



Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 04:42 PM EDT

PDB ID : 6AZ1
EMDB ID : EMD-7024
Title : Cryo-EM structure of the small subunit of Leishmania ribosome bound to paromomycin
Authors : Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Matzov, D.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : 2017-09-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

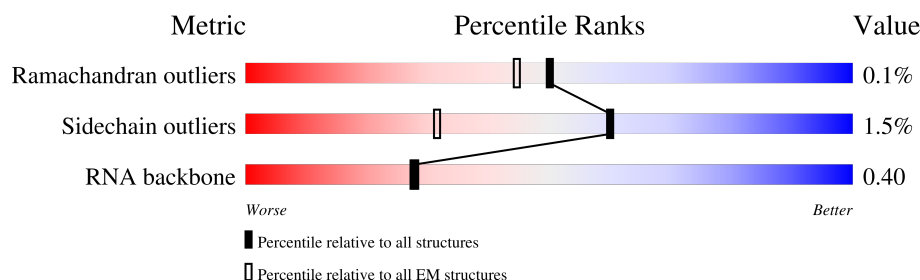
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	264	
2	B	246	
3	C	219	
4	D	190	
5	E	273	
6	F	265	
7	G	249	
8	H	190	

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Mol	Chain	Length	Quality of chain
9	I	200	
10	J	130	
11	K	220	
12	L	149	
13	M	116	
14	N	153	
15	O	144	
16	P	143	
17	Q	141	
18	R	153	
19	S	57	
20	T	151	
21	U	173	
22	V	143	
23	W	152	
24	X	179	
25	Y	159	
26	Z	137	
27	a	120	
28	b	112	
29	c	86	
30	d	87	
31	e	66	
32	f	152	
33	g	312	

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Mol	Chain	Length	Quality of chain
34	1	2203	<div><div></div><div>49%26%5%20%</div></div>
35	2	76	<div><div></div><div>82%57%39%</div></div>
36	3	77	<div><div></div><div>57%70%30%</div></div>
37	4	76	<div><div></div><div>82%49%45%7%</div></div>
38	5	13	<div><div></div><div>8%62%31%8%</div></div>

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein s1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	3	0
			1829	1147	350	320	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	GLY	conflict	UNP E9BRS2

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	211	Total	C	N	O	S	2	0
			1676	1066	306	292	12		

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	212	Total	C	N	O	S	5	0
			1668	1059	307	289	13		

- Molecule 4 is a protein called ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	182	Total	C	N	O	S	1	0
			1504	948	304	244	8		

- Molecule 5 is a protein called ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	2	0
			2029	1292	395	333	9		

- Molecule 6 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	220	Total	C	N	O	S	0	0
			1656	1062	298	286	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	THR	ALA	conflict	UNP E9BNF0
F	8	GLN	-	insertion	UNP E9BNF0
F	10	ALA	ASN	conflict	UNP E9BNF0
F	12	ALA	GLY	conflict	UNP E9BNF0
F	13	ALA	VAL	conflict	UNP E9BNF0
F	14	ASP	GLU	conflict	UNP E9BNF0
F	15	VAL	ALA	conflict	UNP E9BNF0

- Molecule 7 is a protein called ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	238	Total	C	N	O	S	1	0
			1796	1123	366	304	3		

- Molecule 8 is a protein called ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	184	Total	C	N	O	S	1	0
			1438	893	283	255	7		

- Molecule 9 is a protein called ribosomal protein S7e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	200	Total	C	N	O	S	0	0
			1613	1033	303	270	7		

- Molecule 10 is a protein called ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 11 is a protein called ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	183	Total	C	N	O	S	0	0
			1403	885	294	222	2		

- Molecule 12 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1127	724	209	191	3		

- Molecule 13 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	102	Total	C	N	O	S	1	0
			809	505	149	153	2		

- Molecule 14 is a protein called ribosomal protein S10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	91	Total	C	N	O	S	1	0
			728	473	127	123	5		

- Molecule 15 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	137	Total	C	N	O	S	2	0
			1032	637	205	183	7		

- Molecule 16 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	142	Total	C	N	O	S	3	0
			1134	716	229	186	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	18	ARG	CYS	conflict	UNP E9BFB6
P	34	ALA	SER	conflict	UNP E9BFB6
P	36	LYS	ARG	conflict	UNP E9BFB6
P	127	SER	ASN	conflict	UNP E9BFB6

- Molecule 17 is a protein called ribosomal protein S12e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			746	462	130	149	5		

- Molecule 18 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1080	680	210	186	4		

- Molecule 19 is a protein called ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	54	Total	C	N	O	S	0	0
			441	272	90	73	6		

- Molecule 20 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	142	Total	C	N	O	S	0	0
			1153	727	228	190	8		

- Molecule 21 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	156	Total	C	N	O	S	0	0
			1241	786	249	201	5		

- Molecule 22 is a protein called ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	122	Total	C	N	O	S	1	0
			935	587	187	156	5		

- Molecule 23 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			822	530	158	130	4		

- Molecule 24 is a protein called ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	152	Total	C	N	O	S	1	0
			1202	765	235	198	4		

- Molecule 25 is a protein called ribosomal protein S21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	88	Total	C	N	O	S	0	0
			664	409	122	129	4		

- Molecule 26 is a protein called ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	127	Total	C	N	O	S	1	0
			1032	664	199	166	3		

- Molecule 27 is a protein called ribosomal protein S25e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	72	Total	C	N	O	S	0	0
			544	348	94	99	3		

- Molecule 28 is a protein called ribosomal protein S26e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	103	Total	C	N	O	S	0	0
			796	496	164	129	7		

- Molecule 29 is a protein called ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	84	Total	C	N	O	S	0	0
			656	407	128	113	8		

- Molecule 30 is a protein called ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 31 is a protein called ribosomal protein S30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	59	Total	C	N	O	S	0	0
			449	280	97	71	1		

- Molecule 32 is a protein called ribosomal protein S31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	60	Total	C	N	O	S	0	0
			385	242	71	69	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	5	ILE	VAL	conflict	UNP E9BTC5

- Molecule 33 is a protein called LACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	300	Total	C	N	O	S	1	0
			2240	1410	395	423	12		

- Molecule 34 is a RNA chain called ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	1760	Total	C	N	O	P	0	0
			37613	16832	6780	12242	1759		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1539	M1Y	U	conflict	GB 322500086
1	1543	C4J	U	conflict	GB 322500086

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	G	-	expression tag	GB 1229082179

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2	C	-	expression tag	GB 1229082179
2	3	G	-	expression tag	GB 1229082179
2	70	C	G	conflict	GB 1229082179

- Molecule 36 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	77	Total	C	N	O	P	0	0
			1639	732	297	534	76		

- Molecule 37 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	G	-	expression tag	GB 1229082179
4	2	C	-	expression tag	GB 1229082179
4	3	G	-	expression tag	GB 1229082179
4	70	C	G	conflict	GB 1229082179

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	C	1	Total	Mg	0
			1	1	
39	D	1	Total	Mg	0
			1	1	
39	S	1	Total	Mg	0
			1	1	
39	1	20	Total	Mg	0
			20	20	

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Mol	Chain	Residues	Atoms	AltConf
39	5	1	Total Mg 1 1	0

- # PAR

[illegible]

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 41 | D | 2 | Total
2 | O
2 | 0 |
| 41 | E | 1 | Total
1 | O
1 | 0 |



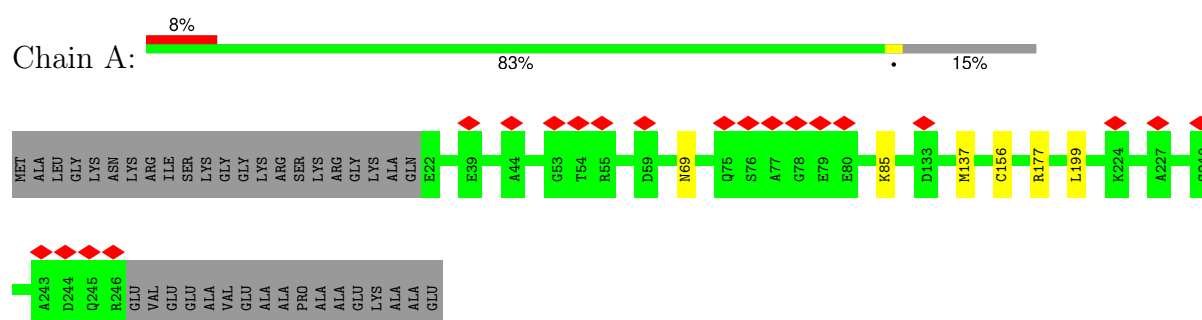
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Mol	Chain	Residues	Atoms		AltConf
41	F	3	Total 3	O 3	0
41	G	1	Total 1	O 1	0
41	H	1	Total 1	O 1	0
41	K	1	Total 1	O 1	0
41	L	1	Total 1	O 1	0
41	M	3	Total 3	O 3	0
41	O	1	Total 1	O 1	0
41	P	6	Total 6	O 6	0
41	R	2	Total 2	O 2	0
41	S	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	X	4	Total 4	O 4	0
41	Y	1	Total 1	O 1	0
41	Z	1	Total 1	O 1	0
41	b	1	Total 1	O 1	0
41	c	2	Total 2	O 2	0
41	f	1	Total 1	O 1	0
41	1	217	Total 217	O 217	0
41	2	2	Total 2	O 2	0
41	3	3	Total 3	O 3	0
41	5	3	Total 3	O 3	0

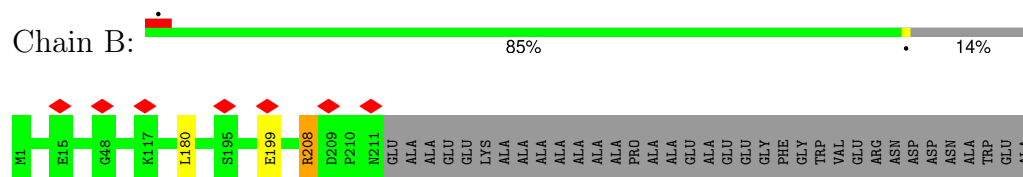
3 Residue-property plots [i](#)

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.

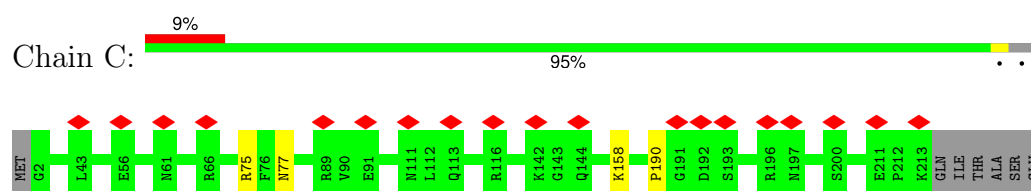
• Molecule 1: Ribosomal protein s1e



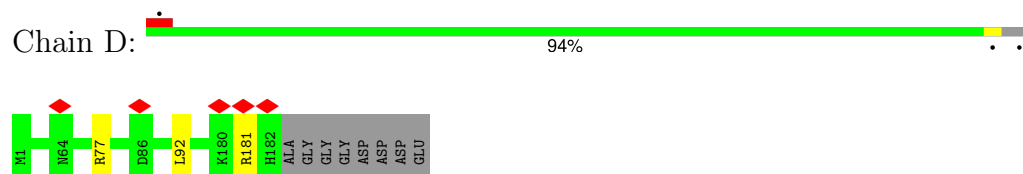
• Molecule 2: ribosomal protein S2



• Molecule 3: ribosomal protein S3

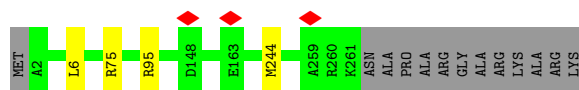


• Molecule 4: ribosomal protein S4



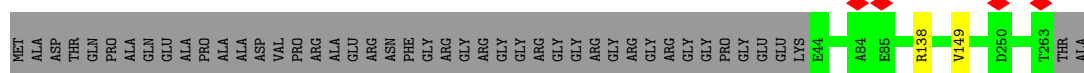
• Molecule 5: ribosomal protein S4e





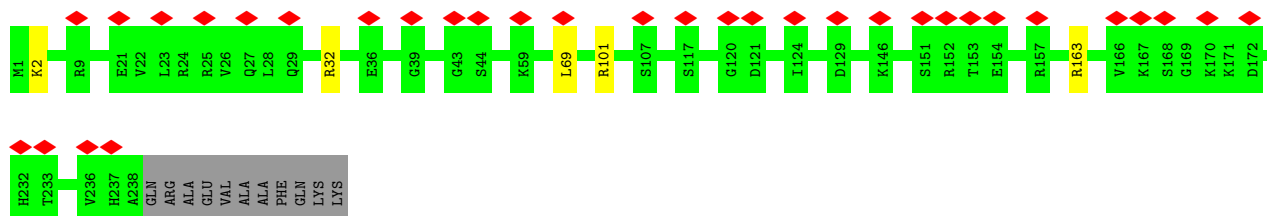
- Molecule 6: ribosomal protein S5

Chain F: 82% 17%



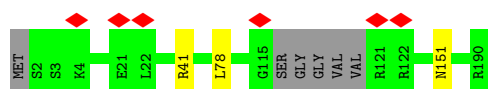
- Molecule 7: ribosomal protein S6e

Chain G: 13% 94%



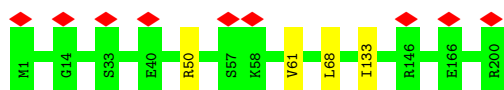
- Molecule 8: ribosomal protein S7

Chain H: 95%



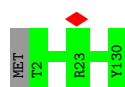
- Molecule 9: ribosomal protein S7e

Chain I: 98%



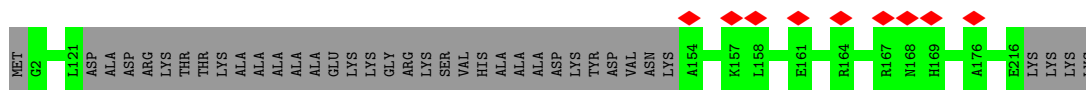
- Molecule 10: ribosomal protein S8

Chain J: 99%

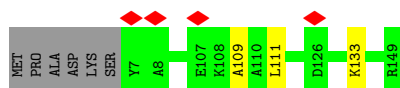


- Molecule 11: ribosomal protein S8e

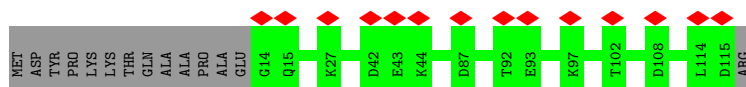
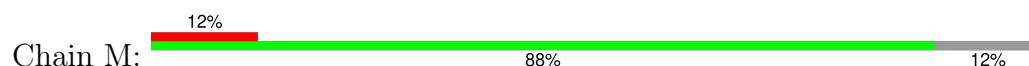
Chain K: 83% 17%



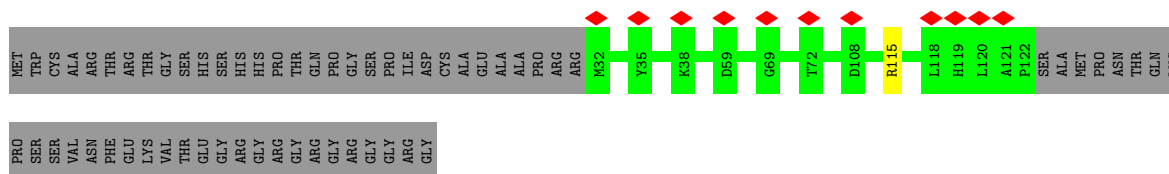
- Molecule 12: ribosomal protein S9



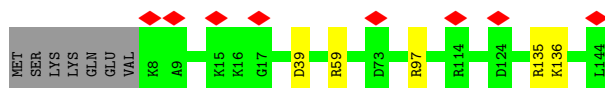
- Molecule 13: ribosomal protein S10



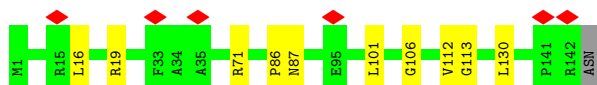
- Molecule 14: ribosomal protein S10e



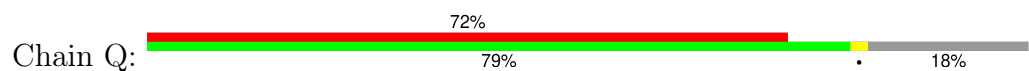
- Molecule 15: ribosomal protein S11

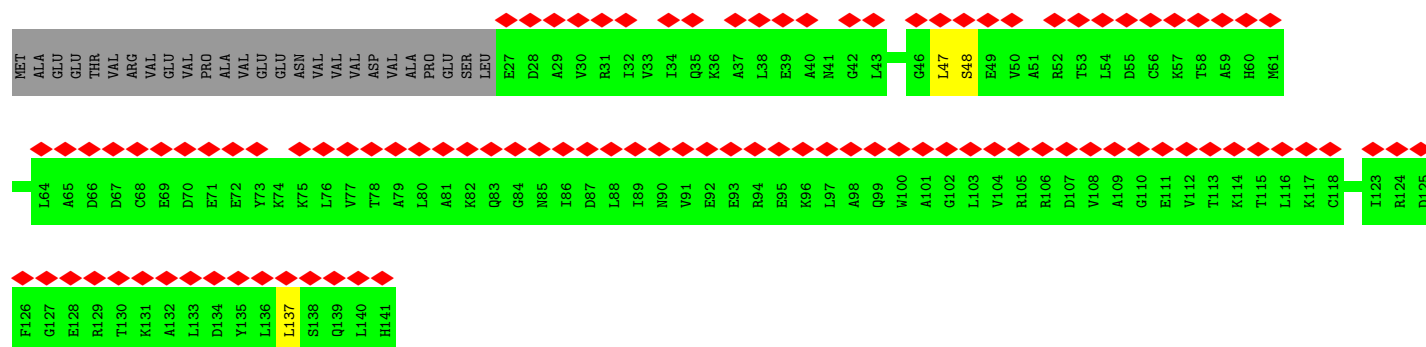


- Molecule 16: ribosomal protein S12

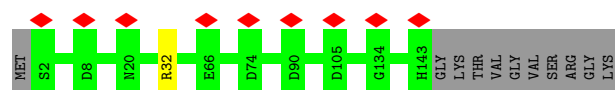


- Molecule 17: ribosomal protein S12e

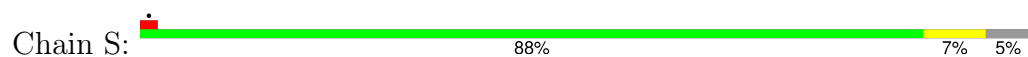




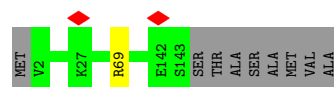
- Molecule 18: ribosomal protein S13



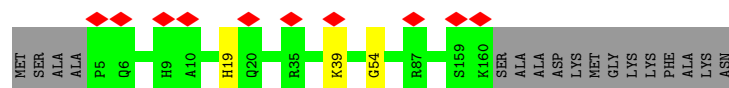
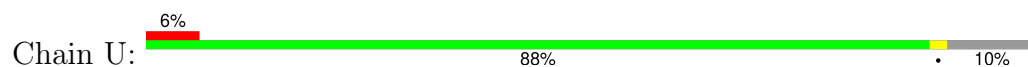
- Molecule 19: ribosomal protein S14



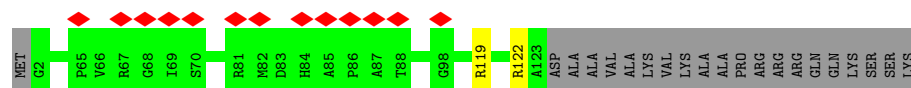
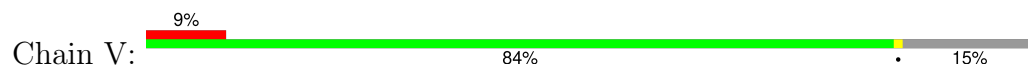
- Molecule 20: ribosomal protein S15



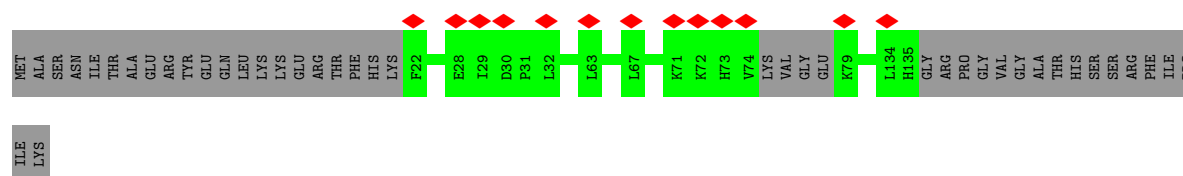
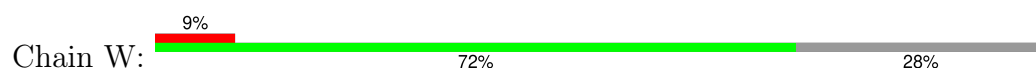
- Molecule 21: ribosomal protein S17



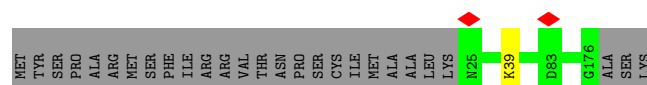
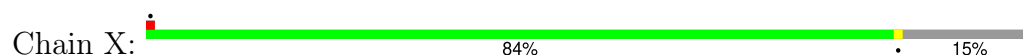
- Molecule 22: ribosomal protein S17e



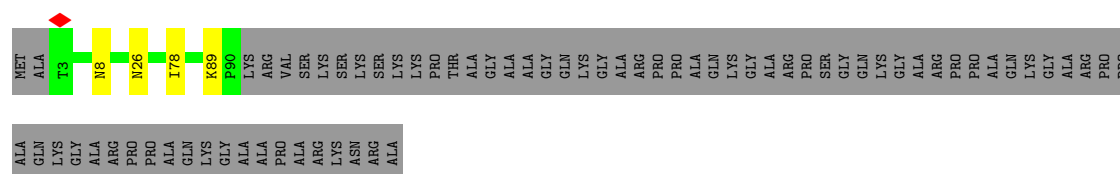
- Molecule 23: ribosomal protein S19



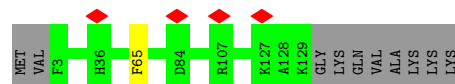
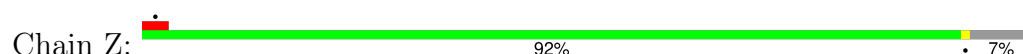
- Molecule 24: ribosomal protein S19e



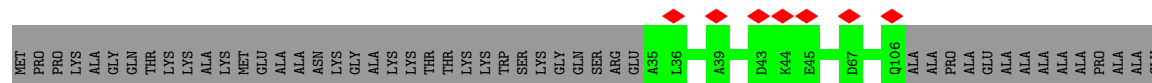
- Molecule 25: ribosomal protein S21e



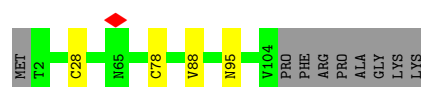
- Molecule 26: ribosomal protein S24e



- Molecule 27: ribosomal protein S25e

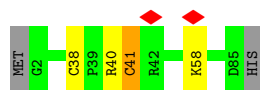


- Molecule 28: ribosomal protein S26e



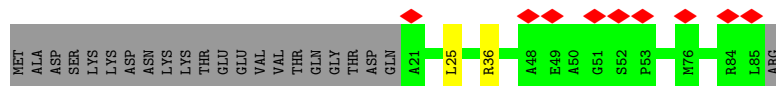
- Molecule 29: ribosomal protein S27e

Chain c:  93%




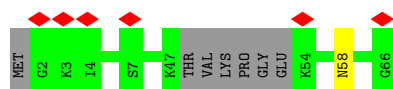
- Molecule 30: ribosomal protein S28e

Chain d:  10% 72% 25%



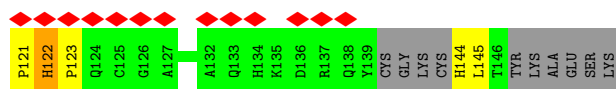
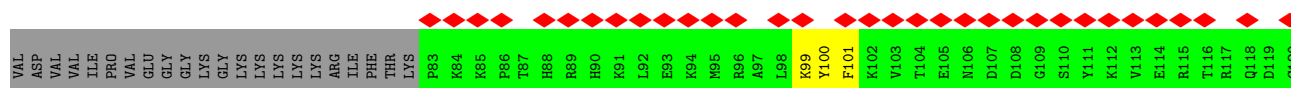
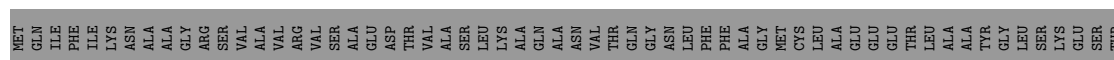
- Molecule 31: ribosomal protein S30e

Chain e:  9% 88% 11%



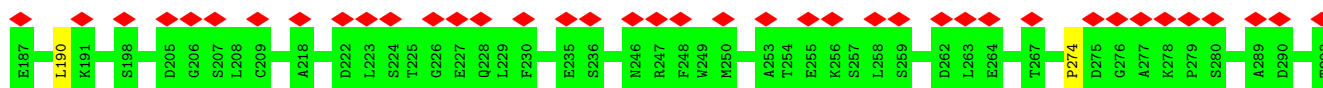
- Molecule 32: ribosomal protein S31e

Chain f:  30% 34% 5% 61%



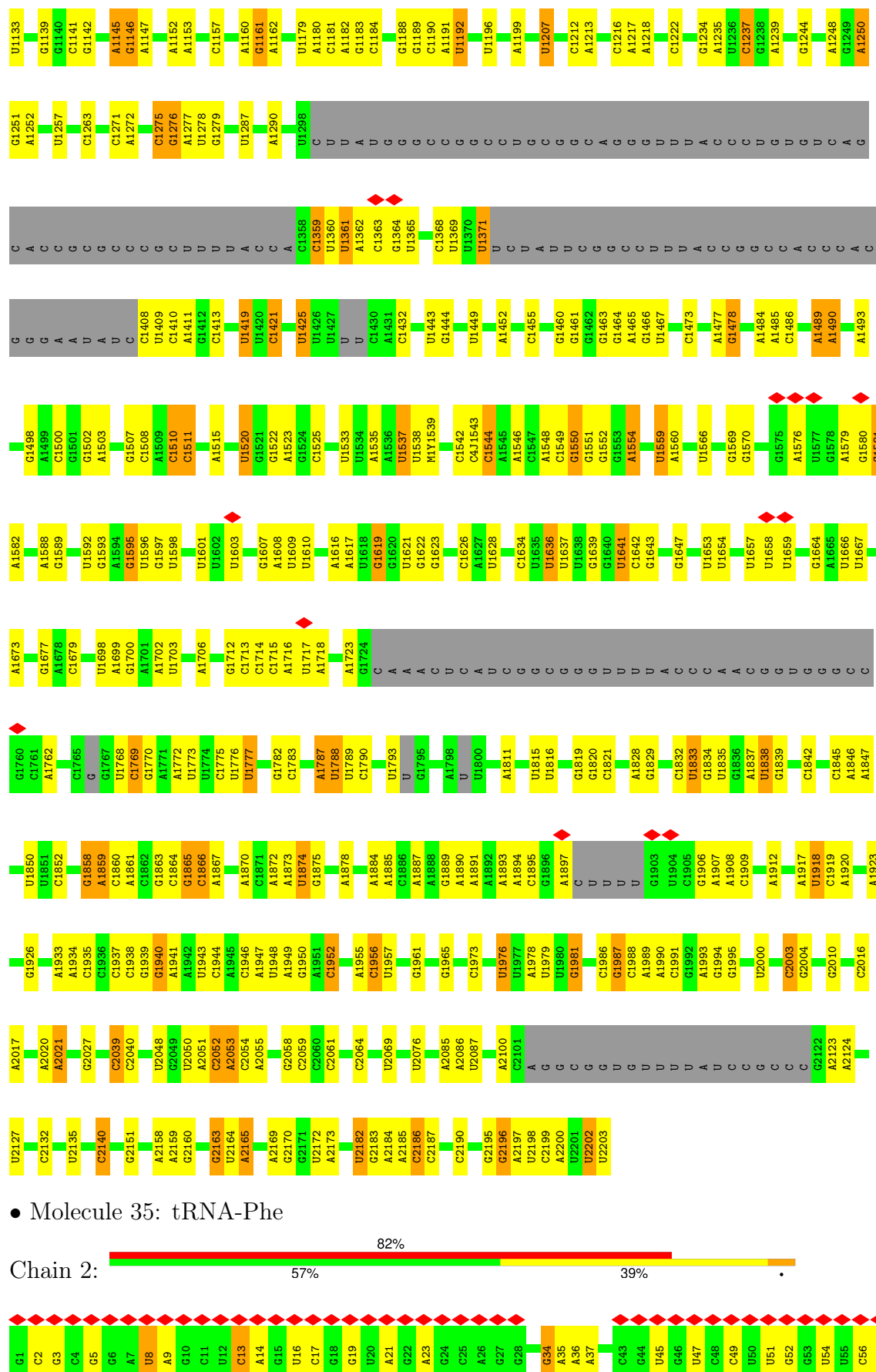
- Molecule 33: LACK1

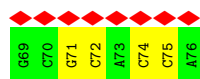
Chain g:  22% 94%



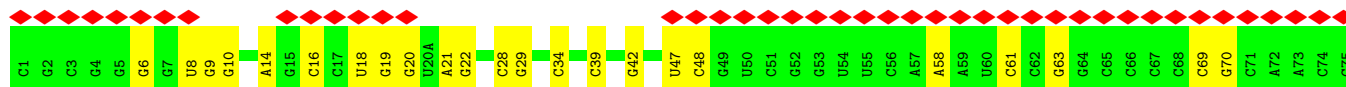
- Molecule 34: ribosomal RNA 18S



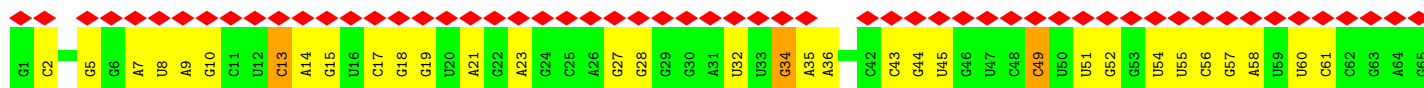
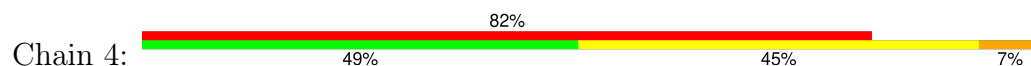




● Molecule 36: P-site tRNA



● Molecule 37: E-site tRNA



● Molecule 38: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	391.68, 391.68, 391.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMG, 5MC, PAR, M1Y, A2M, C4J, MA6, 4OC, OMU, MIA, MG, 7MG

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	0.52	0/1860	0.69	2/2503 (0.1%)
2	B	0.53	0/1713	0.64	1/2316 (0.0%)
3	C	0.46	0/1700	0.64	0/2274
4	D	0.48	0/1533	0.62	1/2057 (0.0%)
5	E	0.50	0/2074	0.70	1/2797 (0.0%)
6	F	0.51	0/1692	0.62	0/2295
7	G	0.41	0/1823	0.65	2/2449 (0.1%)
8	H	0.47	0/1460	0.68	1/1959 (0.1%)
9	I	0.58	0/1644	0.68	1/2217 (0.0%)
10	J	0.64	0/1031	0.64	0/1382
11	K	0.55	0/1425	0.68	0/1916
12	L	0.53	0/1148	0.68	1/1543 (0.1%)
13	M	0.41	0/819	0.69	0/1109
14	N	0.48	0/753	0.62	0/1024
15	O	0.57	0/1047	0.67	1/1408 (0.1%)
16	P	0.51	0/1163	0.75	4/1554 (0.3%)
17	Q	0.30	0/749	0.81	3/1028 (0.3%)
18	R	0.44	0/1099	0.65	0/1489
19	S	0.49	0/446	0.73	0/591
20	T	0.60	0/1176	0.73	0/1577
21	U	0.60	0/1270	0.66	0/1710
22	V	0.40	0/945	0.60	0/1267
23	W	0.40	0/841	0.56	0/1144
24	X	0.51	0/1236	0.67	0/1659
25	Y	0.52	0/674	0.64	0/914
26	Z	0.47	0/1056	0.67	0/1407
27	a	0.45	0/549	0.66	0/743
28	b	0.68	1/813 (0.1%)	0.80	1/1092 (0.1%)
29	c	0.65	0/669	0.72	1/897 (0.1%)
30	d	0.41	0/468	0.76	1/630 (0.2%)
31	e	0.45	0/456	0.57	0/603
32	f	0.29	0/393	0.68	1/540 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.44	0/2294	0.72	3/3131 (0.1%)
34	1	1.06	0/41155	1.23	426/64074 (0.7%)
35	2	0.46	0/1783	0.98	6/2776 (0.2%)
36	3	0.59	0/1831	1.04	8/2853 (0.3%)
37	4	0.43	1/1809 (0.1%)	1.16	22/2819 (0.8%)
38	5	1.00	0/279	1.29	3/431 (0.7%)
All	All	0.82	2/84876 (0.0%)	1.02	490/124178 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
12	L	0	1
15	O	0	1
16	P	0	3
17	Q	0	1
19	S	0	2
21	U	0	2
26	Z	0	1
29	c	0	2
32	f	0	4
33	g	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	78	CYS	CB-SG	6.89	1.94	1.82
37	4	75	C	C1'-N1	5.14	1.56	1.48

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	78	CYS	CA-CB-SG	13.35	138.02	114.00
34	1	1956	C	N1-C2-O2	13.04	126.72	118.90
34	1	1973	C	N1-C2-O2	11.17	125.60	118.90
34	1	1956	C	N3-C2-O2	-10.96	114.23	121.90
34	1	1510	C	C2-N1-C1'	10.23	130.05	118.80
37	4	60	U	C2-N1-C1'	9.95	129.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	354	C	C2-N1-C1'	9.88	129.66	118.80
34	1	1510	C	N3-C2-O2	-9.84	115.02	121.90
34	1	2039	C	C6-N1-C2	-9.58	116.47	120.30
34	1	1510	C	N1-C2-O2	9.32	124.49	118.90
34	1	1838	U	N3-C2-O2	-9.27	115.71	122.20
34	1	775	C	C2-N1-C1'	9.24	128.96	118.80
34	1	1838	U	C2-N1-C1'	9.18	128.72	117.70
34	1	1222	C	C6-N1-C2	-9.16	116.64	120.30
34	1	1212	C	N1-C2-O2	9.01	124.31	118.90
34	1	354	C	N3-C2-O2	-8.91	115.66	121.90
34	1	775	C	N1-C2-O2	8.86	124.21	118.90
34	1	88	C	C6-N1-C2	-8.85	116.76	120.30
34	1	147	U	C2-N1-C1'	8.83	128.30	117.70
34	1	1179	U	N3-C2-O2	-8.78	116.05	122.20
34	1	1222	C	C5-C6-N1	8.76	125.38	121.00
34	1	1408	C	C2-N1-C1'	8.60	128.26	118.80
34	1	1973	C	N3-C2-O2	-8.48	115.96	121.90
34	1	395	U	C2-N1-C1'	8.48	127.88	117.70
17	Q	47	LEU	CA-CB-CG	8.41	134.64	115.30
34	1	1956	C	C2-N1-C1'	8.35	127.98	118.80
34	1	632	C	C5-C6-N1	8.30	125.15	121.00
37	4	49	C	N1-C2-O2	8.28	123.86	118.90
34	1	1626	C	N1-C2-O2	8.26	123.86	118.90
34	1	2039	C	C2-N1-C1'	8.24	127.87	118.80
34	1	1192	U	C5-C6-N1	8.16	126.78	122.70
34	1	1222	C	N1-C2-O2	8.16	123.80	118.90
34	1	1973	C	C2-N1-C1'	8.14	127.76	118.80
37	4	60	U	N1-C2-O2	8.12	128.49	122.80
34	1	741	C	C2-N1-C1'	8.07	127.68	118.80
34	1	1473	C	C6-N1-C2	-8.04	117.09	120.30
34	1	2040	C	C6-N1-C2	-8.02	117.09	120.30
34	1	1408	C	N1-C2-O2	8.01	123.70	118.90
34	1	589	U	N1-C2-O2	7.97	128.38	122.80
34	1	147	U	N3-C2-O2	-7.95	116.63	122.20
34	1	313	G	C4-N9-C1'	7.93	136.81	126.50
34	1	2039	C	N3-C2-O2	-7.92	116.35	121.90
34	1	624	C	C5-C6-N1	7.92	124.96	121.00
34	1	354	C	N1-C2-O2	7.89	123.64	118.90
34	1	85	C	N1-C2-O2	7.89	123.63	118.90
34	1	276	G	OP1-P-O3'	7.84	122.44	105.20
34	1	1359	C	C2-N1-C1'	7.83	127.41	118.80
34	1	2052	C	C6-N1-C2	-7.80	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1595	G	C4-N9-C1'	7.79	136.63	126.50
34	1	2	A	O5'-P-OP1	-7.77	98.71	105.70
34	1	1212	C	C2-N1-C1'	7.76	127.33	118.80
34	1	624	C	C6-N1-C2	-7.66	117.23	120.30
34	1	2040	C	N3-C2-O2	-7.65	116.54	121.90
34	1	1581	G	C4-N9-C1'	7.65	136.45	126.50
34	1	565	U	N3-C2-O2	-7.64	116.85	122.20
34	1	1	G	O4'-C1'-N9	7.62	114.30	108.20
37	4	60	U	N3-C2-O2	-7.59	116.89	122.20
34	1	1510	C	C6-N1-C1'	-7.55	111.75	120.80
29	c	38	CYS	CA-CB-SG	7.54	127.58	114.00
34	1	1489	A	P-O3'-C3'	7.52	128.72	119.70
34	1	319	C	N1-C2-O2	7.44	123.36	118.90
34	1	842	U	N1-C2-O2	7.43	128.00	122.80
34	1	632	C	C6-N1-C2	-7.34	117.36	120.30
37	4	49	C	C2-N1-C1'	7.34	126.87	118.80
34	1	1421	C	C6-N1-C2	-7.33	117.37	120.30
34	1	565	U	N1-C2-O2	7.29	127.90	122.80
37	4	32	U	N1-C2-O2	7.29	127.90	122.80
34	1	1626	C	N3-C2-O2	-7.28	116.81	121.90
34	1	1250	A	P-O3'-C3'	7.27	128.43	119.70
34	1	298	C	N1-C2-O2	7.26	123.26	118.90
34	1	1956	C	C6-N1-C2	-7.26	117.40	120.30
37	4	32	U	C2-N1-C1'	7.26	126.41	117.70
34	1	398	C	C5-C6-N1	7.22	124.61	121.00
34	1	671	G	P-O3'-C3'	7.20	128.34	119.70
34	1	32	U	N3-C2-O2	-7.17	117.18	122.20
34	1	589	U	C2-N1-C1'	7.12	126.25	117.70
34	1	1145	A	P-O3'-C3'	7.11	128.24	119.70
34	1	842	U	C2-N1-C1'	7.10	126.22	117.70
34	1	1287	U	C2-N1-C1'	7.10	126.22	117.70
36	3	28	C	C6-N1-C2	-7.09	117.46	120.30
34	1	775	C	N3-C2-O2	-7.08	116.95	121.90
34	1	592	C	N1-C2-O2	7.07	123.14	118.90
34	1	17	C	C6-N1-C2	-7.04	117.48	120.30
34	1	589	U	N3-C2-O2	-7.03	117.28	122.20
34	1	2040	C	C2-N1-C1'	7.01	126.52	118.80
34	1	689	U	N3-C2-O2	-7.01	117.30	122.20
34	1	689	U	C2-N1-C1'	7.00	126.10	117.70
34	1	741	C	N1-C2-O2	6.99	123.09	118.90
37	4	34	G	P-O3'-C3'	6.98	128.08	119.70
37	4	60	U	C5-C6-N1	6.98	126.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1788	U	C2-N1-C1'	6.98	126.07	117.70
34	1	618	C	N1-C2-O2	6.97	123.08	118.90
34	1	1287	U	N3-C2-O2	-6.96	117.33	122.20
34	1	1275	C	P-O3'-C3'	6.94	128.03	119.70
36	3	28	C	N1-C2-O2	6.93	123.06	118.90
33	g	190	LEU	CA-CB-CG	6.93	131.24	115.30
34	1	1595	G	C8-N9-C1'	-6.92	118.01	127.00
34	1	1222	C	C2-N1-C1'	6.91	126.40	118.80
34	1	1838	U	N1-C2-O2	6.91	127.64	122.80
34	1	354	C	C6-N1-C2	-6.91	117.53	120.30
34	1	147	U	N1-C2-O2	6.88	127.62	122.80
7	G	69	LEU	CA-CB-CG	6.87	131.11	115.30
34	1	1654	U	N3-C2-O2	-6.87	117.39	122.20
34	1	837	G	N3-C2-N2	-6.86	115.09	119.90
36	3	28	C	N3-C2-O2	-6.86	117.10	121.90
34	1	842	U	N3-C2-O2	-6.86	117.40	122.20
2	B	180	LEU	CA-CB-CG	6.86	131.08	115.30
34	1	514	C	N1-C2-O2	6.85	123.01	118.90
34	1	1525	C	C6-N1-C2	-6.85	117.56	120.30
36	3	28	C	C2-N1-C1'	6.84	126.33	118.80
34	1	887	U	C2-N1-C1'	6.83	125.90	117.70
34	1	1610	U	N3-C2-O2	-6.83	117.42	122.20
34	1	395	U	N3-C2-O2	-6.82	117.43	122.20
34	1	1131	C	C6-N1-C2	-6.81	117.58	120.30
34	1	1542	C	N1-C2-O2	6.80	122.98	118.90
34	1	1190	C	C6-N1-C2	-6.80	117.58	120.30
34	1	1222	C	N3-C2-O2	-6.80	117.14	121.90
34	1	354	C	C6-N1-C1'	-6.78	112.67	120.80
34	1	1	G	C4-N9-C1'	-6.77	117.69	126.50
34	1	319	C	C6-N1-C2	-6.77	117.59	120.30
34	1	2182	U	N1-C2-O2	6.76	127.53	122.80
34	1	664	U	N3-C2-O2	-6.75	117.47	122.20
34	1	1131	C	C2-N1-C1'	6.75	126.23	118.80
34	1	1419	U	C5-C6-N1	6.75	126.08	122.70
34	1	1581	G	N7-C8-N9	6.75	116.47	113.10
34	1	2165	A	N9-C1'-C2'	-6.73	104.60	112.00
34	1	1408	C	C5-C6-N1	6.73	124.36	121.00
34	1	398	C	C6-N1-C2	-6.72	117.61	120.30
34	1	485	C	C6-N1-C2	-6.71	117.62	120.30
34	1	1654	U	C2-N1-C1'	6.67	125.70	117.70
34	1	1636	U	P-O3'-C3'	6.67	127.70	119.70
16	P	16	LEU	CA-CB-CG	6.66	130.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1626	C	C2-N1-C1'	6.66	126.13	118.80
34	1	655	U	N3-C2-O2	-6.66	117.54	122.20
34	1	1559	U	P-O3'-C3'	6.66	127.69	119.70
34	1	1131	C	N1-C2-O2	6.61	122.87	118.90
34	1	1361	U	C2-N1-C1'	6.61	125.64	117.70
34	1	1108	A	P-O3'-C3'	6.60	127.62	119.70
34	1	2165	A	C4'-C3'-O3'	6.59	126.18	113.00
34	1	85	C	C6-N1-C2	-6.58	117.67	120.30
34	1	1520	U	N3-C2-O2	-6.57	117.60	122.20
34	1	1619	G	N7-C8-N9	6.56	116.38	113.10
34	1	1520	U	N1-C2-O2	6.55	127.38	122.80
34	1	1511	C	N1-C2-O2	6.55	122.83	118.90
34	1	1944	C	N1-C2-O2	6.55	122.83	118.90
34	1	104	U	N3-C2-O2	-6.54	117.62	122.20
34	1	1276	G	P-O3'-C3'	6.54	127.54	119.70
34	1	85	C	N3-C2-O2	-6.52	117.34	121.90
37	4	49	C	C5-C6-N1	6.51	124.25	121.00
34	1	2003	C	C2-N1-C1'	6.50	125.95	118.80
34	1	1421	C	C5-C6-N1	6.49	124.25	121.00
34	1	1788	U	N1-C2-O2	6.49	127.34	122.80
34	1	1	G	OP1-P-O3'	6.47	119.44	105.20
34	1	592	C	C2-N1-C1'	6.46	125.91	118.80
34	1	1	G	P-O3'-C3'	6.46	127.45	119.70
34	1	759	U	O4'-C1'-N1	6.45	113.36	108.20
34	1	503	C	C2-N1-C1'	6.44	125.89	118.80
34	1	2202	U	N3-C2-O2	-6.42	117.71	122.20
34	1	1542	C	N3-C2-O2	-6.42	117.41	121.90
30	d	25	LEU	CA-CB-CG	6.42	130.06	115.30
34	1	1610	U	N1-C2-O2	6.41	127.29	122.80
34	1	1141	C	N1-C2-O2	6.41	122.75	118.90
34	1	1188	G	N3-C4-N9	6.41	129.85	126.00
34	1	503	C	N1-C2-O2	6.40	122.74	118.90
34	1	95	C	N1-C2-O2	6.39	122.73	118.90
34	1	994	U	N3-C2-O2	-6.39	117.73	122.20
34	1	332	C	N1-C2-O2	6.39	122.73	118.90
34	1	565	U	C2-N1-C1'	6.39	125.36	117.70
17	Q	47	LEU	C-N-CA	6.38	137.64	121.70
37	4	32	U	N3-C2-O2	-6.38	117.74	122.20
34	1	775	C	C6-N1-C1'	-6.37	113.16	120.80
34	1	689	U	N1-C2-O2	6.36	127.25	122.80
34	1	1787	A	P-O3'-C3'	6.35	127.32	119.70
34	1	1533	U	N3-C2-O2	-6.33	117.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1775	C	N1-C2-O2	6.33	122.69	118.90
34	1	2052	C	C5-C6-N1	6.33	124.16	121.00
34	1	1408	C	C6-N1-C2	-6.31	117.77	120.30
34	1	313	G	N3-C4-C5	-6.31	125.44	128.60
34	1	313	G	C8-N9-C1'	-6.31	118.80	127.00
34	1	147	U	C6-N1-C1'	-6.30	112.38	121.20
34	1	1641	U	C5-C6-N1	6.29	125.85	122.70
34	1	372	C	C6-N1-C2	-6.29	117.79	120.30
34	1	297	U	N3-C2-O2	-6.28	117.80	122.20
34	1	1190	C	C5-C6-N1	6.28	124.14	121.00
34	1	1874	U	C2-N1-C1'	6.28	125.24	117.70
34	1	1473	C	C5-C6-N1	6.27	124.14	121.00
34	1	1500	C	C6-N1-C2	-6.27	117.79	120.30
34	1	1538	U	N1-C2-O2	6.27	127.19	122.80
34	1	2182	U	N3-C2-O2	-6.26	117.81	122.20
34	1	1183	G	N1-C6-O6	-6.26	116.14	119.90
34	1	1961	G	N3-C4-N9	-6.26	122.25	126.00
34	1	306	U	P-O3'-C3'	6.24	127.19	119.70
34	1	50	C	C6-N1-C2	-6.24	117.81	120.30
34	1	17	C	C5-C6-N1	6.22	124.11	121.00
34	1	887	U	N1-C2-O2	6.20	127.14	122.80
34	1	915	A	P-O3'-C3'	6.20	127.14	119.70
34	1	1610	U	C2-N1-C1'	6.20	125.14	117.70
38	5	1	C	N1-C2-O2	6.19	122.61	118.90
34	1	335	C	N1-C2-O2	6.19	122.61	118.90
9	I	68	LEU	CA-CB-CG	6.19	129.53	115.30
34	1	1212	C	N3-C2-O2	-6.18	117.57	121.90
34	1	1976	U	N3-C2-O2	-6.17	117.88	122.20
34	1	403	G	O4'-C1'-N9	6.16	113.13	108.20
34	1	403	G	P-O3'-C3'	6.16	127.09	119.70
34	1	1944	C	N3-C2-O2	-6.16	117.59	121.90
17	Q	137	LEU	CA-CB-CG	6.15	129.44	115.30
34	1	2039	C	N1-C2-O2	6.15	122.59	118.90
37	4	60	U	C6-N1-C1'	-6.13	112.61	121.20
34	1	757	C	P-O3'-C3'	6.13	127.05	119.70
34	1	319	C	N3-C2-O2	-6.12	117.62	121.90
34	1	2202	U	P-O3'-C3'	6.11	127.03	119.70
34	1	1619	G	C8-N9-C4	-6.10	103.96	106.40
34	1	454	C	C6-N1-C2	-6.09	117.86	120.30
34	1	775	C	C6-N1-C2	-6.09	117.86	120.30
34	1	1216	C	C6-N1-C2	-6.09	117.86	120.30
34	1	592	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1952	C	C5-C6-N1	6.08	124.04	121.00
34	1	2040	C	N1-C2-O2	6.08	122.55	118.90
34	1	32	U	N1-C2-O2	6.07	127.05	122.80
16	P	113	GLY	N-CA-C	6.07	128.27	113.10
34	1	13	U	C5-C6-N1	6.05	125.72	122.70
37	4	49	C	C6-N1-C2	-6.04	117.88	120.30
32	f	121	PRO	C-N-CA	6.03	136.77	121.70
34	1	789	G	P-O3'-C3'	6.02	126.93	119.70
34	1	1500	C	C5-C6-N1	6.02	124.01	121.00
34	1	1783	C	C6-N1-C2	-6.01	117.90	120.30
34	1	638	C	C6-N1-C2	-6.00	117.90	120.30
34	1	619	A	C6-N1-C2	5.99	122.20	118.60
34	1	2050	U	C5-C6-N1	5.99	125.69	122.70
34	1	381	G	C2-N3-C4	5.98	114.89	111.90
34	1	1473	C	N1-C2-O2	5.97	122.48	118.90
34	1	608	C	C6-N1-C2	-5.97	117.91	120.30
34	1	1419	U	N1-C2-O2	5.97	126.98	122.80
34	1	1538	U	N3-C2-O2	-5.97	118.02	122.20
34	1	514	C	N3-C2-O2	-5.96	117.73	121.90
34	1	372	C	N1-C2-O2	5.95	122.47	118.90
37	4	70	C	N1-C2-O2	5.95	122.47	118.90
34	1	2196	G	OP1-P-O3'	5.95	118.28	105.20
34	1	396	G	P-O3'-C3'	5.94	126.83	119.70
34	1	14	C	C5-C6-N1	5.93	123.97	121.00
34	1	335	C	C2-N1-C1'	5.93	125.32	118.80
34	1	398	C	C2-N3-C4	5.93	122.86	119.90
33	g	104	LEU	CA-CB-CG	5.92	128.91	115.30
34	1	1944	C	C6-N1-C2	-5.91	117.94	120.30
35	2	66	U	N1-C2-O2	5.91	126.94	122.80
34	1	276	G	P-O3'-C3'	5.91	126.79	119.70
34	1	14	C	C6-N1-C2	-5.90	117.94	120.30
16	P	101	LEU	CA-CB-CG	5.90	128.86	115.30
34	1	1991	C	C5-C6-N1	5.89	123.94	121.00
34	1	50	C	N3-C2-O2	-5.89	117.78	121.90
34	1	313	G	N3-C4-N9	5.89	129.53	126.00
34	1	887	U	N3-C2-O2	-5.89	118.08	122.20
34	1	1581	G	C8-N9-C1'	-5.88	119.35	127.00
37	4	49	C	N3-C2-O2	-5.87	117.79	121.90
34	1	31	C	C6-N1-C2	-5.87	117.95	120.30
34	1	1654	U	C6-N1-C2	-5.86	117.48	121.00
34	1	1120	U	C2-N1-C1'	5.86	124.73	117.70
34	1	88	C	C5-C6-N1	5.85	123.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1511	C	N3-C2-O2	-5.84	117.81	121.90
34	1	632	C	C2-N1-C1'	5.83	125.22	118.80
34	1	1642	C	C6-N1-C2	-5.83	117.97	120.30
34	1	624	C	N1-C2-O2	5.82	122.39	118.90
34	1	1987	G	O4'-C1'-N9	5.81	112.85	108.20
34	1	1554	A	C4-N9-C1'	5.81	136.76	126.30
34	1	88	C	N3-C2-O2	-5.81	117.84	121.90
34	1	1131	C	C5-C6-N1	5.80	123.90	121.00
34	1	955	A	O5'-P-OP1	5.79	117.65	110.70
34	1	395	U	N1-C2-O2	5.78	126.85	122.80
34	1	1181	C	C2-N1-C1'	5.78	125.15	118.80
34	1	1473	C	N3-C2-O2	-5.77	117.86	121.90
34	1	433	G	O4'-C1'-N9	5.76	112.81	108.20
34	1	1179	U	N1-C2-O2	5.76	126.83	122.80
34	1	1257	U	N3-C2-O2	-5.75	118.18	122.20
34	1	1257	U	C2-N1-C1'	5.74	124.59	117.70
34	1	319	C	C5-C6-N1	5.74	123.87	121.00
34	1	2187	C	N1-C2-O2	5.74	122.34	118.90
34	1	1188	G	N3-C4-C5	-5.74	125.73	128.60
34	1	1237	C	C5-C6-N1	5.74	123.87	121.00
34	1	1188	G	C6-C5-N7	-5.72	126.97	130.40
34	1	1196	U	N1-C2-O2	5.71	126.80	122.80
34	1	1408	C	C6-N1-C1'	-5.71	113.95	120.80
34	1	1864	C	C2-N1-C1'	5.69	125.05	118.80
34	1	1511	C	C6-N1-C2	-5.68	118.03	120.30
34	1	425	C	C6-N1-C2	-5.68	118.03	120.30
34	1	36	U	C5-C6-N1	5.68	125.54	122.70
34	1	1425	U	N3-C2-O2	-5.66	118.24	122.20
34	1	2053	A	P-O3'-C3'	5.66	126.49	119.70
34	1	367	A	O5'-P-OP2	-5.65	100.61	105.70
34	1	1768	U	C2-N1-C1'	5.65	124.48	117.70
34	1	90	C	C5-C6-N1	5.65	123.83	121.00
34	1	1408	C	N3-C2-O2	-5.65	117.95	121.90
38	5	10	C	N1-C2-O2	5.65	122.29	118.90
34	1	1181	C	N3-C2-O2	-5.64	117.95	121.90
34	1	1276	G	O5'-P-OP1	-5.64	100.62	105.70
34	1	1161	G	C4-N9-C1'	5.64	133.83	126.50
34	1	1131	C	N3-C2-O2	-5.63	117.96	121.90
34	1	1775	C	C6-N1-C2	-5.63	118.05	120.30
34	1	615	C	C6-N1-C2	-5.62	118.05	120.30
34	1	1838	U	C6-N1-C1'	-5.62	113.33	121.20
34	1	659	G	C4-N9-C1'	5.62	133.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1991	C	C6-N1-C2	-5.62	118.05	120.30
16	P	130	LEU	CA-CB-CG	5.60	128.19	115.30
34	1	659	G	N3-C4-N9	5.60	129.36	126.00
34	1	1973	C	C6-N1-C1'	-5.60	114.08	120.80
34	1	1533	U	N1-C2-O2	5.60	126.72	122.80
34	1	994	U	N1-C2-O2	5.59	126.71	122.80
34	1	104	U	N1-C2-O2	5.58	126.71	122.80
34	1	1858	G	P-O3'-C3'	5.57	126.38	119.70
34	1	1609	U	N3-C2-O2	-5.57	118.30	122.20
35	2	66	U	N3-C2-O2	-5.56	118.31	122.20
34	1	1196	U	N3-C2-O2	-5.56	118.31	122.20
34	1	1918	U	N1-C2-O2	5.56	126.69	122.80
34	1	1361	U	C5-C6-N1	5.54	125.47	122.70
34	1	1508	C	N1-C2-O2	5.53	122.22	118.90
34	1	741	C	C6-N1-C1'	-5.53	114.16	120.80
34	1	1874	U	C6-N1-C1'	-5.53	113.46	121.20
34	1	1120	U	N1-C2-O2	5.52	126.67	122.80
15	O	39	ASP	C-N-CA	5.52	135.50	121.70
34	1	297	U	N1-C2-O2	5.52	126.66	122.80
34	1	619	A	N1-C2-N3	-5.51	126.54	129.30
34	1	1460	G	O4'-C1'-N9	5.51	112.61	108.20
34	1	1859	A	C4-N9-C1'	5.51	136.22	126.30
34	1	862	G	O4'-C1'-N9	5.50	112.60	108.20
37	4	13	C	P-O3'-C3'	5.50	126.31	119.70
34	1	332	C	C5-C6-N1	5.50	123.75	121.00
34	1	85	C	C5-C6-N1	5.50	123.75	121.00
34	1	1486	C	C6-N1-C2	-5.50	118.10	120.30
34	1	1359	C	C6-N1-C2	-5.50	118.10	120.30
34	1	1581	G	C8-N9-C4	-5.49	104.20	106.40
34	1	1609	U	N1-C2-O2	5.49	126.64	122.80
34	1	1973	C	C6-N1-C2	-5.49	118.10	120.30
34	1	676	C	N1-C2-O2	5.49	122.19	118.90
1	A	199	LEU	CA-CB-CG	5.48	127.91	115.30
34	1	1788	U	N3-C2-O2	-5.48	118.36	122.20
34	1	659	G	C8-N9-C1'	-5.48	119.88	127.00
34	1	381	G	C4-N9-C1'	5.47	133.62	126.50
7	G	69	LEU	CB-CG-CD1	5.47	120.30	111.00
34	1	503	C	C6-N1-C1'	-5.46	114.25	120.80
34	1	1654	U	N1-C2-O2	5.46	126.62	122.80
33	g	301	ASN	N-CA-C	5.45	125.70	111.00
34	1	1679	C	N1-C2-O2	5.45	122.17	118.90
34	1	836	C	C6-N1-C2	-5.44	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1181	C	N1-C2-O2	5.44	122.17	118.90
34	1	1537	U	C2-N1-C1'	5.44	124.23	117.70
34	1	1146	G	O5'-P-OP1	-5.43	100.81	105.70
37	4	60	U	C6-N1-C2	-5.43	117.74	121.00
34	1	1525	C	N3-C2-O2	-5.43	118.10	121.90
34	1	591	A	P-O3'-C3'	5.43	126.22	119.70
34	1	298	C	C2-N1-C1'	5.43	124.77	118.80
34	1	1161	G	P-O3'-C3'	5.42	126.21	119.70
34	1	99	U	N3-C2-O2	-5.42	118.41	122.20
34	1	417	U	C5-C6-N1	5.42	125.41	122.70
34	1	1	G	C8-N9-C1'	5.42	134.04	127.00
34	1	31	C	C5-C6-N1	5.41	123.70	121.00
34	1	1421	C	C4-C5-C6	-5.41	114.70	117.40
34	1	1769	C	C5-C6-N1	5.41	123.70	121.00
34	1	1525	C	C5-C6-N1	5.41	123.70	121.00
34	1	1212	C	C6-N1-C1'	-5.41	114.31	120.80
37	4	72	C	C6-N1-C2	-5.41	118.14	120.30
34	1	1359	C	C5-C6-N1	5.40	123.70	121.00
34	1	883	G	O4'-C1'-N9	5.40	112.52	108.20
34	1	760	G	C4-N9-C1'	5.39	133.51	126.50
34	1	151	U	N1-C2-O2	5.39	126.57	122.80
34	1	1940	G	N3-C4-N9	5.39	129.23	126.00
34	1	496	A	C2-N3-C4	5.39	113.29	110.60
34	1	454	C	C5-C6-N1	5.39	123.69	121.00
34	1	1359	C	O4'-C1'-N1	5.39	112.51	108.20
34	1	335	C	C6-N1-C2	-5.38	118.15	120.30
34	1	332	C	C2-N1-C1'	5.38	124.72	118.80
34	1	319	C	C2-N1-C1'	5.38	124.72	118.80
34	1	510	G	N9-C1'-C2'	-5.37	106.09	112.00
34	1	951	U	N1-C2-O2	5.37	126.56	122.80
34	1	741	C	C6-N1-C2	-5.37	118.15	120.30
34	1	1698	U	N3-C2-O2	-5.37	118.44	122.20
34	1	2039	C	N3-C4-C5	-5.36	119.75	121.90
34	1	1419	U	C2-N1-C1'	5.35	124.11	117.70
34	1	1510	C	C6-N1-C2	-5.35	118.16	120.30
34	1	1595	G	N3-C4-N9	5.34	129.21	126.00
34	1	372	C	N3-C2-O2	-5.34	118.16	121.90
34	1	608	C	C5-C6-N1	5.34	123.67	121.00
34	1	2202	U	C2-N1-C1'	5.34	124.10	117.70
34	1	1485	A	C5-C6-N6	-5.33	119.43	123.70
34	1	95	C	N3-C2-O2	-5.33	118.17	121.90
34	1	1628	U	N1-C2-O2	5.33	126.53	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	760	G	O4'-C1'-N9	5.32	112.46	108.20
34	1	1207	U	C5-C6-N1	5.32	125.36	122.70
35	2	8	U	C2-N1-C1'	5.32	124.08	117.70
36	3	39	C	C6-N1-C2	-5.31	118.17	120.30
34	1	14	C	N1-C2-O2	5.31	122.09	118.90
34	1	2186	C	C6-N1-C2	-5.31	118.18	120.30
34	1	238	G	P-O3'-C3'	5.30	126.07	119.70
34	1	355	U	N3-C2-O2	-5.30	118.49	122.20
36	3	34	C	C2-N1-C1'	5.29	124.62	118.80
34	1	1237	C	C6-N1-C2	-5.29	118.19	120.30
34	1	403	G	C5-C6-O6	-5.28	125.43	128.60
34	1	1956	C	C5-C6-N1	5.28	123.64	121.00
34	1	1769	C	C6-N1-C2	-5.28	118.19	120.30
34	1	297	U	C2-N1-C1'	5.28	124.03	117.70
34	1	1654	U	C5-C6-N1	5.28	125.34	122.70
34	1	1371	U	N3-C2-O2	-5.28	118.51	122.20
34	1	1634	C	C6-N1-C2	-5.28	118.19	120.30
34	1	1489	A	OP2-P-O3'	5.27	116.80	105.20
34	1	1554	A	C8-N9-C1'	-5.27	118.21	127.70
34	1	335	C	C5-C6-N1	5.27	123.63	121.00
34	1	342	C	C6-N1-C2	-5.27	118.19	120.30
4	D	92	LEU	CA-CB-CG	5.26	127.41	115.30
34	1	506	U	C5-C6-N1	5.26	125.33	122.70
34	1	1359	C	C6-N1-C1'	-5.26	114.48	120.80
34	1	298	C	N3-C2-O2	-5.25	118.22	121.90
34	1	741	C	N3-C2-O2	-5.25	118.23	121.90
34	1	36	U	N3-C2-O2	-5.25	118.53	122.20
1	A	156	CYS	CA-CB-SG	5.23	123.42	114.00
34	1	1768	U	N3-C2-O2	-5.23	118.54	122.20
34	1	2064	C	C6-N1-C2	-5.22	118.21	120.30
34	1	664	U	N1-C2-O2	5.21	126.45	122.80
37	4	74	C	C2-N1-C1'	5.21	124.53	118.80
8	H	78	LEU	CA-CB-CG	5.21	127.28	115.30
34	1	355	U	N1-C2-O2	5.21	126.45	122.80
34	1	1939	G	C8-N9-C4	5.21	108.48	106.40
37	4	74	C	N1-C2-O2	5.20	122.02	118.90
34	1	1371	U	N1-C2-O2	5.20	126.44	122.80
34	1	2182	U	C5-C6-N1	5.20	125.30	122.70
34	1	664	U	C6-N1-C2	-5.19	117.89	121.00
35	2	13	C	P-O3'-C3'	5.19	125.93	119.70
34	1	1918	U	C2-N1-C1'	5.19	123.92	117.70
34	1	1522	G	N3-C4-N9	5.18	129.11	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1859	A	C8-N9-C1'	-5.18	118.37	127.70
34	1	167	C	C6-N1-C2	-5.18	118.23	120.30
34	1	675	U	C5-C6-N1	5.18	125.29	122.70
34	1	1361	U	C6-N1-C1'	-5.18	113.95	121.20
34	1	618	C	N3-C2-O2	-5.18	118.28	121.90
34	1	1212	C	C5-C6-N1	5.18	123.59	121.00
34	1	1918	U	N3-C2-O2	-5.18	118.58	122.20
34	1	1956	C	C6-N1-C1'	-5.18	114.59	120.80
34	1	90	C	C6-N1-C2	-5.16	118.23	120.30
34	1	1533	U	C2-N1-C1'	5.16	123.89	117.70
34	1	592	C	C6-N1-C1'	-5.16	114.61	120.80
34	1	1525	C	N1-C2-O2	5.16	121.99	118.90
34	1	2186	C	N3-C4-C5	-5.15	119.84	121.90
37	4	13	C	OP1-P-O3'	5.15	116.54	105.20
34	1	313	G	C8-N9-C4	-5.14	104.34	106.40
34	1	2163	G	N9-C1'-C2'	-5.14	106.34	112.00
34	1	676	C	N3-C2-O2	-5.14	118.30	121.90
34	1	2132	C	C6-N1-C2	-5.14	118.24	120.30
34	1	913	G	C2'-C3'-O3'	-5.14	98.19	109.50
34	1	1642	C	N1-C2-O2	5.14	121.98	118.90
34	1	313	G	C2-N3-C4	5.14	114.47	111.90
34	1	2190	C	C6-N1-C2	-5.14	118.24	120.30
34	1	424	C	C6-N1-C2	-5.13	118.25	120.30
34	1	395	U	C6-N1-C1'	-5.13	114.02	121.20
37	4	70	C	N3-C2-O2	-5.13	118.31	121.90
34	1	36	U	N1-C2-O2	5.12	126.38	122.80
34	1	837	G	N1-C2-N2	5.12	120.81	116.20
34	1	1939	G	N9-C4-C5	-5.12	103.35	105.40
34	1	151	U	N3-C2-O2	-5.11	118.62	122.20
12	L	111	LEU	CA-CB-CG	5.11	127.06	115.30
5	E	6	LEU	CA-CB-CG	5.11	127.05	115.30
34	1	381	G	N3-C4-C5	-5.11	126.05	128.60
34	1	787	G	O4'-C1'-N9	5.11	112.29	108.20
34	1	1864	C	N1-C2-O2	5.11	121.96	118.90
34	1	588	G	O4'-C1'-N9	5.10	112.28	108.20
34	1	1838	U	C6-N1-C2	-5.09	117.95	121.00
34	1	426	G	C2-N3-C4	5.08	114.44	111.90
34	1	2202	U	N1-C2-O2	5.08	126.36	122.80
34	1	1698	U	C2-N1-C1'	5.08	123.79	117.70
34	1	675	U	N1-C2-O2	5.07	126.35	122.80
34	1	1467	U	N3-C2-O2	-5.07	118.65	122.20
34	1	741	C	C5-C6-N1	5.06	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1981	G	C4-N9-C1'	5.06	133.08	126.50
38	5	1	C	N3-C2-O2	-5.06	118.36	121.90
34	1	1120	U	N3-C2-O2	-5.05	118.66	122.20
34	1	1455	C	C6-N1-C2	-5.05	118.28	120.30
34	1	1157	C	C6-N1-C2	-5.05	118.28	120.30
34	1	1467	U	N1-C2-O2	5.05	126.34	122.80
34	1	655	U	N1-C2-O2	5.04	126.33	122.80
35	2	34	G	P-O3'-C3'	5.04	125.75	119.70
34	1	1419	U	N3-C2-O2	-5.04	118.67	122.20
34	1	1775	C	C5-C6-N1	5.04	123.52	121.00
34	1	952	U	N1-C2-O2	5.03	126.32	122.80
35	2	60	U	C2-N1-C1'	5.03	123.74	117.70
34	1	159	C	C6-N1-C2	-5.02	118.29	120.30
34	1	755	C	C6-N1-C2	-5.02	118.29	120.30
34	1	50	C	N1-C2-O2	5.02	121.91	118.90
36	3	28	C	C5-C6-N1	5.01	123.51	121.00
34	1	303	C	C4-C5-C6	-5.01	114.90	117.40
34	1	621	C	C6-N1-C2	-5.01	118.30	120.30
34	1	2100	A	C4-N9-C1'	5.01	135.31	126.30
34	1	1184	C	N1-C2-O2	5.00	121.90	118.90
36	3	34	C	C6-N1-C2	-5.00	118.30	120.30
34	1	1490	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208[A]	ARG	Peptide
2	B	208[B]	ARG	Peptide
12	L	109	ALA	Peptide
15	O	97	ARG	Peptide
16	P	106	GLY	Peptide
16	P	112	VAL	Peptide
16	P	86	PRO	Peptide
17	Q	48	SER	Peptide
19	S	5	ASP	Peptide
19	S	6	GLN	Peptide
21	U	19	HIS	Peptide
21	U	54	GLY	Peptide
26	Z	65	PHE	Peptide
29	c	40	ARG	Peptide
29	c	41	CYS	Peptide

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Mol	Chain	Res	Type	Group
32	f	122	HIS	Peptide
32	f	144	HIS	Peptide
32	f	145	LEU	Peptide
32	f	99	LYS	Peptide
33	g	300	ASP	Peptide

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	
1	A	226/264 (86%)	209 (92%)	17 (8%)	0	100	100
2	B	211/246 (86%)	200 (95%)	11 (5%)	0	100	100
3	C	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	25	49
4	D	181/190 (95%)	176 (97%)	5 (3%)	0	100	100
5	E	260/273 (95%)	246 (95%)	14 (5%)	0	100	100
6	F	218/265 (82%)	206 (94%)	12 (6%)	0	100	100
7	G	237/249 (95%)	222 (94%)	15 (6%)	0	100	100
8	H	181/190 (95%)	173 (96%)	8 (4%)	0	100	100
9	I	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
10	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
11	K	179/220 (81%)	170 (95%)	9 (5%)	0	100	100
12	L	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
13	M	101/116 (87%)	94 (93%)	7 (7%)	0	100	100
14	N	90/153 (59%)	85 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	137/144 (95%)	128 (93%)	9 (7%)	0	100	100
16	P	143/143 (100%)	134 (94%)	8 (6%)	1 (1%)	19	42
17	Q	113/141 (80%)	107 (95%)	6 (5%)	0	100	100
18	R	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	S	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
20	T	140/151 (93%)	132 (94%)	8 (6%)	0	100	100
21	U	154/173 (89%)	141 (92%)	13 (8%)	0	100	100
22	V	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
23	W	106/152 (70%)	100 (94%)	6 (6%)	0	100	100
24	X	151/179 (84%)	141 (93%)	10 (7%)	0	100	100
25	Y	86/159 (54%)	85 (99%)	1 (1%)	0	100	100
26	Z	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
27	a	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
28	b	101/112 (90%)	96 (95%)	5 (5%)	0	100	100
29	c	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
30	d	63/87 (72%)	61 (97%)	2 (3%)	0	100	100
31	e	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
32	f	56/152 (37%)	40 (71%)	14 (25%)	2 (4%)	3	6
33	g	295/312 (95%)	264 (90%)	30 (10%)	1 (0%)	37	61
All	All	4756/5531 (86%)	4466 (94%)	285 (6%)	5 (0%)	50	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	87	ASN
32	f	123	PRO
32	f	122	HIS
3	C	190	PRO
33	g	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/223 (88%)	191 (97%)	6 (3%)	36	65
2	B	180/202 (89%)	176 (98%)	4 (2%)	47	76
3	C	176/184 (96%)	172 (98%)	4 (2%)	45	74
4	D	158/164 (96%)	156 (99%)	2 (1%)	65	85
5	E	207/225 (92%)	203 (98%)	4 (2%)	52	79
6	F	170/208 (82%)	168 (99%)	2 (1%)	67	86
7	G	171/208 (82%)	166 (97%)	5 (3%)	37	67
8	H	149/159 (94%)	146 (98%)	3 (2%)	50	78
9	I	173/187 (92%)	170 (98%)	3 (2%)	56	81
10	J	108/111 (97%)	108 (100%)	0	100	100
11	K	130/176 (74%)	130 (100%)	0	100	100
12	L	113/120 (94%)	112 (99%)	1 (1%)	75	90
13	M	93/104 (89%)	93 (100%)	0	100	100
14	N	72/129 (56%)	70 (97%)	2 (3%)	38	68
15	O	103/113 (91%)	98 (95%)	5 (5%)	21	47
16	P	117/116 (101%)	113 (97%)	4 (3%)	32	61
17	Q	60/119 (50%)	60 (100%)	0	100	100
18	R	106/130 (82%)	105 (99%)	1 (1%)	75	90
19	S	47/49 (96%)	45 (96%)	2 (4%)	25	52
20	T	124/132 (94%)	123 (99%)	1 (1%)	79	91
21	U	128/150 (85%)	127 (99%)	1 (1%)	79	91
22	V	91/124 (73%)	88 (97%)	3 (3%)	33	62
23	W	78/131 (60%)	78 (100%)	0	100	100
24	X	122/147 (83%)	120 (98%)	2 (2%)	58	82
25	Y	72/117 (62%)	68 (94%)	4 (6%)	17	41
26	Z	109/118 (92%)	109 (100%)	0	100	100
27	a	58/95 (61%)	58 (100%)	0	100	100
28	b	81/93 (87%)	78 (96%)	3 (4%)	29	58
29	c	72/76 (95%)	70 (97%)	2 (3%)	38	68
30	d	46/75 (61%)	45 (98%)	1 (2%)	47	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	e	43/54 (80%)	42 (98%)	1 (2%)	45	74
32	f	26/126 (21%)	24 (92%)	2 (8%)	10	26
33	g	232/266 (87%)	229 (99%)	3 (1%)	65	85
All	All	3812/4631 (82%)	3741 (98%)	71 (2%)	60	79

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	85	LYS
1	A	137[A]	MET
1	A	137[B]	MET
1	A	177[A]	ARG
1	A	177[B]	ARG
2	B	199[A]	GLU
2	B	199[B]	GLU
2	B	208[A]	ARG
2	B	208[B]	ARG
3	C	75	ARG
3	C	77	ASN
3	C	158[A]	LYS
3	C	158[B]	LYS
4	D	77	ARG
4	D	181	ARG
5	E	75[A]	ARG
5	E	75[B]	ARG
5	E	95	ARG
5	E	244	MET
6	F	138	ARG
6	F	149	VAL
7	G	2[A]	LYS
7	G	2[B]	LYS
7	G	32	ARG
7	G	101	ARG
7	G	163	ARG
8	H	41[A]	ARG
8	H	41[B]	ARG
8	H	151	ASN
9	I	50	ARG
9	I	61	VAL
9	I	133	ILE

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Mol	Chain	Res	Type
12	L	133	LYS
14	N	115[A]	ARG
14	N	115[B]	ARG
15	O	59[A]	ARG
15	O	59[B]	ARG
15	O	135	ARG
15	O	136[A]	LYS
15	O	136[B]	LYS
16	P	19[A]	ARG
16	P	19[B]	ARG
16	P	71[A]	ARG
16	P	71[B]	ARG
18	R	32	ARG
19	S	27	ASN
19	S	43	CYS
20	T	69	ARG
21	U	39	LYS
22	V	119[A]	ARG
22	V	119[B]	ARG
22	V	122	ARG
24	X	39[A]	LYS
24	X	39[B]	LYS
25	Y	8	ASN
25	Y	26	ASN
25	Y	78	ILE
25	Y	89	LYS
28	b	28	CYS
28	b	88	VAL
28	b	95	ASN
29	c	41	CYS
29	c	58	LYS
30	d	36	ARG
31	e	58	ASN
32	f	100	TYR
32	f	101	PHE
33	g	44	ASN
33	g	299[A]	LYS
33	g	299[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
2	B	33	GLN
2	B	96	HIS
2	B	102	HIS
3	C	77	ASN
4	D	65	HIS
4	D	122	HIS
4	D	132	HIS
4	D	138	GLN
5	E	5	HIS
5	E	72	HIS
5	E	185	ASN
5	E	203	ASN
7	G	4	ASN
7	G	99	ASN
7	G	113	ASN
7	G	219	ASN
8	H	151	ASN
9	I	34	HIS
9	I	89	HIS
9	I	113	GLN
9	I	196	GLN
10	J	64	ASN
11	K	64	ASN
11	K	194	GLN
12	L	11	GLN
12	L	32	GLN
12	L	43	GLN
14	N	82	GLN
15	O	31	ASN
16	P	20	ASN
16	P	63	ASN
19	S	27	ASN
19	S	47	ASN
20	T	134	GLN
21	U	24	GLN
21	U	107	HIS
23	W	108	GLN
23	W	110	ASN
24	X	80	GLN
25	Y	8	ASN
25	Y	23	HIS
25	Y	26	ASN

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Mol	Chain	Res	Type
25	Y	71	HIS
26	Z	61	GLN
28	b	84	HIS
28	b	95	ASN
29	c	27	GLN
29	c	50	HIS
30	d	41	GLN
31	e	17	GLN
31	e	58	ASN
31	e	60	GLN
33	g	10	HIS
33	g	44	ASN
33	g	59	HIS
33	g	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	1725/2203 (78%)	551 (31%)	35 (2%)
35	2	74/76 (97%)	29 (39%)	2 (2%)
36	3	76/77 (98%)	20 (26%)	0
37	4	75/76 (98%)	34 (45%)	2 (2%)
38	5	11/13 (84%)	2 (18%)	0
All	All	1961/2445 (80%)	636 (32%)	39 (1%)

All (636) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	2	A
34	1	3	U
34	1	14	C
34	1	17	C
34	1	22	A
34	1	25	C
34	1	34	G
34	1	36	U
34	1	39	A
34	1	42	G
34	1	44	C
34	1	46	U
34	1	47	A

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Mol	Chain	Res	Type
34	1	55	A
34	1	58	C
34	1	59	C
34	1	63	G
34	1	68	A
34	1	71	G
34	1	95	C
34	1	96	U
34	1	98	A2M
34	1	101	A
34	1	102	C
34	1	103	A
34	1	105	C
34	1	112	A
34	1	114	U
34	1	115	OMC
34	1	117	G
34	1	122	A
34	1	124	A
34	1	125	A
34	1	126	A
34	1	128	C
34	1	129	U
34	1	134	G
34	1	144	A
34	1	145	A
34	1	146	U
34	1	152	A
34	1	161	A
34	1	171	C
34	1	174	A
34	1	176	A
34	1	181	A
34	1	185	A
34	1	192	U
34	1	197	U
34	1	230	G
34	1	238	G
34	1	239	C
34	1	249	A
34	1	250	C
34	1	256	A

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Mol	Chain	Res	Type
34	1	262	U
34	1	264	C
34	1	266	U
34	1	274	C
34	1	275	A
34	1	276	G
34	1	277	U
34	1	278	A
34	1	281	A
34	1	282	C
34	1	284	C
34	1	287	C
34	1	288	A
34	1	297	U
34	1	298	C
34	1	304	A
34	1	307	C
34	1	308	C
34	1	309	G
34	1	310	U
34	1	315	A
34	1	316	A
34	1	317	G
34	1	332	C
34	1	335	C
34	1	336	U
34	1	337	U
34	1	339	U
34	1	340	G
34	1	343	G
34	1	348	A
34	1	352	C
34	1	353	C
34	1	356	A
34	1	358	C
34	1	360	G
34	1	371	C
34	1	372	C
34	1	373	G
34	1	377	A
34	1	381	G
34	1	382	A

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Mol	Chain	Res	Type
34	1	396	G
34	1	397	A
34	1	403	G
34	1	404	C
34	1	423	U
34	1	431	G
34	1	432	G
34	1	439	G
34	1	442	A
34	1	443	A
34	1	444	A
34	1	445	U
34	1	447	G
34	1	459	A
34	1	460	C
34	1	462	G
34	1	465	G
34	1	466	G
34	1	467	C
34	1	469	G
34	1	472	G
34	1	473	G
34	1	477	G
34	1	481	A
34	1	482	U
34	1	483	U
34	1	487	C
34	1	488	A
34	1	491	G
34	1	494	A
34	1	495	A
34	1	501	A
34	1	502	A
34	1	503	C
34	1	507	G
34	1	508	A
34	1	516	A
34	1	520	G
34	1	521	A
34	1	523	A
34	1	525	A
34	1	554	U

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Mol	Chain	Res	Type
34	1	557	A
34	1	558	U
34	1	559	G
34	1	562	G
34	1	563	G
34	1	565	U
34	1	566	A
34	1	568	U
34	1	570	A
34	1	572	A
34	1	574	C
34	1	576	A
34	1	578	C
34	1	579	C
34	1	580	A
34	1	588	G
34	1	591	A
34	1	592	C
34	1	593	A
34	1	594	A
34	1	600	G
34	1	602	A
34	1	603	C
34	1	604	A
34	1	606	G
34	1	607	U
34	1	608	C
34	1	614	C
34	1	617	G
34	1	624	C
34	1	626	G
34	1	627	U
34	1	628	A
34	1	629	A
34	1	631	U
34	1	643	A
34	1	657	C
34	1	658	U
34	1	659	G
34	1	660	U
34	1	662	G
34	1	663	C

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Mol	Chain	Res	Type
34	1	668	A2M
34	1	669	A
34	1	670	A
34	1	671	G
34	1	672	G
34	1	685	A
34	1	686	C
34	1	688	G
34	1	690	G
34	1	694	U
34	1	721	U
34	1	722	C
34	1	723	C
34	1	724	A
34	1	728	C
34	1	729	G
34	1	731	A
34	1	740	C
34	1	741	C
34	1	742	C
34	1	751	G
34	1	756	C
34	1	757	C
34	1	758	G
34	1	759	U
34	1	762	A
34	1	771	G
34	1	776	A
34	1	785	G
34	1	787	G
34	1	788	A
34	1	789	G
34	1	790	U
34	1	791	G
34	1	792	G
34	1	834	U
34	1	842	U
34	1	844	U
34	1	845	U
34	1	855	U
34	1	856	A
34	1	862	G

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Mol	Chain	Res	Type
34	1	863	C
34	1	866	G
34	1	867	A
34	1	872	A
34	1	875	A
34	1	876	G
34	1	883	G
34	1	884	A
34	1	890	A
34	1	893	A
34	1	894	G
34	1	895	A
34	1	903	G
34	1	905	A
34	1	906	U
34	1	907	A
34	1	908	A
34	1	911	A
34	1	912	A2M
34	1	913	G
34	1	914	G
34	1	916	G
34	1	918	A
34	1	950	U
34	1	952	U
34	1	954	A
34	1	955	A
34	1	972	A
34	1	981	U
34	1	982	G
34	1	987	A
34	1	990	U
34	1	991	G
34	1	992	C
34	1	994	U
34	1	997	C
34	1	1102	G
34	1	1103	G
34	1	1105	A
34	1	1109	A
34	1	1118	G
34	1	1123	G

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Mol	Chain	Res	Type
34	1	1129	A
34	1	1133	U
34	1	1139	G
34	1	1142	G
34	1	1145	A
34	1	1146	G
34	1	1147	A
34	1	1152	A
34	1	1153	A
34	1	1160	A
34	1	1161	G
34	1	1162	A
34	1	1180	A
34	1	1182	A
34	1	1189	G
34	1	1191	A
34	1	1192	U
34	1	1199	A
34	1	1207	U
34	1	1213	A
34	1	1217	A
34	1	1218	A
34	1	1234	G
34	1	1235	A
34	1	1237	C
34	1	1239	A
34	1	1244	G
34	1	1248	A
34	1	1250	A
34	1	1251	G
34	1	1252	A
34	1	1263	C
34	1	1271	C
34	1	1272	A
34	1	1275	C
34	1	1276	G
34	1	1277	A
34	1	1278	U
34	1	1279	G
34	1	1290	A
34	1	1359	C
34	1	1360	U

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Mol	Chain	Res	Type
34	1	1361	U
34	1	1362	A
34	1	1363	C
34	1	1364	G
34	1	1365	U
34	1	1368	C
34	1	1369	U
34	1	1371	U
34	1	1409	U
34	1	1410	C
34	1	1411	A
34	1	1413	C
34	1	1419	U
34	1	1421	C
34	1	1425	U
34	1	1432	C
34	1	1443	U
34	1	1444	G
34	1	1449	U
34	1	1452	A
34	1	1461	G
34	1	1463	G
34	1	1465	A
34	1	1466	G
34	1	1477	A
34	1	1478	OMG
34	1	1484	A
34	1	1489	A
34	1	1490	A
34	1	1493	A
34	1	1498	G
34	1	1502	G
34	1	1503	A
34	1	1507	G
34	1	1510	C
34	1	1511	C
34	1	1515	A
34	1	1520	U
34	1	1523	A
34	1	1535	A
34	1	1537	U
34	1	1544	5MC

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Mol	Chain	Res	Type
34	1	1546	A
34	1	1548	A
34	1	1549	C
34	1	1550	OMG
34	1	1551	G
34	1	1552	G
34	1	1554	A
34	1	1559	U
34	1	1560	A
34	1	1566	U
34	1	1569	G
34	1	1570	G
34	1	1576	A
34	1	1579	A
34	1	1580	G
34	1	1581	G
34	1	1582	A
34	1	1588	A
34	1	1589	G
34	1	1592	U
34	1	1593	G
34	1	1595	G
34	1	1596	U
34	1	1597	G
34	1	1598	U
34	1	1601	U
34	1	1603	U
34	1	1607	G
34	1	1608	A
34	1	1616	A
34	1	1617	A
34	1	1619	G
34	1	1622	G
34	1	1636	U
34	1	1637	U
34	1	1639	G
34	1	1641	U
34	1	1643	G
34	1	1653	U
34	1	1657	U
34	1	1658	U
34	1	1659	U

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Mol	Chain	Res	Type
34	1	1664	G
34	1	1666	U
34	1	1667	U
34	1	1673	A
34	1	1677	G
34	1	1699	A
34	1	1700	G
34	1	1702	A
34	1	1703	U
34	1	1706	A
34	1	1712	G
34	1	1713	C
34	1	1714	C
34	1	1715	C
34	1	1716	A
34	1	1717	U
34	1	1718	A
34	1	1723	A
34	1	1762	A
34	1	1769	C
34	1	1770	G
34	1	1772	A
34	1	1773	U
34	1	1776	U
34	1	1777	OMU
34	1	1782	G
34	1	1788	U
34	1	1789	U
34	1	1790	C
34	1	1793	U
34	1	1811	A
34	1	1815	U
34	1	1816	U
34	1	1819	G
34	1	1820	G
34	1	1821	C
34	1	1828	A
34	1	1832	C
34	1	1833	OMU
34	1	1834	G
34	1	1835	U
34	1	1837	A

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Mol	Chain	Res	Type
34	1	1838	U
34	1	1839	G
34	1	1842	C
34	1	1845	C
34	1	1846	A
34	1	1847	A
34	1	1850	U
34	1	1852	C
34	1	1858	G
34	1	1859	A
34	1	1860	C
34	1	1861	A
34	1	1863	G
34	1	1865	OMG
34	1	1866	OMC
34	1	1867	A
34	1	1870	A
34	1	1872	A
34	1	1873	A
34	1	1874	U
34	1	1875	G
34	1	1878	A
34	1	1884	A
34	1	1885	A
34	1	1887	A
34	1	1889	G
34	1	1890	A
34	1	1891	A
34	1	1893	A
34	1	1894	A
34	1	1895	C
34	1	1897	A
34	1	1906	G
34	1	1907	A
34	1	1908	A
34	1	1909	C
34	1	1912	A
34	1	1917	A
34	1	1918	U
34	1	1919	C
34	1	1920	A
34	1	1923	A

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Mol	Chain	Res	Type
34	1	1926	G
34	1	1933	A
34	1	1934	A
34	1	1935	C
34	1	1937	C
34	1	1938	C
34	1	1940	G
34	1	1941	A
34	1	1943	U
34	1	1946	C
34	1	1947	A
34	1	1948	U
34	1	1949	A
34	1	1950	G
34	1	1952	C
34	1	1955	A
34	1	1956	C
34	1	1957	U
34	1	1965	G
34	1	1976	U
34	1	1978	A
34	1	1981	G
34	1	1986	C
34	1	1987	G
34	1	1988	C
34	1	1989	A
34	1	1990	A
34	1	1993	A
34	1	1994	G
34	1	2000	U
34	1	2003	C
34	1	2004	G
34	1	2010	G
34	1	2016	C
34	1	2017	A
34	1	2020	A
34	1	2021	A2M
34	1	2027	G
34	1	2039	C
34	1	2051	A
34	1	2052	C
34	1	2053	A

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Mol	Chain	Res	Type
34	1	2054	C
34	1	2055	A
34	1	2058	G
34	1	2069	U
34	1	2076	U
34	1	2085	A
34	1	2086	A
34	1	2087	U
34	1	2123	A
34	1	2124	A
34	1	2127	U
34	1	2135	U
34	1	2140	OMC
34	1	2158	A
34	1	2159	A
34	1	2160	G
34	1	2163	G
34	1	2164	U
34	1	2165	A
34	1	2169	A
34	1	2170	G
34	1	2172	U
34	1	2173	A
34	1	2182	U
34	1	2183	G
34	1	2186	C
34	1	2195	G
34	1	2196	G
34	1	2197	A
34	1	2198	U
34	1	2199	C
34	1	2200	A
34	1	2202	U
34	1	2203	U
35	2	2	C
35	2	3	G
35	2	5	G
35	2	8	U
35	2	9	A
35	2	14	A
35	2	16	U
35	2	17	C

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Mol	Chain	Res	Type
35	2	19	G
35	2	21	A
35	2	23	A
35	2	34	G
35	2	35	A
35	2	36	A
35	2	45	U
35	2	47	U
35	2	49	C
35	2	51	U
35	2	52	G
35	2	54	U
35	2	56	C
35	2	57	G
35	2	59	U
35	2	61	C
35	2	65	G
35	2	71	G
35	2	72	C
35	2	74	C
35	2	75	C
36	3	6	G
36	3	8	U
36	3	9	G
36	3	10	G
36	3	14	A
36	3	16	C
36	3	18	U
36	3	19	G
36	3	20	G
36	3	21	A
36	3	22	G
36	3	29	G
36	3	42	G
36	3	47	U
36	3	48	C
36	3	58	A
36	3	61	C
36	3	63	G
36	3	69	C
36	3	70	G
37	4	2	C

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Mol	Chain	Res	Type
37	4	5	G
37	4	7	A
37	4	8	U
37	4	9	A
37	4	10	G
37	4	14	A
37	4	15	G
37	4	17	C
37	4	18	G
37	4	19	G
37	4	21	A
37	4	23	A
37	4	27	G
37	4	28	G
37	4	34	G
37	4	35	A
37	4	36	A
37	4	43	C
37	4	44	G
37	4	45	U
37	4	49	C
37	4	51	U
37	4	52	G
37	4	54	U
37	4	55	U
37	4	56	C
37	4	57	G
37	4	58	A
37	4	61	C
37	4	69	G
37	4	70	C
37	4	74	C
37	4	76	A
38	5	5	A
38	5	8	U

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	1	1	G
34	1	238	G
34	1	276	G

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Mol	Chain	Res	Type
34	1	306	U
34	1	381	G
34	1	396	G
34	1	403	G
34	1	494	A
34	1	576	A
34	1	591	A
34	1	602	A
34	1	603	C
34	1	671	G
34	1	757	C
34	1	789	G
34	1	905	A
34	1	913	G
34	1	915	A
34	1	1108	A
34	1	1145	A
34	1	1161	G
34	1	1250	A
34	1	1275	C
34	1	1276	G
34	1	1489	A
34	1	1550	OMG
34	1	1551	G
34	1	1559	U
34	1	1636	U
34	1	1787	A
34	1	1858	G
34	1	1926	G
34	1	2053	A
34	1	2164	U
34	1	2202	U
35	2	13	C
35	2	34	G
37	4	13	C
37	4	34	G

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

37 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	OMC	1	38	34	19,22,23	0.95	1 (5%)	25,31,34	1.16	3 (12%)
34	5MC	1	2061	34	19,22,23	1.47	4 (21%)	26,32,35	1.35	5 (19%)
34	7MG	1	1995	36,34	23,26,27	1.35	2 (8%)	27,39,42	1.45	6 (22%)
34	C4J	1	1543	34	25,29,30	2.01	7 (28%)	28,42,45	1.43	4 (14%)
34	OMC	1	115	34	19,22,23	1.02	1 (5%)	25,31,34	1.11	3 (12%)
34	A2M	1	2021	34	18,25,26	1.59	2 (11%)	20,36,39	1.56	4 (20%)
34	A2M	1	28	34	18,25,26	1.63	4 (22%)	20,36,39	1.05	0
34	MA6	1	2185	34	19,26,27	1.68	2 (10%)	18,38,41	3.10	3 (16%)
34	OMG	1	1550	34	19,26,27	0.95	1 (5%)	21,38,41	1.35	4 (19%)
34	OMG	1	1829	34	19,26,27	1.33	2 (10%)	21,38,41	1.43	3 (14%)
34	OMC	1	18	34	19,22,23	0.86	0	25,31,34	1.12	2 (8%)
34	OMU	1	33	34	19,22,23	0.53	0	25,31,34	1.05	2 (8%)
34	OMU	1	2048	34	19,22,23	0.57	0	25,31,34	0.98	2 (8%)
34	A2M	1	98	34	18,25,26	1.55	3 (16%)	20,36,39	1.09	1 (5%)
34	OMU	1	1621	34	19,22,23	0.64	0	25,31,34	1.32	2 (8%)
34	OMU	1	1777	34	19,22,23	0.73	0	25,31,34	0.98	1 (4%)
34	OMG	1	1464	34	19,26,27	1.26	2 (10%)	21,38,41	1.76	6 (28%)
34	OMU	1	661	34	19,22,23	0.78	0	25,31,34	1.00	2 (8%)
34	A2M	1	479	34	18,25,26	1.68	3 (16%)	20,36,39	1.04	1 (5%)
34	OMU	1	8	34	19,22,23	0.90	0	25,31,34	1.14	2 (8%)
34	5MC	1	1544	34	19,22,23	1.55	5 (26%)	26,32,35	1.31	4 (15%)
34	OMU	1	1979	34	19,22,23	0.57	0	25,31,34	0.88	1 (4%)
34	OMG	1	2151	34	19,26,27	1.26	2 (10%)	21,38,41	1.49	4 (19%)
34	MA6	1	2184	34	19,26,27	1.78	3 (15%)	18,38,41	2.64	3 (16%)
34	OMG	1	1478	34	19,26,27	1.25	2 (10%)	21,38,41	1.51	5 (23%)
34	OMG	1	1623	34	19,26,27	1.24	2 (10%)	21,38,41	1.51	4 (19%)
34	OMC	1	2140	34	19,22,23	1.03	1 (5%)	25,31,34	1.12	3 (12%)
34	OMG	1	1865	34	19,26,27	1.29	2 (10%)	21,38,41	1.54	6 (28%)
34	OMG	1	1647	34	19,26,27	1.33	2 (10%)	21,38,41	1.59	6 (28%)
34	OMG	1	509	34	19,26,27	1.11	1 (5%)	21,38,41	1.23	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	OMC	1	1866	34	19,22,23	1.26	2 (10%)	25,31,34	1.31	3 (12%)
34	M1Y	1	1539	34	19,22,23	1.18	3 (15%)	21,32,35	2.06	4 (19%)
34	4OC	1	2059	34	20,23,24	0.51	0	25,32,35	1.02	2 (8%)
34	A2M	1	912	34	18,25,26	0.75	0	20,36,39	1.33	2 (10%)
34	OMU	1	1833	34	19,22,23	0.83	1 (5%)	25,31,34	1.23	3 (12%)
34	A2M	1	668	34	18,25,26	1.98	4 (22%)	20,36,39	1.34	2 (10%)
35	MIA	2	37	35	24,31,32	2.01	4 (16%)	22,44,47	2.71	6 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	OMC	1	38	34	-	0/9/27/28	0/2/2/2
34	5MC	1	2061	34	-	0/7/25/26	0/2/2/2
34	7MG	1	1995	36,34	-	2/7/37/38	0/3/3/3
34	C4J	1	1543	34	-	1/16/34/35	0/2/2/2
34	OMC	1	115	34	-	2/9/27/28	0/2/2/2
34	A2M	1	2021	34	-	0/5/27/28	0/3/3/3
34	A2M	1	28	34	-	0/5/27/28	0/3/3/3
34	MA6	1	2185	34	-	2/7/29/30	0/3/3/3
34	OMG	1	1550	34	-	2/5/27/28	0/3/3/3
34	OMG	1	1829	34	-	0/5/27/28	0/3/3/3
34	OMC	1	18	34	-	0/9/27/28	0/2/2/2
34	OMU	1	33	34	-	0/9/27/28	0/2/2/2
34	OMU	1	2048	34	-	0/9/27/28	0/2/2/2
34	A2M	1	98	34	-	2/5/27/28	0/3/3/3
34	OMU	1	1621	34	-	2/9/27/28	0/2/2/2
34	OMU	1	1777	34	-	2/9/27/28	0/2/2/2
34	OMG	1	1464	34	-	1/5/27/28	0/3/3/3
34	OMU	1	661	34	-	0/9/27/28	0/2/2/2
34	A2M	1	479	34	-	0/5/27/28	0/3/3/3
34	OMU	1	8	34	-	5/9/27/28	0/2/2/2
34	5MC	1	1544	34	-	0/7/25/26	0/2/2/2
34	OMU	1	1979	34	-	1/9/27/28	0/2/2/2
34	OMG	1	2151	34	-	0/5/27/28	0/3/3/3
34	MA6	1	2184	34	-	2/7/29/30	0/3/3/3
34	OMG	1	1478	34	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	OMG	1	1623	34	-	0/5/27/28	0/3/3/3
34	OMC	1	2140	34	-	1/9/27/28	0/2/2/2
34	OMG	1	1865	34	-	2/5/27/28	0/3/3/3
34	OMG	1	1647	34	-	0/5/27/28	0/3/3/3
34	OMG	1	509	34	-	0/5/27/28	0/3/3/3
34	OMC	1	1866	34	-	2/9/27/28	0/2/2/2
34	M1Y	1	1539	34	-	2/7/25/26	0/2/2/2
34	4OC	1	2059	34	-	2/9/29/30	0/2/2/2
34	A2M	1	912	34	-	2/5/27/28	0/3/3/3
34	OMU	1	1833	34	-	5/9/27/28	0/2/2/2
34	A2M	1	668	34	-	2/5/27/28	0/3/3/3
35	MIA	2	37	35	-	5/11/33/34	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	2	37	MIA	C13-C14	6.99	1.53	1.32
34	1	2184	MA6	C6-C5	-5.69	1.36	1.44
34	1	2185	MA6	C6-C5	-5.36	1.36	1.44
34	1	1543	C4J	C4-C5	-5.22	1.35	1.47
34	1	1543	C4J	C4-N3	-5.21	1.31	1.40
34	1	668	A2M	O5'-C5'	-4.90	1.30	1.44
35	2	37	MIA	C6-C5	-4.34	1.38	1.44
34	1	2021	A2M	O5'-C5'	-4.33	1.31	1.44
34	1	98	A2M	O5'-C5'	-4.29	1.31	1.44
34	1	28	A2M	O5'-C5'	-4.24	1.31	1.44
34	1	1995	7MG	C5-N7	4.22	1.41	1.35
34	1	479	A2M	O5'-C5'	-4.04	1.32	1.44
34	1	668	A2M	O4'-C4'	-3.99	1.36	1.45
34	1	2185	MA6	C6-N6	3.90	1.46	1.37
34	1	2184	MA6	C6-N6	3.89	1.46	1.37
34	1	1829	OMG	C6-N1	3.71	1.43	1.37
34	1	1623	OMG	C6-N1	3.69	1.43	1.37
34	1	1647	OMG	C6-N1	3.62	1.43	1.37
34	1	1995	7MG	C8-N9	3.60	1.48	1.45
34	1	2151	OMG	C6-N1	3.56	1.43	1.37
34	1	479	A2M	O4'-C4'	-3.53	1.37	1.45
34	1	1866	OMC	C2-N1	3.50	1.47	1.40
34	1	1544	5MC	C6-N1	-3.46	1.32	1.38
34	1	1865	OMG	C6-N1	3.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	2140	OMC	C2-N1	3.41	1.47	1.40
34	1	1544	5MC	C2-N1	3.30	1.47	1.40
34	1	1543	C4J	O4'-C1'	-3.29	1.39	1.43
34	1	1464	OMG	C6-N1	3.28	1.42	1.37
34	1	1478	OMG	C6-N1	3.23	1.42	1.37
35	2	37	MIA	C6-N1	3.22	1.37	1.33
34	1	1464	OMG	C5-C6	-3.12	1.41	1.47
34	1	509	OMG	C6-N1	-3.09	1.33	1.37
34	1	115	OMC	C4-N3	-3.06	1.28	1.34
34	1	1865	OMG	C5-C6	-3.03	1.41	1.47
34	1	2061	5MC	C2-N1	2.98	1.46	1.40
34	1	1647	OMG	C5-C6	-2.96	1.41	1.47
34	1	1478	OMG	C5-C6	-2.94	1.41	1.47
34	1	1539	M1Y	O4'-C1'	-2.93	1.39	1.43
34	1	1829	OMG	C5-C6	-2.93	1.41	1.47
34	1	2061	5MC	C6-N1	-2.91	1.33	1.38
34	1	2151	OMG	C5-C6	-2.87	1.41	1.47
34	1	1866	OMC	C4-N3	-2.73	1.29	1.34
34	1	668	A2M	C1'-N9	-2.61	1.43	1.49
34	1	1550	OMG	C6-N1	-2.54	1.33	1.37
34	1	1544	5MC	C2-N3	2.53	1.41	1.36
34	1	2021	A2M	O2'-C2'	-2.52	1.36	1.42
34	1	1539	M1Y	C1-N1	2.49	1.51	1.46
34	1	1543	C4J	C6-N1	-2.49	1.31	1.36
34	1	28	A2M	O3'-C3'	-2.49	1.36	1.43
34	1	98	A2M	O4'-C4'	-2.48	1.39	1.45
34	1	1623	OMG	C5-C6	-2.45	1.42	1.47
34	1	1833	OMU	C2-N1	2.45	1.42	1.38
35	2	37	MIA	C2-N1	2.43	1.37	1.34
34	1	1543	C4J	O2-C2	-2.43	1.18	1.22
34	1	2061	5MC	O2-C2	-2.40	1.19	1.23
34	1	1543	C4J	C2-N3	-2.40	1.34	1.38
34	1	1544	5MC	O2-C2	-2.36	1.19	1.23
34	1	2061	5MC	C2-N3	2.33	1.41	1.36
34	1	28	A2M	C1'-N9	-2.27	1.44	1.49
34	1	668	A2M	O4'-C1'	-2.22	1.38	1.40
34	1	98	A2M	C1'-N9	-2.14	1.44	1.49
34	1	479	A2M	C1'-N9	-2.13	1.44	1.49
34	1	1543	C4J	O4-C4	-2.13	1.18	1.23
34	1	1544	5MC	CM5-C5	-2.08	1.45	1.50
34	1	2184	MA6	C5-N7	-2.07	1.32	1.39
34	1	28	A2M	O4'-C4'	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	1539	M1Y	C2'-C1'	-2.03	1.51	1.53
34	1	38	OMC	C4-N3	-2.01	1.30	1.34

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	37	MIA	C12-C13-C14	-10.10	108.89	127.01
34	1	2185	MA6	N1-C6-N6	-9.83	105.47	116.83
34	1	2184	MA6	N1-C6-N6	-8.34	107.20	116.83
34	1	2185	MA6	N3-C2-N1	-7.22	118.87	128.67
34	1	2184	MA6	N3-C2-N1	-6.19	120.27	128.67
34	1	1539	M1Y	C4-N3-C2	-5.75	119.80	127.34
34	1	1539	M1Y	N3-C2-N1	5.09	120.14	115.22
34	1	1621	OMU	CM2-O2'-C2'	-4.39	103.21	114.47
34	1	668	A2M	O4'-C1'-N9	-4.29	103.05	108.75
34	1	2021	A2M	O4'-C1'-N9	-4.26	103.10	108.75
34	1	2185	MA6	C2-N1-C6	4.04	120.80	116.84
35	2	37	MIA	C16-C14-C13	-4.03	110.55	122.66
35	2	37	MIA	C15-C14-C13	-4.03	110.56	122.66
34	1	1543	C4J	C4-N3-C2	-3.99	120.71	125.62
34	1	1623	OMG	O6-C6-N1	-3.78	116.14	120.62
34	1	912	A2M	N3-C2-N1	-3.75	123.59	128.67
34	1	1544	5MC	C5-C4-N3	3.64	125.48	121.75
34	1	1623	OMG	O6-C6-C5	3.60	131.45	124.32
34	1	1995	7MG	C5-C4-N9	3.58	110.93	106.33
34	1	1464	OMG	O6-C6-N1	-3.47	116.50	120.62
34	1	1829	OMG	O6-C6-C5	3.45	131.15	124.32
34	1	1995	7MG	O6-C6-N1	-3.43	113.67	120.11
34	1	1829	OMG	O6-C6-N1	-3.42	116.56	120.62
34	1	2151	OMG	O6-C6-N1	-3.39	116.60	120.62
34	1	1647	OMG	O6-C6-N1	-3.39	116.60	120.62
34	1	2151	OMG	O6-C6-C5	3.38	131.03	124.32
34	1	1464	OMG	O6-C6-C5	3.31	130.88	124.32
34	1	2184	MA6	C2-N1-C6	3.30	120.08	116.84
34	1	2061	5MC	C5-C4-N3	3.26	125.10	121.75
34	1	1478	OMG	O6-C6-C5	3.26	130.79	124.32
34	1	1866	OMC	C5-C4-N3	3.23	126.76	121.32
34	1	1647	OMG	O6-C6-C5	3.23	130.72	124.32
34	1	1478	OMG	O6-C6-N1	-3.20	116.83	120.62
34	1	1464	OMG	CM2-O2'-C2'	3.13	122.51	114.47
34	1	1865	OMG	O6-C6-N1	-3.10	116.94	120.62
34	1	1865	OMG	O6-C6-C5	3.09	130.45	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	18	OMC	C5-C4-N3	3.09	126.52	121.32
34	1	1544	5MC	C5-C4-N4	-3.07	117.06	121.39
34	1	2140	OMC	C5-C4-N3	3.02	126.40	121.32
34	1	509	OMG	C8-N7-C5	2.92	107.53	102.55
34	1	38	OMC	C5-C4-N3	2.92	126.24	121.32
34	1	115	OMC	C5-C4-N3	2.89	126.19	121.32
34	1	1539	M1Y	C1-N1-C2	2.87	121.06	117.83
34	1	1478	OMG	CM2-O2'-C2'	-2.84	107.18	114.47
34	1	2140	OMC	CM2-O2'-C2'	-2.83	107.21	114.47
34	1	1647	OMG	CM2-O2'-C2'	-2.80	107.28	114.47
34	1	1543	C4J	C1'-C5-C4	2.73	121.74	117.61
34	1	1550	OMG	C8-N7-C5	2.71	107.16	102.55
34	1	38	OMC	CM2-O2'-C2'	-2.71	107.53	114.47
35	2	37	MIA	C16-C14-C15	-2.70	108.37	114.59
34	1	8	OMU	C4-N3-C2	-2.68	123.28	126.61
34	1	115	OMC	CM2-O2'-C2'	-2.68	107.59	114.47
34	1	2061	5MC	C5-C4-N4	-2.63	117.69	121.39
34	1	1777	OMU	CM2-O2'-C2'	-2.61	107.77	114.47
34	1	1464	OMG	N1-C2-N3	2.61	128.09	123.32
34	1	1544	5MC	N1-C2-N3	-2.56	114.36	118.80
34	1	2061	5MC	N1-C2-N3	-2.55	114.37	118.80
34	1	1865	OMG	CM2-O2'-C2'	-2.55	107.94	114.47
34	1	1550	OMG	C2'-C1'-N9	-2.53	106.95	112.56
34	1	661	OMU	CM2-O2'-C2'	-2.52	108.01	114.47
34	1	912	A2M	C4-C5-N7	-2.51	106.69	109.34
34	1	2151	OMG	N1-C2-N3	2.47	127.84	123.32
34	1	115	OMC	N4-C4-N3	-2.45	113.52	117.91
34	1	1543	C4J	N3-C2-N1	2.45	119.71	116.72
34	1	18	OMC	CM2-O2'-C2'	-2.42	108.27	114.47
34	1	1621	OMU	C4-N3-C2	-2.42	123.61	126.61
34	1	33	OMU	CM2-O2'-C2'	-2.41	108.28	114.47
34	1	1995	7MG	C4-C5-N7	2.40	108.21	105.38
34	1	1464	OMG	C2-N1-C6	-2.39	120.73	125.11
35	2	37	MIA	C4-C5-N7	2.38	111.85	109.34
34	1	8	OMU	CM2-O2'-C2'	-2.37	108.39	114.47
34	1	1866	OMC	CM2-O2'-C2'	-2.34	108.45	114.47
34	1	1833	OMU	C1'-N1-C2	2.34	121.80	117.59
34	1	1478	OMG	N1-C2-N3	2.34	127.61	123.32
34	1	1979	OMU	C4-N3-C2	-2.32	123.73	126.61
34	1	2061	5MC	C1'-N1-C2	-2.32	113.31	118.44
34	1	1647	OMG	N2-C2-N3	-2.32	115.15	119.67
34	1	1543	C4J	C5-C4-N3	2.32	120.36	116.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	661	OMU	C4-N3-C2	-2.31	123.74	126.61
34	1	2021	A2M	C4'-O4'-C1'	2.31	112.04	109.92
34	1	1995	7MG	C5-C4-N3	-2.29	123.83	128.13
34	1	2048	OMU	CM2-O2'-C2'	-2.29	108.59	114.47
34	1	1833	OMU	CM2-O2'-C2'	-2.26	108.68	114.47
35	2	37	MIA	N3-C2-N1	2.25	131.14	127.03
34	1	1865	OMG	C2-N1-C6	-2.24	121.00	125.11
34	1	1829	OMG	N2-C2-N3	-2.24	115.30	119.67
34	1	1464	OMG	O2'-C2'-C1'	2.24	113.33	109.00
34	1	1550	OMG	C5-C6-N1	2.23	118.33	114.07
34	1	1865	OMG	N1-C2-N3	2.23	127.40	123.32
34	1	33	OMU	C4-N3-C2	-2.22	123.86	126.61
34	1	1995	7MG	O6-C6-C5	2.21	133.05	127.62
34	1	1866	OMC	N4-C4-N3	-2.20	113.97	117.91
34	1	479	A2M	O4'-C1'-N9	-2.19	105.84	108.75
34	1	1623	OMG	N1-C2-N3	2.18	127.31	123.32
34	1	1865	OMG	N2-C2-N3	-2.16	115.45	119.67
34	1	2059	4OC	C4-N3-C2	-2.16	117.25	120.11
34	1	2151	OMG	C2-N1-C6	-2.13	121.21	125.11
34	1	38	OMC	C4-N3-C2	-2.12	116.92	120.26
34	1	668	A2M	C4-C5-N7	2.11	111.56	109.34
34	1	509	OMG	C5-C6-N1	2.10	118.08	114.07
34	1	1539	M1Y	O2-C2-N1	-2.09	120.66	122.78
34	1	1647	OMG	C2-N1-C6	-2.09	121.28	125.11
34	1	1550	OMG	O6-C6-C5	-2.08	120.19	124.32
34	1	1833	OMU	O2-C2-N1	2.08	125.50	122.80
34	1	2061	5MC	C1'-N1-C6	2.07	124.56	121.15
34	1	1647	OMG	N1-C2-N3	2.07	127.10	123.32
34	1	2140	OMC	C4-N3-C2	-2.07	117.01	120.26
34	1	1995	7MG	C2-N1-C6	-2.05	121.39	125.11
34	1	1544	5MC	O2-C2-N1	2.05	122.92	118.90
34	1	98	A2M	C4-C5-N7	2.05	111.50	109.34
34	1	2021	A2M	O4'-C4'-C3'	2.04	109.20	105.15
34	1	1478	OMG	C2-N1-C6	-2.03	121.39	125.11
34	1	509	OMG	O2'-C2'-C1'	-2.03	105.08	109.00
34	1	1623	OMG	C2-N1-C6	-2.03	121.40	125.11
34	1	2021	A2M	C4-C5-N7	2.02	111.47	109.34
34	1	2059	4OC	O2-C2-N3	-2.01	119.16	122.33
34	1	2048	OMU	C4-N3-C2	-2.01	124.12	126.61

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	1	115	OMC	O4'-C4'-C5'-O5'
34	1	912	A2M	O4'-C4'-C5'-O5'
34	1	1464	OMG	C1'-C2'-O2'-CM2
34	1	1833	OMU	O4'-C1'-N1-C2
34	1	1833	OMU	O4'-C1'-N1-C6
34	1	1833	OMU	C4'-C5'-O5'-P
34	1	1865	OMG	O4'-C4'-C5'-O5'
34	1	2184	MA6	C5-C6-N6-C9
35	2	37	MIA	C12-C13-C14-C16
34	1	1539	M1Y	C3'-C4'-C5'-O5'
34	1	1539	M1Y	O4'-C4'-C5'-O5'
34	1	98	A2M	O4'-C4'-C5'-O5'
34	1	115	OMC	C3'-C4'-C5'-O5'
34	1	668	A2M	C3'-C4'-C5'-O5'
34	1	1777	OMU	O4'-C4'-C5'-O5'
34	1	1833	OMU	C3'-C4'-C5'-O5'
34	1	1865	OMG	C3'-C4'-C5'-O5'
34	1	1866	OMC	C3'-C4'-C5'-O5'
34	1	1866	OMC	O4'-C4'-C5'-O5'
35	2	37	MIA	O4'-C4'-C5'-O5'
35	2	37	MIA	C3'-C4'-C5'-O5'
34	1	668	A2M	O4'-C4'-C5'-O5'
34	1	912	A2M	C3'-C4'-C5'-O5'
34	1	1478	OMG	C3'-C4'-C5'-O5'
34	1	1833	OMU	O4'-C4'-C5'-O5'
34	1	2059	4OC	O4'-C4'-C5'-O5'
34	1	2184	MA6	N1-C6-N6-C9
34	1	1543	C4J	C4'-C5'-O5'-P
34	1	8	OMU	C2'-C1'-N1-C6
34	1	1550	OMG	C3'-C4'-C5'-O5'
34	1	1777	OMU	C3'-C4'-C5'-O5'
34	1	1995	7MG	O4'-C4'-C5'-O5'
34	1	1995	7MG	C3'-C4'-C5'-O5'
35	2	37	MIA	N1-C6-N6-C12
34	1	8	OMU	O4'-C4'-C5'-O5'
34	1	1478	OMG	O4'-C4'-C5'-O5'
34	1	1979	OMU	C1'-C2'-O2'-CM2
34	1	98	A2M	C3'-C4'-C5'-O5'
34	1	1550	OMG	O4'-C4'-C5'-O5'
34	1	8	OMU	O4'-C1'-N1-C6
34	1	2185	MA6	C5-C6-N6-C9
34	1	8	OMU	C2'-C1'-N1-C2
34	1	8	OMU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
34	1	2140	OMC	C4'-C5'-O5'-P
34	1	1478	OMG	C4'-C5'-O5'-P
34	1	1621	OMU	C3'-C2'-O2'-CM2
34	1	2059	4OC	C3'-C4'-C5'-O5'
35	2	37	MIA	C5-C6-N6-C12
34	1	1621	OMU	O4'-C4'-C5'-O5'
34	1	2185	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 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
40	PAR	1	2307	-	44,45,45	3.64	10 (22%)	63,67,67	1.07	2 (3%)
40	PAR	1	2304	-	44,45,45	3.72	9 (20%)	63,67,67	1.62	10 (15%)
40	PAR	1	2305	-	44,45,45	3.50	7 (15%)	63,67,67	1.53	10 (15%)
40	PAR	1	2302	-	44,45,45	3.68	10 (22%)	63,67,67	1.59	14 (22%)
40	PAR	1	2306	-	44,45,45	3.59	8 (18%)	63,67,67	1.35	9 (14%)
40	PAR	1	2303	34	44,45,45	3.58	10 (22%)	63,67,67	1.72	13 (20%)

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
40	PAR	1	2307	-	-	5/18/94/94	0/4/4/4
40	PAR	1	2304	-	-	9/18/94/94	0/4/4/4
40	PAR	1	2305	-	-	8/18/94/94	0/4/4/4
40	PAR	1	2302	-	-	4/18/94/94	0/4/4/4
40	PAR	1	2306	-	-	10/18/94/94	0/4/4/4
40	PAR	1	2303	34	-	5/18/94/94	0/4/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2304	PAR	C13-C23	-17.36	1.30	1.52
40	1	2302	PAR	C13-C23	-16.79	1.31	1.52
40	1	2307	PAR	C13-C23	-16.64	1.31	1.52
40	1	2303	PAR	C13-C23	-16.20	1.32	1.52
40	1	2306	PAR	C13-C23	-16.19	1.32	1.52
40	1	2305	PAR	C13-C23	-15.54	1.33	1.52
40	1	2302	PAR	O43-C13	12.69	1.64	1.41
40	1	2304	PAR	O43-C13	12.55	1.63	1.41
40	1	2305	PAR	O43-C13	12.48	1.63	1.41
40	1	2307	PAR	O43-C13	12.45	1.63	1.41
40	1	2306	PAR	O43-C13	12.10	1.63	1.41
40	1	2303	PAR	O43-C13	11.92	1.62	1.41
40	1	2303	PAR	O43-C43	-7.48	1.28	1.45
40	1	2306	PAR	O43-C43	-6.90	1.29	1.45
40	1	2305	PAR	O43-C43	-6.77	1.29	1.45
40	1	2304	PAR	O43-C43	-6.70	1.30	1.45
40	1	2307	PAR	O43-C43	-6.57	1.30	1.45
40	1	2302	PAR	O43-C43	-6.52	1.30	1.45
40	1	2302	PAR	C31-C21	-5.50	1.46	1.53
40	1	2304	PAR	C31-C21	-4.98	1.47	1.53
40	1	2306	PAR	C31-C21	-4.96	1.47	1.53
40	1	2307	PAR	C31-C21	-4.45	1.48	1.53
40	1	2306	PAR	C34-C24	-4.43	1.48	1.53
40	1	2305	PAR	C31-C21	-4.37	1.48	1.53
40	1	2305	PAR	C34-C24	-4.26	1.48	1.53
40	1	2307	PAR	C34-C24	-4.17	1.48	1.53
40	1	2307	PAR	O54-C14	4.10	1.52	1.41
40	1	2303	PAR	C34-C24	-4.07	1.48	1.53
40	1	2302	PAR	O54-C14	4.03	1.52	1.41
40	1	2303	PAR	C31-C21	-4.02	1.48	1.53
40	1	2306	PAR	O54-C14	3.88	1.51	1.41
40	1	2304	PAR	O54-C14	3.83	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2304	PAR	C34-C24	-3.79	1.48	1.53
40	1	2303	PAR	O54-C14	3.77	1.51	1.41
40	1	2305	PAR	O54-C14	3.63	1.51	1.41
40	1	2303	PAR	O33-C33	-3.53	1.34	1.43
40	1	2304	PAR	O33-C33	-3.42	1.35	1.43
40	1	2302	PAR	C34-C24	-3.37	1.49	1.53
40	1	2302	PAR	O33-C33	-3.19	1.35	1.43
40	1	2306	PAR	O33-C33	-3.06	1.36	1.43
40	1	2307	PAR	O33-C33	-3.02	1.36	1.43
40	1	2305	PAR	O51-C11	2.90	1.49	1.41
40	1	2307	PAR	O51-C11	2.88	1.49	1.41
40	1	2303	PAR	O51-C11	2.86	1.49	1.41
40	1	2306	PAR	O51-C11	2.81	1.49	1.41
40	1	2304	PAR	O51-C11	2.53	1.48	1.41
40	1	2302	PAR	O51-C11	2.51	1.48	1.41
40	1	2302	PAR	C21-N21	-2.23	1.43	1.47
40	1	2303	PAR	O11-C42	2.17	1.49	1.43
40	1	2302	PAR	C22-C12	-2.06	1.49	1.53
40	1	2307	PAR	O51-C51	2.05	1.49	1.44
40	1	2307	PAR	C22-C12	-2.04	1.49	1.53
40	1	2303	PAR	O51-C51	2.03	1.49	1.44
40	1	2304	PAR	C21-N21	-2.01	1.44	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2303	PAR	C14-O33-C33	-6.67	102.17	117.98
40	1	2302	PAR	C44-C34-C24	4.49	118.45	110.99
40	1	2304	PAR	O51-C51-C41	4.43	117.69	109.70
40	1	2305	PAR	C13-C23-C33	4.38	107.37	102.10
40	1	2303	PAR	C31-C41-C51	-4.31	102.41	110.23
40	1	2303	PAR	O11-C42-C52	4.26	118.24	107.42
40	1	2304	PAR	C44-C34-C24	4.22	118.00	110.99
40	1	2306	PAR	C13-C23-C33	4.09	107.02	102.10
40	1	2304	PAR	C31-C41-C51	4.00	117.48	110.23
40	1	2302	PAR	O11-C11-C21	-3.85	101.78	108.08
40	1	2304	PAR	C14-O33-C33	-3.82	108.93	117.98
40	1	2304	PAR	C41-C31-C21	3.76	117.23	110.99
40	1	2304	PAR	C13-O52-C52	-3.22	110.34	117.98
40	1	2302	PAR	C52-C62-C12	3.12	117.45	109.93
40	1	2303	PAR	O33-C14-C24	3.06	113.09	108.08
40	1	2303	PAR	O41-C41-C51	3.02	116.76	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2306	PAR	C14-O33-C33	-2.96	110.96	117.98
40	1	2302	PAR	C31-C21-N21	-2.90	105.10	111.05
40	1	2302	PAR	O54-C14-C24	2.89	116.48	110.08
40	1	2305	PAR	O54-C54-C44	2.88	114.89	109.70
40	1	2302	PAR	C22-C12-C62	2.87	114.38	110.08
40	1	2306	PAR	C52-C62-C12	2.87	116.85	109.93
40	1	2305	PAR	O52-C13-O43	-2.83	108.48	111.37
40	1	2305	PAR	O33-C33-C23	2.78	120.26	111.32
40	1	2303	PAR	C41-C31-C21	2.75	115.56	110.99
40	1	2305	PAR	O33-C14-C24	2.64	112.40	108.08
40	1	2302	PAR	C14-O33-C33	-2.60	111.81	117.98
40	1	2307	PAR	C13-O52-C52	-2.60	111.82	117.98
40	1	2305	PAR	C13-O52-C52	-2.59	111.83	117.98
40	1	2304	PAR	O34-C34-C24	-2.52	105.69	110.22
40	1	2303	PAR	C11-O51-C51	2.49	118.59	113.72
40	1	2304	PAR	C61-C51-C41	-2.44	107.03	113.02
40	1	2302	PAR	C14-C24-C34	2.40	116.31	110.29
40	1	2306	PAR	C62-C12-N12	-2.37	106.25	110.94
40	1	2305	PAR	O33-C14-O54	-2.33	104.57	110.69
40	1	2306	PAR	C31-C21-N21	-2.32	106.29	111.05
40	1	2303	PAR	O51-C11-C21	2.31	115.19	110.08
40	1	2303	PAR	C31-C21-N21	-2.31	106.33	111.05
40	1	2302	PAR	C53-C43-C33	-2.24	107.78	114.84
40	1	2304	PAR	C62-C12-N12	-2.23	106.53	110.94
40	1	2303	PAR	C11-C21-C31	2.23	115.88	110.29
40	1	2302	PAR	O62-C62-C12	-2.23	105.74	109.90
40	1	2304	PAR	O31-C31-C21	-2.20	106.26	110.22
40	1	2306	PAR	O33-C14-C24	2.17	111.62	108.08
40	1	2305	PAR	C14-O33-C33	2.16	123.09	117.98
40	1	2305	PAR	C31-C41-C51	-2.14	106.36	110.23
40	1	2303	PAR	O43-C43-C33	-2.12	100.45	104.92
40	1	2307	PAR	C14-O33-C33	-2.11	112.97	117.98
40	1	2306	PAR	C62-C52-C42	2.11	116.46	111.72
40	1	2302	PAR	C34-C44-C54	2.10	114.04	110.23
40	1	2306	PAR	C52-C42-C32	2.08	115.16	111.31
40	1	2302	PAR	C11-C21-N21	-2.07	106.47	110.20
40	1	2305	PAR	C14-C24-C34	2.06	115.46	110.29
40	1	2302	PAR	C62-C12-N12	-2.04	106.91	110.94
40	1	2302	PAR	O11-C42-C32	-2.03	104.32	109.18
40	1	2306	PAR	C34-C24-N24	-2.03	106.89	111.05
40	1	2303	PAR	O34-C34-C24	-2.03	106.58	110.22
40	1	2303	PAR	O54-C54-C44	2.00	113.31	109.70

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	2303	PAR	C52-C42-O11-C11
40	1	2303	PAR	C23-C13-O52-C52
40	1	2304	PAR	C23-C13-O52-C52
40	1	2304	PAR	O54-C54-C64-N64
40	1	2305	PAR	C24-C14-O33-C33
40	1	2305	PAR	C33-C43-C53-O53
40	1	2305	PAR	O43-C43-C53-O53
40	1	2306	PAR	C23-C13-O52-C52
40	1	2306	PAR	O43-C13-O52-C52
40	1	2306	PAR	C24-C14-O33-C33
40	1	2306	PAR	C44-C54-C64-N64
40	1	2306	PAR	O54-C54-C64-N64
40	1	2307	PAR	C23-C13-O52-C52
40	1	2307	PAR	O43-C13-O52-C52
40	1	2302	PAR	O54-C14-O33-C33
40	1	2307	PAR	O54-C14-O33-C33
40	1	2302	PAR	O43-C43-C53-O53
40	1	2304	PAR	O51-C51-C61-O61
40	1	2305	PAR	O51-C51-C61-O61
40	1	2302	PAR	C33-C43-C53-O53
40	1	2305	PAR	C41-C51-C61-O61
40	1	2304	PAR	C41-C51-C61-O61
40	1	2306	PAR	C41-C51-C61-O61
40	1	2306	PAR	C33-C43-C53-O53
40	1	2306	PAR	O43-C43-C53-O53
40	1	2303	PAR	O51-C51-C61-O61
40	1	2306	PAR	O51-C51-C61-O61
40	1	2304	PAR	O43-C13-O52-C52
40	1	2305	PAR	O51-C11-O11-C42
40	1	2303	PAR	C21-C11-O11-C42
40	1	2307	PAR	C44-C54-C64-N64
40	1	2305	PAR	O54-C54-C64-N64
40	1	2302	PAR	C43-C33-O33-C14
40	1	2304	PAR	O51-C11-O11-C42
40	1	2306	PAR	O51-C11-O11-C42
40	1	2304	PAR	C33-C43-C53-O53
40	1	2307	PAR	C41-C51-C61-O61
40	1	2303	PAR	C43-C33-O33-C14
40	1	2304	PAR	C23-C33-O33-C14
40	1	2304	PAR	C43-C33-O33-C14

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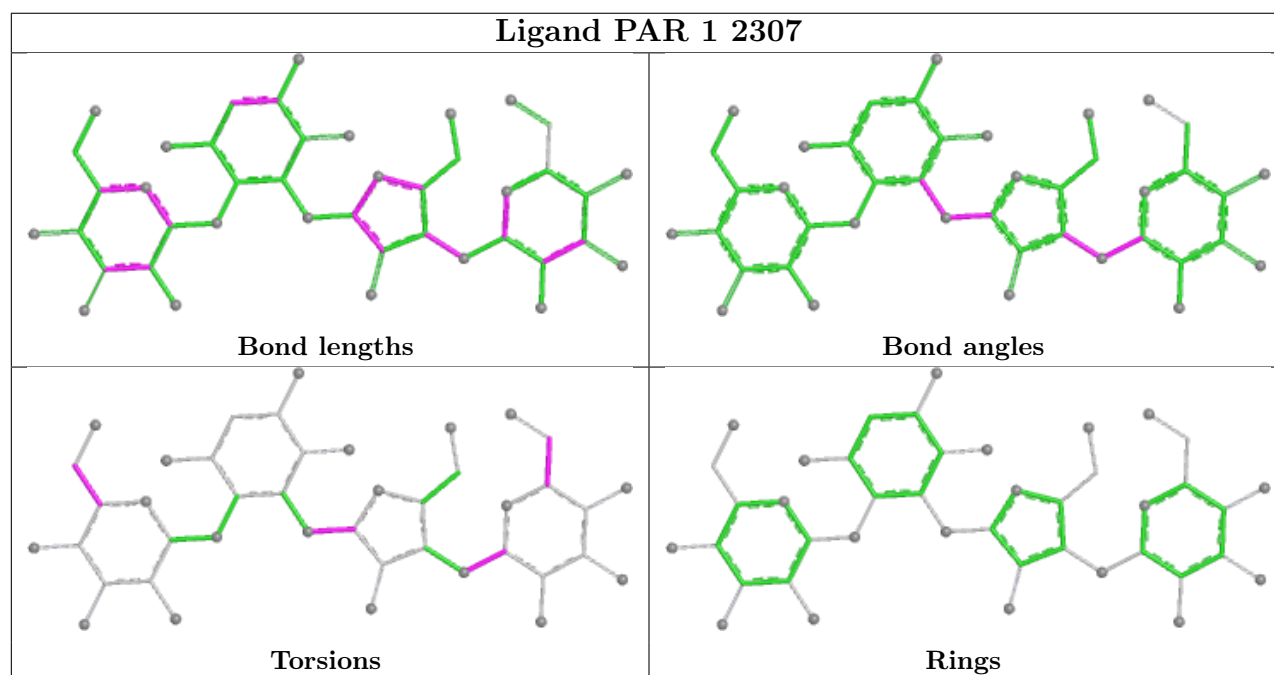
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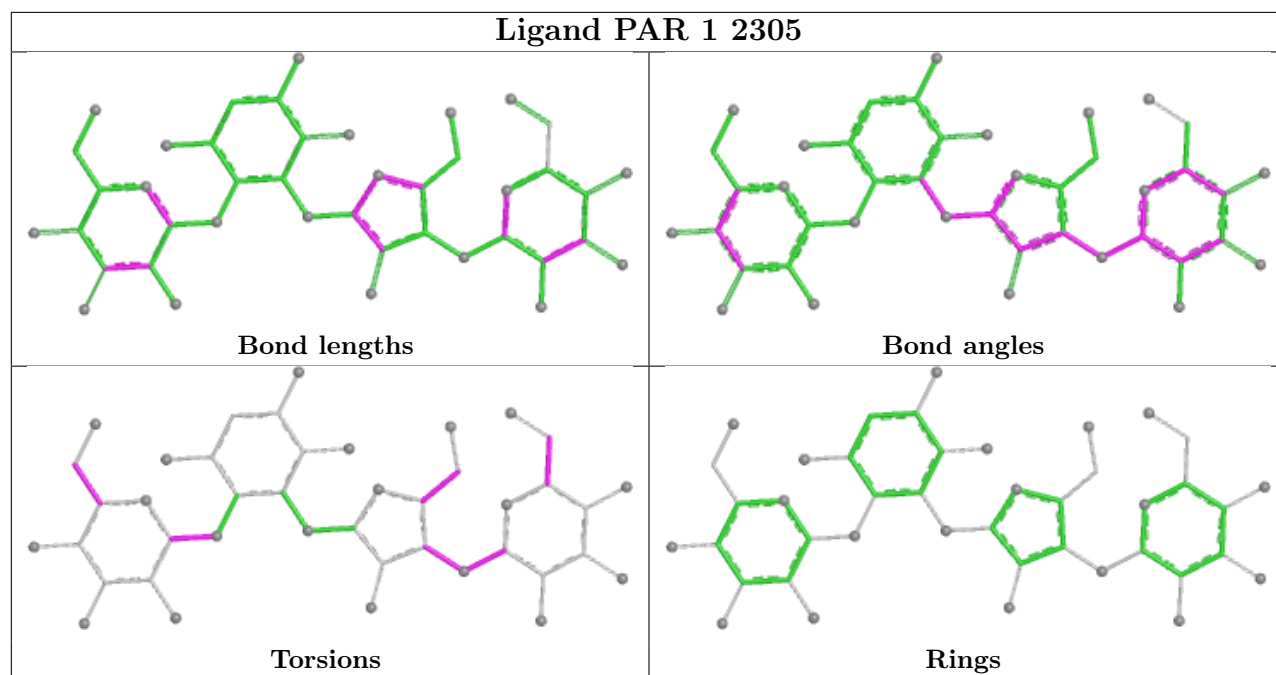
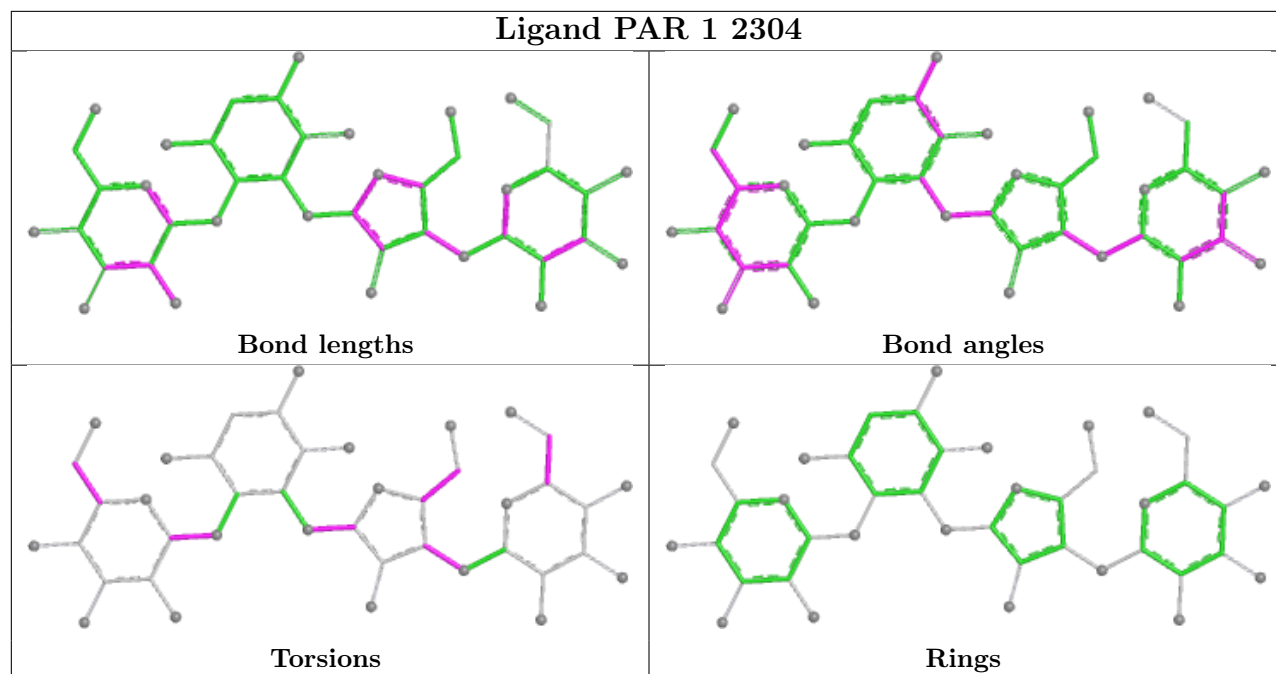
Mol	Chain	Res	Type	Atoms
40	1	2305	PAR	C43-C33-O33-C14

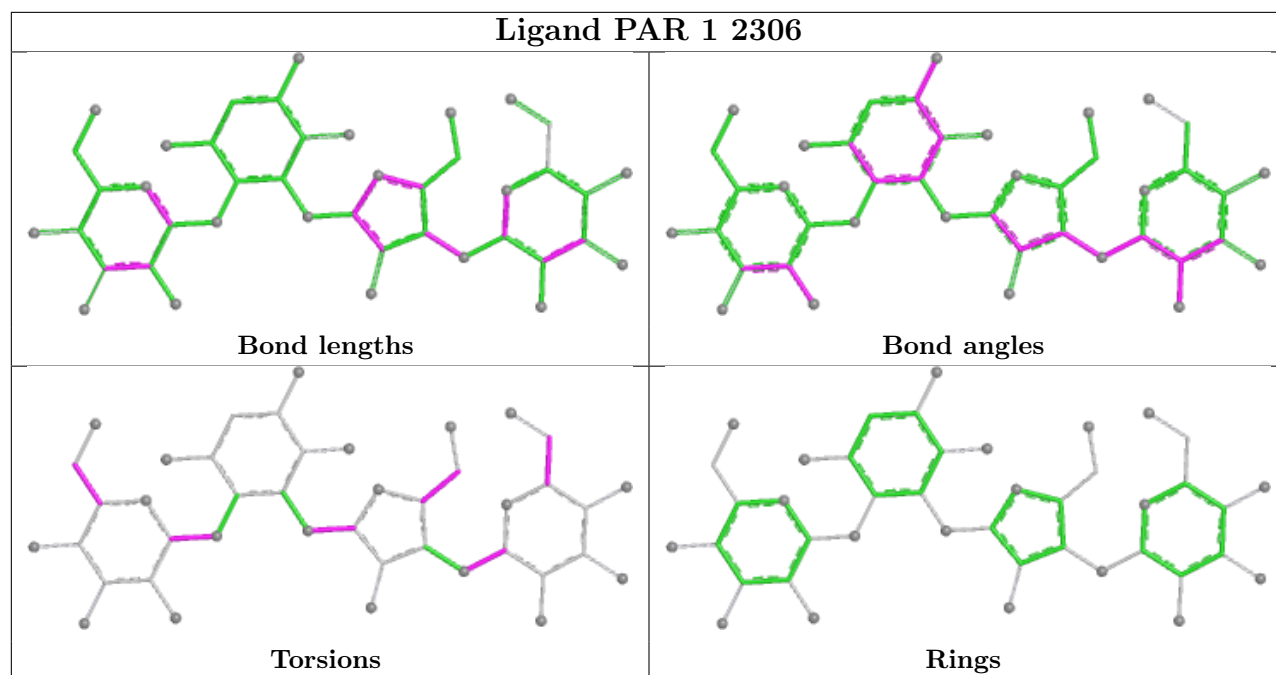
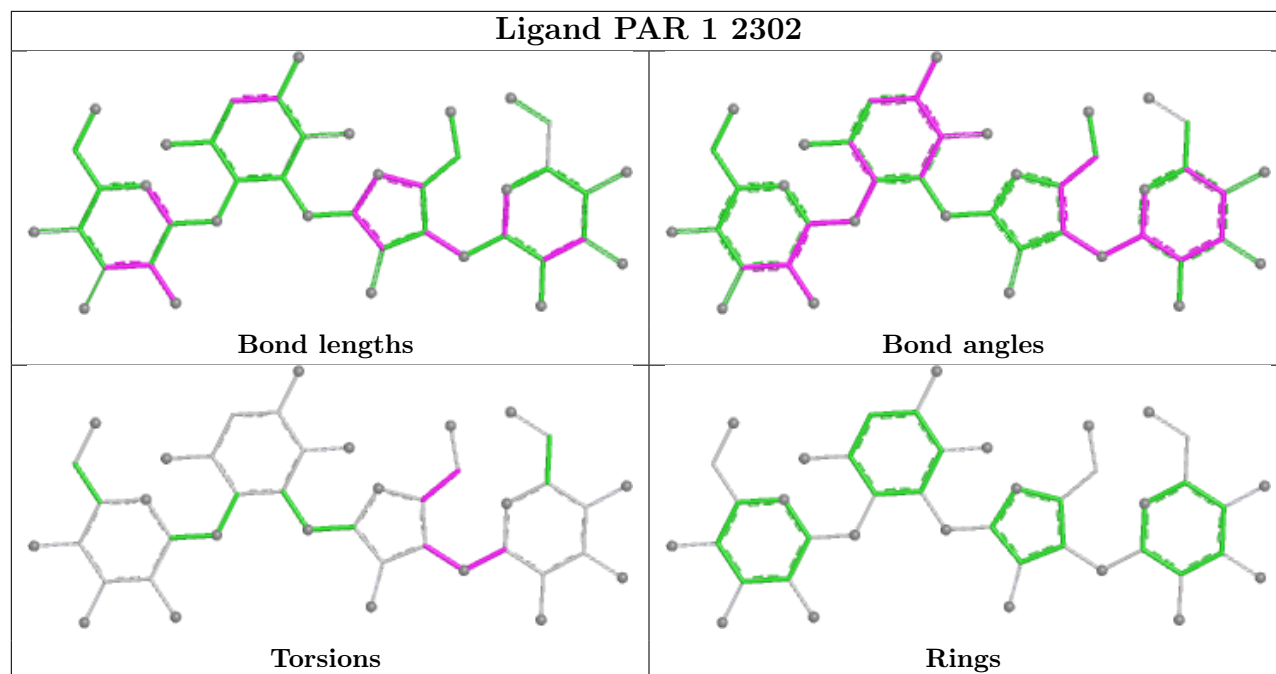
There are no ring outliers.

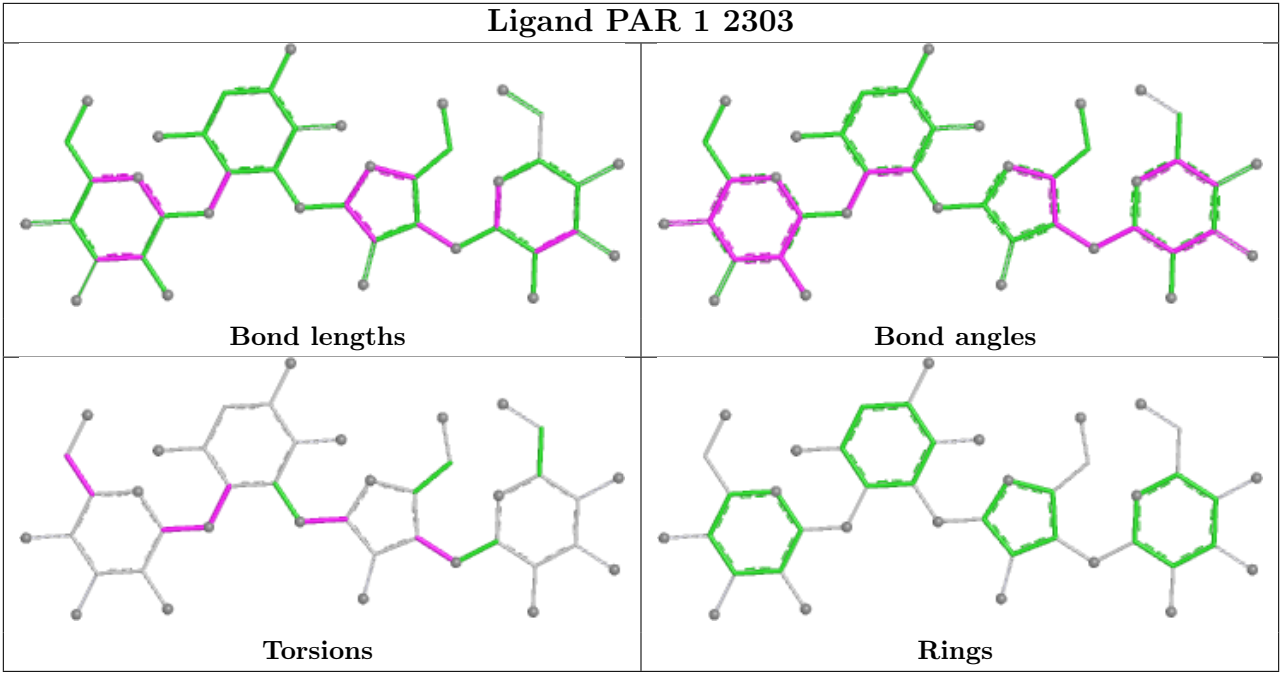
No monomer is involved in short contacts.

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	960:C	O3'	961:U	P	10.63

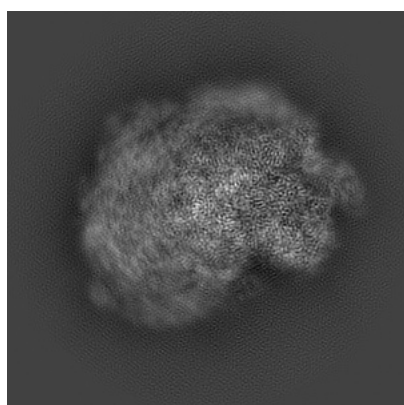
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7024. These allow visual inspection of the internal detail of the map and identification of artifacts.

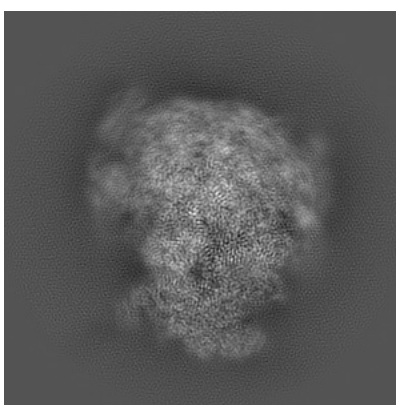
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

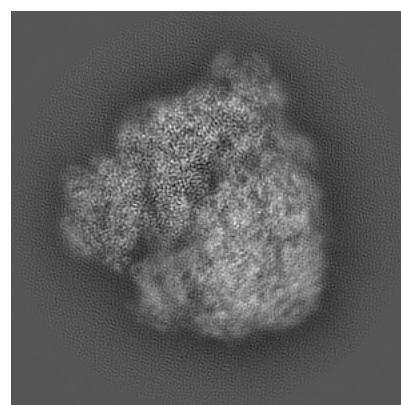
6.1.1 Primary map



X



Y

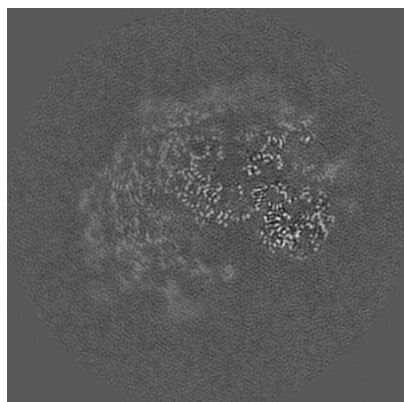


Z

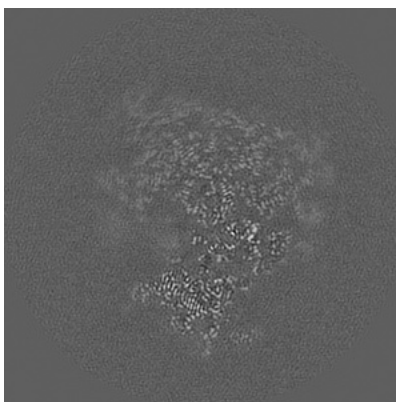
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

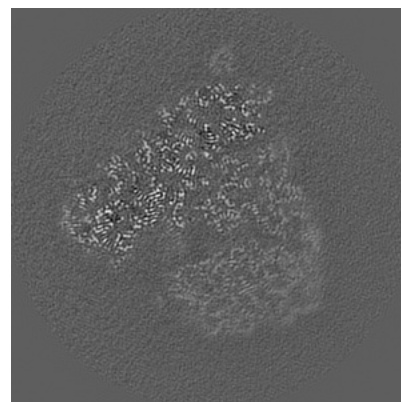
6.2.1 Primary map



X Index: 192



Y Index: 192

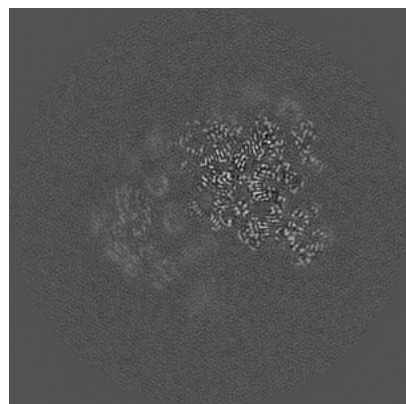


Z Index: 192

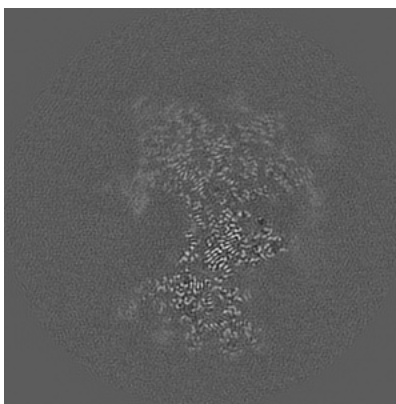
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

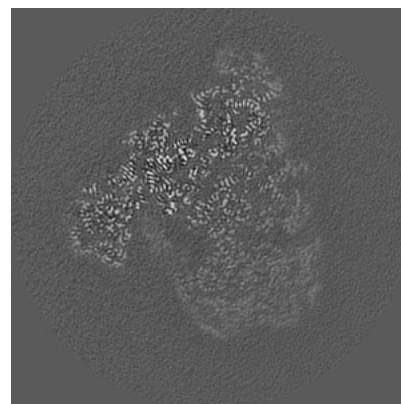
6.3.1 Primary map



X Index: 165



Y Index: 211

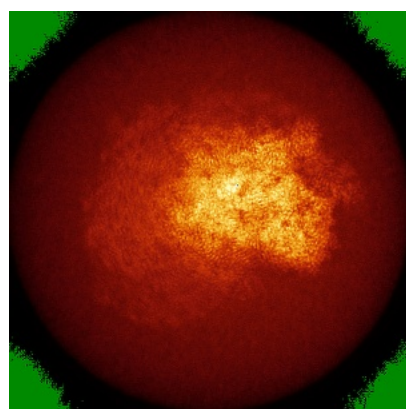


Z Index: 203

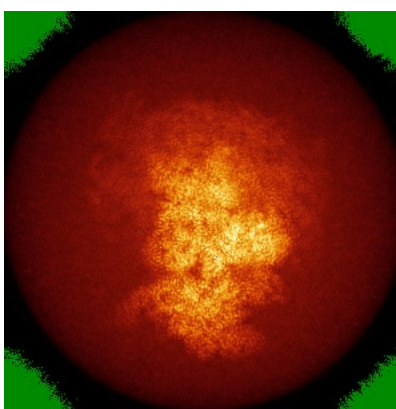
The images above show the largest variance slices of the map in three orthogonal directions.

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

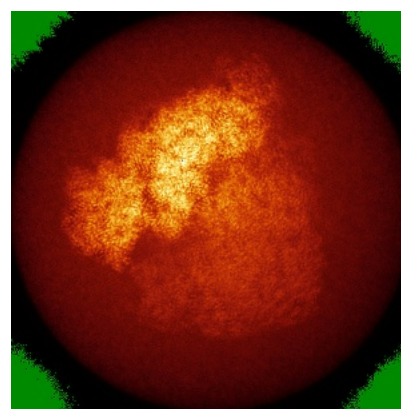
6.4.1 Primary map



X



Y

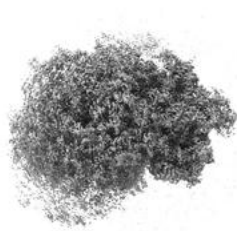


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

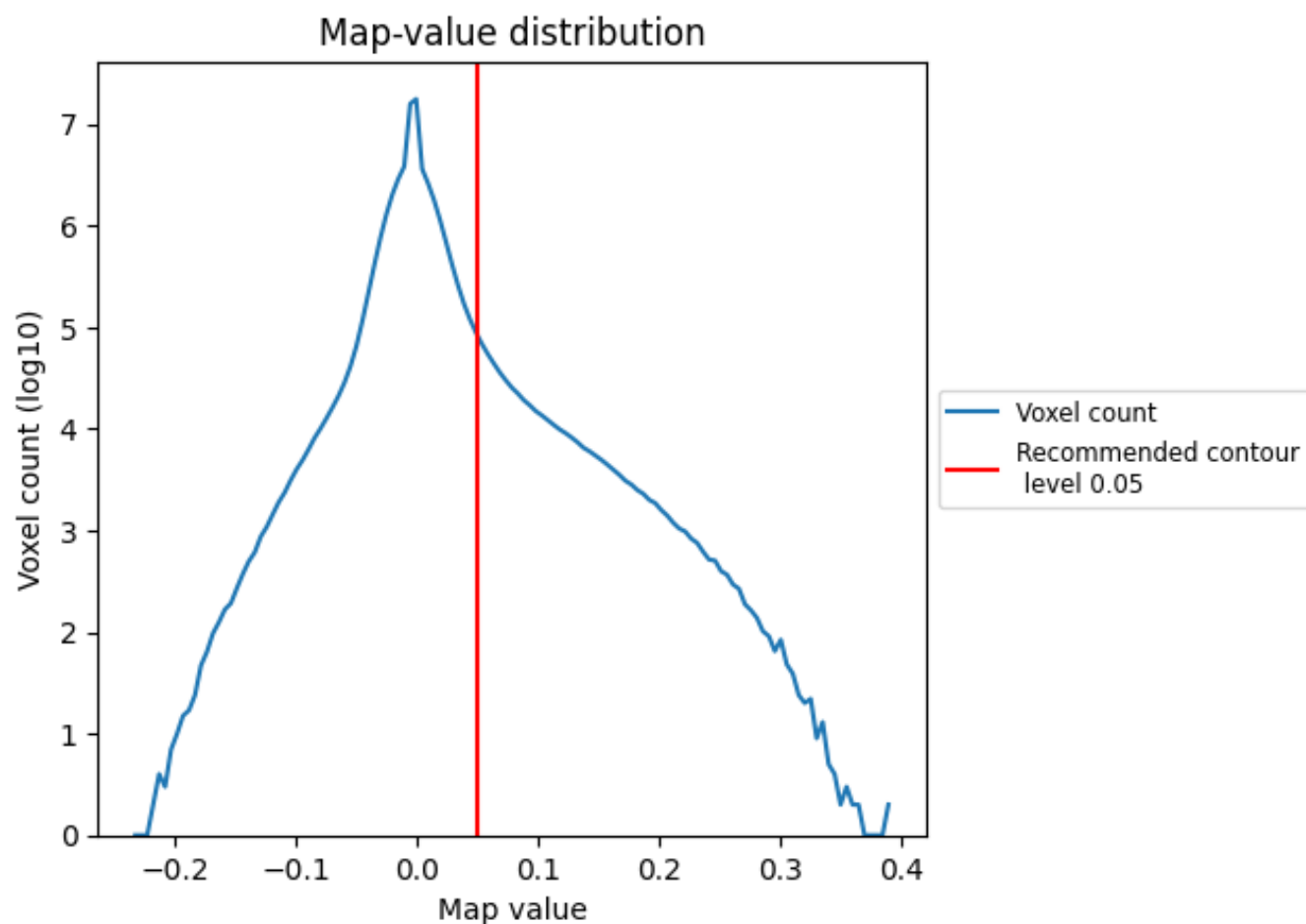
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

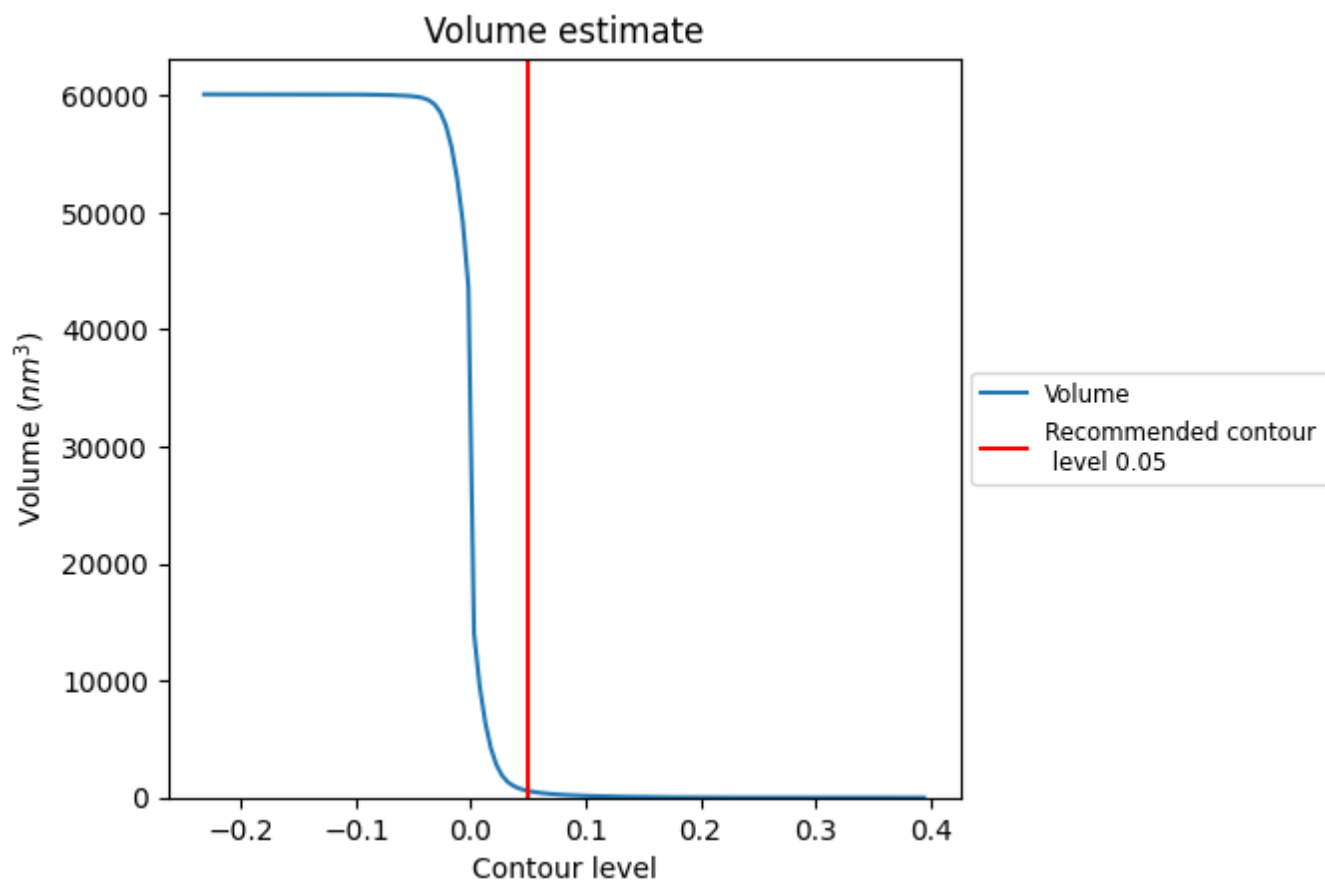
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

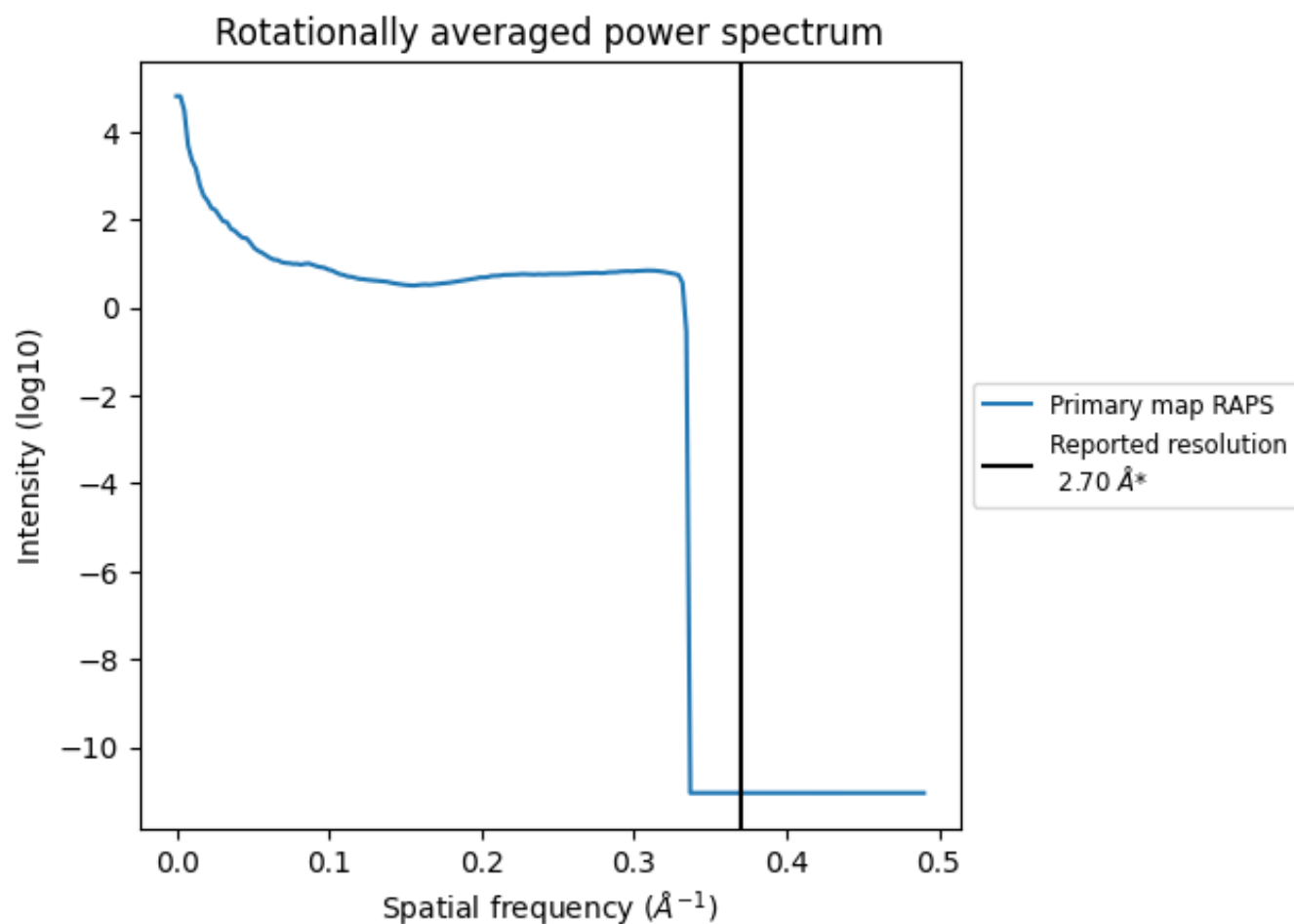
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm³; this corresponds to an approximate mass of 516 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

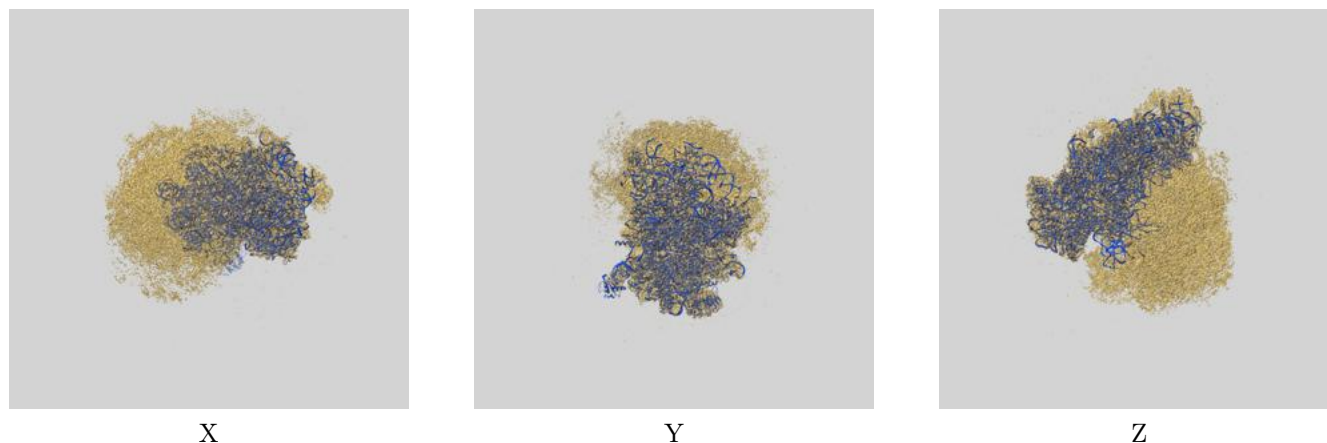
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

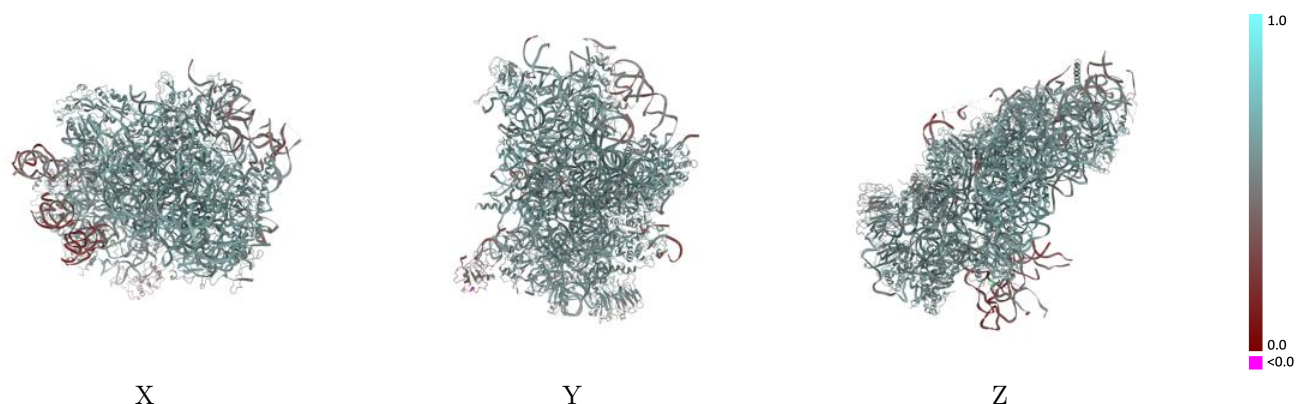
This section contains information regarding the fit between EMDB map EMD-7024 and PDB model 6AZ1. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



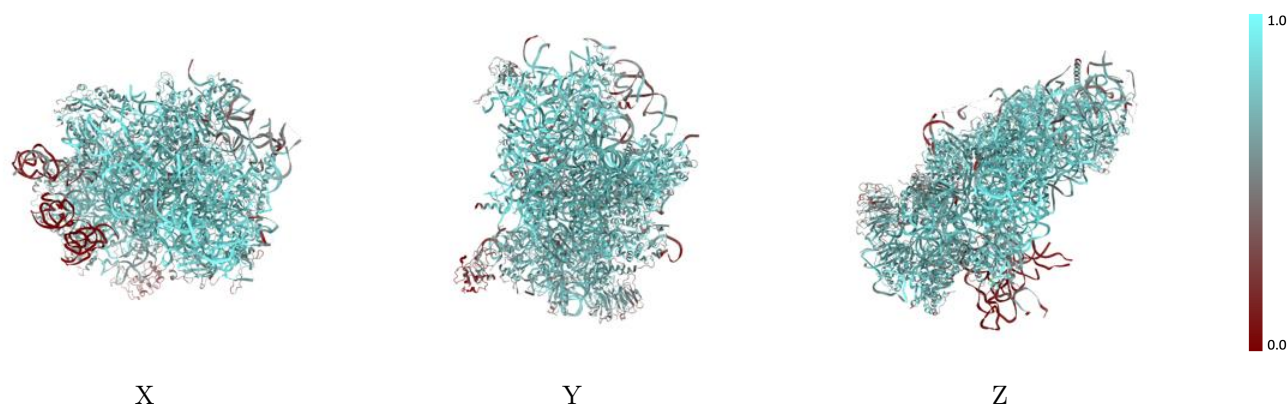
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



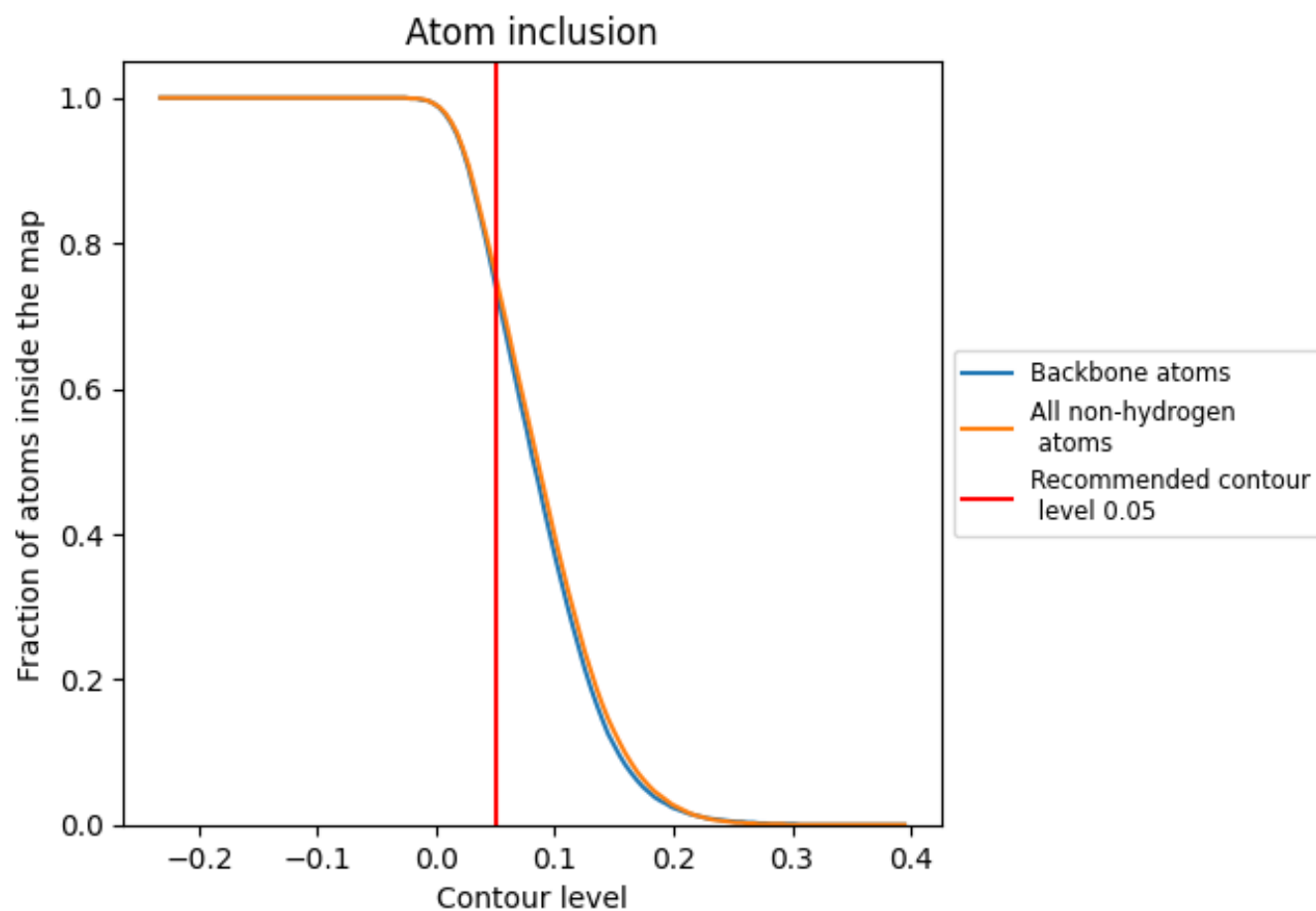
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.5660
1	 0.8600	 0.5900
2	 0.1860	 0.3080
3	 0.3610	 0.4230
4	 0.2070	 0.3470
5	 0.8180	 0.5890
A	 0.7300	 0.5800
B	 0.7890	 0.5900
C	 0.6850	 0.5590
D	 0.7690	 0.5800
E	 0.8000	 0.5930
F	 0.8210	 0.6020
G	 0.6440	 0.5480
H	 0.7360	 0.5740
I	 0.7700	 0.5730
J	 0.8410	 0.6100
K	 0.7630	 0.5800
L	 0.7740	 0.5870
M	 0.6690	 0.5590
N	 0.6890	 0.5490
O	 0.7530	 0.5810
P	 0.7720	 0.5830
Q	 0.1690	 0.3570
R	 0.7010	 0.5680
S	 0.7930	 0.5860
T	 0.8110	 0.5950
U	 0.7830	 0.5960
V	 0.6880	 0.5600
W	 0.6670	 0.5630
X	 0.7930	 0.5830
Y	 0.7750	 0.5820
Z	 0.7580	 0.5770
a	 0.7020	 0.5630
b	 0.8210	 0.6060
c	 0.7910	 0.5920



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Chain	Atom inclusion	Q-score
d	 0.6340	 0.5650
e	 0.7160	 0.5800
f	 0.2730	 0.3930
g	 0.5700	 0.5200