



## Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 09:54 pm BST

PDB ID : 28UN / pdb\_000028un  
EMDB ID : EMD-56833  
Title : E. coli 70S ribosome, conformational excited state mutation in SSU-h41, with A/P- and P/E-site tRNA  
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.  
Deposited on : 2026-02-20  
Resolution : 2.48 Å(reported)  
Based on initial model : 7K00

This is a Full wwPDB EM Validation 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:

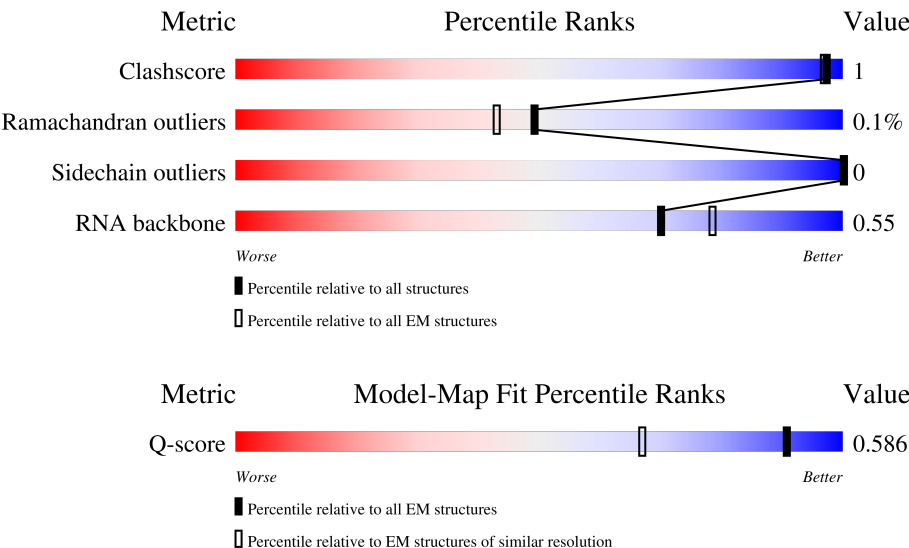
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 2.48 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	6178 ( 1.98 - 2.98 )

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	3	38	
2	4	70	
3	K	129	

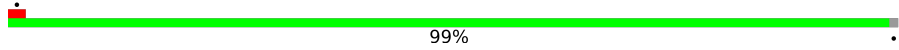
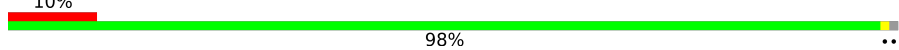
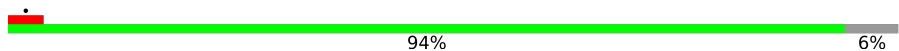


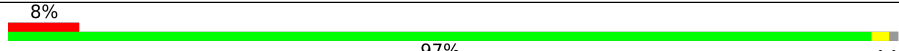
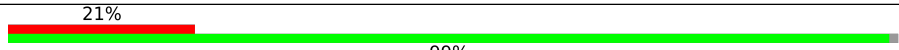

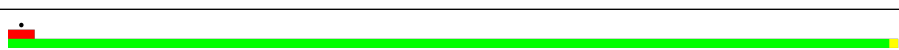
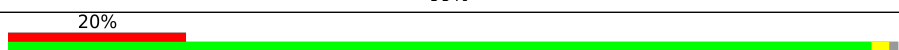
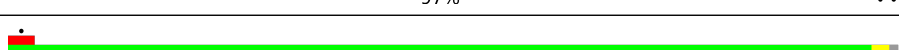
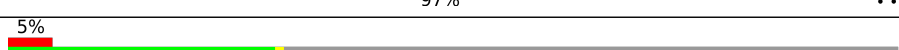

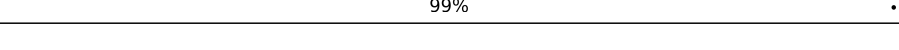
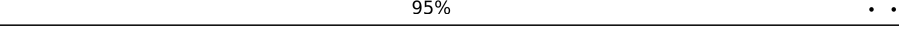
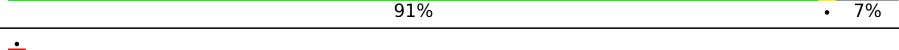
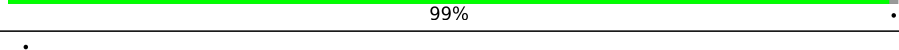
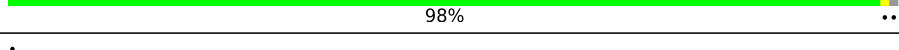
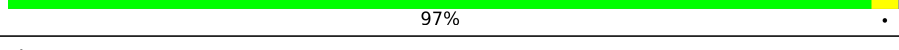
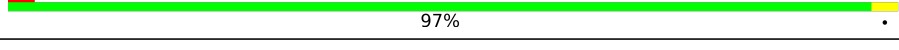
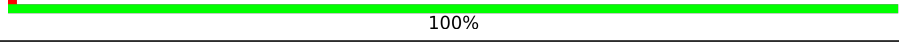
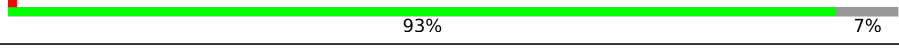
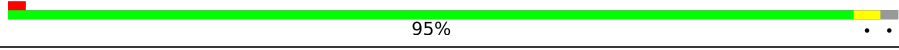
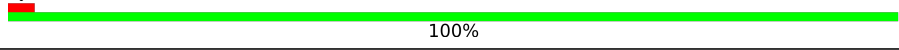

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Mol	Chain	Length	Quality of chain
4	L	124	
5	b	120	
6	c	273	
7	d	209	
8	k	144	
9	l	136	
10	z	57	
11	A	1542	
12	Y	76	
13	Z	78	
14	a	2904	
15	0	55	
16	1	46	
17	2	65	
18	B	241	
19	C	233	
20	D	206	
21	E	167	
22	F	135	
23	G	179	
24	H	130	
25	I	130	
26	J	103	
27	M	118	
28	N	101	

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Mol	Chain	Length	Quality of chain
29	O	89	
30	P	82	
31	Q	84	
32	R	75	
33	S	92	
34	T	87	
35	U	71	
36	X	10	
37	e	201	
38	f	179	
39	g	177	
40	h	149	
41	i	142	
42	j	123	
43	m	127	
44	n	117	
45	o	115	
46	p	118	
47	q	103	
48	r	110	
49	s	100	
50	t	104	
51	u	94	
52	v	85	
53	w	78	

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Mol	Chain	Length	Quality of chain
54	x	63	<div><div></div><div>97%</div><div>.</div></div>
55	y	59	<div><div></div><div>98%</div><div>.</div></div>

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146325 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 Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 3 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 4 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 10 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1519	Total	C	N	O	P	0	0
			32610	14551	5983	10557	1519		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	C	A	engineered mutation	GB 2971391267
A	1262	U	C	engineered mutation	GB 2971391267

- Molecule 12 is a RNA chain called A/P-site Val-tRNA<sup>Val</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	72	Total	C	N	O	P	S	0	0
			1539	689	280	498	71	1		

- Molecule 13 is a RNA chain called P/E-site tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Z	72	Total	C	N	O	P	S	0	0
			1546	690	285	498	72	1		

- Molecule 14 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	a	2757	Total	C	N	O	P		0	0
			59216	26422	10911	19126	2757			

- Molecule 15 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 16 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 17 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 18 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS3.



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

- Molecule 20 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 23 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 30 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 31 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 32 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 34 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 35 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 36 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	X	10	Total	C	N	O	P	0	0
			216	97	41	68	10		

- Molecule 37 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 38 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 40 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	46	Total	C	N	O	S	0	0
			348	224	61	62	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 43 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 44 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 47 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 48 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 49 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 51 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 55 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

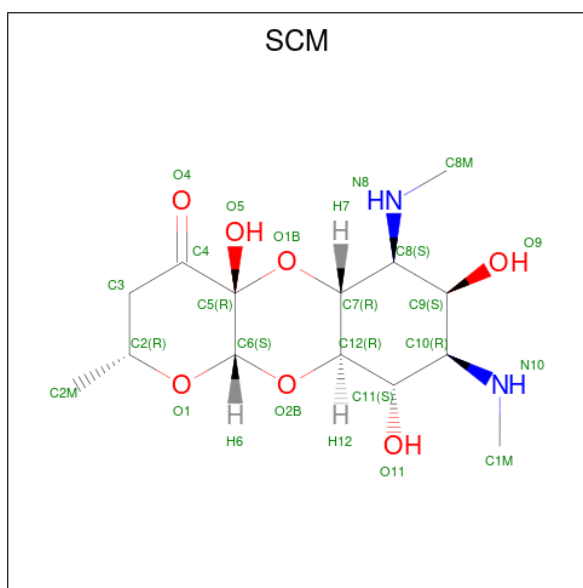
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	b	3	Total	Mg	0
			3	3	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	27	Total	Mg	0
			27	27	
57	a	150	Total	Mg	0
			150	150	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

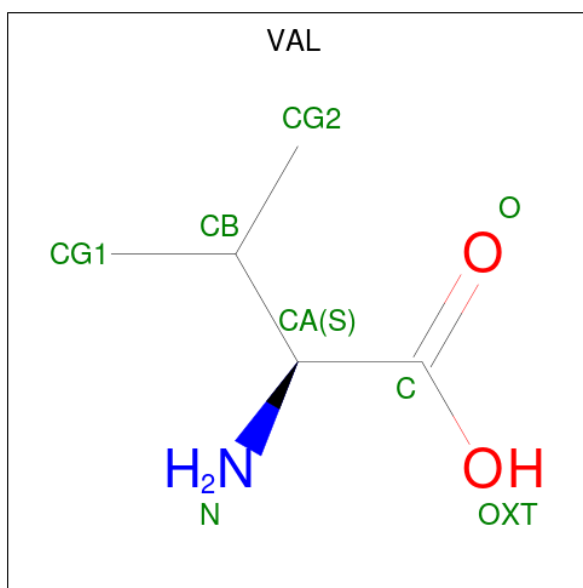
Mol	Chain	Residues	Atoms		AltConf
58	c	2	Total	K	0
			2	2	
58	A	13	Total	K	0
			13	13	
58	a	50	Total	K	0
			50	50	

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula:  $C_{14}H_{24}N_2O_7$ ).



Mol	Chain	Residues	Atoms				AltConf
59	A	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 60 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
60	Y	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	3	8	Total 8	O 8	0
61	K	8	Total 8	O 8	0
61	L	4	Total 4	O 4	0
61	b	68	Total 68	O 68	0
61	c	73	Total 73	O 73	0
61	d	40	Total 40	O 40	0
61	k	38	Total 38	O 38	0
61	l	21	Total 21	O 21	0
61	z	25	Total 25	O 25	0
61	A	837	Total 837	O 837	0
61	Y	10	Total 10	O 10	0
61	Z	12	Total 12	O 12	0
61	a	3165	Total 3165	O 3165	0
61	0	4	Total 4	O 4	0
61	1	14	Total 14	O 14	0
61	2	18	Total 18	O 18	0
61	B	5	Total 5	O 5	0
61	C	4	Total 4	O 4	0
61	D	3	Total 3	O 3	0
61	E	5	Total 5	O 5	0
61	F	3	Total 3	O 3	0
61	G	3	Total 3	O 3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
61	H	7	Total 7	O 7	0
61	I	2	Total 2	O 2	0
61	J	1	Total 1	O 1	0
61	M	1	Total 1	O 1	0
61	N	1	Total 1	O 1	0
61	O	5	Total 5	O 5	0
61	P	3	Total 3	O 3	0
61	Q	4	Total 4	O 4	0
61	R	3	Total 3	O 3	0
61	T	4	Total 4	O 4	0
61	U	7	Total 7	O 7	0
61	X	7	Total 7	O 7	0
61	e	56	Total 56	O 56	0
61	f	3	Total 3	O 3	0
61	g	3	Total 3	O 3	0
61	h	4	Total 4	O 4	0
61	i	23	Total 23	O 23	0
61	j	11	Total 11	O 11	0
61	m	17	Total 17	O 17	0
61	n	8	Total 8	O 8	0
61	o	18	Total 18	O 18	0

*Continued on next page...*

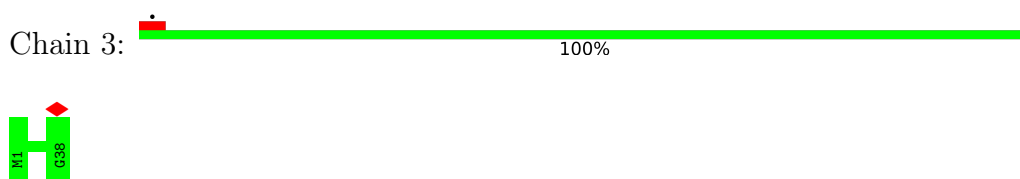
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
61	p	25	Total 25	O 25	0
61	q	22	Total 22	O 22	0
61	r	23	Total 23	O 23	0
61	s	7	Total 7	O 7	0
61	t	9	Total 9	O 9	0
61	u	9	Total 9	O 9	0
61	v	17	Total 17	O 17	0
61	w	13	Total 13	O 13	0
61	x	5	Total 5	O 5	0
61	y	11	Total 11	O 11	0

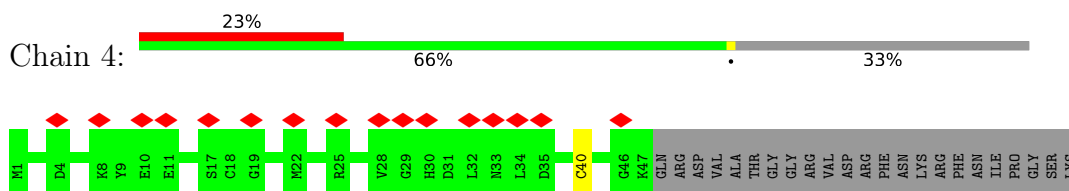
### 3 Residue-property plots [i](#)

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.

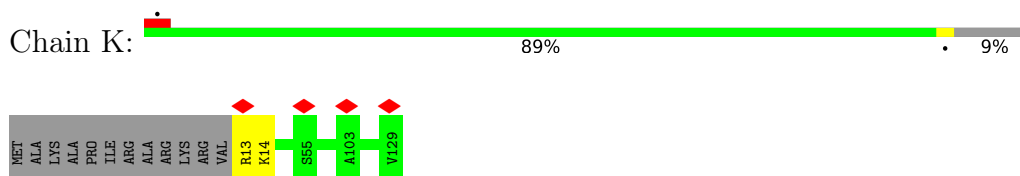
- Molecule 1: Large ribosomal subunit protein bL36A



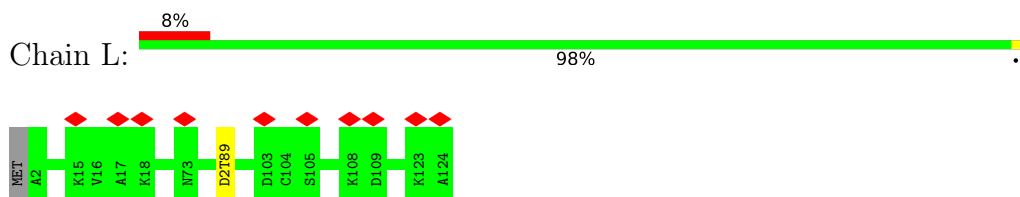
- Molecule 2: Large ribosomal subunit protein bL31



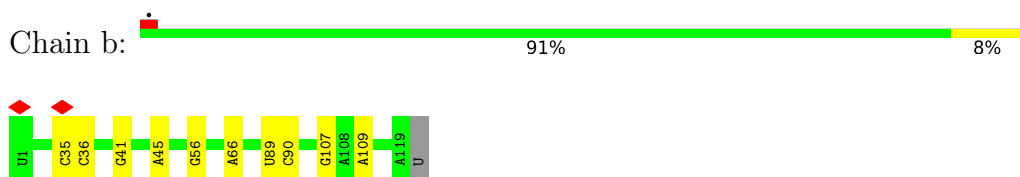
- Molecule 3: Small ribosomal subunit protein uS11



- Molecule 4: Small ribosomal subunit protein uS12



- Molecule 5: 5S rRNA



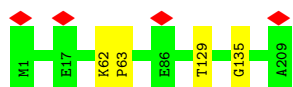
- Molecule 6: Large ribosomal subunit protein uL2

Chain c:  97%



- Molecule 7: Large ribosomal subunit protein uL3

Chain d:  98%



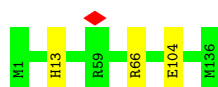
- Molecule 8: Large ribosomal subunit protein uL15

Chain k:  98%

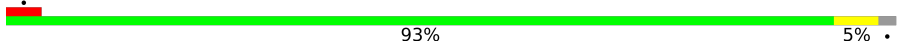


- Molecule 9: Large ribosomal subunit protein uL16

Chain l:  98%




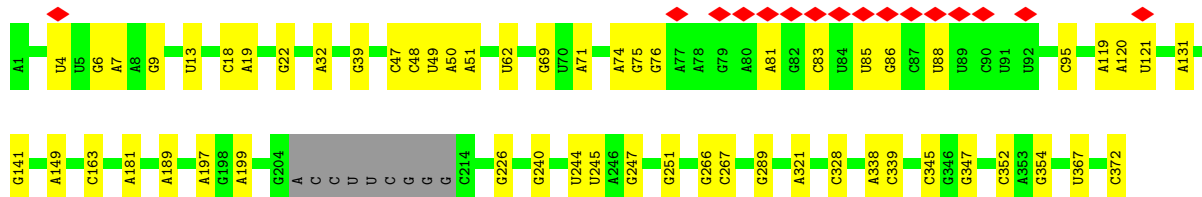
- Molecule 10: Large ribosomal subunit protein bL32

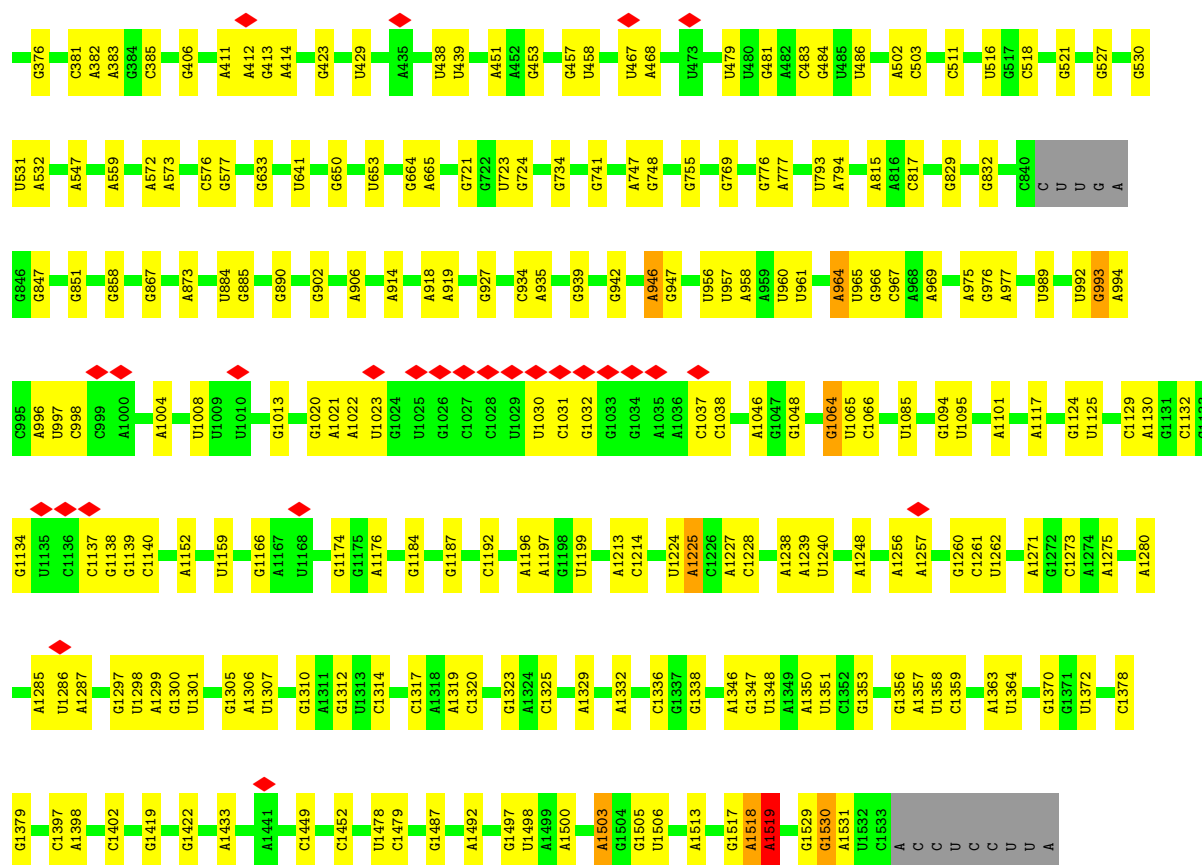
Chain z:  93% 5%



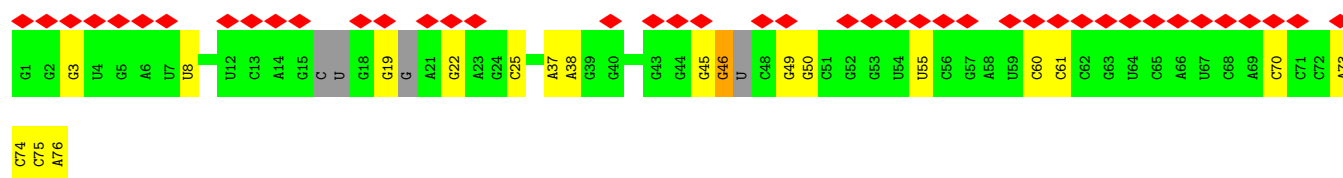
- Molecule 11: 16S rRNA

Chain A:  80% 18%





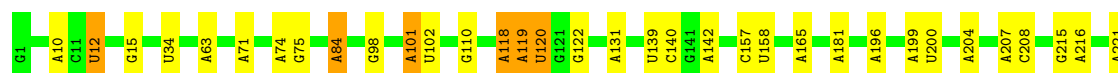
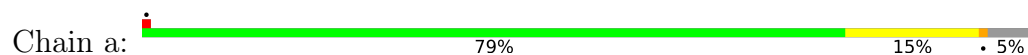
• Molecule 12: A/P-site Val-tRNA<sup>Val</sup>



• Molecule 13: P/E-site tRNA<sup>fMet</sup>



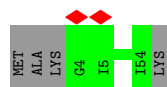
• Molecule 14: 23S rRNA



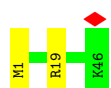
A2518	U2519	U2522	G2529	A2547	U2548	A2566	G2567	C2573	U2580	C2601	G2603	U2604	U2605	U2609	U2613	G2627	C2628	U2629	U2647	G2661	A2662	G2663	A2682	U2689	U2690	G2709	G2714	C2715	C2716	A2726	G2744	G2747	A2748	C2755	U2756	A2757	A2765																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A2328	U2329	A2333	U2334	A2335	C2339	C2347	C2350	G2351	A2352	U2361	A2366	G2383	U2384	C2385	U2402	A2406	C2424	A2425	G2429	A2430	U2431	A2432	A2435	U2441	G2447	A2448	U2449	A2450	U2457	G2470	A2476	C2486	U2491	C2501	G2502	A2503	U2504	G2505																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
U	U	U	A	U	G	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G	G	G	G	G	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A504	A505	C509	G530	C531	A532	U534	U545	G548	G549	A563	U568	U573	A574	A575	U580	A586	A603	U615	G620	A621	A627	A637	G638	U639	C640	A644	C645	U646	G647	U653	A654	A655	G656	U657	U658	U667	A668	U686	G711																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U714	C717	G723	U724	G729	A730	G738	A743	U746	U747	A752	A764	C765	G775	G776	A782	A783	G784	G785	A788	A789	U790	C791	A792	G805	G809	U810	U811	C812	U827	U828	U846	G858	G859	U860	A861	G862	A877	A878	G879	G880																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C883	U884	C885	A886	U887	C888	C889	C890	C891	A892	C893	U894	U895	A896	C897	C898	A899	A910	G914	C915	A927	U931	A936	A947	C948	U955	C961	G962	A972	A973	G974	A983	A984	C985	A996	C1005	U1012	C1013	A1020	A1021	G1022	G1026	A1027	A1028	U1033																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A1040	G1047	C1052	C	A	G	G	A	U	U	U	U	G	U	U	U	A	A	C	A	G	C	C	A	U	C	A	A	A	G	C	C	U	A	U	A	A	G	A	C	C	U	G																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1107	U1108	G1109	A1110	A1111	G1112	G1115	G1116	G1125	G1128	A1129	U1132	A1133	A1134	C1135	U1141	A1142	G1171	C1172	U	A	U	G1177	G1182	U1183	U1184	G1187	U1188	G1223	G1227	A1253	G1256	G1271	A1272	A1275	A1286	A1287	C1295	G1296	G1300	A1301	A1302																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1321	U1352	C1357	G1358	A1365	A1378	U1379	G1380	A1383	C1386	U1394	U1405	U1406	G1416	G1421	G1422	C1428	A1434	G1435	G1452	A1453	G1482	C1493	A1508	A1509	A1515	A1535	C1536	G1537	C1558	U1559	G1560	A1566	A1569	U1578	U1584																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
C1585	A1603	C1607	A1608	A1609	G1622	A1637	C1638	C1644	U1647	U1648	G1649	A1650	G1674	G1702	G1715	U1729	C1730	G1731	C1732	G1738	G1750	U1758	A1759	C1760	C1764	A1773	U1778	U1782	A1783	A1784	A1791	C1800	A1801	G1807	A1808	C1816	U1827																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1828	A1829	G1842	A1848	A1853	A1858	G1862	G1869	A1872	G1873	U1882	A1890	C1902	G1906	G1907	G1910	U1911	A1912	A1913	C1914	3TD1915	A1916	U1917	A1918	A1919	C1925	G1930	U1931	A1932	G1933	A1937	A1938	U1939	U1955	A1966	C1967	U1970	U1971	G1972	U1991	G1992																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U1993	C1997	C2000	A2014	A2020	C2021	U2022	C2023	G2027	A2030	A2031	G2032	A2033	G2038	U2039	C2043	C2055	G2056	A2060	G2061	A2062	C2063	G2069	G2087	G2093	U2099	G2100	A	C	C	U	U	U	G	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U



- Molecule 15: Large ribosomal subunit protein bL33



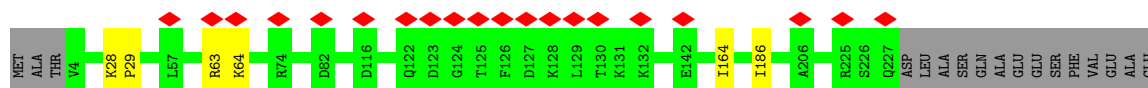
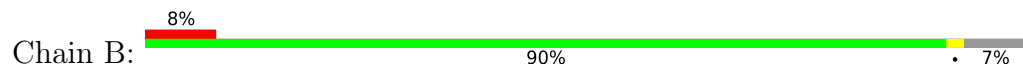
- Molecule 16: Large ribosomal subunit protein bL34



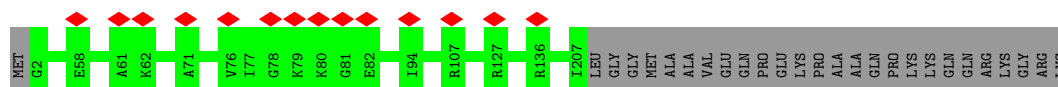
- Molecule 17: Large ribosomal subunit protein bL35



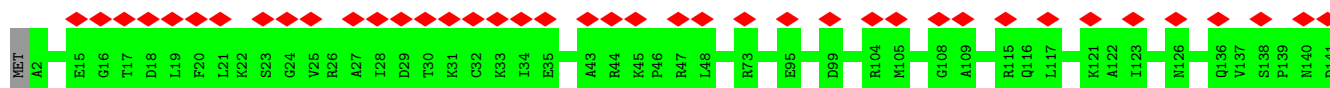
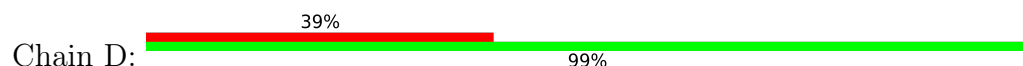
- Molecule 18: Small ribosomal subunit protein uS2

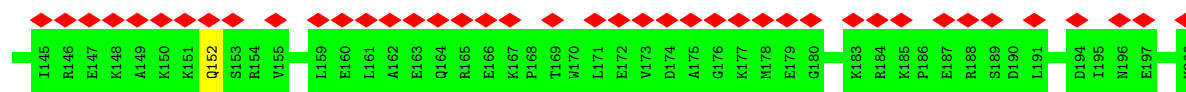


- Molecule 19: Small ribosomal subunit protein uS3

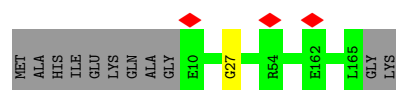
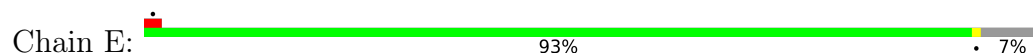


- Molecule 20: Small ribosomal subunit protein uS4





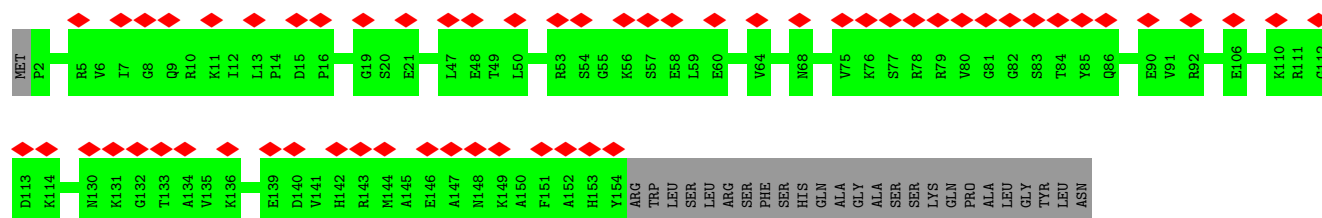
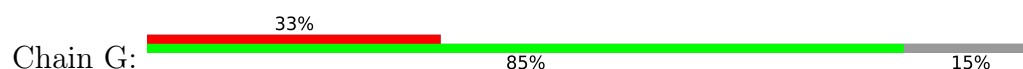
- Molecule 21: Small ribosomal subunit protein uS5



- Molecule 22: Small ribosomal subunit protein bS6, fully modified isoform



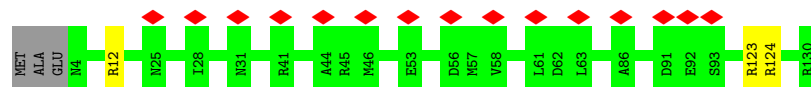
- Molecule 23: Small ribosomal subunit protein uS7



- Molecule 24: Small ribosomal subunit protein uS8



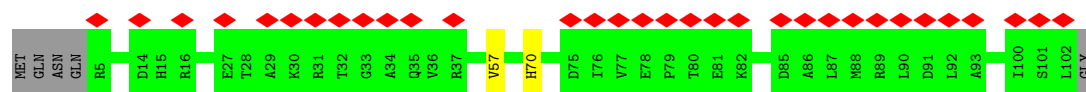
- Molecule 25: Small ribosomal subunit protein uS9



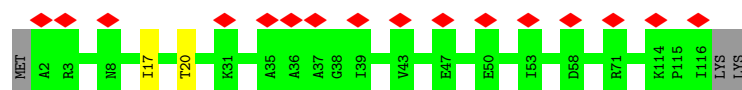
- Molecule 26: Small ribosomal subunit protein uS10



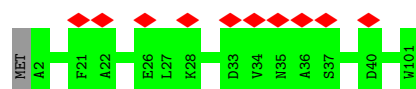




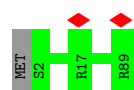
- Molecule 27: Small ribosomal subunit protein uS13



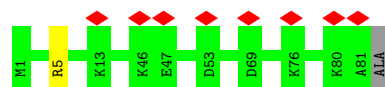
- Molecule 28: Small ribosomal subunit protein uS14



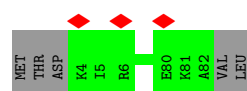
- Molecule 29: Small ribosomal subunit protein uS15



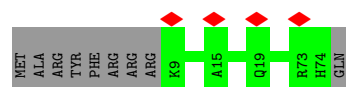
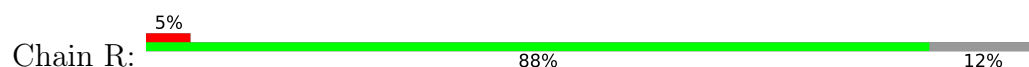
- Molecule 30: Small ribosomal subunit protein bS16



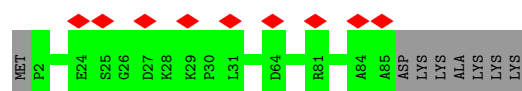
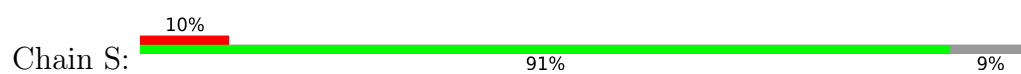
- Molecule 31: Small ribosomal subunit protein uS17



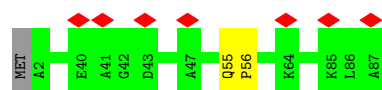
- Molecule 32: Small ribosomal subunit protein bS18



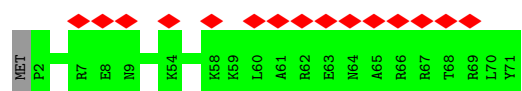
- Molecule 33: Small ribosomal subunit protein uS19



- Molecule 34: Small ribosomal subunit protein bS20



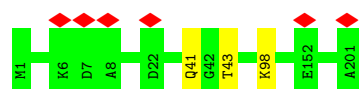
- Molecule 35: Small ribosomal subunit protein bS21



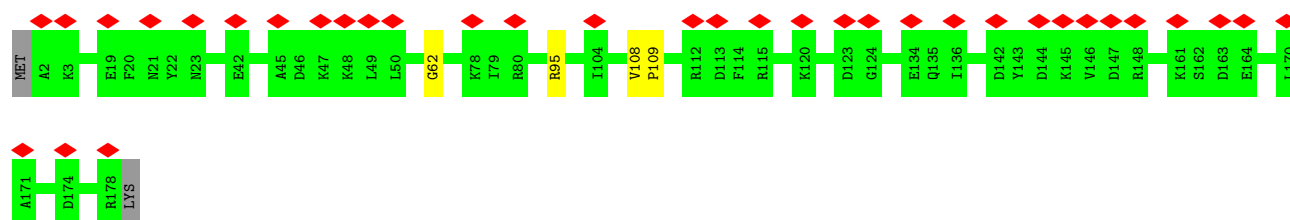
- Molecule 36: mRNA



- Molecule 37: Large ribosomal subunit protein uL4



- Molecule 38: Large ribosomal subunit protein uL5



- Molecule 39: Large ribosomal subunit protein uL6





- Molecule 46: Large ribosomal subunit protein bL20

Chain p:  97%



- Molecule 47: Large ribosomal subunit protein bL21

Chain q:  97%




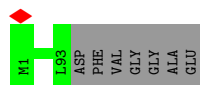
- Molecule 48: Large ribosomal subunit protein uL22

Chain r:  100%



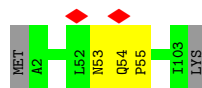
- Molecule 49: Large ribosomal subunit protein uL23

Chain s:  93%



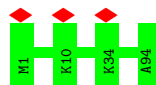
- Molecule 50: Large ribosomal subunit protein uL24

Chain t:  95%




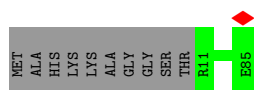
- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  100%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  88%



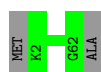
- Molecule 53: Large ribosomal subunit protein bL28

Chain w:  99%



- Molecule 54: Large ribosomal subunit protein uL29

Chain x:  97%



- Molecule 55: Large ribosomal subunit protein uL30

Chain y:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14786	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.88	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0761	Depositor
Map size (Å)	436.32, 436.32, 436.32	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7575, 0.7575, 0.7575	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, 5MC, K, MG, 6MZ, 2MA, ZN, OMG, UR3, 4D4, 4SU, MS6, SCM, 5MU, OMC, 2MG, MEQ, 1MG, H2U, OMU, 3TD, G7M, 4OC, MA6, IAS, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	3	0.48	0/303	0.81	0/397
2	4	0.48	0/371	0.80	0/496
3	K	0.50	0/884	0.84	0/1191
4	L	0.46	0/960	0.83	0/1286
5	b	0.53	0/2850	0.80	0/4444
6	c	0.48	0/2121	0.83	0/2852
7	d	0.46	0/1576	0.79	0/2119
8	k	0.47	0/1062	0.84	0/1413
9	l	0.46	0/1073	0.82	0/1433
10	z	0.47	0/450	0.88	0/599
11	A	0.52	1/36233 (0.0%)	0.79	0/56515
12	Y	0.57	1/1596 (0.1%)	0.76	0/2478
13	Z	0.56	1/1608 (0.1%)	0.79	1/2500 (0.0%)
14	a	0.50	1/65747 (0.0%)	0.82	12/102563 (0.0%)
15	0	0.45	0/424	0.82	0/565
16	1	0.47	0/380	0.90	0/498
17	2	0.50	0/513	0.88	0/676
18	B	0.45	0/1784	0.89	0/2403
19	C	0.46	0/1651	0.84	0/2225
20	D	0.44	0/1665	0.90	0/2227
21	E	0.46	0/1165	0.81	0/1568
22	F	0.45	0/858	0.84	0/1160
23	G	0.46	0/1219	0.93	0/1635
24	H	0.46	0/989	0.86	0/1326
25	I	0.45	0/1034	0.89	0/1375
26	J	0.45	0/796	0.85	0/1077
27	M	0.46	0/900	0.93	0/1204
28	N	0.46	0/817	0.90	0/1088
29	O	0.43	0/722	0.95	0/964
30	P	0.45	0/653	0.83	0/877
31	Q	0.45	0/650	0.80	0/871

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	R	0.45	0/553	0.90	0/742
33	S	0.49	0/685	0.83	0/922
34	T	0.46	0/676	0.98	0/895
35	U	0.47	0/598	0.95	0/792
36	X	0.54	0/242	0.83	0/375
37	e	0.44	0/1571	0.84	0/2113
38	f	0.45	0/1434	0.88	0/1926
39	g	0.47	0/1333	0.82	0/1805
40	h	0.48	0/352	0.81	0/474
41	i	0.45	0/1152	0.84	0/1551
42	j	0.45	0/956	0.83	0/1279
43	m	0.45	0/958	0.88	0/1281
44	n	0.46	0/902	0.89	0/1209
45	o	0.45	0/929	0.77	0/1242
46	p	0.45	0/960	0.91	0/1278
47	q	0.44	0/829	0.71	0/1107
48	r	0.46	0/864	0.86	0/1156
49	s	0.44	0/744	0.79	0/994
50	t	0.46	0/787	0.78	0/1051
51	u	0.45	0/766	0.80	0/1025
52	v	0.47	0/582	0.78	0/769
53	w	0.45	0/635	0.83	0/848
54	x	0.41	0/496	0.91	0/660
55	y	0.45	0/453	0.88	0/605
All	All	0.50	4/152511 (0.0%)	0.82	13/228124 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	2	0	1
25	I	0	1
45	o	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	8	4SU	O3'-P	5.11	1.61	1.56
12	Y	8	4SU	O3'-P	5.07	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1498	UR3	O3'-P	5.03	1.61	1.56
14	a	2069	G7M	O3'-P	5.02	1.61	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	2022	U	O3'-P-O5'	-6.84	93.73	104.00
14	a	1142	A	O3'-P-O5'	-5.95	95.08	104.00
14	a	1966	A	O3'-P-O5'	-5.62	95.58	104.00
14	a	2519	U	O3'-P-O5'	-5.52	95.72	104.00
14	a	1650	A	O3'-P-O5'	-5.17	96.24	104.00
14	a	1638	C	O3'-P-O5'	-5.16	96.25	104.00
14	a	204	A	O3'-P-O5'	-5.16	96.27	104.00
14	a	627	A	O3'-P-O5'	-5.12	96.32	104.00
14	a	621	A	O3'-P-O5'	-5.12	96.32	104.00
14	a	2277	G	O3'-P-O5'	-5.11	96.33	104.00
14	a	2501	C	O3'-P-O5'	-5.09	96.37	104.00
13	Z	37	A	O3'-P-O5'	-5.07	96.39	104.00
14	a	972	A	O3'-P-O5'	-5.03	96.46	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	2	13	ARG	Sidechain
25	I	12	ARG	Sidechain
45	o	53	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	302	0	340	0	0
2	4	364	0	362	0	0
3	K	877	0	884	1	0
4	L	957	0	1017	0	0
5	b	2549	0	1291	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	c	2082	0	2153	6	0
7	d	1566	0	1618	3	0
8	k	1053	0	1129	2	0
9	l	1075	0	1145	2	0
10	z	444	0	458	2	0
11	A	32610	0	16430	27	0
12	Y	1539	0	791	1	0
13	Z	1546	0	794	1	0
14	a	59216	0	29795	84	0
15	0	417	0	451	0	0
16	1	377	0	418	2	0
17	2	504	0	572	1	0
18	B	1753	0	1780	3	0
19	C	1624	0	1696	0	0
20	D	1643	0	1707	0	0
21	E	1152	0	1196	1	0
22	F	839	0	833	1	0
23	G	1203	0	1254	0	0
24	H	979	0	1031	0	0
25	I	1022	0	1070	1	0
26	J	786	0	828	1	0
27	M	891	0	952	1	0
28	N	805	0	844	0	0
29	O	714	0	734	0	0
30	P	643	0	661	1	0
31	Q	641	0	682	0	0
32	R	544	0	565	0	0
33	S	668	0	693	0	0
34	T	670	0	719	1	0
35	U	590	0	629	0	0
36	X	216	0	108	1	0
37	e	1552	0	1619	2	0
38	f	1410	0	1444	3	0
39	g	1313	0	1358	2	0
40	h	348	0	372	1	0
41	i	1129	0	1162	1	0
42	j	947	0	1023	4	0
43	m	945	0	989	3	0
44	n	892	0	923	0	0
45	o	917	0	962	0	0
46	p	947	0	1019	3	0
47	q	816	0	839	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	r	857	0	922	0	0
49	s	738	0	807	0	0
50	t	779	0	831	1	0
51	u	753	0	780	0	0
52	v	575	0	592	0	0
53	w	625	0	652	0	0
54	x	495	0	526	0	0
55	y	449	0	488	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	27	0	0	0	0
57	a	150	0	0	0	0
57	b	3	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	A	13	0	0	0	0
58	a	50	0	0	0	0
58	c	2	0	0	0	0
59	A	23	0	24	4	0
60	Y	7	0	8	0	0
61	0	4	0	0	0	0
61	1	14	0	0	1	0
61	2	18	0	0	0	0
61	3	8	0	0	0	0
61	A	837	0	0	0	0
61	B	5	0	0	0	0
61	C	4	0	0	0	0
61	D	3	0	0	0	0
61	E	5	0	0	0	0
61	F	3	0	0	0	0
61	G	3	0	0	0	0
61	H	7	0	0	0	0
61	I	2	0	0	0	0
61	J	1	0	0	0	0
61	K	8	0	0	0	0
61	L	4	0	0	0	0
61	M	1	0	0	0	0
61	N	1	0	0	0	0
61	O	5	0	0	0	0
61	P	3	0	0	0	0
61	Q	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	R	3	0	0	0	0
61	T	4	0	0	0	0
61	U	7	0	0	0	0
61	X	7	0	0	0	0
61	Y	10	0	0	0	0
61	Z	12	0	0	0	0
61	a	3165	0	0	1	0
61	b	68	0	0	0	0
61	c	73	0	0	0	0
61	d	40	0	0	0	0
61	e	56	0	0	0	0
61	f	3	0	0	0	0
61	g	3	0	0	0	0
61	h	4	0	0	0	0
61	i	23	0	0	0	0
61	j	11	0	0	0	0
61	k	38	0	0	0	0
61	l	21	0	0	0	0
61	m	17	0	0	1	0
61	n	8	0	0	0	0
61	o	18	0	0	0	0
61	p	25	0	0	1	0
61	q	22	0	0	0	0
61	r	23	0	0	0	0
61	s	7	0	0	0	0
61	t	9	0	0	0	0
61	u	9	0	0	0	0
61	v	17	0	0	0	0
61	w	13	0	0	0	0
61	x	5	0	0	0	0
61	y	11	0	0	0	0
61	z	25	0	0	0	0
All	All	146325	0	94970	145	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 1.

All (145) 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)
14:a:12:U:H2'	14:a:12:U:O2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:568:U:H1'	14:a:2030:6MZ:H9C1	1.82	0.62
14:a:534:U:O2'	46:p:49:ASP:OD2	2.19	0.60
11:A:1518:MA6:H103	11:A:1519:MA6:H102	1.84	0.59
14:a:2780:G:OP2	41:i:120:ARG:HD3	2.03	0.59
11:A:664:G:H22	11:A:741:G:H1	1.50	0.59
50:t:54:GLN:N	50:t:55:PRO:HD2	2.18	0.58
14:a:1115:G:O2'	14:a:1116:G:O5'	2.23	0.56
14:a:1939:5MU:OP1	14:a:2604:PSU:O2'	2.24	0.56
10:z:9:THR:CG2	14:a:2020:A:H5'	2.37	0.55
14:a:12:U:O2	14:a:12:U:C2'	2.55	0.55
14:a:1020:A:N1	14:a:1141:U:O2'	2.33	0.54
11:A:1066:C:O2	59:A:1601:SCM:N10	2.39	0.53
11:A:964:A:OP1	11:A:1199:U:OP1	2.27	0.53
46:p:28:ARG:NH2	61:p:201:HOH:O	2.41	0.53
14:a:84:A:N1	14:a:98:G:O2'	2.34	0.53
11:A:1064:G:N7	59:A:1601:SCM:O11	2.40	0.52
11:A:338:A:OP2	42:j:98:ARG:NH2	2.43	0.52
11:A:1225:A:H2'	11:A:1225:A:N3	2.25	0.52
14:a:1378:A:O2'	14:a:1380:G:N7	2.43	0.52
14:a:1637:A:H5'	14:a:1760:C:O2'	2.11	0.51
14:a:1508:A:HO2'	14:a:1509:A:C4'	2.23	0.51
11:A:993:G:H2'	11:A:993:G:N3	2.25	0.51
14:a:2522:U:O2'	14:a:2647:U:OP1	2.26	0.50
14:a:639:U:H2'	14:a:640:C:C6	2.47	0.50
5:b:66:A:H61	5:b:107:G:H2'	1.77	0.49
14:a:2038:G:H2'	14:a:2039:U:O4'	2.12	0.49
14:a:1508:A:O2'	14:a:1509:A:O4'	2.24	0.49
14:a:548:G:H2'	14:a:549:G:O4'	2.12	0.49
14:a:644:A:H2'	14:a:645:C:O4'	2.12	0.49
38:f:108:VAL:N	38:f:109:PRO:CD	2.76	0.48
11:A:769:G:H4'	11:A:1513:A:H4'	1.94	0.48
14:a:2328:A:H2'	14:a:2329:U:C6	2.48	0.48
14:a:2547:A:H2'	14:a:2548:U:C6	2.48	0.48
14:a:2273:A:H2'	14:a:2274:A:C8	2.48	0.48
8:k:21:ARG:HA	14:a:811:U:H2'	1.95	0.48
14:a:1932:A:H2'	14:a:1933:G:O4'	2.13	0.48
5:b:66:A:N6	5:b:107:G:H2'	2.29	0.48
11:A:1152:A:OP1	26:J:70:HIS:ND1	2.47	0.48
14:a:788:A:OP1	14:a:790:U:H5	1.97	0.47
18:B:28:LYS:N	18:B:29:PRO:CD	2.78	0.47
6:c:242:LYS:O	14:a:1902:C:H4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:493:G:H2'	14:a:494:G:O4'	2.15	0.46
14:a:1607:C:H4'	14:a:1608:A:O5'	2.14	0.46
14:a:1906:G:H2'	14:a:1907:G:O4'	2.16	0.46
14:a:2627:G:O2'	14:a:2781:A:N1	2.44	0.46
34:T:55:GLN:N	34:T:56:PRO:HD2	2.30	0.46
14:a:2063:C:O2	14:a:2450:A:N1	2.49	0.46
25:I:123:ARG:NH2	25:I:124:ARG:O	2.49	0.46
11:A:381:C:H2'	11:A:382:A:O4'	2.16	0.45
14:a:2000:C:OP1	43:m:5:LYS:NZ	2.47	0.45
9:l:66:ARG:NH2	9:l:104:GLU:OE2	2.48	0.45
6:c:242:LYS:HE2	61:a:3818:HOH:O	2.17	0.45
36:X:14:A:H2'	36:X:14:A:N3	2.32	0.45
14:a:1434:A:H2'	14:a:1435:G:C8	2.52	0.45
14:a:586:A:N1	14:a:809:G:O2'	2.47	0.45
14:a:620:G:O6	37:e:98:LYS:NZ	2.49	0.45
14:a:1778:U:H2'	14:a:1784:A:N6	2.32	0.45
38:f:62:GLY:O	38:f:95:ARG:NH1	2.49	0.45
8:k:57:LEU:HD22	17:2:54:ASP:HB3	1.99	0.44
6:c:271:ARG:O	6:c:272:SER:C	2.61	0.44
7:d:62:LYS:N	7:d:63:PRO:HD2	2.32	0.44
14:a:118:A:C8	14:a:119:A:C8	3.05	0.44
12:Y:37:6MZ:O2'	14:a:1913:A:N1	2.45	0.44
37:e:41:GLN:HG2	37:e:43:THR:HG23	1.98	0.44
11:A:1530:G:H2'	11:A:1531:A:C8	2.53	0.44
14:a:1296:G:OP1	14:a:2709:G:O2'	2.27	0.44
14:a:120:U:H5''	14:a:122:G:OP2	2.18	0.44
14:a:157:C:H2'	14:a:158:U:O4'	2.18	0.44
42:j:4:GLU:O	42:j:5:GLN:HB2	2.18	0.44
14:a:1028:A:N6	14:a:1125:G:H2'	2.33	0.44
11:A:918:A:H2'	11:A:919:A:O4'	2.18	0.43
14:a:667:U:H2'	14:a:668:A:O4'	2.18	0.43
14:a:2812:G:H2'	14:a:2813:A:O4'	2.18	0.43
47:q:5:PHE:HB3	47:q:59:ILE:HD12	2.00	0.43
11:A:1518:MA6:H103	11:A:1519:MA6:C10	2.48	0.43
14:a:948:C:H1'	14:a:984:A:C8	2.52	0.43
38:f:108:VAL:HG12	38:f:109:PRO:HD3	2.00	0.43
7:d:135:GLY:HA2	14:a:743:A:OP1	2.18	0.43
11:A:62:U:OP1	11:A:385:C:O2'	2.35	0.43
14:a:1275:A:N1	14:a:1295:C:O2'	2.50	0.43
42:j:1:MET:HE3	42:j:32:TYR:CZ	2.54	0.43
6:c:221:ARG:HD2	14:a:1827:U:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:1182:G:H2'	14:a:1183:U:O4'	2.18	0.43
11:A:946:A:H2'	11:A:947:G:C8	2.53	0.43
6:c:31:ALA:N	6:c:32:PRO:CD	2.81	0.43
11:A:376:G:H5''	30:P:5:ARG:HB2	2.01	0.43
39:g:175:LYS:O	39:g:176:LYS:C	2.62	0.43
11:A:1356:G:H2'	11:A:1357:A:C8	2.54	0.42
14:a:1558:C:O4'	14:a:1560:G:C8	2.72	0.42
14:a:723:C:H2'	14:a:724:U:O4'	2.18	0.42
14:a:1028:A:N3	14:a:2486:C:O2'	2.48	0.42
14:a:861:A:H2'	14:a:862:G:O4'	2.19	0.42
14:a:2566:A:N1	42:j:28:SER:OG	2.48	0.42
39:g:94:TYR:HA	39:g:106:SER:O	2.18	0.42
14:a:476:G:H4'	14:a:502:A:N1	2.34	0.42
14:a:1853:A:N1	14:a:2087:G:H1'	2.35	0.42
14:a:2291:U:H2'	14:a:2292:U:C6	2.54	0.42
14:a:2709:G:OP1	43:m:18:GLN:NE2	2.53	0.42
11:A:244:U:O4	11:A:906:A:H1'	2.19	0.42
43:m:45:ARG:NH2	61:m:201:HOH:O	2.34	0.42
14:a:2243:U:H2'	14:a:2244:U:C6	2.55	0.42
18:B:63:ARG:O	18:B:64:LYS:C	2.62	0.42
14:a:1405:U:H2'	14:a:1406:U:C6	2.55	0.42
14:a:207:A:H2'	14:a:208:C:O4'	2.20	0.42
14:a:1394:U:H4'	14:a:1603:A:H4'	2.02	0.42
14:a:1750:G:O2'	14:a:2860:A:N1	2.52	0.41
14:a:2747:G:O6	14:a:2755:C:H5''	2.20	0.41
47:q:74:ILE:N	47:q:74:ILE:HD12	2.35	0.41
6:c:207:LYS:HB2	14:a:729:G:C6	2.56	0.41
11:A:481:G:O2'	11:A:483:C:N4	2.52	0.41
5:b:41:G:N2	14:a:2339:C:O3'	2.53	0.41
10:z:43:ILE:HG22	10:z:49:TYR:HB2	2.02	0.41
14:a:878:A:N6	14:a:899:A:O2'	2.53	0.41
14:a:1183:U:H2'	14:a:1184:U:C6	2.54	0.41
27:M:17:ILE:O	27:M:20:THR:OG1	2.34	0.41
14:a:1021:A:N3	14:a:1021:A:H3'	2.35	0.41
11:A:18:C:H2'	11:A:19:A:O4'	2.21	0.41
59:A:1601:SCM:H2M1	21:E:27:GLY:HA2	2.03	0.41
18:B:164:ILE:O	18:B:186:ILE:HB	2.19	0.41
14:a:101:A:N3	14:a:101:A:H2'	2.36	0.41
14:a:1357:C:H2'	14:a:1358:G:O4'	2.20	0.41
14:a:2327:A:H2'	14:a:2328:A:C8	2.56	0.41
14:a:2352:A:C4	14:a:2366:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:18:VAL:HB	22:F:19:PRO:HD3	2.03	0.41
7:d:129:THR:OG1	14:a:1997:C:OP2	2.31	0.41
11:A:867:G:O2'	11:A:873:A:N1	2.49	0.41
11:A:1192:C:N3	59:A:1601:SCM:O5	2.46	0.41
11:A:1402:4OC:O2	11:A:1500:A:N1	2.54	0.41
14:a:244:A:C2	14:a:255:A:C4	3.09	0.41
14:a:1421:G:C2	14:a:1422:G:C8	3.09	0.41
40:h:31:VAL:N	40:h:32:PRO:HD2	2.36	0.41
11:A:502:A:H2'	11:A:503:C:O4'	2.21	0.41
14:a:580:U:O3'	46:p:31:VAL:HG13	2.21	0.41
16:l:19:ARG:NH2	61:l:101:HOH:O	2.43	0.41
14:a:747:5MU:O2	14:a:2014:A:H1'	2.21	0.40
3:K:13:ARG:O	3:K:14:LYS:C	2.64	0.40
14:a:263:G:H2'	14:a:264:C:O4'	2.22	0.40
14:a:752:A:H3'	16:l:1:MET:SD	2.61	0.40
14:a:657:U:H2'	14:a:658:U:C6	2.57	0.40
11:A:1306:A:H2'	11:A:1307:U:O4'	2.22	0.40
13:Z:75:C:O4'	14:a:2432:A:H1'	2.20	0.40
14:a:1223:G:C6	14:a:1227:G:C6	3.10	0.40
9:l:13:HIS:CE1	14:a:910:A:C4	3.09	0.40
11:A:927:G:O2'	11:A:1503:A:N7	2.45	0.40

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	
1	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
2	4	45/70 (64%)	39 (87%)	5 (11%)	1 (2%)	5	8
3	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
4	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
7	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
8	k	142/144 (99%)	140 (99%)	1 (1%)	1 (1%)	18	32
9	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
10	z	54/57 (95%)	54 (100%)	0	0	100	100
15	0	49/55 (89%)	49 (100%)	0	0	100	100
16	1	44/46 (96%)	44 (100%)	0	0	100	100
17	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
18	B	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
19	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
20	D	203/206 (98%)	190 (94%)	12 (6%)	1 (0%)	24	40
21	E	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
22	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
23	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
24	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
25	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
26	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	22
27	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
28	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
29	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
30	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
31	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
32	R	64/75 (85%)	64 (100%)	0	0	100	100
33	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
34	T	84/87 (97%)	84 (100%)	0	0	100	100
35	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
37	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
38	f	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
39	g	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
40	h	44/149 (30%)	40 (91%)	4 (9%)	0	100	100
41	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	j	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	28
43	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
44	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
45	o	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
46	p	115/118 (98%)	115 (100%)	0	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	91 (100%)	0	0	100	100
50	t	100/104 (96%)	94 (94%)	5 (5%)	1 (1%)	12	22
51	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
54	x	59/63 (94%)	59 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5470/5913 (92%)	5266 (96%)	198 (4%)	6 (0%)	49	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	40	CYS
26	J	57	VAL
50	t	53	ASN
8	k	29	LYS
42	j	5	GLN
20	D	152	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4	43/62 (69%)	43 (100%)	0	100	100
3	K	89/98 (91%)	89 (100%)	0	100	100
4	L	102/103 (99%)	102 (100%)	0	100	100
6	c	216/218 (99%)	216 (100%)	0	100	100
7	d	163/163 (100%)	163 (100%)	0	100	100
8	k	103/103 (100%)	103 (100%)	0	100	100
9	l	107/107 (100%)	107 (100%)	0	100	100
10	z	47/48 (98%)	47 (100%)	0	100	100
15	0	46/49 (94%)	46 (100%)	0	100	100
16	1	38/38 (100%)	38 (100%)	0	100	100
17	2	51/52 (98%)	51 (100%)	0	100	100
18	B	186/199 (94%)	186 (100%)	0	100	100
19	C	170/190 (90%)	170 (100%)	0	100	100
20	D	172/173 (99%)	172 (100%)	0	100	100
21	E	119/126 (94%)	119 (100%)	0	100	100
22	F	90/116 (78%)	90 (100%)	0	100	100
23	G	126/147 (86%)	126 (100%)	0	100	100
24	H	104/105 (99%)	104 (100%)	0	100	100
25	I	105/107 (98%)	105 (100%)	0	100	100
26	J	86/90 (96%)	86 (100%)	0	100	100
27	M	93/96 (97%)	93 (100%)	0	100	100
28	N	83/84 (99%)	83 (100%)	0	100	100
29	O	76/77 (99%)	76 (100%)	0	100	100
30	P	65/65 (100%)	65 (100%)	0	100	100
31	Q	73/78 (94%)	73 (100%)	0	100	100
32	R	57/65 (88%)	57 (100%)	0	100	100
33	S	72/79 (91%)	72 (100%)	0	100	100
34	T	65/66 (98%)	65 (100%)	0	100	100
35	U	60/61 (98%)	60 (100%)	0	100	100
37	e	165/165 (100%)	165 (100%)	0	100	100
38	f	148/150 (99%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	g	136/138 (99%)	136 (100%)	0	100	100
40	h	37/114 (32%)	37 (100%)	0	100	100
41	i	116/116 (100%)	116 (100%)	0	100	100
42	j	104/104 (100%)	104 (100%)	0	100	100
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	86 (100%)	0	100	100
45	o	99/100 (99%)	99 (100%)	0	100	100
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	84 (100%)	0	100	100
48	r	93/93 (100%)	93 (100%)	0	100	100
49	s	80/84 (95%)	80 (100%)	0	100	100
50	t	83/85 (98%)	83 (100%)	0	100	100
51	u	78/78 (100%)	78 (100%)	0	100	100
52	v	57/63 (90%)	57 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
All	All	4563/4825 (95%)	4563 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	40	ASN
3	K	118	HIS
4	L	72	HIS
4	L	75	GLN
6	c	60	GLN
6	c	134	ASN
7	d	185	ASN
9	l	22	GLN
9	l	60	GLN
9	l	97	GLN
18	B	19	GLN
18	B	58	ASN

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Mol	Chain	Res	Type
20	D	40	GLN
20	D	54	GLN
20	D	89	ASN
21	E	82	GLN
21	E	121	HIS
21	E	132	ASN
21	E	148	ASN
22	F	17	GLN
22	F	46	GLN
22	F	94	HIS
23	G	68	ASN
23	G	130	ASN
23	G	142	HIS
24	H	21	ASN
25	I	4	ASN
26	J	58	ASN
28	N	60	GLN
30	P	59	HIS
32	R	54	GLN
33	S	57	HIS
34	T	82	GLN
39	g	73	ASN
39	g	115	HIS
41	i	47	HIS
41	i	86	GLN
41	i	128	ASN
43	m	31	HIS
45	o	52	ASN
45	o	66	ASN
46	p	52	GLN
47	q	86	GLN
51	u	12	GLN
53	w	17	ASN
53	w	36	HIS
54	x	58	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1516/1542 (98%)	239 (15%)	29 (1%)
12	Y	68/76 (89%)	16 (23%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	Z	68/78 (87%)	10 (14%)	2 (2%)
14	a	2753/2904 (94%)	323 (11%)	0
36	X	9/10 (90%)	3 (33%)	1 (11%)
5	b	118/120 (98%)	7 (5%)	0
All	All	4532/4730 (95%)	598 (13%)	34 (0%)

All (598) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	35	C
5	b	36	C
5	b	45	A
5	b	56	G
5	b	89	U
5	b	90	C
5	b	109	A
11	A	4	U
11	A	6	G
11	A	7	A
11	A	9	G
11	A	22	G
11	A	32	A
11	A	39	G
11	A	47	C
11	A	48	C
11	A	49	U
11	A	50	A
11	A	51	A
11	A	69	G
11	A	71	A
11	A	74	A
11	A	75	G
11	A	76	G
11	A	81	A
11	A	83	C
11	A	85	U
11	A	86	G
11	A	88	U
11	A	95	C
11	A	119	A
11	A	120	A
11	A	121	U

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Mol	Chain	Res	Type
11	A	131	A
11	A	141	G
11	A	149	A
11	A	163	C
11	A	189	A
11	A	197	A
11	A	226	G
11	A	240	G
11	A	245	U
11	A	247	G
11	A	251	G
11	A	266	G
11	A	267	C
11	A	289	G
11	A	321	A
11	A	328	C
11	A	339	C
11	A	345	C
11	A	347	G
11	A	352	C
11	A	354	G
11	A	367	U
11	A	372	C
11	A	383	A
11	A	406	G
11	A	411	A
11	A	412	A
11	A	413	G
11	A	414	A
11	A	423	G
11	A	429	U
11	A	438	U
11	A	439	U
11	A	451	A
11	A	453	G
11	A	457	G
11	A	458	U
11	A	467	U
11	A	468	A
11	A	479	U
11	A	484	G
11	A	486	U

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Mol	Chain	Res	Type
11	A	511	C
11	A	518	C
11	A	521	G
11	A	530	G
11	A	531	U
11	A	532	A
11	A	547	A
11	A	559	A
11	A	572	A
11	A	573	A
11	A	576	C
11	A	577	G
11	A	633	G
11	A	650	G
11	A	653	U
11	A	665	A
11	A	721	G
11	A	723	U
11	A	724	G
11	A	734	G
11	A	747	A
11	A	748	G
11	A	755	G
11	A	777	A
11	A	793	U
11	A	794	A
11	A	815	A
11	A	817	C
11	A	829	G
11	A	832	G
11	A	847	G
11	A	851	G
11	A	884	U
11	A	885	G
11	A	890	G
11	A	902	G
11	A	914	A
11	A	934	C
11	A	935	A
11	A	939	G
11	A	942	G
11	A	946	A

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Mol	Chain	Res	Type
11	A	956	U
11	A	957	U
11	A	958	A
11	A	960	U
11	A	961	U
11	A	964	A
11	A	965	U
11	A	966	2MG
11	A	967	5MC
11	A	969	A
11	A	975	A
11	A	976	G
11	A	977	A
11	A	989	U
11	A	992	U
11	A	993	G
11	A	994	A
11	A	996	A
11	A	997	U
11	A	998	C
11	A	1004	A
11	A	1008	U
11	A	1013	G
11	A	1020	G
11	A	1021	A
11	A	1022	A
11	A	1023	U
11	A	1030	U
11	A	1031	C
11	A	1032	G
11	A	1037	C
11	A	1038	C
11	A	1046	A
11	A	1048	G
11	A	1064	G
11	A	1065	U
11	A	1085	U
11	A	1094	G
11	A	1095	U
11	A	1101	A
11	A	1117	A
11	A	1124	G

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Mol	Chain	Res	Type
11	A	1125	U
11	A	1129	C
11	A	1130	A
11	A	1132	C
11	A	1134	G
11	A	1137	C
11	A	1138	G
11	A	1139	G
11	A	1140	C
11	A	1159	U
11	A	1166	G
11	A	1174	G
11	A	1176	A
11	A	1184	G
11	A	1196	A
11	A	1197	A
11	A	1213	A
11	A	1214	C
11	A	1224	U
11	A	1225	A
11	A	1227	A
11	A	1228	C
11	A	1238	A
11	A	1239	A
11	A	1240	U
11	A	1248	A
11	A	1256	A
11	A	1257	A
11	A	1260	G
11	A	1261	C
11	A	1262	U
11	A	1271	A
11	A	1273	C
11	A	1275	A
11	A	1280	A
11	A	1285	A
11	A	1286	U
11	A	1287	A
11	A	1297	G
11	A	1298	U
11	A	1299	A
11	A	1300	G

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Mol	Chain	Res	Type
11	A	1301	U
11	A	1305	G
11	A	1310	G
11	A	1312	G
11	A	1314	C
11	A	1317	C
11	A	1319	A
11	A	1320	C
11	A	1323	G
11	A	1325	C
11	A	1329	A
11	A	1332	A
11	A	1336	C
11	A	1338	G
11	A	1346	A
11	A	1347	G
11	A	1348	U
11	A	1350	A
11	A	1351	U
11	A	1353	G
11	A	1358	U
11	A	1359	C
11	A	1363	A
11	A	1364	U
11	A	1370	G
11	A	1372	U
11	A	1378	C
11	A	1379	G
11	A	1398	A
11	A	1419	G
11	A	1422	G
11	A	1433	A
11	A	1449	C
11	A	1452	C
11	A	1479	C
11	A	1487	G
11	A	1492	A
11	A	1497	G
11	A	1503	A
11	A	1505	G
11	A	1506	U
11	A	1517	G

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Mol	Chain	Res	Type
11	A	1519	MA6
11	A	1529	G
11	A	1530	G
12	Y	3	G
12	Y	19	G
12	Y	22	G
12	Y	25	C
12	Y	38	A
12	Y	45	G
12	Y	46	G7M
12	Y	49	G
12	Y	50	G
12	Y	60	C
12	Y	61	C
12	Y	70	C
12	Y	73	A
12	Y	74	C
12	Y	75	C
12	Y	76	A
13	Z	8	4SU
13	Z	9	G
13	Z	15	G
13	Z	23	C
13	Z	45	G
13	Z	46	G7M
13	Z	58	A
13	Z	60	U
13	Z	61	C
13	Z	76	A
14	a	10	A
14	a	12	U
14	a	15	G
14	a	34	U
14	a	63	A
14	a	71	A
14	a	74	A
14	a	75	G
14	a	84	A
14	a	101	A
14	a	102	U
14	a	110	G
14	a	118	A

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Mol	Chain	Res	Type
14	a	119	A
14	a	120	U
14	a	131	A
14	a	139	U
14	a	140	C
14	a	142	A
14	a	165	A
14	a	181	A
14	a	196	A
14	a	199	A
14	a	200	U
14	a	215	G
14	a	216	A
14	a	221	A
14	a	222	A
14	a	230	G
14	a	248	G
14	a	272	A
14	a	276	U
14	a	277	G
14	a	278	A
14	a	279	A
14	a	282	A
14	a	285	G
14	a	288	U
14	a	289	G
14	a	291	G
14	a	310	A
14	a	311	A
14	a	330	A
14	a	353	C
14	a	361	G
14	a	386	G
14	a	404	A
14	a	405	U
14	a	411	G
14	a	412	A
14	a	451	U
14	a	481	G
14	a	491	G
14	a	503	A
14	a	504	A

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Mol	Chain	Res	Type
14	a	505	A
14	a	509	C
14	a	530	G
14	a	531	C
14	a	532	A
14	a	533	G
14	a	545	U
14	a	548	G
14	a	549	G
14	a	563	A
14	a	573	U
14	a	574	A
14	a	575	A
14	a	586	A
14	a	603	A
14	a	615	U
14	a	627	A
14	a	637	A
14	a	645	C
14	a	646	U
14	a	647	G
14	a	654	A
14	a	655	A
14	a	686	U
14	a	711	G
14	a	714	U
14	a	717	C
14	a	730	A
14	a	738	G
14	a	747	5MU
14	a	764	A
14	a	765	C
14	a	775	G
14	a	776	G
14	a	782	A
14	a	784	G
14	a	785	G
14	a	789	A
14	a	792	A
14	a	805	G
14	a	812	C
14	a	827	U

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Mol	Chain	Res	Type
14	a	828	U
14	a	846	U
14	a	858	G
14	a	859	G
14	a	877	A
14	a	883	G
14	a	884	U
14	a	888	C
14	a	890	C
14	a	891	G
14	a	895	U
14	a	896	A
14	a	897	C
14	a	899	A
14	a	910	A
14	a	914	G
14	a	915	C
14	a	927	A
14	a	931	U
14	a	946	C
14	a	961	C
14	a	962	G
14	a	974	G
14	a	983	A
14	a	984	A
14	a	985	C
14	a	996	A
14	a	1005	C
14	a	1012	U
14	a	1013	C
14	a	1022	G
14	a	1026	G
14	a	1033	U
14	a	1040	A
14	a	1047	G
14	a	1108	U
14	a	1110	G
14	a	1111	A
14	a	1112	G
14	a	1116	G
14	a	1128	G
14	a	1129	A

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Mol	Chain	Res	Type
14	a	1132	U
14	a	1133	A
14	a	1135	C
14	a	1142	A
14	a	1171	G
14	a	1187	G
14	a	1188	U
14	a	1253	A
14	a	1256	G
14	a	1271	G
14	a	1272	A
14	a	1286	A
14	a	1287	A
14	a	1300	G
14	a	1301	A
14	a	1302	A
14	a	1321	A
14	a	1352	U
14	a	1365	A
14	a	1383	A
14	a	1386	C
14	a	1416	G
14	a	1428	C
14	a	1452	G
14	a	1453	A
14	a	1482	G
14	a	1493	C
14	a	1508	A
14	a	1515	A
14	a	1535	A
14	a	1536	C
14	a	1537	G
14	a	1566	A
14	a	1569	A
14	a	1578	U
14	a	1584	U
14	a	1585	C
14	a	1608	A
14	a	1609	A
14	a	1622	G
14	a	1644	C
14	a	1647	U

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Mol	Chain	Res	Type
14	a	1648	U
14	a	1649	G
14	a	1674	G
14	a	1702	G
14	a	1715	G
14	a	1729	U
14	a	1730	C
14	a	1732	C
14	a	1738	G
14	a	1758	U
14	a	1764	C
14	a	1773	A
14	a	1782	U
14	a	1791	A
14	a	1800	C
14	a	1801	A
14	a	1807	G
14	a	1808	A
14	a	1816	C
14	a	1829	A
14	a	1842	G
14	a	1848	A
14	a	1858	A
14	a	1862	G
14	a	1869	G
14	a	1872	A
14	a	1873	G
14	a	1882	U
14	a	1890	A
14	a	1907	G
14	a	1910	G
14	a	1911	PSU
14	a	1912	A
14	a	1918	A
14	a	1919	A
14	a	1925	C
14	a	1930	G
14	a	1931	U
14	a	1937	A
14	a	1938	A
14	a	1955	U
14	a	1967	C

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Mol	Chain	Res	Type
14	a	1970	A
14	a	1971	U
14	a	1972	G
14	a	1991	U
14	a	1993	U
14	a	2023	C
14	a	2027	G
14	a	2031	A
14	a	2033	A
14	a	2043	C
14	a	2055	C
14	a	2056	G
14	a	2060	A
14	a	2061	G
14	a	2062	A
14	a	2069	G7M
14	a	2093	G
14	a	2099	U
14	a	2198	A
14	a	2204	G
14	a	2211	A
14	a	2225	A
14	a	2238	G
14	a	2239	G
14	a	2268	A
14	a	2279	G
14	a	2282	G
14	a	2283	C
14	a	2286	G
14	a	2287	A
14	a	2288	A
14	a	2305	U
14	a	2307	G
14	a	2309	A
14	a	2310	C
14	a	2311	A
14	a	2312	U
14	a	2317	A
14	a	2322	A
14	a	2325	G
14	a	2333	A
14	a	2335	A

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Mol	Chain	Res	Type
14	a	2347	C
14	a	2350	C
14	a	2361	G
14	a	2383	G
14	a	2385	C
14	a	2402	U
14	a	2406	A
14	a	2424	C
14	a	2425	A
14	a	2429	G
14	a	2430	A
14	a	2431	U
14	a	2435	A
14	a	2441	U
14	a	2447	G
14	a	2448	A
14	a	2470	G
14	a	2476	A
14	a	2491	U
14	a	2502	G
14	a	2505	G
14	a	2518	A
14	a	2529	G
14	a	2547	A
14	a	2566	A
14	a	2567	G
14	a	2573	C
14	a	2601	C
14	a	2602	A
14	a	2603	G
14	a	2609	U
14	a	2613	U
14	a	2629	U
14	a	2661	G
14	a	2663	G
14	a	2682	A
14	a	2689	U
14	a	2690	U
14	a	2714	G
14	a	2716	C
14	a	2726	A
14	a	2744	G

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Mol	Chain	Res	Type
14	a	2748	A
14	a	2757	A
14	a	2765	A
14	a	2778	A
14	a	2790	U
14	a	2797	U
14	a	2800	A
14	a	2801	G
14	a	2818	U
14	a	2820	A
14	a	2821	A
14	a	2861	U
14	a	2880	C
14	a	2883	A
14	a	2884	U
14	a	2903	U
36	X	14	A
36	X	15	A
36	X	16	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	7	A
11	A	13	U
11	A	119	A
11	A	181	A
11	A	199	A
11	A	438	U
11	A	530	G
11	A	559	A
11	A	641	U
11	A	776	G
11	A	793	U
11	A	858	G
11	A	884	U
11	A	964	A
11	A	966	2MG
11	A	993	G
11	A	1124	G
11	A	1129	C
11	A	1187	G

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Mol	Chain	Res	Type
11	A	1224	U
11	A	1225	A
11	A	1239	A
11	A	1240	U
11	A	1297	G
11	A	1319	A
11	A	1320	C
11	A	1363	A
11	A	1397	C
11	A	1478	U
12	Y	60	C
12	Y	74	C
13	Z	22	G
13	Z	60	U
36	X	14	A

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

50 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	$\# Z  > 2$
11	G7M	A	527	11	23,26,27	0.72	1 (4%)	35,39,42	0.67	0
11	UR3	A	1498	11	19,22,23	0.27	0	26,32,35	0.62	0
11	MA6	A	1519	11	23,26,27	0.27	0	34,38,41	0.76	1 (2%)
14	PSU	a	746	57,14	18,21,22	0.87	1 (5%)	22,30,33	0.66	0
13	OMC	Z	32	13	19,22,23	0.28	0	26,31,34	0.36	0
12	5MU	Y	54	12	19,22,23	0.26	0	28,32,35	0.30	0
9	MS6	l	82	9	5,7,8	0.21	0	2,7,9	0.09	0
12	4SU	Y	8	12	18,21,22	0.38	0	26,30,33	1.22	3 (11%)
14	OMU	a	2552	14	19,22,23	0.21	0	26,31,34	0.34	0
14	1MG	a	745	14	22,26,27	0.55	0	33,39,42	0.52	0
14	5MU	a	747	14	19,22,23	0.22	0	28,32,35	0.33	0
14	PSU	a	2504	58,14	18,21,22	0.88	1 (5%)	22,30,33	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	OMG	a	2251	14,12	23,26,27	0.31	0	33,38,41	0.43	0
4	D2T	L	89	4	7,9,10	0.92	0	6,11,13	1.73	2 (33%)
13	G7M	Z	46	13	23,26,27	0.73	1 (4%)	35,39,42	0.65	0
14	5MC	a	1962	58,14	18,22,23	0.34	0	26,32,35	0.48	0
11	MA6	A	1518	11	23,26,27	0.26	0	34,38,41	0.68	1 (2%)
14	PSU	a	2580	14	18,21,22	0.94	1 (5%)	22,30,33	0.72	1 (4%)
13	4SU	Z	8	13	18,21,22	0.38	0	26,30,33	1.19	3 (11%)
14	PSU	a	2605	14	18,21,22	0.90	1 (5%)	22,30,33	0.83	1 (4%)
14	2MG	a	1835	14	23,26,27	0.37	0	32,38,41	0.35	0
14	G7M	a	2069	14	23,26,27	0.72	1 (4%)	35,39,42	0.63	1 (2%)
12	6MZ	Y	37	12	22,25,26	0.38	0	30,36,39	0.55	0
14	PSU	a	1917	14	18,21,22	0.90	1 (5%)	22,30,33	0.56	0
3	IAS	K	119	3	6,7,8	0.88	0	6,8,10	0.93	0
14	OMC	a	2498	57,14	19,22,23	0.26	0	26,31,34	0.53	0
14	6MZ	a	1618	14	22,25,26	0.32	0	30,36,39	0.55	0
11	5MC	A	967	11	18,22,23	0.32	0	26,32,35	0.53	0
14	3TD	a	1915	14	18,22,23	0.96	1 (5%)	22,32,35	0.68	0
11	4OC	A	1402	11	20,23,24	0.35	0	26,32,35	0.48	0
14	PSU	a	1911	14	18,21,22	0.89	1 (5%)	22,30,33	0.55	0
12	G7M	Y	46	12	23,26,27	0.72	1 (4%)	35,39,42	0.54	0
11	5MC	A	1407	11	18,22,23	0.32	0	26,32,35	0.59	0
14	6MZ	a	2030	14	22,25,26	0.33	0	30,36,39	0.63	0
14	2MA	a	2503	57,58,14	22,25,26	0.26	0	33,37,40	0.67	2 (6%)
11	PSU	A	516	11	18,21,22	0.89	1 (5%)	22,30,33	0.81	1 (4%)
14	5MU	a	1939	58,14	19,22,23	0.27	0	28,32,35	0.43	0
14	2MG	a	2445	14	23,26,27	0.37	0	32,38,41	0.41	0
11	2MG	A	1207	11	23,26,27	0.39	0	32,38,41	0.41	0
12	PSU	Y	55	12	18,21,22	0.92	1 (5%)	22,30,33	0.63	0
13	PSU	Z	55	13	18,21,22	0.92	1 (5%)	22,30,33	0.64	0
13	5MU	Z	54	13	19,22,23	0.26	0	28,32,35	0.27	0
14	PSU	a	955	14	18,21,22	0.90	1 (5%)	22,30,33	0.67	0
14	H2U	a	2449	14	18,21,22	0.55	0	21,30,33	0.84	1 (4%)
7	MEQ	d	150	7	8,9,10	0.42	0	5,10,12	0.87	0
14	PSU	a	2457	14	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
11	2MG	A	966	11	23,26,27	0.41	0	32,38,41	0.39	0
14	PSU	a	2604	14	18,21,22	0.94	1 (5%)	22,30,33	0.73	0
9	4D4	l	81	9	9,11,12	0.50	0	8,13,15	0.61	0
11	2MG	A	1516	11	23,26,27	0.35	0	32,38,41	0.50	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
11	G7M	A	527	11	-	1/7/25/26	0/3/3/3
11	UR3	A	1498	11	-	0/7/25/26	0/2/2/2
11	MA6	A	1519	11	-	3/11/29/30	0/3/3/3
14	PSU	a	746	57,14	-	1/7/25/26	0/2/2/2
13	OMC	Z	32	13	-	0/9/27/28	0/2/2/2
12	5MU	Y	54	12	-	0/7/25/26	0/2/2/2
9	MS6	l	82	9	-	1/4/6/8	-
12	4SU	Y	8	12	-	0/7/25/26	0/2/2/2
14	OMU	a	2552	14	-	0/9/27/28	0/2/2/2
14	1MG	a	745	14	-	0/7/25/26	0/3/3/3
14	5MU	a	747	14	-	0/7/25/26	0/2/2/2
14	PSU	a	2504	58,14	-	0/7/25/26	0/2/2/2
14	OMG	a	2251	14,12	-	0/9/27/28	0/3/3/3
4	D2T	L	89	4	-	5/7/12/14	-
13	G7M	Z	46	13	-	3/7/25/26	0/3/3/3
14	5MC	a	1962	58,14	-	1/7/25/26	0/2/2/2
11	MA6	A	1518	11	-	0/11/29/30	0/3/3/3
14	PSU	a	2580	14	-	0/7/25/26	0/2/2/2
13	4SU	Z	8	13	-	0/7/25/26	0/2/2/2
14	PSU	a	2605	14	-	0/7/25/26	0/2/2/2
14	2MG	a	1835	14	-	0/9/27/28	0/3/3/3
14	G7M	a	2069	14	-	2/7/25/26	0/3/3/3
12	6MZ	Y	37	12	-	0/9/27/28	0/3/3/3
14	PSU	a	1917	14	-	0/7/25/26	0/2/2/2
3	IAS	K	119	3	-	0/7/7/8	-
14	OMC	a	2498	57,14	-	0/9/27/28	0/2/2/2
14	6MZ	a	1618	14	-	0/9/27/28	0/3/3/3
11	5MC	A	967	11	-	0/7/25/26	0/2/2/2
14	3TD	a	1915	14	-	0/7/25/26	0/2/2/2
11	4OC	A	1402	11	-	0/9/29/30	0/2/2/2
14	PSU	a	1911	14	-	3/7/25/26	0/2/2/2
12	G7M	Y	46	12	-	3/7/25/26	0/3/3/3
11	5MC	A	1407	11	-	0/7/25/26	0/2/2/2
14	6MZ	a	2030	14	-	2/9/27/28	0/3/3/3
14	2MA	a	2503	57,58,14	-	2/7/25/26	0/3/3/3
11	PSU	A	516	11	-	0/7/25/26	0/2/2/2
14	5MU	a	1939	58,14	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	2MG	a	2445	14	-	0/9/27/28	0/3/3/3
11	2MG	A	1207	11	-	0/9/27/28	0/3/3/3
12	PSU	Y	55	12	-	0/7/25/26	0/2/2/2
13	PSU	Z	55	13	-	1/7/25/26	0/2/2/2
13	5MU	Z	54	13	-	0/7/25/26	0/2/2/2
14	PSU	a	955	14	-	0/7/25/26	0/2/2/2
14	H2U	a	2449	14	-	0/7/38/39	0/2/2/2
7	MEQ	d	150	7	-	2/8/9/11	-
14	PSU	a	2457	14	-	0/7/25/26	0/2/2/2
11	2MG	A	966	11	-	3/9/27/28	0/3/3/3
14	PSU	a	2604	14	-	0/7/25/26	0/2/2/2
9	4D4	l	81	9	-	3/11/12/14	-
11	2MG	A	1516	11	-	0/9/27/28	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	2604	PSU	C6-C5	3.64	1.39	1.35
14	a	1915	3TD	C6-C5	3.63	1.39	1.35
14	a	2580	PSU	C6-C5	3.63	1.39	1.35
12	Y	55	PSU	C6-C5	3.62	1.39	1.35
13	Z	55	PSU	C6-C5	3.61	1.39	1.35
14	a	1917	PSU	C6-C5	3.55	1.39	1.35
11	A	516	PSU	C6-C5	3.51	1.39	1.35
14	a	1911	PSU	C6-C5	3.51	1.39	1.35
14	a	955	PSU	C6-C5	3.43	1.39	1.35
14	a	2504	PSU	C6-C5	3.41	1.39	1.35
14	a	2605	PSU	C6-C5	3.41	1.39	1.35
14	a	746	PSU	C6-C5	3.41	1.39	1.35
14	a	2457	PSU	C6-C5	3.38	1.39	1.35
12	Y	46	G7M	C8-N7	2.64	1.37	1.33
11	A	527	G7M	C8-N7	2.62	1.37	1.33
13	Z	46	G7M	C8-N7	2.55	1.37	1.33
14	a	2069	G7M	C8-N7	2.47	1.37	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	8	4SU	C4-N3-C2	-4.34	123.12	127.34
13	Z	8	4SU	C4-N3-C2	-4.34	123.12	127.34
11	A	1518	MA6	C2-N1-C6	2.90	118.59	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1519	MA6	C2-N1-C6	2.85	118.49	111.75
12	Y	8	4SU	C5-C4-N3	2.78	117.27	114.69
13	Z	8	4SU	C5-C4-N3	2.77	117.26	114.69
11	A	516	PSU	C3'-C2'-C1'	2.69	104.77	101.64
4	L	89	D2T	OD1-CG-CB	-2.55	117.09	122.44
14	a	2449	H2U	O2-C2-N1	-2.29	120.23	123.11
14	a	2503	2MA	C5-C4-N3	-2.29	124.62	127.19
14	a	2580	PSU	C3'-C2'-C1'	2.20	104.20	101.64
12	Y	8	4SU	N3-C2-N1	2.19	117.79	114.89
13	Z	8	4SU	N3-C2-N1	2.18	117.78	114.89
4	L	89	D2T	OD2-CG-CB	2.11	117.71	113.15
14	a	2069	G7M	N9-C8-N7	-2.08	107.07	112.21
14	a	2605	PSU	C2'-C3'-C4'	-2.04	98.67	102.64
14	a	2503	2MA	N3-C4-N9	2.00	129.77	126.99

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	89	D2T	CG-CB-SB-CB1
4	L	89	D2T	CA-CB-CG-OD1
4	L	89	D2T	CA-CB-CG-OD2
11	A	1519	MA6	O4'-C4'-C5'-O5'
14	a	2030	6MZ	O4'-C4'-C5'-O5'
12	Y	46	G7M	C4'-C5'-O5'-P
11	A	966	2MG	O4'-C4'-C5'-O5'
11	A	966	2MG	C3'-C4'-C5'-O5'
11	A	1519	MA6	C3'-C4'-C5'-O5'
14	a	1911	PSU	C3'-C4'-C5'-O5'
14	a	1911	PSU	O4'-C4'-C5'-O5'
14	a	2030	6MZ	C3'-C4'-C5'-O5'
12	Y	46	G7M	O4'-C4'-C5'-O5'
12	Y	46	G7M	C3'-C4'-C5'-O5'
13	Z	46	G7M	C3'-C4'-C5'-O5'
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
13	Z	46	G7M	O4'-C4'-C5'-O5'
9	l	81	4D4	OB-CB-CG-CD
14	a	1911	PSU	C4'-C5'-O5'-P
13	Z	46	G7M	C4'-C5'-O5'-P
11	A	966	2MG	C4'-C5'-O5'-P
14	a	2503	2MA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
9	l	82	MS6	CB-CG-SD-CE
14	a	2069	G7M	C4'-C5'-O5'-P
13	Z	55	PSU	O4'-C1'-C5-C4
9	l	81	4D4	CA-CB-CG-CD
4	L	89	D2T	CA-CB-SB-CB1
4	L	89	D2T	SB-CB-CG-OD2
14	a	746	PSU	O4'-C1'-C5-C6
11	A	1519	MA6	C4'-C5'-O5'-P
14	a	2069	G7M	O4'-C4'-C5'-O5'
14	a	2503	2MA	O4'-C4'-C5'-O5'
11	A	527	G7M	C3'-C4'-C5'-O5'
14	a	1962	5MC	O4'-C1'-N1-C6
9	l	81	4D4	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1519	MA6	2	0
14	a	747	5MU	1	0
11	A	1518	MA6	2	0
12	Y	37	6MZ	1	0
11	A	1402	4OC	1	0
14	a	2030	6MZ	1	0
14	a	1939	5MU	1	0
14	a	2604	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 252 ligands modelled in this entry, 250 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	VAL	Y	101	12	4,6,7	0.57	0	6,7,9	0.59	0
59	SCM	A	1601	-	23,25,25	0.27	0	26,39,39	0.60	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
60	VAL	Y	101	12	-	0/5/6/8	-
59	SCM	A	1601	-	-	2/4/57/57	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	1601	SCM	C7-C8-N8-C8M
59	A	1601	SCM	C9-C8-N8-C8M

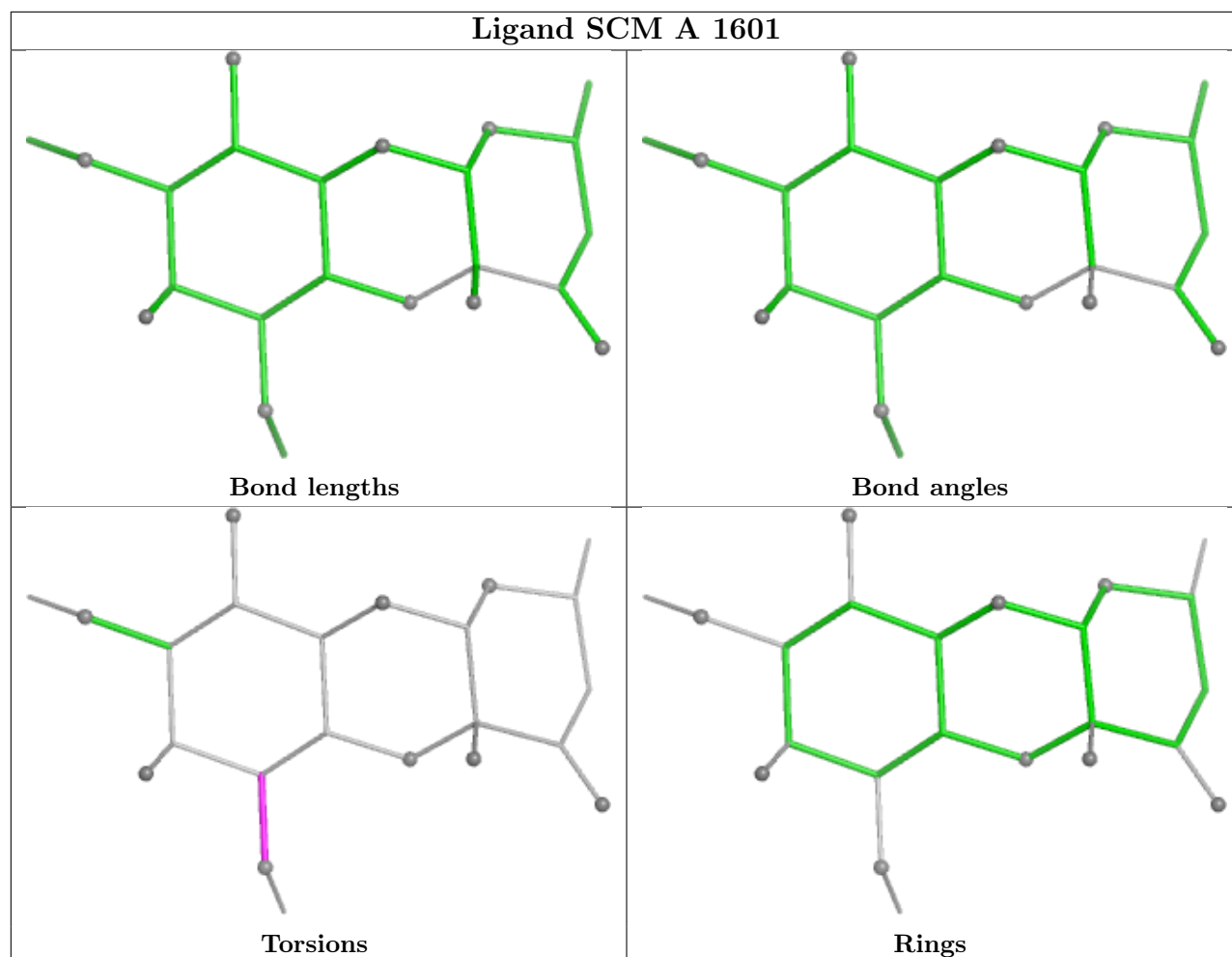
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	A	1601	SCM	4	0

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

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

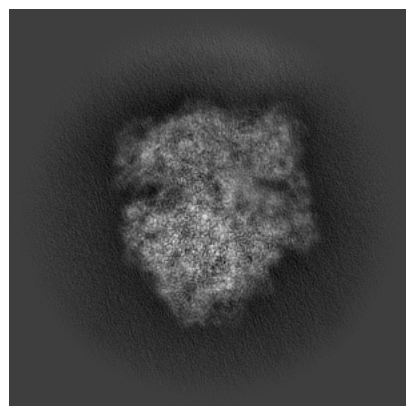
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56833. These allow visual inspection of the internal detail of the map and identification of artifacts.

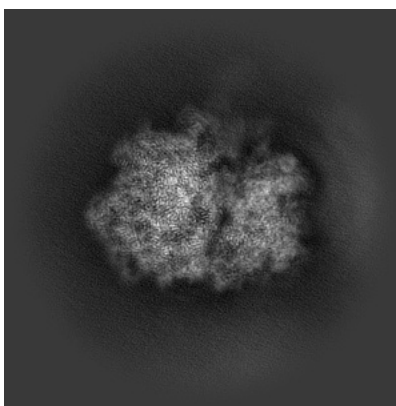
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

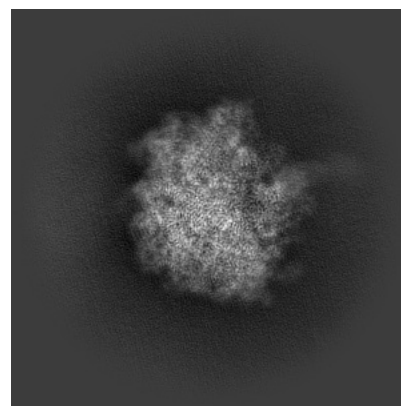
#### 6.1.1 Primary map



X

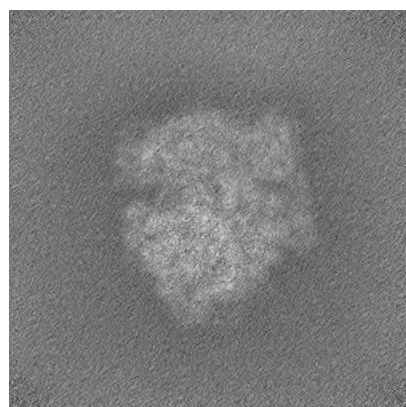


Y

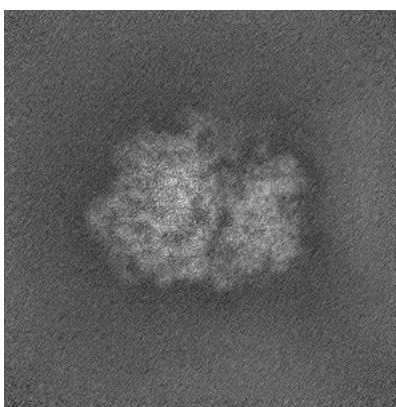


Z

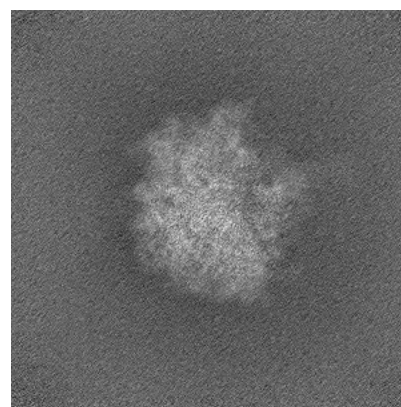
#### 6.1.2 Raw map



X



Y



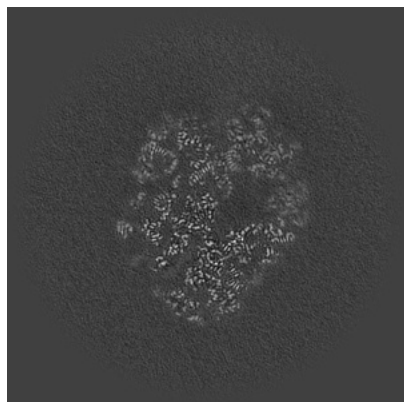
Z

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

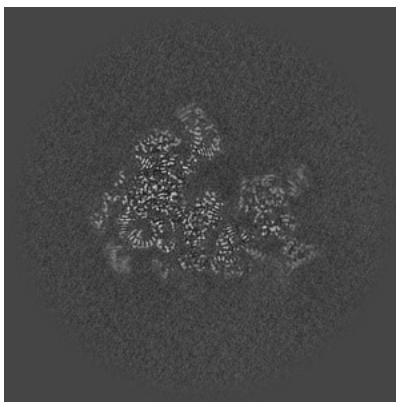


## 6.2 Central slices [i](#)

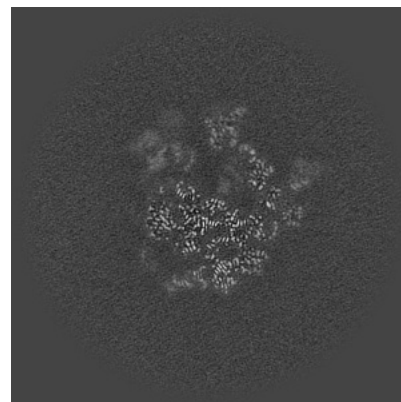
### 6.2.1 Primary map



X Index: 288

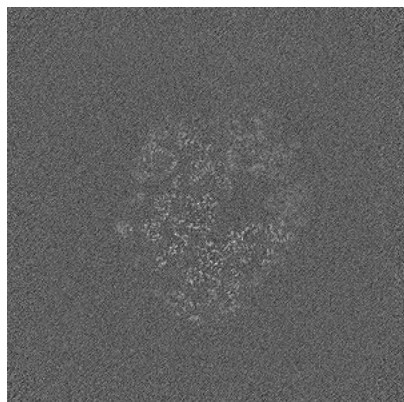


Y Index: 288

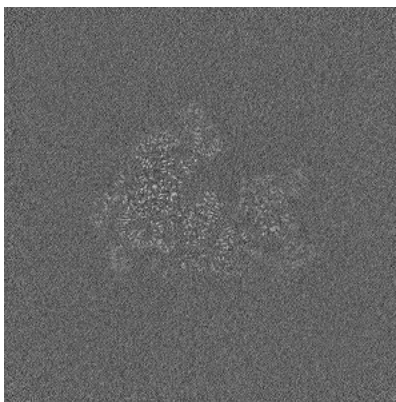


Z Index: 288

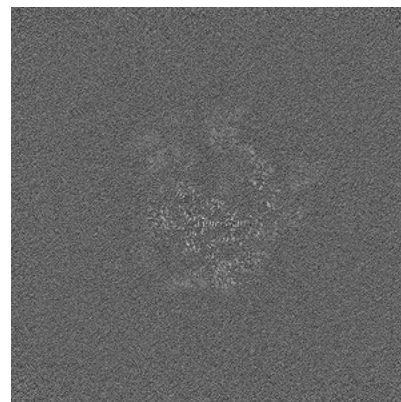
### 6.2.2 Raw map



X Index: 288



Y Index: 288

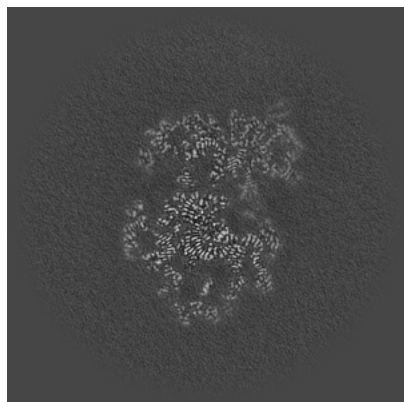


Z Index: 288

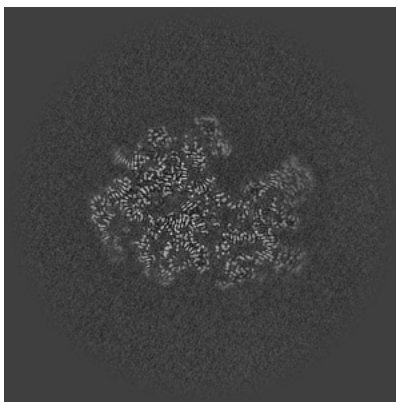
The images above show central slices of the map in three orthogonal directions.

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

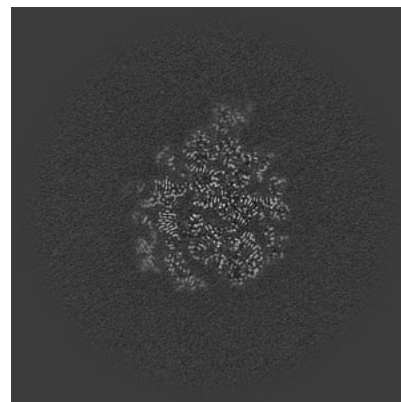
### 6.3.1 Primary map



X Index: 264

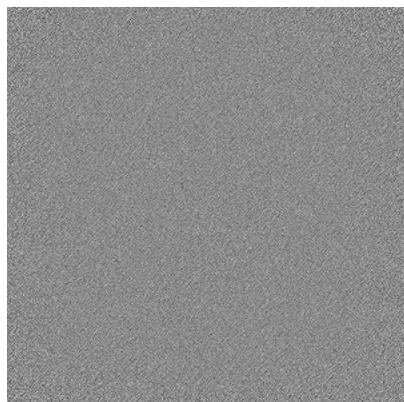


Y Index: 272

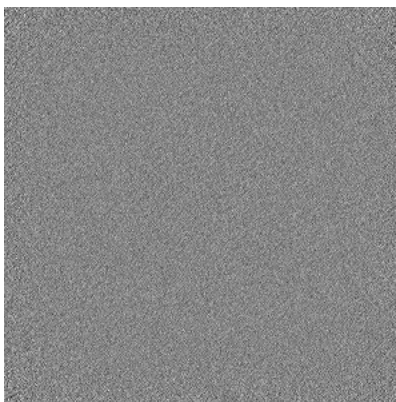


Z Index: 234

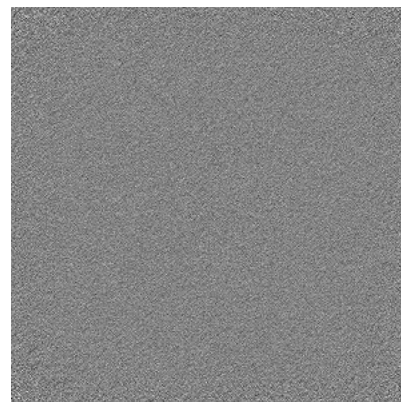
### 6.3.2 Raw map



X Index: 0



Y Index: 0

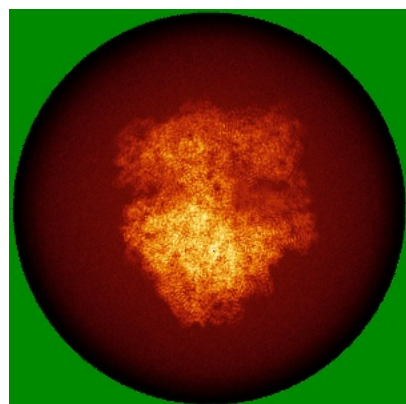


Z Index: 0

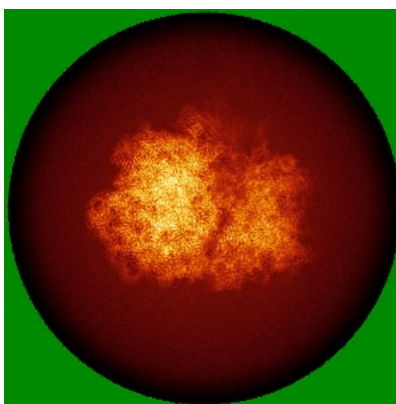
The images above show the largest variance slices of the map in three orthogonal directions.

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

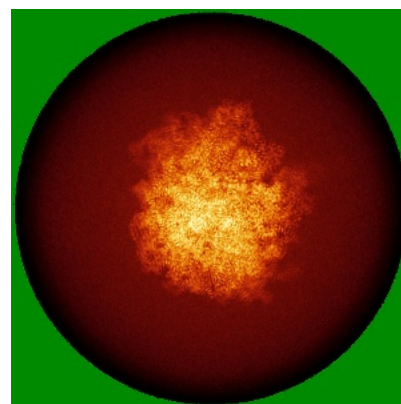
### 6.4.1 Primary map



X

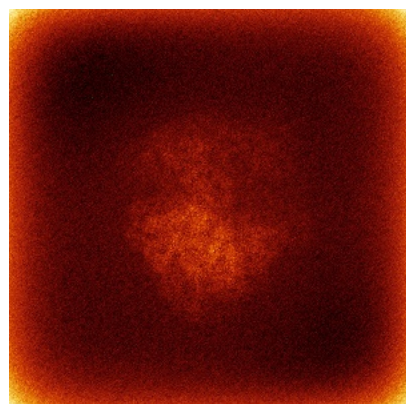


Y

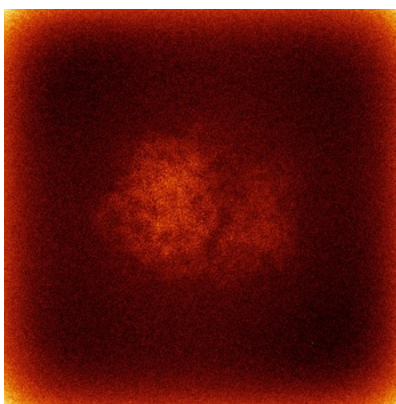


Z

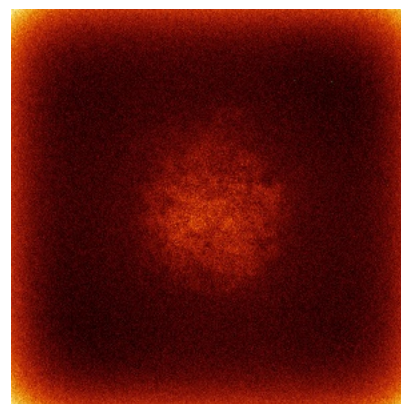
### 6.4.2 Raw map



X



Y



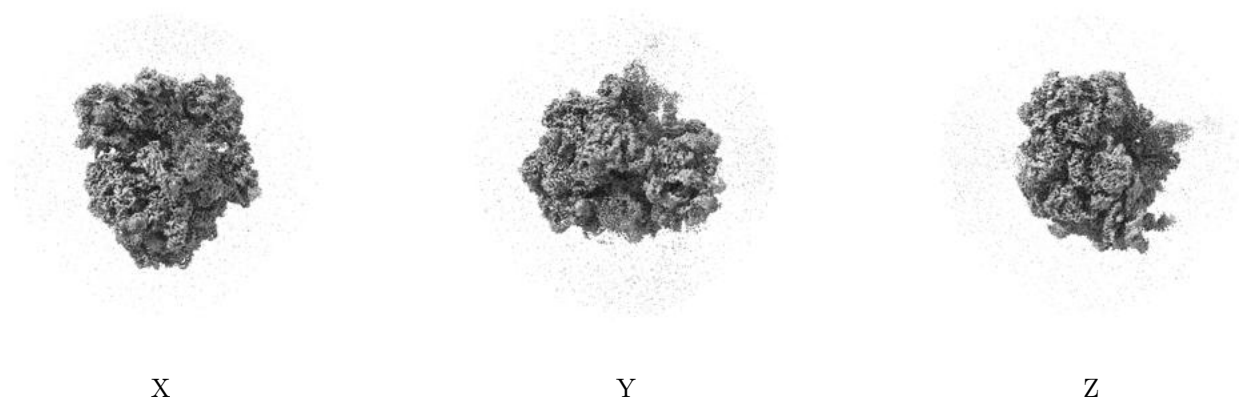
Z

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.



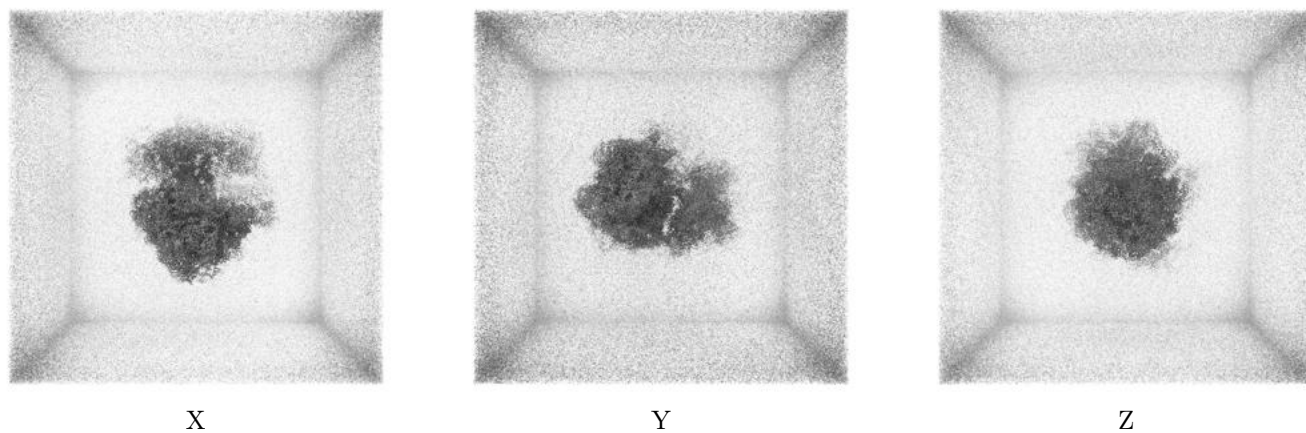
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0761. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

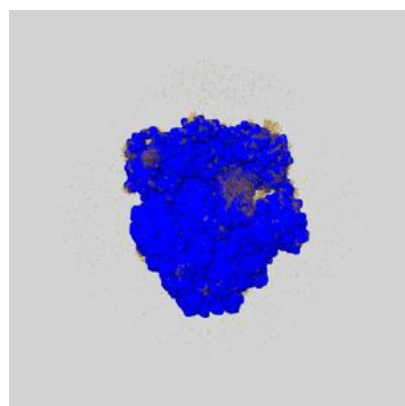
## 6.6 Mask visualisation [i](#)

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

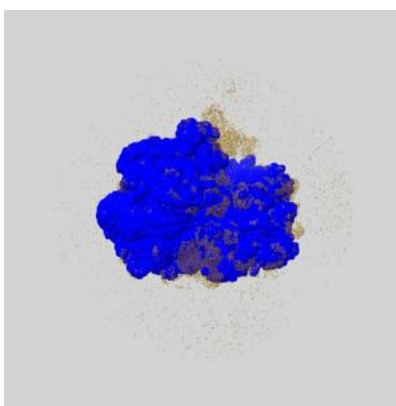
A mask typically either:

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

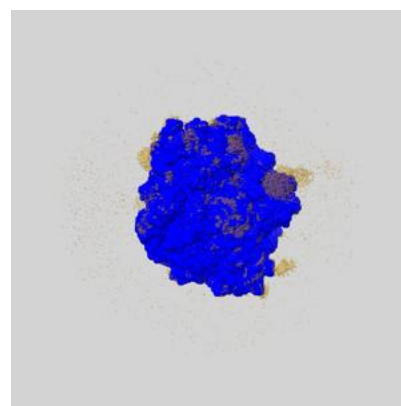
### 6.6.1 emd\_56833\_msk\_1.map [i](#)



X



Y

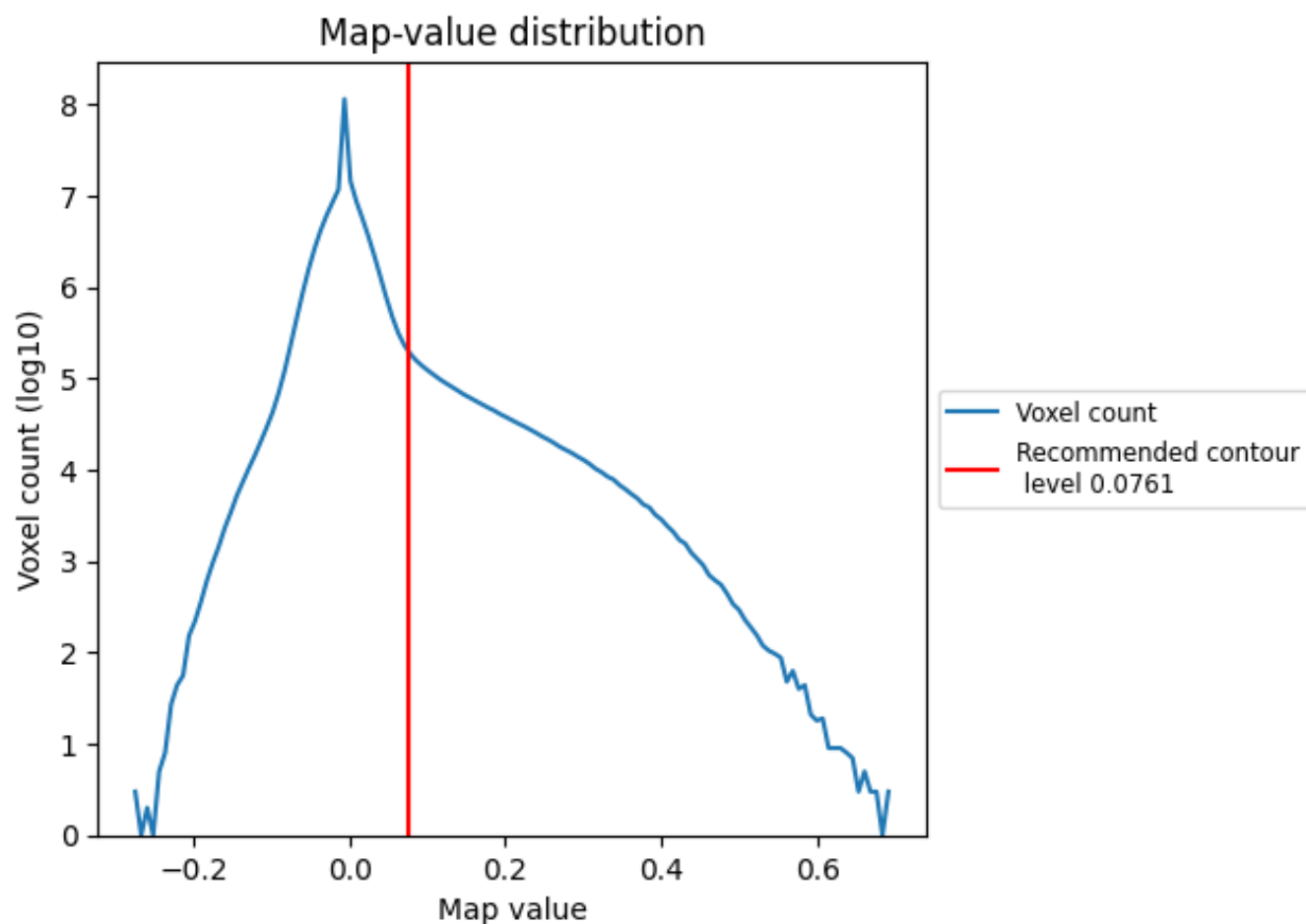


Z

## 7 Map analysis [i](#)

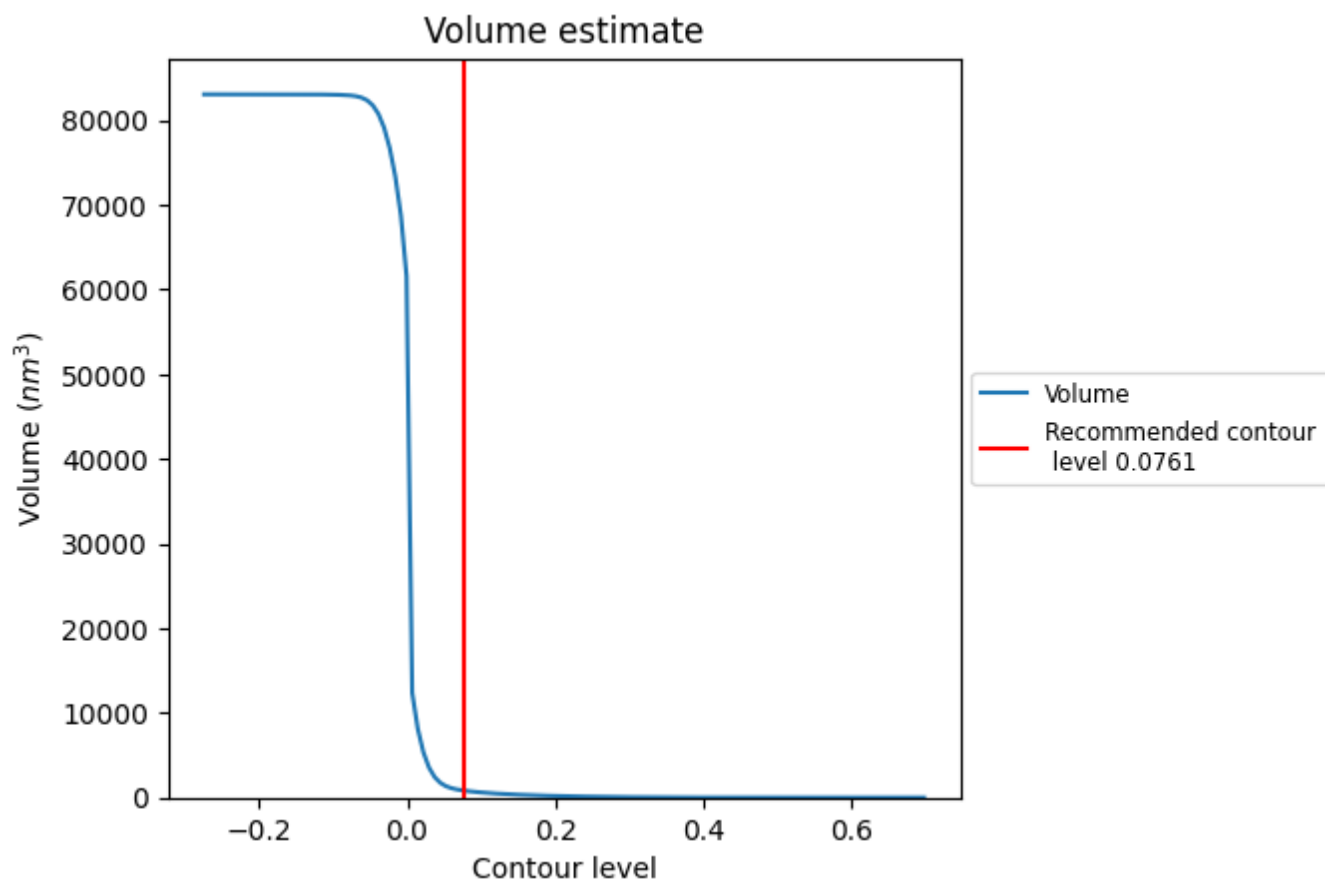
This section contains the results of statistical analysis of the map.

### 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.

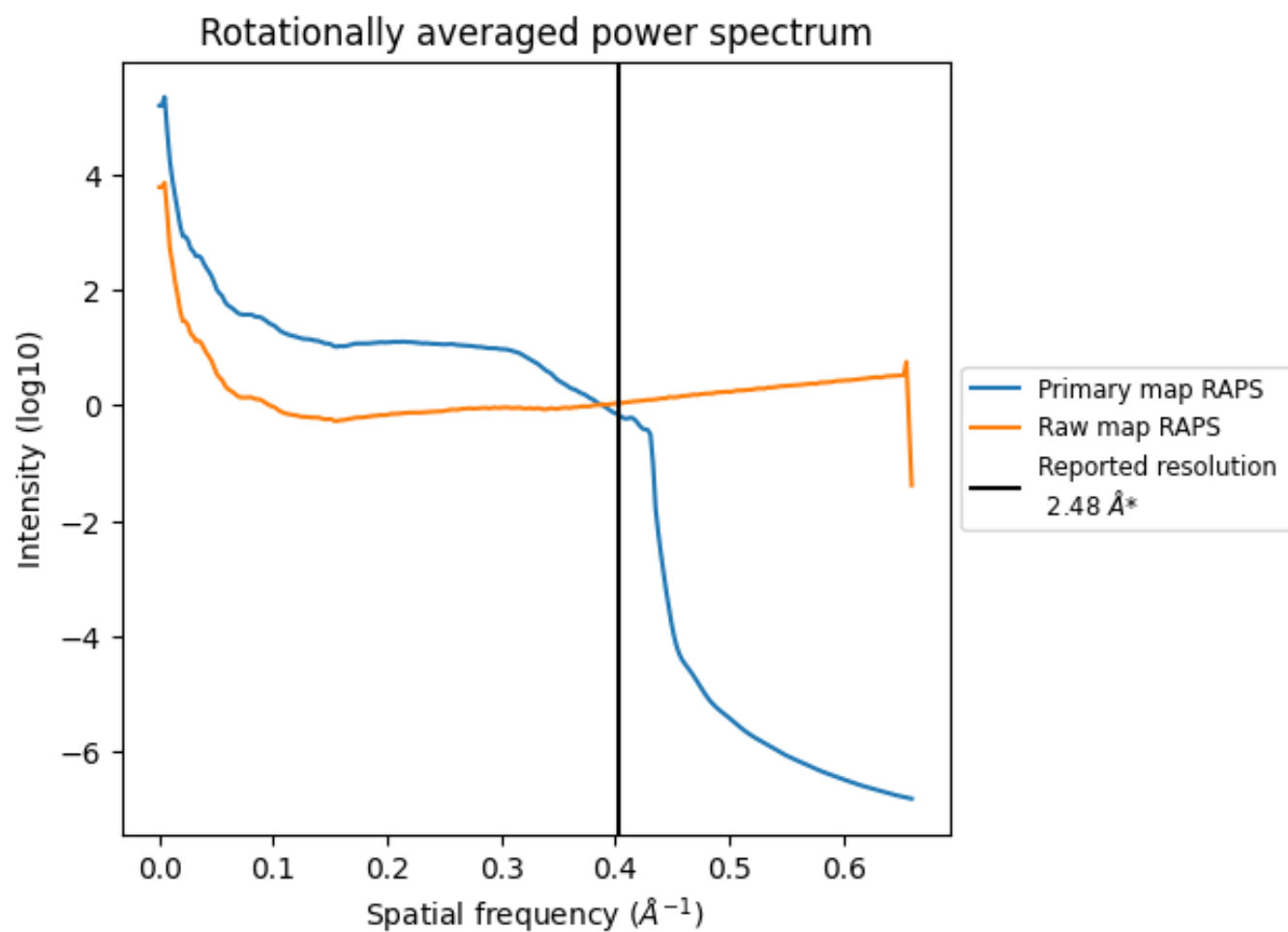
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 831 nm<sup>3</sup>; this corresponds to an approximate mass of 751 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

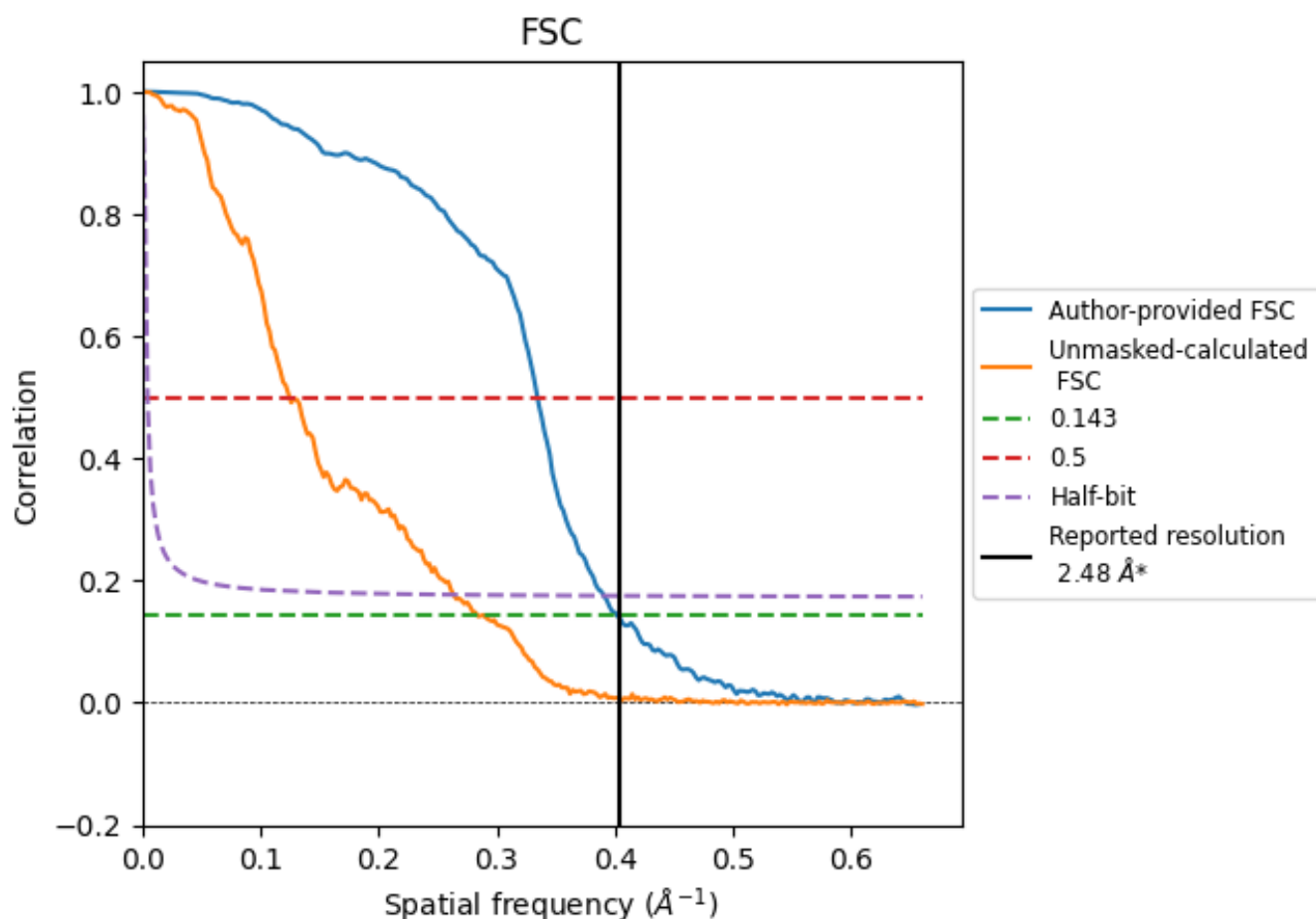


\*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.403  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

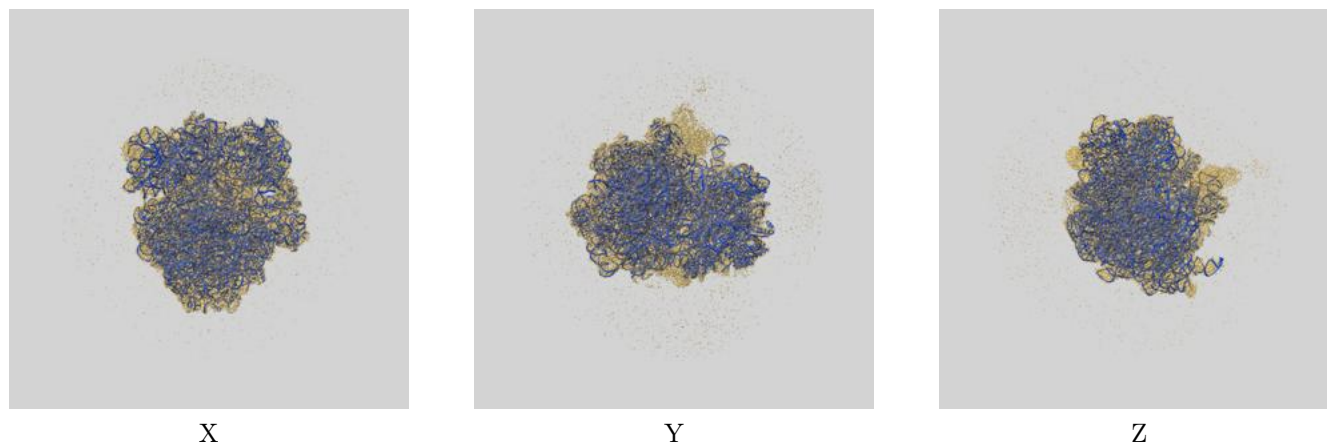
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.49	2.99	2.56
Unmasked-calculated*	3.53	8.03	3.80

\*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 3.53 differs from the reported value 2.48 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-56833 and PDB model 28UN. Per-residue inclusion information can be found in section [3](#) on page [19](#).

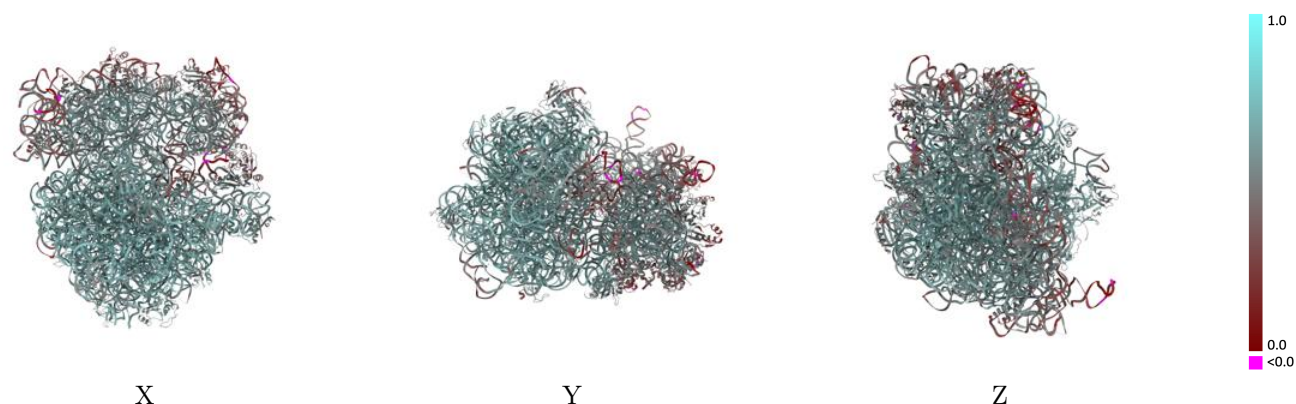
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0761 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.

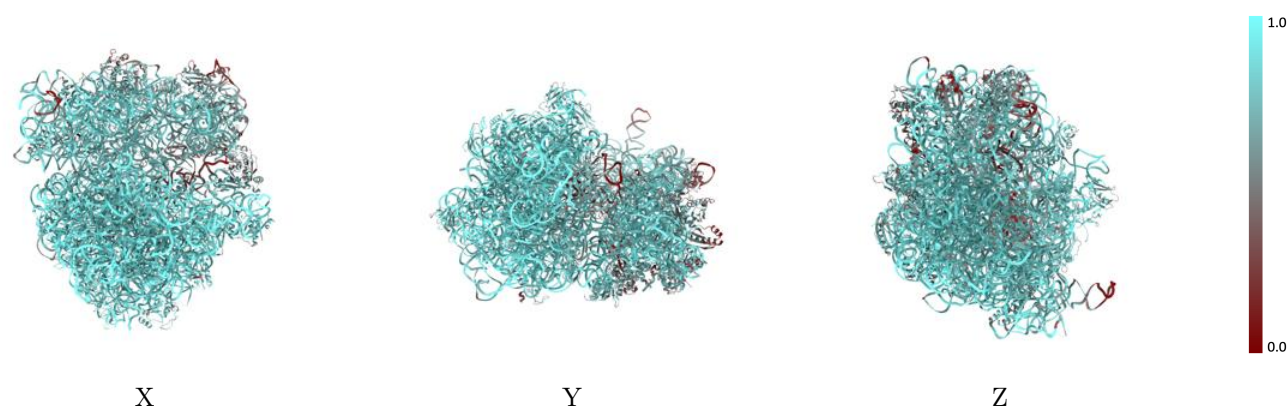


## 9.2 Q-score mapped to coordinate model [i](#)



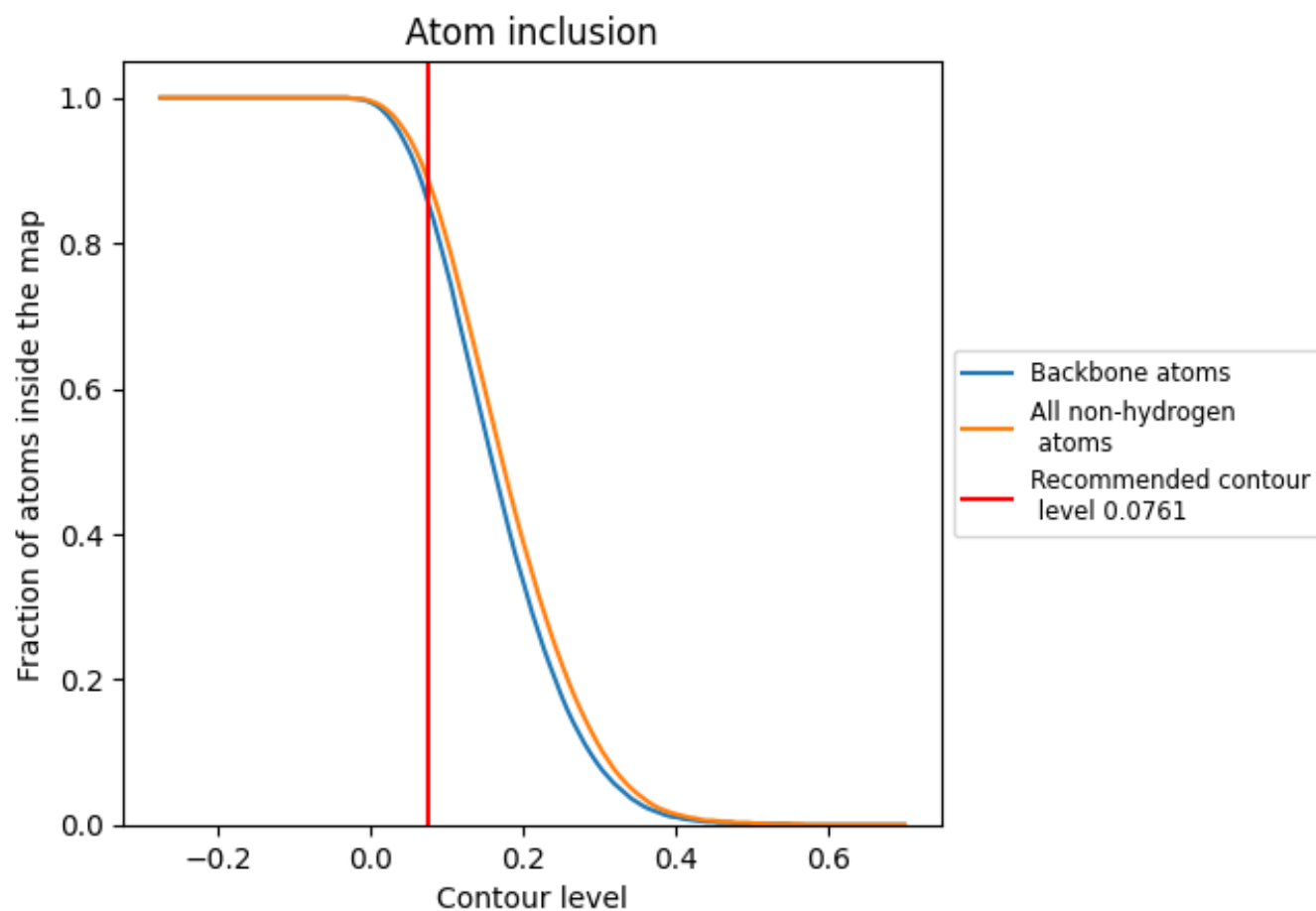
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0761).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 88% 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 (0.0761) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.5860
0	 0.8260	 0.5970
1	 0.9410	 0.6720
2	 0.9570	 0.6670
3	 0.9080	 0.6220
4	 0.5170	 0.3440
A	 0.8960	 0.5500
B	 0.6920	 0.4920
C	 0.6970	 0.5200
D	 0.5110	 0.3930
E	 0.8270	 0.5930
F	 0.7420	 0.5200
G	 0.4610	 0.3580
H	 0.8580	 0.6040
I	 0.6610	 0.4690
J	 0.5160	 0.4120
K	 0.8200	 0.5780
L	 0.7490	 0.5350
M	 0.6270	 0.4510
N	 0.6940	 0.4890
O	 0.8320	 0.5810
P	 0.7250	 0.5060
Q	 0.7310	 0.5310
R	 0.8160	 0.5630
S	 0.6550	 0.4570
T	 0.7020	 0.4640
U	 0.6570	 0.4860
X	 0.7680	 0.5150
Y	 0.4220	 0.3130
Z	 0.8100	 0.4830
a	 0.9680	 0.6370
b	 0.9330	 0.5890
c	 0.9370	 0.6650
d	 0.9180	 0.6400
e	 0.8650	 0.6050



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Chain	Atom inclusion	Q-score
f	 0.6210	 0.4410
g	 0.7610	 0.5150
h	 0.6410	 0.4880
i	 0.9250	 0.6390
j	 0.8860	 0.6370
k	 0.9070	 0.6330
l	 0.9000	 0.6380
m	 0.9600	 0.6610
n	 0.8060	 0.5340
o	 0.8440	 0.6070
p	 0.9550	 0.6680
q	 0.8960	 0.6270
r	 0.9040	 0.6370
s	 0.8570	 0.5980
t	 0.8450	 0.5770
u	 0.8320	 0.5790
v	 0.9050	 0.6330
w	 0.9200	 0.6320
x	 0.8120	 0.5660
y	 0.8830	 0.6300
z	 0.8860	 0.6300