



## wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 04:34 pm BST

PDB ID : 8CAS  
EMDB ID : EMD-16533  
Title : Cryo-EM structure of native Otu2-bound ubiquitinated 48S initiation complex (partial)  
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2023-01-24  
Resolution : 3.30 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](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:

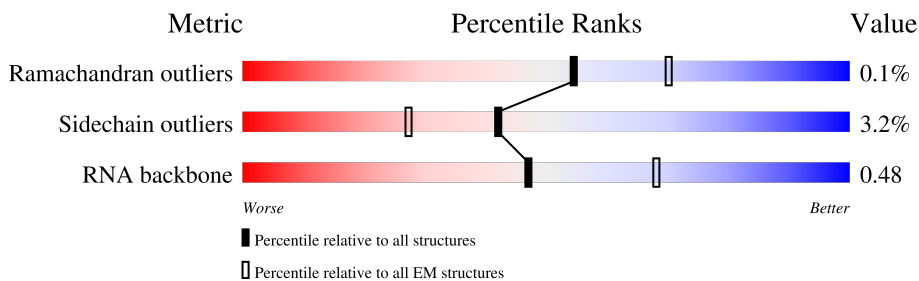
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



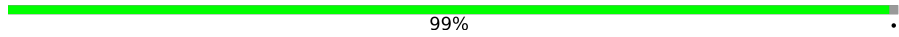
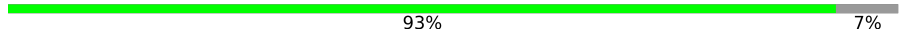
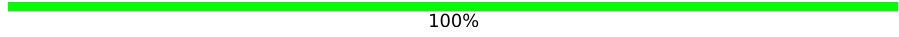
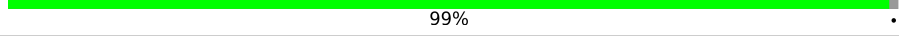
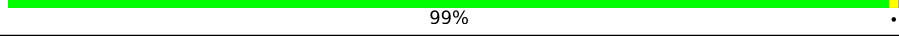
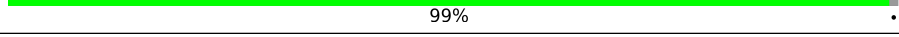

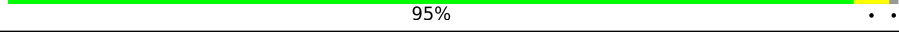
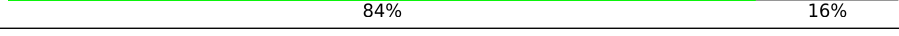

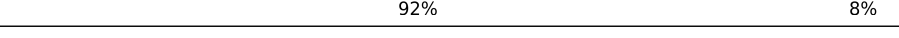
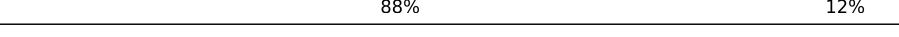

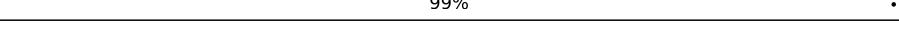

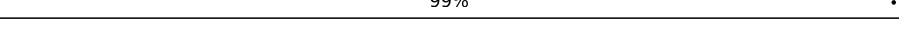
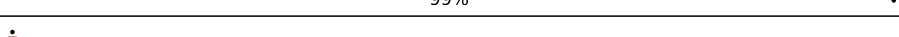

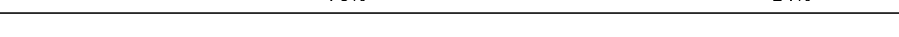



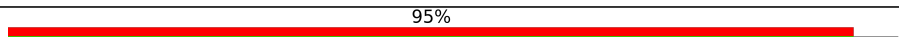


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	P	252	
2	Q	255	
3	R	254	
4	S	261	
5	T	236	
6	V	200	
7	W	197	
8	X	156	

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Mol	Chain	Length	Quality of chain
9	Y	151	 99%
10	Z	137	 93% 7%
11	a	87	 100%
12	b	130	 99%
13	c	145	 99%
14	d	135	 99%
15	e	119	 82% 18%
16	f	82	 26% 95%
17	g	63	 84% 16%
18	E	142	 82% 18%
19	B	240	 92% 8%
20	D	105	 88% 12%
21	F	143	 84% 15%
22	H	143	 99%
23	I	136	 89% 11%
24	J	146	 99%
25	K	144	 99%
26	L	121	 83% 17%
27	M	108	 6% 76% 24%
28	N	56	 95% 5%
29	O	76	 96%
30	h	319	 98%
31	i	67	 94% 6%
32	l	347	 95% 95% 5%
33	r	274	 19% 19% 81%

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Mol	Chain	Length	Quality of chain
34	1	75	61% 23% 16%
35	m	405	6% 36% 64%
36	o	964	13% 55% 45%
37	p	763	39% 84% 15%
38	q	812	16% 78% 22%
39	3	8	12% 88% 12%
40	A	153	65% 34%
41	k	608	75% 95% 5%
42	2	1800	65% 29%
43	C	225	92% 8%
44	y	76	7% 100%
45	n	25	72% 28%
46	j	304	35% 77% 5% 18%
47	G	527	50% 73% 25%
48	s	285	36% 44% 55%
49	x	307	84% 16%
50	U	190	89% 7%

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 86738 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	P	206	1020	608	206	206	0	0

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	Q	226	1119	667	226	226	0	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	R	216	1058	626	216	216	0	0

- Molecule 4 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	S	258	1267	751	258	258	0	0

- Molecule 5 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	T	228	1123	667	228	228	0	0

- Molecule 6 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	V	187	919	545	187	187	0	0

- Molecule 7 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	W	184	910	542	184	184	0	0

- Molecule 8 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	X	142	702	418	142	142	0	0

- Molecule 9 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Y	150	742	442	150	150	0	0

- Molecule 10 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	Z	127	620	366	127	127	0	0

- Molecule 11 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	a	87	429	255	87	87	0	0

- Molecule 12 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	b	129	634	376	129	129	0	0

- Molecule 13 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	c	144	704	416	144	144	0	0

- Molecule 14 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	d	134	Total	C	N	O	0	0
			661	393	134	134		

- Molecule 15 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	97	Total	C	N	O	0	0
			482	288	97	97		

- Molecule 16 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	81	Total	C	N	O	0	0
			400	238	81	81		

- Molecule 17 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 18 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	E	117	Total	C	N	O	0	0
			576	342	117	117		

- Molecule 19 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	B	222	Total	C	N	O	0	0
			1093	649	222	222		

- Molecule 20 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	D	92	Total	C	N	O	0	0
			456	272	92	92		

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms			AltConf	Trace	
21	F	121	Total	C	N	O	0	0
			595	353	121	121		

- Molecule 22 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
22	H	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 23 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
23	I	121	Total	C	N	O	0	0
			600	358	121	121		

- Molecule 24 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
24	J	145	Total	C	N	O	0	0
			715	425	145	145		

- Molecule 25 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
25	K	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms			AltConf	Trace	
26	L	100	Total	C	N	O	0	0
			496	296	100	100		

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
27	M	82	Total	C	N	O	0	0
			407	243	82	82		

- Molecule 28 is a protein called RPS29A isoform 1.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	N	53	Total	C	N	O	0	0
			260	154	53	53		

- Molecule 29 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	O	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 30 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	h	312	Total	C	N	O	0	0
			1538	914	312	312		

- Molecule 31 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	i	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 32 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	l	330	Total	C	N	O	0	0
			1624	964	330	330		

- Molecule 33 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 34 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 35 is a protein called TIF5 isoform 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
35	m	147	Total	C	N	O	0	0
			726	432	147	147		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
36	o	529	Total	C	N	O	0	0
			2632	1574	529	529		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms			AltConf	Trace	
37	p	646	Total	C	N	O	0	0
			3201	1909	646	646		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms			AltConf	Trace	
38	q	636	Total	C	N	O	0	0
			3169	1897	636	636		

- Molecule 39 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
39	3	8	Total	C	N	O	P	0	0
			171	77	32	54	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms			AltConf	Trace	
40	A	101	Total	C	N	O	0	0
			497	295	101	101		

- Molecule 41 is a protein called RLI1 isoform 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
41	k	579	Total	C	N	O	0	0
			2860	1702	579	579		

- Molecule 42 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	2	1763	37577	16799	6661	12354	1763	0	0

- Molecule 43 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	C	206	1020	608	206	206	0	0

- Molecule 44 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	y	76	374	222	76	76	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	19	PRO	SER	conflict	UNP P0CH08
y	24	GLU	ASP	conflict	UNP P0CH08
y	28	ALA	SER	conflict	UNP P0CH08

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	n	18	175	107	48	19	1	0	0

- Molecule 46 is a protein called SUI2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	j	249	2006	1283	333	382	8	0	0

- Molecule 47 is a protein called protein-synthesizing GTPase.

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

- Molecule 48 is a protein called SUI3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	s	128	1036	661	186	182	7	0	0

- Molecule 49 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	x	259	1289	770	259	260	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	178	SER	CYS	engineered mutation	UNP P38747

- Molecule 50 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	U	184	1473	946	263	264	0	0

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	N	1	Total 1	Zn 1	0
51	O	1	Total 1	Zn 1	0
51	m	1	Total 1	Zn 1	0
51	s	1	Total 1	Zn 1	0

- Molecule 52 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	k	1	27	10	5	10	2	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

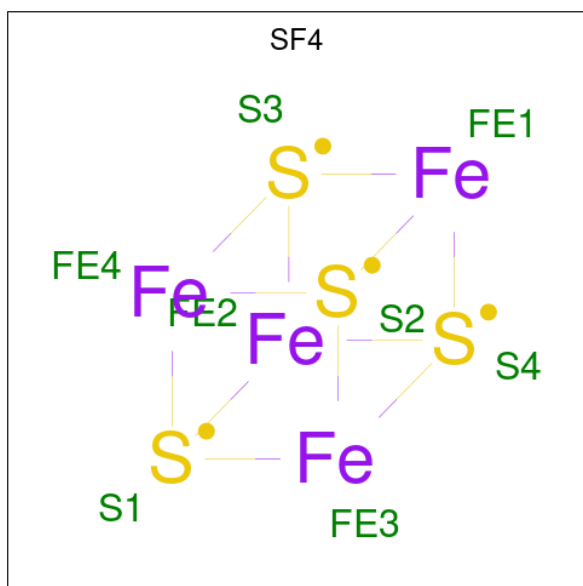
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	k	2	2	2	0
53	2	2	2	2	0
53	G	1	1	1	0

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



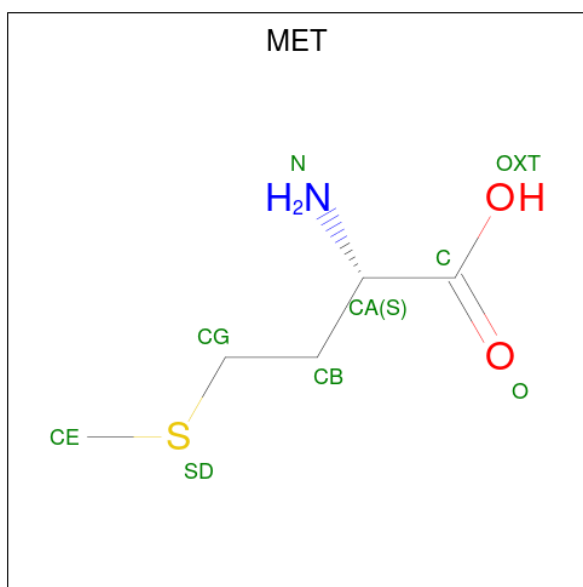
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	k	1	31	10	5	13	3	0

- Molecule 55 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



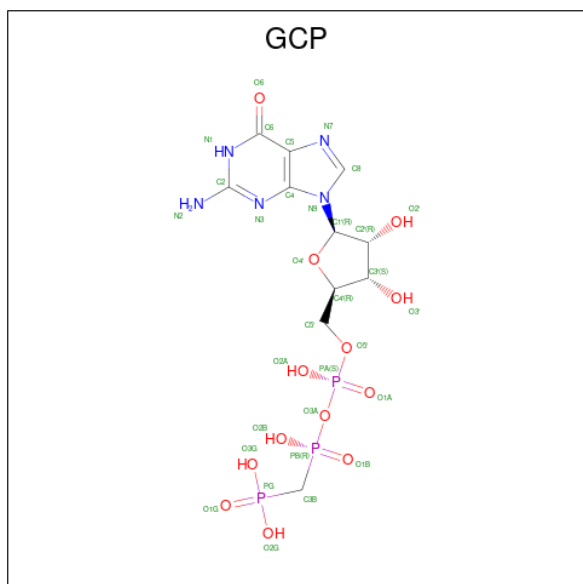
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
55	k	1	8	4	4	0
55	k	1	8	4	4	0

- Molecule 56 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
56	G	1	8	5	1	1	1	0

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).

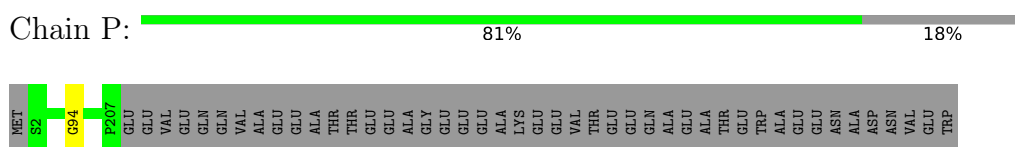


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	G	1	32	11	5	13	3	0

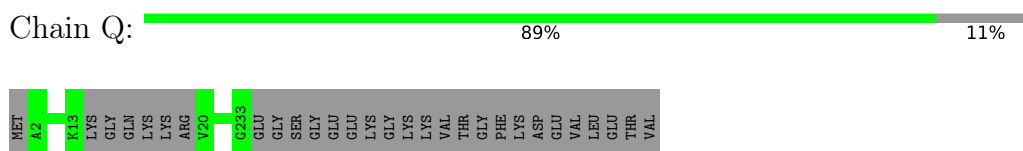
### 3 Residue-property plots [i](#)

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.

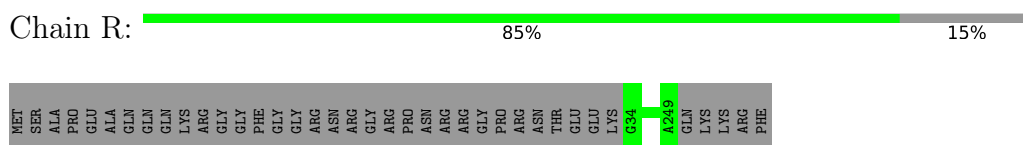
- Molecule 1: 40S ribosomal protein S0-A



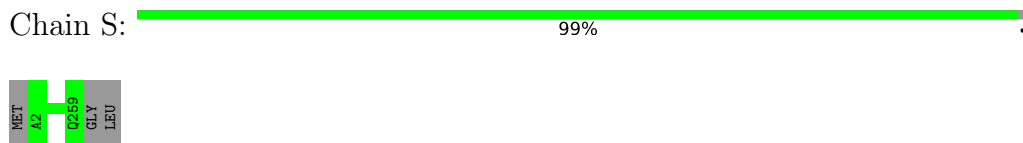
- Molecule 2: 40S ribosomal protein S1-A



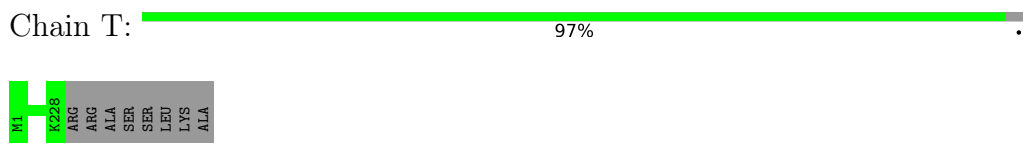
- Molecule 3: 40S ribosomal protein S2



- Molecule 4: 40S ribosomal protein S4-B



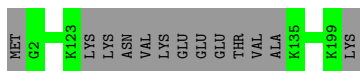
- Molecule 5: 40S ribosomal protein S6-B



- Molecule 6: 40S ribosomal protein S8-A

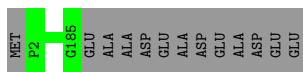


Chain V:  94% 6%



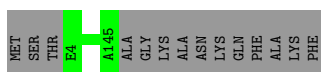
- Molecule 7: 40S ribosomal protein S9-A

Chain W:  93% 7%



- Molecule 8: 40S ribosomal protein S11-A

Chain X:  91% 9%



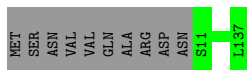
- Molecule 9: 40S ribosomal protein S13

Chain Y:  99% .



- Molecule 10: 40S ribosomal protein S14-A

Chain Z:  93% 7%



- Molecule 11: 40S ribosomal protein S21-A

Chain a:  100%

There are no outlier residues recorded for this chain.

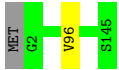
- Molecule 12: 40S ribosomal protein S22-A

Chain b:  99% .



- Molecule 13: 40S ribosomal protein S23-A

Chain c:  99% ..



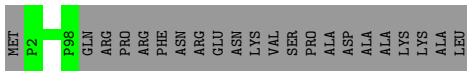
- Molecule 14: 40S ribosomal protein S24-A

Chain d: 99%



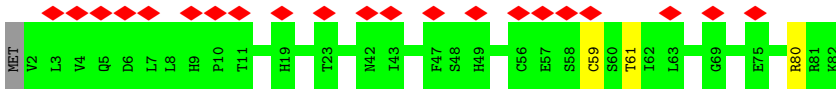
- Molecule 15: 40S ribosomal protein S26-A

Chain e: 82%



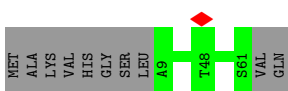
- Molecule 16: 40S ribosomal protein S27-A

Chain f: 26%



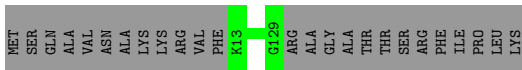
- Molecule 17: 40S ribosomal protein S30-A

Chain g: 84%



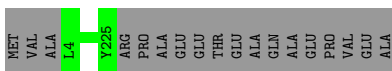
- Molecule 18: RPS15 isoform 1

Chain E: 82%



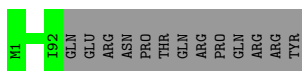
- Molecule 19: 40S ribosomal protein S3

Chain B: 92%

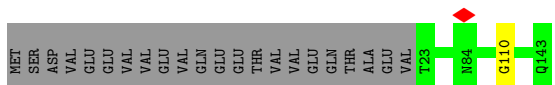
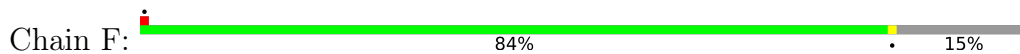


- Molecule 20: 40S ribosomal protein S10-A

Chain D: 88%



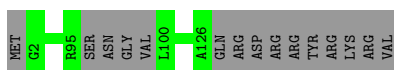
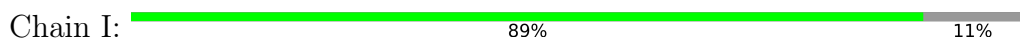
- Molecule 21: 40S ribosomal protein S12



- Molecule 22: 40S ribosomal protein S16-A



- Molecule 23: 40S ribosomal protein S17-A



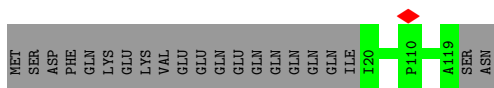
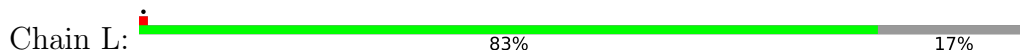
- Molecule 24: 40S ribosomal protein S18-A



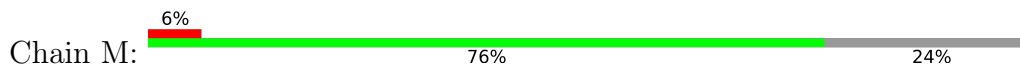
- Molecule 25: 40S ribosomal protein S19-A

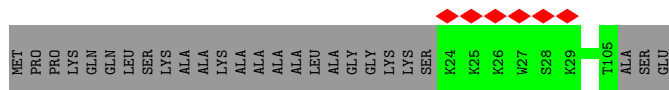


- Molecule 26: 40S ribosomal protein S20

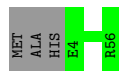


- Molecule 27: 40S ribosomal protein S25-A





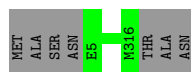
- Molecule 28: RPS29A isoform 1



- Molecule 29: 40S ribosomal protein S31



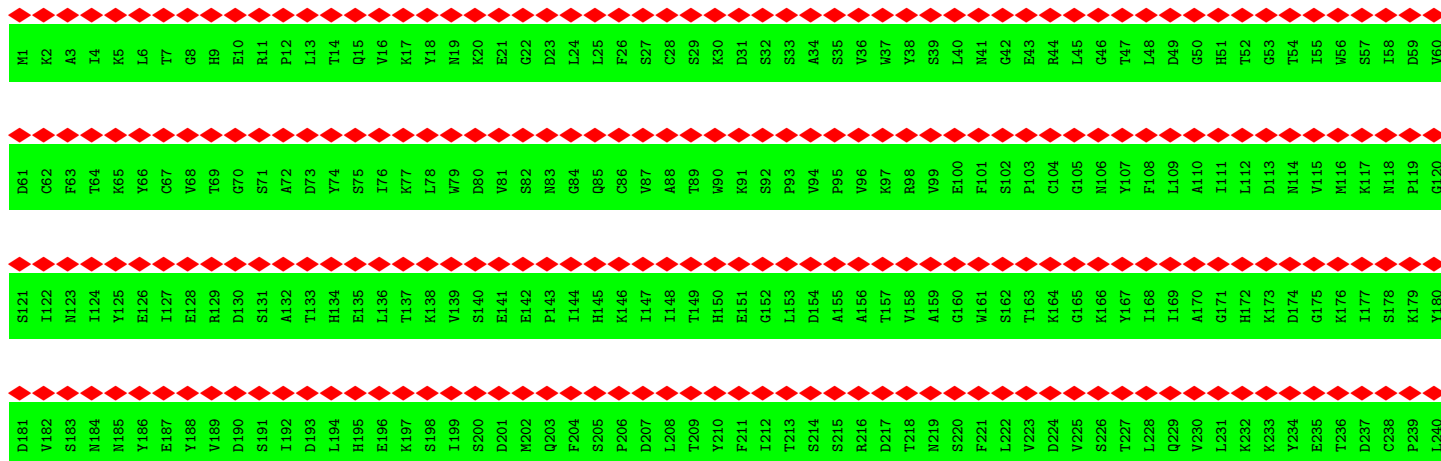
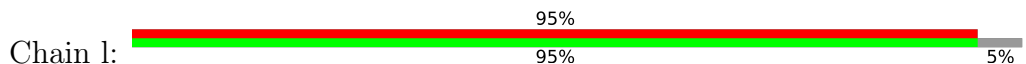
- Molecule 30: Guanine nucleotide-binding protein subunit beta-like protein

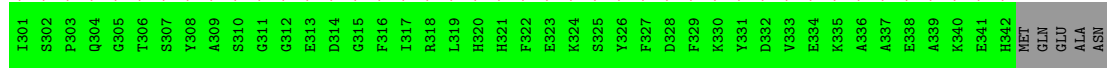
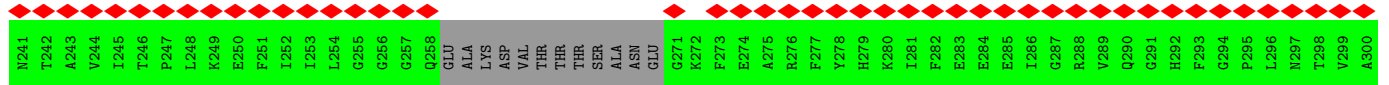


- Molecule 31: 40S ribosomal protein S28-A

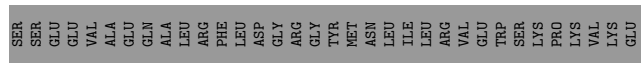
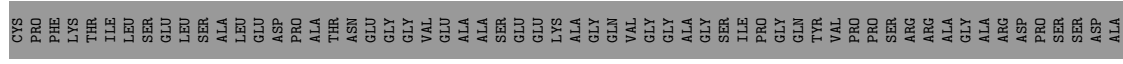
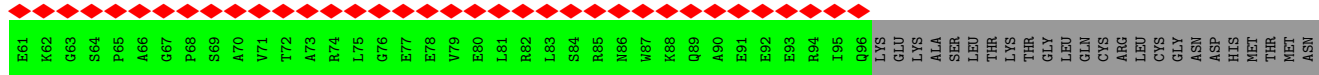


- Molecule 32: Eukaryotic translation initiation factor 3 subunit I

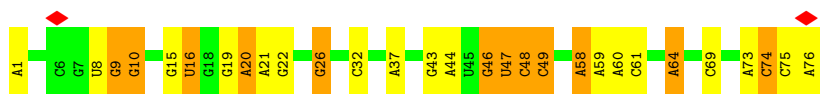




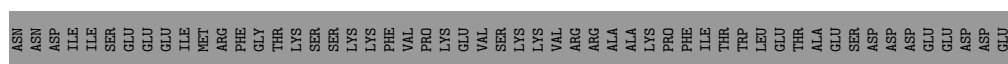
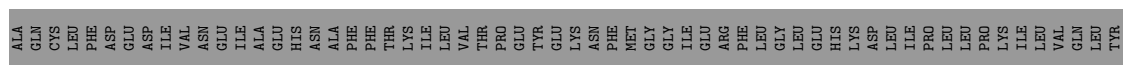
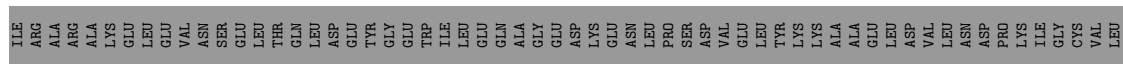
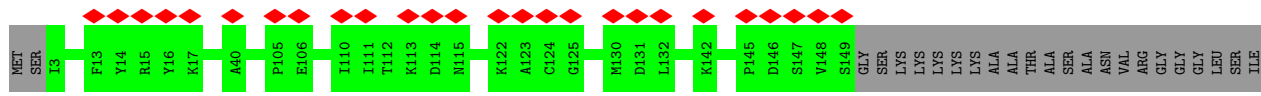
• Molecule 33: Eukaryotic translation initiation factor 3 subunit G



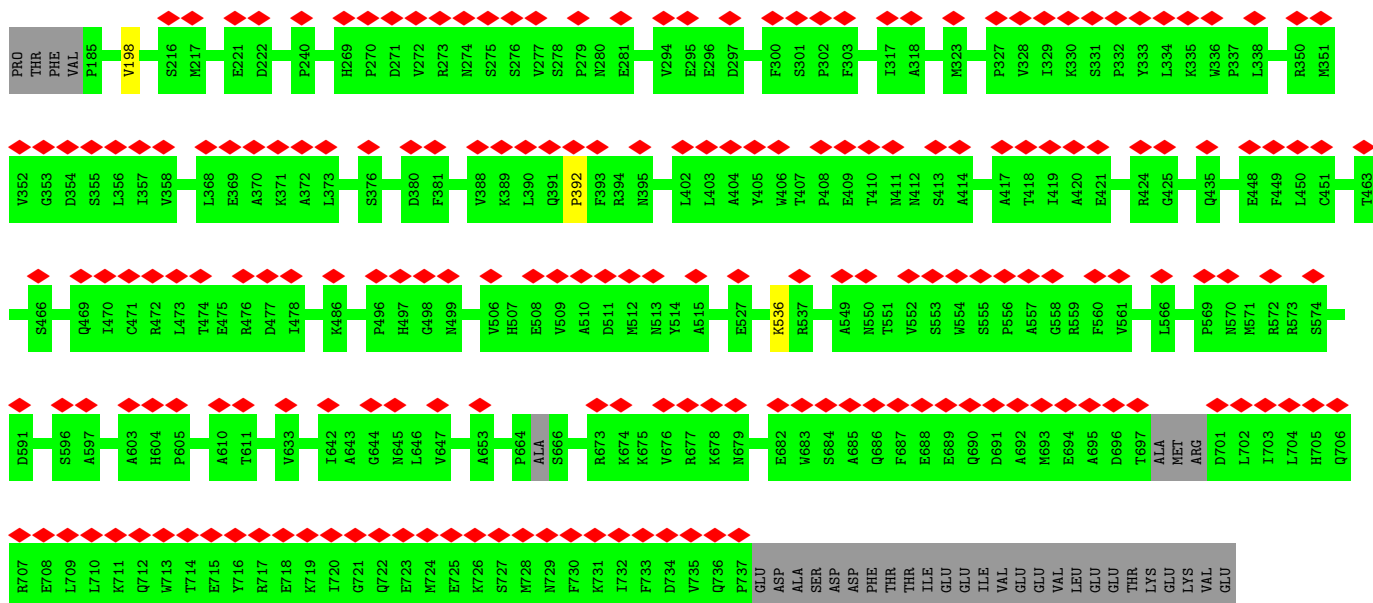
• Molecule 34: tRNA



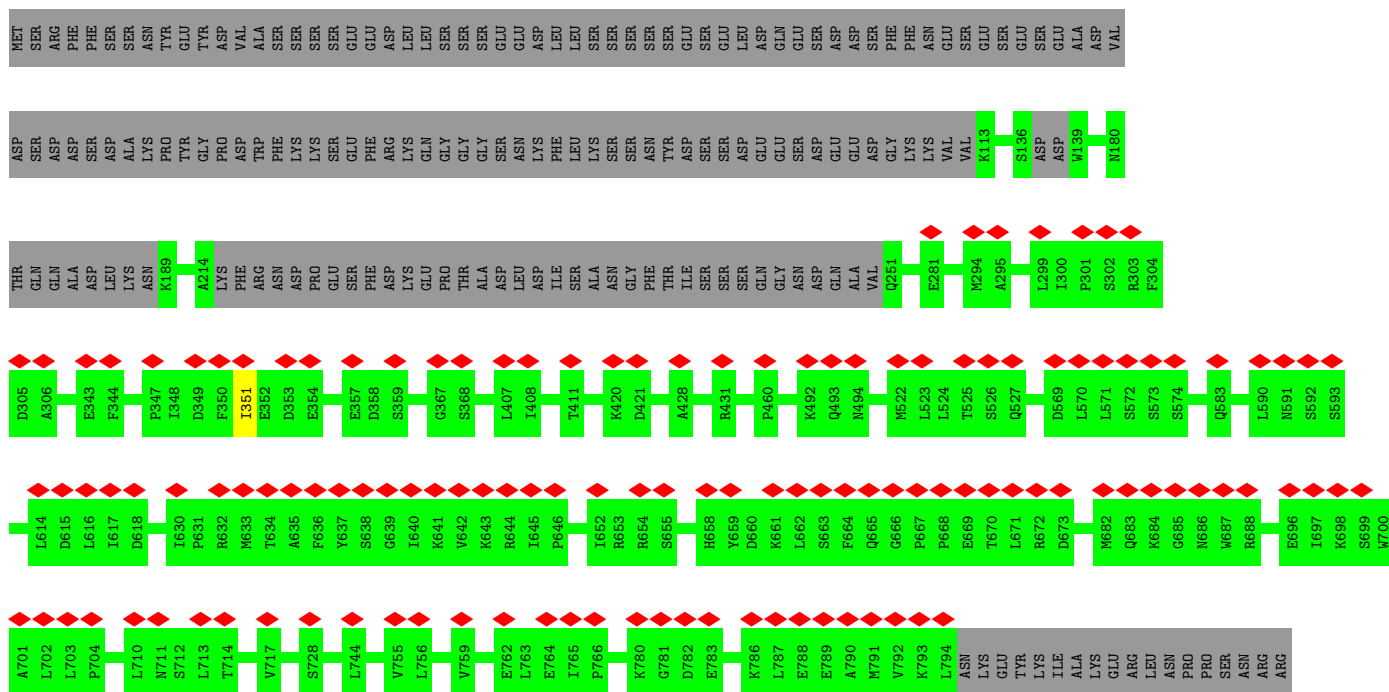
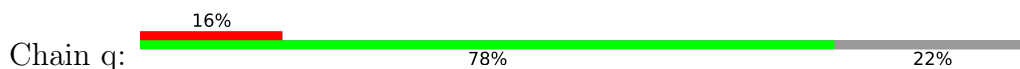
• Molecule 35: TIF5 isoform 1



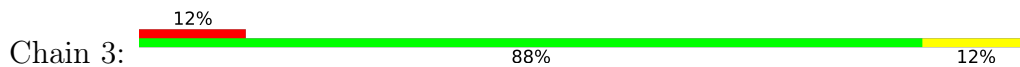




• Molecule 38: Eukaryotic translation initiation factor 3 subunit C



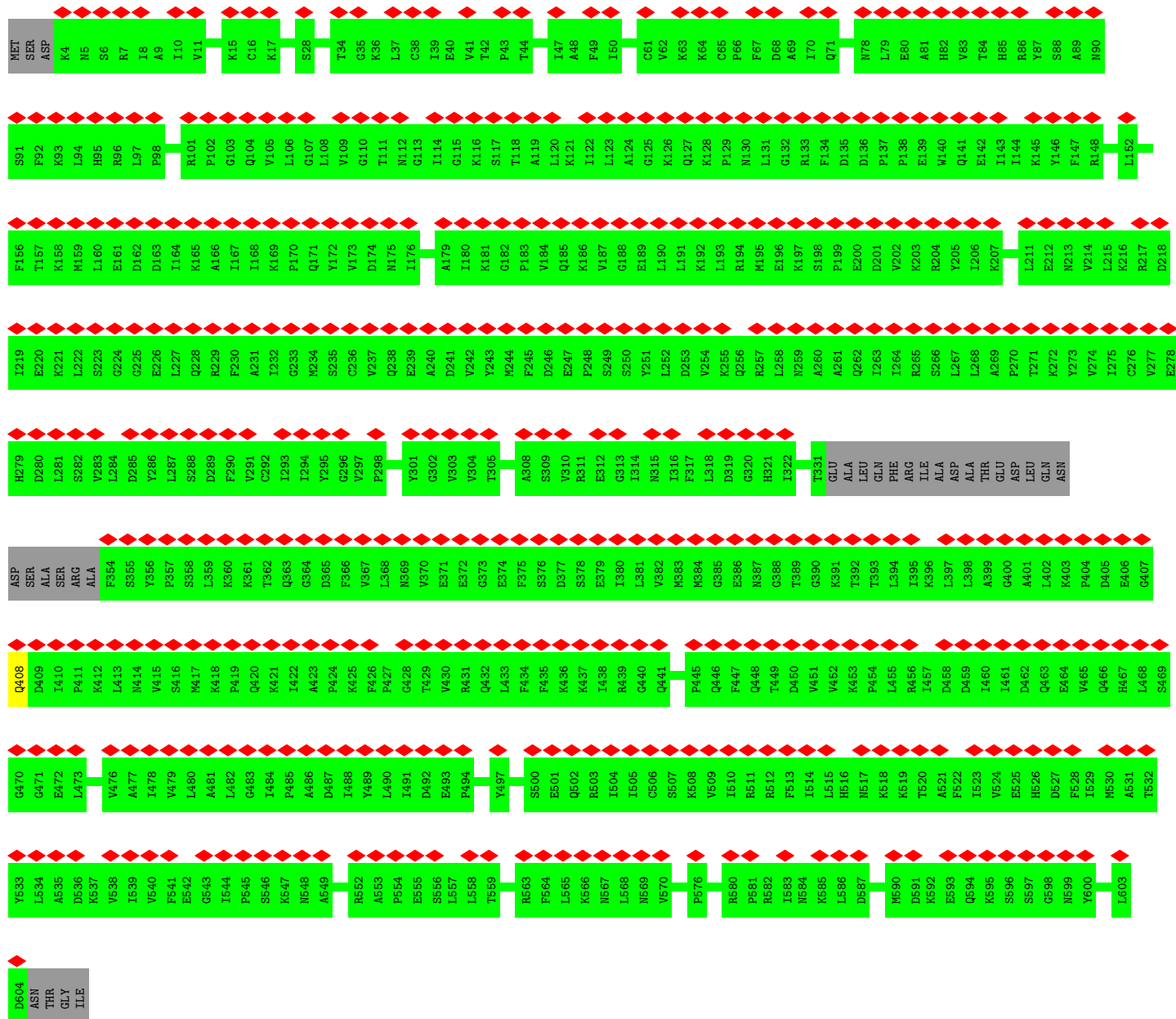
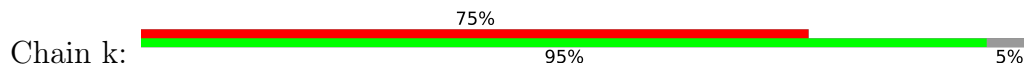
• Molecule 39: mRNA



• Molecule 40: Eukaryotic translation initiation factor 4C



• Molecule 41: RLI1 isoform 1



• Molecule 42: 18S ribosomal RNA



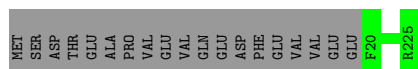


U1535	G1536	C1537	G1540	A1543	U1544	G1545	U1557	A1558	U1559	U1560	U1566	A1570	C1571	G1572	A1573	G1574	G1575	A1576	A1583	G1584	G1590	G1596	G1601	C1602	A1611	A1614	G1615	G1616	C1619	C1620	U1621	G1622	A1631	C1632	A1633	C1634	A1635	C1636	C1637	U1657	G1658	C1674	A1678						
U1307	G1308	U1314	U1315	G1316	C1317	G1318	A1321	A1322	A1325	C1332	G1344	A1345	A1346	U1347	A1348	G1349	G1354	C1355	A1360	U1361	U1362	U1363	G1364	G1367	U1370	A1371	U1372	C1373	A1382	G1383	C1389	U1390	U1398	C1399	A1400	A1401	G1402	A1410	G1411	G1412	U1413	U1414	G1418	A1421					
G1170	U1182	U1185	A1194	C1195	A1196	G1199	U1200	G1201	A1202	U1207	A1208	G1212	G1213	U1214	A1217	G1218	A1226	A1227	G1228	G1229	C1236	G1241	A1242	G1243	A1244	G1245	C1246	U1247	U1251	C1252	A1256	U1257	U1258	G1273	C1274	A1275	C1284	U1285	U1286	G1291	U1301								
U1028	U1029	A1030	C1033	A1039	U1052	G1053	U1058	U1059	U1060	A1061	U1063	C1066	C1075	A1076	C1077	U1080	A1081	C1082	U1092	C1096	U1097	U1098	G1100	A1108	A1113	C1121	C1134	A1138	A1139	U1145	G1150	C1156	A1157	C1158	G1159	A1160	G1164	G1167											
G901	G902	U903	U912	G913	U916	U917	U918	U919	U928	A929	U932	A934	C934	U935	G942	U945	A951	U959	U960	A963	U964	U965	A966	A970	A971	A988	A992	A993	U996	A998	A1003	U1004	A1005	U1012	A1020	C1021	C1022	A1023	U1024	A1026	A1027								
U698	U699	C700	U701	G702	U703	C704	U705	A706	A707	C708	U709	A791	U710	U711	G712	U713	A714	U715	U716	U717	U718	U726	U727	U728	G729	U730	C731	G732	U733	A734	C735	C736	A737	G738	U739	C740	U742	U743	U745	A755	A756	U758	U765	U767	A774	G775			
G778	U779	A780	U781	U782	G783	G787	U790	A791	U792	A812	U813	A814	C815	G816	U819	U820	U821	U822	G823	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U846	C849	A850	U851	C852	A855	A856	U857	U861	A862	U864	U876	U886	U893	G899					
A520	A525	A526	A527	C530	C531	A534	A538	G539	G540	A541	A542	C543	A544	A545	U546	U547	G548	G549	A550	G551	A555	A556	A557	U558	C565	G568	G569	C572	A579	A580	C583	A594	G595	U598	A606	G607	U608	U609	G610	U611	C614	U617	U618	A619					
A620	A621	A623	A624	C625	U626	U633	G634	A635	U638	U639	U640	A641	C642	C643	C644	C645	U648	G649	C653	C654	G655	U657	C658	C659	C664	C665	C668	C676	C677	A678	U679	U680	U681	C682	U686	U689	U691	C692	C693	C694	C697								
C435	A436	U439	C444	A445	A446	U447	C448	A452	U453	U454	G459	A460	C461	A464	A468	C469	A470	A471	U472	A485	G486	U487	A490	C491	A492	U493	C494	C495	C496	C497	G498	U499	C500	U501	G422	C423	C424	A425	C426	C427	A428	C431	C432	C433	C434				
U121	A126	G127	U128	U129	C	C	U	U	U	A	C	U	A138	C139	A140	U141	G142	U143	A144	A147	A148	C149	U155	U159	C160	U161	C166	A169	U170	A171	C172	U178	A179	A180	C184	U185	C186	A188	C189	C190	C191	U192	U193	U194	G195	U216	A217	A218	A219
A220	U223	C224	U225	A226	U227	G228	C230	U231	U232	C233	G234	G235	A236	C237	A240	U241	G243	C250	A257	C258	U259	U260	U261	U267	C268	A269	U270	C273	C274	C275	C276	U277	U278	C279	C281	U282	U283	G287	A299	U302	C309	U313	C314	A315	A316				
G322	A323	G330	G334	G337	C338	A352	A353	C354	A359	A360	C361	A370	G373	C381	A385	G386	C388	C393	C394	A400	A401	A402	G403	G404	C405	C411	C415	A416	A417	G418	G419	U422	C423	C424	A425	G426	C427	A428	C431	C432	C433	C434	G435						

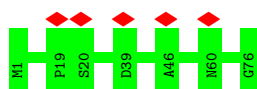


A

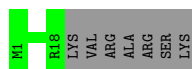
- Molecule 43: 40S ribosomal protein S5



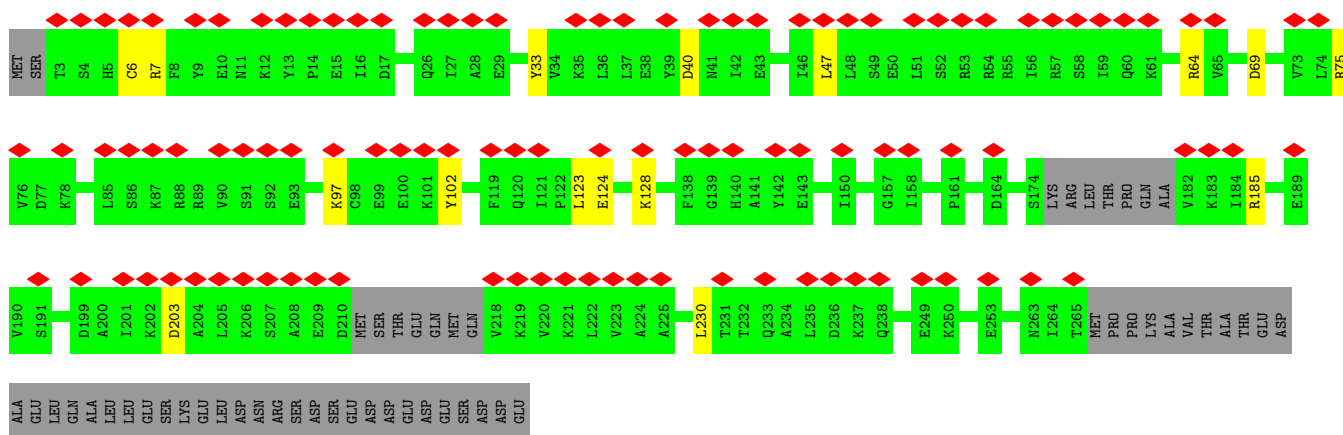
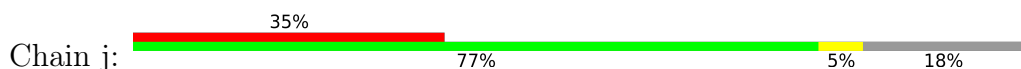
- Molecule 44: 60S ribosomal protein L40-A



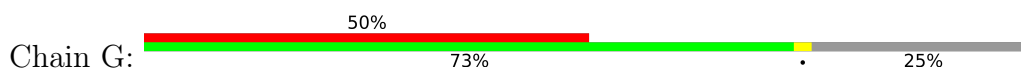
- Molecule 45: 60S ribosomal protein L41-A

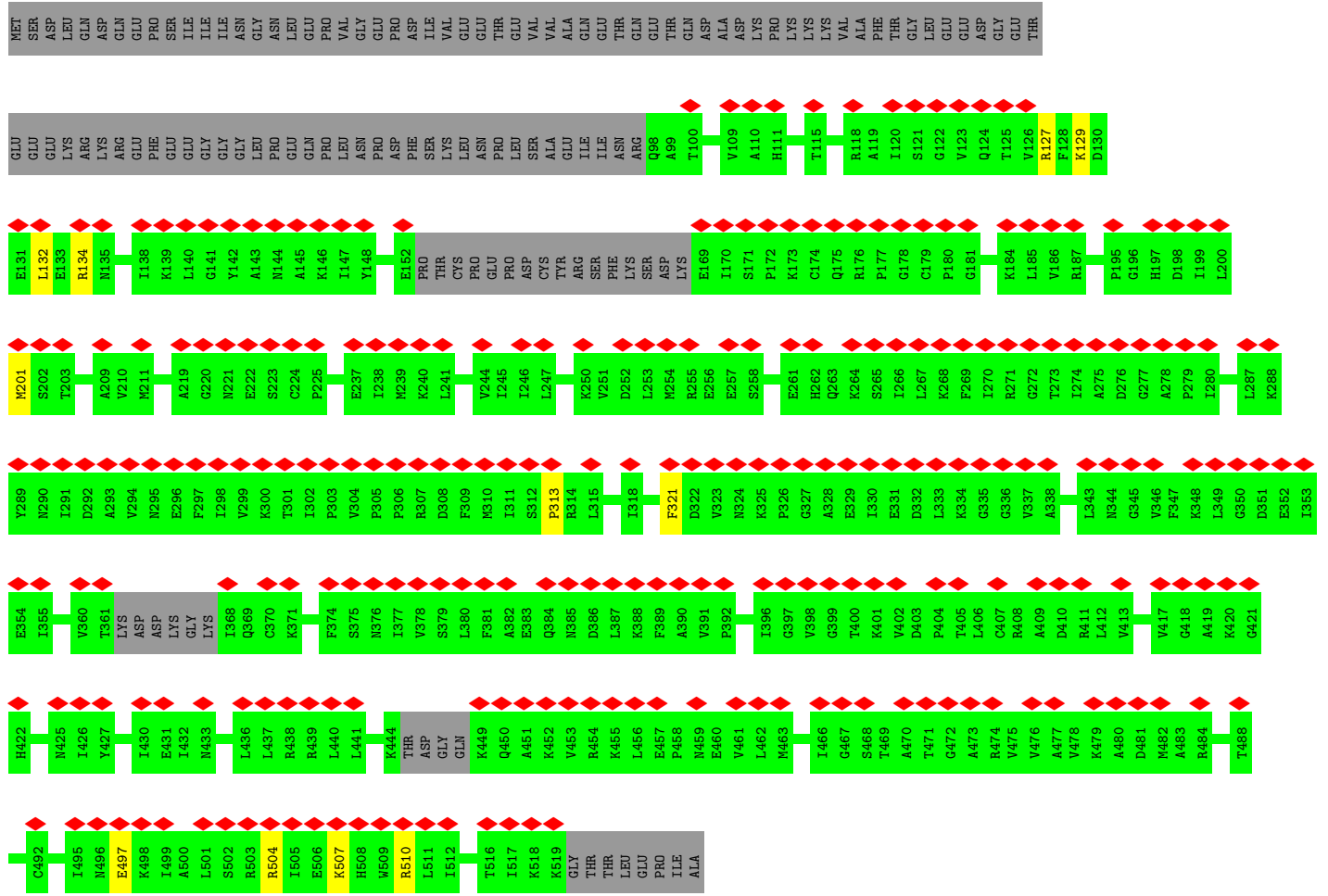


- Molecule 46: SUI2 isoform 1

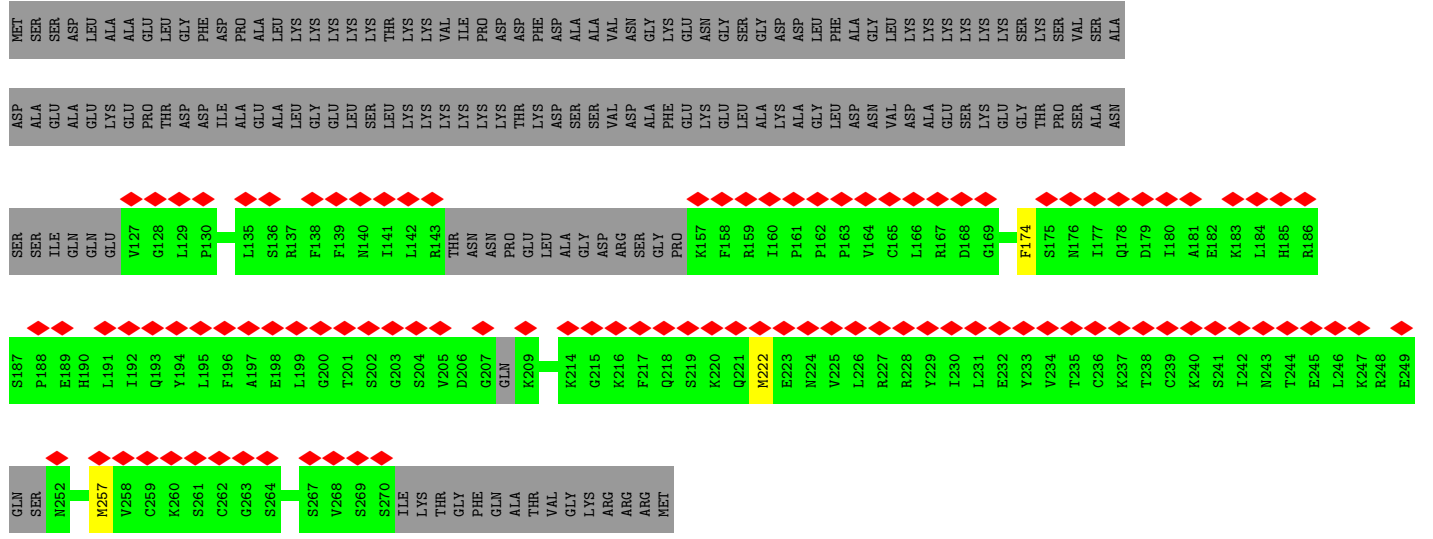


- Molecule 47: protein-synthesizing GTPase






• Molecule 48: SUI3 isoform 1




• Molecule 49: OTU domain-containing protein 2

Chain x:  84% 16%



- Molecule 50: 40S ribosomal protein S7-A

Chain U:  89% 7% . . .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12059	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 ( $e^-/\text{\AA}^2$ )	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.596	Depositor
Minimum map value	-1.857	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: G7M, MG, RIA, ZN, 1MA, ADP, GCP, 5MC, 2MG, H2U, 1MG, ATP, T6A, M2G, SF4

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	P	0.27	0/1019	0.50	0/1419
2	Q	0.26	0/1117	0.50	0/1554
3	R	0.28	0/1057	0.53	0/1465
4	S	0.29	0/1266	0.56	0/1757
5	T	0.28	0/1122	0.48	0/1559
6	V	0.29	0/917	0.50	0/1271
7	W	0.27	0/909	0.50	0/1265
8	X	0.29	0/701	0.53	0/975
9	Y	0.28	0/741	0.48	0/1031
10	Z	0.28	0/619	0.51	0/856
11	a	0.27	0/428	0.52	0/594
12	b	0.30	0/633	0.54	0/878
13	c	0.32	0/703	0.55	0/973
14	d	0.31	0/660	0.49	0/917
15	e	0.27	0/481	0.53	0/670
16	f	0.29	0/399	0.62	0/554
17	g	0.27	0/260	0.45	0/360
18	E	0.25	0/575	0.43	0/798
19	B	0.27	0/1092	0.47	0/1517
20	D	0.25	0/455	0.47	0/633
21	F	0.25	0/594	0.54	0/824
22	H	0.27	0/692	0.48	0/960
23	I	0.25	0/598	0.39	0/831
24	J	0.25	0/714	0.48	0/992
25	K	0.25	0/699	0.44	0/968
26	L	0.26	0/495	0.45	0/689
27	M	0.25	0/406	0.46	0/565
28	N	0.25	0/259	0.49	0/358
29	O	0.26	0/360	0.58	0/500
30	h	0.26	0/1537	0.51	0/2137
31	i	0.27	0/309	0.50	0/428
32	l	0.25	0/1622	0.49	0/2252

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	r	0.23	0/260	0.40	0/360
34	1	0.50	1/1529 (0.1%)	1.21	14/2376 (0.6%)
35	m	0.25	0/725	0.43	0/1008
36	o	0.23	0/2627	0.33	0/3662
37	p	0.26	0/3197	0.46	0/4452
38	q	0.23	0/3163	0.35	0/4412
39	3	0.50	0/191	0.95	0/295
40	A	0.26	0/495	0.46	0/685
41	k	0.24	0/2858	0.46	0/3977
42	2	0.94	2/42031 (0.0%)	1.19	328/65492 (0.5%)
43	C	0.25	0/1019	0.46	0/1419
44	y	0.24	0/373	0.48	0/517
45	n	0.43	0/176	0.96	0/225
46	j	0.32	0/2034	0.71	4/2737 (0.1%)
47	G	0.27	0/3079	0.61	3/4157 (0.1%)
48	s	0.28	0/1051	0.57	0/1402
49	x	0.24	0/1286	0.36	0/1790
50	U	0.47	0/1498	0.91	9/2019 (0.4%)
All	All	0.67	3/91031 (0.0%)	0.92	358/133535 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
13	c	0	1
16	f	0	2
21	F	0	1
47	G	0	1
50	U	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	1	A	OP3-P	-10.59	1.48	1.61
42	2	555	A	N7-C5	-5.50	1.35	1.39
42	2	555	A	N3-C4	-5.20	1.31	1.34

The worst 5 of 358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	74	C	N1-C2-O2	12.66	126.50	118.90
34	1	74	C	C2-N1-C1'	11.25	131.18	118.80
42	2	653	C	N1-C2-O2	11.14	125.58	118.90
42	2	555	A	N7-C8-N9	10.71	119.16	113.80
42	2	1527	C	C2-N1-C1'	10.50	130.35	118.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	F	110	GLY	Peptide
1	P	94	GLY	Peptide
13	c	96	VAL	Peptide
16	f	61	THR	Peptide
16	f	80	ARG	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
1	P	204/252 (81%)	179 (88%)	25 (12%)	0	100	100
2	Q	222/255 (87%)	206 (93%)	16 (7%)	0	100	100
3	R	214/254 (84%)	203 (95%)	11 (5%)	0	100	100
4	S	256/261 (98%)	236 (92%)	20 (8%)	0	100	100
5	T	226/236 (96%)	216 (96%)	10 (4%)	0	100	100
6	V	183/200 (92%)	166 (91%)	17 (9%)	0	100	100
7	W	182/197 (92%)	171 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	X	140/156 (90%)	129 (92%)	11 (8%)	0	100	100
9	Y	148/151 (98%)	136 (92%)	12 (8%)	0	100	100
10	Z	125/137 (91%)	114 (91%)	11 (9%)	0	100	100
11	a	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
12	b	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
13	c	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
14	d	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
15	e	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
16	f	79/82 (96%)	65 (82%)	13 (16%)	1 (1%)	12	40
17	g	51/63 (81%)	44 (86%)	7 (14%)	0	100	100
18	E	115/142 (81%)	105 (91%)	10 (9%)	0	100	100
19	B	220/240 (92%)	211 (96%)	9 (4%)	0	100	100
20	D	90/105 (86%)	81 (90%)	9 (10%)	0	100	100
21	F	119/143 (83%)	98 (82%)	21 (18%)	0	100	100
22	H	139/143 (97%)	125 (90%)	14 (10%)	0	100	100
23	I	117/136 (86%)	113 (97%)	4 (3%)	0	100	100
24	J	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
25	K	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
26	L	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
27	M	80/108 (74%)	77 (96%)	3 (4%)	0	100	100
28	N	51/56 (91%)	51 (100%)	0	0	100	100
29	O	71/76 (93%)	54 (76%)	17 (24%)	0	100	100
30	h	310/319 (97%)	287 (93%)	23 (7%)	0	100	100
31	i	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
32	l	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
33	r	51/274 (19%)	49 (96%)	2 (4%)	0	100	100
35	m	145/405 (36%)	134 (92%)	11 (8%)	0	100	100
36	o	519/964 (54%)	509 (98%)	10 (2%)	0	100	100
37	p	638/763 (84%)	613 (96%)	22 (3%)	3 (0%)	29	61
38	q	624/812 (77%)	597 (96%)	26 (4%)	1 (0%)	47	77
40	A	97/153 (63%)	90 (93%)	6 (6%)	1 (1%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	575/608 (95%)	552 (96%)	22 (4%)	1 (0%)	47	77
43	C	204/225 (91%)	188 (92%)	16 (8%)	0	100	100
44	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	n	16/25 (64%)	16 (100%)	0	0	100	100
46	j	243/304 (80%)	222 (91%)	20 (8%)	1 (0%)	34	66
47	G	388/527 (74%)	357 (92%)	28 (7%)	3 (1%)	19	51
48	s	120/285 (42%)	117 (98%)	3 (2%)	0	100	100
49	x	253/307 (82%)	251 (99%)	2 (1%)	0	100	100
50	U	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
All	All	8821/11071 (80%)	8283 (94%)	527 (6%)	11 (0%)	54	81

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	f	59	CYS
37	p	392	PRO
37	p	536	LYS
47	G	497	GLU
40	A	118	THR

### 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	
45	n	17/23 (74%)	17 (100%)	0	100	100
46	j	224/274 (82%)	213 (95%)	11 (5%)	25	56
47	G	332/449 (74%)	328 (99%)	4 (1%)	71	83
48	s	119/246 (48%)	116 (98%)	3 (2%)	47	72
50	U	163/170 (96%)	154 (94%)	9 (6%)	21	52
All	All	855/1162 (74%)	828 (97%)	27 (3%)	42	67

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	G	510	ARG
48	s	257	MET
50	U	123	ASP
48	s	222	MET
50	U	19	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
47	G	344	ASN
50	U	29	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	72/75 (96%)	25 (34%)	2 (2%)
39	3	7/8 (87%)	1 (14%)	0
42	2	1759/1800 (97%)	499 (28%)	40 (2%)
All	All	1838/1883 (97%)	525 (28%)	42 (2%)

5 of 525 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	8	U
34	1	9	1MG
34	1	10	2MG
34	1	15	G
34	1	16	H2U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
42	2	1108	G
42	2	1430	U
42	2	1226	A
42	2	1274	C
42	2	1573	A

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

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
34	RIA	1	64	34	31,38,39	4.48	19 (61%)	39,57,60	2.29	5 (12%)
34	1MG	1	9	34	18,26,27	2.87	6 (33%)	19,39,42	1.52	3 (15%)
34	H2U	1	47	34	18,21,22	0.46	0	21,30,33	1.30	2 (9%)
34	M2G	1	26	34	20,27,28	1.17	2 (10%)	22,40,43	0.82	0
34	H2U	1	16	34	18,21,22	0.49	0	21,30,33	1.09	1 (4%)
34	5MC	1	49	34	18,22,23	0.55	0	26,32,35	1.15	2 (7%)
34	G7M	1	46	34	20,26,27	2.47	7 (35%)	17,39,42	1.22	2 (11%)
34	T6A	1	37	34	27,34,35	2.03	5 (18%)	29,49,52	2.66	8 (27%)
34	1MA	1	58	34	16,25,26	0.88	2 (12%)	18,37,40	1.24	3 (16%)
34	5MC	1	48	34	18,22,23	0.53	0	26,32,35	0.79	1 (3%)
34	2MG	1	10	34	18,26,27	1.08	2 (11%)	16,38,41	0.88	1 (6%)

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
34	RIA	1	64	34	-	3/13/51/52	0/4/4/4
34	1MG	1	9	34	-	3/3/25/26	0/3/3/3
34	H2U	1	47	34	-	5/7/38/39	0/2/2/2
34	M2G	1	26	34	-	2/7/29/30	0/3/3/3
34	H2U	1	16	34	-	2/7/38/39	0/2/2/2
34	5MC	1	49	34	-	2/7/25/26	0/2/2/2
34	G7M	1	46	34	-	1/3/25/26	0/3/3/3
34	T6A	1	37	34	-	8/19/41/42	0/3/3/3
34	1MA	1	58	34	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	5MC	1	48	34	-	3/7/25/26	0/2/2/2
34	2MG	1	10	34	-	2/5/27/28	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	64	RIA	C3A-C2A	-12.91	1.24	1.52
34	1	64	RIA	C1'-C2'	11.29	1.67	1.52
34	1	64	RIA	C3'-C2'	-10.44	1.24	1.53
34	1	64	RIA	O4'-C1A	-7.35	1.30	1.41
34	1	9	1MG	C2-N3	7.17	1.47	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	64	RIA	C5-C6-N6	8.63	133.47	120.35
34	1	37	T6A	C12-N11-C10	6.56	132.87	121.94
34	1	64	RIA	N3-C2-N1	-6.12	119.11	128.68
34	1	37	T6A	N3-C2-N1	-6.10	119.14	128.68
34	1	37	T6A	N6-C10-N11	5.95	122.08	113.76

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	1	9	1MG	O4'-C4'-C5'-O5'
34	1	9	1MG	C3'-C4'-C5'-O5'
34	1	10	2MG	O4'-C4'-C5'-O5'
34	1	16	H2U	C4'-C5'-O5'-P
34	1	26	M2G	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
57	GCP	G	603	-	27,34,34	2.39	4 (14%)	34,54,54	2.32	6 (17%)
55	SF4	k	706	-	0,12,12	-	-	-	-	-
55	SF4	k	705	-	0,12,12	-	-	-	-	-
54	ATP	k	703	53	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
56	MET	G	601	-	6,7,8	0.50	0	2,7,9	0.33	0
52	ADP	k	701	53	24,29,29	0.97	1 (4%)	29,45,45	1.47	4 (13%)

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
57	GCP	G	603	-	-	4/15/38/38	0/3/3/3
55	SF4	k	706	-	-	-	0/6/5/5
55	SF4	k	705	-	-	-	0/6/5/5
54	ATP	k	703	53	-	5/18/38/38	0/3/3/3
56	MET	G	601	-	-	0/5/6/8	-
52	ADP	k	701	53	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	G	603	GCP	PB-O3A	10.40	1.70	1.58
57	G	603	GCP	C6-N1	4.30	1.40	1.33
52	k	701	ADP	C5-C4	2.51	1.47	1.40
57	G	603	GCP	C8-N7	-2.48	1.30	1.34
57	G	603	GCP	PB-O2B	-2.27	1.51	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	G	603	GCP	C5-C6-N1	-9.43	110.53	123.43
57	G	603	GCP	C2-N1-C6	6.40	126.11	115.93
52	k	701	ADP	PA-O3A-PB	-3.60	120.49	132.83
52	k	701	ADP	C3'-C2'-C1'	3.34	106.01	100.98
52	k	701	ADP	N3-C2-N1	-3.17	123.73	128.68

There are no chirality outliers.

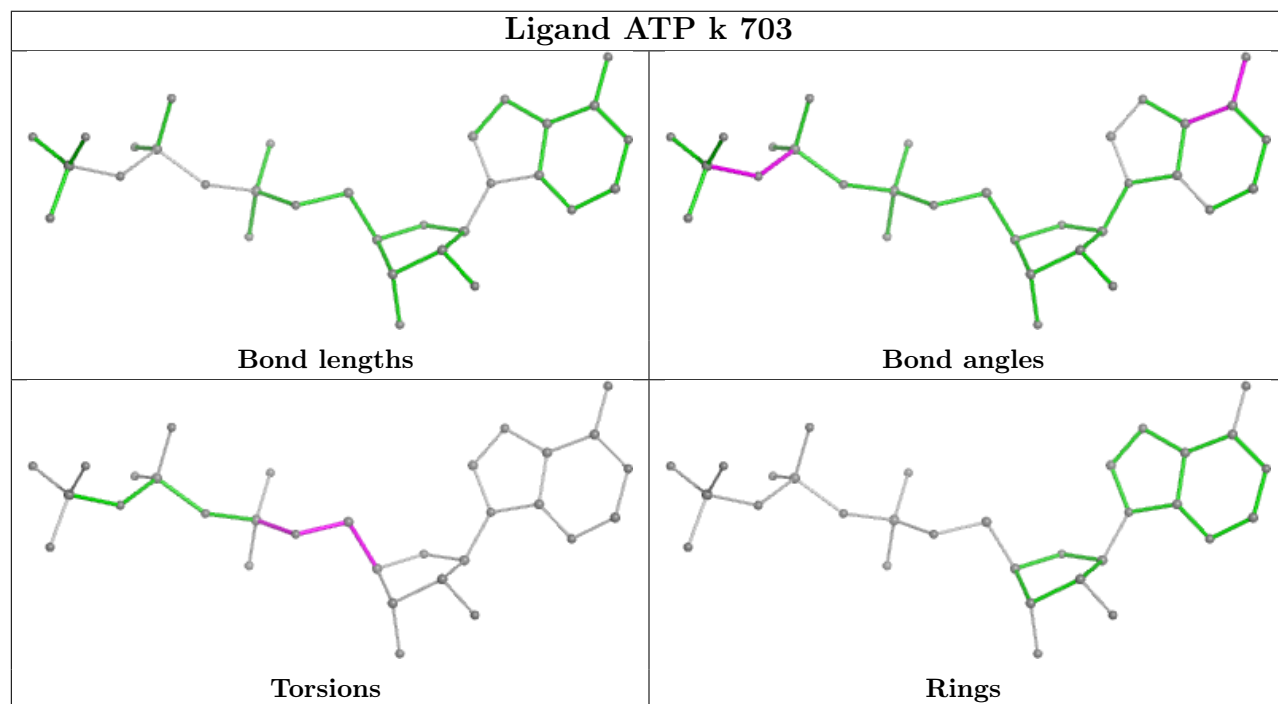
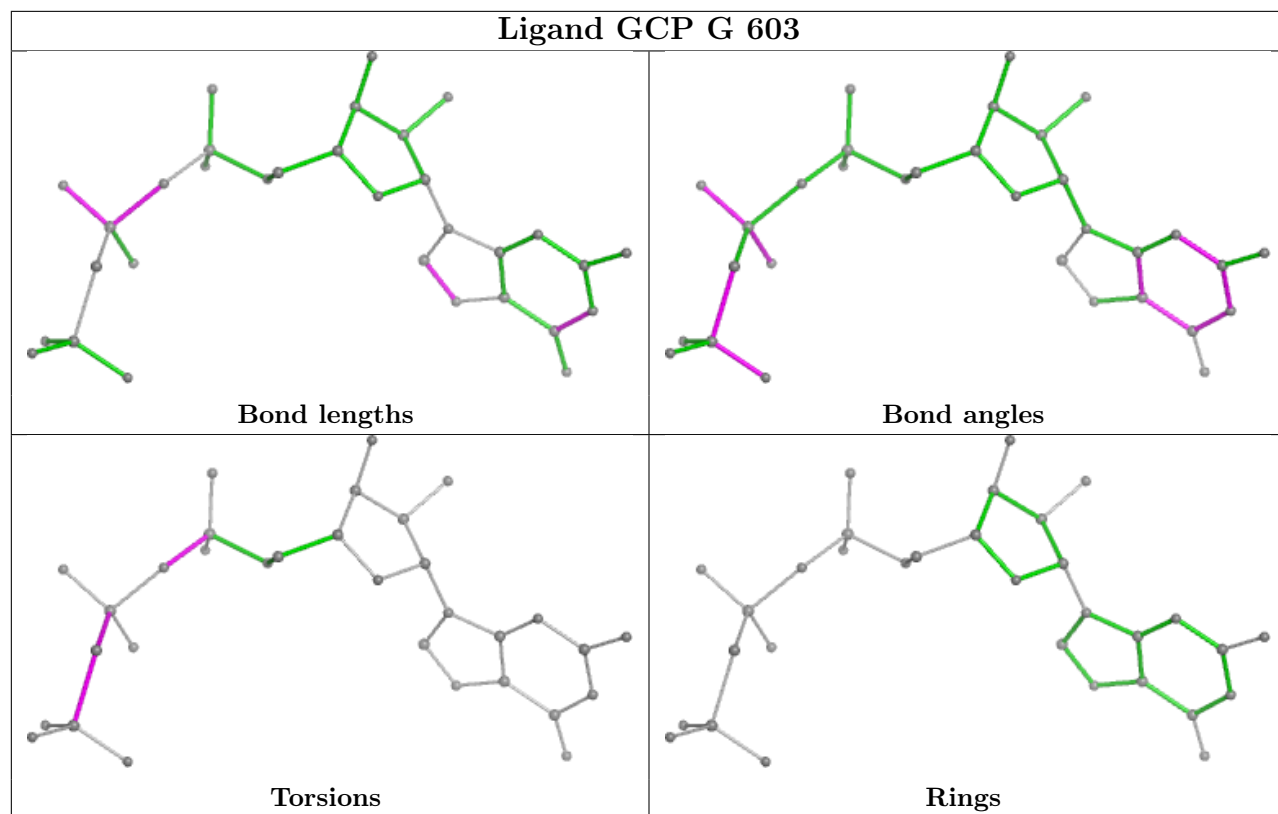
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	k	701	ADP	O4'-C4'-C5'-O5'
54	k	703	ATP	C5'-O5'-PA-O2A
54	k	703	ATP	C5'-O5'-PA-O3A
57	G	603	GCP	PB-C3B-PG-O1G
57	G	603	GCP	PG-C3B-PB-O2B

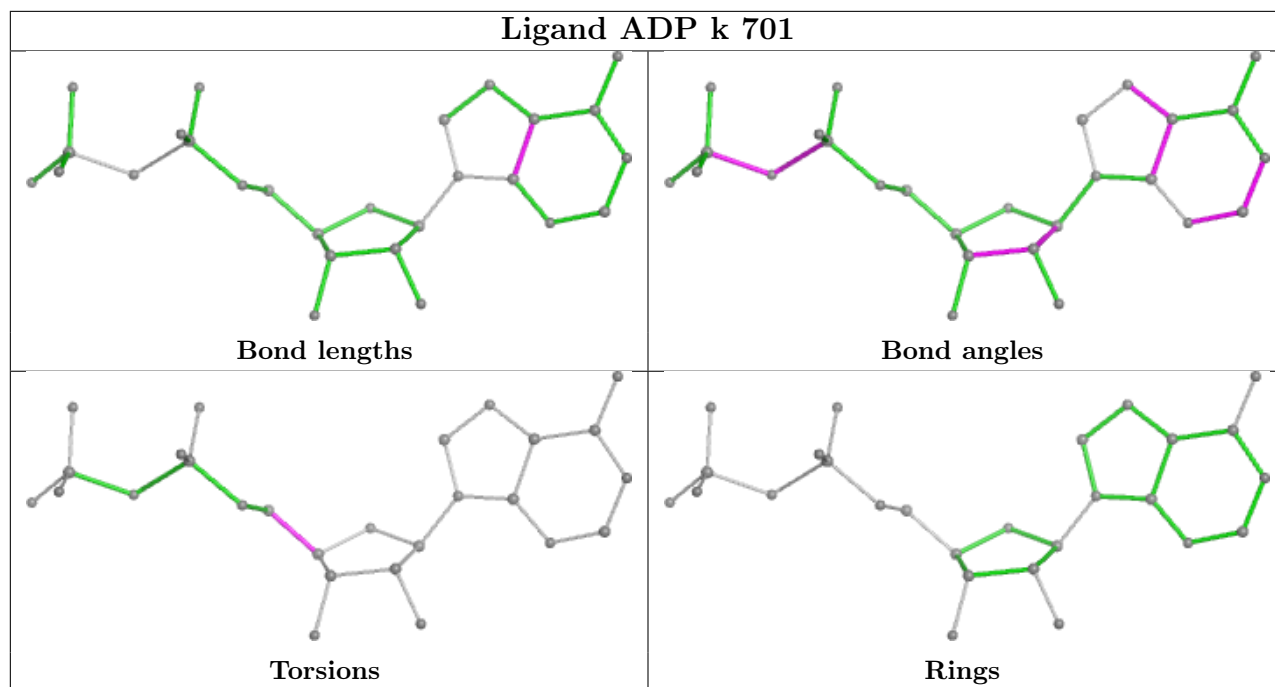
There are no ring outliers.

No monomer is involved in short contacts.

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	q	2
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	582:GLN	C	583:GLN	N	4.38
1	q	605:CYS	C	606:LEU	N	4.22
1	1	16:H2U	O3'	18:G	P	4.10

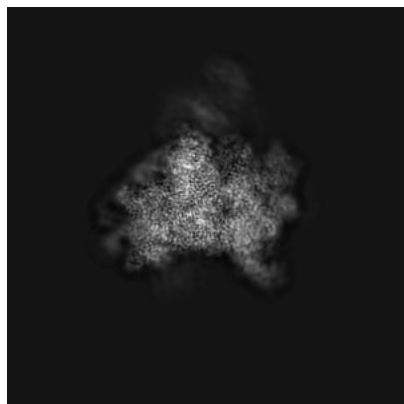
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16533. These allow visual inspection of the internal detail of the map and identification of artifacts.

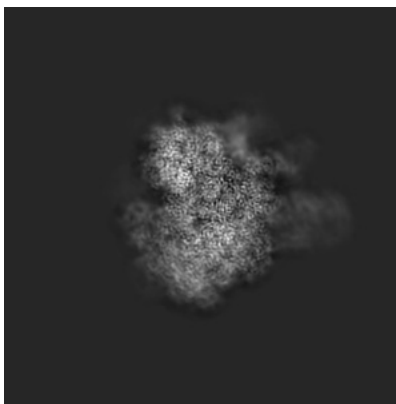
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

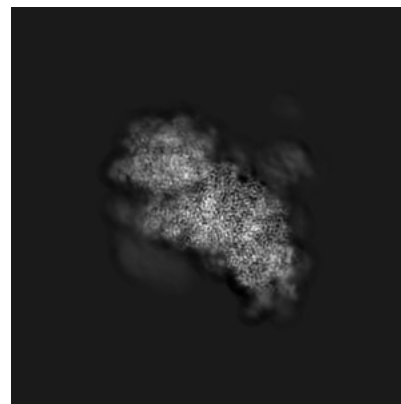
#### 6.1.1 Primary map



X

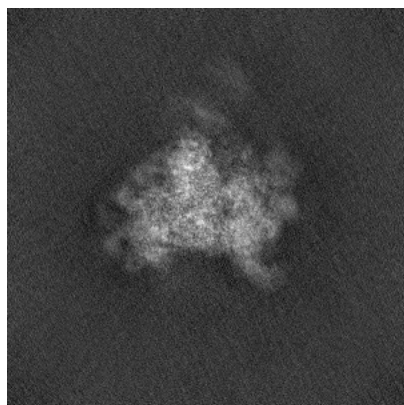


Y

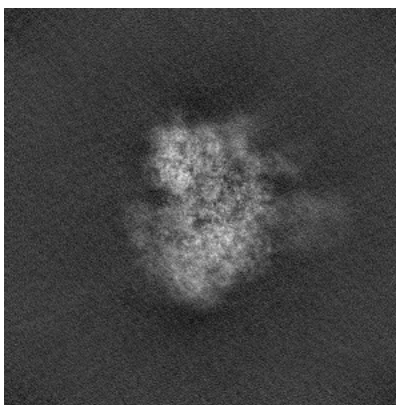


Z

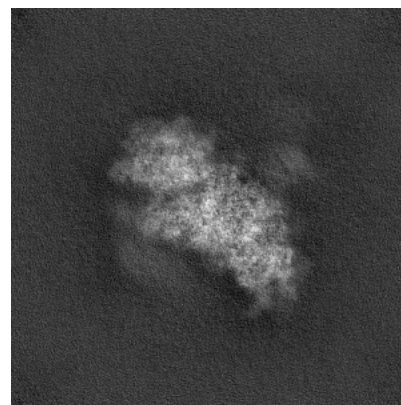
#### 6.1.2 Raw map



X



Y

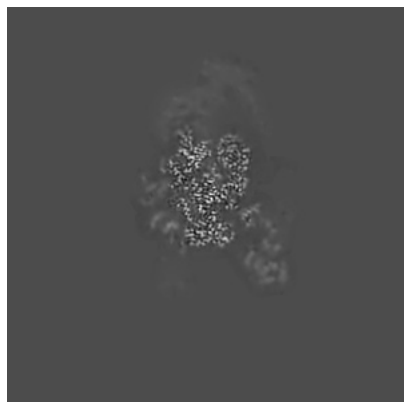


Z

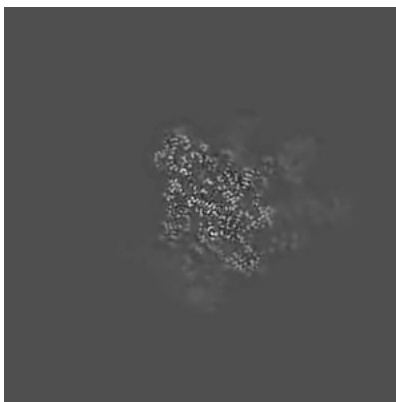
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

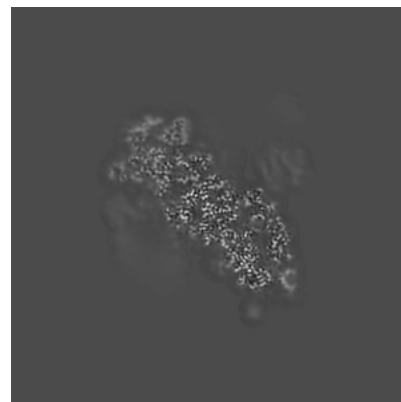
### 6.2.1 Primary map



X Index: 210

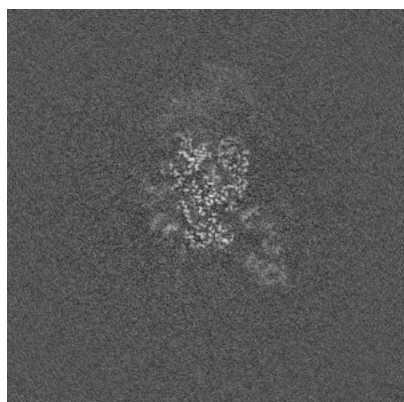


Y Index: 210

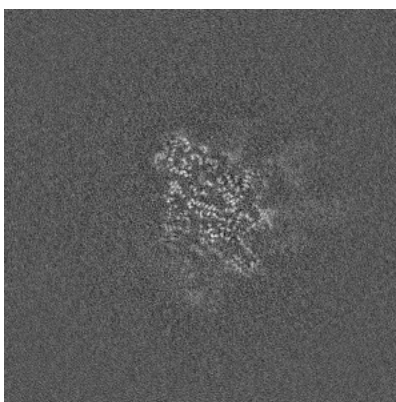


Z Index: 210

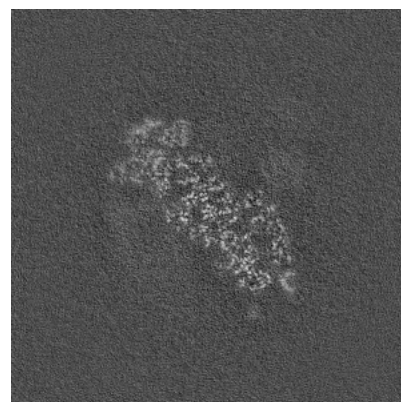
### 6.2.2 Raw map



X Index: 210



Y Index: 210

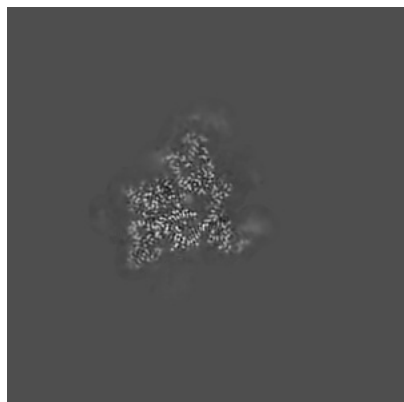


Z Index: 210

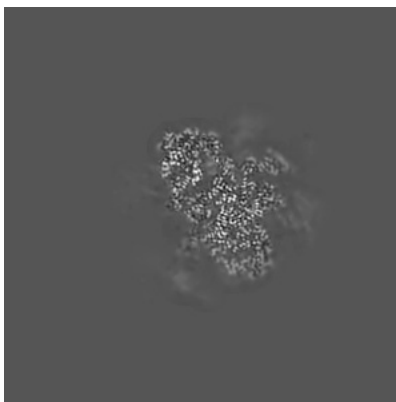
The images above show central slices of the map in three orthogonal directions.

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

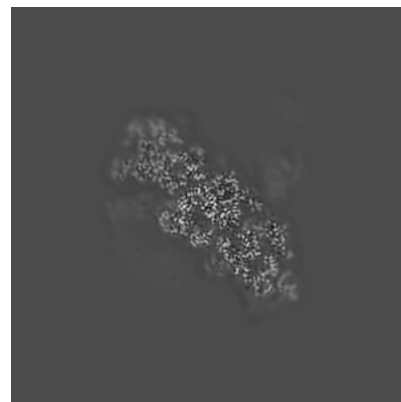
### 6.3.1 Primary map



X Index: 245

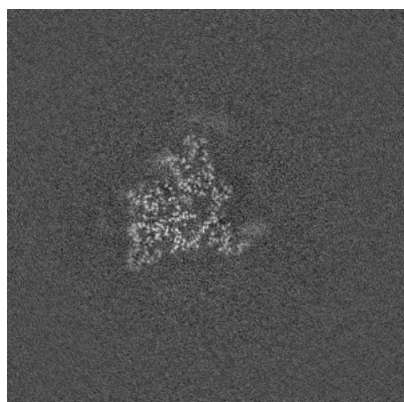


Y Index: 189

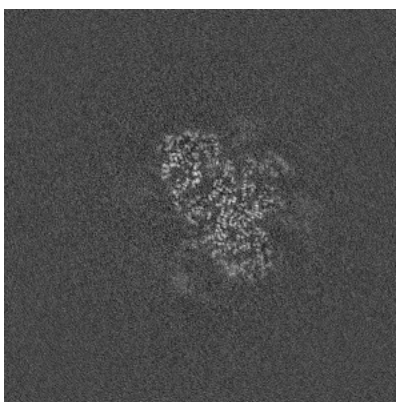


Z Index: 218

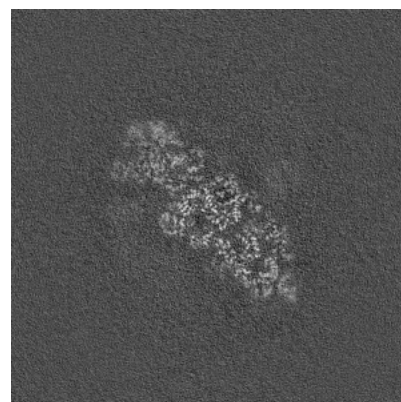
### 6.3.2 Raw map



X Index: 245



Y Index: 189

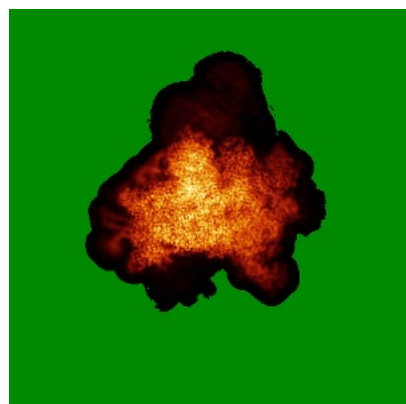


Z Index: 217

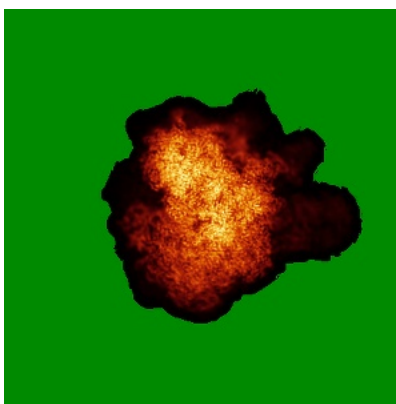
The images above show the largest variance slices of the map in three orthogonal directions.

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

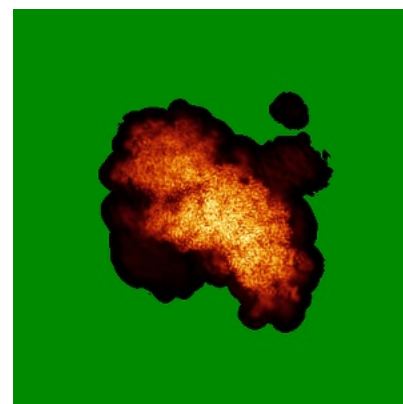
### 6.4.1 Primary map



X

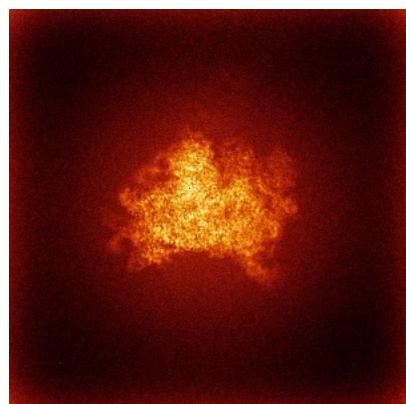


Y

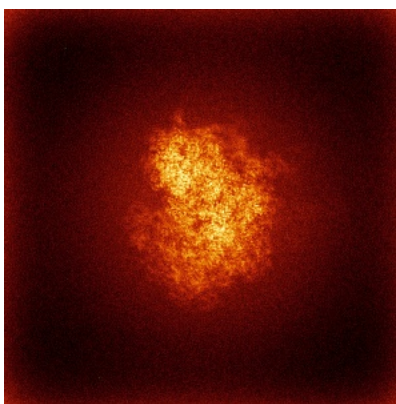


Z

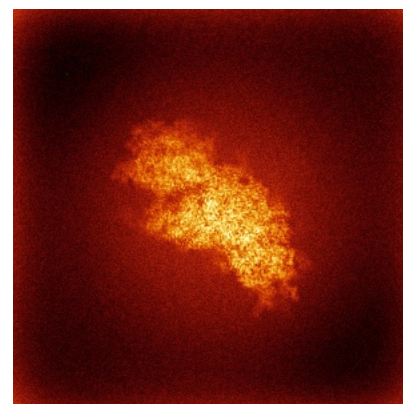
### 6.4.2 Raw map



X



Y

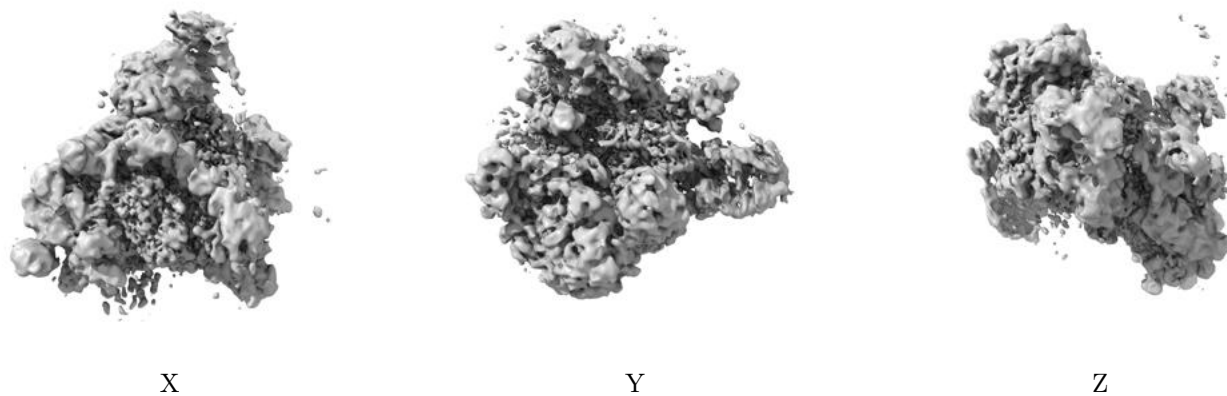


Z

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.

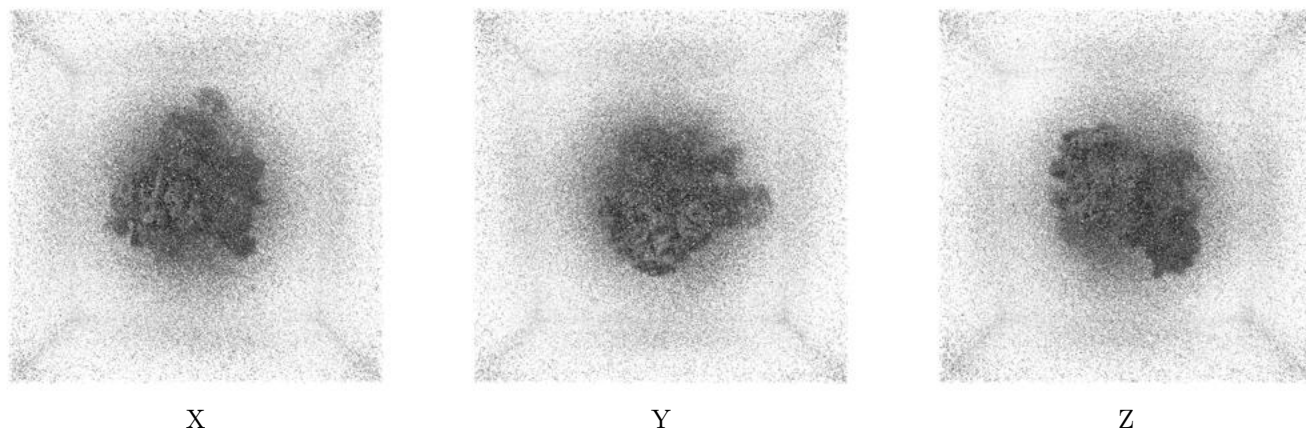
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

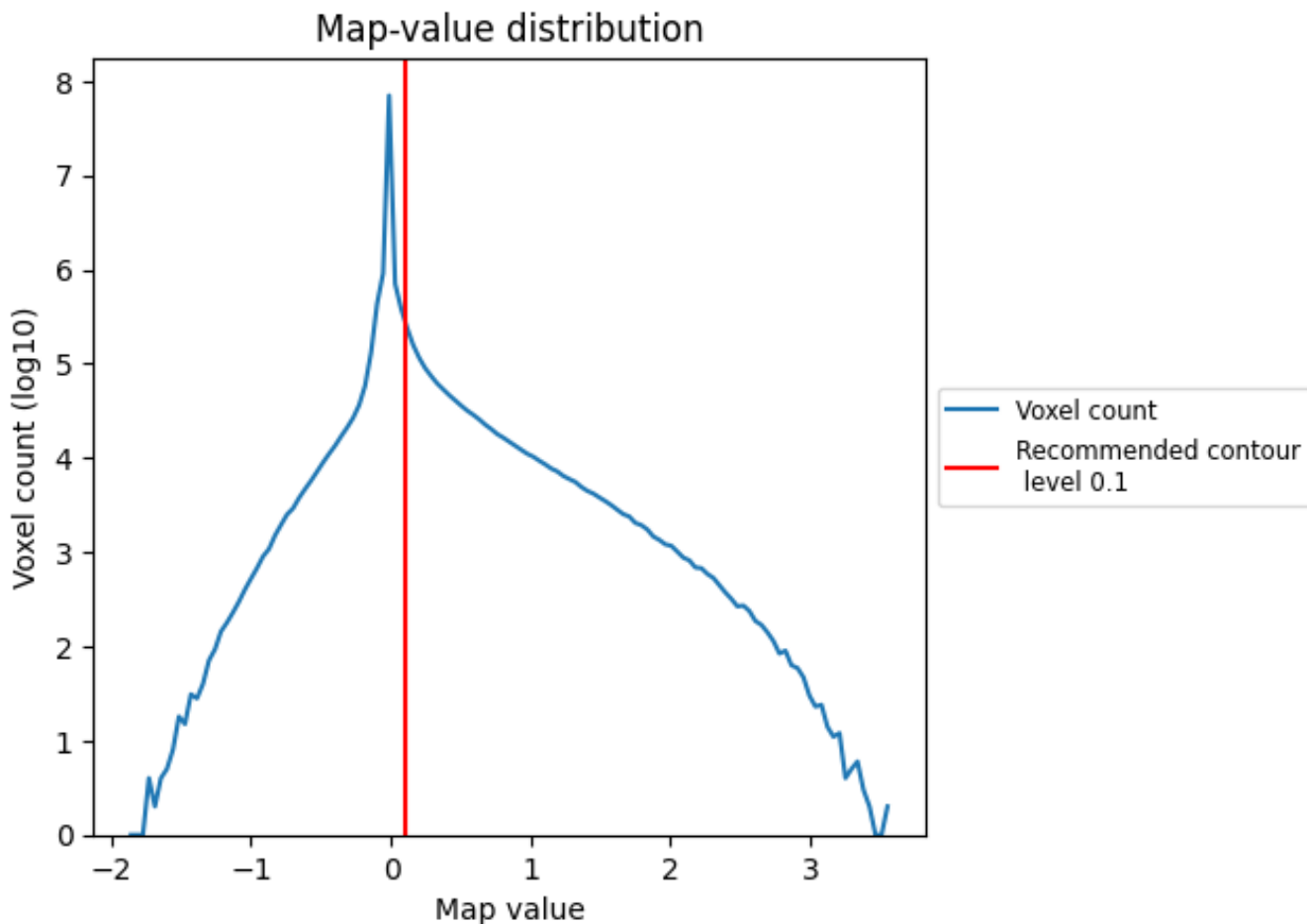
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

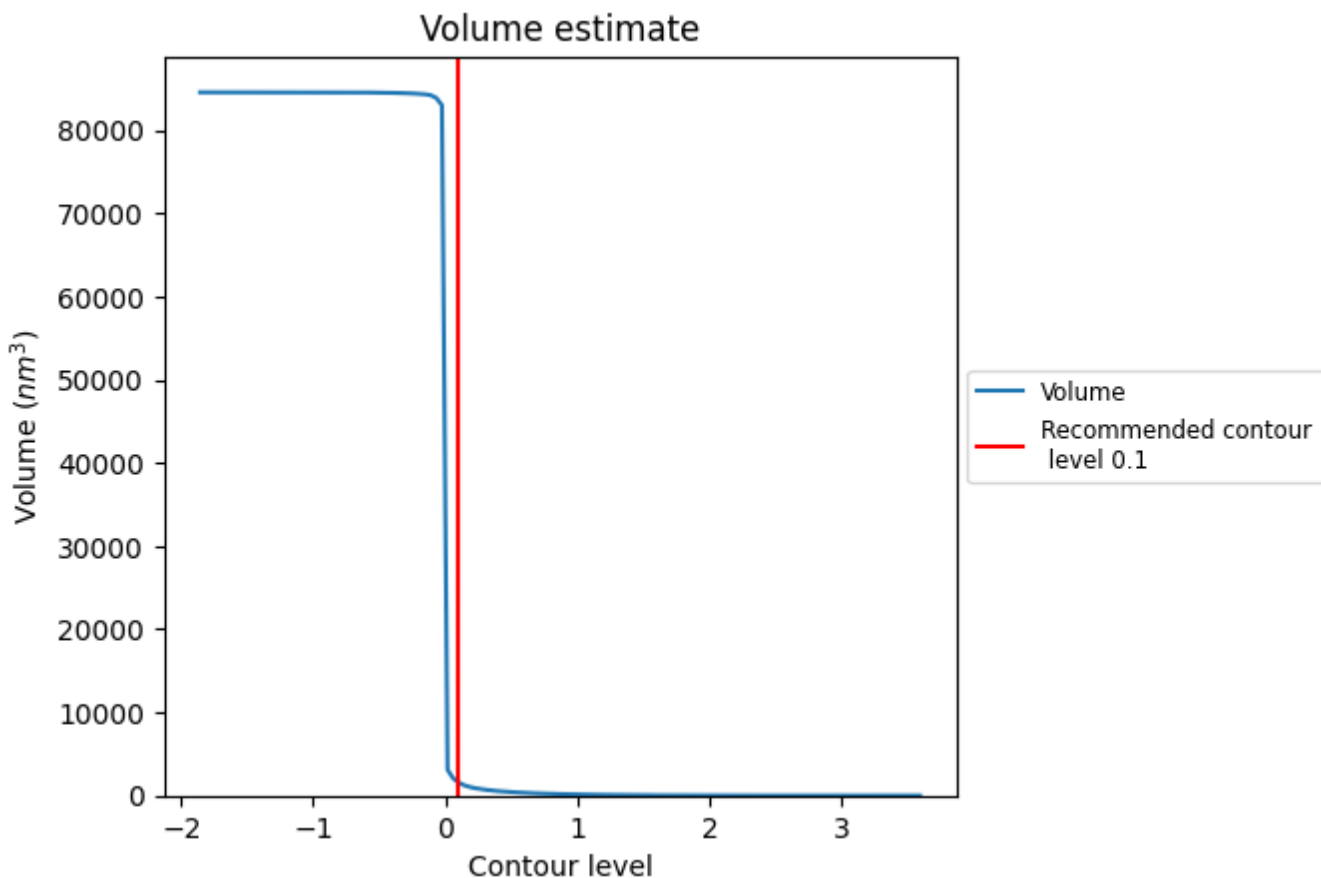
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

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

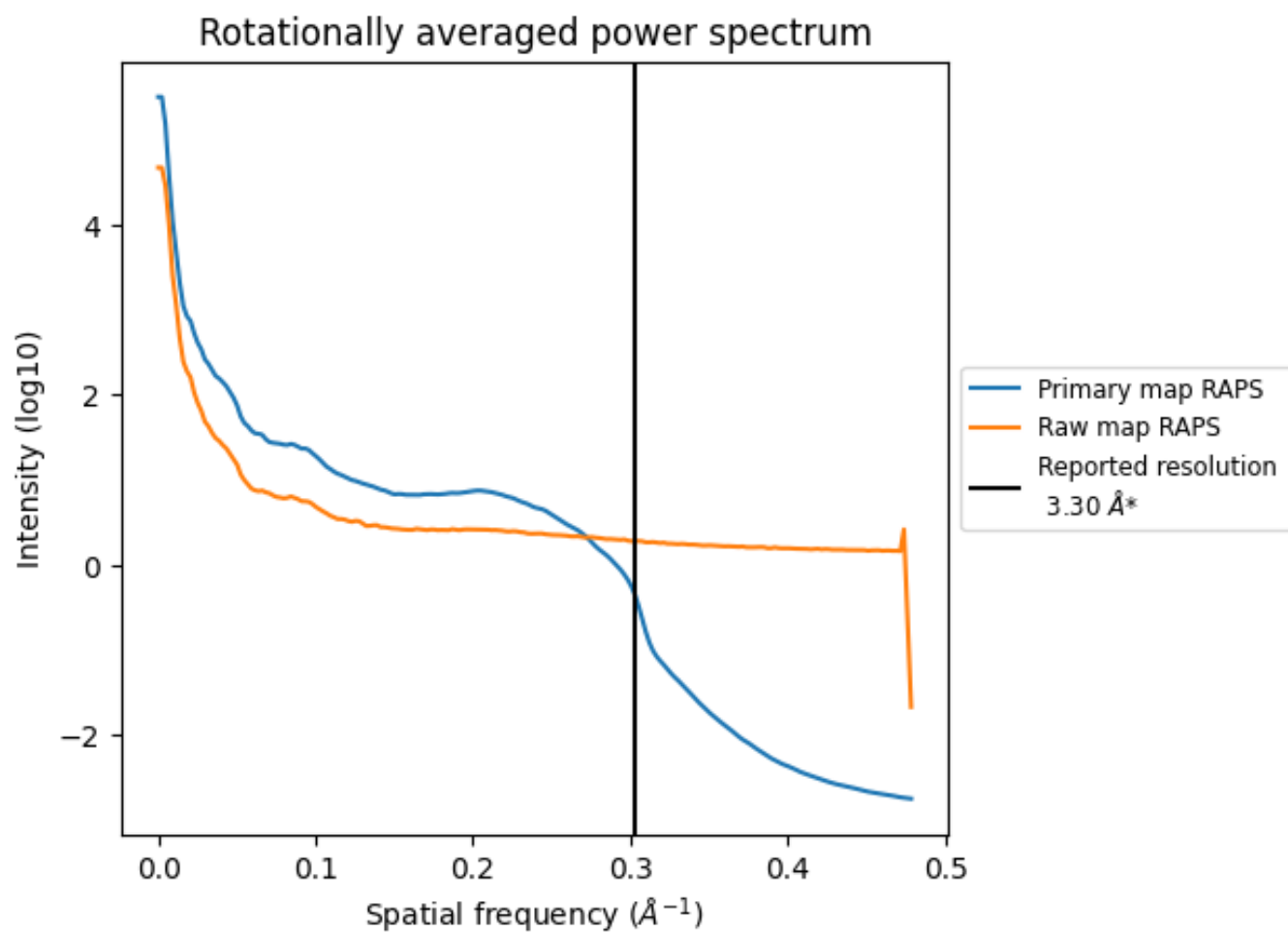


The volume at the recommended contour level is 1582 nm<sup>3</sup>; this corresponds to an approximate mass of 1429 kDa.

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

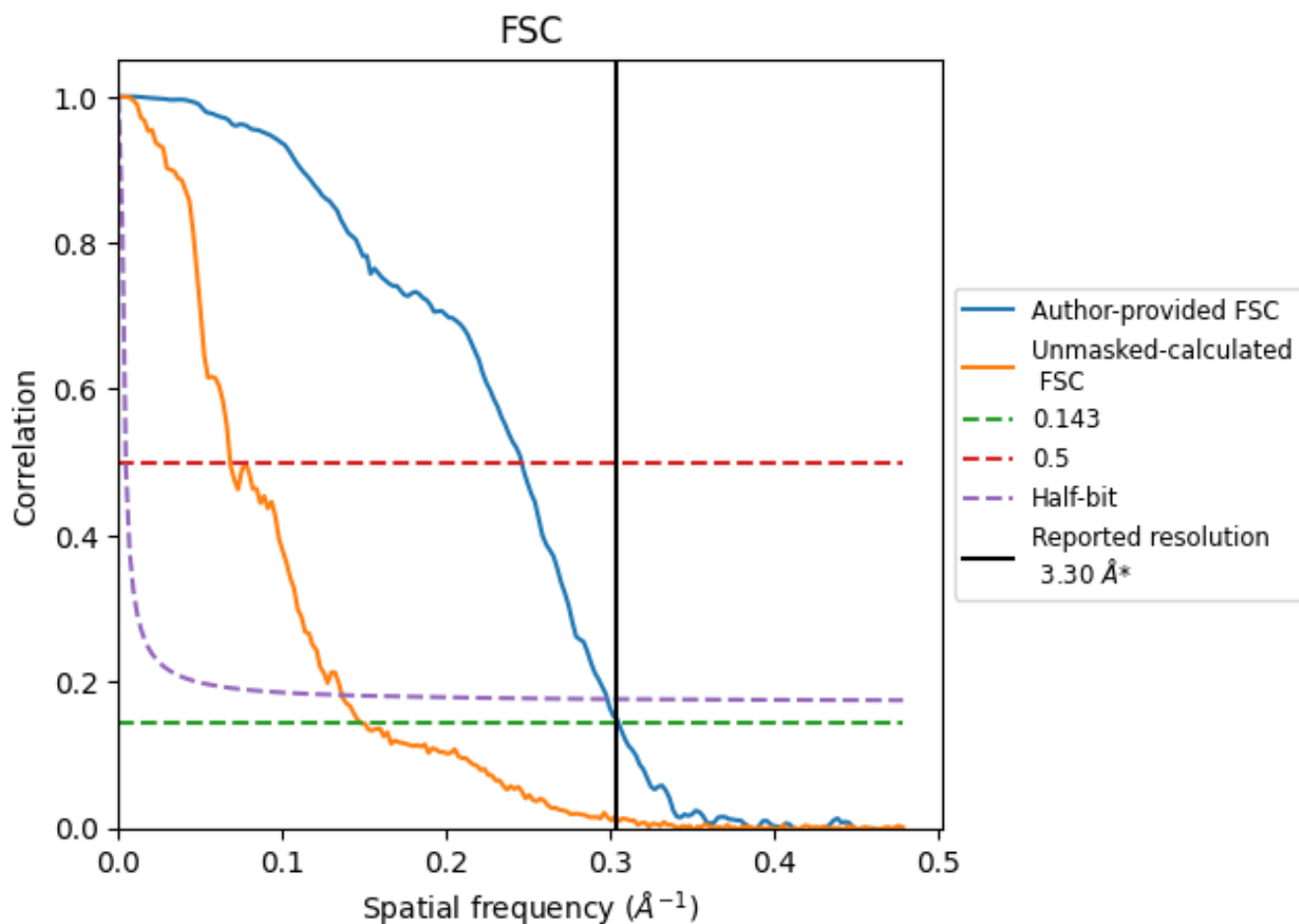


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

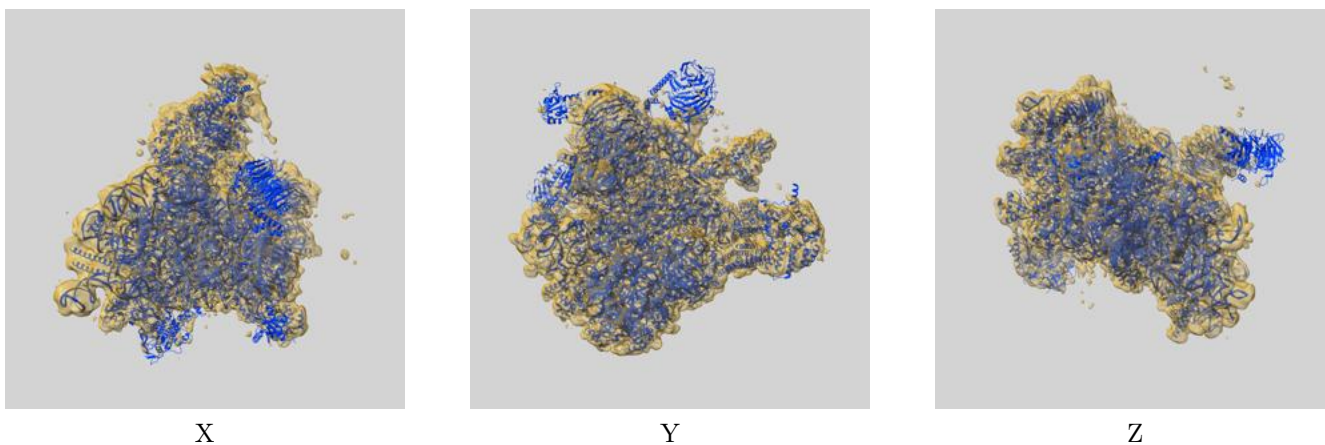
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	4.07	3.35
Unmasked-calculated*	6.76	14.66	7.34

\*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 6.76 differs from the reported value 3.3 by more than 10 %

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

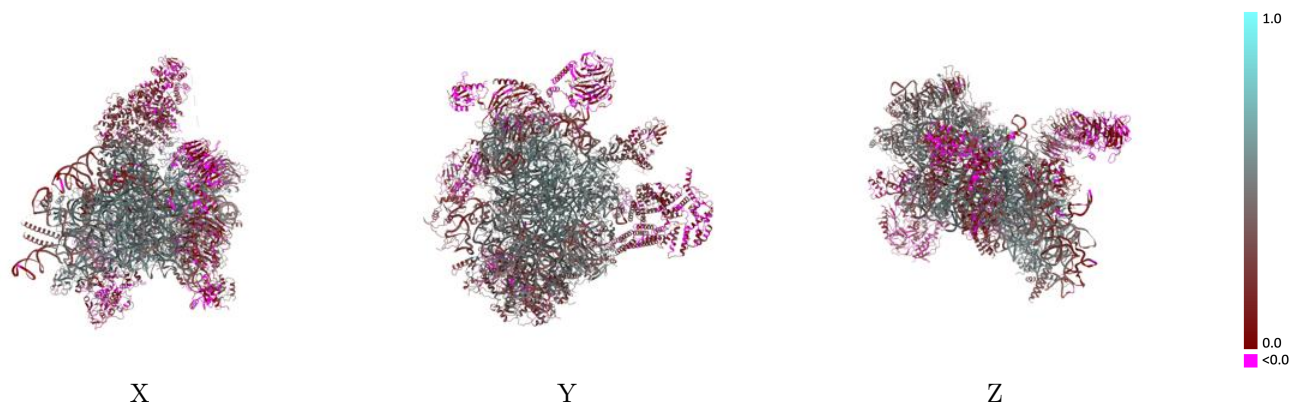
This section contains information regarding the fit between EMDB map EMD-16533 and PDB model 8CAS. Per-residue inclusion information can be found in section 3 on page 16.

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



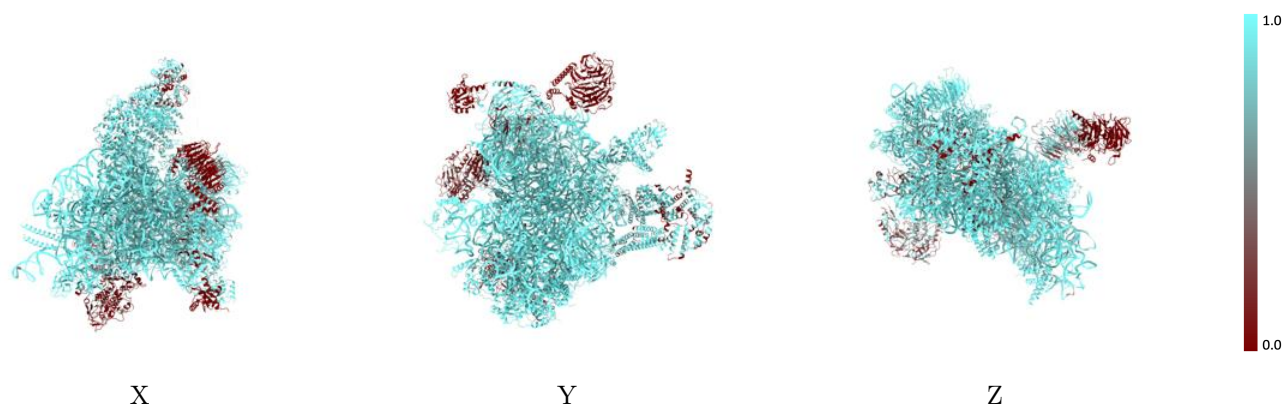
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



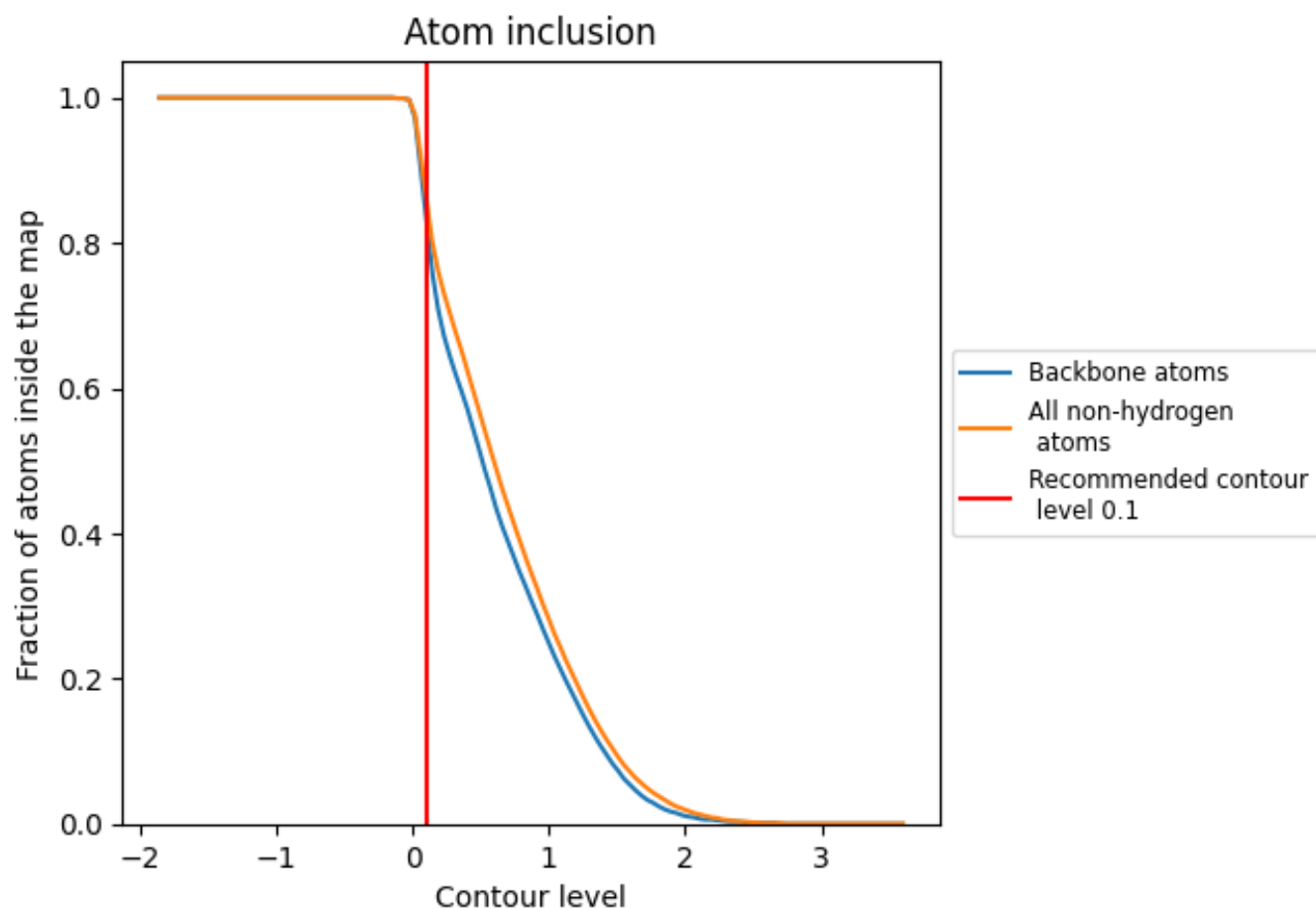
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.3660
1	 0.8970	 0.1700
2	 0.9950	 0.4560
3	 0.8770	 0.3510
A	 0.9840	 0.4580
B	 0.9960	 0.4670
C	 0.9940	 0.4380
D	 1.0000	 0.4090
E	 0.9950	 0.3860
F	 0.9770	 0.2600
G	 0.3010	 0.0530
H	 0.9970	 0.4410
I	 0.9950	 0.4820
J	 0.9870	 0.3810
K	 0.9970	 0.4090
L	 0.9940	 0.4540
M	 0.9160	 0.3250
N	 1.0000	 0.5360
O	 0.9890	 0.2910
P	 0.9950	 0.5290
Q	 0.9970	 0.4820
R	 0.9970	 0.5590
S	 0.9990	 0.5610
T	 0.9990	 0.4860
U	 0.9770	 0.4130
V	 0.9960	 0.5250
W	 0.9980	 0.5270
X	 0.9990	 0.5560
Y	 0.9920	 0.5240
Z	 0.9940	 0.5120
a	 1.0000	 0.5510
b	 0.9970	 0.5750
c	 0.9960	 0.5710
d	 0.9890	 0.5200
e	 0.9980	 0.5470



*Continued on next page...*

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Chain	Atom inclusion	Q-score
f	 0.7150	 0.1730
g	 0.9660	 0.4990
h	 0.9990	 0.3600
i	 0.9940	 0.4810
j	 0.4980	 0.0910
k	 0.2220	 0.1230
l	 0.0050	 0.0130
m	 0.7990	 0.2220
n	 0.9870	 0.4940
o	 0.7280	 0.1310
p	 0.5190	 0.1320
q	 0.7760	 0.1620
r	 0.0000	 0.0060
s	 0.1870	 0.0400
x	 0.9830	 0.2410
y	 0.9090	 0.1660