



# wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 02:39 AM UTC

PDB ID : 9H9H / pdb\_00009h9h  
EMDB ID : EMD-51964  
Title : Complex 1 30S-IF1-IF2-IF3-GE81112  
Authors : Schedlbauer, A.; Han, X.; van Bakel, W.; Kaminishi, T.; Ochoa-Lizarralde, B.; Iturrioz, I.; Capuni, R.; Parry, R.; Zegarra, R.; Gil-Carton, D.; Lopez-Alonso, J.P.; Barragan Sanz, K.; Brandi, L.; Gualerzi, C.O.; Fucini, P.; Connell, S.R.  
Deposited on : 2024-10-31  
Resolution : 3.80 Å(reported)  
Based on initial model : 4YBB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

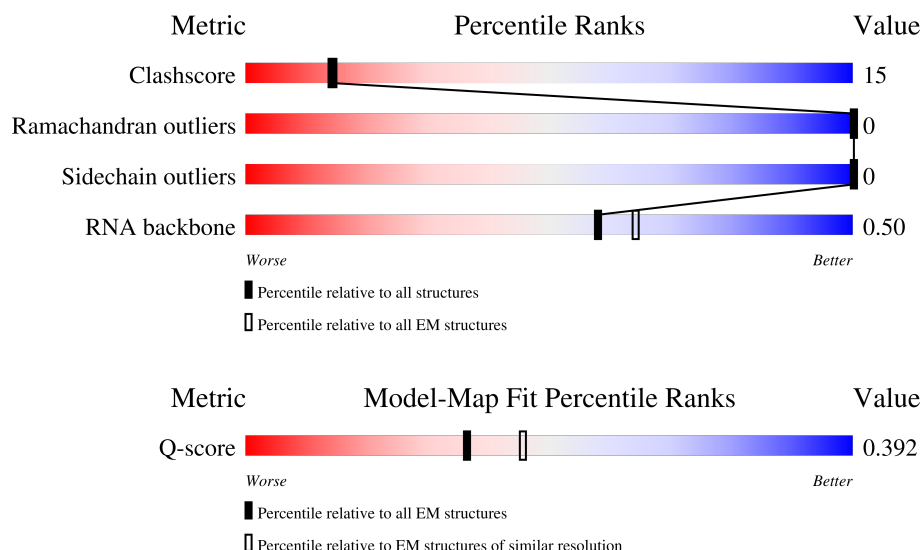
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

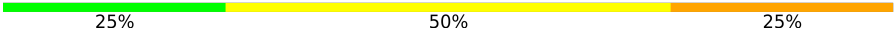

The reported resolution of this entry is 3.80 Å.

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.






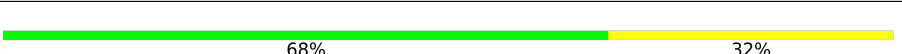
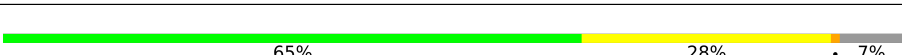
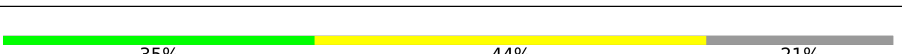

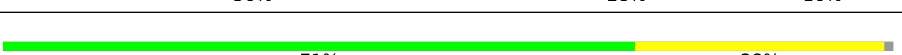
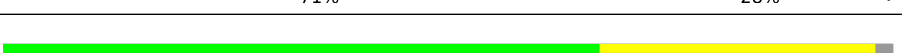
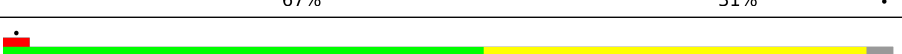


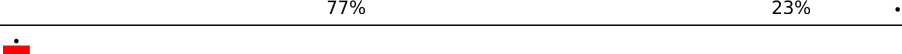
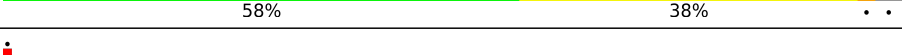
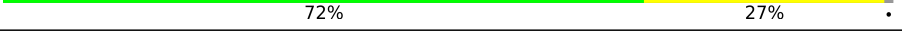



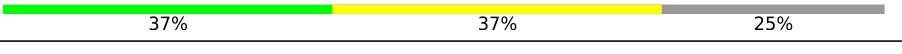
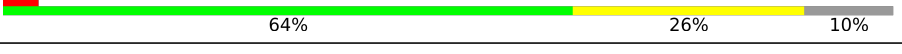


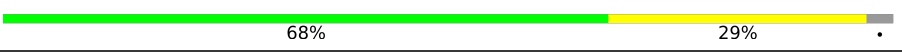

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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  $\geq 3$ , 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	4	 25% 50% 25%
2	3	77	 26% 40% 34%

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Mol	Chain	Length	Quality of chain
3	A	1542	
4	B	241	
5	C	233	
6	D	206	
7	E	167	
8	F	135	
9	G	179	
10	H	130	
11	I	130	
12	J	103	
13	K	129	
14	L	124	
15	M	118	
16	N	101	
17	O	89	
18	P	82	
19	Q	84	
20	R	75	
21	S	92	
22	T	87	
23	U	71	
24	X	72	
25	Y	890	
26	Z	180	

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 58815 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 mRNA (5'-R(P\*AP\*AP\*UP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	4	Total	C	N	O	P	0	0
			87	39	17	27	4		

- Molecule 2 is a RNA chain called t-RNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	77	Total	C	N	O	P	0	0
			1646	732	293	544	77		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	34	C	G	conflict	GB 2208028712
3	35	A	-	insertion	GB 2208028712
3	37	A	C	conflict	GB 2208028712
3	?	-	G	deletion	GB 2208028712
3	69	U	C	conflict	GB 2208028712

- Molecule 3 is a RNA chain called 16S RNA (1534-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 4 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 6 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 8 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 11 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	56	Total	C	N	O	S	0	0
			464	293	88	83			

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 22 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	52	Total	C	N	O	S	0	0
			430	269	89	71	1		

- Molecule 24 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	70	Total	C	N	O	S	0	0
			563	353	102	105	3		

- Molecule 25 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	488	Total	C	N	O	S	0	0
			3651	2278	640	716	17		

- Molecule 26 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	112	Total	C	N	O	S	0	0
			923	586	166	167	4		

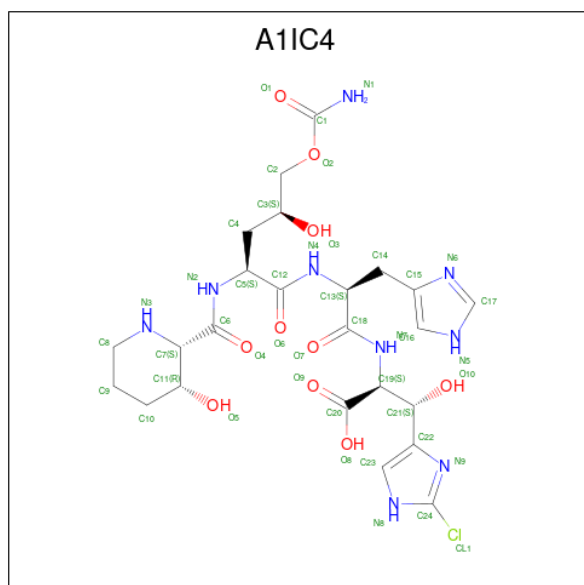
- Molecule 27 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
27	2	1	Total	K	0
			1	1	
27	A	4	Total	K	0
			4	4	

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	3	3	Total	Mg	0
			3	3	
28	A	148	Total	Mg	0
			148	148	
28	K	1	Total	Mg	0
			1	1	

- Molecule 29 is (2S,3S)-2-[[[(2S)-2-[[[(2S,4S)-5-aminocarbonyloxy-4-oxidanyl-2-[[[(2S,3R)-3-oxidanylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-3-(1H-imidazol-4-yl)propanoyl]amino]-3-(2-chloranyl-1H-imidazol-4-yl)-3-oxidanyl-propanoic acid (CCD ID: A1IC4) (formula: C<sub>24</sub>H<sub>34</sub>ClN<sub>9</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Cl	N	O	0
			44	24	1	9	10	

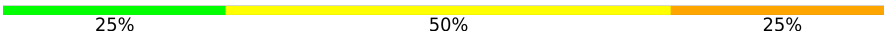
- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

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

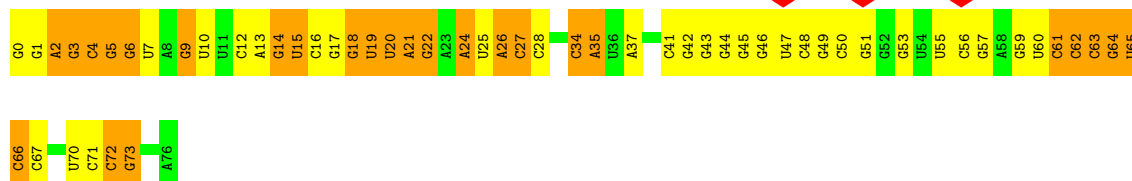
- Molecule 1: mRNA (5'-R(P\*AP\*AP\*UP\*G)-3')

Chain 2: 



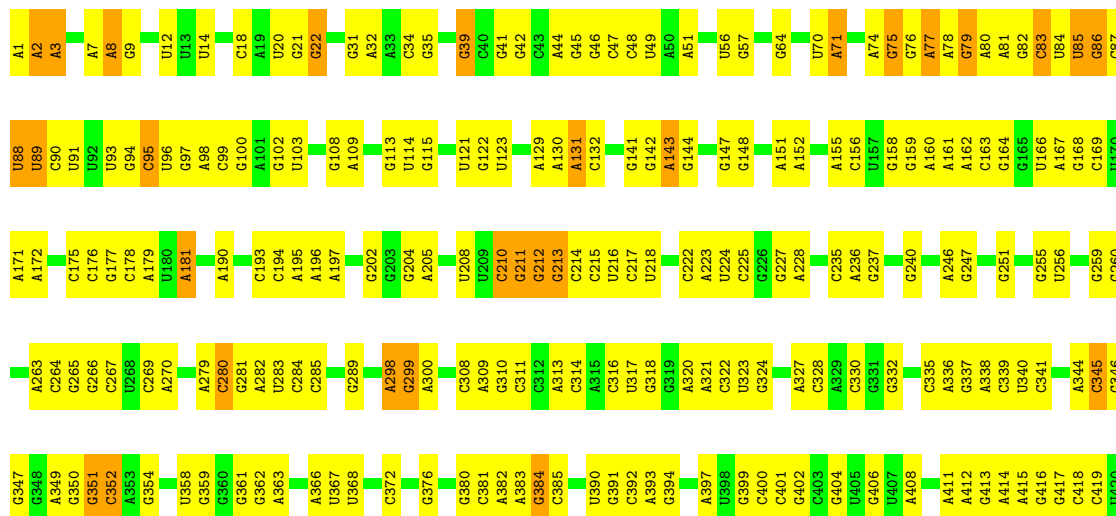
- Molecule 2: t-RNA (77-MER)

Chain 3: 



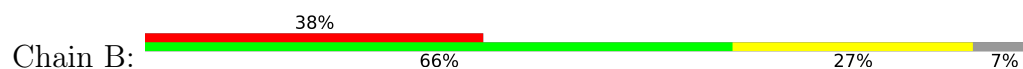
- Molecule 3: 16S RNA (1534-MER)

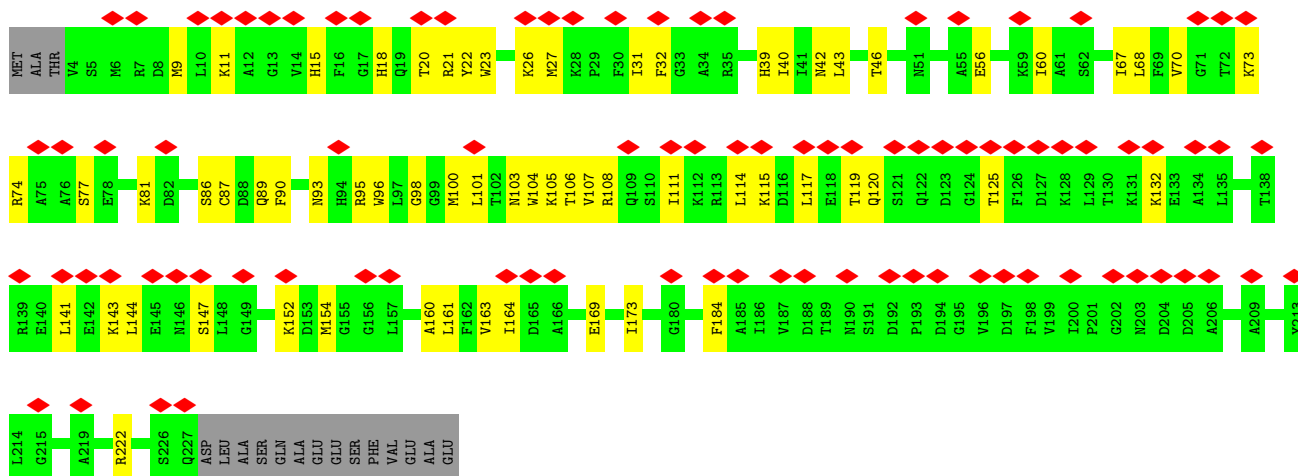
Chain A: 



U1495	C1496	G1497	U1498	A1499	A1503	G1504	G1505	U1506	A1507	A1508	U1512	A1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	U1522	G1523	C1524	G1525	G1526	A1527	U1528	G1529	G1530	A1531	U1532	C1533	A1534	C	C	U	C	U	U	A																
G1421	U1425	G1426	C1427	A1428	A1429	A1430	A1434	G1435	U1438	A1439	A1441	G1442	C1443	A1446	A1447	C1448	G1449	C1450	U1451	C1452	G1453	G1454	A1456	C1460	G1461	U1464	A1465	A1468	C1469	C1470	U1471	U1473	C1474	C1475	U1476	U1477	U1478	C1479	A1480	U1481	G1482	A1483	C1484	U1485	C1486	G1487	G1488	G1489	U1490	G1491	A1492	C1493	G1494			
C1328	G1331	A1340	U1341	C1342	G1343	C1344	G1347	U1348	A1349	A1350	G1353	C1359	A1360	A1368	C1369	G1370	G1373	A1374	C1375	G1379	U1380	U1381	G1385	C1386	G1387	C1391	U1392	C1400	G1401	C1402	C1403	C1404	C1407	A1408	C1409	A1410	C1411	C1412	A1413	A1418	G1419	A1420														
A1236	C1237	A1238	U1239	U1240	G1241	A1250	G1253	A1254	G1255	G1258	C1259	G1260	G1266	C1267	A1268	A1269	G1279	A1280	C1281	C1282	U1283	C1284	A1285	U1286	A1287	G1290	U1291	G1292	C1296	U1297	U1298	A1299	G1300	U1301	C1302	C1303	G1304	A1305	U1307	U1313	C1314	G1315	G1316	C1317	A1318	A1319	C1320	U1321	C1322	U1323	U1324	U1325				
U1159	A1163	G1164	U1165	G1166	U1167	U1168	A1169	A1170	A1171	G1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	U1183	G1184	U1185	U1186	A1187	U1188	C1119	C1120	U1121	U1122	U1123	U1124	U1125	U1126	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	C1136	C1137	G1138	G1139	C1141	G1142	G1143	U1144	A1145	U1070	G1071	G1072	U1078	G1079	A1080	A1081	C1158
A1004	A1005	G1006	U1007	U1008	U1009	G1013	A1014	G1015	A1016	G1020	A1021	A1022	U1023	G1024	U1025	G1026	C1027	C1028	U1029	U1030	C1031	G1032	A1036	C1037	C1038	G1039	U1040	G1041	A1042	A1044	C1045	A1046	G1047	G1048	U1049	G1050	G1053	C1054	A1055	U1060	U1065	C1066	U1070	G1071	G1072	U1078	G1079	A1080	A1081	C1158						
G922	A923	C924	G925	C926	G927	C930	C931	C932	G933	C934	A935	G939	C940	G941	G947	C948	A949	U950	G951	G954	U957	U959	U961	U962	C962	G963	A964	U965	G966	C967	A968	A969	C970	G971	C972	A975	G976	A977	A978	C980	A900	A901	C902	U986	G987	U992	G993	A994	A1000	C1001	G1002	G1003				
U835	G836	U837	G838	C839	C840	C841	U842	U843	G844	A845	G846	G847	C848	G849	U850	G851	G852	U855	G859	A864	A865	C866	C867	G868	C869	U870	U871	A872	A873	G874	C883	U884	A889	G890	C899	A900	A901	C902	U986	G987	U992	G993	A994	A1000	C1001	G1002	G1003									
G752	A753	G754	G755	C758	G765	G771	U772	A777	G778	C779	G780	A781	A790	G791	A792	U793	A794	G795	C796	C797	U798	G799	U800	U801	A802	A803	A873	G874	C883	U884	A889	G890	C899	A900	A901	C902	U986	G987	U992	G993	A994	A1000	C1001	G1002	G1003											
A673	G674	A675	U677	U678	G683	U684	G685	U686	G690	G691	U692	G693	U694	A695	U696	U697	G698	A790	G791	A792	U793	A794	G795	C796	C797	U798	G799	U800	U801	A802	A803	A873	G874	C883	U884	A889	G890	C899	A900	A901	C902	U986	G987	U992	G993	A994	A1000	C1001	G1002	G1003						
U421	C422	G423	G424	G425	U426	U429	A430	A431	A432	G433	U434	A435	C436	U437	C440	A441	G444	G447	C452	A453	C454	C455	C456	G457	G458	A459	A460	A461	U467	A468	C469	C470	U471	U472	U473	G474	C475	U476	C477	A478	A481	A482	U483	G484	U486	C489	U490	G491	C492	A493	G494					

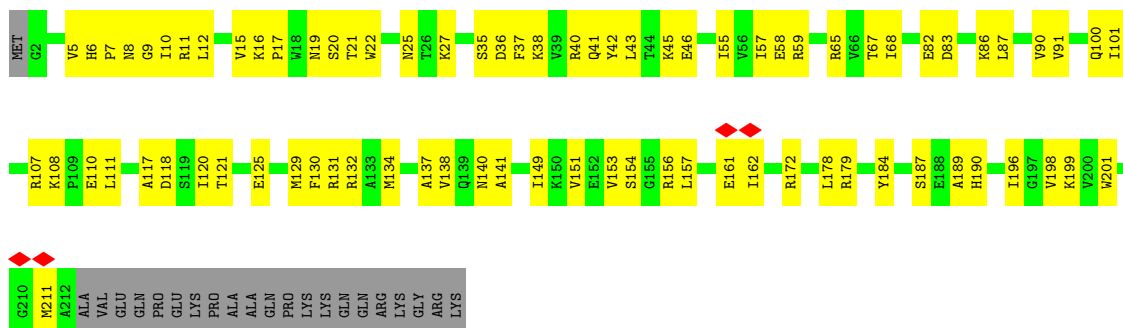
● Molecule 4: Small ribosomal subunit protein uS2





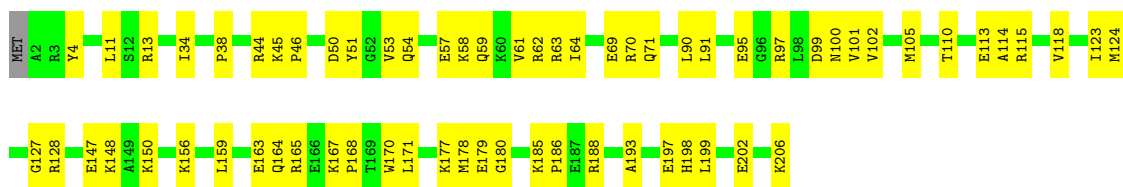
- Molecule 5: Small ribosomal subunit protein uS3

Chain C: 56% 34% 9%



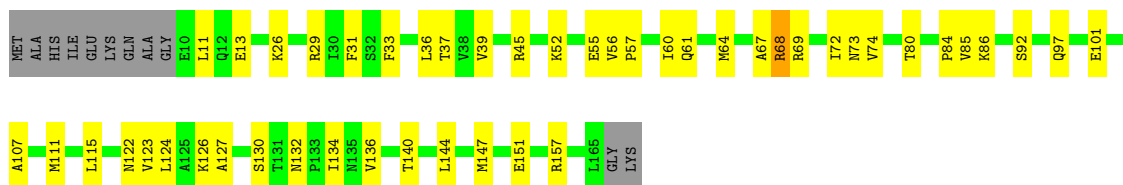
- Molecule 6: Small ribosomal subunit protein uS4

Chain D: 68% 32%



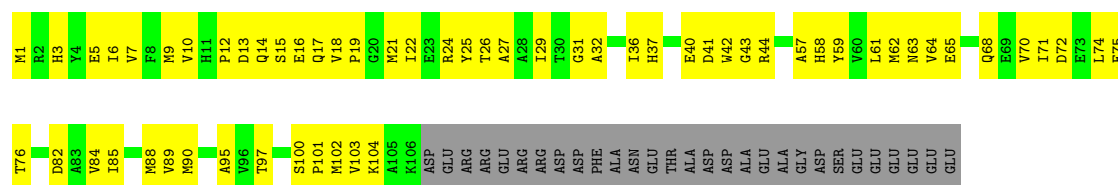
- Molecule 7: Small ribosomal subunit protein uS5

Chain E: 65% 28% 7%



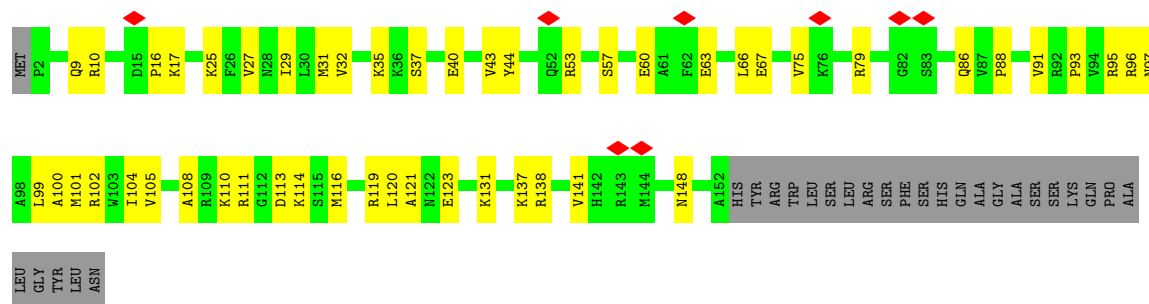
- Molecule 8: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  35% 44% 21%



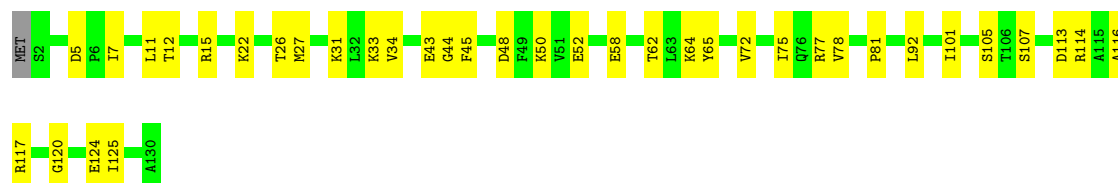
• Molecule 9: Small ribosomal subunit protein uS7

Chain G:  56% 28% 16%



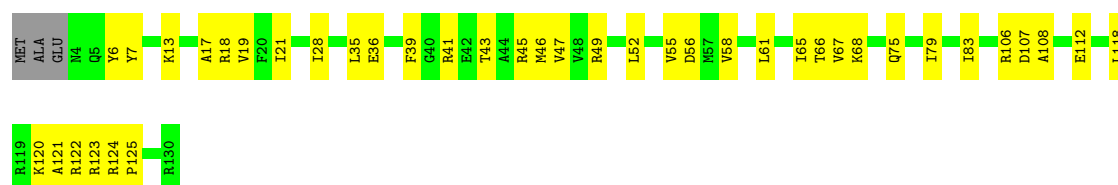
• Molecule 10: Small ribosomal subunit protein uS8

Chain H:  71% 28%



• Molecule 11: Small ribosomal subunit protein uS9

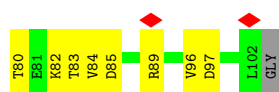
Chain I:  67% 31%



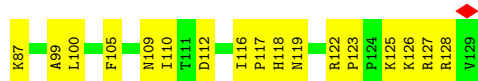
• Molecule 12: Small ribosomal subunit protein uS10

Chain J:  54% 43%





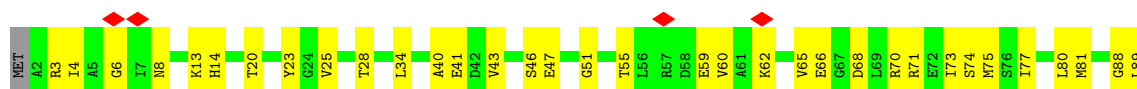
- Molecule 13: Small ribosomal subunit protein uS11



- Molecule 14: Small ribosomal subunit protein uS12



- Molecule 15: Small ribosomal subunit protein uS13



- Molecule 16: Small ribosomal subunit protein uS14

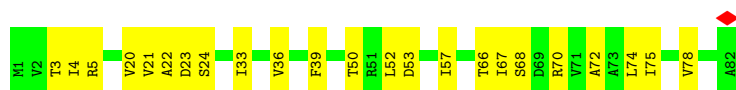


- Molecule 17: Small ribosomal subunit protein uS15



- Molecule 18: Small ribosomal subunit protein bS16





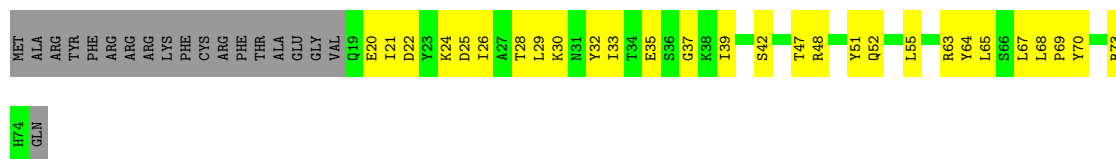
- Molecule 19: Small ribosomal subunit protein uS17

Chain Q: 64% 30% 5%



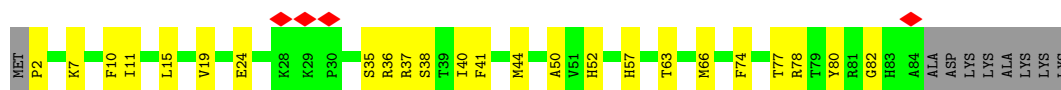
- Molecule 20: Small ribosomal subunit protein bS18

Chain R: 37% 37% 25%



- Molecule 21: Small ribosomal subunit protein uS19

Chain S: 64% 26% 10%



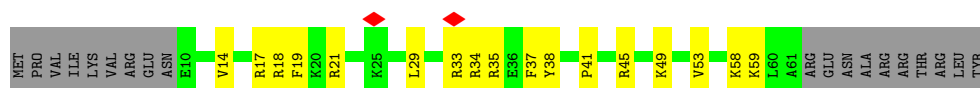
- Molecule 22: Small ribosomal subunit protein bS20

Chain T: 60% 39% 1%



- Molecule 23: Small ribosomal subunit protein bS21

Chain U: 49% 24% 27%



- Molecule 24: Translation initiation factor IF-1

Chain X: 68% 29% 3%



- Molecule 25: Translation initiation factor IF-2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	325.8, 325.8, 325.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.086, 1.086, 1.086	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, PSU, 4OC, MA6, K, G7M, 5MC, 2MG, A1IC4, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.40	0/97	0.45	0/149
2	3	0.19	0/1838	0.33	0/2863
3	A	0.25	0/36593	0.31	0/57081
4	B	0.25	0/1784	0.47	0/2403
5	C	0.22	0/1680	0.40	0/2263
6	D	0.31	0/1665	0.48	0/2227
7	E	0.33	0/1165	0.53	0/1568
8	F	0.22	0/881	0.49	0/1189
9	G	0.24	0/1195	0.46	0/1602
10	H	0.28	0/989	0.52	0/1326
11	I	0.21	0/1033	0.49	1/1375 (0.1%)
12	J	0.38	0/813	0.59	0/1100
13	K	0.48	0/893	0.63	0/1205
14	L	0.49	0/969	0.60	0/1300
15	M	0.37	0/900	0.58	0/1204
16	N	0.15	0/817	0.42	0/1088
17	O	0.34	0/722	0.55	0/964
18	P	0.47	0/659	0.55	0/884
19	Q	0.57	0/657	0.72	0/881
20	R	0.43	0/471	0.63	0/633
21	S	0.20	0/680	0.47	0/915
22	T	0.26	0/676	0.46	0/895
23	U	0.34	0/436	0.54	0/577
24	X	0.42	0/570	0.67	0/766
25	Y	0.43	0/3691	0.59	0/4988
26	Z	0.28	0/934	0.58	0/1238
All	All	0.29	0/62808	0.41	1/92684 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	E	0	2
15	M	0	2
19	Q	0	1
20	R	0	1
25	Y	0	2
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	13	LYS	CB-CA-C	-5.36	110.38	116.54

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	68	ARG	Sidechain
7	E	69	ARG	Sidechain
15	M	92	ARG	Sidechain
15	M	93	ARG	Sidechain
19	Q	65	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	87	0	44	4	0
2	3	1646	0	832	41	0
3	A	32930	0	16588	630	0
4	B	1753	0	1780	56	0
5	C	1653	0	1722	61	0
6	D	1643	0	1707	60	0
7	E	1152	0	1192	39	0
8	F	862	0	864	51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	1181	0	1238	42	0
10	H	979	0	1031	29	0
11	I	1021	0	1070	31	0
12	J	803	0	842	38	0
13	K	877	0	887	50	0
14	L	955	0	1016	28	0
15	M	891	0	952	38	0
16	N	805	0	844	24	0
17	O	714	0	734	24	0
18	P	649	0	666	18	0
19	Q	648	0	691	19	0
20	R	464	0	486	27	0
21	S	663	0	688	21	0
22	T	670	0	719	26	0
23	U	430	0	458	25	0
24	X	563	0	581	15	0
25	Y	3651	0	3726	162	0
26	Z	923	0	976	46	0
27	2	1	0	0	0	0
27	A	4	0	0	0	0
28	3	3	0	0	0	0
28	A	148	0	0	0	0
28	K	1	0	0	0	0
29	A	44	0	0	2	0
30	B	1	0	0	0	0
All	All	58815	0	42334	1472	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 15.

The worst 5 of 1472 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:35:THR:HG22	13:K:41:ALA:HA	1.18	1.16
13:K:21:ALA:HB3	13:K:84:VAL:HG22	1.39	1.00
15:M:4:ILE:HD11	15:M:60:VAL:HG21	1.48	0.94
18:P:3:THR:HG22	18:P:66:THR:OG1	1.69	0.93
6:D:110:THR:HG23	6:D:113:GLU:H	1.34	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	222/241 (92%)	215 (97%)	7 (3%)	0	100	100
5	C	209/233 (90%)	206 (99%)	3 (1%)	0	100	100
6	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
7	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
8	F	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
9	G	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
10	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
11	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
12	J	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
13	K	115/129 (89%)	112 (97%)	3 (3%)	0	100	100
14	L	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
16	N	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
17	O	86/89 (97%)	86 (100%)	0	0	100	100
18	P	80/82 (98%)	80 (100%)	0	0	100	100
19	Q	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
20	R	54/75 (72%)	53 (98%)	1 (2%)	0	100	100
21	S	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
22	T	84/87 (97%)	84 (100%)	0	0	100	100
23	U	50/71 (70%)	50 (100%)	0	0	100	100
24	X	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	Y	486/890 (55%)	466 (96%)	20 (4%)	0	100	100
26	Z	110/180 (61%)	105 (96%)	5 (4%)	0	100	100
All	All	3015/3718 (81%)	2935 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
4	B	186/199 (94%)	186 (100%)	0	100	100
5	C	172/190 (90%)	172 (100%)	0	100	100
6	D	172/173 (99%)	172 (100%)	0	100	100
7	E	119/126 (94%)	119 (100%)	0	100	100
8	F	92/116 (79%)	92 (100%)	0	100	100
9	G	124/147 (84%)	124 (100%)	0	100	100
10	H	104/105 (99%)	104 (100%)	0	100	100
11	I	105/107 (98%)	105 (100%)	0	100	100
12	J	88/90 (98%)	88 (100%)	0	100	100
13	K	90/99 (91%)	90 (100%)	0	100	100
14	L	103/104 (99%)	103 (100%)	0	100	100
15	M	93/96 (97%)	93 (100%)	0	100	100
16	N	83/84 (99%)	83 (100%)	0	100	100
17	O	76/77 (99%)	76 (100%)	0	100	100
18	P	65/65 (100%)	65 (100%)	0	100	100
19	Q	74/78 (95%)	74 (100%)	0	100	100
20	R	49/65 (75%)	49 (100%)	0	100	100
21	S	72/79 (91%)	72 (100%)	0	100	100
22	T	65/66 (98%)	65 (100%)	0	100	100
23	U	43/61 (70%)	43 (100%)	0	100	100
24	X	64/65 (98%)	64 (100%)	0	100	100
25	Y	386/713 (54%)	386 (100%)	0	100	100
26	Z	101/156 (65%)	101 (100%)	0	100	100
All	All	2526/3061 (82%)	2526 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
17	O	20	ASN
22	T	75	HIS
25	Y	773	ASN
17	O	38	HIS
20	R	54	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	3/4 (75%)	1 (33%)	0
2	3	76/77 (98%)	38 (50%)	6 (7%)
3	A	1533/1542 (99%)	249 (16%)	13 (0%)
All	All	1612/1623 (99%)	288 (17%)	19 (1%)

5 of 288 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	18	G
2	3	2	A
2	3	3	G
2	3	4	C
2	3	5	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	790	A
3	A	1240	U
3	A	1484	C
3	A	1183	U
3	A	298	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 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
3	2MG	A	1516	3	23,26,27	1.27	4 (17%)	33,38,41	2.17	10 (30%)
3	5MC	A	967	3	19,22,23	1.63	3 (15%)	26,32,35	1.14	3 (11%)
3	2MG	A	966	3	23,26,27	1.24	4 (17%)	33,38,41	2.19	7 (21%)
3	MA6	A	1519	3	23,26,27	1.45	4 (17%)	33,38,41	2.41	13 (39%)
3	4OC	A	1402	3	20,23,24	0.76	0	25,32,35	0.92	1 (4%)
3	2MG	A	1207	3	23,26,27	1.26	4 (17%)	33,38,41	2.19	5 (15%)
3	G7M	A	527	3	23,26,27	0.54	0	34,39,42	0.93	1 (2%)
3	PSU	A	516	3	18,21,22	1.41	4 (22%)	21,30,33	2.05	4 (19%)
3	5MC	A	1407	3	19,22,23	1.48	3 (15%)	26,32,35	1.17	3 (11%)
3	UR3	A	1498	3	19,22,23	0.92	0	26,32,35	1.71	2 (7%)
3	MA6	A	1518	3	23,26,27	1.49	5 (21%)	33,38,41	2.34	11 (33%)

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
3	2MG	A	1516	3	-	0/9/27/28	0/3/3/3
3	5MC	A	967	3	-	1/7/25/26	0/2/2/2
3	2MG	A	966	3	-	0/9/27/28	0/3/3/3
3	MA6	A	1519	3	-	3/11/29/30	0/3/3/3
3	4OC	A	1402	3	-	0/9/29/30	0/2/2/2
3	2MG	A	1207	3	-	0/9/27/28	0/3/3/3
3	G7M	A	527	3	-	2/7/25/26	0/3/3/3
3	PSU	A	516	3	-	4/7/25/26	0/2/2/2
3	5MC	A	1407	3	-	0/7/25/26	0/2/2/2
3	UR3	A	1498	3	-	1/7/25/26	0/2/2/2
3	MA6	A	1518	3	-	1/11/29/30	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	967	5MC	C5-C4	5.87	1.48	1.44
3	A	1407	5MC	C5-C4	5.07	1.48	1.44
3	A	1518	MA6	C5-C4	4.44	1.47	1.39
3	A	1519	MA6	C5-C4	4.36	1.46	1.39
3	A	1207	2MG	C5-C4	3.13	1.47	1.38

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1207	2MG	C2-N3-C4	7.15	120.94	112.00
3	A	966	2MG	C2-N3-C4	7.15	120.94	112.00
3	A	1498	UR3	C4-N3-C2	-6.98	118.96	124.58
3	A	1516	2MG	C2-N3-C4	6.74	120.43	112.00
3	A	516	PSU	N1-C2-N3	6.37	121.89	115.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	516	PSU	C2'-C1'-C5-C4
3	A	516	PSU	C2'-C1'-C5-C6
3	A	527	G7M	O4'-C4'-C5'-O5'
3	A	1519	MA6	O4'-C4'-C5'-O5'
3	A	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1516	2MG	1	0
3	A	1519	MA6	4	0
3	A	1402	4OC	1	0
3	A	516	PSU	1	0
3	A	1518	MA6	4	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 159 ligands modelled in this entry, 158 are monoatomic - leaving 1 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
29	A1IC4	A	1601	-	42,46,46	2.29	12 (28%)	47,63,63	1.70	7 (14%)

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
29	A1IC4	A	1601	-	-	19/49/60/60	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)
29	A	1601	A1IC4	C1-N1	6.63	1.45	1.33
29	A	1601	A1IC4	C12-N4	5.45	1.45	1.34
29	A	1601	A1IC4	C6-N2	5.24	1.45	1.34
29	A	1601	A1IC4	C18-N7	5.15	1.45	1.34
29	A	1601	A1IC4	C22-N9	-3.53	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	1601	A1IC4	O2-C1-N1	7.26	120.14	111.11
29	A	1601	A1IC4	O1-C1-N1	-3.73	119.69	125.58
29	A	1601	A1IC4	C23-C22-N9	-3.17	106.65	110.75
29	A	1601	A1IC4	O2-C1-O1	-3.16	120.16	123.08
29	A	1601	A1IC4	C13-C14-C15	-2.41	108.09	113.75

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

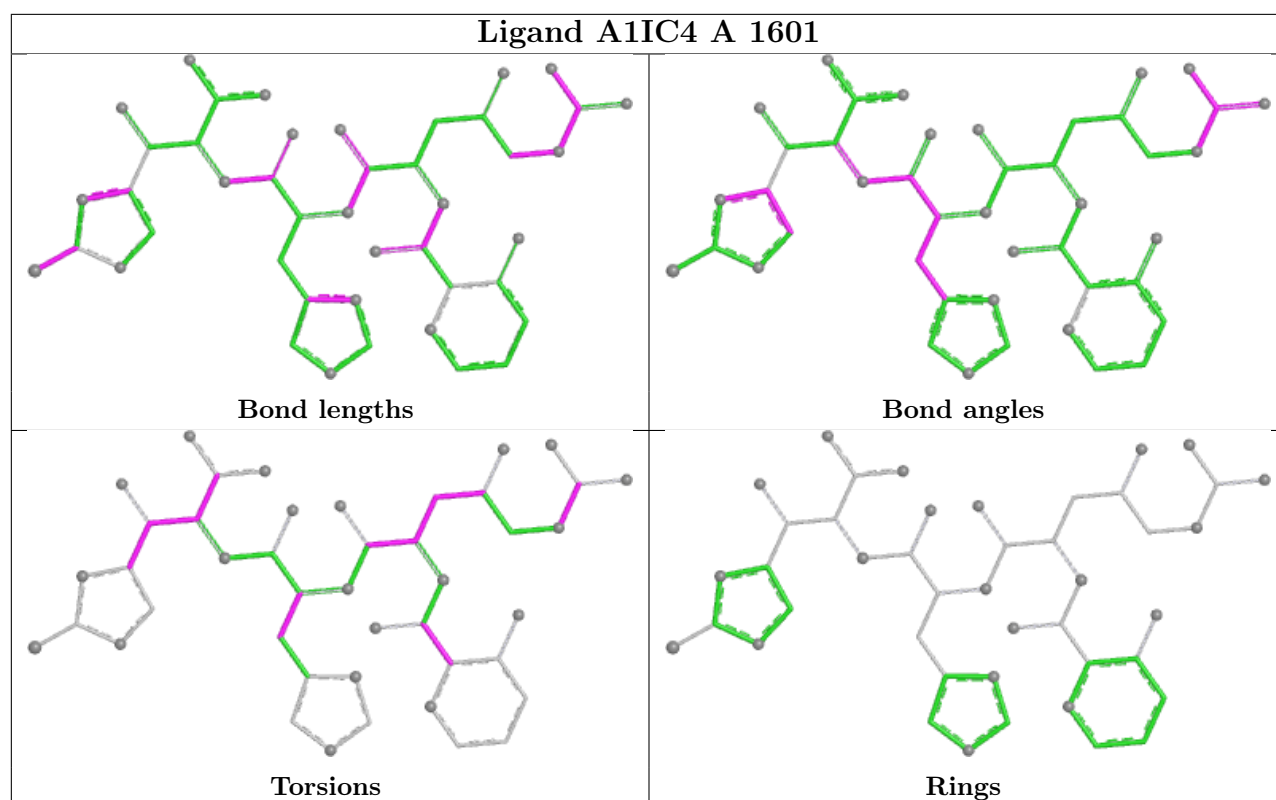
Mol	Chain	Res	Type	Atoms
29	A	1601	A1IC4	N1-C1-O2-C2
29	A	1601	A1IC4	O1-C1-O2-C2
29	A	1601	A1IC4	C2-C3-C4-C5
29	A	1601	A1IC4	O3-C3-C4-C5
29	A	1601	A1IC4	C18-C13-C14-C15

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	1601	A1IC4	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](#)

There are no chain breaks in this entry.

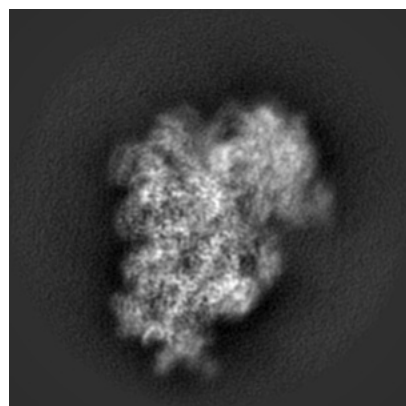
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51964. These allow visual inspection of the internal detail of the map and identification of artifacts.

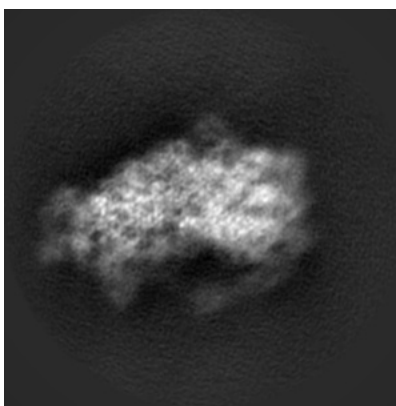
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

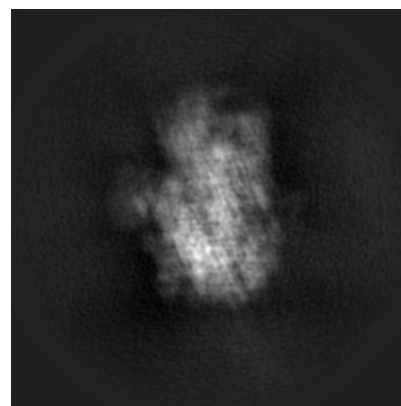
#### 6.1.1 Primary map



X

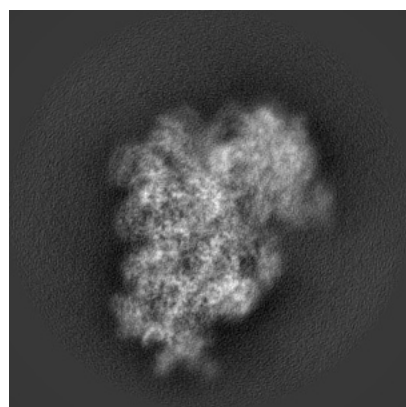


Y

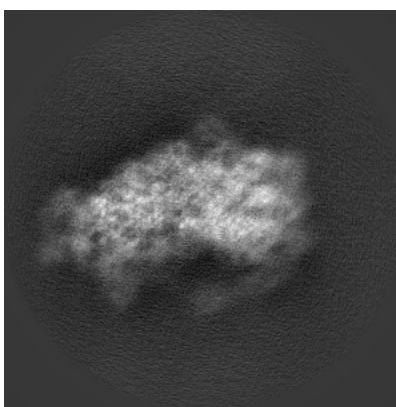


Z

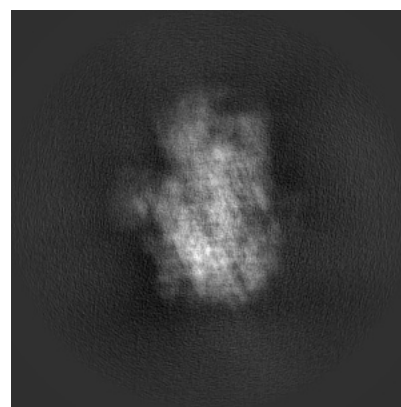
#### 6.1.2 Raw map



X



Y

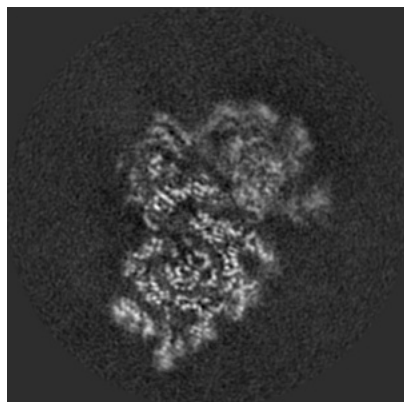


Z

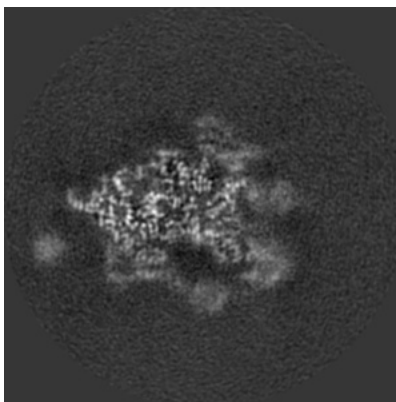
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

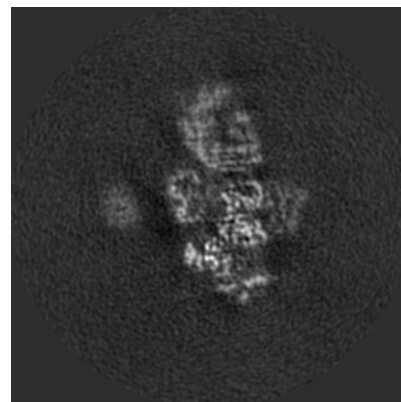
### 6.2.1 Primary map



X Index: 150

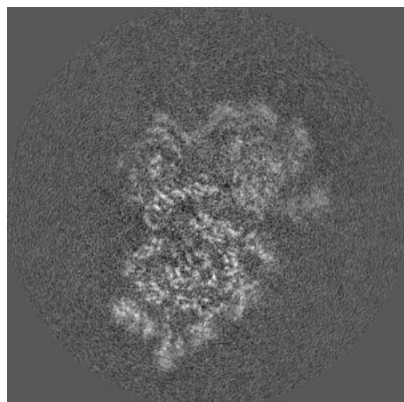


Y Index: 150

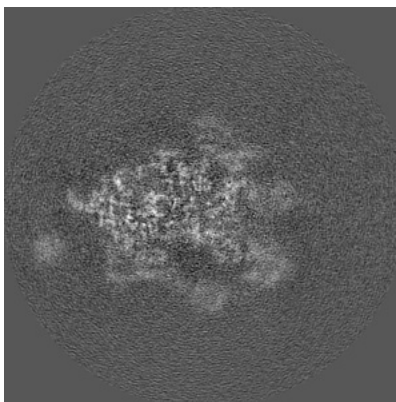


Z Index: 150

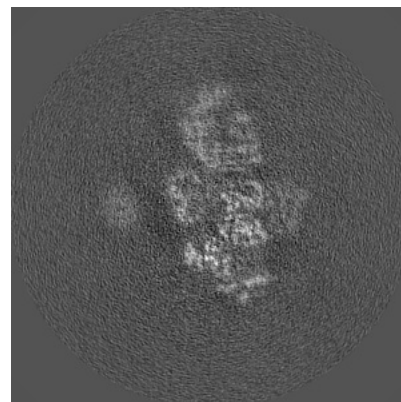
### 6.2.2 Raw map



X Index: 150



Y Index: 150



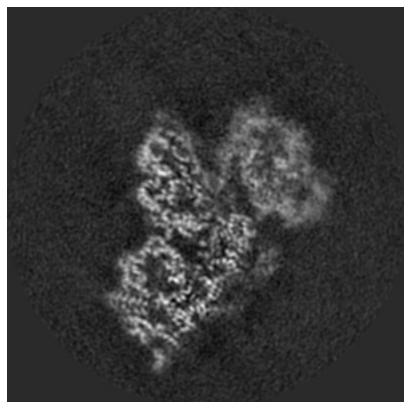
Z Index: 150

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

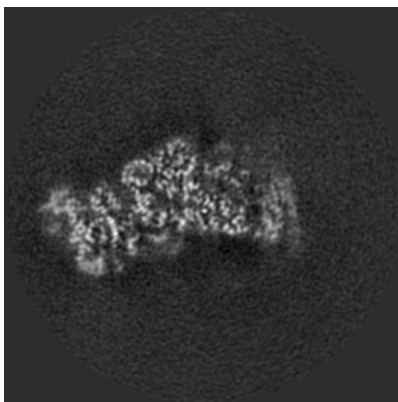


## 6.3 Largest variance slices [i](#)

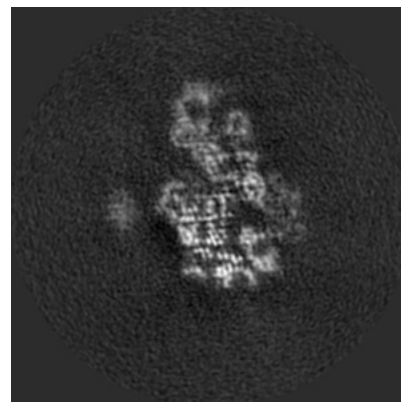
### 6.3.1 Primary map



X Index: 141

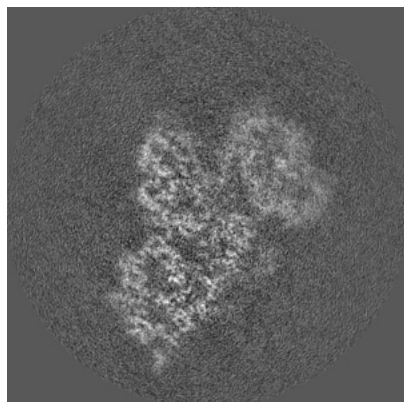


Y Index: 120

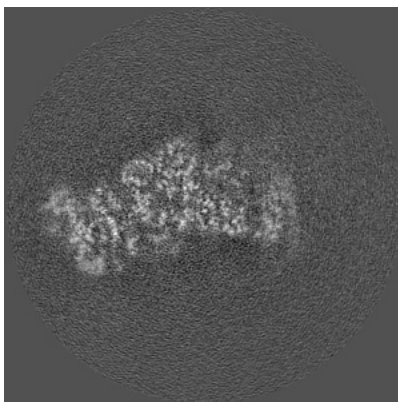


Z Index: 161

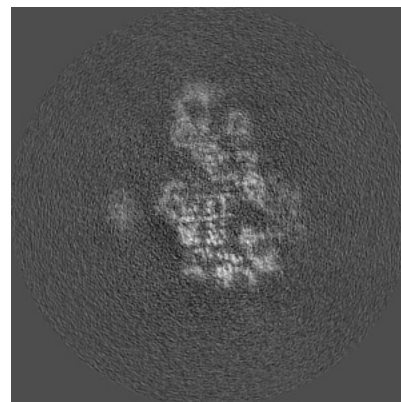
### 6.3.2 Raw map



X Index: 141



Y Index: 120



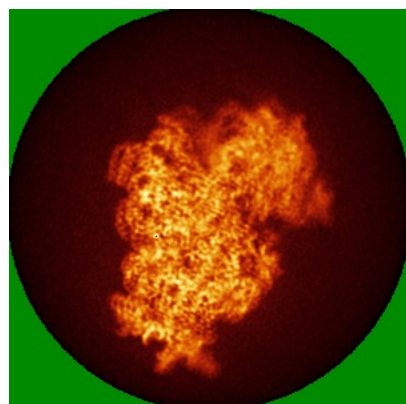
Z Index: 161

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

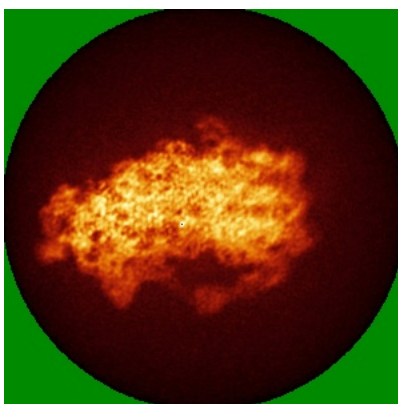


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

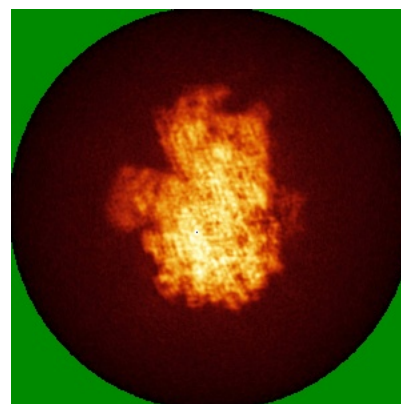
### 6.4.1 Primary map



X

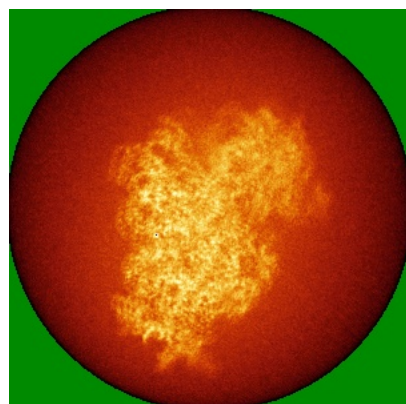


Y

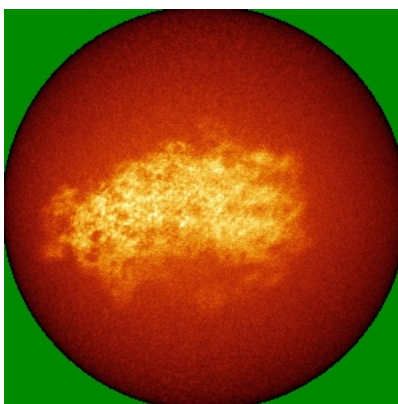


Z

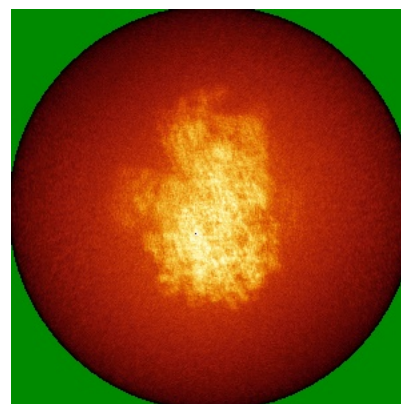
### 6.4.2 Raw map



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



X



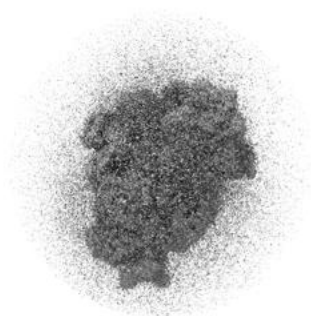
Y



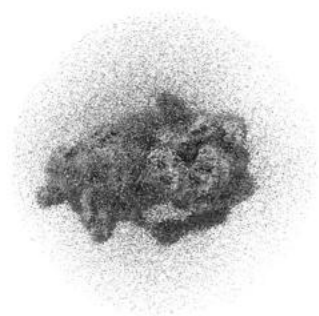
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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



X



Y



Z

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.

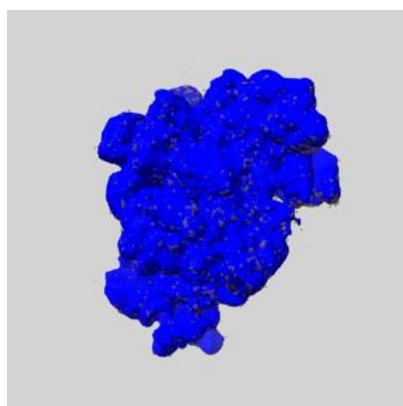
## 6.6 Mask visualisation [i](#)

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

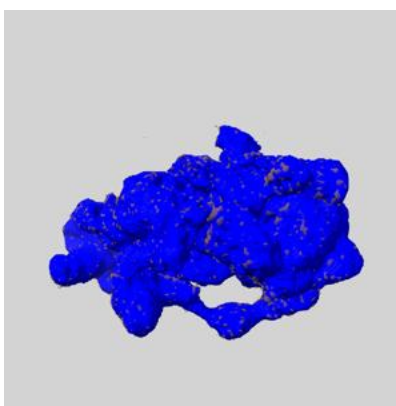
A mask typically either:

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

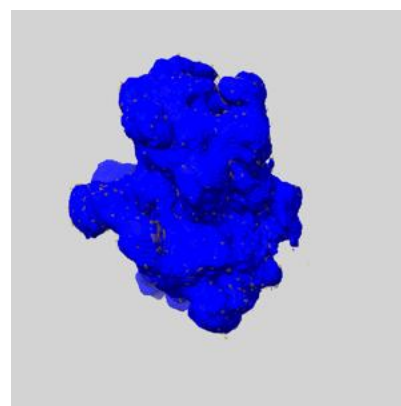
### 6.6.1 emd\_51964\_msk\_1.map [i](#)



X



Y

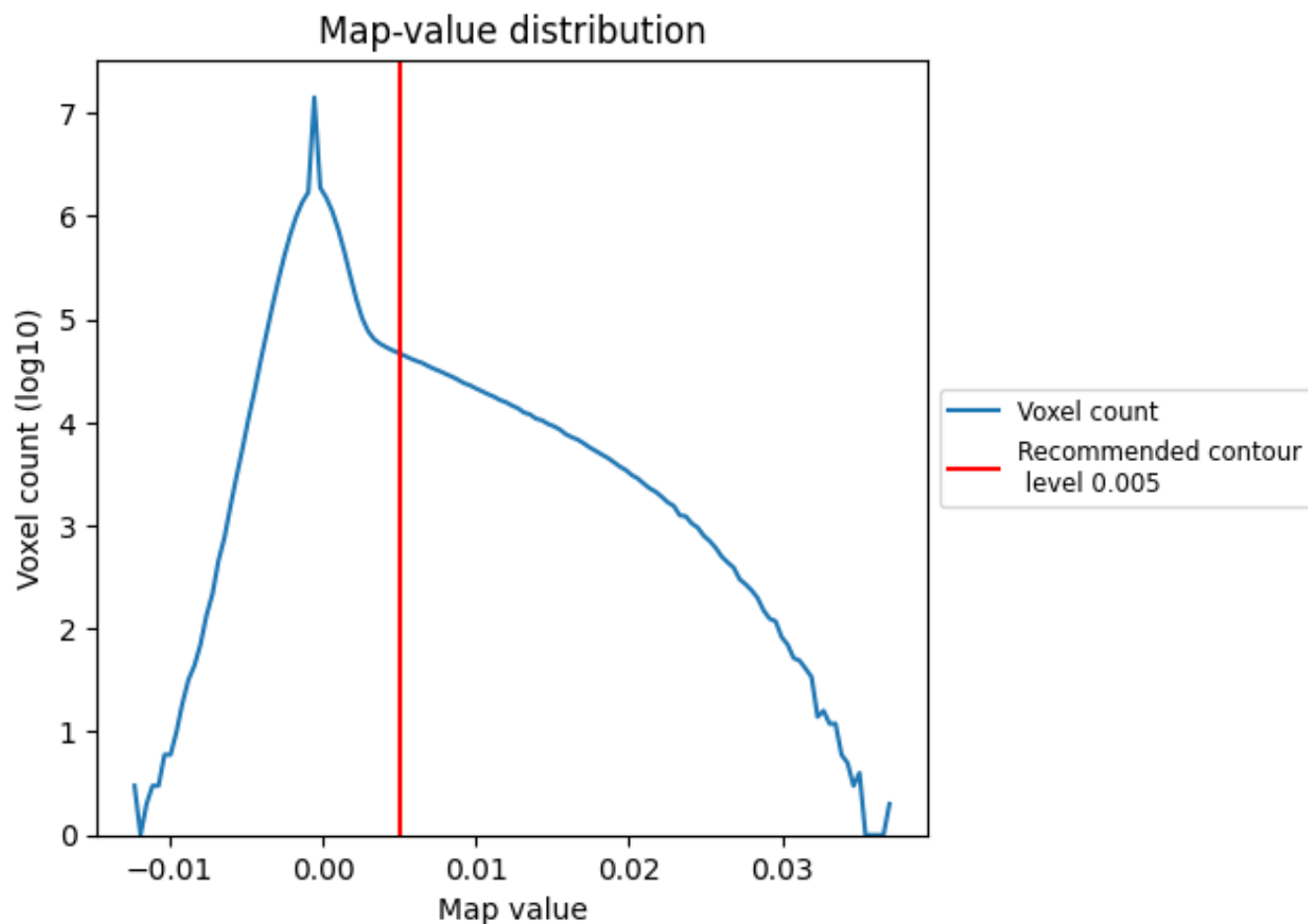


Z

## 7 Map analysis [i](#)

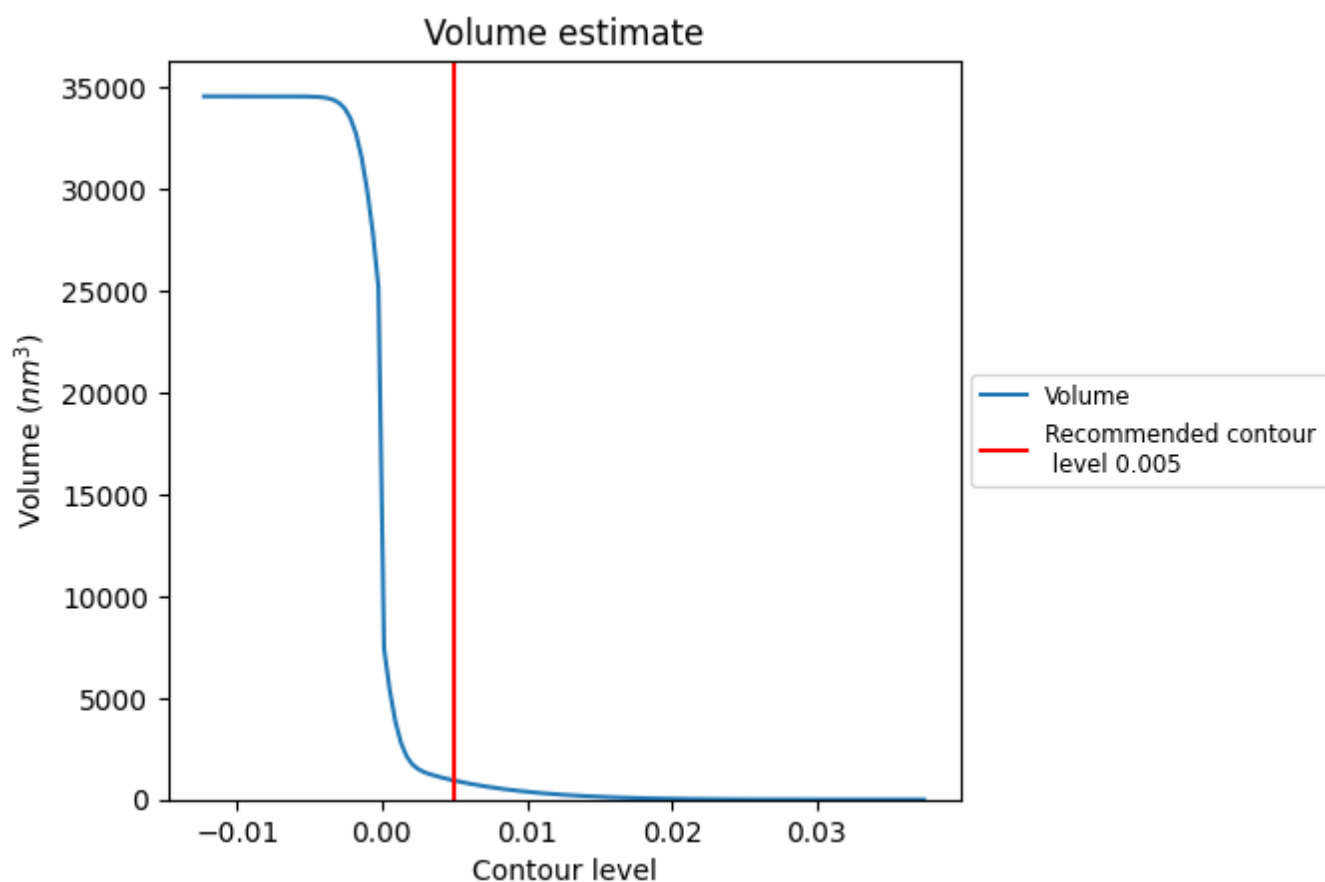
This section contains the results of statistical analysis of the map.

### 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.

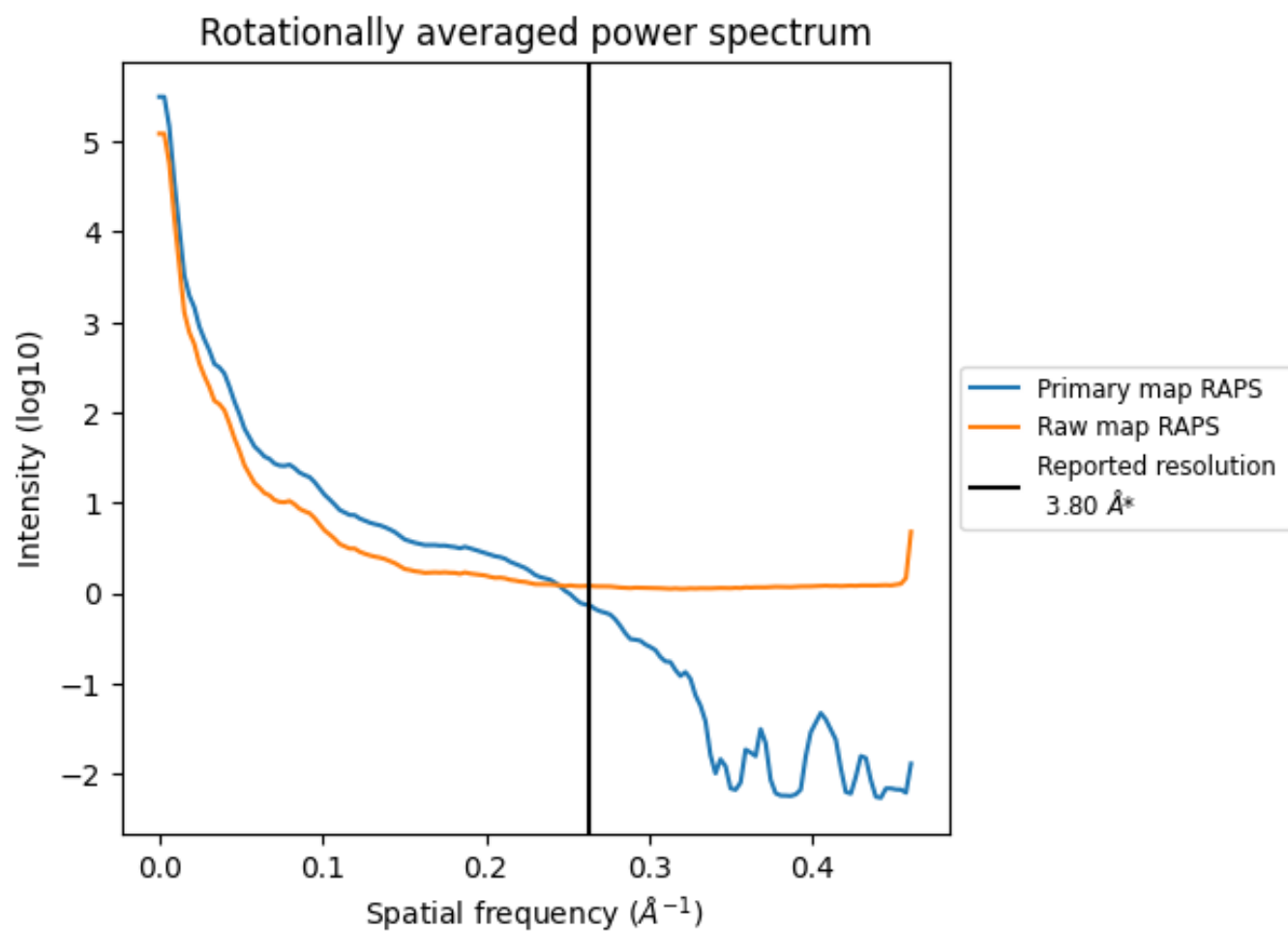
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 934 nm<sup>3</sup>; this corresponds to an approximate mass of 844 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 ⓘ

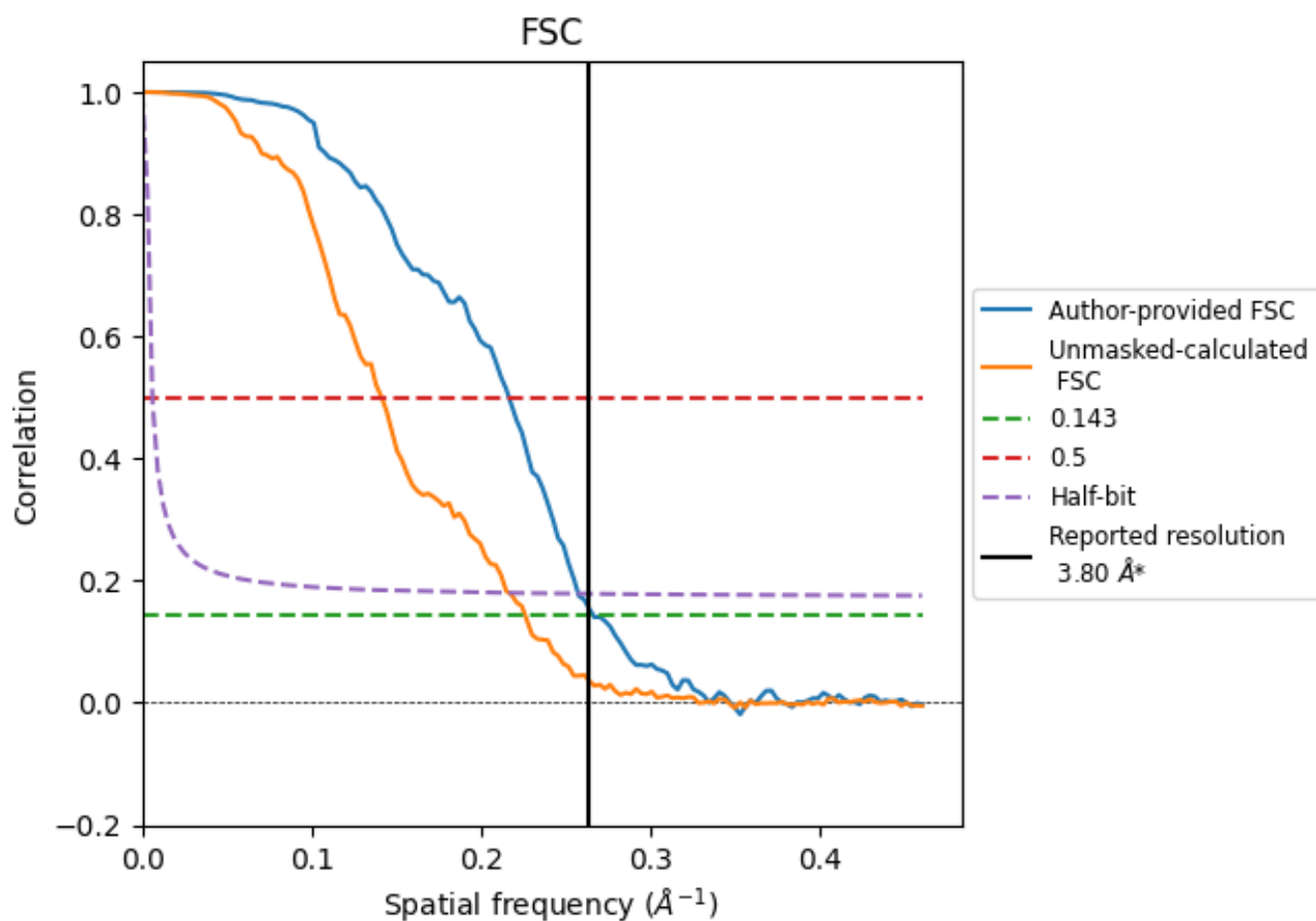


\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.75	4.62	3.89
Unmasked-calculated*	4.42	7.07	4.62

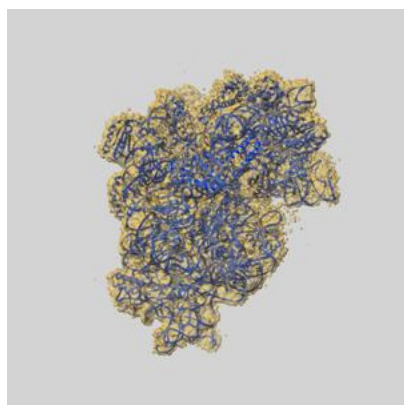
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.8 by more than 10 %



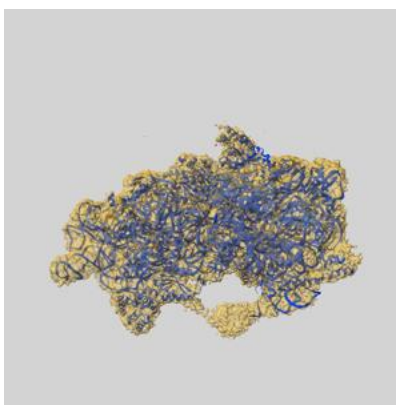
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51964 and PDB model 9H9H. Per-residue inclusion information can be found in section [3](#) on page [10](#).

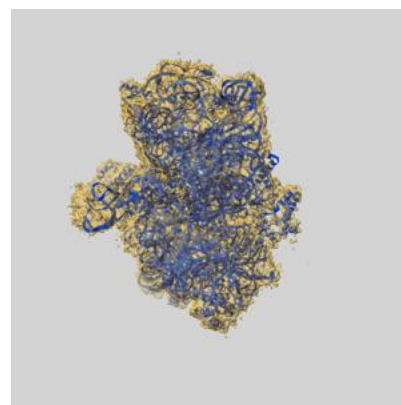
### 9.1 Map-model overlay [i](#)



X



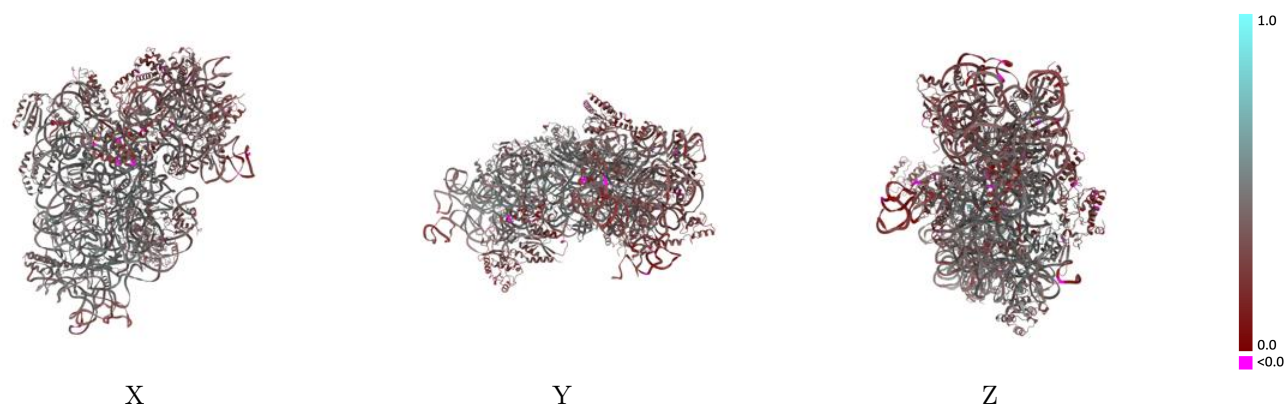
Y



Z

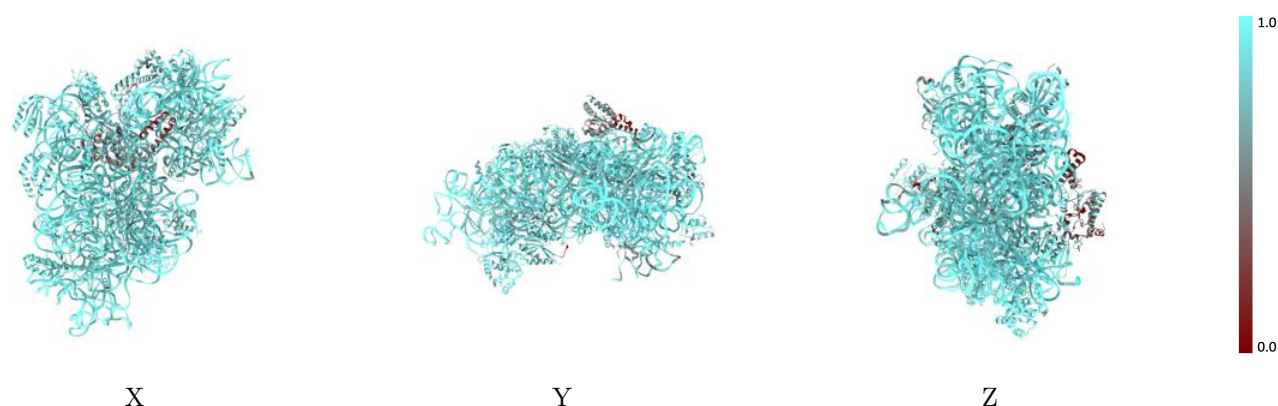
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



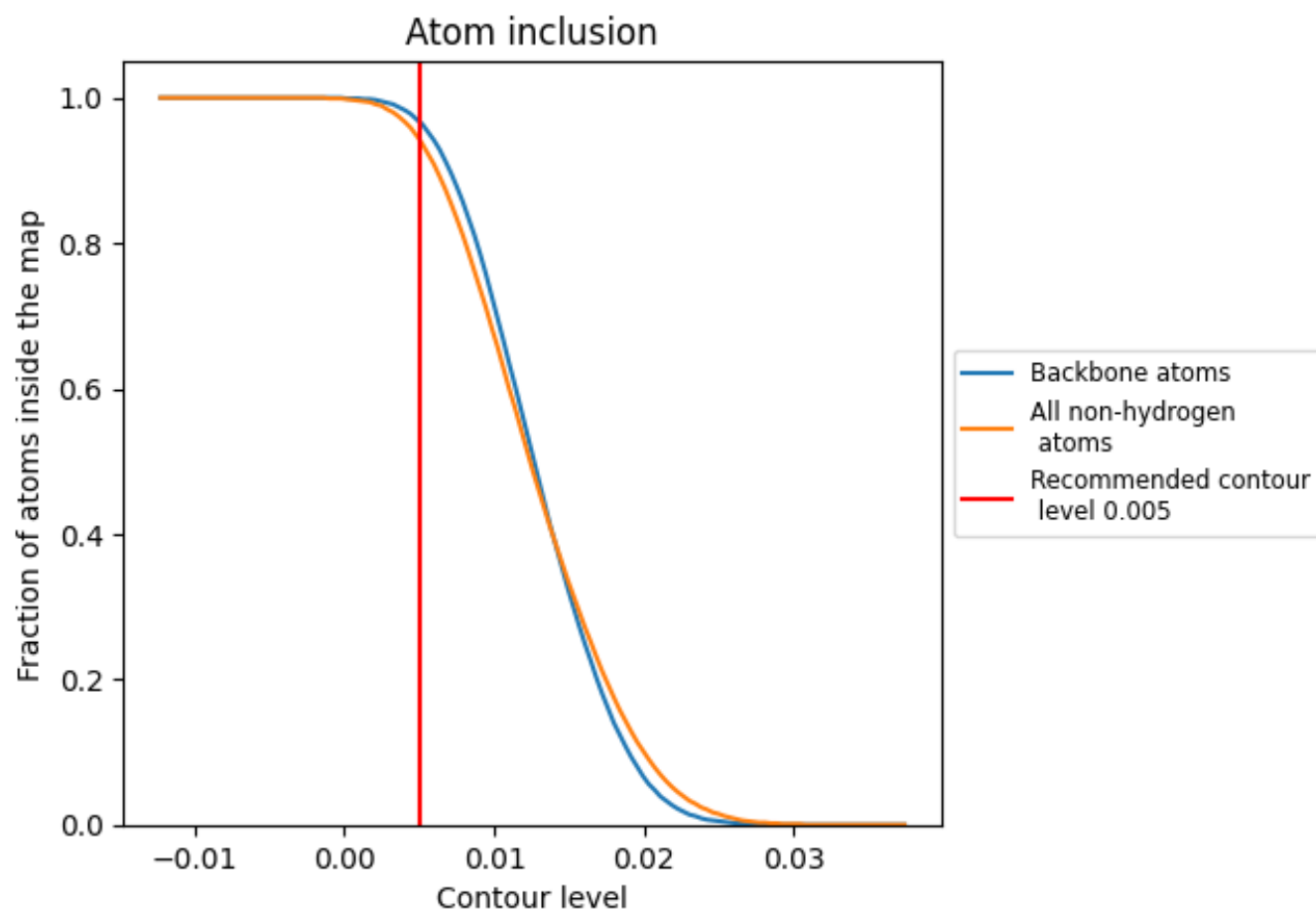
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.3920
2	 0.8980	 0.3100
3	 0.8670	 0.2470
A	 0.9910	 0.4200
B	 0.4820	 0.2690
C	 0.8870	 0.3820
D	 0.9480	 0.4200
E	 0.9440	 0.4470
F	 0.9510	 0.3890
G	 0.8140	 0.2440
H	 0.9530	 0.4520
I	 0.9530	 0.3450
J	 0.8520	 0.3360
K	 0.9460	 0.3840
L	 0.9360	 0.4690
M	 0.8870	 0.2790
N	 0.9520	 0.3660
O	 0.9590	 0.4220
P	 0.9550	 0.4650
Q	 0.9780	 0.4510
R	 0.9460	 0.4080
S	 0.8620	 0.3240
T	 0.9590	 0.4130
U	 0.8420	 0.3650
X	 0.9580	 0.4350
Y	 0.8720	 0.3030
Z	 0.8520	 0.3490

