



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 8S8F / pdb_00008s8f
EMDB ID : EMD-19803
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation
(model py48S-AUC-3.2)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 3.95 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:

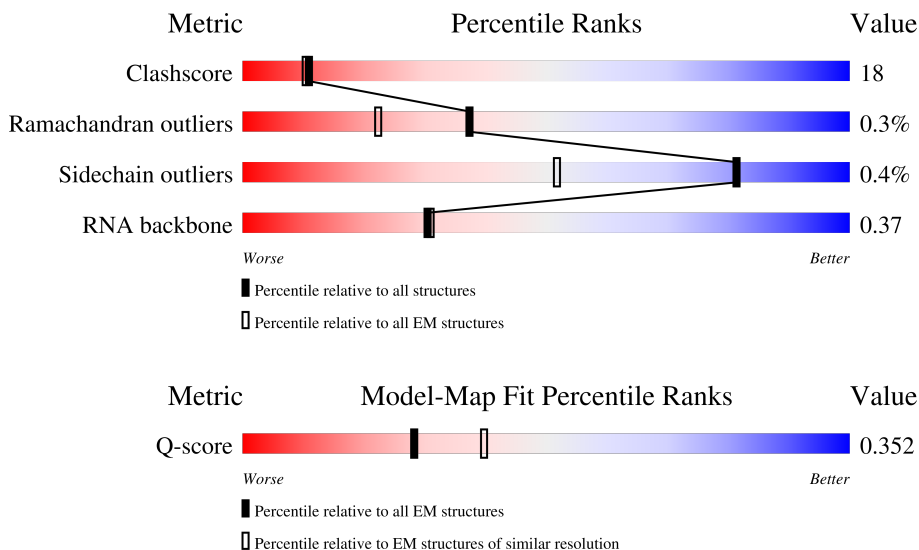
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.95 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	7707 (3.45 - 4.45)

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	
2	A	254	
3	B	255	




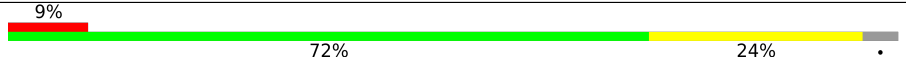
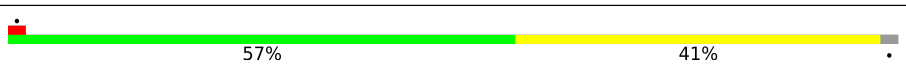
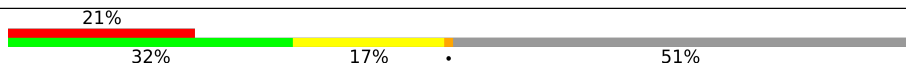
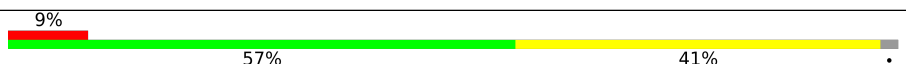
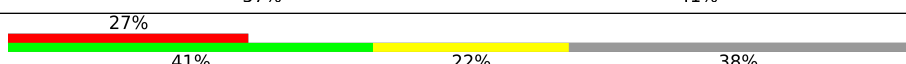
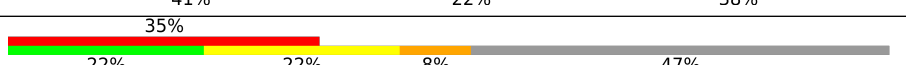
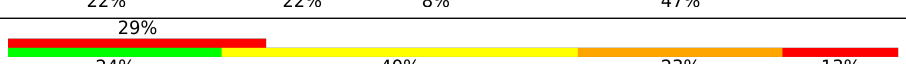

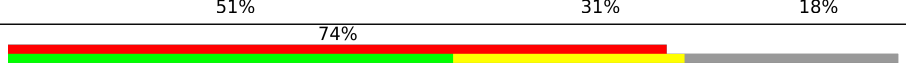

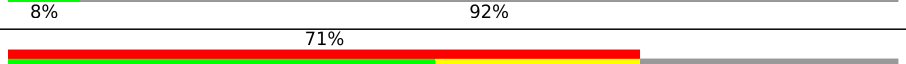
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Mol	Chain	Length	Quality of chain
4	C	259	54% 31% 15%
5	E	261	54% 45%
6	G	236	63% 34%
7	H	190	10% 57% 38%
8	I	201	6% 59% 34% 6%
9	J	188	52% 45%
10	L	156	13% 65% 33%
11	N	151	62% 38%
12	O	137	52% 42% 6%
13	V	87	54% 46%
14	W	130	55% 43%
15	X	145	57% 42%
16	Y	135	64% 36%
17	a	119	50% 36% 14%
18	b	82	68% 30%
19	e	63	14% 54% 41% 5%
20	h	25	96% 80% 20%
21	D	237	73% 23%
22	F	227	8% 52% 37% 9%
23	K	106	6% 39% 52% 9%
24	M	134	51% 52% 34% 13%
25	P	142	6% 54% 28% 18%
26	Q	143	53% 44%
27	R	136	10% 60% 35%
28	S	146	5% 54% 45%

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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	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	519	
41	l	285	
42	m	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	M2G	1	26	-	-	X	-
38	5MC	1	48	-	-	X	-

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 85732 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
			Total	C	N	O	P		
1	2	1789	38003	16989	6694	12531	1789	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	225	1796	1135	330	328	3	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	182	1464	923	287	253	1	0	0

- Molecule 10 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	155	1248	798	237	210	3	0	0

- Molecule 11 is a protein called KLLA0F18040p.

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

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

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

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

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

- 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 40S 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
			885	553	161	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
			Total	C	N	O	S		
28	S	145	1189	739	239	209	2	0	0

- Molecule 29 is a protein called KLLA0A07194p.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called KLLA0E12277p.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	95	Total	C	N	O	S	0	0
			764	474	142	143	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total	C	N	O	P	0	0
			536	242	84	184	26		

- 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	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			190	124	32	34		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	77	Total	C	N	O	S	0	0
			619	395	109	111	4		

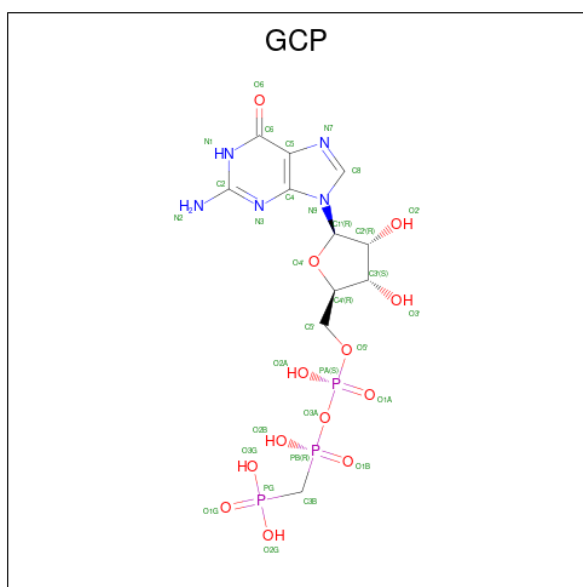
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
43	2	111	Total	Mg	0
			111	111	
43	S	1	Total	Mg	0
			1	1	
43	T	2	Total	Mg	0
			2	2	
43	i	1	Total	Mg	0
			1	1	
43	k	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

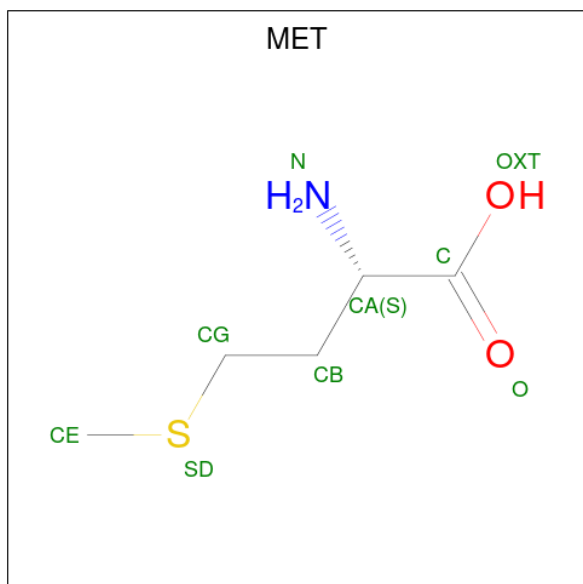
Mol	Chain	Residues	Atoms		AltConf
44	a	1	Total	Zn	0
			1	1	
44	b	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	
44	k	1	Total	Zn	0
			1	1	

- Molecule 45 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 46 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S) (labeled as "Ligand of Interest" by depositor).



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

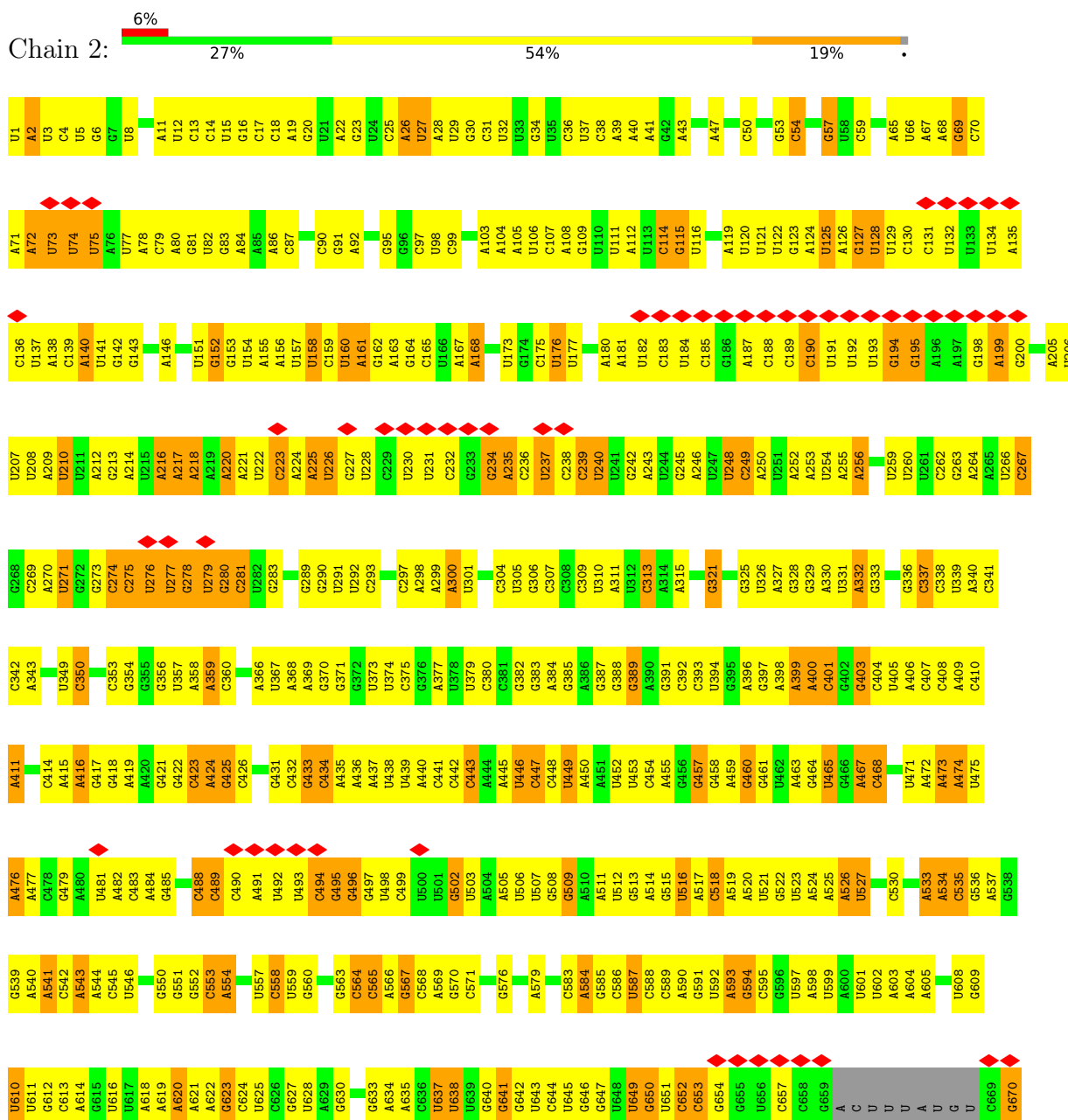
- Molecule 47 is water.

Mol	Chain	Residues	Atoms		AltConf
47	2	3	Total 3	O 3	0

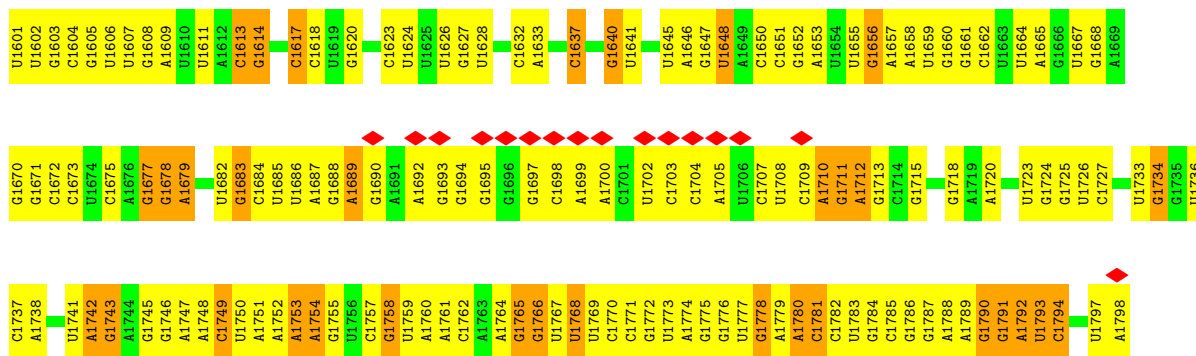
3 Residue-property plots

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

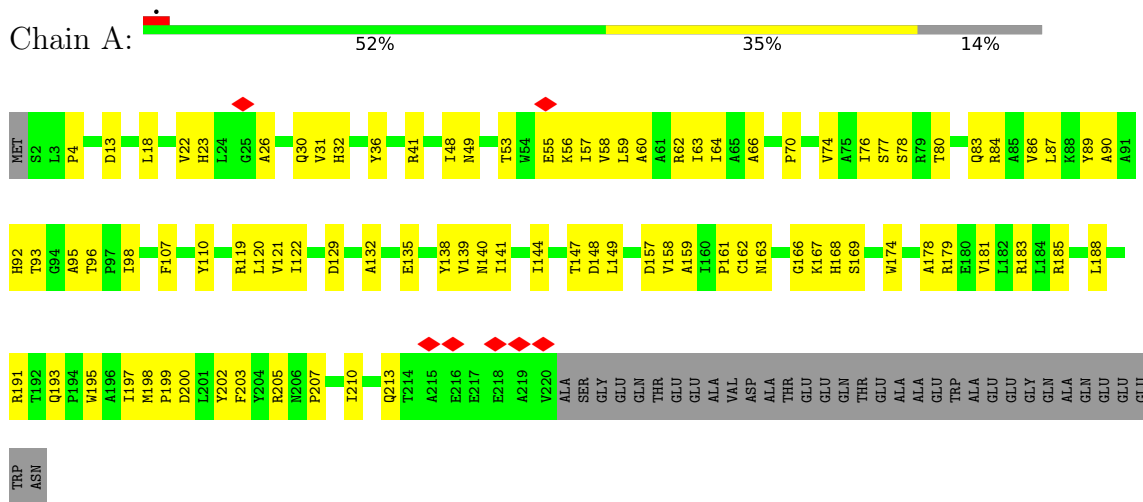
• Molecule 1: 18S ribosomal RNA



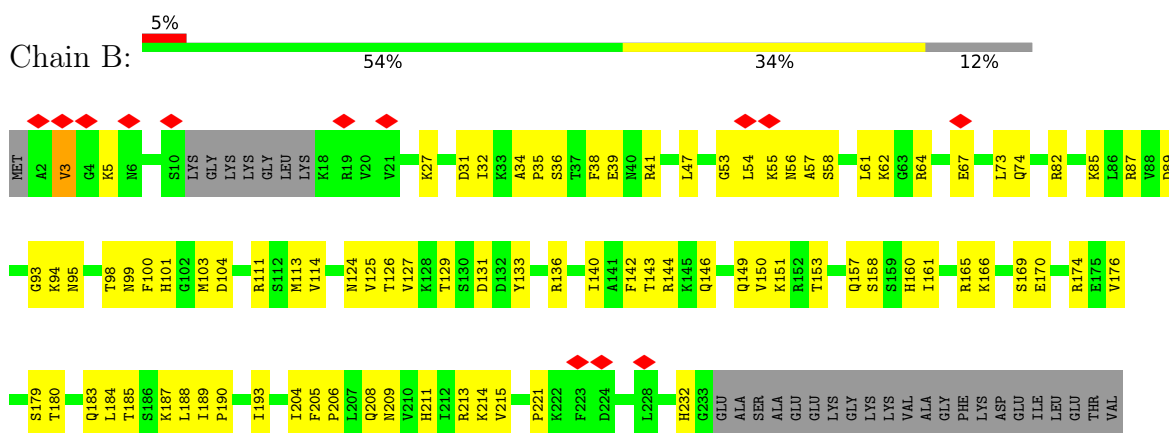
G1539	G1540	A1541	G1542	A1543	G1544	A1545	G1546	C1547	A1548	G1549	A1550	G1551	A1552	G1553	A1554	G1555	A1556	G1557	A1558	C1559	G1560	A1561	G1562	A1563	G1564	A1565	G1566	A1567	G1568	A1569	G1570	A1571	G1572	G1573	A1574	A1575	G1576	A1577	G1578	C1579	G1580	A1581	G1582	A1583	A1584	A1585	G1586	A1587	G1588	A1589	A1590	A1591	G1592	G1593	A1594	A1595	G1596	C1597	A1598	G1599	C1600
G1472	A1473	G1474	G1475	A1476	G1477	A1478	G1479	C1480	A1481	G1482	A1483	G1484	A1485	G1486	A1487	A1488	A1489	A1490	A1491	C1492	G1493	A1494	G1497	G1498	A1499	G1500	G1504	G1505	G1506	C1507	G1510	G1511	G1512	A1513	A1514	A1515	G1516	G1517	G1518	G1521	A1522	A1523	C1527	G1528	G1529	G1530	G1531	G1532	A1533	G1534	C1535	G1536	A1537	G1538	A1539	G1540					
C1391	G1392	G1396	C1397	A1398	G1399	C1331	A1332	A1333	A1334	A1335	A1336	C1337	A1338	A1339	A1340	A1343	A1344	A1345	A1346	A1347	G1350	G1351	G1352	G1353	C1354	G1355	G1356	G1357	G1358	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1373	A1374	G1375	G1376	C1377	G1378	G1379	A1380	G1381	A1382	G1383	G1384	G1385	A1386	G1387	A1388	C1322	G1323					
U1259	G1260	U1261	G1262	G1263	G1264	U1265	U1268	G1269	G1270	U1271	G1272	U1275	G1276	G1277	G1278	C1279	G1280	U1281	U1282	C1283	U1284	U1285	A1286	U1289	G1290	G1291	U1292	G1293	G1294	A1295	G1296	U1297	G1298	A1299	U1302	G1303	U1304	U1305	U1306	G1307	C1308	U1309	A1312	U1313	U1314	G1315	C1316	G1317	A1318	U1319	A1320	A1321	U1256	G1258							
C1196	G1197	G1198	G1199	G1200	A1201	U1205	C1206	A1207	C1208	C1209	A1210	G1211	G1212	U1213	C1214	A1215	A1216	G1217	A1218	C1219	A1220	C1221	A1222	A1223	U1224	A1225	G1226	A1227	A1228	A1229	U1230	A1233	C1234	A1235	G1236	A1237	U1238	U1239	G1240	A1241	G1242	A1243	G1244	C1245	U1246	C1247	U1248	U1249	G1251	U1252	U1253	G1254	A1255	U1256	G1258						
G1052	U1053	U1054	U1055	U1056	U1057	C1058	U1059	U1062	G1063	A1064	C1065	C1066	C1067	A1068	C1069	U1070	C1071	A1075	C1076	G1077	U1078	C1081	G1082	G1083	G1084	A1085	A1086	A1087	A1091	U1094	C1095	U1096	U1097	U1098	G1099	G1100	G1101	U1102	U1103	C1104	U1105	A1182	A1183	U1184	U1185	U1186	A1187	A1188	C1189	B801190	A1193	C1194	A1195								
G989	G990	A991	A992	A993	A994	U995	G996	A997	U998	C999	A1000	G1001	A1002	U1003	A1004	C1005	C1006	G1007	U1008	C1009	U1010	U1011	C948	C949	A950	A951	G952	G953	U954	G955	U956	U957	U958	U959	U960	C961	A962	A965	A966	U967	C968	A969	A970	G971	A972	G975	A976	A977	A978	C979	U981	A982	G983	U984	G985	G986	A987	U988	U989	A992	A993
U859	U860	A861	A862	A863	A864	G865	G866	A867	A868	G870	G871	U872	C873	G874	G875	G876	G877	G878	C879	A880	A883	G884	U885	A886	U887	U888	C889	A890	A891	U892	U893	G894	C895	U896	U897	U898	U899	U900	U901	U902	G903	A904	A905	U911	G912	G913	A914	U915	U916	U917	A918	U919	U920	A921	A922	A923					
G824	A825	C926	U927	A928	A929	C930	U931	A932	C933	C934	G935	A938	A939	A940	G941	U944	U945	U946	G947	C948	C949	A950	A951	G952	G953	U954	G955	U956	U957	U958	U959	U960	C961	A962	A965	A966	U967	C968	A969	A970	G971	A972	G975	A976	A977	A978	C979	U981	A982	G983	U984	G985	G986	A987	U988	U989	A992	A993			
U796	C797	A798	G801	C735	A802	A803	U804	A805	U806	U807	G808	G809	A810	A811	A812	A813	G814	G815	A816	U817	U818	A819	U820	U821	U822	U823	U824	U825	C826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U840	U842	U843	G844	G845	A846	C847	C848	U849	G852	U853	A854	U855	U856	U857	A858					
U732	A733	A734	C735	A736	A737	C738	G739	A740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	A752	A753	A754	A755	A756	A757	A760	A761	A762	G765	U766	U767	C768	A769	A770	A771	C772	C773	A774	G775	G776	C777	C778	A779	A780	A781	G782	C783	U784	U785	U786	U787	U788	A789	U790	U791	A792	U793				
C671	G672	C673	A674	C675	U676	G677	G678	U679	U680	U681	A684	A685	C686	C687	G688	G689	A690	U691	C692	U693	U694	U695	U696	U697	U698	U699	C700	U701	G702	G703	C704	U705	A706	A707	C708	C709	U710	G711	U712	U713	C714	U715	C716	C717	U718	U719	G720	U721	G722	G723	G724	U725	G726	C727	A728	G729	C730				



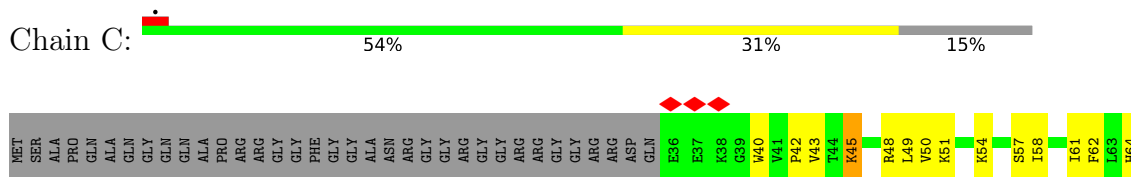
• Molecule 2: Small ribosomal subunit protein uS2

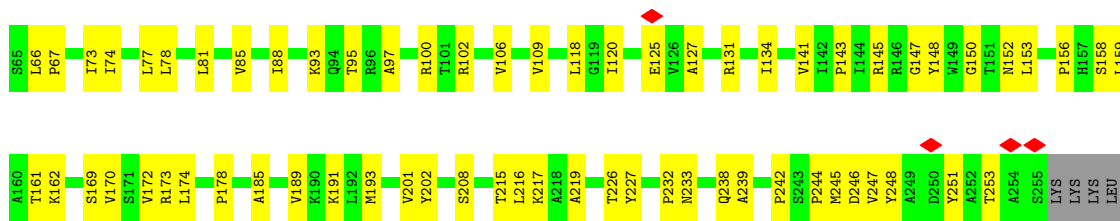


• Molecule 3: Small ribosomal subunit protein eS1

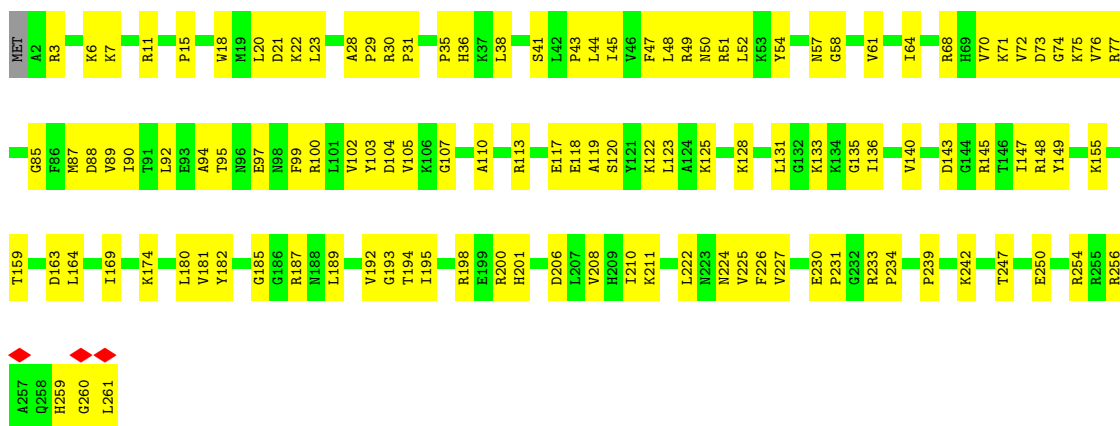


• Molecule 4: Small ribosomal subunit protein uS5

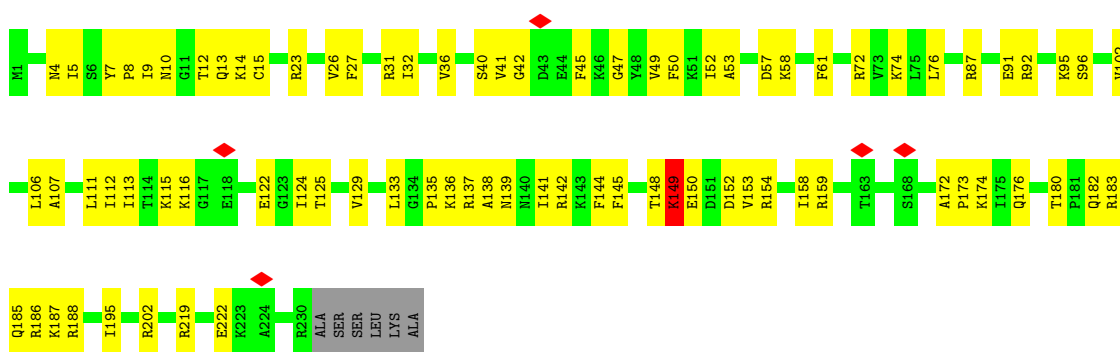




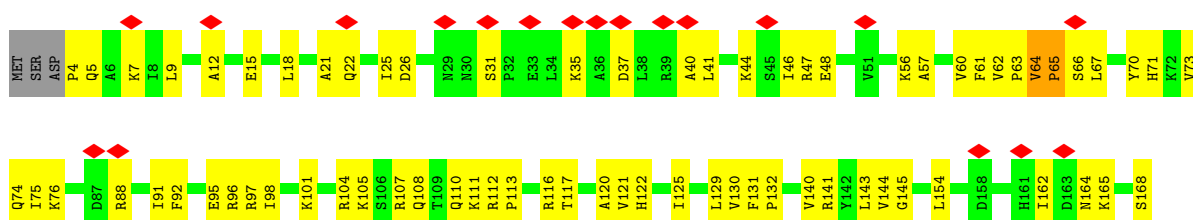
• Molecule 5: 40S ribosomal protein S4

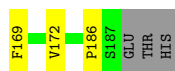


• Molecule 6: Small ribosomal subunit protein eS6

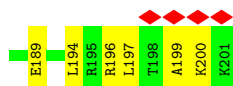
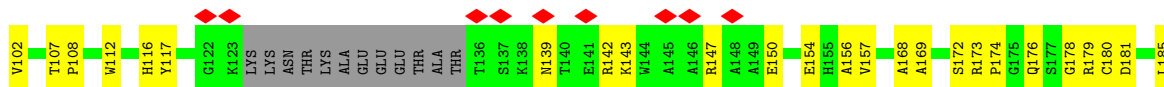
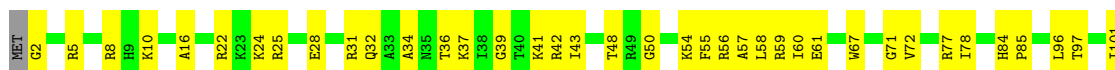


• Molecule 7: 40S ribosomal protein S7

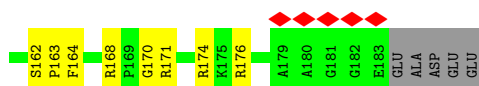
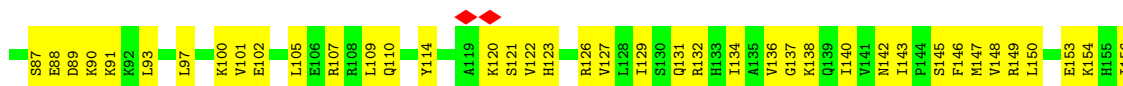




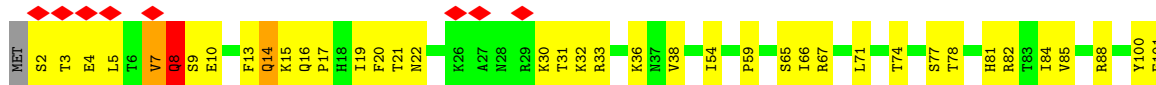
• Molecule 8: 40S ribosomal protein S8



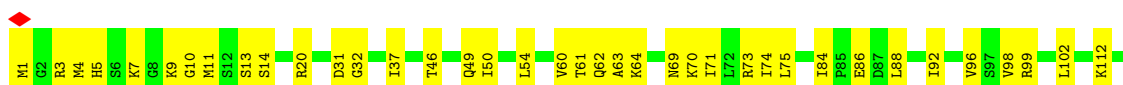
• Molecule 9: KLLA0E23673p



• Molecule 10: KLLA0A10483p

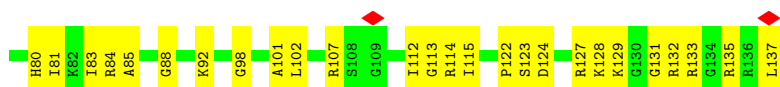


• Molecule 11: KLLA0F18040p

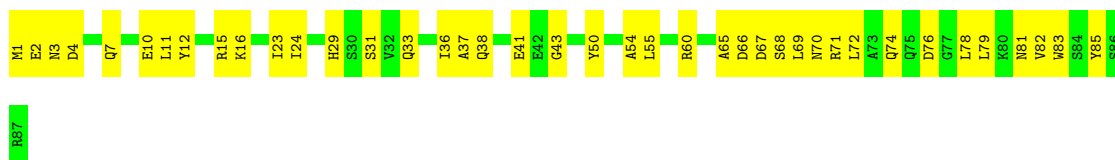




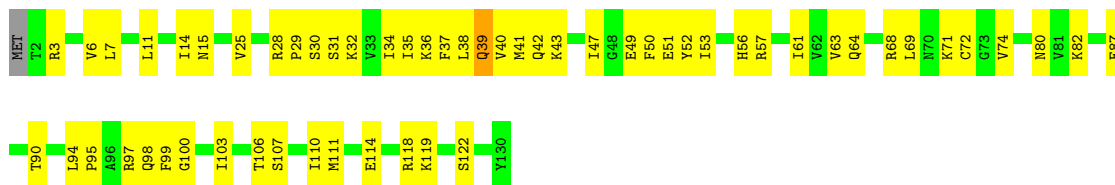
- Molecule 12: Small ribosomal subunit protein uS11



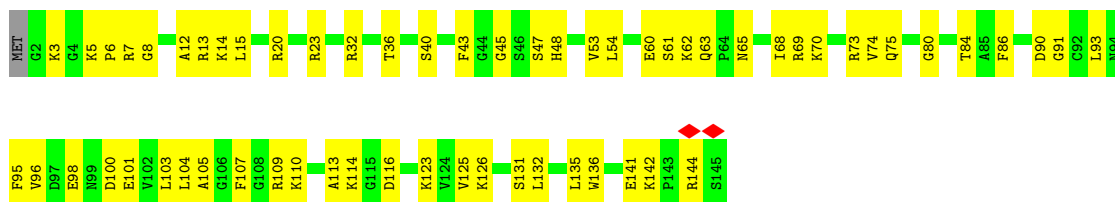
- Molecule 13: 40S ribosomal protein S21



- Molecule 14: Small ribosomal subunit protein uS8

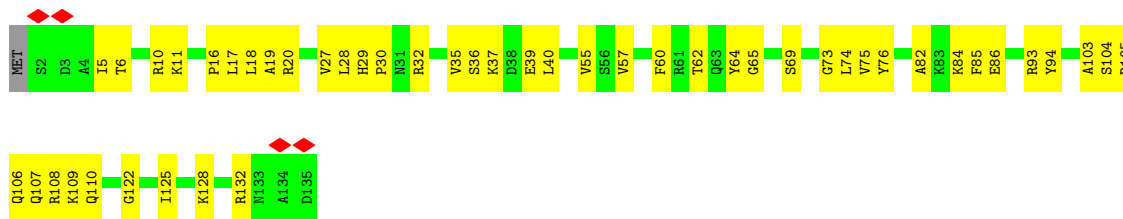


- Molecule 15: KLLA0B11231p

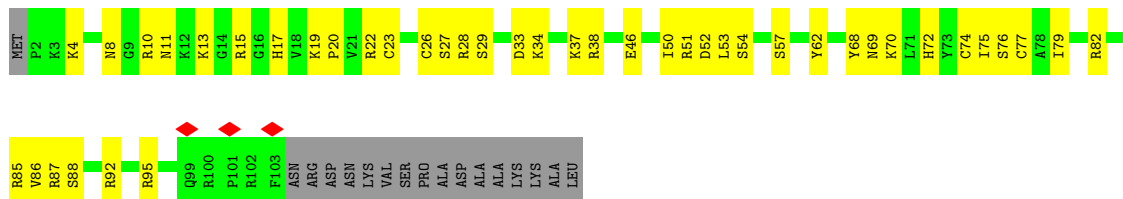


- Molecule 16: 40S ribosomal protein S24





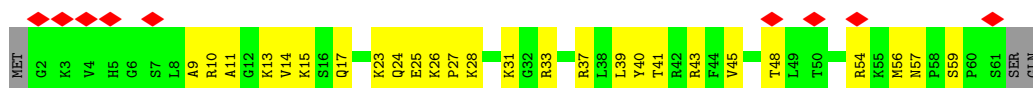
- Molecule 17: 40S ribosomal protein S26



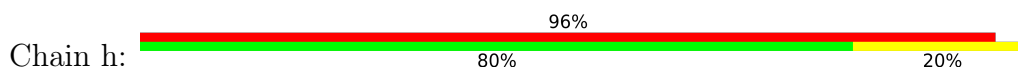
- Molecule 18: 40S ribosomal protein S27



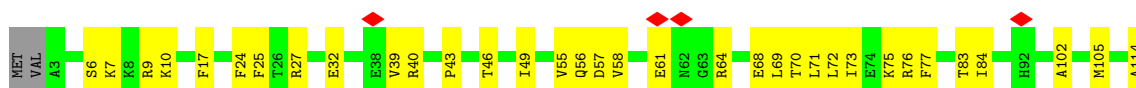
- Molecule 19: 40S ribosomal protein S30

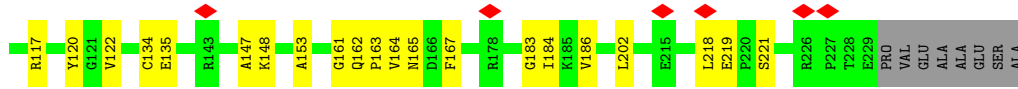


- Molecule 20: 40S ribosomal protein L41-A

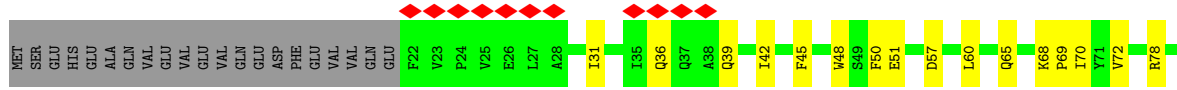


- Molecule 21: 40S ribosomal protein S3

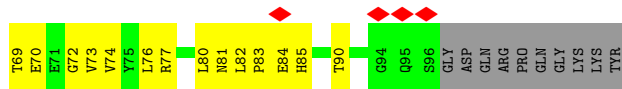
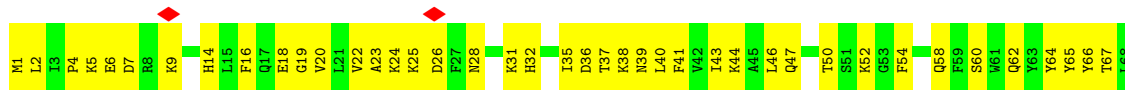




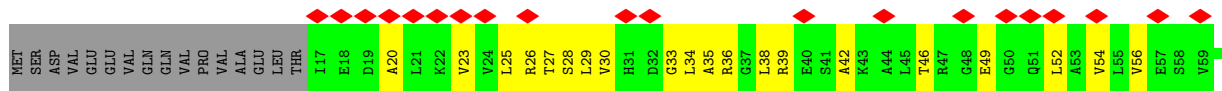
• Molecule 22: KLLA0D10659p



• Molecule 23: KLLA0B08173p

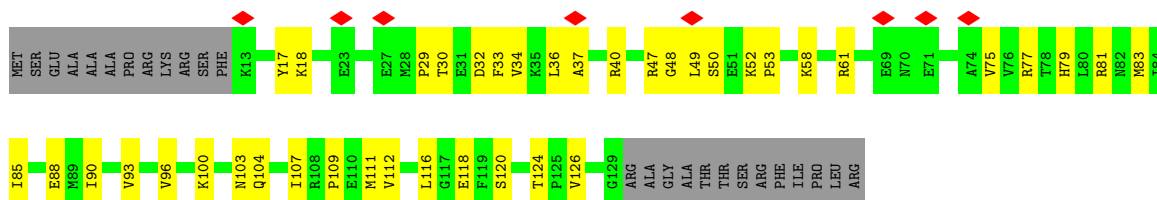


• Molecule 24: 40S ribosomal protein S12

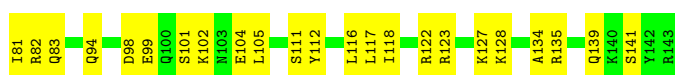
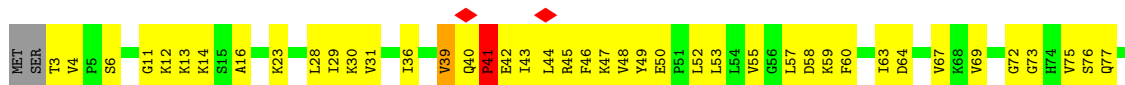


• Molecule 25: KLLA0F07843p

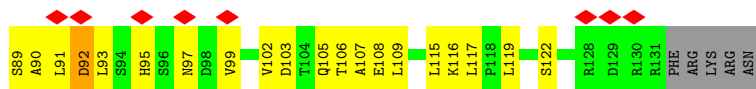
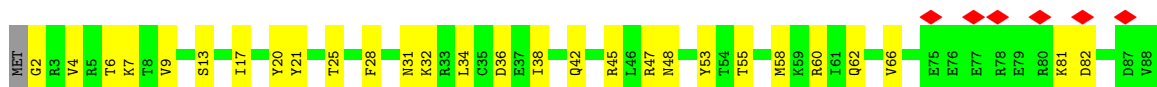




• Molecule 26: Small ribosomal subunit protein uS9



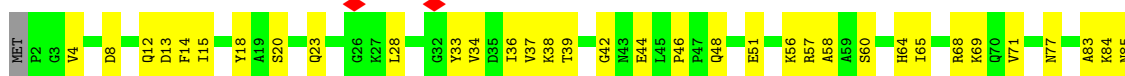
• Molecule 27: KLLA0B01474p



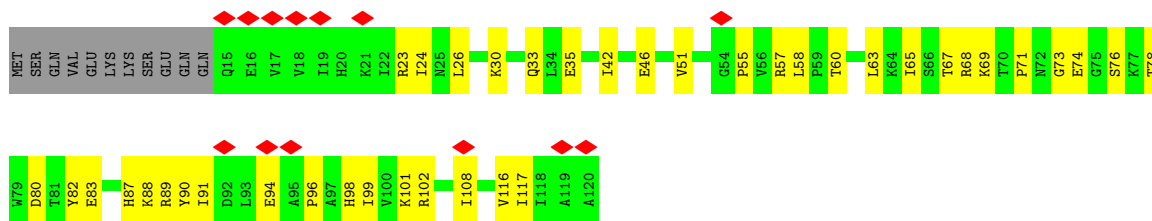
• Molecule 28: KLLA0B01562p



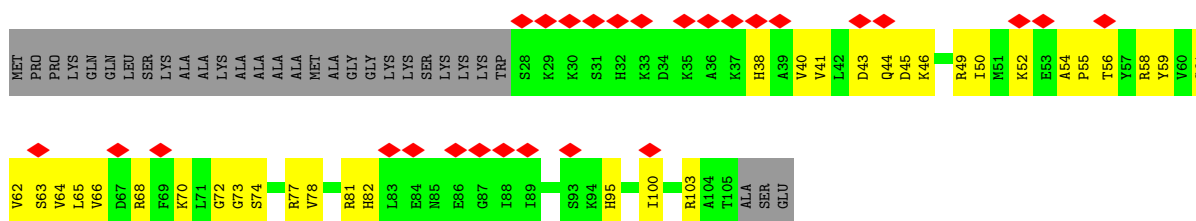
• Molecule 29: KLLA0A07194p



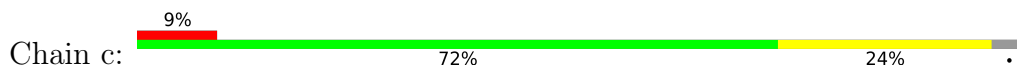
• Molecule 30: Small ribosomal subunit protein uS10



• Molecule 31: 40S ribosomal protein S25



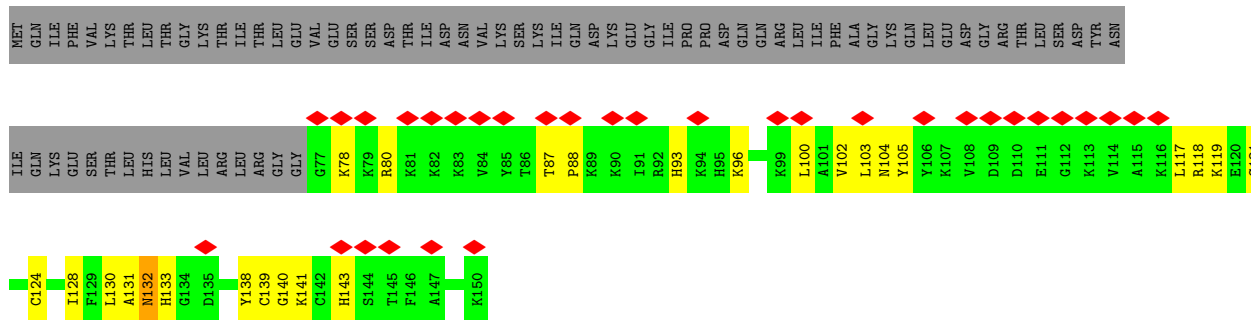
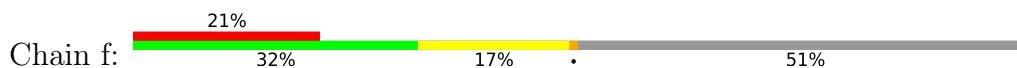
• Molecule 32: Small ribosomal subunit protein eS28



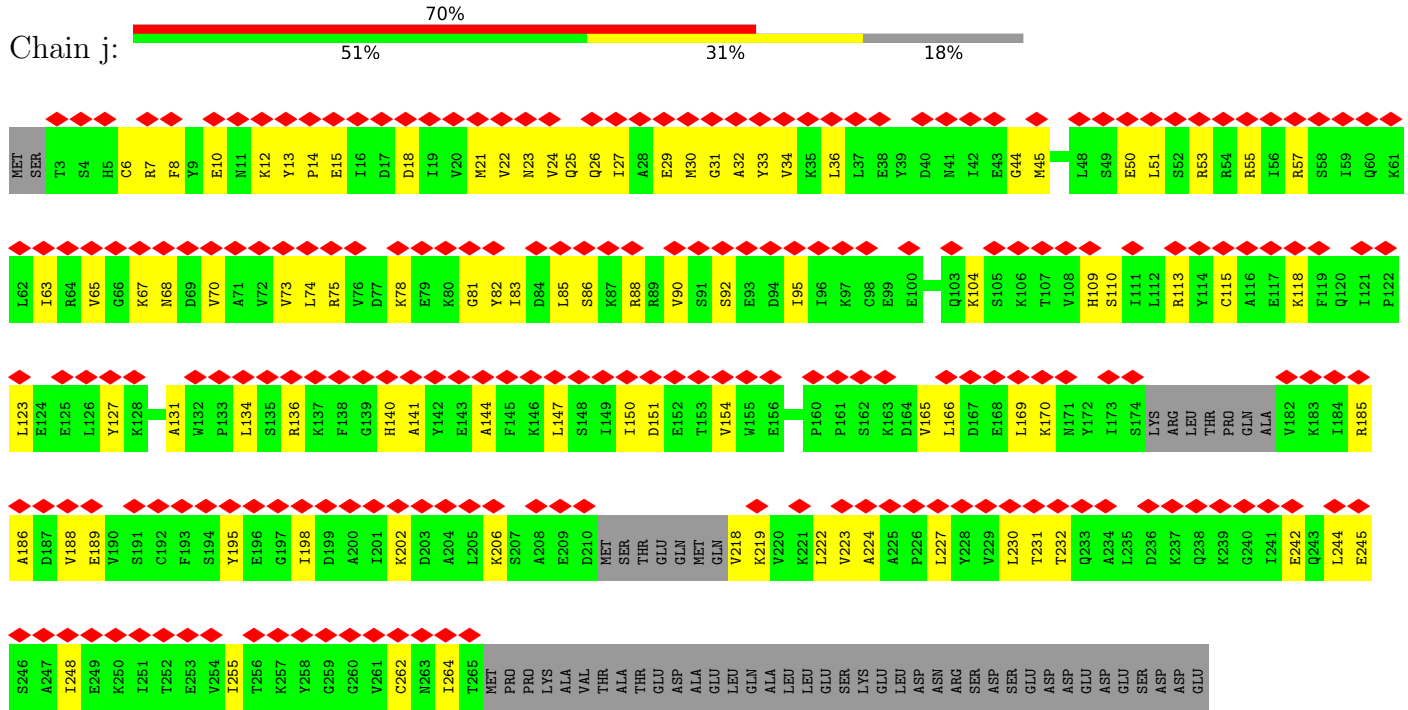
• Molecule 33: Small ribosomal subunit protein uS14



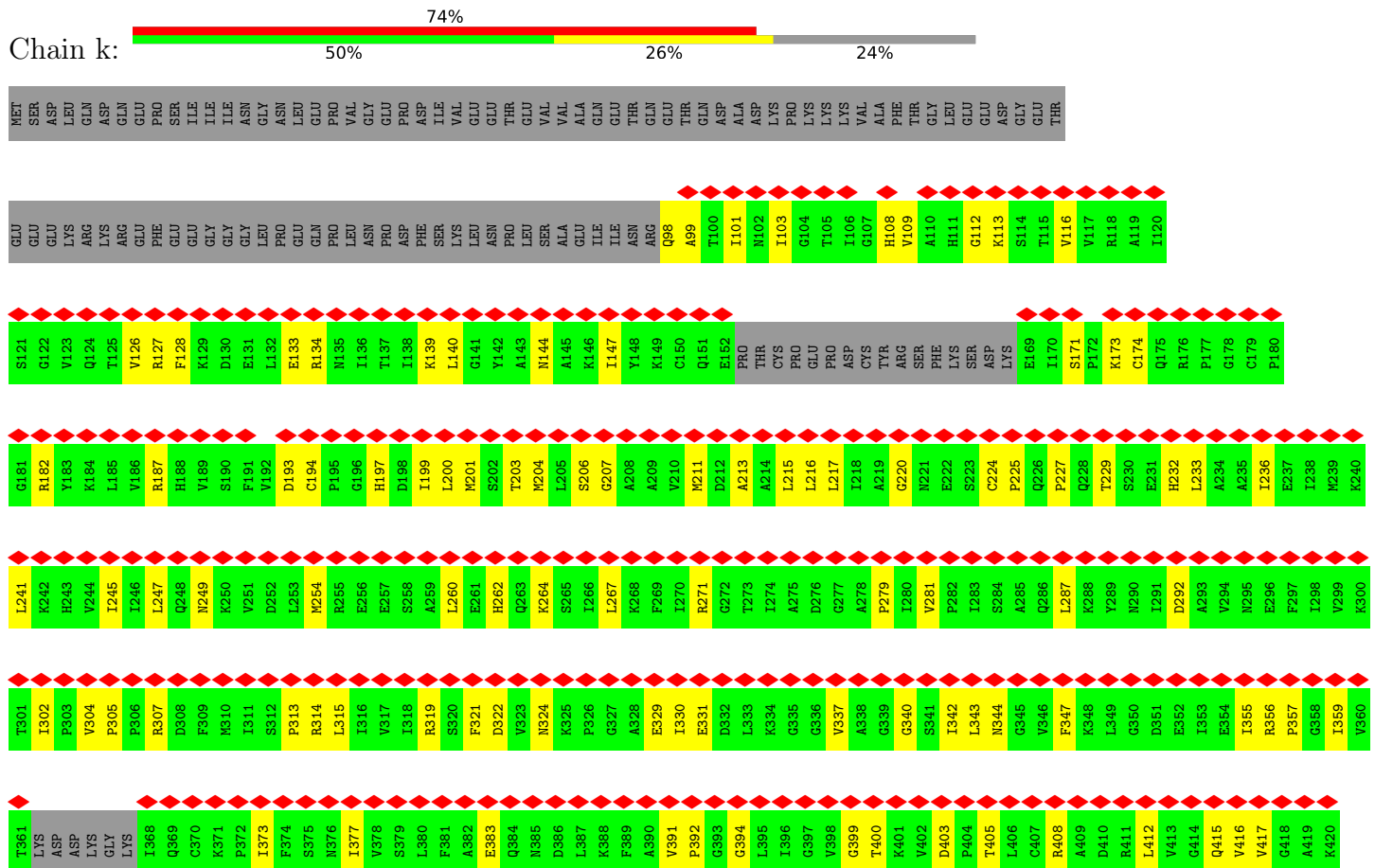
• Molecule 34: Small ribosomal subunit protein eS31



● Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha



● Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39886	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	0.467	Depositor
Minimum map value	-0.252	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	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: 1MA, T6A, M2G, PSU, RIA, MG, 7MG, H2U, 5MC, ZN, 1MG, GCP, MA6, B8N, 2MG

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	0.14	0/42201	0.32	0/65752
2	A	0.17	0/1742	0.41	0/2383
3	B	0.23	0/1820	0.53	1/2448 (0.0%)
4	C	0.17	0/1678	0.42	0/2277
5	E	0.17	0/2122	0.44	0/2861
6	G	0.16	0/1855	0.41	0/2479
7	H	0.22	0/1507	0.50	0/2028
8	I	0.16	0/1515	0.42	0/2029
9	J	0.24	0/1487	0.64	4/1990 (0.2%)
10	L	0.23	0/1276	0.43	0/1718
11	N	0.17	0/1218	0.42	0/1638
12	O	0.17	0/966	0.47	0/1297
13	V	0.16	0/696	0.40	0/938
14	W	0.21	0/1039	0.47	0/1399
15	X	0.19	0/1137	0.48	0/1516
16	Y	0.17	0/1075	0.44	0/1433
17	a	0.17	0/810	0.47	0/1087
18	b	0.18	0/619	0.46	0/837
19	e	0.19	0/480	0.61	0/640
20	h	0.11	0/234	0.29	0/300
21	D	0.14	0/1800	0.38	0/2421
22	F	0.24	0/1628	0.68	2/2198 (0.1%)
23	K	0.22	0/831	0.62	0/1123
24	M	0.23	0/891	0.52	0/1201
25	P	0.17	0/942	0.51	2/1269 (0.2%)
26	Q	0.26	0/1125	0.59	0/1510
27	R	0.26	0/1044	0.56	0/1402
28	S	0.18	0/1208	0.49	0/1624
29	T	0.17	0/1129	0.40	0/1520
30	U	0.14	0/857	0.38	0/1158
31	Z	0.14	0/603	0.38	0/814
32	c	0.13	0/501	0.39	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.17	0/473	0.49	0/629
34	f	0.16	0/597	0.50	0/795
35	g	0.19	0/2523	0.45	0/3434
36	i	0.15	0/773	0.49	0/1031
37	3	0.08	0/595	0.19	0/920
38	1	0.30	1/1529 (0.1%)	0.57	4/2376 (0.2%)
39	j	0.14	0/2034	0.41	0/2737
40	k	0.13	0/3079	0.41	0/4157
41	l	0.12	0/194	0.33	0/263
42	m	0.13	0/626	0.37	0/835
All	All	0.17	1/90459 (0.0%)	0.40	13/131140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	26	M2G	O3'-P	7.62	1.72	1.61

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	104	ARG	N-CA-C	-19.00	90.65	111.36
9	J	19	TYR	N-CA-C	10.88	125.12	112.72
22	F	102	ASN	N-CA-C	-10.83	95.90	111.17
38	1	26	M2G	P-O3'-C3'	9.74	134.81	120.20
3	B	190	PRO	CA-N-CD	-9.18	99.15	112.00

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	38003	0	19120	1124	0
2	A	1702	0	1695	86	0
3	B	1796	0	1874	70	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1648	0	1727	74	0
5	E	2078	0	2157	108	0
6	G	1832	0	1919	73	0
7	H	1483	0	1579	76	0
8	I	1489	0	1504	53	0
9	J	1464	0	1547	74	0
10	L	1248	0	1311	43	0
11	N	1195	0	1263	43	0
12	O	955	0	987	61	0
13	V	687	0	682	36	0
14	W	1021	0	1056	67	0
15	X	1119	0	1198	60	0
16	Y	1061	0	1111	51	0
17	a	797	0	835	44	0
18	b	609	0	628	19	0
19	e	472	0	508	27	0
20	h	233	0	284	6	0
21	D	1774	0	1855	42	0
22	F	1609	0	1679	102	0
23	K	809	0	810	55	0
24	M	885	0	917	38	0
25	P	923	0	960	38	0
26	Q	1105	0	1170	68	0
27	R	1033	0	1082	46	0
28	S	1189	0	1211	68	0
29	T	1110	0	1124	55	0
30	U	845	0	913	35	0
31	Z	594	0	590	29	0
32	c	499	0	536	14	0
33	d	461	0	448	34	0
34	f	584	0	600	29	0
35	g	2469	0	2403	101	0
36	i	764	0	763	29	0
37	3	536	0	277	5	0
38	1	1639	0	852	94	0
39	j	2006	0	2066	68	0
40	k	3034	0	3195	98	0
41	l	190	0	191	1	0
42	m	619	0	646	24	0
43	2	111	0	0	0	0
43	S	1	0	0	0	0
43	T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	i	1	0	0	0	0
43	k	1	0	0	0	0
44	a	1	0	0	0	0
44	b	1	0	0	0	0
44	f	1	0	0	0	0
44	k	1	0	0	0	0
45	k	32	0	13	2	0
46	k	8	0	8	1	0
47	2	3	0	0	0	0
All	All	85732	0	67294	2764	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 18.

The worst 5 of 2764 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)
38:1:48:5MC:HM52	38:1:59:A:N1	1.41	1.32
38:1:48:5MC:CM5	38:1:59:A:N1	2.16	1.08
38:1:14:A:C2	38:1:48:5MC:N4	2.24	1.04
17:a:26:CYS:HB3	17:a:77:CYS:SG	2.01	1.01
3:B:144:ARG:HB2	3:B:208:GLN:HB2	1.45	0.98

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%)	195 (90%)	22 (10%)	0	100 100
3	B	221/255 (87%)	197 (89%)	22 (10%)	2 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	218/259 (84%)	201 (92%)	16 (7%)	1 (0%)	24	60
5	E	258/261 (99%)	232 (90%)	26 (10%)	0	100	100
6	G	228/236 (97%)	217 (95%)	10 (4%)	1 (0%)	30	65
7	H	182/190 (96%)	160 (88%)	21 (12%)	1 (0%)	24	60
8	I	184/201 (92%)	162 (88%)	22 (12%)	0	100	100
9	J	180/188 (96%)	156 (87%)	22 (12%)	2 (1%)	11	44
10	L	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	53
11	N	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
12	O	127/137 (93%)	114 (90%)	13 (10%)	0	100	100
13	V	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
14	W	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
15	X	142/145 (98%)	125 (88%)	17 (12%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	82 (82%)	18 (18%)	0	100	100
18	b	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
19	e	58/63 (92%)	48 (83%)	10 (17%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	215 (96%)	10 (4%)	0	100	100
22	F	204/227 (90%)	181 (89%)	21 (10%)	2 (1%)	12	45
23	K	94/106 (89%)	77 (82%)	17 (18%)	0	100	100
24	M	113/134 (84%)	94 (83%)	19 (17%)	0	100	100
25	P	115/142 (81%)	95 (83%)	20 (17%)	0	100	100
26	Q	139/143 (97%)	125 (90%)	13 (9%)	1 (1%)	18	53
27	R	128/136 (94%)	104 (81%)	21 (16%)	3 (2%)	5	31
28	S	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
29	T	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
30	U	104/117 (89%)	96 (92%)	8 (8%)	0	100	100
31	Z	76/108 (70%)	70 (92%)	6 (8%)	0	100	100
32	c	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
33	d	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
34	f	72/150 (48%)	58 (81%)	14 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	g	314/326 (96%)	289 (92%)	24 (8%)	1 (0%)	36	69
36	i	93/153 (61%)	81 (87%)	12 (13%)	0	100	100
39	j	243/304 (80%)	221 (91%)	22 (9%)	0	100	100
40	k	388/519 (75%)	352 (91%)	36 (9%)	0	100	100
41	l	21/285 (7%)	21 (100%)	0	0	100	100
42	m	73/108 (68%)	68 (93%)	5 (7%)	0	100	100
All	All	5664/6682 (85%)	5090 (90%)	559 (10%)	15 (0%)	37	69

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	65	PRO
9	J	101	VAL
10	L	8	GLN
3	B	221	PRO
6	G	149	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	200 (99%)	2 (1%)	68	76
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%)	191 (100%)	1 (0%)	81	82
7	H	164/170 (96%)	163 (99%)	1 (1%)	78	81
8	I	147/159 (92%)	147 (100%)	0	100	100
9	J	152/158 (96%)	150 (99%)	2 (1%)	61	72
10	L	136/137 (99%)	132 (97%)	4 (3%)	37	58
11	N	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	108 (98%)	2 (2%)	51	67
15	X	119/120 (99%)	119 (100%)	0	100	100
16	Y	108/109 (99%)	108 (100%)	0	100	100
17	a	83/100 (83%)	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%)	188 (100%)	0	100	100
22	F	174/194 (90%)	173 (99%)	1 (1%)	78	81
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	91 (98%)	2 (2%)	45	64
25	P	99/119 (83%)	99 (100%)	0	100	100
26	Q	117/119 (98%)	115 (98%)	2 (2%)	53	68
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%)	55 (100%)	0	100	100
33	d	47/48 (98%)	47 (100%)	0	100	100
34	f	60/133 (45%)	59 (98%)	1 (2%)	53	68
35	g	264/272 (97%)	263 (100%)	1 (0%)	84	84
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	224/274 (82%)	224 (100%)	0	100	100
40	k	332/443 (75%)	332 (100%)	0	100	100
41	l	22/246 (9%)	22 (100%)	0	100	100
42	m	69/96 (72%)	69 (100%)	0	100	100
All	All	4863/5685 (86%)	4844 (100%)	19 (0%)	81	84

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	M	121	THR
34	f	132	ASN
35	g	122	LYS
26	Q	41	PRO
10	L	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
39	j	23	ASN
39	j	103	GLN
42	m	79	GLN
13	V	29	HIS
13	V	21	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1787/1798 (99%)	570 (31%)	26 (1%)
37	3	25/49 (51%)	13 (52%)	0
38	1	72/75 (96%)	31 (43%)	7 (9%)
All	All	1884/1922 (98%)	614 (32%)	33 (1%)

5 of 614 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	23	G
1	2	26	A
1	2	27	U

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	1	43	G
38	1	44	A
38	1	74	C
1	2	828	A
1	2	781	A

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	2MG	2	1570	1	23,26,27	2.91	8 (34%)	33,38,41	2.19	11 (33%)
1	MA6	2	1780	1	23,26,27	1.39	4 (17%)	33,38,41	3.28	12 (36%)
38	2MG	1	10	38	23,26,27	2.94	8 (34%)	33,38,41	2.17	11 (33%)
38	7MG	1	46	38	23,26,27	3.64	11 (47%)	27,39,42	2.18	9 (33%)
38	H2U	1	16	38	18,21,22	3.15	4 (22%)	19,30,33	1.49	4 (21%)
1	PSU	2	1289	1	18,21,22	4.46	7 (38%)	21,30,33	1.81	5 (23%)
1	5MC	2	1006	1	19,22,23	3.78	8 (42%)	26,32,35	1.15	2 (7%)
38	M2G	1	26	38	24,27,28	2.68	8 (33%)	33,40,43	1.70	7 (21%)
38	1MA	1	58	38	21,25,26	3.14	6 (28%)	30,37,40	2.30	8 (26%)
38	5MC	1	49	38	19,22,23	3.95	8 (42%)	26,32,35	1.00	1 (3%)
1	2MG	2	1426	1,43	23,26,27	2.90	8 (34%)	33,38,41	2.18	9 (27%)
38	RIA	1	64	38	35,38,39	4.61	14 (40%)	50,57,60	2.00	13 (26%)
1	B8N	2	1190	1	25,29,30	3.38	7 (28%)	28,42,45	2.00	7 (25%)
1	PSU	2	766	1	18,21,22	4.48	8 (44%)	21,30,33	2.07	6 (28%)
1	PSU	2	998	1	18,21,22	4.38	8 (44%)	21,30,33	1.91	4 (19%)
38	T6A	1	37	38	31,34,35	1.78	7 (22%)	43,49,52	2.09	15 (34%)
38	H2U	1	47	38	18,21,22	3.15	4 (22%)	19,30,33	1.45	4 (21%)
1	7MG	2	1573	1	23,26,27	3.59	10 (43%)	27,39,42	2.29	9 (33%)
1	5MC	2	1637	1	19,22,23	3.86	8 (42%)	26,32,35	1.11	2 (7%)
38	1MG	1	9	38	23,26,27	3.32	7 (30%)	33,39,42	2.33	8 (24%)
1	PSU	2	465	1	18,21,22	4.41	7 (38%)	21,30,33	1.91	5 (23%)
38	5MC	1	48	38	19,22,23	3.99	9 (47%)	26,32,35	1.71	5 (19%)
1	PSU	2	120	1	18,21,22	4.50	7 (38%)	21,30,33	1.89	6 (28%)

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	2MG	2	1570	1	-	0/9/27/28	0/3/3/3
1	MA6	2	1780	1	-	3/11/29/30	0/3/3/3
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
38	H2U	1	16	38	-	3/7/38/39	0/2/2/2
1	PSU	2	1289	1	-	3/7/25/26	0/2/2/2
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
38	M2G	1	26	38	-	3/11/29/30	0/3/3/3
38	1MA	1	58	38	-	1/7/25/26	0/3/3/3
38	5MC	1	49	38	-	3/7/25/26	0/2/2/2
1	2MG	2	1426	1,43	-	1/9/27/28	0/3/3/3
38	RIA	1	64	38	-	9/17/51/52	0/4/4/4
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2
1	PSU	2	998	1	-	3/7/25/26	0/2/2/2
38	T6A	1	37	38	-	6/23/41/42	0/3/3/3
38	H2U	1	47	38	-	3/7/38/39	0/2/2/2
1	7MG	2	1573	1	-	2/7/37/38	0/3/3/3
1	5MC	2	1637	1	-	3/7/25/26	0/2/2/2
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
1	PSU	2	120	1	-	2/7/25/26	0/2/2/2

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.12	1.32	1.52
1	2	120	PSU	C6-C5	11.94	1.48	1.35
1	2	1289	PSU	C6-C5	11.79	1.48	1.35
1	2	465	PSU	C6-C5	11.74	1.48	1.35
1	2	766	PSU	C6-C5	11.72	1.48	1.35

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-12.07	102.15	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	C5-C6-N6	7.95	137.92	125.33
38	1	9	1MG	C1'-N9-C4	-6.77	106.48	126.49
1	2	1570	2MG	C2-N3-C4	6.46	120.09	112.00
38	1	10	2MG	C2-N3-C4	6.46	120.08	112.00

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	998	PSU	C2'-C1'-C5-C4
1	2	998	PSU	C2'-C1'-C5-C6
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1573	7MG	O4'-C4'-C5'-O5'
1	2	1637	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1780	MA6	3	0
38	1	10	2MG	8	0
38	1	46	7MG	3	0
38	1	16	H2U	5	0
38	1	26	M2G	17	0
38	1	58	1MA	1	0
38	1	49	5MC	1	0
1	2	1426	2MG	2	0
38	1	64	RIA	2	0
38	1	37	T6A	2	0
38	1	47	H2U	3	0
1	2	1573	7MG	2	0
38	1	9	1MG	7	0
1	2	465	PSU	1	0
38	1	48	5MC	13	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 122 ligands modelled in this entry, 120 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
46	MET	k	604	-	6,7,8	0.50	0	2,7,9	0.18	0
45	GCP	k	601	-	32,34,34	3.21	12 (37%)	49,54,54	1.64	9 (18%)

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
46	MET	k	604	-	-	0/5/6/8	-
45	GCP	k	601	-	-	2/19/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	k	601	GCP	O4'-C1'	8.73	1.62	1.42
45	k	601	GCP	C2'-C1'	-7.17	1.31	1.53
45	k	601	GCP	PB-O3A	6.32	1.65	1.58
45	k	601	GCP	O4'-C4'	-6.25	1.31	1.45
45	k	601	GCP	PA-O3A	5.58	1.65	1.59

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	601	GCP	C5-C4-N3	-5.38	119.82	128.39
45	k	601	GCP	C2-N3-C4	4.46	119.99	112.30
45	k	601	GCP	N9-C4-N3	3.20	132.35	125.95
45	k	601	GCP	C2-N1-C6	-2.84	119.96	125.11
45	k	601	GCP	N9-C8-N7	-2.70	108.39	113.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

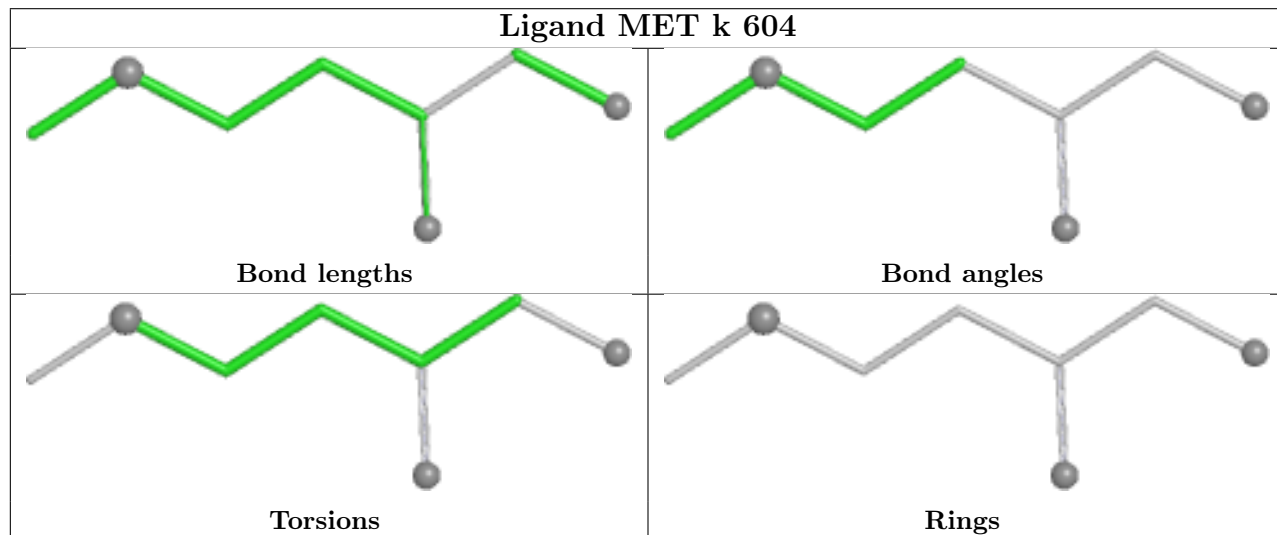
Mol	Chain	Res	Type	Atoms
45	k	601	GCP	O4'-C4'-C5'-O5'
45	k	601	GCP	C3'-C4'-C5'-O5'

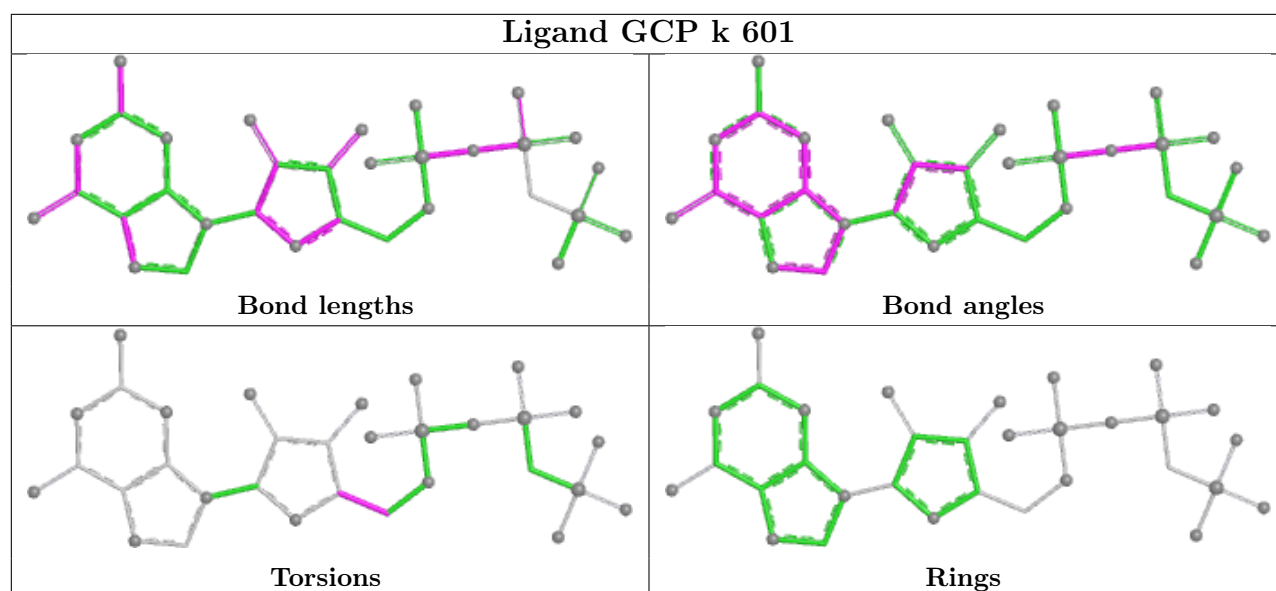
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	k	604	MET	1	0
45	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

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	7.48
1	1	63:G	O3'	64:RIA	P	5.09
1	1	16:H2U	O3'	18:G	P	3.37

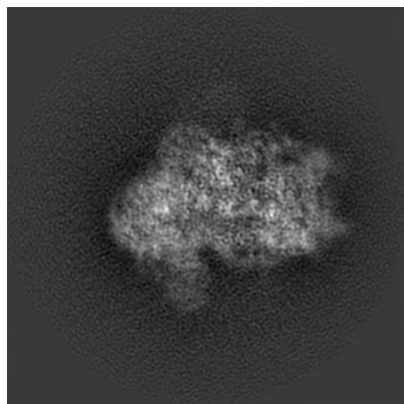
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19803. These allow visual inspection of the internal detail of the map and identification of artifacts.

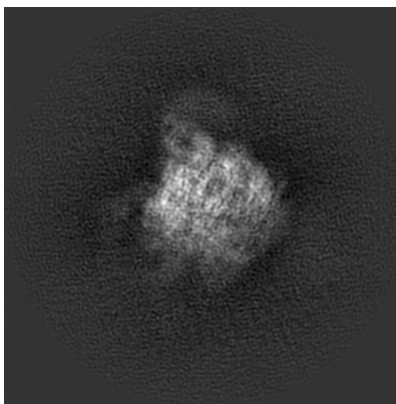
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

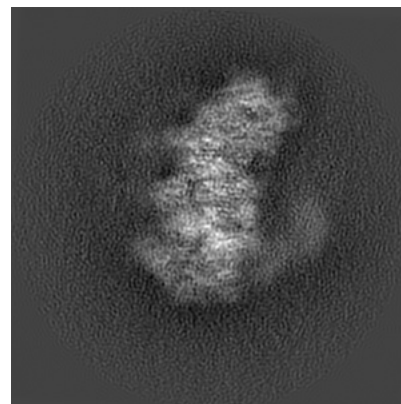
6.1.1 Primary map



X

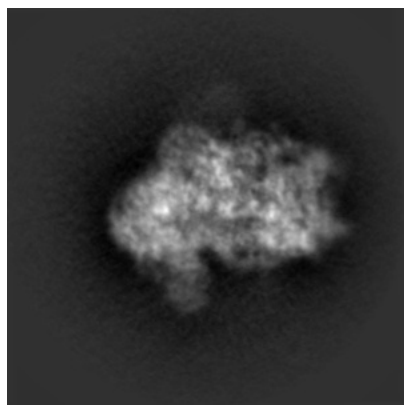


Y

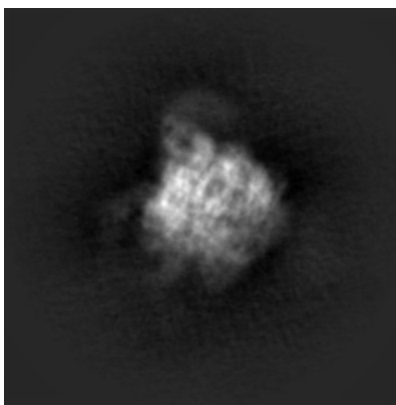


Z

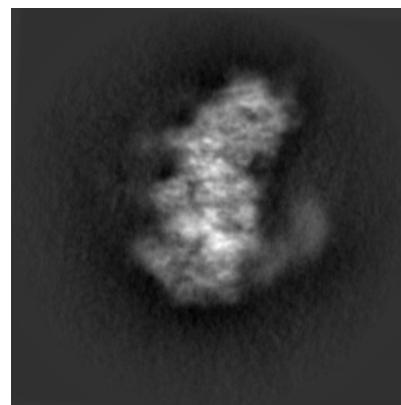
6.1.2 Raw map



X



Y

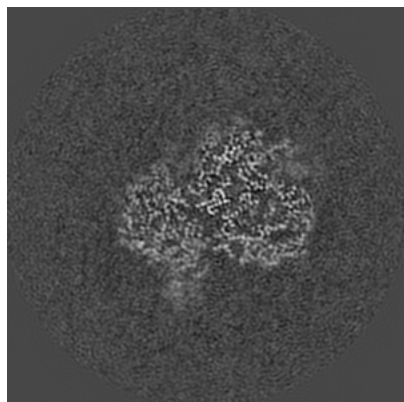


Z

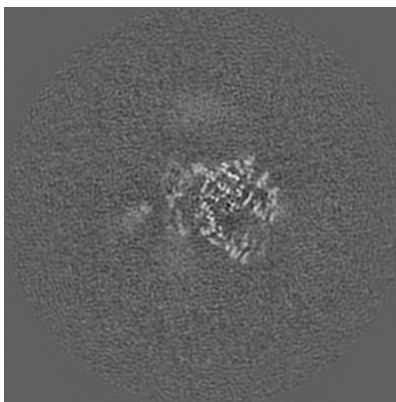
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

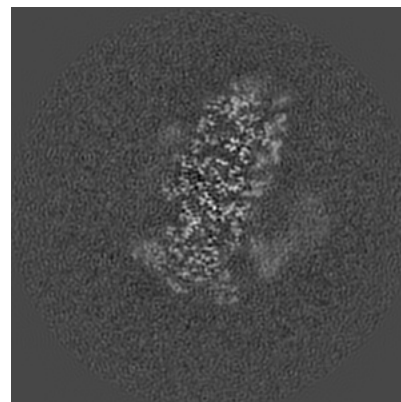
6.2.1 Primary map



X Index: 150

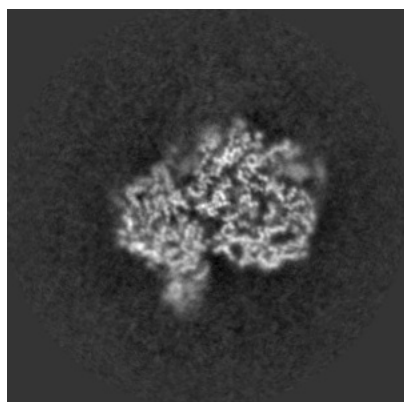


Y Index: 150

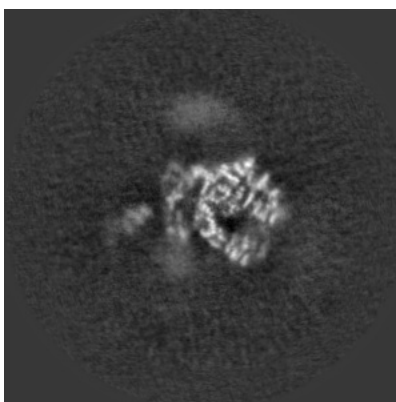


Z Index: 150

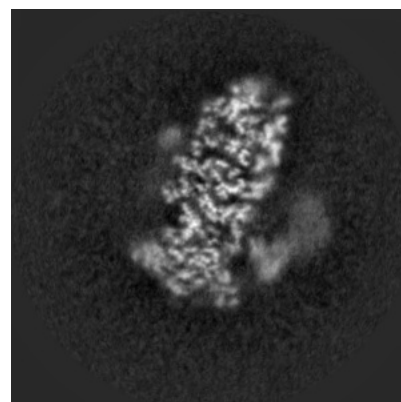
6.2.2 Raw map



X Index: 150



Y Index: 150

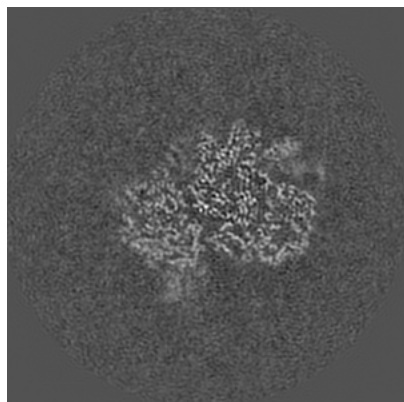


Z Index: 150

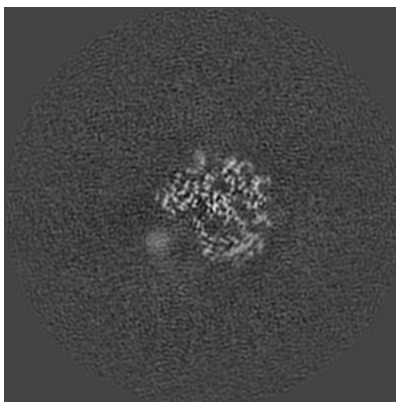
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

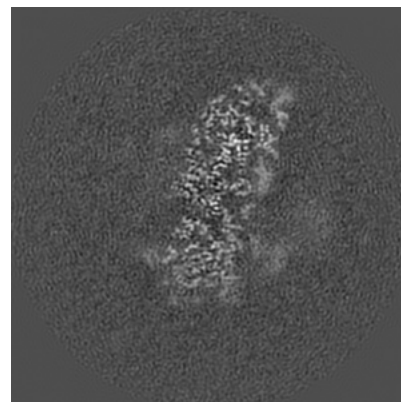
6.3.1 Primary map



X Index: 152

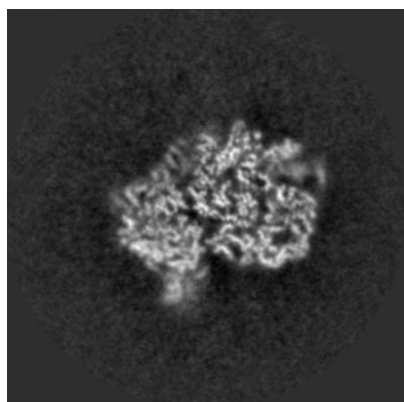


Y Index: 162

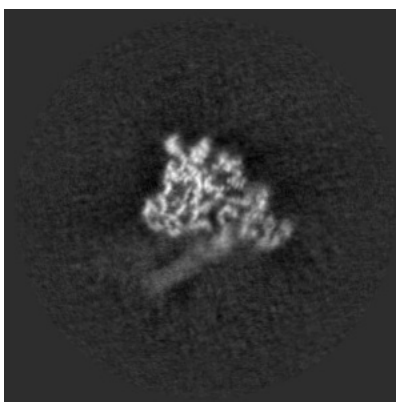


Z Index: 146

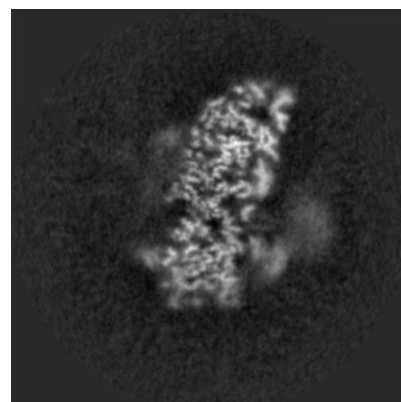
6.3.2 Raw map



X Index: 152



Y Index: 198

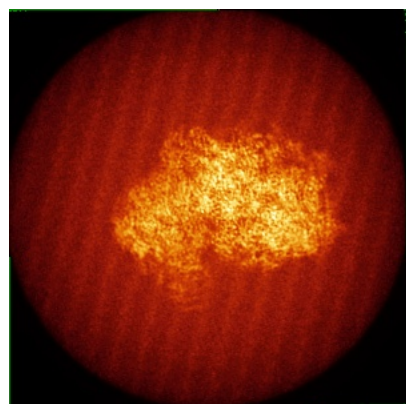


Z Index: 146

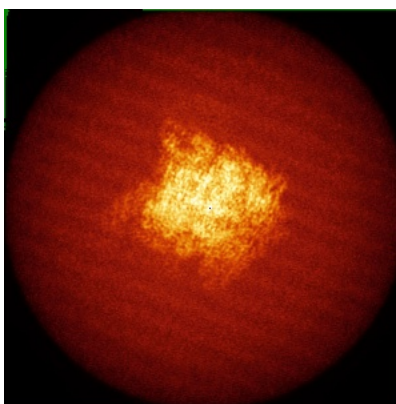
The images above show the largest variance slices of the map in three orthogonal directions.

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

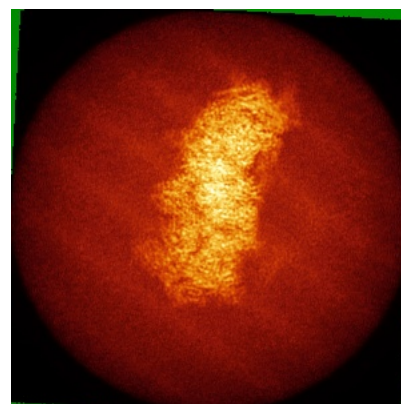
6.4.1 Primary map



X

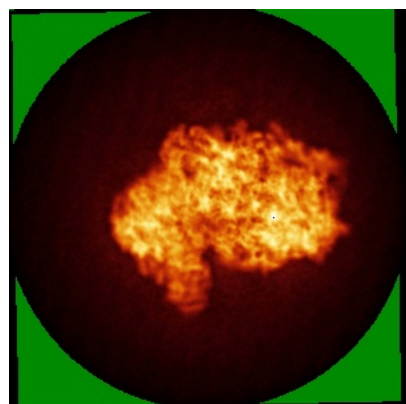


Y

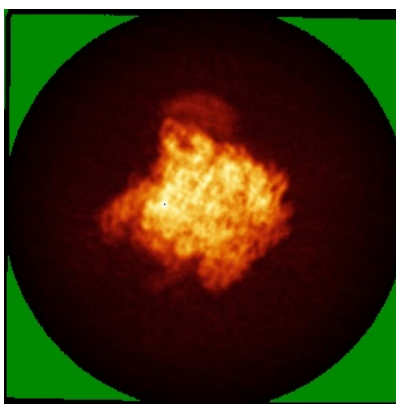


Z

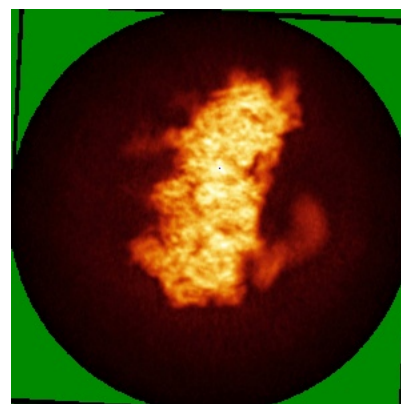
6.4.2 Raw map



X



Y

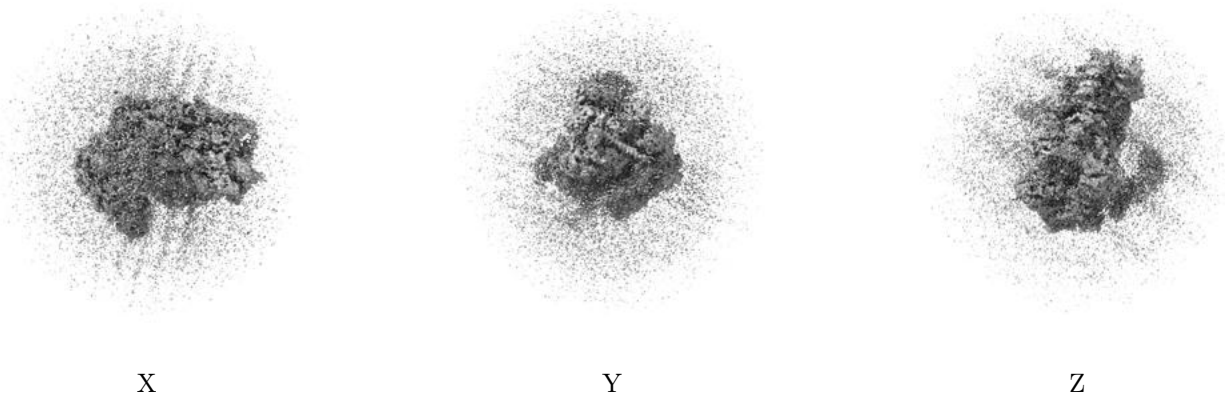


Z

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.

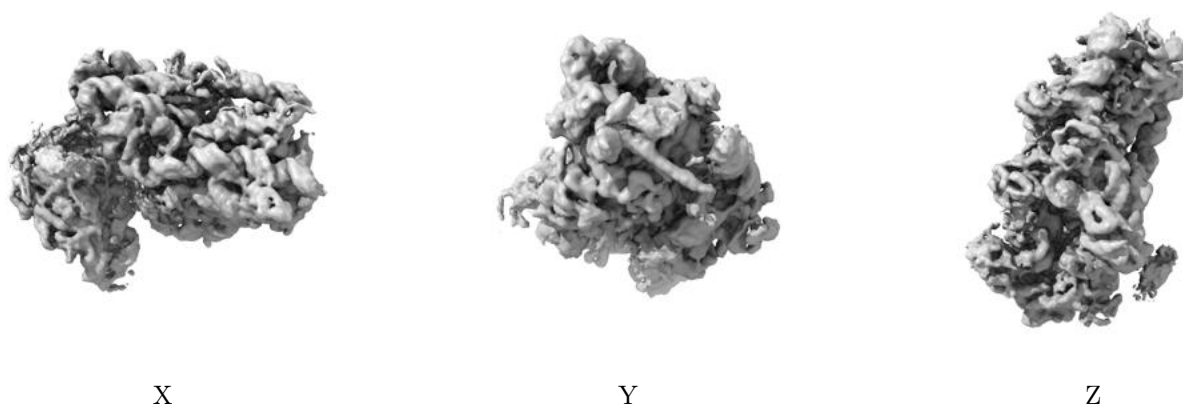
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

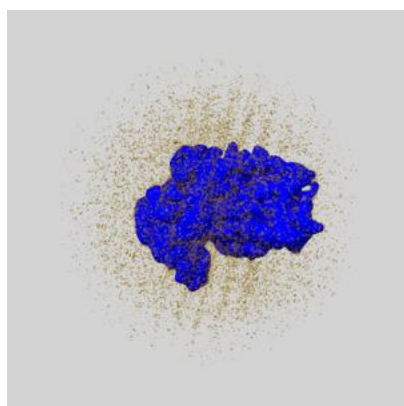
6.6 Mask visualisation [i](#)

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

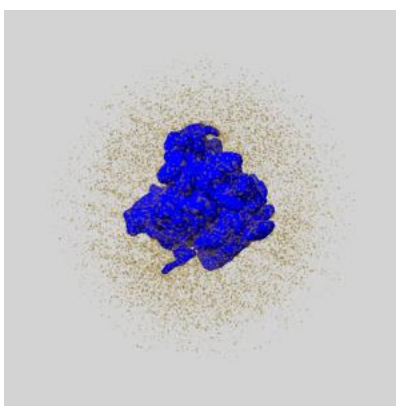
A mask typically either:

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

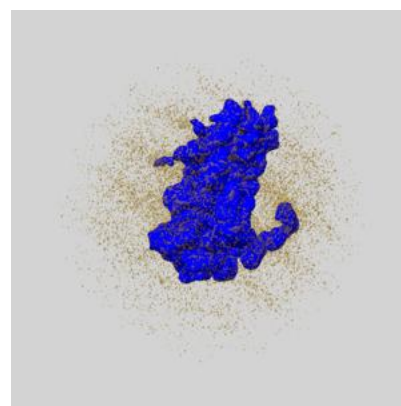
6.6.1 emd_19803_msk_1.map [i](#)



X



Y

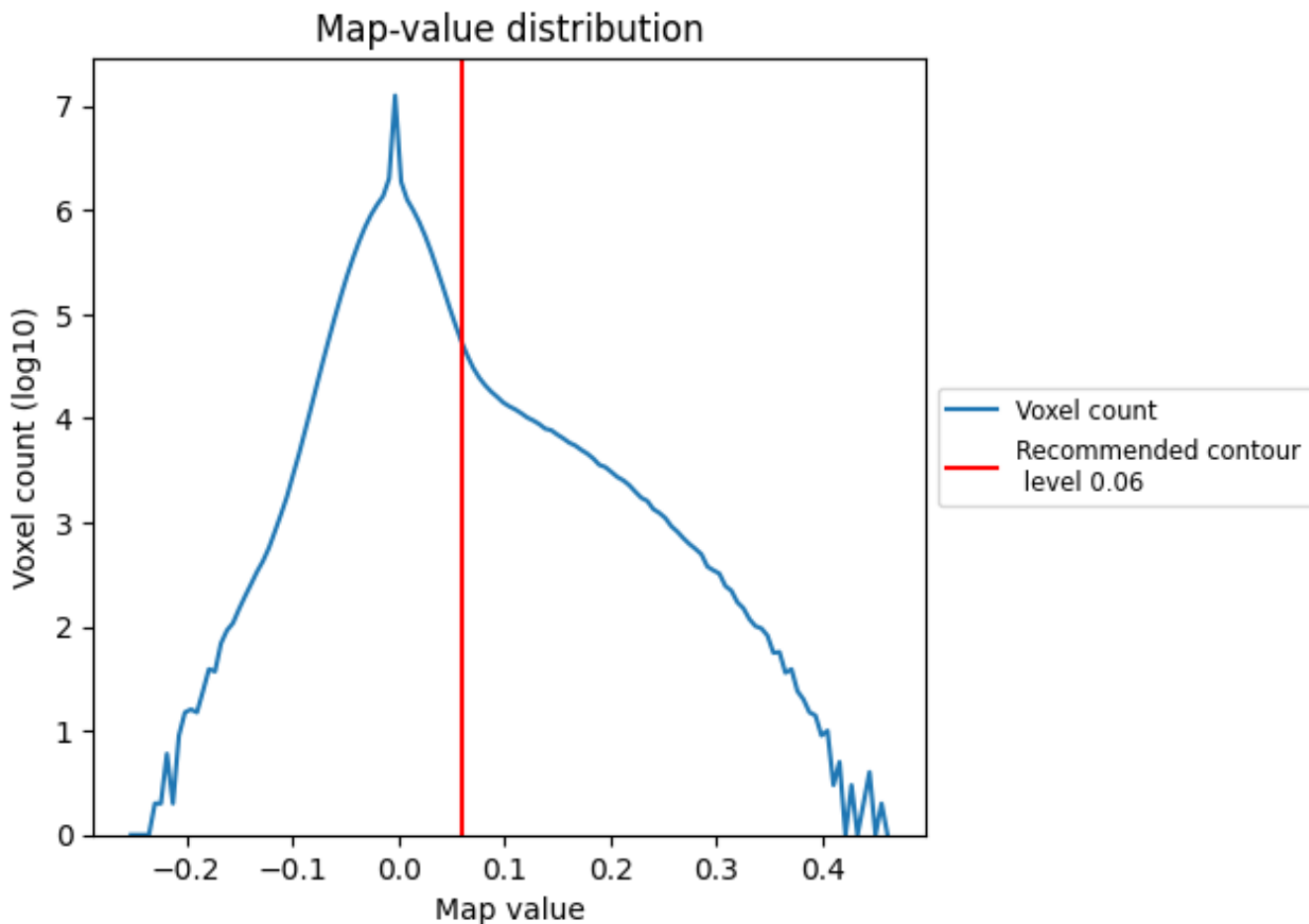


Z

7 Map analysis [i](#)

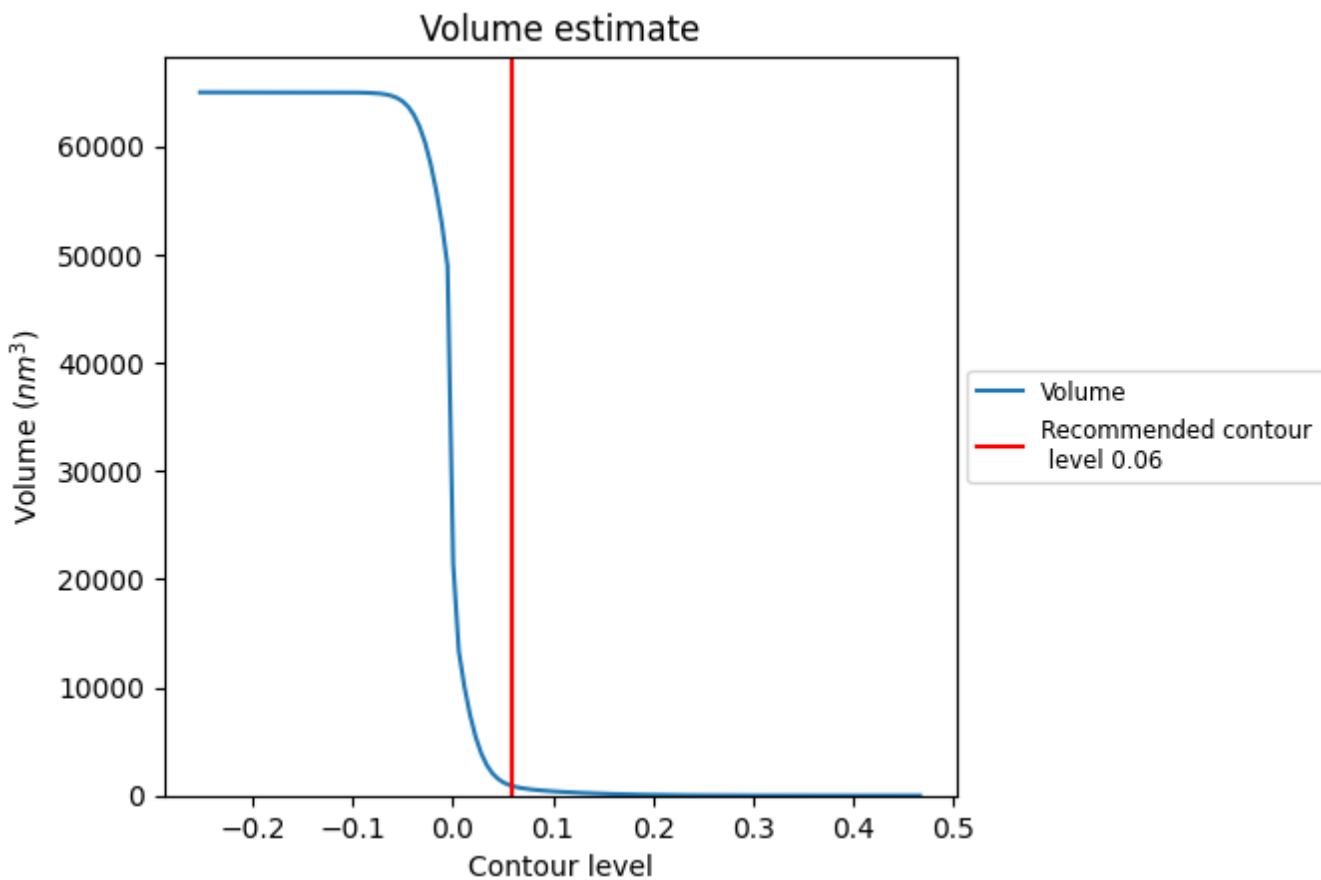
This section contains the results of statistical analysis of the map.

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.

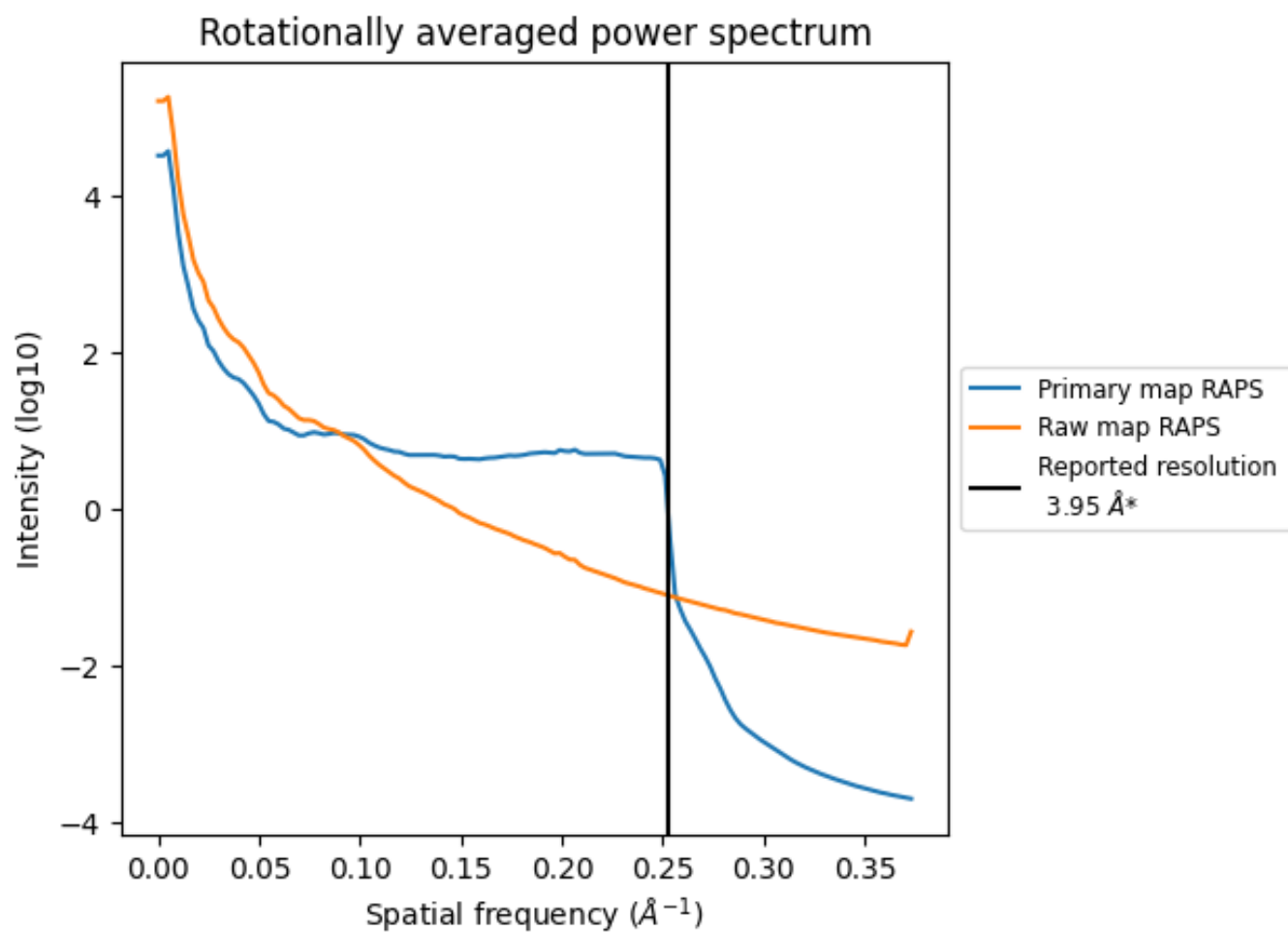
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 878 nm³; this corresponds to an approximate mass of 793 kDa.

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

7.3 Rotationally averaged power spectrum i

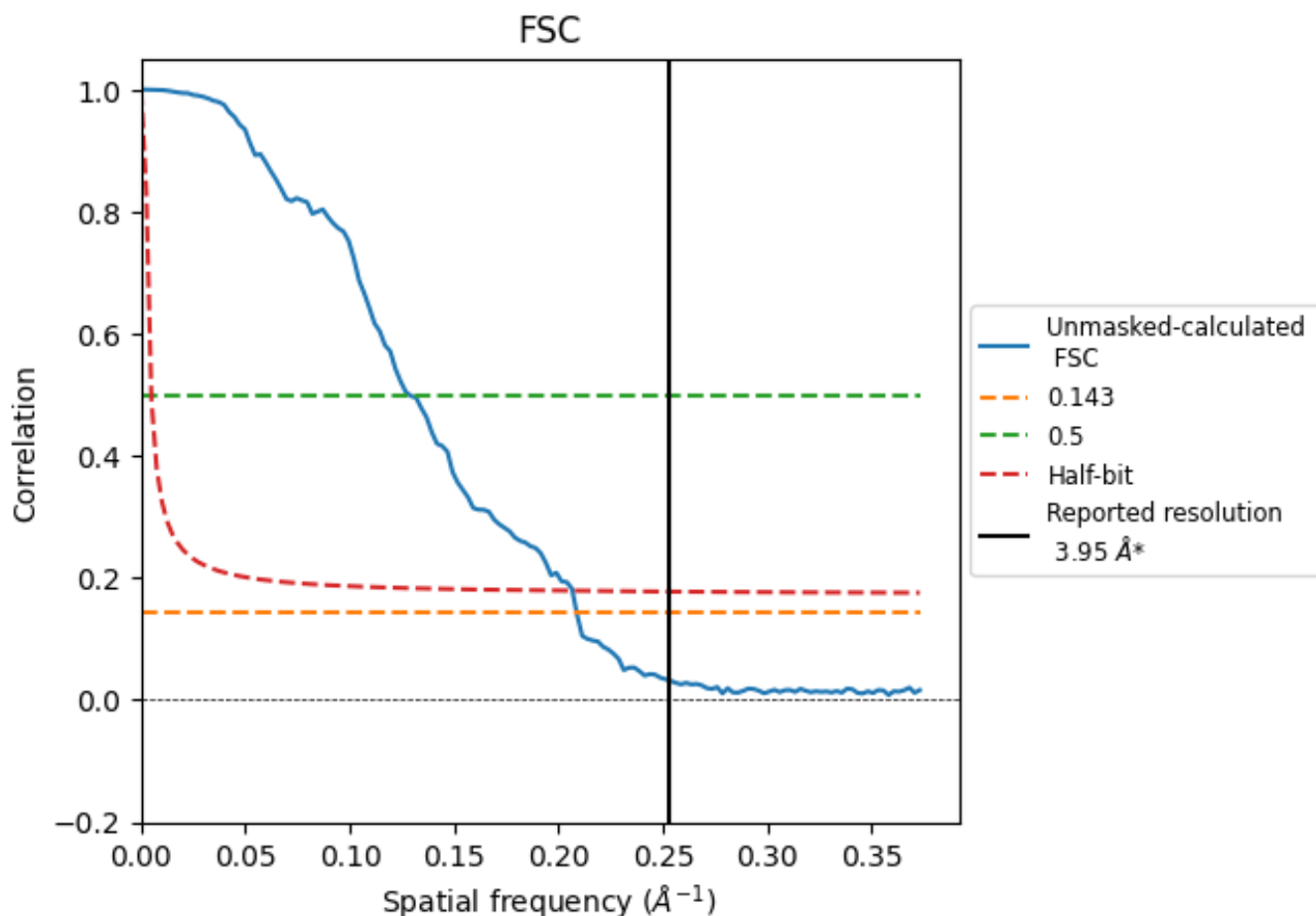


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

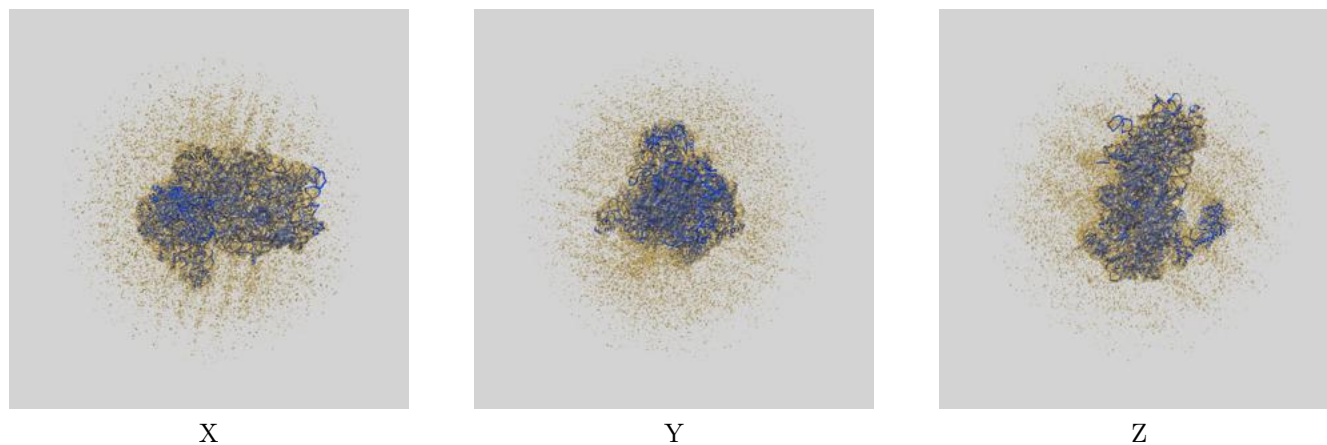
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.79	7.78	4.84

*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 4.79 differs from the reported value 3.95 by more than 10 %

9 Map-model fit [i](#)

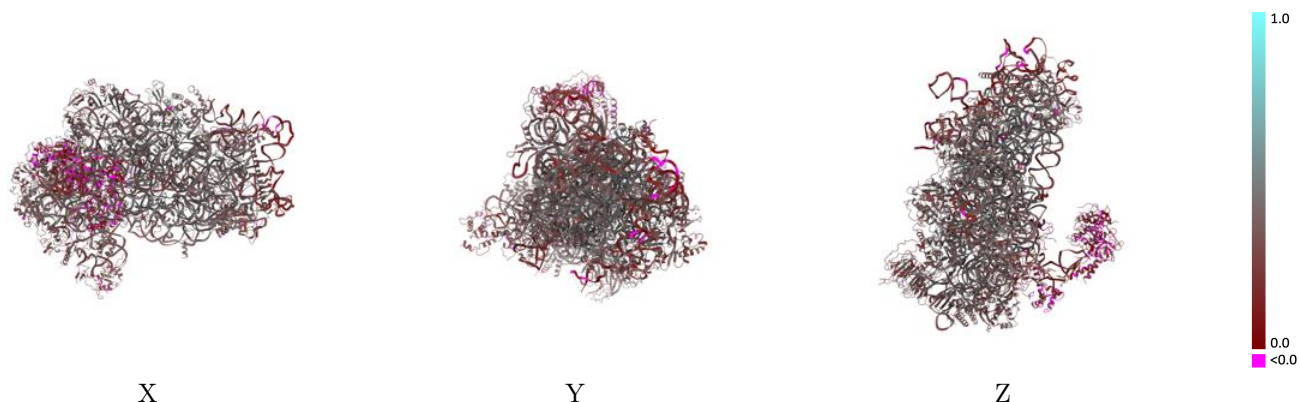
This section contains information regarding the fit between EMDB map EMD-19803 and PDB model 8S8F. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



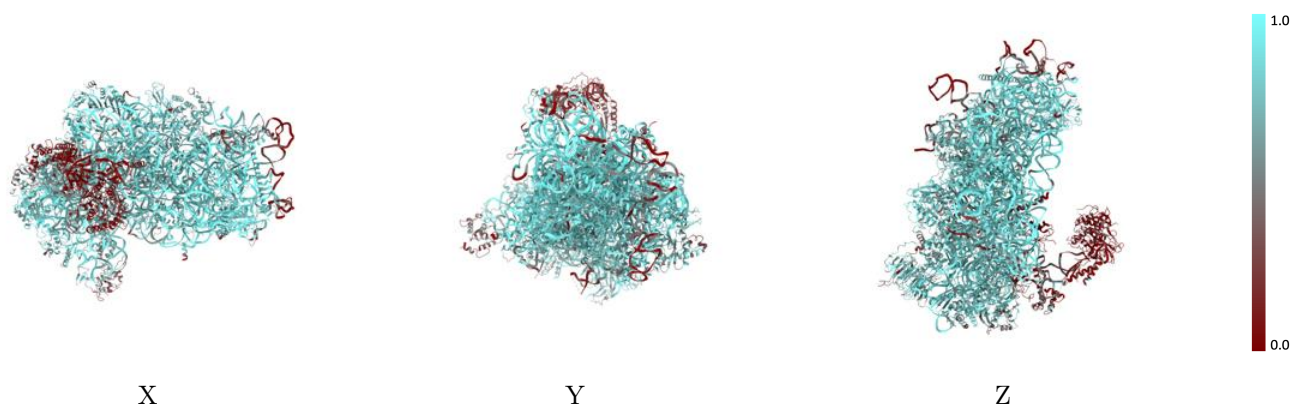
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



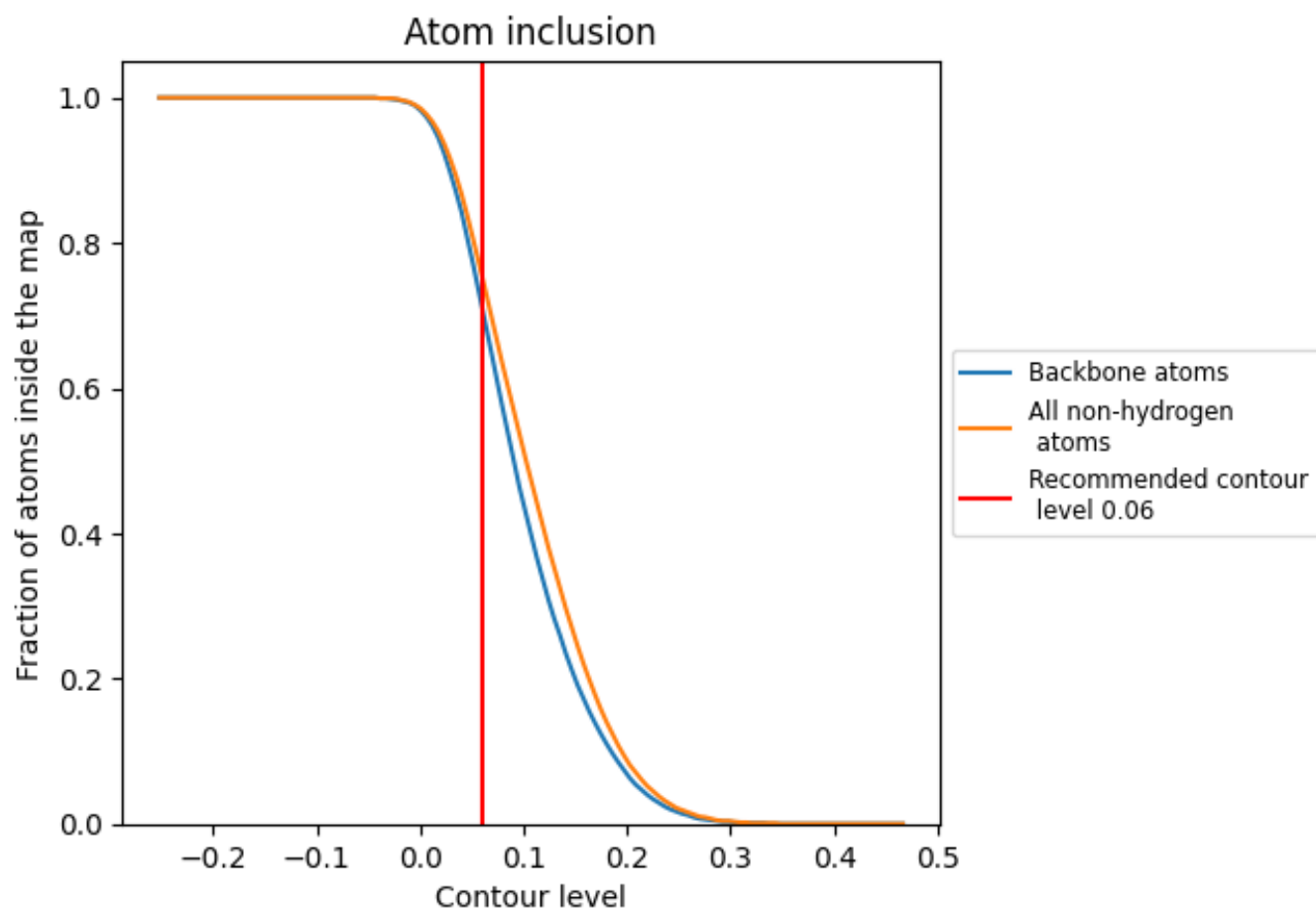
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 75% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.3520
1	 0.5570	 0.2260
2	 0.8740	 0.3620
3	 0.3470	 0.2790
A	 0.8160	 0.3950
B	 0.7740	 0.3740
C	 0.8090	 0.4270
D	 0.7620	 0.3810
E	 0.8430	 0.4260
F	 0.7390	 0.3810
G	 0.8070	 0.3530
H	 0.6840	 0.3430
I	 0.8030	 0.4060
J	 0.7890	 0.4000
K	 0.7570	 0.3290
L	 0.7540	 0.4000
M	 0.3430	 0.2270
N	 0.8310	 0.4110
O	 0.7930	 0.3800
P	 0.7710	 0.3190
Q	 0.8040	 0.3840
R	 0.7090	 0.3610
S	 0.7670	 0.3370
T	 0.8300	 0.3570
U	 0.6870	 0.3540
V	 0.8700	 0.4020
W	 0.8170	 0.4360
X	 0.8260	 0.4390
Y	 0.8370	 0.3940
Z	 0.5230	 0.3140
a	 0.8220	 0.4370
b	 0.8060	 0.4130
c	 0.7660	 0.4360
d	 0.8510	 0.4150
e	 0.7210	 0.3820



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Chain	Atom inclusion	Q-score
f	 0.4890	 0.2520
g	 0.7360	 0.3310
h	 0.1790	 0.3130
i	 0.4460	 0.3480
j	 0.1700	 0.1730
k	 0.0850	 0.1480
l	 0.0590	 0.0490
m	 0.0520	 0.1940