



Full wwPDB EM Validation Report ⓘ

Feb 4, 2025 – 10:58 AM EST

PDB ID : 5WDT
EMDB ID : EMD-8813
Title : 70S ribosome-EF-Tu H84A complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-06
Resolution : 3.00 Å(reported)

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

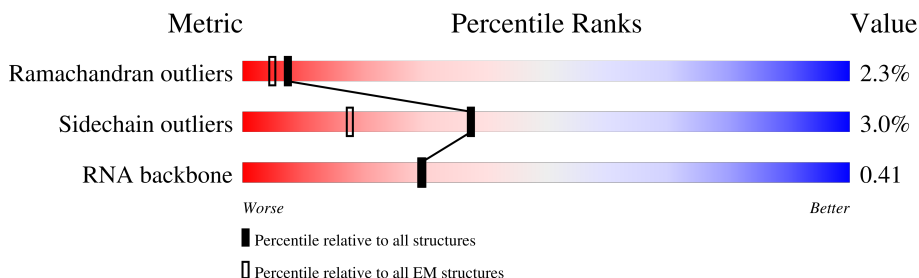
1 Overall quality at a glance

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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	


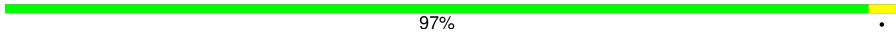
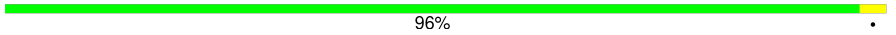
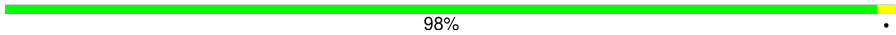

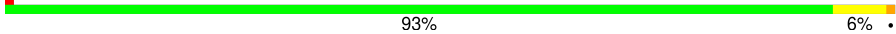
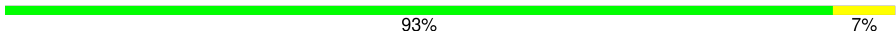
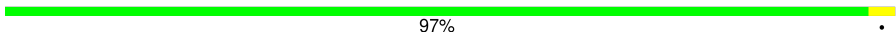
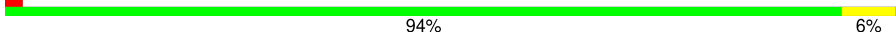



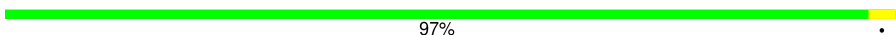
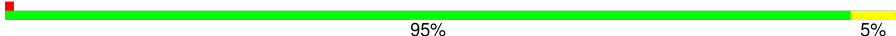

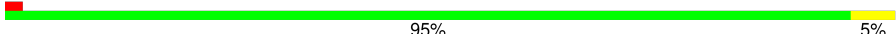
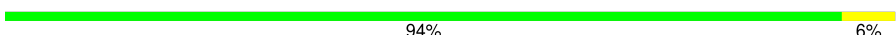

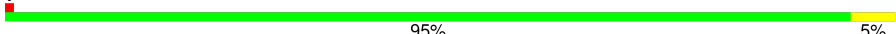






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Mol	Chain	Length	Quality of chain
9	I	141	<div> <div>26%</div> <div>95%</div> <div>5%</div> </div>
10	J	141	<div> <div>97%</div> <div>.</div> </div>
11	K	122	<div> <div>93%</div> <div>7%</div> </div>
12	L	143	<div> <div>90%</div> <div>10%</div> </div>
13	M	136	<div> <div>99%</div> <div>.</div> </div>
14	N	119	<div> <div>97%</div> <div>..</div> </div>
15	O	116	<div> <div>99%</div> <div>.</div> </div>
16	P	114	<div> <div>100%</div> </div>
17	Q	115	<div> <div>97%</div> <div>.</div> </div>
18	R	102	<div> <div>95%</div> <div>5%</div> </div>
19	S	109	<div> <div>95%</div> <div>5%</div> </div>
20	T	92	<div> <div>96%</div> <div>.</div> </div>
21	U	102	<div> <div>95%</div> <div>5%</div> </div>
22	V	92	<div> <div>98%</div> <div>..</div> </div>
23	W	75	<div> <div>97%</div> <div>.</div> </div>
24	X	77	<div> <div>97%</div> <div>.</div> </div>
25	Y	60	<div> <div>98%</div> <div>.</div> </div>
26	Z	56	<div> <div>98%</div> <div>.</div> </div>
27	0	55	<div> <div>98%</div> <div>.</div> </div>
28	1	51	<div> <div>98%</div> <div>.</div> </div>
29	2	45	<div> <div>93%</div> <div>..</div> </div>
30	3	64	<div> <div>95%</div> <div>5%</div> </div>
31	4	38	<div> <div>97%</div> <div>.</div> </div>
32	5	131	<div> <div>77%</div> <div>92%</div> <div>8%</div> </div>
33	6	66	<div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	

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Mol	Chain	Length	Quality of chain
58	z	393	<div><div></div><div>95%</div><div>5%</div></div>

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1174070234

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O		0	0
			933	595	190	148			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	51	Total	C	N	O	S	0	0
			417	269	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	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	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	42	85	12		

- Molecule 57 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		

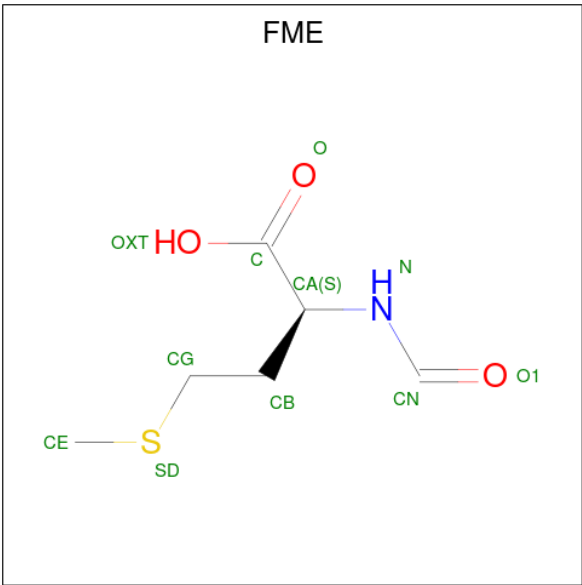
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	521	582	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

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

Mol	Chain	Residues	Atoms		AltConf
60	A	1325	Total	Mg	0
			1325	1325	
60	B	36	Total	Mg	0
			36	36	
60	C	3	Total	Mg	0
			3	3	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	L	2	Total	Mg	0
			2	2	
60	M	1	Total	Mg	0
			1	1	
60	N	1	Total	Mg	0
			1	1	
60	Q	2	Total	Mg	0
			2	2	
60	R	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	

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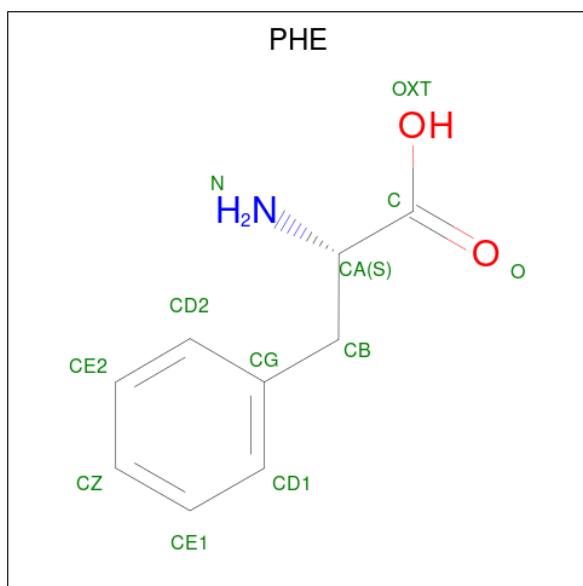
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Mol	Chain	Residues	Atoms		AltConf
60	T	1	Total 1	Mg 1	0
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	2	Total 2	Mg 2	0
60	0	2	Total 2	Mg 2	0
60	3	3	Total 3	Mg 3	0
60	4	1	Total 1	Mg 1	0
60	a	481	Total 481	Mg 481	0
60	d	1	Total 1	Mg 1	0
60	h	1	Total 1	Mg 1	0
60	i	3	Total 3	Mg 3	0
60	s	1	Total 1	Mg 1	0
60	t	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	12	Total 12	Mg 12	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0
60	y	8	Total 8	Mg 8	0
60	z	4	Total 4	Mg 4	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

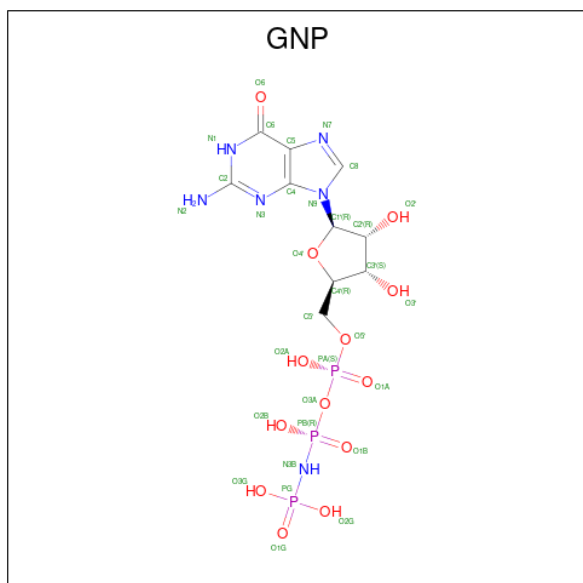
Mol	Chain	Residues	Atoms		AltConf
61	A	5	Total 5	K 5	0

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: $\text{C}_9\text{H}_{11}\text{NO}_2$).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	653	Total	O	0
			653	653	
64	B	22	Total	O	0
			22	22	
64	C	7	Total	O	0
			7	7	
64	D	6	Total	O	0
			6	6	
64	E	6	Total	O	0
			6	6	
64	G	1	Total	O	0
			1	1	
64	J	1	Total	O	0
			1	1	
64	L	6	Total	O	0
			6	6	
64	M	1	Total	O	0
			1	1	
64	N	3	Total	O	0
			3	3	
64	P	1	Total	O	0
			1	1	
64	Q	4	Total	O	0
			4	4	
64	S	2	Total	O	0
			2	2	
64	U	3	Total	O	0
			3	3	
64	W	1	Total	O	0
			1	1	
64	X	3	Total	O	0
			3	3	
64	Y	1	Total	O	0
			1	1	
64	Z	2	Total	O	0
			2	2	
64	0	1	Total	O	0
			1	1	

Continued on next page...

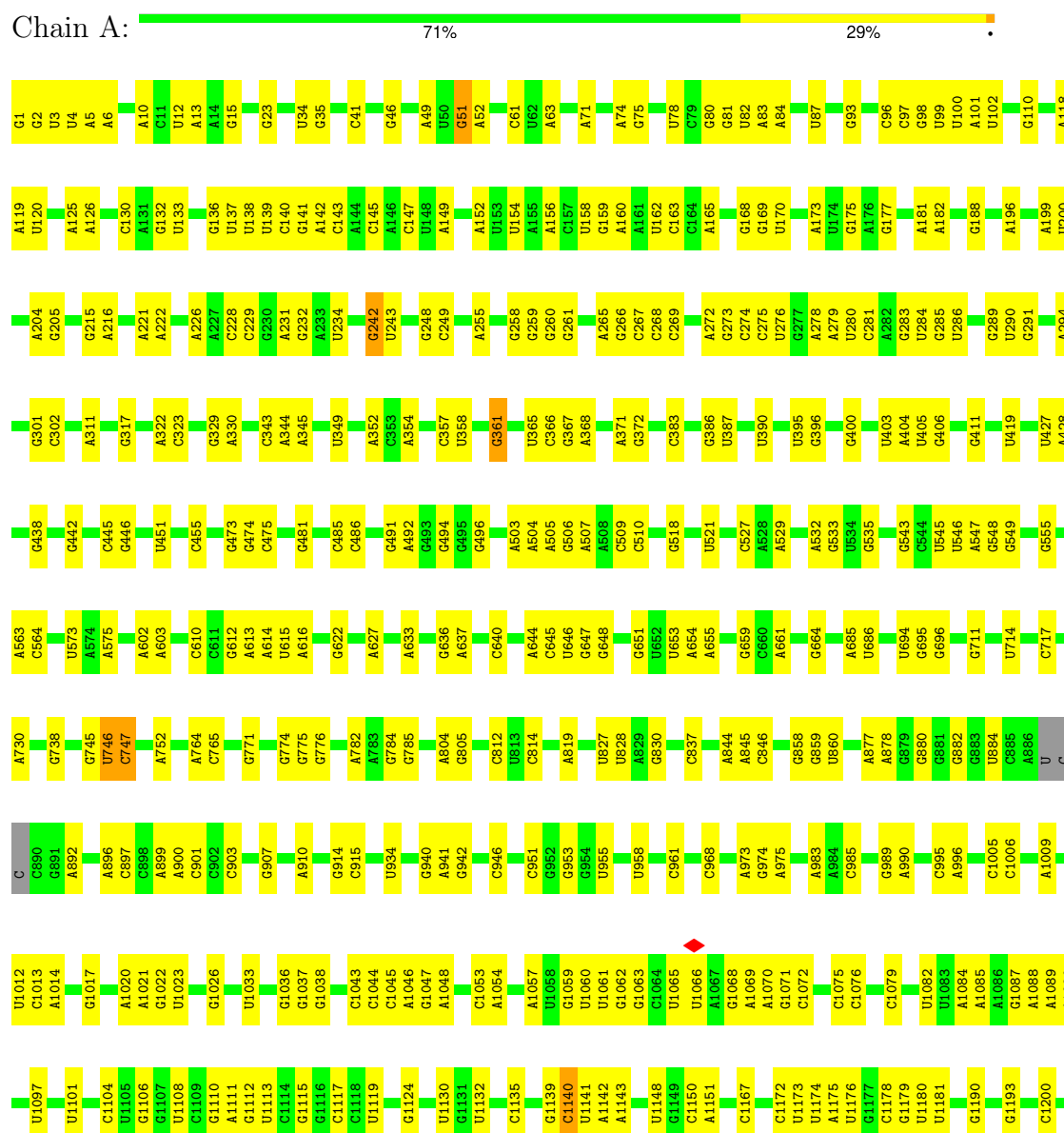
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Mol	Chain	Residues	Atoms		AltConf
64	2	4	Total 4	O 4	0
64	3	1	Total 1	O 1	0
64	4	1	Total 1	O 1	0
64	a	163	Total 163	O 163	0
64	d	1	Total 1	O 1	0
64	h	2	Total 2	O 2	0
64	k	1	Total 1	O 1	0
64	m	3	Total 3	O 3	0
64	o	1	Total 1	O 1	0
64	s	2	Total 2	O 2	0
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	v	9	Total 9	O 9	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	y	2	Total 2	O 2	0
64	z	2	Total 2	O 2	0

3 Residue-property plots

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: 23S rRNA



A1204	A1365	G1478	G1567	U1716	G1857	C1967	A2108	G2330	G2399	G2535		A2826
G1210	A1366	G1479	G1568	G1721	A1858	A1970	U2109	G2338	G2400	A2542	U2720	G2844
G1212	U1211	G1482	A1569	G1724	G1862	U1971	U2110	G2238	U2401	A2547	U2724	A2856
G1218	G1368	G1483	G1368	G1725	A1572	G1972	G1212	G2251	U2404	G2552	A2726	A2861
G1225	A1378	G1485	A1579	G1726	A1866	U1976	U2118	A2278	G2405	G2553	A2727	
G1227	U1379	U1485	A1580	G1727	C1868	U1991	A2119	C2283	A2406	U2554	U2728	G2867
G1236	A1383	U1486	C1582	C1728	C1870	U1992	G2120	C2283	A2407	U2555	A2733	A2868
	A1390	U1487	C1583	C1729	A1871	U1993	G2121	G2286	U2408	G2556	A2734	
	U1391	A1490	A1584	U1730	A1872		G2127	A2287	U2423	A2566	G2735	A2872
	A1392	G1491	C1585	G1731	G1873	C1987		A2288	U2424	G2567		C2874
		C1493		C1732			U2131		A2425		G2742	
	U1240	A1494	G1588	U1735	A1876	A2020	U2132	U2296	G2428	A2572	U2743	C2880
		A1495	A1591	U1736	C1879	C2021	G2133	A2297	G2429	C2573	C2744	
	A1247	A1496	A1592	G1737	A1593	C2022	A2134		A2430		U2745	A2883
	G1248	U1402	A1593	U1738	G1884	C2023	G2141	U2305		U2580	G2746	U2884
	A1403	A1404		G1739	A1885	G2027		U2309	A2435	G2581	G2747	G2885
	C1404	A1504		G1740			G2145	A2309	U2441		A2748	A2886
		C1507	C1605	C1741	A1890	A2030	C2146	G2310	G2445	U2586	C2752	
	G1256	A1508	A1608	A1746	C1895	A2033	A2147	A2311	C2446	U2586	A2753	C2896
	U1258	A1515	A1610	G1750	U1898	U2039	G2157	G2318	G2447	A2602	U2754	U2897
	A1262	G1516	A1616	U1758	G1906	C2043	G2162	G2319	U2448	G2603	A2758	A2899
	A1269	G1519	C1617	C1764	G1907	C2043	A2163	G2325	U2449	U2604	C2762	C36
	G1270	A1618	A1618		C1908	C2055	C2164	G2326		U2605	G2763	C37
	C1271	U1523		A1634	G1909	G2056		C2332	C2452	U2609	A2764	C38
	A1272	G1524			G1910		A2170	A2333	U2457	U2613	A2765	
	U1273		G1527	U1776	A1911	A2059	A2171	A2334		G2624	U2768	
		C1289	A1528	U1647	A1912	A2060	U2172	U2335	C2465	G2629	A2776	
	C1290	A1529	G1649	U1648	A1913	G2061	A2173	A2336	A2469	U2629	G2777	
	C1291	C1428		A1654	3TD1915	A2062		C2339	C2475	A2634	A2778	
				C1531	A1916		U2180	U2340	A2476			G2791
	U1294	G1432	A1532	G1659	U1917	G2069	G2186	U2344	C2480	C2651		
		G1436	C1533		A1918	C2072	U2192	G2345		G2652	U2794	
	G1300	A1301	U1534	G1674	A1801	A2077	G2193	U2346	C2484	U2653		
		G1441	A1535	C1536	A1808		U2194	C2350	G2484	A2654	G2799	
	C1305	G1449	C1537	G1538	A1809	A2080	U2195	G2357	G2494	G2655	A2800	
	C1306				G1923					U2656	G2801	
				G1546	U1692		A2198	G2387			A2802	
	C1320	G1452	U1693		C1816	U2092	G2204	G2361	C2498	G2673	U2807	
	A1321	A1453	C1694	A1549	G1817	G2093	G2205		C2499	G2674	G2808	
	G1342	G1455	G1695		U1818	C2096	C2206	U2372	G2502	U2689	A2809	
				U1554	A1829	A2097			A2503	U2690		
	U1344	U1458	G1555		C1941	U2098	A2211	A2378	U2504	C2691		
	C1345	G1459	C1556		C1833	G2100	A2212	G2379	G2505			
		U1460	C1557		G1835	A2101	U2213	G2383	U2506	U2707		
	C1349	C1461	U1558			G2102	G2221	U2384			G2812	
			U1559			C2103		C2385	C2517	C2712		
	U1352	U1468		U1563	U1712	C2104	A2225	G2391	A2518	U2713	U2818	
		G1475	C1564		A1713	U2105	C2226	G2392		G2714	G2819	
	G1355	U1476			G1715			A2392	G2529	C2715	A2820	
	A1359	A1477	A1566							C2716		

• Molecule 2: 5S rRNA

Chain B:  70% 30%

U1	G2	C3	C4	U5		G9		C12	G13	U14		C17		G20	G21	U22		U25	G26	C27		U32	G33	A34	C35	C36	C37	C38		G41	C42	G43	G44		G56		C63	G64	U65	A66	G67		G84		U89	C90		G102		G105		A108	A109	C110		C118	A119	A120
----	----	----	----	----	--	----	--	-----	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	--	-----	--	-----	-----	-----	-----	-----	--	-----	--	-----	-----	--	------	--	------	--	------	------	------	--	------	------	------

- Molecule 3: 50S ribosomal protein L2

Chain C:  96%



- Molecule 4: 50S ribosomal protein L3

Chain D:  94%



- Molecule 5: 50S ribosomal protein L4

Chain E:  97%



- Molecule 6: 50S ribosomal protein L5

Chain F:  97%



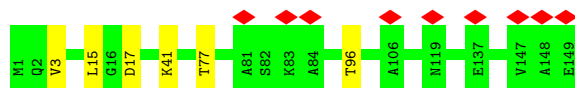
- Molecule 7: 50S ribosomal protein L6

Chain G:  98%

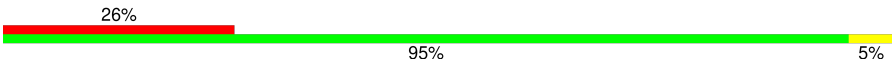


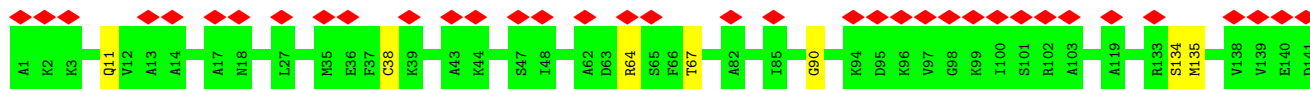
- Molecule 8: 50S ribosomal protein L9

Chain H:  96%



- Molecule 9: 50S ribosomal protein L11

Chain I:  95%



- Molecule 10: 50S ribosomal protein L13

Chain J:  97% .




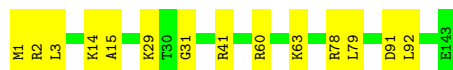
- Molecule 11: 50S ribosomal protein L14

Chain K:  93% 7%



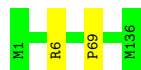
- Molecule 12: 50S ribosomal protein L15

Chain L:  90% 10%



- Molecule 13: 50S ribosomal protein L16

Chain M:  99% .



- Molecule 14: 50S ribosomal protein L17

Chain N:  97% ..



- Molecule 15: 50S ribosomal protein L18

Chain O:  99% .



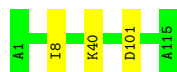
- Molecule 16: 50S ribosomal protein L19

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L20

Chain Q:  97% .



- Molecule 18: 50S ribosomal protein L21

Chain R:  95% 5%



- Molecule 19: 50S ribosomal protein L22

Chain S:  95% 5%



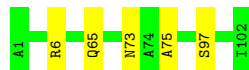
- Molecule 20: 50S ribosomal protein L23

Chain T:  96% .



- Molecule 21: 50S ribosomal protein L24

Chain U:  95% 5%



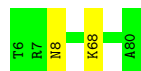
- Molecule 22: 50S ribosomal protein L25

Chain V:  98% ..




- Molecule 23: 50S ribosomal protein L27

Chain W:  97% .



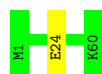
- Molecule 24: 50S ribosomal protein L28

Chain X:  97% .



- Molecule 25: 50S ribosomal protein L29

Chain Y:  98% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  98% .



- Molecule 27: 50S ribosomal protein L32

Chain 0:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  98% .



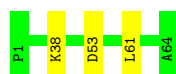
- Molecule 29: 50S ribosomal protein L34

Chain 2:  93% . .

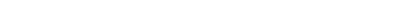


- Molecule 30: 50S ribosomal protein L35

Chain 3:  95% 5%



- Molecule 31: 50S ribosomal protein L36

- Chain 5:  77% 92% 8%

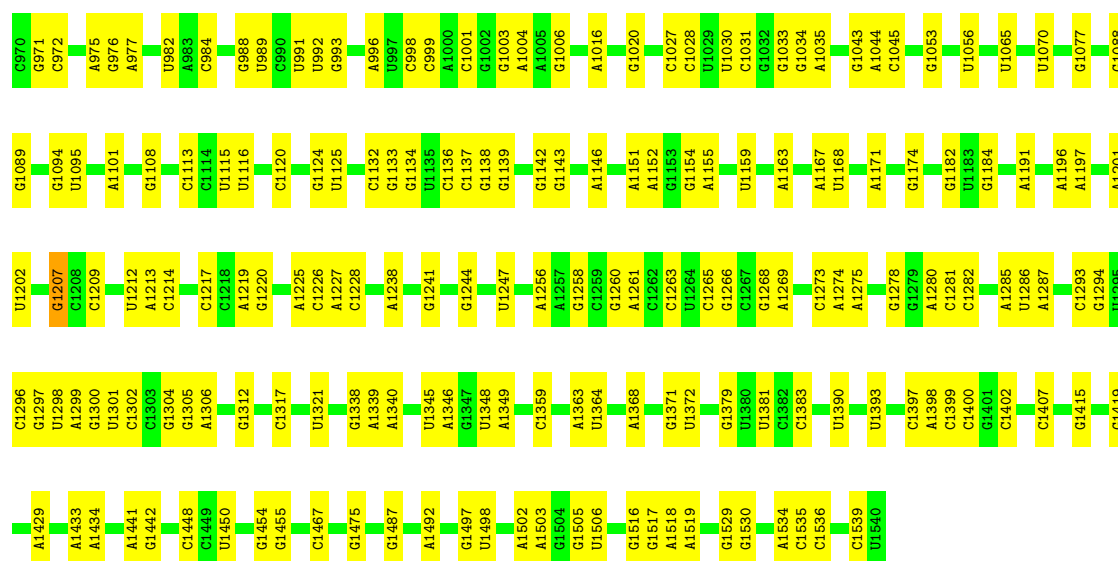
P79	T80	L81	I82	A83	Y84	S85	M86	E87	H88	P89	G90	A91	A92	A93	R94	L95	F96	K97	E98	F99	A100	K101	A102	A103	A104	K105	F106	E107	V108	K109	A110	A111	A112	F113	E114	G115	E116	L117	I118	P119	A120	S121	Q122	I123	D124	R125	A126	L127	T128	L129	P130	T131	
H1	Q9	A10	T11	V12	A13	E14	V15	S16	E17	V18	A19	K20	G21	A22	L23	S24	A25	V26	V27	A28	D29	T34	E40	K43	A44	G45	R46	E47	A48	G49	V50	V51	H52	H53	V54	V55	L60	H61	V64	E65	G66	T67	P68	F69	E70	C71	L72	K73	D74	A75	F76	V77	C78

- Chain 6:  97%

A diagram showing a sequence of five residues: M1, D4, C37, A52, and I66. The residues are represented by colored blocks: M1 (green), D4 (yellow), C37 (yellow), A52 (green), and I66 (green). They are connected by horizontal lines. A red diamond is positioned above the A52 residue.

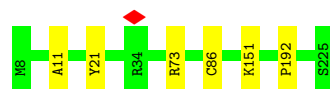
- Chain a: 71% 29%

A777	A595	U467	C362	G212	G107	A1
A596	A468	A353	A353	C215	G108	A2
U793	G354	G469	G354	U216	A109	A3
A794	G615	C470	C355			U4
					G115	U5
A802	G618	G474	U865	C222	A116	G6
		C475	A366			A7
A814	G633	U476	U367	G226	A120	A8
A815		C477		G227	U121	G9
A816	U638		C372			
C817	G639	G484	A373	G230	G128	A32
G818		U485			A129	
A819	A642	U486	G376	U245	A130	G38
				A246	A131	G39
G829	A648	G491	C381	G247		C40
					G141	
G832	G654	A496	G388	G251	G142	G45
			A389		A143	G46
G836	G661	A499	U390	G254	G144	C47
U837			G391		G145	C48
G838	A665	A509	C392	G259	U46	U49
C839					G147	A50
C840	G671	C514	A397	G266	G148	A51
		G515	U398	C267	A149	
U843	A687	U516	G399		U150	G64
G844		G517		A279	A151	A65
A845	A695	C518	G404	C280		A66
G846			U405	G281		C67
		G521	G406		U154	G68
U850	G700			G289	A161	G69
G851	U701	G524	A411		A162	U70
	A702	C525	A412	A300	C163	A71
U871	G703	C526	G413		G164	A72
A872	A704	G527		G305	G165	C73
	G713		U420	A306	U166	A74
		A532	U421		A167	G75
G902			C422	U317		G76
	C720	C536	G423		U173	A77
A914	G721		G424	A321		A78
	G722	G542	G425		A181	G79
G924	U723			A325	A182	A80
G925	G724	C545	U429	G326	C183	
G926		A546		A327	G184	C83
	C731	A547	U434	C328		U84
C931	G732		A435	A329	A189	U85
G934	G733	G550	C436	C330	A190	G86
A935			U437		C87	C87
	C737	U665	U438		G191	U88
				C335		
G939	G742				A197	U89
		A572	C443	C339	G198	
G954	C754	A573	U340	U340	A199	G94
	G755	A574	G446	C341		C95
					G202	U96
U960		G575		C345	G203	G97
U961	C758	C576	G457	G345		A98
	A759	G577	U458	G347	C207	C99
U965			A459	G348	U208	G100
G966	G769	U591	A460	G349	U209	
C967		G592	A461	A349		
	G776	U593	G462	G350	C210	G105
A968	C775	U594		C351	C211	C106
G969						



• Molecule 35: 30S ribosomal protein S2

Chain b:  97%



• Molecule 36: 30S ribosomal protein S3

Chain c:  96%



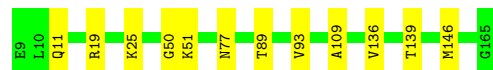
• Molecule 37: 30S ribosomal protein S4

Chain d:  98%



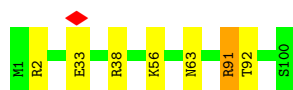
• Molecule 38: 30S ribosomal protein S5

Chain e:  92%



• Molecule 39: 30S ribosomal protein S6

Chain f:  93%



- Molecule 40: 30S ribosomal protein S7

Chain g: 93% 7%



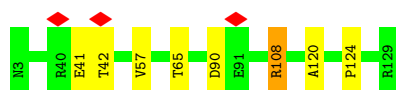
- Molecule 41: 30S ribosomal protein S8

Chain h: 97% .



- Molecule 42: 30S ribosomal protein S9

Chain i: 94% 6% .



- Molecule 43: 30S ribosomal protein S10

Chain j: 93% 7%



- Molecule 44: 30S ribosomal protein S11

Chain k: 93% 7%



- Molecule 45: 30S ribosomal protein S12

Chain l: 92% 7% .



- Molecule 46: 30S ribosomal protein S13

Chain m: 97% .



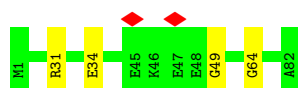
- Molecule 47: 30S ribosomal protein S14



- Molecule 48: 30S ribosomal protein S15



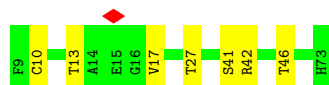
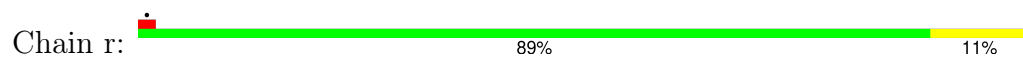
- Molecule 49: 30S ribosomal protein S16



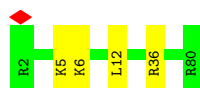
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18

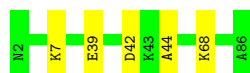


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

Chain t:  94% 6%



- Molecule 54: 30S ribosomal protein S21

Chain u:  82% 17% •



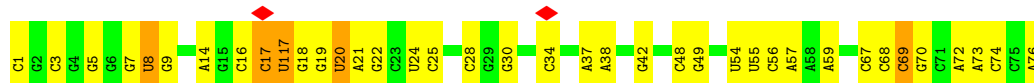
- Molecule 55: tRNA-fMet

Chain v:  74% 23% •



- Molecule 55: tRNA-fMet

Chain w:  51% 43% 6%



- Molecule 56: mRNA

Chain x:  92% 8%



- Molecule 57: tRNA-Phe

Chain y:  54% 42% •



- Molecule 58: Elongation factor Tu 2

Chain z:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.00558	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, MG, 5MC, 6MZ, 4OC, OMC, 3TD, 4SU, UR3, H2U, OMU, 5MU, 2MG, PSU, MA6, K, 2MA, FME, 7MG, 1MG, OMG, GNP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	1/69174 (0.0%)	0.70	11/107907 (0.0%)
2	B	0.31	1/2876 (0.0%)	0.69	0/4483
3	C	0.34	0/2121	0.66	0/2852
4	D	0.35	0/1578	0.59	0/2124
5	E	0.35	0/1563	0.61	0/2103
6	F	0.37	0/1434	0.59	0/1926
7	G	0.35	0/1324	0.54	0/1794
8	H	0.37	0/1122	0.51	0/1515
9	I	0.41	0/1046	0.60	0/1410
10	J	0.34	0/1143	0.60	0/1540
11	K	0.35	0/947	0.66	0/1268
12	L	0.36	0/1052	0.68	0/1401
13	M	0.36	0/1093	0.61	0/1460
14	N	0.39	0/964	0.68	0/1289
15	O	0.38	0/902	0.63	0/1209
16	P	0.35	0/929	0.63	0/1242
17	Q	0.37	0/946	0.67	0/1260
18	R	0.34	0/823	0.58	0/1100
19	S	0.34	0/852	0.67	0/1142
20	T	0.35	0/736	0.60	0/984
21	U	0.35	0/787	0.57	0/1051
22	V	0.36	0/752	0.57	1/1008 (0.1%)
23	W	0.35	0/579	0.64	0/767
24	X	0.36	0/635	0.65	0/848
25	Y	0.37	0/495	0.61	0/658
26	Z	0.37	0/438	0.59	0/586
27	0	0.35	0/440	0.69	0/588
28	1	0.35	0/424	0.54	0/565
29	2	0.39	0/370	0.77	0/487
30	3	0.35	0/513	0.62	0/676
31	4	0.32	0/303	0.66	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.42	0/1001	0.61	0/1350
33	6	0.39	0/531	0.54	0/709
34	a	0.24	0/36725	0.70	3/57285 (0.0%)
35	b	0.37	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.58	0/2225
37	d	0.37	0/1665	0.59	0/2227
38	e	0.36	0/1180	0.61	0/1587
39	f	0.36	0/835	0.65	2/1128 (0.2%)
40	g	0.36	0/1195	0.61	0/1602
41	h	0.34	0/989	0.59	0/1326
42	i	0.39	0/1034	0.68	0/1375
43	j	0.36	0/796	0.65	0/1077
44	k	0.36	0/885	0.60	0/1195
45	l	0.36	0/954	0.69	0/1282
46	m	0.37	0/900	0.64	0/1204
47	n	0.38	0/822	0.65	0/1095
48	o	0.38	0/722	0.74	1/964 (0.1%)
49	p	0.36	0/659	0.61	0/884
50	q	0.37	0/657	0.63	0/881
51	r	0.40	0/544	0.64	0/731
52	s	0.36	0/652	0.61	0/877
53	t	0.37	0/671	0.63	0/888
54	u	0.44	0/550	0.78	0/728
55	v	0.34	1/1747 (0.1%)	0.69	0/2721
55	w	0.46	3/1747 (0.2%)	0.90	5/2721 (0.2%)
56	x	0.21	0/280	0.64	0/433
57	y	0.32	1/1607 (0.1%)	0.67	0/2501
58	z	0.35	0/3086	0.58	0/4175
All	All	0.29	7/164181 (0.0%)	0.68	23/245149 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	y	1	G	OP3-P	-10.19	1.49	1.61
55	v	0	C	OP3-P	-10.18	1.49	1.61
2	B	1	U	OP3-P	-10.16	1.49	1.61
55	w	1	C	OP3-P	-10.14	1.49	1.61
55	w	117	U	O3'-P	-9.83	1.49	1.61
1	A	1	G	OP3-P	-9.79	1.49	1.61
55	w	17	C	O3'-P	8.11	1.70	1.61

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	23.18	148.04	104.00
55	w	17	C	P-O3'-C3'	-13.48	103.52	119.70
55	w	17	C	OP1-P-O3'	-10.56	81.96	105.20
48	o	88	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	A	2712	C	C2'-C3'-O3'	8.01	127.11	109.50
1	A	1140	C	C2'-C3'-O3'	7.06	125.03	109.50
1	A	242	G	C2'-C3'-O3'	6.86	124.68	113.70
1	A	2407	A	C2'-C3'-O3'	6.74	124.49	113.70
34	a	141	G	O4'-C1'-N9	6.48	113.38	108.20
55	w	69	C	C2'-C3'-O3'	6.44	124.01	113.70
55	w	17	C	OP2-P-O3'	-6.37	91.18	105.20
1	A	51	G	C2'-C3'-O3'	6.31	123.80	113.70
1	A	361	G	N9-C1'-C2'	6.08	121.90	114.00
1	A	361	G	O4'-C1'-N9	5.83	112.86	108.20
1	A	1735	G	N9-C1'-C2'	-5.70	105.73	112.00
39	f	91	ARG	NE-CZ-NH1	5.41	123.01	120.30
34	a	246	A	C4'-C3'-O3'	5.29	123.57	113.00
34	a	142	G	N9-C1'-C2'	5.20	120.75	114.00
1	A	1530	G	C4-N9-C1'	5.15	133.19	126.50
39	f	2	ARG	NE-CZ-NH1	5.07	122.84	120.30
22	V	21	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	1727	A	C4-N9-C1'	-5.01	117.28	126.30
1	A	1725	C	C2-N1-C1'	-5.01	113.29	118.80

There are no chirality outliers.

There are no planarity outliers.

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	242 (90%)	25 (9%)	2 (1%)	19	54
4	D	206/208 (99%)	191 (93%)	14 (7%)	1 (0%)	25	61
5	E	198/200 (99%)	179 (90%)	17 (9%)	2 (1%)	13	46
6	F	175/177 (99%)	155 (89%)	19 (11%)	1 (1%)	22	57
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	6	29
9	I	139/141 (99%)	112 (81%)	24 (17%)	3 (2%)	5	27
10	J	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	54
11	K	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	3	18
12	L	141/143 (99%)	117 (83%)	20 (14%)	4 (3%)	4	21
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	36
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	33
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	49
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	20
19	S	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	31
20	T	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	5	27
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	20
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	12	44
23	W	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	33
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	48 (91%)	4 (8%)	1 (2%)	6	31
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5	26
30	3	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
31	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	5	129/131 (98%)	99 (77%)	22 (17%)	8 (6%)	1	7
33	6	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	8	34
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	184 (90%)	15 (7%)	5 (2%)	4	24
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	13	46
38	e	156/157 (99%)	131 (84%)	19 (12%)	6 (4%)	2	15
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	130 (87%)	12 (8%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	2	14
43	j	96/98 (98%)	73 (76%)	17 (18%)	6 (6%)	1	6
44	k	114/116 (98%)	99 (87%)	10 (9%)	5 (4%)	2	12
45	l	119/121 (98%)	98 (82%)	13 (11%)	8 (7%)	1	5
46	m	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	7	32
47	n	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	1	10
48	o	86/88 (98%)	78 (91%)	5 (6%)	3 (4%)	3	16
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	24
50	q	78/80 (98%)	70 (90%)	6 (8%)	2 (3%)	4	23
51	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	5	25
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	1
58	z	391/393 (100%)	352 (90%)	29 (7%)	10 (3%)	4	23
All	All	6219/6322 (98%)	5477 (88%)	602 (10%)	140 (2%)	7	26

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	83	VAL
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
40	g	64	ALA
42	i	90	ASP
43	j	57	VAL
44	k	88	PRO

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Mol	Chain	Res	Type
44	k	94	SER
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
5	E	8	ALA
9	I	64	ARG
10	J	81	ILE
15	O	66	GLY
18	R	54	VAL
18	R	55	ASP
20	T	37	ASP
20	T	38	ALA
32	5	60	LEU
33	6	4	ASP
38	e	77	ASN
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
45	l	42	LYS
45	l	75	GLU
45	l	88	ASP
46	m	7	ASN
47	n	22	LYS
47	n	55	SER
47	n	90	ARG
51	r	17	VAL
54	u	30	GLU
54	u	37	TYR
58	z	161	ASP
12	L	15	ALA
12	L	29	LYS
12	L	31	GLY
13	M	69	PRO
21	U	6	ARG
22	V	58	SER
25	Y	24	GLU
27	0	2	VAL
32	5	48	ALA
32	5	88	HIS
35	b	73	ARG

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Mol	Chain	Res	Type
35	b	86	CYS
37	d	191	SER
39	f	63	ASN
40	g	20	GLU
42	i	124	PRO
43	j	35	GLN
44	k	13	LYS
44	k	103	GLY
47	n	2	LYS
47	n	38	ASP
49	p	64	GLY
51	r	10	CYS
51	r	46	THR
54	u	9	GLU
54	u	11	PHE
54	u	12	ASP
58	z	249	GLU
3	C	13	ARG
3	C	120	ASP
4	D	31	ALA
6	F	20	ASN
8	H	15	LEU
8	H	41	LYS
9	I	38	CYS
11	K	110	GLU
14	N	59	SER
14	N	117	ASP
21	U	97	SER
29	2	2	LYS
32	5	118	ILE
36	c	95	GLY
37	d	166	LYS
38	e	89	THR
38	e	93	VAL
38	e	109	ALA
39	f	33	GLU
40	g	19	SER
45	l	33	CYS
45	l	46	SER
46	m	102	LYS
48	o	13	GLU
48	o	45	HIS

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Mol	Chain	Res	Type
49	p	49	GLY
54	u	65	ARG
58	z	332	PHE
8	H	3	VAL
11	K	35	VAL
12	L	92	LEU
13	M	6	ARG
19	S	3	THR
19	S	65	ASP
21	U	75	ALA
32	5	113	PHE
35	b	192	PRO
38	e	146	MET
39	f	92	THR
40	g	56	SER
45	l	77	SER
48	o	2	LEU
50	q	49	ASN
50	q	79	GLU
53	t	44	ALA
58	z	9	LYS
58	z	82	PRO
58	z	126	GLY
58	z	207	ASP
32	5	108	VAL
35	b	11	ALA
35	b	151	LYS
39	f	56	LYS
40	g	112	ASP
42	i	120	ALA
43	j	6	ILE
43	j	75	ASP
45	l	21	PRO
45	l	35	ARG
54	u	24	LYS
58	z	2	LYS
36	c	147	GLY
43	j	41	PRO
58	z	180	GLY
36	c	144	GLY
58	z	52	ALA
18	R	100	GLY

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Mol	Chain	Res	Type
38	e	50	GLY
40	g	111	GLY
9	I	90	GLY
11	K	93	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	208 (96%)	8 (4%)	29	63
4	D	163/163 (100%)	152 (93%)	11 (7%)	13	43
5	E	164/164 (100%)	160 (98%)	4 (2%)	44	74
6	F	148/148 (100%)	144 (97%)	4 (3%)	40	71
7	G	135/135 (100%)	132 (98%)	3 (2%)	47	76
8	H	114/114 (100%)	111 (97%)	3 (3%)	41	72
9	I	109/109 (100%)	105 (96%)	4 (4%)	29	63
10	J	115/115 (100%)	112 (97%)	3 (3%)	41	72
11	K	103/103 (100%)	98 (95%)	5 (5%)	21	54
12	L	102/102 (100%)	92 (90%)	10 (10%)	6	26
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	99/99 (100%)	97 (98%)	2 (2%)	50	78
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	66
18	R	84/84 (100%)	82 (98%)	2 (2%)	44	74
19	S	92/92 (100%)	89 (97%)	3 (3%)	33	67
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	73
21	U	83/83 (100%)	81 (98%)	2 (2%)	44	74
22	V	77/77 (100%)	76 (99%)	1 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	57/57 (100%)	55 (96%)	2 (4%)	31	65
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	69
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	48	77
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	47	76
29	2	37/37 (100%)	34 (92%)	3 (8%)	9	34
30	3	51/51 (100%)	48 (94%)	3 (6%)	16	47
31	4	34/34 (100%)	33 (97%)	1 (3%)	37	70
32	5	100/100 (100%)	98 (98%)	2 (2%)	50	78
33	6	59/59 (100%)	58 (98%)	1 (2%)	56	81
35	b	180/180 (100%)	179 (99%)	1 (1%)	84	93
36	c	170/170 (100%)	166 (98%)	4 (2%)	44	74
37	d	172/172 (100%)	169 (98%)	3 (2%)	56	81
38	e	120/119 (101%)	114 (95%)	6 (5%)	20	53
39	f	87/87 (100%)	85 (98%)	2 (2%)	45	75
40	g	124/124 (100%)	121 (98%)	3 (2%)	44	74
41	h	104/104 (100%)	100 (96%)	4 (4%)	28	62
42	i	105/105 (100%)	101 (96%)	4 (4%)	28	62
43	j	86/86 (100%)	85 (99%)	1 (1%)	67	86
44	k	89/89 (100%)	86 (97%)	3 (3%)	32	66
45	l	102/102 (100%)	98 (96%)	4 (4%)	27	61
46	m	93/93 (100%)	91 (98%)	2 (2%)	47	76
47	n	83/83 (100%)	83 (100%)	0	100	100
48	o	76/76 (100%)	73 (96%)	3 (4%)	27	61
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	68
50	q	74/74 (100%)	71 (96%)	3 (4%)	26	60
51	r	56/56 (100%)	52 (93%)	4 (7%)	12	40
52	s	70/70 (100%)	66 (94%)	4 (6%)	17	49
53	t	65/65 (100%)	62 (95%)	3 (5%)	23	56
54	u	55/55 (100%)	51 (93%)	4 (7%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	z	325/325 (100%)	317 (98%)	8 (2%)	42	73
All	All	5165/5164 (100%)	5011 (97%)	154 (3%)	37	69

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	42	ARG
3	C	58	LYS
3	C	69	ASN
3	C	85	ASN
3	C	200	MET
3	C	212	TRP
3	C	241	LYS
4	D	12	THR
4	D	51	THR
4	D	56	LYS
4	D	58	ASN
4	D	77	ARG
4	D	150	GLN
4	D	151	THR
4	D	157	LYS
4	D	169	ARG
4	D	176	ASP
4	D	204	LYS
5	E	69	ARG
5	E	117	ARG
5	E	141	MET
5	E	150	THR
6	F	67	THR
6	F	87	LYS
6	F	91	ARG
6	F	112	ASP
7	G	34	ARG
7	G	121	THR
7	G	152	ARG
8	H	17	ASP
8	H	77	THR
8	H	96	THR
9	I	11	GLN
9	I	67	THR
9	I	134	SER

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Mol	Chain	Res	Type
9	I	135	MET
10	J	2	LYS
10	J	85	LYS
10	J	138	GLN
11	K	7	MET
11	K	23	LYS
11	K	31	ARG
11	K	58	LEU
11	K	67	LYS
12	L	1	MET
12	L	2	ARG
12	L	3	LEU
12	L	14	LYS
12	L	41	ARG
12	L	60	ARG
12	L	63	LYS
12	L	78	ARG
12	L	79	LEU
12	L	91	ASP
14	N	2	ARG
14	N	117	ASP
17	Q	8	ILE
17	Q	40	LYS
17	Q	101	ASP
18	R	66	HIS
18	R	73	LYS
19	S	29	VAL
19	S	86	MET
19	S	108	SER
20	T	69	ARG
20	T	91	GLN
21	U	65	GLN
21	U	73	ASN
22	V	21	ARG
23	W	8	ASN
23	W	68	LYS
24	X	16	ASN
24	X	59	ASP
26	Z	10	ARG
28	1	31	GLU
29	2	2	LYS
29	2	22	MET

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Mol	Chain	Res	Type
29	2	34	ARG
30	3	38	LYS
30	3	53	ASP
30	3	61	LEU
31	4	4	ARG
32	5	29	ASP
32	5	34	THR
33	6	37	CYS
35	b	21	TYR
36	c	121	SER
36	c	138	GLN
36	c	156	LEU
36	c	182	ASP
37	d	30	LYS
37	d	54	LEU
37	d	140	ASP
38	e	11	GLN
38	e	19	ARG
38	e	25	LYS
38	e	51	LYS
38	e	136	VAL
38	e	139	THR
39	f	38	ARG
39	f	91	ARG
40	g	2	ARG
40	g	11	ILE
40	g	78	ARG
41	h	2	MET
41	h	59	GLU
41	h	111	THR
41	h	120	LEU
42	i	41	GLU
42	i	42	THR
42	i	65	THR
42	i	108	ARG
43	j	45	ARG
44	k	28	ASN
44	k	126	ARG
44	k	127	ARG
45	l	9	LYS
45	l	77	SER
45	l	88	ASP

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Mol	Chain	Res	Type
45	l	93	ARG
46	m	57	ASP
46	m	89	ARG
48	o	71	ARG
48	o	87	ARG
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	52	CYS
50	q	63	CYS
51	r	13	THR
51	r	27	THR
51	r	41	SER
51	r	42	ARG
52	s	5	LYS
52	s	6	LYS
52	s	12	LEU
52	s	36	ARG
53	t	7	LYS
53	t	42	ASP
53	t	68	LYS
54	u	9	GLU
54	u	32	ARG
54	u	35	GLU
54	u	62	GLU
58	z	22	HIS
58	z	47	ASP
58	z	65	SER
58	z	112	MET
58	z	136	LYS
58	z	181	ASP
58	z	204	ARG
58	z	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	59	GLN
4	D	36	GLN
15	O	100	HIS
18	R	11	GLN

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Mol	Chain	Res	Type
20	T	70	HIS
45	l	72	ASN
53	t	69	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2892/2903 (99%)	793 (27%)	79 (2%)
2	B	119/120 (99%)	33 (27%)	4 (3%)
34	a	1536/1540 (99%)	435 (28%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	35 (46%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	74/76 (97%)	28 (37%)	0
All	All	4784/4805 (99%)	1342 (28%)	83 (1%)

All (1342) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U
1	A	13	A
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	41	C
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	61	C
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G

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Mol	Chain	Res	Type
1	A	78	U
1	A	80	G
1	A	81	G
1	A	82	U
1	A	83	A
1	A	84	A
1	A	87	U
1	A	93	G
1	A	96	C
1	A	97	C
1	A	98	G
1	A	99	U
1	A	100	U
1	A	101	A
1	A	102	U
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	126	A
1	A	130	C
1	A	132	G
1	A	133	U
1	A	136	G
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	142	A
1	A	143	C
1	A	145	C
1	A	147	C
1	A	149	A
1	A	152	A
1	A	154	U
1	A	156	A
1	A	158	U
1	A	159	G
1	A	160	A
1	A	162	U
1	A	163	C

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Mol	Chain	Res	Type
1	A	165	A
1	A	168	G
1	A	169	G
1	A	170	U
1	A	173	A
1	A	175	G
1	A	181	A
1	A	188	G
1	A	196	A
1	A	199	A
1	A	200	U
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	226	A
1	A	228	C
1	A	229	C
1	A	231	A
1	A	232	G
1	A	234	U
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	258	G
1	A	259	G
1	A	260	G
1	A	261	G
1	A	265	A
1	A	266	G
1	A	267	C
1	A	268	C
1	A	269	C
1	A	272	A
1	A	273	G
1	A	274	C
1	A	275	C
1	A	276	U
1	A	278	A

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Mol	Chain	Res	Type
1	A	279	A
1	A	280	U
1	A	281	C
1	A	283	G
1	A	284	U
1	A	285	G
1	A	286	U
1	A	289	G
1	A	290	U
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C
1	A	311	A
1	A	317	G
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	343	C
1	A	344	A
1	A	345	A
1	A	349	U
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	365	U
1	A	366	C
1	A	367	G
1	A	368	A
1	A	371	A
1	A	372	G
1	A	383	C
1	A	386	G
1	A	387	U
1	A	390	U
1	A	395	U
1	A	396	G
1	A	400	G
1	A	403	U

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Mol	Chain	Res	Type
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	419	U
1	A	427	U
1	A	428	A
1	A	438	G
1	A	442	G
1	A	445	C
1	A	451	U
1	A	455	C
1	A	473	G
1	A	475	C
1	A	481	G
1	A	485	C
1	A	486	C
1	A	491	G
1	A	492	A
1	A	494	G
1	A	496	G
1	A	503	A
1	A	504	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	518	G
1	A	521	U
1	A	527	C
1	A	529	A
1	A	532	A
1	A	533	G
1	A	535	G
1	A	543	G
1	A	545	U
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	563	A
1	A	564	C

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Mol	Chain	Res	Type
1	A	573	U
1	A	575	A
1	A	602	A
1	A	603	A
1	A	610	C
1	A	612	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	633	A
1	A	636	G
1	A	637	A
1	A	640	C
1	A	644	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	648	G
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	661	A
1	A	664	G
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	730	A
1	A	738	G
1	A	747	5MC
1	A	752	A
1	A	764	A
1	A	765	C

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Mol	Chain	Res	Type
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	804	A
1	A	805	G
1	A	812	C
1	A	814	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	837	C
1	A	844	A
1	A	845	A
1	A	846	C
1	A	858	G
1	A	860	U
1	A	877	A
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	934	U
1	A	940	G
1	A	941	A
1	A	942	G
1	A	946	C
1	A	951	C
1	A	953	G

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Mol	Chain	Res	Type
1	A	958	U
1	A	961	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	985	C
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1006	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1014	A
1	A	1017	G
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1036	G
1	A	1037	G
1	A	1038	G
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G

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Mol	Chain	Res	Type
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1082	U
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1097	U
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1115	G
1	A	1117	C
1	A	1119	U
1	A	1130	U
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1141	U
1	A	1142	A
1	A	1143	A
1	A	1148	U
1	A	1150	C
1	A	1151	A
1	A	1167	C
1	A	1172	C
1	A	1173	U
1	A	1174	U

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Mol	Chain	Res	Type
1	A	1175	A
1	A	1176	U
1	A	1178	C
1	A	1179	G
1	A	1180	U
1	A	1181	U
1	A	1193	G
1	A	1200	C
1	A	1204	A
1	A	1210	G
1	A	1212	G
1	A	1218	G
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1258	U
1	A	1262	A
1	A	1269	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1289	C
1	A	1290	C
1	A	1291	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1306	C
1	A	1320	C
1	A	1321	A
1	A	1332	G
1	A	1344	U
1	A	1345	C
1	A	1349	C
1	A	1352	U
1	A	1355	G
1	A	1359	A

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Mol	Chain	Res	Type
1	A	1365	A
1	A	1367	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1390	U
1	A	1392	A
1	A	1402	U
1	A	1403	A
1	A	1404	C
1	A	1407	G
1	A	1411	U
1	A	1412	U
1	A	1414	C
1	A	1415	U
1	A	1416	G
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1436	G
1	A	1441	G
1	A	1449	G
1	A	1452	G
1	A	1453	A
1	A	1454	C
1	A	1455	G
1	A	1458	U
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1468	U
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1487	U

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Mol	Chain	Res	Type
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1495	A
1	A	1497	U
1	A	1504	A
1	A	1507	C
1	A	1508	A
1	A	1515	A
1	A	1516	G
1	A	1519	G
1	A	1523	U
1	A	1524	G
1	A	1527	G
1	A	1528	A
1	A	1529	G
1	A	1530	G
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1546	G
1	A	1549	A
1	A	1554	U
1	A	1555	G
1	A	1556	C
1	A	1559	U
1	A	1563	U
1	A	1565	C
1	A	1567	G
1	A	1569	A
1	A	1572	A
1	A	1579	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1588	G

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Mol	Chain	Res	Type
1	A	1591	A
1	A	1592	C
1	A	1593	A
1	A	1605	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1659	G
1	A	1674	G
1	A	1675	C
1	A	1691	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1700	A
1	A	1705	A
1	A	1706	C
1	A	1709	U
1	A	1712	U
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1721	G
1	A	1724	G
1	A	1725	C
1	A	1729	U
1	A	1730	U
1	A	1731	G
1	A	1732	C
1	A	1736	U
1	A	1738	G
1	A	1739	A
1	A	1741	C
1	A	1746	A
1	A	1750	G
1	A	1758	U

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Mol	Chain	Res	Type
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1809	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1841	U
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1867	G
1	A	1868	C
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1876	A
1	A	1879	C
1	A	1884	G
1	A	1885	A
1	A	1890	A
1	A	1895	C
1	A	1898	U
1	A	1906	G
1	A	1907	G
1	A	1909	C
1	A	1913	A
1	A	1914	C
1	A	1916	A
1	A	1917	PSU
1	A	1927	A
1	A	1929	G
1	A	1930	G

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Mol	Chain	Res	Type
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1955	U
1	A	1962	5MC
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2033	A
1	A	2039	U
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2100	G
1	A	2102	G
1	A	2104	C
1	A	2106	U

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Mol	Chain	Res	Type
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2180	U
1	A	2186	G
1	A	2192	U
1	A	2193	G
1	A	2195	U
1	A	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2221	G
1	A	2225	A
1	A	2226	C
1	A	2230	G
1	A	2238	G
1	A	2239	G
1	A	2278	A
1	A	2283	C
1	A	2286	G

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Mol	Chain	Res	Type
1	A	2287	A
1	A	2288	A
1	A	2296	U
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2332	C
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2340	A
1	A	2344	U
1	A	2345	G
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2372	U
1	A	2378	A
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2399	G
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A
1	A	2408	U
1	A	2423	U
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2445	2MG

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Mol	Chain	Res	Type
1	A	2447	G
1	A	2448	A
1	A	2452	C
1	A	2465	C
1	A	2469	A
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2484	G
1	A	2494	G
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2556	C
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2613	U
1	A	2624	G
1	A	2629	U
1	A	2634	A
1	A	2651	C
1	A	2653	U
1	A	2654	A
1	A	2656	U
1	A	2673	G
1	A	2674	G
1	A	2689	U

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Mol	Chain	Res	Type
1	A	2690	U
1	A	2691	C
1	A	2707	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2720	U
1	A	2724	U
1	A	2726	A
1	A	2728	U
1	A	2733	A
1	A	2734	A
1	A	2735	G
1	A	2742	G
1	A	2744	G
1	A	2745	C
1	A	2746	U
1	A	2748	A
1	A	2752	C
1	A	2754	U
1	A	2758	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2768	U
1	A	2776	A
1	A	2778	A
1	A	2791	G
1	A	2794	U
1	A	2799	G
1	A	2800	A
1	A	2801	G
1	A	2803	G
1	A	2805	C
1	A	2807	U
1	A	2809	A
1	A	2812	G
1	A	2818	U
1	A	2820	A
1	A	2826	A
1	A	2844	G
1	A	2856	A

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Mol	Chain	Res	Type
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2874	C
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2886	A
1	A	2896	C
1	A	2898	U
1	A	2899	A
1	A	2901	C
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	5	U
2	B	9	G
2	B	12	C
2	B	13	G
2	B	14	U
2	B	17	C
2	B	20	G
2	B	21	G
2	B	22	U
2	B	25	U
2	B	27	C
2	B	32	U
2	B	33	G
2	B	35	C
2	B	37	C
2	B	38	C
2	B	41	G
2	B	42	C
2	B	44	G
2	B	63	C
2	B	65	U
2	B	66	A
2	B	67	G
2	B	84	G
2	B	89	U
2	B	90	C

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Mol	Chain	Res	Type
2	B	102	G
2	B	105	G
2	B	108	A
2	B	109	A
2	B	110	C
2	B	118	C
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	32	A
34	a	38	G
34	a	39	G
34	a	40	C
34	a	45	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	64	G
34	a	66	A
34	a	68	G
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A
34	a	74	A
34	a	76	G
34	a	77	A
34	a	78	A
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G

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Mol	Chain	Res	Type
34	a	95	C
34	a	96	U
34	a	97	G
34	a	98	A
34	a	99	C
34	a	100	G
34	a	105	G
34	a	107	G
34	a	109	A
34	a	115	G
34	a	116	A
34	a	120	A
34	a	121	U
34	a	128	G
34	a	130	A
34	a	131	A
34	a	142	G
34	a	143	A
34	a	144	G
34	a	145	G
34	a	146	G
34	a	147	G
34	a	149	A
34	a	151	A
34	a	154	U
34	a	161	A
34	a	162	A
34	a	163	C
34	a	165	G
34	a	167	A
34	a	173	U
34	a	181	A
34	a	182	A
34	a	183	C
34	a	184	G
34	a	189	A
34	a	190	A
34	a	191	G
34	a	197	A
34	a	199	A
34	a	202	G
34	a	203	G

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Mol	Chain	Res	Type
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	215	C
34	a	216	U
34	a	222	C
34	a	226	G
34	a	227	G
34	a	230	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	254	G
34	a	259	G
34	a	266	G
34	a	267	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	325	A
34	a	326	G
34	a	328	C
34	a	330	C
34	a	335	C
34	a	339	C
34	a	341	C
34	a	345	C
34	a	346	G
34	a	347	G
34	a	348	G
34	a	349	A
34	a	351	G
34	a	352	C
34	a	354	G

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Mol	Chain	Res	Type
34	a	355	C
34	a	365	U
34	a	367	U
34	a	372	C
34	a	373	A
34	a	376	G
34	a	381	C
34	a	388	G
34	a	390	U
34	a	392	C
34	a	397	A
34	a	398	U
34	a	399	G
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	420	U
34	a	422	C
34	a	424	G
34	a	425	G
34	a	429	U
34	a	434	U
34	a	436	C
34	a	437	U
34	a	438	U
34	a	443	C
34	a	446	G
34	a	457	G
34	a	458	U
34	a	459	A
34	a	461	A
34	a	462	G
34	a	467	U
34	a	468	A
34	a	470	C
34	a	474	G
34	a	475	C
34	a	476	U
34	a	477	C

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Mol	Chain	Res	Type
34	a	484	G
34	a	485	U
34	a	486	U
34	a	491	G
34	a	496	A
34	a	499	A
34	a	509	A
34	a	514	C
34	a	518	C
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	532	A
34	a	536	C
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	550	G
34	a	565	U
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	591	U
34	a	592	G
34	a	594	U
34	a	596	A
34	a	615	G
34	a	618	C
34	a	633	G
34	a	638	U
34	a	639	G
34	a	642	A
34	a	648	A
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	687	A

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Mol	Chain	Res	Type
34	a	695	A
34	a	700	G
34	a	701	U
34	a	703	G
34	a	704	A
34	a	713	G
34	a	720	C
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	737	C
34	a	742	G
34	a	754	C
34	a	755	G
34	a	758	C
34	a	759	A
34	a	769	G
34	a	775	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	814	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	829	G
34	a	832	G
34	a	836	G
34	a	838	G
34	a	840	C
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	850	U
34	a	851	G
34	a	871	U

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Mol	Chain	Res	Type
34	a	872	A
34	a	902	G
34	a	914	A
34	a	924	C
34	a	926	G
34	a	931	C
34	a	934	C
34	a	935	A
34	a	939	G
34	a	954	G
34	a	960	U
34	a	961	U
34	a	965	U
34	a	966	2MG
34	a	969	A
34	a	971	G
34	a	972	C
34	a	975	A
34	a	976	G
34	a	977	A
34	a	982	U
34	a	984	C
34	a	988	G
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	996	A
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G

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Mol	Chain	Res	Type
34	a	1035	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1077	G
34	a	1088	G
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1108	G
34	a	1113	C
34	a	1115	U
34	a	1116	U
34	a	1120	C
34	a	1124	G
34	a	1125	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1155	A
34	a	1159	U
34	a	1163	A
34	a	1167	A
34	a	1168	U
34	a	1171	A
34	a	1174	G
34	a	1182	G

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Mol	Chain	Res	Type
34	a	1184	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1207	2MG
34	a	1209	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1238	A
34	a	1241	G
34	a	1244	G
34	a	1247	U
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1263	C
34	a	1265	C
34	a	1266	G
34	a	1268	G
34	a	1269	A
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1293	C

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Mol	Chain	Res	Type
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1299	A
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1312	G
34	a	1317	C
34	a	1321	U
34	a	1338	G
34	a	1339	A
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1349	A
34	a	1359	C
34	a	1363	A
34	a	1364	U
34	a	1368	A
34	a	1371	G
34	a	1372	U
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1390	U
34	a	1393	U
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1415	G
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1441	A

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Mol	Chain	Res	Type
34	a	1442	G
34	a	1448	C
34	a	1450	U
34	a	1454	G
34	a	1455	G
34	a	1467	C
34	a	1475	G
34	a	1487	G
34	a	1492	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
34	a	1505	G
34	a	1506	U
34	a	1517	G
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	47	U
55	v	50	U
55	v	52	G
55	v	70	G
55	v	76	A
55	w	3	C
55	w	5	G
55	w	7	G
55	w	8	4SU

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Mol	Chain	Res	Type
55	w	9	G
55	w	14	A
55	w	16	C
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A
55	w	67	C
55	w	68	C
55	w	69	C
55	w	70	G
55	w	72	A
55	w	73	A
55	w	74	C
55	w	76	A
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	17	C
57	y	18	G
57	y	20	H2U

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Mol	Chain	Res	Type
57	y	21	A
57	y	24	G
57	y	33	U
57	y	36	A
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	59	U
57	y	61	C
57	y	65	G
57	y	68	C
57	y	69	G
57	y	72	C
57	y	75	C
57	y	76	A

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	51	G
1	A	97	C
1	A	141	G
1	A	163	C
1	A	177	G
1	A	182	A
1	A	199	A
1	A	204	A
1	A	231	A
1	A	242	G
1	A	265	A
1	A	278	A
1	A	285	G
1	A	301	G
1	A	403	U
1	A	446	G
1	A	474	G
1	A	506	G
1	A	546	U

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Mol	Chain	Res	Type
1	A	555	G
1	A	645	C
1	A	746	PSU
1	A	752	A
1	A	764	A
1	A	774	G
1	A	784	G
1	A	859	G
1	A	884	U
1	A	983	A
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1070	A
1	A	1089	A
1	A	1111	A
1	A	1124	G
1	A	1140	C
1	A	1141	U
1	A	1190	G
1	A	1240	U
1	A	1378	A
1	A	1399	C
1	A	1419	A
1	A	1432	G
1	A	1454	C
1	A	1459	G
1	A	1475	G
1	A	1493	C
1	A	1555	G
1	A	1558	C
1	A	1608	A
1	A	1647	U
1	A	1706	C
1	A	1730	U
1	A	1738	G
1	A	1818	U
1	A	1857	G
1	A	1913	A
1	A	1918	A
1	A	1939	5MU
1	A	1940	U

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Mol	Chain	Res	Type
1	A	1976	U
1	A	2238	G
1	A	2296	U
1	A	2333	A
1	A	2391	G
1	A	2401	U
1	A	2402	U
1	A	2407	A
1	A	2517	C
1	A	2566	A
1	A	2581	G
1	A	2585	U
1	A	2712	C
1	A	2803	G
1	A	2808	G
1	A	2873	A
1	A	2901	C
2	B	3	C
2	B	14	U
2	B	56	G
2	B	66	A

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

52 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	$\# Z > 2$
57	PSU	y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
57	PSU	y	32	57,60	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)
34	UR3	a	1498	34	19,22,23	1.14	1 (5%)	26,32,35	2.01	5 (19%)
1	H2U	A	2449	1	18,21,22	0.95	2 (11%)	19,30,33	1.74	4 (21%)
34	4OC	a	1402	34	20,23,24	0.85	2 (10%)	25,32,35	1.32	4 (16%)
34	MA6	a	1518	34,60	19,26,27	1.52	4 (21%)	18,38,41	2.56	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.54	4 (15%)
34	5MC	a	967	34	19,22,23	2.04	2 (10%)	26,32,35	1.55	5 (19%)
1	2MG	A	2445	1,60	18,26,27	0.95	1 (5%)	16,38,41	1.53	3 (18%)
34	MA6	a	1519	34	19,26,27	1.45	4 (21%)	18,38,41	2.46	6 (33%)
1	PSU	A	955	1	18,21,22	1.41	2 (11%)	21,30,33	2.06	4 (19%)
1	6MZ	A	1618	1	17,25,26	1.08	2 (11%)	15,36,39	2.38	5 (33%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.22	5 (20%)
1	OMC	A	2498	1,60	19,22,23	0.84	0	25,31,34	1.21	2 (8%)
55	5MU	v	54	55	19,22,23	1.47	4 (21%)	27,32,35	1.94	8 (29%)
1	PSU	A	1917	1	18,21,22	1.45	2 (11%)	21,30,33	2.07	5 (23%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.57	2 (10%)
1	2MG	A	1835	1	18,26,27	1.03	2 (11%)	16,38,41	1.26	2 (12%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	19,30,33	1.38	4 (21%)
1	OMG	A	2251	1,55,60	19,26,27	1.03	2 (10%)	21,38,41	1.09	2 (9%)
1	PSU	A	2457	1,60	18,21,22	1.44	2 (11%)	21,30,33	2.04	5 (23%)
1	PSU	A	2504	1	18,21,22	1.43	2 (11%)	21,30,33	2.05	4 (19%)
55	H2U	v	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.68	3 (15%)
57	H2U	y	20	57	18,21,22	0.87	1 (5%)	19,30,33	1.48	4 (21%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	1.99	4 (19%)
57	MIA	y	37	57	23,30,32	2.31	5 (21%)	22,42,47	2.58	7 (31%)
34	5MC	a	1407	34	19,22,23	2.02	2 (10%)	26,32,35	1.62	5 (19%)
1	PSU	A	2605	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)
55	PSU	v	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	5 (23%)
1	2MA	A	2503	1,60	17,25,26	1.12	2 (11%)	16,37,40	1.32	3 (18%)
34	2MG	a	966	34	18,26,27	1.04	1 (5%)	16,38,41	2.12	5 (31%)
1	5MU	A	1939	1	19,22,23	1.48	4 (21%)	27,32,35	2.05	8 (29%)
1	PSU	A	2580	1	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
1	6MZ	A	2030	1,60	17,25,26	1.07	2 (11%)	15,36,39	2.38	5 (33%)
55	5MU	w	54	55	19,22,23	1.50	4 (21%)	27,32,35	2.07	10 (37%)
1	7MG	A	2069	1,60	23,26,27	1.43	2 (8%)	27,39,42	2.53	11 (40%)
1	5MC	A	747	1	19,22,23	1.91	2 (10%)	26,32,35	1.54	5 (19%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.36	6 (24%)
57	4SU	y	8	57	18,21,22	1.85	5 (27%)	25,30,33	2.38	7 (28%)
34	2MG	a	1207	34	18,26,27	0.93	1 (5%)	16,38,41	2.68	5 (31%)
1	PSU	A	2604	1	18,21,22	1.44	2 (11%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	5MU	y	54	57	19,22,23	1.43	4 (21%)	27,32,35	2.08	7 (25%)
1	PSU	A	746	1,60	18,21,22	1.42	2 (11%)	21,30,33	1.99	4 (19%)
1	OMU	A	2552	1,60	19,22,23	1.31	3 (15%)	25,31,34	2.04	9 (36%)
34	7MG	a	527	34,60	23,26,27	1.41	2 (8%)	27,39,42	2.52	7 (25%)
34	PSU	a	516	34	18,21,22	1.38	2 (11%)	21,30,33	2.16	5 (23%)
34	2MG	a	1516	34	18,26,27	0.96	1 (5%)	16,38,41	1.57	4 (25%)
57	7MG	y	46	57	23,26,27	1.41	3 (13%)	27,39,42	2.46	7 (25%)
55	PSU	w	55	55	18,21,22	1.32	2 (11%)	21,30,33	2.07	5 (23%)
1	3TD	A	1915	1	19,22,23	7.08	14 (73%)	23,32,35	2.02	5 (21%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.16	4 (19%)
1	1MG	A	745	1	19,26,27	1.33	3 (15%)	18,39,42	1.84	5 (27%)

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
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
57	PSU	y	32	57,60	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	MA6	a	1518	34,60	-	3/7/29/30	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,60	-	2/5/27/28	0/3/3/3
34	MA6	a	1519	34	-	2/7/29/30	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	2251	1,55,60	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1,60	-	2/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/10/32/34	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	3/3/25/26	0/3/3/3
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1,60	-	3/5/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.51	1.66	1.43
1	A	1915	3TD	C6-C5	15.64	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C2'-C1'	-14.44	1.34	1.53
1	A	1915	3TD	C2-N1	8.58	1.47	1.37
34	a	967	5MC	C5-C4	7.69	1.49	1.44
34	a	1407	5MC	C5-C4	7.66	1.49	1.44
1	A	1962	5MC	C5-C4	7.51	1.49	1.44
1	A	747	5MC	C5-C4	7.23	1.49	1.44
57	y	37	MIA	C13-C14	6.86	1.52	1.32
57	y	37	MIA	C2-S10	-6.35	1.70	1.75
1	A	1915	3TD	C2-N3	6.28	1.51	1.38
1	A	1915	3TD	O4'-C4'	-6.01	1.31	1.45
1	A	1915	3TD	C6-N1	5.26	1.44	1.36
55	v	7	4SU	C4-S4	-4.99	1.59	1.68
57	y	8	4SU	C4-S4	-4.92	1.60	1.68
55	w	8	4SU	C4-S4	-4.89	1.60	1.68
1	A	2580	PSU	C6-C5	4.72	1.40	1.35
1	A	1917	PSU	C6-C5	4.44	1.40	1.35
1	A	1911	PSU	C6-C5	4.42	1.40	1.35
57	y	39	PSU	C6-C5	4.41	1.40	1.35
1	A	746	PSU	C6-C5	4.34	1.40	1.35
1	A	2605	PSU	C6-C5	4.32	1.40	1.35
1	A	2604	PSU	C6-C5	4.30	1.40	1.35
1	A	2504	PSU	C6-C5	4.27	1.40	1.35
57	y	55	PSU	C6-C5	4.26	1.40	1.35
1	A	955	PSU	C6-C5	4.26	1.40	1.35
1	A	2457	PSU	C6-C5	4.25	1.40	1.35
34	a	516	PSU	C6-C5	4.24	1.40	1.35
57	y	32	PSU	C6-C5	4.19	1.39	1.35
55	w	55	PSU	C6-C5	4.00	1.39	1.35
1	A	2069	7MG	C4-N9	-3.96	1.33	1.37
55	v	55	PSU	C6-C5	3.76	1.39	1.35
34	a	1518	MA6	C6-C5	3.57	1.50	1.44
57	y	46	7MG	C5-C4	3.50	1.48	1.37
55	v	54	5MU	C6-C5	3.44	1.40	1.34
1	A	745	1MG	C2-N1	3.44	1.43	1.37
34	a	527	7MG	C5-C4	3.43	1.48	1.37
34	a	1519	MA6	C6-C5	3.40	1.50	1.44
34	a	527	7MG	C4-N9	-3.34	1.33	1.37
1	A	1939	5MU	C6-C5	3.25	1.39	1.34
1	A	2069	7MG	C5-C4	3.24	1.47	1.37
57	y	46	7MG	C4-N9	-3.22	1.33	1.37
1	A	1962	5MC	C6-C5	3.20	1.39	1.34
57	y	8	4SU	C4-N3	-3.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	967	5MC	C6-C5	3.18	1.39	1.34
34	a	1407	5MC	C6-C5	3.13	1.39	1.34
55	w	54	5MU	C2-N1	3.12	1.43	1.38
55	w	54	5MU	C6-C5	3.11	1.39	1.34
55	w	8	4SU	C2-N1	3.06	1.43	1.38
57	y	54	5MU	C2-N1	3.05	1.43	1.38
1	A	1915	3TD	O2'-C2'	3.01	1.50	1.43
55	v	54	5MU	C4-N3	-2.98	1.33	1.38
55	w	8	4SU	C4-N3	-2.94	1.34	1.37
1	A	747	5MC	C6-C5	2.93	1.39	1.34
57	y	37	MIA	C6-C5	2.90	1.49	1.44
1	A	2552	OMU	C2-N1	2.89	1.43	1.38
55	v	7	4SU	C2-N1	2.88	1.43	1.38
57	y	8	4SU	C2-N1	2.86	1.42	1.38
57	y	54	5MU	C6-C5	2.84	1.39	1.34
34	a	1518	MA6	C6-N1	2.83	1.36	1.32
55	w	54	5MU	C4-C5	2.82	1.49	1.44
1	A	1939	5MU	C4-C5	2.79	1.49	1.44
1	A	1915	3TD	C4-N3	2.78	1.46	1.40
1	A	1915	3TD	C10-N3	-2.75	1.42	1.47
1	A	2552	OMU	C4-N3	-2.74	1.33	1.38
55	v	7	4SU	C4-N3	-2.68	1.34	1.37
34	a	1519	MA6	C6-N1	2.67	1.36	1.32
34	a	1498	UR3	C2-N1	2.65	1.42	1.38
34	a	966	2MG	O4'-C1'	2.64	1.44	1.40
1	A	1939	5MU	C2-N1	2.62	1.42	1.38
1	A	1915	3TD	O2-C2	-2.59	1.18	1.23
1	A	1618	6MZ	C6-C5	2.53	1.48	1.44
1	A	2580	PSU	C4-N3	-2.53	1.34	1.38
34	a	1518	MA6	C6-N6	2.52	1.43	1.37
1	A	1835	2MG	O4'-C1'	2.52	1.44	1.40
57	y	37	MIA	C6-N1	2.52	1.36	1.33
57	y	8	4SU	C5-C4	-2.52	1.39	1.42
55	v	7	4SU	C5-C4	-2.51	1.39	1.42
1	A	2030	6MZ	C6-C5	2.48	1.48	1.44
1	A	1915	3TD	O3'-C3'	-2.46	1.36	1.43
57	y	54	5MU	C4-C5	2.45	1.48	1.44
1	A	2457	PSU	C4-N3	-2.44	1.34	1.38
34	a	1519	MA6	C6-N6	2.43	1.43	1.37
1	A	2604	PSU	C4-N3	-2.42	1.34	1.38
1	A	2504	PSU	C4-N3	-2.42	1.34	1.38
57	y	37	MIA	O4'-C1'	2.41	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	8	4SU	C5-C4	-2.41	1.39	1.42
1	A	2449	H2U	C2-N3	-2.40	1.33	1.38
55	v	55	PSU	C4-N3	-2.40	1.34	1.38
1	A	1917	PSU	C4-N3	-2.39	1.34	1.38
1	A	2503	2MA	C2-N3	2.38	1.36	1.31
1	A	1939	5MU	C4-N3	-2.38	1.34	1.38
1	A	2449	H2U	C4-N3	-2.35	1.33	1.37
1	A	2605	PSU	C4-N3	-2.33	1.34	1.38
55	v	54	5MU	C2-N3	-2.32	1.33	1.38
1	A	746	PSU	C4-N3	-2.32	1.34	1.38
57	y	55	PSU	C4-N3	-2.31	1.34	1.38
55	v	54	5MU	C4-C5	2.31	1.48	1.44
1	A	2251	OMG	O4'-C1'	2.29	1.43	1.40
55	w	54	5MU	C4-N3	-2.27	1.34	1.38
1	A	1915	3TD	C3'-C4'	2.26	1.58	1.53
57	y	54	5MU	C4-N3	-2.25	1.34	1.38
34	a	1519	MA6	O4'-C1'	2.25	1.43	1.40
57	y	32	PSU	C4-N3	-2.25	1.34	1.38
34	a	516	PSU	C4-N3	-2.23	1.34	1.38
57	y	39	PSU	C4-N3	-2.22	1.34	1.38
55	w	55	PSU	C4-N3	-2.19	1.34	1.38
1	A	1915	3TD	O4-C4	-2.18	1.18	1.23
1	A	745	1MG	O4'-C1'	2.18	1.43	1.40
34	a	1516	2MG	O4'-C1'	2.18	1.43	1.40
34	a	1518	MA6	O4'-C1'	2.16	1.43	1.40
57	y	20	H2U	C2-N3	-2.16	1.34	1.38
1	A	1835	2MG	C6-N1	-2.15	1.34	1.37
1	A	955	PSU	C4-N3	-2.13	1.34	1.38
1	A	2445	2MG	O4'-C1'	2.12	1.43	1.40
1	A	2251	OMG	C6-N1	-2.12	1.34	1.37
1	A	1911	PSU	C4-N3	-2.12	1.34	1.38
57	y	8	4SU	C6-C5	2.09	1.39	1.35
57	y	16	H2U	C2-N3	-2.08	1.34	1.38
55	v	20	H2U	C2-N3	-2.08	1.34	1.38
1	A	2552	OMU	C6-C5	2.06	1.39	1.35
57	y	46	7MG	C5-C6	2.06	1.48	1.43
34	a	1402	4OC	C6-C5	2.05	1.39	1.35
34	a	1207	2MG	O4'-C1'	2.04	1.43	1.40
55	w	8	4SU	C6-C5	2.04	1.39	1.35
34	a	1402	4OC	C4-N3	2.02	1.36	1.32
55	w	20	H2U	C2-N3	-2.02	1.34	1.38
1	A	1618	6MZ	O4'-C1'	2.02	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	1MG	C2-N3	2.02	1.37	1.33
1	A	2503	2MA	C6-N6	2.02	1.35	1.27
1	A	2030	6MZ	O4'-C1'	2.00	1.43	1.40

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.12	137.35	125.46
57	y	46	7MG	N9-C4-N3	8.09	137.32	125.46
34	a	1207	2MG	N1-C2-N2	7.72	124.44	116.56
57	y	37	MIA	C12-C13-C14	-7.51	113.53	127.01
1	A	2069	7MG	N9-C4-N3	7.39	136.29	125.46
34	a	1518	MA6	C2-N1-C6	7.17	123.87	116.84
34	a	1498	UR3	C4-N3-C2	-6.94	119.00	124.58
34	a	1519	MA6	C2-N1-C6	6.62	123.33	116.84
1	A	2030	6MZ	C2-N1-C6	6.59	121.71	116.60
1	A	1618	6MZ	C2-N1-C6	6.58	121.71	116.60
55	v	7	4SU	C4-N3-C2	-6.50	121.08	127.31
57	y	8	4SU	C4-N3-C2	-6.49	121.09	127.31
1	A	2504	PSU	N1-C2-N3	6.25	121.77	115.17
55	w	55	PSU	N1-C2-N3	6.18	121.69	115.17
1	A	1911	PSU	N1-C2-N3	6.17	121.68	115.17
55	w	8	4SU	C4-N3-C2	-6.12	121.45	127.31
1	A	746	PSU	N1-C2-N3	6.11	121.61	115.17
57	y	32	PSU	N1-C2-N3	6.08	121.58	115.17
57	y	39	PSU	N1-C2-N3	6.07	121.57	115.17
1	A	955	PSU	N1-C2-N3	6.05	121.55	115.17
57	y	55	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	2457	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	2605	PSU	N1-C2-N3	5.98	121.48	115.17
1	A	2580	PSU	N1-C2-N3	5.96	121.46	115.17
1	A	2604	PSU	N1-C2-N3	5.96	121.45	115.17
34	a	516	PSU	N1-C2-N3	5.94	121.44	115.17
1	A	1917	PSU	N1-C2-N3	5.94	121.43	115.17
55	v	54	5MU	N3-C2-N1	5.92	122.60	114.89
55	v	55	PSU	N1-C2-N3	5.87	121.36	115.17
55	v	20	H2U	O4'-C1'-N1	5.64	116.99	109.30
34	a	966	2MG	N1-C2-N2	5.60	122.28	116.56
55	v	7	4SU	C5-C4-N3	5.38	119.75	114.75
1	A	1915	3TD	N1-C2-N3	5.35	120.02	116.13
57	y	8	4SU	N3-C2-N1	5.23	121.70	114.89
34	a	1207	2MG	N2-C2-N3	-5.21	113.88	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1939	5MU	N3-C2-N1	5.20	121.66	114.89
55	w	8	4SU	C5-C4-N3	5.16	119.55	114.75
34	a	527	7MG	C5-C4-N3	-5.11	118.54	128.13
57	y	8	4SU	C5-C4-N3	5.09	119.48	114.75
1	A	1915	3TD	C4-N3-C2	-5.05	119.27	124.61
57	y	46	7MG	C5-C4-N3	-5.04	118.67	128.13
1	A	2069	7MG	C5-C4-N3	-4.91	118.92	128.13
55	w	54	5MU	N3-C2-N1	4.90	121.28	114.89
1	A	2069	7MG	C2-N3-C4	4.86	120.67	112.30
1	A	2552	OMU	N3-C2-N1	4.79	121.13	114.89
1	A	1939	5MU	C4-N3-C2	-4.74	121.13	127.34
1	A	2069	7MG	N9-C8-N7	-4.65	96.79	103.37
1	A	2552	OMU	C4-N3-C2	-4.63	120.86	126.61
57	y	54	5MU	N3-C2-N1	4.60	120.88	114.89
57	y	46	7MG	C2-N3-C4	4.60	120.22	112.30
34	a	527	7MG	C2-N3-C4	4.57	120.17	112.30
55	v	7	4SU	C5-C4-S4	-4.56	119.10	124.31
55	w	8	4SU	N3-C2-N1	4.55	120.82	114.89
55	w	20	H2U	O4'-C1'-N1	4.55	115.50	109.30
1	A	1911	PSU	O2-C2-N1	-4.53	118.12	122.79
57	y	46	7MG	N9-C8-N7	-4.51	96.99	103.37
55	v	7	4SU	N3-C2-N1	4.50	120.75	114.89
57	y	37	MIA	C16-C14-C13	-4.48	109.21	122.66
34	a	1518	MA6	N3-C2-N1	-4.44	122.65	128.67
55	w	54	5MU	C4-N3-C2	-4.43	121.53	127.34
34	a	527	7MG	N9-C8-N7	-4.41	97.13	103.37
57	y	54	5MU	C4-N3-C2	-4.38	121.59	127.34
55	v	54	5MU	C4-N3-C2	-4.16	121.88	127.34
57	y	54	5MU	C5-C4-N3	4.15	118.93	115.32
1	A	2605	PSU	C4-N3-C2	-4.12	120.69	126.37
1	A	2449	H2U	N3-C2-N1	4.12	120.79	116.65
1	A	1939	5MU	C5-C4-N3	4.11	118.90	115.32
34	a	1519	MA6	C4-C5-N7	-4.11	105.00	109.34
1	A	1915	3TD	C1'-C5-C4	4.10	123.84	117.61
57	y	55	PSU	C4-N3-C2	-4.09	120.73	126.37
55	w	54	5MU	C5-C4-N3	4.06	118.85	115.32
34	a	1518	MA6	O4'-C1'-N9	4.02	114.08	108.75
1	A	747	5MC	CM5-C5-C6	-3.98	117.46	122.85
1	A	2504	PSU	C4-N3-C2	-3.93	120.96	126.37
1	A	1911	PSU	C4-N3-C2	-3.91	120.99	126.37
1	A	955	PSU	C4-N3-C2	-3.90	120.99	126.37
55	w	55	PSU	C4-N3-C2	-3.89	121.02	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	967	5MC	CM5-C5-C6	-3.89	117.59	122.85
57	y	54	5MU	O4-C4-C5	-3.85	120.51	124.92
34	a	516	PSU	C4-N3-C2	-3.84	121.08	126.37
57	y	32	PSU	C4-N3-C2	-3.83	121.09	126.37
57	y	39	PSU	C4-N3-C2	-3.82	121.11	126.37
34	a	1407	5MC	CM5-C5-C6	-3.80	117.70	122.85
1	A	746	PSU	C4-N3-C2	-3.78	121.16	126.37
34	a	1519	MA6	N3-C2-N1	-3.78	123.54	128.67
57	y	37	MIA	O4'-C1'-N9	3.78	113.76	108.75
34	a	1407	5MC	C5-C4-N3	-3.75	117.91	121.75
1	A	2457	PSU	C4-N3-C2	-3.75	121.21	126.37
55	w	8	4SU	C5-C4-S4	-3.71	120.07	124.31
1	A	2580	PSU	C6-C5-C4	-3.71	115.67	118.17
1	A	2449	H2U	O4'-C1'-N1	3.71	114.35	109.30
1	A	955	PSU	O2-C2-N1	-3.71	118.97	122.79
1	A	2030	6MZ	N3-C2-N1	-3.68	123.68	128.67
1	A	1618	6MZ	N3-C2-N1	-3.64	123.73	128.67
1	A	1917	PSU	C4-N3-C2	-3.63	121.37	126.37
55	v	55	PSU	C4-N3-C2	-3.61	121.40	126.37
1	A	1962	5MC	C5-C4-N3	-3.59	118.07	121.75
1	A	747	5MC	C5-C4-N3	-3.59	118.07	121.75
34	a	1498	UR3	C1'-N1-C2	3.59	122.91	117.04
1	A	2552	OMU	C5-C4-N3	3.59	119.82	114.80
55	v	55	PSU	C6-C5-C4	-3.58	115.76	118.17
1	A	1962	5MC	CM5-C5-C6	-3.58	118.00	122.85
55	w	55	PSU	O2-C2-N1	-3.57	119.11	122.79
57	y	8	4SU	C5-C4-S4	-3.57	120.23	124.31
1	A	2604	PSU	C4-N3-C2	-3.56	121.46	126.37
1	A	955	PSU	C6-C5-C4	-3.56	115.77	118.17
1	A	2449	H2U	C5-C4-N3	3.56	120.48	116.69
1	A	1917	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A	2504	PSU	O2-C2-N1	-3.52	119.16	122.79
57	y	39	PSU	O2-C2-N1	-3.52	119.16	122.79
34	a	967	5MC	C5-C4-N3	-3.51	118.16	121.75
34	a	516	PSU	O2-C2-N1	-3.49	119.19	122.79
1	A	2605	PSU	O2-C2-N1	-3.47	119.21	122.79
57	y	37	MIA	C15-C14-C13	-3.46	112.28	122.66
57	y	32	PSU	O2-C2-N1	-3.45	119.23	122.79
1	A	745	1MG	N2-C2-N1	3.45	121.56	118.79
1	A	2580	PSU	C4-N3-C2	-3.42	121.66	126.37
34	a	1518	MA6	C4-C5-N7	-3.41	105.73	109.34
1	A	2457	PSU	O2-C2-N1	-3.41	119.28	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	55	PSU	O2-C2-N1	-3.40	119.28	122.79
34	a	966	2MG	N2-C2-N3	-3.40	116.19	120.51
34	a	1498	UR3	C5-C4-N3	3.39	119.50	115.04
1	A	2445	2MG	N1-C2-N2	3.38	120.01	116.56
57	y	8	4SU	C6-N1-C2	-3.38	116.89	121.00
57	y	54	5MU	C5M-C5-C4	3.36	122.37	118.78
1	A	746	PSU	O2-C2-N1	-3.36	119.33	122.79
34	a	516	PSU	C3'-C2'-C1'	3.35	105.64	101.69
1	A	2604	PSU	O2-C2-N1	-3.34	119.34	122.79
55	w	54	5MU	C5M-C5-C4	3.32	122.33	118.78
55	v	55	PSU	O2-C2-N1	-3.24	119.44	122.79
1	A	1917	PSU	C6-C5-C4	-3.24	115.98	118.17
1	A	745	1MG	O6-C6-C5	-3.24	118.85	124.18
57	y	37	MIA	C2-N1-C6	3.24	123.18	117.42
1	A	2605	PSU	C6-C5-C4	-3.21	116.00	118.17
1	A	1939	5MU	O4-C4-C5	-3.21	121.25	124.92
1	A	1911	PSU	C6-C5-C4	-3.17	116.03	118.17
1	A	2580	PSU	C3'-C2'-C1'	3.15	105.40	101.69
55	w	54	5MU	O4-C4-C5	-3.15	121.32	124.92
55	v	54	5MU	C5-C4-N3	3.15	118.06	115.32
1	A	1962	5MC	O2-C2-N3	-3.13	117.40	122.33
1	A	2552	OMU	C1'-N1-C2	3.10	123.15	117.59
34	a	966	2MG	C8-N7-C5	3.07	107.78	102.55
1	A	2503	2MA	C8-N7-C5	3.06	107.75	102.55
1	A	1618	6MZ	C9-N6-C6	-3.05	120.02	122.85
34	a	1207	2MG	C8-N7-C5	3.04	107.73	102.55
1	A	2445	2MG	C8-N7-C5	3.04	107.73	102.55
57	y	37	MIA	C4-C5-N7	-3.04	106.13	109.34
1	A	2030	6MZ	C9-N6-C6	-3.04	120.03	122.85
34	a	1516	2MG	N1-C2-N2	3.03	119.65	116.56
34	a	1516	2MG	C8-N7-C5	3.03	107.70	102.55
57	y	55	PSU	C6-C5-C4	-3.02	116.14	118.17
34	a	1407	5MC	O2-C2-N3	-3.02	117.58	122.33
1	A	745	1MG	C8-N7-C5	3.01	107.67	102.55
1	A	2069	7MG	C5-C6-N1	3.01	116.24	110.94
1	A	2498	OMC	O2-C2-N3	-3.00	117.60	122.33
55	v	54	5MU	C6-N1-C2	-2.97	118.35	121.30
34	a	527	7MG	C5-C6-N1	2.96	116.14	110.94
34	a	516	PSU	C6-C5-C4	-2.95	116.18	118.17
34	a	967	5MC	O2-C2-N3	-2.94	117.69	122.33
57	y	46	7MG	C5-C6-N1	2.92	116.08	110.94
55	w	55	PSU	C3'-C2'-C1'	2.92	105.13	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	745	1MG	C5-C6-N1	2.91	118.16	113.96
34	a	1519	MA6	C10-N6-C6	-2.90	111.41	119.40
55	w	20	H2U	C5-C6-N1	-2.88	102.80	111.52
34	a	1519	MA6	O4'-C1'-N9	2.86	112.54	108.75
1	A	2504	PSU	C6-C5-C4	-2.86	116.24	118.17
57	y	37	MIA	N3-C2-N1	-2.84	121.83	127.03
57	y	20	H2U	C3'-C2'-C1'	2.82	106.79	101.46
1	A	2552	OMU	O4-C4-C5	-2.79	120.34	125.16
1	A	1835	2MG	C8-N7-C5	2.78	107.28	102.55
1	A	1939	5MU	C5-C6-N1	-2.76	120.32	123.31
34	a	1402	4OC	C6-C5-C4	2.76	120.32	117.00
55	w	8	4SU	C6-N1-C2	-2.75	117.65	121.00
34	a	1518	MA6	C9-N6-C6	-2.75	111.82	119.40
1	A	1917	PSU	C3'-C2'-C1'	2.73	104.91	101.69
1	A	2457	PSU	C6-C5-C4	-2.72	116.34	118.17
1	A	2580	PSU	O2-C2-N1	-2.70	120.00	122.79
57	y	20	H2U	C5-C4-N3	2.70	119.56	116.69
1	A	2503	2MA	C4-N3-C2	-2.68	121.24	123.30
57	y	20	H2U	O4'-C1'-N1	2.64	112.90	109.30
1	A	2030	6MZ	C4-C5-N7	-2.62	106.57	109.34
55	v	20	H2U	C5-C4-N3	2.59	119.44	116.69
1	A	2251	OMG	C8-N7-C5	2.58	106.94	102.55
1	A	1618	6MZ	C4-C5-N7	-2.58	106.61	109.34
57	y	39	PSU	C6-C5-C4	-2.57	116.44	118.17
57	y	16	H2U	C5-C4-N3	2.56	119.41	116.69
1	A	745	1MG	O4'-C1'-N9	2.55	112.13	108.75
1	A	2498	OMC	O4'-C1'-N1	2.55	114.14	108.36
1	A	1915	3TD	C10-N3-C4	2.55	121.60	117.64
34	a	1402	4OC	C5-C4-N3	-2.54	118.63	122.60
57	y	8	4SU	O2-C2-N3	-2.53	116.83	121.49
57	y	32	PSU	C6-C5-C4	-2.52	116.47	118.17
34	a	966	2MG	C5-C6-N1	2.52	118.88	114.07
1	A	746	PSU	C6-C5-C4	-2.50	116.49	118.17
1	A	747	5MC	C5-C6-N1	-2.49	120.61	123.31
1	A	1915	3TD	C3'-C2'-C1'	2.49	104.63	101.69
1	A	1939	5MU	C5M-C5-C4	2.49	121.44	118.78
57	y	32	PSU	C3'-C2'-C1'	2.49	104.62	101.69
1	A	2552	OMU	C6-N1-C2	-2.48	117.98	121.00
55	v	7	4SU	C6-N1-C2	-2.48	117.98	121.00
34	a	1207	2MG	C5-C6-N1	2.47	118.78	114.07
34	a	1516	2MG	O4'-C1'-N9	2.46	112.01	108.75
34	a	1407	5MC	O4'-C1'-N1	2.45	113.91	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	54	5MU	O4-C4-C5	-2.44	122.13	124.92
34	a	1498	UR3	C3U-N3-C2	2.42	121.55	117.33
1	A	2604	PSU	C6-C5-C4	-2.41	116.55	118.17
1	A	2552	OMU	O4'-C1'-N1	2.40	113.81	108.36
1	A	2552	OMU	O2-C2-N3	-2.39	117.07	121.49
57	y	16	H2U	O4'-C1'-N1	2.38	112.55	109.30
55	v	54	5MU	C5-C6-N1	-2.38	120.72	123.31
34	a	967	5MC	CM5-C5-C4	2.38	124.42	120.51
34	a	1402	4OC	O4'-C1'-N1	2.37	113.74	108.36
34	a	1402	4OC	O2-C2-N3	-2.37	118.59	122.33
1	A	2445	2MG	C5-C6-N1	2.35	118.56	114.07
55	v	54	5MU	O2-C2-N1	-2.35	119.74	122.80
34	a	1519	MA6	C10-N6-C9	-2.34	108.65	116.18
34	a	1498	UR3	C6-N1-C2	-2.34	119.89	121.80
1	A	2552	OMU	C2'-C1'-N1	-2.33	109.81	114.24
34	a	527	7MG	O4'-C1'-N9	2.33	112.47	109.30
55	w	54	5MU	C5M-C5-C6	-2.32	119.70	122.85
1	A	2069	7MG	O4'-C1'-N9	2.31	112.45	109.30
1	A	2503	2MA	C5-C6-N1	2.29	118.39	114.12
1	A	2069	7MG	C6-C5-C4	-2.27	118.40	122.40
1	A	1835	2MG	C5-C6-N1	2.27	118.41	114.07
1	A	2069	7MG	O6-C6-C5	-2.25	122.09	127.62
1	A	1939	5MU	O2-C2-N1	-2.23	119.89	122.80
57	y	54	5MU	C5M-C5-C6	-2.23	119.83	122.85
34	a	966	2MG	C4'-O4'-C1'	2.23	111.96	109.92
1	A	2069	7MG	N2-C2-N1	2.21	121.43	116.76
34	a	1516	2MG	C5-C6-N1	2.20	118.28	114.07
34	a	527	7MG	O6-C6-C5	-2.20	122.22	127.62
55	w	54	5MU	O4'-C1'-N1	2.19	113.33	108.36
1	A	1939	5MU	O4'-C1'-N1	2.19	113.32	108.36
55	w	54	5MU	C3'-C2'-C1'	2.17	105.57	101.46
34	a	1407	5MC	CM5-C5-C4	2.17	124.07	120.51
1	A	747	5MC	O2-C2-N3	-2.17	118.91	122.33
55	v	55	PSU	C3'-C2'-C1'	2.15	104.22	101.69
57	y	16	H2U	C5-C6-N1	-2.15	105.03	111.52
57	y	55	PSU	C3'-C2'-C1'	2.14	104.22	101.69
57	y	20	H2U	C5-C6-N1	-2.14	105.05	111.52
1	A	2457	PSU	C3'-C2'-C1'	2.13	104.21	101.69
57	y	46	7MG	C6-C5-C4	-2.13	118.66	122.40
57	y	16	H2U	C3'-C2'-C1'	2.13	105.49	101.46
34	a	1207	2MG	O6-C6-C5	-2.13	120.10	124.32
57	y	54	5MU	C1'-N1-C2	2.13	121.41	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	967	5MC	C3'-C2'-C1'	2.12	105.48	101.46
55	v	7	4SU	O4'-C1'-N1	2.12	113.16	108.36
57	y	8	4SU	C1'-N1-C2	2.11	121.39	117.59
1	A	1618	6MZ	C4'-O4'-C1'	2.10	111.85	109.92
1	A	1962	5MC	CM5-C5-C4	2.10	123.96	120.51
1	A	2449	H2U	O4-C4-C5	-2.10	117.91	122.20
55	w	54	5MU	C5-C6-N1	-2.10	121.04	123.31
1	A	747	5MC	O4'-C1'-N1	2.09	113.09	108.36
1	A	2030	6MZ	C4'-O4'-C1'	2.08	111.83	109.92
57	y	46	7MG	O6-C6-C5	-2.08	122.52	127.62
55	v	54	5MU	O2-C2-N3	-2.07	117.66	121.49
55	w	55	PSU	C6-C5-C4	-2.07	116.78	118.17
55	w	54	5MU	O2-C2-N3	-2.07	117.68	121.49
1	A	2069	7MG	N2-C2-N3	-2.06	115.65	119.67
55	v	20	H2U	C5-C6-N1	-2.04	105.35	111.52
1	A	2251	OMG	C5-C6-N1	2.04	117.95	114.07
1	A	2069	7MG	C6-C5-N7	2.04	135.09	131.93

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
34	a	1519	MA6	N1-C6-N6-C10
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	O4'-C4'-C5'-O5'
57	y	20	H2U	O4'-C1'-N1-C2
57	y	20	H2U	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
57	y	37	MIA	O4'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
55	w	8	4SU	C3'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
57	y	37	MIA	C3'-C4'-C5'-O5'
34	a	1518	MA6	N1-C6-N6-C9
55	w	8	4SU	C2'-C1'-N1-C6
1	A	1917	PSU	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
57	y	37	MIA	C12-C13-C14-C16
55	v	7	4SU	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C2
57	y	46	7MG	C2'-C1'-N9-C8
34	a	527	7MG	C3'-C4'-C5'-O5'
55	v	54	5MU	C3'-C4'-C5'-O5'
34	a	1207	2MG	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
34	a	1518	MA6	C5-C6-N6-C10
55	w	8	4SU	O4'-C1'-N1-C2
34	a	527	7MG	C4'-C5'-O5'-P
34	a	516	PSU	O4'-C1'-C5-C4
57	y	32	PSU	O4'-C1'-C5-C4
55	w	20	H2U	C2'-C1'-N1-C6
1	A	1939	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	2457	PSU	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
55	w	55	PSU	O4'-C1'-C5-C6
57	y	32	PSU	O4'-C1'-C5-C6
57	y	46	7MG	O4'-C1'-N9-C8
57	y	8	4SU	C2'-C1'-N1-C2
1	A	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1912 ligands modelled in this entry, 1909 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	FME	A	3001	-	8,9,10	0.63	0	8,9,11	1.92	2 (25%)
63	GNP	z	402	60	29,34,34	2.58	6 (20%)	33,54,54	1.93	9 (27%)
62	PHE	z	401	-	10,11,12	0.45	0	8,13,15	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	A	3001	-	-	2/7/9/11	-
63	GNP	z	402	60	-	2/14/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	10.09	1.61	1.46
63	z	402	GNP	C5-C6	4.46	1.49	1.41
63	z	402	GNP	PG-N3B	4.42	1.74	1.63
63	z	402	GNP	PB-N3B	4.23	1.74	1.63
63	z	402	GNP	PG-O2G	-3.25	1.48	1.56
63	z	402	GNP	O4'-C1'	2.02	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GNP	C2-N3-C4	5.32	121.22	115.48
63	z	402	GNP	C2-N1-C6	4.14	121.71	115.96
59	A	3001	FME	C-CA-N	4.03	117.28	109.50
63	z	402	GNP	N3-C2-N1	-3.56	122.68	127.21
63	z	402	GNP	C5-C6-N1	-3.33	118.96	123.42
63	z	402	GNP	C4-C5-C6	-3.01	116.63	121.23
63	z	402	GNP	O4'-C1'-N9	2.85	112.53	108.75
63	z	402	GNP	O1B-PB-N3B	-2.84	107.58	111.77
63	z	402	GNP	C4-C5-N7	-2.55	106.64	109.34
59	A	3001	FME	O1-CN-N	-2.17	119.72	125.32
63	z	402	GNP	O3A-PB-N3B	2.04	112.24	106.59

There are no chirality outliers.

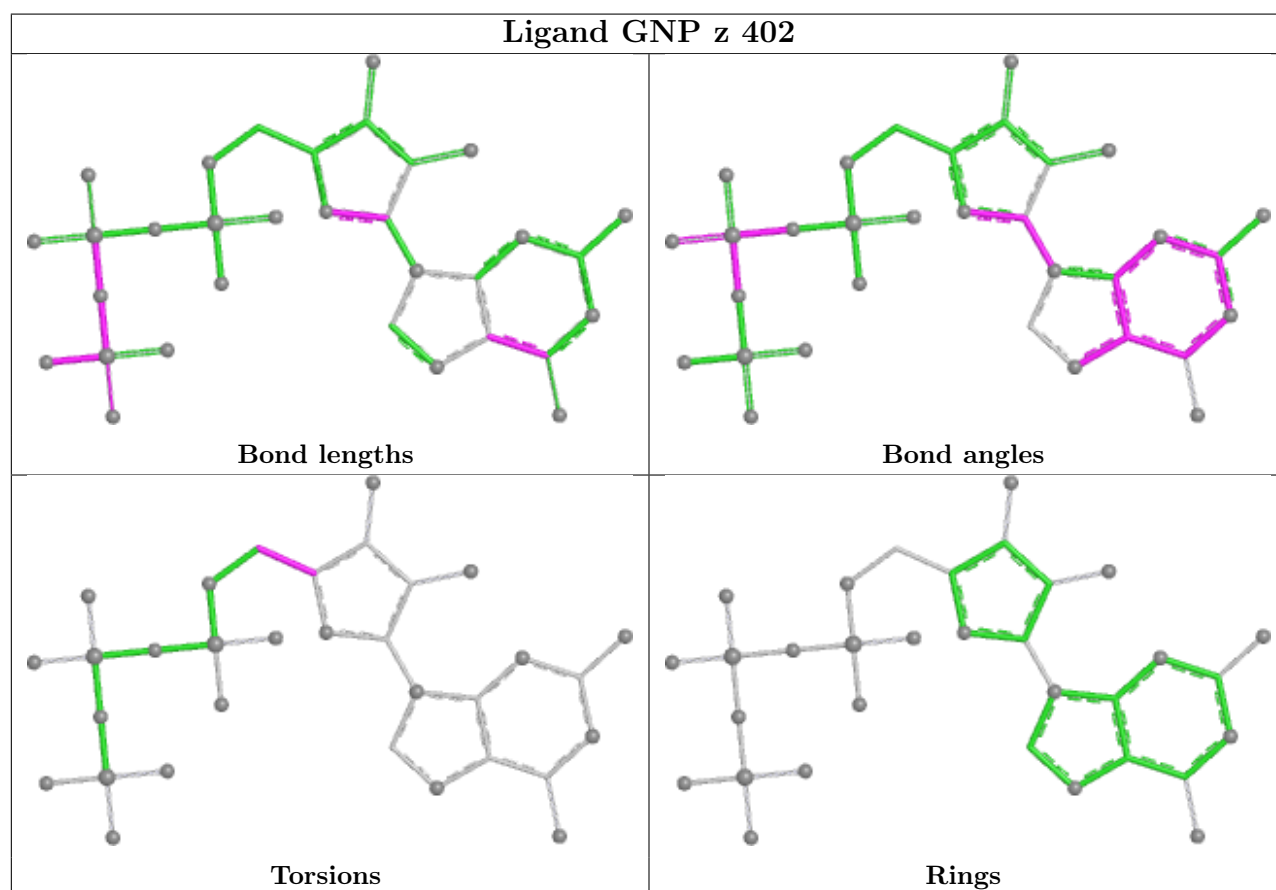
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB
63	z	402	GNP	O4'-C4'-C5'-O5'
63	z	402	GNP	C3'-C4'-C5'-O5'
59	A	3001	FME	CA-CB-CG-SD

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2030:6MZ	O3'	2031:A	P	2.28
1	A	1618:6MZ	O3'	1619:G	P	1.81

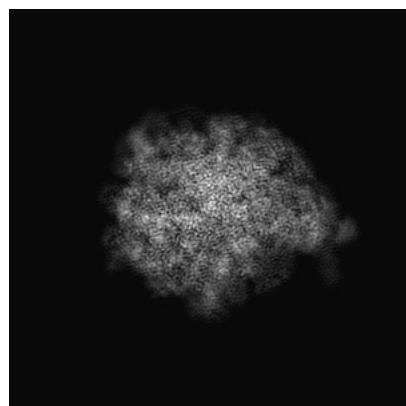
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8813. These allow visual inspection of the internal detail of the map and identification of artifacts.

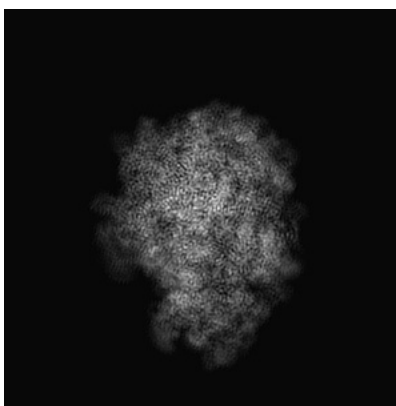
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

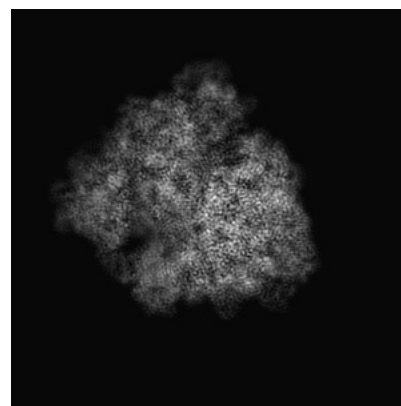
6.1.1 Primary map



X

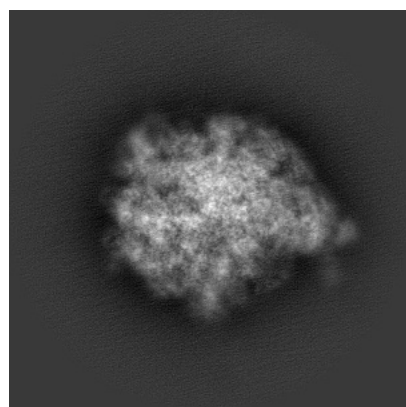


Y

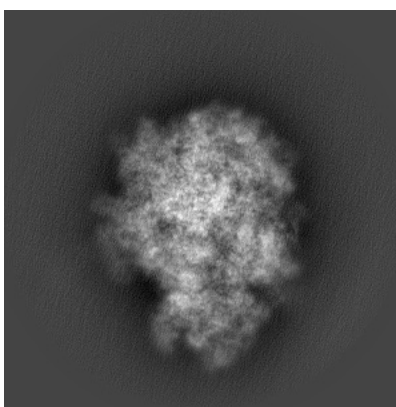


Z

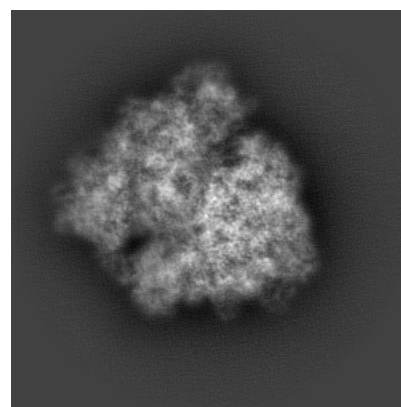
6.1.2 Raw map



X



Y

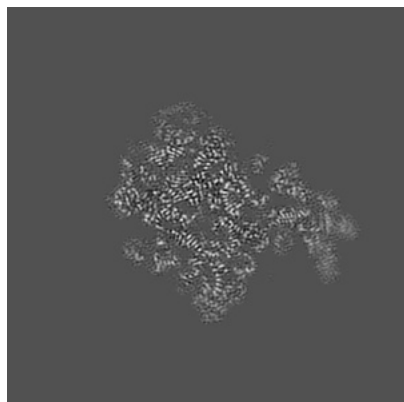


Z

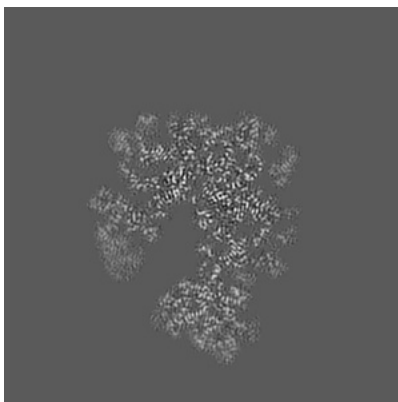
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

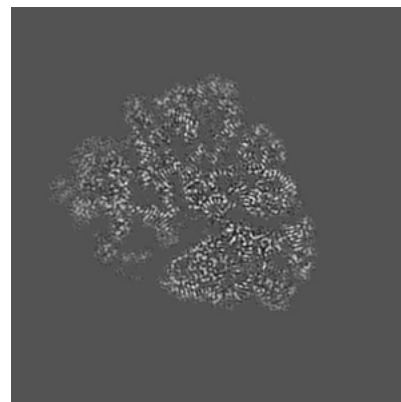
6.2.1 Primary map



X Index: 199

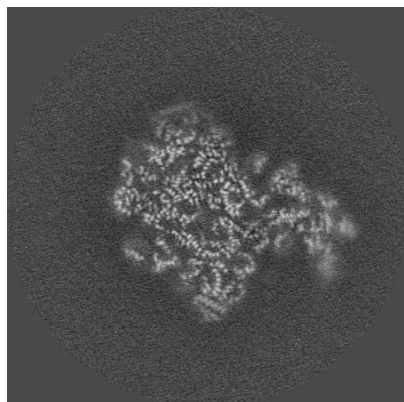


Y Index: 199

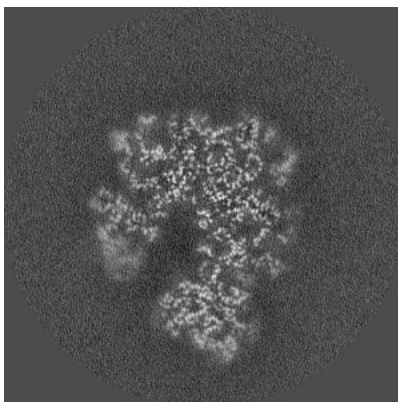


Z Index: 199

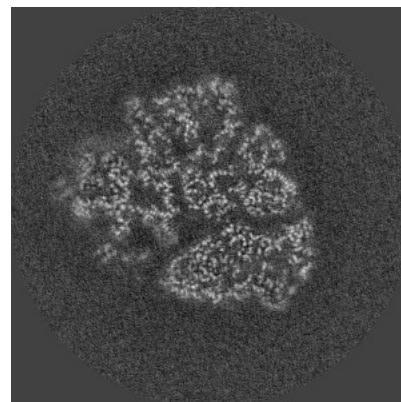
6.2.2 Raw map



X Index: 199



Y Index: 199

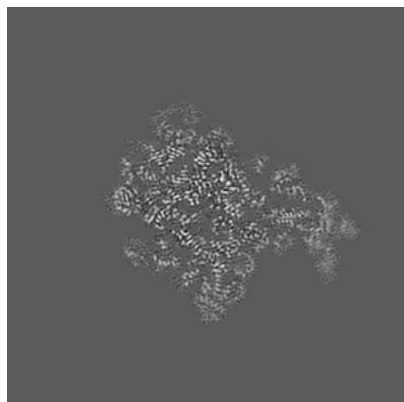


Z Index: 199

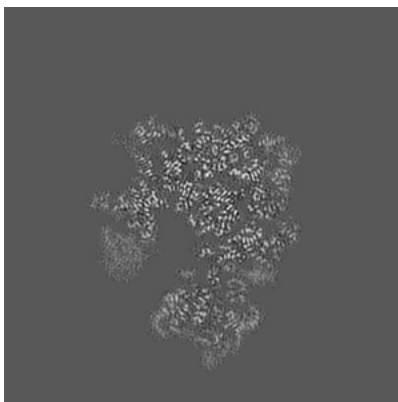
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

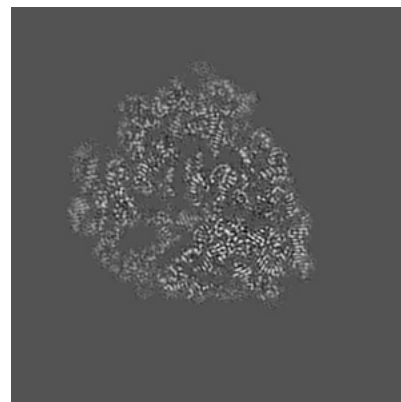
6.3.1 Primary map



X Index: 200

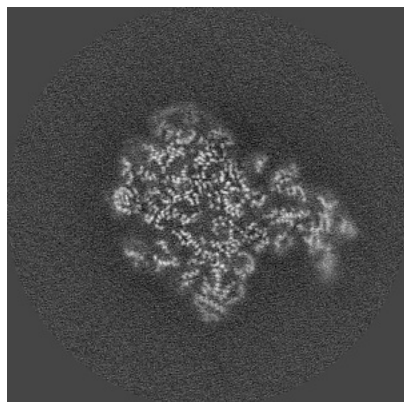


Y Index: 208

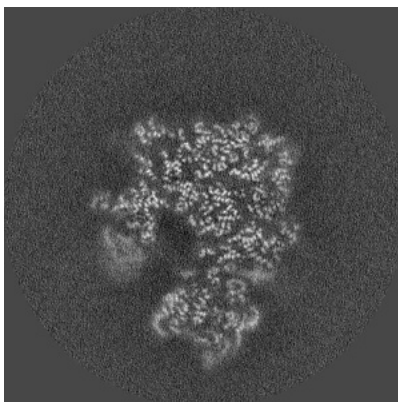


Z Index: 191

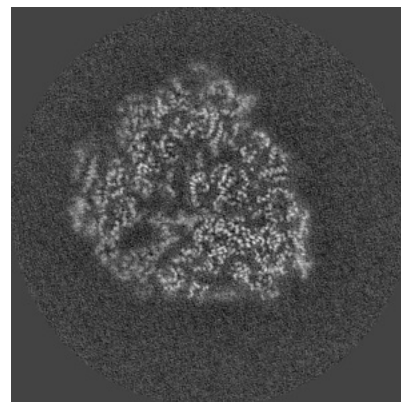
6.3.2 Raw map



X Index: 200



Y Index: 208

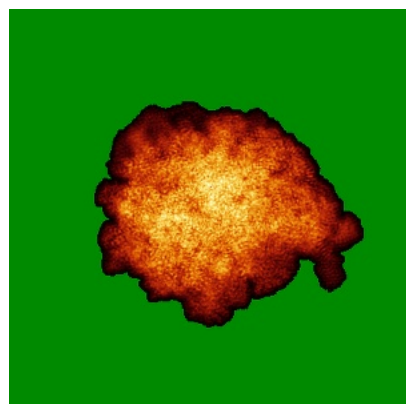


Z Index: 190

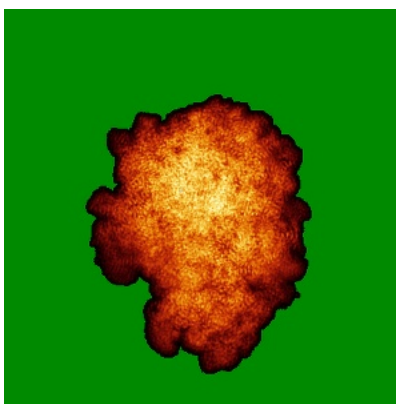
The images above show the largest variance slices of the map in three orthogonal directions.

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

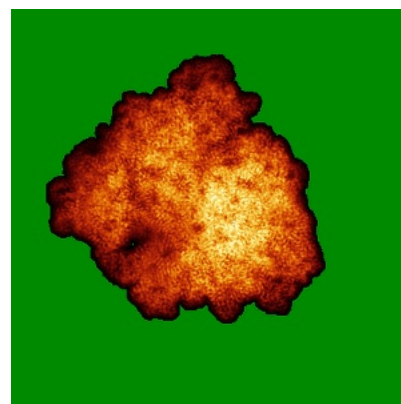
6.4.1 Primary map



X

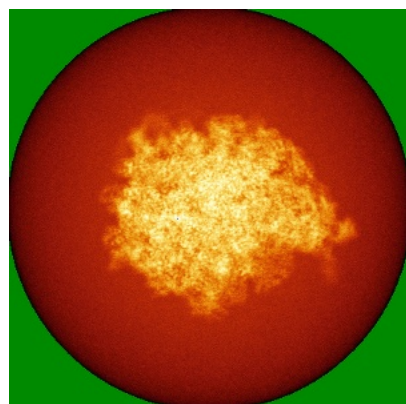


Y

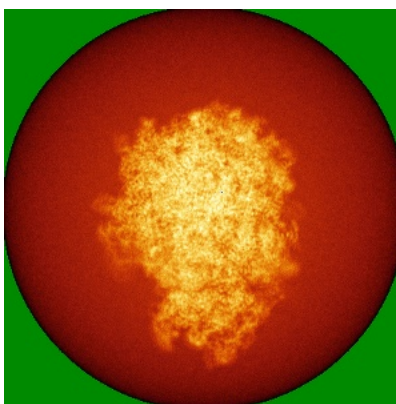


Z

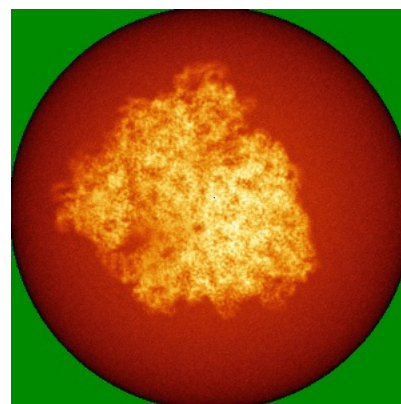
6.4.2 Raw map



X



Y



Z

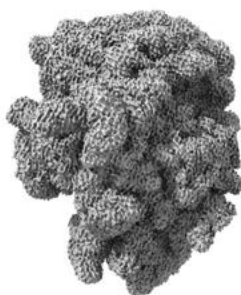
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

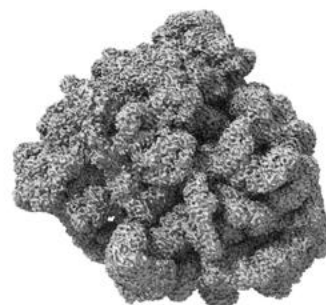
6.5.1 Primary map



X



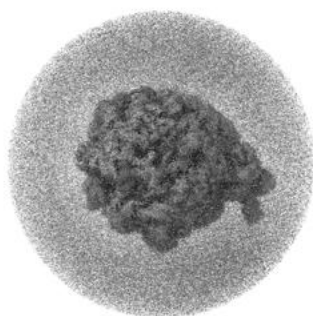
Y



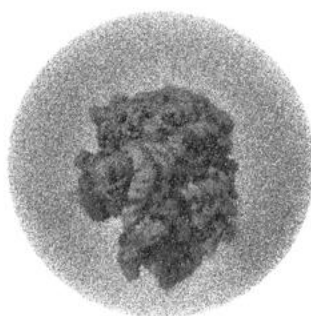
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00558. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

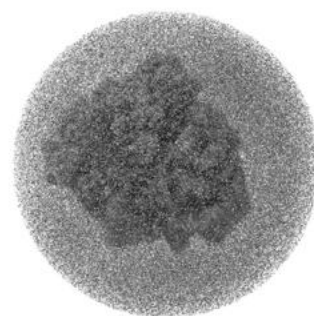
6.5.2 Raw map



X



Y



Z

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

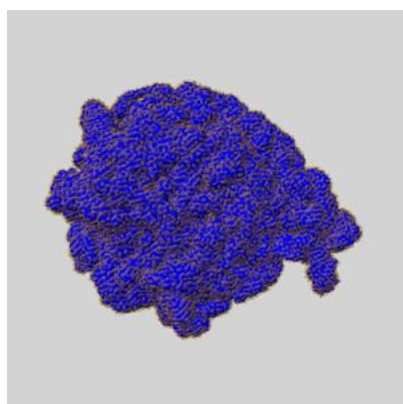
6.6 Mask visualisation [i](#)

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

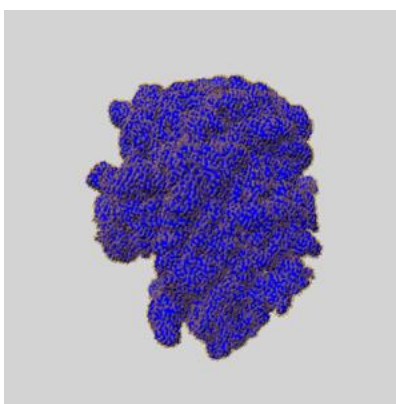
A mask typically either:

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

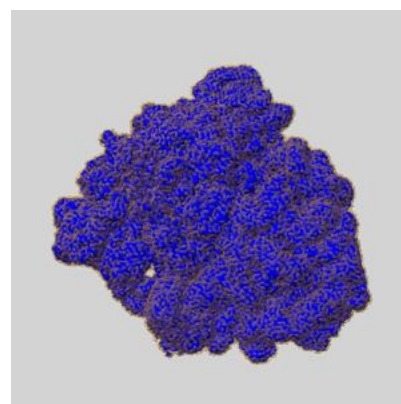
6.6.1 emd_8813_msk_1.map [i](#)



X



Y

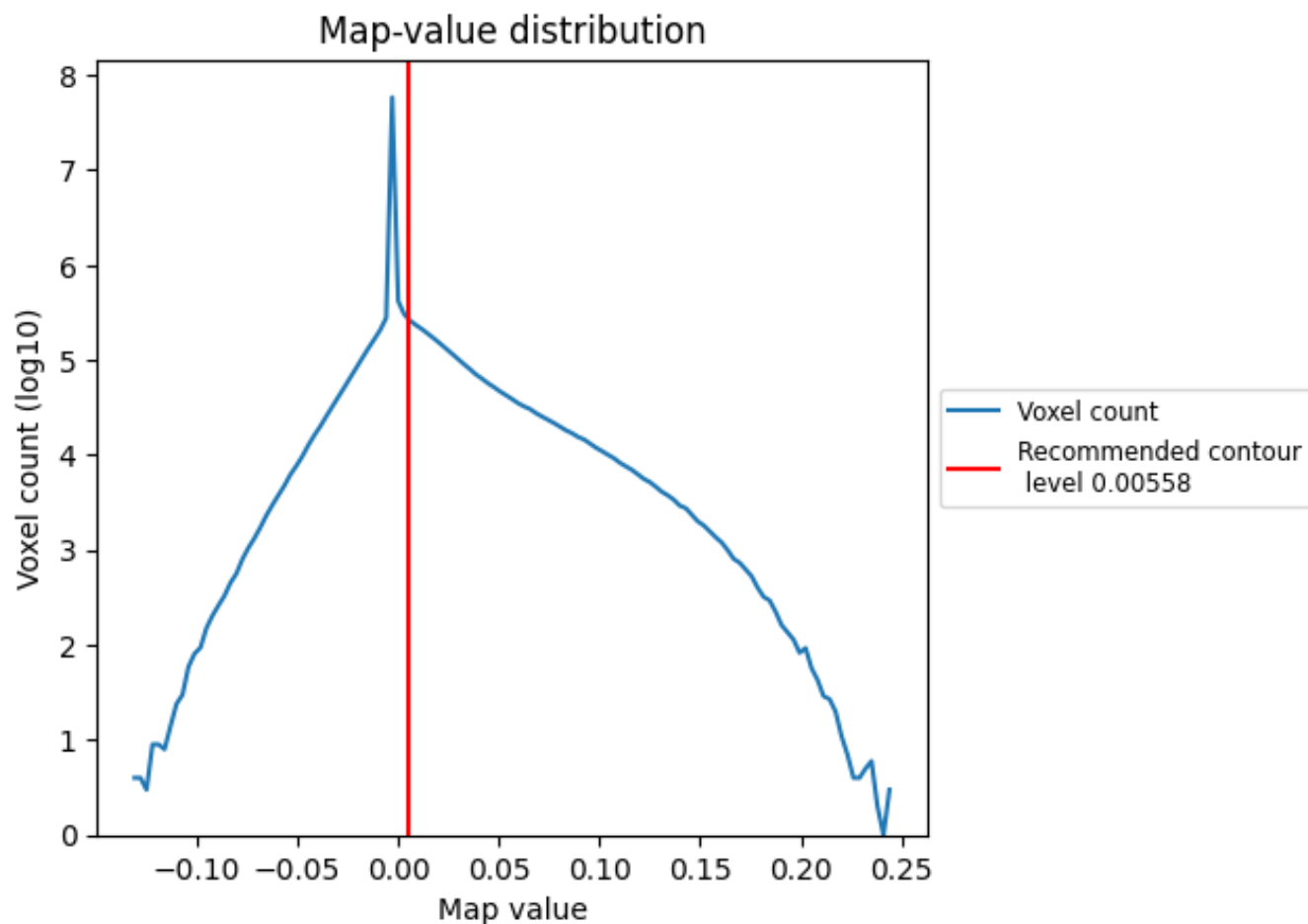


Z

7 Map analysis [i](#)

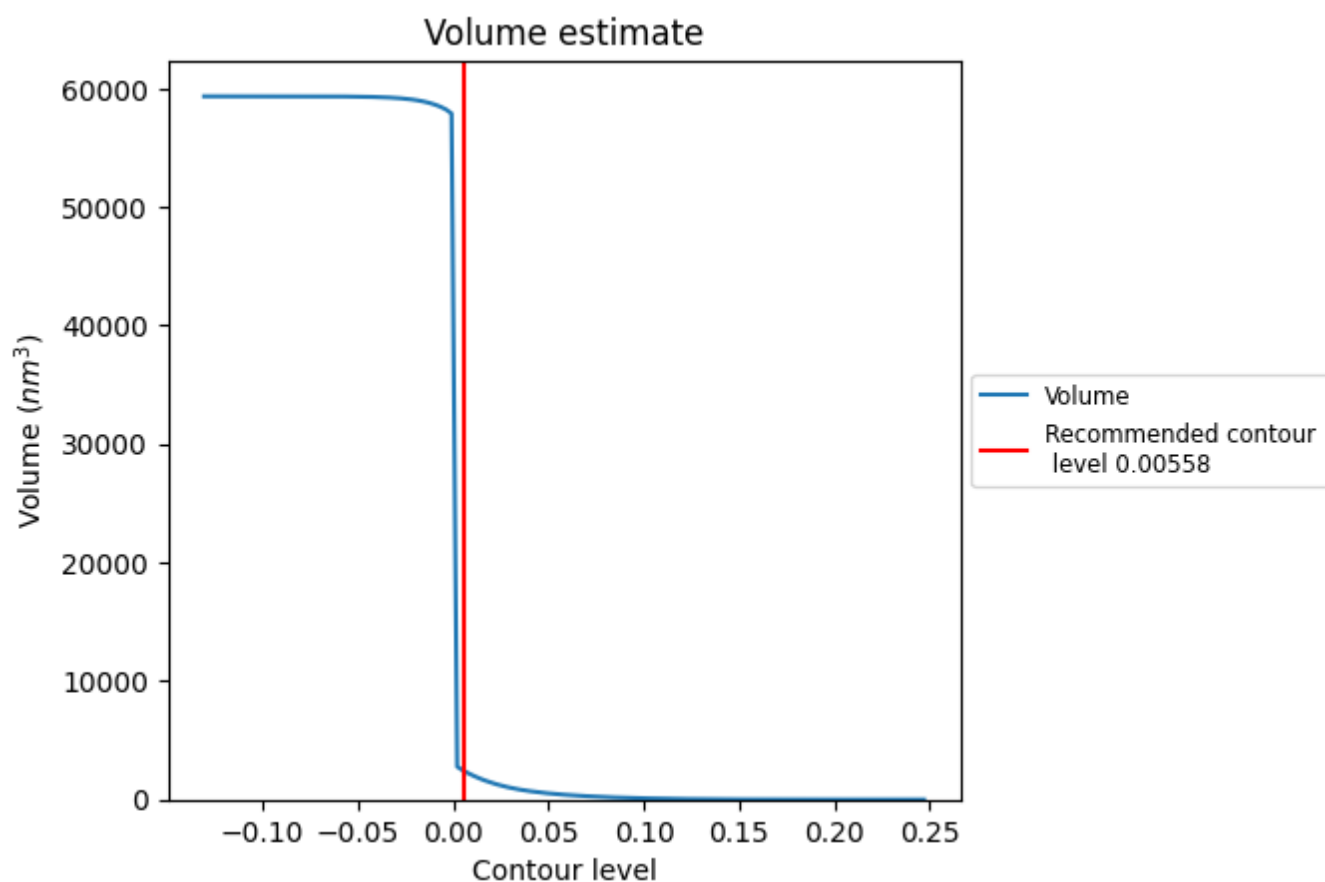
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

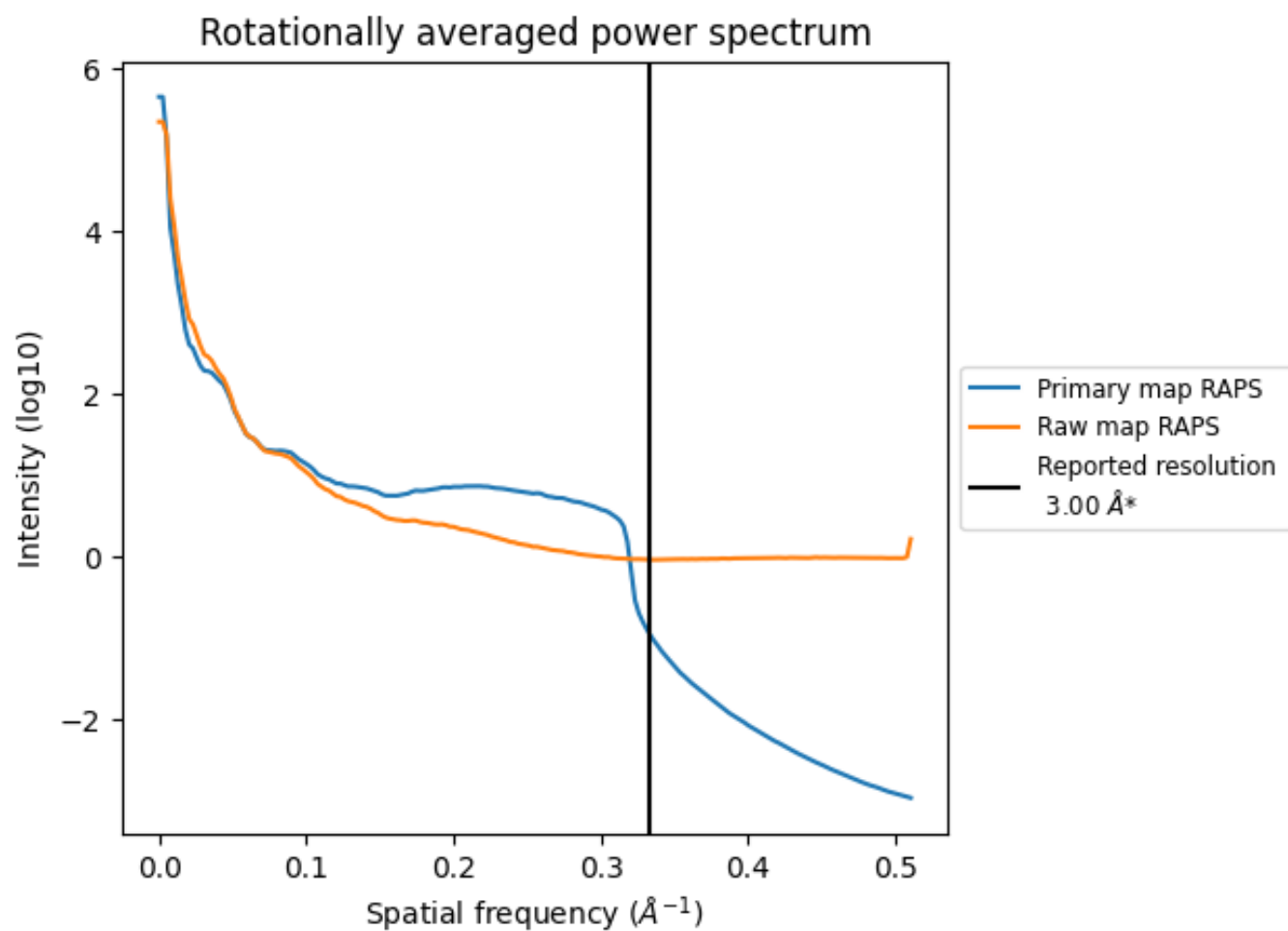
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2421 nm³; this corresponds to an approximate mass of 2187 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 ⓘ

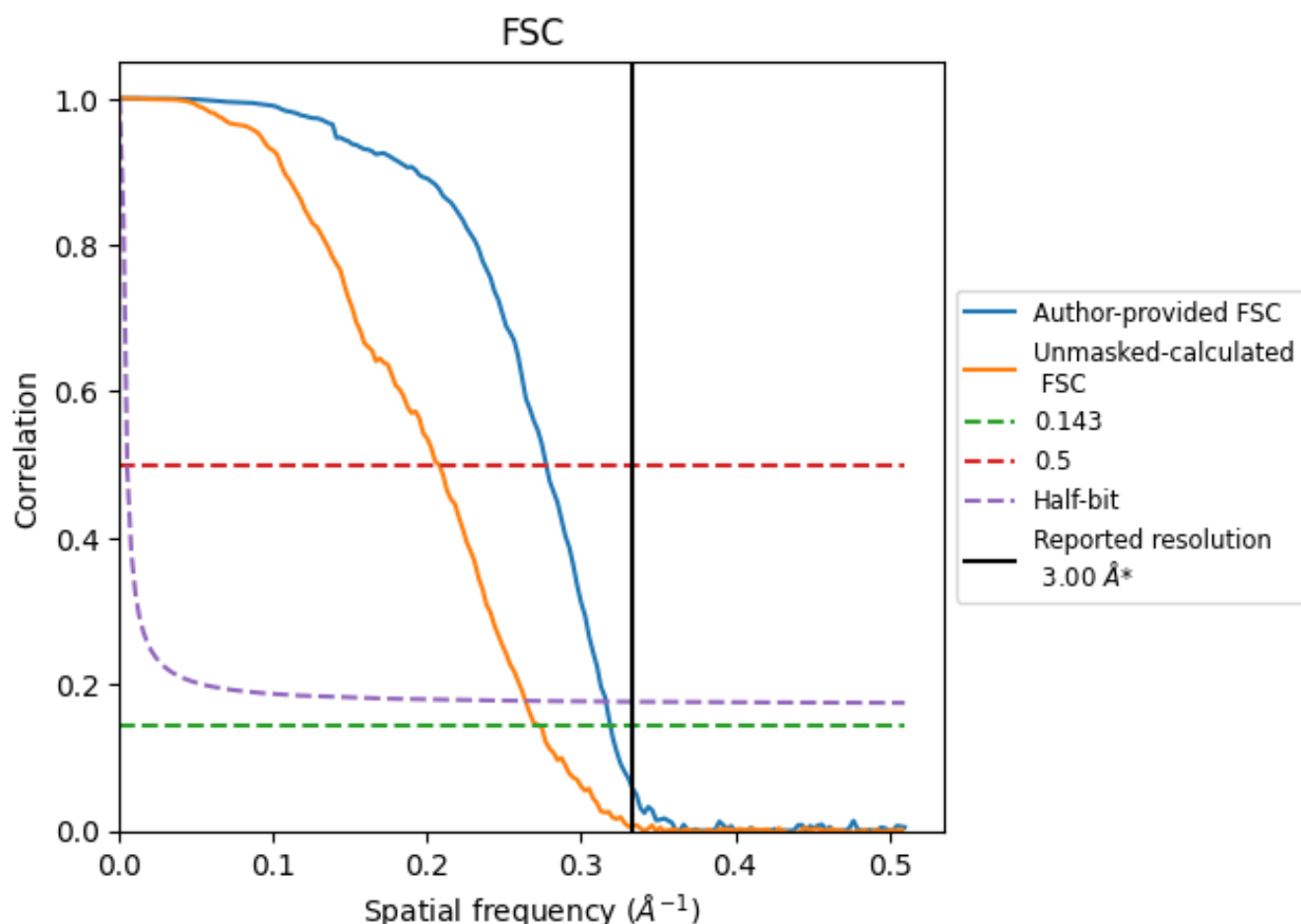


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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](#)

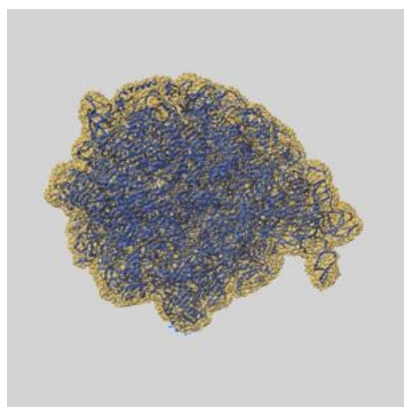
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.13	3.61	3.16
Unmasked-calculated*	3.66	4.82	3.79

*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 3.66 differs from the reported value 3.0 by more than 10 %

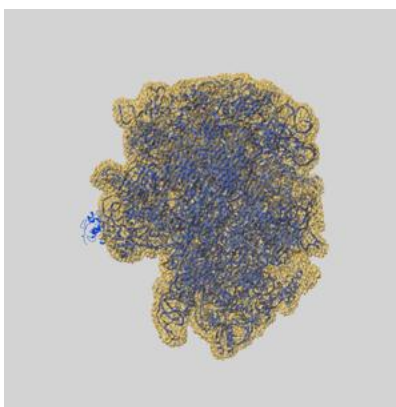
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8813 and PDB model 5WDT. Per-residue inclusion information can be found in section [3](#) on page [20](#).

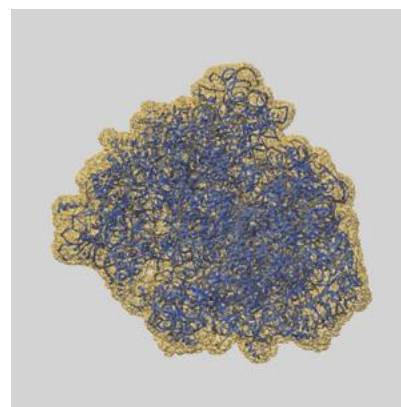
9.1 Map-model overlay [i](#)



X



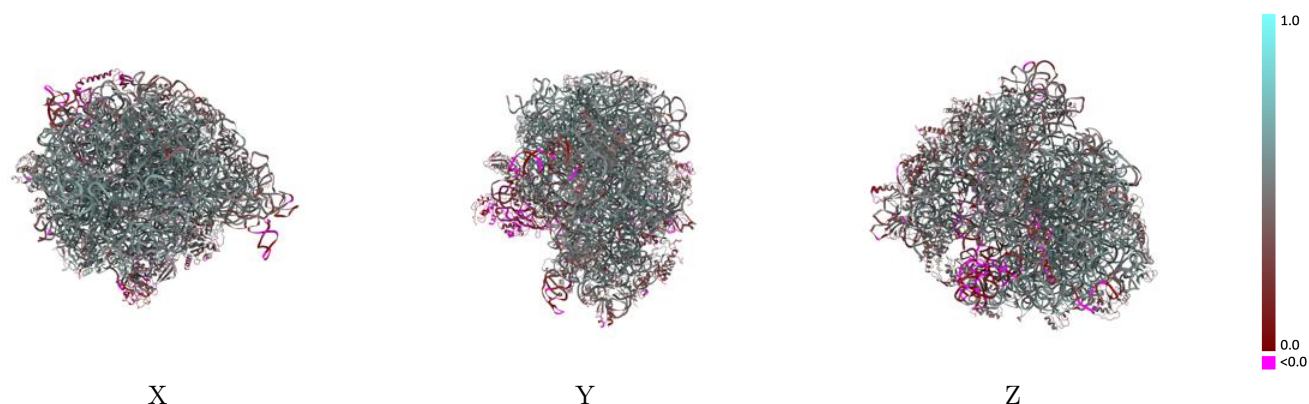
Y



Z

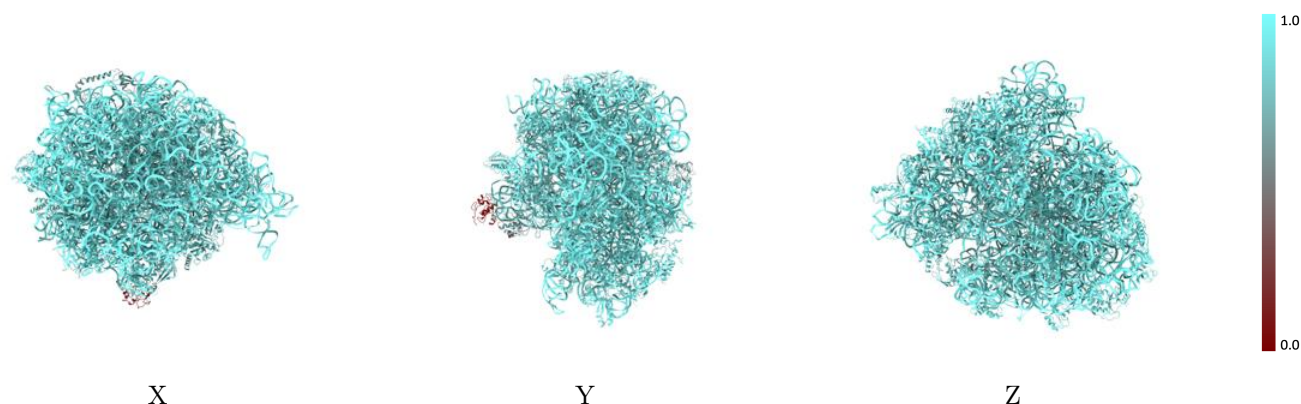
The images above show the 3D surface view of the map at the recommended contour level 0.00558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



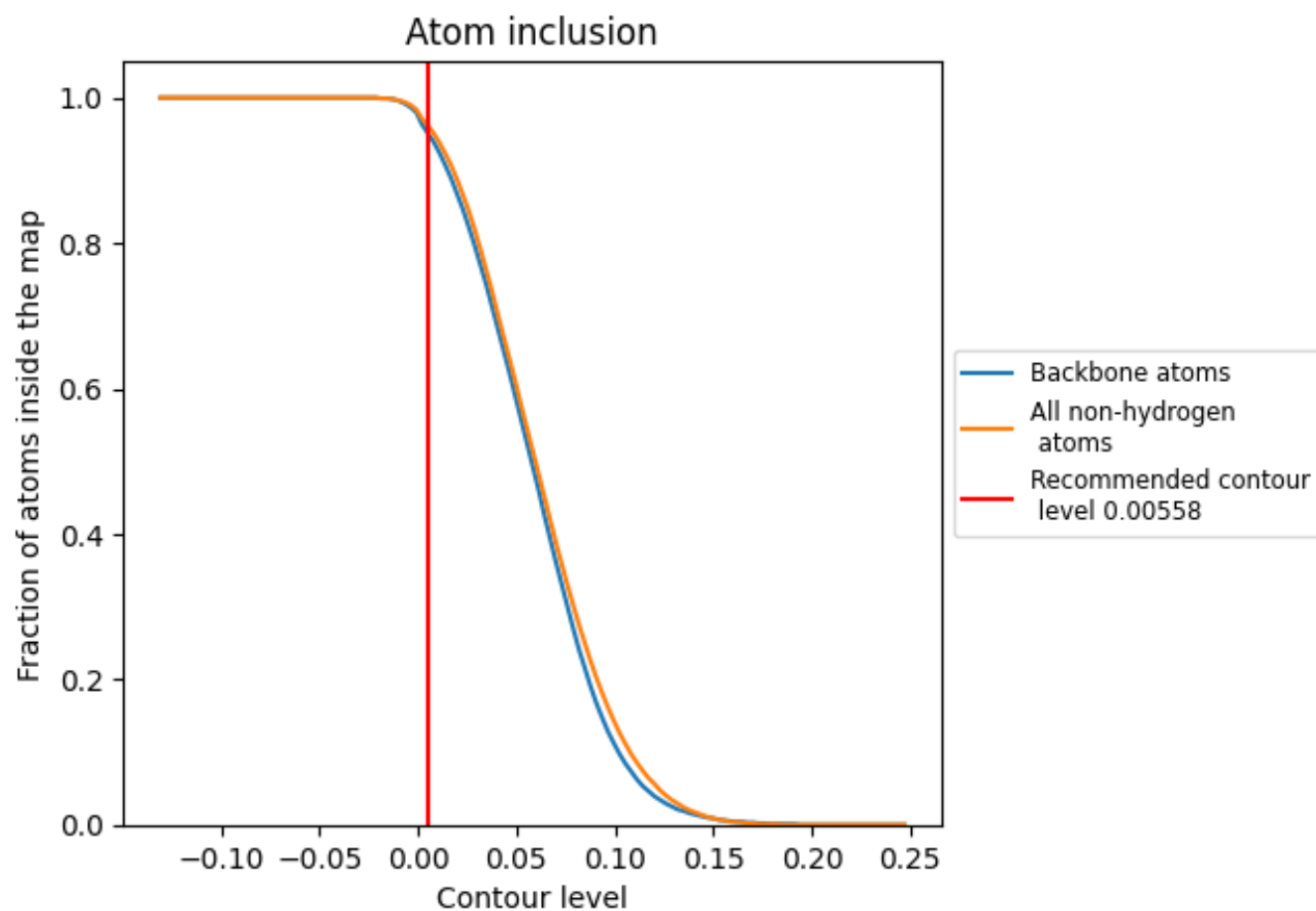
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00558).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.00558) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.4690
0	 0.9430	 0.4710
1	 0.9540	 0.4730
2	 0.9680	 0.5660
3	 0.9680	 0.5520
4	 0.9760	 0.5170
5	 0.1950	 0.0080
6	 0.8810	 0.2830
A	 0.9860	 0.5100
B	 0.9950	 0.5060
C	 0.9660	 0.5260
D	 0.9680	 0.5190
E	 0.9510	 0.4730
F	 0.9270	 0.3960
G	 0.9410	 0.3910
H	 0.7410	 0.1690
I	 0.6250	 0.0170
J	 0.9720	 0.5140
K	 0.9380	 0.4980
L	 0.9460	 0.4800
M	 0.9550	 0.4980
N	 0.9690	 0.5250
O	 0.9570	 0.4340
P	 0.9400	 0.4850
Q	 0.9720	 0.5400
R	 0.9390	 0.4660
S	 0.9430	 0.5010
T	 0.9300	 0.4440
U	 0.9480	 0.4300
V	 0.9380	 0.4460
W	 0.9680	 0.5310
X	 0.9520	 0.5040
Y	 0.9300	 0.4080
Z	 0.9510	 0.4930
a	 0.9900	 0.4890



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Chain	Atom inclusion	Q-score
b	 0.9040	 0.3380
c	 0.9450	 0.4310
d	 0.9350	 0.4110
e	 0.9440	 0.4610
f	 0.9150	 0.3890
g	 0.9150	 0.3550
h	 0.9510	 0.4730
i	 0.9220	 0.3720
j	 0.9260	 0.3410
k	 0.9470	 0.4480
l	 0.9450	 0.4870
m	 0.9400	 0.4100
n	 0.9550	 0.4370
o	 0.9540	 0.4570
p	 0.9310	 0.4280
q	 0.9290	 0.4380
r	 0.9180	 0.4040
s	 0.9530	 0.4390
t	 0.9430	 0.4210
u	 0.8110	 0.2700
v	 0.9680	 0.4680
w	 0.8190	 0.1030
x	 0.9840	 0.4830
y	 0.9490	 0.3620
z	 0.8850	 0.3280