



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 8S8K / pdb_00008s8k
EMDB ID : EMD-19808
Title : Structure of a yeast 48S-AUC preinitiation complex in swivelled conformation
(model py48S-AUC-swiv-eIF1)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary 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:

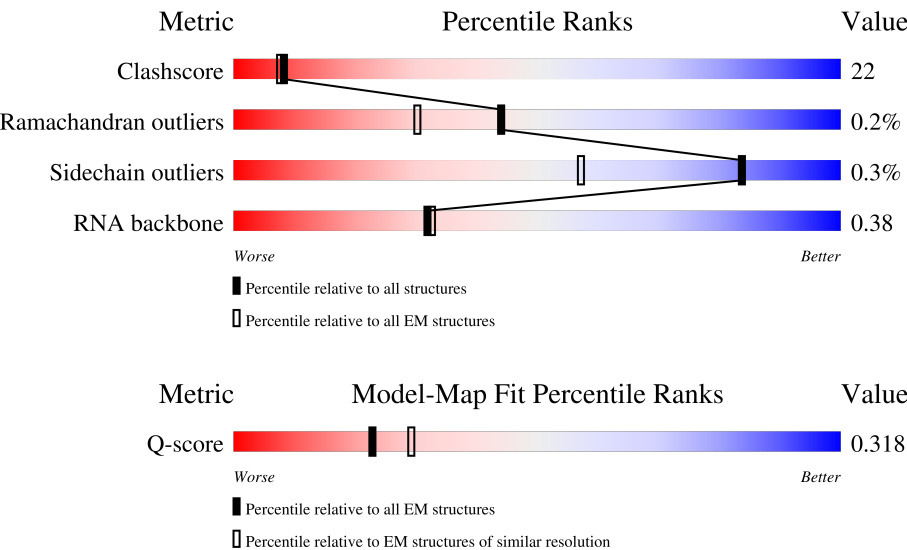
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.00 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.



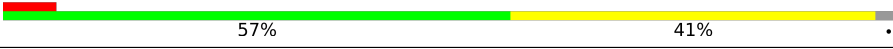
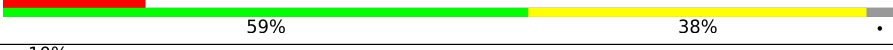
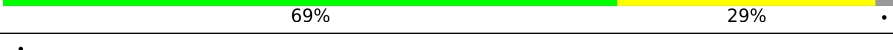
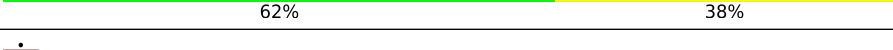
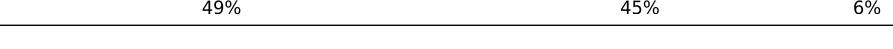
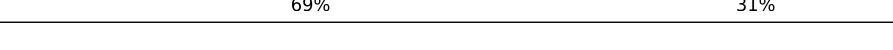
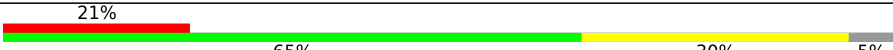
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	2	1798	10% 27% 56% 17%
2	A	254	6% 46% 40% 14%
3	B	255	9% 56% 34% 10%

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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	103	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	

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Mol	Chain	Length	Quality of chain
29	T	144	
30	U	117	
31	Z	108	
32	c	67	
33	d	56	
34	f	150	
35	i	153	
36	m	108	
37	3	49	
38	1	75	
39	j	304	
40	k	527	
41	l	270	
42	n	812	
43	g	326	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 87738 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total	C	N	O	P	0	0
			38190	17073	6722	12597	1798		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	229	Total	C	N	O	S	0	0
			1809	1143	331	332	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 5 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 9 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 10 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1235	791	235	206	3		

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	102	Total	C	N	O	S	0	0
			797	492	168	132	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 20 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 22 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 23 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	117	Total	C	N	O		0	0
			867	544	152	171			

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 29 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	143	Total	C	N	O		0	0
			1110	693	210	207			

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	96	Total	C	N	O	S	0	0
			769	477	143	144	5		

- Molecule 36 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	6	Total	C	N	O	P	6	0
			256	116	50	78	12		

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	267	Total	C	N	O	S	0	0
			2139	1366	355	407	11		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total	C	N	O	S	0	0
			3596	2279	633	666	18		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	134	Total	C	N	O	S	0	0
			1083	689	194	193	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	n	93	Total	C	N	O	0	0
			464	278	93	93		

- Molecule 43 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

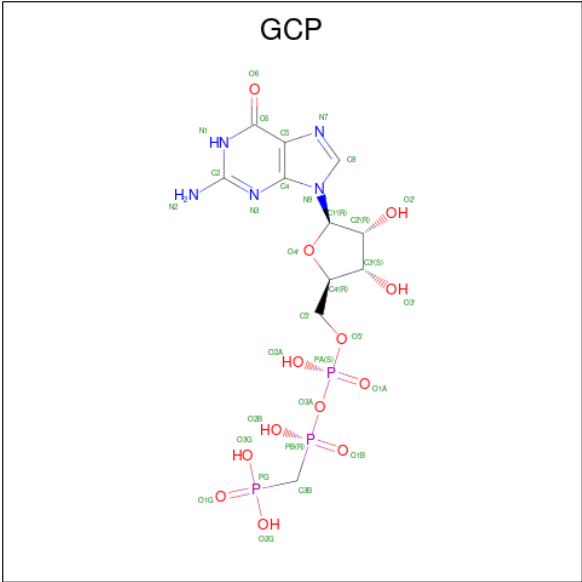
- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	2	94	Total	Mg	0
			94	94	
44	X	1	Total	Mg	0
			1	1	
44	k	1	Total	Mg	0
			1	1	

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

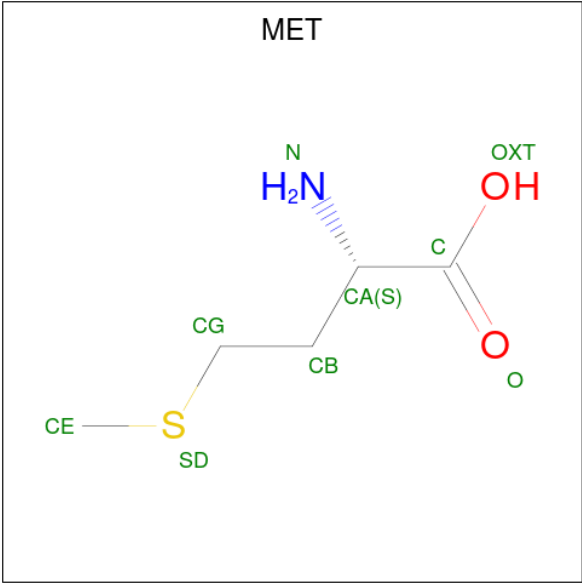
Mol	Chain	Residues	Atoms		AltConf
45	a	1	Total	Zn	0
			1	1	
45	b	1	Total	Zn	0
			1	1	
45	f	1	Total	Zn	0
			1	1	
45	l	1	Total	Zn	0
			1	1	

- Molecule 46 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 47 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S) (labeled as "Ligand of Interest" by depositor).

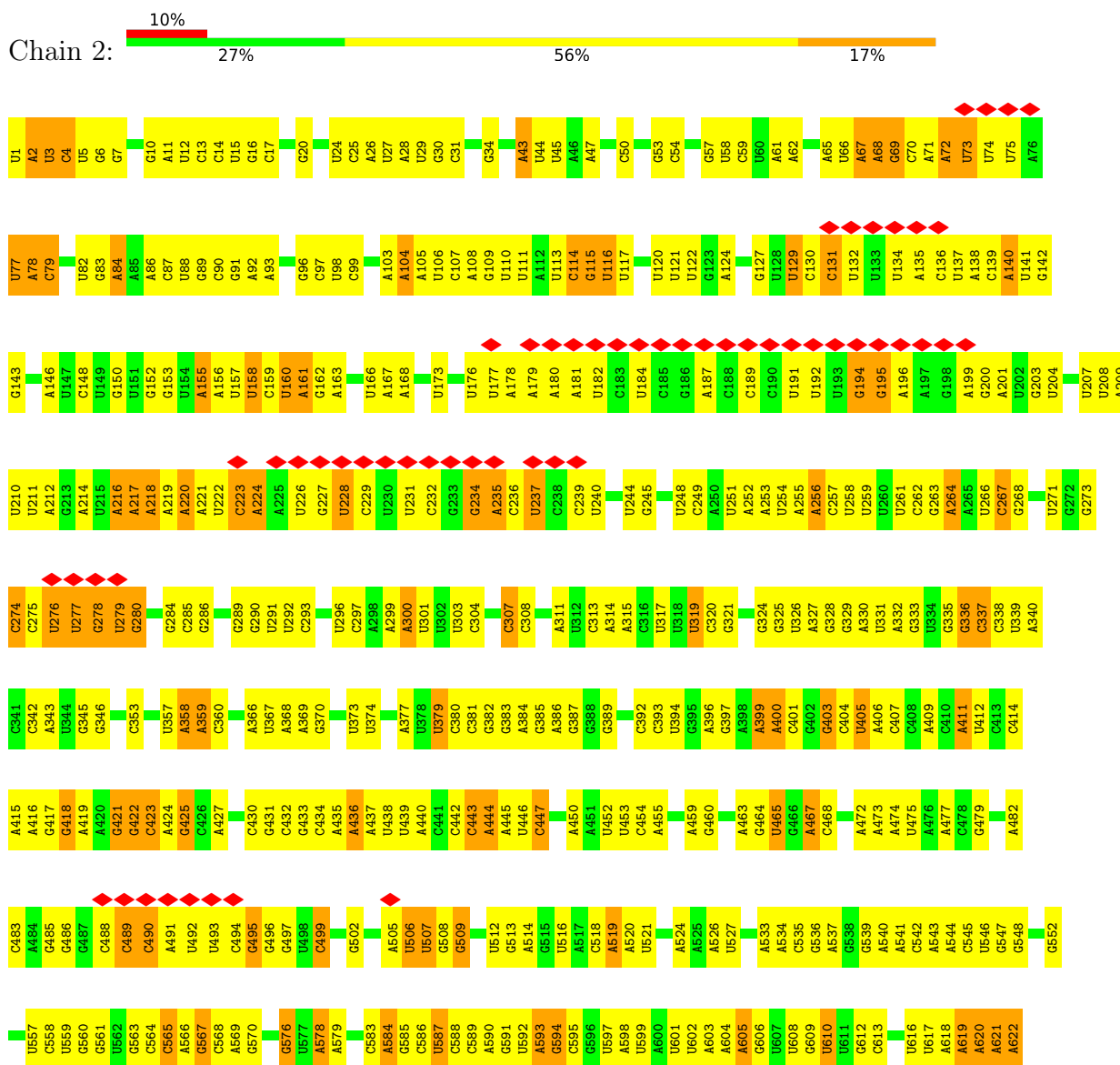


Mol	Chain	Residues	Atoms					AltConf
47	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

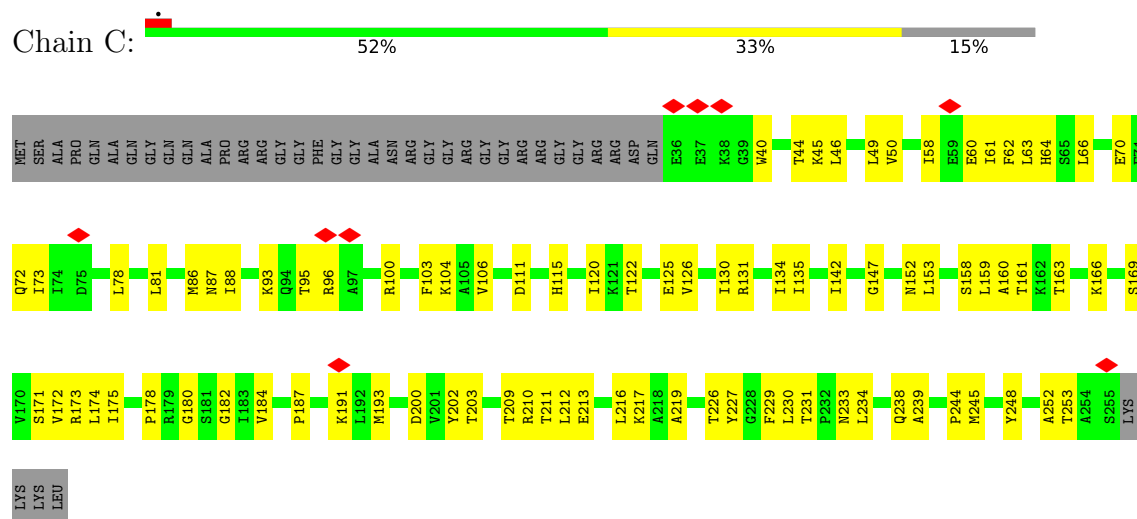
3 Residue-property plots

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.

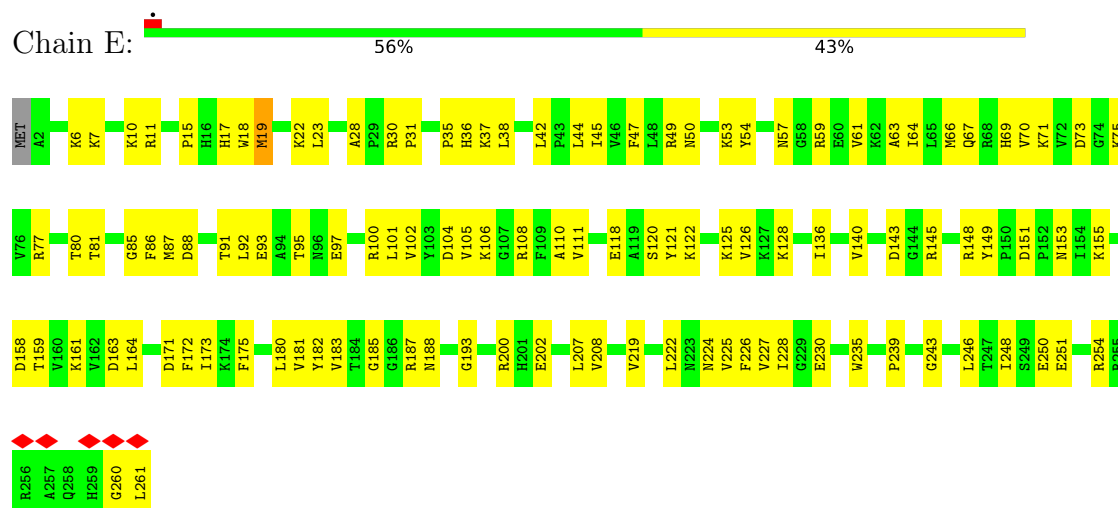
• Molecule 1: 18S ribosomal RNA



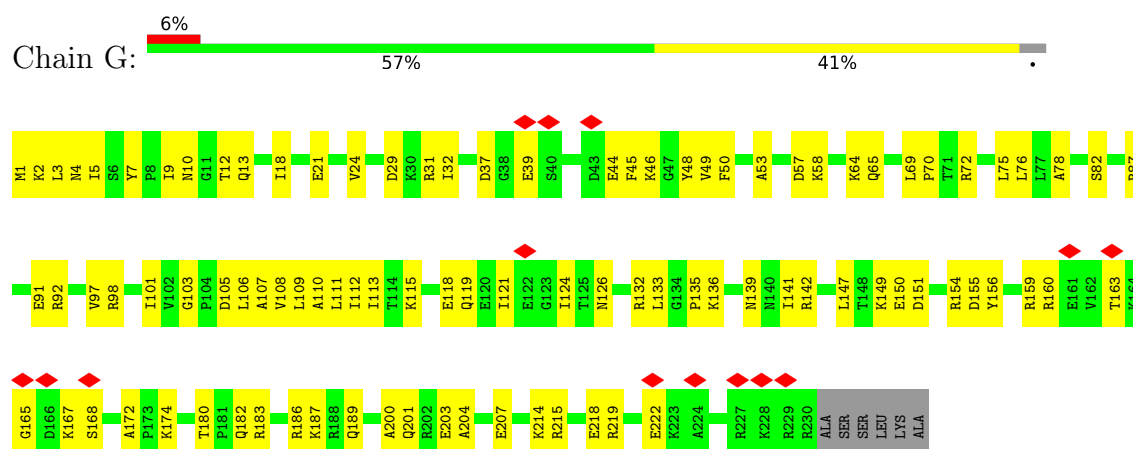
A1477	G1478	C1479	C1480	A1481	G1482	C1483	G1484	A1485	G1486	A1487	A1488	C1489	A1490	A1491	C1492	C1493	A1494	U1495	G1496	C1497	C1498	C1499	G1500	A1501	G1502	A1503	U1506	C1507	G1510	G1511	U1512	A1513	A1514	U1515	C1516	U1517	U1518	G1519	U1520	G1521	A1522	A1523	A1524	C1525	U1526	C1527	C1528	G1529	U1530	C1531	G1532	U1533	G1534	C1535	U1536	G1537	G1538									
G1410	U1411	U1412	U1413	U1414	U1415	G1416	G1417	C1418	U1421	A1422	A1423	C1424	A1425	G1426	U1427	C1428	U1429	U1495	U1496	U1497	U1498	U1499	A1434	U1435	G1436	C1437	C1438	C1439	U1440	U1441	A1442	G1443	A1444	A1445	G1446	U1447	U1448	G1453	U1454	G1455	C1456	C1457	A1458	C1459	G1460	C1461	U1464	C1465	U1469	C1470	U1471	G1472	A1473	C1474	G1475	A1408	A1409									
A1347	G1348	G1349	G1350	U1351	U1352	C1353	C1354	U1355	U1356	G1357	C1358	A1359	C1360	U1361	U1362	C1363	C1364	C1365	G1366	G1367	U1368	U1369	G1370	U1371	U1374	U1375	U1376	C1377	U1378	C1379	A1380	G1381	A1382	G1383	C1384	G1385	A1386	C1387	U1388	A1389	U1390	C1391	G1392	U1395	U1396	C1397	A1398	U1399	G1400	C1401	C1402	G1403	A1404	U1407	U1408	A1409										
G1276	G1277	C1278	C1279	G1280	C1283	C1284	U1284	U1285	U1288	U1289	G1290	C1291	U1292	U1293	G1294	A1295	C1296	U1297	G1298	U1299	U1300	U1301	U1302	U1303	U1304	C1305	U1306	U1313	U1314	G1315	C1316	G1317	U1318	U1319	A1320	A1321	G1322	G1323	A1324	U1328	G1329	A1330	C1331	C1332	U1333	U1334	A1335	C1336	C1337	U1338	U1339	G1400	A1343	A1344	A1345	U1346										
U1213	A1216	G1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	A1225	U1226	G1227	U1228	U1229	U1230	U1231	G1232	U1233	U1234	A1235	G1236	U1237	U1238	U1239	U1240	U1241	U1242	A1243	G1244	C1245	U1246	C1247	U1248	U1249	U1250	C1251	U1252	U1253	G1254	A1255	U1256	U1257	U1258	U1259	G1260	U1261	G1262	G1263	U1264	U1265	G1266	U1267	U1268	G1269	U1270	U1271	G1272									
G1145	A1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	A1182	U1183	U1184	U1185	U1186	U1187	U1188	C1189	B8N1190	U1193	C1194	A1195	U1196	G1198	G1199	G1200	A1201	A1202	A1203	C1204	U1205	U1206	A1207	C1208	C1209	A1141	A1142	U1143	G1211	G1212
G1073	C1074	U1075	C1076	C1077	U1078	U1079	U1080	C1081	G1082	A1083	U1084	A1085	U1086	A1087	U1091	C1095	U1096	U1097	U1098	U1099	U1100	G1101	U1102	U1103	C1104	U1105	G1106	A1042	U1043	C1107	U1044	G1045	G1109	G1110	U1113	U1114	U1119	C1120	G1121	A1124	C1127	U1057	U1128	C1058	U1059	A1131	A1132	C1133	U1061	U1062	G1063	A1064	C1065	C1066	C1067	A1141	A1142	U1143	U1144							
U1011	A1012	G1013	U1014	C1015	U1016	U1017	U1018	A1019	C1020	C1021	U1022	U1023	A1024	A1025	A1026	C1027	U1028	A1029	U1030	G1031	C1032	A1035	C1036	U1037	A1038	G1039	G1040	U1041	A1042	U1043	C1044	G1045	U1046	G1047	U1048	G1049	G1050	U1051	G1052	U1053	U1054	U1055	U1056	U1057	C1058	U1059	A1131	A1132	C1133	U1061	U1062	G1063	A1064	C1065	C1066	C1067	A1141	A1142	U1143	U1144						
G947	C948	C949	U881	A951	G952	G953	A954	C955	C956	U957	U958	U959	U960	C961	A965	U967	C968	A969	U970	G971	A972	G975	A976	A977	A978	U981	G912	G913	A914	U915	U916	G986	U987	U988	U989	U920	G921	A922	A923	G924	A925	C926	U927	C930	U931	A932	G933	U934	A938	A939	C1006	G1007	U1008	C1009	G1010											
G814	G815	A816	C817	G818	U819	U820	U821	G822	G823	U824	U825	C826	U827	U828	U829	U830	U831	U832	U833	U834	U835	G836	G837	U838	U839	U840	U841	U842	U843	G844	U845	A846	C847	C848	U853	A854	A855	U856	C857	U858	U859	U860	U861	A862	U863	U864	U865	A866	U867	U868	U869	G870	U871	G872	U873	U874	U875									
A884	A885	C886	C887	C888	U891	C892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	A905	A906	U911	G912	G913	A914	U915	U916	U917	U918	U919	U920	G921	A922	A923	G924	A925	C926	U927	C930	U931	A932	G933	U934	A938	A939	C1006	G1007	U1008	C1009	G1010																			
G777	A880	C881	C882	C883	C884	U885	U886	U887	U888	C889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	G901	U902	A905	A906	U911	G912	G913	A914	U915	U916	U917	U918	U919	U920	G921	A922	A923	G924	A925	C926	U927	C930	U931	A932	G933	U934	A938	A939	C1006	G1007	U1008	C1009	G1010													
C747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U803	G808	G809	A810	U811	G812	U813						
U691	C692	U693	U694	U695	C696	U697	U698	U699	C700	U701	G642	G702	G703	C704	U705	A706	U707	C708	U709	U710	U711	U712	U713	U714	U715	U716	C717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	C731	G732	A733	C734	U735	C736	U737	U738	G739	A740	U741	U742	U743	U744												
A684	A685	C686	C687	C688	U691	C692	U693	U694	U695	C696	U697	U698	U699	C700	U701	G642	G702	G703	C704	U705	A706	U707	C708	U709	U710	U711	U712	U713	U714	U715	U716	C717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	C731	G732	A733	C734	U735	C736	U737	U738	G739	A740	U741	U742	U743	U744							
G623	C624	U625	C626	G627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	A660	C661	U662	U663	U664	U665	U666	U667	U668	C669	G670	C671	G672	C673	A674	C675	U676	U677	G678	U679	U680	U681	U682	C683						



• Molecule 5: 40S ribosomal protein S4

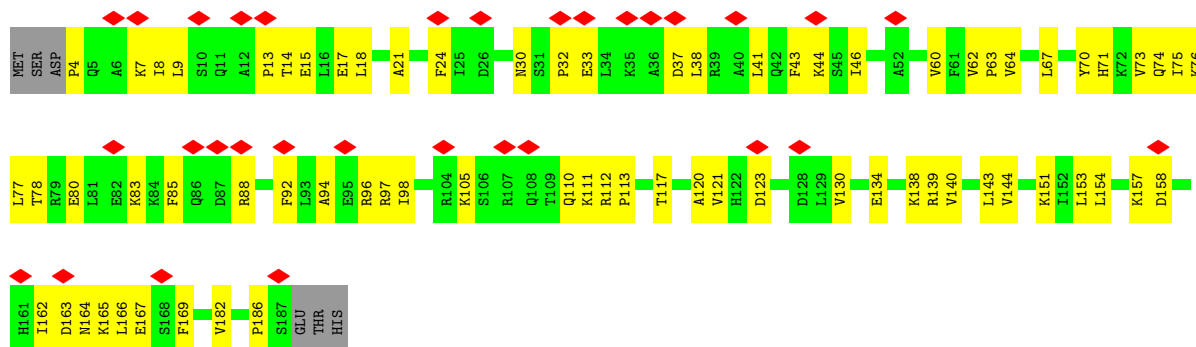


• Molecule 6: Small ribosomal subunit protein eS6

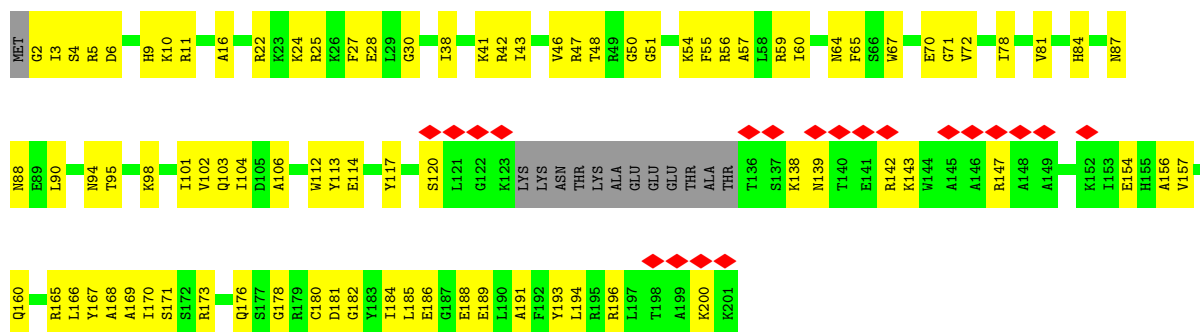


• Molecule 7: 40S ribosomal protein S7





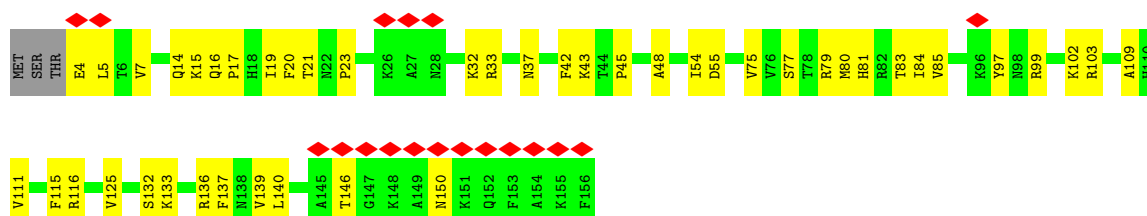
• Molecule 8: 40S ribosomal protein S8



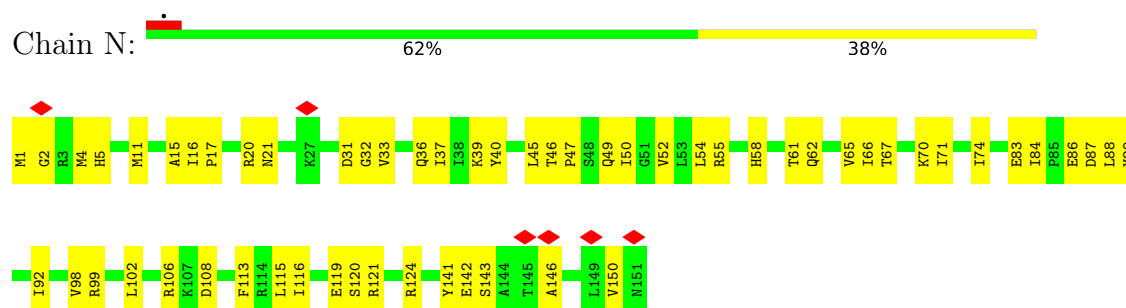
• Molecule 9: KLLA0E23673p



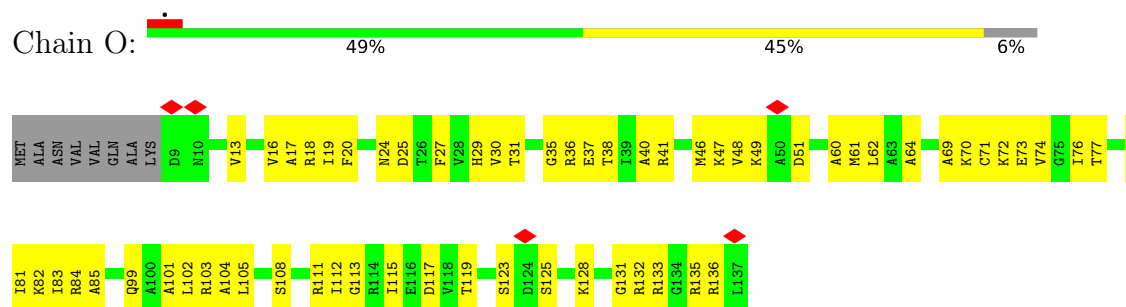
• Molecule 10: KLLA0A10483p



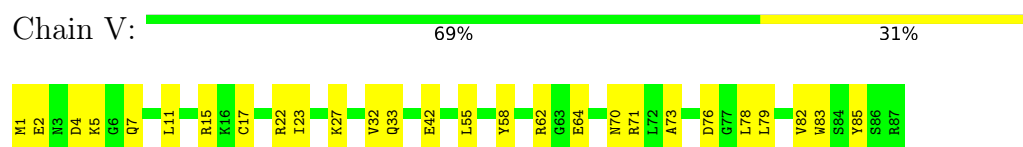
- Molecule 11: KLLA0F18040p



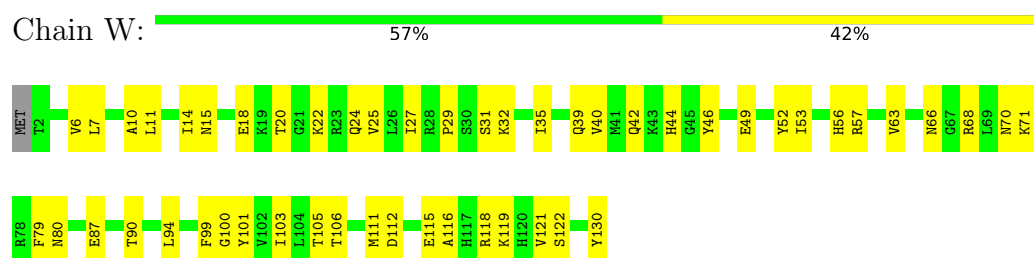
- Molecule 12: Small ribosomal subunit protein uS11



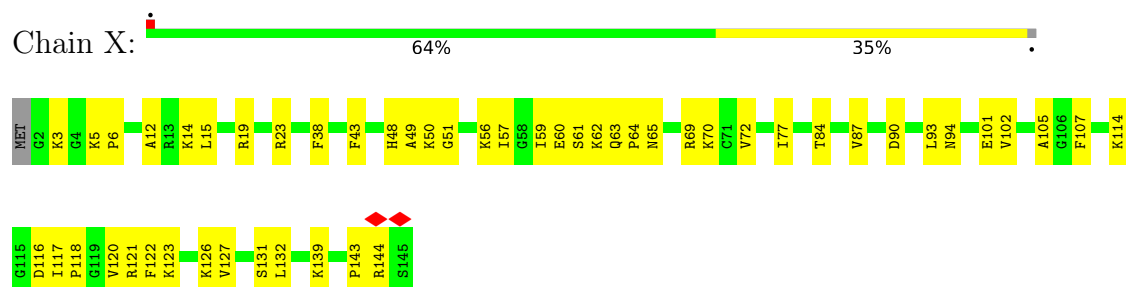
- Molecule 13: 40S ribosomal protein S21



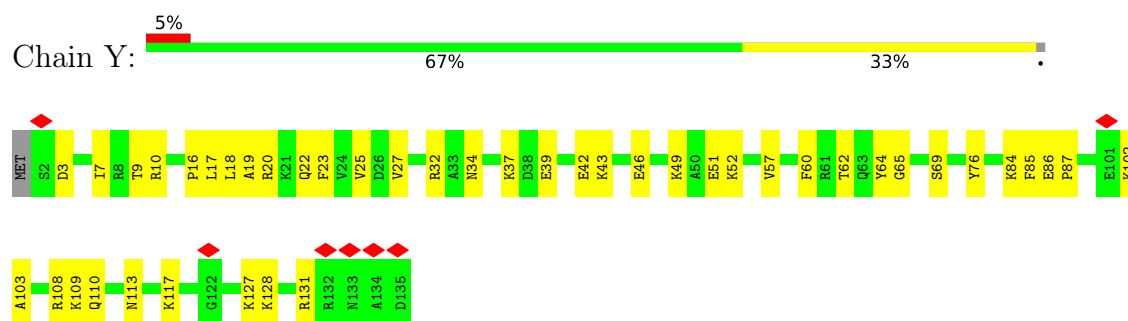
- Molecule 14: Small ribosomal subunit protein uS8



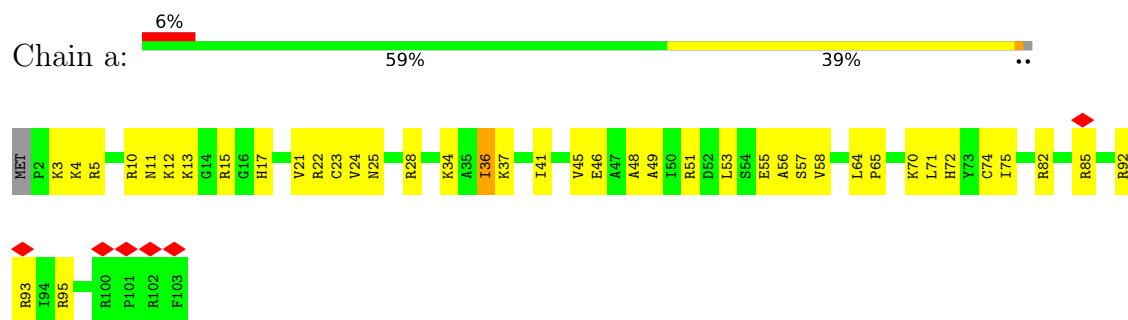
- Molecule 15: KLLA0B11231p



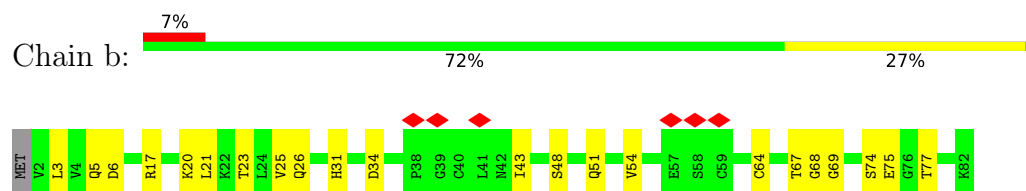
- Molecule 16: 40S ribosomal protein S24



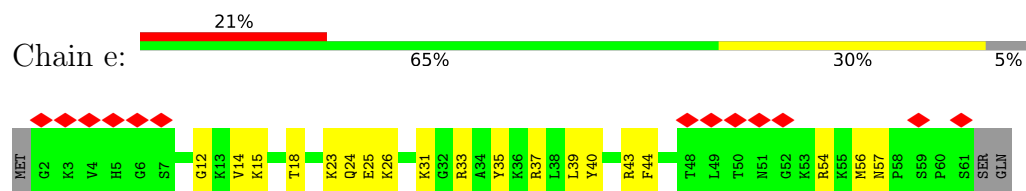
- Molecule 17: 40S ribosomal protein S26



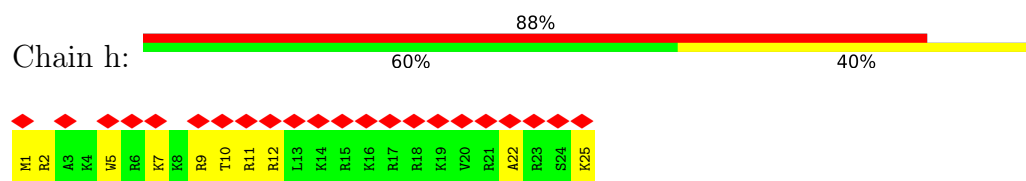
- Molecule 18: 40S ribosomal protein S27



- Molecule 19: 40S ribosomal protein S30

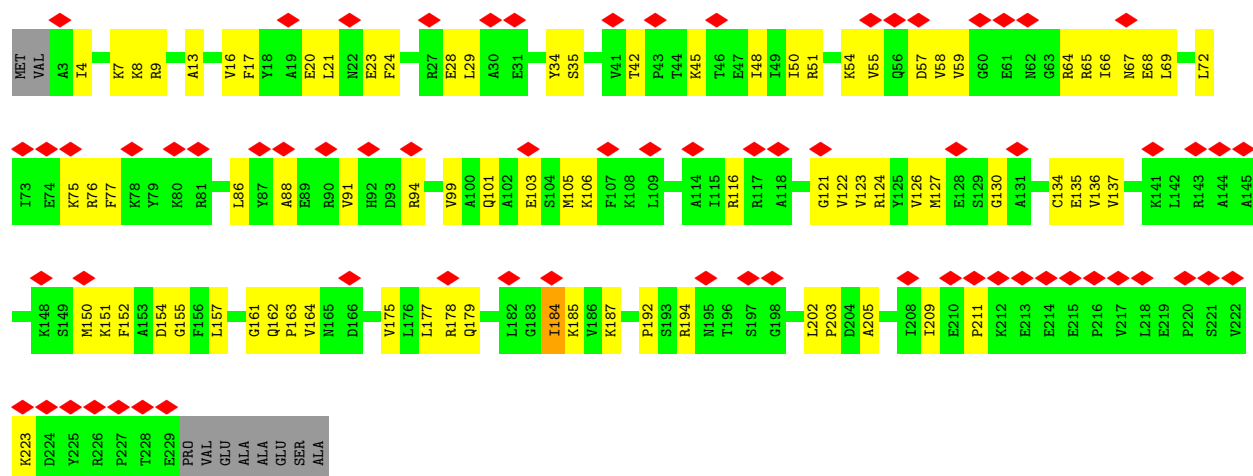


- Molecule 20: 60S ribosomal protein L41-A

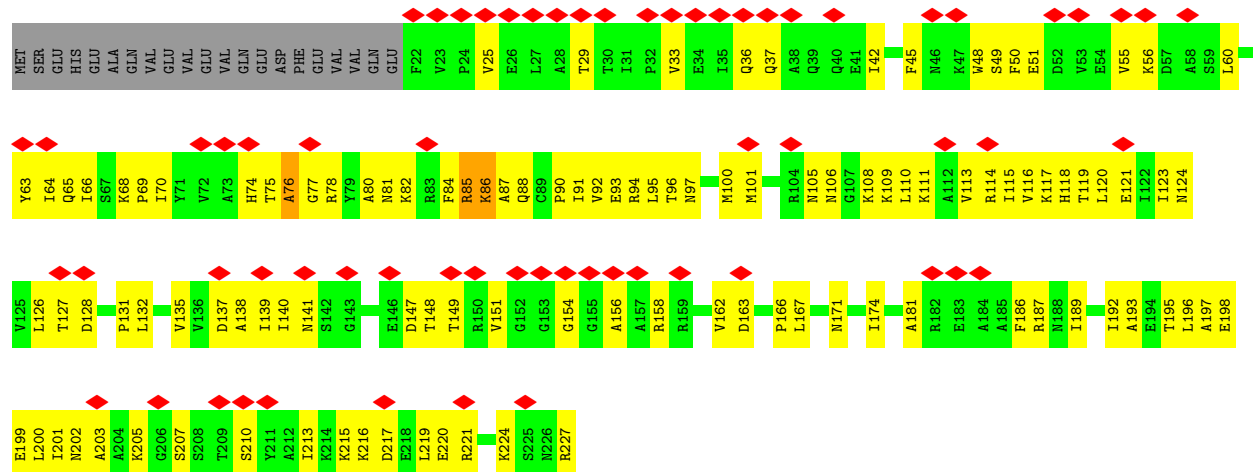
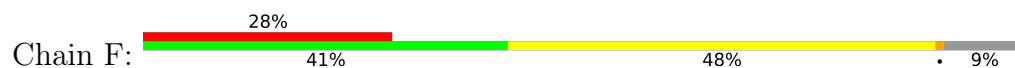


- Molecule 21: 40S ribosomal protein S3

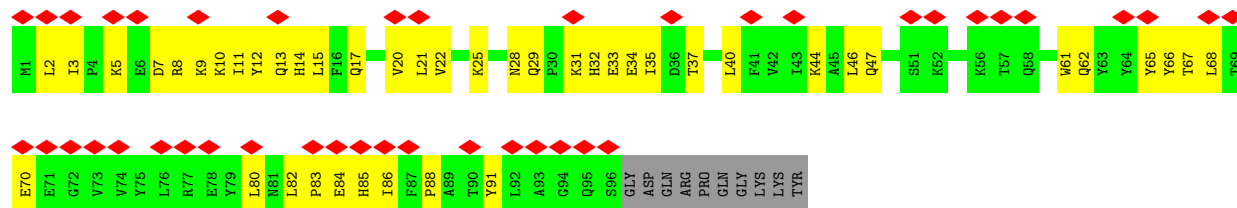
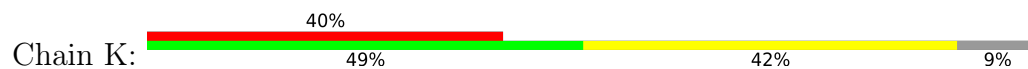




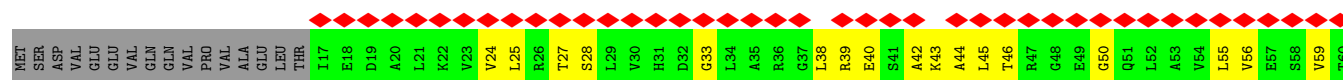
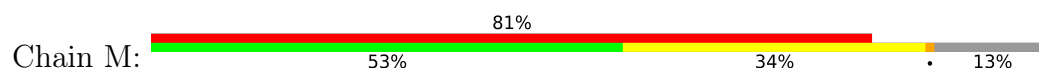
• Molecule 22: KLLA0D10659p

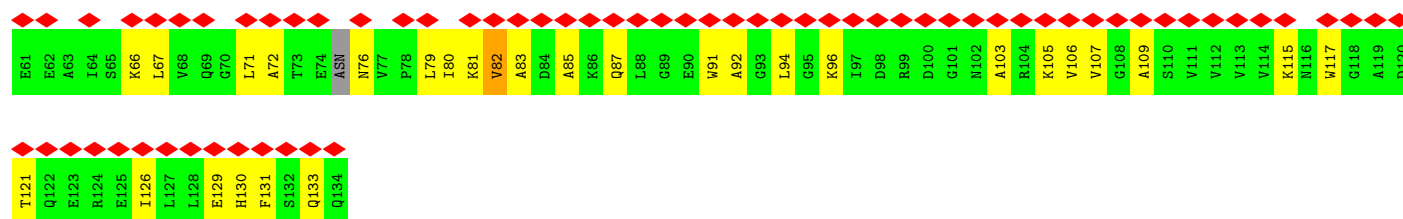


• Molecule 23: KLLA0B08173p

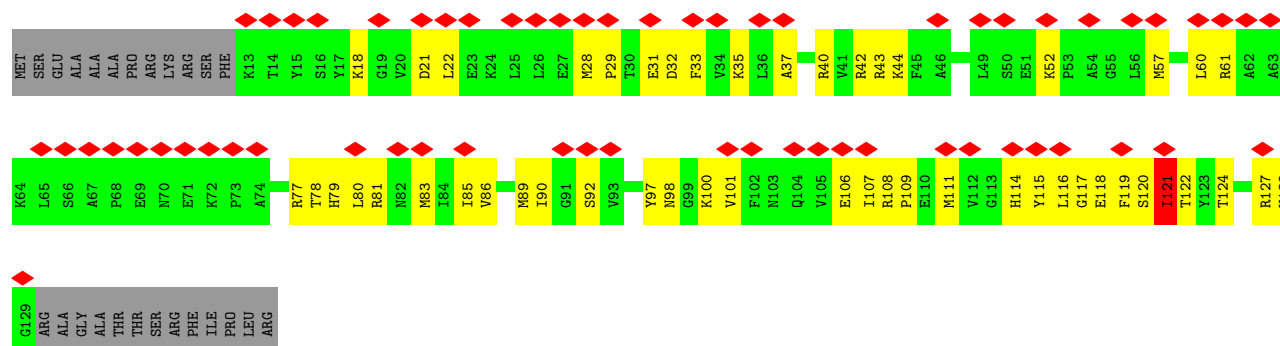
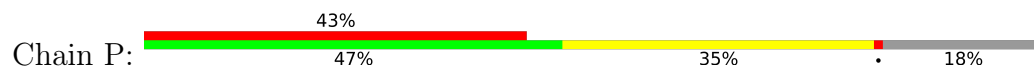


• Molecule 24: 40S ribosomal protein S12

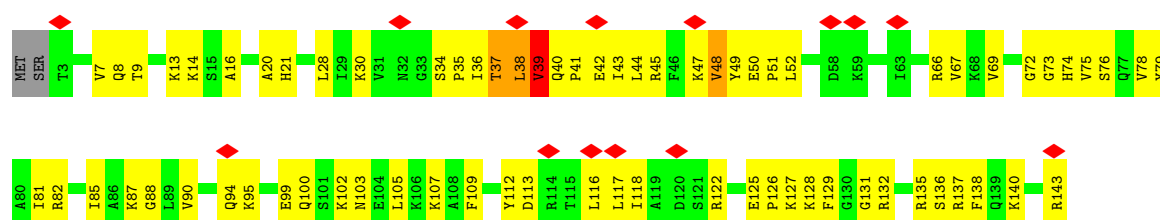




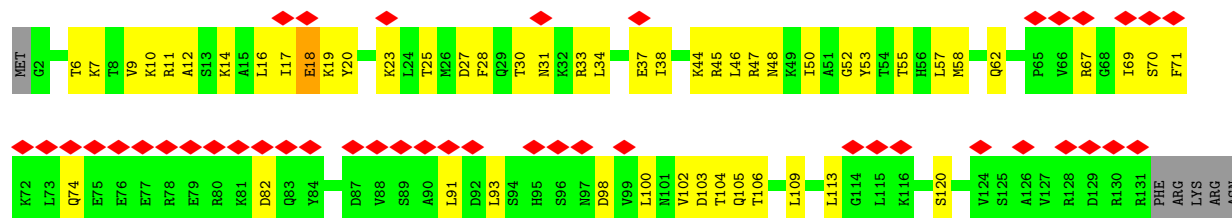
• Molecule 25: KLLA0F07843p



• Molecule 26: Small ribosomal subunit protein uS9

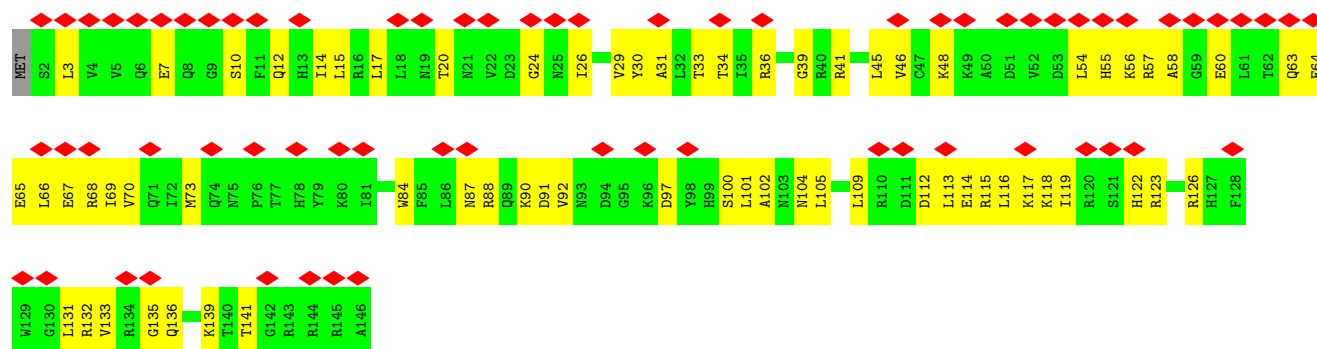


• Molecule 27: KLLA0B01474p

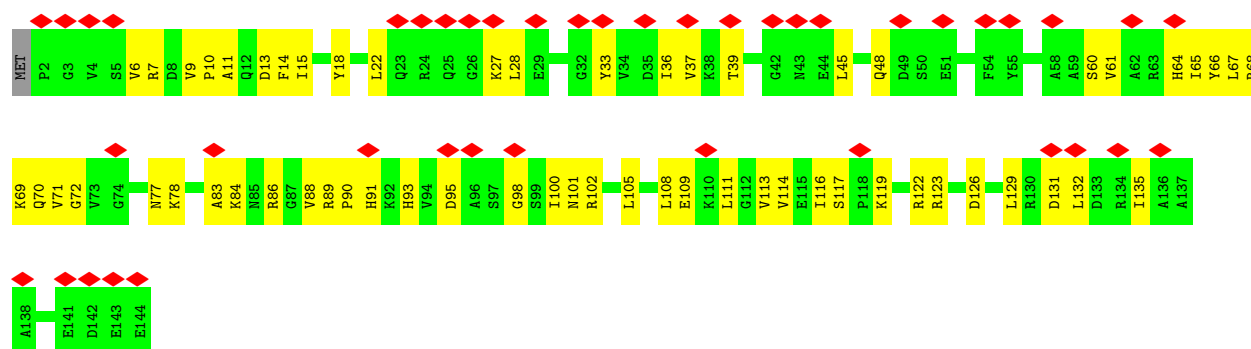


• Molecule 28: KLLA0B01562p

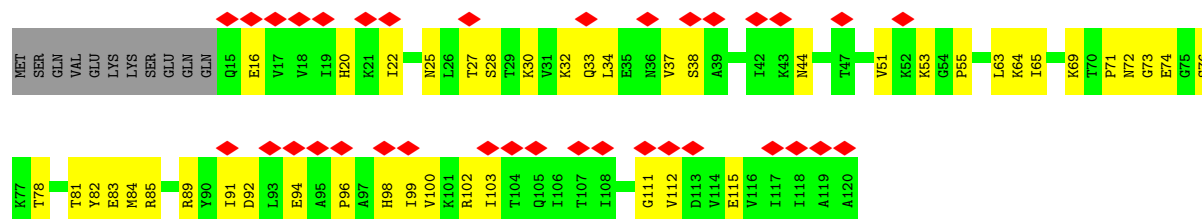




• Molecule 29: KLLA0A07194p



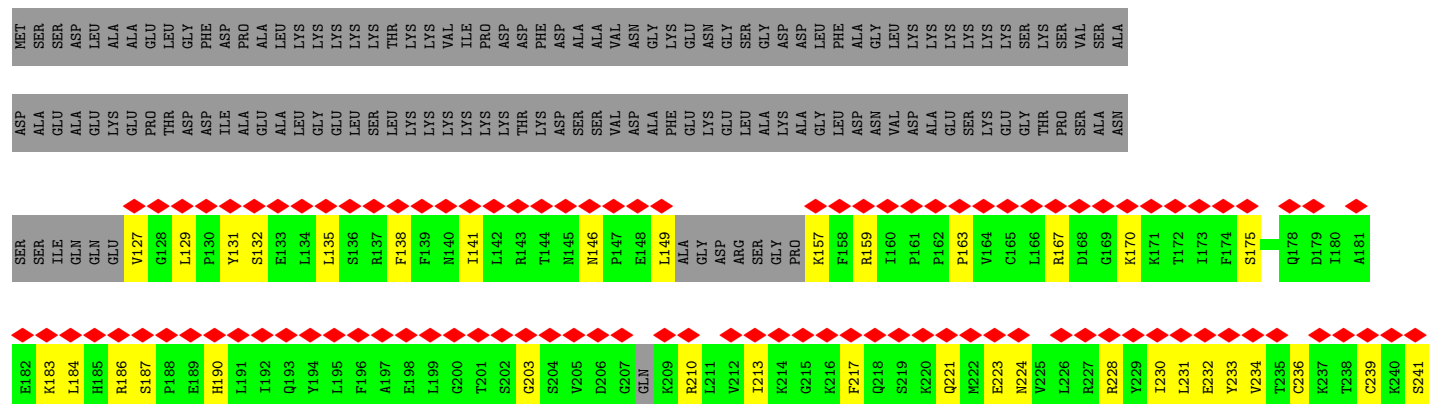
• Molecule 30: Small ribosomal subunit protein uS10



• Molecule 31: 40S ribosomal protein S25



• Molecule 32: Small ribosomal subunit protein eS28







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66217	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	-0.320	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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, MA6, RIA, 1MG, B8N, 5MC, M2G, T6A, GCP, 1MA, MG, 7MG, 2MG, H2U, PSU

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	2	0.23	0/42410	0.33	0/66079
2	A	0.31	0/1742	0.50	0/2383
3	B	0.24	0/1833	0.46	0/2467
4	C	0.29	0/1678	0.46	0/2277
5	E	0.30	0/2122	0.50	1/2861 (0.0%)
6	G	0.21	0/1855	0.44	0/2479
7	H	0.24	0/1507	0.44	0/2028
8	I	0.27	0/1515	0.44	0/2029
9	J	0.27	0/1495	0.48	0/2001
10	L	0.27	0/1263	0.43	0/1700
11	N	0.24	0/1218	0.39	0/1638
12	O	0.32	0/966	0.47	0/1297
13	V	0.25	0/696	0.40	0/938
14	W	0.32	0/1039	0.49	0/1399
15	X	0.26	0/1137	0.44	0/1516
16	Y	0.22	0/1075	0.41	0/1433
17	a	0.72	2/810 (0.2%)	0.55	1/1087 (0.1%)
18	b	0.21	0/619	0.40	0/837
19	e	0.24	0/480	0.40	0/640
20	h	0.17	0/234	0.34	0/300
21	D	0.19	0/1800	0.41	0/2421
22	F	0.20	0/1628	0.45	0/2198
23	K	0.15	0/831	0.41	0/1123
24	M	0.18	0/873	0.49	0/1180
25	P	0.23	0/942	0.45	0/1269
26	Q	0.25	0/1125	0.50	0/1510
27	R	0.25	0/1044	0.51	1/1402 (0.1%)
28	S	0.21	0/1208	0.39	0/1624
29	T	0.24	0/1129	0.43	0/1520
30	U	0.20	0/857	0.45	0/1158
31	Z	0.13	0/603	0.36	0/814
32	c	0.20	0/501	0.61	1/673 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.22	0/473	0.52	0/629
34	f	0.18	0/597	0.52	1/795 (0.1%)
35	i	0.25	0/778	0.57	0/1038
36	m	0.32	0/703	0.52	0/938
37	3	0.07	0/286	0.17	0/440
38	1	0.18	0/1529	0.36	0/2376
39	j	0.18	0/2171	0.48	1/2924 (0.0%)
40	k	0.16	0/3657	0.38	0/4946
41	l	0.12	0/1099	0.33	0/1469
42	n	0.10	0/461	0.25	0/640
43	g	0.22	0/2523	0.49	1/3434 (0.0%)
All	All	0.24	2/92512 (0.0%)	0.40	7/133910 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	25	ASN	C-N	17.08	1.57	1.33
17	a	74	CYS	C-N	-8.72	1.22	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	j	223	VAL	N-CA-C	-6.10	107.55	113.53
17	a	74	CYS	O-C-N	-5.97	115.37	122.65
5	E	19	MET	CB-CG-SD	-5.73	95.52	112.70
27	R	18	GLU	CA-CB-CG	-5.67	102.75	114.10
34	f	133	HIS	CB-CA-C	-5.27	110.48	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	38190	0	19213	1136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1702	0	1695	109	0
3	B	1809	0	1872	81	0
4	C	1648	0	1727	93	0
5	E	2078	0	2157	95	0
6	G	1832	0	1919	102	0
7	H	1483	0	1579	75	0
8	I	1489	0	1504	83	0
9	J	1471	0	1554	76	0
10	L	1235	0	1299	43	0
11	N	1195	0	1263	64	0
12	O	955	0	987	82	0
13	V	687	0	682	35	0
14	W	1021	0	1056	61	0
15	X	1119	0	1198	57	0
16	Y	1061	0	1111	46	0
17	a	797	0	835	60	0
18	b	609	0	629	25	0
19	e	472	0	508	27	0
20	h	233	0	284	10	0
21	D	1774	0	1855	100	0
22	F	1609	0	1679	128	0
23	K	809	0	810	62	0
24	M	867	0	884	39	0
25	P	923	0	960	62	0
26	Q	1105	0	1170	124	0
27	R	1033	0	1082	64	0
28	S	1189	0	1211	90	0
29	T	1110	0	1124	65	0
30	U	845	0	913	60	0
31	Z	594	0	590	19	0
32	c	499	0	536	46	0
33	d	461	0	448	48	0
34	f	584	0	602	104	0
35	i	769	0	765	54	0
36	m	695	0	729	45	0
37	3	256	0	132	4	0
38	1	1639	0	852	35	0
39	j	2139	0	2205	92	0
40	k	3596	0	3713	136	0
41	l	1083	0	1120	40	0
42	n	464	0	207	1	0
43	g	2469	0	2403	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2	94	0	0	0	0
44	X	1	0	0	0	0
44	k	1	0	0	0	0
45	a	1	0	0	0	0
45	b	1	0	0	0	0
45	f	1	0	0	0	0
45	l	1	0	0	0	0
46	k	32	0	14	2	0
47	k	8	0	8	0	0
All	All	87738	0	69084	3375	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 22.

The worst 5 of 3375 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)
34:f:116:LYS:HG3	34:f:129:PHE:CE1	1.53	1.41
21:D:75:LYS:HZ2	23:K:22:VAL:CB	1.35	1.39
34:f:116:LYS:CG	34:f:129:PHE:HE1	1.40	1.33
21:D:75:LYS:NZ	23:K:22:VAL:HB	1.44	1.31
34:f:116:LYS:CG	34:f:129:PHE:CE1	2.11	1.30

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	217/254 (85%)	203 (94%)	14 (6%)	0	100	100
3	B	225/255 (88%)	215 (96%)	9 (4%)	1 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	218/259 (84%)	206 (94%)	11 (5%)	1 (0%)	24	60
5	E	258/261 (99%)	245 (95%)	13 (5%)	0	100	100
6	G	228/236 (97%)	223 (98%)	5 (2%)	0	100	100
7	H	182/190 (96%)	174 (96%)	8 (4%)	0	100	100
8	I	184/201 (92%)	172 (94%)	12 (6%)	0	100	100
9	J	180/188 (96%)	176 (98%)	4 (2%)	0	100	100
10	L	151/156 (97%)	141 (93%)	9 (6%)	1 (1%)	18	54
11	N	149/151 (99%)	143 (96%)	6 (4%)	0	100	100
12	O	127/137 (93%)	122 (96%)	5 (4%)	0	100	100
13	V	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
14	W	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
15	X	142/145 (98%)	132 (93%)	10 (7%)	0	100	100
16	Y	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
17	a	100/103 (97%)	91 (91%)	8 (8%)	1 (1%)	12	45
18	b	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
19	e	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	218 (97%)	6 (3%)	1 (0%)	30	65
22	F	204/227 (90%)	183 (90%)	18 (9%)	3 (2%)	8	38
23	K	94/106 (89%)	88 (94%)	6 (6%)	0	100	100
24	M	113/134 (84%)	104 (92%)	8 (7%)	1 (1%)	14	48
25	P	115/142 (81%)	106 (92%)	8 (7%)	1 (1%)	14	48
26	Q	139/143 (97%)	122 (88%)	16 (12%)	1 (1%)	18	54
27	R	128/136 (94%)	122 (95%)	6 (5%)	0	100	100
28	S	143/146 (98%)	134 (94%)	9 (6%)	0	100	100
29	T	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
30	U	104/117 (89%)	99 (95%)	5 (5%)	0	100	100
31	Z	76/108 (70%)	71 (93%)	5 (7%)	0	100	100
32	c	62/67 (92%)	56 (90%)	6 (10%)	0	100	100
33	d	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
34	f	72/150 (48%)	55 (76%)	16 (22%)	1 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	i	94/153 (61%)	84 (89%)	10 (11%)	0	100	100
36	m	84/108 (78%)	76 (90%)	8 (10%)	0	100	100
39	j	263/304 (86%)	246 (94%)	16 (6%)	1 (0%)	30	65
40	k	468/527 (89%)	437 (93%)	30 (6%)	1 (0%)	43	75
41	l	126/270 (47%)	123 (98%)	3 (2%)	0	100	100
42	n	87/812 (11%)	87 (100%)	0	0	100	100
43	g	314/326 (96%)	284 (90%)	30 (10%)	0	100	100
All	All	5970/7471 (80%)	5605 (94%)	351 (6%)	14 (0%)	44	75

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	j	55	ARG
3	B	21	VAL
22	F	86	LYS
26	Q	39	VAL
10	L	7	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	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	201/228 (88%)	201 (100%)	0	100	100
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	223 (100%)	0	100	100
6	G	192/200 (96%)	192 (100%)	0	100	100
7	H	164/170 (96%)	164 (100%)	0	100	100
8	I	147/159 (92%)	147 (100%)	0	100	100
9	J	153/158 (97%)	153 (100%)	0	100	100
10	L	134/137 (98%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	N	128/128 (100%)	128 (100%)	0	100	100
12	O	97/104 (93%)	97 (100%)	0	100	100
13	V	73/73 (100%)	73 (100%)	0	100	100
14	W	110/111 (99%)	109 (99%)	1 (1%)	70	76
15	X	119/120 (99%)	119 (100%)	0	100	100
16	Y	108/109 (99%)	108 (100%)	0	100	100
17	a	83/88 (94%)	83 (100%)	0	100	100
18	b	71/72 (99%)	71 (100%)	0	100	100
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	23 (100%)	0	100	100
21	D	188/196 (96%)	187 (100%)	1 (0%)	81	82
22	F	174/194 (90%)	173 (99%)	1 (1%)	78	81
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	90/109 (83%)	90 (100%)	0	100	100
25	P	99/119 (83%)	98 (99%)	1 (1%)	68	76
26	Q	117/119 (98%)	113 (97%)	4 (3%)	32	55
27	R	116/124 (94%)	116 (100%)	0	100	100
28	S	127/129 (98%)	127 (100%)	0	100	100
29	T	117/118 (99%)	117 (100%)	0	100	100
30	U	96/107 (90%)	96 (100%)	0	100	100
31	Z	59/88 (67%)	59 (100%)	0	100	100
32	c	55/59 (93%)	54 (98%)	1 (2%)	51	68
33	d	47/48 (98%)	47 (100%)	0	100	100
34	f	60/133 (45%)	57 (95%)	3 (5%)	22	45
35	i	80/130 (62%)	79 (99%)	1 (1%)	61	72
36	m	77/96 (80%)	77 (100%)	0	100	100
39	j	239/274 (87%)	238 (100%)	1 (0%)	84	84
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	125/234 (53%)	125 (100%)	0	100	100
43	g	264/272 (97%)	263 (100%)	1 (0%)	84	84
All	All	5045/5667 (89%)	5030 (100%)	15 (0%)	84	85

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Q	48	VAL
39	j	233	GLN
32	c	22	ARG
43	g	54	GLN
34	f	141	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
36	m	81	GLN
39	j	41	ASN
40	k	433	ASN
14	W	42	GLN
13	V	70	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	581 (32%)	29 (1%)
37	3	0/49	-	-
38	1	72/75 (96%)	26 (36%)	4 (5%)
All	All	1869/1922 (97%)	607 (32%)	33 (1%)

5 of 607 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	17	C
1	2	25	C

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1797	U
38	1	8	U
38	1	74	C
1	2	781	A

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Mol	Chain	Res	Type
1	2	700	C

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

23 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8N	2	1190	1	25,29,30	3.37	7 (28%)	28,42,45	1.98	9 (32%)
1	MA6	2	1780	1	23,26,27	1.36	4 (17%)	33,38,41	4.20	14 (42%)
38	5MC	1	49	38	19,22,23	3.62	8 (42%)	26,32,35	1.17	4 (15%)
38	1MA	1	58	38	21,25,26	2.91	5 (23%)	30,37,40	2.41	8 (26%)
1	7MG	2	1573	38,1	23,26,27	3.42	11 (47%)	27,39,42	2.17	10 (37%)
1	PSU	2	998	1	18,21,22	4.45	8 (44%)	21,30,33	2.00	6 (28%)
1	PSU	2	465	1	18,21,22	4.49	7 (38%)	21,30,33	1.95	5 (23%)
1	2MG	2	1570	1	23,26,27	2.90	8 (34%)	33,38,41	3.12	12 (36%)
38	T6A	1	37	38	31,34,35	2.03	8 (25%)	43,49,52	2.57	14 (32%)
38	H2U	1	47	38	18,21,22	3.16	5 (27%)	19,30,33	1.51	4 (21%)
38	RIA	1	64	38	35,38,39	4.30	20 (57%)	50,57,60	3.50	19 (38%)
38	H2U	1	16	38	18,21,22	3.13	5 (27%)	19,30,33	1.46	4 (21%)
38	2MG	1	10	38	23,26,27	2.87	9 (39%)	33,38,41	3.22	12 (36%)
1	5MC	2	1637	1	19,22,23	3.45	8 (42%)	26,32,35	0.98	2 (7%)
38	M2G	1	26	38	24,27,28	2.71	8 (33%)	33,40,43	2.52	10 (30%)
1	PSU	2	1289	1	18,21,22	4.50	7 (38%)	21,30,33	2.09	5 (23%)
38	1MG	1	9	38	23,26,27	3.04	7 (30%)	33,39,42	2.13	9 (27%)
38	7MG	1	46	38	23,26,27	3.64	11 (47%)	27,39,42	2.20	9 (33%)
1	5MC	2	1006	1	19,22,23	3.42	8 (42%)	26,32,35	0.98	2 (7%)
1	PSU	2	120	1	18,21,22	4.53	7 (38%)	21,30,33	1.96	5 (23%)
1	PSU	2	766	1	18,21,22	4.41	8 (44%)	21,30,33	2.12	6 (28%)
1	2MG	2	1426	44,1	23,26,27	2.84	9 (39%)	33,38,41	3.23	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	5MC	1	48	38	19,22,23	3.69	8 (42%)	26,32,35	1.00	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8N	2	1190	1	-	4/16/34/35	0/2/2/2
1	MA6	2	1780	1	-	3/11/29/30	0/3/3/3
38	5MC	1	49	38	-	3/7/25/26	0/2/2/2
38	1MA	1	58	38	-	2/7/25/26	0/3/3/3
1	7MG	2	1573	38,1	-	0/7/37/38	0/3/3/3
1	PSU	2	998	1	-	1/7/25/26	0/2/2/2
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1570	1	-	1/9/27/28	0/3/3/3
38	T6A	1	37	38	-	5/23/41/42	0/3/3/3
38	H2U	1	47	38	-	1/7/38/39	0/2/2/2
38	RIA	1	64	38	-	6/17/51/52	0/4/4/4
38	H2U	1	16	38	-	7/7/38/39	0/2/2/2
38	2MG	1	10	38	-	4/9/27/28	0/3/3/3
1	5MC	2	1637	1	-	0/7/25/26	0/2/2/2
38	M2G	1	26	38	-	2/11/29/30	0/3/3/3
1	PSU	2	1289	1	-	0/7/25/26	0/2/2/2
38	1MG	1	9	38	-	3/7/25/26	0/3/3/3
38	7MG	1	46	38	-	2/7/37/38	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
1	PSU	2	120	1	-	1/7/25/26	0/2/2/2
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2
1	2MG	2	1426	44,1	-	1/9/27/28	0/3/3/3
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2

The worst 5 of 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C3A-C2A	-12.88	1.24	1.53
1	2	120	PSU	C6-C5	11.19	1.47	1.35
1	2	465	PSU	C6-C5	11.01	1.47	1.35
1	2	1289	PSU	C6-C5	10.95	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	998	PSU	C6-C5	10.89	1.47	1.35

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	64	RIA	C1A-N9-C8	-12.96	98.34	127.09
1	2	1780	MA6	N1-C6-N6	-11.98	102.26	116.86
38	1	64	RIA	C4-N9-C1A	11.67	153.91	126.63
1	2	1780	MA6	C1'-N9-C8	-11.23	102.18	127.09
38	1	10	2MG	C1'-N9-C8	-10.42	97.13	126.73

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	766	PSU	O4'-C4'-C5'-O5'
1	2	1780	MA6	O4'-C4'-C5'-O5'
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	10	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1780	MA6	4	0
38	1	49	5MC	1	0
1	2	1573	7MG	4	0
1	2	998	PSU	2	0
1	2	465	PSU	1	0
1	2	1570	2MG	3	0
38	1	64	RIA	1	0
38	1	16	H2U	3	0
38	1	10	2MG	2	0
1	2	1637	5MC	2	0
38	1	26	M2G	2	0
1	2	1289	PSU	2	0
38	1	9	1MG	2	0
1	2	1006	5MC	1	0
1	2	766	PSU	1	0
1	2	1426	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 100 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	MET	k	603	-	6,7,8	0.48	0	2,7,9	0.13	0
46	GCP	k	601	-	32,34,34	2.09	3 (9%)	49,54,54	0.88	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	MET	k	603	-	-	2/5/6/8	-
46	GCP	k	601	-	-	3/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	k	601	GCP	PB-O3A	10.53	1.70	1.58
46	k	601	GCP	PA-O3A	2.90	1.62	1.59
46	k	601	GCP	PB-O2B	-2.20	1.51	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	k	601	GCP	O2B-PB-O1B	2.85	119.22	109.95
46	k	601	GCP	O1G-PG-C3B	-2.15	106.69	111.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

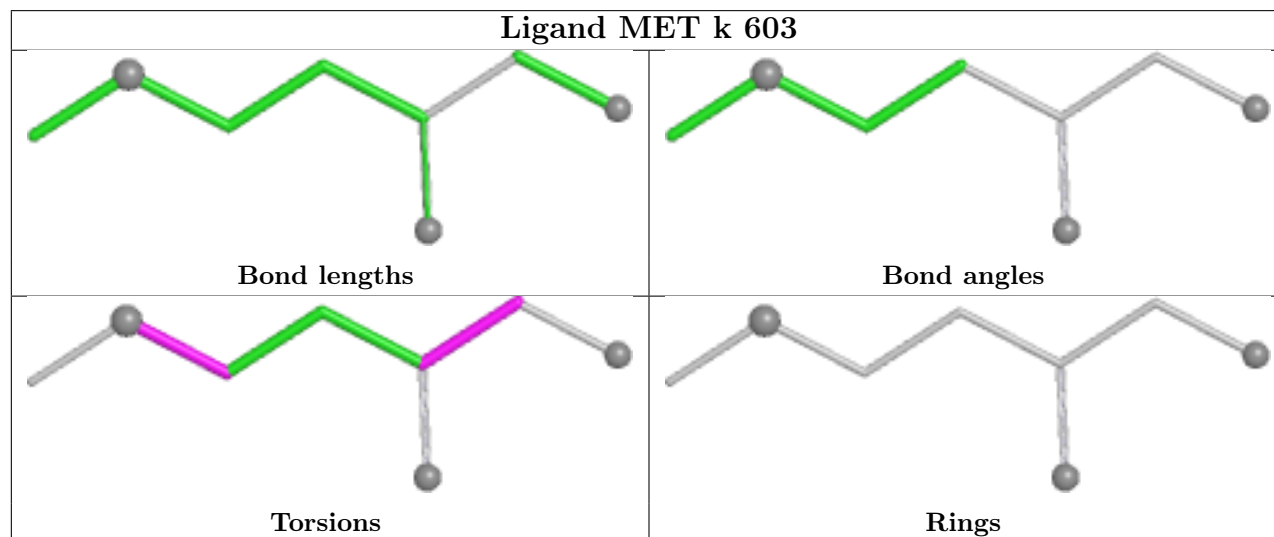
Mol	Chain	Res	Type	Atoms
46	k	601	GCP	C5'-O5'-PA-O3A
47	k	603	MET	O-C-CA-CB
46	k	601	GCP	O4'-C4'-C5'-O5'
46	k	601	GCP	C3'-C4'-C5'-O5'
47	k	603	MET	CB-CG-SD-CE

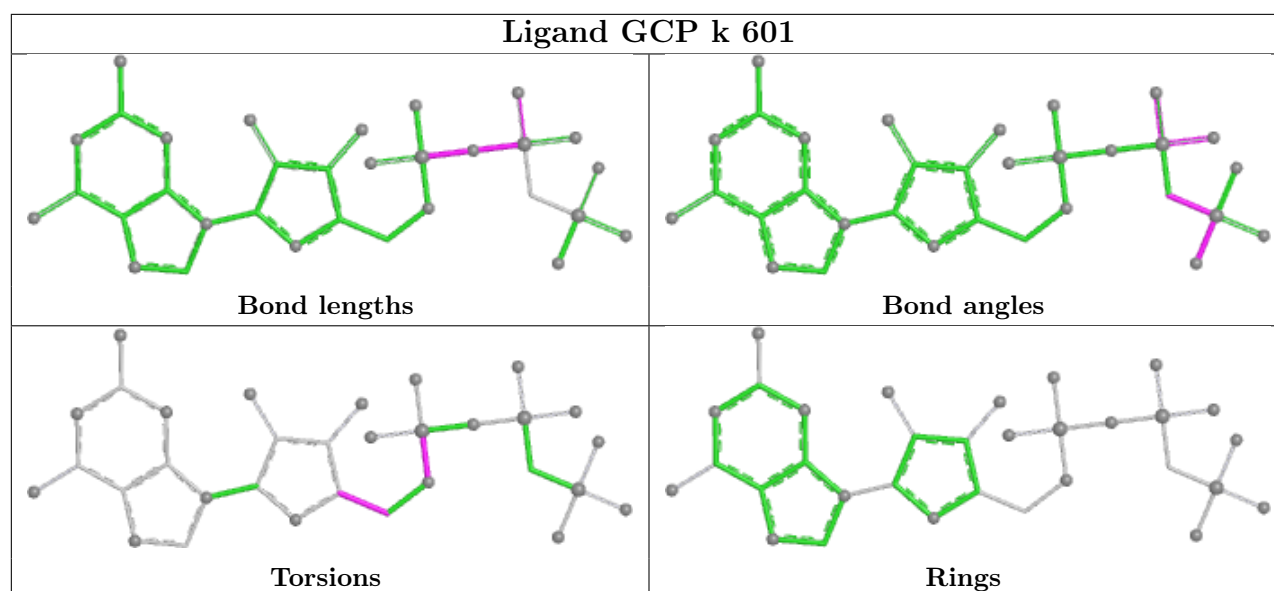
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	k	601	GCP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	1	3
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3'	65:G	P	8.59
1	1	63:G	O3'	64:RIA	P	4.32
1	2	1190:B8N	O3'	1191:C	P	3.40
1	1	16:H2U	O3'	18:G	P	3.29

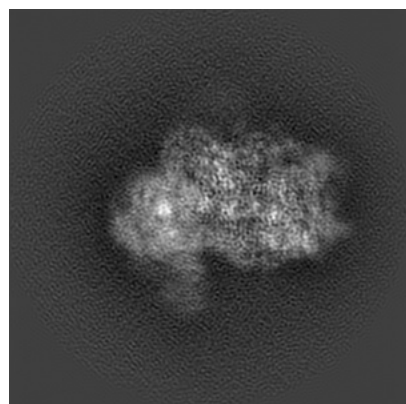
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19808. These allow visual inspection of the internal detail of the map and identification of artifacts.

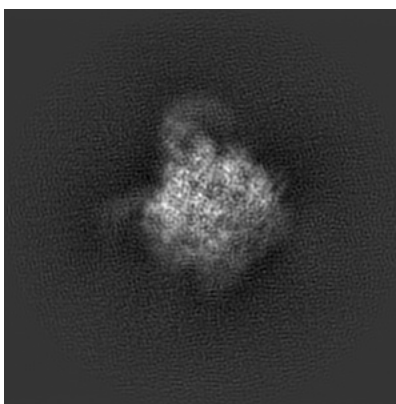
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

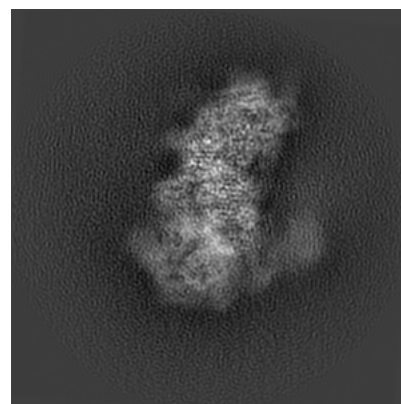
6.1.1 Primary map



X

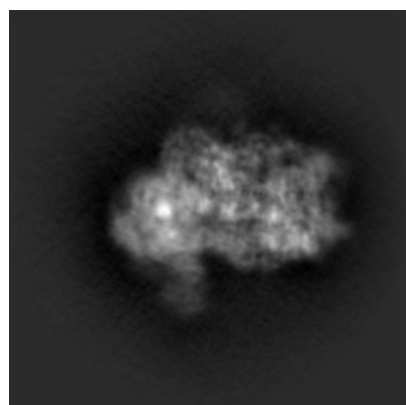


Y

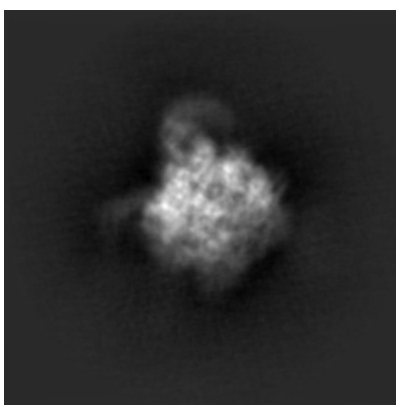


Z

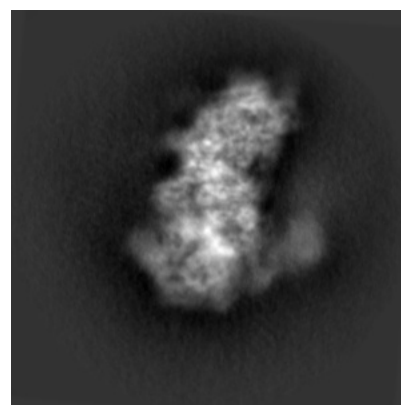
6.1.2 Raw map



X



Y

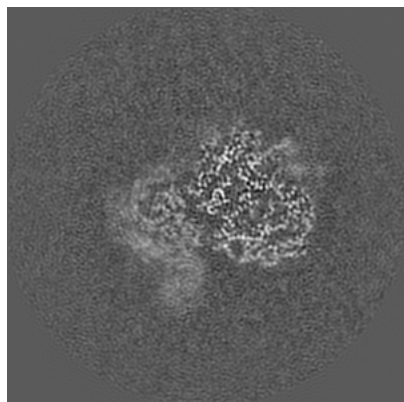


Z

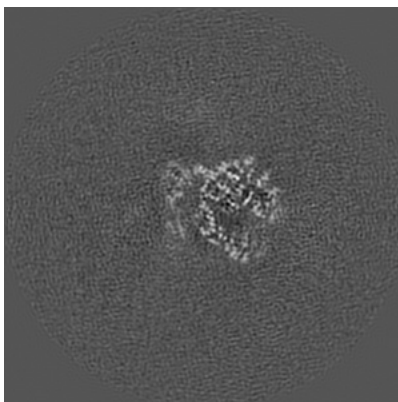
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

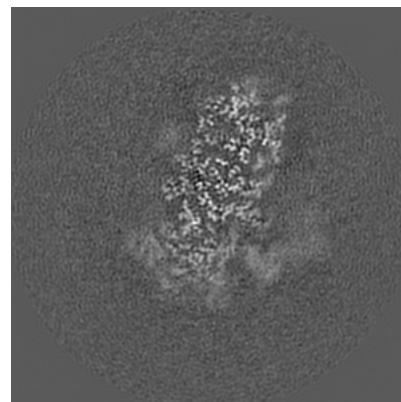
6.2.1 Primary map



X Index: 150

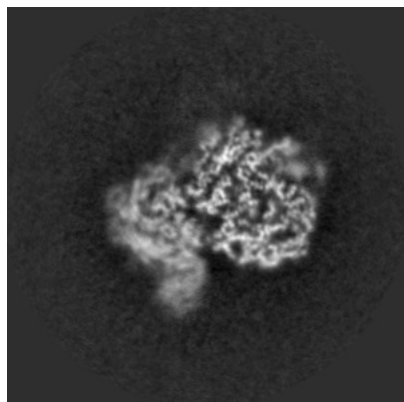


Y Index: 150

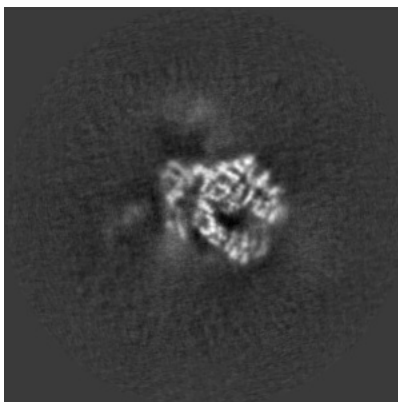


Z Index: 150

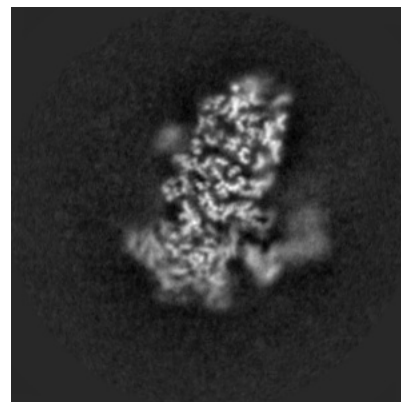
6.2.2 Raw map



X Index: 150



Y Index: 150

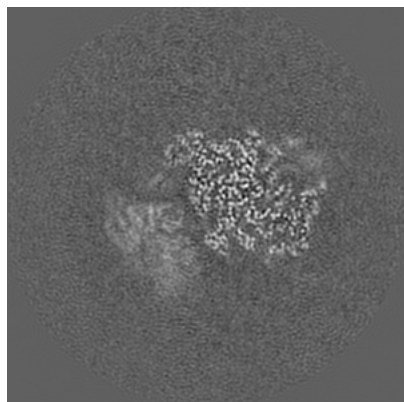


Z Index: 150

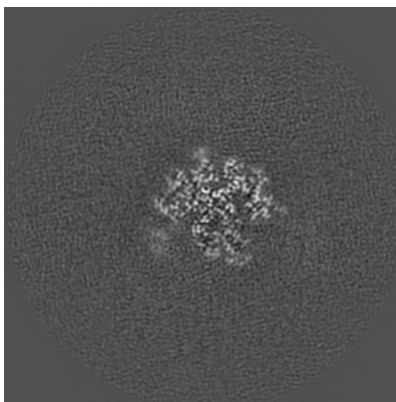
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

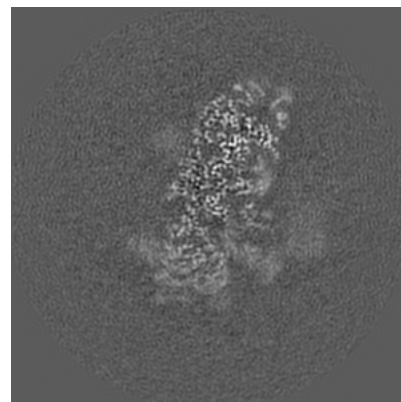
6.3.1 Primary map



X Index: 157

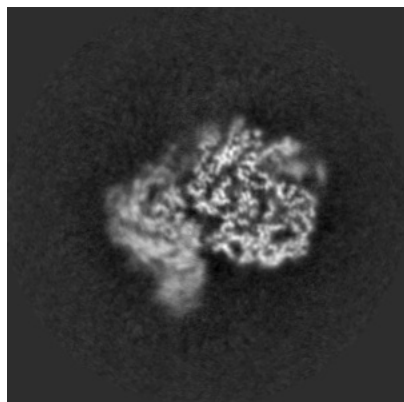


Y Index: 166

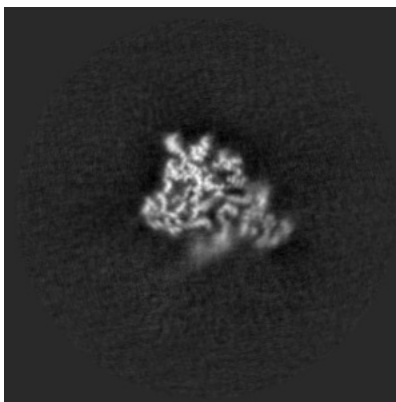


Z Index: 147

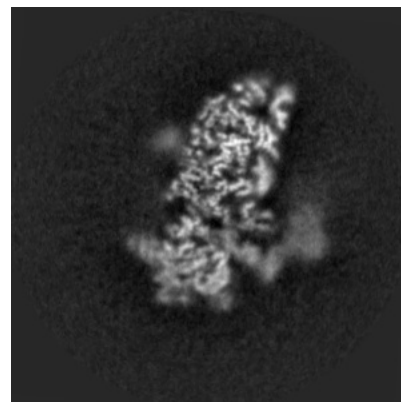
6.3.2 Raw map



X Index: 151



Y Index: 198

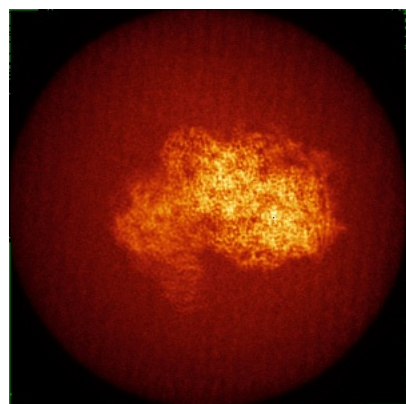


Z Index: 146

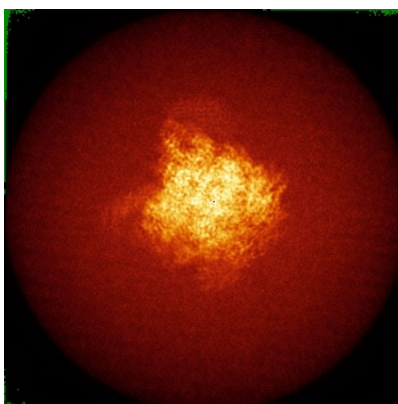
The images above show the largest variance slices of the map in three orthogonal directions.

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

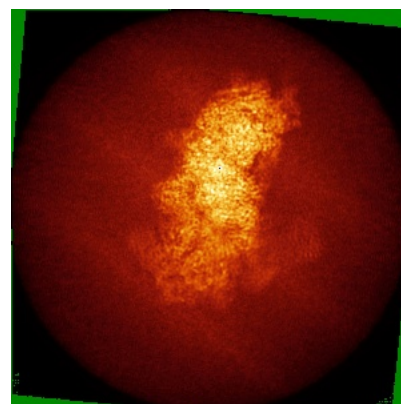
6.4.1 Primary map



X

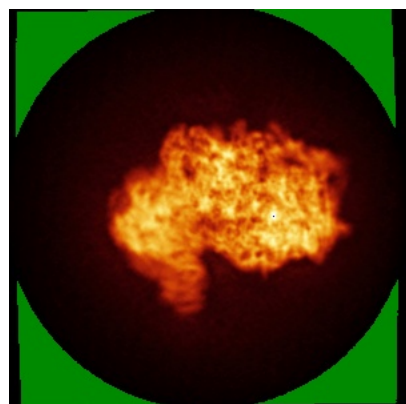


Y

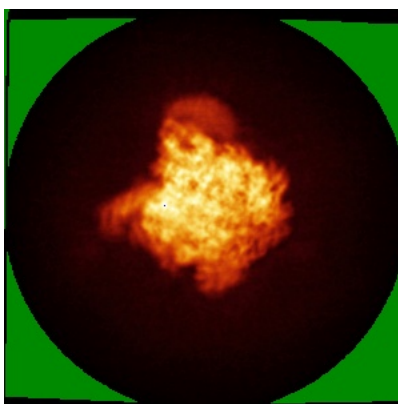


Z

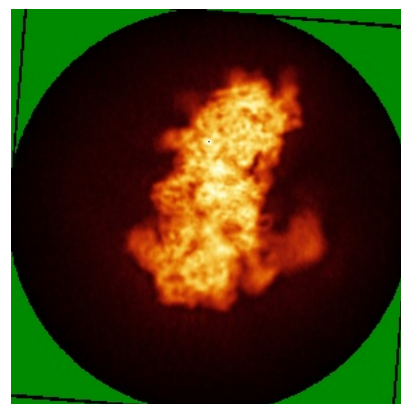
6.4.2 Raw map



X



Y

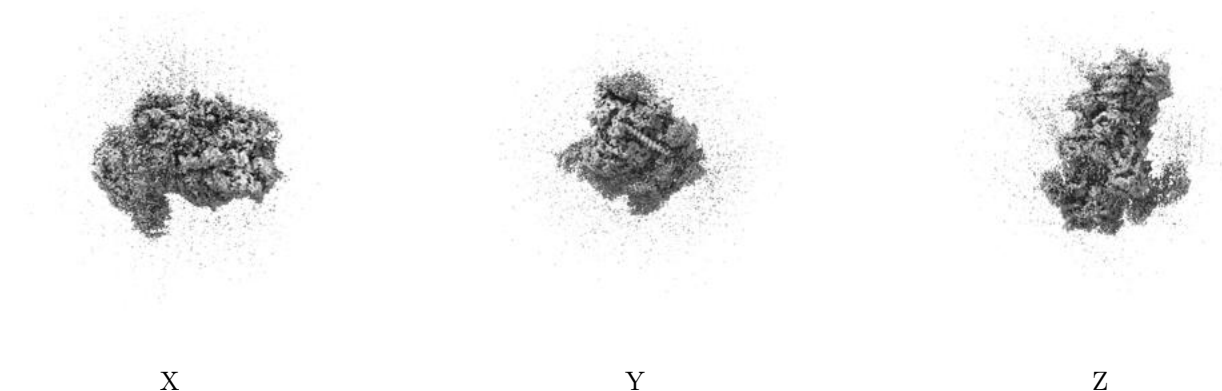


Z

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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

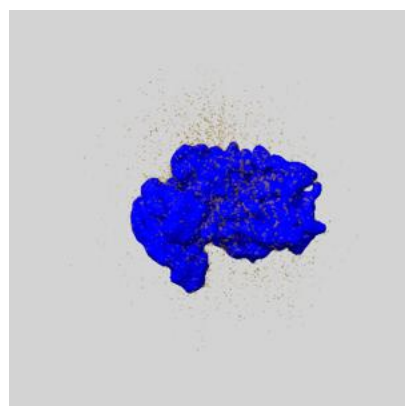
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

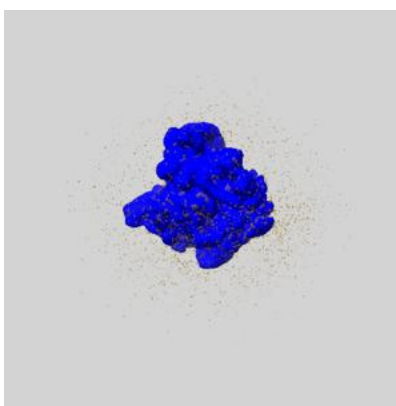
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

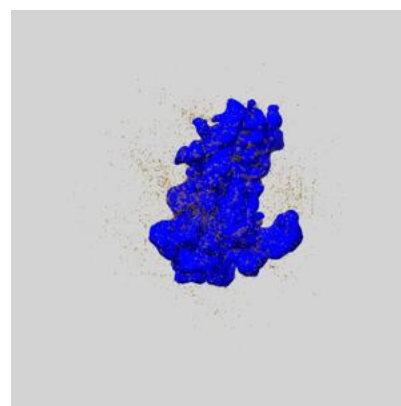
6.6.1 emd_19808_msk_1.map [i](#)



X



Y

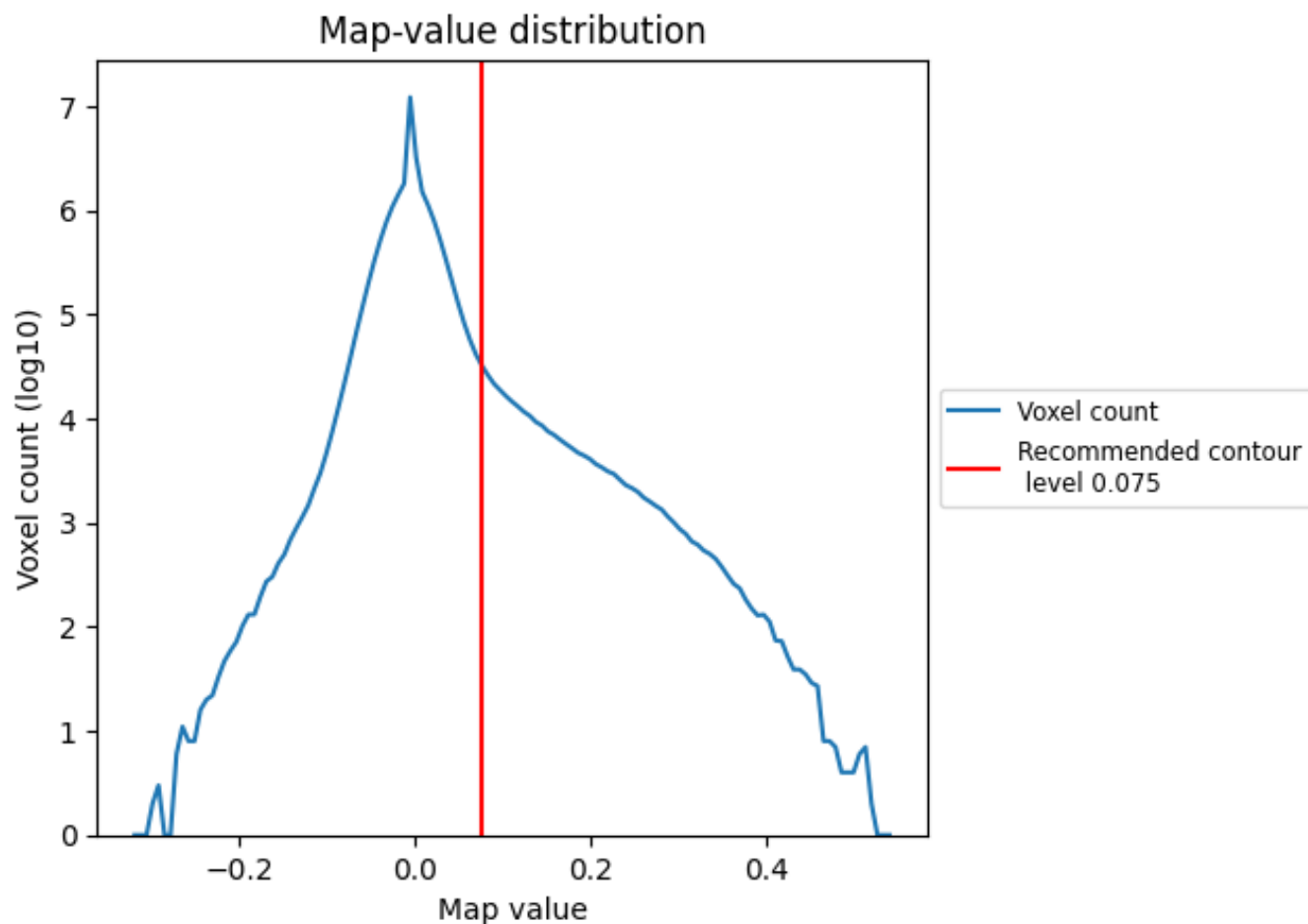


Z

7 Map analysis [i](#)

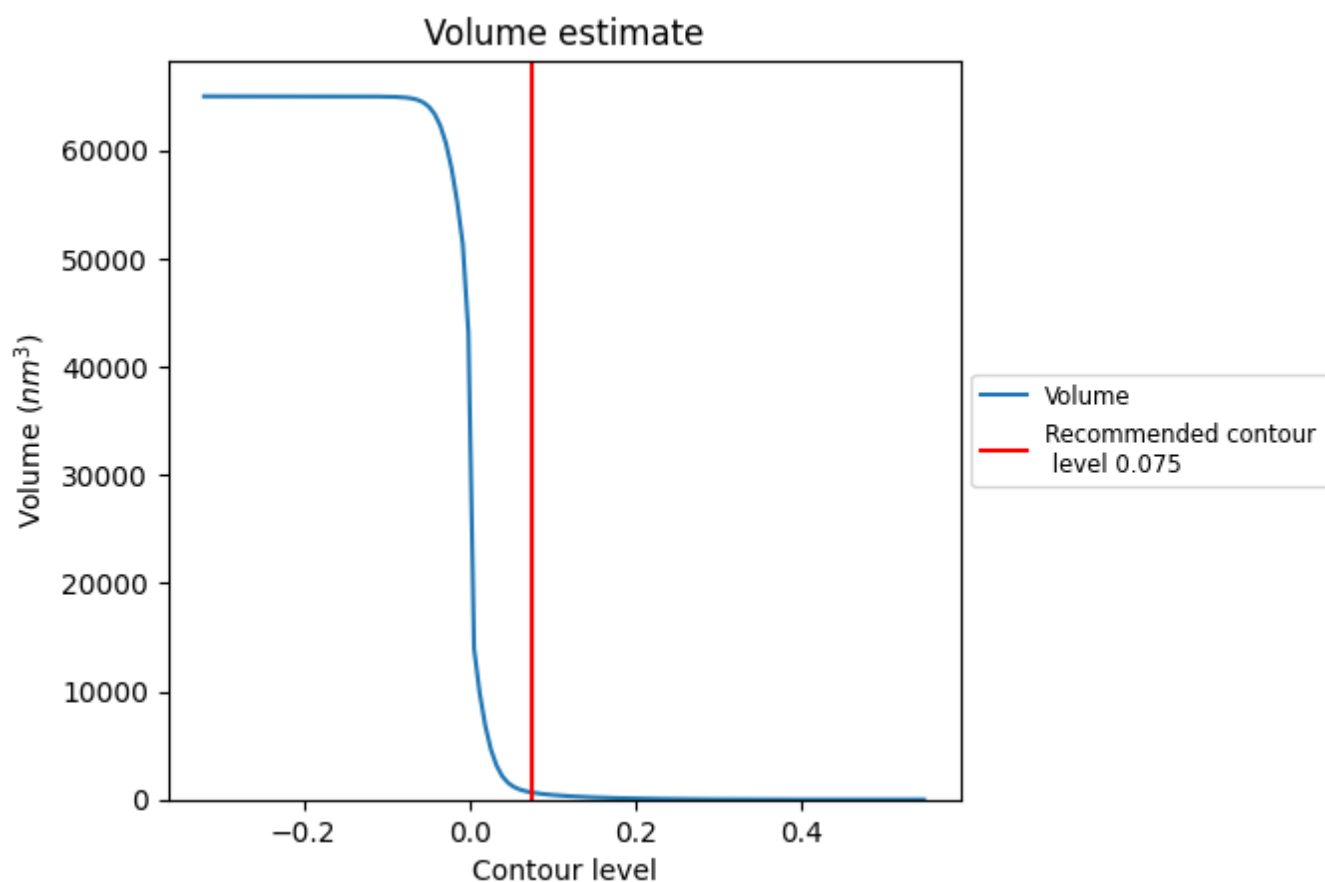
This section contains the results of statistical analysis of the map.

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.

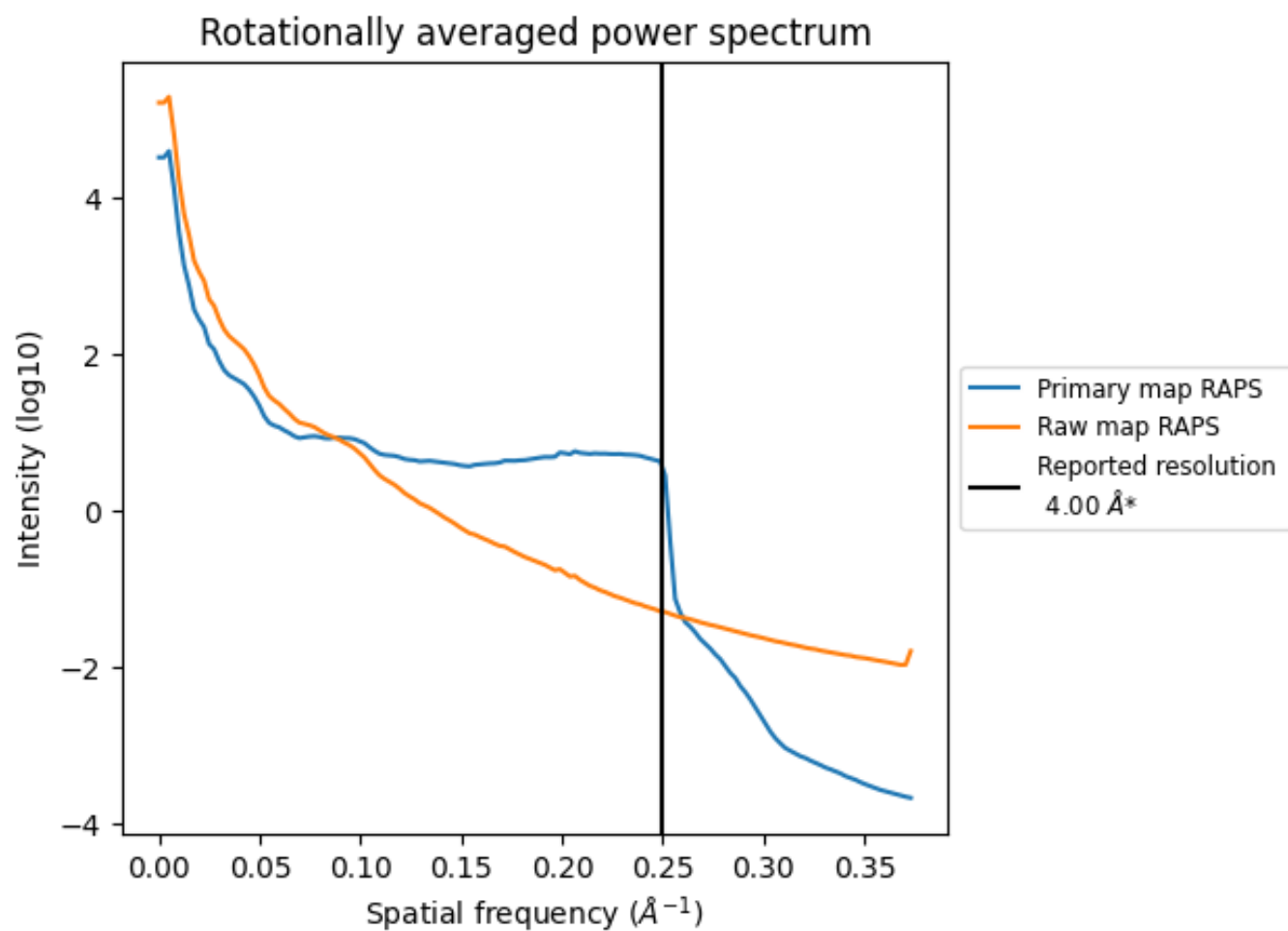
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm³; this corresponds to an approximate mass of 591 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 ⓘ

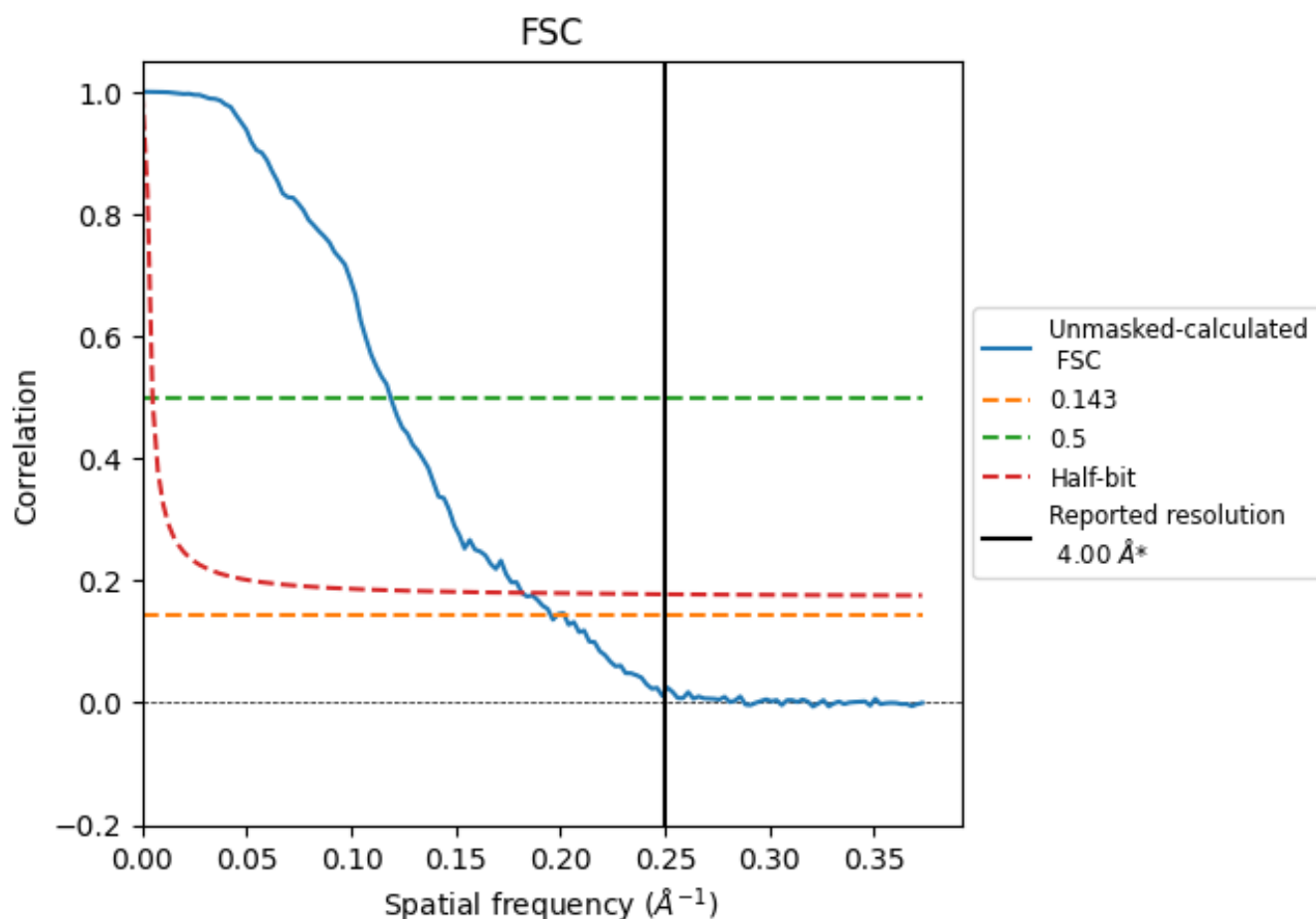


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

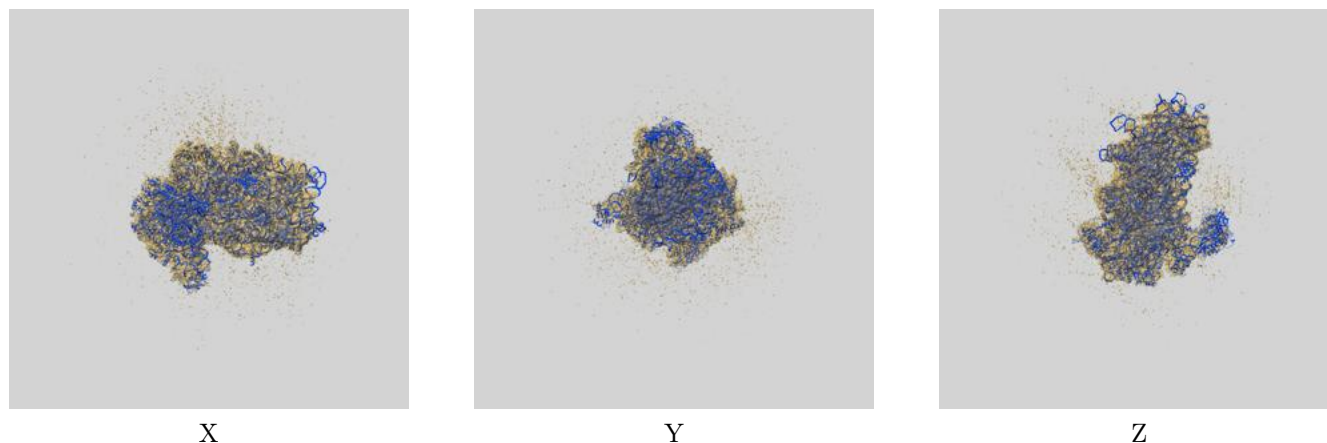
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.12	8.42	5.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.12 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

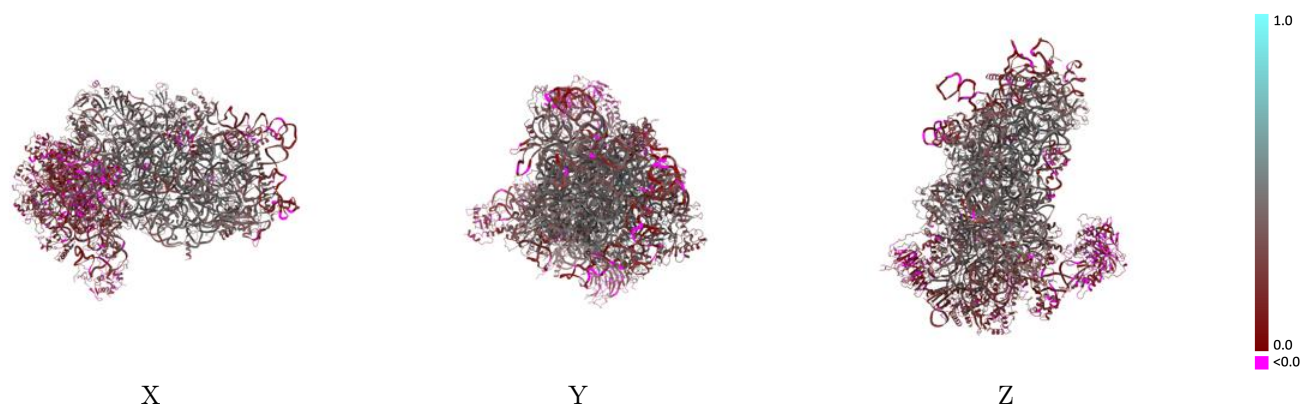
This section contains information regarding the fit between EMDB map EMD-19808 and PDB model 8S8K. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.075 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](#)

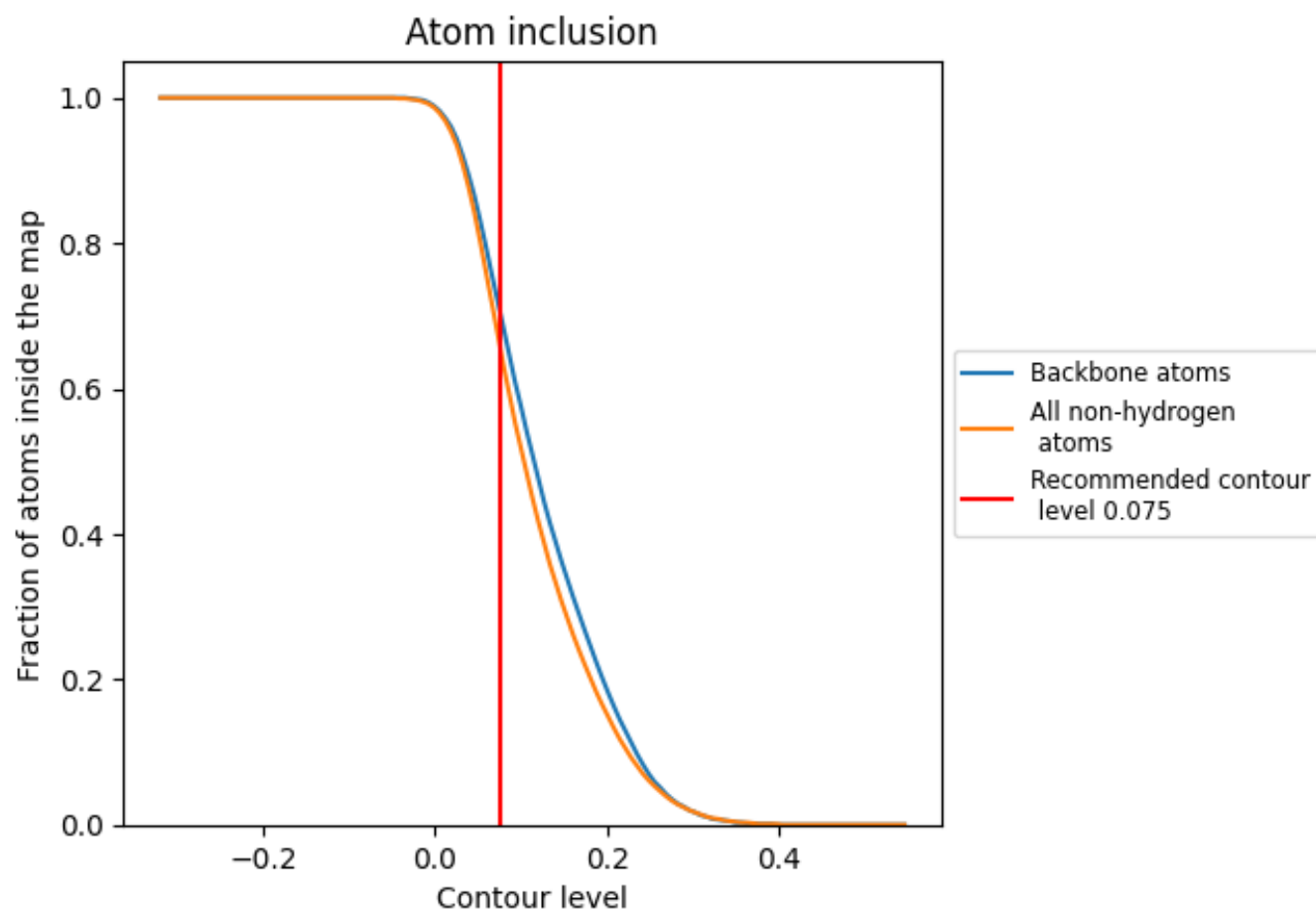


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6620	 0.3180
1	 0.4670	 0.1460
2	 0.8210	 0.3410
3	 0.0780	 0.2130
A	 0.7500	 0.3960
B	 0.7210	 0.3770
C	 0.7810	 0.4330
D	 0.5230	 0.2950
E	 0.8140	 0.4440
F	 0.5360	 0.2530
G	 0.7530	 0.3620
H	 0.6030	 0.3550
I	 0.7520	 0.4020
J	 0.8050	 0.4250
K	 0.4520	 0.2250
L	 0.7370	 0.4230
M	 0.1110	 0.1130
N	 0.7860	 0.4160
O	 0.7450	 0.3920
P	 0.3890	 0.1870
Q	 0.6170	 0.2770
R	 0.5210	 0.3110
S	 0.4530	 0.1950
T	 0.5610	 0.2320
U	 0.4810	 0.2990
V	 0.8130	 0.4260
W	 0.7960	 0.4530
X	 0.8000	 0.4530
Y	 0.8080	 0.4160
Z	 0.1500	 0.1930
a	 0.7870	 0.4330
b	 0.7080	 0.4110
c	 0.5260	 0.3150
d	 0.6020	 0.3040
e	 0.6790	 0.3990



Continued on next page...

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Chain	Atom inclusion	Q-score
f	 0.2250	 0.1520
g	 0.3520	 0.1570
h	 0.1840	 0.2910
i	 0.5530	 0.3620
j	 0.1580	 0.1750
k	 0.0610	 0.1030
l	 0.0990	 0.1340
m	 0.4830	 0.3130
n	 0.0350	 0.2020