



Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 09:21 PM EDT

PDB ID : 5WF0
EMDB ID : EMD-8826
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C2)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-11
Resolution : 3.60 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

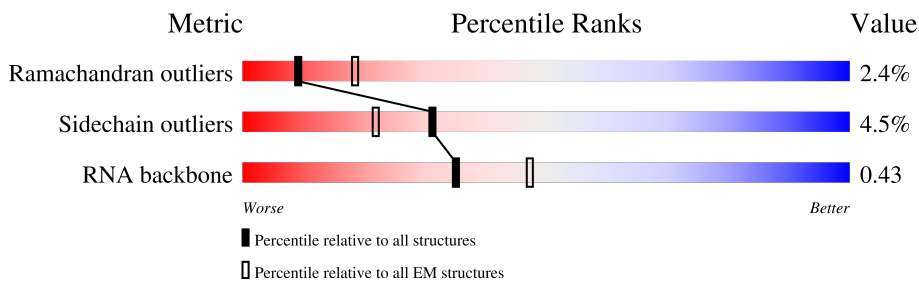
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	


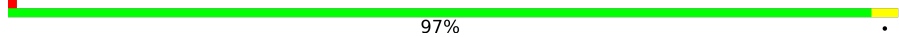
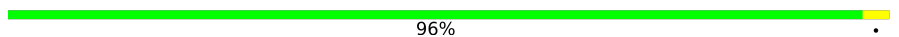
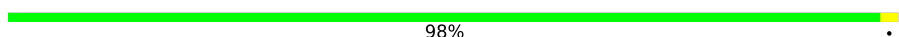

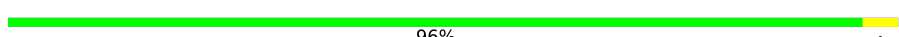




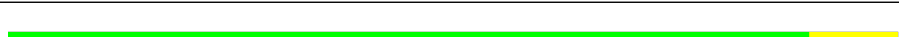


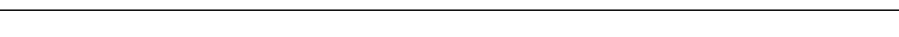
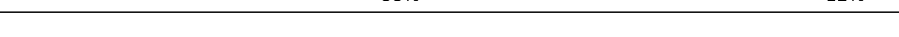
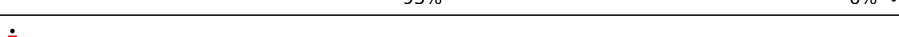
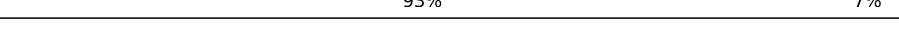

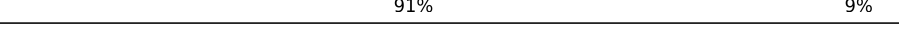
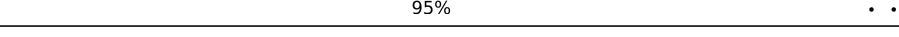





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Mol	Chain	Length	Quality of chain
9	I	141	16% 91% 9%
10	J	141	94% 6%
11	K	122	92% 7%
12	L	143	92% 8%
13	M	136	94% 6%
14	N	119	95% ..
15	O	116	97% ..
16	P	114	99% .
17	Q	115	97% .
18	R	102	92% 7%
19	S	109	95% 5%
20	T	92	92% 8%
21	U	102	91% 9%
22	V	92	98% .
23	W	75	92% 8%
24	X	77	100%
25	Y	60	97% .
26	Z	56	96% .
27	0	55	98% .
28	1	51	92% 8%
29	2	45	91% 9%
30	3	64	95% 5%
31	4	38	100%
32	5	131	76% 92% 8%
33	6	66	89% 11%

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Mol	Chain	Length	Quality of chain
34	a	1540	 69% 30%
35	b	218	 97%
36	c	206	 96%
37	d	205	 98%
38	e	157	 95% 5%
39	f	100	 96%
40	g	151	 91% 8%
41	h	129	 95% 5%
42	i	127	 92% 7%
43	j	98	 90% 10%
44	k	116	 90% 10%
45	l	121	 91% 8%
46	m	115	 92% 8%
47	n	101	 88% 12%
48	o	88	 93% 6%
49	p	82	 93% 7%
50	q	80	 88% 12%
51	r	65	 91% 9%
52	s	79	 95%
53	t	85	 87% 13%
54	u	65	 77% 22%
55	v	77	 73% 25%
55	w	77	 52% 42% 6%
56	x	12	 75% 25%
57	y	76	 92% 54% 41% 5%

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Mol	Chain	Length	Quality of chain
58	z	393	 <p>96% 97%</p>

2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 154600 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
			Total	C	N	O	P		
1	A	2900	62277	27788	11459	20130	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	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 1.

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	0	0
			1156	719	218	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
			Total	C	N	O	S		
47	n	101	810	502	165	140	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

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

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

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

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

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

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

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

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

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

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

- 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	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
55	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- 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	43	84	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	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	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

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



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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	A	1001	1001	1001	0
60	B	34	34	34	0
60	D	2	2	2	0
60	E	2	2	2	0
60	L	3	3	3	0
60	M	1	1	1	0
60	N	2	2	2	0
60	Q	2	2	2	0
60	T	1	1	1	0
60	W	2	2	2	0
60	X	2	2	2	0

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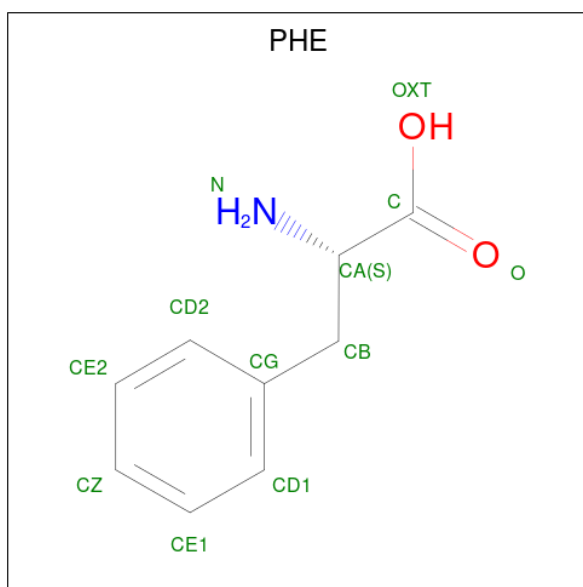
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Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	a	402	Total 402	Mg 402	0
60	d	3	Total 3	Mg 3	0
60	g	1	Total 1	Mg 1	0
60	i	2	Total 2	Mg 2	0
60	k	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	o	2	Total 2	Mg 2	0
60	t	3	Total 3	Mg 3	0
60	v	8	Total 8	Mg 8	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0

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

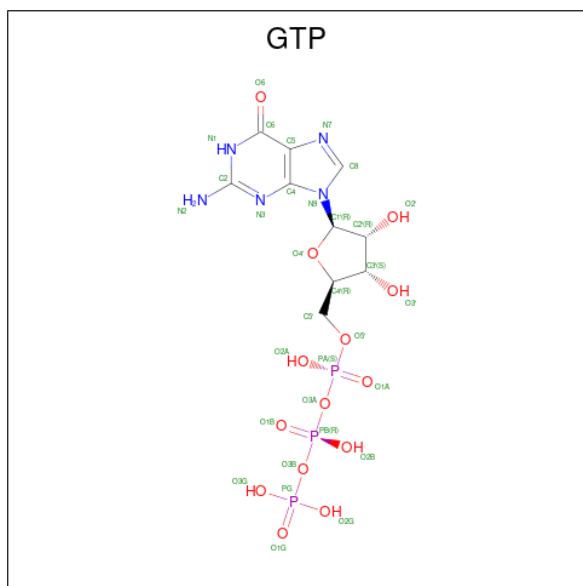
Mol	Chain	Residues	Atoms		AltConf
61	A	4	Total 4	K 4	0
61	a	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



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

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	5	14	3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	463	Total O 463 463	0
64	B	11	Total O 11 11	0
64	C	5	Total O 5 5	0
64	D	1	Total O 1 1	0
64	E	1	Total O 1 1	0
64	G	3	Total O 3 3	0
64	J	2	Total O 2 2	0
64	L	3	Total O 3 3	0
64	M	2	Total O 2 2	0
64	N	4	Total O 4 4	0
64	O	1	Total O 1 1	0
64	Q	2	Total O 2 2	0
64	S	1	Total O 1 1	0
64	W	2	Total O 2 2	0
64	X	1	Total O 1 1	0
64	Z	2	Total O 2 2	0
64	0	1	Total O 1 1	0
64	3	2	Total O 2 2	0
64	a	160	Total O 160 160	0
64	d	1	Total O 1 1	0
64	i	1	Total O 1 1	0
64	s	3	Total O 3 3	0

Continued on next page...

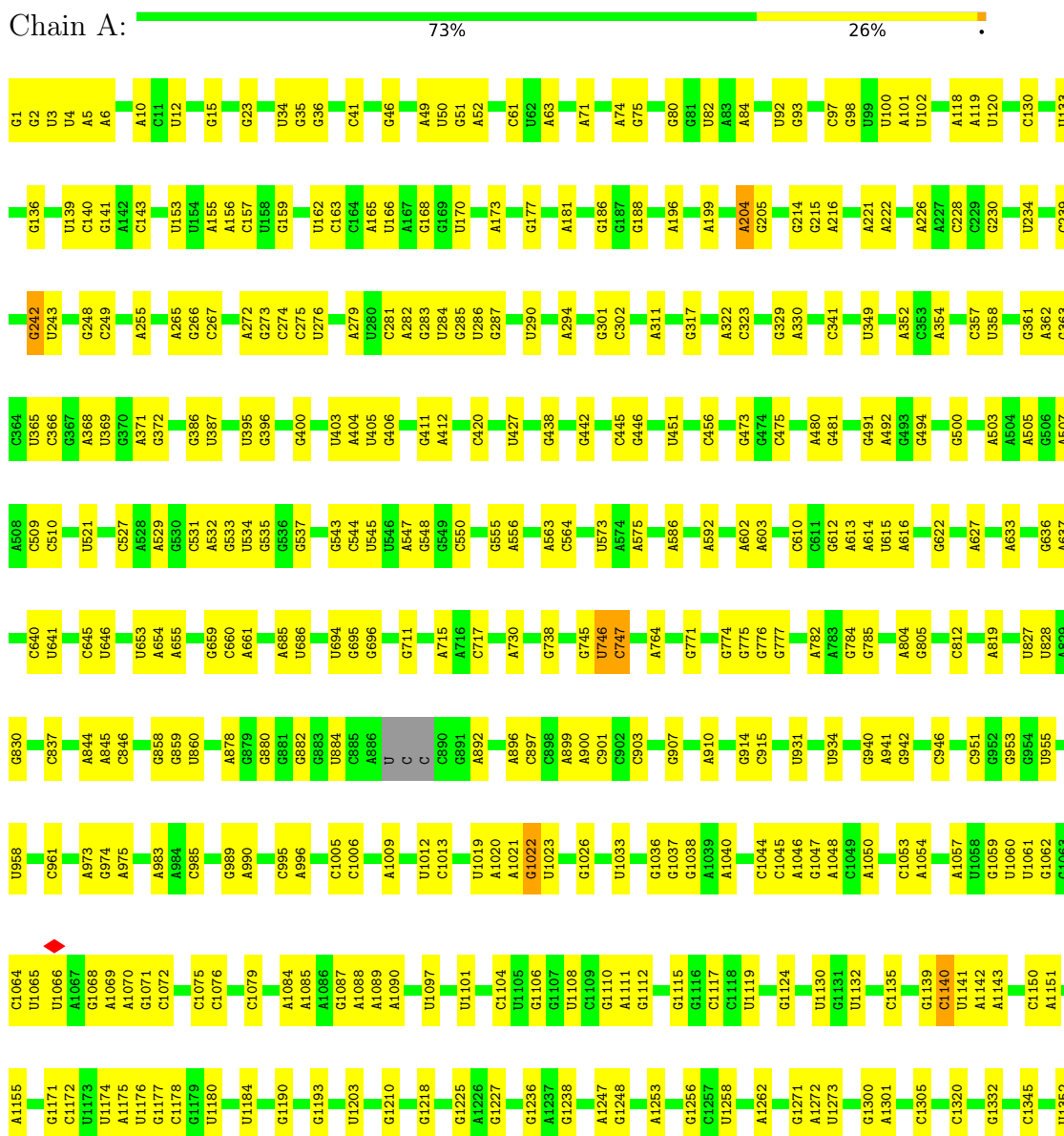
Continued from previous page...

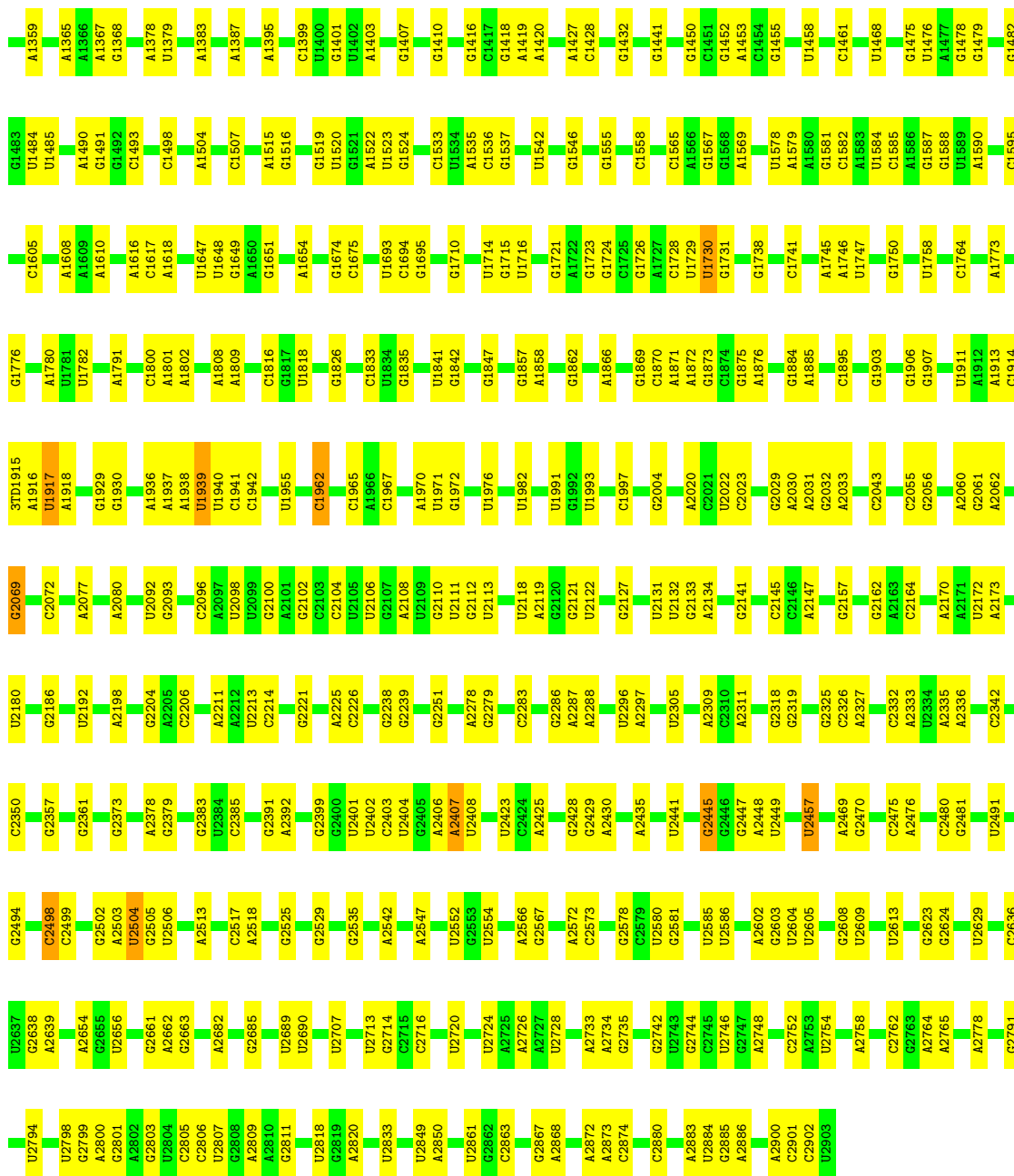
Mol	Chain	Residues	Atoms		AltConf
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	w	2	Total 2	O 2	0

3 Residue-property plots i

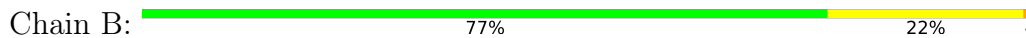
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA





• Molecule 2: 5S rRNA

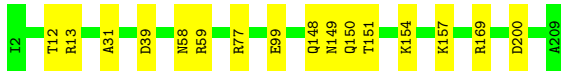


• Molecule 3: 50S ribosomal protein L2





- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



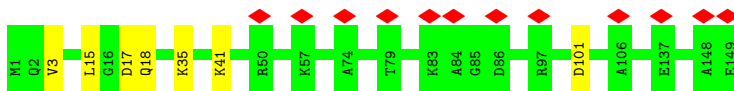
- Molecule 6: 50S ribosomal protein L5



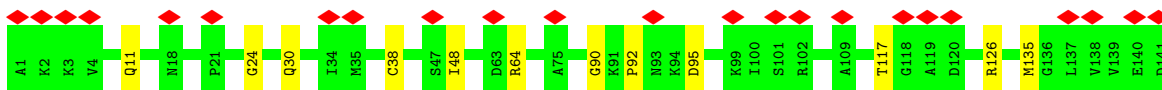
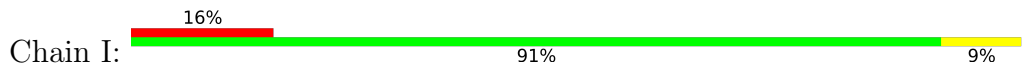
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9

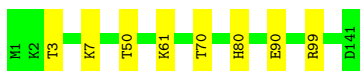


- Molecule 9: 50S ribosomal protein L11



- Molecule 10: 50S ribosomal protein L13





- Molecule 11: 50S ribosomal protein L14

Chain K: 92% 7%



- Molecule 12: 50S ribosomal protein L15

Chain L: 92% 8%



- Molecule 13: 50S ribosomal protein L16

Chain M: 94% 6%



- Molecule 14: 50S ribosomal protein L17

Chain N: 95% 2%



- Molecule 15: 50S ribosomal protein L18

Chain O: 97% 2%



- Molecule 16: 50S ribosomal protein L19

Chain P: 99% 1%



- Molecule 17: 50S ribosomal protein L20

Chain Q: 97% 2%



- Molecule 18: 50S ribosomal protein L21

Chain R: 92% 7%



- Molecule 19: 50S ribosomal protein L22

Chain S: 95% 5%



- Molecule 20: 50S ribosomal protein L23

Chain T: 92% 8%



- Molecule 21: 50S ribosomal protein L24

Chain U: 91% 9%



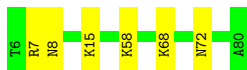
- Molecule 22: 50S ribosomal protein L25

Chain V: 98%



- Molecule 23: 50S ribosomal protein L27

Chain W: 92% 8%



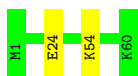
- Molecule 24: 50S ribosomal protein L28

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L29

Chain Y:  97%



- Molecule 26: 50S ribosomal protein L30

Chain Z:  96%



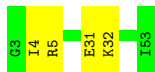
- Molecule 27: 50S ribosomal protein L32

Chain 0:  98%




- Molecule 28: 50S ribosomal protein L33

Chain 1:  92%



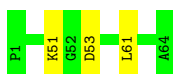
- Molecule 29: 50S ribosomal protein L34

Chain 2:  91%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  95%

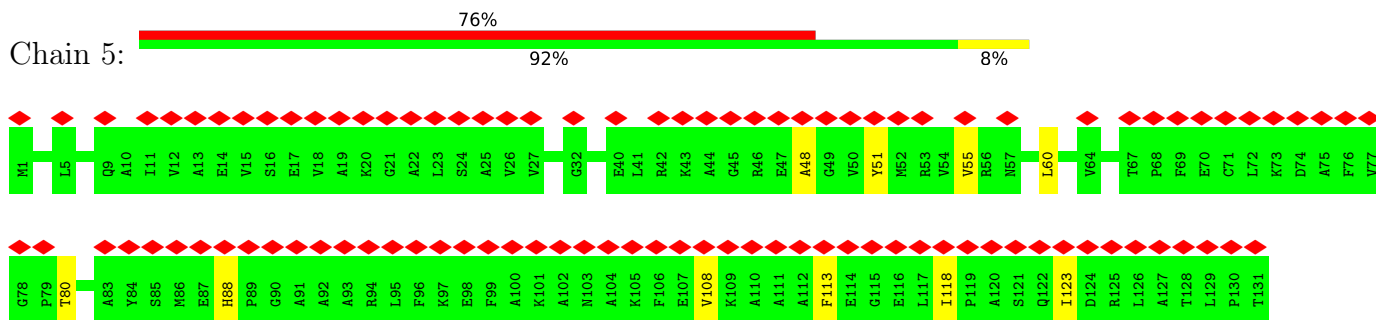


- Molecule 31: 50S ribosomal protein L36 1

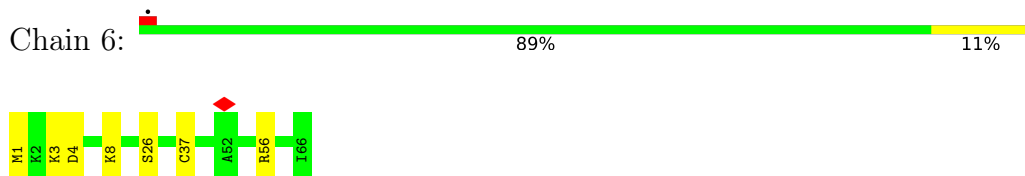
Chain 4:  100%

There are no outlier residues recorded for this chain.

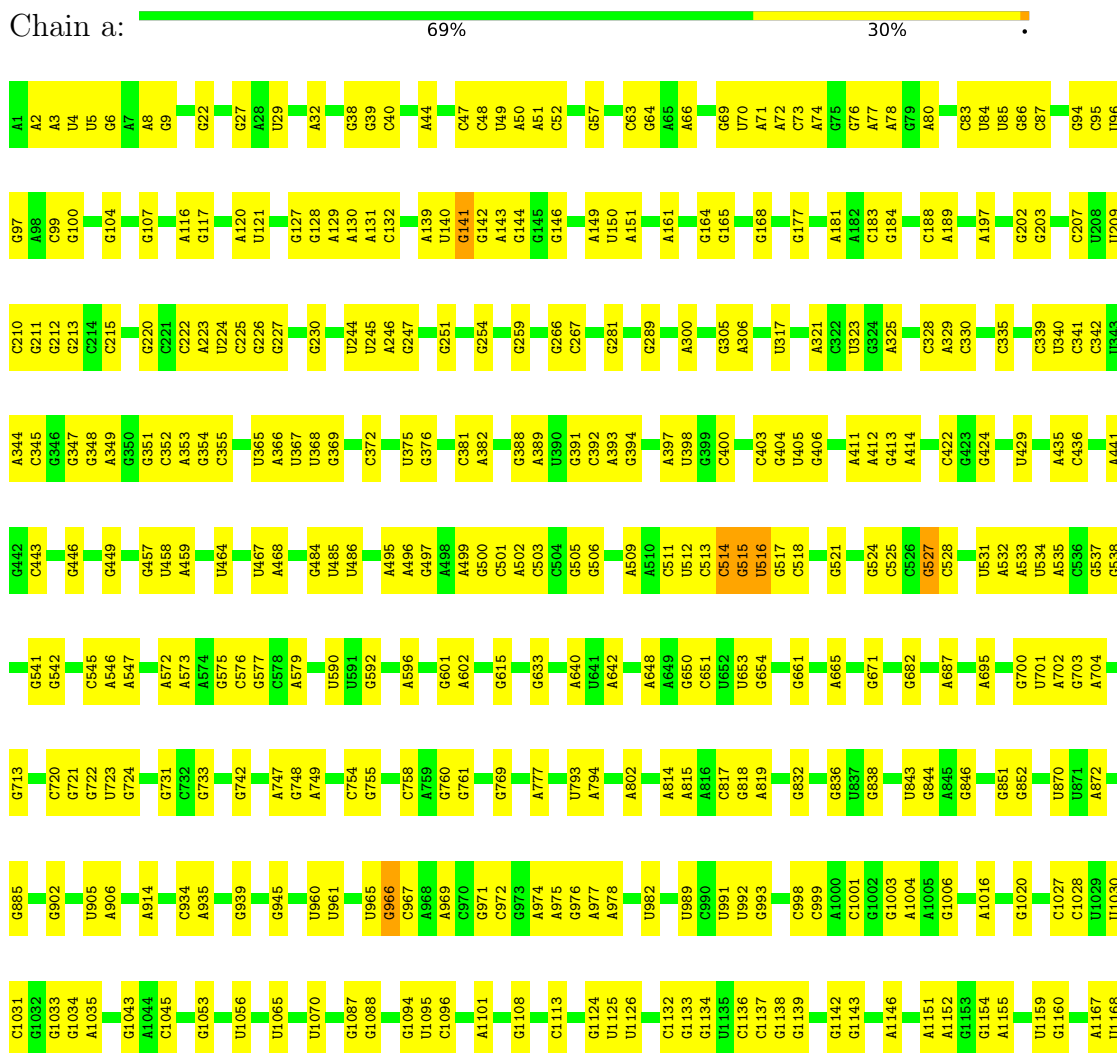
- Molecule 32: 50S ribosomal protein L10

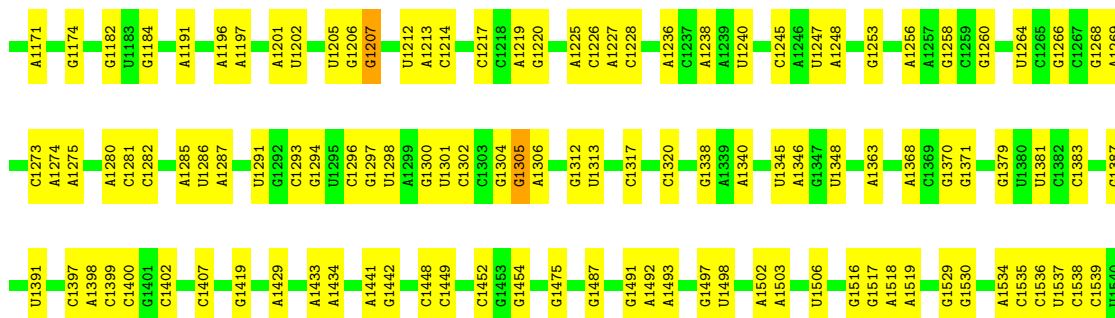


• Molecule 33: 50S ribosomal protein L31

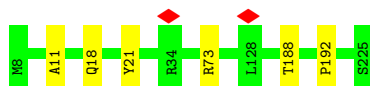


• Molecule 34: 16S rRNA





- Molecule 35: 30S ribosomal protein S2



- Molecule 36: 30S ribosomal protein S3



- Molecule 37: 30S ribosomal protein S4



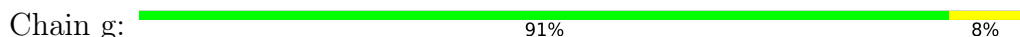
- Molecule 38: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7

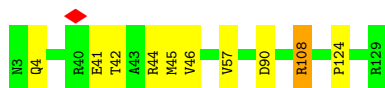
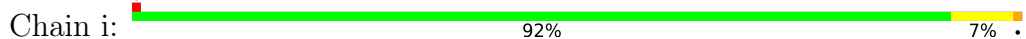




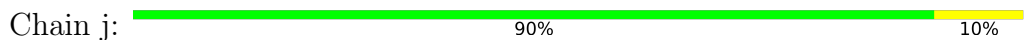
- Molecule 41: 30S ribosomal protein S8



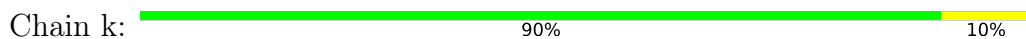
- Molecule 42: 30S ribosomal protein S9



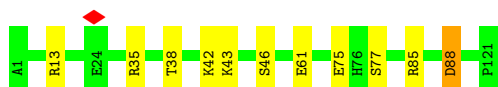
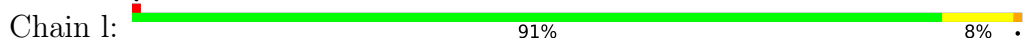
- Molecule 43: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S11



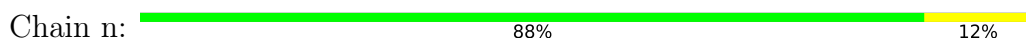
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14

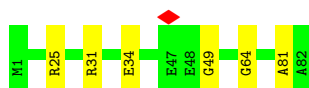




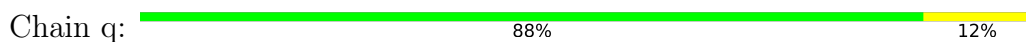
- Molecule 48: 30S ribosomal protein S15



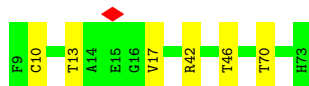
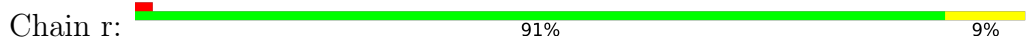
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17



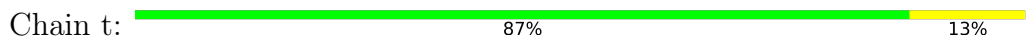
- Molecule 51: 30S ribosomal protein S18



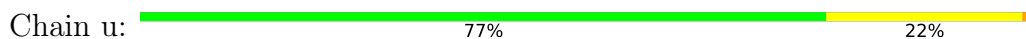
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

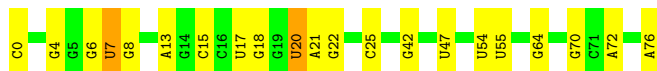


- Molecule 54: 30S ribosomal protein S21

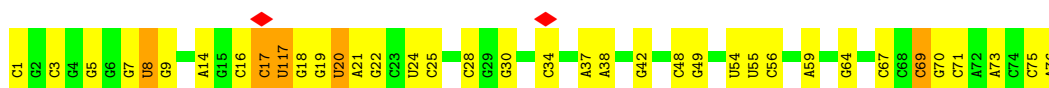




• Molecule 55: tRNA-fMet



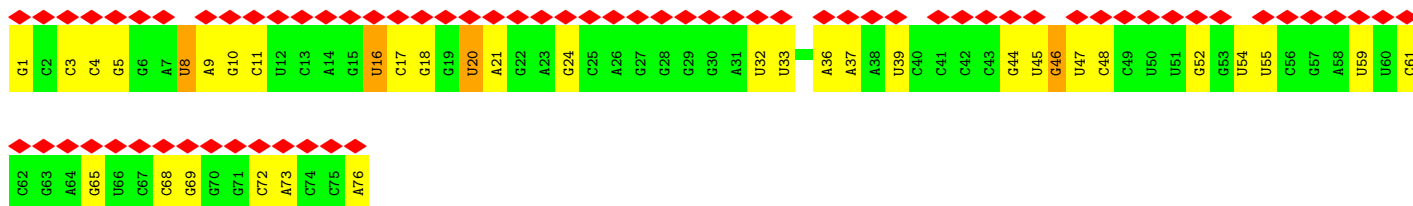
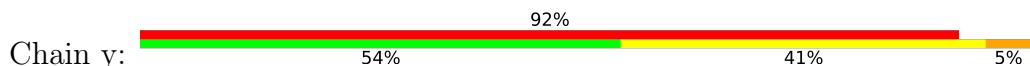
• Molecule 55: tRNA-fMet



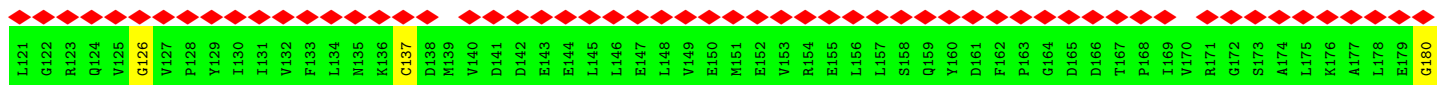
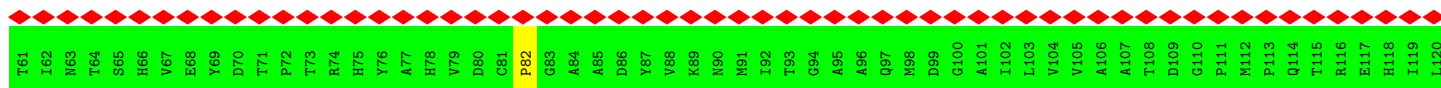
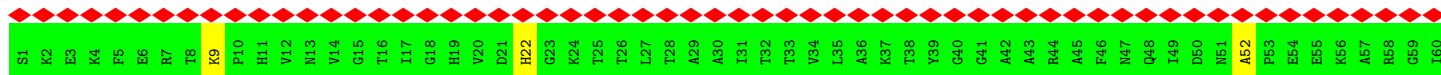
• Molecule 56: mRNA



• Molecule 57: Phe-tRNA-Phe



• Molecule 58: Elongation factor Tu 2



D181	A182	E183	W184	E185	A186	K187	I188	L189	E190	L191	A192	G193	F194	L195	D196	S197	Y198	I199	P200	E201	P202	E203	R204	A205	I206	D207	K208	P209	F210	L211	L212	P213	I214	E215	D216	V217	F218	S219	G222	T225	V226	V227	T228	G229	R230	V231	R233	G234	I235	I236	K237	V238	G239	E240	E241	V242			
E243	I244	V245	G246	I247	K248	E249	T250	Q251	K252	S253	T254	C255	T256	G257	V258	E259	M260	F261	R262	K263	L264	L265	D266	E267	G268	R269	A270	G271	E272	N273	V274	G275	V276	L277	L278	I281	K282	R283	E284	E285	I286	E287	R288	G289	Q290	V291	L292	A293	K294	P295	G296	T297	I298	K299	P300	H301	T302	K303	
F304	E305	S306	E307	V308	Y309	I310	L311	S312	K313	D314	E315	G316	G317	R318	H319	T320	P321	F322	F323	K324	G325	Y326	R327	P328	Q329	F330	Y331	F332	R333	T334	T335	D336	V337	T338	G339	T340	I341	E342	L343	P344	E345	G346	V347	E348	M349	V350	M351	P352	G353	D354	M355	I356	K357	M358	V359	V360	T361	L362	I363
H364	P365	I366	A367	M368	D369	D370	G371	L372	R373	F374	A375	I376	R377	E378	G379	G380	R381	T382	V383	G384	A385	G386	V387	V388	A389	K390	V391	L392	S393																														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30623	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)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.00371	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: 4SU, 6MZ, OMU, 4OC, 7MG, 5MC, 5MU, PSU, MG, 3TD, MIA, 2MA, K, GTP, OMG, UR3, H2U, MA6, OMC, FME, 2MG, 1MG

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	0.22	1/69174 (0.0%)	0.68	6/107907 (0.0%)
2	B	0.27	1/2876 (0.0%)	0.67	1/4483 (0.0%)
3	C	0.34	0/2121	0.65	0/2852
4	D	0.35	0/1578	0.59	0/2124
5	E	0.35	0/1563	0.59	0/2103
6	F	0.37	0/1434	0.62	0/1926
7	G	0.36	0/1324	0.55	0/1794
8	H	0.37	0/1122	0.51	0/1515
9	I	0.42	0/1046	0.63	0/1410
10	J	0.34	0/1143	0.58	0/1540
11	K	0.35	0/947	0.64	0/1268
12	L	0.36	0/1052	0.70	2/1401 (0.1%)
13	M	0.36	0/1093	0.64	0/1460
14	N	0.39	0/964	0.72	0/1289
15	O	0.37	0/902	0.64	0/1209
16	P	0.35	0/929	0.63	0/1242
17	Q	0.37	0/946	0.69	1/1260 (0.1%)
18	R	0.36	0/823	0.75	2/1100 (0.2%)
19	S	0.33	0/852	0.66	0/1142
20	T	0.36	0/736	0.67	0/984
21	U	0.35	0/787	0.60	0/1051
22	V	0.36	0/752	0.56	0/1008
23	W	0.34	0/579	0.64	0/767
24	X	0.36	0/635	0.60	0/848
25	Y	0.37	0/495	0.60	0/658
26	Z	0.37	0/438	0.62	0/586
27	0	0.33	0/440	0.64	0/588
28	1	0.34	0/424	0.57	0/565
29	2	0.40	0/370	0.75	0/487
30	3	0.33	0/513	0.57	0/676
31	4	0.33	0/303	0.64	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.42	0/1001	0.59	0/1350
33	6	0.40	0/531	0.58	0/709
34	a	0.23	0/36725	0.70	7/57285 (0.0%)
35	b	0.37	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.57	0/2225
37	d	0.37	0/1665	0.60	0/2227
38	e	0.35	0/1169	0.60	0/1573
39	f	0.37	0/835	0.59	0/1128
40	g	0.36	0/1195	0.61	0/1602
41	h	0.35	0/989	0.61	0/1326
42	i	0.38	0/1034	0.67	0/1375
43	j	0.37	0/796	0.64	0/1077
44	k	0.37	0/885	0.64	0/1195
45	l	0.37	0/954	0.67	0/1282
46	m	0.38	0/900	0.66	0/1204
47	n	0.39	0/822	0.65	0/1095
48	o	0.36	0/722	0.63	1/964 (0.1%)
49	p	0.37	0/659	0.66	0/884
50	q	0.37	0/657	0.65	0/881
51	r	0.39	0/544	0.59	0/731
52	s	0.37	0/652	0.61	0/877
53	t	0.36	0/671	0.62	0/888
54	u	0.45	0/550	0.78	0/728
55	v	0.32	1/1747 (0.1%)	0.68	0/2721
55	w	0.38	2/1747 (0.1%)	0.80	6/2721 (0.2%)
56	x	0.27	0/280	0.68	0/433
57	y	0.33	1/1607 (0.1%)	0.66	0/2501
58	z	0.36	0/3086	0.55	0/4175
All	All	0.28	6/164170 (0.0%)	0.67	26/245135 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
34	a	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	C	OP3-P	-10.20	1.49	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	0	C	OP3-P	-10.18	1.49	1.61
57	y	1	G	OP3-P	-10.18	1.49	1.61
2	B	1	U	OP3-P	-10.15	1.49	1.61
1	A	1	G	OP3-P	-10.10	1.49	1.61
55	w	117	U	O3'-P	-8.00	1.51	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	P-O3'-C3'	14.22	136.76	119.70
55	w	17	C	O3'-P-O5'	12.87	128.46	104.00
18	R	80	ARG	NE-CZ-NH1	9.52	125.06	120.30
34	a	515	G	C2'-C3'-O3'	7.58	126.16	109.50
1	A	242	G	C2'-C3'-O3'	7.44	125.88	109.50
1	A	2407	A	C2'-C3'-O3'	7.34	125.65	109.50
55	w	117	U	OP2-P-O3'	-6.70	90.45	105.20
12	L	78	ARG	NE-CZ-NH2	6.65	123.62	120.30
34	a	1305	G	C2'-C3'-O3'	6.53	124.15	113.70
34	a	63	C	C2'-C3'-O3'	6.49	124.08	113.70
12	L	78	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	1022	G	C2'-C3'-O3'	6.06	123.40	113.70
48	o	88	ARG	NE-CZ-NH2	6.04	123.32	120.30
18	R	80	ARG	NE-CZ-NH2	-6.01	117.30	120.30
17	Q	10	ARG	NE-CZ-NH1	5.88	123.24	120.30
55	w	17	C	OP2-P-O3'	-5.59	92.89	105.20
55	w	117	U	O3'-P-O5'	5.50	114.45	104.00
34	a	515	G	N9-C1'-C2'	5.41	121.03	114.00
34	a	141	G	O4'-C1'-N9	5.40	112.52	108.20
34	a	514	C	C4'-C3'-O3'	5.28	123.57	113.00
2	B	66	A	C4'-C3'-O3'	5.28	123.55	113.00
34	a	500	G	O4'-C1'-C2'	-5.24	100.56	105.80
1	A	1140	C	C2'-C3'-O3'	5.19	122.01	113.70
55	w	69	C	C2'-C3'-O3'	5.03	121.75	113.70
1	A	204	A	C4'-C3'-O3'	5.01	123.03	113.00
1	A	1730	U	C2'-C3'-O3'	5.01	121.71	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	a	502	A	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [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%)	241 (90%)	26 (10%)	2 (1%)	22	61
4	D	206/208 (99%)	187 (91%)	15 (7%)	4 (2%)	8	42
5	E	198/200 (99%)	181 (91%)	13 (7%)	4 (2%)	7	41
6	F	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
7	G	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	25	64
8	H	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	7	41
9	I	139/141 (99%)	110 (79%)	24 (17%)	5 (4%)	3	29
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	104 (87%)	12 (10%)	4 (3%)	4	31
12	L	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	34
13	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6	39
14	N	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9	45
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	57
16	P	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
17	Q	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	R	100/102 (98%)	83 (83%)	13 (13%)	4 (4%)	3	26
19	S	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	57
20	T	90/92 (98%)	77 (86%)	11 (12%)	2 (2%)	6	39
21	U	100/102 (98%)	84 (84%)	12 (12%)	4 (4%)	3	26
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	14	53
23	W	73/75 (97%)	65 (89%)	7 (10%)	1 (1%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	55 (95%)	2 (3%)	1 (2%)	9	45
26	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
27	0	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	8	42
28	1	49/51 (96%)	41 (84%)	6 (12%)	2 (4%)	3	26
29	2	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	98 (76%)	21 (16%)	10 (8%)	1	11
33	6	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	9	46
35	b	216/218 (99%)	187 (87%)	25 (12%)	4 (2%)	8	42
36	c	204/206 (99%)	184 (90%)	14 (7%)	6 (3%)	4	33
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	15	55
38	e	155/157 (99%)	129 (83%)	23 (15%)	3 (2%)	8	42
39	f	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	7	41
40	g	149/151 (99%)	132 (89%)	12 (8%)	5 (3%)	3	31
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/127 (98%)	96 (77%)	24 (19%)	5 (4%)	3	26
43	j	96/98 (98%)	73 (76%)	16 (17%)	7 (7%)	1	13
44	k	114/116 (98%)	100 (88%)	9 (8%)	5 (4%)	2	23
45	l	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	1	18
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	8	43
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	2	20
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	22
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	3	27
50	q	78/80 (98%)	71 (91%)	4 (5%)	3 (4%)	3	27
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1	17
52	s	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	12	50
53	t	83/85 (98%)	73 (88%)	7 (8%)	3 (4%)	3	29
54	u	63/65 (97%)	41 (65%)	13 (21%)	9 (14%)	0	4
58	z	391/393 (100%)	348 (89%)	32 (8%)	11 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6218/6322 (98%)	5461 (88%)	605 (10%)	152 (2%)	9	37

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	31	GLY
18	R	51	VAL
20	T	37	ASP
21	U	6	ARG
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
42	i	90	ASP
43	j	57	VAL
43	j	89	ARG
44	k	88	PRO
48	o	45	HIS
48	o	47	LYS
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
4	D	58	ASN
5	E	8	ALA
5	E	83	VAL
7	G	60	GLY
9	I	24	GLY
11	K	89	ASN
18	R	49	ILE
18	R	54	VAL
18	R	55	ASP
20	T	6	ARG
32	5	60	LEU
38	e	77	ASN
40	g	20	GLU
40	g	64	ALA
40	g	129	ASN
42	i	46	VAL
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE

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Mol	Chain	Res	Type
44	k	94	SER
45	l	42	LYS
45	l	75	GLU
45	l	88	ASP
46	m	7	ASN
47	n	2	LYS
47	n	22	LYS
47	n	38	ASP
47	n	90	ARG
49	p	64	GLY
51	r	10	CYS
51	r	17	VAL
54	u	36	PHE
58	z	180	GLY
58	z	222	GLY
3	C	13	ARG
4	D	31	ALA
4	D	154	LYS
9	I	64	ARG
11	K	110	GLU
11	K	111	LYS
12	L	15	ALA
14	N	59	SER
14	N	117	ASP
22	V	58	SER
23	W	72	ASN
27	0	2	VAL
28	1	5	ARG
32	5	88	HIS
35	b	73	ARG
37	d	191	SER
39	f	63	ASN
42	i	124	PRO
43	j	35	GLN
44	k	13	LYS
45	l	35	ARG
47	n	55	SER
49	p	81	ALA
50	q	69	THR
53	t	5	SER
54	u	9	GLU
54	u	24	LYS

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Mol	Chain	Res	Type
54	u	30	GLU
58	z	249	GLU
3	C	204	LEU
5	E	122	GLU
8	H	15	LEU
8	H	41	LYS
9	I	38	CYS
12	L	29	LYS
13	M	58	LYS
13	M	69	PRO
15	O	100	HIS
19	S	65	ASP
21	U	75	ALA
21	U	97	SER
25	Y	24	GLU
32	5	48	ALA
32	5	55	VAL
32	5	118	ILE
33	6	4	ASP
36	c	147	GLY
37	d	166	LYS
40	g	19	SER
40	g	112	ASP
43	j	41	PRO
45	l	43	LYS
45	l	46	SER
45	l	77	SER
46	m	102	LYS
48	o	2	LEU
48	o	13	GLU
50	q	17	GLU
51	r	46	THR
52	s	36	ARG
53	t	44	ALA
4	D	149	ASN
5	E	69	ARG
8	H	3	VAL
12	L	91	ASP
13	M	6	ARG
32	5	51	TYR
32	5	80	THR
32	5	113	PHE

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Mol	Chain	Res	Type
35	b	11	ALA
35	b	192	PRO
38	e	93	VAL
43	j	75	ASP
49	p	49	GLY
50	q	79	GLU
51	r	70	THR
54	u	11	PHE
54	u	22	CYS
58	z	207	ASP
58	z	248	LYS
58	z	332	PHE
11	K	35	VAL
21	U	38	ILE
32	5	108	VAL
35	b	18	GLN
36	c	95	GLY
36	c	148	ILE
38	e	89	THR
39	f	33	GLU
43	j	6	ILE
44	k	103	GLY
58	z	9	LYS
58	z	126	GLY
58	z	137	CYS
28	1	4	ILE
36	c	144	GLY
9	I	90	GLY
58	z	82	PRO
9	I	48	ILE
58	z	52	ALA

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	204 (94%)	12 (6%)	21	56
4	D	163/163 (100%)	151 (93%)	12 (7%)	13	46
5	E	164/164 (100%)	157 (96%)	7 (4%)	29	63
6	F	148/148 (100%)	142 (96%)	6 (4%)	30	64
7	G	135/135 (100%)	132 (98%)	3 (2%)	52	77
8	H	114/114 (100%)	110 (96%)	4 (4%)	36	68
9	I	109/109 (100%)	102 (94%)	7 (6%)	17	52
10	J	115/115 (100%)	107 (93%)	8 (7%)	15	48
11	K	103/103 (100%)	96 (93%)	7 (7%)	16	50
12	L	102/102 (100%)	94 (92%)	8 (8%)	12	44
13	M	109/109 (100%)	104 (95%)	5 (5%)	27	61
14	N	99/99 (100%)	94 (95%)	5 (5%)	24	58
15	O	86/86 (100%)	83 (96%)	3 (4%)	36	68
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	88
17	Q	88/88 (100%)	86 (98%)	2 (2%)	50	76
18	R	84/84 (100%)	80 (95%)	4 (5%)	25	60
19	S	92/92 (100%)	88 (96%)	4 (4%)	29	63
20	T	79/79 (100%)	74 (94%)	5 (6%)	18	53
21	U	83/83 (100%)	78 (94%)	5 (6%)	19	54
22	V	77/77 (100%)	76 (99%)	1 (1%)	69	86
23	W	57/57 (100%)	52 (91%)	5 (9%)	10	40
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	59	81
26	Z	47/47 (100%)	45 (96%)	2 (4%)	29	63
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	44 (96%)	2 (4%)	29	63
29	2	37/37 (100%)	33 (89%)	4 (11%)	6	32
30	3	51/51 (100%)	48 (94%)	3 (6%)	19	55
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	6	59/59 (100%)	53 (90%)	6 (10%)	7	34
35	b	180/180 (100%)	178 (99%)	2 (1%)	73	88
36	c	170/170 (100%)	167 (98%)	3 (2%)	59	81
37	d	172/172 (100%)	169 (98%)	3 (2%)	60	82
38	e	119/119 (100%)	114 (96%)	5 (4%)	30	63
39	f	87/87 (100%)	85 (98%)	2 (2%)	50	76
40	g	124/124 (100%)	115 (93%)	9 (7%)	14	46
41	h	104/104 (100%)	98 (94%)	6 (6%)	20	55
42	i	105/105 (100%)	99 (94%)	6 (6%)	20	55
43	j	86/86 (100%)	83 (96%)	3 (4%)	36	68
44	k	89/89 (100%)	82 (92%)	7 (8%)	12	44
45	l	102/102 (100%)	97 (95%)	5 (5%)	25	59
46	m	93/93 (100%)	86 (92%)	7 (8%)	13	45
47	n	83/83 (100%)	76 (92%)	7 (8%)	11	42
48	o	76/76 (100%)	74 (97%)	2 (3%)	46	74
49	p	65/65 (100%)	62 (95%)	3 (5%)	27	61
50	q	74/74 (100%)	67 (90%)	7 (10%)	8	37
51	r	56/56 (100%)	54 (96%)	2 (4%)	35	67
52	s	70/70 (100%)	66 (94%)	4 (6%)	20	55
53	t	65/65 (100%)	57 (88%)	8 (12%)	4	26
54	u	55/55 (100%)	48 (87%)	7 (13%)	4	24
58	z	325/325 (100%)	324 (100%)	1 (0%)	92	97
All	All	5164/5164 (100%)	4933 (96%)	231 (4%)	31	62

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	42	ARG
3	C	69	ASN
3	C	131	MET
3	C	147	PRO
3	C	183	VAL
3	C	212	TRP

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Mol	Chain	Res	Type
3	C	241	LYS
3	C	249	VAL
3	C	263	ASP
3	C	268	ARG
3	C	269	ARG
4	D	12	THR
4	D	13	ARG
4	D	39	ASP
4	D	59	ARG
4	D	77	ARG
4	D	99	GLU
4	D	148	GLN
4	D	150	GLN
4	D	151	THR
4	D	157	LYS
4	D	169	ARG
4	D	200	ASP
5	E	21	ARG
5	E	47	LYS
5	E	80	SER
5	E	88	ARG
5	E	117	ARG
5	E	140	ASP
5	E	141	MET
6	F	32	LYS
6	F	70	ARG
6	F	87	LYS
6	F	94	ARG
6	F	112	ASP
6	F	132	ARG
7	G	59	ASP
7	G	113	ASP
7	G	165	ASP
8	H	17	ASP
8	H	18	GLN
8	H	35	LYS
8	H	101	ASP
9	I	11	GLN
9	I	30	GLN
9	I	92	PRO
9	I	95	ASP
9	I	117	THR

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Mol	Chain	Res	Type
9	I	126	ARG
9	I	135	MET
10	J	3	THR
10	J	7	LYS
10	J	50	THR
10	J	61	LYS
10	J	70	THR
10	J	80	HIS
10	J	90	GLU
10	J	99	ARG
11	K	12	ASP
11	K	58	LEU
11	K	61	VAL
11	K	84	CYS
11	K	97	THR
11	K	109	SER
11	K	111	LYS
12	L	1	MET
12	L	13	LYS
12	L	14	LYS
12	L	60	ARG
12	L	79	LEU
12	L	91	ASP
12	L	126	ARG
12	L	129	LYS
13	M	40	ARG
13	M	59	ARG
13	M	110	GLU
13	M	118	LYS
13	M	134	THR
14	N	17	ARG
14	N	46	ARG
14	N	71	ARG
14	N	103	ARG
14	N	117	ASP
15	O	9	ARG
15	O	16	ARG
15	O	100	HIS
16	P	38	ARG
17	Q	29	ARG
17	Q	74	SER
18	R	1	MET

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Mol	Chain	Res	Type
18	R	66	HIS
18	R	80	ARG
18	R	95	ASP
19	S	57	ASN
19	S	62	ASP
19	S	72	THR
19	S	101	SER
20	T	5	GLU
20	T	12	ARG
20	T	69	ARG
20	T	70	HIS
20	T	93	LEU
21	U	3	LYS
21	U	16	LYS
21	U	18	LYS
21	U	34	ILE
21	U	65	GLN
22	V	35	GLU
23	W	7	ARG
23	W	8	ASN
23	W	15	LYS
23	W	58	LYS
23	W	68	LYS
25	Y	54	LYS
26	Z	44	ARG
26	Z	56	VAL
28	1	31	GLU
28	1	32	LYS
29	2	11	LYS
29	2	25	LYS
29	2	41	ARG
29	2	43	THR
30	3	51	LYS
30	3	53	ASP
30	3	61	LEU
33	6	1	MET
33	6	3	LYS
33	6	8	LYS
33	6	26	SER
33	6	37	CYS
33	6	56	ARG
35	b	21	TYR

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Mol	Chain	Res	Type
35	b	188	THR
36	c	82	ASP
36	c	156	LEU
36	c	182	ASP
37	d	72	ARG
37	d	119	HIS
37	d	189	ASP
38	e	9	GLU
38	e	11	GLN
38	e	12	GLU
38	e	111	ARG
38	e	136	VAL
39	f	38	ARG
39	f	91	ARG
40	g	2	ARG
40	g	9	ARG
40	g	11	ILE
40	g	20	GLU
40	g	47	GLU
40	g	55	LYS
40	g	76	SER
40	g	78	ARG
40	g	124	SER
41	h	59	GLU
41	h	79	ARG
41	h	89	ASP
41	h	106	SER
41	h	110	MET
41	h	120	LEU
42	i	4	GLN
42	i	41	GLU
42	i	42	THR
42	i	44	ARG
42	i	45	MET
42	i	108	ARG
43	j	45	ARG
43	j	87	LEU
43	j	88	MET
44	k	12	ARG
44	k	54	SER
44	k	58	THR
44	k	71	ASP

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Mol	Chain	Res	Type
44	k	118	ASN
44	k	120	CYS
44	k	126	ARG
45	l	13	ARG
45	l	38	THR
45	l	61	GLU
45	l	85	ARG
45	l	88	ASP
46	m	15	VAL
46	m	41	ASP
46	m	45	SER
46	m	47	LEU
46	m	75	SER
46	m	84	CYS
46	m	89	ARG
47	n	10	VAL
47	n	15	LEU
47	n	23	ARG
47	n	37	SER
47	n	54	ASP
47	n	56	SER
47	n	63	ARG
48	o	46	LYS
48	o	88	ARG
49	p	25	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	4	ILE
50	q	15	LYS
50	q	16	MET
50	q	52	CYS
50	q	61	ARG
50	q	66	LEU
51	r	13	THR
51	r	42	ARG
52	s	5	LYS
52	s	12	LEU
52	s	13	HIS
52	s	36	ARG
53	t	4	LYS
53	t	8	LYS

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Mol	Chain	Res	Type
53	t	15	LYS
53	t	29	THR
53	t	42	ASP
53	t	43	LYS
53	t	56	ILE
53	t	63	LYS
54	u	17	ARG
54	u	32	ARG
54	u	34	ARG
54	u	37	TYR
54	u	43	GLU
54	u	62	GLU
54	u	66	ARG
58	z	22	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	231	HIS
5	E	30	GLN
5	E	41	GLN
5	E	62	GLN
7	G	63	GLN
21	U	39	ASN
21	U	65	GLN
38	e	121	ASN
48	o	36	ASN
48	o	45	HIS
58	z	135	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	718 (24%)	74 (2%)
2	B	119/120 (99%)	25 (21%)	5 (4%)
34	a	1536/1540 (99%)	461 (30%)	0
55	v	76/77 (98%)	18 (23%)	0
55	w	76/77 (98%)	34 (44%)	0
56	x	11/12 (91%)	3 (27%)	0
57	y	74/76 (97%)	29 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4785/4805 (99%)	1288 (26%)	79 (1%)

All (1288) 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	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	41	C
1	A	46	G
1	A	49	A
1	A	50	U
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
1	A	80	G
1	A	82	U
1	A	84	A
1	A	92	U
1	A	93	G
1	A	97	C
1	A	98	G
1	A	100	U
1	A	101	A
1	A	102	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	130	C

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Mol	Chain	Res	Type
1	A	133	U
1	A	136	G
1	A	139	U
1	A	140	C
1	A	141	G
1	A	143	C
1	A	153	U
1	A	155	A
1	A	156	A
1	A	157	C
1	A	159	G
1	A	162	U
1	A	163	C
1	A	165	A
1	A	166	U
1	A	168	G
1	A	170	U
1	A	173	A
1	A	181	A
1	A	186	G
1	A	188	G
1	A	196	A
1	A	205	G
1	A	214	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	230	G
1	A	234	U
1	A	239	C
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	273	G

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Mol	Chain	Res	Type
1	A	274	C
1	A	275	C
1	A	276	U
1	A	279	A
1	A	281	C
1	A	282	A
1	A	283	G
1	A	284	U
1	A	285	G
1	A	286	U
1	A	287	G
1	A	290	U
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	349	U
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	362	A
1	A	363	G
1	A	365	U
1	A	366	C
1	A	368	A
1	A	369	U
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	395	U
1	A	396	G
1	A	400	G
1	A	403	U
1	A	404	A

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Mol	Chain	Res	Type
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	420	C
1	A	427	U
1	A	438	G
1	A	442	G
1	A	445	C
1	A	451	U
1	A	456	C
1	A	473	G
1	A	475	C
1	A	480	A
1	A	481	G
1	A	491	G
1	A	492	A
1	A	494	G
1	A	503	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	521	U
1	A	527	C
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	535	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	556	A
1	A	563	A
1	A	564	C
1	A	573	U
1	A	575	A
1	A	586	A

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Mol	Chain	Res	Type
1	A	592	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	645	C
1	A	646	U
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	660	C
1	A	661	A
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	715	A
1	A	717	C
1	A	730	A
1	A	738	G
1	A	747	5MC
1	A	764	A
1	A	771	G
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G

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Mol	Chain	Res	Type
1	A	785	G
1	A	804	A
1	A	805	G
1	A	812	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	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	931	U
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
1	A	958	U
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A

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Mol	Chain	Res	Type
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	1019	U
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	1040	A
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1050	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	1064	C
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

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Mol	Chain	Res	Type
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	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	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	1150	C
1	A	1151	A
1	A	1155	A
1	A	1171	G
1	A	1172	C
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1184	U
1	A	1193	G
1	A	1203	U
1	A	1210	G

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Mol	Chain	Res	Type
1	A	1218	G
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1238	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	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1320	C
1	A	1332	G
1	A	1345	C
1	A	1352	U
1	A	1359	A
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	1387	A
1	A	1395	A
1	A	1401	G
1	A	1403	A
1	A	1407	G
1	A	1410	G
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	1441	G
1	A	1450	G

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Mol	Chain	Res	Type
1	A	1452	G
1	A	1453	A
1	A	1455	G
1	A	1458	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	1490	A
1	A	1491	G
1	A	1493	C
1	A	1498	C
1	A	1504	A
1	A	1507	C
1	A	1515	A
1	A	1516	G
1	A	1519	G
1	A	1520	U
1	A	1522	A
1	A	1523	U
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1542	U
1	A	1546	G
1	A	1555	G
1	A	1565	C
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1582	C
1	A	1584	U
1	A	1585	C

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Mol	Chain	Res	Type
1	A	1587	G
1	A	1588	G
1	A	1590	A
1	A	1595	C
1	A	1605	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1710	G
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1721	G
1	A	1723	G
1	A	1724	G
1	A	1726	G
1	A	1728	C
1	A	1729	U
1	A	1731	G
1	A	1738	G
1	A	1741	C
1	A	1745	A
1	A	1746	A
1	A	1747	U
1	A	1750	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U

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Mol	Chain	Res	Type
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1809	A
1	A	1816	C
1	A	1826	G
1	A	1833	C
1	A	1841	U
1	A	1842	G
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1884	G
1	A	1885	A
1	A	1895	C
1	A	1903	G
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1916	A
1	A	1917	PSU
1	A	1929	G
1	A	1930	G
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

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Mol	Chain	Res	Type
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	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2029	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
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
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U

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Mol	Chain	Res	Type
1	A	2119	A
1	A	2121	G
1	A	2122	U
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	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2213	U
1	A	2214	C
1	A	2221	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G

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Mol	Chain	Res	Type
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2332	C
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2342	C
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2373	G
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
1	A	2447	G
1	A	2448	A
1	A	2457	PSU
1	A	2469	A
1	A	2470	G
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2481	G
1	A	2491	U

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Mol	Chain	Res	Type
1	A	2494	G
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2513	A
1	A	2518	A
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2578	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2623	G
1	A	2624	G
1	A	2629	U
1	A	2636	C
1	A	2639	A
1	A	2654	A
1	A	2656	U
1	A	2661	G
1	A	2662	A
1	A	2663	G
1	A	2682	A
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2707	U

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Mol	Chain	Res	Type
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	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	2778	A
1	A	2791	G
1	A	2794	U
1	A	2798	U
1	A	2799	G
1	A	2800	A
1	A	2801	G
1	A	2803	G
1	A	2805	C
1	A	2806	C
1	A	2807	U
1	A	2809	A
1	A	2811	G
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2850	A
1	A	2861	U
1	A	2863	C
1	A	2867	G
1	A	2868	A
1	A	2872	A

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Mol	Chain	Res	Type
1	A	2874	C
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2900	A
1	A	2901	C
1	A	2902	C
2	B	4	C
2	B	12	C
2	B	13	G
2	B	21	G
2	B	26	C
2	B	28	C
2	B	31	C
2	B	33	G
2	B	35	C
2	B	36	C
2	B	42	C
2	B	44	G
2	B	65	U
2	B	66	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	91	C
2	B	105	G
2	B	108	A
2	B	109	A
2	B	111	U
2	B	113	C
2	B	114	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	8	A
34	a	9	G
34	a	22	G

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Mol	Chain	Res	Type
34	a	27	G
34	a	29	U
34	a	32	A
34	a	38	G
34	a	39	G
34	a	40	C
34	a	44	A
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	52	C
34	a	57	G
34	a	64	G
34	a	66	A
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A
34	a	73	C
34	a	74	A
34	a	76	G
34	a	77	A
34	a	78	A
34	a	80	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	99	C
34	a	100	G
34	a	104	G
34	a	107	G
34	a	116	A
34	a	117	G
34	a	120	A

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Mol	Chain	Res	Type
34	a	121	U
34	a	127	G
34	a	128	G
34	a	129	A
34	a	130	A
34	a	131	A
34	a	132	C
34	a	139	A
34	a	140	U
34	a	141	G
34	a	142	G
34	a	143	A
34	a	144	G
34	a	146	G
34	a	149	A
34	a	150	U
34	a	151	A
34	a	161	A
34	a	164	G
34	a	165	G
34	a	168	G
34	a	177	G
34	a	181	A
34	a	183	C
34	a	184	G
34	a	188	C
34	a	189	A
34	a	197	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	215	C
34	a	220	G
34	a	222	C
34	a	223	A
34	a	224	U
34	a	225	C

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Mol	Chain	Res	Type
34	a	226	G
34	a	227	G
34	a	230	G
34	a	244	U
34	a	245	U
34	a	246	A
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	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	323	U
34	a	325	A
34	a	328	C
34	a	329	A
34	a	330	C
34	a	335	C
34	a	339	C
34	a	340	U
34	a	341	C
34	a	342	C
34	a	344	A
34	a	345	C
34	a	347	G
34	a	348	G
34	a	349	A
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	355	C
34	a	365	U
34	a	366	A
34	a	367	U

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Mol	Chain	Res	Type
34	a	368	U
34	a	369	G
34	a	372	C
34	a	375	U
34	a	376	G
34	a	381	C
34	a	382	A
34	a	388	G
34	a	389	A
34	a	391	G
34	a	392	C
34	a	393	A
34	a	394	G
34	a	397	A
34	a	398	U
34	a	400	C
34	a	403	C
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	414	A
34	a	422	C
34	a	424	G
34	a	429	U
34	a	435	A
34	a	436	C
34	a	441	A
34	a	443	C
34	a	446	G
34	a	449	G
34	a	457	G
34	a	458	U
34	a	459	A
34	a	464	U
34	a	467	U
34	a	468	A
34	a	484	G
34	a	485	U
34	a	486	U

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Mol	Chain	Res	Type
34	a	495	A
34	a	496	A
34	a	497	G
34	a	499	A
34	a	501	C
34	a	503	C
34	a	505	G
34	a	506	G
34	a	509	A
34	a	511	C
34	a	512	U
34	a	513	C
34	a	514	C
34	a	515	G
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	528	C
34	a	531	U
34	a	532	A
34	a	533	A
34	a	534	U
34	a	535	A
34	a	537	G
34	a	538	G
34	a	541	G
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	579	A
34	a	590	U
34	a	592	G

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Mol	Chain	Res	Type
34	a	596	A
34	a	601	G
34	a	602	A
34	a	615	G
34	a	633	G
34	a	640	A
34	a	642	A
34	a	648	A
34	a	650	G
34	a	651	C
34	a	653	U
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	682	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	701	U
34	a	702	A
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	742	G
34	a	747	A
34	a	748	G
34	a	749	A
34	a	754	C
34	a	755	G
34	a	758	C
34	a	760	G
34	a	761	G
34	a	769	G
34	a	777	A

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Mol	Chain	Res	Type
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	832	G
34	a	836	G
34	a	838	G
34	a	843	U
34	a	844	G
34	a	846	G
34	a	851	G
34	a	852	G
34	a	870	U
34	a	872	A
34	a	885	G
34	a	902	G
34	a	905	U
34	a	906	A
34	a	914	A
34	a	934	C
34	a	935	A
34	a	939	G
34	a	945	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	974	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	978	A
34	a	982	U
34	a	989	U
34	a	991	U

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Mol	Chain	Res	Type
34	a	992	U
34	a	993	G
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
34	a	1035	A
34	a	1043	G
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1087	G
34	a	1088	G
34	a	1094	G
34	a	1095	U
34	a	1096	C
34	a	1101	A
34	a	1108	G
34	a	1113	C
34	a	1124	G
34	a	1125	U
34	a	1126	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

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Mol	Chain	Res	Type
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	1160	G
34	a	1167	A
34	a	1168	U
34	a	1171	A
34	a	1174	G
34	a	1182	G
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	1205	U
34	a	1206	G
34	a	1207	2MG
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	1236	A
34	a	1238	A
34	a	1240	U
34	a	1245	C
34	a	1247	U
34	a	1248	A
34	a	1253	G
34	a	1256	A
34	a	1258	G
34	a	1260	G

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Mol	Chain	Res	Type
34	a	1264	U
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	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1291	U
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
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	1313	U
34	a	1317	C
34	a	1320	C
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1363	A
34	a	1368	A
34	a	1370	G
34	a	1371	G
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1387	G

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Mol	Chain	Res	Type
34	a	1391	U
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1448	C
34	a	1449	C
34	a	1452	C
34	a	1454	G
34	a	1475	G
34	a	1487	G
34	a	1491	G
34	a	1492	A
34	a	1493	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
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	1537	U
34	a	1538	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	20	H2U

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Mol	Chain	Res	Type
55	v	21	A
55	v	22	G
55	v	25	C
55	v	42	G
55	v	47	U
55	v	64	G
55	v	70	G
55	v	72	A
55	v	76	A
55	w	3	C
55	w	5	G
55	w	7	G
55	w	8	4SU
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	59	A
55	w	64	G
55	w	67	C
55	w	69	C
55	w	70	G
55	w	71	C
55	w	73	A
55	w	75	C

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Mol	Chain	Res	Type
55	w	76	A
56	x	14	C
56	x	20	U
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	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U
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	73	A
57	y	76	A

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	141	G
1	A	162	U
1	A	177	G
1	A	199	A

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Mol	Chain	Res	Type
1	A	204	A
1	A	242	G
1	A	265	A
1	A	301	G
1	A	341	C
1	A	362	A
1	A	404	A
1	A	446	G
1	A	500	G
1	A	534	U
1	A	537	G
1	A	555	G
1	A	613	A
1	A	641	U
1	A	653	U
1	A	746	PSU
1	A	764	A
1	A	774	G
1	A	775	G
1	A	784	G
1	A	827	U
1	A	859	G
1	A	884	U
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1064	C
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	1378	A
1	A	1399	C
1	A	1432	G
1	A	1475	G
1	A	1491	G
1	A	1523	U
1	A	1555	G
1	A	1558	C

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Mol	Chain	Res	Type
1	A	1567	G
1	A	1608	A
1	A	1647	U
1	A	1730	U
1	A	1745	A
1	A	1818	U
1	A	1857	G
1	A	1913	A
1	A	1918	A
1	A	1939	5MU
1	A	1940	U
1	A	1976	U
1	A	2238	G
1	A	2296	U
1	A	2319	G
1	A	2326	C
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	2638	G
1	A	2798	U
1	A	2849	U
1	A	2873	A
2	B	34	A
2	B	56	G
2	B	66	A
2	B	89	U
2	B	108	A

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

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
55	5MU	v	54	55	19,22,23	1.48	4 (21%)	28,32,35	1.93	8 (28%)
34	5MC	a	967	34	18,22,23	1.04	1 (5%)	26,32,35	1.43	3 (11%)
57	PSU	y	39	57	18,21,22	1.38	2 (11%)	22,30,33	1.87	4 (18%)
34	UR3	a	1498	34	19,22,23	1.12	2 (10%)	26,32,35	1.70	4 (15%)
57	PSU	y	32	57	18,21,22	1.32	2 (11%)	22,30,33	1.96	5 (22%)
55	H2U	v	20	55,60	18,21,22	0.82	1 (5%)	21,30,33	1.65	4 (19%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	21,30,33	1.49	4 (19%)
1	PSU	A	955	1	18,21,22	1.39	2 (11%)	22,30,33	1.93	4 (18%)
1	6MZ	A	1618	1	18,25,26	1.02	1 (5%)	16,36,39	2.29	5 (31%)
1	OMU	A	2552	1	19,22,23	1.27	3 (15%)	26,31,34	1.93	8 (30%)
1	7MG	A	2069	1	22,26,27	1.48	2 (9%)	29,39,42	2.42	10 (34%)
34	5MC	a	1407	34	18,22,23	1.04	1 (5%)	26,32,35	1.51	4 (15%)
55	PSU	v	55	55	18,21,22	1.34	3 (16%)	22,30,33	1.86	4 (18%)
57	MIA	y	37	57	24,31,32	2.30	7 (29%)	26,44,47	2.63	11 (42%)
1	OMC	A	2498	60,1	19,22,23	0.87	0	26,31,34	1.21	2 (7%)
1	H2U	A	2449	1	18,21,22	0.93	2 (11%)	21,30,33	1.61	4 (19%)
34	2MG	a	1516	34	18,26,27	0.94	0	16,38,41	1.16	2 (12%)
1	OMG	A	2251	55,1	18,26,27	1.06	2 (11%)	19,38,41	1.07	2 (10%)
34	MA6	a	1518	34	19,26,27	1.26	3 (15%)	18,38,41	1.77	4 (22%)
55	4SU	w	8	55	18,21,22	1.72	5 (27%)	26,30,33	2.19	6 (23%)
1	6MZ	A	2030	60,1	18,25,26	1.02	1 (5%)	16,36,39	2.29	5 (31%)
34	2MG	a	1207	34	18,26,27	0.92	0	16,38,41	1.34	4 (25%)
1	PSU	A	2457	1	18,21,22	1.41	2 (11%)	22,30,33	1.97	5 (22%)
1	PSU	A	2504	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
55	4SU	v	7	55	18,21,22	1.71	4 (22%)	26,30,33	2.25	6 (23%)
1	5MU	A	1939	1	19,22,23	1.46	4 (21%)	28,32,35	2.07	9 (32%)
1	PSU	A	2605	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	1MG	A	745	1	18,26,27	1.02	0	19,39,42	1.43	3 (15%)
1	2MG	A	2445	1	18,26,27	0.97	1 (5%)	16,38,41	1.17	2 (12%)
1	PSU	A	2604	60,1	18,21,22	1.40	2 (11%)	22,30,33	1.81	4 (18%)
57	4SU	y	8	57	18,21,22	1.73	5 (27%)	26,30,33	2.29	7 (26%)
57	5MU	y	54	57	19,22,23	1.46	4 (21%)	28,32,35	2.01	8 (28%)
1	PSU	A	2580	1	18,21,22	1.41	2 (11%)	22,30,33	1.90	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	747	1	18,22,23	0.97	1 (5%)	26,32,35	1.52	3 (11%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	21,30,33	1.58	3 (14%)
34	2MG	a	966	34	18,26,27	0.99	1 (5%)	16,38,41	1.40	3 (18%)
34	PSU	a	516	34	18,21,22	1.32	2 (11%)	22,30,33	1.98	5 (22%)
1	2MG	A	1835	1	18,26,27	1.05	2 (11%)	16,38,41	1.18	2 (12%)
57	PSU	y	55	57	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
55	5MU	w	54	55	19,22,23	1.48	4 (21%)	28,32,35	1.99	10 (35%)
57	7MG	y	46	57	22,26,27	1.42	4 (18%)	29,39,42	2.38	7 (24%)
1	PSU	A	1911	1	18,21,22	1.38	2 (11%)	22,30,33	2.00	5 (22%)
1	PSU	A	746	60,1	18,21,22	1.36	2 (11%)	22,30,33	1.91	5 (22%)
34	7MG	a	527	60,34	22,26,27	1.43	3 (13%)	29,39,42	2.45	8 (27%)
55	PSU	w	55	55	18,21,22	1.29	2 (11%)	22,30,33	1.93	5 (22%)
1	3TD	A	1915	1	18,22,23	7.25	13 (72%)	22,32,35	1.72	4 (18%)
34	4OC	a	1402	34	20,23,24	0.83	1 (5%)	26,32,35	1.30	5 (19%)
55	H2U	w	20	55	18,21,22	0.80	0	21,30,33	1.42	4 (19%)
1	PSU	A	1917	1	18,21,22	1.40	2 (11%)	22,30,33	1.93	5 (22%)
34	MA6	a	1519	34	19,26,27	1.23	3 (15%)	18,38,41	1.78	4 (22%)
1	2MA	A	2503	60,1	17,25,26	1.12	1 (5%)	17,37,40	1.19	3 (17%)
1	5MC	A	1962	1	18,22,23	1.03	1 (5%)	26,32,35	1.42	3 (11%)

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
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
55	H2U	v	20	55,60	-	0/7/38/39	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	3/5/27/28	0/3/3/3
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/11/33/34	0/3/3/3
1	OMC	A	2498	60,1	-	1/9/27/28	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
1	OMG	A	2251	55,1	-	0/5/27/28	0/3/3/3
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	6MZ	A	2030	60,1	-	3/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	2/5/27/28	0/3/3/3
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	A	2604	60,1	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	2/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
34	PSU	a	516	34	-	4/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	746	60,1	-	1/7/25/26	0/2/2/2
34	7MG	a	527	60,34	-	2/7/37/38	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	5/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
1	2MA	A	2503	60,1	-	2/3/25/26	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.87	1.66	1.43
1	A	1915	3TD	C6-C5	15.04	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.89	1.34	1.53
1	A	1915	3TD	C2-N1	8.11	1.47	1.37
57	y	37	MIA	C13-C14	7.17	1.53	1.32
57	y	37	MIA	C2-S10	-6.12	1.70	1.75
1	A	1915	3TD	O4'-C4'	-5.99	1.31	1.45
1	A	1915	3TD	C2-N3	5.98	1.51	1.38
1	A	1915	3TD	C6-N1	5.18	1.44	1.36
55	v	7	4SU	C4-S4	-4.49	1.59	1.68
55	w	8	4SU	C4-S4	-4.44	1.60	1.68
57	y	8	4SU	C4-S4	-4.41	1.60	1.68
57	y	39	PSU	C6-C5	4.19	1.40	1.35
1	A	2069	7MG	C4-N9	-4.18	1.32	1.37
1	A	2580	PSU	C6-C5	4.13	1.40	1.35
1	A	1911	PSU	C6-C5	4.09	1.40	1.35
1	A	2604	PSU	C6-C5	4.09	1.40	1.35
1	A	955	PSU	C6-C5	4.09	1.40	1.35
1	A	2457	PSU	C6-C5	4.09	1.40	1.35
1	A	1917	PSU	C6-C5	4.08	1.40	1.35
1	A	746	PSU	C6-C5	4.07	1.40	1.35
57	y	55	PSU	C6-C5	3.98	1.40	1.35
55	v	55	PSU	C6-C5	3.97	1.39	1.35
34	a	516	PSU	C6-C5	3.97	1.39	1.35
1	A	2605	PSU	C6-C5	3.94	1.39	1.35
57	y	32	PSU	C6-C5	3.90	1.39	1.35
1	A	2504	PSU	C6-C5	3.79	1.39	1.35
55	w	55	PSU	C6-C5	3.78	1.39	1.35
34	a	527	7MG	C4-N9	-3.20	1.34	1.37
55	v	54	5MU	C6-C5	3.17	1.39	1.34
34	a	1407	5MC	C6-C5	3.17	1.39	1.34
57	y	46	7MG	C5-C4	3.16	1.48	1.38
34	a	527	7MG	C5-C4	3.14	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	967	5MC	C6-C5	3.13	1.39	1.34
57	y	46	7MG	C4-N9	-3.13	1.34	1.37
55	w	54	5MU	C6-C5	3.13	1.39	1.34
1	A	1939	5MU	C6-C5	3.11	1.39	1.34
1	A	1915	3TD	O2'-C2'	3.11	1.50	1.43
57	y	54	5MU	C2-N1	3.08	1.43	1.38
1	A	1962	5MC	C6-C5	3.06	1.39	1.34
57	y	54	5MU	C6-C5	2.98	1.39	1.34
57	y	8	4SU	C2-N1	2.94	1.43	1.38
55	w	54	5MU	C2-N1	2.92	1.43	1.38
1	A	2069	7MG	C5-C4	2.91	1.47	1.38
55	w	8	4SU	C2-N1	2.91	1.43	1.38
34	a	1518	MA6	C5-C4	2.89	1.48	1.40
1	A	747	5MC	C6-C5	2.88	1.39	1.34
1	A	2552	OMU	C2-N1	2.87	1.43	1.38
55	w	8	4SU	C4-N3	-2.85	1.34	1.37
55	v	54	5MU	C2-N1	2.85	1.43	1.38
57	y	8	4SU	C4-N3	-2.79	1.34	1.37
1	A	1915	3TD	C10-N3	-2.79	1.41	1.47
1	A	1915	3TD	C4-N3	2.78	1.46	1.40
57	y	37	MIA	C5-C4	2.75	1.48	1.40
55	v	7	4SU	C2-N1	2.72	1.42	1.38
34	a	1519	MA6	C5-C4	2.72	1.48	1.40
57	y	37	MIA	C6-N1	2.70	1.36	1.32
55	w	54	5MU	C4-C5	2.67	1.49	1.44
1	A	1939	5MU	C4-C5	2.65	1.49	1.44
55	v	54	5MU	C4-C5	2.62	1.49	1.44
55	v	7	4SU	C4-N3	-2.59	1.34	1.37
1	A	1939	5MU	C2-N1	2.57	1.42	1.38
1	A	2552	OMU	C4-N3	-2.55	1.34	1.38
57	y	54	5MU	C4-C5	2.54	1.49	1.44
34	a	1498	UR3	C2-N1	2.53	1.42	1.38
1	A	1915	3TD	O3'-C3'	-2.53	1.37	1.43
1	A	1618	6MZ	C5-C4	2.51	1.47	1.40
1	A	2030	6MZ	C5-C4	2.51	1.47	1.40
1	A	2457	PSU	C4-N3	-2.50	1.34	1.38
1	A	1939	5MU	C4-N3	-2.47	1.34	1.38
1	A	2580	PSU	C4-N3	-2.46	1.34	1.38
1	A	1835	2MG	O4'-C1'	2.46	1.44	1.41
1	A	2604	PSU	C4-N3	-2.45	1.34	1.38
1	A	2504	PSU	C4-N3	-2.45	1.34	1.38
1	A	2605	PSU	C4-N3	-2.44	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1917	PSU	C4-N3	-2.43	1.34	1.38
55	w	54	5MU	C4-N3	-2.42	1.34	1.38
1	A	2503	2MA	C2-N3	2.42	1.36	1.31
55	v	54	5MU	C4-N3	-2.41	1.34	1.38
55	v	7	4SU	C5-C4	-2.41	1.39	1.42
1	A	1915	3TD	O2-C2	-2.38	1.18	1.23
1	A	2449	H2U	C2-N3	-2.38	1.33	1.38
57	y	8	4SU	C5-C4	-2.37	1.39	1.42
34	a	1518	MA6	C6-N1	2.35	1.36	1.33
1	A	1835	2MG	C6-N1	-2.33	1.34	1.37
1	A	1915	3TD	C3'-C4'	2.33	1.58	1.53
1	A	2449	H2U	C4-N3	-2.31	1.33	1.37
57	y	55	PSU	C4-N3	-2.28	1.34	1.38
57	y	54	5MU	C4-N3	-2.28	1.34	1.38
57	y	39	PSU	C4-N3	-2.26	1.34	1.38
34	a	1519	MA6	O4'-C1'	2.25	1.44	1.41
34	a	516	PSU	C4-N3	-2.25	1.34	1.38
1	A	746	PSU	C4-N3	-2.24	1.34	1.38
55	w	8	4SU	C5-C4	-2.23	1.39	1.42
55	w	55	PSU	C4-N3	-2.22	1.34	1.38
34	a	966	2MG	O4'-C1'	2.21	1.44	1.41
57	y	37	MIA	O4'-C1'	2.21	1.44	1.41
1	A	2552	OMU	C6-C5	2.20	1.40	1.35
1	A	2251	OMG	C6-N1	-2.20	1.34	1.37
57	y	32	PSU	C4-N3	-2.20	1.34	1.38
55	v	55	PSU	C4-N3	-2.20	1.34	1.38
1	A	955	PSU	C4-N3	-2.17	1.34	1.38
34	a	527	7MG	C6-N1	-2.17	1.34	1.38
1	A	1911	PSU	C4-N3	-2.17	1.34	1.38
34	a	1519	MA6	C6-N1	2.14	1.36	1.33
1	A	2251	OMG	O4'-C1'	2.12	1.44	1.41
57	y	46	7MG	C8-N9	2.11	1.47	1.46
34	a	1498	UR3	C6-C5	2.11	1.39	1.35
57	y	37	MIA	C2-N1	2.10	1.37	1.34
57	y	20	H2U	C2-N3	-2.09	1.34	1.38
55	w	8	4SU	C6-C5	2.08	1.39	1.35
57	y	8	4SU	C6-C5	2.06	1.39	1.35
57	y	16	H2U	C2-N3	-2.06	1.34	1.38
55	v	20	H2U	C2-N3	-2.05	1.34	1.38
34	a	1402	4OC	C6-C5	2.02	1.39	1.35
57	y	37	MIA	C2-N3	2.02	1.37	1.34
57	y	46	7MG	C5-C6	2.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	55	PSU	C4-C5	2.01	1.49	1.44
1	A	2445	2MG	C6-N1	-2.01	1.34	1.37
34	a	1518	MA6	O4'-C1'	2.01	1.43	1.41

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.24	137.79	125.47
57	y	46	7MG	N9-C4-N3	8.01	137.45	125.47
57	y	37	MIA	C12-C13-C14	-7.46	112.63	127.14
1	A	2069	7MG	N9-C4-N3	7.16	136.18	125.47
57	y	8	4SU	C4-N3-C2	-6.36	121.16	127.34
55	v	7	4SU	C4-N3-C2	-6.36	121.17	127.34
55	w	8	4SU	C4-N3-C2	-6.29	121.23	127.34
1	A	1618	6MZ	C2-N1-C6	5.99	121.73	116.59
1	A	2030	6MZ	C2-N1-C6	5.99	121.73	116.59
1	A	2457	PSU	N1-C2-N3	5.99	121.91	115.13
1	A	2504	PSU	N1-C2-N3	5.98	121.90	115.13
57	y	55	PSU	N1-C2-N3	5.86	121.77	115.13
34	a	1498	UR3	C4-N3-C2	-5.84	119.07	124.56
57	y	32	PSU	N1-C2-N3	5.80	121.70	115.13
55	w	55	PSU	N1-C2-N3	5.78	121.68	115.13
55	v	55	PSU	N1-C2-N3	5.76	121.66	115.13
34	a	516	PSU	N1-C2-N3	5.74	121.64	115.13
1	A	1911	PSU	N1-C2-N3	5.72	121.61	115.13
1	A	1917	PSU	N1-C2-N3	5.71	121.60	115.13
57	y	39	PSU	N1-C2-N3	5.70	121.59	115.13
1	A	746	PSU	N1-C2-N3	5.70	121.59	115.13
1	A	2605	PSU	N1-C2-N3	5.66	121.55	115.13
1	A	955	PSU	N1-C2-N3	5.60	121.48	115.13
1	A	2604	PSU	N1-C2-N3	5.60	121.47	115.13
55	v	7	4SU	C5-C4-N3	5.51	119.80	114.69
55	w	8	4SU	C5-C4-N3	5.48	119.77	114.69
57	y	8	4SU	C5-C4-N3	5.42	119.72	114.69
1	A	2580	PSU	N1-C2-N3	5.26	121.09	115.13
34	a	527	7MG	C5-C4-N3	-5.17	118.28	128.13
57	y	46	7MG	C5-C4-N3	-5.09	118.43	128.13
55	v	20	H2U	O4'-C1'-N1	5.04	116.16	109.30
1	A	1939	5MU	N3-C2-N1	5.00	121.52	114.89
1	A	2069	7MG	C5-C4-N3	-4.93	118.73	128.13
1	A	2552	OMU	N3-C2-N1	4.93	121.43	114.89
55	w	54	5MU	N3-C2-N1	4.84	121.31	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1939	5MU	C4-N3-C2	-4.83	121.10	127.35
1	A	1915	3TD	N1-C2-N3	4.79	119.92	116.14
55	v	54	5MU	N3-C2-N1	4.79	121.25	114.89
1	A	2069	7MG	C2-N3-C4	4.73	120.73	112.30
57	y	8	4SU	N3-C2-N1	4.66	121.08	114.89
57	y	54	5MU	N3-C2-N1	4.65	121.06	114.89
57	y	37	MIA	C2-N3-C4	4.62	121.69	115.32
1	A	2069	7MG	N9-C8-N7	-4.61	96.78	103.38
57	y	46	7MG	C2-N3-C4	4.55	120.41	112.30
55	w	8	4SU	N3-C2-N1	4.47	120.83	114.89
57	y	54	5MU	C4-N3-C2	-4.44	121.61	127.35
1	A	2552	OMU	C4-N3-C2	-4.42	120.75	126.58
34	a	527	7MG	C2-N3-C4	4.40	120.14	112.30
57	y	46	7MG	N9-C8-N7	-4.39	97.11	103.38
34	a	527	7MG	N9-C8-N7	-4.37	97.12	103.38
55	w	54	5MU	C4-N3-C2	-4.36	121.71	127.35
57	y	37	MIA	C5-C6-N1	-4.35	117.19	120.81
1	A	1915	3TD	C4-N3-C2	-4.33	119.91	124.61
1	A	1939	5MU	C5-C4-N3	4.27	118.96	115.31
55	v	7	4SU	N3-C2-N1	4.25	120.53	114.89
34	a	1519	MA6	C4-C5-N7	-4.22	105.00	109.40
57	y	54	5MU	C5-C4-N3	4.20	118.90	115.31
55	v	54	5MU	C4-N3-C2	-4.20	121.92	127.35
1	A	747	5MC	CM5-C5-C6	-4.17	117.28	122.85
55	v	7	4SU	C5-C4-S4	-4.16	119.11	124.47
57	y	37	MIA	C16-C14-C13	-4.11	110.77	122.65
1	A	1911	PSU	O2-C2-N1	-4.02	118.36	122.79
55	w	54	5MU	C5-C4-N3	3.98	118.71	115.31
1	A	2605	PSU	C4-N3-C2	-3.96	120.64	126.34
55	v	54	5MU	C5-C4-N3	3.95	118.68	115.31
34	a	1518	MA6	N3-C2-N1	-3.89	122.60	128.68
34	a	1407	5MC	CM5-C5-C6	-3.84	117.72	122.85
57	y	37	MIA	C15-C14-C13	-3.83	111.59	122.65
1	A	1962	5MC	CM5-C5-C6	-3.82	117.74	122.85
57	y	20	H2U	O4'-C1'-N1	3.80	114.48	109.30
34	a	967	5MC	CM5-C5-C6	-3.80	117.78	122.85
57	y	55	PSU	C4-N3-C2	-3.79	120.88	126.34
1	A	2504	PSU	C4-N3-C2	-3.78	120.90	126.34
1	A	955	PSU	C4-N3-C2	-3.77	120.90	126.34
1	A	955	PSU	C6-C5-C4	-3.77	115.56	118.20
57	y	32	PSU	C4-N3-C2	-3.71	120.99	126.34
1	A	2457	PSU	C4-N3-C2	-3.70	121.00	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	55	PSU	C4-N3-C2	-3.70	121.01	126.34
34	a	516	PSU	C4-N3-C2	-3.70	121.01	126.34
57	y	39	PSU	C4-N3-C2	-3.69	121.02	126.34
1	A	746	PSU	C4-N3-C2	-3.69	121.03	126.34
1	A	1911	PSU	C4-N3-C2	-3.68	121.03	126.34
57	y	8	4SU	C5-C4-S4	-3.66	119.75	124.47
55	v	55	PSU	C4-N3-C2	-3.63	121.11	126.34
34	a	1407	5MC	C5-C4-N3	-3.59	117.80	121.67
1	A	1917	PSU	C4-N3-C2	-3.57	121.19	126.34
1	A	2449	H2U	N3-C2-N1	3.53	120.39	116.65
1	A	747	5MC	C5-C4-N3	-3.53	117.87	121.67
34	a	1518	MA6	C4-C5-N7	-3.53	105.72	109.40
1	A	2604	PSU	C4-N3-C2	-3.50	121.30	126.34
34	a	1519	MA6	N3-C2-N1	-3.50	123.22	128.68
55	v	20	H2U	C4-N3-C2	-3.49	122.90	125.79
1	A	2504	PSU	O2-C2-N1	-3.48	118.96	122.79
57	y	54	5MU	O4-C4-C5	-3.44	120.92	124.90
1	A	2030	6MZ	C3'-C2'-C1'	3.42	106.13	100.98
1	A	1618	6MZ	C3'-C2'-C1'	3.41	106.12	100.98
55	w	8	4SU	C5-C4-S4	-3.41	120.08	124.47
1	A	2580	PSU	C6-C5-C4	-3.39	115.83	118.20
1	A	746	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	1618	6MZ	C9-N6-C6	-3.36	119.98	122.87
1	A	2457	PSU	O2-C2-N1	-3.35	119.10	122.79
55	w	55	PSU	O2-C2-N1	-3.35	119.11	122.79
57	y	20	H2U	C4-N3-C2	-3.34	123.02	125.79
1	A	1917	PSU	O2-C2-N1	-3.33	119.13	122.79
57	y	16	H2U	C4-N3-C2	-3.32	123.03	125.79
1	A	2580	PSU	C4-N3-C2	-3.32	121.56	126.34
1	A	2605	PSU	O2-C2-N1	-3.31	119.14	122.79
57	y	32	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A	2030	6MZ	C9-N6-C6	-3.31	120.02	122.87
34	a	967	5MC	C5-C4-N3	-3.31	118.11	121.67
1	A	2449	H2U	O4'-C1'-N1	3.30	113.80	109.30
34	a	516	PSU	O2-C2-N1	-3.30	119.16	122.79
57	y	55	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A	2552	OMU	C5-C4-N3	3.29	119.77	114.84
57	y	39	PSU	O2-C2-N1	-3.27	119.19	122.79
57	y	32	PSU	C3'-C2'-C1'	3.24	105.41	101.64
55	v	55	PSU	O2-C2-N1	-3.20	119.27	122.79
1	A	1911	PSU	C6-C5-C4	-3.20	115.96	118.20
1	A	1618	6MZ	N3-C2-N1	-3.19	123.69	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2030	6MZ	N3-C2-N1	-3.19	123.69	128.68
1	A	2449	H2U	C5-C4-N3	3.18	120.23	116.65
34	a	1518	MA6	C3'-C2'-C1'	3.18	105.77	100.98
1	A	955	PSU	O2-C2-N1	-3.18	119.29	122.79
34	a	1498	UR3	C1'-N1-C2	3.18	122.35	116.99
1	A	1962	5MC	C5-C4-N3	-3.17	118.25	121.67
57	y	37	MIA	C2-N1-C6	3.15	122.83	117.19
57	y	37	MIA	C4-C5-N7	-3.14	106.12	109.40
1	A	1939	5MU	O4-C4-C5	-3.14	121.27	124.90
1	A	2498	OMC	O2-C2-N3	-3.09	117.31	122.33
1	A	1939	5MU	C5-C6-N1	-3.08	120.17	123.34
57	y	54	5MU	C5M-C5-C4	3.07	122.14	118.77
55	w	54	5MU	C5M-C5-C4	3.06	122.13	118.77
1	A	1962	5MC	O2-C2-N3	-3.04	117.39	122.33
1	A	1915	3TD	C10-N3-C4	3.03	122.34	117.69
55	w	55	PSU	C3'-C2'-C1'	3.02	105.16	101.64
1	A	2604	PSU	O2-C2-N1	-3.01	119.48	122.79
1	A	2605	PSU	C6-C5-C4	-3.00	116.10	118.20
55	v	54	5MU	O4-C4-C5	-2.97	121.45	124.90
34	a	516	PSU	C3'-C2'-C1'	2.97	105.09	101.64
34	a	527	7MG	C5-C6-N1	2.94	116.18	110.99
57	y	46	7MG	C5-C6-N1	2.94	116.16	110.99
1	A	745	1MG	O6-C6-C5	-2.92	119.02	124.19
57	y	37	MIA	C3'-C2'-C1'	2.91	105.36	100.98
1	A	2069	7MG	C5-C6-N1	2.90	116.11	110.99
1	A	2552	OMU	C1'-N1-C2	2.89	122.81	117.57
34	a	1407	5MC	O2-C2-N3	-2.89	117.63	122.33
1	A	1939	5MU	O4'-C1'-N1	2.88	114.95	108.36
1	A	1917	PSU	C6-C5-C4	-2.88	116.19	118.20
1	A	2449	H2U	C4-N3-C2	-2.86	123.42	125.79
55	v	54	5MU	C5M-C5-C4	2.85	121.91	118.77
55	w	20	H2U	C4-N3-C2	-2.85	123.43	125.79
55	w	54	5MU	O4-C4-C5	-2.82	121.64	124.90
34	a	1518	MA6	C9-N6-C6	-2.80	111.05	119.51
34	a	1498	UR3	C6-N1-C2	-2.80	119.28	121.79
34	a	966	2MG	C3'-C2'-C1'	2.76	105.14	100.98
57	y	8	4SU	C6-N1-C2	-2.76	117.46	120.99
57	y	37	MIA	N3-C2-N1	-2.76	121.90	126.98
34	a	1207	2MG	C5-C6-N1	2.76	118.82	113.95
34	a	966	2MG	C5-C6-N1	2.75	118.81	113.95
1	A	747	5MC	C5-C6-N1	-2.75	120.51	123.34
1	A	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	20	H2U	C5-C4-N3	2.74	119.72	116.65
34	a	1402	4OC	C6-C5-C4	2.71	120.28	116.96
55	w	20	H2U	O4'-C1'-N1	2.71	112.99	109.30
1	A	745	1MG	C5-C6-N1	2.69	117.94	113.90
1	A	2030	6MZ	C4-C5-N7	-2.68	106.60	109.40
34	a	967	5MC	O2-C2-N3	-2.68	117.97	122.33
1	A	1618	6MZ	C4-C5-N7	-2.67	106.61	109.40
1	A	2445	2MG	C5-C6-N1	2.66	118.65	113.95
1	A	1917	PSU	C3'-C2'-C1'	2.65	104.72	101.64
34	a	1519	MA6	C10-N6-C6	-2.63	111.54	119.51
1	A	1835	2MG	C5-C6-N1	2.62	118.57	113.95
1	A	2580	PSU	O2-C2-N1	-2.59	119.93	122.79
1	A	746	PSU	C6-C5-C4	-2.57	116.40	118.20
34	a	1519	MA6	C10-N6-C9	-2.54	107.92	116.12
1	A	1915	3TD	C3'-C2'-C1'	2.54	104.59	101.64
57	y	16	H2U	C5-C4-N3	2.53	119.49	116.65
34	a	1407	5MC	O4'-C1'-N1	2.52	114.13	108.36
34	a	1516	2MG	C5-C6-N1	2.52	118.39	113.95
1	A	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
34	a	966	2MG	C8-N7-C5	2.50	107.75	102.99
1	A	2457	PSU	C3'-C2'-C1'	2.49	104.54	101.64
1	A	1939	5MU	C5M-C5-C4	2.49	121.50	118.77
1	A	2498	OMC	O4'-C1'-N1	2.48	114.04	108.36
1	A	2503	2MA	C8-N7-C5	2.46	107.67	102.99
1	A	2552	OMU	O2-C2-N3	-2.45	116.94	121.50
55	v	20	H2U	C5-C4-N3	2.45	119.40	116.65
34	a	1402	4OC	O4'-C1'-N1	2.45	113.96	108.36
1	A	2445	2MG	C8-N7-C5	2.44	107.64	102.99
1	A	745	1MG	C8-N7-C5	2.43	107.62	102.99
34	a	1498	UR3	C3U-N3-C2	2.43	121.57	117.31
1	A	2503	2MA	C5-C6-N1	2.43	118.21	114.02
55	w	8	4SU	C6-N1-C2	-2.42	117.89	120.99
34	a	1402	4OC	C5-C4-N3	-2.42	118.70	122.59
34	a	1516	2MG	C8-N7-C5	2.41	107.59	102.99
1	A	2552	OMU	C6-N1-C2	-2.41	117.91	120.99
55	v	54	5MU	O4'-C1'-N1	2.40	113.85	108.36
1	A	2069	7MG	N2-C2-N3	-2.40	115.06	119.73
57	y	39	PSU	C6-C5-C4	-2.38	116.53	118.20
1	A	2251	OMG	C5-C6-N1	2.37	118.14	113.95
34	a	1207	2MG	C3'-C2'-C1'	2.37	104.54	100.98
34	a	1207	2MG	C8-N7-C5	2.36	107.49	102.99
34	a	1207	2MG	O6-C6-C5	-2.35	119.78	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2069	7MG	O4'-C1'-N9	2.35	112.50	109.30
55	v	55	PSU	C6-C5-C4	-2.35	116.56	118.20
1	A	746	PSU	C3'-C2'-C1'	2.33	104.36	101.64
1	A	2069	7MG	N2-C2-N1	2.33	121.68	116.71
1	A	2457	PSU	C6-C5-C4	-2.33	116.57	118.20
57	y	16	H2U	O4'-C1'-N1	2.32	112.46	109.30
57	y	16	H2U	C3'-C2'-C1'	2.31	105.81	101.43
1	A	2604	PSU	C6-C5-C4	-2.30	116.59	118.20
34	a	527	7MG	CM7-N7-C5	2.30	132.33	126.40
34	a	527	7MG	O4'-C1'-N9	2.25	112.37	109.30
55	w	54	5MU	C3'-C2'-C1'	2.25	105.69	101.43
57	y	46	7MG	CM7-N7-C5	2.24	132.18	126.40
55	w	20	H2U	C2'-C3'-C4'	2.23	106.97	102.64
55	v	7	4SU	O4'-C1'-N1	2.23	113.45	108.36
55	w	54	5MU	C5M-C5-C6	-2.22	119.88	122.85
34	a	1402	4OC	O2-C2-N3	-2.21	118.74	122.33
1	A	1835	2MG	C8-N7-C5	2.19	107.17	102.99
1	A	2251	OMG	C8-N7-C5	2.19	107.16	102.99
55	w	55	PSU	C6-C5-C4	-2.18	116.67	118.20
34	a	1402	4OC	C2'-C1'-N1	-2.18	110.00	114.22
1	A	1939	5MU	O2-C2-N1	-2.18	119.89	122.79
57	y	8	4SU	O2-C2-N3	-2.15	117.49	121.50
1	A	1911	PSU	C3'-C2'-C1'	2.15	104.14	101.64
1	A	2069	7MG	O6-C6-C5	-2.14	122.29	127.54
55	w	54	5MU	C5-C6-N1	-2.14	121.14	123.34
55	w	54	5MU	C6-N1-C2	-2.13	119.14	121.30
1	A	2504	PSU	C6-C5-C4	-2.13	116.71	118.20
55	v	54	5MU	C6-N1-C2	-2.13	119.14	121.30
57	y	54	5MU	C1'-N1-C2	2.12	121.42	117.57
57	y	55	PSU	C3'-C2'-C1'	2.12	104.11	101.64
55	v	54	5MU	C5-C6-N1	-2.12	121.16	123.34
1	A	2503	2MA	C3'-C2'-C1'	2.11	104.16	100.98
55	v	7	4SU	C6-N1-C2	-2.11	118.29	120.99
34	a	527	7MG	O6-C6-C5	-2.10	122.38	127.54
57	y	54	5MU	C5M-C5-C6	-2.09	120.06	122.85
55	w	54	5MU	O2-C2-N3	-2.08	117.62	121.50
57	y	37	MIA	C11-S10-C2	2.08	103.82	102.27
57	y	46	7MG	O6-C6-C5	-2.08	122.44	127.54
57	y	8	4SU	C3'-C2'-C1'	2.08	105.37	101.43
1	A	2069	7MG	C6-C5-N7	2.07	135.17	131.91
55	v	20	H2U	C5-C6-N1	-2.07	104.79	111.61
57	y	54	5MU	C6-N1-C2	-2.07	119.20	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	C6-C5-C4	-2.07	116.75	118.20
1	A	2552	OMU	O4'-C1'-N1	2.06	113.07	108.36
55	w	20	H2U	C5-C4-N3	2.05	118.95	116.65
57	y	32	PSU	C6-C5-C4	-2.05	116.77	118.20
57	y	37	MIA	C16-C14-C15	-2.04	110.09	114.60
55	w	8	4SU	O2-C2-N3	-2.01	117.77	121.50
1	A	1939	5MU	C5M-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
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'
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	2503	2MA	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	516	PSU	C2'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
34	a	1402	4OC	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-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'

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Mol	Chain	Res	Type	Atoms
57	y	37	MIA	C3'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
57	y	37	MIA	C12-C13-C14-C16
34	a	1498	UR3	O4'-C1'-N1-C2
1	A	1917	PSU	C3'-C4'-C5'-O5'
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
34	a	516	PSU	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
57	y	55	PSU	C3'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
1	A	1939	5MU	C3'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
1	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	516	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
34	a	1207	2MG	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
1	A	2069	7MG	O4'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
57	y	55	PSU	O4'-C4'-C5'-O5'
34	a	1519	MA6	C5-C6-N6-C9
1	A	2504	PSU	O4'-C4'-C5'-O5'
34	a	527	7MG	C3'-C4'-C5'-O5'
34	a	1207	2MG	O4'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
55	w	8	4SU	O4'-C1'-N1-C6
55	w	8	4SU	C2'-C1'-N1-C2
1	A	1618	6MZ	C4'-C5'-O5'-P
55	v	7	4SU	C3'-C4'-C5'-O5'
34	a	527	7MG	C4'-C5'-O5'-P
55	w	8	4SU	O4'-C1'-N1-C2
34	a	1519	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A	2504	PSU	C3'-C4'-C5'-O5'
57	y	32	PSU	O4'-C1'-C5-C4
57	y	46	7MG	O4'-C1'-N9-C8
55	w	20	H2U	O4'-C4'-C5'-O5'
55	w	20	H2U	C3'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C6
55	w	55	PSU	O4'-C1'-C5-C6
57	y	8	4SU	O4'-C4'-C5'-O5'
57	y	8	4SU	C2'-C1'-N1-C2
1	A	2498	OMC	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 1488 ligands modelled in this entry, 1485 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	$\# Z > 2$
63	GTP	z	402	-	26,34,34	0.92	0	32,54,54	1.45	5 (15%)
62	PHE	z	401	-	10,11,12	0.45	0	10,13,15	0.27	0
59	FME	A	3001	-	8,9,10	0.50	0	7,9,11	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GTP	z	402	-	-	1/18/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
59	FME	A	3001	-	-	1/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C3'-C2'-C1'	3.22	105.82	100.98
63	z	402	GTP	PB-O3B-PG	-3.18	121.93	132.83
63	z	402	GTP	PA-O3A-PB	-3.06	122.32	132.83
63	z	402	GTP	C5-C6-N1	2.51	118.39	113.95
63	z	402	GTP	C8-N7-C5	2.47	107.69	102.99

There are no chirality outliers.

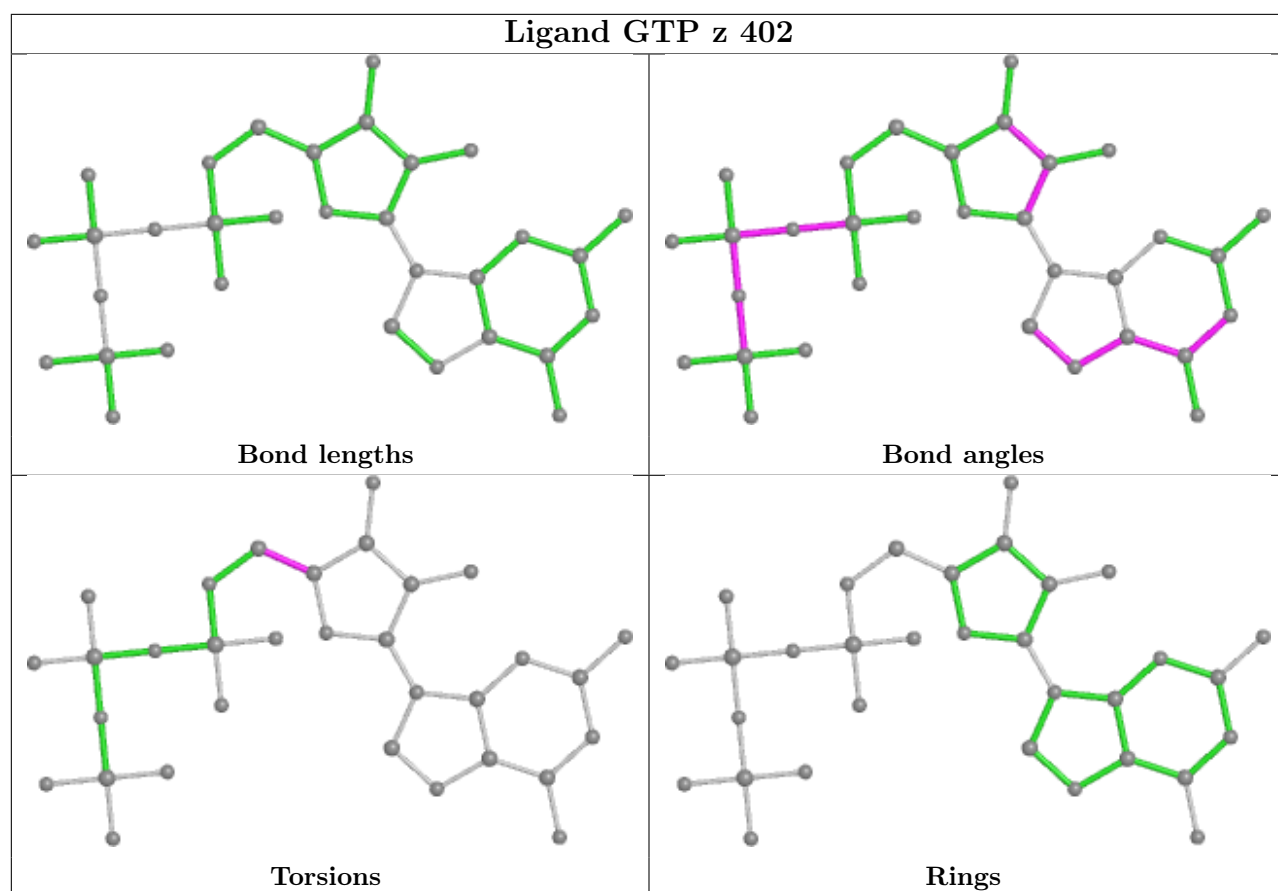
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O-C-CA-CB
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

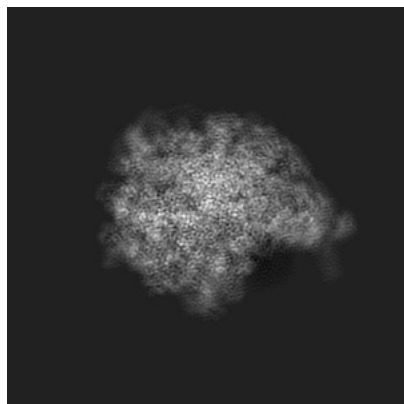
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8826. These allow visual inspection of the internal detail of the map and identification of artifacts.

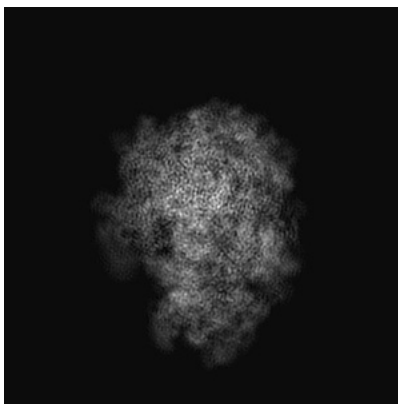
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

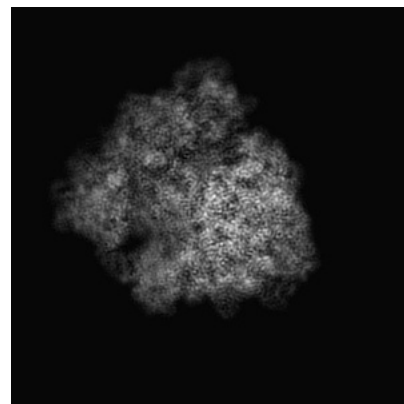
6.1.1 Primary map



X

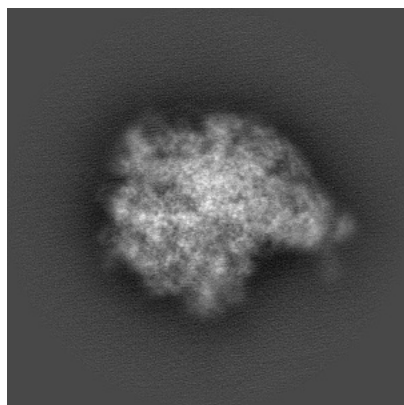


Y

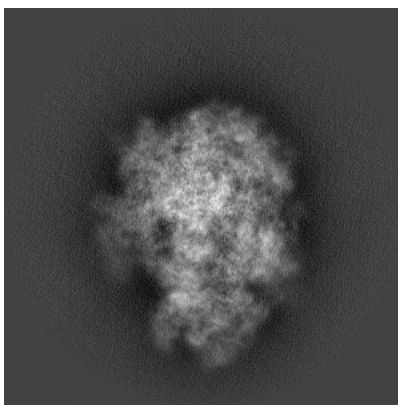


Z

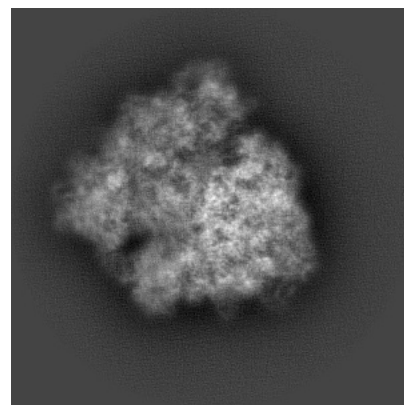
6.1.2 Raw map



X



Y

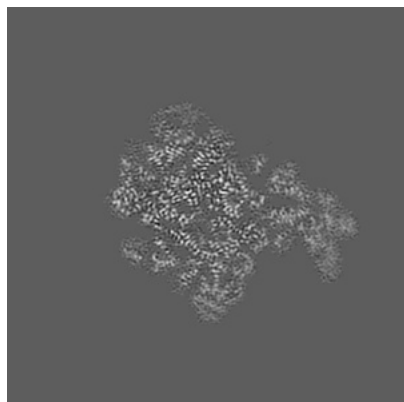


Z

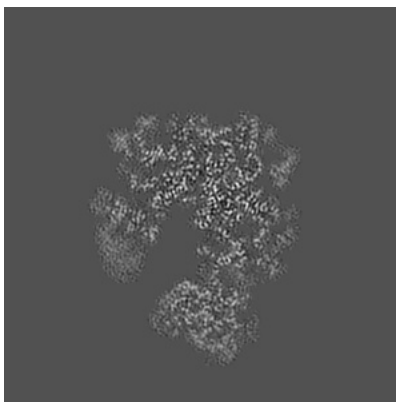
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

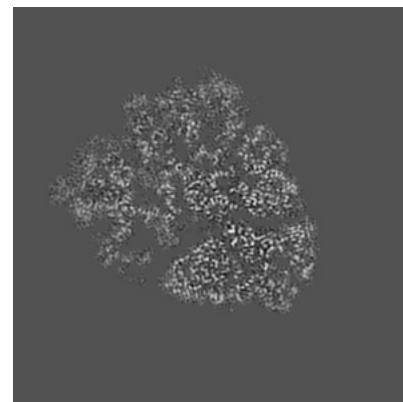
6.2.1 Primary map



X Index: 199

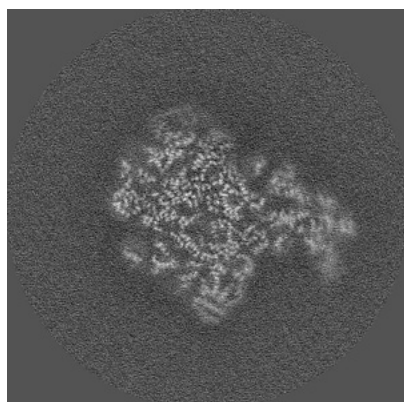


Y Index: 199

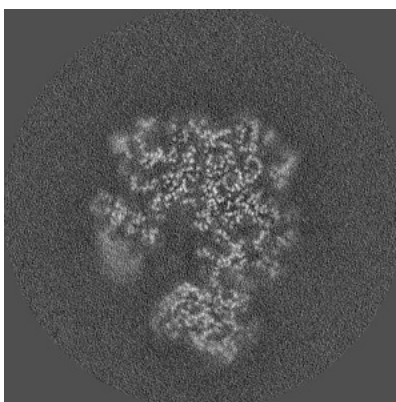


Z Index: 199

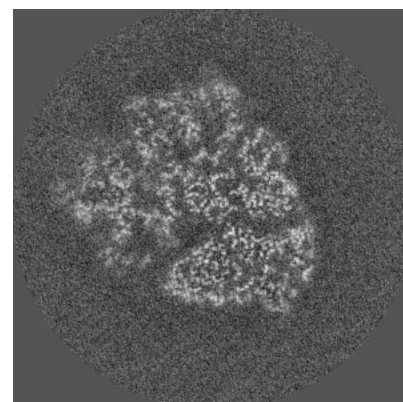
6.2.2 Raw map



X Index: 199



Y Index: 199

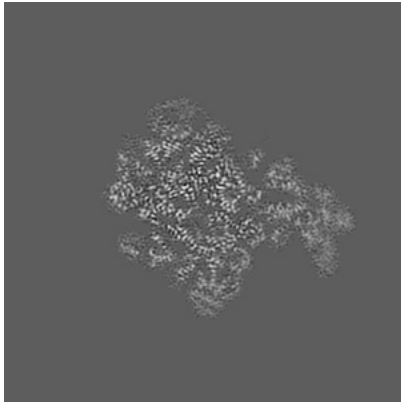


Z Index: 199

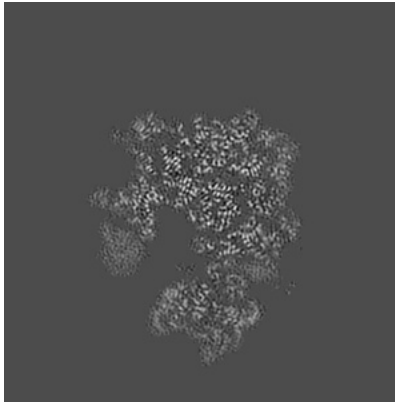
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

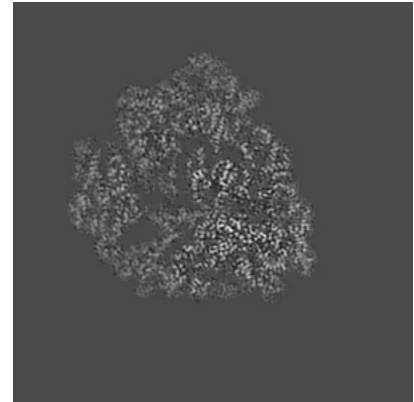
6.3.1 Primary map



X Index: 199

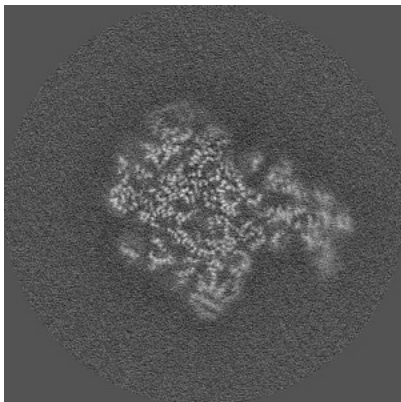


Y Index: 207

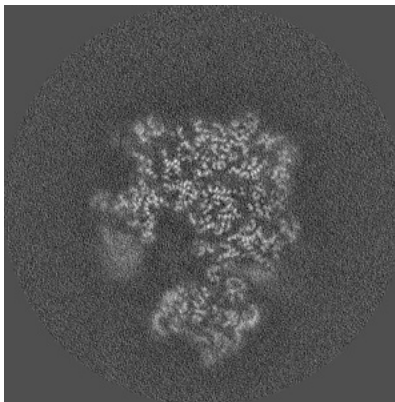


Z Index: 190

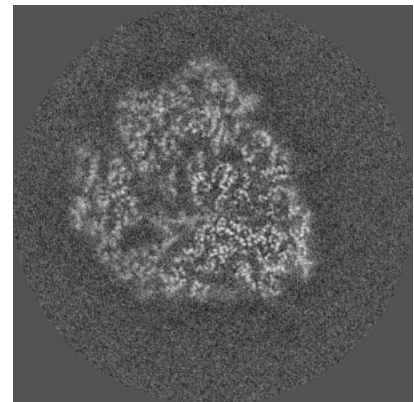
6.3.2 Raw map



X Index: 199



Y Index: 207

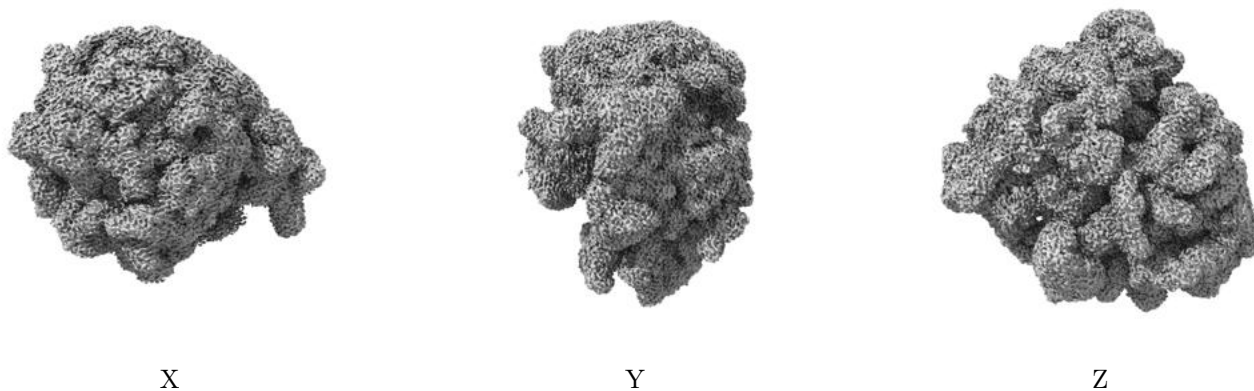


Z Index: 190

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

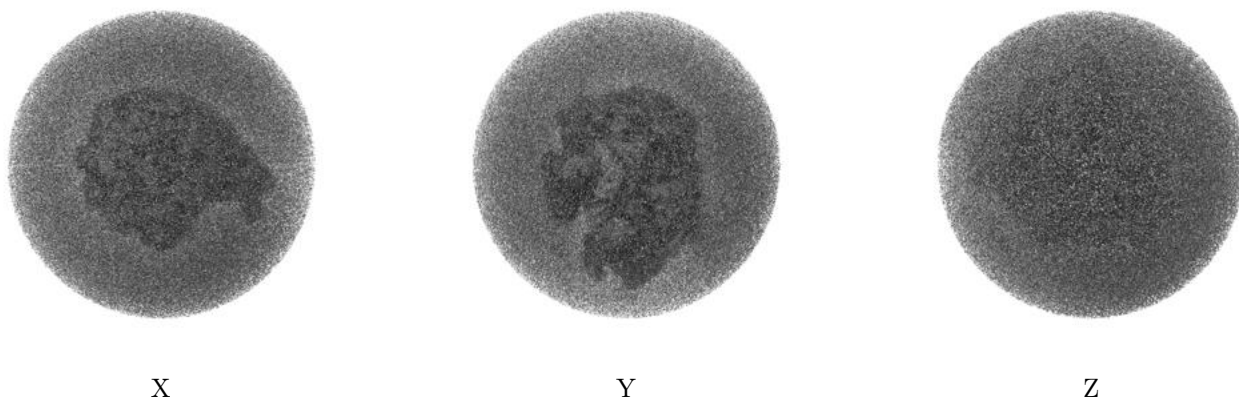
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00371. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

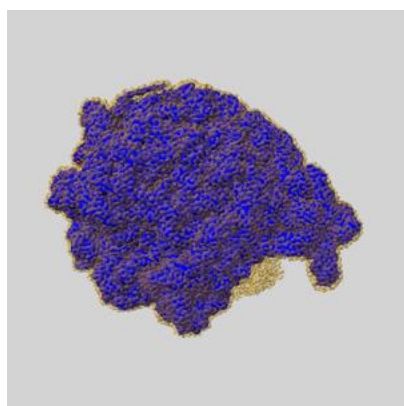
6.5 Mask visualisation [i](#)

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

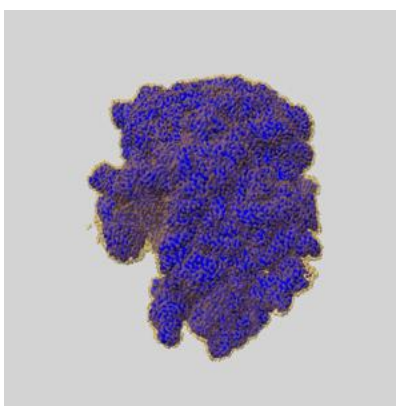
A mask typically either:

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

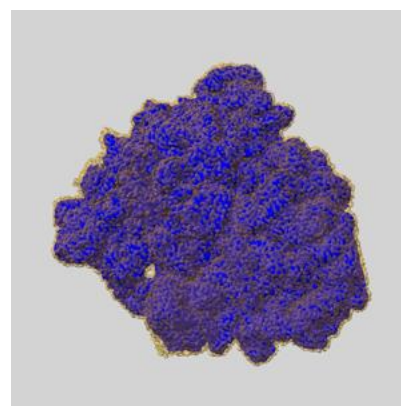
6.5.1 emd_8826_msk_1.map [i](#)



X



Y

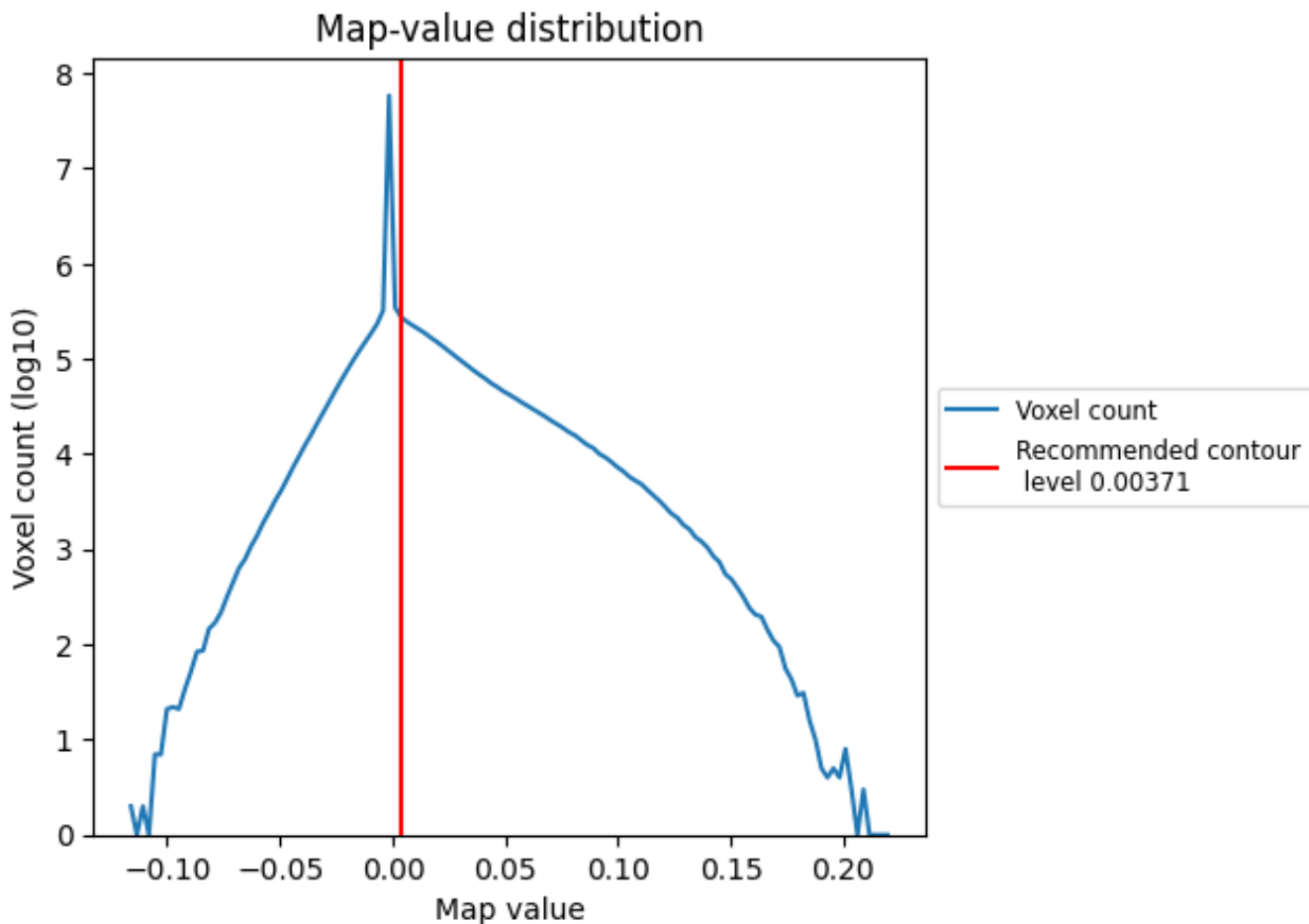


Z

7 Map analysis [i](#)

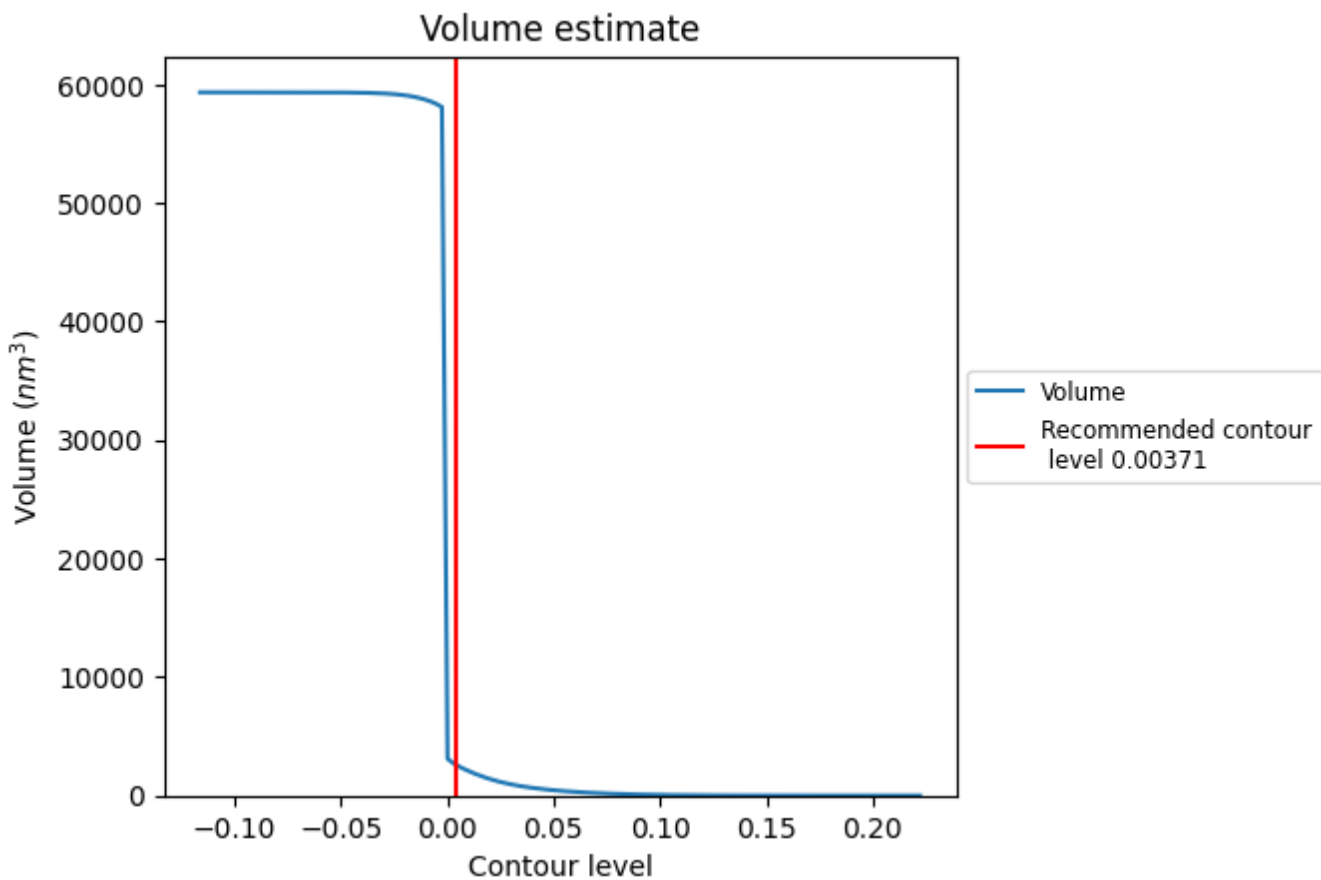
This section contains the results of statistical analysis of the map.

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.

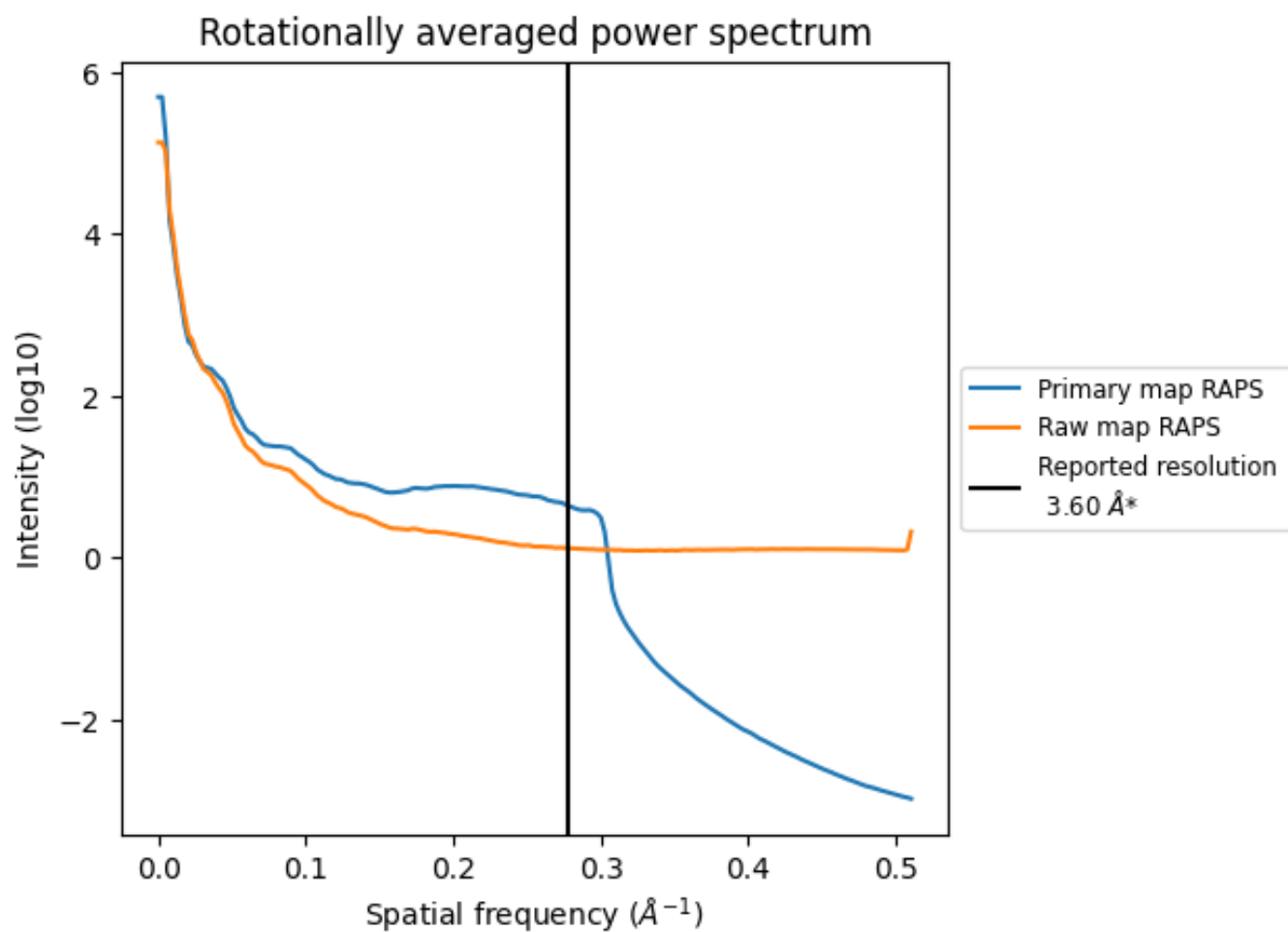
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2650 nm³; this corresponds to an approximate mass of 2393 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](#)

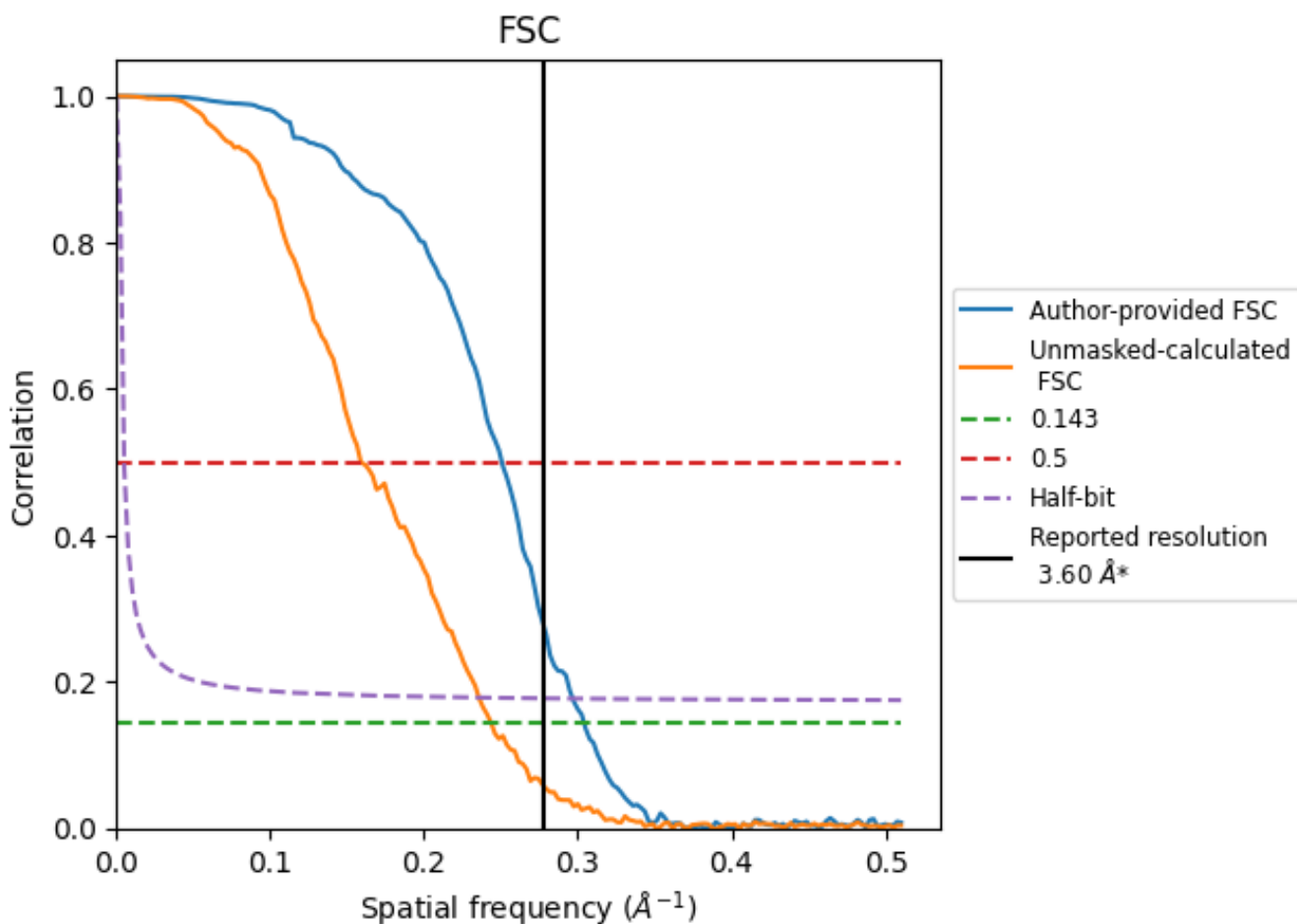


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

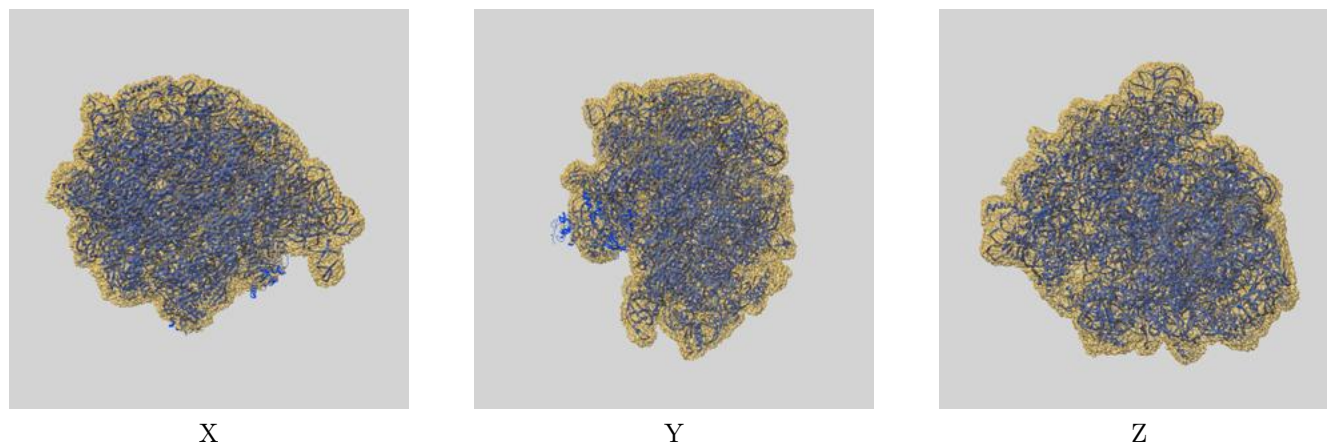
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.29	3.99	3.37
Unmasked-calculated*	4.10	6.29	4.24

*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 4.10 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

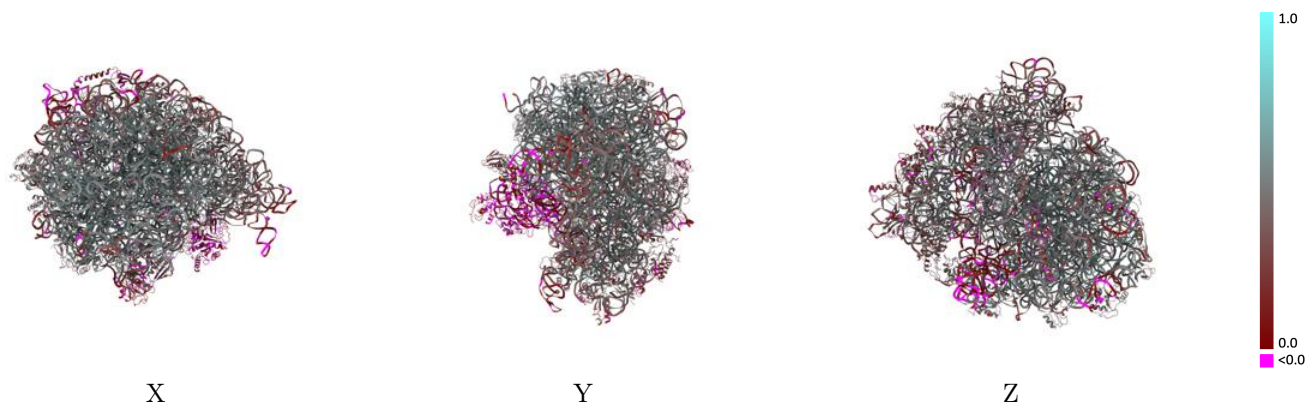
This section contains information regarding the fit between EMDB map EMD-8826 and PDB model 5WF0. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



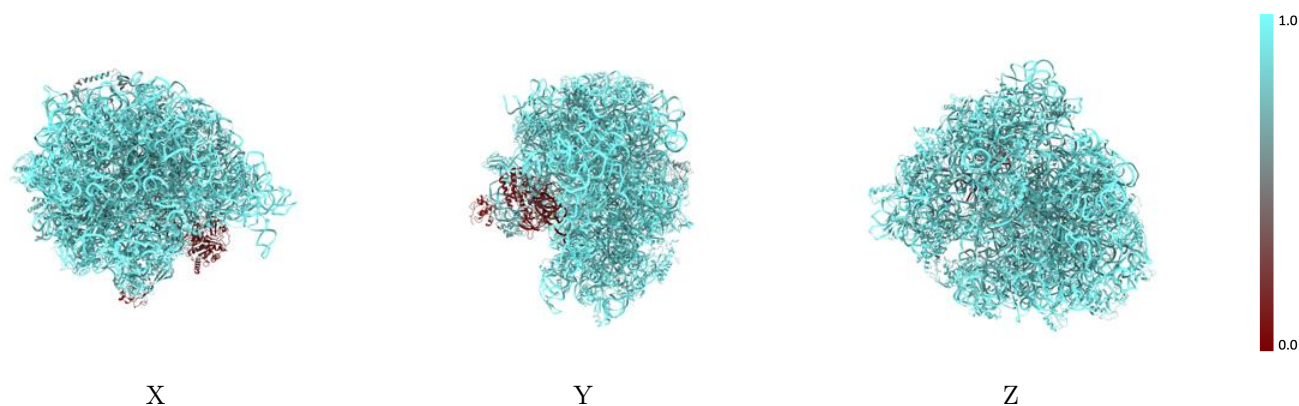
The images above show the 3D surface view of the map at the recommended contour level 0.00371 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



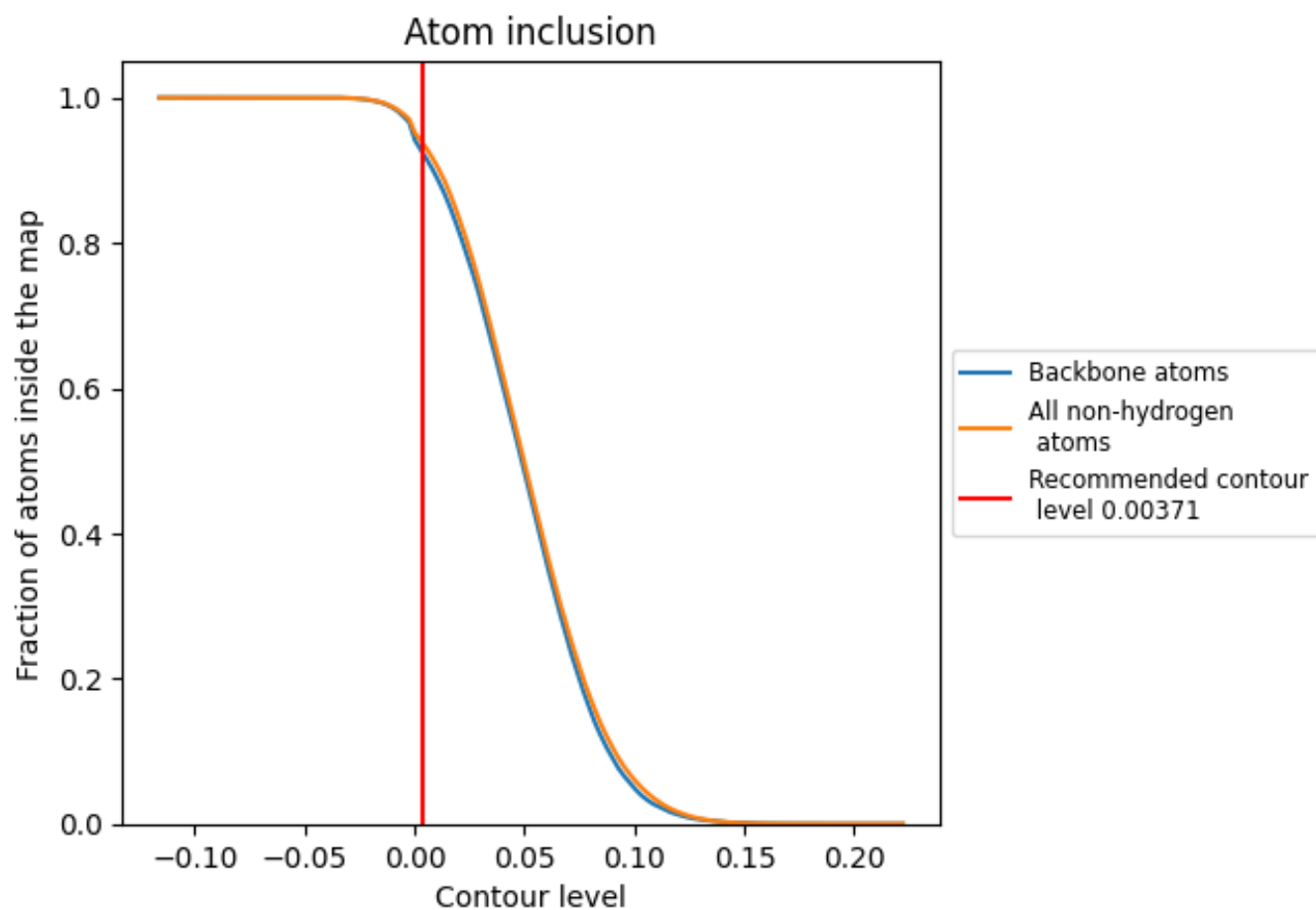
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00371).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.00371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9374	 0.4130
0	 0.9547	 0.4680
1	 0.9633	 0.4550
2	 0.9797	 0.5340
3	 0.9735	 0.5360
4	 0.9693	 0.5040
5	 0.1963	 0.0000
6	 0.9061	 0.2600
A	 0.9840	 0.4570
B	 0.9919	 0.4280
C	 0.9598	 0.5020
D	 0.9621	 0.4850
E	 0.9551	 0.4560
F	 0.9417	 0.3720
G	 0.9413	 0.3460
H	 0.7500	 0.1730
I	 0.6791	 0.0210
J	 0.9633	 0.4730
K	 0.9551	 0.4780
L	 0.9666	 0.4740
M	 0.9636	 0.4860
N	 0.9727	 0.5000
O	 0.9699	 0.4120
P	 0.9606	 0.4690
Q	 0.9777	 0.5090
R	 0.9545	 0.4510
S	 0.9637	 0.4960
T	 0.9608	 0.4470
U	 0.9752	 0.4220
V	 0.9420	 0.4060
W	 0.9588	 0.5090
X	 0.9685	 0.4850
Y	 0.9336	 0.3890
Z	 0.9668	 0.4970
a	 0.9881	 0.4270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9110	 0.3010
c	 0.9366	 0.3800
d	 0.9379	 0.3590
e	 0.9594	 0.4440
f	 0.9372	 0.3760
g	 0.9205	 0.3330
h	 0.9510	 0.4390
i	 0.9348	 0.3430
j	 0.9330	 0.3240
k	 0.9551	 0.4270
l	 0.9382	 0.4240
m	 0.9337	 0.3490
n	 0.9487	 0.3720
o	 0.9566	 0.4110
p	 0.9298	 0.3780
q	 0.9383	 0.4060
r	 0.9261	 0.3890
s	 0.9436	 0.3650
t	 0.9479	 0.3790
u	 0.8259	 0.2460
v	 0.9685	 0.3980
w	 0.8243	 0.0890
x	 0.9249	 0.3220
y	 0.1164	 -0.0070
z	 0.1167	 -0.0010