



Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 09:04 PM EDT

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

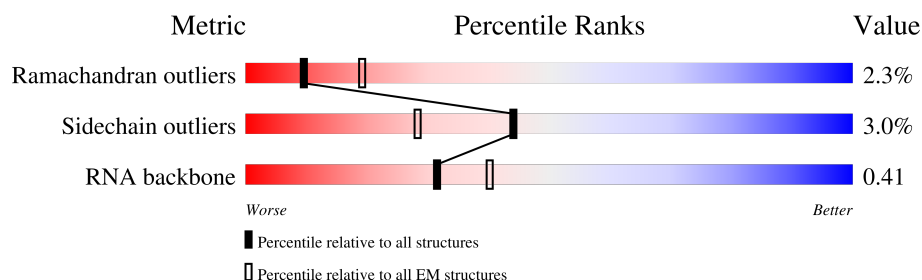
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	


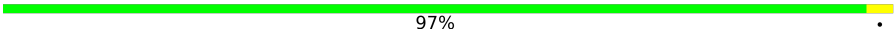
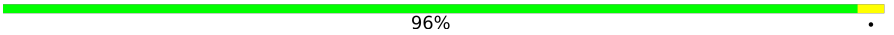
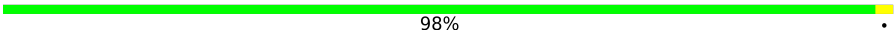

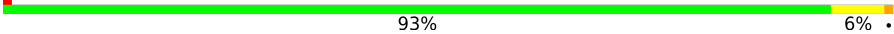
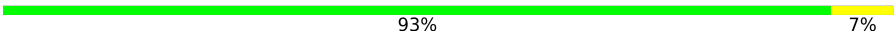
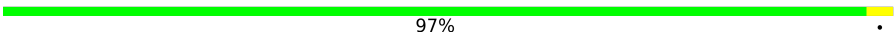
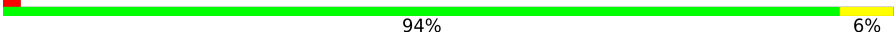
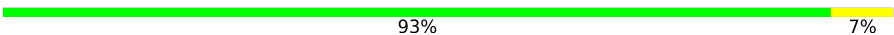
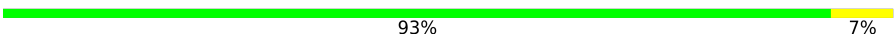

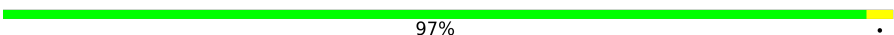
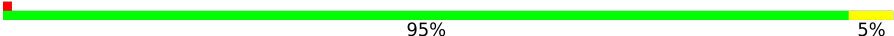

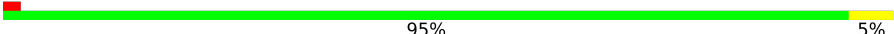
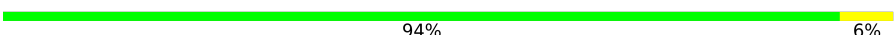

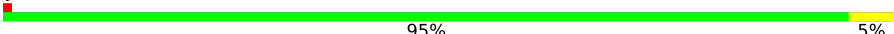
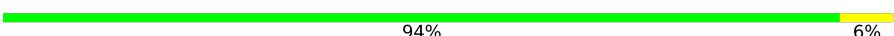





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Mol	Chain	Length	Quality of chain
9	I	141	
10	J	141	
11	K	122	
12	L	143	
13	M	136	
14	N	119	
15	O	116	
16	P	114	
17	Q	115	
18	R	102	
19	S	109	
20	T	92	
21	U	102	
22	V	92	
23	W	75	
24	X	77	
25	Y	60	
26	Z	56	
27	0	55	
28	1	51	
29	2	45	
30	3	64	
31	4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

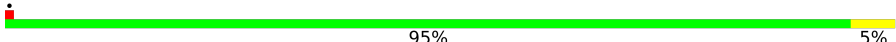
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Mol	Chain	Length	Quality of chain
34	a	1540	 71% 29%
35	b	218	 97% .
36	c	206	 96% .
37	d	205	 98% .
38	e	157	 92% 8%
39	f	100	 93% 6% .
40	g	151	 93% 7%
41	h	129	 97% .
42	i	127	 94% 6% .
43	j	98	 93% 7%
44	k	116	 93% 7%
45	l	121	 92% 7% .
46	m	115	 97% .
47	n	101	 95% 5%
48	o	88	 93% 6% .
49	p	82	 95% 5%
50	q	80	 94% 6%
51	r	65	 89% 11%
52	s	79	 95% 5%
53	t	85	 94% 6%
54	u	65	 82% 17% .
55	v	77	 74% 23% .
55	w	77	 51% 43% 6%
56	x	12	 92% 8%
57	y	76	 54% 42% .

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Mol	Chain	Length	Quality of chain
58	z	393	 A horizontal bar chart showing the quality of chain 58 (chain z, length 393). The bar is green, indicating a high quality score. The bar is labeled with '95%' in the center and '5%' at the right end. A small red dot is visible at the left end of the bar.

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		

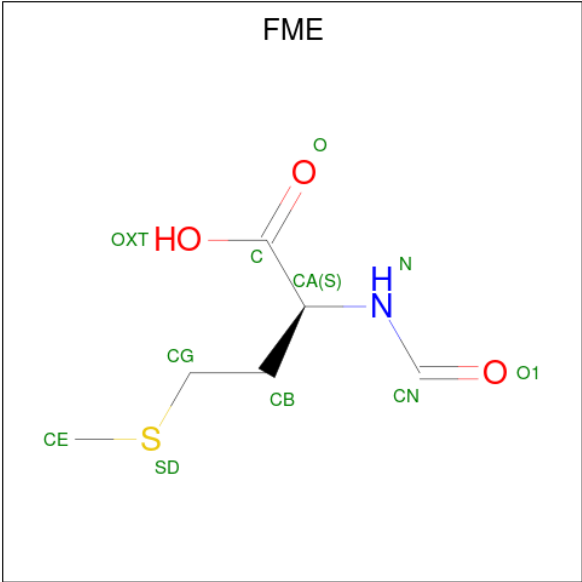
- Molecule 58 is a protein called Elongation factor Tu 2.

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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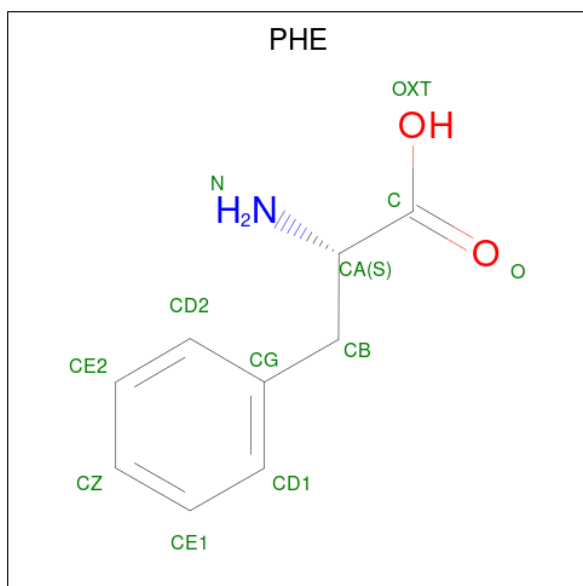
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Mol	Chain	Residues	Atoms		AltConf
60	T	1	Total 1	Mg 1	0
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	2	Total 2	Mg 2	0
60	0	2	Total 2	Mg 2	0
60	3	3	Total 3	Mg 3	0
60	4	1	Total 1	Mg 1	0
60	a	481	Total 481	Mg 481	0
60	d	1	Total 1	Mg 1	0
60	h	1	Total 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).

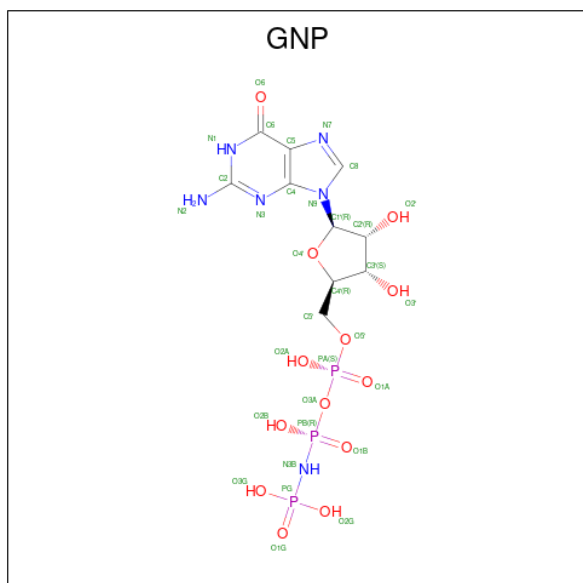
Mol	Chain	Residues	Atoms			AltConf
61	A	5	Total	K		0
			5	5		

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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: $C_{10}H_{17}N_6O_{13}P_3$).



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	

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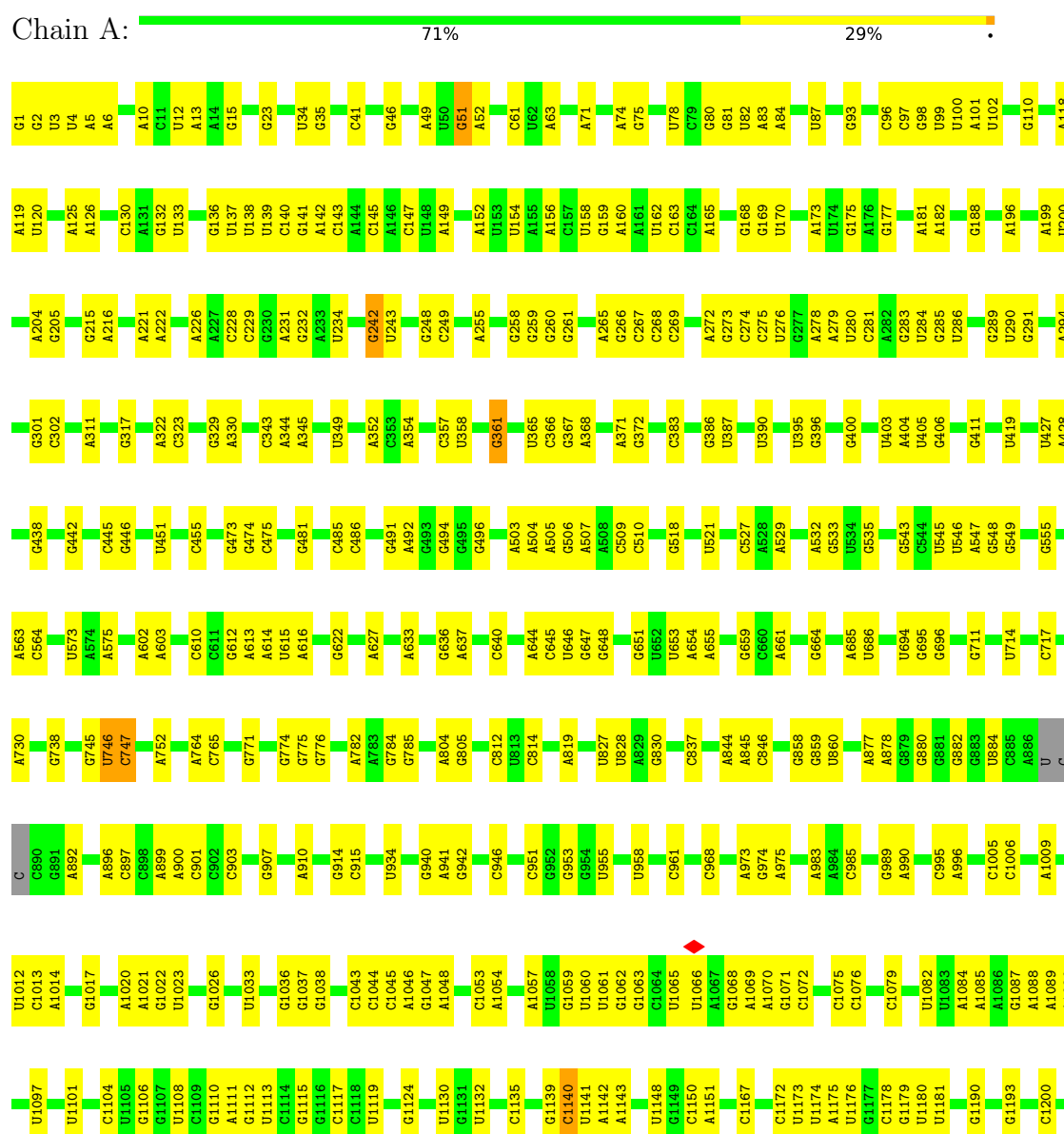
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Mol	Chain	Residues	Atoms		AltConf
64	2	4	Total 4	O 4	0
64	3	1	Total 1	O 1	0
64	4	1	Total 1	O 1	0
64	a	163	Total 163	O 163	0
64	d	1	Total 1	O 1	0
64	h	2	Total 2	O 2	0
64	k	1	Total 1	O 1	0
64	m	3	Total 3	O 3	0
64	o	1	Total 1	O 1	0
64	s	2	Total 2	O 2	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



A2826	U2720	G2535	G2399	G2230	A2108	C1967	G1857	U1716	G1567	G1478	A1204
G2844	A2542	A2542	G2401	G2238	U2109	A1858	A1858	G1479	G1568	G1479	A1365
A2856	A2547	A2547	U2402	G2239	G2110	A1970	G1862	G1721	A1569	G1482	G1210
U2861	A2726	A2547	U2404	G2251	U2113	G1972	A1866	G1724	A1572	G1483	G1211
G2867	A2727	U2552	G2405	A2278	U2118	U1976	G1867	C1725	A1579	U1484	G1218
A2868	U2728	G2553	A2406	G2278	U2119	U1991	C1868	A1727	A1580	U1485	A1378
A2872	A2733	U2554	A2407	C2283	A2119	U1992	C1869	G1728	C1728	U1486	G1225
A2873	A2734	C2556	U2408	G2286	G2120	G1992	C1870	U1729	G1581	U1487	G1226
C2874	G2735	C2566	U2423	G2286	G2121	U1993	A1871	U1730	A1583	A1490	G1227
C2880	G2742	A2566	C2424	A2288	G2127	C1997	A1872	G1731	U1584	G1491	U1390
A2883	U2743	G2567	A2425	A2288	U2131	A2020	G1873	C1732	C1585	G1492	U1391
U2884	G2744	A2572	G2428	U2296	U2132	C2021	A1876	G1735	G1588	C1493	A1392
G2885	C2745	C2573	G2429	A2297	G2133	U2022	C1879	U1736	U1368	A1494	U1240
A2886	U2746	U2580	A2430	A2297	A2134	C2023	G1884	G1738	A1591	A1495	A1247
C2896	G2747	G2581	A2435	U2305	G2141	G2027	A1885	A1739	C1592	A1496	G1248
U2897	A2748	U2586	U2441	A2309	G2145	A2030	A1890	C1741	A1593	A1504	A1253
A2898	U2752	U2586	U2445	A2311	C2146	A2033	C1895	A1746	A1605	C1507	G1256
A2899	U2754	G2445	G2445	G2318	A2147	A2039	C1895	A1608	A1608	A1508	G1257
A2900	A2758	G2603	G2446	G2319	G2157	U2039	U1898	G1750	A1610	U1411	U1258
C2901	U2762	U2604	A2448	G2325	G2162	C2043	G1906	U1758	A1616	A1413	A1262
C2902	G2763	U2605	U2449	C2326	G2163	C2055	G1907	C1764	C1617	C1414	A1269
U2903	A2764	U2609	C2452	C2332	C2164	G2056	C1968	A1634	A1618	G1519	G1270
	A2765	U2613	U2457	A2333	A2170	G2056	G1909	A1773	A1634	U1523	G1271
	U2768	G2624	C2465	U2334	A2171	A2059	G1910	G1776	U1647	G1524	A1272
A2776	A2776	U2629	A2469	A2335	U2172	A2060	A1912	A1780	U1648	A1527	C1289
G2777	G2777	U2629	A2469	A2336	A2173	G2061	C1913	A1780	G1649	G1529	C1290
A2778	A2778	A2634	C2475	C2339	U2180	A2062	3TD1915	A1791	A1654	G1530	C1291
G2791	U2791	C2651	A2476	A2340	G2186	G2069	A1916	A1800	G1659	C1531	U1294
U2794	U2794	C2652	C2480	U2344	U2192	C2072	U1917	A1801	C1533	A1532	G1432
G2799	U2803	U2653	G2484	G2345	G2193	A2077	A1918	A1808	G1659	U1534	G1300
A2800	U2804	A2654	G2484	C2340	U2194	A1928	A1936	A1809	G1674	A1535	A1301
G2801	G2801	U2656	G2494	G2357	U2195	A2080	A1937	G1811	C1675	C1536	C1306
A2802	A2802	G2673	C2498	G2361	A2198	U2092	A1936	G1816	G1691	G1537	G1305
G2803	U2804	G2674	C2499	U2372	G2204	G2093	A1937	G1817	U1692	U1538	C1306
C2805	C2805	A2805	G2502	U2372	A2205	C2096	A1938	U1818	G1895	A1549	G1332
C2806	U2806	U2689	G2503	G2378	C2206	A2097	U1939	A1829	A1700	U1554	
U2807	U2807	U2690	A2502	A2378	A2206	U2098	U1940	A1829	A1705	G1555	U1344
G2808	G2808	C2691	U2504	G2379	A2211	U2099	C1941	A1829	C1706	C1459	C1345
A2809	A2809	G2707	G2505	G2383	A2212	G2100	C1942	C1833	C1706	C1557	U1460
			U2506	U2383	U2213	A2101	U1945	U1834	U1709	C1558	C1349
G2812	G2812	C2712	C2517	U2394	U2213	G2102	U1945	G1835	U1709	U1559	
U2818	U2818	U2713	A2518	C2385	G2221	C2103	C1962	U1841	U1712	U1563	U1352
G2819	G2819	G2714	G2518	G2385	A2225	U2105	C1962	U1841	A1713	G1475	G1355
A2820	A2820	C2715	G2529	A2392	C2226	U2106	C1965	G1847	U1714	C1454	U1476
		C2716				C2107	A1966		C1715	G1455	A1359

• 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	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% 6%



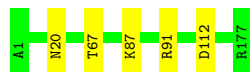
- Molecule 5: 50S ribosomal protein L4

Chain E:  97%



- Molecule 6: 50S ribosomal protein L5

Chain F:  97%



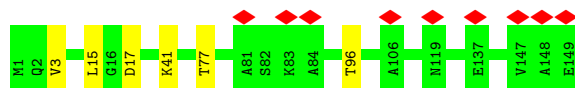
- Molecule 7: 50S ribosomal protein L6

Chain G:  98%




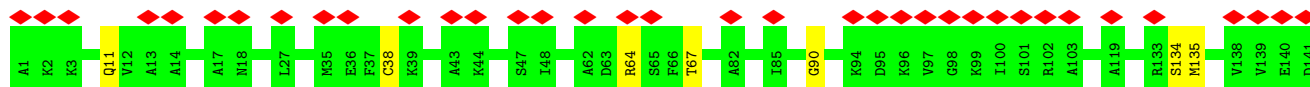
- Molecule 8: 50S ribosomal protein L9

Chain H:  6% 96%



- Molecule 9: 50S ribosomal protein L11

Chain I:  26% 95% 5%



- Molecule 10: 50S ribosomal protein L13

Chain J:  97% .




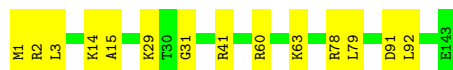
- Molecule 11: 50S ribosomal protein L14

Chain K:  93% 7%



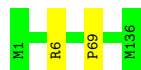
- Molecule 12: 50S ribosomal protein L15

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% .



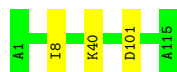
- Molecule 16: 50S ribosomal protein L19

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%



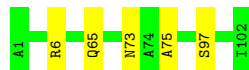
- Molecule 20: 50S ribosomal protein L23

Chain T:  96% .



- Molecule 21: 50S ribosomal protein L24

Chain U:  95% 5%



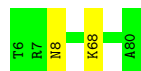
- Molecule 22: 50S ribosomal protein L25

Chain V:  98% ..



- Molecule 23: 50S ribosomal protein L27

Chain W:  97% .



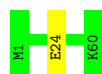
- Molecule 24: 50S ribosomal protein L28

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% .



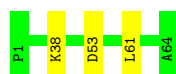
- Molecule 29: 50S ribosomal protein L34

Chain 2:  93% . .



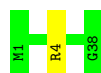
- Molecule 30: 50S ribosomal protein L35

Chain 3:  95% 5%




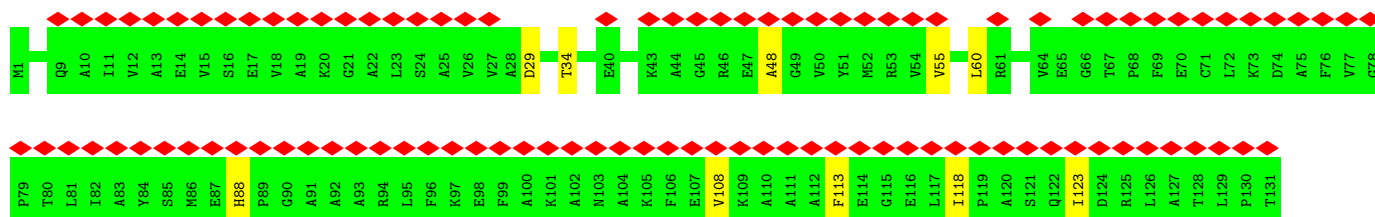
- Molecule 31: 50S ribosomal protein L36

Chain 4:  97% .



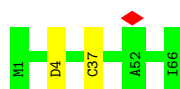
- Molecule 32: 50S ribosomal protein L10

Chain 5:  77% 92% 8%



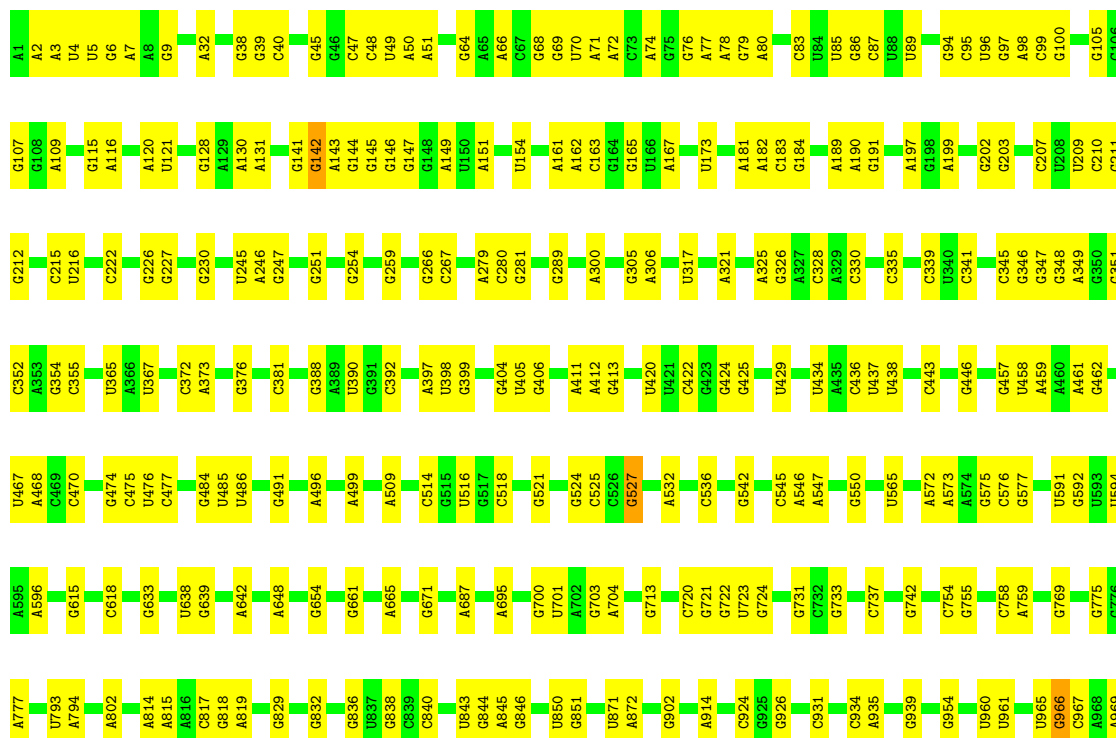
- Molecule 33: 50S ribosomal protein L31

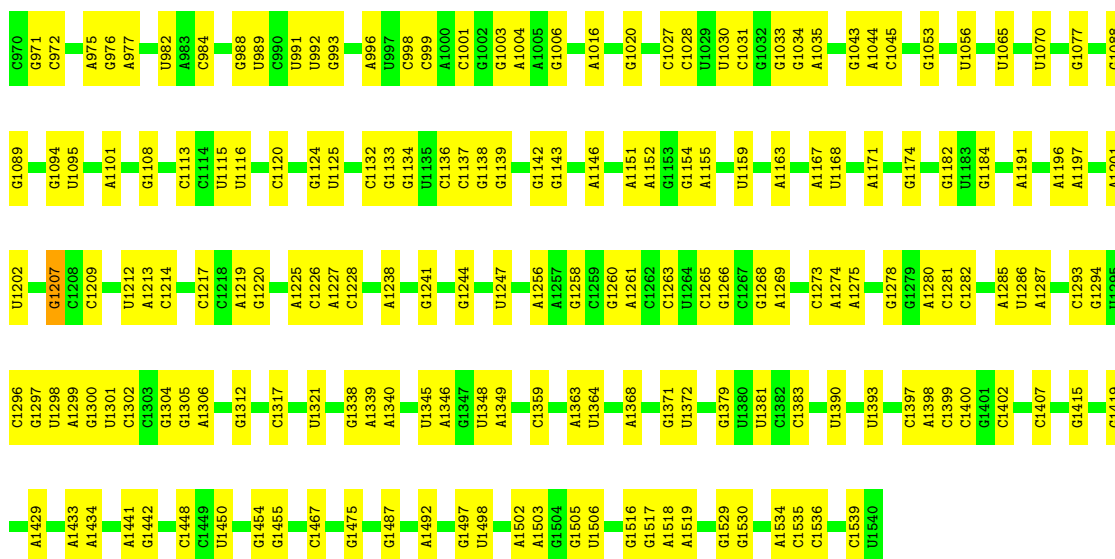
Chain 6:  97% .



- Molecule 34: 16S rRNA

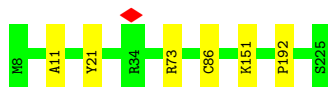
Chain a:  71% 29%





• 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%



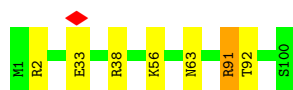
• Molecule 38: 30S ribosomal protein S5

Chain e:  92%



• Molecule 39: 30S ribosomal protein S6

Chain f:  93%



- Molecule 40: 30S ribosomal protein S7

Chain g: 93% 7%



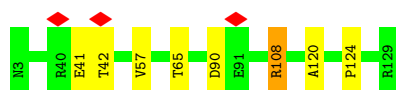
- Molecule 41: 30S ribosomal protein S8

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% .



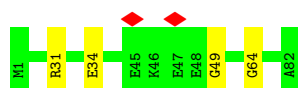
- Molecule 47: 30S ribosomal protein S14



- Molecule 48: 30S ribosomal protein S15



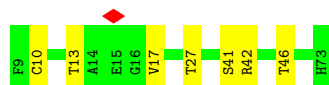
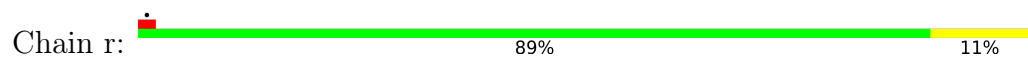
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17




- Molecule 51: 30S ribosomal protein S18

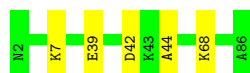


- Molecule 52: 30S ribosomal protein S19




- Molecule 53: 30S ribosomal protein S20

Chain t:  94% 6%



- Molecule 54: 30S ribosomal protein S21

Chain u:  82% 17% .



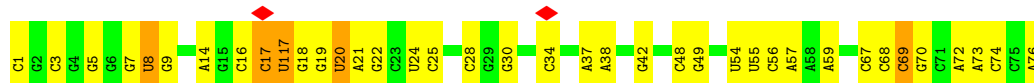
- Molecule 55: tRNA-fMet

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: 5MU, MIA, MG, 7MG, GNP, K, 2MG, OMC, FME, 4SU, PSU, 5MC, 6MZ, 4OC, OMU, 2MA, 1MG, OMG, 3TD, MA6, UR3, H2U

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%)	22	60
4	D	206/208 (99%)	191 (93%)	14 (7%)	1 (0%)	29	68
5	E	198/200 (99%)	179 (90%)	17 (9%)	2 (1%)	15	53
6	F	175/177 (99%)	155 (89%)	19 (11%)	1 (1%)	25	64
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	7	34
9	I	139/141 (99%)	112 (81%)	24 (17%)	3 (2%)	6	31
10	J	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	60
11	K	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	4	21
12	L	141/143 (99%)	117 (83%)	20 (14%)	4 (3%)	5	25
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	10	42
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	9	39
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	55
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%)	4	24
19	S	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	8	36
20	T	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	6	31
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	4	24
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	14	50
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%)	9	39
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	48 (91%)	4 (8%)	1 (2%)	8	36
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	6	30
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	8
33	6	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	9	40
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	184 (90%)	15 (7%)	5 (2%)	5	28
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	15	53
38	e	156/157 (99%)	131 (84%)	19 (12%)	6 (4%)	3	18
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	3	16
40	g	149/151 (99%)	130 (87%)	12 (8%)	7 (5%)	2	14
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	3	17
43	j	96/98 (98%)	73 (76%)	17 (18%)	6 (6%)	1	7
44	k	114/116 (98%)	99 (87%)	10 (9%)	5 (4%)	2	15
45	l	119/121 (98%)	98 (82%)	13 (11%)	8 (7%)	1	6
46	m	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	8	37
47	n	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	2	12
48	o	86/88 (98%)	78 (91%)	5 (6%)	3 (4%)	3	20
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	5	28
50	q	78/80 (98%)	70 (90%)	6 (8%)	2 (3%)	5	27
51	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	13
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	29
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	1
58	z	391/393 (100%)	352 (90%)	29 (7%)	10 (3%)	5	27
All	All	6219/6322 (98%)	5477 (88%)	602 (10%)	140 (2%)	9	30

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%)	34	70
4	D	163/163 (100%)	152 (93%)	11 (7%)	16	49
5	E	164/164 (100%)	160 (98%)	4 (2%)	49	79
6	F	148/148 (100%)	144 (97%)	4 (3%)	44	77
7	G	135/135 (100%)	132 (98%)	3 (2%)	52	81
8	H	114/114 (100%)	111 (97%)	3 (3%)	46	78
9	I	109/109 (100%)	105 (96%)	4 (4%)	34	70
10	J	115/115 (100%)	112 (97%)	3 (3%)	46	78
11	K	103/103 (100%)	98 (95%)	5 (5%)	25	61
12	L	102/102 (100%)	92 (90%)	10 (10%)	8	30
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	99/99 (100%)	97 (98%)	2 (2%)	55	83
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%)	37	72
18	R	84/84 (100%)	82 (98%)	2 (2%)	49	79
19	S	92/92 (100%)	89 (97%)	3 (3%)	38	73
20	T	79/79 (100%)	77 (98%)	2 (2%)	47	79
21	U	83/83 (100%)	81 (98%)	2 (2%)	49	79
22	V	77/77 (100%)	76 (99%)	1 (1%)	69	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	57/57 (100%)	55 (96%)	2 (4%)	36	71
24	X	67/67 (100%)	65 (97%)	2 (3%)	41	75
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	53	82
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	52	81
29	2	37/37 (100%)	34 (92%)	3 (8%)	11	40
30	3	51/51 (100%)	48 (94%)	3 (6%)	19	54
31	4	34/34 (100%)	33 (97%)	1 (3%)	42	76
32	5	100/100 (100%)	98 (98%)	2 (2%)	55	83
33	6	59/59 (100%)	58 (98%)	1 (2%)	60	85
35	b	180/180 (100%)	179 (99%)	1 (1%)	86	95
36	c	170/170 (100%)	166 (98%)	4 (2%)	49	79
37	d	172/172 (100%)	169 (98%)	3 (2%)	60	85
38	e	120/119 (101%)	114 (95%)	6 (5%)	24	60
39	f	87/87 (100%)	85 (98%)	2 (2%)	50	80
40	g	124/124 (100%)	121 (98%)	3 (2%)	49	79
41	h	104/104 (100%)	100 (96%)	4 (4%)	33	69
42	i	105/105 (100%)	101 (96%)	4 (4%)	33	69
43	j	86/86 (100%)	85 (99%)	1 (1%)	71	90
44	k	89/89 (100%)	86 (97%)	3 (3%)	37	72
45	l	102/102 (100%)	98 (96%)	4 (4%)	32	69
46	m	93/93 (100%)	91 (98%)	2 (2%)	52	81
47	n	83/83 (100%)	83 (100%)	0	100	100
48	o	76/76 (100%)	73 (96%)	3 (4%)	32	69
49	p	65/65 (100%)	63 (97%)	2 (3%)	40	75
50	q	74/74 (100%)	71 (96%)	3 (4%)	30	67
51	r	56/56 (100%)	52 (93%)	4 (7%)	14	46
52	s	70/70 (100%)	66 (94%)	4 (6%)	20	56
53	t	65/65 (100%)	62 (95%)	3 (5%)	27	64
54	u	55/55 (100%)	51 (93%)	4 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	z	325/325 (100%)	317 (98%)	8 (2%)	47	79
All	All	5165/5164 (100%)	5011 (97%)	154 (3%)	44	75

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	$\# Z > 2$
34	MA6	a	1518	34,60	19,26,27	1.26	2 (10%)	18,38,41	1.75	4 (22%)
34	PSU	a	516	34	18,21,22	1.34	2 (11%)	22,30,33	2.03	5 (22%)
1	5MC	A	747	1	18,22,23	0.98	1 (5%)	26,32,35	1.47	5 (19%)
1	3TD	A	1915	1	18,22,23	7.24	14 (77%)	22,32,35	1.77	4 (18%)
34	5MC	a	1407	34	18,22,23	1.03	1 (5%)	26,32,35	1.54	4 (15%)
55	5MU	v	54	55	19,22,23	1.46	4 (21%)	28,32,35	1.91	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	A	2498	1,60	19,22,23	0.85	0	26,31,34	1.17	2 (7%)
1	PSU	A	2457	1,60	18,21,22	1.41	2 (11%)	22,30,33	1.89	5 (22%)
57	7MG	y	46	57	22,26,27	1.42	3 (13%)	29,39,42	2.36	7 (24%)
1	OMG	A	2251	1,60,55	18,26,27	1.05	2 (11%)	19,38,41	1.02	2 (10%)
55	H2U	v	20	55	18,21,22	0.82	1 (5%)	21,30,33	1.75	3 (14%)
55	4SU	w	8	55	18,21,22	1.72	5 (27%)	26,30,33	2.15	5 (19%)
1	PSU	A	2605	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
34	4OC	a	1402	34	20,23,24	0.85	1 (5%)	26,32,35	1.28	4 (15%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	21,30,33	1.48	5 (23%)
55	H2U	w	20	55	18,21,22	0.81	0	21,30,33	1.69	3 (14%)
1	5MU	A	1939	1	19,22,23	1.47	4 (21%)	28,32,35	2.02	8 (28%)
1	7MG	A	2069	1,60	22,26,27	1.45	2 (9%)	29,39,42	2.44	12 (41%)
57	H2U	y	20	57	18,21,22	0.86	1 (5%)	21,30,33	1.58	4 (19%)
1	2MG	A	2445	1,60	18,26,27	0.95	0	16,38,41	1.15	2 (12%)
34	2MG	a	966	34	18,26,27	1.01	1 (5%)	16,38,41	1.34	3 (18%)
1	PSU	A	2604	1	18,21,22	1.41	2 (11%)	22,30,33	1.81	4 (18%)
1	PSU	A	1911	1	18,21,22	1.40	2 (11%)	22,30,33	2.02	4 (18%)
1	PSU	A	955	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	4 (18%)
1	H2U	A	2449	1	18,21,22	0.94	2 (11%)	21,30,33	1.71	4 (19%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	22,30,33	1.89	4 (18%)
55	PSU	w	55	55	18,21,22	1.29	2 (11%)	22,30,33	1.93	5 (22%)
34	UR3	a	1498	34	19,22,23	1.13	1 (5%)	26,32,35	1.73	4 (15%)
57	4SU	y	8	57	18,21,22	1.76	5 (27%)	26,30,33	2.30	7 (26%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	22,30,33	1.92	5 (22%)
34	5MC	a	967	34	18,22,23	1.05	1 (5%)	26,32,35	1.47	4 (15%)
57	PSU	y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.95	5 (22%)
57	MIA	y	37	57	24,30,32	2.28	5 (20%)	25,42,47	2.65	9 (36%)
34	2MG	a	1516	34	18,26,27	0.96	0	16,38,41	1.15	2 (12%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	28,32,35	2.04	10 (35%)
1	PSU	A	2580	1	18,21,22	1.48	2 (11%)	22,30,33	1.99	5 (22%)
1	PSU	A	746	1,60	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
57	5MU	y	54	57	19,22,23	1.42	4 (21%)	28,32,35	2.04	7 (25%)
34	MA6	a	1519	34	19,26,27	1.19	2 (10%)	18,38,41	1.71	4 (22%)
57	PSU	y	32	57,60	18,21,22	1.34	2 (11%)	22,30,33	1.90	5 (22%)
1	2MA	A	2503	1,60	17,25,26	1.11	1 (5%)	17,37,40	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MG	A	745	1	18,26,27	1.05	0	19,39,42	1.46	4 (21%)
34	2MG	a	1207	34	18,26,27	0.92	0	16,38,41	1.26	3 (18%)
1	5MC	A	1962	1	18,22,23	1.05	1 (5%)	26,32,35	1.45	3 (11%)
57	PSU	y	39	57	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
55	PSU	v	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.88	5 (22%)
1	2MG	A	1835	1	18,26,27	1.02	2 (11%)	16,38,41	1.18	2 (12%)
55	4SU	v	7	55	18,21,22	1.71	4 (22%)	26,30,33	2.27	6 (23%)
1	OMU	A	2552	1,60	19,22,23	1.28	3 (15%)	26,31,34	1.94	9 (34%)
34	7MG	a	527	34,60	22,26,27	1.42	2 (9%)	29,39,42	2.43	8 (27%)
1	6MZ	A	1618	1	18,25,26	1.02	1 (5%)	16,36,39	2.28	5 (31%)
1	6MZ	A	2030	1,60	18,25,26	1.03	1 (5%)	16,36,39	2.29	5 (31%)

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
34	MA6	a	1518	34,60	-	2/7/29/30	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	5/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
1	PSU	A	2457	1,60	-	2/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	OMG	A	2251	1,60,55	-	0/5/27/28	0/3/3/3
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	2445	1,60	-	2/5/27/28	0/3/3/3
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	2/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/10/32/34	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	2/7/29/30	0/3/3/3
57	PSU	y	32	57,60	-	2/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	3/3/25/26	0/3/3/3
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
34	2MG	a	1207	34	-	1/5/27/28	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	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
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
1	6MZ	A	2030	1,60	-	3/5/27/28	0/3/3/3

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.78	1.66	1.43
1	A	1915	3TD	C2'-C1'	-15.07	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C6-C5	14.85	1.52	1.35
1	A	1915	3TD	C2-N1	8.13	1.47	1.37
57	y	37	MIA	C13-C14	7.16	1.52	1.32
57	y	37	MIA	C2-S10	-6.16	1.70	1.75
1	A	1915	3TD	O4'-C4'	-5.98	1.31	1.45
1	A	1915	3TD	C2-N3	5.96	1.51	1.38
1	A	1915	3TD	C6-N1	5.23	1.44	1.36
55	v	7	4SU	C4-S4	-4.50	1.59	1.68
1	A	2580	PSU	C6-C5	4.46	1.40	1.35
57	y	8	4SU	C4-S4	-4.44	1.60	1.68
55	w	8	4SU	C4-S4	-4.41	1.60	1.68
1	A	1917	PSU	C6-C5	4.19	1.40	1.35
1	A	1911	PSU	C6-C5	4.17	1.40	1.35
57	y	39	PSU	C6-C5	4.16	1.40	1.35
1	A	746	PSU	C6-C5	4.10	1.40	1.35
1	A	2605	PSU	C6-C5	4.08	1.40	1.35
1	A	2069	7MG	C4-N9	-4.06	1.33	1.37
1	A	2604	PSU	C6-C5	4.06	1.40	1.35
1	A	2504	PSU	C6-C5	4.03	1.40	1.35
57	y	55	PSU	C6-C5	4.03	1.40	1.35
1	A	955	PSU	C6-C5	4.02	1.40	1.35
1	A	2457	PSU	C6-C5	4.02	1.40	1.35
34	a	516	PSU	C6-C5	4.01	1.40	1.35
57	y	32	PSU	C6-C5	3.96	1.39	1.35
55	w	55	PSU	C6-C5	3.77	1.39	1.35
55	v	55	PSU	C6-C5	3.55	1.39	1.35
55	v	54	5MU	C6-C5	3.43	1.40	1.34
34	a	527	7MG	C4-N9	-3.41	1.33	1.37
57	y	46	7MG	C4-N9	-3.29	1.33	1.37
1	A	1939	5MU	C6-C5	3.23	1.39	1.34
1	A	1962	5MC	C6-C5	3.19	1.39	1.34
34	a	967	5MC	C6-C5	3.16	1.39	1.34
1	A	1915	3TD	O2'-C2'	3.16	1.50	1.43
57	y	46	7MG	C5-C4	3.15	1.48	1.38
34	a	1407	5MC	C6-C5	3.11	1.39	1.34
55	w	54	5MU	C6-C5	3.10	1.39	1.34
34	a	527	7MG	C5-C4	3.09	1.48	1.38
57	y	8	4SU	C4-N3	-3.08	1.34	1.37
55	w	54	5MU	C2-N1	3.05	1.43	1.38
55	v	54	5MU	C4-N3	-3.00	1.33	1.38
55	w	8	4SU	C2-N1	3.00	1.43	1.38
57	y	54	5MU	C2-N1	2.99	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	5MC	C6-C5	2.92	1.39	1.34
1	A	2069	7MG	C5-C4	2.92	1.47	1.38
55	w	8	4SU	C4-N3	-2.84	1.34	1.37
34	a	1518	MA6	C5-C4	2.83	1.48	1.40
1	A	2552	OMU	C2-N1	2.83	1.43	1.38
55	v	7	4SU	C2-N1	2.82	1.43	1.38
57	y	54	5MU	C6-C5	2.82	1.39	1.34
57	y	8	4SU	C2-N1	2.80	1.42	1.38
55	w	54	5MU	C4-C5	2.79	1.49	1.44
1	A	1939	5MU	C4-C5	2.76	1.49	1.44
1	A	2503	2MA	C2-N3	2.68	1.36	1.31
1	A	1915	3TD	C4-N3	2.68	1.46	1.40
1	A	1915	3TD	C10-N3	-2.67	1.42	1.47
57	y	37	MIA	C6-N1	2.65	1.36	1.32
34	a	1519	MA6	C5-C4	2.64	1.47	1.40
57	y	37	MIA	C5-C4	2.62	1.47	1.40
55	v	7	4SU	C4-N3	-2.60	1.34	1.37
1	A	1915	3TD	O3'-C3'	-2.59	1.36	1.43
1	A	2552	OMU	C4-N3	-2.59	1.33	1.38
1	A	1939	5MU	C2-N1	2.57	1.42	1.38
1	A	2580	PSU	C4-N3	-2.54	1.34	1.38
34	a	1498	UR3	C2-N1	2.54	1.42	1.38
1	A	2030	6MZ	C5-C4	2.51	1.47	1.40
1	A	1915	3TD	O2-C2	-2.50	1.18	1.23
1	A	1618	6MZ	C5-C4	2.49	1.47	1.40
1	A	2457	PSU	C4-N3	-2.46	1.34	1.38
1	A	2604	PSU	C4-N3	-2.44	1.34	1.38
1	A	2504	PSU	C4-N3	-2.44	1.34	1.38
57	y	54	5MU	C4-C5	2.43	1.48	1.44
55	v	55	PSU	C4-N3	-2.41	1.34	1.38
1	A	1917	PSU	C4-N3	-2.40	1.34	1.38
1	A	1939	5MU	C4-N3	-2.39	1.34	1.38
57	y	8	4SU	C5-C4	-2.38	1.39	1.42
55	v	7	4SU	C5-C4	-2.38	1.39	1.42
34	a	1518	MA6	C6-N1	2.37	1.36	1.33
34	a	966	2MG	O4'-C1'	2.35	1.44	1.41
1	A	2449	H2U	C2-N3	-2.35	1.33	1.38
1	A	2605	PSU	C4-N3	-2.34	1.34	1.38
1	A	746	PSU	C4-N3	-2.33	1.34	1.38
57	y	55	PSU	C4-N3	-2.33	1.34	1.38
1	A	2449	H2U	C4-N3	-2.32	1.33	1.37
55	v	54	5MU	C4-C5	2.29	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	8	4SU	C5-C4	-2.28	1.39	1.42
55	w	54	5MU	C4-N3	-2.28	1.34	1.38
55	v	54	5MU	C2-N3	-2.27	1.33	1.38
57	y	54	5MU	C4-N3	-2.27	1.34	1.38
1	A	1835	2MG	C6-N1	-2.26	1.34	1.37
57	y	32	PSU	C4-N3	-2.26	1.34	1.38
1	A	1915	3TD	C3'-C4'	2.25	1.58	1.53
34	a	516	PSU	C4-N3	-2.24	1.34	1.38
1	A	1835	2MG	O4'-C1'	2.24	1.44	1.41
34	a	1519	MA6	C6-N1	2.23	1.36	1.33
57	y	39	PSU	C4-N3	-2.23	1.34	1.38
1	A	2251	OMG	C6-N1	-2.22	1.34	1.37
55	w	55	PSU	C4-N3	-2.20	1.34	1.38
1	A	955	PSU	C4-N3	-2.14	1.34	1.38
1	A	1915	3TD	O4-C4	-2.13	1.18	1.23
57	y	37	MIA	O4'-C1'	2.13	1.44	1.41
1	A	1911	PSU	C4-N3	-2.13	1.34	1.38
57	y	8	4SU	C6-C5	2.11	1.39	1.35
57	y	20	H2U	C2-N3	-2.11	1.34	1.38
1	A	2552	OMU	C6-C5	2.09	1.39	1.35
34	a	1402	4OC	C6-C5	2.08	1.39	1.35
55	w	8	4SU	C6-C5	2.06	1.39	1.35
57	y	46	7MG	C8-N9	2.06	1.47	1.46
57	y	16	H2U	C2-N3	-2.04	1.34	1.38
55	v	20	H2U	C2-N3	-2.03	1.34	1.38
1	A	2251	OMG	O4'-C1'	2.02	1.43	1.41

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	7.95	137.35	125.47
57	y	46	7MG	N9-C4-N3	7.92	137.32	125.47
1	A	2069	7MG	N9-C4-N3	7.23	136.29	125.47
57	y	37	MIA	C12-C13-C14	-7.00	113.53	127.14
55	v	7	4SU	C4-N3-C2	-6.44	121.08	127.34
57	y	8	4SU	C4-N3-C2	-6.43	121.09	127.34
55	w	8	4SU	C4-N3-C2	-6.07	121.45	127.34
1	A	2030	6MZ	C2-N1-C6	5.97	121.71	116.59
1	A	1618	6MZ	C2-N1-C6	5.97	121.71	116.59
34	a	1498	UR3	C4-N3-C2	-5.91	119.00	124.56
1	A	2504	PSU	N1-C2-N3	5.86	121.77	115.13
55	v	54	5MU	N3-C2-N1	5.81	122.60	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	55	PSU	N1-C2-N3	5.79	121.69	115.13
1	A	1911	PSU	N1-C2-N3	5.78	121.68	115.13
1	A	746	PSU	N1-C2-N3	5.72	121.61	115.13
57	y	32	PSU	N1-C2-N3	5.69	121.58	115.13
57	y	39	PSU	N1-C2-N3	5.69	121.57	115.13
1	A	955	PSU	N1-C2-N3	5.67	121.55	115.13
55	v	20	H2U	O4'-C1'-N1	5.64	116.99	109.30
57	y	55	PSU	N1-C2-N3	5.63	121.51	115.13
1	A	2457	PSU	N1-C2-N3	5.63	121.51	115.13
1	A	2605	PSU	N1-C2-N3	5.60	121.48	115.13
1	A	2580	PSU	N1-C2-N3	5.58	121.46	115.13
1	A	2604	PSU	N1-C2-N3	5.58	121.45	115.13
34	a	516	PSU	N1-C2-N3	5.57	121.44	115.13
1	A	1917	PSU	N1-C2-N3	5.56	121.43	115.13
55	v	55	PSU	N1-C2-N3	5.50	121.36	115.13
55	v	7	4SU	C5-C4-N3	5.46	119.75	114.69
55	w	8	4SU	C5-C4-N3	5.24	119.55	114.69
57	y	8	4SU	C5-C4-N3	5.17	119.48	114.69
57	y	8	4SU	N3-C2-N1	5.13	121.70	114.89
1	A	1939	5MU	N3-C2-N1	5.10	121.66	114.89
34	a	527	7MG	C5-C4-N3	-5.03	118.54	128.13
57	y	46	7MG	C5-C4-N3	-4.96	118.67	128.13
1	A	1915	3TD	C4-N3-C2	-4.92	119.27	124.61
1	A	1915	3TD	N1-C2-N3	4.92	120.02	116.14
1	A	2069	7MG	C5-C4-N3	-4.83	118.92	128.13
55	w	54	5MU	N3-C2-N1	4.81	121.28	114.89
1	A	1939	5MU	C4-N3-C2	-4.80	121.13	127.35
1	A	2552	OMU	N3-C2-N1	4.70	121.13	114.89
1	A	2069	7MG	C2-N3-C4	4.70	120.67	112.30
57	y	37	MIA	C16-C14-C13	-4.65	109.21	122.65
1	A	2069	7MG	N9-C8-N7	-4.60	96.79	103.38
55	w	20	H2U	O4'-C1'-N1	4.55	115.50	109.30
57	y	37	MIA	C5-C6-N1	-4.52	117.06	120.81
57	y	54	5MU	N3-C2-N1	4.51	120.88	114.89
55	w	54	5MU	C4-N3-C2	-4.50	121.53	127.35
55	w	8	4SU	N3-C2-N1	4.47	120.82	114.89
57	y	46	7MG	N9-C8-N7	-4.46	96.99	103.38
57	y	54	5MU	C4-N3-C2	-4.45	121.59	127.35
57	y	46	7MG	C2-N3-C4	4.45	120.22	112.30
34	a	527	7MG	C2-N3-C4	4.42	120.17	112.30
55	v	7	4SU	N3-C2-N1	4.42	120.75	114.89
34	a	527	7MG	N9-C8-N7	-4.37	97.13	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2552	OMU	C4-N3-C2	-4.33	120.86	126.58
57	y	37	MIA	C2-N3-C4	4.32	121.28	115.32
1	A	1911	PSU	O2-C2-N1	-4.25	118.12	122.79
57	y	54	5MU	C5-C4-N3	4.24	118.93	115.31
55	v	54	5MU	C4-N3-C2	-4.22	121.88	127.35
34	a	1519	MA6	C4-C5-N7	-4.22	105.00	109.40
1	A	1939	5MU	C5-C4-N3	4.20	118.90	115.31
55	v	7	4SU	C5-C4-S4	-4.17	119.10	124.47
55	w	54	5MU	C5-C4-N3	4.15	118.85	115.31
1	A	747	5MC	CM5-C5-C6	-4.04	117.46	122.85
34	a	967	5MC	CM5-C5-C6	-3.94	117.59	122.85
1	A	2605	PSU	C4-N3-C2	-3.92	120.69	126.34
1	A	2449	H2U	N3-C2-N1	3.91	120.79	116.65
57	y	55	PSU	C4-N3-C2	-3.89	120.73	126.34
55	w	20	H2U	C4-N3-C2	-3.86	122.59	125.79
34	a	1518	MA6	N3-C2-N1	-3.86	122.65	128.68
34	a	1407	5MC	CM5-C5-C6	-3.85	117.70	122.85
57	y	54	5MU	O4-C4-C5	-3.79	120.51	124.90
1	A	2504	PSU	C4-N3-C2	-3.74	120.96	126.34
1	A	1911	PSU	C4-N3-C2	-3.71	120.99	126.34
1	A	955	PSU	C4-N3-C2	-3.71	120.99	126.34
1	A	2449	H2U	O4'-C1'-N1	3.71	114.35	109.30
55	w	55	PSU	C4-N3-C2	-3.69	121.02	126.34
34	a	516	PSU	C4-N3-C2	-3.65	121.08	126.34
57	y	32	PSU	C4-N3-C2	-3.64	121.09	126.34
57	y	39	PSU	C4-N3-C2	-3.63	121.11	126.34
1	A	1962	5MC	CM5-C5-C6	-3.63	118.00	122.85
1	A	2580	PSU	C6-C5-C4	-3.61	115.67	118.20
1	A	746	PSU	C4-N3-C2	-3.60	121.16	126.34
57	y	37	MIA	C15-C14-C13	-3.59	112.28	122.65
1	A	2457	PSU	C4-N3-C2	-3.56	121.21	126.34
34	a	1518	MA6	C4-C5-N7	-3.52	105.73	109.40
34	a	1498	UR3	C1'-N1-C2	3.51	122.91	116.99
57	y	20	H2U	C4-N3-C2	-3.51	122.88	125.79
55	v	55	PSU	C6-C5-C4	-3.49	115.76	118.20
34	a	1407	5MC	C5-C4-N3	-3.49	117.91	121.67
1	A	955	PSU	C6-C5-C4	-3.47	115.77	118.20
1	A	955	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A	1618	6MZ	C3'-C2'-C1'	3.46	106.19	100.98
57	y	16	H2U	C4-N3-C2	-3.46	122.92	125.79
1	A	1917	PSU	C4-N3-C2	-3.45	121.37	126.34
1	A	2030	6MZ	C3'-C2'-C1'	3.45	106.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	C3'-C2'-C1'	3.44	105.64	101.64
55	v	55	PSU	C4-N3-C2	-3.43	121.40	126.34
55	w	8	4SU	C5-C4-S4	-3.42	120.07	124.47
55	v	20	H2U	C4-N3-C2	-3.41	122.96	125.79
1	A	2449	H2U	C5-C4-N3	3.41	120.48	116.65
1	A	2604	PSU	C4-N3-C2	-3.39	121.46	126.34
34	a	1518	MA6	C3'-C2'-C1'	3.38	106.07	100.98
57	y	37	MIA	C2-N1-C6	3.35	123.18	117.19
55	w	55	PSU	O2-C2-N1	-3.35	119.11	122.79
1	A	1962	5MC	C5-C4-N3	-3.34	118.07	121.67
1	A	747	5MC	C5-C4-N3	-3.34	118.07	121.67
1	A	2552	OMU	C5-C4-N3	3.33	119.82	114.84
1	A	1917	PSU	O2-C2-N1	-3.32	119.14	122.79
1	A	1618	6MZ	C9-N6-C6	-3.31	120.02	122.87
1	A	2504	PSU	O2-C2-N1	-3.30	119.16	122.79
57	y	39	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A	2030	6MZ	C9-N6-C6	-3.29	120.03	122.87
34	a	1519	MA6	N3-C2-N1	-3.29	123.54	128.68
57	y	8	4SU	C5-C4-S4	-3.29	120.23	124.47
57	y	54	5MU	C5M-C5-C4	3.27	122.37	118.77
34	a	516	PSU	O2-C2-N1	-3.27	119.19	122.79
34	a	967	5MC	C5-C4-N3	-3.26	118.16	121.67
1	A	2605	PSU	O2-C2-N1	-3.25	119.21	122.79
1	A	2580	PSU	C4-N3-C2	-3.24	121.66	126.34
55	w	54	5MU	C5M-C5-C4	3.24	122.33	118.77
57	y	32	PSU	O2-C2-N1	-3.23	119.23	122.79
1	A	2580	PSU	C3'-C2'-C1'	3.23	105.40	101.64
55	v	54	5MU	C5-C4-N3	3.22	118.06	115.31
57	y	8	4SU	C6-N1-C2	-3.21	116.89	120.99
1	A	2030	6MZ	N3-C2-N1	-3.20	123.68	128.68
1	A	2457	PSU	O2-C2-N1	-3.19	119.28	122.79
57	y	55	PSU	O2-C2-N1	-3.19	119.28	122.79
1	A	1618	6MZ	N3-C2-N1	-3.17	123.73	128.68
1	A	1917	PSU	C6-C5-C4	-3.17	115.98	118.20
1	A	1939	5MU	O4-C4-C5	-3.15	121.25	124.90
1	A	746	PSU	O2-C2-N1	-3.15	119.33	122.79
57	y	37	MIA	C4-C5-N7	-3.14	106.13	109.40
1	A	2605	PSU	C6-C5-C4	-3.14	116.00	118.20
1	A	2604	PSU	O2-C2-N1	-3.13	119.34	122.79
1	A	1911	PSU	C6-C5-C4	-3.10	116.03	118.20
55	w	54	5MU	O4-C4-C5	-3.09	121.32	124.90
1	A	2552	OMU	C1'-N1-C2	3.08	123.15	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	55	PSU	O2-C2-N1	-3.04	119.44	122.79
1	A	1962	5MC	O2-C2-N3	-3.03	117.40	122.33
1	A	745	1MG	O6-C6-C5	-3.02	118.85	124.19
55	w	55	PSU	C3'-C2'-C1'	3.00	105.13	101.64
1	A	2069	7MG	C5-C6-N1	2.98	116.24	110.99
57	y	37	MIA	C3'-C2'-C1'	2.96	105.43	100.98
57	y	55	PSU	C6-C5-C4	-2.95	116.14	118.20
1	A	1939	5MU	C5-C6-N1	-2.93	120.32	123.34
34	a	527	7MG	C5-C6-N1	2.93	116.14	110.99
34	a	1407	5MC	O2-C2-N3	-2.92	117.58	122.33
1	A	2498	OMC	O2-C2-N3	-2.91	117.60	122.33
55	v	54	5MU	C6-N1-C2	-2.91	118.35	121.30
57	y	46	7MG	C5-C6-N1	2.89	116.08	110.99
34	a	516	PSU	C6-C5-C4	-2.88	116.18	118.20
34	a	967	5MC	O2-C2-N3	-2.85	117.69	122.33
1	A	745	1MG	C5-C6-N1	2.83	118.16	113.90
57	y	20	H2U	C3'-C2'-C1'	2.82	106.79	101.43
1	A	1917	PSU	C3'-C2'-C1'	2.81	104.91	101.64
57	y	37	MIA	N3-C2-N1	-2.80	121.83	126.98
1	A	2504	PSU	C6-C5-C4	-2.80	116.24	118.20
34	a	966	2MG	C5-C6-N1	2.79	118.88	113.95
34	a	1402	4OC	C6-C5-C4	2.75	120.32	116.96
1	A	2552	OMU	O4-C4-C5	-2.74	120.34	125.16
34	a	1207	2MG	C5-C6-N1	2.74	118.78	113.95
1	A	2030	6MZ	C4-C5-N7	-2.71	106.57	109.40
34	a	1519	MA6	C10-N6-C6	-2.68	111.41	119.51
55	w	20	H2U	C5-C6-N1	-2.68	102.80	111.61
1	A	2449	H2U	C4-N3-C2	-2.68	123.57	125.79
1	A	1618	6MZ	C4-C5-N7	-2.67	106.61	109.40
1	A	2457	PSU	C6-C5-C4	-2.66	116.34	118.20
1	A	747	5MC	C5-C6-N1	-2.66	120.61	123.34
57	y	20	H2U	O4'-C1'-N1	2.64	112.90	109.30
55	w	8	4SU	C6-N1-C2	-2.62	117.65	120.99
1	A	2445	2MG	C5-C6-N1	2.61	118.56	113.95
57	y	20	H2U	C5-C4-N3	2.59	119.56	116.65
1	A	1915	3TD	C3'-C2'-C1'	2.57	104.63	101.64
57	y	32	PSU	C3'-C2'-C1'	2.56	104.62	101.64
1	A	1915	3TD	C10-N3-C4	2.55	121.60	117.69
34	a	1518	MA6	C9-N6-C6	-2.54	111.82	119.51
55	v	54	5MU	C5-C6-N1	-2.54	120.72	123.34
1	A	2503	2MA	C5-C6-N1	2.53	118.39	114.02
1	A	2580	PSU	O2-C2-N1	-2.53	120.00	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2498	OMC	O4'-C1'-N1	2.53	114.14	108.36
1	A	1835	2MG	C5-C6-N1	2.52	118.41	113.95
57	y	39	PSU	C6-C5-C4	-2.52	116.44	118.20
34	a	966	2MG	C8-N7-C5	2.51	107.78	102.99
57	y	8	4SU	O2-C2-N3	-2.51	116.83	121.50
1	A	2503	2MA	C8-N7-C5	2.50	107.75	102.99
34	a	1207	2MG	C8-N7-C5	2.49	107.73	102.99
1	A	2445	2MG	C8-N7-C5	2.49	107.73	102.99
55	v	20	H2U	C5-C4-N3	2.48	119.44	116.65
34	a	1516	2MG	C8-N7-C5	2.47	107.70	102.99
57	y	32	PSU	C6-C5-C4	-2.47	116.47	118.20
34	a	1402	4OC	C5-C4-N3	-2.46	118.63	122.59
1	A	745	1MG	C8-N7-C5	2.46	107.67	102.99
57	y	16	H2U	C5-C4-N3	2.46	119.41	116.65
34	a	1516	2MG	C5-C6-N1	2.45	118.28	113.95
1	A	746	PSU	C6-C5-C4	-2.44	116.49	118.20
1	A	1939	5MU	C5M-C5-C4	2.43	121.44	118.77
34	a	1407	5MC	O4'-C1'-N1	2.43	113.91	108.36
34	a	1498	UR3	C3U-N3-C2	2.42	121.55	117.31
34	a	966	2MG	C3'-C2'-C1'	2.41	104.60	100.98
34	a	527	7MG	CM7-N7-C5	2.40	132.59	126.40
55	v	54	5MU	O4-C4-C5	-2.39	122.13	124.90
57	y	16	H2U	O4'-C1'-N1	2.38	112.55	109.30
1	A	2552	OMU	O4'-C1'-N1	2.38	113.81	108.36
1	A	2552	OMU	O2-C2-N3	-2.38	117.07	121.50
1	A	2604	PSU	C6-C5-C4	-2.36	116.55	118.20
1	A	2552	OMU	C6-N1-C2	-2.36	117.98	120.99
55	v	7	4SU	C6-N1-C2	-2.35	117.98	120.99
55	w	54	5MU	C5M-C5-C6	-2.35	119.70	122.85
34	a	1402	4OC	O4'-C1'-N1	2.35	113.74	108.36
34	a	527	7MG	O4'-C1'-N9	2.33	112.47	109.30
34	a	1519	MA6	C10-N6-C9	-2.32	108.65	116.12
1	A	2069	7MG	O4'-C1'-N9	2.31	112.45	109.30
57	y	46	7MG	CM7-N7-C5	2.30	132.34	126.40
34	a	1402	4OC	O2-C2-N3	-2.30	118.59	122.33
55	v	54	5MU	O2-C2-N1	-2.29	119.74	122.79
1	A	2552	OMU	C2'-C1'-N1	-2.27	109.81	114.22
1	A	2251	OMG	C5-C6-N1	2.27	117.95	113.95
57	y	54	5MU	C5M-C5-C6	-2.26	119.83	122.85
1	A	1835	2MG	C8-N7-C5	2.25	107.28	102.99
55	w	54	5MU	C5-C6-N1	-2.24	121.04	123.34
55	v	55	PSU	C3'-C2'-C1'	2.22	104.22	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2069	7MG	O6-C6-C5	-2.22	122.09	127.54
57	y	55	PSU	C3'-C2'-C1'	2.22	104.22	101.64
1	A	2069	7MG	N2-C2-N1	2.21	121.43	116.71
1	A	2457	PSU	C3'-C2'-C1'	2.21	104.21	101.64
34	a	1207	2MG	O6-C6-C5	-2.19	120.10	124.37
55	w	54	5MU	C3'-C2'-C1'	2.18	105.57	101.43
1	A	1939	5MU	O2-C2-N1	-2.18	119.89	122.79
55	w	54	5MU	O4'-C1'-N1	2.17	113.33	108.36
34	a	527	7MG	O6-C6-C5	-2.17	122.22	127.54
1	A	1939	5MU	O4'-C1'-N1	2.17	113.32	108.36
57	y	16	H2U	C3'-C2'-C1'	2.14	105.49	101.43
34	a	967	5MC	C3'-C2'-C1'	2.13	105.48	101.43
57	y	54	5MU	C1'-N1-C2	2.12	121.41	117.57
34	a	1498	UR3	C6-N1-C2	-2.12	119.89	121.79
57	y	8	4SU	C1'-N1-C2	2.11	121.39	117.57
1	A	747	5MC	O2-C2-N3	-2.10	118.91	122.33
55	v	7	4SU	O4'-C1'-N1	2.10	113.16	108.36
1	A	2069	7MG	N2-C2-N3	-2.10	115.65	119.73
1	A	2251	OMG	C8-N7-C5	2.08	106.94	102.99
1	A	747	5MC	O4'-C1'-N1	2.07	113.09	108.36
1	A	2069	7MG	CM7-N7-C5	2.06	131.72	126.40
55	v	54	5MU	O2-C2-N3	-2.06	117.66	121.50
55	w	54	5MU	O2-C2-N3	-2.05	117.68	121.50
57	y	46	7MG	O6-C6-C5	-2.05	122.52	127.54
1	A	2069	7MG	C6-C5-C4	-2.05	118.40	122.62
55	w	55	PSU	C6-C5-C4	-2.03	116.78	118.20
1	A	745	1MG	C3'-C2'-C1'	2.03	104.03	100.98
1	A	2069	7MG	C6-C5-N7	2.02	135.09	131.91
57	y	16	H2U	C5-C6-N1	-2.00	105.03	111.61

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	C2'-C1'-C5-C6
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	1962	5MC	C3'-C4'-C5'-O5'

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

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Mol	Chain	Res	Type	Atoms
1	A	2457	PSU	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
34	a	527	7MG	C4'-C5'-O5'-P
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	20	H2U	C2'-C1'-N1-C6
55	w	8	4SU	O4'-C1'-N1-C2
1	A	2457	PSU	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
34	a	516	PSU	O4'-C1'-C5-C4
57	y	32	PSU	O4'-C1'-C5-C4
57	y	16	H2U	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C1'-N9-C8
1	A	1939	5MU	O4'-C4'-C5'-O5'
57	y	8	4SU	C2'-C1'-N1-C2
1	A	746	PSU	O4'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
55	w	20	H2U	C2'-C1'-N1-C2
55	w	55	PSU	O4'-C1'-C5-C6
57	y	32	PSU	O4'-C1'-C5-C6
1	A	1939	5MU	C3'-C4'-C5'-O5'
57	y	8	4SU	O4'-C4'-C5'-O5'
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 monosaccharides 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
62	PHE	z	401	-	10,11,12	0.43	0	10,13,15	0.33	0
63	GNP	z	402	60	29,34,34	2.53	6 (20%)	33,54,54	2.00	9 (27%)
59	FME	A	3001	-	8,9,10	0.65	0	7,9,11	2.06	2 (28%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	9.63	1.61	1.46
63	z	402	GNP	C5-C6	4.52	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	-3.18	1.48	1.56
63	z	402	GNP	C5-C4	2.42	1.47	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	5.14	121.22	115.36
63	z	402	GNP	C4-C5-C6	-4.37	116.63	120.80
59	A	3001	FME	C-CA-N	4.18	117.28	109.73
63	z	402	GNP	C2-N1-C6	3.64	121.71	115.93
63	z	402	GNP	PB-O3A-PA	-3.53	120.19	132.62
63	z	402	GNP	N3-C2-N1	-3.40	122.68	127.22
63	z	402	GNP	C5-C6-N1	-3.27	118.96	123.43
63	z	402	GNP	O1B-PB-N3B	-2.84	107.58	111.77
63	z	402	GNP	C4-C5-N7	-2.65	106.64	109.40
59	A	3001	FME	O1-CN-N	-2.11	119.72	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
63	z	402	GNP	O3A-PB-N3B	2.04	112.24	106.59

There are no chirality outliers.

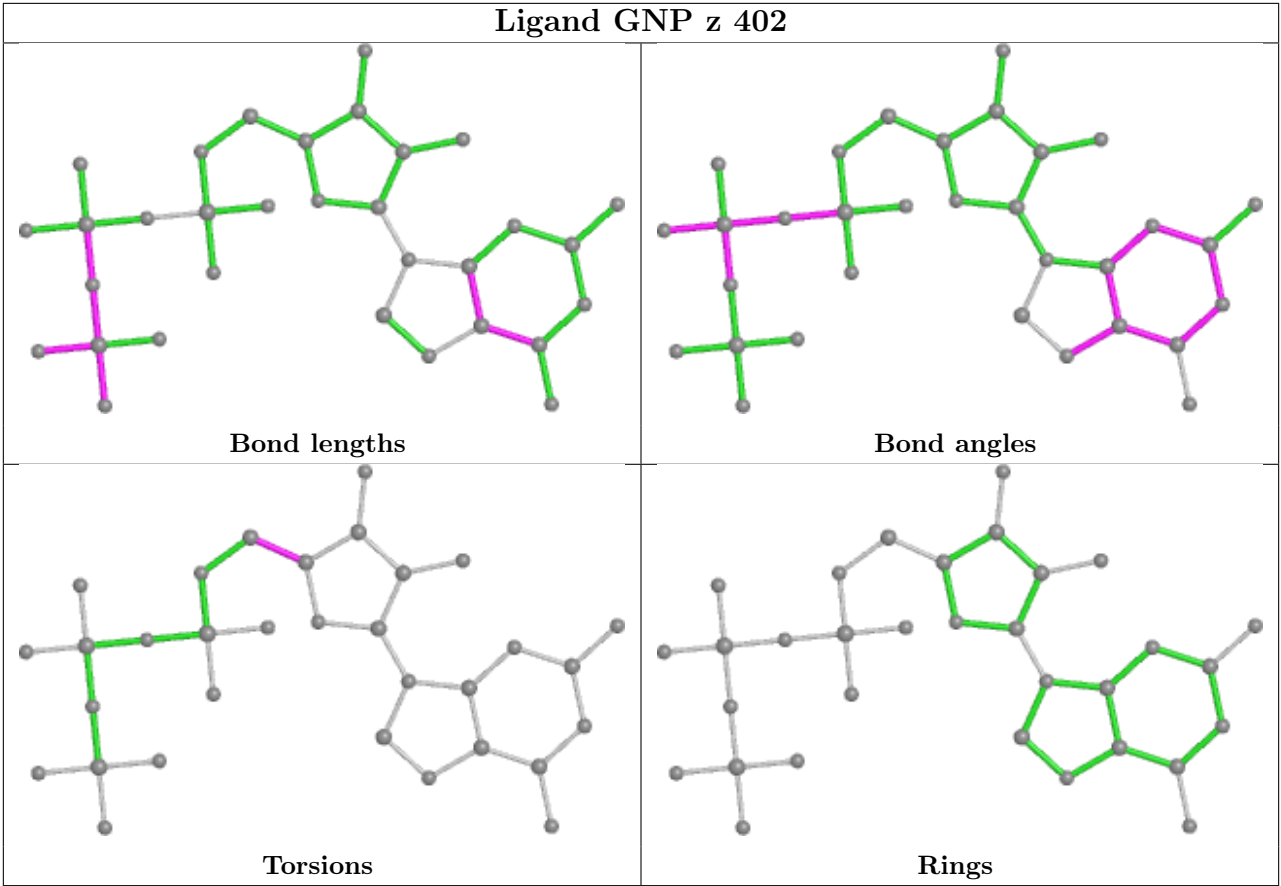
All (5) torsion outliers are listed below:

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'
59	A	3001	FME	CA-CB-CG-SD
63	z	402	GNP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

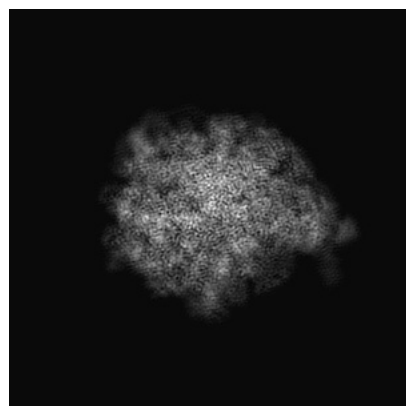
6 Map visualisation [i](#)

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.

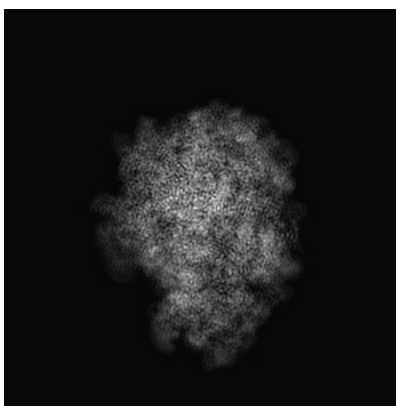
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

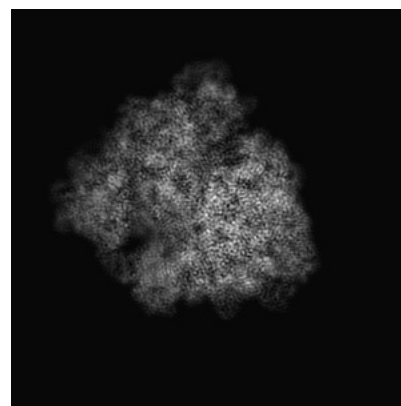
6.1.1 Primary map



X

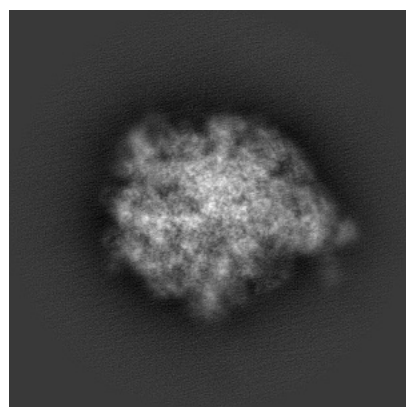


Y

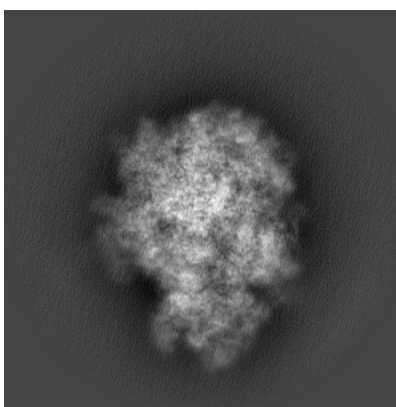


Z

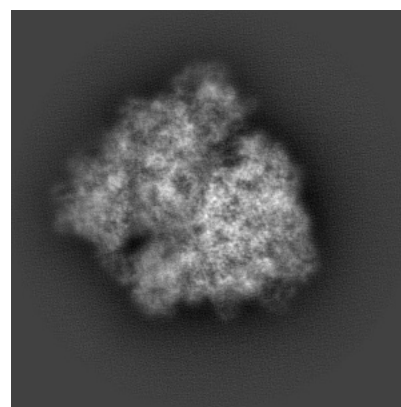
6.1.2 Raw map



X



Y

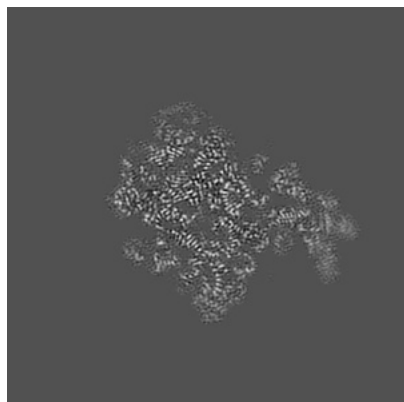


Z

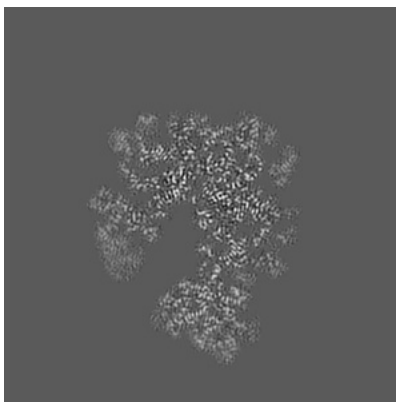
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

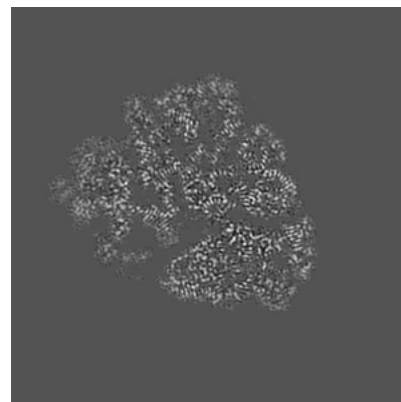
6.2.1 Primary map



X Index: 199

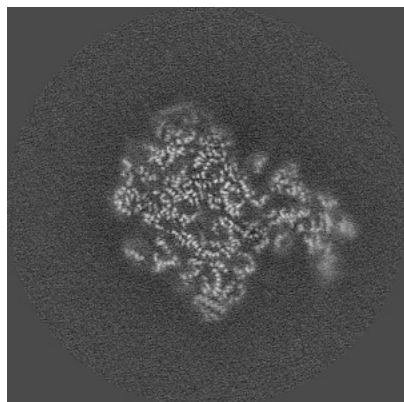


Y Index: 199

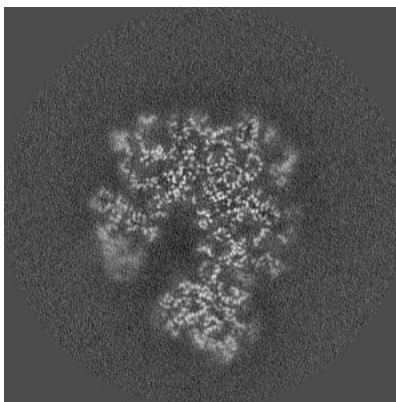


Z Index: 199

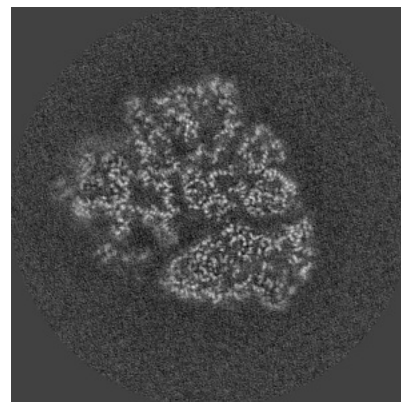
6.2.2 Raw map



X Index: 199



Y Index: 199

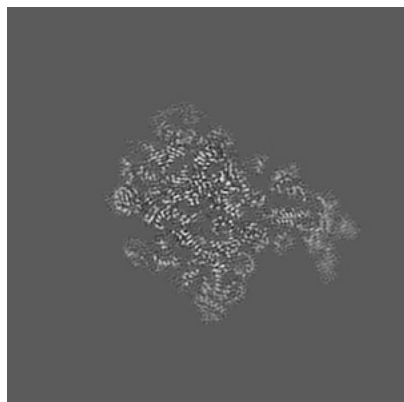


Z Index: 199

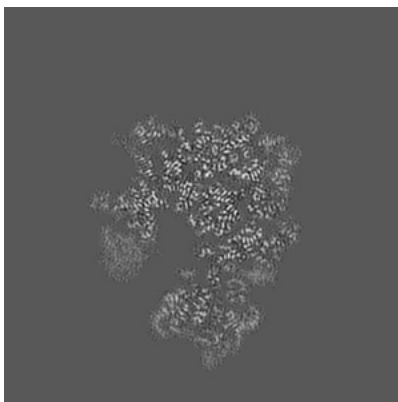
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

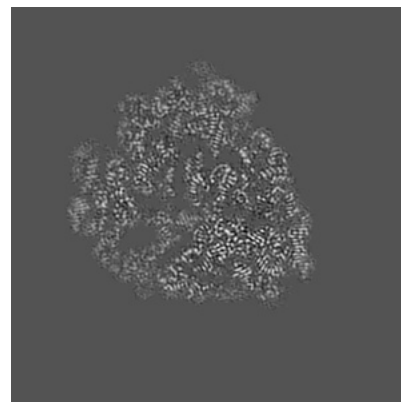
6.3.1 Primary map



X Index: 200

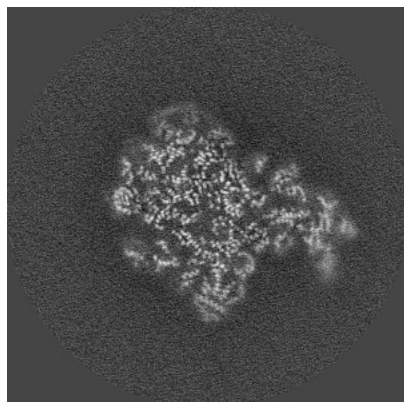


Y Index: 208

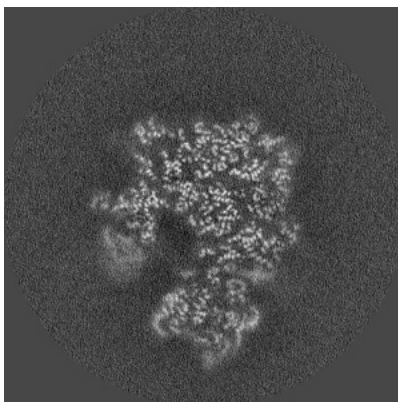


Z Index: 191

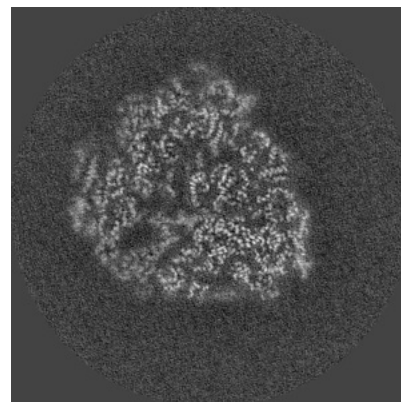
6.3.2 Raw map



X Index: 200



Y Index: 208



Z Index: 190

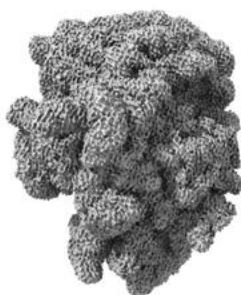
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

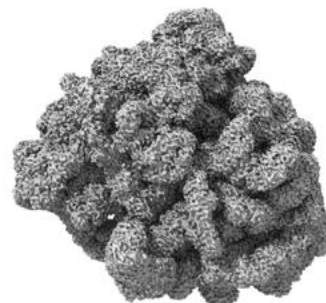
6.4.1 Primary map



X



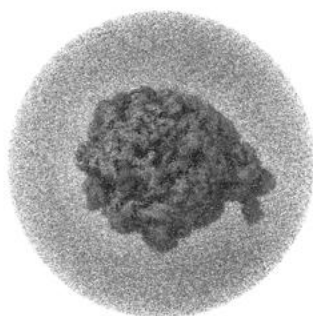
Y



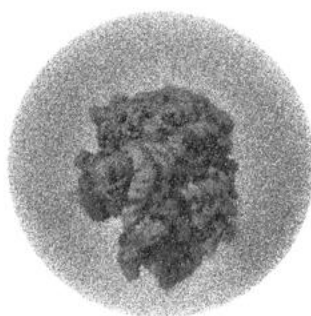
Z

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.

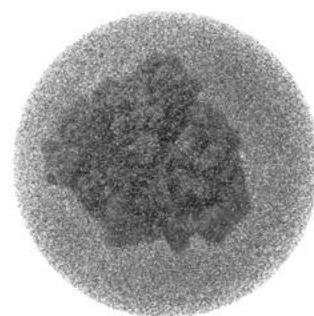
6.4.2 Raw map



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.

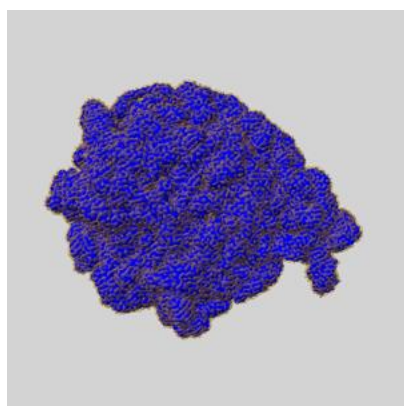
6.5 Mask visualisation [i](#)

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

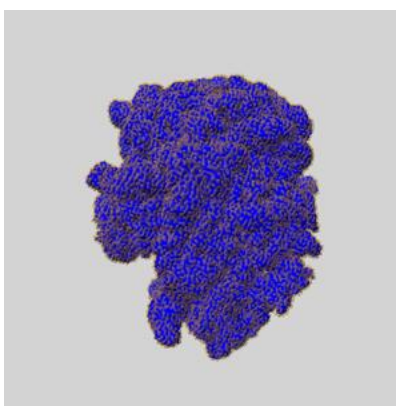
A mask typically either:

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

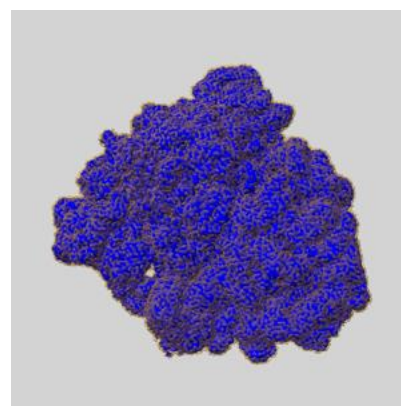
6.5.1 emd_8813_msk_1.map [i](#)



X



Y

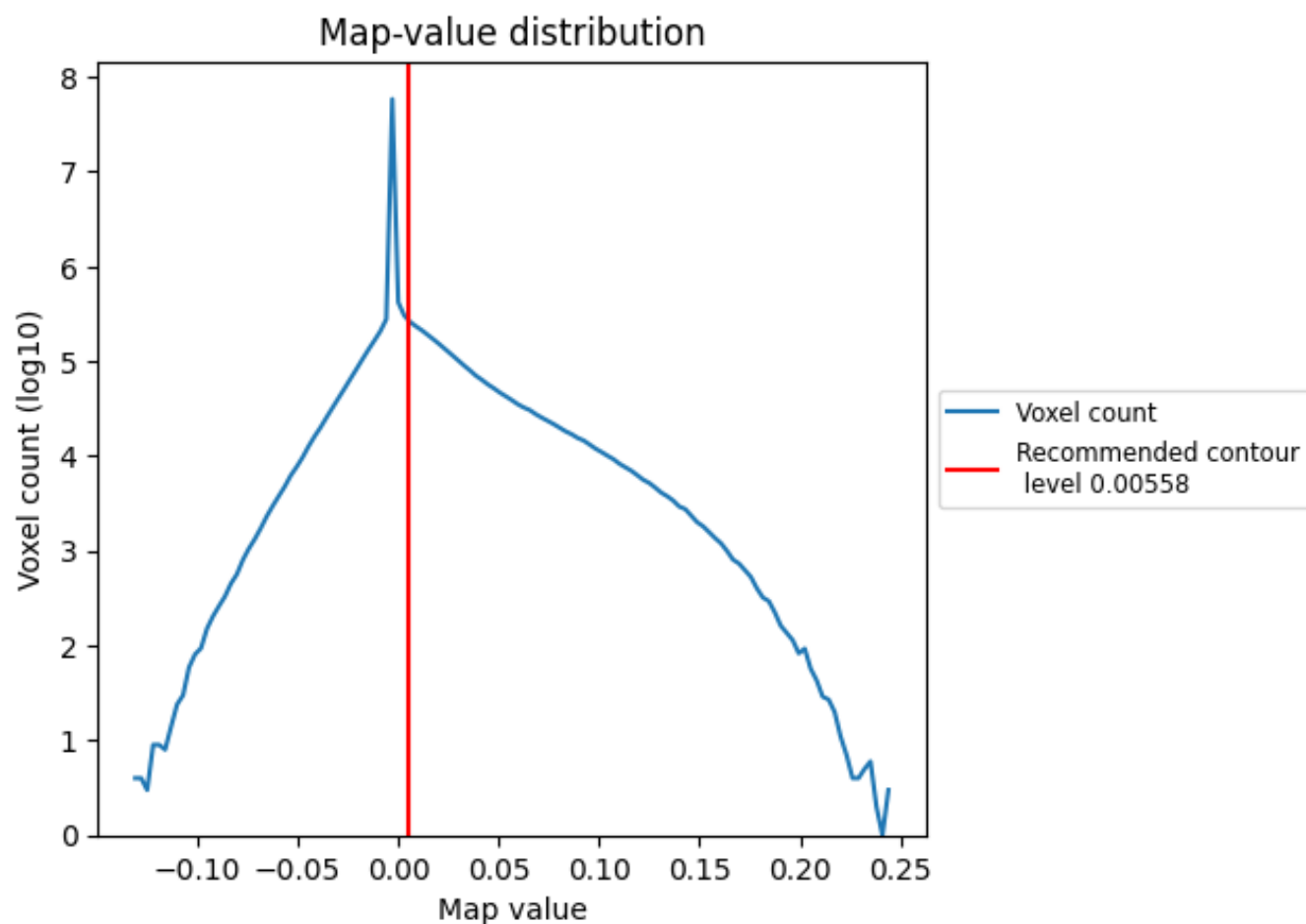


Z

7 Map analysis [i](#)

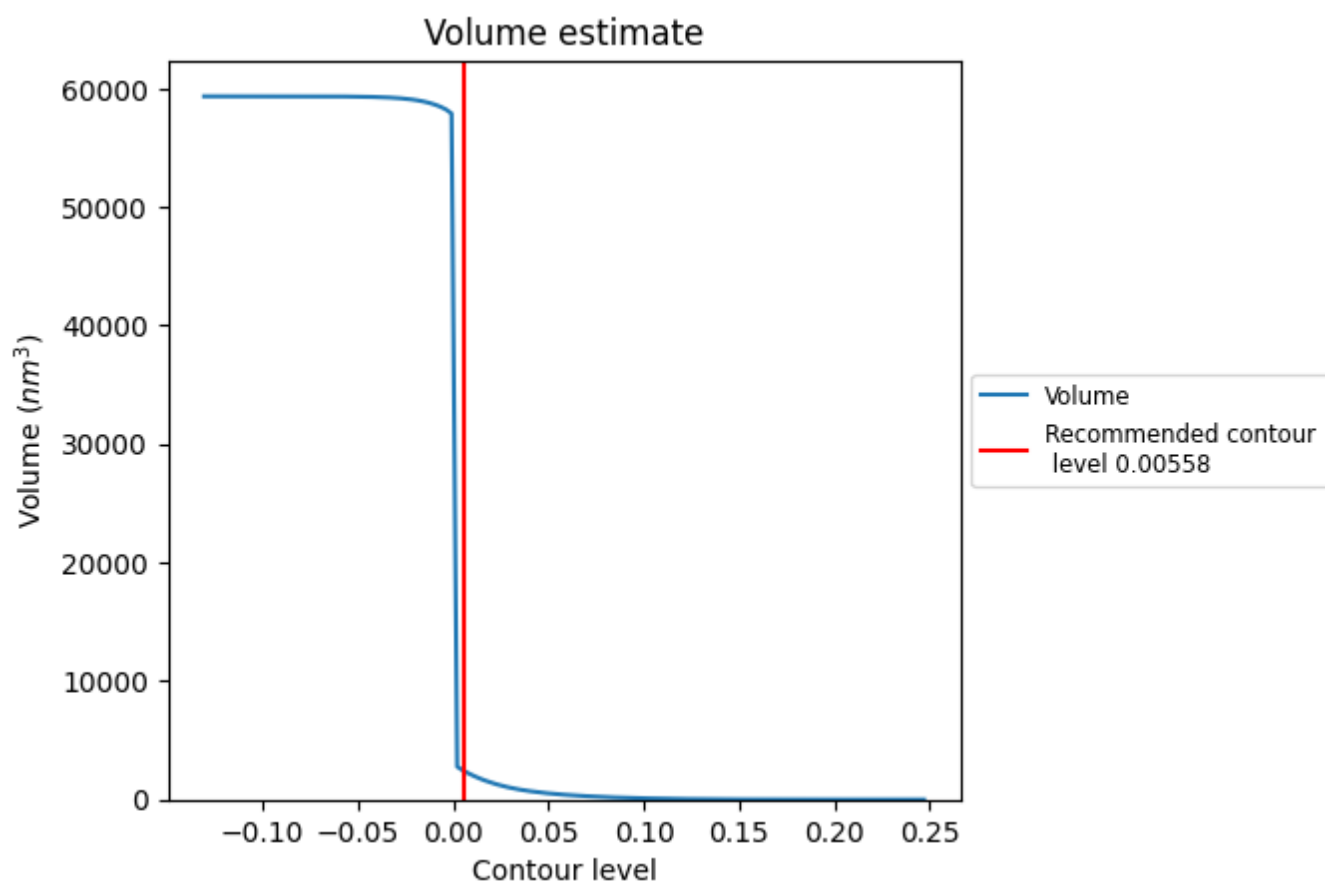
This section contains the results of statistical analysis of the map.

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.

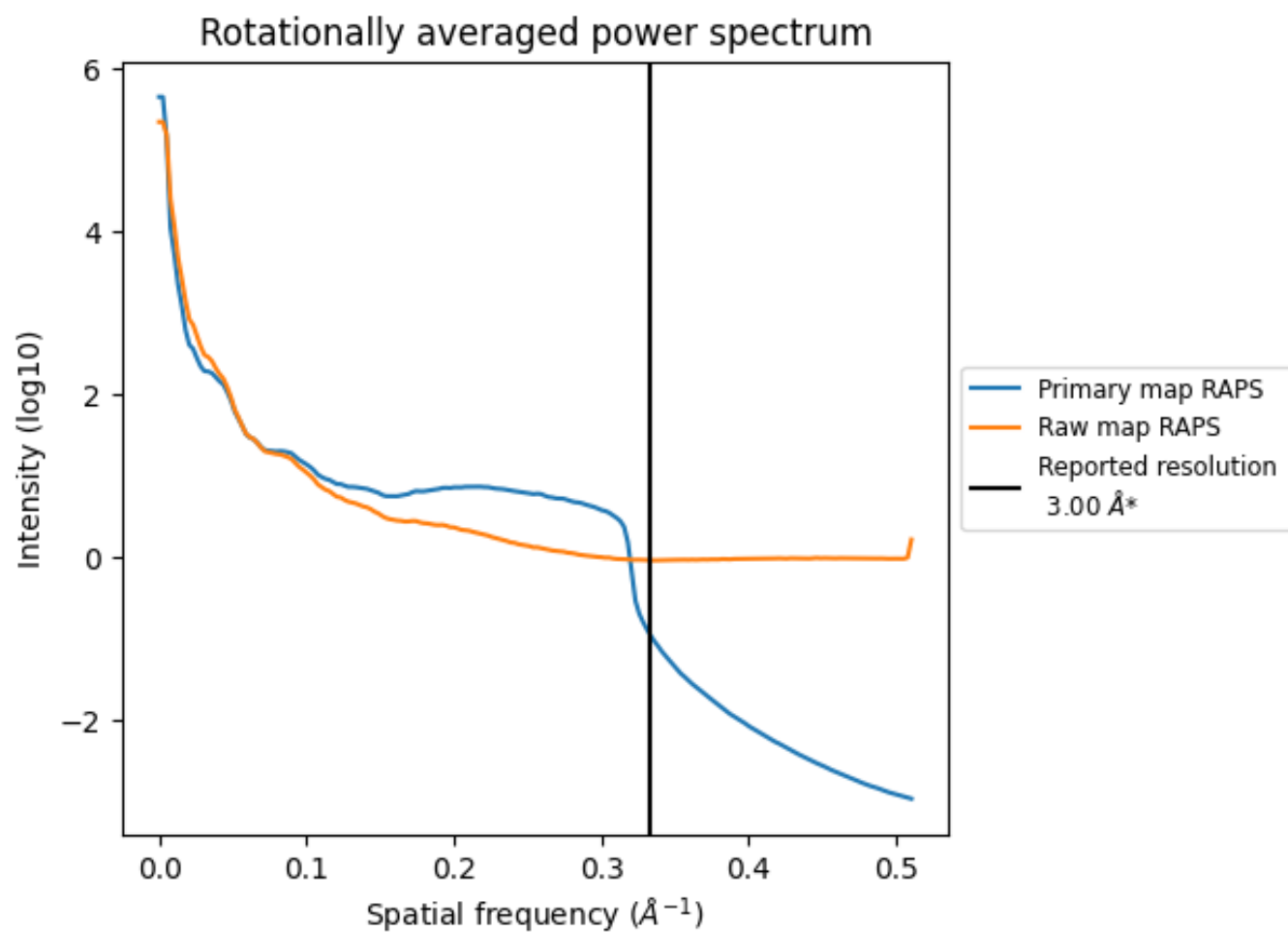
7.2 Volume estimate [i](#)



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 [i](#)

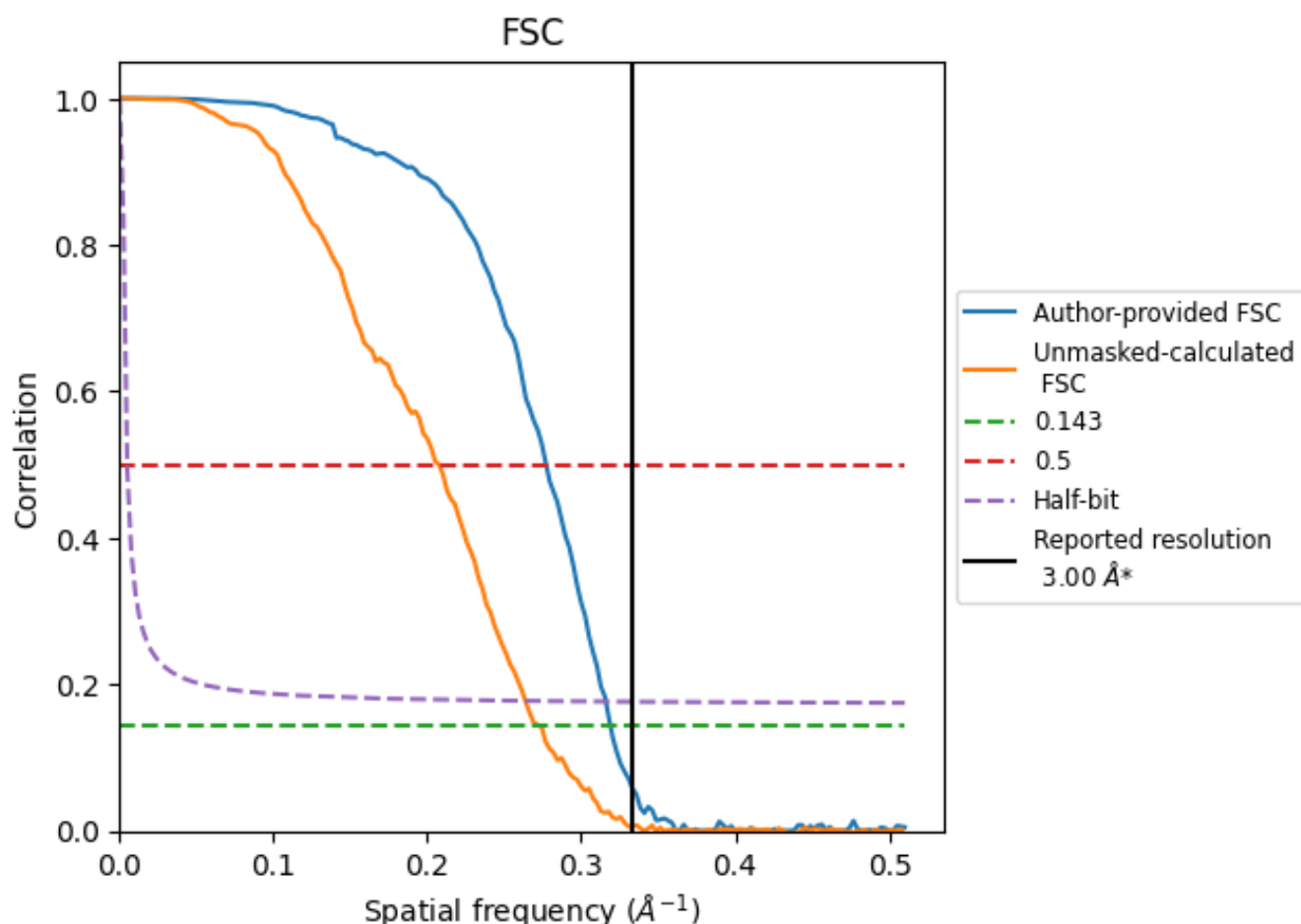


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

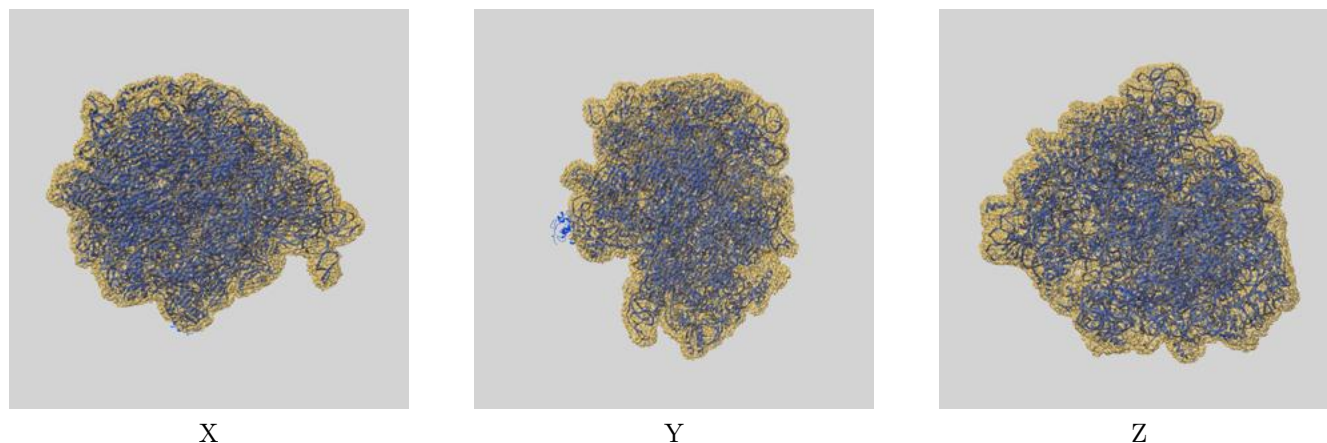
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.13	3.61	3.16
Unmasked-calculated*	3.66	4.82	3.79

*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](#)

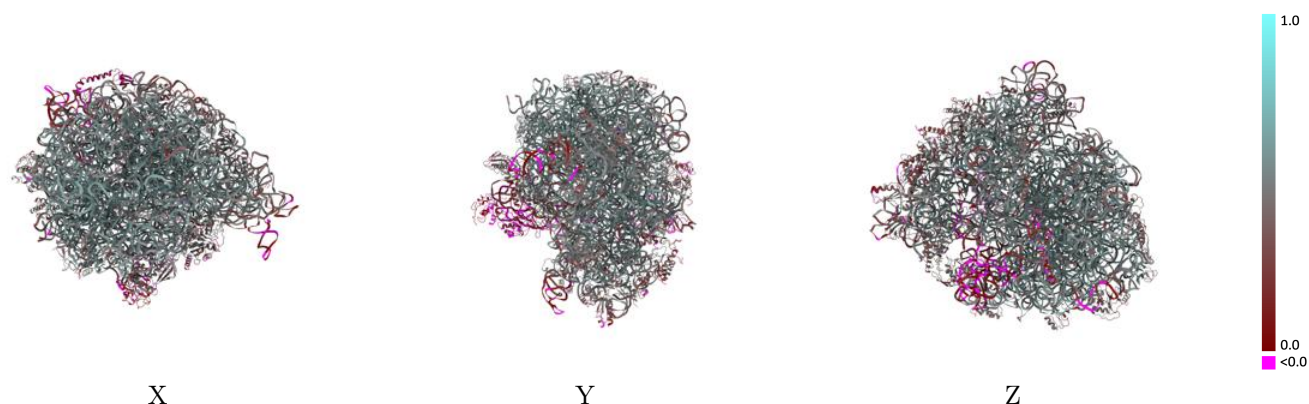
This section contains information regarding the fit between EMDB map EMD-8813 and PDB model 5WDT. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



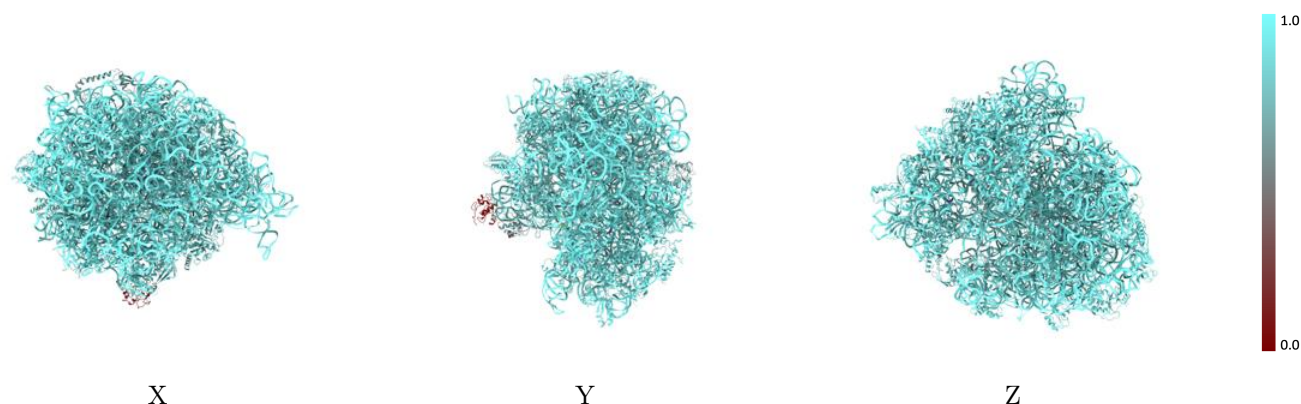
The images above show the 3D surface view of the map at the recommended contour level 0.00558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



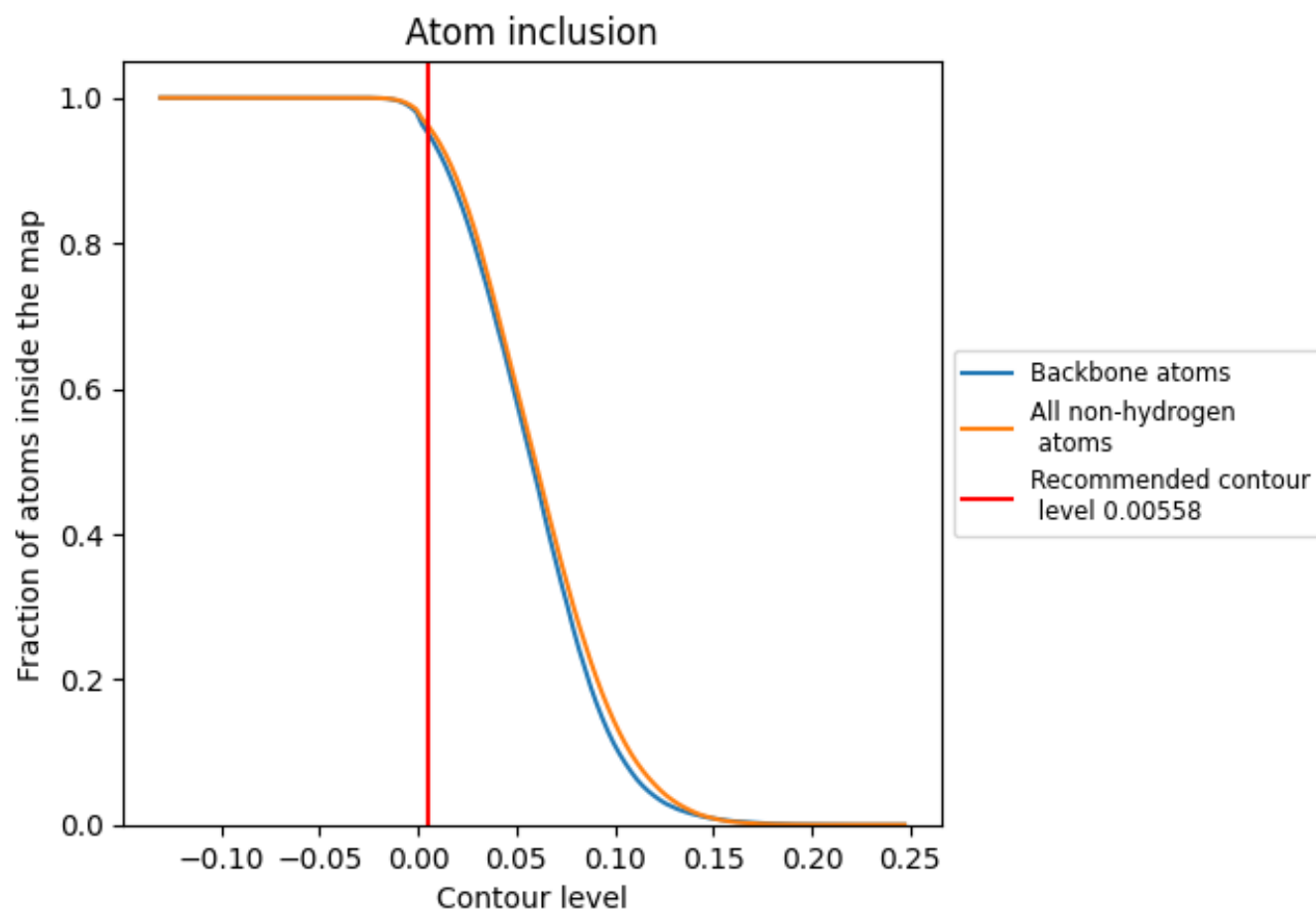
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.9429	 0.4710
1	 0.9535	 0.4730
2	 0.9681	 0.5660
3	 0.9676	 0.5520
4	 0.9761	 0.5170
5	 0.1952	 0.0080
6	 0.8806	 0.2830
A	 0.9857	 0.5100
B	 0.9950	 0.5060
C	 0.9658	 0.5260
D	 0.9680	 0.5190
E	 0.9505	 0.4730
F	 0.9272	 0.3960
G	 0.9405	 0.3910
H	 0.7409	 0.1690
I	 0.6252	 0.0170
J	 0.9716	 0.5140
K	 0.9376	 0.4980
L	 0.9459	 0.4800
M	 0.9549	 0.4980
N	 0.9694	 0.5250
O	 0.9571	 0.4340
P	 0.9403	 0.4850
Q	 0.9721	 0.5400
R	 0.9394	 0.4660
S	 0.9432	 0.5010
T	 0.9301	 0.4440
U	 0.9478	 0.4300
V	 0.9378	 0.4460
W	 0.9676	 0.5310
X	 0.9518	 0.5040
Y	 0.9296	 0.4080
Z	 0.9505	 0.4930
a	 0.9897	 0.4890



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Chain	Atom inclusion	Q-score
b	 0.9039	 0.3380
c	 0.9449	 0.4310
d	 0.9346	 0.4110
e	 0.9444	 0.4610
f	 0.9146	 0.3890
g	 0.9152	 0.3550
h	 0.9511	 0.4730
i	 0.9216	 0.3720
j	 0.9264	 0.3410
k	 0.9467	 0.4480
l	 0.9448	 0.4870
m	 0.9395	 0.4100
n	 0.9551	 0.4370
o	 0.9536	 0.4570
p	 0.9314	 0.4280
q	 0.9288	 0.4380
r	 0.9183	 0.4040
s	 0.9534	 0.4390
t	 0.9432	 0.4210
u	 0.8108	 0.2700
v	 0.9680	 0.4680
w	 0.8188	 0.1030
x	 0.9842	 0.4830
y	 0.9487	 0.3620
z	 0.8848	 0.3280