



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:54 PM UTC

PDB ID : 9T0Y / pdb\_00009t0y  
EMDB ID : EMD-55415  
Title : E. coli 70S ribosome from delta-9 strain  
Authors : Larsson, D.S.D.; Selmer, M.  
Deposited on : 2025-10-20  
Resolution : 1.87 Å(reported)  
Based on initial model : 9SYH

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

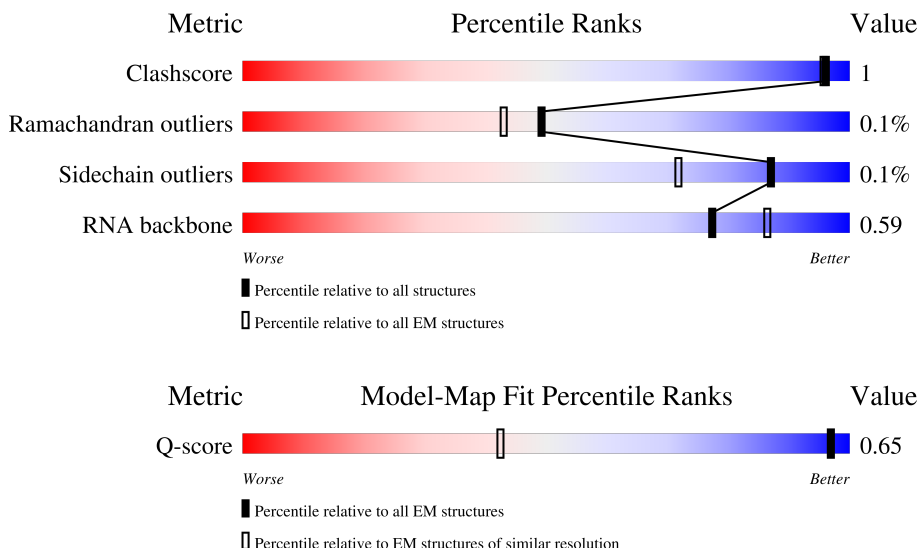
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 1.87 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	985 ( 1.37 - 2.37 )

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

Mol	Chain	Length	Quality of chain
1	A	1542	<div> <div>11%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	B	241	<div> <div>58%</div> <div>87%</div> <div>11%</div> </div>
3	C	233	<div> <div>11%</div> <div>87%</div> <div>12%</div> </div>



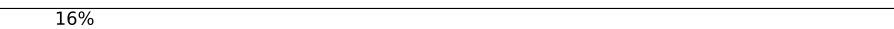
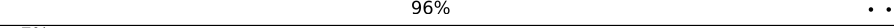


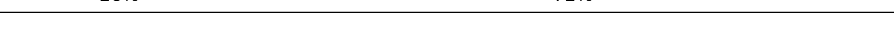
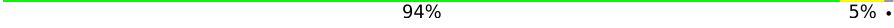


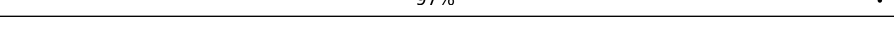


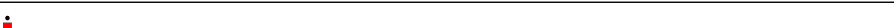
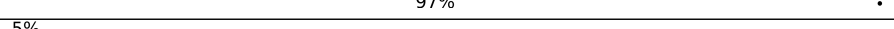
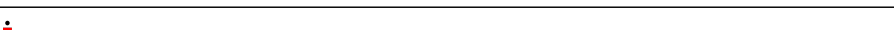

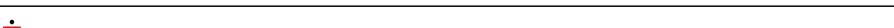
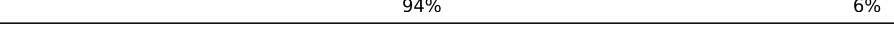
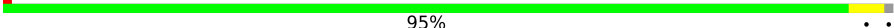


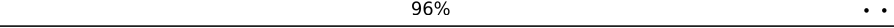
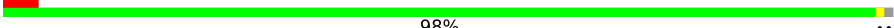

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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	X	120	
23	Y	76	
24	5	77	
24	Z	77	
25	a	2904	
26	b	120	
27	c	273	

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Mol	Chain	Length	Quality of chain
28	d	209	 94% . .
29	e	201	 11% 91% 8% .
30	f	179	 16% 96% . .
31	g	177	 7% 92% . 5%
32	h	149	 8% 26% . 72%
33	i	142	 94% 5% .
34	j	123	 94% 6%
35	k	144	 97% .
36	l	136	 91% 8% .
37	m	127	 87% 6% 7%
38	n	117	 97% . .
39	o	115	 5% 97% . .
40	p	118	 87% 12% .
41	q	103	 94% 6%
42	r	110	 95% . .
43	s	100	 87% 6% 7%
44	t	104	 7% 96% . .
45	u	94	 98% . .
46	v	85	 11% 93% 6% .
47	w	78	 96% . .
48	x	63	 90% . . 5%
49	y	59	 90% 7% . .
50	z	57	 86% 9% 5%
51	0	55	 85% 5% 9%
52	1	46	 96% . .

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Mol	Chain	Length	Quality of chain
53	2	65	<div><div></div><div>91%</div><div>8%</div><div></div></div>
54	3	38	<div><div></div><div>92%</div><div>8%</div><div></div></div>
55	4	70	<div><div></div><div>41%</div><div>83%</div><div></div><div>13%</div></div>

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151117 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1519	Total	C	N	O	P	0	0
			32602	14549	5979	10555	1519		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1693	1071	305	309	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.



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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	22	Total	C	N	O	P	0	0
			474	212	88	152	22		

- Molecule 23 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	73	Total	C	N	O	P	S	0	0
			1572	704	283	510	73	2		

- Molecule 24 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	73	Total	C	N	O	P	S	0	0
			1565	698	288	505	73	1		
24	5	71	Total	C	N	O	P	S	3	0
			1583	708	294	507	73	1		

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	2853	Total	C	N	O	P	14	0
			61561	27466	11327	19901	2867		

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	201	Total	C	N	O	S	19	0
			1692	1057	316	314	5		

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	168	Total	C	N	O	S	0	0
			1255	791	228	234	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 34 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A7ZSK2

- Molecule 37 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 49 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 51 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 52 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 53 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	61	Total	C	N	O	S	0	0
			487	304	91	86	6		

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	28	Total	K	0
			28	28	
56	F	1	Total	K	0
			1	1	
56	M	1	Total	K	0
			1	1	
56	a	107	Total	K	0
			107	107	
56	b	1	Total	K	0
			1	1	
56	c	3	Total	K	0
			3	3	
56	e	1	Total	K	0
			1	1	
56	v	1	Total	K	0
			1	1	

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

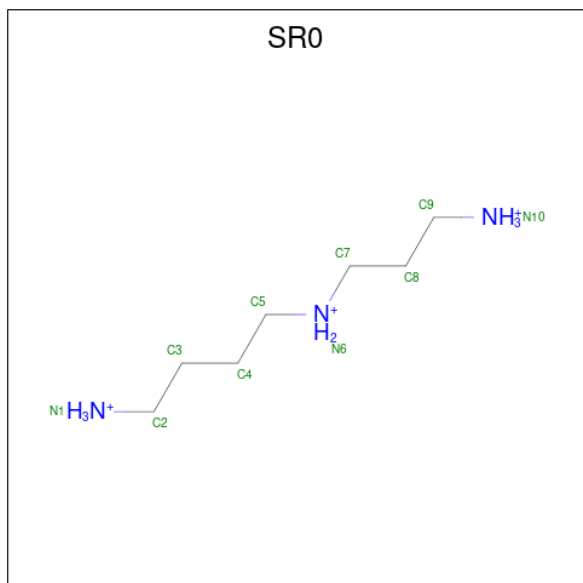
Mol	Chain	Residues	Atoms		AltConf
57	A	78	Total	Mg	0
			78	78	
57	a	247	Total	Mg	0
			247	247	
57	b	5	Total	Mg	0
			5	5	
57	c	3	Total	Mg	0
			3	3	
57	d	1	Total	Mg	0
			1	1	

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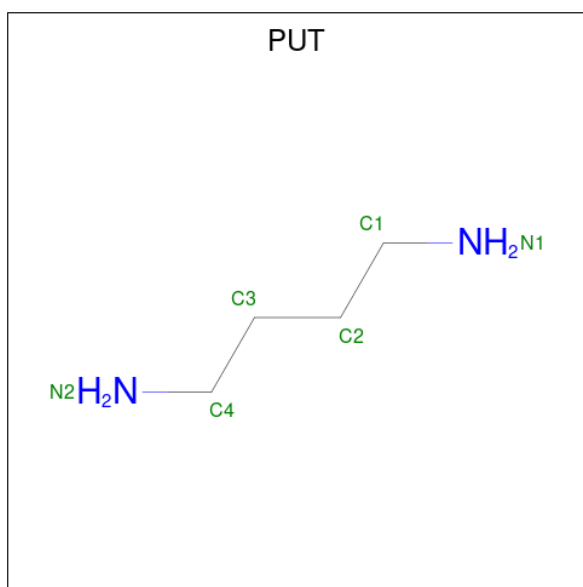
Mol	Chain	Residues	Atoms		AltConf
57	p	1	Total	Mg	0
			1	1	
57	z	2	Total	Mg	0
			2	2	

- Molecule 58 is N 1 -(3-azaniumylpropyl)butane-1,4-diaminium (CCD ID: SR0) (formula:  $C_7H_{22}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	
58	a	1	Total	C	N	0
			10	7	3	

- Molecule 59 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

- Molecule 61 is water.



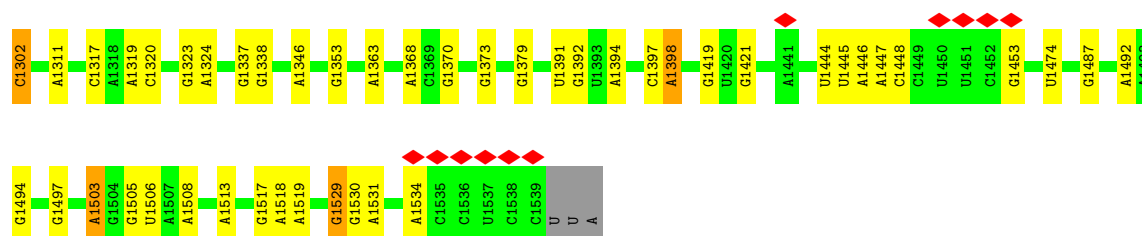
Mol	Chain	Residues	Atoms		AltConf
61	A	288	Total 288	O 288	0
61	D	1	Total 1	O 1	0
61	E	1	Total 1	O 1	0
61	G	1	Total 1	O 1	0
61	H	2	Total 2	O 2	0
61	J	1	Total 1	O 1	0
61	K	1	Total 1	O 1	0
61	L	3	Total 3	O 3	0
61	N	1	Total 1	O 1	0
61	O	2	Total 2	O 2	0
61	P	2	Total 2	O 2	0
61	R	1	Total 1	O 1	0
61	a	3739	Total 3739	O 3739	0
61	b	1	Total 1	O 1	0
61	c	116	Total 116	O 116	0
61	d	77	Total 77	O 77	0
61	e	45	Total 45	O 45	0
61	g	2	Total 2	O 2	0
61	h	1	Total 1	O 1	0
61	i	44	Total 44	O 44	0
61	j	30	Total 30	O 30	0
61	k	55	Total 55	O 55	0

*Continued on next page...*

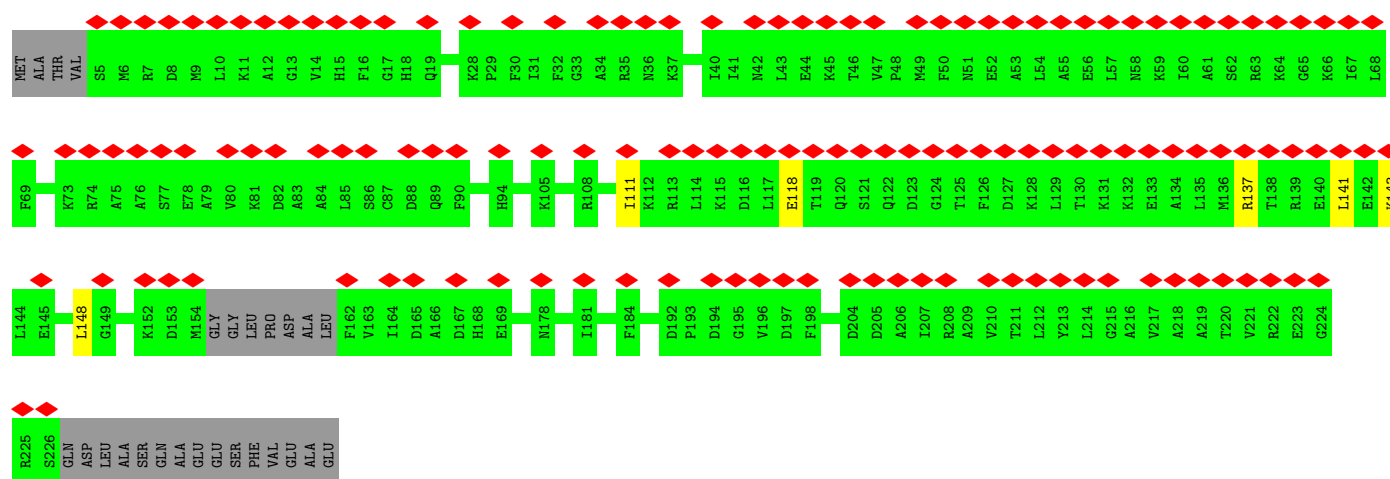
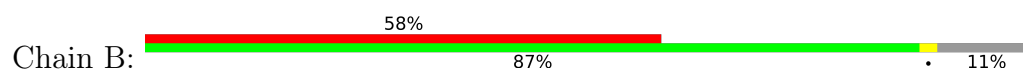
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
61	l	49	Total 49	O 49	0
61	m	47	Total 47	O 47	0
61	o	28	Total 28	O 28	0
61	p	60	Total 60	O 60	0
61	q	30	Total 30	O 30	0
61	r	50	Total 50	O 50	0
61	s	22	Total 22	O 22	0
61	t	13	Total 13	O 13	0
61	u	17	Total 17	O 17	0
61	v	19	Total 19	O 19	0
61	w	28	Total 28	O 28	0
61	x	8	Total 8	O 8	0
61	y	19	Total 19	O 19	0
61	z	39	Total 39	O 39	0
61	0	7	Total 7	O 7	0
61	1	34	Total 34	O 34	0
61	2	31	Total 31	O 31	0
61	3	7	Total 7	O 7	0

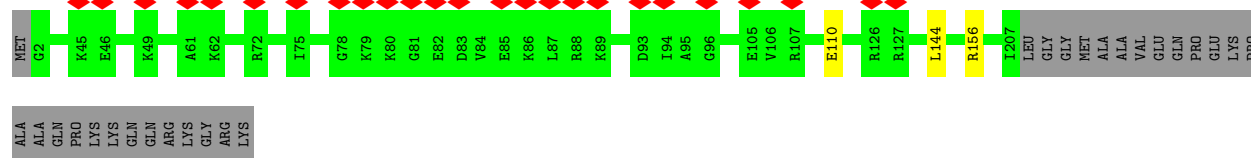
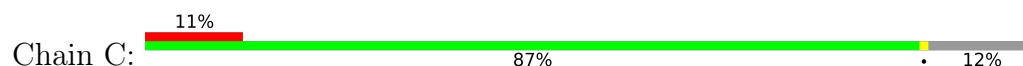




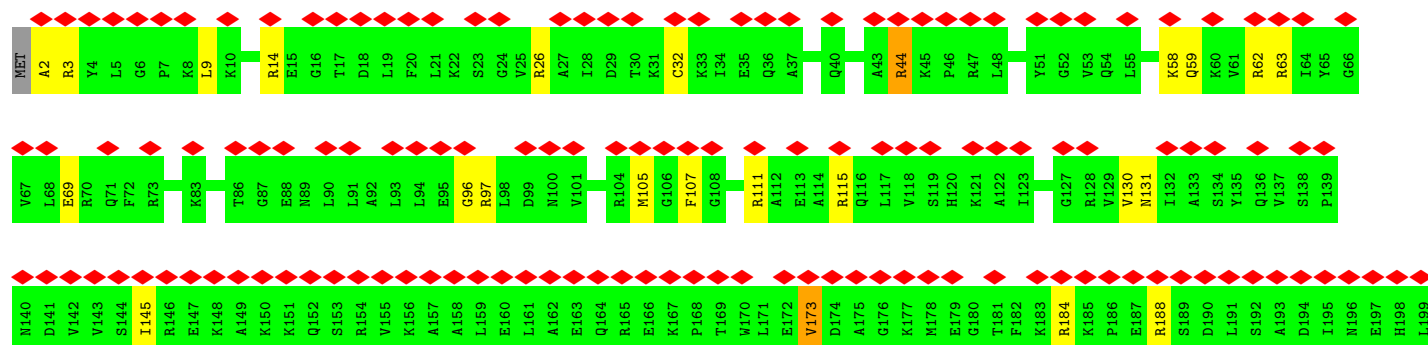
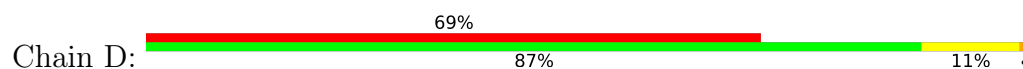
• Molecule 2: Small ribosomal subunit protein uS2

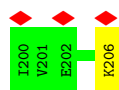


• Molecule 3: Small ribosomal subunit protein uS3

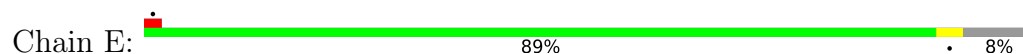


• Molecule 4: Small ribosomal subunit protein uS4

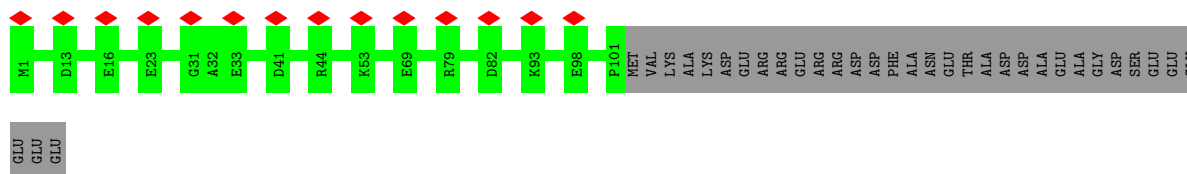
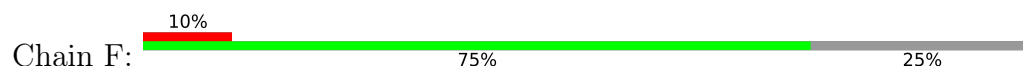




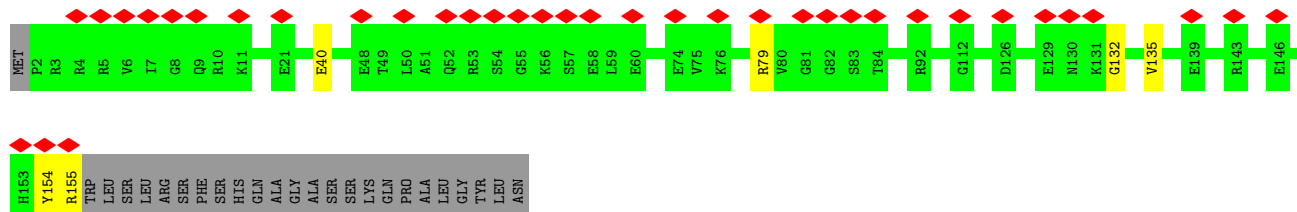
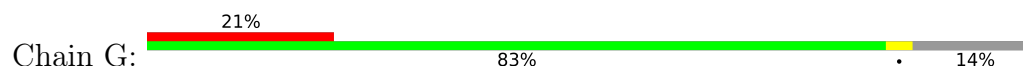
- Molecule 5: Small ribosomal subunit protein uS5



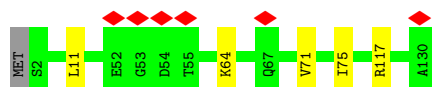
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



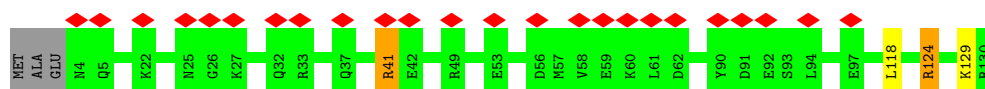
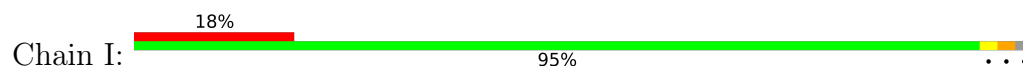
- Molecule 7: Small ribosomal subunit protein uS7



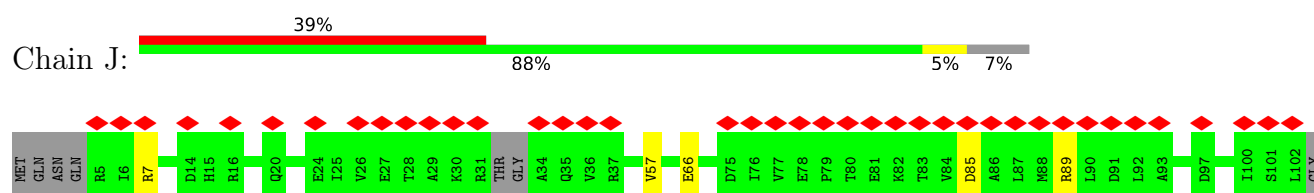
- Molecule 8: Small ribosomal subunit protein uS8



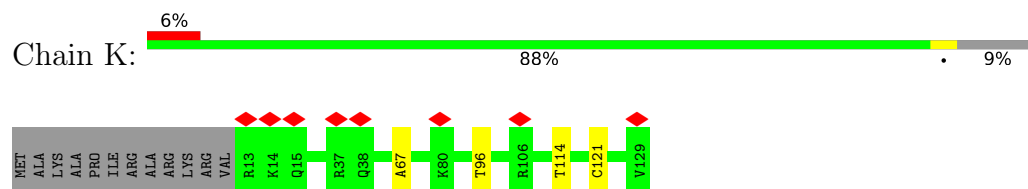
- Molecule 9: Small ribosomal subunit protein uS9



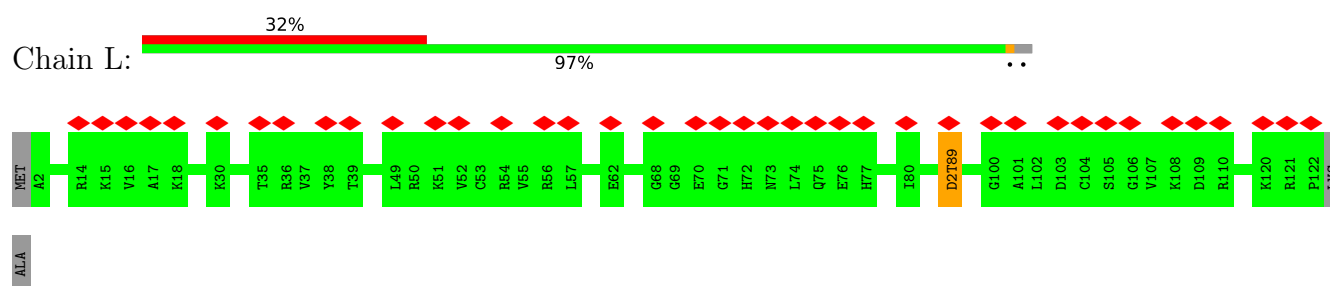
- Molecule 10: Small ribosomal subunit protein uS10



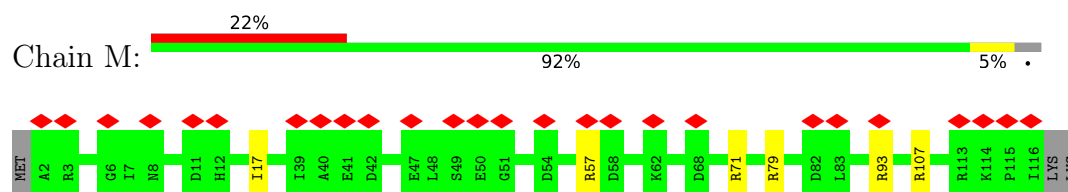
- Molecule 11: Small ribosomal subunit protein uS11



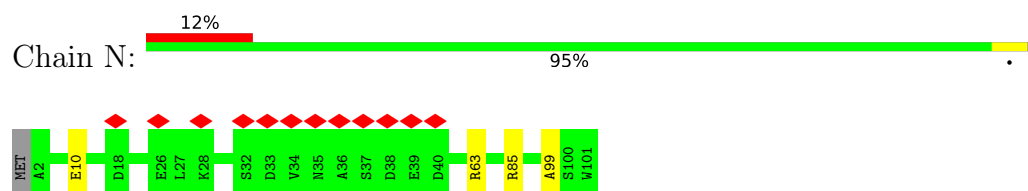
- Molecule 12: Small ribosomal subunit protein uS12



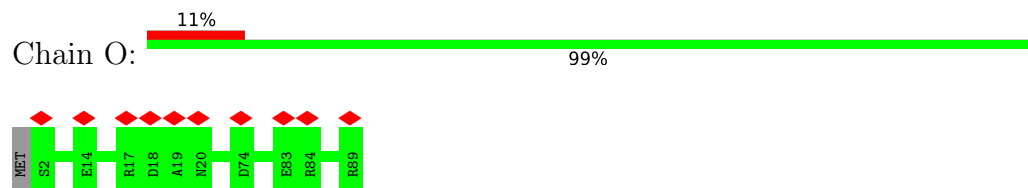
- Molecule 13: Small ribosomal subunit protein uS13



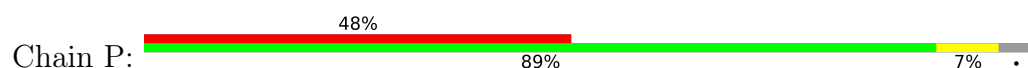
- Molecule 14: Small ribosomal subunit protein uS14

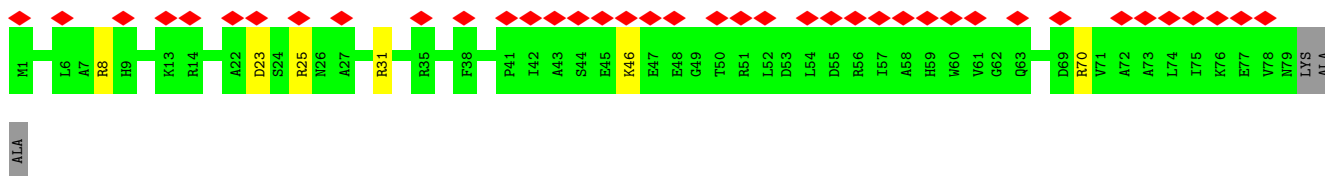


- Molecule 15: Small ribosomal subunit protein uS15

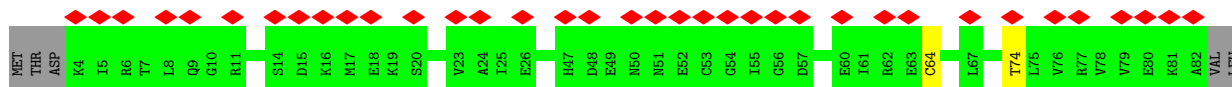
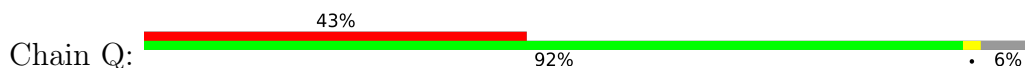


- Molecule 16: Small ribosomal subunit protein bS16

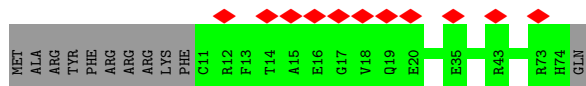
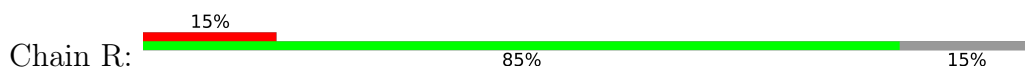




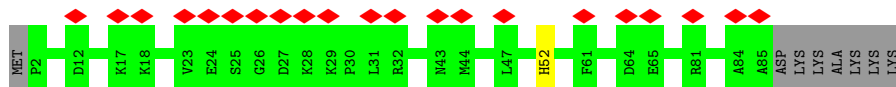
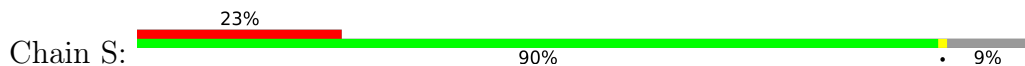
- Molecule 17: Small ribosomal subunit protein uS17



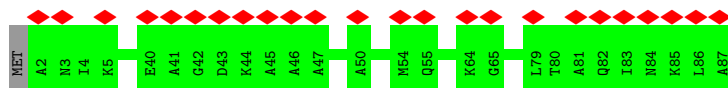
- Molecule 18: Small ribosomal subunit protein bS18



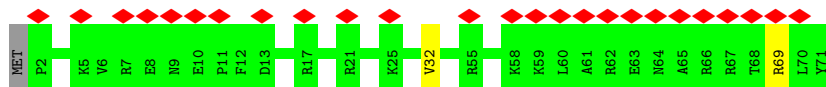
- Molecule 19: Small ribosomal subunit protein uS19



- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein bS21



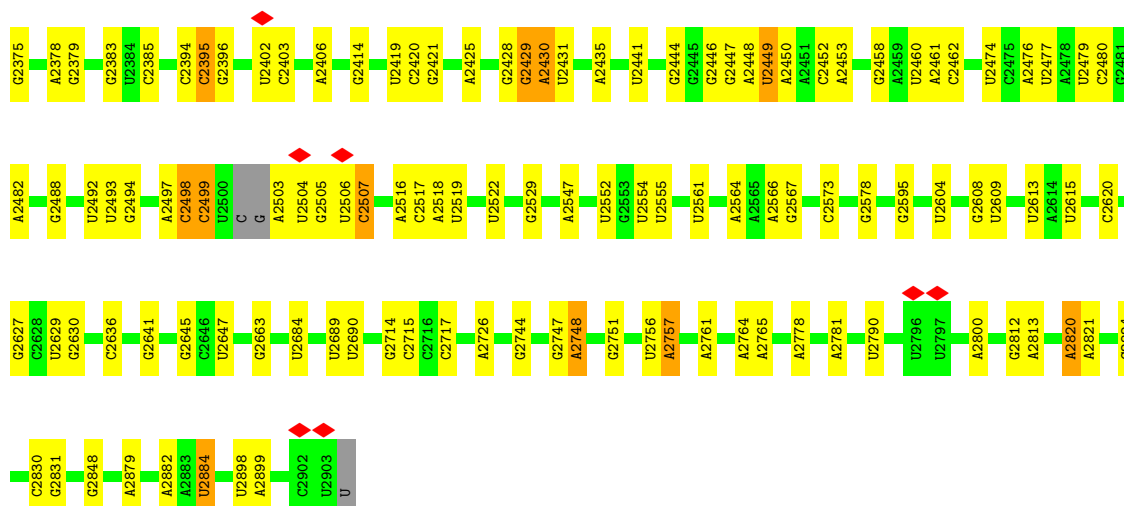
- Molecule 22: mRNA



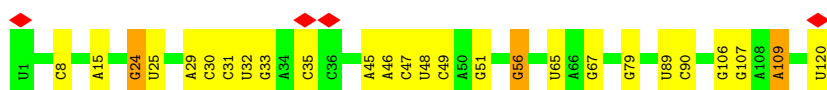
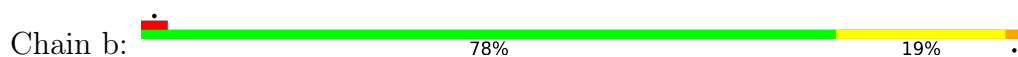








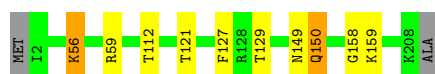
• Molecule 26: 5S rRNA



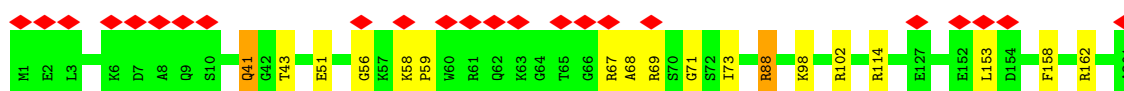
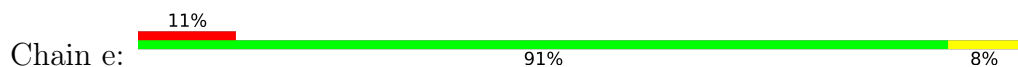
• Molecule 27: Large ribosomal subunit protein uL2



• Molecule 28: Large ribosomal subunit protein uL3



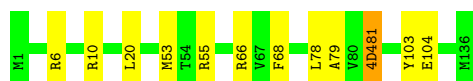
• Molecule 29: Large ribosomal subunit protein uL4



• Molecule 30: Large ribosomal subunit protein uL5







- Molecule 37: Large ribosomal subunit protein bL17

Chain m: 87% 6% 7%



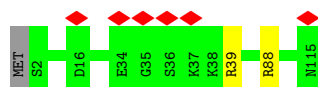
- Molecule 38: Large ribosomal subunit protein uL18

Chain n: 97% ..



- Molecule 39: Large ribosomal subunit protein bL19

Chain o: 5% 97% ..



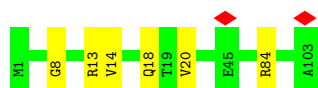
- Molecule 40: Large ribosomal subunit protein bL20

Chain p: 87% 12% .



- Molecule 41: Large ribosomal subunit protein bL21

Chain q: 94% 6% .

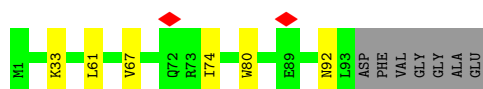
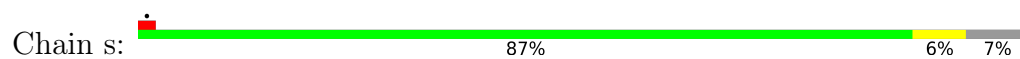


- Molecule 42: Large ribosomal subunit protein uL22

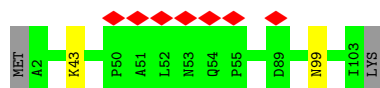
Chain r: 95% . .



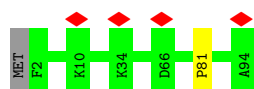
- Molecule 43: Large ribosomal subunit protein uL23



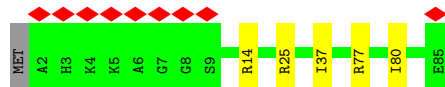
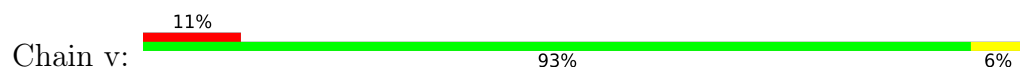
- Molecule 44: Large ribosomal subunit protein uL24



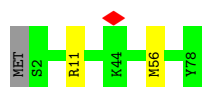
- Molecule 45: Large ribosomal subunit protein bL25



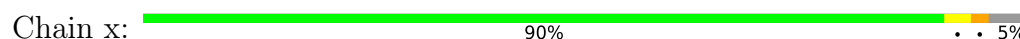
- Molecule 46: Large ribosomal subunit protein bL27



- Molecule 47: Large ribosomal subunit protein bL28




- Molecule 48: Large ribosomal subunit protein uL29



- Molecule 49: Large ribosomal subunit protein uL30




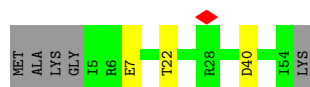
- Molecule 50: Large ribosomal subunit protein bL32

Chain z:  86% 9% 5%



- Molecule 51: Large ribosomal subunit protein bL33

Chain 0:  85% 5% 9%



- Molecule 52: Large ribosomal subunit protein bL34

Chain 1:  96% ..



- Molecule 53: Large ribosomal subunit protein bL35

Chain 2:  91% 8% .




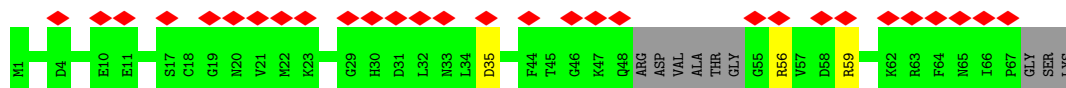
- Molecule 54: Large ribosomal subunit protein bL36A

Chain 3:  92% 8%



- Molecule 55: Large ribosomal subunit protein bL31A

Chain 4:  41% 83% 13%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	910722	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 ( $e^-/\text{\AA}^2$ )	30.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	420.608, 420.608, 420.608	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8215, 0.8215, 0.8215	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 5MC, ZN, MG, G7M, 3TD, 1MG, 2MG, PUT, 4OC, IAS, 4SU, 4D4, OMC, MEQ, PSU, D2T, SR0, OMU, 6MZ, K, 5MU, MIA, H2U, MA6, MS6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.55	0/36223	0.96	68/56497 (0.1%)
2	B	0.51	0/1722	1.01	0/2316
3	C	0.50	0/1651	0.89	0/2225
4	D	0.51	0/1665	1.08	0/2227
5	E	0.55	0/1148	0.95	1/1545 (0.1%)
6	F	0.50	0/843	0.86	0/1140
7	G	0.51	0/1230	0.99	0/1649
8	H	0.51	0/989	0.91	0/1326
9	I	0.50	0/1034	0.94	0/1375
10	J	0.51	0/784	0.97	0/1059
11	K	0.56	0/884	0.93	0/1191
12	L	0.54	0/945	0.95	0/1268
13	M	0.51	0/900	0.97	0/1204
14	N	0.51	0/817	0.93	0/1088
15	O	0.50	0/722	0.96	0/964
16	P	0.63	0/639	1.13	2/859 (0.2%)
17	Q	0.54	0/650	0.93	0/871
18	R	0.52	0/532	0.92	0/715
19	S	0.51	0/685	0.91	0/922
20	T	0.54	0/676	1.07	0/895
21	U	0.53	0/597	1.03	0/792
22	X	0.60	0/530	0.90	0/822
23	Y	0.61	1/1560 (0.1%)	0.86	1/2421 (0.0%)
24	5	0.60	1/1675 (0.1%)	0.80	0/2601
24	Z	0.59	1/1656 (0.1%)	0.95	4/2575 (0.2%)
25	a	0.65	4/68589 (0.0%)	1.07	212/106994 (0.2%)
26	b	0.58	0/2872	1.06	8/4478 (0.2%)
27	c	0.86	0/2121	1.18	5/2852 (0.2%)
28	d	0.81	0/1562	1.06	3/2102 (0.1%)
29	e	0.66	0/1714	1.02	2/2301 (0.1%)
30	f	0.48	0/1434	1.00	1/1926 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	g	0.54	0/1273	0.95	0/1725
32	h	0.49	0/306	0.92	0/413
33	i	0.80	0/1144	1.13	3/1541 (0.2%)
34	j	0.72	0/955	1.10	2/1279 (0.2%)
35	k	0.83	1/1062 (0.1%)	1.13	0/1413
36	l	0.73	0/1073	1.12	1/1433 (0.1%)
37	m	0.89	0/958	1.23	5/1281 (0.4%)
38	n	0.59	0/902	1.00	2/1209 (0.2%)
39	o	0.68	0/929	1.03	0/1242
40	p	0.89	0/960	1.20	7/1278 (0.5%)
41	q	0.71	0/829	1.09	1/1107 (0.1%)
42	r	0.85	0/852	1.05	0/1142
43	s	0.65	0/744	1.02	0/994
44	t	0.60	0/787	0.98	0/1051
45	u	0.63	0/758	1.02	0/1015
46	v	0.80	0/642	1.12	2/848 (0.2%)
47	w	0.79	0/635	1.11	1/848 (0.1%)
48	x	0.52	0/492	0.98	2/655 (0.3%)
49	y	0.72	0/453	0.99	1/605 (0.2%)
50	z	0.82	0/435	1.28	2/581 (0.3%)
51	0	0.65	0/420	0.97	1/560 (0.2%)
52	1	1.00	0/370	1.34	0/487
53	2	0.94	0/513	1.19	1/676 (0.1%)
54	3	0.87	0/303	1.20	2/397 (0.5%)
55	4	0.49	0/496	0.93	0/661
All	All	0.63	8/157340 (0.0%)	1.03	340/235641 (0.1%)

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
2	B	0	1
4	D	0	10
7	G	0	1
8	H	0	1
9	I	0	2
10	J	0	1
13	M	0	3
14	N	0	1
16	P	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
21	U	0	1
25	a	0	35
27	c	0	2
28	d	0	1
29	e	0	5
31	g	0	1
33	i	0	2
35	k	0	1
36	l	0	4
38	n	0	1
39	o	0	2
40	p	0	2
41	q	0	1
46	v	0	1
48	x	0	1
53	2	0	1
54	3	0	2
55	4	0	1
All	All	0	86

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	574	A	O5'-C5'	-7.68	1.31	1.42
25	a	1187	G	O5'-C5'	-6.91	1.32	1.42
25	a	2499	C	P-O5'	6.16	1.69	1.59
25	a	196	A	O5'-C5'	-5.59	1.34	1.42
24	Z	8	4SU	O3'-P	5.31	1.61	1.56
35	k	47	ARG	NE-CZ	-5.15	1.27	1.33
24	5	8	4SU	O3'-P	5.14	1.61	1.56
23	Y	8	4SU	O3'-P	5.12	1.61	1.56

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	980	A	O3'-P-O5'	-17.86	77.22	104.00
25	a	980	A	C4'-C3'-O3'	13.45	133.17	113.00
25	a	1971	U	O3'-P-O5'	-12.25	85.62	104.00
25	a	2498	C	O3'-P-O5'	-11.07	87.40	104.00
25	a	1246	A	O3'-P-O5'	-10.60	88.10	104.00
25	a	2222	C	O3'-P-O5'	-10.35	88.47	104.00
25	a	124	G	O3'-P-O5'	-10.03	88.96	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	1974	C	O3'-P-O5'	-10.01	88.98	104.00
25	a	1905	C	O3'-P-O5'	-9.98	89.03	104.00
25	a	204	A	O3'-P-O5'	-9.88	89.18	104.00
25	a	1643	G	O3'-P-O5'	-9.51	89.74	104.00
25	a	1186	G	O3'-P-O5'	-9.45	89.82	104.00
38	n	20	GLU	CB-CA-C	-9.28	95.96	110.81
25	a	737	C	O3'-P-O5'	-8.97	90.54	104.00
25	a	1565	C	O3'-P-O5'	-8.94	90.59	104.00
25	a	1408	G	O3'-P-O5'	-8.85	90.73	104.00
25	a	2395	C	O3'-P-O5'	-8.83	90.75	104.00
25	a	2494	G	O3'-P-O5'	-8.73	90.90	104.00
25	a	2820	A	C4'-C3'-O3'	-8.60	100.09	113.00
1	A	339	C	O3'-P-O5'	-8.58	91.13	104.00
25	a	130	C	O3'-P-O5'	-8.30	91.55	104.00
1	A	107	G	O3'-P-O5'	-8.27	91.60	104.00
25	a	2224	G	O3'-P-O5'	8.24	116.36	104.00
1	A	1529	G	O3'-P-O5'	-8.22	91.67	104.00
25	a	1959	G	O3'-P-O5'	-8.06	91.91	104.00
40	p	31	VAL	N-CA-CB	-8.05	101.31	111.46
25	a	2761	A	O3'-P-O5'	-8.04	91.93	104.00
25	a	574	A	O5'-P-OP2	8.04	132.11	108.00
25	a	2331	G	C2'-C3'-O3'	-7.91	101.83	113.70
25	a	2479	U	O3'-P-O5'	-7.78	92.33	104.00
25	a	2223	G	C4'-C3'-O3'	-7.57	101.64	113.00
25	a	2458	G	O3'-P-O5'	-7.54	92.70	104.00
25	a	1305	C	O3'-P-O5'	-7.47	92.80	104.00
25	a	1373	A	O3'-P-O5'	-7.46	92.80	104.00
25	a	621	A	O3'-P-O5'	-7.45	92.82	104.00
40	p	11	ARG	NE-CZ-NH2	7.40	125.86	119.20
25	a	146	A	O3'-P-O5'	-7.38	92.93	104.00
26	b	46	A	O3'-P-O5'	-7.37	92.95	104.00
16	P	23	ASP	CA-CB-CG	7.31	119.91	112.60
25	a	2250	G	C1'-C2'-O2'	7.30	122.75	111.80
25	a	2203	U	C4'-C3'-O3'	-7.25	102.12	113.00
1	A	652	U	O3'-P-O5'	-7.23	93.15	104.00
26	b	32	U	O3'-P-O5'	-7.13	93.31	104.00
25	a	781	A	O3'-P-O5'	-7.10	93.35	104.00
25	a	1359	A	O3'-P-O5'	-7.09	93.37	104.00
1	A	835	U	O3'-P-O5'	-7.04	93.44	104.00
25	a	187	G	O3'-P-O5'	-7.00	93.50	104.00
25	a	1857	G	O3'-P-O5'	-6.99	93.51	104.00
37	m	21	PHE	CA-CB-CG	-6.98	106.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	770	G	C4'-C3'-C2'	-6.97	95.63	102.60
27	c	52	ARG	NE-CZ-NH2	6.95	125.45	119.20
25	a	134	G	O3'-P-O5'	-6.90	93.65	104.00
25	a	57	C	O3'-P-O5'	-6.87	93.69	104.00
25	a	2884	U	C2'-C3'-O3'	-6.86	103.41	113.70
33	i	3	THR	CA-CB-OG1	-6.85	99.33	109.60
25	a	622	G	C4'-C3'-O3'	-6.83	102.76	113.00
25	a	676	A	O3'-P-O5'	-6.80	93.81	104.00
25	a	2331	G	O5'-P-OP2	-6.78	87.65	108.00
1	A	786	G	O3'-P-O5'	-6.71	93.94	104.00
25	a	38	A	O3'-P-O5'	-6.68	93.97	104.00
25	a	54	G	O3'-P-O5'	-6.63	94.05	104.00
25	a	2278	A	O3'-P-O5'	-6.62	94.06	104.00
25	a	1866	A	O3'-P-O5'	-6.62	94.07	104.00
1	A	921	U	O3'-P-O5'	-6.60	94.11	104.00
1	A	1474	U	O3'-P-O5'	-6.59	94.11	104.00
25	a	1254	A	C4'-C3'-O3'	-6.57	103.14	113.00
1	A	379	C	O3'-P-O5'	-6.55	94.17	104.00
25	a	982	C	C2'-C3'-O3'	-6.54	103.89	113.70
25	a	1807	G	O3'-P-O5'	-6.53	94.21	104.00
36	l	68	PHE	CA-CB-CG	-6.53	107.28	113.80
1	A	773	G	O3'-P-O5'	-6.52	94.22	104.00
25	a	2050	C	O3'-P-O5'	-6.51	94.24	104.00
40	p	11	ARG	NE-CZ-NH1	-6.50	115.00	121.50
25	a	1434	A	O3'-P-O5'	-6.48	94.28	104.00
25	a	1025	G	O3'-P-O5'	-6.46	94.31	104.00
25	a	41	C	O3'-P-O5'	-6.43	94.35	104.00
25	a	2421	G	O3'-P-O5'	6.41	113.61	104.00
25	a	1410	G	O3'-P-O5'	-6.40	94.40	104.00
1	A	352	C	O3'-P-O5'	-6.38	94.44	104.00
25	a	1154	G	C4'-C3'-O3'	-6.33	103.51	113.00
25	a	1187	G	C5'-C4'-C3'	-6.32	106.52	116.00
25	a	1810	A	O3'-P-O5'	-6.32	94.53	104.00
25	a	868	U	O3'-P-O5'	-6.31	94.53	104.00
1	A	106	C	O3'-P-O5'	-6.28	94.58	104.00
1	A	53	A	O3'-P-O5'	-6.26	94.61	104.00
25	a	271	G	C2'-C3'-O3'	6.26	118.89	109.50
25	a	2045	C	O3'-P-O5'	-6.24	94.64	104.00
25	a	22	C	O3'-P-O5'	-6.24	94.64	104.00
25	a	1485	U	O3'-P-O5'	-6.24	94.64	104.00
16	P	23	ASP	CB-CA-C	6.21	119.59	109.90
27	c	257	THR	CA-CB-OG1	-6.21	100.29	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	8	C	O3'-P-O5'	-6.20	94.70	104.00
1	A	105	G	O4'-C4'-C3'	-6.19	97.81	104.00
25	a	674	G	O3'-P-O5'	-6.18	94.73	104.00
1	A	181	A	O3'-P-O5'	-6.18	94.73	104.00
25	a	906	U	O3'-P-O5'	-6.17	94.74	104.00
24	Z	70	G	O3'-P-O5'	-6.17	94.75	104.00
25	a	1936	A	O4'-C1'-C2'	-6.17	99.63	105.80
25	a	2507	C	C2'-C3'-O3'	-6.15	104.48	113.70
25	a	221	A	O3'-P-O5'	-6.14	94.79	104.00
1	A	362	G	O3'-P-O5'	-6.14	94.80	104.00
28	d	56	LYS	CB-CA-C	-6.13	100.34	109.90
40	p	53	ARG	NE-CZ-NH2	-6.11	113.70	119.20
25	a	574	A	O5'-P-OP1	-6.10	89.70	108.00
37	m	103	ARG	N-CA-CB	-6.10	101.00	109.97
25	a	1606	C	O3'-P-O5'	-6.10	94.85	104.00
1	A	107	G	C3'-C2'-O2'	6.09	119.83	110.70
25	a	1358	G	O3'-P-O5'	-6.07	94.89	104.00
25	a	2884	U	C1'-C2'-O2'	-6.06	99.31	108.40
25	a	2356	U	O3'-P-O5'	-6.04	94.94	104.00
1	A	389	A	C3'-C2'-O2'	6.03	119.75	110.70
25	a	2324	U	C4'-C3'-O3'	-6.02	103.97	113.00
25	a	528	A	O3'-P-O5'	-6.00	95.00	104.00
25	a	2429	G	O3'-P-O5'	-6.00	95.00	104.00
1	A	977	A	O3'-P-O5'	-6.00	95.01	104.00
25	a	510	C	O3'-P-O5'	5.98	112.97	104.00
54	3	24	ARG	NE-CZ-NH1	-5.97	115.53	121.50
25	a	2242	G	O3'-P-O5'	-5.96	95.05	104.00
33	i	111	LYS	CB-CA-C	5.96	119.71	109.51
25	a	1689	A	O3'-P-O5'	-5.94	95.09	104.00
40	p	28	ARG	CG-CD-NE	-5.94	98.93	112.00
25	a	2240	U	O3'-P-O5'	5.94	112.91	104.00
1	A	599	C	O3'-P-O5'	-5.93	95.11	104.00
25	a	1394	U	O3'-P-O5'	-5.91	95.14	104.00
25	a	2027	G	O5'-P-OP2	-5.91	90.28	108.00
25	a	2444	G	O3'-P-O5'	-5.90	95.15	104.00
25	a	2460	U	C2'-C3'-O3'	-5.90	104.85	113.70
25	a	570	G	C4'-C3'-O3'	-5.89	104.16	113.00
37	m	17	ARG	CB-CA-C	-5.89	101.64	110.88
25	a	2223	G	C2'-C3'-O3'	5.88	122.52	113.70
28	d	129	THR	CA-CB-OG1	-5.87	100.80	109.60
25	a	1328	A	O3'-P-O5'	-5.87	95.20	104.00
25	a	1757	A	C4'-C3'-O3'	-5.85	104.23	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	681	G	O3'-P-O5'	-5.83	95.25	104.00
25	a	241	A	O3'-P-O5'	-5.83	95.25	104.00
1	A	886	G	O3'-P-O5'	-5.83	95.26	104.00
1	A	510	A	O3'-P-O5'	-5.82	95.27	104.00
25	a	1261	C	O3'-P-O5'	-5.82	95.27	104.00
38	n	20	GLU	N-CA-CB	5.82	118.61	109.94
1	A	1232	U	O3'-P-O5'	-5.81	95.28	104.00
25	a	2277	G	O3'-P-O5'	-5.81	95.28	104.00
46	v	25	ARG	CG-CD-NE	-5.79	99.26	112.00
40	p	53	ARG	NE-CZ-NH1	5.79	127.29	121.50
27	c	52	ARG	NE-CZ-NH1	-5.78	115.72	121.50
25	a	2715	C	O3'-P-O5'	-5.77	95.34	104.00
46	v	77	ARG	CA-CB-CG	-5.77	102.56	114.10
25	a	1992	G	O3'-P-O5'	-5.76	95.36	104.00
25	a	2019	A	O3'-P-O5'	-5.75	95.37	104.00
1	A	339	C	C4'-C3'-O3'	-5.75	104.37	113.00
25	a	1140	C	C4'-C3'-O3'	-5.74	104.39	113.00
25	a	558	U	O5'-P-OP1	-5.74	90.78	108.00
25	a	1454	C	O3'-P-O5'	-5.73	95.40	104.00
1	A	1065	U	O3'-P-O5'	-5.73	95.41	104.00
50	z	10	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	A	780	A	O3'-P-O5'	-5.71	95.43	104.00
25	a	856	G	C1'-C2'-O2'	5.71	116.97	108.40
25	a	266	G	O3'-P-O5'	-5.70	95.45	104.00
26	b	79	G	C4'-C3'-O3'	-5.70	104.45	113.00
25	a	867	C	O3'-P-O5'	-5.70	95.45	104.00
1	A	112	G	O3'-P-O5'	-5.69	95.46	104.00
25	a	60	G	O3'-P-O5'	-5.69	95.46	104.00
1	A	1235	U	O3'-P-O5'	-5.69	95.47	104.00
25	a	827	U	C2'-C3'-O3'	-5.68	100.98	109.50
25	a	1847	A	O3'-P-O5'	-5.67	95.49	104.00
25	a	379	G	O3'-P-O5'	-5.67	95.49	104.00
25	a	1960	A	C4'-C3'-O3'	-5.67	104.50	113.00
25	a	866	A	O3'-P-O5'	-5.66	95.50	104.00
25	a	2747	G	O3'-P-O5'	-5.66	95.50	104.00
25	a	784	G	P-O3'-C3'	5.66	128.69	120.20
25	a	2879	A	O3'-P-O5'	-5.66	95.51	104.00
48	x	52	ARG	CB-CA-C	-5.64	102.02	110.88
50	z	10	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	8	A	O3'-P-O5'	-5.62	95.58	104.00
25	a	664	G	C4'-C3'-C2'	-5.60	97.00	102.60
25	a	2010	G	C4'-C3'-C2'	-5.60	97.00	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	1969	A	O3'-P-O5'	-5.60	95.60	104.00
25	a	256	A	C2'-C3'-O3'	-5.60	105.31	113.70
1	A	790	A	O3'-P-O5'	-5.59	95.62	104.00
25	a	2764	A	O3'-P-O5'	-5.59	95.62	104.00
25	a	1313	U	C2'-C3'-O3'	-5.57	105.34	113.70
25	a	2279	G	O3'-P-O5'	-5.56	95.67	104.00
26	b	65	U	O3'-P-O5'	-5.55	95.67	104.00
53	2	45	ARG	CB-CA-C	-5.55	103.99	113.04
1	A	598	U	O3'-P-O5'	-5.55	95.68	104.00
25	a	1467	U	O3'-P-O5'	-5.54	95.69	104.00
1	A	576	C	O3'-P-O5'	-5.54	95.69	104.00
25	a	2330	G	O3'-P-O5'	5.54	112.31	104.00
25	a	418	C	O3'-P-O5'	5.53	112.30	104.00
25	a	2365	G	O3'-P-O5'	-5.53	95.71	104.00
25	a	1284	A	O3'-P-O5'	-5.53	95.71	104.00
25	a	2717	C	O3'-P-O5'	-5.52	95.73	104.00
25	a	13	A	C3'-C2'-O2'	-5.51	106.33	114.60
25	a	1331	G	O3'-P-O5'	-5.51	95.73	104.00
1	A	1043	G	O3'-P-O5'	-5.51	95.74	104.00
25	a	1659	G	O3'-P-O5'	-5.50	95.74	104.00
25	a	2477	U	O3'-P-O5'	-5.50	95.75	104.00
25	a	62	U	O3'-P-O5'	-5.49	95.77	104.00
25	a	1895	C	O3'-P-O5'	-5.49	95.77	104.00
29	e	98	LYS	CB-CA-C	-5.49	101.36	110.68
25	a	1607	C	C2'-C3'-O3'	5.48	117.72	109.50
1	A	1247	U	O3'-P-O5'	-5.48	95.78	104.00
48	x	52	ARG	CG-CD-NE	-5.48	99.94	112.00
25	a	495	G	O3'-P-O5'	-5.47	95.79	104.00
25	a	2041	U	C2'-C3'-O3'	-5.47	105.49	113.70
27	c	217	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	1190	G	O3'-P-O5'	-5.47	95.79	104.00
1	A	652	U	C2'-C3'-O3'	5.47	117.70	109.50
25	a	1251	C	O3'-P-O5'	-5.47	95.80	104.00
40	p	57	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	297	G	O3'-P-O5'	-5.46	95.81	104.00
1	A	938	A	O3'-P-O5'	-5.46	95.81	104.00
1	A	1398	A	P-O5'-C5'	-5.46	112.71	120.90
1	A	353	A	O3'-P-O5'	-5.45	95.82	104.00
25	a	12	U	O3'-P-O5'	-5.45	95.82	104.00
25	a	2203	U	O3'-P-O5'	-5.45	95.82	104.00
1	A	65	A	C2'-C3'-O3'	5.45	117.67	109.50
37	m	49	GLU	CB-CG-CD	5.45	121.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1311	A	O3'-P-O5'	-5.45	95.83	104.00
1	A	563	A	O3'-P-O5'	-5.45	95.83	104.00
25	a	2414	G	C4'-C3'-C2'	-5.45	97.15	102.60
25	a	1168	G	O3'-P-O5'	-5.44	95.84	104.00
25	a	2561	U	O3'-P-O5'	-5.44	95.84	104.00
26	b	48	U	O3'-P-O5'	-5.43	95.86	104.00
1	A	1044	A	O3'-P-O5'	-5.42	95.87	104.00
25	a	1755	A	O3'-P-O5'	5.42	112.14	104.00
25	a	2331	G	C3'-C2'-C1'	5.42	106.72	101.30
25	a	2378	A	O3'-P-O5'	-5.42	95.88	104.00
25	a	980	A	C5'-C4'-O4'	-5.41	101.68	109.80
25	a	2012	G	O3'-P-O5'	-5.40	95.90	104.00
24	Z	45	G	O3'-P-O5'	-5.40	95.91	104.00
1	A	338	A	O3'-P-O5'	-5.39	95.91	104.00
24	Z	59	A	O3'-P-O5'	-5.39	95.91	104.00
1	A	365	U	O3'-P-O5'	-5.39	95.92	104.00
25	a	1187	G	C4'-C3'-O3'	-5.39	104.92	113.00
25	a	2051	A	O3'-P-O5'	-5.39	95.92	104.00
1	A	1421	G	O3'-P-O5'	-5.38	95.93	104.00
25	a	2824	C	O3'-P-O5'	-5.38	95.93	104.00
1	A	1373	G	O3'-P-O5'	-5.37	95.94	104.00
25	a	1633	G	O3'-P-O5'	-5.37	95.94	104.00
25	a	2360	G	C4'-C3'-O3'	-5.36	104.96	113.00
25	a	2079	U	O3'-P-O5'	-5.36	95.96	104.00
49	y	47	MET	CG-SD-CE	-5.36	89.11	100.90
25	a	2420	C	O5'-P-OP2	-5.35	91.95	108.00
25	a	2882	A	O3'-P-O5'	-5.34	95.99	104.00
25	a	538	A	C4'-C3'-C2'	-5.34	97.26	102.60
25	a	998	C	O3'-P-O5'	-5.34	95.99	104.00
1	A	107	G	C2'-C3'-O3'	5.33	121.70	113.70
25	a	573	U	O3'-P-O5'	-5.32	96.01	104.00
25	a	2831	G	O3'-P-O5'	-5.32	96.02	104.00
34	j	20	MET	CG-SD-CE	-5.32	89.19	100.90
26	b	49	C	O3'-P-O5'	-5.32	96.02	104.00
1	A	176	C	O3'-P-O5'	-5.32	96.02	104.00
25	a	1151	A	C1'-C2'-O2'	5.32	116.38	108.40
25	a	1351	C	O3'-P-O5'	-5.32	96.03	104.00
25	a	1016	G	O3'-P-O5'	-5.31	96.03	104.00
47	w	11	ARG	NE-CZ-NH2	5.31	123.98	119.20
25	a	2519	U	O3'-P-O5'	-5.30	96.05	104.00
25	a	748	G	C1'-O4'-C4'	-5.30	104.60	109.90
1	A	869	G	O3'-P-O5'	-5.30	96.05	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	125	LYS	N-CA-CB	-5.30	102.16	111.17
25	a	2048	G	O3'-P-O5'	-5.30	96.05	104.00
28	d	112	THR	CA-CB-OG1	-5.30	101.66	109.60
25	a	548	G	O3'-P-O5'	5.29	111.94	104.00
25	a	310	A	O3'-P-O5'	-5.29	96.07	104.00
25	a	2620	C	O3'-P-O5'	-5.29	96.07	104.00
25	a	2898	U	O3'-P-O5'	-5.29	96.07	104.00
51	0	7	GLU	N-CA-CB	-5.29	102.02	110.63
25	a	1452	G	O3'-P-O5'	-5.28	96.08	104.00
25	a	334	C	O3'-P-O5'	-5.28	96.08	104.00
25	a	150	U	O3'-P-O5'	-5.27	96.10	104.00
29	e	41	GLN	N-CA-CB	-5.27	102.43	110.33
1	A	694	A	O3'-P-O5'	-5.26	96.11	104.00
1	A	455	G	O3'-P-O5'	-5.26	96.11	104.00
25	a	1301	A	C4'-C3'-C2'	-5.26	97.34	102.60
25	a	2636	C	O3'-P-O5'	-5.25	96.12	104.00
33	i	138	GLN	N-CA-CB	-5.24	101.74	110.23
1	A	340	U	O5'-P-OP2	5.24	123.72	108.00
25	a	109	C	O3'-P-O5'	-5.24	96.14	104.00
34	j	5	GLN	CB-CA-C	-5.24	104.64	109.83
1	A	378	G	O3'-P-O5'	-5.23	96.15	104.00
25	a	2351	G	O3'-P-O5'	-5.23	96.15	104.00
25	a	2608	G	O3'-P-O5'	-5.23	96.16	104.00
25	a	757	G	C4'-C3'-C2'	-5.22	97.38	102.60
1	A	376	G	C4'-C3'-C2'	-5.22	97.38	102.60
37	m	4	ARG	CG-CD-NE	-5.21	100.53	112.00
25	a	1301	A	C5'-C4'-C3'	-5.21	107.38	115.20
1	A	1131	G	O3'-P-O5'	-5.21	96.19	104.00
25	a	696	G	C4'-C3'-C2'	-5.21	97.39	102.60
25	a	1138	G	O3'-P-O5'	-5.21	96.19	104.00
41	q	18	GLN	CB-CA-C	5.20	118.41	109.51
25	a	385	C	O3'-P-O5'	-5.19	96.22	104.00
1	A	1180	A	O3'-P-O5'	-5.17	96.24	104.00
25	a	1648	U	O3'-P-O5'	-5.17	96.24	104.00
25	a	2641	G	C4'-C3'-C2'	-5.17	97.43	102.60
25	a	938	G	C4'-C3'-C2'	-5.17	97.43	102.60
25	a	73	A	O3'-P-O5'	-5.17	96.25	104.00
24	Z	30	G	O3'-P-O5'	-5.16	96.25	104.00
25	a	1612	C	O3'-P-O5'	-5.16	96.25	104.00
1	A	108	G	O4'-C1'-C2'	-5.16	102.44	107.60
54	3	24	ARG	NE-CZ-NH2	5.16	123.84	119.20
25	a	912	C	C4'-C3'-O3'	-5.16	105.26	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	254	G	O3'-P-O5'	-5.15	96.27	104.00
25	a	1009	A	C4'-C3'-O3'	-5.15	105.28	113.00
25	a	1029	A	C3'-C2'-O2'	5.15	118.42	110.70
1	A	347	G	O3'-P-O5'	-5.14	96.30	104.00
25	a	1650	A	O3'-P-O5'	-5.14	96.30	104.00
25	a	1977	A	C2'-C3'-O3'	-5.14	106.00	113.70
25	a	2428	G	C2'-C3'-O3'	-5.13	106.00	113.70
25	a	763	G	C4'-C3'-O3'	-5.13	105.31	113.00
25	a	1812	U	C3'-C2'-O2'	-5.12	103.02	110.70
25	a	871	U	O3'-P-O5'	-5.11	96.33	104.00
25	a	127	A	C4'-C3'-O3'	-5.11	105.33	113.00
1	A	319	G	C4'-C3'-C2'	-5.10	97.50	102.60
1	A	124	C	O3'-P-O5'	-5.09	96.36	104.00
25	a	1930	G	C3'-C2'-C1'	-5.09	96.41	101.50
25	a	1996	C	OP2-P-O3'	-5.09	92.74	108.00
5	E	26	LYS	CB-CA-C	-5.08	102.30	110.74
25	a	2578	G	C4'-C3'-O3'	-5.08	105.38	113.00
30	f	63	GLN	N-CA-CB	-5.08	102.28	110.71
25	a	2316	G	O3'-P-O5'	-5.07	96.39	104.00
1	A	262	A	O3'-P-O5'	-5.06	96.41	104.00
1	A	780	A	C4'-C3'-O3'	-5.06	105.41	113.00
1	A	333	U	O3'-P-O5'	-5.06	96.42	104.00
25	a	1783	A	C4'-C3'-O3'	-5.05	105.42	113.00
25	a	2379	G	O3'-P-O5'	-5.05	96.42	104.00
25	a	2899	A	O3'-P-O5'	-5.05	96.42	104.00
23	Y	40	C	O3'-P-O5'	-5.05	96.42	104.00
25	a	1270	C	C2'-C3'-O3'	-5.05	106.12	113.70
25	a	26	G	C4'-C3'-O3'	-5.04	105.43	113.00
1	A	112	G	C1'-C2'-O2'	5.04	115.96	108.40
1	A	360	G	O3'-P-O5'	-5.04	96.44	104.00
25	a	694	U	O3'-P-O5'	-5.04	96.44	104.00
25	a	2001	C	O3'-P-O5'	-5.04	96.44	104.00
25	a	2292	U	O3'-P-O5'	-5.04	96.45	104.00
25	a	1630	A	C4'-C3'-C2'	-5.03	97.57	102.60
25	a	1929	G	O3'-P-O5'	-5.03	96.45	104.00
26	b	24	G	O3'-P-O5'	-5.03	96.46	104.00
1	A	372	C	O3'-P-O5'	-5.02	96.47	104.00
25	a	1117	C	O3'-P-O5'	-5.02	96.47	104.00
25	a	569	U	C3'-C2'-O2'	5.01	118.22	110.70

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	2	13	ARG	Sidechain
54	3	19	ARG	Sidechain
54	3	36	ARG	Sidechain
55	4	59	ARG	Sidechain
2	B	137	ARG	Sidechain
4	D	111	ARG	Sidechain
4	D	115	ARG	Sidechain
4	D	14	ARG	Sidechain
4	D	184	ARG	Sidechain
4	D	188	ARG	Sidechain
4	D	26	ARG	Sidechain
4	D	3	ARG	Sidechain
4	D	44	ARG	Sidechain
4	D	62	ARG	Sidechain
4	D	63	ARG	Sidechain
7	G	79	ARG	Sidechain
8	H	117	ARG	Sidechain
9	I	124	ARG	Sidechain
9	I	41	ARG	Sidechain
10	J	7	ARG	Sidechain
13	M	107	ARG	Sidechain
13	M	71	ARG	Sidechain
13	M	93	ARG	Sidechain
14	N	85	ARG	Sidechain
16	P	25	ARG	Sidechain
16	P	70	ARG	Sidechain
21	U	69	ARG	Sidechain
25	a	1025	G	Sidechain
25	a	1142	A	Sidechain
25	a	1153	C	Sidechain
25	a	1225	G	Sidechain
25	a	1253	A	Sidechain
25	a	126	A	Sidechain
25	a	1645	G	Sidechain
25	a	1952	A	Sidechain
25	a	2037	A	Sidechain
25	a	2074	U	Sidechain
25	a	2078	C	Sidechain
25	a	2267	A	Sidechain
25	a	2375	G	Sidechain
25	a	249	C	Sidechain
25	a	250	G	Sidechain
25	a	2516	A	Sidechain

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Mol	Chain	Res	Type	Group
25	a	2517	C	Sidechain
25	a	2564	A	Sidechain
25	a	2595	G	Sidechain
25	a	2645	G	Sidechain
25	a	27	G	Sidechain
25	a	2848	G	Sidechain
25	a	395	U	Sidechain
25	a	463	G	Sidechain
25	a	512	G	Sidechain
25	a	555	G	Sidechain
25	a	581	C	Sidechain
25	a	666	A	Sidechain
25	a	675	A	Sidechain
25	a	683	U	Sidechain
25	a	704	G	Sidechain
25	a	795	C	Sidechain
25	a	980	A	Sidechain
25	a	982	C	Sidechain
25	a	984	A	Sidechain
27	c	156	ARG	Sidechain
27	c	217	ARG	Sidechain
28	d	59	ARG	Sidechain
29	e	102	ARG	Sidechain
29	e	114	ARG	Sidechain
29	e	162	ARG	Sidechain
29	e	69[A]	ARG	Sidechain
29	e	88	ARG	Sidechain
31	g	95	ARG	Sidechain
33	i	120	ARG	Sidechain
33	i	96	ARG	Sidechain
35	k	78	ARG	Sidechain
36	l	10	ARG	Sidechain
36	l	55	ARG	Sidechain
36	l	6	ARG	Sidechain
36	l	81	4D4	Mainchain
38	n	16	ARG	Sidechain
39	o	39	ARG	Sidechain
39	o	88	ARG	Sidechain
40	p	13	ARG	Sidechain
40	p	51	ARG	Sidechain
41	q	84	ARG	Sidechain
46	v	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
48	x	52	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32602	0	16421	37	0
2	B	1693	0	1718	2	0
3	C	1624	0	1696	2	0
4	D	1643	0	1707	13	0
5	E	1135	0	1179	2	0
6	F	824	0	815	0	0
7	G	1214	0	1267	3	0
8	H	979	0	1031	2	0
9	I	1022	0	1070	3	0
10	J	775	0	817	2	0
11	K	877	0	884	3	0
12	L	942	0	999	1	0
13	M	891	0	952	3	0
14	N	805	0	844	2	0
15	O	714	0	734	0	0
16	P	629	0	643	2	0
17	Q	641	0	682	1	0
18	R	524	0	543	0	0
19	S	668	0	693	1	0
20	T	670	0	719	0	0
21	U	589	0	629	1	0
22	X	474	0	238	3	0
23	Y	1572	0	811	2	0
24	5	1583	0	814	3	0
24	Z	1565	0	802	0	0
25	a	61561	0	30951	94	0
26	b	2569	0	1301	6	0
27	c	2082	0	2153	5	0
28	d	1552	0	1601	4	0
29	e	1692	0	1763	7	0
30	f	1410	0	1444	2	0
31	g	1255	0	1296	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	h	303	0	327	2	0
33	i	1121	0	1150	1	0
34	j	946	0	1023	3	0
35	k	1053	0	1129	2	0
36	l	1075	0	1145	4	0
37	m	945	0	989	1	0
38	n	892	0	923	1	0
39	o	917	0	962	0	0
40	p	947	0	1019	5	0
41	q	816	0	839	3	0
42	r	845	0	909	2	0
43	s	738	0	807	3	0
44	t	779	0	830	2	0
45	u	745	0	768	1	0
46	v	634	0	653	1	0
47	w	625	0	652	1	0
48	x	491	0	523	1	0
49	y	449	0	488	3	0
50	z	429	0	440	5	0
51	0	413	0	448	2	0
52	1	367	0	404	1	0
53	2	504	0	572	3	0
54	3	302	0	340	0	0
55	4	487	0	485	2	0
56	A	28	0	0	0	0
56	F	1	0	0	0	0
56	M	1	0	0	0	0
56	a	107	0	0	0	0
56	b	1	0	0	0	0
56	c	3	0	0	0	0
56	e	1	0	0	0	0
56	v	1	0	0	0	0
57	A	78	0	0	0	0
57	a	247	0	0	0	0
57	b	5	0	0	0	0
57	c	3	0	0	0	0
57	d	1	0	0	0	0
57	p	1	0	0	0	0
57	z	2	0	0	0	0
58	a	60	0	0	0	0
59	a	54	0	108	2	0
60	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	4	1	0	0	0	0
61	0	7	0	0	0	0
61	1	34	0	0	0	0
61	2	31	0	0	0	0
61	3	7	0	0	0	0
61	A	288	0	0	0	0
61	D	1	0	0	0	0
61	E	1	0	0	0	0
61	G	1	0	0	0	0
61	H	2	0	0	0	0
61	J	1	0	0	0	0
61	K	1	0	0	0	0
61	L	3	0	0	0	0
61	N	1	0	0	0	0
61	O	2	0	0	0	0
61	P	2	0	0	0	0
61	R	1	0	0	0	0
61	a	3739	0	0	5	0
61	b	1	0	0	0	0
61	c	116	0	0	0	0
61	d	77	0	0	0	0
61	e	45	0	0	0	0
61	g	2	0	0	0	0
61	h	1	0	0	0	0
61	i	44	0	0	0	0
61	j	30	0	0	0	0
61	k	55	0	0	0	0
61	l	49	0	0	0	0
61	m	47	0	0	0	0
61	o	28	0	0	0	0
61	p	60	0	0	0	0
61	q	30	0	0	0	0
61	r	50	0	0	0	0
61	s	22	0	0	0	0
61	t	13	0	0	0	0
61	u	17	0	0	0	0
61	v	19	0	0	0	0
61	w	28	0	0	0	0
61	x	8	0	0	0	0
61	y	19	0	0	0	0
61	z	39	0	0	0	0
All	All	151117	0	97150	215	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 (215) 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)
1:A:664:G:H22	1:A:741:G:H1	1.42	0.65
29:e:56[B]:GLY:HA2	29:e:73:ILE:HG12	1.82	0.61
29:e:59[A]:PRO:HG3	29:e:73:ILE:HG23	1.82	0.61
25:a:2447[B]:G:N2	25:a:2450[B]:A:H62	1.98	0.61
25:a:2063:C:H2'	25:a:2064:C:C6	2.35	0.60
25:a:568:U:H1'	25:a:2030:6MZ:H9C1	1.84	0.59
25:a:1939:5MU:OP1	25:a:2604:U:O2'	2.22	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.39	0.57
25:a:1182:G:H2'	25:a:1183:U:O4'	2.06	0.56
1:A:769:G:H4'	1:A:1513:A:H4'	1.87	0.56
25:a:2830:C:H5''	28:d:56:LYS:HE3	1.89	0.55
25:a:1427:A:OP1	61:a:3401:HOH:O	2.18	0.55
25:a:2031:A:C6	25:a:2498:C:H1'	2.43	0.54
25:a:548:G:H3'	25:a:549:G:H5''	1.90	0.53
24:5:35:A:H2'	24:5:37:A:C8	2.44	0.53
25:a:1027:A:C2	25:a:2488:G:H5'	2.44	0.53
31:g:89:LEU:HD22	31:g:162:VAL:HG22	1.90	0.52
25:a:1304:A:N3	61:a:3421:HOH:O	2.34	0.51
25:a:1738:G:HO2'	25:a:1739:A:H8	1.57	0.51
25:a:2552:OMU:H6	25:a:2552:OMU:O5'	2.10	0.51
36:l:66:ARG:NH1	36:l:104:GLU:OE2	2.44	0.51
7:G:154:TYR:O	7:G:155:ARG:C	2.53	0.51
1:A:1397:C:N4	22:X:26:A:H8	2.09	0.50
7:G:132:GLY:O	7:G:135:VAL:HG22	2.12	0.50
13:M:79:ARG:NH2	55:4:56:ARG:NE	2.59	0.50
25:a:1932:A:H2'	25:a:1933:G:O4'	2.11	0.50
1:A:404:G:N7	4:D:2:ALA:HB3	2.26	0.50
25:a:2331:G:H2'	25:a:2332:C:C6	2.47	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.47	0.50
31:g:99:LYS:HD2	31:g:104:ASN:HD22	1.77	0.50
35:k:57:LEU:HD22	53:2:54:ASP:HB3	1.94	0.50
25:a:2394:C:N4	24:5:76[A]:A:C2	2.80	0.49
1:A:677:U:H3	1:A:713:G:H22	1.59	0.49
9:I:118:LEU:HD22	9:I:124:ARG:HG2	1.95	0.49
48:x:9:LYS:O	48:x:60:LYS:NZ	2.45	0.49
3:C:110:GLU:HB2	3:C:144:LEU:HD12	1.94	0.49
25:a:2030:6MZ:C2	25:a:2499:C:H5''	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:267:ILE:HG21	27:c:270:ARG:HD2	1.94	0.49
25:a:2110:G:H3'	25:a:2111:U:H5'	1.94	0.49
25:a:1050:A:C2	25:a:2751:G:C4	3.00	0.48
26:b:24:G:N7	26:b:56:G:H2'	2.27	0.48
1:A:8:A:N6	4:D:206:LYS:HA	2.28	0.48
25:a:1433:A:O2'	25:a:1434:A:H5'	2.13	0.48
25:a:2446[B]:G:H2'	25:a:2447[B]:G:O4'	2.13	0.48
25:a:667:U:O2	53:2:2:PRO:HD2	2.14	0.48
26:b:30:C:H2'	26:b:31:C:H5'	1.95	0.48
1:A:966:2MG:O2'	9:I:129:LYS:O	2.31	0.47
40:p:76:TYR:CZ	40:p:80:ILE:HG13	2.48	0.47
1:A:429:U:H3'	4:D:9:LEU:HD12	1.95	0.47
25:a:2020:A:H5'	50:z:9:THR:CG2	2.45	0.47
22:X:11:G:H2'	22:X:12:G:C8	2.49	0.47
32:h:15:LEU:C	32:h:15:LEU:HD13	2.39	0.47
27:c:29:PRO:HG2	27:c:34:LEU:HD11	1.95	0.47
34:j:107:LEU:O	34:j:109:SER:N	2.47	0.47
25:a:2273:A:H2'	25:a:2274:A:C8	2.50	0.47
25:a:2395:C:H2'	25:a:2396:G:O4'	2.15	0.47
61:a:6659:HOH:O	34:j:67:LYS:HE2	2.15	0.47
40:p:97:ASP:OD2	41:q:13:ARG:NE	2.48	0.47
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.97	0.46
12:L:89:D2T:OD1	12:L:89:D2T:C	2.63	0.46
33:i:114:LEU:HG	33:i:118:MET:HE3	1.96	0.46
1:A:439:U:O2'	4:D:131:ASN:ND2	2.47	0.46
25:a:811:U:H2'	35:k:21:ARG:HA	1.97	0.46
25:a:1840:G:C6	25:a:1841:U:C4	3.04	0.46
10:J:66:GLU:HB2	14:N:99:ALA:HB2	1.98	0.46
17:Q:64:CYS:SG	17:Q:74:THR:HG23	2.55	0.46
28:d:121:THR:HB	28:d:127:PHE:CD2	2.51	0.46
49:y:25:LEU:C	49:y:25:LEU:HD13	2.41	0.46
25:a:1161:C:O2'	41:q:8:GLY:HA2	2.16	0.46
29:e:58[A]:LYS:HG3	29:e:71[A]:GLY:HA2	1.98	0.46
40:p:91:ASP:OD2	40:p:91:ASP:C	2.57	0.46
25:a:1028:A:N6	25:a:1125:G:H2'	2.30	0.46
25:a:1209:U:O2'	25:a:1237:A:N1	2.44	0.46
1:A:1302:C:C5	13:M:17:ILE:HG13	2.51	0.46
29:e:41:GLN:HG2	29:e:43:THR:HG23	1.98	0.46
25:a:2615:U:C2	50:z:4:GLN:HA	2.51	0.45
25:a:2812:G:H2'	25:a:2813:A:O4'	2.16	0.45
1:A:51:A:N7	1:A:114:U:O2'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:ARG:NH2	55:4:35:ASP:HB3	2.31	0.45
25:a:723:C:H2'	25:a:724:U:O4'	2.17	0.45
25:a:2447[B]:G:H22	25:a:2450[B]:A:H62	1.64	0.45
4:D:105:MET:HA	4:D:173:VAL:HG21	1.98	0.45
25:a:2684:U:H4'	34:j:76:VAL:CG2	2.47	0.45
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.99	0.45
36:l:20:LEU:HD13	45:u:81:PRO:HG2	1.99	0.45
1:A:142:G:O2'	1:A:196:A:N1	2.49	0.45
25:a:493:G:H2'	25:a:494:G:O4'	2.16	0.45
27:c:107:PRO:HD2	27:c:110:LEU:HD22	1.99	0.45
32:h:9:VAL:O	32:h:10:ALA:C	2.59	0.45
1:A:125:U:H2'	1:A:126:G:O4'	2.17	0.45
1:A:502:A:H2'	1:A:503:C:O4'	2.17	0.45
10:J:85:ASP:HB3	10:J:89:ARG:HH21	1.82	0.45
43:s:33:LYS:HG2	43:s:80:TRP:CZ3	2.52	0.45
4:D:58:LYS:HG3	4:D:59:GLN:N	2.31	0.44
4:D:107:PHE:HB3	4:D:145:ILE:HD11	2.00	0.44
11:K:114:THR:HG21	21:U:32:VAL:HG21	2.00	0.44
2:B:111:ILE:HD13	2:B:148:LEU:HB3	1.99	0.44
25:a:988:A:OP2	59:a:3014:PUT:H11	2.16	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	0.44
1:A:619:U:O2	4:D:130:VAL:HA	2.17	0.44
25:a:499:U:H5''	44:t:43:LYS:HE2	1.99	0.44
44:t:99:ASN:C	44:t:99:ASN:OD1	2.60	0.44
25:a:639:U:H2'	25:a:640:C:C6	2.53	0.44
25:a:2627:G:O2'	25:a:2781:A:N1	2.44	0.44
1:A:502:A:C2	1:A:544:G:C2	3.06	0.44
1:A:512:U:OP1	4:D:44:ARG:NH2	2.49	0.44
25:a:2498:C:C2'	25:a:2499:C:O5'	2.66	0.44
25:a:2497:A:N3	25:a:2498:C:N4	2.65	0.44
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.99	0.43
25:a:1739:A:H2'	25:a:1740:G:O4'	2.17	0.43
25:a:2522:U:O2'	25:a:2647:U:OP1	2.33	0.43
1:A:927:G:O2'	1:A:1503:A:N7	2.48	0.43
25:a:460:A:OP1	52:1:41:ARG:NH1	2.51	0.43
28:d:149:ASN:OD1	28:d:150:MEQ:N	2.51	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.43
4:D:9:LEU:HD13	4:D:32:CYS:HB3	2.00	0.43
27:c:78:VAL:HG21	27:c:110:LEU:HD21	2.00	0.43
28:d:158:GLY:O	28:d:159:LYS:C	2.61	0.43
1:A:1220:G:O2'	19:S:52:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:157:C:H2'	25:a:158:U:O4'	2.19	0.43
36:l:53:MET:HE1	36:l:103:TYR:CG	2.54	0.43
25:a:642:U:O2'	25:a:644:A:N7	2.51	0.43
25:a:1607:C:H4'	25:a:1608:A:O5'	2.18	0.43
1:A:986:U:H2'	1:A:987:G:O4'	2.19	0.43
25:a:265:A:N1	25:a:427:U:O2'	2.49	0.43
25:a:570:G:H2'	25:a:2030:6MZ:N7	2.34	0.43
25:a:2291:U:H2'	25:a:2292:U:C6	2.54	0.43
1:A:778:G:O2'	11:K:121:CYS:HB3	2.19	0.42
50:z:55:ILE:HG13	50:z:55:ILE:O	2.17	0.42
1:A:546:A:P	4:D:69:GLU:HB3	2.59	0.42
1:A:1444:U:H2'	1:A:1445:U:C6	2.54	0.42
25:a:2030:6MZ:N3	25:a:2499:C:H5''	2.34	0.42
25:a:677:A:OP1	59:a:3008:PUT:N2	2.51	0.42
25:a:1263:U:O2'	50:z:8:PRO:HD2	2.19	0.42
25:a:2110:G:H3'	25:a:2111:U:C5'	2.48	0.42
36:l:78:LEU:O	36:l:79:ALA:HB3	2.19	0.42
40:p:41:LYS:HA	40:p:44:GLN:HE21	1.84	0.42
1:A:392:C:OP1	16:P:8:ARG:NH2	2.52	0.42
25:a:118:A:N3	25:a:178:G:H1'	2.34	0.42
25:a:1048:A:N7	25:a:1111:A:C6	2.88	0.42
5:E:38:VAL:HG11	5:E:114:VAL:HG22	2.01	0.42
25:a:479:A:N3	25:a:481:G:H5''	2.34	0.42
25:a:2748:A:O2'	31:g:63:ALA:O	2.33	0.42
25:a:2020:A:H5'	50:z:9:THR:HG21	2.01	0.42
29:e:67[B]:ARG:O	29:e:68[B]:ALA:HB2	2.20	0.42
51:0:40:ASP:OD1	51:0:40:ASP:C	2.63	0.42
25:a:1736:U:H2'	25:a:1737:G:O4'	2.19	0.42
25:a:2756:U:H1'	25:a:2757:A:H5''	2.02	0.42
41:q:14:VAL:HG11	41:q:20:VAL:HG21	2.00	0.42
37:m:55:ALA:HA	37:m:80:PHE:CE2	2.55	0.42
25:a:1199:U:H1'	40:p:4:VAL:HG22	2.02	0.41
7:G:40:GLU:CD	9:I:41:ARG:HH22	2.27	0.41
25:a:207:A:H2'	25:a:208:C:O4'	2.20	0.41
25:a:1853:A:N1	25:a:2087:G:H1'	2.35	0.41
25:a:2448[A]:A:H4'	25:a:2449[A]:H2U:OP2	2.20	0.41
43:s:61:LEU:HD12	43:s:61:LEU:C	2.45	0.41
1:A:134:G:H1'	1:A:325:A:C5	2.55	0.41
23:Y:1:G:C2	23:Y:73:A:C4	3.08	0.41
23:Y:63:G:O2'	25:a:2482:A:H4'	2.20	0.41
25:a:120:U:H5''	25:a:122:G:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:2061:G:C2	25:a:2503:A:O4'	2.73	0.41
43:s:67:VAL:CG1	43:s:74:ILE:HD11	2.50	0.41
1:A:1004:A:H2'	1:A:1005:A:O4'	2.20	0.41
61:a:4405:HOH:O	42:r:98:LYS:HE2	2.21	0.41
30:f:101:GLU:O	30:f:102:ARG:C	2.63	0.41
49:y:44:ILE:HD13	49:y:47:MET:CE	2.51	0.41
22:X:16:A:N6	24:5:34:C:C4	2.89	0.41
25:a:948:C:H1'	25:a:984:A:C8	2.55	0.41
25:a:1021:A:H3'	25:a:1021:A:N3	2.35	0.41
25:a:2238:G:N3	25:a:2238:G:H2'	2.36	0.41
25:a:2461:A:H2'	25:a:2462:C:C6	2.56	0.41
25:a:634:C:H2'	25:a:635:C:C6	2.56	0.41
49:y:24:LEU:HD11	49:y:54:MET:CE	2.50	0.41
25:a:2419:U:H4'	51:0:22:THR:HG21	2.03	0.41
29:e:51:GLU:OE2	29:e:88:ARG:NH1	2.54	0.41
1:A:673:A:H2'	1:A:674:G:C8	2.56	0.41
1:A:1323:G:H2'	1:A:1324:A:C8	2.56	0.41
5:E:56:VAL:N	5:E:57:PRO:HD2	2.36	0.41
25:a:614:A:H3'	25:a:615:U:H5''	2.02	0.41
25:a:1313:U:O2	25:a:1313:U:C2'	2.69	0.41
25:a:1720:U:H2'	25:a:1721:G:O4'	2.20	0.41
25:a:1878:G:H2'	25:a:1879:C:O4'	2.21	0.41
25:a:2554:U:H2'	25:a:2555:U:C6	2.56	0.41
26:b:15:A:O4'	26:b:109:A:C8	2.74	0.41
26:b:51:G:OP1	38:n:63:LYS:HE3	2.21	0.41
42:r:20:VAL:HG11	42:r:44:ALA:HA	2.03	0.41
1:A:310:G:H5''	16:P:31:ARG:HB2	2.02	0.41
1:A:1288:A:H2'	1:A:1289:A:O4'	2.22	0.41
11:K:67:ALA:HB2	11:K:96:THR:HG23	2.03	0.41
25:a:460:A:H2'	25:a:461:C:O4'	2.21	0.41
25:a:2430:A:N3	25:a:2430:A:H2'	2.35	0.41
1:A:8:A:C6	4:D:206:LYS:HA	2.57	0.40
25:a:476:G:H4'	25:a:502:A:N1	2.36	0.40
25:a:844:A:N3	61:a:3431:HOH:O	2.37	0.40
25:a:1370:C:H2'	25:a:1371:G:O4'	2.22	0.40
25:a:2492[B]:U:H2'	25:a:2493:U:C6	2.55	0.40
26:b:106:G:H2'	26:b:107:G:O4'	2.21	0.40
30:f:40:VAL:HB	30:f:85:ILE:O	2.20	0.40
47:w:56:MET:HE3	47:w:56:MET:HB2	1.86	0.40
1:A:1055:A:H2'	3:C:156:ARG:HD2	2.03	0.40
2:B:118:GLU:HA	2:B:141:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:242:G:H5''	53:2:64:TYR:CE2	2.56	0.40
25:a:2038:G:H2'	25:a:2039:U:O4'	2.20	0.40
25:a:2343:U:O2'	25:a:2373:G:O2'	2.35	0.40
25:a:2498:C:H2'	25:a:2499:C:O5'	2.21	0.40
29:e:153:LEU:HD11	29:e:158:PHE:HB2	2.02	0.40
25:a:644:A:H2'	25:a:645:C:O4'	2.21	0.40
25:a:1980:G:O2'	25:a:1982:U:OP2	2.36	0.40
25:a:2452[A]:C:C4	25:a:2453[A]:A:C6	3.09	0.40
27:c:37:ASN:HB2	27:c:62:TYR:HB2	2.02	0.40
1:A:918:A:H2'	1:A:919:A:O4'	2.22	0.40
25:a:2169:A:H2'	25:a:2170:A:C8	2.56	0.40
26:b:29:A:H2'	26:b:30:C:O4'	2.21	0.40
46:v:37:ILE:HG21	46:v:80:ILE:HG21	2.03	0.40
4:D:96:GLY:O	4:D:97:ARG:C	2.65	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	211/241 (88%)	199 (94%)	12 (6%)	0	100	100
3	C	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
4	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	E	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
6	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
7	G	152/179 (85%)	149 (98%)	3 (2%)	0	100	100
8	H	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
9	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	J	92/103 (89%)	90 (98%)	1 (1%)	1 (1%)	11	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
12	L	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
13	M	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
14	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	77/82 (94%)	74 (96%)	2 (3%)	1 (1%)	9	2
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	62/75 (83%)	59 (95%)	3 (5%)	0	100	100
19	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
27	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
28	d	204/209 (98%)	199 (98%)	5 (2%)	0	100	100
29	e	218/201 (108%)	208 (95%)	10 (5%)	0	100	100
30	f	175/179 (98%)	160 (91%)	15 (9%)	0	100	100
31	g	164/177 (93%)	159 (97%)	5 (3%)	0	100	100
32	h	39/149 (26%)	33 (85%)	6 (15%)	0	100	100
33	i	139/142 (98%)	139 (100%)	0	0	100	100
34	j	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	5
35	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
36	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
37	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
38	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
39	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
40	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
42	r	107/110 (97%)	104 (97%)	2 (2%)	1 (1%)	14	4
43	s	91/100 (91%)	87 (96%)	3 (3%)	1 (1%)	11	3
44	t	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
45	u	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
46	v	82/85 (96%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	w	75/78 (96%)	75 (100%)	0	0	100	100
48	x	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
49	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	z	52/57 (91%)	52 (100%)	0	0	100	100
51	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
52	1	43/46 (94%)	43 (100%)	0	0	100	100
53	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	3	36/38 (95%)	36 (100%)	0	0	100	100
55	4	57/70 (81%)	55 (96%)	2 (4%)	0	100	100
All	All	5462/5913 (92%)	5298 (97%)	159 (3%)	5 (0%)	49	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
16	P	46	LYS
34	j	108	ARG
43	s	92	ASN
42	r	12	SER

### 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	
2	B	180/199 (90%)	179 (99%)	1 (1%)	78	72
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	171 (99%)	1 (1%)	78	72
5	E	117/126 (93%)	117 (100%)	0	100	100
6	F	88/116 (76%)	88 (100%)	0	100	100
7	G	127/147 (86%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	85/90 (94%)	85 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	101/103 (98%)	101 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	64/65 (98%)	64 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	55/65 (85%)	55 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
27	c	216/218 (99%)	216 (100%)	0	100	100
28	d	162/163 (99%)	162 (100%)	0	100	100
29	e	178/165 (108%)	178 (100%)	0	100	100
30	f	148/150 (99%)	147 (99%)	1 (1%)	76	69
31	g	130/138 (94%)	130 (100%)	0	100	100
32	h	32/114 (28%)	32 (100%)	0	100	100
33	i	115/116 (99%)	115 (100%)	0	100	100
34	j	104/104 (100%)	104 (100%)	0	100	100
35	k	103/103 (100%)	103 (100%)	0	100	100
36	l	107/107 (100%)	107 (100%)	0	100	100
37	m	98/103 (95%)	98 (100%)	0	100	100
38	n	86/87 (99%)	86 (100%)	0	100	100
39	o	99/100 (99%)	99 (100%)	0	100	100
40	p	89/90 (99%)	89 (100%)	0	100	100
41	q	84/84 (100%)	84 (100%)	0	100	100
42	r	92/93 (99%)	92 (100%)	0	100	100
43	s	80/84 (95%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	t	83/85 (98%)	83 (100%)	0	100	100
45	u	77/78 (99%)	77 (100%)	0	100	100
46	v	62/63 (98%)	62 (100%)	0	100	100
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	54/55 (98%)	54 (100%)	0	100	100
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	46/48 (96%)	46 (100%)	0	100	100
51	0	46/49 (94%)	46 (100%)	0	100	100
52	1	37/38 (97%)	37 (100%)	0	100	100
53	2	51/52 (98%)	51 (100%)	0	100	100
54	3	34/34 (100%)	34 (100%)	0	100	100
55	4	56/62 (90%)	56 (100%)	0	100	100
All	All	4563/4825 (95%)	4560 (100%)	3 (0%)	87	85

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

Mol	Chain	Res	Type
2	B	143	LYS
4	D	173	VAL
30	f	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	ASN
2	B	168	HIS
2	B	177	ASN
2	B	178	ASN
3	C	102	ASN
3	C	139	GLN
3	C	140	ASN
4	D	36	GLN
4	D	40	GLN
4	D	41	HIS
4	D	71	GLN
5	E	82	GLN
5	E	132	ASN

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Mol	Chain	Res	Type
5	E	148	ASN
6	F	46	GLN
6	F	68	GLN
7	G	68	ASN
7	G	148	ASN
8	H	21	ASN
9	I	4	ASN
9	I	5	GLN
9	I	31	ASN
9	I	75	GLN
10	J	56	HIS
10	J	58	ASN
12	L	112	GLN
13	M	8	ASN
14	N	4	GLN
14	N	60	GLN
15	O	35	GLN
15	O	40	GLN
15	O	80	GLN
17	Q	9	GLN
19	S	14	HIS
19	S	52	HIS
19	S	83	HIS
20	T	3	ASN
20	T	13	GLN
27	c	90	ASN
27	c	134	ASN
29	e	92	HIS
29	e	94	GLN
30	f	81	GLN
31	g	22	GLN
31	g	30	ASN
31	g	104	ASN
33	i	80	HIS
35	k	35	HIS
35	k	104	GLN
37	m	9	GLN
37	m	18	GLN
38	n	116	GLN
39	o	66	ASN
39	o	115	ASN
40	p	44	GLN

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Mol	Chain	Res	Type
40	p	59	GLN
40	p	72	ASN
40	p	81	ASN
41	q	66	HIS
42	r	9	HIS
43	s	28	ASN
46	v	76	ASN
48	x	15	ASN
48	x	27	ASN
48	x	45	GLN
55	4	20	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1514/1542 (98%)	178 (11%)	23 (1%)
22	X	20/120 (16%)	6 (30%)	0
23	Y	69/76 (90%)	10 (14%)	2 (2%)
24	5	63/77 (81%)	9 (14%)	0
24	Z	70/77 (90%)	11 (15%)	2 (2%)
25	a	2835/2904 (97%)	279 (9%)	0
26	b	119/120 (99%)	11 (9%)	0
All	All	4690/4916 (95%)	504 (10%)	27 (0%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	69	G
1	A	71	A
1	A	72	A
1	A	74	A
1	A	81	A

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Mol	Chain	Res	Type
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	91	U
1	A	94	G
1	A	95	C
1	A	121	U
1	A	131	A
1	A	164	G
1	A	182	A
1	A	183	C
1	A	197	A
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	330	C
1	A	342	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	376	G
1	A	384	G
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C

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Mol	Chain	Res	Type
1	A	423	G
1	A	429	U
1	A	436	C
1	A	445	G
1	A	446	G
1	A	451	A
1	A	453	G
1	A	457	G
1	A	467	U
1	A	468	A
1	A	469	C
1	A	481	G
1	A	484	G
1	A	486	U
1	A	511	C
1	A	518	C
1	A	531	U
1	A	547	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	633	G
1	A	650	G
1	A	653	U
1	A	661	G
1	A	665	A
1	A	723	U
1	A	724	G
1	A	734	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	884	U
1	A	885	G
1	A	890	G
1	A	926	G

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Mol	Chain	Res	Type
1	A	931	C
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G
1	A	994	A
1	A	1003	G
1	A	1004	A
1	A	1024	G
1	A	1025	U
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1039	G
1	A	1042	A
1	A	1043	G
1	A	1044	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1137	C
1	A	1139	G
1	A	1159	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1227	A
1	A	1238	A

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Mol	Chain	Res	Type
1	A	1256	A
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1398	A
1	A	1419	G
1	A	1446	A
1	A	1447	A
1	A	1448	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1534	A
22	X	9	G
22	X	13	U
22	X	22	U
22	X	27	A

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Mol	Chain	Res	Type
22	X	28	G
22	X	29	U
23	Y	5	G
23	Y	7	A
23	Y	8	4SU
23	Y	19	G
23	Y	38	A
23	Y	46	G7M
23	Y	62	C
23	Y	65	G
23	Y	69	G
23	Y	75	C
24	Z	5	G
24	Z	6	G
24	Z	9	G
24	Z	16	C
24	Z	22	G
24	Z	31	G
24	Z	43	A
24	Z	46	G
24	Z	49	G
24	Z	60	U
24	Z	61	C
25	a	10	A
25	a	14	A
25	a	34	U
25	a	71	A
25	a	74	A
25	a	75	G
25	a	101	A
25	a	102	U
25	a	118	A
25	a	119	A
25	a	120	U
25	a	136	G
25	a	140	C
25	a	141	G
25	a	142	A
25	a	147	C
25	a	181	A
25	a	196	A
25	a	199	A

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Mol	Chain	Res	Type
25	a	200	U
25	a	215	G
25	a	216	A
25	a	221	A
25	a	222	A
25	a	248	G
25	a	249	C
25	a	250	G
25	a	272	A
25	a	276	U
25	a	287	G
25	a	291	G
25	a	311	A
25	a	329	G
25	a	330	A
25	a	345	A
25	a	361	G
25	a	362	A
25	a	386	G
25	a	411	G
25	a	412	A
25	a	451	U
25	a	456	C
25	a	481	G
25	a	491	G
25	a	503	A
25	a	504	A
25	a	505	A
25	a	509	C
25	a	532	A
25	a	533	G
25	a	546	U
25	a	547	A
25	a	548	G
25	a	549	G
25	a	563	A
25	a	573	U
25	a	575	A
25	a	603	A
25	a	615	U
25	a	627	A
25	a	637	A

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Mol	Chain	Res	Type
25	a	645	C
25	a	646	U
25	a	647	G
25	a	653	U
25	a	654	A
25	a	686	U
25	a	730	A
25	a	747	5MU
25	a	764	A
25	a	765	C
25	a	775	G
25	a	776	G
25	a	777	G
25	a	782	A
25	a	784	G
25	a	785	G
25	a	805	G
25	a	812	C
25	a	827	U
25	a	828	U
25	a	846	U
25	a	847	U
25	a	858	G
25	a	859	G
25	a	888	C
25	a	890	C
25	a	891	G
25	a	893	C
25	a	897	C
25	a	900	A
25	a	910	A
25	a	914	G
25	a	915	C
25	a	933	A
25	a	934	U
25	a	946	C
25	a	961	C
25	a	974	G
25	a	981	A
25	a	983	A
25	a	984	A
25	a	985	C

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Mol	Chain	Res	Type
25	a	996	A
25	a	1012	U
25	a	1013	C
25	a	1022	G
25	a	1026	G
25	a	1033	U
25	a	1040	A
25	a	1045	C
25	a	1047	G
25	a	1105	U
25	a	1107	G
25	a	1110	G
25	a	1112	G
25	a	1116	G
25	a	1132	U
25	a	1133	A
25	a	1135	C
25	a	1142	A
25	a	1143	A
25	a	1176	U
25	a	1253	A
25	a	1256	G
25	a	1271	G
25	a	1272	A
25	a	1273	U
25	a	1300	G
25	a	1301	A
25	a	1352	U
25	a	1365	A
25	a	1379	U
25	a	1380	G
25	a	1383	A
25	a	1409	U
25	a	1411	U
25	a	1416	G
25	a	1428	C
25	a	1452	G
25	a	1453	A
25	a	1460	U
25	a	1482	G
25	a	1490	A
25	a	1493	C

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Mol	Chain	Res	Type
25	a	1497	U
25	a	1508	A
25	a	1509	A
25	a	1515	A
25	a	1529	G
25	a	1535	A
25	a	1536	C
25	a	1537	G
25	a	1569	A
25	a	1578	U
25	a	1583	A
25	a	1584	U
25	a	1608	A
25	a	1647	U
25	a	1648	U
25	a	1649	G
25	a	1674	G
25	a	1715	G
25	a	1729	U
25	a	1730	C
25	a	1732	C
25	a	1738	G
25	a	1764	C
25	a	1773	A
25	a	1782	U
25	a	1800	C
25	a	1801	A
25	a	1808	A
25	a	1816	C
25	a	1829	A
25	a	1847	A
25	a	1848	A
25	a	1858	A
25	a	1872	A
25	a	1873	G
25	a	1906	G
25	a	1913	A
25	a	1929	G
25	a	1930	G
25	a	1937	A
25	a	1938	A
25	a	1955	U

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Mol	Chain	Res	Type
25	a	1967	C
25	a	1970	A
25	a	1971	U
25	a	1972	G
25	a	1991	U
25	a	1993	U
25	a	2023	C
25	a	2031	A
25	a	2033	A
25	a	2043	C
25	a	2055	C
25	a	2056	G
25	a	2062	A
25	a	2063	C
25	a	2069	G
25	a	2110	G
25	a	2111	U
25	a	2119	A
25	a	2123	G
25	a	2125	G
25	a	2126	A
25	a	2132	U
25	a	2133	G
25	a	2148	G
25	a	2157	G
25	a	2169	A
25	a	2171	A
25	a	2172	U
25	a	2198	A
25	a	2204	G
25	a	2211	A
25	a	2225	A
25	a	2226	C
25	a	2238	G
25	a	2239	G
25	a	2268	A
25	a	2283	C
25	a	2287	A
25	a	2305	U
25	a	2308	G
25	a	2312	U
25	a	2322	A

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Mol	Chain	Res	Type
25	a	2324	U
25	a	2325	G
25	a	2333	A
25	a	2335	A
25	a	2347	C
25	a	2366	A
25	a	2372	U
25	a	2383	G
25	a	2385	C
25	a	2402	U
25	a	2403	C
25	a	2406	A
25	a	2425	A
25	a	2429	G
25	a	2430	A
25	a	2431	U
25	a	2435	A
25	a	2441	U
25	a	2474	U
25	a	2476	A
25	a	2480	C
25	a	2504	U
25	a	2505	G
25	a	2506	U
25	a	2507	C
25	a	2518	A
25	a	2529	G
25	a	2547	A
25	a	2566	A
25	a	2567	G
25	a	2573	C
25	a	2609	U
25	a	2613	U
25	a	2629	U
25	a	2630	G
25	a	2663	G
25	a	2689	U
25	a	2690	U
25	a	2714	G
25	a	2726	A
25	a	2744	G
25	a	2748	A

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Mol	Chain	Res	Type
25	a	2757	A
25	a	2765	A
25	a	2778	A
25	a	2790	U
25	a	2800	A
25	a	2820	A
25	a	2821	A
25	a	2884	U
26	b	25	U
26	b	33	G
26	b	35	C
26	b	45	A
26	b	47	C
26	b	56	G
26	b	67	G
26	b	89	U
26	b	90	C
26	b	109	A
26	b	120	U
24	5	5	G
24	5	6	G
24	5	7	G
24	5	8	4SU
24	5	19	G
24	5	33	U
24	5	38	A
24	5	39	C
24	5	56	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	70	U
1	A	84	U
1	A	85	U
1	A	94	G
1	A	107	G
1	A	199	A
1	A	361	G
1	A	412	A
1	A	776	G

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Mol	Chain	Res	Type
1	A	793	U
1	A	827	U
1	A	884	U
1	A	993	G
1	A	1024	G
1	A	1035	A
1	A	1042	A
1	A	1124	G
1	A	1225	A
1	A	1281	C
1	A	1319	A
1	A	1505	G
1	A	1508	A
23	Y	60	U
23	Y	68	C
24	Z	48	C
24	Z	60	U

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

47 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	$\# Z  > 2$
25	5MC	a	1962	25,56	19,22,23	0.78	0	26,32,35	0.57	0
24	5MU	5	54	24	19,22,23	0.20	0	27,32,35	0.25	0
1	MA6	A	1518	1	23,26,27	0.32	0	33,38,41	0.64	1 (3%)
1	2MG	A	966	1	23,26,27	0.48	0	33,38,41	0.50	0
23	MIA	Y	37	23	28,31,32	0.38	0	38,44,47	0.49	0
36	4D4	l	81	36	9,11,12	1.81	2 (22%)	7,13,15	1.09	1 (14%)
23	5MU	Y	54	23	19,22,23	0.24	0	27,32,35	0.38	0
25	OMU	a	2552	25,57	19,22,23	0.61	0	25,31,34	0.47	0
1	PSU	A	516	1	18,21,22	0.31	0	21,30,33	0.42	0
24	OMC	Z	32	24	19,22,23	0.36	0	25,31,34	0.41	0
25	PSU	a	955	25	18,21,22	0.78	0	21,30,33	0.68	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	Y	8	23	18,21,22	0.16	0	25,30,33	0.23	0
24	OMC	5	32	24	19,22,23	0.19	0	25,31,34	0.59	0
25	6MZ	a	2030	25	22,25,26	0.70	0	29,36,39	0.66	0
1	4OC	A	1402	57,1	20,23,24	0.47	0	25,32,35	0.64	0
25	5MU	a	1939	25,56	19,22,23	0.77	0	27,32,35	0.61	0
12	D2T	L	89	12	8,9,10	1.07	0	6,11,13	1.58	1 (16%)
23	G7M	Y	46	23	23,26,27	1.52	2 (8%)	34,39,42	1.52	4 (11%)
25	PSU	a	1911	25	18,21,22	0.27	0	21,30,33	0.38	0
24	PSU	Z	55	24	18,21,22	0.24	0	21,30,33	0.44	0
1	2MG	A	1207	56,1	23,26,27	0.34	0	33,38,41	0.44	0
1	UR3	A	1498	1	19,22,23	0.49	0	26,32,35	0.41	0
1	5MC	A	967	1	19,22,23	0.27	0	26,32,35	0.45	0
28	MEQ	d	150	28	8,9,10	0.67	0	5,10,12	1.71	2 (40%)
25	1MG	a	745	25	23,26,27	0.82	1 (4%)	33,39,42	0.93	2 (6%)
25	2MG	a	1835	25	23,26,27	0.61	0	33,38,41	0.46	0
1	MA6	A	1519	1	23,26,27	0.49	0	33,38,41	0.69	1 (3%)
25	PSU	a	746	25,57	18,21,22	0.40	0	21,30,33	0.56	0
1	G7M	A	527	1	23,26,27	0.32	0	34,39,42	0.72	0
23	PSU	Y	32	23	18,21,22	0.21	0	21,30,33	0.31	0
25	PSU	a	1917	25	18,21,22	0.27	0	21,30,33	0.40	0
25	3TD	a	1915	25	19,22,23	0.20	0	23,32,35	0.33	0
24	4SU	5	8	24	18,21,22	0.20	0	25,30,33	0.28	0
25	5MU	a	747	25	19,22,23	0.59	0	27,32,35	0.74	0
24	5MU	Z	54	24	19,22,23	0.22	0	27,32,35	0.30	0
25	H2U	a	2449[A]	25	18,21,22	0.54	0	19,30,33	1.00	1 (5%)
23	PSU	Y	55	23	18,21,22	0.24	0	21,30,33	0.30	0
23	PSU	Y	39	23	18,21,22	0.24	0	21,30,33	0.44	0
23	H2U	Y	16	23	18,21,22	0.24	0	19,30,33	0.42	0
25	H2U	a	2449[B]	25	18,21,22	0.36	0	19,30,33	0.91	1 (5%)
36	MS6	l	82	36	5,7,8	0.50	0	2,7,9	0.10	0
24	PSU	5	55	24	18,21,22	0.26	0	21,30,33	0.35	0
1	5MC	A	1407	1	19,22,23	0.40	0	26,32,35	0.60	0
1	2MG	A	1516	1	23,26,27	0.50	0	33,38,41	0.50	0
11	IAS	K	119	11	6,7,8	0.87	0	3,8,10	0.92	0
25	6MZ	a	1618	25	22,25,26	0.42	0	29,36,39	0.52	0
24	4SU	Z	8	24	18,21,22	0.23	0	25,30,33	0.32	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
25	5MC	a	1962	25,56	-	2/7/25/26	0/2/2/2
24	5MU	5	54	24	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
23	MIA	Y	37	23	-	0/15/33/34	0/3/3/3
36	4D4	l	81	36	-	1/11/12/14	-
23	5MU	Y	54	23	-	0/7/25/26	0/2/2/2
25	OMU	a	2552	25,57	-	0/9/27/28	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
24	OMC	Z	32	24	-	0/9/27/28	0/2/2/2
25	PSU	a	955	25	-	0/7/25/26	0/2/2/2
23	4SU	Y	8	23	-	0/7/25/26	0/2/2/2
24	OMC	5	32	24	-	0/9/27/28	0/2/2/2
25	6MZ	a	2030	25	-	2/9/27/28	0/3/3/3
1	4OC	A	1402	57,1	-	0/9/29/30	0/2/2/2
25	5MU	a	1939	25,56	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	4/7/12/14	-
23	G7M	Y	46	23	-	1/7/25/26	0/3/3/3
25	PSU	a	1911	25	-	0/7/25/26	0/2/2/2
24	PSU	Z	55	24	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	56,1	-	0/9/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
28	MEQ	d	150	28	-	3/8/9/11	-
25	1MG	a	745	25	-	0/7/25/26	0/3/3/3
25	2MG	a	1835	25	-	0/9/27/28	0/3/3/3
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
25	PSU	a	746	25,57	-	2/7/25/26	0/2/2/2
1	G7M	A	527	1	-	0/7/25/26	0/3/3/3
23	PSU	Y	32	23	-	0/7/25/26	0/2/2/2
25	PSU	a	1917	25	-	1/7/25/26	0/2/2/2
25	3TD	a	1915	25	-	0/7/25/26	0/2/2/2
24	4SU	5	8	24	-	0/7/25/26	0/2/2/2
25	5MU	a	747	25	-	0/7/25/26	0/2/2/2
24	5MU	Z	54	24	-	0/7/25/26	0/2/2/2
25	H2U	a	2449[A]	25	-	0/7/38/39	0/2/2/2
23	PSU	Y	55	23	-	0/7/25/26	0/2/2/2
23	PSU	Y	39	23	-	0/7/25/26	0/2/2/2
23	H2U	Y	16	23	-	1/7/38/39	0/2/2/2
25	H2U	a	2449[B]	25	-	4/7/38/39	0/2/2/2
36	MS6	l	82	36	-	1/4/6/8	-
24	PSU	5	55	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
11	IAS	K	119	11	-	1/7/7/8	-
25	6MZ	a	1618	25	-	0/9/27/28	0/3/3/3
24	4SU	Z	8	24	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	46	G7M	C8-N7	5.85	1.43	1.33
36	l	81	4D4	CZ-NE	3.90	1.40	1.33
23	Y	46	G7M	C8-N9	3.70	1.45	1.35
36	l	81	4D4	CZ-NH1	3.21	1.46	1.34
25	a	745	1MG	CM1-N1	2.21	1.50	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	46	G7M	N9-C8-N7	-4.72	101.02	112.48
23	Y	46	G7M	C8-N7-C5	4.54	113.46	107.78
23	Y	46	G7M	CN7-N7-C8	-4.01	118.72	124.79
25	a	2449[A]	H2U	O4'-C1'-N1	3.80	114.47	109.30
25	a	745	1MG	C6-C5-C4	-3.79	115.68	119.97
28	d	150	MEQ	CG-CD-NE2	2.72	120.20	116.39
36	l	81	4D4	O-C-CA	-2.67	117.91	124.77
1	A	1518	MA6	C2-N1-C6	2.54	118.05	111.83
12	L	89	D2T	O-C-CA	-2.46	118.45	124.77
1	A	1519	MA6	C2-N1-C6	2.42	117.75	111.83
23	Y	46	G7M	C2'-C1'-N9	2.38	119.87	113.25
28	d	150	MEQ	OE1-CD-CG	-2.15	118.12	122.02
25	a	2449[B]	H2U	O4'-C1'-N1	-2.12	106.41	109.30
25	a	745	1MG	C6-C5-N7	2.05	133.91	129.36

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
28	d	150	MEQ	C-CA-CB-CG
25	a	746	PSU	C2'-C1'-C5-C6
25	a	746	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
25	a	2449[B]	H2U	O4'-C1'-N1-C6
25	a	2449[B]	H2U	C2'-C1'-N1-C2
25	a	2449[B]	H2U	C2'-C1'-N1-C6
1	A	1519	MA6	O4'-C4'-C5'-O5'
28	d	150	MEQ	NE2-CD-CG-CB
28	d	150	MEQ	OE1-CD-CG-CB
25	a	2030	6MZ	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
25	a	1962	5MC	C2'-C1'-N1-C6
12	L	89	D2T	SB-CB-CG-OD1
25	a	2030	6MZ	O4'-C4'-C5'-O5'
25	a	2449[B]	H2U	O4'-C1'-N1-C2
25	a	1962	5MC	O4'-C1'-N1-C6
36	l	82	MS6	CB-CG-SD-CE
23	Y	16	H2U	C4'-C5'-O5'-P
36	l	81	4D4	OB-CB-CG-CD
23	Y	46	G7M	O4'-C4'-C5'-O5'
25	a	1917	PSU	O4'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD2
11	K	119	IAS	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	2MG	1	0
25	a	2552	OMU	1	0
25	a	2030	6MZ	4	0
25	a	1939	5MU	1	0
12	L	89	D2T	1	0
28	d	150	MEQ	1	0
25	a	2449[A]	H2U	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 497 ligands modelled in this entry, 482 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	SR0	a	3006	-	9,9,9	0.77	0	8,8,8	0.85	0
58	SR0	a	3003	-	9,9,9	0.54	0	8,8,8	0.57	0
58	SR0	a	3004	-	9,9,9	0.61	0	8,8,8	0.27	0
58	SR0	a	3001	-	9,9,9	0.32	0	8,8,8	0.47	0
59	PUT	a	3008	-	5,5,5	0.39	0	4,4,4	0.56	0
59	PUT	a	3011	-	5,5,5	0.63	0	4,4,4	0.54	0
59	PUT	a	3013	-	5,5,5	0.45	0	4,4,4	0.36	0
59	PUT	a	3010	-	5,5,5	0.55	0	4,4,4	0.08	0
59	PUT	a	3012	-	5,5,5	0.35	0	4,4,4	0.22	0
59	PUT	a	3014	-	5,5,5	0.60	0	4,4,4	0.34	0
59	PUT	a	3007	-	5,5,5	0.39	0	4,4,4	0.25	0
59	PUT	a	3009	-	5,5,5	0.34	0	4,4,4	0.35	0
58	SR0	a	3002	-	9,9,9	0.64	0	8,8,8	0.75	0
58	SR0	a	3005	-	9,9,9	0.55	0	8,8,8	0.26	0
59	PUT	a	3015	-	5,5,5	0.36	0	4,4,4	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SR0	a	3006	-	-	3/7/7/7	-
58	SR0	a	3003	-	-	1/7/7/7	-
58	SR0	a	3004	-	-	0/7/7/7	-
58	SR0	a	3001	-	-	3/7/7/7	-
59	PUT	a	3008	-	-	0/3/3/3	-
59	PUT	a	3011	-	-	0/3/3/3	-
59	PUT	a	3013	-	-	1/3/3/3	-
59	PUT	a	3010	-	-	0/3/3/3	-
59	PUT	a	3012	-	-	1/3/3/3	-
59	PUT	a	3014	-	-	2/3/3/3	-
59	PUT	a	3007	-	-	0/3/3/3	-
59	PUT	a	3009	-	-	1/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SR0	a	3002	-	-	4/7/7/7	-
58	SR0	a	3005	-	-	3/7/7/7	-
59	PUT	a	3015	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	a	3006	SR0	N6-C7-C8-C9
58	a	3002	SR0	N6-C7-C8-C9
58	a	3006	SR0	C8-C7-N6-C5
58	a	3005	SR0	C3-C4-C5-N6
59	a	3014	PUT	N1-C1-C2-C3
58	a	3001	SR0	C3-C4-C5-N6
59	a	3009	PUT	C1-C2-C3-C4
58	a	3006	SR0	C2-C3-C4-C5
59	a	3014	PUT	C1-C2-C3-C4
59	a	3013	PUT	N1-C1-C2-C3
58	a	3002	SR0	C8-C7-N6-C5
58	a	3005	SR0	C2-C3-C4-C5
58	a	3001	SR0	C2-C3-C4-C5
58	a	3001	SR0	C8-C7-N6-C5
58	a	3002	SR0	C3-C4-C5-N6
58	a	3002	SR0	C4-C5-N6-C7
59	a	3012	PUT	C2-C3-C4-N2
58	a	3003	SR0	C4-C5-N6-C7
58	a	3005	SR0	C7-C8-C9-N10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	a	3008	PUT	1	0
59	a	3014	PUT	1	0

## 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.

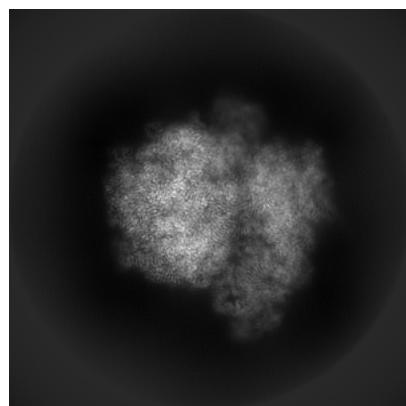
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55415. These allow visual inspection of the internal detail of the map and identification of artifacts.

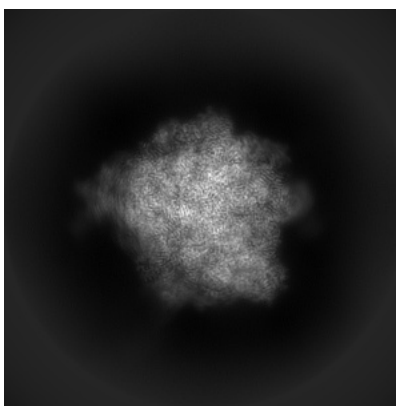
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

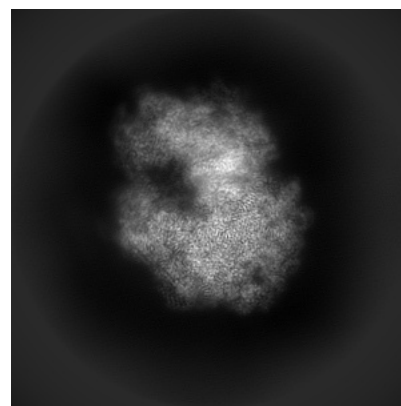
#### 6.1.1 Primary map



X

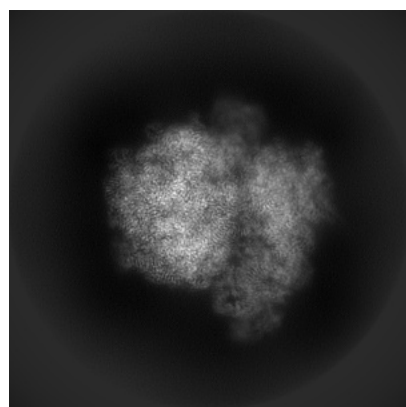


Y

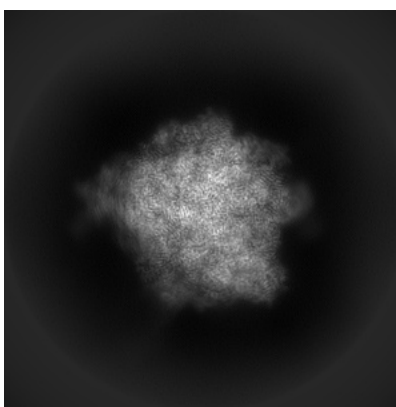


Z

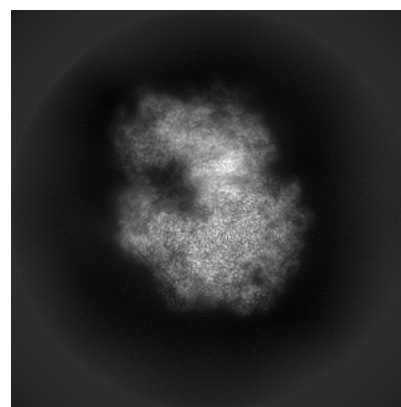
#### 6.1.2 Raw map



X



Y



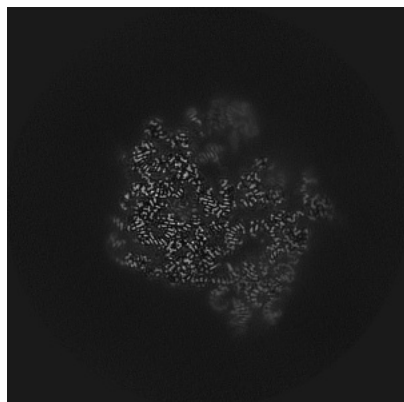
Z

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

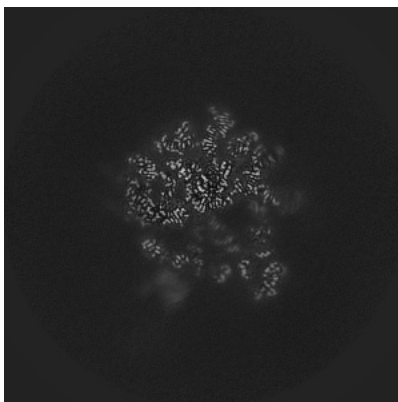


## 6.2 Central slices [i](#)

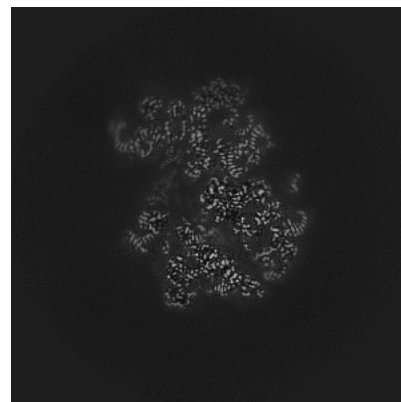
### 6.2.1 Primary map



X Index: 256

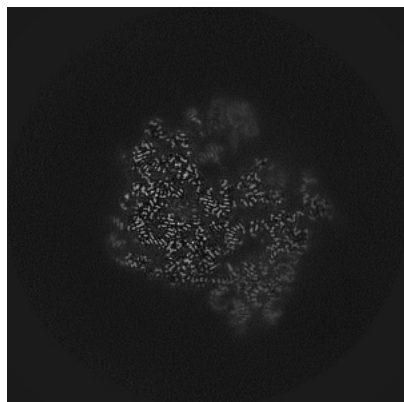


Y Index: 256

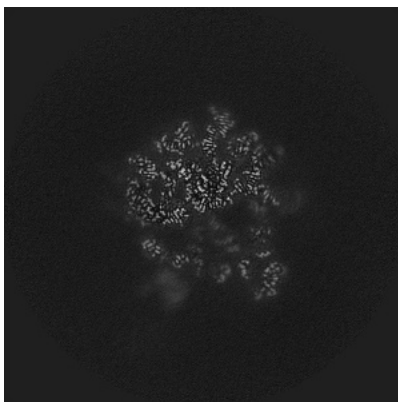


Z Index: 256

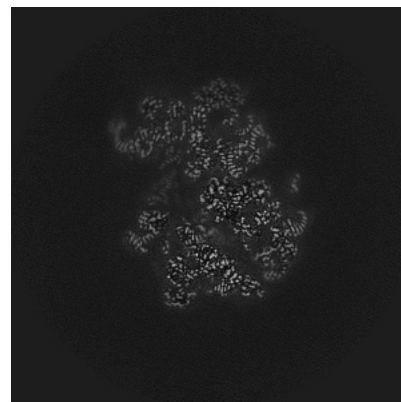
### 6.2.2 Raw map



X Index: 256



Y Index: 256

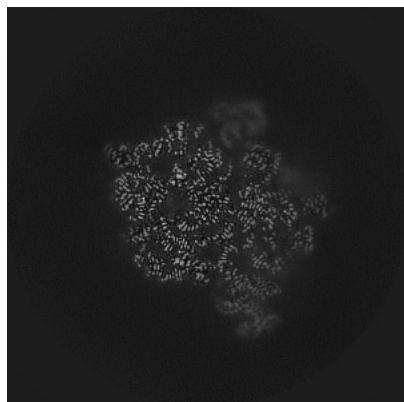


Z Index: 256

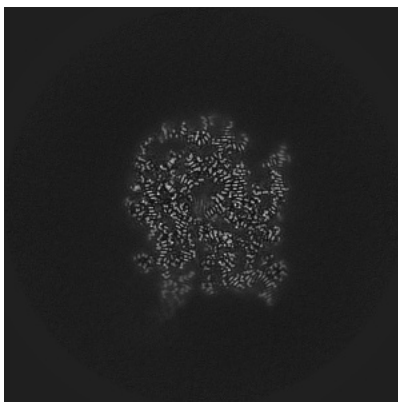
The images above show central slices of the map in three orthogonal directions.

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

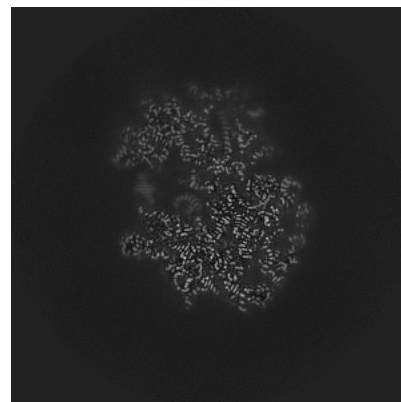
### 6.3.1 Primary map



X Index: 279

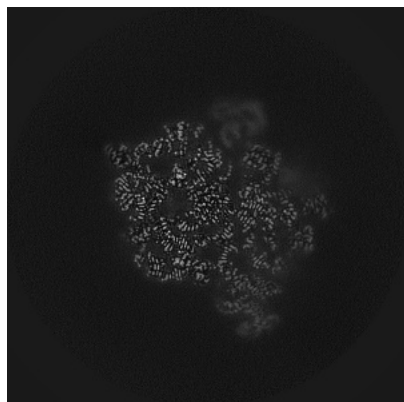


Y Index: 221

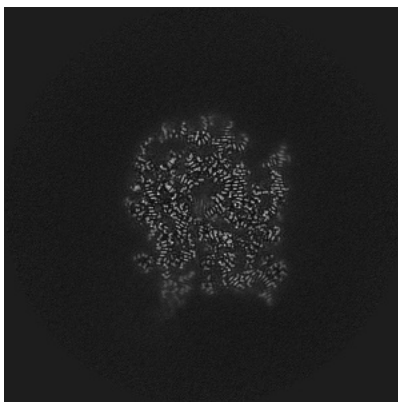


Z Index: 270

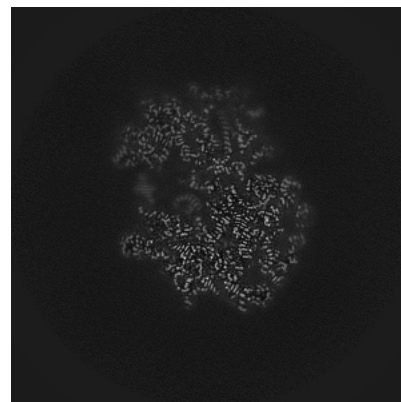
### 6.3.2 Raw map



X Index: 279



Y Index: 221

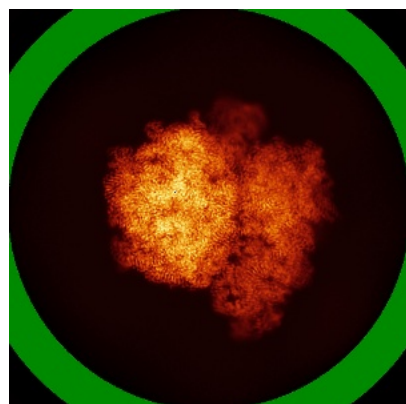


Z Index: 270

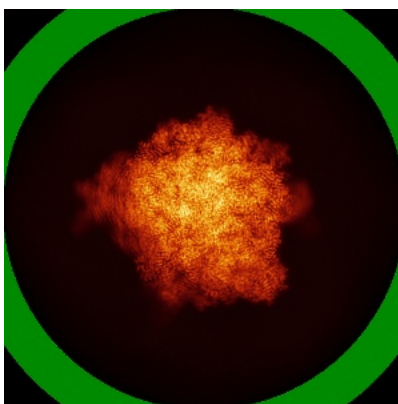
The images above show the largest variance slices of the map in three orthogonal directions.

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

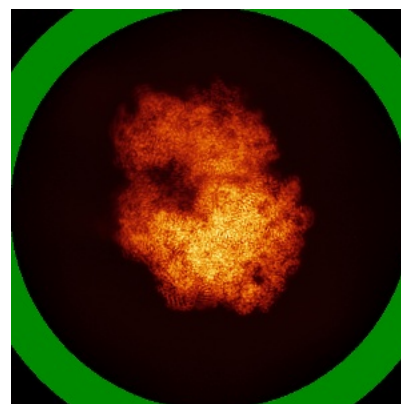
### 6.4.1 Primary map



X

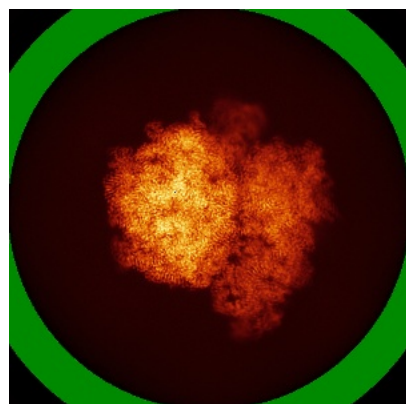


Y

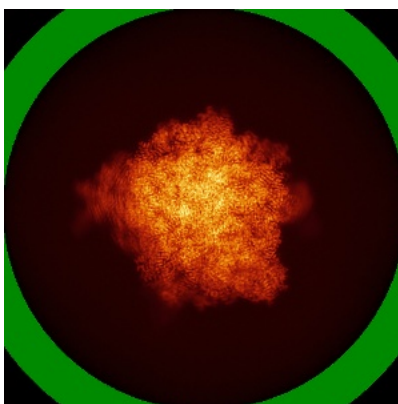


Z

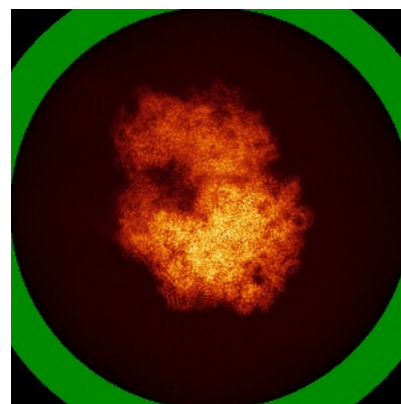
### 6.4.2 Raw map



X



Y

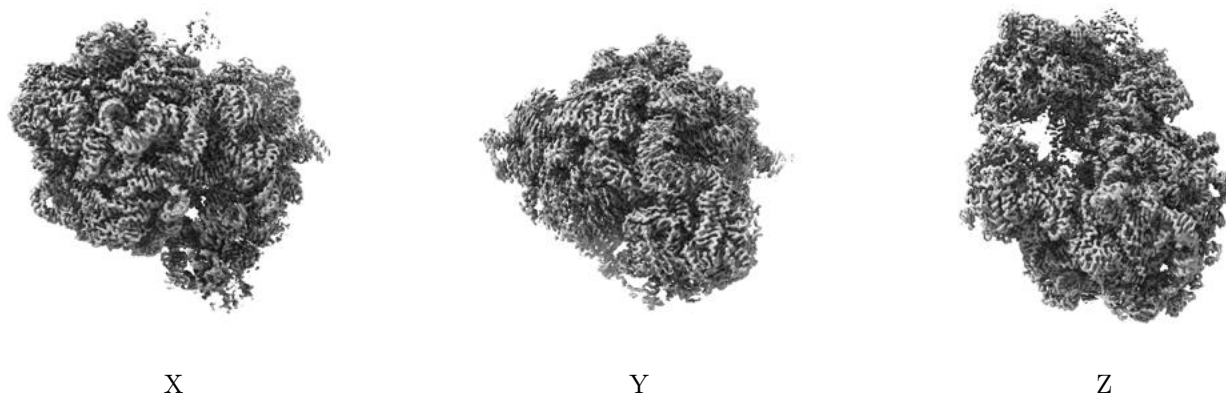


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

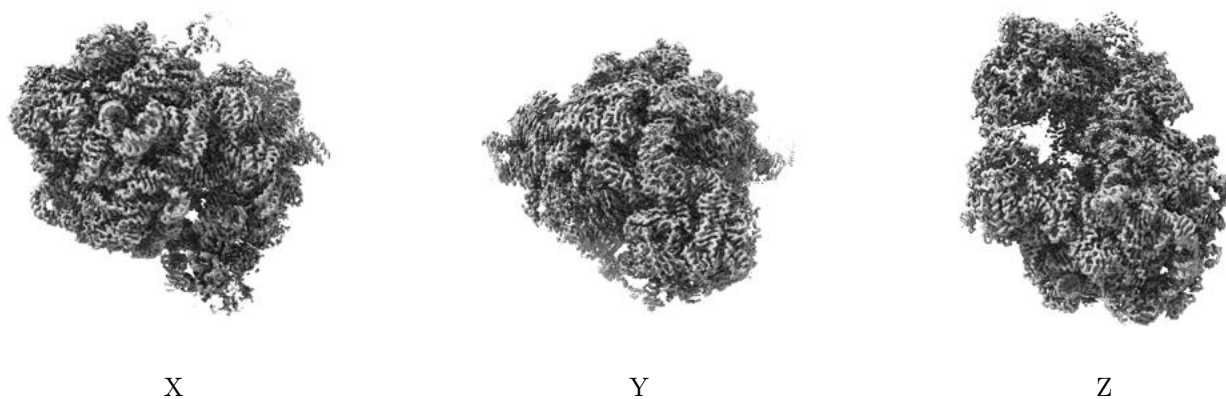
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

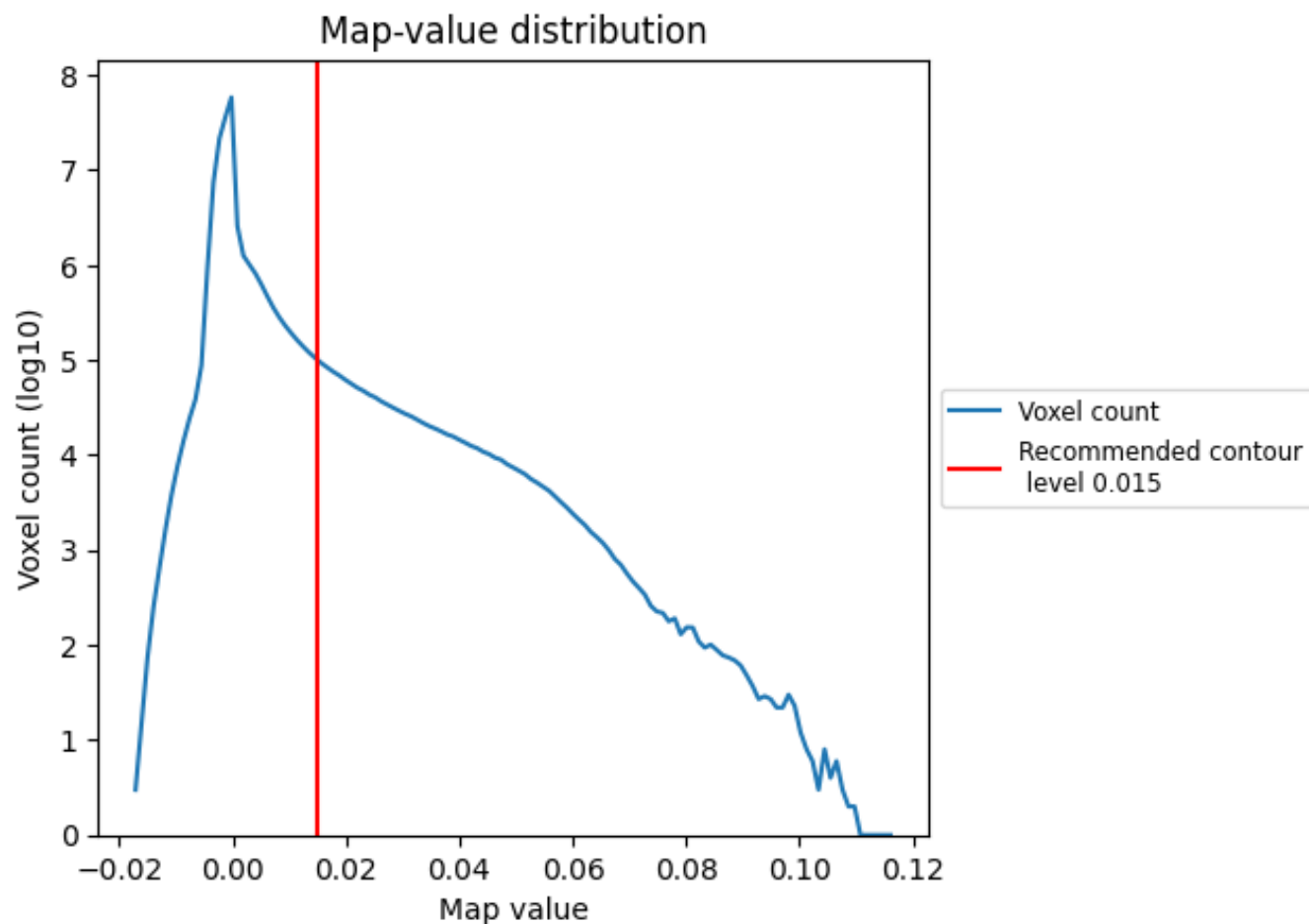
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

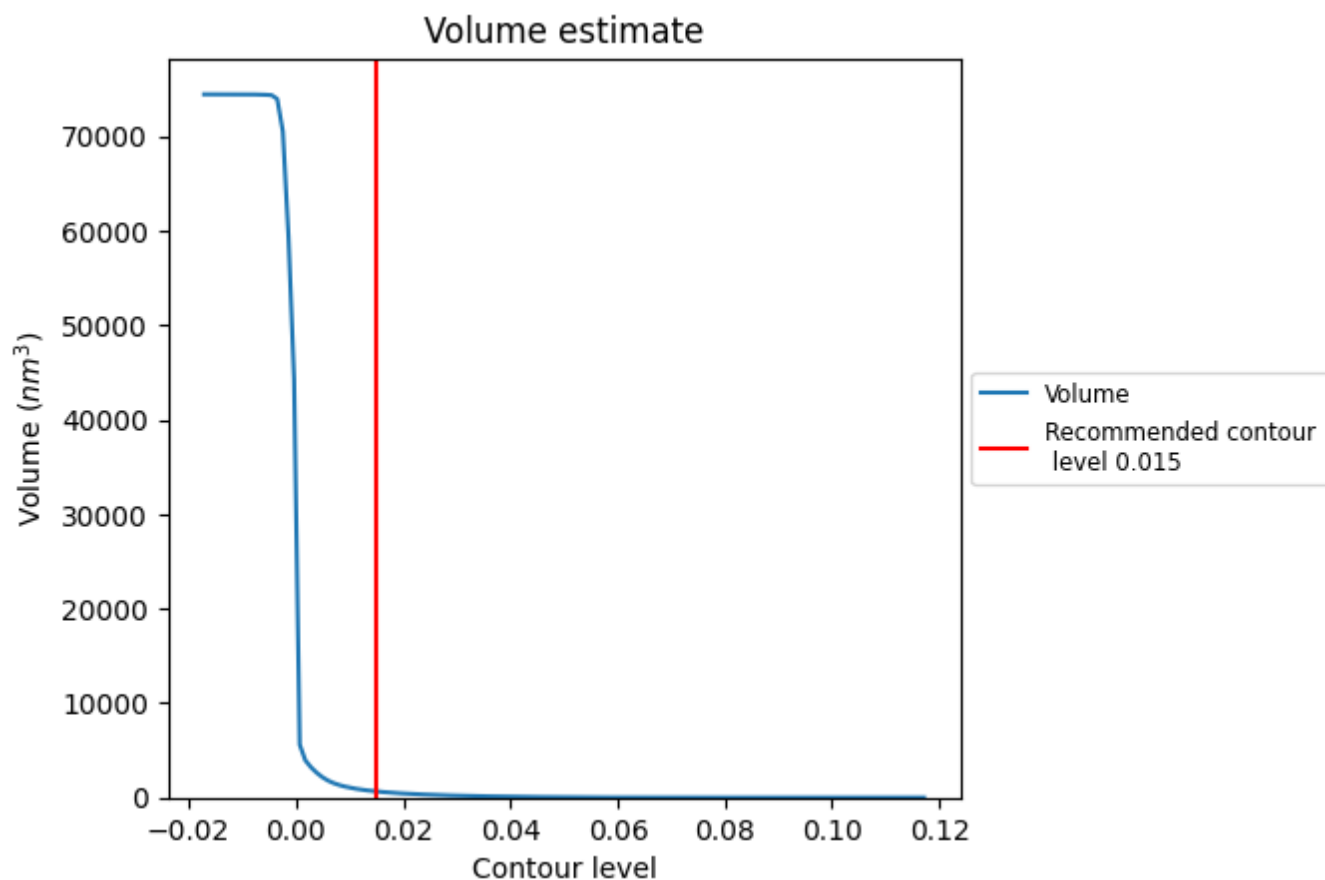
This section contains the results of statistical analysis of the map.

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



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

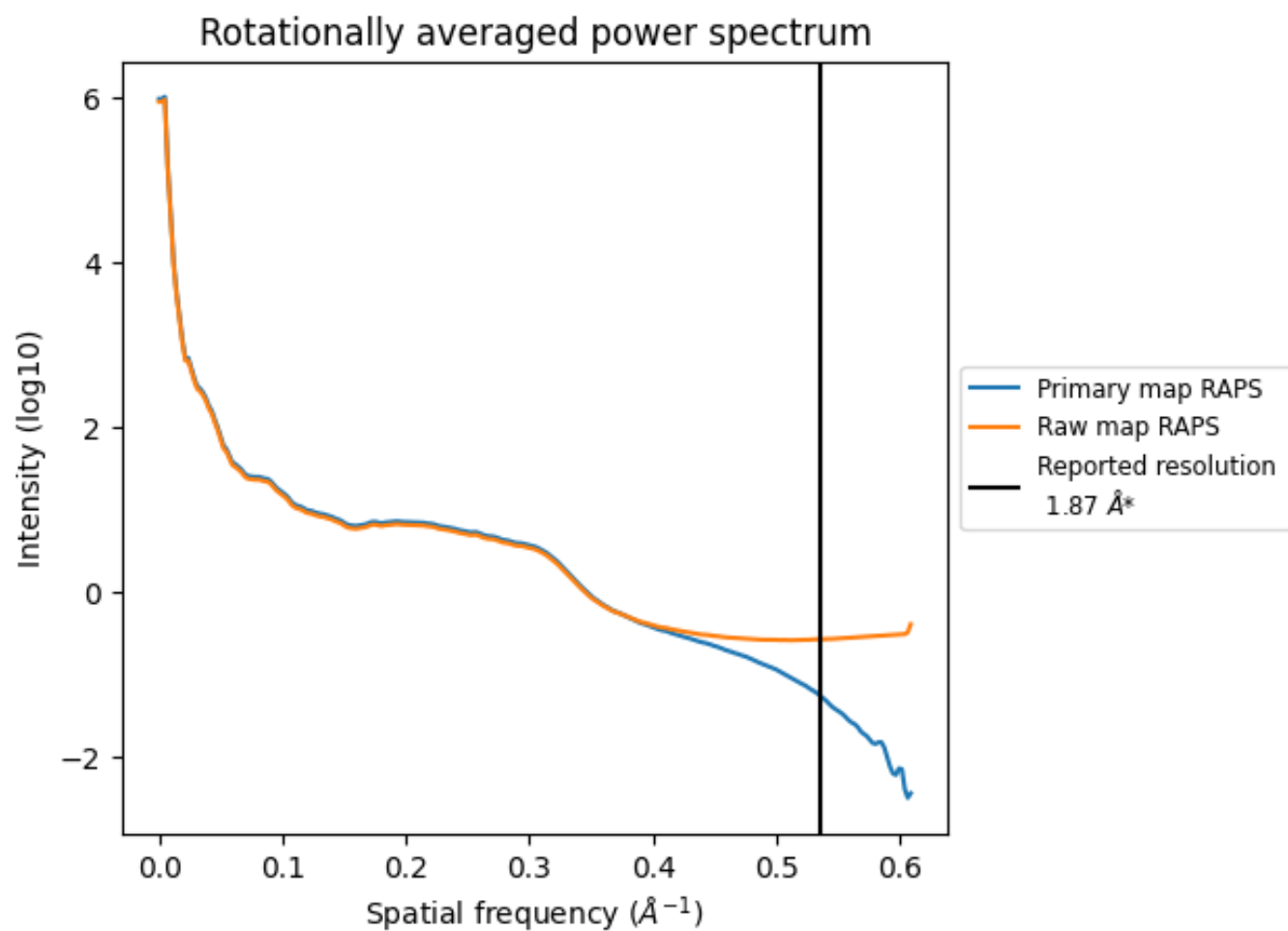
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm<sup>3</sup>; this corresponds to an approximate mass of 587 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 ⓘ



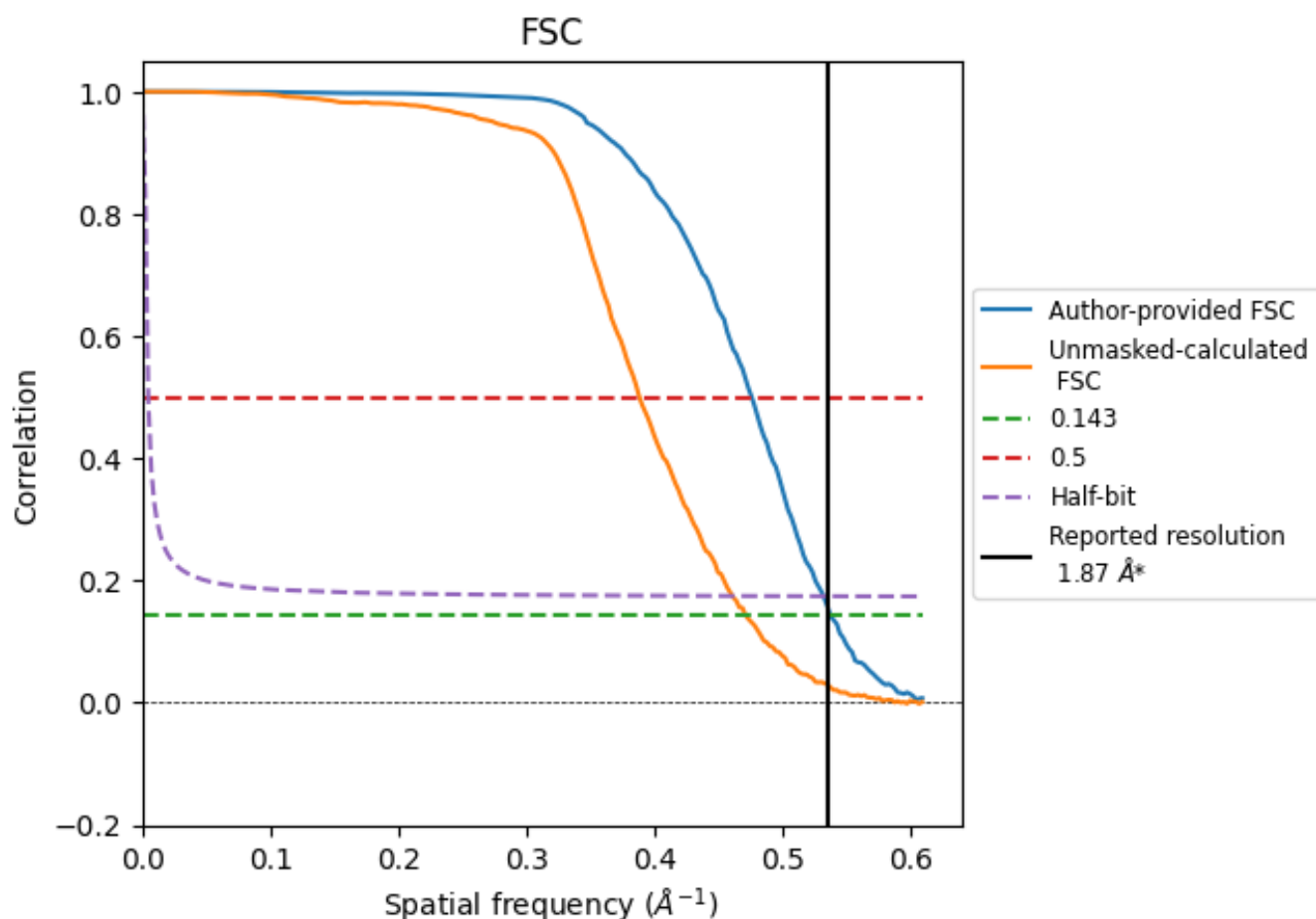
\*Reported resolution corresponds to spatial frequency of 0.535  $\text{\AA}^{-1}$



## 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 0.535  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

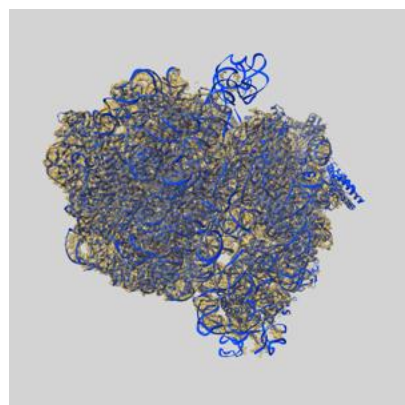
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.87	-	-
Author-provided FSC curve	1.86	2.10	1.88
Unmasked-calculated*	2.12	2.58	2.17

\*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 2.12 differs from the reported value 1.87 by more than 10 %

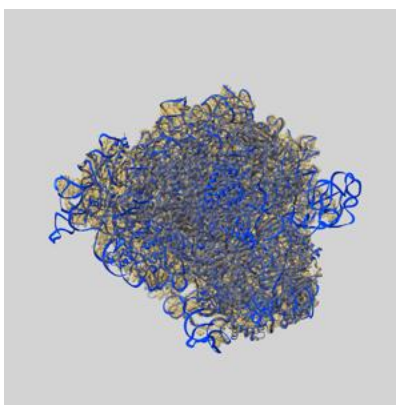
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55415 and PDB model 9T0Y. Per-residue inclusion information can be found in section [3](#) on page [19](#).

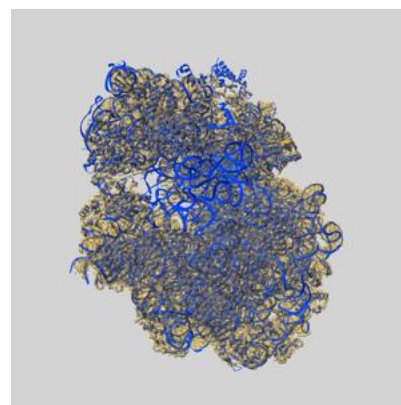
### 9.1 Map-model overlay [i](#)



X



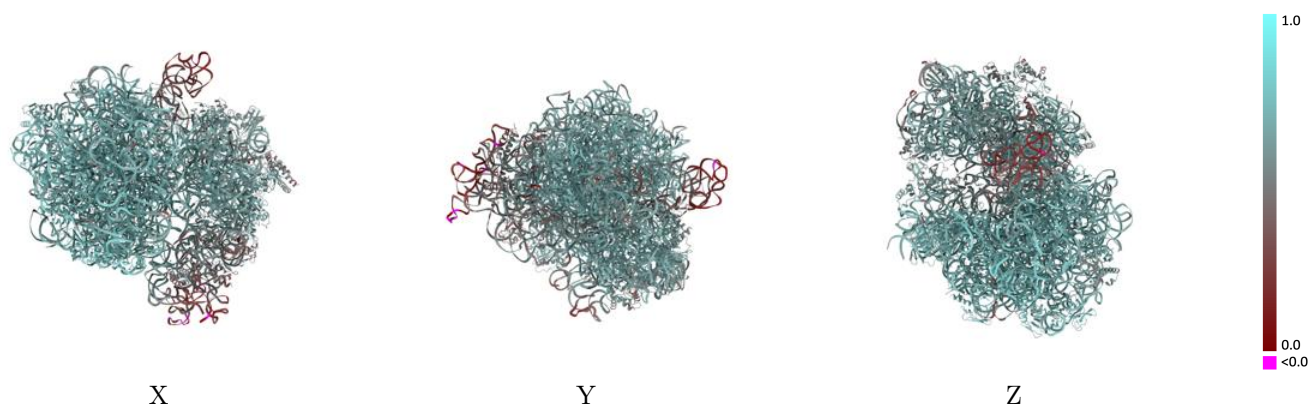
Y



Z

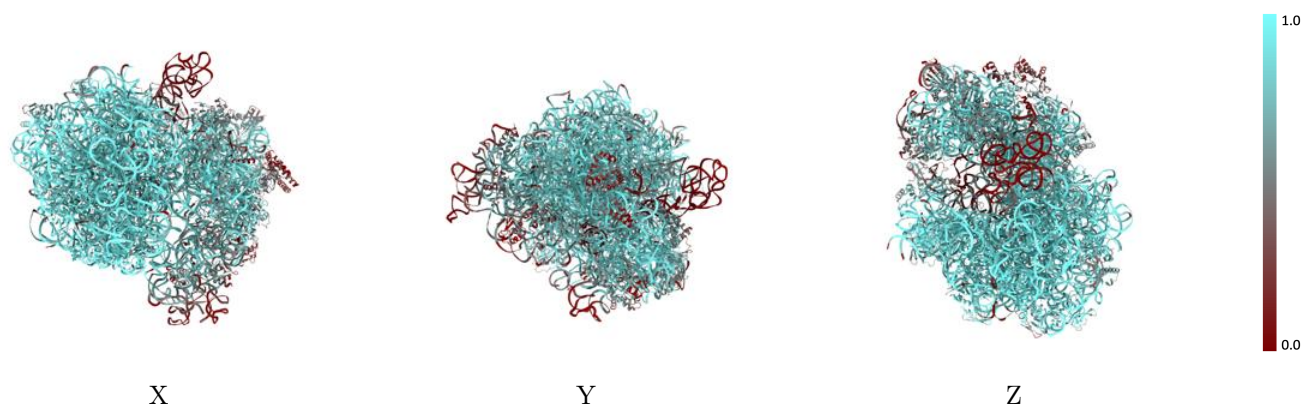
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



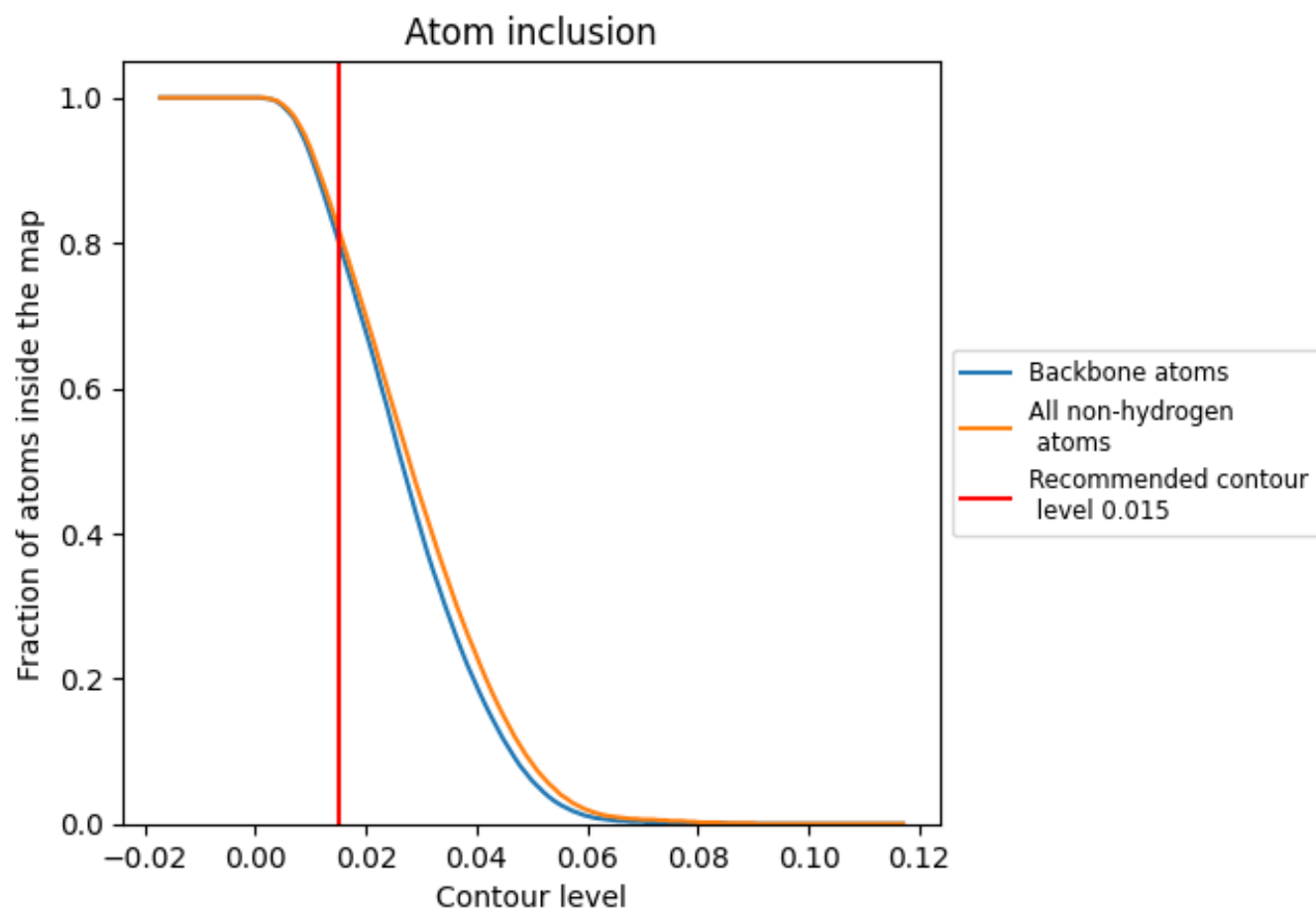
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.6500
0	 0.8670	 0.7060
1	 0.9880	 0.7640
2	 0.9720	 0.7550
3	 0.9210	 0.7030
4	 0.4550	 0.5480
5	 0.1120	 0.4080
A	 0.8070	 0.5910
B	 0.3070	 0.5390
C	 0.6730	 0.6210
D	 0.2800	 0.4430
E	 0.8090	 0.6540
F	 0.6360	 0.6050
G	 0.5600	 0.5820
H	 0.7580	 0.6430
I	 0.6620	 0.6110
J	 0.4970	 0.5650
K	 0.7540	 0.6440
L	 0.5370	 0.5920
M	 0.6380	 0.6130
N	 0.7180	 0.6300
O	 0.7260	 0.6290
P	 0.3860	 0.4300
Q	 0.4830	 0.4670
R	 0.7280	 0.6240
S	 0.5920	 0.5970
T	 0.5270	 0.4690
U	 0.4990	 0.5510
X	 0.3520	 0.4590
Y	 0.0780	 0.5280
Z	 0.5720	 0.6040
a	 0.9300	 0.6930
b	 0.9390	 0.6710
c	 0.9500	 0.7410
d	 0.9400	 0.7350



*Continued on next page...*

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Chain	Atom inclusion	Q-score
e	 0.7760	 0.6900
f	 0.6450	 0.5960
g	 0.7240	 0.6240
h	 0.5930	 0.6240
i	 0.9410	 0.7330
j	 0.9080	 0.7190
k	 0.9220	 0.7240
l	 0.9220	 0.7200
m	 0.9750	 0.7520
n	 0.8700	 0.6760
o	 0.8780	 0.7110
p	 0.9660	 0.7540
q	 0.8810	 0.7090
r	 0.9240	 0.7320
s	 0.8680	 0.6960
t	 0.8200	 0.6770
u	 0.8370	 0.6730
v	 0.8500	 0.7220
w	 0.9280	 0.7230
x	 0.8040	 0.6670
y	 0.9060	 0.7130
z	 0.9400	 0.7390