



## wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 06:27 PM EDT

PDB ID : 5WE6 / pdb\_00005we6  
EMDB ID : EMD-8815  
Title : 70S ribosome-EF-Tu H84A complex with GTP and cognate tRNA  
Authors : Fislage, M.; Frank, J.  
Deposited on : 2017-07-07  
Resolution : 3.40 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:

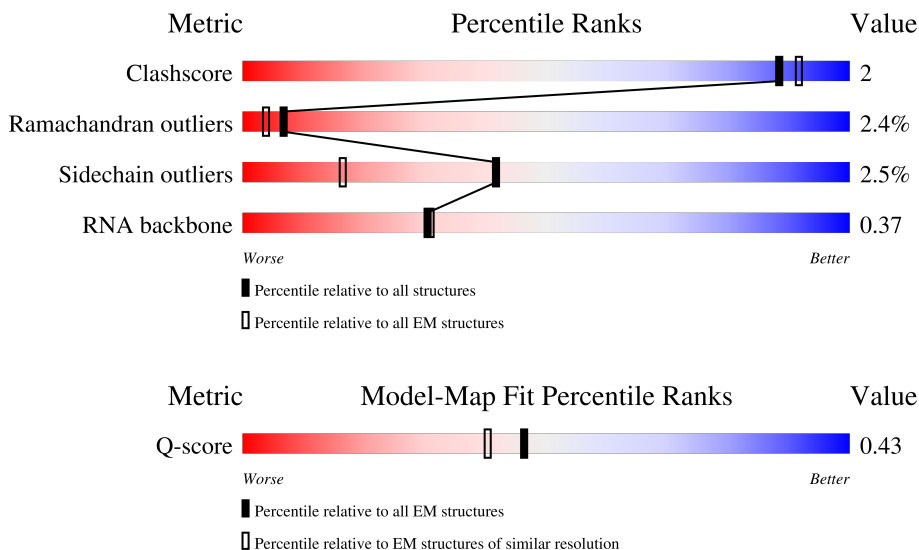
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.40 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	14717 ( 2.90 - 3.90 )

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	A	2903	
2	B	120	
3	C	271	

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Mol	Chain	Length	Quality of chain
4	D	208	95% .
5	E	200	92% 8% .
6	F	177	98% ..
7	G	174	97% .
8	H	149	10% 94% 6% .
9	I	141	16% 94% 5% .
10	J	141	92% 8% .
11	K	122	88% 10% .
12	L	142	90% 10% .
13	M	136	96% .
14	N	119	96% ..
15	O	116	95% 5% .
16	P	114	96% .
17	Q	115	95% 5% .
18	R	102	94% 6% .
19	S	109	94% 6% .
20	T	92	95% 5% .
21	U	102	97% .
22	V	92	98% .
23	W	75	95% 5% .
24	X	77	97% .
25	Y	60	98% .
26	Z	56	95% . .
27	0	55	95% 5% .
28	1	51	96% .

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Mol	Chain	Length	Quality of chain
29	2	45	96%
30	3	64	98%
31	4	38	95%
32	5	131	44% 89% 11%
33	6	66	9% 94% 6%
34	a	1539	62% 32% 5%
35	b	218	93% 7%
36	c	206	94% 6%
37	d	205	98%
38	e	157	94% 5%
39	f	100	85% 11%
40	g	151	95% 5%
41	h	129	94% 5%
42	i	127	91% 9%
43	j	98	87% 12%
44	k	116	91% 9%
45	l	121	90% 10%
46	m	114	93% 6%
47	n	101	95%
48	o	88	94% 6%
49	p	82	90% 10%
50	q	80	94% 5%
51	r	65	92% 5%
52	s	79	91% 8%
53	t	85	94% 6%

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Mol	Chain	Length	Quality of chain
54	u	65	 91% 9%
55	v	77	 73% 23%
55	w	77	 58% 35% 5%
56	x	12	 67% 33%
57	y	76	 58% 38%
58	z	393	 94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	1618	-	-	X	-
1	6MZ	A	2030	-	-	X	-

## 2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 153233 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62278	27789	11459	20130	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	conflict	GB 1174070234

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1557	974	287	293	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	200	1544	969	282	289	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	177	1410	899	249	256	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	174	1304	820	239	243	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1111	699	197	214	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	141	1032	651	179	196	6	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	141	1120	708	211	197	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	122	938	587	180	165	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	142	1035	644	205	185	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	136	1074	686	205	177	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	119	951	588	195	163	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	116	892	552	178	162	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	114	917	574	179	163	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	115	933	595	190	148	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	102	810	513	152	143	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	109	845	526	162	154	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	92	730	461	138	130	1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	102	779	492	146	141	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	92	739	471	135	131	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	75	572	355	116	100	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	77	625	388	129	106	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	60	494	305	96	91	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	i	127	1022	634	206	179	3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	j	98	786	493	150	142	1	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	k	116	869	535	173	158	3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	l	121	940	581	193	162	4	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	m	114	883	546	178	156	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	n	101	810	502	165	140	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	r	65	535	339	100	95	1	0	0

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s	79	637	408	120	107	2	0	0

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	t	85	665	411	137	114	3	0	0

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	u	65	544	335	117	91	1	0	0

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
55	v	77	1644	733	297	536	77	1	0	0
55	w	77	1644	733	297	536	77	1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	x	12	252	113	42	85	12	0	0

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
57	y	76	1632	731	290	533	76	2	0	0

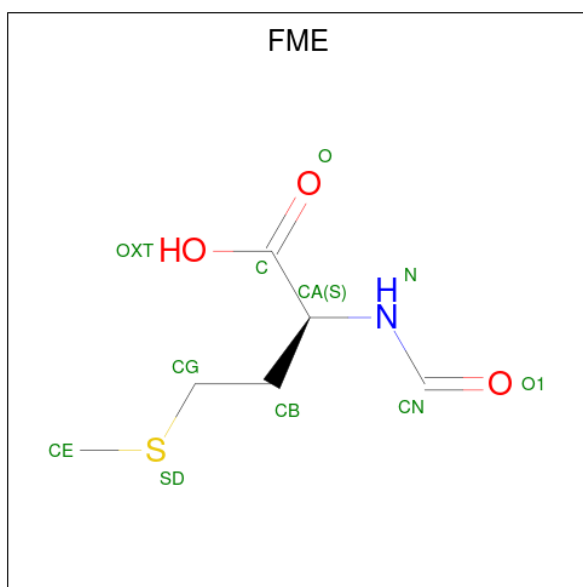
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	z	393	3031	1915	522	581	13	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	A	1	10	6	1	2	1	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	A	404	404	404	0
60	B	6	6	6	0
60	C	2	2	2	0
60	D	1	1	1	0
60	E	1	1	1	0
60	J	1	1	1	0
60	L	1	1	1	0
60	N	3	3	3	0
60	O	1	1	1	0
60	S	1	1	1	0
60	T	2	2	2	0

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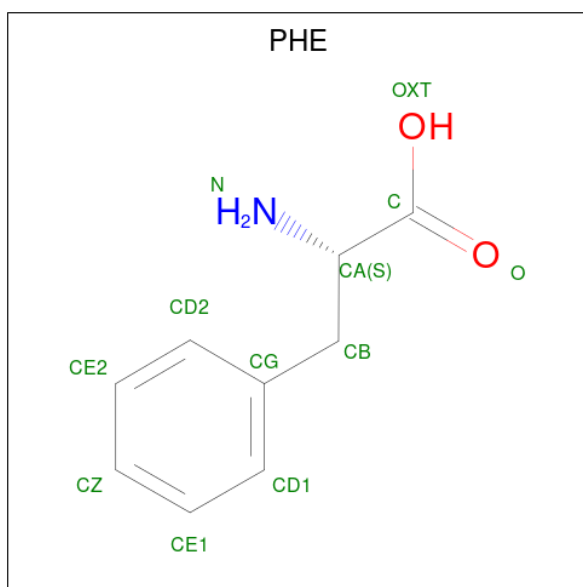
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Mol	Chain	Residues	Atoms		AltConf
60	0	3	Total 3	Mg 3	0
60	3	2	Total 2	Mg 2	0
60	4	1	Total 1	Mg 1	0
60	a	221	Total 221	Mg 221	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	t	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	2	Total 2	Mg 2	0
60	y	4	Total 4	Mg 4	0
60	z	2	Total 2	Mg 2	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

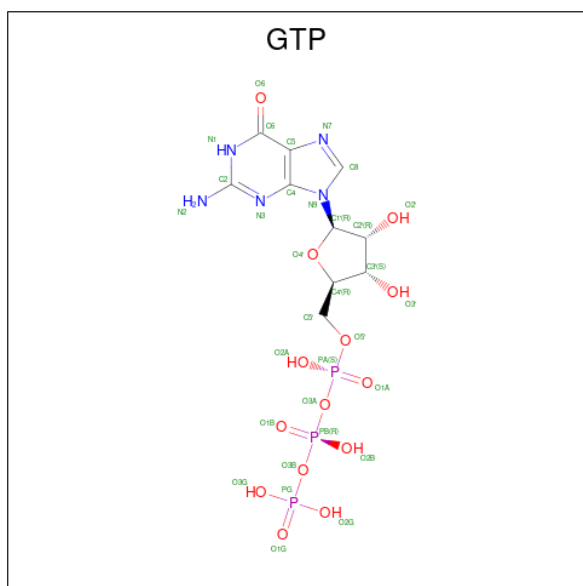
Mol	Chain	Residues	Atoms		AltConf
61	A	7	Total 7	K 7	0
61	v	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
62	y	1	11	9	1	1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	5	14	3	0

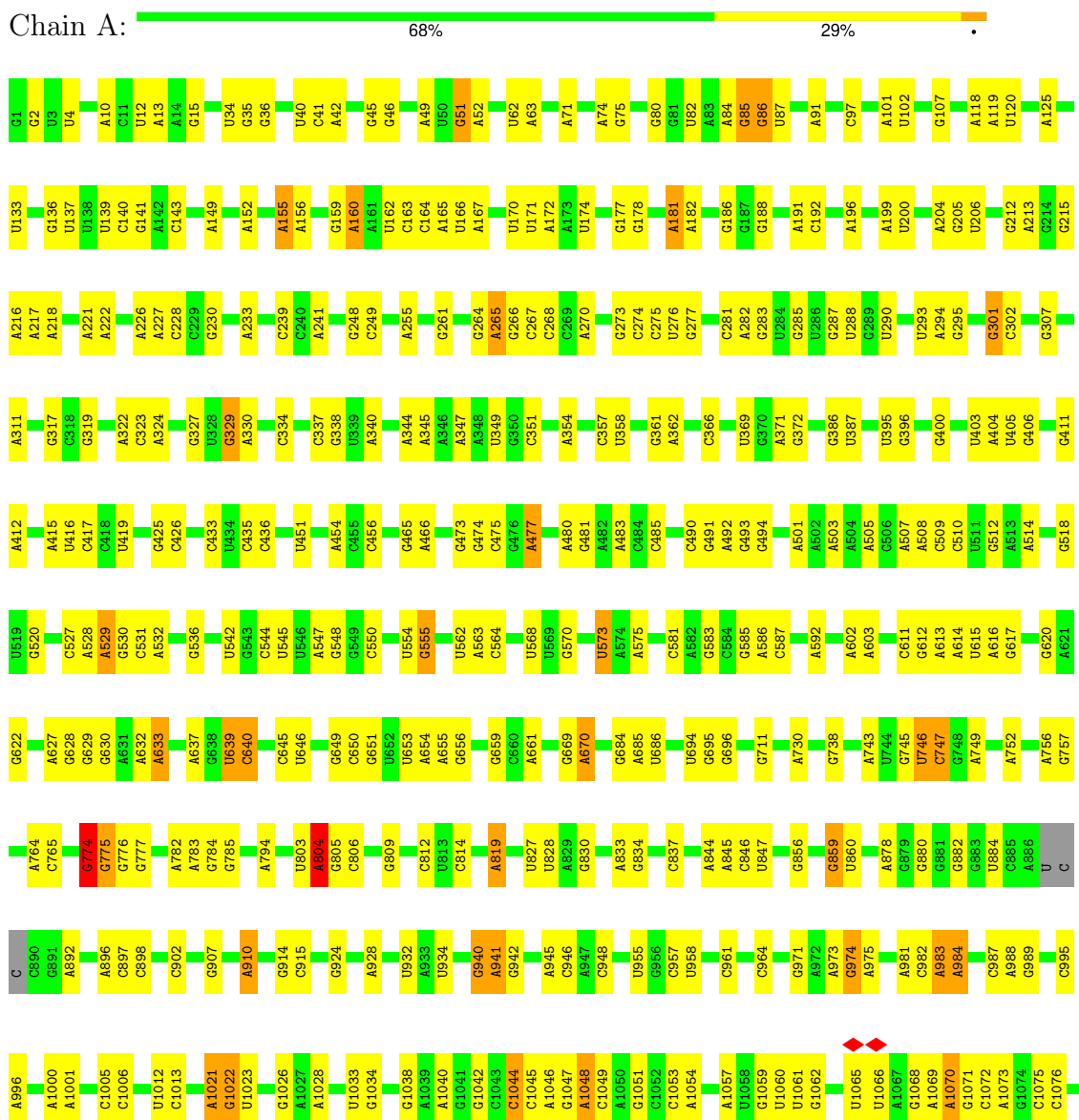
- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	83	Total 83	O 83	0
64	B	3	Total 3	O 3	0
64	C	3	Total 3	O 3	0
64	E	1	Total 1	O 1	0
64	L	1	Total 1	O 1	0
64	Q	1	Total 1	O 1	0
64	U	1	Total 1	O 1	0
64	W	3	Total 3	O 3	0
64	X	2	Total 2	O 2	0
64	Z	2	Total 2	O 2	0
64	0	1	Total 1	O 1	0
64	2	1	Total 1	O 1	0
64	a	46	Total 46	O 46	0
64	k	1	Total 1	O 1	0
64	q	2	Total 2	O 2	0
64	s	2	Total 2	O 2	0

### 3 Residue-property plots

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

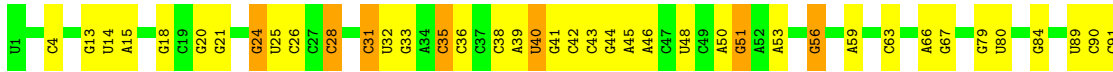
- Molecule 1: 23S rRNA



C1079	C1196	A1321	G1482	A1593	G1725	G1857	G1992	G2103	A2212	G2332	G2445	G2553	G2715
A1084	G1197	A1328	U1485	U1594	G1726	A1858	U1993	C2104	U2219	A2333	G2446	U2554	C2716
A1085	U1203	U1329	U1486	C1607	A1727	G1867	C1997	C2105	U2220	U2334	G2447	A2566	U2720
A1086	A1204	A1608	U1487	C1608	C1728	C1868	G1997	U2106	A2225	A2335	A2448	A2567	A2721
G1087	A1205	G1331	U1488	A1609	U1730	G1869	G2004	G2110	G2226	A2336	U2449	U2568	G2722
A1088	G1206	U1331	A1490	A1610	G1731	C1870	A2013	G2111	G2238	C2342	U2457	A2572	A2726
A1089	U1207	G1341	G1491	G1613	A1738	A1871	A2013	G2112	G2239	G2345	G2464	C2573	A2733
A1090	C1208	U1344	G1492	A1614	A1739	C1874	A2020	U2113	G2243	G2346	G2465	C2574	A2733
U1097	U1209	C1345	A1493	A1615	G1740	U1882	U2022	G2116	U2243	C2350	A2469	G2578	U2743
U1098	G1210	U1346	A1494	C1616	A1741	U1883	C2023	A2117	G2250	U2356	G2470	C2579	U2743
U1099	U1211	U1352	A1503	C1617	U1742	U1884	G2023	A2118	G2251	G2357	C2471	U2580	G2744
C1104	G1212	U1352	A1504	A1618	A1755	G1884	G2029	A2119	C2251	A2358	U2474	U2580	A2748
U1105	U1218	U1365	C1507	G1619	A1756	A1890	A2030	G2120	U2262	A2359	G2475	U2585	A2749
G1106	U1219	A1366	A1508	G1622	U1758	A1891	A2031	C2121	C2263	C2359	C2476	C2586	A2750
G1110	G1227	A1367	A1509	G1627	U1759	C1895	G2032	U2122	C2264	G2360	A2477	U2586	A2751
A1111	G1227	G1368	G1510	G1627	C1764	G1895	A2033	U2123	U2268	G2361	C2480	C2587	G2752
G1112	G1232	G1369	G1511	G1633	A1773	C1905	G2033	U2124	A2268	G2362	G2481	G2602	A2753
U1113	U1232	C1370	G1512	G1633	A1774	G1906	G2033	U2125	A2269	A2377	G2482	G2603	A2753
C1114	U1236	G1371	G1513	G1633	G1776	G1907	U2039	U2126	A2270	A2378	G2483	U2604	U2754
C1117	A1237	U1378	G1514	C1639	G1777	G1908	G2043	U2127	A2271	A2379	G2484	U2605	A2758
U1118	G1238	U1379	G1515	C1646	U1779	A1913	C2043	U2128	A2272	A2380	G2485	U2606	A2764
U1119	U1244	U1383	G1516	U1647	A1780	A1914	G2046	U2129	A2273	A2381	G2486	U2607	A2765
G1124	G1245	A1383	G1517	U1648	U1781	C1915	G2046	U2130	A2274	G2382	C2487	U2608	A2765
U1130	A1247	C1399	G1518	G1649	U1782	3TD1915	G2049	U2131	A2275	U2383	G2488	U2609	A2765
G1131	G1248	G1416	G1519	G1659	A1783	U1916	C2055	U2132	C2275	U2384	U2491	U2610	A2765
U1132	U1249	U1416	G1520	G1660	A1784	A1918	G2056	U2133	A2276	A2385	U2492	U2611	A2765
C1135	G1250	U1419	G1521	G1660	A1789	A1918	G2056	U2134	A2277	A2386	G2494	U2612	A2765
G1139	C1251	A1420	G1522	G1666	C1790	G1929	A2060	U2135	A2278	G2387	G2495	U2613	A2765
C1140	A1252	A1420	G1523	G1666	A1791	U1930	G2061	U2136	A2279	A2388	G2496	U2614	A2765
U1141	A1253	G1425	G1524	G1667	A1792	U1931	A2062	U2137	A2280	G2389	G2497	U2615	A2765
A1142	U1253	G1425	G1525	A1668	A1793	U1931	A2063	U2138	A2281	U2393	G2498	U2616	A2765
A1144	G1256	U1428	G1526	A1669	A1794	U1937	C2063	U2139	A2282	U2394	G2499	U2617	A2765
C1170	U1256	C1428	G1527	G1674	C1795	A1938	G2069	U2140	A2283	G2399	G2500	U2618	A2765
G1171	A1265	G1429	G1528	C1674	U1796	U1938	A2070	U2141	A2284	U2406	U2501	C2620	A2765
C1172	A1268	A1430	G1529	C1675	U1796	U1939	A2071	U2142	A2285	A2407	G2502	U2621	A2765
U1173	A1268	A1433	G1530	C1685	C1800	U1940	C2072	U2143	A2286	A2408	G2503	U2622	A2765
U1174	A1275	G1452	G1531	U1693	A1801	C1941	A2077	U2144	A2287	U2409	U2504	U2623	A2765
A1175	A1275	A1453	G1532	G1695	A1802	C1942	C2078	U2145	A2288	G2310	G2505	U2624	A2765
U1176	A1275	C1454	G1533	G1695	A1803	U1944	U2079	U2146	A2289	A2311	U2506	U2625	A2765
G1177	G1281	U1458	G1534	A1698	A1808	U1955	A2080	U2147	A2290	G2315	A2518	U2626	A2765
C1178	U1288	U1460	G1535	A1698	A1809	C1962	U2086	U2148	A2291	G2318	G2519	U2627	A2765
G1179	G1288	U1461	G1536	G1703	A1810	C1962	G2087	U2149	A2292	U2319	G2520	A2634	A2765
U1180	C1297	U1466	G1537	G1703	A1816	C1965	U2092	U2150	A2293	G2321	U2521	U2635	A2765
G1181	G1297	U1466	G1538	G1710	C1833	C1966	G2093	U2151	A2294	A2322	U2522	U2636	A2765
G1182	C1297	U1467	G1539	U1714	U1835	C1967	G2093	U2152	A2295	A2323	U2523	U2637	A2765
U1183	U1468	U1468	G1540	U1715	G1835	A1970	C2096	U2153	A2296	U2324	G2524	U2638	A2765
U1184	G1300	U1468	A1579	U1716	G1842	U1971	U2097	U2154	A2297	U2325	A2430	U2639	A2765
A1189	A1301	U1468	A1580	A1717	G1847	G1972	U2098	U2155	A2298	C2326	U2431	C2699	A2765
G1190	C1314	G1471	G1581	G1721	U1847	U1982	U2099	U2156	A2299	A2327	A2432	C2710	A2765
C1320	U1476	U1476	A1590	G1724	A1853	U1991	G2102	A2211	A2300	A2328	U2435	G2714	A2765



- Molecule 2: 5S rRNA



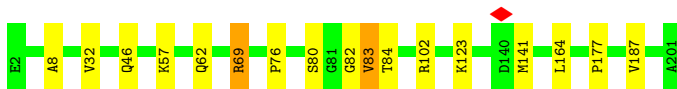
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



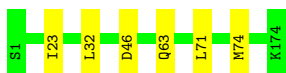
- Molecule 5: 50S ribosomal protein L4



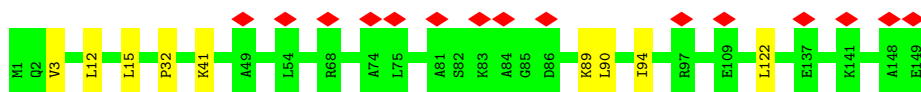
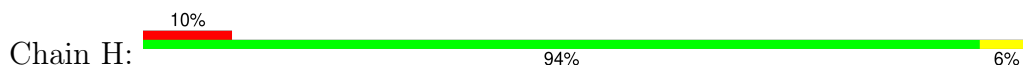
- Molecule 6: 50S ribosomal protein L5



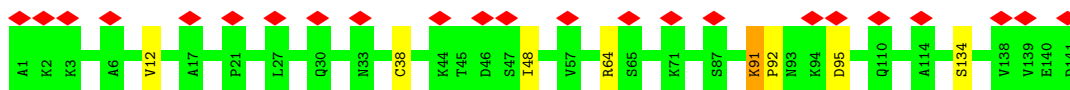
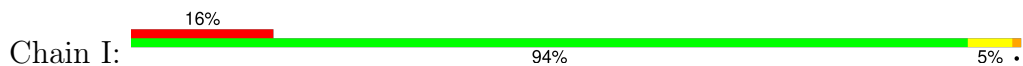
- Molecule 7: 50S ribosomal protein L6



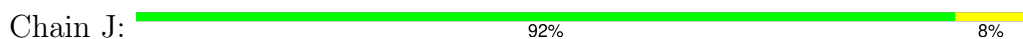
- Molecule 8: 50S ribosomal protein L9



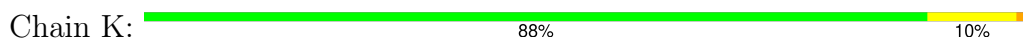
- Molecule 9: 50S ribosomal protein L11



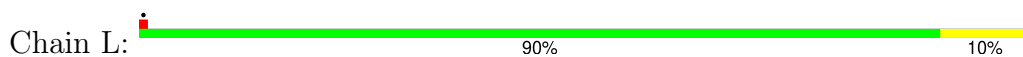
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



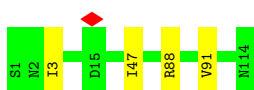
- Molecule 15: 50S ribosomal protein L18

Chain O:  95% 5%



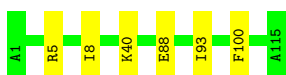
- Molecule 16: 50S ribosomal protein L19

Chain P:  96% .



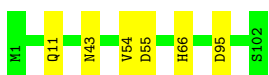
- Molecule 17: 50S ribosomal protein L20

Chain Q:  95% 5%



- Molecule 18: 50S ribosomal protein L21

Chain R:  94% 6%



- Molecule 19: 50S ribosomal protein L22

Chain S:  94% 6%



- Molecule 20: 50S ribosomal protein L23

Chain T:  95% 5%



- Molecule 21: 50S ribosomal protein L24

Chain U:  97% .



- Molecule 22: 50S ribosomal protein L25

Chain V:  98%



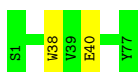
- Molecule 23: 50S ribosomal protein L27

Chain W:  95%



- Molecule 24: 50S ribosomal protein L28

Chain X:  97%



- Molecule 25: 50S ribosomal protein L29

Chain Y:  98%



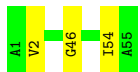
- Molecule 26: 50S ribosomal protein L30

Chain Z:  95%



- Molecule 27: 50S ribosomal protein L32

Chain 0:  95%



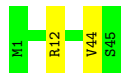
- Molecule 28: 50S ribosomal protein L33

Chain 1:  96%



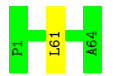
- Molecule 29: 50S ribosomal protein L34

Chain 2:  96%



• Molecule 30: 50S ribosomal protein L35

Chain 3:  98%

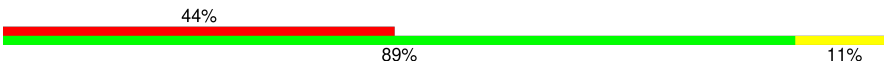


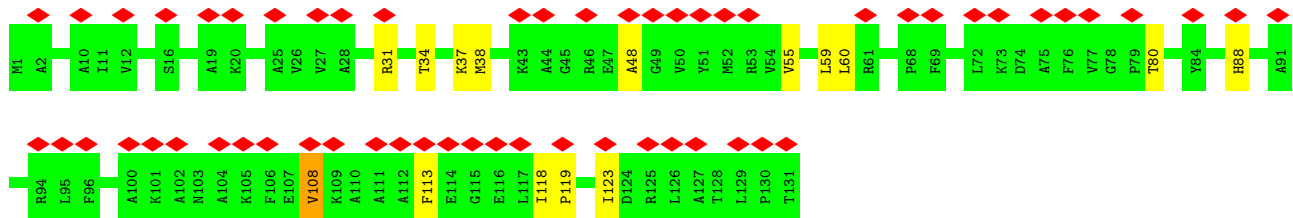
• Molecule 31: 50S ribosomal protein L36

Chain 4:  95%



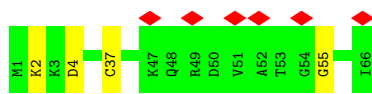
• Molecule 32: 50S ribosomal protein L10

Chain 5:  44% 89% 11%



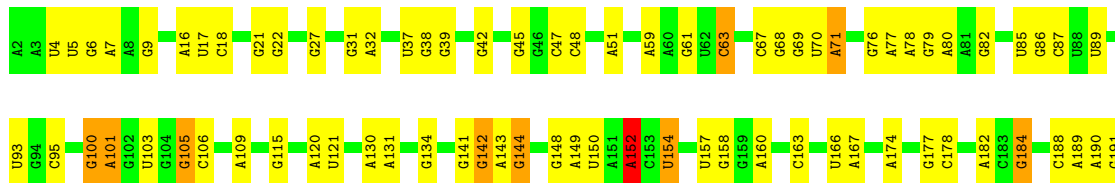
• Molecule 33: 50S ribosomal protein L31

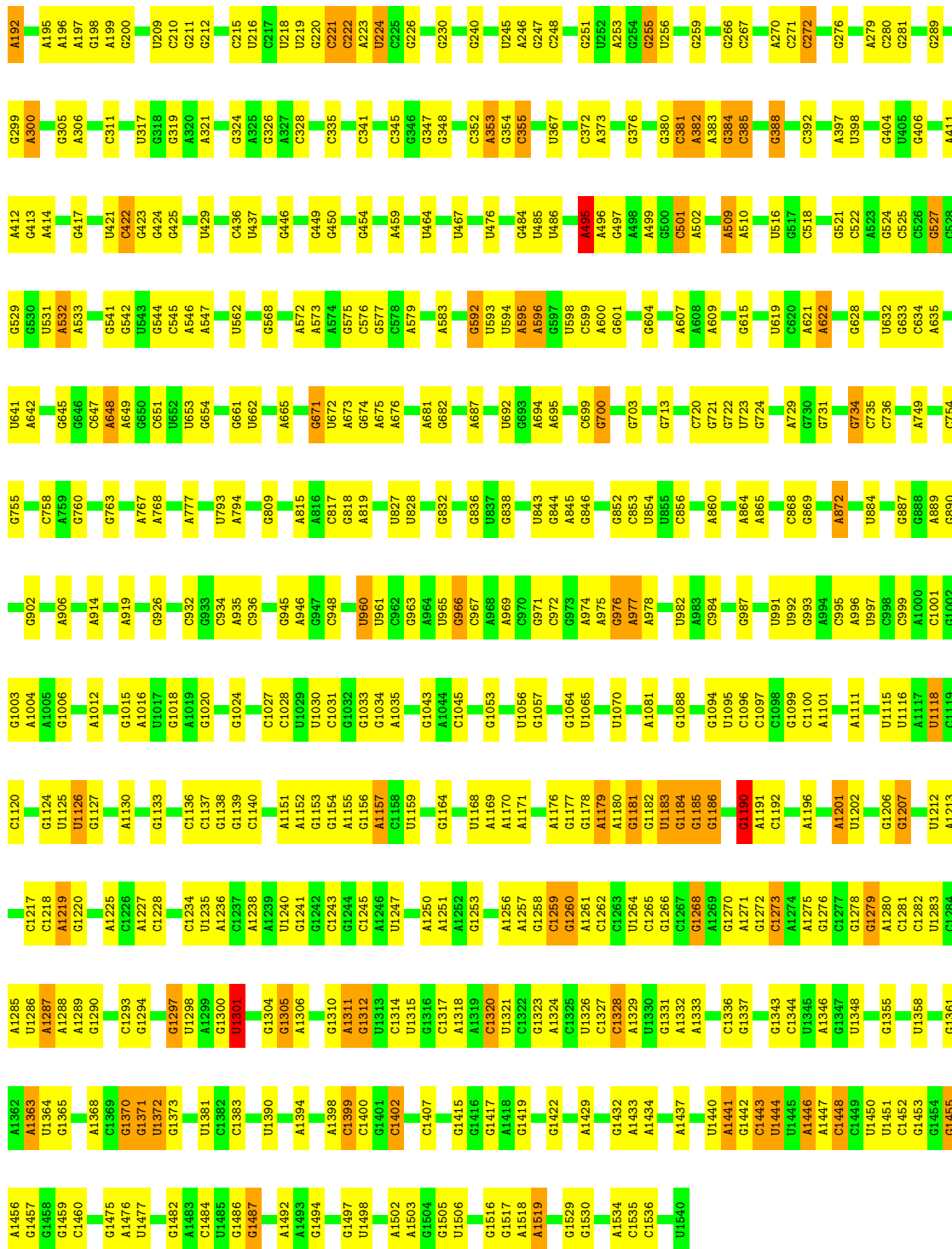
Chain 6:  9% 94% 6%



• Molecule 34: 16S rRNA

Chain a:  62% 32% 5%





• Molecule 35: 30S ribosomal protein S2



- Molecule 36: 30S ribosomal protein S3

Chain c:  94% 6%



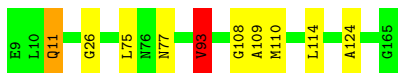
- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .




- Molecule 38: 30S ribosomal protein S5

Chain e:  94% 5% ..



- Molecule 39: 30S ribosomal protein S6

Chain f:  85% 11% .



- Molecule 40: 30S ribosomal protein S7

Chain g:  95% 5%



- Molecule 41: 30S ribosomal protein S8

Chain h:  94% 5% .

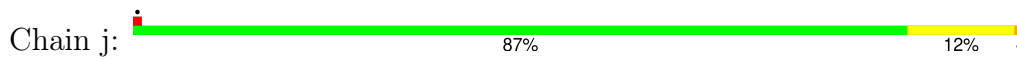


- Molecule 42: 30S ribosomal protein S9

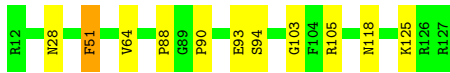
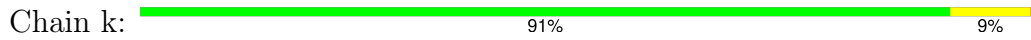
Chain i:  91% 9%



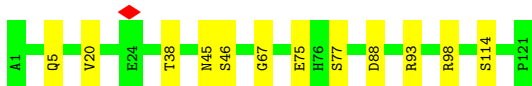
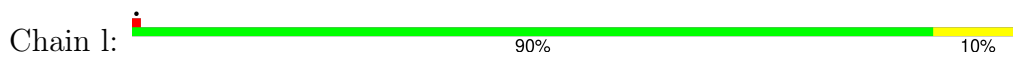
- Molecule 43: 30S ribosomal protein S10



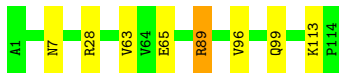
- Molecule 44: 30S ribosomal protein S11



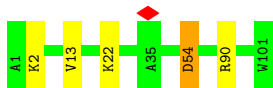
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



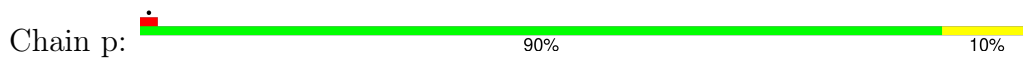
- Molecule 47: 30S ribosomal protein S14

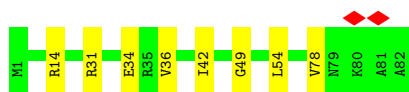


- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

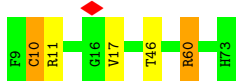
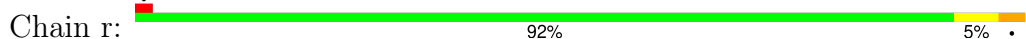




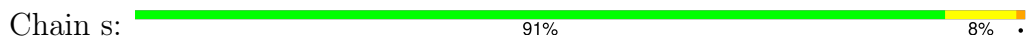
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



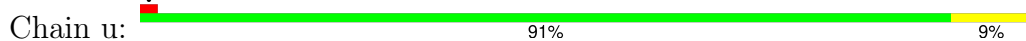
- Molecule 52: 30S ribosomal protein S19



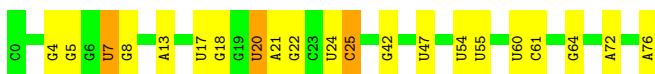
- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21



- Molecule 55: tRNA-fMet



- Molecule 55: tRNA-fMet





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5200	Depositor
Magnification	39683	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.012	Depositor
Map size ( $\text{\AA}$ )	384.4, 384.4, 384.4	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.24, 1.24, 1.24	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: 4OC, 1MG, 2MA, H2U, FME, PSU, GTP, 2MG, K, OMC, 5MC, MG, MIA, 3TD, OMU, 4SU, 6MZ, 7MG, UR3, MA6, 5MU, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/69177	0.71	29/107915 (0.0%)
2	B	0.40	0/2876	0.72	0/4483
3	C	0.49	0/2121	0.74	0/2852
4	D	0.49	0/1578	0.74	0/2124
5	E	0.49	0/1563	0.80	0/2103
6	F	0.56	1/1434 (0.1%)	0.81	0/1926
7	G	0.53	0/1324	0.73	0/1794
8	H	0.57	0/1122	0.78	0/1515
9	I	0.67	0/1046	0.87	2/1410 (0.1%)
10	J	0.51	0/1143	0.82	2/1540 (0.1%)
11	K	0.51	0/947	0.77	1/1268 (0.1%)
12	L	0.49	0/1044	0.81	0/1391
13	M	0.48	0/1093	0.79	0/1460
14	N	0.53	0/964	0.83	0/1289
15	O	0.53	0/902	0.84	0/1209
16	P	0.51	0/929	0.74	0/1242
17	Q	0.51	0/946	0.85	0/1260
18	R	0.50	0/823	0.69	0/1100
19	S	0.49	0/852	0.83	0/1142
20	T	0.49	0/736	0.72	0/984
21	U	0.53	0/787	0.77	0/1051
22	V	0.50	0/752	0.76	0/1008
23	W	0.44	0/579	0.65	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.51	0/495	0.84	0/658
26	Z	0.54	0/438	0.87	0/586
27	0	0.49	0/440	0.83	0/588
28	1	0.48	0/424	0.70	0/565
29	2	0.50	0/370	0.99	0/487
30	3	0.47	0/513	0.81	0/676
31	4	0.45	0/303	0.75	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	5	0.68	0/1001	0.88	0/1350
33	6	0.57	0/531	0.82	0/709
34	a	0.38	0/36700	0.72	19/57246 (0.0%)
35	b	0.56	0/1735	0.80	0/2338
36	c	0.54	0/1651	0.78	0/2225
37	d	0.56	0/1665	0.79	0/2227
38	e	0.54	0/1180	0.82	0/1587
39	f	0.57	1/835 (0.1%)	0.79	0/1128
40	g	0.54	0/1195	0.82	0/1602
41	h	0.51	0/989	0.81	0/1326
42	i	0.56	0/1034	0.79	0/1375
43	j	0.60	0/796	0.79	0/1077
44	k	0.52	0/885	0.78	0/1195
45	l	0.54	0/954	0.79	1/1282 (0.1%)
46	m	0.57	0/892	0.85	0/1193
47	n	0.55	0/822	0.78	0/1095
48	o	0.52	0/722	0.86	0/964
49	p	0.55	0/659	0.79	0/884
50	q	0.54	0/657	0.73	0/881
51	r	0.57	0/544	0.77	0/731
52	s	0.56	0/652	0.77	0/877
53	t	0.54	0/671	0.89	0/888
54	u	0.61	0/550	0.84	0/728
55	v	0.40	1/1747 (0.1%)	0.71	0/2721
55	w	0.67	1/1746 (0.1%)	0.90	5/2717 (0.2%)
56	x	0.39	0/280	0.72	0/433
57	y	0.39	0/1607	0.71	1/2501 (0.0%)
58	z	0.57	0/3086	0.77	0/4175
All	All	0.44	4/164142 (0.0%)	0.74	60/245093 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-22.64	1.27	1.61
39	f	18	VAL	CA-CB	5.99	1.57	1.54
6	F	107	VAL	CA-CB	5.73	1.56	1.54
55	v	7	4SU	O3'-P	5.16	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	P-O3'-C3'	21.78	152.87	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	O3'-P-O5'	14.89	126.33	104.00
1	A	1022	G	C2'-C3'-O3'	11.13	126.20	109.50
1	A	1378	A	C4'-C3'-O3'	10.12	124.58	109.40
55	w	117	U	OP2-P-O3'	-9.56	79.33	108.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62278	0	31344	162	0
2	B	2572	0	1302	21	0
3	C	2082	0	2157	4	0
4	D	1557	0	1604	4	0
5	E	1544	0	1607	2	0
6	F	1410	0	1447	0	0
7	G	1304	0	1348	2	0
8	H	1111	0	1148	2	0
9	I	1032	0	1088	1	0
10	J	1120	0	1151	3	0
11	K	938	0	1012	6	0
12	L	1035	0	1111	4	0
13	M	1074	0	1157	0	0
14	N	951	0	994	3	0
15	O	892	0	923	5	0
16	P	917	0	965	1	0
17	Q	933	0	1006	2	0
18	R	810	0	834	1	0
19	S	845	0	909	0	0
20	T	730	0	795	0	0
21	U	779	0	834	0	0
22	V	739	0	763	0	0
23	W	572	0	593	1	0
24	X	625	0	655	2	0
25	Y	494	0	530	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	434	0	477	1	0
27	0	434	0	448	1	0
28	1	417	0	451	0	0
29	2	367	0	405	1	0
30	3	504	0	574	0	0
31	4	302	0	343	1	0
32	5	988	0	1025	2	0
33	6	522	0	524	1	0
34	a	33028	0	16644	205	0
35	b	1704	0	1732	3	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	0	0
38	e	1164	0	1212	3	0
39	f	817	0	808	11	0
40	g	1181	0	1240	1	0
41	h	979	0	1034	3	0
42	i	1022	0	1070	2	0
43	j	786	0	828	3	0
44	k	869	0	878	1	0
45	l	940	0	1001	3	0
46	m	883	0	944	1	0
47	n	810	0	852	0	0
48	o	714	0	737	0	0
49	p	649	0	666	3	0
50	q	648	0	691	2	0
51	r	535	0	552	2	0
52	s	637	0	665	2	0
53	t	665	0	714	0	0
54	u	544	0	579	1	0
55	v	1644	0	840	1	0
55	w	1644	0	841	2	0
56	x	252	0	129	0	0
57	y	1632	0	843	1	0
58	z	3031	0	3050	5	0
59	A	10	0	10	0	0
60	0	3	0	0	0	0
60	3	2	0	0	0	0
60	4	1	0	0	0	0
60	A	404	0	0	0	0
60	B	6	0	0	0	0
60	C	2	0	0	0	0
60	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	E	1	0	0	0	0
60	J	1	0	0	0	0
60	L	1	0	0	0	0
60	N	3	0	0	0	0
60	O	1	0	0	0	0
60	S	1	0	0	0	0
60	T	2	0	0	0	0
60	a	221	0	0	0	0
60	e	1	0	0	0	0
60	i	1	0	0	0	0
60	t	1	0	0	0	0
60	u	1	0	0	0	0
60	v	2	0	0	0	0
60	y	4	0	0	0	0
60	z	2	0	0	0	0
61	A	7	0	0	0	0
61	v	1	0	0	0	0
62	y	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	2	1	0	0	0	0
64	A	83	0	0	0	0
64	B	3	0	0	0	0
64	C	3	0	0	0	0
64	E	1	0	0	0	0
64	L	1	0	0	0	0
64	Q	1	0	0	0	0
64	U	1	0	0	0	0
64	W	3	0	0	0	0
64	X	2	0	0	0	0
64	Z	2	0	0	0	0
64	a	46	0	0	0	0
64	k	1	0	0	0	0
64	q	2	0	0	0	0
64	s	2	0	0	0	0
All	All	153233	0	103513	462	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 2.

The worst 5 of 462 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:827:U:O4	34:a:872:A:N1	1.68	1.25
1:A:1021:A:N1	1:A:1141:U:O4	1.73	1.20
1:A:2013:A:N1	1:A:2613:U:O4	1.75	1.18
1:A:2030:6MZ:O3'	1:A:2031:A:P	2.02	1.17
34:a:101:A:N1	34:a:152:A:H4'	1.58	1.17

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	235 (87%)	31 (12%)	3 (1%)	11	38
4	D	206/208 (99%)	189 (92%)	14 (7%)	3 (2%)	8	30
5	E	198/200 (99%)	170 (86%)	20 (10%)	8 (4%)	2	15
6	F	175/177 (99%)	159 (91%)	15 (9%)	1 (1%)	21	50
7	G	172/174 (99%)	161 (94%)	10 (6%)	1 (1%)	21	50
8	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	17
9	I	139/141 (99%)	112 (81%)	22 (16%)	5 (4%)	2	16
10	J	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
11	K	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	21
12	L	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	2	16
13	M	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	18	47
14	N	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	42
15	O	114/116 (98%)	105 (92%)	7 (6%)	2 (2%)	6	26
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	14	42
18	R	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	6	26
20	T	90/92 (98%)	78 (87%)	9 (10%)	3 (3%)	3	17
21	U	100/102 (98%)	86 (86%)	12 (12%)	2 (2%)	6	25
22	V	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	38
23	W	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	31
24	X	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
25	Y	58/60 (97%)	51 (88%)	6 (10%)	1 (2%)	7	28
26	Z	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
27	0	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	2	15
28	1	49/51 (96%)	43 (88%)	5 (10%)	1 (2%)	6	25
29	2	43/45 (96%)	39 (91%)	4 (9%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	19
32	5	129/131 (98%)	102 (79%)	17 (13%)	10 (8%)	1	4
33	6	64/66 (97%)	55 (86%)	7 (11%)	2 (3%)	3	18
35	b	216/218 (99%)	184 (85%)	28 (13%)	4 (2%)	6	26
36	c	204/206 (99%)	181 (89%)	17 (8%)	6 (3%)	3	19
37	d	203/205 (99%)	177 (87%)	23 (11%)	3 (2%)	8	30
38	e	156/157 (99%)	128 (82%)	24 (15%)	4 (3%)	4	21
39	f	98/100 (98%)	84 (86%)	11 (11%)	3 (3%)	3	18
40	g	149/151 (99%)	125 (84%)	19 (13%)	5 (3%)	3	17
41	h	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	29
42	i	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2	11
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	10
44	k	114/116 (98%)	94 (82%)	15 (13%)	5 (4%)	2	13
45	l	119/121 (98%)	96 (81%)	19 (16%)	4 (3%)	3	17
46	m	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	4	20
47	n	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2	15
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	12
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	21
50	q	78/80 (98%)	67 (86%)	10 (13%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	8 (10%)	2 (3%)	4	21
53	t	83/85 (98%)	78 (94%)	2 (2%)	3 (4%)	2	16
54	u	63/65 (97%)	43 (68%)	16 (25%)	4 (6%)	1	7
58	z	391/393 (100%)	351 (90%)	34 (9%)	6 (2%)	8	30
All	All	6217/6320 (98%)	5428 (87%)	642 (10%)	147 (2%)	7	22

5 of 147 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	5	123	ILE
33	6	4	ASP
36	c	96	VAL
36	c	156	LEU
38	e	93	VAL

### 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	
3	C	216/216 (100%)	212 (98%)	4 (2%)	50	66
4	D	163/163 (100%)	160 (98%)	3 (2%)	51	67
5	E	164/164 (100%)	157 (96%)	7 (4%)	26	51
6	F	148/148 (100%)	145 (98%)	3 (2%)	48	65
7	G	135/135 (100%)	134 (99%)	1 (1%)	76	78
8	H	114/114 (100%)	113 (99%)	1 (1%)	70	76
9	I	109/109 (100%)	108 (99%)	1 (1%)	70	76
10	J	115/115 (100%)	110 (96%)	5 (4%)	26	51
11	K	103/103 (100%)	98 (95%)	5 (5%)	22	49
12	L	101/101 (100%)	98 (97%)	3 (3%)	36	59
13	M	109/109 (100%)	105 (96%)	4 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	99/99 (100%)	96 (97%)	3 (3%)	36	59
15	O	86/86 (100%)	84 (98%)	2 (2%)	44	63
16	P	99/99 (100%)	96 (97%)	3 (3%)	36	59
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	57
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	62
19	S	92/92 (100%)	88 (96%)	4 (4%)	26	51
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	62
21	U	83/83 (100%)	82 (99%)	1 (1%)	63	72
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	71
23	W	57/57 (100%)	56 (98%)	1 (2%)	51	67
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	45 (96%)	2 (4%)	26	51
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	63
29	2	37/37 (100%)	37 (100%)	0	100	100
30	3	51/51 (100%)	50 (98%)	1 (2%)	48	65
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	98 (98%)	2 (2%)	48	65
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	67
35	b	180/180 (100%)	174 (97%)	6 (3%)	33	57
36	c	170/170 (100%)	167 (98%)	3 (2%)	51	67
37	d	172/172 (100%)	171 (99%)	1 (1%)	78	80
38	e	120/119 (101%)	116 (97%)	4 (3%)	33	57
39	f	87/87 (100%)	83 (95%)	4 (5%)	24	50
40	g	124/124 (100%)	123 (99%)	1 (1%)	73	77
41	h	104/104 (100%)	102 (98%)	2 (2%)	50	66
42	i	105/105 (100%)	103 (98%)	2 (2%)	50	66
43	j	86/86 (100%)	82 (95%)	4 (5%)	23	50
44	k	89/89 (100%)	84 (94%)	5 (6%)	19	46
45	l	102/102 (100%)	99 (97%)	3 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	m	92/92 (100%)	88 (96%)	4 (4%)	26	51
47	n	83/83 (100%)	81 (98%)	2 (2%)	43	62
48	o	76/76 (100%)	75 (99%)	1 (1%)	61	71
49	p	65/65 (100%)	64 (98%)	1 (2%)	57	69
50	q	74/74 (100%)	72 (97%)	2 (3%)	39	60
51	r	56/56 (100%)	55 (98%)	1 (2%)	51	67
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	51
53	t	65/65 (100%)	63 (97%)	2 (3%)	35	59
54	u	55/55 (100%)	55 (100%)	0	100	100
58	z	325/325 (100%)	314 (97%)	11 (3%)	32	57
All	All	5163/5162 (100%)	5035 (98%)	128 (2%)	42	62

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	t	24	ARG
58	z	50	ASP
18	R	66	HIS
17	Q	88	GLU
58	z	81	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
25	Y	31	GLN
58	z	124	GLN
33	6	61	ASN
58	z	22	HIS
49	p	79	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2898/2903 (99%)	757 (26%)	50 (1%)
2	B	119/120 (99%)	34 (28%)	3 (2%)
34	a	1538/1539 (99%)	455 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	v	76/77 (98%)	18 (23%)	0
55	w	76/77 (98%)	29 (38%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	75/76 (98%)	23 (30%)	0
All	All	4793/4804 (99%)	1320 (27%)	53 (1%)

5 of 1320 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	4	U
1	A	10	A
1	A	12	U
1	A	13	A

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1314	C
1	A	1555	G
1	A	2873	A
1	A	1331	G
1	A	1432	G

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

52 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$
57	PSU	y	32	57	18,21,22	1.32	2 (11%)	21,30,33	2.06	5 (23%)
55	H2U	v	20	55	18,21,22	0.80	1 (5%)	19,30,33	1.57	3 (15%)
57	7MG	y	46	57	23,26,27	1.44	4 (17%)	27,39,42	2.52	7 (25%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.28	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	2MG	a	1516	34	23,26,27	1.28	4 (17%)	33,38,41	2.26	9 (27%)
1	PSU	A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.13	4 (19%)
55	5MU	v	54	55	19,22,23	1.46	4 (21%)	27,32,35	2.01	7 (25%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	19,30,33	1.62	3 (15%)
1	H2U	A	2449	1	18,21,22	0.97	2 (11%)	19,30,33	1.40	3 (15%)
1	OMC	A	2498	60,1	19,22,23	0.84	0	25,31,34	1.30	2 (8%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.07	10 (37%)
57	PSU	y	39	57	18,21,22	1.44	2 (11%)	21,30,33	2.03	4 (19%)
34	5MC	a	1407	34	19,22,23	1.72	2 (10%)	26,32,35	1.52	5 (19%)
1	7MG	A	2069	1	23,26,27	1.45	3 (13%)	27,39,42	2.52	10 (37%)
1	PSU	A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.15	4 (19%)
34	2MG	a	1207	34	23,26,27	1.27	3 (13%)	33,38,41	2.79	10 (30%)
1	PSU	A	955	1	18,21,22	1.39	4 (22%)	21,30,33	2.10	4 (19%)
34	MA6	a	1519	34	23,26,27	1.68	5 (21%)	33,38,41	2.35	10 (30%)
55	H2U	w	20	55	18,21,22	0.80	0	19,30,33	1.58	3 (15%)
1	5MC	A	747	1	19,22,23	1.98	2 (10%)	26,32,35	1.58	4 (15%)
34	7MG	a	527	34	23,26,27	1.45	3 (13%)	27,39,42	2.58	7 (25%)
1	2MG	A	2445	1	23,26,27	1.26	3 (13%)	33,38,41	2.37	10 (30%)
1	2MA	A	2503	60,1	22,25,26	1.59	5 (22%)	32,37,40	2.14	8 (25%)
1	PSU	A	2504	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.08	5 (23%)
1	3TD	A	1915	1	19,22,23	7.09	13 (68%)	23,32,35	2.04	5 (21%)
55	PSU	v	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	5MU	A	1939	1	19,22,23	1.44	4 (21%)	27,32,35	2.07	8 (29%)
34	5MC	a	967	34	19,22,23	2.01	2 (10%)	26,32,35	1.42	4 (15%)
57	PSU	y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
1	2MG	A	1835	1	23,26,27	1.34	4 (17%)	33,38,41	2.25	8 (24%)
55	4SU	v	7	55	18,21,22	1.78	4 (22%)	25,30,33	2.39	5 (20%)
57	4SU	y	8	57	18,21,22	1.81	4 (22%)	25,30,33	2.33	6 (24%)
1	OMG	A	2251	55,1	23,26,27	1.29	3 (13%)	32,38,41	1.98	6 (18%)
1	1MG	A	745	1	23,26,27	1.28	3 (13%)	33,39,42	2.03	7 (21%)
1	5MC	A	1962	1	19,22,23	1.70	2 (10%)	26,32,35	1.42	4 (15%)
1	PSU	A	2604	1	18,21,22	1.42	2 (11%)	21,30,33	1.96	4 (19%)
57	5MU	y	54	57	19,22,23	1.48	4 (21%)	27,32,35	2.05	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.26	6 (24%)
1	OMU	A	2552	1	19,22,23	1.31	4 (21%)	25,31,34	2.01	8 (32%)
1	PSU	A	746	1	18,21,22	1.40	2 (11%)	21,30,33	1.97	4 (19%)
1	PSU	A	2457	1	18,21,22	1.48	3 (16%)	21,30,33	2.05	4 (19%)
34	MA6	a	1518	34	23,26,27	1.74	6 (26%)	33,38,41	2.26	11 (33%)
57	MIA	y	37	60,57	28,31,32	2.39	7 (25%)	38,44,47	2.87	14 (36%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.35	3 (15%)
55	PSU	w	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
1	PSU	A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.13	5 (23%)
34	PSU	a	516	34	18,21,22	1.39	2 (11%)	21,30,33	2.12	5 (23%)
34	UR3	a	1498	34	19,22,23	1.09	1 (5%)	26,32,35	1.97	5 (19%)
34	2MG	a	966	34,60	23,26,27	1.29	3 (13%)	33,38,41	2.68	10 (30%)
34	4OC	a	1402	34	20,23,24	0.82	0	25,32,35	1.40	5 (20%)

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	PSU	y	32	57	-	3/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	OMC	A	2498	60,1	-	0/9/27/28	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	3/9/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
34	7MG	a	527	34	-	3/7/37/38	0/3/3/3
1	2MG	A	2445	1	-	3/9/27/28	0/3/3/3
1	2MA	A	2503	60,1	-	2/7/25/26	0/3/3/3
1	PSU	A	2504	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
55	4SU	v	7	55	-	1/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	OMG	A	2251	55,1	-	1/9/27/28	0/3/3/3
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
1	PSU	A	746	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
57	MIA	y	37	60,57	-	3/15/33/34	0/3/3/3
57	H2U	y	16	57	-	0/7/38/39	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34,60	-	3/9/27/28	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.58	1.66	1.43
1	A	1915	3TD	C6-C5	15.69	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.48	1.34	1.53
1	A	1915	3TD	C2-N1	8.50	1.47	1.37
1	A	747	5MC	C5-C4	7.60	1.49	1.44

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.56	138.01	125.46
34	a	966	2MG	C2-N3-C4	8.50	122.63	112.00
34	a	1207	2MG	C2-N3-C4	8.47	122.59	112.00
57	y	46	7MG	N9-C4-N3	8.29	137.61	125.46
57	y	37	MIA	C5-C4-N3	-8.22	118.52	127.18

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2030	6MZ	13	0
1	A	2504	PSU	1	0
1	A	1915	3TD	1	0
1	A	1618	6MZ	9	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 673 ligands modelled in this entry, 670 are monoatomic - leaving 3 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
59	FME	A	3001	-	8,9,10	0.49	0	8,9,11	1.02	0
63	GTP	z	401	60	33,34,34	1.21	4 (12%)	50,54,54	1.79	8 (16%)
62	PHE	y	101	-	10,11,12	0.51	0	8,13,15	0.16	0

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
59	FME	A	3001	-	-	0/7/9/11	-
63	GTP	z	401	60	-	3/22/38/38	0/3/3/3
62	PHE	y	101	-	-	2/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	401	GTP	C5-C4	3.24	1.47	1.38
63	z	401	GTP	C5-N7	-2.18	1.34	1.39
63	z	401	GTP	PA-O3A	2.14	1.61	1.59
63	z	401	GTP	C6-N1	-2.10	1.34	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	401	GTP	C5-C4-N3	-6.15	118.60	128.39
63	z	401	GTP	C2-N3-C4	5.21	121.27	112.30
63	z	401	GTP	N9-C4-N3	4.59	135.13	125.95
63	z	401	GTP	C6-C5-N7	3.33	136.35	130.29
63	z	401	GTP	C3'-C2'-C1'	2.60	106.38	101.46

There are no chirality outliers.

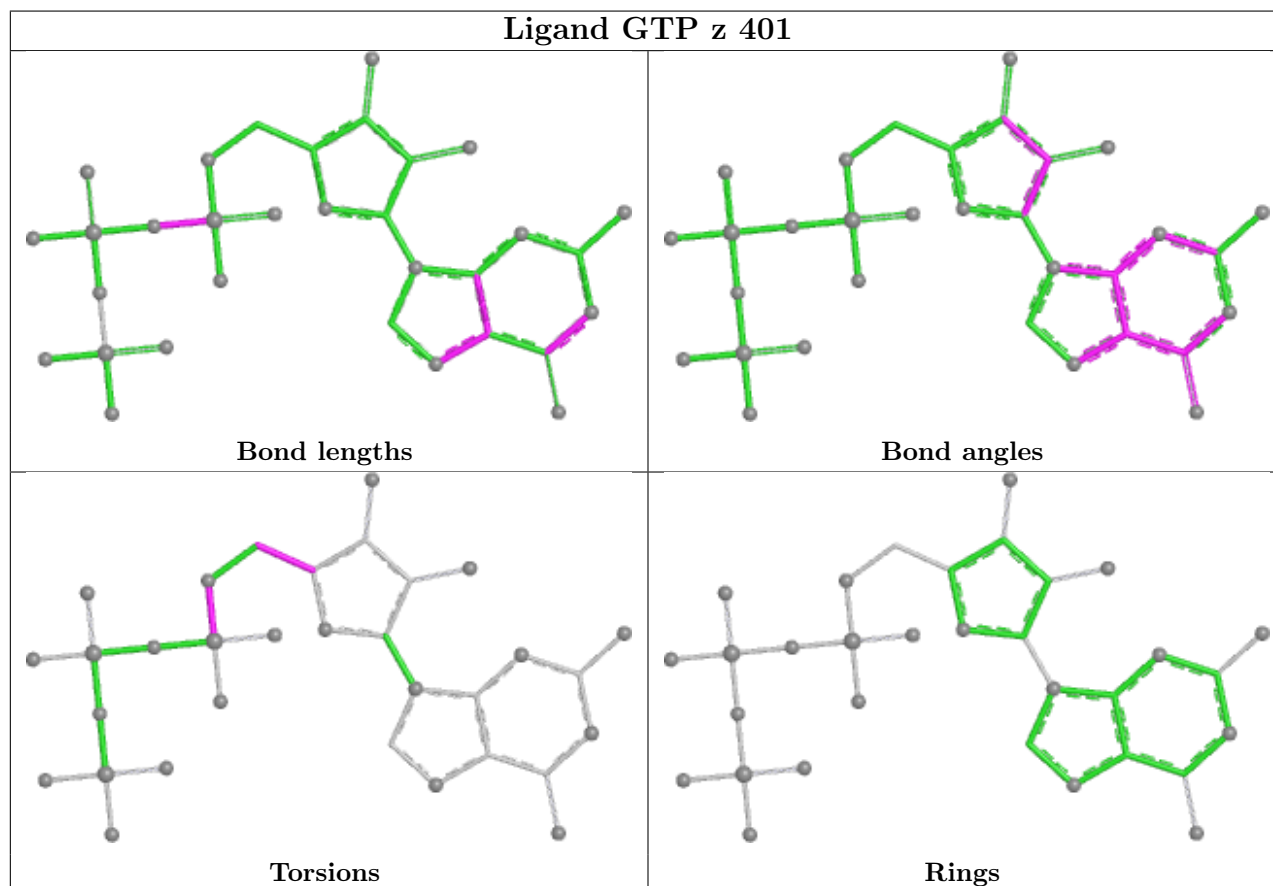
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	z	401	GTP	C5'-O5'-PA-O3A
63	z	401	GTP	C5'-O5'-PA-O1A
63	z	401	GTP	C3'-C4'-C5'-O5'
62	y	101	PHE	N-CA-CB-CG
62	y	101	PHE	C-CA-CB-CG

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
55	w	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	17:C	O3'	117:U	P	2.27
1	A	2030:6MZ	O3'	2031:A	P	2.02
1	A	1618:6MZ	O3'	1619:G	P	1.90
1	w	117:U	O3'	18:G	P	1.27

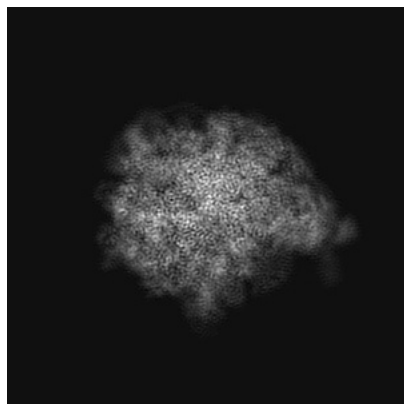
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8815. These allow visual inspection of the internal detail of the map and identification of artifacts.

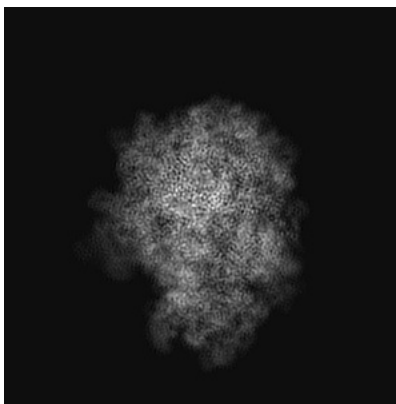
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

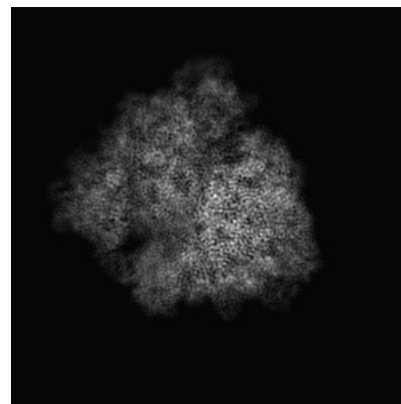
#### 6.1.1 Primary map



X

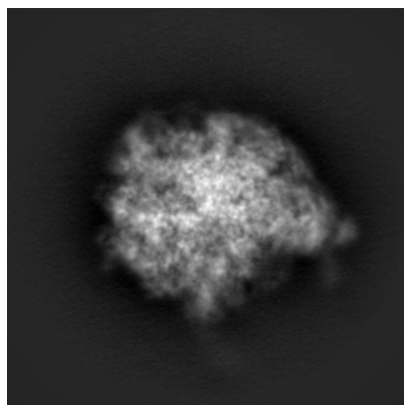


Y

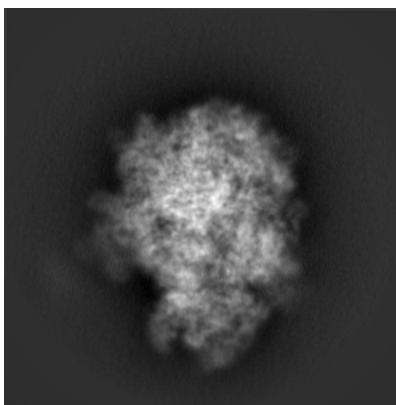


Z

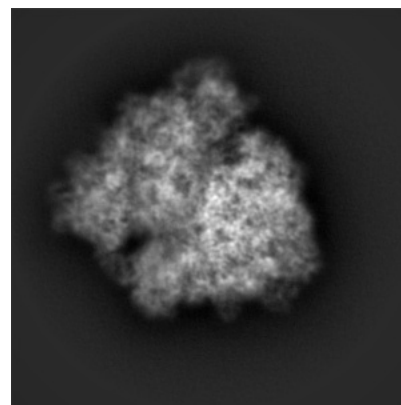
#### 6.1.2 Raw map



X



Y

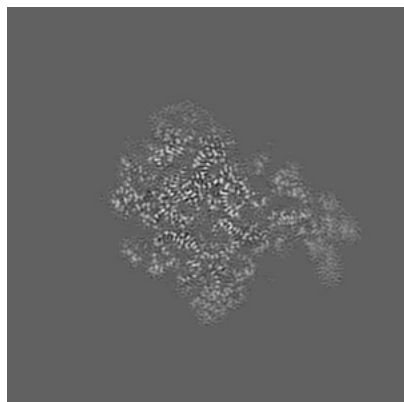


Z

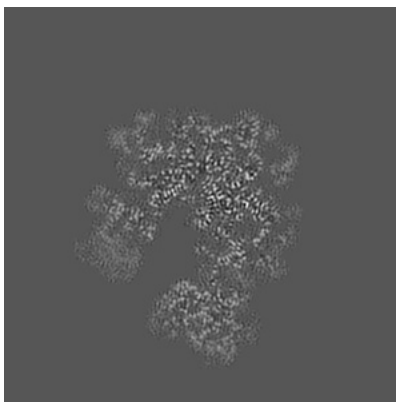
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

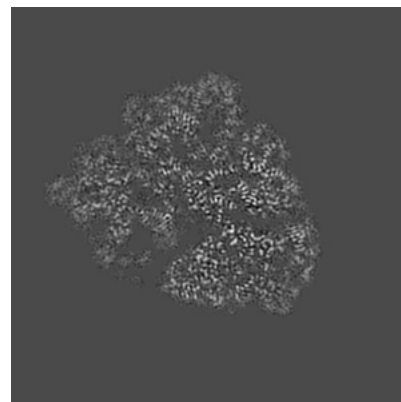
### 6.2.1 Primary map



X Index: 155

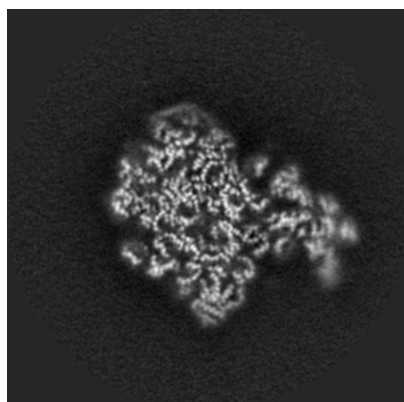


Y Index: 155

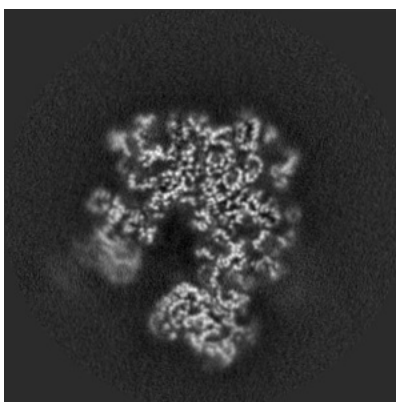


Z Index: 155

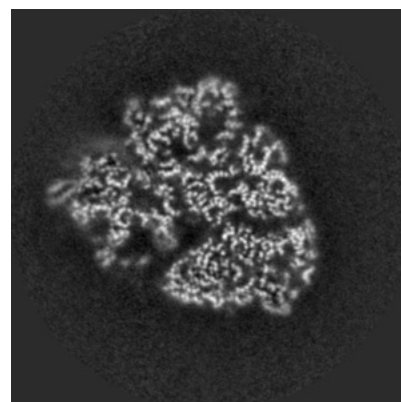
### 6.2.2 Raw map



X Index: 155



Y Index: 155

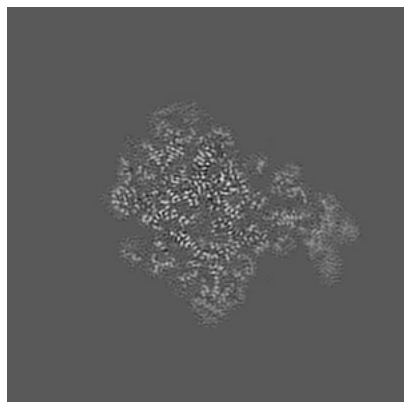


Z Index: 155

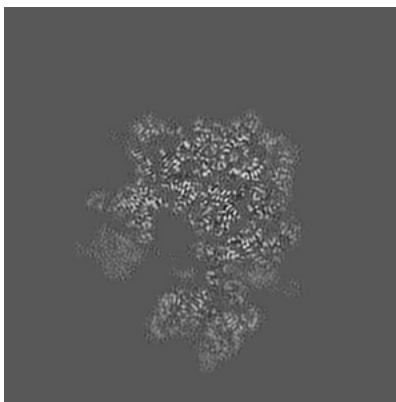
The images above show central slices of the map in three orthogonal directions.

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

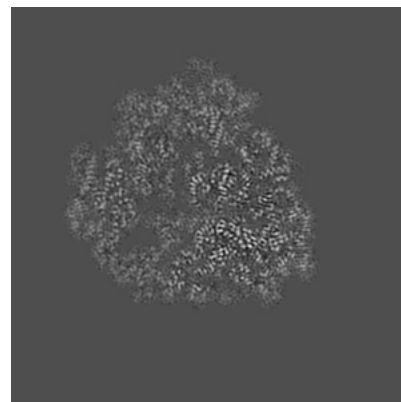
### 6.3.1 Primary map



X Index: 156

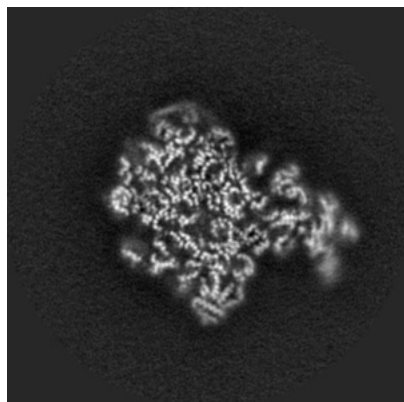


Y Index: 162

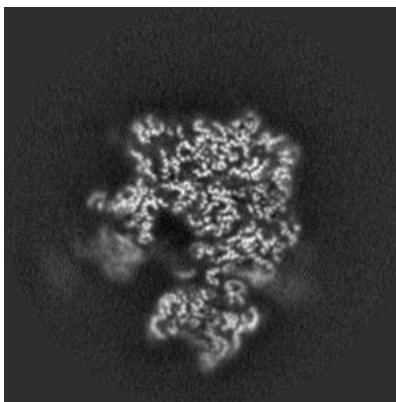


Z Index: 147

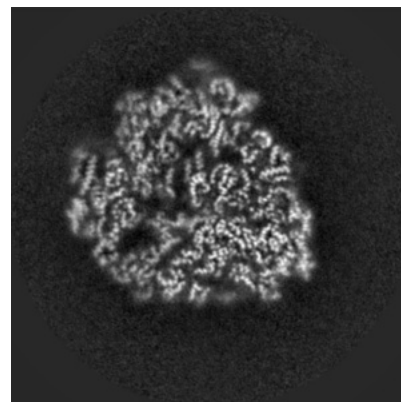
### 6.3.2 Raw map



X Index: 156



Y Index: 162

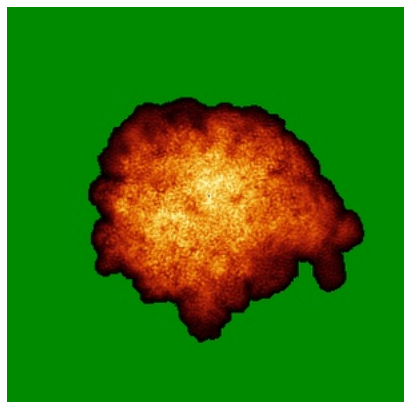


Z Index: 147

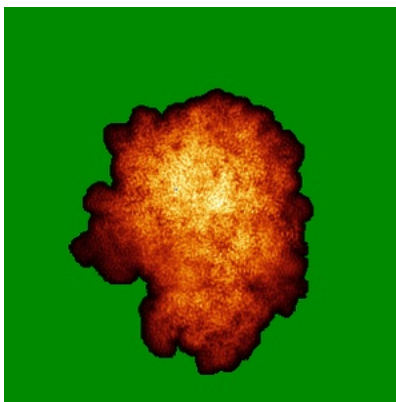
The images above show the largest variance slices of the map in three orthogonal directions.

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

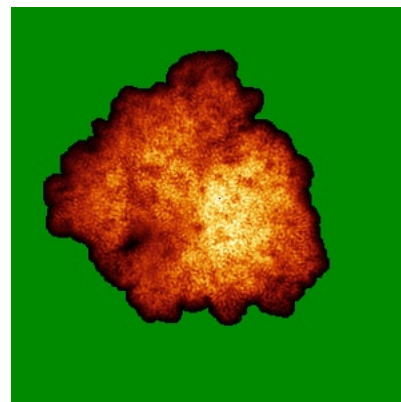
### 6.4.1 Primary map



X

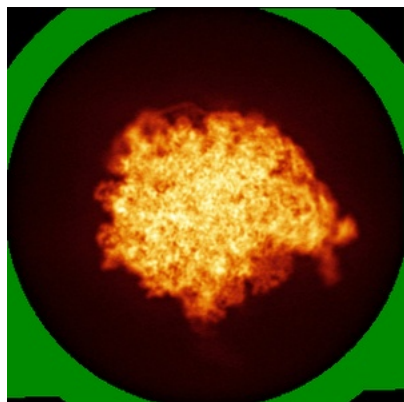


Y

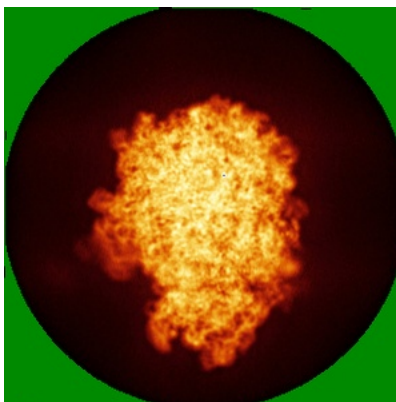


Z

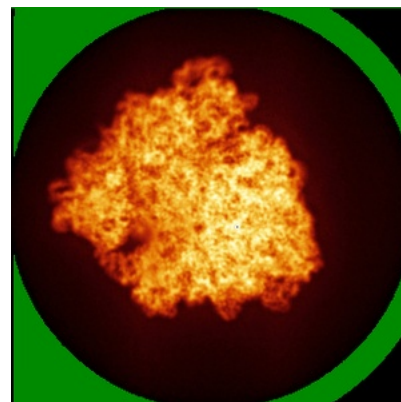
### 6.4.2 Raw map



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](#)

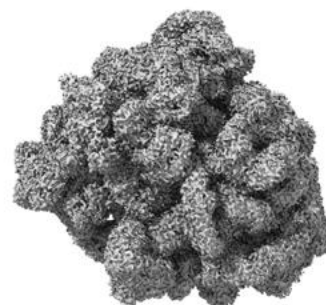
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

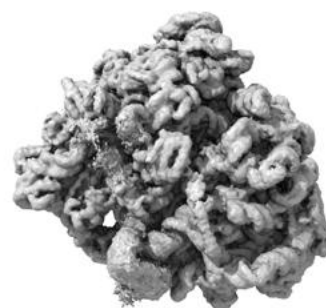
### 6.5.2 Raw map



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.

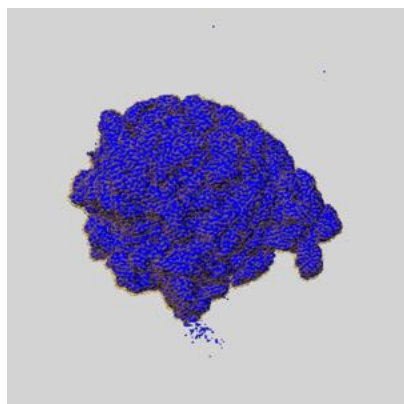
## 6.6 Mask visualisation [i](#)

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

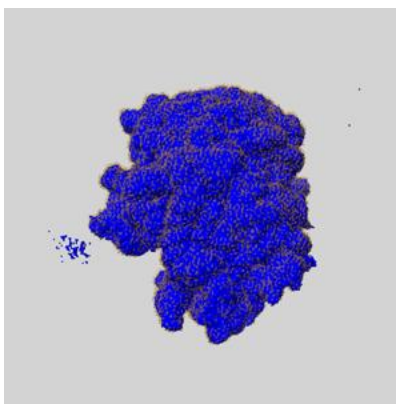
A mask typically either:

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

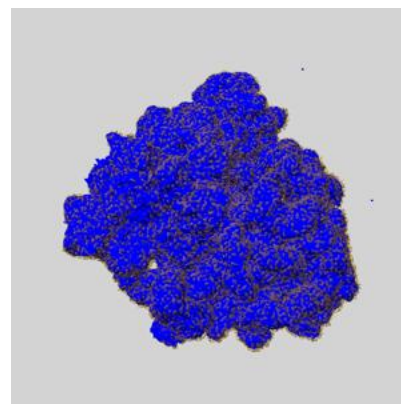
### 6.6.1 emd\_8815\_msk\_1.map [i](#)



X



Y

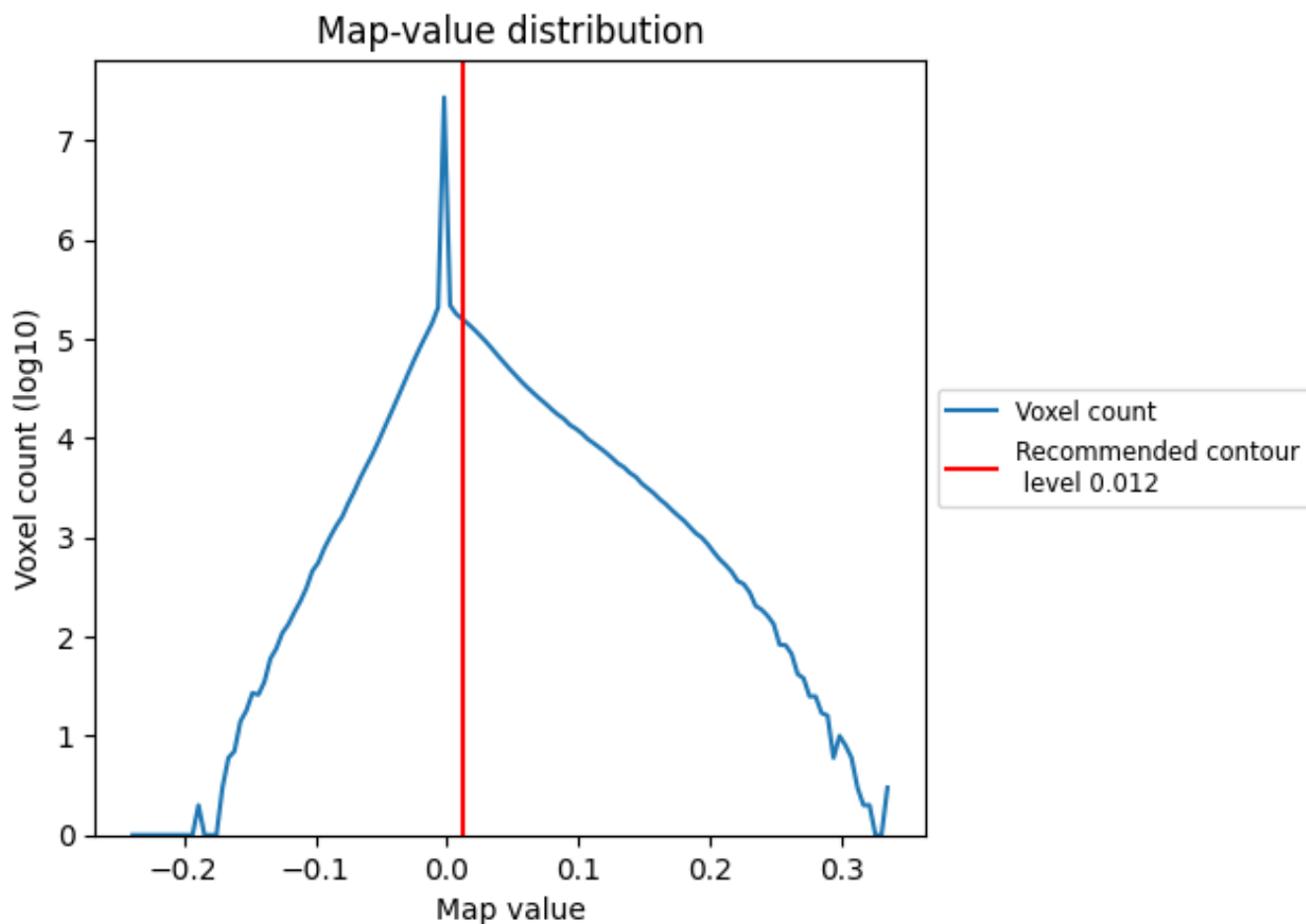


Z

## 7 Map analysis [i](#)

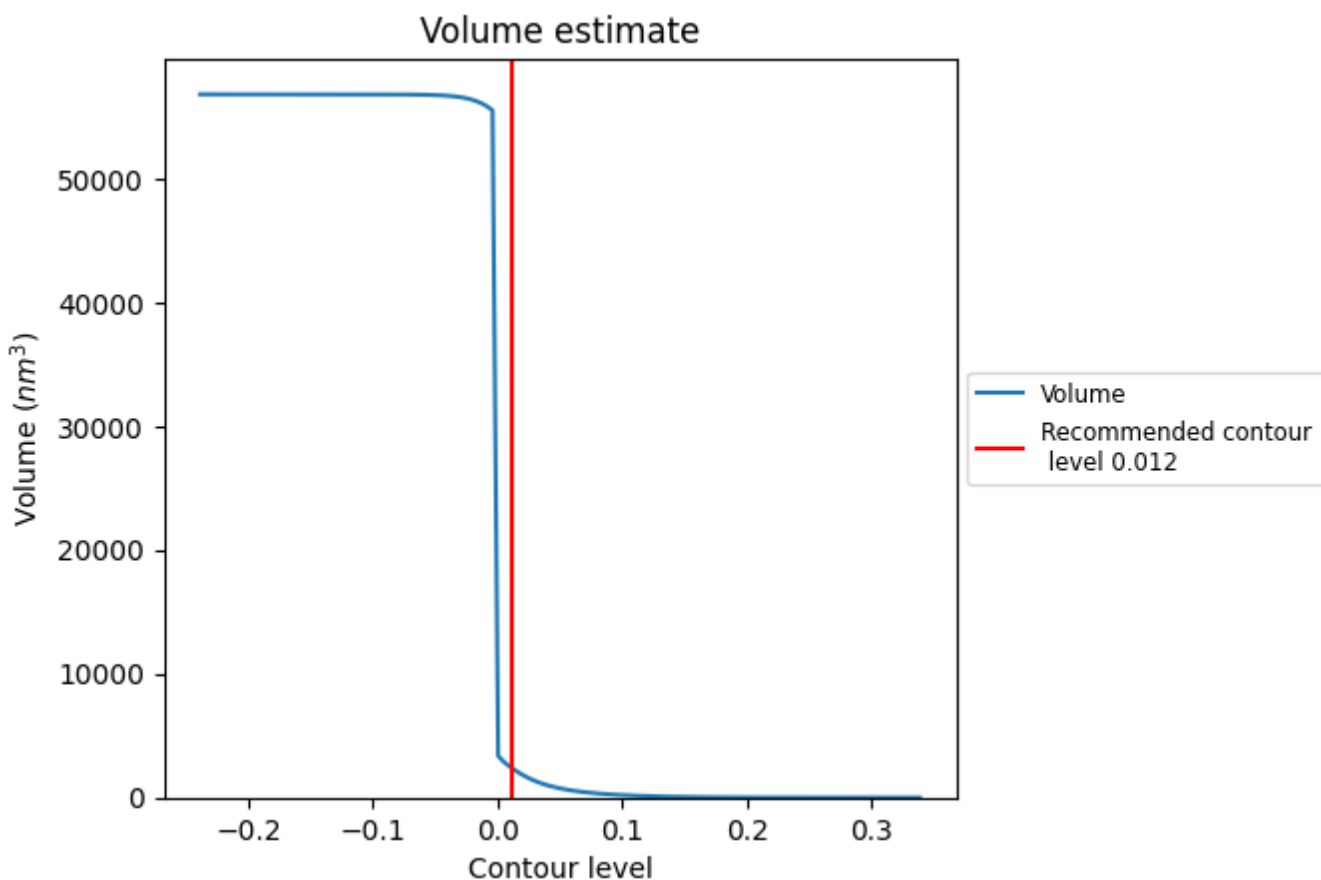
This section contains the results of statistical analysis of the map.

### 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.

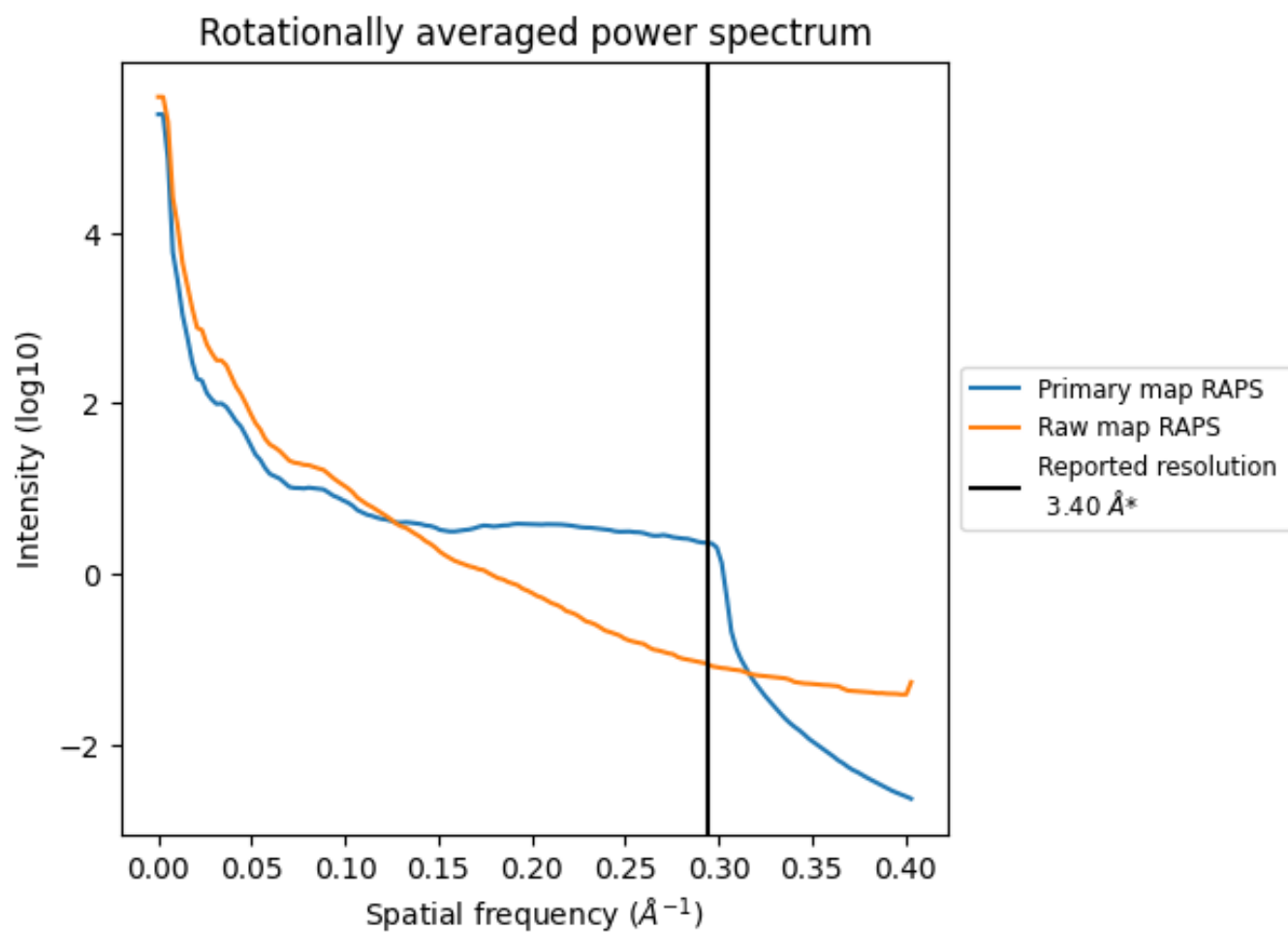
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2345  $\text{nm}^3$ ; this corresponds to an approximate mass of 2119 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

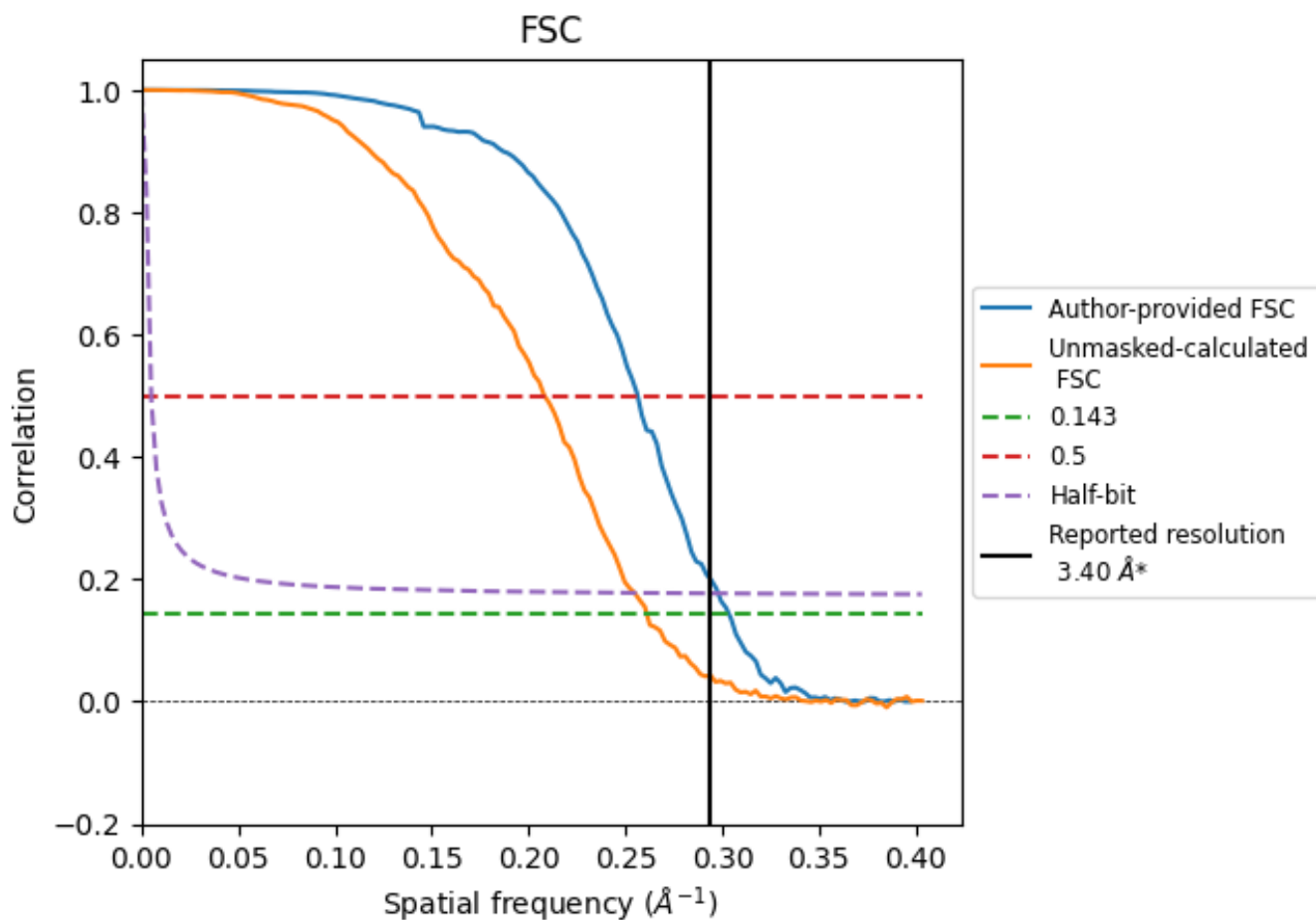


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

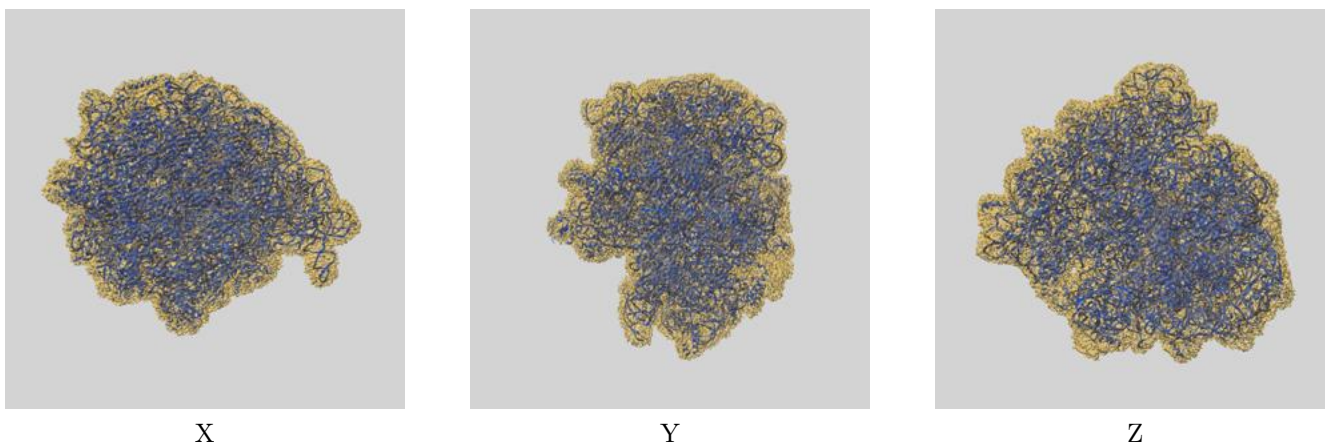
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.29	3.90	3.36
Unmasked-calculated*	3.83	4.80	3.92

\*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 3.83 differs from the reported value 3.4 by more than 10 %

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

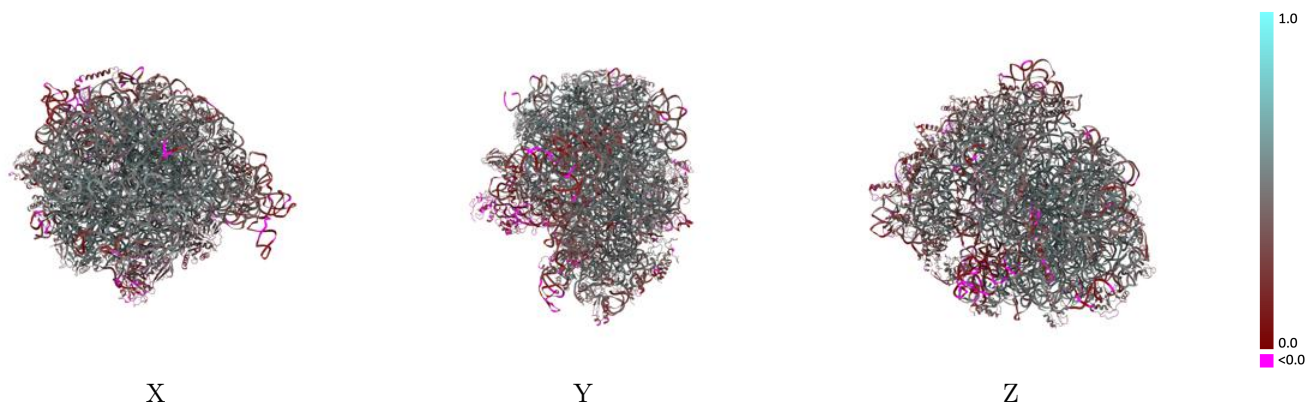
This section contains information regarding the fit between EMDB map EMD-8815 and PDB model 5WE6. Per-residue inclusion information can be found in section 3 on page 19.

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



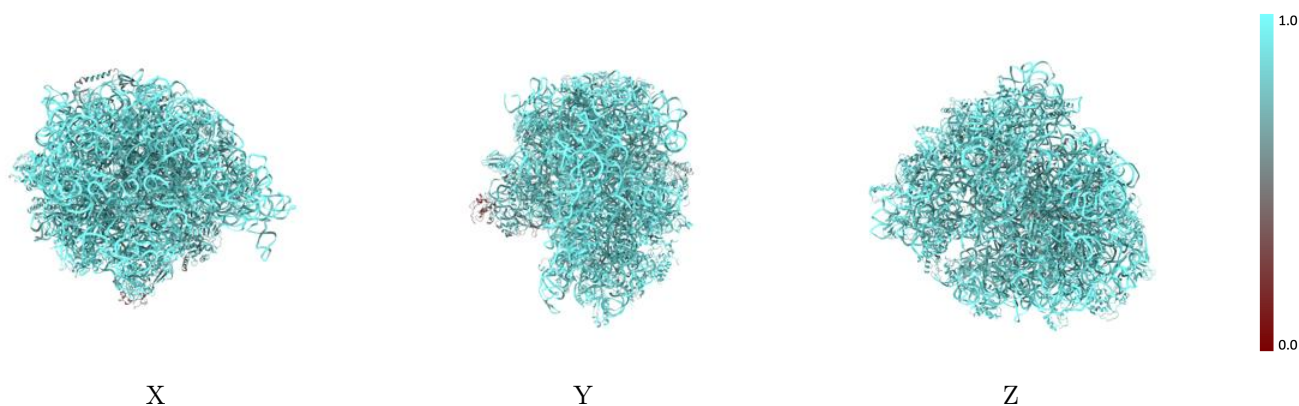
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



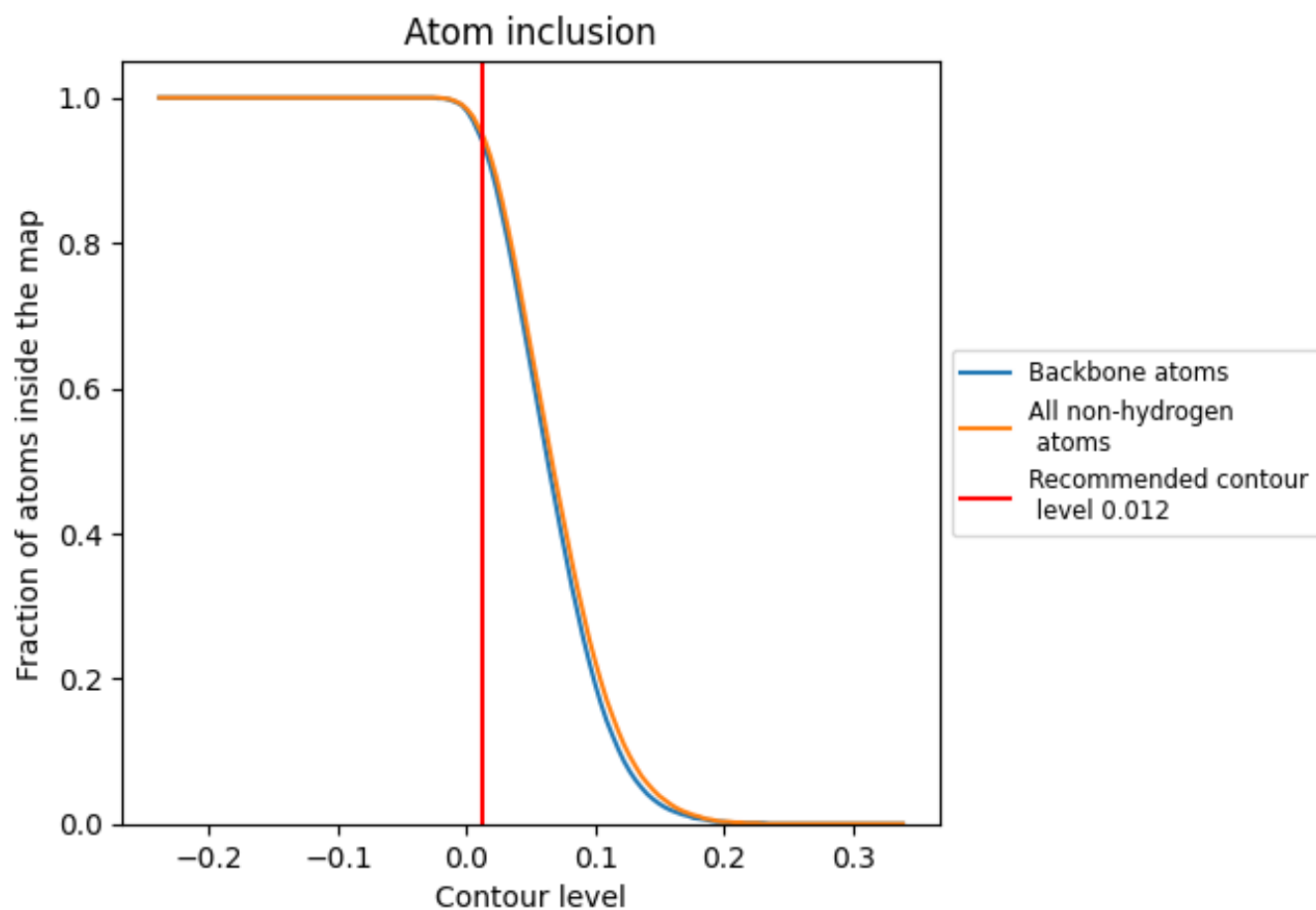
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.4300
0	 0.9550	 0.4670
1	 0.9360	 0.4560
2	 0.9680	 0.5380
3	 0.9660	 0.5360
4	 0.9520	 0.4900
5	 0.4510	 0.0600
6	 0.8160	 0.2270
A	 0.9770	 0.4660
B	 0.9880	 0.4460
C	 0.9540	 0.5210
D	 0.9510	 0.4850
E	 0.9300	 0.4370
F	 0.9180	 0.3760
G	 0.9260	 0.3680
H	 0.7450	 0.2170
I	 0.6590	 0.0620
J	 0.9540	 0.4880
K	 0.9330	 0.4840
L	 0.9440	 0.4660
M	 0.9590	 0.4920
N	 0.9710	 0.5000
O	 0.9410	 0.4150
P	 0.9300	 0.4700
Q	 0.9500	 0.5030
R	 0.9300	 0.4500
S	 0.9470	 0.4840
T	 0.9440	 0.4340
U	 0.9320	 0.3930
V	 0.9250	 0.4200
W	 0.9590	 0.5040
X	 0.9600	 0.4980
Y	 0.9150	 0.3980
Z	 0.9530	 0.4760
a	 0.9790	 0.4320



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Chain	Atom inclusion	Q-score
b	 0.8970	 0.3290
c	 0.9190	 0.4030
d	 0.9000	 0.3200
e	 0.9440	 0.4660
f	 0.9060	 0.3880
g	 0.9110	 0.3490
h	 0.9380	 0.4540
i	 0.8990	 0.3540
j	 0.8870	 0.3190
k	 0.9530	 0.4630
l	 0.9240	 0.4540
m	 0.9240	 0.3980
n	 0.9230	 0.4110
o	 0.9450	 0.4440
p	 0.9190	 0.3680
q	 0.9260	 0.4080
r	 0.9160	 0.4050
s	 0.9210	 0.3740
t	 0.9290	 0.3720
u	 0.8280	 0.3150
v	 0.9680	 0.4300
w	 0.8360	 0.1220
x	 0.9560	 0.4200
y	 0.8940	 0.2930
z	 0.8150	 0.2890