



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 11:56 pm BST

PDB ID : 28UH / pdb_000028uh
EMDB ID : EMD-56827
Title : E. coli 70S ribosome, trapped conformational ground 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 : 2.06 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:

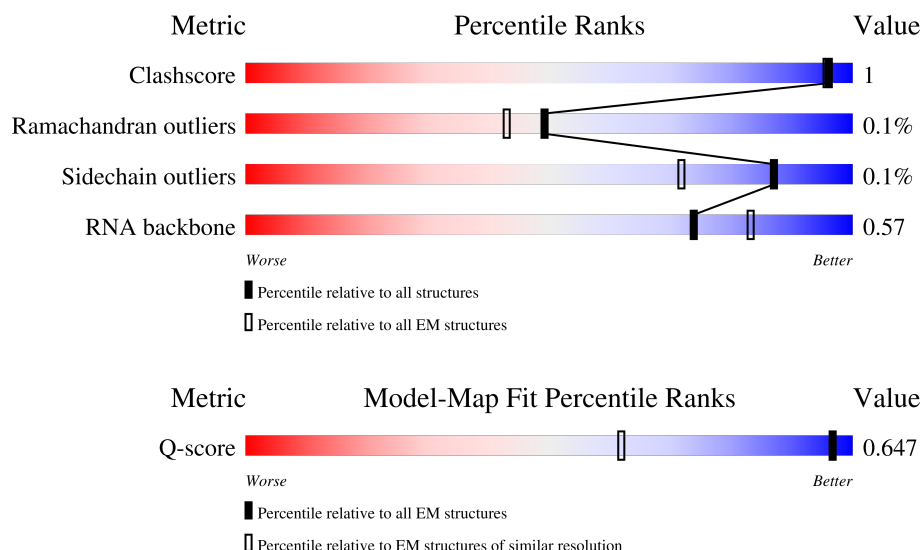
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.06 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.



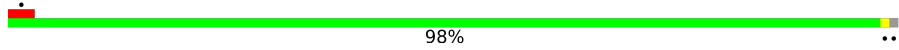
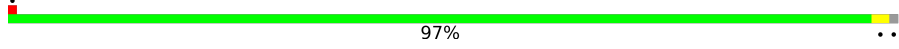

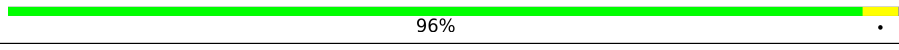
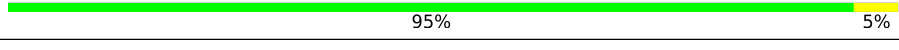
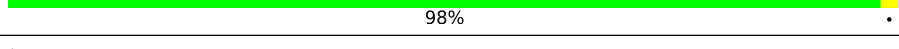
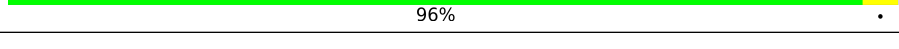
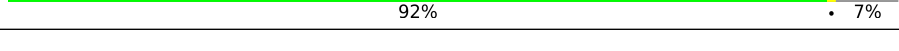
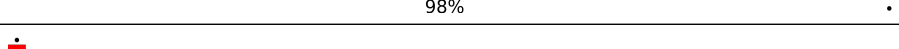
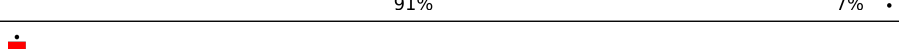
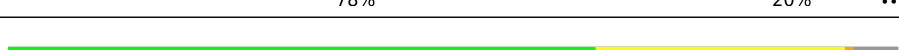

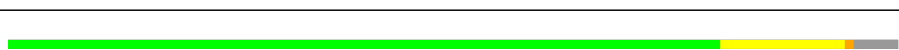
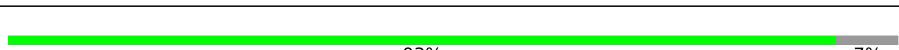
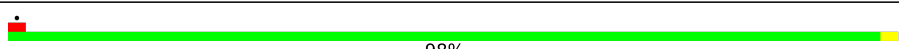

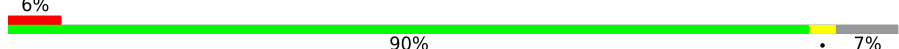

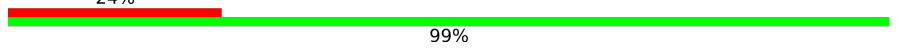
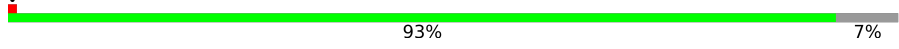
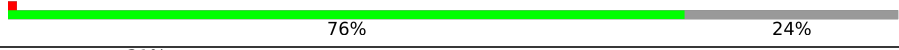
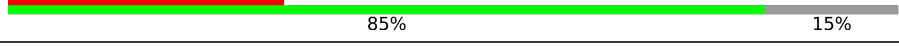
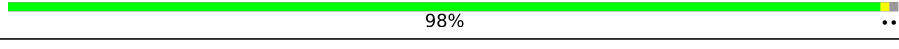
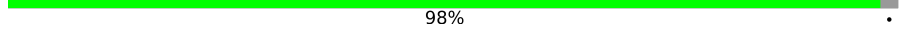

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1895 (1.56 - 2.56)

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	
2	4	70	
3	K	129	

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Mol	Chain	Length	Quality of chain
4	L	124	
5	N	101	
6	b	120	
7	c	273	
8	d	209	
9	k	144	
10	l	136	
11	m	127	
12	r	110	
13	z	57	
14	A	1544	
15	Y	76	
16	Z	78	
17	a	2904	
18	0	55	
19	1	46	
20	2	65	
21	B	241	
22	C	233	
23	D	206	
24	E	167	
25	F	135	
26	G	179	
27	H	130	
28	I	130	

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Mol	Chain	Length	Quality of chain
29	J	103	
30	M	118	
31	O	89	
32	P	82	
33	Q	84	
34	R	75	
35	S	92	
36	T	87	
37	U	71	
38	X	10	
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	<div><div></div><div>97%</div><div>.</div></div>
55	y	59	<div><div></div><div>98%</div><div>.</div></div>

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 150006 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 protein called Small ribosomal subunit protein uS14.

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

- Molecule 6 is a RNA chain called 5S rRNA.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 14 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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	1454A	C	-	insertion	GB 2971070070

- Molecule 15 is a RNA chain called A/P-site Val-tRNA^{Val}.

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

- Molecule 16 is a RNA chain called P/E-site tRNA^{fMet}.

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

- Molecule 17 is a RNA chain called 23S rRNA.

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

- Molecule 18 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 19 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 31 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 32 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 34 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 36 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 37 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 38 is a RNA chain called mRNA.

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

- 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	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	49	Total	Mg	0
			49	49	
57	a	217	Total	Mg	0
			217	217	
57	p	1	Total	Mg	0
			1	1	

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

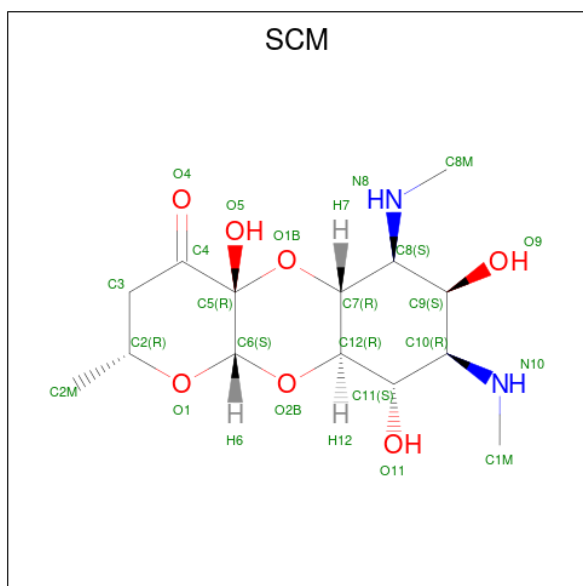
Mol	Chain	Residues	Atoms		AltConf
58	c	1	Total	K	0
			1	1	
58	A	8	Total	K	0
			8	8	

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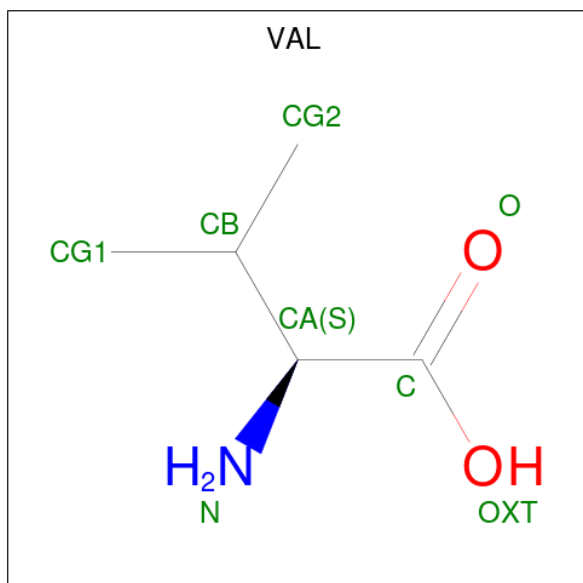
Mol	Chain	Residues	Atoms		AltConf
58	a	56	Total	K	0
			56	56	

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



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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms				AltConf
61	3	11	Total	O			0
			11	11			
61	4	2	Total	O			0
			2	2			
61	K	18	Total	O			0
			18	18			
61	L	11	Total	O			0
			11	11			
61	N	5	Total	O			0
			5	5			
61	b	131	Total	O			0
			131	131			
61	c	123	Total	O			0
			123	123			
61	d	67	Total	O			0
			67	67			
61	k	48	Total	O			0
			48	48			
61	l	46	Total	O			0
			46	46			
61	m	23	Total	O			0
			23	23			
61	r	37	Total	O			0
			37	37			
61	z	32	Total	O			0
			32	32			
61	A	1554	Total	O			0
			1554	1554			
61	Y	17	Total	O			0
			17	17			
61	Z	36	Total	O			0
			36	36			
61	a	4613	Total	O			0
			4613	4613			
61	0	9	Total	O			0
			9	9			
61	1	23	Total	O			0
			23	23			

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Mol	Chain	Residues	Atoms		AltConf
61	2	22	Total 22	O 22	0
61	B	22	Total 22	O 22	0
61	C	21	Total 21	O 21	0
61	D	14	Total 14	O 14	0
61	E	17	Total 17	O 17	0
61	F	3	Total 3	O 3	0
61	G	12	Total 12	O 12	0
61	H	27	Total 27	O 27	0
61	I	13	Total 13	O 13	0
61	J	16	Total 16	O 16	0
61	M	11	Total 11	O 11	0
61	O	16	Total 16	O 16	0
61	P	10	Total 10	O 10	0
61	Q	9	Total 9	O 9	0
61	R	3	Total 3	O 3	0
61	S	3	Total 3	O 3	0
61	T	3	Total 3	O 3	0
61	U	16	Total 16	O 16	0
61	X	9	Total 9	O 9	0
61	e	75	Total 75	O 75	0
61	f	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
61	g	15	Total 15	O 15	0
61	h	8	Total 8	O 8	0
61	i	33	Total 33	O 33	0
61	j	33	Total 33	O 33	0
61	n	18	Total 18	O 18	0
61	o	28	Total 28	O 28	0
61	p	44	Total 44	O 44	0
61	q	37	Total 37	O 37	0
61	s	21	Total 21	O 21	0
61	t	20	Total 20	O 20	0
61	u	10	Total 10	O 10	0
61	v	22	Total 22	O 22	0
61	w	25	Total 25	O 25	0
61	x	7	Total 7	O 7	0
61	y	19	Total 19	O 19	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.

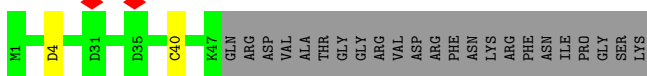
- Molecule 1: Large ribosomal subunit protein bL36A

Chain 3:  95% 5%



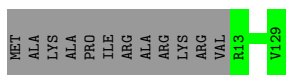
- Molecule 2: Large ribosomal subunit protein bL31

Chain 4:  64% 33%



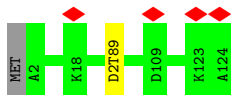
- Molecule 3: Small ribosomal subunit protein uS11

Chain K:  91% 9%



- Molecule 4: Small ribosomal subunit protein uS12

Chain L:  98%


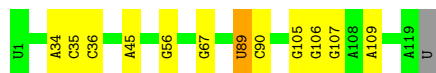


- Molecule 5: Small ribosomal subunit protein uS14

Chain N:  97%



• Molecule 6: 5S rRNA

Chain b:  89% 9% ..

• Molecule 7: Large ribosomal subunit protein uL2

Chain c:  96% . .

• Molecule 8: Large ribosomal subunit protein uL3

Chain d:  95% 5%

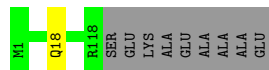
• Molecule 9: Large ribosomal subunit protein uL15

Chain k:  98% .

• Molecule 10: Large ribosomal subunit protein uL16

Chain l:  96% .


• Molecule 11: Large ribosomal subunit protein bL17

Chain m:  92% . 7%

• Molecule 12: Large ribosomal subunit protein uL22


Chain r:  98% .

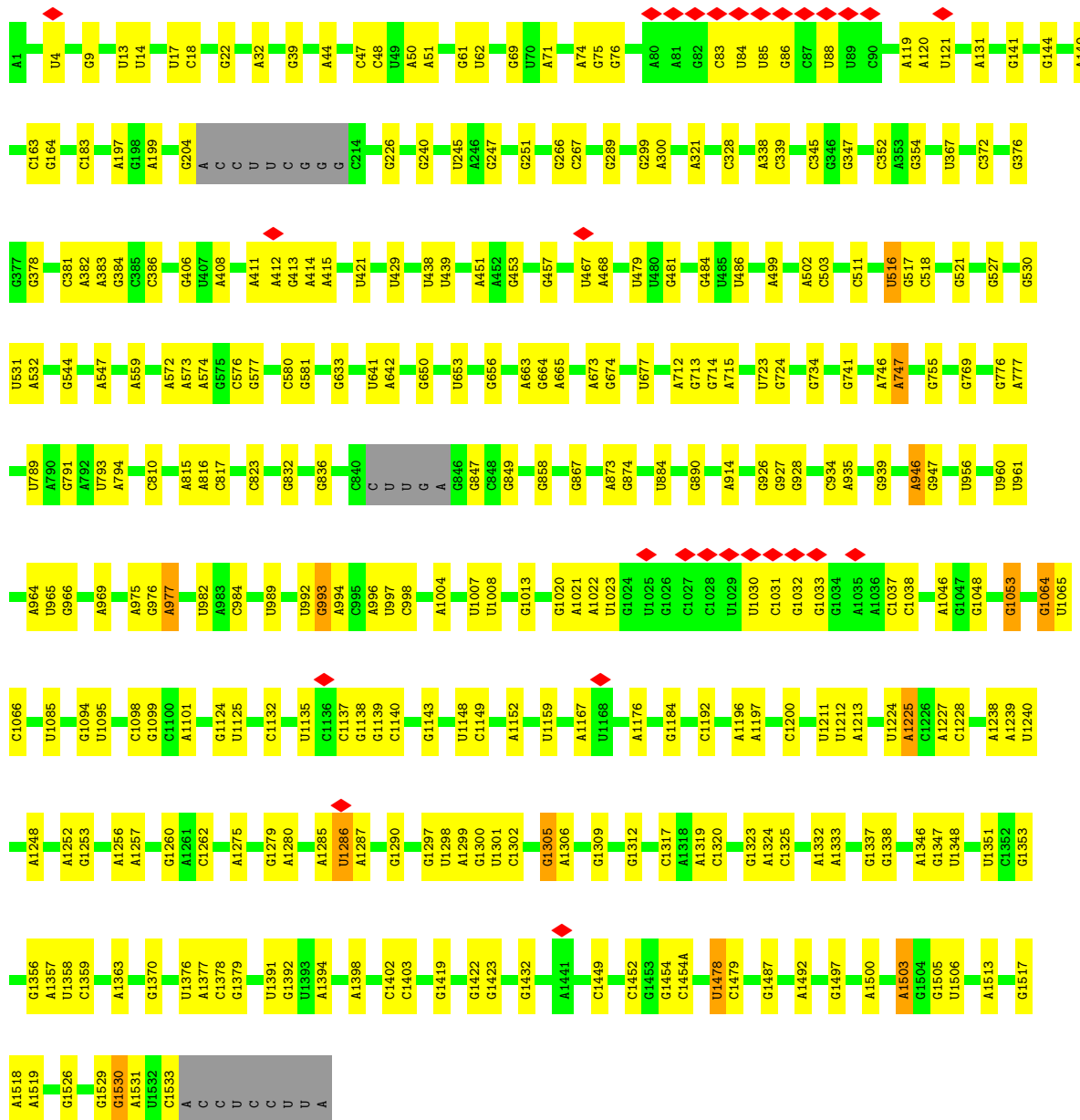
- Molecule 13: Large ribosomal subunit protein bL32

Chain z:  91% 7%



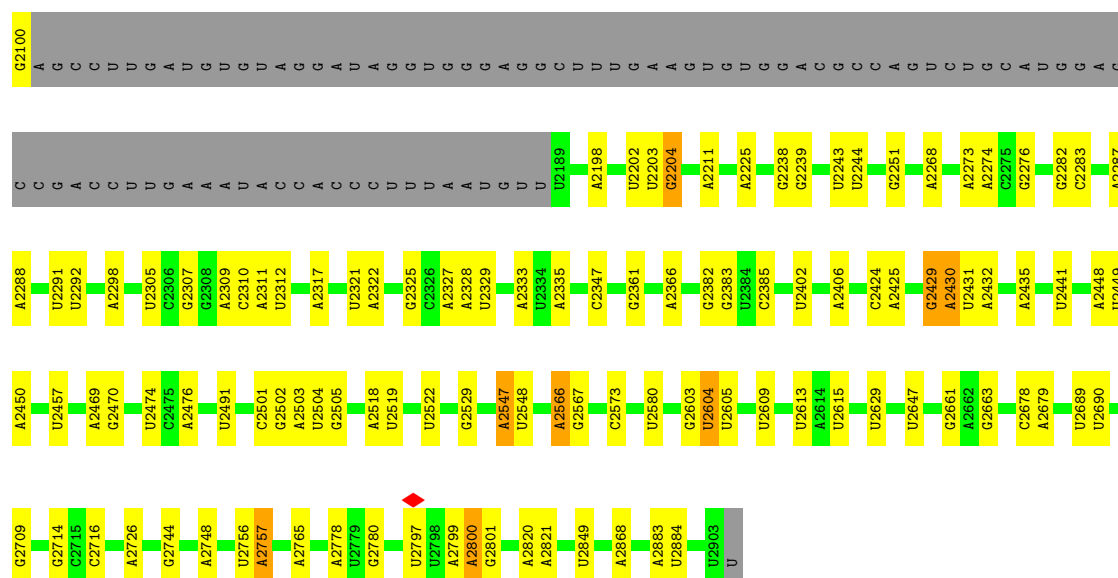
- Molecule 14: 16S rRNA

Chain A:  78% 20%



- Molecule 15: A/P-site Val-tRNA^{Val}

Chain Y:  66% 28% 5%



• Molecule 18: Large ribosomal subunit protein bL33

Chain 0: 93% 7%



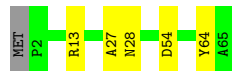
• Molecule 19: Large ribosomal subunit protein bL34

Chain 1: 98%



• Molecule 20: Large ribosomal subunit protein bL35

Chain 2: 91% 8%



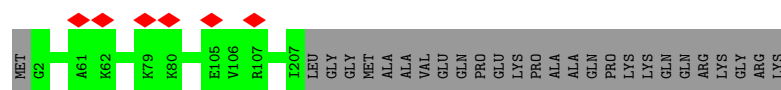
• Molecule 21: Small ribosomal subunit protein uS2

Chain B: 6% 90% 7%

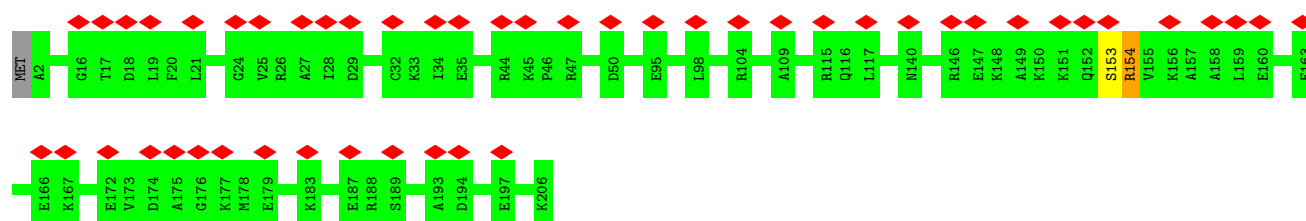


• Molecule 22: Small ribosomal subunit protein uS3

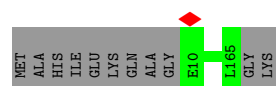
Chain C: 88% 12%



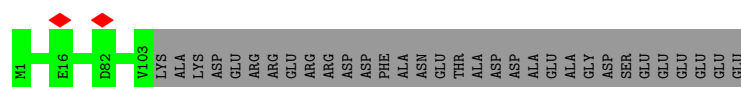
- Molecule 23: Small ribosomal subunit protein uS4



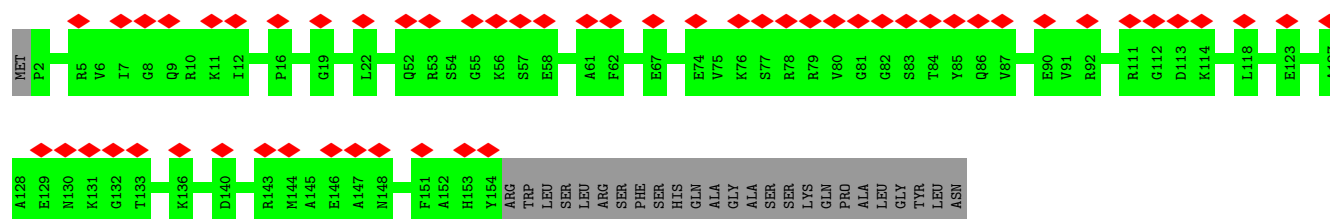
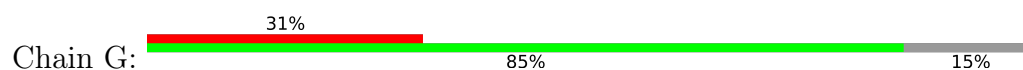
- Molecule 24: Small ribosomal subunit protein uS5



- Molecule 25: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 26: Small ribosomal subunit protein uS7

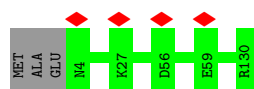


- Molecule 27: Small ribosomal subunit protein uS8



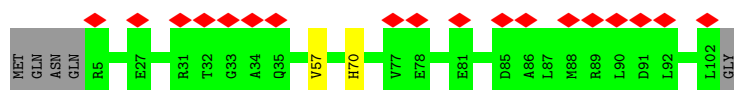
- Molecule 28: Small ribosomal subunit protein uS9

Chain I:  98%



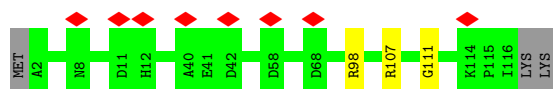
- Molecule 29: Small ribosomal subunit protein uS10

Chain J:  17% 93% 5%



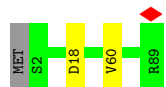
- Molecule 30: Small ribosomal subunit protein uS13

Chain M:  7% 95%



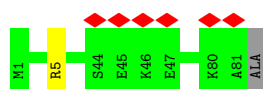
- Molecule 31: Small ribosomal subunit protein uS15

Chain O:  97%



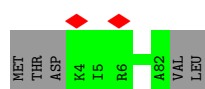
- Molecule 32: Small ribosomal subunit protein bS16

Chain P:  7% 98%




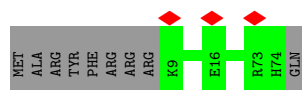
- Molecule 33: Small ribosomal subunit protein uS17

Chain Q:  94% 6%




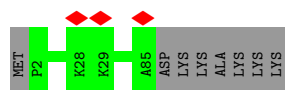
- Molecule 34: Small ribosomal subunit protein bS18

Chain R:  88% 12%



- Molecule 35: Small ribosomal subunit protein uS19

Chain S:  91% 9%



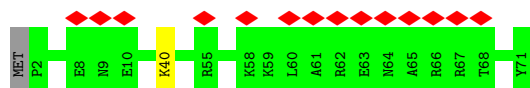
- Molecule 36: Small ribosomal subunit protein bS20

Chain T:  6% 94% 5%



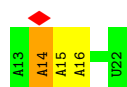
- Molecule 37: Small ribosomal subunit protein bS21

Chain U:  20% 97%



- Molecule 38: mRNA

Chain X:  10% 70% 20% 10%



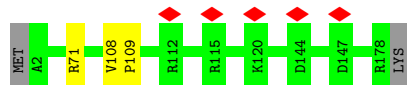
- Molecule 39: Large ribosomal subunit protein uL4

Chain e:  97%



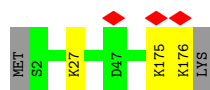
- Molecule 40: Large ribosomal subunit protein uL5

Chain f:  97%

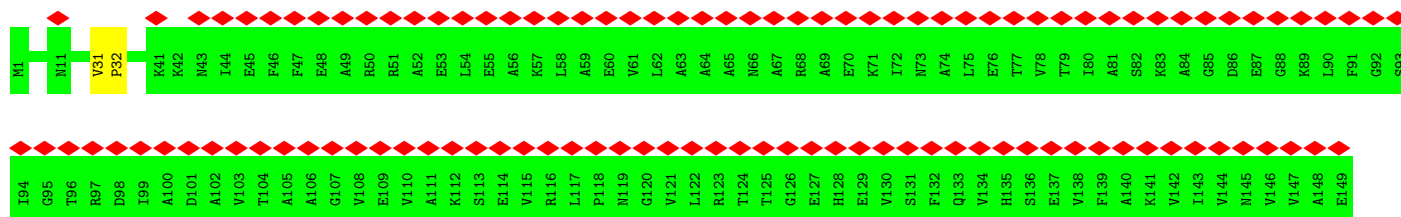
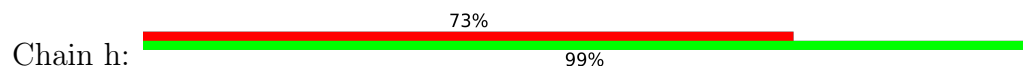


- Molecule 41: Large ribosomal subunit protein uL6

Chain g:  97%



- Molecule 42: Large ribosomal subunit protein bL9



- Molecule 43: Large ribosomal subunit protein uL13



- Molecule 44: Large ribosomal subunit protein uL14



- Molecule 45: Large ribosomal subunit protein uL18



- Molecule 46: Large ribosomal subunit protein bL19



- Molecule 47: Large ribosomal subunit protein bL20




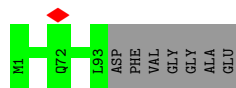
- Molecule 48: Large ribosomal subunit protein bL21

Chain q:  96%



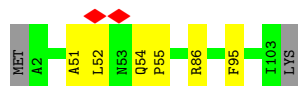
- Molecule 49: Large ribosomal subunit protein uL23

Chain s:  93%



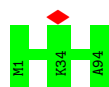
- Molecule 50: Large ribosomal subunit protein uL24

Chain t:  92%




- Molecule 51: Large ribosomal subunit protein bL25

Chain u:  100%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  84%



- 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	75660	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	0.599	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0484	Depositor
Map size (Å)	436.896, 436.896, 436.896	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MS6, PSU, 2MA, 6MZ, IAS, D2T, 5MU, K, OMU, MA6, H2U, 3TD, ZN, MG, OMG, UR3, OMC, MEQ, 4D4, 5MC, 1MG, 4SU, 4OC, G7M, 2MG, SCM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3	0.48	0/303	0.84	0/397
2	4	0.48	0/371	0.82	0/496
3	K	0.50	0/884	0.85	0/1191
4	L	0.47	0/960	0.84	0/1286
5	N	0.46	0/817	0.91	0/1088
6	b	0.51	0/2850	0.82	0/4444
7	c	0.48	0/2121	0.85	0/2852
8	d	0.45	0/1576	0.80	0/2119
9	k	0.47	0/1062	0.84	0/1413
10	l	0.46	0/1073	0.84	0/1433
11	m	0.46	0/958	0.90	0/1281
12	r	0.46	0/864	0.85	0/1156
13	z	0.47	0/450	0.88	0/599
14	A	0.51	0/36284	0.81	2/56595 (0.0%)
15	Y	0.57	0/1596	0.80	0/2478
16	Z	0.55	0/1608	0.81	1/2500 (0.0%)
17	a	0.49	1/65747 (0.0%)	0.85	10/102563 (0.0%)
18	0	0.45	0/424	0.82	0/565
19	1	0.46	0/380	0.93	0/498
20	2	0.49	0/513	0.88	0/676
21	B	0.45	0/1784	0.91	0/2403
22	C	0.46	0/1651	0.85	0/2225
23	D	0.44	0/1665	0.90	0/2227
24	E	0.46	0/1165	0.83	0/1568
25	F	0.45	0/858	0.85	0/1160
26	G	0.47	0/1219	0.93	0/1635
27	H	0.46	0/989	0.86	0/1326
28	I	0.45	0/1034	0.90	0/1375
29	J	0.46	0/796	0.86	0/1077
30	M	0.48	0/900	0.93	0/1204
31	O	0.43	0/722	0.96	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	P	0.45	0/653	0.85	0/877
33	Q	0.45	0/650	0.82	0/871
34	R	0.44	0/553	0.91	0/742
35	S	0.49	0/685	0.84	0/922
36	T	0.46	0/676	0.99	0/895
37	U	0.46	0/598	0.97	0/792
38	X	0.54	0/242	0.84	0/375
39	e	0.45	0/1571	0.86	0/2113
40	f	0.45	0/1434	0.89	0/1926
41	g	0.47	0/1333	0.84	0/1805
42	h	0.46	0/1122	0.83	0/1515
43	i	0.45	0/1152	0.85	0/1551
44	j	0.45	0/956	0.83	0/1279
45	n	0.46	0/902	0.89	0/1209
46	o	0.45	0/929	0.78	0/1242
47	p	0.45	0/960	0.92	0/1278
48	q	0.45	0/829	0.74	0/1107
49	s	0.44	0/744	0.78	0/994
50	t	0.46	0/787	0.79	0/1051
51	u	0.45	0/766	0.82	0/1025
52	v	0.47	0/582	0.81	0/769
53	w	0.46	0/635	0.87	0/848
54	x	0.41	0/496	0.92	0/660
55	y	0.45	0/453	0.86	0/605
All	All	0.49	1/153332 (0.0%)	0.84	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
20	2	0	1
47	p	0	1
52	v	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	2069	G7M	O3'-P	5.27	1.61	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	2429	G	O3'-P-O5'	-8.51	91.23	104.00
17	a	1971	U	O3'-P-O5'	-7.13	93.30	104.00
17	a	204	A	O3'-P-O5'	-6.82	93.77	104.00
17	a	2519	U	O3'-P-O5'	-6.13	94.80	104.00
17	a	781	A	O3'-P-O5'	-5.84	95.24	104.00
14	A	1478	U	C2'-C3'-O3'	5.79	122.39	113.70
16	Z	37	A	O3'-P-O5'	-5.70	95.45	104.00
17	a	2050	C	O3'-P-O5'	-5.37	95.95	104.00
17	a	763	G	O3'-P-O5'	-5.32	96.02	104.00
17	a	2501	C	O3'-P-O5'	-5.27	96.09	104.00
17	a	1025	G	O3'-P-O5'	5.24	111.86	104.00
14	A	1359	C	O3'-P-O5'	-5.20	96.20	104.00
17	a	2382	G	O3'-P-O5'	-5.03	96.46	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	2	13	ARG	Sidechain
47	p	13	ARG	Sidechain
52	v	25	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	N	805	0	844	1	0
6	b	2549	0	1291	2	0
7	c	2082	0	2153	8	0
8	d	1566	0	1618	7	0
9	k	1053	0	1129	3	0
10	l	1075	0	1145	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	945	0	989	1	0
12	r	857	0	922	1	0
13	z	444	0	458	3	0
14	A	32655	0	16453	50	0
15	Y	1539	0	791	2	0
16	Z	1546	0	794	3	0
17	a	59216	0	29790	101	0
18	0	417	0	451	0	0
19	1	377	0	418	1	0
20	2	504	0	572	3	0
21	B	1753	0	1780	4	0
22	C	1624	0	1696	0	0
23	D	1643	0	1707	1	0
24	E	1152	0	1196	0	0
25	F	839	0	833	0	0
26	G	1203	0	1254	0	0
27	H	979	0	1031	1	0
28	I	1022	0	1070	0	0
29	J	786	0	828	1	0
30	M	891	0	952	2	0
31	O	714	0	734	1	0
32	P	643	0	661	1	0
33	Q	641	0	682	0	0
34	R	544	0	565	0	0
35	S	668	0	693	0	0
36	T	670	0	719	2	0
37	U	590	0	629	1	0
38	X	216	0	108	1	0
39	e	1552	0	1619	3	0
40	f	1410	0	1444	3	0
41	g	1313	0	1358	1	0
42	h	1111	0	1148	1	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	1	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	w	625	0	652	0	0
54	x	495	0	526	0	0
55	y	449	0	488	0	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	49	0	0	0	0
57	a	217	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	8	0	0	0	0
58	a	56	0	0	0	0
58	c	1	0	0	0	0
59	A	23	0	24	3	0
60	Y	7	0	8	0	0
61	0	9	0	0	0	0
61	1	23	0	0	0	0
61	2	22	0	0	0	0
61	3	11	0	0	0	0
61	4	2	0	0	0	0
61	A	1554	0	0	0	0
61	B	22	0	0	0	0
61	C	21	0	0	0	0
61	D	14	0	0	0	0
61	E	17	0	0	0	0
61	F	3	0	0	0	0
61	G	12	0	0	0	0
61	H	27	0	0	0	0
61	I	13	0	0	0	0
61	J	16	0	0	0	0
61	K	18	0	0	0	0
61	L	11	0	0	0	0
61	M	11	0	0	0	0
61	N	5	0	0	0	0
61	O	16	0	0	0	0
61	P	10	0	0	0	0
61	Q	9	0	0	0	0
61	R	3	0	0	0	0
61	S	3	0	0	0	0
61	T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	U	16	0	0	0	0
61	X	9	0	0	0	0
61	Y	17	0	0	0	0
61	Z	36	0	0	0	0
61	a	4613	0	0	11	0
61	b	131	0	0	0	0
61	c	123	0	0	1	0
61	d	67	0	0	0	0
61	e	75	0	0	0	0
61	f	11	0	0	0	0
61	g	15	0	0	0	0
61	h	8	0	0	0	0
61	i	33	0	0	0	0
61	j	33	0	0	0	0
61	k	48	0	0	1	0
61	l	46	0	0	1	0
61	m	23	0	0	0	0
61	n	18	0	0	0	0
61	o	28	0	0	0	0
61	p	44	0	0	0	0
61	q	37	0	0	1	0
61	r	37	0	0	0	0
61	s	21	0	0	0	0
61	t	20	0	0	0	0
61	u	10	0	0	0	0
61	v	22	0	0	0	0
61	w	25	0	0	0	0
61	x	7	0	0	0	0
61	y	19	0	0	0	0
61	z	32	0	0	0	0
All	All	150006	0	95764	201	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 (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:664:G:H22	14:A:741:G:H1	1.39	0.71
17:a:568:U:H1'	17:a:2030:6MZ:H9C1	1.75	0.69
17:a:12:U:H2'	17:a:12:U:O2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:1508:A:O2'	17:a:1509:A:O4'	2.13	0.64
7:c:271:ARG:O	7:c:272:SER:C	2.44	0.60
17:a:1434:A:H2'	17:a:1435:G:C8	2.37	0.60
13:z:9:THR:CG2	17:a:2020:A:H5'	2.32	0.59
7:c:39:LYS:NZ	61:c:401:HOH:O	2.31	0.59
17:a:1434:A:H2'	17:a:1435:G:H8	1.69	0.58
14:A:823:C:HO2'	27:H:2:SER:N	2.02	0.58
14:A:964:A:H5'	14:A:965:U:OP2	2.03	0.58
17:a:2780:G:OP2	43:i:120:ARG:HD3	2.04	0.58
14:A:928:G:O2'	14:A:1533:C:OP1	2.22	0.58
48:q:71:LYS:NZ	61:q:201:HOH:O	2.37	0.57
14:A:1064:G:N7	59:A:1602:SCM:O11	2.34	0.57
17:a:2547:A:H2'	17:a:2548:U:C6	2.40	0.57
23:D:153:SER:O	23:D:154:ARG:C	2.48	0.57
17:a:1115:G:O2'	17:a:1116:G:O5'	2.21	0.56
17:a:983:A:OP1	61:a:3303:HOH:O	2.18	0.56
6:b:89:U:C2	17:a:958:U:H2'	2.41	0.55
14:A:1391:U:H2'	14:A:1392:G:C8	2.41	0.55
50:t:54:GLN:N	50:t:55:PRO:CD	2.70	0.55
9:k:57:LEU:HD22	20:2:54:ASP:HB3	1.88	0.54
17:a:12:U:O2	17:a:12:U:C2'	2.56	0.53
17:a:1182:G:H2'	17:a:1183:U:O4'	2.09	0.53
14:A:1286:U:O2	14:A:1286:U:O4'	2.28	0.52
17:a:1932:A:H2'	17:a:1933:G:O4'	2.10	0.52
17:a:1939:5MU:OP1	17:a:2604:PSU:O2'	2.26	0.52
44:j:1:MET:HE3	44:j:32:TYR:CZ	2.45	0.52
17:a:1427:A:OP1	61:a:3302:HOH:O	2.18	0.52
14:A:677:U:H3	14:A:713:G:H22	1.57	0.52
9:k:21:ARG:HA	17:a:811:U:H2'	1.92	0.51
17:a:493:G:H2'	17:a:494:G:O4'	2.12	0.50
17:a:2756:U:H1'	17:a:2757:A:H5''	1.94	0.50
16:Z:75:C:O4'	17:a:2432:A:H1'	2.11	0.50
17:a:84:A:N1	17:a:98:G:O2'	2.41	0.50
14:A:1225:A:H2'	14:A:1225:A:N3	2.27	0.50
14:A:1066:C:O2	59:A:1602:SCM:N10	2.43	0.49
10:l:55:ARG:CD	17:a:2469:A:H4'	2.42	0.49
17:a:1607:C:N4	17:a:1622:G:OP2	2.33	0.49
15:Y:37:6MZ:O2'	17:a:1913:A:N1	2.42	0.49
8:d:140:HIS:CD2	61:a:3902:HOH:O	2.65	0.49
17:a:811:U:H5'	61:a:3344:HOH:O	2.13	0.49
14:A:673:A:H2'	14:A:674:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:q:74:ILE:N	48:q:74:ILE:HD12	2.28	0.48
17:a:2328:A:H2'	17:a:2329:U:C6	2.48	0.48
8:d:156:PHE:CE1	43:i:81:ILE:HD13	2.49	0.48
14:A:977:A:H1'	14:A:982:U:O4	2.14	0.48
17:a:1296:G:OP1	17:a:2709:G:O2'	2.29	0.48
8:d:208:LYS:O	8:d:209:ALA:C	2.57	0.48
17:a:1508:A:HO2'	17:a:1509:A:C4'	2.24	0.48
17:a:644:A:H2'	17:a:645:C:O4'	2.13	0.47
9:k:39:LYS:HG3	61:k:201:HOH:O	2.14	0.47
14:A:1053:G:N7	14:A:1200:C:H5''	2.30	0.47
7:c:207:LYS:HB2	17:a:729:G:C6	2.50	0.47
17:a:1906:G:H2'	17:a:1907:G:O4'	2.14	0.47
40:f:108:VAL:HG12	40:f:109:PRO:HD3	1.96	0.47
40:f:108:VAL:N	40:f:109:PRO:CD	2.77	0.47
10:l:76:LYS:HE2	61:l:202:HOH:O	2.14	0.47
17:a:645:C:H2'	17:a:647:G:C8	2.50	0.47
17:a:2273:A:H2'	17:a:2274:A:C8	2.49	0.47
52:v:25:ARG:NH2	52:v:31:VAL:HG12	2.30	0.47
14:A:502:A:H2'	14:A:503:C:O4'	2.14	0.46
14:A:1305:G:O2'	14:A:1306:A:H8	1.98	0.46
17:a:653:U:O2	17:a:653:U:O4'	2.33	0.46
17:a:2243:U:H2'	17:a:2244:U:C6	2.50	0.46
17:a:586:A:N1	17:a:809:G:O2'	2.47	0.46
14:A:376:G:H5''	32:P:5:ARG:HB2	1.97	0.46
10:l:53:MET:HE1	10:l:103:TYR:CG	2.51	0.46
17:a:747:5MU:O2	17:a:2014:A:H1'	2.15	0.46
17:a:1754:A:C8	46:o:94:LYS:HE3	2.50	0.46
21:B:94:HIS:O	21:B:95:ARG:C	2.56	0.46
14:A:17:U:H2'	14:A:18:C:C6	2.50	0.46
50:t:54:GLN:N	50:t:55:PRO:HD2	2.30	0.46
17:a:1028:A:N6	17:a:1125:G:H2'	2.31	0.46
17:a:1378:A:O2'	17:a:1380:G:N7	2.48	0.46
17:a:2799:A:O2'	17:a:2800:A:O5'	2.27	0.46
41:g:175:LYS:O	41:g:176:LYS:C	2.58	0.46
14:A:516:PSU:C2	14:A:517:G:C6	3.04	0.46
14:A:789:U:O2'	14:A:791:G:N7	2.48	0.46
14:A:1402:4OC:O2	14:A:1500:A:N1	2.49	0.46
14:A:1526:G:N7	37:U:40:LYS:NZ	2.63	0.46
7:c:180:GLU:OE2	17:a:1799:G:O2'	2.30	0.46
8:d:121:THR:HB	8:d:127:PHE:CD2	2.51	0.46
17:a:788:A:OP1	17:a:790:U:H5	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:1778:U:H2'	17:a:1784:A:N6	2.31	0.46
14:A:946:A:H2'	14:A:947:G:C8	2.51	0.46
21:B:164:ILE:O	21:B:186:ILE:HB	2.16	0.45
8:d:62:LYS:N	8:d:63:PRO:HD2	2.30	0.45
17:a:810:U:H5''	61:a:3344:HOH:O	2.16	0.45
14:A:769:G:H4'	14:A:1513:A:H4'	1.97	0.45
14:A:927:G:O2'	14:A:1503:A:N7	2.42	0.45
17:a:476:G:H4'	17:a:502:A:N1	2.32	0.45
17:a:2327:A:H2'	17:a:2328:A:C8	2.52	0.45
7:c:138:GLY:HA3	14:A:712:A:H5'	1.99	0.45
7:c:242:LYS:HE2	61:a:6706:HOH:O	2.17	0.45
13:z:4:GLN:HA	17:a:2615:U:C2	2.52	0.45
17:a:2038:G:H2'	17:a:2039:U:O4'	2.17	0.45
10:l:53:MET:HE1	10:l:103:TYR:CD1	2.52	0.45
14:A:1309:G:N7	30:M:98:ARG:NH1	2.65	0.45
17:a:58:G:O2'	17:a:73:A:N1	2.50	0.44
20:2:27:ALA:O	20:2:28:ASN:HB2	2.16	0.44
21:B:28:LYS:N	21:B:29:PRO:CD	2.81	0.44
52:v:38:VAL:HG12	52:v:59:LEU:HB2	1.99	0.44
14:A:1323:G:H2'	14:A:1324:A:C8	2.51	0.44
17:a:1020:A:C2	17:a:1141:U:C2	3.06	0.44
17:a:1754:A:C8	46:o:94:LYS:CE	3.00	0.44
47:p:76:TYR:CZ	47:p:80:ILE:HG13	2.52	0.44
14:A:299:G:H2'	14:A:300:A:C8	2.52	0.44
14:A:663:A:H5'	14:A:836:G:OP1	2.17	0.44
14:A:1403:C:O5'	14:A:1403:C:H6	2.00	0.44
17:a:715:A:C8	31:O:60:VAL:HG11	2.53	0.44
17:a:2202:U:O2'	17:a:2204:G:OP1	2.29	0.44
17:a:642:U:O2'	17:a:644:A:N7	2.47	0.44
16:Z:8:4SU:H5'	16:Z:8:4SU:C6	2.48	0.44
17:a:2063:C:O2	17:a:2450:A:N1	2.50	0.44
10:l:66:ARG:NH2	10:l:104:GLU:OE2	2.51	0.43
14:A:502:A:C2	14:A:544:G:C2	3.06	0.43
14:A:993:G:H2'	14:A:993:G:N3	2.31	0.43
14:A:1530:G:H2'	14:A:1531:A:C8	2.53	0.43
21:B:130:THR:O	21:B:132:LYS:N	2.49	0.43
14:A:867:G:O2'	14:A:873:A:N1	2.49	0.43
17:a:242:G:H5''	20:2:64:TYR:CE2	2.54	0.43
17:a:2276:G:H3'	61:a:7314:HOH:O	2.18	0.43
17:a:2849:U:H4'	17:a:2868:A:C2	2.53	0.43
7:c:29:PRO:HG2	7:c:34:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:1730:C:O2	17:a:1730:C:O4'	2.36	0.43
17:a:2291:U:H2'	17:a:2292:U:C6	2.53	0.43
17:a:1405:U:H2'	17:a:1406:U:C6	2.54	0.43
17:a:1853:A:N1	17:a:2087:G:H1'	2.32	0.43
36:T:48:GLN:O	36:T:52:ASN:ND2	2.52	0.43
17:a:819:A:C4	17:a:1189:A:C2	3.07	0.43
14:A:381:C:H2'	14:A:382:A:O4'	2.19	0.43
17:a:2065:C:H4'	17:a:2251:OMG:HM22	2.01	0.43
17:a:1607:C:H4'	17:a:1608:A:O5'	2.19	0.43
38:X:14:A:H2'	38:X:14:A:N3	2.33	0.43
14:A:746:A:H2'	14:A:747:A:C8	2.54	0.42
16:Z:3:C:O2'	17:a:1851:U:OP1	2.36	0.42
17:a:126:A:OP1	19:1:45:SER:OG	2.32	0.42
17:a:2099:U:H2'	17:a:2100:G:C8	2.55	0.42
11:m:18:GLN:NE2	17:a:2709:G:OP1	2.52	0.42
17:a:1021:A:N3	17:a:1021:A:H3'	2.34	0.42
39:e:41:GLN:HG2	39:e:43:THR:HG23	2.01	0.42
17:a:2298:A:OP1	40:f:71:ARG:NH2	2.49	0.42
17:a:1585:C:H2'	17:a:1586:A:O4'	2.20	0.42
17:a:2014:A:H2'	17:a:2015:A:C8	2.55	0.42
17:a:2522:U:O2'	17:a:2647:U:OP1	2.35	0.42
17:a:577:G:H5''	61:a:6688:HOH:O	2.20	0.42
8:d:135:GLY:HA2	17:a:743:A:OP1	2.20	0.42
39:e:49:ARG:O	39:e:74:LYS:HD3	2.20	0.42
17:a:639:U:H2'	17:a:640:C:C6	2.55	0.41
17:a:1914:C:H2'	17:a:1915:3TD:O4'	2.19	0.41
17:a:2678:C:H2'	17:a:2679:A:O4'	2.20	0.41
15:Y:18:G:HO2'	15:Y:57:G:H22	1.68	0.41
14:A:1423:G:C8	14:A:1423:G:H5''	2.55	0.41
17:a:576:U:H5''	61:a:3352:HOH:O	2.19	0.41
17:a:857:G:H2'	17:a:858:G:O4'	2.21	0.41
42:h:31:VAL:N	42:h:32:PRO:HD2	2.36	0.41
17:a:247:G:H4'	17:a:386:G:C5	2.56	0.41
14:A:816:A:OP1	14:A:1526:G:O2'	2.35	0.41
14:A:1356:G:H2'	14:A:1357:A:C8	2.54	0.41
17:a:2566:A:N1	44:j:28:SER:OG	2.51	0.41
17:a:588:U:H2'	17:a:589:U:C6	2.55	0.41
17:a:1180:U:H2'	17:a:1181:U:O4'	2.20	0.41
14:A:1394:A:N1	14:A:1500:A:O2'	2.50	0.41
17:a:1450:G:C6	17:a:1451:C:N4	2.89	0.41
36:T:55:GLN:N	36:T:56:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:580:C:H2'	14:A:581:G:O4'	2.21	0.41
17:a:1657:U:H5''	61:a:3902:HOH:O	2.21	0.41
7:c:221:ARG:HD2	17:a:1827:U:OP2	2.20	0.41
14:A:1098:C:H2'	14:A:1099:G:O4'	2.21	0.41
14:A:1152:A:OP1	29:J:70:HIS:ND1	2.54	0.41
17:a:223:A:N1	17:a:407:G:O2'	2.49	0.41
17:a:1149:G:H2'	17:a:1150:C:C6	2.56	0.41
17:a:1266:G:O2'	17:a:2012:G:O6	2.31	0.41
8:d:35:THR:HG22	8:d:73:VAL:HG21	2.03	0.41
12:r:4:ILE:HG12	12:r:106:VAL:HG22	2.03	0.41
14:A:1192:C:N3	59:A:1602:SCM:O5	2.43	0.41
17:a:1338:G:O2'	17:a:1393:A:N1	2.41	0.41
17:a:2040:G:H2'	17:a:2041:U:O4'	2.20	0.41
5:N:73:PHE:CZ	5:N:78:GLY:HA2	2.56	0.40
14:A:378:G:C2	14:A:386:C:O2	2.74	0.40
17:a:2430:A:H2'	17:a:2430:A:N3	2.36	0.40
14:A:61:G:H2'	14:A:62:U:O4'	2.20	0.40
17:a:478:A:N1	17:a:500:G:H4'	2.36	0.40
17:a:984:A:H2'	17:a:984:A:N3	2.36	0.40
50:t:86:ARG:HG3	50:t:95:PHE:CE1	2.57	0.40
17:a:1205:A:C6	39:e:165:HIS:HB2	2.56	0.40
30:M:107:ARG:O	30:M:111:GLY:N	2.53	0.40
43:i:125:TYR:OH	43:i:132:HIS:NE2	2.34	0.40
1:3:16:ILE:HD13	1:3:25:VAL:HG22	2.03	0.40
6:b:106:G:H2'	6:b:107:G:O4'	2.22	0.40
13:z:43:ILE:HG22	13:z:49:TYR:HB2	2.02	0.40
14:A:714:G:H2'	14:A:715:A:C8	2.56	0.40
14:A:1148:U:H2'	14:A:1149:C:O4'	2.21	0.40
14:A:1376:U:H2'	14:A:1377:A:C8	2.56	0.40
17:a:1223:G:C6	17:a:1227:G:C6	3.10	0.40
14:A:338:A:OP2	44:j:98:ARG:NH2	2.51	0.40
17:a:581:C:H5''	61:a:3491:HOH:O	2.22	0.40
17:a:620:G:H5'	17:a:620:G:N3	2.36	0.40
48:q:5:PHE:HB3	48:q:59:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	36/38 (95%)	36 (100%)	0	0	100	100
2	4	45/70 (64%)	40 (89%)	3 (7%)	2 (4%)	2	0
3	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
4	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
5	N	98/101 (97%)	98 (100%)	0	0	100	100
7	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
8	d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
9	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
10	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
11	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
12	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
13	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
18	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
19	1	44/46 (96%)	44 (100%)	0	0	100	100
20	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
21	B	222/241 (92%)	214 (96%)	8 (4%)	0	100	100
22	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
23	D	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	24	17
24	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
25	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
26	G	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
27	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
28	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
29	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	5
30	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
32	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
33	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
34	R	64/75 (85%)	64 (100%)	0	0	100	100
35	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
36	T	84/87 (97%)	84 (100%)	0	0	100	100
37	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
39	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
40	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
41	g	173/177 (98%)	164 (95%)	9 (5%)	0	100	100
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%)	113 (99%)	1 (1%)	0	100	100
46	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
47	p	115/118 (98%)	115 (100%)	0	0	100	100
48	q	101/103 (98%)	101 (100%)	0	0	100	100
49	s	91/100 (91%)	91 (100%)	0	0	100	100
50	t	100/104 (96%)	95 (95%)	4 (4%)	1 (1%)	12	5
51	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
54	x	59/63 (94%)	59 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
All	All	5573/5913 (94%)	5391 (97%)	177 (3%)	5 (0%)	49	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	40	CYS
23	D	154	ARG
29	J	57	VAL
50	t	51	ALA
2	4	4	ASP

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
2	4	43/62 (69%)	43 (100%)	0	100	100
3	K	89/98 (91%)	89 (100%)	0	100	100
4	L	102/103 (99%)	102 (100%)	0	100	100
5	N	83/84 (99%)	83 (100%)	0	100	100
7	c	216/218 (99%)	216 (100%)	0	100	100
8	d	163/163 (100%)	163 (100%)	0	100	100
9	k	103/103 (100%)	103 (100%)	0	100	100
10	l	107/107 (100%)	107 (100%)	0	100	100
11	m	98/103 (95%)	98 (100%)	0	100	100
12	r	93/93 (100%)	93 (100%)	0	100	100
13	z	47/48 (98%)	47 (100%)	0	100	100
18	0	46/49 (94%)	46 (100%)	0	100	100
19	1	38/38 (100%)	38 (100%)	0	100	100
20	2	51/52 (98%)	51 (100%)	0	100	100
21	B	186/199 (94%)	186 (100%)	0	100	100
22	C	170/190 (90%)	170 (100%)	0	100	100
23	D	172/173 (99%)	172 (100%)	0	100	100
24	E	119/126 (94%)	119 (100%)	0	100	100
25	F	90/116 (78%)	90 (100%)	0	100	100
26	G	126/147 (86%)	126 (100%)	0	100	100
27	H	104/105 (99%)	104 (100%)	0	100	100
28	I	105/107 (98%)	105 (100%)	0	100	100
29	J	86/90 (96%)	86 (100%)	0	100	100
30	M	93/96 (97%)	93 (100%)	0	100	100
31	O	76/77 (99%)	75 (99%)	1 (1%)	61	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	P	65/65 (100%)	65 (100%)	0	100	100
33	Q	73/78 (94%)	73 (100%)	0	100	100
34	R	57/65 (88%)	57 (100%)	0	100	100
35	S	72/79 (91%)	72 (100%)	0	100	100
36	T	65/66 (98%)	65 (100%)	0	100	100
37	U	60/61 (98%)	60 (100%)	0	100	100
39	e	165/165 (100%)	164 (99%)	1 (1%)	78	82
40	f	148/150 (99%)	148 (100%)	0	100	100
41	g	136/138 (99%)	135 (99%)	1 (1%)	76	79
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%)	82 (99%)	1 (1%)	63	65
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%)	4636 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	O	18	ASP
39	e	88	ARG
41	g	27	LYS
50	t	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50)

such sidechains are listed below:

Mol	Chain	Res	Type
4	L	75	GLN
7	c	60	GLN
10	l	97	GLN
11	m	9	GLN
11	m	31	HIS
11	m	73	ASN
12	r	9	HIS
12	r	40	ASN
13	z	6	ASN
21	B	58	ASN
23	D	54	GLN
23	D	89	ASN
23	D	126	ASN
23	D	196	ASN
23	D	198	HIS
24	E	82	GLN
24	E	121	HIS
24	E	132	ASN
24	E	148	ASN
26	G	68	ASN
26	G	130	ASN
27	H	4	GLN
27	H	21	ASN
28	I	25	ASN
28	I	110	GLN
30	M	8	ASN
32	P	59	HIS
35	S	14	HIS
36	T	48	GLN
36	T	52	ASN
37	U	64	ASN
39	e	165	HIS
41	g	22	GLN
41	g	73	ASN
42	h	66	ASN
42	h	145	ASN
43	i	47	HIS
43	i	80	HIS
43	i	128	ASN
44	j	3	GLN
45	n	29	HIS
46	o	10	GLN

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Mol	Chain	Res	Type
46	o	66	ASN
50	t	53	ASN
53	w	36	HIS
54	x	25	GLN
54	x	27	ASN
54	x	38	GLN
54	x	39	GLN
54	x	58	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	A	1518/1544 (98%)	232 (15%)	27 (1%)
15	Y	68/76 (89%)	17 (25%)	3 (4%)
16	Z	69/78 (88%)	15 (21%)	3 (4%)
17	a	2753/2904 (94%)	295 (10%)	0
38	X	9/10 (90%)	3 (33%)	0
6	b	118/120 (98%)	10 (8%)	0
All	All	4535/4732 (95%)	572 (12%)	33 (0%)

All (572) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
14	A	47	C
14	A	48	C
14	A	50	A
14	A	51	A
14	A	69	G
14	A	71	A
14	A	74	A
14	A	75	G
14	A	76	G
14	A	83	C
14	A	84	U
14	A	85	U
14	A	86	G
14	A	88	U
14	A	119	A
14	A	120	A
14	A	121	U
14	A	131	A
14	A	141	G
14	A	144	G
14	A	149	A
14	A	163	C
14	A	164	G
14	A	183	C
14	A	197	A
14	A	204	G
14	A	226	G
14	A	240	G
14	A	245	U
14	A	247	G
14	A	251	G
14	A	266	G
14	A	267	C
14	A	289	G
14	A	321	A
14	A	328	C
14	A	339	C
14	A	345	C
14	A	347	G
14	A	352	C
14	A	354	G
14	A	367	U

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Mol	Chain	Res	Type
14	A	372	C
14	A	383	A
14	A	384	G
14	A	406	G
14	A	408	A
14	A	411	A
14	A	412	A
14	A	413	G
14	A	414	A
14	A	415	A
14	A	429	U
14	A	438	U
14	A	439	U
14	A	451	A
14	A	453	G
14	A	457	G
14	A	467	U
14	A	468	A
14	A	479	U
14	A	481	G
14	A	484	G
14	A	486	U
14	A	499	A
14	A	511	C
14	A	518	C
14	A	521	G
14	A	530	G
14	A	531	U
14	A	532	A
14	A	547	A
14	A	559	A
14	A	572	A
14	A	573	A
14	A	576	C
14	A	577	G
14	A	633	G
14	A	642	A
14	A	650	G
14	A	653	U
14	A	656	G
14	A	665	A
14	A	723	U

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Mol	Chain	Res	Type
14	A	724	G
14	A	734	G
14	A	747	A
14	A	755	G
14	A	777	A
14	A	793	U
14	A	794	A
14	A	810	C
14	A	815	A
14	A	817	C
14	A	832	G
14	A	847	G
14	A	849	G
14	A	874	G
14	A	890	G
14	A	914	A
14	A	926	G
14	A	934	C
14	A	935	A
14	A	939	G
14	A	946	A
14	A	956	U
14	A	960	U
14	A	961	U
14	A	966	2MG
14	A	969	A
14	A	975	A
14	A	976	G
14	A	977	A
14	A	984	C
14	A	989	U
14	A	992	U
14	A	993	G
14	A	994	A
14	A	996	A
14	A	997	U
14	A	998	C
14	A	1004	A
14	A	1007	U
14	A	1008	U
14	A	1013	G
14	A	1020	G

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Mol	Chain	Res	Type
14	A	1021	A
14	A	1022	A
14	A	1023	U
14	A	1030	U
14	A	1031	C
14	A	1032	G
14	A	1033	G
14	A	1037	C
14	A	1038	C
14	A	1048	G
14	A	1053	G
14	A	1064	G
14	A	1065	U
14	A	1085	U
14	A	1094	G
14	A	1095	U
14	A	1101	A
14	A	1124	G
14	A	1125	U
14	A	1132	C
14	A	1135	U
14	A	1137	C
14	A	1138	G
14	A	1139	G
14	A	1140	C
14	A	1143	G
14	A	1159	U
14	A	1167	A
14	A	1176	A
14	A	1184	G
14	A	1196	A
14	A	1197	A
14	A	1211	U
14	A	1212	U
14	A	1213	A
14	A	1224	U
14	A	1225	A
14	A	1227	A
14	A	1228	C
14	A	1238	A
14	A	1239	A
14	A	1240	U

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Mol	Chain	Res	Type
14	A	1248	A
14	A	1252	A
14	A	1253	G
14	A	1256	A
14	A	1257	A
14	A	1260	G
14	A	1262	C
14	A	1275	A
14	A	1279	G
14	A	1280	A
14	A	1285	A
14	A	1286	U
14	A	1287	A
14	A	1290	G
14	A	1297	G
14	A	1298	U
14	A	1299	A
14	A	1300	G
14	A	1301	U
14	A	1302	C
14	A	1305	G
14	A	1312	G
14	A	1317	C
14	A	1319	A
14	A	1320	C
14	A	1325	C
14	A	1332	A
14	A	1333	A
14	A	1337	G
14	A	1338	G
14	A	1346	A
14	A	1347	G
14	A	1348	U
14	A	1351	U
14	A	1353	G
14	A	1358	U
14	A	1363	A
14	A	1370	G
14	A	1378	C
14	A	1379	G
14	A	1398	A
14	A	1419	G

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Mol	Chain	Res	Type
14	A	1422	G
14	A	1449	C
14	A	1452	C
14	A	1454(A)	C
14	A	1479	C
14	A	1487	G
14	A	1492	A
14	A	1497	G
14	A	1503	A
14	A	1505	G
14	A	1506	U
14	A	1517	G
14	A	1529	G
14	A	1530	G
15	Y	2	G
15	Y	3	G
15	Y	5	G
15	Y	19	G
15	Y	22	G
15	Y	25	C
15	Y	45	G
15	Y	46	G7M
15	Y	49	G
15	Y	50	G
15	Y	60	C
15	Y	61	C
15	Y	70	C
15	Y	73	A
15	Y	74	C
15	Y	75	C
15	Y	76	A
16	Z	8	4SU
16	Z	9	G
16	Z	14	A
16	Z	15	G
16	Z	22	G
16	Z	23	C
16	Z	37	A
16	Z	38	A
16	Z	45	G
16	Z	46	G7M
16	Z	49	G

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Mol	Chain	Res	Type
16	Z	58	A
16	Z	60	U
16	Z	61	C
16	Z	76	A
17	a	10	A
17	a	34	U
17	a	63	A
17	a	71	A
17	a	74	A
17	a	75	G
17	a	101	A
17	a	102	U
17	a	118	A
17	a	119	A
17	a	120	U
17	a	139	U
17	a	140	C
17	a	142	A
17	a	165	A
17	a	181	A
17	a	196	A
17	a	199	A
17	a	200	U
17	a	215	G
17	a	216	A
17	a	221	A
17	a	222	A
17	a	248	G
17	a	272	A
17	a	276	U
17	a	278	A
17	a	279	A
17	a	282	A
17	a	285	G
17	a	287	G
17	a	289	G
17	a	311	A
17	a	330	A
17	a	361	G
17	a	386	G
17	a	404	A
17	a	405	U

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Mol	Chain	Res	Type
17	a	411	G
17	a	412	A
17	a	420	C
17	a	451	U
17	a	455	C
17	a	481	G
17	a	491	G
17	a	503	A
17	a	504	A
17	a	505	A
17	a	509	C
17	a	530	G
17	a	531	C
17	a	532	A
17	a	533	G
17	a	538	A
17	a	545	U
17	a	548	G
17	a	549	G
17	a	563	A
17	a	573	U
17	a	574	A
17	a	575	A
17	a	586	A
17	a	603	A
17	a	615	U
17	a	627	A
17	a	637	A
17	a	645	C
17	a	646	U
17	a	647	G
17	a	654	A
17	a	655	A
17	a	686	U
17	a	711	G
17	a	717	C
17	a	730	A
17	a	738	G
17	a	747	5MU
17	a	764	A
17	a	765	C
17	a	775	G

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Mol	Chain	Res	Type
17	a	776	G
17	a	777	G
17	a	782	A
17	a	784	G
17	a	785	G
17	a	805	G
17	a	812	C
17	a	827	U
17	a	828	U
17	a	846	U
17	a	858	G
17	a	859	G
17	a	883	G
17	a	884	U
17	a	888	C
17	a	890	C
17	a	891	G
17	a	896	A
17	a	897	C
17	a	899	A
17	a	907	G
17	a	910	A
17	a	914	G
17	a	915	C
17	a	931	U
17	a	934	U
17	a	946	C
17	a	961	C
17	a	974	G
17	a	983	A
17	a	984	A
17	a	985	C
17	a	996	A
17	a	1012	U
17	a	1013	C
17	a	1022	G
17	a	1026	G
17	a	1033	U
17	a	1040	A
17	a	1047	G
17	a	1108	U
17	a	1110	G

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Mol	Chain	Res	Type
17	a	1111	A
17	a	1112	G
17	a	1116	G
17	a	1128	G
17	a	1129	A
17	a	1132	U
17	a	1133	A
17	a	1135	C
17	a	1141	U
17	a	1142	A
17	a	1172	C
17	a	1253	A
17	a	1256	G
17	a	1271	G
17	a	1272	A
17	a	1273	U
17	a	1286	A
17	a	1287	A
17	a	1300	G
17	a	1301	A
17	a	1306	C
17	a	1352	U
17	a	1365	A
17	a	1379	U
17	a	1383	A
17	a	1416	G
17	a	1428	C
17	a	1452	G
17	a	1453	A
17	a	1482	G
17	a	1493	C
17	a	1508	A
17	a	1515	A
17	a	1529	G
17	a	1535	A
17	a	1536	C
17	a	1537	G
17	a	1569	A
17	a	1578	U
17	a	1584	U
17	a	1585	C
17	a	1608	A

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Mol	Chain	Res	Type
17	a	1609	A
17	a	1647	U
17	a	1648	U
17	a	1649	G
17	a	1674	G
17	a	1715	G
17	a	1730	C
17	a	1732	C
17	a	1738	G
17	a	1764	C
17	a	1773	A
17	a	1782	U
17	a	1800	C
17	a	1801	A
17	a	1808	A
17	a	1809	A
17	a	1816	C
17	a	1829	A
17	a	1847	A
17	a	1848	A
17	a	1858	A
17	a	1869	G
17	a	1872	A
17	a	1873	G
17	a	1907	G
17	a	1909	C
17	a	1910	G
17	a	1911	PSU
17	a	1917	PSU
17	a	1918	A
17	a	1919	A
17	a	1925	C
17	a	1930	G
17	a	1931	U
17	a	1937	A
17	a	1938	A
17	a	1955	U
17	a	1965	C
17	a	1967	C
17	a	1970	A
17	a	1971	U
17	a	1972	G

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Mol	Chain	Res	Type
17	a	1987	A
17	a	1991	U
17	a	1993	U
17	a	2023	C
17	a	2027	G
17	a	2031	A
17	a	2033	A
17	a	2043	C
17	a	2055	C
17	a	2056	G
17	a	2060	A
17	a	2061	G
17	a	2062	A
17	a	2069	G7M
17	a	2099	U
17	a	2198	A
17	a	2203	U
17	a	2204	G
17	a	2211	A
17	a	2225	A
17	a	2238	G
17	a	2239	G
17	a	2268	A
17	a	2282	G
17	a	2283	C
17	a	2287	A
17	a	2288	A
17	a	2305	U
17	a	2307	G
17	a	2309	A
17	a	2310	C
17	a	2311	A
17	a	2312	U
17	a	2317	A
17	a	2321	U
17	a	2322	A
17	a	2325	G
17	a	2333	A
17	a	2335	A
17	a	2347	C
17	a	2361	G
17	a	2366	A

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Mol	Chain	Res	Type
17	a	2383	G
17	a	2385	C
17	a	2402	U
17	a	2406	A
17	a	2424	C
17	a	2425	A
17	a	2429	G
17	a	2430	A
17	a	2431	U
17	a	2435	A
17	a	2441	U
17	a	2448	A
17	a	2470	G
17	a	2474	U
17	a	2476	A
17	a	2491	U
17	a	2502	G
17	a	2505	G
17	a	2518	A
17	a	2529	G
17	a	2547	A
17	a	2566	A
17	a	2567	G
17	a	2573	C
17	a	2603	G
17	a	2609	U
17	a	2613	U
17	a	2629	U
17	a	2661	G
17	a	2663	G
17	a	2689	U
17	a	2690	U
17	a	2714	G
17	a	2716	C
17	a	2726	A
17	a	2744	G
17	a	2748	A
17	a	2757	A
17	a	2765	A
17	a	2778	A
17	a	2797	U
17	a	2800	A

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Mol	Chain	Res	Type
17	a	2801	G
17	a	2820	A
17	a	2821	A
17	a	2883	A
17	a	2884	U
38	X	14	A
38	X	15	A
38	X	16	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	A	13	U
14	A	119	A
14	A	199	A
14	A	421	U
14	A	438	U
14	A	530	G
14	A	532	A
14	A	574	A
14	A	641	U
14	A	776	G
14	A	793	U
14	A	858	G
14	A	884	U
14	A	993	G
14	A	1046	A
14	A	1124	G
14	A	1211	U
14	A	1224	U
14	A	1225	A
14	A	1239	A
14	A	1297	G
14	A	1319	A
14	A	1337	G
14	A	1432	G
14	A	1454	G
14	A	1478	U
14	A	1505	G
15	Y	49	G
15	Y	60	C
15	Y	74	C

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Mol	Chain	Res	Type
16	Z	48	C
16	Z	58	A
16	Z	60	U

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

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	$\# Z > 2$
17	OMU	a	2552	17	19,22,23	0.23	0	26,31,34	0.40	0
14	4OC	A	1402	14,57	20,23,24	0.37	0	26,32,35	0.53	0
17	2MG	a	2445	17	23,26,27	0.36	0	32,38,41	0.45	0
10	4D4	l	81	10	9,11,12	0.44	0	8,13,15	0.73	0
14	5MC	A	1407	14	18,22,23	0.31	0	26,32,35	0.65	0
17	PSU	a	2457	17	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
14	2MG	A	1207	14	23,26,27	0.38	0	32,38,41	0.36	0
14	PSU	A	516	14	18,21,22	0.92	1 (5%)	22,30,33	0.74	1 (4%)
16	4SU	Z	8	16	18,21,22	0.39	0	26,30,33	1.21	2 (7%)
17	PSU	a	1911	17	18,21,22	0.89	1 (5%)	22,30,33	0.65	0
14	UR3	A	1498	14	19,22,23	0.26	0	26,32,35	0.66	0
17	2MG	a	1835	17	23,26,27	0.37	0	32,38,41	0.41	0
17	H2U	a	2449	58,17	18,21,22	0.59	0	21,30,33	0.78	1 (4%)
17	6MZ	a	1618	17	22,25,26	0.31	0	30,36,39	0.55	0
14	MA6	A	1518	14	23,26,27	0.25	0	34,38,41	0.68	1 (2%)
17	G7M	a	2069	17	23,26,27	0.74	1 (4%)	35,39,42	0.66	0
14	MA6	A	1519	14	23,26,27	0.25	0	34,38,41	0.81	2 (5%)
14	G7M	A	527	14	23,26,27	0.74	1 (4%)	35,39,42	0.64	0
17	3TD	a	1915	17	18,22,23	0.94	1 (5%)	22,32,35	0.67	0
17	PSU	a	2605	17	18,21,22	0.87	1 (5%)	22,30,33	0.81	1 (4%)
17	5MC	a	1962	58,17	18,22,23	0.33	0	26,32,35	0.50	0
15	4SU	Y	8	15	18,21,22	0.36	0	26,30,33	1.20	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	OMC	Z	32	16	19,22,23	0.26	0	26,31,34	0.41	0
4	D2T	L	89	4	7,9,10	0.93	0	6,11,13	1.72	2 (33%)
14	2MG	A	1516	14	23,26,27	0.35	0	32,38,41	0.54	0
17	PSU	a	955	58,17	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
17	2MA	a	2503	58,57,17	22,25,26	0.26	0	33,37,40	0.68	2 (6%)
15	5MU	Y	54	15	19,22,23	0.27	0	28,32,35	0.32	0
17	6MZ	a	2030	17	22,25,26	0.34	0	30,36,39	0.61	0
17	1MG	a	745	17	22,26,27	0.50	0	33,39,42	0.48	0
16	G7M	Z	46	16	23,26,27	0.71	1 (4%)	35,39,42	0.63	0
17	PSU	a	1917	17	18,21,22	0.90	1 (5%)	22,30,33	0.58	0
16	5MU	Z	54	16	19,22,23	0.27	0	28,32,35	0.28	0
15	6MZ	Y	37	15	22,25,26	0.37	0	30,36,39	0.50	0
17	PSU	a	746	57,17	18,21,22	0.92	1 (5%)	22,30,33	0.63	0
16	PSU	Z	55	16	18,21,22	0.93	1 (5%)	22,30,33	0.62	0
17	OMC	a	2498	57,17	19,22,23	0.26	0	26,31,34	0.51	0
15	PSU	Y	55	15	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
17	5MU	a	747	17	19,22,23	0.28	0	28,32,35	0.39	0
15	G7M	Y	46	15	23,26,27	0.73	1 (4%)	35,39,42	0.54	0
10	MS6	l	82	10	5,7,8	0.22	0	2,7,9	0.17	0
8	MEQ	d	150	8	8,9,10	0.43	0	5,10,12	0.73	0
17	PSU	a	2504	58,17	18,21,22	0.87	1 (5%)	22,30,33	0.79	1 (4%)
17	PSU	a	2580	17	18,21,22	0.95	1 (5%)	22,30,33	0.78	1 (4%)
3	IAS	K	119	3	6,7,8	0.88	0	6,8,10	0.97	0
17	5MU	a	1939	17	19,22,23	0.28	0	28,32,35	0.35	0
17	PSU	a	2604	17	18,21,22	0.91	1 (5%)	22,30,33	0.87	1 (4%)
17	OMG	a	2251	15,17	23,26,27	0.31	0	33,38,41	0.43	0
14	2MG	A	966	14	23,26,27	0.40	0	32,38,41	0.39	0
14	5MC	A	967	14	18,22,23	0.32	0	26,32,35	0.52	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
17	OMU	a	2552	17	-	0/9/27/28	0/2/2/2
14	4OC	A	1402	14,57	-	0/9/29/30	0/2/2/2
17	2MG	a	2445	17	-	0/9/27/28	0/3/3/3
10	4D4	l	81	10	-	1/11/12/14	-
14	5MC	A	1407	14	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PSU	a	2457	17	-	0/7/25/26	0/2/2/2
14	2MG	A	1207	14	-	0/9/27/28	0/3/3/3
14	PSU	A	516	14	-	0/7/25/26	0/2/2/2
16	4SU	Z	8	16	-	4/7/25/26	0/2/2/2
17	PSU	a	1911	17	-	2/7/25/26	0/2/2/2
14	UR3	A	1498	14	-	0/7/25/26	0/2/2/2
17	2MG	a	1835	17	-	0/9/27/28	0/3/3/3
17	H2U	a	2449	58,17	-	0/7/38/39	0/2/2/2
17	6MZ	a	1618	17	-	0/9/27/28	0/3/3/3
14	MA6	A	1518	14	-	0/11/29/30	0/3/3/3
17	G7M	a	2069	17	-	2/7/25/26	0/3/3/3
14	MA6	A	1519	14	-	3/11/29/30	0/3/3/3
14	G7M	A	527	14	-	0/7/25/26	0/3/3/3
17	3TD	a	1915	17	-	0/7/25/26	0/2/2/2
17	PSU	a	2605	17	-	0/7/25/26	0/2/2/2
17	5MC	a	1962	58,17	-	0/7/25/26	0/2/2/2
15	4SU	Y	8	15	-	0/7/25/26	0/2/2/2
16	OMC	Z	32	16	-	0/9/27/28	0/2/2/2
4	D2T	L	89	4	-	4/7/12/14	-
14	2MG	A	1516	14	-	0/9/27/28	0/3/3/3
17	PSU	a	955	58,17	-	0/7/25/26	0/2/2/2
17	2MA	a	2503	58,57,17	-	2/7/25/26	0/3/3/3
15	5MU	Y	54	15	-	0/7/25/26	0/2/2/2
17	6MZ	a	2030	17	-	2/9/27/28	0/3/3/3
17	1MG	a	745	17	-	0/7/25/26	0/3/3/3
16	G7M	Z	46	16	-	3/7/25/26	0/3/3/3
17	PSU	a	1917	17	-	2/7/25/26	0/2/2/2
16	5MU	Z	54	16	-	0/7/25/26	0/2/2/2
15	6MZ	Y	37	15	-	0/9/27/28	0/3/3/3
17	PSU	a	746	57,17	-	2/7/25/26	0/2/2/2
16	PSU	Z	55	16	-	2/7/25/26	0/2/2/2
17	OMC	a	2498	57,17	-	0/9/27/28	0/2/2/2
15	PSU	Y	55	15	-	0/7/25/26	0/2/2/2
17	5MU	a	747	17	-	1/7/25/26	0/2/2/2
15	G7M	Y	46	15	-	3/7/25/26	0/3/3/3
10	MS6	l	82	10	-	1/4/6/8	-
8	MEQ	d	150	8	-	2/8/9/11	-
17	PSU	a	2504	58,17	-	0/7/25/26	0/2/2/2
17	PSU	a	2580	17	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IAS	K	119	3	-	0/7/7/8	-
17	5MU	a	1939	17	-	0/7/25/26	0/2/2/2
17	PSU	a	2604	17	-	0/7/25/26	0/2/2/2
17	OMG	a	2251	15,17	-	0/9/27/28	0/3/3/3
14	2MG	A	966	14	-	2/9/27/28	0/3/3/3
14	5MC	A	967	14	-	0/7/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	2580	PSU	C6-C5	3.69	1.39	1.35
16	Z	55	PSU	C6-C5	3.67	1.39	1.35
17	a	2457	PSU	C6-C5	3.63	1.39	1.35
17	a	746	PSU	C6-C5	3.62	1.39	1.35
14	A	516	PSU	C6-C5	3.61	1.39	1.35
17	a	1917	PSU	C6-C5	3.59	1.39	1.35
15	Y	55	PSU	C6-C5	3.59	1.39	1.35
17	a	955	PSU	C6-C5	3.58	1.39	1.35
17	a	1915	3TD	C6-C5	3.56	1.39	1.35
17	a	1911	PSU	C6-C5	3.50	1.39	1.35
17	a	2504	PSU	C6-C5	3.39	1.39	1.35
17	a	2604	PSU	C6-C5	3.36	1.39	1.35
17	a	2605	PSU	C6-C5	3.34	1.39	1.35
17	a	2069	G7M	C8-N7	2.84	1.38	1.33
14	A	527	G7M	C8-N7	2.69	1.37	1.33
15	Y	46	G7M	C8-N7	2.66	1.37	1.33
16	Z	46	G7M	C8-N7	2.46	1.37	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	8	4SU	C4-N3-C2	-4.48	122.99	127.34
15	Y	8	4SU	C4-N3-C2	-4.28	123.19	127.34
14	A	1519	MA6	C2-N1-C6	2.88	118.56	111.75
14	A	1518	MA6	C2-N1-C6	2.85	118.48	111.75
15	Y	8	4SU	C5-C4-N3	2.76	117.25	114.69
16	Z	8	4SU	C5-C4-N3	2.66	117.15	114.69
4	L	89	D2T	OD1-CG-CB	-2.60	117.00	122.44
17	a	2503	2MA	C5-C4-N3	-2.38	124.51	127.19
17	a	2604	PSU	C2'-C3'-C4'	-2.38	98.02	102.64
17	a	2580	PSU	C3'-C2'-C1'	2.36	104.38	101.64
14	A	516	PSU	C3'-C2'-C1'	2.28	104.29	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	8	4SU	N3-C2-N1	2.21	117.83	114.89
17	a	2503	2MA	N3-C4-N9	2.17	130.00	126.99
4	L	89	D2T	OD2-CG-CB	2.09	117.66	113.15
17	a	2504	PSU	C2'-C3'-C4'	-2.04	98.67	102.64
14	A	1519	MA6	C2'-C3'-C4'	-2.03	98.69	102.64
17	a	2449	H2U	O2-C2-N1	-2.03	120.56	123.11
17	a	2605	PSU	C2'-C3'-C4'	-2.02	98.72	102.64

There are no chirality outliers.

All (38) 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
14	A	966	2MG	O4'-C4'-C5'-O5'
14	A	966	2MG	C3'-C4'-C5'-O5'
15	Y	46	G7M	C4'-C5'-O5'-P
17	a	746	PSU	C2'-C1'-C5-C4
17	a	1911	PSU	O4'-C4'-C5'-O5'
17	a	1917	PSU	C3'-C4'-C5'-O5'
17	a	1917	PSU	O4'-C4'-C5'-O5'
14	A	1519	MA6	O4'-C4'-C5'-O5'
17	a	1911	PSU	C3'-C4'-C5'-O5'
8	d	150	MEQ	NE2-CD-CG-CB
8	d	150	MEQ	OE1-CD-CG-CB
14	A	1519	MA6	C3'-C4'-C5'-O5'
15	Y	46	G7M	C3'-C4'-C5'-O5'
16	Z	8	4SU	C3'-C4'-C5'-O5'
16	Z	46	G7M	C3'-C4'-C5'-O5'
17	a	2030	6MZ	O4'-C4'-C5'-O5'
16	Z	46	G7M	O4'-C4'-C5'-O5'
15	Y	46	G7M	O4'-C4'-C5'-O5'
10	l	82	MS6	CB-CG-SD-CE
16	Z	46	G7M	C4'-C5'-O5'-P
16	Z	8	4SU	O4'-C4'-C5'-O5'
16	Z	8	4SU	C2'-C1'-N1-C2
17	a	2069	G7M	C4'-C5'-O5'-P
16	Z	8	4SU	C2'-C1'-N1-C6
16	Z	55	PSU	O4'-C1'-C5-C4
17	a	2030	6MZ	C3'-C4'-C5'-O5'
4	L	89	D2T	SB-CB-CG-OD2
4	L	89	D2T	CG-CB-SB-CB1

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Mol	Chain	Res	Type	Atoms
16	Z	55	PSU	O4'-C1'-C5-C6
17	a	746	PSU	O4'-C1'-C5-C6
17	a	2069	G7M	O4'-C4'-C5'-O5'
17	a	2503	2MA	O4'-C4'-C5'-O5'
10	l	81	4D4	O-C-CA-CB
14	A	1519	MA6	C4'-C5'-O5'-P
17	a	2503	2MA	C4'-C5'-O5'-P
17	a	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1402	4OC	1	0
14	A	516	PSU	1	0
16	Z	8	4SU	1	0
17	a	1915	3TD	1	0
17	a	2030	6MZ	1	0
15	Y	37	6MZ	1	0
17	a	747	5MU	1	0
17	a	1939	5MU	1	0
17	a	2604	PSU	1	0
17	a	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 341 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
59	SCM	A	1602	-	23,25,25	0.26	0	26,39,39	0.62	0
60	VAL	Y	101	15	4,6,7	0.58	0	6,7,9	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SCM	A	1602	-	-	4/4/57/57	0/3/3/3
60	VAL	Y	101	15	-	0/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	1602	SCM	C7-C8-N8-C8M
59	A	1602	SCM	C9-C8-N8-C8M
59	A	1602	SCM	C9-C10-N10-C1M
59	A	1602	SCM	C11-C10-N10-C1M

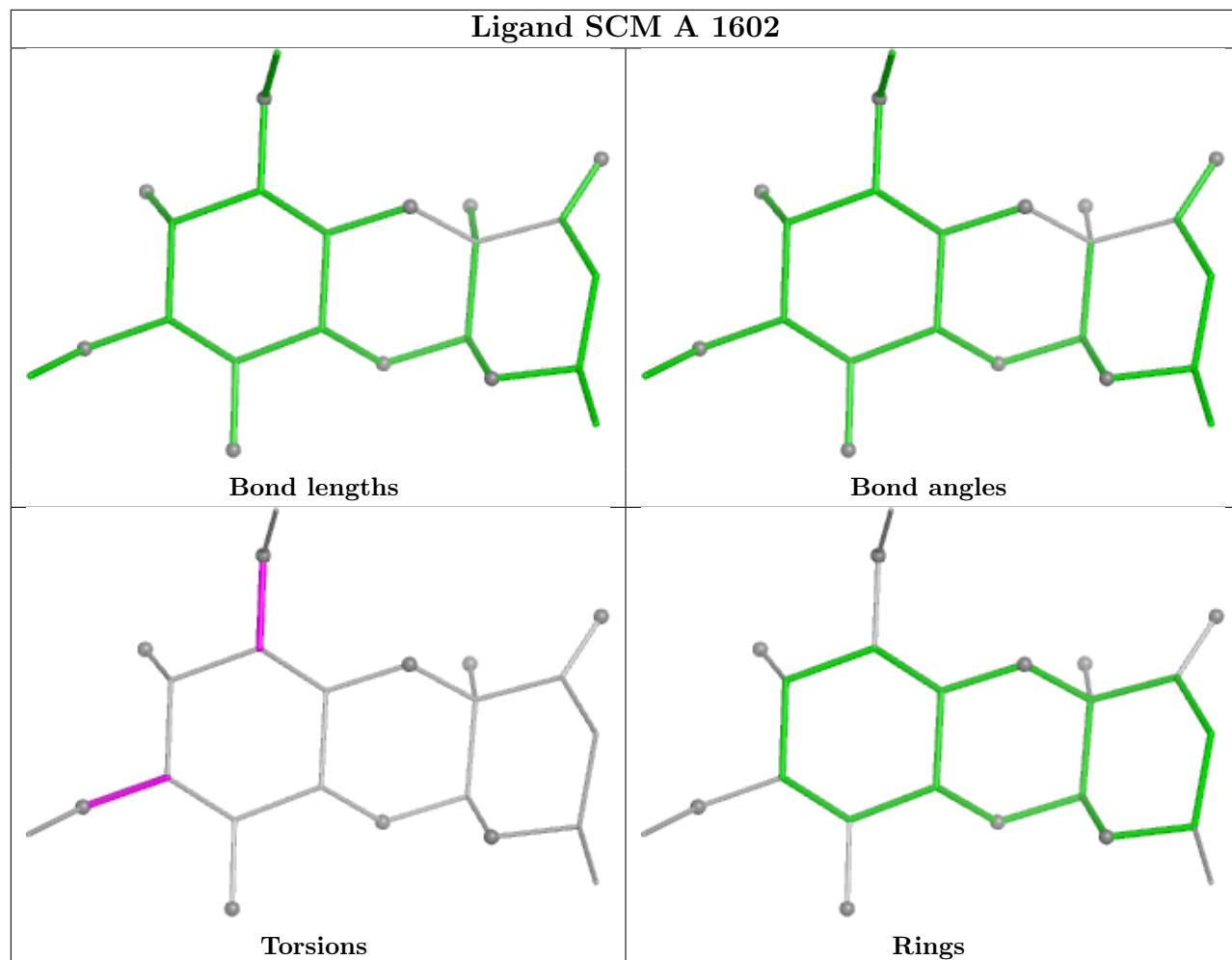
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	A	1602	SCM	3	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.

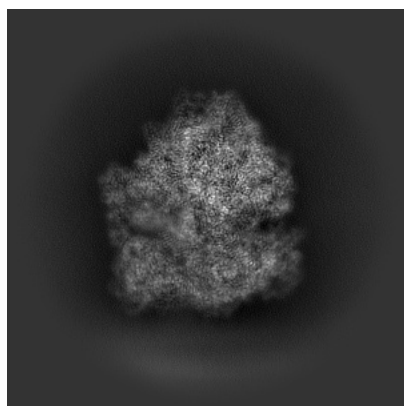
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56827. These allow visual inspection of the internal detail of the map and identification of artifacts.

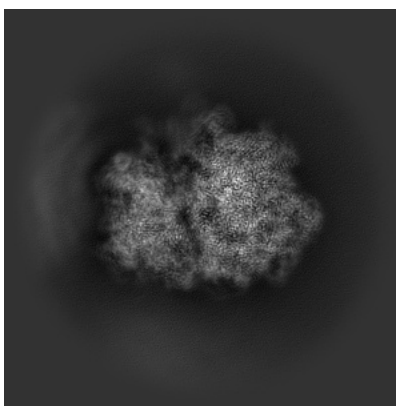
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

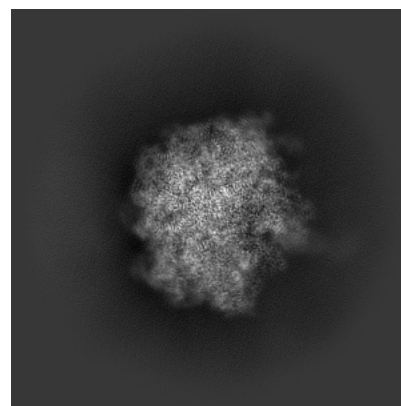
6.1.1 Primary map



X

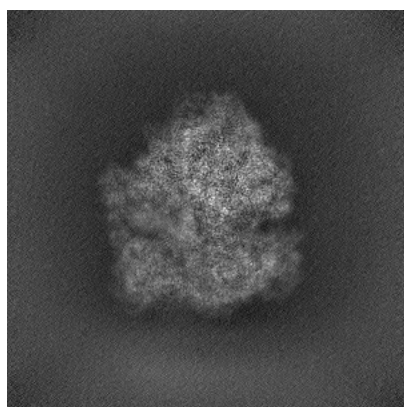


Y

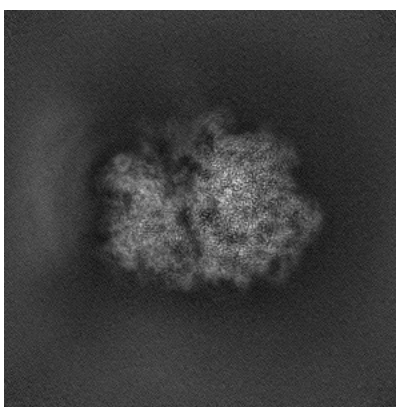


Z

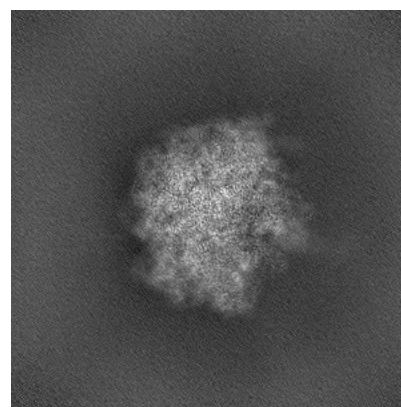
6.1.2 Raw map



X



Y

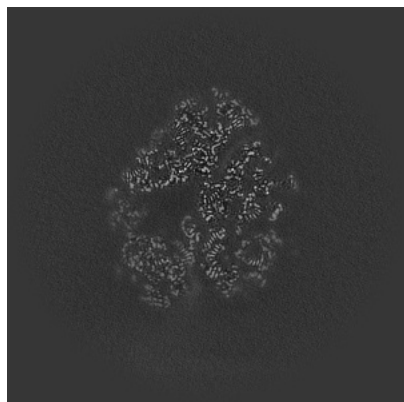


Z

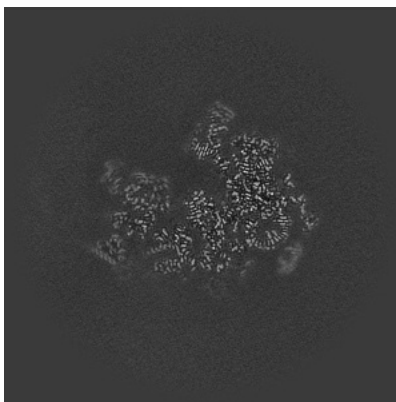
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

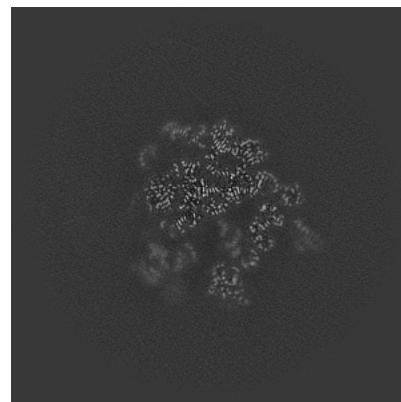
6.2.1 Primary map



X Index: 288

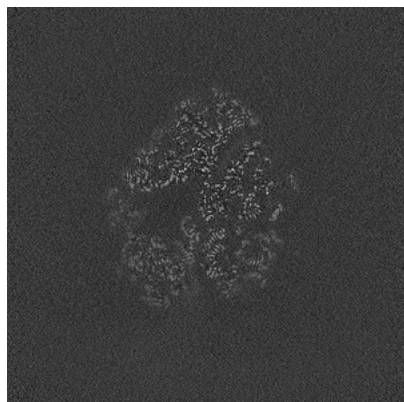


Y Index: 288

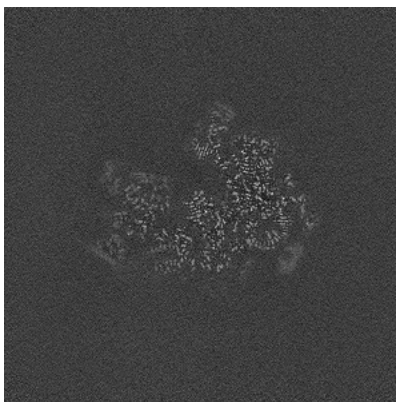


Z Index: 288

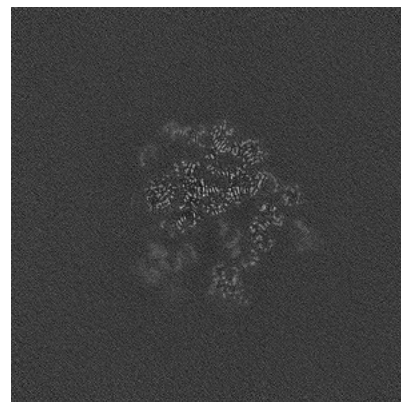
6.2.2 Raw map



X Index: 288



Y Index: 288

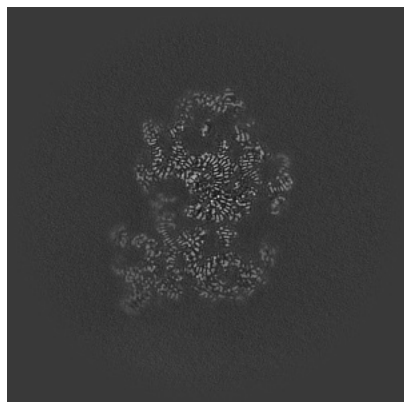


Z Index: 288

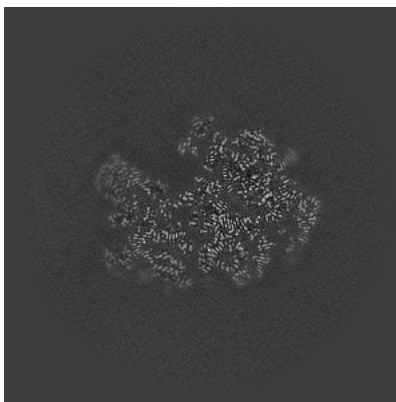
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

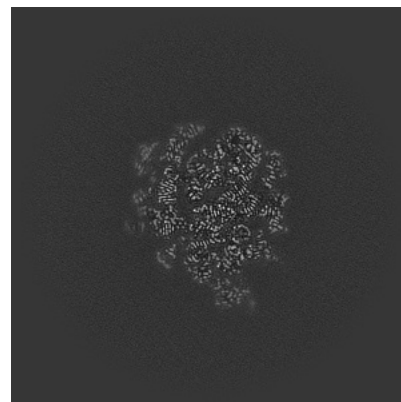
6.3.1 Primary map



X Index: 264

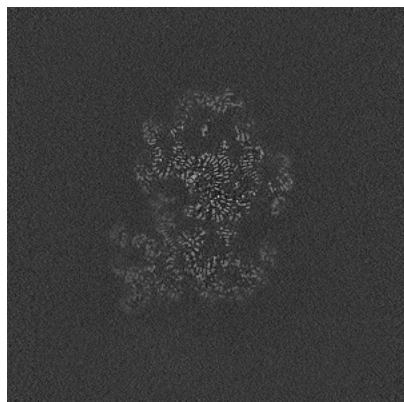


Y Index: 303

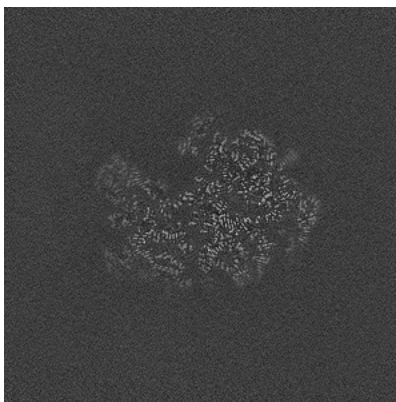


Z Index: 342

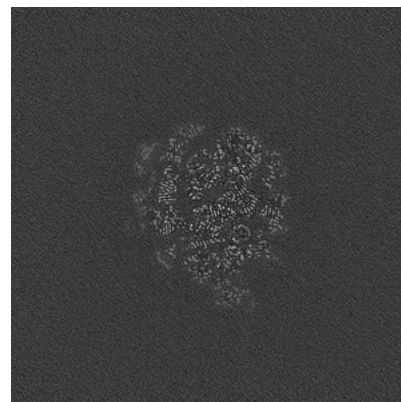
6.3.2 Raw map



X Index: 264



Y Index: 303

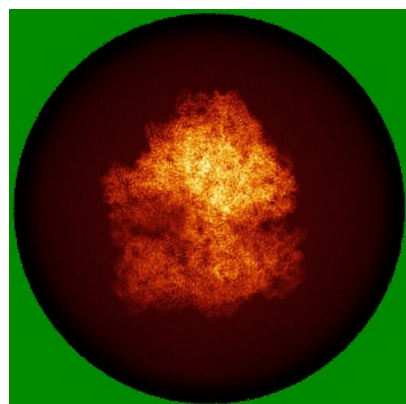


Z Index: 342

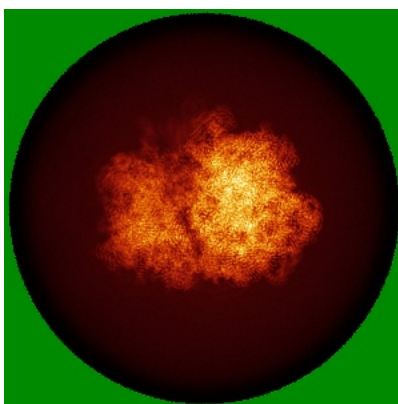
The images above show the largest variance slices of the map in three orthogonal directions.

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

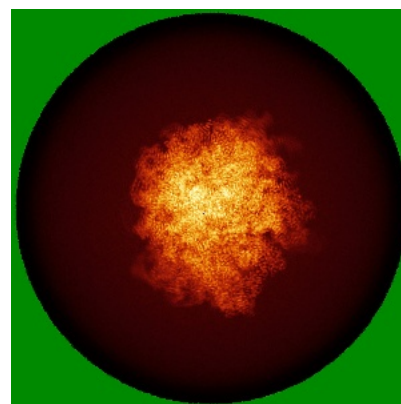
6.4.1 Primary map



X

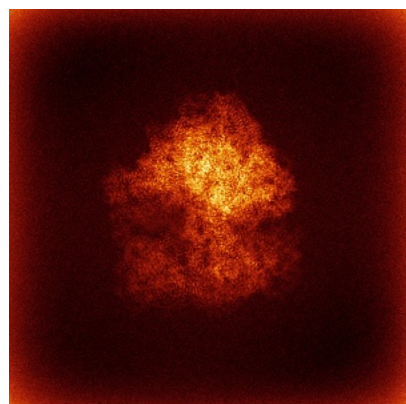


Y

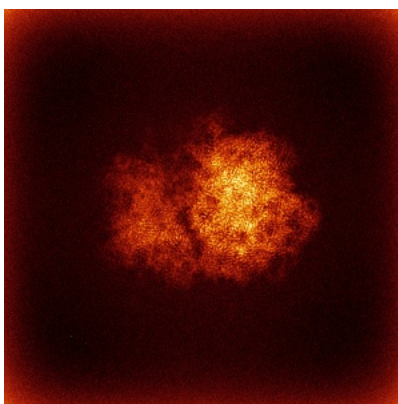


Z

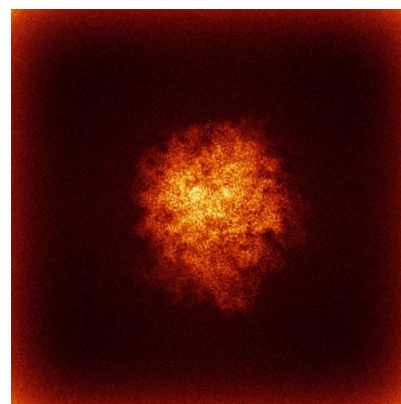
6.4.2 Raw map



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



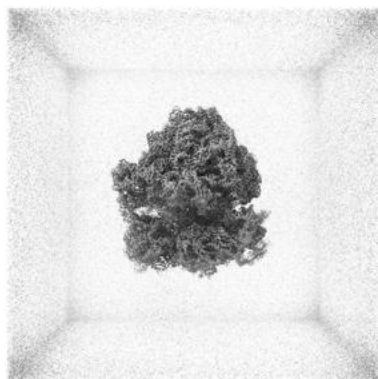
Y



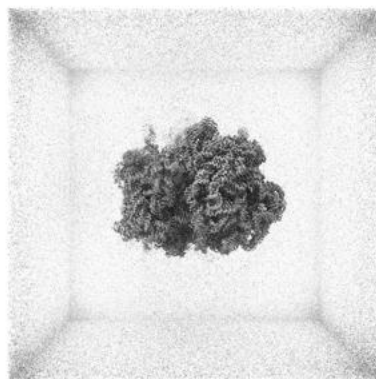
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0484. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

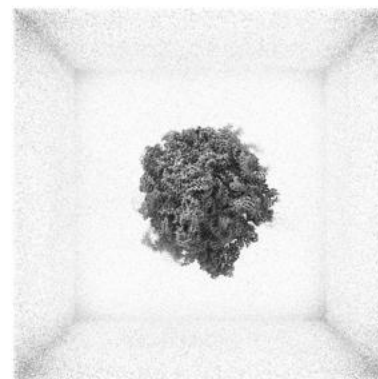
6.5.2 Raw map



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.

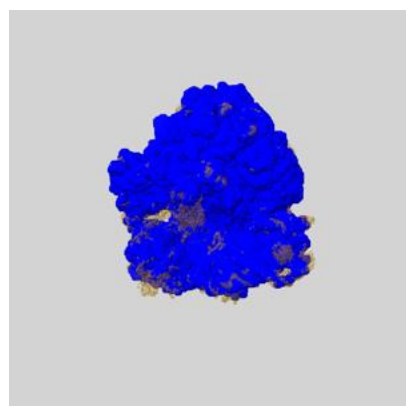
6.6 Mask visualisation [i](#)

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

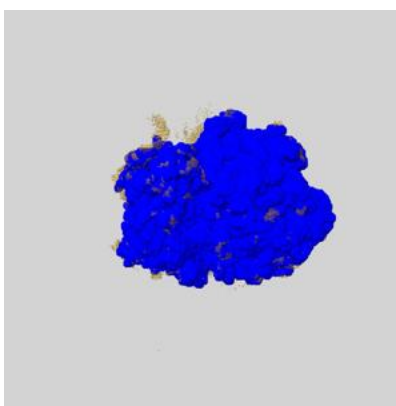
A mask typically either:

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

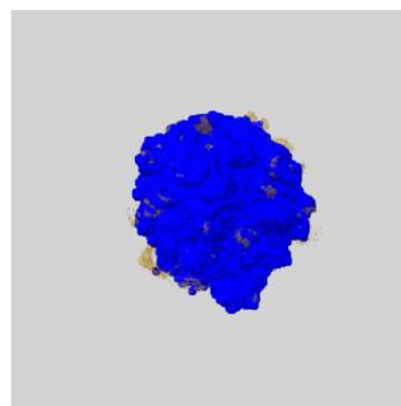
6.6.1 emd_56827_msk_1.map [i](#)



X



Y

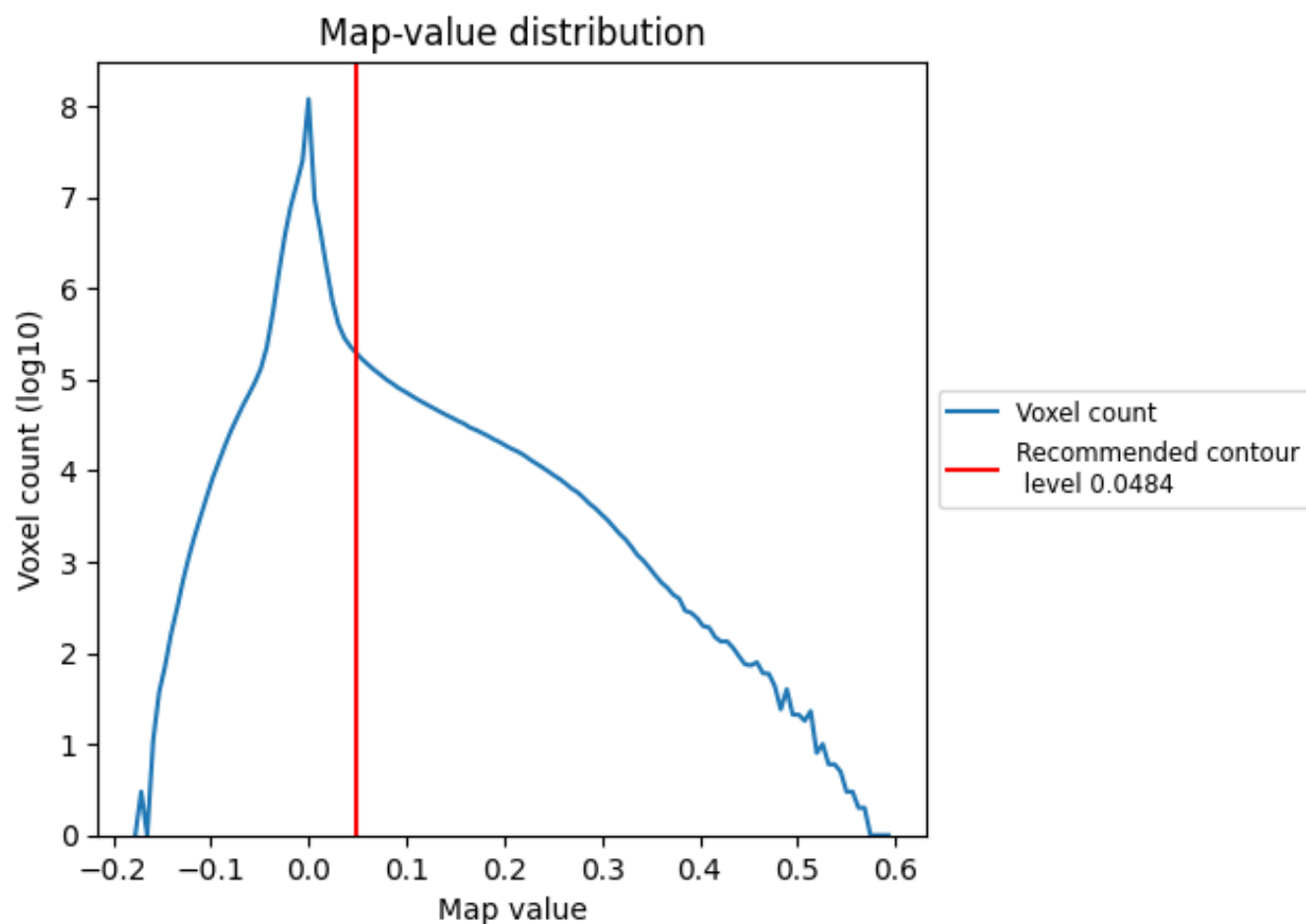


Z

7 Map analysis [i](#)

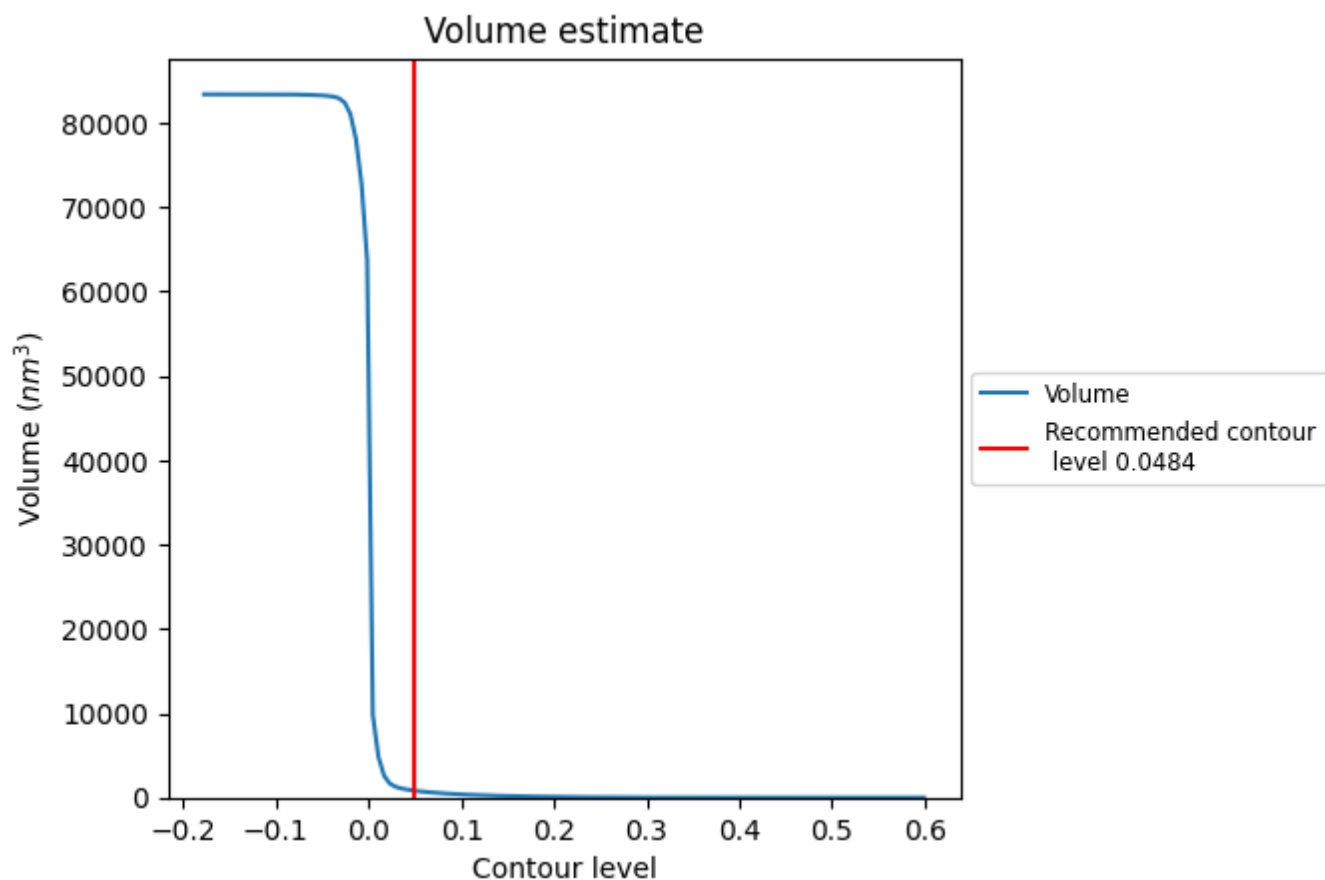
This section contains the results of statistical analysis of the map.

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.

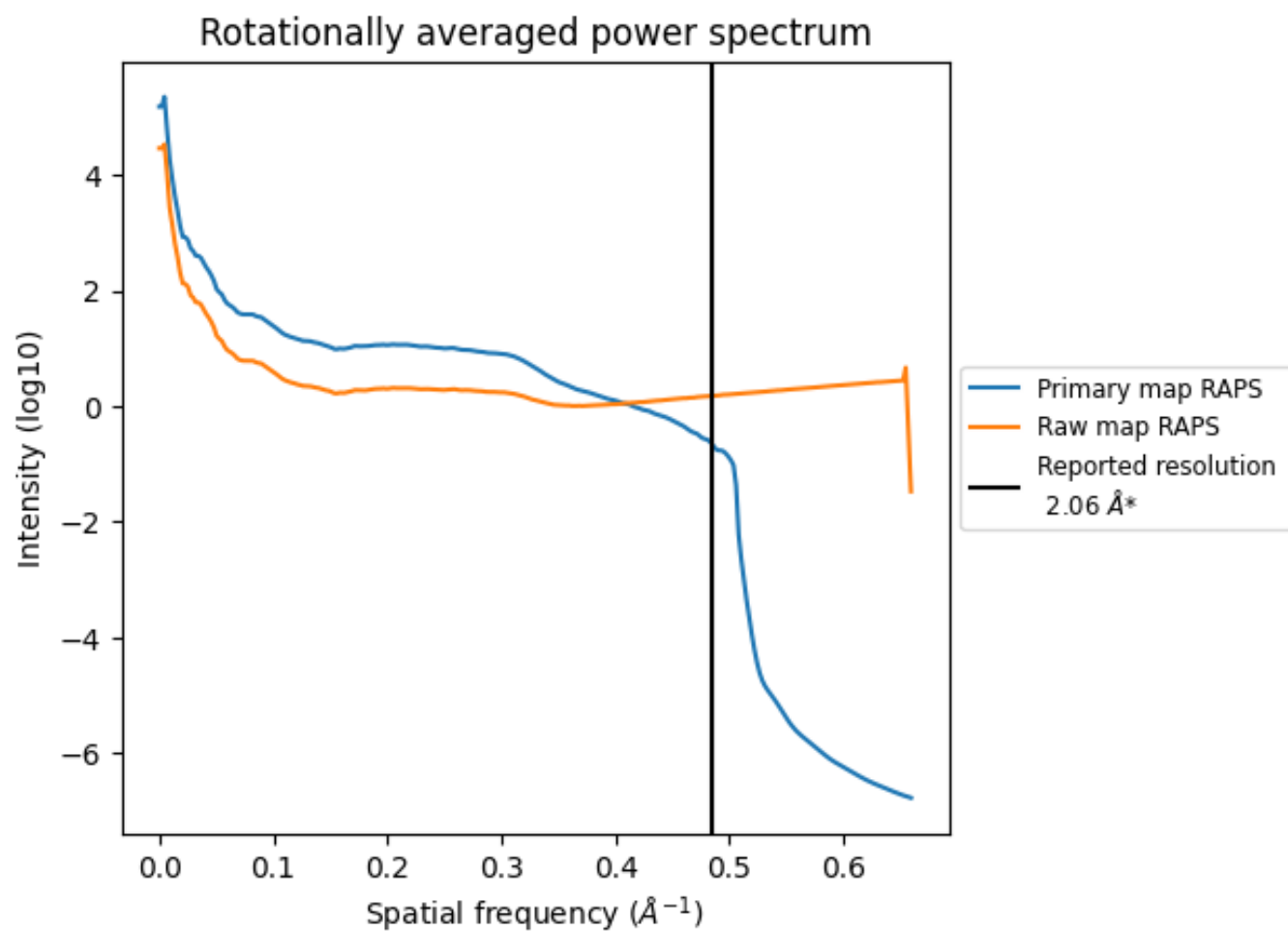
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 835 nm³; this corresponds to an approximate mass of 755 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 ⓘ

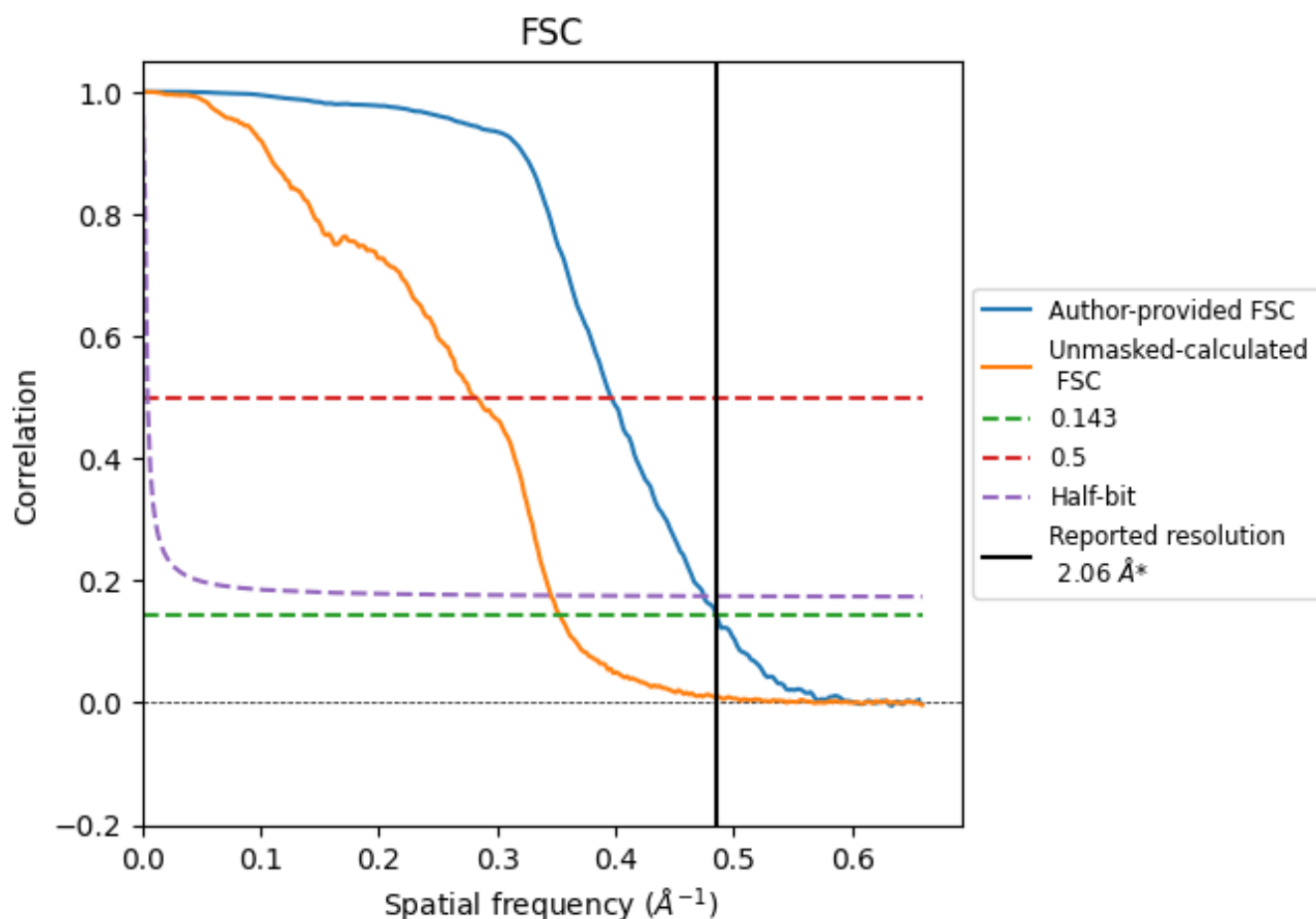


*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

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 0.485 \AA^{-1}

8.2 Resolution estimates [i](#)

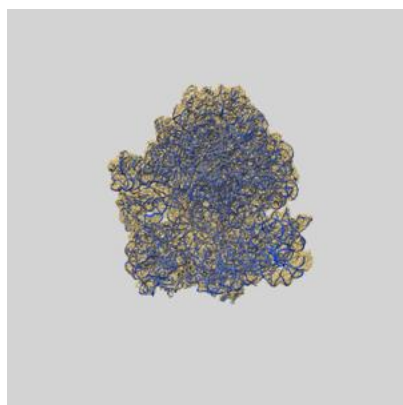
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.52	2.11
Unmasked-calculated*	2.83	3.55	2.90

*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 2.83 differs from the reported value 2.06 by more than 10 %

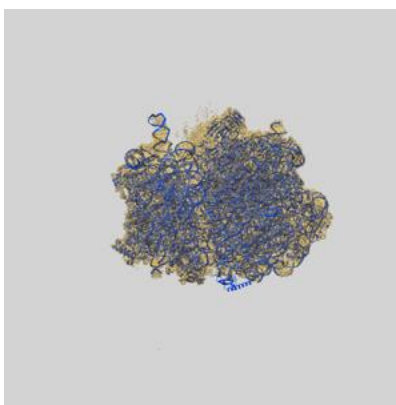
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56827 and PDB model 28UH. Per-residue inclusion information can be found in section [3](#) on page [19](#).

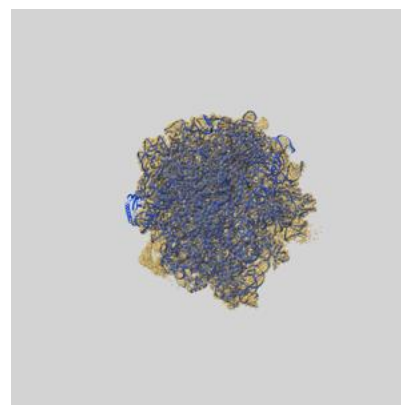
9.1 Map-model overlay [i](#)



X



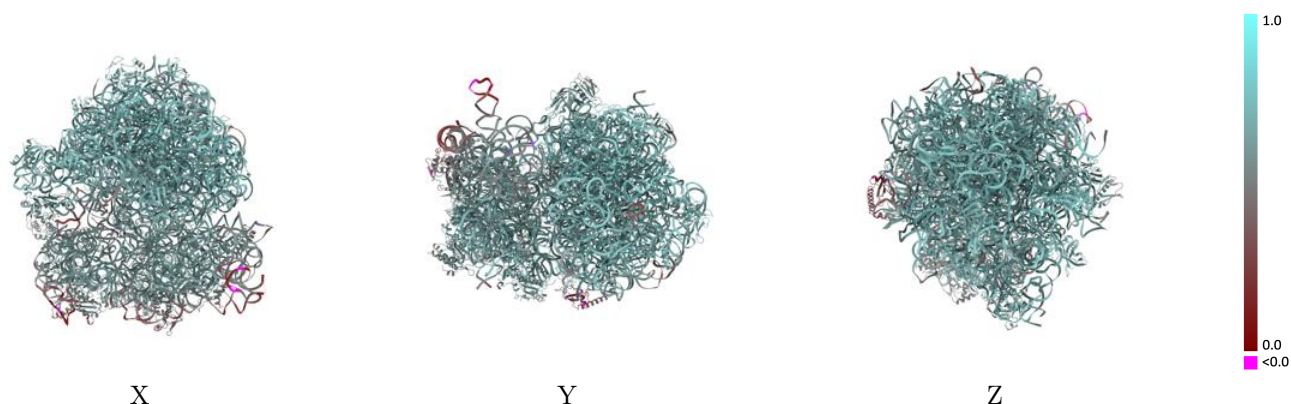
Y



Z

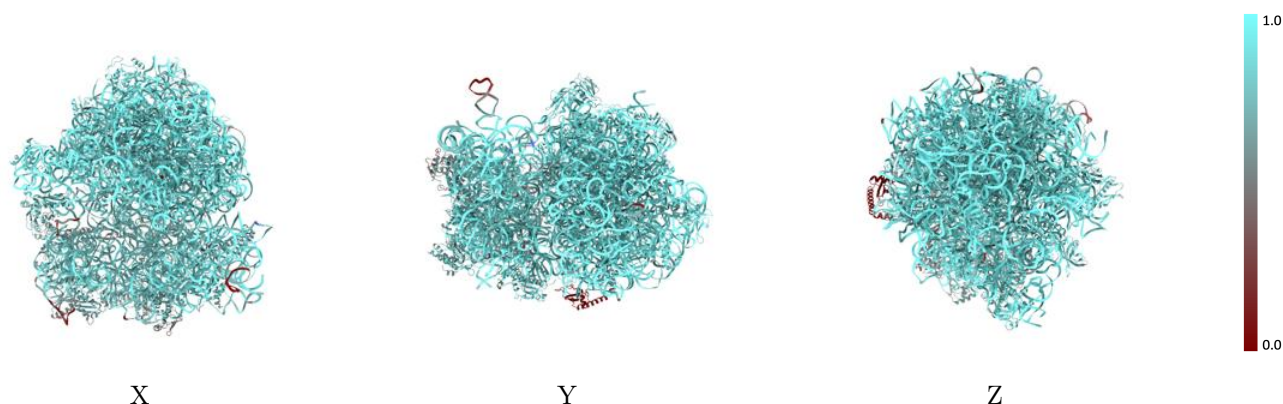
The images above show the 3D surface view of the map at the recommended contour level 0.0484 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



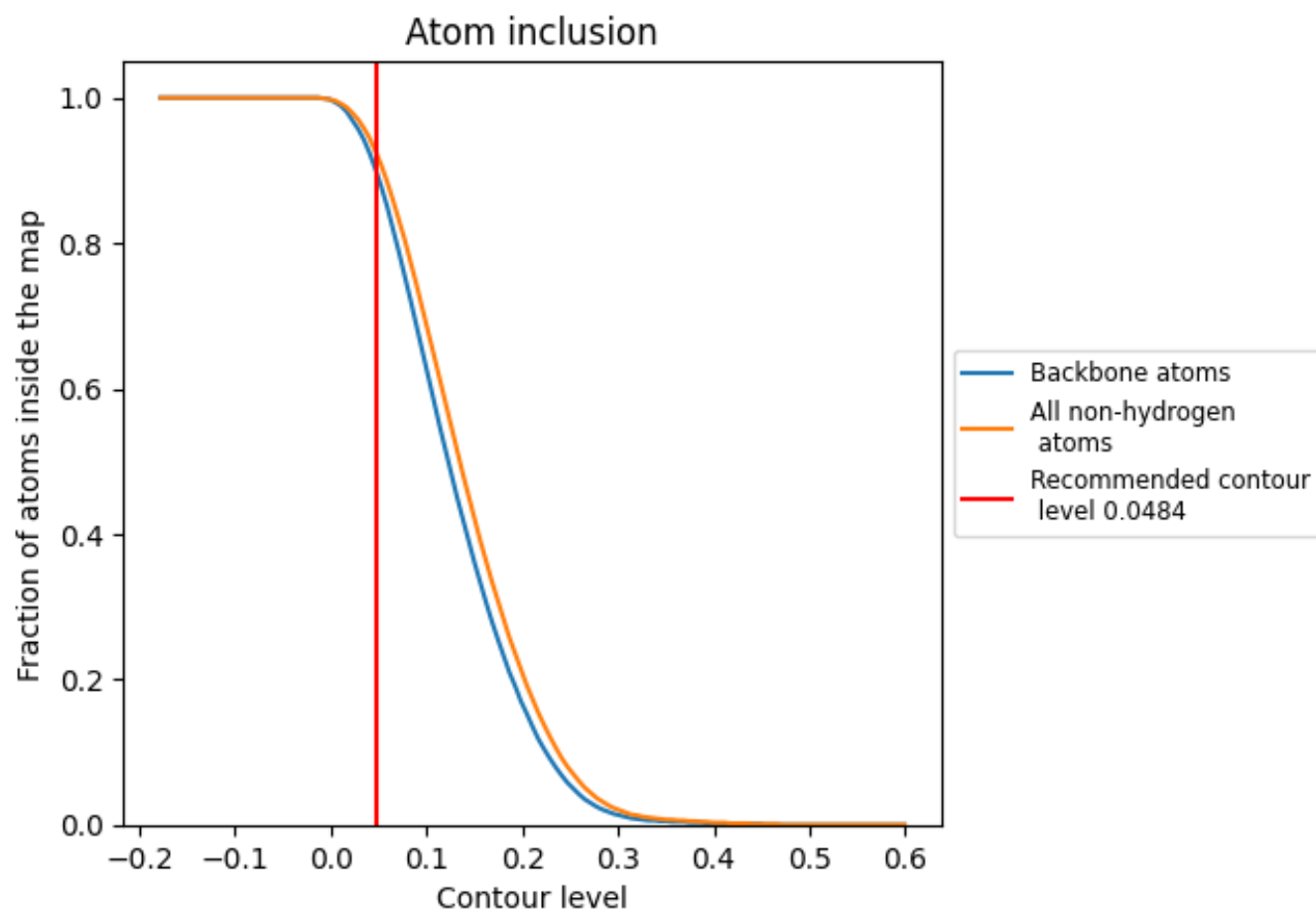
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0484).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.0484) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9220	 0.6470
0	 0.9070	 0.6760
1	 0.9720	 0.7330
2	 0.9800	 0.7290
3	 0.9450	 0.6910
4	 0.7210	 0.5330
A	 0.9340	 0.6070
B	 0.7380	 0.5550
C	 0.8030	 0.6020
D	 0.6180	 0.4740
E	 0.9020	 0.6600
F	 0.8150	 0.5900
G	 0.4930	 0.4510
H	 0.9190	 0.6710
I	 0.7810	 0.5580
J	 0.6700	 0.5210
K	 0.8940	 0.6430
L	 0.8150	 0.5960
M	 0.7300	 0.5580
N	 0.8320	 0.6040
O	 0.9040	 0.6580
P	 0.8070	 0.5630
Q	 0.8220	 0.6090
R	 0.8620	 0.6290
S	 0.7840	 0.5880
T	 0.7710	 0.5610
U	 0.6520	 0.5430
X	 0.8190	 0.5810
Y	 0.8180	 0.5180
Z	 0.8830	 0.5690
a	 0.9820	 0.6870
b	 0.9790	 0.6550
c	 0.9660	 0.7230
d	 0.9560	 0.7110
e	 0.9200	 0.6770



Continued on next page...

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Chain	Atom inclusion	Q-score
f	 0.8050	 0.5850
g	 0.8490	 0.5960
h	 0.2380	 0.3730
i	 0.9510	 0.7090
j	 0.9480	 0.7100
k	 0.9550	 0.7010
l	 0.9450	 0.7040
m	 0.9840	 0.7250
n	 0.9140	 0.6500
o	 0.8940	 0.6790
p	 0.9790	 0.7310
q	 0.9330	 0.6900
r	 0.9350	 0.7050
s	 0.9040	 0.6700
t	 0.8980	 0.6530
u	 0.9000	 0.6630
v	 0.9360	 0.7030
w	 0.9520	 0.6980
x	 0.8820	 0.6490
y	 0.9270	 0.6980
z	 0.9390	 0.7020