



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:58 pm GMT

PDB ID : 5IQR
EMDB ID : EMD-8107
Title : Structure of RelA bound to the 70S ribosome
Authors : Brown, A.; Fernandez, I.S.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-03-11
Resolution : 3.00 Å(reported)
Based on initial model : 4YBB

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

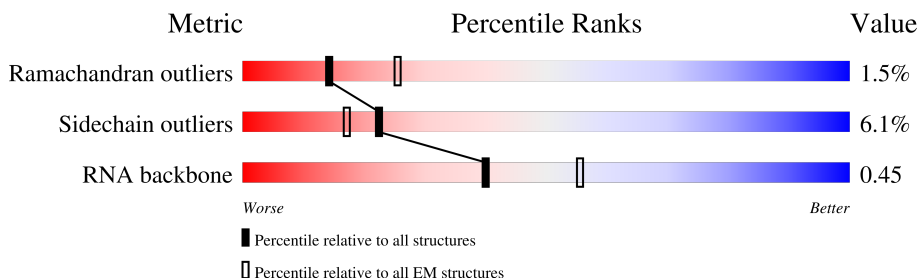
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



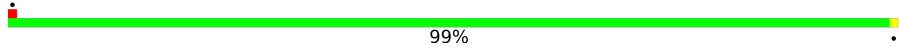
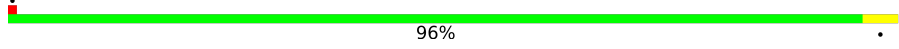
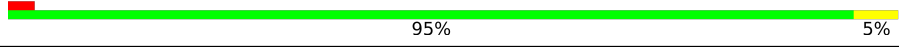
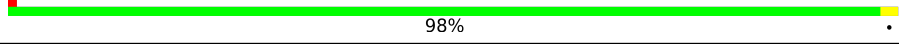
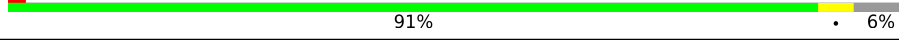
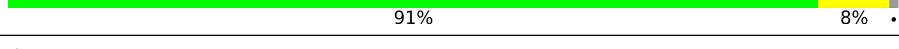
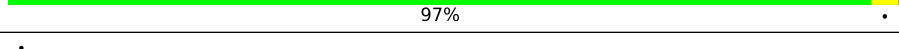
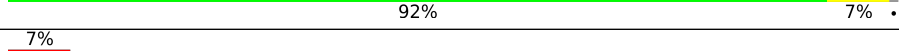
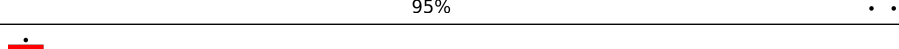
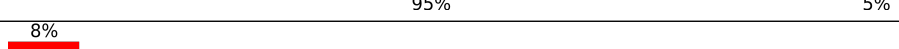
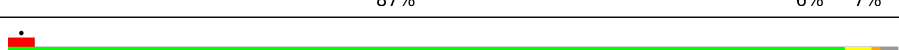
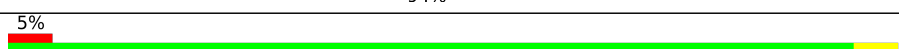
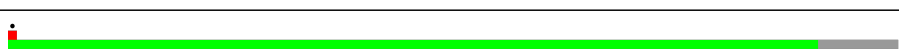
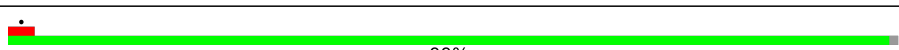

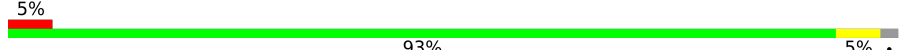
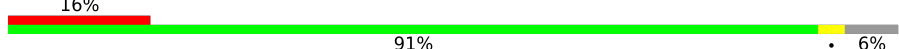
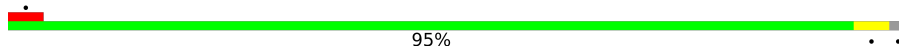


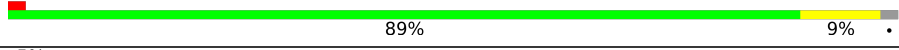
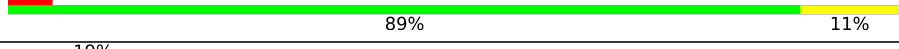



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	B	273	
2	C	209	
3	D	201	
4	E	179	
5	F	177	
6	G	149	
7	H	165	
8	I	142	

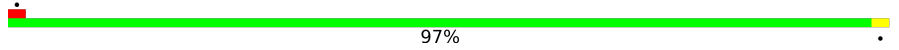



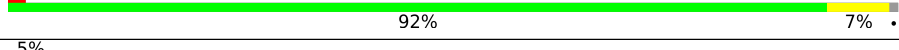
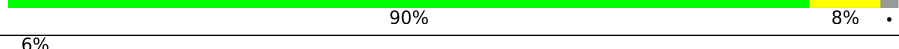
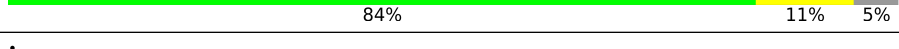
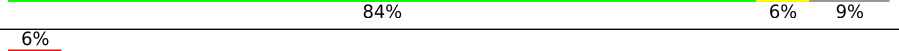
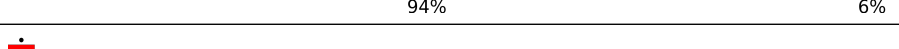
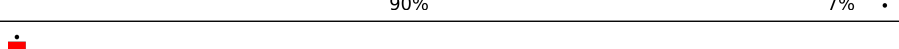
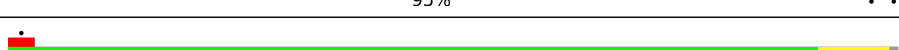
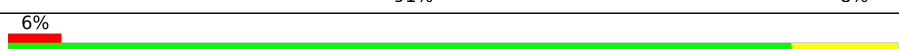
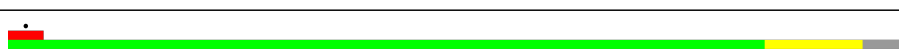

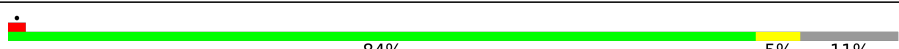







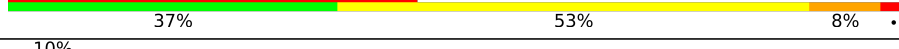
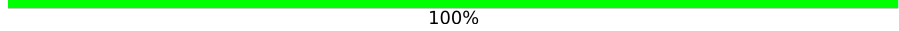

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Mol	Chain	Length	Quality of chain
9	J	142	
10	K	123	
11	L	144	
12	M	136	
13	N	127	
14	O	117	
15	P	115	
16	Q	118	
17	R	103	
18	S	110	
19	T	100	
20	U	104	
21	V	94	
22	W	85	
23	X	78	
24	Y	63	
25	Z	59	
26	a	70	
27	b	57	
28	c	55	
29	d	46	
30	e	65	
31	f	38	
32	g	241	
33	h	233	

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Mol	Chain	Length	Quality of chain
34	i	206	
35	j	167	
36	k	135	
37	l	179	
38	m	130	
39	n	130	
40	o	103	
41	p	129	
42	q	124	
43	r	118	
44	s	101	
45	t	89	
46	u	82	
47	v	84	
48	w	75	
49	x	92	
50	y	87	
51	z	71	
52	1	2904	
53	2	1533	
54	3	118	
55	4	76	
56	5	78	
57	6	76	
58	7	10	

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Mol	Chain	Length	Quality of chain
59	8	744	<div> <div>64%</div> <div>68%</div> <div>12%</div> <div>17%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	H2U	6	16	X	-	-	-
57	H2U	6	20	X	-	-	-
57	PSU	6	32	X	-	-	-
57	6IA	6	37	X	-	-	-
57	PSU	6	55	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	50	Total	C	N	O	0	0
			409	263	75	71		

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

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

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

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

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

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	207	Total	C	N	O	S	0	0
			1628	1030	306	289	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	207	LEU	ILE	conflict	UNP P0A7V3
h	208	GLY	LEU	conflict	UNP P0A7V3

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

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

- Molecule 37 is a protein called 30S ribosomal protein S7.

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

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

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

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 52 is a RNA chain called LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	2904	Total	C	N	O	P	0	0
			62356	27825	11472	20155	2904		

- Molecule 53 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	1533	Total	C	N	O	P	0	0
			32907	14683	6036	10655	1533		

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 55 is a RNA chain called E-site tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 56 is a RNA chain called P-site fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	5	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 57 is a RNA chain called A/T tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
57	6	76	Total	C	N	O	P	S	0	0
			1637	734	290	536	76	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	7	10	Total	C	N	O	P	0	0
			211	95	36	70	10		

- Molecule 59 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	8	615	Total	C	N	O	S	0	0
			4792	3010	875	885	22		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	B	1	Total	Mg	0
			1	1	
60	C	1	Total	Mg	0
			1	1	
60	L	2	Total	Mg	0
			2	2	

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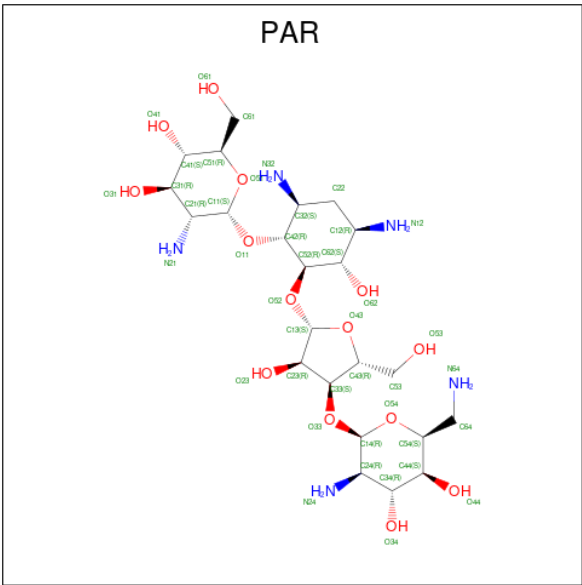
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	N	1	Total 1	Mg 1	0
60	U	1	Total 1	Mg 1	0
60	r	1	Total 1	Mg 1	0
60	s	1	Total 1	Mg 1	0
60	1	220	Total 220	Mg 220	0
60	2	64	Total 64	Mg 64	0
60	3	6	Total 6	Mg 6	0
60	8	1	Total 1	Mg 1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

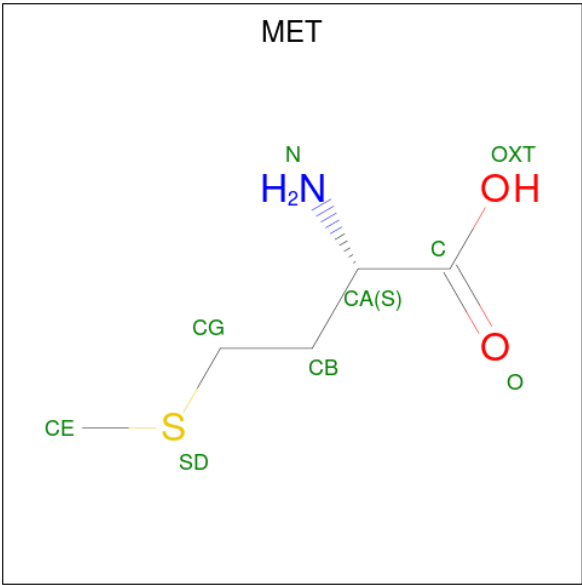
Mol	Chain	Residues	Atoms		AltConf
61	a	1	Total 1	Zn 1	0
61	f	1	Total 1	Zn 1	0
61	8	1	Total 1	Zn 1	0

- Molecule 62 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
62	2	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 63 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
63	5	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	B	2	Total	O	0
			2	2	

3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L2

Chain B: 

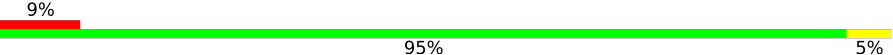


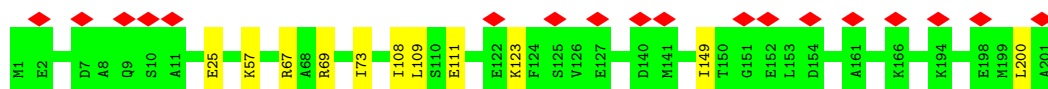
- Molecule 2: 50S ribosomal protein L3

Chain C: 



- Molecule 3: 50S ribosomal protein L4

Chain D: 



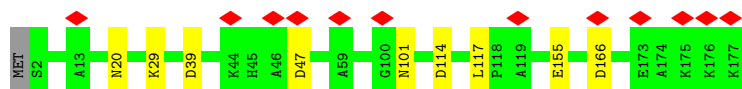
- Molecule 4: 50S ribosomal protein L5

Chain E: 

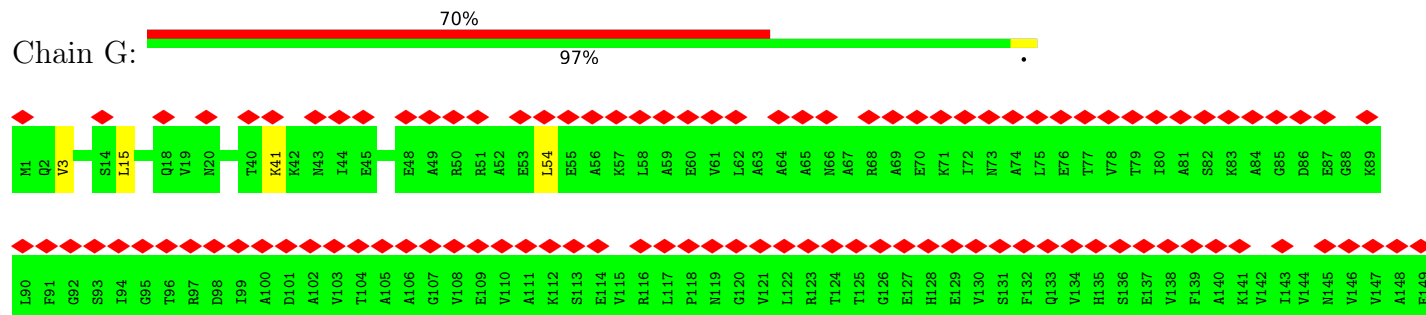


- Molecule 5: 50S ribosomal protein L6

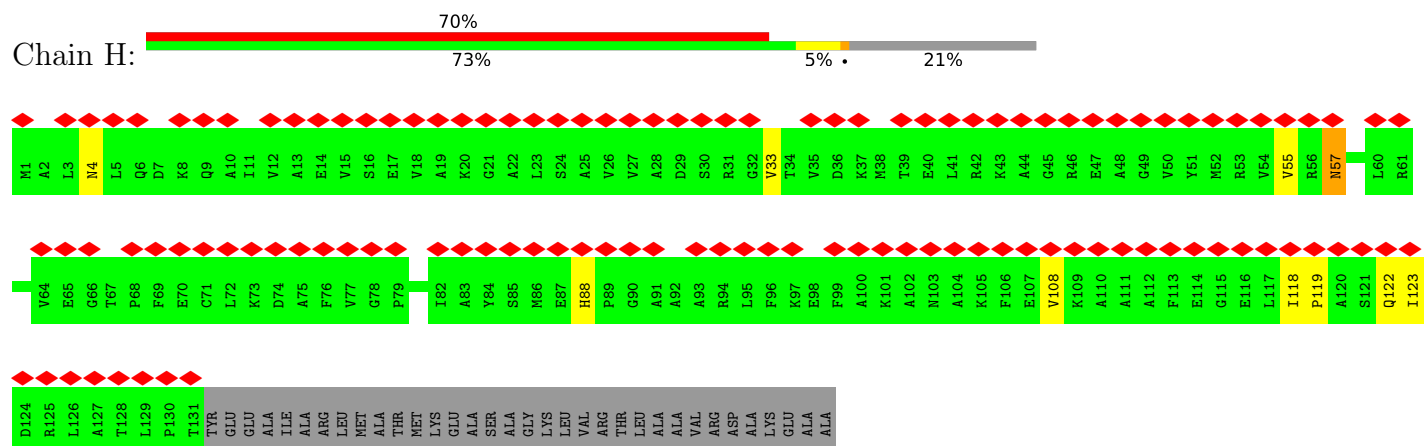
Chain F: 



- Molecule 6: 50S ribosomal protein L9



- Molecule 7: 50S ribosomal protein L10

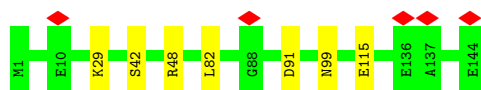


Chain K:  96%



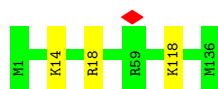
- Molecule 11: 50S ribosomal protein L15

Chain L:  95%



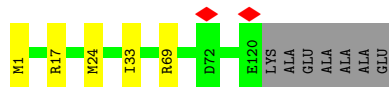
- Molecule 12: 50S ribosomal protein L16

Chain M:  98%



- Molecule 13: 50S ribosomal protein L17

Chain N:  91%



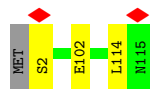
- Molecule 14: 50S ribosomal protein L18

Chain O:  91%




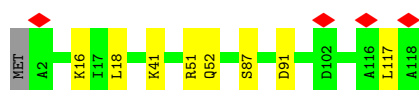
- Molecule 15: 50S ribosomal protein L19

Chain P:  97%

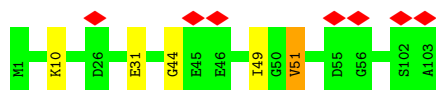


- Molecule 16: 50S ribosomal protein L20

Chain Q:  92%



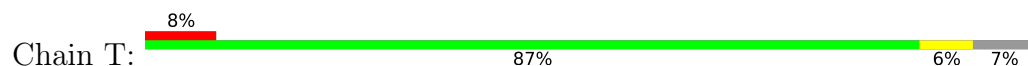
- Molecule 17: 50S ribosomal protein L21



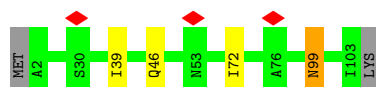
- Molecule 18: 50S ribosomal protein L22



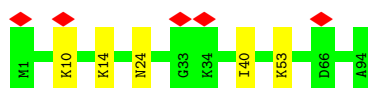
- Molecule 19: 50S ribosomal protein L23



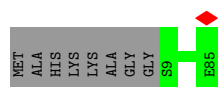
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

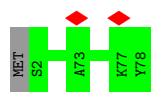


- Molecule 22: 50S ribosomal protein L27

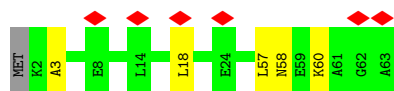
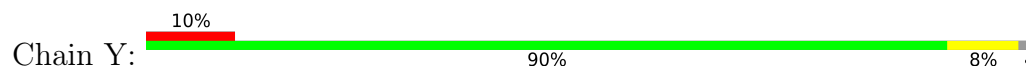


- Molecule 23: 50S ribosomal protein L28





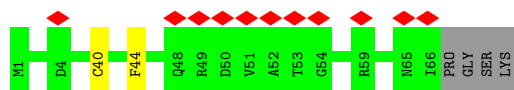
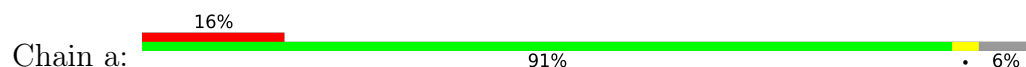
- Molecule 24: 50S ribosomal protein L29



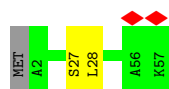
- Molecule 25: 50S ribosomal protein L30



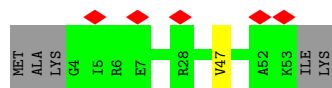
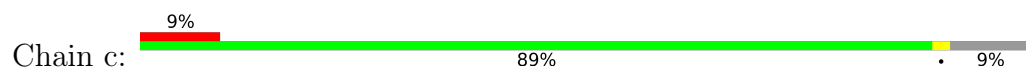
- Molecule 26: 50S ribosomal protein L31



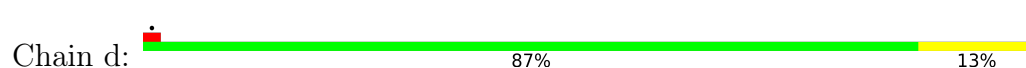
- Molecule 27: 50S ribosomal protein L32



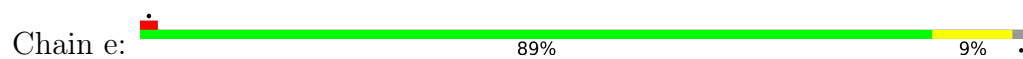
- Molecule 28: 50S ribosomal protein L33



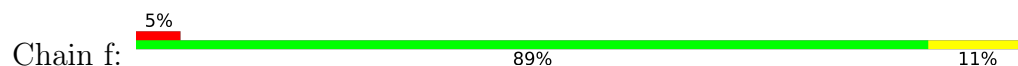
- Molecule 29: 50S ribosomal protein L34



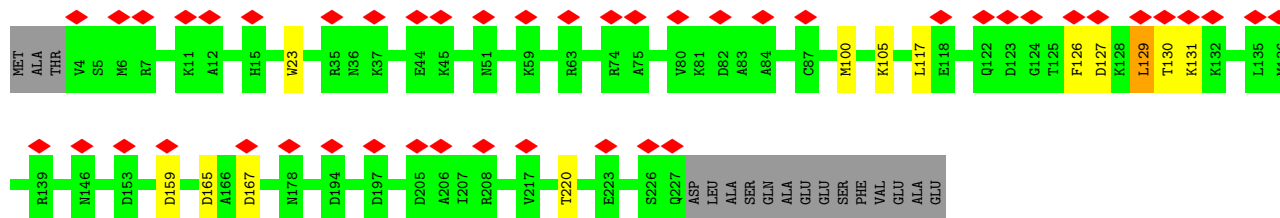
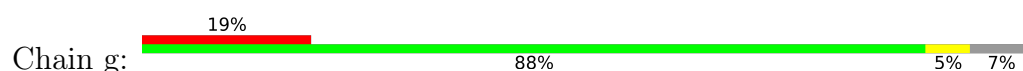
- Molecule 30: 50S ribosomal protein L35



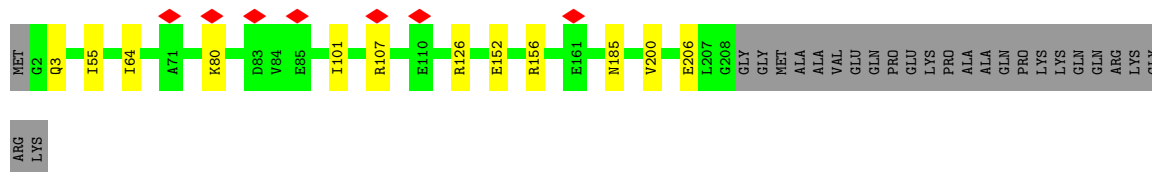
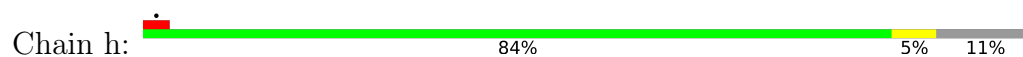
- Molecule 31: 50S ribosomal protein L36



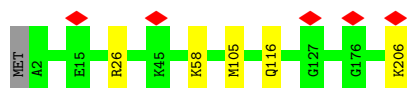
- Molecule 32: 30S ribosomal protein S2



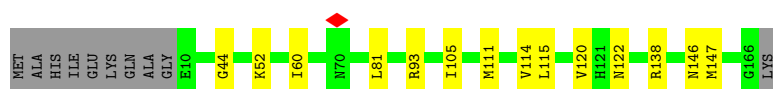
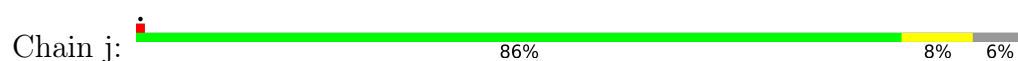
- Molecule 33: 30S ribosomal protein S3



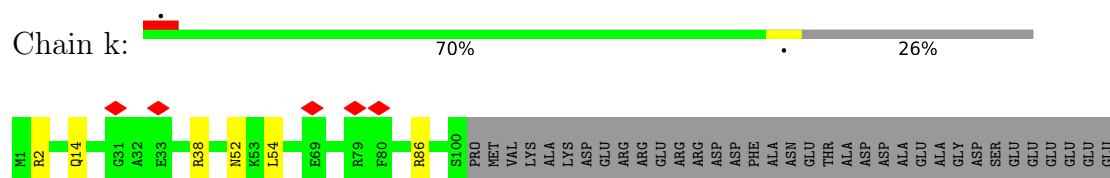
- Molecule 34: 30S ribosomal protein S4



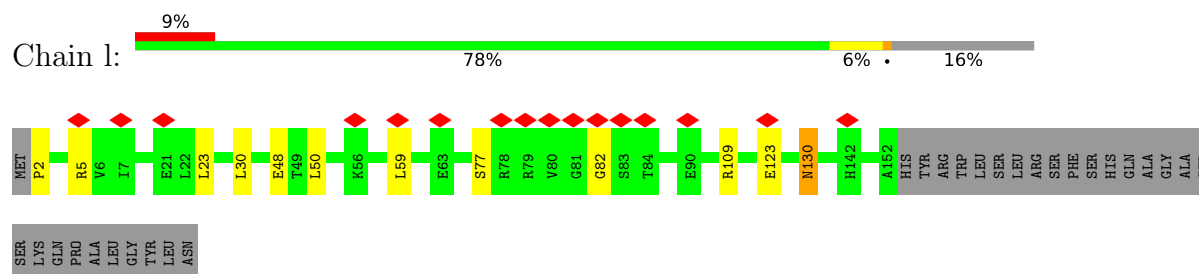
- Molecule 35: 30S ribosomal protein S5



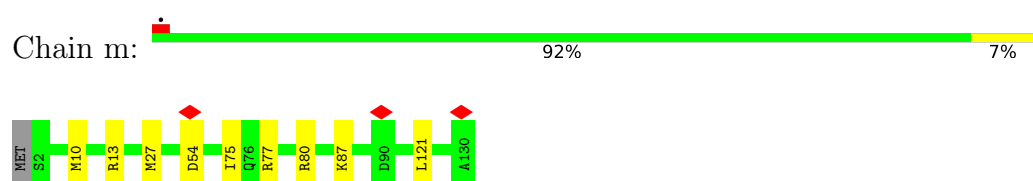
- Molecule 36: 30S ribosomal protein S6



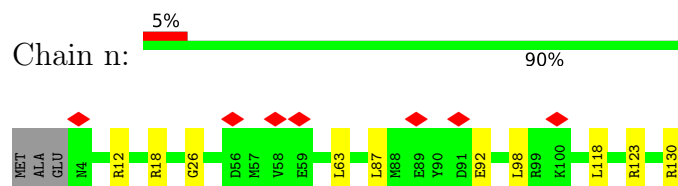
- Molecule 37: 30S ribosomal protein S7



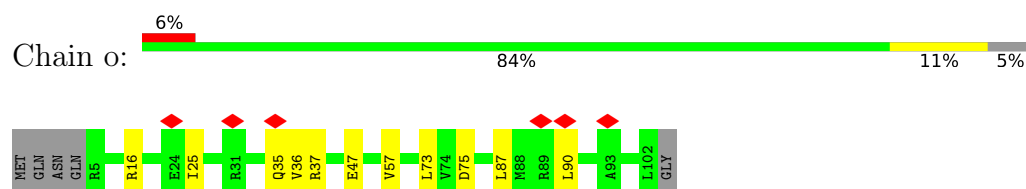
- Molecule 38: 30S ribosomal protein S8



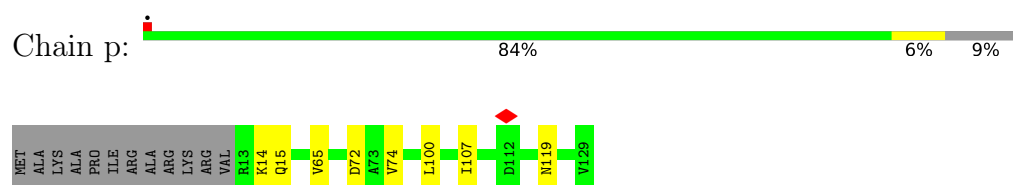
- Molecule 39: 30S ribosomal protein S9



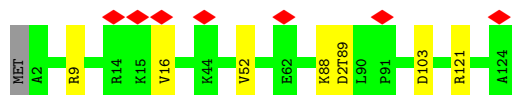
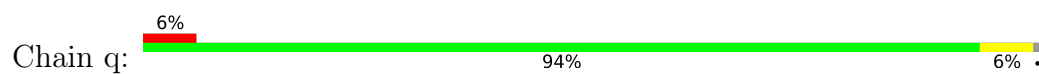
- Molecule 40: 30S ribosomal protein S10



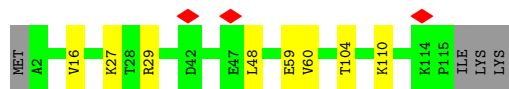
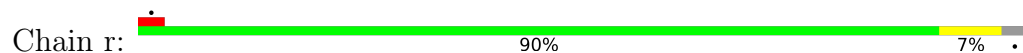
- Molecule 41: 30S ribosomal protein S11



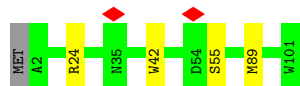
- Molecule 42: 30S ribosomal protein S12



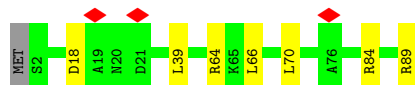
- Molecule 43: 30S ribosomal protein S13



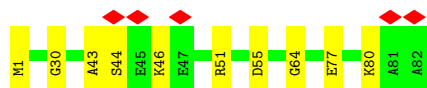
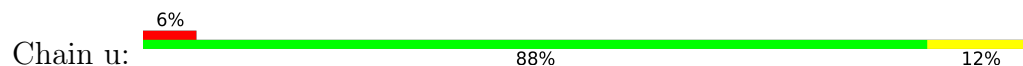
- Molecule 44: 30S ribosomal protein S14



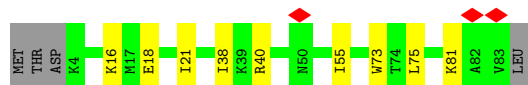
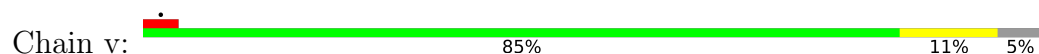
- Molecule 45: 30S ribosomal protein S15



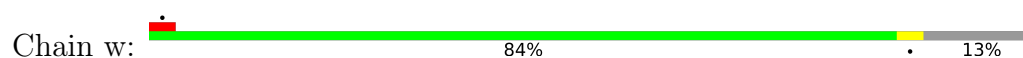
- Molecule 46: 30S ribosomal protein S16

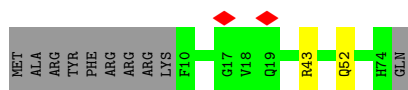


- Molecule 47: 30S ribosomal protein S17

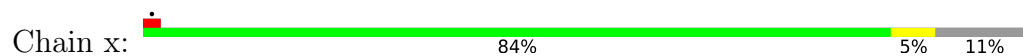


- Molecule 48: 30S ribosomal protein S18

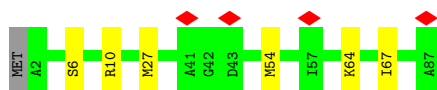
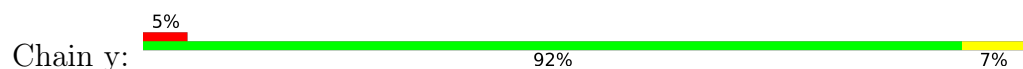




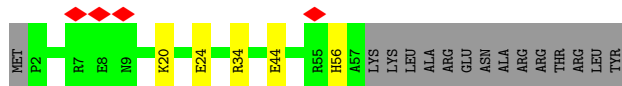
- Molecule 49: 30S ribosomal protein S19



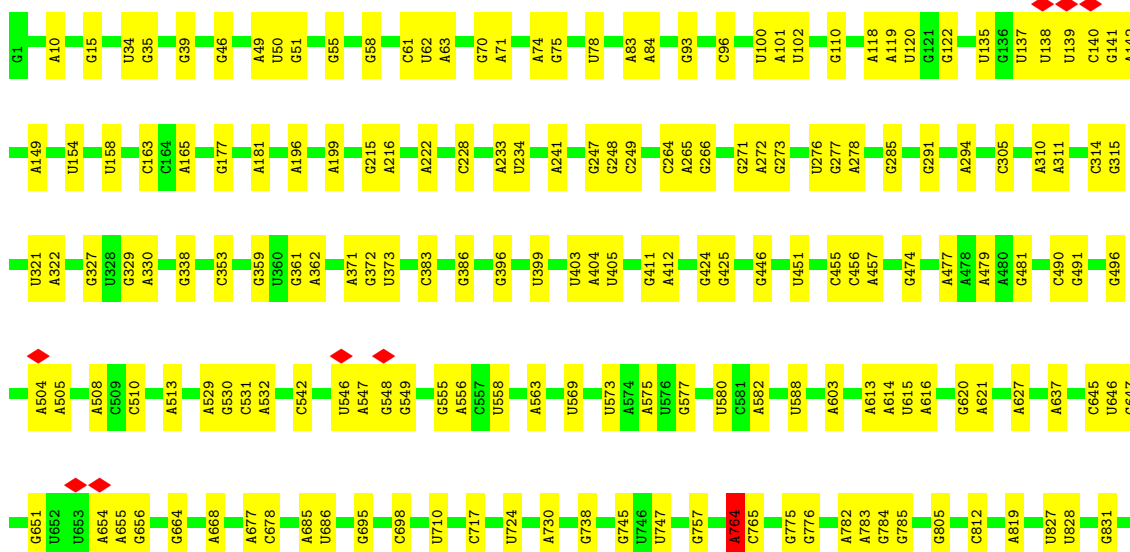
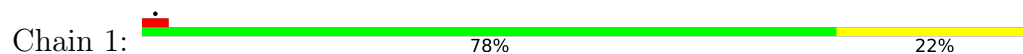
- Molecule 50: 30S ribosomal protein S20

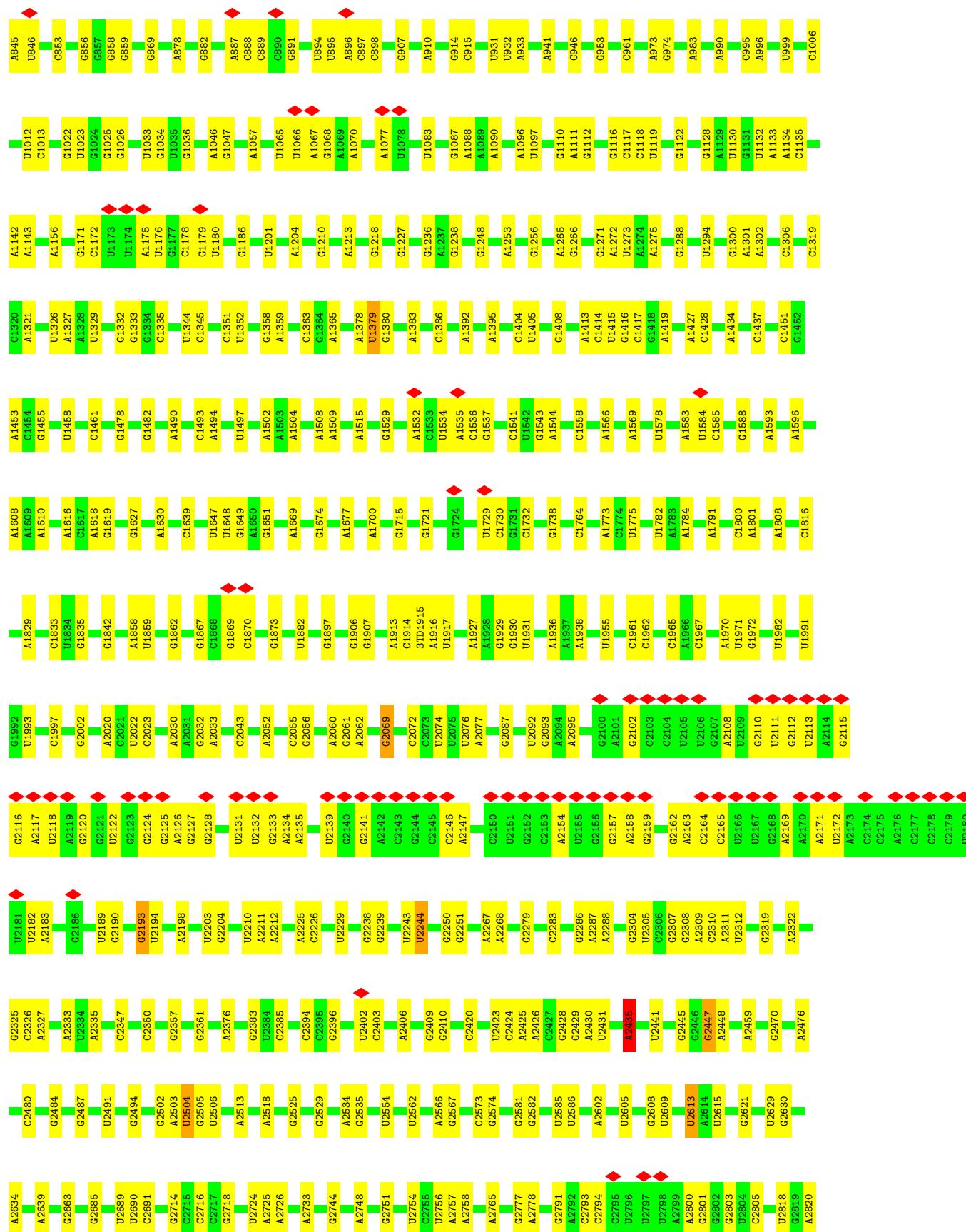


- Molecule 51: 30S ribosomal protein S21



- Molecule 52: LSU rRNA

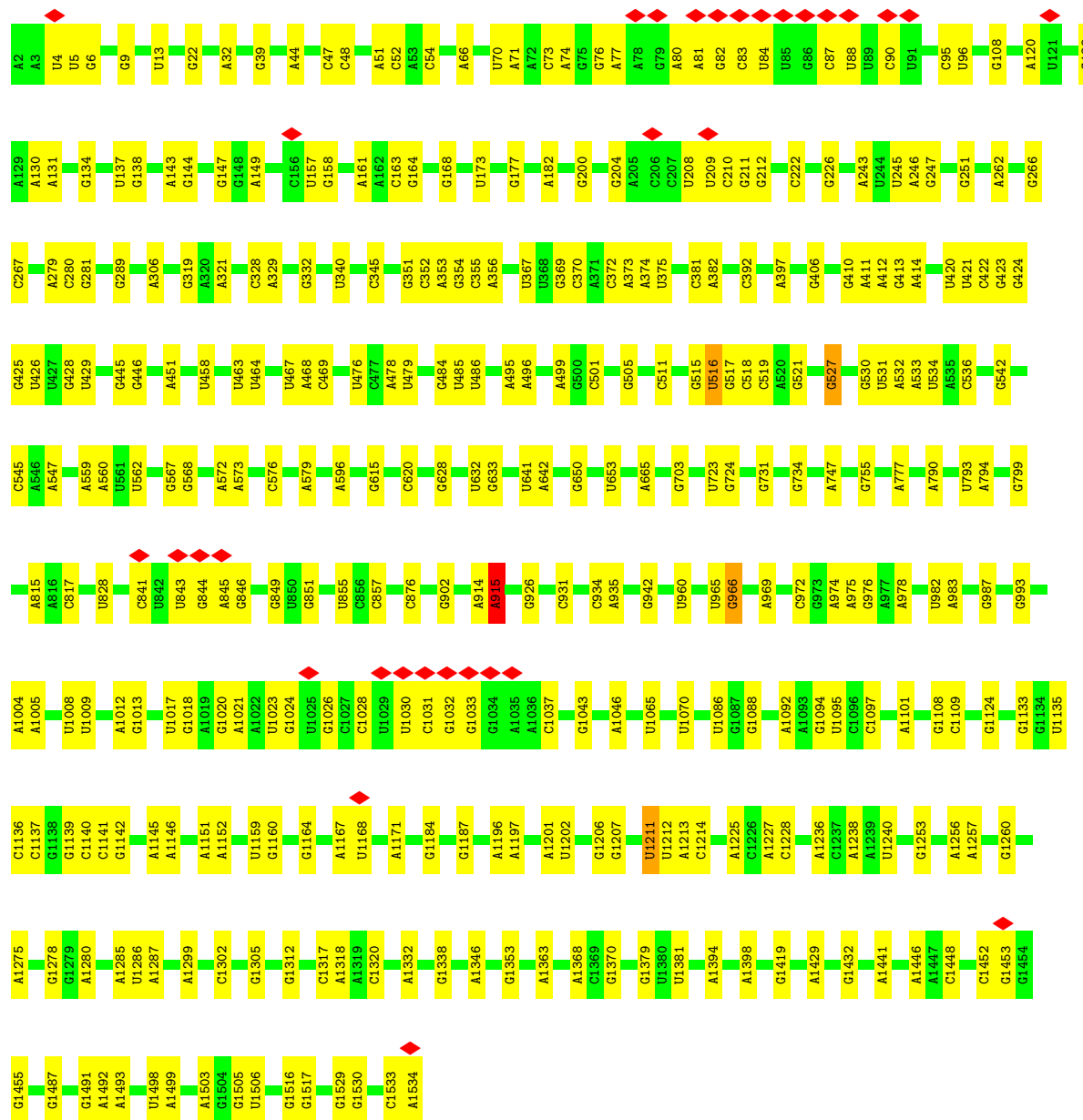






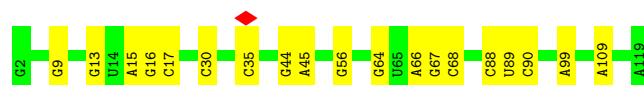
• Molecule 53: SSU rRNA

Chain 2: 78% 22%

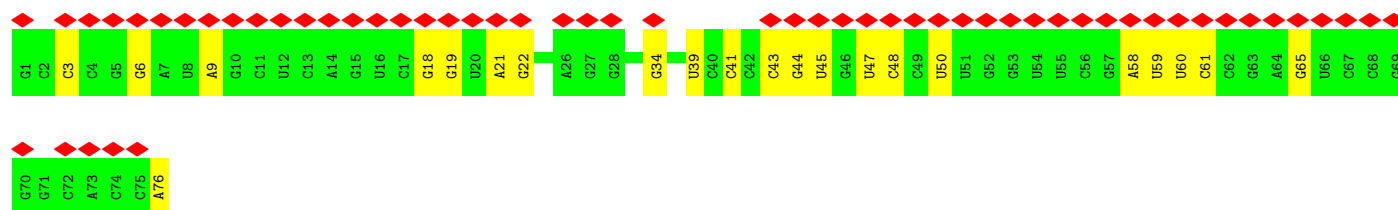
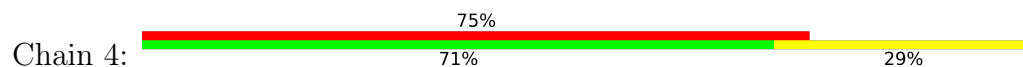


• Molecule 54: 5S rRNA

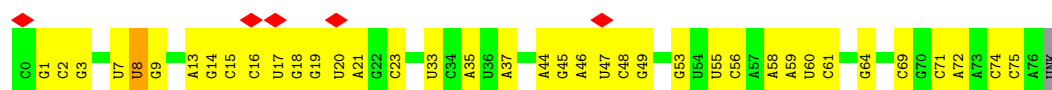
Chain 3: 84% 16%



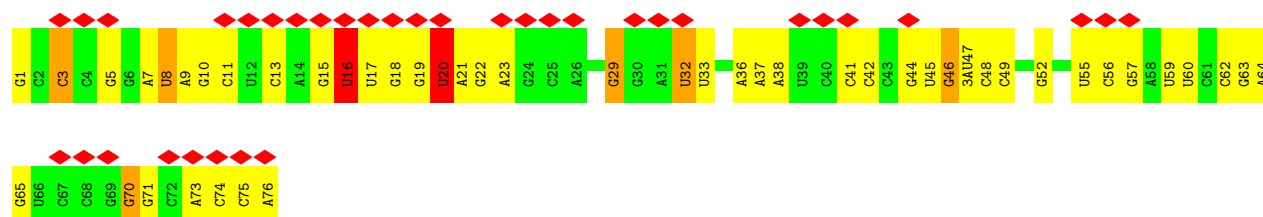
- Molecule 55: E-site tRNA(Phe)



- Molecule 56: P-site fMet-tRNA(fMet)



- Molecule 57: A/T tRNA(Phe)



- Molecule 58: mRNA



- Molecule 59: GTP pyrophosphokinase



D734	V735	I736	D737	A738	R739	L740	LEU	HIS	GLY	SER	A663	G664	Y665	S666	L667	R670	N674	D675	R676	S677	G678	L679	L680	R681	D682	I683	L687	A688	R689	E690	K691	V692	R693	V694	L695	S699	R700	S701	D702	T703	K704	Q705	Q706	L707	A708	D711	I716	Y717	N718	L719	Q720	V721	L722	G723	R724	V725	L726	G727	K728	L729	N730	Q731	V732	P733
PHE	ASN	LYS	PRO	SER	A553	E554	E555	Q556	D557	A558	A559	A560	L561	K562	Q563	L564	Q565	Q566	K567	S568	Y569	T570	P571	GLN	ASN	ARG	SER	LYS	ASP	N594	G595	B596	G601	V602	R611	I616	D619	V622	R629	S632	R635	L641	E650	G658	E659	S660	V661	S662																
LYS	ASN	ILE	LEU	ALA	GLY	ARG	GLN	ILE	LEU	ASP	ASP	GLU	LEU	HIS	GLY	ILE	SER	LEU	LYS	GLU	ALA	GLY	GLU	LYS	HIS	LEU	PRO	ARG	TYR	ASN	PHE	ASN	ASP	VAL	ASP	GLU	LEU	A539	A540	G543	G544	D545	I546	R547	L548	N549	GLN	MET	VAL	ASN	PHE	LEU	GLN	SER	GLN									
ALA	ALA	GLY	GLY	ALA	ARG	SER	GLY	HIS	GLU	ASP	ARG	ILE	ALA	TRP	N313	P314	K315	P316	N317	G318	Y319	Q320	S321	I322	H323	T324	V325	V326	L327	G328	P329	G330	G331	K332	T333	V334	E335	I336	Q337	I338	R339	T340	K341	Q342	M343	H344	E345	D346	A347	E348	L349	G350	V351	A352	A353	HIS	TRP	LYS	TYR	LYS	GLY	GLY		
K241	A242	E243	G244	V245	K246	A247	E248	V249	Y250	G251	R252	P253	K254	H255	I256	Y257	S258	I259	W260	R261	K262	M263	Q264	K265	K266	N267	L268	A269	F270	F271	E272	L273	F274	D275	V276	R277	A278	V279	R280	I281	V282	A283	E284	R285	L286	Q287	D288	C289	Y290	A291	A292	L293	G294	I295	V296	T298	Y299	H299						
I181	Y182	A183	P184	L185	A186	N187	R188	L189	G190	I191	G192	Q193	L194	K195	W196	E197	L198	E199	D200	Y201	C202	F203	R204	Y205	L206	H207	P208	T209	E210	Y211	K212	R213	I214	A215	K216	L217	L218	H219	E220	R221	R222	L223	D224	R225	E226	H227	Y228	I229	E230	E231	F232	V233	G234	A235	L236	R237	A238	E239	W240					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	1.341	Depositor
Minimum map value	-0.666	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, OMU, 5MU, MG, 3AU, UR3, D2T, OMG, 6IA, 7MG, PSU, 5MC, 6MZ, OMC, MA6, PAR, 2MG, ZN, G7M, 1MG, 4OC, 3TD, 2MA, 4SU

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	B	0.35	0/2121	0.70	0/2852
2	C	0.35	0/1586	0.65	0/2134
3	D	0.43	0/1571	0.74	1/2113 (0.0%)
4	E	0.45	0/1434	0.73	0/1926
5	F	0.39	0/1343	0.65	0/1816
6	G	0.42	0/1122	0.63	0/1515
7	H	0.46	0/1001	0.66	0/1350
8	I	0.42	0/1046	0.62	0/1410
9	J	0.44	0/1152	0.72	0/1551
10	K	0.35	0/955	0.72	0/1279
11	L	0.38	0/1062	0.74	0/1413
12	M	0.41	0/1093	0.72	0/1460
13	N	0.49	0/973	0.82	0/1301
14	O	0.47	0/902	0.81	0/1209
15	P	0.36	0/929	0.69	0/1242
16	Q	0.55	0/960	0.93	0/1278
17	R	0.33	0/829	0.66	0/1107
18	S	0.42	0/864	0.78	0/1156
19	T	0.41	0/744	0.68	0/994
20	U	0.35	0/787	0.61	0/1051
21	V	0.39	0/766	0.64	0/1025
22	W	0.34	0/595	0.64	0/787
23	X	0.42	0/635	0.75	0/848
24	Y	0.53	0/502	0.83	0/667
25	Z	0.44	0/453	0.71	0/605
26	a	0.43	0/531	0.66	0/709
27	b	0.41	0/450	0.73	0/599
28	c	0.34	0/416	0.62	0/554
29	d	0.52	0/380	0.95	0/498
30	e	0.42	0/513	0.81	0/676
31	f	0.34	0/303	0.71	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.47	0/1784	0.71	0/2403
33	h	0.43	0/1655	0.72	0/2230
34	i	0.45	0/1665	0.72	0/2227
35	j	0.43	0/1169	0.76	0/1573
36	k	0.42	0/835	0.72	0/1128
37	l	0.48	0/1195	0.78	0/1602
38	m	0.41	0/989	0.71	0/1326
39	n	0.43	0/1034	0.77	0/1375
40	o	0.42	0/796	0.74	0/1077
41	p	0.40	0/893	0.71	0/1205
42	q	0.35	0/960	0.72	0/1286
43	r	0.46	0/892	0.86	0/1193
44	s	0.47	0/817	0.78	0/1088
45	t	0.54	0/722	0.85	0/964
46	u	0.44	0/659	0.75	0/884
47	v	0.35	0/657	0.64	0/881
48	w	0.45	0/548	0.73	0/736
49	x	0.41	0/675	0.70	0/908
50	y	0.58	0/676	0.88	0/895
51	z	0.51	0/472	0.89	0/627
52	1	0.34	11/69300 (0.0%)	0.74	21/108089 (0.0%)
53	2	0.27	2/36561 (0.0%)	0.72	2/57019 (0.0%)
54	3	0.24	0/2828	0.70	0/4410
55	4	0.25	0/1808	0.70	0/2815
56	5	0.35	0/1716	0.83	0/2672
57	6	0.42	1/1606 (0.1%)	0.80	1/2497 (0.0%)
58	7	0.31	0/235	0.71	0/363
59	8	0.62	0/4878	1.14	30/6606 (0.5%)
All	All	0.36	14/166043 (0.0%)	0.75	55/247601 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
52	1	0	9
53	2	0	2
57	6	8	3
59	8	0	19
All	All	8	33

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	2244	U	C2-N3	19.23	1.51	1.37
52	1	2244	U	N3-C4	17.42	1.54	1.38
52	1	2435	A	C6-N1	-15.77	1.24	1.35
52	1	2244	U	N1-C2	13.64	1.50	1.38
52	1	1775	U	C2-N3	12.29	1.46	1.37
57	6	1	G	OP3-P	-10.15	1.49	1.61
52	1	1775	U	N3-C4	8.99	1.46	1.38
52	1	1596	A	N1-C2	7.23	1.40	1.34
52	1	1405	U	C2-N3	7.15	1.42	1.37
52	1	2435	A	N1-C2	6.21	1.40	1.34
53	2	13	U	C2-N3	6.08	1.42	1.37
53	2	915	A	C6-N1	-5.73	1.31	1.35
52	1	2244	U	O4'-C1'	5.49	1.48	1.41
52	1	764	A	C6-N1	-5.39	1.31	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	2244	U	C2-N3-C4	-18.02	116.19	127.00
52	1	2435	A	N1-C6-N6	-14.25	110.05	118.60
52	1	2244	U	C2-N1-C1'	13.09	133.41	117.70
52	1	2244	U	C6-N1-C1'	-11.39	105.26	121.20
52	1	2244	U	C5-C4-O4	-10.87	119.38	125.90
59	8	171	ARG	NE-CZ-NH2	10.07	125.34	120.30
52	1	1775	U	C2-N3-C4	-10.05	120.97	127.00
59	8	213	ARG	NE-CZ-NH2	9.31	124.95	120.30
52	1	2435	A	C5-C6-N6	8.63	130.60	123.70
59	8	277	ARG	NE-CZ-NH2	8.37	124.48	120.30
59	8	204	ARG	NE-CZ-NH2	7.82	124.21	120.30
59	8	221	ARG	NE-CZ-NH1	-7.66	116.47	120.30
52	1	2244	U	C4-C5-C6	7.55	124.23	119.70
59	8	58	ARG	NE-CZ-NH2	7.29	123.94	120.30
59	8	130	GLU	CB-CA-C	7.20	124.80	110.40
52	1	1596	A	C6-N1-C2	-7.03	114.38	118.60
59	8	221	ARG	NE-CZ-NH2	6.93	123.76	120.30
59	8	196	TRP	CA-CB-CG	6.84	126.69	113.70
59	8	161	ARG	NE-CZ-NH2	6.80	123.70	120.30
59	8	121	ALA	CB-CA-C	6.74	120.22	110.10
52	1	1405	U	C2-N3-C4	-6.73	122.96	127.00
52	1	1775	U	N1-C1'-C2'	6.49	122.44	114.00
52	1	2193	G	C2'-C3'-O3'	6.46	124.03	113.70
59	8	339	ARG	NE-CZ-NH2	6.35	123.47	120.30
53	2	1211	U	C2'-C3'-O3'	6.33	123.83	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	8	261	ARG	NE-CZ-NH2	6.17	123.38	120.30
57	6	70	G	C2'-C3'-O3'	6.02	123.33	113.70
59	8	222	ARG	NE-CZ-NH2	5.99	123.29	120.30
59	8	319	TYR	CB-CG-CD2	-5.74	117.56	121.00
59	8	163	VAL	CA-CB-CG1	5.72	119.48	110.90
59	8	96	ARG	NE-CZ-NH2	5.67	123.13	120.30
52	1	2244	U	C5'-C4'-O4'	5.60	115.82	109.10
52	1	2244	U	C3'-C2'-C1'	5.55	105.94	101.50
59	8	117	ARG	NE-CZ-NH2	5.53	123.06	120.30
52	1	1379	U	C2'-C3'-O3'	5.47	122.45	113.70
52	1	2244	U	N3-C4-O4	5.45	123.22	119.40
59	8	156	ARG	NE-CZ-NH2	5.41	123.00	120.30
59	8	571	PRO	N-CA-CB	5.40	109.78	103.30
59	8	41	TYR	CB-CG-CD2	-5.39	117.77	121.00
59	8	124	THR	C-N-CA	5.39	135.17	121.70
53	2	632	U	N1-C1'-C2'	5.38	120.99	114.00
59	8	132	VAL	CG1-CB-CG2	-5.37	102.31	110.90
59	8	120	LYS	CB-CA-C	5.24	120.89	110.40
59	8	147	ARG	NE-CZ-NH2	5.20	122.90	120.30
59	8	261	ARG	N-CA-CB	-5.18	101.28	110.60
52	1	2447	G	C2'-C3'-O3'	-5.14	98.18	109.50
52	1	2613	U	O4'-C1'-N1	5.13	112.30	108.20
59	8	201	TYR	CB-CG-CD2	-5.12	117.93	121.00
59	8	222	ARG	CD-NE-CZ	5.10	130.74	123.60
59	8	237	ARG	NE-CZ-NH2	5.08	122.84	120.30
52	1	2074	U	N1-C1'-C2'	5.05	120.56	114.00
59	8	301	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	D	67	ARG	NE-CZ-NH1	5.04	122.82	120.30
52	1	2244	U	N1-C2-O2	-5.00	119.30	122.80
52	1	2613	U	N1-C1'-C2'	5.00	120.50	114.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C1',C3',C2'
57	6	20	H2U	C1',C2'
57	6	32	PSU	C1'
57	6	37	6IA	C3'
57	6	55	PSU	C1'

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	1	1319	C	Sidechain
52	1	1335	C	Sidechain
52	1	1351	C	Sidechain
52	1	1363	C	Sidechain
52	1	2244	U	Sidechain
52	1	2435	A	Sidechain
52	1	305	C	Sidechain
52	1	314	C	Sidechain
52	1	764	A	Sidechain
53	2	915	A	Sidechain
53	2	931	C	Sidechain
57	6	29	G	Sidechain
57	6	3	C	Sidechain
57	6	42	C	Sidechain
59	8	116	ILE	Peptide
59	8	121	ALA	Peptide
59	8	123	HIS	Peptide
59	8	127	VAL	Peptide
59	8	133	ASP	Peptide
59	8	135	VAL	Peptide
59	8	136	ARG	Peptide
59	8	138	MET	Peptide
59	8	163	VAL	Peptide
59	8	166	ALA	Peptide
59	8	170	GLU	Peptide
59	8	171	ARG	Sidechain
59	8	211	TYR	Sidechain
59	8	252	ARG	Sidechain
59	8	264	GLN	Peptide
59	8	300	TYR	Sidechain
59	8	332	LYS	Peptide
59	8	77	ARG	Sidechain
59	8	96	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/273 (98%)	249 (93%)	18 (7%)	2 (1%)	22	60
2	C	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	29	68
3	D	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	29	68
4	E	175/179 (98%)	158 (90%)	13 (7%)	4 (2%)	6	30
5	F	174/177 (98%)	156 (90%)	17 (10%)	1 (1%)	25	64
6	G	147/149 (99%)	126 (86%)	17 (12%)	4 (3%)	5	26
7	H	129/165 (78%)	103 (80%)	18 (14%)	8 (6%)	1	8
8	I	139/142 (98%)	113 (81%)	20 (14%)	6 (4%)	2	15
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
10	K	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
11	L	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	11	43
12	M	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
13	N	118/127 (93%)	107 (91%)	10 (8%)	1 (1%)	19	57
14	O	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	8	37
15	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
16	Q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	17	55
17	R	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	7	34
18	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
19	T	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
20	U	100/104 (96%)	91 (91%)	7 (7%)	2 (2%)	7	34
21	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
22	W	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
23	X	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
24	Y	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	9	39
25	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	64/70 (91%)	51 (80%)	12 (19%)	1 (2%)	9	40
27	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	c	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
29	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	e	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	40
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	g	222/241 (92%)	200 (90%)	15 (7%)	7 (3%)	4	22
33	h	205/233 (88%)	185 (90%)	18 (9%)	2 (1%)	15	53
34	i	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
35	j	155/167 (93%)	142 (92%)	10 (6%)	3 (2%)	8	36
36	k	98/135 (73%)	88 (90%)	9 (9%)	1 (1%)	15	53
37	l	149/179 (83%)	140 (94%)	7 (5%)	2 (1%)	12	45
38	m	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	57
39	n	125/130 (96%)	113 (90%)	10 (8%)	2 (2%)	9	40
40	o	96/103 (93%)	82 (85%)	11 (12%)	3 (3%)	4	23
41	p	115/129 (89%)	98 (85%)	15 (13%)	2 (2%)	9	39
42	q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	19	57
43	r	112/118 (95%)	106 (95%)	6 (5%)	0	100	100
44	s	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	t	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	u	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	2	12
47	v	78/84 (93%)	72 (92%)	4 (5%)	2 (3%)	5	27
48	w	63/75 (84%)	60 (95%)	3 (5%)	0	100	100
49	x	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	5	28
50	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
51	z	54/71 (76%)	52 (96%)	1 (2%)	1 (2%)	8	36
59	8	604/744 (81%)	528 (87%)	55 (9%)	21 (4%)	3	20
All	All	6455/6964 (93%)	5874 (91%)	487 (8%)	94 (2%)	14	42

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	175	PHE

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Mol	Chain	Res	Type
7	H	4	ASN
7	H	123	ILE
11	L	99	ASN
17	R	51	VAL
32	g	130	THR
32	g	131	LYS
46	u	43	ALA
59	8	117	ARG
59	8	125	ASP
59	8	136	ARG
59	8	137	ARG
59	8	167	PRO
59	8	596	ARG
59	8	616	ILE
6	G	15	LEU
6	G	41	LYS
11	L	29	LYS
26	a	40	CYS
32	g	127	ASP
37	l	130	ASN
40	o	57	VAL
47	v	18	GLU
59	8	115	ALA
59	8	131	GLN
59	8	168	GLU
59	8	350	GLY
4	E	41	GLY
4	E	174	ASP
5	F	47	ASP
8	I	64	ARG
16	Q	87	SER
20	U	99	ASN
24	Y	3	ALA
32	g	100	MET
33	h	80	LYS
35	j	111	MET
35	j	147	MET
36	k	52	ASN
41	p	14	LYS
42	q	16	VAL
47	v	16	LYS
59	8	120	LYS

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Mol	Chain	Res	Type
59	8	124	THR
59	8	126	SER
59	8	133	ASP
1	B	158	ALA
6	G	54	LEU
7	H	57	ASN
7	H	108	VAL
7	H	118	ILE
7	H	119	PRO
8	I	38	CYS
32	g	126	PHE
32	g	129	LEU
49	x	29	LYS
59	8	666	SER
6	G	3	VAL
7	H	88	HIS
8	I	12	VAL
8	I	92	PRO
13	N	33	ILE
14	O	99	TYR
32	g	165	ASP
38	m	75	ILE
40	o	36	VAL
40	o	75	ASP
46	u	64	GLY
51	z	56	HIS
59	8	268	LEU
59	8	635	ARG
59	8	660	SER
2	C	151	THR
3	D	69	ARG
33	h	101	ILE
39	n	92	GLU
46	u	44	SER
30	e	32	ILE
7	H	55	VAL
49	x	67	VAL
59	8	331	GLY
4	E	84	PRO
17	R	44	GLY
20	U	39	ILE
37	l	82	GLY

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Mol	Chain	Res	Type
39	n	26	GLY
59	8	89	VAL
1	B	56	GLY
8	I	22	PRO
8	I	136	GLY
35	j	44	GLY
14	O	114	GLY
41	p	74	VAL
46	u	30	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/218 (99%)	205 (95%)	11 (5%)	24	60
2	C	164/164 (100%)	159 (97%)	5 (3%)	41	75
3	D	165/165 (100%)	156 (94%)	9 (6%)	21	57
4	E	148/150 (99%)	138 (93%)	10 (7%)	16	48
5	F	137/138 (99%)	129 (94%)	8 (6%)	20	55
6	G	114/114 (100%)	114 (100%)	0	100	100
7	H	100/123 (81%)	97 (97%)	3 (3%)	41	75
8	I	109/110 (99%)	106 (97%)	3 (3%)	43	77
9	J	116/116 (100%)	114 (98%)	2 (2%)	60	85
10	K	104/104 (100%)	99 (95%)	5 (5%)	25	62
11	L	103/103 (100%)	98 (95%)	5 (5%)	25	61
12	M	109/109 (100%)	106 (97%)	3 (3%)	43	77
13	N	100/103 (97%)	96 (96%)	4 (4%)	31	68
14	O	86/87 (99%)	79 (92%)	7 (8%)	11	40
15	P	99/100 (99%)	96 (97%)	3 (3%)	41	75
16	Q	89/90 (99%)	82 (92%)	7 (8%)	12	41
17	R	84/84 (100%)	80 (95%)	4 (5%)	25	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	93/93 (100%)	87 (94%)	6 (6%)	17	50
19	T	80/84 (95%)	74 (92%)	6 (8%)	13	43
20	U	83/85 (98%)	80 (96%)	3 (4%)	35	70
21	V	78/78 (100%)	73 (94%)	5 (6%)	17	51
22	W	59/63 (94%)	59 (100%)	0	100	100
23	X	67/68 (98%)	67 (100%)	0	100	100
24	Y	54/55 (98%)	50 (93%)	4 (7%)	13	44
25	Z	48/49 (98%)	45 (94%)	3 (6%)	18	51
26	a	59/62 (95%)	58 (98%)	1 (2%)	60	85
27	b	47/48 (98%)	45 (96%)	2 (4%)	29	66
28	c	45/49 (92%)	44 (98%)	1 (2%)	52	81
29	d	38/38 (100%)	32 (84%)	6 (16%)	2	12
30	e	51/52 (98%)	46 (90%)	5 (10%)	8	30
31	f	34/34 (100%)	30 (88%)	4 (12%)	5	22
32	g	186/199 (94%)	179 (96%)	7 (4%)	33	69
33	h	170/189 (90%)	160 (94%)	10 (6%)	19	54
34	i	172/173 (99%)	167 (97%)	5 (3%)	42	76
35	j	119/126 (94%)	108 (91%)	11 (9%)	9	34
36	k	87/116 (75%)	82 (94%)	5 (6%)	20	56
37	l	124/147 (84%)	113 (91%)	11 (9%)	9	35
38	m	104/105 (99%)	96 (92%)	8 (8%)	13	42
39	n	105/107 (98%)	97 (92%)	8 (8%)	13	43
40	o	86/90 (96%)	78 (91%)	8 (9%)	9	33
41	p	90/99 (91%)	84 (93%)	6 (7%)	16	49
42	q	102/103 (99%)	97 (95%)	5 (5%)	25	61
43	r	92/96 (96%)	84 (91%)	8 (9%)	10	37
44	s	83/84 (99%)	79 (95%)	4 (5%)	25	62
45	t	76/77 (99%)	69 (91%)	7 (9%)	9	34
46	u	65/65 (100%)	59 (91%)	6 (9%)	9	34
47	v	74/78 (95%)	67 (90%)	7 (10%)	8	32
48	w	57/66 (86%)	55 (96%)	2 (4%)	36	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	x	72/79 (91%)	69 (96%)	3 (4%)	30 66
50	y	65/66 (98%)	59 (91%)	6 (9%)	9 34
51	z	48/61 (79%)	44 (92%)	4 (8%)	11 39
59	8	500/629 (80%)	438 (88%)	62 (12%)	4 20
All	All	5356/5691 (94%)	5028 (94%)	328 (6%)	22 53

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	ARG
1	B	105	LEU
1	B	130	LEU
1	B	156	ARG
1	B	195	VAL
1	B	202	LEU
1	B	203	ARG
1	B	204	VAL
1	B	205	LEU
1	B	242	LYS
1	B	271	ARG
2	C	13	ARG
2	C	32	ASN
2	C	43	ASP
2	C	149	ASN
2	C	170	VAL
3	D	25	GLU
3	D	57	LYS
3	D	73	ILE
3	D	108	ILE
3	D	109	LEU
3	D	111	GLU
3	D	123	LYS
3	D	149	ILE
3	D	200	LEU
4	E	50	LEU
4	E	64	LYS
4	E	80	ARG
4	E	94	GLU
4	E	106	ILE
4	E	117	LEU
4	E	123	ASP

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Mol	Chain	Res	Type
4	E	137	ILE
4	E	140	GLU
4	E	175	PHE
5	F	20	ASN
5	F	29	LYS
5	F	39	ASP
5	F	101	ASN
5	F	114	ASP
5	F	117	LEU
5	F	155	GLU
5	F	166	ASP
7	H	33	VAL
7	H	57	ASN
7	H	122	GLN
8	I	10	LEU
8	I	11	GLN
8	I	48	ILE
9	J	30	THR
9	J	128	ASN
10	K	17	ARG
10	K	32	TYR
10	K	58	LEU
10	K	67	LYS
10	K	123	LEU
11	L	42	SER
11	L	48	ARG
11	L	82	LEU
11	L	91	ASP
11	L	115	GLU
12	M	14	LYS
12	M	18	ARG
12	M	118	LYS
13	N	1	MET
13	N	17	ARG
13	N	24	MET
13	N	69	ARG
14	O	7	ARG
14	O	17	LYS
14	O	18	LEU
14	O	19	GLN
14	O	31	THR
14	O	53	THR

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Mol	Chain	Res	Type
14	O	104	GLN
15	P	2	SER
15	P	102	GLU
15	P	114	LEU
16	Q	16	LYS
16	Q	18	LEU
16	Q	41	LYS
16	Q	51	ARG
16	Q	52	GLN
16	Q	91	ASP
16	Q	117	LEU
17	R	10	LYS
17	R	31	GLU
17	R	49	ILE
17	R	51	VAL
18	S	7	HIS
18	S	22	ASP
18	S	28	LYS
18	S	41	LYS
18	S	95	ARG
18	S	96	ILE
19	T	2	ILE
19	T	3	ARG
19	T	30	ILE
19	T	49	LYS
19	T	50	LEU
19	T	77	ARG
20	U	46	GLN
20	U	72	ILE
20	U	99	ASN
21	V	10	LYS
21	V	14	LYS
21	V	24	ASN
21	V	40	ILE
21	V	53	LYS
24	Y	18	LEU
24	Y	57	LEU
24	Y	58	ASN
24	Y	60	LYS
25	Z	4	THR
25	Z	31	ARG
25	Z	45	ARG

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Mol	Chain	Res	Type
26	a	44	PHE
27	b	27	SER
27	b	28	LEU
28	c	47	VAL
29	d	1	MET
29	d	3	ARG
29	d	22	MET
29	d	24	THR
29	d	41	ARG
29	d	44	VAL
30	e	13	ARG
30	e	30	ARG
30	e	47	LYS
30	e	54	ASP
30	e	55	LEU
31	f	3	VAL
31	f	4	ARG
31	f	12	ARG
31	f	26	ILE
32	g	23	TRP
32	g	105	LYS
32	g	117	LEU
32	g	129	LEU
32	g	159	ASP
32	g	167	ASP
32	g	220	THR
33	h	3	GLN
33	h	55	ILE
33	h	64	ILE
33	h	107	ARG
33	h	126	ARG
33	h	152	GLU
33	h	156	ARG
33	h	185	ASN
33	h	200	VAL
33	h	206	GLU
34	i	26	ARG
34	i	58	LYS
34	i	105	MET
34	i	116	GLN
34	i	206	LYS
35	j	52	LYS

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Mol	Chain	Res	Type
35	j	60	ILE
35	j	81	LEU
35	j	93	ARG
35	j	105	ILE
35	j	114	VAL
35	j	115	LEU
35	j	120	VAL
35	j	122	ASN
35	j	138	ARG
35	j	146	ASN
36	k	2	ARG
36	k	14	GLN
36	k	38	ARG
36	k	54	LEU
36	k	86	ARG
37	l	2	PRO
37	l	5	ARG
37	l	23	LEU
37	l	30	LEU
37	l	48	GLU
37	l	50	LEU
37	l	59	LEU
37	l	77	SER
37	l	109	ARG
37	l	123	GLU
37	l	130	ASN
38	m	10	MET
38	m	13	ARG
38	m	27	MET
38	m	54	ASP
38	m	77	ARG
38	m	80	ARG
38	m	87	LYS
38	m	121	LEU
39	n	12	ARG
39	n	18	ARG
39	n	63	LEU
39	n	87	LEU
39	n	98	LEU
39	n	118	LEU
39	n	123	ARG
39	n	130	ARG

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Mol	Chain	Res	Type
40	o	16	ARG
40	o	25	ILE
40	o	35	GLN
40	o	37	ARG
40	o	47	GLU
40	o	73	LEU
40	o	87	LEU
40	o	90	LEU
41	p	15	GLN
41	p	65	VAL
41	p	72	ASP
41	p	100	LEU
41	p	107	ILE
41	p	119	ASN
42	q	9	ARG
42	q	52	VAL
42	q	88	LYS
42	q	103	ASP
42	q	121	ARG
43	r	16	VAL
43	r	27	LYS
43	r	29	ARG
43	r	48	LEU
43	r	59	GLU
43	r	60	VAL
43	r	104	THR
43	r	110	LYS
44	s	24	ARG
44	s	42	TRP
44	s	55	SER
44	s	89	MET
45	t	18	ASP
45	t	39	LEU
45	t	64	ARG
45	t	66	LEU
45	t	70	LEU
45	t	84	ARG
45	t	89	ARG
46	u	1	MET
46	u	46	LYS
46	u	51	ARG
46	u	55	ASP

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Mol	Chain	Res	Type
46	u	77	GLU
46	u	80	LYS
47	v	21	ILE
47	v	38	ILE
47	v	40	ARG
47	v	55	ILE
47	v	73	TRP
47	v	75	LEU
47	v	81	LYS
48	w	43	ARG
48	w	52	GLN
49	x	13	LEU
49	x	32	ARG
49	x	49	ILE
50	y	6	SER
50	y	10	ARG
50	y	27	MET
50	y	54	MET
50	y	64	LYS
50	y	67	ILE
51	z	20	LYS
51	z	24	GLU
51	z	34	ARG
51	z	44	GLU
59	8	15	PHE
59	8	16	ASP
59	8	18	GLU
59	8	39	TRP
59	8	41	TYR
59	8	49	HIS
59	8	84	LEU
59	8	88	ASN
59	8	112	ASP
59	8	116	ILE
59	8	122	THR
59	8	125	ASP
59	8	128	SER
59	8	134	ASN
59	8	135	VAL
59	8	159	HIS
59	8	163	VAL
59	8	164	LYS

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Mol	Chain	Res	Type
59	8	179	THR
59	8	187	ASN
59	8	191	ILE
59	8	194	LEU
59	8	204	ARG
59	8	205	TYR
59	8	214	ILE
59	8	220	GLU
59	8	246	LYS
59	8	264	GLN
59	8	265	LYS
59	8	275	ASP
59	8	299	HIS
59	8	313	ASN
59	8	339	ARG
59	8	344	HIS
59	8	396	GLU
59	8	410	THR
59	8	430	HIS
59	8	457	MET
59	8	467	LYS
59	8	470	ASN
59	8	487	ARG
59	8	594	ASN
59	8	602	VAL
59	8	611	ARG
59	8	616	ILE
59	8	622	VAL
59	8	629	ARG
59	8	632	SER
59	8	635	ARG
59	8	650	GLU
59	8	665	TYR
59	8	667	LEU
59	8	676	ARG
59	8	679	LEU
59	8	681	ARG
59	8	682	ASP
59	8	690	GLU
59	8	691	LYS
59	8	700	ARG
59	8	711	ASP

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Mol	Chain	Res	Type
59	8	716	ILE
59	8	740	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	GLN
2	C	149	ASN
3	D	24	ASN
4	E	37	ASN
21	V	24	ASN
23	X	16	ASN
45	t	46	HIS
50	y	21	ASN
50	y	68	HIS
59	8	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	1	2891/2904 (99%)	610 (21%)	61 (2%)
53	2	1524/1533 (99%)	324 (21%)	24 (1%)
54	3	117/118 (99%)	19 (16%)	0
55	4	74/76 (97%)	22 (29%)	0
56	5	75/78 (96%)	37 (49%)	14 (18%)
57	6	73/76 (96%)	42 (57%)	11 (15%)
58	7	9/10 (90%)	0	0
All	All	4763/4795 (99%)	1054 (22%)	110 (2%)

All (1054) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	1	10	A
52	1	15	G
52	1	34	U
52	1	35	G
52	1	39	G
52	1	46	G
52	1	49	A
52	1	50	U

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Mol	Chain	Res	Type
52	1	51	G
52	1	55	G
52	1	58	G
52	1	61	C
52	1	62	U
52	1	63	A
52	1	70	G
52	1	71	A
52	1	74	A
52	1	75	G
52	1	78	U
52	1	83	A
52	1	84	A
52	1	93	G
52	1	96	C
52	1	101	A
52	1	102	U
52	1	110	G
52	1	118	A
52	1	119	A
52	1	120	U
52	1	122	G
52	1	135	U
52	1	137	U
52	1	138	U
52	1	139	U
52	1	140	C
52	1	141	G
52	1	142	A
52	1	149	A
52	1	154	U
52	1	158	U
52	1	163	C
52	1	165	A
52	1	181	A
52	1	196	A
52	1	199	A
52	1	215	G
52	1	216	A
52	1	222	A
52	1	228	C
52	1	233	A

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Mol	Chain	Res	Type
52	1	234	U
52	1	241	A
52	1	248	G
52	1	249	C
52	1	264	C
52	1	265	A
52	1	266	G
52	1	271	G
52	1	272	A
52	1	273	G
52	1	276	U
52	1	277	G
52	1	278	A
52	1	285	G
52	1	291	G
52	1	294	A
52	1	311	A
52	1	315	G
52	1	321	U
52	1	322	A
52	1	327	G
52	1	329	G
52	1	330	A
52	1	338	G
52	1	353	C
52	1	359	G
52	1	361	G
52	1	362	A
52	1	371	A
52	1	372	G
52	1	373	U
52	1	383	C
52	1	386	G
52	1	396	G
52	1	399	U
52	1	403	U
52	1	404	A
52	1	405	U
52	1	411	G
52	1	412	A
52	1	424	G
52	1	425	G

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Mol	Chain	Res	Type
52	1	451	U
52	1	455	C
52	1	456	C
52	1	457	A
52	1	477	A
52	1	479	A
52	1	481	G
52	1	490	C
52	1	491	G
52	1	496	G
52	1	504	A
52	1	505	A
52	1	508	A
52	1	510	C
52	1	513	A
52	1	529	A
52	1	530	G
52	1	531	C
52	1	532	A
52	1	542	C
52	1	546	U
52	1	547	A
52	1	548	G
52	1	549	G
52	1	555	G
52	1	556	A
52	1	558	U
52	1	563	A
52	1	569	U
52	1	573	U
52	1	575	A
52	1	577	G
52	1	580	U
52	1	582	A
52	1	588	U
52	1	603	A
52	1	613	A
52	1	614	A
52	1	615	U
52	1	616	A
52	1	620	G
52	1	621	A

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Mol	Chain	Res	Type
52	1	627	A
52	1	637	A
52	1	645	C
52	1	646	U
52	1	647	G
52	1	651	G
52	1	654	A
52	1	655	A
52	1	656	G
52	1	664	G
52	1	668	A
52	1	677	A
52	1	678	C
52	1	685	A
52	1	686	U
52	1	695	G
52	1	698	C
52	1	710	U
52	1	717	C
52	1	724	U
52	1	730	A
52	1	738	G
52	1	747	5MU
52	1	757	G
52	1	764	A
52	1	765	C
52	1	775	G
52	1	776	G
52	1	782	A
52	1	783	A
52	1	784	G
52	1	785	G
52	1	805	G
52	1	812	C
52	1	819	A
52	1	827	U
52	1	828	U
52	1	831	G
52	1	845	A
52	1	846	U
52	1	853	C
52	1	856	G

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Mol	Chain	Res	Type
52	1	858	G
52	1	859	G
52	1	869	G
52	1	878	A
52	1	882	G
52	1	887	A
52	1	888	C
52	1	889	C
52	1	891	G
52	1	895	U
52	1	896	A
52	1	897	C
52	1	898	C
52	1	907	G
52	1	910	A
52	1	914	G
52	1	915	C
52	1	931	U
52	1	932	U
52	1	933	A
52	1	941	A
52	1	946	C
52	1	953	G
52	1	961	C
52	1	973	A
52	1	974	G
52	1	983	A
52	1	990	A
52	1	995	C
52	1	996	A
52	1	999	U
52	1	1006	C
52	1	1012	U
52	1	1013	C
52	1	1022	G
52	1	1023	U
52	1	1025	G
52	1	1026	G
52	1	1033	U
52	1	1034	G
52	1	1036	G
52	1	1046	A

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Mol	Chain	Res	Type
52	1	1047	G
52	1	1057	A
52	1	1065	U
52	1	1066	U
52	1	1067	A
52	1	1068	G
52	1	1070	A
52	1	1077	A
52	1	1083	U
52	1	1087	G
52	1	1088	A
52	1	1090	A
52	1	1096	A
52	1	1097	U
52	1	1110	G
52	1	1111	A
52	1	1112	G
52	1	1116	G
52	1	1117	C
52	1	1118	C
52	1	1119	U
52	1	1122	G
52	1	1128	G
52	1	1130	U
52	1	1132	U
52	1	1133	A
52	1	1134	A
52	1	1135	C
52	1	1142	A
52	1	1143	A
52	1	1156	A
52	1	1171	G
52	1	1172	C
52	1	1175	A
52	1	1176	U
52	1	1178	C
52	1	1179	G
52	1	1180	U
52	1	1186	G
52	1	1201	U
52	1	1204	A
52	1	1210	G

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Mol	Chain	Res	Type
52	1	1213	A
52	1	1218	G
52	1	1227	G
52	1	1236	G
52	1	1238	G
52	1	1248	G
52	1	1253	A
52	1	1256	G
52	1	1265	A
52	1	1266	G
52	1	1271	G
52	1	1272	A
52	1	1273	U
52	1	1275	A
52	1	1294	U
52	1	1300	G
52	1	1301	A
52	1	1302	A
52	1	1306	C
52	1	1321	A
52	1	1326	U
52	1	1327	A
52	1	1329	U
52	1	1332	G
52	1	1333	G
52	1	1344	U
52	1	1345	C
52	1	1352	U
52	1	1359	A
52	1	1365	A
52	1	1378	A
52	1	1379	U
52	1	1380	G
52	1	1383	A
52	1	1386	C
52	1	1392	A
52	1	1395	A
52	1	1404	C
52	1	1408	G
52	1	1413	A
52	1	1414	C
52	1	1416	G

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Mol	Chain	Res	Type
52	1	1417	C
52	1	1419	A
52	1	1427	A
52	1	1428	C
52	1	1434	A
52	1	1437	C
52	1	1451	C
52	1	1453	A
52	1	1455	G
52	1	1458	U
52	1	1461	C
52	1	1478	G
52	1	1482	G
52	1	1490	A
52	1	1493	C
52	1	1494	A
52	1	1497	U
52	1	1502	A
52	1	1504	A
52	1	1508	A
52	1	1509	A
52	1	1515	A
52	1	1529	G
52	1	1532	A
52	1	1534	U
52	1	1535	A
52	1	1536	C
52	1	1537	G
52	1	1541	C
52	1	1544	A
52	1	1558	C
52	1	1566	A
52	1	1569	A
52	1	1578	U
52	1	1583	A
52	1	1584	U
52	1	1585	C
52	1	1588	G
52	1	1593	A
52	1	1608	A
52	1	1610	A
52	1	1616	A

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Mol	Chain	Res	Type
52	1	1619	G
52	1	1627	G
52	1	1630	A
52	1	1639	C
52	1	1647	U
52	1	1648	U
52	1	1649	G
52	1	1651	G
52	1	1669	A
52	1	1674	G
52	1	1677	A
52	1	1700	A
52	1	1715	G
52	1	1721	G
52	1	1729	U
52	1	1730	C
52	1	1732	C
52	1	1738	G
52	1	1764	C
52	1	1773	A
52	1	1782	U
52	1	1791	A
52	1	1800	C
52	1	1801	A
52	1	1808	A
52	1	1816	C
52	1	1829	A
52	1	1833	C
52	1	1842	G
52	1	1858	A
52	1	1859	U
52	1	1862	G
52	1	1867	G
52	1	1869	G
52	1	1870	C
52	1	1873	G
52	1	1882	U
52	1	1897	G
52	1	1906	G
52	1	1907	G
52	1	1913	A
52	1	1914	C

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Mol	Chain	Res	Type
52	1	1916	A
52	1	1917	PSU
52	1	1927	A
52	1	1929	G
52	1	1930	G
52	1	1931	U
52	1	1936	A
52	1	1938	A
52	1	1955	U
52	1	1961	C
52	1	1962	5MC
52	1	1965	C
52	1	1967	C
52	1	1970	A
52	1	1971	U
52	1	1972	G
52	1	1982	U
52	1	1991	U
52	1	1993	U
52	1	1997	C
52	1	2002	G
52	1	2020	A
52	1	2022	U
52	1	2023	C
52	1	2032	G
52	1	2033	A
52	1	2043	C
52	1	2052	A
52	1	2055	C
52	1	2056	G
52	1	2060	A
52	1	2061	G
52	1	2062	A
52	1	2069	G7M
52	1	2072	C
52	1	2076	U
52	1	2077	A
52	1	2087	G
52	1	2092	U
52	1	2093	G
52	1	2095	A
52	1	2102	G

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Mol	Chain	Res	Type
52	1	2108	A
52	1	2110	G
52	1	2111	U
52	1	2112	G
52	1	2113	U
52	1	2115	G
52	1	2116	G
52	1	2117	A
52	1	2118	U
52	1	2120	G
52	1	2122	U
52	1	2124	G
52	1	2125	G
52	1	2126	A
52	1	2127	G
52	1	2128	G
52	1	2131	U
52	1	2132	U
52	1	2133	G
52	1	2134	A
52	1	2135	A
52	1	2139	U
52	1	2141	G
52	1	2146	C
52	1	2147	A
52	1	2154	A
52	1	2157	G
52	1	2158	A
52	1	2159	G
52	1	2162	G
52	1	2163	A
52	1	2164	C
52	1	2165	C
52	1	2169	A
52	1	2171	A
52	1	2172	U
52	1	2182	U
52	1	2183	A
52	1	2189	U
52	1	2190	G
52	1	2193	G
52	1	2194	U

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Mol	Chain	Res	Type
52	1	2198	A
52	1	2203	U
52	1	2204	G
52	1	2210	U
52	1	2211	A
52	1	2212	A
52	1	2225	A
52	1	2226	C
52	1	2229	U
52	1	2238	G
52	1	2239	G
52	1	2243	U
52	1	2250	G
52	1	2267	A
52	1	2268	A
52	1	2279	G
52	1	2283	C
52	1	2287	A
52	1	2288	A
52	1	2304	G
52	1	2305	U
52	1	2307	G
52	1	2309	A
52	1	2310	C
52	1	2311	A
52	1	2312	U
52	1	2322	A
52	1	2325	G
52	1	2326	C
52	1	2327	A
52	1	2333	A
52	1	2335	A
52	1	2347	C
52	1	2350	C
52	1	2357	G
52	1	2361	G
52	1	2376	A
52	1	2383	G
52	1	2385	C
52	1	2394	C
52	1	2396	G
52	1	2402	U

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Mol	Chain	Res	Type
52	1	2403	C
52	1	2406	A
52	1	2409	G
52	1	2410	G
52	1	2420	C
52	1	2423	U
52	1	2424	C
52	1	2425	A
52	1	2426	A
52	1	2428	G
52	1	2429	G
52	1	2430	A
52	1	2431	U
52	1	2435	A
52	1	2441	U
52	1	2447	G
52	1	2448	A
52	1	2459	A
52	1	2470	G
52	1	2476	A
52	1	2480	C
52	1	2484	G
52	1	2487	G
52	1	2491	U
52	1	2494	G
52	1	2502	G
52	1	2504	PSU
52	1	2505	G
52	1	2506	U
52	1	2513	A
52	1	2518	A
52	1	2525	G
52	1	2529	G
52	1	2534	A
52	1	2535	G
52	1	2554	U
52	1	2562	U
52	1	2566	A
52	1	2567	G
52	1	2573	C
52	1	2574	G
52	1	2582	G

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Mol	Chain	Res	Type
52	1	2585	U
52	1	2586	U
52	1	2602	A
52	1	2608	G
52	1	2609	U
52	1	2613	U
52	1	2615	U
52	1	2621	G
52	1	2629	U
52	1	2630	G
52	1	2634	A
52	1	2639	A
52	1	2663	G
52	1	2685	G
52	1	2689	U
52	1	2690	U
52	1	2691	C
52	1	2714	G
52	1	2716	C
52	1	2718	G
52	1	2724	U
52	1	2725	A
52	1	2726	A
52	1	2733	A
52	1	2744	G
52	1	2748	A
52	1	2754	U
52	1	2757	A
52	1	2758	A
52	1	2765	A
52	1	2777	G
52	1	2778	A
52	1	2791	G
52	1	2793	C
52	1	2794	C
52	1	2800	A
52	1	2801	G
52	1	2803	G
52	1	2805	C
52	1	2818	U
52	1	2820	A
52	1	2821	A

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Mol	Chain	Res	Type
52	1	2825	G
52	1	2830	C
52	1	2835	A
52	1	2850	A
52	1	2860	A
52	1	2867	G
52	1	2874	C
52	1	2880	C
52	1	2884	U
52	1	2891	U
52	1	2893	A
52	1	2894	G
52	1	2902	C
52	1	2904	U
53	2	4	U
53	2	5	U
53	2	6	G
53	2	9	G
53	2	22	G
53	2	32	A
53	2	39	G
53	2	44	A
53	2	47	C
53	2	48	C
53	2	51	A
53	2	52	C
53	2	54	C
53	2	66	A
53	2	70	U
53	2	71	A
53	2	73	C
53	2	74	A
53	2	76	G
53	2	77	A
53	2	80	A
53	2	81	A
53	2	82	G
53	2	83	C
53	2	84	U
53	2	87	C
53	2	88	U
53	2	90	C

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Mol	Chain	Res	Type
53	2	95	C
53	2	96	U
53	2	108	G
53	2	120	A
53	2	128	G
53	2	130	A
53	2	131	A
53	2	134	G
53	2	137	U
53	2	138	G
53	2	143	A
53	2	144	G
53	2	147	G
53	2	149	A
53	2	157	U
53	2	158	G
53	2	161	A
53	2	163	C
53	2	164	G
53	2	168	G
53	2	173	U
53	2	177	G
53	2	182	A
53	2	200	G
53	2	204	G
53	2	208	U
53	2	209	U
53	2	210	C
53	2	211	G
53	2	212	G
53	2	222	C
53	2	226	G
53	2	245	U
53	2	246	A
53	2	247	G
53	2	251	G
53	2	262	A
53	2	266	G
53	2	267	C
53	2	279	A
53	2	280	C
53	2	281	G

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Mol	Chain	Res	Type
53	2	289	G
53	2	306	A
53	2	319	G
53	2	321	A
53	2	328	C
53	2	329	A
53	2	332	G
53	2	340	U
53	2	345	C
53	2	351	G
53	2	352	C
53	2	353	A
53	2	354	G
53	2	355	C
53	2	356	A
53	2	367	U
53	2	369	G
53	2	370	C
53	2	372	C
53	2	373	A
53	2	374	A
53	2	375	U
53	2	381	C
53	2	382	A
53	2	392	C
53	2	397	A
53	2	406	G
53	2	410	G
53	2	411	A
53	2	412	A
53	2	413	G
53	2	414	A
53	2	420	U
53	2	421	U
53	2	422	C
53	2	423	G
53	2	424	G
53	2	425	G
53	2	426	U
53	2	429	U
53	2	445	G
53	2	446	G

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Mol	Chain	Res	Type
53	2	451	A
53	2	458	U
53	2	463	U
53	2	464	U
53	2	467	U
53	2	468	A
53	2	469	C
53	2	476	U
53	2	478	A
53	2	479	U
53	2	484	G
53	2	485	U
53	2	486	U
53	2	495	A
53	2	496	A
53	2	499	A
53	2	501	C
53	2	505	G
53	2	511	C
53	2	515	G
53	2	516	PSU
53	2	517	G
53	2	518	C
53	2	519	C
53	2	521	G
53	2	527	G7M
53	2	530	G
53	2	531	U
53	2	532	A
53	2	533	A
53	2	534	U
53	2	536	C
53	2	542	G
53	2	545	C
53	2	547	A
53	2	559	A
53	2	560	A
53	2	562	U
53	2	567	G
53	2	568	G
53	2	572	A
53	2	573	A

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Mol	Chain	Res	Type
53	2	576	C
53	2	579	A
53	2	596	A
53	2	615	G
53	2	620	C
53	2	628	G
53	2	633	G
53	2	642	A
53	2	650	G
53	2	653	U
53	2	665	A
53	2	703	G
53	2	723	U
53	2	724	G
53	2	731	G
53	2	734	G
53	2	747	A
53	2	755	G
53	2	777	A
53	2	790	A
53	2	793	U
53	2	794	A
53	2	799	G
53	2	815	A
53	2	817	C
53	2	828	U
53	2	841	C
53	2	843	U
53	2	844	G
53	2	845	A
53	2	846	G
53	2	849	G
53	2	851	G
53	2	855	U
53	2	857	C
53	2	876	C
53	2	902	G
53	2	914	A
53	2	915	A
53	2	926	G
53	2	934	C
53	2	935	A

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Mol	Chain	Res	Type
53	2	942	G
53	2	960	U
53	2	966	2MG
53	2	969	A
53	2	972	C
53	2	975	A
53	2	976	G
53	2	978	A
53	2	982	U
53	2	983	A
53	2	987	G
53	2	993	G
53	2	1004	A
53	2	1005	A
53	2	1008	U
53	2	1009	U
53	2	1012	A
53	2	1013	G
53	2	1017	U
53	2	1018	G
53	2	1020	G
53	2	1021	A
53	2	1023	U
53	2	1024	G
53	2	1026	G
53	2	1028	C
53	2	1030	U
53	2	1031	C
53	2	1032	G
53	2	1033	G
53	2	1037	C
53	2	1043	G
53	2	1046	A
53	2	1065	U
53	2	1070	U
53	2	1086	U
53	2	1088	G
53	2	1092	A
53	2	1094	G
53	2	1095	U
53	2	1097	C
53	2	1101	A

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Mol	Chain	Res	Type
53	2	1108	G
53	2	1124	G
53	2	1133	G
53	2	1135	U
53	2	1136	C
53	2	1137	C
53	2	1139	G
53	2	1140	C
53	2	1141	C
53	2	1142	G
53	2	1145	A
53	2	1146	A
53	2	1151	A
53	2	1152	A
53	2	1159	U
53	2	1160	G
53	2	1164	G
53	2	1167	A
53	2	1168	U
53	2	1171	A
53	2	1184	G
53	2	1187	G
53	2	1196	A
53	2	1197	A
53	2	1201	A
53	2	1202	U
53	2	1206	G
53	2	1212	U
53	2	1213	A
53	2	1214	C
53	2	1225	A
53	2	1227	A
53	2	1228	C
53	2	1236	A
53	2	1238	A
53	2	1240	U
53	2	1253	G
53	2	1256	A
53	2	1257	A
53	2	1260	G
53	2	1275	A
53	2	1278	G

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Mol	Chain	Res	Type
53	2	1280	A
53	2	1285	A
53	2	1286	U
53	2	1287	A
53	2	1299	A
53	2	1302	C
53	2	1305	G
53	2	1312	G
53	2	1317	C
53	2	1318	A
53	2	1320	C
53	2	1332	A
53	2	1338	G
53	2	1346	A
53	2	1353	G
53	2	1363	A
53	2	1368	A
53	2	1370	G
53	2	1379	G
53	2	1381	U
53	2	1394	A
53	2	1398	A
53	2	1419	G
53	2	1429	A
53	2	1432	G
53	2	1441	A
53	2	1446	A
53	2	1448	C
53	2	1452	C
53	2	1453	G
53	2	1455	G
53	2	1487	G
53	2	1491	G
53	2	1492	A
53	2	1493	A
53	2	1499	A
53	2	1503	A
53	2	1505	G
53	2	1506	U
53	2	1517	G
53	2	1529	G
53	2	1530	G

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Mol	Chain	Res	Type
53	2	1533	C
53	2	1534	A
54	3	9	G
54	3	13	G
54	3	15	A
54	3	16	G
54	3	17	C
54	3	30	C
54	3	35	C
54	3	44	G
54	3	45	A
54	3	56	G
54	3	64	G
54	3	66	A
54	3	67	G
54	3	68	C
54	3	88	C
54	3	89	U
54	3	90	C
54	3	99	A
54	3	109	A
55	4	3	C
55	4	6	G
55	4	9	A
55	4	18	G
55	4	19	G
55	4	21	A
55	4	22	G
55	4	34	G
55	4	39	U
55	4	41	C
55	4	43	C
55	4	44	G
55	4	45	U
55	4	47	U
55	4	48	C
55	4	50	U
55	4	58	A
55	4	59	U
55	4	60	U
55	4	61	C
55	4	65	G

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Mol	Chain	Res	Type
55	4	76	A
56	5	1	G
56	5	2	C
56	5	3	G
56	5	7	U
56	5	8	4SU
56	5	9	G
56	5	13	A
56	5	14	G
56	5	15	C
56	5	16	C
56	5	18	G
56	5	19	G
56	5	20	H2U
56	5	21	A
56	5	23	C
56	5	33	U
56	5	35	A
56	5	37	A
56	5	44	A
56	5	45	G
56	5	46	A
56	5	47	U
56	5	48	C
56	5	49	G
56	5	53	G
56	5	55	PSU
56	5	56	C
56	5	58	A
56	5	59	A
56	5	60	U
56	5	61	C
56	5	64	G
56	5	69	C
56	5	71	C
56	5	72	A
56	5	74	C
56	5	75	C
57	6	3	C
57	6	5	G
57	6	7	A
57	6	8	4SU

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Mol	Chain	Res	Type
57	6	9	A
57	6	10	G
57	6	11	C
57	6	13	C
57	6	15	G
57	6	16	H2U
57	6	17	U
57	6	18	G
57	6	19	G
57	6	20	H2U
57	6	21	A
57	6	22	G
57	6	23	A
57	6	29	G
57	6	32	PSU
57	6	33	U
57	6	36	A
57	6	38	A
57	6	41	C
57	6	44	G
57	6	45	U
57	6	46	7MG
57	6	48	C
57	6	49	C
57	6	52	G
57	6	57	G
57	6	59	U
57	6	60	U
57	6	62	C
57	6	63	G
57	6	64	A
57	6	65	G
57	6	70	G
57	6	71	G
57	6	73	A
57	6	74	C
57	6	75	C
57	6	76	A

All (110) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
52	1	62	U
52	1	70	G
52	1	84	A
52	1	100	U
52	1	102	U
52	1	177	G
52	1	199	A
52	1	247	G
52	1	271	G
52	1	272	A
52	1	310	A
52	1	403	U
52	1	404	A
52	1	446	G
52	1	474	G
52	1	504	A
52	1	529	A
52	1	555	G
52	1	614	A
52	1	620	G
52	1	645	C
52	1	685	A
52	1	784	G
52	1	894	U
52	1	896	A
52	1	974	G
52	1	995	C
52	1	1065	U
52	1	1067	A
52	1	1070	A
52	1	1288	G
52	1	1332	G
52	1	1344	U
52	1	1358	G
52	1	1379	U
52	1	1415	U
52	1	1508	A
52	1	1509	A
52	1	1543	G
52	1	1608	A
52	1	1784	A

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Mol	Chain	Res	Type
52	1	2133	G
52	1	2146	C
52	1	2162	G
52	1	2182	U
52	1	2193	G
52	1	2211	A
52	1	2225	A
52	1	2286	G
52	1	2308	G
52	1	2311	A
52	1	2319	G
52	1	2326	C
52	1	2425	A
52	1	2447	G
52	1	2581	G
52	1	2629	U
52	1	2751	G
52	1	2756	U
52	1	2830	C
52	1	2873	A
53	2	73	C
53	2	243	A
53	2	246	A
53	2	279	A
53	2	280	C
53	2	328	C
53	2	329	A
53	2	351	G
53	2	428	G
53	2	517	G
53	2	518	C
53	2	530	G
53	2	531	U
53	2	532	A
53	2	533	A
53	2	641	U
53	2	965	U
53	2	974	A
53	2	982	U
53	2	1109	C
53	2	1145	A
53	2	1201	A

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Mol	Chain	Res	Type
53	2	1211	U
53	2	1363	A
56	5	8	4SU
56	5	14	G
56	5	15	C
56	5	16	C
56	5	17	U
56	5	18	G
56	5	19	G
56	5	20	H2U
56	5	21	A
56	5	47	U
56	5	48	C
56	5	58	A
56	5	59	A
56	5	60	U
57	6	10	G
57	6	16	H2U
57	6	17	U
57	6	18	G
57	6	19	G
57	6	32	PSU
57	6	45	U
57	6	56	C
57	6	59	U
57	6	70	G
57	6	75	C

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

48 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	$\# Z > 2$
52	1MG	1	745	52	18,26,27	0.94	2 (11%)	19,39,42	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	2MG	2	966	53	18,26,27	1.00	1 (5%)	16,38,41	0.80	0
57	6IA	6	37	58,57	22,29,30	0.59	0	22,41,44	1.74	5 (22%)
52	G7M	1	2069	52	20,26,27	0.88	1 (5%)	17,39,42	0.58	0
52	PSU	1	1917	52	18,21,22	0.49	0	22,30,33	0.68	0
57	PSU	6	32	57	18,21,22	0.56	0	22,30,33	1.37	2 (9%)
57	5MU	6	54	57	19,22,23	0.26	0	28,32,35	0.56	0
56	4SU	5	8	56	18,21,22	0.50	0	26,30,33	1.77	5 (19%)
52	OMG	1	2251	52,56	18,26,27	1.03	2 (11%)	19,38,41	0.60	0
53	5MC	2	1407	53	18,22,23	0.32	0	26,32,35	0.84	0
52	PSU	1	2457	52	18,21,22	0.50	0	22,30,33	0.78	0
52	2MA	1	2503	52,60	17,25,26	0.74	0	17,37,40	0.88	1 (5%)
56	PSU	5	55	56	18,21,22	0.49	0	22,30,33	0.81	0
52	PSU	1	2605	52	18,21,22	0.54	0	22,30,33	0.88	1 (4%)
53	5MC	2	967	53	18,22,23	0.41	0	26,32,35	0.70	0
56	4OC	5	32	56	20,23,24	0.22	0	26,32,35	0.51	0
57	H2U	6	20	57	18,21,22	0.59	0	21,30,33	1.77	4 (19%)
42	D2T	q	89	42	7,9,10	1.10	0	6,11,13	2.12	3 (50%)
53	PSU	2	516	53	18,21,22	0.50	0	22,30,33	1.16	1 (4%)
52	5MU	1	747	52	19,22,23	0.26	0	28,32,35	0.67	0
53	2MG	2	1516	53	18,26,27	1.01	1 (5%)	16,38,41	0.68	0
53	MA6	2	1519	53	19,26,27	0.70	0	18,38,41	0.75	0
57	H2U	6	16	57	18,21,22	0.53	0	21,30,33	2.68	7 (33%)
52	2MG	1	1835	52	18,26,27	1.02	2 (11%)	16,38,41	0.72	0
52	2MG	1	2445	52	18,26,27	1.06	3 (16%)	16,38,41	0.91	0
53	MA6	2	1518	53	19,26,27	0.67	0	18,38,41	0.72	0
57	3AU	6	47	57	25,28,29	0.54	0	32,40,43	0.77	1 (3%)
53	UR3	2	1498	53	19,22,23	0.35	0	26,32,35	0.73	1 (3%)
56	5MU	5	54	56	19,22,23	0.26	0	28,32,35	0.60	0
57	PSU	6	55	57	18,21,22	0.58	0	22,30,33	1.27	2 (9%)
52	6MZ	1	1618	52	18,25,26	0.61	0	16,36,39	0.93	1 (6%)
53	G7M	2	527	53	20,26,27	0.88	1 (5%)	17,39,42	0.51	0
52	PSU	1	2580	52	18,21,22	0.53	0	22,30,33	0.79	0
52	PSU	1	746	52,60	18,21,22	0.47	0	22,30,33	0.82	0
57	7MG	6	46	57	22,26,27	0.89	1 (4%)	29,39,42	0.94	3 (10%)
52	PSU	1	955	52	18,21,22	0.51	0	22,30,33	0.74	0
52	5MC	1	1962	52	18,22,23	0.40	0	26,32,35	0.64	0
56	H2U	5	20	56	18,21,22	0.50	0	21,30,33	0.71	0
52	6MZ	1	2030	52	18,25,26	0.66	0	16,36,39	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	1	2504	52	18,21,22	0.51	0	22,30,33	0.89	1 (4%)
53	2MG	2	1207	53	18,26,27	1.01	1 (5%)	16,38,41	0.93	0
53	4OC	2	1402	53	20,23,24	0.22	0	26,32,35	0.68	0
52	3TD	1	1915	52	18,22,23	0.38	0	22,32,35	1.07	1 (4%)
52	5MU	1	1939	52	19,22,23	0.26	0	28,32,35	0.62	0
52	OMC	1	2498	52,60	19,22,23	0.26	0	26,31,34	0.57	0
52	OMU	1	2552	52,60	19,22,23	0.23	0	26,31,34	0.60	0
52	PSU	1	1911	52	18,21,22	0.47	0	22,30,33	0.81	0
57	4SU	6	8	57	18,21,22	0.47	0	26,30,33	1.66	2 (7%)

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
52	1MG	1	745	52	-	0/3/25/26	0/3/3/3
57	6IA	6	37	58,57	1/1/6/7	6/9/31/32	0/3/3/3
53	2MG	2	966	53	-	0/5/27/28	0/3/3/3
52	G7M	1	2069	52	-	2/3/25/26	0/3/3/3
52	PSU	1	1917	52	-	2/7/25/26	0/2/2/2
57	PSU	6	32	57	1/1/5/5	1/7/25/26	0/2/2/2
57	5MU	6	54	57	-	0/7/25/26	0/2/2/2
56	4SU	5	8	56	-	4/7/25/26	0/2/2/2
52	OMG	1	2251	52,56	-	0/5/27/28	0/3/3/3
53	5MC	2	1407	53	-	0/7/25/26	0/2/2/2
52	PSU	1	2457	52	-	0/7/25/26	0/2/2/2
52	2MA	1	2503	52,60	-	1/3/25/26	0/3/3/3
56	PSU	5	55	56	-	3/7/25/26	0/2/2/2
52	PSU	1	2605	52	-	0/7/25/26	0/2/2/2
53	5MC	2	967	53	-	0/7/25/26	0/2/2/2
56	4OC	5	32	56	-	0/9/29/30	0/2/2/2
57	H2U	6	20	57	2/2/8/9	6/7/38/39	0/2/2/2
42	D2T	q	89	42	-	2/7/12/14	-
53	PSU	2	516	53	-	2/7/25/26	0/2/2/2
52	5MU	1	747	52	-	0/7/25/26	0/2/2/2
53	2MG	2	1516	53	-	0/5/27/28	0/3/3/3
53	MA6	2	1519	53	-	6/7/29/30	0/3/3/3
57	H2U	6	16	57	3/3/8/9	5/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	2MG	1	1835	52	-	2/5/27/28	0/3/3/3
52	2MG	1	2445	52	-	1/5/27/28	0/3/3/3
53	MA6	2	1518	53	-	0/7/29/30	0/3/3/3
57	3AU	6	47	57	-	3/16/34/35	0/2/2/2
53	UR3	2	1498	53	-	0/7/25/26	0/2/2/2
56	5MU	5	54	56	-	0/7/25/26	0/2/2/2
57	PSU	6	55	57	1/1/5/5	2/7/25/26	0/2/2/2
52	6MZ	1	1618	52	-	3/5/27/28	0/3/3/3
53	G7M	2	527	53	-	2/3/25/26	0/3/3/3
52	PSU	1	2580	52	-	0/7/25/26	0/2/2/2
52	PSU	1	746	52,60	-	1/7/25/26	0/2/2/2
57	7MG	6	46	57	-	1/7/37/38	0/3/3/3
52	PSU	1	955	52	-	0/7/25/26	0/2/2/2
52	5MC	1	1962	52	-	0/7/25/26	0/2/2/2
56	H2U	5	20	56	-	3/7/38/39	0/2/2/2
52	6MZ	1	2030	52	-	1/5/27/28	0/3/3/3
52	PSU	1	2504	52	-	2/7/25/26	0/2/2/2
53	2MG	2	1207	53	-	2/5/27/28	0/3/3/3
53	4OC	2	1402	53	-	0/9/29/30	0/2/2/2
52	3TD	1	1915	52	-	1/7/25/26	0/2/2/2
52	5MU	1	1939	52	-	0/7/25/26	0/2/2/2
52	OMC	1	2498	52,60	-	1/9/27/28	0/2/2/2
52	OMU	1	2552	52,60	-	0/9/27/28	0/2/2/2
52	PSU	1	1911	52	-	0/7/25/26	0/2/2/2
57	4SU	6	8	57	-	4/7/25/26	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	6	46	7MG	C5-N7	3.57	1.39	1.35
52	1	2251	OMG	C5-C6	-2.83	1.41	1.47
52	1	2445	2MG	C5-C6	-2.81	1.41	1.47
52	1	1835	2MG	C5-C6	-2.63	1.42	1.47
53	2	1207	2MG	C5-C6	-2.46	1.42	1.47
53	2	1516	2MG	C5-C6	-2.37	1.42	1.47
53	2	966	2MG	C5-C6	-2.35	1.42	1.47
53	2	527	G7M	C8-N9	2.32	1.37	1.33
52	1	2069	G7M	C8-N9	2.32	1.37	1.33
52	1	745	1MG	C5-C4	-2.18	1.37	1.43
52	1	2251	OMG	C8-N7	-2.12	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	1835	2MG	C8-N7	-2.05	1.31	1.35
52	1	745	1MG	C8-N7	-2.03	1.31	1.35
52	1	2445	2MG	C8-N7	-2.01	1.31	1.35
52	1	2445	2MG	C5-C4	-2.01	1.38	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	6	16	H2U	O3'-C3'-C4'	6.75	130.56	111.05
57	6	8	4SU	C4-N3-C2	-6.66	120.87	127.34
57	6	16	H2U	O2'-C2'-C1'	5.37	127.99	110.02
56	5	8	4SU	C4-N3-C2	-5.20	122.29	127.34
57	6	16	H2U	O4'-C1'-N1	5.07	116.20	109.30
57	6	20	H2U	O2'-C2'-C1'	4.83	126.18	110.02
57	6	37	6IA	O3'-C3'-C2'	4.60	126.70	111.82
57	6	37	6IA	O3'-C3'-C4'	4.57	124.28	111.05
57	6	16	H2U	O2'-C2'-C3'	4.13	125.18	111.82
57	6	55	PSU	C3'-C2'-C1'	-4.04	96.93	101.64
53	2	516	PSU	C3'-C2'-C1'	4.00	106.30	101.64
57	6	32	PSU	C3'-C2'-C1'	-3.87	97.13	101.64
57	6	20	H2U	O4'-C1'-N1	3.84	114.53	109.30
56	5	8	4SU	C2'-C1'-N1	3.64	123.54	113.22
57	6	20	H2U	O2'-C2'-C3'	3.62	123.54	111.82
56	5	8	4SU	O4'-C1'-C2'	-3.62	98.76	106.64
57	6	16	H2U	C3'-C2'-C1'	-3.59	94.61	101.43
57	6	32	PSU	O3'-C3'-C4'	3.49	121.13	111.05
42	q	89	D2T	CB-CA-N	3.33	116.20	109.10
57	6	8	4SU	C5-C4-N3	3.27	117.73	114.69
56	5	8	4SU	C5-C4-N3	3.27	117.72	114.69
57	6	16	H2U	O3'-C3'-C2'	3.04	121.66	111.82
52	1	1915	3TD	C4-N3-C2	-2.99	121.36	124.61
52	1	1618	6MZ	C2-N1-C6	2.77	118.96	116.59
57	6	37	6IA	C12-N6-C6	2.76	127.53	122.89
52	1	2030	6MZ	C2-N1-C6	2.74	118.94	116.59
53	2	1498	UR3	C4-N3-C2	-2.73	121.99	124.56
57	6	37	6IA	C2-N1-C6	2.48	118.72	116.59
57	6	46	7MG	C2-N3-C4	2.45	116.67	112.30
57	6	55	PSU	O3'-C3'-C4'	2.35	117.85	111.05
56	5	8	4SU	N3-C2-N1	2.34	118.00	114.89
57	6	47	3AU	C4-N3-C2	-2.28	121.77	124.63
42	q	89	D2T	CB1-SB-CB	-2.19	98.47	102.44
57	6	20	H2U	O4'-C1'-C2'	2.18	111.38	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	2503	2MA	CM2-C2-N1	2.17	121.05	116.23
52	1	2504	PSU	C2'-C3'-C4'	-2.15	98.46	102.64
57	6	16	H2U	O4'-C1'-C2'	2.14	111.30	106.64
57	6	37	6IA	C2'-C3'-C4'	2.13	106.79	102.64
57	6	46	7MG	C5-C4-N9	2.09	109.06	106.35
52	1	2605	PSU	C2'-C3'-C4'	-2.06	98.64	102.64
42	q	89	D2T	O-C-CA	-2.05	119.40	124.78
57	6	46	7MG	C5-C4-N3	-2.04	124.25	128.13

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	6	16	H2U	C1'
57	6	16	H2U	C3'
57	6	16	H2U	C2'
57	6	20	H2U	C1'
57	6	20	H2U	C2'
57	6	32	PSU	C1'
57	6	37	6IA	C3'
57	6	55	PSU	C1'

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	q	89	D2T	SB-CB-CG-OD2
52	1	1618	6MZ	N1-C6-N6-C9
52	1	1618	6MZ	O4'-C4'-C5'-O5'
52	1	1618	6MZ	C3'-C4'-C5'-O5'
52	1	1835	2MG	N1-C2-N2-CM2
52	1	1835	2MG	N3-C2-N2-CM2
52	1	1917	PSU	O4'-C4'-C5'-O5'
53	2	516	PSU	O4'-C4'-C5'-O5'
53	2	527	G7M	O4'-C4'-C5'-O5'
53	2	527	G7M	C3'-C4'-C5'-O5'
53	2	1207	2MG	N1-C2-N2-CM2
53	2	1207	2MG	N3-C2-N2-CM2
53	2	1519	MA6	O4'-C4'-C5'-O5'
53	2	1519	MA6	C5-C6-N6-C9
53	2	1519	MA6	C5-C6-N6-C10
56	5	20	H2U	O4'-C1'-N1-C6
56	5	55	PSU	C3'-C4'-C5'-O5'
57	6	8	4SU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
57	6	8	4SU	O4'-C4'-C5'-O5'
57	6	16	H2U	C3'-C4'-C5'-O5'
57	6	16	H2U	C2'-C1'-N1-C2
57	6	20	H2U	O4'-C4'-C5'-O5'
57	6	20	H2U	C3'-C4'-C5'-O5'
57	6	20	H2U	O4'-C1'-N1-C6
57	6	37	6IA	C3'-C4'-C5'-O5'
57	6	37	6IA	C5-C6-N6-C12
57	6	37	6IA	N6-C12-C13-C14
57	6	55	PSU	O4'-C1'-C5-C6
56	5	8	4SU	C2'-C1'-N1-C2
52	1	1917	PSU	C3'-C4'-C5'-O5'
52	1	2504	PSU	O4'-C4'-C5'-O5'
53	2	516	PSU	C3'-C4'-C5'-O5'
53	2	1519	MA6	C3'-C4'-C5'-O5'
56	5	8	4SU	O4'-C4'-C5'-O5'
57	6	16	H2U	O4'-C4'-C5'-O5'
57	6	37	6IA	O4'-C4'-C5'-O5'
56	5	8	4SU	C2'-C1'-N1-C6
52	1	2504	PSU	C3'-C4'-C5'-O5'
56	5	8	4SU	C3'-C4'-C5'-O5'
53	2	1519	MA6	N1-C6-N6-C10
57	6	16	H2U	C2'-C1'-N1-C6
57	6	20	H2U	C2'-C1'-N1-C6
57	6	37	6IA	N1-C6-N6-C12
56	5	55	PSU	O4'-C4'-C5'-O5'
52	1	2069	G7M	C4'-C5'-O5'-P
57	6	16	H2U	C4'-C5'-O5'-P
52	1	2445	2MG	C3'-C4'-C5'-O5'
56	5	20	H2U	O4'-C4'-C5'-O5'
57	6	47	3AU	C10-C11-C12-C13
57	6	20	H2U	C2'-C1'-N1-C2
56	5	55	PSU	C4'-C5'-O5'-P
53	2	1519	MA6	C4'-C5'-O5'-P
57	6	37	6IA	C4'-C5'-O5'-P
57	6	47	3AU	N40-C12-C13-O31
57	6	32	PSU	C4'-C5'-O5'-P
57	6	8	4SU	C2'-C1'-N1-C6
56	5	20	H2U	O4'-C1'-N1-C2
52	1	1915	3TD	O4'-C1'-C5-C4
57	6	55	PSU	O4'-C1'-C5-C4
52	1	2498	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
57	6	47	3AU	N40-C12-C13-O30
52	1	2503	2MA	O4'-C4'-C5'-O5'
57	6	46	7MG	C4'-C5'-O5'-P
42	q	89	D2T	CG-CB-SB-CB1
52	1	746	PSU	O4'-C1'-C5-C6
57	6	8	4SU	C2'-C1'-N1-C2
52	1	2069	G7M	O4'-C4'-C5'-O5'
57	6	20	H2U	O4'-C1'-N1-C2
52	1	2030	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 302 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	PAR	2	1665	-	45,45,45	0.81	2 (4%)	64,67,67	0.67	1 (1%)
63	MET	5	101	-	6,7,8	0.53	0	2,7,9	0.43	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
62	PAR	2	1665	-	-	3/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	MET	5	101	-	-	2/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	2	1665	PAR	O51-C11	-3.78	1.32	1.41
62	2	1665	PAR	C14-C24	-2.17	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	2	1665	PAR	O51-C11-C21	2.36	115.36	110.06

There are no chirality outliers.

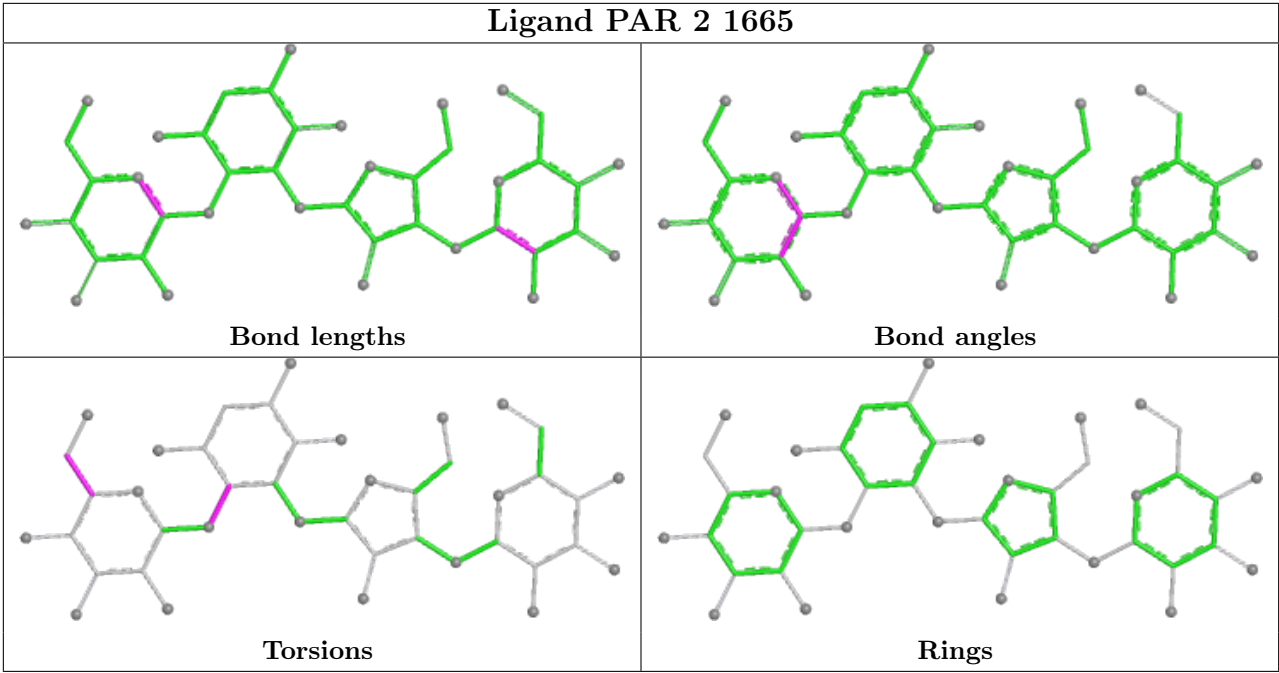
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	2	1665	PAR	C41-C51-C61-O61
63	5	101	MET	CA-CB-CG-SD
63	5	101	MET	CB-CG-SD-CE
62	2	1665	PAR	O51-C51-C61-O61
62	2	1665	PAR	C52-C42-O11-C11

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	1	8
53	2	4
55	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1588:G	O3'	1589:U	P	4.95
1	4	1:G	O3'	2:C	P	4.28
1	1	2098:U	O3'	2099:U	P	3.58
1	2	480:U	O3'	481:G	P	3.44
1	1	1408:G	O3'	1409:U	P	3.41
1	1	1169:A	O3'	1170:C	P	3.38
1	2	147:G	O3'	148:G	P	3.36
1	1	2314:A	O3'	2315:G	P	3.34
1	1	1579:A	O3'	1580:A	P	3.31
1	1	1167:C	O3'	1168:G	P	3.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	197:A	O3'	198:G	P	3.24
1	1	2196:C	O3'	2197:U	P	3.12
1	2	1383:C	O3'	1384:C	P	3.09

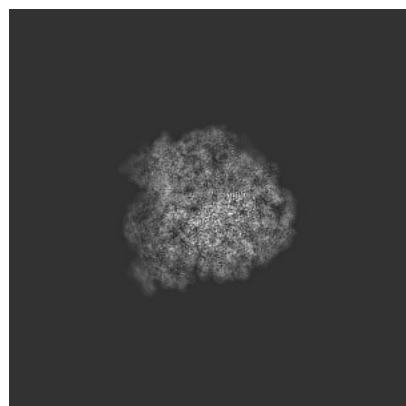
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8107. These allow visual inspection of the internal detail of the map and identification of artifacts.

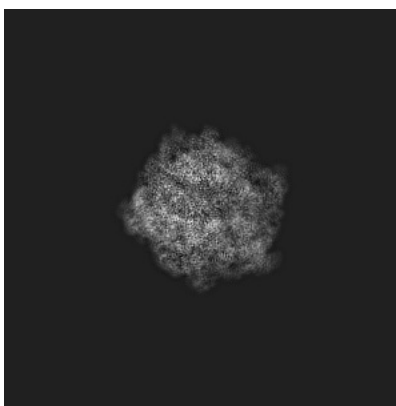
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

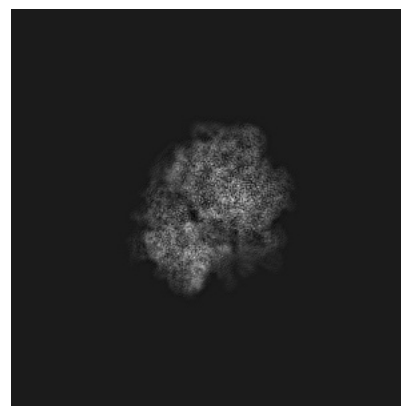
6.1.1 Primary map



X

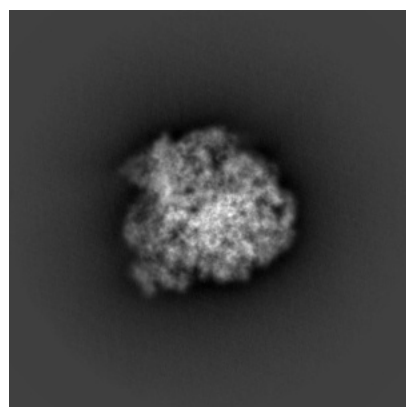


Y

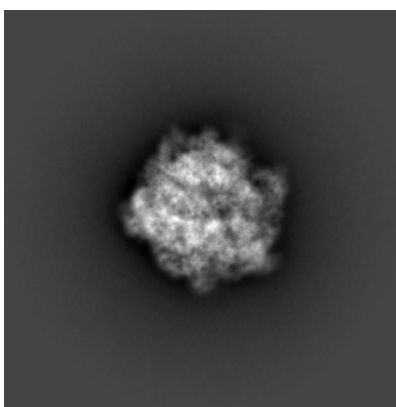


Z

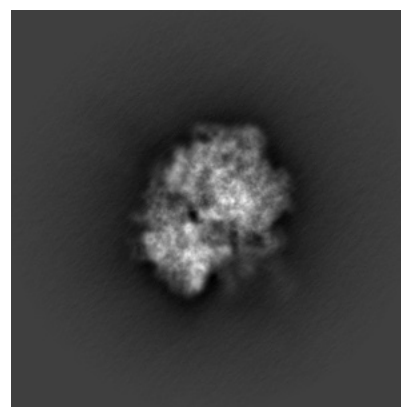
6.1.2 Raw map



X



Y

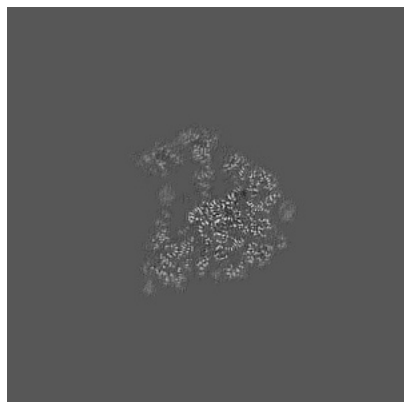


Z

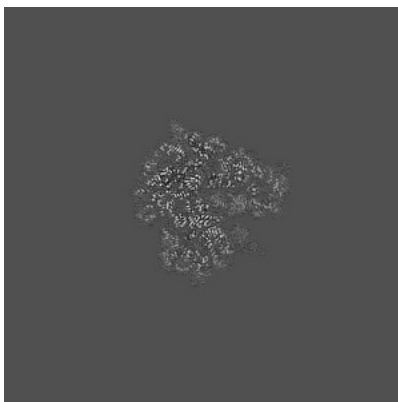
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

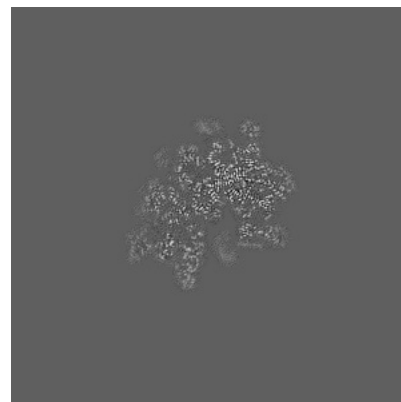
6.2.1 Primary map



X Index: 200

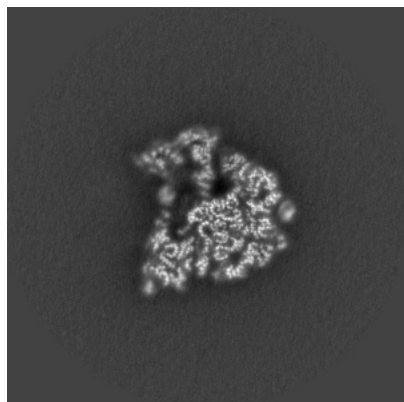


Y Index: 200

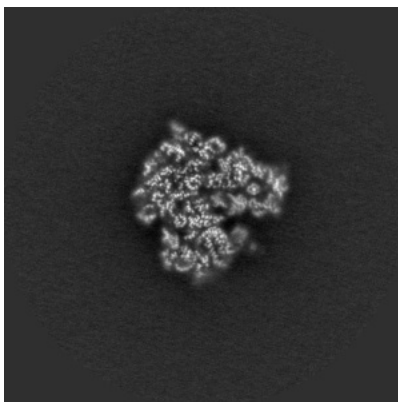


Z Index: 200

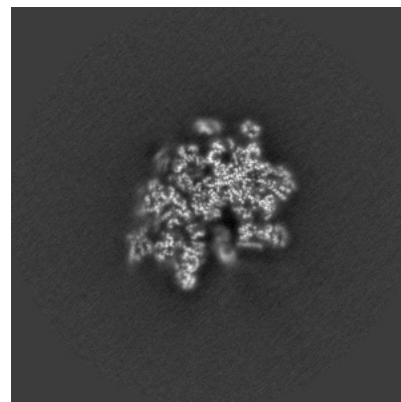
6.2.2 Raw map



X Index: 200



Y Index: 200

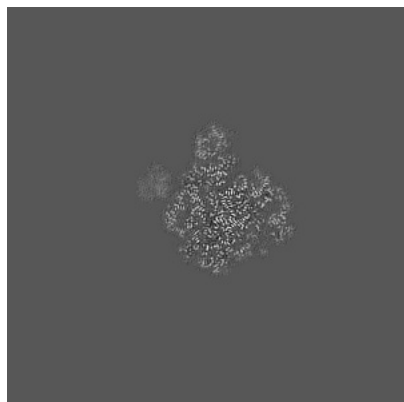


Z Index: 200

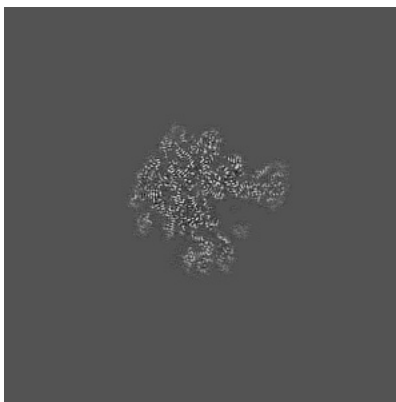
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

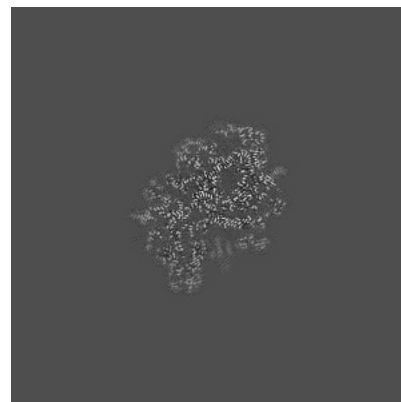
6.3.1 Primary map



X Index: 233

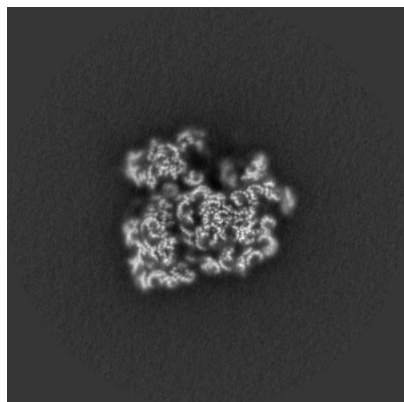


Y Index: 209

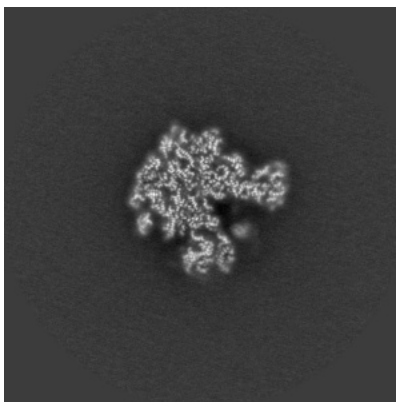


Z Index: 185

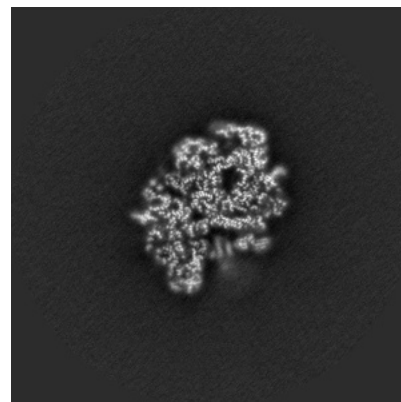
6.3.2 Raw map



X Index: 188



Y Index: 209

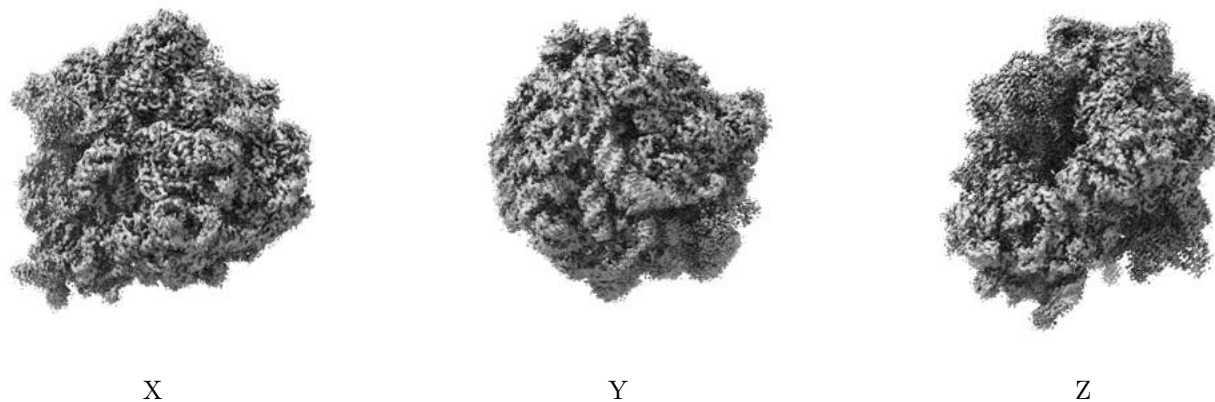


Z Index: 185

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

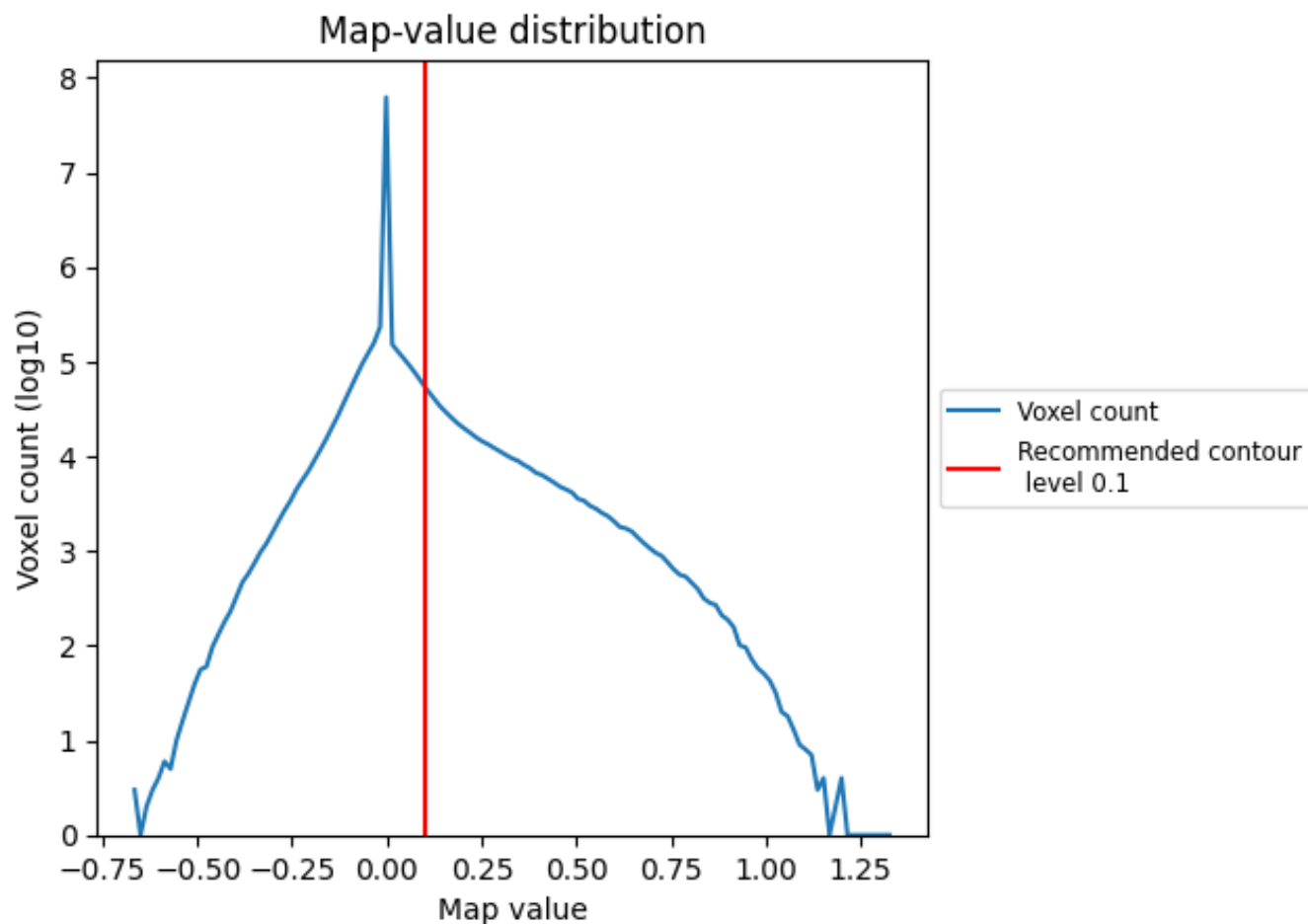
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

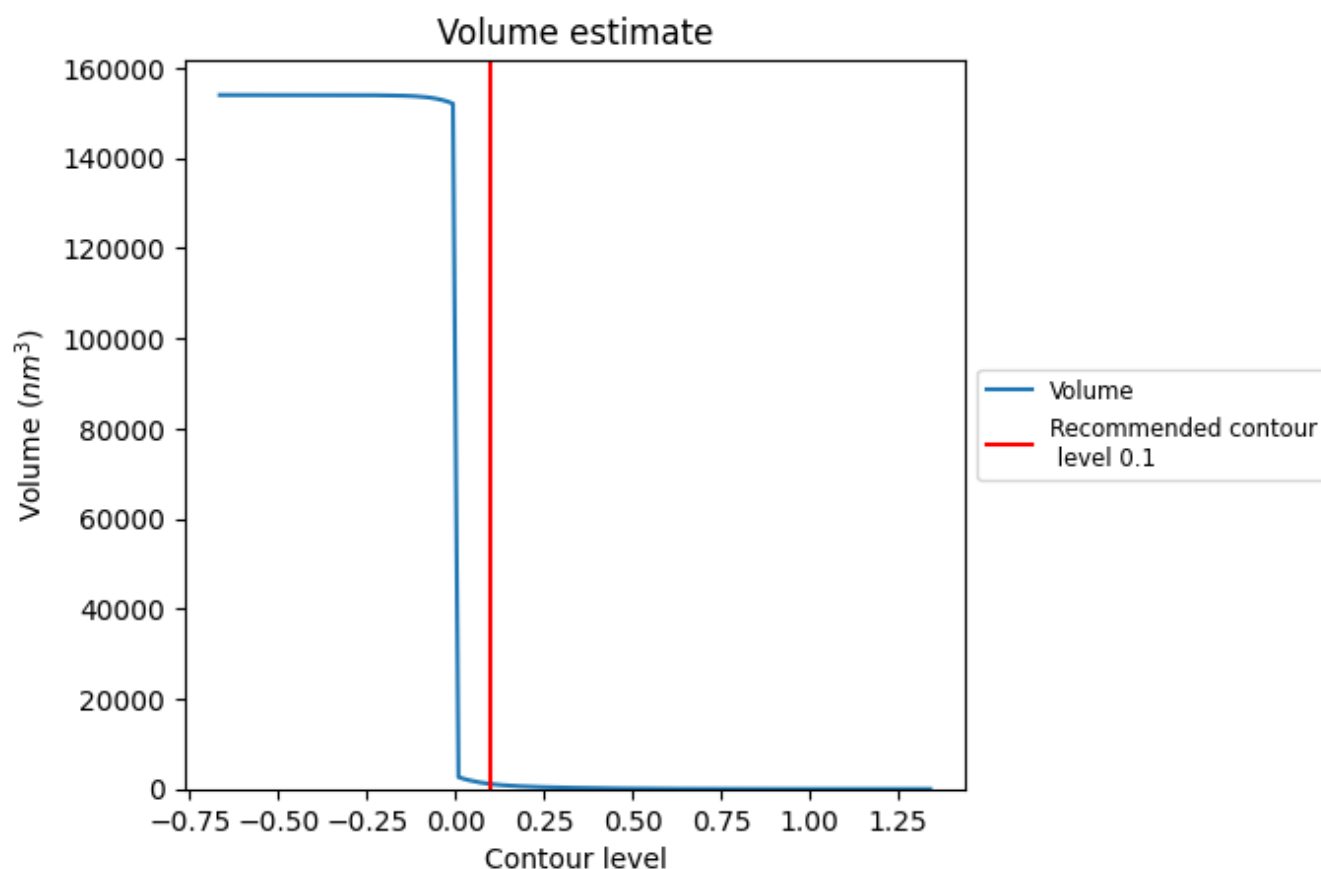
This section contains the results of statistical analysis of the map.

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.

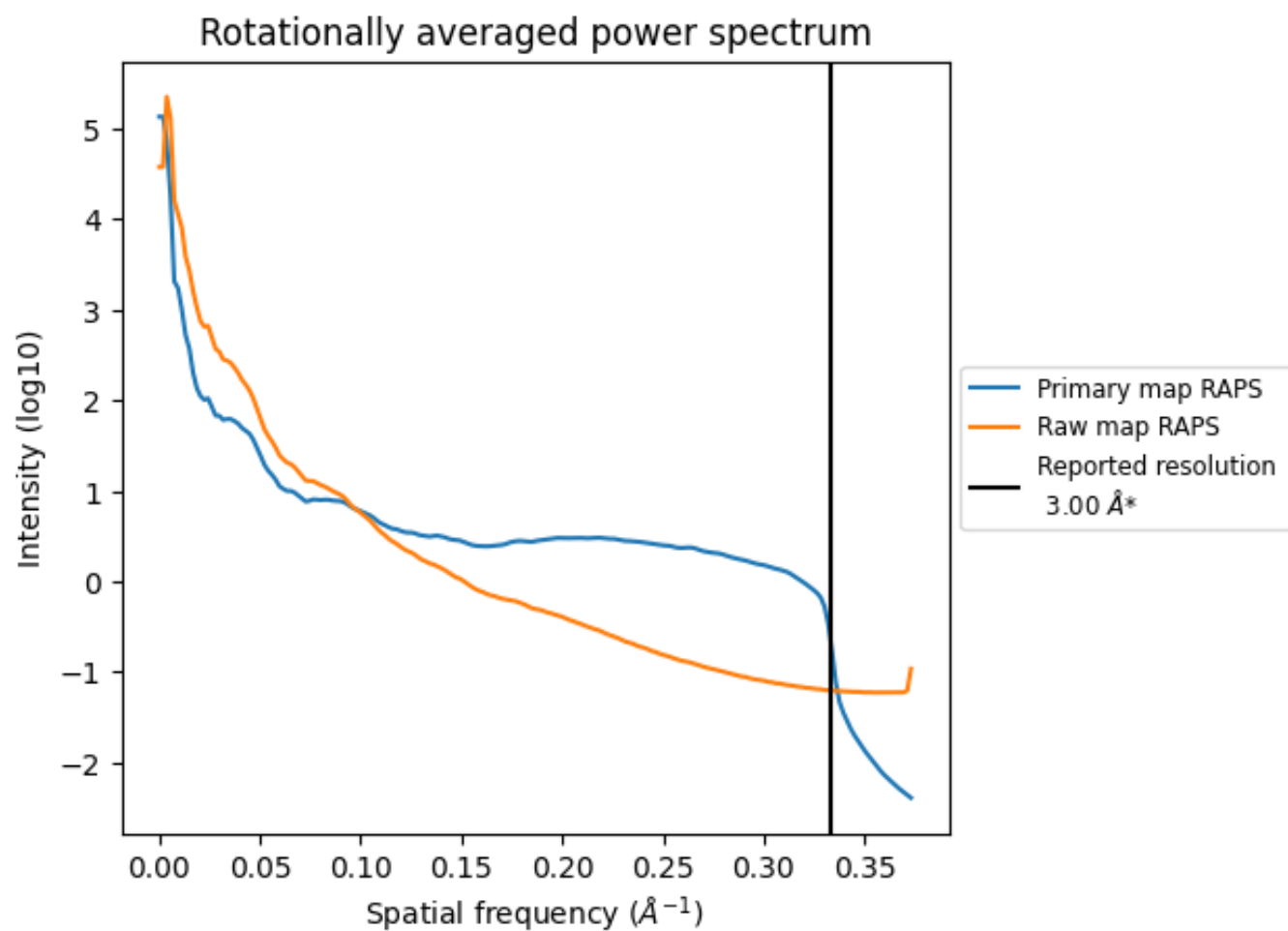
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1094 nm^3 ; this corresponds to an approximate mass of 988 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 ⓘ

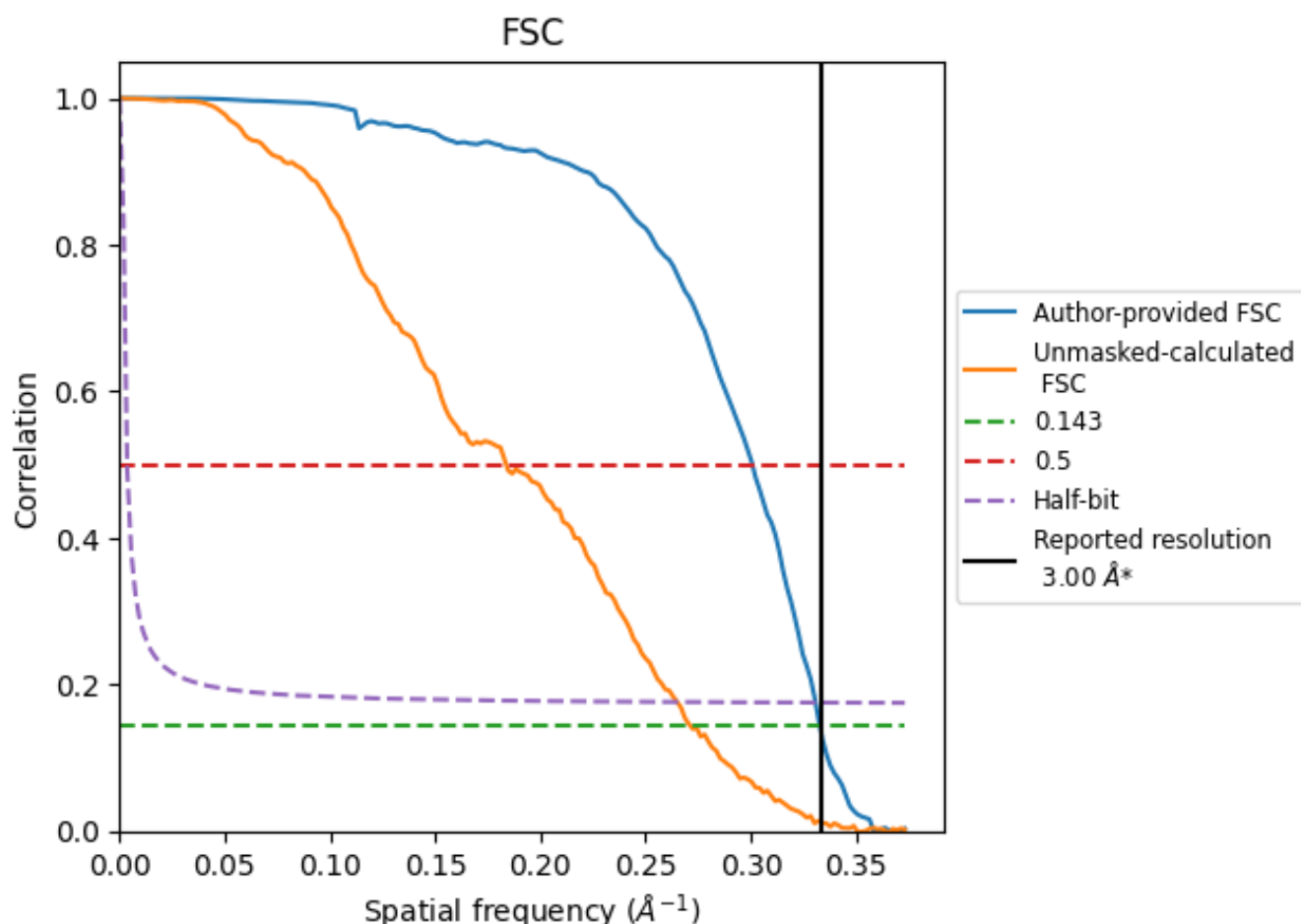


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

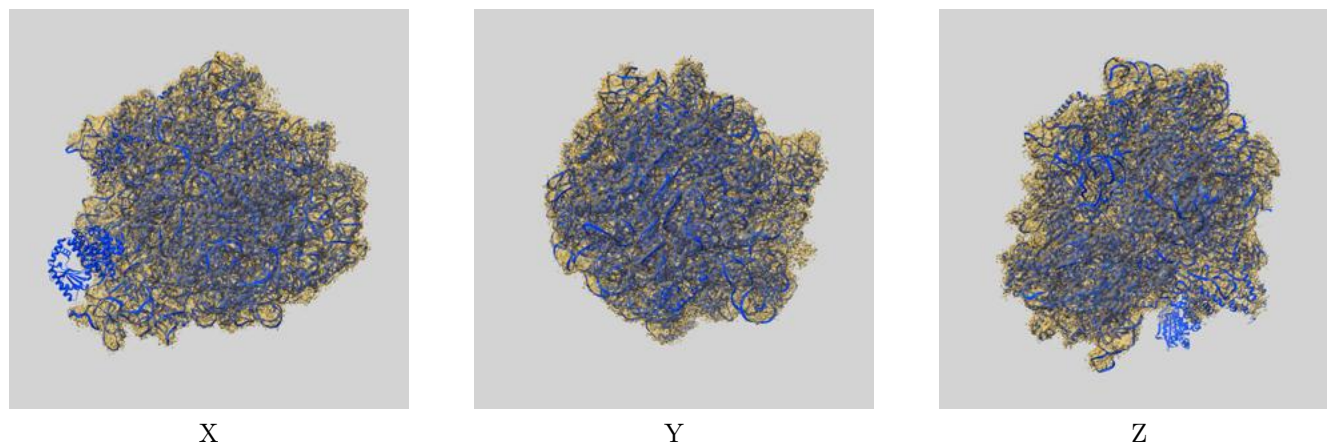
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.33	3.02
Unmasked-calculated*	3.69	5.44	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.69 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

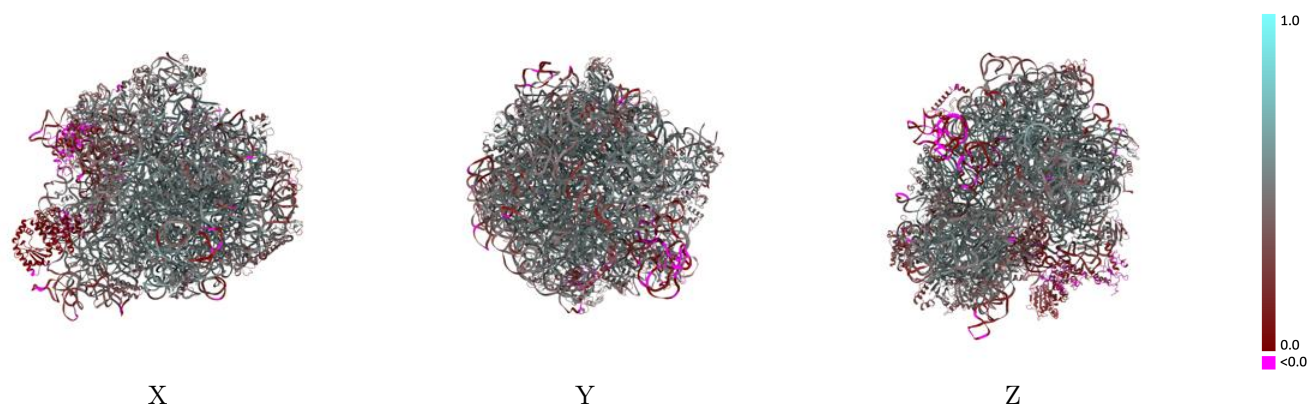
This section contains information regarding the fit between EMDB map EMD-8107 and PDB model 5IQR. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



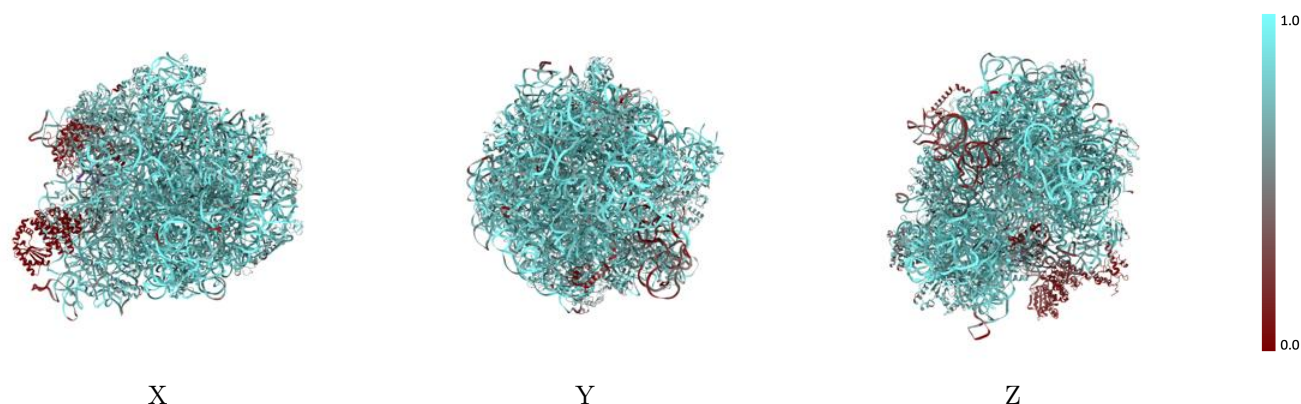
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



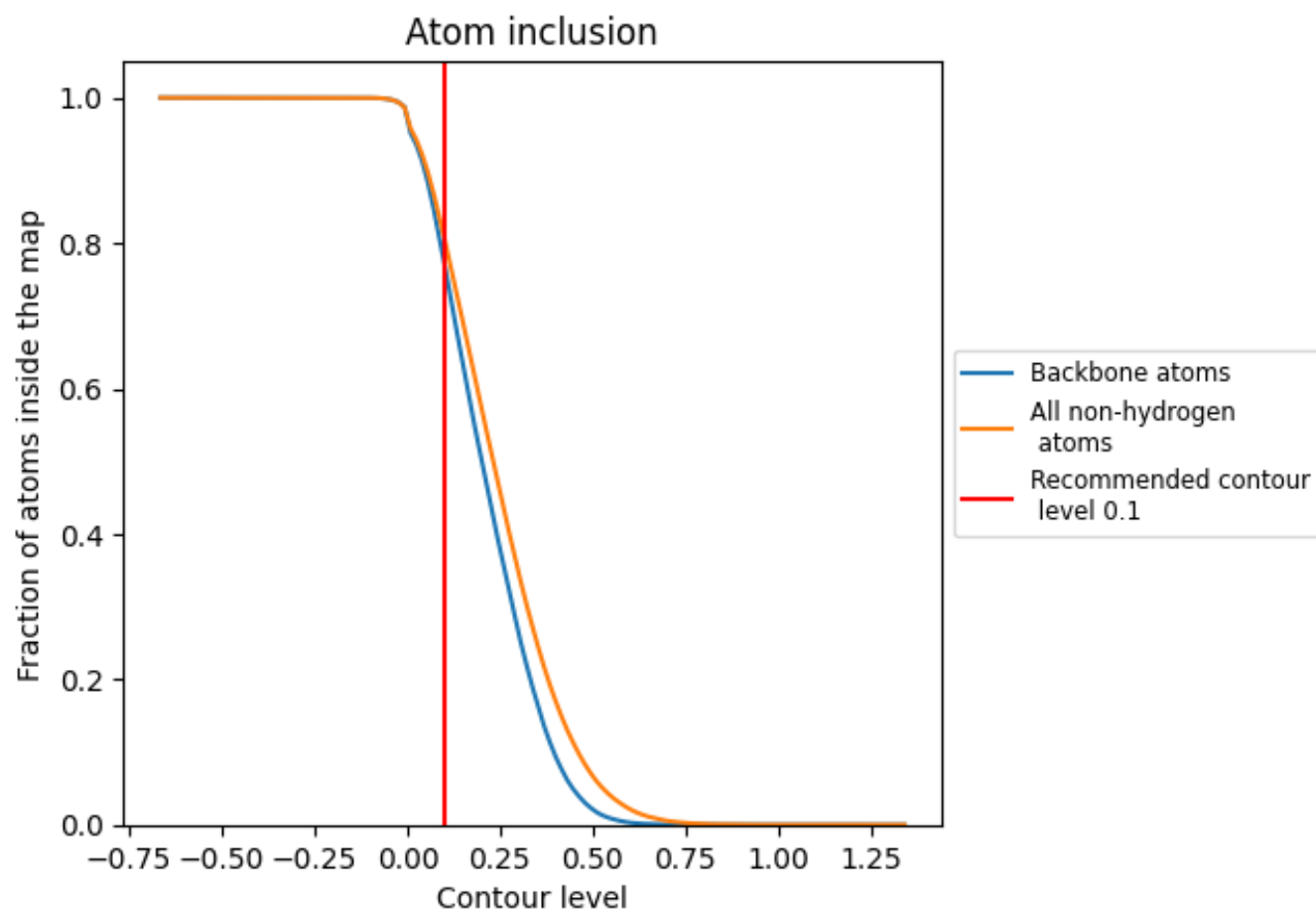
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 81% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8067	 0.4500
1	 0.8940	 0.4900
2	 0.8930	 0.4730
3	 0.9116	 0.4820
4	 0.2792	 0.1370
5	 0.8136	 0.4620
6	 0.4264	 0.1880
7	 0.7630	 0.4750
8	 0.1788	 0.1070
B	 0.8314	 0.5430
C	 0.8343	 0.5140
D	 0.7434	 0.4050
E	 0.7393	 0.4090
F	 0.7255	 0.4090
G	 0.2984	 0.1910
H	 0.1333	 0.0520
I	 0.1673	 0.0780
J	 0.8136	 0.5080
K	 0.8208	 0.5330
L	 0.7914	 0.4820
M	 0.8234	 0.5250
N	 0.8418	 0.4970
O	 0.7914	 0.4290
P	 0.8063	 0.4990
Q	 0.8161	 0.4890
R	 0.7942	 0.4680
S	 0.7871	 0.4790
T	 0.7299	 0.4260
U	 0.7331	 0.4160
V	 0.7764	 0.4630
W	 0.8444	 0.5360
X	 0.8203	 0.5060
Y	 0.6769	 0.3200
Z	 0.7963	 0.4800
a	 0.6309	 0.3090



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Chain	Atom inclusion	Q-score
b	 0.8294	 0.4960
c	 0.7382	 0.4780
d	 0.8169	 0.5370
e	 0.8595	 0.5470
f	 0.8396	 0.5240
g	 0.5935	 0.3550
h	 0.7503	 0.4520
i	 0.7352	 0.4100
j	 0.7945	 0.4840
k	 0.7525	 0.4300
l	 0.6871	 0.3920
m	 0.7906	 0.4900
n	 0.7600	 0.4160
o	 0.7280	 0.4060
p	 0.8101	 0.4930
q	 0.7432	 0.4770
r	 0.7653	 0.4440
s	 0.7806	 0.4650
t	 0.7565	 0.4430
u	 0.7656	 0.4420
v	 0.7421	 0.4420
w	 0.7838	 0.4710
x	 0.7850	 0.4690
y	 0.7496	 0.3950
z	 0.6622	 0.3940