



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 08:38 pm BST

PDB ID : 28UJ / pdb_000028uj
EMDB ID : EMD-56829
Title : E. coli 70S ribosome, trapped conformational excited state of SSU-h44 apical loop, with A/P- and P/E-site tRNA
Authors : Steinmetzger, C.; Riad, M.; Petzold, K.
Deposited on : 2026-02-20
Resolution : 2.16 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

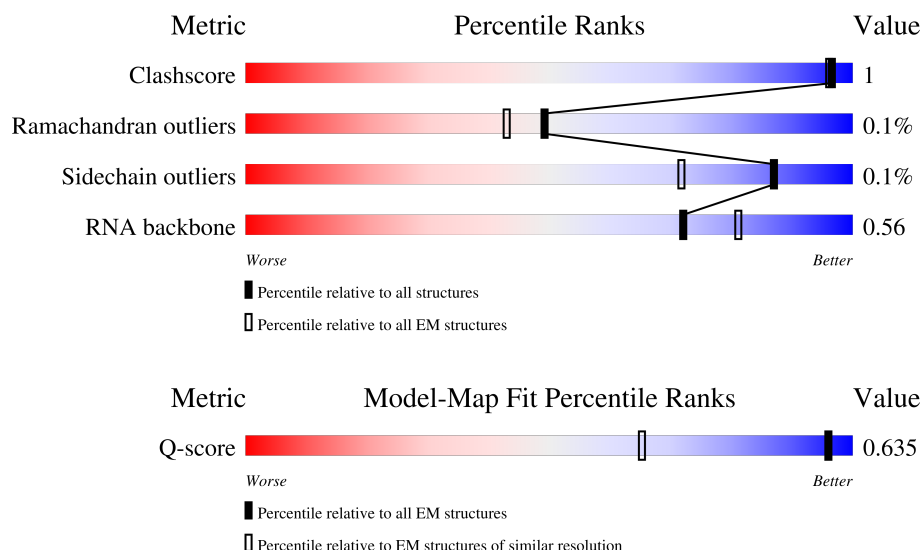
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

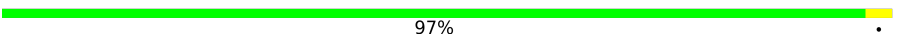


The reported resolution of this entry is 2.16 Å.

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.



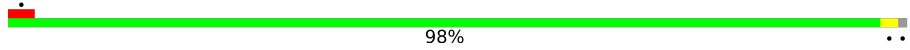

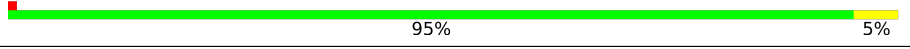
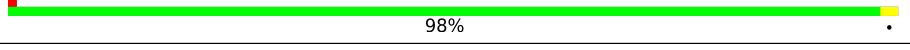
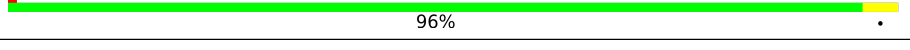
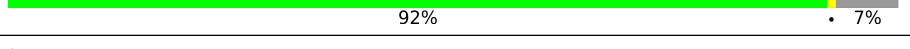
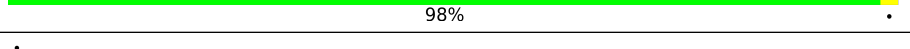
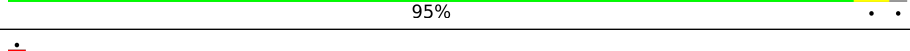
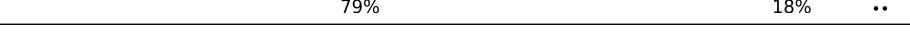
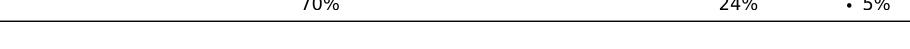
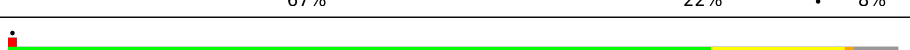

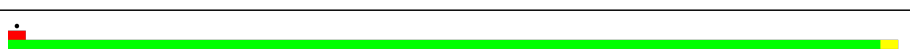
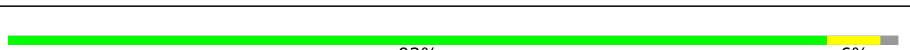
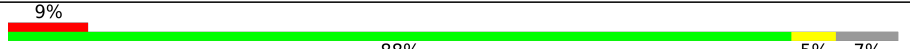





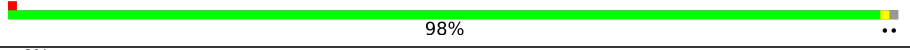
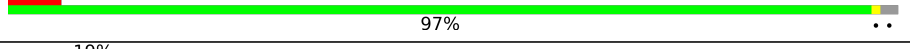
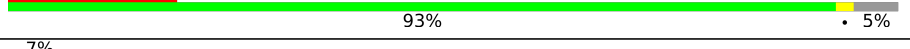
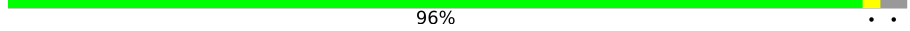

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2609 (1.67 - 2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	38	 97%
2	4	70	 66% 33%
3	K	129	 91% 9%

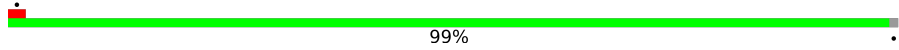
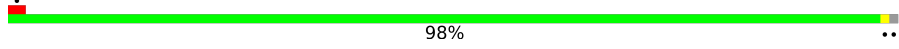
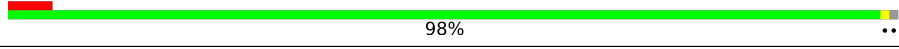
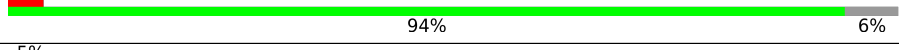

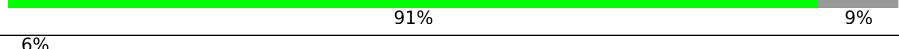
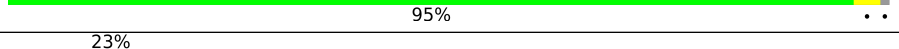
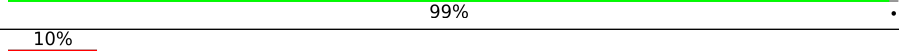
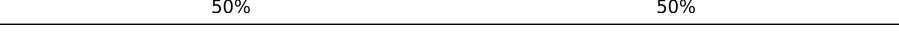
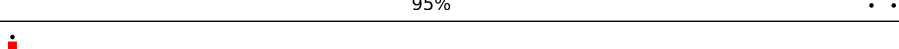
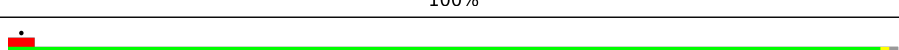
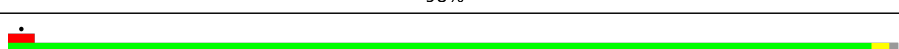

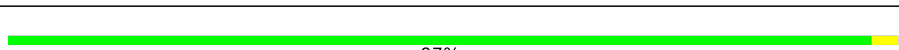
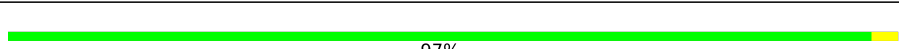
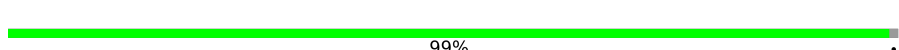

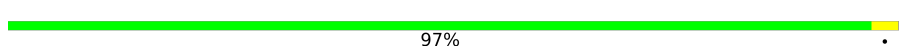
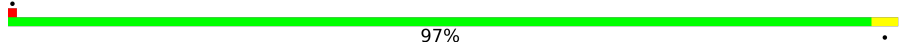
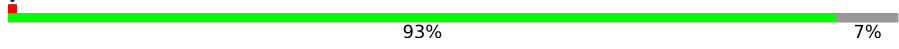
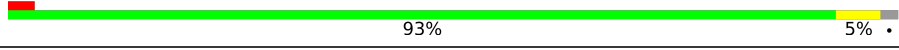
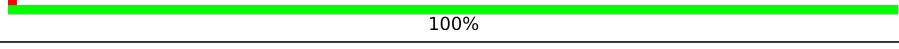

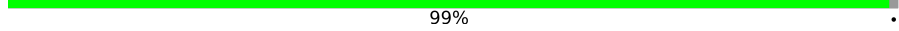

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Mol	Chain	Length	Quality of chain
4	L	124	
5	b	120	
6	d	209	
7	k	144	
8	l	136	
9	m	127	
10	r	110	
11	z	57	
12	A	1544	
13	Y	76	
14	Z	78	
15	a	2904	
16	0	55	
17	1	46	
18	2	65	
19	B	241	
20	C	233	
21	D	206	
22	E	167	
23	F	135	
24	G	179	
25	H	130	
26	I	130	
27	J	103	
28	M	118	

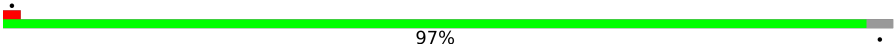
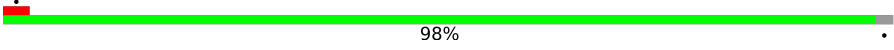
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Mol	Chain	Length	Quality of chain
29	N	101	
30	O	89	
31	P	82	
32	Q	84	
33	R	75	
34	S	92	
35	T	87	
36	U	71	
37	X	10	
38	c	273	
39	e	201	
40	f	179	
41	g	177	
42	h	149	
43	i	142	
44	j	123	
45	n	117	
46	o	115	
47	p	118	
48	q	103	
49	s	100	
50	t	104	
51	u	94	
52	v	85	
53	w	78	

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Mol	Chain	Length	Quality of chain
54	x	63	 97%
55	y	59	 98%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149221 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 uL3.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 9 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 12 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1521	Total	C	N	O	P	0	0
			32655	14571	5994	10569	1521		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1448A	G	-	insertion	GB 2971070070
A	1453A	C	-	insertion	GB 2971070070

- Molecule 13 is a RNA chain called A/P-site Val-tRNA^{Val}.

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

- Molecule 14 is a RNA chain called P/E-site tRNA^{fMet}.

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

- Molecule 15 is a RNA chain called 23S rRNA.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 17 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 18 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 31 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 33 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 35 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 36 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 37 is a RNA chain called mRNA.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL21.

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

- 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	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		

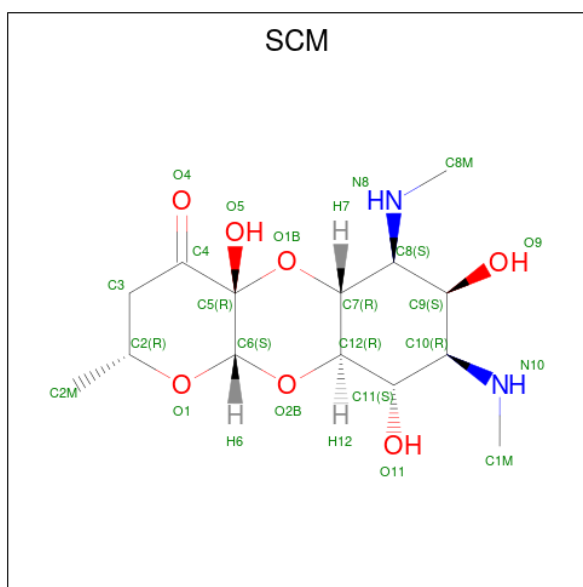
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	4	Total	Mg	0
			4	4	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	48	Total	Mg	0
			48	48	
57	a	195	Total	Mg	0
			195	195	
57	c	1	Total	Mg	0
			1	1	
57	p	1	Total	Mg	0
			1	1	

- Molecule 58 is SPECTINOMYCIN (CCD ID: SCM) (formula: C₁₄H₂₄N₂O₇).

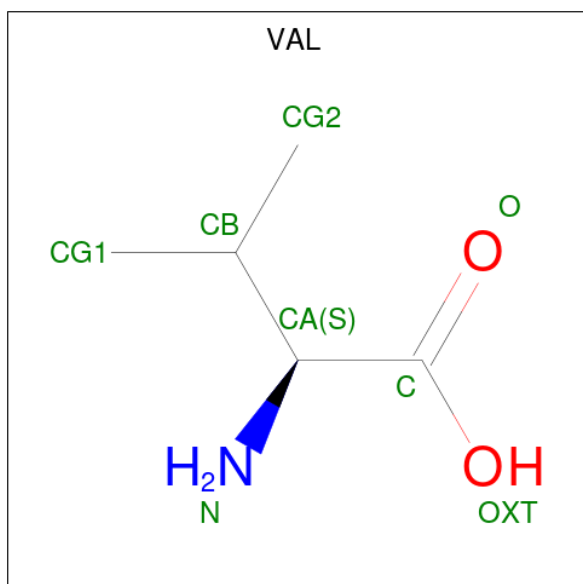


Mol	Chain	Residues	Atoms				AltConf
58	A	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	A	11	Total	K	0
			11	11	
59	a	36	Total	K	0
			36	36	

- Molecule 60 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



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	9	Total	O			0
			9	9			
61	4	3	Total	O			0
			3	3			
61	K	18	Total	O			0
			18	18			
61	L	14	Total	O			0
			14	14			
61	b	103	Total	O			0
			103	103			
61	d	74	Total	O			0
			74	74			
61	k	46	Total	O			0
			46	46			
61	l	44	Total	O			0
			44	44			
61	m	28	Total	O			0
			28	28			
61	r	44	Total	O			0
			44	44			
61	z	35	Total	O			0
			35	35			
61	A	1331	Total	O			0
			1331	1331			
61	Y	13	Total	O			0
			13	13			
61	Z	37	Total	O			0
			37	37			
61	a	4252	Total	O			0
			4252	4252			
61	0	7	Total	O			0
			7	7			
61	1	18	Total	O			0
			18	18			
61	2	21	Total	O			0
			21	21			
61	B	15	Total	O			0
			15	15			

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Mol	Chain	Residues	Atoms		AltConf
61	C	13	Total 13	O 13	0
61	D	7	Total 7	O 7	0
61	E	14	Total 14	O 14	0
61	F	2	Total 2	O 2	0
61	G	6	Total 6	O 6	0
61	H	17	Total 17	O 17	0
61	I	9	Total 9	O 9	0
61	J	11	Total 11	O 11	0
61	M	5	Total 5	O 5	0
61	N	6	Total 6	O 6	0
61	O	19	Total 19	O 19	0
61	P	9	Total 9	O 9	0
61	Q	8	Total 8	O 8	0
61	R	4	Total 4	O 4	0
61	S	3	Total 3	O 3	0
61	T	3	Total 3	O 3	0
61	U	10	Total 10	O 10	0
61	X	8	Total 8	O 8	0
61	c	106	Total 106	O 106	0
61	e	66	Total 66	O 66	0
61	f	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
61	g	11	Total 11	O 11	0
61	h	10	Total 10	O 10	0
61	i	25	Total 25	O 25	0
61	j	32	Total 32	O 32	0
61	n	10	Total 10	O 10	0
61	o	26	Total 26	O 26	0
61	p	35	Total 35	O 35	0
61	q	32	Total 32	O 32	0
61	s	21	Total 21	O 21	0
61	t	15	Total 15	O 15	0
61	u	13	Total 13	O 13	0
61	v	16	Total 16	O 16	0
61	w	19	Total 19	O 19	0
61	x	10	Total 10	O 10	0
61	y	14	Total 14	O 14	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.

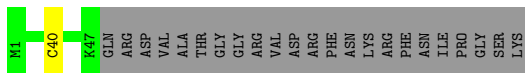
- Molecule 1: Large ribosomal subunit protein bL36A

Chain 3:  97%



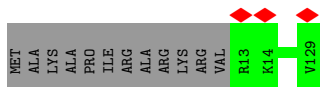
- Molecule 2: Large ribosomal subunit protein bL31

Chain 4:  66% 33%



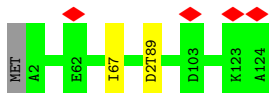
- Molecule 3: Small ribosomal subunit protein uS11

Chain K:  91% 9%




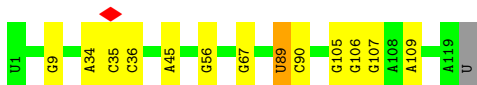
- Molecule 4: Small ribosomal subunit protein uS12

Chain L:  98% ..



- Molecule 5: 5S rRNA

Chain b:  88% 10% ..



- Molecule 6: Large ribosomal subunit protein uL3

Chain d:  95% 5%



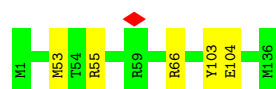
- Molecule 7: Large ribosomal subunit protein uL15

Chain k:  98%



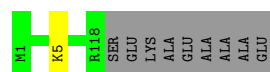
- Molecule 8: Large ribosomal subunit protein uL16

Chain l:  96%



- Molecule 9: Large ribosomal subunit protein bL17

Chain m:  92% 7%



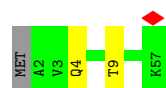
- Molecule 10: Large ribosomal subunit protein uL22

Chain r:  98%




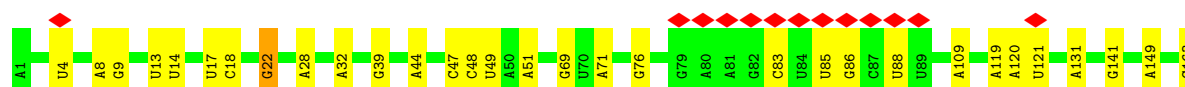
- Molecule 11: Large ribosomal subunit protein bL32

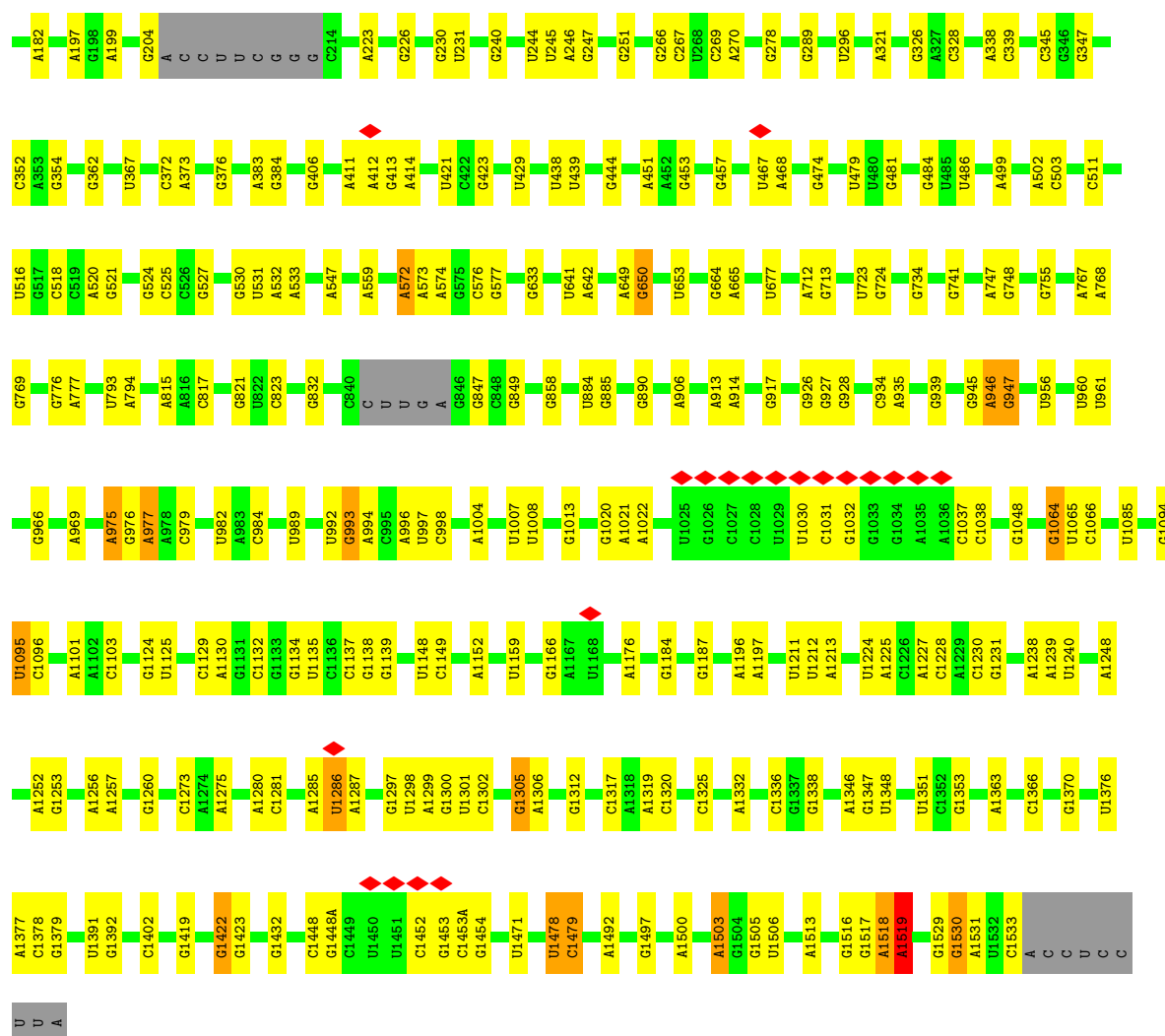
Chain z:  95%



- Molecule 12: 16S rRNA

Chain A:  79% 18%





• Molecule 13: A/P-site Val-tRNA^{Val}

Chain Y: 70% 24% 5%



• Molecule 14: P/E-site tRNA^{fMet}

Chain Z: 67% 22% 8%



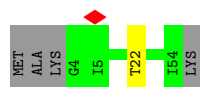
• Molecule 15: 23S rRNA

Chain a: 79% 15% 5%

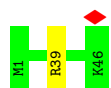
C2558	C2350	U	G	U1993	A1808	A1515	G1256	G	A996	G818	A627	G424	G1
A2566	G2382	G	A	C2000	C1816	G1529	G1271	C	C1005	A819	A627	G425	A10
G2567	G2383	U	G	G	A1272	G1529	A1272	U	U1012	U827	A637	U451	C11
C2573	U2384	C	C	A2014	A1829	A1535	A1286	A	U1013	U828	U639	A466	U12
U2580	C2385	U	U	A2020	G1846	C1536	A1287	U	A1020	A829	U641	G467	G26
A2602	U2402	U	U	G	A1847	G1537	G1300	A	A1021	U846	U642	G468	G26
G2603	A2406	G	G	U	A1848	C1558	A1301	G	G1022	U847	U643	G476	U34
U2604	A2211	A	A	A2030	A1858	U1559	G1338	U	G1026	G857	A643	A477	A56
U2605	A2225	G	G	G2032	G1560	G1560	U1352	C	A1027	G858	C645	A478	C57
U2609	G2238	U	U	A2033	A1566	A1566	U1352	C	A1028	U860	G847	G481	G58
U2613	G2239	U	U	G	A1569	A1569	C1357	G	U1033	A861	U653	G491	A71
U2430	G2239	G	G	U	A1578	A1578	G1358	U	A1040	A877	A654	A492	U72
U2431	U2243	A	A	U	U1578	U1578	A1365	U	G1047	G883	A655	G493	A73
A2432	U2244	C	C	G	U1584	C1585	C1370	U	C1052	U884	U656	G494	G75
A2435	C2248	G	G	C	C1607	C1585	G1371	U	C	C885	U656	G500	A84
U2441	A2268	C	C	G	A1608	A1608	U1378	U	A	U886	G711	A501	A84
A2448	A2273	U	U	U	A1609	A1609	U1379	U	G	U887	G712	A502	G98
U2449	A2274	C	C	G	A1610	A1610	G1380	U	A	C888	C717	A503	A101
G2661	G2282	G	G	A2060	A1912	A1912	A1383	U	G	C889	G729	A504	U102
A2662	C2283	C	C	G2061	C1914	C1914	A1383	U	U	C890	A730	A505	G110
G2663	G2286	A	A	A2062	3TD1915	A1916	A1393	U	U	G891	G738	A514	A118
U2689	A2287	U	U	C2063	U1647	U1647	U1405	U	G	C892	G738	G530	A119
U2690	A2288	G	G	U	U1648	U1648	U1406	U	G	C893	G738	C531	U120
G2714	U2291	A	A	G	G1674	G1674	G1416	U	C	A896	A743	G532	A131
C2715	U2292	C	C	U	G1715	G1715	C1417	U	U	A899	U746	G533	U138
C2716	U2305	C	C	A	C1730	C1730	G1428	U	A	A910	U747	G534	U139
A2726	G2306	G	G	G	G1731	G1731	C1428	U	G	G914	C765	U545	U138
G2744	G2307	C	C	C	C1732	C1732	A1434	U	A	C915	G775	U546	C140
G2747	G2308	U	U	U	G1738	G1738	G1435	U	G	G916	G776	G548	G141
A2748	C2310	U	U	G	A1754	A1754	G1452	U	A	A917	G777	G549	C157
G2751	A2317	A	A	A	U1758	U1758	A1453	U	C	A827	A781	A563	U158
C2755	A2322	A	A	G	G1764	G1764	U1474	U	C	A782	A782	U588	A165
U2756	G2325	U	U	U	A1773	A1773	G1475	U	A	U931	A783	U573	A181
A2757	C2326	C	C	A	U1778	U1778	G1482	U	U	A945	G785	U574	A196
A2765	A2327	A	A	G	U1782	U1782	A1490	U	A	C946	A788	A575	A199
G2778	U2329	C	C	U	A1783	A1783	C1493	U	U	U955	A789	A586	U200
G2780	A2333	C	C	A	A1784	A1784	U1497	A	A	U958	U790	A603	A204
C2788	A2335	U	U	G	G1799	G1799	C1498	G	A	C961	G795	U607	A207
U2789	C2347	U	U	U	C1800	C1800	A1508	A	A	G974	U811	U615	C208
U2790	G2557	A	A	G	A1801	A1801	A1509	A	A	A983	C812	G620	G215
										A984			A216
										C985			



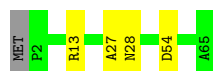
- Molecule 16: Large ribosomal subunit protein bL33



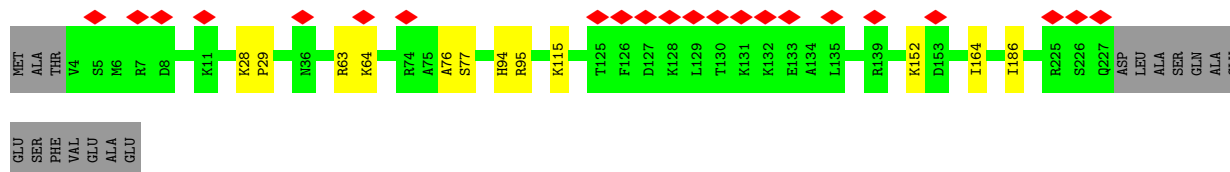
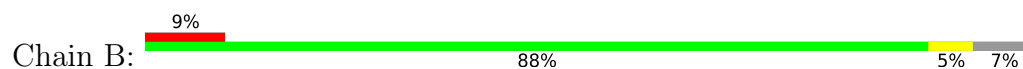
- Molecule 17: Large ribosomal subunit protein bL34



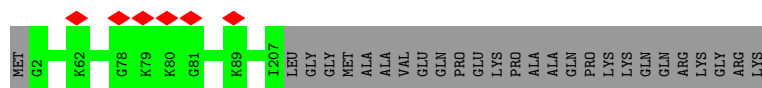
- Molecule 18: Large ribosomal subunit protein bL35



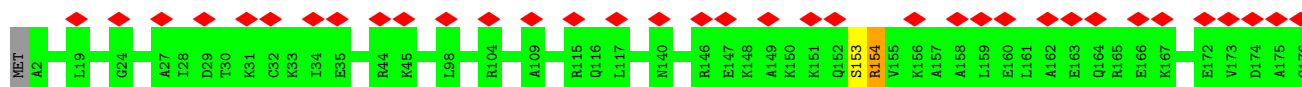
- Molecule 19: Small ribosomal subunit protein uS2

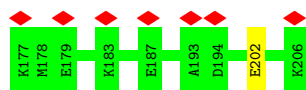


- Molecule 20: Small ribosomal subunit protein uS3

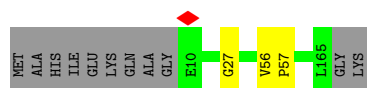
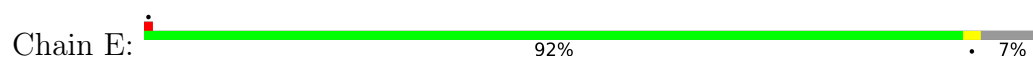


- Molecule 21: Small ribosomal subunit protein uS4

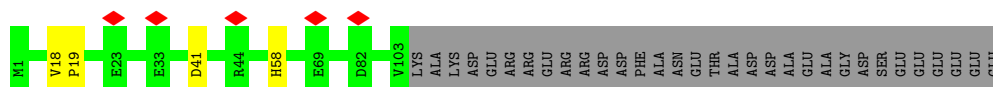




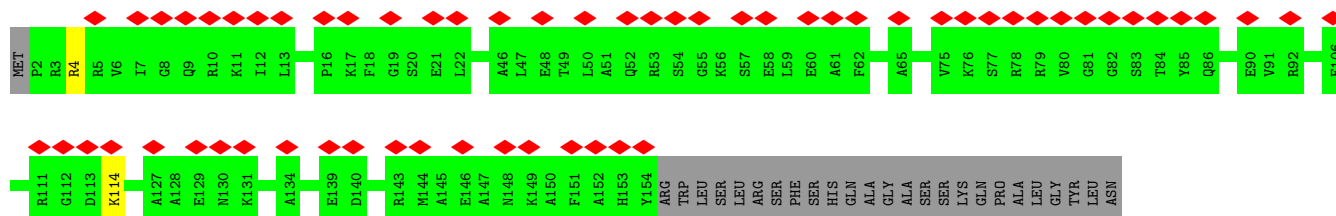
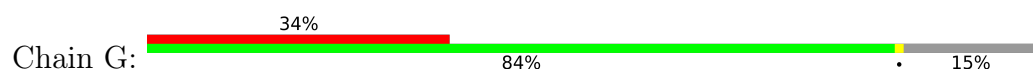
- Molecule 22: Small ribosomal subunit protein uS5



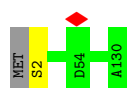
- Molecule 23: Small ribosomal subunit protein bS6, fully modified isoform



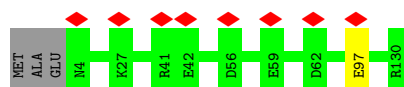
- Molecule 24: Small ribosomal subunit protein uS7



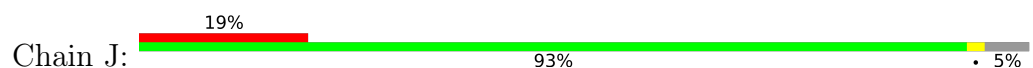
- Molecule 25: Small ribosomal subunit protein uS8

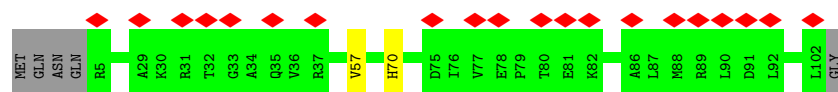


- Molecule 26: Small ribosomal subunit protein uS9

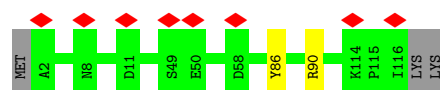


- Molecule 27: Small ribosomal subunit protein uS10

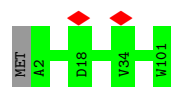




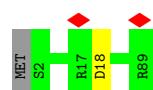
- Molecule 28: Small ribosomal subunit protein uS13



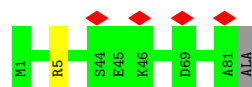
- Molecule 29: Small ribosomal subunit protein uS14



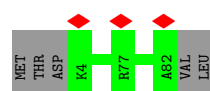
- Molecule 30: Small ribosomal subunit protein uS15



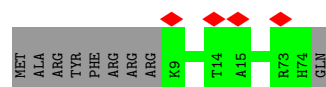
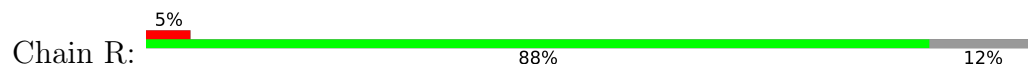
- Molecule 31: Small ribosomal subunit protein bS16




- Molecule 32: Small ribosomal subunit protein uS17

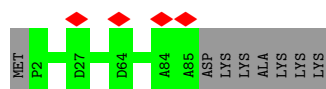


- Molecule 33: Small ribosomal subunit protein bS18



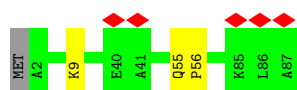
- Molecule 34: Small ribosomal subunit protein uS19

Chain S:  91% 9%



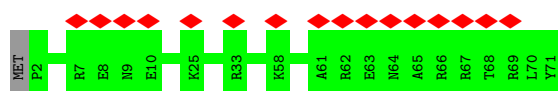
- Molecule 35: Small ribosomal subunit protein bS20

Chain T:  6% 95% ..



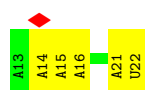
- Molecule 36: Small ribosomal subunit protein bS21

Chain U:  23% 99% .



- Molecule 37: mRNA

Chain X:  10% 50% 50%



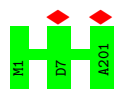
- Molecule 38: Large ribosomal subunit protein uL2

Chain c:  95% ..



- Molecule 39: Large ribosomal subunit protein uL4

Chain e:  100%



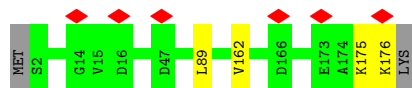
- Molecule 40: Large ribosomal subunit protein uL5

Chain f:  98% ..




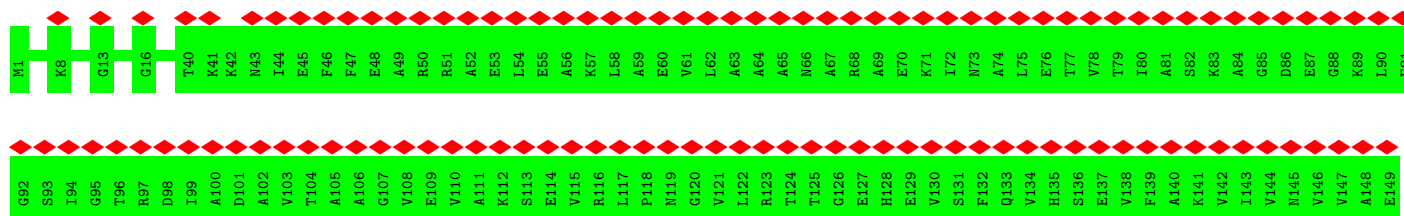
- Molecule 41: Large ribosomal subunit protein uL6

Chain g:  97%



- Molecule 42: Large ribosomal subunit protein bL9

Chain h:  75%
100%



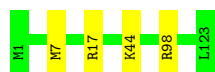
- Molecule 43: Large ribosomal subunit protein uL13

Chain i:  97%



- Molecule 44: Large ribosomal subunit protein uL14

Chain j:  97%



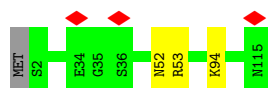
- Molecule 45: Large ribosomal subunit protein uL18

Chain n:  99%



- Molecule 46: Large ribosomal subunit protein bL19

Chain o:  97%



- Molecule 47: Large ribosomal subunit protein bL20

Chain p:  97% ..




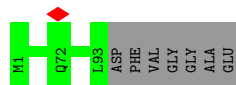
- Molecule 48: Large ribosomal subunit protein bL21

Chain q:  97% .



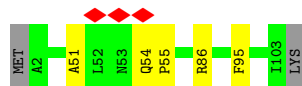
- Molecule 49: Large ribosomal subunit protein uL23

Chain s:  93% 7%



- Molecule 50: Large ribosomal subunit protein uL24

Chain t:  93% 5% .




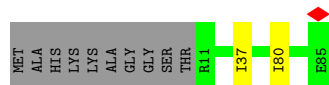
- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  100%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  86% 12%



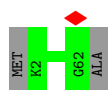
- Molecule 53: Large ribosomal subunit protein bL28

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	62030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	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	0.733	Depositor
Minimum map value	-0.229	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0642	Depositor
Map size (\AA)	436.896, 436.896, 436.896	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.7585, 0.7585, 0.7585	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/303	0.82	0/397
2	4	0.48	0/371	0.80	0/496
3	K	0.49	0/884	0.87	0/1191
4	L	0.47	0/960	0.84	0/1286
5	b	0.52	0/2850	0.81	0/4444
6	d	0.45	0/1576	0.80	0/2119
7	k	0.47	0/1062	0.83	0/1413
8	l	0.46	0/1073	0.84	0/1433
9	m	0.45	0/958	0.88	0/1281
10	r	0.46	0/864	0.85	0/1156
11	z	0.47	0/450	0.88	0/599
12	A	0.52	1/36284 (0.0%)	0.81	2/56595 (0.0%)
13	Y	0.57	0/1596	0.79	0/2478
14	Z	0.56	0/1608	0.83	1/2500 (0.0%)
15	a	0.49	0/65747	0.83	10/102563 (0.0%)
16	0	0.45	0/424	0.81	0/565
17	1	0.48	0/380	0.92	0/498
18	2	0.49	0/513	0.89	0/676
19	B	0.46	0/1784	0.91	0/2403
20	C	0.46	0/1651	0.85	0/2225
21	D	0.44	0/1665	0.89	0/2227
22	E	0.46	0/1165	0.82	0/1568
23	F	0.45	0/858	0.85	0/1160
24	G	0.47	0/1219	0.93	0/1635
25	H	0.47	0/989	0.86	0/1326
26	I	0.45	0/1034	0.89	0/1375
27	J	0.46	0/796	0.86	0/1077
28	M	0.47	0/900	0.92	0/1204
29	N	0.46	0/817	0.92	0/1088
30	O	0.43	0/722	0.95	0/964
31	P	0.45	0/653	0.84	0/877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Q	0.45	0/650	0.79	0/871
33	R	0.44	0/553	0.91	0/742
34	S	0.49	0/685	0.83	0/922
35	T	0.46	0/676	0.99	0/895
36	U	0.47	0/598	0.98	0/792
37	X	0.53	0/242	0.87	0/375
38	c	0.48	0/2121	0.84	0/2852
39	e	0.44	0/1571	0.86	0/2113
40	f	0.44	0/1434	0.89	0/1926
41	g	0.47	0/1333	0.84	0/1805
42	h	0.46	0/1122	0.84	0/1515
43	i	0.45	0/1152	0.84	0/1551
44	j	0.45	0/956	0.83	0/1279
45	n	0.46	0/902	0.88	0/1209
46	o	0.45	0/929	0.78	0/1242
47	p	0.45	0/960	0.93	0/1278
48	q	0.44	0/829	0.72	0/1107
49	s	0.44	0/744	0.80	0/994
50	t	0.46	0/787	0.78	0/1051
51	u	0.45	0/766	0.81	0/1025
52	v	0.46	0/582	0.80	0/769
53	w	0.47	0/635	0.86	0/848
54	x	0.41	0/496	0.90	0/660
55	y	0.45	0/453	0.84	0/605
All	All	0.49	1/153332 (0.0%)	0.83	13/229245 (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
18	2	0	1
46	o	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	527	G7M	O3'-P	5.13	1.61	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Z	37	A	O3'-P-O5'	-8.11	91.84	104.00
15	a	2429	G	O3'-P-O5'	-7.48	92.78	104.00
15	a	204	A	O3'-P-O5'	-6.79	93.81	104.00
15	a	781	A	O3'-P-O5'	-6.59	94.12	104.00
15	a	1971	U	O3'-P-O5'	-5.93	95.10	104.00
12	A	1230	C	O3'-P-O5'	-5.63	95.56	104.00
15	a	2501	C	O3'-P-O5'	-5.57	95.65	104.00
15	a	2382	G	O3'-P-O5'	-5.33	96.00	104.00
12	A	1422	G	O3'-P-O5'	-5.25	96.13	104.00
15	a	2879	A	O3'-P-O5'	-5.20	96.21	104.00
15	a	73	A	O3'-P-O5'	-5.14	96.30	104.00
15	a	1378	A	O3'-P-O5'	-5.04	96.43	104.00
15	a	1929	G	O3'-P-O5'	-5.01	96.48	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	2	13	ARG	Sidechain
46	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	1	0
2	4	364	0	362	0	0
3	K	877	0	884	0	0
4	L	957	0	1017	0	0
5	b	2549	0	1291	2	0
6	d	1566	0	1618	7	0
7	k	1053	0	1129	3	0
8	l	1075	0	1145	3	0
9	m	945	0	989	1	0
10	r	857	0	921	1	0
11	z	444	0	458	2	0
12	A	32655	0	16453	49	0
13	Y	1539	0	791	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	Z	1546	0	794	2	0
15	a	59216	0	29794	95	0
16	0	417	0	451	1	0
17	1	377	0	418	1	0
18	2	504	0	572	2	0
19	B	1753	0	1780	7	0
20	C	1624	0	1696	0	0
21	D	1643	0	1707	2	0
22	E	1152	0	1196	2	0
23	F	839	0	833	2	0
24	G	1203	0	1254	1	0
25	H	979	0	1031	1	0
26	I	1022	0	1070	0	0
27	J	786	0	828	1	0
28	M	891	0	952	1	0
29	N	805	0	844	0	0
30	O	714	0	734	0	0
31	P	643	0	661	1	0
32	Q	641	0	682	0	0
33	R	544	0	565	0	0
34	S	668	0	693	0	0
35	T	670	0	719	2	0
36	U	590	0	629	0	0
37	X	216	0	108	0	0
38	c	2082	0	2154	9	0
39	e	1552	0	1619	0	0
40	f	1410	0	1444	2	0
41	g	1313	0	1358	2	0
42	h	1111	0	1148	0	0
43	i	1129	0	1162	3	0
44	j	947	0	1023	3	0
45	n	892	0	923	0	0
46	o	917	0	962	2	0
47	p	947	0	1019	2	0
48	q	816	0	839	3	0
49	s	738	0	807	0	0
50	t	779	0	831	3	0
51	u	753	0	780	0	0
52	v	575	0	592	1	0
53	w	625	0	652	0	0
54	x	495	0	526	0	0
55	y	449	0	488	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	48	0	0	0	0
57	a	195	0	0	0	0
57	b	4	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	p	1	0	0	0	0
57	z	1	0	0	0	0
58	A	23	0	24	3	0
59	A	11	0	0	0	0
59	a	36	0	0	0	0
60	Y	7	0	8	1	0
61	0	7	0	0	0	0
61	1	18	0	0	0	0
61	2	21	0	0	0	0
61	3	9	0	0	1	0
61	4	3	0	0	0	0
61	A	1331	0	0	0	0
61	B	15	0	0	0	0
61	C	13	0	0	0	0
61	D	7	0	0	0	0
61	E	14	0	0	0	0
61	F	2	0	0	0	0
61	G	6	0	0	1	0
61	H	17	0	0	0	0
61	I	9	0	0	0	0
61	J	11	0	0	0	0
61	K	18	0	0	0	0
61	L	14	0	0	0	0
61	M	5	0	0	0	0
61	N	6	0	0	0	0
61	O	19	0	0	0	0
61	P	9	0	0	0	0
61	Q	8	0	0	0	0
61	R	4	0	0	0	0
61	S	3	0	0	0	0
61	T	3	0	0	1	0
61	U	10	0	0	0	0
61	X	8	0	0	0	0
61	Y	13	0	0	0	0
61	Z	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	a	4252	0	0	3	0
61	b	103	0	0	0	0
61	c	106	0	0	0	0
61	d	74	0	0	0	0
61	e	66	0	0	0	0
61	f	8	0	0	0	0
61	g	11	0	0	0	0
61	h	10	0	0	0	0
61	i	25	0	0	0	0
61	j	32	0	0	0	0
61	k	46	0	0	1	0
61	l	44	0	0	0	0
61	m	28	0	0	0	0
61	n	10	0	0	0	0
61	o	26	0	0	0	0
61	p	35	0	0	0	0
61	q	32	0	0	1	0
61	r	44	0	0	0	0
61	s	21	0	0	0	0
61	t	15	0	0	0	0
61	u	13	0	0	0	0
61	v	16	0	0	0	0
61	w	19	0	0	0	0
61	x	10	0	0	0	0
61	y	14	0	0	0	0
61	z	35	0	0	0	0
All	All	149221	0	95768	191	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 (191) 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)
15:a:12:U:H2'	15:a:12:U:O2	1.91	0.69
15:a:568:U:H1'	15:a:2030:6MZ:H9C1	1.77	0.67
12:A:664:G:H22	12:A:741:G:H1	1.43	0.67
15:a:1508:A:O2'	15:a:1509:A:O4'	2.09	0.65
15:a:1020:A:N1	15:a:1141:U:O2'	2.27	0.64
12:A:1518:MA6:H103	12:A:1519:MA6:H102	1.81	0.61
38:c:271:ARG:O	38:c:272:SER:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1391:U:H2'	12:A:1392:G:C8	2.38	0.59
43:i:125:TYR:OH	43:i:132:HIS:NE2	2.36	0.58
24:G:4:ARG:NH2	61:G:201:HOH:O	2.37	0.57
48:q:84:ARG:NH2	61:q:201:HOH:O	2.37	0.56
12:A:823:C:HO2'	25:H:2:SER:N	2.04	0.56
15:a:221:A:N1	15:a:265:A:O2'	2.38	0.56
15:a:1115:G:O2'	15:a:1116:G:O5'	2.22	0.56
12:A:1286:U:O2	12:A:1286:U:O4'	2.25	0.56
15:a:818:G:N2	61:a:3303:HOH:O	2.23	0.56
15:a:2780:G:OP2	43:i:120:ARG:HD3	2.06	0.55
12:A:1064:G:N7	58:A:1601:SCM:O11	2.39	0.54
50:t:54:GLN:N	50:t:55:PRO:CD	2.71	0.54
15:a:12:U:O2	15:a:12:U:C2'	2.55	0.54
12:A:572:A:H5''	12:A:917:G:H4'	1.90	0.52
21:D:153:SER:O	21:D:154:ARG:C	2.53	0.52
7:k:21:ARG:HA	15:a:811:U:H2'	1.92	0.52
12:A:927:G:O2'	12:A:1503:A:N7	2.38	0.52
15:a:2273:A:H2'	15:a:2274:A:C8	2.45	0.52
11:z:9:THR:CG2	15:a:2020:A:H5'	2.40	0.52
12:A:677:U:H3	12:A:713:G:H22	1.59	0.51
15:a:1434:A:H2'	15:a:1435:G:C8	2.46	0.51
61:a:4091:HOH:O	38:c:242:LYS:HE2	2.10	0.50
7:k:57:LEU:HD22	18:2:54:ASP:HB3	1.93	0.50
15:a:493:G:H2'	15:a:494:G:O4'	2.12	0.50
15:a:1799:G:O2'	38:c:180:GLU:OE2	2.21	0.49
15:a:1188:U:H3'	61:a:3303:HOH:O	2.11	0.49
15:a:2547:A:H2'	15:a:2548:U:C6	2.47	0.49
15:a:1021:A:N3	15:a:1021:A:H3'	2.27	0.49
12:A:1305:G:HO2'	12:A:1306:A:H8	1.55	0.49
40:f:108:VAL:N	40:f:109:PRO:CD	2.75	0.49
47:p:76:TYR:CZ	47:p:80:ILE:HG13	2.48	0.49
52:v:37:ILE:HG21	52:v:80:ILE:HG21	1.95	0.49
12:A:338:A:OP2	44:j:98:ARG:NH2	2.46	0.49
12:A:1103:C:OP1	19:B:95:ARG:NH1	2.46	0.49
6:d:62:LYS:N	6:d:63:PRO:HD2	2.28	0.48
7:k:17:LYS:NZ	61:k:201:HOH:O	2.33	0.48
15:a:747:5MU:O2	15:a:2014:A:H1'	2.13	0.48
15:a:2328:A:H2'	15:a:2329:U:C6	2.48	0.48
8:l:66:ARG:NH2	8:l:104:GLU:OE2	2.45	0.48
58:A:1601:SCM:H2M1	22:E:27:GLY:HA2	1.96	0.48
15:a:2327:A:H2'	15:a:2328:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:g:175:LYS:O	41:g:176:LYS:C	2.57	0.48
14:Z:75:C:O4'	15:a:2432:A:H1'	2.12	0.48
12:A:246:A:N1	12:A:278:G:O2'	2.43	0.47
15:a:534:U:O2'	47:p:49:ASP:OD2	2.24	0.47
12:A:946:A:H2'	12:A:947:G:C8	2.49	0.47
15:a:639:U:H2'	15:a:640:C:C6	2.50	0.47
12:A:977:A:H1'	12:A:982:U:O4	2.13	0.47
15:a:2038:G:H2'	15:a:2039:U:O4'	2.15	0.47
15:a:1182:G:H2'	15:a:1183:U:O4'	2.15	0.47
15:a:1754:A:C8	46:o:94:LYS:CE	2.98	0.47
15:a:1607:C:H4'	15:a:1608:A:O5'	2.15	0.47
13:Y:37:6MZ:O2'	15:a:1913:A:N1	2.43	0.46
15:a:247:G:H4'	15:a:386:G:C5	2.50	0.46
41:g:89:LEU:HD22	41:g:162:VAL:HG22	1.97	0.46
15:a:1028:A:N6	15:a:1125:G:H2'	2.31	0.46
19:B:28:LYS:N	19:B:29:PRO:CD	2.79	0.46
19:B:164:ILE:O	19:B:186:ILE:HB	2.16	0.46
12:A:993:G:H2'	12:A:993:G:N3	2.30	0.46
15:a:263:G:H2'	15:a:264:C:O4'	2.15	0.46
12:A:182:A:N1	12:A:223:A:O2'	2.49	0.46
12:A:502:A:H2'	12:A:503:C:O4'	2.16	0.46
12:A:769:G:H4'	12:A:1513:A:H4'	1.96	0.46
12:A:28:A:O2'	12:A:296:U:OP1	2.23	0.45
15:a:784:G:H5'	15:a:785:G:OP1	2.15	0.45
15:a:1338:G:O2'	15:a:1393:A:N1	2.37	0.45
9:m:5:LYS:NZ	15:a:2000:C:OP1	2.43	0.45
15:a:157:C:H2'	15:a:158:U:O4'	2.17	0.45
15:a:1474:U:C4	15:a:1475:G:C6	3.03	0.45
15:a:2756:U:H1'	15:a:2757:A:H5''	1.99	0.45
6:d:135:GLY:HA2	15:a:743:A:OP1	2.17	0.45
15:a:644:A:H2'	15:a:645:C:O4'	2.16	0.45
15:a:2522:U:O2'	15:a:2647:U:OP1	2.32	0.45
12:A:767:A:H2'	12:A:768:A:O4'	2.16	0.45
15:a:1778:U:H2'	15:a:1784:A:N6	2.32	0.45
15:a:2747:G:O6	15:a:2755:C:H5''	2.17	0.45
15:a:476:G:H4'	15:a:502:A:N1	2.32	0.45
15:a:1730:C:O2	15:a:1730:C:O4'	2.34	0.45
38:c:29:PRO:HG2	38:c:34:LEU:HD11	1.96	0.45
12:A:244:U:O4	12:A:906:A:H1'	2.17	0.45
12:A:928:G:O2'	12:A:1533:C:OP1	2.33	0.45
12:A:975:A:N1	12:A:1366:C:O2'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:642:U:O2'	15:a:644:A:N7	2.48	0.45
60:Y:101:VAL:HG23	15:a:2451:A:H2	1.82	0.44
15:a:2788:C:O2'	15:a:2809:A:N3	2.45	0.44
12:A:1471:U:OP1	44:j:17:ARG:NH2	2.51	0.44
12:A:1530:G:H2'	12:A:1531:A:C8	2.52	0.44
15:a:857:G:H2'	15:a:858:G:O4'	2.18	0.44
12:A:376:G:H5''	31:P:5:ARG:HB2	2.00	0.44
15:a:1902:C:H4'	38:c:242:LYS:O	2.17	0.44
35:T:9:LYS:NZ	61:T:101:HOH:O	2.51	0.44
38:c:72:ASP:OD2	38:c:189:ARG:NH1	2.46	0.44
5:b:106:G:H2'	5:b:107:G:O4'	2.17	0.44
15:a:2063:C:O2	15:a:2450:A:N1	2.50	0.44
15:a:2419:U:H4'	16:0:22:THR:HG21	1.99	0.44
8:l:53:MET:HE1	8:l:103:TYR:CG	2.53	0.44
12:A:17:U:H2'	12:A:18:C:C6	2.52	0.44
12:A:1066:C:O2	58:A:1601:SCM:N10	2.46	0.44
15:a:1846:G:C6	15:a:1847:A:C6	3.06	0.44
19:B:94:HIS:O	19:B:95:ARG:C	2.60	0.44
50:t:86:ARG:HG3	50:t:95:PHE:CE1	2.53	0.44
8:l:55:ARG:CD	15:a:2469:A:H4'	2.47	0.43
12:A:1402:4OC:O2	12:A:1500:A:N1	2.51	0.43
19:B:76:ALA:O	19:B:77:SER:C	2.61	0.43
15:a:1370:C:H2'	15:a:1371:G:O4'	2.16	0.43
15:a:84:A:N1	15:a:98:G:O2'	2.45	0.43
15:a:1405:U:H2'	15:a:1406:U:C6	2.54	0.43
15:a:2243:U:H2'	15:a:2244:U:C6	2.54	0.43
15:a:788:A:OP1	15:a:790:U:H5	2.02	0.43
11:z:4:GLN:HA	15:a:2615:U:C2	2.54	0.43
40:f:108:VAL:HG12	40:f:109:PRO:HD3	2.00	0.43
12:A:22:G:O2'	12:A:913:A:N1	2.47	0.43
15:a:466:A:N1	15:a:795:C:O2'	2.51	0.43
15:a:2845:U:H5''	46:o:52:ASN:O	2.18	0.43
15:a:729:G:C6	38:c:207:LYS:HB2	2.54	0.43
15:a:1378:A:O2'	15:a:1380:G:N7	2.51	0.43
15:a:56:A:H2'	15:a:57:C:O4'	2.19	0.43
15:a:373:U:O2'	15:a:423:A:H1'	2.19	0.43
15:a:2291:U:H2'	15:a:2292:U:C6	2.53	0.43
5:b:89:U:C2	15:a:958:U:H2'	2.54	0.42
12:A:8:A:N6	21:D:202:GLU:O	2.48	0.42
12:A:109:A:H2'	12:A:326:G:N2	2.34	0.42
15:a:244:A:C2	15:a:255:A:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:j:7:MET:HE1	44:j:44:LYS:HG3	2.01	0.42
6:d:1:MET:HB3	6:d:205:PRO:HG2	2.00	0.42
15:a:1932:A:H2'	15:a:1933:G:O4'	2.19	0.42
15:a:478:A:N1	15:a:500:G:H4'	2.35	0.42
15:a:620:G:H5'	15:a:620:G:N3	2.35	0.42
12:A:1148:U:H2'	12:A:1149:C:O4'	2.20	0.42
15:a:2040:G:H2'	15:a:2041:U:O4'	2.19	0.42
50:t:54:GLN:N	50:t:55:PRO:HD2	2.34	0.42
14:Z:21:A:O2'	14:Z:22:G:O5'	2.37	0.42
15:a:468:G:N7	17:1:39:ARG:NH1	2.59	0.42
12:A:945:G:H2'	12:A:945:G:N3	2.35	0.42
15:a:829:A:N7	15:a:2248:C:H5'	2.35	0.42
23:F:18:VAL:HB	23:F:19:PRO:HD3	2.01	0.42
38:c:31:ALA:N	38:c:32:PRO:CD	2.82	0.42
15:a:945:A:C4	15:a:2448:A:C2	3.08	0.41
22:E:56:VAL:HB	22:E:57:PRO:HD3	2.02	0.41
15:a:207:A:H2'	15:a:208:C:O4'	2.20	0.41
15:a:2030:6MZ:C2	15:a:2499:C:H5''	2.50	0.41
12:A:524:G:H2'	12:A:525:C:C6	2.55	0.41
15:a:861:A:C2	15:a:917:A:C4	3.08	0.41
15:a:1161:C:O2'	48:q:8:GLY:HA2	2.19	0.41
12:A:49:U:O2	12:A:362:G:H1'	2.20	0.41
19:B:115:LYS:NZ	19:B:152:LYS:O	2.52	0.41
12:A:649:A:H2'	12:A:650:G:O4'	2.19	0.41
18:2:27:ALA:O	18:2:28:ASN:HB2	2.20	0.41
12:A:1516:2MG:N1	12:A:1519:MA6:OP2	2.52	0.41
15:a:58:G:O2'	15:a:73:A:N1	2.52	0.41
15:a:299:A:N1	15:a:322:A:O2'	2.45	0.41
15:a:1558:C:O4'	15:a:1560:G:C8	2.74	0.41
35:T:55:GLN:N	35:T:56:PRO:HD2	2.35	0.41
6:d:121:THR:HB	6:d:127:PHE:CD2	2.56	0.41
12:A:712:A:H5'	38:c:138:GLY:HA3	2.02	0.41
12:A:269:C:H2'	12:A:270:A:C8	2.55	0.41
12:A:977:A:O2'	12:A:979:C:OP2	2.32	0.41
12:A:1376:U:H2'	12:A:1377:A:C8	2.56	0.41
15:a:819:A:C4	15:a:1189:A:C2	3.09	0.41
15:a:1417:C:H2'	15:a:1418:G:O4'	2.20	0.41
15:a:2849:U:H4'	15:a:2868:A:C2	2.56	0.41
48:q:74:ILE:N	48:q:74:ILE:HD12	2.36	0.41
6:d:152:PRO:HG3	6:d:156:PHE:CZ	2.56	0.41
12:A:1518:MA6:H103	12:A:1519:MA6:C10	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:18:LYS:NZ	61:3:201:HOH:O	2.54	0.40
12:A:1152:A:OP1	27:J:70:HIS:ND1	2.51	0.40
15:a:26:G:H1'	15:a:514:A:N6	2.36	0.40
15:a:1239:G:H2'	15:a:1240:U:O4'	2.21	0.40
15:a:1357:C:H2'	15:a:1358:G:O4'	2.21	0.40
23:F:41:ASP:OD1	23:F:58:HIS:NE2	2.52	0.40
28:M:86:TYR:O	28:M:90:ARG:HG2	2.20	0.40
6:d:83:ARG:NH1	15:a:2638:G:OP2	2.54	0.40
12:A:945:G:C2	12:A:946:A:C8	3.08	0.40
12:A:1478:U:H2'	12:A:1479:C:C6	2.57	0.40
15:a:653:U:O2	15:a:653:U:O4'	2.38	0.40
10:r:20:VAL:HG11	10:r:44:ALA:HA	2.03	0.40
15:a:607:U:O4	15:a:620:G:H5''	2.21	0.40
6:d:156:PHE:CE1	43:i:81:ILE:HD13	2.57	0.40
12:A:230:G:H2'	12:A:231:U:O4'	2.22	0.40
12:A:1095:U:H2'	12:A:1096:C:O4'	2.22	0.40
15:a:548:G:H2'	15:a:549:G:O4'	2.22	0.40
15:a:1906:G:H2'	15:a:1907:G:O4'	2.21	0.40
19:B:63:ARG:O	19:B:64:LYS:C	2.65	0.40
15:a:2557:G:H2'	15:a:2558:C:C6	2.56	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%)	36 (100%)	0	0	100	100
2	4	45/70 (64%)	38 (84%)	6 (13%)	1 (2%)	5	1
3	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
4	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
7	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
8	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
9	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
10	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
11	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
16	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
17	1	44/46 (96%)	44 (100%)	0	0	100	100
18	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
19	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
20	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
21	D	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	24	20
22	E	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
23	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
24	G	151/179 (84%)	144 (95%)	6 (4%)	1 (1%)	18	13
25	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
26	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
27	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	8
28	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
29	N	98/101 (97%)	98 (100%)	0	0	100	100
30	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
31	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
32	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
33	R	64/75 (85%)	64 (100%)	0	0	100	100
34	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
35	T	84/87 (97%)	84 (100%)	0	0	100	100
36	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
38	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
39	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
40	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
41	g	173/177 (98%)	169 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	h	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
43	i	140/142 (99%)	140 (100%)	0	0	100	100
44	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
45	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
46	o	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
47	p	115/118 (98%)	115 (100%)	0	0	100	100
48	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	12	8
51	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
52	v	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
53	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
54	x	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5573/5913 (94%)	5386 (97%)	182 (3%)	5 (0%)	49	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	40	CYS
27	J	57	VAL
24	G	114	LYS
50	t	51	ALA
21	D	154	ARG

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%)	101 (99%)	1 (1%)	68	75
6	d	163/163 (100%)	163 (100%)	0	100	100
7	k	103/103 (100%)	103 (100%)	0	100	100
8	l	107/107 (100%)	107 (100%)	0	100	100
9	m	98/103 (95%)	98 (100%)	0	100	100
10	r	93/93 (100%)	93 (100%)	0	100	100
11	z	47/48 (98%)	47 (100%)	0	100	100
16	0	46/49 (94%)	46 (100%)	0	100	100
17	1	38/38 (100%)	38 (100%)	0	100	100
18	2	51/52 (98%)	51 (100%)	0	100	100
19	B	186/199 (94%)	186 (100%)	0	100	100
20	C	170/190 (90%)	170 (100%)	0	100	100
21	D	172/173 (99%)	172 (100%)	0	100	100
22	E	119/126 (94%)	119 (100%)	0	100	100
23	F	90/116 (78%)	90 (100%)	0	100	100
24	G	126/147 (86%)	126 (100%)	0	100	100
25	H	104/105 (99%)	104 (100%)	0	100	100
26	I	105/107 (98%)	104 (99%)	1 (1%)	68	75
27	J	86/90 (96%)	86 (100%)	0	100	100
28	M	93/96 (97%)	93 (100%)	0	100	100
29	N	83/84 (99%)	83 (100%)	0	100	100
30	O	76/77 (99%)	75 (99%)	1 (1%)	61	68
31	P	65/65 (100%)	65 (100%)	0	100	100
32	Q	73/78 (94%)	73 (100%)	0	100	100
33	R	57/65 (88%)	57 (100%)	0	100	100
34	S	72/79 (91%)	72 (100%)	0	100	100
35	T	65/66 (98%)	65 (100%)	0	100	100
36	U	60/61 (98%)	60 (100%)	0	100	100
38	c	216/218 (99%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	e	165/165 (100%)	165 (100%)	0	100	100
40	f	148/150 (99%)	148 (100%)	0	100	100
41	g	136/138 (99%)	136 (100%)	0	100	100
42	h	114/114 (100%)	114 (100%)	0	100	100
43	i	116/116 (100%)	116 (100%)	0	100	100
44	j	104/104 (100%)	104 (100%)	0	100	100
45	n	86/87 (99%)	86 (100%)	0	100	100
46	o	99/100 (99%)	99 (100%)	0	100	100
47	p	89/90 (99%)	89 (100%)	0	100	100
48	q	84/84 (100%)	84 (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	4640/4825 (96%)	4637 (100%)	3 (0%)	87	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	67	ILE
26	I	97	GLU
30	O	18	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	15	GLN
3	K	118	HIS
4	L	75	GLN
6	d	173	GLN
8	l	60	GLN
9	m	9	GLN

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Mol	Chain	Res	Type
9	m	73	ASN
11	z	6	ASN
16	0	45	GLN
19	B	58	ASN
19	B	120	GLN
21	D	40	GLN
21	D	54	GLN
21	D	89	ASN
22	E	82	GLN
22	E	132	ASN
22	E	148	ASN
23	F	17	GLN
23	F	94	HIS
24	G	68	ASN
24	G	130	ASN
25	H	21	ASN
25	H	67	GLN
26	I	4	ASN
26	I	25	ASN
27	J	58	ASN
28	M	14	HIS
29	N	60	GLN
31	P	59	HIS
33	R	54	GLN
38	c	117	GLN
38	c	153	GLN
39	e	94	GLN
40	f	21	ASN
41	g	73	ASN
41	g	115	HIS
42	h	66	ASN
42	h	145	ASN
43	i	47	HIS
43	i	128	ASN
44	j	3	GLN
44	j	5	GLN
46	o	66	ASN
47	p	52	GLN
48	q	86	GLN
50	t	53	ASN
51	u	49	ASN
53	w	17	ASN

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Mol	Chain	Res	Type
53	w	36	HIS
54	x	27	ASN
54	x	38	GLN
54	x	58	ASN
55	y	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	A	1518/1544 (98%)	227 (14%)	30 (1%)
13	Y	68/76 (89%)	16 (23%)	1 (1%)
14	Z	69/78 (88%)	14 (20%)	3 (4%)
15	a	2753/2904 (94%)	309 (11%)	0
37	X	9/10 (90%)	5 (55%)	0
5	b	118/120 (98%)	11 (9%)	0
All	All	4535/4732 (95%)	582 (12%)	34 (0%)

All (582) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	9	G
5	b	34	A
5	b	35	C
5	b	36	C
5	b	45	A
5	b	56	G
5	b	67	G
5	b	89	U
5	b	90	C
5	b	105	G
5	b	109	A
12	A	4	U
12	A	9	G
12	A	13	U
12	A	14	U
12	A	22	G
12	A	32	A
12	A	39	G
12	A	44	A
12	A	47	C
12	A	48	C

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Mol	Chain	Res	Type
12	A	51	A
12	A	69	G
12	A	71	A
12	A	76	G
12	A	83	C
12	A	85	U
12	A	86	G
12	A	88	U
12	A	120	A
12	A	121	U
12	A	131	A
12	A	141	G
12	A	149	A
12	A	163	C
12	A	197	A
12	A	204	G
12	A	226	G
12	A	240	G
12	A	245	U
12	A	247	G
12	A	251	G
12	A	266	G
12	A	267	C
12	A	289	G
12	A	321	A
12	A	328	C
12	A	339	C
12	A	345	C
12	A	347	G
12	A	352	C
12	A	354	G
12	A	367	U
12	A	372	C
12	A	373	A
12	A	383	A
12	A	384	G
12	A	406	G
12	A	411	A
12	A	412	A
12	A	413	G
12	A	414	A
12	A	423	G

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Mol	Chain	Res	Type
12	A	429	U
12	A	438	U
12	A	439	U
12	A	444	G
12	A	451	A
12	A	453	G
12	A	457	G
12	A	467	U
12	A	468	A
12	A	474	G
12	A	479	U
12	A	481	G
12	A	484	G
12	A	486	U
12	A	499	A
12	A	511	C
12	A	518	C
12	A	520	A
12	A	521	G
12	A	530	G
12	A	531	U
12	A	532	A
12	A	533	A
12	A	547	A
12	A	559	A
12	A	572	A
12	A	573	A
12	A	576	C
12	A	577	G
12	A	633	G
12	A	642	A
12	A	650	G
12	A	653	U
12	A	665	A
12	A	723	U
12	A	724	G
12	A	734	G
12	A	747	A
12	A	748	G
12	A	755	G
12	A	777	A
12	A	793	U

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Mol	Chain	Res	Type
12	A	794	A
12	A	815	A
12	A	817	C
12	A	821	G
12	A	832	G
12	A	847	G
12	A	849	G
12	A	884	U
12	A	885	G
12	A	890	G
12	A	914	A
12	A	926	G
12	A	934	C
12	A	935	A
12	A	939	G
12	A	946	A
12	A	947	G
12	A	956	U
12	A	960	U
12	A	961	U
12	A	966	2MG
12	A	969	A
12	A	975	A
12	A	976	G
12	A	977	A
12	A	984	C
12	A	989	U
12	A	992	U
12	A	993	G
12	A	994	A
12	A	996	A
12	A	997	U
12	A	998	C
12	A	1004	A
12	A	1007	U
12	A	1008	U
12	A	1013	G
12	A	1020	G
12	A	1021	A
12	A	1022	A
12	A	1030	U
12	A	1031	C

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Mol	Chain	Res	Type
12	A	1032	G
12	A	1037	C
12	A	1038	C
12	A	1048	G
12	A	1064	G
12	A	1065	U
12	A	1085	U
12	A	1094	G
12	A	1095	U
12	A	1101	A
12	A	1124	G
12	A	1125	U
12	A	1129	C
12	A	1130	A
12	A	1132	C
12	A	1134	G
12	A	1135	U
12	A	1137	C
12	A	1138	G
12	A	1139	G
12	A	1159	U
12	A	1166	G
12	A	1176	A
12	A	1184	G
12	A	1196	A
12	A	1197	A
12	A	1211	U
12	A	1212	U
12	A	1213	A
12	A	1224	U
12	A	1225	A
12	A	1227	A
12	A	1228	C
12	A	1231	G
12	A	1238	A
12	A	1239	A
12	A	1240	U
12	A	1248	A
12	A	1252	A
12	A	1253	G
12	A	1256	A
12	A	1257	A

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Mol	Chain	Res	Type
12	A	1260	G
12	A	1273	C
12	A	1275	A
12	A	1280	A
12	A	1285	A
12	A	1286	U
12	A	1287	A
12	A	1297	G
12	A	1298	U
12	A	1299	A
12	A	1300	G
12	A	1301	U
12	A	1302	C
12	A	1305	G
12	A	1312	G
12	A	1317	C
12	A	1319	A
12	A	1320	C
12	A	1325	C
12	A	1332	A
12	A	1336	C
12	A	1338	G
12	A	1346	A
12	A	1347	G
12	A	1348	U
12	A	1351	U
12	A	1353	G
12	A	1363	A
12	A	1370	G
12	A	1378	C
12	A	1379	G
12	A	1419	G
12	A	1422	G
12	A	1423	G
12	A	1448(A)	G
12	A	1452	C
12	A	1453	G
12	A	1453(A)	C
12	A	1454	G
12	A	1479	C
12	A	1492	A
12	A	1497	G

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Mol	Chain	Res	Type
12	A	1503	A
12	A	1505	G
12	A	1506	U
12	A	1517	G
12	A	1519	MA6
12	A	1529	G
12	A	1530	G
13	Y	2	G
13	Y	3	G
13	Y	5	G
13	Y	19	G
13	Y	22	G
13	Y	43	G
13	Y	45	G
13	Y	46	G7M
13	Y	49	G
13	Y	50	G
13	Y	70	C
13	Y	72	C
13	Y	73	A
13	Y	74	C
13	Y	75	C
13	Y	76	A
14	Z	5	G
14	Z	8	4SU
14	Z	9	G
14	Z	14	A
14	Z	15	G
14	Z	23	C
14	Z	38	A
14	Z	45	G
14	Z	46	G7M
14	Z	49	G
14	Z	58	A
14	Z	60	U
14	Z	61	C
14	Z	76	A
15	a	10	A
15	a	12	U
15	a	34	U
15	a	71	A
15	a	74	A

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Mol	Chain	Res	Type
15	a	75	G
15	a	101	A
15	a	102	U
15	a	110	G
15	a	118	A
15	a	119	A
15	a	120	U
15	a	131	A
15	a	138	U
15	a	139	U
15	a	140	C
15	a	141	G
15	a	142	A
15	a	158	U
15	a	165	A
15	a	181	A
15	a	196	A
15	a	199	A
15	a	200	U
15	a	215	G
15	a	216	A
15	a	221	A
15	a	222	A
15	a	248	G
15	a	272	A
15	a	276	U
15	a	278	A
15	a	279	A
15	a	282	A
15	a	285	G
15	a	287	G
15	a	288	U
15	a	289	G
15	a	291	G
15	a	305	C
15	a	311	A
15	a	330	A
15	a	361	G
15	a	362	A
15	a	367	G
15	a	386	G
15	a	404	A

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Mol	Chain	Res	Type
15	a	405	U
15	a	411	G
15	a	412	A
15	a	420	C
15	a	425	G
15	a	451	U
15	a	481	G
15	a	491	G
15	a	503	A
15	a	504	A
15	a	505	A
15	a	509	C
15	a	530	G
15	a	531	C
15	a	532	A
15	a	533	G
15	a	545	U
15	a	547	A
15	a	548	G
15	a	563	A
15	a	573	U
15	a	574	A
15	a	575	A
15	a	586	A
15	a	603	A
15	a	615	U
15	a	627	A
15	a	637	A
15	a	645	C
15	a	646	U
15	a	647	G
15	a	654	A
15	a	655	A
15	a	686	U
15	a	711	G
15	a	712	G
15	a	717	C
15	a	730	A
15	a	738	G
15	a	747	5MU
15	a	764	A
15	a	765	C

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Mol	Chain	Res	Type
15	a	775	G
15	a	776	G
15	a	777	G
15	a	782	A
15	a	784	G
15	a	785	G
15	a	805	G
15	a	812	C
15	a	827	U
15	a	828	U
15	a	846	U
15	a	847	U
15	a	858	G
15	a	859	G
15	a	877	A
15	a	883	G
15	a	884	U
15	a	888	C
15	a	891	G
15	a	896	A
15	a	899	A
15	a	910	A
15	a	914	G
15	a	915	C
15	a	927	A
15	a	931	U
15	a	946	C
15	a	961	C
15	a	974	G
15	a	983	A
15	a	984	A
15	a	985	C
15	a	996	A
15	a	1005	C
15	a	1012	U
15	a	1013	C
15	a	1022	G
15	a	1026	G
15	a	1033	U
15	a	1040	A
15	a	1047	G
15	a	1108	U

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Mol	Chain	Res	Type
15	a	1110	G
15	a	1111	A
15	a	1112	G
15	a	1116	G
15	a	1128	G
15	a	1129	A
15	a	1132	U
15	a	1133	A
15	a	1135	C
15	a	1136	G
15	a	1141	U
15	a	1142	A
15	a	1253	A
15	a	1256	G
15	a	1271	G
15	a	1272	A
15	a	1286	A
15	a	1287	A
15	a	1300	G
15	a	1301	A
15	a	1352	U
15	a	1365	A
15	a	1379	U
15	a	1383	A
15	a	1416	G
15	a	1428	C
15	a	1434	A
15	a	1452	G
15	a	1453	A
15	a	1482	G
15	a	1490	A
15	a	1493	C
15	a	1497	U
15	a	1498	C
15	a	1508	A
15	a	1509	A
15	a	1515	A
15	a	1529	G
15	a	1535	A
15	a	1536	C
15	a	1537	G
15	a	1566	A

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Mol	Chain	Res	Type
15	a	1569	A
15	a	1578	U
15	a	1584	U
15	a	1585	C
15	a	1608	A
15	a	1609	A
15	a	1610	A
15	a	1644	C
15	a	1647	U
15	a	1648	U
15	a	1674	G
15	a	1715	G
15	a	1732	C
15	a	1738	G
15	a	1758	U
15	a	1764	C
15	a	1773	A
15	a	1782	U
15	a	1800	C
15	a	1801	A
15	a	1808	A
15	a	1816	C
15	a	1829	A
15	a	1847	A
15	a	1848	A
15	a	1858	A
15	a	1862	G
15	a	1869	G
15	a	1872	A
15	a	1873	G
15	a	1907	G
15	a	1910	G
15	a	1911	PSU
15	a	1912	A
15	a	1917	PSU
15	a	1918	A
15	a	1919	A
15	a	1925	C
15	a	1930	G
15	a	1931	U
15	a	1937	A
15	a	1938	A

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Mol	Chain	Res	Type
15	a	1955	U
15	a	1965	C
15	a	1967	C
15	a	1970	A
15	a	1971	U
15	a	1972	G
15	a	1987	A
15	a	1991	U
15	a	1993	U
15	a	2023	C
15	a	2031	A
15	a	2033	A
15	a	2043	C
15	a	2049	G
15	a	2055	C
15	a	2056	G
15	a	2060	A
15	a	2061	G
15	a	2062	A
15	a	2069	G7M
15	a	2099	U
15	a	2198	A
15	a	2204	G
15	a	2211	A
15	a	2225	A
15	a	2238	G
15	a	2239	G
15	a	2268	A
15	a	2282	G
15	a	2283	C
15	a	2286	G
15	a	2287	A
15	a	2288	A
15	a	2305	U
15	a	2307	G
15	a	2309	A
15	a	2310	C
15	a	2317	A
15	a	2322	A
15	a	2325	G
15	a	2333	A
15	a	2335	A

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Mol	Chain	Res	Type
15	a	2347	C
15	a	2350	C
15	a	2383	G
15	a	2385	C
15	a	2402	U
15	a	2406	A
15	a	2425	A
15	a	2429	G
15	a	2430	A
15	a	2431	U
15	a	2435	A
15	a	2441	U
15	a	2448	A
15	a	2470	G
15	a	2476	A
15	a	2478	A
15	a	2491	U
15	a	2502	G
15	a	2505	G
15	a	2518	A
15	a	2529	G
15	a	2535	G
15	a	2547	A
15	a	2566	A
15	a	2567	G
15	a	2573	C
15	a	2602	A
15	a	2609	U
15	a	2613	U
15	a	2629	U
15	a	2661	G
15	a	2663	G
15	a	2689	U
15	a	2690	U
15	a	2714	G
15	a	2716	C
15	a	2726	A
15	a	2744	G
15	a	2748	A
15	a	2751	G
15	a	2757	A
15	a	2765	A

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Mol	Chain	Res	Type
15	a	2778	A
15	a	2790	U
15	a	2797	U
15	a	2800	A
15	a	2801	G
15	a	2820	A
15	a	2821	A
15	a	2861	U
15	a	2883	A
15	a	2884	U
37	X	14	A
37	X	15	A
37	X	16	A
37	X	21	A
37	X	22	U

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	A	13	U
12	A	119	A
12	A	199	A
12	A	367	U
12	A	421	U
12	A	438	U
12	A	530	G
12	A	532	A
12	A	574	A
12	A	641	U
12	A	776	G
12	A	793	U
12	A	858	G
12	A	884	U
12	A	993	G
12	A	1124	G
12	A	1129	C
12	A	1187	G
12	A	1211	U
12	A	1224	U
12	A	1225	A
12	A	1239	A
12	A	1240	U

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Mol	Chain	Res	Type
12	A	1281	C
12	A	1297	G
12	A	1319	A
12	A	1432	G
12	A	1448	C
12	A	1478	U
12	A	1505	G
13	Y	74	C
14	Z	22	G
14	Z	48	C
14	Z	60	U

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	$\# Z > 2$
12	5MC	A	1407	12	18,22,23	0.31	0	26,32,35	0.61	0
15	G7M	a	2069	15	23,26,27	0.69	1 (4%)	35,39,42	0.64	0
12	5MC	A	967	12	18,22,23	0.32	0	26,32,35	0.53	0
8	4D4	l	81	8	9,11,12	0.50	0	8,13,15	0.76	0
13	5MU	Y	54	13	19,22,23	0.26	0	28,32,35	0.31	0
15	OMU	a	2552	15	19,22,23	0.21	0	26,31,34	0.39	0
13	PSU	Y	55	13	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
8	MS6	l	82	8	5,7,8	0.18	0	2,7,9	0.16	0
15	5MU	a	1939	15	19,22,23	0.28	0	28,32,35	0.37	0
15	PSU	a	746	15,57	18,21,22	0.89	1 (5%)	22,30,33	0.58	0
13	G7M	Y	46	13	23,26,27	0.73	1 (4%)	35,39,42	0.54	0
14	G7M	Z	46	14	23,26,27	0.72	1 (4%)	35,39,42	0.60	0
15	PSU	a	2457	15	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
12	UR3	A	1498	12	19,22,23	0.26	0	26,32,35	0.66	0
3	IAS	K	119	3	6,7,8	0.88	0	6,8,10	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PSU	a	955	15	18,21,22	0.93	1 (5%)	22,30,33	0.64	0
15	3TD	a	1915	15	18,22,23	0.97	1 (5%)	22,32,35	0.67	0
15	PSU	a	1917	15	18,21,22	0.93	1 (5%)	22,30,33	0.62	0
15	PSU	a	2504	15,59	18,21,22	0.88	1 (5%)	22,30,33	0.72	0
12	G7M	A	527	12	23,26,27	0.73	1 (4%)	35,39,42	0.66	0
15	PSU	a	2580	15	18,21,22	0.93	1 (5%)	22,30,33	0.79	1 (4%)
12	MA6	A	1519	12	23,26,27	0.24	0	34,38,41	0.75	1 (2%)
15	5MC	a	1962	15,59	18,22,23	0.34	0	26,32,35	0.50	0
12	4OC	A	1402	12,57	20,23,24	0.37	0	26,32,35	0.55	0
15	OMC	a	2498	15,57	19,22,23	0.27	0	26,31,34	0.51	0
12	2MG	A	1207	12	23,26,27	0.38	0	32,38,41	0.36	0
15	PSU	a	2605	15	18,21,22	0.90	1 (5%)	22,30,33	0.85	1 (4%)
14	5MU	Z	54	14	19,22,23	0.26	0	28,32,35	0.27	0
15	5MU	a	747	15	19,22,23	0.29	0	28,32,35	0.48	0
15	PSU	a	2604	15	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
15	1MG	a	745	15	22,26,27	0.52	0	33,39,42	0.51	0
13	4SU	Y	8	13	18,21,22	0.37	0	26,30,33	1.22	3 (11%)
15	6MZ	a	2030	15	22,25,26	0.34	0	30,36,39	0.61	0
12	2MG	A	1516	12	23,26,27	0.37	0	32,38,41	0.53	0
14	4SU	Z	8	14	18,21,22	0.37	0	26,30,33	1.19	3 (11%)
15	2MG	a	1835	15	23,26,27	0.37	0	32,38,41	0.38	0
15	2MA	a	2503	15,57	22,25,26	0.25	0	33,37,40	0.68	2 (6%)
15	PSU	a	1911	15	18,21,22	0.90	1 (5%)	22,30,33	0.56	0
15	2MG	a	2445	15	23,26,27	0.38	0	32,38,41	0.44	0
4	D2T	L	89	4	7,9,10	0.94	0	6,11,13	1.69	2 (33%)
12	PSU	A	516	12	18,21,22	0.91	1 (5%)	22,30,33	0.75	1 (4%)
14	PSU	Z	55	14	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
12	2MG	A	966	12	23,26,27	0.41	0	32,38,41	0.39	0
15	H2U	a	2449	15,59	18,21,22	0.58	0	21,30,33	0.77	1 (4%)
6	MEQ	d	150	6	8,9,10	0.44	0	5,10,12	0.75	0
12	MA6	A	1518	12	23,26,27	0.25	0	34,38,41	0.67	1 (2%)
15	OMG	a	2251	13,15	23,26,27	0.30	0	33,38,41	0.48	0
15	6MZ	a	1618	15	22,25,26	0.34	0	30,36,39	0.57	0
13	6MZ	Y	37	13	22,25,26	0.37	0	30,36,39	0.53	0
14	OMC	Z	32	14	19,22,23	0.26	0	26,31,34	0.36	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
12	5MC	A	1407	12	-	0/7/25/26	0/2/2/2
15	G7M	a	2069	15	-	2/7/25/26	0/3/3/3
12	5MC	A	967	12	-	0/7/25/26	0/2/2/2
8	4D4	l	81	8	-	0/11/12/14	-
13	5MU	Y	54	13	-	0/7/25/26	0/2/2/2
15	OMU	a	2552	15	-	0/9/27/28	0/2/2/2
13	PSU	Y	55	13	-	0/7/25/26	0/2/2/2
8	MS6	l	82	8	-	1/4/6/8	-
15	5MU	a	1939	15	-	0/7/25/26	0/2/2/2
15	PSU	a	746	15,57	-	3/7/25/26	0/2/2/2
13	G7M	Y	46	13	-	3/7/25/26	0/3/3/3
14	G7M	Z	46	14	-	3/7/25/26	0/3/3/3
15	PSU	a	2457	15	-	0/7/25/26	0/2/2/2
12	UR3	A	1498	12	-	0/7/25/26	0/2/2/2
3	IAS	K	119	3	-	0/7/7/8	-
15	PSU	a	955	15	-	0/7/25/26	0/2/2/2
15	3TD	a	1915	15	-	0/7/25/26	0/2/2/2
15	PSU	a	1917	15	-	2/7/25/26	0/2/2/2
15	PSU	a	2504	15,59	-	0/7/25/26	0/2/2/2
12	G7M	A	527	12	-	1/7/25/26	0/3/3/3
15	PSU	a	2580	15	-	0/7/25/26	0/2/2/2
12	MA6	A	1519	12	-	2/11/29/30	0/3/3/3
15	5MC	a	1962	15,59	-	1/7/25/26	0/2/2/2
12	4OC	A	1402	12,57	-	1/9/29/30	0/2/2/2
15	OMC	a	2498	15,57	-	0/9/27/28	0/2/2/2
12	2MG	A	1207	12	-	0/9/27/28	0/3/3/3
15	PSU	a	2605	15	-	0/7/25/26	0/2/2/2
14	5MU	Z	54	14	-	0/7/25/26	0/2/2/2
15	5MU	a	747	15	-	1/7/25/26	0/2/2/2
15	PSU	a	2604	15	-	0/7/25/26	0/2/2/2
15	1MG	a	745	15	-	0/7/25/26	0/3/3/3
13	4SU	Y	8	13	-	0/7/25/26	0/2/2/2
15	6MZ	a	2030	15	-	2/9/27/28	0/3/3/3
12	2MG	A	1516	12	-	0/9/27/28	0/3/3/3
14	4SU	Z	8	14	-	1/7/25/26	0/2/2/2
15	2MG	a	1835	15	-	0/9/27/28	0/3/3/3
15	2MA	a	2503	15,57	-	1/7/25/26	0/3/3/3
15	PSU	a	1911	15	-	2/7/25/26	0/2/2/2
15	2MG	a	2445	15	-	0/9/27/28	0/3/3/3
4	D2T	L	89	4	-	4/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PSU	A	516	12	-	0/7/25/26	0/2/2/2
14	PSU	Z	55	14	-	0/7/25/26	0/2/2/2
12	2MG	A	966	12	-	3/9/27/28	0/3/3/3
15	H2U	a	2449	15,59	-	0/7/38/39	0/2/2/2
6	MEQ	d	150	6	-	3/8/9/11	-
12	MA6	A	1518	12	-	0/11/29/30	0/3/3/3
15	OMG	a	2251	13,15	-	1/9/27/28	0/3/3/3
15	6MZ	a	1618	15	-	0/9/27/28	0/3/3/3
13	6MZ	Y	37	13	-	0/9/27/28	0/3/3/3
14	OMC	Z	32	14	-	0/9/27/28	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	1917	PSU	C6-C5	3.64	1.39	1.35
15	a	2580	PSU	C6-C5	3.64	1.39	1.35
15	a	955	PSU	C6-C5	3.62	1.39	1.35
15	a	1915	3TD	C6-C5	3.61	1.39	1.35
14	Z	55	PSU	C6-C5	3.60	1.39	1.35
15	a	1911	PSU	C6-C5	3.58	1.39	1.35
12	A	516	PSU	C6-C5	3.58	1.39	1.35
13	Y	55	PSU	C6-C5	3.56	1.39	1.35
15	a	2457	PSU	C6-C5	3.55	1.39	1.35
15	a	2604	PSU	C6-C5	3.52	1.39	1.35
15	a	746	PSU	C6-C5	3.45	1.39	1.35
15	a	2605	PSU	C6-C5	3.41	1.39	1.35
15	a	2504	PSU	C6-C5	3.39	1.39	1.35
13	Y	46	G7M	C8-N7	2.64	1.37	1.33
12	A	527	G7M	C8-N7	2.64	1.37	1.33
15	a	2069	G7M	C8-N7	2.52	1.37	1.33
14	Z	46	G7M	C8-N7	2.51	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Z	8	4SU	C4-N3-C2	-4.41	123.06	127.34
13	Y	8	4SU	C4-N3-C2	-4.34	123.12	127.34
12	A	1519	MA6	C2-N1-C6	2.96	118.74	111.75
12	A	1518	MA6	C2-N1-C6	2.93	118.67	111.75
13	Y	8	4SU	C5-C4-N3	2.74	117.23	114.69
14	Z	8	4SU	C5-C4-N3	2.70	117.20	114.69
4	L	89	D2T	OD1-CG-CB	-2.57	117.06	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	2580	PSU	C3'-C2'-C1'	2.53	104.58	101.64
15	a	2503	2MA	C5-C4-N3	-2.49	124.39	127.19
12	A	516	PSU	C3'-C2'-C1'	2.36	104.39	101.64
13	Y	8	4SU	N3-C2-N1	2.25	117.88	114.89
15	a	2605	PSU	C2'-C3'-C4'	-2.24	98.29	102.64
15	a	2503	2MA	N3-C4-N9	2.17	130.00	126.99
15	a	2449	H2U	O2-C2-N1	-2.09	120.48	123.11
4	L	89	D2T	OD2-CG-CB	2.08	117.65	113.15
14	Z	8	4SU	N3-C2-N1	2.04	117.59	114.89

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	89	D2T	CA-CB-CG-OD1
4	L	89	D2T	CA-CB-CG-OD2
12	A	966	2MG	O4'-C4'-C5'-O5'
12	A	966	2MG	C3'-C4'-C5'-O5'
12	A	1519	MA6	O4'-C4'-C5'-O5'
13	Y	46	G7M	C4'-C5'-O5'-P
15	a	746	PSU	C2'-C1'-C5-C4
15	a	1911	PSU	C3'-C4'-C5'-O5'
15	a	1911	PSU	O4'-C4'-C5'-O5'
15	a	1917	PSU	C3'-C4'-C5'-O5'
15	a	1917	PSU	O4'-C4'-C5'-O5'
15	a	2030	6MZ	O4'-C4'-C5'-O5'
12	A	1519	MA6	C3'-C4'-C5'-O5'
14	Z	46	G7M	O4'-C4'-C5'-O5'
13	Y	46	G7M	O4'-C4'-C5'-O5'
13	Y	46	G7M	C3'-C4'-C5'-O5'
15	a	2030	6MZ	C3'-C4'-C5'-O5'
6	d	150	MEQ	NE2-CD-CG-CB
6	d	150	MEQ	OE1-CD-CG-CB
14	Z	46	G7M	C3'-C4'-C5'-O5'
12	A	966	2MG	C4'-C5'-O5'-P
8	l	82	MS6	CB-CG-SD-CE
15	a	747	5MU	C3'-C4'-C5'-O5'
15	a	2069	G7M	C4'-C5'-O5'-P
15	a	746	PSU	O4'-C1'-C5-C4
12	A	527	G7M	C4'-C5'-O5'-P
6	d	150	MEQ	C-CA-CB-CG
4	L	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
15	a	2251	OMG	C1'-C2'-O2'-CM2
4	L	89	D2T	CG-CB-SB-CB1
15	a	746	PSU	O4'-C1'-C5-C6
14	Z	8	4SU	C2'-C1'-N1-C2
15	a	2069	G7M	O4'-C4'-C5'-O5'
12	A	1402	4OC	O4'-C4'-C5'-O5'
15	a	2503	2MA	O4'-C4'-C5'-O5'
14	Z	46	G7M	C4'-C5'-O5'-P
15	a	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1519	MA6	3	0
12	A	1402	4OC	1	0
15	a	747	5MU	1	0
15	a	2030	6MZ	2	0
12	A	1516	2MG	1	0
12	A	1518	MA6	2	0
13	Y	37	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 302 ligands modelled in this entry, 300 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	$\# Z > 2$
58	SCM	A	1601	-	23,25,25	0.27	0	26,39,39	0.56	0
60	VAL	Y	101	13	4,6,7	0.59	0	6,7,9	0.99	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
58	SCM	A	1601	-	-	4/4/57/57	0/3/3/3
60	VAL	Y	101	13	-	1/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

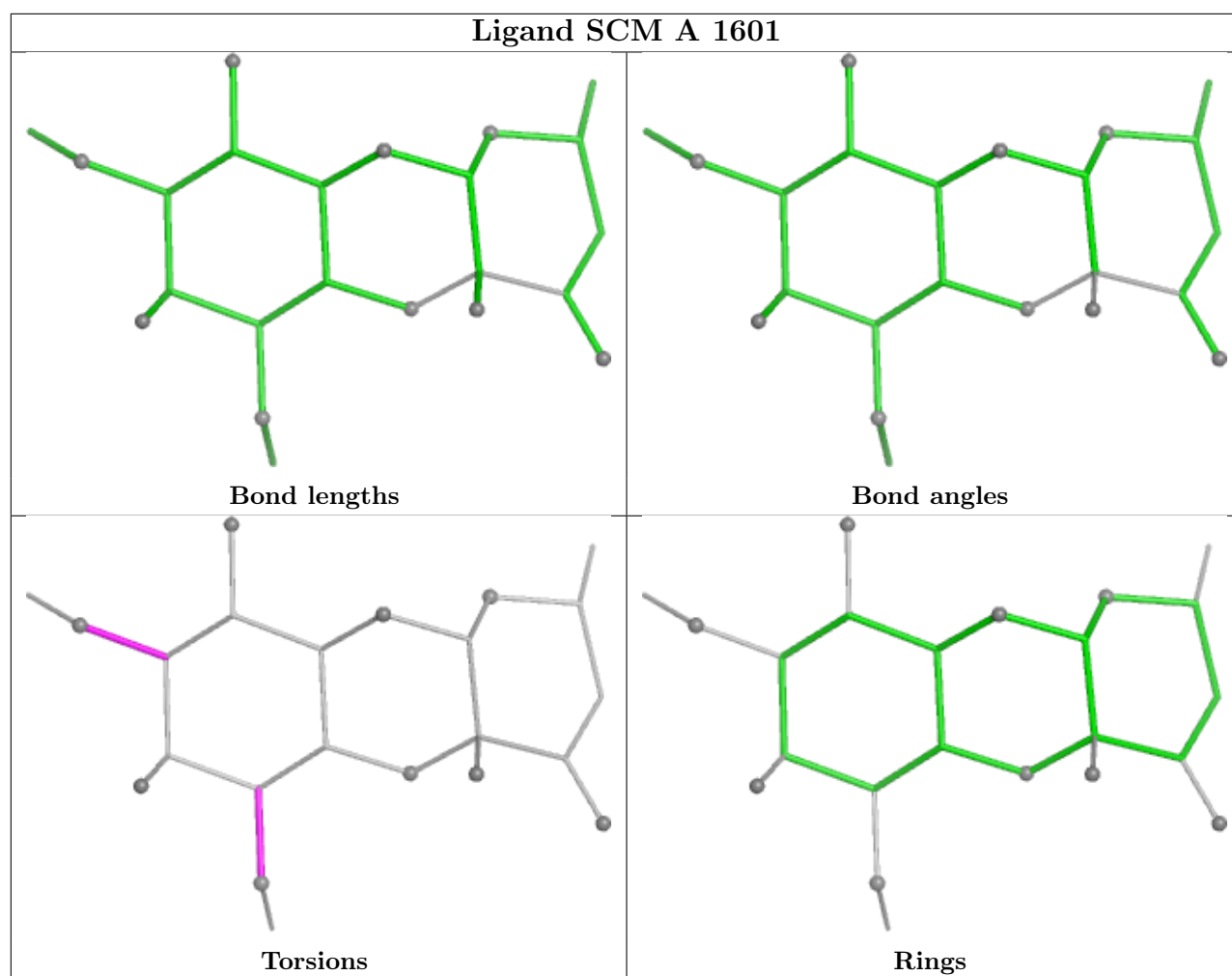
Mol	Chain	Res	Type	Atoms
58	A	1601	SCM	C9-C8-N8-C8M
58	A	1601	SCM	C7-C8-N8-C8M
60	Y	101	VAL	O-C-CA-CB
58	A	1601	SCM	C9-C10-N10-C1M
58	A	1601	SCM	C11-C10-N10-C1M

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	A	1601	SCM	3	0
60	Y	101	VAL	1	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.

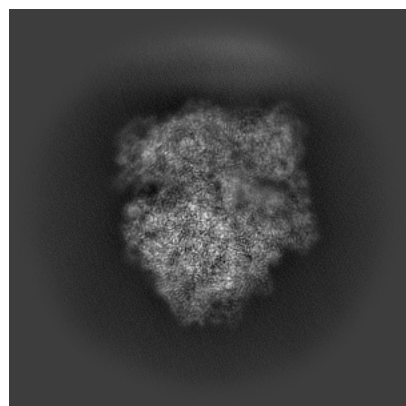
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56829. These allow visual inspection of the internal detail of the map and identification of artifacts.

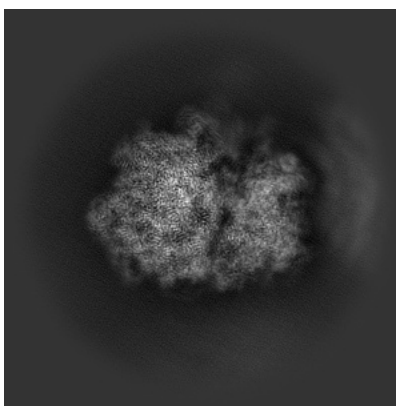
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

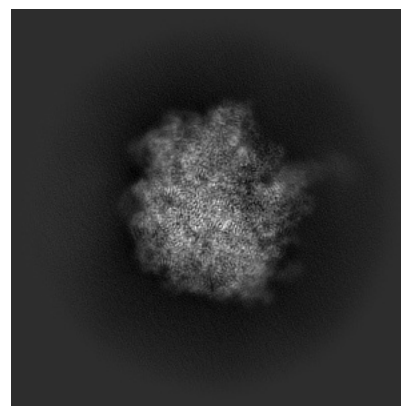
6.1.1 Primary map



X

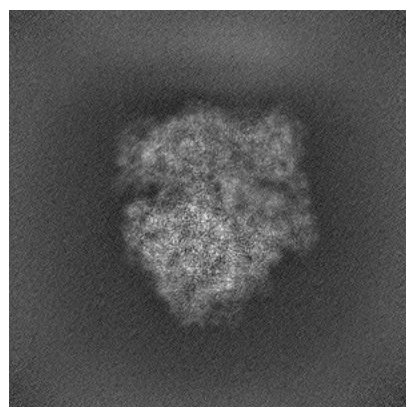


Y

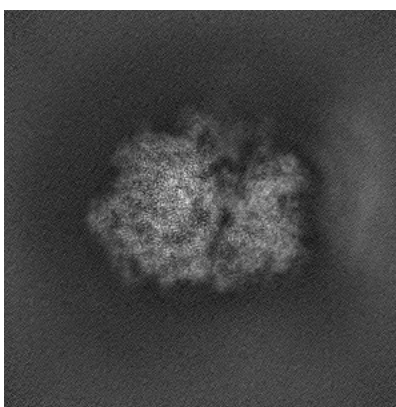


Z

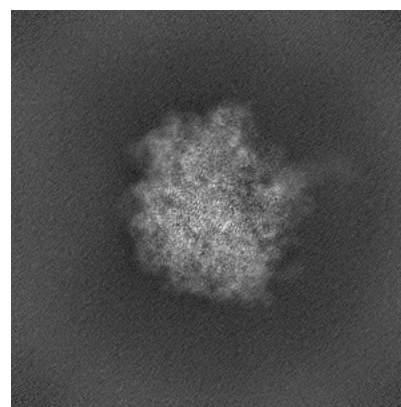
6.1.2 Raw map



X



Y

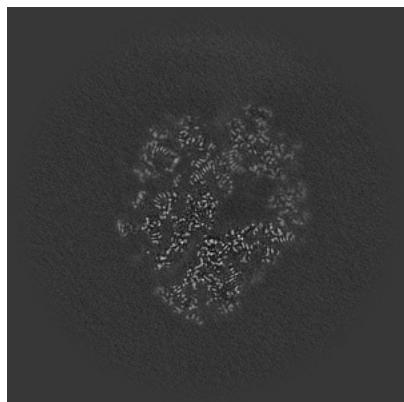


Z

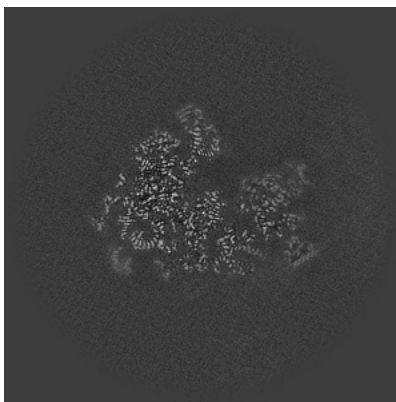
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

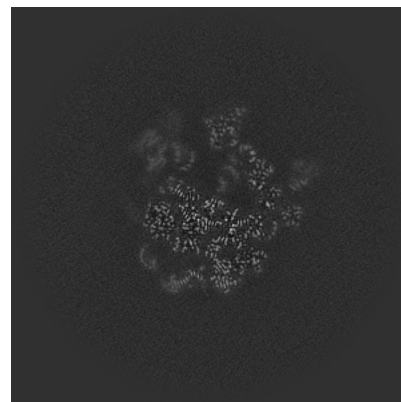
6.2.1 Primary map



X Index: 288

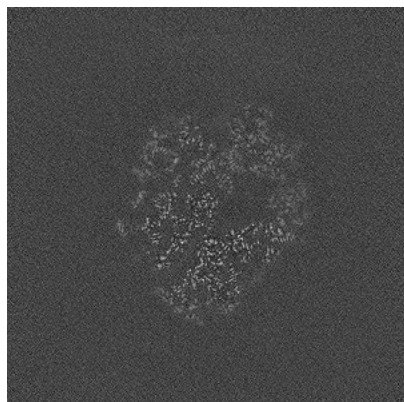


Y Index: 288

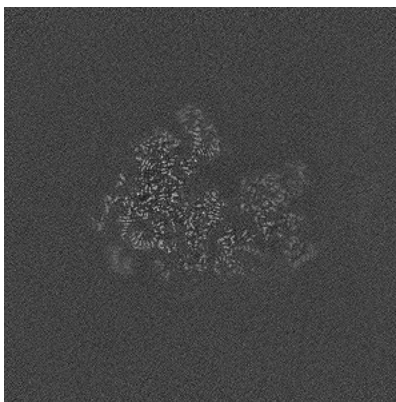


Z Index: 288

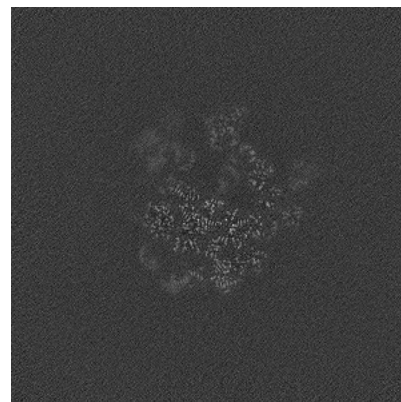
6.2.2 Raw map



X Index: 288



Y Index: 288

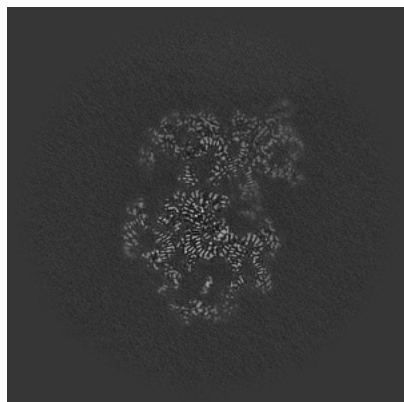


Z Index: 288

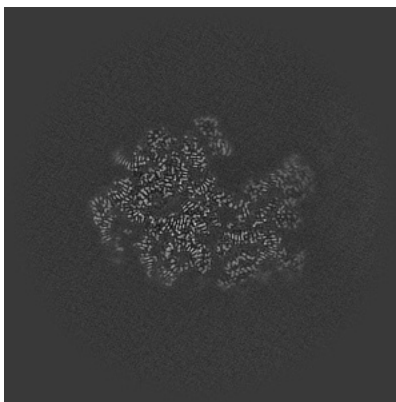
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

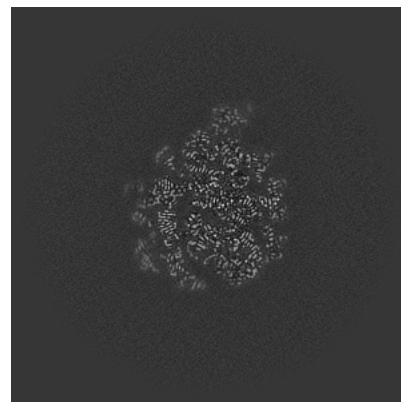
6.3.1 Primary map



X Index: 263

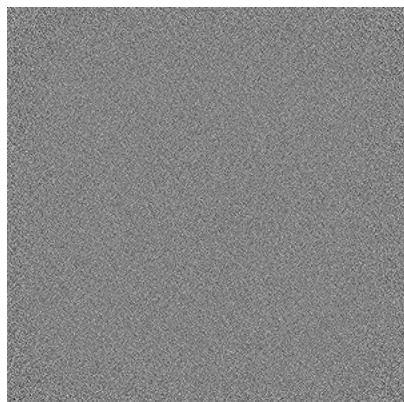


Y Index: 272

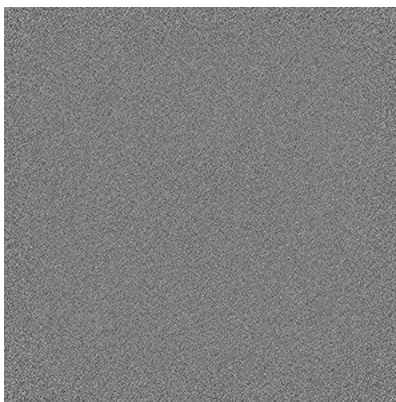


Z Index: 235

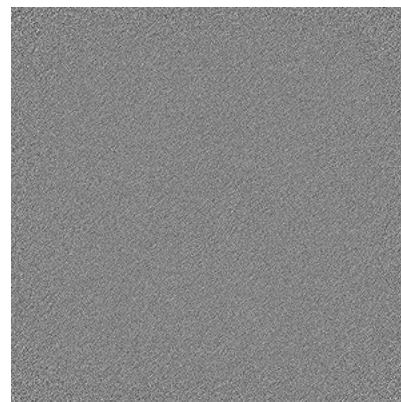
6.3.2 Raw map



X Index: 0



Y Index: 0

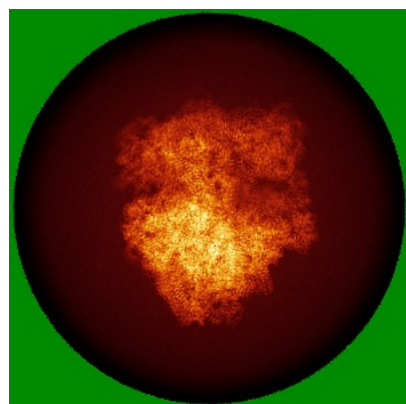


Z Index: 0

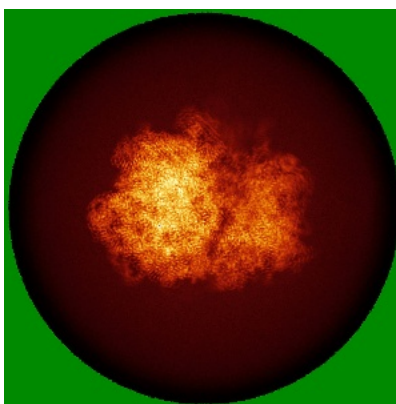
The images above show the largest variance slices of the map in three orthogonal directions.

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

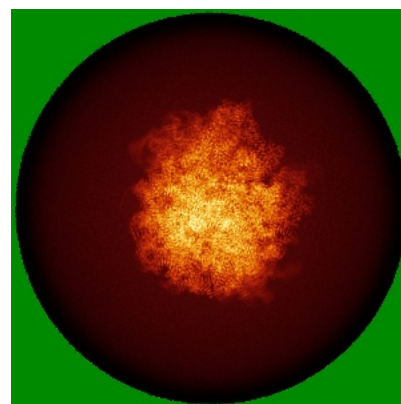
6.4.1 Primary map



X

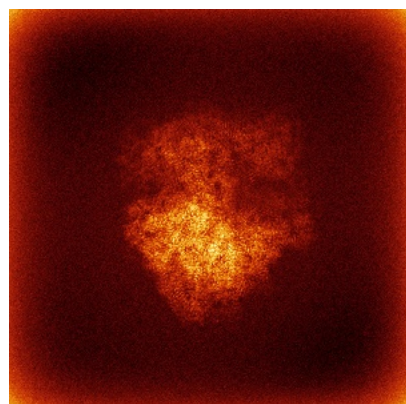


Y

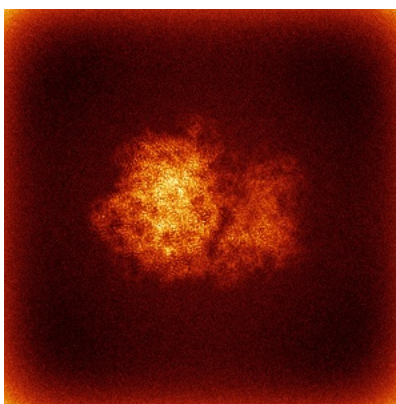


Z

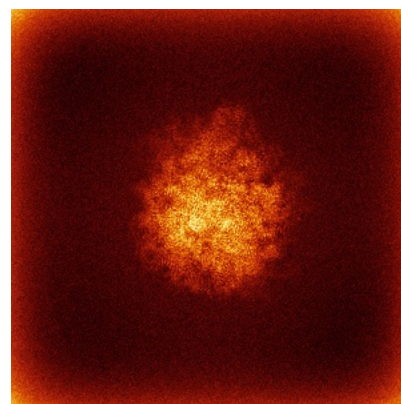
6.4.2 Raw map



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



X



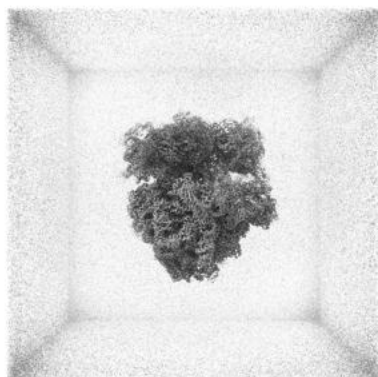
Y



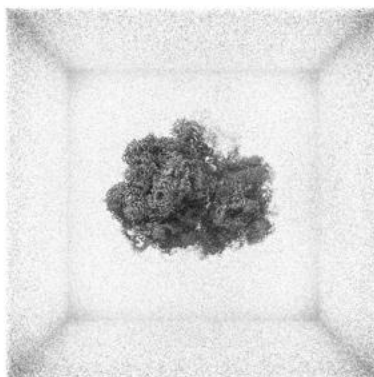
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0642. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

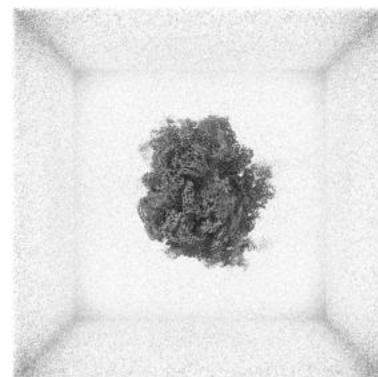
6.5.2 Raw map



X



Y



Z

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

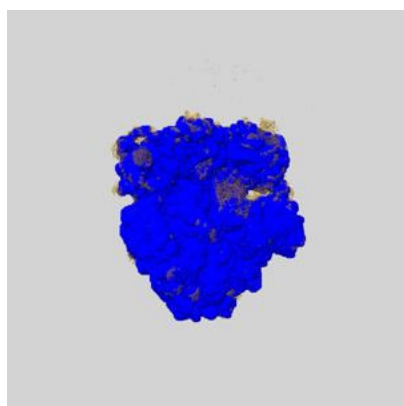
6.6 Mask visualisation [i](#)

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

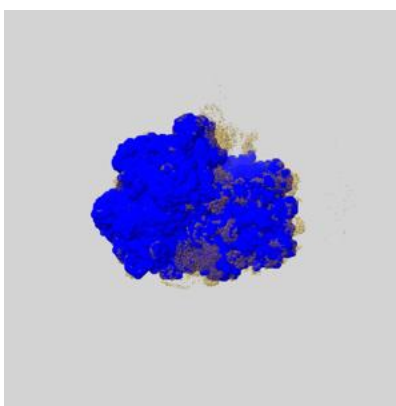
A mask typically either:

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

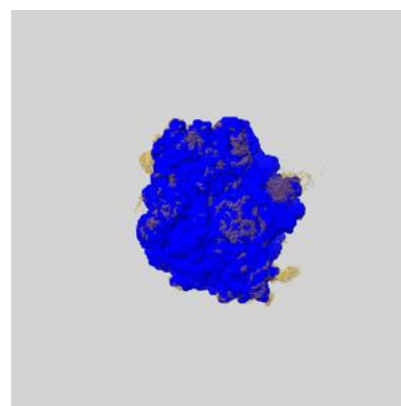
6.6.1 emd_56829_msk_1.map [i](#)



X



Y

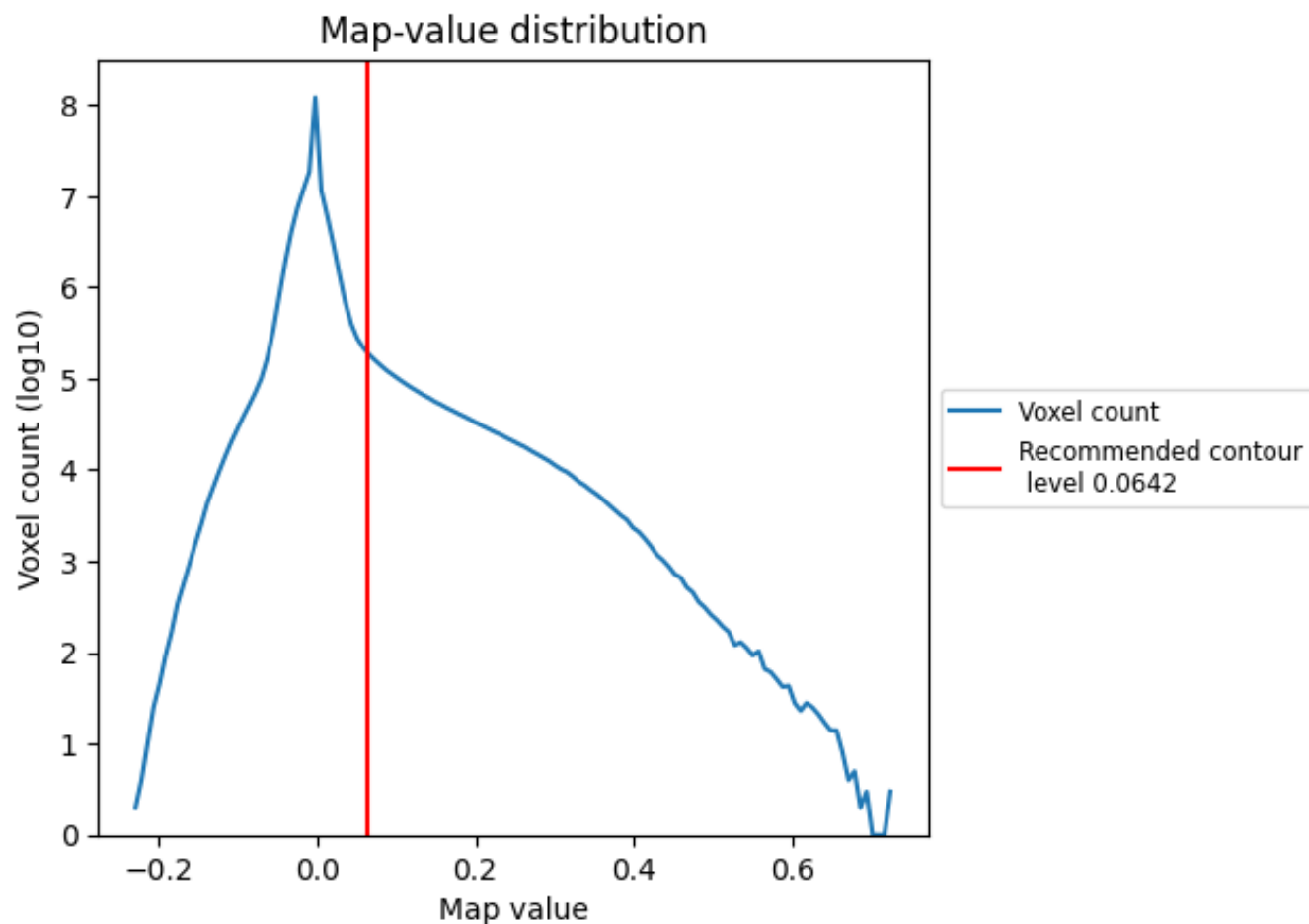


Z

7 Map analysis [i](#)

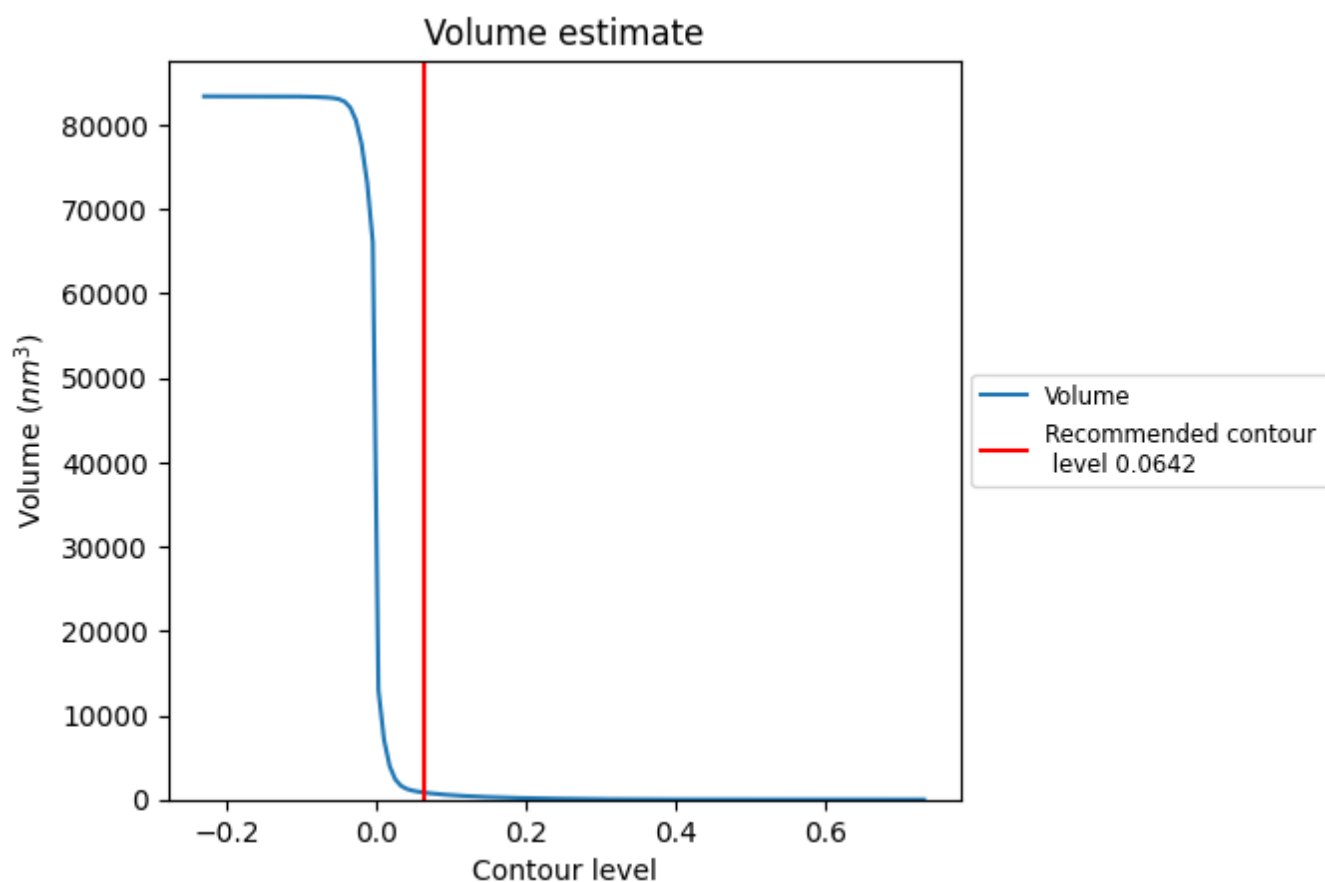
This section contains the results of statistical analysis of the map.

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.

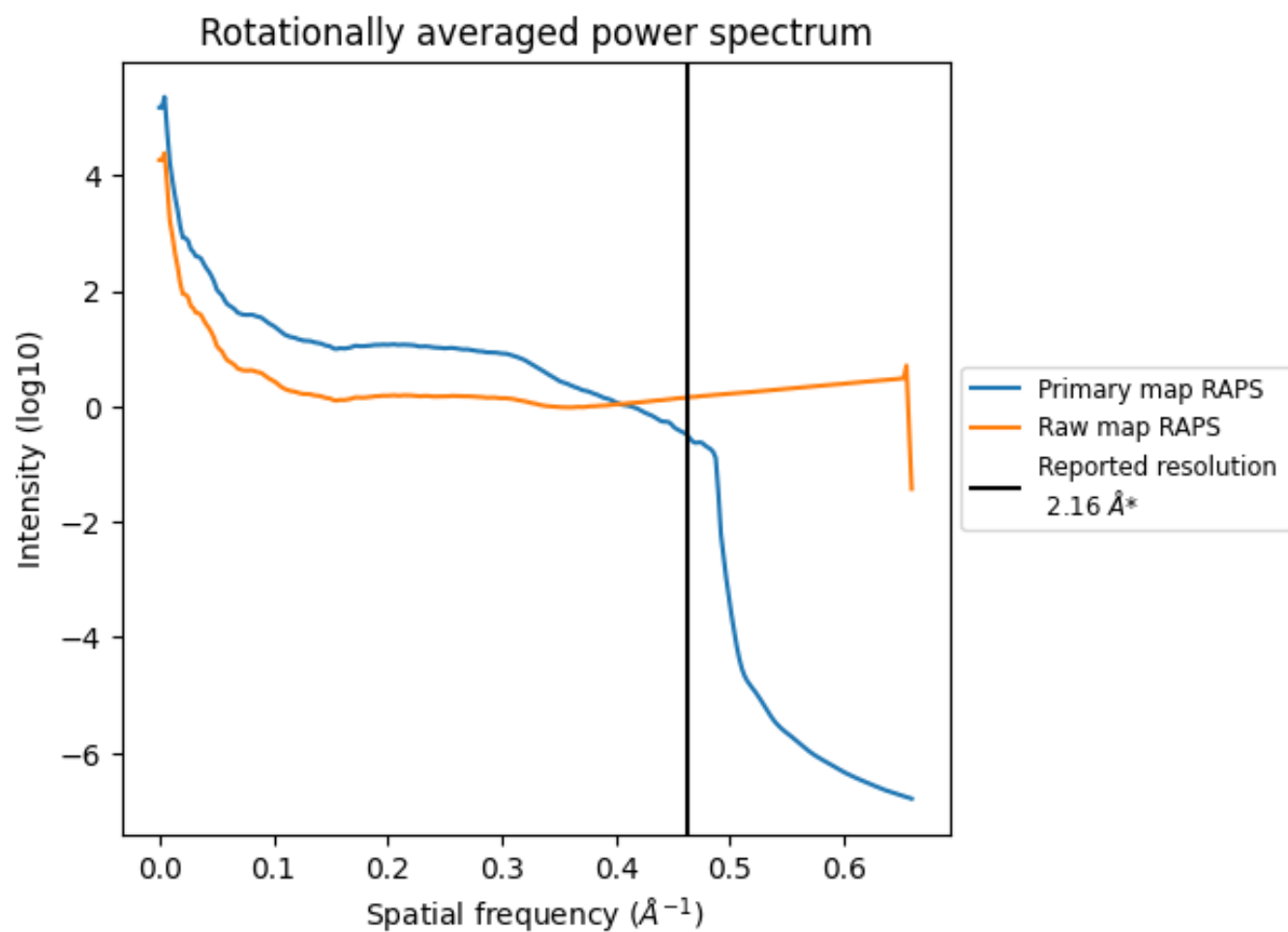
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 835 nm³; this corresponds to an approximate mass of 754 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 ⓘ

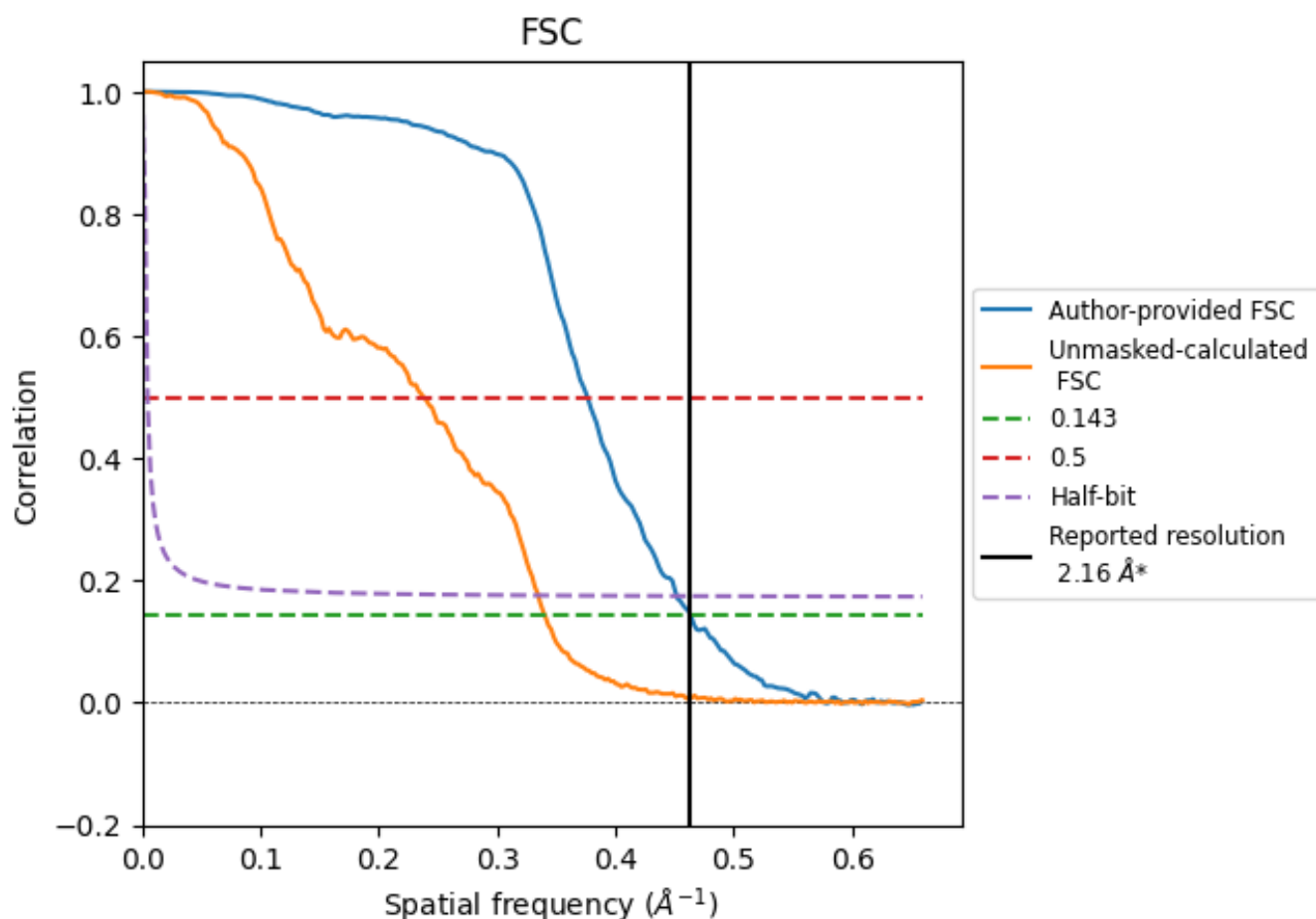


*Reported resolution corresponds to spatial frequency of 0.463 Å⁻¹

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 0.463 \AA^{-1}

8.2 Resolution estimates [i](#)

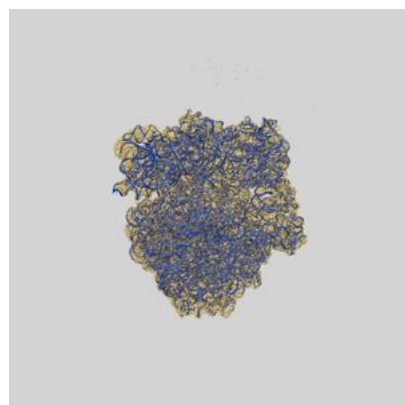
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.16	-	-
Author-provided FSC curve	2.16	2.66	2.21
Unmasked-calculated*	2.94	4.21	2.99

*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 2.94 differs from the reported value 2.16 by more than 10 %

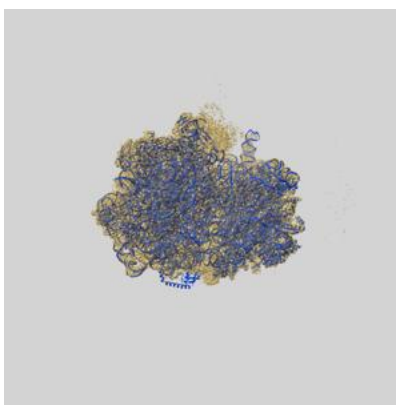
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56829 and PDB model 28UJ. Per-residue inclusion information can be found in section [3](#) on page [19](#).

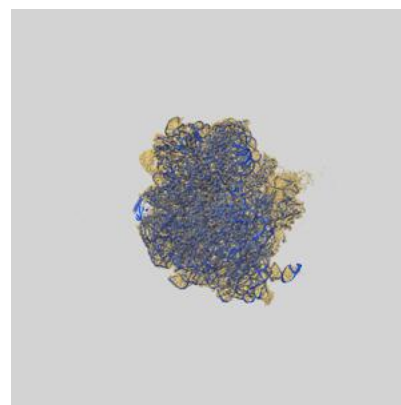
9.1 Map-model overlay [i](#)



X



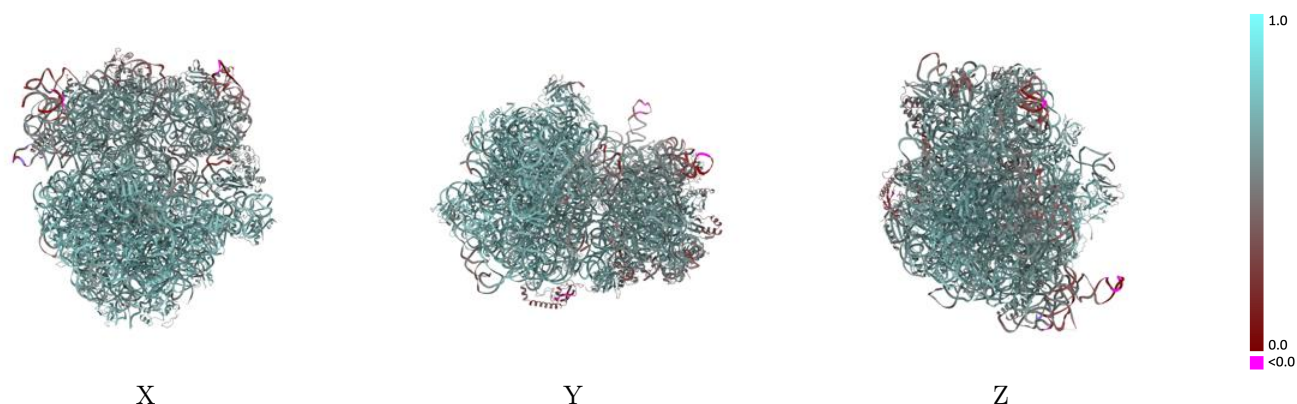
Y



Z

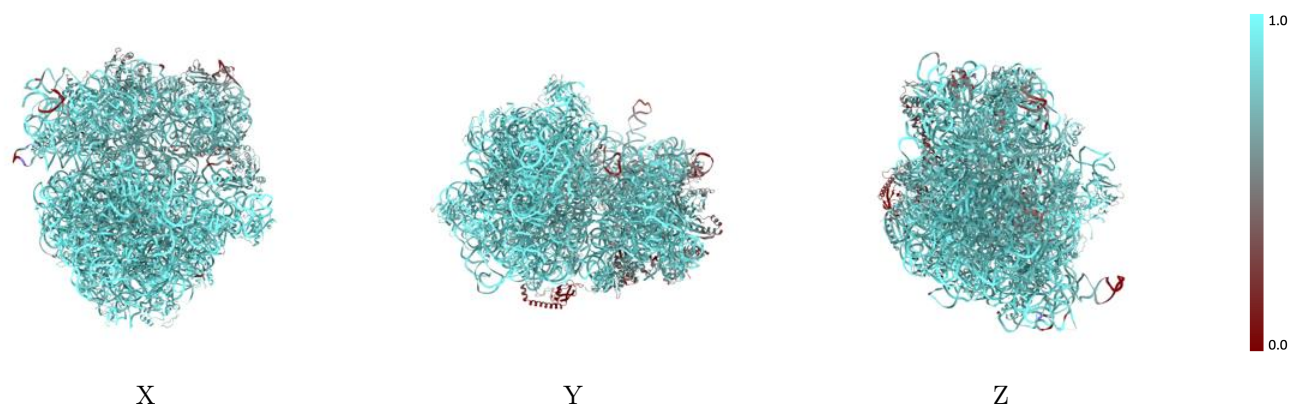
The images above show the 3D surface view of the map at the recommended contour level 0.0642 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



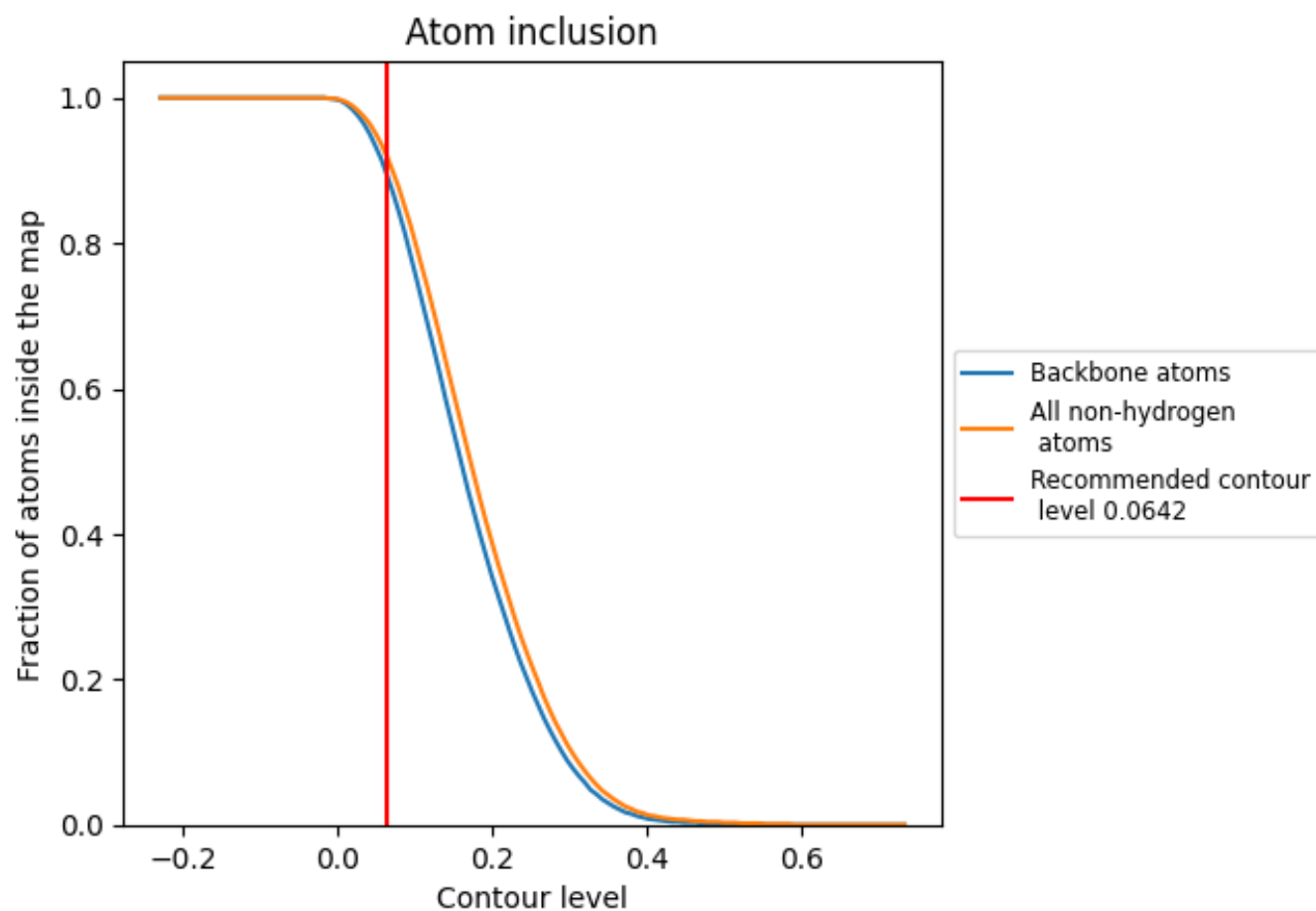
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0642).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 92% 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 (0.0642) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.6350
0	 0.8900	 0.6660
1	 0.9630	 0.7200
2	 0.9720	 0.7170
3	 0.9320	 0.6770
4	 0.7240	 0.5000
A	 0.9280	 0.5960
B	 0.7110	 0.5370
C	 0.7880	 0.5920
D	 0.6040	 0.4680
E	 0.8930	 0.6470
F	 0.7760	 0.5640
G	 0.4780	 0.4280
H	 0.9090	 0.6500
I	 0.7560	 0.5380
J	 0.6600	 0.4980
K	 0.8750	 0.6260
L	 0.8050	 0.5780
M	 0.7210	 0.5400
N	 0.8300	 0.5940
O	 0.8960	 0.6350
P	 0.7940	 0.5570
Q	 0.8130	 0.5860
R	 0.8550	 0.6170
S	 0.7880	 0.5750
T	 0.7850	 0.5410
U	 0.6210	 0.5340
X	 0.8330	 0.5640
Y	 0.7990	 0.5010
Z	 0.8800	 0.5600
a	 0.9800	 0.6760
b	 0.9730	 0.6440
c	 0.9650	 0.7110
d	 0.9480	 0.6970
e	 0.9140	 0.6640



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Chain	Atom inclusion	Q-score
f	 0.7740	 0.5740
g	 0.8310	 0.5940
h	 0.2280	 0.3540
i	 0.9520	 0.6970
j	 0.9390	 0.6960
k	 0.9520	 0.6900
l	 0.9380	 0.6910
m	 0.9890	 0.7140
n	 0.9110	 0.6430
o	 0.8780	 0.6650
p	 0.9780	 0.7190
q	 0.9230	 0.6820
r	 0.9370	 0.6930
s	 0.8990	 0.6590
t	 0.8870	 0.6380
u	 0.8920	 0.6430
v	 0.9360	 0.6930
w	 0.9430	 0.6870
x	 0.8900	 0.6330
y	 0.9220	 0.6810
z	 0.9390	 0.6930