



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 01:13 AM EDT

PDB ID : 5WFK / pdb_00005wfk
EMDB ID : EMD-8828
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C3)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-12
Resolution : 3.40 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:

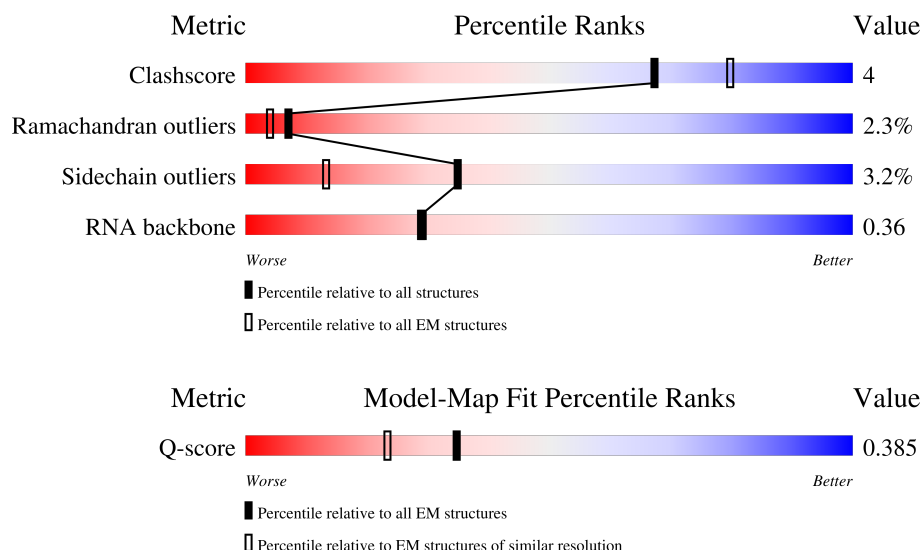
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



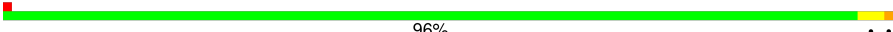
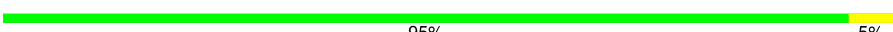
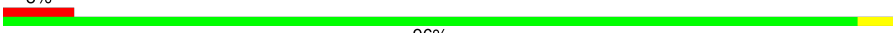
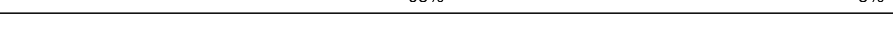
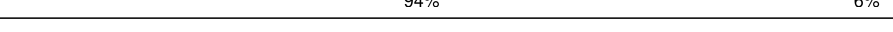
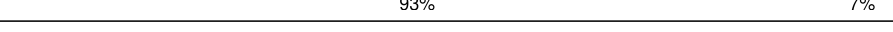
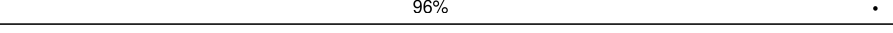
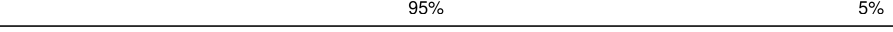
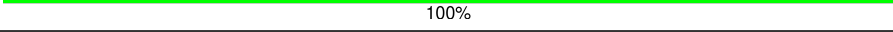
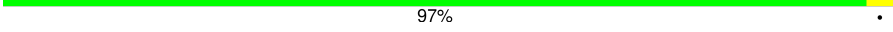
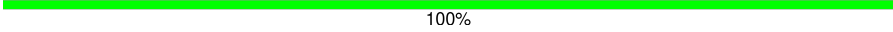
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	2903	 67% 28% 5%
2	B	120	 72% 27% 1%
3	C	271	 92% 7%

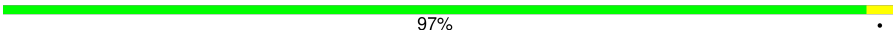
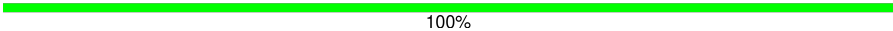
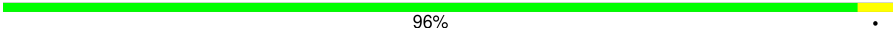
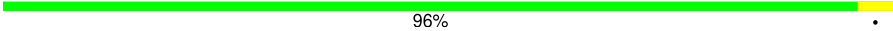
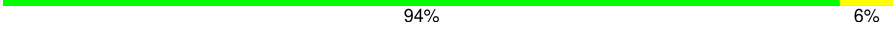
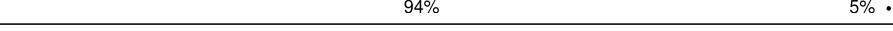
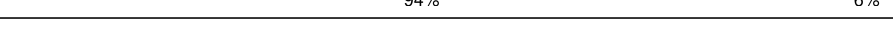
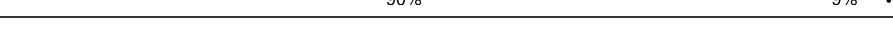
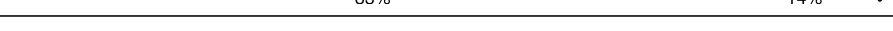
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Mol	Chain	Length	Quality of chain
4	D	208	 92% 6% .
5	E	200	 94% 6% .
6	F	177	 96% ..
7	G	174	 95% 5%
8	H	149	 8% 96% .
9	I	141	 19% 83% 15% .
10	J	141	 91% 9%
11	K	122	 85% 13% .
12	L	143	 92% 8%
13	M	136	 96% .
14	N	119	 94% 5% .
15	O	116	 97% ..
16	P	114	 95% 5%
17	Q	115	 95% 5%
18	R	102	 90% 8% ..
19	S	109	 94% 6%
20	T	92	 93% 7%
21	U	102	 96% .
22	V	92	 95% 5%
23	W	75	 91% 9%
24	X	77	 100%
25	Y	60	 97% .
26	Z	56	 100%
27	0	55	 91% 9%
28	1	51	 96% .

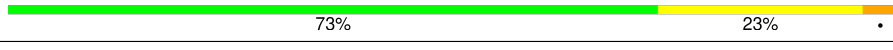
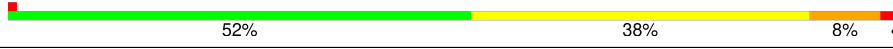
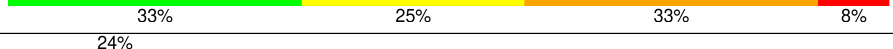
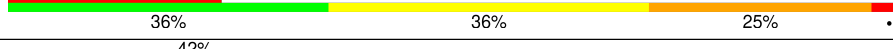
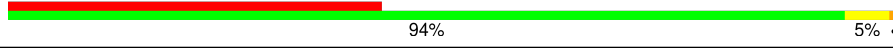
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Mol	Chain	Length	Quality of chain
29	2	45	 87% 13%
30	3	64	 97% .
31	4	38	 100%
32	5	131	 72% 85% 15%
33	6	66	 95% 5%
34	a	1540	 56% 35% 9% .
35	b	218	 96% .
36	c	206	 96% .
37	d	205	 96% .
38	e	157	 91% 8% .
39	f	100	 89% 9% .
40	g	151	 94% 6%
41	h	129	 94% 5% .
42	i	127	 85% 12% .
43	j	98	 86% 10% .
44	k	116	 91% 7% .
45	l	121	 85% 13% .
46	m	115	 94% 5% .
47	n	101	 92% 8%
48	o	88	 90% 7% .
49	p	82	 94% 6%
50	q	80	 90% 9% .
51	r	65	 83% 14% .
52	s	79	 90% 10%
53	t	85	 88% 12%

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	
58	z	393	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	2030	-	-	X	-
57	MIA	y	37	-	-	X	-

2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 154325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	expression tag	GB 1324665466

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	2	0
			33095	14768	6067	10718	1542		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

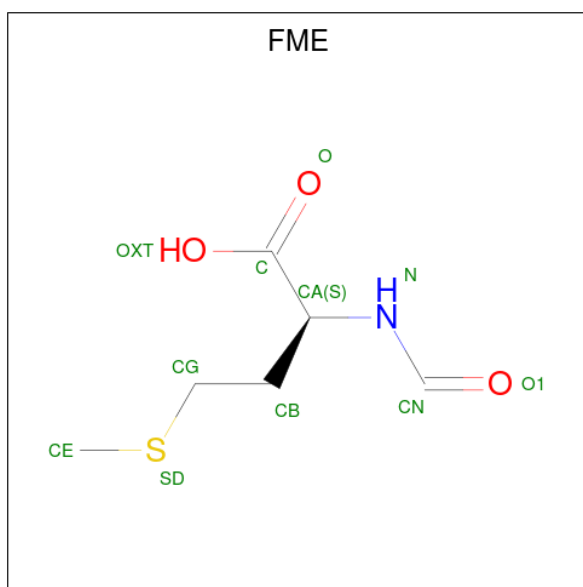
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



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

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	965	Total	Mg	0
			965	965	
60	B	27	Total	Mg	0
			27	27	
60	C	2	Total	Mg	0
			2	2	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	H	1	Total	Mg	0
			1	1	
60	L	3	Total	Mg	0
			3	3	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	
60	U	1	Total	Mg	0
			1	1	

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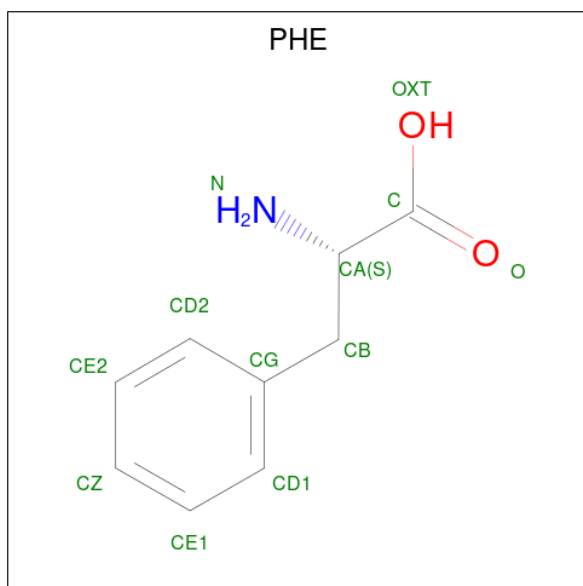
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Mol	Chain	Residues	Atoms		AltConf
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	1	Total 1	Mg 1	0
60	0	1	Total 1	Mg 1	0
60	2	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	a	375	Total 375	Mg 375	0
60	c	1	Total 1	Mg 1	0
60	d	1	Total 1	Mg 1	0
60	e	1	Total 1	Mg 1	0
60	f	1	Total 1	Mg 1	0
60	g	1	Total 1	Mg 1	0
60	i	2	Total 2	Mg 2	0
60	k	1	Total 1	Mg 1	0
60	l	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	q	1	Total 1	Mg 1	0
60	v	9	Total 9	Mg 9	0
60	w	3	Total 3	Mg 3	0
60	x	1	Total 1	Mg 1	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

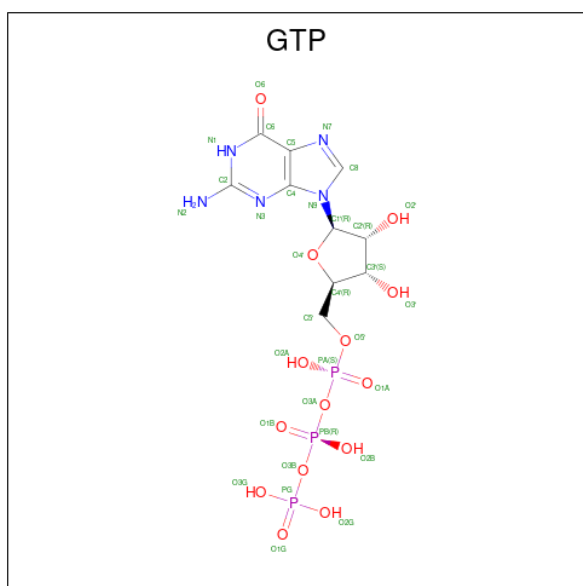
Mol	Chain	Residues	Atoms			AltConf
61	A	1	Total	K		0
			1	1		

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



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

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



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

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	293	Total	O	0
			293	293	
64	B	8	Total	O	0
			8	8	
64	C	3	Total	O	0
			3	3	
64	D	3	Total	O	0
			3	3	
64	L	1	Total	O	0
			1	1	
64	N	1	Total	O	0
			1	1	
64	O	1	Total	O	0
			1	1	
64	Q	1	Total	O	0
			1	1	
64	V	1	Total	O	0
			1	1	
64	W	1	Total	O	0
			1	1	
64	0	1	Total	O	0
			1	1	
64	2	1	Total	O	0
			1	1	
64	3	1	Total	O	0
			1	1	
64	a	93	Total	O	0
			93	93	
64	l	1	Total	O	0
			1	1	
64	m	1	Total	O	0
			1	1	
64	o	1	Total	O	0
			1	1	
64	s	3	Total	O	0
			3	3	
64	t	1	Total	O	0
			1	1	

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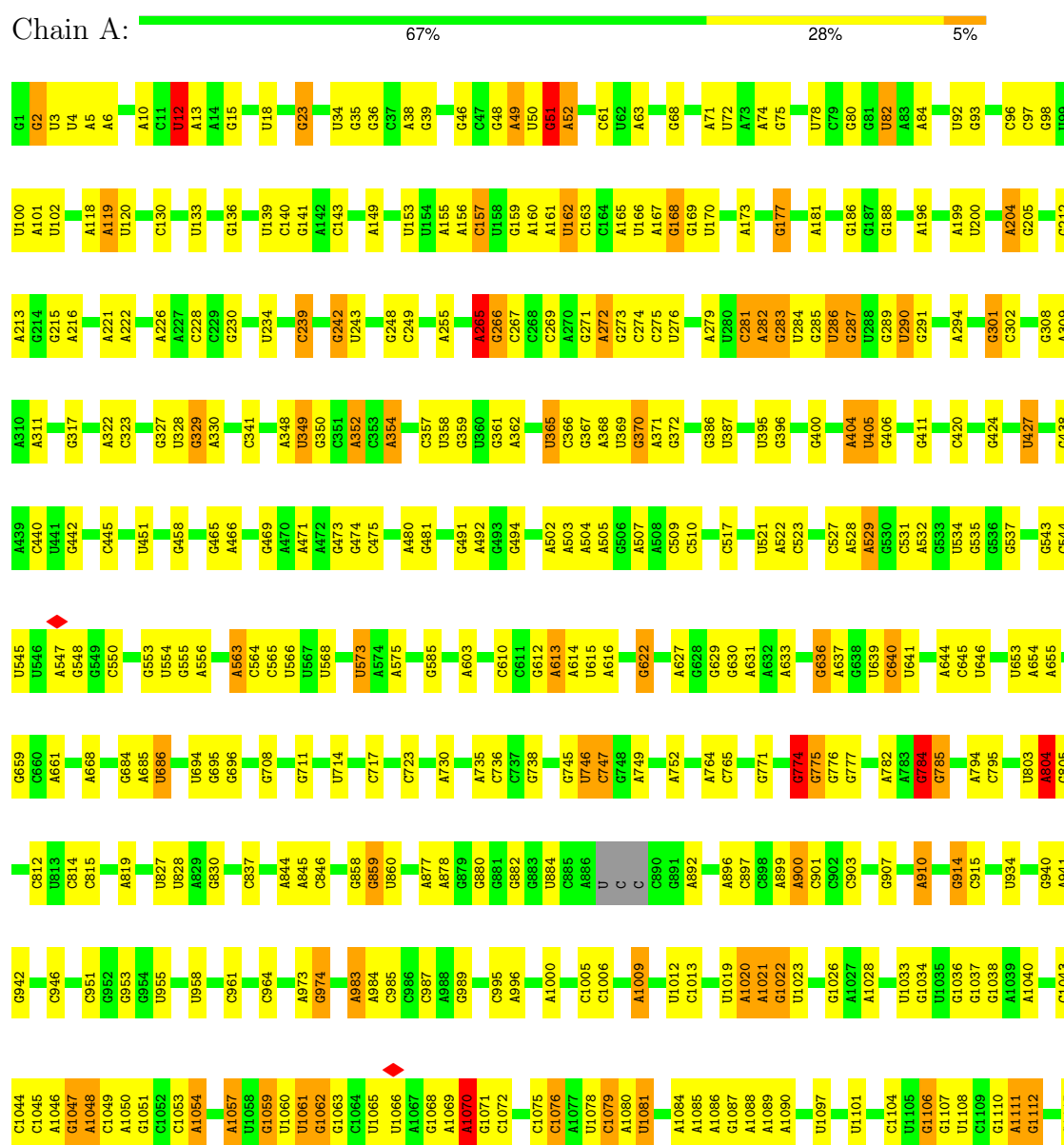
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Mol	Chain	Residues	Atoms		AltConf
64	u	1	Total 1	O 1	0
64	v	1	Total 1	O 1	0
64	w	1	Total 1	O 1	0

3 Residue-property plots

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

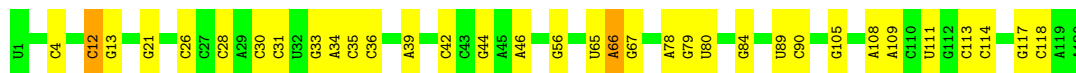
• Molecule 1: 23S rRNA



C2819	U2724	G2578	G2446	C2332	U2192	A2077	U1955	C1833	U1716	A1583	C1490	A1392	G1238	G1116
A2820	A2725	C2579	G2447	C2333	U2193	C2078	U1962	U1834	U1720	U1584	A1490	A1395	G1247	C1117
A2823	A2726	U2580	U2448	U2334	A2198	U2079	C1962	C1835	G1721	C1585	A1505	C1398	G1248	U1118
A2826	U2728	C2582	U2449	A2335	A2335	A2080	C1965	U1841	A1722	G1587	A1504	C1399	A1253	U1119
U2833	G2732	U2585	U2457	A2336	G2204	U2092	A1966	G1842	G1723	A1590	A1506	A1403	A1253	G1124
U2837	A2733	U2586	A2469	C2342	C2206	G2093	C1967	G1847	G1724	A1591	U1506	A1403	G1256	U1130
G2838	G2735	A2602	G2470	C2350	C2207	C2096	A1971	G1853	C1726	C1592	C1507	G1407	G1257	G1131
G2839	G2742	G2603	C2475	G2357	A2211	A2097	A1971	A1853	A1727	C1595	A1508	G1410	U1258	U1132
C2840	U2743	U2604	A2476	G2361	A2212	U2098	G1972	A1854	C1728	A1596	A1509	A1410	A1262	C1135
G2844	G2744	U2605	C2480	G2370	U2213	U2099	U1976	G1857	U1730	C1605	G1510	G1416	A1269	G1139
U2845	U2745	G2608	G2481	G2370	A2211	G2100	U1980	A1858	C1732	A1608	A1515	C1417	G1270	C1140
U2849	G2747	U2609	C2486	G2370	G2221	A2102	G1980	A1858	C1732	A1608	A1515	C1417	G1270	U1141
A2850	A2748	U2613	U2491	G2373	A2225	C2104	U1982	G1862	G1738	A1609	A1519	A1419	A1272	A1142
A2856	C2752	U2615	G2494	G2373	C2226	U2106	U1991	A1866	A1739	A1610	U1520	A1420	U1273	A1143
U2861	U2753	G2624	G2494	A2378	G2238	G2107	G1992	G1869	G1740	C1615	U1523	A1427	G1300	U1148
G2867	A2757	U2629	C2498	G2379	G2239	A2108	U1993	A1870	C1741	A1616	G1524	C1428	A1301	U1149
A2868	A2758	G2630	C2499	G2383	G2242	U2109	C1996	A1871	A1746	A1617	G1524	G1429	C1305	C1150
A2872	C2762	C2846	G2502	G2385	U2243	G2112	C1997	A1872	G1750	G1619	A1528	A1431	G1311	C1151
A2873	G2763	U2653	A2503	G2391	G2251	U2113	G2004	A1875	U1758	G1642	C1533	A1433	G1320	C1152
C2874	A2764	A2654	U2504	A2392	C2264	A2118	A2013	A1876	C1764	U1647	U1534	A1434	C1327	G1154
C2880	A2778	U2656	G2513	G2399	A2278	U2119	A2020	G1884	A1773	U1648	A1536	G1441	A1328	A1155
A2883	C2788	G2673	U2514	U2401	A2274	G2121	C2021	G1885	G1776	G1649	G1537	C1447	U1329	G1171
U2884	A2790	A2681	C2515	U2402	G2278	U2132	U2022	G1906	U1779	A1654	U1542	G1450	G1330	U1172
A2889	G2791	A2682	A2516	U2403	G2279	G2133	C2023	G1907	A1780	A1654	G1543	C1451	G1332	C1173
A2900	A2792	U2688	U2517	G2405	C2283	G2133	A2031	U1911	U1782	G1674	A1544	A1453	C1345	A1175
C2901	C2793	U2689	A2411	U2408	G2286	A2134	A2032	A1912	A1783	C1675	A1545	C1454	U1352	G1176
C2902	U2794	U2690	G2412	A2407	A2287	G2134	A2033	A1913	U1784	U1688	A1549	A1454	U1352	C1177
U2903	C2796	G2698	U2413	U2408	A2288	G2141	A2033	A1914	A1791	C1691	U1547	G1455	U1352	C1178
A2909	U2797	A2700	G2414	A2411	U2296	C2145	G2038	A1916	U1791	U1692	G1555	C1461	C1363	U1184
A2909	U2798	A2705	G2414	G2415	A2297	C2146	U2039	U1917	C1795	U1693	C1557	U1466	G1364	G1190
A2909	U2799	A2706	G2415	G2415	A2297	C2146	U2039	A1918	U1796	C1694	C1557	U1467	G1365	G1210
A2909	U2800	A2707	U2423	U2423	U2305	G2157	A2042	A1919	C1800	C1695	U1559	U1468	A1366	C1196
A2909	U2801	U2707	U2423	U2423	U2305	G2157	A2042	A1919	A1801	A1698	G1560	A1469	A1367	G1197
A2909	U2802	C2712	U2552	A2424	A2309	G2162	C2055	A1927	A1802	G1699	C1565	A1470	G1368	C1197
A2909	A2803	G2713	G2553	A2425	A2311	A2163	G2056	A1928	A1803	A1700	C1565	G1475	G1369	G1210
A2909	U2804	U2713	U2554	A2425	A2311	C2164	G2056	A1928	A1803	A1700	C1565	G1475	G1370	G1210
A2909	C2805	G2714	A2566	G2428	G2318	C2164	A2059	G1929	A1808	G1702	A1566	A1476	G1371	G1218
A2909	C2806	C2715	G2567	G2429	G2319	A2170	A2060	G1930	A1809	G1703	C1567	A1477	A1378	G1218
A2909	U2807	C2716	U2568	A2430	G2319	A2171	G2061	A1936	A1810	G1706	U1578	G1478	U1379	G1225
A2909	G2808	C2717	G2569	A2434	G2323	A2172	A2062	A1937	C1816	G1706	U1578	G1479	U1379	A1226
A2909	C2809	G2718	G2570	A2435	G2323	A2173	A2062	A1938	G1817	G1710	A1579	G1482	A1383	G1227
A2909	U2810	U2720	U2571	A2435	G2325	A2173	A2062	A1938	U1818	G1710	A1579	G1482	A1383	G1227
A2909	C2812	A2721	A2572	U2441	C2326	U2180	G2069	U1939	U1818	G1710	A1579	G1482	A1383	G1227
A2909	A2813	C2722	C2573	U2441	C2327	U2180	A2070	U1940	U1818	G1710	A1579	G1482	A1383	G1227
A2909	U2818	C2723	A2573	G2445	A2328	G2186	C2072	C1942	G1826	G1715	C1582	U1485	A1387	A1237

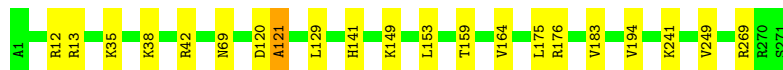
- Molecule 2: 5S rRNA

Chain B:  72% 27%



- Molecule 3: 50S ribosomal protein L2

Chain C:  92% 7%



- Molecule 4: 50S ribosomal protein L3

Chain D:  92% 6%

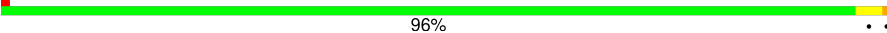


- Molecule 5: 50S ribosomal protein L4

Chain E:  94% 6%

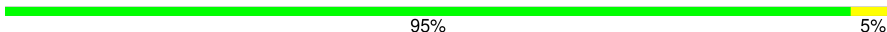


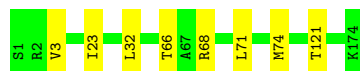
- Molecule 6: 50S ribosomal protein L5

Chain F:  96%

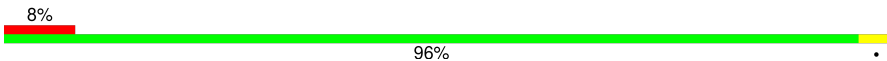


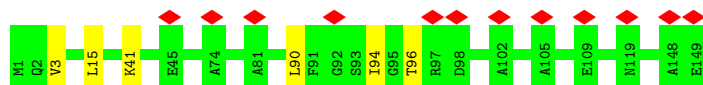
- Molecule 7: 50S ribosomal protein L6

Chain G:  95% 5%

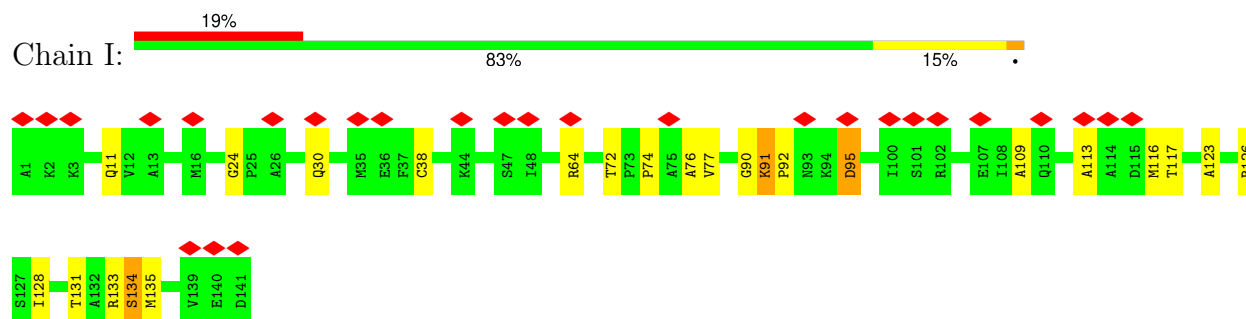


- Molecule 8: 50S ribosomal protein L9

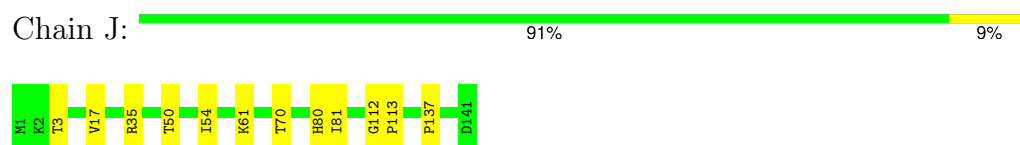
Chain H:  8% 96%



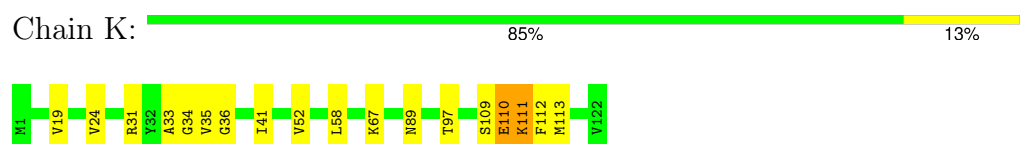
- Molecule 9: 50S ribosomal protein L11



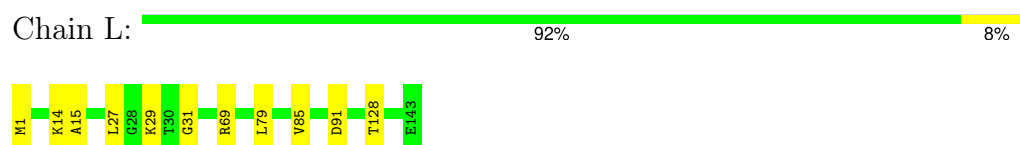
- Molecule 10: 50S ribosomal protein L13



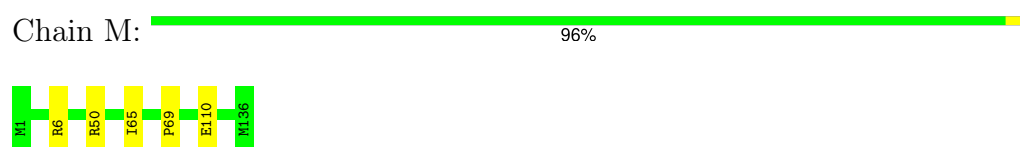
- Molecule 11: 50S ribosomal protein L14



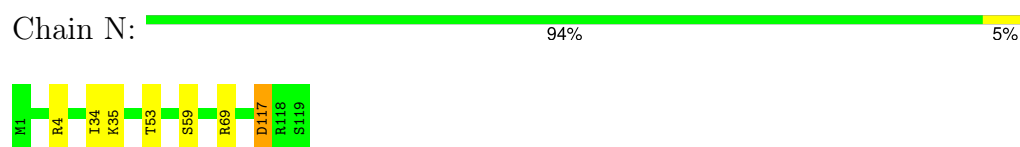
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18





- Molecule 16: 50S ribosomal protein L19

Chain P: 95% 5%



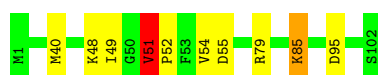
- Molecule 17: 50S ribosomal protein L20

Chain Q: 95% 5%



- Molecule 18: 50S ribosomal protein L21

Chain R: 90% 8% ..



- Molecule 19: 50S ribosomal protein L22

Chain S: 94% 6%



- Molecule 20: 50S ribosomal protein L23

Chain T: 93% 7%



- Molecule 21: 50S ribosomal protein L24

Chain U: 96% .



- Molecule 22: 50S ribosomal protein L25

Chain V: 95% 5%



- Molecule 23: 50S ribosomal protein L27

Chain W: 91% 9%



- Molecule 24: 50S ribosomal protein L28

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L29

Chain Y: 97% .



- Molecule 26: 50S ribosomal protein L30

Chain Z: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain 0: 91% 9%



- Molecule 28: 50S ribosomal protein L33

Chain 1: 96% .

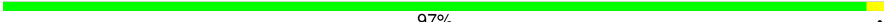


- Molecule 29: 50S ribosomal protein L34

Chain 2: 87% 13%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  97% .



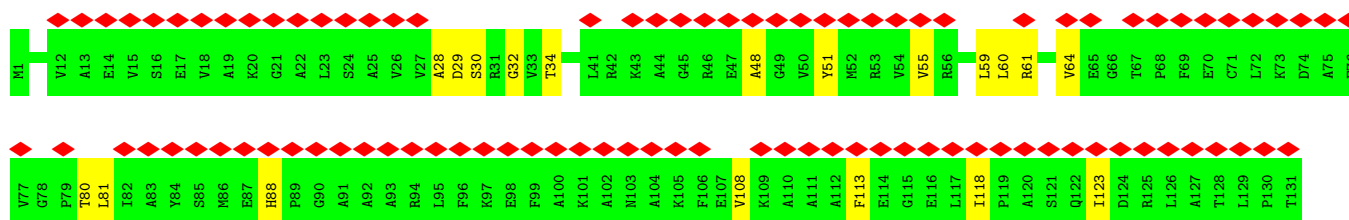
- Molecule 31: 50S ribosomal protein L36

Chain 4:  100%

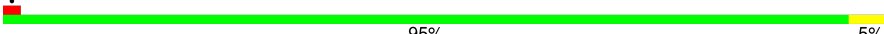
There are no outlier residues recorded for this chain.

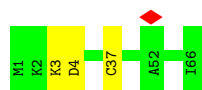
- Molecule 32: 50S ribosomal protein L10

Chain 5:  72% 85% 15%



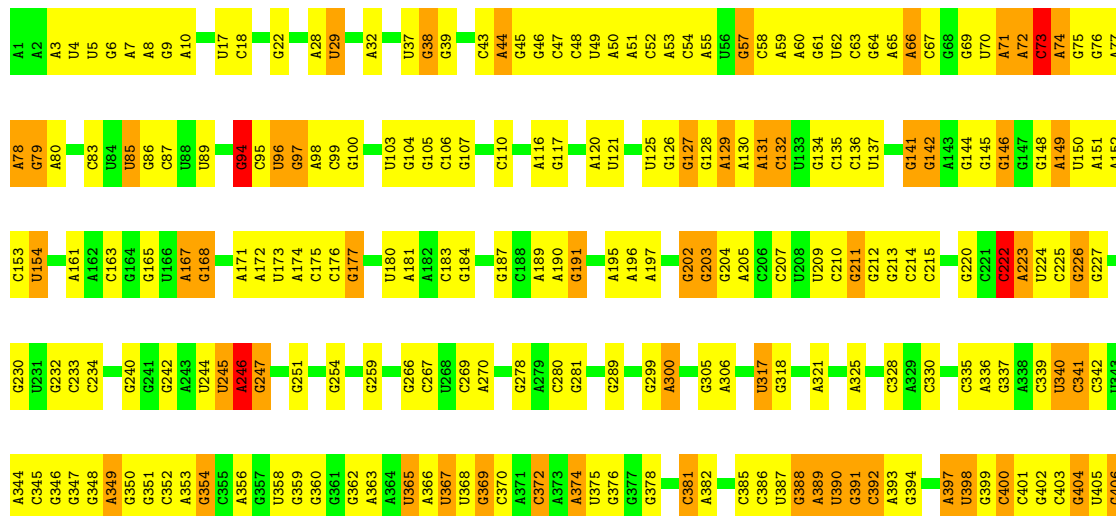
- Molecule 33: 50S ribosomal protein L31

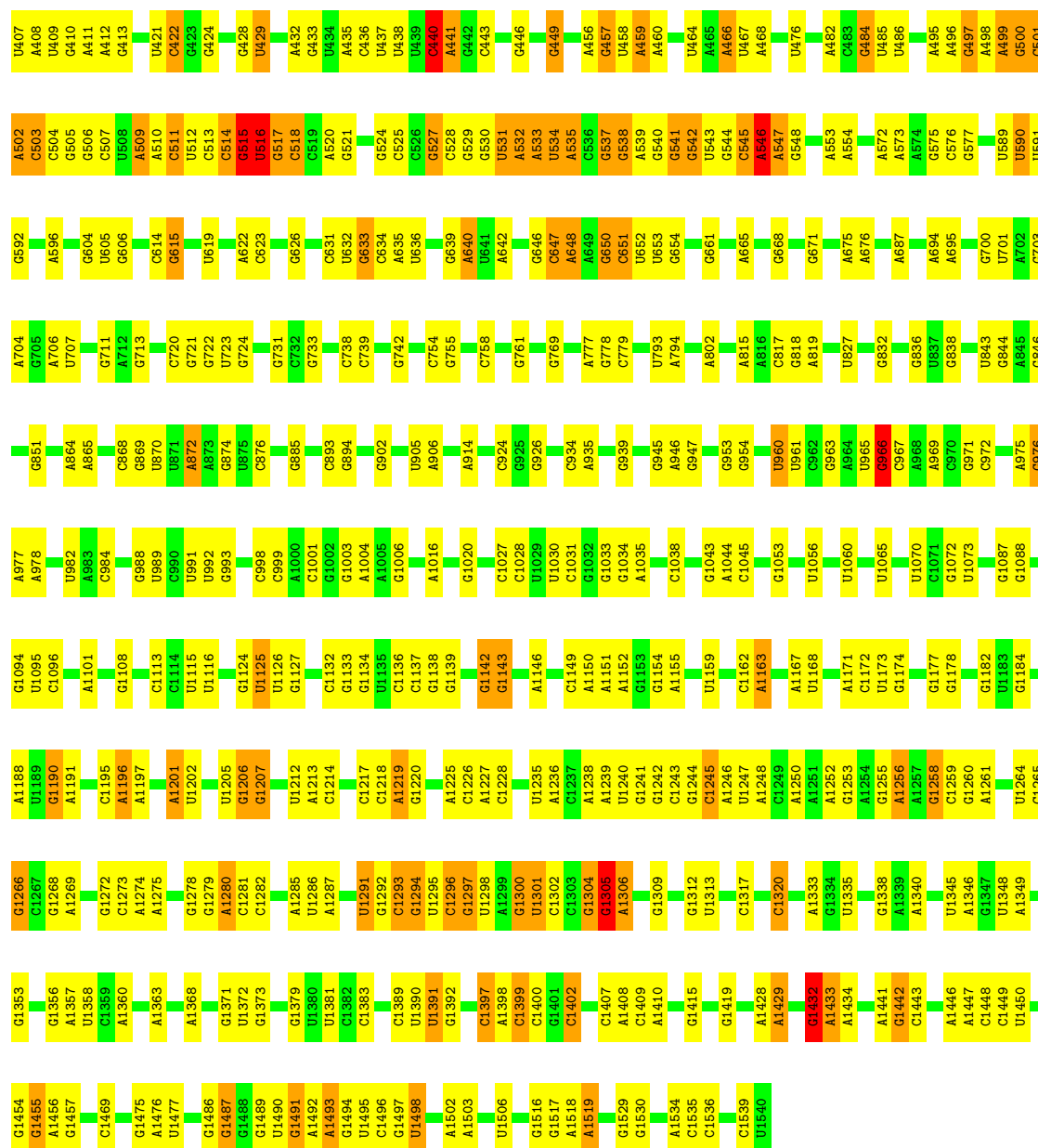
Chain 6:  95% 5%



- Molecule 34: 16S rRNA

Chain a:  56% 35% 9%





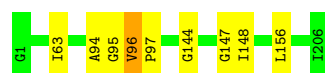
• Molecule 35: 30S ribosomal protein S2

Chain b: 96%

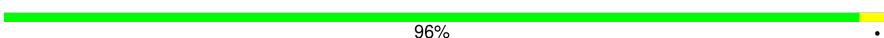


• Molecule 36: 30S ribosomal protein S3

Chain c: 96%



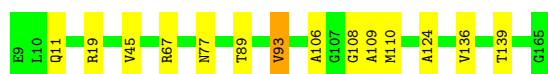
- Molecule 37: 30S ribosomal protein S4

Chain d:  96% .



- Molecule 38: 30S ribosomal protein S5

Chain e:  91% 8% .

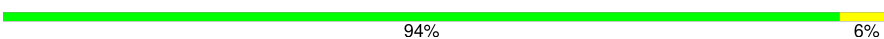


- Molecule 39: 30S ribosomal protein S6

Chain f:  89% 9% .

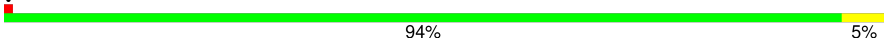


- Molecule 40: 30S ribosomal protein S7

Chain g:  94% 6% .



- Molecule 41: 30S ribosomal protein S8

Chain h:  94% 5% .



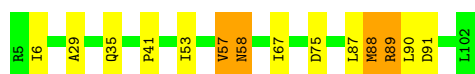
- Molecule 42: 30S ribosomal protein S9

Chain i:  85% 12% .

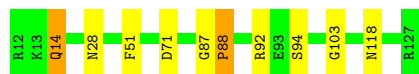


- Molecule 43: 30S ribosomal protein S10

Chain j:  86% 10% .



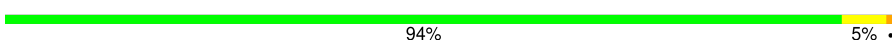
• Molecule 44: 30S ribosomal protein S11

Chain k:  91% 7%

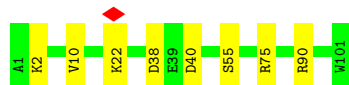
• Molecule 45: 30S ribosomal protein S12

Chain l:  85% 13%

• Molecule 46: 30S ribosomal protein S13

Chain m:  94% 5%

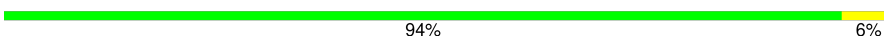
• Molecule 47: 30S ribosomal protein S14

Chain n:  92% 8%

• Molecule 48: 30S ribosomal protein S15

Chain o:  90% 7%

• Molecule 49: 30S ribosomal protein S16

Chain p:  94% 6%

• Molecule 50: 30S ribosomal protein S17

Chain q:  90% 9%

- Molecule 51: 30S ribosomal protein S18

Chain r:  83% 14%



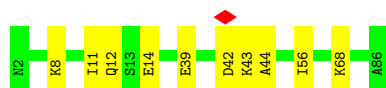
- Molecule 52: 30S ribosomal protein S19

Chain s:  90% 10%



- Molecule 53: 30S ribosomal protein S20

Chain t:  88% 12%



- Molecule 54: 30S ribosomal protein S21

Chain u:  72% 18% 9%



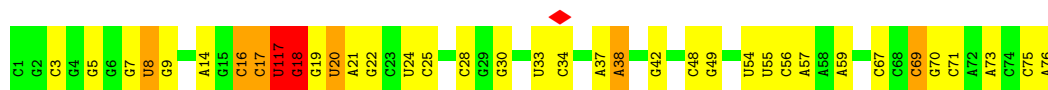
- Molecule 55: tRNA-fMet

Chain v:  73% 23%

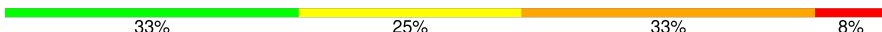


- Molecule 55: tRNA-fMet

Chain w:  52% 38% 8%

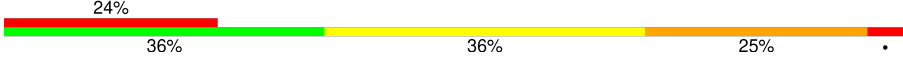


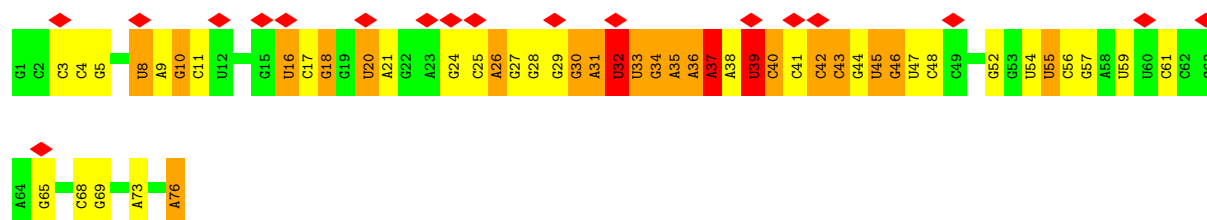
- Molecule 56: mRNA

Chain x:  33% 25% 33% 8%

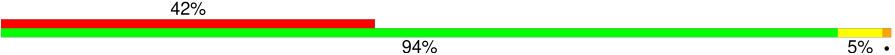


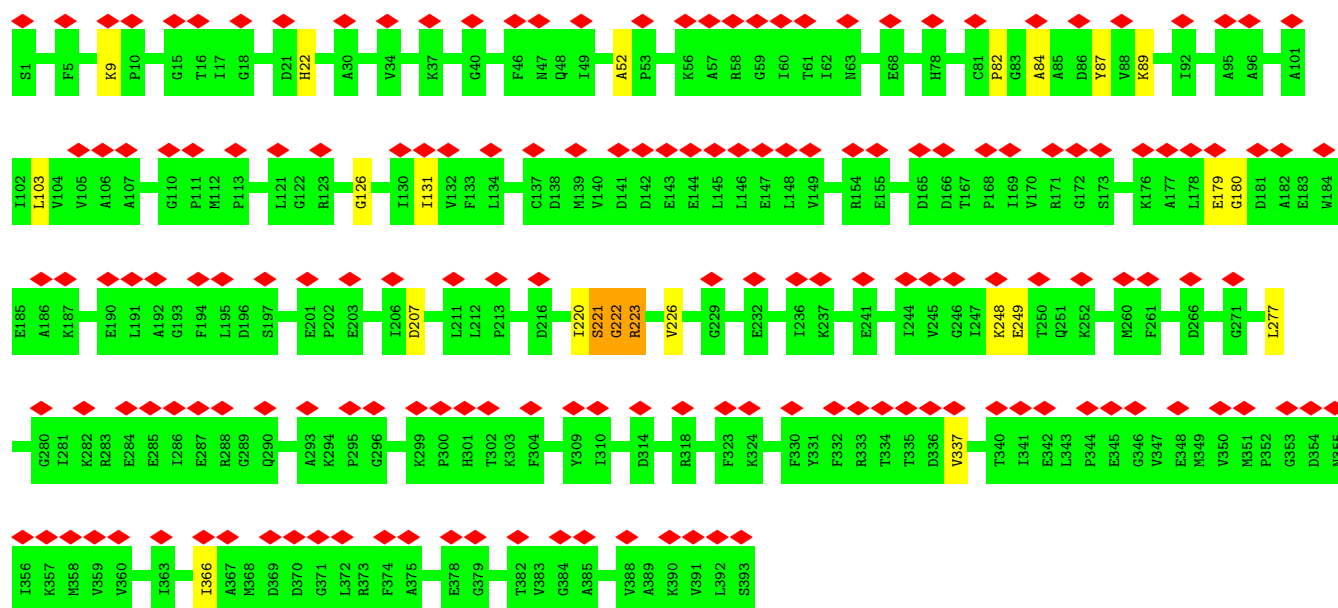
- Molecule 57: Phe-tRNA-Phe

Chain y: 



- Molecule 58: Elongation factor Tu 2

Chain z: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.00651	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/69174	0.71	32/107907 (0.0%)
2	B	0.37	0/2876	0.69	2/4483 (0.0%)
3	C	0.53	0/2121	0.74	0/2852
4	D	0.53	0/1578	0.78	2/2124 (0.1%)
5	E	0.51	0/1563	0.82	0/2103
6	F	0.55	0/1434	0.81	1/1926 (0.1%)
7	G	0.54	0/1324	0.75	0/1794
8	H	0.56	0/1122	0.76	0/1515
9	I	0.68	0/1046	0.91	2/1410 (0.1%)
10	J	0.52	0/1143	0.81	2/1540 (0.1%)
11	K	0.53	0/947	0.73	0/1268
12	L	0.55	0/1052	0.85	0/1401
13	M	0.50	0/1093	0.78	0/1460
14	N	0.57	0/964	0.87	0/1289
15	O	0.54	0/902	0.86	0/1209
16	P	0.50	0/929	0.73	0/1242
17	Q	0.54	0/946	0.91	0/1260
18	R	0.52	0/823	0.74	2/1100 (0.2%)
19	S	0.51	0/852	0.83	0/1142
20	T	0.53	0/736	0.76	0/984
21	U	0.51	0/787	0.75	0/1051
22	V	0.50	0/752	0.75	0/1008
23	W	0.49	0/579	0.68	0/767
24	X	0.51	0/635	0.74	0/848
25	Y	0.55	0/495	0.87	0/658
26	Z	0.57	0/438	0.82	0/586
27	0	0.50	0/440	0.81	0/588
28	1	0.47	0/424	0.66	0/565
29	2	0.58	0/370	1.00	0/487
30	3	0.50	0/513	0.87	0/676
31	4	0.48	0/303	0.71	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.65	0/1001	0.86	0/1350
33	6	0.57	0/531	0.81	0/709
34	a	0.38	0/36776	0.74	32/57365 (0.1%)
35	b	0.57	0/1735	0.80	0/2338
36	c	0.55	0/1651	0.80	0/2225
37	d	0.55	0/1665	0.82	0/2227
38	e	0.55	0/1180	0.83	0/1587
39	f	0.58	0/835	0.82	0/1128
40	g	0.54	0/1195	0.82	0/1602
41	h	0.53	0/989	0.83	0/1326
42	i	0.56	0/1034	0.77	0/1375
43	j	0.56	0/796	0.74	0/1077
44	k	0.54	0/885	0.79	0/1195
45	l	0.57	0/954	0.77	1/1282 (0.1%)
46	m	0.58	0/900	0.87	0/1204
47	n	0.55	0/822	0.81	0/1095
48	o	0.52	0/722	0.85	0/964
49	p	0.55	0/659	0.79	0/884
50	q	0.56	0/657	0.72	0/881
51	r	0.57	0/544	0.82	0/731
52	s	0.57	0/652	0.77	0/877
53	t	0.56	0/671	0.88	0/888
54	u	0.66	0/550	0.98	0/728
55	v	0.40	1/1747 (0.1%)	0.71	0/2721
55	w	0.84	1/1747 (0.1%)	0.86	5/2721 (0.2%)
56	x	0.37	0/280	0.74	1/433 (0.2%)
57	y	0.39	0/1607	0.70	0/2501
58	z	0.56	0/3086	0.76	0/4175
All	All	0.44	2/164232 (0.0%)	0.74	82/245229 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-31.02	1.14	1.61
55	v	7	4SU	O3'-P	5.11	1.61	1.56

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	P-O3'-C3'	18.64	148.16	120.20
55	w	117	U	O3'-P-O5'	10.76	120.13	104.00
1	A	51	G	C2'-C3'-O3'	9.48	123.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1305	G	C2'-C3'-O3'	9.24	123.36	109.50
1	A	242	G	C2'-C3'-O3'	9.18	123.27	109.50
1	A	204	A	C4'-C3'-O3'	8.66	122.40	109.40
1	A	1022	G	C2'-C3'-O3'	8.66	122.49	109.50
1	A	1730	U	C2'-C3'-O3'	8.34	122.01	109.50
1	A	1378	A	C4'-C3'-O3'	8.15	121.62	109.40
34	a	515	G	C2'-C3'-O3'	8.13	125.90	113.70
55	w	117	U	OP2-P-O3'	-7.95	84.14	108.00
1	A	2712	C	C2'-C3'-O3'	7.94	121.41	109.50
1	A	2407	A	C2'-C3'-O3'	7.74	125.31	113.70
34	a	1432	G	C2'-C3'-O3'	7.61	120.91	109.50
1	A	265	A	C4'-C3'-O3'	7.51	120.67	109.40
1	A	613	A	C4'-C3'-O3'	7.08	120.02	109.40
2	B	66	A	C4'-C3'-O3'	6.97	123.46	113.00
34	a	141	G	C4'-C3'-O3'	-6.89	99.06	109.40
34	a	1190	G	C2'-C3'-O3'	6.79	119.69	109.50
1	A	859	G	C2'-C3'-O3'	6.76	119.65	109.50
1	A	1857	G	C4'-C3'-O3'	6.72	119.48	109.40
55	w	18	G	C2'-C3'-O3'	6.65	119.48	109.50
34	a	440	C	C4'-C3'-O3'	-6.63	103.05	113.00
34	a	246	A	C4'-C3'-O3'	6.56	119.23	109.40
1	A	2296	U	C4'-C3'-O3'	6.55	119.23	109.40
34	a	63	C	C2'-C3'-O3'	6.48	123.42	113.70
34	a	500	G	O4'-C1'-C2'	-6.47	101.13	107.60
1	A	774	G	C2'-C3'-O3'	6.44	119.16	109.50
34	a	1201	A	C2'-C3'-O3'	6.42	119.14	109.50
1	A	1020	A	C4'-C3'-O3'	6.39	118.99	109.40
1	A	2391	G	C4'-C3'-O3'	6.31	122.47	113.00
1	A	1475	G	C2'-C3'-O3'	6.28	118.92	109.50
34	a	428	G	C4'-C3'-O3'	6.27	118.81	109.40
4	D	152	PRO	N-CA-C	-6.24	105.39	113.57
1	A	301	G	C4'-C3'-O3'	6.14	118.61	109.40
1	A	1070	A	C2'-C3'-O3'	6.14	118.71	109.50
34	a	374	A	C2'-C3'-O3'	-6.07	104.60	113.70
1	A	1130	U	C4'-C3'-O3'	-6.06	103.91	113.00
34	a	280	C	C2'-C3'-O3'	6.05	118.58	109.50
34	a	515	G	N9-C1'-C2'	6.02	121.02	112.00
1	A	2566	A	C4'-C3'-O3'	5.95	118.33	109.40
34	a	1297	G	C2'-C3'-O3'	5.94	118.41	109.50
1	A	1940	U	C4'-C3'-O3'	5.93	118.29	109.40
18	R	51	VAL	CA-C-N	-5.86	112.51	119.84
18	R	51	VAL	C-N-CA	-5.86	112.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	440	C	C2'-C3'-O3'	5.82	122.43	113.70
1	A	1140	C	C2'-C3'-O3'	5.79	122.38	113.70
34	a	222	C	N1-C1'-C2'	5.76	120.64	112.00
34	a	1399	C	C4'-C3'-O3'	5.72	117.99	109.40
1	A	1475	G	C4'-C3'-O3'	5.70	117.95	109.40
34	a	960	U	C4'-C3'-O3'	5.70	117.94	109.40
34	a	85	U	C2'-C3'-O3'	-5.68	105.17	113.70
1	A	96	C	C4'-C3'-O3'	-5.65	104.53	113.00
34	a	214	C	C2'-C3'-O3'	5.64	122.17	113.70
1	A	784	G	C2'-C3'-O3'	-5.62	105.27	113.70
9	I	91	LYS	CA-C-N	5.62	126.86	119.84
9	I	91	LYS	C-N-CA	5.62	126.86	119.84
34	a	94	G	C2'-C3'-O3'	5.58	117.87	109.50
56	x	23	C	C1'-C2'-O2'	5.58	116.77	108.40
1	A	1081	U	C3'-C2'-O2'	5.56	119.04	110.70
1	A	301	G	C2'-C3'-O3'	5.55	117.83	109.50
34	a	73	C	N1-C1'-C2'	5.54	120.31	112.00
1	A	1078	U	C2'-C3'-O3'	-5.49	105.47	113.70
34	a	1272	G	C4'-C3'-O3'	-5.47	104.79	113.00
2	B	66	A	C2'-C3'-O3'	-5.46	105.50	113.70
1	A	804	A	C4'-C3'-O3'	-5.46	104.81	113.00
34	a	960	U	C2'-C3'-O3'	5.40	117.60	109.50
55	w	69	C	C2'-C3'-O3'	5.40	121.80	113.70
34	a	421	U	C4'-C3'-O3'	5.34	117.41	109.40
34	a	546	A	N9-C1'-C2'	5.30	119.95	112.00
1	A	1047	G	C2'-C3'-O3'	5.26	117.39	109.50
34	a	1399	C	C2'-C3'-O3'	5.26	117.39	109.50
4	D	151	THR	O-C-N	5.23	124.51	120.38
34	a	1201	A	C4'-C3'-O3'	5.23	117.25	109.40
34	a	67	C	C4'-C3'-O3'	-5.18	105.23	113.00
34	a	63	C	C3'-C2'-O2'	5.18	118.47	110.70
34	a	422	C	C2'-C3'-O3'	-5.13	106.00	113.70
45	l	20	VAL	N-CA-C	5.11	113.21	108.15
6	F	105	ILE	N-CA-C	5.09	116.40	112.12
10	J	112	GLY	CA-C-N	5.02	124.46	119.24
10	J	112	GLY	C-N-CA	5.02	124.46	119.24
1	A	12	U	N1-C1'-C2'	5.01	119.52	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31339	268	0
2	B	2572	0	1302	4	0
3	C	2082	0	2157	5	0
4	D	1557	0	1604	6	0
5	E	1544	0	1607	4	0
6	F	1410	0	1447	1	0
7	G	1304	0	1348	5	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	11	0
10	J	1120	0	1151	3	0
11	K	938	0	1012	12	0
12	L	1043	0	1123	1	0
13	M	1074	0	1157	1	0
14	N	951	0	994	2	0
15	O	892	0	923	1	0
16	P	917	0	965	2	0
17	Q	933	0	1006	3	0
18	R	810	0	834	6	0
19	S	845	0	909	1	0
20	T	730	0	795	2	0
21	U	779	0	834	0	0
22	V	739	0	763	2	0
23	W	572	0	593	1	0
24	X	625	0	655	0	0
25	Y	494	0	530	1	0
26	Z	434	0	477	0	0
27	0	434	0	448	2	0
28	1	417	0	451	2	0
29	2	367	0	405	3	0
30	3	504	0	574	0	0
31	4	302	0	343	0	0
32	5	988	0	1025	7	0
33	6	522	0	524	0	0
34	a	33095	0	16676	386	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1164	0	1212	7	0
39	f	817	0	808	4	0
40	g	1181	0	1240	2	0
41	h	979	0	1034	3	0
42	i	1022	0	1070	16	0
43	j	786	0	828	7	0
44	k	869	0	878	2	0
45	l	940	0	1001	5	0
46	m	891	0	955	2	0
47	n	810	0	852	0	0
48	o	714	0	736	8	0
49	p	649	0	666	1	0
50	q	648	0	691	2	0
51	r	535	0	552	3	0
52	s	637	0	665	4	0
53	t	665	0	714	6	0
54	u	544	0	579	7	0
55	v	1644	0	840	4	0
55	w	1644	0	841	16	0
56	x	252	0	130	38	0
57	y	1632	0	843	127	0
58	z	3031	0	3052	13	0
59	A	10	0	10	0	0
60	0	1	0	0	0	0
60	2	1	0	0	0	0
60	4	1	0	0	0	0
60	A	965	0	0	0	0
60	B	27	0	0	0	0
60	C	2	0	0	0	0
60	D	3	0	0	0	0
60	E	3	0	0	0	0
60	H	1	0	0	0	0
60	L	3	0	0	0	0
60	N	1	0	0	0	0
60	Q	1	0	0	0	0
60	S	1	0	0	0	0
60	U	1	0	0	0	0
60	X	1	0	0	0	0
60	Y	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	375	0	0	0	0
60	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	f	1	0	0	0	0
60	g	1	0	0	0	0
60	i	2	0	0	0	0
60	k	1	0	0	0	0
60	l	1	0	0	0	0
60	m	1	0	0	0	0
60	q	1	0	0	0	0
60	v	9	0	0	0	0
60	w	3	0	0	0	0
60	x	1	0	0	0	0
61	A	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	2	1	0	0	0	0
64	3	1	0	0	0	0
64	A	293	0	0	0	0
64	B	8	0	0	0	0
64	C	3	0	0	0	0
64	D	3	0	0	0	0
64	L	1	0	0	0	0
64	N	1	0	0	0	0
64	O	1	0	0	0	0
64	Q	1	0	0	0	0
64	V	1	0	0	0	0
64	W	1	0	0	0	0
64	a	93	0	0	0	0
64	l	1	0	0	0	0
64	m	1	0	0	0	0
64	o	1	0	0	0	0
64	s	3	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	v	1	0	0	0	0
64	w	1	0	0	0	0
All	All	154325	0	103565	929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (929) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:117:U:O3'	55:w:18:G:P	1.14	1.54
57:y:25:C:C2'	57:y:26:A:H5''	1.46	1.46
1:A:1913:A:H2'	34:a:1492[A]:A:N1	1.36	1.38
57:y:30:G:C2	57:y:31:A:N6	1.90	1.37
57:y:41:C:H2'	57:y:42:C:O4'	1.20	1.36
57:y:41:C:C4	57:y:42:C:C5	2.13	1.35
57:y:25:C:H2'	57:y:26:A:C5'	1.58	1.33
34:a:511:C:O2	34:a:541:G:N2	1.63	1.30
55:w:117:U:HO3'	55:w:18:G:P	1.03	1.29
57:y:41:C:N4	57:y:42:C:N4	1.80	1.28
1:A:1913:A:C2'	34:a:1492[A]:A:N1	1.97	1.27
34:a:1410:A:C6	34:a:1491:G:C6	2.22	1.26
56:x:20:U:H5	56:x:21:C:N4	1.35	1.25
57:y:41:C:C4	57:y:42:C:C4	2.22	1.25
56:x:20:U:C5	56:x:21:C:C4	2.25	1.24
1:A:2013:A:N1	1:A:2613:U:O4	1.69	1.24
42:i:129:ARG:O	55:v:35:A:OP1	1.53	1.22
1:A:1913:A:H2'	34:a:1492[A]:A:C6	1.74	1.22
34:a:539:A:N6	34:a:540:G:C2	2.07	1.22
56:x:20:U:C5	56:x:21:C:N4	2.07	1.22
34:a:502:A:N1	34:a:544:G:N3	1.88	1.19
43:j:88:MET:O	43:j:90:LEU:N	1.76	1.19
57:y:41:C:N3	57:y:42:C:C4	2.12	1.18
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.14
34:a:511:C:C2	34:a:541:G:N2	2.16	1.12
34:a:1490:U:H2'	34:a:1491:G:H5''	1.31	1.11
34:a:374:A:N1	34:a:391:G:H1'	1.65	1.10
48:o:44:GLU:HG2	48:o:45:HIS:HD2	1.12	1.10
57:y:25:C:N3	57:y:26:A:C8	2.20	1.08
57:y:41:C:C2	57:y:42:C:C6	2.40	1.08
57:y:41:C:H2'	57:y:42:C:C1'	1.83	1.08
34:a:539:A:N6	34:a:540:G:N1	2.02	1.08
57:y:27:G:N1	57:y:45:U:O4	1.86	1.08
1:A:1916:A:N6	34:a:1408:A:O3'	1.87	1.07
57:y:41:C:C2'	57:y:42:C:O4'	2.03	1.07
34:a:1493:A:H2	56:x:20:U:H1'	1.07	1.07
57:y:27:G:N2	57:y:45:U:C4	2.23	1.06
57:y:30:G:N2	57:y:31:A:H61	1.51	1.06
57:y:41:C:C5	57:y:42:C:C5	2.43	1.06
57:y:31:A:C2	57:y:40:C:O2	2.08	1.05
57:y:31:A:H2	57:y:40:C:O2	1.35	1.05
34:a:1493:A:C2	56:x:20:U:H1'	1.93	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:67[B]:ARG:HG2	38:e:67[B]:ARG:HH11	1.19	1.04
57:y:25:C:C3'	57:y:26:A:H5''	1.86	1.04
1:A:2030:6MZ:OP1	1:A:2031:A:C8	2.10	1.03
57:y:25:C:C4	57:y:26:A:C8	2.45	1.03
34:a:1410:A:N6	34:a:1491:G:C6	2.26	1.02
34:a:1490:U:H2'	34:a:1491:G:C5'	1.88	1.02
11:K:110:GLU:O	11:K:112:PHE:N	1.92	1.02
55:w:117:U:C3'	55:w:18:G:P	2.47	1.02
34:a:502:A:N6	34:a:544:G:C2	2.27	1.02
55:w:117:U:O3'	55:w:18:G:OP2	1.78	1.01
34:a:502:A:N1	34:a:544:G:C2	2.29	1.00
34:a:1492[B]:A:O4'	34:a:1493:A:OP1	1.78	1.00
56:x:19:C:O2	57:y:37:MIA:H111	1.61	1.00
57:y:41:C:N3	57:y:42:C:C5	2.28	1.00
34:a:1410:A:C5	34:a:1491:G:N1	2.30	0.99
56:x:19:C:O2	57:y:37:MIA:C11	2.10	0.99
57:y:43:C:C2	57:y:45:U:C5	2.48	0.99
34:a:500:G:N2	34:a:501:C:O2	1.96	0.99
39:f:38:ARG:HG3	39:f:63:ASN:HB3	1.44	0.98
57:y:41:C:H42	57:y:42:C:N4	1.62	0.98
57:y:41:C:N4	57:y:42:C:H41	1.58	0.98
57:y:26:A:N6	57:y:45:U:H3	1.61	0.97
48:o:44:GLU:HG2	48:o:45:HIS:CD2	1.98	0.97
34:a:668:G:H21	48:o:45:HIS:HE1	1.13	0.96
57:y:26:A:N6	57:y:45:U:N3	2.12	0.96
1:A:2791:G:N2	1:A:2805:C:O2	1.99	0.96
34:a:591:U:O4	34:a:648:A:N1	1.99	0.96
56:x:22:A:C8	56:x:23:C:C5	2.54	0.95
34:a:437:U:N3	34:a:495:A:N6	2.14	0.94
1:A:2793:C:N3	1:A:2803:G:O6	2.00	0.94
34:a:1410:A:N6	34:a:1491:G:O6	2.00	0.94
1:A:1912:A:N7	1:A:1917:PSU:N3	2.16	0.92
57:y:27:G:N1	57:y:43:C:N3	2.16	0.92
34:a:1410:A:C6	34:a:1491:G:C5	2.59	0.90
57:y:27:G:N2	57:y:43:C:O2	2.05	0.90
57:y:25:C:H2'	57:y:26:A:C4'	2.02	0.90
1:A:1913:A:H2'	34:a:1492[A]:A:N6	1.84	0.90
34:a:404:G:N2	34:a:498:A:N3	2.20	0.90
57:y:27:G:C2	57:y:45:U:C4	2.59	0.89
57:y:43:C:O2	57:y:45:U:C5	2.24	0.89
34:a:58:C:N3	34:a:354:G:O6	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:17:C:H4'	55:w:117:U:OP2	1.73	0.88
34:a:1490:U:O4	34:a:1491:G:N7	2.07	0.88
57:y:25:C:H2'	57:y:26:A:H5''	0.88	0.88
42:i:45:MET:O	42:i:48:ARG:N	2.07	0.87
1:A:2030:6MZ:OP1	1:A:2031:A:H8	1.58	0.87
1:A:1913:A:O2'	34:a:1492[A]:A:N1	2.08	0.86
34:a:517:G:C6	34:a:531:U:O4'	2.28	0.86
57:y:41:C:C4	57:y:42:C:N4	2.39	0.86
34:a:502:A:N6	34:a:544:G:N2	2.23	0.86
34:a:369:G:H2'	34:a:393:A:C2	2.11	0.86
34:a:827:U:N3	34:a:872:A:N6	2.23	0.86
1:A:1912:A:C8	1:A:1918:A:C2	2.63	0.85
34:a:502:A:C6	34:a:544:G:N2	2.45	0.85
1:A:2030:6MZ:O2'	1:A:2031:A:OP2	1.93	0.85
34:a:1410:A:C5	34:a:1491:G:C6	2.65	0.85
34:a:502:A:C6	34:a:544:G:C2	2.64	0.84
57:y:28:G:N2	57:y:43:C:O2	2.10	0.84
57:y:30:G:N3	57:y:31:A:N6	2.25	0.84
57:y:41:C:C2	57:y:42:C:C5	2.65	0.84
38:e:67[B]:ARG:HH11	38:e:67[B]:ARG:CG	1.91	0.83
34:a:605:U:O2	34:a:633:G:O6	1.97	0.83
34:a:1492[B]:A:C1'	34:a:1493:A:OP1	2.25	0.83
1:A:1916:A:H5''	1:A:1916:A:H8	1.43	0.83
1:A:1916:A:H61	34:a:1408:A:C3'	1.92	0.83
34:a:437:U:C4	34:a:495:A:C6	2.67	0.83
34:a:1409:C:N4	34:a:1491:G:O6	2.12	0.83
56:x:20:U:C4	56:x:21:C:N3	2.48	0.81
57:y:31:A:C2	57:y:40:C:C2	2.67	0.81
57:y:41:C:N1	57:y:42:C:C6	2.48	0.81
56:x:20:U:C5	56:x:21:C:N3	2.49	0.81
1:A:2796:C:O2	1:A:2801:G:N2	2.13	0.81
1:A:1048:A:N1	1:A:1111:A:C6	2.49	0.80
56:x:20:U:H5	56:x:21:C:H42	1.28	0.80
1:A:2805:C:H2'	1:A:2806:C:O4'	1.81	0.80
39:f:38:ARG:CG	39:f:63:ASN:HB3	2.12	0.80
1:A:2028:U:H2'	1:A:2029:G:C8	2.17	0.80
34:a:539:A:C6	34:a:540:G:C2	2.70	0.80
57:y:41:C:N4	57:y:42:C:C4	2.41	0.79
34:a:142:G:H22	34:a:222:C:H1'	1.48	0.79
34:a:1410:A:C4	34:a:1491:G:C2	2.70	0.79
34:a:437:U:C4	34:a:495:A:N6	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2013:A:N1	1:A:2613:U:C4	2.52	0.78
57:y:43:C:O2	57:y:45:U:C4	2.27	0.78
57:y:41:C:C5	57:y:42:C:H5	1.98	0.78
57:y:25:C:N4	57:y:26:A:N7	2.30	0.78
34:a:827:U:C4	34:a:872:A:N6	2.52	0.78
34:a:1495:U:O2'	34:a:1496:C:H5'	1.84	0.77
11:K:110:GLU:O	11:K:113:MET:N	2.17	0.77
34:a:500:G:O4'	34:a:547:A:N6	2.17	0.77
55:w:117:U:C3'	55:w:18:G:OP2	2.32	0.77
57:y:25:C:C4	57:y:26:A:H8	2.04	0.76
57:y:31:A:H2	57:y:40:C:C2	2.03	0.76
56:x:22:A:N7	56:x:23:C:C5	2.52	0.76
34:a:500:G:N2	34:a:501:C:C2	2.53	0.76
4:D:153:GLY:O	4:D:154:LYS:HB3	1.85	0.75
53:t:8:LYS:O	53:t:11:ILE:HG12	1.85	0.75
34:a:501:C:C2	34:a:502:A:N7	2.55	0.75
57:y:41:C:C2	57:y:42:C:N1	2.54	0.75
34:a:1410:A:N1	34:a:1491:G:C5	2.55	0.75
56:x:19:C:H2'	57:y:37:MIA:H111	1.68	0.75
34:a:437:U:N3	34:a:495:A:C6	2.54	0.75
57:y:25:C:C2	57:y:26:A:O4'	2.40	0.75
48:o:44:GLU:O	48:o:46:LYS:N	2.19	0.74
34:a:539:A:H61	34:a:540:G:N2	1.85	0.74
57:y:27:G:C2	57:y:45:U:O4	2.38	0.74
57:y:30:G:N2	57:y:31:A:N6	2.20	0.74
1:A:2795:C:N3	1:A:2801:G:O6	2.20	0.74
34:a:74:A:C2	34:a:97:G:N2	2.56	0.74
57:y:32:PSU:H2'	57:y:33:U:C4	2.23	0.74
57:y:43:C:C2	57:y:45:U:H5	2.06	0.73
1:A:2013:A:C2	1:A:2613:U:O4	2.41	0.73
34:a:500:G:C2	34:a:501:C:C2	2.76	0.73
34:a:223:A:C2	34:a:224:U:C4	2.76	0.73
48:o:44:GLU:CG	48:o:45:HIS:HD2	1.97	0.73
34:a:437:U:O4	34:a:495:A:C5	2.41	0.72
1:A:2028:U:C4	1:A:2029:G:C6	2.77	0.72
34:a:1409:C:N3	34:a:1491:G:N1	2.38	0.72
57:y:41:C:C6	57:y:42:C:C5	2.77	0.72
34:a:149:A:O2'	34:a:1446:A:N3	2.22	0.72
34:a:145:G:N1	34:a:177:G:O6	2.18	0.72
34:a:246:A:N1	34:a:278:G:O2'	2.23	0.72
34:a:367:U:H5	34:a:394:G:N3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:G:N7	1:A:352:A:N1	2.38	0.72
42:i:45:MET:O	42:i:47:VAL:N	2.23	0.72
58:z:220:ILE:HD12	58:z:226:VAL:HG21	1.71	0.72
57:y:25:C:O2	57:y:26:A:O4'	2.08	0.71
34:a:511:C:H5	34:a:534:U:HO2'	1.37	0.71
34:a:530[A]:G:H2'	34:a:530[A]:G:N3	2.04	0.71
1:A:2030:6MZ:O2'	1:A:2031:A:P	2.48	0.71
42:i:129:ARG:O	55:v:35:A:P	2.48	0.71
57:y:29:G:H3'	57:y:30:G:H5''	1.73	0.70
57:y:25:C:C3'	57:y:26:A:C5'	2.68	0.70
34:a:1256:A:N6	34:a:1278:G:O4'	2.24	0.70
57:y:32:PSU:H2'	57:y:33:U:N3	2.06	0.70
34:a:1256:A:N6	34:a:1279:G:N2	2.39	0.70
34:a:141:G:H1'	34:a:142:G:C8	2.27	0.69
57:y:31:A:N1	57:y:40:C:N3	2.39	0.69
42:i:128:LYS:O	42:i:129:ARG:HB2	1.92	0.69
55:w:17:C:H6	55:w:17:C:C5'	2.04	0.69
56:x:20:U:C6	56:x:21:C:C4	2.79	0.69
34:a:512:U:OP1	37:d:43:ARG:NH2	2.25	0.69
1:A:1528:A:N6	1:A:1543:G:O2'	2.26	0.69
34:a:515:G:O6	34:a:517:G:N1	2.26	0.69
1:A:1048:A:N7	1:A:1049:C:C5	2.61	0.69
34:a:511:C:H5	34:a:534:U:O2'	1.76	0.69
55:w:16:C:H5''	55:w:17:C:OP2	1.92	0.69
1:A:1479:G:O2'	1:A:1560:G:O2'	2.12	0.68
34:a:29:U:O4	34:a:554:A:N1	2.26	0.68
34:a:66:A:O4'	34:a:173:U:N3	2.27	0.68
34:a:374:A:N1	34:a:391:G:C1'	2.53	0.68
34:a:827:U:N3	34:a:872:A:C6	2.60	0.68
53:t:11:ILE:HG13	53:t:12:GLN:N	2.08	0.68
38:e:67[B]:ARG:HG2	38:e:67[B]:ARG:NH1	2.01	0.68
34:a:406:G:C2	34:a:495:A:N6	2.61	0.68
34:a:1492[B]:A:H4'	34:a:1492[B]:A:OP2	1.92	0.68
34:a:148:G:N2	34:a:1446:A:C2	2.61	0.67
1:A:1913:A:H2'	34:a:1492[A]:A:H61	1.58	0.67
1:A:1916:A:OP1	1:A:1916:A:H4'	1.93	0.67
1:A:2030:6MZ:HA	1:A:2031:A:P	2.16	0.67
34:a:512:U:C4	34:a:540:G:N2	2.62	0.67
34:a:1256:A:O4'	34:a:1258:G:H1'	1.93	0.67
34:a:1495:U:O2'	34:a:1496:C:C5'	2.42	0.67
57:y:37:MIA:H132	57:y:37:MIA:N7	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:543:U:N3	34:a:544:G:N3	2.34	0.67
57:y:37:MIA:C5	57:y:37:MIA:H153	2.25	0.66
34:a:1408:A:C4	34:a:1494:G:N2	2.64	0.66
55:w:117:U:H3'	55:w:18:G:OP2	1.96	0.66
42:i:45:MET:O	42:i:46:VAL:C	2.37	0.66
56:x:22:A:O2'	56:x:23:C:H5'	1.94	0.66
57:y:28:G:C2	57:y:43:C:O2	2.48	0.66
56:x:20:U:C2	57:y:35:A:N1	2.63	0.66
1:A:2013:A:N6	1:A:2613:U:N3	2.43	0.66
34:a:378:G:N2	34:a:386:C:O2	2.27	0.66
34:a:141:G:H1'	34:a:142:G:H8	1.60	0.66
34:a:668:G:H21	48:o:45:HIS:CE1	2.04	0.66
57:y:25:C:C2'	57:y:26:A:C5'	2.36	0.66
1:A:2795:C:O2	1:A:2801:G:N1	2.28	0.65
55:w:17:C:C4'	55:w:117:U:OP2	2.44	0.65
57:y:25:C:N3	57:y:26:A:H8	1.90	0.65
57:y:39:PSU:H3'	57:y:40:C:C5	2.31	0.65
34:a:1241:G:H2'	34:a:1242:G:C8	2.31	0.65
34:a:1492[B]:A:H2	56:x:20:U:HO2'	1.42	0.65
46:m:15:VAL:HG23	46:m:16:ILE:HD12	1.78	0.65
34:a:532:A:N6	34:a:1206:G:O2'	2.30	0.65
57:y:30:G:C2	57:y:31:A:C6	2.84	0.65
57:y:26:A:N6	57:y:45:U:C4	2.61	0.65
34:a:369:G:N2	34:a:393:A:N7	2.45	0.64
57:y:39:PSU:C3'	57:y:40:C:C6	2.80	0.64
34:a:367:U:H5	34:a:394:G:C4	2.16	0.64
34:a:1258:G:H2'	34:a:1259:C:C6	2.32	0.64
53:t:11:ILE:CG1	53:t:12:GLN:N	2.60	0.64
34:a:515:G:O2'	34:a:537:G:N1	2.30	0.64
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.79	0.64
1:A:286:U:C2	1:A:354:A:N6	2.66	0.64
1:A:2013:A:N6	1:A:2613:U:H3	1.95	0.64
11:K:110:GLU:CG	11:K:111:LYS:N	2.57	0.64
57:y:26:A:N1	57:y:45:U:O2	2.31	0.64
34:a:223:A:H2'	34:a:224:U:C6	2.33	0.64
34:a:500:G:C2	34:a:501:C:N3	2.66	0.64
34:a:392:C:H2'	34:a:393:A:C8	2.33	0.64
57:y:39:PSU:C3'	57:y:40:C:H6	2.11	0.64
34:a:223:A:C2	34:a:224:U:N3	2.66	0.63
34:a:1490:U:C4	34:a:1491:G:N7	2.66	0.63
1:A:160:A:N3	1:A:2208:C:O2'	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:500:G:C8	34:a:500:G:H5''	2.33	0.63
57:y:39:PSU:H3'	57:y:40:C:C6	2.34	0.63
1:A:1914:C:OP2	34:a:1492[A]:A:N6	2.32	0.63
23:W:71:LYS:HB2	23:W:73:ARG:HG3	1.80	0.63
34:a:509:A:N7	34:a:510:A:C6	2.67	0.62
34:a:367:U:C5	34:a:394:G:N3	2.67	0.62
34:a:1490:U:C4	34:a:1491:G:C8	2.86	0.62
1:A:287:G:O4'	1:A:354:A:C6	2.52	0.62
55:w:17:C:H6	55:w:17:C:H5''	1.64	0.62
34:a:97:G:H2'	34:a:98:A:O4'	2.00	0.62
34:a:437:U:C2	34:a:495:A:N6	2.67	0.62
34:a:1243:C:N3	34:a:1294:G:O6	2.33	0.62
57:y:41:C:C6	57:y:42:C:C6	2.86	0.62
1:A:803:U:H2'	1:A:804:A:H5'	1.81	0.62
11:K:110:GLU:HG3	11:K:111:LYS:N	2.15	0.62
34:a:1410:A:C5	34:a:1491:G:C2	2.88	0.62
42:i:94:ARG:O	42:i:98:ARG:HB2	1.99	0.62
34:a:369:G:C2	34:a:393:A:C5	2.88	0.62
34:a:633:G:H2'	34:a:634:C:O4'	2.00	0.61
1:A:686:U:O4	29:2:12:ARG:HG2	2.00	0.61
34:a:73:C:H2'	34:a:74:A:C8	2.35	0.61
53:t:11:ILE:CG1	53:t:12:GLN:H	2.12	0.61
1:A:1048:A:C2	1:A:1111:A:C6	2.88	0.61
34:a:1494:G:O5'	34:a:1494:G:H8	1.84	0.61
57:y:27:G:C2	57:y:45:U:N3	2.67	0.61
1:A:1028:A:N3	1:A:2486:C:O2'	2.26	0.61
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.83	0.61
11:K:110:GLU:CG	11:K:111:LYS:H	2.14	0.61
1:A:585:G:N7	17:Q:5:ARG:NH1	2.49	0.61
34:a:372:C:N4	34:a:389:A:N7	2.49	0.61
34:a:17:U:H2'	34:a:18:C:C6	2.36	0.60
50:q:63:CYS:SG	50:q:64:ARG:N	2.73	0.60
57:y:41:C:N3	57:y:42:C:N3	2.48	0.60
34:a:369:G:N2	34:a:393:A:C5	2.68	0.60
34:a:1492[B]:A:H1'	34:a:1493:A:OP1	2.00	0.60
1:A:1688:U:O2'	1:A:1700:A:N7	2.32	0.60
1:A:2030:6MZ:OP1	1:A:2031:A:N7	2.34	0.60
34:a:515:G:O2'	34:a:516:PSU:OP1	2.16	0.60
56:x:20:U:H4'	56:x:20:U:OP1	2.00	0.60
34:a:500:G:N1	34:a:501:C:N3	2.50	0.60
34:a:515:G:H3'	34:a:515:G:N3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:G:N2	1:A:1452:G:O6	2.35	0.60
34:a:1490:U:C2'	34:a:1491:G:C5'	2.74	0.60
43:j:88:MET:C	43:j:90:LEU:H	1.97	0.60
1:A:1048:A:C8	1:A:1049:C:C5	2.89	0.60
34:a:223:A:H2'	34:a:224:U:H6	1.66	0.60
34:a:1410:A:C6	34:a:1491:G:N1	2.62	0.60
38:e:67[B]:ARG:CG	38:e:67[B]:ARG:NH1	2.55	0.60
34:a:946:A:O2'	34:a:1333:A:N3	2.31	0.59
1:A:290:U:C2	1:A:291:G:C8	2.90	0.59
1:A:49:A:N6	1:A:177:G:H2'	2.17	0.59
1:A:51:G:O2'	1:A:52:A:OP2	2.14	0.59
34:a:515:G:N1	34:a:517:G:C6	2.68	0.59
34:a:1490:U:H2'	34:a:1491:G:O5'	2.02	0.59
34:a:437:U:O4	34:a:495:A:C6	2.55	0.59
57:y:25:C:H3'	57:y:26:A:H5''	1.83	0.59
34:a:142:G:N2	34:a:222:C:H1'	2.15	0.59
34:a:530[A]:G:N3	34:a:530[A]:G:C2'	2.65	0.59
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.83	0.59
1:A:2030:6MZ:OP1	1:A:2030:6MZ:H4'	2.01	0.59
1:A:2791:G:N1	1:A:2805:C:N3	2.44	0.59
11:K:110:GLU:C	11:K:112:PHE:N	2.61	0.59
57:y:41:C:H2'	57:y:42:C:C6	2.37	0.59
1:A:1466:U:O2'	1:A:1546:G:O2'	2.17	0.59
57:y:41:C:O5'	57:y:41:C:H6	1.85	0.59
57:y:31:A:N1	57:y:40:C:C2	2.71	0.59
1:A:1916:A:H5''	1:A:1916:A:C8	2.32	0.58
34:a:129:A:N1	34:a:232:G:C6	2.70	0.58
43:j:88:MET:C	43:j:90:LEU:N	2.60	0.58
11:K:110:GLU:O	11:K:111:LYS:C	2.45	0.58
34:a:222:C:O2	34:a:222:C:H2'	2.02	0.58
34:a:1410:A:C2	34:a:1491:G:C4	2.91	0.58
57:y:28:G:O5'	57:y:28:G:H8	1.85	0.58
1:A:1916:A:N1	34:a:1409:C:C5'	2.67	0.58
57:y:41:C:C2	57:y:42:C:C2	2.92	0.58
34:a:513:C:H2'	34:a:514:C:C6	2.39	0.58
1:A:2334:U:O3'	15:O:13:ARG:NH1	2.37	0.58
57:y:25:C:N4	57:y:26:A:C8	2.68	0.58
5:E:46:GLN:HB3	5:E:83:VAL:HG11	1.86	0.58
34:a:369:G:C2	34:a:393:A:C6	2.92	0.57
34:a:502:A:H61	34:a:544:G:N2	1.91	0.57
1:A:749:A:C8	1:A:1618:6MZ:N6	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:C:O2'	1:A:1809:A:N3	2.36	0.57
34:a:539:A:N6	34:a:540:G:C6	2.73	0.57
1:A:1107:G:OP1	32:5:59:LEU:N	2.37	0.57
34:a:500:G:H1'	34:a:547:A:N7	2.18	0.57
34:a:1492[B]:A:C4'	34:a:1493:A:OP1	2.50	0.57
48:o:46:LYS:HG2	48:o:52:ARG:HH22	1.69	0.57
57:y:18:G:O2'	57:y:57:G:N2	2.38	0.57
57:y:42:C:H5'	57:y:43:C:OP2	2.04	0.57
34:a:367:U:C5	34:a:394:G:C2	2.93	0.57
56:x:22:A:C8	56:x:23:C:H5	2.21	0.57
57:y:34:G:N3	57:y:34:G:H2'	2.20	0.57
34:a:125:U:O3'	34:a:633:G:N2	2.38	0.57
54:u:32:ARG:HD3	54:u:33:ARG:HD3	1.86	0.57
43:j:57:VAL:HG12	43:j:58:ASN:H	1.70	0.57
1:A:1271:G:O2'	1:A:1618:6MZ:H8	2.04	0.57
34:a:37:U:H2'	34:a:38:G:O4'	2.05	0.57
34:a:46:G:O2'	34:a:365:U:H1'	2.05	0.57
34:a:1300:G:N2	34:a:1301:U:O4	2.20	0.57
1:A:465:G:H2'	1:A:466:A:C8	2.40	0.56
34:a:441:A:C2	34:a:497:G:C5	2.93	0.56
34:a:515:G:O6	34:a:517:G:C6	2.58	0.56
34:a:354:G:H21	34:a:388:G:C2'	2.18	0.56
34:a:553:A:H2'	34:a:554:A:C8	2.40	0.56
57:y:26:A:N1	57:y:45:U:C2	2.73	0.56
34:a:827:U:N3	34:a:874:G:C2	2.73	0.56
34:a:354:G:N2	34:a:388:G:O2'	2.34	0.56
40:g:107:ALA:HB1	40:g:115:MET:HE1	1.87	0.56
42:i:44:ARG:O	42:i:47:VAL:HG22	2.05	0.56
1:A:23:G:OP1	1:A:504:A:N6	2.39	0.55
1:A:749:A:O2'	1:A:1618:6MZ:OP1	2.13	0.55
54:u:9:GLU:HB2	54:u:10:PRO:CD	2.36	0.55
34:a:675:A:H2'	34:a:676:A:O4'	2.06	0.55
1:A:1061:U:H2'	1:A:1061:U:O2	2.07	0.55
34:a:590:U:C1'	34:a:650:G:N2	2.70	0.55
56:x:19:C:C2'	57:y:37:MIA:H111	2.33	0.55
56:x:20:U:O2	57:y:35:A:N1	2.40	0.55
34:a:75:G:N2	34:a:96:U:C4	2.75	0.55
34:a:369:G:H2'	34:a:393:A:H2	1.70	0.55
34:a:502:A:C6	34:a:544:G:N3	2.70	0.55
34:a:1410:A:N1	34:a:1491:G:C4	2.75	0.55
1:A:1063:G:N2	9:I:134:SER:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1218:C:H2'	34:a:1219:A:C8	2.42	0.55
1:A:1912:A:C8	1:A:1918:A:N1	2.74	0.55
34:a:72:A:N7	34:a:73:C:C5	2.75	0.55
55:w:17:C:H5''	55:w:17:C:C6	2.41	0.55
34:a:437:U:H2'	34:a:437:U:O2	2.07	0.54
34:a:544:G:H2'	34:a:545:C:O4'	2.06	0.54
34:a:864:A:H2'	34:a:865:A:C8	2.41	0.54
34:a:976:G:C8	34:a:1358:U:O2	2.60	0.54
34:a:1127:G:H1'	34:a:1280:A:C6	2.42	0.54
38:e:93:VAL:HG13	38:e:110:MET:HE3	1.88	0.54
1:A:12:U:H2'	1:A:12:U:O2	2.08	0.54
1:A:49:A:H61	1:A:177:G:H2'	1.72	0.54
2:B:78:A:OP2	22:V:18:ARG:NH2	2.40	0.54
16:P:59:THR:HG22	16:P:72:VAL:HG22	1.89	0.54
1:A:1181:U:H2'	1:A:1182:G:C8	2.42	0.54
1:A:517:C:OP1	27:0:12:ARG:NH2	2.40	0.54
34:a:1235:U:H2'	34:a:1236:A:O4'	2.06	0.54
1:A:2838:G:H2'	1:A:2839:G:O4'	2.08	0.54
34:a:1256:A:N6	34:a:1279:G:C2	2.74	0.54
1:A:51:G:HO2'	1:A:119:A:H61	1.56	0.54
1:A:636:G:H3'	12:L:128:THR:HG21	1.90	0.54
1:A:2370:G:H1'	28:1:43:ARG:HH12	1.72	0.54
34:a:129:A:C2	34:a:233:C:O2	2.61	0.54
34:a:171:A:H2'	34:a:172:A:C8	2.43	0.54
57:y:37:MIA:H153	57:y:37:MIA:C6	2.37	0.54
1:A:1106:G:N3	32:5:81:LEU:HD12	2.23	0.54
34:a:59:A:H1'	34:a:354:G:C2	2.43	0.54
34:a:440:C:N4	34:a:497:G:N1	2.56	0.54
57:y:33:U:H3'	57:y:33:U:H6	1.73	0.54
56:x:19:C:O2	56:x:19:C:H2'	2.07	0.54
57:y:42:C:H2'	57:y:42:C:O2	2.08	0.54
1:A:2572:A:P	4:D:151:THR:HG1	2.31	0.53
1:A:2734:A:C3'	1:A:2735:G:H5'	2.39	0.53
34:a:57:G:H2'	34:a:58:C:O4'	2.07	0.53
34:a:362:G:OP1	45:l:57:THR:OG1	2.26	0.53
34:a:141:G:N2	34:a:223:A:C8	2.74	0.53
34:a:203:G:N2	34:a:204:G:O6	2.41	0.53
51:r:10:CYS:SG	51:r:11:ARG:N	2.76	0.53
57:y:40:C:O2	57:y:40:C:H2'	2.08	0.53
1:A:1466:U:HO2'	1:A:1546:G:HO2'	1.55	0.53
34:a:503:C:O2'	34:a:504:C:O4'	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:x:20:U:O2	57:y:35:A:C2	2.61	0.53
57:y:31:A:O5'	57:y:31:A:H8	1.92	0.53
34:a:129:A:N1	34:a:233:C:C2	2.76	0.53
34:a:541:G:H2'	34:a:542:G:O4'	2.09	0.53
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.38	0.53
34:a:539:A:C6	34:a:540:G:N3	2.75	0.53
34:a:1162:C:H2'	34:a:1163:A:C8	2.44	0.53
57:y:30:G:N2	57:y:31:A:C6	2.76	0.53
1:A:1618:6MZ:H2'	1:A:1618:6MZ:N3	2.23	0.53
1:A:1809:A:H2'	1:A:1810:A:C8	2.44	0.53
1:A:1916:A:N1	34:a:1409:C:H5'	2.24	0.53
1:A:2038:G:H2'	1:A:2039:U:O4'	2.09	0.53
56:x:19:C:H1'	57:y:37:MIA:H112	1.91	0.52
1:A:2796:C:O2	1:A:2801:G:C2	2.61	0.52
10:J:35:ARG:HB2	10:J:54:ILE:HD11	1.91	0.52
34:a:55:A:C2	58:z:222:GLY:HA2	2.44	0.52
34:a:126:G:OP1	34:a:605:U:O2'	2.27	0.52
34:a:129:A:C2	34:a:233:C:C2	2.97	0.52
34:a:175:C:H2'	34:a:176:C:C6	2.44	0.52
34:a:778:G:H2'	34:a:779:C:O4'	2.10	0.52
34:a:71:A:N1	34:a:94:G:O6	2.42	0.52
56:x:19:C:O2	57:y:37:MIA:H113	2.04	0.52
57:y:39:PSU:O3'	57:y:40:C:H6	1.93	0.52
1:A:1430:G:H2'	1:A:1431:A:O4'	2.09	0.52
34:a:499:A:O2'	34:a:547:A:N6	2.43	0.52
34:a:517:G:C5	34:a:531:U:O4'	2.61	0.52
1:A:1721:G:O2'	1:A:1739:A:N6	2.43	0.52
1:A:1642:G:H2'	1:A:1643:G:O4'	2.09	0.52
1:A:2327:A:H2'	1:A:2328:A:C8	2.45	0.52
1:A:2794:U:C2	1:A:2803:G:C2	2.98	0.52
34:a:55:A:H2	58:z:222:GLY:HA2	1.75	0.52
1:A:1595:C:H2'	1:A:1596:A:O4'	2.10	0.52
34:a:175:C:O2'	34:a:1447:A:N1	2.41	0.52
34:a:543:U:C5	34:a:544:G:N1	2.64	0.52
1:A:1737:G:H2'	1:A:1738:G:H1'	1.93	0.51
1:A:1912:A:C8	1:A:1917:PSU:O2	2.63	0.51
34:a:533:A:N3	34:a:535:A:OP2	2.44	0.51
1:A:157:C:C4	1:A:169:G:C6	2.99	0.51
1:A:286:U:O2	1:A:354:A:C6	2.64	0.51
32:5:59:LEU:O	32:5:61:ARG:N	2.43	0.51
34:a:1250:A:N1	34:a:1353:G:N2	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:C:H2'	1:A:1050:A:H5'	1.91	0.51
34:a:651:C:H3'	34:a:652:U:C6	2.46	0.51
1:A:1447:C:O2'	1:A:1544:A:N3	2.36	0.51
1:A:348:A:H2'	1:A:349:U:O4'	2.10	0.51
1:A:2793:C:C4	1:A:2803:G:O6	2.63	0.51
55:w:17:C:C5'	55:w:17:C:C6	2.91	0.51
1:A:2405:G:O2'	1:A:2412:A:N6	2.44	0.51
11:K:110:GLU:C	11:K:112:PHE:H	2.19	0.51
34:a:1244:G:N1	34:a:1293:C:N4	2.59	0.51
56:x:21:C:O5'	56:x:21:C:H6	1.94	0.51
57:y:30:G:N3	57:y:31:A:C6	2.79	0.51
1:A:1048:A:C2	1:A:1111:A:N1	2.79	0.51
1:A:1111:A:C2	1:A:1112:G:H1'	2.45	0.51
1:A:1912:A:N7	1:A:1917:PSU:C2	2.79	0.51
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.92	0.51
1:A:914:G:N3	1:A:914:G:H3'	2.26	0.51
34:a:167:A:H2'	34:a:168:G:O4'	2.10	0.51
34:a:1397:C:N4	56:x:22:A:OP2	2.43	0.51
1:A:774:G:O2'	1:A:775:G:O5'	2.29	0.50
1:A:1737:G:H2'	1:A:1738:G:C1'	2.41	0.50
34:a:129:A:C6	34:a:232:G:O6	2.64	0.50
34:a:440:C:N3	34:a:497:G:N2	2.59	0.50
34:a:223:A:N3	34:a:224:U:C6	2.80	0.50
34:a:1456:A:H2'	34:a:1457:G:O4'	2.11	0.50
1:A:1050:A:H2'	1:A:1051:G:O4'	2.11	0.50
51:r:72:ARG:C	51:r:72:ARG:HD3	2.37	0.50
1:A:2029:G:O5'	1:A:2029:G:H8	1.94	0.50
19:S:5:ALA:HB3	19:S:54:ALA:HB2	1.94	0.50
34:a:876:C:H1'	41:h:11:THR:HG21	1.91	0.50
1:A:287:G:O4'	1:A:354:A:N1	2.45	0.50
1:A:1702:G:N2	34:a:1428:A:O2'	2.45	0.50
34:a:180:U:O2	34:a:195:A:N7	2.45	0.50
34:a:518:C:O4'	34:a:518:C:O2	2.28	0.50
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.76	0.50
34:a:29:U:O4	34:a:554:A:C6	2.64	0.50
34:a:223:A:C2	34:a:224:U:C2	3.00	0.50
34:a:246:A:H4'	34:a:247:G:OP1	2.11	0.50
40:g:76:SER:HB2	55:w:33:U:H5'	1.94	0.50
34:a:437:U:C4	34:a:495:A:C5	2.99	0.50
34:a:606:G:C6	34:a:631:C:N4	2.80	0.50
34:a:946:A:H2'	34:a:947:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:543:U:C5	34:a:544:G:C6	3.00	0.49
1:A:1062:G:N2	9:I:131:THR:O	2.46	0.49
1:A:82:U:O2	1:A:82:U:O4'	2.29	0.49
34:a:45:G:C2	34:a:398:U:O4	2.64	0.49
34:a:827:U:C2	34:a:874:G:N2	2.81	0.49
1:A:1059:G:H1'	9:I:116:MET:HE1	1.94	0.49
34:a:127:G:O6	34:a:234:C:N3	2.45	0.49
34:a:537:G:H2'	34:a:538:G:C8	2.47	0.49
34:a:1255:G:C5	34:a:1279:G:C2	3.00	0.49
34:a:1409:C:N3	34:a:1491:G:C6	2.81	0.49
34:a:1498:UR3:H3U2	56:x:17:U:H4'	1.95	0.49
57:y:27:G:N2	57:y:45:U:N3	2.57	0.49
57:y:30:G:N1	57:y:31:A:N6	2.54	0.49
1:A:283:G:N2	1:A:359:G:N2	2.60	0.49
34:a:242:G:C2	34:a:245:U:C4	3.00	0.49
34:a:1244:G:H2'	34:a:1245:C:C6	2.48	0.49
34:a:1490:U:C2'	34:a:1491:G:O5'	2.60	0.49
1:A:287:G:C4	1:A:354:A:N6	2.81	0.49
1:A:370:G:O6	1:A:424:G:C5	2.66	0.49
1:A:1548:A:H2'	1:A:1549:A:C8	2.48	0.49
34:a:317:U:C2	34:a:337:G:N2	2.81	0.49
34:a:694:A:O2'	55:w:38:A:O2'	2.09	0.49
41:h:77:VAL:HG11	41:h:124:ILE:HD12	1.95	0.49
18:R:51:VAL:HG12	18:R:52:PRO:HD3	1.95	0.49
34:a:1256:A:O4'	34:a:1258:G:C1'	2.58	0.49
53:t:11:ILE:HG13	53:t:12:GLN:H	1.73	0.49
34:a:1244:G:C6	34:a:1293:C:N4	2.81	0.49
1:A:1182:G:H2'	1:A:1183:U:O4'	2.13	0.49
1:A:2020:A:N7	27:0:5:ASN:ND2	2.60	0.49
34:a:509:A:N7	34:a:510:A:C5	2.81	0.49
44:k:88:PRO:HG3	54:u:28:LEU:HD23	1.95	0.49
1:A:1509:A:H2'	1:A:1510:G:C8	2.48	0.48
1:A:1874:C:H2'	1:A:1875:G:O4'	2.12	0.48
57:y:41:C:C2'	57:y:42:C:C1'	2.75	0.48
13:M:50:ARG:HD3	13:M:65:ILE:HD11	1.95	0.48
34:a:43:C:H2'	34:a:44:A:O4'	2.13	0.48
1:A:309:A:N3	1:A:329:G:O2'	2.43	0.48
1:A:1615:C:C6	1:A:1617:C:C5	3.00	0.48
1:A:2028:U:C2'	1:A:2029:G:C8	2.93	0.48
56:x:22:A:N7	56:x:23:C:C4	2.81	0.48
57:y:25:C:C2	57:y:26:A:C8	2.99	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:A:N7	1:A:1049:C:H5	2.09	0.48
1:A:2788:C:H2'	1:A:2789:C:C6	2.48	0.48
1:A:2794:U:O2	1:A:2803:G:N2	2.47	0.48
11:K:19:VAL:HB	11:K:41:ILE:HG23	1.95	0.48
56:x:20:U:H3	57:y:35:A:N6	2.11	0.48
57:y:27:G:O6	57:y:43:C:N4	2.45	0.48
1:A:2514:U:H2'	1:A:2515:C:C6	2.49	0.48
1:A:1919:A:N1	34:a:1495:U:O2'	2.39	0.48
34:a:65:A:H2'	34:a:381:C:N4	2.29	0.48
34:a:408:A:C6	34:a:409:U:C4	3.02	0.48
36:c:63:ILE:HD13	36:c:94:ALA:HB1	1.95	0.48
1:A:282:A:C6	1:A:359:G:N2	2.81	0.48
1:A:2028:U:H2'	1:A:2029:G:H8	1.74	0.48
34:a:1292:G:C6	34:a:1293:C:N4	2.82	0.48
42:i:45:MET:C	42:i:47:VAL:N	2.72	0.48
34:a:55:A:C2	58:z:222:GLY:CA	2.97	0.48
34:a:110:C:O2'	49:p:25:ARG:O	2.28	0.48
34:a:401:C:H2'	34:a:402:G:C8	2.48	0.48
34:a:868:C:H2'	34:a:869:G:O4'	2.14	0.48
1:A:2:G:O6	1:A:2901:C:O2	2.32	0.48
1:A:427:U:O2	1:A:427:U:H5''	2.14	0.48
34:a:211:G:N3	34:a:211:G:H2'	2.28	0.48
34:a:340:U:C4	34:a:341:C:N3	2.82	0.48
42:i:129:ARG:C	55:v:35:A:OP1	2.48	0.48
34:a:501:C:C2	34:a:502:A:C8	3.03	0.47
34:a:501:C:N3	34:a:502:A:N7	2.60	0.47
57:y:27:G:N2	57:y:45:U:C5	2.79	0.47
1:A:1469:A:H2'	1:A:1470:A:C8	2.49	0.47
1:A:1980:G:O2'	1:A:1982:U:OP2	2.32	0.47
7:G:3:VAL:HG12	7:G:68:ARG:HG2	1.96	0.47
20:T:61:LEU:HG	20:T:82:LYS:HG2	1.96	0.47
34:a:515:G:C6	34:a:517:G:C6	3.02	0.47
34:a:1295:U:H2'	34:a:1296:C:O4'	2.14	0.47
34:a:1486:G:H2'	34:a:1487:G:O4'	2.14	0.47
57:y:10:G:N1	57:y:26:A:H1'	2.29	0.47
1:A:1432:G:H2'	1:A:1433:A:C8	2.48	0.47
1:A:2370:G:O2'	28:l:43:ARG:NH1	2.48	0.47
34:a:74:A:C2	34:a:97:G:C2	3.02	0.47
34:a:437:U:O4	34:a:438:U:N3	2.47	0.47
34:a:513:C:H6	34:a:513:C:O5'	1.98	0.47
34:a:1492[B]:A:H2	56:x:20:U:O2'	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2273:A:H2'	1:A:2274:A:C8	2.49	0.47
39:f:29:ILE:HG21	39:f:64:VAL:HG21	1.96	0.47
34:a:57:G:O6	34:a:356:A:C6	2.67	0.47
34:a:341:C:N3	34:a:349:A:N6	2.62	0.47
34:a:367:U:O2	34:a:367:U:C2'	2.62	0.47
34:a:1177:G:H2'	34:a:1178:G:O4'	2.14	0.47
56:x:22:A:H2'	56:x:23:C:O4'	2.14	0.47
1:A:2800:A:H3'	1:A:2801:G:C5'	2.44	0.47
34:a:530[B]:G:H3'	34:a:530[B]:G:OP1	2.15	0.47
1:A:1720:U:O2	1:A:1740:G:O6	2.33	0.47
34:a:129:A:C2	34:a:232:G:N1	2.83	0.47
34:a:1305:G:O2'	34:a:1306:A:OP2	2.29	0.47
34:a:590:U:C2	34:a:650:G:C2	3.03	0.47
58:z:220:ILE:HG22	58:z:222:GLY:HA3	1.97	0.47
34:a:1432:G:O2'	34:a:1433:A:OP2	2.23	0.47
57:y:30:G:N2	57:y:31:A:N1	2.63	0.47
1:A:2567:G:H2'	1:A:2568:U:C6	2.50	0.47
34:a:370:C:C2	34:a:393:A:N1	2.83	0.46
34:a:650:G:H2'	34:a:651:C:C6	2.49	0.46
1:A:573:U:O4	1:A:2030:6MZ:H3'	2.15	0.46
34:a:53:A:H2'	34:a:54:C:O4'	2.15	0.46
44:k:87:GLY:O	44:k:92:ARG:NH1	2.48	0.46
3:C:121:ALA:HB3	3:C:129:LEU:HD21	1.98	0.46
34:a:299:G:H2'	34:a:300:A:C8	2.51	0.46
34:a:632:U:H3'	34:a:633:G:H5''	1.97	0.46
34:a:1309:G:N7	46:m:97:ARG:NH2	2.64	0.46
57:y:28:G:N2	57:y:43:C:C2	2.83	0.46
34:a:1495:U:C2'	34:a:1496:C:O5'	2.64	0.46
42:i:83:THR:HG21	42:i:102:PHE:HB3	1.97	0.46
1:A:48:G:N2	1:A:49:A:N1	2.64	0.46
1:A:466:A:OP1	29:2:34:ARG:NH1	2.49	0.46
1:A:529:A:OP2	10:J:113:PRO:HD3	2.16	0.46
2:B:39:A:O2'	2:B:46:A:N1	2.38	0.46
34:a:222:C:O2	34:a:223:A:C8	2.68	0.46
57:y:34:G:P	57:y:34:G:C8	3.09	0.46
1:A:910:A:N3	1:A:2264:C:O2'	2.46	0.46
1:A:1272:A:C2	1:A:1618:6MZ:C2	2.99	0.46
1:A:1483:G:O6	1:A:1506:U:O2	2.34	0.46
1:A:1802:A:H2'	1:A:1803:A:C8	2.51	0.46
34:a:233:C:H2'	34:a:234:C:C6	2.51	0.46
36:c:148:ILE:O	36:c:148:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:r:20:ILE:HG21	51:r:54:LEU:HA	1.97	0.46
34:a:1125:U:H2'	34:a:1126:U:H2'	1.98	0.46
1:A:18:U:O2'	1:A:554:U:OP1	2.33	0.46
1:A:157:C:C4	1:A:169:G:O6	2.69	0.46
11:K:34:GLY:O	11:K:36:GLY:N	2.48	0.46
34:a:61:G:H2'	34:a:62:U:O4'	2.15	0.46
1:A:1916:A:C6	34:a:1409:C:H5'	2.50	0.46
2:B:12:C:O4'	2:B:12:C:O2	2.34	0.46
34:a:1490:U:N3	34:a:1491:G:C8	2.84	0.46
42:i:34:LEU:HD11	42:i:47:VAL:HG21	1.97	0.46
1:A:2242:G:H2'	1:A:2243:U:O4'	2.16	0.45
18:R:51:VAL:HB	18:R:52:PRO:CD	2.45	0.45
53:t:11:ILE:O	53:t:14:GLU:N	2.49	0.45
1:A:327:G:H2'	1:A:328:U:O4'	2.17	0.45
34:a:10:A:O2'	34:a:507:C:H4'	2.16	0.45
34:a:187:G:N2	34:a:191:G:C5	2.84	0.45
34:a:1408:A:N9	34:a:1494:G:N2	2.64	0.45
1:A:803:U:C2'	1:A:804:A:H5'	2.46	0.45
1:A:1730:U:O2'	1:A:1731:G:OP2	2.34	0.45
34:a:103:U:O2'	34:a:172:A:N1	2.37	0.45
34:a:1060:U:H4'	43:j:53:ILE:HG23	1.97	0.45
1:A:72:U:OP2	25:Y:54:LYS:NZ	2.50	0.45
1:A:289:G:C2	1:A:290:U:H1'	2.51	0.45
1:A:1196:C:H2'	1:A:1197:G:O4'	2.16	0.45
4:D:151:THR:CB	4:D:152:PRO:HD3	2.46	0.45
43:j:57:VAL:HG12	43:j:58:ASN:N	2.30	0.45
1:A:271:G:C2	1:A:367:G:C2	3.05	0.45
52:s:10:ILE:HD12	52:s:40:PHE:CE2	2.51	0.45
1:A:1111:A:H2'	1:A:1112:G:H4'	1.98	0.45
34:a:46:G:O2'	34:a:365:U:O2	2.31	0.45
34:a:372:C:C4	34:a:387:U:C5	3.04	0.45
34:a:545:C:C5	34:a:546:A:N7	2.85	0.45
34:a:1356:G:H2'	34:a:1357:A:C8	2.51	0.45
34:a:1408:A:C4	34:a:1494:G:C2	3.04	0.45
1:A:639:U:H2'	1:A:640:C:C6	2.52	0.45
1:A:2757:A:N1	7:G:66:THR:OG1	2.45	0.45
18:R:40:MET:HG3	18:R:48:LYS:HG2	1.98	0.45
34:a:397:A:H3'	34:a:397:A:N3	2.32	0.45
34:a:510:A:H1'	34:a:543:U:H1'	1.99	0.45
34:a:1244:G:C2	34:a:1294:G:C4	3.04	0.45
34:a:1495:U:H2'	34:a:1496:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1591:A:H2'	1:A:1592:C:C6	2.52	0.45
1:A:2734:A:H2'	1:A:2735:G:H5'	1.98	0.45
34:a:127:G:N1	34:a:234:C:O2	2.47	0.45
34:a:173:U:O2'	34:a:174:A:H5'	2.18	0.45
34:a:406:G:C6	34:a:495:A:N7	2.85	0.45
34:a:635:A:H2'	34:a:636:U:O4'	2.17	0.45
54:u:9:GLU:HB2	54:u:10:PRO:HD3	1.98	0.45
56:x:21:C:O5'	56:x:21:C:C6	2.70	0.45
57:y:76:A:O4'	58:z:220:ILE:HD11	2.17	0.45
1:A:573:U:O4	1:A:2029:G:O2'	2.31	0.44
1:A:2722:G:H4'	14:N:4:ARG:HB2	2.00	0.44
34:a:539:A:C6	34:a:540:G:C4	3.04	0.44
45:l:98:ARG:HB2	45:l:116:TYR:HA	1.99	0.44
57:y:34:G:C8	57:y:34:G:OP2	2.70	0.44
1:A:281:C:H2'	1:A:282:A:C8	2.52	0.44
34:a:72:A:H2'	34:a:72:A:N3	2.32	0.44
1:A:553:G:H2'	1:A:554:U:O4'	2.17	0.44
34:a:126:G:H5'	34:a:633:G:N2	2.32	0.44
34:a:367:U:C5	34:a:394:G:C4	3.03	0.44
34:a:440:C:N4	34:a:497:G:H1	2.15	0.44
34:a:515:G:N3	34:a:515:G:C3'	2.80	0.44
1:A:2840:C:H5''	14:N:53:THR:CG2	2.48	0.44
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.98	0.44
7:G:32:LEU:HB3	7:G:74:MET:HE3	1.98	0.44
34:a:1196:A:C8	56:x:23:C:H1'	2.52	0.44
52:s:10:ILE:HD12	52:s:40:PHE:CD2	2.52	0.44
58:z:84:ALA:HB3	58:z:87:TYR:CD2	2.53	0.44
1:A:1370:C:H2'	1:A:1371:G:O4'	2.18	0.44
1:A:2070:A:H2'	1:A:2071:A:O4'	2.18	0.44
34:a:55:A:C2	58:z:222:GLY:N	2.85	0.44
34:a:72:A:C5	34:a:73:C:C6	3.05	0.44
34:a:75:G:C2	34:a:96:U:C4	3.06	0.44
34:a:615:G:C2	34:a:626:G:C5	3.06	0.44
34:a:966:2MG:O2'	42:i:129:ARG:HB2	2.18	0.44
34:a:1455:G:H8	34:a:1455:G:H5''	1.83	0.44
57:y:40:C:C6	57:y:40:C:P	3.11	0.44
1:A:265:A:H4'	1:A:266:G:OP1	2.16	0.44
57:y:39:PSU:C2'	57:y:40:C:C6	3.00	0.44
1:A:1062:G:H1'	9:I:76:ALA:HB3	2.00	0.44
1:A:1149:G:H2'	1:A:1150:C:C6	2.52	0.44
9:I:91:LYS:O	9:I:95:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:456:A:H2'	34:a:457:G:O4'	2.17	0.44
34:a:541:G:H2'	34:a:542:G:C1'	2.48	0.44
34:a:1476:A:H2'	34:a:1477:U:O4'	2.18	0.44
57:y:31:A:O5'	57:y:31:A:C8	2.70	0.44
57:y:41:C:C5	57:y:41:C:OP2	2.70	0.44
22:V:30:ILE:HG23	22:V:72:VAL:HG11	2.00	0.44
34:a:223:A:C2	34:a:224:U:C5	3.05	0.44
34:a:1304:G:C6	34:a:1305:G:N1	2.86	0.44
57:y:10:G:C2	57:y:26:A:H1'	2.53	0.44
34:a:369:G:N2	34:a:393:A:C8	2.85	0.43
34:a:441:A:C2	34:a:497:G:C4	3.06	0.43
34:a:1300:G:O6	34:a:1335:U:C6	2.71	0.43
1:A:1086:A:H2'	1:A:1086:A:N3	2.32	0.43
34:a:62:U:OP1	34:a:385:C:O2'	2.37	0.43
34:a:223:A:N3	34:a:224:U:C5	2.86	0.43
34:a:893:C:N4	34:a:894:G:O6	2.51	0.43
1:A:1795:C:H2'	1:A:1796:U:O4'	2.19	0.43
9:I:74:PRO:HG2	9:I:77:VAL:HG22	2.00	0.43
9:I:109:ALA:HA	9:I:128:ILE:HG21	2.00	0.43
34:a:153:C:C4	34:a:154:U:C5	3.05	0.43
34:a:202:G:H21	34:a:466:A:H61	1.67	0.43
34:a:225:C:H2'	34:a:226:G:O4'	2.18	0.43
34:a:359:G:H2'	34:a:360:G:O4'	2.19	0.43
56:x:22:A:C8	56:x:23:C:C6	3.03	0.43
58:z:223:ARG:HB3	58:z:277:LEU:HD21	2.00	0.43
1:A:684:G:C2	1:A:794:A:C2	3.07	0.43
1:A:987:C:O2'	1:A:1000:A:N3	2.49	0.43
1:A:1076:C:O2	9:I:92:PRO:HD2	2.18	0.43
34:a:318:G:C6	34:a:336:A:C6	3.06	0.43
34:a:1196:A:C8	56:x:23:C:O2'	2.58	0.43
57:y:40:C:H6	57:y:40:C:P	2.42	0.43
1:A:1271:G:O2'	1:A:1618:6MZ:C8	2.67	0.43
34:a:136:C:H2'	34:a:137:U:O4'	2.18	0.43
34:a:530[B]:G:P	34:a:530[B]:G:H2'	2.59	0.43
34:a:604:G:H2'	34:a:605:U:O4'	2.18	0.43
34:a:1409:C:C4	34:a:1491:G:O6	2.71	0.43
34:a:28:A:N6	34:a:29:U:C4	2.87	0.43
34:a:75:G:N3	34:a:97:G:N2	2.67	0.43
34:a:622:A:C8	34:a:623:C:C6	3.07	0.43
1:A:2078:C:H2'	1:A:2079:U:O4'	2.19	0.43
1:A:2743:U:H2'	1:A:2744:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:410:G:H2'	34:a:429:U:C4	2.54	0.43
34:a:589:U:C2	34:a:650:G:O6	2.72	0.43
1:A:1057:A:N6	1:A:1080:A:N1	2.67	0.43
3:C:159:THR:HG23	3:C:176:ARG:HG3	2.01	0.43
34:a:1489:G:H2'	34:a:1490:U:O4'	2.19	0.43
34:a:1492[B]:A:C2	56:x:20:U:O2'	2.71	0.43
38:e:106:ALA:HB2	38:e:124:ALA:HB3	2.01	0.43
1:A:2323:G:H2'	1:A:2324:U:O4'	2.19	0.43
34:a:173:U:O2	34:a:173:U:O4'	2.37	0.43
34:a:1265:C:H3'	34:a:1266:G:H5''	2.01	0.43
1:A:404:A:H4'	1:A:405:U:H5'	2.00	0.43
34:a:1239:A:C2	34:a:1296:C:N3	2.87	0.43
43:j:88:MET:HB3	43:j:89:ARG:H	1.51	0.43
1:A:308:G:H2'	1:A:309:A:C8	2.54	0.42
3:C:141:HIS:CD2	3:C:194:VAL:HG22	2.54	0.42
6:F:91:ARG:HA	6:F:95:MET:HB2	2.01	0.42
1:A:877:A:C2	1:A:900:A:N7	2.87	0.42
1:A:2405:G:O2'	1:A:2411:A:N6	2.53	0.42
1:A:2900:A:C6	1:A:2901:C:O2	2.73	0.42
57:y:41:C:C2'	57:y:42:C:C6	3.01	0.42
57:y:41:C:O2	57:y:42:C:N1	2.52	0.42
1:A:271:G:C2	1:A:367:G:N2	2.88	0.42
1:A:2794:U:O2	1:A:2803:G:C2	2.72	0.42
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.01	0.42
34:a:148:G:C2	34:a:1446:A:C2	3.07	0.42
34:a:233:C:H2'	34:a:234:C:O4'	2.18	0.42
55:w:17:C:O2'	55:w:117:U:P	2.77	0.42
1:A:157:C:N4	1:A:169:G:C6	2.87	0.42
1:A:1482:G:O2'	1:A:1509:A:N1	2.51	0.42
34:a:1320:C:O2	52:s:35:ARG:NH1	2.53	0.42
58:z:337:VAL:HG11	58:z:366:ILE:HD12	2.01	0.42
1:A:239:C:HO2'	1:A:622:G:HO2'	1.67	0.42
1:A:735:A:C8	1:A:736:C:C5	3.07	0.42
1:A:1049:C:H5''	1:A:1049:C:H6	1.84	0.42
1:A:1722:A:H2'	1:A:1723:G:O4'	2.20	0.42
1:A:2899:A:C6	1:A:2900:A:C6	3.08	0.42
32:5:29:ASP:HB3	32:5:32:GLY:HA3	2.02	0.42
34:a:75:G:N2	34:a:97:G:N1	2.67	0.42
34:a:390:U:H2'	34:a:391:G:O4'	2.19	0.42
34:a:1252:A:H2'	34:a:1253:G:O4'	2.19	0.42
58:z:103:LEU:N	58:z:131:ILE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:A:H2'	1:A:1506:U:O4'	2.19	0.42
1:A:2900:A:N6	1:A:2901:C:O2	2.52	0.42
34:a:437:U:O4	34:a:438:U:C2	2.72	0.42
34:a:640:A:N3	41:h:106:SER:HB2	2.35	0.42
34:a:711:G:OP2	39:f:53:LYS:NZ	2.53	0.42
34:a:1246:A:N1	34:a:1291:U:O4	2.52	0.42
1:A:815:C:OP2	18:R:85:LYS:HE3	2.20	0.42
1:A:1997:C:O5'	4:D:129:THR:HG22	2.19	0.42
34:a:152:A:H2'	34:a:153:C:O4'	2.19	0.42
34:a:224:U:O2	34:a:225:C:C6	2.73	0.42
34:a:459:A:H2'	34:a:460:A:O4'	2.20	0.42
34:a:1442:G:H2'	34:a:1443:C:C6	2.55	0.42
42:i:43:ALA:HB3	42:i:46:VAL:HG13	2.00	0.42
1:A:266:G:C6	1:A:427:U:C5	3.07	0.42
1:A:629:G:H2'	1:A:630:G:O4'	2.20	0.42
1:A:1727:A:C2	1:A:1728:C:C2	3.07	0.42
1:A:2412:A:H2'	1:A:2413:G:O4'	2.20	0.42
1:A:2646:C:OP2	1:A:2732:G:O2'	2.30	0.42
1:A:2734:A:H3'	1:A:2735:G:H5'	2.00	0.42
34:a:55:A:C2	58:z:221:SER:C	2.98	0.42
1:A:964:C:O2'	1:A:2273:A:N3	2.48	0.42
1:A:1048:A:N1	1:A:1111:A:C5	2.88	0.42
1:A:2798:U:OP2	1:A:2799:G:N2	2.53	0.42
8:H:90:LEU:CD2	8:H:94:ILE:HD11	2.49	0.42
34:a:105:G:H2'	34:a:106:C:O4'	2.20	0.42
34:a:738:C:H2'	34:a:739:C:C6	2.55	0.42
34:a:1149:C:H2'	34:a:1150:A:C8	2.54	0.42
34:a:1172:C:H2'	34:a:1173:U:C6	2.55	0.42
34:a:1391:U:H2'	34:a:1392:G:C8	2.54	0.42
1:A:471:A:OP1	5:E:79:ARG:NH2	2.53	0.42
1:A:749:A:C8	1:A:1618:6MZ:C6	3.03	0.42
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.42
32:5:28:ALA:HA	32:5:81:LEU:CD2	2.50	0.42
34:a:346:G:N3	34:a:346:G:H3'	2.35	0.42
34:a:605:U:O2	34:a:633:G:C6	2.70	0.42
1:A:1271:G:HO2'	1:A:1618:6MZ:H8	1.83	0.41
34:a:1372:U:H2'	34:a:1373:G:O4'	2.19	0.41
1:A:1528:A:H2'	1:A:1529:G:O4'	2.20	0.41
1:A:2570:G:H2'	1:A:2571:U:O4'	2.20	0.41
34:a:340:U:C4	34:a:350:G:N2	2.89	0.41
45:l:109:ARG:HB2	45:l:118:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:y:33:U:C3'	57:y:33:U:C6	3.03	0.41
1:A:38:A:H2'	1:A:39:G:O4'	2.20	0.41
1:A:212:G:H2'	1:A:213:A:O4'	2.20	0.41
1:A:1021:A:N6	1:A:1141:U:H3	2.18	0.41
1:A:1050:A:C5	1:A:1051:G:N7	2.88	0.41
1:A:1779:U:H5	1:A:1784:A:N7	2.19	0.41
50:q:29:LYS:HA	50:q:36:PHE:HA	2.01	0.41
57:y:43:C:C1'	57:y:45:U:H5	2.33	0.41
7:G:23:ILE:HD13	7:G:71:LEU:HD21	2.03	0.41
10:J:17:VAL:HG23	10:J:137:PRO:HB2	2.02	0.41
17:Q:104:ALA:O	18:R:48:LYS:NZ	2.53	0.41
34:a:187:G:N2	34:a:190:A:C8	2.88	0.41
34:a:513:C:O5'	34:a:513:C:C6	2.73	0.41
55:v:18:G:C6	55:v:57:A:N6	2.87	0.41
1:A:272:A:C2	1:A:365:U:O4	2.73	0.41
1:A:1176:U:H2'	1:A:1177:G:C8	2.56	0.41
1:A:1327:A:N6	1:A:1328:A:C2	2.88	0.41
1:A:1739:A:C4	1:A:1740:G:H1'	2.56	0.41
1:A:2028:U:C4	1:A:2029:G:C5	3.09	0.41
34:a:1256:A:N7	34:a:1278:G:C8	2.88	0.41
42:i:128:LYS:O	42:i:129:ARG:CB	2.62	0.41
54:u:34:ARG:NH2	54:u:36:PHE:HA	2.34	0.41
1:A:458:G:O2'	1:A:469:G:O6	2.34	0.41
1:A:631:A:N3	1:A:2415:G:O2'	2.43	0.41
1:A:1615:C:C2	1:A:1617:C:C6	3.09	0.41
34:a:432:A:H2'	34:a:433:G:O4'	2.20	0.41
34:a:953:G:H2'	34:a:954:G:O4'	2.20	0.41
1:A:1061:U:H4'	1:A:1070:A:C4	2.56	0.41
1:A:1853:A:H2'	1:A:1854:A:O4'	2.20	0.41
1:A:2844:G:H2'	1:A:2845:U:O4'	2.21	0.41
9:I:113:ALA:HA	9:I:116:MET:HB2	2.03	0.41
32:5:64:VAL:HG12	32:5:64:VAL:O	2.20	0.41
34:a:632:U:C3'	34:a:633:G:H5''	2.51	0.41
34:a:1125:U:O2	34:a:1125:U:C2'	2.68	0.41
58:z:223:ARG:HB2	58:z:277:LEU:CD1	2.50	0.41
1:A:565:C:H2'	1:A:566:U:O4'	2.20	0.41
1:A:784:G:H5'	1:A:785:G:OP1	2.21	0.41
1:A:1582:C:O2'	1:A:1585:C:N3	2.53	0.41
1:A:2794:U:C2	1:A:2803:G:N2	2.89	0.41
34:a:646:G:C6	34:a:647:C:C4	3.08	0.41
34:a:706:A:H2'	34:a:707:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:l:54:VAL:HG11	45:l:81:ILE:HG13	2.03	0.41
57:y:27:G:H2'	57:y:28:G:C8	2.56	0.41
1:A:290:U:C4	1:A:350:G:O6	2.74	0.41
1:A:974:G:H2'	1:A:974:G:N3	2.36	0.41
1:A:983:A:C6	1:A:984:A:C2	3.09	0.41
1:A:1328:A:H2'	1:A:1330:C:C5	2.55	0.41
1:A:1615:C:H2'	1:A:1617:C:C5	2.56	0.41
1:A:1918:A:O2'	1:A:1920:C:N4	2.54	0.41
1:A:2029:G:C8	1:A:2029:G:O5'	2.72	0.41
1:A:2705:A:H2'	1:A:2706:A:O4'	2.20	0.41
5:E:59:PRO:HB2	5:E:60:TRP:CE3	2.56	0.41
34:a:269:C:H2'	34:a:270:A:C8	2.55	0.41
34:a:529:G:O6	45:l:45:ASN:HA	2.20	0.41
34:a:1072:G:H2'	34:a:1073:U:O4'	2.21	0.41
34:a:1142:G:C5	34:a:1143:G:H1'	2.56	0.41
37:d:23:GLY:HA2	37:d:108:ALA:HB1	2.03	0.41
57:y:37:MIA:N7	57:y:37:MIA:C13	2.81	0.41
1:A:161:A:H3'	1:A:162:U:H5''	2.02	0.41
1:A:1079:C:O2'	9:I:133:ARG:NH1	2.53	0.41
1:A:1081:U:O2'	9:I:123:ALA:HB1	2.21	0.41
1:A:1467:U:H2'	1:A:1468:U:O4'	2.20	0.41
2:B:79:G:H2'	2:B:80:U:O4'	2.21	0.41
34:a:29:U:C4	34:a:554:A:N1	2.88	0.41
34:a:71:A:N1	34:a:98:A:N1	2.69	0.41
34:a:399:G:H2'	34:a:400:C:C6	2.56	0.41
1:A:2688:G:N1	1:A:2720:U:OP2	2.47	0.40
34:a:58:C:C2	34:a:354:G:O6	2.72	0.40
34:a:78:A:H2'	34:a:79:G:O4'	2.22	0.40
34:a:146:G:C2	34:a:177:G:C5	3.09	0.40
34:a:504:C:O2	34:a:543:U:O2	2.39	0.40
34:a:966:2MG:H1'	42:i:129:ARG:HD3	2.03	0.40
54:u:12:ASP:O	54:u:14:ALA:N	2.54	0.40
1:A:167:A:H2'	1:A:168:G:O4'	2.20	0.40
1:A:528:A:C2	1:A:2042:A:H2'	2.55	0.40
1:A:1009:A:N3	1:A:1153:C:O2'	2.50	0.40
1:A:1054:A:O2'	32:5:30:SER:HA	2.21	0.40
1:A:1703:G:O3'	34:a:1429:A:O2'	2.39	0.40
1:A:2079:U:H2'	1:A:2080:A:O4'	2.21	0.40
34:a:134:G:H2'	34:a:135:C:O4'	2.21	0.40
34:a:614:C:C4	34:a:615:G:C8	3.09	0.40
34:a:1389:C:H2'	34:a:1390:U:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1495:U:H2'	34:a:1496:C:O5'	2.21	0.40
57:y:33:U:H1'	57:y:36:A:N7	2.36	0.40
1:A:1048:A:C2	1:A:1111:A:N6	2.90	0.40
1:A:1433:A:H2'	1:A:1434:A:C8	2.56	0.40
4:D:77:ARG:NH1	4:D:200:ASP:OD2	2.55	0.40
11:K:24:VAL:HG13	11:K:33:ALA:HB2	2.02	0.40
20:T:80:TRP:CZ3	20:T:82:LYS:HB3	2.56	0.40
34:a:131:A:H2'	34:a:132:C:C6	2.57	0.40
1:A:794:A:H2'	1:A:795:C:O4'	2.21	0.40
1:A:1996:C:OP1	11:K:31:ARG:HD3	2.22	0.40
7:G:3:VAL:HG12	7:G:68:ARG:CG	2.51	0.40
16:P:113:LEU:HD21	34:a:1442:G:O2'	2.21	0.40
34:a:408:A:C5	34:a:409:U:C5	3.10	0.40
34:a:547:A:H1'	34:a:548:G:O4'	2.21	0.40
48:o:46:LYS:HB3	48:o:47:LYS:H	1.51	0.40
54:u:36:PHE:O	54:u:38:GLU:N	2.54	0.40
1:A:522:A:H2'	1:A:523:C:C6	2.56	0.40
1:A:563:A:OP2	18:R:79:ARG:NH2	2.54	0.40
1:A:1311:G:N3	1:A:1311:G:H2'	2.36	0.40
1:A:1801:A:OP2	3:C:149:LYS:NZ	2.55	0.40
1:A:2812:G:H2'	1:A:2813:A:C8	2.57	0.40
34:a:126:G:H2'	34:a:127:G:O4'	2.21	0.40
34:a:449:G:O6	34:a:484:G:O6	2.39	0.40
38:e:108:GLY:O	38:e:109:ALA:HB3	2.22	0.40
56:x:20:U:H3	57:y:35:A:H61	1.69	0.40
57:y:27:G:N2	57:y:28:G:N3	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	240 (89%)	26 (10%)	3 (1%)	11	38
4	D	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	8	30
5	E	198/200 (99%)	181 (91%)	15 (8%)	2 (1%)	12	40
6	F	175/177 (99%)	157 (90%)	18 (10%)	0	100	100
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100	100
8	H	147/149 (99%)	127 (86%)	17 (12%)	3 (2%)	6	25
9	I	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	3	19
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	21
12	L	141/143 (99%)	116 (82%)	20 (14%)	5 (4%)	3	16
13	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	30
14	N	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	28
15	O	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
16	P	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	80 (80%)	16 (16%)	4 (4%)	2	15
19	S	107/109 (98%)	96 (90%)	10 (9%)	1 (1%)	14	42
20	T	90/92 (98%)	81 (90%)	8 (9%)	1 (1%)	11	38
21	U	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	18
22	V	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	11	38
23	W	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	9	31
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	49 (92%)	3 (6%)	1 (2%)	6	26
28	1	49/51 (96%)	42 (86%)	6 (12%)	1 (2%)	6	25
29	2	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	98 (76%)	21 (16%)	10 (8%)	1	4
33	6	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	7	29
35	b	216/218 (99%)	187 (87%)	23 (11%)	6 (3%)	4	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	187 (92%)	12 (6%)	5 (2%)	4	21
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	12	40
38	e	156/157 (99%)	133 (85%)	20 (13%)	3 (2%)	6	26
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	15
40	g	149/151 (99%)	132 (89%)	13 (9%)	4 (3%)	4	20
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/127 (98%)	94 (75%)	26 (21%)	5 (4%)	2	15
43	j	96/98 (98%)	73 (76%)	15 (16%)	8 (8%)	0	4
44	k	114/116 (98%)	100 (88%)	9 (8%)	5 (4%)	2	13
45	l	119/121 (98%)	96 (81%)	15 (13%)	8 (7%)	1	6
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6	26
47	n	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	1	10
48	o	86/88 (98%)	79 (92%)	2 (2%)	5 (6%)	1	8
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	2	15
50	q	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	9	33
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1	7
52	s	77/79 (98%)	67 (87%)	9 (12%)	1 (1%)	9	33
53	t	83/85 (98%)	75 (90%)	6 (7%)	2 (2%)	4	22
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	0
58	z	391/393 (100%)	349 (89%)	32 (8%)	10 (3%)	4	21
All	All	6219/6322 (98%)	5471 (88%)	605 (10%)	143 (2%)	7	23

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	89	ASN
11	K	111	LYS
12	L	31	GLY
18	R	51	VAL
21	U	6	ARG
32	5	60	LEU
32	5	123	ILE
36	c	96	VAL
40	g	64	ALA
42	i	46	VAL

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Mol	Chain	Res	Type
42	i	90	ASP
43	j	57	VAL
43	j	89	ARG
44	k	88	PRO
44	k	94	SER
48	o	45	HIS
48	o	47	LYS
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
4	D	58	ASN
5	E	8	ALA
5	E	83	VAL
9	I	24	GLY
18	R	49	ILE
18	R	54	VAL
18	R	55	ASP
20	T	37	ASP
36	c	156	LEU
38	e	77	ASN
40	g	20	GLU
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
45	l	42	LYS
45	l	75	GLU
45	l	88	ASP
46	m	7	ASN
47	n	2	LYS
47	n	22	LYS
47	n	38	ASP
47	n	55	SER
47	n	90	ARG
49	p	81	ALA
51	r	10	CYS
51	r	17	VAL
54	u	9	GLU
54	u	36	PHE
3	C	13	ARG

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Mol	Chain	Res	Type
4	D	31	ALA
4	D	154	LYS
9	I	38	CYS
9	I	64	ARG
12	L	15	ALA
14	N	59	SER
22	V	58	SER
27	0	2	VAL
32	5	88	HIS
33	6	4	ASP
35	b	73	ARG
37	d	191	SER
40	g	19	SER
42	i	124	PRO
43	j	35	GLN
43	j	41	PRO
44	k	14	GLN
44	k	103	GLY
45	l	35	ARG
49	p	64	GLY
50	q	17	GLU
51	r	46	THR
52	s	36	ARG
54	u	24	LYS
54	u	30	GLU
58	z	249	GLU
8	H	15	LEU
8	H	41	LYS
12	L	29	LYS
12	L	91	ASP
13	M	69	PRO
14	N	117	ASP
21	U	97	SER
32	5	48	ALA
32	5	55	VAL
32	5	80	THR
32	5	118	ILE
35	b	192	PRO
36	c	147	GLY
37	d	166	LYS
38	e	89	THR
39	f	33	GLU

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Mol	Chain	Res	Type
39	f	63	ASN
43	j	58	ASN
45	l	43	LYS
45	l	77	SER
46	m	102	LYS
48	o	13	GLU
51	r	70	THR
54	u	11	PHE
54	u	12	ASP
58	z	180	GLY
58	z	221	SER
58	z	222	GLY
8	H	3	VAL
11	K	35	VAL
13	M	6	ARG
19	S	65	ASP
23	W	72	ASN
32	5	51	TYR
32	5	113	PHE
35	b	11	ALA
35	b	86	CYS
36	c	95	GLY
38	e	93	VAL
39	f	92	THR
43	j	75	ASP
45	l	46	SER
48	o	2	LEU
48	o	48	ASP
49	p	49	GLY
53	t	44	ALA
58	z	9	LYS
58	z	207	ASP
3	C	120	ASP
3	C	121	ALA
32	5	108	VAL
35	b	63	LYS
35	b	151	LYS
39	f	99	ALA
43	j	6	ILE
45	l	33	CYS
58	z	126	GLY
58	z	248	LYS

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Mol	Chain	Res	Type
36	c	144	GLY
58	z	52	ALA
12	L	85	VAL
21	U	38	ILE
28	1	4	ILE
58	z	82	PRO
9	I	90	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	206 (95%)	10 (5%)	24	50
4	D	163/163 (100%)	154 (94%)	9 (6%)	19	46
5	E	164/164 (100%)	160 (98%)	4 (2%)	43	62
6	F	148/148 (100%)	143 (97%)	5 (3%)	32	57
7	G	135/135 (100%)	134 (99%)	1 (1%)	76	78
8	H	114/114 (100%)	113 (99%)	1 (1%)	70	76
9	I	109/109 (100%)	101 (93%)	8 (7%)	13	39
10	J	115/115 (100%)	109 (95%)	6 (5%)	21	48
11	K	103/103 (100%)	97 (94%)	6 (6%)	18	45
12	L	102/102 (100%)	97 (95%)	5 (5%)	22	49
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	76
14	N	99/99 (100%)	95 (96%)	4 (4%)	28	53
15	O	86/86 (100%)	82 (95%)	4 (5%)	23	50
16	P	99/99 (100%)	96 (97%)	3 (3%)	36	59
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	57
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	62
19	S	92/92 (100%)	88 (96%)	4 (4%)	26	51
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	83/83 (100%)	82 (99%)	1 (1%)	63	72
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	71
23	W	57/57 (100%)	53 (93%)	4 (7%)	14	40
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51	67
26	Z	47/47 (100%)	47 (100%)	0	100	100
27	0	46/46 (100%)	44 (96%)	2 (4%)	26	51
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	34 (92%)	3 (8%)	11	36
30	3	51/51 (100%)	49 (96%)	2 (4%)	28	53
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	99 (99%)	1 (1%)	68	75
33	6	59/59 (100%)	57 (97%)	2 (3%)	32	57
35	b	180/180 (100%)	178 (99%)	2 (1%)	65	74
36	c	170/170 (100%)	170 (100%)	0	100	100
37	d	172/172 (100%)	169 (98%)	3 (2%)	53	67
38	e	120/119 (101%)	115 (96%)	5 (4%)	26	52
39	f	87/87 (100%)	83 (95%)	4 (5%)	24	50
40	g	124/124 (100%)	122 (98%)	2 (2%)	55	68
41	h	104/104 (100%)	99 (95%)	5 (5%)	23	50
42	i	105/105 (100%)	100 (95%)	5 (5%)	23	50
43	j	86/86 (100%)	82 (95%)	4 (5%)	23	50
44	k	89/89 (100%)	85 (96%)	4 (4%)	24	51
45	l	102/102 (100%)	99 (97%)	3 (3%)	37	60
46	m	93/93 (100%)	90 (97%)	3 (3%)	34	58
47	n	83/83 (100%)	80 (96%)	3 (4%)	31	56
48	o	76/76 (100%)	74 (97%)	2 (3%)	40	61
49	p	65/65 (100%)	64 (98%)	1 (2%)	57	69
50	q	74/74 (100%)	70 (95%)	4 (5%)	20	47
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	39
52	s	70/70 (100%)	68 (97%)	2 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	t	65/65 (100%)	61 (94%)	4 (6%)	16	43
54	u	55/55 (100%)	50 (91%)	5 (9%)	9	30
58	z	325/325 (100%)	321 (99%)	4 (1%)	63	72
All	All	5165/5164 (100%)	5001 (97%)	164 (3%)	35	58

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	35	LYS
3	C	38	LYS
3	C	42	ARG
3	C	69	ASN
3	C	164	VAL
3	C	183	VAL
3	C	241	LYS
3	C	249	VAL
3	C	269	ARG
4	D	12	THR
4	D	39	ASP
4	D	77	ARG
4	D	99	GLU
4	D	148	GLN
4	D	150	GLN
4	D	151	THR
4	D	160	LYS
4	D	200	ASP
5	E	47	LYS
5	E	117	ARG
5	E	139	LYS
5	E	141	MET
6	F	70	ARG
6	F	87	LYS
6	F	91	ARG
6	F	112	ASP
6	F	116	LEU
7	G	121	THR
8	H	96	THR
9	I	11	GLN
9	I	30	GLN
9	I	72	THR

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Mol	Chain	Res	Type
9	I	95	ASP
9	I	117	THR
9	I	126	ARG
9	I	134	SER
9	I	135	MET
10	J	3	THR
10	J	50	THR
10	J	61	LYS
10	J	70	THR
10	J	80	HIS
10	J	81	ILE
11	K	52	VAL
11	K	58	LEU
11	K	67	LYS
11	K	97	THR
11	K	109	SER
11	K	110	GLU
12	L	1	MET
12	L	14	LYS
12	L	27	LEU
12	L	69	ARG
12	L	79	LEU
13	M	110	GLU
14	N	34	ILE
14	N	35	LYS
14	N	69	ARG
14	N	117	ASP
15	O	13	ARG
15	O	28	VAL
15	O	62	LEU
15	O	76	LYS
16	P	47	ILE
16	P	79	VAL
16	P	88	ARG
17	Q	8	ILE
17	Q	40	LYS
17	Q	108	LEU
18	R	85	LYS
18	R	95	ASP
19	S	19	LEU
19	S	29	VAL
19	S	57	ASN

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Mol	Chain	Res	Type
19	S	72	THR
20	T	12	ARG
20	T	93	LEU
21	U	65	GLN
22	V	42	LEU
23	W	8	ASN
23	W	15	LYS
23	W	67	VAL
23	W	68	LYS
25	Y	28	LEU
27	0	52	LYS
27	0	53	VAL
29	2	22	MET
29	2	41	ARG
29	2	43	THR
30	3	51	LYS
30	3	61	LEU
32	5	34	THR
33	6	3	LYS
33	6	37	CYS
35	b	21	TYR
35	b	67	LEU
37	d	90	LEU
37	d	120	LYS
37	d	190	LEU
38	e	11	GLN
38	e	19	ARG
38	e	45	VAL
38	e	136	VAL
38	e	139	THR
39	f	38	ARG
39	f	39	LEU
39	f	44	ARG
39	f	91	ARG
40	g	2	ARG
40	g	11	ILE
41	h	54	THR
41	h	79	ARG
41	h	106	SER
41	h	110	MET
41	h	120	LEU
42	i	41	GLU

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Mol	Chain	Res	Type
42	i	42	THR
42	i	44	ARG
42	i	98	ARG
42	i	129	ARG
43	j	67	ILE
43	j	87	LEU
43	j	88	MET
43	j	91	ASP
44	k	14	GLN
44	k	28	ASN
44	k	71	ASP
44	k	118	ASN
45	l	23	LEU
45	l	77	SER
45	l	88	ASP
46	m	15	VAL
46	m	47	LEU
46	m	89	ARG
47	n	10	VAL
47	n	40	ASP
47	n	75	ARG
48	o	46	LYS
48	o	88	ARG
49	p	34	GLU
50	q	3	LYS
50	q	4	ILE
50	q	63	CYS
50	q	66	LEU
51	r	13	THR
51	r	42	ARG
51	r	60	ARG
51	r	72	ARG
52	s	5	LYS
52	s	12	LEU
53	t	42	ASP
53	t	43	LYS
53	t	56	ILE
53	t	68	LYS
54	u	31	VAL
54	u	33	ARG
54	u	34	ARG
54	u	43	GLU

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Mol	Chain	Res	Type
54	u	62	GLU
58	z	22	HIS
58	z	89	LYS
58	z	179	GLU
58	z	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	59	GLN
3	C	133	ASN
3	C	142	ASN
3	C	196	ASN
4	D	67	HIS
4	D	136	ASN
4	D	140	HIS
5	E	41	GLN
5	E	94	GLN
5	E	115	GLN
7	G	37	ASN
8	H	2	GLN
8	H	18	GLN
8	H	135	HIS
9	I	5	GLN
10	J	47	HIS
10	J	58	ASN
10	J	77	HIS
10	J	128	ASN
10	J	131	ASN
10	J	132	HIS
10	J	136	GLN
11	K	3	GLN
11	K	9	ASN
14	N	62	ASN
16	P	65	ASN
18	R	12	HIS
21	U	45	GLN
23	W	8	ASN
33	6	61	ASN
33	6	65	ASN
35	b	23	ASN
35	b	38	HIS

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Mol	Chain	Res	Type
36	c	5	HIS
36	c	7	ASN
36	c	122	GLN
37	d	35	GLN
37	d	70	GLN
37	d	119	HIS
38	e	96	GLN
38	e	121	ASN
40	g	129	ASN
40	g	141	HIS
42	i	30	ASN
42	i	125	GLN
44	k	39	ASN
44	k	63	GLN
45	l	71	HIS
45	l	72	ASN
45	l	95	HIS
48	o	19	ASN
48	o	27	GLN
48	o	36	ASN
48	o	45	HIS
50	q	49	ASN
52	s	56	HIS
53	t	12	GLN
53	t	51	ASN
54	u	63	ASN
58	z	13	ASN
58	z	51	ASN
58	z	329	GLN
58	z	355	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	735 (25%)	73 (2%)
2	B	119/120 (99%)	27 (22%)	4 (3%)
34	a	1537/1540 (99%)	465 (30%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	34 (44%)	0
56	x	11/12 (91%)	7 (63%)	0
57	y	75/76 (98%)	42 (56%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4791/4805 (99%)	1327 (27%)	77 (1%)

All (1327) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U
1	A	13	A
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	G
1	A	49	A
1	A	50	U
1	A	51	G
1	A	52	A
1	A	61	C
1	A	63	A
1	A	68	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	78	U
1	A	80	G
1	A	82	U
1	A	84	A
1	A	92	U
1	A	93	G
1	A	97	C
1	A	98	G
1	A	100	U
1	A	101	A
1	A	102	U
1	A	118	A
1	A	119	A

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Mol	Chain	Res	Type
1	A	120	U
1	A	130	C
1	A	133	U
1	A	136	G
1	A	139	U
1	A	140	C
1	A	141	G
1	A	143	C
1	A	149	A
1	A	153	U
1	A	155	A
1	A	156	A
1	A	157	C
1	A	159	G
1	A	162	U
1	A	163	C
1	A	165	A
1	A	166	U
1	A	168	G
1	A	170	U
1	A	173	A
1	A	181	A
1	A	186	G
1	A	188	G
1	A	196	A
1	A	199	A
1	A	200	U
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	226	A
1	A	228	C
1	A	230	G
1	A	234	U
1	A	239	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A

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Mol	Chain	Res	Type
1	A	265	A
1	A	266	G
1	A	267	C
1	A	269	C
1	A	272	A
1	A	273	G
1	A	274	C
1	A	275	C
1	A	276	U
1	A	279	A
1	A	281	C
1	A	282	A
1	A	283	G
1	A	284	U
1	A	285	G
1	A	286	U
1	A	287	G
1	A	290	U
1	A	294	A
1	A	301	G
1	A	302	C
1	A	311	A
1	A	317	G
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	349	U
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	362	A
1	A	365	U
1	A	366	C
1	A	368	A
1	A	369	U
1	A	370	G
1	A	371	A
1	A	372	G
1	A	386	G

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Mol	Chain	Res	Type
1	A	387	U
1	A	395	U
1	A	396	G
1	A	400	G
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	420	C
1	A	427	U
1	A	438	G
1	A	442	G
1	A	445	C
1	A	451	U
1	A	473	G
1	A	475	C
1	A	480	A
1	A	481	G
1	A	491	G
1	A	492	A
1	A	494	G
1	A	503	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	521	U
1	A	527	C
1	A	529	A
1	A	531	C
1	A	532	A
1	A	535	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	556	A
1	A	563	A
1	A	564	C

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Mol	Chain	Res	Type
1	A	573	U
1	A	575	A
1	A	603	A
1	A	610	C
1	A	612	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	633	A
1	A	636	G
1	A	637	A
1	A	640	C
1	A	644	A
1	A	645	C
1	A	646	U
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	661	A
1	A	668	A
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	708	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	723	C
1	A	730	A
1	A	738	G
1	A	746	PSU
1	A	747	5MC
1	A	752	A
1	A	764	A
1	A	765	C
1	A	771	G

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Mol	Chain	Res	Type
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	804	A
1	A	805	G
1	A	812	C
1	A	814	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	837	C
1	A	844	A
1	A	845	A
1	A	846	C
1	A	858	G
1	A	860	U
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	934	U
1	A	940	G
1	A	941	A
1	A	942	G
1	A	946	C
1	A	951	C
1	A	953	G
1	A	958	U

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Mol	Chain	Res	Type
1	A	961	C
1	A	973	A
1	A	974	G
1	A	983	A
1	A	985	C
1	A	989	G
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1006	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1019	U
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1034	G
1	A	1036	G
1	A	1037	G
1	A	1038	G
1	A	1040	A
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A

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Mol	Chain	Res	Type
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1097	U
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1117	C
1	A	1119	U
1	A	1130	U
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1141	U
1	A	1142	A
1	A	1143	A
1	A	1148	U
1	A	1150	C
1	A	1151	A
1	A	1155	A
1	A	1157	G
1	A	1171	G
1	A	1172	C
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C

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Mol	Chain	Res	Type
1	A	1180	U
1	A	1184	U
1	A	1210	G
1	A	1218	G
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1238	G
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1258	U
1	A	1262	A
1	A	1269	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1320	C
1	A	1332	G
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1365	A
1	A	1367	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1387	A
1	A	1392	A
1	A	1395	A
1	A	1398	C
1	A	1403	A
1	A	1407	G
1	A	1410	G
1	A	1416	G
1	A	1418	G
1	A	1419	A

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Mol	Chain	Res	Type
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1441	G
1	A	1450	G
1	A	1452	G
1	A	1453	A
1	A	1455	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1468	U
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1504	A
1	A	1507	C
1	A	1515	A
1	A	1516	G
1	A	1519	G
1	A	1520	U
1	A	1523	U
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1541	C
1	A	1542	U
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1565	C
1	A	1567	G
1	A	1569	A

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Mol	Chain	Res	Type
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1582	C
1	A	1584	U
1	A	1585	C
1	A	1587	G
1	A	1590	A
1	A	1595	C
1	A	1605	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1618	6MZ
1	A	1619	G
1	A	1643	G
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1691	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1698	A
1	A	1706	C
1	A	1710	G
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1721	G
1	A	1723	G
1	A	1724	G
1	A	1725	C
1	A	1726	G
1	A	1728	C
1	A	1729	U
1	A	1730	U

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Mol	Chain	Res	Type
1	A	1731	G
1	A	1732	C
1	A	1738	G
1	A	1740	G
1	A	1741	C
1	A	1746	A
1	A	1750	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1809	A
1	A	1816	C
1	A	1826	G
1	A	1833	C
1	A	1841	U
1	A	1842	G
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1884	G
1	A	1885	A
1	A	1895	C
1	A	1906	G
1	A	1907	G
1	A	1912	A
1	A	1913	A

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Mol	Chain	Res	Type
1	A	1914	C
1	A	1915	3TD
1	A	1916	A
1	A	1917	PSU
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1955	U
1	A	1962	5MC
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2029	G
1	A	2030	6MZ
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG

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Mol	Chain	Res	Type
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2100	G
1	A	2102	G
1	A	2104	C
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2180	U
1	A	2186	G
1	A	2192	U
1	A	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2212	A
1	A	2213	U

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Mol	Chain	Res	Type
1	A	2221	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2332	C
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2342	C
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2373	G
1	A	2378	A
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2399	G
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2408	U
1	A	2423	U
1	A	2425	A
1	A	2428	G

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Mol	Chain	Res	Type
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2435	A
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2457	PSU
1	A	2469	A
1	A	2470	G
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2481	G
1	A	2491	U
1	A	2494	G
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2503	2MA
1	A	2505	G
1	A	2506	U
1	A	2513	A
1	A	2517	C
1	A	2518	A
1	A	2519	U
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2578	G
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2608	G

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Mol	Chain	Res	Type
1	A	2609	U
1	A	2613	U
1	A	2615	U
1	A	2624	G
1	A	2629	U
1	A	2630	G
1	A	2653	U
1	A	2654	A
1	A	2656	U
1	A	2673	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2700	A
1	A	2707	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2720	U
1	A	2724	U
1	A	2726	A
1	A	2728	U
1	A	2733	A
1	A	2734	A
1	A	2735	G
1	A	2742	G
1	A	2744	G
1	A	2746	U
1	A	2748	A
1	A	2752	C
1	A	2754	U
1	A	2758	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2791	G
1	A	2794	U
1	A	2798	U
1	A	2799	G
1	A	2800	A

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Mol	Chain	Res	Type
1	A	2801	G
1	A	2803	G
1	A	2805	C
1	A	2806	C
1	A	2807	U
1	A	2809	A
1	A	2812	G
1	A	2818	U
1	A	2820	A
1	A	2823	A
1	A	2826	A
1	A	2837	A
1	A	2849	U
1	A	2850	A
1	A	2856	A
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2874	C
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2901	C
1	A	2902	C
2	B	4	C
2	B	12	C
2	B	13	G
2	B	21	G
2	B	26	C
2	B	28	C
2	B	30	C
2	B	31	C
2	B	33	G
2	B	35	C
2	B	36	C
2	B	42	C
2	B	44	G
2	B	65	U
2	B	66	A
2	B	67	G

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Mol	Chain	Res	Type
2	B	84	G
2	B	89	U
2	B	90	C
2	B	105	G
2	B	108	A
2	B	109	A
2	B	111	U
2	B	113	C
2	B	114	C
2	B	117	G
2	B	118	C
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	8	A
34	a	9	G
34	a	22	G
34	a	29	U
34	a	32	A
34	a	38	G
34	a	39	G
34	a	44	A
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	52	C
34	a	57	G
34	a	60	A
34	a	64	G
34	a	66	A
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A
34	a	73	C
34	a	74	A
34	a	76	G
34	a	77	A

Continued on next page...

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Mol	Chain	Res	Type
34	a	78	A
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	99	C
34	a	100	G
34	a	104	G
34	a	107	G
34	a	116	A
34	a	117	G
34	a	120	A
34	a	121	U
34	a	127	G
34	a	128	G
34	a	129	A
34	a	130	A
34	a	131	A
34	a	132	C
34	a	142	G
34	a	144	G
34	a	146	G
34	a	149	A
34	a	150	U
34	a	151	A
34	a	154	U
34	a	161	A
34	a	163	C
34	a	165	G
34	a	167	A
34	a	168	G
34	a	177	G
34	a	181	A
34	a	183	C
34	a	184	G

Continued on next page...

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Mol	Chain	Res	Type
34	a	189	A
34	a	191	G
34	a	196	A
34	a	197	A
34	a	202	G
34	a	203	G
34	a	205	A
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	215	C
34	a	220	G
34	a	222	C
34	a	223	A
34	a	226	G
34	a	227	G
34	a	230	G
34	a	240	G
34	a	244	U
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	254	G
34	a	259	G
34	a	266	G
34	a	267	C
34	a	281	G
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	325	A
34	a	328	C
34	a	330	C
34	a	335	C
34	a	339	C

Continued on next page...

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Mol	Chain	Res	Type
34	a	340	U
34	a	341	C
34	a	342	C
34	a	344	A
34	a	345	C
34	a	347	G
34	a	348	G
34	a	349	A
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	358	U
34	a	363	A
34	a	365	U
34	a	366	A
34	a	367	U
34	a	368	U
34	a	369	G
34	a	372	C
34	a	375	U
34	a	376	G
34	a	381	C
34	a	382	A
34	a	388	G
34	a	389	A
34	a	390	U
34	a	391	G
34	a	392	C
34	a	397	A
34	a	398	U
34	a	400	C
34	a	403	C
34	a	404	G
34	a	405	U
34	a	406	G
34	a	407	U
34	a	411	A
34	a	412	A
34	a	413	G
34	a	422	C
34	a	424	G

Continued on next page...

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Mol	Chain	Res	Type
34	a	429	U
34	a	435	A
34	a	436	C
34	a	440	C
34	a	441	A
34	a	443	C
34	a	446	G
34	a	449	G
34	a	457	G
34	a	458	U
34	a	459	A
34	a	464	U
34	a	466	A
34	a	467	U
34	a	468	A
34	a	476	U
34	a	482	A
34	a	484	G
34	a	485	U
34	a	486	U
34	a	496	A
34	a	497	G
34	a	499	A
34	a	501	C
34	a	502	A
34	a	503	C
34	a	505	G
34	a	506	G
34	a	509	A
34	a	511	C
34	a	514	C
34	a	515	G
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	520	A
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	528	C
34	a	531	U

Continued on next page...

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Mol	Chain	Res	Type
34	a	532	A
34	a	533	A
34	a	534	U
34	a	535	A
34	a	537	G
34	a	538	G
34	a	541	G
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	590	U
34	a	592	G
34	a	596	A
34	a	615	G
34	a	619	U
34	a	633	G
34	a	639	G
34	a	640	A
34	a	642	A
34	a	647	C
34	a	648	A
34	a	650	G
34	a	651	C
34	a	653	U
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	701	U
34	a	703	G
34	a	704	A
34	a	713	G
34	a	720	C

Continued on next page...

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Mol	Chain	Res	Type
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	742	G
34	a	754	C
34	a	755	G
34	a	758	C
34	a	761	G
34	a	769	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	832	G
34	a	836	G
34	a	838	G
34	a	843	U
34	a	844	G
34	a	846	G
34	a	851	G
34	a	870	U
34	a	872	A
34	a	885	G
34	a	902	G
34	a	905	U
34	a	906	A
34	a	914	A
34	a	924	C
34	a	926	G
34	a	934	C
34	a	935	A
34	a	939	G
34	a	945	G
34	a	960	U
34	a	961	U

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Mol	Chain	Res	Type
34	a	963	G
34	a	965	U
34	a	966	2MG
34	a	969	A
34	a	971	G
34	a	972	C
34	a	975	A
34	a	976	G
34	a	977	A
34	a	978	A
34	a	982	U
34	a	984	C
34	a	988	G
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1038	C
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1087	G
34	a	1088	G

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Mol	Chain	Res	Type
34	a	1094	G
34	a	1095	U
34	a	1096	C
34	a	1101	A
34	a	1108	G
34	a	1113	C
34	a	1115	U
34	a	1116	U
34	a	1124	G
34	a	1125	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1155	A
34	a	1159	U
34	a	1163	A
34	a	1167	A
34	a	1168	U
34	a	1171	A
34	a	1174	G
34	a	1182	G
34	a	1184	G
34	a	1188	A
34	a	1190	G
34	a	1191	A
34	a	1195	C
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1205	U
34	a	1206	G

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Mol	Chain	Res	Type
34	a	1207	2MG
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1238	A
34	a	1240	U
34	a	1245	C
34	a	1247	U
34	a	1248	A
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1264	U
34	a	1266	G
34	a	1268	G
34	a	1269	A
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1291	U
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C

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Mol	Chain	Res	Type
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1312	G
34	a	1313	U
34	a	1317	C
34	a	1320	C
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1349	A
34	a	1360	A
34	a	1363	A
34	a	1368	A
34	a	1371	G
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1391	U
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1402	4OC
34	a	1415	G
34	a	1419	G
34	a	1429	A
34	a	1432	G
34	a	1433	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1448	C
34	a	1449	C
34	a	1450	U
34	a	1454	G
34	a	1455	G
34	a	1469	C
34	a	1475	G
34	a	1487	G

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Mol	Chain	Res	Type
34	a	1491	G
34	a	1493	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1519	MA6
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	25	C
55	v	42	G
55	v	47	U
55	v	70	G
55	v	72	A
55	v	76	A
55	w	3	C
55	w	5	G
55	w	7	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G

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Mol	Chain	Res	Type
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A
55	w	67	C
55	w	69	C
55	w	70	G
55	w	71	C
55	w	73	A
55	w	75	C
55	w	76	A
56	x	14	C
56	x	19	C
56	x	20	U
56	x	21	C
56	x	22	A
56	x	23	C
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U
57	y	21	A

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Mol	Chain	Res	Type
57	y	24	G
57	y	26	A
57	y	30	G
57	y	31	A
57	y	32	PSU
57	y	33	U
57	y	34	G
57	y	35	A
57	y	36	A
57	y	37	MIA
57	y	38	A
57	y	39	PSU
57	y	40	C
57	y	42	C
57	y	43	C
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	55	PSU
57	y	56	C
57	y	59	U
57	y	61	C
57	y	65	G
57	y	68	C
57	y	69	G
57	y	73	A
57	y	76	A

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	51	G
1	A	162	U
1	A	177	G
1	A	199	A
1	A	204	A
1	A	242	G
1	A	265	A

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Mol	Chain	Res	Type
1	A	301	G
1	A	341	C
1	A	440	C
1	A	474	G
1	A	502	A
1	A	534	U
1	A	537	G
1	A	555	G
1	A	613	A
1	A	641	U
1	A	653	U
1	A	746	PSU
1	A	752	A
1	A	764	A
1	A	774	G
1	A	775	G
1	A	784	G
1	A	827	U
1	A	859	G
1	A	884	U
1	A	1020	A
1	A	1022	G
1	A	1033	U
1	A	1046	A
1	A	1070	A
1	A	1089	A
1	A	1111	A
1	A	1124	G
1	A	1140	C
1	A	1190	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1475	G
1	A	1523	U
1	A	1555	G
1	A	1558	C
1	A	1567	G
1	A	1608	A
1	A	1647	U
1	A	1706	C
1	A	1730	U

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Mol	Chain	Res	Type
1	A	1818	U
1	A	1857	G
1	A	1918	A
1	A	1939	5MU
1	A	1940	U
1	A	1976	U
1	A	2238	G
1	A	2296	U
1	A	2319	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2401	U
1	A	2402	U
1	A	2407	A
1	A	2517	C
1	A	2566	A
1	A	2581	G
1	A	2681	C
1	A	2798	U
1	A	2833	U
1	A	2849	U
1	A	2873	A
2	B	34	A
2	B	56	G
2	B	66	A
2	B	108	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	7MG	A	2069	60,1	23,26,27	1.46	4 (17%)	27,39,42	2.52	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	MA6	a	1518	34	23,26,27	1.77	5 (21%)	33,38,41	2.40	11 (33%)
57	PSU	y	32	57	18,21,22	1.33	2 (11%)	21,30,33	2.27	5 (23%)
1	PSU	A	746	60,1	18,21,22	1.42	2 (11%)	21,30,33	2.05	5 (23%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.18	5 (23%)
55	H2U	w	20	55	18,21,22	0.81	1 (5%)	19,30,33	1.56	3 (15%)
1	5MC	A	747	1	19,22,23	1.96	2 (10%)	26,32,35	1.54	5 (19%)
1	OMC	A	2498	60,1	19,22,23	0.86	0	25,31,34	1.25	3 (12%)
1	2MA	A	2503	60,1	22,25,26	1.59	4 (18%)	32,37,40	2.27	9 (28%)
1	2MG	A	2445	1	23,26,27	1.25	3 (13%)	33,38,41	2.35	10 (30%)
55	4SU	v	7	55	18,21,22	1.79	4 (22%)	25,30,33	2.33	6 (24%)
57	5MU	y	54	57	19,22,23	1.46	4 (21%)	27,32,35	2.07	8 (29%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.30	10 (34%)
1	PSU	A	2605	1	18,21,22	1.41	2 (11%)	21,30,33	2.04	4 (19%)
1	1MG	A	745	1	23,26,27	1.42	3 (13%)	33,39,42	2.05	8 (24%)
57	4SU	y	8	57	18,21,22	1.83	5 (27%)	25,30,33	2.37	7 (28%)
34	MA6	a	1519	34	23,26,27	1.74	5 (21%)	33,38,41	2.47	15 (45%)
1	H2U	A	2449	1	18,21,22	0.92	2 (11%)	19,30,33	1.56	3 (15%)
34	4OC	a	1402	34	20,23,24	0.85	1 (5%)	25,32,35	1.30	4 (16%)
1	OMG	A	2251	55,1	23,26,27	1.25	3 (13%)	32,38,41	2.01	6 (18%)
1	2MG	A	1835	1	23,26,27	1.32	4 (17%)	33,38,41	2.28	7 (21%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.08	5 (23%)
1	PSU	A	955	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
55	5MU	v	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.96	9 (33%)
1	5MU	A	1939	1	19,22,23	1.49	4 (21%)	27,32,35	2.08	8 (29%)
34	PSU	a	516	34	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
1	OMU	A	2552	60,1	19,22,23	1.30	3 (15%)	25,31,34	2.03	8 (32%)
57	7MG	y	46	57	23,26,27	1.42	3 (13%)	27,39,42	2.47	7 (25%)
57	PSU	y	55	57	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.40	4 (21%)
1	6MZ	A	1618	1	22,25,26	1.52	4 (18%)	29,36,39	2.28	10 (34%)
55	PSU	v	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
57	MIA	y	37	57	28,31,32	2.35	6 (21%)	38,44,47	2.86	15 (39%)
34	2MG	a	966	34	23,26,27	1.29	4 (17%)	33,38,41	2.63	11 (33%)
57	PSU	y	39	57	18,21,22	1.33	2 (11%)	21,30,33	2.28	5 (23%)
1	PSU	A	2580	1	18,21,22	1.48	2 (11%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2457	1	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.07	10 (37%)
1	PSU	A	2504	1	18,21,22	1.41	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	A	1917	1	18,21,22	1.43	2 (11%)	21,30,33	2.07	5 (23%)
34	2MG	a	1516	34	23,26,27	1.29	4 (17%)	33,38,41	2.30	8 (24%)
34	2MG	a	1207	34	23,26,27	1.26	3 (13%)	33,38,41	2.77	10 (30%)
34	5MC	a	1407	34	19,22,23	2.05	2 (10%)	26,32,35	1.65	6 (23%)
1	5MC	A	1962	1	19,22,23	2.01	2 (10%)	26,32,35	1.48	4 (15%)
1	3TD	A	1915	1	19,22,23	7.12	14 (73%)	23,32,35	1.86	4 (17%)
34	UR3	a	1498	34	19,22,23	1.16	2 (10%)	26,32,35	1.98	5 (19%)
1	PSU	A	2604	1	18,21,22	1.43	2 (11%)	21,30,33	2.01	5 (23%)
57	H2U	y	20	57	18,21,22	0.86	1 (5%)	19,30,33	1.48	4 (21%)
34	5MC	a	967	34	19,22,23	2.06	2 (10%)	26,32,35	1.52	4 (15%)
55	4SU	w	8	55	18,21,22	1.83	5 (27%)	25,30,33	2.23	5 (20%)
55	H2U	v	20	55	18,21,22	0.83	1 (5%)	19,30,33	1.59	3 (15%)
34	7MG	a	527	34	23,26,27	1.40	2 (8%)	27,39,42	2.58	7 (25%)

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
1	7MG	A	2069	60,1	-	2/7/37/38	0/3/3/3
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
57	PSU	y	32	57	-	0/7/25/26	0/2/2/2
1	PSU	A	746	60,1	-	1/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	0/9/27/28	0/2/2/2
1	2MA	A	2503	60,1	-	2/7/25/26	0/3/3/3
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
1	OMG	A	2251	55,1	-	0/9/27/28	0/3/3/3
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
34	PSU	a	516	34	-	3/7/25/26	0/2/2/2
1	OMU	A	2552	60,1	-	2/9/27/28	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	8/15/33/34	0/3/3/3
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
34	2MG	a	1207	34	-	2/9/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.24	1.66	1.43
1	A	1915	3TD	C2'-C1'	-15.57	1.32	1.53
1	A	1915	3TD	C6-C5	15.33	1.52	1.35
1	A	1915	3TD	C2-N1	8.61	1.47	1.37
34	a	967	5MC	C5-C4	7.81	1.50	1.44
34	a	1407	5MC	C5-C4	7.76	1.50	1.44
1	A	1962	5MC	C5-C4	7.54	1.49	1.44
1	A	747	5MC	C5-C4	7.52	1.49	1.44
57	y	37	MIA	C2-S10	-7.02	1.69	1.75
57	y	37	MIA	C13-C14	6.84	1.52	1.32
1	A	1915	3TD	O4'-C4'	-6.13	1.31	1.45
1	A	1915	3TD	C2-N3	5.82	1.50	1.38
34	a	1518	MA6	C5-C4	5.30	1.48	1.39
1	A	1915	3TD	C6-N1	5.25	1.44	1.36
34	a	1519	MA6	C5-C4	5.17	1.48	1.39
55	v	7	4SU	C4-S4	-4.93	1.60	1.68
55	w	8	4SU	C4-S4	-4.90	1.60	1.68
57	y	8	4SU	C4-S4	-4.89	1.60	1.68
1	A	2030	6MZ	C5-C4	4.77	1.47	1.39
57	y	37	MIA	C5-C4	4.75	1.47	1.39
1	A	1618	6MZ	C5-C4	4.70	1.47	1.39
1	A	2503	2MA	C5-C4	4.68	1.47	1.39
1	A	2580	PSU	C6-C5	4.56	1.40	1.35
1	A	1911	PSU	C6-C5	4.48	1.40	1.35
1	A	746	PSU	C6-C5	4.40	1.40	1.35
1	A	2604	PSU	C6-C5	4.37	1.40	1.35
1	A	2605	PSU	C6-C5	4.35	1.40	1.35
1	A	2457	PSU	C6-C5	4.34	1.40	1.35
1	A	1917	PSU	C6-C5	4.34	1.40	1.35
1	A	955	PSU	C6-C5	4.29	1.40	1.35
1	A	2504	PSU	C6-C5	4.28	1.40	1.35
55	v	55	PSU	C6-C5	4.16	1.39	1.35
34	a	516	PSU	C6-C5	4.11	1.39	1.35
57	y	55	PSU	C6-C5	4.11	1.39	1.35
55	w	55	PSU	C6-C5	4.11	1.39	1.35
1	A	2069	7MG	C4-N9	-4.00	1.33	1.37
1	A	1915	3TD	C10-N3	-3.61	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1518	MA6	C5-C6	3.55	1.50	1.41
34	a	1519	MA6	C5-C6	3.54	1.50	1.41
1	A	745	1MG	C2-N1	3.54	1.43	1.37
34	a	527	7MG	C5-C4	3.49	1.48	1.37
57	y	46	7MG	C5-C4	3.49	1.48	1.37
57	y	39	PSU	C6-C5	3.42	1.39	1.35
57	y	32	PSU	C6-C5	3.36	1.39	1.35
34	a	1407	5MC	C6-C5	3.35	1.40	1.34
1	A	2251	OMG	C5-C4	3.33	1.47	1.38
1	A	1939	5MU	C6-C5	3.32	1.40	1.34
1	A	745	1MG	C5-C4	3.27	1.47	1.38
1	A	2069	7MG	C5-C4	3.26	1.47	1.37
1	A	1835	2MG	C5-C4	3.25	1.47	1.38
55	v	54	5MU	C6-C5	3.23	1.39	1.34
57	y	46	7MG	C4-N9	-3.23	1.33	1.37
1	A	1962	5MC	C6-C5	3.23	1.39	1.34
34	a	966	2MG	C5-C4	3.18	1.47	1.38
34	a	1516	2MG	C5-C4	3.15	1.47	1.38
34	a	967	5MC	C6-C5	3.14	1.39	1.34
34	a	1207	2MG	C5-C4	3.12	1.47	1.38
57	y	54	5MU	C2-N1	3.09	1.43	1.38
55	w	8	4SU	C2-N1	3.08	1.43	1.38
55	w	54	5MU	C2-N1	3.08	1.43	1.38
55	w	54	5MU	C6-C5	3.07	1.39	1.34
34	a	527	7MG	C4-N9	-3.04	1.34	1.37
1	A	2445	2MG	C5-C4	3.01	1.47	1.38
57	y	8	4SU	C2-N1	2.99	1.43	1.38
1	A	2552	OMU	C2-N1	2.95	1.43	1.38
57	y	8	4SU	C4-N3	-2.95	1.34	1.37
1	A	747	5MC	C6-C5	2.93	1.39	1.34
55	w	8	4SU	C4-N3	-2.92	1.34	1.37
57	y	54	5MU	C6-C5	2.92	1.39	1.34
1	A	2503	2MA	C5-C6	2.90	1.49	1.41
1	A	1915	3TD	O2'-C2'	2.90	1.50	1.43
34	a	1498	UR3	C2-N1	2.84	1.42	1.38
1	A	1618	6MZ	C5-C6	2.83	1.48	1.41
1	A	1915	3TD	O3'-C3'	-2.81	1.36	1.43
55	v	54	5MU	C2-N1	2.80	1.42	1.38
57	y	37	MIA	C5-C6	2.80	1.48	1.41
1	A	2030	6MZ	C5-C6	2.79	1.48	1.41
55	w	54	5MU	C4-C5	2.79	1.49	1.44
1	A	1939	5MU	C2-N1	2.77	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	C4-C5	2.77	1.49	1.44
55	v	7	4SU	C2-N1	2.76	1.42	1.38
55	v	54	5MU	C4-C5	2.64	1.49	1.44
1	A	1915	3TD	O2-C2	-2.62	1.18	1.23
55	v	7	4SU	C4-N3	-2.62	1.34	1.37
57	y	32	PSU	C4-N3	-2.61	1.34	1.38
57	y	54	5MU	C4-C5	2.61	1.49	1.44
57	y	39	PSU	C4-N3	-2.58	1.34	1.38
1	A	2552	OMU	C4-N3	-2.56	1.34	1.38
1	A	1835	2MG	C2-N3	2.55	1.36	1.32
34	a	966	2MG	C2-N3	2.54	1.36	1.32
34	a	1516	2MG	C2-N3	2.53	1.36	1.32
55	v	54	5MU	C4-N3	-2.47	1.34	1.38
57	y	8	4SU	C5-C4	-2.47	1.39	1.42
1	A	2457	PSU	C4-N3	-2.46	1.34	1.38
55	v	7	4SU	C5-C4	-2.46	1.39	1.42
1	A	2580	PSU	C4-N3	-2.44	1.34	1.38
55	w	8	4SU	C5-C4	-2.44	1.39	1.42
1	A	2503	2MA	C8-N7	2.44	1.36	1.31
34	a	1518	MA6	C6-N6	2.43	1.43	1.36
1	A	1939	5MU	C4-N3	-2.42	1.34	1.38
1	A	2604	PSU	C4-N3	-2.40	1.34	1.38
34	a	1519	MA6	C5-N7	-2.40	1.34	1.39
34	a	1518	MA6	C5-N7	-2.37	1.34	1.39
1	A	2251	OMG	C5-N7	-2.36	1.34	1.39
1	A	2504	PSU	C4-N3	-2.36	1.34	1.38
1	A	1917	PSU	C4-N3	-2.35	1.34	1.38
57	y	37	MIA	C8-N7	2.35	1.36	1.31
1	A	1618	6MZ	C8-N7	2.35	1.36	1.31
34	a	1519	MA6	C6-N6	2.35	1.43	1.36
1	A	2605	PSU	C4-N3	-2.34	1.34	1.38
1	A	2030	6MZ	C8-N7	2.33	1.36	1.31
1	A	2449	H2U	C2-N3	-2.33	1.33	1.38
34	a	1207	2MG	C2-N3	2.32	1.36	1.32
57	y	55	PSU	C4-N3	-2.32	1.34	1.38
34	a	1207	2MG	C5-N7	-2.31	1.34	1.39
57	y	54	5MU	C4-N3	-2.30	1.34	1.38
1	A	1835	2MG	C6-N1	-2.30	1.34	1.38
1	A	2503	2MA	C5-N7	-2.29	1.34	1.39
1	A	2449	H2U	C4-N3	-2.29	1.33	1.37
1	A	2445	2MG	C2-N3	2.29	1.36	1.32
34	a	516	PSU	C4-N3	-2.27	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1835	2MG	C5-N7	-2.25	1.34	1.39
1	A	746	PSU	C4-N3	-2.25	1.34	1.38
57	y	37	MIA	C5-N7	-2.24	1.35	1.39
34	a	1519	MA6	C8-N7	2.24	1.36	1.31
55	w	54	5MU	C4-N3	-2.24	1.34	1.38
1	A	1618	6MZ	C5-N7	-2.24	1.35	1.39
1	A	2251	OMG	C6-N1	-2.23	1.34	1.38
1	A	955	PSU	C4-N3	-2.21	1.34	1.38
1	A	2030	6MZ	C5-N7	-2.21	1.35	1.39
34	a	1518	MA6	C8-N7	2.20	1.35	1.31
55	w	55	PSU	C4-N3	-2.20	1.34	1.38
34	a	966	2MG	C5-N7	-2.19	1.34	1.39
55	v	55	PSU	C4-N3	-2.18	1.34	1.38
1	A	1915	3TD	C3'-C4'	2.18	1.58	1.53
1	A	745	1MG	C5-N7	-2.17	1.34	1.39
1	A	2445	2MG	C5-N7	-2.15	1.34	1.39
57	y	20	H2U	C2-N3	-2.15	1.34	1.38
34	a	1516	2MG	C5-N7	-2.14	1.34	1.39
1	A	1911	PSU	C4-N3	-2.12	1.34	1.38
34	a	1498	UR3	C6-C5	2.10	1.40	1.35
57	y	16	H2U	C2-N3	-2.09	1.34	1.38
1	A	2069	7MG	C8-N9	2.08	1.47	1.45
55	v	20	H2U	C2-N3	-2.08	1.34	1.38
57	y	46	7MG	C5-C6	2.07	1.48	1.43
1	A	2552	OMU	C6-C5	2.06	1.39	1.35
1	A	2069	7MG	C5-C6	2.05	1.48	1.43
34	a	1402	4OC	C6-C5	2.04	1.39	1.35
55	w	8	4SU	C6-C5	2.03	1.39	1.35
57	y	8	4SU	C6-C5	2.01	1.39	1.35
1	A	1915	3TD	O4-C4	-2.01	1.19	1.23
1	A	1915	3TD	C4-N3	2.01	1.44	1.40
55	w	20	H2U	C2-N3	-2.01	1.34	1.38
34	a	966	2MG	C6-N1	-2.00	1.35	1.38
34	a	1516	2MG	C6-N1	-2.00	1.35	1.38

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	37	MIA	C12-C13-C14	-8.94	110.97	127.01
34	a	527	7MG	N9-C4-N3	8.47	137.88	125.46
34	a	966	2MG	C2-N3-C4	8.36	122.46	112.00
34	a	1207	2MG	C2-N3-C4	8.31	122.40	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	46	7MG	N9-C4-N3	8.12	137.35	125.46
57	y	37	MIA	C5-C4-N3	-7.91	118.84	127.18
1	A	1835	2MG	C2-N3-C4	7.91	121.89	112.00
1	A	2445	2MG	C2-N3-C4	7.89	121.87	112.00
34	a	1516	2MG	C2-N3-C4	7.67	121.59	112.00
1	A	2503	2MA	C5-C4-N3	-7.64	119.14	127.18
1	A	2069	7MG	N9-C4-N3	7.28	136.13	125.46
34	a	1207	2MG	N1-C2-N2	7.27	123.98	116.56
34	a	1498	UR3	C4-N3-C2	-6.94	118.99	124.58
34	a	966	2MG	C5-C4-N3	-6.50	118.05	128.39
57	y	8	4SU	C4-N3-C2	-6.43	121.15	127.31
1	A	2251	OMG	C5-C4-N3	-6.42	118.18	128.39
55	v	7	4SU	C4-N3-C2	-6.41	121.17	127.31
57	y	39	PSU	N1-C2-N3	6.39	121.91	115.17
1	A	1835	2MG	C5-C4-N3	-6.38	118.24	128.39
57	y	32	PSU	N1-C2-N3	6.34	121.86	115.17
57	y	55	PSU	N1-C2-N3	6.31	121.82	115.17
34	a	1207	2MG	C5-C4-N3	-6.24	118.46	128.39
55	w	55	PSU	N1-C2-N3	6.23	121.74	115.17
1	A	2457	PSU	N1-C2-N3	6.20	121.71	115.17
1	A	1911	PSU	N1-C2-N3	6.20	121.71	115.17
57	y	37	MIA	N3-C4-N9	6.20	134.86	126.99
55	w	8	4SU	C4-N3-C2	-6.19	121.38	127.31
1	A	746	PSU	N1-C2-N3	6.19	121.69	115.17
1	A	2504	PSU	N1-C2-N3	6.18	121.69	115.17
34	a	516	PSU	N1-C2-N3	6.14	121.64	115.17
1	A	1917	PSU	N1-C2-N3	6.12	121.62	115.17
55	v	55	PSU	N1-C2-N3	6.09	121.59	115.17
1	A	2605	PSU	N1-C2-N3	6.08	121.58	115.17
34	a	1516	2MG	C5-C4-N3	-6.05	118.76	128.39
1	A	2604	PSU	N1-C2-N3	6.04	121.54	115.17
1	A	2580	PSU	N1-C2-N3	5.97	121.46	115.17
1	A	955	PSU	N1-C2-N3	5.96	121.46	115.17
1	A	2030	6MZ	C5-C4-N3	-5.89	118.60	126.72
1	A	2445	2MG	C5-C4-N3	-5.85	119.08	128.39
34	a	1519	MA6	C5-C4-N3	-5.84	118.67	126.72
1	A	1618	6MZ	C5-C4-N3	-5.80	118.73	126.72
1	A	2503	2MA	N3-C4-N9	5.79	134.33	126.99
34	a	1518	MA6	C5-C4-N3	-5.66	118.93	126.72
34	a	966	2MG	N1-C2-N2	5.59	122.27	116.56
1	A	1915	3TD	N1-C2-N3	5.50	120.13	116.13
1	A	745	1MG	C5-C4-N3	-5.47	119.69	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	7	4SU	C5-C4-N3	5.36	119.74	114.75
34	a	527	7MG	C5-C4-N3	-5.26	118.26	128.13
57	y	8	4SU	C5-C4-N3	5.25	119.63	114.75
55	w	8	4SU	C5-C4-N3	5.25	119.63	114.75
1	A	2251	OMG	C2-N3-C4	5.16	121.19	112.30
55	v	20	H2U	O4'-C1'-N1	5.15	116.32	109.30
1	A	1939	5MU	N3-C2-N1	5.12	121.56	114.89
57	y	46	7MG	C5-C4-N3	-5.09	118.58	128.13
55	v	54	5MU	N3-C2-N1	4.98	121.38	114.89
34	a	1518	MA6	C2-N1-C6	4.92	123.84	111.83
57	y	8	4SU	N3-C2-N1	4.90	121.26	114.89
1	A	2069	7MG	C5-C4-N3	-4.89	118.94	128.13
1	A	2069	7MG	C2-N3-C4	4.88	120.71	112.30
34	a	1519	MA6	C4-C5-N7	-4.88	105.00	110.58
1	A	2552	OMU	N3-C2-N1	4.88	121.24	114.89
55	w	54	5MU	N3-C2-N1	4.87	121.24	114.89
34	a	1207	2MG	N2-C2-N3	-4.85	114.33	120.51
34	a	1519	MA6	C2-N1-C6	4.82	123.59	111.83
1	A	745	1MG	C2-N3-C4	4.78	122.72	111.98
57	y	54	5MU	N3-C2-N1	4.74	121.06	114.89
1	A	2251	OMG	N9-C4-N3	4.72	135.38	125.95
34	a	966	2MG	N9-C4-N3	4.67	135.29	125.95
1	A	2030	6MZ	N3-C4-N9	4.66	135.09	127.17
1	A	1939	5MU	C4-N3-C2	-4.65	121.25	127.34
57	y	46	7MG	C2-N3-C4	4.64	120.29	112.30
1	A	2069	7MG	N9-C8-N7	-4.64	96.80	103.37
34	a	527	7MG	C2-N3-C4	4.62	120.26	112.30
1	A	1618	6MZ	N3-C4-N9	4.57	134.94	127.17
34	a	1518	MA6	C4-C5-N7	-4.55	105.39	110.58
1	A	2552	OMU	C4-N3-C2	-4.53	120.99	126.61
55	w	8	4SU	N3-C2-N1	4.52	120.78	114.89
55	v	7	4SU	C5-C4-S4	-4.52	119.15	124.31
55	w	20	H2U	O4'-C1'-N1	4.50	115.43	109.30
1	A	1835	2MG	N9-C4-N3	4.50	134.95	125.95
57	y	46	7MG	N9-C8-N7	-4.48	97.02	103.37
55	v	7	4SU	N3-C2-N1	4.43	120.66	114.89
57	y	54	5MU	C4-N3-C2	-4.43	121.53	127.34
55	w	54	5MU	C4-N3-C2	-4.42	121.55	127.34
34	a	527	7MG	N9-C8-N7	-4.39	97.16	103.37
1	A	1911	PSU	O2-C2-N1	-4.29	118.36	122.79
55	v	54	5MU	C4-N3-C2	-4.18	121.86	127.34
57	y	54	5MU	C5-C4-N3	4.17	118.95	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	39	PSU	C4-N3-C2	-4.17	120.62	126.37
34	a	1207	2MG	N9-C4-N3	4.14	134.22	125.95
57	y	32	PSU	C4-N3-C2	-4.13	120.69	126.37
1	A	1939	5MU	C5-C4-N3	4.13	118.91	115.32
1	A	1915	3TD	C4-N3-C2	-4.13	120.25	124.61
34	a	1519	MA6	N3-C4-N9	4.11	134.16	127.17
1	A	747	5MC	CM5-C5-C6	-4.11	117.29	122.85
1	A	745	1MG	N9-C4-N3	4.08	134.11	125.95
34	a	1516	2MG	N9-C4-N3	4.07	134.09	125.95
55	w	54	5MU	C5-C4-N3	4.03	118.83	115.32
1	A	2605	PSU	C4-N3-C2	-4.03	120.82	126.37
1	A	955	PSU	C4-N3-C2	-4.01	120.85	126.37
34	a	1407	5MC	C5-C4-N3	-4.00	117.65	121.75
57	y	55	PSU	C4-N3-C2	-3.99	120.87	126.37
34	a	516	PSU	C4-N3-C2	-3.98	120.88	126.37
1	A	1911	PSU	C4-N3-C2	-3.96	120.91	126.37
34	a	1518	MA6	N3-C4-N9	3.94	133.87	127.17
1	A	2504	PSU	C4-N3-C2	-3.93	120.96	126.37
55	w	55	PSU	C4-N3-C2	-3.92	120.97	126.37
57	y	37	MIA	C16-C14-C13	-3.89	110.97	122.66
1	A	746	PSU	C4-N3-C2	-3.89	121.01	126.37
57	y	37	MIA	C15-C14-C13	-3.89	110.99	122.66
1	A	2445	2MG	N9-C4-N3	3.88	133.72	125.95
1	A	745	1MG	N2-C2-N1	3.88	121.91	118.79
1	A	2445	2MG	C6-C5-N7	3.87	137.33	130.29
57	y	8	4SU	C5-C4-S4	-3.86	119.89	124.31
1	A	2604	PSU	C4-N3-C2	-3.81	121.13	126.37
34	a	1518	MA6	N1-C2-N3	-3.81	122.82	128.58
1	A	2457	PSU	C4-N3-C2	-3.80	121.14	126.37
57	y	32	PSU	C3'-C2'-C1'	3.79	106.17	101.69
55	v	54	5MU	C5-C4-N3	3.79	118.62	115.32
57	y	39	PSU	C3'-C2'-C1'	3.79	106.16	101.69
34	a	1518	MA6	C2-N3-C4	3.79	121.08	111.83
34	a	967	5MC	CM5-C5-C6	-3.77	117.75	122.85
34	a	1519	MA6	C2-N3-C4	3.76	121.01	111.83
1	A	2503	2MA	C4-C5-N7	-3.75	106.30	110.58
55	v	55	PSU	C4-N3-C2	-3.74	121.21	126.37
1	A	1917	PSU	C4-N3-C2	-3.74	121.21	126.37
1	A	2030	6MZ	C2-N3-C4	3.72	120.93	111.83
55	w	8	4SU	C5-C4-S4	-3.71	120.07	124.31
1	A	1618	6MZ	C2-N3-C4	3.69	120.84	111.83
34	a	1519	MA6	C10-N6-C6	-3.65	111.23	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	54	5MU	O4-C4-C5	-3.64	120.76	124.92
34	a	1516	2MG	C6-C5-N7	3.63	136.89	130.29
57	y	32	PSU	O2-C2-N1	-3.61	119.06	122.79
57	y	39	PSU	O2-C2-N1	-3.61	119.07	122.79
1	A	955	PSU	O2-C2-N1	-3.59	119.08	122.79
34	a	1519	MA6	N1-C2-N3	-3.59	123.15	128.58
57	y	55	PSU	O2-C2-N1	-3.59	119.09	122.79
1	A	746	PSU	O2-C2-N1	-3.58	119.09	122.79
1	A	2580	PSU	C4-N3-C2	-3.57	121.45	126.37
1	A	2445	2MG	N1-C2-N2	3.56	120.20	116.56
34	a	516	PSU	O2-C2-N1	-3.56	119.12	122.79
1	A	747	5MC	C5-C4-N3	-3.56	118.11	121.75
1	A	2449	H2U	N3-C2-N1	3.56	120.22	116.65
34	a	967	5MC	C5-C4-N3	-3.56	118.11	121.75
55	w	55	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A	1917	PSU	O2-C2-N1	-3.54	119.14	122.79
34	a	1518	MA6	C9-N6-C6	-3.53	111.55	120.52
1	A	2030	6MZ	C4-C5-N7	-3.52	106.55	110.58
55	v	55	PSU	O2-C2-N1	-3.52	119.16	122.79
34	a	1519	MA6	C5-N7-C8	3.51	108.97	103.45
57	y	37	MIA	C4-C5-N7	-3.50	106.58	110.58
1	A	2504	PSU	O2-C2-N1	-3.47	119.21	122.79
1	A	1962	5MC	C5-C4-N3	-3.47	118.20	121.75
34	a	1407	5MC	CM5-C5-C6	-3.46	118.16	122.85
34	a	1207	2MG	C6-C5-N7	3.46	136.59	130.29
1	A	1962	5MC	CM5-C5-C6	-3.46	118.17	122.85
1	A	1618	6MZ	C4-C5-N7	-3.46	106.63	110.58
1	A	2552	OMU	C5-C4-N3	3.44	119.62	114.80
1	A	2457	PSU	O2-C2-N1	-3.42	119.26	122.79
34	a	966	2MG	N2-C2-N3	-3.41	116.16	120.51
1	A	955	PSU	C6-C5-C4	-3.41	115.88	118.17
1	A	2030	6MZ	C6-C5-N7	3.40	136.14	132.43
57	y	37	MIA	C2-N3-C4	3.39	121.18	112.29
1	A	1835	2MG	C6-C5-N7	3.39	136.46	130.29
1	A	1618	6MZ	C6-C5-N7	3.38	136.12	132.43
1	A	2604	PSU	O2-C2-N1	-3.38	119.31	122.79
1	A	2580	PSU	C6-C5-C4	-3.36	115.91	118.17
1	A	2605	PSU	O2-C2-N1	-3.35	119.33	122.79
34	a	1498	UR3	C1'-N1-C2	3.35	122.53	117.04
57	y	20	H2U	O4'-C1'-N1	3.35	113.86	109.30
55	w	54	5MU	C5M-C5-C4	3.33	122.33	118.78
57	y	37	MIA	C6-C5-N7	3.31	136.03	132.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C6-C5-N7	3.31	136.31	130.29
1	A	2449	H2U	O4'-C1'-N1	3.30	113.80	109.30
34	a	1498	UR3	C5-C4-N3	3.29	119.37	115.04
1	A	2552	OMU	C1'-N1-C2	3.25	123.44	117.59
57	y	54	5MU	C5M-C5-C4	3.24	122.24	118.78
1	A	1618	6MZ	N1-C2-N3	-3.22	123.71	128.58
1	A	2030	6MZ	N1-C2-N3	-3.21	123.73	128.58
1	A	1962	5MC	O2-C2-N3	-3.18	117.32	122.33
34	a	1518	MA6	O4'-C1'-N9	3.17	114.18	108.09
34	a	1518	MA6	C5-N7-C8	3.16	108.42	103.45
34	a	1407	5MC	O2-C2-N3	-3.16	117.36	122.33
1	A	1911	PSU	C6-C5-C4	-3.14	116.06	118.17
55	w	54	5MU	O4-C4-C5	-3.12	121.35	124.92
1	A	1939	5MU	O4-C4-C5	-3.08	121.39	124.92
1	A	2449	H2U	C5-C4-N3	3.08	119.97	116.69
57	y	8	4SU	C6-N1-C2	-3.07	117.26	121.00
1	A	2030	6MZ	C9-N6-C6	-3.07	120.01	122.85
1	A	2498	OMC	O2-C2-N3	-3.06	117.50	122.33
1	A	1618	6MZ	C9-N6-C6	-3.04	120.03	122.85
1	A	2069	7MG	C5-C6-N1	3.02	116.25	110.94
34	a	527	7MG	C5-C6-N1	2.98	116.18	110.94
57	y	37	MIA	C11-S10-C2	-2.96	100.03	102.25
1	A	1917	PSU	C3'-C2'-C1'	2.93	105.15	101.69
55	w	55	PSU	C3'-C2'-C1'	2.92	105.14	101.69
57	y	46	7MG	C5-C6-N1	2.92	116.08	110.94
1	A	2552	OMU	O4-C4-C5	-2.92	120.13	125.16
1	A	1939	5MU	O4'-C1'-N1	2.91	114.96	108.36
1	A	2251	OMG	C6-C5-N7	2.90	135.56	130.29
34	a	1516	2MG	C4-C5-N7	-2.89	106.08	110.67
1	A	2605	PSU	C6-C5-C4	-2.88	116.23	118.17
55	v	54	5MU	O4-C4-C5	-2.86	121.64	124.92
55	v	54	5MU	C5M-C5-C4	2.86	121.84	118.78
1	A	2580	PSU	O2-C2-N1	-2.85	119.85	122.79
1	A	2503	2MA	C2-N1-C6	2.85	122.47	118.10
1	A	2445	2MG	C4-C5-N7	-2.84	106.17	110.67
55	w	20	H2U	C5-C6-N1	-2.84	102.93	111.52
1	A	2580	PSU	C3'-C2'-C1'	2.82	105.02	101.69
34	a	967	5MC	O2-C2-N3	-2.82	117.88	122.33
1	A	2503	2MA	C5-N7-C8	2.80	107.85	103.45
1	A	2552	OMU	C6-N1-C2	-2.80	117.59	121.00
1	A	2503	2MA	C4-N9-C8	2.78	108.65	105.74
57	y	20	H2U	C5-C4-N3	2.76	119.63	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1498	UR3	C6-N1-C2	-2.73	119.57	121.80
34	a	1207	2MG	C4-C5-N7	-2.71	106.37	110.67
34	a	1407	5MC	O4'-C1'-N1	2.71	114.50	108.36
1	A	1939	5MU	C5-C6-N1	-2.71	120.38	123.31
1	A	745	1MG	C4-C5-N7	-2.69	106.41	110.67
34	a	1402	4OC	C6-C5-C4	2.67	120.21	117.00
55	w	8	4SU	C6-N1-C2	-2.66	117.76	121.00
1	A	745	1MG	C6-C5-N7	2.66	135.26	129.36
34	a	1498	UR3	C3U-N3-C2	2.65	121.95	117.33
57	y	16	H2U	C5-C4-N3	2.64	119.50	116.69
34	a	1207	2MG	O6-C6-C5	-2.63	119.60	126.53
1	A	2030	6MZ	C4-N9-C8	2.62	108.49	105.74
1	A	2457	PSU	C6-C5-C4	-2.62	116.41	118.17
1	A	2503	2MA	C6-C5-N7	2.62	137.14	132.09
57	y	37	MIA	C4-N9-C8	2.62	108.48	105.74
1	A	2498	OMC	O4'-C1'-N1	2.61	114.27	108.36
1	A	1939	5MU	C5M-C5-C4	2.60	121.56	118.78
34	a	966	2MG	C4-C5-N7	-2.59	106.56	110.67
1	A	1835	2MG	C4-C5-N7	-2.59	106.56	110.67
1	A	746	PSU	C6-C5-C4	-2.57	116.44	118.17
57	y	37	MIA	C5-N7-C8	2.57	107.49	103.45
34	a	1516	2MG	N1-C2-N2	2.56	119.18	116.56
1	A	1618	6MZ	C4-N9-C8	2.56	108.43	105.74
55	v	20	H2U	C5-C4-N3	2.56	119.41	116.69
1	A	2457	PSU	C3'-C2'-C1'	2.56	104.71	101.69
1	A	2030	6MZ	C5-N7-C8	2.55	107.46	103.45
1	A	1917	PSU	C6-C5-C4	-2.55	116.45	118.17
1	A	1618	6MZ	C5-N7-C8	2.54	107.44	103.45
1	A	2069	7MG	O4'-C1'-N9	2.53	112.74	109.30
1	A	2604	PSU	C6-C5-C4	-2.52	116.47	118.17
55	v	55	PSU	C6-C5-C4	-2.51	116.48	118.17
34	a	527	7MG	O4'-C1'-N9	2.51	112.72	109.30
57	y	37	MIA	C3'-C2'-C1'	2.49	106.18	101.46
34	a	1402	4OC	O2-C2-N3	-2.49	118.41	122.33
34	a	516	PSU	C6-C5-C4	-2.48	116.50	118.17
1	A	2504	PSU	C6-C5-C4	-2.48	116.50	118.17
1	A	1618	6MZ	C3'-C2'-C1'	2.48	106.15	101.46
34	a	1519	MA6	C10-N6-C9	-2.47	108.24	116.18
1	A	2030	6MZ	C3'-C2'-C1'	2.47	106.14	101.46
34	a	1402	4OC	C5-C4-N3	-2.47	118.74	122.60
1	A	2552	OMU	O2-C2-N3	-2.43	117.00	121.49
1	A	2251	OMG	C4-C5-N7	-2.43	106.81	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	16	H2U	O4'-C1'-N1	2.43	112.61	109.30
55	v	54	5MU	O4'-C1'-N1	2.42	113.84	108.36
34	a	1519	MA6	O4'-C1'-N9	2.36	112.62	108.09
57	y	37	MIA	N3-C2-N1	-2.35	122.70	127.00
1	A	2069	7MG	N2-C2-N1	2.35	121.72	116.76
34	a	1402	4OC	O4'-C1'-N1	2.34	113.67	108.36
57	y	37	MIA	C2-N1-C6	2.34	121.98	117.54
1	A	1911	PSU	C3'-C2'-C1'	2.34	104.44	101.69
34	a	516	PSU	C3'-C2'-C1'	2.33	104.43	101.69
57	y	8	4SU	O2-C2-N3	-2.32	117.21	121.49
1	A	747	5MC	C5-C6-N1	-2.32	120.80	123.31
55	v	7	4SU	C6-N1-C2	-2.32	118.18	121.00
55	w	54	5MU	C5M-C5-C6	-2.31	119.72	122.85
34	a	1519	MA6	C6-C5-N7	2.31	137.12	133.43
1	A	2503	2MA	N9-C8-N7	-2.30	110.67	113.94
1	A	1915	3TD	C3'-C2'-C1'	2.30	104.41	101.69
34	a	1519	MA6	C4-N9-C8	2.30	108.16	105.74
34	a	966	2MG	O6-C6-C5	-2.29	120.49	126.53
1	A	2069	7MG	C6-C5-C4	-2.29	118.38	122.40
34	a	1519	MA6	N9-C8-N7	-2.28	110.70	113.94
1	A	2069	7MG	N2-C2-N3	-2.28	115.22	119.67
55	w	54	5MU	C3'-C2'-C1'	2.27	105.77	101.46
1	A	2445	2MG	O6-C6-C5	-2.27	120.55	126.53
34	a	1519	MA6	C9-N6-C6	-2.27	114.76	120.52
34	a	967	5MC	CM5-C5-C4	2.27	124.23	120.51
1	A	2069	7MG	O6-C6-C5	-2.26	122.08	127.62
34	a	1518	MA6	C6-C5-N7	2.25	137.02	133.43
1	A	2498	OMC	C2'-C1'-N1	-2.25	109.98	114.24
34	a	1207	2MG	C2-N1-C6	-2.23	121.85	124.55
57	y	16	H2U	C3'-C2'-C1'	2.23	105.68	101.46
34	a	1519	MA6	C2'-C1'-N9	-2.22	107.78	113.30
57	y	20	H2U	C3'-C2'-C1'	2.21	105.65	101.46
55	w	54	5MU	O4'-C1'-N1	2.21	113.37	108.36
1	A	2251	OMG	O6-C6-C5	-2.21	120.69	126.53
34	a	527	7MG	O6-C6-C5	-2.20	122.22	127.62
55	v	54	5MU	C6-N1-C2	-2.20	119.12	121.30
55	v	20	H2U	C5-C6-N1	-2.19	104.89	111.52
57	y	39	PSU	C5-C6-N1	-2.18	119.11	122.14
57	y	32	PSU	C5-C6-N1	-2.18	119.12	122.14
55	v	7	4SU	O4'-C1'-N1	2.17	113.28	108.36
1	A	747	5MC	CM5-C5-C4	2.17	124.07	120.51
1	A	2503	2MA	N6-C6-N1	2.17	119.95	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	55	PSU	C3'-C2'-C1'	2.16	104.23	101.69
57	y	54	5MU	C1'-N1-C2	2.15	121.46	117.59
1	A	745	1MG	O6-C6-C5	-2.15	119.05	124.59
57	y	8	4SU	C1'-N1-C2	2.15	121.45	117.59
34	a	966	2MG	C5-C6-N1	2.14	118.71	113.25
1	A	1939	5MU	O2-C2-N1	-2.14	120.01	122.80
34	a	1516	2MG	O6-C6-C5	-2.14	120.89	126.53
34	a	1518	MA6	C3'-C2'-C1'	2.13	105.49	101.46
1	A	746	PSU	C3'-C2'-C1'	2.12	104.19	101.69
57	y	54	5MU	C6-N1-C2	-2.11	119.20	121.30
1	A	1835	2MG	C5-C6-N1	2.10	118.61	113.25
1	A	2552	OMU	O4'-C1'-N1	2.10	113.12	108.36
1	A	2445	2MG	C5-C6-N1	2.10	118.59	113.25
57	y	46	7MG	C6-C5-C4	-2.10	118.71	122.40
55	w	54	5MU	C5-C6-N1	-2.10	121.04	123.31
34	a	1207	2MG	C5-C6-N1	2.09	118.58	113.25
57	y	54	5MU	C5M-C5-C6	-2.09	120.02	122.85
1	A	2069	7MG	C6-C5-N7	2.09	135.17	131.93
57	y	46	7MG	O6-C6-C5	-2.09	122.49	127.62
1	A	2604	PSU	C3'-C2'-C1'	2.09	104.15	101.69
55	w	54	5MU	O2-C2-N3	-2.08	117.65	121.49
1	A	1915	3TD	C1'-C5-C4	2.08	120.76	117.61
55	w	55	PSU	C6-C5-C4	-2.07	116.78	118.17
34	a	1407	5MC	C5-C4-N4	2.06	124.30	121.39
1	A	745	1MG	C8-N7-C5	2.06	107.93	104.26
34	a	1516	2MG	C2-N1-C6	-2.05	122.08	124.55
1	A	1962	5MC	CM5-C5-C4	2.05	123.87	120.51
55	v	54	5MU	C5-C6-N1	-2.04	121.09	123.31
34	a	966	2MG	C2-N1-C6	-2.04	122.08	124.55
57	y	16	H2U	C5-C6-N1	-2.04	105.34	111.52
57	y	20	H2U	C5-C6-N1	-2.04	105.35	111.52
1	A	2445	2MG	C2-N1-C6	-2.04	122.09	124.55
1	A	1835	2MG	O6-C6-C5	-2.03	121.17	126.53
34	a	966	2MG	C3'-C2'-C1'	2.03	105.29	101.46
1	A	2445	2MG	N2-C2-N3	-2.02	117.94	120.51
57	y	37	MIA	N6-C6-N1	2.02	121.04	118.33
1	A	747	5MC	O2-C2-N3	-2.01	119.16	122.33
55	w	20	H2U	C5-C4-N3	2.01	118.82	116.69
34	a	1407	5MC	CM5-C5-C4	2.00	123.80	120.51
55	v	54	5MU	O2-C2-N3	-2.00	117.80	121.49

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1402	4OC	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2503	2MA	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
57	y	20	H2U	O4'-C1'-N1-C2
57	y	20	H2U	O4'-C1'-N1-C6
57	y	37	MIA	N6-C12-C13-C14
57	y	37	MIA	C12-C13-C14-C15
57	y	37	MIA	C12-C13-C14-C16
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
57	y	39	PSU	C3'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
55	v	7	4SU	O4'-C4'-C5'-O5'
1	A	1917	PSU	C3'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2503	2MA	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
57	y	39	PSU	O4'-C4'-C5'-O5'
57	y	55	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	a	1518	MA6	O4'-C1'-N9-C4
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
34	a	1402	4OC	C3'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C6
34	a	1207	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C8
1	A	2069	7MG	O4'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
57	y	55	PSU	O4'-C4'-C5'-O5'
57	y	37	MIA	N1-C6-N6-C12
1	A	2504	PSU	C3'-C4'-C5'-O5'
55	v	7	4SU	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
34	a	1207	2MG	O4'-C4'-C5'-O5'
57	y	37	MIA	C5-C6-N6-C12
57	y	37	MIA	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
55	w	8	4SU	C2'-C1'-N1-C2
1	A	1618	6MZ	C2'-C1'-N9-C4
34	a	516	PSU	O4'-C4'-C5'-O5'
1	A	1939	5MU	O4'-C4'-C5'-O5'
57	y	37	MIA	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C2'-C1'-N9-C8
34	a	516	PSU	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C2
34	a	527	7MG	C4'-C5'-O5'-P
1	A	1618	6MZ	C4'-C5'-O5'-P
34	a	527	7MG	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
57	y	46	7MG	O4'-C1'-N9-C8
34	a	516	PSU	O4'-C1'-C5-C6
55	w	55	PSU	O4'-C1'-C5-C6
1	A	746	PSU	O4'-C1'-C5-C6
1	A	1939	5MU	C3'-C4'-C5'-O5'
55	w	20	H2U	C2'-C1'-N1-C6
57	y	37	MIA	C2'-C1'-N9-C8

Continued on next page...

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Mol	Chain	Res	Type	Atoms
57	y	8	4SU	C2'-C1'-N1-C2
1	A	2580	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	y	32	PSU	2	0
1	A	2030	6MZ	9	0
34	a	516	PSU	1	0
1	A	1618	6MZ	8	0
57	y	37	MIA	10	0
34	a	966	2MG	2	0
57	y	39	PSU	6	0
1	A	1917	PSU	3	0
1	A	1915	3TD	1	0
34	a	1498	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1417 ligands modelled in this entry, 1414 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	FME	A	3001	-	8,9,10	0.50	0	8,9,11	0.95	0
62	PHE	z	401	-	10,11,12	0.48	0	8,13,15	0.16	0
63	GTP	z	402	-	33,34,34	1.20	3 (9%)	50,54,54	1.73	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	A	3001	-	-	1/7/9/11	-
62	PHE	z	401	-	-	0/5/6/8	0/1/1/1
63	GTP	z	402	-	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.30	1.47	1.38
63	z	402	GTP	C5-N7	-2.18	1.34	1.39
63	z	402	GTP	C6-N1	-2.07	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C5-C4-N3	-6.11	118.67	128.39
63	z	402	GTP	C2-N3-C4	5.13	121.13	112.30
63	z	402	GTP	N9-C4-N3	4.58	135.11	125.95
63	z	402	GTP	C6-C5-N7	3.29	136.28	130.29
63	z	402	GTP	C4-C5-N7	-2.57	106.60	110.67
63	z	402	GTP	O6-C6-C5	-2.27	120.54	126.53
63	z	402	GTP	C3'-C2'-C1'	2.23	105.68	101.46
63	z	402	GTP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

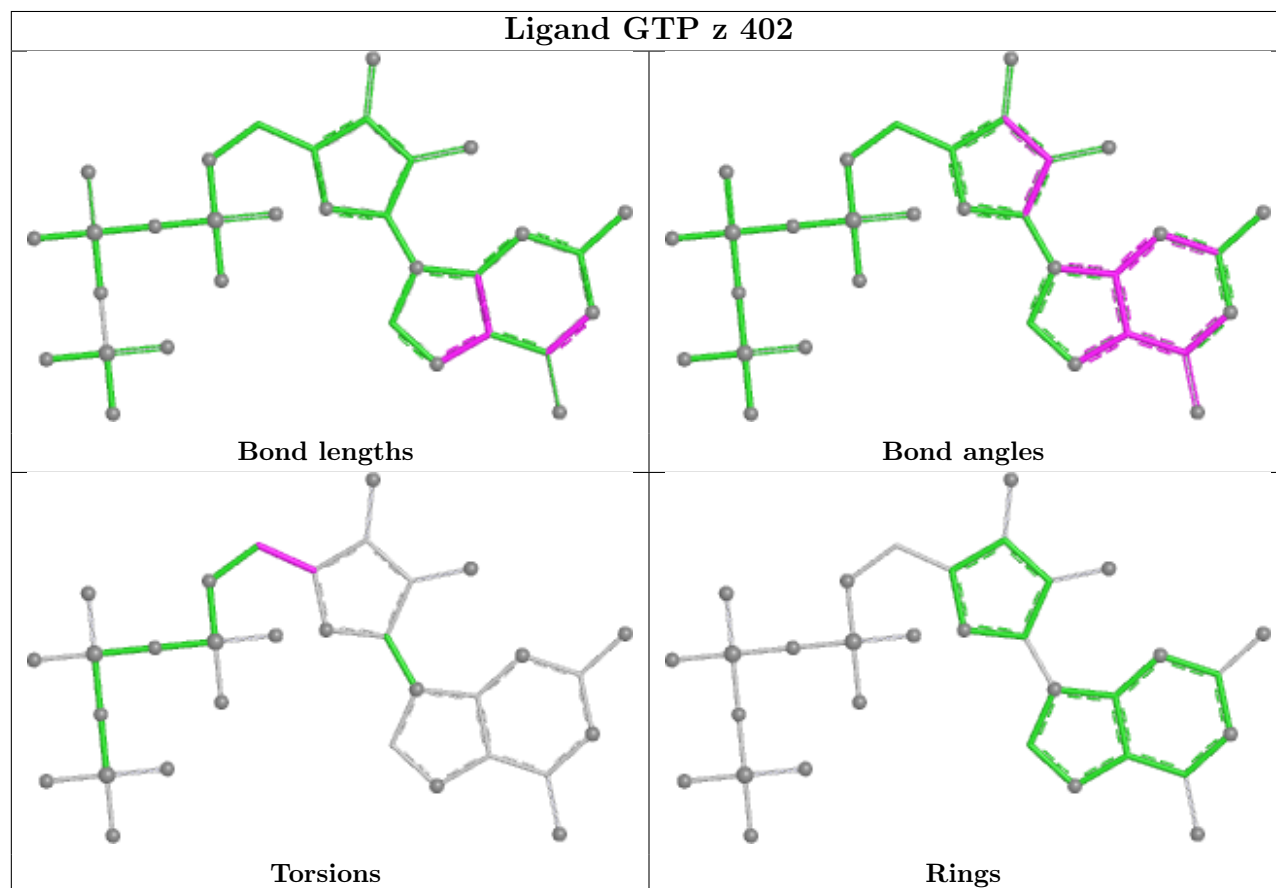
Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O-C-CA-CB
63	z	402	GTP	C3'-C4'-C5'-O5'
63	z	402	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	w	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	117:U	O3'	18:G	P	1.14

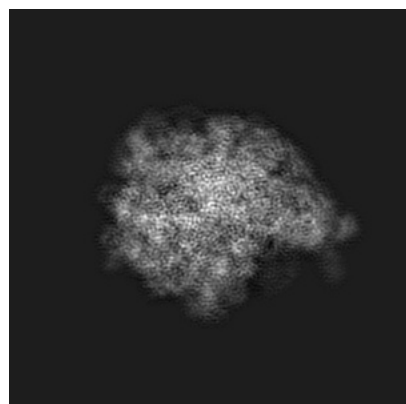
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8828. These allow visual inspection of the internal detail of the map and identification of artifacts.

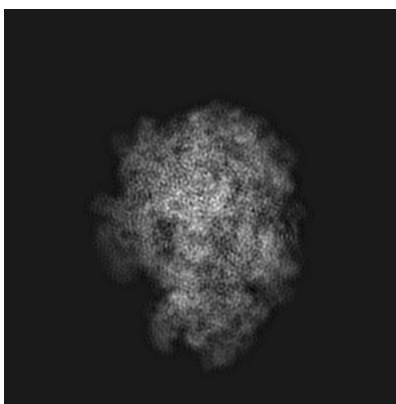
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

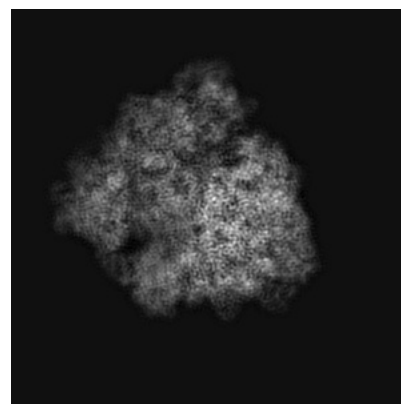
6.1.1 Primary map



X

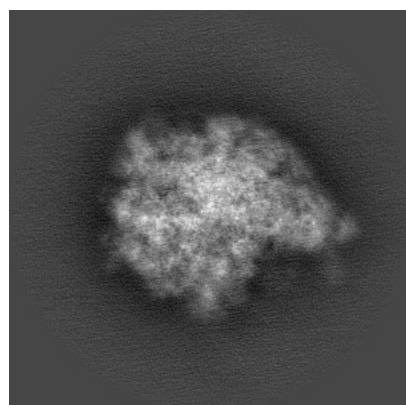


Y

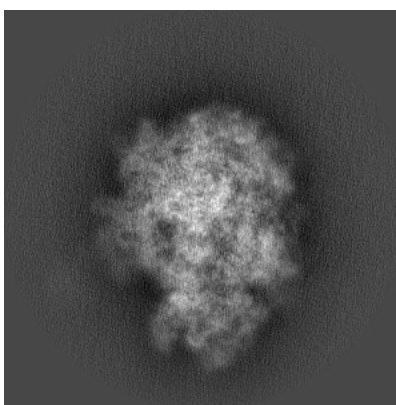


Z

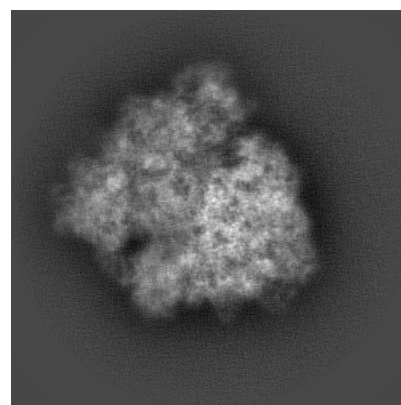
6.1.2 Raw map



X



Y

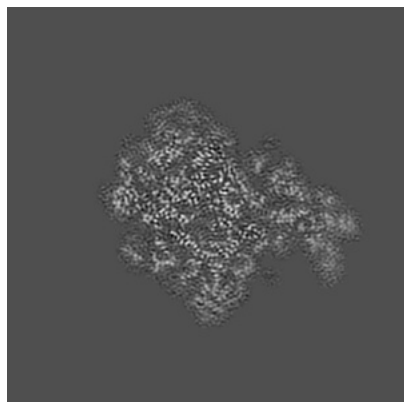


Z

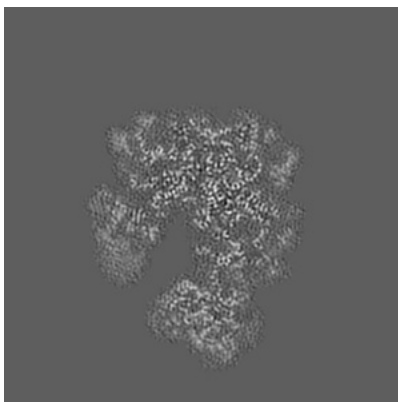
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

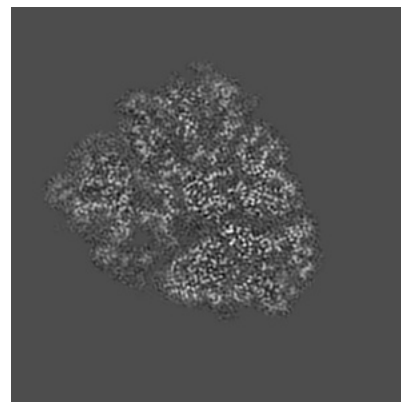
6.2.1 Primary map



X Index: 199

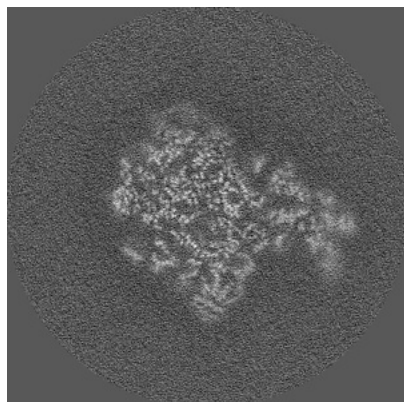


Y Index: 199

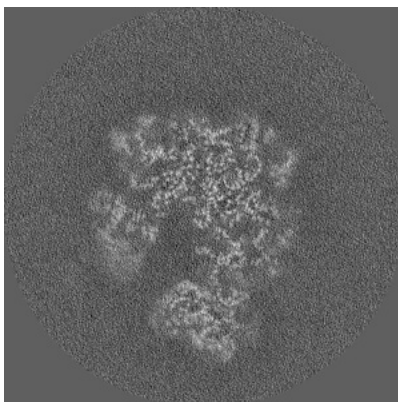


Z Index: 199

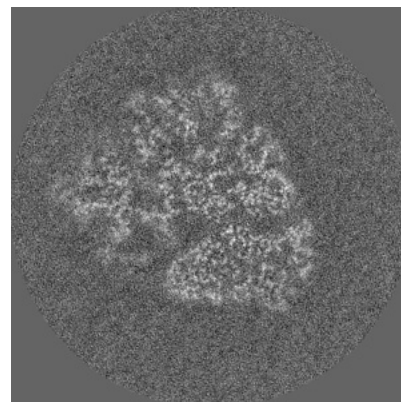
6.2.2 Raw map



X Index: 199



Y Index: 199

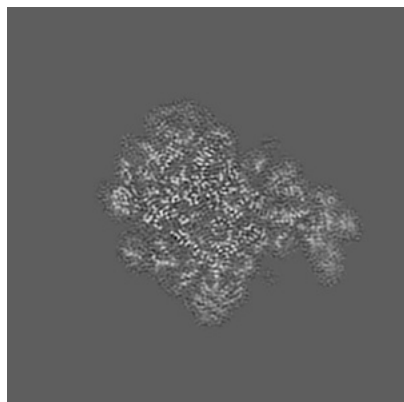


Z Index: 199

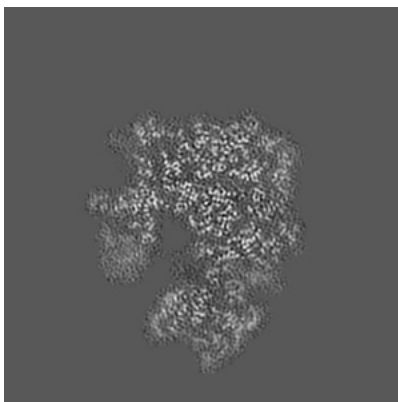
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

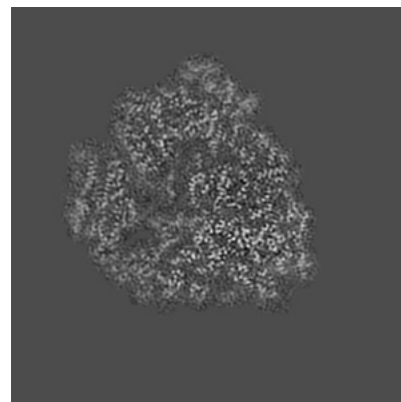
6.3.1 Primary map



X Index: 200

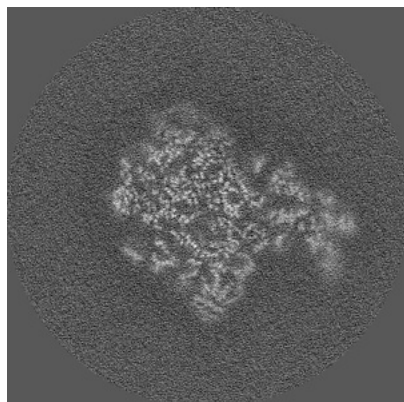


Y Index: 207

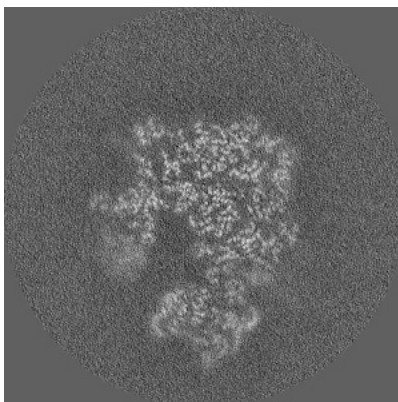


Z Index: 189

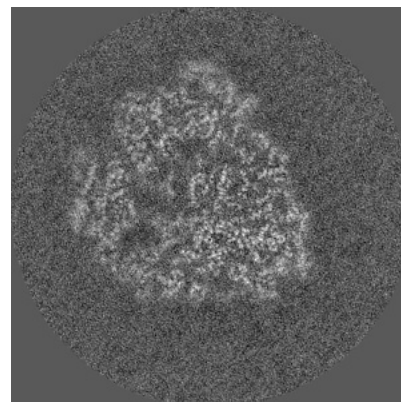
6.3.2 Raw map



X Index: 199



Y Index: 207

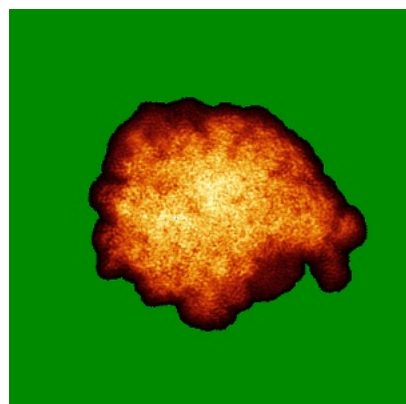


Z Index: 189

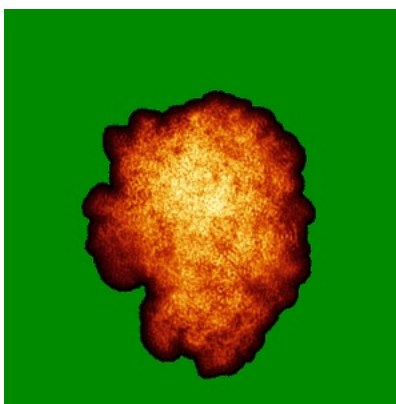
The images above show the largest variance slices of the map in three orthogonal directions.

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

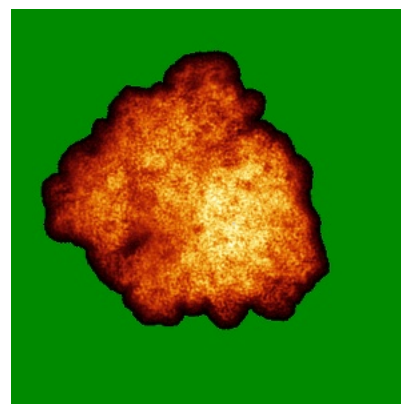
6.4.1 Primary map



X

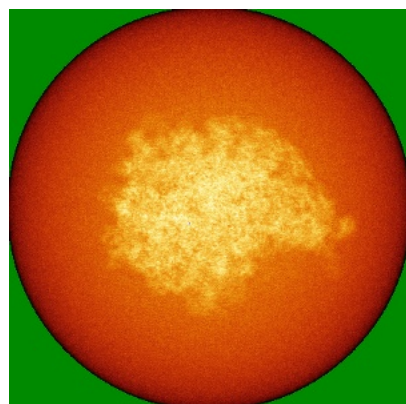


Y

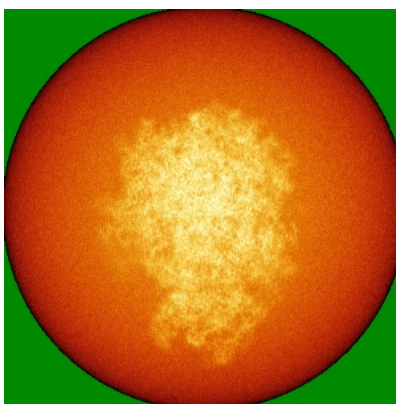


Z

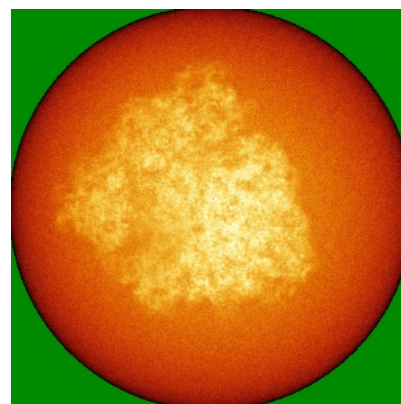
6.4.2 Raw map



X



Y



Z

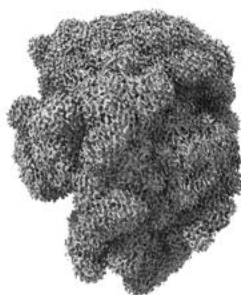
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



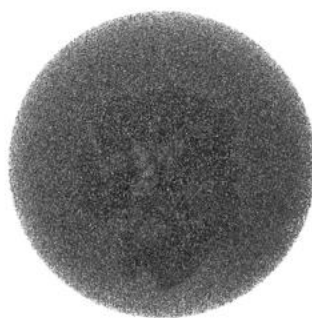
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00651. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

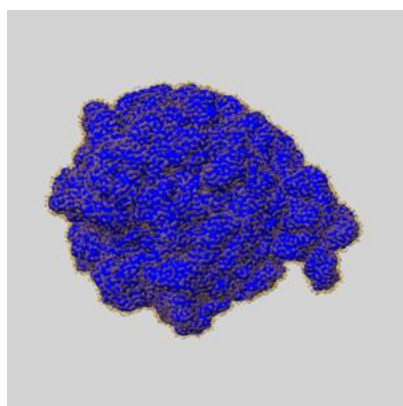
6.6 Mask visualisation [i](#)

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

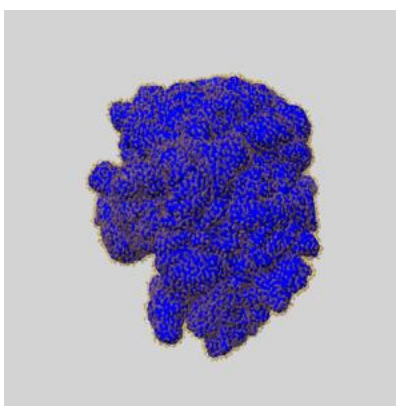
A mask typically either:

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

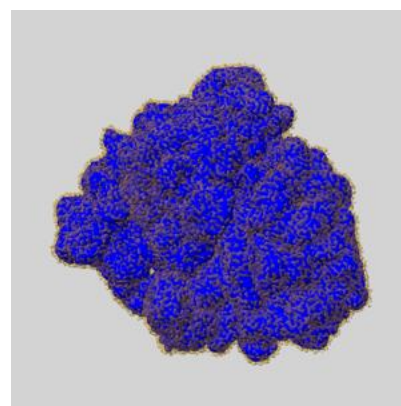
6.6.1 emd_8828_msk_1.map [i](#)



X



Y

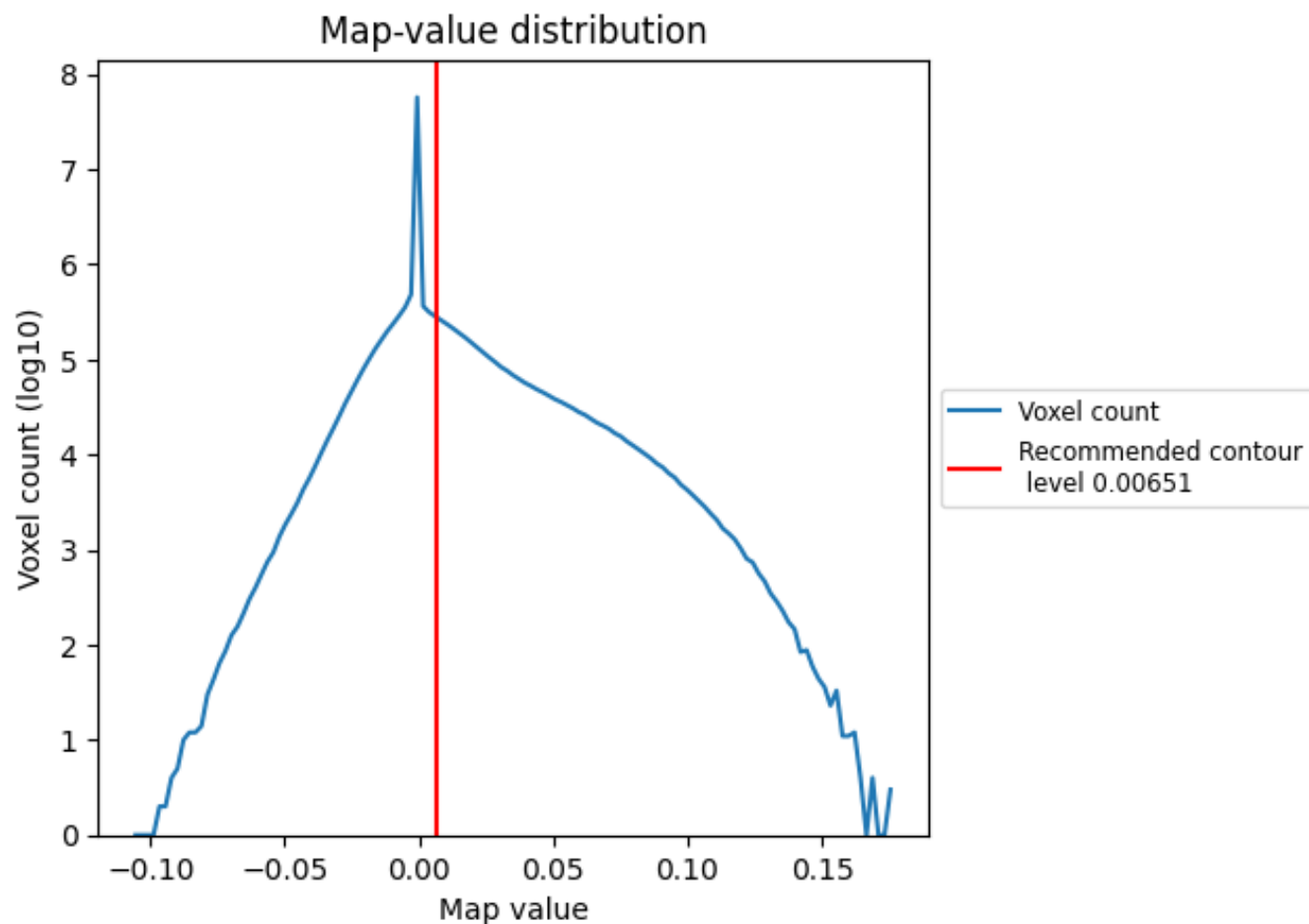


Z

7 Map analysis [i](#)

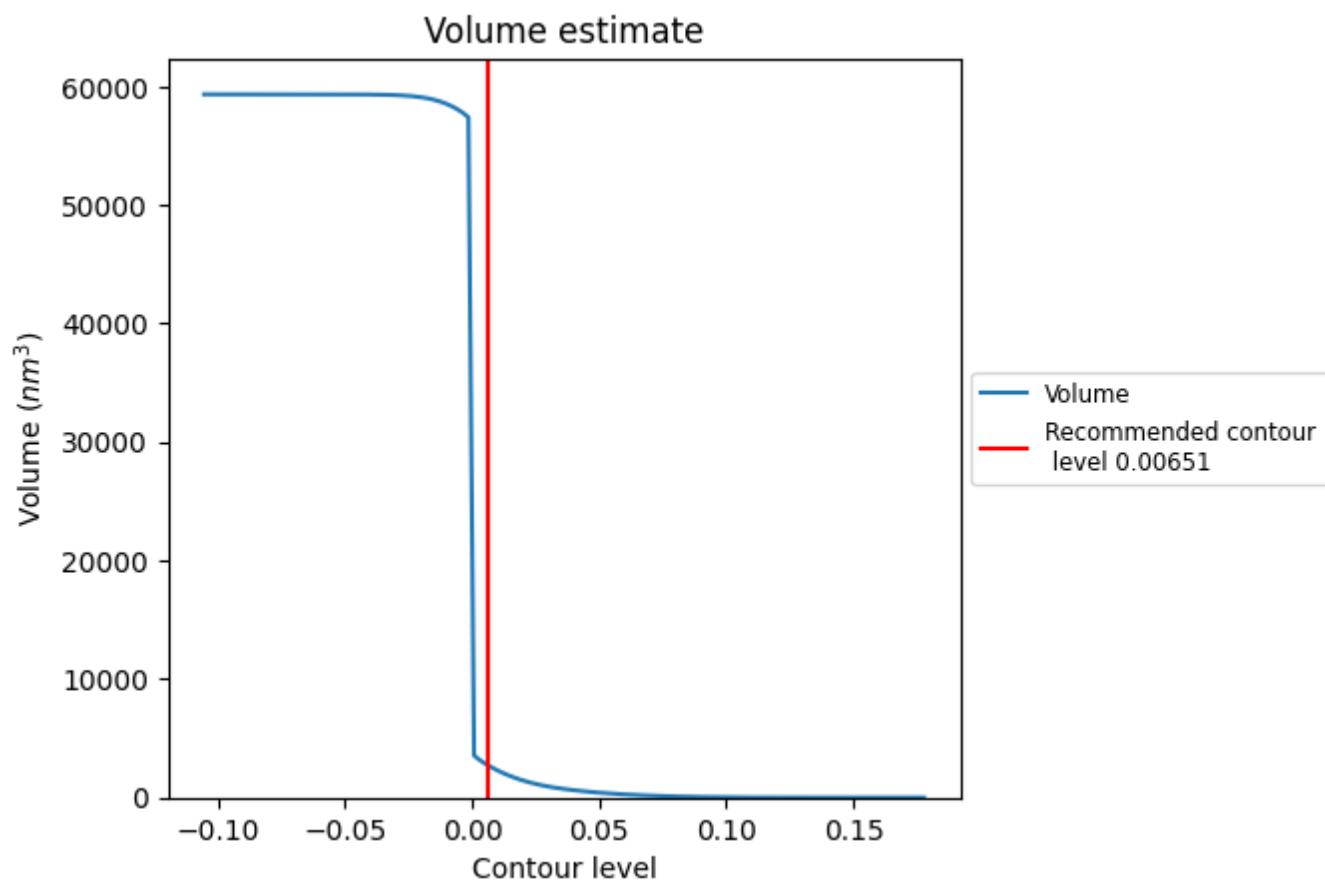
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

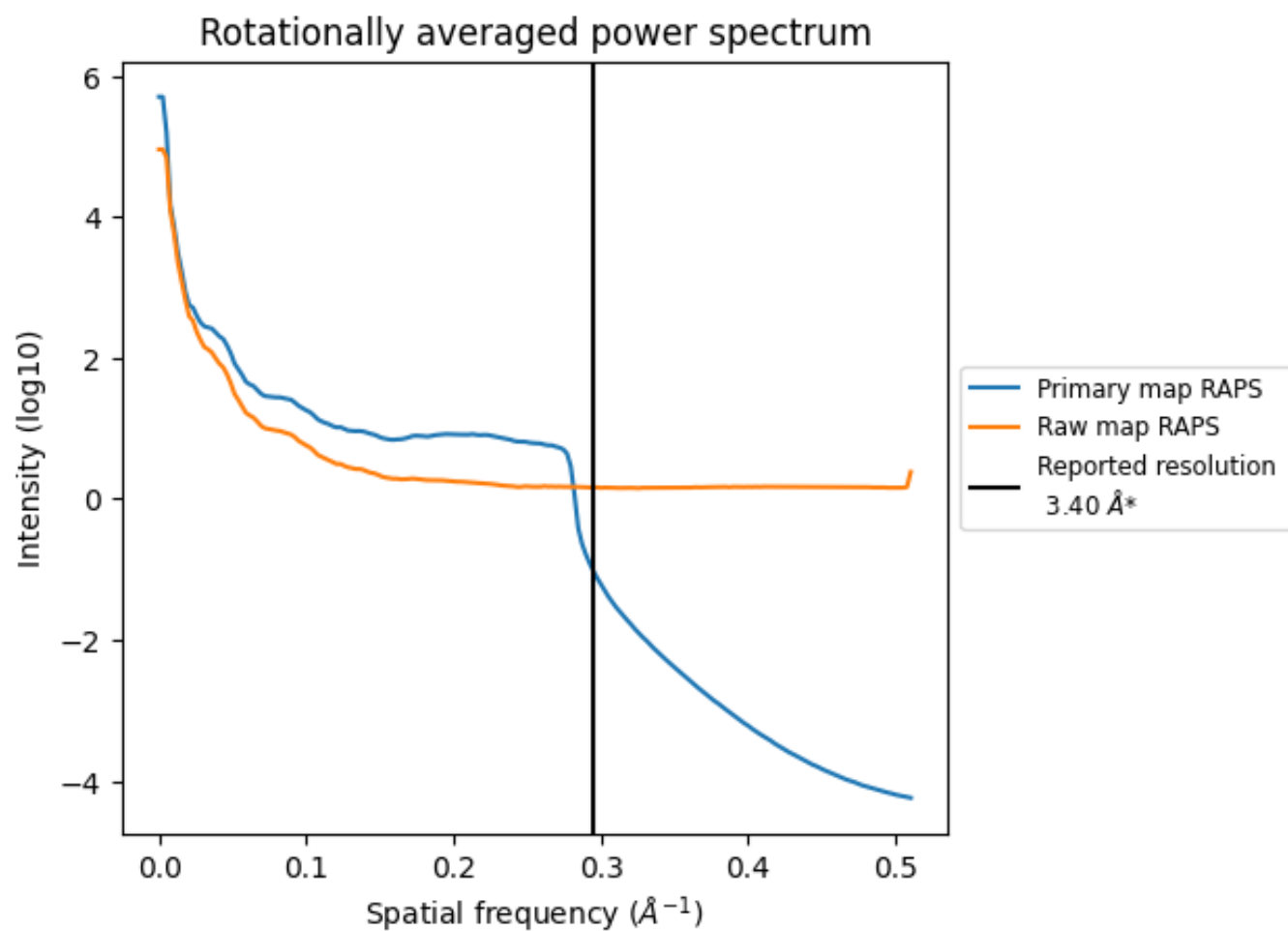
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2690 nm³; this corresponds to an approximate mass of 2430 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 ⓘ

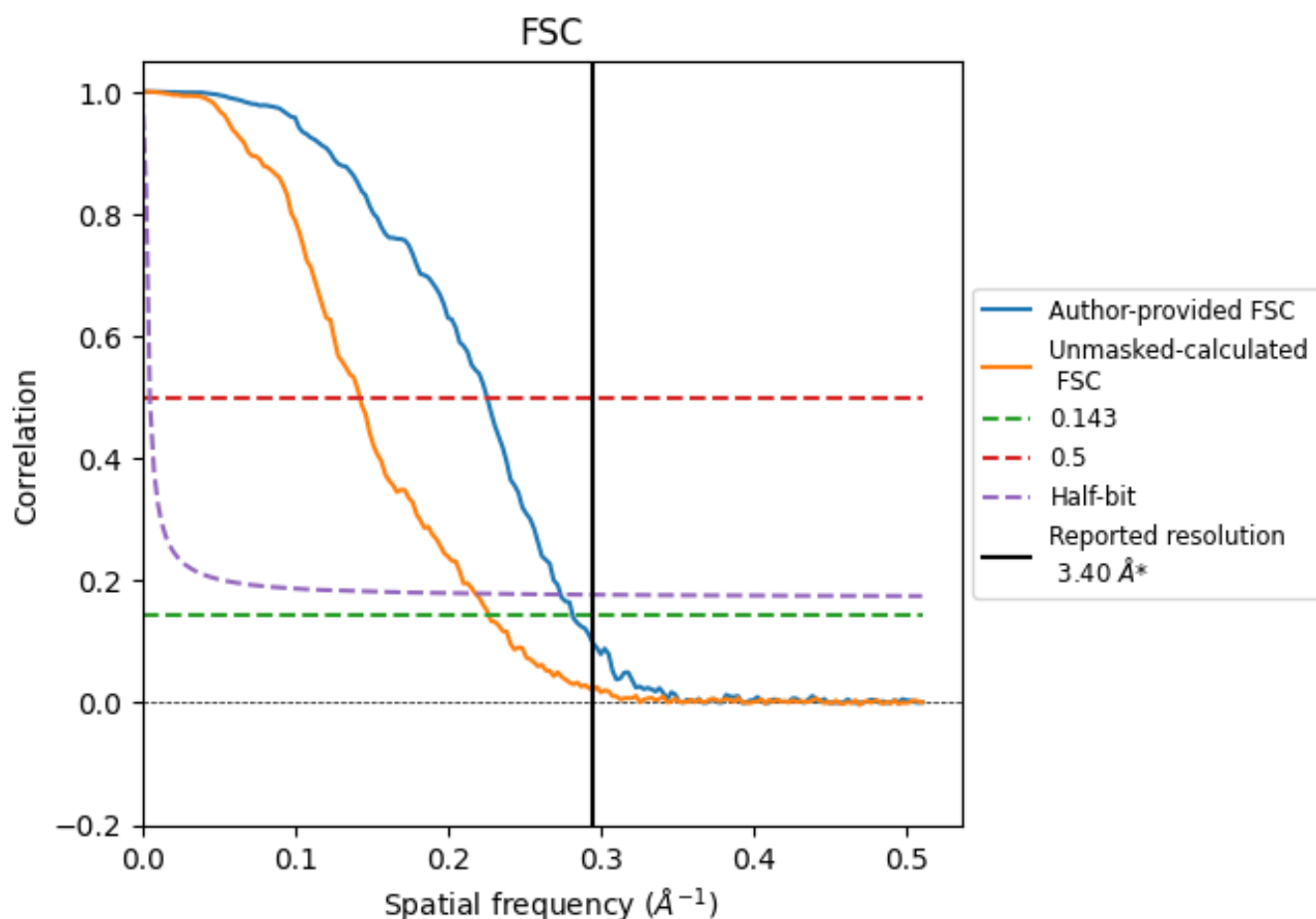


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

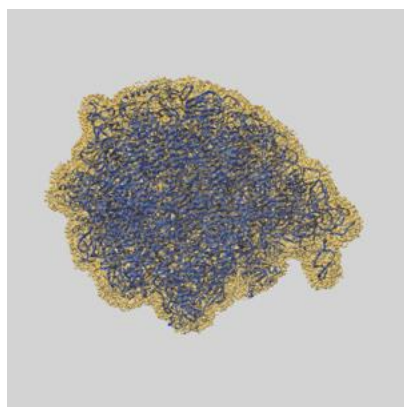
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.55	4.43	3.65
Unmasked-calculated*	4.41	7.03	4.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.4 by more than 10 %

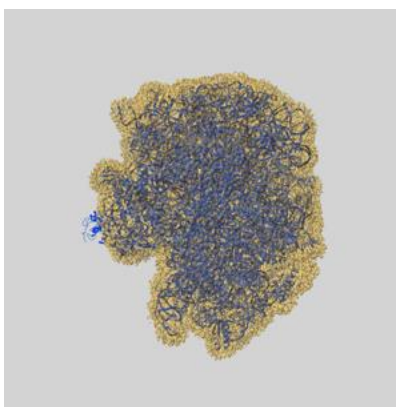
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8828 and PDB model 5WFK. Per-residue inclusion information can be found in section [3](#) on page [20](#).

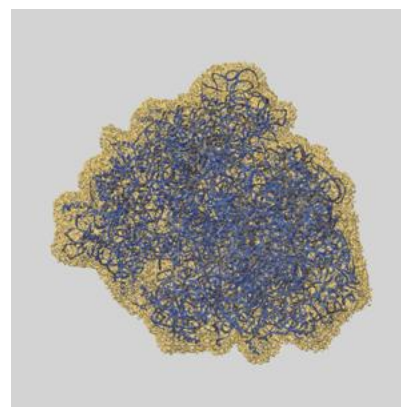
9.1 Map-model overlay [i](#)



X



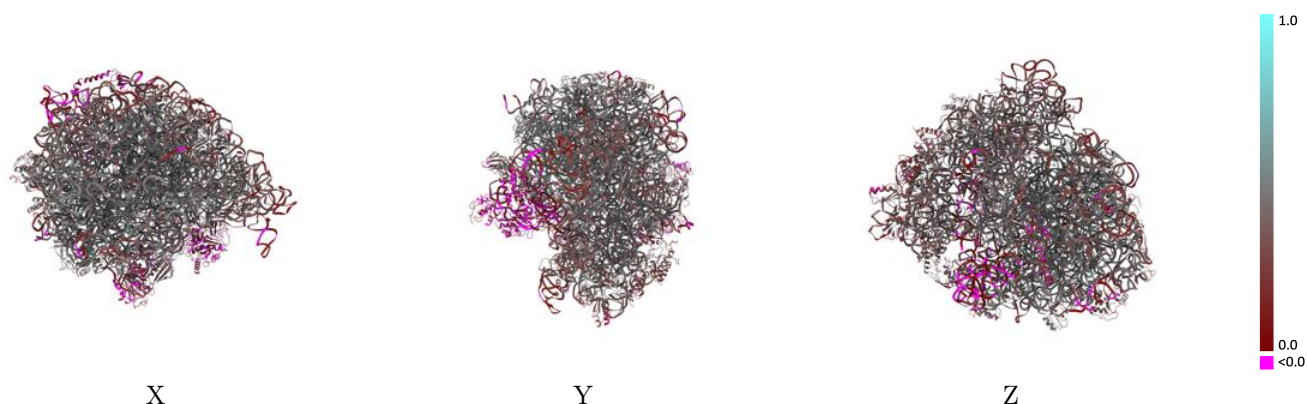
Y



Z

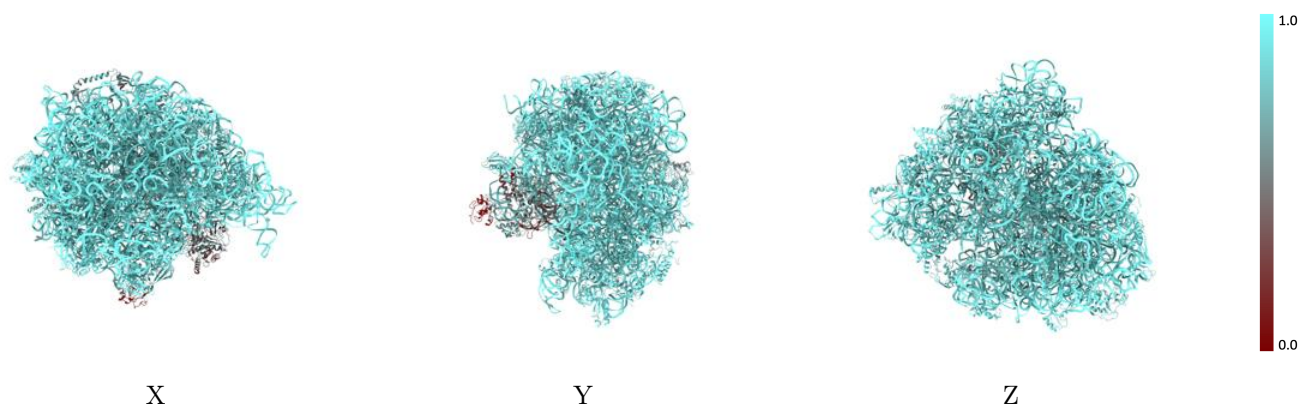
The images above show the 3D surface view of the map at the recommended contour level 0.00651 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



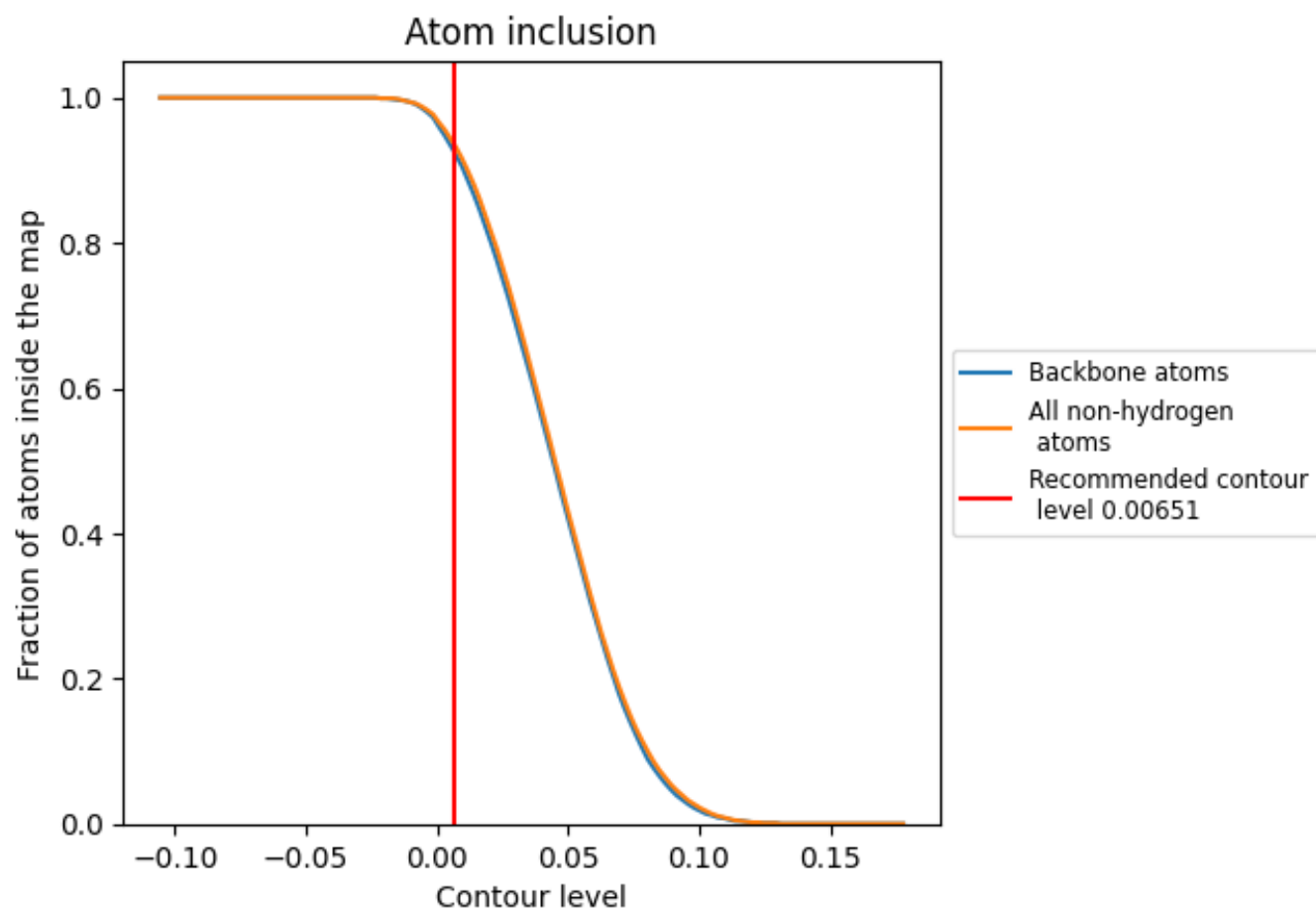
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00651).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00651) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.3850
0	 0.9570	 0.4610
1	 0.9490	 0.4460
2	 0.9420	 0.4890
3	 0.9550	 0.5060
4	 0.9420	 0.4720
5	 0.2240	 0.0090
6	 0.8750	 0.2840
A	 0.9750	 0.4110
B	 0.9820	 0.3850
C	 0.9430	 0.4790
D	 0.9510	 0.4630
E	 0.9360	 0.4350
F	 0.9180	 0.3570
G	 0.9190	 0.3330
H	 0.6960	 0.1660
I	 0.6220	 0.0280
J	 0.9360	 0.4550
K	 0.9110	 0.4420
L	 0.9520	 0.4600
M	 0.9540	 0.4540
N	 0.9540	 0.4660
O	 0.9560	 0.4010
P	 0.9490	 0.4570
Q	 0.9650	 0.4790
R	 0.9460	 0.4430
S	 0.9470	 0.4680
T	 0.9220	 0.4040
U	 0.9480	 0.4070
V	 0.9350	 0.4100
W	 0.9530	 0.4760
X	 0.9390	 0.4610
Y	 0.9400	 0.3860
Z	 0.9650	 0.4830
a	 0.9790	 0.3950



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Chain	Atom inclusion	Q-score
b	 0.8980	 0.3220
c	 0.9120	 0.3800
d	 0.9210	 0.3730
e	 0.9290	 0.4330
f	 0.9100	 0.3760
g	 0.9140	 0.3330
h	 0.9170	 0.4230
i	 0.9010	 0.3380
j	 0.9030	 0.3210
k	 0.9470	 0.4200
l	 0.9160	 0.4290
m	 0.9220	 0.3680
n	 0.9180	 0.3640
o	 0.9360	 0.4000
p	 0.9360	 0.4140
q	 0.9370	 0.3840
r	 0.9030	 0.3720
s	 0.9450	 0.3970
t	 0.9140	 0.3650
u	 0.8180	 0.2530
v	 0.9550	 0.3780
w	 0.7960	 0.0760
x	 0.9330	 0.3390
y	 0.5280	 0.0470
z	 0.4550	 0.0680