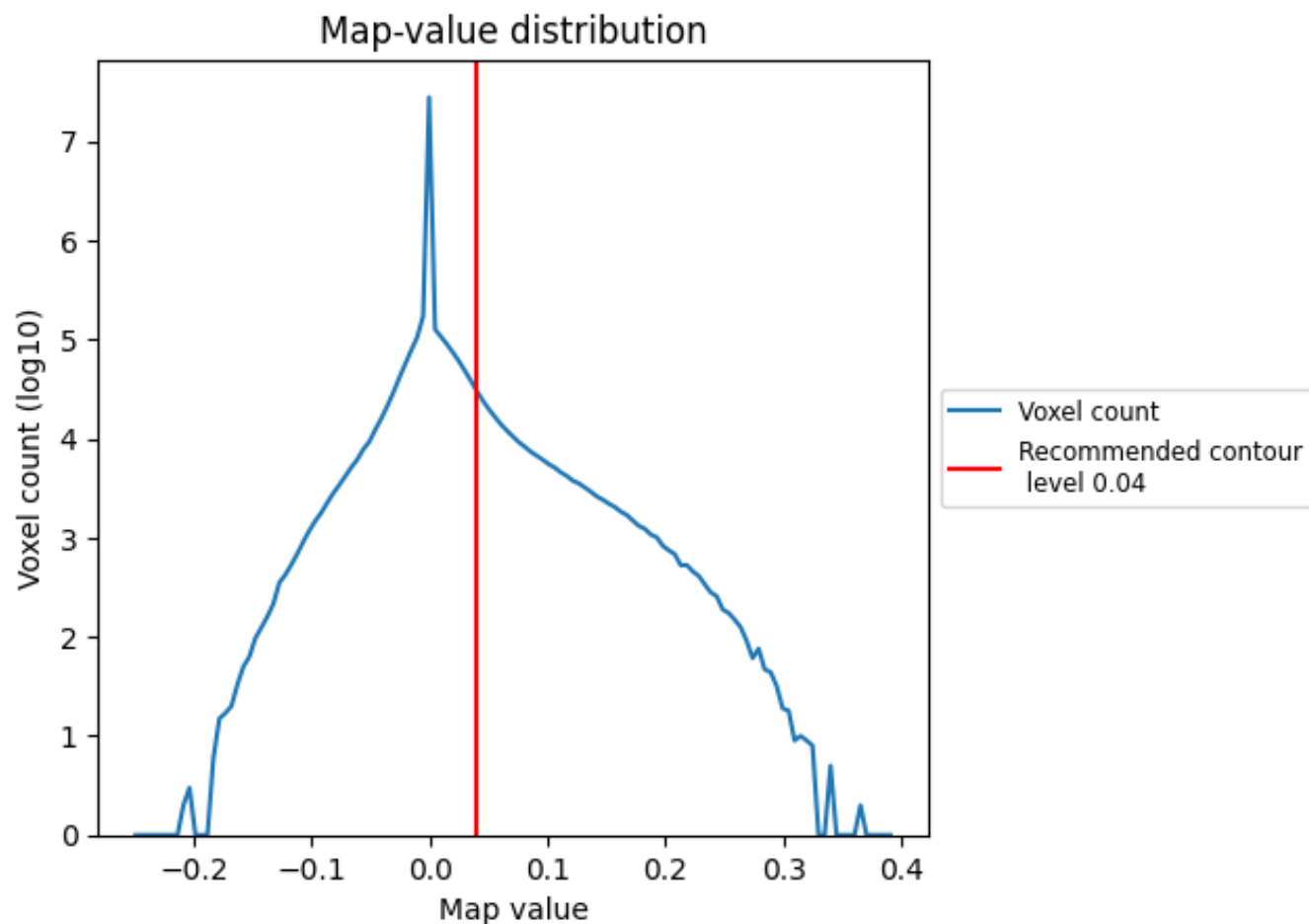
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

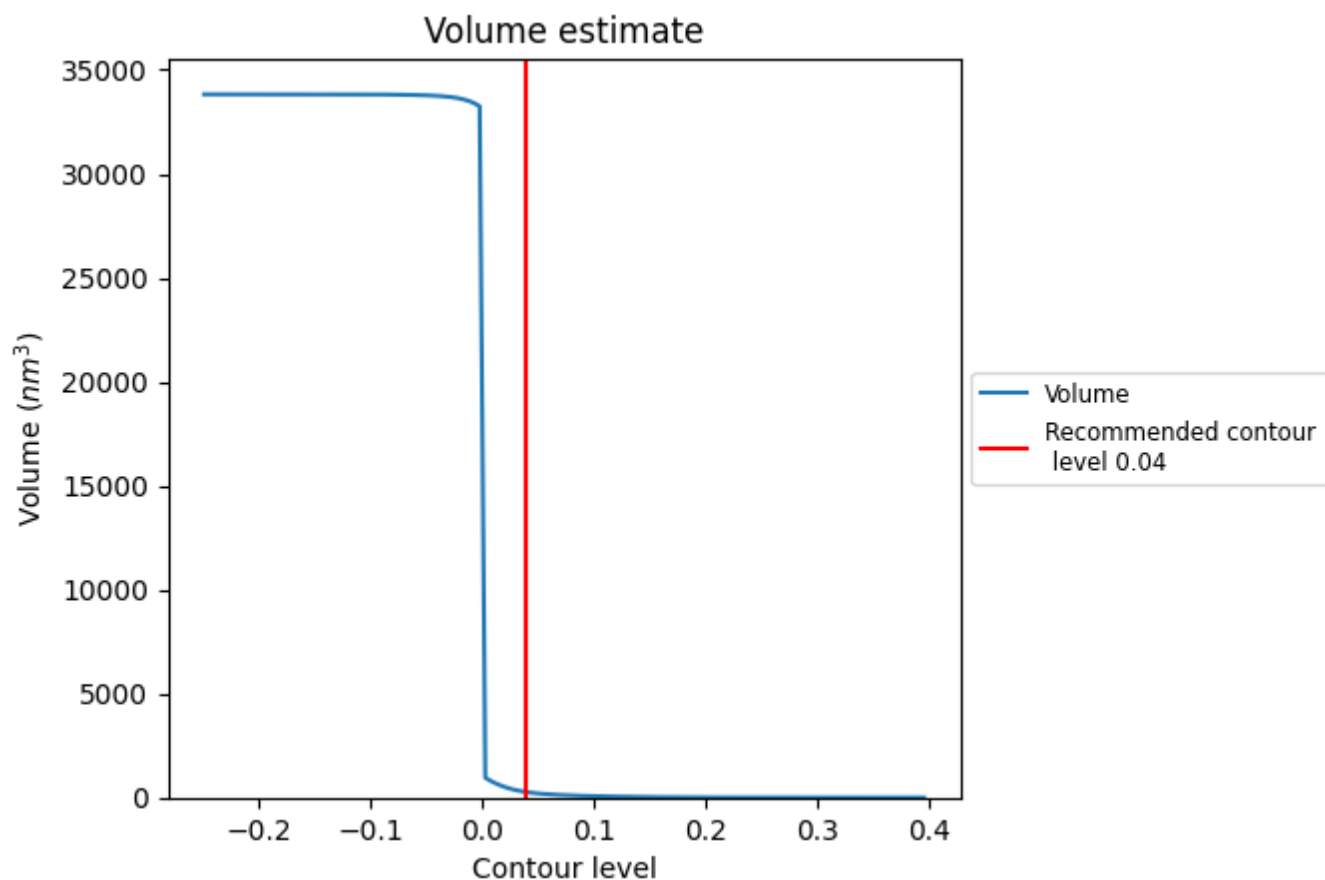
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

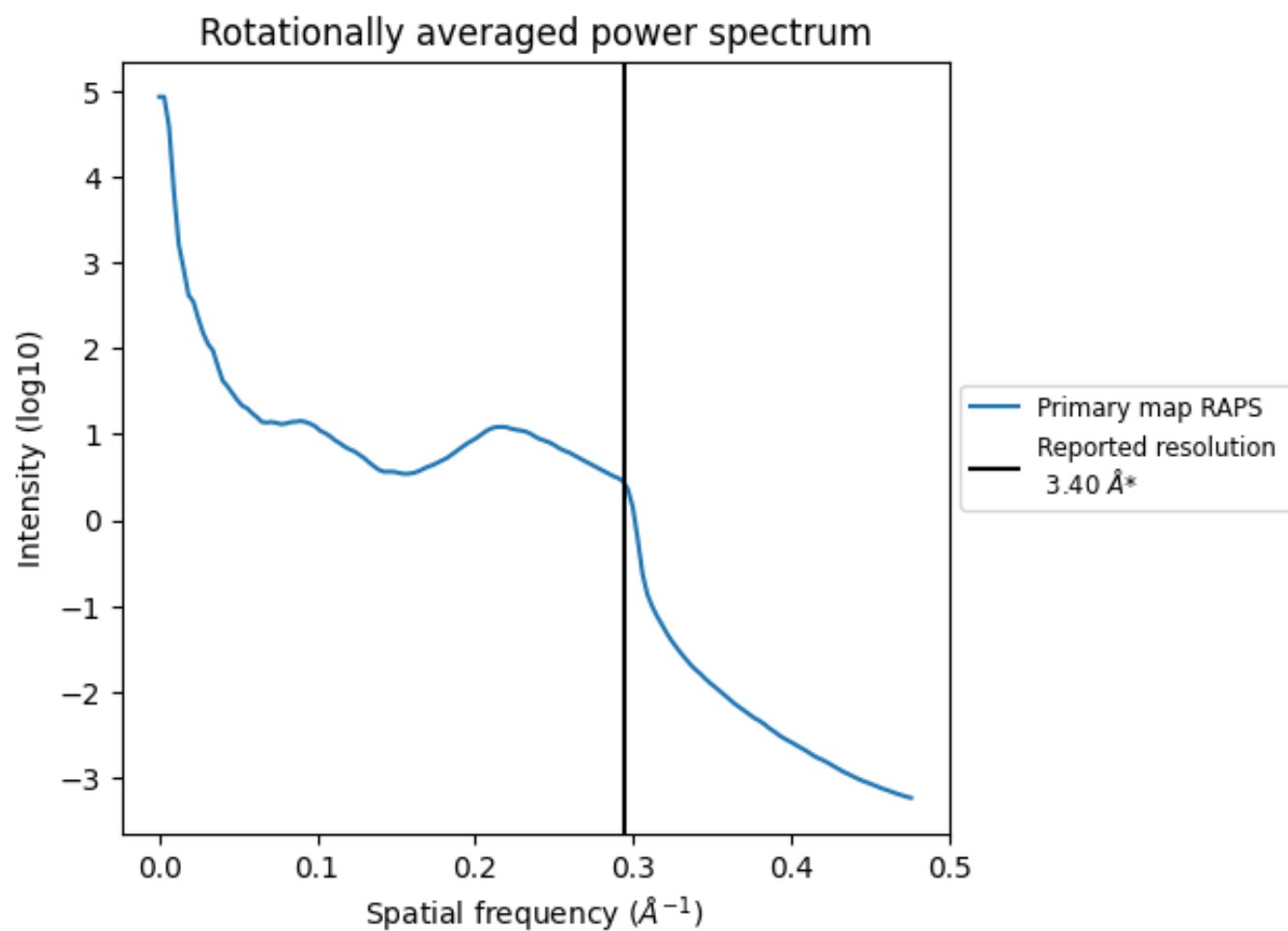
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm^3 ; this corresponds to an approximate mass of 236 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 ⓘ

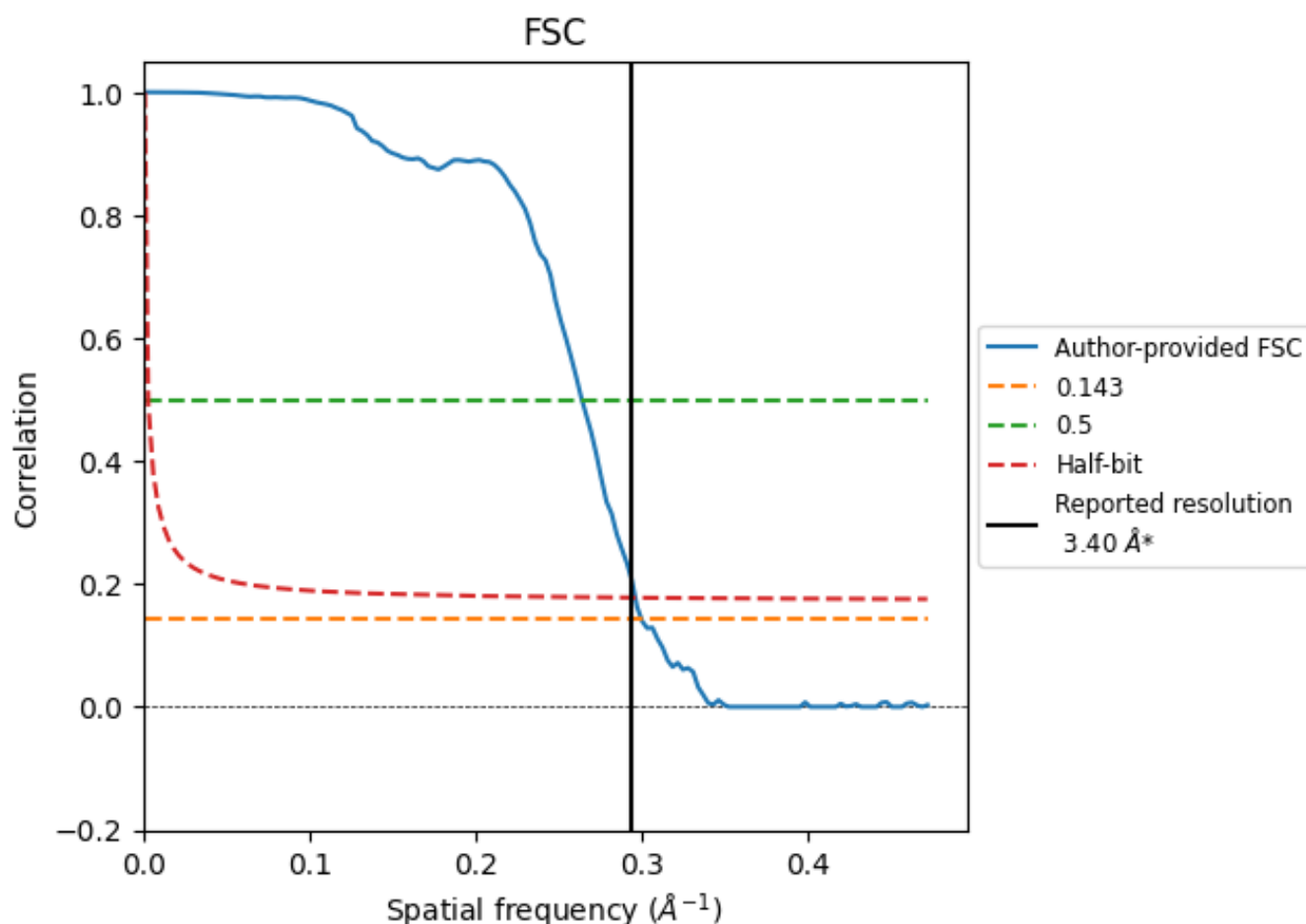


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

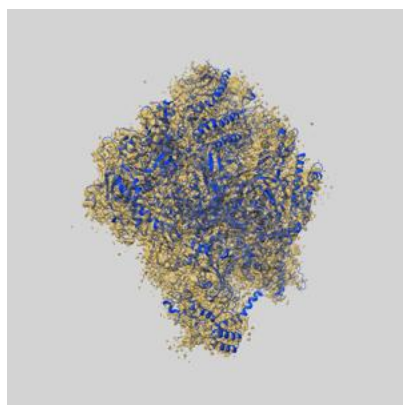
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.79	3.38
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

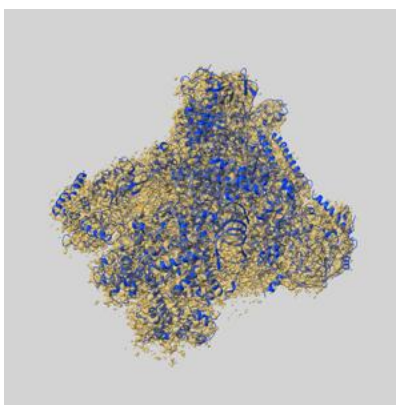
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3956 and PDB model 6EU1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

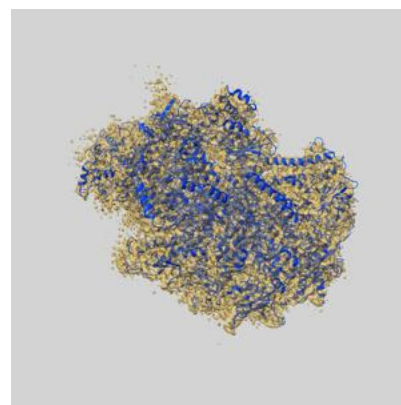
9.1 Map-model overlay [i](#)



X



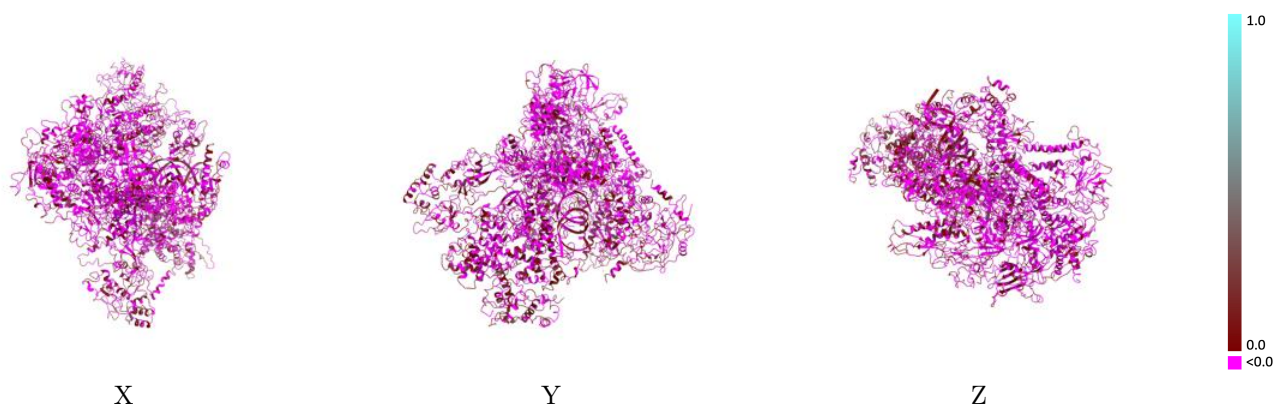
Y



Z

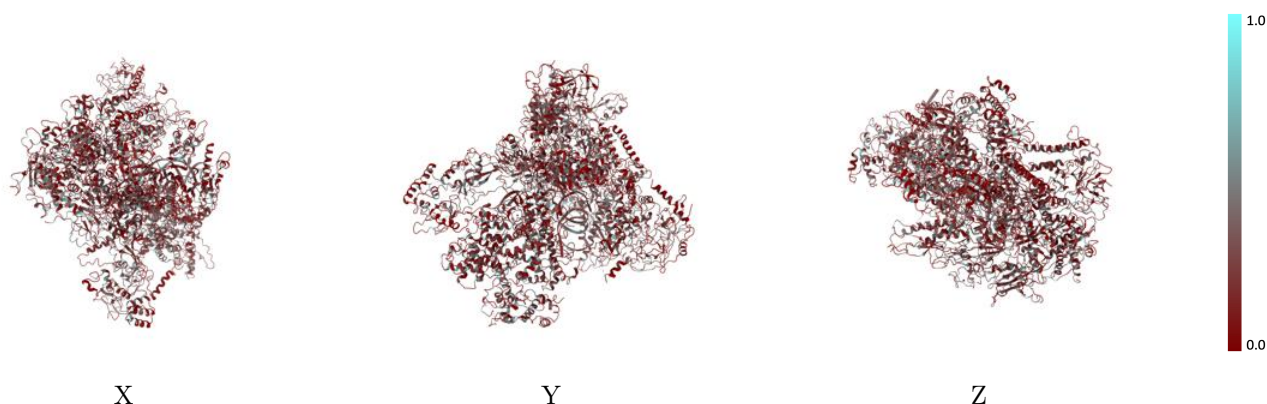
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



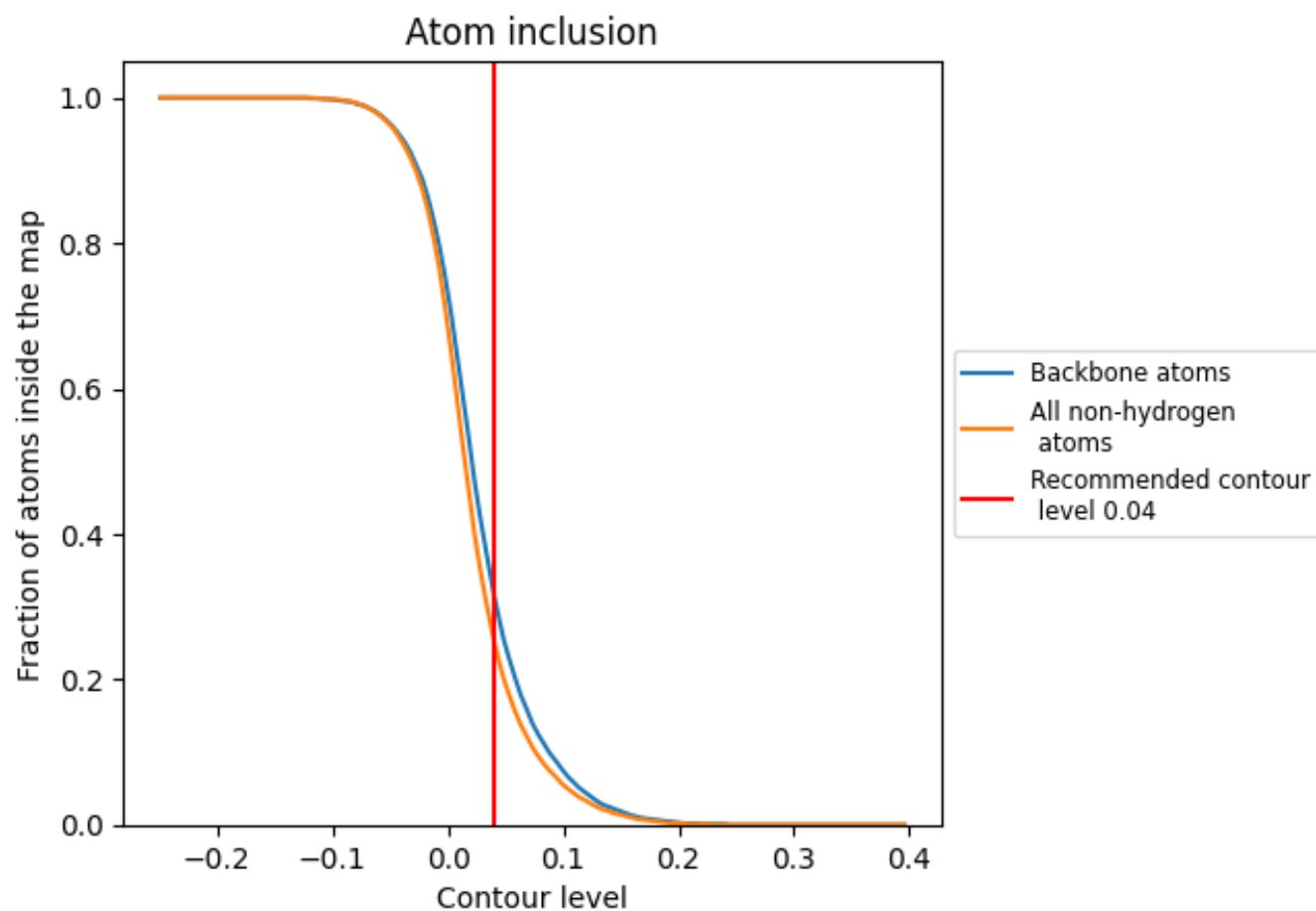
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 25% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.2530	 -0.0420
A	 0.2480	 -0.0590
B	 0.2650	 -0.0660
C	 0.2610	 -0.0710
D	 0.2520	 0.0570
E	 0.2590	 -0.0370
F	 0.2590	 -0.0480
G	 0.2450	 -0.0030
H	 0.2070	 -0.0950
I	 0.1670	 -0.0310
J	 0.2810	 -0.0860
K	 0.2670	 -0.0810
L	 0.3120	 -0.0520
M	 0.2320	 0.0280
N	 0.1760	 -0.0700
O	 0.2590	 -0.0070
P	 0.2430	 0.0380
Q	 0.2040	 0.0100
R	 0.3080	 0.0380
S	 0.3270	 0.0370

