Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 09:25 am GMT

PDB ID	:	4UE5
EMDB ID	:	EMD-2844
Title	:	Structural basis for targeting and elongation arrest of Bacillus signal recognition particle
Authors	:	Beckert, B.; Kedrov, A.; Sohmen, D.; Kempf, G.; Wild, K.; Sinning, I.; Stahlberg, H.; Wilson, D.N.; Beckmann, R.
Deposited on	:	2014-12-15
Resolution	:	9.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

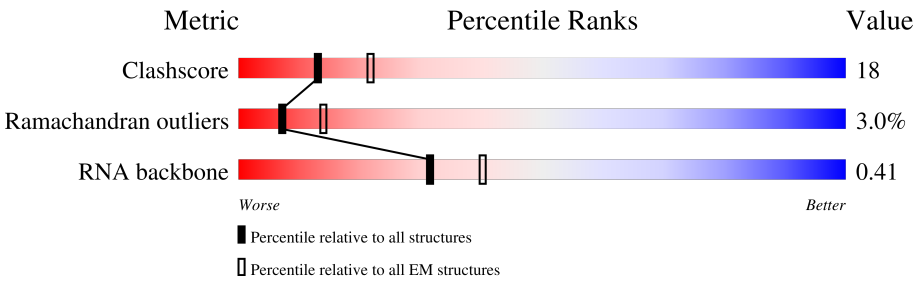
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
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	299	33%; • 45% 37% 15%
2	B	75	61%; 87% 12% •
3	C	195	56%; 88% • 8%
4	D	433	26%; 70% 28% •
5	E	74	59%; 81% 18% •
6	F	107	55%; 81% 19%
7	S	18	83%; 100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9948 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 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	299	6403	2852	1167	2086	298	0	0

- Molecule 2 is a protein called SRP14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	75	300	150	75	75	0	0

- Molecule 3 is a protein called SIGNAL RECOGNITION PARTICLE SUBUNIT SRP68.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	179	716	358	179	179	0	0

- Molecule 4 is a protein called SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	433	1732	866	433	433	0	0

- Molecule 5 is a protein called SRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	74	296	148	74	74	0	0

- Molecule 6 is a protein called SIGNAL RECOGNITION PARTICLE 9 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	107	429	214	107	108	0	0

- Molecule 7 is a protein called SIGNAL SEQUENCE.

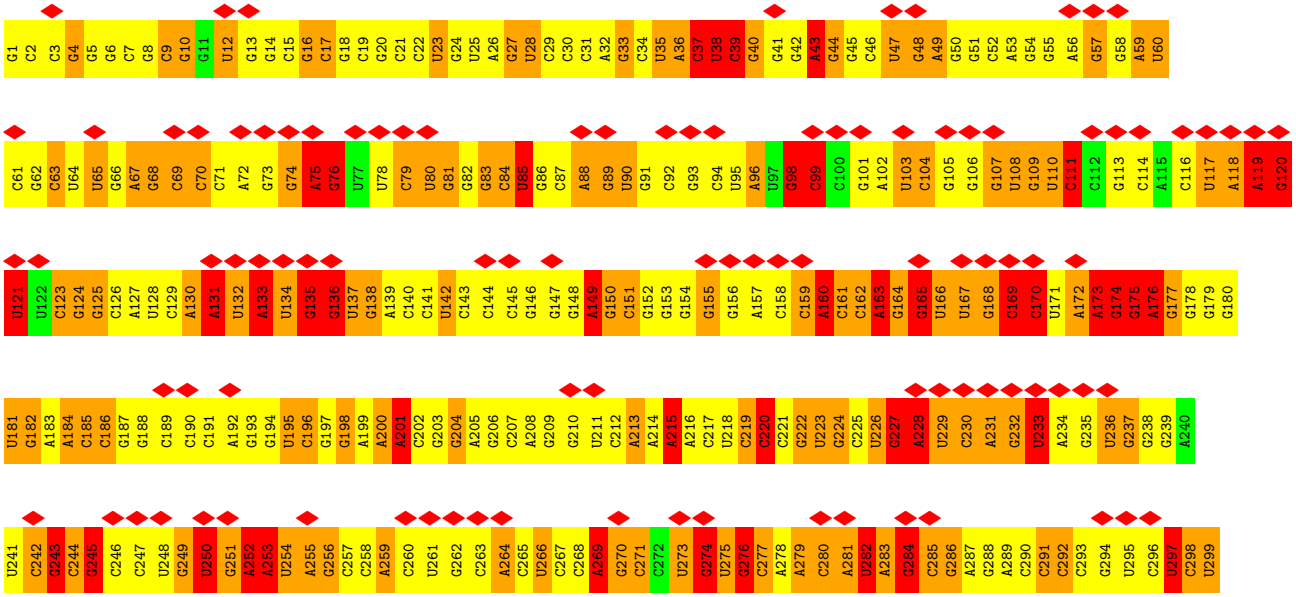
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S	18	72	36	18	18	0	0

3 Residue-property plots (i)

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

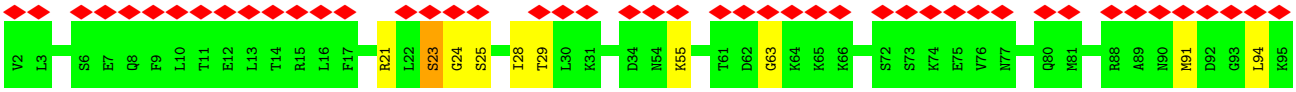
- Molecule 1: 7S RNA

Chain A:



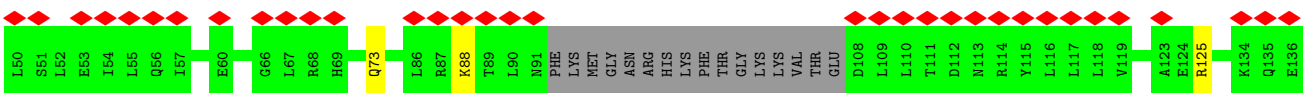
- Molecule 2: SRP14

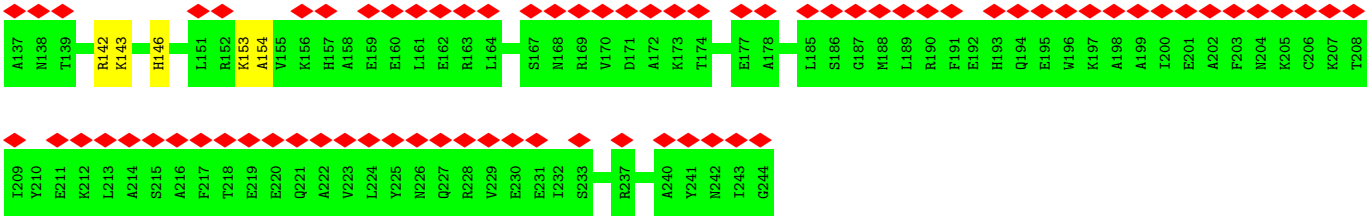
Chain B:



- Molecule 3: SIGNAL RECOGNITION PARTICLE SUBUNIT SRP68

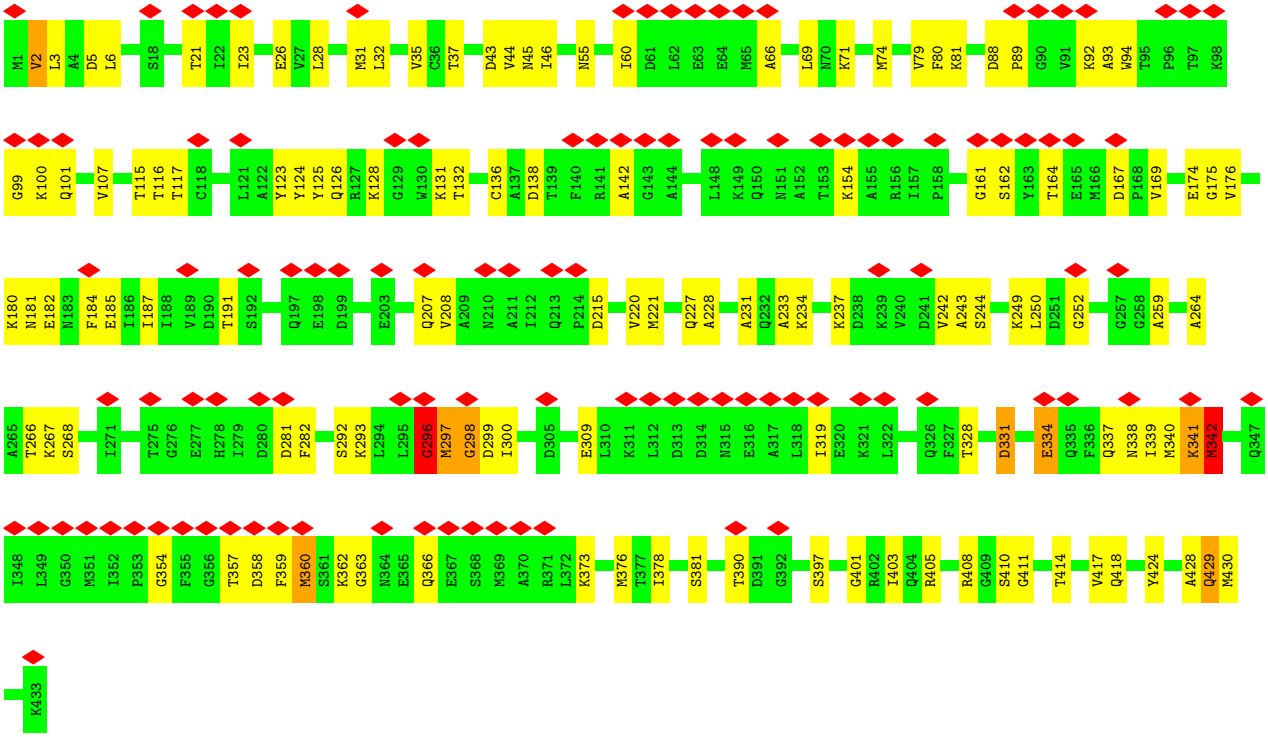
Chain C:





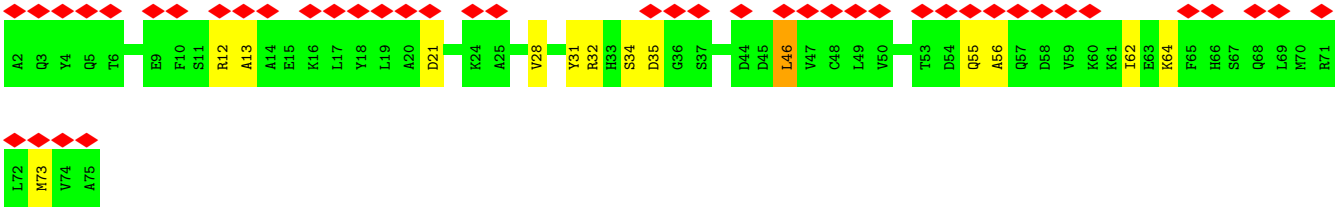
• Molecule 4: SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN

Chain D:



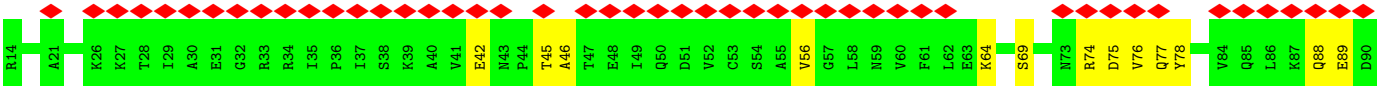
• Molecule 5: SRP9

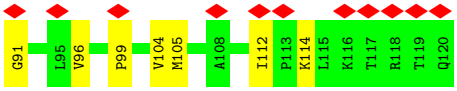
Chain E:



• Molecule 6: SIGNAL RECOGNITION PARTICLE 9 KDA PROTEIN

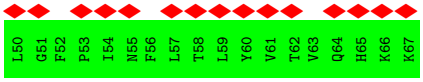
Chain F:





- Molecule 7: SIGNAL SEQUENCE

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19096	Depositor
Resolution determination method	Not provided	
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	0.651	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.119	Depositor
Map size (Å)	520.8, 520.8, 520.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.55	31/7161 (0.4%)	2.59	812/11171 (7.3%)
2	B	0.40	0/298	0.74	0/369
3	C	0.25	0/714	0.48	0/889
4	D	0.73	0/1731	0.94	0/2162
5	E	0.37	0/295	0.73	0/367
6	F	0.40	0/428	0.68	0/532
7	S	0.44	0/71	0.72	0/87
All	All	1.31	31/10698 (0.3%)	2.23	812/15577 (5.2%)

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	0	38
4	D	0	108
All	All	0	146

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	C	O3'-P	-8.07	1.51	1.61
1	A	229	U	O3'-P	-7.93	1.51	1.61
1	A	198	G	C2-N3	7.58	1.38	1.32
1	A	131	A	C6-N6	6.36	1.39	1.33
1	A	201	A	N7-C5	-6.30	1.35	1.39
1	A	118	A	C6-N6	6.09	1.38	1.33
1	A	88	A	C6-N6	5.93	1.38	1.33
1	A	283	A	C6-N6	5.79	1.38	1.33
1	A	259	A	C6-N6	5.76	1.38	1.33
1	A	287	A	C6-N6	5.67	1.38	1.33
1	A	133	A	N7-C5	-5.65	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	A	C6-N6	5.64	1.38	1.33
1	A	37	C	O3'-P	5.61	1.67	1.61
1	A	43	A	C6-N6	5.47	1.38	1.33
1	A	135	G	C2'-C1'	-5.36	1.47	1.53
1	A	255	A	C6-N6	5.30	1.38	1.33
1	A	96	A	C6-N6	5.29	1.38	1.33
1	A	253	A	C6-N6	5.24	1.38	1.33
1	A	130	A	C6-N6	5.22	1.38	1.33
1	A	48	G	C2'-C1'	-5.18	1.47	1.53
1	A	67	A	O3'-P	-5.16	1.54	1.61
1	A	251	G	C2-N3	5.09	1.36	1.32
1	A	243	G	C2-N3	5.09	1.36	1.32
1	A	72	A	C6-N6	5.08	1.38	1.33
1	A	187	G	C2-N3	5.07	1.36	1.32
1	A	96	A	N7-C5	-5.07	1.36	1.39
1	A	105	G	O3'-P	5.07	1.67	1.61
1	A	157	A	N9-C4	-5.06	1.34	1.37
1	A	280	C	O3'-P	5.04	1.67	1.61
1	A	237	G	C2-N3	5.00	1.36	1.32
1	A	49	A	C6-N6	5.00	1.38	1.33

All (812) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	G	O5'-P-OP2	-25.39	80.23	110.70
1	A	59	A	C4'-C3'-O3'	20.59	154.17	113.00
1	A	59	A	P-O3'-C3'	-18.37	97.66	119.70
1	A	201	A	N1-C6-N6	17.49	129.09	118.60
1	A	47	U	P-O3'-C3'	17.26	140.41	119.70
1	A	176	A	P-O3'-C3'	16.41	139.40	119.70
1	A	270	G	C4'-C3'-O3'	15.17	143.34	113.00
1	A	176	A	N1-C6-N6	14.93	127.56	118.60
1	A	215	A	N1-C6-N6	14.53	127.32	118.60
1	A	17	C	P-O5'-C5'	13.76	142.91	120.90
1	A	216	A	N1-C6-N6	13.64	126.79	118.60
1	A	270	G	O5'-P-OP1	13.58	127.00	110.70
1	A	83	G	N1-C6-O6	13.39	127.93	119.90
1	A	53	A	N1-C6-N6	13.29	126.57	118.60
1	A	149	A	N1-C6-N6	13.15	126.49	118.60
1	A	127	A	N1-C6-N6	12.99	126.39	118.60
1	A	57	G	C4'-C3'-O3'	12.98	138.97	113.00
1	A	253	A	N1-C6-N6	12.93	126.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	C	P-O5'-C5'	12.89	141.53	120.90
1	A	43	A	P-O3'-C3'	12.81	135.07	119.70
1	A	16	G	C4'-C3'-O3'	12.77	138.54	113.00
1	A	68	G	P-O5'-C5'	12.69	141.21	120.90
1	A	69	C	O4'-C1'-N1	12.58	118.26	108.20
1	A	60	U	O4'-C1'-N1	12.51	118.21	108.20
1	A	164	G	N1-C6-O6	12.50	127.40	119.90
1	A	172	A	P-O3'-C3'	12.49	134.69	119.70
1	A	252	A	P-O3'-C3'	12.48	134.68	119.70
1	A	200	A	N1-C6-N6	12.45	126.07	118.60
1	A	192	A	N1-C6-N6	12.42	126.05	118.60
1	A	36	A	C4'-C3'-O3'	-12.41	83.34	109.40
1	A	199	A	N1-C6-N6	12.37	126.02	118.60
1	A	96	A	N1-C6-N6	12.31	125.99	118.60
1	A	35	U	C4'-C3'-O3'	-12.27	83.63	109.40
1	A	166	U	O4'-C1'-N1	12.23	117.99	108.20
1	A	60	U	C4'-C3'-O3'	12.11	137.21	113.00
1	A	208	A	N1-C6-N6	12.10	125.86	118.60
1	A	173	A	N1-C6-N6	12.06	125.83	118.60
1	A	32	A	N1-C6-N6	11.95	125.77	118.60
1	A	185	C	P-O3'-C3'	11.94	134.02	119.70
1	A	76	G	C4'-C3'-O3'	11.91	136.82	113.00
1	A	49	A	N1-C6-N6	11.89	125.73	118.60
1	A	105	G	O4'-C1'-N9	11.78	117.62	108.20
1	A	58	G	O4'-C1'-N9	11.69	117.55	108.20
1	A	214	A	N1-C6-N6	11.64	125.58	118.60
1	A	139	A	N1-C6-N6	11.63	125.58	118.60
1	A	157	A	N1-C6-N6	11.61	125.57	118.60
1	A	61	C	P-O5'-C5'	-11.51	102.48	120.90
1	A	75	A	N1-C6-N6	11.50	125.50	118.60
1	A	183	A	N1-C6-N6	11.42	125.45	118.60
1	A	102	A	N1-C6-N6	11.36	125.42	118.60
1	A	294	G	N1-C6-O6	11.36	126.71	119.90
1	A	255	A	N1-C6-N6	11.35	125.41	118.60
1	A	160	A	N1-C6-N6	11.31	125.39	118.60
1	A	252	A	N1-C6-N6	11.28	125.37	118.60
1	A	259	A	N1-C6-N6	11.27	125.36	118.60
1	A	172	A	N1-C6-N6	11.22	125.33	118.60
1	A	83	G	C5-C6-O6	-11.21	121.88	128.60
1	A	26	A	N1-C6-N6	11.14	125.29	118.60
1	A	285	C	O4'-C1'-N1	11.13	117.10	108.20
1	A	205	A	N1-C6-N6	11.02	125.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	C	O5'-C5'-C4'	-11.02	90.77	111.70
1	A	213	A	N1-C6-N6	10.99	125.19	118.60
1	A	184	A	N1-C6-N6	10.97	125.19	118.60
1	A	283	A	N1-C6-N6	10.97	125.18	118.60
1	A	72	A	N1-C6-N6	10.96	125.17	118.60
1	A	24	G	N1-C6-O6	10.92	126.45	119.90
1	A	165	G	N1-C6-O6	10.91	126.45	119.90
1	A	86	G	N1-C6-O6	10.91	126.44	119.90
1	A	168	G	N1-C6-O6	10.88	126.43	119.90
1	A	234	A	N1-C6-N6	10.88	125.13	118.60
1	A	264	A	N1-C6-N6	10.82	125.09	118.60
1	A	161	C	O4'-C1'-N1	10.76	116.81	108.20
1	A	48	G	N1-C6-O6	10.65	126.29	119.90
1	A	88	A	N1-C6-N6	10.59	124.95	118.60
1	A	50	G	N1-C6-O6	10.58	126.25	119.90
1	A	51	G	N1-C6-O6	10.53	126.22	119.90
1	A	230	C	P-O5'-C5'	10.51	137.72	120.90
1	A	276	G	O4'-C1'-N9	10.39	116.51	108.20
1	A	81	G	N1-C6-O6	10.36	126.12	119.90
1	A	44	G	N1-C6-O6	10.35	126.11	119.90
1	A	282	U	O4'-C1'-N1	10.32	116.46	108.20
1	A	60	U	C5'-C4'-O4'	10.30	121.46	109.10
1	A	219	C	O4'-C1'-N1	10.29	116.43	108.20
1	A	159	C	O4'-C1'-N1	10.26	116.41	108.20
1	A	63	C	O4'-C1'-N1	10.24	116.39	108.20
1	A	131	A	C5-C6-N1	-10.21	112.60	117.70
1	A	237	G	N1-C6-O6	10.19	126.01	119.90
1	A	130	A	N1-C6-N6	10.16	124.69	118.60
1	A	187	G	N1-C6-O6	10.15	125.99	119.90
1	A	117	U	O4'-C1'-N1	10.11	116.29	108.20
1	A	61	C	O4'-C1'-N1	10.10	116.28	108.20
1	A	94	C	O4'-C1'-N1	10.00	116.20	108.20
1	A	254	U	O4'-C1'-N1	9.98	116.19	108.20
1	A	164	G	C5-C6-O6	-9.91	122.65	128.60
1	A	276	G	N1-C6-O6	9.88	125.83	119.90
1	A	162	C	O4'-C1'-N1	9.77	116.02	108.20
1	A	65	U	O4'-C1'-N1	9.77	116.02	108.20
1	A	227	G	N1-C6-O6	9.76	125.76	119.90
1	A	280	C	O3'-P-O5'	9.74	122.50	104.00
1	A	118	A	N1-C6-N6	9.70	124.42	118.60
1	A	242	C	C2'-C3'-O3'	9.66	130.75	109.50
1	A	243	G	N1-C6-O6	9.64	125.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	A	P-O3'-C3'	9.63	131.26	119.70
1	A	9	C	O4'-C1'-N1	9.58	115.87	108.20
1	A	257	C	O4'-C1'-N1	9.54	115.83	108.20
1	A	251	G	N1-C6-O6	9.53	125.62	119.90
1	A	20	G	N1-C6-O6	9.53	125.62	119.90
1	A	178	G	N1-C6-O6	9.52	125.61	119.90
1	A	286	G	O4'-C1'-N9	9.52	115.81	108.20
1	A	230	C	C5'-C4'-C3'	-9.51	100.78	116.00
1	A	87	C	O4'-C1'-N1	9.47	115.78	108.20
1	A	274	G	N1-C6-O6	9.45	125.57	119.90
1	A	140	C	O4'-C1'-N1	9.45	115.76	108.20
1	A	175	G	N1-C6-O6	9.41	125.55	119.90
1	A	201	A	C5-C6-N6	-9.39	116.19	123.70
1	A	52	C	O4'-C1'-N1	9.38	115.71	108.20
1	A	64	U	O4'-C1'-N1	9.37	115.70	108.20
1	A	223	U	O4'-C1'-N1	9.36	115.69	108.20
1	A	258	C	O4'-C1'-N1	9.35	115.68	108.20
1	A	105	G	C5'-C4'-O4'	9.32	120.28	109.10
1	A	209	G	N1-C6-O6	9.32	125.49	119.90
1	A	225	C	O4'-C1'-N1	9.31	115.65	108.20
1	A	43	A	N1-C6-N6	9.29	124.17	118.60
1	A	293	C	O4'-C1'-N1	9.27	115.62	108.20
1	A	4	G	N1-C6-O6	9.27	125.46	119.90
1	A	88	A	C5-C6-N1	-9.24	113.08	117.70
1	A	268	C	O4'-C1'-N1	9.22	115.58	108.20
1	A	158	C	O4'-C1'-N1	9.22	115.57	108.20
1	A	105	G	C5'-C4'-C3'	-9.21	101.26	116.00
1	A	118	A	C5-C6-N1	-9.21	113.09	117.70
1	A	287	A	N1-C6-N6	9.19	124.12	118.60
1	A	5	G	N1-C6-O6	9.13	125.38	119.90
1	A	24	G	C5-C6-O6	-9.11	123.13	128.60
1	A	167	U	O4'-C1'-N1	9.11	115.49	108.20
1	A	181	U	O4'-C1'-N1	9.10	115.48	108.20
1	A	215	A	C5-C6-N6	-9.10	116.42	123.70
1	A	6	G	N1-C6-O6	9.10	125.36	119.90
1	A	283	A	C5-C6-N1	-9.09	113.15	117.70
1	A	144	C	O4'-C1'-N1	9.07	115.46	108.20
1	A	207	C	O4'-C1'-N1	9.06	115.45	108.20
1	A	141	C	O4'-C1'-N1	9.06	115.45	108.20
1	A	204	G	N1-C6-O6	9.05	125.33	119.90
1	A	260	C	O4'-C1'-N1	9.04	115.43	108.20
1	A	96	A	C5-C6-N1	-9.03	113.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	G	N1-C6-O6	9.00	125.30	119.90
1	A	22	C	O4'-C1'-N1	8.99	115.39	108.20
1	A	40	G	N1-C6-O6	8.98	125.29	119.90
1	A	198	G	N1-C6-O6	8.98	125.29	119.90
1	A	234	A	C5-C6-N1	-8.97	113.22	117.70
1	A	106	G	N1-C6-O6	8.96	125.27	119.90
1	A	221	C	O4'-C1'-N1	8.95	115.36	108.20
1	A	95	U	O4'-C1'-N1	8.94	115.35	108.20
1	A	36	A	P-O5'-C5'	-8.93	106.61	120.90
1	A	152	G	N1-C6-O6	8.93	125.26	119.90
1	A	259	A	C5-C6-N1	-8.93	113.23	117.70
1	A	263	C	O4'-C1'-N1	8.92	115.34	108.20
1	A	91	G	O4'-C1'-N9	8.89	115.32	108.20
1	A	108	U	O4'-C1'-N1	8.89	115.31	108.20
1	A	147	G	N1-C6-O6	8.87	125.22	119.90
1	A	151	C	O4'-C1'-N1	8.87	115.30	108.20
1	A	206	G	N1-C6-O6	8.83	125.20	119.90
1	A	253	A	O4'-C1'-N9	8.83	115.27	108.20
1	A	28	U	O4'-C1'-N1	8.83	115.27	108.20
1	A	245	G	N1-C6-O6	8.83	125.20	119.90
1	A	182	G	N1-C6-O6	8.82	125.19	119.90
1	A	93	G	O4'-C1'-N9	8.81	115.25	108.20
1	A	266	U	O4'-C1'-N1	8.81	115.25	108.20
1	A	34	C	O4'-C1'-N1	8.80	115.24	108.20
1	A	217	C	O4'-C1'-N1	8.80	115.24	108.20
1	A	292	C	O4'-C1'-N1	8.80	115.24	108.20
1	A	232	G	N1-C6-O6	8.78	125.17	119.90
1	A	8	G	N1-C6-O6	8.75	125.15	119.90
1	A	284	G	O4'-C1'-N9	8.74	115.19	108.20
1	A	128	U	O4'-C1'-N1	8.73	115.19	108.20
1	A	135	G	O4'-C1'-N9	8.72	115.18	108.20
1	A	148	G	N1-C6-O6	8.72	125.13	119.90
1	A	60	U	C2'-C3'-O3'	-8.72	90.31	109.50
1	A	246	C	O4'-C1'-N1	8.71	115.17	108.20
1	A	41	G	N1-C6-O6	8.69	125.11	119.90
1	A	23	U	O4'-C1'-N1	8.69	115.15	108.20
1	A	267	C	O4'-C1'-N1	8.69	115.15	108.20
1	A	250	U	O4'-C1'-N1	8.67	115.14	108.20
1	A	287	A	C5-C6-N1	-8.65	113.37	117.70
1	A	247	C	O4'-C1'-N1	8.65	115.12	108.20
1	A	262	G	N1-C6-O6	8.64	125.08	119.90
1	A	33	G	N1-C6-O6	8.63	125.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	G	N1-C6-O6	8.62	125.07	119.90
1	A	92	C	O4'-C1'-N1	8.61	115.09	108.20
1	A	291	C	O4'-C1'-N1	8.60	115.08	108.20
1	A	126	C	O4'-C1'-N1	8.59	115.08	108.20
1	A	294	G	C5-C6-O6	-8.57	123.46	128.60
1	A	180	G	N1-C6-O6	8.56	125.04	119.90
1	A	228	A	C4'-C3'-O3'	8.56	130.12	113.00
1	A	284	G	N1-C6-O6	8.53	125.02	119.90
1	A	145	C	O4'-C1'-N1	8.52	115.02	108.20
1	A	18	G	N1-C6-O6	8.52	125.01	119.90
1	A	134	U	O4'-C1'-N1	8.50	115.00	108.20
1	A	107	G	O4'-C1'-N9	8.50	115.00	108.20
1	A	146	G	N1-C6-O6	8.50	125.00	119.90
1	A	226	U	O4'-C1'-N1	8.50	115.00	108.20
1	A	4	G	O4'-C1'-N9	8.45	114.96	108.20
1	A	42	G	N1-C6-O6	8.45	124.97	119.90
1	A	131	A	N1-C6-N6	8.44	123.67	118.60
1	A	1	G	N1-C6-O6	8.44	124.96	119.90
1	A	45	G	N1-C6-O6	8.44	124.96	119.90
1	A	19	C	O4'-C1'-N1	8.43	114.95	108.20
1	A	31	C	O4'-C1'-N1	8.42	114.94	108.20
1	A	79	C	P-O3'-C3'	-8.41	109.61	119.70
1	A	29	C	O4'-C1'-N1	8.39	114.91	108.20
1	A	244	C	O4'-C1'-N1	8.39	114.91	108.20
1	A	107	G	N1-C6-O6	8.37	124.92	119.90
1	A	296	C	O4'-C1'-N1	8.37	114.90	108.20
1	A	119	A	N1-C6-N6	8.37	123.62	118.60
1	A	54	G	N1-C6-O6	8.36	124.92	119.90
1	A	156	G	N1-C6-O6	8.36	124.92	119.90
1	A	58	G	C4'-C3'-O3'	-8.36	91.85	109.40
1	A	224	G	N1-C6-O6	8.36	124.92	119.90
1	A	21	C	O4'-C1'-N1	8.36	114.88	108.20
1	A	189	C	O4'-C1'-N1	8.34	114.87	108.20
1	A	277	C	O4'-C1'-N1	8.34	114.87	108.20
1	A	46	C	O4'-C1'-N1	8.32	114.85	108.20
1	A	70	C	O4'-C1'-N1	8.30	114.84	108.20
1	A	12	U	C4'-C3'-O3'	-8.28	92.02	109.40
1	A	220	C	O4'-C1'-N1	8.28	114.82	108.20
1	A	190	C	O4'-C1'-N1	8.28	114.82	108.20
1	A	120	G	N1-C6-O6	8.27	124.86	119.90
1	A	298	C	O4'-C1'-N1	8.27	114.82	108.20
1	A	218	U	O4'-C1'-N1	8.27	114.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	G	C5-C6-O6	-8.27	123.64	128.60
1	A	269	A	C4'-C3'-O3'	8.27	129.54	113.00
1	A	106	G	P-O5'-C5'	-8.26	107.68	120.90
1	A	252	A	O4'-C1'-N9	8.26	114.81	108.20
1	A	27	G	N1-C6-O6	8.25	124.85	119.90
1	A	177	G	N1-C6-O6	8.24	124.84	119.90
1	A	249	G	O4'-C1'-N9	8.24	114.79	108.20
1	A	39	C	O4'-C1'-N1	8.21	114.77	108.20
1	A	176	A	C5-C6-N6	-8.21	117.14	123.70
1	A	106	G	O4'-C1'-N9	8.20	114.76	108.20
1	A	93	G	N1-C6-O6	8.20	124.82	119.90
1	A	136	G	O4'-C1'-N9	8.20	114.76	108.20
1	A	62	G	N1-C6-O6	8.20	124.82	119.90
1	A	265	C	O4'-C1'-N1	8.19	114.75	108.20
1	A	74	G	N1-C6-O6	8.19	124.81	119.90
1	A	50	G	C5-C6-O6	-8.19	123.69	128.60
1	A	215	A	O4'-C1'-N9	8.18	114.74	108.20
1	A	129	C	O4'-C1'-N1	8.18	114.74	108.20
1	A	235	G	N1-C6-O6	8.18	124.81	119.90
1	A	188	G	N1-C6-O6	8.16	124.79	119.90
1	A	182	G	O4'-C1'-N9	8.15	114.72	108.20
1	A	248	U	O4'-C1'-N1	8.13	114.70	108.20
1	A	271	C	P-O5'-C5'	8.12	133.89	120.90
1	A	273	U	O4'-C1'-N1	8.11	114.69	108.20
1	A	295	U	O4'-C1'-N1	8.11	114.69	108.20
1	A	136	G	N1-C6-O6	8.09	124.76	119.90
1	A	203	G	N1-C6-O6	8.09	124.75	119.90
1	A	242	C	P-O3'-C3'	8.08	129.40	119.70
1	A	48	G	C5-C6-O6	-8.08	123.75	128.60
1	A	86	G	C5-C6-O6	-8.07	123.76	128.60
1	A	58	G	O4'-C4'-C3'	-8.06	95.94	104.00
1	A	62	G	O4'-C1'-N9	8.05	114.64	108.20
1	A	103	U	C4'-C3'-O3'	8.05	129.10	113.00
1	A	89	G	N1-C6-O6	8.04	124.72	119.90
1	A	253	A	C5-C6-N1	-8.04	113.68	117.70
1	A	37	C	C5'-C4'-C3'	8.03	128.85	116.00
1	A	82	G	N1-C6-O6	8.03	124.72	119.90
1	A	243	G	C5-C6-O6	-8.02	123.79	128.60
1	A	281	A	C4'-C3'-O3'	8.01	129.01	113.00
1	A	51	G	C5-C6-O6	-7.99	123.81	128.60
1	A	197	G	O4'-C1'-N9	7.99	114.59	108.20
1	A	256	G	O4'-C1'-N9	7.96	114.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	C	O4'-C1'-N1	7.96	114.56	108.20
1	A	154	G	O4'-C1'-N9	7.95	114.56	108.20
1	A	59	A	C2'-C3'-O3'	-7.95	92.01	109.50
1	A	120	G	O4'-C1'-N9	7.93	114.55	108.20
1	A	7	C	O4'-C1'-N1	7.92	114.53	108.20
1	A	283	A	O4'-C1'-N9	7.91	114.53	108.20
1	A	142	U	O4'-C1'-N1	7.90	114.52	108.20
1	A	290	C	O5'-C5'-C4'	7.90	126.71	111.70
1	A	79	C	C2'-C3'-O3'	7.90	126.88	109.50
1	A	71	C	O4'-C1'-N1	7.89	114.51	108.20
1	A	121	U	C4'-C3'-O3'	7.88	128.75	113.00
1	A	261	U	O4'-C1'-N1	7.88	114.50	108.20
1	A	255	A	O4'-C1'-N9	7.87	114.50	108.20
1	A	155	G	N1-C6-O6	7.87	124.62	119.90
1	A	90	U	O4'-C1'-N1	7.85	114.48	108.20
1	A	137	U	O4'-C1'-N1	7.85	114.48	108.20
1	A	160	A	O4'-C1'-N9	7.85	114.48	108.20
1	A	2	C	O4'-C1'-N1	7.85	114.48	108.20
1	A	125	G	N1-C6-O6	7.85	124.61	119.90
1	A	73	G	N1-C6-O6	7.84	124.60	119.90
1	A	33	G	O4'-C1'-N9	7.83	114.46	108.20
1	A	154	G	N1-C6-O6	7.82	124.59	119.90
1	A	290	C	P-O5'-C5'	-7.81	108.40	120.90
1	A	124	G	O4'-C1'-N9	7.81	114.45	108.20
1	A	256	G	N1-C6-O6	7.80	124.58	119.90
1	A	42	G	O4'-C1'-N9	7.80	114.44	108.20
1	A	210	G	N1-C6-O6	7.80	124.58	119.90
1	A	202	C	O4'-C1'-N1	7.77	114.42	108.20
1	A	193	G	O4'-C1'-N9	7.74	114.39	108.20
1	A	212	C	O4'-C1'-N1	7.73	114.38	108.20
1	A	236	U	O4'-C1'-N1	7.73	114.38	108.20
1	A	211	U	O4'-C1'-N1	7.72	114.38	108.20
1	A	119	A	O4'-C1'-N9	7.71	114.37	108.20
1	A	80	U	C4'-C3'-O3'	7.71	128.42	113.00
1	A	143	C	O4'-C1'-N1	7.70	114.36	108.20
1	A	3	C	O4'-C1'-N1	7.70	114.36	108.20
1	A	185	C	O4'-C1'-N1	7.70	114.36	108.20
1	A	165	G	O4'-C1'-N9	7.69	114.35	108.20
1	A	138	G	N1-C6-O6	7.69	124.51	119.90
1	A	5	G	O4'-C1'-N9	7.67	114.34	108.20
1	A	54	G	O4'-C1'-N9	7.67	114.34	108.20
1	A	224	G	O4'-C1'-N9	7.66	114.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	G	O4'-C1'-N9	7.61	114.29	108.20
1	A	198	G	O4'-C1'-N9	7.61	114.29	108.20
1	A	287	A	O4'-C1'-N9	7.61	114.29	108.20
1	A	168	G	C5-C6-O6	-7.59	124.04	128.60
1	A	195	U	O4'-C1'-N1	7.59	114.27	108.20
1	A	255	A	C5-C6-N1	-7.59	113.90	117.70
1	A	165	G	C5-C6-O6	-7.58	124.05	128.60
1	A	196	C	O4'-C1'-N1	7.58	114.27	108.20
1	A	55	G	N1-C6-O6	7.58	124.45	119.90
1	A	191	C	O4'-C1'-N1	7.56	114.25	108.20
1	A	153	G	N1-C6-O6	7.55	124.43	119.90
1	A	157	A	O4'-C1'-N9	7.54	114.23	108.20
1	A	251	G	C5-C6-O6	-7.53	124.08	128.60
1	A	200	A	O4'-C1'-N9	7.52	114.22	108.20
1	A	109	G	N1-C6-O6	7.51	124.41	119.90
1	A	73	G	O4'-C1'-N9	7.49	114.19	108.20
1	A	104	C	P-O3'-C3'	-7.48	110.72	119.70
1	A	170	C	O4'-C1'-N1	7.47	114.18	108.20
1	A	89	G	O4'-C1'-N9	7.47	114.17	108.20
1	A	98	G	C4'-C3'-O3'	7.45	127.90	113.00
1	A	88	A	O4'-C1'-N9	7.40	114.12	108.20
1	A	198	G	N3-C2-N2	7.39	125.07	119.90
1	A	36	A	O5'-C5'-C4'	7.39	125.73	111.70
1	A	39	C	N3-C4-N4	7.37	123.16	118.00
1	A	116	C	O4'-C1'-N1	7.37	114.10	108.20
1	A	17	C	C5'-C4'-C3'	-7.35	104.24	116.00
1	A	81	G	C5-C6-O6	-7.33	124.20	128.60
1	A	187	G	C5-C6-O6	-7.33	124.20	128.60
1	A	55	G	O4'-C1'-N9	7.30	114.04	108.20
1	A	155	G	O4'-C1'-N9	7.27	114.01	108.20
1	A	193	G	N1-C6-O6	7.26	124.26	119.90
1	A	44	G	C5-C6-O6	-7.25	124.25	128.60
1	A	91	G	N1-C6-O6	7.25	124.25	119.90
1	A	47	U	O4'-C1'-N1	7.23	113.98	108.20
1	A	233	U	O4'-C1'-N1	7.22	113.98	108.20
1	A	194	G	N1-C6-O6	7.21	124.23	119.90
1	A	74	G	O4'-C1'-N9	7.20	113.96	108.20
1	A	186	C	C2-N1-C1'	7.19	126.71	118.80
1	A	85	U	O4'-C1'-N1	7.19	113.95	108.20
1	A	160	A	C5-C6-N1	-7.16	114.12	117.70
1	A	71	C	N3-C4-N4	7.16	123.01	118.00
1	A	185	C	C2-N1-C1'	7.12	126.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	C	O4'-C1'-N1	7.12	113.89	108.20
1	A	130	A	C5-C6-N1	-7.11	114.14	117.70
1	A	204	G	C5-C6-O6	-7.11	124.33	128.60
1	A	201	A	O4'-C1'-N9	7.11	113.89	108.20
1	A	157	A	C5-C6-N1	-7.10	114.15	117.70
1	A	84	C	O4'-C1'-N1	7.09	113.88	108.20
1	A	153	G	O4'-C1'-N9	7.09	113.87	108.20
1	A	201	A	C4-C5-C6	7.08	120.54	117.00
1	A	133	A	O4'-C1'-N9	7.08	113.86	108.20
1	A	39	C	C5-C4-N4	-7.07	115.25	120.20
1	A	6	G	C5-C6-O6	-7.07	124.36	128.60
1	A	244	C	N3-C4-C5	-7.07	119.07	121.90
1	A	237	G	N1-C2-N3	-7.06	119.66	123.90
1	A	123	C	C4'-C3'-O3'	7.06	127.12	113.00
1	A	222	G	O4'-C1'-N9	7.05	113.84	108.20
1	A	242	C	P-O5'-C5'	-7.04	109.63	120.90
1	A	276	G	C5-C6-O6	-7.04	124.38	128.60
1	A	58	G	P-O5'-C5'	7.04	132.16	120.90
1	A	72	A	C5-C6-N1	-7.02	114.19	117.70
1	A	290	C	C5'-C4'-C3'	7.02	127.23	116.00
1	A	243	G	O4'-C1'-N9	6.98	113.78	108.20
1	A	127	A	C5-C6-N1	-6.98	114.21	117.70
1	A	16	G	C2'-C3'-O3'	-6.97	94.17	109.50
1	A	132	U	O4'-C1'-N1	6.96	113.77	108.20
1	A	20	G	C5-C6-O6	-6.96	124.42	128.60
1	A	8	G	O4'-C1'-N9	6.96	113.76	108.20
1	A	71	C	N3-C4-C5	-6.93	119.13	121.90
1	A	232	G	C5-C6-O6	-6.92	124.44	128.60
1	A	129	C	N3-C4-C5	-6.90	119.14	121.90
1	A	299	U	O4'-C1'-N1	6.89	113.71	108.20
1	A	285	C	N3-C4-C5	-6.88	119.15	121.90
1	A	222	G	N1-C6-O6	6.88	124.03	119.90
1	A	43	A	O4'-C1'-N9	6.88	113.70	108.20
1	A	174	G	N1-C6-O6	6.88	124.03	119.90
1	A	245	G	O4'-C1'-N9	6.87	113.70	108.20
1	A	25	U	O4'-C1'-N1	6.87	113.69	108.20
1	A	203	G	O4'-C1'-N9	6.86	113.69	108.20
1	A	177	G	O4'-C1'-N9	6.86	113.69	108.20
1	A	197	G	N1-C6-O6	6.85	124.01	119.90
1	A	79	C	N1-C1'-C2'	6.83	122.88	114.00
1	A	125	G	O4'-C1'-N9	6.83	113.66	108.20
1	A	51	G	O4'-C1'-N9	6.82	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	G	O4'-C1'-N9	6.82	113.66	108.20
1	A	259	A	O4'-C1'-N9	6.82	113.66	108.20
1	A	69	C	N3-C4-C5	-6.81	119.17	121.90
1	A	3	C	N3-C4-C5	-6.81	119.18	121.90
1	A	206	G	C5-C6-O6	-6.81	124.52	128.60
1	A	18	G	O4'-C1'-N9	6.81	113.64	108.20
1	A	140	C	N3-C4-N4	6.80	122.76	118.00
1	A	43	A	C5-C6-N1	-6.80	114.30	117.70
1	A	232	G	O4'-C1'-N9	6.79	113.63	108.20
1	A	298	C	N3-C4-C5	-6.79	119.19	121.90
1	A	147	G	C5-C6-O6	-6.78	124.53	128.60
1	A	179	G	N1-C6-O6	6.78	123.97	119.90
1	A	169	C	O4'-C1'-N1	6.78	113.62	108.20
1	A	148	G	C5-C6-O6	-6.77	124.54	128.60
1	A	274	G	N3-C2-N2	6.77	124.64	119.90
1	A	63	C	N3-C4-C5	-6.77	119.19	121.90
1	A	221	C	N3-C4-C5	-6.77	119.19	121.90
1	A	49	A	C5-C6-N1	-6.77	114.32	117.70
1	A	139	A	O4'-C1'-N9	6.76	113.61	108.20
1	A	291	C	N3-C4-C5	-6.76	119.19	121.90
1	A	27	G	O4'-C1'-N9	6.75	113.60	108.20
1	A	219	C	N3-C4-C5	-6.75	119.20	121.90
1	A	209	G	C5-C6-O6	-6.74	124.55	128.60
1	A	178	G	C5-C6-O6	-6.74	124.56	128.60
1	A	227	G	C5-C6-O6	-6.74	124.56	128.60
1	A	135	G	N1-C6-O6	6.72	123.93	119.90
1	A	130	A	O4'-C1'-N9	6.71	113.57	108.20
1	A	146	G	O4'-C1'-N9	6.71	113.57	108.20
1	A	175	G	O4'-C1'-N9	6.71	113.56	108.20
1	A	109	G	O4'-C1'-N9	6.70	113.56	108.20
1	A	5	G	C5-C6-O6	-6.70	124.58	128.60
1	A	216	A	O4'-C1'-N9	6.69	113.56	108.20
1	A	216	A	C5-C6-N6	-6.69	118.35	123.70
1	A	16	G	P-O5'-C5'	6.68	131.59	120.90
1	A	105	G	O4'-C4'-C3'	-6.67	97.33	104.00
1	A	48	G	O4'-C1'-N9	6.66	113.53	108.20
1	A	212	C	N3-C4-C5	-6.66	119.24	121.90
1	A	150	G	C5-C6-O6	-6.65	124.61	128.60
1	A	202	C	N3-C4-C5	-6.65	119.24	121.90
1	A	182	G	C5-C6-O6	-6.64	124.61	128.60
1	A	33	G	C5-C6-O6	-6.64	124.62	128.60
1	A	135	G	N3-C2-N2	6.63	124.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	G	O4'-C4'-C3'	-6.62	97.38	104.00
1	A	80	U	O5'-C5'-C4'	-6.61	99.14	111.70
1	A	149	A	C5-C6-N6	-6.61	118.41	123.70
1	A	118	A	C4-C5-C6	6.61	120.30	117.00
1	A	52	C	N3-C4-C5	-6.60	119.26	121.90
1	A	196	C	N3-C4-C5	-6.59	119.26	121.90
1	A	106	G	O5'-C5'-C4'	6.59	124.23	111.70
1	A	161	C	N3-C4-C5	-6.59	119.26	121.90
1	A	39	C	C4'-C3'-C2'	-6.58	96.02	102.60
1	A	41	G	O4'-C1'-N9	6.58	113.46	108.20
1	A	294	G	O4'-C1'-N9	6.57	113.46	108.20
1	A	159	C	N3-C4-C5	-6.56	119.28	121.90
1	A	124	G	O5'-C5'-C4'	6.56	124.16	111.70
1	A	225	C	N3-C4-C5	-6.56	119.28	121.90
1	A	192	A	O4'-C1'-N9	6.55	113.44	108.20
1	A	150	G	P-O5'-C5'	6.53	131.35	120.90
1	A	4	G	C5-C6-O6	-6.52	124.69	128.60
1	A	26	A	O4'-C1'-N9	6.51	113.41	108.20
1	A	267	C	N3-C4-C5	-6.49	119.30	121.90
1	A	180	G	O4'-C1'-N9	6.49	113.39	108.20
1	A	106	G	C5-C6-O6	-6.48	124.71	128.60
1	A	210	G	O4'-C1'-N9	6.47	113.38	108.20
1	A	38	U	C5'-C4'-C3'	6.46	126.34	116.00
1	A	264	A	C4-C5-C6	6.46	120.23	117.00
1	A	262	G	O4'-C1'-N9	6.45	113.36	108.20
1	A	274	G	P-O3'-C3'	6.45	127.44	119.70
1	A	175	G	C5-C6-O6	-6.45	124.73	128.60
1	A	8	G	C5-C6-O6	-6.44	124.74	128.60
1	A	263	C	N3-C4-C5	-6.43	119.33	121.90
1	A	59	A	P-O5'-C5'	-6.43	110.61	120.90
1	A	192	A	C5-C6-N6	-6.41	118.57	123.70
1	A	127	A	C4-C5-C6	6.41	120.20	117.00
1	A	268	C	N3-C4-C5	-6.40	119.34	121.90
1	A	40	G	C5-C6-O6	-6.39	124.76	128.60
1	A	143	C	N3-C4-N4	6.37	122.46	118.00
1	A	241	U	C4'-C3'-O3'	6.36	125.72	113.00
1	A	179	G	O4'-C1'-N9	6.35	113.28	108.20
1	A	58	G	C5'-C4'-O4'	6.35	116.72	109.10
1	A	258	C	N3-C4-C5	-6.35	119.36	121.90
1	A	185	C	C6-N1-C1'	-6.34	113.19	120.80
1	A	130	A	C4-C5-C6	6.34	120.17	117.00
1	A	216	A	C4-C5-C6	6.34	120.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	A	O4'-C1'-N9	6.32	113.26	108.20
1	A	244	C	N3-C4-N4	6.32	122.43	118.00
1	A	150	G	O4'-C1'-N9	6.32	113.25	108.20
1	A	207	C	N3-C4-N4	6.32	122.42	118.00
1	A	291	C	N3-C4-N4	6.31	122.42	118.00
1	A	162	C	N3-C4-C5	-6.30	119.38	121.90
1	A	72	A	O4'-C1'-N9	6.30	113.24	108.20
1	A	194	G	O4'-C1'-N9	6.30	113.24	108.20
1	A	180	G	C5-C6-O6	-6.29	124.82	128.60
1	A	205	A	O4'-C1'-N9	6.29	113.23	108.20
1	A	61	C	N3-C4-C5	-6.29	119.38	121.90
1	A	29	C	N3-C4-C5	-6.29	119.39	121.90
1	A	82	G	O4'-C1'-N9	6.29	113.23	108.20
1	A	200	A	C4-C5-C6	6.28	120.14	117.00
1	A	17	C	C5'-C4'-O4'	6.28	116.63	109.10
1	A	53	A	C5-C6-N6	-6.28	118.68	123.70
1	A	275	U	O4'-C1'-N1	6.28	113.22	108.20
1	A	7	C	N3-C4-N4	6.27	122.39	118.00
1	A	138	G	O4'-C1'-N9	6.27	113.21	108.20
1	A	44	G	O4'-C1'-N9	6.26	113.21	108.20
1	A	199	A	C4-C5-C6	6.26	120.13	117.00
1	A	184	A	C4-C5-C6	6.26	120.13	117.00
1	A	260	C	N3-C4-C5	-6.25	119.40	121.90
1	A	188	G	O4'-C1'-N9	6.25	113.20	108.20
1	A	165	G	O4'-C4'-C3'	-6.25	97.75	104.00
1	A	152	G	C5-C6-O6	-6.24	124.86	128.60
1	A	205	A	C5-C6-N1	-6.24	114.58	117.70
1	A	279	A	P-O3'-C3'	6.23	127.18	119.70
1	A	20	G	O4'-C1'-N9	6.23	113.19	108.20
1	A	38	U	P-O3'-C3'	6.23	127.18	119.70
1	A	144	C	N3-C4-C5	-6.23	119.41	121.90
1	A	41	G	C5-C6-O6	-6.23	124.86	128.60
1	A	249	G	N1-C6-O6	6.23	123.64	119.90
1	A	298	C	C2-N3-C4	6.22	123.01	119.90
1	A	276	G	C5'-C4'-C3'	-6.22	106.04	116.00
1	A	158	C	N3-C4-N4	6.21	122.35	118.00
1	A	293	C	N3-C4-N4	6.21	122.35	118.00
1	A	30	C	N3-C4-C5	-6.21	119.42	121.90
1	A	94	C	N3-C4-C5	-6.20	119.42	121.90
1	A	264	A	C5-C6-N1	-6.20	114.60	117.70
1	A	198	G	C5-C6-O6	-6.20	124.88	128.60
1	A	235	G	O4'-C1'-N9	6.19	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	C	N3-C4-C5	-6.19	119.42	121.90
1	A	151	C	N3-C4-C5	-6.19	119.42	121.90
1	A	96	A	O4'-C1'-N9	6.18	113.15	108.20
1	A	139	A	C5-C6-N1	-6.18	114.61	117.70
1	A	270	G	P-O3'-C3'	-6.18	112.29	119.70
1	A	156	G	O4'-C1'-N9	6.17	113.14	108.20
1	A	145	C	N3-C4-C5	-6.17	119.43	121.90
1	A	296	C	N3-C4-C5	-6.16	119.43	121.90
1	A	262	G	C5-C6-O6	-6.16	124.90	128.60
1	A	168	G	O4'-C1'-N9	6.16	113.13	108.20
1	A	27	G	C5-C6-O6	-6.15	124.91	128.60
1	A	292	C	N3-C4-C5	-6.15	119.44	121.90
1	A	131	A	C6-N1-C2	6.15	122.29	118.60
1	A	173	A	C4-C5-C6	6.14	120.07	117.00
1	A	257	C	N3-C4-C5	-6.14	119.44	121.90
1	A	141	C	N3-C4-C5	-6.13	119.45	121.90
1	A	171	U	O4'-C1'-N1	6.12	113.10	108.20
1	A	297	U	O4'-C1'-N1	6.12	113.10	108.20
1	A	286	G	C5-C6-O6	-6.12	124.93	128.60
1	A	264	A	O4'-C1'-N9	6.12	113.09	108.20
1	A	32	A	C4-C5-C6	6.12	120.06	117.00
1	A	18	G	C5-C6-O6	-6.11	124.93	128.60
1	A	205	A	C4-C5-C6	6.11	120.06	117.00
1	A	255	A	C4-C5-C6	6.11	120.06	117.00
1	A	49	A	C4-C5-C6	6.11	120.05	117.00
1	A	283	A	C4-C5-C6	6.10	120.05	117.00
1	A	289	A	C4'-C3'-O3'	-6.09	96.62	109.40
1	A	277	C	N3-C4-C5	-6.08	119.47	121.90
1	A	206	G	O4'-C1'-N9	6.08	113.06	108.20
1	A	42	G	C5-C6-O6	-6.07	124.96	128.60
1	A	253	A	C4-C5-C6	6.07	120.04	117.00
1	A	102	A	C4-C5-C6	6.07	120.03	117.00
1	A	96	A	C4-C5-C6	6.06	120.03	117.00
1	A	178	G	O4'-C1'-N9	6.06	113.05	108.20
1	A	204	G	O4'-C1'-N9	6.06	113.05	108.20
1	A	208	A	C5-C6-N6	-6.04	118.87	123.70
1	A	47	U	C2'-C3'-O3'	6.04	123.36	113.70
1	A	173	A	C5-C6-N1	-6.03	114.69	117.70
1	A	45	G	O4'-C1'-N9	6.03	113.02	108.20
1	A	70	C	N3-C4-N4	6.03	122.22	118.00
1	A	72	A	C4-C5-C6	6.02	120.01	117.00
1	A	220	C	N3-C4-C5	-6.02	119.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	C	N3-C4-N4	6.02	122.21	118.00
1	A	199	A	C5-C6-N6	-6.01	118.89	123.70
1	A	186	C	C6-N1-C1'	-6.01	113.59	120.80
1	A	146	G	C5-C6-O6	-6.00	125.00	128.60
1	A	6	G	O4'-C1'-N9	6.00	113.00	108.20
1	A	192	A	C4-C5-C6	6.00	120.00	117.00
1	A	200	A	C5-C6-N6	-6.00	118.90	123.70
1	A	79	C	P-O5'-C5'	5.99	130.49	120.90
1	A	92	C	N3-C4-N4	5.99	122.19	118.00
1	A	183	A	C4-C5-C6	5.99	119.99	117.00
1	A	45	G	C5-C6-O6	-5.99	125.01	128.60
1	A	7	C	N3-C4-C5	-5.98	119.51	121.90
1	A	71	C	C2-N3-C4	5.98	122.89	119.90
1	A	261	U	C2-N3-C4	5.98	130.59	127.00
1	A	102	A	C5-C6-N1	-5.97	114.71	117.70
1	A	93	G	C5-C6-O6	-5.97	125.02	128.60
1	A	63	C	C2-N3-C4	5.97	122.89	119.90
1	A	201	A	C5-C6-N1	-5.97	114.72	117.70
1	A	46	C	N3-C4-C5	-5.96	119.52	121.90
1	A	3	C	C2-N3-C4	5.96	122.88	119.90
1	A	53	A	C4-C5-C6	5.95	119.98	117.00
1	A	160	A	C4-C5-C6	5.94	119.97	117.00
1	A	208	A	O4'-C1'-N9	5.94	112.95	108.20
1	A	292	C	N3-C4-N4	5.93	122.15	118.00
1	A	15	C	P-O5'-C5'	-5.93	111.41	120.90
1	A	227	G	O4'-C1'-N9	5.93	112.94	108.20
1	A	43	A	C4-C5-C6	5.93	119.96	117.00
1	A	58	G	O3'-P-O5'	-5.93	92.74	104.00
1	A	231	A	P-O5'-C5'	-5.93	111.42	120.90
1	A	17	C	O4'-C1'-N1	5.92	112.94	108.20
1	A	107	G	C5-C6-O6	-5.92	125.05	128.60
1	A	143	C	N3-C4-C5	-5.92	119.53	121.90
1	A	9	C	N3-C4-C5	-5.92	119.53	121.90
1	A	87	C	N3-C4-C5	-5.92	119.53	121.90
1	A	246	C	N3-C4-C5	-5.92	119.53	121.90
1	A	287	A	C4-C5-C6	5.92	119.96	117.00
1	A	189	C	N3-C4-C5	-5.91	119.53	121.90
1	A	19	C	N3-C4-C5	-5.91	119.54	121.90
1	A	32	A	O4'-C1'-N9	5.90	112.92	108.20
1	A	164	G	P-O5'-C5'	5.90	130.34	120.90
1	A	53	A	C5-C6-N1	-5.90	114.75	117.70
1	A	126	C	N3-C4-C5	-5.90	119.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	A	C4-C5-C6	5.90	119.95	117.00
1	A	119	A	C5-C6-N1	-5.90	114.75	117.70
1	A	258	C	N3-C4-N4	5.89	122.12	118.00
1	A	208	A	C4-C5-C6	5.89	119.94	117.00
1	A	22	C	N3-C4-N4	5.89	122.12	118.00
1	A	259	A	C6-N1-C2	5.89	122.13	118.60
1	A	17	C	O4'-C4'-C3'	-5.87	98.13	104.00
1	A	48	G	P-O3'-C3'	5.87	126.75	119.70
1	A	229	U	O4'-C4'-C3'	-5.87	98.13	104.00
1	A	64	U	C2-N3-C4	5.86	130.52	127.00
1	A	224	G	C5-C6-O6	-5.86	125.08	128.60
1	A	234	A	C4-C5-C6	5.86	119.93	117.00
1	A	187	G	O4'-C1'-N9	5.86	112.88	108.20
1	A	274	G	C5-C6-O6	-5.86	125.09	128.60
1	A	96	A	C6-N1-C2	5.85	122.11	118.60
1	A	75	A	C4-C5-C6	5.84	119.92	117.00
1	A	190	C	N3-C4-C5	-5.84	119.56	121.90
1	A	281	A	C2'-C3'-O3'	-5.83	96.67	109.50
1	A	140	C	N3-C4-C5	-5.83	119.57	121.90
1	A	21	C	N3-C4-N4	5.83	122.08	118.00
1	A	101	G	C5'-C4'-C3'	5.83	125.32	116.00
1	A	235	G	C5-C6-O6	-5.83	125.11	128.60
1	A	209	G	O4'-C1'-N9	5.81	112.85	108.20
1	A	88	A	C6-N1-C2	5.81	122.08	118.60
1	A	152	G	O4'-C1'-N9	5.80	112.84	108.20
1	A	1	G	C5-C6-O6	-5.79	125.12	128.60
1	A	101	G	P-O5'-C5'	-5.79	111.64	120.90
1	A	188	G	C5-C6-O6	-5.79	125.13	128.60
1	A	214	A	C4-C5-C6	5.77	119.89	117.00
1	A	201	A	C4'-C3'-C2'	-5.76	96.84	102.60
1	A	118	A	C6-N1-C2	5.76	122.06	118.60
1	A	2	C	N3-C4-C5	-5.75	119.60	121.90
1	A	279	A	C4'-C3'-O3'	5.75	124.50	113.00
1	A	1	G	O4'-C1'-N9	5.74	112.79	108.20
1	A	176	A	C4-C5-C6	5.74	119.87	117.00
1	A	216	A	C5-C6-N1	-5.73	114.83	117.70
1	A	26	A	C4-C5-C6	5.72	119.86	117.00
1	A	252	A	C5-C6-N6	-5.71	119.13	123.70
1	A	217	C	N3-C4-C5	-5.70	119.62	121.90
1	A	166	U	C4'-C3'-C2'	-5.69	96.91	102.60
1	A	138	G	N3-C2-N2	5.69	123.89	119.90
1	A	48	G	N1-C2-N3	-5.69	120.49	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	C	N3-C4-N4	5.69	121.98	118.00
1	A	247	C	N3-C4-N4	5.68	121.98	118.00
1	A	34	C	N3-C4-N4	5.68	121.98	118.00
1	A	196	C	N3-C4-N4	5.68	121.97	118.00
1	A	191	C	N3-C4-N4	5.67	121.97	118.00
1	A	212	C	C2-N3-C4	5.67	122.73	119.90
1	A	247	C	N3-C4-C5	-5.67	119.63	121.90
1	A	186	C	N3-C4-C5	-5.67	119.63	121.90
1	A	214	A	C5-C6-N1	-5.67	114.87	117.70
1	A	283	A	C6-N1-C2	5.67	122.00	118.60
1	A	185	C	N3-C4-N4	5.66	121.96	118.00
1	A	57	G	O3'-P-O5'	5.65	114.74	104.00
1	A	118	A	O4'-C1'-N9	5.65	112.72	108.20
1	A	22	C	N3-C4-C5	-5.64	119.64	121.90
1	A	245	G	C5-C6-O6	-5.63	125.22	128.60
1	A	259	A	C4-C5-C6	5.63	119.81	117.00
1	A	242	C	C5'-C4'-O4'	-5.62	102.35	109.10
1	A	177	G	C5-C6-O6	-5.62	125.23	128.60
1	A	172	A	C4-C5-C6	5.62	119.81	117.00
1	A	155	G	C5-C6-O6	-5.61	125.23	128.60
1	A	257	C	N3-C4-N4	5.61	121.93	118.00
1	A	148	G	O4'-C1'-N9	5.61	112.69	108.20
1	A	52	C	C2-N3-C4	5.61	122.70	119.90
1	A	83	G	O4'-C1'-N9	5.61	112.69	108.20
1	A	184	A	O4'-C1'-N9	5.61	112.68	108.20
1	A	133	A	C5-C6-N1	-5.60	114.90	117.70
1	A	156	G	C5-C6-O6	-5.60	125.24	128.60
1	A	32	A	C5-C6-N6	-5.60	119.22	123.70
1	A	149	A	O4'-C1'-N9	5.59	112.68	108.20
1	A	24	G	O4'-C1'-N9	5.59	112.67	108.20
1	A	296	C	N3-C4-N4	5.59	121.91	118.00
1	A	198	G	C6-C5-N7	-5.59	127.05	130.40
1	A	246	C	N3-C4-N4	5.58	121.91	118.00
1	A	199	A	O4'-C1'-N9	5.58	112.67	108.20
1	A	37	C	P-O3'-C3'	5.57	126.39	119.70
1	A	263	C	C2-N3-C4	5.57	122.69	119.90
1	A	69	C	C2-N3-C4	5.56	122.68	119.90
1	A	293	C	N3-C4-C5	-5.56	119.67	121.90
1	A	92	C	N3-C4-C5	-5.55	119.68	121.90
1	A	40	G	O4'-C1'-N9	5.55	112.64	108.20
1	A	99	C	O4'-C1'-N1	5.54	112.63	108.20
1	A	149	A	C4-C5-C6	5.54	119.77	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	G	C5-C6-O6	-5.54	125.28	128.60
1	A	75	A	C5-C6-N6	-5.54	119.27	123.70
1	A	86	G	O4'-C1'-N9	5.53	112.62	108.20
1	A	38	U	O4'-C1'-N1	5.52	112.62	108.20
1	A	131	A	C4-C5-C6	5.52	119.76	117.00
1	A	164	G	O4'-C1'-N9	5.50	112.60	108.20
1	A	231	A	C4-C5-C6	5.50	119.75	117.00
1	A	280	C	N1-C1'-C2'	5.50	121.15	114.00
1	A	139	A	C4-C5-C6	5.49	119.75	117.00
1	A	44	G	N1-C2-N3	-5.48	120.61	123.90
1	A	186	C	N3-C4-N4	5.48	121.83	118.00
1	A	50	G	O4'-C1'-N9	5.48	112.58	108.20
1	A	21	C	N3-C4-C5	-5.47	119.71	121.90
1	A	189	C	N3-C4-N4	5.47	121.83	118.00
1	A	119	A	P-O3'-C3'	5.46	126.26	119.70
1	A	281	A	P-O5'-C5'	5.46	129.64	120.90
1	A	277	C	N3-C4-N4	5.46	121.82	118.00
1	A	131	A	O4'-C1'-N9	5.45	112.56	108.20
1	A	127	A	C5-C6-N6	-5.45	119.34	123.70
1	A	288	G	C4'-C3'-O3'	5.45	123.90	113.00
1	A	9	C	N3-C4-N4	5.44	121.81	118.00
1	A	119	A	C4-C5-C6	5.43	119.72	117.00
1	A	89	G	C5-C6-O6	-5.43	125.34	128.60
1	A	30	C	N3-C4-N4	5.43	121.80	118.00
1	A	68	G	O5'-C5'-C4'	-5.43	101.39	111.70
1	A	81	G	N1-C2-N3	-5.43	120.64	123.90
1	A	270	G	C2'-C3'-O3'	-5.43	97.56	109.50
1	A	193	G	C5-C6-O6	-5.41	125.36	128.60
1	A	158	C	N3-C4-C5	-5.41	119.74	121.90
1	A	269	A	P-O3'-C3'	-5.40	113.22	119.70
1	A	32	A	C5-C6-N1	-5.39	115.00	117.70
1	A	228	A	P-O3'-C3'	5.38	126.16	119.70
1	A	111	C	P-O5'-C5'	5.38	129.51	120.90
1	A	184	A	C5-C6-N1	-5.38	115.01	117.70
1	A	185	C	N3-C4-C5	-5.38	119.75	121.90
1	A	86	G	N1-C2-N3	-5.38	120.67	123.90
1	A	120	G	C5-C6-O6	-5.38	125.37	128.60
1	A	219	C	C2-N3-C4	5.37	122.59	119.90
1	A	280	C	C5'-C4'-O4'	5.37	115.55	109.10
1	A	253	A	P-O3'-C3'	5.37	126.14	119.70
1	A	187	G	N1-C2-N3	-5.37	120.68	123.90
1	A	251	G	P-O5'-C5'	5.37	129.48	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	C	N3-C4-C5	-5.36	119.75	121.90
1	A	284	G	C5-C6-O6	-5.36	125.38	128.60
1	A	151	C	N3-C4-N4	5.36	121.75	118.00
1	A	200	A	C5-C6-N1	-5.35	115.03	117.70
1	A	84	C	N3-C4-C5	-5.35	119.76	121.90
1	A	183	A	C5-C6-N6	-5.33	119.44	123.70
1	A	170	C	N3-C4-N4	5.31	121.72	118.00
1	A	176	A	C5-C6-N1	-5.30	115.05	117.70
1	A	116	C	N3-C4-C5	-5.29	119.78	121.90
1	A	82	G	C5-C6-O6	-5.29	125.42	128.60
1	A	294	G	N1-C2-N3	-5.29	120.73	123.90
1	A	234	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	1	G	N3-C2-N2	5.29	123.60	119.90
1	A	70	C	N3-C4-C5	-5.29	119.79	121.90
1	A	88	A	C4-C5-C6	5.28	119.64	117.00
1	A	173	A	C5-C6-N6	-5.28	119.48	123.70
1	A	34	C	N3-C4-C5	-5.25	119.80	121.90
1	A	210	G	C5-C6-O6	-5.25	125.45	128.60
1	A	172	A	C5-C6-N6	-5.25	119.50	123.70
1	A	221	C	N3-C4-N4	5.25	121.67	118.00
1	A	46	C	N3-C4-N4	5.24	121.67	118.00
1	A	170	C	N3-C4-C5	-5.24	119.80	121.90
1	A	54	G	C5-C6-O6	-5.24	125.46	128.60
1	A	116	C	N3-C4-N4	5.24	121.66	118.00
1	A	199	A	C5-C6-N1	-5.24	115.08	117.70
1	A	281	A	C5'-C4'-O4'	5.24	115.38	109.10
1	A	229	U	N1-C1'-C2'	-5.23	106.25	112.00
1	A	230	C	O4'-C1'-N1	5.23	112.38	108.20
1	A	285	C	C2-N3-C4	5.22	122.51	119.90
1	A	168	G	N1-C2-N3	-5.22	120.77	123.90
1	A	276	G	N1-C2-N3	-5.21	120.77	123.90
1	A	291	C	C2-N3-C4	5.21	122.50	119.90
1	A	149	A	C5-C6-N1	-5.21	115.10	117.70
1	A	166	U	N3-C4-C5	-5.20	111.48	114.60
1	A	234	A	C6-N1-C2	5.20	121.72	118.60
1	A	147	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	274	G	O4'-C1'-N9	5.19	112.35	108.20
1	A	214	A	C5-C6-N6	-5.19	119.55	123.70
1	A	256	G	C5-C6-O6	-5.19	125.48	128.60
1	A	183	A	C5-C6-N1	-5.18	115.11	117.70
1	A	227	G	N1-C2-N3	-5.18	120.79	123.90
1	A	26	A	C5-C6-N1	-5.16	115.12	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	C	N3-C4-N4	5.16	121.61	118.00
1	A	15	C	C4'-C3'-O3'	-5.13	98.62	109.40
1	A	26	A	C5-C6-N6	-5.13	119.59	123.70
1	A	268	C	C2-N3-C4	5.13	122.47	119.90
1	A	191	C	N3-C4-C5	-5.13	119.85	121.90
1	A	265	C	N3-C4-C5	-5.12	119.85	121.90
1	A	105	G	P-O3'-C3'	-5.12	113.56	119.70
1	A	49	A	O4'-C1'-N9	5.12	112.29	108.20
1	A	74	G	C5-C6-O6	-5.11	125.53	128.60
1	A	75	A	C5-C6-N1	-5.11	115.14	117.70
1	A	136	G	C5-C6-O6	-5.11	125.53	128.60
1	A	105	G	C1'-O4'-C4'	-5.11	105.81	109.90
1	A	62	G	C5-C6-O6	-5.10	125.54	128.60
1	A	190	C	N3-C4-N4	5.10	121.57	118.00
1	A	60	U	N1-C1'-C2'	5.10	120.63	114.00
1	A	159	C	C2-N3-C4	5.09	122.45	119.90
1	A	213	A	C5-C6-N6	-5.09	119.63	123.70
1	A	60	U	C1'-O4'-C4'	-5.09	105.83	109.90
1	A	172	A	C5-C6-N1	-5.09	115.16	117.70
1	A	174	G	C5-C6-O6	-5.09	125.55	128.60
1	A	55	G	N3-C2-N2	5.08	123.45	119.90
1	A	125	G	C5-C6-O6	-5.08	125.55	128.60
1	A	29	C	N3-C4-N4	5.07	121.55	118.00
1	A	76	G	C2'-C3'-O3'	-5.07	98.36	109.50
1	A	265	C	N3-C4-N4	5.05	121.54	118.00
1	A	213	A	C5-C6-N1	-5.05	115.18	117.70
1	A	129	C	C2-N3-C4	5.04	122.42	119.90
1	A	105	G	C2'-C3'-O3'	-5.03	98.43	109.50
1	A	225	C	C2-N3-C4	5.03	122.41	119.90
1	A	163	A	C5-C6-N1	-5.03	115.19	117.70
1	A	267	C	C2-N3-C4	5.03	122.41	119.90
1	A	274	G	C4'-C3'-C2'	-5.02	97.58	102.60
1	A	2	C	N3-C4-N4	5.02	121.51	118.00
1	A	163	A	O4'-C1'-N9	5.02	112.22	108.20
1	A	166	U	C5-C4-O4	5.01	128.91	125.90
1	A	203	G	C5-C6-O6	-5.01	125.59	128.60
1	A	260	C	N3-C4-N4	5.01	121.51	118.00
1	A	182	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (146) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	U	Sidechain
1	A	119	A	Sidechain
1	A	131	A	Sidechain
1	A	133	A	Sidechain
1	A	134	U	Sidechain
1	A	135	G	Sidechain
1	A	136	G	Sidechain
1	A	137	U	Sidechain
1	A	138	G	Sidechain
1	A	149	A	Sidechain
1	A	163	A	Sidechain
1	A	165	G	Sidechain
1	A	166	U	Sidechain
1	A	167	U	Sidechain
1	A	168	G	Sidechain
1	A	175	G	Sidechain
1	A	201	A	Sidechain
1	A	215	A	Sidechain
1	A	233	U	Sidechain
1	A	237	G	Sidechain
1	A	245	G	Sidechain
1	A	250	U	Sidechain
1	A	251	G	Sidechain
1	A	252	A	Sidechain
1	A	253	A	Sidechain
1	A	254	U	Sidechain
1	A	255	A	Sidechain
1	A	274	G	Sidechain
1	A	276	G	Sidechain
1	A	282	U	Sidechain
1	A	284	G	Sidechain
1	A	297	U	Sidechain
1	A	39	C	Sidechain
1	A	43	A	Sidechain
1	A	75	A	Sidechain
1	A	83	G	Sidechain
1	A	85	U	Sidechain
1	A	96	A	Sidechain
4	D	100	LYS	Mainchain
4	D	107	VAL	Mainchain
4	D	115	THR	Mainchain
4	D	116	THR	Mainchain
4	D	117	THR	Mainchain

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Mol	Chain	Res	Type	Group
4	D	123	TYR	Mainchain
4	D	124	TYR	Mainchain
4	D	125	TYR	Mainchain
4	D	126	GLN	Mainchain
4	D	128	LYS	Mainchain
4	D	131	LYS	Mainchain
4	D	132	THR	Mainchain
4	D	136	CYS	Mainchain
4	D	138	ASP	Mainchain
4	D	142	ALA	Mainchain
4	D	154	LYS	Mainchain
4	D	162	SER	Mainchain
4	D	167	ASP	Mainchain
4	D	169	VAL	Mainchain
4	D	174	GLU	Mainchain
4	D	175	GLY	Mainchain
4	D	176	VAL	Mainchain
4	D	180	LYS	Mainchain
4	D	181	ASN	Mainchain
4	D	182	GLU	Mainchain
4	D	184	PHE	Mainchain
4	D	185	GLU	Mainchain
4	D	187	ILE	Mainchain
4	D	191	THR	Mainchain
4	D	2	VAL	Mainchain
4	D	207	GLN	Mainchain
4	D	208	VAL	Mainchain
4	D	21	THR	Mainchain
4	D	215	ASP	Mainchain
4	D	220	VAL	Mainchain
4	D	221	MET	Mainchain
4	D	227	GLN	Mainchain
4	D	228	ALA	Mainchain
4	D	23	ILE	Mainchain
4	D	231	ALA	Mainchain
4	D	237	LYS	Mainchain
4	D	242	VAL	Mainchain
4	D	243	ALA	Mainchain
4	D	244	SER	Mainchain
4	D	249	LYS	Mainchain
4	D	250	LEU	Mainchain
4	D	252	GLY	Mainchain

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Mol	Chain	Res	Type	Group
4	D	259	ALA	Mainchain
4	D	26	GLU	Mainchain
4	D	264	ALA	Mainchain
4	D	266	THR	Mainchain
4	D	268	SER	Mainchain
4	D	28	LEU	Mainchain
4	D	281	ASP	Mainchain
4	D	282	PHE	Mainchain
4	D	292	SER	Mainchain
4	D	293	LYS	Mainchain
4	D	296	GLY	Mainchain
4	D	298	GLY	Mainchain,Peptide
4	D	3	LEU	Mainchain
4	D	309	GLU	Mainchain
4	D	31	MET	Mainchain
4	D	319	ILE	Mainchain
4	D	32	LEU	Mainchain
4	D	331	ASP	Mainchain
4	D	334	GLU	Mainchain
4	D	342	MET	Peptide
4	D	35	VAL	Mainchain
4	D	357	THR	Mainchain
4	D	358	ASP	Mainchain
4	D	360	MET	Mainchain
4	D	366	GLN	Mainchain
4	D	37	THR	Mainchain
4	D	376	MET	Mainchain
4	D	378	ILE	Mainchain
4	D	381	SER	Mainchain
4	D	390	THR	Mainchain
4	D	397	SER	Mainchain
4	D	401	GLY	Mainchain
4	D	403	ILE	Mainchain
4	D	405	ARG	Mainchain
4	D	408	ARG	Mainchain
4	D	417	VAL	Mainchain
4	D	418	GLN	Mainchain
4	D	424	TYR	Mainchain
4	D	428	ALA	Mainchain
4	D	429	GLN	Mainchain
4	D	43	ASP	Mainchain
4	D	44	VAL	Mainchain

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Mol	Chain	Res	Type	Group
4	D	45	ASN	Mainchain
4	D	46	ILE	Mainchain
4	D	5	ASP	Mainchain
4	D	55	ASN	Mainchain
4	D	6	LEU	Mainchain
4	D	60	ILE	Mainchain
4	D	66	ALA	Mainchain
4	D	69	LEU	Mainchain
4	D	71	LYS	Mainchain
4	D	74	MET	Mainchain
4	D	79	VAL	Mainchain
4	D	80	PHE	Mainchain
4	D	81	LYS	Mainchain
4	D	89	PRO	Mainchain
4	D	92	LYS	Mainchain
4	D	93	ALA	Mainchain
4	D	94	TRP	Mainchain
4	D	99	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6403	0	3239	205	0
2	B	300	0	74	22	0
3	C	716	0	184	28	0
4	D	1732	0	488	27	0
5	E	296	0	71	26	0
6	F	429	0	109	11	0
7	S	72	0	18	0	0
All	All	9948	0	4183	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LEU:CA	5:E:55:GLN:CA	1.96	1.43
1:A:174:G:O3'	3:C:146:HIS:CA	1.71	1.38
2:B:94:LEU:N	5:E:56:ALA:H	1.26	1.31
2:B:94:LEU:H	5:E:56:ALA:N	1.30	1.28
1:A:196:C:H4'	6:F:69:SER:CA	1.65	1.26
2:B:94:LEU:CA	5:E:56:ALA:H	1.49	1.25
2:B:94:LEU:N	5:E:56:ALA:N	1.84	1.22
1:A:174:G:H5"	3:C:146:HIS:O	1.08	1.21
1:A:195:U:C5'	4:D:411:GLY:HA3	1.71	1.20
2:B:94:LEU:CA	5:E:56:ALA:N	2.03	1.19
1:A:195:U:H5"	4:D:411:GLY:HA3	1.20	1.15
1:A:174:G:C5'	3:C:146:HIS:O	1.93	1.15
1:A:175:G:C5'	3:C:146:HIS:H	1.62	1.12
1:A:175:G:C5'	3:C:143:LYS:O	2.03	1.07
1:A:175:G:H5'	3:C:146:HIS:N	1.68	1.07
1:A:175:G:H5'	3:C:146:HIS:H	1.16	1.06
1:A:278:A:C2	1:A:280:C:N4	2.24	1.06
1:A:278:A:H2	1:A:280:C:N4	1.56	1.04
1:A:174:G:H5"	3:C:146:HIS:C	1.80	1.01
2:B:94:LEU:CA	5:E:55:GLN:C	2.31	0.99
1:A:175:G:H5'	3:C:143:LYS:O	1.64	0.95
1:A:175:G:H5'	3:C:146:HIS:CA	1.98	0.93
1:A:195:U:H4'	4:D:411:GLY:HA2	1.49	0.93
2:B:23:SER:CA	5:E:35:ASP:CA	2.34	0.92
1:A:175:G:H4'	3:C:143:LYS:O	1.67	0.92
1:A:67:A:C2	1:A:281:A:N6	2.38	0.91
1:A:173:A:OP2	3:C:153:LYS:CA	2.19	0.91
1:A:66:G:N2	1:A:283:A:C1'	2.34	0.91
1:A:173:A:OP2	3:C:153:LYS:C	2.10	0.90
1:A:16:G:H5"	1:A:17:C:C5	2.07	0.90
1:A:66:G:H21	1:A:283:A:C1'	1.86	0.89
1:A:196:C:C4'	6:F:69:SER:CA	2.50	0.87
1:A:109:G:P	1:A:238:G:OP2	2.32	0.87
1:A:79:C:H42	1:A:270:G:H1	1.16	0.86
1:A:110:U:H3'	1:A:111:C:H5	1.41	0.86
1:A:124:G:O2'	1:A:125:G:H5'	1.76	0.86
1:A:175:G:C5'	3:C:146:HIS:N	2.34	0.85
1:A:195:U:C5'	4:D:411:GLY:CA	2.54	0.84
4:D:362:LYS:N	4:D:363:GLY:HA3	1.92	0.84
1:A:173:A:OP2	3:C:154:ALA:N	2.09	0.84
1:A:175:G:C4'	3:C:143:LYS:O	2.25	0.83
1:A:79:C:N4	1:A:270:G:H1	1.75	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:A:H2'	1:A:59:A:N3	1.95	0.81
1:A:278:A:N6	1:A:279:A:N1	2.27	0.81
1:A:74:G:H1	1:A:271:C:H42	1.25	0.81
1:A:174:G:C3'	3:C:146:HIS:CA	2.60	0.80
1:A:195:U:H4'	4:D:411:GLY:CA	2.12	0.80
2:B:28:ILE:C	5:E:28:VAL:C	2.40	0.79
1:A:278:A:H2	1:A:280:C:C4	2.01	0.79
1:A:59:A:C2	1:A:60:U:H5'	2.17	0.79
1:A:291:C:O4'	5:E:46:LEU:CA	2.31	0.78
2:B:21:ARG:O	5:E:34:SER:C	2.25	0.75
1:A:111:C:N4	1:A:239:G:O6	2.20	0.75
1:A:37:C:O2'	1:A:38:U:H5'	1.86	0.74
1:A:229:U:H3'	1:A:230:C:H6	1.52	0.74
4:D:296:GLY:HA2	4:D:297:MET:C	2.09	0.74
1:A:37:C:H2'	1:A:38:U:O4'	1.89	0.73
1:A:66:G:N2	1:A:283:A:N9	2.37	0.73
1:A:226:U:H2'	1:A:227:G:H5"	1.71	0.72
2:B:91:MET:O	5:E:56:ALA:CA	2.37	0.72
1:A:109:G:OP2	1:A:238:G:OP2	2.08	0.72
1:A:74:G:H1	1:A:271:C:N4	1.88	0.72
1:A:16:G:H5"	1:A:17:C:H5	1.51	0.72
1:A:123:C:O2'	1:A:124:G:H5'	1.89	0.72
1:A:66:G:N2	1:A:283:A:C8	2.58	0.71
1:A:110:U:C2'	1:A:111:C:OP1	2.39	0.71
1:A:98:G:C8	1:A:98:G:H5"	2.25	0.71
2:B:21:ARG:O	5:E:35:ASP:N	2.24	0.70
1:A:175:G:C5'	3:C:146:HIS:CA	2.69	0.70
1:A:13:G:H1	1:A:37:C:H42	1.40	0.69
1:A:278:A:O2'	1:A:279:A:H5'	1.93	0.69
1:A:175:G:C5'	3:C:143:LYS:C	2.49	0.68
1:A:175:G:H5"	3:C:143:LYS:C	2.14	0.68
1:A:37:C:C2'	1:A:38:U:H5'	2.25	0.67
1:A:281:A:C5	1:A:282:U:H1'	2.30	0.67
1:A:195:U:H5'	4:D:410:SER:O	1.95	0.66
2:B:24:GLY:C	5:E:32:ARG:CA	2.64	0.66
1:A:23:U:O4	2:B:63:GLY:O	2.13	0.66
2:B:55:LYS:N	5:E:73:MET:O	2.29	0.66
1:A:110:U:H2'	1:A:111:C:OP1	1.95	0.65
1:A:124:G:HO2'	1:A:125:G:H5'	1.61	0.64
2:B:29:THR:N	5:E:28:VAL:CA	2.61	0.63
1:A:223:U:OP1	3:C:73:GLN:CA	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:U:C2'	1:A:227:G:H5"	2.29	0.63
4:D:339:ILE:O	4:D:342:MET:N	2.30	0.62
1:A:181:U:H2'	1:A:182:G:H5'	1.79	0.62
1:A:66:G:H21	1:A:283:A:H1'	1.63	0.62
1:A:103:U:C6	1:A:104:C:C6	2.88	0.61
1:A:103:U:C5	1:A:104:C:C5	2.88	0.61
1:A:111:C:H6	1:A:111:C:O5'	1.83	0.61
1:A:195:U:C4'	4:D:411:GLY:CA	2.79	0.61
1:A:9:C:C2'	1:A:10:G:H5'	2.31	0.61
1:A:135:G:H2'	1:A:136:G:H5'	1.81	0.61
1:A:37:C:H2'	1:A:38:U:C5'	2.31	0.61
1:A:59:A:N3	1:A:60:U:H5'	2.16	0.60
4:D:296:GLY:CA	4:D:297:MET:C	2.69	0.60
1:A:66:G:N2	1:A:283:A:H1'	2.13	0.60
1:A:242:C:O2	1:A:242:C:H5"	2.02	0.60
1:A:269:A:H2'	1:A:270:G:O5'	2.01	0.60
1:A:229:U:C6	1:A:230:C:C6	2.90	0.60
1:A:278:A:N6	1:A:279:A:C6	2.70	0.60
1:A:66:G:N2	1:A:283:A:O4'	2.32	0.59
1:A:67:A:C2	1:A:281:A:C6	2.90	0.59
4:D:340:MET:C	4:D:342:MET:N	2.56	0.59
1:A:78:U:H2'	1:A:78:U:O2	2.02	0.59
1:A:291:C:C1'	5:E:46:LEU:CA	2.80	0.59
1:A:280:C:O2	1:A:280:C:H2'	2.02	0.59
1:A:278:A:C6	1:A:279:A:C2	2.90	0.59
1:A:175:G:H5"	3:C:142:ARG:O	2.01	0.59
1:A:162:C:H2'	1:A:163:A:H5'	1.84	0.59
1:A:195:U:H5'	4:D:411:GLY:HA3	1.74	0.58
2:B:25:SER:C	5:E:31:TYR:C	2.60	0.58
1:A:68:G:H2'	1:A:69:C:O4'	2.04	0.58
1:A:278:A:H2'	1:A:279:A:O4'	2.03	0.58
4:D:340:MET:C	4:D:342:MET:H	2.06	0.58
1:A:175:G:H5"	3:C:146:HIS:H	1.62	0.58
1:A:278:A:N6	1:A:279:A:C2	2.72	0.58
1:A:163:A:H2'	1:A:164:G:C8	2.39	0.57
1:A:227:G:C2	1:A:228:A:H1'	2.39	0.57
1:A:104:C:H2'	1:A:104:C:O2	2.04	0.57
1:A:14:G:H1'	1:A:38:U:H3	1.69	0.56
1:A:37:C:C2'	1:A:38:U:C5'	2.83	0.56
1:A:195:U:H5"	4:D:411:GLY:CA	2.13	0.56
1:A:224:G:H5"	3:C:125:ARG:CA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:A:C5	1:A:279:A:C5	2.94	0.55
1:A:291:C:H1'	5:E:46:LEU:CA	2.36	0.55
1:A:16:G:H5"	1:A:17:C:C6	2.42	0.55
1:A:79:C:H5'	1:A:80:U:OP2	2.08	0.54
4:D:337:GLN:O	4:D:340:MET:N	2.40	0.54
1:A:76:G:N3	1:A:76:G:H2'	2.23	0.54
1:A:67:A:N3	1:A:281:A:C6	2.76	0.54
1:A:269:A:H2'	1:A:270:G:C5'	2.38	0.54
1:A:98:G:C2	1:A:253:A:C5	2.96	0.53
1:A:79:C:P	1:A:264:A:H5"	2.48	0.53
1:A:103:U:C6	1:A:104:C:C5	2.96	0.53
1:A:67:A:H3'	1:A:68:G:H8	1.73	0.53
1:A:182:G:H1'	1:A:215:A:H61	1.73	0.53
1:A:103:U:C5	1:A:104:C:C6	2.97	0.52
1:A:113:G:OP2	1:A:114:C:H5	1.92	0.52
2:B:94:LEU:N	5:E:55:GLN:CA	2.70	0.52
1:A:229:U:O5'	1:A:230:C:H5	1.93	0.51
6:F:88:GLN:O	6:F:91:GLY:N	2.42	0.51
1:A:75:A:C5	1:A:76:G:H1'	2.45	0.51
1:A:133:A:N1	1:A:163:A:N1	2.58	0.51
6:F:112:ILE:C	6:F:114:LYS:H	2.13	0.51
1:A:162:C:C2'	1:A:163:A:H5'	2.41	0.51
1:A:278:A:C2	1:A:280:C:C4	2.86	0.51
1:A:198:G:H1'	1:A:201:A:N6	2.25	0.51
1:A:135:G:C2'	1:A:136:G:H5'	2.41	0.51
1:A:79:C:H2'	1:A:79:C:O2	2.10	0.50
1:A:150:G:H2'	1:A:151:C:H5'	1.91	0.50
1:A:67:A:H3'	1:A:68:G:C8	2.47	0.50
1:A:249:G:H2'	1:A:250:U:C6	2.47	0.50
1:A:270:G:OP2	1:A:271:C:C5	2.65	0.50
2:B:94:LEU:N	5:E:55:GLN:C	2.52	0.49
1:A:67:A:C6	1:A:68:G:C2	3.00	0.49
1:A:229:U:H3'	1:A:230:C:C6	2.40	0.49
1:A:119:A:H3'	1:A:120:G:H5"	1.95	0.49
1:A:56:A:N6	1:A:57:G:C2	2.81	0.49
1:A:59:A:N3	1:A:59:A:C2'	2.72	0.49
1:A:131:A:C2	1:A:132:U:H1'	2.48	0.49
1:A:229:U:P	1:A:230:C:H5	2.36	0.49
4:D:360:MET:O	4:D:362:LYS:N	2.41	0.48
1:A:159:C:H2'	1:A:160:A:H5'	1.95	0.48
1:A:123:C:C2'	1:A:124:G:H5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:A:N6	1:A:68:G:N1	2.62	0.48
1:A:110:U:H3'	1:A:111:C:C5	2.33	0.48
4:D:337:GLN:C	4:D:340:MET:H	2.17	0.48
1:A:111:C:O5'	1:A:111:C:C6	2.65	0.47
4:D:340:MET:O	4:D:342:MET:N	2.47	0.47
4:D:341:LYS:O	4:D:342:MET:O	2.32	0.47
1:A:9:C:H2'	1:A:10:G:H5'	1.95	0.47
1:A:160:A:H2'	1:A:161:C:O4'	2.14	0.47
1:A:98:G:H5"	1:A:98:G:H8	1.72	0.47
1:A:67:A:C5	1:A:68:G:C5	3.02	0.47
1:A:227:G:H2'	1:A:228:A:O4'	2.14	0.47
1:A:270:G:OP2	1:A:271:C:H5	1.98	0.47
1:A:35:U:O2'	1:A:36:A:H5'	2.15	0.47
4:D:429:GLN:O	4:D:430:MET:C	2.53	0.47
1:A:75:A:C4	1:A:76:G:H1'	2.50	0.47
1:A:79:C:OP1	1:A:264:A:H5"	2.16	0.46
1:A:173:A:P	3:C:153:LYS:C	2.93	0.46
1:A:67:A:N6	1:A:68:G:C2	2.83	0.46
1:A:228:A:OP2	3:C:88:LYS:CA	2.64	0.46
1:A:277:C:H2'	1:A:278:A:C8	2.50	0.46
2:B:94:LEU:H	5:E:56:ALA:CA	2.18	0.46
6:F:76:VAL:C	6:F:78:TYR:N	2.69	0.46
1:A:278:A:H2'	1:A:279:A:O5'	2.16	0.46
1:A:110:U:O2'	1:A:111:C:OP1	2.32	0.46
1:A:124:G:C2'	1:A:125:G:H5'	2.46	0.45
1:A:181:U:C2'	1:A:182:G:H5'	2.45	0.45
1:A:269:A:H2'	1:A:270:G:H5'	1.98	0.45
1:A:278:A:N7	1:A:279:A:C5	2.84	0.45
2:B:25:SER:CA	5:E:32:ARG:N	2.79	0.45
1:A:281:A:C4	1:A:282:U:H1'	2.51	0.45
6:F:76:VAL:O	6:F:78:TYR:N	2.50	0.45
1:A:79:C:C5'	1:A:80:U:OP2	2.65	0.45
1:A:119:A:N1	1:A:231:A:C2	2.85	0.45
1:A:281:A:C6	1:A:282:U:H1'	2.52	0.45
1:A:113:G:OP2	1:A:114:C:C5	2.70	0.45
4:D:362:LYS:N	4:D:363:GLY:CA	2.72	0.45
1:A:169:C:H3'	1:A:170:C:C5'	2.47	0.45
1:A:242:C:H4'	1:A:243:G:H8	1.82	0.45
1:A:98:G:C8	1:A:98:G:C5'	2.99	0.44
1:A:79:C:OP1	1:A:264:A:OP1	2.35	0.44
1:A:164:G:C5	1:A:165:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:G:H1'	1:A:201:A:H61	1.82	0.44
1:A:229:U:OP2	1:A:230:C:C5	2.70	0.44
6:F:45:THR:O	6:F:46:ALA:C	2.56	0.44
4:D:233:ALA:O	4:D:234:LYS:C	2.56	0.44
1:A:108:U:O3'	1:A:238:G:OP2	2.35	0.44
1:A:229:U:OP2	1:A:230:C:H5	2.01	0.44
1:A:230:C:H2'	1:A:231:A:O5'	2.18	0.44
5:E:12:ARG:O	5:E:13:ALA:C	2.57	0.43
1:A:75:A:C6	1:A:76:G:H1'	2.53	0.43
1:A:163:A:C2	1:A:164:G:C6	3.06	0.43
1:A:16:G:H1'	1:A:39:C:N4	2.33	0.43
1:A:123:C:H2'	1:A:124:G:C5'	2.49	0.42
1:A:243:G:H2'	1:A:244:C:C6	2.53	0.42
1:A:13:G:H1	1:A:37:C:N4	2.12	0.42
4:D:414:THR:H	6:F:74:ARG:CA	2.32	0.42
1:A:12:U:O2'	1:A:14:G:N7	2.45	0.42
1:A:37:C:H3'	1:A:37:C:O2	2.20	0.42
1:A:182:G:H1'	1:A:215:A:N6	2.32	0.42
1:A:219:C:C2'	1:A:220:C:H5'	2.49	0.42
1:A:174:G:H3'	3:C:146:HIS:CA	2.47	0.42
4:D:334:GLU:O	4:D:338:ASN:N	2.48	0.42
4:D:337:GLN:C	4:D:339:ILE:N	2.73	0.42
1:A:159:C:C2'	1:A:160:A:H5'	2.49	0.42
1:A:269:A:C2'	1:A:270:G:O5'	2.68	0.41
1:A:273:U:H2'	1:A:274:G:C8	2.55	0.41
4:D:328:THR:O	4:D:331:ASP:N	2.34	0.41
1:A:65:U:O2'	1:A:66:G:H5'	2.20	0.41
1:A:164:G:C6	1:A:165:G:C8	3.08	0.41
6:F:88:GLN:O	6:F:89:GLU:C	2.58	0.41
1:A:56:A:N6	1:A:57:G:N1	2.69	0.41
1:A:222:G:H2'	1:A:223:U:H5'	2.03	0.41
1:A:252:A:H4'	1:A:253:A:H5'	2.03	0.41
1:A:278:A:C6	1:A:279:A:C6	3.09	0.41
1:A:278:A:O5'	1:A:278:A:H8	2.04	0.41
1:A:297:U:H2'	1:A:298:C:C6	2.56	0.41
1:A:99:C:C5	1:A:252:A:N6	2.89	0.41
6:F:104:VAL:O	6:F:105:MET:C	2.60	0.41
6:F:112:ILE:C	6:F:114:LYS:N	2.74	0.41
1:A:276:G:H2'	1:A:277:C:C6	2.56	0.41
5:E:62:ILE:C	5:E:64:LYS:N	2.74	0.41
1:A:224:G:H5'	3:C:125:ARG:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:U:H2'	1:A:81:G:C8	2.56	0.40
1:A:79:C:O2	1:A:79:C:C2'	2.68	0.40
1:A:120:G:O2'	1:A:121:U:H5'	2.22	0.40
1:A:110:U:O2'	1:A:111:C:P	2.79	0.40
1:A:132:U:H2'	1:A:133:A:C8	2.57	0.40
2:B:25:SER:N	5:E:32:ARG:CA	2.84	0.40
1:A:165:G:N7	1:A:176:A:C6	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	71/75 (95%)	61 (86%)	9 (13%)	1 (1%)	11 46
3	C	175/195 (90%)	168 (96%)	7 (4%)	0	100 100
4	D	431/433 (100%)	360 (84%)	55 (13%)	16 (4%)	3 24
5	E	72/74 (97%)	61 (85%)	9 (12%)	2 (3%)	5 30
6	F	105/107 (98%)	87 (83%)	11 (10%)	7 (7%)	1 15
7	S	16/18 (89%)	14 (88%)	2 (12%)	0	100 100
All	All	870/902 (96%)	751 (86%)	93 (11%)	26 (3%)	7 28

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	342	MET
6	F	42	GLU
6	F	75	ASP
4	D	296	GLY
4	D	297	MET

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Mol	Chain	Res	Type
4	D	298	GLY
4	D	299	ASP
6	F	99	PRO
2	B	23	SER
4	D	2	VAL
4	D	88	ASP
4	D	161	GLY
4	D	300	ILE
4	D	359	PHE
5	E	46	LEU
4	D	267	LYS
6	F	64	LYS
6	F	77	GLN
4	D	164	THR
4	D	341	LYS
4	D	373	LYS
4	D	101	GLN
4	D	354	GLY
5	E	21	ASP
6	F	56	VAL
6	F	96	VAL

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	298/299 (99%)	69 (23%)	10 (3%)

All (69) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	G
1	A	10	G
1	A	27	G
1	A	28	U
1	A	33	G
1	A	38	U
1	A	40	G

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Mol	Chain	Res	Type
1	A	43	A
1	A	44	G
1	A	47	U
1	A	48	G
1	A	49	A
1	A	63	C
1	A	70	C
1	A	75	A
1	A	76	G
1	A	84	C
1	A	85	U
1	A	88	A
1	A	89	G
1	A	90	U
1	A	99	C
1	A	107	G
1	A	111	C
1	A	118	A
1	A	119	A
1	A	120	G
1	A	121	U
1	A	130	A
1	A	136	G
1	A	142	U
1	A	149	A
1	A	155	G
1	A	160	A
1	A	163	A
1	A	169	C
1	A	170	C
1	A	173	A
1	A	174	G
1	A	175	G
1	A	176	A
1	A	177	G
1	A	184	A
1	A	185	C
1	A	186	C
1	A	201	A
1	A	204	G
1	A	213	A
1	A	220	C

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Mol	Chain	Res	Type
1	A	227	G
1	A	228	A
1	A	232	G
1	A	233	U
1	A	236	U
1	A	243	G
1	A	245	G
1	A	253	A
1	A	256	G
1	A	259	A
1	A	266	U
1	A	269	A
1	A	275	U
1	A	276	G
1	A	282	U
1	A	284	G
1	A	285	C
1	A	286	G
1	A	292	C
1	A	299	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	37	C
1	A	43	A
1	A	47	U
1	A	98	G
1	A	110	U
1	A	172	A
1	A	176	A
1	A	185	C
1	A	200	A
1	A	252	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	34:ASP	C	54:ASN	N	9.50

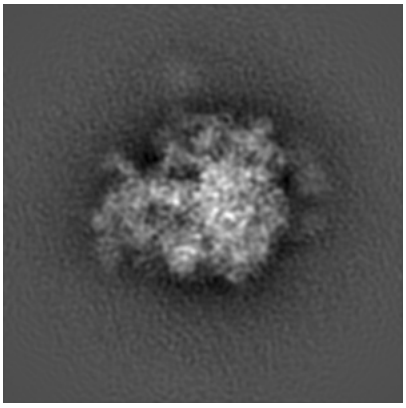
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2844. These allow visual inspection of the internal detail of the map and identification of artifacts.

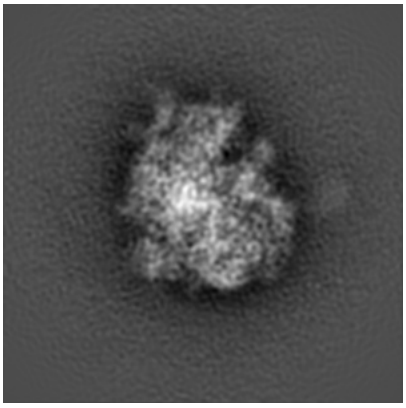
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

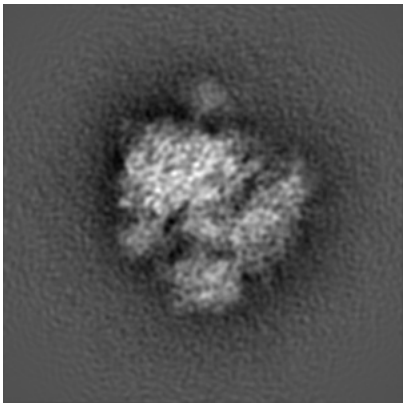
6.1.1 Primary map



X



Y

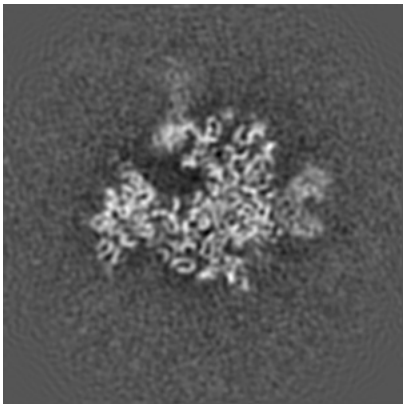


Z

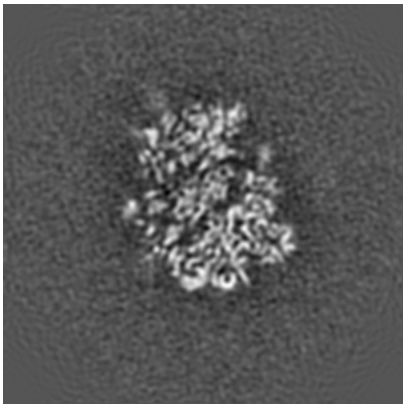
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

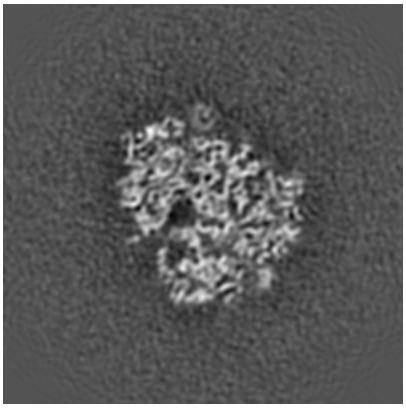
6.2.1 Primary map



X Index: 210



Y Index: 210

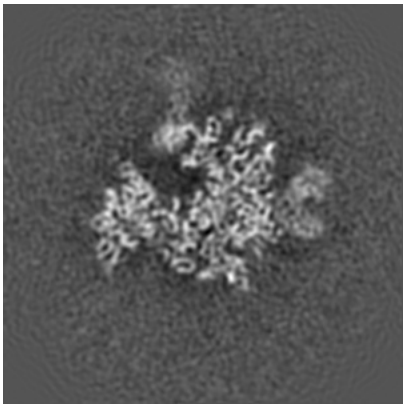


Z Index: 210

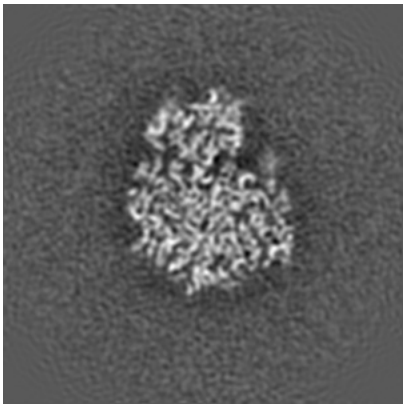
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

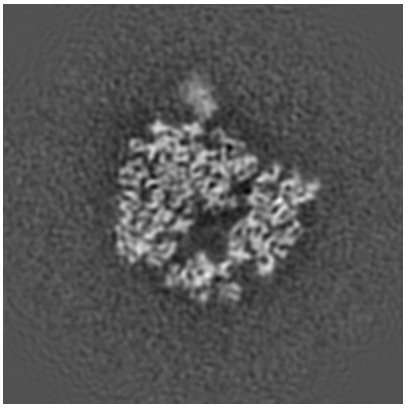
6.3.1 Primary map



X Index: 211



Y Index: 223



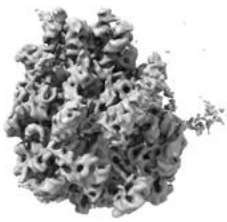
Z Index: 224

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

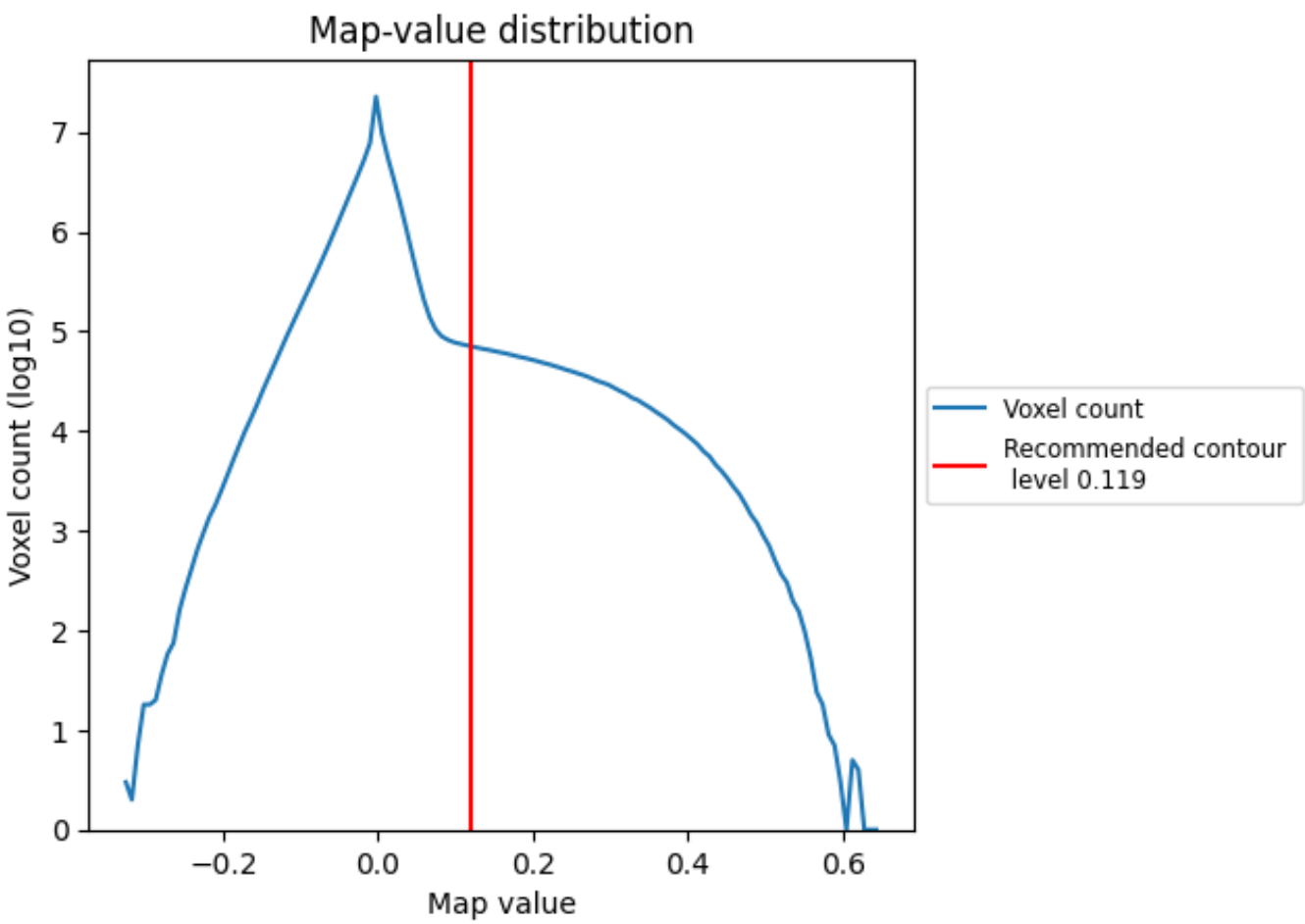
6.5 Mask visualisation (i)

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

7 Map analysis (i)

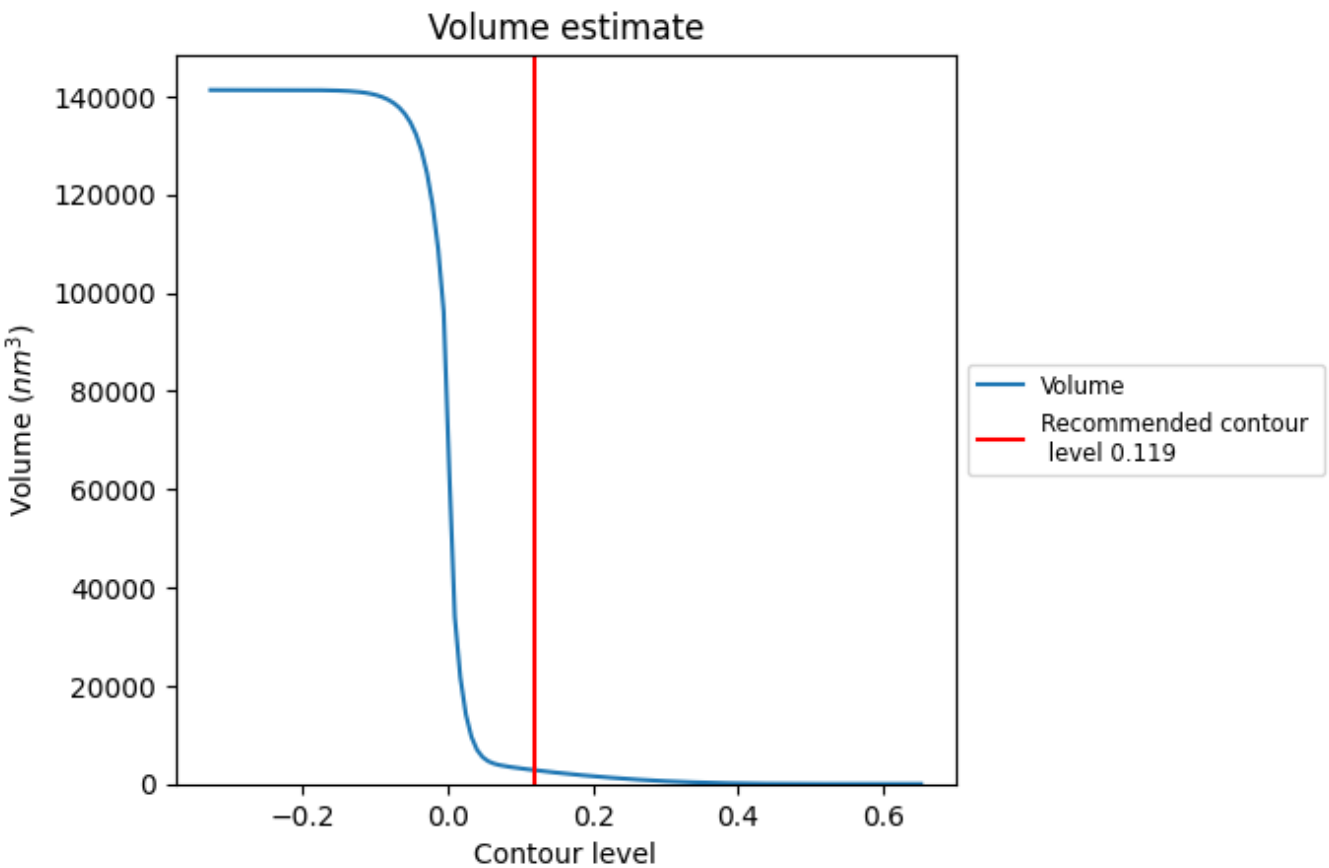
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

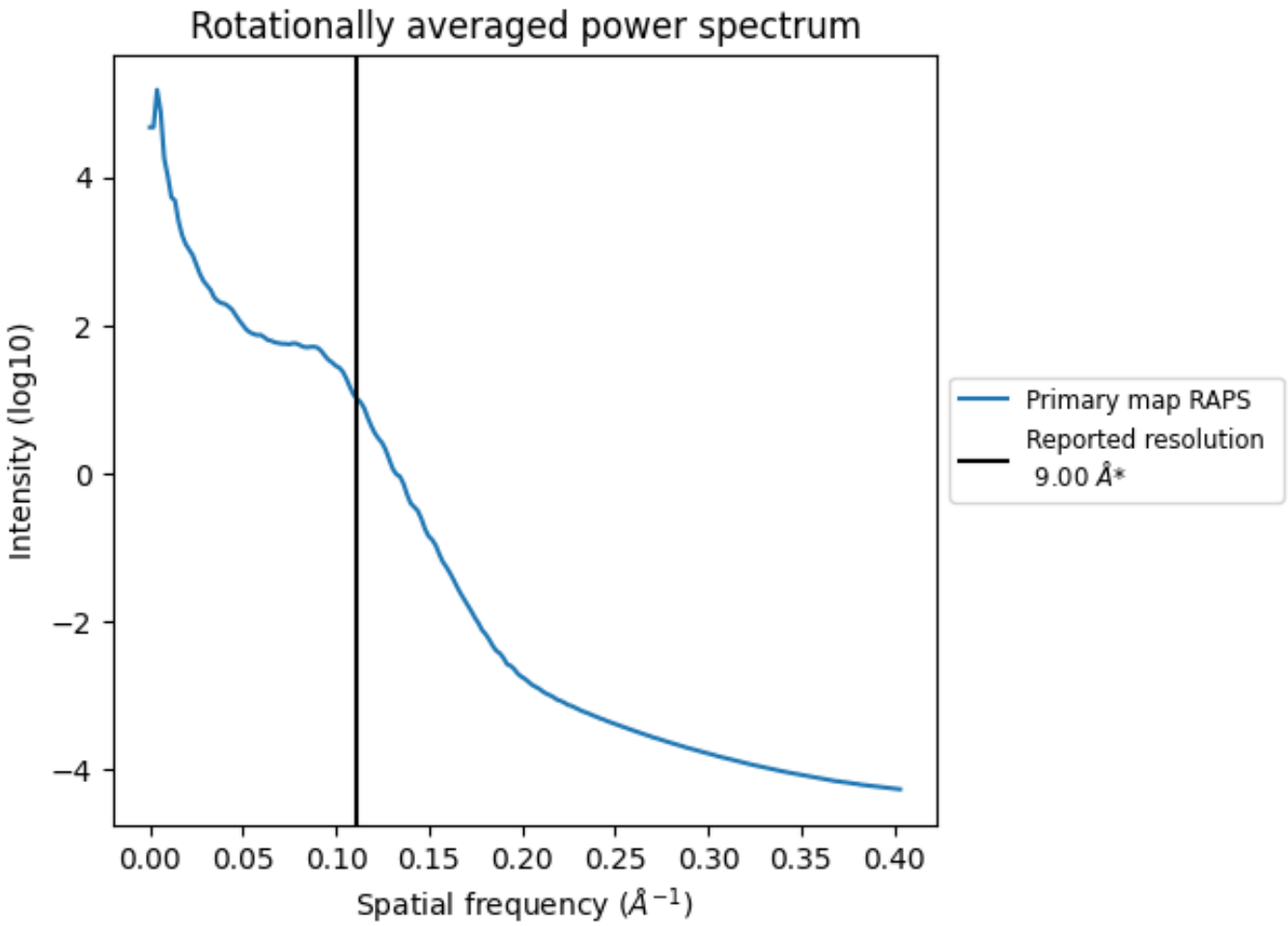
7.2 Volume estimate (i)



The volume at the recommended contour level is 2828 nm^3; this corresponds to an approximate mass of 2554 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

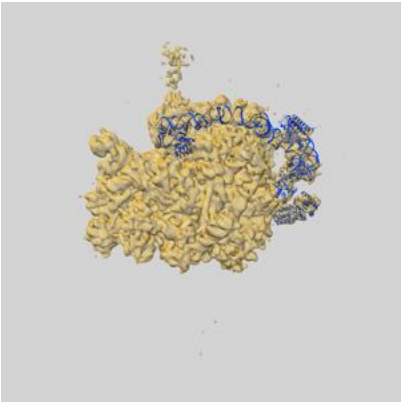
8 Fourier-Shell correlation (i)

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

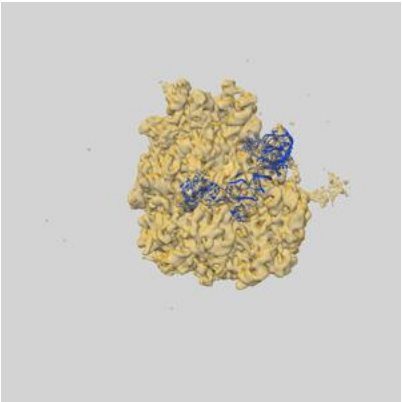
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2844 and PDB model 4UE5. Per-residue inclusion information can be found in section 3 on page 5.

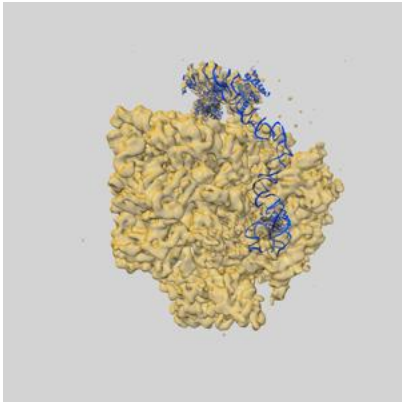
9.1 Map-model overlay (i)



X



Y



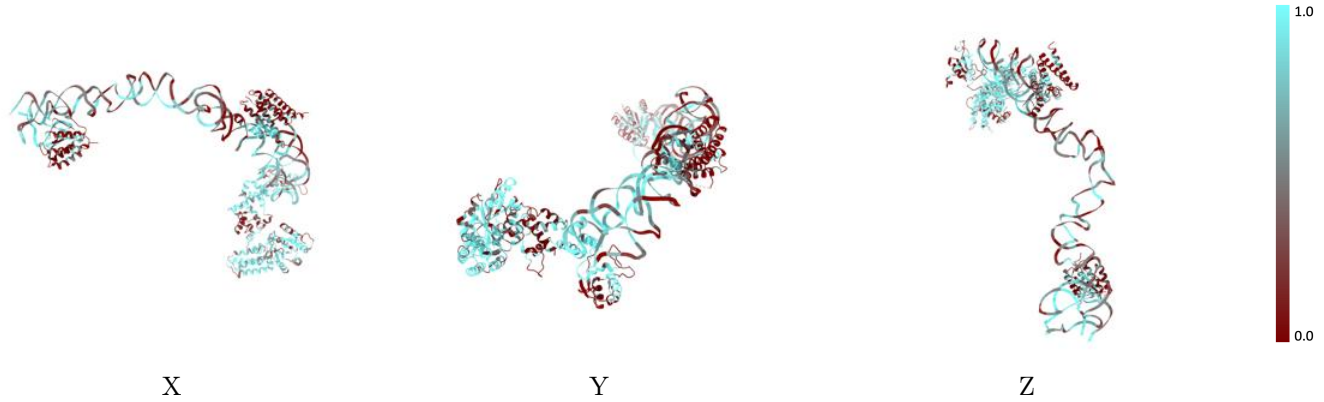
Z

The images above show the 3D surface view of the map at the recommended contour level 0.119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

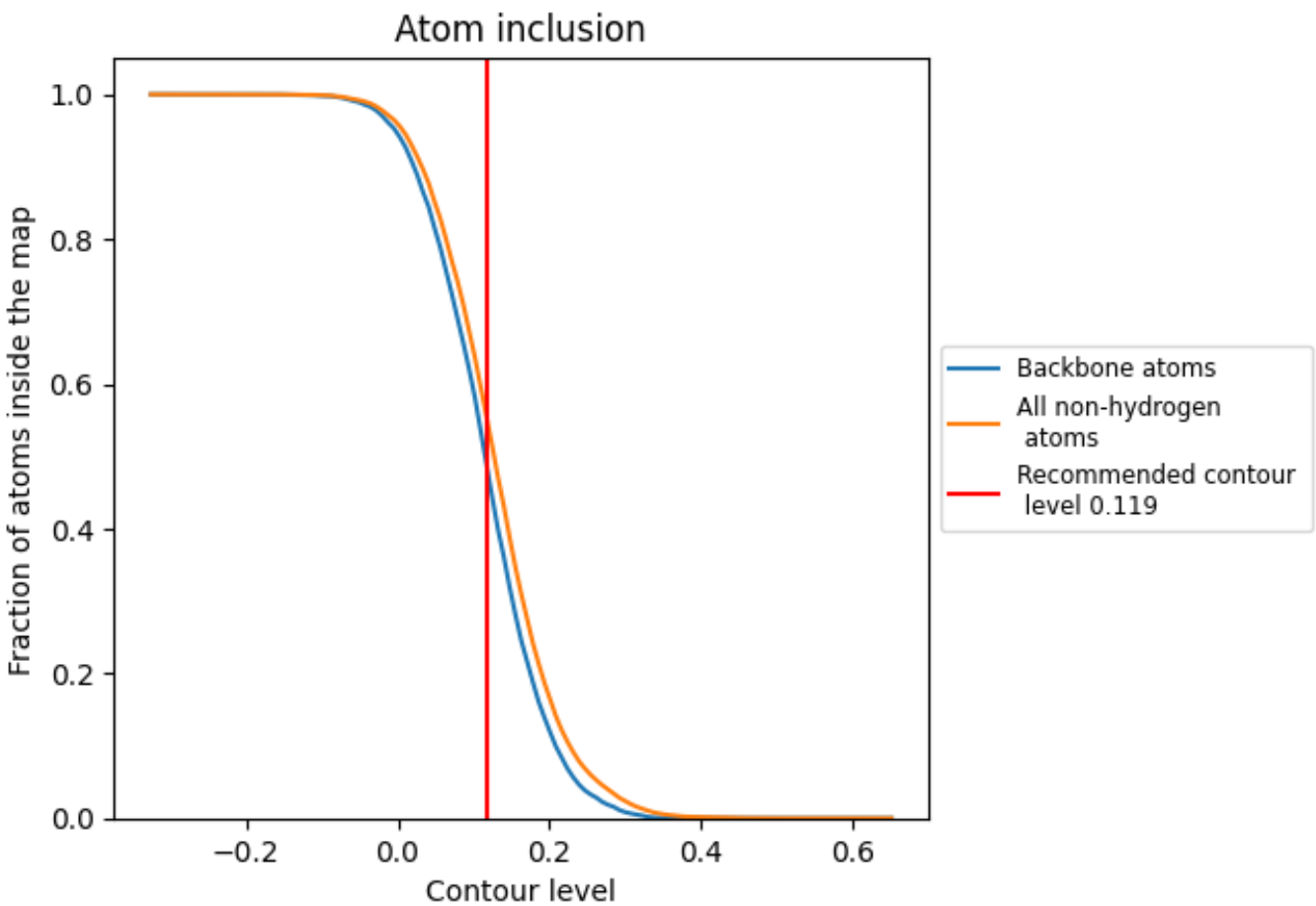
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.119).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5437	0.0840
A	0.5568	0.0600
B	0.3133	0.0600
C	0.3561	0.0440
D	0.6871	0.1810
E	0.3784	0.1670
F	0.4289	0.0640
S	0.1250	0.1150