



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 05:58 PM BST

PDB ID : 3OFA
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol. This file contains the 30S subunit of the first 70S ribosome.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-14
Resolution : 3.19 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

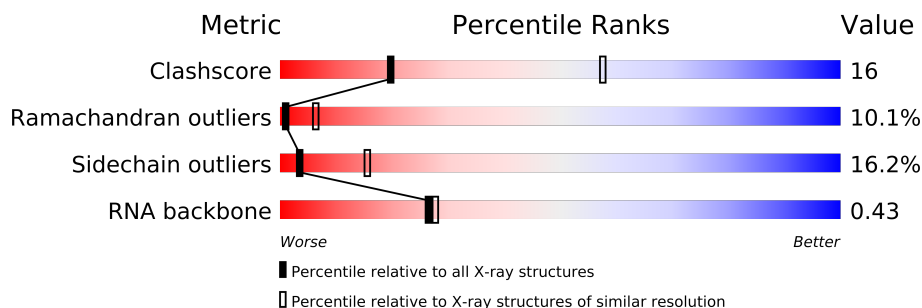
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.19 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RNA backbone	1838	1002 (3.72-2.68)


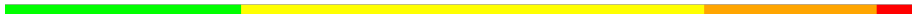




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1533	
2	B	218	
3	C	206	
4	D	205	
5	E	150	
6	F	100	
7	G	151	
8	H	129	
9	I	127	
10	J	98	
11	K	117	
12	L	123	
13	M	114	
14	N	100	
15	O	88	

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Mol	Chain	Length	Quality of chain
16	P	82	
17	Q	80	
18	R	55	
19	S	79	
20	T	85	
21	U	51	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51700 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	55	Total	C	N	O	0	0	0
			456	288	86	82			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	42	Total	Mg	0	0
			42	42		
22	N	1	Total	Mg	0	0
			1	1		

- Molecule 23 is water.

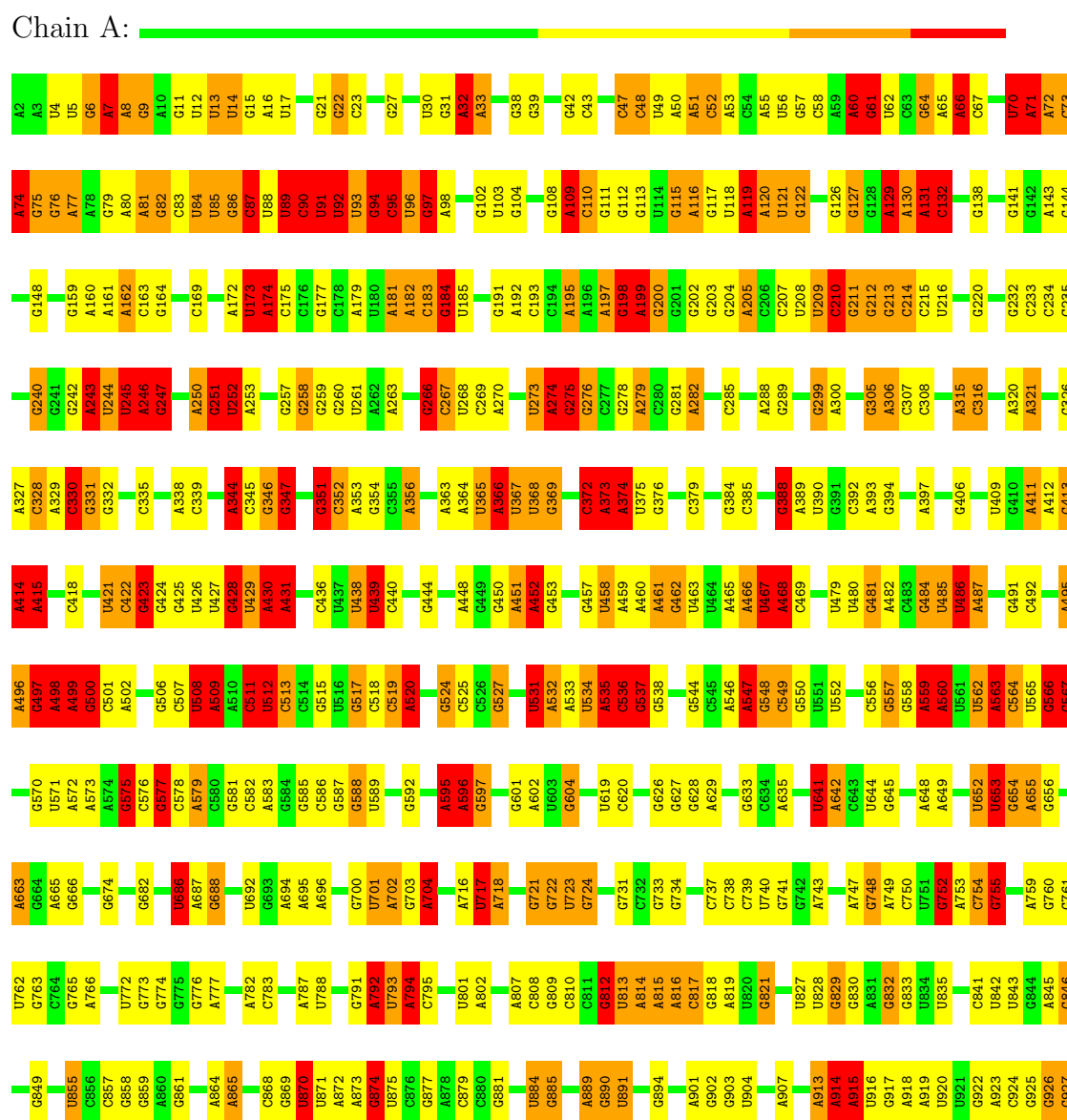
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	201	Total	O	0	0
			201	201		
23	L	1	Total	O	0	0
			1	1		
23	N	5	Total	O	0	0
			5	5		
23	U	1	Total	O	0	0
			1	1		

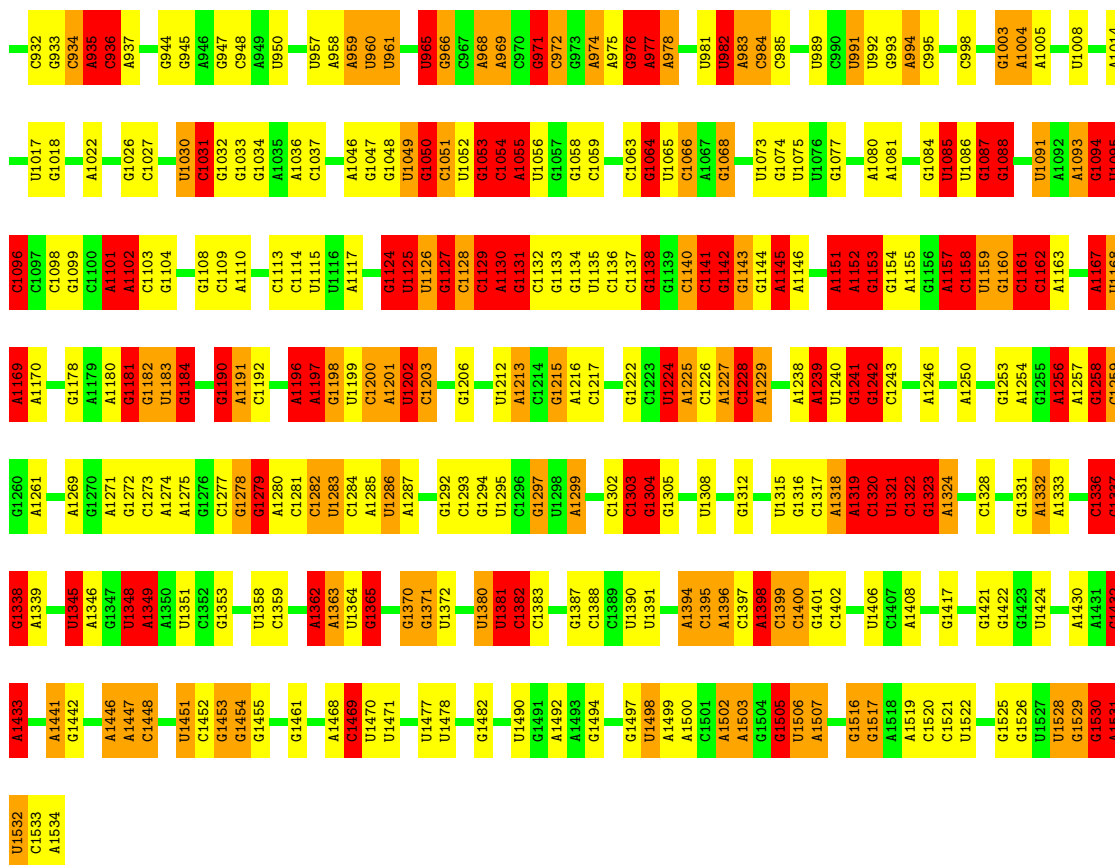
3 Residue-property plots

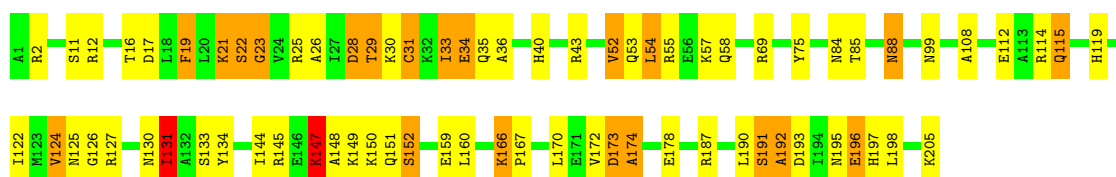
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: 16S rRNA

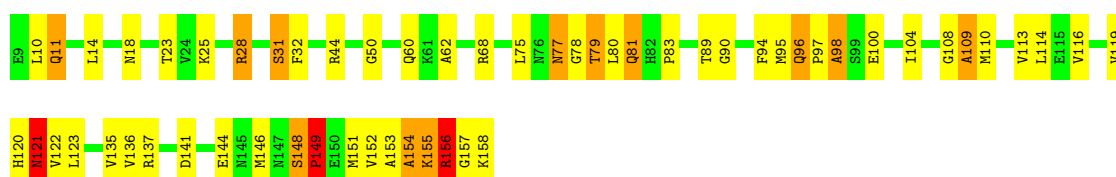






- Molecule 5: 30S ribosomal protein S5

Chain E:



- Molecule 6: 30S ribosomal protein S6

Chain F:



- Molecule 7: 30S ribosomal protein S7

Chain G:



- Molecule 8: 30S ribosomal protein S8

Chain H:



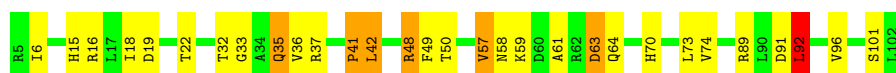
- Molecule 9: 30S ribosomal protein S9

Chain I:



- Molecule 10: 30S ribosomal protein S10

Chain J:



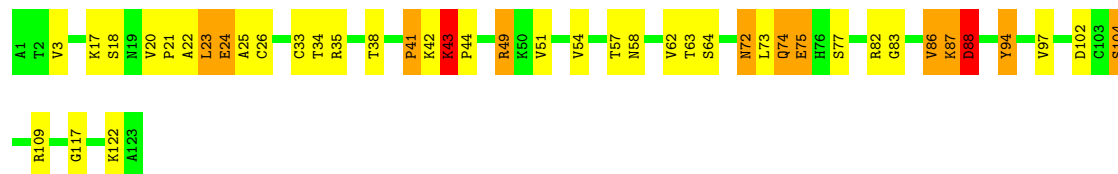
- Molecule 11: 30S ribosomal protein S11

Chain K:



- Molecule 12: 30S ribosomal protein S12

Chain L:



- Molecule 13: 30S ribosomal protein S13

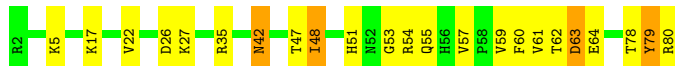
Chain M:





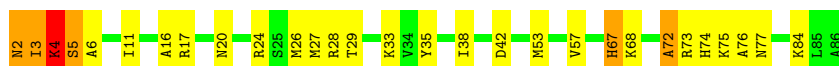
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein S21

Chain U:



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19	Depositor
% Data completeness (in resolution range)	75.8 (82.15-3.19)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.252	Depositor
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.366	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 759111 reflections	Xtriage
Total number of atoms	51700	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.50	6/36834 (0.0%)	1.27	532/57462 (0.9%)
2	B	0.40	2/1736 (0.1%)	0.57	4/2338 (0.2%)
3	C	0.26	0/1652	0.50	0/2225
4	D	0.29	0/1665	0.52	0/2227
5	E	0.37	1/1119 (0.1%)	0.59	0/1504
6	F	0.28	0/836	0.49	0/1128
7	G	0.23	0/1196	0.46	0/1602
8	H	0.29	0/989	0.54	0/1326
9	I	0.23	0/1034	0.47	0/1375
10	J	0.24	0/797	0.49	0/1077
11	K	0.27	0/893	0.52	0/1205
12	L	0.36	0/969	0.67	0/1300
13	M	0.22	0/893	0.47	0/1193
14	N	0.25	0/785	0.49	0/1043
15	O	0.27	0/722	0.47	0/964
16	P	0.28	0/659	0.49	0/884
17	Q	0.35	0/658	0.56	0/881
18	R	0.28	0/463	0.50	0/621
19	S	0.23	0/653	0.47	0/877
20	T	0.30	0/671	0.57	0/888
21	U	0.28	0/431	0.49	0/570
All	All	0.44	9/55655 (0.0%)	1.10	536/82690 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1047	G	O3'-P	-14.49	1.43	1.61
2	B	107	ARG	C-N	11.33	1.60	1.34
1	A	1390	U	O3'-P	9.48	1.72	1.61
1	A	557	G	O3'-P	-7.45	1.52	1.61
2	B	146	SER	C-N	6.53	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	G	O3'-P	5.81	1.68	1.61
1	A	925	G	O3'-P	5.78	1.68	1.61
5	E	149	PRO	C-N	-5.67	1.21	1.34
1	A	8	A	O3'-P	-5.48	1.54	1.61

All (536) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	C	N1-C1'-C2'	-14.16	95.59	114.00
1	A	1202	U	N1-C1'-C2'	-13.63	96.28	114.00
1	A	972	C	N1-C1'-C2'	-12.58	97.65	114.00
1	A	1283	U	N1-C1'-C2'	-12.51	97.74	114.00
1	A	1162	C	N1-C1'-C2'	-12.26	98.06	114.00
1	A	512	U	N1-C1'-C2'	-12.03	98.36	114.00
1	A	1228	C	N1-C1'-C2'	-11.93	98.49	114.00
1	A	1399	C	P-O3'-C3'	11.62	133.64	119.70
1	A	1047	G	P-O3'-C3'	-11.54	105.85	119.70
1	A	330	C	N1-C1'-C2'	-11.45	99.11	114.00
1	A	422	C	P-O3'-C3'	11.41	133.39	119.70
1	A	352	C	N1-C1'-C2'	-11.34	99.25	114.00
1	A	1303	C	N1-C1'-C2'	-11.34	99.26	114.00
1	A	1141	C	N1-C1'-C2'	-11.33	99.27	114.00
1	A	267	C	N1-C1'-C2'	-11.33	99.27	114.00
1	A	913	A	P-O3'-C3'	11.24	133.19	119.70
1	A	431	A	P-O3'-C3'	-11.10	106.38	119.70
1	A	119	A	P-O3'-C3'	11.06	132.97	119.70
1	A	641	U	P-O3'-C3'	11.04	132.95	119.70
1	A	1345	U	O4'-C1'-N1	10.97	116.97	108.20
1	A	891	U	N1-C1'-C2'	-10.90	99.82	114.00
1	A	1348	U	N1-C1'-C2'	-10.89	99.84	114.00
1	A	547	A	P-O3'-C3'	10.83	132.69	119.70
1	A	961	U	N1-C1'-C2'	-10.53	100.31	114.00
1	A	132	C	N1-C1'-C2'	-10.48	100.38	114.00
1	A	173	U	O4'-C1'-N1	10.27	116.42	108.20
1	A	1320	C	N1-C1'-C2'	-10.27	100.65	114.00
1	A	87	C	N1-C1'-C2'	-10.24	100.68	114.00
1	A	1095	U	N1-C1'-C2'	-10.17	100.78	114.00
1	A	984	C	N1-C1'-C2'	-10.05	100.94	114.00
1	A	1336	C	P-O3'-C3'	10.01	131.71	119.70
1	A	724	G	P-O3'-C3'	-9.98	107.72	119.70
1	A	279	A	P-O3'-C3'	9.98	131.68	119.70
1	A	1381	U	N1-C1'-C2'	-9.95	101.05	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	A	P-O3'-C3'	-9.94	107.77	119.70
1	A	536	C	N1-C1'-C2'	-9.86	101.15	112.00
1	A	7	A	P-O3'-C3'	9.86	131.53	119.70
1	A	889	A	P-O3'-C3'	9.80	131.46	119.70
1	A	812	G	P-O3'-C3'	9.76	131.41	119.70
1	A	14	U	N1-C1'-C2'	-9.74	101.28	112.00
1	A	1088	G	P-O3'-C3'	-9.70	108.06	119.70
1	A	132	C	P-O3'-C3'	-9.63	108.14	119.70
1	A	115	G	P-O3'-C3'	9.58	131.19	119.70
1	A	1282	C	N1-C1'-C2'	-9.57	101.47	112.00
1	A	66	A	P-O3'-C3'	-9.56	108.23	119.70
1	A	315	A	P-O3'-C3'	9.55	131.16	119.70
1	A	642	A	P-O3'-C3'	-9.53	108.26	119.70
1	A	969	A	P-O3'-C3'	-9.52	108.28	119.70
1	A	1228	C	P-O3'-C3'	-9.39	108.43	119.70
1	A	1053	G	P-O3'-C3'	9.38	130.96	119.70
1	A	1157	A	P-O3'-C3'	9.35	130.92	119.70
1	A	1224	U	O4'-C1'-N1	9.32	115.66	108.20
1	A	960	U	P-O3'-C3'	9.32	130.88	119.70
1	A	415	A	P-O3'-C3'	-9.30	108.54	119.70
1	A	1432	G	P-O3'-C3'	9.30	130.87	119.70
1	A	1167	A	P-O3'-C3'	9.29	130.84	119.70
1	A	1382	C	N1-C1'-C2'	-9.28	101.79	112.00
1	A	109	A	P-O3'-C3'	9.25	130.80	119.70
1	A	1224	U	P-O3'-C3'	9.23	130.77	119.70
1	A	874	G	P-O3'-C3'	-9.18	108.68	119.70
1	A	915	A	P-O3'-C3'	-9.15	108.72	119.70
1	A	1398	A	P-O3'-C3'	-9.10	108.78	119.70
1	A	1528	U	P-O3'-C3'	9.05	130.56	119.70
1	A	305	G	P-O3'-C3'	9.03	130.54	119.70
1	A	1095	U	O4'-C1'-N1	9.03	115.42	108.20
1	A	577	G	P-O3'-C3'	-9.00	108.90	119.70
1	A	792	A	O4'-C1'-N9	9.00	115.40	108.20
1	A	1506	U	P-O3'-C3'	8.93	130.41	119.70
1	A	813	U	P-O3'-C3'	-8.87	109.06	119.70
1	A	1201	A	P-O3'-C3'	8.82	130.29	119.70
1	A	1258	G	P-O3'-C3'	-8.74	109.21	119.70
1	A	717	U	P-O3'-C3'	8.74	130.19	119.70
1	A	1229	A	P-O3'-C3'	-8.72	109.23	119.70
1	A	974	A	P-O3'-C3'	8.70	130.15	119.70
1	A	32	A	P-O3'-C3'	-8.69	109.27	119.70
1	A	1064	G	P-O3'-C3'	8.68	130.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	U	P-O5'-C5'	-8.67	107.03	120.90
1	A	870	U	P-O3'-C3'	8.57	129.98	119.70
1	A	1190	G	P-O3'-C3'	8.57	129.99	119.70
1	A	1196	A	P-O3'-C3'	8.53	129.94	119.70
1	A	991	U	P-O3'-C3'	8.49	129.88	119.70
1	A	1153	G	P-O3'-C3'	-8.48	109.53	119.70
1	A	968	A	P-O3'-C3'	8.47	129.87	119.70
1	A	512	U	P-O3'-C3'	-8.44	109.57	119.70
1	A	1125	U	P-O3'-C3'	8.44	129.82	119.70
1	A	388	G	P-O3'-C3'	8.43	129.81	119.70
1	A	1322	C	P-O3'-C3'	8.35	129.72	119.70
1	A	316	C	P-O3'-C3'	-8.32	109.72	119.70
1	A	245	U	P-O3'-C3'	-8.28	109.77	119.70
1	A	595	A	P-O3'-C3'	8.28	129.63	119.70
1	A	1152	A	P-O3'-C3'	-8.26	109.79	119.70
1	A	13	U	P-O3'-C3'	8.25	129.60	119.70
1	A	1332	A	P-O3'-C3'	-8.25	109.80	119.70
1	A	531	U	P-O3'-C3'	8.21	129.55	119.70
1	A	1382	C	P-O3'-C3'	-8.19	109.88	119.70
1	A	815	A	P-O3'-C3'	8.12	129.45	119.70
1	A	1380	U	P-O3'-C3'	8.11	129.43	119.70
1	A	373	A	P-O3'-C3'	-8.03	110.06	119.70
1	A	282	A	P-O3'-C3'	-8.01	110.09	119.70
1	A	537	G	P-O3'-C3'	-8.00	110.11	119.70
1	A	451	A	P-O3'-C3'	7.98	129.28	119.70
1	A	1162	C	P-O3'-C3'	-7.96	110.14	119.70
1	A	935	A	P-O3'-C3'	-7.92	110.20	119.70
1	A	884	U	P-O3'-C3'	7.91	129.19	119.70
1	A	1448	C	N1-C1'-C2'	-7.91	103.30	112.00
1	A	821	G	P-O3'-C3'	-7.88	110.25	119.70
1	A	500	G	P-O3'-C3'	-7.86	110.27	119.70
1	A	85	U	P-O3'-C3'	7.86	129.13	119.70
1	A	9	G	P-O3'-C3'	-7.84	110.29	119.70
1	A	95	C	P-O3'-C3'	-7.83	110.31	119.70
1	A	480	U	O4'-C1'-N1	7.83	114.46	108.20
1	A	1320	C	P-O3'-C3'	-7.81	110.32	119.70
1	A	374	A	P-O3'-C3'	-7.79	110.35	119.70
1	A	1124	G	P-O3'-C3'	7.79	129.04	119.70
1	A	972	C	O4'-C1'-N1	7.79	114.43	108.20
2	B	146	SER	O-C-N	-7.75	110.29	122.70
1	A	1362	A	O4'-C1'-N9	7.75	114.40	108.20
1	A	1502	A	P-O3'-C3'	7.74	128.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	816	A	P-O3'-C3'	-7.72	110.43	119.70
1	A	486	U	N1-C1'-C2'	-7.71	103.53	112.00
1	A	216	U	P-O3'-C3'	-7.66	110.50	119.70
1	A	439	U	P-O3'-C3'	-7.64	110.53	119.70
1	A	1161	C	N1-C1'-C2'	-7.63	103.61	112.00
1	A	1256	A	P-O3'-C3'	7.62	128.84	119.70
1	A	94	G	P-O3'-C3'	7.60	128.82	119.70
1	A	960	U	N1-C1'-C2'	7.56	123.83	114.00
1	A	575	G	P-O3'-C3'	7.55	128.76	119.70
1	A	174	A	P-O3'-C3'	-7.55	110.64	119.70
1	A	347	G	P-O3'-C3'	-7.53	110.66	119.70
1	A	564	C	N1-C1'-C2'	-7.52	103.73	112.00
1	A	1087	G	P-O3'-C3'	-7.50	110.70	119.70
1	A	1200	C	P-O3'-C3'	7.50	128.70	119.70
1	A	91	U	N1-C1'-C2'	-7.48	103.77	112.00
1	A	1433	A	P-O3'-C3'	-7.47	110.74	119.70
1	A	275	G	P-O3'-C3'	-7.47	110.74	119.70
1	A	511	C	P-O3'-C3'	7.45	128.64	119.70
1	A	534	U	N1-C1'-C2'	-7.42	103.84	112.00
1	A	1336	C	O4'-C1'-N1	7.42	114.13	108.20
1	A	1345	U	P-O3'-C3'	7.41	128.59	119.70
1	A	1183	U	N1-C1'-C2'	-7.41	103.85	112.00
2	B	107	ARG	O-C-N	-7.41	110.85	122.70
1	A	754	C	N1-C1'-C2'	-7.39	103.87	112.00
1	A	1181	G	P-O3'-C3'	7.38	128.55	119.70
1	A	245	U	N1-C1'-C2'	-7.35	103.91	112.00
1	A	1505	G	P-O3'-C3'	-7.34	110.89	119.70
1	A	1101	A	P-O3'-C3'	7.34	128.51	119.70
1	A	722	G	P-O3'-C3'	-7.31	110.93	119.70
1	A	1054	C	P-O3'-C3'	7.29	128.44	119.70
1	A	686	U	P-O3'-C3'	7.25	128.40	119.70
1	A	1085	U	P-O3'-C3'	7.23	128.38	119.70
1	A	934	C	O4'-C1'-N1	7.23	113.98	108.20
1	A	485	U	P-O3'-C3'	7.20	128.34	119.70
1	A	519	C	N1-C1'-C2'	-7.20	104.08	112.00
1	A	1068	G	P-O3'-C3'	-7.20	111.07	119.70
1	A	73	C	N1-C1'-C2'	-7.19	104.09	112.00
1	A	467	U	O4'-C1'-N1	7.18	113.95	108.20
1	A	122	G	P-O3'-C3'	-7.18	111.08	119.70
1	A	1394	A	P-O3'-C3'	7.17	128.31	119.70
1	A	173	U	P-O3'-C3'	7.14	128.26	119.70
1	A	961	U	P-O3'-C3'	-7.13	111.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	G	N9-C1'-C2'	-7.12	104.17	112.00
1	A	934	C	P-O3'-C3'	7.09	128.22	119.70
1	A	422	C	N1-C1'-C2'	7.09	123.21	114.00
1	A	439	U	N1-C1'-C2'	-7.05	104.24	112.00
1	A	372	C	P-O3'-C3'	7.00	128.10	119.70
1	A	267	C	P-O5'-C5'	-6.99	109.72	120.90
1	A	452	A	P-O3'-C3'	-6.95	111.36	119.70
1	A	704	A	P-O3'-C3'	-6.95	111.36	119.70
1	A	14	U	P-O5'-C5'	-6.92	109.83	120.90
1	A	1094	G	P-O3'-C3'	6.92	128.00	119.70
1	A	535	A	P-O3'-C3'	6.91	127.99	119.70
1	A	1297	G	P-O3'-C3'	6.90	127.98	119.70
1	A	1131	G	P-O3'-C3'	-6.90	111.42	119.70
1	A	1055	A	P-O3'-C3'	-6.90	111.42	119.70
1	A	110	C	N1-C1'-C2'	-6.89	104.42	112.00
1	A	1145	A	P-O3'-C3'	6.88	127.95	119.70
1	A	519	C	P-O3'-C3'	-6.87	111.45	119.70
1	A	216	U	N1-C1'-C2'	-6.87	104.44	112.00
1	A	1184	G	P-O3'-C3'	-6.82	111.52	119.70
1	A	266	G	P-O3'-C3'	6.80	127.86	119.70
1	A	1202	U	O4'-C1'-N1	6.79	113.63	108.20
1	A	792	A	P-O3'-C3'	6.78	127.84	119.70
1	A	509	A	P-O3'-C3'	-6.77	111.58	119.70
1	A	566	G	P-O3'-C3'	6.77	127.82	119.70
1	A	1337	G	P-O3'-C3'	-6.74	111.61	119.70
1	A	116	A	P-O3'-C3'	-6.74	111.62	119.70
1	A	411	A	P-O3'-C3'	6.73	127.78	119.70
1	A	131	A	P-O3'-C3'	-6.70	111.66	119.70
1	A	1399	C	O4'-C1'-N1	6.70	113.56	108.20
1	A	1140	C	O4'-C1'-N1	6.70	113.56	108.20
1	A	1395	C	P-O5'-C5'	-6.66	110.24	120.90
1	A	688	G	N9-C1'-C2'	-6.66	104.67	112.00
1	A	1162	C	O4'-C1'-N1	6.65	113.52	108.20
1	A	306	A	P-O3'-C3'	-6.64	111.74	119.70
1	A	653	U	O4'-C1'-N1	6.63	113.51	108.20
1	A	344	A	P-O3'-C3'	6.62	127.64	119.70
1	A	1507	A	P-O3'-C3'	-6.59	111.79	119.70
1	A	653	U	P-O3'-C3'	6.59	127.61	119.70
1	A	1530	G	N9-C1'-C2'	-6.59	104.75	112.00
1	A	351	G	O4'-C1'-N9	6.58	113.47	108.20
1	A	1401	G	P-O3'-C3'	-6.58	111.80	119.70
1	A	243	A	P-O3'-C3'	6.58	127.59	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	G	P-O3'-C3'	-6.58	111.81	119.70
1	A	14	U	P-O3'-C3'	-6.58	111.81	119.70
1	A	74	A	P-O3'-C3'	-6.56	111.82	119.70
1	A	984	C	P-O3'-C3'	-6.55	111.84	119.70
1	A	252	U	N1-C1'-C2'	-6.54	104.80	112.00
1	A	184	G	P-O3'-C3'	-6.52	111.88	119.70
1	A	552	U	P-O3'-C3'	-6.52	111.88	119.70
1	A	1213	A	P-O3'-C3'	6.50	127.50	119.70
1	A	1447	A	P-O3'-C3'	6.50	127.50	119.70
1	A	801	U	O4'-C1'-N1	6.50	113.40	108.20
1	A	70	U	P-O3'-C3'	6.49	127.49	119.70
1	A	1066	C	N1-C1'-C2'	-6.48	104.88	112.00
1	A	60	A	P-O3'-C3'	6.47	127.47	119.70
1	A	1239	A	P-O3'-C3'	6.46	127.45	119.70
1	A	85	U	N1-C1'-C2'	6.46	122.40	114.00
1	A	891	U	P-O3'-C3'	-6.45	111.96	119.70
1	A	1478	U	P-O5'-C5'	-6.43	110.61	120.90
1	A	48	C	O4'-C1'-N1	6.42	113.33	108.20
1	A	331	G	P-O3'-C3'	-6.40	112.02	119.70
1	A	438	U	P-O3'-C3'	6.40	127.38	119.70
1	A	1129	C	N1-C1'-C2'	6.40	122.32	114.00
1	A	547	A	O4'-C1'-N9	6.39	113.31	108.20
1	A	428	G	P-O3'-C3'	6.36	127.33	119.70
1	A	1095	U	C3'-C2'-C1'	6.35	106.58	101.50
1	A	686	U	N1-C1'-C2'	6.34	122.24	114.00
1	A	47	C	P-O3'-C3'	6.33	127.30	119.70
1	A	688	G	P-O3'-C3'	-6.32	112.12	119.70
1	A	1068	G	N9-C1'-C2'	-6.31	105.06	112.00
1	A	982	U	P-O3'-C3'	6.30	127.27	119.70
1	A	1202	U	C3'-C2'-C1'	6.30	106.54	101.50
1	A	1131	G	N9-C1'-C2'	-6.30	105.07	112.00
1	A	977	A	P-O3'-C3'	-6.29	112.16	119.70
1	A	1349	A	P-O3'-C3'	-6.29	112.16	119.70
1	A	90	C	O4'-C1'-N1	6.28	113.23	108.20
1	A	721	G	P-O3'-C3'	6.28	127.24	119.70
1	A	1282	C	P-O3'-C3'	-6.28	112.16	119.70
1	A	344	A	O4'-C1'-N9	6.26	113.21	108.20
1	A	368	U	N1-C1'-C2'	-6.25	105.12	112.00
1	A	1451	U	N1-C1'-C2'	6.25	122.13	114.00
1	A	1046	A	O4'-C1'-N9	6.25	113.20	108.20
1	A	1200	C	N1-C1'-C2'	6.23	122.10	114.00
1	A	1319	A	P-O3'-C3'	6.22	127.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	A	O4'-C1'-N9	-6.22	103.22	108.20
1	A	559	A	P-O3'-C3'	6.21	127.16	119.70
1	A	81	A	P-O3'-C3'	6.21	127.15	119.70
1	A	965	U	P-O3'-C3'	6.21	127.15	119.70
1	A	1283	U	P-O3'-C3'	-6.20	112.26	119.70
1	A	1498	U	P-O3'-C3'	6.19	127.13	119.70
1	A	1127	G	P-O3'-C3'	-6.19	112.27	119.70
1	A	1064	G	O4'-C1'-N9	6.18	113.15	108.20
1	A	365	U	C5-C6-N1	-6.18	119.61	122.70
1	A	1129	C	P-O3'-C3'	6.17	127.11	119.70
1	A	914	A	C3'-C2'-C1'	6.17	106.44	101.50
1	A	1141	C	O4'-C1'-N1	6.15	113.12	108.20
1	A	971	G	O4'-C1'-N9	6.15	113.12	108.20
1	A	91	U	C3'-C2'-C1'	6.14	106.41	101.50
1	A	169	C	O4'-C1'-N1	6.14	113.11	108.20
1	A	1302	C	N1-C1'-C2'	-6.12	105.26	112.00
1	A	97	G	C3'-C2'-C1'	6.12	106.40	101.50
1	A	198	G	C3'-C2'-C1'	6.10	106.38	101.50
1	A	559	A	O4'-C1'-N9	6.09	113.07	108.20
1	A	479	U	O4'-C1'-N1	6.08	113.07	108.20
1	A	279	A	O4'-C1'-N9	-6.07	103.34	108.20
1	A	429	U	P-O3'-C3'	6.07	126.98	119.70
1	A	1142	G	P-O3'-C3'	-6.07	112.42	119.70
1	A	1320	C	O4'-C1'-N1	6.07	113.05	108.20
1	A	508	U	P-O3'-C3'	6.06	126.97	119.70
1	A	884	U	O4'-C1'-N1	6.06	113.05	108.20
1	A	1506	U	O4'-C1'-N1	6.06	113.05	108.20
1	A	1365	G	P-O3'-C3'	-6.05	112.44	119.70
1	A	935	A	C3'-C2'-C1'	6.04	106.34	101.50
1	A	95	C	N1-C1'-C2'	-6.04	105.36	112.00
1	A	654	G	C3'-C2'-C1'	6.04	106.33	101.50
1	A	52	C	P-O3'-C3'	-6.03	112.46	119.70
1	A	794	A	P-O3'-C3'	-6.02	112.47	119.70
1	A	184	G	C3'-C2'-C1'	6.01	106.31	101.50
1	A	976	G	C3'-C2'-C1'	6.01	106.31	101.50
1	A	816	A	C3'-C2'-C1'	6.00	106.30	101.50
1	A	654	G	P-O3'-C3'	-6.00	112.50	119.70
1	A	500	G	N9-C1'-C2'	-6.00	105.40	112.00
1	A	520	A	P-O3'-C3'	-6.00	112.51	119.70
1	A	199	A	C3'-C2'-C1'	5.99	106.29	101.50
1	A	1323	G	C3'-C2'-C1'	5.99	106.29	101.50
1	A	517	G	P-O3'-C3'	5.99	126.89	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1282	C	C3'-C2'-C1'	5.99	106.29	101.50
1	A	966	G	P-O3'-C3'	-5.98	112.53	119.70
1	A	793	U	P-O3'-C3'	-5.98	112.53	119.70
1	A	1380	U	O4'-C1'-N1	5.97	112.98	108.20
1	A	423	G	C3'-C2'-C1'	5.97	106.27	101.50
1	A	1169	A	C3'-C2'-C1'	5.96	106.27	101.50
1	A	1091	U	O4'-C1'-N1	5.96	112.97	108.20
1	A	1453	G	P-O3'-C3'	-5.95	112.56	119.70
1	A	330	C	P-O3'-C3'	-5.95	112.56	119.70
1	A	794	A	C3'-C2'-C1'	5.95	106.26	101.50
1	A	596	A	C3'-C2'-C1'	5.95	106.26	101.50
1	A	162	A	P-O3'-C3'	5.93	126.82	119.70
1	A	497	G	C3'-C2'-C1'	5.93	106.24	101.50
1	A	718	A	P-O3'-C3'	-5.93	112.58	119.70
1	A	121	U	N1-C1'-C2'	-5.93	105.48	112.00
1	A	372	C	O4'-C1'-N1	5.93	112.94	108.20
1	A	1323	G	P-O3'-C3'	-5.92	112.59	119.70
1	A	213	G	P-O3'-C3'	5.91	126.79	119.70
1	A	1151	A	P-O3'-C3'	5.91	126.79	119.70
1	A	1381	U	C3'-C2'-C1'	5.90	106.22	101.50
1	A	468	A	P-O3'-C3'	-5.90	112.62	119.70
1	A	1241	G	C3'-C2'-C1'	5.88	106.20	101.50
1	A	89	U	O4'-C1'-N1	5.87	112.89	108.20
1	A	972	C	P-O3'-C3'	-5.85	112.69	119.70
1	A	1087	G	C3'-C2'-C1'	5.84	106.17	101.50
1	A	1158	C	N1-C1'-C2'	-5.84	105.57	112.00
1	A	1531	A	P-O3'-C3'	-5.84	112.69	119.70
1	A	368	U	C3'-C2'-C1'	5.84	106.17	101.50
1	A	567	G	C3'-C2'-C1'	5.84	106.17	101.50
1	A	132	C	O4'-C1'-N1	5.83	112.87	108.20
1	A	414	A	C3'-C2'-C1'	5.83	106.17	101.50
1	A	972	C	C3'-C2'-C1'	5.83	106.17	101.50
1	A	90	C	N1-C1'-C2'	-5.82	105.59	112.00
1	A	549	C	C3'-C2'-C1'	5.82	106.16	101.50
1	A	857	C	O4'-C1'-N1	5.82	112.86	108.20
1	A	51	A	P-O3'-C3'	5.82	126.69	119.70
1	A	366	A	P-O3'-C3'	5.82	126.68	119.70
1	A	247	G	P-O3'-C3'	-5.81	112.73	119.70
1	A	1469	C	P-O5'-C5'	-5.81	111.61	120.90
1	A	950	U	O4'-C1'-N1	5.79	112.84	108.20
1	A	13	U	O4'-C1'-N1	5.78	112.82	108.20
1	A	210	C	P-O3'-C3'	5.78	126.63	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1365	G	N9-C1'-C2'	-5.78	105.65	112.00
1	A	116	A	N9-C1'-C2'	-5.77	105.66	112.00
1	A	266	G	O3'-P-O5'	5.77	114.96	104.00
1	A	652	U	P-O3'-C3'	5.76	126.61	119.70
1	A	562	U	O4'-C1'-N1	-5.76	103.59	108.20
1	A	1047	G	OP2-P-O3'	5.75	117.84	105.20
1	A	74	A	N9-C1'-C2'	-5.74	105.68	112.00
1	A	251	G	O4'-C1'-N9	-5.74	103.61	108.20
1	A	1424	U	O4'-C1'-N1	5.73	112.79	108.20
1	A	1141	C	C3'-C2'-C1'	5.73	106.08	101.50
1	A	1055	A	N9-C1'-C2'	-5.73	105.70	112.00
1	A	984	C	C3'-C2'-C1'	5.72	106.08	101.50
1	A	1066	C	P-O3'-C3'	-5.72	112.83	119.70
1	A	914	A	P-O3'-C3'	-5.71	112.84	119.70
1	A	92	U	P-O3'-C3'	-5.71	112.85	119.70
1	A	9	G	N9-C1'-C2'	-5.70	105.73	112.00
1	A	1283	U	O4'-C1'-N1	5.70	112.76	108.20
1	A	486	U	P-O3'-C3'	-5.70	112.86	119.70
1	A	1184	G	N9-C1'-C2'	-5.69	105.74	112.00
1	A	1283	U	C3'-C2'-C1'	5.69	106.05	101.50
1	A	564	C	P-O3'-C3'	-5.68	112.88	119.70
1	A	772	U	P-O3'-C3'	-5.68	112.89	119.70
1	A	468	A	C3'-C2'-C1'	5.68	106.04	101.50
1	A	686	U	O4'-C1'-N1	5.68	112.74	108.20
1	A	1095	U	P-O3'-C3'	-5.67	112.89	119.70
1	A	865	A	P-O3'-C3'	5.67	126.51	119.70
1	A	915	A	O4'-C1'-N9	5.65	112.72	108.20
1	A	267	C	C3'-C2'-C1'	5.65	106.02	101.50
1	A	817	C	N1-C1'-C2'	5.64	121.33	114.00
1	A	813	U	N1-C1'-C2'	-5.64	105.80	112.00
1	A	1383	C	C6-N1-C2	5.63	122.55	120.30
1	A	439	U	C3'-C2'-C1'	5.63	106.00	101.50
1	A	198	G	P-O3'-C3'	-5.62	112.95	119.70
1	A	436	C	O4'-C1'-N1	5.62	112.70	108.20
1	A	509	A	C3'-C2'-C1'	5.62	106.00	101.50
1	A	173	U	N1-C1'-C2'	5.62	121.30	114.00
1	A	487	A	P-O3'-C3'	-5.62	112.96	119.70
1	A	498	A	C3'-C2'-C1'	5.61	105.99	101.50
1	A	998	C	O4'-C1'-N1	5.61	112.69	108.20
1	A	1477	U	P-O5'-C5'	-5.61	111.92	120.90
1	A	1168	U	O4'-C1'-N1	5.60	112.68	108.20
1	A	316	C	P-O5'-C5'	-5.59	111.95	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	C	C3'-C2'-C1'	5.59	105.97	101.50
1	A	1088	G	N9-C1'-C2'	-5.59	105.85	112.00
1	A	110	C	C3'-C2'-C1'	5.58	105.97	101.50
1	A	718	A	C3'-C2'-C1'	5.58	105.97	101.50
1	A	1031	C	P-O3'-C3'	5.58	126.40	119.70
1	A	512	U	C3'-C2'-C1'	5.58	105.96	101.50
1	A	497	G	P-O3'-C3'	-5.58	113.00	119.70
1	A	1215	G	P-O3'-C3'	-5.58	113.01	119.70
1	A	704	A	C3'-C2'-C1'	5.56	105.95	101.50
1	A	379	C	O4'-C1'-N1	5.56	112.64	108.20
1	A	1054	C	P-O5'-C5'	-5.56	112.01	120.90
1	A	1395	C	C3'-C2'-C1'	5.56	105.95	101.50
1	A	971	G	C4-N9-C1'	-5.55	119.28	126.50
1	A	1348	U	P-O3'-C3'	-5.55	113.04	119.70
1	A	61	G	C3'-C2'-C1'	5.54	105.94	101.50
1	A	641	U	N1-C1'-C2'	5.54	121.21	114.00
1	A	537	G	N9-C1'-C2'	-5.54	105.91	112.00
1	A	1242	G	P-O3'-C3'	-5.54	113.06	119.70
1	A	1152	A	C3'-C2'-C1'	5.53	105.93	101.50
1	A	1349	A	C3'-C2'-C1'	5.53	105.92	101.50
1	A	1365	G	C3'-C2'-C1'	5.53	105.92	101.50
1	A	1530	G	P-O3'-C3'	-5.52	113.07	119.70
1	A	339	C	O4'-C1'-N1	5.52	112.62	108.20
1	A	275	G	N9-C1'-C2'	-5.52	105.93	112.00
1	A	1228	C	C3'-C2'-C1'	5.51	105.91	101.50
1	A	870	U	N1-C1'-C2'	5.51	121.16	114.00
1	A	306	A	C3'-C2'-C1'	5.51	105.91	101.50
1	A	534	U	C3'-C2'-C1'	5.50	105.90	101.50
1	A	1258	G	C3'-C2'-C1'	5.50	105.90	101.50
1	A	110	C	P-O3'-C3'	-5.49	113.11	119.70
1	A	131	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	1338	G	P-O3'-C3'	-5.48	113.12	119.70
1	A	724	G	N9-C1'-C2'	-5.48	105.97	112.00
1	A	250	A	P-O3'-C3'	5.48	126.27	119.70
1	A	74	A	C3'-C2'-C1'	5.48	105.88	101.50
1	A	752	G	P-O3'-C3'	5.47	126.27	119.70
1	A	549	C	N1-C1'-C2'	-5.47	105.99	112.00
1	A	1169	A	P-O3'-C3'	-5.46	113.15	119.70
1	A	414	A	P-O3'-C3'	-5.46	113.15	119.70
1	A	1530	G	C3'-C2'-C1'	5.46	105.86	101.50
1	A	64	G	P-O3'-C3'	5.45	126.24	119.70
1	A	92	U	C3'-C2'-C1'	5.45	105.86	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	C	C3'-C2'-C1'	5.45	105.86	101.50
1	A	1243	C	O4'-C1'-N1	5.45	112.56	108.20
1	A	755	G	C3'-C2'-C1'	5.44	105.86	101.50
1	A	499	A	P-O3'-C3'	5.44	126.22	119.70
1	A	1454	G	C3'-C2'-C1'	5.44	105.85	101.50
1	A	982	U	N1-C1'-C2'	5.42	121.05	114.00
1	A	1241	G	N9-C1'-C2'	-5.42	106.03	112.00
1	A	1142	G	C3'-C2'-C1'	5.42	105.84	101.50
1	A	52	C	C3'-C2'-C1'	5.42	105.83	101.50
1	A	274	A	O4'-C1'-N9	5.42	112.53	108.20
1	A	116	A	C3'-C2'-C1'	5.42	105.83	101.50
1	A	1304	G	C3'-C2'-C1'	5.41	105.83	101.50
1	A	1381	U	P-O3'-C3'	-5.41	113.20	119.70
1	A	1451	U	P-O3'-C3'	5.41	126.19	119.70
1	A	365	U	O4'-C1'-N1	5.40	112.52	108.20
1	A	1348	U	C3'-C2'-C1'	5.40	105.82	101.50
1	A	885	G	C3'-C2'-C1'	5.39	105.81	101.50
1	A	994	A	C3'-C2'-C1'	5.39	105.81	101.50
1	A	1303	C	C3'-C2'-C1'	5.39	105.81	101.50
1	A	1130	A	P-O3'-C3'	-5.34	113.29	119.70
1	A	411	A	O4'-C1'-N9	5.34	112.47	108.20
1	A	885	G	N9-C1'-C2'	-5.33	106.13	112.00
1	A	1158	C	C3'-C2'-C1'	5.33	105.76	101.50
1	A	891	U	P-O5'-C5'	-5.33	112.38	120.90
1	A	919	A	P-O3'-C3'	5.32	126.08	119.70
1	A	421	U	P-O3'-C3'	5.32	126.08	119.70
1	A	1303	C	P-O3'-C3'	-5.32	113.32	119.70
1	A	1153	G	C3'-C2'-C1'	5.31	105.75	101.50
1	A	977	A	C3'-C2'-C1'	5.31	105.75	101.50
1	A	816	A	N9-C1'-C2'	-5.31	106.16	112.00
1	A	430	A	C3'-C2'-C1'	5.30	105.74	101.50
1	A	61	G	P-O3'-C3'	-5.30	113.34	119.70
2	B	146	SER	CA-C-N	5.30	128.86	117.20
1	A	1337	G	C3'-C2'-C1'	5.30	105.74	101.50
1	A	1478	U	O4'-C1'-N1	-5.29	103.97	108.20
1	A	452	A	C3'-C2'-C1'	5.29	105.73	101.50
1	A	438	U	O4'-C1'-N1	5.29	112.43	108.20
1	A	246	A	P-O3'-C3'	5.29	126.04	119.70
1	A	53	A	O5'-P-OP2	-5.28	100.95	105.70
1	A	874	G	C3'-C2'-C1'	5.28	105.72	101.50
1	A	1286	U	N1-C1'-C2'	5.28	120.86	114.00
1	A	1318	A	P-O3'-C3'	5.28	126.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	G	C3'-C2'-C1'	5.27	105.72	101.50
1	A	717	U	N1-C1'-C2'	5.27	120.85	114.00
1	A	1321	U	P-O3'-C3'	-5.27	113.38	119.70
1	A	352	C	C3'-C2'-C1'	5.27	105.71	101.50
1	A	351	G	C4-N9-C1'	5.26	133.34	126.50
1	A	467	U	N1-C1'-C2'	-5.26	106.21	112.00
1	A	267	C	P-O3'-C3'	-5.26	113.39	119.70
1	A	500	G	C3'-C2'-C1'	5.26	105.71	101.50
1	A	129	A	P-O3'-C3'	5.26	126.01	119.70
1	A	1127	G	C3'-C2'-C1'	5.26	105.71	101.50
1	A	1225	A	P-O5'-C5'	-5.26	112.49	120.90
1	A	174	A	C3'-C2'-C1'	5.25	105.70	101.50
1	A	1362	A	P-O3'-C3'	5.25	126.00	119.70
1	A	1448	C	C3'-C2'-C1'	5.25	105.70	101.50
1	A	306	A	N9-C1'-C2'	-5.24	106.23	112.00
1	A	511	C	N1-C1'-C2'	5.24	120.82	114.00
1	A	536	C	C3'-C2'-C1'	5.24	105.69	101.50
1	A	879	C	N1-C1'-C2'	-5.23	106.25	112.00
1	A	1400	C	O4'-C1'-N1	-5.23	104.02	108.20
1	A	548	G	C3'-C2'-C1'	5.22	105.68	101.50
1	A	373	A	C3'-C2'-C1'	5.22	105.67	101.50
1	A	1152	A	N9-C1'-C2'	-5.22	106.26	112.00
1	A	1197	A	P-O3'-C3'	-5.21	113.45	119.70
1	A	936	C	P-O3'-C3'	-5.21	113.45	119.70
1	A	567	G	P-O5'-C5'	-5.20	112.58	120.90
1	A	331	G	C3'-C2'-C1'	5.20	105.66	101.50
1	A	1050	G	N9-C1'-C2'	-5.20	106.29	112.00
1	A	267	C	O4'-C1'-N1	5.19	112.36	108.20
1	A	552	U	O4'-C1'-N1	5.19	112.35	108.20
1	A	252	U	P-O3'-C3'	-5.19	113.47	119.70
2	B	146	SER	C-N-CA	5.19	134.67	121.70
1	A	346	G	P-O5'-C5'	-5.18	112.62	120.90
1	A	330	C	C3'-C2'-C1'	5.17	105.64	101.50
1	A	1321	U	N1-C1'-C2'	-5.17	106.32	112.00
1	A	84	U	N1-C1'-C2'	5.17	120.72	114.00
1	A	497	G	N9-C1'-C2'	-5.16	106.33	112.00
1	A	1050	G	C3'-C2'-C1'	5.16	105.63	101.50
1	A	108	G	O4'-C1'-N9	5.15	112.32	108.20
1	A	1161	C	P-O3'-C3'	-5.15	113.52	119.70
1	A	273	U	P-O3'-C3'	-5.15	113.52	119.70
1	A	1229	A	C3'-C2'-C1'	5.15	105.62	101.50
1	A	1398	A	N9-C1'-C2'	-5.15	106.34	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	C	C3'-C2'-C1'	5.15	105.62	101.50
1	A	1184	G	C3'-C2'-C1'	5.14	105.61	101.50
1	A	1096	C	O4'-C1'-N1	5.14	112.31	108.20
1	A	1153	G	N9-C1'-C2'	-5.14	106.35	112.00
1	A	1505	G	C3'-C2'-C1'	5.14	105.61	101.50
1	A	1102	A	C3'-C2'-C1'	5.13	105.60	101.50
1	A	117	G	O5'-P-OP2	-5.12	101.09	105.70
1	A	1191	A	C3'-C2'-C1'	5.12	105.60	101.50
1	A	1453	G	C3'-C2'-C1'	5.12	105.59	101.50
1	A	245	U	C3'-C2'-C1'	5.12	105.59	101.50
1	A	722	G	C3'-C2'-C1'	5.11	105.59	101.50
1	A	1406	U	P-O3'-C3'	-5.11	113.57	119.70
1	A	1526	G	P-O5'-C5'	-5.11	112.72	120.90
1	A	534	U	P-O3'-C3'	-5.11	113.57	119.70
1	A	51	A	C3'-C2'-C1'	5.11	105.58	101.50
1	A	183	C	O4'-C1'-N1	5.10	112.28	108.20
1	A	431	A	P-O5'-C5'	-5.10	112.74	120.90
1	A	801	U	P-O3'-C3'	-5.10	113.58	119.70
1	A	817	C	P-O3'-C3'	5.10	125.82	119.70
1	A	891	U	C3'-C2'-C1'	5.10	105.58	101.50
1	A	4	U	C2-N1-C1'	5.10	123.81	117.70
1	A	560	A	P-O3'-C3'	-5.09	113.59	119.70
1	A	835	U	P-O3'-C3'	-5.08	113.60	119.70
1	A	373	A	N9-C1'-C2'	-5.08	106.42	112.00
1	A	959	A	P-O3'-C3'	5.07	125.78	119.70
1	A	642	A	N9-C1'-C2'	-5.06	106.43	112.00
1	A	1278	G	P-O3'-C3'	5.06	125.77	119.70
1	A	71	A	C3'-C2'-C1'	5.06	105.55	101.50
1	A	794	A	N9-C1'-C2'	-5.05	106.44	112.00
1	A	1517	G	P-O3'-C3'	-5.05	113.64	119.70
1	A	422	C	O4'-C1'-N1	5.04	112.23	108.20
1	A	1279	G	P-O3'-C3'	-5.04	113.66	119.70
1	A	1516	G	P-O3'-C3'	5.03	125.73	119.70
1	A	484	G	P-O3'-C3'	5.02	125.73	119.70
1	A	1168	U	P-O3'-C3'	5.02	125.73	119.70
1	A	467	U	P-O3'-C3'	-5.02	113.68	119.70
1	A	563	A	C3'-C2'-C1'	5.02	105.52	101.50
1	A	916	U	C2-N1-C1'	5.02	123.72	117.70
1	A	1138	G	C3'-C2'-C1'	5.01	105.51	101.50
1	A	1338	G	C3'-C2'-C1'	5.01	105.51	101.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32895	0	44	492	0
2	B	1705	0	0	21	0
3	C	1625	0	0	14	0
4	D	1643	0	0	35	0
5	E	1106	0	75	45	0
6	F	818	0	0	8	0
7	G	1182	0	0	8	0
8	H	979	0	0	16	0
9	I	1022	0	0	9	0
10	J	787	0	0	10	0
11	K	877	0	0	10	0
12	L	955	0	0	16	0
13	M	884	0	0	7	0
14	N	774	0	0	17	0
15	O	714	0	0	14	0
16	P	649	0	0	12	0
17	Q	649	0	691	74	0
18	R	456	0	0	5	0
19	S	638	0	0	8	0
20	T	665	0	0	10	0
21	U	426	0	0	9	0
22	A	42	0	0	0	0
22	N	1	0	0	0	0
23	A	201	0	0	6	0
23	L	1	0	0	0	0
23	N	5	0	0	0	0
23	U	1	0	0	1	0
All	All	51700	0	810	805	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (805) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:16:MET:HB2	17:Q:19:SER:HB3	1.28	1.08
17:Q:18:LYS:HA	17:Q:47:ASP:HB2	1.38	0.99
17:Q:45:VAL:HG21	17:Q:60:ILE:HD13	1.42	0.99
5:E:155:LYS:HA	5:E:158:LYS:NZ	1.83	0.91
1:A:274:A:O2'	1:A:275:G:C8	2.24	0.90
5:E:155:LYS:HA	5:E:158:LYS:HZ1	1.42	0.82
1:A:366:A:O2'	1:A:394:G:N2	2.13	0.82
1:A:338:A:N1	1:A:351:G:O6	2.13	0.82
17:Q:12:VAL:HG13	17:Q:13:SER:N	1.97	0.80
1:A:1336:C:O2'	1:A:1337:G:OP2	2.00	0.80
5:E:153:ALA:HA	5:E:156:ARG:HB2	1.64	0.79
1:A:15:G:O4'	5:E:28:ARG:NH1	2.15	0.79
17:Q:51:GLU:HG3	17:Q:74:LEU:HD21	1.67	0.77
1:A:792:A:O2'	1:A:794:A:N7	2.18	0.76
1:A:181:A:N6	1:A:195:A:OP2	2.20	0.73
1:A:686:U:O2'	1:A:687:A:C8	2.41	0.73
1:A:1239:A:N6	1:A:1299:A:N6	2.35	0.73
8:H:76:ARG:NE	8:H:78:SER:O	2.22	0.73
5:E:156:ARG:O	5:E:158:LYS:N	2.22	0.71
5:E:155:LYS:HD2	5:E:156:ARG:H	1.56	0.70
2:B:22:TRP:O	2:B:22:TRP:CG	2.42	0.70
17:Q:11:VAL:HG12	17:Q:12:VAL:N	2.07	0.70
1:A:1160:G:O6	1:A:1181:G:C6	2.44	0.69
13:M:10:ASP:CG	13:M:11:HIS:N	2.46	0.69
1:A:111:G:O6	1:A:330:C:N4	2.26	0.69
1:A:1095:U:O2'	1:A:1096:C:O4'	2.10	0.69
1:A:1141:C:O2'	1:A:1142:G:O5'	2.11	0.69
1:A:958:A:C6	1:A:959:A:N1	2.61	0.68
1:A:182:A:N3	1:A:184:G:C8	2.62	0.68
1:A:1167:A:C8	1:A:1169:A:N6	2.62	0.68
17:Q:55:GLY:HA3	17:Q:82:VAL:HG11	1.76	0.68
5:E:152:VAL:HB	5:E:155:LYS:HZ2	1.58	0.67
5:E:155:LYS:HA	5:E:158:LYS:HZ3	1.60	0.67
1:A:1533:C:H3'	1:A:1534:A:H5''	1.77	0.67
8:H:81:GLY:O	17:Q:35:LYS:HE2	1.95	0.67
17:Q:29:LYS:HB2	17:Q:36:PHE:CZ	2.31	0.65
1:A:596:A:N6	1:A:645:G:C6	2.65	0.65
17:Q:22:VAL:HG21	17:Q:60:ILE:HD11	1.79	0.65
1:A:82:G:N2	1:A:84:U:N3	2.44	0.65
1:A:701:U:O2'	1:A:702:A:OP2	2.15	0.65
1:A:1094:G:O2'	1:A:1095:U:OP2	2.15	0.64
1:A:1433:A:OP2	23:A:1715:HOH:O	2.15	0.64
17:Q:12:VAL:HG13	17:Q:13:SER:H	1.62	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:A:O2'	1:A:198:G:C8	2.50	0.63
5:E:153:ALA:HA	5:E:156:ARG:CB	2.28	0.63
1:A:413:G:N2	1:A:428:G:O2'	2.31	0.63
3:C:10:ARG:O	3:C:13:ILE:O	2.16	0.63
17:Q:10:ARG:O	17:Q:22:VAL:HG13	1.97	0.63
17:Q:18:LYS:HA	17:Q:47:ASP:CB	2.21	0.63
17:Q:37:ILE:H	17:Q:37:ILE:HD12	1.63	0.63
1:A:86:G:C2	1:A:87:C:N4	2.66	0.63
1:A:872:A:C4	1:A:874:G:N7	2.66	0.62
12:L:49:ARG:CG	12:L:49:ARG:NH1	2.61	0.62
5:E:153:ALA:CA	5:E:156:ARG:HB2	2.30	0.62
1:A:508:U:O2'	1:A:509:A:C8	2.52	0.62
1:A:1432:G:O2'	1:A:1433:A:OP2	2.17	0.62
12:L:23:LEU:O	12:L:25:ALA:N	2.32	0.62
17:Q:12:VAL:CG1	17:Q:13:SER:N	2.63	0.62
5:E:79:THR:OG1	5:E:80:LEU:N	2.32	0.62
17:Q:18:LYS:C	17:Q:47:ASP:OD2	2.38	0.62
20:T:5:SER:OG	20:T:6:ALA:N	2.33	0.61
1:A:579:A:O2'	15:O:53:ARG:NH1	2.34	0.61
17:Q:45:VAL:HG13	17:Q:72:TRP:O	2.01	0.61
1:A:242:G:C2	1:A:245:U:C4	2.88	0.61
3:C:13:ILE:O	3:C:15:LYS:N	2.34	0.61
1:A:1058:G:C5	1:A:1059:C:C5	2.89	0.60
1:A:1530:G:O2'	1:A:1531:A:C8	2.54	0.60
1:A:1222:G:OP1	1:A:1321:U:O2'	2.18	0.60
13:M:10:ASP:OD1	13:M:11:HIS:N	2.34	0.60
1:A:198:G:O2'	1:A:199:A:C8	2.55	0.60
17:Q:13:SER:O	17:Q:16:MET:SD	2.59	0.60
17:Q:67:SER:OG	17:Q:70:LYS:HB3	2.02	0.60
1:A:1241:G:C2	1:A:1242:G:C5	2.90	0.60
1:A:374:A:OP1	1:A:452:A:N1	2.35	0.60
1:A:582:C:C2	1:A:583:A:C8	2.90	0.60
1:A:261:U:OP2	20:T:73:ARG:NH2	2.35	0.60
1:A:1381:U:O2'	1:A:1382:C:C5'	2.49	0.60
1:A:1084:G:C5	1:A:1085:U:C4	2.91	0.59
1:A:1151:A:O2'	1:A:1152:A:C8	2.55	0.59
14:N:63:CYS:SG	14:N:66:THR:OG1	2.61	0.59
1:A:1053:G:O2'	1:A:1054:C:OP2	2.21	0.59
1:A:762:U:C2	1:A:763:G:C8	2.90	0.59
1:A:1241:G:O2'	1:A:1242:G:C8	2.56	0.59
1:A:1520:C:C2	1:A:1521:C:C5	2.91	0.59
1:A:450:G:N7	1:A:481:G:O6	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:U:O2'	1:A:93:U:O4'	2.21	0.58
9:I:6:TYR:CG	9:I:7:GLY:N	2.69	0.58
17:Q:60:ILE:HG22	17:Q:72:TRP:HE3	1.68	0.58
12:L:82:ARG:NH1	12:L:83:GLY:O	2.36	0.58
1:A:1094:G:O2'	1:A:1095:U:P	2.61	0.58
1:A:144:G:C4	1:A:179:A:C2	2.92	0.58
16:P:59:HIS:CE1	16:P:63:GLN:NE2	2.71	0.58
14:N:60:ARG:O	14:N:61:ASN:CB	2.50	0.58
5:E:152:VAL:HG12	5:E:155:LYS:HZ1	1.68	0.58
1:A:1167:A:C8	1:A:1169:A:C6	2.92	0.58
1:A:428:G:O4'	1:A:430:A:C8	2.57	0.58
11:K:126:ARG:CB	21:U:33:ARG:NH1	2.67	0.58
1:A:397:A:N7	1:A:547:A:O2'	2.36	0.58
1:A:1261:A:N1	1:A:1274:A:C2	2.72	0.57
5:E:89:THR:CG2	5:E:90:GLY:N	2.67	0.57
1:A:1160:G:C6	1:A:1181:G:O6	2.57	0.57
1:A:497:G:N2	1:A:498:A:C6	2.72	0.57
1:A:1277:C:O2'	1:A:1279:G:C8	2.57	0.57
1:A:1064:G:N2	1:A:1190:G:O2'	2.36	0.57
17:Q:51:GLU:HG2	17:Q:52:CYS:SG	2.45	0.57
1:A:512:U:O2'	1:A:513:C:O4'	2.22	0.57
1:A:1250:A:N3	1:A:1370:G:O2'	2.37	0.57
17:Q:20:ILE:N	17:Q:47:ASP:OD1	2.37	0.57
17:Q:80:LYS:HB2	17:Q:80:LYS:NZ	2.19	0.57
17:Q:51:GLU:O	17:Q:52:CYS:O	2.22	0.57
1:A:75:G:C5	1:A:76:G:C8	2.91	0.57
1:A:258:G:C4	1:A:259:G:C8	2.92	0.57
4:D:133:SER:O	4:D:134:TYR:C	2.43	0.57
1:A:466:A:O2'	1:A:467:U:C5	2.58	0.57
1:A:198:G:C4	1:A:199:A:N7	2.72	0.57
1:A:92:U:C2'	1:A:93:U:C6	2.88	0.56
1:A:872:A:C8	1:A:874:G:C8	2.93	0.56
1:A:49:U:O4	1:A:365:U:C5	2.57	0.56
17:Q:12:VAL:CG1	17:Q:13:SER:H	2.18	0.56
1:A:914:A:N3	1:A:915:A:C8	2.73	0.56
20:T:2:ASN:O	20:T:3:ILE:C	2.43	0.56
4:D:16:THR:CG2	4:D:17:ASP:N	2.69	0.56
3:C:166:TRP:N	3:C:166:TRP:CE3	2.74	0.56
1:A:827:U:C4	1:A:870:U:C2	2.94	0.56
1:A:199:A:O2'	1:A:200:G:O4'	2.22	0.56
1:A:1151:A:O2'	1:A:1152:A:C5'	2.53	0.56
1:A:563:A:N3	1:A:563:A:C2'	2.67	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:31:PRO:HB2	17:Q:32:ILE:HD12	1.87	0.56
1:A:367:U:C6	1:A:394:G:N2	2.74	0.56
1:A:109:A:C6	1:A:326:G:C6	2.93	0.56
1:A:86:G:N2	1:A:87:C:N4	2.53	0.56
1:A:414:A:O2'	1:A:415:A:O4'	2.24	0.56
1:A:596:A:N6	1:A:645:G:N1	2.54	0.55
1:A:903:G:C5	1:A:904:U:C5	2.94	0.55
5:E:120:HIS:O	5:E:121:ASN:CB	2.53	0.55
1:A:511:C:O2'	1:A:512:U:C5'	2.55	0.55
1:A:868:C:N4	1:A:869:G:C2	2.73	0.55
10:J:48:ARG:NH2	14:N:100:TRP:CD2	2.74	0.55
1:A:1161:C:O2'	1:A:1162:C:C6	2.59	0.55
1:A:937:A:N6	1:A:1345:U:O4	2.39	0.55
1:A:1319:A:C8	1:A:1323:G:C6	2.94	0.55
1:A:765:G:N1	1:A:812:G:O2'	2.40	0.55
1:A:1533:C:O5'	1:A:1533:C:H6	1.89	0.55
1:A:428:G:C1'	1:A:430:A:C8	2.89	0.55
5:E:109:ALA:O	5:E:110:MET:CG	2.55	0.55
12:L:74:GLN:O	12:L:75:GLU:C	2.45	0.55
1:A:74:A:C6	1:A:97:G:O6	2.60	0.55
1:A:269:C:N4	1:A:270:A:N6	2.55	0.55
4:D:173:ASP:O	4:D:174:ALA:CB	2.54	0.55
1:A:923:A:O4'	1:A:1398:A:C2	2.60	0.55
1:A:70:U:O2'	1:A:71:A:C8	2.61	0.55
1:A:172:A:C5	1:A:174:A:N7	2.75	0.55
1:A:1500:A:OP2	23:A:1751:HOH:O	2.18	0.55
12:L:82:ARG:NH1	12:L:82:ARG:CG	2.70	0.54
1:A:1162:C:O2'	1:A:1163:A:O4'	2.25	0.54
1:A:1503:A:C8	1:A:1531:A:H1'	2.42	0.54
1:A:1441:A:N6	1:A:1461:G:N2	2.54	0.54
15:O:78:THR:O	15:O:82:GLU:OE1	2.24	0.54
1:A:1138:G:N3	1:A:1138:G:C2'	2.71	0.54
17:Q:20:ILE:H	17:Q:47:ASP:CG	2.10	0.54
18:R:24:ASP:O	18:R:27:THR:N	2.40	0.54
5:E:155:LYS:HD2	5:E:156:ARG:N	2.21	0.54
1:A:914:A:C4	1:A:915:A:C8	2.96	0.54
4:D:130:ASN:O	4:D:131:ILE:C	2.45	0.54
1:A:247:G:C6	1:A:278:G:C2	2.96	0.54
4:D:151:GLN:O	4:D:152:SER:C	2.46	0.54
1:A:204:G:C1'	1:A:465:A:C2	2.90	0.54
1:A:57:G:C6	1:A:356:A:N1	2.76	0.54
2:B:49:PHE:CG	2:B:212:TYR:OH	2.60	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:A:C2	1:A:184:G:C8	2.96	0.54
1:A:49:U:C4	1:A:364:A:C6	2.96	0.54
1:A:652:U:O2'	1:A:653:U:O5'	2.26	0.54
1:A:11:G:C5	1:A:12:U:C5	2.96	0.54
2:B:14:HIS:O	2:B:14:HIS:CG	2.61	0.54
1:A:1363:A:O2'	1:A:1365:G:N7	2.41	0.53
1:A:958:A:C5	1:A:959:A:C6	2.96	0.53
1:A:1279:G:C2'	1:A:1279:G:N3	2.71	0.53
17:Q:18:LYS:CA	17:Q:47:ASP:HB2	2.26	0.53
1:A:792:A:C4	1:A:794:A:N6	2.77	0.53
1:A:66:A:N6	1:A:104:G:C2	2.77	0.53
1:A:1052:U:C5'	1:A:1053:G:OP2	2.56	0.53
1:A:430:A:C4	1:A:431:A:C8	2.96	0.53
1:A:563:A:N6	23:A:1696:HOH:O	2.41	0.53
1:A:1387:G:C6	1:A:1388:C:N4	2.77	0.53
17:Q:46:HIS:HA	17:Q:70:LYS:HE3	1.91	0.53
4:D:147:LYS:O	4:D:149:LYS:N	2.42	0.53
1:A:427:U:C4	1:A:428:G:C6	2.96	0.53
1:A:566:G:C4'	1:A:567:G:OP1	2.56	0.53
1:A:66:A:O4'	1:A:173:U:C4	2.62	0.53
1:A:335:C:O2'	1:A:1433:A:N3	2.42	0.52
1:A:299:G:C6	1:A:300:A:C6	2.96	0.52
1:A:978:A:OP2	1:A:1362:A:N6	2.42	0.52
17:Q:40:THR:HG22	17:Q:41:THR:N	2.25	0.52
1:A:809:G:C6	1:A:810:C:C5	2.97	0.52
1:A:76:G:C2	1:A:95:C:N3	2.77	0.52
1:A:373:A:C2	1:A:374:A:C8	2.97	0.52
1:A:1098:C:C2	1:A:1099:G:C8	2.97	0.52
1:A:1084:G:C6	1:A:1085:U:O4	2.62	0.52
1:A:1053:G:C6	1:A:1199:U:C2	2.98	0.52
1:A:89:U:O2'	1:A:90:C:C5'	2.57	0.52
1:A:1073:U:O2'	2:B:102:ASN:ND2	2.43	0.52
17:Q:45:VAL:HG21	17:Q:60:ILE:CD1	2.27	0.52
8:H:25:THR:O	8:H:26:MET:CB	2.57	0.52
8:H:1:SER:C	8:H:3:GLN:N	2.62	0.52
1:A:945:G:C6	1:A:1337:G:C5	2.98	0.52
1:A:1158:C:O2	1:A:1158:C:C2'	2.58	0.52
1:A:71:A:O2'	1:A:72:A:O5'	2.28	0.52
21:U:16:ARG:NH1	21:U:19:LYS:CG	2.73	0.52
17:Q:60:ILE:HG22	17:Q:61:ARG:N	2.25	0.52
5:E:158:LYS:HE2	8:H:63:LYS:NZ	2.25	0.52
11:K:33:ILE:O	11:K:41:LEU:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:G:C6	1:A:525:C:N4	2.78	0.52
1:A:1530:G:O2'	1:A:1531:A:H8	1.92	0.51
1:A:499:A:O2'	1:A:500:G:C8	2.62	0.51
1:A:414:A:N3	1:A:415:A:C8	2.78	0.51
1:A:914:A:O2'	1:A:915:A:C5'	2.58	0.51
1:A:626:G:C4	1:A:627:G:C8	2.99	0.51
1:A:15:G:C4'	5:E:28:ARG:NH1	2.73	0.51
1:A:791:G:C6	1:A:792:A:N7	2.78	0.51
1:A:1533:C:H3'	1:A:1534:A:C5'	2.40	0.51
1:A:1303:C:O2'	1:A:1304:G:C5'	2.58	0.51
1:A:1124:G:OP1	10:J:37:ARG:C	2.49	0.51
6:F:85:ILE:O	6:F:86:ARG:C	2.48	0.51
1:A:1151:A:C4	1:A:1152:A:N7	2.79	0.51
17:Q:20:ILE:HB	17:Q:47:ASP:OD1	2.11	0.51
1:A:792:A:N3	1:A:794:A:C5	2.79	0.51
1:A:1320:C:N3	19:S:35:ARG:NH1	2.58	0.51
5:E:152:VAL:CB	5:E:155:LYS:NZ	2.74	0.51
1:A:1161:C:O2'	1:A:1162:C:C5'	2.58	0.51
1:A:55:A:C4	1:A:56:U:C6	2.99	0.51
3:C:164:THR:O	3:C:165:GLU:C	2.49	0.51
10:J:15:HIS:CG	10:J:16:ARG:N	2.78	0.51
1:A:1157:A:C5	1:A:1180:A:C6	2.98	0.51
1:A:958:A:C6	1:A:959:A:C6	2.99	0.51
1:A:570:G:C4	1:A:571:U:C5	2.99	0.51
1:A:373:A:O2'	1:A:374:A:C5'	2.58	0.51
2:B:17:HIS:CD2	2:B:202:ASN:ND2	2.78	0.51
17:Q:79:GLU:C	17:Q:80:LYS:HD3	2.32	0.51
1:A:977:A:C2'	1:A:977:A:N3	2.73	0.51
1:A:1196:A:O2'	1:A:1197:A:OP2	2.29	0.50
1:A:1468:A:C2'	1:A:1469:C:C5'	2.88	0.50
14:N:51:PRO:O	14:N:52:ARG:CB	2.59	0.50
1:A:321:A:N7	1:A:328:C:O2'	2.43	0.50
17:Q:11:VAL:HG12	17:Q:12:VAL:H	1.76	0.50
17:Q:33:TYR:O	17:Q:35:LYS:N	2.44	0.50
12:L:62:VAL:CG2	12:L:94:TYR:CE2	2.93	0.50
7:G:96:ASN:N	7:G:96:ASN:OD1	2.44	0.50
2:B:20:ARG:O	2:B:22:TRP:N	2.44	0.50
1:A:1074:G:C6	1:A:1075:U:C4	2.99	0.50
1:A:1159:U:N3	1:A:1182:G:C5	2.80	0.50
14:N:22:LYS:CG	14:N:23:ARG:N	2.74	0.50
1:A:119:A:C2	1:A:240:G:C8	3.00	0.50
17:Q:29:LYS:HB2	17:Q:36:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:373:A:N3	1:A:374:A:C8	2.79	0.50
1:A:628:G:C2	1:A:629:A:C4	3.00	0.50
1:A:1421:G:C6	1:A:1422:G:N7	2.79	0.50
1:A:1417:G:C6	1:A:1482:G:C6	3.00	0.50
1:A:1160:G:O6	1:A:1181:G:C5	2.64	0.50
1:A:903:G:C4	1:A:904:U:C5	3.00	0.50
4:D:124:VAL:O	4:D:126:GLY:N	2.45	0.50
11:K:76:TYR:CD1	11:K:76:TYR:N	2.80	0.50
5:E:152:VAL:HB	5:E:155:LYS:NZ	2.26	0.50
1:A:1091:U:C2	1:A:1095:U:N3	2.80	0.50
1:A:259:G:C4	1:A:260:G:C8	3.00	0.50
1:A:243:A:C4'	1:A:244:U:C5'	2.90	0.50
8:H:48:PHE:O	8:H:49:LYS:CB	2.59	0.50
1:A:716:A:C6	1:A:717:U:N3	2.79	0.50
6:F:52:ASN:O	6:F:53:LYS:CB	2.60	0.50
1:A:94:G:C4'	1:A:95:C:O5'	2.59	0.50
1:A:922:G:C6	1:A:923:A:C6	2.99	0.50
14:N:90:GLY:O	14:N:92:ILE:N	2.44	0.50
1:A:531:U:C4'	1:A:532:A:O5'	2.59	0.50
5:E:149:PRO:O	5:E:152:VAL:HG22	2.12	0.49
5:E:152:VAL:CB	5:E:155:LYS:HZ2	2.25	0.49
17:Q:29:LYS:HG2	17:Q:34:GLY:HA2	1.92	0.49
1:A:739:C:C4	1:A:740:U:C5	3.00	0.49
17:Q:21:VAL:HA	17:Q:43:LEU:O	2.12	0.49
12:L:23:LEU:CB	12:L:58:ASN:ND2	2.75	0.49
1:A:832:G:C6	1:A:833:G:N7	2.80	0.49
16:P:43:ALA:O	16:P:44:SER:OG	2.30	0.49
7:G:146:ALA:C	7:G:148:LYS:N	2.65	0.49
1:A:596:A:C6	1:A:645:G:C2	3.00	0.49
1:A:57:G:N1	1:A:356:A:C2	2.81	0.49
1:A:1468:A:C3'	1:A:1469:C:C5'	2.90	0.49
1:A:520:A:C2	1:A:536:C:O2	2.65	0.49
12:L:43:LYS:CB	12:L:44:PRO:CD	2.90	0.49
1:A:588:G:C2	1:A:589:U:C2	3.00	0.49
3:C:22:PHE:C	3:C:22:PHE:CD2	2.85	0.49
5:E:152:VAL:O	5:E:156:ARG:HB2	2.13	0.49
1:A:1322:C:O2'	1:A:1323:G:P	2.70	0.49
1:A:81:A:O2'	1:A:89:U:O2	2.31	0.49
4:D:28:ASP:C	4:D:29:THR:O	2.49	0.49
1:A:1338:G:C2'	1:A:1339:A:C8	2.95	0.49
11:K:13:LYS:O	11:K:14:GLN:CB	2.61	0.49
1:A:198:G:C6	1:A:220:G:C2	3.01	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:66:LEU:O	17:Q:67:SER:HB3	2.13	0.49
1:A:1319:A:C4'	1:A:1320:C:OP1	2.61	0.49
1:A:663:A:N1	1:A:743:A:C2	2.81	0.49
17:Q:45:VAL:O	17:Q:47:ASP:OD1	2.31	0.49
1:A:819:A:N7	1:A:1529:G:C2	2.80	0.49
1:A:74:A:C2	1:A:75:G:C4	3.01	0.49
1:A:191:G:C4	1:A:192:A:C8	3.00	0.49
1:A:198:G:O2'	1:A:199:A:C5'	2.61	0.48
1:A:1441:A:N7	1:A:1442:G:N7	2.61	0.48
2:B:186:VAL:N	2:B:199:ILE:O	2.46	0.48
15:O:2:LEU:O	15:O:3:SER:C	2.51	0.48
7:G:94:ARG:O	7:G:95:ARG:C	2.52	0.48
1:A:977:A:N6	1:A:1224:U:OP1	2.47	0.48
1:A:1421:G:C2	1:A:1422:G:C8	3.01	0.48
1:A:1160:G:O6	1:A:1181:G:O6	2.31	0.48
12:L:58:ASN:OD1	12:L:58:ASN:C	2.51	0.48
1:A:80:A:C2	1:A:90:C:N3	2.80	0.48
1:A:558:G:C4	1:A:559:A:C2	3.02	0.48
1:A:1055:A:N6	1:A:1206:G:C6	2.81	0.48
17:Q:80:LYS:HZ3	17:Q:80:LYS:HB2	1.78	0.48
1:A:57:G:C5	1:A:58:C:C4	3.02	0.48
1:A:251:G:N1	1:A:266:G:O6	2.46	0.48
10:J:91:ASP:O	10:J:92:LEU:O	2.31	0.48
5:E:155:LYS:CD	5:E:155:LYS:H	2.27	0.48
1:A:246:A:C4	1:A:282:A:N6	2.82	0.48
17:Q:7:LEU:HD22	17:Q:72:TRP:CZ3	2.48	0.48
17:Q:7:LEU:HD23	17:Q:24:ILE:CD1	2.43	0.48
12:L:24:GLU:O	12:L:25:ALA:C	2.51	0.48
1:A:563:A:C1'	1:A:566:G:O2'	2.61	0.48
1:A:585:G:C6	1:A:586:C:C4	3.01	0.48
1:A:877:G:N3	8:H:1:SER:N	2.62	0.48
1:A:1371:G:C6	1:A:1372:U:C4	3.02	0.48
5:E:81:GLN:NE2	5:E:146:MET:SD	2.87	0.48
16:P:11:ALA:O	16:P:12:LYS:C	2.52	0.48
4:D:34:GLU:O	4:D:36:ALA:N	2.46	0.48
17:Q:30:HIS:N	17:Q:35:LYS:O	2.42	0.48
1:A:701:U:O2	1:A:701:U:C2'	2.62	0.48
5:E:121:ASN:ND2	5:E:122:VAL:N	2.62	0.48
1:A:944:G:N1	1:A:1338:G:OP2	2.47	0.48
1:A:595:A:C5	1:A:641:U:C5	3.01	0.48
3:C:6:PRO:CG	3:C:183:TYR:CG	2.97	0.48
1:A:1319:A:C8	1:A:1323:G:C5	3.02	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:52:VAL:CG2	4:D:53:GLN:N	2.77	0.48
17:Q:50:ASN:N	17:Q:50:ASN:OD1	2.47	0.48
1:A:161:A:N1	1:A:347:G:O2'	2.46	0.48
1:A:1087:G:N2	1:A:1088:G:C4	2.82	0.48
1:A:829:G:C6	1:A:858:G:C2	3.01	0.48
17:Q:6:THR:O	17:Q:7:LEU:HD12	2.13	0.47
1:A:1160:G:O2'	1:A:1161:C:O5'	2.31	0.47
1:A:595:A:C6	1:A:641:U:C6	3.01	0.47
6:F:55:HIS:O	6:F:56:LYS:CB	2.61	0.47
1:A:506:G:C6	1:A:507:C:C4	3.02	0.47
20:T:4:LYS:O	20:T:5:SER:C	2.52	0.47
1:A:1003:G:C6	1:A:1036:A:N6	2.82	0.47
1:A:6:G:O2'	1:A:7:A:C8	2.67	0.47
4:D:75:TYR:C	4:D:75:TYR:CD1	2.87	0.47
1:A:209:U:C5'	1:A:210:C:OP2	2.63	0.47
14:N:42:ASN:O	14:N:44:VAL:N	2.47	0.47
1:A:1202:U:O2'	1:A:1203:C:C5'	2.62	0.47
2:B:49:PHE:CD1	2:B:49:PHE:C	2.88	0.47
1:A:1055:A:C6	1:A:1206:G:C5	3.02	0.47
1:A:1108:G:C5	1:A:1109:C:C5	3.02	0.47
1:A:491:G:C6	1:A:492:C:C4	3.03	0.47
4:D:191:SER:OG	4:D:192:ALA:N	2.48	0.47
19:S:47:THR:O	19:S:48:ILE:C	2.53	0.47
17:Q:16:MET:HG3	17:Q:19:SER:C	2.35	0.47
1:A:1158:C:O2'	1:A:1160:G:OP1	2.33	0.47
20:T:4:LYS:O	20:T:6:ALA:N	2.48	0.47
1:A:976:G:OP1	14:N:70:HIS:ND1	2.48	0.47
1:A:7:A:N6	5:E:96:GLN:OE1	2.48	0.47
1:A:515:G:N1	1:A:537:G:C6	2.83	0.47
4:D:114:ARG:O	4:D:115:GLN:C	2.53	0.47
1:A:666:G:C2	1:A:741:G:C4	3.02	0.47
19:S:79:TYR:CG	19:S:80:ARG:N	2.81	0.47
1:A:1328:C:OP1	13:M:27:THR:OG1	2.32	0.47
1:A:1095:U:O2'	1:A:1096:C:C5'	2.63	0.47
17:Q:11:VAL:HB	17:Q:55:GLY:H	1.80	0.47
1:A:557:G:C6	1:A:558:G:N1	2.82	0.47
19:S:51:HIS:CD2	19:S:53:GLY:N	2.83	0.47
13:M:113:LYS:N	13:M:114:PRO:CD	2.77	0.47
8:H:63:LYS:C	8:H:64:TYR:CD1	2.88	0.47
11:K:34:THR:OG1	11:K:39:ASN:N	2.48	0.47
18:R:50:TYR:O	18:R:54:LEU:N	2.48	0.47
15:O:16:ARG:O	15:O:17:ASP:CB	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:242:G:C2	1:A:245:U:C5	3.04	0.46
1:A:1256:A:C1'	1:A:1258:G:C5	2.98	0.46
13:M:45:SER:O	13:M:46:GLU:CB	2.62	0.46
1:A:428:G:C1'	1:A:430:A:N7	2.79	0.46
1:A:119:A:C4	1:A:240:G:N7	2.83	0.46
1:A:1048:G:OP1	14:N:3:GLN:N	2.48	0.46
2:B:185:ILE:CG1	2:B:185:ILE:O	2.63	0.46
4:D:19:PHE:N	4:D:19:PHE:CD1	2.84	0.46
1:A:597:G:C2	1:A:644:U:C2	3.04	0.46
1:A:1152:A:O2'	1:A:1153:G:C5'	2.64	0.46
1:A:1261:A:C2	1:A:1274:A:C2	3.02	0.46
12:L:86:VAL:CG1	12:L:86:VAL:O	2.62	0.46
1:A:1181:G:C2	1:A:1182:G:N2	2.83	0.46
15:O:67:ASP:OD1	15:O:87:ARG:NH2	2.48	0.46
1:A:1351:U:O4	9:I:119:LYS:NZ	2.49	0.46
5:E:77:ASN:CG	5:E:78:GLY:N	2.67	0.46
21:U:10:PRO:O	21:U:11:PHE:CB	2.63	0.46
1:A:957:U:O2	1:A:959:A:C8	2.68	0.46
1:A:1154:G:C2	1:A:1155:A:C8	3.04	0.46
1:A:1521:C:C2	1:A:1522:U:C6	3.04	0.46
1:A:94:G:C4'	1:A:95:C:C5'	2.94	0.46
5:E:60:GLN:C	5:E:62:ALA:N	2.68	0.46
1:A:1049:U:O2'	1:A:1050:G:P	2.74	0.46
1:A:570:G:C6	1:A:873:A:C2	3.04	0.46
1:A:369:G:C4	1:A:393:A:C2	3.03	0.46
16:P:28:ARG:NE	16:P:29:ASN:ND2	2.63	0.46
1:A:829:G:C2	1:A:830:G:C8	3.03	0.46
1:A:920:U:O4'	1:A:1080:A:C2	2.69	0.46
1:A:131:A:O2'	1:A:132:C:O4'	2.33	0.46
1:A:198:G:O2'	1:A:199:A:O5'	2.33	0.46
1:A:872:A:C5	1:A:874:G:C8	3.04	0.46
1:A:565:U:C4	1:A:566:G:C5	3.04	0.46
7:G:101:ARG:O	7:G:105:GLU:N	2.48	0.46
1:A:372:C:C4'	1:A:373:A:OP1	2.64	0.46
1:A:91:U:C2'	1:A:92:U:O4'	2.64	0.46
1:A:257:G:C2	1:A:258:G:C5	3.04	0.46
1:A:1525:G:OP1	11:K:121:ARG:NH2	2.49	0.46
15:O:23:SER:O	15:O:24:THR:C	2.54	0.46
1:A:1131:G:C2'	1:A:1132:C:O5'	2.63	0.46
17:Q:45:VAL:CG2	17:Q:60:ILE:HD13	2.31	0.45
12:L:21:PRO:O	12:L:23:LEU:N	2.50	0.45
1:A:1053:G:N2	1:A:1056:U:C4	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:971:G:O2'	1:A:1365:G:O2'	2.34	0.45
12:L:42:LYS:O	12:L:43:LYS:C	2.55	0.45
1:A:1258:G:C4	1:A:1259:C:C5	3.04	0.45
1:A:1253:G:N3	1:A:1254:A:C8	2.85	0.45
1:A:577:G:O2'	1:A:578:C:C5'	2.64	0.45
2:B:81:ASP:OD1	2:B:83:ALA:N	2.48	0.45
1:A:1127:G:O2'	1:A:1128:C:C5'	2.65	0.45
2:B:74:ALA:O	2:B:75:ALA:CB	2.64	0.45
17:Q:12:VAL:HG12	17:Q:21:VAL:O	2.16	0.45
1:A:275:G:C4	1:A:276:G:C8	3.04	0.45
1:A:1160:G:N2	1:A:1161:C:C2	2.85	0.45
1:A:112:G:C6	1:A:330:C:N4	2.85	0.45
11:K:125:LYS:O	11:K:126:ARG:CB	2.64	0.45
10:J:91:ASP:N	10:J:91:ASP:OD1	2.49	0.45
16:P:10:GLY:O	16:P:11:ALA:CB	2.64	0.45
20:T:16:ALA:O	20:T:17:ARG:C	2.55	0.45
18:R:63:TYR:CD1	18:R:69:TYR:OH	2.70	0.45
12:L:87:LYS:O	12:L:88:ASP:CB	2.65	0.45
9:I:56:MET:SD	9:I:57:VAL:N	2.90	0.45
4:D:22:SER:O	4:D:23:GLY:C	2.55	0.45
1:A:502:A:C2	1:A:544:G:C2	3.05	0.45
1:A:1320:C:O2'	1:A:1321:U:O4'	2.35	0.45
1:A:557:G:C6	1:A:558:G:C2	3.05	0.45
1:A:748:G:C6	1:A:749:A:C6	3.04	0.45
17:Q:56:ASP:OD2	17:Q:80:LYS:HA	2.17	0.45
1:A:1093:A:N3	1:A:1109:C:O2'	2.49	0.45
1:A:1154:G:C2	1:A:1155:A:C5	3.05	0.45
1:A:74:A:C6	1:A:97:G:C6	3.05	0.45
1:A:6:G:O6	5:E:98:ALA:CB	2.64	0.45
1:A:750:C:O2'	15:O:20:ASP:OD1	2.34	0.45
17:Q:12:VAL:CB	17:Q:21:VAL:HG22	2.46	0.45
1:A:414:A:N6	1:A:431:A:C4	2.84	0.45
2:B:132:GLU:O	2:B:136:ARG:CB	2.65	0.45
1:A:1129:C:C5'	9:I:17:ARG:NH2	2.79	0.45
1:A:129:A:O2'	1:A:130:A:C5'	2.63	0.45
17:Q:16:MET:O	17:Q:17:GLU:C	2.54	0.45
17:Q:47:ASP:C	17:Q:51:GLU:OE2	2.55	0.45
1:A:1322:C:O4'	1:A:1322:C:O2	2.32	0.45
1:A:1371:G:C5	1:A:1372:U:C4	3.05	0.45
2:B:72:LYS:O	2:B:74:ALA:N	2.50	0.45
1:A:495:A:C4'	1:A:496:A:O5'	2.64	0.45
17:Q:24:ILE:HG22	17:Q:24:ILE:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:791:G:C5	1:A:792:A:N7	2.84	0.45
1:A:1157:A:C6	1:A:1180:A:C5	3.05	0.45
1:A:1241:G:N2	1:A:1242:G:C5	2.84	0.45
1:A:500:G:C6	1:A:546:A:C2	3.04	0.45
2:B:49:PHE:CB	2:B:212:TYR:OH	2.65	0.45
1:A:747:A:C5'	1:A:748:G:OP2	2.65	0.45
10:J:63:ASP:OD2	14:N:97:LYS:NZ	2.50	0.45
1:A:439:U:C6	4:D:119:HIS:CD2	3.05	0.45
1:A:1077:G:N1	1:A:1081:A:C6	2.85	0.45
1:A:1126:U:O4'	1:A:1281:C:O2	2.34	0.45
20:T:72:ALA:O	20:T:73:ARG:C	2.55	0.45
1:A:1338:G:O2'	1:A:1339:A:O4'	2.34	0.45
7:G:128:GLU:O	7:G:129:ASN:C	2.56	0.45
20:T:20:ASN:O	20:T:24:ARG:N	2.49	0.45
1:A:62:U:OP1	1:A:385:C:O2'	2.33	0.45
1:A:1196:A:O2'	1:A:1197:A:P	2.75	0.45
1:A:161:A:N6	1:A:162:A:C6	2.85	0.45
1:A:1258:G:C2	1:A:1259:C:C5	3.05	0.45
4:D:108:ALA:N	4:D:112:GLU:OE2	2.50	0.45
16:P:16:PHE:O	16:P:16:PHE:CD1	2.70	0.45
5:E:149:PRO:C	5:E:151:MET:H	2.19	0.44
14:N:19:TYR:O	14:N:22:LYS:CB	2.66	0.44
1:A:773:G:C4	1:A:774:G:C8	3.05	0.44
1:A:596:A:N3	1:A:597:G:C8	2.85	0.44
1:A:450:G:N7	1:A:481:G:C6	2.85	0.44
1:A:1363:A:C8	1:A:1365:G:C5	3.06	0.44
1:A:244:U:C6	1:A:894:G:N2	2.85	0.44
5:E:153:ALA:O	5:E:154:ALA:C	2.56	0.44
8:H:77:VAL:O	8:H:78:SER:C	2.56	0.44
11:K:39:ASN:O	11:K:40:ALA:CB	2.65	0.44
1:A:1294:G:C6	1:A:1295:U:C4	3.05	0.44
21:U:39:LYS:N	21:U:40:PRO:CD	2.80	0.44
1:A:423:G:N3	1:A:423:G:C2'	2.80	0.44
4:D:88:ASN:N	4:D:88:ASN:OD1	2.50	0.44
1:A:1108:G:C5	1:A:1109:C:C6	3.06	0.44
1:A:198:G:N3	1:A:199:A:C8	2.85	0.44
1:A:363:A:C2	1:A:364:A:C4	3.06	0.44
5:E:31:SER:O	5:E:32:PHE:CD2	2.70	0.44
1:A:1430:A:C2	1:A:1471:U:C2	3.05	0.44
4:D:54:LEU:CD2	4:D:54:LEU:C	2.86	0.44
2:B:209:VAL:O	2:B:211:LEU:N	2.50	0.44
8:H:64:TYR:N	8:H:64:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:U:OP1	4:D:12:ARG:NH2	2.50	0.44
5:E:83:PRO:CB	5:E:96:GLN:NE2	2.80	0.44
1:A:527:G:O2'	1:A:535:A:N1	2.50	0.44
19:S:42:ASN:ND2	19:S:42:ASN:C	2.70	0.44
17:Q:20:ILE:CB	17:Q:47:ASP:OD1	2.65	0.44
1:A:935:A:O2'	1:A:936:C:O4'	2.36	0.44
9:I:49:GLN:C	9:I:51:LEU:N	2.70	0.44
8:H:4:ASP:OD1	8:H:76:ARG:NH1	2.51	0.44
1:A:1322:C:O2'	1:A:1323:G:O5'	2.36	0.44
1:A:766:A:OP2	1:A:812:G:N2	2.50	0.44
1:A:1505:G:P	23:A:1751:HOH:O	2.76	0.44
1:A:1124:G:O2'	1:A:1125:U:C6	2.71	0.44
1:A:1216:A:C2	1:A:1217:C:C4	3.06	0.44
4:D:21:LYS:O	4:D:23:GLY:N	2.51	0.44
1:A:760:G:N7	1:A:761:G:C8	2.85	0.44
1:A:1320:C:O2'	1:A:1321:U:O5'	2.36	0.44
1:A:1261:A:C2	1:A:1275:A:C6	3.05	0.44
1:A:560:A:OP2	1:A:566:G:N2	2.50	0.44
1:A:1269:A:C2	1:A:1312:G:N3	2.85	0.44
6:F:10:VAL:CG1	6:F:11:HIS:N	2.80	0.44
1:A:1084:G:C6	1:A:1085:U:C4	3.06	0.44
1:A:92:U:O2'	1:A:93:U:C5'	2.65	0.44
1:A:96:U:O2'	1:A:97:G:C8	2.71	0.44
1:A:258:G:C6	1:A:259:G:C5	3.06	0.44
1:A:247:G:C5	1:A:278:G:N2	2.85	0.44
1:A:737:C:C2	1:A:738:C:C5	3.06	0.44
1:A:981:U:C2	1:A:982:U:C5	3.06	0.44
1:A:160:A:O2'	1:A:344:A:C6	2.71	0.44
1:A:807:A:C5	1:A:808:C:C5	3.06	0.44
1:A:1117:A:C6	1:A:1184:G:O6	2.71	0.44
1:A:32:A:C2'	1:A:33:A:C8	3.01	0.44
1:A:127:G:N2	1:A:235:C:C2	2.86	0.44
1:A:864:A:C3'	1:A:865:A:C8	3.00	0.44
1:A:1142:G:C2'	1:A:1143:G:O4'	2.66	0.43
1:A:199:A:N3	1:A:200:G:C8	2.86	0.43
1:A:57:G:C2	1:A:356:A:C2	3.06	0.43
1:A:192:A:C6	1:A:193:C:C4	3.06	0.43
1:A:1055:A:C8	1:A:1055:A:O5'	2.71	0.43
7:G:83:THR:O	7:G:84:TYR:C	2.55	0.43
19:S:78:THR:O	19:S:78:THR:OG1	2.34	0.43
4:D:196:GLU:C	4:D:198:LEU:N	2.71	0.43
5:E:155:LYS:HD2	5:E:155:LYS:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:A:N6	1:A:90:C:C4	2.85	0.43
1:A:32:A:C2	1:A:33:A:C5	3.06	0.43
6:F:38:ARG:CG	6:F:39:LEU:N	2.81	0.43
6:F:3:HIS:O	6:F:92:THR:OG1	2.36	0.43
19:S:62:THR:O	19:S:63:ASP:C	2.56	0.43
1:A:842:U:O2'	1:A:846:G:N1	2.50	0.43
1:A:782:A:C8	1:A:783:C:C5	3.07	0.43
1:A:923:A:OP1	5:E:25:LYS:CG	2.66	0.43
14:N:50:LEU:O	14:N:52:ARG:N	2.51	0.43
5:E:81:GLN:NE2	5:E:81:GLN:N	2.66	0.43
1:A:131:A:C2	1:A:132:C:C4	3.07	0.43
1:A:1054:C:O4'	1:A:1054:C:O2	2.33	0.43
1:A:933:G:C5	1:A:935:A:C8	3.06	0.43
1:A:425:G:C6	1:A:426:U:C2	3.07	0.43
1:A:118:U:C4	1:A:288:A:C2	3.06	0.43
3:C:139:ASN:C	3:C:139:ASN:ND2	2.71	0.43
1:A:692:U:O2'	1:A:694:A:N7	2.50	0.43
1:A:15:G:N7	1:A:1396:A:C2	2.87	0.43
1:A:976:G:N1	1:A:1363:A:C2	2.86	0.43
1:A:748:G:C6	1:A:749:A:C5	3.07	0.43
1:A:418:C:N4	23:A:1593:HOH:O	2.51	0.43
1:A:701:U:O2'	1:A:702:A:P	2.76	0.43
1:A:173:U:C2	1:A:197:A:N1	2.86	0.43
1:A:1516:G:N2	1:A:1519:A:OP2	2.51	0.43
17:Q:58:VAL:HG22	17:Q:59:GLU:N	2.33	0.43
17:Q:58:VAL:HG23	17:Q:77:VAL:HG22	2.00	0.43
1:A:1227:A:N3	1:A:1227:A:C2'	2.81	0.43
1:A:792:A:C4	1:A:794:A:C6	3.07	0.43
14:N:62:ARG:O	14:N:63:CYS:C	2.55	0.43
1:A:558:G:C5	1:A:559:A:C2	3.07	0.43
13:M:3:ILE:O	13:M:5:GLY:N	2.52	0.43
21:U:35:GLU:O	21:U:36:PHE:CB	2.66	0.43
1:A:787:A:C5	1:A:788:U:C5	3.07	0.43
7:G:144:ALA:C	7:G:146:ALA:N	2.72	0.43
17:Q:49:ASN:O	17:Q:50:ASN:C	2.56	0.43
1:A:210:C:C4'	1:A:211:G:N2	2.82	0.43
8:H:8:ASP:O	8:H:9:MET:C	2.57	0.43
16:P:17:TYR:CD1	16:P:17:TYR:N	2.86	0.43
16:P:48:GLU:CG	16:P:49:GLY:N	2.82	0.43
1:A:1134:G:N1	1:A:1141:C:C4	2.87	0.43
1:A:1154:G:N1	1:A:1155:A:C5	2.87	0.43
1:A:917:G:C6	1:A:918:A:C6	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:8:ASN:ND2	21:U:8:ASN:N	2.67	0.43
2:B:110:ILE:CD1	2:B:147:LEU:CD1	2.97	0.43
1:A:481:G:C8	1:A:481:G:C3'	3.01	0.43
17:Q:58:VAL:HG23	17:Q:76:ARG:O	2.19	0.43
9:I:112:ARG:NH2	10:J:64:GLN:NE2	2.66	0.43
1:A:27:G:C5	1:A:557:G:C2	3.07	0.42
1:A:1055:A:N6	1:A:1206:G:C5	2.87	0.42
4:D:191:SER:O	4:D:192:ALA:CB	2.67	0.42
1:A:1227:A:O2'	1:A:1228:C:O5'	2.37	0.42
3:C:33:ASP:O	3:C:37:LYS:CB	2.67	0.42
7:G:14:ASP:OD2	7:G:14:ASP:C	2.58	0.42
1:A:923:A:C4	1:A:924:C:C5	3.08	0.42
14:N:20:PHE:C	14:N:22:LYS:N	2.73	0.42
1:A:126:G:C2'	1:A:127:G:O5'	2.67	0.42
9:I:121:ARG:O	9:I:122:ARG:C	2.55	0.42
1:A:375:U:C4	1:A:376:G:N7	2.87	0.42
1:A:1026:G:C6	1:A:1027:C:N4	2.87	0.42
1:A:695:A:C6	1:A:696:A:C6	3.08	0.42
1:A:181:A:C6	1:A:195:A:N7	2.88	0.42
1:A:199:A:C2	1:A:200:G:C4	3.07	0.42
1:A:1153:G:O2'	1:A:1154:G:O5'	2.37	0.42
1:A:38:G:N1	1:A:397:A:OP1	2.52	0.42
1:A:652:U:O4	1:A:752:G:C2'	2.67	0.42
1:A:524:G:C6	1:A:525:C:C4	3.08	0.42
1:A:1087:G:O2'	1:A:1088:G:C5'	2.68	0.42
1:A:604:G:C2	1:A:635:A:C2	3.08	0.42
1:A:1271:A:C2	1:A:1272:G:C5	3.07	0.42
1:A:1272:G:C5	1:A:1273:C:C4	3.07	0.42
15:O:18:ALA:O	15:O:19:ASN:CB	2.66	0.42
1:A:723:U:O2	1:A:855:U:O3'	2.37	0.42
2:B:123:GLY:O	2:B:125:PHE:CD2	2.72	0.42
1:A:499:A:C6	1:A:547:A:C8	3.08	0.42
1:A:77:A:N6	1:A:90:C:C5	2.88	0.42
1:A:829:G:N3	1:A:830:G:C8	2.88	0.42
1:A:933:G:C4	1:A:935:A:C8	3.07	0.42
1:A:1348:U:O2'	1:A:1349:A:C5'	2.67	0.42
15:O:34:GLN:O	15:O:35:ILE:C	2.58	0.42
17:Q:12:VAL:HB	17:Q:21:VAL:HG22	2.01	0.42
1:A:281:G:O2'	1:A:282:A:OP2	2.38	0.42
1:A:1055:A:C5	1:A:1206:G:C2	3.07	0.42
1:A:266:G:O3'	17:Q:68:LYS:HB2	2.19	0.42
1:A:1087:G:O2'	1:A:1088:G:C8	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:42:ASN:C	14:N:44:VAL:N	2.73	0.42
1:A:1258:G:N3	1:A:1259:C:C5	2.88	0.42
15:O:23:SER:O	15:O:26:VAL:N	2.52	0.42
1:A:460:A:O3'	1:A:462:G:OP2	2.38	0.42
1:A:947:G:C6	1:A:948:C:C4	3.08	0.42
17:Q:60:ILE:CG2	17:Q:61:ARG:N	2.81	0.42
1:A:734:G:N2	18:R:63:TYR:CE1	2.88	0.42
1:A:1358:U:C6	1:A:1359:C:C5	3.08	0.42
2:B:23:ASN:O	2:B:26:MET:N	2.53	0.42
15:O:65:LEU:CD2	15:O:65:LEU:N	2.83	0.42
8:H:112:ASP:O	8:H:113:ARG:C	2.57	0.42
1:A:461:A:C3'	1:A:461:A:N3	2.83	0.42
5:E:152:VAL:O	5:E:155:LYS:HD2	2.19	0.42
1:A:1299:A:C2'	1:A:1299:A:N3	2.82	0.42
1:A:1091:U:O2	1:A:1093:A:C8	2.73	0.42
1:A:1323:G:C2'	1:A:1324:A:C8	3.02	0.42
1:A:926:G:C6	1:A:1505:G:C5	3.06	0.42
1:A:1246:A:N1	1:A:1292:G:C6	2.88	0.42
1:A:102:G:C4	1:A:103:U:C5	3.08	0.42
17:Q:11:VAL:HG23	17:Q:56:ASP:O	2.19	0.42
1:A:198:G:C6	1:A:220:G:C4	3.08	0.42
1:A:1054:C:P	1:A:1197:A:OP2	2.78	0.42
1:A:762:U:O2	1:A:763:G:C8	2.73	0.42
4:D:145:ARG:C	4:D:147:LYS:N	2.70	0.42
1:A:243:A:C2	1:A:246:A:C8	3.08	0.42
1:A:444:G:C2	1:A:491:G:C4	3.08	0.42
1:A:965:U:OP1	1:A:1198:G:C5'	2.67	0.42
17:Q:12:VAL:CG1	17:Q:21:VAL:O	2.68	0.42
1:A:1157:A:C2	1:A:1181:G:C4	3.07	0.42
1:A:66:A:C8	1:A:66:A:O5'	2.73	0.42
1:A:872:A:C4	1:A:874:G:C8	3.07	0.42
11:K:124:LYS:O	21:U:33:ARG:NE	2.53	0.42
12:L:94:TYR:N	12:L:94:TYR:CD2	2.87	0.42
1:A:832:G:C2	1:A:833:G:C8	3.08	0.42
1:A:425:G:C6	1:A:426:U:N3	2.88	0.42
2:B:148:GLY:C	2:B:150:ILE:N	2.73	0.42
1:A:148:G:O2'	1:A:1446:A:O2'	2.38	0.42
3:C:136:ALA:O	3:C:140:ALA:CB	2.68	0.42
1:A:203:G:C2	1:A:215:C:N3	2.88	0.42
1:A:202:G:O2'	1:A:468:A:C8	2.72	0.42
3:C:59:PRO:O	3:C:60:ALA:O	2.37	0.42
17:Q:12:VAL:HG11	17:Q:21:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:A:N1	1:A:195:A:C8	2.88	0.42
1:A:198:G:C2'	1:A:199:A:C8	3.02	0.42
1:A:586:C:O2'	8:H:3:GLN:NE2	2.53	0.42
1:A:575:G:C5	1:A:881:G:C2	3.08	0.42
4:D:190:LEU:O	4:D:191:SER:CB	2.68	0.42
4:D:21:LYS:CD	4:D:21:LYS:O	2.68	0.42
1:A:42:G:C6	1:A:43:C:C4	3.08	0.42
1:A:60:A:C4'	1:A:61:G:O5'	2.68	0.42
1:A:15:G:C5	1:A:1396:A:C2	3.08	0.41
1:A:592:G:C6	1:A:648:A:C6	3.08	0.41
1:A:252:U:O2'	1:A:275:G:N2	2.53	0.41
1:A:687:A:C2	1:A:704:A:C5	3.07	0.41
1:A:1108:G:N7	1:A:1109:C:C5	2.88	0.41
1:A:263:A:OP1	20:T:73:ARG:NH1	2.53	0.41
17:Q:32:ILE:HD12	17:Q:32:ILE:N	2.35	0.41
9:I:49:GLN:O	9:I:51:LEU:N	2.54	0.41
2:B:140:LEU:O	2:B:141:GLU:C	2.59	0.41
1:A:901:A:N7	1:A:902:G:C1'	2.83	0.41
2:B:27:LYS:N	2:B:28:PRO:CD	2.83	0.41
1:A:1014:A:OP1	19:S:17:LYS:NZ	2.53	0.41
17:Q:11:VAL:HG12	17:Q:13:SER:H	1.85	0.41
1:A:428:G:C5	1:A:430:A:C6	3.08	0.41
1:A:1322:C:O2'	1:A:1323:G:C5'	2.68	0.41
1:A:1261:A:N3	1:A:1275:A:C6	2.89	0.41
1:A:914:A:O2'	1:A:915:A:O4'	2.38	0.41
1:A:55:A:C5	1:A:56:U:C5	3.08	0.41
6:F:11:HIS:CD2	6:F:12:PRO:CD	3.03	0.41
3:C:35:ASP:O	3:C:37:LYS:N	2.52	0.41
16:P:77:GLU:C	16:P:79:ASN:N	2.72	0.41
21:U:34:ARG:NH2	23:U:219:HOH:O	2.52	0.41
21:U:52:VAL:CG1	21:U:53:LYS:N	2.83	0.41
10:J:18:ILE:CG2	10:J:19:ASP:N	2.82	0.41
20:T:68:LYS:CB	20:T:68:LYS:NZ	2.83	0.41
1:A:511:C:O2'	1:A:512:U:P	2.79	0.41
5:E:108:GLY:O	5:E:109:ALA:CB	2.69	0.41
4:D:147:LYS:CD	4:D:147:LYS:N	2.84	0.41
5:E:94:PHE:CZ	5:E:96:GLN:CD	2.94	0.41
1:A:369:G:OP2	1:A:388:G:N1	2.53	0.41
1:A:439:U:O2'	1:A:440:C:C5'	2.68	0.41
1:A:1030:U:OP2	1:A:1031:C:O2	2.39	0.41
17:Q:74:LEU:C	17:Q:74:LEU:CD1	2.88	0.41
1:A:1533:C:C3'	1:A:1534:A:H5''	2.48	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:935:A:C2	1:A:936:C:C2	3.09	0.41
1:A:1050:G:O2'	1:A:1051:C:C5'	2.69	0.41
1:A:787:A:C6	1:A:788:U:C4	3.09	0.41
18:R:33:THR:OG1	18:R:34:GLU:N	2.53	0.41
1:A:22:G:C6	1:A:23:C:C4	3.08	0.41
4:D:84:ASN:O	4:D:85:THR:C	2.59	0.41
5:E:149:PRO:C	5:E:151:MET:N	2.74	0.41
5:E:152:VAL:CA	5:E:155:LYS:NZ	2.84	0.41
4:D:144:ILE:O	4:D:145:ARG:C	2.59	0.41
17:Q:48:GLU:O	17:Q:49:ASN:C	2.58	0.41
4:D:187:ARG:NH1	4:D:190:LEU:O	2.54	0.41
12:L:72:ASN:OD1	12:L:104:SER:CB	2.69	0.41
1:A:927:G:N1	1:A:1391:U:C2	2.89	0.41
1:A:1109:C:C2	1:A:1110:A:C8	3.08	0.41
1:A:1101:A:O2'	1:A:1102:A:OP2	2.38	0.41
1:A:674:G:N2	1:A:717:U:O2	2.54	0.41
1:A:515:G:N2	1:A:537:G:C4	2.89	0.41
1:A:1272:G:C6	1:A:1273:C:C4	3.08	0.41
13:M:100:ARG:NH1	13:M:103:THR:OG1	2.54	0.41
1:A:587:G:C2	1:A:755:G:C5	3.09	0.41
15:O:38:LEU:O	15:O:41:HIS:N	2.53	0.41
9:I:54:VAL:O	9:I:55:ASP:O	2.39	0.41
1:A:1319:A:C5	1:A:1323:G:C4	3.09	0.41
1:A:1241:G:C2	1:A:1242:G:N7	2.89	0.41
1:A:1154:G:N3	1:A:1155:A:C8	2.89	0.41
1:A:512:U:O5'	4:D:40:HIS:CE1	2.74	0.41
1:A:628:G:N2	1:A:629:A:N3	2.68	0.41
1:A:601:G:C2	1:A:602:A:C4	3.08	0.41
1:A:655:A:C2	1:A:656:G:C4	3.09	0.41
6:F:76:THR:O	6:F:79:ARG:N	2.54	0.41
1:A:486:U:C5'	1:A:486:U:C6	3.04	0.41
17:Q:16:MET:SD	17:Q:20:ILE:HD12	2.61	0.41
1:A:16:A:O2'	1:A:17:U:C5'	2.69	0.41
1:A:15:G:C4	1:A:16:A:C8	3.09	0.41
1:A:1167:A:N7	1:A:1169:A:C6	2.88	0.41
1:A:198:G:O6	1:A:220:G:C6	2.73	0.41
3:C:10:ARG:O	3:C:13:ILE:N	2.54	0.41
1:A:582:C:C4	1:A:583:A:N7	2.89	0.41
1:A:1261:A:N1	1:A:1274:A:N3	2.68	0.41
1:A:620:C:C2	4:D:131:ILE:CG2	3.03	0.41
1:A:204:G:C3'	1:A:205:A:C5'	2.99	0.41
1:A:1125:U:OP2	1:A:1145:A:N6	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:890:G:N2	1:A:907:A:OP2	2.54	0.41
1:A:1004:A:C6	1:A:1005:A:C4	3.09	0.41
3:C:156:LEU:CD1	3:C:156:LEU:N	2.84	0.41
1:A:1532:U:H2'	1:A:1534:A:H5'	2.03	0.41
16:P:79:ASN:O	16:P:80:LYS:CB	2.68	0.41
3:C:125:ARG:O	3:C:126:ARG:CB	2.69	0.41
8:H:17:GLN:NE2	8:H:71:VAL:CG2	2.83	0.41
17:Q:11:VAL:HG12	17:Q:12:VAL:HG12	2.03	0.40
1:A:792:A:N3	1:A:794:A:C6	2.88	0.40
1:A:181:A:N6	1:A:195:A:C8	2.89	0.40
1:A:76:G:N1	1:A:95:C:N4	2.68	0.40
5:E:110:MET:O	5:E:114:LEU:CB	2.70	0.40
15:O:15:GLY:C	15:O:17:ASP:N	2.75	0.40
15:O:74:VAL:O	15:O:77:TYR:N	2.54	0.40
1:A:1130:A:C5	1:A:1146:A:C6	3.09	0.40
1:A:199:A:C2	1:A:200:G:C8	3.09	0.40
1:A:49:U:C5	1:A:364:A:C6	3.09	0.40
16:P:55:ASP:N	16:P:55:ASP:OD2	2.54	0.40
11:K:28:ASN:OD1	11:K:29:THR:N	2.54	0.40
1:A:112:G:C2	1:A:113:G:C8	3.10	0.40
16:P:56:ARG:NH1	16:P:59:HIS:CD2	2.90	0.40
1:A:257:G:C2	1:A:258:G:N7	2.90	0.40
1:A:619:U:O2	4:D:130:ASN:N	2.54	0.40
1:A:982:U:C4'	1:A:983:A:O5'	2.69	0.40
1:A:21:G:N2	1:A:22:G:C6	2.89	0.40
5:E:148:SER:O	5:E:152:VAL:HG13	2.21	0.40
1:A:414:A:C2	1:A:415:A:C8	3.09	0.40
1:A:1063:C:C2'	1:A:1064:G:C8	3.04	0.40
1:A:258:G:C2	1:A:259:G:N9	2.90	0.40
1:A:258:G:C5	1:A:259:G:C8	3.10	0.40
5:E:121:ASN:N	5:E:121:ASN:ND2	2.69	0.40
14:N:20:PHE:O	14:N:22:LYS:N	2.54	0.40
4:D:33:ILE:O	4:D:34:GLU:CB	2.68	0.40
4:D:2:ARG:CZ	4:D:114:ARG:CD	2.98	0.40
8:H:8:ASP:O	8:H:12:ARG:N	2.55	0.40
10:J:57:VAL:CG2	10:J:58:ASN:N	2.84	0.40
1:A:814:A:P	23:A:1635:HOH:O	2.79	0.40
14:N:46:LYS:C	14:N:48:GLN:N	2.74	0.40
1:A:581:G:N1	1:A:759:A:OP2	2.55	0.40
1:A:233:C:C2	1:A:234:C:C5	3.10	0.40
17:Q:15:LYS:O	17:Q:16:MET:SD	2.79	0.40
1:A:627:G:C4	1:A:628:G:C8	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:920:U:O4'	1:A:1080:A:N1	2.54	0.40
1:A:212:G:C2	1:A:213:G:C5	3.09	0.40
1:A:213:G:C8	1:A:214:C:C5	3.09	0.40
1:A:457:G:C5	1:A:458:U:C5	3.10	0.40
1:A:1114:C:C4	1:A:1115:U:C5	3.09	0.40
10:J:41:PRO:O	10:J:42:LEU:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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%)	132 (61%)	55 (26%)	29 (13%)	0	2
3	C	204/206 (99%)	153 (75%)	34 (17%)	17 (8%)	1	9
4	D	203/205 (99%)	133 (66%)	43 (21%)	27 (13%)	0	2
5	E	148/150 (99%)	103 (70%)	28 (19%)	17 (12%)	1	4
6	F	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	2	13
7	G	149/151 (99%)	108 (72%)	35 (24%)	6 (4%)	5	32
8	H	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	4	27
9	I	125/127 (98%)	84 (67%)	30 (24%)	11 (9%)	1	8
10	J	96/98 (98%)	70 (73%)	16 (17%)	10 (10%)	1	5
11	K	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
12	L	121/123 (98%)	88 (73%)	16 (13%)	17 (14%)	0	2
13	M	112/114 (98%)	84 (75%)	19 (17%)	9 (8%)	1	10
14	N	92/100 (92%)	58 (63%)	22 (24%)	12 (13%)	0	3
15	O	86/88 (98%)	62 (72%)	13 (15%)	11 (13%)	0	3
16	P	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	1	4
17	Q	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	1
18	R	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	77/79 (98%)	59 (77%)	12 (16%)	6 (8%)	1	11
20	T	83/85 (98%)	65 (78%)	10 (12%)	8 (10%)	1	7
21	U	49/51 (96%)	26 (53%)	15 (31%)	8 (16%)	0	1
All	All	2312/2358 (98%)	1628 (70%)	451 (20%)	233 (10%)	1	6

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	ARG
2	B	40	ILE
2	B	72	LYS
2	B	75	ALA
2	B	119	GLN
2	B	133	ALA
2	B	169	HIS
2	B	200	PRO
3	C	16	PRO
3	C	17	TRP
3	C	60	ALA
3	C	205	GLU
4	D	26	ALA
4	D	28	ASP
4	D	29	THR
4	D	34	GLU
4	D	131	ILE
4	D	159	GLU
4	D	191	SER
4	D	192	ALA
5	E	44	ARG
5	E	97	PRO
5	E	137	ARG
5	E	156	ARG
5	E	157	GLY
6	F	54	LEU
6	F	86	ARG
7	G	93	VAL
8	H	26	MET
8	H	49	LYS
8	H	66	GLN
9	I	8	THR
9	I	40	ARG

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Mol	Chain	Res	Type
9	I	43	ALA
9	I	55	ASP
9	I	71	ILE
9	I	128	LYS
10	J	57	VAL
10	J	61	ALA
10	J	92	LEU
11	K	13	LYS
11	K	51	PHE
11	K	125	LYS
11	K	126	ARG
12	L	23	LEU
12	L	24	GLU
12	L	43	LYS
12	L	75	GLU
13	M	46	GLU
14	N	22	LYS
14	N	33	VAL
14	N	51	PRO
14	N	61	ASN
15	O	17	ASP
16	P	11	ALA
16	P	80	LYS
17	Q	12	VAL
17	Q	16	MET
17	Q	52	CYS
17	Q	70	LYS
19	S	48	ILE
19	S	63	ASP
20	T	3	ILE
20	T	4	LYS
20	T	5	SER
21	U	11	PHE
21	U	12	ASP
2	B	17	HIS
2	B	18	GLN
2	B	21	TYR
2	B	22	TRP
2	B	37	VAL
2	B	63	LYS
2	B	125	PHE
2	B	140	LEU

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Mol	Chain	Res	Type
2	B	189	ASN
2	B	210	THR
2	B	211	LEU
3	C	14	VAL
3	C	126	ARG
3	C	165	GLU
4	D	22	SER
4	D	23	GLY
4	D	31	CYS
4	D	33	ILE
4	D	35	GLN
4	D	147	LYS
4	D	148	ALA
4	D	150	LYS
4	D	152	SER
4	D	173	ASP
4	D	174	ALA
5	E	11	GLN
5	E	50	GLY
5	E	98	ALA
5	E	121	ASN
5	E	154	ALA
7	G	95	ARG
7	G	129	ASN
8	H	48	PHE
8	H	77	VAL
8	H	88	LYS
10	J	74	VAL
10	J	101	SER
12	L	33	CYS
12	L	73	LEU
12	L	88	ASP
12	L	97	VAL
12	L	117	GLY
13	M	4	ALA
14	N	27	LYS
14	N	44	VAL
14	N	52	ARG
16	P	10	GLY
16	P	16	PHE
16	P	36	VAL
17	Q	34	GLY

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Mol	Chain	Res	Type
17	Q	75	VAL
18	R	47	ARG
19	S	27	LYS
20	T	67	HIS
21	U	8	ASN
2	B	33	ALA
2	B	58	LYS
2	B	128	LEU
2	B	142	LYS
2	B	150	ILE
2	B	219	THR
3	C	192	TYR
4	D	124	VAL
4	D	167	PRO
4	D	195	ASN
4	D	196	GLU
5	E	109	ALA
5	E	149	PRO
6	F	7	VAL
9	I	119	LYS
11	K	97	ARG
12	L	102	ASP
13	M	3	ILE
13	M	113	LYS
14	N	41	TRP
14	N	43	ALA
15	O	45	HIS
16	P	49	GLY
16	P	78	VAL
17	Q	11	VAL
17	Q	49	ASN
17	Q	50	ASN
17	Q	67	SER
21	U	23	GLU
2	B	96	LEU
3	C	35	ASP
3	C	100	ILE
3	C	139	ASN
3	C	148	ILE
4	D	125	ASN
4	D	197	HIS
5	E	23	THR

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Mol	Chain	Res	Type
6	F	39	LEU
6	F	56	LYS
7	G	130	LYS
9	I	37	TYR
9	I	120	ALA
10	J	36	VAL
11	K	124	LYS
12	L	22	ALA
12	L	72	ASN
12	L	77	SER
13	M	104	ASN
14	N	63	CYS
15	O	16	ARG
15	O	24	THR
15	O	72	LYS
15	O	86	LEU
17	Q	10	ARG
19	S	5	LYS
3	C	65	VAL
3	C	107	LYS
3	C	145	ALA
3	C	191	THR
4	D	166	LYS
5	E	77	ASN
5	E	144	GLU
6	F	15	SER
6	F	63	ASN
7	G	84	TYR
9	I	56	MET
9	I	122	ARG
10	J	35	GLN
11	K	88	PRO
12	L	122	LYS
13	M	6	ILE
13	M	84	CYS
14	N	91	GLU
15	O	43	ALA
15	O	68	TYR
17	Q	5	ARG
18	R	54	LEU
20	T	72	ALA
20	T	74	HIS

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Mol	Chain	Res	Type
21	U	37	TYR
2	B	120	SER
2	B	141	GLU
3	C	173	PRO
5	E	104	ILE
10	J	33	GLY
11	K	40	ALA
13	M	11	HIS
15	O	2	LEU
15	O	35	ILE
19	S	22	VAL
19	S	26	ASP
20	T	76	ALA
21	U	33	ARG
21	U	36	PHE
4	D	172	VAL
5	E	148	SER
10	J	41	PRO
12	L	86	VAL
16	P	42	ILE
21	U	52	VAL
7	G	6	ILE
10	J	42	LEU
11	K	15	VAL
15	O	85	GLY
20	T	57	VAL
2	B	209	VAL
12	L	41	PRO
16	P	15	PRO
12	L	54	VAL
13	M	9	PRO
14	N	81	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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%)	142 (79%)	38 (21%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	170/170 (100%)	142 (84%)	28 (16%)	3	14
4	D	172/172 (100%)	146 (85%)	26 (15%)	4	19
5	E	113/113 (100%)	90 (80%)	23 (20%)	2	8
6	F	87/87 (100%)	75 (86%)	12 (14%)	5	24
7	G	124/124 (100%)	108 (87%)	16 (13%)	6	28
8	H	104/104 (100%)	87 (84%)	17 (16%)	3	15
9	I	105/105 (100%)	84 (80%)	21 (20%)	2	9
10	J	86/86 (100%)	72 (84%)	14 (16%)	3	15
11	K	90/90 (100%)	73 (81%)	17 (19%)	2	11
12	L	103/103 (100%)	82 (80%)	21 (20%)	2	8
13	M	92/92 (100%)	87 (95%)	5 (5%)	31	75
14	N	79/83 (95%)	72 (91%)	7 (9%)	14	49
15	O	76/76 (100%)	67 (88%)	9 (12%)	8	33
16	P	65/65 (100%)	57 (88%)	8 (12%)	7	31
17	Q	74/74 (100%)	58 (78%)	16 (22%)	1	7
18	R	48/48 (100%)	46 (96%)	2 (4%)	40	82
19	S	70/70 (100%)	61 (87%)	9 (13%)	6	28
20	T	65/65 (100%)	49 (75%)	16 (25%)	1	3
21	U	44/44 (100%)	33 (75%)	11 (25%)	1	3
All	All	1947/1951 (100%)	1631 (84%)	316 (16%)	3	15

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LYS
2	B	13	VAL
2	B	15	PHE
2	B	19	THR
2	B	20	ARG
2	B	22	TRP
2	B	30	ILE
2	B	36	LYS
2	B	38	HIS
2	B	42	LEU
2	B	56	LEU

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	67	LEU
2	B	73	ARG
2	B	86	CYS
2	B	87	ASP
2	B	88	GLN
2	B	90	PHE
2	B	94	ARG
2	B	100	LEU
2	B	102	ASN
2	B	108	GLN
2	B	112	ARG
2	B	115	ASP
2	B	116	LEU
2	B	119	GLN
2	B	125	PHE
2	B	128	LEU
2	B	130	LYS
2	B	141	GLU
2	B	143	LEU
2	B	156	LEU
2	B	170	ILE
2	B	185	ILE
2	B	206	ILE
2	B	207	ARG
2	B	209	VAL
2	B	219	THR
3	C	2	GLN
3	C	13	ILE
3	C	17	TRP
3	C	24	ASN
3	C	25	THR
3	C	26	LYS
3	C	28	PHE
3	C	32	LEU
3	C	35	ASP
3	C	36	PHE
3	C	42	LEU
3	C	50	SER
3	C	58	ARG
3	C	69	THR
3	C	79	LYS

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Mol	Chain	Res	Type
3	C	89	VAL
3	C	106	ARG
3	C	119	ILE
3	C	127	VAL
3	C	139	ASN
3	C	143	LEU
3	C	148	ILE
3	C	156	LEU
3	C	161	ILE
3	C	165	GLU
3	C	166	TRP
3	C	184	ASN
3	C	199	VAL
4	D	11	SER
4	D	19	PHE
4	D	21	LYS
4	D	25	ARG
4	D	30	LYS
4	D	31	CYS
4	D	43	ARG
4	D	52	VAL
4	D	54	LEU
4	D	55	ARG
4	D	57	LYS
4	D	58	GLN
4	D	69	ARG
4	D	88	ASN
4	D	99	ASN
4	D	115	GLN
4	D	122	ILE
4	D	127	ARG
4	D	131	ILE
4	D	147	LYS
4	D	160	LEU
4	D	166	LYS
4	D	170	LEU
4	D	178	GLU
4	D	193	ASP
4	D	205	LYS
5	E	10	LEU
5	E	11	GLN
5	E	14	LEU

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Mol	Chain	Res	Type
5	E	18	ASN
5	E	28	ARG
5	E	31	SER
5	E	68	ARG
5	E	75	LEU
5	E	79	THR
5	E	81	GLN
5	E	95	MET
5	E	96	GLN
5	E	100	GLU
5	E	113	VAL
5	E	116	VAL
5	E	119	VAL
5	E	121	ASN
5	E	123	LEU
5	E	135	VAL
5	E	136	VAL
5	E	141	ASP
5	E	155	LYS
5	E	156	ARG
6	F	14	GLN
6	F	17	GLN
6	F	24	ARG
6	F	29	ILE
6	F	38	ARG
6	F	46	GLN
6	F	54	LEU
6	F	55	HIS
6	F	68	GLN
6	F	69	GLU
6	F	77	THR
6	F	86	ARG
7	G	3	ARG
7	G	8	GLN
7	G	12	LEU
7	G	21	LEU
7	G	22	LEU
7	G	37	THR
7	G	47	GLU
7	G	62	GLU
7	G	68	VAL
7	G	83	THR

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Mol	Chain	Res	Type
7	G	85	GLN
7	G	93	VAL
7	G	105	GLU
7	G	117	LEU
7	G	123	LEU
7	G	143	MET
8	H	21	LYS
8	H	29	SER
8	H	30	LYS
8	H	64	TYR
8	H	65	PHE
8	H	72	GLU
8	H	76	ARG
8	H	79	ARG
8	H	82	LEU
8	H	86	LYS
8	H	89	ASP
8	H	98	LEU
8	H	100	ILE
8	H	110	MET
8	H	111	THR
8	H	120	LEU
8	H	128	VAL
9	I	4	GLN
9	I	21	LYS
9	I	28	VAL
9	I	35	GLU
9	I	37	TYR
9	I	42	THR
9	I	44	ARG
9	I	47	VAL
9	I	48	ARG
9	I	54	VAL
9	I	56	MET
9	I	62	LEU
9	I	67	LYS
9	I	87	MET
9	I	88	GLU
9	I	98	ARG
9	I	105	ARG
9	I	106	ASP
9	I	125	GLN

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Mol	Chain	Res	Type
9	I	126	PHE
9	I	128	LYS
10	J	6	ILE
10	J	22	THR
10	J	32	THR
10	J	35	GLN
10	J	48	ARG
10	J	49	PHE
10	J	50	THR
10	J	59	LYS
10	J	63	ASP
10	J	70	HIS
10	J	73	LEU
10	J	89	ARG
10	J	92	LEU
10	J	96	VAL
11	K	17	ASP
11	K	30	ILE
11	K	35	ASP
11	K	51	PHE
11	K	55	ARG
11	K	64	VAL
11	K	76	TYR
11	K	78	ILE
11	K	82	GLU
11	K	96	ILE
11	K	100	ASN
11	K	106	ILE
11	K	118	ASN
11	K	124	LYS
11	K	125	LYS
11	K	127	ARG
11	K	128	VAL
12	L	3	VAL
12	L	17	LYS
12	L	18	SER
12	L	20	VAL
12	L	26	CYS
12	L	34	THR
12	L	35	ARG
12	L	38	THR
12	L	41	PRO

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Mol	Chain	Res	Type
12	L	43	LYS
12	L	49	ARG
12	L	51	VAL
12	L	57	THR
12	L	63	THR
12	L	64	SER
12	L	74	GLN
12	L	87	LYS
12	L	88	ASP
12	L	94	TYR
12	L	104	SER
12	L	109	ARG
13	M	3	ILE
13	M	7	ASN
13	M	42	VAL
13	M	58	GLU
13	M	106	ARG
14	N	13	VAL
14	N	58	ARG
14	N	59	GLN
14	N	61	ASN
14	N	73	LEU
14	N	96	LYS
14	N	99	SER
15	O	16	ARG
15	O	34	GLN
15	O	57	ARG
15	O	63	ARG
15	O	65	LEU
15	O	67	ASP
15	O	80	LEU
15	O	84	LEU
15	O	86	LEU
16	P	6	LEU
16	P	19	VAL
16	P	33	ILE
16	P	46	LYS
16	P	55	ASP
16	P	63	GLN
16	P	68	SER
16	P	77	GLU
17	Q	3	LYS

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Mol	Chain	Res	Type
17	Q	16	MET
17	Q	20	ILE
17	Q	28	VAL
17	Q	29	LYS
17	Q	37	ILE
17	Q	47	ASP
17	Q	49	ASN
17	Q	50	ASN
17	Q	51	GLU
17	Q	54	ILE
17	Q	64	ARG
17	Q	74	LEU
17	Q	75	VAL
17	Q	78	VAL
17	Q	80	LYS
18	R	20	ILE
18	R	54	LEU
19	S	42	ASN
19	S	54	ARG
19	S	55	GLN
19	S	57	VAL
19	S	59	VAL
19	S	60	PHE
19	S	61	VAL
19	S	64	GLU
19	S	79	TYR
20	T	2	ASN
20	T	4	LYS
20	T	11	ILE
20	T	26	MET
20	T	27	MET
20	T	28	ARG
20	T	29	THR
20	T	33	LYS
20	T	35	TYR
20	T	38	ILE
20	T	42	ASP
20	T	53	MET
20	T	67	HIS
20	T	75	LYS
20	T	77	ASN
20	T	84	LYS

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Mol	Chain	Res	Type
21	U	4	LYS
21	U	8	ASN
21	U	9	GLU
21	U	10	PRO
21	U	15	LEU
21	U	18	PHE
21	U	27	VAL
21	U	33	ARG
21	U	37	TYR
21	U	38	GLU
21	U	42	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	44	HIS
17	Q	49	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1533 (99%)	478 (31%)	237 (15%)

All (478) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	7	A
1	A	8	A
1	A	9	G
1	A	14	U
1	A	22	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A

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Mol	Chain	Res	Type
1	A	51	A
1	A	52	C
1	A	61	G
1	A	65	A
1	A	66	A
1	A	67	C
1	A	70	U
1	A	71	A
1	A	72	A
1	A	73	C
1	A	74	A
1	A	75	G
1	A	76	G
1	A	77	A
1	A	79	G
1	A	82	G
1	A	83	C
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	89	U
1	A	90	C
1	A	91	U
1	A	92	U
1	A	93	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	97	G
1	A	98	A
1	A	109	A
1	A	110	C
1	A	116	A
1	A	119	A
1	A	120	A
1	A	121	U
1	A	122	G
1	A	127	G
1	A	130	A
1	A	131	A
1	A	132	C

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Mol	Chain	Res	Type
1	A	138	G
1	A	141	G
1	A	143	A
1	A	159	G
1	A	163	C
1	A	164	G
1	A	174	A
1	A	175	C
1	A	177	G
1	A	181	A
1	A	182	A
1	A	183	C
1	A	184	G
1	A	185	U
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	A
1	A	200	G
1	A	205	A
1	A	207	C
1	A	208	U
1	A	209	U
1	A	210	C
1	A	211	G
1	A	212	G
1	A	214	C
1	A	232	G
1	A	240	G
1	A	243	A
1	A	244	U
1	A	245	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	A
1	A	258	G
1	A	266	G
1	A	267	C
1	A	268	U
1	A	273	U

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Mol	Chain	Res	Type
1	A	274	A
1	A	275	G
1	A	276	G
1	A	279	A
1	A	285	C
1	A	289	G
1	A	299	G
1	A	305	G
1	A	306	A
1	A	307	C
1	A	308	C
1	A	316	C
1	A	320	A
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	368	U
1	A	369	G
1	A	373	A
1	A	374	A
1	A	384	G
1	A	388	G
1	A	389	A
1	A	390	U
1	A	392	C
1	A	406	G
1	A	409	U
1	A	411	A
1	A	412	A
1	A	413	G

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Mol	Chain	Res	Type
1	A	414	A
1	A	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	431	A
1	A	438	U
1	A	439	U
1	A	448	A
1	A	451	A
1	A	452	A
1	A	453	G
1	A	458	U
1	A	459	A
1	A	461	A
1	A	462	G
1	A	463	U
1	A	466	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	U
1	A	486	U
1	A	487	A
1	A	495	A
1	A	496	A
1	A	497	G
1	A	498	A
1	A	499	A
1	A	500	G
1	A	501	C
1	A	508	U
1	A	509	A
1	A	511	C
1	A	512	U

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Mol	Chain	Res	Type
1	A	513	C
1	A	518	C
1	A	519	C
1	A	520	A
1	A	524	G
1	A	527	G
1	A	532	A
1	A	533	A
1	A	534	U
1	A	535	A
1	A	536	C
1	A	537	G
1	A	538	G
1	A	548	G
1	A	549	C
1	A	550	G
1	A	556	C
1	A	559	A
1	A	560	A
1	A	562	U
1	A	563	A
1	A	564	C
1	A	566	G
1	A	567	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	579	A
1	A	588	G
1	A	595	A
1	A	596	A
1	A	597	G
1	A	604	G
1	A	633	G
1	A	642	A
1	A	649	A
1	A	653	U
1	A	654	G
1	A	655	A
1	A	663	A

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Mol	Chain	Res	Type
1	A	665	A
1	A	682	G
1	A	688	G
1	A	700	G
1	A	701	U
1	A	702	A
1	A	703	G
1	A	717	U
1	A	718	A
1	A	721	G
1	A	722	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	G
1	A	748	G
1	A	752	G
1	A	753	A
1	A	754	C
1	A	755	G
1	A	776	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	802	A
1	A	813	U
1	A	814	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	828	U
1	A	829	G
1	A	832	G
1	A	841	C
1	A	843	U
1	A	845	A
1	A	846	G
1	A	849	G
1	A	855	U

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Mol	Chain	Res	Type
1	A	859	G
1	A	861	G
1	A	870	U
1	A	871	U
1	A	874	G
1	A	875	U
1	A	884	U
1	A	885	G
1	A	889	A
1	A	890	G
1	A	914	A
1	A	915	A
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	936	C
1	A	960	U
1	A	961	U
1	A	965	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	983	A
1	A	984	C
1	A	985	C
1	A	989	U
1	A	992	U
1	A	993	G
1	A	995	C
1	A	1003	G
1	A	1004	A
1	A	1008	U

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Mol	Chain	Res	Type
1	A	1017	U
1	A	1018	G
1	A	1022	A
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1037	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1085	U
1	A	1086	U
1	A	1087	G
1	A	1088	G
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1102	A
1	A	1103	C
1	A	1104	G
1	A	1113	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1133	G
1	A	1135	U
1	A	1137	C
1	A	1138	G

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Mol	Chain	Res	Type
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1144	G
1	A	1145	A
1	A	1151	A
1	A	1152	A
1	A	1153	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1162	C
1	A	1167	A
1	A	1168	U
1	A	1169	A
1	A	1170	A
1	A	1178	G
1	A	1181	G
1	A	1182	G
1	A	1183	U
1	A	1184	G
1	A	1191	A
1	A	1192	C
1	A	1196	A
1	A	1197	A
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	U
1	A	1203	C
1	A	1212	U
1	A	1213	A
1	A	1224	U
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1229	A
1	A	1238	A

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Mol	Chain	Res	Type
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1242	G
1	A	1256	A
1	A	1257	A
1	A	1258	G
1	A	1259	C
1	A	1278	G
1	A	1279	G
1	A	1280	A
1	A	1282	C
1	A	1283	U
1	A	1284	C
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1293	C
1	A	1297	G
1	A	1299	A
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1308	U
1	A	1315	U
1	A	1316	G
1	A	1317	C
1	A	1318	A
1	A	1320	C
1	A	1321	U
1	A	1322	C
1	A	1323	G
1	A	1324	A
1	A	1332	A
1	A	1333	A
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1348	U
1	A	1349	A
1	A	1353	G
1	A	1362	A

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Mol	Chain	Res	Type
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1371	G
1	A	1380	U
1	A	1381	U
1	A	1382	C
1	A	1394	A
1	A	1395	C
1	A	1396	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	C
1	A	1402	C
1	A	1408	A
1	A	1432	G
1	A	1433	A
1	A	1441	A
1	A	1446	A
1	A	1448	C
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1455	G
1	A	1469	C
1	A	1470	U
1	A	1490	U
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1529	G
1	A	1530	G

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Mol	Chain	Res	Type
1	A	1531	A
1	A	1532	U

All (237) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	13	U
1	A	30	U
1	A	32	A
1	A	47	C
1	A	51	A
1	A	52	C
1	A	60	A
1	A	61	G
1	A	64	G
1	A	66	A
1	A	71	A
1	A	73	C
1	A	74	A
1	A	85	U
1	A	87	C
1	A	91	U
1	A	92	U
1	A	94	G
1	A	95	C
1	A	97	G
1	A	109	A
1	A	115	G
1	A	116	A
1	A	119	A
1	A	121	U
1	A	129	A
1	A	131	A
1	A	173	U
1	A	174	A
1	A	181	A
1	A	184	G
1	A	197	A
1	A	198	G
1	A	199	A
1	A	243	A

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Mol	Chain	Res	Type
1	A	245	U
1	A	246	A
1	A	250	A
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	274	A
1	A	275	G
1	A	279	A
1	A	305	G
1	A	306	A
1	A	315	A
1	A	327	A
1	A	330	C
1	A	331	G
1	A	344	A
1	A	346	G
1	A	347	G
1	A	351	G
1	A	352	C
1	A	366	A
1	A	368	U
1	A	372	C
1	A	373	A
1	A	388	G
1	A	389	A
1	A	411	A
1	A	414	A
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	U
1	A	451	A
1	A	452	A
1	A	466	A
1	A	468	A
1	A	484	G
1	A	486	U
1	A	487	A

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Mol	Chain	Res	Type
1	A	495	A
1	A	496	A
1	A	497	G
1	A	499	A
1	A	500	G
1	A	508	U
1	A	509	A
1	A	511	C
1	A	512	U
1	A	517	G
1	A	519	C
1	A	531	U
1	A	534	U
1	A	535	A
1	A	536	C
1	A	537	G
1	A	547	A
1	A	548	G
1	A	549	C
1	A	559	A
1	A	563	A
1	A	564	C
1	A	566	G
1	A	575	G
1	A	577	G
1	A	595	A
1	A	596	A
1	A	641	U
1	A	642	A
1	A	653	U
1	A	654	G
1	A	686	U
1	A	688	G
1	A	701	U
1	A	704	A
1	A	717	U
1	A	718	A
1	A	721	G
1	A	722	G
1	A	723	U
1	A	724	G
1	A	752	G

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Mol	Chain	Res	Type
1	A	754	C
1	A	755	G
1	A	792	A
1	A	794	A
1	A	812	G
1	A	813	U
1	A	815	A
1	A	816	A
1	A	817	C
1	A	821	G
1	A	870	U
1	A	874	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	891	U
1	A	913	A
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	965	U
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	991	U
1	A	994	A
1	A	1049	U
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1066	C
1	A	1068	G

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Mol	Chain	Res	Type
1	A	1085	U
1	A	1087	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1136	C
1	A	1138	G
1	A	1141	C
1	A	1142	G
1	A	1151	A
1	A	1152	A
1	A	1157	A
1	A	1158	C
1	A	1161	C
1	A	1168	U
1	A	1169	A
1	A	1181	G
1	A	1183	U
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	A
1	A	1197	A
1	A	1200	C
1	A	1201	A
1	A	1202	U
1	A	1215	G
1	A	1224	U
1	A	1228	C
1	A	1229	A
1	A	1239	A
1	A	1241	G
1	A	1256	A
1	A	1258	G
1	A	1282	C
1	A	1283	U
1	A	1297	G
1	A	1303	C

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Mol	Chain	Res	Type
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1332	A
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1345	U
1	A	1348	U
1	A	1362	A
1	A	1365	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1395	C
1	A	1396	A
1	A	1398	A
1	A	1399	C
1	A	1432	G
1	A	1447	A
1	A	1448	C
1	A	1451	U
1	A	1453	G
1	A	1454	G
1	A	1498	U
1	A	1502	A
1	A	1505	G
1	A	1506	U
1	A	1528	U
1	A	1530	G
1	A	1531	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 43 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.