Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 04:01 am BST

PDB ID	:	5LZB
EMDB ID	:	EMD-4122
Title	:	Structure of SelB-Sec-tRNASec bound to the 70S ribosome in the initial binding state (IB)
Authors	:	Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on	:	2016-09-29
Resolution	:	5.30 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:

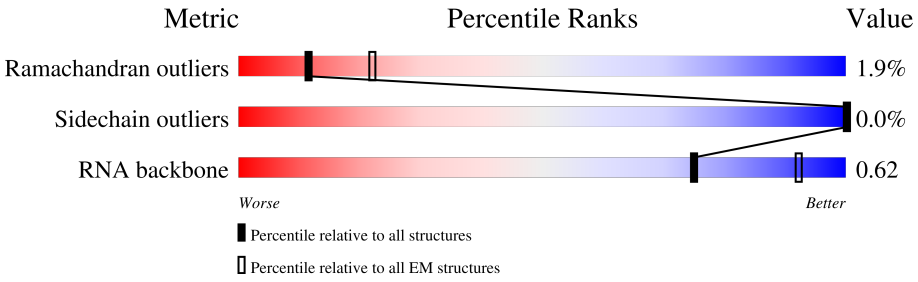
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1539	75% 22%
2	b	218	44% 96%
3	c	206	20% 97%
4	d	205	32% 97%
5	e	157	17% 95% 5%
6	f	100	14% 95% 5%
7	g	151	13% 97%
8	h	129	16% 98%

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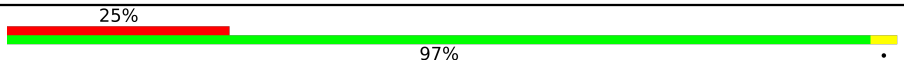
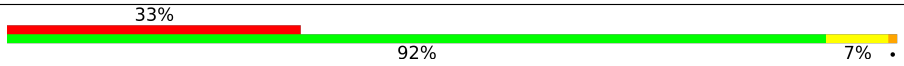
Mol	Chain	Length	Quality of chain
9	i	127	
10	j	98	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152991 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1705	1081	305	312	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	206	1625	1028	305	289	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1157	719	218	214	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	100	818	515	148	149	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called Sec-tRNASec.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	1	0
			4863	3049	904	893	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Q	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total 739	C 466	N 139	O 132	S 2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	U	102	Total 780	C 492	N 146	O 142	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

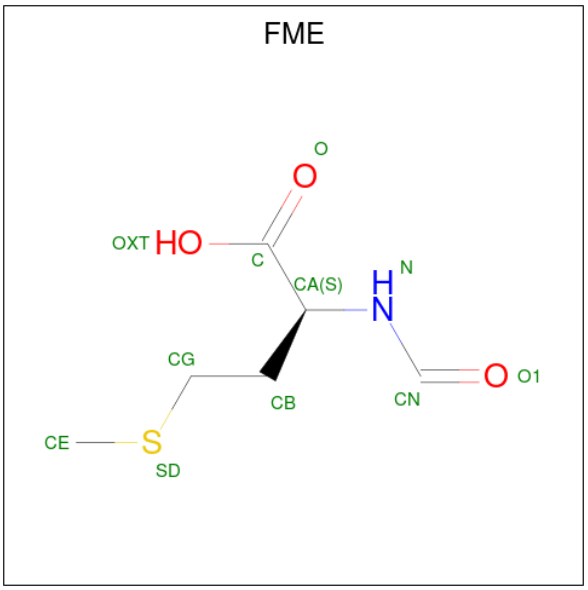
- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNASec (low occupancy).

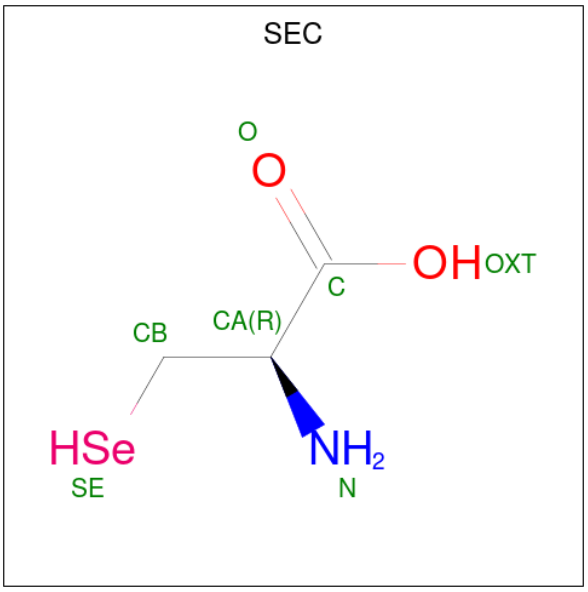
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



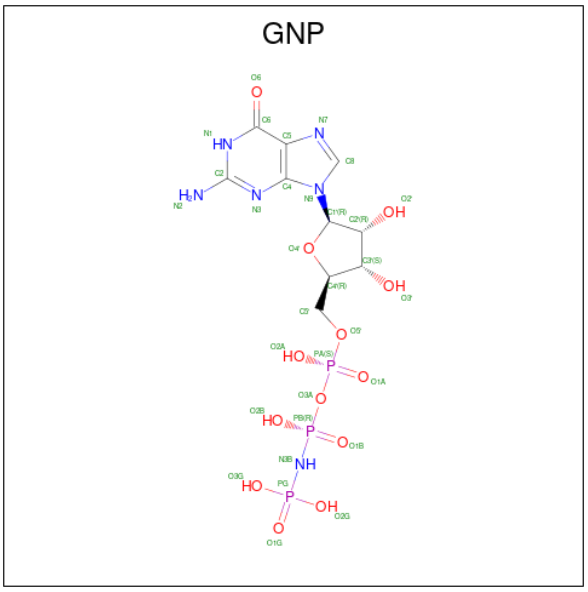
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: $C_3H_7NO_2Se$).



Mol	Chain	Residues	Atoms					AltConf
60	y	1	Total	C	N	O	Se	0
			6	3	1	1	1	

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
62	z	1	Total Mg 1 1	0

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
63	4	1	Total Zn 1 1	0
63	6	1	Total Zn 1 1	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	z	2	Total O 2 2	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.675	Depositor
Minimum map value	-0.887	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, 6IA, 4SU, MA6, UR3, PSU, G7M, OMC, OMU, OMG, MG, 4OC, 2MG, SEC, 3TD, H2U, ZN, 5MC, 5MU, 2MA, 1MG, GNP, FME

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	0.58	3/36701 (0.0%)	1.30	392/57246 (0.7%)
2	b	0.45	0/1736	0.85	4/2338 (0.2%)
3	c	0.41	0/1652	0.76	3/2225 (0.1%)
4	d	0.49	0/1665	0.93	3/2227 (0.1%)
5	e	0.45	0/1170	0.88	0/1573
6	f	0.51	0/836	0.85	1/1128 (0.1%)
7	g	0.46	0/1196	0.81	2/1602 (0.1%)
8	h	0.43	0/989	0.78	1/1326 (0.1%)
9	i	0.47	0/1034	0.84	0/1375
10	j	0.44	0/797	0.87	1/1077 (0.1%)
11	k	0.48	0/886	0.87	3/1195 (0.3%)
12	l	0.43	0/969	0.79	1/1300 (0.1%)
13	m	0.42	0/893	0.90	1/1193 (0.1%)
14	n	0.45	0/806	0.82	1/1074 (0.1%)
15	o	0.42	0/722	0.81	3/964 (0.3%)
16	p	0.55	0/659	0.78	0/884
17	q	0.45	0/658	0.88	0/881
18	r	0.36	0/512	0.67	0/689
19	s	0.37	0/653	0.73	2/877 (0.2%)
20	t	0.43	0/671	0.77	0/888
21	u	0.43	0/501	0.85	1/668 (0.1%)
22	v	0.62	2/1745 (0.1%)	1.33	25/2716 (0.9%)
23	x	0.88	1/1145 (0.1%)	1.84	45/1781 (2.5%)
24	y	0.89	2/2168 (0.1%)	1.92	110/3375 (3.3%)
25	z	0.47	0/4963	0.89	12/6727 (0.2%)
26	A	0.57	13/69240 (0.0%)	1.24	539/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.24	27/4478 (0.6%)
28	C	0.42	0/2122	0.77	1/2852 (0.0%)
29	D	0.45	0/1586	0.75	0/2134
30	E	0.43	0/1571	0.75	2/2113 (0.1%)
31	F	0.52	1/1435 (0.1%)	0.90	4/1926 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	G	0.47	0/1343	0.82	3/1816 (0.2%)
33	I	0.49	0/1046	0.97	5/1410 (0.4%)
34	H	0.40	0/1122	0.74	1/1515 (0.1%)
35	J	0.42	0/1152	0.70	2/1551 (0.1%)
36	K	0.47	0/948	0.75	0/1268
37	L	0.42	0/1054	0.75	0/1403
38	M	0.43	0/1093	0.74	1/1460 (0.1%)
39	N	0.43	0/974	0.68	0/1301
40	O	0.43	0/902	0.72	0/1209
41	P	0.43	0/929	0.72	1/1242 (0.1%)
42	Q	0.41	0/960	0.58	1/1278 (0.1%)
43	R	0.42	0/829	0.79	0/1107
44	S	0.39	0/864	0.80	2/1156 (0.2%)
45	T	0.44	0/745	0.77	0/994
46	U	0.43	0/788	0.91	1/1051 (0.1%)
47	V	0.47	0/766	0.72	0/1025
48	W	0.39	0/582	0.69	0/769
49	X	0.35	0/635	0.70	1/848 (0.1%)
50	Y	0.48	0/510	0.92	2/677 (0.3%)
51	Z	0.40	0/453	0.72	1/605 (0.2%)
52	0	0.44	0/450	0.80	0/599
53	1	0.36	0/417	0.77	0/554
54	2	0.40	0/380	0.69	0/498
55	3	0.40	0/513	0.63	0/676
56	4	0.48	0/303	0.80	1/397 (0.3%)
57	6	0.46	0/532	1.01	5/709 (0.7%)
58	w	0.32	0/68	0.98	0/103
All	All	0.55	23/164912 (0.0%)	1.17	1211/246067 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
2	b	0	2
5	e	0	1
10	j	0	2
11	k	0	1
12	l	0	2
13	m	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	o	0	1
18	r	0	2
25	z	0	3
26	A	2	0
28	C	0	1
33	I	0	2
34	H	0	3
36	K	0	1
38	M	0	1
44	S	0	1
46	U	0	2
55	3	0	1
All	All	4	28

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.71	1.48	1.61
22	v	1	C	OP3-P	-10.67	1.48	1.61
23	x	87	A	OP3-P	-10.65	1.48	1.61
1	a	2	A	OP3-P	-10.60	1.48	1.61
27	B	1	U	OP3-P	-10.57	1.48	1.61
26	A	1	G	OP3-P	-10.57	1.48	1.61
26	A	2169	A	C8-N7	-9.34	1.25	1.31
26	A	571	U	C4-O4	8.22	1.30	1.23
1	a	723	U	C4-O4	-6.98	1.18	1.23
26	A	2059	A	N9-C4	-6.42	1.34	1.37
26	A	1171	G	C6-N1	6.16	1.43	1.39
26	A	2167	U	N1-C2	-6.15	1.33	1.38
26	A	1085	A	N7-C5	-6.04	1.35	1.39
31	F	11	VAL	CB-CG1	-5.89	1.40	1.52
26	A	2169	A	N7-C5	-5.56	1.35	1.39
26	A	1313	U	N1-C2	5.49	1.43	1.38
24	y	61	C	C5-C6	-5.45	1.29	1.34
26	A	574	A	N9-C4	-5.16	1.34	1.37
26	A	1178	C	N3-C4	-5.09	1.30	1.33
26	A	101	A	N9-C4	-5.08	1.34	1.37
22	v	57	A	N7-C5	-5.07	1.36	1.39
26	A	278	A	N9-C4	5.03	1.40	1.37
1	a	80	A	N9-C4	-5.00	1.34	1.37

All (1211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	452	A	O5'-P-OP1	-19.89	86.83	110.70
1	a	450	G	O5'-P-OP1	16.99	131.09	110.70
26	A	1026	G	O5'-P-OP1	-15.92	91.37	105.70
26	A	2169	A	C5-N7-C8	15.84	111.82	103.90
26	A	1178	C	N1-C2-O2	15.82	128.39	118.90
26	A	1178	C	N3-C2-O2	-15.14	111.30	121.90
26	A	120	U	C5-C4-O4	-14.70	117.08	125.90
26	A	2059	A	N1-C2-N3	-14.28	122.16	129.30
26	A	890	C	N1-C2-O2	14.17	127.40	118.90
1	a	1158	C	N1-C2-O2	13.98	127.29	118.90
26	A	1171	G	N3-C2-N2	-13.97	110.12	119.90
26	A	120	U	N3-C4-O4	13.94	129.16	119.40
26	A	1313	U	N1-C2-O2	13.34	132.14	122.80
26	A	1071	G	C5-C6-O6	-13.14	120.72	128.60
1	a	1158	C	N3-C2-O2	-12.84	112.92	121.90
1	a	1304	G	O5'-P-OP2	-12.64	94.32	105.70
26	A	1313	U	N3-C2-O2	-12.56	113.41	122.20
24	y	47(I)	G	O5'-P-OP2	-12.20	94.72	105.70
26	A	2146	C	O5'-P-OP1	12.19	125.33	110.70
26	A	1186	G	O5'-P-OP2	12.09	125.20	110.70
1	a	1198	G	O5'-P-OP2	-11.90	94.99	105.70
24	y	61	C	C6-N1-C2	-11.44	115.72	120.30
26	A	1313	U	C2-N1-C1'	11.27	131.22	117.70
1	a	1197	A	O5'-P-OP1	-11.26	95.57	105.70
26	A	2109	U	C5-C6-N1	11.05	128.23	122.70
46	U	51	LEU	CA-CB-CG	10.88	140.32	115.30
23	x	117	C	N1-C2-O2	10.85	125.41	118.90
26	A	1093	G	C5-C6-O6	-10.75	122.15	128.60
26	A	2169	A	C4-C5-N7	-10.70	105.35	110.70
22	v	51	C	C6-N1-C2	-10.52	116.09	120.30
24	y	61	C	C4-C5-C6	10.45	122.62	117.40
24	y	61	C	N3-C4-C5	-10.39	117.74	121.90
24	y	41	C	C5-C6-N1	10.34	126.17	121.00
26	A	2305	U	C5-C4-O4	-10.29	119.72	125.90
24	y	47(D)	C	C6-N1-C2	-10.19	116.22	120.30
24	y	47(D)	C	C5-C6-N1	10.13	126.06	121.00
26	A	1071	G	N1-C6-O6	10.10	125.96	119.90
1	a	1054	C	O5'-P-OP2	-10.06	96.65	105.70
23	x	117	C	N3-C2-O2	-10.02	114.89	121.90
1	a	968	A	N1-C6-N6	-9.97	112.61	118.60
26	A	647	G	O5'-P-OP1	-9.92	96.77	105.70
1	a	1296	C	C6-N1-C2	-9.89	116.34	120.30
26	A	436	C	O5'-P-OP2	-9.84	96.84	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	51	C	C5-C6-N1	9.80	125.90	121.00
26	A	1993	U	N3-C2-O2	-9.78	115.35	122.20
26	A	2059	A	C6-N1-C2	9.73	124.44	118.60
26	A	1186	G	O5'-P-OP1	-9.71	96.96	105.70
26	A	887	U	N3-C2-O2	-9.71	115.41	122.20
26	A	2637	U	C5-C6-N1	9.70	127.55	122.70
26	A	2583	G	O5'-P-OP2	-9.70	96.97	105.70
24	y	48	G	N1-C6-O6	9.62	125.67	119.90
33	I	32	VAL	CG1-CB-CG2	-9.59	95.56	110.90
1	a	656	G	N3-C2-N2	-9.58	113.19	119.90
24	y	48	G	C5-C6-O6	-9.58	122.85	128.60
24	y	43	G	O4'-C1'-N9	9.54	115.83	108.20
26	A	67	U	C5-C4-O4	-9.48	120.21	125.90
26	A	1539	U	C5-C6-N1	9.46	127.43	122.70
26	A	1093	G	N9-C4-C5	-9.42	101.63	105.40
26	A	1079	C	N1-C2-O2	9.38	124.53	118.90
1	a	414	A	N1-C6-N6	-9.35	112.99	118.60
26	A	2147	A	C8-N9-C4	-9.34	102.06	105.80
1	a	597	G	O5'-P-OP2	-9.30	97.33	105.70
1	a	214	C	C5-C6-N1	9.29	125.65	121.00
1	a	1158	C	C6-N1-C2	-9.27	116.59	120.30
24	y	41	C	C6-N1-C2	-9.22	116.61	120.30
57	6	18	CYS	CA-CB-SG	-9.22	97.40	114.00
26	A	890	C	C2-N3-C4	9.16	124.48	119.90
26	A	2302	U	N3-C2-O2	-9.16	115.79	122.20
26	A	281	C	C5-C6-N1	9.15	125.58	121.00
1	a	214	C	C6-N1-C2	-9.14	116.64	120.30
24	y	47(N)	C	C6-N1-C2	-9.14	116.64	120.30
23	x	117	C	C6-N1-C2	-9.10	116.66	120.30
26	A	1783	A	O5'-P-OP2	-9.09	97.52	105.70
1	a	72	A	O5'-P-OP2	-9.08	97.53	105.70
1	a	1158	C	C2-N1-C1'	9.05	128.75	118.80
26	A	67	U	N3-C4-O4	9.03	125.72	119.40
26	A	545	U	C6-N1-C2	-9.03	115.58	121.00
23	x	125	G	N9-C1'-C2'	-9.02	102.07	112.00
26	A	2150	C	C6-N1-C2	-8.94	116.72	120.30
24	y	61	C	N1-C2-O2	8.94	124.27	118.90
26	A	2428	G	O5'-P-OP1	8.94	121.43	110.70
26	A	1171	G	N9-C4-C5	8.92	108.97	105.40
24	y	47(C)	C	C6-N1-C2	-8.87	116.75	120.30
26	A	2359	C	C6-N1-C2	-8.84	116.76	120.30
26	A	2617	U	N3-C2-O2	-8.79	116.04	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	62	C	N3-C2-O2	-8.79	115.75	121.90
26	A	2325	G	O5'-P-OP1	8.68	121.11	110.70
1	a	1241	G	C2-N3-C4	8.66	116.23	111.90
26	A	281	C	C6-N1-C2	-8.65	116.84	120.30
26	A	647	G	O5'-P-OP2	8.63	121.06	110.70
24	y	61	C	N3-C2-O2	-8.63	115.86	121.90
1	a	528	C	N1-C2-O2	8.60	124.06	118.90
26	A	887	U	N1-C2-O2	8.60	128.82	122.80
1	a	563	A	N9-C4-C5	-8.54	102.38	105.80
24	y	48	G	O4'-C1'-N9	-8.54	101.36	108.20
3	c	33	ASP	CB-CG-OD1	8.52	125.97	118.30
26	A	545	U	C5-C6-N1	8.49	126.95	122.70
24	y	73	G	C4-C5-N7	8.42	114.17	110.80
26	A	1042	G	P-O3'-C3'	8.40	129.78	119.70
1	a	1412	C	C6-N1-C2	-8.37	116.95	120.30
26	A	1104	C	C6-N1-C2	-8.35	116.96	120.30
26	A	546	U	C5-C6-N1	8.35	126.87	122.70
24	y	60	U	N1-C2-O2	-8.32	116.98	122.80
26	A	610	C	C6-N1-C2	-8.32	116.97	120.30
1	a	392	C	C6-N1-C2	-8.32	116.97	120.30
23	x	127	U	P-O3'-C3'	8.31	129.67	119.70
26	A	571	U	N3-C4-C5	-8.31	109.61	114.60
24	y	57	G	O5'-P-OP2	8.24	120.59	110.70
26	A	1093	G	C4-C5-N7	8.24	114.10	110.80
21	u	15	LEU	CA-CB-CG	8.23	134.23	115.30
1	a	1296	C	N1-C2-O2	8.22	123.83	118.90
1	a	972	C	C6-N1-C2	-8.22	117.01	120.30
24	y	30	G	N9-C4-C5	-8.21	102.12	105.40
27	B	24	G	C5-C6-O6	-8.19	123.69	128.60
26	A	2150	C	C5-C6-N1	8.18	125.09	121.00
25	z	328	ALA	N-CA-C	-8.18	88.92	111.00
26	A	1080	A	C8-N9-C4	-8.18	102.53	105.80
26	A	1076	C	C6-N1-C2	-8.14	117.05	120.30
26	A	2714	G	O5'-P-OP2	8.13	120.46	110.70
1	a	1296	C	C5-C6-N1	8.12	125.06	121.00
1	a	723	U	N3-C4-C5	8.12	119.47	114.60
26	A	2109	U	C6-N1-C2	-8.11	116.13	121.00
26	A	2502	G	O5'-P-OP2	8.11	120.43	110.70
26	A	1076	C	C5-C6-N1	8.07	125.04	121.00
15	o	30	LEU	CB-CG-CD2	-8.06	97.30	111.00
1	a	1397	C	C6-N1-C2	8.05	123.52	120.30
24	y	61	C	C2-N1-C1'	8.05	127.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2267	A	C2-N3-C4	8.05	114.63	110.60
26	A	2169	A	N7-C8-N9	-8.05	109.78	113.80
26	A	2147	A	N7-C8-N9	8.02	117.81	113.80
26	A	2109	U	C2-N3-C4	7.99	131.79	127.00
1	a	477	C	C6-N1-C2	-7.97	117.11	120.30
1	a	419	C	C6-N1-C2	-7.96	117.12	120.30
26	A	84	A	C8-N9-C4	7.96	108.98	105.80
26	A	2269	G	O5'-P-OP1	-7.93	98.56	105.70
1	a	799	G	N1-C6-O6	-7.92	115.15	119.90
24	y	61	C	N3-C4-N4	7.90	123.53	118.00
1	a	34	C	C6-N1-C2	-7.89	117.14	120.30
27	B	24	G	N1-C6-O6	7.89	124.63	119.90
1	a	1395	C	N1-C2-O2	7.88	123.63	118.90
26	A	2637	U	C6-N1-C2	-7.88	116.28	121.00
26	A	891	G	C5-C6-O6	-7.87	123.88	128.60
26	A	890	C	C4-C5-C6	-7.85	113.47	117.40
26	A	1047	G	O4'-C1'-N9	7.85	114.48	108.20
23	x	117	C	C2-N1-C1'	7.84	127.43	118.80
26	A	2466	C	O5'-P-OP1	-7.84	98.65	105.70
1	a	750	C	C6-N1-C2	-7.83	117.17	120.30
1	a	392	C	N1-C2-O2	7.82	123.59	118.90
26	A	1386	C	C5-C6-N1	7.79	124.90	121.00
26	A	962	G	O5'-P-OP1	-7.78	98.70	105.70
1	a	513	C	C6-N1-C2	-7.76	117.19	120.30
6	f	72	ASP	CB-CG-OD1	7.76	125.28	118.30
26	A	2758	A	N1-C6-N6	-7.75	113.95	118.60
26	A	669	G	N3-C4-C5	-7.74	124.73	128.60
26	A	885	C	C6-N1-C2	-7.73	117.21	120.30
26	A	1270	C	C5-C6-N1	7.73	124.86	121.00
26	A	883	G	C6-C5-N7	-7.72	125.77	130.40
26	A	1564	C	C5-C6-N1	7.72	124.86	121.00
26	A	2359	C	C5-C6-N1	7.72	124.86	121.00
26	A	1656	C	C5-C6-N1	7.71	124.86	121.00
26	A	2474	U	N3-C2-O2	-7.71	116.80	122.20
33	I	64	ARG	CA-CB-CG	7.71	130.35	113.40
26	A	546	U	C6-N1-C2	-7.70	116.38	121.00
13	m	57	ASP	CB-CG-OD1	7.68	125.21	118.30
1	a	1397	C	N3-C4-N4	-7.65	112.65	118.00
26	A	2166	U	C6-N1-C2	-7.64	116.42	121.00
1	a	924	C	C6-N1-C2	-7.64	117.25	120.30
26	A	2416	C	C5-C6-N1	7.64	124.82	121.00
26	A	571	U	C5-C4-O4	7.63	130.48	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1074	G	N3-C2-N2	-7.62	114.56	119.90
26	A	1656	C	C6-N1-C2	-7.62	117.25	120.30
1	a	754	C	C2-N1-C1'	7.61	127.17	118.80
7	g	139	ASP	CB-CG-OD1	7.61	125.14	118.30
1	a	492	C	C5-C6-N1	7.60	124.80	121.00
1	a	993	G	N9-C4-C5	-7.59	102.36	105.40
4	d	190	LEU	CB-CG-CD1	7.59	123.90	111.00
27	B	11	C	C6-N1-C2	-7.59	117.27	120.30
1	a	430	A	O5'-P-OP1	-7.58	98.88	105.70
1	a	993	G	N3-C4-N9	7.56	130.54	126.00
1	a	34	C	C5-C6-N1	7.56	124.78	121.00
26	A	1271	G	O4'-C1'-N9	7.55	114.24	108.20
26	A	2143	C	C6-N1-C2	-7.53	117.29	120.30
26	A	2896	C	C5-C6-N1	7.53	124.76	121.00
1	a	1034	G	C4-C5-N7	7.51	113.81	110.80
24	y	27	C	C6-N1-C2	-7.49	117.30	120.30
26	A	1171	G	N1-C2-N2	7.49	122.94	116.20
1	a	476	U	C5-C6-N1	7.47	126.44	122.70
24	y	30	G	N3-C4-N9	7.46	130.48	126.00
1	a	737	C	C6-N1-C2	-7.42	117.33	120.30
1	a	1102	A	N9-C4-C5	-7.42	102.83	105.80
26	A	231	A	N9-C4-C5	-7.42	102.83	105.80
26	A	53	A	C5-C6-N6	-7.41	117.77	123.70
26	A	647	G	OP1-P-OP2	-7.41	108.49	119.60
1	a	968	A	O5'-P-OP2	-7.41	99.03	105.70
26	A	890	C	N3-C4-N4	-7.40	112.82	118.00
26	A	1171	G	C6-N1-C2	-7.40	120.66	125.10
26	A	2165	C	O5'-P-OP2	-7.38	99.06	105.70
1	a	563	A	N1-C2-N3	-7.38	125.61	129.30
24	y	47	G	C8-N9-C4	-7.38	103.45	106.40
1	a	490	C	C6-N1-C2	-7.38	117.35	120.30
1	a	878	A	N9-C4-C5	-7.38	102.85	105.80
1	a	1034	G	N9-C4-C5	-7.38	102.45	105.40
26	A	2562	U	N3-C2-O2	-7.37	117.04	122.20
1	a	180	U	C5-C6-N1	7.36	126.38	122.70
26	A	1665	A	O5'-P-OP2	-7.35	99.09	105.70
26	A	669	G	N3-C4-N9	7.34	130.40	126.00
26	A	1982	U	O5'-P-OP2	-7.34	99.09	105.70
1	a	1263	C	C5-C6-N1	7.33	124.67	121.00
1	a	1397	C	N3-C4-C5	7.33	124.83	121.90
14	n	32	ASP	CB-CG-OD1	7.33	124.90	118.30
26	A	1079	C	N3-C2-O2	-7.33	116.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	575	G	N3-C2-N2	-7.32	114.77	119.90
1	a	1027	C	N1-C2-O2	7.30	123.28	118.90
1	a	1262	C	N1-C2-O2	7.29	123.28	118.90
26	A	813	U	N3-C2-O2	-7.29	117.10	122.20
26	A	2473	U	N3-C2-O2	-7.28	117.10	122.20
24	y	59	C	C5-C6-N1	7.27	124.64	121.00
25	z	398	LEU	CA-CB-CG	7.26	132.01	115.30
26	A	2746	U	C5-C6-N1	7.26	126.33	122.70
27	B	60	C	C6-N1-C2	-7.26	117.40	120.30
26	A	1171	G	N3-C4-N9	-7.26	121.65	126.00
26	A	2582	G	OP2-P-O3'	7.25	121.16	105.20
1	a	1071	C	C6-N1-C2	-7.25	117.40	120.30
2	b	81	ASP	CB-CG-OD1	7.24	124.82	118.30
26	A	1386	C	C6-N1-C2	-7.24	117.41	120.30
1	a	1148	U	N3-C2-O2	-7.24	117.14	122.20
24	y	59	C	C6-N1-C2	-7.22	117.41	120.30
24	y	47(B)	G	N7-C8-N9	7.21	116.71	113.10
26	A	1060	U	O5'-P-OP1	-7.20	99.22	105.70
1	a	1493	A	N1-C2-N3	-7.20	125.70	129.30
1	a	620	C	N1-C2-O2	7.19	123.21	118.90
1	a	472	U	C5-C6-N1	7.16	126.28	122.70
26	A	2161	C	N1-C2-O2	-7.15	114.61	118.90
26	A	1476	U	N3-C2-O2	-7.13	117.20	122.20
1	a	217	C	C5-C6-N1	7.13	124.57	121.00
1	a	414	A	C2-N3-C4	7.12	114.16	110.60
26	A	2110	G	N3-C4-N9	-7.12	121.73	126.00
1	a	419	C	N3-C2-O2	-7.11	116.92	121.90
26	A	1080	A	N7-C8-N9	7.11	117.36	113.80
24	y	47(P)	C	C6-N1-C2	-7.11	117.46	120.30
31	F	88	VAL	CG1-CB-CG2	-7.11	99.52	110.90
1	a	80	A	C6-N1-C2	7.11	122.86	118.60
1	a	477	C	C5-C6-N1	7.10	124.55	121.00
24	y	47(N)	C	C5-C6-N1	7.10	124.55	121.00
27	B	60	C	C5-C6-N1	7.10	124.55	121.00
50	Y	49	ASP	CB-CG-OD1	7.08	124.67	118.30
24	y	55	PSU	P-O3'-C3'	7.07	128.19	119.70
1	a	163	C	C6-N1-C2	-7.07	117.47	120.30
1	a	392	C	C5-C6-N1	7.07	124.53	121.00
26	A	183	C	N1-C2-O2	7.07	123.14	118.90
30	E	82	GLY	N-CA-C	7.07	130.76	113.10
1	a	397	A	C2-N3-C4	7.06	114.13	110.60
22	v	39	C	C5-C6-N1	7.05	124.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1202	U	N3-C2-O2	-7.05	117.27	122.20
1	a	397	A	N3-C4-N9	7.04	133.03	127.40
1	a	409	U	C5-C6-N1	7.04	126.22	122.70
26	A	1074	G	N1-C2-N2	7.03	122.53	116.20
1	a	512	U	C5-C6-N1	7.03	126.21	122.70
24	y	30	G	C6-C5-N7	-7.01	126.19	130.40
1	a	492	C	C6-N1-C2	-7.00	117.50	120.30
24	y	47(C)	C	C5-C6-N1	6.97	124.49	121.00
23	x	126	G	P-O3'-C3'	6.97	128.06	119.70
26	A	114	U	N1-C2-O2	6.97	127.68	122.80
26	A	79	C	C6-N1-C2	-6.96	117.52	120.30
25	z	328	ALA	N-CA-CB	6.94	119.82	110.10
1	a	392	C	C2-N1-C1'	6.93	126.43	118.80
24	y	73	G	N9-C4-C5	-6.93	102.63	105.40
26	A	1936	A	N1-C6-N6	-6.92	114.45	118.60
26	A	1313	U	C6-N1-C1'	-6.91	111.52	121.20
26	A	2442	C	N1-C2-O2	6.91	123.05	118.90
26	A	1071	G	N9-C4-C5	-6.91	102.64	105.40
31	F	11	VAL	CG1-CB-CG2	-6.90	99.86	110.90
26	A	2474	U	N1-C2-O2	6.89	127.62	122.80
25	z	445	LEU	CB-CG-CD2	-6.88	99.30	111.00
26	A	1104	C	C5-C6-N1	6.87	124.43	121.00
26	A	2195	U	N3-C2-O2	-6.87	117.39	122.20
26	A	53	A	N1-C6-N6	6.86	122.71	118.60
1	a	1448	C	N1-C2-O2	6.85	123.01	118.90
26	A	2636	C	N1-C2-O2	6.85	123.01	118.90
26	A	445	C	N3-C2-O2	-6.85	117.11	121.90
26	A	2755	C	N1-C2-O2	6.85	123.01	118.90
26	A	1294	U	N3-C2-O2	-6.83	117.42	122.20
26	A	883	G	N7-C8-N9	6.83	116.52	113.10
24	y	48	G	C4-C5-N7	6.83	113.53	110.80
1	a	1296	C	N3-C2-O2	-6.82	117.12	121.90
26	A	884	U	N1-C2-N3	6.82	118.99	114.90
22	v	32	C	N1-C2-O2	6.82	122.99	118.90
33	I	79	LEU	CB-CG-CD2	-6.82	99.41	111.00
1	a	868	C	C6-N1-C2	-6.82	117.57	120.30
22	v	50	U	C5-C6-N1	6.82	126.11	122.70
26	A	2167	U	N1-C2-O2	-6.82	118.03	122.80
1	a	1034	G	N1-C6-O6	6.81	123.99	119.90
24	y	40	C	C5-C6-N1	6.81	124.41	121.00
24	y	47(G)	C	N1-C2-O2	-6.81	114.81	118.90
1	a	88	U	C6-N1-C2	-6.81	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	x	118	G	N7-C8-N9	6.81	116.50	113.10
44	S	64	ALA	N-CA-CB	6.80	119.62	110.10
1	a	1263	C	C6-N1-C2	-6.80	117.58	120.30
26	A	2326	C	C6-N1-C2	-6.79	117.58	120.30
26	A	2512	C	C6-N1-C2	-6.79	117.58	120.30
27	B	120	U	N3-C2-O2	-6.79	117.45	122.20
1	a	407	U	O5'-P-OP2	6.78	118.84	110.70
26	A	2069	G7M	P-O3'-C3'	6.77	127.82	119.70
26	A	84	A	N7-C8-N9	-6.75	110.42	113.80
26	A	140	C	C6-N1-C2	-6.75	117.60	120.30
1	a	428	G	N3-C4-N9	-6.72	121.97	126.00
26	A	1071	G	C4-C5-N7	6.72	113.49	110.80
1	a	429	U	OP1-P-O3'	6.71	119.97	105.20
26	A	546	U	N3-C2-O2	-6.71	117.50	122.20
27	B	55	U	N3-C2-O2	-6.71	117.51	122.20
1	a	923	A	N7-C8-N9	6.71	117.15	113.80
26	A	283	G	N3-C2-N2	-6.69	115.22	119.90
24	y	20	G	C2-N3-C4	-6.69	108.56	111.90
1	a	526	C	C6-N1-C2	-6.68	117.63	120.30
26	A	2080	A	N9-C4-C5	-6.68	103.13	105.80
1	a	407	U	C6-N1-C2	-6.67	117.00	121.00
23	x	133	C	C6-N1-C2	-6.67	117.63	120.30
24	y	48	G	N9-C4-C5	-6.67	102.73	105.40
26	A	2574	G	O5'-P-OP1	6.67	118.71	110.70
26	A	2163	A	O5'-P-OP1	6.66	118.70	110.70
27	B	57	A	N7-C8-N9	6.66	117.13	113.80
26	A	8	C	C5-C6-N1	6.66	124.33	121.00
26	A	2267	A	N1-C6-N6	-6.66	114.60	118.60
1	a	1344	C	C6-N1-C2	-6.64	117.64	120.30
1	a	1466	C	N3-C2-O2	-6.63	117.25	121.90
26	A	1178	C	C6-N1-C2	-6.63	117.65	120.30
22	v	19	G	O4'-C1'-N9	-6.62	102.90	108.20
26	A	890	C	N3-C2-O2	-6.62	117.27	121.90
1	a	397	A	N9-C4-C5	-6.62	103.15	105.80
1	a	1105	A	N9-C4-C5	-6.62	103.15	105.80
22	v	32	C	N3-C2-O2	-6.62	117.27	121.90
26	A	208	C	C5-C6-N1	6.62	124.31	121.00
1	a	88	U	C5-C6-N1	6.61	126.01	122.70
26	A	528	A	N7-C8-N9	6.61	117.11	113.80
26	A	1664	A	O5'-P-OP1	6.61	118.63	110.70
26	A	1083	U	N1-C2-O2	-6.60	118.18	122.80
1	a	1037	C	C6-N1-C2	-6.60	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	42	C	N1-C2-O2	6.60	122.86	118.90
26	A	528	A	C8-N9-C4	-6.60	103.16	105.80
1	a	1393	U	N3-C2-O2	-6.60	117.58	122.20
26	A	642	U	C6-N1-C2	-6.60	117.04	121.00
26	A	399	U	N3-C2-O2	-6.60	117.58	122.20
1	a	443	C	C5-C6-N1	6.59	124.30	121.00
1	a	1109	C	N1-C2-O2	6.59	122.85	118.90
1	a	993	G	C6-C5-N7	-6.59	126.45	130.40
26	A	889	C	N1-C2-O2	6.59	122.85	118.90
23	x	109	C	C6-N1-C2	-6.58	117.67	120.30
26	A	1313	U	C5-C6-N1	6.58	125.99	122.70
1	a	1497	G	N3-C4-N9	6.58	129.95	126.00
24	y	72	C	C2-N1-C1'	6.58	126.03	118.80
1	a	136	C	C2-N1-C1'	6.57	126.02	118.80
1	a	527	G7M	P-O3'-C3'	6.57	127.58	119.70
1	a	611	C	N1-C2-O2	6.57	122.84	118.90
26	A	2626	C	C5-C6-N1	6.56	124.28	121.00
1	a	592	G	C8-N9-C4	-6.56	103.78	106.40
26	A	534	U	C5-C6-N1	6.56	125.98	122.70
1	a	536	C	C6-N1-C2	-6.56	117.68	120.30
26	A	1093	G	C8-N9-C4	6.55	109.02	106.40
1	a	1109	C	C6-N1-C2	-6.55	117.68	120.30
26	A	837	C	N3-C2-O2	-6.55	117.31	121.90
1	a	1195	C	C6-N1-C2	-6.55	117.68	120.30
26	A	231	A	C8-N9-C4	6.55	108.42	105.80
26	A	806	C	C6-N1-C2	-6.54	117.69	120.30
26	A	1072	C	O5'-P-OP2	-6.54	99.81	105.70
1	a	620	C	N3-C2-O2	-6.53	117.33	121.90
26	A	1075	C	N1-C2-O2	6.53	122.82	118.90
26	A	1093	G	N1-C6-O6	6.53	123.82	119.90
26	A	1669	A	N3-C4-N9	6.51	132.61	127.40
1	a	563	A	C4-C5-N7	6.51	113.95	110.70
26	A	2502	G	O5'-P-OP1	-6.50	99.85	105.70
26	A	1064	C	N1-C2-O2	-6.50	115.00	118.90
1	a	136	C	N1-C2-O2	6.50	122.80	118.90
1	a	418	C	C6-N1-C2	-6.49	117.70	120.30
1	a	1427	C	C6-N1-C2	-6.49	117.70	120.30
26	A	2162	G	N1-C6-O6	-6.49	116.01	119.90
1	a	513	C	C5-C6-N1	6.49	124.24	121.00
1	a	1517	G	N3-C2-N2	-6.47	115.37	119.90
26	A	1075	C	C2-N1-C1'	6.47	125.92	118.80
27	B	37	C	N1-C2-O2	6.47	122.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	90	C	C6-N1-C2	-6.47	117.71	120.30
26	A	445	C	N1-C2-O2	6.47	122.78	118.90
26	A	571	U	C4-C5-C6	6.47	123.58	119.70
1	a	661	G	N9-C4-C5	-6.46	102.81	105.40
26	A	2060	A	OP2-P-O3'	6.45	119.39	105.20
1	a	1469	C	N1-C2-O2	6.45	122.77	118.90
56	4	14	CYS	CA-CB-SG	6.45	125.60	114.00
26	A	1956	U	N3-C2-O2	-6.44	117.69	122.20
23	x	109	C	C5-C6-N1	6.44	124.22	121.00
1	a	475	C	C6-N1-C2	-6.43	117.73	120.30
26	A	1056	G	N1-C6-O6	6.43	123.76	119.90
26	A	2702	G	N1-C6-O6	-6.43	116.05	119.90
1	a	656	G	C6-N1-C2	-6.42	121.25	125.10
26	A	183	C	N3-C2-O2	-6.42	117.40	121.90
24	y	30	G	C8-N9-C1'	-6.42	118.65	127.00
26	A	2188	U	C5-C6-N1	6.42	125.91	122.70
1	a	493	A	C8-N9-C4	-6.42	103.23	105.80
1	a	449	G	C4-C5-N7	6.41	113.37	110.80
1	a	744	C	C5-C6-N1	6.41	124.21	121.00
26	A	669	G	C2-N3-C4	6.41	115.11	111.90
26	A	1294	U	N1-C2-O2	6.41	127.29	122.80
1	a	217	C	C6-N1-C2	-6.41	117.74	120.30
1	a	1027	C	C5-C6-N1	6.41	124.20	121.00
26	A	560	C	C5-C6-N1	6.41	124.20	121.00
26	A	891	G	C6-C5-N7	-6.41	126.56	130.40
1	a	963	G	N3-C2-N2	-6.40	115.42	119.90
26	A	1064	C	C6-N1-C2	-6.40	117.74	120.30
33	I	64	ARG	N-CA-CB	-6.39	99.10	110.60
26	A	646	U	OP2-P-O3'	6.39	119.25	105.20
26	A	615	U	C5-C4-O4	-6.39	122.07	125.90
23	x	124	A	N9-C4-C5	-6.38	103.25	105.80
1	a	110	C	N1-C2-O2	6.38	122.73	118.90
1	a	723	U	N1-C2-O2	6.38	127.27	122.80
23	x	104	U	N3-C2-O2	-6.38	117.74	122.20
26	A	399	U	N1-C2-O2	6.37	127.26	122.80
26	A	783	A	C2-N3-C4	6.37	113.79	110.60
26	A	1059	G	C5-C6-O6	-6.37	124.78	128.60
26	A	891	G	N3-C4-N9	6.37	129.82	126.00
1	a	896	C	C5-C6-N1	6.37	124.18	121.00
24	y	56	C	C6-N1-C2	-6.37	117.75	120.30
26	A	1075	C	N3-C2-O2	-6.36	117.45	121.90
26	A	1348	C	N1-C2-O2	6.36	122.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	20	G	N1-C2-N3	6.36	127.72	123.90
26	A	114	U	N3-C2-O2	-6.36	117.75	122.20
1	a	419	C	C6-N1-C1'	6.36	128.43	120.80
26	A	2110	G	C5-C6-O6	6.36	132.41	128.60
24	y	47(K)	G	N3-C4-C5	6.36	131.78	128.60
1	a	307	C	N1-C2-O2	6.35	122.71	118.90
1	a	1326	U	N3-C2-O2	-6.35	117.76	122.20
24	y	65	U	O5'-P-OP1	-6.34	99.99	105.70
26	A	2011	U	N3-C2-O2	-6.34	117.76	122.20
1	a	1202	U	N1-C2-O2	6.34	127.24	122.80
26	A	2305	U	C6-N1-C2	6.34	124.80	121.00
26	A	1025	G	OP1-P-O3'	6.33	119.13	105.20
1	a	754	C	C6-N1-C1'	-6.33	113.20	120.80
1	a	868	C	C5-C6-N1	6.33	124.17	121.00
1	a	1404	C	N1-C2-O2	6.33	122.69	118.90
1	a	968	A	C5-C6-N6	6.32	128.75	123.70
26	A	2840	C	C5-C6-N1	6.32	124.16	121.00
27	B	26	C	N3-C2-O2	-6.32	117.48	121.90
26	A	2160	C	C6-N1-C2	-6.31	117.78	120.30
1	a	177	G	N3-C4-C5	-6.31	125.45	128.60
26	A	2267	A	N1-C2-N3	-6.30	126.15	129.30
26	A	1669	A	N9-C4-C5	-6.30	103.28	105.80
24	y	48	G	C6-C5-N7	-6.29	126.62	130.40
8	h	95	MET	CA-CB-CG	6.29	124.00	113.30
26	A	1539	U	C5-C4-O4	-6.29	122.12	125.90
1	a	177	G	C2-N3-C4	6.29	115.05	111.90
26	A	1101	U	N3-C2-O2	-6.29	117.80	122.20
1	a	1066	C	N3-C2-O2	-6.29	117.50	121.90
2	b	134	LEU	CA-CB-CG	6.29	129.76	115.30
26	A	1200	C	C6-N1-C2	-6.29	117.79	120.30
26	A	1178	C	C5-C4-N4	6.28	124.60	120.20
26	A	2691	C	C5-C6-N1	6.28	124.14	121.00
27	B	49	C	C6-N1-C2	-6.28	117.79	120.30
26	A	2394	C	C6-N1-C2	-6.28	117.79	120.30
25	z	559	ASP	CB-CG-OD1	6.28	123.95	118.30
1	a	1412	C	C5-C6-N1	6.27	124.14	121.00
26	A	1096	A	C8-N9-C4	-6.27	103.29	105.80
26	A	2442	C	N3-C2-O2	-6.27	117.51	121.90
1	a	1302	C	C6-N1-C2	6.26	122.80	120.30
1	a	979	C	N1-C2-O2	6.26	122.65	118.90
26	A	898	C	C6-N1-C2	-6.25	117.80	120.30
1	a	1302	C	OP1-P-O3'	-6.25	91.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	26	C	N1-C2-O2	6.25	122.65	118.90
26	A	357	C	C6-N1-C2	-6.25	117.80	120.30
26	A	1313	U	C6-N1-C2	-6.24	117.26	121.00
11	k	96	ILE	CG1-CB-CG2	-6.24	97.68	111.40
27	B	26	C	C6-N1-C2	-6.24	117.81	120.30
26	A	1787	A	N9-C4-C5	-6.24	103.31	105.80
26	A	140	C	C5-C6-N1	6.23	124.11	121.00
26	A	2572	A	O5'-P-OP1	-6.22	100.10	105.70
26	A	234	U	N3-C2-O2	-6.22	117.85	122.20
26	A	1101	U	N1-C2-O2	6.21	127.15	122.80
26	A	1012	U	N1-C2-O2	-6.20	118.46	122.80
1	a	977	A	C2-N3-C4	6.20	113.70	110.60
26	A	2394	C	N1-C2-O2	6.20	122.62	118.90
23	x	129	U	O4'-C1'-N1	6.20	113.16	108.20
26	A	1096	A	N7-C8-N9	6.18	116.89	113.80
26	A	2044	C	C6-N1-C2	-6.18	117.83	120.30
1	a	516	PSU	O3'-P-O5'	-6.17	92.28	104.00
1	a	795	C	C6-N1-C2	-6.17	117.83	120.30
4	d	189	ASP	CB-CG-OD1	6.16	123.84	118.30
1	a	989	U	N3-C2-O2	-6.16	117.89	122.20
1	a	1296	C	C2-N1-C1'	6.15	125.57	118.80
1	a	660	C	C5-C6-N1	6.14	124.07	121.00
1	a	180	U	C6-N1-C2	-6.14	117.32	121.00
26	A	231	A	C5-C6-N6	-6.14	118.79	123.70
26	A	444	C	C6-N1-C2	-6.14	117.84	120.30
26	A	1611	C	C6-N1-C2	-6.14	117.85	120.30
23	x	121	U	N3-C2-O2	-6.13	117.91	122.20
26	A	1075	C	C6-N1-C2	-6.13	117.85	120.30
24	y	30	G	N1-C6-O6	6.12	123.58	119.90
26	A	2617	U	N1-C2-O2	6.12	127.09	122.80
1	a	1497	G	N3-C4-C5	-6.12	125.54	128.60
26	A	2043	C	C2-N1-C1'	6.12	125.53	118.80
1	a	397	A	N1-C2-N3	-6.12	126.24	129.30
26	A	891	G	N1-C6-O6	6.11	123.57	119.90
23	x	118	G	C6-C5-N7	-6.11	126.73	130.40
26	A	1021	A	C2-N3-C4	6.11	113.66	110.60
1	a	1493	A	C6-N1-C2	6.10	122.26	118.60
24	y	47(D)	C	C2-N3-C4	6.10	122.95	119.90
23	x	104	U	O4'-C1'-N1	6.10	113.08	108.20
26	A	1171	G	C4-C5-N7	-6.09	108.36	110.80
1	a	1284	C	C6-N1-C2	-6.08	117.87	120.30
24	y	45	U	P-O3'-C3'	6.08	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2103	C	N3-C2-O2	-6.08	117.64	121.90
26	A	2766	A	N9-C4-C5	-6.08	103.37	105.80
24	y	50	C	C5-C6-N1	6.08	124.04	121.00
1	a	1109	C	N3-C2-O2	-6.08	117.65	121.90
24	y	40	C	C6-N1-C2	-6.08	117.87	120.30
1	a	679	C	C6-N1-C2	-6.07	117.87	120.30
24	y	56	C	C5-C6-N1	6.07	124.03	121.00
1	a	993	G	C4-C5-N7	6.06	113.23	110.80
26	A	2755	C	N3-C2-O2	-6.06	117.66	121.90
26	A	889	C	N3-C2-O2	-6.06	117.66	121.90
3	c	117	ASP	CB-CG-OD1	6.05	123.75	118.30
1	a	1466	C	N1-C2-O2	6.05	122.53	118.90
23	x	129	U	N3-C2-O2	-6.05	117.97	122.20
26	A	283	G	C6-C5-N7	6.05	134.03	130.40
1	a	1195	C	C5-C6-N1	6.04	124.02	121.00
1	a	536	C	C5-C6-N1	6.03	124.02	121.00
23	x	108	A	O4'-C1'-N9	6.03	113.02	108.20
26	A	1181	U	N3-C2-O2	-6.03	117.98	122.20
24	y	16	C	C6-N1-C1'	6.02	128.03	120.80
22	v	36	U	N3-C2-O2	-6.02	117.99	122.20
26	A	1056	G	C5-C6-O6	-6.01	124.99	128.60
22	v	51	C	C2-N1-C1'	6.01	125.41	118.80
26	A	198	C	C5-C6-N1	6.00	124.00	121.00
24	y	30	G	C4-C5-N7	6.00	113.20	110.80
1	a	207	C	C6-N1-C2	-6.00	117.90	120.30
26	A	1723	G	N1-C6-O6	-5.99	116.31	119.90
1	a	438	U	O4'-C1'-N1	5.99	112.99	108.20
1	a	968	A	O4'-C1'-N9	5.99	112.99	108.20
26	A	1279	G	C4-C5-N7	5.99	113.19	110.80
23	x	131	C	O4'-C1'-N1	5.98	112.99	108.20
1	a	799	G	C2-N3-C4	5.98	114.89	111.90
1	a	1393	U	N1-C2-O2	5.98	126.98	122.80
26	A	435	C	OP1-P-OP2	-5.98	110.63	119.60
1	a	464	U	C5-C6-N1	5.97	125.69	122.70
24	y	46	G	N3-C2-N2	-5.97	115.72	119.90
26	A	2837	A	O5'-P-OP2	-5.97	100.33	105.70
1	a	1326	U	N1-C2-O2	5.97	126.98	122.80
1	a	52	C	C6-N1-C2	-5.96	117.91	120.30
1	a	1262	C	N3-C2-O2	-5.96	117.73	121.90
1	a	968	A	N9-C4-C5	5.96	108.19	105.80
1	a	612	C	N1-C2-O2	5.96	122.47	118.90
26	A	1348	C	C6-N1-C2	-5.96	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	980	C	C6-N1-C2	-5.95	117.92	120.30
12	l	80	LEU	CA-CB-CG	5.95	128.99	115.30
24	y	56	C	OP2-P-O3'	-5.95	92.11	105.20
26	A	1092	C	N1-C2-O2	5.95	122.47	118.90
1	a	354	G	N9-C4-C5	-5.95	103.02	105.40
26	A	2160	C	N3-C2-O2	-5.95	117.74	121.90
49	X	21	LEU	CA-CB-CG	5.94	128.97	115.30
26	A	2394	C	N3-C2-O2	-5.94	117.74	121.90
26	A	1585	C	N1-C2-O2	5.93	122.46	118.90
26	A	2162	G	C5-C6-O6	5.93	132.16	128.60
26	A	2473	U	N1-C2-O2	5.93	126.95	122.80
23	x	128	C	C3'-C2'-C1'	5.92	106.24	101.50
27	B	120	U	N1-C2-O2	5.92	126.95	122.80
23	x	101	A	N1-C2-N3	-5.92	126.34	129.30
26	A	2179	C	C6-N1-C2	-5.92	117.93	120.30
26	A	1775	U	N3-C2-O2	-5.92	118.06	122.20
1	a	578	C	C6-N1-C2	-5.91	117.93	120.30
22	v	34	C	N1-C2-O2	5.91	122.45	118.90
1	a	423	G	C5-C6-O6	-5.91	125.05	128.60
1	a	16	A	C6-N1-C2	5.91	122.14	118.60
24	y	43	G	C4-N9-C1'	-5.90	118.83	126.50
1	a	1027	C	C6-N1-C2	-5.90	117.94	120.30
1	a	1448	C	C2-N1-C1'	5.90	125.29	118.80
26	A	231	A	C4-C5-N7	5.90	113.65	110.70
1	a	528	C	C2-N1-C1'	5.90	125.28	118.80
26	A	130	C	C6-N1-C2	-5.89	117.94	120.30
26	A	687	C	N1-C2-O2	5.89	122.44	118.90
1	a	494	G	C5-C6-O6	-5.89	125.06	128.60
1	a	483	C	C6-N1-C2	-5.89	117.94	120.30
26	A	890	C	C5-C4-N4	5.88	124.32	120.20
26	A	2550	G	O5'-P-OP1	-5.88	100.40	105.70
26	A	885	C	C5-C6-N1	5.88	123.94	121.00
1	a	368	U	N3-C2-O2	-5.88	118.09	122.20
1	a	346	G	C2-N3-C4	5.87	114.84	111.90
11	k	112	VAL	CA-CB-CG1	5.87	119.71	110.90
27	B	49	C	C5-C6-N1	5.87	123.94	121.00
26	A	560	C	C6-N1-C2	-5.86	117.96	120.30
1	a	166	U	N3-C2-O2	-5.86	118.10	122.20
26	A	1093	G	N3-C4-N9	5.85	129.51	126.00
27	B	37	C	N3-C2-O2	-5.85	117.80	121.90
1	a	1162	C	C6-N1-C2	-5.85	117.96	120.30
24	y	48	G	C8-N9-C1'	-5.85	119.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	234	U	N1-C2-O2	5.85	126.89	122.80
26	A	257	C	C6-N1-C2	-5.85	117.96	120.30
1	a	188	C	C6-N1-C2	-5.85	117.96	120.30
1	a	400	C	C5-C6-N1	5.85	123.92	121.00
26	A	1171	G	C8-N9-C4	-5.85	104.06	106.40
1	a	923	A	C6-C5-N7	-5.84	128.21	132.30
25	z	257	LEU	CA-CB-CG	5.84	128.74	115.30
1	a	808	C	C6-N1-C2	-5.84	117.96	120.30
26	A	302	C	C6-N1-C2	-5.84	117.96	120.30
26	A	397	U	C5-C6-N1	5.84	125.62	122.70
26	A	2254	C	N1-C2-O2	5.84	122.40	118.90
1	a	346	G	N3-C4-N9	5.84	129.50	126.00
26	A	1063	G	N3-C4-C5	-5.84	125.68	128.60
1	a	1455	G	N3-C4-N9	5.83	129.50	126.00
26	A	1494	A	N7-C8-N9	5.83	116.72	113.80
44	S	64	ALA	N-CA-C	-5.83	95.25	111.00
24	y	47(G)	C	C6-N1-C2	-5.83	117.97	120.30
24	y	47(B)	G	C8-N9-C4	-5.83	104.07	106.40
26	A	2649	C	C5-C6-N1	5.82	123.91	121.00
1	a	82	G	N3-C4-N9	5.82	129.49	126.00
1	a	879	C	N1-C2-O2	5.82	122.39	118.90
26	A	2606	C	C6-N1-C2	-5.82	117.97	120.30
24	y	27	C	C5-C6-N1	5.82	123.91	121.00
26	A	1049	C	N3-C4-N4	-5.81	113.93	118.00
23	x	130	G	N7-C8-N9	5.81	116.01	113.10
1	a	497	G	N3-C2-N2	-5.81	115.83	119.90
1	a	582	C	C6-N1-C2	-5.81	117.98	120.30
1	a	658	C	N1-C2-O2	5.81	122.39	118.90
1	a	1382	C	N1-C2-O2	5.81	122.39	118.90
26	A	2292	U	C5-C6-N1	5.81	125.60	122.70
1	a	735	C	C6-N1-C2	-5.80	117.98	120.30
22	v	57	A	C5-N7-C8	5.80	106.80	103.90
26	A	1993	U	N1-C2-O2	5.80	126.86	122.80
26	A	2896	C	C6-N1-C2	-5.80	117.98	120.30
1	a	679	C	C5-C6-N1	5.80	123.90	121.00
26	A	383	C	N1-C2-O2	5.80	122.38	118.90
26	A	1081	U	C6-N1-C2	-5.80	117.52	121.00
1	a	980	C	N3-C2-O2	-5.80	117.84	121.90
1	a	684	U	N3-C2-O2	-5.79	118.14	122.20
26	A	229	C	C6-N1-C2	-5.79	117.98	120.30
26	A	1113	U	N3-C2-O2	-5.79	118.14	122.20
26	A	1113	U	N1-C2-O2	5.79	126.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	876	C	C6-N1-C2	-5.79	117.98	120.30
26	A	889	C	C6-N1-C2	-5.79	117.98	120.30
26	A	668	A	N9-C4-C5	-5.79	103.48	105.80
26	A	1314	C	C6-N1-C2	-5.79	117.98	120.30
23	x	118	G	N3-C4-N9	5.79	129.47	126.00
1	a	556	C	C5-C6-N1	5.78	123.89	121.00
24	y	57	G	N1-C2-N2	5.78	121.41	116.20
26	A	1103	A	C2-N3-C4	5.78	113.49	110.60
26	A	2120	G	O5'-P-OP1	-5.78	100.49	105.70
1	a	1494	G	O5'-P-OP1	-5.78	100.50	105.70
24	y	15	C	N1-C2-O2	5.78	122.37	118.90
1	a	90	C	C5-C6-N1	5.78	123.89	121.00
25	z	26	ASP	CB-CG-OD1	5.77	123.50	118.30
26	A	1539	U	N3-C4-O4	5.77	123.44	119.40
26	A	2310	C	N1-C2-O2	5.77	122.36	118.90
24	y	73	G	N1-C6-O6	5.77	123.36	119.90
26	A	2147	A	O5'-P-OP1	-5.77	100.51	105.70
32	G	70	LEU	CA-CB-CG	5.77	128.57	115.30
24	y	56	C	C2-N1-C1'	5.76	125.14	118.80
26	A	2305	U	N3-C4-C5	5.76	118.06	114.60
26	A	2146	C	OP1-P-O3'	-5.76	92.52	105.20
26	A	2215	C	C6-N1-C2	-5.76	118.00	120.30
23	x	115	A	O4'-C1'-N9	-5.76	103.59	108.20
24	y	31	A	OP2-P-O3'	5.76	117.87	105.20
1	a	1034	G	C5-C6-O6	-5.76	125.15	128.60
24	y	47(D)	C	N1-C2-O2	5.75	122.35	118.90
26	A	1905	C	N1-C2-O2	5.75	122.35	118.90
26	A	1494	A	C8-N9-C4	-5.75	103.50	105.80
26	A	1760	C	N1-C2-O2	5.75	122.35	118.90
23	x	126	G	N1-C2-N2	-5.74	111.03	116.20
1	a	1226	C	N3-C2-O2	-5.74	117.88	121.90
24	y	30	G	C5-C6-O6	-5.74	125.16	128.60
26	A	1267	U	N3-C2-O2	-5.74	118.18	122.20
26	A	1380	G	N3-C4-N9	5.74	129.44	126.00
27	B	30	C	C6-N1-C2	-5.74	118.00	120.30
26	A	1054	A	O4'-C1'-N9	5.74	112.79	108.20
1	a	656	G	N9-C4-C5	5.74	107.69	105.40
1	a	1378	C	N1-C2-O2	5.74	122.34	118.90
57	6	40	CYS	N-CA-CB	5.74	120.92	110.60
22	v	32	C	C6-N1-C2	-5.73	118.01	120.30
26	A	1279	G	N9-C4-C5	-5.73	103.11	105.40
1	a	491	G	C8-N9-C1'	-5.73	119.55	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	689	C	C6-N1-C2	-5.73	118.01	120.30
26	A	1270	C	C6-N1-C2	-5.73	118.01	120.30
1	a	866	C	C5-C6-N1	5.72	123.86	121.00
1	a	575	G	N9-C4-C5	5.72	107.69	105.40
24	y	1	G	N9-C4-C5	-5.71	103.11	105.40
26	A	2804	U	N3-C2-O2	-5.71	118.20	122.20
1	a	330	C	N1-C2-O2	5.71	122.33	118.90
1	a	1197	A	N9-C4-C5	-5.71	103.52	105.80
26	A	1565	C	C6-N1-C2	-5.71	118.02	120.30
26	A	2043	C	N1-C2-O2	5.71	122.33	118.90
1	a	1536	C	C6-N1-C2	-5.71	118.02	120.30
26	A	1582	C	C6-N1-C2	-5.71	118.02	120.30
26	A	2103	C	N1-C2-O2	5.71	122.33	118.90
24	y	43	G	C8-N9-C1'	5.71	134.42	127.00
24	y	65	U	OP2-P-O3'	5.71	117.75	105.20
26	A	1083	U	C2-N1-C1'	-5.71	110.85	117.70
28	C	32	LEU	CA-CB-CG	5.71	128.43	115.30
1	a	392	C	N3-C2-O2	-5.70	117.91	121.90
1	a	723	U	N3-C4-O4	-5.70	115.41	119.40
23	x	104	U	OP2-P-O3'	5.70	117.74	105.20
1	a	993	G	C8-N9-C1'	-5.70	119.59	127.00
1	a	1028	C	N1-C2-O2	5.70	122.32	118.90
24	y	10	C	C6-N1-C2	-5.70	118.02	120.30
1	a	14	U	C6-N1-C2	-5.69	117.58	121.00
26	A	2512	C	C5-C6-N1	5.68	123.84	121.00
1	a	87	C	N1-C2-O2	5.68	122.31	118.90
26	A	729	G	C4-N9-C1'	5.68	133.88	126.50
26	A	1257	C	C5-C6-N1	5.68	123.84	121.00
1	a	968	A	N9-C1'-C2'	-5.68	105.75	112.00
35	J	81	ILE	CG1-CB-CG2	-5.68	98.91	111.40
23	x	118	G	C4-C5-N7	5.67	113.07	110.80
26	A	680	C	C5-C6-N1	5.67	123.84	121.00
26	A	1760	C	C5-C6-N1	5.67	123.84	121.00
1	a	426	U	N3-C2-O2	-5.67	118.23	122.20
26	A	2080	A	N1-C2-N3	-5.67	126.46	129.30
1	a	923	A	C5-N7-C8	-5.67	101.07	103.90
1	a	1149	C	C6-N1-C2	-5.66	118.03	120.30
26	A	1380	G	C6-C5-N7	-5.66	127.00	130.40
26	A	2065	C	C6-N1-C2	-5.66	118.04	120.30
26	A	1053	C	C6-N1-C2	-5.65	118.04	120.30
26	A	2558	C	C5-C6-N1	5.65	123.83	121.00
26	A	2765	A	C2-N3-C4	5.65	113.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	60	U	N3-C2-O2	5.65	126.15	122.20
25	z	461	LEU	CB-CG-CD1	-5.65	101.40	111.00
26	A	883	G	C4-C5-N7	5.65	113.06	110.80
26	A	2720	U	N3-C2-O2	-5.65	118.25	122.20
1	a	514	C	C6-N1-C2	-5.64	118.04	120.30
1	a	1317	C	C6-N1-C2	-5.64	118.04	120.30
26	A	209	C	C5-C6-N1	5.64	123.82	121.00
1	a	449	G	C5-C6-O6	-5.64	125.21	128.60
1	a	799	G	N3-C2-N2	-5.64	115.95	119.90
26	A	503	A	C8-N9-C4	5.64	108.06	105.80
26	A	1267	U	N1-C2-O2	5.64	126.75	122.80
24	y	15	C	C2-N1-C1'	5.64	125.00	118.80
26	A	558	U	O5'-P-OP1	-5.64	100.63	105.70
1	a	513	C	N1-C2-O2	5.63	122.28	118.90
23	x	125	G	C3'-C2'-C1'	5.63	106.00	101.50
1	a	407	U	C5-C6-N1	5.62	125.51	122.70
26	A	243	U	N1-C2-O2	5.62	126.73	122.80
26	A	729	G	O4'-C1'-N9	5.62	112.69	108.20
24	y	17	G	N3-C4-N9	-5.61	122.63	126.00
26	A	2180	U	C2-N3-C4	5.61	130.37	127.00
1	a	322	C	C6-N1-C2	-5.61	118.06	120.30
1	a	611	C	N3-C2-O2	-5.61	117.97	121.90
26	A	243	U	N3-C2-O2	-5.61	118.28	122.20
26	A	2710	C	C6-N1-C2	-5.61	118.06	120.30
26	A	2637	U	N3-C2-O2	-5.60	118.28	122.20
1	a	54	C	N1-C2-O2	5.60	122.26	118.90
1	a	1303	C	OP2-P-O3'	5.60	117.53	105.20
24	y	5	G	N3-C2-N2	-5.60	115.98	119.90
27	B	70	C	C6-N1-C2	-5.60	118.06	120.30
1	a	920	U	N3-C2-O2	-5.60	118.28	122.20
26	A	2416	C	C6-N1-C2	-5.60	118.06	120.30
32	G	42	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	a	1469	C	N3-C2-O2	-5.59	117.98	121.90
26	A	2066	C	C6-N1-C2	-5.59	118.06	120.30
26	A	806	C	C5-C6-N1	5.58	123.79	121.00
1	a	1009	U	N3-C4-O4	-5.58	115.50	119.40
26	A	837	C	N1-C2-O2	5.58	122.25	118.90
32	G	173	ALA	C-N-CA	5.58	135.65	121.70
24	y	47(G)	C	C6-N1-C1'	5.58	127.49	120.80
1	a	1133	G	N3-C2-N2	-5.58	116.00	119.90
26	A	279	A	C5-C6-N6	-5.58	119.24	123.70
26	A	1180	U	C2-N1-C1'	5.57	124.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	354	G	N3-C4-N9	5.57	129.34	126.00
1	a	723	U	C4-C5-C6	-5.57	116.36	119.70
1	a	799	G	N9-C4-C5	5.57	107.63	105.40
26	A	2626	C	C6-N1-C2	-5.57	118.07	120.30
1	a	502	A	N9-C4-C5	-5.57	103.57	105.80
24	y	16	C	C2-N1-C1'	-5.57	112.68	118.80
1	a	110	C	N3-C2-O2	-5.56	118.00	121.90
26	A	2044	C	C5-C6-N1	5.56	123.78	121.00
26	A	198	C	C6-N1-C2	-5.55	118.08	120.30
26	A	2214	C	N1-C2-O2	5.55	122.23	118.90
24	y	47(H)	A	O5'-P-OP2	-5.55	100.71	105.70
26	A	1594	U	C5-C6-N1	5.55	125.47	122.70
1	a	647	C	C6-N1-C2	-5.54	118.08	120.30
26	A	1103	A	C5-C6-N1	5.54	120.47	117.70
26	A	84	A	C5-N7-C8	5.54	106.67	103.90
26	A	1076	C	C2-N3-C4	5.54	122.67	119.90
26	A	2179	C	N3-C2-O2	-5.54	118.02	121.90
1	a	443	C	C6-N1-C2	-5.54	118.08	120.30
1	a	956	U	N3-C2-O2	-5.54	118.32	122.20
22	v	1	C	C2-N3-C4	5.54	122.67	119.90
26	A	2276	G	N3-C2-N2	-5.54	116.02	119.90
1	a	312	C	C2-N1-C1'	5.53	124.89	118.80
1	a	1161	C	N1-C2-O2	5.53	122.22	118.90
26	A	610	C	C5-C6-N1	5.53	123.77	121.00
1	a	737	C	C5-C6-N1	5.53	123.77	121.00
1	a	1460	C	C5-C6-N1	5.53	123.77	121.00
26	A	2562	U	N1-C2-O2	5.53	126.67	122.80
51	Z	23	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	a	536	C	C2-N1-C1'	5.53	124.88	118.80
26	A	890	C	N1-C2-N3	-5.53	115.33	119.20
26	A	1971	U	N1-C2-O2	-5.53	118.93	122.80
1	a	90	C	N3-C2-O2	-5.53	118.03	121.90
1	a	960	U	N1-C2-O2	5.53	126.67	122.80
23	x	101	A	N9-C4-C5	-5.52	103.59	105.80
26	A	948	C	C5-C6-N1	5.52	123.76	121.00
26	A	1071	G	OP1-P-O3'	5.52	117.35	105.20
26	A	1564	C	C6-N1-C2	-5.52	118.09	120.30
26	A	1775	U	N1-C2-O2	5.52	126.67	122.80
1	a	307	C	C6-N1-C2	-5.52	118.09	120.30
23	x	125	G	C8-N9-C4	-5.52	104.19	106.40
26	A	2075	U	N3-C4-O4	5.52	123.26	119.40
26	A	2573	C	O5'-P-OP1	5.51	117.32	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2707	U	N1-C2-O2	5.51	126.66	122.80
26	A	231	A	N1-C6-N6	5.51	121.91	118.60
26	A	642	U	N3-C2-O2	-5.51	118.34	122.20
1	a	1395	C	N3-C2-O2	-5.51	118.04	121.90
26	A	393	C	C6-N1-C2	-5.51	118.10	120.30
1	a	662	U	C5-C4-O4	-5.50	122.60	125.90
24	y	47(K)	G	N3-C4-N9	-5.50	122.70	126.00
26	A	559	G	N7-C8-N9	5.50	115.85	113.10
26	A	2462	C	C5-C6-N1	5.50	123.75	121.00
24	y	47(B)	G	C4-N9-C1'	5.49	133.64	126.50
26	A	901	C	N1-C2-O2	5.49	122.20	118.90
1	a	491	G	C4-N9-C1'	5.49	133.64	126.50
1	a	868	C	C2-N1-C1'	5.49	124.84	118.80
1	a	514	C	C5-C6-N1	5.49	123.74	121.00
1	a	1071	C	C2-N1-C1'	5.49	124.84	118.80
26	A	852	U	C5-C4-O4	-5.49	122.61	125.90
1	a	896	C	C6-N1-C2	-5.49	118.11	120.30
23	x	126	G	C2'-C3'-O3'	-5.48	97.44	109.50
26	A	1158	C	O5'-P-OP2	-5.48	100.76	105.70
1	a	513	C	C2-N1-C1'	5.48	124.83	118.80
26	A	2805	C	C6-N1-C2	-5.48	118.11	120.30
1	a	598	U	N3-C2-O2	-5.48	118.36	122.20
26	A	125	A	C8-N9-C4	5.48	107.99	105.80
26	A	1244	A	N9-C4-C5	-5.48	103.61	105.80
26	A	822	G	N7-C8-N9	5.48	115.84	113.10
26	A	2134	A	N1-C6-N6	-5.47	115.32	118.60
1	a	334	C	C6-N1-C2	-5.47	118.11	120.30
26	A	415	A	N9-C4-C5	-5.47	103.61	105.80
26	A	717	C	C6-N1-C2	-5.47	118.11	120.30
1	a	418	C	N1-C2-O2	5.47	122.18	118.90
24	y	47(O)	C	C6-N1-C2	-5.47	118.11	120.30
26	A	1314	C	C5-C6-N1	5.47	123.73	121.00
41	P	113	LEU	CA-CB-CG	5.46	127.87	115.30
1	a	90	C	N1-C2-O2	5.46	122.18	118.90
26	A	1548	A	N9-C4-C5	-5.46	103.61	105.80
1	a	1521	C	C5-C6-N1	5.46	123.73	121.00
22	v	67	C	C6-N1-C2	-5.46	118.12	120.30
26	A	1061	U	OP2-P-O3'	5.46	117.21	105.20
1	a	103	U	N3-C2-O2	-5.45	118.38	122.20
24	y	48	G	C5-N7-C8	-5.45	101.57	104.30
1	a	984	C	C6-N1-C2	-5.45	118.12	120.30
26	A	1578	U	N3-C2-O2	-5.45	118.38	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	6	32	LEU	CB-CG-CD1	5.45	120.26	111.00
1	a	211	G	N3-C4-C5	-5.44	125.88	128.60
1	a	34	C	C2-N1-C1'	5.44	124.78	118.80
1	a	1066	C	C6-N1-C2	-5.44	118.12	120.30
24	y	57	G	N9-C4-C5	5.43	107.57	105.40
26	A	1340	U	N3-C2-O2	-5.43	118.40	122.20
26	A	2766	A	C5-C6-N6	-5.43	119.35	123.70
1	a	610	U	N3-C2-O2	-5.43	118.40	122.20
2	b	56	LEU	CA-CB-CG	5.43	127.78	115.30
26	A	1624	U	N3-C2-O2	-5.42	118.40	122.20
1	a	16	A	N1-C2-N3	-5.42	126.59	129.30
1	a	322	C	C5-C6-N1	5.42	123.71	121.00
22	v	68	C	C6-N1-C2	-5.42	118.13	120.30
26	A	120	U	C4-C5-C6	5.42	122.95	119.70
26	A	669	G	C4-N9-C1'	5.42	133.55	126.50
1	a	1487	G	N3-C2-N2	-5.42	116.11	119.90
1	a	1131	G	C4-C5-N7	5.42	112.97	110.80
24	y	45	U	C6-N1-C2	-5.42	117.75	121.00
24	y	48	G	C4-N9-C1'	5.42	133.54	126.50
1	a	723	U	N3-C2-O2	-5.41	118.41	122.20
24	y	47(E)	G	N1-C6-O6	-5.41	116.65	119.90
57	6	4	ASP	CB-CG-OD1	5.41	123.17	118.30
26	A	1348	C	N3-C2-O2	-5.41	118.11	121.90
26	A	2118	U	C5-C4-O4	-5.41	122.66	125.90
26	A	1070	A	O5'-P-OP2	5.40	117.19	110.70
1	a	87	C	C6-N1-C2	-5.40	118.14	120.30
23	x	124	A	N3-C4-N9	5.40	131.72	127.40
26	A	2254	C	N3-C2-O2	-5.40	118.12	121.90
26	A	2305	U	C6-N1-C1'	-5.40	113.64	121.20
26	A	278	A	C2-N3-C4	5.39	113.30	110.60
26	A	1708	C	C5-C6-N1	5.39	123.70	121.00
1	a	307	C	N3-C2-O2	-5.39	118.13	121.90
26	A	2902	C	C6-N1-C2	-5.39	118.14	120.30
23	x	129	U	C5'-C4'-C3'	5.39	124.62	116.00
27	B	108	A	N1-C6-N6	5.38	121.83	118.60
26	A	2699	C	C5-C6-N1	5.38	123.69	121.00
1	a	680	C	C6-N1-C2	-5.38	118.15	120.30
26	A	1914	C	C6-N1-C2	-5.38	118.15	120.30
26	A	867	C	N1-C2-O2	5.38	122.13	118.90
24	y	47(G)	C	N1-C2-N3	5.38	122.97	119.20
26	A	141	G	N3-C4-N9	5.38	129.23	126.00
1	a	71	A	OP2-P-O3'	5.38	117.03	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	65	U	N3-C2-O2	-5.38	118.44	122.20
23	x	126	G	N3-C2-N2	5.38	123.66	119.90
22	v	62	C	C5-C6-N1	5.37	123.69	121.00
26	A	827	U	O5'-P-OP1	-5.37	100.86	105.70
26	A	365	U	C5-C4-O4	-5.37	122.68	125.90
27	B	25	U	N3-C2-O2	-5.37	118.44	122.20
26	A	1476	U	C2-N1-C1'	5.37	124.14	117.70
1	a	661	G	C4-C5-N7	5.37	112.95	110.80
19	s	15	LEU	CA-CB-CG	5.37	127.64	115.30
26	A	1723	G	C5-C6-N1	5.37	114.18	111.50
1	a	582	C	N1-C2-O2	5.36	122.12	118.90
26	A	1670	C	C6-N1-C2	-5.36	118.16	120.30
26	A	658	U	C5-C6-N1	5.36	125.38	122.70
26	A	1927	A	OP2-P-O3'	5.36	116.99	105.20
1	a	923	A	C4-C5-N7	5.36	113.38	110.70
23	x	110	G	P-O3'-C3'	-5.36	113.27	119.70
1	a	470	C	C6-N1-C2	-5.36	118.16	120.30
1	a	1158	C	C6-N1-C1'	-5.36	114.37	120.80
1	a	979	C	C6-N1-C2	-5.35	118.16	120.30
26	A	1585	C	N3-C2-O2	-5.35	118.15	121.90
1	a	1302	C	N3-C4-C5	5.35	124.04	121.90
26	A	230	G	N9-C4-C5	-5.35	103.26	105.40
26	A	2165	C	N1-C2-O2	5.35	122.11	118.90
22	v	40	C	C6-N1-C2	-5.35	118.16	120.30
1	a	967	5MC	OP2-P-O3'	5.35	116.96	105.20
1	a	1389	C	C6-N1-C2	-5.35	118.16	120.30
26	A	717	C	C5-C6-N1	5.35	123.67	121.00
24	y	41	C	C2-N1-C1'	5.35	124.68	118.80
26	A	1886	U	N3-C2-O2	-5.35	118.46	122.20
1	a	413	G	N3-C4-C5	5.34	131.27	128.60
26	A	1043	C	O4'-C1'-N1	5.34	112.47	108.20
1	a	420	U	C2-N1-C1'	5.34	124.11	117.70
26	A	444	C	C5-C6-N1	5.33	123.67	121.00
1	a	1102	A	C8-N9-C4	5.33	107.93	105.80
1	a	1241	G	C8-N9-C4	-5.33	104.27	106.40
26	A	2428	G	OP1-P-OP2	-5.33	111.60	119.60
1	a	440	C	C6-N1-C2	-5.33	118.17	120.30
26	A	2180	U	C5-C6-N1	5.33	125.36	122.70
1	a	178	C	C6-N1-C2	-5.33	118.17	120.30
1	a	225	C	C6-N1-C2	-5.33	118.17	120.30
1	a	431	A	N1-C6-N6	-5.33	115.40	118.60
1	a	1460	C	C6-N1-C2	-5.33	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	148	U	C5-C4-O4	-5.33	122.70	125.90
24	y	62	C	N3-C4-N4	-5.33	114.27	118.00
25	z	338	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	a	751	U	N3-C2-O2	-5.33	118.47	122.20
26	A	947	A	N9-C4-C5	-5.32	103.67	105.80
23	x	131	C	C3'-C2'-C1'	5.32	105.76	101.50
26	A	2302	U	N1-C2-O2	5.32	126.53	122.80
26	A	1498	C	C5-C6-N1	5.32	123.66	121.00
1	a	610	U	N1-C2-O2	5.32	126.52	122.80
1	a	1382	C	N3-C2-O2	-5.32	118.18	121.90
24	y	53	G	C2-N3-C4	-5.31	109.24	111.90
26	A	1990	C	C6-N1-C2	-5.31	118.17	120.30
33	I	10	LEU	CA-CB-CG	5.31	127.52	115.30
1	a	80	A	C5-C6-N1	-5.31	115.05	117.70
1	a	1138	G	C2-N3-C4	5.31	114.55	111.90
22	v	40	C	N1-C2-O2	5.31	122.08	118.90
26	A	2081	U	C5-C6-N1	5.31	125.35	122.70
1	a	323	U	C5-C4-O4	-5.30	122.72	125.90
1	a	764	C	C5-C6-N1	5.30	123.65	121.00
1	a	878	A	C4-C5-N7	5.30	113.35	110.70
1	a	879	C	C5-C6-N1	5.30	123.65	121.00
1	a	1504	G	N3-C4-N9	-5.30	122.82	126.00
24	y	57	G	N3-C4-N9	-5.30	122.82	126.00
26	A	1629	U	N3-C2-O2	-5.30	118.49	122.20
26	A	2007	U	C5-C6-N1	5.30	125.35	122.70
1	a	924	C	C5-C6-N1	5.29	123.65	121.00
42	Q	108	LEU	CA-CB-CG	5.29	127.47	115.30
24	y	72	C	C6-N1-C2	-5.29	118.19	120.30
26	A	2080	A	N1-C6-N6	5.29	121.77	118.60
26	A	1548	A	N1-C2-N3	-5.29	126.66	129.30
1	a	528	C	C5-C6-N1	5.28	123.64	121.00
26	A	1229	C	C6-N1-C2	-5.28	118.19	120.30
24	y	58	A	O5'-P-OP2	-5.28	100.95	105.70
31	F	162	ASP	CB-CG-OD1	5.28	123.05	118.30
1	a	439	U	N3-C2-O2	-5.27	118.51	122.20
26	A	2231	U	C5-C6-N1	5.27	125.33	122.70
24	y	40	C	C2-N1-C1'	5.27	124.60	118.80
27	B	47	C	C6-N1-C2	-5.27	118.19	120.30
23	x	117	C	C5-C6-N1	5.27	123.63	121.00
26	A	233	A	N9-C4-C5	-5.27	103.69	105.80
1	a	620	C	C6-N1-C2	-5.26	118.19	120.30
26	A	283	G	N3-C4-N9	-5.26	122.84	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	67	C	C5-C6-N1	5.26	123.63	121.00
26	A	302	C	C5-C6-N1	5.26	123.63	121.00
24	y	30	G	C4-N9-C1'	5.25	133.33	126.50
26	A	1512	C	C6-N1-C2	-5.25	118.20	120.30
1	a	968	A	C6-C5-N7	5.25	135.97	132.30
1	a	169	C	N3-C2-O2	-5.25	118.23	121.90
26	A	1399	C	C5-C6-N1	5.25	123.62	121.00
1	a	528	C	N3-C2-O2	-5.24	118.23	121.90
1	a	1263	C	N1-C2-O2	5.24	122.05	118.90
1	a	1410	A	N9-C4-C5	-5.24	103.70	105.80
26	A	2259	U	N3-C2-O2	-5.24	118.53	122.20
1	a	1086	U	C5-C6-N1	5.24	125.32	122.70
26	A	2254	C	C6-N1-C2	-5.24	118.20	120.30
26	A	1059	G	OP1-P-O3'	5.24	116.73	105.20
1	a	552	U	C5-C6-N1	5.24	125.32	122.70
26	A	283	G	N1-C6-O6	-5.24	116.76	119.90
26	A	1644	C	N1-C2-O2	5.24	122.04	118.90
26	A	1118	C	C6-N1-C2	-5.23	118.21	120.30
26	A	209	C	C6-N1-C2	-5.23	118.21	120.30
26	A	1257	C	C6-N1-C2	-5.23	118.21	120.30
25	z	610	LEU	CA-CB-CG	5.23	127.33	115.30
1	a	449	G	N9-C4-C5	-5.23	103.31	105.40
1	a	1317	C	N1-C2-O2	5.23	122.04	118.90
1	a	956	U	N1-C2-O2	5.23	126.46	122.80
26	A	101	A	C2-N3-C4	-5.23	107.99	110.60
10	j	75	ASP	CB-CG-OD1	5.23	123.00	118.30
26	A	2565	A	C8-N9-C4	-5.23	103.71	105.80
26	A	143	C	C6-N1-C2	-5.22	118.21	120.30
1	a	1412	C	C2-N1-C1'	5.22	124.54	118.80
27	B	42	C	C6-N1-C2	-5.22	118.21	120.30
1	a	1464	U	N3-C2-O2	-5.22	118.55	122.20
26	A	1958	C	C6-N1-C2	-5.22	118.21	120.30
1	a	580	C	C6-N1-C2	-5.22	118.21	120.30
1	a	582	C	C5-C6-N1	5.22	123.61	121.00
26	A	56	A	N9-C4-C5	-5.22	103.71	105.80
26	A	898	C	C5-C6-N1	5.21	123.61	121.00
1	a	493	A	N7-C8-N9	5.21	116.41	113.80
26	A	813	U	N1-C2-O2	5.21	126.45	122.80
1	a	920	U	N1-C2-O2	5.21	126.44	122.80
26	A	890	C	C2-N1-C1'	5.21	124.53	118.80
26	A	2086	U	N3-C2-O2	-5.21	118.56	122.20
24	y	73	G	C5-C6-O6	-5.20	125.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	39	C	C6-N1-C2	-5.20	118.22	120.30
26	A	2028	U	C5-C6-N1	5.20	125.30	122.70
57	6	40	CYS	CB-CA-C	-5.20	100.00	110.40
1	a	397	A	C4-C5-N7	5.20	113.30	110.70
25	z	457	LEU	CA-CB-CG	5.20	127.26	115.30
26	A	2556	C	N3-C2-O2	-5.20	118.26	121.90
1	a	866	C	C6-N1-C2	-5.20	118.22	120.30
24	y	40	C	O5'-P-OP2	-5.20	101.02	105.70
1	a	274	A	N1-C2-N3	-5.19	126.70	129.30
1	a	127	G	N9-C4-C5	-5.19	103.32	105.40
24	y	1	G	C4-C5-N7	5.19	112.88	110.80
26	A	435	C	OP2-P-O3'	5.19	116.62	105.20
26	A	891	G	N3-C4-C5	-5.19	126.00	128.60
26	A	933	A	N3-C4-N9	5.19	131.55	127.40
26	A	346	A	OP2-P-O3'	5.19	116.62	105.20
26	A	314	C	C5-C6-N1	5.19	123.59	121.00
26	A	1077	A	C5-C6-N1	5.19	120.29	117.70
26	A	2226	C	N1-C2-O2	5.19	122.01	118.90
50	Y	28	LEU	CA-CB-CG	5.18	127.22	115.30
26	A	1093	G	C6-C5-N7	-5.18	127.29	130.40
26	A	119	A	C4-C5-C6	-5.18	114.41	117.00
26	A	883	G	N1-C6-O6	5.18	123.01	119.90
23	x	119	G	N9-C4-C5	5.18	107.47	105.40
30	E	82	GLY	CA-C-O	-5.18	111.28	120.60
22	v	50	U	C6-N1-C2	-5.18	117.89	121.00
24	y	32	C	O4'-C1'-N1	5.17	112.34	108.20
26	A	2136	G	C5-C6-O6	-5.17	125.50	128.60
26	A	2766	A	N1-C6-N6	5.17	121.70	118.60
1	a	219	U	C5-C6-N1	5.17	125.29	122.70
24	y	47(P)	C	N3-C2-O2	-5.17	118.28	121.90
15	o	55	LEU	CA-CB-CG	5.17	127.19	115.30
26	A	2310	C	N3-C2-O2	-5.17	118.28	121.90
1	a	431	A	O4'-C1'-N9	5.17	112.33	108.20
26	A	1243	C	C6-N1-C2	-5.17	118.23	120.30
23	x	110	G	C4-N9-C1'	5.16	133.21	126.50
31	F	50	ASP	CB-CG-OD1	5.16	122.95	118.30
1	a	1148	U	C6-N1-C2	-5.16	117.90	121.00
1	a	1109	C	C5-C6-N1	5.16	123.58	121.00
24	y	47(F)	C	C6-N1-C2	-5.16	118.24	120.30
26	A	2430	A	C2-N3-C4	5.16	113.18	110.60
1	a	1003	G	C8-N9-C4	-5.16	104.34	106.40
15	o	86	LEU	CA-CB-CG	5.16	127.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	413	G	O4'-C1'-N9	-5.15	104.08	108.20
26	A	888	C	O4'-C1'-N1	5.15	112.32	108.20
1	a	1034	G	C6-C5-N7	-5.15	127.31	130.40
26	A	687	C	N3-C2-O2	-5.15	118.29	121.90
26	A	1075	C	C6-N1-C1'	-5.15	114.62	120.80
1	a	634	C	C6-N1-C2	-5.14	118.24	120.30
26	A	946	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1771	C	C6-N1-C2	-5.14	118.24	120.30
1	a	199	A	N9-C4-C5	-5.14	103.74	105.80
1	a	1241	G	N3-C4-C5	-5.14	126.03	128.60
26	A	314	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1043	C	C6-N1-C2	-5.14	118.24	120.30
26	A	1081	U	C5-C6-N1	5.14	125.27	122.70
26	A	2469	A	C5-C6-N6	-5.14	119.59	123.70
1	a	340	U	N3-C2-O2	-5.14	118.60	122.20
1	a	1411	C	C6-N1-C2	-5.14	118.24	120.30
26	A	897	C	N3-C2-O2	-5.14	118.30	121.90
26	A	2065	C	N1-C2-O2	5.14	121.98	118.90
1	a	414	A	C5-C6-N1	5.14	120.27	117.70
1	a	1237	C	C5-C6-N1	5.13	123.57	121.00
1	a	1263	C	C2-N1-C1'	5.13	124.45	118.80
11	k	84	MET	CA-CB-CG	5.13	122.03	113.30
1	a	1032	G	N3-C4-N9	5.13	129.08	126.00
1	a	418	C	C5-C6-N1	5.13	123.57	121.00
1	a	923	A	N9-C4-C5	-5.13	103.75	105.80
23	x	119	G	N3-C2-N2	-5.13	116.31	119.90
26	A	2146	C	OP1-P-OP2	-5.13	111.90	119.60
27	B	28	C	C6-N1-C2	-5.13	118.25	120.30
23	x	118	G	C5-N7-C8	-5.13	101.73	104.30
1	a	697	U	N3-C2-O2	-5.13	118.61	122.20
26	A	1181	U	C6-N1-C2	-5.13	117.92	121.00
26	A	283	G	N9-C4-C5	5.13	107.45	105.40
26	A	889	C	C2-N1-C1'	5.13	124.44	118.80
25	z	177	LEU	CB-CG-CD2	-5.12	102.29	111.00
4	d	4	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	a	207	C	N3-C2-O2	-5.12	118.32	121.90
1	a	428	G	N3-C4-C5	5.12	131.16	128.60
7	g	39	GLU	CA-CB-CG	5.12	124.66	113.40
26	A	1350	C	N1-C2-O2	5.12	121.97	118.90
26	A	1499	C	C6-N1-C2	-5.12	118.25	120.30
26	A	1990	C	C5-C6-N1	5.12	123.56	121.00
27	B	120	U	C2-N1-C1'	5.12	123.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1524	C	N1-C2-O2	5.11	121.97	118.90
26	A	851	C	C5-C6-N1	5.11	123.56	121.00
24	y	16	C	N3-C4-N4	-5.11	114.42	118.00
1	a	55	A	C2-N3-C4	5.11	113.16	110.60
1	a	1342	C	C6-N1-C2	-5.11	118.26	120.30
26	A	2548	U	C5-C6-N1	5.11	125.26	122.70
34	H	58	LEU	CA-CB-CG	5.11	127.05	115.30
26	A	278	A	N3-C4-C5	-5.11	123.22	126.80
26	A	668	A	N1-C2-N3	-5.11	126.75	129.30
3	c	30	ASP	CB-CG-OD1	5.11	122.89	118.30
26	A	283	G	N1-C2-N2	5.11	120.79	116.20
1	a	409	U	N3-C2-O2	-5.10	118.63	122.20
26	A	665	U	C5-C6-N1	5.10	125.25	122.70
26	A	807	U	N3-C2-O2	-5.10	118.63	122.20
26	A	2656	U	N1-C2-O2	5.10	126.37	122.80
26	A	867	C	N3-C2-O2	-5.10	118.33	121.90
26	A	1680	U	N3-C2-O2	-5.10	118.63	122.20
1	a	1500	A	C6-N1-C2	5.10	121.66	118.60
2	b	17	HIS	N-CA-C	5.10	124.77	111.00
22	v	28	C	C6-N1-C2	-5.10	118.26	120.30
1	a	419	C	N1-C2-N3	5.09	122.76	119.20
26	A	1476	U	C6-N1-C2	-5.09	117.94	121.00
26	A	53	A	C4-C5-N7	5.09	113.25	110.70
26	A	392	U	N3-C2-O2	-5.09	118.64	122.20
26	A	1158	C	C5-C6-N1	5.09	123.55	121.00
1	a	54	C	N3-C2-O2	-5.09	118.34	121.90
26	A	208	C	C6-N1-C2	-5.09	118.27	120.30
26	A	373	U	C6-N1-C2	-5.09	117.95	121.00
26	A	610	C	C2-N1-C1'	5.09	124.40	118.80
26	A	2558	C	C6-N1-C2	-5.09	118.27	120.30
26	A	2756	U	OP1-P-O3'	5.09	116.39	105.20
1	a	294	U	C5-C6-N1	5.08	125.24	122.70
1	a	1489	G	N3-C2-N2	-5.08	116.34	119.90
26	A	1578	U	N1-C2-O2	5.08	126.36	122.80
38	M	65	ILE	CG1-CB-CG2	-5.08	100.21	111.40
26	A	2716	C	N1-C2-O2	5.08	121.95	118.90
26	A	1812	U	N3-C2-O2	-5.08	118.64	122.20
26	A	2086	U	N1-C2-O2	5.08	126.36	122.80
26	A	1830	C	C6-N1-C2	-5.08	118.27	120.30
27	B	57	A	C8-N9-C4	-5.08	103.77	105.80
26	A	2234	G	N7-C8-N9	5.07	115.64	113.10
24	y	35	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	750	C	N1-C2-N3	5.07	122.75	119.20
26	A	1113	U	O4'-C1'-N1	5.07	112.25	108.20
1	a	489	C	C6-N1-C2	-5.07	118.27	120.30
1	a	879	C	C6-N1-C2	-5.07	118.27	120.30
26	A	1093	G	C5-C6-N1	5.07	114.03	111.50
26	A	2103	C	C6-N1-C2	-5.07	118.27	120.30
1	a	418	C	N3-C2-O2	-5.07	118.35	121.90
23	x	118	G	C4-N9-C1'	5.07	133.09	126.50
24	y	32	C	C6-N1-C1'	5.07	126.88	120.80
26	A	2480	C	C6-N1-C2	-5.07	118.27	120.30
1	a	392	C	N3-C4-N4	5.06	121.54	118.00
22	v	57	A	N7-C8-N9	-5.06	111.27	113.80
24	y	47(J)	C	C6-N1-C2	-5.06	118.28	120.30
1	a	796	C	C6-N1-C2	-5.06	118.28	120.30
26	A	1052	C	C5-C6-N1	5.06	123.53	121.00
26	A	2739	U	N3-C2-O2	-5.06	118.66	122.20
35	J	17	VAL	CG1-CB-CG2	-5.06	102.81	110.90
26	A	883	G	C5-N7-C8	-5.05	101.77	104.30
26	A	2119	A	C5-C6-N6	-5.05	119.66	123.70
1	a	1455	G	C5-C6-O6	-5.05	125.57	128.60
26	A	1437	C	C5-C6-N1	5.05	123.53	121.00
26	A	1646	C	OP1-P-O3'	5.05	116.31	105.20
1	a	1226	C	N1-C2-O2	5.05	121.93	118.90
26	A	358	U	N3-C2-O2	-5.05	118.67	122.20
1	a	1448	C	C5-C6-N1	5.05	123.52	121.00
26	A	2636	C	N3-C2-O2	-5.05	118.37	121.90
23	x	101	A	C6-N1-C2	5.04	121.63	118.60
1	a	80	A	N3-C4-C5	5.04	130.33	126.80
1	a	623	C	C6-N1-C2	-5.04	118.28	120.30
1	a	979	C	N3-C2-O2	-5.04	118.37	121.90
23	x	114	C	O5'-P-OP2	-5.04	101.16	105.70
26	A	2895	G	N9-C4-C5	-5.04	103.38	105.40
1	a	1379	G	N3-C2-N2	-5.04	116.37	119.90
22	v	25	C	C6-N1-C2	-5.04	118.28	120.30
26	A	2405	G	OP2-P-O3'	5.04	116.29	105.20
26	A	832	U	N3-C2-O2	-5.04	118.67	122.20
26	A	1716	U	C6-N1-C2	-5.04	117.98	121.00
26	A	2782	G	N3-C4-N9	5.04	129.02	126.00
26	A	2880	C	C6-N1-C2	-5.04	118.28	120.30
1	a	550	G	N3-C4-C5	-5.03	126.08	128.60
26	A	852	U	C5-C6-N1	5.03	125.22	122.70
26	A	1956	U	N1-C2-O2	5.03	126.32	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	88	U	N3-C2-O2	-5.03	118.68	122.20
1	a	817	C	C2-N1-C1'	5.03	124.33	118.80
26	A	141	G	N3-C4-C5	-5.03	126.09	128.60
26	A	1539	U	C2-N1-C1'	5.03	123.73	117.70
26	A	2065	C	N3-C2-O2	-5.03	118.38	121.90
19	s	4	LEU	CA-CB-CG	5.02	126.86	115.30
26	A	193	U	N3-C2-O2	-5.02	118.68	122.20
26	A	915	C	C2-N1-C1'	5.02	124.33	118.80
1	a	71	A	OP1-P-OP2	-5.02	112.07	119.60
26	A	1774	C	N1-C2-O2	5.02	121.91	118.90
26	A	1279	G	N1-C6-O6	5.02	122.91	119.90
26	A	595	C	C5-C6-N1	5.02	123.51	121.00
24	y	72	C	C5-C6-N1	5.02	123.51	121.00
1	a	218	U	C5-C6-N1	5.02	125.21	122.70
26	A	49	A	O4'-C1'-N9	-5.02	104.19	108.20
26	A	2752	C	N1-C2-O2	5.02	121.91	118.90
1	a	905	U	C6-N1-C2	-5.01	117.99	121.00
26	A	2305	U	C2-N3-C4	-5.01	123.99	127.00
26	A	2656	U	N3-C2-O2	-5.01	118.69	122.20
1	a	674	G	N7-C8-N9	5.01	115.61	113.10
1	a	346	G	C5-C6-N1	5.01	114.00	111.50
24	y	47(B)	G	C6-C5-N7	-5.01	127.39	130.40
26	A	2238	G	N3-C4-N9	5.01	129.00	126.00
1	a	1348	U	N1-C2-O2	5.01	126.31	122.80
1	a	94	G	C5-C6-O6	-5.01	125.60	128.60
22	v	17	C	C6-N1-C2	-5.01	118.30	120.30
26	A	2556	C	N1-C2-O2	5.01	121.90	118.90
24	y	67(A)	U	C5-C6-N1	5.00	125.20	122.70
1	a	689	C	C2-N1-C1'	5.00	124.30	118.80
26	A	2110	G	N3-C4-C5	5.00	131.10	128.60
26	A	2279	G	N9-C4-C5	-5.00	103.40	105.40
1	a	136	C	C5-C6-N1	5.00	123.50	121.00
1	a	656	G	N1-C2-N3	5.00	126.90	123.90
26	A	919	U	N1-C2-O2	5.00	126.30	122.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
26	A	2069	G7M	C3',C4'

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
55	3	30	HIS	Peptide
28	C	120	ASP	Peptide
34	H	2	GLN	Peptide
34	H	8	LYS	Mainchain,Peptide
33	I	23	VAL	Peptide
33	I	63	ASP	Peptide
36	K	34	GLY	Peptide
38	M	57	VAL	Mainchain
44	S	63	GLY	Peptide
46	U	5	ARG	Peptide
46	U	50	ALA	Peptide
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
5	e	92	ARG	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Peptide
11	k	91	GLY	Peptide
12	l	100	ALA	Peptide
12	l	74	GLN	Peptide
13	m	3	ILE	Peptide
13	m	4	ALA	Mainchain
15	o	87	ARG	Mainchain
18	r	10	CYS	Peptide
18	r	16	GLY	Peptide
25	z	190	LEU	Peptide
25	z	300	LEU	Peptide
25	z	327	SER	Mainchain

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	b	216/218 (99%)	188 (87%)	24 (11%)	4 (2%)	8 40
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	10 46
4	d	203/205 (99%)	190 (94%)	8 (4%)	5 (2%)	5 34
5	e	155/157 (99%)	142 (92%)	6 (4%)	7 (4%)	2 23
6	f	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	3 25
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	7 39
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19 60
9	i	125/127 (98%)	108 (86%)	13 (10%)	4 (3%)	4 29
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	1 18
11	k	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	8 41
12	l	121/123 (98%)	110 (91%)	7 (6%)	4 (3%)	4 29
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	5 33
14	n	98/100 (98%)	85 (87%)	13 (13%)	0	100 100
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	3 28
16	p	80/82 (98%)	72 (90%)	5 (6%)	3 (4%)	3 26
17	q	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	3 26
18	r	63/65 (97%)	57 (90%)	3 (5%)	3 (5%)	2 23
19	s	77/79 (98%)	69 (90%)	8 (10%)	0	100 100
20	t	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13 50
21	u	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2 23
25	z	613/614 (100%)	587 (96%)	20 (3%)	6 (1%)	15 54
28	C	269/271 (99%)	254 (94%)	13 (5%)	2 (1%)	22 62
29	D	207/209 (99%)	197 (95%)	8 (4%)	2 (1%)	15 54
30	E	199/201 (99%)	189 (95%)	8 (4%)	2 (1%)	15 54
31	F	175/177 (99%)	163 (93%)	9 (5%)	3 (2%)	9 43
32	G	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	4 31
33	I	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	4 31
34	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3 28
35	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	22 62
36	K	120/122 (98%)	116 (97%)	2 (2%)	2 (2%)	9 43
37	L	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11 46
38	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	10 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	N	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	19 60
40	O	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	17 56
41	P	112/114 (98%)	108 (96%)	4 (4%)	0	100 100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100 100
43	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	7 39
44	S	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	8 40
45	T	91/93 (98%)	79 (87%)	11 (12%)	1 (1%)	14 52
46	U	100/102 (98%)	89 (89%)	5 (5%)	6 (6%)	1 18
47	V	92/94 (98%)	88 (96%)	4 (4%)	0	100 100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100 100
49	X	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	9 44
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100 100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	8 40
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	7 38
54	2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6 36
55	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9 44
56	4	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
57	6	64/66 (97%)	57 (89%)	5 (8%)	2 (3%)	4 30
All	All	6330/6431 (98%)	5844 (92%)	368 (6%)	118 (2%)	11 40

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	151	LYS
5	e	89	THR
6	f	94	HIS
9	i	57	VAL
9	i	125	GLN
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU

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Mol	Chain	Res	Type
13	m	4	ALA
13	m	6	ILE
15	o	46	LYS
15	o	87	ARG
16	p	44	SER
17	q	16	MET
17	q	49	ASN
25	z	191	VAL
25	z	301	GLU
25	z	328	ALA
28	C	121	ALA
30	E	83	VAL
32	G	174	LYS
32	G	175	LYS
33	I	64	ARG
34	H	9	VAL
35	J	81	ILE
37	L	36	LYS
38	M	58	LYS
44	S	64	ALA
46	U	51	LEU
46	U	88	ASP
52	0	2	VAL
53	1	4	ILE
55	3	31	ILE
3	c	60	ALA
3	c	79	LYS
4	d	165	GLU
4	d	191	SER
5	e	77	ASN
5	e	93	VAL
8	h	44	PHE
9	i	107	ALA
10	j	42	LEU
11	k	91	GLY
12	l	25	ALA
18	r	11	ARG
18	r	18	GLN
21	u	25	ALA
25	z	487	PHE
32	G	108	PHE
33	I	24	GLY

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Mol	Chain	Res	Type
34	H	3	VAL
34	H	41	LYS
36	K	35	VAL
39	N	117	ASP
43	R	52	PRO
43	R	53	PHE
46	U	6	ARG
46	U	18	LYS
57	6	40	CYS
57	6	43	PHE
4	d	47	LEU
5	e	23	THR
6	f	99	ALA
7	g	129	ASN
9	i	12	LYS
15	o	2	LEU
16	p	43	ALA
21	u	24	LYS
21	u	34	ARG
28	C	204	LEU
29	D	140	HIS
29	D	149	ASN
32	G	118	ALA
33	I	69	VAL
34	H	15	LEU
37	L	29	LYS
2	b	17	HIS
3	c	156	LEU
5	e	122	VAL
7	g	57	GLU
10	j	58	ASN
12	l	2	THR
12	l	46	SER
17	q	72	TRP
20	t	26	MET
31	F	20	ASN
32	G	173	ALA
34	H	89	LYS
44	S	3	THR
45	T	88	LYS
54	2	40	ALA
2	b	120	SER

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Mol	Chain	Res	Type
4	d	150	LYS
5	e	158	LYS
6	f	92	THR
7	g	56	SER
10	j	75	ASP
25	z	345	ARG
30	E	122	GLU
31	F	149	ARG
36	K	92	GLU
40	O	101	GLY
46	U	97	SER
46	U	98	ASN
50	Y	24	GLU
4	d	4	LEU
13	m	11	HIS
38	M	69	PRO
5	e	24	VAL
16	p	49	GLY
18	r	17	VAL
25	z	600	GLY
31	F	135	ILE
6	f	19	PRO
33	I	12	VAL

4.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	86
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	z	502/501 (100%)	502 (100%)	0	100	100
28	C	216/216 (100%)	216 (100%)	0	100	100
29	D	164/164 (100%)	164 (100%)	0	100	100
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	148 (100%)	0	100	100
32	G	137/137 (100%)	137 (100%)	0	100	100
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	103 (100%)	0	100	100
37	L	102/102 (100%)	102 (100%)	0	100	100
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	100 (100%)	0	100	100
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	80 (100%)	0	100	100
46	U	83/83 (100%)	83 (100%)	0	100	100
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100
49	X	67/67 (100%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	55 (100%)	0	100	100
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5230/5252 (100%)	5229 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	138	GLN
5	e	121	ASN
9	i	4	GLN
9	i	109	GLN
9	i	125	GLN
14	n	42	ASN
15	o	36	ASN
15	o	45	HIS
17	q	44	HIS
18	r	51	GLN
19	s	51	HIS
19	s	56	HIS

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Mol	Chain	Res	Type
25	z	47	GLN
25	z	292	HIS
25	z	388	GLN
25	z	483	HIS
25	z	529	GLN
28	C	85	ASN
28	C	89	ASN
28	C	250	GLN
29	D	150	GLN
30	E	90	GLN
31	F	26	GLN
32	G	114	HIS
32	G	138	GLN
34	H	2	GLN
34	H	18	GLN
36	K	29	HIS
37	L	35	HIS
41	P	55	HIS
43	R	91	GLN
44	S	102	HIS
46	U	73	ASN
50	Y	58	ASN
52	0	5	ASN
56	4	33	HIS

4.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	197 (12%)	0
22	v	76/77 (98%)	10 (13%)	0
23	x	47/48 (97%)	29 (61%)	0
24	y	93/95 (97%)	23 (24%)	0
26	A	2898/2903 (99%)	414 (14%)	5 (0%)
27	B	119/120 (99%)	11 (9%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	684 (14%)	5 (0%)

All (684) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	A

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Mol	Chain	Res	Type
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	86	G
1	a	94	G
1	a	95	C
1	a	96	U
1	a	121	U
1	a	127	G
1	a	131	A
1	a	141	G
1	a	164	G
1	a	173	U
1	a	177	G
1	a	183	C
1	a	197	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	237	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	254	G
1	a	266	G
1	a	267	C
1	a	289	G
1	a	298	A
1	a	316	C
1	a	319	G
1	a	328	C
1	a	330	C
1	a	347	G
1	a	352	C

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Mol	Chain	Res	Type
1	a	354	G
1	a	356	A
1	a	367	U
1	a	368	U
1	a	372	C
1	a	392	C
1	a	406	G
1	a	407	U
1	a	411	A
1	a	412	A
1	a	414	A
1	a	420	U
1	a	426	U
1	a	429	U
1	a	430	A
1	a	436	C
1	a	438	U
1	a	439	U
1	a	467	U
1	a	481	G
1	a	482	A
1	a	491	G
1	a	497	G
1	a	499	A
1	a	509	A
1	a	511	C
1	a	512	U
1	a	517	G
1	a	518	C
1	a	524	G
1	a	527	G7M
1	a	528	C
1	a	531	U
1	a	532	A
1	a	546	A
1	a	547	A
1	a	551	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	575	G
1	a	576	C

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Mol	Chain	Res	Type
1	a	577	G
1	a	633	G
1	a	642	A
1	a	653	U
1	a	661	G
1	a	665	A
1	a	686	U
1	a	723	U
1	a	724	G
1	a	733	G
1	a	748	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	816	A
1	a	817	C
1	a	819	A
1	a	832	G
1	a	841	C
1	a	842	U
1	a	843	U
1	a	844	G
1	a	845	A
1	a	876	C
1	a	878	A
1	a	889	A
1	a	890	G
1	a	926	G
1	a	934	C
1	a	935	A
1	a	942	G
1	a	960	U
1	a	966	2MG
1	a	968	A
1	a	969	A
1	a	974	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	993	G

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Mol	Chain	Res	Type
1	a	1004	A
1	a	1020	G
1	a	1032	G
1	a	1034	G
1	a	1043	G
1	a	1065	U
1	a	1085	U
1	a	1089	G
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1105	A
1	a	1134	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1158	C
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1169	A
1	a	1182	G
1	a	1196	A
1	a	1197	A
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1260	G
1	a	1278	G
1	a	1280	A
1	a	1287	A
1	a	1297	G
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C

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Mol	Chain	Res	Type
1	a	1338	G
1	a	1345	U
1	a	1346	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1396	A
1	a	1397	C
1	a	1398	A
1	a	1406	U
1	a	1419	G
1	a	1429	A
1	a	1441	A
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1497	G
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1520	C
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1536	C
1	a	1537	U
22	v	9	G
22	v	18	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	31	G
22	v	52	G
22	v	54	5MU
22	v	59	A
22	v	75	C
23	x	88	A
23	x	90	G
23	x	96	C
23	x	98	U

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Mol	Chain	Res	Type
23	x	104	U
23	x	108	A
23	x	109	C
23	x	110	G
23	x	111	G
23	x	112	C
23	x	113	C
23	x	114	C
23	x	115	A
23	x	116	U
23	x	117	C
23	x	118	G
23	x	119	G
23	x	120	U
23	x	121	U
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	133	C
23	x	134	C
24	y	8	G
24	y	15	C
24	y	18	G
24	y	20	G
24	y	29	G
24	y	31	A
24	y	40	C
24	y	45	U
24	y	46	G
24	y	47(F)	C
24	y	47(G)	C
24	y	47(H)	A
24	y	47(I)	G
24	y	47(J)	C
24	y	49	G
24	y	54	5MU
24	y	55	PSU

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Mol	Chain	Res	Type
24	y	56	C
24	y	60	U
24	y	61	C
24	y	64	G
24	y	66	G
24	y	73	G
26	A	10	A
26	A	15	G
26	A	23	G
26	A	27	G
26	A	34	U
26	A	60	G
26	A	63	A
26	A	71	A
26	A	74	A
26	A	75	G
26	A	91	A
26	A	101	A
26	A	102	U
26	A	118	A
26	A	120	U
26	A	125	A
26	A	131	A
26	A	138	U
26	A	139	U
26	A	142	A
26	A	181	A
26	A	196	A
26	A	199	A
26	A	204	A
26	A	205	G
26	A	216	A
26	A	222	A
26	A	228	C
26	A	230	G
26	A	232	G
26	A	248	G
26	A	255	A
26	A	277	G
26	A	278	A
26	A	279	A
26	A	285	G

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Mol	Chain	Res	Type
26	A	311	A
26	A	322	A
26	A	329	G
26	A	330	A
26	A	362	A
26	A	367	G
26	A	372	G
26	A	386	G
26	A	396	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	448	U
26	A	451	U
26	A	456	C
26	A	473	G
26	A	479	A
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A
26	A	508	A
26	A	509	C
26	A	529	A
26	A	530	G
26	A	531	C
26	A	532	A
26	A	533	G
26	A	549	G
26	A	562	U
26	A	563	A
26	A	573	U
26	A	603	A
26	A	614	A
26	A	615	U
26	A	616	A
26	A	622	G
26	A	637	A
26	A	646	U
26	A	647	G

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Mol	Chain	Res	Type
26	A	655	A
26	A	664	G
26	A	668	A
26	A	675	A
26	A	686	U
26	A	695	G
26	A	711	G
26	A	717	C
26	A	726	G
26	A	730	A
26	A	747	5MU
26	A	748	G
26	A	765	C
26	A	775	G
26	A	782	A
26	A	784	G
26	A	789	A
26	A	805	G
26	A	812	C
26	A	819	A
26	A	827	U
26	A	830	G
26	A	846	U
26	A	859	G
26	A	869	G
26	A	885	C
26	A	887	U
26	A	888	C
26	A	889	C
26	A	890	C
26	A	910	A
26	A	932	U
26	A	941	A
26	A	946	C
26	A	959	A
26	A	961	C
26	A	965	C
26	A	973	A
26	A	974	G
26	A	983	A
26	A	990	A
26	A	1009	A

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Mol	Chain	Res	Type
26	A	1012	U
26	A	1013	C
26	A	1022	G
26	A	1023	U
26	A	1026	G
26	A	1033	U
26	A	1040	A
26	A	1042	G
26	A	1043	C
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1057	A
26	A	1058	U
26	A	1059	G
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1067	A
26	A	1068	G
26	A	1069	A
26	A	1070	A
26	A	1071	G
26	A	1073	A
26	A	1076	C
26	A	1077	A
26	A	1078	U
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1092	C
26	A	1094	U
26	A	1100	C
26	A	1101	U
26	A	1110	G
26	A	1112	G
26	A	1119	U
26	A	1132	U
26	A	1133	A
26	A	1134	A

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Mol	Chain	Res	Type
26	A	1135	C
26	A	1142	A
26	A	1143	A
26	A	1157	G
26	A	1171	G
26	A	1175	A
26	A	1178	C
26	A	1180	U
26	A	1206	G
26	A	1210	G
26	A	1211	C
26	A	1236	G
26	A	1248	G
26	A	1253	A
26	A	1255	U
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1300	G
26	A	1301	A
26	A	1311	G
26	A	1314	C
26	A	1325	U
26	A	1329	U
26	A	1345	C
26	A	1359	A
26	A	1365	A
26	A	1378	A
26	A	1379	U
26	A	1383	A
26	A	1392	A
26	A	1394	U
26	A	1395	A
26	A	1401	G
26	A	1403	A
26	A	1407	G
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1437	C

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Mol	Chain	Res	Type
26	A	1452	G
26	A	1455	G
26	A	1458	U
26	A	1460	U
26	A	1468	U
26	A	1482	G
26	A	1490	A
26	A	1493	C
26	A	1497	U
26	A	1509	A
26	A	1515	A
26	A	1532	A
26	A	1534	U
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1566	A
26	A	1569	A
26	A	1578	U
26	A	1583	A
26	A	1608	A
26	A	1609	A
26	A	1619	G
26	A	1639	C
26	A	1646	C
26	A	1648	U
26	A	1649	G
26	A	1654	A
26	A	1660	G
26	A	1674	G
26	A	1675	C
26	A	1715	G
26	A	1738	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1784	A
26	A	1791	A
26	A	1799	G
26	A	1800	C
26	A	1801	A
26	A	1808	A

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Mol	Chain	Res	Type
26	A	1816	C
26	A	1829	A
26	A	1833	C
26	A	1847	A
26	A	1870	C
26	A	1871	A
26	A	1876	A
26	A	1906	G
26	A	1913	A
26	A	1927	A
26	A	1929	G
26	A	1930	G
26	A	1937	A
26	A	1941	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1992	G
26	A	1993	U
26	A	1997	C
26	A	2002	G
26	A	2021	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2032	G
26	A	2043	C
26	A	2051	A
26	A	2052	A
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	G7M
26	A	2070	A

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Mol	Chain	Res	Type
26	A	2080	A
26	A	2100	G
26	A	2105	U
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2116	G
26	A	2118	U
26	A	2119	A
26	A	2120	G
26	A	2125	G
26	A	2127	G
26	A	2129	C
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2134	A
26	A	2146	C
26	A	2147	A
26	A	2157	G
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2168	G
26	A	2171	A
26	A	2172	U
26	A	2173	A
26	A	2177	C
26	A	2178	C
26	A	2179	C
26	A	2182	U
26	A	2198	A
26	A	2204	G
26	A	2210	U
26	A	2211	A
26	A	2212	A
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G

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Mol	Chain	Res	Type
26	A	2251	OMG
26	A	2268	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2305	U
26	A	2308	G
26	A	2310	C
26	A	2312	U
26	A	2319	G
26	A	2322	A
26	A	2333	A
26	A	2334	U
26	A	2335	A
26	A	2336	A
26	A	2342	C
26	A	2347	C
26	A	2350	C
26	A	2354	C
26	A	2357	G
26	A	2383	G
26	A	2385	C
26	A	2402	U
26	A	2403	C
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2434	A
26	A	2436	G
26	A	2441	U
26	A	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2470	G
26	A	2476	A
26	A	2478	A
26	A	2480	C
26	A	2484	G
26	A	2494	G
26	A	2502	G
26	A	2504	PSU
26	A	2505	G

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Mol	Chain	Res	Type
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2520	C
26	A	2525	G
26	A	2529	G
26	A	2547	A
26	A	2554	U
26	A	2567	G
26	A	2581	G
26	A	2582	G
26	A	2585	U
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2629	U
26	A	2630	G
26	A	2639	A
26	A	2663	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2718	G
26	A	2726	A
26	A	2733	A
26	A	2744	G
26	A	2755	C
26	A	2758	A
26	A	2764	A
26	A	2765	A
26	A	2778	A
26	A	2791	G
26	A	2793	C
26	A	2797	U
26	A	2809	A
26	A	2818	U
26	A	2821	A
26	A	2833	U
26	A	2849	U
26	A	2872	A
26	A	2879	A
26	A	2884	U

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Mol	Chain	Res	Type
27	B	24	G
27	B	26	C
27	B	35	C
27	B	38	C
27	B	42	C
27	B	45	A
27	B	57	A
27	B	87	U
27	B	90	C
27	B	108	A
27	B	109	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	818	G
26	A	960	A
26	A	1042	G
26	A	1358	G
26	A	1875	G

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	a	967	1	18,22,23	0.89	2 (11%)	26,32,35	1.00	3 (11%)
26	6MZ	A	2030	26	18,25,26	0.99	1 (5%)	16,36,39	1.77	5 (31%)
26	PSU	A	2605	26	18,21,22	1.36	3 (16%)	22,30,33	1.94	4 (18%)
26	PSU	A	955	26	18,21,22	1.45	3 (16%)	22,30,33	2.07	3 (13%)
26	3TD	A	1915	26	18,22,23	4.08	7 (38%)	22,32,35	1.90	3 (13%)
26	PSU	A	1917	26	18,21,22	1.46	4 (22%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MU	v	54	22	19,22,23	1.45	6 (31%)	28,32,35	2.08	9 (32%)
1	4OC	a	1402	1	20,23,24	0.77	1 (5%)	26,32,35	1.15	2 (7%)
24	6IA	y	37	24	22,29,30	0.85	1 (4%)	22,41,44	2.11	3 (13%)
22	PSU	v	55	22	18,21,22	1.48	3 (16%)	22,30,33	1.93	4 (18%)
26	G7M	A	2069	26	20,26,27	1.58	4 (20%)	17,39,42	1.66	4 (23%)
22	4SU	v	8	22	18,21,22	1.77	5 (27%)	26,30,33	2.25	5 (19%)
26	2MG	A	1835	26	18,26,27	0.91	1 (5%)	16,38,41	1.32	3 (18%)
26	PSU	A	2604	26	18,21,22	1.43	2 (11%)	22,30,33	2.01	3 (13%)
22	H2U	v	20	22	18,21,22	1.01	2 (11%)	21,30,33	1.44	2 (9%)
26	PSU	A	2580	26	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)
1	MA6	a	1518	1	18,26,27	0.92	1 (5%)	19,38,41	2.02	6 (31%)
26	5MC	A	1962	26	18,22,23	0.89	1 (5%)	26,32,35	1.49	4 (15%)
26	OMG	A	2251	26,22	18,26,27	1.00	1 (5%)	19,38,41	1.09	2 (10%)
26	5MU	A	747	26	19,22,23	1.52	5 (26%)	28,32,35	1.95	6 (21%)
1	G7M	a	527	1	20,26,27	1.61	3 (15%)	17,39,42	1.77	5 (29%)
26	1MG	A	745	26	18,26,27	0.93	1 (5%)	19,39,42	1.23	2 (10%)
26	H2U	A	2449	26	18,21,22	1.16	3 (16%)	21,30,33	1.54	3 (14%)
26	2MG	A	2445	26	18,26,27	0.96	1 (5%)	16,38,41	1.22	3 (18%)
26	2MA	A	2503	26	17,25,26	1.06	2 (11%)	17,37,40	0.89	1 (5%)
1	2MG	a	1516	1	18,26,27	0.92	1 (5%)	16,38,41	1.13	2 (12%)
1	PSU	a	516	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	4 (18%)
1	UR3	a	1498	1	19,22,23	1.05	1 (5%)	26,32,35	1.90	5 (19%)
26	PSU	A	2457	26	18,21,22	1.35	2 (11%)	22,30,33	1.95	5 (22%)
1	2MG	a	966	1	18,26,27	0.94	1 (5%)	16,38,41	1.06	2 (12%)
1	2MG	a	1207	1	18,26,27	0.93	1 (5%)	16,38,41	1.15	2 (12%)
26	6MZ	A	1618	26	18,25,26	0.95	1 (5%)	16,36,39	2.21	4 (25%)
26	PSU	A	1911	26	18,21,22	1.42	3 (16%)	22,30,33	1.92	4 (18%)
1	MA6	a	1519	1	18,26,27	0.99	2 (11%)	19,38,41	1.89	4 (21%)
26	PSU	A	2504	26	18,21,22	1.42	4 (22%)	22,30,33	1.93	3 (13%)
24	5MU	y	54	24	19,22,23	1.51	4 (21%)	28,32,35	2.61	8 (28%)
26	PSU	A	746	26	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
24	H2U	y	19	24	18,21,22	1.25	3 (16%)	21,30,33	2.79	5 (23%)
1	5MC	a	1407	1	18,22,23	0.96	2 (11%)	26,32,35	1.31	3 (11%)
26	OMU	A	2552	26	19,22,23	1.22	3 (15%)	26,31,34	1.88	7 (26%)
24	PSU	y	55	24	18,21,22	1.38	3 (16%)	22,30,33	2.88	9 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	5MU	A	1939	26	19,22,23	1.40	6 (31%)	28,32,35	2.11	6 (21%)
26	OMC	A	2498	26	19,22,23	0.91	0	26,31,34	1.29	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	6MZ	A	2030	26	-	4/5/27/28	0/3/3/3
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	5/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	2/7/25/26	0/2/2/2
22	5MU	v	54	22	-	2/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
24	6IA	y	37	24	-	1/9/31/32	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
26	G7M	A	2069	26	2/2/5/5	2/3/25/26	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3
26	5MC	A	1962	26	-	5/7/25/26	0/2/2/2
26	OMG	A	2251	26,22	-	1/5/27/28	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
26	2MA	A	2503	26	-	2/3/25/26	0/3/3/3
1	2MG	a	1516	1	-	2/5/27/28	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	a	1207	1	-	1/5/27/28	0/3/3/3
26	6MZ	A	1618	26	-	2/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/7/29/30	0/3/3/3
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
24	5MU	y	54	24	-	3/7/25/26	0/2/2/2
26	PSU	A	746	26	-	1/7/25/26	0/2/2/2
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
24	PSU	y	55	24	-	5/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/9/27/28	0/2/2/2

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	11.65	1.48	1.35
26	A	1915	3TD	C2-N1	9.25	1.49	1.37
26	A	1915	3TD	C6-N1	5.96	1.46	1.36
1	a	527	G7M	C5-C4	4.74	1.48	1.39
22	v	8	4SU	C4-S4	-4.65	1.59	1.68
26	A	2069	G7M	C5-C4	4.40	1.47	1.39
24	y	54	5MU	C2-N1	3.86	1.44	1.38
24	y	55	PSU	C2-N1	-3.85	1.31	1.36
26	A	1915	3TD	O4-C4	-3.49	1.15	1.23
26	A	955	PSU	C6-C5	3.49	1.39	1.35
26	A	1911	PSU	C6-C5	3.47	1.39	1.35
26	A	1917	PSU	C6-C5	3.44	1.39	1.35
26	A	2504	PSU	C6-C5	3.37	1.39	1.35
1	a	516	PSU	C6-C5	3.36	1.39	1.35
22	v	55	PSU	C6-C5	3.36	1.39	1.35
26	A	1915	3TD	C2-N3	3.35	1.46	1.38
24	y	19	H2U	C2-N3	-3.34	1.32	1.38
26	A	2604	PSU	C6-C5	3.30	1.39	1.35
26	A	2580	PSU	C6-C5	3.20	1.39	1.35
22	v	55	PSU	C4-N3	-3.20	1.32	1.38
22	v	8	4SU	C5-C4	-3.16	1.38	1.42
26	A	2457	PSU	C6-C5	3.08	1.38	1.35
26	A	746	PSU	C6-C5	3.07	1.38	1.35
26	A	2604	PSU	C4-N3	-3.00	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	747	5MU	C6-C5	2.98	1.39	1.34
26	A	1618	6MZ	C5-C4	2.97	1.48	1.40
22	v	8	4SU	C4-N3	-2.96	1.34	1.37
26	A	747	5MU	C2-N1	2.95	1.43	1.38
26	A	2030	6MZ	C5-C4	2.94	1.48	1.40
26	A	2449	H2U	C2-N3	-2.92	1.32	1.38
26	A	2605	PSU	C4-N3	-2.91	1.33	1.38
24	y	54	5MU	C4-N3	-2.90	1.33	1.38
26	A	2605	PSU	C6-C5	2.89	1.38	1.35
22	v	54	5MU	C2-N1	2.81	1.42	1.38
26	A	747	5MU	C4-N3	-2.81	1.33	1.38
1	a	527	G7M	C6-N1	-2.79	1.33	1.37
22	v	54	5MU	C4-N3	-2.79	1.33	1.38
26	A	2504	PSU	C4-N3	-2.78	1.33	1.38
26	A	1911	PSU	C4-N3	-2.78	1.33	1.38
26	A	955	PSU	C4-N3	-2.77	1.33	1.38
1	a	1498	UR3	C2-N1	2.76	1.42	1.38
26	A	1939	5MU	C6-C5	2.75	1.39	1.34
1	a	966	2MG	C6-N1	-2.73	1.33	1.37
26	A	746	PSU	C4-N3	-2.71	1.33	1.38
26	A	1939	5MU	C4-N3	-2.69	1.33	1.38
26	A	2457	PSU	C4-N3	-2.67	1.33	1.38
26	A	2445	2MG	C6-N1	-2.65	1.33	1.37
1	a	1518	MA6	C5-C4	2.64	1.47	1.40
22	v	20	H2U	C2-N3	-2.63	1.33	1.38
24	y	55	PSU	C6-N1	-2.63	1.31	1.36
26	A	2580	PSU	C4-N3	-2.62	1.34	1.38
26	A	2069	G7M	C6-N1	-2.62	1.34	1.37
26	A	2449	H2U	C4-N3	-2.60	1.33	1.37
26	A	1917	PSU	C4-N3	-2.60	1.34	1.38
1	a	1519	MA6	C5-C4	2.59	1.47	1.40
1	a	1407	5MC	C6-C5	2.58	1.38	1.34
1	a	527	G7M	O2'-C2'	-2.57	1.36	1.43
26	A	2069	G7M	O2'-C2'	-2.57	1.36	1.43
24	y	37	6IA	C5-C4	2.56	1.47	1.40
24	y	19	H2U	O4-C4	-2.54	1.18	1.23
26	A	1915	3TD	O2-C2	-2.54	1.18	1.23
26	A	2552	OMU	C4-N3	-2.53	1.34	1.38
1	a	1207	2MG	C6-N1	-2.52	1.34	1.37
22	v	55	PSU	C2-N3	-2.51	1.33	1.37
26	A	2251	OMG	C6-N1	-2.46	1.34	1.37
26	A	1962	5MC	C6-N1	-2.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	54	5MU	C6-C5	2.43	1.38	1.34
1	a	967	5MC	C6-C5	2.42	1.38	1.34
22	v	20	H2U	C4-N3	-2.39	1.33	1.37
26	A	2449	H2U	C2-N1	-2.39	1.32	1.35
24	y	55	PSU	C4-N3	-2.38	1.34	1.38
1	a	1516	2MG	C6-N1	-2.38	1.34	1.37
26	A	747	5MU	C4-C5	2.36	1.48	1.44
24	y	54	5MU	C6-C5	2.36	1.38	1.34
1	a	516	PSU	C4-N3	-2.35	1.34	1.38
24	y	19	H2U	C4-N3	-2.31	1.33	1.37
26	A	1835	2MG	C6-N1	-2.28	1.34	1.37
26	A	1939	5MU	C4-C5	2.24	1.48	1.44
24	y	54	5MU	C6-N1	-2.24	1.34	1.38
22	v	54	5MU	C6-N1	-2.22	1.34	1.38
26	A	1939	5MU	C6-N1	-2.22	1.34	1.38
26	A	2503	2MA	C2-N3	2.22	1.35	1.31
26	A	1915	3TD	C4-N3	2.21	1.45	1.40
26	A	745	1MG	C5-C4	2.20	1.48	1.43
26	A	2552	OMU	C2-N3	-2.15	1.34	1.38
26	A	1917	PSU	C4-C5	2.14	1.50	1.44
26	A	2069	G7M	C8-N9	2.14	1.37	1.33
26	A	2503	2MA	C5-C4	2.13	1.48	1.43
26	A	2605	PSU	C2-N3	-2.13	1.33	1.37
26	A	1939	5MU	C2-N1	2.12	1.41	1.38
22	v	54	5MU	C2-N3	-2.11	1.34	1.38
1	a	1407	5MC	C6-N1	-2.10	1.34	1.38
26	A	1939	5MU	C2-N3	-2.09	1.34	1.38
26	A	2504	PSU	C2-N3	-2.09	1.33	1.37
1	a	967	5MC	C6-N1	-2.09	1.34	1.38
22	v	54	5MU	C4-C5	2.09	1.48	1.44
1	a	1519	MA6	C6-N1	2.08	1.36	1.33
26	A	2504	PSU	C4-C5	2.07	1.50	1.44
26	A	747	5MU	C2-N3	-2.04	1.34	1.38
26	A	1917	PSU	C2-N1	-2.04	1.34	1.36
26	A	1911	PSU	C2-N3	-2.04	1.34	1.37
26	A	2552	OMU	C2-N1	2.03	1.41	1.38
26	A	955	PSU	C2-N1	-2.02	1.34	1.36
22	v	8	4SU	C2-N3	-2.02	1.34	1.38
22	v	8	4SU	C2-N1	2.01	1.41	1.38
1	a	1402	4OC	C6-C5	2.00	1.39	1.35

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	19	H2U	C4-N3-C2	-8.63	118.63	125.79
24	y	37	6IA	C2-N1-C6	7.92	123.38	116.59
24	y	55	PSU	C6-C5-C4	-6.71	113.51	118.20
26	A	955	PSU	N1-C2-N3	6.62	122.63	115.13
26	A	2604	PSU	N1-C2-N3	6.61	122.62	115.13
24	y	19	H2U	C5-C4-N3	6.49	123.94	116.65
26	A	1618	6MZ	C2-N1-C6	6.29	121.99	116.59
26	A	2504	PSU	N1-C2-N3	6.24	122.20	115.13
26	A	2457	PSU	N1-C2-N3	6.08	122.02	115.13
1	a	1498	UR3	C4-N3-C2	-6.06	118.86	124.56
26	A	2580	PSU	N1-C2-N3	6.05	121.98	115.13
26	A	2605	PSU	N1-C2-N3	6.05	121.98	115.13
22	v	55	PSU	N1-C2-N3	6.03	121.97	115.13
22	v	8	4SU	C4-N3-C2	-5.97	121.55	127.34
26	A	746	PSU	N1-C2-N3	5.91	121.83	115.13
26	A	1917	PSU	N1-C2-N3	5.86	121.76	115.13
22	v	8	4SU	C5-C4-N3	5.83	120.10	114.69
24	y	54	5MU	O4-C4-C5	-5.81	118.17	124.90
26	A	1911	PSU	N1-C2-N3	5.75	121.65	115.13
24	y	55	PSU	O2-C2-N1	-5.61	116.61	122.79
24	y	55	PSU	N1-C2-N3	5.50	121.36	115.13
1	a	516	PSU	N1-C2-N3	5.42	121.27	115.13
26	A	2449	H2U	C4-N3-C2	-5.38	121.33	125.79
22	v	8	4SU	C5-C4-S4	-5.35	117.57	124.47
26	A	1939	5MU	C4-N3-C2	-5.28	120.52	127.35
24	y	54	5MU	C5-C4-N3	5.23	119.78	115.31
24	y	54	5MU	C1'-N1-C2	5.19	126.96	117.57
26	A	747	5MU	N3-C2-N1	5.07	121.62	114.89
26	A	1915	3TD	N1-C2-N3	4.98	120.07	116.14
26	A	1939	5MU	N3-C2-N1	4.86	121.34	114.89
26	A	1939	5MU	C5-C4-N3	4.77	119.38	115.31
24	y	54	5MU	C4-N3-C2	-4.70	121.26	127.35
24	y	55	PSU	C4-N3-C2	-4.67	119.61	126.34
26	A	1915	3TD	C4-N3-C2	-4.66	119.56	124.61
26	A	747	5MU	C4-N3-C2	-4.66	121.32	127.35
24	y	54	5MU	N3-C2-N1	4.61	121.01	114.89
24	y	19	H2U	O4-C4-C5	-4.59	112.36	122.17
22	v	54	5MU	C4-N3-C2	-4.58	121.42	127.35
1	a	1519	MA6	C4-C5-N7	-4.55	104.65	109.40
26	A	2030	6MZ	C4-C5-N7	-4.48	104.73	109.40
22	v	54	5MU	N3-C2-N1	4.43	120.78	114.89
22	v	54	5MU	C5-C4-N3	4.43	119.09	115.31
26	A	2552	OMU	N3-C2-N1	4.38	120.70	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	955	PSU	O2-C2-N1	-4.35	118.00	122.79
26	A	1618	6MZ	C9-N6-C6	-4.31	119.16	122.87
26	A	2605	PSU	C4-N3-C2	-4.27	120.18	126.34
1	a	1498	UR3	C1'-N1-C2	4.23	124.14	116.99
26	A	1911	PSU	C4-N3-C2	-4.17	120.33	126.34
26	A	1962	5MC	C5-C6-N1	-4.11	119.11	123.34
26	A	2552	OMU	C1'-N1-C2	4.09	124.97	117.57
1	a	1518	MA6	C4-C5-N7	-4.08	105.15	109.40
26	A	1939	5MU	O4-C4-C5	-4.06	120.19	124.90
1	a	1518	MA6	C9-N6-C6	-4.05	107.25	119.51
24	y	54	5MU	O2-C2-N3	-4.04	113.97	121.50
26	A	2457	PSU	C4-N3-C2	-4.04	120.52	126.34
26	A	1915	3TD	O4-C4-N3	-4.04	112.90	120.30
26	A	746	PSU	C4-N3-C2	-4.03	120.53	126.34
26	A	747	5MU	C5-C4-N3	4.02	118.74	115.31
26	A	1939	5MU	C5-C6-N1	-3.98	119.25	123.34
26	A	2604	PSU	C4-N3-C2	-3.96	120.64	126.34
26	A	2552	OMU	C4-N3-C2	-3.92	121.41	126.58
22	v	20	H2U	C4-N3-C2	-3.92	122.54	125.79
24	y	37	6IA	N3-C2-N1	-3.91	122.56	128.68
26	A	2069	G7M	O3'-C3'-C4'	3.91	122.36	111.05
26	A	2504	PSU	C4-N3-C2	-3.89	120.73	126.34
22	v	55	PSU	C4-N3-C2	-3.88	120.74	126.34
24	y	55	PSU	O4-C4-C5	-3.88	113.90	124.05
26	A	2498	OMC	O2-C2-N3	-3.86	116.05	122.33
26	A	955	PSU	C4-N3-C2	-3.86	120.78	126.34
1	a	1519	MA6	N3-C2-N1	-3.77	122.78	128.68
1	a	1519	MA6	C10-N6-C6	-3.77	108.10	119.51
1	a	516	PSU	C4-N3-C2	-3.77	120.91	126.34
1	a	1518	MA6	N1-C6-N6	-3.75	113.11	117.06
24	y	54	5MU	C1'-N1-C6	-3.74	114.89	121.12
26	A	2580	PSU	C4-N3-C2	-3.74	120.95	126.34
26	A	1917	PSU	O2-C2-N1	-3.73	118.69	122.79
22	v	8	4SU	N3-C2-N1	3.71	119.81	114.89
22	v	54	5MU	O4-C4-C5	-3.69	120.62	124.90
26	A	2604	PSU	O2-C2-N1	-3.66	118.76	122.79
1	a	1518	MA6	N3-C2-N1	-3.64	122.99	128.68
26	A	2457	PSU	O2-C2-N1	-3.57	118.86	122.79
1	a	1498	UR3	O2-C2-N3	-3.53	116.36	121.34
1	a	1407	5MC	O2-C2-N3	-3.51	116.61	122.33
1	a	1519	MA6	C10-N6-C9	-3.45	105.01	116.12
26	A	2580	PSU	O2-C2-N1	-3.39	119.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	746	PSU	O2-C2-N1	-3.36	119.09	122.79
1	a	527	G7M	O3'-C3'-C4'	3.27	120.50	111.05
22	v	54	5MU	C1'-N1-C2	3.26	123.48	117.57
1	a	527	G7M	O3'-C3'-C2'	3.26	122.37	111.82
26	A	747	5MU	O4-C4-C5	-3.25	121.14	124.90
26	A	2552	OMU	C5-C4-N3	3.23	119.68	114.84
24	y	54	5MU	C6-N1-C2	-3.23	118.03	121.30
1	a	1402	4OC	O2-C2-N3	-3.21	117.11	122.33
24	y	55	PSU	C6-N1-C2	-3.14	119.47	122.68
26	A	1618	6MZ	N3-C2-N1	-3.14	123.78	128.68
26	A	1917	PSU	C4-N3-C2	-3.11	121.86	126.34
1	a	1498	UR3	C6-N1-C2	-3.07	119.03	121.79
26	A	2605	PSU	O2-C2-N1	-3.04	119.44	122.79
26	A	747	5MU	C5-C6-N1	-3.04	120.21	123.34
26	A	2504	PSU	O2-C2-N1	-3.01	119.48	122.79
26	A	1962	5MC	N4-C4-N3	3.00	123.95	118.48
1	a	516	PSU	O2-C2-N1	-2.96	119.54	122.79
26	A	1962	5MC	C5-C4-N4	-2.94	117.08	121.48
26	A	1911	PSU	O2-C2-N1	-2.92	119.57	122.79
26	A	2030	6MZ	C9-N6-C6	-2.92	120.36	122.87
26	A	2552	OMU	O2-C2-N3	-2.88	116.14	121.50
24	y	55	PSU	O4-C4-N3	2.86	125.60	120.12
22	v	54	5MU	C1'-N1-C6	-2.81	116.44	121.12
1	a	1407	5MC	C5-C6-N1	-2.80	120.46	123.34
26	A	1835	2MG	C5-C6-N1	2.78	118.87	113.95
22	v	54	5MU	C5-C6-N1	-2.78	120.48	123.34
26	A	1835	2MG	CM2-N2-C2	-2.78	117.73	123.86
26	A	2069	G7M	O3'-C3'-C2'	2.75	120.71	111.82
26	A	747	5MU	O2-C2-N3	-2.69	116.49	121.50
26	A	745	1MG	C8-N7-C5	2.65	108.05	102.99
22	v	54	5MU	O2-C2-N3	-2.64	116.59	121.50
24	y	37	6IA	C4-C5-N7	-2.63	106.65	109.40
1	a	527	G7M	C5'-C4'-C3'	2.63	125.03	115.18
22	v	55	PSU	C6-C5-C4	-2.61	116.37	118.20
1	a	1407	5MC	C5-C4-N3	-2.60	118.87	121.67
26	A	1917	PSU	C6-C5-C4	-2.58	116.39	118.20
26	A	2552	OMU	O4-C4-C5	-2.57	120.64	125.16
26	A	1939	5MU	O2-C2-N1	-2.57	119.37	122.79
26	A	2030	6MZ	C2-N1-C6	2.56	118.79	116.59
26	A	2445	2MG	CM2-N2-C2	-2.56	118.21	123.86
26	A	1962	5MC	C5-C4-N3	-2.56	118.91	121.67
26	A	1618	6MZ	C4-C5-N7	-2.56	106.73	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2498	OMC	O2-C2-N1	2.56	124.17	118.89
22	v	55	PSU	O2-C2-N3	-2.53	117.05	121.82
1	a	527	G7M	C3'-C2'-C1'	2.48	104.71	100.98
24	y	19	H2U	C5-C6-N1	-2.43	103.61	111.61
26	A	2498	OMC	CM2-O2'-C2'	-2.42	108.18	114.52
26	A	2445	2MG	C8-N7-C5	2.41	107.59	102.99
26	A	2030	6MZ	C1'-N9-C4	2.39	130.84	126.64
26	A	2251	OMG	C8-N7-C5	2.38	107.53	102.99
26	A	2445	2MG	C5-C6-N1	2.37	118.14	113.95
26	A	2069	G7M	C5'-C4'-C3'	2.37	124.07	115.18
1	a	1207	2MG	C5-C6-N1	2.37	118.14	113.95
1	a	967	5MC	C5-C6-N1	-2.36	120.91	123.34
1	a	1402	4OC	C6-C5-C4	2.35	119.83	116.96
26	A	746	PSU	C5-C6-N1	-2.35	118.59	122.11
26	A	2498	OMC	C1'-N1-C2	2.35	123.66	118.42
1	a	1498	UR3	C3U-N3-C4	2.34	121.24	117.89
1	a	1518	MA6	C10-N6-C9	-2.33	108.61	116.12
26	A	745	1MG	C5-C6-N1	2.32	117.39	113.90
1	a	527	G7M	O4'-C4'-C5'	2.32	117.01	109.37
26	A	1835	2MG	C8-N7-C5	2.32	107.41	102.99
1	a	1516	2MG	C5-C6-N1	2.29	117.99	113.95
24	y	55	PSU	C5-C6-N1	2.29	125.53	122.11
26	A	2069	G7M	C3'-C2'-C1'	2.28	104.41	100.98
1	a	1518	MA6	C3'-C2'-C1'	2.28	104.41	100.98
1	a	1207	2MG	C8-N7-C5	2.27	107.32	102.99
1	a	516	PSU	C6-C5-C4	-2.27	116.61	118.20
22	v	54	5MU	C5M-C5-C4	2.26	121.26	118.77
1	a	966	2MG	C5-C6-N1	2.25	117.93	113.95
26	A	2449	H2U	C5-C6-N1	-2.25	104.21	111.61
26	A	2457	PSU	C5-C6-N1	-2.24	118.75	122.11
1	a	1516	2MG	C8-N7-C5	2.24	107.25	102.99
26	A	2605	PSU	C5-C6-N1	-2.22	118.77	122.11
26	A	2552	OMU	C6-N1-C2	-2.22	118.15	120.99
26	A	1911	PSU	C6-C5-C4	-2.19	116.66	118.20
26	A	2503	2MA	C8-N7-C5	2.17	107.12	102.99
22	v	8	4SU	S4-C4-N3	2.16	122.33	120.21
24	y	19	H2U	O4-C4-N3	2.16	123.70	120.28
26	A	2251	OMG	C5-C6-N1	2.15	117.74	113.95
26	A	2580	PSU	O4'-C1'-C2'	2.14	108.16	105.14
26	A	2449	H2U	O2-C2-N1	-2.13	120.43	123.11
26	A	2030	6MZ	N3-C2-N1	-2.12	125.37	128.68
24	y	55	PSU	O4'-C1'-C2'	2.12	108.13	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	20	H2U	C5-C4-N3	2.09	119.00	116.65
1	a	966	2MG	C8-N7-C5	2.08	106.96	102.99
1	a	967	5MC	C5-C4-N3	-2.08	119.43	121.67
1	a	967	5MC	CM5-C5-C6	-2.06	120.10	122.85
26	A	2457	PSU	O4'-C1'-C2'	2.00	107.97	105.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
26	A	2069	G7M	C3'
26	A	2069	G7M	C4'

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
22	v	54	5MU	C3'-C4'-C5'-O5'
22	v	54	5MU	O4'-C4'-C5'-O5'
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	y	19	H2U	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C6
24	y	55	PSU	O4'-C4'-C5'-O5'
26	A	1618	6MZ	O4'-C4'-C5'-O5'
26	A	1618	6MZ	C3'-C4'-C5'-O5'
26	A	1915	3TD	O4'-C1'-C5-C4
26	A	1915	3TD	C2'-C1'-C5-C6
26	A	1915	3TD	O4'-C1'-C5-C6
26	A	1917	PSU	O4'-C4'-C5'-O5'
26	A	1962	5MC	C2'-C1'-N1-C2
26	A	1962	5MC	C2'-C1'-N1-C6
26	A	2030	6MZ	N1-C6-N6-C9
26	A	2445	2MG	O4'-C4'-C5'-O5'
26	A	2445	2MG	C3'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
26	A	2552	OMU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
26	A	2552	OMU	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C2
26	A	1915	3TD	O4'-C4'-C5'-O5'
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2069	G7M	O4'-C4'-C5'-O5'
26	A	2504	PSU	C3'-C4'-C5'-O5'
24	y	55	PSU	C3'-C4'-C5'-O5'
26	A	1915	3TD	C3'-C4'-C5'-O5'
26	A	1917	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C10
1	a	1516	2MG	O4'-C4'-C5'-O5'
24	y	54	5MU	C4'-C5'-O5'-P
1	a	1519	MA6	C5-C6-N6-C9
26	A	2030	6MZ	O4'-C4'-C5'-O5'
26	A	2069	G7M	C3'-C4'-C5'-O5'
24	y	37	6IA	N6-C12-C13-C14
26	A	2503	2MA	C4'-C5'-O5'-P
24	y	19	H2U	O4'-C1'-N1-C2
22	v	20	H2U	C4'-C5'-O5'-P
24	y	55	PSU	C4'-C5'-O5'-P
24	y	54	5MU	C2'-C1'-N1-C6
26	A	1962	5MC	O4'-C1'-N1-C6
26	A	2030	6MZ	C4'-C5'-O5'-P
1	a	1207	2MG	C3'-C4'-C5'-O5'
26	A	2251	OMG	O4'-C4'-C5'-O5'
24	y	55	PSU	O4'-C1'-C5-C4
1	a	1516	2MG	C3'-C4'-C5'-O5'
24	y	54	5MU	C2'-C1'-N1-C2
24	y	55	PSU	O4'-C1'-C5-C6
26	A	746	PSU	O4'-C1'-C5-C6
26	A	1962	5MC	O4'-C1'-N1-C2
26	A	2503	2MA	O4'-C4'-C5'-O5'
26	A	1962	5MC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
61	GNP	z	701	62	29,34,34	1.52	4 (13%)	33,54,54	1.73	8 (24%)
60	SEC	y	701	24	2,5,6	0.63	0	0,5,7	-	-
59	FME	v	101	22	8,9,10	1.01	0	7,9,11	1.31	1 (14%)

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
61	GNP	z	701	62	-	6/14/38/38	0/3/3/3
60	SEC	y	701	24	-	0/0/4/6	-
59	FME	v	101	22	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	PB-N3B	4.30	1.74	1.63
61	z	701	GNP	PG-N3B	4.05	1.74	1.63
61	z	701	GNP	C5-C6	3.25	1.47	1.41
61	z	701	GNP	C5-C4	2.03	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	z	701	GNP	C2-N3-C4	5.09	121.17	115.36
61	z	701	GNP	C4-C5-C6	-4.07	116.91	120.80
61	z	701	GNP	C3'-C2'-C1'	3.04	105.56	100.98
61	z	701	GNP	N3-C2-N1	-2.99	123.24	127.22
61	z	701	GNP	C2-N1-C6	2.88	120.50	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	z	701	GNP	O3G-PG-O1G	-2.83	106.34	113.45
59	v	101	FME	CA-N-CN	2.51	126.68	122.82
61	z	701	GNP	C5-C6-N1	-2.43	120.11	123.43
61	z	701	GNP	PB-O3A-PA	-2.14	125.07	132.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

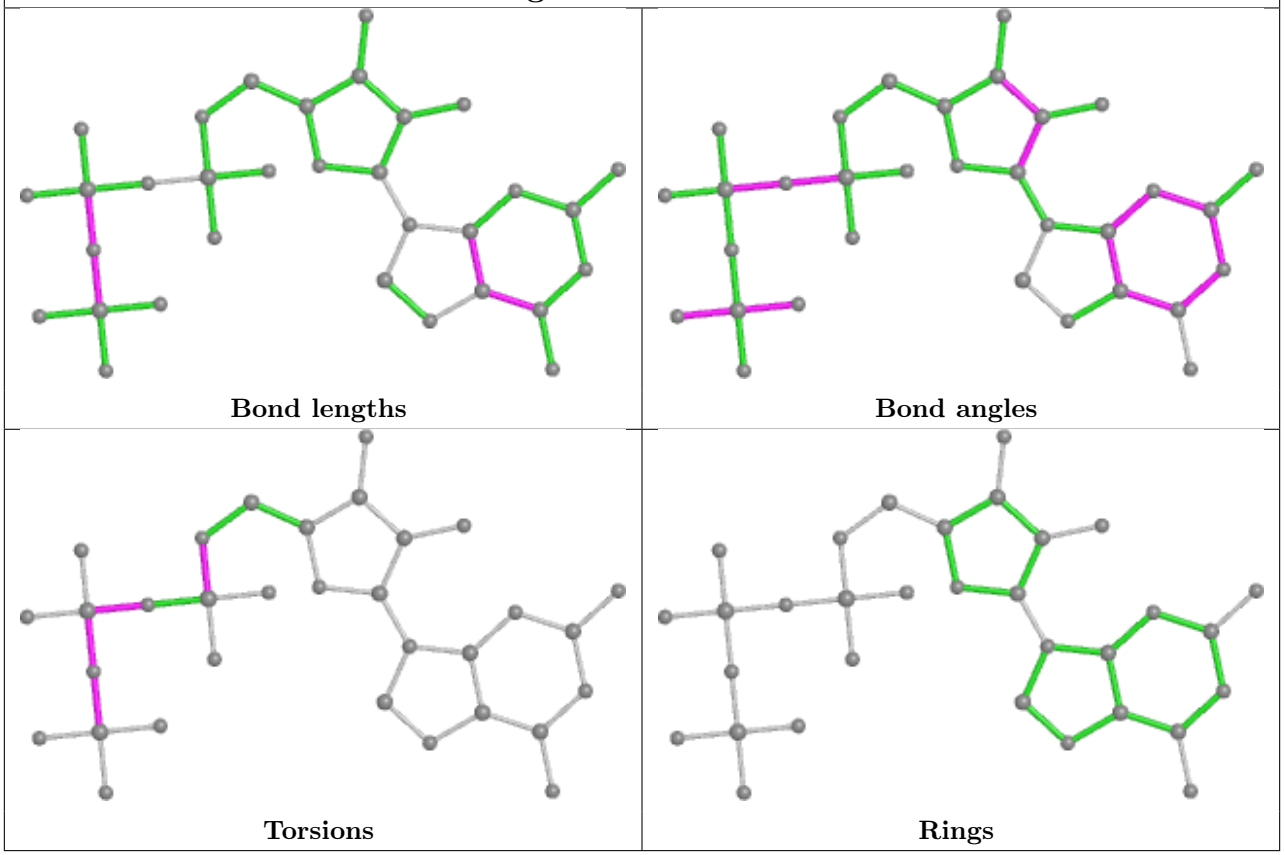
Mol	Chain	Res	Type	Atoms
59	v	101	FME	O1-CN-N-CA
59	v	101	FME	CA-CB-CG-SD
61	z	701	GNP	PB-N3B-PG-O1G
61	z	701	GNP	PG-N3B-PB-O1B
61	z	701	GNP	PA-O3A-PB-O1B
61	z	701	GNP	PA-O3A-PB-O2B
61	z	701	GNP	C5'-O5'-PA-O1A
59	v	101	FME	CB-CG-SD-CE
61	z	701	GNP	C5'-O5'-PA-O3A

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 then 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.

Ligand GNP z 701



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

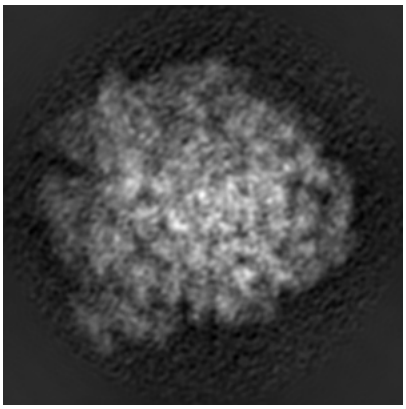
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-4122. These allow visual inspection of the internal detail of the map and identification of artifacts.

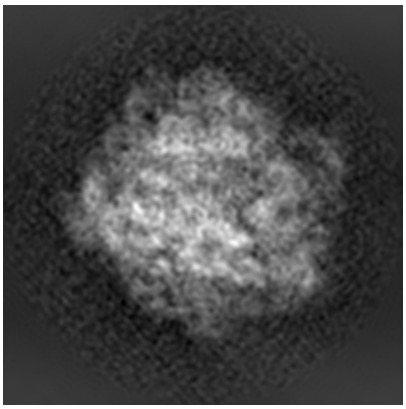
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

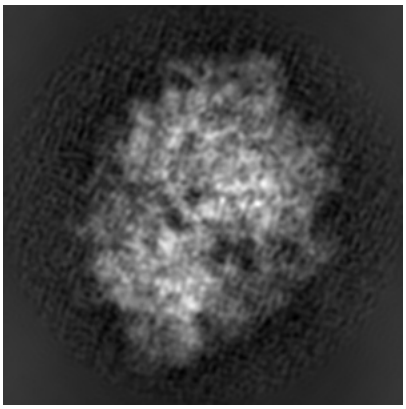
5.1.1 Primary map



X

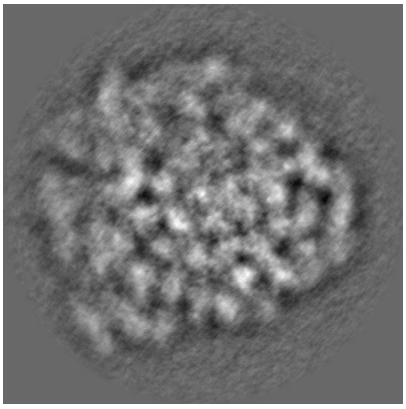


Y

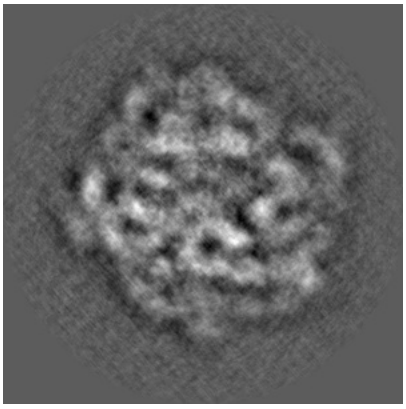


Z

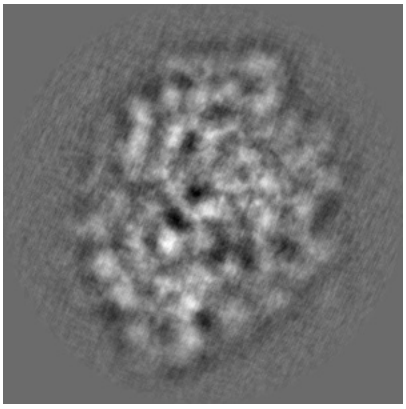
5.1.2 Raw map



X



Y

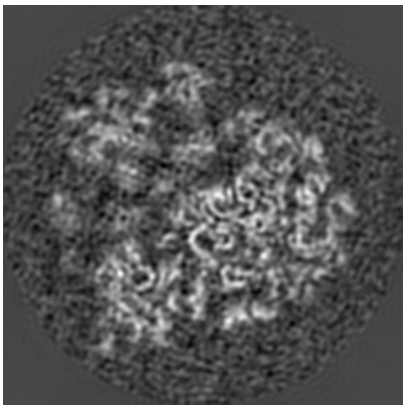


Z

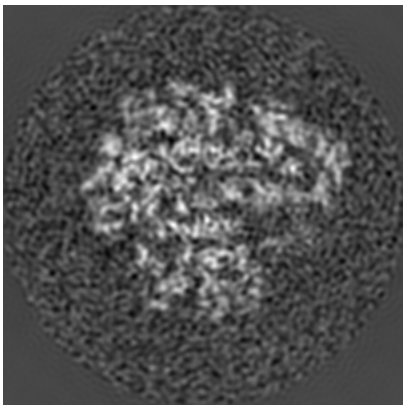
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

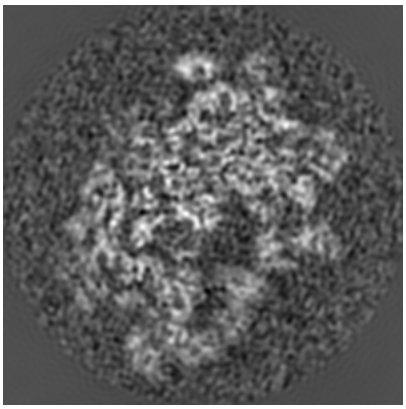
5.2.1 Primary map



X Index: 136

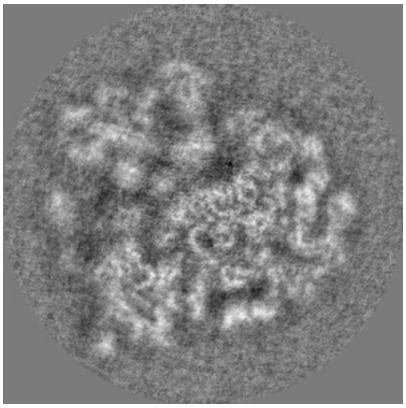


Y Index: 136

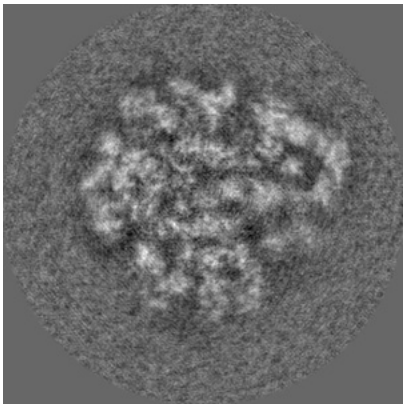


Z Index: 136

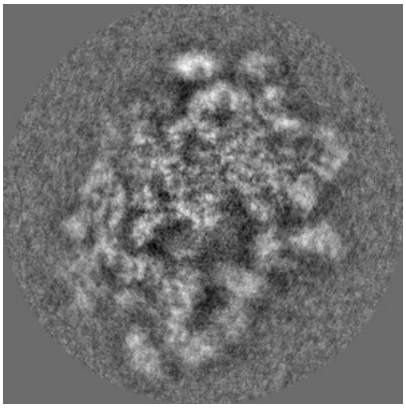
5.2.2 Raw map



X Index: 136



Y Index: 136

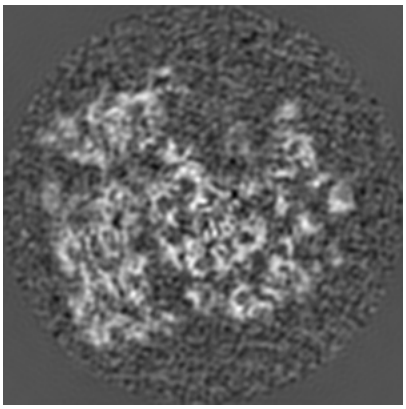


Z Index: 136

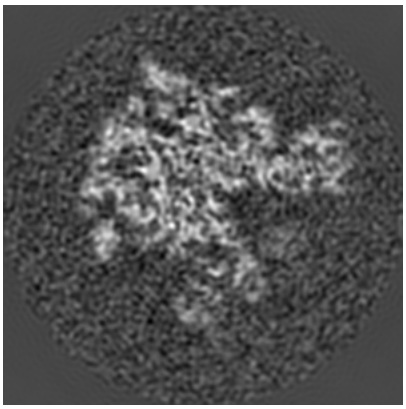
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

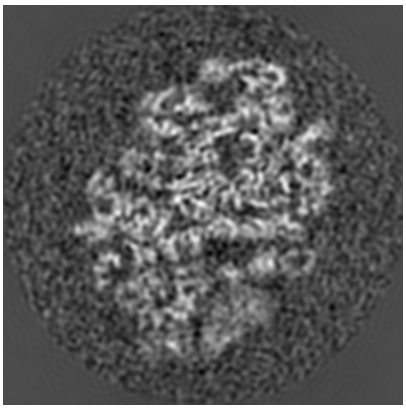
5.3.1 Primary map



X Index: 125

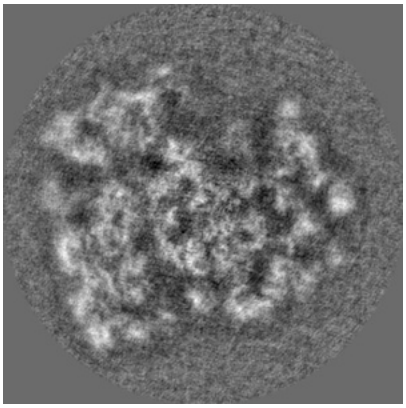


Y Index: 148

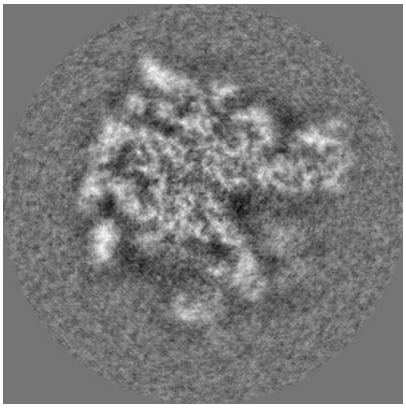


Z Index: 121

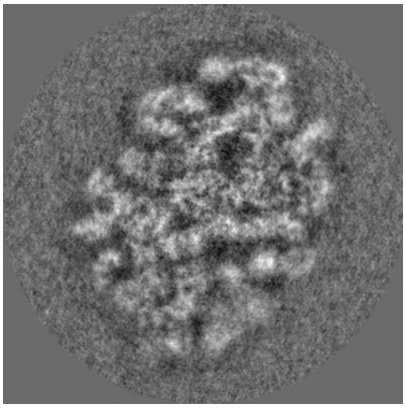
5.3.2 Raw map



X Index: 126



Y Index: 149

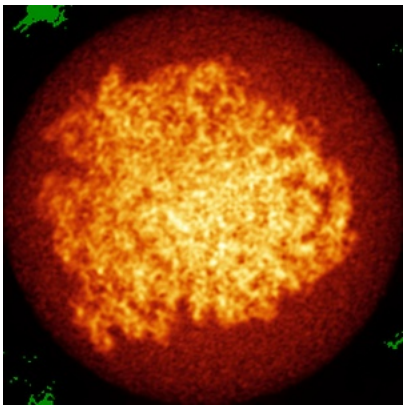


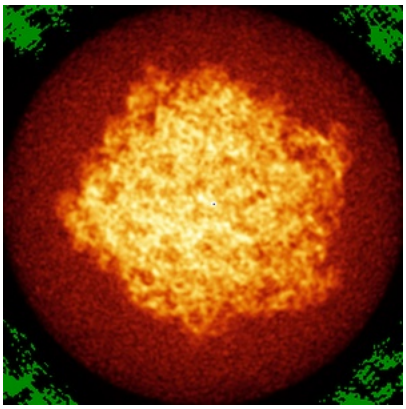
Z Index: 121

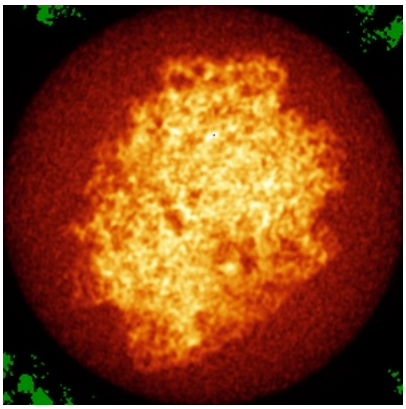
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

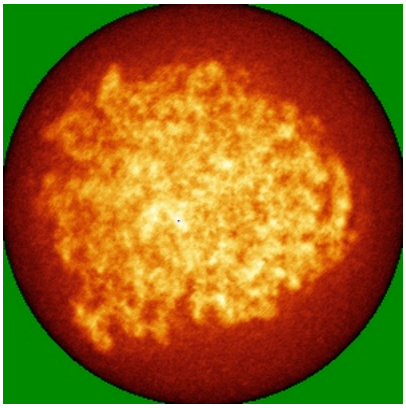
5.4.1 Primary map

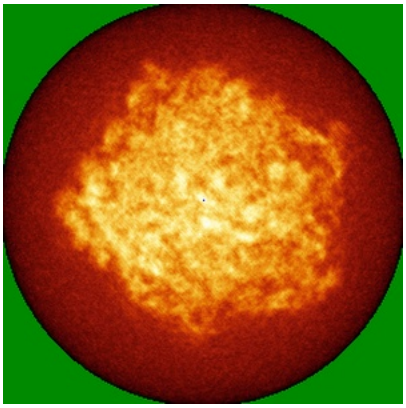

X

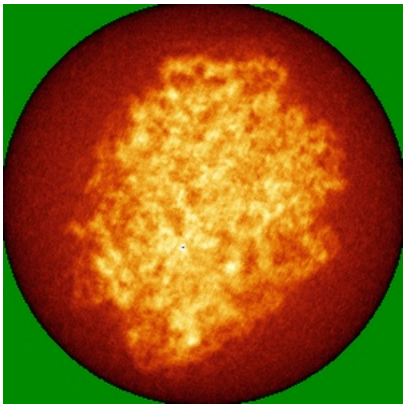

Y


Z

5.4.2 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.

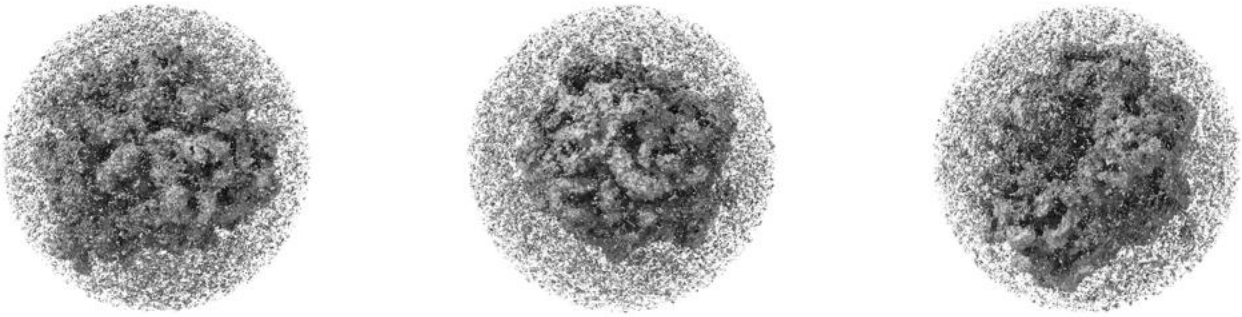
5.5 Orthogonal surface views (i)

5.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

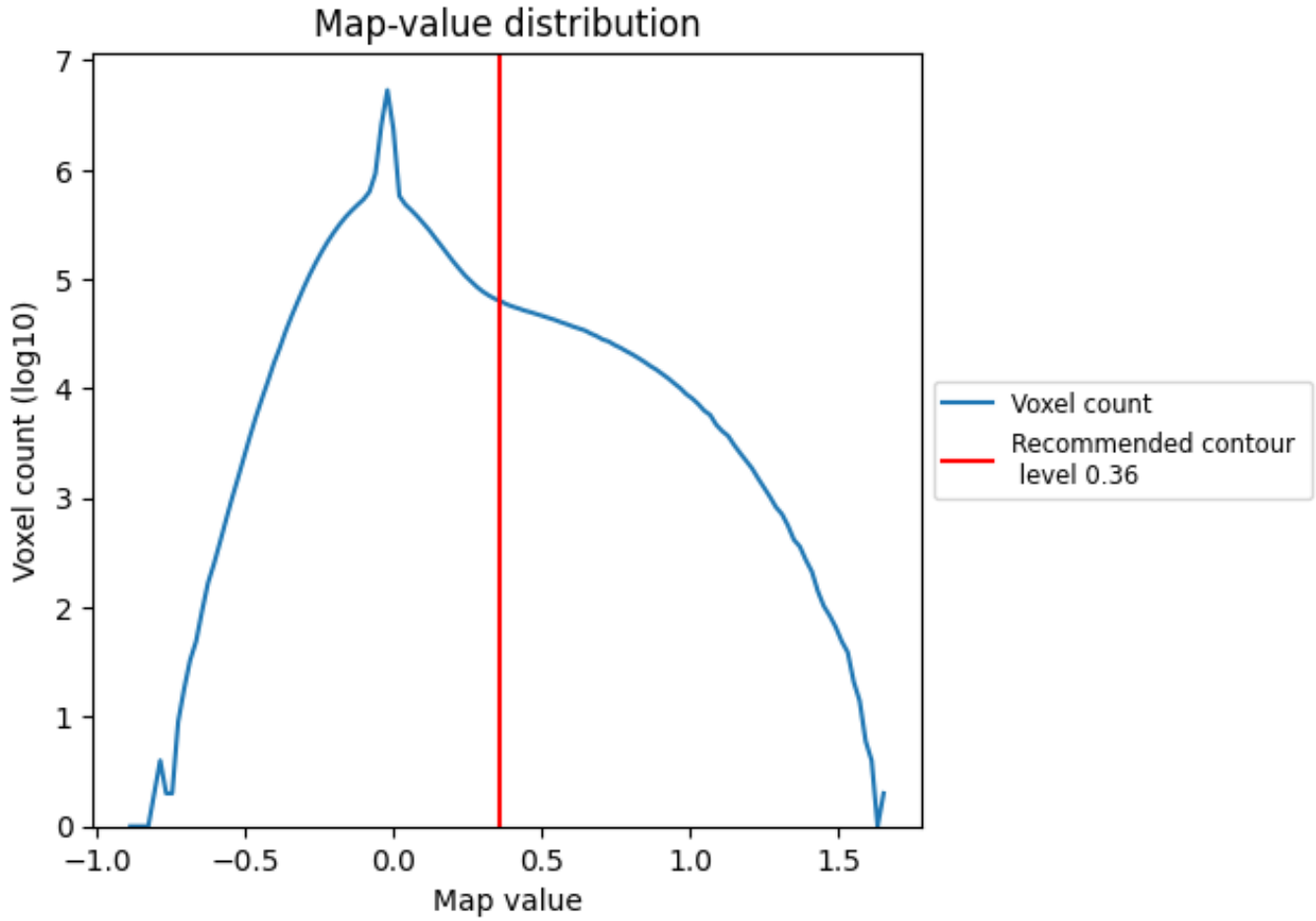
5.6 Mask visualisation (i)

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

6 Map analysis

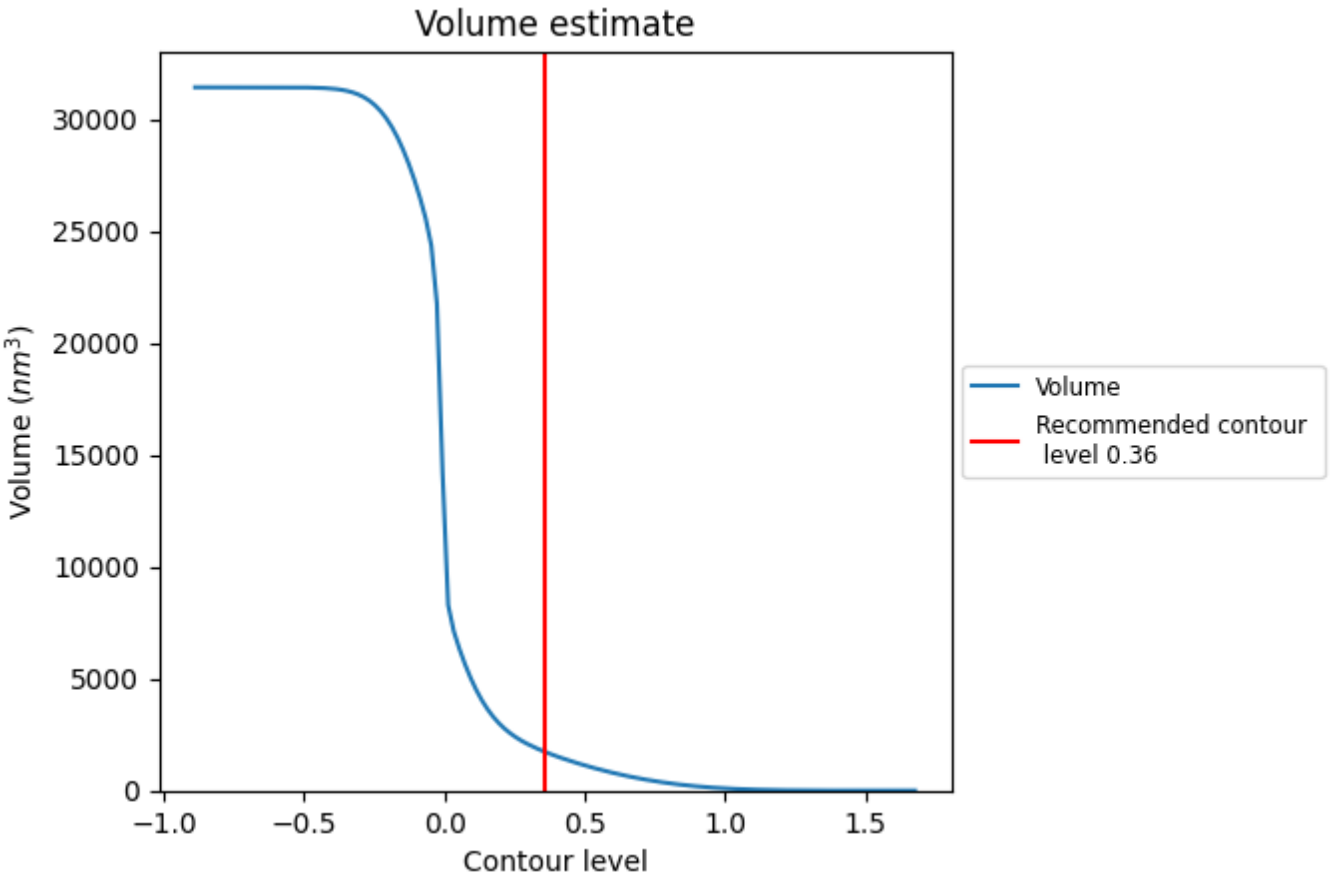
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



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.

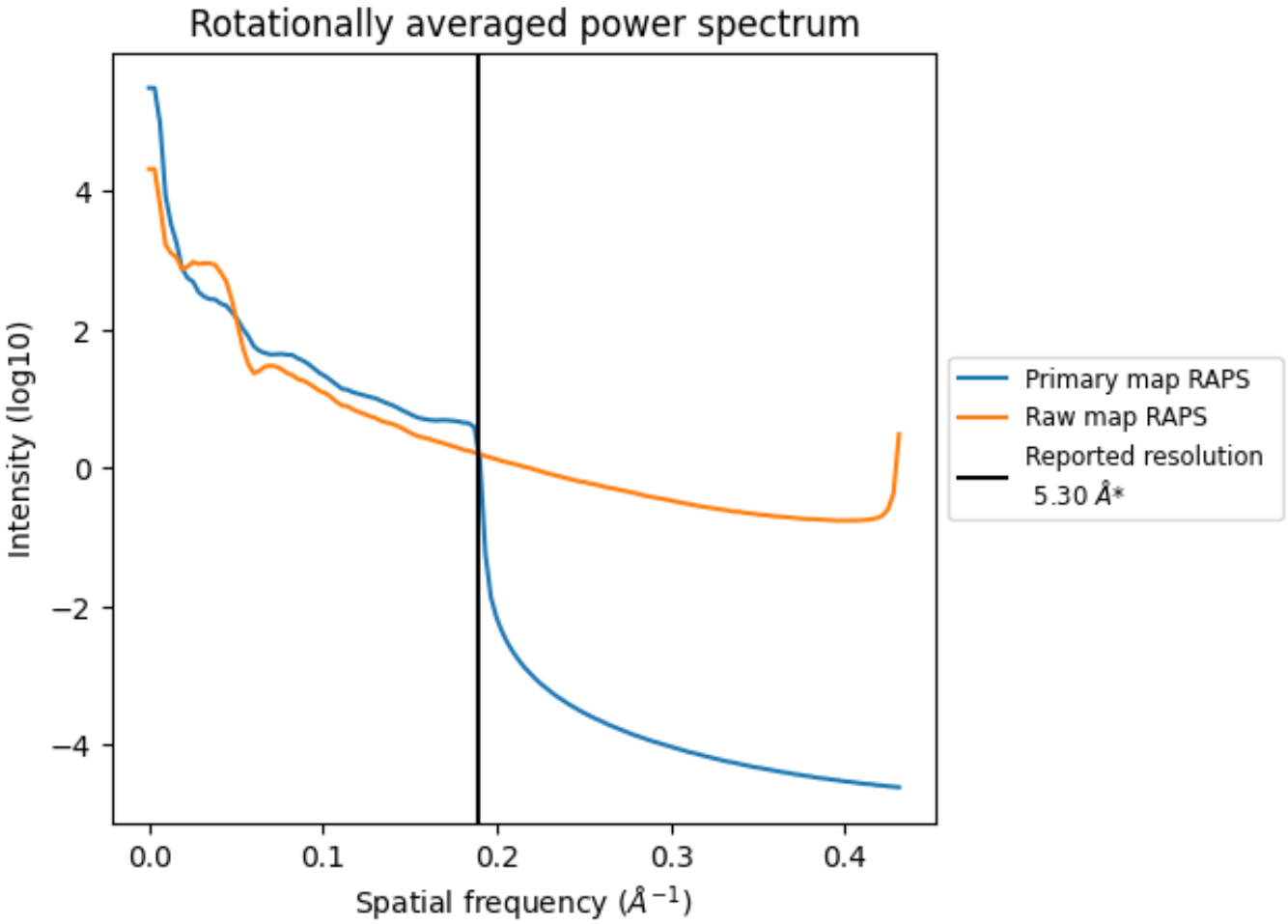
6.2 Volume estimate



The volume at the recommended contour level is 1719 nm^3; this corresponds to an approximate mass of 1553 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.

6.3 Rotationally averaged power spectrum (i)

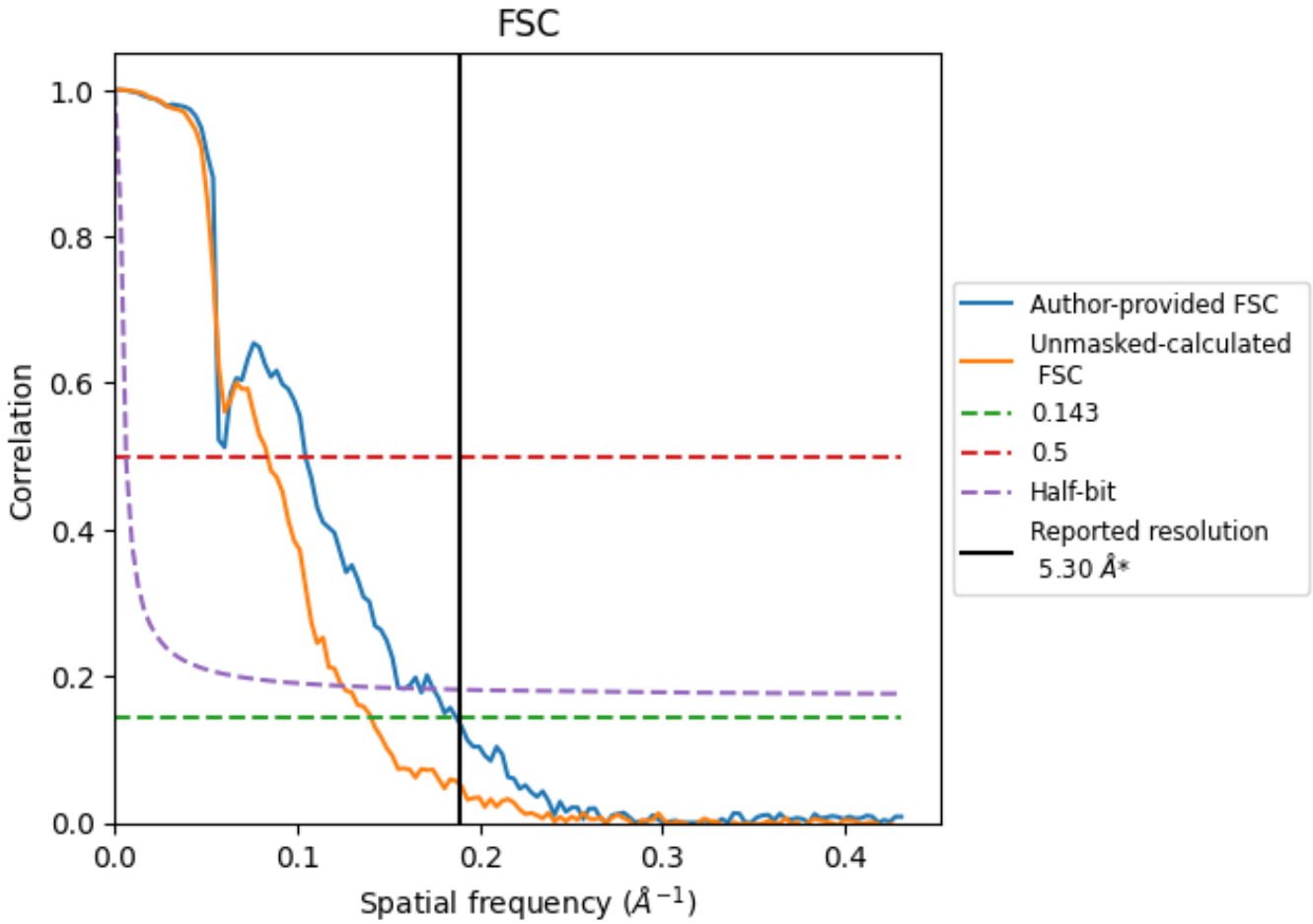


*Reported resolution corresponds to spatial frequency of 0.189 $Å^{-1}$

7 Fourier-Shell correlation

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.

7.1 FSC



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

7.2 Resolution estimates (i)

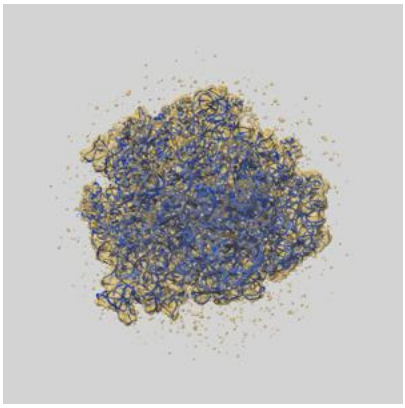
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.34	9.57	6.36
Unmasked-calculated*	7.12	11.95	8.01

*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 7.12 differs from the reported value 5.3 by more than 10 %

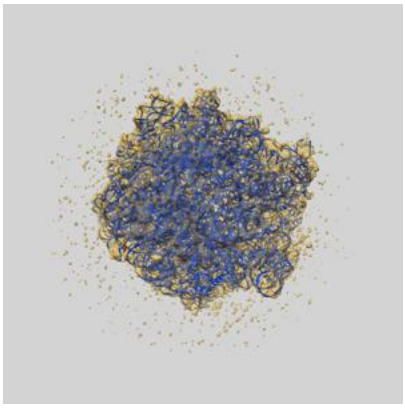
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4122 and PDB model 5LZB. Per-residue inclusion information can be found in section ?? on page ??.

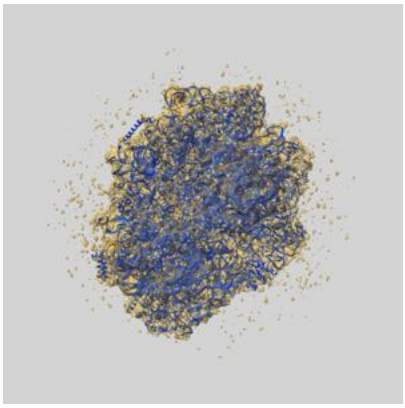
8.1 Map-model overlay



X



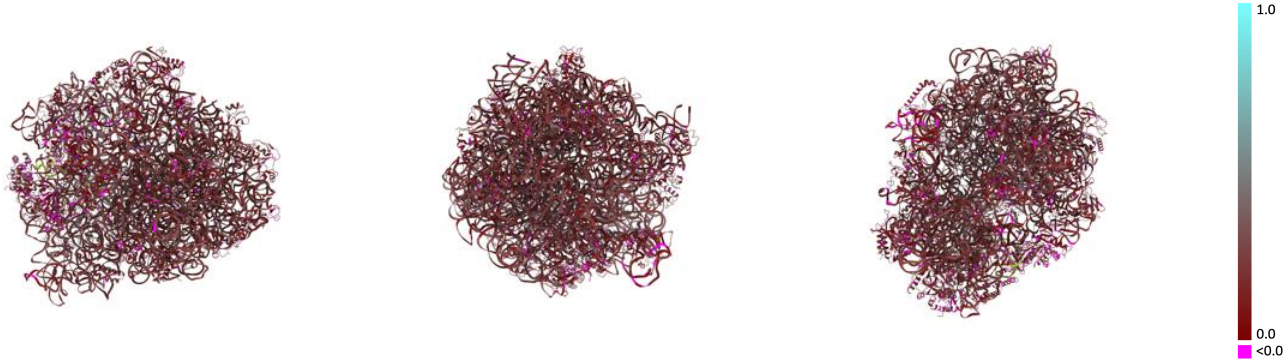
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.36 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.

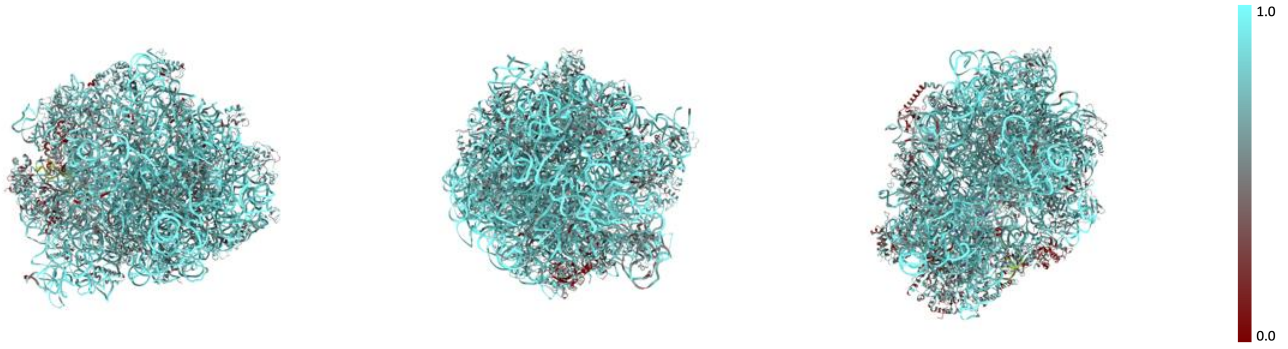
8.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

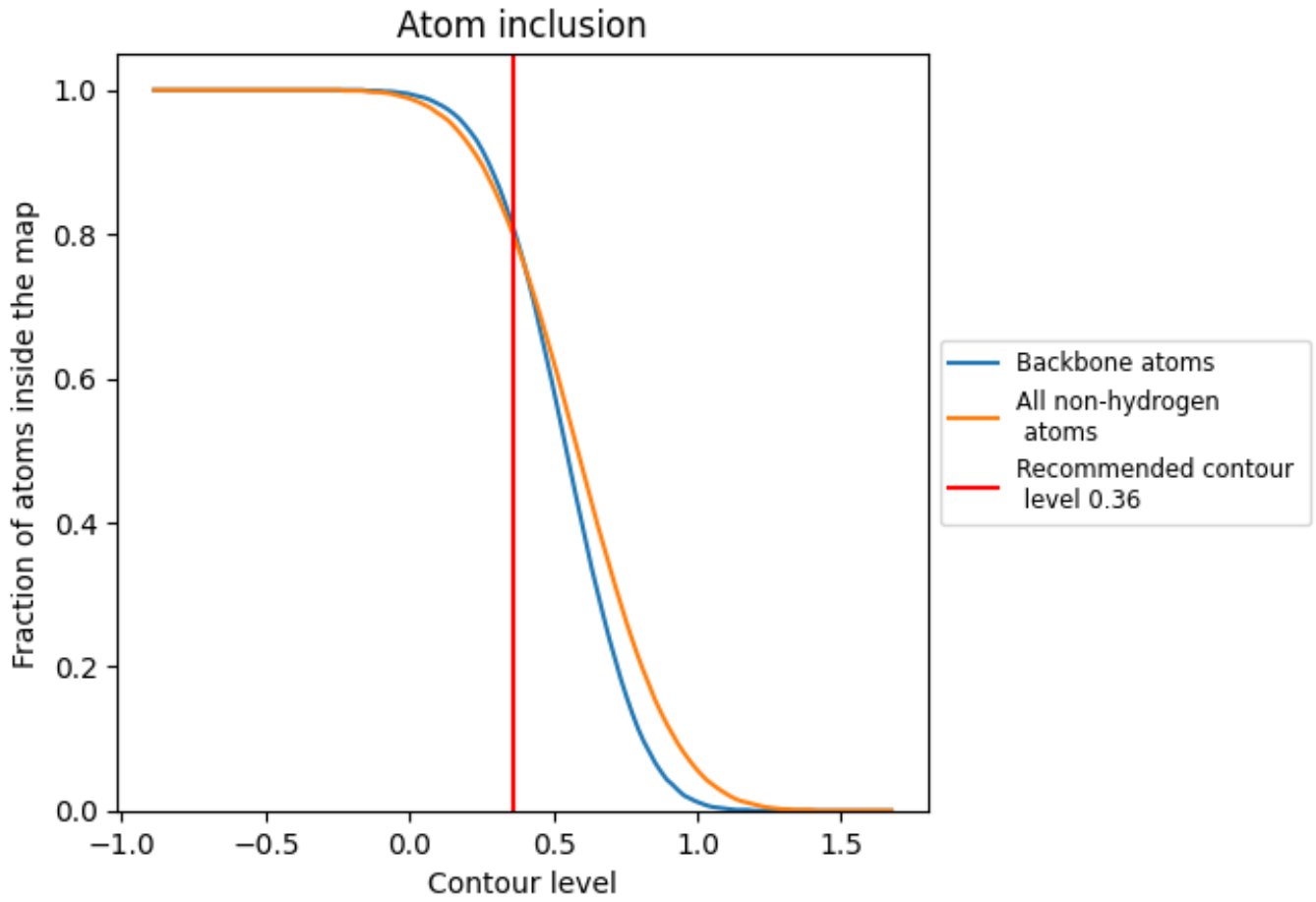
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.36).

8.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.2200
0	0.5890	0.1780
1	0.4500	0.1530
2	0.6370	0.1500
3	0.6070	0.1680
4	0.6080	0.1660
6	0.6610	0.1960
A	0.9110	0.2470
B	0.9160	0.2390
C	0.6350	0.1900
D	0.6070	0.1810
E	0.6130	0.1840
F	0.6400	0.1610
G	0.6710	0.1990
H	0.2440	0.1300
I	0.2240	0.0830
J	0.6570	0.1850
K	0.5550	0.1880
L	0.6190	0.2010
M	0.6450	0.1970
N	0.6280	0.1700
O	0.6280	0.1680
P	0.6120	0.1760
Q	0.6340	0.1690
R	0.6250	0.1760
S	0.6240	0.1700
T	0.6060	0.1810
U	0.6380	0.1720
V	0.6250	0.1730
W	0.6240	0.1840
X	0.6490	0.1950
Y	0.6420	0.1650
Z	0.6450	0.1800
a	0.9080	0.2430
b	0.4710	0.1670

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Chain	Atom inclusion	Q-score
c	0.5780	0.1860
d	0.5310	0.1750
e	0.6060	0.1940
f	0.6340	0.1880
g	0.6410	0.1780
h	0.6060	0.1730
i	0.5860	0.1640
j	0.5410	0.1670
k	0.6420	0.1680
l	0.5680	0.1910
m	0.6540	0.1750
n	0.6020	0.1610
o	0.6710	0.1630
p	0.6190	0.1840
q	0.6940	0.1740
r	0.6580	0.1920
s	0.6320	0.1750
t	0.6520	0.1690
u	0.5390	0.1590
v	0.8960	0.2380
w	0.6770	0.2190
x	0.6290	0.1880
y	0.8100	0.1590
z	0.5460	0.1390