



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:51 AM UTC

PDB ID : 6EU3 / pdb_00006eu3
EMDB ID : EMD-3958
Title : Apo RNA Polymerase III - closed conformation (cPOL3)
Authors : Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A.
Deposited on : 2017-10-27
Resolution : 3.30 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

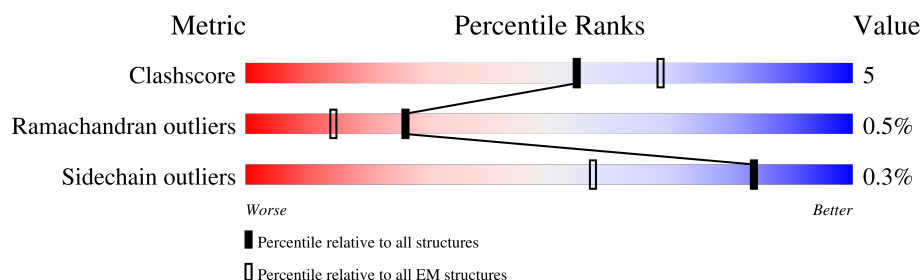
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	74% 82% 14% .
2	B	1149	74% 81% 15% ..
3	C	335	73% 86% 13%
4	D	161	51% 64% 10% 26%
5	E	215	78% 81% 19%
6	F	155	40% 45% 8% 46%
7	G	212	67% 75% 16% 10%
8	H	146	82% 77% 18% .

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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	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 38330 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	1402	Total	C	N	O	S	0	0
			10980	6924	1930	2068	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	119	Total	C	N	O	S	0	0
			977	628	156	187	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	191	Total	C	N	O	S	0	0
			1544	1007	250	281	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	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	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	68	Total	C	N	O	S	0	0
			558	356	97	99	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	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	0	0
			358	221	71	62	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	165	Total	C	N	O	S	0	0
			1347	862	229	255	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	537	Total	C	N	O	S	0	0
			4316	2748	739	810	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	123	Total	C	N	O	S	0	0
			1024	667	161	192	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	40	Total	C	N	O	0	0
			311	204	50	57		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

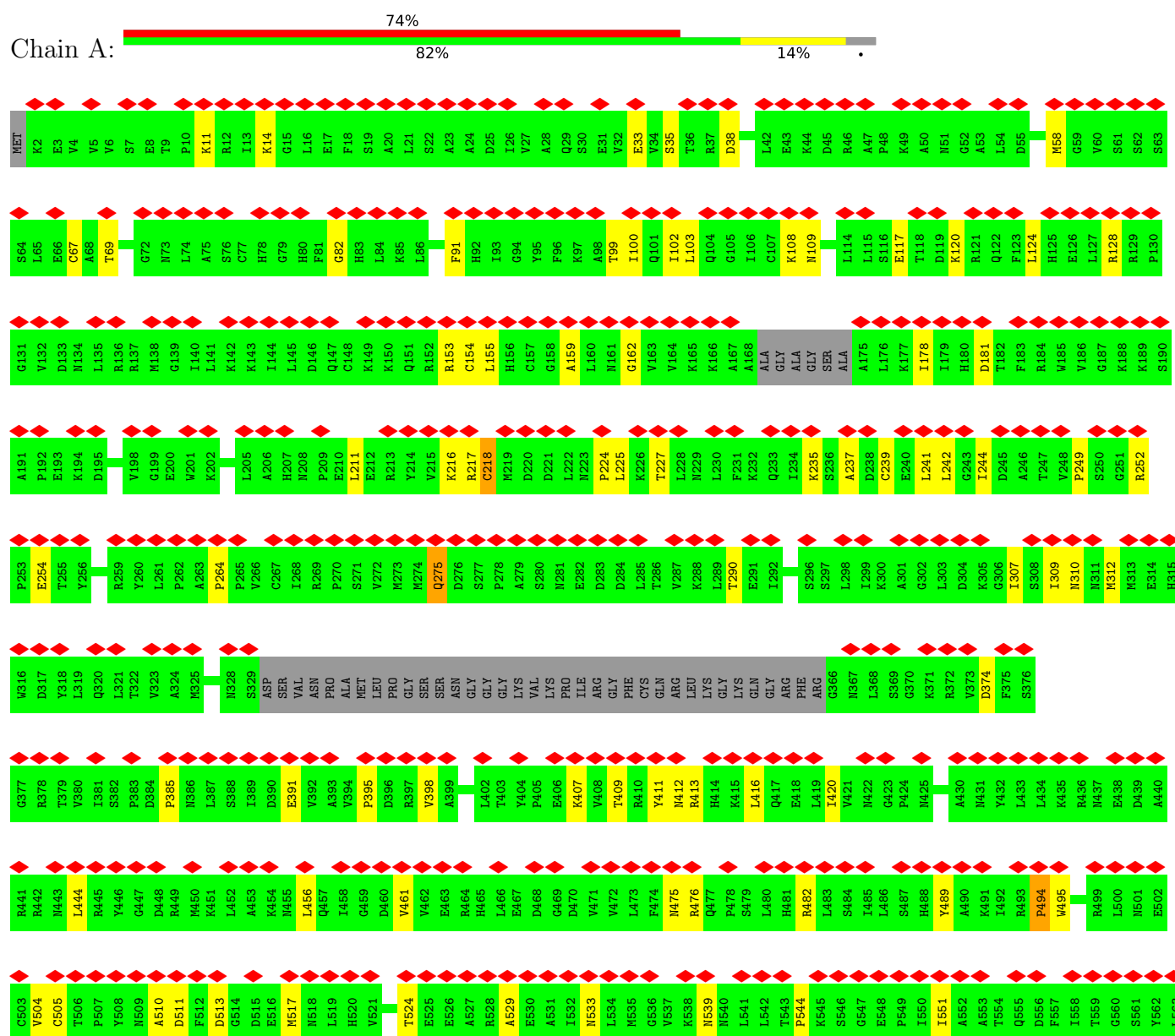
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

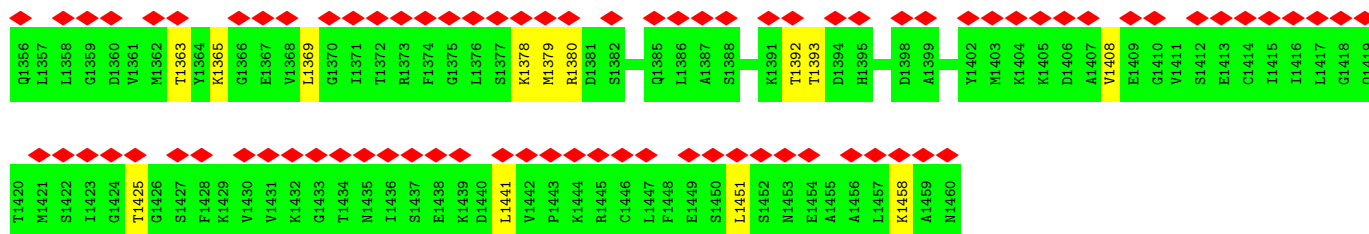
3 Residue-property plots

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.

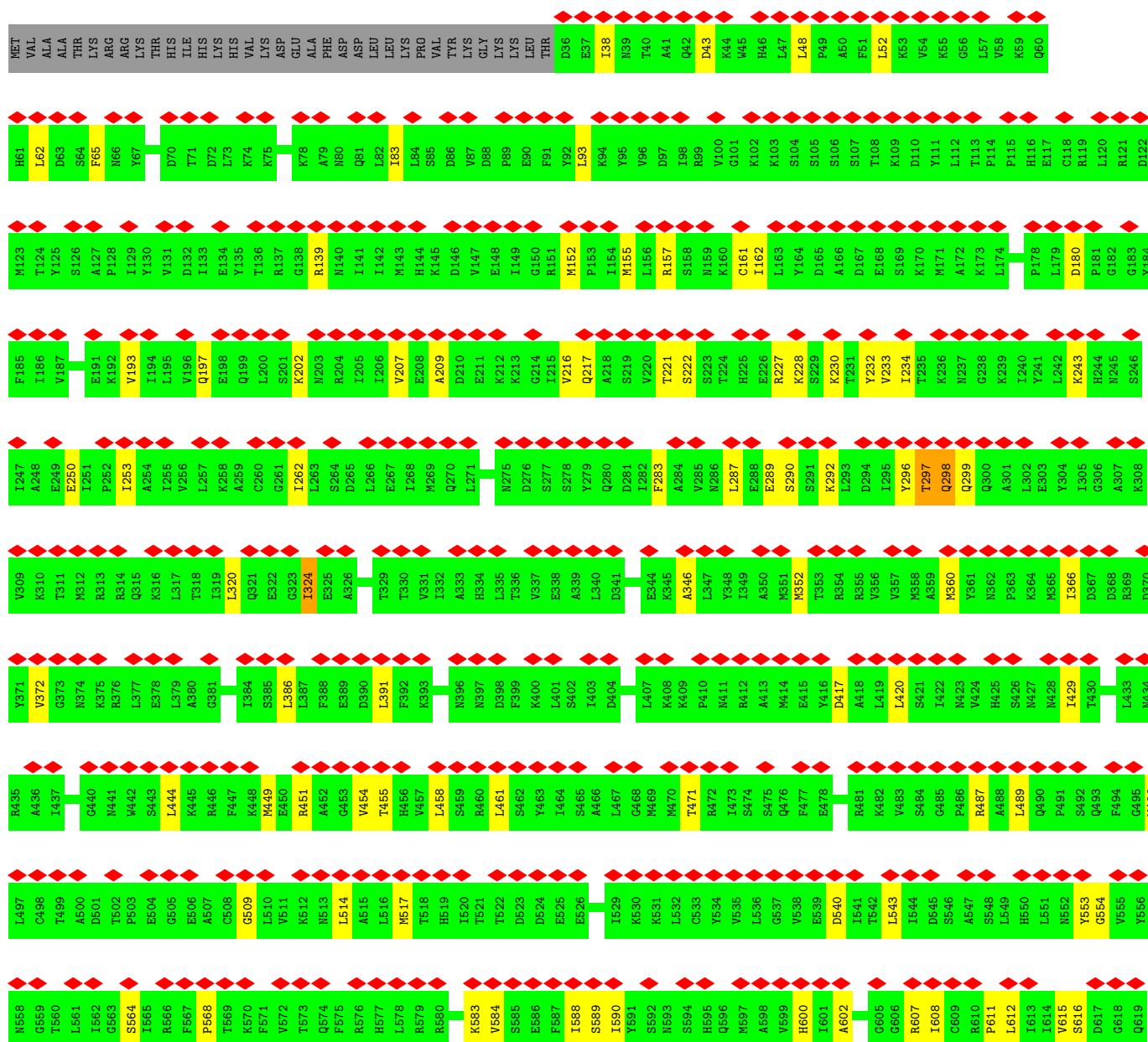
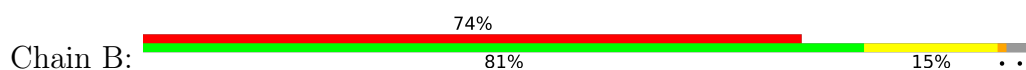
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

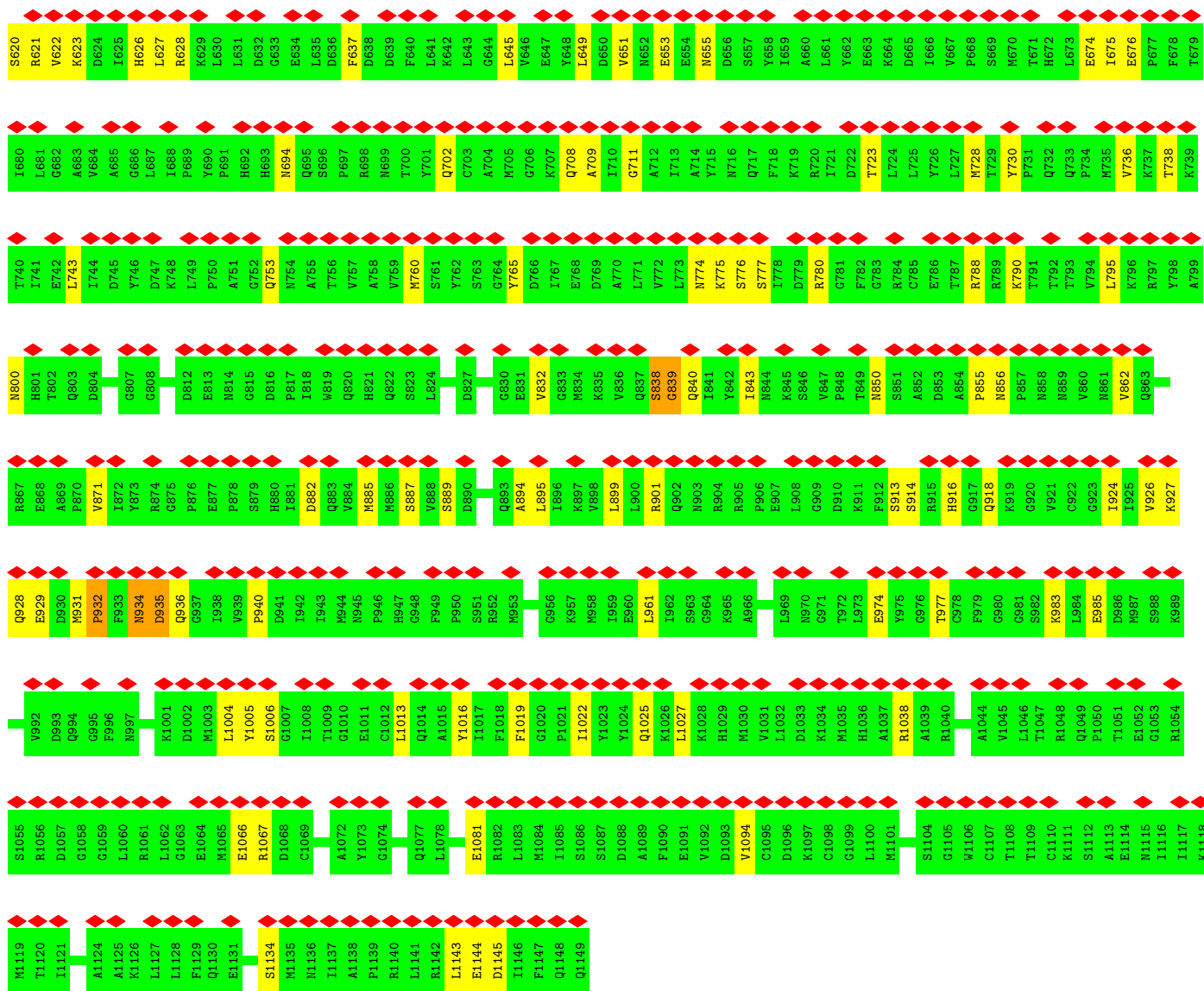


E1296	G1297	Y1298	T1299	L1300	R1301	D1302	V1303	G1304	M1305	T1306	D1307	G1308	V1309	I1310	G1311	S1312	R1313	T1314	T1315	T1316	H1317	H1318	V1319	E1320	E1321	F1322	F1323	S1324	L1325	P1268	D1269	G1327	I1328	E1329	A1330	A1331	R1332	I1333	I1335	R1336	R1337	E1338	I1339	M1340	Y1341	T1342	M1343	S1344	M1345	H1346	G1347	M1348	S1349	V1350	D1351	P1352	R1353	H1354	I1355
F1236	GLU	GLY	TYR	LYS	ALA	LYS	SER	SER	ILE	THR	ALA	LYS	GLU	PRO	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	D1277	I1278	S1279	R1280	A1281	V1282	I1283	N1284	R1285	R1286	D1287	D1288	G1289	K1290	R1291	E1292	L1293	L1294	V1295	
V1173	Q1174	D1175	V1176	Y1177	K1178	D1179	N1180	L1181	S1182	F1183	I1184	Q1185	V1186	R1187	I1188	D1189	G1190	G1191	T1192	I1193	D1194	K1195	L1196	Q1197	L1198	E1199	L1200	T1201	I1202	E1203	N1204	A1205	A1206	I1209	A1212	S1213	K1214	L1215	K1216	I1217	Q1218	D1221	V1222	M1223	I1224	I1225	G1226	K1227	R1228	R1229	I1230	A1231	I1232	D1168	V1169	A1170	F1171	Y1172	
H1110	F1111	A1112	G1113	V1114	A1115	S1116	M1117	N1118	V1119	T1120	L1121	G1122	V1123	P1124	R1125	E1128	I1129	I1130	N1131	A1132	S1133	K1134	V1135	I1136	S1137	T1138	P1139	I1140	I1141	N1142	A1143	V1144	L1145	V1146	N1147	D1148	N1149	D1150	E1151	R1152	A1153	A1154	R1155	V1156	V1157	K1158	G1159	R1160	V1161	E1162	L1165	D1168	V1169	A1170	F1171	Y1172			
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N990	K991	A992	E993	Y994	V995	D996	Q997	Y998	D999	A1000	E1001	D1002	F1004	Y1005	H1006	S1007	L1008	R1009	E1010	Y1011	I1012	N1013	G1014	L1015	A1016	T1017	A1018	L1019	A1020	M1021	L1022	R1023	K1024	S1025	R1026	G1027	M1028	L1029	G1030	L1031	L1032	E1033	P1034	V1035	A1036	K1037	E1038	L1039	Q1040	G1041	I1042	D1043	P1044	D1045	E1046	T1047	P1049		
A930	Q931	P932	V933	N934	P935	N936	S937	S938	N939	D940	H941	A942	Y943	N944	Y945	T946	F947	N948	N949	Q950	D951	K952	G953	L954	L955	P956	Y957	A958	I959	N960	E961	T962	A963	N964	E965	P966	L967	G968	P969	L970	E971	E972	R973	L974	V975	R976	Y977	D978	N979	S980	G981	L982	Y984	K985	R986	D988	L989		
R869	E870	G871	L872	V873	D874	T875	A876	V877	K878	T879	R880	E881	T882	G883	Y884	H885	S886	R887	R888	L889	N890	K891	S892	L893	E894	D895	L896	S897	C898	Q899	Y900	D901	N902	T903	V904	R905	T906	S907	A908	N909	G910	N911	V912	Q913	F914	T915	Y916	G917	G918	D919	L921	S922	P923	L924	E925	G928	N929		
M809	V810	A811	V812	V813	G814	Q815	Q816	I817	S818	S819	G820	N821	R822	V823	P824	D825	G826	F827	Q828	D829	R830	S831	L832	P833	H834	F835	P836	K837	N838	S839	K840	T841	P842	Q843	S844	K845	G846	F847	V848	R849	N850	S851	F852	P853	S854	G855	L856	S857	P858	R859	E860	F861	L862	F863	H864	A865	L866	G867	
G748	E749	L750	E751	T752	Q753	P754	G755	T756	N757	E758	Q760	T761	E763	A764	K765	I766	G767	G768	L769	L770	S771	T772	V773	R774	E775	E776	V777	D778	T779	R780	K781	D782	L783	E784	L785	D786	N787	W788	A789	A790	F791	L792	I793	W794	A795	T796	S799	K800	G801	S802	T803	L804	N805	L806	V806	S807	Q808		
E689	A690	A691	N692	A693	M694	N695	R696	M697	A698	K699	L700	C701	A702	R703	F704	L705	G706	N707	R708	G709	F710	S711	T712	G713	T714	N715	D716	V717	P718	P719	A720	D721	K722	L723	K724	Q725	K726	K727	E728	E729	L730	V731	E732	I733	A734	Y735	K736	K737	D738	E739	E740	L741	T742	T743	L744	F745	L882	R883	D884
N625	L626	D627	A628	K629	N630	K631	F632	F633	V634	P635	P636	K637	S638	K639	S640	L641	P642	N643	E644	M645	S646	Q647	N648	D649	G650	F651	V652	I653	I654	G655	S657	Q658	I659	L660	S661	G662	V663	M664	D665	K666	S667	V668	L669	G670	D671	F610	G672	K673	K674	H675	S676	V677	F678	Y679	T680	I681	L682	R683	D684
I564	S565	H566	K567	S569	F570	Y571	D572	R573	A574	T575	L576	T577	Q578	L579	L580	P581	M582	S583	S584	D585	G586	I587	E588	H589	F590	D591	P594	P595	A596	I597	M598	K599	P600	Y601	Y602	L603	M604	T605	G606	K607	Q608	P609	F610	S611	L612	L613	I614	K615	P616	N617	H618	N619	S620	P621	V622	I624			

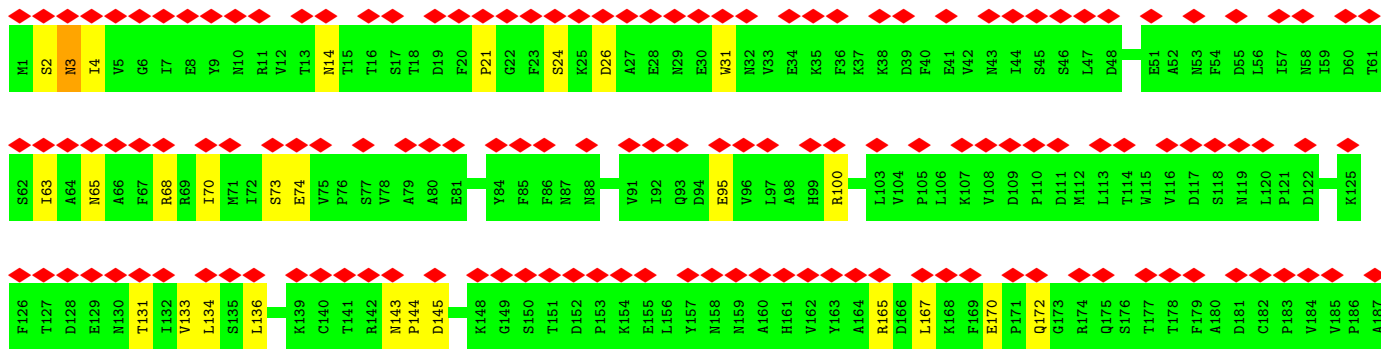
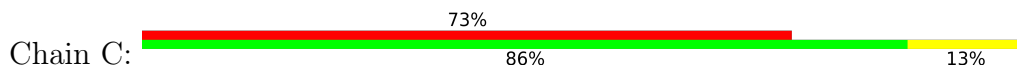


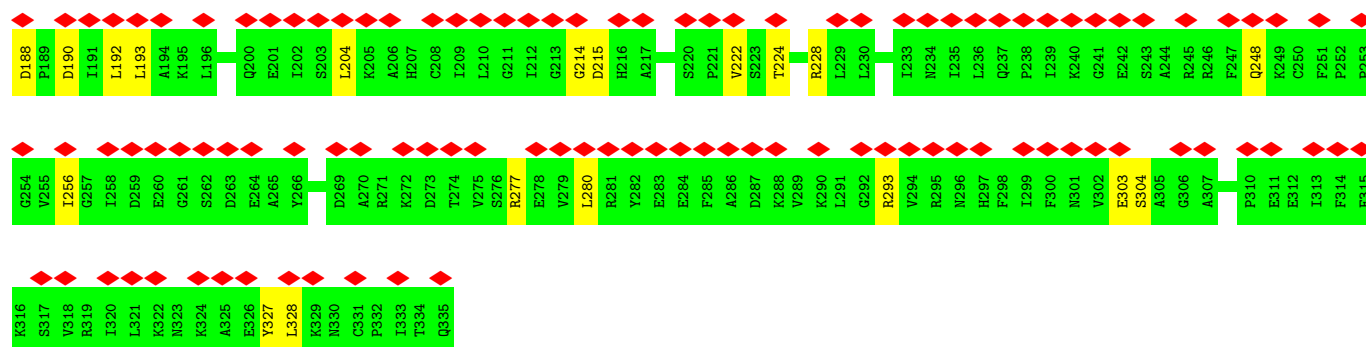
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2



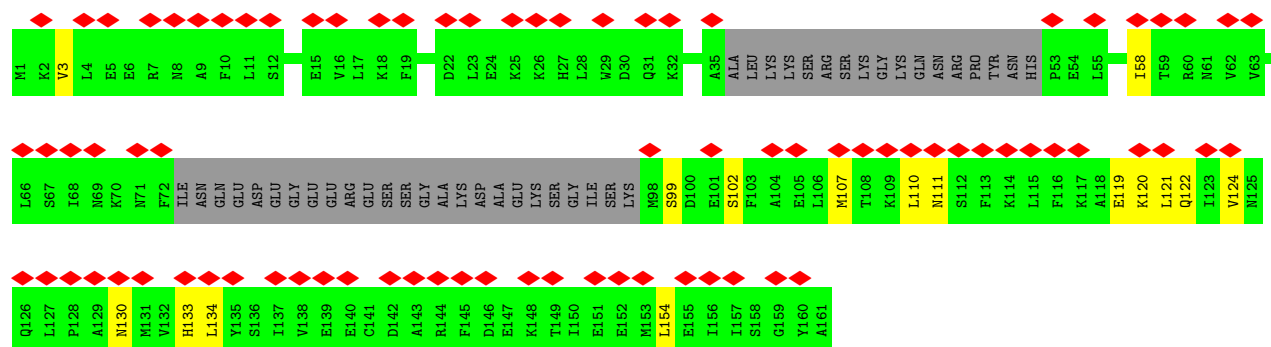


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

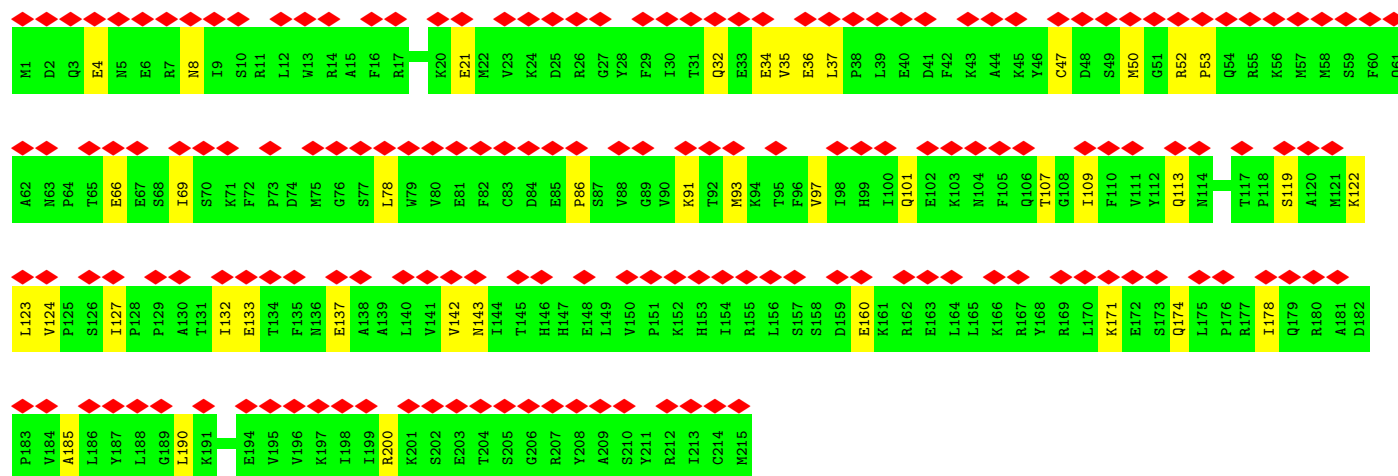
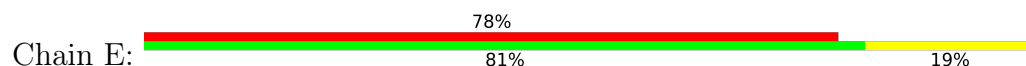




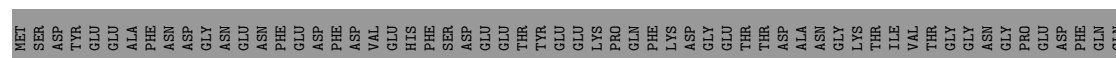
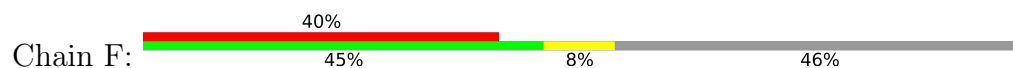
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

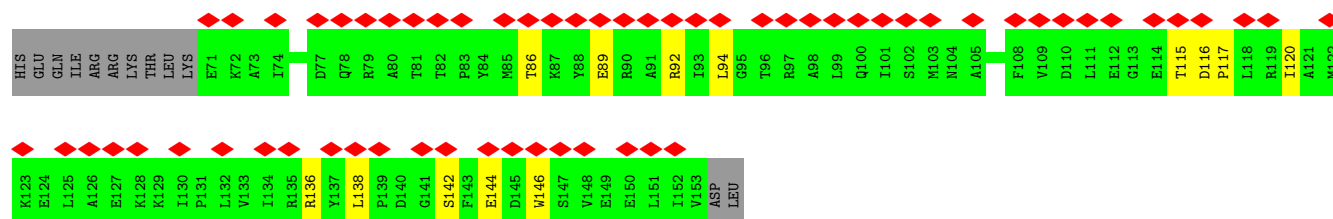


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

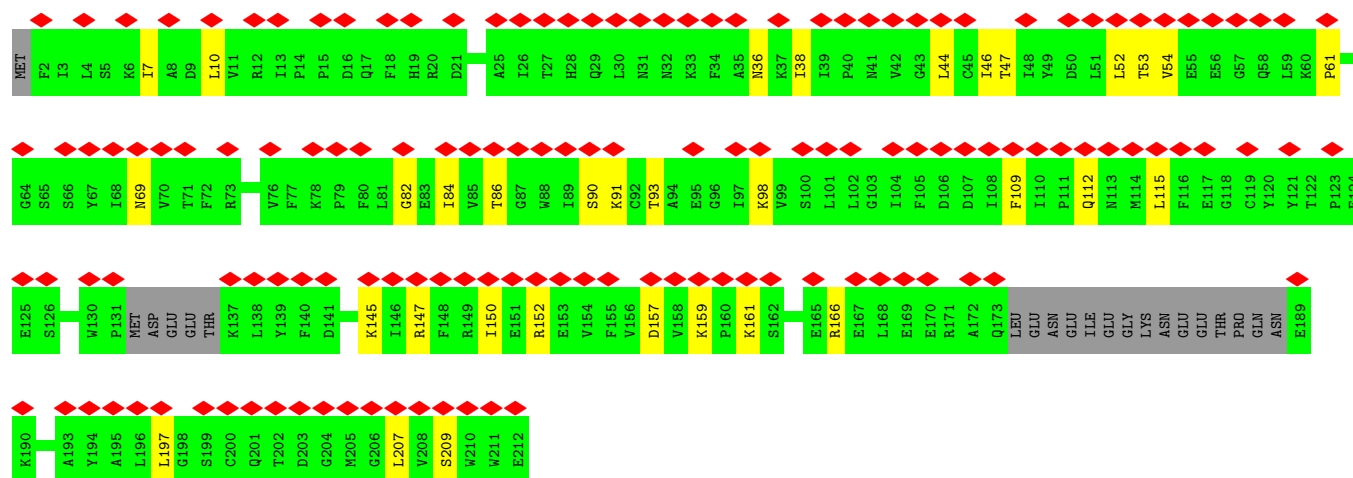
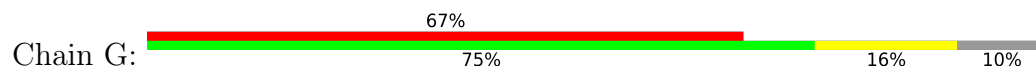


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

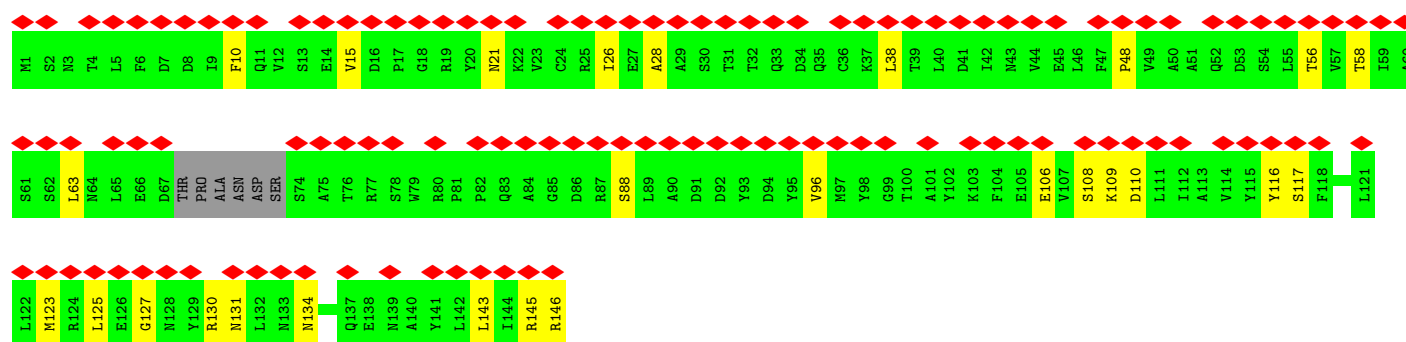
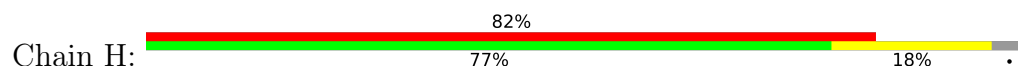




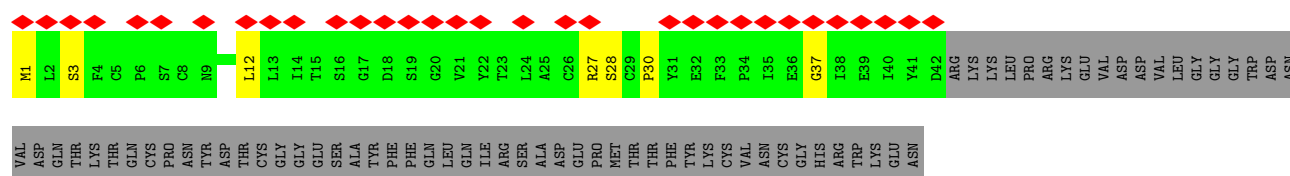
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



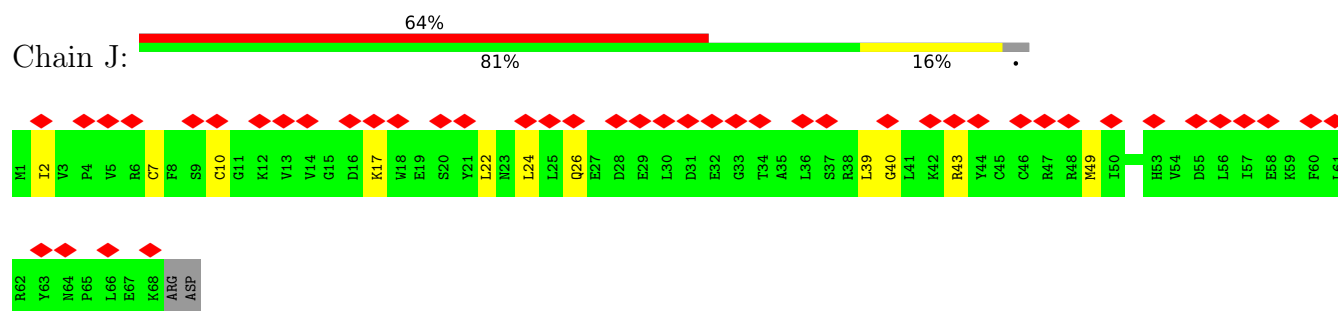
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



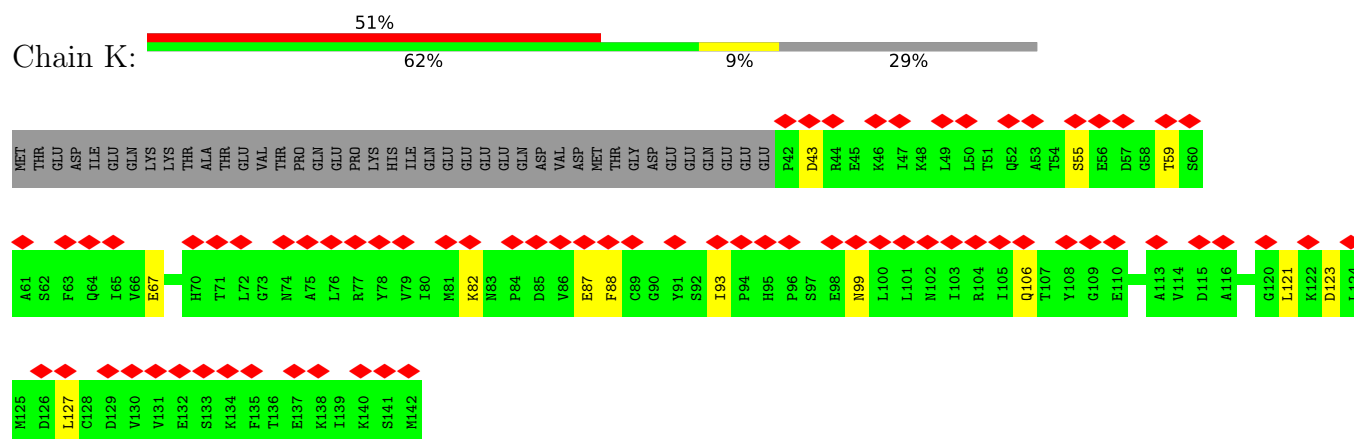
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10



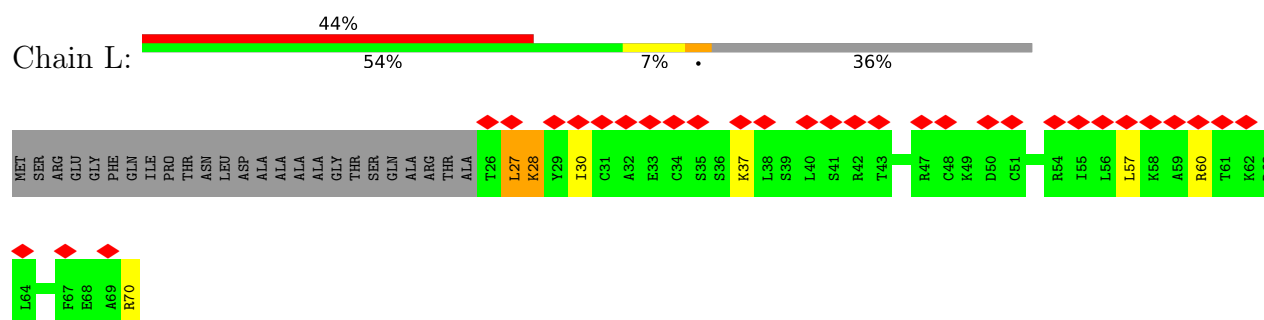
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



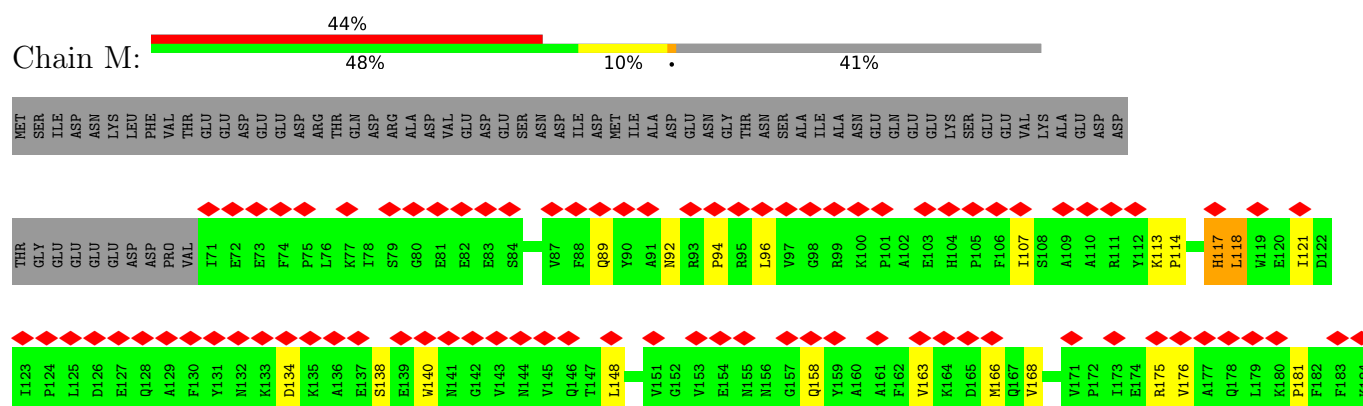
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

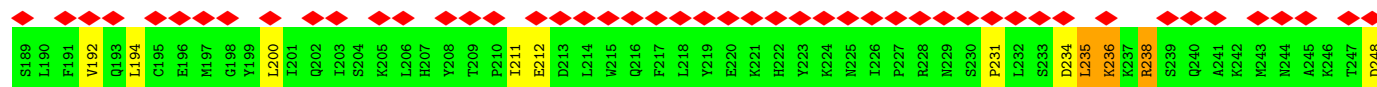


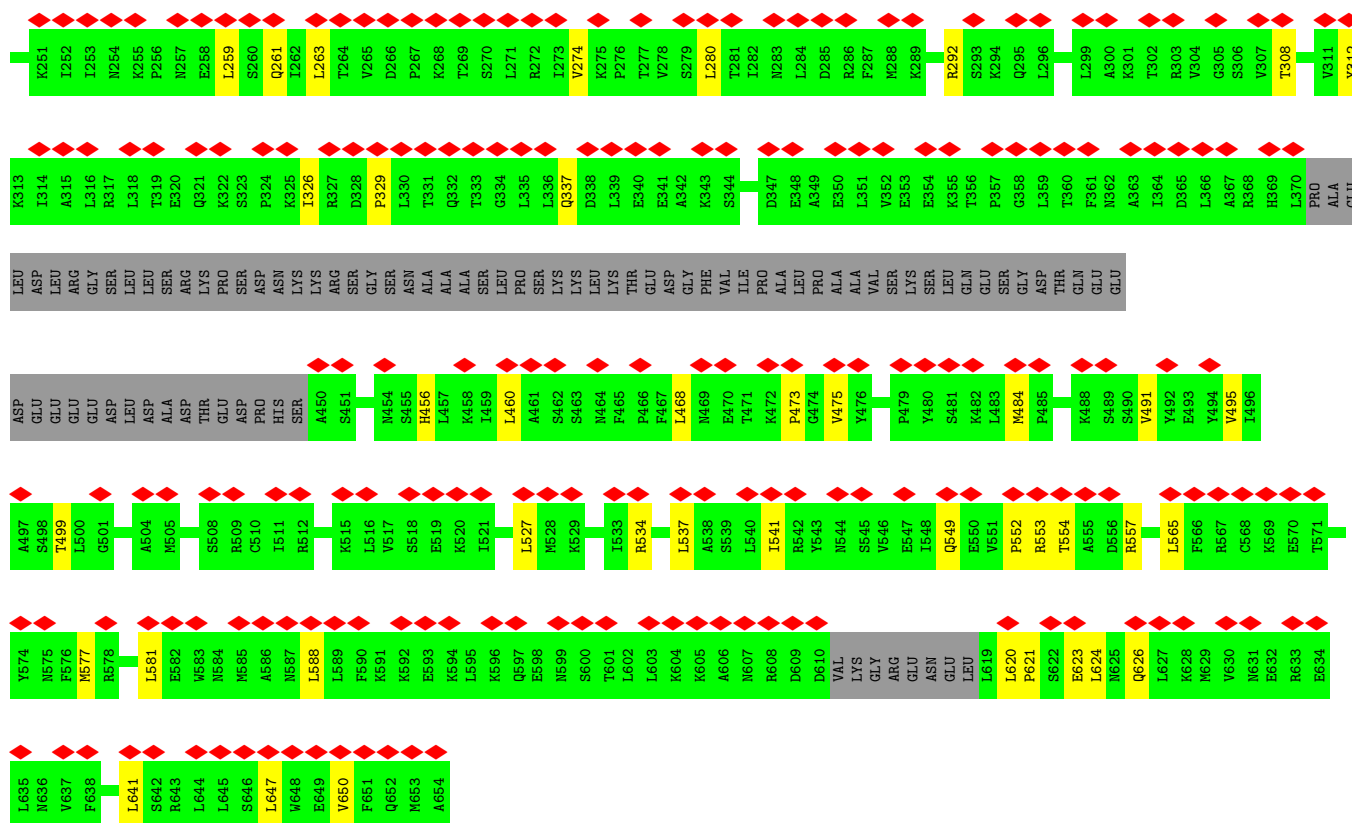
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



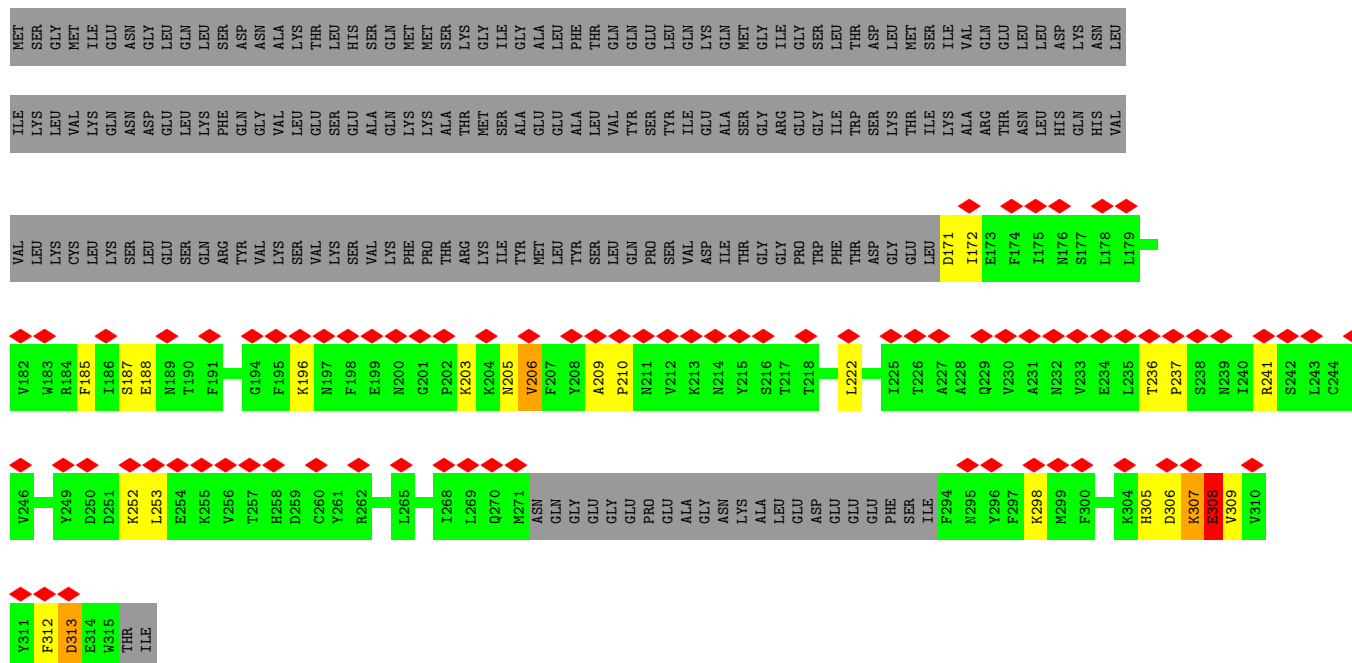
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



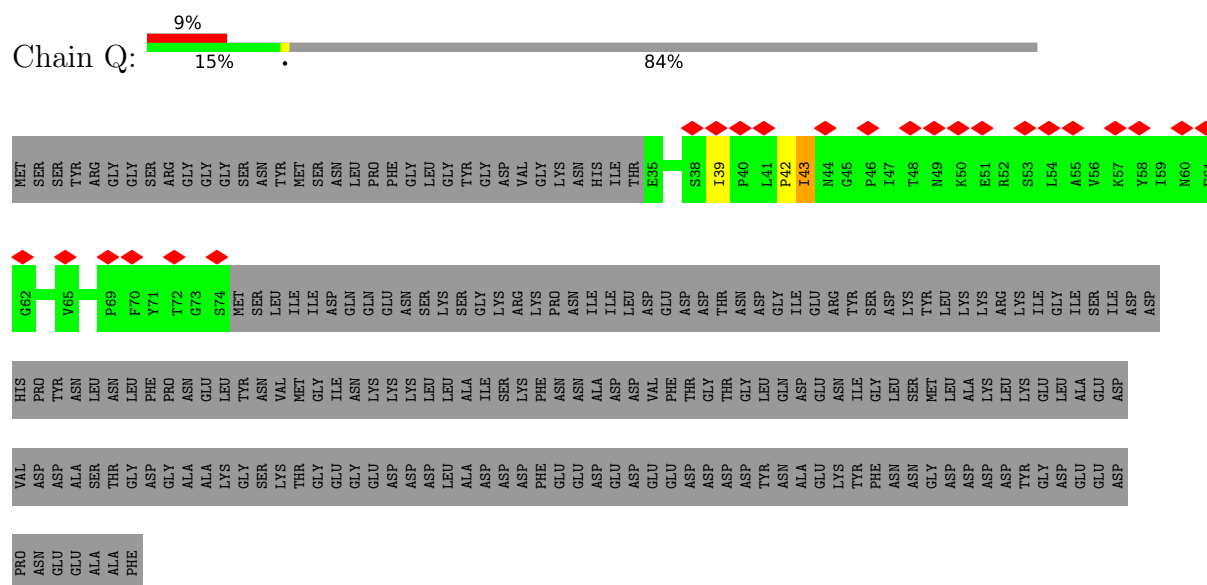




• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62306	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	0.385	Depositor
Minimum map value	-0.237	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/11176	0.59	6/15104 (0.0%)
2	B	0.21	0/8943	0.59	8/12068 (0.1%)
3	C	0.20	0/2711	0.58	0/3676
4	D	0.19	0/991	0.55	0/1328
5	E	0.21	0/1795	0.51	0/2416
6	F	0.22	0/683	0.61	0/923
7	G	0.20	0/1583	0.57	0/2146
8	H	0.21	0/1138	0.62	2/1540 (0.1%)
9	I	0.17	0/328	0.53	0/445
10	J	0.23	0/567	0.74	2/761 (0.3%)
11	K	0.21	0/803	0.61	0/1083
12	L	0.20	0/360	0.64	2/478 (0.4%)
13	M	0.23	0/1378	0.70	2/1863 (0.1%)
14	N	0.26	0/810	0.79	1/1088 (0.1%)
15	O	0.21	0/4380	0.61	0/5908
16	P	0.34	0/1050	0.93	5/1424 (0.4%)
17	Q	0.38	0/320	0.98	3/434 (0.7%)
All	All	0.22	0/39016	0.61	31/52685 (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	6
2	B	0	8
3	C	0	1
8	H	0	1
12	L	0	1
13	M	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	3
15	O	0	3
16	P	0	8
17	Q	0	1
All	All	0	36

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	409	LEU	N-CA-C	-8.60	92.49	110.80
1	A	275	GLN	CA-C-N	6.88	134.69	121.54
1	A	275	GLN	C-N-CA	6.88	134.69	121.54
17	Q	43	ILE	CA-C-N	6.26	133.49	121.54
17	Q	43	ILE	C-N-CA	6.26	133.49	121.54
16	P	308	GLU	CA-C-N	6.11	132.97	121.97
16	P	308	GLU	C-N-CA	6.11	132.97	121.97
2	B	324	ILE	N-CA-C	-5.69	107.95	113.53
16	P	210	PRO	N-CA-C	5.66	120.11	111.11
17	Q	39	ILE	CB-CA-C	5.63	115.97	109.89
2	B	637	PHE	CA-C-N	5.56	132.17	121.54
2	B	637	PHE	C-N-CA	5.56	132.17	121.54
2	B	296	TYR	CA-C-N	5.49	132.02	121.54
2	B	296	TYR	C-N-CA	5.49	132.02	121.54
8	H	109	LYS	CA-C-N	5.39	130.06	122.46
8	H	109	LYS	C-N-CA	5.39	130.06	122.46
16	P	252	LYS	CA-C-N	5.26	131.59	121.54
16	P	252	LYS	C-N-CA	5.26	131.59	121.54
2	B	839	GLY	N-CA-C	5.25	125.64	113.18
13	M	114	PRO	CA-C-N	5.24	131.55	121.54
13	M	114	PRO	C-N-CA	5.24	131.55	121.54
12	L	28	LYS	CA-C-N	5.14	131.35	121.54
12	L	28	LYS	C-N-CA	5.14	131.35	121.54
1	A	584	SER	CA-C-N	5.09	131.27	121.54
1	A	584	SER	C-N-CA	5.09	131.27	121.54
1	A	218	CYS	CA-C-N	5.08	131.24	121.54
1	A	218	CYS	C-N-CA	5.08	131.24	121.54
2	B	139	ARG	CA-C-N	5.03	129.54	122.46
2	B	139	ARG	C-N-CA	5.03	129.54	122.46
10	J	40	GLY	CA-C-N	5.01	128.21	121.05
10	J	40	GLY	C-N-CA	5.01	128.21	121.05

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1351	ASP	Peptide
1	A	218	CYS	Peptide
1	A	275	GLN	Peptide
1	A	494	PRO	Peptide
1	A	511	ASP	Peptide
1	A	631	LYS	Peptide
2	B	297	THR	Peptide
2	B	298	GLN	Peptide
2	B	583	LYS	Peptide
2	B	838	SER	Peptide
2	B	856	ASN	Peptide
2	B	889	SER	Peptide
2	B	932	PRO	Peptide
2	B	934	ASN	Peptide
3	C	3	ASN	Peptide
8	H	108	SER	Peptide
12	L	28	LYS	Peptide
13	M	107	ILE	Peptide
13	M	117	HIS	Peptide
13	M	166	MET	Peptide
13	M	96	LEU	Peptide
14	N	377	ASN	Peptide
14	N	379	VAL	Peptide
14	N	410	GLY	Peptide
15	O	238	ARG	Peptide
15	O	248	ASP	Peptide
15	O	326	ILE	Peptide
16	P	205	ASN	Peptide
16	P	209	ALA	Peptide
16	P	236	THR	Peptide
16	P	306	ASP	Peptide
16	P	307	LYS	Peptide
16	P	308	GLU	Peptide
16	P	312	PHE	Peptide
16	P	313	ASP	Peptide
17	Q	43	ILE	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	10980	0	11096	123	0
2	B	8788	0	8903	110	0
3	C	2655	0	2628	30	0
4	D	977	0	983	10	0
5	E	1759	0	1788	24	0
6	F	671	0	692	9	0
7	G	1544	0	1540	19	0
8	H	1120	0	1089	17	0
9	I	321	0	306	5	0
10	J	558	0	573	5	0
11	K	792	0	790	11	0
12	L	358	0	382	4	0
13	M	1347	0	1315	17	0
14	N	802	0	851	16	0
15	O	4316	0	4485	45	0
16	P	1024	0	992	7	0
17	Q	311	0	315	1	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	38330	0	38728	390	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 5.

All (390) 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)
1:A:162:GLY:HA3	1:A:181:ASP:O	1.86	0.75
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.73	0.70
15:O:107:LEU:O	15:O:119:TYR:HB2	1.92	0.69
1:A:475:ASN:HD21	2:B:1066:GLU:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.79	0.65
7:G:90:SER:HB2	7:G:98:LYS:HG3	1.80	0.64
2:B:589:SER:HB3	2:B:653:GLU:HG3	1.81	0.63
2:B:607:ARG:HH11	2:B:651:VAL:HB	1.64	0.63
4:D:58:ILE:HD12	7:G:36:ASN:HD21	1.64	0.63
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.81	0.63
2:B:887:SER:HB2	2:B:895:LEU:HB3	1.81	0.62
1:A:869:ARG:HH21	2:B:509:GLY:HA2	1.62	0.62
15:O:552:PRO:HG3	15:O:557:ARG:HA	1.80	0.62
1:A:1328:ILE:HD13	5:E:178:ILE:HG13	1.83	0.61
1:A:235:LYS:HG3	1:A:237:ALA:H	1.64	0.61
1:A:216:LYS:HD3	1:A:217:ARG:HG3	1.83	0.61
3:C:277:ARG:HB2	3:C:280:LEU:HD12	1.83	0.60
15:O:40:ARG:NH2	16:P:313:ASP:OD1	2.34	0.60
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.66	0.60
2:B:694:ASN:HD21	2:B:916:HIS:HD2	1.49	0.60
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.84	0.59
2:B:52:LEU:HD22	2:B:743:LEU:HD23	1.84	0.59
1:A:38:ASP:HB2	1:A:290:THR:HG23	1.83	0.59
9:I:1:MET:HE1	9:I:37:GLY:HA3	1.84	0.59
1:A:1369:LEU:HD11	1:A:1378:LYS:HB3	1.85	0.59
1:A:1152:ARG:NH1	1:A:1197:GLN:OE1	2.36	0.59
1:A:573:ARG:HH22	11:K:87:GLU:HB3	1.67	0.58
3:C:63:ILE:HD13	11:K:127:LEU:HD21	1.85	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.36	0.58
2:B:675:ILE:HG22	2:B:676:GLU:HG3	1.83	0.58
2:B:776:SER:O	2:B:780:ARG:NH1	2.37	0.58
3:C:2:SER:O	3:C:14:ASN:ND2	2.37	0.58
1:A:252:ARG:NH2	1:A:254:GLU:OE2	2.36	0.58
1:A:652:VAL:HG22	1:A:662:GLY:HA3	1.87	0.57
1:A:154:CYS:SG	1:A:155:LEU:N	2.77	0.57
1:A:1184:ILE:HD12	1:A:1232:ILE:HB	1.86	0.57
10:J:24:LEU:HD12	10:J:39:LEU:HD12	1.86	0.57
1:A:103:LEU:O	1:A:108:LYS:NZ	2.37	0.57
2:B:612:LEU:HD12	2:B:649:LEU:HD12	1.84	0.57
10:J:22:LEU:O	10:J:26:GLN:NE2	2.38	0.57
2:B:788:ARG:NH1	2:B:882:ASP:OD2	2.38	0.56
2:B:588:ILE:HA	2:B:602:ALA:O	2.05	0.56
1:A:869:ARG:HD3	2:B:489:LEU:HB2	1.88	0.56
1:A:1206:ALA:HB2	1:A:1224:ILE:HD11	1.87	0.56
2:B:496:MET:HB3	2:B:608:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:VAL:HB	2:B:931:MET:HE3	1.88	0.56
15:O:620:LEU:HD22	15:O:623:GLU:HG2	1.87	0.56
6:F:92:ARG:HH21	7:G:61:PRO:HG3	1.69	0.56
1:A:505:CYS:HB2	1:A:510:ALA:HB3	1.88	0.56
8:H:58:THR:HB	8:H:143:LEU:HB2	1.88	0.56
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.86	0.56
1:A:1185:GLN:OE1	1:A:1229:ARG:NH1	2.39	0.56
15:O:292:ARG:HD2	15:O:484:MET:HE1	1.87	0.56
16:P:203:LYS:HB2	16:P:206:VAL:HG22	1.87	0.55
2:B:299:GLN:HG3	13:M:190:ASN:HD22	1.71	0.55
1:A:533:ASN:O	1:A:539:ASN:ND2	2.40	0.55
2:B:622:VAL:HG22	2:B:645:LEU:HD23	1.88	0.55
15:O:137:ILE:HA	15:O:140:ILE:HG22	1.89	0.55
4:D:110:LEU:HD21	4:D:120:LYS:HB2	1.87	0.55
9:I:28:SER:O	13:M:185:TYR:OH	2.25	0.55
2:B:202:LYS:HB3	2:B:222:SER:HB2	1.89	0.55
2:B:882:ASP:HB3	2:B:901:ARG:HE	1.72	0.54
14:N:304:PHE:CE1	14:N:409:LEU:HB3	2.41	0.54
7:G:84:ILE:HD11	7:G:147:ARG:HB3	1.90	0.54
7:G:86:THR:HG22	7:G:145:LYS:HD2	1.89	0.54
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.90	0.54
1:A:654:ILE:HG12	1:A:659:ILE:HG13	1.90	0.54
1:A:1059:LEU:HD11	8:H:106:GLU:HB2	1.89	0.54
1:A:1441:LEU:HD21	7:G:54:VAL:HG22	1.89	0.54
2:B:838:SER:O	2:B:840:GLN:N	2.39	0.54
14:N:409:LEU:N	14:N:409:LEU:HD12	2.23	0.54
1:A:1055:SER:HB2	8:H:131:ASN:HD22	1.73	0.53
6:F:89:GLU:OE2	6:F:136:ARG:NH2	2.41	0.53
1:A:1023:ARG:NH2	1:A:1045:ASP:OD1	2.41	0.53
15:O:43:ASN:HB2	15:O:47:PHE:HB2	1.90	0.53
15:O:312:TYR:HB2	15:O:460:LEU:HD21	1.89	0.53
3:C:143:ASN:HD22	3:C:144:PRO:HD2	1.73	0.53
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.40	0.53
1:A:391:GLU:HG2	1:A:489:TYR:HB2	1.91	0.53
2:B:207:VAL:HG22	2:B:217:GLN:HG3	1.90	0.53
1:A:504:VAL:HG12	1:A:551:ILE:HD11	1.91	0.53
2:B:774:ASN:ND2	2:B:775:LYS:O	2.42	0.53
1:A:1278:ILE:HG13	1:A:1297:GLY:HA3	1.89	0.53
5:E:4:GLU:O	5:E:8:ASN:ND2	2.38	0.53
6:F:117:PRO:HA	6:F:120:ILE:HG12	1.91	0.52
2:B:209:ALA:HB2	2:B:366:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:LYS:NZ	7:G:93:THR:OG1	2.42	0.52
7:G:98:LYS:HB3	7:G:109:PHE:HD1	1.74	0.52
14:N:303:ARG:HG3	14:N:411:ARG:HB2	1.91	0.52
8:H:123:MET:HE2	8:H:125:LEU:HD23	1.91	0.52
15:O:194:LEU:HD22	15:O:200:LEU:HG	1.91	0.52
1:A:1332:ARG:HB3	1:A:1363:THR:HG21	1.92	0.52
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.91	0.52
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.92	0.52
8:H:48:PRO:O	8:H:146:ARG:NH2	2.42	0.52
14:N:409:LEU:N	14:N:409:LEU:CD1	2.73	0.52
1:A:1304:MET:HG2	5:E:142:VAL:HG11	1.90	0.52
2:B:927:LYS:NZ	3:C:214:GLY:O	2.43	0.52
13:M:230:SER:O	13:M:234:HIS:ND1	2.41	0.52
2:B:612:LEU:HD22	2:B:674:GLU:HA	1.90	0.51
15:O:150:GLU:HG2	15:O:151:GLU:HG3	1.92	0.51
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.91	0.51
1:A:224:PRO:HA	1:A:227:THR:HG22	1.91	0.51
1:A:1253:GLU:OE2	9:I:27:ARG:NH1	2.44	0.51
1:A:1425:THR:HG22	6:F:92:ARG:HD2	1.91	0.51
2:B:736:VAL:HG12	2:B:974:GLU:HB2	1.92	0.51
14:N:380:MET:SD	14:N:421:GLN:NE2	2.83	0.51
1:A:873:VAL:HG21	2:B:487:ARG:HB3	1.92	0.51
1:A:1329:GLU:OE2	5:E:200:ARG:NE	2.44	0.51
7:G:161:LYS:HZ2	7:G:166:ARG:HA	1.76	0.51
2:B:553:TYR:HD2	2:B:568:PRO:HG2	1.76	0.51
14:N:372:SER:HB2	14:N:382:ILE:HG22	1.91	0.51
15:O:102:ARG:O	15:O:123:ASN:ND2	2.43	0.51
1:A:1351:ASP:O	1:A:1353:ARG:N	2.44	0.51
1:A:894:GLU:OE2	2:B:1067:ARG:NH1	2.44	0.51
2:B:623:LYS:H	2:B:626:HIS:HD2	1.58	0.51
1:A:307:ILE:HD11	1:A:312:MET:HG2	1.91	0.50
1:A:808:GLN:HE21	1:A:813:VAL:HG13	1.77	0.50
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.93	0.50
2:B:197:GLN:HE22	2:B:454:VAL:HG22	1.75	0.50
1:A:813:VAL:HG23	1:A:851:SER:HA	1.92	0.50
2:B:616:SER:HG	2:B:621:ARG:HH21	1.57	0.50
1:A:413:ARG:NH1	1:A:456:LEU:O	2.41	0.50
2:B:372:VAL:HB	2:B:651:VAL:HG11	1.93	0.50
2:B:554:GLY:HA2	2:B:564:SER:HA	1.93	0.50
3:C:100:ARG:NH1	3:C:193:LEU:O	2.45	0.50
1:A:1323:PHE:HE1	1:A:1328:ILE:HG13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:ASN:ND2	3:C:145:ASP:OD1	2.44	0.50
15:O:308:THR:HG23	15:O:456:HIS:HB3	1.94	0.50
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.93	0.50
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.93	0.50
1:A:124:LEU:HD23	1:A:128:ARG:HH12	1.77	0.50
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.77	0.49
1:A:1160:ARG:NH1	1:A:1307:ASP:O	2.45	0.49
2:B:738:THR:HG23	2:B:977:THR:HA	1.95	0.49
1:A:124:LEU:HD12	1:A:241:LEU:HD21	1.94	0.49
1:A:788:TRP:NE1	8:H:21:ASN:OD1	2.45	0.49
2:B:543:LEU:O	13:M:89:GLN:NE2	2.43	0.49
14:N:304:PHE:CE1	14:N:409:LEU:CB	2.96	0.49
9:I:3:SER:HB2	9:I:12:LEU:HD11	1.95	0.49
1:A:1258:TYR:O	1:A:1262:GLN:NE2	2.45	0.49
5:E:50:MET:SD	5:E:52:ARG:NH1	2.79	0.49
13:M:113:LYS:HE3	13:M:118:LEU:HB3	1.93	0.49
1:A:623:VAL:HG13	1:A:656:GLY:HA2	1.95	0.48
1:A:1223:ASN:HD21	1:A:1231:ALA:HB3	1.78	0.48
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.46	0.48
2:B:216:VAL:HG22	2:B:233:VAL:HG23	1.94	0.48
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.32	0.48
2:B:800:ASN:HD22	2:B:855:PRO:HG2	1.78	0.48
2:B:1005:TYR:OH	3:C:293:ARG:NH1	2.47	0.48
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.94	0.48
12:L:27:LEU:HD11	12:L:37:LYS:HD2	1.95	0.48
1:A:14:LYS:HD3	2:B:1144:GLU:HB3	1.96	0.48
1:A:1120:THR:HG22	1:A:1125:ARG:HB2	1.96	0.48
1:A:1194:ASP:O	1:A:1197:GLN:NE2	2.46	0.48
2:B:901:ARG:NH1	3:C:95:GLU:OE1	2.38	0.48
5:E:47:CYS:HA	5:E:53:PRO:HA	1.94	0.48
5:E:32:GLN:HE21	5:E:36:GLU:HG3	1.79	0.48
5:E:171:LYS:H	5:E:174:GLN:HE21	1.61	0.48
1:A:109:ASN:HD22	1:A:159:ALA:HB2	1.79	0.48
1:A:249:PRO:HB2	15:O:42:LEU:HD22	1.94	0.48
2:B:243:LYS:HA	2:B:250:GLU:HG2	1.96	0.48
3:C:224:THR:OG1	3:C:303:GLU:OE1	2.30	0.48
3:C:327:TYR:OH	11:K:43:ASP:OD2	2.32	0.48
1:A:409:THR:HG23	1:A:411:TYR:H	1.78	0.48
1:A:1136:ILE:HD11	1:A:1139:PRO:HB3	1.96	0.48
5:E:93:MET:HE2	5:E:123:LEU:HD23	1.96	0.48
1:A:1451:LEU:HD13	4:D:107:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLY:HA2	2:B:728:MET:HB2	1.96	0.48
2:B:929:GLU:OE2	3:C:73:SER:OG	2.25	0.47
2:B:940:PRO:HG3	2:B:1019:PHE:HE1	1.78	0.47
7:G:152:ARG:HB3	7:G:197:LEU:HD12	1.96	0.47
1:A:211:LEU:O	15:O:553:ARG:NH2	2.48	0.47
1:A:476:ARG:HD2	1:A:517:MET:HE2	1.96	0.47
2:B:760:MET:HE1	2:B:932:PRO:HD2	1.96	0.47
16:P:222:LEU:HB2	16:P:241:ARG:NH1	2.28	0.47
2:B:38:ILE:HG13	2:B:628:ARG:HG2	1.96	0.47
4:D:130:ASN:H	4:D:133:HIS:CE1	2.33	0.47
2:B:161:CYS:SG	2:B:162:ILE:N	2.87	0.47
1:A:117:GLU:HG3	15:O:212:GLU:HG3	1.96	0.47
5:E:119:SER:O	5:E:122:LYS:NZ	2.47	0.47
13:M:134:ASP:O	13:M:138:SER:CB	2.63	0.47
15:O:495:VAL:HG21	15:O:577:MET:HE1	1.96	0.47
1:A:832:LEU:HD21	1:A:862:LEU:HD23	1.97	0.47
2:B:43:ASP:HB3	2:B:627:LEU:HD13	1.97	0.47
2:B:217:GLN:HB3	2:B:232:TYR:HB3	1.96	0.47
3:C:188:ASP:OD1	3:C:188:ASP:N	2.46	0.47
5:E:91:LYS:HE3	15:O:231:PRO:HG2	1.96	0.47
15:O:499:THR:HG23	17:Q:42:PRO:HA	1.97	0.47
15:O:581:LEU:HD11	15:O:647:LEU:HD12	1.97	0.47
2:B:227:ARG:NH2	2:B:449:MET:SD	2.88	0.47
14:N:287:HIS:HB3	14:N:371:LEU:HD13	1.96	0.47
15:O:140:ILE:HD11	15:O:194:LEU:HD21	1.96	0.47
1:A:1058:GLN:NE2	8:H:134:ASN:O	2.48	0.47
2:B:234:ILE:HD13	2:B:360:MET:HE2	1.97	0.47
14:N:374:LYS:HA	14:N:380:MET:HG2	1.97	0.47
1:A:385:PRO:HD2	2:B:765:TYR:CD1	2.50	0.46
2:B:931:MET:HB3	2:B:940:PRO:HD2	1.97	0.46
16:P:187:SER:C	16:P:196:LYS:HZ1	2.23	0.46
1:A:790:ALA:HB1	1:A:794:MET:HE2	1.97	0.46
2:B:193:VAL:HG21	2:B:458:LEU:HD23	1.96	0.46
2:B:702:GLN:HE22	2:B:1025:GLN:HE22	1.63	0.46
2:B:850:ASN:ND2	2:B:862:VAL:O	2.45	0.46
15:O:552:PRO:HB2	15:O:554:THR:HG22	1.96	0.46
1:A:33:GLU:HG2	1:A:35:SER:H	1.80	0.46
2:B:788:ARG:HB3	2:B:899:LEU:HD11	1.98	0.46
13:M:245:LEU:HD21	14:N:404:SER:HA	1.96	0.46
5:E:97:VAL:HG13	5:E:127:ILE:HD11	1.97	0.46
4:D:119:GLU:HA	4:D:122:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:117:HIS:CE1	13:M:175:ARG:HH12	2.34	0.46
15:O:549:GLN:O	15:O:565:LEU:HB2	2.15	0.46
2:B:62:LEU:HA	2:B:155:MET:HE1	1.96	0.46
2:B:776:SER:HB2	2:B:928:GLN:HB2	1.98	0.46
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.98	0.46
1:A:264:PRO:HG3	2:B:1134:SER:HB2	1.98	0.46
1:A:529:ALA:O	1:A:533:ASN:ND2	2.49	0.46
1:A:890:MET:HE3	1:A:894:GLU:HG3	1.98	0.46
2:B:65:PHE:HE1	2:B:152:MET:HE1	1.81	0.46
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.98	0.46
7:G:10:LEU:HA	7:G:69:ASN:HA	1.97	0.46
13:M:158:GLN:HE22	14:N:415:LYS:HE3	1.81	0.46
1:A:967:LEU:HD22	1:A:1009:ARG:HH21	1.81	0.46
2:B:262:ILE:HG12	2:B:346:ALA:HB1	1.98	0.46
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.96	0.46
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.84	0.46
15:O:52:LEU:O	15:O:56:HIS:ND1	2.47	0.46
2:B:832:VAL:HB	12:L:60:ARG:HA	1.98	0.45
7:G:112:GLN:HG2	7:G:115:LEU:HD22	1.98	0.45
7:G:157:ASP:HB3	7:G:159:LYS:HG3	1.97	0.45
15:O:621:PRO:HA	15:O:624:LEU:HD23	1.97	0.45
1:A:374:ASP:OD1	2:B:1038:ARG:NH1	2.36	0.45
2:B:934:ASN:O	2:B:936:GLN:N	2.48	0.45
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.99	0.45
14:N:303:ARG:C	14:N:304:PHE:HD1	2.25	0.45
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.98	0.45
1:A:1332:ARG:HA	1:A:1335:ILE:HG22	1.98	0.45
2:B:1094:VAL:HG23	2:B:1143:LEU:HD11	1.97	0.45
13:M:121:ILE:HG22	13:M:148:LEU:HB2	1.98	0.45
1:A:1112:ALA:HB1	1:A:1116:SER:HB3	1.99	0.45
1:A:978:ASP:HB3	1:A:984:VAL:HG12	1.98	0.45
1:A:1458:LYS:NZ	4:D:111:ASN:O	2.45	0.45
5:E:124:VAL:HG23	5:E:132:ILE:HG13	1.99	0.45
14:N:304:PHE:N	14:N:304:PHE:CD1	2.85	0.45
14:N:382:ILE:HG12	14:N:421:GLN:HB3	1.99	0.45
15:O:100:GLN:NE2	15:O:166:LEU:O	2.48	0.45
15:O:588:LEU:HD23	15:O:641:LEU:HD23	1.97	0.45
3:C:215:ASP:OD1	12:L:70:ARG:NH2	2.50	0.45
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.99	0.45
1:A:225:LEU:HD23	15:O:541:ILE:HG22	1.99	0.45
1:A:895:ASP:OD2	1:A:1380:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:LEU:HB3	1:A:958:ALA:HB3	1.98	0.45
1:A:980:SER:HB3	5:E:160:GLU:HG2	1.98	0.45
2:B:157:ARG:NH2	2:B:180:ASP:OD1	2.50	0.45
2:B:461:LEU:HD23	2:B:708:GLN:HA	1.99	0.45
4:D:99:SER:HA	4:D:102:SER:HB2	1.98	0.45
5:E:101:GLN:HE21	5:E:127:ILE:HG13	1.82	0.45
1:A:239:CYS:HB3	1:A:244:ILE:HB	1.98	0.44
2:B:253:ILE:HD11	2:B:283:PHE:HE1	1.81	0.44
7:G:38:ILE:HG12	7:G:44:LEU:HD13	1.99	0.44
16:P:171:ASP:HA	16:P:172:ILE:HA	1.65	0.44
1:A:420:ILE:HG23	1:A:444:LEU:HD21	1.99	0.44
1:A:1209:ILE:HA	1:A:1212:ALA:HB2	2.00	0.44
15:O:235:LEU:HD13	15:O:238:ARG:HB2	1.99	0.44
1:A:703:ARG:NH2	11:K:93:ILE:O	2.50	0.44
1:A:1084:GLU:HB3	6:F:86:THR:HG23	1.98	0.44
12:L:30:ILE:N	12:L:57:LEU:O	2.51	0.44
15:O:200:LEU:HB3	15:O:280:LEU:HD12	1.99	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
1:A:533:ASN:HD21	6:F:94:LEU:HD23	1.82	0.44
1:A:1198:LEU:HD23	1:A:1273:LYS:HD3	1.99	0.44
2:B:765:TYR:HD2	2:B:924:ILE:HB	1.82	0.44
10:J:7:CYS:HA	10:J:49:MET:HE3	1.98	0.44
11:K:67:GLU:N	11:K:99:ASN:O	2.50	0.44
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.82	0.44
15:O:53:VAL:HG11	15:O:65:ILE:HG21	1.99	0.44
2:B:709:ALA:HA	2:B:1027:LEU:HA	1.98	0.44
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.00	0.44
2:B:935:ASP:HB2	3:C:228:ARG:HB3	1.99	0.44
3:C:100:ARG:NH2	3:C:192:LEU:O	2.50	0.44
14:N:304:PHE:HD1	14:N:304:PHE:N	2.15	0.44
15:O:192:VAL:HG23	15:O:274:VAL:HG13	1.99	0.44
1:A:58:MET:HE2	1:A:82:GLY:HA3	1.99	0.44
1:A:948:ASN:HB3	1:A:951:ASP:HB2	1.99	0.44
2:B:289:GLU:HA	2:B:292:LYS:HD3	1.99	0.44
2:B:386:LEU:HB3	2:B:444:LEU:HD21	2.00	0.44
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.98	0.44
8:H:96:VAL:HG12	8:H:143:LEU:HD23	1.99	0.44
1:A:1161:VAL:HG11	1:A:1295:VAL:HG11	1.98	0.44
1:A:1175:ASP:HA	1:A:1183:PHE:O	2.18	0.44
4:D:121:LEU:HA	4:D:124:VAL:HG12	2.00	0.44
16:P:222:LEU:HD21	16:P:237:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HB3	15:O:337:GLN:HB3	1.99	0.43
1:A:1026:ARG:HH22	8:H:110:ASP:H	1.66	0.43
2:B:417:ASP:HA	2:B:420:LEU:HB2	2.00	0.43
3:C:136:LEU:HB3	3:C:204:LEU:HG	2.00	0.43
4:D:134:LEU:HD13	4:D:154:LEU:HD11	2.00	0.43
8:H:10:PHE:HD2	8:H:38:LEU:HD22	1.83	0.43
2:B:197:GLN:OE1	2:B:451:ARG:NH1	2.51	0.43
2:B:391:LEU:HD23	2:B:429:ILE:HA	1.99	0.43
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.99	0.43
1:A:719:PRO:HB3	1:A:723:LEU:HD23	2.00	0.43
1:A:966:ILE:HA	1:A:970:LEU:HD12	2.01	0.43
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.43
1:A:91:PHE:HE1	1:A:99:THR:HG21	1.83	0.43
1:A:309:ILE:HG13	1:A:310:ASN:H	1.83	0.43
3:C:70:ILE:HB	3:C:74:GLU:HB2	2.01	0.43
3:C:131:THR:O	3:C:172:GLN:NE2	2.51	0.43
5:E:113:GLN:NE2	5:E:137:GLU:OE2	2.51	0.43
6:F:115:THR:HG22	6:F:116:ASP:H	1.84	0.43
13:M:134:ASP:O	13:M:138:SER:HB3	2.18	0.43
15:O:259:LEU:HG	15:O:261:GLN:H	1.83	0.43
1:A:67:CYS:SG	1:A:69:THR:OG1	2.72	0.43
1:A:612:LEU:HD23	1:A:616:PRO:HA	2.00	0.43
2:B:961:LEU:HD11	2:B:1022:ILE:HD11	2.00	0.43
3:C:133:VAL:HG23	3:C:170:GLU:HB2	2.01	0.43
5:E:34:GLU:HA	5:E:37:LEU:HD23	2.01	0.43
1:A:1213:SER:OG	1:A:1218:GLN:NE2	2.52	0.43
2:B:843:ILE:HB	2:B:871:VAL:HG12	2.01	0.43
15:O:134:GLY:HA2	15:O:137:ILE:HG12	2.01	0.43
2:B:935:ASP:HB3	2:B:1005:TYR:HE2	1.84	0.43
11:K:55:SER:OG	11:K:59:THR:O	2.36	0.43
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.93	0.43
3:C:24:SER:OG	3:C:26:ASP:OD1	2.33	0.43
1:A:1346:HIS:HB3	1:A:1348:MET:HE2	2.00	0.42
2:B:723:THR:HA	2:B:790:LYS:HB3	2.01	0.42
7:G:46:ILE:HG22	7:G:47:THR:HG23	2.00	0.42
1:A:524:THR:HG22	2:B:1081:GLU:HG3	2.01	0.42
2:B:730:TYR:O	2:B:753:GLN:NE2	2.40	0.42
15:O:211:ILE:HG23	15:O:329:PRO:HB3	2.01	0.42
2:B:885:MET:SD	2:B:887:SER:OG	2.76	0.42
15:O:154:GLN:HG2	15:O:155:LEU:HD22	2.02	0.42
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:LEU:HB3	11:K:121:LEU:HD21	2.01	0.42
15:O:623:GLU:HA	15:O:626:GLN:HB3	2.01	0.42
2:B:517:MET:HE2	2:B:611:PRO:HG2	2.01	0.42
4:D:3:VAL:HA	7:G:7:ILE:HG22	2.01	0.42
5:E:35:VAL:HG13	5:E:36:GLU:HG2	2.01	0.42
8:H:28:ALA:HB3	8:H:38:LEU:HB3	2.02	0.42
2:B:320:LEU:HA	2:B:324:ILE:HB	2.02	0.42
2:B:471:THR:HG22	2:B:514:LEU:HB2	2.02	0.42
2:B:615:VAL:HG12	2:B:620:SER:HA	2.01	0.42
9:I:30:PRO:HG3	13:M:140:TRP:HZ2	1.84	0.42
16:P:185:PHE:HA	16:P:188:GLU:HG2	2.02	0.42
1:A:102:ILE:HG13	1:A:242:LEU:HD22	2.01	0.41
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.84	0.41
2:B:983:LYS:HG3	2:B:985:GLU:H	1.84	0.41
8:H:15:VAL:HG22	8:H:26:ILE:HG22	2.02	0.41
2:B:774:ASN:HB3	2:B:777:SER:HB3	2.02	0.41
1:A:1392:THR:HG22	1:A:1393:THR:H	1.85	0.41
2:B:913:SER:HB2	2:B:1027:LEU:HD11	2.01	0.41
3:C:26:ASP:OD1	3:C:26:ASP:N	2.52	0.41
5:E:78:LEU:HB3	5:E:107:THR:HG23	2.03	0.41
5:E:86:PRO:HA	5:E:113:GLN:HG2	2.02	0.41
1:A:953:GLY:HA2	1:A:1063:SER:HA	2.02	0.41
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	2.01	0.41
13:M:227:LEU:HB3	13:M:231:LEU:HB2	2.03	0.41
15:O:62:ALA:HA	15:O:65:ILE:HG22	2.03	0.41
2:B:932:PRO:HB2	2:B:1004:LEU:HD13	2.01	0.41
1:A:100:ILE:HD11	1:A:178:ILE:HD12	2.01	0.41
2:B:287:LEU:O	2:B:290:SER:OG	2.33	0.41
3:C:248:GLN:HA	3:C:256:ILE:HD11	2.01	0.41
7:G:207:LEU:HD23	7:G:209:SER:H	1.85	0.41
1:A:11:LYS:HA	2:B:1145:ASP:HA	2.02	0.41
1:A:908:ALA:HB3	1:A:1379:MET:HE2	2.03	0.41
2:B:590:ILE:HA	2:B:600:HIS:O	2.20	0.41
3:C:134:LEU:HD12	3:C:167:LEU:HB3	2.02	0.41
3:C:222:VAL:HA	3:C:304:SER:HA	2.03	0.41
6:F:144:GLU:HG2	6:F:146:TRP:CD1	2.56	0.41
13:M:92:ASN:HD21	13:M:181:PRO:HD3	1.86	0.41
2:B:193:VAL:O	2:B:455:THR:HA	2.21	0.41
2:B:230:LYS:NZ	2:B:352:MET:SD	2.89	0.41
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.56	0.41
15:O:491:VAL:HG11	15:O:650:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:ASP:O	1:A:1155:ARG:NH1	2.54	0.40
15:O:235:LEU:HD12	15:O:236:LYS:H	1.86	0.40
1:A:939:TRP:HZ2	1:A:1062:ILE:HD12	1.85	0.40
2:B:83:ILE:HD11	2:B:93:LEU:HD13	2.02	0.40
1:A:412:ASN:HB2	1:A:416:LEU:HD13	2.03	0.40
1:A:660:LEU:HD12	8:H:117:SER:HB3	2.03	0.40
1:A:816:GLN:NE2	1:A:867:SER:OG	2.51	0.40
2:B:935:ASP:HB3	2:B:1005:TYR:CE2	2.57	0.40
7:G:82:GLY:H	7:G:150:ILE:HB	1.86	0.40
15:O:473:PRO:HG2	15:O:475:VAL:HG12	2.02	0.40
15:O:534:ARG:HD3	15:O:537:LEU:HD12	2.03	0.40
1:A:711:SER:OG	2:B:1016:TYR:O	2.39	0.40
1:A:826:GLY:H	1:A:831:SER:HA	1.86	0.40
2:B:221:THR:HB	2:B:228:LYS:HB2	2.03	0.40
2:B:932:PRO:HG3	2:B:1006:SER:HA	2.04	0.40
8:H:56:THR:HB	8:H:145:ARG:HB3	2.04	0.40
15:O:231:PRO:HB3	15:O:234:ASP:HA	2.04	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	1394/1460 (96%)	1213 (87%)	174 (12%)	7 (0%)	24	55
2	B	1112/1149 (97%)	979 (88%)	128 (12%)	5 (0%)	30	60
3	C	333/335 (99%)	299 (90%)	32 (10%)	2 (1%)	21	52
4	D	113/161 (70%)	96 (85%)	17 (15%)	0	100	100
5	E	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	68 (84%)	13 (16%)	0	100	100
7	G	185/212 (87%)	162 (88%)	23 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	35 (88%)	5 (12%)	0	100	100
10	J	66/70 (94%)	56 (85%)	10 (15%)	0	100	100
11	K	99/142 (70%)	88 (89%)	11 (11%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
13	M	161/282 (57%)	123 (76%)	36 (22%)	2 (1%)	10	37
14	N	101/422 (24%)	82 (81%)	18 (18%)	1 (1%)	12	40
15	O	531/654 (81%)	470 (88%)	60 (11%)	1 (0%)	43	71
16	P	119/317 (38%)	82 (69%)	31 (26%)	6 (5%)	1	11
17	Q	38/251 (15%)	28 (74%)	10 (26%)	0	100	100
All	All	4765/6151 (78%)	4127 (87%)	614 (13%)	24 (0%)	26	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	839	GLY
2	B	935	ASP
1	A	495	TRP
2	B	297	THR
16	P	309	VAL
1	A	513	ASP
2	B	298	GLN
3	C	4	ILE
13	M	118	LEU
16	P	206	VAL
1	A	494	PRO
1	A	1179	ASP
15	O	236	LYS
16	P	307	LYS
1	A	1352	PRO
13	M	94	PRO
16	P	253	LEU
16	P	305	HIS
16	P	308	GLU
1	A	599	LYS
1	A	636	PRO
3	C	3	ASN
2	B	584	VAL
14	N	378	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	1215/1257 (97%)	1212 (100%)	3 (0%)	87	88
2	B	975/1006 (97%)	974 (100%)	1 (0%)	88	90
3	C	296/296 (100%)	296 (100%)	0	100	100
4	D	110/145 (76%)	110 (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	170/190 (90%)	170 (100%)	0	100	100
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	38 (100%)	0	100	100
10	J	63/65 (97%)	62 (98%)	1 (2%)	55	72
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	39 (98%)	1 (2%)	42	64
13	M	143/249 (57%)	143 (100%)	0	100	100
14	N	88/360 (24%)	88 (100%)	0	100	100
15	O	493/593 (83%)	489 (99%)	4 (1%)	73	79
16	P	116/285 (41%)	115 (99%)	1 (1%)	70	78
17	Q	35/212 (16%)	35 (100%)	0	100	100
All	All	4266/5405 (79%)	4255 (100%)	11 (0%)	84	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	LEU
1	A	1032	LEU
1	A	1408	VAL
2	B	48	LEU
10	J	2	ILE
12	L	27	LEU
15	O	235	LEU

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Mol	Chain	Res	Type
15	O	263	LEU
15	O	468	LEU
15	O	527	LEU
16	P	298	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	109	ASN
1	A	161	ASN
1	A	229	ASN
1	A	523	GLN
1	A	533	ASN
1	A	566	HIS
1	A	618	HIS
1	A	643	ASN
1	A	808	GLN
1	A	816	GLN
1	A	899	GLN
1	A	931	GLN
1	A	941	HIS
1	A	948	ASN
1	A	990	ASN
1	A	1218	GLN
1	A	1233	ASN
1	A	1254	ASN
1	A	1262	GLN
1	A	1354	HIS
1	A	1419	GLN
1	A	1453	ASN
2	B	39	ASN
2	B	116	HIS
2	B	362	ASN
2	B	396	ASN
2	B	626	HIS
2	B	655	ASN
2	B	694	ASN
2	B	702	GLN
2	B	774	ASN
2	B	916	HIS
2	B	997	ASN

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Mol	Chain	Res	Type
2	B	1029	HIS
3	C	137	ASN
3	C	143	ASN
3	C	161	HIS
3	C	200	GLN
3	C	207	HIS
3	C	301	ASN
4	D	31	GLN
4	D	71	ASN
4	D	130	ASN
5	E	5	ASN
5	E	32	GLN
5	E	54	GLN
5	E	101	GLN
5	E	113	GLN
5	E	136	ASN
5	E	174	GLN
7	G	32	ASN
7	G	36	ASN
8	H	35	GLN
9	I	10	ASN
13	M	86	HIS
13	M	89	GLN
13	M	92	ASN
13	M	104	HIS
13	M	117	HIS
13	M	132	ASN
13	M	155	ASN
13	M	158	GLN
13	M	190	ASN
14	N	287	HIS
14	N	421	GLN
15	O	202	GLN
15	O	216	GLN
15	O	244	ASN
15	O	254	ASN
15	O	332	GLN
15	O	362	ASN
15	O	469	ASN
15	O	544	ASN
15	O	575	ASN
15	O	579	GLN

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Mol	Chain	Res	Type
15	O	584	ASN
15	O	631	ASN
15	O	652	GLN
16	P	176	ASN
17	Q	49	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.

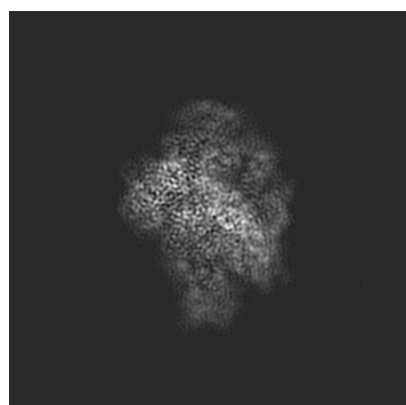
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3958. These allow visual inspection of the internal detail of the map and identification of artifacts.

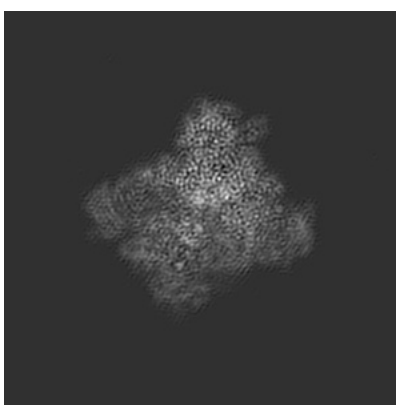
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

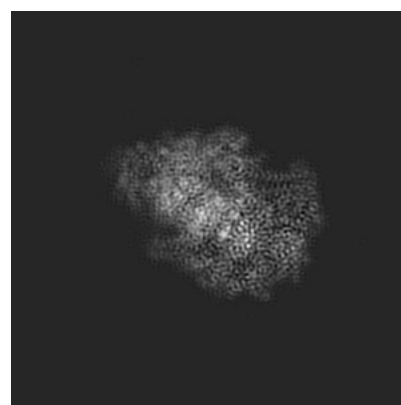
6.1.1 Primary map



X



Y

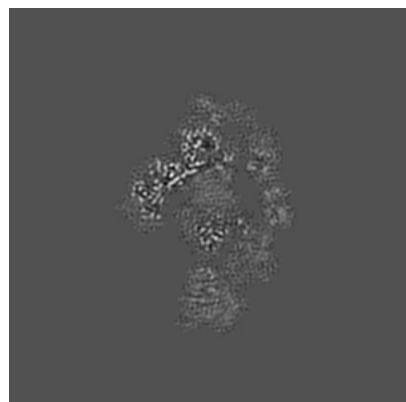


Z

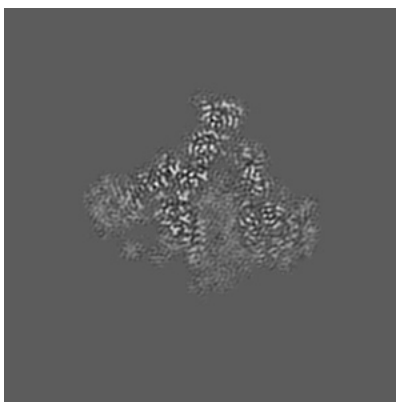
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

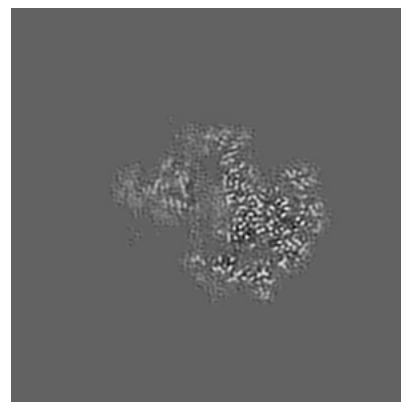
6.2.1 Primary map



X Index: 154



Y Index: 154

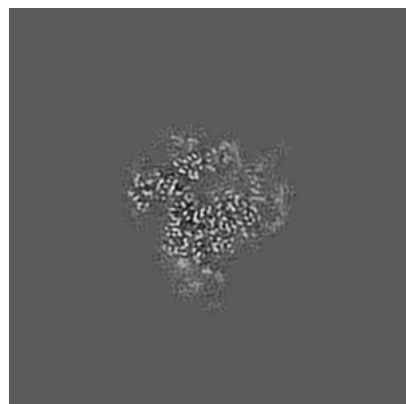


Z Index: 154

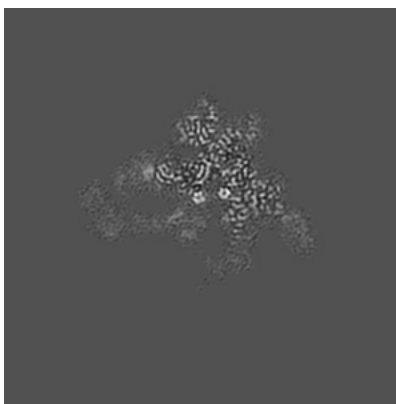
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

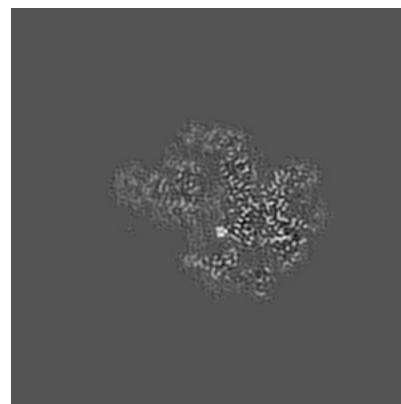
6.3.1 Primary map



X Index: 178



Y Index: 135

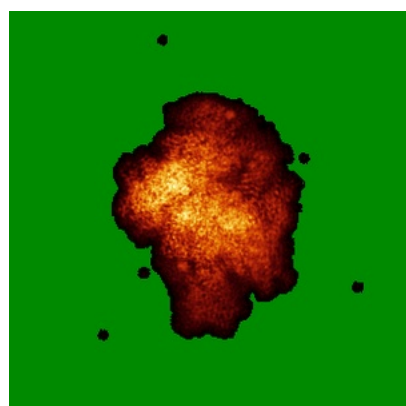


Z Index: 151

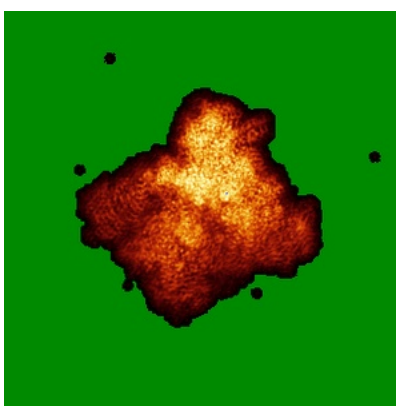
The images above show the largest variance slices of the map in three orthogonal directions.

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

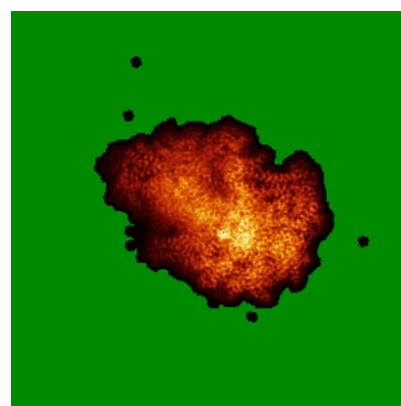
6.4.1 Primary map



X



Y

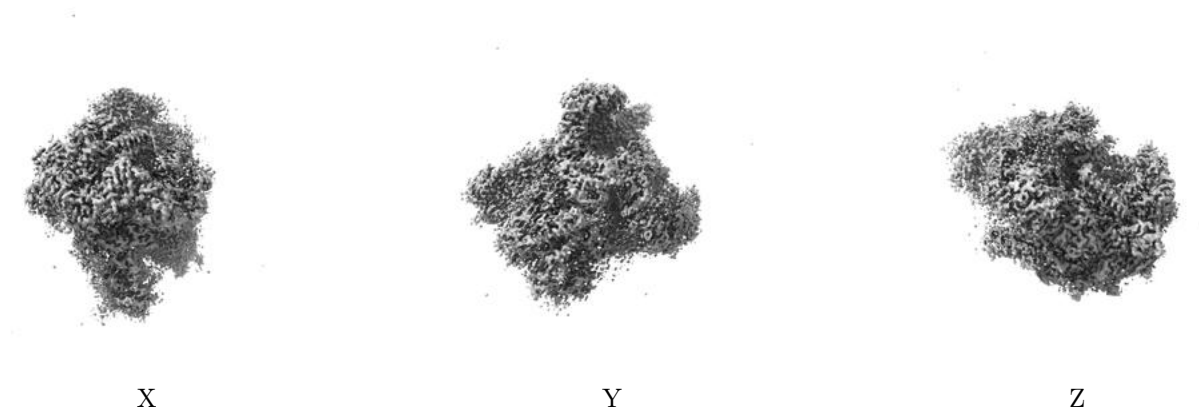


Z

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.

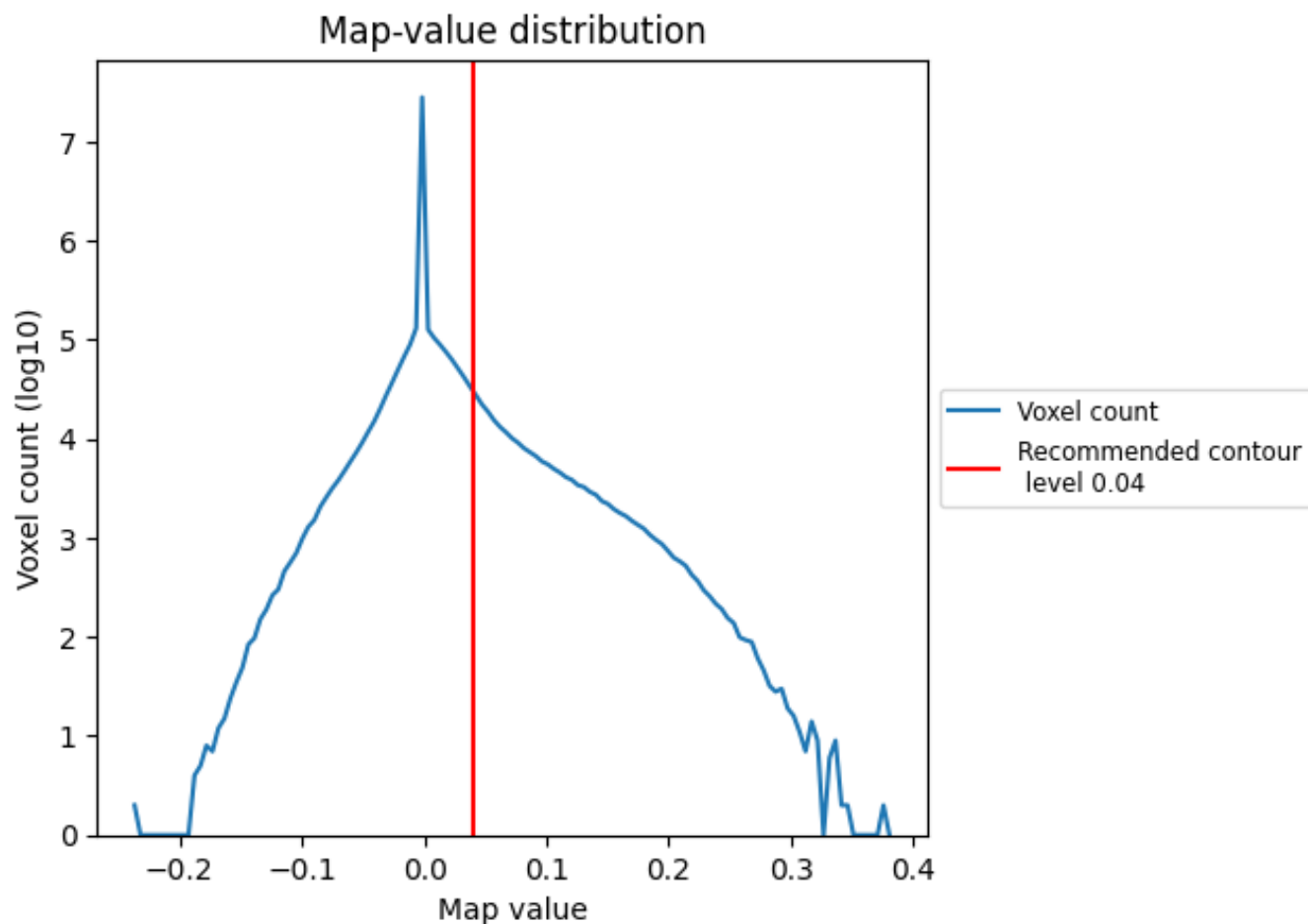
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

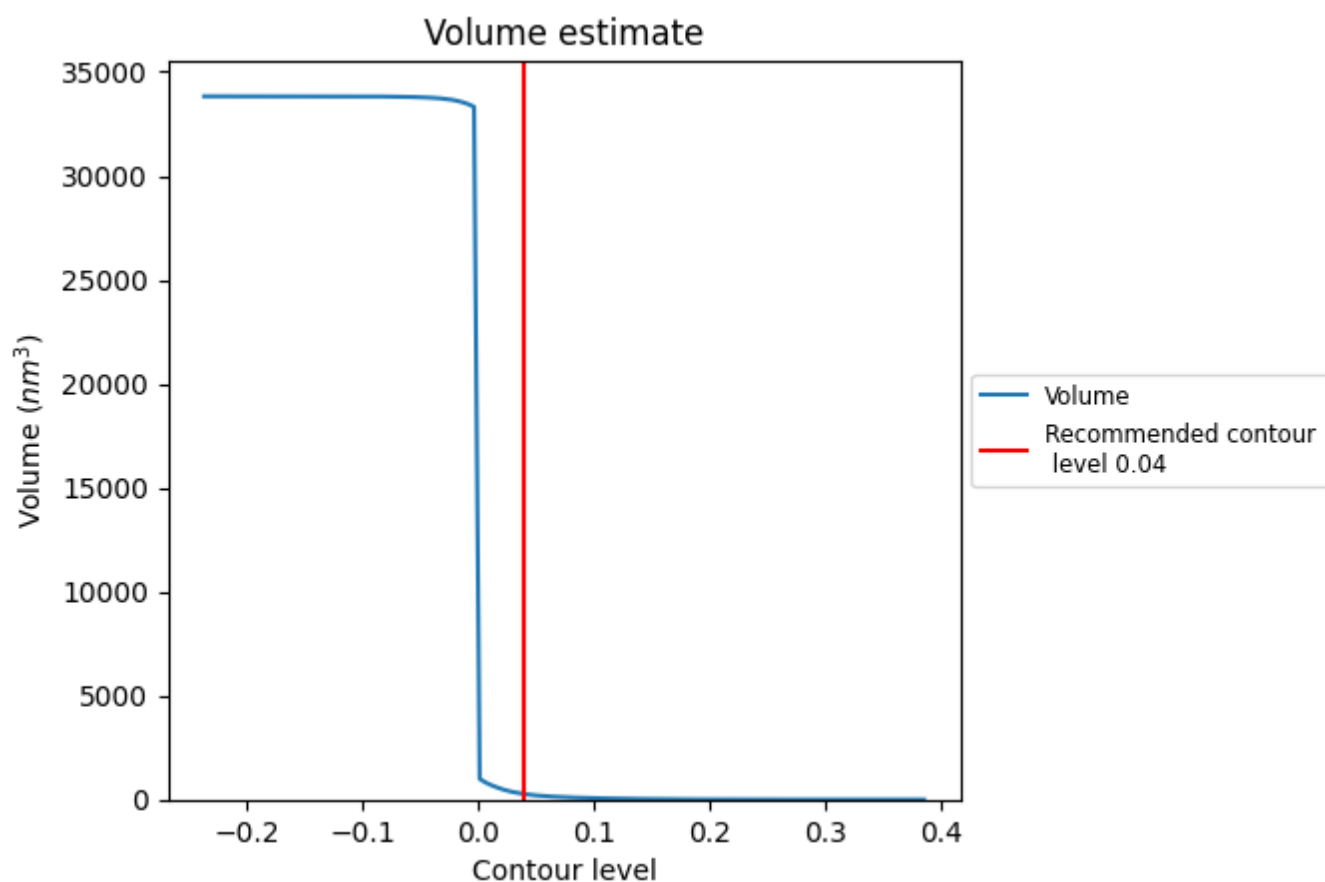
This section contains the results of statistical analysis of the map.

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.

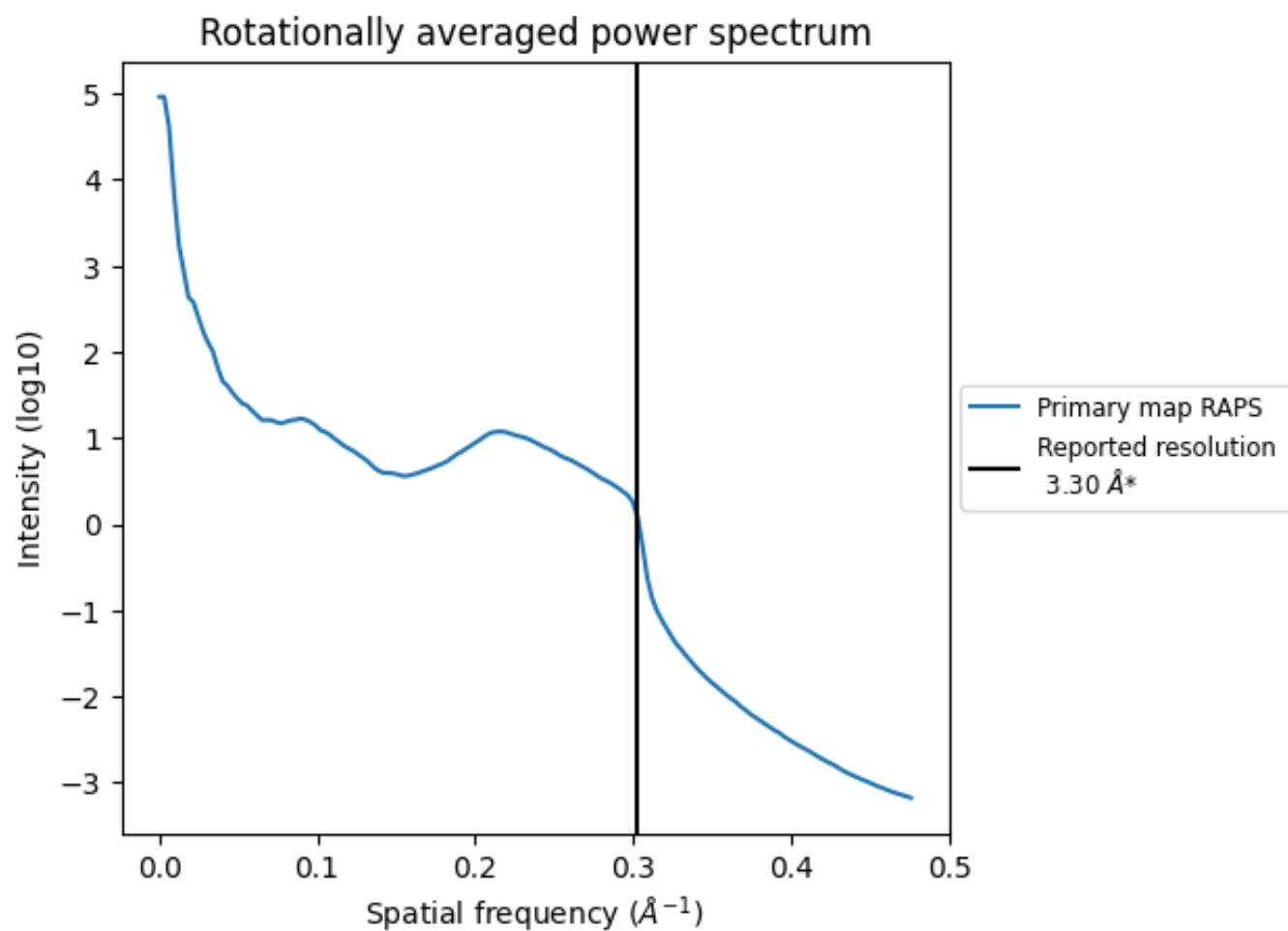
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm³; this corresponds to an approximate mass of 239 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 ⓘ

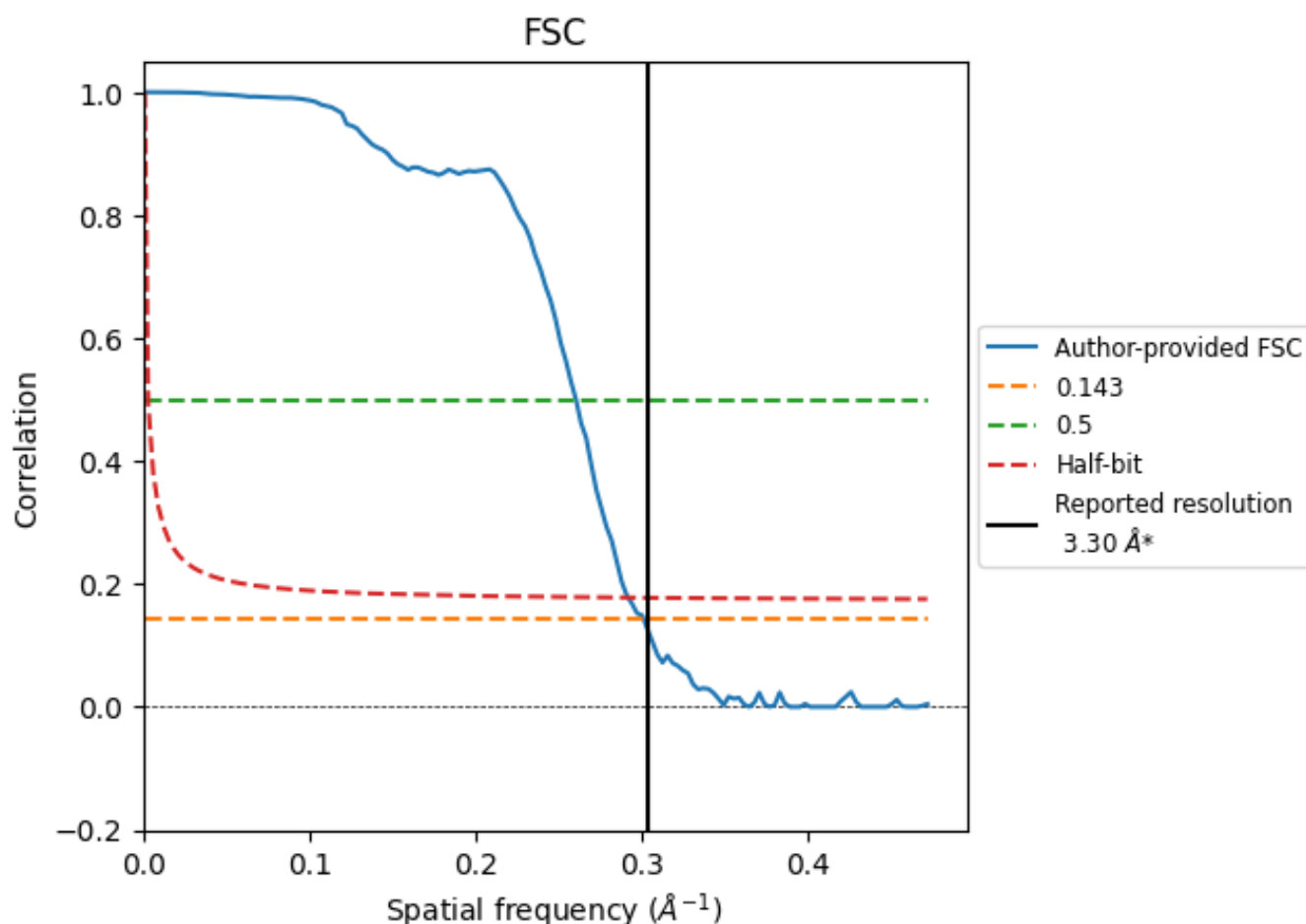


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

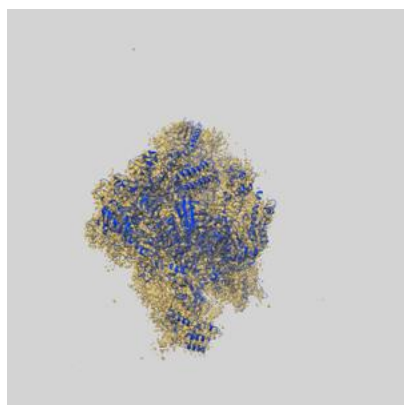
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.84	3.43
Unmasked-calculated*	-	-	-

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

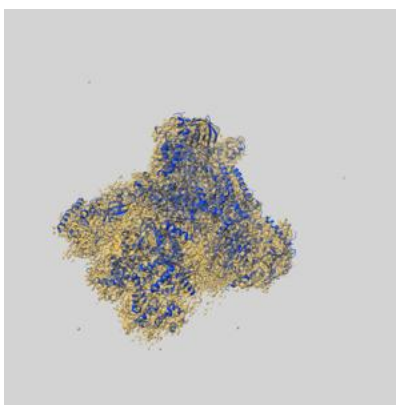
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3958 and PDB model 6EU3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

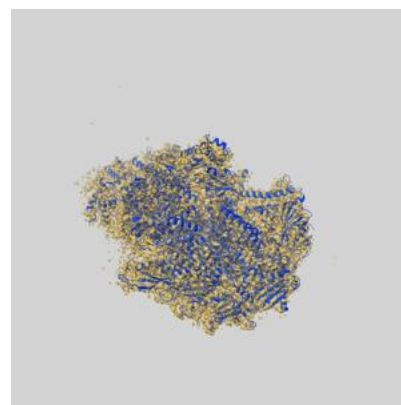
9.1 Map-model overlay [i](#)



X



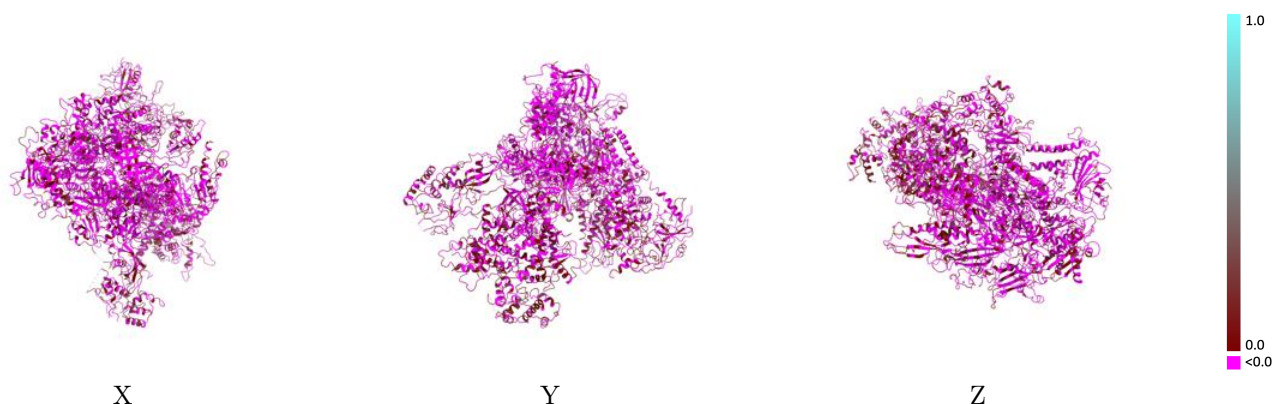
Y



Z

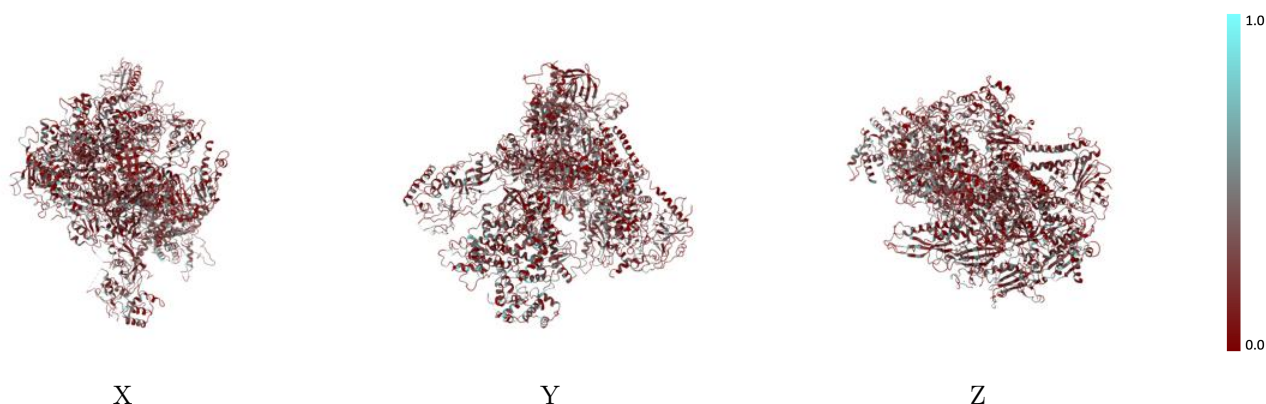
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



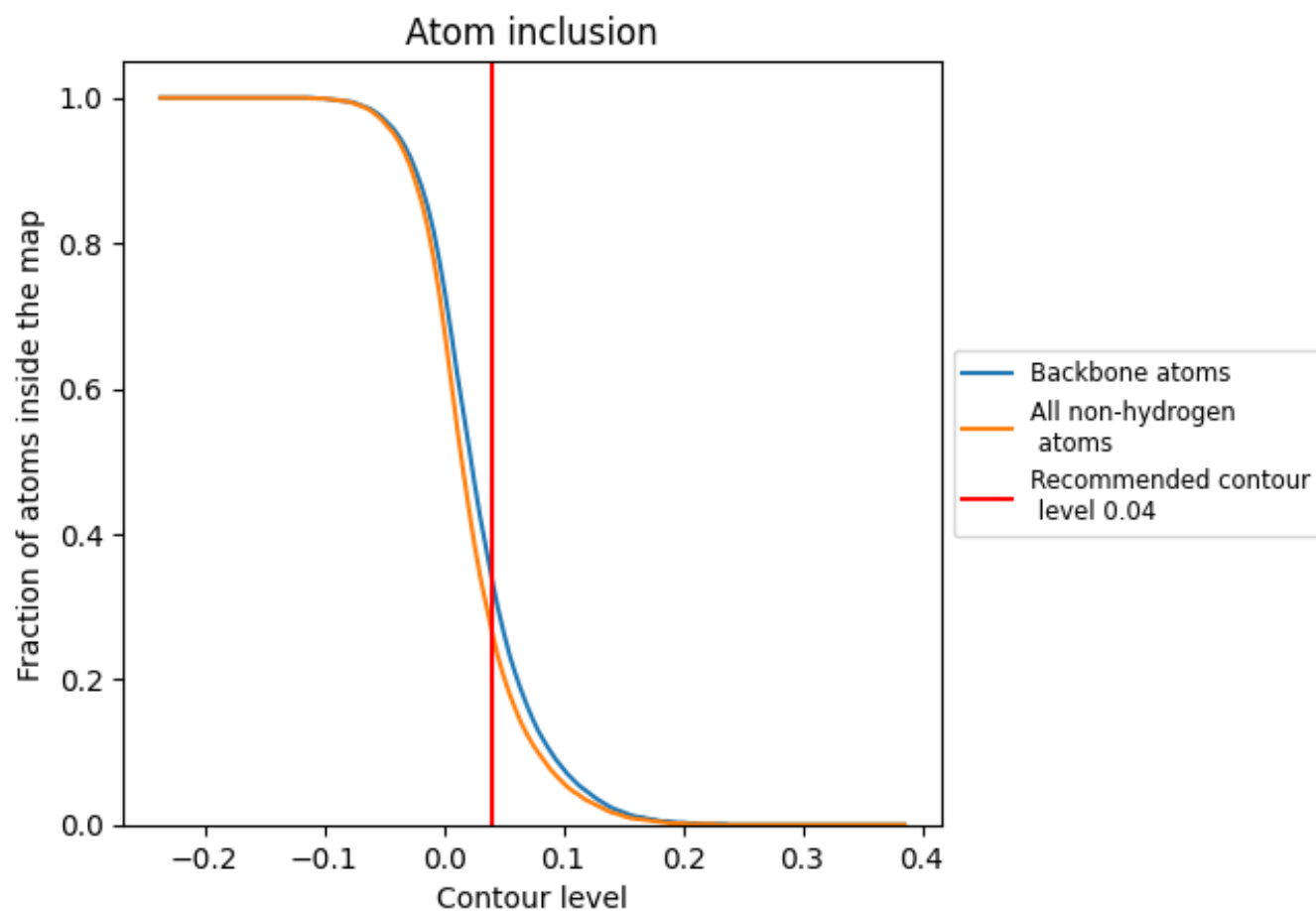
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 34% of all backbone atoms, 27% 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	 0.2670	 -0.0440
A	 0.2540	 -0.0610
B	 0.2600	 -0.0660
C	 0.2800	 -0.0740
D	 0.3030	 0.0660
E	 0.2480	 -0.0450
F	 0.2800	 -0.0660
G	 0.2680	 -0.0140
H	 0.2140	 -0.0990
I	 0.2020	 0.0320
J	 0.2930	 -0.0740
K	 0.2580	 -0.0830
L	 0.3300	 -0.0170
M	 0.2500	 0.0190
N	 0.2120	 -0.0360
O	 0.3070	 0.0000
P	 0.3250	 0.0430
Q	 0.4100	 0.0330

