



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 04:52 PM EDT

PDB ID : 5WDT / pdb_00005wdt
EMDB ID : EMD-8813
Title : 70S ribosome-EF-Tu H84A complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

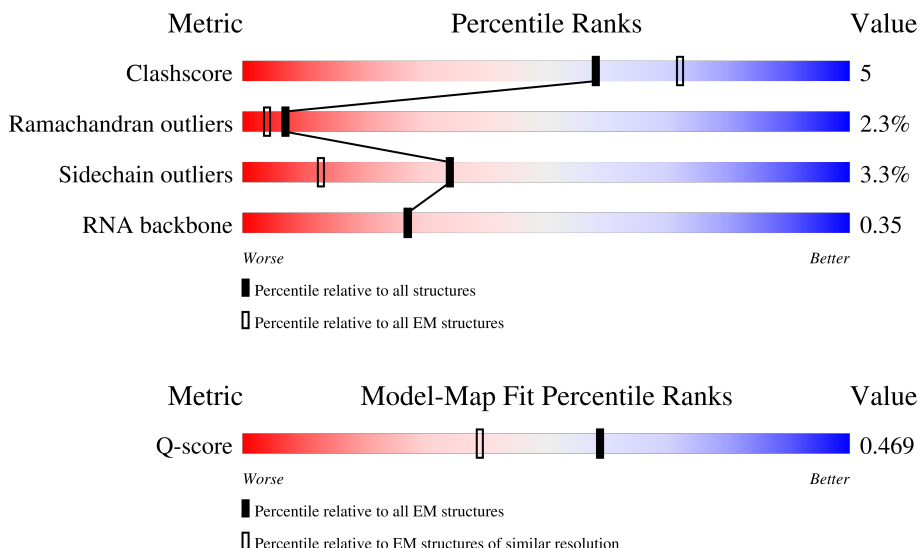
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 Å.

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



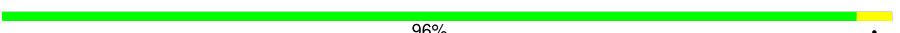
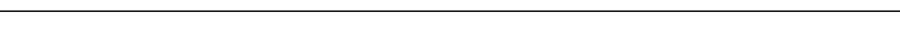
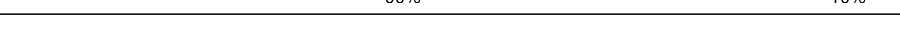
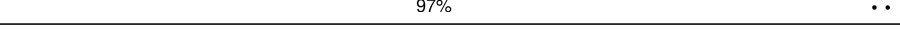
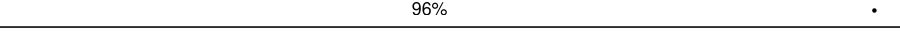
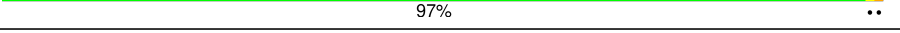
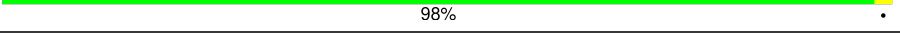
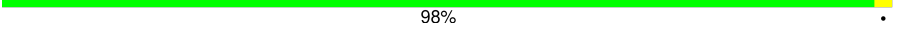
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	

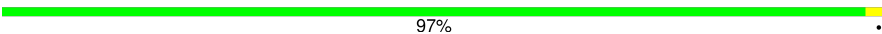
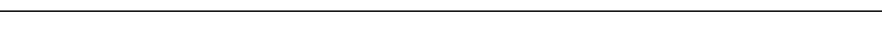
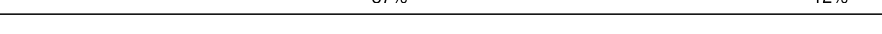
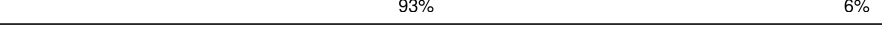
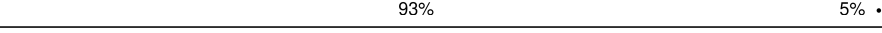
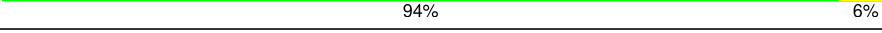
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Mol	Chain	Length	Quality of chain
4	D	208	 92% 7% .
5	E	200	 94% 6%
6	F	177	 95% 5%
7	G	174	 96% .
8	H	149	 6% 95% 5%
9	I	141	 26% 85% 12% .
10	J	141	 98% .
11	K	122	 85% 15%
12	L	143	 88% 10% .
13	M	136	 95% 5%
14	N	119	 97% .
15	O	116	 94% 6%
16	P	114	 91% 9%
17	Q	115	 90% 10% .
18	R	102	 90% 10%
19	S	109	 91% 9%
20	T	92	 92% 8%
21	U	102	 92% 8%
22	V	92	 97% ..
23	W	75	 96% .
24	X	77	 97% ..
25	Y	60	 98% .
26	Z	56	 98% .
27	0	55	 91% 9%
28	1	51	 100%

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Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	72% 25% • •
55	v	77	66% 26% 8%
55	w	77	44% 36% 17% •
56	x	12	83% 17%
57	y	76	51% 39% 8% •
58	z	393	93% 6% •

2 Entry composition

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called mRNA.

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

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

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

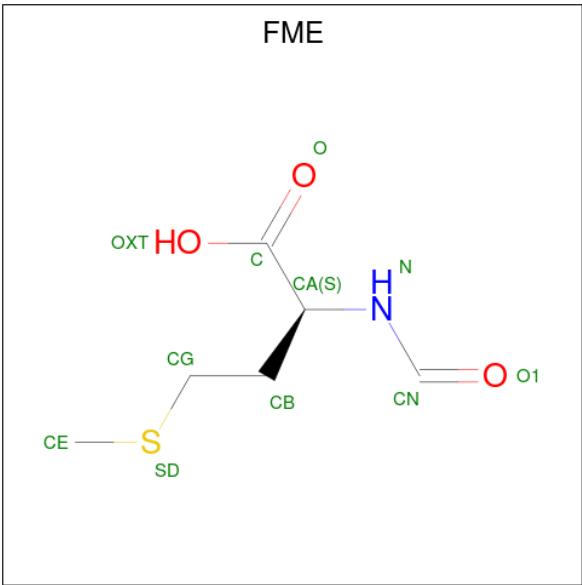
- Molecule 58 is a protein called Elongation factor Tu 2.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 59 is N-FORMYLMETHIONINE (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	1325	Total	Mg	0
			1325	1325	
60	B	36	Total	Mg	0
			36	36	
60	C	3	Total	Mg	0
			3	3	
60	D	3	Total	Mg	0
			3	3	
60	E	3	Total	Mg	0
			3	3	
60	L	2	Total	Mg	0
			2	2	
60	M	1	Total	Mg	0
			1	1	
60	N	1	Total	Mg	0
			1	1	
60	Q	2	Total	Mg	0
			2	2	
60	R	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	

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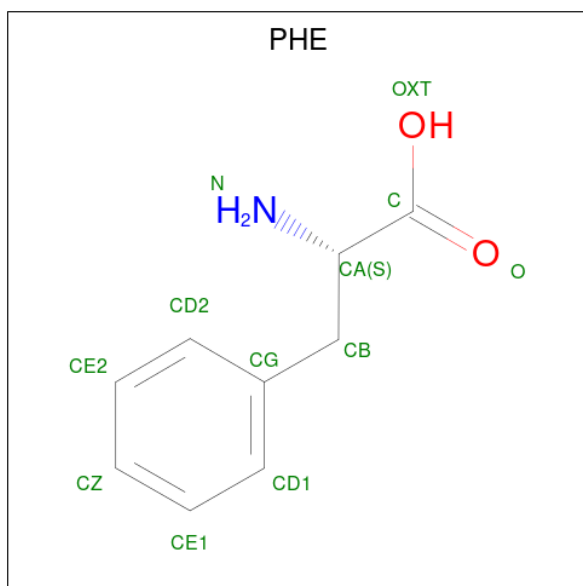
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Mol	Chain	Residues	Atoms		AltConf
60	T	1	Total 1	Mg 1	0
60	X	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	2	Total 2	Mg 2	0
60	0	2	Total 2	Mg 2	0
60	3	3	Total 3	Mg 3	0
60	4	1	Total 1	Mg 1	0
60	a	481	Total 481	Mg 481	0
60	d	1	Total 1	Mg 1	0
60	h	1	Total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

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

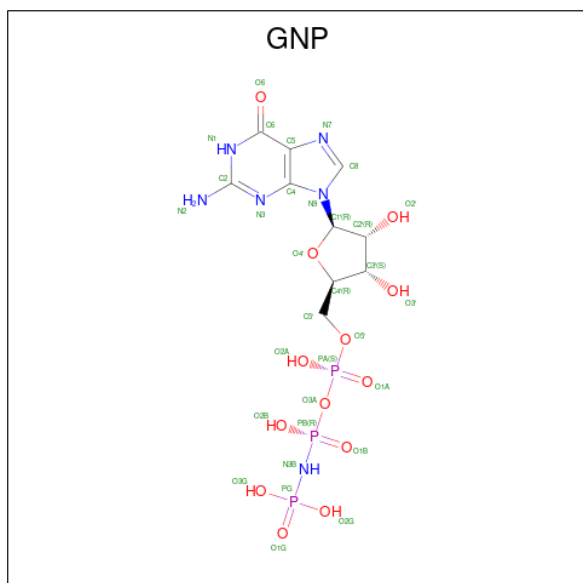
Mol	Chain	Residues	Atoms			AltConf
61	A	5	Total	K		0
			5	5		

- 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 PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 64 is water.

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

Continued on next page...

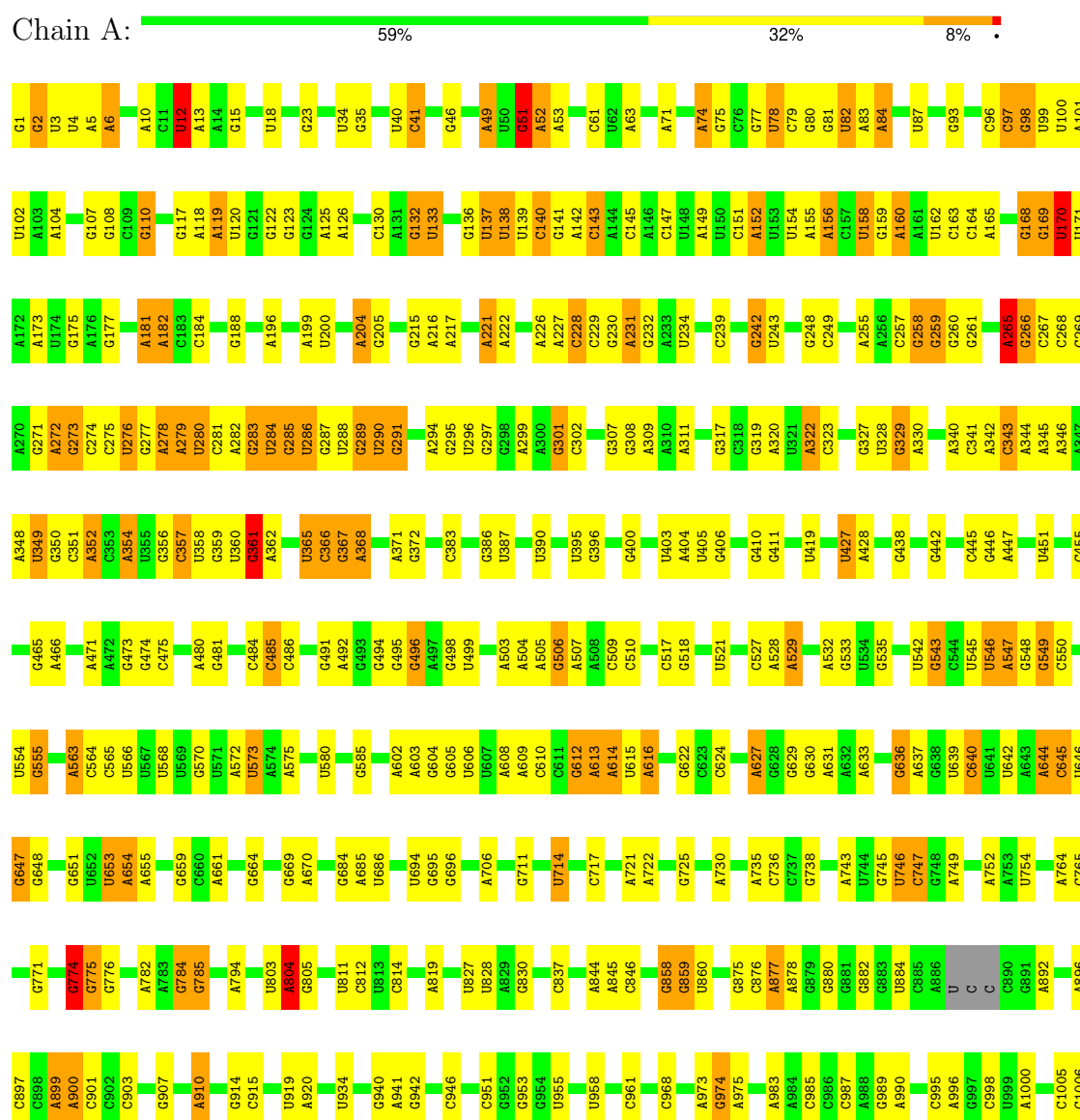
Continued from previous page...

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

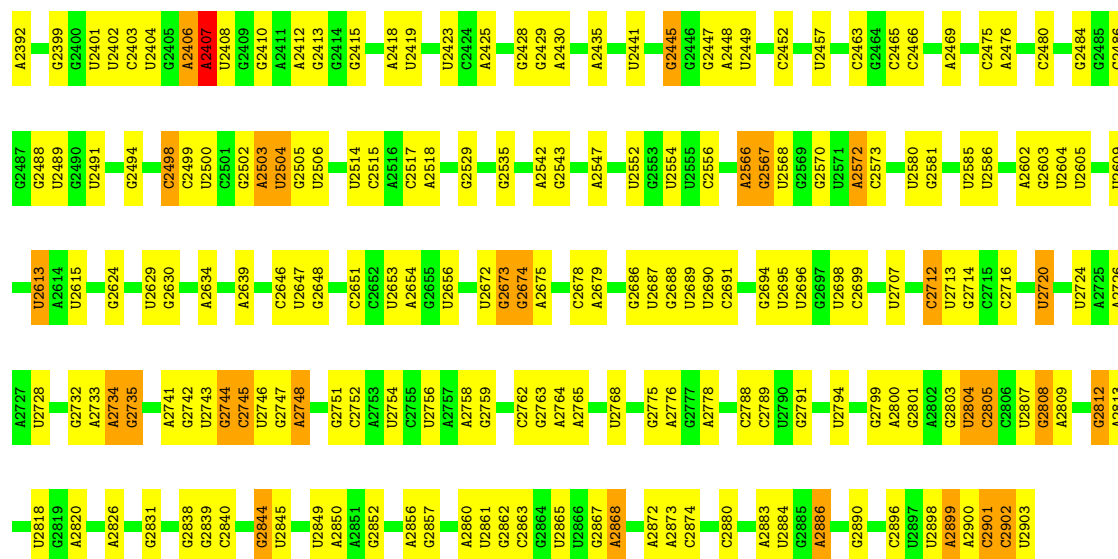
3 Residue-property plots

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

• Molecule 1: 23S rRNA

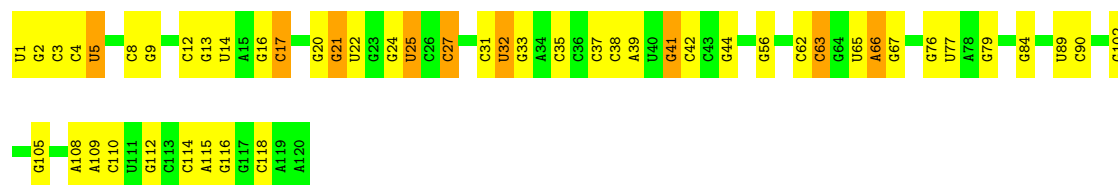


A2287	U2172	A2062	A1937	A1854	U1736	C1617	C1541	U1476	A1392	C1289	C1167	U1078	A1009
A2288	A2173	G2069	A1938	G1857	G1737	A1618	A1544	A1477	A1393	C1290	C1171	C1079	U1012
G2289	U2180	A2070	U1939	A1858	A1739	G1619	A1545	G1479	U1394	C1291	G1172	A1080	U1081
G2290	G2196	C2072	C1941	U1859	G1741	G1622	C1547	U1482	C1399	U1294	U1173	U1082	A1014
U2291	G2196		C1942		U1742	A1634	A1548	G1483	U1402	G1300	U1174	A1084	G1017
G2294	U2182	A2077	U1955	G1862	G1743	G1743	A1549	U1484	A1403	A1301	U1175	A1085	U1018
G2296	G2193	C2078	U1962	G1863	A1744	G1642	U1554	U1485	C1404	G1306	U1176	A1086	G1019
A2297	U2194	A2080	C1963	U1866	A1746	G1643	U1555	U1487	U1405	C1305	G1177	A1087	A1020
U2305	U2195		U1963	G1867	G1746	U1647	C1556	G1488	U1407	C1306	G1179	A1089	A1021
G2305	G2198	U2092	G1964	G1868	G1750	U1648	C1557	U1490	G1408	C1320	U1180	A1090	G1022
A2309	A2199	G2093	C1965	G1869	G1755	G1649	C1558	U1491		A1321	U1181		U1023
C2310	C2200		C1967	C1870	A1755		U1559	G1492	U1412	G1190		G1026	
A2311	G2201	C2096	A1871	G1872	U1758	A1654	U1560	U1493	A1413	G1191	U1101	G1027	A1028
U2320	U2202	A2097	U1970	G1873	U1764	G1659	U1563	U1494	A1414	U1328	U1102		
G2320	G2203	U2098	U1971	G1874	C1764		C1564	U1495	C1330	G1193	A1103		
U2321	A2205	U2099	G1972	G1875	A1773	G1674	U1565	U1496	C1331	C1196	U1104		U1033
	G2206	G2100	U1976	A1876	U1776	C1675	A1566	U1497	G1332	G1197	U1105		G1034
	C2207	A2101	G1776	G1682	U1779	G1675	G1567	U1498	G1338	C1200	G1106		U1035
G2325	C2208	C2103	G1779	G1691	U1780	G1682	G1568	U1499	G1339	C1200	U1108		G1036
C2326	C2104	U2105	U1883	U1692	A1780	C1691	A1569	G1500	G1421	A1204	C1109		G1037
A2327	A2112	U2106	G1884	U1693	A1784	U1692	A1572	U1501	G1426	G1343	G1110		G1038
A2328	U2213	G2107	A1885	G1694	U1784	U1693	A1579	U1503	A1427	U1210	A1111		C1043
	G2216	A2108	A1890	G1695	A1789	G1695	G1580	U1504	C1428	U1211	C1044		C1044
U2334	U2220	G2110	C1895	G1699	C1790	G1699	G1581	U1505	G1429	G1212	U1113		C1045
A2335	G2221	C2111	U1896	A1700	A1791	A1700	A1583	U1506	A1431	G1218	C1114		A1046
G2337	U2224	U2118	G1906	A1705	C1795	A1705	U1584	U1507	U1352	G1225	G1115		G1047
C2338	C2226	A2119	G1907	A1706	U1796	C1706	A1586	U1508	A1353	A1226	C1117		A1048
A2340	G2230	G2120	C1908	U1709	G1800	U1709	G1587	G1510	G1355	G1227	U1119		A1050
	G2238	G2121	C1909	U1712	A1801	U1712	G1588	A1515	G1357	G1236	G1124		G1051
A2346	G2239	G2127	U1910	A1713	A1808	A1713	U1589	G1516	G1441	U1240			G1053
C2350	U2131	U2131	U1911	G1714	A1809	G1714	A1591	G1517	G1449	A1247	A1127		A1054
U2356	G2242	G2132	A1913	G1715	A1810	G1715	C1592	U1520	G1450	G1248	U1130		G1055
G2357	U2243	G2133	C1914	U1716	G1811	U1716	U1593	U1523	C1451	U1249	G1131		A1057
	G2250	A2134	A1916	A1717	C1816	A1717	C1595	G1524	G1452	G1250	U1132		G1059
G2361	G2251	G2141	U1917	A1721	G1817	A1721	A1596	G1525	A1453	A1253	C1135		U1060
U2372	C2264	C2145	U1918	G1722	U1818	G1722	U1597	G1526	C1454	G1262	U1061		U1062
A2378	A2268	C2146	U1923	G1723	A1829	G1723	A1603	U1527	G1455	G1368	G1139		G1063
G2379	C2273	A2147	C1924	G1725	U1833	G1725	C1604	G1528	U1458	C1370	U1140		G1064
C2380	A2274	G2157	A1927	G1726	U1835	G1726	C1605	G1529	U1459	G1371	U1141		U1065
A2381	G2274	G2162	U1928	A1727	G1836	A1727	C1606	G1530	A1461	U1258	A1142		U1066
G2382	G2278	G2163	G1930	U1729	U1841	U1729	C1607	U1531	U1466	A1262	A1143		A1067
G2383	A2278	G2164	U1931	G1730	U1847	G1730	A1610	U1532	U1467	G1266	C1146		A1069
U2384	C2283	C2164	A1932	G1731	G1847	G1731	G1613	U1533	U1468	G1269	U1147		A1070
C2385	A2170	A2171	G1933	U1733	U1852	U1733	A1614	U1534	U1469	A1272	U1149		G1071
G2391	G2286	A2171	A1936	G1735	A1853	G1735	A1616	G1537	A1470	U1273	C1150		G1072



• Molecule 2: 5S rRNA

Chain B: 58% 34% 8%



• Molecule 3: 50S ribosomal protein L2

Chain C: 92% 8%



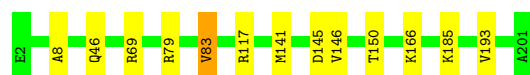
• Molecule 4: 50S ribosomal protein L3

Chain D: 92% 7%

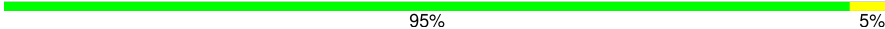


• Molecule 5: 50S ribosomal protein L4

Chain E: 94% 6%

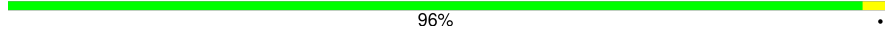


• Molecule 6: 50S ribosomal protein L5

Chain F:  95% 5%

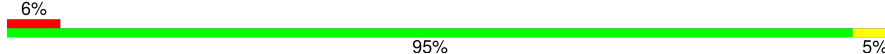


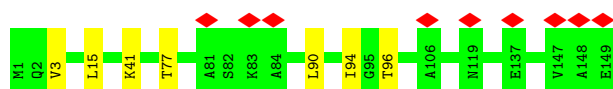
- Molecule 7: 50S ribosomal protein L6

Chain G:  96% .



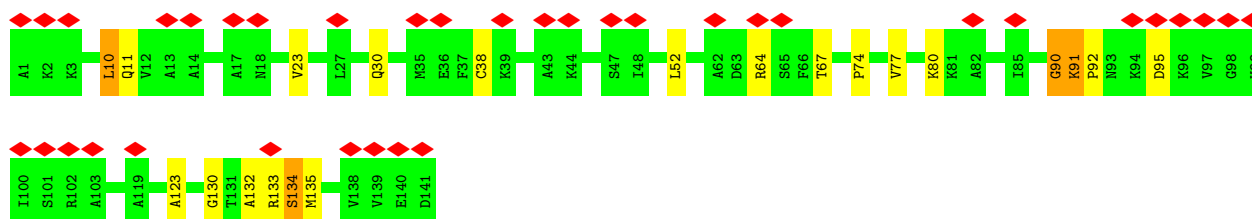
- Molecule 8: 50S ribosomal protein L9

Chain H:  6% 95% 5%

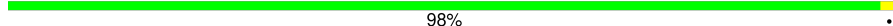


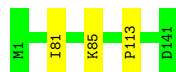
- Molecule 9: 50S ribosomal protein L11

Chain I:  26% 85% 12% .



- Molecule 10: 50S ribosomal protein L13

Chain J:  98% .



- Molecule 11: 50S ribosomal protein L14

Chain K:  85% 15%



- Molecule 12: 50S ribosomal protein L15

Chain L:  88% 10% .



- Molecule 13: 50S ribosomal protein L16

Chain M: 95% 5%



- Molecule 14: 50S ribosomal protein L17

Chain N: 97% .



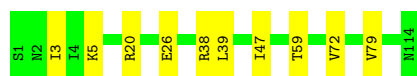
- Molecule 15: 50S ribosomal protein L18

Chain O: 94% 6%



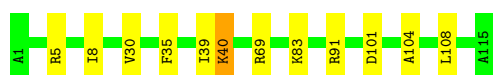
- Molecule 16: 50S ribosomal protein L19

Chain P: 91% 9%



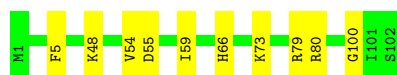
- Molecule 17: 50S ribosomal protein L20

Chain Q: 90% 10% .



- Molecule 18: 50S ribosomal protein L21

Chain R: 90% 10%



- Molecule 19: 50S ribosomal protein L22

Chain S: 91% 9%



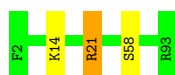
- Molecule 20: 50S ribosomal protein L23



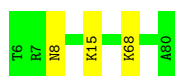
- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



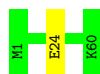
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

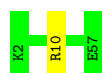


- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30





- Molecule 27: 50S ribosomal protein L32

Chain 0: 91% 9%



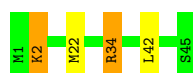
- Molecule 28: 50S ribosomal protein L33

Chain 1: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 2: 91% . .



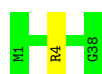
- Molecule 30: 50S ribosomal protein L35

Chain 3: 97% .



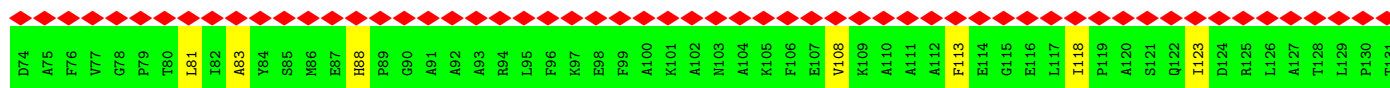
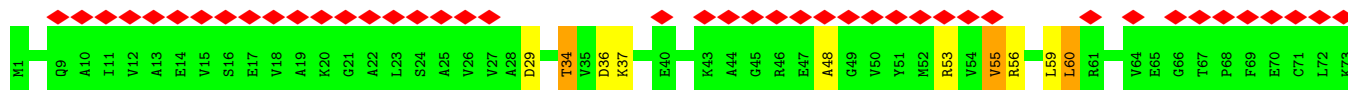
- Molecule 31: 50S ribosomal protein L36

Chain 4: 97% .



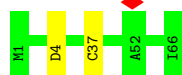
- Molecule 32: 50S ribosomal protein L10

Chain 5: 77% 87% 11% .



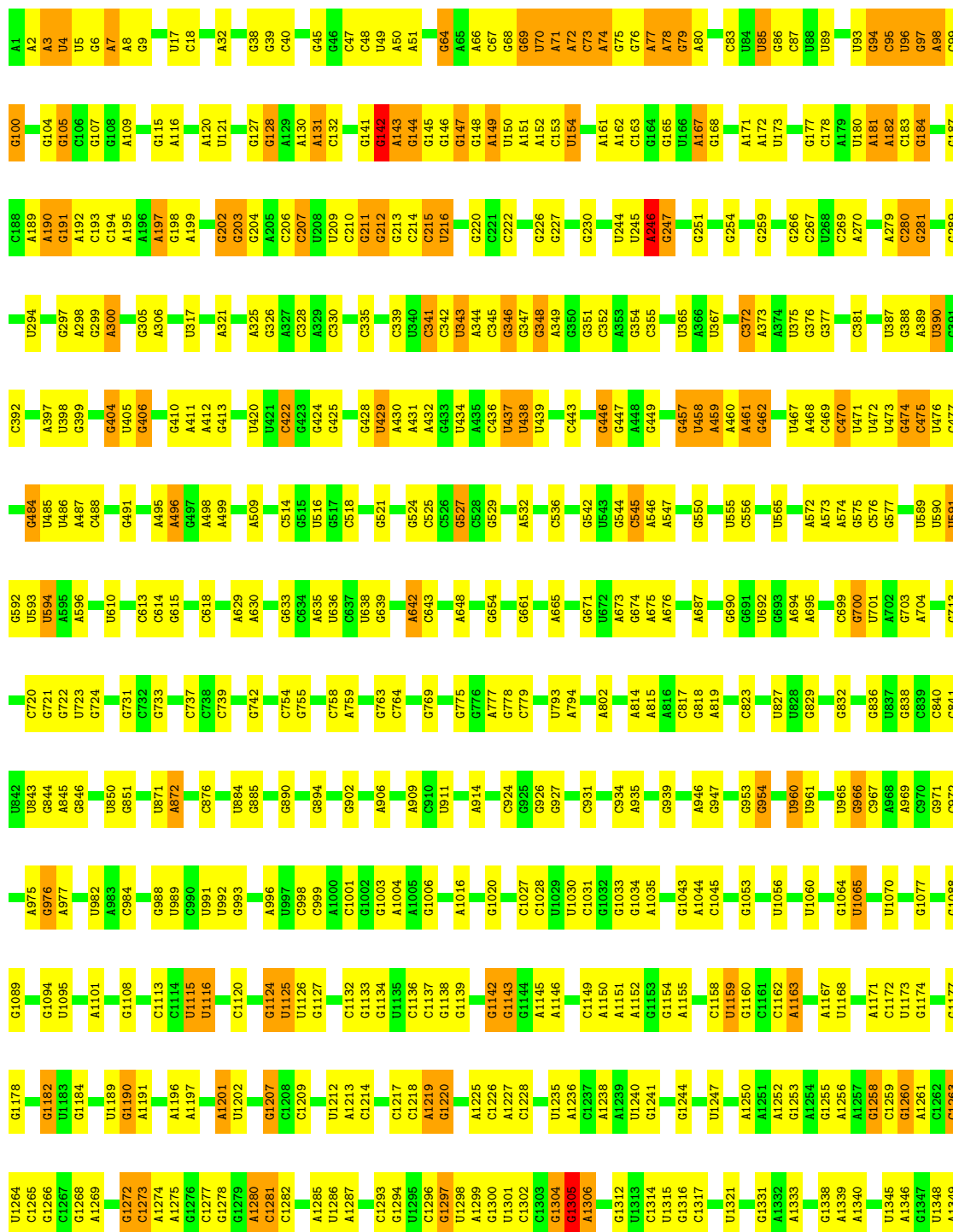
- Molecule 33: 50S ribosomal protein L31

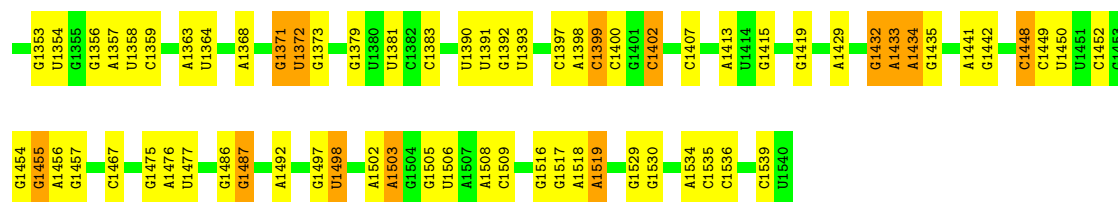
Chain 6:  97%.



• Molecule 34: 16S rRNA

Chain a:  61% 31% 8%





- Molecule 35: 30S ribosomal protein S2

Chain b: 98% .



- Molecule 36: 30S ribosomal protein S3

Chain c: 93% 6% .



- Molecule 37: 30S ribosomal protein S4

Chain d: 95% 5% .



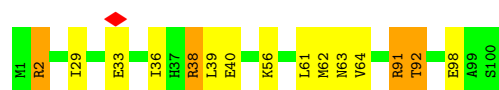
- Molecule 38: 30S ribosomal protein S5

Chain e: 89% 10% .



- Molecule 39: 30S ribosomal protein S6

Chain f: 85% 11% .

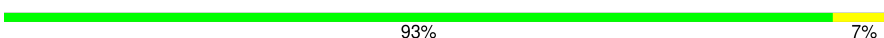


- Molecule 40: 30S ribosomal protein S7

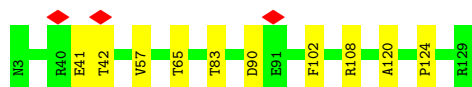
Chain g: 91% 9% .



• Molecule 41: 30S ribosomal protein S8

Chain h:  93% 7%

• Molecule 42: 30S ribosomal protein S9

Chain i:  92% 8%

• Molecule 43: 30S ribosomal protein S10

Chain j:  87% 12%

• Molecule 44: 30S ribosomal protein S11

Chain k:  90% 10%

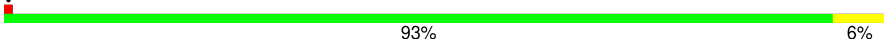
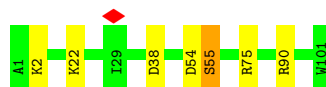
• Molecule 45: 30S ribosomal protein S12

Chain l:  85% 12%

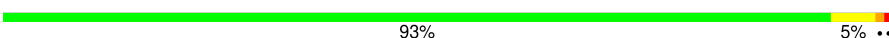
• Molecule 46: 30S ribosomal protein S13

Chain m:  90% 9%

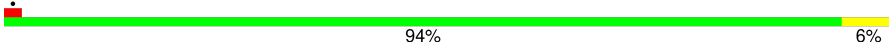
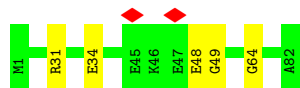
• Molecule 47: 30S ribosomal protein S14

Chain n:  93% 6%

• Molecule 48: 30S ribosomal protein S15

Chain o:  93% 5% ..

• Molecule 49: 30S ribosomal protein S16

Chain p:  94% 6%

• Molecule 50: 30S ribosomal protein S17

Chain q:  89% 11%

• Molecule 51: 30S ribosomal protein S18

Chain r:  85% 14% .

• Molecule 52: 30S ribosomal protein S19

Chain s:  87% 11% .

• Molecule 53: 30S ribosomal protein S20

Chain t:  89% 9% .

• Molecule 54: 30S ribosomal protein S21

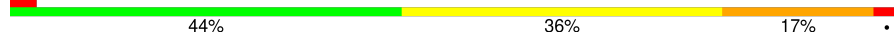
Chain u:  72% 25% ..

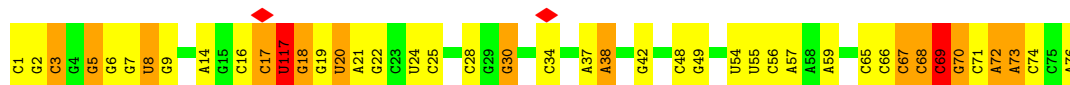
- Molecule 55: tRNA-fMet

Chain v:  66% 26% 8%



- Molecule 55: tRNA-fMet

Chain w:  44% 36% 17%



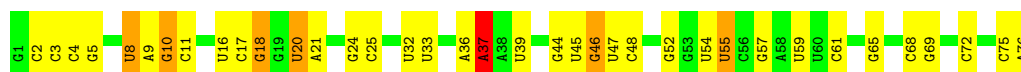
- Molecule 56: mRNA

Chain x:  83% 17%



- Molecule 57: tRNA-Phe

Chain y:  51% 39% 8%



- Molecule 58: Elongation factor Tu 2

Chain z:  93% 6%



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/69174	0.73	39/107907 (0.0%)
2	B	0.39	0/2876	0.72	2/4483 (0.0%)
3	C	0.52	0/2121	0.76	0/2852
4	D	0.51	0/1578	0.77	0/2124
5	E	0.52	0/1563	0.82	0/2103
6	F	0.54	0/1434	0.81	0/1926
7	G	0.54	0/1324	0.74	0/1794
8	H	0.57	0/1122	0.77	0/1515
9	I	0.67	0/1046	0.92	2/1410 (0.1%)
10	J	0.52	0/1143	0.80	0/1540
11	K	0.53	0/947	0.75	0/1268
12	L	0.53	0/1052	0.85	0/1401
13	M	0.50	0/1093	0.78	0/1460
14	N	0.55	0/964	0.85	0/1289
15	O	0.54	0/902	0.85	0/1209
16	P	0.51	0/929	0.73	0/1242
17	Q	0.52	0/946	0.90	0/1260
18	R	0.49	0/823	0.66	0/1100
19	S	0.53	0/852	0.87	0/1142
20	T	0.52	0/736	0.76	0/984
21	U	0.51	0/787	0.74	0/1051
22	V	0.51	0/752	0.76	0/1008
23	W	0.47	0/579	0.70	0/767
24	X	0.49	0/635	0.74	0/848
25	Y	0.54	0/495	0.84	0/658
26	Z	0.55	0/438	0.79	0/586
27	0	0.49	0/440	0.81	0/588
28	1	0.50	0/424	0.68	0/565
29	2	0.53	0/370	1.00	0/487
30	3	0.52	0/513	0.86	0/676
31	4	0.47	0/303	0.71	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.64	0/1001	0.85	0/1350
33	6	0.56	0/531	0.78	0/709
34	a	0.38	0/36725	0.73	20/57285 (0.0%)
35	b	0.57	0/1735	0.78	0/2338
36	c	0.54	0/1651	0.80	0/2225
37	d	0.55	0/1665	0.80	0/2227
38	e	0.54	0/1180	0.82	0/1587
39	f	0.54	0/835	0.78	0/1128
40	g	0.54	0/1195	0.84	0/1602
41	h	0.53	0/989	0.81	0/1326
42	i	0.57	0/1034	0.78	0/1375
43	j	0.56	0/796	0.77	0/1077
44	k	0.54	0/885	0.79	0/1195
45	l	0.54	0/954	0.78	0/1282
46	m	0.57	0/900	0.84	0/1204
47	n	0.55	0/822	0.78	0/1095
48	o	0.54	0/722	0.91	1/964 (0.1%)
49	p	0.53	0/659	0.76	0/884
50	q	0.57	0/657	0.74	0/881
51	r	0.60	0/544	0.81	0/731
52	s	0.54	0/652	0.75	0/877
53	t	0.55	0/671	0.87	0/888
54	u	0.64	0/550	0.93	0/728
55	v	0.40	1/1747 (0.1%)	0.72	0/2721
55	w	0.47	2/1747 (0.1%)	1.01	6/2721 (0.2%)
56	x	0.36	0/280	0.67	0/433
57	y	0.39	0/1607	0.71	1/2501 (0.0%)
58	z	0.54	0/3086	0.79	0/4175
All	All	0.43	3/164181 (0.0%)	0.75	71/245149 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-7.86	1.49	1.61
55	w	17	C	O3'-P	6.49	1.70	1.61
55	v	7	4SU	O3'-P	5.27	1.61	1.56

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	29.36	148.04	104.00
1	A	2712	C	C2'-C3'-O3'	11.74	127.11	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	P-O3'-C3'	-11.12	103.52	120.20
1	A	242	G	C2'-C3'-O3'	10.12	124.68	109.50
1	A	51	G	C2'-C3'-O3'	9.53	123.80	109.50
34	a	246	A	C4'-C3'-O3'	9.45	123.57	109.40
55	w	17	C	OP1-P-O3'	-8.68	81.96	108.00
1	A	1378	A	C4'-C3'-O3'	8.68	122.42	109.40
1	A	204	A	C4'-C3'-O3'	8.14	121.61	109.40
1	A	774	G	C2'-C3'-O3'	7.83	121.25	109.50
34	a	1305	G	C2'-C3'-O3'	7.74	121.10	109.50
1	A	1730	U	C2'-C3'-O3'	7.72	121.08	109.50
34	a	428	G	C4'-C3'-O3'	7.56	120.74	109.40
1	A	1140	C	C2'-C3'-O3'	7.55	125.03	113.70
34	a	1432	G	C2'-C3'-O3'	7.48	120.72	109.50
1	A	1020	A	C4'-C3'-O3'	7.37	120.45	109.40
1	A	1130	U	C4'-C3'-O3'	-7.35	101.97	113.00
1	A	265	A	C4'-C3'-O3'	7.32	120.37	109.40
1	A	2407	A	C2'-C3'-O3'	7.19	124.49	113.70
34	a	1201	A	C2'-C3'-O3'	7.13	120.20	109.50
1	A	1022	G	C2'-C3'-O3'	7.04	120.06	109.50
1	A	859	G	C2'-C3'-O3'	6.94	119.91	109.50
1	A	301	G	C4'-C3'-O3'	6.89	119.74	109.40
55	w	69	C	C2'-C3'-O3'	6.87	124.01	113.70
1	A	1857	G	C4'-C3'-O3'	6.82	119.62	109.40
55	w	18	G	C2'-C3'-O3'	6.62	119.43	109.50
48	o	88	ARG	NE-CZ-NH2	6.53	125.08	119.20
1	A	1735	G	C4'-C3'-O3'	6.43	119.05	109.40
34	a	1297	G	C4'-C3'-O3'	6.40	119.00	109.40
34	a	375	U	C4'-C3'-O3'	-6.33	103.50	113.00
1	A	1070	A	C2'-C3'-O3'	6.32	118.98	109.50
9	I	91	LYS	CA-C-N	6.31	127.73	119.84
9	I	91	LYS	C-N-CA	6.31	127.73	119.84
1	A	1475	G	C2'-C3'-O3'	6.30	118.94	109.50
1	A	2391	G	C4'-C3'-O3'	6.28	122.43	113.00
2	B	66	A	C4'-C3'-O3'	6.03	122.05	113.00
1	A	1800	C	C4'-C3'-O3'	5.99	118.38	109.40
34	a	1399	C	C2'-C3'-O3'	5.98	118.47	109.50
1	A	1735	G	C1'-C2'-O2'	5.96	120.75	111.80
34	a	343	U	C3'-C2'-O2'	5.88	119.51	110.70
1	A	1940	U	C2'-C3'-O3'	5.88	118.31	109.50
1	A	2296	U	C4'-C3'-O3'	5.86	118.18	109.40
34	a	142	G	N9-C1'-C2'	5.84	120.75	112.00
1	A	1078	U	C2'-C3'-O3'	-5.81	104.99	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	574	A	C4'-C3'-O3'	-5.80	104.31	113.00
34	a	85	U	C2'-C3'-O3'	-5.70	105.15	113.70
1	A	2566	A	C4'-C3'-O3'	5.65	117.87	109.40
55	w	17	C	OP2-P-O3'	-5.61	91.18	108.00
1	A	804	A	C4'-C3'-O3'	-5.59	104.62	113.00
34	a	1190	G	C4'-C3'-O3'	5.57	117.76	109.40
1	A	1735	G	N9-C1'-C2'	-5.51	105.73	114.00
34	a	73	C	N1-C1'-C2'	5.49	120.23	112.00
1	A	1475	G	C4'-C3'-O3'	5.48	117.62	109.40
1	A	1047	G	C2'-C3'-O3'	5.48	117.72	109.50
1	A	282	A	C2'-C3'-O3'	5.42	117.63	109.50
34	a	960	U	C4'-C3'-O3'	5.42	117.53	109.40
34	a	422	C	C2'-C3'-O3'	-5.38	105.63	113.70
1	A	361	G	N9-C1'-C2'	5.27	121.90	114.00
1	A	12	U	N1-C1'-C2'	5.26	119.89	112.00
1	A	170	U	N1-C1'-C2'	5.26	119.89	112.00
1	A	1530	G	N9-C1'-C2'	5.25	119.87	112.00
34	a	960	U	C2'-C3'-O3'	5.23	117.34	109.50
34	a	1272	G	C4'-C3'-O3'	-5.19	105.22	113.00
1	A	1970	A	C2'-C3'-O3'	5.16	117.24	109.50
57	y	2	C	C2'-C3'-O3'	5.13	121.39	113.70
34	a	1399	C	C4'-C3'-O3'	5.13	117.09	109.40
1	A	1940	U	C4'-C3'-O3'	5.12	117.07	109.40
2	B	39	A	C1'-C2'-O2'	5.04	115.96	108.40
34	a	1190	G	C2'-C3'-O3'	5.04	117.06	109.50
1	A	1022	G	C4'-C3'-O3'	5.03	116.94	109.40
1	A	301	G	C2'-C3'-O3'	5.02	117.04	109.50

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	31340	646	0
2	B	2572	0	1302	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2082	0	2157	5	0
4	D	1557	0	1604	7	0
5	E	1544	0	1607	4	0
6	F	1410	0	1447	1	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	13	0
10	J	1120	0	1151	1	0
11	K	938	0	1012	4	0
12	L	1043	0	1123	8	0
13	M	1074	0	1157	2	0
14	N	951	0	994	1	0
15	O	892	0	923	3	0
16	P	917	0	965	5	0
17	Q	933	0	1006	7	0
18	R	810	0	834	4	0
19	S	845	0	909	2	0
20	T	730	0	795	2	0
21	U	779	0	834	1	0
22	V	739	0	763	4	0
23	W	572	0	593	0	0
24	X	625	0	655	1	0
25	Y	494	0	530	0	0
26	Z	434	0	477	0	0
27	0	434	0	448	3	0
28	1	417	0	451	0	0
29	2	367	0	405	1	0
30	3	504	0	574	0	0
31	4	302	0	343	1	0
32	5	988	0	1025	8	0
33	6	522	0	524	0	0
34	a	33050	0	16656	274	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	4	0
37	d	1643	0	1710	5	0
38	e	1164	0	1212	2	0
39	f	817	0	808	17	0
40	g	1181	0	1240	2	0
41	h	979	0	1034	5	0
42	i	1022	0	1070	1	0
43	j	786	0	828	4	0
44	k	869	0	878	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	l	940	0	1001	5	0
46	m	891	0	955	4	0
47	n	810	0	852	1	0
48	o	714	0	737	3	0
49	p	649	0	666	0	0
50	q	648	0	691	2	0
51	r	535	0	552	2	0
52	s	637	0	665	6	0
53	t	665	0	714	4	0
54	u	544	0	579	6	0
55	v	1644	0	840	11	0
55	w	1644	0	840	67	0
56	x	252	0	129	1	0
57	y	1631	0	843	4	0
58	z	3031	0	3049	5	0
59	A	10	0	10	0	0
60	0	2	0	0	0	0
60	3	3	0	0	0	0
60	4	1	0	0	0	0
60	A	1325	0	0	0	0
60	B	36	0	0	0	0
60	C	3	0	0	0	0
60	D	3	0	0	0	0
60	E	3	0	0	0	0
60	L	2	0	0	0	0
60	M	1	0	0	0	0
60	N	1	0	0	0	0
60	Q	2	0	0	0	0
60	R	1	0	0	0	0
60	S	1	0	0	0	0
60	T	1	0	0	0	0
60	X	1	0	0	0	0
60	Y	1	0	0	0	0
60	Z	2	0	0	0	0
60	a	481	0	0	0	0
60	d	1	0	0	0	0
60	h	1	0	0	0	0
60	i	3	0	0	0	0
60	s	1	0	0	0	0
60	t	1	0	0	0	0
60	u	1	0	0	0	0
60	v	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	w	1	0	0	0	0
60	x	1	0	0	0	0
60	y	8	0	0	0	0
60	z	4	0	0	0	0
61	A	5	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	13	0	0
64	0	1	0	0	0	0
64	2	4	0	0	0	0
64	3	1	0	0	0	0
64	4	1	0	0	0	0
64	A	653	0	0	0	0
64	B	22	0	0	0	0
64	C	7	0	0	0	0
64	D	6	0	0	0	0
64	E	6	0	0	0	0
64	G	1	0	0	0	0
64	J	1	0	0	0	0
64	L	6	0	0	0	0
64	M	1	0	0	0	0
64	N	3	0	0	0	0
64	P	1	0	0	0	0
64	Q	4	0	0	0	0
64	S	2	0	0	0	0
64	U	3	0	0	0	0
64	W	1	0	0	0	0
64	X	3	0	0	0	0
64	Y	1	0	0	0	0
64	Z	2	0	0	0	0
64	a	163	0	0	0	0
64	d	1	0	0	0	0
64	h	2	0	0	0	0
64	k	1	0	0	0	0
64	m	3	0	0	0	0
64	o	1	0	0	0	0
64	s	2	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	v	9	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
64	y	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	z	2	0	0	0	0
All	All	155275	0	103543	1133	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 5.

All (1133) 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)
1:A:1048:A:N1	1:A:1111:A:C6	1.73	1.54
1:A:1048:A:C2	1:A:1111:A:C6	1.97	1.49
1:A:283:G:N7	1:A:284:U:C2	1.87	1.40
1:A:1867:G:N1	1:A:1874:C:N3	1.68	1.38
1:A:1048:A:C2	1:A:1111:A:N1	1.90	1.38
55:w:1:C:N3	55:w:72:A:N6	1.80	1.30
34:a:459:A:N6	34:a:473:U:H3	1.29	1.29
34:a:207:C:N3	34:a:212:G:N2	1.81	1.28
1:A:1:G:C6	1:A:2902:C:O2	1.86	1.27
55:w:3:C:N4	55:w:70:G:O6	1.69	1.25
34:a:459:A:N6	34:a:473:U:N3	1.82	1.24
1:A:2013:A:N1	1:A:2613:U:O4	1.71	1.23
1:A:1724:G:O6	1:A:1736:U:C4	1.91	1.22
1:A:1724:G:O6	1:A:1736:U:N3	1.72	1.22
1:A:1048:A:C2	1:A:1111:A:N6	2.06	1.21
1:A:1867:G:C6	1:A:1874:C:N3	2.09	1.21
1:A:283:G:O6	1:A:356:G:O6	1.57	1.20
39:f:38:ARG:NH1	39:f:98:GLU:O	1.75	1.19
1:A:278:A:C6	1:A:361:G:C8	2.31	1.19
1:A:2489:U:O2	1:A:2491:U:O4	1.62	1.18
1:A:1733:U:H2'	1:A:1734:C:C6	1.78	1.18
1:A:277:G:C4	1:A:361:G:C8	2.32	1.17
1:A:1416:G:O2'	1:A:1587:G:N2	1.74	1.17
2:B:5:U:O4	2:B:115:A:N1	1.76	1.16
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.16
1:A:2294:G:C2	1:A:2339:C:O2	2.00	1.15
1:A:1722:A:N7	1:A:1738:G:N2	1.95	1.14
1:A:290:U:C4	1:A:350:G:O6	2.01	1.14
39:f:36:ILE:HG21	39:f:39:LEU:CD2	1.78	1.14
1:A:1048:A:N1	1:A:1111:A:C5	2.17	1.11
1:A:287:G:C8	1:A:354:A:N6	2.18	1.11
55:w:2:G:C6	55:w:71:C:C4	2.38	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:2:G:N1	55:w:71:C:N3	1.99	1.10
1:A:1416:G:N2	1:A:1582:C:O2	1.84	1.09
1:A:278:A:N1	1:A:361:G:H1'	1.65	1.09
1:A:1724:G:O6	1:A:1736:U:O4	1.69	1.07
34:a:462:G:N2	34:a:470:C:N3	2.03	1.07
1:A:278:A:N1	1:A:361:G:C8	2.22	1.07
1:A:1:G:O6	1:A:2902:C:O2	1.71	1.06
1:A:283:G:N7	1:A:284:U:N3	2.04	1.06
1:A:2028:U:H2'	1:A:2029:G:C8	1.90	1.06
1:A:287:G:C8	1:A:354:A:C6	2.44	1.05
1:A:280:U:O4	1:A:360:U:O2	1.74	1.05
1:A:290:U:C4	1:A:350:G:C6	2.45	1.05
34:a:437:U:C4	34:a:495:A:C6	2.45	1.04
55:w:66:C:C4	55:w:67:C:C2	2.45	1.04
39:f:36:ILE:HG21	39:f:39:LEU:HD21	1.07	1.04
1:A:1867:G:N1	1:A:1874:C:C2	2.13	1.03
1:A:289:G:N2	1:A:351:C:O2	1.91	1.03
34:a:341:C:N3	34:a:348:G:O6	1.93	1.02
34:a:437:U:N3	34:a:495:A:N6	2.09	1.01
1:A:1867:G:O6	1:A:1874:C:C4	2.13	1.01
39:f:38:ARG:O	39:f:62:MET:O	1.77	1.01
1:A:706:A:N6	1:A:725:G:N3	2.09	1.00
1:A:1048:A:H2	1:A:1111:A:N6	1.51	1.00
1:A:1727:A:N1	1:A:1733:U:O4	1.95	0.99
1:A:107:G:N2	1:A:346:A:N1	2.10	0.99
1:A:1417:C:N3	1:A:1581:G:N1	2.11	0.98
55:w:65:C:C4	55:w:66:C:N4	2.30	0.98
1:A:257:C:H2'	1:A:258:G:H5'	1.43	0.98
1:A:1735:G:HO2'	1:A:1736:U:H6	1.09	0.98
55:w:66:C:N4	55:w:67:C:C2	2.32	0.98
1:A:271:G:N2	1:A:366:C:O2	1.96	0.97
1:A:1735:G:O2'	1:A:1736:U:H6	1.46	0.97
1:A:285:G:N2	1:A:356:G:C5	2.32	0.97
1:A:287:G:H8	1:A:354:A:C5	1.81	0.97
1:A:484:C:N4	1:A:496:G:O6	1.97	0.97
34:a:437:U:O4	34:a:495:A:C5	2.18	0.97
1:A:1867:G:O6	1:A:1874:C:N4	1.97	0.96
39:f:36:ILE:CG2	39:f:39:LEU:HD21	1.94	0.96
55:w:2:G:C2	55:w:71:C:N3	2.34	0.96
1:A:283:G:C8	1:A:284:U:C2	2.53	0.96
1:A:290:U:N3	1:A:350:G:N1	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:C:N3	1:A:1735:G:N2	2.13	0.95
34:a:1160:G:O6	34:a:1182:G:N2	1.99	0.94
1:A:1867:G:N2	1:A:1874:C:O2	2.00	0.94
1:A:277:G:C8	1:A:361:G:N7	2.36	0.94
1:A:271:G:N2	1:A:366:C:C2	2.35	0.94
2:B:5:U:C4	2:B:115:A:N1	2.37	0.93
1:A:290:U:O4	1:A:350:G:C6	2.22	0.93
1:A:1867:G:O6	1:A:1874:C:N3	2.02	0.92
55:w:66:C:N4	55:w:67:C:N3	2.17	0.91
55:w:3:C:C4	55:w:70:G:O6	2.23	0.91
1:A:1416:G:N2	1:A:1582:C:C2	2.37	0.91
1:A:2030:6MZ:O3'	1:A:2031:A:P	2.28	0.91
55:w:2:G:C6	55:w:71:C:N4	2.38	0.91
1:A:221:A:N7	1:A:427:U:O4	2.03	0.91
1:A:290:U:N3	1:A:350:G:C6	2.39	0.90
1:A:277:G:N1	1:A:360:U:O2'	2.04	0.90
1:A:1726:G:O6	1:A:1734:C:N3	2.04	0.90
2:B:8:C:O2	2:B:112:G:N2	2.04	0.90
34:a:1160:G:O6	34:a:1182:G:N1	2.04	0.90
1:A:1733:U:H2'	1:A:1734:C:C5	2.05	0.90
34:a:430:A:OP2	37:d:21:LYS:NZ	2.04	0.90
1:A:278:A:N6	1:A:362:A:N7	2.19	0.90
1:A:289:G:N1	1:A:351:C:N3	2.19	0.90
1:A:277:G:C2	1:A:361:G:O4'	2.25	0.90
1:A:289:G:N1	1:A:351:C:C2	2.40	0.90
34:a:1160:G:O6	34:a:1182:G:C2	2.25	0.89
34:a:207:C:C2	34:a:212:G:N2	2.40	0.89
1:A:221:A:C8	1:A:427:U:O4	2.26	0.89
34:a:69:G:N2	34:a:100:G:O6	2.05	0.89
34:a:437:U:C4	34:a:495:A:C5	2.61	0.89
55:w:6:G:N1	55:w:68:C:O2	2.06	0.89
1:A:1857:G:N2	1:A:1884:G:H2'	1.88	0.88
34:a:827:U:H3	34:a:872:A:H61	1.20	0.88
34:a:461:A:C2	34:a:472:U:C2	2.60	0.88
34:a:827:U:H3	34:a:872:A:N6	1.71	0.88
1:A:277:G:N7	1:A:361:G:C5	2.42	0.88
1:A:1417:C:N4	1:A:1581:G:O6	2.06	0.88
1:A:272:A:C2	1:A:366:C:C2	2.62	0.88
1:A:277:G:C8	1:A:361:G:C5	2.62	0.88
1:A:285:G:C2	1:A:356:G:C6	2.62	0.88
1:A:627:A:OP1	12:L:78:ARG:NH1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:G:N9	1:A:361:G:N7	2.22	0.88
39:f:36:ILE:CG2	39:f:39:LEU:CD2	2.51	0.88
1:A:1615:C:OP2	1:A:1617:C:N4	2.08	0.87
1:A:283:G:N1	1:A:357:C:O2	2.06	0.87
1:A:289:G:C2	1:A:351:C:C2	2.63	0.86
34:a:459:A:N1	34:a:473:U:O2	2.09	0.86
39:f:39:LEU:O	39:f:61:LEU:O	1.93	0.86
1:A:2028:U:C4	1:A:2029:G:C6	2.64	0.86
1:A:49:A:H5'	1:A:51:G:H5'	1.56	0.85
55:w:2:G:C5	55:w:71:C:N4	2.44	0.85
55:w:2:G:C6	55:w:70:G:O6	2.30	0.85
1:A:283:G:C6	1:A:357:C:O2	2.30	0.85
1:A:277:G:N1	1:A:361:G:O4'	2.10	0.85
1:A:1857:G:O2'	1:A:1884:G:N2	2.09	0.84
1:A:2:G:N2	1:A:2901:C:O2	2.11	0.84
1:A:228:C:N4	1:A:2407:A:N3	2.24	0.84
1:A:1867:G:N1	1:A:1874:C:O2	2.08	0.84
34:a:1263:C:N4	34:a:1272:G:O6	2.10	0.84
1:A:257:C:C2'	1:A:258:G:H5'	2.06	0.83
55:w:66:C:C5	55:w:67:C:C6	2.65	0.83
1:A:1048:A:H2	1:A:1111:A:C6	1.68	0.83
1:A:1538:G:H2'	1:A:1539:U:C6	2.13	0.83
1:A:2294:G:N2	1:A:2339:C:O2	2.11	0.83
34:a:437:U:N3	34:a:495:A:C6	2.45	0.83
34:a:1258:G:O6	34:a:1277:C:N4	2.11	0.83
1:A:285:G:H3'	1:A:286:U:C6	2.13	0.83
1:A:278:A:C6	1:A:362:A:C8	2.66	0.83
1:A:1450:G:N2	1:A:1452:G:O6	2.11	0.82
1:A:283:G:O6	1:A:357:C:O2	1.96	0.82
1:A:1733:U:H2'	1:A:1734:C:H6	1.42	0.82
34:a:404:G:C2	34:a:498:A:N3	2.48	0.82
34:a:462:G:C2	34:a:470:C:N3	2.47	0.82
1:A:287:G:C8	1:A:354:A:C5	2.66	0.81
1:A:295:G:O6	1:A:343:C:N3	2.14	0.81
1:A:1048:A:H2	1:A:1111:A:H61	1.23	0.81
34:a:74:A:C2	34:a:97:G:N2	2.48	0.81
1:A:1727:A:H2	1:A:1733:U:H3	1.28	0.81
1:A:1013:C:O2	1:A:1149:G:N2	2.13	0.81
1:A:277:G:C2	1:A:360:U:O2'	2.33	0.81
34:a:341:C:O2	34:a:348:G:N1	2.14	0.81
1:A:1408:G:N1	1:A:1594:U:O2	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:5:G:N2	55:w:69:C:O2	2.14	0.80
34:a:1258:G:N1	34:a:1277:C:N3	2.28	0.80
55:w:66:C:C2	55:w:67:C:H1'	2.16	0.80
55:w:2:G:N1	55:w:71:C:C4	2.45	0.80
1:A:563:A:OP1	17:Q:40:LYS:NZ	2.12	0.80
1:A:1518:C:H3'	1:A:1519:G:H5''	1.65	0.79
1:A:289:G:C2	1:A:351:C:O2	2.36	0.79
34:a:462:G:N2	34:a:470:C:C2	2.49	0.79
1:A:271:G:N1	1:A:366:C:N3	2.29	0.79
1:A:1048:A:N1	1:A:1111:A:N6	2.23	0.79
1:A:1417:C:N3	1:A:1581:G:C6	2.50	0.79
1:A:1595:C:H2'	1:A:1596:A:O4'	1.83	0.79
1:A:1755:A:N6	1:A:2694:G:O2'	2.16	0.78
1:A:290:U:O4	1:A:350:G:O6	1.99	0.78
34:a:1115:U:H2'	34:a:1116:U:H5'	1.65	0.78
1:A:287:G:H8	1:A:354:A:C6	1.93	0.78
34:a:458:U:O4	34:a:459:A:N6	2.16	0.78
1:A:289:G:H2'	1:A:290:U:H4'	1.65	0.78
1:A:1867:G:C2	1:A:1874:C:O2	2.36	0.78
55:w:2:G:O6	55:w:70:G:C6	2.38	0.77
1:A:498:G:N1	1:A:506:G:O6	2.15	0.77
1:A:1020:A:C6	1:A:1141:U:O2	2.38	0.77
1:A:278:A:N6	1:A:362:A:C8	2.52	0.77
1:A:283:G:N7	1:A:284:U:O2	2.17	0.77
34:a:827:U:O4	34:a:872:A:N1	2.17	0.77
34:a:207:C:N4	34:a:212:G:H1	1.82	0.77
34:a:437:U:C4	34:a:495:A:N6	2.52	0.77
1:A:278:A:N1	1:A:361:G:C1'	2.48	0.76
34:a:182:A:N1	34:a:194:C:N3	2.33	0.76
1:A:107:G:N2	1:A:346:A:C2	2.53	0.76
34:a:207:C:C4	34:a:212:G:N2	2.38	0.76
34:a:462:G:O6	34:a:469:C:N4	2.19	0.76
55:w:66:C:C5	55:w:67:C:N1	2.54	0.76
34:a:461:A:C2	34:a:472:U:O2	2.39	0.75
1:A:1479:G:O2'	1:A:1560:G:O2'	2.05	0.75
55:w:2:G:O6	55:w:70:G:O6	2.05	0.75
55:w:66:C:C4	55:w:67:C:N1	2.54	0.75
1:A:2013:A:N6	1:A:2613:U:H3	1.85	0.75
34:a:1316:G:O6	52:s:6:LYS:NZ	2.18	0.75
1:A:289:G:N2	1:A:351:C:C2	2.55	0.74
1:A:2013:A:N1	1:A:2613:U:C4	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2338:C:H2'	1:A:2339:C:H5''	1.68	0.74
34:a:1158:C:H2'	34:a:1160:G:C8	2.22	0.74
1:A:289:G:N3	1:A:290:U:H1'	2.03	0.74
1:A:1417:C:C4	1:A:1581:G:O6	2.39	0.74
1:A:277:G:C5	1:A:361:G:C5	2.76	0.73
34:a:203:G:N2	34:a:204:G:O6	2.21	0.73
1:A:1589:U:H2'	1:A:1590:A:C8	2.22	0.73
1:A:2013:A:C2	1:A:2613:U:O4	2.41	0.73
1:A:277:G:C4	1:A:361:G:N7	2.56	0.73
1:A:2028:U:H2'	1:A:2029:G:H8	1.52	0.73
1:A:749:A:O2'	1:A:1618:6MZ:OP1	2.05	0.73
1:A:2030:6MZ:O2'	1:A:2031:A:P	2.46	0.73
1:A:484:C:N3	1:A:496:G:N1	2.34	0.72
34:a:437:U:C2	34:a:495:A:N6	2.57	0.72
1:A:283:G:N1	1:A:357:C:C2	2.52	0.72
1:A:1868:C:H3'	1:A:1869:G:H5''	1.70	0.72
1:A:2030:6MZ:O3'	1:A:2031:A:OP2	2.08	0.72
1:A:278:A:C2	1:A:361:G:C8	2.77	0.72
1:A:277:G:C5	1:A:361:G:C8	2.77	0.72
1:A:1:G:O6	1:A:2902:C:C2	2.43	0.71
34:a:3:A:C5'	34:a:4:U:H5'	2.20	0.71
34:a:1115:U:C2'	34:a:1116:U:H5'	2.20	0.71
34:a:206:C:O2	34:a:213:G:N2	2.23	0.71
55:w:1:C:H1'	55:w:73:A:N1	2.05	0.71
1:A:1048:A:H2	1:A:1111:A:N1	1.66	0.71
1:A:2028:U:C2'	1:A:2029:G:C8	2.72	0.71
34:a:71:A:N1	34:a:94:G:O6	2.23	0.71
34:a:459:A:H2'	34:a:460:A:C8	2.26	0.71
34:a:141:G:O2'	34:a:142:G:O4'	2.09	0.71
34:a:127:G:H2'	34:a:128:G:H5'	1.72	0.71
55:w:66:C:N1	55:w:67:C:H1'	2.06	0.71
1:A:272:A:N1	1:A:365:U:C4	2.59	0.70
1:A:1725:C:C2	1:A:1735:G:N2	2.57	0.70
34:a:1250:A:N1	34:a:1353:G:N2	2.39	0.70
1:A:272:A:C2	1:A:366:C:O2	2.43	0.70
1:A:283:G:N2	1:A:359:G:C2	2.60	0.70
34:a:437:U:O4	34:a:495:A:C6	2.37	0.70
1:A:277:G:C5	1:A:361:G:C4	2.80	0.70
1:A:283:G:C8	1:A:284:U:N1	2.59	0.70
1:A:743:A:O2'	1:A:1659:G:OP1	2.10	0.70
1:A:1048:A:N1	1:A:1111:A:N1	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:3:A:H5'	34:a:4:U:H5'	1.73	0.70
55:v:75:C:H2'	55:v:76:A:O4'	1.91	0.70
1:A:257:C:C3'	1:A:258:G:H5'	2.21	0.69
34:a:3:A:C4'	34:a:4:U:H5'	2.23	0.69
1:A:2674:G:H2'	1:A:2675:A:O4'	1.91	0.69
1:A:278:A:C2	1:A:361:G:H8	2.11	0.69
55:w:3:C:N3	55:w:70:G:O6	2.25	0.69
55:w:2:G:N1	55:w:71:C:C2	2.60	0.69
55:w:6:G:N2	55:w:68:C:O4'	2.26	0.69
1:A:278:A:N1	1:A:361:G:N9	2.42	0.68
55:w:66:C:C6	55:w:67:C:H1'	2.28	0.68
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.26	0.68
1:A:289:G:C6	1:A:351:C:C4	2.81	0.68
34:a:127:G:C2'	34:a:128:G:H5'	2.23	0.68
1:A:1518:C:C3'	1:A:1519:G:H5''	2.23	0.68
1:A:79:C:O2'	1:A:346:A:N3	2.25	0.68
1:A:1047:G:O2'	1:A:1110:G:O6	2.11	0.68
1:A:277:G:N9	1:A:361:G:C8	2.62	0.68
1:A:1530:G:O6	1:A:1541:C:N3	2.27	0.68
1:A:2406:A:C2	12:L:69:ARG:NH2	2.62	0.68
34:a:97:G:H2'	34:a:98:A:O4'	1.94	0.67
46:m:15:VAL:HG23	46:m:16:ILE:HD12	1.75	0.67
55:w:5:G:C2	55:w:69:C:O2	2.46	0.67
1:A:1727:A:H2	1:A:1733:U:N3	1.92	0.67
55:w:117:U:O5'	55:w:117:U:H6	1.78	0.67
1:A:2192:U:C4	1:A:2193:G:N7	2.63	0.67
1:A:2648:G:O6	1:A:2672:U:O2	2.12	0.67
34:a:1162:C:H2'	34:a:1163:A:C8	2.30	0.67
57:y:18:G:O2'	57:y:57:G:N2	2.28	0.67
1:A:295:G:N1	1:A:343:C:O2	2.23	0.67
1:A:2648:G:O6	1:A:2672:U:C2	2.48	0.67
1:A:612:G:N2	1:A:616:A:C8	2.63	0.66
1:A:289:G:H2'	1:A:290:U:C4'	2.26	0.66
1:A:289:G:C6	1:A:351:C:N3	2.62	0.66
1:A:2020:A:N7	27:O:5:ASN:ND2	2.44	0.66
1:A:132:G:C2'	1:A:133:U:H5'	2.25	0.66
1:A:283:G:O6	1:A:356:G:C6	2.47	0.66
1:A:2831:G:OP2	4:D:59:ARG:NH1	2.26	0.66
34:a:459:A:N1	34:a:473:U:C2	2.64	0.66
1:A:2647:U:C2	1:A:2673:G:O6	2.49	0.66
34:a:459:A:N6	34:a:473:U:C4	2.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:1:C:C4	55:w:72:A:N6	2.62	0.66
34:a:3:A:H4'	34:a:4:U:H5'	1.78	0.66
1:A:296:U:O4	1:A:342:A:N1	2.29	0.65
1:A:1618:6MZ:H2'	1:A:1618:6MZ:N3	2.11	0.65
34:a:458:U:O4	34:a:473:U:O4	2.14	0.65
1:A:49:A:C5'	1:A:51:G:H5'	2.26	0.65
1:A:754:U:H4'	1:A:1618:6MZ:H2	1.79	0.65
34:a:472:U:H2'	34:a:473:U:O4'	1.97	0.65
34:a:142:G:C4	34:a:143:A:C8	2.85	0.64
34:a:207:C:N3	34:a:213:G:C2	2.65	0.64
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.77	0.64
34:a:1255:G:O2'	34:a:1258:G:N3	2.31	0.64
55:w:1:C:C2	55:w:73:A:C6	2.85	0.64
1:A:1421:G:O2'	1:A:1494:A:N6	2.31	0.64
1:A:277:G:N3	1:A:361:G:C8	2.66	0.64
34:a:142:G:H3'	34:a:143:A:H8	1.64	0.63
55:w:66:C:N4	55:w:67:C:C4	2.65	0.63
1:A:284:U:N3	1:A:285:G:N7	2.47	0.63
1:A:289:G:C4	1:A:290:U:H1'	2.33	0.63
1:A:277:G:N7	1:A:361:G:C6	2.66	0.63
1:A:1466:U:O2'	1:A:1546:G:O2'	2.15	0.62
1:A:1:G:N2	1:A:2902:C:O2'	2.33	0.62
1:A:2013:A:N6	1:A:2613:U:N3	2.45	0.62
1:A:1383:A:H2	1:A:1405:U:O2	1.81	0.62
1:A:277:G:N2	1:A:360:U:O2'	2.31	0.62
2:B:5:U:O4	2:B:115:A:C6	2.51	0.62
1:A:221:A:N7	1:A:427:U:C4	2.67	0.62
1:A:2199:A:N6	1:A:2224:G:O2'	2.33	0.62
34:a:461:A:H2	34:a:472:U:C2	2.15	0.62
34:a:1158:C:H2'	34:a:1160:G:H8	1.63	0.62
40:g:143:MET:SD	55:w:30:G:N2	2.73	0.62
54:u:9:GLU:HB2	54:u:10:PRO:CD	2.30	0.62
1:A:1858:A:H62	1:A:1884:G:H1'	1.64	0.62
34:a:437:U:O2'	37:d:153:ARG:NH1	2.33	0.62
55:w:2:G:C6	55:w:70:G:C6	2.87	0.62
1:A:289:G:C6	1:A:290:U:C6	2.87	0.61
1:A:1492:G:C2	1:A:1499:C:C2	2.88	0.61
55:w:1:C:H42	55:w:72:A:H62	1.47	0.61
34:a:461:A:C2	34:a:472:U:N3	2.68	0.61
1:A:284:U:C2	1:A:285:G:N7	2.68	0.61
34:a:206:C:N3	34:a:207:C:N4	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:472:U:C2	34:a:473:U:H1'	2.36	0.61
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.82	0.61
1:A:585:G:N7	17:Q:5:ARG:NH1	2.48	0.61
34:a:459:A:C6	34:a:473:U:N3	2.64	0.61
55:w:66:C:C6	55:w:67:C:C1'	2.83	0.61
43:j:57:VAL:HG12	43:j:58:ASN:H	1.65	0.61
1:A:1294:U:H5''	1:A:1294:U:H6	1.65	0.61
2:B:5:U:N3	2:B:116:G:C2	2.69	0.61
34:a:71:A:N1	34:a:98:A:N1	2.48	0.61
1:A:612:G:H3'	1:A:614:A:N7	2.16	0.61
1:A:803:U:H2'	1:A:804:A:H5'	1.82	0.61
1:A:1338:G:N3	1:A:1393:A:H2	1.99	0.61
1:A:2647:U:O2	1:A:2673:G:O6	2.19	0.60
51:r:10:CYS:SG	51:r:11:ARG:N	2.74	0.60
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.81	0.60
34:a:459:A:N6	34:a:473:U:C2	2.67	0.60
1:A:1430:G:H2'	1:A:1431:A:O4'	2.01	0.60
1:A:1725:C:H42	1:A:1735:G:H1	1.47	0.60
34:a:182:A:N6	34:a:194:C:O2	2.31	0.60
39:f:38:ARG:CG	39:f:38:ARG:HH21	2.13	0.60
1:A:2204:G:O6	1:A:2220:U:O2	2.20	0.60
5:E:46:GLN:HB3	5:E:83:VAL:HG11	1.82	0.60
1:A:2572:A:P	4:D:151:THR:HG1	2.25	0.60
1:A:2648:G:C6	1:A:2672:U:O2	2.54	0.60
3:C:159:THR:HG23	3:C:176:ARG:HG3	1.84	0.59
1:A:2852:G:O6	1:A:2865:U:O2	2.19	0.59
34:a:73:C:H2'	34:a:74:A:C8	2.36	0.59
34:a:142:G:C5	34:a:143:A:C5	2.89	0.59
34:a:406:G:N3	34:a:495:A:N6	2.49	0.59
1:A:272:A:N3	1:A:366:C:O2	2.35	0.59
1:A:1493:C:H5''	1:A:1493:C:C6	2.37	0.59
16:P:59:THR:HG22	16:P:72:VAL:HG22	1.84	0.59
34:a:404:G:N3	34:a:498:A:C2	2.71	0.59
34:a:529:G:O6	45:l:45:ASN:HA	2.02	0.59
2:B:5:U:C4	2:B:115:A:C2	2.90	0.59
34:a:642:A:H2'	34:a:643:C:O4'	2.02	0.59
1:A:1852:U:OP1	55:w:71:C:O2'	2.21	0.59
39:f:38:ARG:NH2	39:f:38:ARG:HG3	2.17	0.59
1:A:271:G:C2	1:A:366:C:N3	2.70	0.59
1:A:132:G:H2'	1:A:133:U:H5'	1.83	0.59
1:A:2489:U:O2	1:A:2491:U:C4	2.52	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:946:A:O2'	34:a:1333:A:N3	2.33	0.59
34:a:1455:G:H8	34:a:1455:G:H5''	1.68	0.59
34:a:1240:U:O4	40:g:108:ARG:NH1	2.36	0.59
1:A:1048:A:N7	1:A:1049:C:C5	2.71	0.58
1:A:1642:G:H2'	1:A:1643:G:O4'	2.03	0.58
1:A:1028:A:N3	1:A:2486:C:O2'	2.25	0.58
1:A:2294:G:C2	1:A:2339:C:C2	2.89	0.58
34:a:387:U:C2	34:a:389:A:N1	2.71	0.58
1:A:1735:G:O2'	1:A:1736:U:C6	2.39	0.58
34:a:94:G:H4'	34:a:95:C:O5'	2.04	0.58
34:a:1127:G:H1'	34:a:1280:A:C6	2.38	0.58
1:A:2788:C:H2'	1:A:2789:C:C6	2.39	0.58
39:f:36:ILE:CG2	39:f:39:LEU:HD23	2.34	0.58
48:o:87:ARG:HE	48:o:87:ARG:HA	1.67	0.58
1:A:277:G:C8	1:A:361:G:C6	2.91	0.58
1:A:572:A:OP2	18:R:80:ARG:NH2	2.37	0.58
1:A:1020:A:C6	1:A:1141:U:C2	2.91	0.58
1:A:1779:U:H5	1:A:1784:A:N7	2.01	0.58
55:w:6:G:C2	55:w:68:C:O2	2.57	0.58
1:A:170:U:H5''	1:A:170:U:H6	1.68	0.58
1:A:271:G:C2	1:A:367:G:C2	2.92	0.58
1:A:1050:A:C5	1:A:1051:G:N7	2.72	0.58
1:A:272:A:C2	1:A:365:U:C4	2.92	0.58
1:A:2:G:N1	1:A:2901:C:N3	2.52	0.57
1:A:348:A:H2'	1:A:349:U:O4'	2.04	0.57
1:A:1394:U:H4'	1:A:1603:A:H4'	1.85	0.57
1:A:327:G:H2'	1:A:328:U:O4'	2.04	0.57
1:A:2030:6MZ:H4'	1:A:2030:6MZ:OP2	2.03	0.57
2:B:27:C:OP1	15:O:34:HIS:NE2	2.35	0.57
34:a:462:G:N1	34:a:470:C:N4	2.52	0.57
34:a:341:C:C2	34:a:348:G:O6	2.56	0.57
1:A:1483:G:O6	1:A:1506:U:O2	2.22	0.57
1:A:1727:A:C2	1:A:1733:U:N3	2.69	0.57
1:A:271:G:N1	1:A:367:G:C2	2.72	0.57
2:B:5:U:N3	2:B:115:A:C2	2.72	0.57
55:w:65:C:C5	55:w:66:C:N4	2.73	0.57
1:A:2688:G:N1	1:A:2720:U:OP2	2.36	0.57
34:a:457:G:O6	34:a:474:G:O6	2.23	0.57
52:s:10:ILE:HD12	52:s:40:PHE:CD2	2.39	0.57
34:a:8:A:N6	37:d:201:GLU:O	2.35	0.57
1:A:78:U:O2	1:A:108:G:O6	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:7:A:H5'	34:a:298:A:O4'	2.05	0.56
1:A:278:A:N6	1:A:362:A:C5	2.73	0.56
1:A:1054:A:O2'	32:5:29:ASP:O	2.23	0.56
1:A:1417:C:N3	1:A:1581:G:O6	2.36	0.56
1:A:2734:A:C3'	1:A:2735:G:H5'	2.35	0.56
1:A:350:G:C6	1:A:351:C:C6	2.94	0.56
1:A:158:U:O2	1:A:168:G:O6	2.23	0.56
1:A:283:G:C8	1:A:284:U:C6	2.94	0.56
34:a:17:U:H2'	34:a:18:C:C6	2.40	0.56
1:A:132:G:C5	1:A:133:U:C5	2.94	0.56
1:A:278:A:C6	1:A:361:G:N7	2.70	0.56
1:A:774:G:O2'	1:A:775:G:O5'	2.22	0.56
1:A:1469:A:H2'	1:A:1470:A:C8	2.41	0.56
1:A:2038:G:H2'	1:A:2039:U:O4'	2.06	0.56
1:A:653:U:H2'	1:A:653:U:O2	2.06	0.56
55:w:65:C:N3	55:w:66:C:C4	2.74	0.56
1:A:1061:U:H2'	1:A:1061:U:O2	2.05	0.56
34:a:1065:U:C5	34:a:1189:U:C4	2.94	0.56
1:A:1050:A:H2'	1:A:1051:G:O4'	2.06	0.56
1:A:1717:A:C2	1:A:1743:G:N2	2.69	0.56
1:A:82:U:H5	1:A:104:A:H61	1.54	0.55
1:A:289:G:C2	1:A:290:U:H1'	2.41	0.55
1:A:289:G:O6	1:A:351:C:C4	2.59	0.55
1:A:517:C:OP1	27:0:12:ARG:NH2	2.40	0.55
1:A:278:A:C2	1:A:361:G:H1'	2.37	0.55
1:A:284:U:C2	1:A:285:G:C5	2.95	0.55
1:A:2029:G:H8	1:A:2029:G:O5'	1.88	0.55
55:w:65:C:C4	55:w:66:C:C4	2.94	0.55
34:a:976:G:C8	34:a:1358:U:O2	2.60	0.55
1:A:276:U:C2'	1:A:277:G:H5''	2.37	0.55
1:A:1516:G:O6	1:A:1732:C:N3	2.40	0.55
34:a:437:U:H2'	34:a:437:U:O2	2.07	0.55
1:A:714:U:OP2	48:o:88:ARG:NH1	2.40	0.55
1:A:1727:A:H2'	1:A:1728:C:C6	2.41	0.55
36:c:63:ILE:HD13	36:c:94:ALA:HB1	1.89	0.55
1:A:1418:G:H1'	1:A:1580:A:H61	1.71	0.55
1:A:1857:G:H22	1:A:1884:G:H2'	1.69	0.55
1:A:1527:G:N2	1:A:1544:A:C8	2.75	0.55
34:a:739:C:P	39:f:2:ARG:HH22	2.30	0.55
55:v:52:G:N2	55:v:63:G:C4	2.74	0.55
1:A:1079:C:O2'	9:I:130:GLY:HA3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:437:U:O4	34:a:495:A:C4	2.59	0.54
34:a:459:A:C6	34:a:473:U:C2	2.95	0.54
1:A:279:A:C2	1:A:362:A:H4'	2.42	0.54
1:A:276:U:H2'	1:A:277:G:H5''	1.89	0.54
1:A:12:U:H2'	1:A:12:U:O2	2.07	0.54
1:A:285:G:N2	1:A:356:G:N7	2.51	0.54
1:A:1418:G:C2	1:A:1579:A:N7	2.75	0.54
1:A:2734:A:H2'	1:A:2735:G:H5'	1.89	0.54
1:A:1454:C:O2'	1:A:1455:G:N7	2.40	0.54
1:A:642:U:O2'	1:A:644:A:N7	2.33	0.54
1:A:1615:C:H2'	1:A:1617:C:C5	2.43	0.54
1:A:2204:G:C6	1:A:2220:U:O2	2.61	0.54
55:w:67:C:N3	55:w:68:C:N3	2.54	0.54
1:A:2:G:C2	1:A:2901:C:O2	2.61	0.54
1:A:1175:A:H3'	1:A:1175:A:N3	2.23	0.54
1:A:2838:G:H2'	1:A:2839:G:O4'	2.08	0.54
34:a:1126:U:O4'	34:a:1281:C:O2	2.25	0.54
34:a:1264:U:C2	34:a:1272:G:N2	2.75	0.54
39:f:38:ARG:HH21	39:f:38:ARG:HG3	1.73	0.54
55:w:1:C:N1	55:w:73:A:N6	2.56	0.54
1:A:2:G:N1	1:A:2901:C:O2	2.41	0.54
34:a:470:C:N4	34:a:471:U:O4	2.40	0.54
55:w:66:C:H3'	55:w:67:C:C4'	2.38	0.54
34:a:343:U:O2'	34:a:344:A:C8	2.61	0.53
34:a:778:G:H2'	34:a:779:C:O4'	2.09	0.53
1:A:1076:C:H1'	9:I:92:PRO:HD2	1.90	0.53
1:A:1305:C:H5''	1:A:1305:C:H6	1.73	0.53
1:A:1417:C:O2'	1:A:1587:G:O2'	2.01	0.53
1:A:2850:A:N7	1:A:2868:A:O2'	2.37	0.53
1:A:998:C:O5'	1:A:998:C:H6	1.91	0.53
1:A:2647:U:O2	1:A:2673:G:C6	2.62	0.53
55:w:65:C:H2'	55:w:66:C:C6	2.43	0.53
16:P:38:ARG:NE	34:a:346:G:OP1	2.40	0.53
34:a:406:G:C4	34:a:495:A:N6	2.76	0.53
34:a:447:G:N2	34:a:487:A:C8	2.76	0.53
34:a:589:U:H2'	34:a:590:U:C6	2.44	0.53
1:A:132:G:C6	1:A:133:U:N3	2.77	0.53
2:B:21:G:N1	2:B:62:C:O2	2.40	0.53
32:5:56:ARG:HD3	32:5:81:LEU:HD11	1.91	0.53
34:a:449:G:O6	34:a:484:G:O6	2.27	0.53
1:A:1495:A:H2'	1:A:1496:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.90	0.53
32:5:56:ARG:HG3	32:5:83:ALA:HB2	1.90	0.53
1:A:169:G:H2'	1:A:170:U:H5''	1.91	0.53
1:A:277:G:C5	1:A:361:G:N9	2.78	0.53
1:A:1:G:C6	1:A:2:G:C5	2.97	0.52
1:A:1021:A:N6	1:A:1141:U:H3	2.07	0.52
34:a:74:A:C2	34:a:97:G:C2	2.97	0.52
34:a:71:A:C2	34:a:94:G:O6	2.62	0.52
34:a:1264:U:O2	34:a:1272:G:N2	2.42	0.52
1:A:285:G:C2	1:A:356:G:C5	2.92	0.52
1:A:498:G:C2	1:A:506:G:O6	2.62	0.52
1:A:283:G:H5'	1:A:284:U:OP2	2.09	0.52
1:A:283:G:H8	1:A:284:U:C6	2.27	0.52
1:A:471:A:OP1	5:E:79:ARG:NH2	2.42	0.52
34:a:187:G:N2	34:a:190:A:C8	2.77	0.52
1:A:542:U:H2'	1:A:543:G:H5'	1.91	0.52
1:A:1009:A:N3	1:A:1153:C:O2'	2.36	0.52
1:A:1127:A:N1	1:A:2463:C:O2'	2.43	0.52
58:z:220:ILE:HD12	58:z:226:VAL:HG21	1.91	0.52
1:A:654:A:H5''	1:A:654:A:N3	2.23	0.52
1:A:2327:A:H2'	1:A:2328:A:C8	2.45	0.52
34:a:171:A:H2'	34:a:172:A:C8	2.45	0.52
1:A:2639:A:N6	1:A:2775:G:O2'	2.42	0.52
1:A:368:A:H5''	1:A:368:A:H8	1.75	0.52
1:A:1019:U:H3	1:A:1142:A:H62	1.58	0.52
1:A:1272:A:C2	1:A:1618:6MZ:C2	2.93	0.52
34:a:3:A:H5'	34:a:4:U:C5'	2.40	0.52
34:a:94:G:C4'	34:a:95:C:O5'	2.58	0.52
34:a:187:G:N2	34:a:191:G:C5	2.77	0.52
34:a:1235:U:H2'	34:a:1236:A:O4'	2.09	0.52
1:A:546:U:H2'	1:A:547:A:H4'	1.92	0.52
1:A:1021:A:H61	1:A:1141:U:H3	1.58	0.52
34:a:404:G:N3	34:a:498:A:H2	2.07	0.52
55:w:65:C:N4	55:w:66:C:N4	2.56	0.52
55:w:66:C:C5	55:w:67:C:C1'	2.93	0.52
1:A:1737:G:O5'	1:A:1737:G:H8	1.92	0.51
2:B:31:C:H2'	2:B:32:U:O4'	2.10	0.51
55:v:75:C:H2'	55:v:76:A:C1'	2.39	0.51
1:A:288:U:H2'	1:A:289:G:H5'	1.92	0.51
1:A:465:G:H2'	1:A:466:A:C8	2.45	0.51
1:A:1049:C:H2'	1:A:1050:A:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:C:O2'	1:A:1809:A:N3	2.34	0.51
1:A:1616:A:H4'	1:A:1617:C:OP2	2.10	0.51
2:B:77:U:C5'	22:V:21:ARG:HH22	2.24	0.51
1:A:910:A:N3	1:A:2264:C:O2'	2.40	0.51
1:A:2028:U:C5	1:A:2029:G:C6	2.98	0.51
1:A:2743:U:H2'	1:A:2744:G:O4'	2.10	0.51
34:a:430:A:P	37:d:21:LYS:NZ	2.83	0.51
34:a:675:A:H2'	34:a:676:A:O4'	2.10	0.51
34:a:1258:G:C6	34:a:1277:C:N3	2.78	0.51
1:A:714:U:H5''	1:A:714:U:H6	1.76	0.51
1:A:1050:A:C6	1:A:1051:G:C5	2.98	0.51
1:A:2093:G:O2'	1:A:2198:A:N1	2.36	0.51
34:a:1218:C:H2'	34:a:1219:A:C8	2.46	0.51
55:w:1:C:N4	55:w:71:C:N4	2.58	0.51
1:A:285:G:N1	1:A:356:G:O6	2.44	0.51
55:w:66:C:H3'	55:w:67:C:H4'	1.91	0.51
1:A:877:A:C2	1:A:900:A:N7	2.79	0.51
1:A:1509:A:H2'	1:A:1510:G:C8	2.46	0.51
34:a:1391:U:H2'	34:a:1392:G:C8	2.46	0.51
1:A:2:G:N1	1:A:2901:C:C2	2.78	0.51
1:A:132:G:N1	1:A:133:U:C2	2.79	0.51
1:A:1130:U:O2'	1:A:1131:G:OP1	2.26	0.51
1:A:2844:G:H2'	1:A:2845:U:O4'	2.11	0.51
34:a:297:G:N2	34:a:300:A:OP2	2.44	0.51
1:A:570:G:H2'	1:A:2030:6MZ:N7	2.25	0.51
1:A:636:G:H3'	12:L:128:THR:HG21	1.92	0.51
1:A:684:G:C2	1:A:794:A:C2	2.99	0.51
1:A:1250:G:OP2	12:L:21:ARG:NH2	2.44	0.51
34:a:152:A:H2'	34:a:153:C:O4'	2.10	0.51
34:a:1060:U:H4'	43:j:53:ILE:HG23	1.92	0.51
34:a:1258:G:N2	34:a:1277:C:O2	2.43	0.51
1:A:155:A:H2'	1:A:156:A:C8	2.46	0.50
1:A:1070:A:N1	9:I:10:LEU:HD13	2.26	0.50
1:A:1339:G:O4'	1:A:1393:A:C2	2.64	0.50
34:a:177:G:OP2	53:t:59:ARG:HD3	2.10	0.50
55:w:71:C:H2'	55:w:71:C:O2	2.11	0.50
1:A:1:G:H1	1:A:2902:C:H1'	1.75	0.50
48:o:87:ARG:HA	48:o:87:ARG:NE	2.25	0.50
1:A:1019:U:OP1	1:A:1035:U:O2'	2.20	0.50
1:A:1482:G:O2'	1:A:1509:A:N1	2.44	0.50
55:w:2:G:O6	55:w:71:C:C4	2.61	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:C:H3'	2:B:32:U:H5''	1.92	0.50
34:a:692:U:O2'	34:a:694:A:N7	2.40	0.50
39:f:38:ARG:CG	39:f:38:ARG:NH2	2.73	0.50
1:A:573:U:O4	1:A:2030:6MZ:H3'	2.12	0.50
1:A:1489:C:C2	1:A:1501:G:N2	2.80	0.50
1:A:1726:G:C6	1:A:1734:C:N3	2.79	0.50
1:A:1914:C:O2	1:A:1914:C:O4'	2.27	0.50
34:a:377:G:C2	34:a:387:U:O2	2.64	0.50
34:a:1356:G:H2'	34:a:1357:A:C8	2.46	0.50
1:A:132:G:C4	1:A:133:U:C6	2.99	0.50
1:A:1413:A:N6	1:A:1589:U:H3	2.09	0.50
12:L:78:ARG:HG3	12:L:113:ALA:CB	2.42	0.50
34:a:590:U:OP1	41:h:30:LYS:N	2.41	0.50
34:a:1159:U:O4'	34:a:1182:G:N2	2.45	0.50
39:f:39:LEU:O	39:f:40:GLU:HB3	2.12	0.50
41:h:10:LEU:HD22	41:h:74:ILE:HD11	1.93	0.50
1:A:485:C:H5''	1:A:485:C:C6	2.47	0.49
7:G:32:LEU:HB3	7:G:74:MET:HE3	1.94	0.49
1:A:283:G:C6	1:A:356:G:O6	2.55	0.49
1:A:1320:C:N3	1:A:1331:G:O6	2.45	0.49
32:5:53:ARG:HB3	32:5:55:VAL:HG23	1.94	0.49
1:A:158:U:C2	1:A:168:G:O6	2.65	0.49
1:A:1048:A:N1	1:A:1111:A:C2	2.80	0.49
1:A:1721:G:C6	1:A:1738:G:C6	3.01	0.49
2:B:114:C:H2'	2:B:115:A:C8	2.47	0.49
34:a:460:A:H2'	34:a:461:A:O4'	2.12	0.49
34:a:1305:G:O2'	34:a:1306:A:OP2	2.26	0.49
1:A:297:G:C6	1:A:342:A:C2	3.00	0.49
1:A:877:A:C6	1:A:899:A:C2	3.00	0.49
34:a:458:U:N3	34:a:474:G:N1	2.61	0.49
1:A:1048:A:C8	1:A:1049:C:C5	3.00	0.49
1:A:2646:C:OP2	1:A:2732:G:O2'	2.29	0.49
34:a:153:C:C4	34:a:154:U:C5	3.00	0.49
34:a:203:G:C2	34:a:215:C:N3	2.80	0.49
34:a:430:A:P	37:d:21:LYS:HZ3	2.35	0.49
2:B:16:G:H2'	2:B:17:C:H5''	1.95	0.49
15:O:100:HIS:O	15:O:104:GLN:NE2	2.37	0.49
1:A:1503:A:H5'	1:A:1504:A:OP2	2.12	0.49
34:a:180:U:O2	34:a:195:A:N7	2.45	0.49
34:a:343:U:O3'	34:a:344:A:C8	2.65	0.49
34:a:1372:U:H2'	34:a:1373:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:1:C:N4	55:w:72:A:H62	2.11	0.49
55:w:1:C:C6	55:w:73:A:N6	2.81	0.49
1:A:289:G:N1	1:A:351:C:C4	2.81	0.49
1:A:289:G:O6	1:A:351:C:N4	2.46	0.49
1:A:1492:G:C2	1:A:1499:C:O2	2.66	0.49
1:A:2031:A:C6	1:A:2498:OMC:H1'	2.47	0.49
34:a:72:A:N7	34:a:73:C:C5	2.80	0.49
34:a:75:G:C2	34:a:96:U:C4	3.01	0.49
34:a:211:G:N3	34:a:211:G:H2'	2.28	0.49
34:a:343:U:O2'	34:a:344:A:H8	1.95	0.49
55:w:66:C:C3'	55:w:67:C:H4'	2.42	0.49
1:A:278:A:N6	1:A:361:G:C8	2.78	0.48
1:A:285:G:C2	1:A:356:G:O6	2.66	0.48
1:A:287:G:H2'	1:A:288:U:C6	2.48	0.48
1:A:288:U:C4	1:A:352:A:N1	2.81	0.48
34:a:244:U:C6	34:a:894:G:N2	2.81	0.48
34:a:299:G:H2'	34:a:300:A:C8	2.49	0.48
1:A:1149:G:H2'	1:A:1150:C:C6	2.48	0.48
1:A:1406:U:H2'	1:A:1407:G:O4'	2.12	0.48
1:A:1589:U:N3	1:A:1590:A:C5	2.81	0.48
1:A:2273:A:H2'	1:A:2274:A:C8	2.47	0.48
34:a:75:G:N2	34:a:96:U:C4	2.82	0.48
34:a:591:U:H5''	34:a:591:U:H6	1.78	0.48
58:z:16:THR:HB	58:z:24:LYS:HG3	1.95	0.48
1:A:132:G:C6	1:A:133:U:C4	3.00	0.48
1:A:1056:G:H5'	32:5:34:THR:HG23	1.95	0.48
1:A:1418:G:N2	1:A:1579:A:C8	2.82	0.48
1:A:2741:A:N6	1:A:2763:G:H1'	2.29	0.48
1:A:2744:G:C2'	1:A:2745:C:H5'	2.44	0.48
55:v:53:G:H3'	55:v:54:5MU:H73	1.95	0.48
1:A:277:G:C6	1:A:361:G:C4	3.01	0.48
1:A:1528:A:H2'	1:A:1529:G:O4'	2.13	0.48
1:A:1870:C:O2	1:A:1871:A:C2	2.67	0.48
1:A:2204:G:O6	1:A:2220:U:C2	2.65	0.48
11:K:24:VAL:HG13	11:K:33:ALA:HB2	1.95	0.48
34:a:342:C:C2	34:a:348:G:C2	3.01	0.48
34:a:447:G:O2'	34:a:487:A:N6	2.45	0.48
34:a:613:C:H2'	34:a:614:C:C6	2.48	0.48
1:A:1532:A:H2	1:A:1539:U:H3	1.61	0.48
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.95	0.48
1:A:277:G:C5	1:A:361:G:N7	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:U:C2	2:B:116:G:C2	3.02	0.48
34:a:142:G:C6	34:a:143:A:C6	3.01	0.48
34:a:1498:UR3:H3U2	56:x:17:U:H4'	1.95	0.48
55:w:2:G:C2	55:w:71:C:C2	3.01	0.48
1:A:79:C:N3	1:A:107:G:O6	2.46	0.48
1:A:1338:G:O2'	1:A:1393:A:N1	2.45	0.48
1:A:1432:G:H2'	1:A:1433:A:C8	2.48	0.48
1:A:2886:A:H8	1:A:2886:A:H5''	1.79	0.48
34:a:182:A:C2	34:a:184:G:C6	3.01	0.48
34:a:629:A:H2'	34:a:630:A:O4'	2.13	0.48
34:a:1126:U:O2'	34:a:1280:A:C8	2.66	0.48
1:A:184:C:H4'	1:A:217:A:C2	2.49	0.48
1:A:351:C:C2	1:A:352:A:C8	3.02	0.48
1:A:2747:G:C2	1:A:2748:A:C2	3.01	0.48
34:a:1149:C:H2'	34:a:1150:A:C8	2.49	0.48
34:a:1486:G:H2'	34:a:1487:G:O4'	2.14	0.48
1:A:82:U:H5	1:A:104:A:N6	2.12	0.48
1:A:365:U:H2'	1:A:365:U:O2	2.13	0.48
1:A:605:G:H2'	1:A:606:U:O4'	2.13	0.48
1:A:608:A:H2'	1:A:609:A:C8	2.49	0.48
1:A:2337:G:C2	1:A:2338:C:C2	3.01	0.48
1:A:239:C:C2	1:A:259:G:C2	3.02	0.48
1:A:563:A:OP2	18:R:79:ARG:NH2	2.43	0.48
1:A:1385:A:C2	1:A:1386:C:C2	3.02	0.48
1:A:2862:G:H2'	1:A:2863:C:O4'	2.13	0.48
2:B:31:C:C5	2:B:32:U:C5	3.02	0.48
41:h:77:VAL:HG11	41:h:124:ILE:HD12	1.95	0.48
1:A:77:G:C6	1:A:110:G:C2	3.02	0.47
1:A:1492:G:N2	1:A:1499:C:C2	2.82	0.47
6:F:91:ARG:HA	6:F:95:MET:HB2	1.94	0.47
39:f:29:ILE:HG21	39:f:64:VAL:HG21	1.95	0.47
1:A:1868:C:N4	1:A:1869:G:C4	2.82	0.47
34:a:207:C:N4	34:a:212:G:N1	2.56	0.47
1:A:645:C:H2'	1:A:647:G:C8	2.50	0.47
1:A:1020:A:N1	1:A:1141:U:H1'	2.29	0.47
1:A:2734:A:C2'	1:A:2735:G:H5'	2.44	0.47
34:a:147:G:H2'	34:a:148:G:C8	2.49	0.47
34:a:472:U:C4	34:a:473:U:C2	3.03	0.47
1:A:181:A:H2'	1:A:182:A:C8	2.50	0.47
1:A:271:G:C2	1:A:367:G:N3	2.82	0.47
1:A:284:U:N3	1:A:285:G:C5	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:U:C2'	1:A:1734:C:H6	2.22	0.47
11:K:19:VAL:HB	11:K:41:ILE:HG23	1.94	0.47
34:a:294:U:OP1	34:a:610:U:O2'	2.31	0.47
34:a:406:G:C5	34:a:495:A:N7	2.83	0.47
34:a:470:C:C4	34:a:471:U:O4	2.67	0.47
34:a:946:A:H2'	34:a:947:G:C8	2.50	0.47
1:A:288:U:C4	1:A:352:A:C2	3.02	0.47
1:A:803:U:C2'	1:A:804:A:H5'	2.45	0.47
1:A:1047:G:O2'	1:A:1110:G:C6	2.58	0.47
1:A:1179:G:H3'	1:A:1180:U:H4'	1.95	0.47
1:A:1434:A:H2'	1:A:1435:G:C8	2.50	0.47
34:a:212:G:H2'	34:a:213:G:C8	2.49	0.47
34:a:214:C:H6	34:a:214:C:O5'	1.96	0.47
34:a:462:G:C6	34:a:470:C:N4	2.82	0.47
34:a:690:G:O6	44:k:52:ARG:NH2	2.48	0.47
34:a:694:A:O2'	55:w:38:A:O2'	2.24	0.47
34:a:1172:C:H2'	34:a:1173:U:C6	2.49	0.47
58:z:98:MET:HE3	58:z:101:ALA:HB2	1.96	0.47
1:A:40:U:C2'	1:A:41:C:H5'	2.44	0.47
1:A:277:G:N2	1:A:361:G:O4'	2.48	0.47
1:A:283:G:H5''	1:A:284:U:C5	2.50	0.47
1:A:1725:C:N4	1:A:1735:G:H1	2.11	0.47
12:L:79:LEU:HD21	12:L:116:VAL:HG23	1.97	0.47
34:a:911:U:OP2	45:l:93:ARG:NH2	2.47	0.47
1:A:278:A:N3	1:A:278:A:H2'	2.28	0.47
1:A:283:G:C8	1:A:284:U:N3	2.74	0.47
1:A:290:U:O2	1:A:290:U:H2'	2.14	0.47
1:A:549:G:H2'	1:A:550:C:C6	2.50	0.47
1:A:1467:U:C5	1:A:1546:G:H2'	2.49	0.47
1:A:1980:G:O2'	1:A:1982:U:OP2	2.31	0.47
3:C:75:ALA:HB1	3:C:93:VAL:CG1	2.45	0.47
34:a:104:G:C2'	34:a:105:G:H5''	2.45	0.47
34:a:446:G:O6	34:a:488:C:N3	2.48	0.47
1:A:287:G:C8	1:A:354:A:N7	2.82	0.47
1:A:639:U:H2'	1:A:640:C:C6	2.50	0.47
34:a:1142:G:C5	34:a:1143:G:H1'	2.50	0.47
54:u:9:GLU:HB2	54:u:10:PRO:HD3	1.96	0.47
1:A:143:C:H6	1:A:143:C:H5''	1.80	0.47
1:A:858:G:O2'	1:A:2268:A:O2'	2.29	0.47
1:A:1412:U:H2'	1:A:1413:A:H8	1.79	0.47
39:f:91:ARG:NH1	39:f:92:THR:HG23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:U:O4	1:A:2029:G:O2'	2.32	0.47
55:w:6:G:N2	55:w:68:C:C1'	2.78	0.47
1:A:495:G:H2'	1:A:496:G:O4'	2.15	0.46
1:A:1853:A:H2'	1:A:1854:A:O4'	2.15	0.46
9:I:134:SER:O	9:I:134:SER:OG	2.33	0.46
34:a:167:A:H2'	34:a:168:G:O4'	2.15	0.46
34:a:1220:G:OP1	52:s:36:ARG:NH1	2.48	0.46
55:w:65:C:N4	55:w:66:C:H42	2.13	0.46
1:A:271:G:C4	1:A:367:G:N2	2.84	0.46
1:A:631:A:N3	1:A:2415:G:O2'	2.41	0.46
1:A:1017:G:N2	1:A:1146:C:C2	2.83	0.46
1:A:1858:A:O4'	1:A:1885:A:C6	2.68	0.46
1:A:286:U:C2	1:A:354:A:N6	2.83	0.46
1:A:288:U:O4	1:A:352:A:C6	2.68	0.46
1:A:308:G:H2'	1:A:309:A:C8	2.50	0.46
1:A:1418:G:N2	1:A:1579:A:N7	2.63	0.46
1:A:2345:G:N3	1:A:2381:A:H2'	2.31	0.46
1:A:2747:G:C2	1:A:2748:A:N1	2.83	0.46
2:B:79:G:N7	22:V:14:LYS:NZ	2.63	0.46
55:w:65:C:C2	55:w:66:C:C4	3.03	0.46
34:a:487:A:H2'	34:a:488:C:O4'	2.15	0.46
34:a:1305:G:O2'	34:a:1331:G:N2	2.49	0.46
1:A:721:A:H2'	1:A:722:A:C8	2.51	0.46
1:A:1050:A:C6	1:A:1051:G:N7	2.83	0.46
1:A:1106:G:H21	32:5:81:LEU:HD13	1.81	0.46
1:A:2514:U:H2'	1:A:2515:C:C6	2.50	0.46
34:a:215:C:H3'	34:a:216:U:H5''	1.97	0.46
34:a:269:C:H2'	34:a:270:A:C8	2.50	0.46
34:a:341:C:O2	34:a:348:G:C6	2.67	0.46
34:a:876:C:H1'	41:h:11:THR:HG21	1.96	0.46
45:l:74:GLN:O	45:l:76:HIS:N	2.49	0.46
1:A:52:A:H2'	1:A:53:A:C8	2.50	0.46
1:A:278:A:C5	1:A:361:G:C8	2.97	0.46
1:A:1020:A:C5	1:A:1141:U:O2	2.68	0.46
1:A:1591:A:H2'	1:A:1592:C:C5	2.51	0.46
1:A:1858:A:H2'	1:A:1859:U:O4'	2.15	0.46
34:a:93:U:H2'	34:a:95:C:N1	2.31	0.46
34:a:197:A:N1	34:a:220:G:O2'	2.46	0.46
34:a:1314:C:H2'	34:a:1315:U:O4'	2.15	0.46
55:v:75:C:C2'	55:v:76:A:O4'	2.61	0.46
1:A:271:G:C6	1:A:367:G:C2	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:A:N6	1:A:322:A:O2'	2.49	0.46
1:A:1086:A:H2'	1:A:1086:A:N3	2.30	0.46
34:a:431:A:H2'	34:a:432:A:O4'	2.15	0.46
55:v:51:C:C4	55:v:52:G:C8	3.03	0.46
1:A:784:G:H5'	1:A:785:G:OP1	2.15	0.46
1:A:1548:A:H2'	1:A:1549:A:C8	2.50	0.46
2:B:31:C:C3'	2:B:32:U:H5''	2.46	0.46
34:a:105:G:H5'	34:a:105:G:H8	1.81	0.46
44:k:108:ASN:HB3	54:u:6:ARG:HG2	1.98	0.46
55:w:2:G:N2	55:w:71:C:O2	2.48	0.46
1:A:546:U:O2	1:A:546:U:O4'	2.33	0.46
1:A:1048:A:C2	1:A:1111:A:C2	2.91	0.46
34:a:1432:G:O2'	34:a:1433:A:OP2	2.26	0.46
1:A:1589:U:O4	1:A:1590:A:N6	2.49	0.46
34:a:75:G:N2	34:a:97:G:N1	2.64	0.46
34:a:149:A:H2'	34:a:150:U:O4'	2.16	0.46
1:A:2840:C:H5''	14:N:53:THR:CG2	2.46	0.45
34:a:212:G:H8	34:a:212:G:H5''	1.81	0.45
52:s:10:ILE:HD12	52:s:40:PHE:CE2	2.51	0.45
57:y:18:G:O6	57:y:55:PSU:H1'	2.16	0.45
34:a:389:A:N7	34:a:390:U:C2	2.84	0.45
34:a:763:G:H2'	34:a:764:C:C6	2.50	0.45
1:A:77:G:C5	1:A:110:G:N2	2.85	0.45
1:A:1048:A:N7	1:A:1049:C:H5	2.13	0.45
1:A:1727:A:C2	1:A:1733:U:O4	2.68	0.45
34:a:890:G:O2'	34:a:906:A:N6	2.49	0.45
34:a:927:G:O2'	34:a:1503:A:N7	2.45	0.45
43:j:42:LEU:HD11	43:j:73:LEU:HG	1.98	0.45
1:A:151:C:C2'	1:A:152:A:H5'	2.47	0.45
1:A:1538:G:H2'	1:A:1539:U:C5	2.50	0.45
34:a:131:A:H2'	34:a:132:C:C6	2.52	0.45
1:A:40:U:H2'	1:A:41:C:H5'	1.97	0.45
1:A:77:G:C5	1:A:110:G:C2	3.03	0.45
1:A:629:G:H2'	1:A:630:G:O4'	2.17	0.45
34:a:470:C:N3	34:a:471:U:C4	2.85	0.45
36:c:140:ALA:HB3	36:c:148:ILE:HD12	1.97	0.45
1:A:132:G:C6	1:A:133:U:C2	3.04	0.45
1:A:1589:U:C2	1:A:1590:A:C5	3.05	0.45
1:A:2756:U:C5	1:A:2759:G:C5	3.05	0.45
34:a:142:G:C6	34:a:143:A:C5	3.04	0.45
46:m:94:LEU:HD22	46:m:101:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2615:U:C2	27:0:3:GLN:HA	2.52	0.45
1:A:2857:G:N2	1:A:2860:A:C8	2.85	0.45
34:a:202:G:N2	34:a:216:U:H1'	2.32	0.45
55:v:24:U:C4	55:v:25:C:C5	3.04	0.45
1:A:307:G:N2	1:A:309:A:H3'	2.32	0.45
1:A:1433:A:H2'	1:A:1434:A:C8	2.52	0.45
46:m:3:ILE:HD11	46:m:18:LEU:HD22	1.99	0.45
1:A:290:U:C2	1:A:291:G:C8	3.05	0.45
1:A:875:G:C6	1:A:876:C:C4	3.05	0.45
1:A:1594:U:H2'	1:A:1595:C:C6	2.52	0.45
2:B:21:G:C2	2:B:63:C:O2	2.70	0.45
34:a:93:U:H3'	34:a:95:C:C5	2.51	0.45
34:a:104:G:H2'	34:a:105:G:H5''	1.99	0.45
1:A:278:A:C6	1:A:361:G:N9	2.79	0.45
36:c:148:ILE:O	36:c:148:ILE:HG23	2.16	0.45
1:A:228:C:N4	1:A:2407:A:C4	2.85	0.44
1:A:319:G:H2'	1:A:320:A:O4'	2.17	0.44
1:A:604:G:O6	1:A:624:C:N3	2.49	0.44
1:A:1110:G:O6	32:5:59:LEU:HD11	2.16	0.44
1:A:1717:A:C8	1:A:1744:A:C6	3.05	0.44
1:A:1874:C:H2'	1:A:1875:G:O4'	2.16	0.44
1:A:2340:A:OP1	2:B:41:G:N2	2.50	0.44
2:B:5:U:N3	2:B:115:A:H2	2.15	0.44
34:a:72:A:H2'	34:a:72:A:N3	2.32	0.44
34:a:75:G:C2	34:a:96:U:N3	2.85	0.44
55:v:52:G:C2	55:v:63:G:C4	3.05	0.44
1:A:273:G:C6	1:A:365:U:C4	3.05	0.44
1:A:2572:A:N7	4:D:150:GLN:HB2	2.33	0.44
1:A:2751:G:OP2	7:G:2:ARG:HD2	2.17	0.44
1:A:2812:G:H2'	1:A:2813:A:C8	2.52	0.44
34:a:1064:G:O2'	34:a:1190:G:N2	2.49	0.44
1:A:283:G:C5	1:A:284:U:O2	2.70	0.44
1:A:735:A:C8	1:A:736:C:C5	3.06	0.44
1:A:2250:G:O5'	1:A:2250:G:H8	2.00	0.44
1:A:2698:U:H2'	1:A:2699:C:C6	2.52	0.44
1:A:2630:G:O6	1:A:2788:C:N3	2.50	0.44
2:B:1:U:H3'	2:B:2:G:H8	1.83	0.44
8:H:90:LEU:CD2	8:H:94:ILE:HD11	2.47	0.44
55:v:52:G:C2	55:v:63:G:C5	3.06	0.44
1:A:613:A:H1'	1:A:614:A:C8	2.53	0.44
11:K:34:GLY:O	11:K:36:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:50:ARG:HD3	13:M:65:ILE:HD11	2.00	0.44
34:a:203:G:N2	34:a:215:C:C2	2.86	0.44
34:a:872:A:H2'	34:a:872:A:N3	2.32	0.44
1:A:160:A:N3	1:A:2208:C:O2'	2.47	0.44
1:A:290:U:O4	1:A:350:G:C5	2.68	0.44
1:A:480:A:N3	1:A:499:U:O2'	2.47	0.44
1:A:974:G:H2'	1:A:974:G:N3	2.32	0.44
1:A:1056:G:N2	1:A:1102:C:C5	2.86	0.44
1:A:1476:U:C2	1:A:1516:G:C6	3.06	0.44
1:A:1913:A:N1	57:y:37:MIA:O2'	2.51	0.44
24:X:16:ASN:O	24:X:16:ASN:ND2	2.50	0.44
1:A:6:A:H8	1:A:6:A:H5''	1.83	0.44
1:A:227:A:N6	1:A:410:G:O2'	2.51	0.44
1:A:285:G:N2	1:A:356:G:C4	2.84	0.44
1:A:1075:C:O2'	9:I:90:GLY:O	2.34	0.44
1:A:1416:G:N1	1:A:1582:C:N3	2.66	0.44
1:A:1426:G:O2'	1:A:1572:A:N6	2.49	0.44
1:A:1727:A:C2	1:A:1733:U:C4	3.06	0.44
34:a:142:G:C5	34:a:143:A:N7	2.85	0.44
34:a:1124:G:O2'	34:a:1145:A:N6	2.50	0.44
1:A:299:A:N3	1:A:319:G:O2'	2.43	0.44
2:B:5:U:O4	2:B:116:G:C6	2.71	0.44
20:T:80:TRP:CZ3	20:T:82:LYS:HB3	2.52	0.44
34:a:1258:G:H2'	34:a:1259:C:C6	2.52	0.44
57:y:10:G:N1	57:y:25:C:O2	2.42	0.44
1:A:84:A:N1	1:A:98:G:O2'	2.49	0.44
1:A:342:A:H2'	1:A:343:C:O4'	2.18	0.44
1:A:1061:U:O2	1:A:1061:U:C2'	2.66	0.44
1:A:1111:A:C2	1:A:1112:G:H1'	2.53	0.44
1:A:2695:U:H2'	1:A:2696:U:C6	2.52	0.44
19:S:5:ALA:HB3	19:S:54:ALA:HB2	1.99	0.44
21:U:33:VAL:HG13	21:U:66:VAL:HG22	2.00	0.44
54:u:44:ARG:HB3	54:u:48:LYS:HE3	1.99	0.44
1:A:565:C:H2'	1:A:566:U:O4'	2.18	0.43
1:A:1063:G:O3'	9:I:80:LYS:HD3	2.17	0.43
1:A:2028:U:C5	1:A:2029:G:O6	2.71	0.43
1:A:2356:U:H2'	1:A:2357:G:O4'	2.18	0.43
1:A:2899:A:H2'	1:A:2900:A:C8	2.53	0.43
1:A:290:U:C4	1:A:291:G:C5	3.07	0.43
1:A:2412:A:H2'	1:A:2413:G:O4'	2.18	0.43
17:Q:104:ALA:O	18:R:48:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1273:C:H5''	34:a:1273:C:H6	1.82	0.43
1:A:1370:C:H2'	1:A:1371:G:O4'	2.17	0.43
1:A:2687:U:O4	1:A:2688:G:N1	2.51	0.43
34:a:143:A:H5'	34:a:144:G:H5'	2.00	0.43
42:i:83:THR:HG21	42:i:102:PHE:HB3	2.00	0.43
1:A:137:U:H3'	1:A:138:U:H5''	1.99	0.43
1:A:278:A:N6	1:A:361:G:C5	2.87	0.43
1:A:1615:C:H2'	1:A:1617:C:C6	2.53	0.43
34:a:593:U:H2'	34:a:594:U:C6	2.53	0.43
53:t:66:ILE:HG23	53:t:70:LYS:HD2	2.00	0.43
1:A:82:U:O2	1:A:82:U:O4'	2.37	0.43
1:A:257:C:H2'	1:A:258:G:C5'	2.31	0.43
1:A:278:A:N1	1:A:362:A:C8	2.85	0.43
1:A:278:A:N6	1:A:361:G:C4	2.87	0.43
1:A:1171:G:H22	1:A:1177:G:H1	1.66	0.43
1:A:1964:G:H4'	1:A:1965:C:OP2	2.19	0.43
1:A:2567:G:H2'	1:A:2568:U:C6	2.53	0.43
34:a:104:G:C3'	34:a:105:G:H5''	2.48	0.43
55:w:2:G:O6	55:w:71:C:C5	2.72	0.43
1:A:278:A:C6	1:A:362:A:N9	2.87	0.43
2:B:77:U:P	22:V:21:ARG:HH22	2.41	0.43
34:a:589:U:H2'	34:a:590:U:H6	1.84	0.43
38:e:108:GLY:O	38:e:109:ALA:HB3	2.18	0.43
1:A:2:G:N3	1:A:2:G:H2'	2.33	0.43
1:A:122:G:H2'	1:A:123:G:O4'	2.18	0.43
1:A:271:G:C6	1:A:367:G:N1	2.87	0.43
1:A:1081:U:O3'	9:I:123:ALA:HB1	2.18	0.43
1:A:1868:C:H3'	1:A:1869:G:C5'	2.43	0.43
2:B:76:G:O3'	22:V:21:ARG:NH2	2.51	0.43
3:C:209:ALA:HA	3:C:212:TRP:CE2	2.53	0.43
9:I:132:ALA:O	9:I:133:ARG:C	2.62	0.43
34:a:142:G:C4	34:a:143:A:N7	2.87	0.43
34:a:180:U:C2	34:a:181:A:C8	3.06	0.43
34:a:635:A:H2'	34:a:636:U:O4'	2.18	0.43
1:A:158:U:O2	1:A:168:G:C6	2.72	0.43
1:A:1027:A:C2	1:A:2488:G:H5'	2.53	0.43
12:L:78:ARG:HE	12:L:78:ARG:HB2	1.67	0.43
34:a:1177:G:H2'	34:a:1178:G:O4'	2.18	0.43
1:A:1864:U:OP1	1:A:2410:G:O2'	2.33	0.43
1:A:2500:U:O2	1:A:2504:PSU:C2	2.71	0.43
34:a:1252:A:H2'	34:a:1253:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1272:G:H3'	34:a:1273:C:H5''	2.00	0.43
55:v:51:C:N4	55:v:52:G:N7	2.66	0.43
34:a:699:C:H2'	34:a:700:G:H5''	2.01	0.43
50:q:22:VAL:HG11	50:q:60:ILE:HD11	2.00	0.43
1:A:279:A:N1	1:A:362:A:O5'	2.52	0.42
1:A:580:U:O3'	17:Q:30:VAL:HG13	2.19	0.42
1:A:811:U:H2'	12:L:21:ARG:HA	2.01	0.42
1:A:1111:A:HO2'	1:A:1112:G:H4'	1.84	0.42
1:A:2029:G:C8	1:A:2029:G:O5'	2.70	0.42
1:A:2678:C:H2'	1:A:2679:A:O4'	2.19	0.42
5:E:146:VAL:HG12	5:E:185:LYS:HB2	2.01	0.42
34:a:472:U:C5	34:a:473:U:C6	3.07	0.42
1:A:2466:C:OP1	31:4:4:ARG:HB2	2.18	0.42
13:M:53:MET:HG3	13:M:120:ALA:HB2	2.01	0.42
34:a:198:G:C5	34:a:220:G:C2	3.07	0.42
1:A:230:G:H2'	1:A:231:A:H5''	2.00	0.42
34:a:206:C:C4	34:a:207:C:N4	2.87	0.42
34:a:280:C:H4'	34:a:281:G:OP2	2.19	0.42
34:a:460:A:N1	34:a:473:U:O2	2.53	0.42
1:A:987:C:O2'	1:A:1000:A:N3	2.51	0.42
1:A:2734:A:H3'	1:A:2735:G:H5'	2.01	0.42
1:A:2741:A:H61	1:A:2763:G:H1'	1.83	0.42
9:I:91:LYS:O	9:I:95:ASP:N	2.47	0.42
55:v:18:G:O2'	55:v:60:U:C4	2.70	0.42
1:A:1589:U:N3	1:A:1590:A:C6	2.87	0.42
11:K:61:VAL:HG13	11:K:87:LEU:HD11	2.02	0.42
34:a:1124:G:HO2'	34:a:1145:A:N6	2.18	0.42
44:k:87:GLY:O	44:k:92:ARG:NH1	2.52	0.42
45:l:54:VAL:HG11	45:l:81:ILE:HG13	2.00	0.42
1:A:1266:G:O2'	1:A:2012:G:O6	2.35	0.42
1:A:2031:A:C8	1:A:2498:OMC:HM21	2.54	0.42
34:a:64:G:C2	34:a:67:C:N4	2.88	0.42
34:a:78:A:H2'	34:a:79:G:O4'	2.19	0.42
34:a:372:C:N3	34:a:389:A:N6	2.67	0.42
34:a:404:G:C2	34:a:498:A:C2	3.06	0.42
34:a:437:U:C4	34:a:438:U:C2	3.08	0.42
34:a:1258:G:O6	34:a:1277:C:C4	2.72	0.42
34:a:1304:G:C6	34:a:1305:G:N1	2.88	0.42
44:k:125:LYS:HE3	54:u:33:ARG:HB3	2.02	0.42
1:A:18:U:O2'	1:A:554:U:OP1	2.35	0.42
1:A:170:U:H2'	1:A:171:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:G:C8	1:A:647:G:H5''	2.54	0.42
1:A:1328:A:H2'	1:A:1330:C:C5	2.54	0.42
1:A:1795:C:H2'	1:A:1796:U:O4'	2.20	0.42
34:a:75:G:N2	34:a:96:U:C5	2.86	0.42
34:a:1508:A:H2'	34:a:1509:C:O4'	2.20	0.42
38:e:12:GLU:HB2	38:e:38:VAL:HG12	2.01	0.42
1:A:529:A:OP2	10:J:113:PRO:HD3	2.20	0.42
34:a:246:A:H4'	34:a:247:G:OP1	2.19	0.42
50:q:29:LYS:HA	50:q:36:PHE:HA	2.01	0.42
52:s:49:ALA:HB1	52:s:56:HIS:HB3	2.02	0.42
1:A:1613:G:C2	1:A:1619:G:C5	3.08	0.42
1:A:1868:C:N4	1:A:1869:G:C5	2.87	0.42
34:a:495:A:C2	34:a:496:A:N6	2.88	0.42
1:A:51:G:N3	1:A:119:A:C2	2.88	0.42
1:A:366:C:H2'	1:A:367:G:O4'	2.19	0.42
19:S:24:ILE:HD11	19:S:36:LEU:HG	2.01	0.42
34:a:471:U:O5'	34:a:471:U:H6	2.02	0.42
54:u:28:LEU:HD13	54:u:29:ALA:N	2.35	0.42
1:A:265:A:H4'	1:A:266:G:OP1	2.18	0.41
1:A:554:U:O4	1:A:555:G:C6	2.72	0.41
34:a:673:A:H2'	34:a:674:G:C8	2.55	0.41
34:a:823:C:O2'	41:h:1:SER:HB3	2.20	0.41
45:l:79:ILE:HD12	45:l:96:THR:HG22	2.01	0.41
1:A:288:U:N3	1:A:352:A:C2	2.89	0.41
1:A:1075:C:H2'	9:I:90:GLY:O	2.21	0.41
1:A:1809:A:H2'	1:A:1810:A:C8	2.55	0.41
1:A:2747:G:N2	1:A:2748:A:C6	2.88	0.41
34:a:1125:U:O2	34:a:1125:U:C2'	2.68	0.41
34:a:1434:A:H2'	34:a:1435:G:O4'	2.20	0.41
34:a:1456:A:H2'	34:a:1457:G:O4'	2.19	0.41
51:r:20:ILE:HG21	51:r:54:LEU:HA	2.01	0.41
58:z:337:VAL:HG11	58:z:366:ILE:HD12	2.01	0.41
1:A:97:C:H2'	1:A:97:C:O2	2.19	0.41
1:A:289:G:C2'	1:A:290:U:H4'	2.44	0.41
1:A:1020:A:H4'	1:A:1021:A:O5'	2.18	0.41
1:A:1058:U:C4	1:A:1059:G:N7	2.88	0.41
1:A:1536:C:O2	1:A:1536:C:H2'	2.20	0.41
1:A:2028:U:C4	1:A:2029:G:C5	3.07	0.41
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.02	0.41
17:Q:35:PHE:CZ	17:Q:39:ILE:HD11	2.55	0.41
34:a:203:G:C6	34:a:215:C:N4	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:555:U:H2'	34:a:556:C:C6	2.55	0.41
55:w:71:C:O2	55:w:71:C:C2'	2.69	0.41
1:A:170:U:H6	1:A:170:U:C5'	2.33	0.41
1:A:528:A:C2	1:A:2042:A:H2'	2.55	0.41
1:A:919:U:H2'	1:A:920:A:O4'	2.20	0.41
1:A:1050:A:C4	1:A:1051:G:C8	3.09	0.41
1:A:1519:G:H3'	1:A:1520:U:C6	2.56	0.41
1:A:1725:C:O2	1:A:1725:C:C2'	2.67	0.41
1:A:2192:U:H3'	1:A:2193:G:O4'	2.21	0.41
1:A:2744:G:H2'	1:A:2745:C:H5'	2.02	0.41
4:D:62:LYS:N	4:D:63:PRO:CD	2.84	0.41
9:I:74:PRO:HG2	9:I:77:VAL:HG22	2.03	0.41
34:a:180:U:H2'	34:a:181:A:O4'	2.20	0.41
34:a:1476:A:H2'	34:a:1477:U:O4'	2.20	0.41
55:w:2:G:O6	55:w:70:G:C5	2.71	0.41
1:A:289:G:C2	1:A:351:C:N3	2.82	0.41
1:A:669:G:H2'	1:A:670:A:N7	2.35	0.41
1:A:1343:G:O4'	1:A:1597:A:H2'	2.21	0.41
7:G:36:LEU:HD11	7:G:67:ALA:HB2	2.02	0.41
34:a:71:A:H61	34:a:98:A:H61	1.68	0.41
34:a:1452:C:H2'	34:a:1452:C:O2	2.20	0.41
55:w:66:C:C5	55:w:67:C:H1'	2.55	0.41
1:A:132:G:C5	1:A:133:U:C4	3.08	0.41
1:A:271:G:C5	1:A:367:G:N2	2.89	0.41
1:A:2242:G:H2'	1:A:2243:U:O4'	2.21	0.41
1:A:2418:A:H2'	1:A:2419:U:O4'	2.21	0.41
1:A:2491:U:H5'	1:A:2570:G:C5'	2.50	0.41
34:a:70:U:H2'	34:a:95:C:N4	2.36	0.41
55:w:66:C:N3	55:w:67:C:C2	2.86	0.41
58:z:160:TYR:O	58:z:161:ASP:HB2	2.20	0.41
1:A:340:A:H2'	1:A:341:C:O4'	2.21	0.41
1:A:1017:G:N2	1:A:1146:C:O2	2.54	0.41
1:A:1306:C:H5''	1:A:1606:C:N4	2.35	0.41
1:A:1525:A:H2'	1:A:1526:C:O4'	2.21	0.41
1:A:1867:G:C6	1:A:1874:C:C4	2.82	0.41
1:A:1932:A:H2'	1:A:1933:G:O4'	2.21	0.41
1:A:2543:G:N2	1:A:2646:C:H5''	2.36	0.41
34:a:75:G:N3	34:a:97:G:N2	2.68	0.41
34:a:406:G:C4	34:a:495:A:C6	3.09	0.41
34:a:470:C:C4	34:a:471:U:C4	3.08	0.41
34:a:1353:G:N2	34:a:1354:U:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:U:O4	1:A:352:A:N1	2.54	0.41
1:A:1883:U:O4	1:A:1884:G:C2	2.74	0.41
1:A:2078:C:H2'	1:A:2079:U:O4'	2.21	0.41
20:T:61:LEU:HG	20:T:82:LYS:HG2	2.01	0.41
34:a:77:A:N1	34:a:78:A:N6	2.68	0.41
34:a:475:C:H2'	34:a:475:C:O2	2.21	0.41
34:a:1259:C:N4	34:a:1260:G:C4	2.89	0.41
34:a:1371:G:C6	34:a:1372:U:C4	3.09	0.41
1:A:117:G:C6	1:A:119:A:N6	2.89	0.41
1:A:140:C:H6	1:A:140:C:H5''	1.86	0.41
1:A:309:A:N3	1:A:329:G:O2'	2.49	0.41
1:A:1012:U:OP2	17:Q:69:ARG:NH2	2.40	0.41
1:A:1076:C:O2	9:I:92:PRO:HD2	2.20	0.41
1:A:1416:G:C2	1:A:1582:C:N3	2.88	0.41
1:A:1682:G:OP2	1:A:1699:G:N2	2.54	0.41
1:A:1789:A:H2'	1:A:1790:C:O4'	2.20	0.41
1:A:1858:A:N6	1:A:1884:G:H1'	2.33	0.41
1:A:2070:A:H2'	1:A:2071:A:O4'	2.20	0.41
1:A:2201:G:C6	1:A:2202:U:N3	2.88	0.41
1:A:2290:G:H2'	1:A:2291:U:O4'	2.21	0.41
1:A:2346:A:O4'	1:A:2383:G:C8	2.74	0.41
1:A:2849:U:O4	16:P:20:ARG:NH2	2.54	0.41
2:B:24:G:H4'	2:B:25:U:C5	2.56	0.41
3:C:203:VAL:O	3:C:205:GLY:N	2.54	0.41
32:5:34:THR:HG22	32:5:37:LYS:HD3	2.03	0.41
34:a:178:C:OP2	53:t:59:ARG:NH2	2.54	0.41
34:a:410:G:H2'	34:a:429:U:C4	2.55	0.41
1:A:74:A:H5''	1:A:74:A:N3	2.35	0.41
1:A:1196:C:H2'	1:A:1197:G:O4'	2.21	0.41
1:A:1353:A:C8	1:A:1378:A:N6	2.89	0.41
1:A:1923:U:H2'	1:A:1924:C:C6	2.56	0.41
29:2:34:ARG:HB2	29:2:42:LEU:HD12	2.03	0.41
1:A:132:G:H2'	1:A:133:U:O4'	2.21	0.40
1:A:612:G:H3'	1:A:614:A:C8	2.56	0.40
1:A:2208:C:N3	1:A:2216:G:O6	2.54	0.40
1:A:2297:A:N1	1:A:2321:U:O4	2.54	0.40
4:D:193:VAL:HG21	4:D:201:LEU:HD13	2.03	0.40
18:R:5:PHE:HB3	18:R:59:ILE:HD12	2.02	0.40
34:a:460:A:C2	34:a:473:U:O2	2.74	0.40
34:a:461:A:H2	34:a:472:U:O2	1.96	0.40
34:a:953:G:H2'	34:a:954:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1448:C:O2	34:a:1448:C:H2'	2.21	0.40
47:n:54:ASP:O	47:n:55:SER:CB	2.69	0.40
55:w:1:C:H2'	55:w:2:G:O4'	2.20	0.40
1:A:295:G:C6	1:A:343:C:N3	2.87	0.40
1:A:367:G:H2'	1:A:368:A:O4'	2.21	0.40
1:A:1417:C:N4	1:A:1581:G:C6	2.87	0.40
1:A:1607:C:N4	1:A:1622:G:OP2	2.45	0.40
1:A:2686:G:H2'	1:A:2687:U:O4'	2.21	0.40
1:A:2808:G:O2'	1:A:2890:G:O6	2.27	0.40
34:a:192:A:H2'	34:a:193:C:O4'	2.21	0.40
34:a:198:G:C6	34:a:220:G:C2	3.09	0.40
39:f:29:ILE:HG21	39:f:64:VAL:CG2	2.51	0.40
43:j:40:ILE:HB	43:j:73:LEU:HB2	2.02	0.40
46:m:89:ARG:HG2	46:m:96:VAL:HA	2.01	0.40
1:A:280:U:O4	1:A:360:U:C2	2.66	0.40
1:A:1357:C:H2'	1:A:1358:G:O4'	2.21	0.40
1:A:1589:U:C4	1:A:1590:A:N6	2.89	0.40
1:A:1725:C:O2	1:A:1725:C:H2'	2.21	0.40
1:A:2804:U:H2'	1:A:2805:C:C6	2.57	0.40
2:B:1:U:H2'	2:B:2:G:O4'	2.21	0.40
15:O:51:ALA:HB3	15:O:78:VAL:HG22	2.02	0.40
1:A:1735:G:N3	1:A:1736:U:C6	2.89	0.40
1:A:1863:G:H2'	1:A:1864:U:O4'	2.20	0.40
34:a:909:A:N3	34:a:1413:A:O2'	2.52	0.40
1:A:151:C:H2'	1:A:152:A:H5'	2.04	0.40
1:A:272:A:C2	1:A:365:U:N3	2.90	0.40
1:A:485:C:H5''	1:A:485:C:H6	1.85	0.40
1:A:1079:C:C5	1:A:1080:A:C6	3.09	0.40
4:D:186:LEU:HD21	16:P:3:ILE:HG23	2.03	0.40
9:I:10:LEU:HD11	9:I:23:VAL:HG13	2.03	0.40
16:P:38:ARG:HG3	16:P:39:LEU:N	2.36	0.40
34:a:544:G:H2'	34:a:545:C:O4'	2.22	0.40
34:a:841:C:O2	34:a:841:C:H2'	2.20	0.40
34:a:1219:A:H2'	34:a:1220:G:O4'	2.20	0.40
53:t:26:MET:HE3	53:t:56:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5	25
30	3	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
31	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	5	129/131 (98%)	99 (77%)	22 (17%)	8 (6%)	1	6
33	6	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	7	34
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	5	25
36	c	204/206 (99%)	184 (90%)	15 (7%)	5 (2%)	4	23
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	12	45
38	e	156/157 (99%)	131 (84%)	19 (12%)	6 (4%)	2	15
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	130 (87%)	12 (8%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	2	14
43	j	96/98 (98%)	73 (76%)	17 (18%)	6 (6%)	1	6
44	k	114/116 (98%)	99 (87%)	10 (9%)	5 (4%)	2	12
45	l	119/121 (98%)	98 (82%)	13 (11%)	8 (7%)	1	5
46	m	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	6	31
47	n	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	1	10
48	o	86/88 (98%)	78 (91%)	5 (6%)	3 (4%)	3	16
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	23
50	q	78/80 (98%)	70 (90%)	6 (8%)	2 (3%)	4	23
51	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	24
54	u	63/65 (97%)	40 (64%)	14 (22%)	9 (14%)	0	1
58	z	391/393 (100%)	352 (90%)	29 (7%)	10 (3%)	4	23
All	All	6219/6322 (98%)	5477 (88%)	602 (10%)	140 (2%)	7	25

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	83	VAL

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Mol	Chain	Res	Type
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
40	g	64	ALA
42	i	90	ASP
43	j	57	VAL
44	k	88	PRO
44	k	94	SER
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
5	E	8	ALA
9	I	64	ARG
10	J	81	ILE
15	O	66	GLY
18	R	54	VAL
18	R	55	ASP
20	T	37	ASP
20	T	38	ALA
32	5	60	LEU
33	6	4	ASP
38	e	77	ASN
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
45	l	42	LYS
45	l	75	GLU
45	l	88	ASP
46	m	7	ASN
47	n	22	LYS
47	n	55	SER
47	n	90	ARG
51	r	17	VAL
54	u	30	GLU
54	u	37	TYR
58	z	161	ASP
12	L	15	ALA
12	L	29	LYS

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Mol	Chain	Res	Type
12	L	31	GLY
13	M	69	PRO
21	U	6	ARG
22	V	58	SER
25	Y	24	GLU
27	0	2	VAL
32	5	48	ALA
32	5	88	HIS
35	b	73	ARG
35	b	86	CYS
37	d	191	SER
39	f	63	ASN
40	g	20	GLU
42	i	124	PRO
43	j	35	GLN
44	k	13	LYS
44	k	103	GLY
47	n	2	LYS
47	n	38	ASP
49	p	64	GLY
51	r	10	CYS
51	r	46	THR
54	u	9	GLU
54	u	11	PHE
54	u	12	ASP
58	z	249	GLU
3	C	13	ARG
3	C	120	ASP
4	D	31	ALA
6	F	20	ASN
8	H	15	LEU
8	H	41	LYS
9	I	38	CYS
11	K	110	GLU
14	N	59	SER
14	N	117	ASP
21	U	97	SER
29	2	2	LYS
32	5	118	ILE
36	c	95	GLY
37	d	166	LYS
38	e	89	THR

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Mol	Chain	Res	Type
38	e	93	VAL
38	e	109	ALA
39	f	33	GLU
40	g	19	SER
45	l	33	CYS
45	l	46	SER
46	m	102	LYS
48	o	13	GLU
48	o	45	HIS
49	p	49	GLY
54	u	65	ARG
58	z	332	PHE
8	H	3	VAL
11	K	35	VAL
12	L	92	LEU
13	M	6	ARG
19	S	3	THR
19	S	65	ASP
21	U	75	ALA
32	5	113	PHE
35	b	192	PRO
38	e	146	MET
39	f	92	THR
40	g	56	SER
45	l	77	SER
48	o	2	LEU
50	q	49	ASN
50	q	79	GLU
53	t	44	ALA
58	z	9	LYS
58	z	82	PRO
58	z	126	GLY
58	z	207	ASP
32	5	108	VAL
35	b	11	ALA
35	b	151	LYS
39	f	56	LYS
40	g	112	ASP
42	i	120	ALA
43	j	6	ILE
43	j	75	ASP
45	l	21	PRO

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Mol	Chain	Res	Type
45	l	35	ARG
54	u	24	LYS
58	z	2	LYS
36	c	147	GLY
43	j	41	PRO
58	z	180	GLY
36	c	144	GLY
58	z	52	ALA
18	R	100	GLY
38	e	50	GLY
40	g	111	GLY
9	I	90	GLY
11	K	93	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	206 (95%)	10 (5%)	24	58
4	D	163/163 (100%)	154 (94%)	9 (6%)	19	53
5	E	164/164 (100%)	159 (97%)	5 (3%)	36	69
6	F	148/148 (100%)	143 (97%)	5 (3%)	32	66
7	G	135/135 (100%)	133 (98%)	2 (2%)	57	80
8	H	114/114 (100%)	112 (98%)	2 (2%)	51	77
9	I	109/109 (100%)	102 (94%)	7 (6%)	16	48
10	J	115/115 (100%)	114 (99%)	1 (1%)	70	85
11	K	103/103 (100%)	97 (94%)	6 (6%)	18	51
12	L	102/102 (100%)	94 (92%)	8 (8%)	11	39
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	85
14	N	99/99 (100%)	98 (99%)	1 (1%)	68	84
15	O	86/86 (100%)	85 (99%)	1 (1%)	63	82
16	P	99/99 (100%)	95 (96%)	4 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	88/88 (100%)	83 (94%)	5 (6%)	18	52
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	73
19	S	92/92 (100%)	88 (96%)	4 (4%)	26	60
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	72
21	U	83/83 (100%)	80 (96%)	3 (4%)	31	65
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	81
23	W	57/57 (100%)	54 (95%)	3 (5%)	20	54
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	69
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	47	75
27	0	46/46 (100%)	45 (98%)	1 (2%)	45	74
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	34 (92%)	3 (8%)	11	38
30	3	51/51 (100%)	49 (96%)	2 (4%)	28	62
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	97 (97%)	3 (3%)	36	69
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	78
35	b	180/180 (100%)	180 (100%)	0	100	100
36	c	170/170 (100%)	165 (97%)	5 (3%)	37	70
37	d	172/172 (100%)	167 (97%)	5 (3%)	37	70
38	e	120/119 (101%)	111 (92%)	9 (8%)	12	41
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	66
40	g	124/124 (100%)	119 (96%)	5 (4%)	28	62
41	h	104/104 (100%)	102 (98%)	2 (2%)	50	76
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	70
43	j	86/86 (100%)	84 (98%)	2 (2%)	44	74
44	k	89/89 (100%)	87 (98%)	2 (2%)	45	74
45	l	102/102 (100%)	97 (95%)	5 (5%)	22	56
46	m	93/93 (100%)	91 (98%)	2 (2%)	45	74
47	n	83/83 (100%)	82 (99%)	1 (1%)	63	82
48	o	76/76 (100%)	73 (96%)	3 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	p	65/65 (100%)	62 (95%)	3 (5%)	24	58
50	q	74/74 (100%)	71 (96%)	3 (4%)	27	61
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	43
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	60
53	t	65/65 (100%)	62 (95%)	3 (5%)	24	58
54	u	55/55 (100%)	51 (93%)	4 (7%)	13	42
58	z	325/325 (100%)	317 (98%)	8 (2%)	42	72
All	All	5165/5164 (100%)	4995 (97%)	170 (3%)	34	67

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	35	LYS
3	C	58	LYS
3	C	69	ASN
3	C	164	VAL
3	C	183	VAL
3	C	200	MET
3	C	241	LYS
3	C	249	VAL
3	C	260	LYS
4	D	12	THR
4	D	51	THR
4	D	56	LYS
4	D	58	ASN
4	D	150	GLN
4	D	151	THR
4	D	157	LYS
4	D	169	ARG
4	D	189	VAL
5	E	69	ARG
5	E	117	ARG
5	E	141	MET
5	E	150	THR
5	E	193	VAL
6	F	67	THR
6	F	87	LYS
6	F	107	VAL
6	F	112	ASP

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Mol	Chain	Res	Type
6	F	116	LEU
7	G	121	THR
7	G	152	ARG
8	H	77	THR
8	H	96	THR
9	I	10	LEU
9	I	11	GLN
9	I	30	GLN
9	I	52	LEU
9	I	67	THR
9	I	134	SER
9	I	135	MET
10	J	85	LYS
11	K	7	MET
11	K	23	LYS
11	K	31	ARG
11	K	52	VAL
11	K	58	LEU
11	K	67	LYS
12	L	1	MET
12	L	3	LEU
12	L	14	LYS
12	L	27	LEU
12	L	60	ARG
12	L	63	LYS
12	L	78	ARG
12	L	79	LEU
13	M	75	GLU
14	N	65	LEU
15	O	28	VAL
16	P	5	LYS
16	P	26	GLU
16	P	47	ILE
16	P	79	VAL
17	Q	8	ILE
17	Q	40	LYS
17	Q	83	LYS
17	Q	101	ASP
17	Q	108	LEU
18	R	66	HIS
18	R	73	LYS
19	S	19	LEU

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Mol	Chain	Res	Type
19	S	29	VAL
19	S	42	LYS
19	S	108	SER
20	T	69	ARG
20	T	91	GLN
21	U	18	LYS
21	U	65	GLN
21	U	73	ASN
22	V	21	ARG
23	W	8	ASN
23	W	15	LYS
23	W	68	LYS
24	X	16	ASN
24	X	59	ASP
26	Z	10	ARG
27	0	49	ARG
29	2	2	LYS
29	2	22	MET
29	2	34	ARG
30	3	38	LYS
30	3	61	LEU
32	5	34	THR
32	5	36	ASP
32	5	60	LEU
33	6	37	CYS
36	c	99	GLN
36	c	121	SER
36	c	138	GLN
36	c	156	LEU
36	c	182	ASP
37	d	30	LYS
37	d	54	LEU
37	d	130	ASN
37	d	140	ASP
37	d	190	LEU
38	e	11	GLN
38	e	19	ARG
38	e	25	LYS
38	e	45	VAL
38	e	51	LYS
38	e	93	VAL
38	e	114	LEU

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Mol	Chain	Res	Type
38	e	136	VAL
38	e	139	THR
39	f	2	ARG
39	f	38	ARG
39	f	91	ARG
40	g	11	ILE
40	g	78	ARG
40	g	89	GLU
40	g	137	ARG
40	g	147	ASN
41	h	2	MET
41	h	111	THR
42	i	41	GLU
42	i	42	THR
42	i	65	THR
43	j	45	ARG
43	j	67	ILE
44	k	28	ASN
44	k	126	ARG
45	l	9	LYS
45	l	38	THR
45	l	77	SER
45	l	88	ASP
45	l	93	ARG
46	m	57	ASP
46	m	89	ARG
47	n	75	ARG
48	o	71	ARG
48	o	87	ARG
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
49	p	48	GLU
50	q	3	LYS
50	q	37	ILE
50	q	52	CYS
51	r	13	THR
51	r	27	THR
51	r	41	SER
51	r	42	ARG
52	s	5	LYS
52	s	6	LYS

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Mol	Chain	Res	Type
52	s	12	LEU
53	t	42	ASP
53	t	56	ILE
53	t	68	LYS
54	u	9	GLU
54	u	28	LEU
54	u	35	GLU
54	u	62	GLU
58	z	22	HIS
58	z	24	LYS
58	z	47	ASP
58	z	89	LYS
58	z	136	LYS
58	z	179	GLU
58	z	204	ARG
58	z	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	59	GLN
4	D	140	HIS
5	E	46	GLN
5	E	90	GLN
5	E	92	HIS
5	E	94	GLN
6	F	4	HIS
6	F	80	GLN
7	G	37	ASN
8	H	11	ASN
8	H	28	ASN
8	H	33	GLN
10	J	47	HIS
10	J	58	ASN
10	J	77	HIS
10	J	86	GLN
10	J	128	ASN
11	K	3	GLN
11	K	9	ASN
12	L	104	GLN
14	N	62	ASN
15	O	100	HIS

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Mol	Chain	Res	Type
16	P	65	ASN
18	R	6	GLN
19	S	9	HIS
19	S	102	HIS
20	T	70	HIS
20	T	92	ASN
23	W	8	ASN
24	X	5	GLN
28	1	44	GLN
31	4	37	GLN
32	5	4	ASN
33	6	41	HIS
33	6	61	ASN
33	6	65	ASN
35	b	23	ASN
35	b	93	HIS
35	b	145	ASN
35	b	189	ASN
36	c	7	ASN
36	c	101	ASN
36	c	122	GLN
37	d	35	GLN
37	d	39	GLN
37	d	84	ASN
37	d	163	GLN
37	d	197	HIS
39	f	55	HIS
40	g	129	ASN
42	i	30	ASN
43	j	20	GLN
44	k	100	ASN
45	l	71	HIS
45	l	111	GLN
48	o	19	ASN
48	o	27	GLN
49	p	9	HIS
50	q	49	ASN
51	r	51	GLN
52	s	56	HIS
53	t	20	ASN
58	z	13	ASN
58	z	251	GLN

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Mol	Chain	Res	Type
58	z	273	ASN
58	z	301	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	806 (27%)	79 (2%)
2	B	119/120 (99%)	33 (27%)	4 (3%)
34	a	1539/1540 (99%)	442 (28%)	0
55	v	76/77 (98%)	17 (22%)	0
55	w	76/77 (98%)	35 (46%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	75/76 (98%)	29 (38%)	0
All	All	4793/4805 (99%)	1363 (28%)	83 (1%)

All (1363) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U
1	A	13	A
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	41	C
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	61	C
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	78	U

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Mol	Chain	Res	Type
1	A	80	G
1	A	81	G
1	A	82	U
1	A	83	A
1	A	84	A
1	A	87	U
1	A	93	G
1	A	96	C
1	A	97	C
1	A	98	G
1	A	99	U
1	A	100	U
1	A	101	A
1	A	102	U
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	126	A
1	A	130	C
1	A	132	G
1	A	133	U
1	A	136	G
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	142	A
1	A	143	C
1	A	145	C
1	A	147	C
1	A	149	A
1	A	152	A
1	A	154	U
1	A	156	A
1	A	158	U
1	A	159	G
1	A	160	A
1	A	162	U
1	A	163	C
1	A	164	C

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

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

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Mol	Chain	Res	Type
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	419	U
1	A	427	U
1	A	428	A
1	A	438	G
1	A	442	G
1	A	445	C
1	A	446	G
1	A	447	A
1	A	451	U
1	A	455	C
1	A	473	G
1	A	475	C
1	A	481	G
1	A	485	C
1	A	486	C
1	A	491	G
1	A	492	A
1	A	494	G
1	A	496	G
1	A	503	A
1	A	504	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	518	G
1	A	521	U
1	A	527	C
1	A	529	A
1	A	532	A
1	A	533	G
1	A	535	G
1	A	543	G
1	A	545	U
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G

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Mol	Chain	Res	Type
1	A	563	A
1	A	564	C
1	A	573	U
1	A	575	A
1	A	602	A
1	A	603	A
1	A	610	C
1	A	612	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	633	A
1	A	636	G
1	A	637	A
1	A	640	C
1	A	644	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	648	G
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	661	A
1	A	664	G
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	730	A
1	A	738	G
1	A	746	PSU
1	A	747	5MC

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Mol	Chain	Res	Type
1	A	752	A
1	A	764	A
1	A	765	C
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	804	A
1	A	805	G
1	A	812	C
1	A	814	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	837	C
1	A	844	A
1	A	845	A
1	A	846	C
1	A	858	G
1	A	860	U
1	A	877	A
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	934	U
1	A	940	G
1	A	941	A
1	A	942	G

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Mol	Chain	Res	Type
1	A	946	C
1	A	951	C
1	A	953	G
1	A	958	U
1	A	961	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	985	C
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1006	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1014	A
1	A	1017	G
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1036	G
1	A	1037	G
1	A	1038	G
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U

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Mol	Chain	Res	Type
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1082	U
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1097	U
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1115	G
1	A	1117	C
1	A	1119	U
1	A	1130	U
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1141	U
1	A	1142	A
1	A	1143	A
1	A	1148	U
1	A	1150	C
1	A	1151	A
1	A	1167	C

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Mol	Chain	Res	Type
1	A	1172	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1178	C
1	A	1179	G
1	A	1180	U
1	A	1181	U
1	A	1193	G
1	A	1200	C
1	A	1204	A
1	A	1210	G
1	A	1212	G
1	A	1218	G
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1258	U
1	A	1262	A
1	A	1269	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1289	C
1	A	1290	C
1	A	1291	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1306	C
1	A	1320	C
1	A	1321	A
1	A	1332	G
1	A	1344	U
1	A	1345	C
1	A	1349	C

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Mol	Chain	Res	Type
1	A	1352	U
1	A	1355	G
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	1390	U
1	A	1392	A
1	A	1402	U
1	A	1403	A
1	A	1404	C
1	A	1407	G
1	A	1411	U
1	A	1412	U
1	A	1414	C
1	A	1415	U
1	A	1416	G
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1436	G
1	A	1441	G
1	A	1449	G
1	A	1452	G
1	A	1453	A
1	A	1454	C
1	A	1455	G
1	A	1458	U
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1468	U
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1482	G

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Mol	Chain	Res	Type
1	A	1484	U
1	A	1485	U
1	A	1487	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1495	A
1	A	1497	U
1	A	1504	A
1	A	1507	C
1	A	1508	A
1	A	1515	A
1	A	1516	G
1	A	1519	G
1	A	1523	U
1	A	1524	G
1	A	1527	G
1	A	1528	A
1	A	1529	G
1	A	1530	G
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1546	G
1	A	1549	A
1	A	1554	U
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1563	U
1	A	1565	C
1	A	1567	G
1	A	1569	A
1	A	1572	A
1	A	1579	A
1	A	1581	G

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Mol	Chain	Res	Type
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1588	G
1	A	1591	A
1	A	1592	C
1	A	1593	A
1	A	1605	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1618	6MZ
1	A	1619	G
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1659	G
1	A	1674	G
1	A	1675	C
1	A	1691	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1700	A
1	A	1705	A
1	A	1706	C
1	A	1709	U
1	A	1712	U
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1721	G
1	A	1724	G
1	A	1725	C
1	A	1729	U
1	A	1730	U
1	A	1731	G
1	A	1732	C
1	A	1736	U

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Mol	Chain	Res	Type
1	A	1738	G
1	A	1739	A
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	1791	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1809	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1841	U
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1867	G
1	A	1868	C
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1876	A
1	A	1879	C
1	A	1884	G
1	A	1885	A
1	A	1890	A
1	A	1895	C
1	A	1898	U
1	A	1906	G
1	A	1907	G
1	A	1909	C
1	A	1913	A

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Mol	Chain	Res	Type
1	A	1914	C
1	A	1915	3TD
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	1991	U
1	A	1993	U
1	A	1997	C
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2030	6MZ
1	A	2031	A
1	A	2033	A
1	A	2039	U
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A

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Mol	Chain	Res	Type
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	2193	G
1	A	2195	U
1	A	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2221	G

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Mol	Chain	Res	Type
1	A	2225	A
1	A	2226	C
1	A	2230	G
1	A	2238	G
1	A	2239	G
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2296	U
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2332	C
1	A	2333	A
1	A	2334	U
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2340	A
1	A	2344	U
1	A	2345	G
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2372	U
1	A	2378	A
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2399	G
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A

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Mol	Chain	Res	Type
1	A	2408	U
1	A	2423	U
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2452	C
1	A	2465	C
1	A	2469	A
1	A	2475	C
1	A	2476	A
1	A	2480	C
1	A	2484	G
1	A	2494	G
1	A	2499	C
1	A	2502	G
1	A	2503	2MA
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2556	C
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2613	U
1	A	2624	G

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Mol	Chain	Res	Type
1	A	2629	U
1	A	2634	A
1	A	2651	C
1	A	2653	U
1	A	2654	A
1	A	2656	U
1	A	2673	G
1	A	2674	G
1	A	2689	U
1	A	2690	U
1	A	2691	C
1	A	2707	U
1	A	2712	C
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2720	U
1	A	2724	U
1	A	2726	A
1	A	2728	U
1	A	2733	A
1	A	2734	A
1	A	2735	G
1	A	2742	G
1	A	2744	G
1	A	2745	C
1	A	2746	U
1	A	2748	A
1	A	2752	C
1	A	2754	U
1	A	2758	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2768	U
1	A	2776	A
1	A	2778	A
1	A	2791	G
1	A	2794	U
1	A	2799	G
1	A	2800	A
1	A	2801	G

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Mol	Chain	Res	Type
1	A	2803	G
1	A	2804	U
1	A	2805	C
1	A	2807	U
1	A	2809	A
1	A	2812	G
1	A	2818	U
1	A	2820	A
1	A	2826	A
1	A	2844	G
1	A	2856	A
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	2886	A
1	A	2896	C
1	A	2898	U
1	A	2899	A
1	A	2901	C
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	5	U
2	B	9	G
2	B	12	C
2	B	13	G
2	B	14	U
2	B	17	C
2	B	20	G
2	B	21	G
2	B	22	U
2	B	25	U
2	B	27	C
2	B	32	U
2	B	33	G
2	B	35	C

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Mol	Chain	Res	Type
2	B	37	C
2	B	38	C
2	B	41	G
2	B	42	C
2	B	44	G
2	B	63	C
2	B	65	U
2	B	66	A
2	B	67	G
2	B	84	G
2	B	89	U
2	B	90	C
2	B	102	G
2	B	105	G
2	B	108	A
2	B	109	A
2	B	110	C
2	B	118	C
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	32	A
34	a	38	G
34	a	39	G
34	a	40	C
34	a	45	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	64	G
34	a	66	A
34	a	68	G
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A

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Mol	Chain	Res	Type
34	a	74	A
34	a	76	G
34	a	77	A
34	a	78	A
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	98	A
34	a	99	C
34	a	100	G
34	a	105	G
34	a	107	G
34	a	109	A
34	a	115	G
34	a	116	A
34	a	120	A
34	a	121	U
34	a	128	G
34	a	130	A
34	a	131	A
34	a	142	G
34	a	143	A
34	a	144	G
34	a	145	G
34	a	146	G
34	a	147	G
34	a	149	A
34	a	151	A
34	a	154	U
34	a	161	A
34	a	162	A
34	a	163	C
34	a	165	G
34	a	167	A

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Mol	Chain	Res	Type
34	a	173	U
34	a	181	A
34	a	182	A
34	a	183	C
34	a	184	G
34	a	189	A
34	a	190	A
34	a	191	G
34	a	197	A
34	a	199	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	215	C
34	a	216	U
34	a	222	C
34	a	226	G
34	a	227	G
34	a	230	G
34	a	245	U
34	a	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	279	A
34	a	280	C
34	a	281	G
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	325	A
34	a	326	G

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Mol	Chain	Res	Type
34	a	328	C
34	a	330	C
34	a	335	C
34	a	339	C
34	a	341	C
34	a	345	C
34	a	346	G
34	a	347	G
34	a	348	G
34	a	349	A
34	a	351	G
34	a	352	C
34	a	354	G
34	a	355	C
34	a	365	U
34	a	367	U
34	a	372	C
34	a	373	A
34	a	376	G
34	a	381	C
34	a	388	G
34	a	390	U
34	a	392	C
34	a	397	A
34	a	398	U
34	a	399	G
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	420	U
34	a	422	C
34	a	424	G
34	a	425	G
34	a	429	U
34	a	434	U
34	a	436	C
34	a	437	U
34	a	438	U
34	a	439	U

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Mol	Chain	Res	Type
34	a	443	C
34	a	446	G
34	a	457	G
34	a	458	U
34	a	459	A
34	a	461	A
34	a	462	G
34	a	467	U
34	a	468	A
34	a	470	C
34	a	474	G
34	a	475	C
34	a	476	U
34	a	477	C
34	a	484	G
34	a	485	U
34	a	486	U
34	a	491	G
34	a	496	A
34	a	499	A
34	a	509	A
34	a	514	C
34	a	518	C
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	532	A
34	a	536	C
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	550	G
34	a	565	U
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	591	U
34	a	592	G

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Mol	Chain	Res	Type
34	a	594	U
34	a	596	A
34	a	615	G
34	a	618	C
34	a	633	G
34	a	638	U
34	a	639	G
34	a	642	A
34	a	648	A
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	701	U
34	a	703	G
34	a	704	A
34	a	713	G
34	a	720	C
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	737	C
34	a	742	G
34	a	754	C
34	a	755	G
34	a	758	C
34	a	759	A
34	a	769	G
34	a	775	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	814	A
34	a	815	A
34	a	817	C

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Mol	Chain	Res	Type
34	a	818	G
34	a	819	A
34	a	829	G
34	a	832	G
34	a	836	G
34	a	838	G
34	a	840	C
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	850	U
34	a	851	G
34	a	871	U
34	a	872	A
34	a	884	U
34	a	885	G
34	a	902	G
34	a	914	A
34	a	924	C
34	a	926	G
34	a	931	C
34	a	934	C
34	a	935	A
34	a	939	G
34	a	954	G
34	a	960	U
34	a	961	U
34	a	965	U
34	a	966	2MG
34	a	969	A
34	a	971	G
34	a	972	C
34	a	975	A
34	a	976	G
34	a	977	A
34	a	982	U
34	a	984	C
34	a	988	G
34	a	989	U
34	a	991	U
34	a	992	U

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Mol	Chain	Res	Type
34	a	993	G
34	a	996	A
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1077	G
34	a	1088	G
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1108	G
34	a	1113	C
34	a	1115	U
34	a	1116	U
34	a	1120	C
34	a	1124	G
34	a	1125	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C

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Mol	Chain	Res	Type
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	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1207	2MG
34	a	1209	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1238	A
34	a	1241	G
34	a	1244	G
34	a	1247	U
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1261	A

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Mol	Chain	Res	Type
34	a	1263	C
34	a	1265	C
34	a	1266	G
34	a	1268	G
34	a	1269	A
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1299	A
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1312	G
34	a	1317	C
34	a	1321	U
34	a	1338	G
34	a	1339	A
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1349	A
34	a	1359	C
34	a	1363	A
34	a	1364	U
34	a	1368	A
34	a	1371	G

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Mol	Chain	Res	Type
34	a	1372	U
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1390	U
34	a	1393	U
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1402	4OC
34	a	1415	G
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1448	C
34	a	1449	C
34	a	1450	U
34	a	1454	G
34	a	1455	G
34	a	1467	C
34	a	1475	G
34	a	1487	G
34	a	1492	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
34	a	1505	G
34	a	1506	U
34	a	1517	G
34	a	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

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Mol	Chain	Res	Type
55	v	7	4SU
55	v	8	G
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	47	U
55	v	50	U
55	v	52	G
55	v	70	G
55	v	76	A
55	w	3	C
55	w	5	G
55	w	7	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A

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Mol	Chain	Res	Type
55	w	67	C
55	w	68	C
55	w	69	C
55	w	70	G
55	w	72	A
55	w	73	A
55	w	74	C
55	w	76	A
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	17	C
57	y	18	G
57	y	20	H2U
57	y	21	A
57	y	24	G
57	y	33	U
57	y	36	A
57	y	37	MIA
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	59	U
57	y	61	C
57	y	65	G
57	y	68	C
57	y	69	G
57	y	72	C
57	y	75	C
57	y	76	A

All (83) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	12	U
1	A	51	G
1	A	97	C
1	A	141	G
1	A	163	C
1	A	177	G
1	A	182	A
1	A	199	A
1	A	204	A
1	A	231	A
1	A	242	G
1	A	265	A
1	A	278	A
1	A	285	G
1	A	301	G
1	A	403	U
1	A	446	G
1	A	474	G
1	A	506	G
1	A	546	U
1	A	555	G
1	A	645	C
1	A	746	PSU
1	A	752	A
1	A	764	A
1	A	774	G
1	A	784	G
1	A	859	G
1	A	884	U
1	A	983	A
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1070	A
1	A	1089	A
1	A	1111	A
1	A	1124	G
1	A	1140	C
1	A	1141	U
1	A	1190	G
1	A	1240	U

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Mol	Chain	Res	Type
1	A	1378	A
1	A	1399	C
1	A	1419	A
1	A	1432	G
1	A	1454	C
1	A	1459	G
1	A	1475	G
1	A	1493	C
1	A	1555	G
1	A	1558	C
1	A	1608	A
1	A	1647	U
1	A	1706	C
1	A	1730	U
1	A	1738	G
1	A	1818	U
1	A	1857	G
1	A	1913	A
1	A	1918	A
1	A	1939	5MU
1	A	1940	U
1	A	1976	U
1	A	2238	G
1	A	2296	U
1	A	2333	A
1	A	2391	G
1	A	2401	U
1	A	2402	U
1	A	2407	A
1	A	2517	C
1	A	2566	A
1	A	2581	G
1	A	2585	U
1	A	2712	C
1	A	2803	G
1	A	2808	G
1	A	2873	A
1	A	2901	C
2	B	3	C
2	B	14	U
2	B	56	G
2	B	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
57	PSU	y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
1	3TD	A	1915	1	19,22,23	7.08	14 (73%)	23,32,35	2.02	5 (21%)
55	PSU	w	55	55	18,21,22	1.32	2 (11%)	21,30,33	2.07	5 (23%)
55	5MU	w	54	55	19,22,23	1.50	4 (21%)	27,32,35	2.07	10 (37%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	19,30,33	1.38	4 (21%)
1	PSU	A	746	1,60	18,21,22	1.42	2 (11%)	21,30,33	1.99	4 (19%)
1	7MG	A	2069	1,60	23,26,27	1.43	2 (8%)	27,39,42	2.53	11 (40%)
1	2MA	A	2503	1,60	22,25,26	1.62	4 (18%)	32,37,40	2.38	9 (28%)
1	OMG	A	2251	1,55,60	23,26,27	1.26	3 (13%)	32,38,41	1.95	6 (18%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	1.99	4 (19%)
1	PSU	A	2504	1	18,21,22	1.43	2 (11%)	21,30,33	2.05	4 (19%)
34	2MG	a	1207	34	23,26,27	1.24	3 (13%)	33,38,41	2.84	10 (30%)
34	2MG	a	1516	34	23,26,27	1.27	3 (13%)	33,38,41	2.31	8 (24%)
1	PSU	A	2605	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)
34	4OC	a	1402	34	20,23,24	0.85	2 (10%)	25,32,35	1.32	4 (16%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.57	2 (10%)
57	4SU	y	8	57	18,21,22	1.85	5 (27%)	25,30,33	2.38	7 (28%)
1	OMU	A	2552	1,60	19,22,23	1.31	3 (15%)	25,31,34	2.04	9 (36%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.54	4 (15%)
1	5MC	A	747	1	19,22,23	1.91	2 (10%)	26,32,35	1.54	5 (19%)
1	2MG	A	1835	1	23,26,27	1.32	4 (17%)	33,38,41	2.27	7 (21%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.22	5 (20%)
1	PSU	A	2457	1,60	18,21,22	1.44	2 (11%)	21,30,33	2.04	5 (23%)
1	PSU	A	2580	1	18,21,22	1.53	2 (11%)	21,30,33	2.13	5 (23%)
34	UR3	a	1498	34	19,22,23	1.14	1 (5%)	26,32,35	2.01	5 (19%)
57	5MU	y	54	57	19,22,23	1.43	4 (21%)	27,32,35	2.08	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	2445	1,60	23,26,27	1.25	4 (17%)	33,38,41	2.32	8 (24%)
55	PSU	v	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	5 (23%)
34	2MG	a	966	34	23,26,27	1.32	4 (17%)	33,38,41	2.66	10 (30%)
34	7MG	a	527	34,60	23,26,27	1.41	2 (8%)	27,39,42	2.52	7 (25%)
1	PSU	A	2604	1	18,21,22	1.44	2 (11%)	21,30,33	1.94	4 (19%)
34	MA6	a	1518	34,60	23,26,27	1.76	6 (26%)	33,38,41	2.33	11 (33%)
1	PSU	A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.16	4 (19%)
1	OMC	A	2498	1,60	19,22,23	0.84	0	25,31,34	1.21	2 (8%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.28	10 (34%)
1	1MG	A	745	1	23,26,27	1.41	4 (17%)	33,39,42	2.02	7 (21%)
34	5MC	a	1407	34	19,22,23	2.02	2 (10%)	26,32,35	1.62	5 (19%)
57	H2U	y	20	57	18,21,22	0.87	1 (5%)	19,30,33	1.48	4 (21%)
55	5MU	v	54	55	19,22,23	1.47	4 (21%)	27,32,35	1.94	8 (29%)
57	MIA	y	37	57	27,30,32	2.40	6 (22%)	38,42,47	2.81	16 (42%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.36	6 (24%)
1	PSU	A	955	1	18,21,22	1.41	2 (11%)	21,30,33	2.06	4 (19%)
1	6MZ	A	2030	1,60	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
34	PSU	a	516	34	18,21,22	1.38	2 (11%)	21,30,33	2.16	5 (23%)
57	PSU	y	32	57,60	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)
34	MA6	a	1519	34	23,26,27	1.71	6 (26%)	33,38,41	2.41	16 (48%)
55	H2U	v	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.68	3 (15%)
34	5MC	a	967	34	19,22,23	2.04	2 (10%)	26,32,35	1.55	5 (19%)
1	PSU	A	1917	1	18,21,22	1.45	2 (11%)	21,30,33	2.07	5 (23%)
1	5MU	A	1939	1	19,22,23	1.48	4 (21%)	27,32,35	2.05	8 (29%)
57	7MG	y	46	57	23,26,27	1.41	3 (13%)	27,39,42	2.46	7 (25%)
1	H2U	A	2449	1	18,21,22	0.95	2 (11%)	19,30,33	1.74	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
1	2MA	A	2503	1,60	-	3/7/25/26	0/3/3/3
1	OMG	A	2251	1,55,60	-	0/9/27/28	0/3/3/3
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/9/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	PSU	A	2457	1,60	-	2/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,60	-	2/9/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34,60	-	4/11/29/30	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
1	6MZ	A	1618	1	-	2/9/27/28	0/3/3/3
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/14/32/34	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1,60	-	3/9/27/28	0/3/3/3
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
57	PSU	y	32	57,60	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	2/11/29/30	0/3/3/3
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.51	1.66	1.43
1	A	1915	3TD	C6-C5	15.64	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.44	1.34	1.53
1	A	1915	3TD	C2-N1	8.58	1.47	1.37
34	a	967	5MC	C5-C4	7.69	1.49	1.44
34	a	1407	5MC	C5-C4	7.66	1.49	1.44
1	A	1962	5MC	C5-C4	7.51	1.49	1.44
1	A	747	5MC	C5-C4	7.23	1.49	1.44
57	y	37	MIA	C13-C14	6.86	1.52	1.32
57	y	37	MIA	C2-S10	-6.35	1.70	1.75
1	A	1915	3TD	C2-N3	6.28	1.51	1.38
1	A	1915	3TD	O4'-C4'	-6.01	1.31	1.45
1	A	1915	3TD	C6-N1	5.26	1.44	1.36
34	a	1518	MA6	C5-C4	5.23	1.48	1.39
55	v	7	4SU	C4-S4	-4.99	1.59	1.68
34	a	1519	MA6	C5-C4	4.96	1.47	1.39
57	y	8	4SU	C4-S4	-4.92	1.60	1.68
57	y	37	MIA	C5-C4	4.91	1.47	1.39
55	w	8	4SU	C4-S4	-4.89	1.60	1.68
1	A	2503	2MA	C5-C4	4.81	1.47	1.39
1	A	2030	6MZ	C5-C4	4.76	1.47	1.39
1	A	1618	6MZ	C5-C4	4.72	1.47	1.39
1	A	2580	PSU	C6-C5	4.72	1.40	1.35
1	A	1917	PSU	C6-C5	4.44	1.40	1.35
1	A	1911	PSU	C6-C5	4.42	1.40	1.35
57	y	39	PSU	C6-C5	4.41	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	PSU	C6-C5	4.34	1.40	1.35
1	A	2605	PSU	C6-C5	4.32	1.40	1.35
1	A	2604	PSU	C6-C5	4.30	1.40	1.35
1	A	2504	PSU	C6-C5	4.27	1.40	1.35
57	y	55	PSU	C6-C5	4.26	1.40	1.35
1	A	955	PSU	C6-C5	4.26	1.40	1.35
1	A	2457	PSU	C6-C5	4.25	1.40	1.35
34	a	516	PSU	C6-C5	4.24	1.40	1.35
57	y	32	PSU	C6-C5	4.19	1.39	1.35
55	w	55	PSU	C6-C5	4.00	1.39	1.35
1	A	2069	7MG	C4-N9	-3.96	1.33	1.37
55	v	55	PSU	C6-C5	3.76	1.39	1.35
57	y	46	7MG	C5-C4	3.50	1.48	1.37
34	a	1518	MA6	C5-C6	3.49	1.50	1.41
55	v	54	5MU	C6-C5	3.44	1.40	1.34
1	A	745	1MG	C2-N1	3.44	1.43	1.37
34	a	527	7MG	C5-C4	3.43	1.48	1.37
34	a	1519	MA6	C5-C6	3.38	1.50	1.41
1	A	2251	OMG	C5-C4	3.36	1.48	1.38
34	a	527	7MG	C4-N9	-3.34	1.33	1.37
1	A	745	1MG	C5-C4	3.33	1.47	1.38
1	A	1835	2MG	C5-C4	3.28	1.47	1.38
1	A	1939	5MU	C6-C5	3.25	1.39	1.34
1	A	2069	7MG	C5-C4	3.24	1.47	1.37
34	a	966	2MG	C5-C4	3.24	1.47	1.38
57	y	46	7MG	C4-N9	-3.22	1.33	1.37
1	A	1962	5MC	C6-C5	3.20	1.39	1.34
57	y	8	4SU	C4-N3	-3.18	1.34	1.37
34	a	967	5MC	C6-C5	3.18	1.39	1.34
34	a	1407	5MC	C6-C5	3.13	1.39	1.34
34	a	1516	2MG	C5-C4	3.12	1.47	1.38
55	w	54	5MU	C2-N1	3.12	1.43	1.38
55	w	54	5MU	C6-C5	3.11	1.39	1.34
57	y	37	MIA	C5-C6	3.07	1.49	1.41
55	w	8	4SU	C2-N1	3.06	1.43	1.38
34	a	1207	2MG	C5-C4	3.06	1.47	1.38
57	y	54	5MU	C2-N1	3.05	1.43	1.38
1	A	1915	3TD	O2'-C2'	3.01	1.50	1.43
1	A	2445	2MG	C5-C4	2.99	1.46	1.38
55	v	54	5MU	C4-N3	-2.98	1.33	1.38
55	w	8	4SU	C4-N3	-2.94	1.34	1.37
1	A	747	5MC	C6-C5	2.93	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2552	OMU	C2-N1	2.89	1.43	1.38
55	v	7	4SU	C2-N1	2.88	1.43	1.38
1	A	2503	2MA	C5-C6	2.88	1.49	1.41
57	y	8	4SU	C2-N1	2.86	1.42	1.38
1	A	1618	6MZ	C5-C6	2.84	1.48	1.41
57	y	54	5MU	C6-C5	2.84	1.39	1.34
55	w	54	5MU	C4-C5	2.82	1.49	1.44
1	A	2030	6MZ	C5-C6	2.80	1.48	1.41
1	A	1939	5MU	C4-C5	2.79	1.49	1.44
1	A	1915	3TD	C4-N3	2.78	1.46	1.40
1	A	1915	3TD	C10-N3	-2.75	1.42	1.47
1	A	2552	OMU	C4-N3	-2.74	1.33	1.38
34	a	966	2MG	C2-N3	2.69	1.37	1.32
55	v	7	4SU	C4-N3	-2.68	1.34	1.37
34	a	1498	UR3	C2-N1	2.65	1.42	1.38
1	A	1939	5MU	C2-N1	2.62	1.42	1.38
34	a	1519	MA6	C5-N7	-2.60	1.34	1.39
1	A	1915	3TD	O2-C2	-2.59	1.18	1.23
1	A	2580	PSU	C4-N3	-2.53	1.34	1.38
57	y	8	4SU	C5-C4	-2.52	1.39	1.42
55	v	7	4SU	C5-C4	-2.51	1.39	1.42
1	A	1835	2MG	C2-N3	2.50	1.36	1.32
1	A	1915	3TD	O3'-C3'	-2.46	1.36	1.43
1	A	2251	OMG	C5-N7	-2.45	1.34	1.39
57	y	54	5MU	C4-C5	2.45	1.48	1.44
1	A	2457	PSU	C4-N3	-2.44	1.34	1.38
1	A	2604	PSU	C4-N3	-2.42	1.34	1.38
1	A	2504	PSU	C4-N3	-2.42	1.34	1.38
55	w	8	4SU	C5-C4	-2.41	1.39	1.42
1	A	1835	2MG	C5-N7	-2.40	1.34	1.39
1	A	2449	H2U	C2-N3	-2.40	1.33	1.38
55	v	55	PSU	C4-N3	-2.40	1.34	1.38
1	A	1917	PSU	C4-N3	-2.39	1.34	1.38
57	y	37	MIA	C8-N7	2.39	1.36	1.31
34	a	1518	MA6	C6-N6	2.38	1.43	1.36
1	A	1939	5MU	C4-N3	-2.38	1.34	1.38
1	A	2030	6MZ	C8-N7	2.37	1.36	1.31
1	A	2503	2MA	C5-N7	-2.36	1.34	1.39
57	y	37	MIA	C5-N7	-2.36	1.34	1.39
1	A	1618	6MZ	C8-N7	2.35	1.36	1.31
1	A	2449	H2U	C4-N3	-2.35	1.33	1.37
34	a	1516	2MG	C2-N3	2.35	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1518	MA6	C5-N7	-2.33	1.34	1.39
1	A	2605	PSU	C4-N3	-2.33	1.34	1.38
1	A	1835	2MG	C6-N1	-2.32	1.34	1.38
55	v	54	5MU	C2-N3	-2.32	1.33	1.38
1	A	746	PSU	C4-N3	-2.32	1.34	1.38
1	A	2503	2MA	C8-N7	2.32	1.36	1.31
57	y	55	PSU	C4-N3	-2.31	1.34	1.38
55	v	54	5MU	C4-C5	2.31	1.48	1.44
34	a	1519	MA6	C6-N6	2.31	1.43	1.36
1	A	2445	2MG	C2-N3	2.30	1.36	1.32
1	A	2251	OMG	C6-N1	-2.29	1.34	1.38
55	w	54	5MU	C4-N3	-2.27	1.34	1.38
1	A	1915	3TD	C3'-C4'	2.26	1.58	1.53
1	A	1618	6MZ	C5-N7	-2.26	1.35	1.39
57	y	54	5MU	C4-N3	-2.25	1.34	1.38
57	y	32	PSU	C4-N3	-2.25	1.34	1.38
34	a	1207	2MG	C2-N3	2.23	1.36	1.32
1	A	2030	6MZ	C5-N7	-2.23	1.35	1.39
34	a	516	PSU	C4-N3	-2.23	1.34	1.38
57	y	39	PSU	C4-N3	-2.22	1.34	1.38
1	A	745	1MG	C5-N7	-2.22	1.34	1.39
34	a	966	2MG	C5-N7	-2.20	1.34	1.39
34	a	1518	MA6	C8-N7	2.19	1.35	1.31
55	w	55	PSU	C4-N3	-2.19	1.34	1.38
34	a	1519	MA6	C8-N7	2.19	1.35	1.31
1	A	1915	3TD	O4-C4	-2.18	1.18	1.23
57	y	20	H2U	C2-N3	-2.16	1.34	1.38
1	A	955	PSU	C4-N3	-2.13	1.34	1.38
34	a	1516	2MG	C5-N7	-2.13	1.34	1.39
1	A	2445	2MG	C5-N7	-2.13	1.34	1.39
1	A	1911	PSU	C4-N3	-2.12	1.34	1.38
34	a	1207	2MG	C5-N7	-2.10	1.34	1.39
57	y	8	4SU	C6-C5	2.09	1.39	1.35
57	y	16	H2U	C2-N3	-2.08	1.34	1.38
55	v	20	H2U	C2-N3	-2.08	1.34	1.38
1	A	2552	OMU	C6-C5	2.06	1.39	1.35
57	y	46	7MG	C5-C6	2.06	1.48	1.43
34	a	1402	4OC	C6-C5	2.05	1.39	1.35
34	a	1519	MA6	C4-N9	-2.05	1.33	1.37
55	w	8	4SU	C6-C5	2.04	1.39	1.35
34	a	966	2MG	C6-N1	-2.03	1.35	1.38
1	A	2445	2MG	C6-N1	-2.02	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1402	4OC	C4-N3	2.02	1.36	1.32
55	w	20	H2U	C2-N3	-2.02	1.34	1.38
1	A	745	1MG	C2-N3	2.02	1.37	1.33
34	a	1518	MA6	C4-N9	-2.00	1.33	1.37

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C2-N3-C4	8.49	122.62	112.00
34	a	1207	2MG	C2-N3-C4	8.32	122.41	112.00
1	A	2503	2MA	C5-C4-N3	-8.12	118.62	127.18
34	a	527	7MG	N9-C4-N3	8.12	137.35	125.46
57	y	46	7MG	N9-C4-N3	8.09	137.32	125.46
1	A	1835	2MG	C2-N3-C4	7.90	121.88	112.00
1	A	2445	2MG	C2-N3-C4	7.80	121.75	112.00
34	a	1207	2MG	N1-C2-N2	7.72	124.44	116.56
34	a	1516	2MG	C2-N3-C4	7.60	121.50	112.00
57	y	37	MIA	C5-C4-N3	-7.56	119.21	127.18
57	y	37	MIA	C12-C13-C14	-7.51	113.53	127.01
1	A	2069	7MG	N9-C4-N3	7.39	136.29	125.46
34	a	1498	UR3	C4-N3-C2	-6.94	119.00	124.58
34	a	966	2MG	C5-C4-N3	-6.67	117.78	128.39
1	A	2503	2MA	N3-C4-N9	6.65	135.44	126.99
55	v	7	4SU	C4-N3-C2	-6.50	121.08	127.31
57	y	8	4SU	C4-N3-C2	-6.49	121.09	127.31
1	A	1835	2MG	C5-C4-N3	-6.46	118.11	128.39
1	A	2251	OMG	C5-C4-N3	-6.28	118.40	128.39
1	A	2504	PSU	N1-C2-N3	6.25	121.77	115.17
55	w	55	PSU	N1-C2-N3	6.18	121.69	115.17
1	A	1911	PSU	N1-C2-N3	6.17	121.68	115.17
55	w	8	4SU	C4-N3-C2	-6.12	121.45	127.31
1	A	746	PSU	N1-C2-N3	6.11	121.61	115.17
57	y	32	PSU	N1-C2-N3	6.08	121.58	115.17
57	y	39	PSU	N1-C2-N3	6.07	121.57	115.17
1	A	955	PSU	N1-C2-N3	6.05	121.55	115.17
34	a	1207	2MG	C5-C4-N3	-6.05	118.76	128.39
57	y	55	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	2457	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	2605	PSU	N1-C2-N3	5.98	121.48	115.17
1	A	2580	PSU	N1-C2-N3	5.96	121.46	115.17
1	A	2604	PSU	N1-C2-N3	5.96	121.45	115.17
34	a	516	PSU	N1-C2-N3	5.94	121.44	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1917	PSU	N1-C2-N3	5.94	121.43	115.17
55	v	54	5MU	N3-C2-N1	5.92	122.60	114.89
34	a	1516	2MG	C5-C4-N3	-5.88	119.03	128.39
55	v	55	PSU	N1-C2-N3	5.87	121.36	115.17
1	A	1618	6MZ	C5-C4-N3	-5.84	118.67	126.72
1	A	2030	6MZ	C5-C4-N3	-5.84	118.68	126.72
1	A	2445	2MG	C5-C4-N3	-5.81	119.14	128.39
57	y	37	MIA	N3-C4-N9	5.76	134.30	126.99
1	A	745	1MG	C5-C4-N3	-5.71	119.31	128.39
55	v	20	H2U	O4'-C1'-N1	5.64	116.99	109.30
34	a	966	2MG	N1-C2-N2	5.60	122.28	116.56
34	a	1519	MA6	C5-C4-N3	-5.55	119.08	126.72
34	a	1518	MA6	C5-C4-N3	-5.39	119.30	126.72
55	v	7	4SU	C5-C4-N3	5.38	119.75	114.75
1	A	1915	3TD	N1-C2-N3	5.35	120.02	116.13
57	y	8	4SU	N3-C2-N1	5.23	121.70	114.89
34	a	1207	2MG	N2-C2-N3	-5.21	113.88	120.51
1	A	1939	5MU	N3-C2-N1	5.20	121.66	114.89
55	w	8	4SU	C5-C4-N3	5.16	119.55	114.75
34	a	527	7MG	C5-C4-N3	-5.11	118.54	128.13
57	y	8	4SU	C5-C4-N3	5.09	119.48	114.75
1	A	1915	3TD	C4-N3-C2	-5.05	119.27	124.61
57	y	46	7MG	C5-C4-N3	-5.04	118.67	128.13
1	A	2251	OMG	C2-N3-C4	5.03	120.96	112.30
34	a	1518	MA6	C2-N1-C6	4.93	123.87	111.83
1	A	2069	7MG	C5-C4-N3	-4.91	118.92	128.13
55	w	54	5MU	N3-C2-N1	4.90	121.28	114.89
34	a	1519	MA6	C4-C5-N7	-4.88	105.00	110.58
1	A	2069	7MG	C2-N3-C4	4.86	120.67	112.30
34	a	966	2MG	N9-C4-N3	4.82	135.59	125.95
1	A	745	1MG	C2-N3-C4	4.81	122.79	111.98
1	A	2552	OMU	N3-C2-N1	4.79	121.13	114.89
1	A	1939	5MU	C4-N3-C2	-4.74	121.13	127.34
34	a	1519	MA6	C2-N1-C6	4.71	123.33	111.83
1	A	2069	7MG	N9-C8-N7	-4.65	96.79	103.37
1	A	2552	OMU	C4-N3-C2	-4.63	120.86	126.61
1	A	2251	OMG	N9-C4-N3	4.61	135.18	125.95
1	A	2030	6MZ	N3-C4-N9	4.60	135.00	127.17
57	y	54	5MU	N3-C2-N1	4.60	120.88	114.89
57	y	46	7MG	C2-N3-C4	4.60	120.22	112.30
1	A	1618	6MZ	N3-C4-N9	4.60	134.99	127.17
1	A	1835	2MG	N9-C4-N3	4.59	135.13	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	C2-N3-C4	4.57	120.17	112.30
55	v	7	4SU	C5-C4-S4	-4.56	119.10	124.31
55	w	8	4SU	N3-C2-N1	4.55	120.82	114.89
55	w	20	H2U	O4'-C1'-N1	4.55	115.50	109.30
1	A	1911	PSU	O2-C2-N1	-4.53	118.12	122.79
57	y	46	7MG	N9-C8-N7	-4.51	96.99	103.37
55	v	7	4SU	N3-C2-N1	4.50	120.75	114.89
57	y	37	MIA	C16-C14-C13	-4.48	109.21	122.66
55	w	54	5MU	C4-N3-C2	-4.43	121.53	127.34
34	a	527	7MG	N9-C8-N7	-4.41	97.13	103.37
57	y	54	5MU	C4-N3-C2	-4.38	121.59	127.34
1	A	745	1MG	N9-C4-N3	4.37	134.69	125.95
34	a	1518	MA6	C4-C5-N7	-4.24	105.73	110.58
55	v	54	5MU	C4-N3-C2	-4.16	121.88	127.34
57	y	54	5MU	C5-C4-N3	4.15	118.93	115.32
1	A	2605	PSU	C4-N3-C2	-4.12	120.69	126.37
1	A	2449	H2U	N3-C2-N1	4.12	120.79	116.65
1	A	1939	5MU	C5-C4-N3	4.11	118.90	115.32
1	A	1915	3TD	C1'-C5-C4	4.10	123.84	117.61
57	y	55	PSU	C4-N3-C2	-4.09	120.73	126.37
55	w	54	5MU	C5-C4-N3	4.06	118.85	115.32
1	A	747	5MC	CM5-C5-C6	-3.98	117.46	122.85
1	A	2445	2MG	N9-C4-N3	3.95	133.86	125.95
34	a	1207	2MG	N9-C4-N3	3.94	133.83	125.95
1	A	2504	PSU	C4-N3-C2	-3.93	120.96	126.37
34	a	1518	MA6	N1-C2-N3	-3.92	122.65	128.58
1	A	1911	PSU	C4-N3-C2	-3.91	120.99	126.37
1	A	955	PSU	C4-N3-C2	-3.90	120.99	126.37
57	y	37	MIA	C4-C5-N7	-3.90	106.13	110.58
55	w	55	PSU	C4-N3-C2	-3.89	121.02	126.37
34	a	967	5MC	CM5-C5-C6	-3.89	117.59	122.85
34	a	1516	2MG	N9-C4-N3	3.87	133.69	125.95
57	y	54	5MU	O4-C4-C5	-3.85	120.51	124.92
34	a	1207	2MG	C6-C5-N7	3.85	137.30	130.29
34	a	516	PSU	C4-N3-C2	-3.84	121.08	126.37
57	y	32	PSU	C4-N3-C2	-3.83	121.09	126.37
57	y	39	PSU	C4-N3-C2	-3.82	121.11	126.37
34	a	1407	5MC	CM5-C5-C6	-3.80	117.70	122.85
1	A	2445	2MG	C6-C5-N7	3.79	137.19	130.29
34	a	1519	MA6	N3-C4-N9	3.79	133.61	127.17
34	a	1518	MA6	N3-C4-N9	3.78	133.60	127.17
1	A	746	PSU	C4-N3-C2	-3.78	121.16	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1516	2MG	C6-C5-N7	3.77	137.16	130.29
34	a	1407	5MC	C5-C4-N3	-3.75	117.91	121.75
34	a	1518	MA6	C2-N3-C4	3.75	120.99	111.83
1	A	2457	PSU	C4-N3-C2	-3.75	121.21	126.37
55	w	8	4SU	C5-C4-S4	-3.71	120.07	124.31
1	A	2580	PSU	C6-C5-C4	-3.71	115.67	118.17
1	A	2449	H2U	O4'-C1'-N1	3.71	114.35	109.30
1	A	1618	6MZ	C2-N3-C4	3.71	120.88	111.83
1	A	955	PSU	O2-C2-N1	-3.71	118.97	122.79
1	A	2030	6MZ	C2-N3-C4	3.71	120.88	111.83
57	y	37	MIA	C6-C5-N7	3.68	136.44	132.43
1	A	1917	PSU	C4-N3-C2	-3.63	121.37	126.37
55	v	55	PSU	C4-N3-C2	-3.61	121.40	126.37
1	A	1962	5MC	C5-C4-N3	-3.59	118.07	121.75
1	A	747	5MC	C5-C4-N3	-3.59	118.07	121.75
34	a	1498	UR3	C1'-N1-C2	3.59	122.91	117.04
1	A	2552	OMU	C5-C4-N3	3.59	119.82	114.80
34	a	1519	MA6	C10-N6-C6	-3.58	111.41	120.52
55	v	55	PSU	C6-C5-C4	-3.58	115.76	118.17
1	A	1962	5MC	CM5-C5-C6	-3.58	118.00	122.85
55	w	55	PSU	O2-C2-N1	-3.57	119.11	122.79
34	a	1519	MA6	C2-N3-C4	3.57	120.55	111.83
57	y	8	4SU	C5-C4-S4	-3.57	120.23	124.31
1	A	2604	PSU	C4-N3-C2	-3.56	121.46	126.37
1	A	955	PSU	C6-C5-C4	-3.56	115.77	118.17
1	A	2449	H2U	C5-C4-N3	3.56	120.48	116.69
1	A	1917	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A	2504	PSU	O2-C2-N1	-3.52	119.16	122.79
57	y	39	PSU	O2-C2-N1	-3.52	119.16	122.79
34	a	967	5MC	C5-C4-N3	-3.51	118.16	121.75
1	A	2030	6MZ	C4-C5-N7	-3.51	106.57	110.58
34	a	1519	MA6	C5-N7-C8	3.50	108.94	103.45
34	a	516	PSU	O2-C2-N1	-3.49	119.19	122.79
1	A	1618	6MZ	C4-C5-N7	-3.47	106.61	110.58
1	A	2605	PSU	O2-C2-N1	-3.47	119.21	122.79
57	y	37	MIA	C15-C14-C13	-3.46	112.28	122.66
57	y	32	PSU	O2-C2-N1	-3.45	119.23	122.79
1	A	745	1MG	N2-C2-N1	3.45	121.56	118.79
1	A	2503	2MA	C4-C5-N7	-3.44	106.65	110.58
57	y	37	MIA	C2-N3-C4	3.43	121.28	112.29
34	a	1518	MA6	C9-N6-C6	-3.42	111.82	120.52
1	A	2580	PSU	C4-N3-C2	-3.42	121.66	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2457	PSU	O2-C2-N1	-3.41	119.28	122.79
1	A	2030	6MZ	C6-C5-N7	3.41	136.14	132.43
57	y	55	PSU	O2-C2-N1	-3.40	119.28	122.79
34	a	966	2MG	N2-C2-N3	-3.40	116.19	120.51
34	a	1498	UR3	C5-C4-N3	3.39	119.50	115.04
1	A	2445	2MG	N1-C2-N2	3.38	120.01	116.56
57	y	8	4SU	C6-N1-C2	-3.38	116.89	121.00
57	y	54	5MU	C5M-C5-C4	3.36	122.37	118.78
1	A	746	PSU	O2-C2-N1	-3.36	119.33	122.79
34	a	516	PSU	C3'-C2'-C1'	3.35	105.64	101.69
1	A	1618	6MZ	C6-C5-N7	3.35	136.08	132.43
1	A	2604	PSU	O2-C2-N1	-3.34	119.34	122.79
34	a	1519	MA6	N1-C2-N3	-3.33	123.54	128.58
55	w	54	5MU	C5M-C5-C4	3.32	122.33	118.78
34	a	966	2MG	C6-C5-N7	3.31	136.31	130.29
55	v	55	PSU	O2-C2-N1	-3.24	119.44	122.79
1	A	1917	PSU	C6-C5-C4	-3.24	115.98	118.17
1	A	2030	6MZ	N1-C2-N3	-3.24	123.68	128.58
1	A	2605	PSU	C6-C5-C4	-3.21	116.00	118.17
1	A	1939	5MU	O4-C4-C5	-3.21	121.25	124.92
1	A	1618	6MZ	N1-C2-N3	-3.21	123.73	128.58
1	A	1835	2MG	C6-C5-N7	3.20	136.11	130.29
1	A	1911	PSU	C6-C5-C4	-3.17	116.03	118.17
1	A	2580	PSU	C3'-C2'-C1'	3.15	105.40	101.69
55	w	54	5MU	O4-C4-C5	-3.15	121.32	124.92
55	v	54	5MU	C5-C4-N3	3.15	118.06	115.32
1	A	1962	5MC	O2-C2-N3	-3.13	117.40	122.33
34	a	1518	MA6	O4'-C1'-N9	3.12	114.08	108.09
1	A	2552	OMU	C1'-N1-C2	3.10	123.15	117.59
57	y	37	MIA	N6-C6-N1	3.09	122.48	118.33
1	A	1618	6MZ	C9-N6-C6	-3.05	120.02	122.85
1	A	2030	6MZ	C9-N6-C6	-3.04	120.03	122.85
34	a	1516	2MG	N1-C2-N2	3.03	119.65	116.56
1	A	2503	2MA	C4-N9-C8	3.02	108.91	105.74
57	y	55	PSU	C6-C5-C4	-3.02	116.14	118.17
34	a	1407	5MC	O2-C2-N3	-3.02	117.58	122.33
1	A	2069	7MG	C5-C6-N1	3.01	116.24	110.94
1	A	2498	OMC	O2-C2-N3	-3.00	117.60	122.33
57	y	37	MIA	C2-N1-C6	2.97	123.18	117.54
55	v	54	5MU	C6-N1-C2	-2.97	118.35	121.30
34	a	527	7MG	C5-C6-N1	2.96	116.14	110.94
57	y	37	MIA	O4'-C1'-N9	2.95	113.76	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	C6-C5-C4	-2.95	116.18	118.17
34	a	967	5MC	O2-C2-N3	-2.94	117.69	122.33
34	a	1516	2MG	C4-C5-N7	-2.93	106.03	110.67
57	y	46	7MG	C5-C6-N1	2.92	116.08	110.94
55	w	55	PSU	C3'-C2'-C1'	2.92	105.13	101.69
34	a	1518	MA6	C5-N7-C8	2.92	108.03	103.45
34	a	1207	2MG	C4-C5-N7	-2.91	106.05	110.67
55	w	20	H2U	C5-C6-N1	-2.88	102.80	111.52
1	A	2504	PSU	C6-C5-C4	-2.86	116.24	118.17
1	A	2251	OMG	C6-C5-N7	2.85	135.47	130.29
1	A	2503	2MA	N6-C6-N1	2.85	120.87	117.03
57	y	37	MIA	C5-N7-C8	2.84	107.92	103.45
57	y	37	MIA	N3-C2-N1	-2.83	121.83	127.00
57	y	20	H2U	C3'-C2'-C1'	2.82	106.79	101.46
1	A	2552	OMU	O4-C4-C5	-2.79	120.34	125.16
1	A	1939	5MU	C5-C6-N1	-2.76	120.32	123.31
34	a	1402	4OC	C6-C5-C4	2.76	120.32	117.00
55	w	8	4SU	C6-N1-C2	-2.75	117.65	121.00
1	A	2445	2MG	C4-C5-N7	-2.75	106.31	110.67
1	A	2503	2MA	C5-N7-C8	2.74	107.75	103.45
1	A	1917	PSU	C3'-C2'-C1'	2.73	104.91	101.69
1	A	2457	PSU	C6-C5-C4	-2.72	116.34	118.17
1	A	2503	2MA	C2-N1-C6	2.71	122.27	118.10
1	A	2580	PSU	O2-C2-N1	-2.70	120.00	122.79
57	y	20	H2U	C5-C4-N3	2.70	119.56	116.69
57	y	37	MIA	C4-N9-C8	2.65	108.52	105.74
57	y	20	H2U	O4'-C1'-N1	2.64	112.90	109.30
34	a	966	2MG	C4-C5-N7	-2.62	106.51	110.67
1	A	2030	6MZ	C4-N9-C8	2.62	108.49	105.74
55	v	20	H2U	C5-C4-N3	2.59	119.44	116.69
57	y	39	PSU	C6-C5-C4	-2.57	116.44	118.17
1	A	1618	6MZ	C4-N9-C8	2.56	108.43	105.74
57	y	16	H2U	C5-C4-N3	2.56	119.41	116.69
1	A	2498	OMC	O4'-C1'-N1	2.55	114.14	108.36
1	A	1915	3TD	C10-N3-C4	2.55	121.60	117.64
1	A	2030	6MZ	C5-N7-C8	2.55	107.46	103.45
1	A	1618	6MZ	C5-N7-C8	2.54	107.45	103.45
34	a	1402	4OC	C5-C4-N3	-2.54	118.63	122.60
57	y	8	4SU	O2-C2-N3	-2.53	116.83	121.49
57	y	32	PSU	C6-C5-C4	-2.52	116.47	118.17
1	A	745	1MG	C4-C5-N7	-2.52	106.68	110.67
1	A	1835	2MG	C4-C5-N7	-2.50	106.70	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1618	6MZ	C3'-C2'-C1'	2.50	106.19	101.46
1	A	746	PSU	C6-C5-C4	-2.50	116.49	118.17
1	A	747	5MC	C5-C6-N1	-2.49	120.61	123.31
1	A	1915	3TD	C3'-C2'-C1'	2.49	104.63	101.69
1	A	1939	5MU	C5M-C5-C4	2.49	121.44	118.78
1	A	2030	6MZ	C3'-C2'-C1'	2.49	106.17	101.46
57	y	32	PSU	C3'-C2'-C1'	2.49	104.62	101.69
1	A	2552	OMU	C6-N1-C2	-2.48	117.98	121.00
55	v	7	4SU	C6-N1-C2	-2.48	117.98	121.00
1	A	745	1MG	C6-C5-N7	2.47	134.85	129.36
34	a	1519	MA6	C2'-C1'-N9	-2.47	107.17	113.30
34	a	1407	5MC	O4'-C1'-N1	2.45	113.91	108.36
55	v	54	5MU	O4-C4-C5	-2.44	122.13	124.92
34	a	1518	MA6	C3'-C2'-C1'	2.44	106.07	101.46
34	a	1207	2MG	O6-C6-C5	-2.44	120.10	126.53
34	a	1498	UR3	C3U-N3-C2	2.42	121.55	117.33
1	A	2604	PSU	C6-C5-C4	-2.41	116.55	118.17
1	A	2552	OMU	O4'-C1'-N1	2.40	113.81	108.36
1	A	2552	OMU	O2-C2-N3	-2.39	117.07	121.49
57	y	16	H2U	O4'-C1'-N1	2.38	112.55	109.30
55	v	54	5MU	C5-C6-N1	-2.38	120.72	123.31
34	a	1519	MA6	N9-C8-N7	-2.38	110.56	113.94
34	a	967	5MC	CM5-C5-C4	2.38	124.42	120.51
34	a	1402	4OC	O4'-C1'-N1	2.37	113.74	108.36
34	a	1402	4OC	O2-C2-N3	-2.37	118.59	122.33
1	A	2251	OMG	C4-C5-N7	-2.35	106.95	110.67
55	v	54	5MU	O2-C2-N1	-2.35	119.74	122.80
34	a	1519	MA6	C10-N6-C9	-2.34	108.65	116.18
34	a	1207	2MG	C2-N1-C6	-2.34	121.72	124.55
34	a	1498	UR3	C6-N1-C2	-2.34	119.89	121.80
1	A	2552	OMU	C2'-C1'-N1	-2.33	109.81	114.24
34	a	527	7MG	O4'-C1'-N9	2.33	112.47	109.30
34	a	1519	MA6	C4-N9-C8	2.33	108.18	105.74
55	w	54	5MU	C5M-C5-C6	-2.32	119.70	122.85
34	a	1519	MA6	O4'-C1'-N9	2.32	112.54	108.09
1	A	2069	7MG	O4'-C1'-N9	2.31	112.45	109.30
1	A	2069	7MG	C6-C5-C4	-2.27	118.40	122.40
34	a	966	2MG	O6-C6-C5	-2.26	120.58	126.53
1	A	2069	7MG	O6-C6-C5	-2.25	122.09	127.62
1	A	2503	2MA	N9-C8-N7	-2.25	110.74	113.94
34	a	1519	MA6	C6-C5-N7	2.24	137.01	133.43
1	A	1939	5MU	O2-C2-N1	-2.23	119.89	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	54	5MU	C5M-C5-C6	-2.23	119.83	122.85
1	A	745	1MG	O6-C6-C5	-2.23	118.85	124.59
34	a	966	2MG	C5-C6-N1	2.21	118.88	113.25
1	A	2069	7MG	N2-C2-N1	2.21	121.43	116.76
34	a	527	7MG	O6-C6-C5	-2.20	122.22	127.62
1	A	2445	2MG	O6-C6-C5	-2.20	120.72	126.53
34	a	1518	MA6	C6-C5-N7	2.20	136.95	133.43
1	A	2503	2MA	C6-C5-N7	2.20	136.33	132.09
55	w	54	5MU	O4'-C1'-N1	2.19	113.33	108.36
1	A	1939	5MU	O4'-C1'-N1	2.19	113.32	108.36
34	a	1207	2MG	C5-C6-N1	2.17	118.78	113.25
55	w	54	5MU	C3'-C2'-C1'	2.17	105.57	101.46
34	a	1407	5MC	CM5-C5-C4	2.17	124.07	120.51
1	A	747	5MC	O2-C2-N3	-2.17	118.91	122.33
34	a	1516	2MG	O6-C6-C5	-2.16	120.82	126.53
1	A	2251	OMG	O6-C6-C5	-2.15	120.85	126.53
55	v	55	PSU	C3'-C2'-C1'	2.15	104.22	101.69
57	y	16	H2U	C5-C6-N1	-2.15	105.03	111.52
57	y	55	PSU	C3'-C2'-C1'	2.14	104.22	101.69
57	y	20	H2U	C5-C6-N1	-2.14	105.05	111.52
1	A	2457	PSU	C3'-C2'-C1'	2.13	104.21	101.69
57	y	46	7MG	C6-C5-C4	-2.13	118.66	122.40
57	y	16	H2U	C3'-C2'-C1'	2.13	105.49	101.46
57	y	54	5MU	C1'-N1-C2	2.13	121.41	117.59
34	a	967	5MC	C3'-C2'-C1'	2.12	105.48	101.46
55	v	7	4SU	O4'-C1'-N1	2.12	113.16	108.36
34	a	966	2MG	C2-N1-C6	-2.11	122.00	124.55
57	y	8	4SU	C1'-N1-C2	2.11	121.39	117.59
57	y	37	MIA	N9-C8-N7	-2.11	110.95	113.94
1	A	1962	5MC	CM5-C5-C4	2.10	123.96	120.51
1	A	2449	H2U	O4-C4-C5	-2.10	117.91	122.20
57	y	37	MIA	C3'-C2'-C1'	2.10	105.43	101.46
55	w	54	5MU	C5-C6-N1	-2.10	121.04	123.31
1	A	747	5MC	O4'-C1'-N1	2.09	113.09	108.36
1	A	2445	2MG	C5-C6-N1	2.09	118.56	113.25
34	a	1519	MA6	C9-N6-C6	-2.09	115.22	120.52
57	y	46	7MG	O6-C6-C5	-2.08	122.52	127.62
55	v	54	5MU	O2-C2-N3	-2.07	117.66	121.49
34	a	1516	2MG	C2-N1-C6	-2.07	122.04	124.55
55	w	55	PSU	C6-C5-C4	-2.07	116.78	118.17
55	w	54	5MU	O2-C2-N3	-2.07	117.68	121.49
1	A	2069	7MG	N2-C2-N3	-2.06	115.65	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	20	H2U	C5-C6-N1	-2.04	105.35	111.52
1	A	1835	2MG	O6-C6-C5	-2.04	121.16	126.53
1	A	2069	7MG	C6-C5-N7	2.04	135.09	131.93
1	A	1835	2MG	C5-C6-N1	2.02	118.41	113.25
34	a	1519	MA6	C4-C5-C6	2.01	117.99	115.91

There are no chirality outliers.

All (75) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
57	y	37	MIA	C3'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C4
34	a	1518	MA6	N1-C6-N6-C9
55	w	8	4SU	C2'-C1'-N1-C6
1	A	1917	PSU	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
57	y	37	MIA	C12-C13-C14-C16
55	v	7	4SU	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C2'-C1'-N9-C4
34	a	1518	MA6	O4'-C1'-N9-C8
1	A	2457	PSU	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C2
57	y	46	7MG	C2'-C1'-N9-C8
34	a	527	7MG	C3'-C4'-C5'-O5'
55	v	54	5MU	C3'-C4'-C5'-O5'
34	a	1207	2MG	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
1	A	1618	6MZ	C2'-C1'-N9-C8
55	w	8	4SU	O4'-C1'-N1-C2
34	a	527	7MG	C4'-C5'-O5'-P
34	a	516	PSU	O4'-C1'-C5-C4
57	y	32	PSU	O4'-C1'-C5-C4
55	w	20	H2U	C2'-C1'-N1-C6
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
55	w	55	PSU	O4'-C1'-C5-C6
57	y	32	PSU	O4'-C1'-C5-C6
57	y	46	7MG	O4'-C1'-N9-C8
57	y	8	4SU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	A	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	y	55	PSU	1	0
1	A	1915	3TD	1	0
1	A	2504	PSU	1	0
34	a	1498	UR3	1	0
1	A	2498	OMC	2	0
1	A	1618	6MZ	4	0
55	v	54	5MU	1	0
57	y	37	MIA	1	0
1	A	2030	6MZ	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
63	GNP	z	402	60	34,34,34	2.41	7 (20%)	47,54,54	1.84	9 (19%)
62	PHE	z	401	-	10,11,12	0.45	0	8,13,15	0.17	0
59	FME	A	3001	-	8,9,10	0.63	0	8,9,11	1.92	2 (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
63	GNP	z	402	60	-	2/18/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
59	FME	A	3001	-	-	2/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	10.09	1.61	1.46
63	z	402	GNP	PG-N3B	4.42	1.74	1.63
63	z	402	GNP	PB-N3B	4.23	1.74	1.63
63	z	402	GNP	PG-O2G	-3.25	1.48	1.56
63	z	402	GNP	C5-C4	3.12	1.47	1.38
63	z	402	GNP	C6-N1	-2.27	1.34	1.38
63	z	402	GNP	C5-N7	-2.05	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GNP	C5-C4-N3	-6.03	118.79	128.39
63	z	402	GNP	C2-N3-C4	5.18	121.22	112.30
63	z	402	GNP	N9-C4-N3	4.49	134.94	125.95
59	A	3001	FME	C-CA-N	4.03	117.28	109.50
63	z	402	GNP	C6-C5-N7	3.54	136.73	130.29
63	z	402	GNP	O1B-PB-N3B	-2.84	107.58	111.77
63	z	402	GNP	C4-C5-N7	-2.54	106.64	110.67
63	z	402	GNP	C5-C6-N1	2.24	118.96	113.25
63	z	402	GNP	O6-C6-C5	-2.18	120.79	126.53
59	A	3001	FME	O1-CN-N	-2.17	119.72	125.32
63	z	402	GNP	O3A-PB-N3B	2.04	112.24	106.59

There are no chirality outliers.

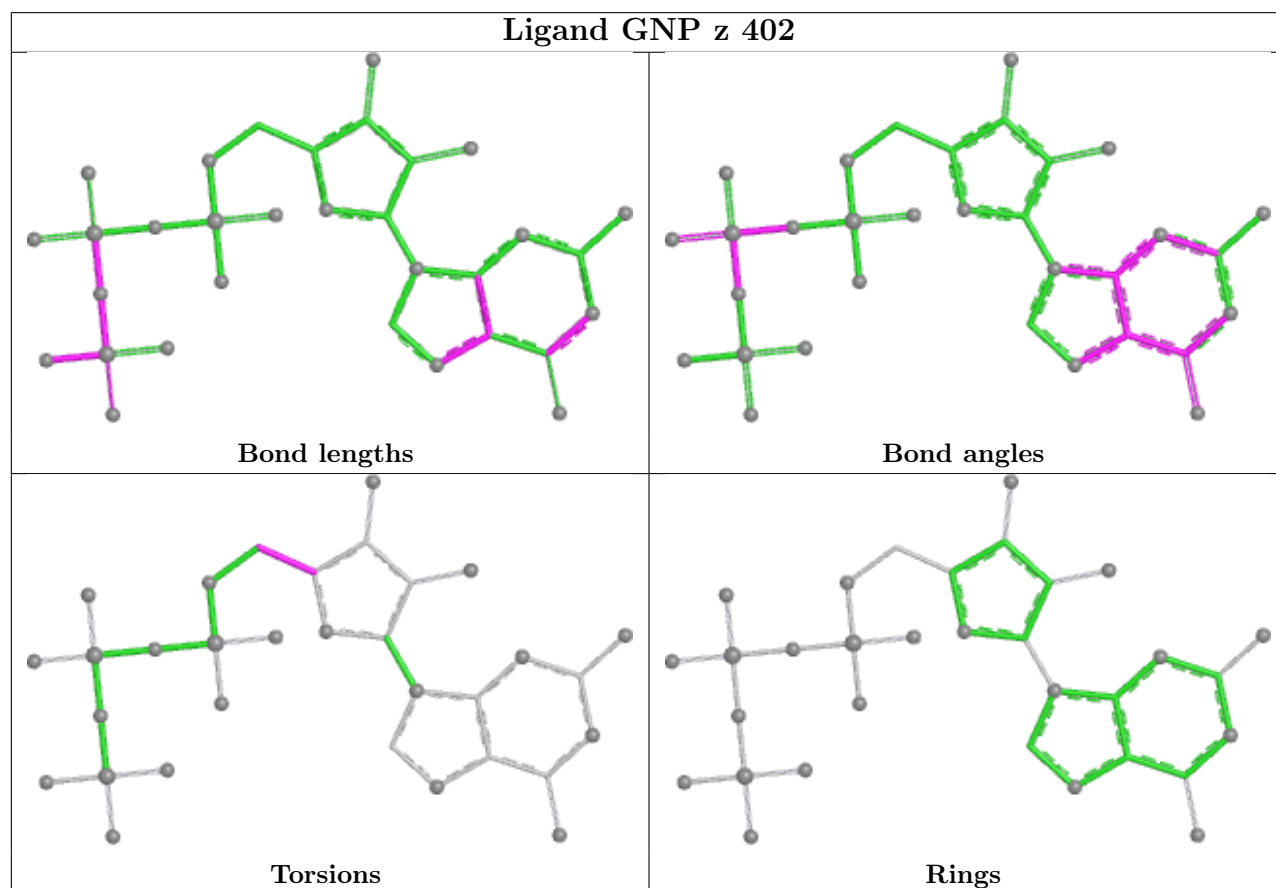
All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

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

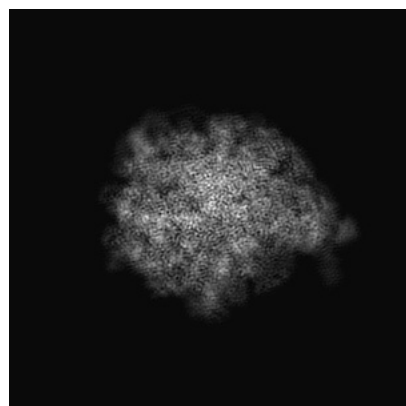
6 Map visualisation [i](#)

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

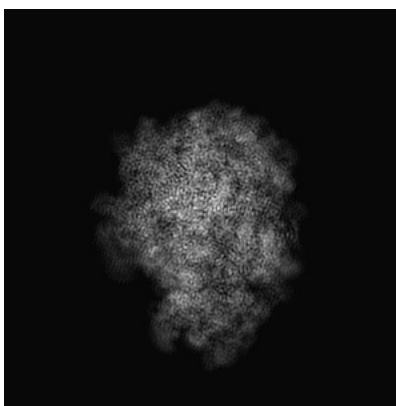
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

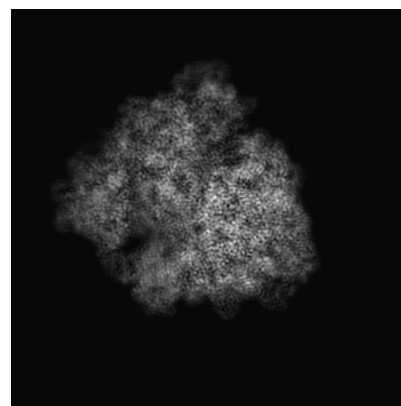
6.1.1 Primary map



X

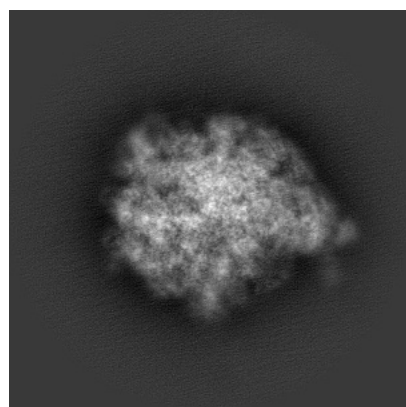


Y

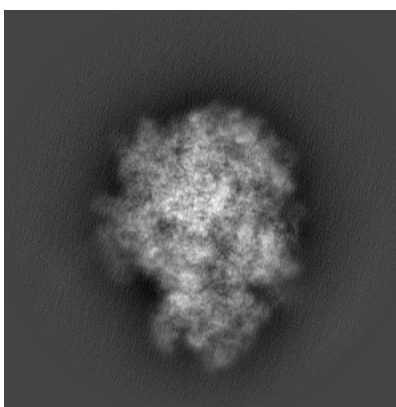


Z

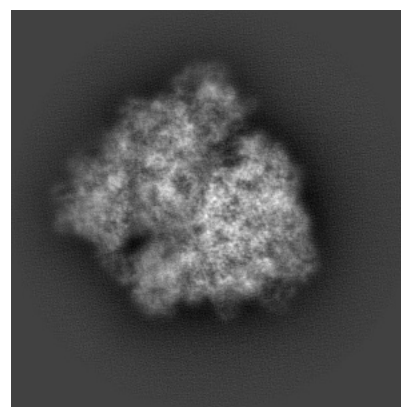
6.1.2 Raw map



X



Y

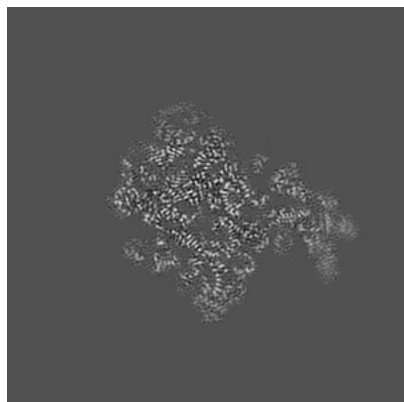


Z

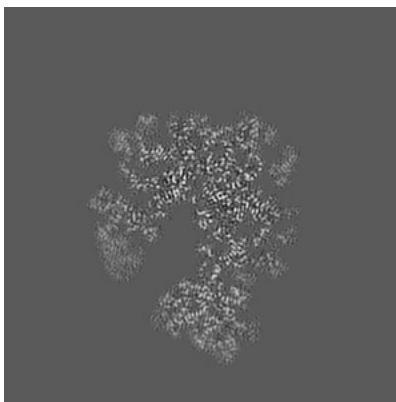
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

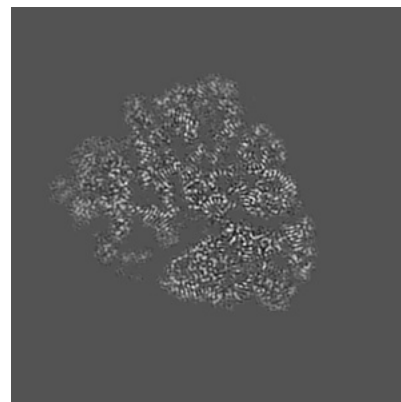
6.2.1 Primary map



X Index: 199

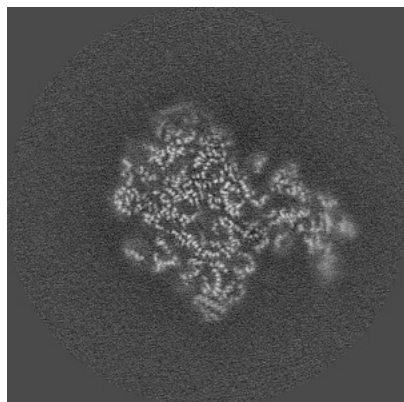


Y Index: 199

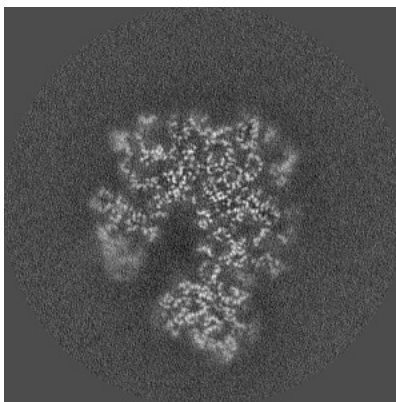


Z Index: 199

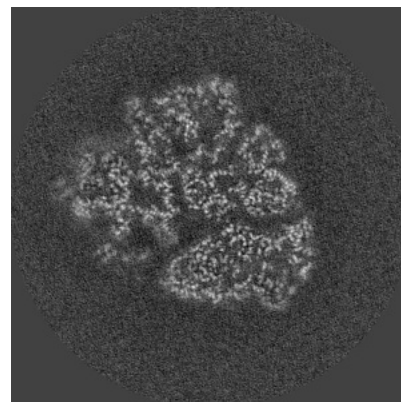
6.2.2 Raw map



X Index: 199



Y Index: 199

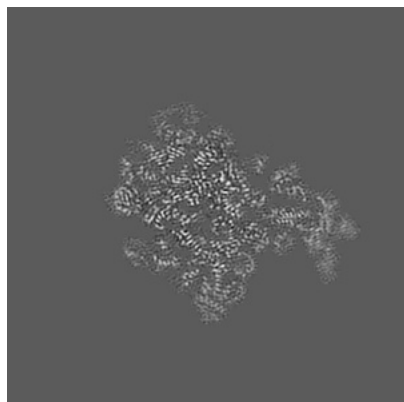


Z Index: 199

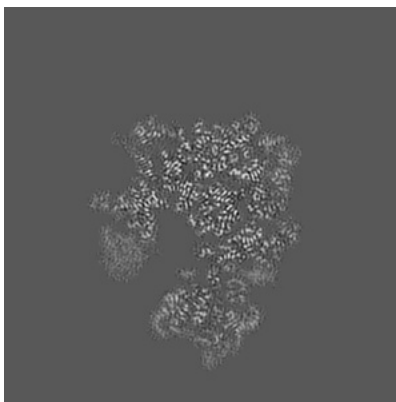
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

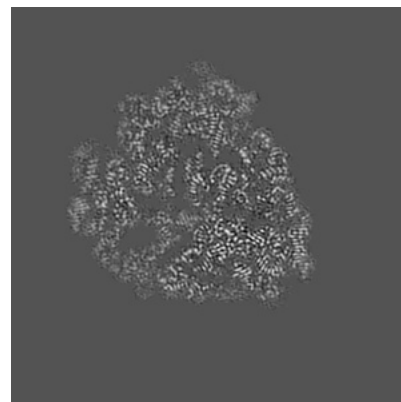
6.3.1 Primary map



X Index: 200

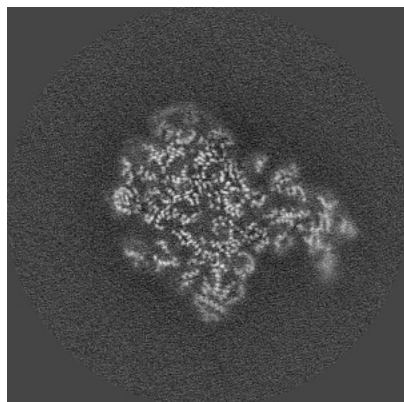


Y Index: 208

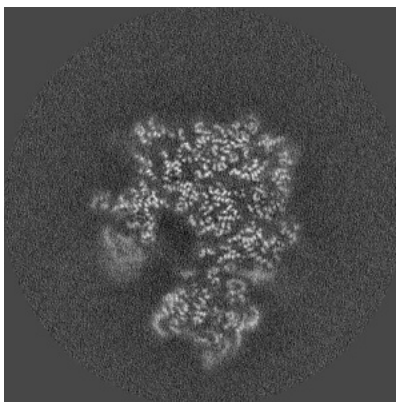


Z Index: 191

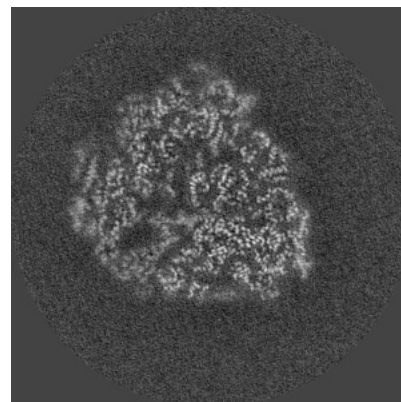
6.3.2 Raw map



X Index: 200



Y Index: 208

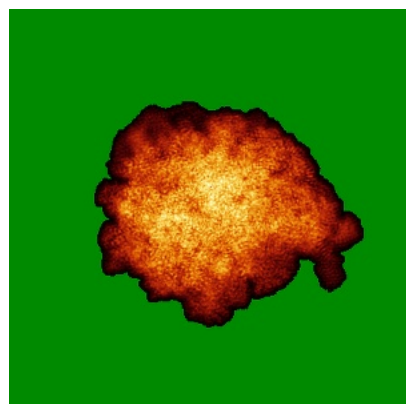


Z Index: 190

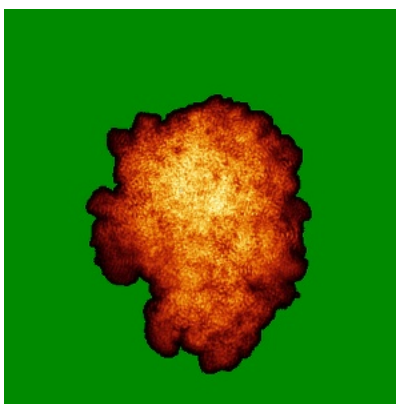
The images above show the largest variance slices of the map in three orthogonal directions.

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

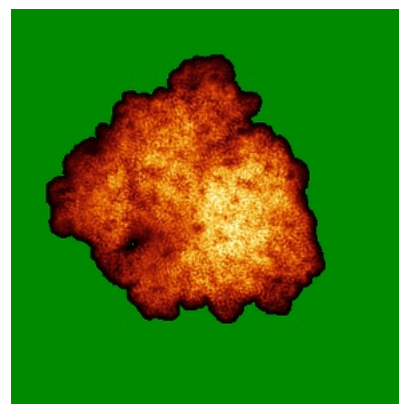
6.4.1 Primary map



X

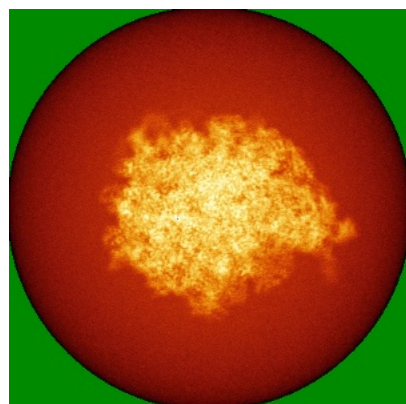


Y

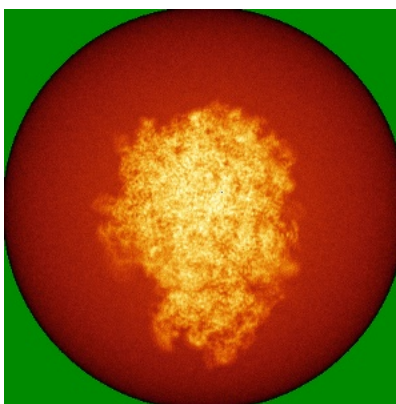


Z

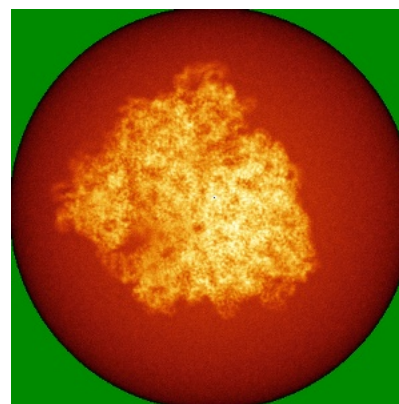
6.4.2 Raw map



X



Y



Z

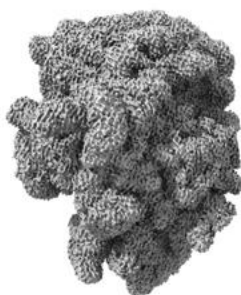
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

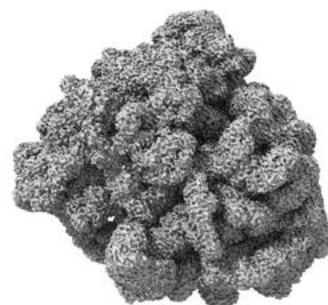
6.5.1 Primary map



X



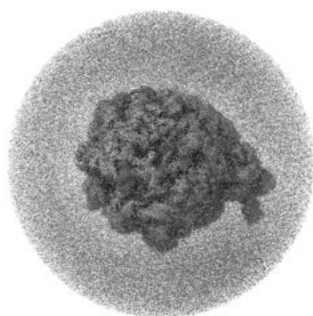
Y



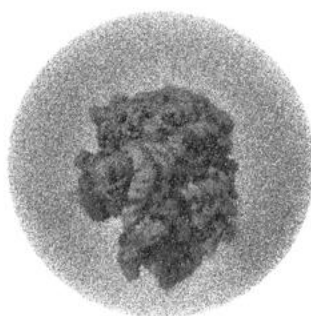
Z

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

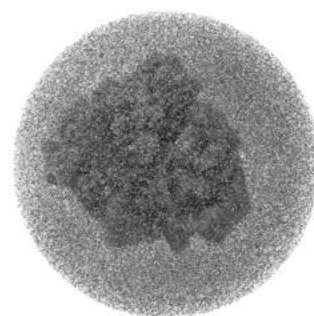
6.5.2 Raw map



X



Y



Z

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

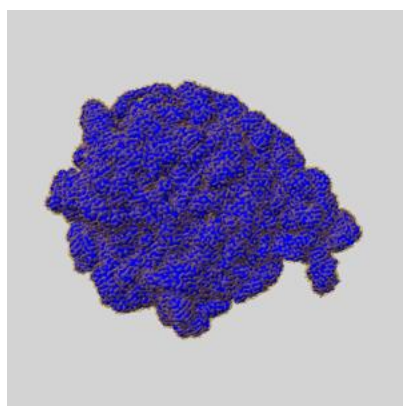
6.6 Mask visualisation [i](#)

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

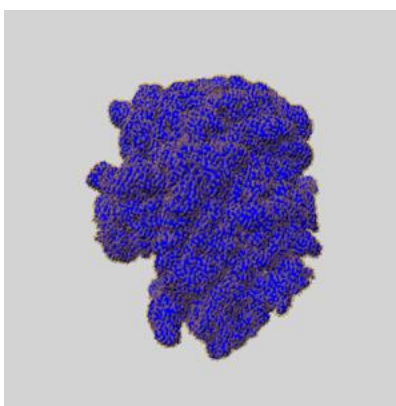
A mask typically either:

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

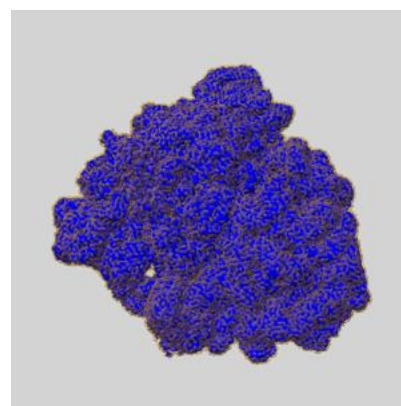
6.6.1 emd_8813_msk_1.map [i](#)



X



Y

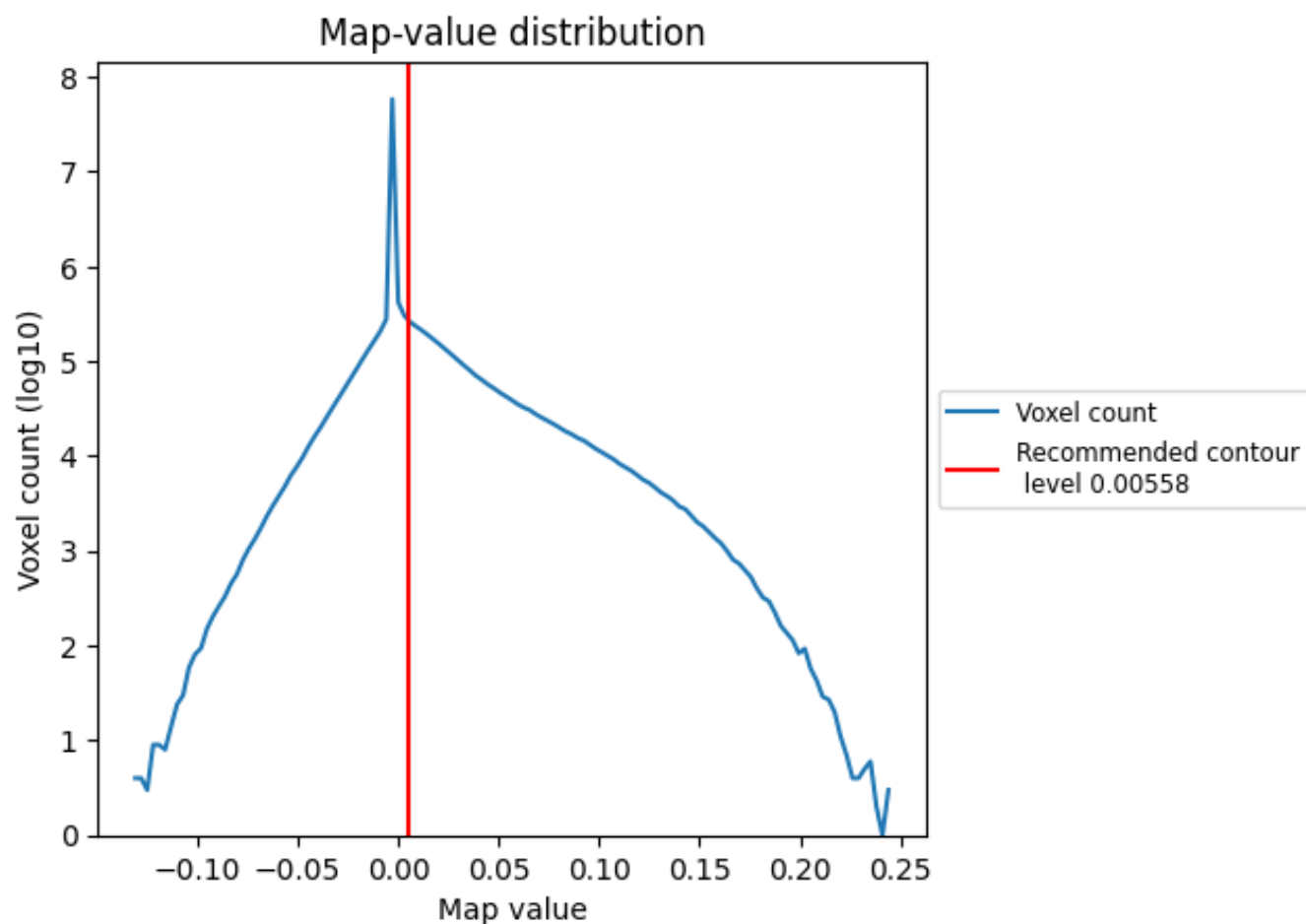


Z

7 Map analysis [i](#)

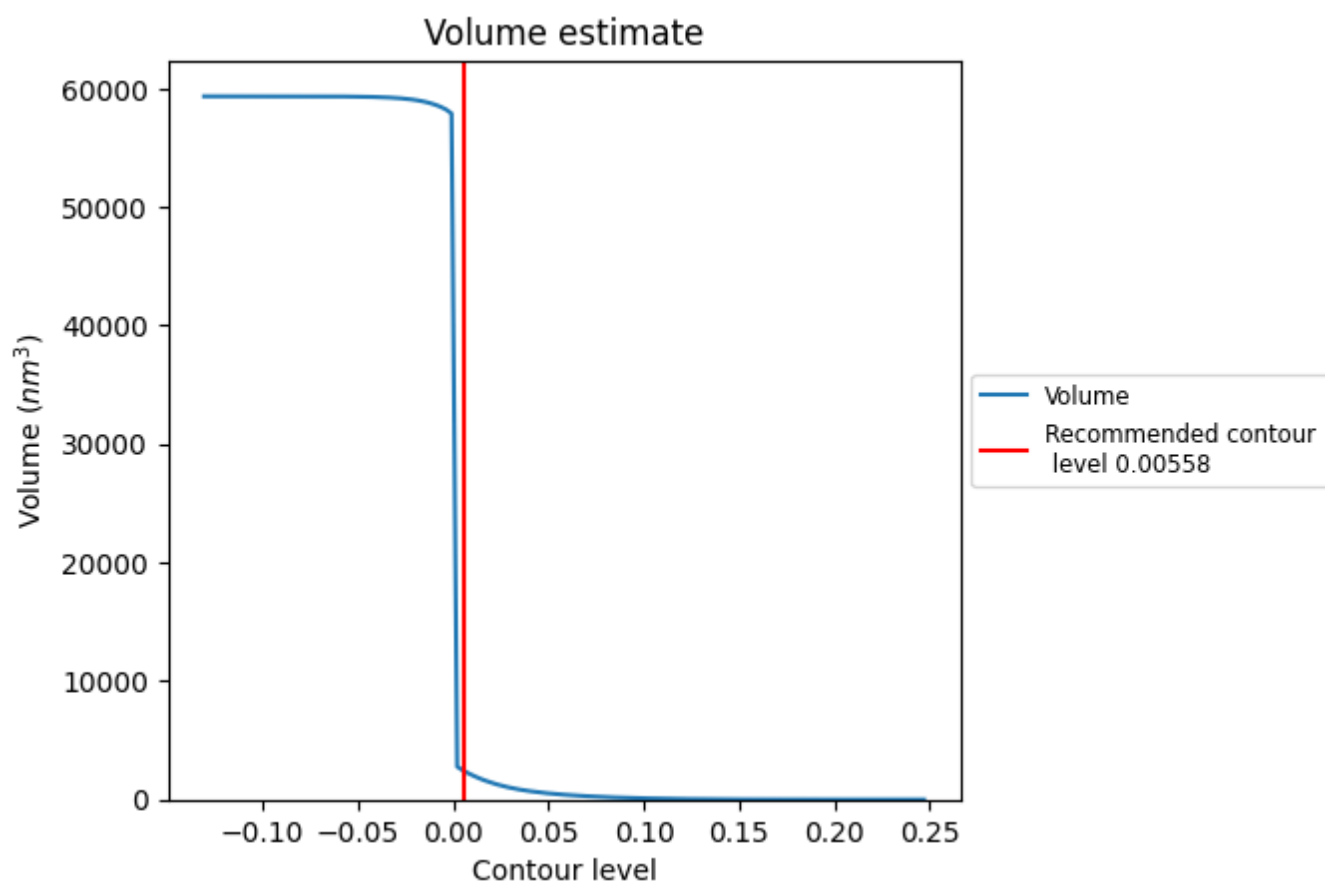
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

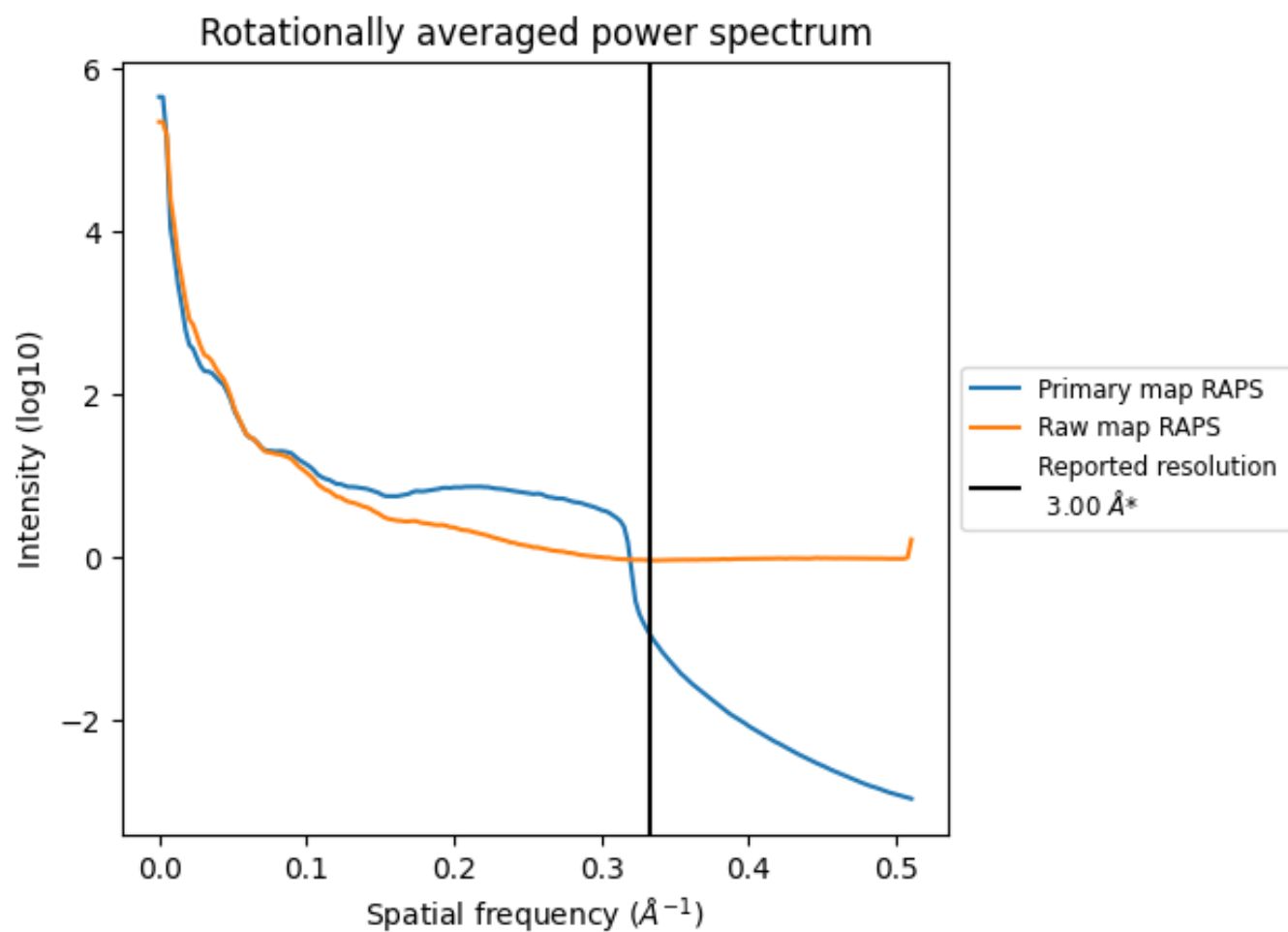
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum [i](#)

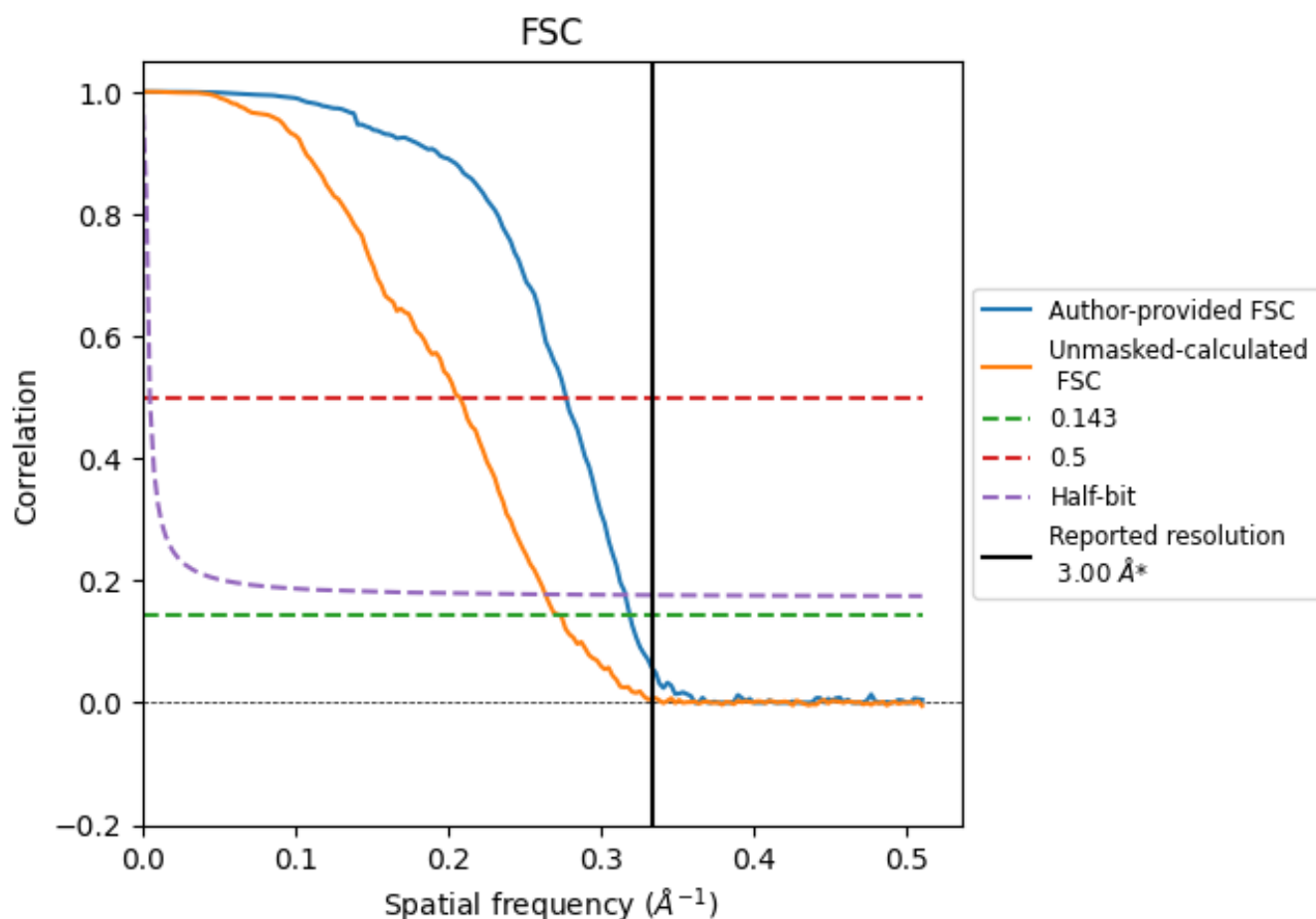


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

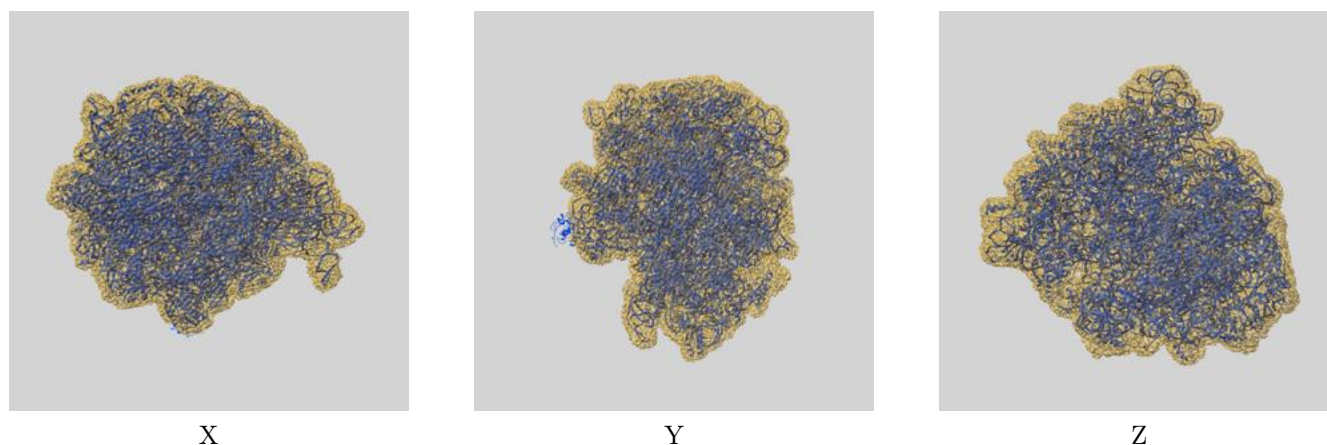
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.13	3.61	3.16
Unmasked-calculated*	3.66	4.82	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

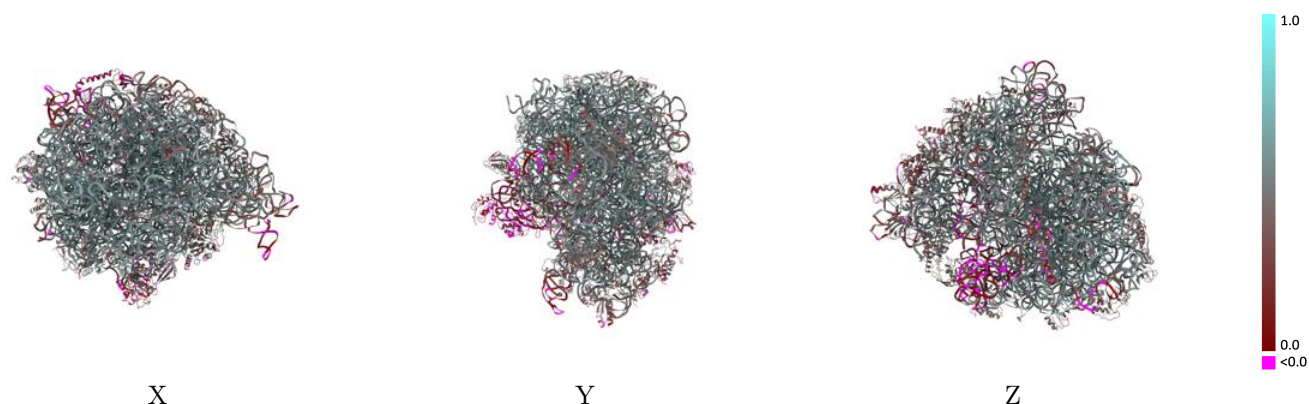
This section contains information regarding the fit between EMDB map EMD-8813 and PDB model 5WDT. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



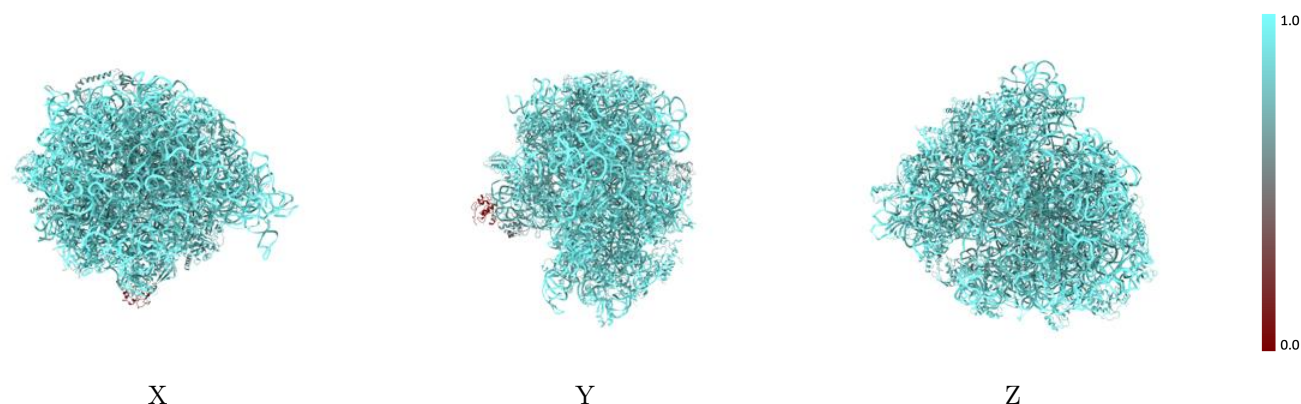
The images above show the 3D surface view of the map at the recommended contour level 0.00558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



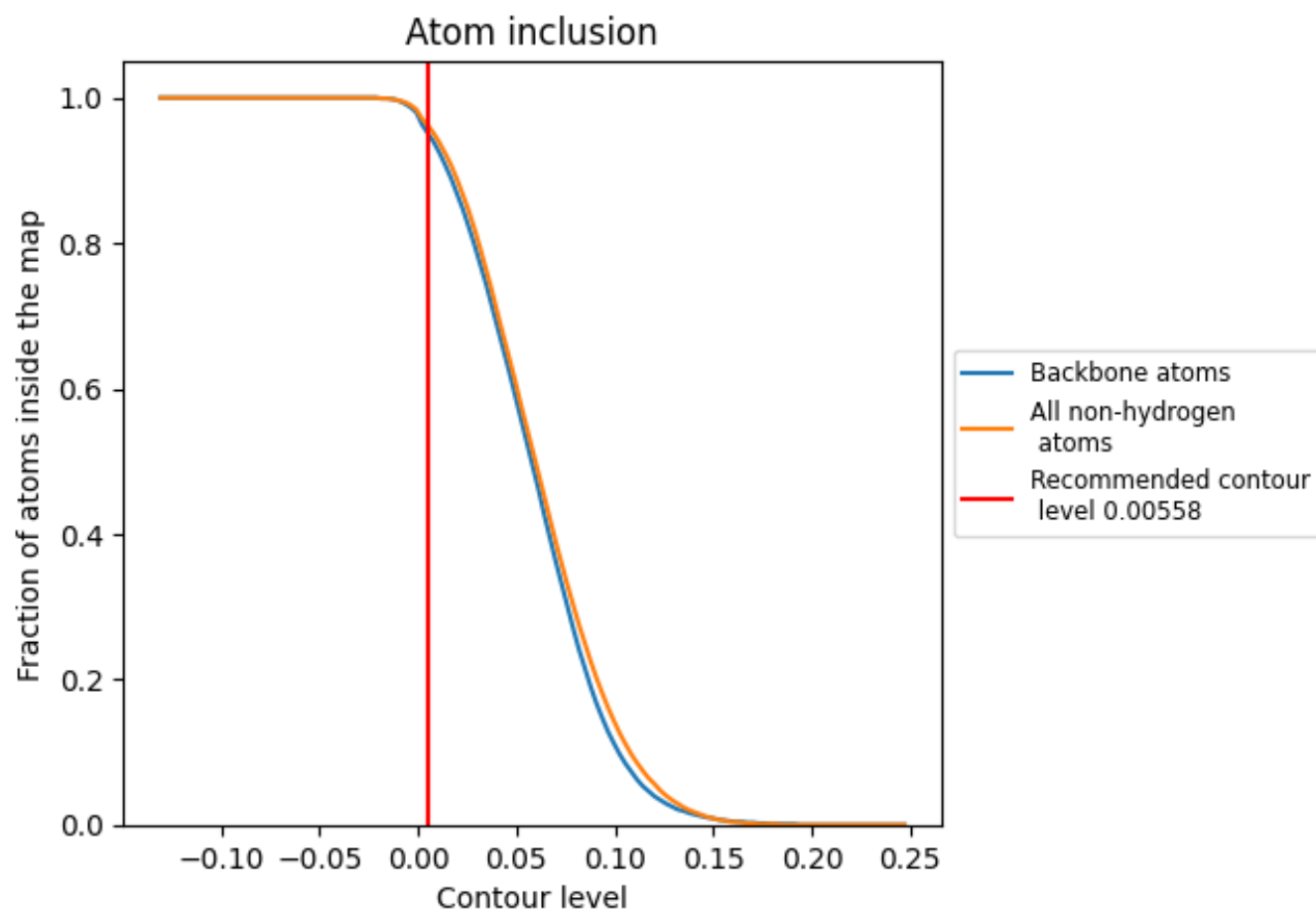
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00558).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00558) and Q-score for the entire model and for each chain.

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



Continued on next page...

Continued from previous page...

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