Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2014 – 03:52 PM EDT

PDB ID   : 4KTG
Title   : Crystal structure of double-helical GGC-repetitive RNA 19mer complexed with RSS p19
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Deposited on : 2013-05-20
Resolution : 1.92 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 1.92 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		13
Ramachandran outliers		0.9%
Sidechain outliers		2.8%
RSRZ outliers		6.8%
RNA backbone		0.58

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
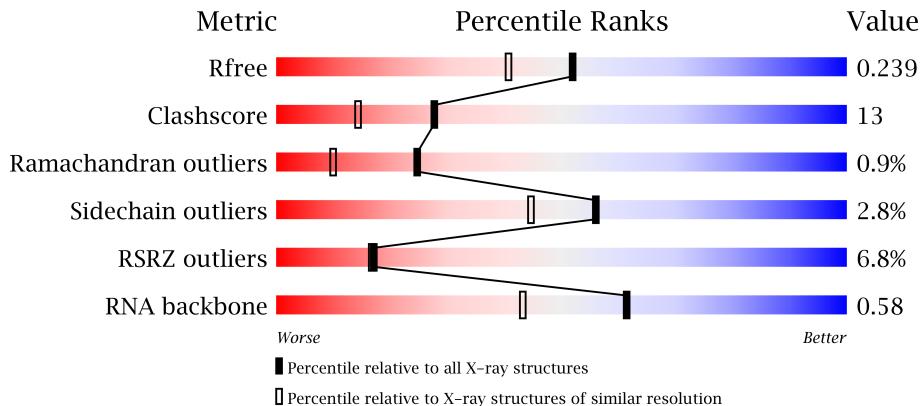
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)
RNA backbone	1838	1001 (2.92-0.96)

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.

Mol	Chain	Length	Quality of chain
1	A	127	
2	B	19	
2	E	19	
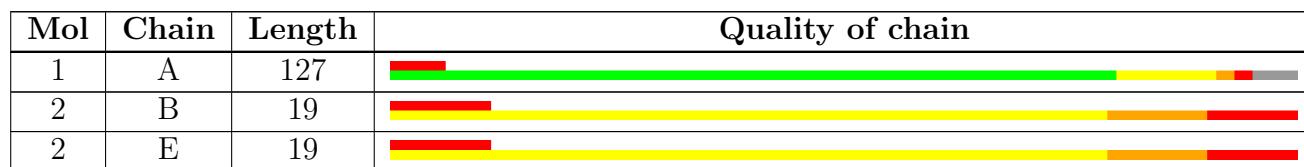
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	601	-	X
3	SO4	A	602	-	X
3	SO4	A	603	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1994 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 protein called RNA silencing suppressor p19.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	5	0
			993	628	176	185	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P69517
A	2	SER	-	EXPRESSION TAG	UNP P69517
A	3	HIS	-	EXPRESSION TAG	UNP P69517
A	4	MET	-	EXPRESSION TAG	UNP P69517

- Molecule 2 is a RNA chain called 5'-R(P*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP* GP*GP*CP*GP*GP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	P	0	1	0
			430	188	81	141	20			
2	E	19	Total	C	N	O	P	0	1	0
			430	188	81	141	20			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻——S——O⁻ O4

S

O

O2
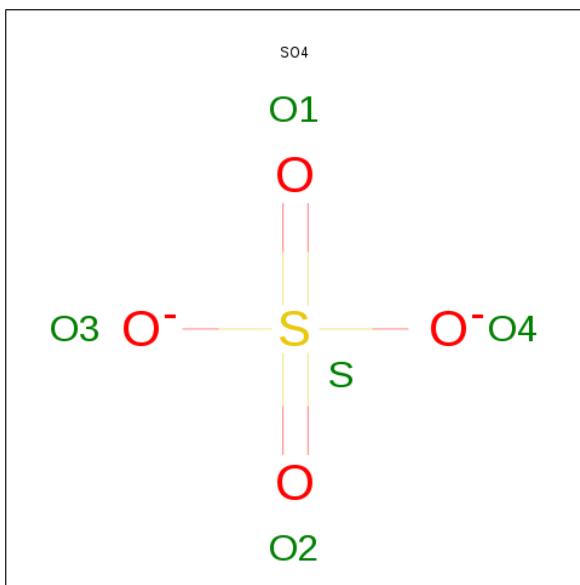
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total O S 5 4 1			0	0
3	A	1	Total O S 5 4 1			0	0
3	A	1	Total O S 5 4 1			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total O 101 101		0	0
4	B	22	Total O 22 22		0	0
4	E	3	Total O 3 3		0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

3 Residue-property plots (i)

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.

• Molecule 1: RNA silencing suppressor p19

Chain A:
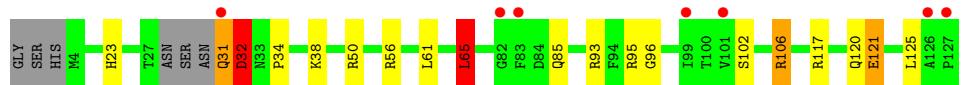
• Molecule 2: 5'-R(P*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP *GP*C)-3'

Chain B:

• Molecule 2: 5'-R(P*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP*GP*GP*CP *GP*C)-3'

Chain E:
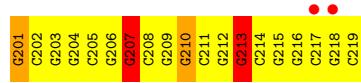
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	91.09Å 91.09Å 148.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 1.92 38.11 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-1.92) 99.1 (38.11-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.235 0.195 , 0.239	Depositor DCC
R_{free} test set	933 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Outliers	0 of 18239 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1994	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.19	0/1044	1.09	5/1406 (0.4%)
2	B	0.73	2/493 (0.4%)	0.95	2/767 (0.3%)
2	E	0.73	2/493 (0.4%)	0.97	2/767 (0.3%)
All	All	0.99	4/2030 (0.2%)	1.03	9/2940 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201[A]	G	OP3-P	-9.30	1.50	1.61
2	E	201[B]	G	OP3-P	-9.30	1.50	1.61
2	B	201[A]	G	OP3-P	-9.28	1.50	1.61
2	B	201[B]	G	OP3-P	-9.28	1.50	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	G	O5'-P-OP1	-9.91	96.78	105.70
2	E	213	G	O5'-P-OP1	-9.86	96.83	105.70
1	A	65	LEU	CB-CG-CD1	6.77	122.51	111.00
1	A	93	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	32	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	106	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	B	207	G	C2'-C3'-O3'	5.27	122.13	113.70
2	E	207	G	C2'-C3'-O3'	5.22	122.05	113.70
1	A	106	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	993	0	960	26	0
2	B	430	0	213	10	1420
2	E	430	0	213	5	1422
3	A	15	0	0	3	0
4	A	101	0	0	8	1
4	B	22	0	0	2	1
4	E	3	0	0	0	0
All	All	1994	0	1386	40	1422

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 13.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:201[B]:G:OP1	4:B:314:HOH:O	1.73	1.04
1:A:38[B]:LYS:NZ	4:A:744:HOH:O	2.04	0.91
1:A:31:GLN:HG2	1:A:95:ARG:HA	1.53	0.91
1:A:38[B]:LYS:CE	4:A:744:HOH:O	2.30	0.79
1:A:85:GLN:HE21	1:A:106:ARG:H	1.30	0.78
2:E:213:G:N3	2:E:213:G:H5"	1.99	0.78
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.50	0.77
1:A:31:GLN:HG3	1:A:34:PRO:HG3	1.67	0.77
4:A:744:HOH:O	2:B:201[B]:G:OP3	2.05	0.75
2:B:213:G:N3	2:B:213:G:H5"	2.01	0.74
1:A:31:GLN:OE1	3:A:603:SO4:O2	2.07	0.71
2:B:201[B]:G:P	4:B:314:HOH:O	2.42	0.68
1:A:96:GLY:N	3:A:603:SO4:O2	2.26	0.65
1:A:23:HIS:HD2	4:A:710:HOH:O	1.86	0.59
1:A:38[B]:LYS:HE2	4:A:744:HOH:O	1.98	0.58
1:A:31:GLN:O	1:A:32:ASP:HB2	2.04	0.57
1:A:31:GLN:HG2	1:A:95:ARG:CA	2.29	0.57
2:E:213:G:N3	2:E:213:G:C5'	2.68	0.57
1:A:85:GLN:NE2	1:A:106:ARG:HB2	2.21	0.55
2:B:204:G:H2'	2:B:205:C:H5'	1.87	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:GLN:HB2	1:A:34:PRO:HB3	1.88	0.54
2:B:213:G:N3	2:B:213:G:C5'	2.70	0.53
1:A:61:LEU:HG	1:A:65:LEU:HD22	1.91	0.52
1:A:31:GLN:OE1	3:A:603:SO4:S	2.69	0.51
2:E:204:G:H2'	2:E:205:C:H5'	1.95	0.48
1:A:95:ARG:NH2	1:A:125:LEU:O	2.47	0.47
2:B:204:G:C2'	2:B:205:C:H5'	2.44	0.47
1:A:117:ARG:HH11	1:A:117:ARG:CG	2.25	0.46
1:A:38[A]:LYS:HD2	1:A:50:ARG:O	2.15	0.46
1:A:56:ARG:HD3	4:A:750:HOH:O	2.16	0.44
1:A:32:ASP:HA	1:A:95:ARG:CD	2.48	0.43
1:A:121:GLU:CD	4:A:794:HOH:O	2.57	0.43
2:E:212:G:H2'	2:E:213:G:H5"	2.00	0.43
2:B:212:G:H2'	2:B:213:G:H5"	2.01	0.42
1:A:102[B]:SER:HB2	2:B:212:G:H4'	2.01	0.42
2:B:209:G:H2'	2:B:210:G:C8	2.55	0.41
1:A:65:LEU:HD11	1:A:120[B]:GLN:HG3	2.02	0.41
1:A:117:ARG:NH1	1:A:117:ARG:HG3	2.28	0.41
1:A:38[A]:LYS:NZ	4:A:737:HOH:O	2.51	0.41
2:E:204:G:N3	2:E:204:G:O4'	2.55	0.40

All (1422) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:201[A]:G:OP1	2:E:201[A]:G:OP1[4_555]	0.04	2.16
2:B:201[A]:G:P	2:E:201[A]:G:P[4_555]	0.05	2.15
2:B:201[A]:G:O5'	2:E:201[A]:G:O5'[4_555]	0.05	2.15
2:B:201[A]:G:OP3	2:E:201[A]:G:OP3[4_555]	0.06	2.14
2:B:201[B]:G:OP1	2:E:201[B]:G:OP1[4_555]	0.06	2.14
2:B:201[A]:G:OP2	2:E:201[A]:G:OP2[4_555]	0.06	2.14
2:B:201[A]:G:C5'	2:E:201[A]:G:C5'[4_555]	0.06	2.14
2:B:201[A]:G:O4'	2:E:201[A]:G:O4'[4_555]	0.06	2.14
2:B:201[B]:G:O4'	2:E:201[B]:G:O4'[4_555]	0.06	2.14
2:B:201[A]:G:C1'	2:E:201[A]:G:C1'[4_555]	0.06	2.14
2:B:201[B]:G:C1'	2:E:201[B]:G:C1'[4_555]	0.06	2.14
2:B:201[B]:G:P	2:E:201[B]:G:P[4_555]	0.07	2.13
2:B:201[B]:G:O5'	2:E:201[B]:G:O5'[4_555]	0.07	2.13
2:B:201[B]:G:C5'	2:E:201[B]:G:C5'[4_555]	0.07	2.13
2:B:201[A]:G:C4'	2:E:201[A]:G:C4'[4_555]	0.07	2.13
2:B:201[B]:G:C4'	2:E:201[B]:G:C4'[4_555]	0.07	2.13
2:B:201[A]:G:C3'	2:E:201[A]:G:C3'[4_555]	0.07	2.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:201[B]:G:C3'	2:E:201[B]:G:C3'[4_555]	0.07	2.13
2:B:201[A]:G:O3'	2:E:201[A]:G:O3'[4_555]	0.07	2.13
2:B:201[B]:G:O3'	2:E:201[B]:G:O3'[4_555]	0.07	2.13
2:B:201[A]:G:C2'	2:E:201[A]:G:C2'[4_555]	0.07	2.13
2:B:201[B]:G:C2'	2:E:201[B]:G:C2'[4_555]	0.07	2.13
2:B:201[A]:G:O2'	2:E:201[A]:G:O2'[4_555]	0.07	2.13
2:B:201[B]:G:O2'	2:E:201[B]:G:O2'[4_555]	0.07	2.13
2:B:202:C:OP2	2:E:202:C:OP2[4_555]	0.07	2.13
2:B:203:G:OP2	2:E:203:G:OP2[4_555]	0.07	2.13
2:B:209:G:O6	2:E:209:G:O6[4_555]	0.07	2.13
2:B:214:C:OP1	2:E:214:C:OP1[4_555]	0.07	2.13
2:B:201[B]:G:OP3	2:E:201[B]:G:OP3[4_555]	0.08	2.12
2:B:201[B]:G:OP2	2:E:201[B]:G:OP2[4_555]	0.08	2.12
2:B:202:C:P	2:E:202:C:P[4_555]	0.08	2.12
2:B:202:C:OP1	2:E:202:C:OP1[4_555]	0.08	2.12
2:B:202:C:O5'	2:E:202:C:O5'[4_555]	0.08	2.12
2:B:202:C:C5'	2:E:202:C:C5'[4_555]	0.08	2.12
2:B:202:C:C4'	2:E:202:C:C4'[4_555]	0.08	2.12
2:B:202:C:O4'	2:E:202:C:O4'[4_555]	0.08	2.12
2:B:202:C:C3'	2:E:202:C:C3'[4_555]	0.08	2.12
2:B:202:C:O3'	2:E:202:C:O3'[4_555]	0.08	2.12
2:B:202:C:C2'	2:E:202:C:C2'[4_555]	0.08	2.12
2:B:202:C:O2'	2:E:202:C:O2'[4_555]	0.08	2.12
2:B:202:C:C1'	2:E:202:C:C1'[4_555]	0.08	2.12
2:B:202:C:N1	2:E:202:C:N1[4_555]	0.08	2.12
2:B:202:C:C2	2:E:202:C:C2[4_555]	0.08	2.12
2:B:202:C:O2	2:E:202:C:O2[4_555]	0.08	2.12
2:B:202:C:N3	2:E:202:C:N3[4_555]	0.08	2.12
2:B:202:C:C4	2:E:202:C:C4[4_555]	0.08	2.12
2:B:202:C:N4	2:E:202:C:N4[4_555]	0.08	2.12
2:B:202:C:C5	2:E:202:C:C5[4_555]	0.08	2.12
2:B:202:C:C6	2:E:202:C:C6[4_555]	0.08	2.12
2:B:203:G:P	2:E:203:G:P[4_555]	0.08	2.12
2:B:203:G:OP1	2:E:203:G:OP1[4_555]	0.08	2.12
2:B:203:G:O5'	2:E:203:G:O5'[4_555]	0.08	2.12
2:B:203:G:C5'	2:E:203:G:C5'[4_555]	0.08	2.12
2:B:203:G:C8	2:E:203:G:C8[4_555]	0.08	2.12
2:B:203:G:N7	2:E:203:G:N7[4_555]	0.08	2.12
2:B:203:G:C5	2:E:203:G:C5[4_555]	0.08	2.12
2:B:203:G:C6	2:E:203:G:C6[4_555]	0.08	2.12
2:B:203:G:O6	2:E:203:G:O6[4_555]	0.08	2.12
2:B:203:G:N1	2:E:203:G:N1[4_555]	0.08	2.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:204:G:OP2	2:E:204:G:OP2[4_555]	0.08	2.12
2:B:204:G:C5	2:E:204:G:C5[4_555]	0.08	2.12
2:B:204:G:C6	2:E:204:G:C6[4_555]	0.08	2.12
2:B:204:G:O6	2:E:204:G:O6[4_555]	0.08	2.12
2:B:204:G:N1	2:E:204:G:N1[4_555]	0.08	2.12
2:B:204:G:C2	2:E:204:G:C2[4_555]	0.08	2.12
2:B:205:C:N4	2:E:205:C:N4[4_555]	0.08	2.12
2:B:207:G:O6	2:E:207:G:O6[4_555]	0.08	2.12
2:B:209:G:C5'	2:E:209:G:C5'[4_555]	0.08	2.12
2:B:209:G:N9	2:E:209:G:N9[4_555]	0.08	2.12
2:B:209:G:N7	2:E:209:G:N7[4_555]	0.08	2.12
2:B:209:G:C5	2:E:209:G:C5[4_555]	0.08	2.12
2:B:209:G:C6	2:E:209:G:C6[4_555]	0.08	2.12
2:B:209:G:N1	2:E:209:G:N1[4_555]	0.08	2.12
2:B:209:G:C2	2:E:209:G:C2[4_555]	0.08	2.12
2:B:209:G:N2	2:E:209:G:N2[4_555]	0.08	2.12
2:B:219:C:O5'	2:E:219:C:O5'[4_555]	0.08	2.12
2:B:203:G:C4'	2:E:203:G:C4'[4_555]	0.09	2.11
2:B:203:G:O4'	2:E:203:G:O4'[4_555]	0.09	2.11
2:B:203:G:C3'	2:E:203:G:C3'[4_555]	0.09	2.11
2:B:203:G:O3'	2:E:203:G:O3'[4_555]	0.09	2.11
2:B:203:G:C2'	2:E:203:G:C2'[4_555]	0.09	2.11
2:B:203:G:O2'	2:E:203:G:O2'[4_555]	0.09	2.11
2:B:203:G:C1'	2:E:203:G:C1'[4_555]	0.09	2.11
2:B:203:G:N9	2:E:203:G:N9[4_555]	0.09	2.11
2:B:203:G:C2	2:E:203:G:C2[4_555]	0.09	2.11
2:B:203:G:N2	2:E:203:G:N2[4_555]	0.09	2.11
2:B:203:G:N3	2:E:203:G:N3[4_555]	0.09	2.11
2:B:203:G:C4	2:E:203:G:C4[4_555]	0.09	2.11
2:B:204:G:P	2:E:204:G:P[4_555]	0.09	2.11
2:B:204:G:OP1	2:E:204:G:OP1[4_555]	0.09	2.11
2:B:204:G:O5'	2:E:204:G:O5'[4_555]	0.09	2.11
2:B:204:G:C5'	2:E:204:G:C5'[4_555]	0.09	2.11
2:B:204:G:C4'	2:E:204:G:C4'[4_555]	0.09	2.11
2:B:204:G:O4'	2:E:204:G:O4'[4_555]	0.09	2.11
2:B:204:G:O3'	2:E:204:G:O3'[4_555]	0.09	2.11
2:B:204:G:C1'	2:E:204:G:C1'[4_555]	0.09	2.11
2:B:204:G:N9	2:E:204:G:N9[4_555]	0.09	2.11
2:B:204:G:C8	2:E:204:G:C8[4_555]	0.09	2.11
2:B:204:G:N7	2:E:204:G:N7[4_555]	0.09	2.11
2:B:204:G:N2	2:E:204:G:N2[4_555]	0.09	2.11
2:B:204:G:N3	2:E:204:G:N3[4_555]	0.09	2.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:204:G:C4	2:E:204:G:C4[4_555]	0.09	2.11
2:B:205:C:OP2	2:E:205:C:OP2[4_555]	0.09	2.11
2:B:206:G:N7	2:E:206:G:N7[4_555]	0.09	2.11
2:B:206:G:C5	2:E:206:G:C5[4_555]	0.09	2.11
2:B:206:G:C6	2:E:206:G:C6[4_555]	0.09	2.11
2:B:206:G:O6	2:E:206:G:O6[4_555]	0.09	2.11
2:B:207:G:C8	2:E:207:G:C8[4_555]	0.09	2.11
2:B:207:G:N7	2:E:207:G:N7[4_555]	0.09	2.11
2:B:207:G:C5	2:E:207:G:C5[4_555]	0.09	2.11
2:B:207:G:C6	2:E:207:G:C6[4_555]	0.09	2.11
2:B:207:G:N1	2:E:207:G:N1[4_555]	0.09	2.11
2:B:207:G:C2	2:E:207:G:C2[4_555]	0.09	2.11
2:B:207:G:N2	2:E:207:G:N2[4_555]	0.09	2.11
2:B:207:G:C4	2:E:207:G:C4[4_555]	0.09	2.11
2:B:208:C:N1	2:E:208:C:N1[4_555]	0.09	2.11
2:B:208:C:C4	2:E:208:C:C4[4_555]	0.09	2.11
2:B:208:C:N4	2:E:208:C:N4[4_555]	0.09	2.11
2:B:209:G:C4'	2:E:209:G:C4'[4_555]	0.09	2.11
2:B:209:G:O4'	2:E:209:G:O4'[4_555]	0.09	2.11
2:B:209:G:C8	2:E:209:G:C8[4_555]	0.09	2.11
2:B:209:G:N3	2:E:209:G:N3[4_555]	0.09	2.11
2:B:209:G:C4	2:E:209:G:C4[4_555]	0.09	2.11
2:B:210:G:P	2:E:210:G:P[4_555]	0.09	2.11
2:B:212:G:P	2:E:212:G:P[4_555]	0.09	2.11
2:B:212:G:OP2	2:E:212:G:OP2[4_555]	0.09	2.11
2:B:212:G:C5'	2:E:212:G:C5'[4_555]	0.09	2.11
2:B:212:G:C4'	2:E:212:G:C4'[4_555]	0.09	2.11
2:B:212:G:O4'	2:E:212:G:O4'[4_555]	0.09	2.11
2:B:213:G:O4'	2:E:213:G:O4'[4_555]	0.09	2.11
2:B:213:G:O3'	2:E:213:G:O3'[4_555]	0.09	2.11
2:B:213:G:C6	2:E:213:G:C6[4_555]	0.09	2.11
2:B:213:G:O6	2:E:213:G:O6[4_555]	0.09	2.11
2:B:213:G:N1	2:E:213:G:N1[4_555]	0.09	2.11
2:B:213:G:C2	2:E:213:G:C2[4_555]	0.09	2.11
2:B:213:G:N2	2:E:213:G:N2[4_555]	0.09	2.11
2:B:214:C:P	2:E:214:C:P[4_555]	0.09	2.11
2:B:215:G:O6	2:E:215:G:O6[4_555]	0.09	2.11
2:B:217:C:N3	2:E:217:C:N3[4_555]	0.09	2.11
2:B:217:C:N4	2:E:217:C:N4[4_555]	0.09	2.11
2:B:218:G:C6	2:E:218:G:C6[4_555]	0.09	2.11
2:B:218:G:O6	2:E:218:G:O6[4_555]	0.09	2.11
2:B:219:C:C2	2:E:219:C:C2[4_555]	0.09	2.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:219:C:O2	2:E:219:C:O2[4_555]	0.09	2.11
2:B:219:C:N3	2:E:219:C:N3[4_555]	0.09	2.11
2:B:219:C:N4	2:E:219:C:N4[4_555]	0.09	2.11
2:B:204:G:C3'	2:E:204:G:C3'[4_555]	0.10	2.10
2:B:204:G:C2'	2:E:204:G:C2'[4_555]	0.10	2.10
2:B:204:G:O2'	2:E:204:G:O2'[4_555]	0.10	2.10
2:B:205:C:P	2:E:205:C:P[4_555]	0.10	2.10
2:B:205:C:OP1	2:E:205:C:OP1[4_555]	0.10	2.10
2:B:206:G:O4'	2:E:206:G:O4'[4_555]	0.10	2.10
2:B:206:G:C2'	2:E:206:G:C2'[4_555]	0.10	2.10
2:B:206:G:C1'	2:E:206:G:C1'[4_555]	0.10	2.10
2:B:206:G:N9	2:E:206:G:N9[4_555]	0.10	2.10
2:B:206:G:C8	2:E:206:G:C8[4_555]	0.10	2.10
2:B:206:G:N1	2:E:206:G:N1[4_555]	0.10	2.10
2:B:206:G:C2	2:E:206:G:C2[4_555]	0.10	2.10
2:B:206:G:N2	2:E:206:G:N2[4_555]	0.10	2.10
2:B:206:G:N3	2:E:206:G:N3[4_555]	0.10	2.10
2:B:206:G:C4	2:E:206:G:C4[4_555]	0.10	2.10
2:B:207:G:OP2	2:E:207:G:OP2[4_555]	0.10	2.10
2:B:207:G:O4'	2:E:207:G:O4'[4_555]	0.10	2.10
2:B:207:G:C3'	2:E:207:G:C3'[4_555]	0.10	2.10
2:B:207:G:C2'	2:E:207:G:C2'[4_555]	0.10	2.10
2:B:207:G:C1'	2:E:207:G:C1'[4_555]	0.10	2.10
2:B:207:G:N9	2:E:207:G:N9[4_555]	0.10	2.10
2:B:207:G:N3	2:E:207:G:N3[4_555]	0.10	2.10
2:B:208:C:C5'	2:E:208:C:C5'[4_555]	0.10	2.10
2:B:208:C:C4'	2:E:208:C:C4'[4_555]	0.10	2.10
2:B:208:C:O4'	2:E:208:C:O4'[4_555]	0.10	2.10
2:B:208:C:C3'	2:E:208:C:C3'[4_555]	0.10	2.10
2:B:208:C:O3'	2:E:208:C:O3'[4_555]	0.10	2.10
2:B:208:C:C2'	2:E:208:C:C2'[4_555]	0.10	2.10
2:B:208:C:O2'	2:E:208:C:O2'[4_555]	0.10	2.10
2:B:208:C:C1'	2:E:208:C:C1'[4_555]	0.10	2.10
2:B:208:C:C2	2:E:208:C:C2[4_555]	0.10	2.10
2:B:208:C:O2	2:E:208:C:O2[4_555]	0.10	2.10
2:B:208:C:N3	2:E:208:C:N3[4_555]	0.10	2.10
2:B:208:C:C5	2:E:208:C:C5[4_555]	0.10	2.10
2:B:208:C:C6	2:E:208:C:C6[4_555]	0.10	2.10
2:B:209:G:P	2:E:209:G:P[4_555]	0.10	2.10
2:B:209:G:OP1	2:E:209:G:OP1[4_555]	0.10	2.10
2:B:209:G:O5'	2:E:209:G:O5'[4_555]	0.10	2.10
2:B:211:C:O5'	2:E:211:C:O5'[4_555]	0.10	2.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:211:C:C5'	2:E:211:C:C5'[4_555]	0.10	2.10
2:B:211:C:C4'	2:E:211:C:C4'[4_555]	0.10	2.10
2:B:211:C:O4'	2:E:211:C:O4'[4_555]	0.10	2.10
2:B:211:C:C3'	2:E:211:C:C3'[4_555]	0.10	2.10
2:B:211:C:O3'	2:E:211:C:O3'[4_555]	0.10	2.10
2:B:211:C:C2'	2:E:211:C:C2'[4_555]	0.10	2.10
2:B:211:C:C1'	2:E:211:C:C1'[4_555]	0.10	2.10
2:B:211:C:N1	2:E:211:C:N1[4_555]	0.10	2.10
2:B:211:C:C2	2:E:211:C:C2[4_555]	0.10	2.10
2:B:211:C:O2	2:E:211:C:O2[4_555]	0.10	2.10
2:B:211:C:N3	2:E:211:C:N3[4_555]	0.10	2.10
2:B:211:C:C4	2:E:211:C:C4[4_555]	0.10	2.10
2:B:211:C:N4	2:E:211:C:N4[4_555]	0.10	2.10
2:B:211:C:C5	2:E:211:C:C5[4_555]	0.10	2.10
2:B:211:C:C6	2:E:211:C:C6[4_555]	0.10	2.10
2:B:212:G:OP1	2:E:212:G:OP1[4_555]	0.10	2.10
2:B:212:G:O5'	2:E:212:G:O5'[4_555]	0.10	2.10
2:B:212:G:C3'	2:E:212:G:C3'[4_555]	0.10	2.10
2:B:212:G:C2'	2:E:212:G:C2'[4_555]	0.10	2.10
2:B:212:G:O2'	2:E:212:G:O2'[4_555]	0.10	2.10
2:B:212:G:C1'	2:E:212:G:C1'[4_555]	0.10	2.10
2:B:212:G:N9	2:E:212:G:N9[4_555]	0.10	2.10
2:B:212:G:C8	2:E:212:G:C8[4_555]	0.10	2.10
2:B:212:G:N7	2:E:212:G:N7[4_555]	0.10	2.10
2:B:212:G:C5	2:E:212:G:C5[4_555]	0.10	2.10
2:B:212:G:C6	2:E:212:G:C6[4_555]	0.10	2.10
2:B:212:G:O6	2:E:212:G:O6[4_555]	0.10	2.10
2:B:212:G:N1	2:E:212:G:N1[4_555]	0.10	2.10
2:B:212:G:C2	2:E:212:G:C2[4_555]	0.10	2.10
2:B:212:G:N2	2:E:212:G:N2[4_555]	0.10	2.10
2:B:212:G:N3	2:E:212:G:N3[4_555]	0.10	2.10
2:B:212:G:C4	2:E:212:G:C4[4_555]	0.10	2.10
2:B:213:G:C5'	2:E:213:G:C5'[4_555]	0.10	2.10
2:B:213:G:C4'	2:E:213:G:C4'[4_555]	0.10	2.10
2:B:213:G:C3'	2:E:213:G:C3'[4_555]	0.10	2.10
2:B:213:G:C2'	2:E:213:G:C2'[4_555]	0.10	2.10
2:B:213:G:C1'	2:E:213:G:C1'[4_555]	0.10	2.10
2:B:213:G:N9	2:E:213:G:N9[4_555]	0.10	2.10
2:B:213:G:C8	2:E:213:G:C8[4_555]	0.10	2.10
2:B:213:G:N7	2:E:213:G:N7[4_555]	0.10	2.10
2:B:213:G:C5	2:E:213:G:C5[4_555]	0.10	2.10
2:B:213:G:N3	2:E:213:G:N3[4_555]	0.10	2.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:213:G:C4	2:E:213:G:C4[4_555]	0.10	2.10
2:B:214:C:O5'	2:E:214:C:O5'[4_555]	0.10	2.10
2:B:215:G:C8	2:E:215:G:C8[4_555]	0.10	2.10
2:B:215:G:N7	2:E:215:G:N7[4_555]	0.10	2.10
2:B:215:G:C5	2:E:215:G:C5[4_555]	0.10	2.10
2:B:215:G:C6	2:E:215:G:C6[4_555]	0.10	2.10
2:B:215:G:N1	2:E:215:G:N1[4_555]	0.10	2.10
2:B:216:G:C6	2:E:216:G:C6[4_555]	0.10	2.10
2:B:216:G:O6	2:E:216:G:O6[4_555]	0.10	2.10
2:B:216:G:N1	2:E:216:G:N1[4_555]	0.10	2.10
2:B:216:G:C2	2:E:216:G:C2[4_555]	0.10	2.10
2:B:216:G:N2	2:E:216:G:N2[4_555]	0.10	2.10
2:B:216:G:N3	2:E:216:G:N3[4_555]	0.10	2.10
2:B:217:C:O4'	2:E:217:C:O4'[4_555]	0.10	2.10
2:B:217:C:C3'	2:E:217:C:C3'[4_555]	0.10	2.10
2:B:217:C:O3'	2:E:217:C:O3'[4_555]	0.10	2.10
2:B:217:C:C2'	2:E:217:C:C2'[4_555]	0.10	2.10
2:B:217:C:C1'	2:E:217:C:C1'[4_555]	0.10	2.10
2:B:217:C:N1	2:E:217:C:N1[4_555]	0.10	2.10
2:B:217:C:C2	2:E:217:C:C2[4_555]	0.10	2.10
2:B:217:C:O2	2:E:217:C:O2[4_555]	0.10	2.10
2:B:217:C:C4	2:E:217:C:C4[4_555]	0.10	2.10
2:B:217:C:C5	2:E:217:C:C5[4_555]	0.10	2.10
2:B:217:C:C6	2:E:217:C:C6[4_555]	0.10	2.10
2:B:218:G:P	2:E:218:G:P[4_555]	0.10	2.10
2:B:218:G:OP1	2:E:218:G:OP1[4_555]	0.10	2.10
2:B:218:G:OP2	2:E:218:G:OP2[4_555]	0.10	2.10
2:B:218:G:O5'	2:E:218:G:O5'[4_555]	0.10	2.10
2:B:218:G:C5'	2:E:218:G:C5'[4_555]	0.10	2.10
2:B:218:G:N9	2:E:218:G:N9[4_555]	0.10	2.10
2:B:218:G:C8	2:E:218:G:C8[4_555]	0.10	2.10
2:B:218:G:N7	2:E:218:G:N7[4_555]	0.10	2.10
2:B:218:G:C5	2:E:218:G:C5[4_555]	0.10	2.10
2:B:218:G:N1	2:E:218:G:N1[4_555]	0.10	2.10
2:B:218:G:C2	2:E:218:G:C2[4_555]	0.10	2.10
2:B:218:G:N2	2:E:218:G:N2[4_555]	0.10	2.10
2:B:218:G:N3	2:E:218:G:N3[4_555]	0.10	2.10
2:B:218:G:C4	2:E:218:G:C4[4_555]	0.10	2.10
2:B:219:C:C5'	2:E:219:C:C5'[4_555]	0.10	2.10
2:B:219:C:C4'	2:E:219:C:C4'[4_555]	0.10	2.10
2:B:219:C:O4'	2:E:219:C:O4'[4_555]	0.10	2.10
2:B:219:C:C3'	2:E:219:C:C3'[4_555]	0.10	2.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:219:C:O3'	2:E:219:C:O3'[4_555]	0.10	2.10
2:B:219:C:C2'	2:E:219:C:C2'[4_555]	0.10	2.10
2:B:219:C:O2'	2:E:219:C:O2'[4_555]	0.10	2.10
2:B:219:C:C1'	2:E:219:C:C1'[4_555]	0.10	2.10
2:B:219:C:N1	2:E:219:C:N1[4_555]	0.10	2.10
2:B:219:C:C4	2:E:219:C:C4[4_555]	0.10	2.10
2:B:219:C:C5	2:E:219:C:C5[4_555]	0.10	2.10
2:B:219:C:C6	2:E:219:C:C6[4_555]	0.10	2.10
2:B:205:C:C4	2:E:205:C:C4[4_555]	0.11	2.09
2:B:206:G:C5'	2:E:206:G:C5'[4_555]	0.11	2.09
2:B:206:G:C4'	2:E:206:G:C4'[4_555]	0.11	2.09
2:B:206:G:C3'	2:E:206:G:C3'[4_555]	0.11	2.09
2:B:206:G:O3'	2:E:206:G:O3'[4_555]	0.11	2.09
2:B:206:G:O2'	2:E:206:G:O2'[4_555]	0.11	2.09
2:B:207:G:P	2:E:207:G:P[4_555]	0.11	2.09
2:B:207:G:O5'	2:E:207:G:O5'[4_555]	0.11	2.09
2:B:207:G:C5'	2:E:207:G:C5'[4_555]	0.11	2.09
2:B:207:G:C4'	2:E:207:G:C4'[4_555]	0.11	2.09
2:B:207:G:O3'	2:E:207:G:O3'[4_555]	0.11	2.09
2:B:207:G:O2'	2:E:207:G:O2'[4_555]	0.11	2.09
2:B:208:C:P	2:E:208:C:P[4_555]	0.11	2.09
2:B:208:C:OP1	2:E:208:C:OP1[4_555]	0.11	2.09
2:B:208:C:OP2	2:E:208:C:OP2[4_555]	0.11	2.09
2:B:208:C:O5'	2:E:208:C:O5'[4_555]	0.11	2.09
2:B:209:G:C1'	2:E:209:G:C1'[4_555]	0.11	2.09
2:B:212:G:O3'	2:E:212:G:O3'[4_555]	0.11	2.09
2:B:213:G:P	2:E:213:G:P[4_555]	0.11	2.09
2:B:213:G:OP2	2:E:213:G:OP2[4_555]	0.11	2.09
2:B:213:G:O5'	2:E:213:G:O5'[4_555]	0.11	2.09
2:B:214:C:C5'	2:E:214:C:C5'[4_555]	0.11	2.09
2:B:215:G:OP2	2:E:215:G:OP2[4_555]	0.11	2.09
2:B:215:G:O5'	2:E:215:G:O5'[4_555]	0.11	2.09
2:B:215:G:C5'	2:E:215:G:C5'[4_555]	0.11	2.09
2:B:215:G:C4'	2:E:215:G:C4'[4_555]	0.11	2.09
2:B:215:G:O4'	2:E:215:G:O4'[4_555]	0.11	2.09
2:B:215:G:C3'	2:E:215:G:C3'[4_555]	0.11	2.09
2:B:215:G:O3'	2:E:215:G:O3'[4_555]	0.11	2.09
2:B:215:G:C2'	2:E:215:G:C2'[4_555]	0.11	2.09
2:B:215:G:C1'	2:E:215:G:C1'[4_555]	0.11	2.09
2:B:215:G:N9	2:E:215:G:N9[4_555]	0.11	2.09
2:B:215:G:C2	2:E:215:G:C2[4_555]	0.11	2.09
2:B:215:G:N2	2:E:215:G:N2[4_555]	0.11	2.09

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:215:G:N3	2:E:215:G:N3[4_555]	0.11	2.09
2:B:215:G:C4	2:E:215:G:C4[4_555]	0.11	2.09
2:B:216:G:P	2:E:216:G:P[4_555]	0.11	2.09
2:B:216:G:OP1	2:E:216:G:OP1[4_555]	0.11	2.09
2:B:216:G:OP2	2:E:216:G:OP2[4_555]	0.11	2.09
2:B:216:G:O5'	2:E:216:G:O5'[4_555]	0.11	2.09
2:B:216:G:C5'	2:E:216:G:C5'[4_555]	0.11	2.09
2:B:216:G:C4'	2:E:216:G:C4'[4_555]	0.11	2.09
2:B:216:G:O4'	2:E:216:G:O4'[4_555]	0.11	2.09
2:B:216:G:C3'	2:E:216:G:C3'[4_555]	0.11	2.09
2:B:216:G:O3'	2:E:216:G:O3'[4_555]	0.11	2.09
2:B:216:G:C2'	2:E:216:G:C2'[4_555]	0.11	2.09
2:B:216:G:C1'	2:E:216:G:C1'[4_555]	0.11	2.09
2:B:216:G:N9	2:E:216:G:N9[4_555]	0.11	2.09
2:B:216:G:C8	2:E:216:G:C8[4_555]	0.11	2.09
2:B:216:G:N7	2:E:216:G:N7[4_555]	0.11	2.09
2:B:216:G:C5	2:E:216:G:C5[4_555]	0.11	2.09
2:B:216:G:C4	2:E:216:G:C4[4_555]	0.11	2.09
2:B:217:C:P	2:E:217:C:P[4_555]	0.11	2.09
2:B:217:C:OP1	2:E:217:C:OP1[4_555]	0.11	2.09
2:B:217:C:OP2	2:E:217:C:OP2[4_555]	0.11	2.09
2:B:217:C:O5'	2:E:217:C:O5'[4_555]	0.11	2.09
2:B:217:C:C5'	2:E:217:C:C5'[4_555]	0.11	2.09
2:B:217:C:C4'	2:E:217:C:C4'[4_555]	0.11	2.09
2:B:217:C:O2'	2:E:217:C:O2'[4_555]	0.11	2.09
2:B:218:G:O4'	2:E:218:G:O4'[4_555]	0.11	2.09
2:B:205:C:N3	2:E:205:C:N3[4_555]	0.12	2.08
2:B:205:C:C5	2:E:205:C:C5[4_555]	0.12	2.08
2:B:207:G:OP1	2:E:207:G:OP1[4_555]	0.12	2.08
2:B:209:G:OP2	2:E:209:G:OP2[4_555]	0.12	2.08
2:B:211:C:OP2	2:E:211:C:OP2[4_555]	0.12	2.08
2:B:211:C:O2'	2:E:211:C:O2'[4_555]	0.12	2.08
2:B:213:G:OP1	2:E:213:G:OP1[4_555]	0.12	2.08
2:B:213:G:O2'	2:E:213:G:O2'[4_555]	0.12	2.08
2:B:214:C:OP2	2:E:214:C:OP2[4_555]	0.12	2.08
2:B:214:C:C4'	2:E:214:C:C4'[4_555]	0.12	2.08
2:B:215:G:O2'	2:E:215:G:O2'[4_555]	0.12	2.08
2:B:216:G:O2'	2:E:216:G:O2'[4_555]	0.12	2.08
2:B:218:G:C4'	2:E:218:G:C4'[4_555]	0.12	2.08
2:B:218:G:C1'	2:E:218:G:C1'[4_555]	0.12	2.08
2:B:205:C:O5'	2:E:205:C:O5'[4_555]	0.13	2.07
2:B:206:G:O5'	2:E:206:G:O5'[4_555]	0.13	2.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:G:C3'	2:E:210:G:C3'[4_555]	0.13	2.07
2:B:211:C:P	2:E:211:C:P[4_555]	0.13	2.07
2:B:214:C:C3'	2:E:214:C:C3'[4_555]	0.13	2.07
2:B:214:C:O3'	2:E:214:C:O3'[4_555]	0.13	2.07
2:B:214:C:N4	2:E:214:C:N4[4_555]	0.13	2.07
2:B:215:G:P	2:E:215:G:P[4_555]	0.13	2.07
2:B:218:G:C2'	2:E:218:G:C2'[4_555]	0.13	2.07
2:B:206:G:OP2	2:E:206:G:OP2[4_555]	0.14	2.06
2:B:209:G:C3'	2:E:209:G:C3'[4_555]	0.14	2.06
2:B:209:G:O3'	2:E:209:G:O3'[4_555]	0.14	2.06
2:B:211:C:OP1	2:E:211:C:OP1[4_555]	0.14	2.06
2:B:214:C:O2'	2:E:214:C:O2'[4_555]	0.14	2.06
2:B:218:G:C3'	2:E:218:G:C3'[4_555]	0.14	2.06
2:B:205:C:O2'	2:E:205:C:O2'[4_555]	0.15	2.05
2:B:205:C:C2	2:E:205:C:C2[4_555]	0.15	2.05
2:B:205:C:C6	2:E:205:C:C6[4_555]	0.15	2.05
2:B:206:G:P	2:E:206:G:P[4_555]	0.15	2.05
2:B:206:G:OP1	2:E:206:G:OP1[4_555]	0.15	2.05
2:B:210:G:OP2	2:E:210:G:OP2[4_555]	0.15	2.05
2:B:214:C:O4'	2:E:214:C:O4'[4_555]	0.15	2.05
2:B:214:C:C2'	2:E:214:C:C2'[4_555]	0.15	2.05
2:B:214:C:C4	2:E:214:C:C4[4_555]	0.15	2.05
2:B:214:C:C5	2:E:214:C:C5[4_555]	0.15	2.05
2:B:215:G:OP1	2:E:215:G:OP1[4_555]	0.15	2.05
2:B:218:G:O2'	2:E:218:G:O2'[4_555]	0.15	2.05
2:B:214:C:N3	2:E:214:C:N3[4_555]	0.16	2.04
2:B:205:C:C5'	2:E:205:C:C5'[4_555]	0.17	2.03
2:B:205:C:O3'	2:E:205:C:O3'[4_555]	0.17	2.03
2:B:205:C:O2	2:E:205:C:O2[4_555]	0.17	2.03
2:B:210:G:O3'	2:E:210:G:O3'[4_555]	0.17	2.03
2:B:214:C:C6	2:E:214:C:C6[4_555]	0.17	2.03
2:B:205:C:N1	2:E:205:C:N1[4_555]	0.18	2.02
2:B:209:G:C2'	2:E:209:G:C2'[4_555]	0.18	2.02
2:B:214:C:C1'	2:E:214:C:C1'[4_555]	0.18	2.02
2:B:214:C:C2	2:E:214:C:C2[4_555]	0.18	2.02
2:B:205:C:C3'	2:E:205:C:C3'[4_555]	0.19	2.01
2:B:205:C:C2'	2:E:205:C:C2'[4_555]	0.19	2.01
2:B:210:G:C4'	2:E:210:G:C4'[4_555]	0.19	2.01
2:B:214:C:O2	2:E:214:C:O2[4_555]	0.19	2.01
2:B:205:C:C4'	2:E:205:C:C4'[4_555]	0.20	2.00
2:B:210:G:OP1	2:E:210:G:OP1[4_555]	0.20	2.00
2:B:219:C:P	2:E:219:C:P[4_555]	0.20	2.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:205:C:C1'	2:E:205:C:C1'[4_555]	0.21	1.99
2:B:219:C:OP1	2:E:219:C:OP1[4_555]	0.21	1.99
2:B:214:C:N1	2:E:214:C:N1[4_555]	0.24	1.96
2:B:219:C:OP2	2:E:219:C:OP2[4_555]	0.24	1.96
2:B:210:G:C1'	2:E:210:G:C1'[4_555]	0.25	1.95
2:B:205:C:O4'	2:E:205:C:O4'[4_555]	0.26	1.94
2:B:210:G:C5'	2:E:210:G:C5'[4_555]	0.26	1.94
2:B:218:G:O3'	2:E:218:G:O3'[4_555]	0.27	1.93
2:B:210:G:O5'	2:E:210:G:O5'[4_555]	0.28	1.92
2:B:210:G:C2'	2:E:210:G:C2'[4_555]	0.31	1.89
2:B:210:G:C8	2:E:210:G:N3[4_555]	0.38	1.82
2:B:210:G:O6	2:E:210:G:O6[4_555]	0.43	1.77
2:B:209:G:O2'	2:E:209:G:O2'[4_555]	0.44	1.76
2:B:210:G:O2'	2:E:210:G:O2'[4_555]	0.44	1.76
2:B:210:G:O4'	2:E:210:G:O4'[4_555]	0.45	1.75
2:B:210:G:N3	2:E:210:G:C8[4_555]	0.56	1.64
2:B:210:G:C5	2:E:210:G:C5[4_555]	0.62	1.58
2:B:210:G:C6	2:E:210:G:C6[4_555]	0.66	1.54
2:B:210:G:N7	2:E:210:G:C2[4_555]	0.79	1.41
2:B:210:G:N9	2:E:210:G:N9[4_555]	0.80	1.40
2:B:210:G:N3	2:E:210:G:N7[4_555]	0.80	1.40
2:B:210:G:C2	2:E:210:G:N7[4_555]	0.87	1.33
2:B:210:G:N9	2:E:210:G:C4[4_555]	0.96	1.24
2:B:210:G:C4	2:E:210:G:C4[4_555]	0.98	1.22
2:B:210:G:N7	2:E:210:G:N3[4_555]	1.01	1.19
2:B:210:G:C6	2:E:210:G:O6[4_555]	1.02	1.18
2:B:210:G:C4	2:E:210:G:C5[4_555]	1.04	1.16
2:B:210:G:O2'	2:E:210:G:C2'[4_555]	1.16	1.04
2:B:210:G:C5	2:E:210:G:C6[4_555]	1.17	1.03
2:B:210:G:C4	2:E:210:G:N9[4_555]	1.17	1.03
2:B:211:C:C2	2:E:211:C:O2[4_555]	1.18	1.02
2:B:202:C:C2	2:E:202:C:O2[4_555]	1.20	1.00
2:B:209:G:C6	2:E:209:G:O6[4_555]	1.20	1.00
2:B:214:C:C2	2:E:214:C:O2[4_555]	1.20	1.00
2:B:218:G:C6	2:E:218:G:O6[4_555]	1.20	1.00
2:B:203:G:O6	2:E:203:G:C6[4_555]	1.21	0.99
2:B:212:G:O6	2:E:212:G:C6[4_555]	1.21	0.99
2:B:204:G:O6	2:E:204:G:C6[4_555]	1.22	0.98
2:B:207:G:C6	2:E:207:G:O6[4_555]	1.22	0.98
2:B:208:C:O2	2:E:208:C:C2[4_555]	1.22	0.98
2:B:215:G:O6	2:E:215:G:C6[4_555]	1.22	0.98
2:B:206:G:C6	2:E:206:G:O6[4_555]	1.23	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:G:O6	2:E:210:G:C6[4_555]	1.23	0.97
2:B:213:G:O6	2:E:213:G:C6[4_555]	1.23	0.97
2:B:217:C:O2	2:E:217:C:C2[4_555]	1.23	0.97
2:B:219:C:O2	2:E:219:C:C2[4_555]	1.23	0.97
2:B:210:G:C8	2:E:210:G:C4[4_555]	1.24	0.96
2:B:216:G:C6	2:E:216:G:O6[4_555]	1.24	0.96
2:B:205:C:C2	2:E:205:C:O2[4_555]	1.25	0.95
2:B:205:C:O2	2:E:205:C:C2[4_555]	1.25	0.95
2:B:206:G:O6	2:E:206:G:C6[4_555]	1.25	0.95
2:B:213:G:C6	2:E:213:G:O6[4_555]	1.25	0.95
2:B:216:G:O6	2:E:216:G:C6[4_555]	1.25	0.95
2:B:204:G:C6	2:E:204:G:O6[4_555]	1.26	0.94
2:B:207:G:O6	2:E:207:G:C6[4_555]	1.26	0.94
2:B:208:C:C2	2:E:208:C:O2[4_555]	1.26	0.94
2:B:210:G:C5	2:E:210:G:C4[4_555]	1.26	0.94
2:B:212:G:C6	2:E:212:G:O6[4_555]	1.26	0.94
2:B:215:G:C6	2:E:215:G:O6[4_555]	1.26	0.94
2:B:217:C:C2	2:E:217:C:O2[4_555]	1.26	0.94
2:B:219:C:C2	2:E:219:C:O2[4_555]	1.26	0.94
2:B:203:G:C6	2:E:203:G:O6[4_555]	1.27	0.93
2:B:209:G:C8	2:E:209:G:N7[4_555]	1.27	0.93
2:B:211:C:C4	2:E:211:C:N3[4_555]	1.27	0.93
2:B:213:G:C2	2:E:213:G:N3[4_555]	1.27	0.93
2:B:202:C:O2	2:E:202:C:C2[4_555]	1.28	0.92
2:B:203:G:N7	2:E:203:G:C8[4_555]	1.28	0.92
2:B:204:G:N7	2:E:204:G:C8[4_555]	1.28	0.92
2:B:209:G:O6	2:E:209:G:C6[4_555]	1.28	0.92
2:B:209:G:N3	2:E:209:G:C2[4_555]	1.28	0.92
2:B:210:G:C1'	2:E:210:G:O4'[4_555]	1.28	0.92
2:B:213:G:N7	2:E:213:G:C8[4_555]	1.28	0.92
2:B:214:C:N4	2:E:214:C:C4[4_555]	1.28	0.92
2:B:214:C:C5	2:E:214:C:C6[4_555]	1.28	0.92
2:B:215:G:N7	2:E:215:G:C8[4_555]	1.28	0.92
2:B:218:G:C8	2:E:218:G:N7[4_555]	1.28	0.92
2:B:218:G:O6	2:E:218:G:C6[4_555]	1.28	0.92
2:B:219:C:C4	2:E:219:C:N4[4_555]	1.28	0.92
2:B:202:C:C4	2:E:202:C:N3[4_555]	1.29	0.91
2:B:205:C:N4	2:E:205:C:C4[4_555]	1.29	0.91
2:B:207:G:C8	2:E:207:G:N7[4_555]	1.29	0.91
2:B:210:G:O3'	2:E:210:G:C3'[4_555]	1.29	0.91
2:B:212:G:C2	2:E:212:G:N2[4_555]	1.29	0.91
2:B:213:G:N2	2:E:213:G:C2[4_555]	1.29	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:214:C:N3	2:E:214:C:C2[4_555]	1.29	0.91
2:B:214:C:C4	2:E:214:C:N3[4_555]	1.29	0.91
2:B:219:C:C6	2:E:219:C:C5[4_555]	1.29	0.91
2:B:204:G:C2	2:E:204:G:N3[4_555]	1.30	0.90
2:B:205:C:C5	2:E:205:C:C6[4_555]	1.30	0.90
2:B:208:C:C4	2:E:208:C:N4[4_555]	1.30	0.90
2:B:211:C:C6	2:E:211:C:N1[4_555]	1.30	0.90
2:B:212:G:N7	2:E:212:G:C8[4_555]	1.30	0.90
2:B:212:G:C4	2:E:212:G:N3[4_555]	1.30	0.90
2:B:213:G:N3	2:E:213:G:C4[4_555]	1.30	0.90
2:B:216:G:N7	2:E:216:G:C8[4_555]	1.30	0.90
2:B:218:G:N3	2:E:218:G:C2[4_555]	1.30	0.90
2:B:219:C:C2	2:E:219:C:N3[4_555]	1.30	0.90
2:B:202:C:N4	2:E:202:C:C4[4_555]	1.31	0.89
2:B:203:G:C2	2:E:203:G:N3[4_555]	1.31	0.89
2:B:205:C:N3	2:E:205:C:C2[4_555]	1.31	0.89
2:B:206:G:C8	2:E:206:G:N7[4_555]	1.31	0.89
2:B:206:G:N7	2:E:206:G:C8[4_555]	1.31	0.89
2:B:208:C:C6	2:E:208:C:C5[4_555]	1.31	0.89
2:B:211:C:O2	2:E:211:C:C2[4_555]	1.31	0.89
2:B:212:G:N3	2:E:212:G:C2[4_555]	1.31	0.89
2:B:214:C:O2	2:E:214:C:C2[4_555]	1.31	0.89
2:B:215:G:C2	2:E:215:G:N3[4_555]	1.31	0.89
2:B:202:C:C5	2:E:202:C:C6[4_555]	1.32	0.88
2:B:206:G:C2	2:E:206:G:N3[4_555]	1.32	0.88
2:B:207:G:N7	2:E:207:G:C8[4_555]	1.32	0.88
2:B:207:G:N3	2:E:207:G:C2[4_555]	1.32	0.88
2:B:208:C:C2	2:E:208:C:N3[4_555]	1.32	0.88
2:B:208:C:N3	2:E:208:C:C4[4_555]	1.32	0.88
2:B:210:G:C4	2:E:210:G:C8[4_555]	1.32	0.88
2:B:212:G:C8	2:E:212:G:N7[4_555]	1.32	0.88
2:B:213:G:C4	2:E:213:G:N9[4_555]	1.32	0.88
2:B:216:G:C8	2:E:216:G:N7[4_555]	1.32	0.88
2:B:216:G:C2	2:E:216:G:N3[4_555]	1.32	0.88
2:B:217:C:N3	2:E:217:C:C4[4_555]	1.32	0.88
2:B:217:C:C4	2:E:217:C:N4[4_555]	1.32	0.88
2:B:217:C:C6	2:E:217:C:C5[4_555]	1.32	0.88
2:B:219:C:N3	2:E:219:C:C4[4_555]	1.32	0.88
2:B:202:C:N3	2:E:202:C:C2[4_555]	1.33	0.87
2:B:202:C:C6	2:E:202:C:N1[4_555]	1.33	0.87
2:B:203:G:C8	2:E:203:G:N7[4_555]	1.33	0.87
2:B:203:G:C2	2:E:203:G:N2[4_555]	1.33	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:203:G:C4	2:E:203:G:N3[4_555]	1.33	0.87
2:B:204:G:N2	2:E:204:G:C2[4_555]	1.33	0.87
2:B:205:C:O3'	2:E:205:C:C3'[4_555]	1.33	0.87
2:B:206:G:N2	2:E:206:G:C2[4_555]	1.33	0.87
2:B:207:G:N2	2:E:207:G:C2[4_555]	1.33	0.87
2:B:208:C:O3'	2:E:208:C:C3'[4_555]	1.33	0.87
2:B:210:G:C2'	2:E:210:G:C1'[4_555]	1.33	0.87
2:B:211:C:C5	2:E:211:C:C6[4_555]	1.33	0.87
2:B:212:G:C8	2:E:212:G:N9[4_555]	1.33	0.87
2:B:213:G:C5	2:E:213:G:N7[4_555]	1.33	0.87
2:B:214:C:C6	2:E:214:C:N1[4_555]	1.33	0.87
2:B:216:G:N2	2:E:216:G:C2[4_555]	1.33	0.87
2:B:217:C:C2	2:E:217:C:N3[4_555]	1.33	0.87
2:B:218:G:N2	2:E:218:G:C2[4_555]	1.33	0.87
2:B:218:G:N3	2:E:218:G:C4[4_555]	1.33	0.87
2:B:219:C:O3'	2:E:219:C:C3'[4_555]	1.33	0.87
2:B:203:G:N3	2:E:203:G:C2[4_555]	1.34	0.86
2:B:204:G:C8	2:E:204:G:N7[4_555]	1.34	0.86
2:B:204:G:N3	2:E:204:G:C4[4_555]	1.34	0.86
2:B:205:C:C1'	2:E:205:C:O4'[4_555]	1.34	0.86
2:B:205:C:N3	2:E:205:C:C4[4_555]	1.34	0.86
2:B:205:C:C4	2:E:205:C:N3[4_555]	1.34	0.86
2:B:206:G:N3	2:E:206:G:C2[4_555]	1.34	0.86
2:B:206:G:N3	2:E:206:G:C4[4_555]	1.34	0.86
2:B:207:G:O3'	2:E:207:G:C3'[4_555]	1.34	0.86
2:B:207:G:C2	2:E:207:G:N3[4_555]	1.34	0.86
2:B:207:G:N3	2:E:207:G:C4[4_555]	1.34	0.86
2:B:209:G:C2'	2:E:209:G:O2'[4_555]	1.34	0.86
2:B:209:G:N9	2:E:209:G:C4[4_555]	1.34	0.86
2:B:209:G:N7	2:E:209:G:C8[4_555]	1.34	0.86
2:B:209:G:C2	2:E:209:G:N1[4_555]	1.34	0.86
2:B:209:G:C2	2:E:209:G:N2[4_555]	1.34	0.86
2:B:211:C:N1	2:E:211:C:C2[4_555]	1.34	0.86
2:B:211:C:N4	2:E:211:C:C4[4_555]	1.34	0.86
2:B:212:G:N7	2:E:212:G:C5[4_555]	1.34	0.86
2:B:212:G:C6	2:E:212:G:N1[4_555]	1.34	0.86
2:B:213:G:C8	2:E:213:G:N7[4_555]	1.34	0.86
2:B:213:G:N1	2:E:213:G:C6[4_555]	1.34	0.86
2:B:214:C:O3'	2:E:214:C:C3'[4_555]	1.34	0.86
2:B:215:G:C8	2:E:215:G:N7[4_555]	1.34	0.86
2:B:215:G:N2	2:E:215:G:C2[4_555]	1.34	0.86
2:B:215:G:N3	2:E:215:G:C2[4_555]	1.34	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:216:G:N3	2:E:216:G:C2[4_555]	1.34	0.86
2:B:216:G:N3	2:E:216:G:C4[4_555]	1.34	0.86
2:B:217:C:O3'	2:E:217:C:C3'[4_555]	1.34	0.86
2:B:218:G:N7	2:E:218:G:C8[4_555]	1.34	0.86
2:B:218:G:C2	2:E:218:G:N1[4_555]	1.34	0.86
2:B:218:G:C4	2:E:218:G:C5[4_555]	1.34	0.86
2:B:203:G:C8	2:E:203:G:N9[4_555]	1.35	0.85
2:B:203:G:C5	2:E:203:G:C4[4_555]	1.35	0.85
2:B:203:G:N1	2:E:203:G:C2[4_555]	1.35	0.85
2:B:204:G:N3	2:E:204:G:C2[4_555]	1.35	0.85
2:B:204:G:C4	2:E:204:G:N9[4_555]	1.35	0.85
2:B:205:C:O5'	2:E:205:C:C5'[4_555]	1.35	0.85
2:B:205:C:C3'	2:E:205:C:C4'[4_555]	1.35	0.85
2:B:207:G:C5'	2:E:207:G:O5'[4_555]	1.35	0.85
2:B:207:G:C2	2:E:207:G:N1[4_555]	1.35	0.85
2:B:208:C:N1	2:E:208:C:C6[4_555]	1.35	0.85
2:B:209:G:N2	2:E:209:G:C2[4_555]	1.35	0.85
2:B:209:G:C4	2:E:209:G:C5[4_555]	1.35	0.85
2:B:209:G:C4	2:E:209:G:N3[4_555]	1.35	0.85
2:B:210:G:C4	2:E:210:G:N7[4_555]	1.35	0.85
2:B:211:C:N3	2:E:211:C:C2[4_555]	1.35	0.85
2:B:211:C:C4	2:E:211:C:N4[4_555]	1.35	0.85
2:B:212:G:C2'	2:E:212:G:O2'[4_555]	1.35	0.85
2:B:212:G:N9	2:E:212:G:C4[4_555]	1.35	0.85
2:B:212:G:C5	2:E:212:G:C4[4_555]	1.35	0.85
2:B:212:G:N1	2:E:212:G:C2[4_555]	1.35	0.85
2:B:212:G:C2	2:E:212:G:N3[4_555]	1.35	0.85
2:B:213:G:N9	2:E:213:G:C8[4_555]	1.35	0.85
2:B:215:G:C2	2:E:215:G:N2[4_555]	1.35	0.85
2:B:215:G:N3	2:E:215:G:C4[4_555]	1.35	0.85
2:B:215:G:C4	2:E:215:G:N9[4_555]	1.35	0.85
2:B:215:G:C4	2:E:215:G:N3[4_555]	1.35	0.85
2:B:216:G:O3'	2:E:216:G:C3'[4_555]	1.35	0.85
2:B:218:G:C4'	2:E:218:G:O4'[4_555]	1.35	0.85
2:B:218:G:N9	2:E:218:G:C8[4_555]	1.35	0.85
2:B:218:G:C2	2:E:218:G:N3[4_555]	1.35	0.85
2:B:219:C:C4	2:E:219:C:N3[4_555]	1.35	0.85
2:B:202:C:C4	2:E:202:C:N4[4_555]	1.36	0.84
2:B:203:G:N2	2:E:203:G:C2[4_555]	1.36	0.84
2:B:204:G:N1	2:E:204:G:C2[4_555]	1.36	0.84
2:B:204:G:C2	2:E:204:G:N2[4_555]	1.36	0.84
2:B:204:G:C4	2:E:204:G:N3[4_555]	1.36	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:205:C:C4'	2:E:205:C:O4'[4_555]	1.36	0.84
2:B:205:C:C2	2:E:205:C:N1[4_555]	1.36	0.84
2:B:206:G:O3'	2:E:206:G:C3'[4_555]	1.36	0.84
2:B:206:G:N9	2:E:206:G:C8[4_555]	1.36	0.84
2:B:206:G:C2	2:E:206:G:N2[4_555]	1.36	0.84
2:B:206:G:C4	2:E:206:G:N9[4_555]	1.36	0.84
2:B:207:G:C4'	2:E:207:G:O4'[4_555]	1.36	0.84
2:B:207:G:N9	2:E:207:G:C8[4_555]	1.36	0.84
2:B:207:G:C2	2:E:207:G:N2[4_555]	1.36	0.84
2:B:207:G:C4	2:E:207:G:C5[4_555]	1.36	0.84
2:B:208:C:C4	2:E:208:C:N3[4_555]	1.36	0.84
2:B:209:G:C4'	2:E:209:G:O4'[4_555]	1.36	0.84
2:B:209:G:O3'	2:E:209:G:C3'[4_555]	1.36	0.84
2:B:209:G:N3	2:E:209:G:C4[4_555]	1.36	0.84
2:B:211:C:C2'	2:E:211:C:O2'[4_555]	1.36	0.84
2:B:211:C:C2	2:E:211:C:N3[4_555]	1.36	0.84
2:B:211:C:C6	2:E:211:C:C5[4_555]	1.36	0.84
2:B:214:C:C1'	2:E:214:C:O4'[4_555]	1.36	0.84
2:B:215:G:O3'	2:E:215:G:C3'[4_555]	1.36	0.84
2:B:215:G:C5	2:E:215:G:C4[4_555]	1.36	0.84
2:B:215:G:N1	2:E:215:G:C2[4_555]	1.36	0.84
2:B:216:G:C2	2:E:216:G:N2[4_555]	1.36	0.84
2:B:216:G:C4	2:E:216:G:N9[4_555]	1.36	0.84
2:B:217:C:N1	2:E:217:C:C6[4_555]	1.36	0.84
2:B:217:C:C4	2:E:217:C:N3[4_555]	1.36	0.84
2:B:217:C:N4	2:E:217:C:C4[4_555]	1.36	0.84
2:B:217:C:C5	2:E:217:C:C6[4_555]	1.36	0.84
2:B:218:G:N9	2:E:218:G:C4[4_555]	1.36	0.84
2:B:218:G:C2	2:E:218:G:N2[4_555]	1.36	0.84
2:B:219:C:C4'	2:E:219:C:O4'[4_555]	1.36	0.84
2:B:219:C:N1	2:E:219:C:C2[4_555]	1.36	0.84
2:B:219:C:N1	2:E:219:C:C6[4_555]	1.36	0.84
2:B:202:C:C2'	2:E:202:C:O2'[4_555]	1.37	0.83
2:B:202:C:N3	2:E:202:C:C4[4_555]	1.37	0.83
2:B:202:C:C6	2:E:202:C:C5[4_555]	1.37	0.83
2:B:203:G:C6	2:E:203:G:N1[4_555]	1.37	0.83
2:B:203:G:N3	2:E:203:G:C4[4_555]	1.37	0.83
2:B:203:G:C4	2:E:203:G:N9[4_555]	1.37	0.83
2:B:204:G:O3'	2:E:204:G:C3'[4_555]	1.37	0.83
2:B:204:G:C2'	2:E:204:G:O2'[4_555]	1.37	0.83
2:B:204:G:C5	2:E:204:G:N7[4_555]	1.37	0.83
2:B:204:G:C5	2:E:204:G:C4[4_555]	1.37	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:206:G:C5	2:E:206:G:N7[4_555]	1.37	0.83
2:B:206:G:C2	2:E:206:G:N1[4_555]	1.37	0.83
2:B:206:G:C4	2:E:206:G:C5[4_555]	1.37	0.83
2:B:206:G:C4	2:E:206:G:N3[4_555]	1.37	0.83
2:B:207:G:C4	2:E:207:G:N3[4_555]	1.37	0.83
2:B:208:C:C4'	2:E:208:C:O4'[4_555]	1.37	0.83
2:B:208:C:N4	2:E:208:C:C4[4_555]	1.37	0.83
2:B:209:G:N9	2:E:209:G:C8[4_555]	1.37	0.83
2:B:209:G:C2	2:E:209:G:N3[4_555]	1.37	0.83
2:B:210:G:C5'	2:E:210:G:O5'[4_555]	1.37	0.83
2:B:211:C:OP1	2:E:211:C:P[4_555]	1.37	0.83
2:B:211:C:O5'	2:E:211:C:C5'[4_555]	1.37	0.83
2:B:211:C:O4'	2:E:211:C:C1'[4_555]	1.37	0.83
2:B:211:C:C5	2:E:211:C:C4[4_555]	1.37	0.83
2:B:213:G:C4'	2:E:213:G:O4'[4_555]	1.37	0.83
2:B:213:G:C6	2:E:213:G:C5[4_555]	1.37	0.83
2:B:213:G:N1	2:E:213:G:C2[4_555]	1.37	0.83
2:B:214:C:O5'	2:E:214:C:C5'[4_555]	1.37	0.83
2:B:215:G:C8	2:E:215:G:N9[4_555]	1.37	0.83
2:B:216:G:C4'	2:E:216:G:O4'[4_555]	1.37	0.83
2:B:216:G:N9	2:E:216:G:C8[4_555]	1.37	0.83
2:B:216:G:C5	2:E:216:G:N7[4_555]	1.37	0.83
2:B:216:G:N1	2:E:216:G:C6[4_555]	1.37	0.83
2:B:216:G:C2	2:E:216:G:N1[4_555]	1.37	0.83
2:B:216:G:C4	2:E:216:G:N3[4_555]	1.37	0.83
2:B:217:C:C4'	2:E:217:C:O4'[4_555]	1.37	0.83
2:B:218:G:O3'	2:E:218:G:C3'[4_555]	1.37	0.83
2:B:218:G:N1	2:E:218:G:C6[4_555]	1.37	0.83
2:B:218:G:C4	2:E:218:G:N3[4_555]	1.37	0.83
2:B:201[A]:G:C2'	2:E:201[A]:G:O2'[4_555]	1.38	0.82
2:B:202:C:O3'	2:E:202:C:C3'[4_555]	1.38	0.82
2:B:202:C:N1	2:E:202:C:C2[4_555]	1.38	0.82
2:B:202:C:C2	2:E:202:C:N3[4_555]	1.38	0.82
2:B:203:G:O3'	2:E:203:G:C3'[4_555]	1.38	0.82
2:B:203:G:N9	2:E:203:G:C4[4_555]	1.38	0.82
2:B:203:G:N7	2:E:203:G:C5[4_555]	1.38	0.82
2:B:204:G:C4'	2:E:204:G:O4'[4_555]	1.38	0.82
2:B:204:G:N9	2:E:204:G:C8[4_555]	1.38	0.82
2:B:204:G:C8	2:E:204:G:N9[4_555]	1.38	0.82
2:B:204:G:N1	2:E:204:G:C6[4_555]	1.38	0.82
2:B:205:C:C2'	2:E:205:C:C1'[4_555]	1.38	0.82
2:B:205:C:N1	2:E:205:C:C6[4_555]	1.38	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:205:C:C4	2:E:205:C:N4[4_555]	1.38	0.82
2:B:205:C:C6	2:E:205:C:N1[4_555]	1.38	0.82
2:B:206:G:C1'	2:E:206:G:O4'[4_555]	1.38	0.82
2:B:206:G:N1	2:E:206:G:C6[4_555]	1.38	0.82
2:B:207:G:N9	2:E:207:G:C4[4_555]	1.38	0.82
2:B:207:G:C5	2:E:207:G:N7[4_555]	1.38	0.82
2:B:207:G:N1	2:E:207:G:C6[4_555]	1.38	0.82
2:B:208:C:C5	2:E:208:C:C6[4_555]	1.38	0.82
2:B:209:G:C8	2:E:209:G:N9[4_555]	1.38	0.82
2:B:209:G:N7	2:E:209:G:C5[4_555]	1.38	0.82
2:B:209:G:C5	2:E:209:G:C6[4_555]	1.38	0.82
2:B:210:G:C1'	2:E:210:G:N9[4_555]	1.38	0.82
2:B:210:G:C6	2:E:210:G:C5[4_555]	1.38	0.82
2:B:211:C:C4'	2:E:211:C:O4'[4_555]	1.38	0.82
2:B:211:C:O3'	2:E:211:C:C3'[4_555]	1.38	0.82
2:B:212:G:O5'	2:E:212:G:C5'[4_555]	1.38	0.82
2:B:212:G:O3'	2:E:212:G:C3'[4_555]	1.38	0.82
2:B:213:G:O3'	2:E:213:G:C3'[4_555]	1.38	0.82
2:B:213:G:C2'	2:E:213:G:O2'[4_555]	1.38	0.82
2:B:213:G:C2	2:E:213:G:N1[4_555]	1.38	0.82
2:B:213:G:N3	2:E:213:G:C2[4_555]	1.38	0.82
2:B:213:G:C4	2:E:213:G:C5[4_555]	1.38	0.82
2:B:215:G:C5	2:E:215:G:N7[4_555]	1.38	0.82
2:B:216:G:C4	2:E:216:G:C5[4_555]	1.38	0.82
2:B:217:C:N3	2:E:217:C:C2[4_555]	1.38	0.82
2:B:218:G:C5	2:E:218:G:N7[4_555]	1.38	0.82
2:B:219:C:C6	2:E:219:C:N1[4_555]	1.38	0.82
2:B:201[A]:G:O3'	2:E:201[A]:G:C3'[4_555]	1.39	0.81
2:B:201[B]:G:O3'	2:E:201[B]:G:C3'[4_555]	1.39	0.81
2:B:201[B]:G:C2'	2:E:201[B]:G:O2'[4_555]	1.39	0.81
2:B:203:G:C2'	2:E:203:G:O2'[4_555]	1.39	0.81
2:B:204:G:C5'	2:E:204:G:O5'[4_555]	1.39	0.81
2:B:204:G:C6	2:E:204:G:C5[4_555]	1.39	0.81
2:B:204:G:C2	2:E:204:G:N1[4_555]	1.39	0.81
2:B:205:C:C4	2:E:205:C:C5[4_555]	1.39	0.81
2:B:205:C:C6	2:E:205:C:C5[4_555]	1.39	0.81
2:B:206:G:C4'	2:E:206:G:O4'[4_555]	1.39	0.81
2:B:206:G:N9	2:E:206:G:C4[4_555]	1.39	0.81
2:B:206:G:C8	2:E:206:G:N9[4_555]	1.39	0.81
2:B:206:G:C5	2:E:206:G:C4[4_555]	1.39	0.81
2:B:206:G:N1	2:E:206:G:C2[4_555]	1.39	0.81
2:B:207:G:C4	2:E:207:G:N9[4_555]	1.39	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:208:C:N1	2:E:208:C:C2[4_555]	1.39	0.81
2:B:208:C:N3	2:E:208:C:C2[4_555]	1.39	0.81
2:B:208:C:C6	2:E:208:C:N1[4_555]	1.39	0.81
2:B:209:G:C6	2:E:209:G:N1[4_555]	1.39	0.81
2:B:209:G:N1	2:E:209:G:C6[4_555]	1.39	0.81
2:B:212:G:C4'	2:E:212:G:O4'[4_555]	1.39	0.81
2:B:213:G:C5'	2:E:213:G:O5'[4_555]	1.39	0.81
2:B:213:G:C5	2:E:213:G:C4[4_555]	1.39	0.81
2:B:214:C:C4'	2:E:214:C:O4'[4_555]	1.39	0.81
2:B:214:C:C2'	2:E:214:C:C1'[4_555]	1.39	0.81
2:B:214:C:C2	2:E:214:C:N1[4_555]	1.39	0.81
2:B:215:G:C4'	2:E:215:G:O4'[4_555]	1.39	0.81
2:B:215:G:C1'	2:E:215:G:O4'[4_555]	1.39	0.81
2:B:215:G:N9	2:E:215:G:C8[4_555]	1.39	0.81
2:B:215:G:N9	2:E:215:G:C4[4_555]	1.39	0.81
2:B:215:G:N1	2:E:215:G:C6[4_555]	1.39	0.81
2:B:215:G:C2	2:E:215:G:N1[4_555]	1.39	0.81
2:B:216:G:C1'	2:E:216:G:O4'[4_555]	1.39	0.81
2:B:216:G:N9	2:E:216:G:C4[4_555]	1.39	0.81
2:B:216:G:C8	2:E:216:G:N9[4_555]	1.39	0.81
2:B:216:G:C5	2:E:216:G:C4[4_555]	1.39	0.81
2:B:216:G:N1	2:E:216:G:C2[4_555]	1.39	0.81
2:B:217:C:N1	2:E:217:C:C2[4_555]	1.39	0.81
2:B:217:C:C6	2:E:217:C:N1[4_555]	1.39	0.81
2:B:218:G:C4	2:E:218:G:N9[4_555]	1.39	0.81
2:B:219:C:O2'	2:E:219:C:C2'[4_555]	1.39	0.81
2:B:219:C:N4	2:E:219:C:C4[4_555]	1.39	0.81
2:B:219:C:C5	2:E:219:C:C4[4_555]	1.39	0.81
2:B:219:C:C5	2:E:219:C:C6[4_555]	1.39	0.81
2:B:201[A]:G:O4'	2:E:201[A]:G:C1'[4_555]	1.40	0.80
2:B:203:G:C4'	2:E:203:G:O4'[4_555]	1.40	0.80
2:B:204:G:C6	2:E:204:G:N1[4_555]	1.40	0.80
2:B:204:G:C4	2:E:204:G:C5[4_555]	1.40	0.80
2:B:205:C:C2'	2:E:205:C:O2'[4_555]	1.40	0.80
2:B:207:G:C8	2:E:207:G:N9[4_555]	1.40	0.80
2:B:207:G:N7	2:E:207:G:C5[4_555]	1.40	0.80
2:B:207:G:N1	2:E:207:G:C2[4_555]	1.40	0.80
2:B:208:C:O2'	2:E:208:C:C2'[4_555]	1.40	0.80
2:B:209:G:OP1	2:E:209:G:P[4_555]	1.40	0.80
2:B:210:G:OP1	2:E:210:G:P[4_555]	1.40	0.80
2:B:210:G:N7	2:E:210:G:N1[4_555]	1.40	0.80
2:B:211:C:N3	2:E:211:C:C4[4_555]	1.40	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:212:G:N2	2:E:212:G:C2[4_555]	1.40	0.80
2:B:213:G:O5'	2:E:213:G:C5'[4_555]	1.40	0.80
2:B:213:G:O4'	2:E:213:G:C1'[4_555]	1.40	0.80
2:B:213:G:C2	2:E:213:G:N2[4_555]	1.40	0.80
2:B:213:G:C4	2:E:213:G:N3[4_555]	1.40	0.80
2:B:214:C:C2'	2:E:214:C:O2'[4_555]	1.40	0.80
2:B:214:C:N3	2:E:214:C:C4[4_555]	1.40	0.80
2:B:215:G:C2'	2:E:215:G:O2'[4_555]	1.40	0.80
2:B:215:G:N7	2:E:215:G:C5[4_555]	1.40	0.80
2:B:215:G:C6	2:E:215:G:C5[4_555]	1.40	0.80
2:B:215:G:C6	2:E:215:G:N1[4_555]	1.40	0.80
2:B:215:G:C4	2:E:215:G:C5[4_555]	1.40	0.80
2:B:217:C:C2	2:E:217:C:N1[4_555]	1.40	0.80
2:B:218:G:C2'	2:E:218:G:O2'[4_555]	1.40	0.80
2:B:218:G:N7	2:E:218:G:C5[4_555]	1.40	0.80
2:B:218:G:C5	2:E:218:G:C6[4_555]	1.40	0.80
2:B:219:C:OP2	2:E:219:C:P[4_555]	1.40	0.80
2:B:201[B]:G:O5'	2:E:201[B]:G:C5'[4_555]	1.41	0.79
2:B:201[A]:G:C4'	2:E:201[A]:G:O4'[4_555]	1.41	0.79
2:B:201[B]:G:C4'	2:E:201[B]:G:O4'[4_555]	1.41	0.79
2:B:201[B]:G:O4'	2:E:201[B]:G:C1'[4_555]	1.41	0.79
2:B:202:C:O5'	2:E:202:C:C5'[4_555]	1.41	0.79
2:B:202:C:C4'	2:E:202:C:O4'[4_555]	1.41	0.79
2:B:202:C:N1	2:E:202:C:C6[4_555]	1.41	0.79
2:B:202:C:C2	2:E:202:C:N1[4_555]	1.41	0.79
2:B:202:C:C5	2:E:202:C:C4[4_555]	1.41	0.79
2:B:203:G:O5'	2:E:203:G:C5'[4_555]	1.41	0.79
2:B:203:G:C1'	2:E:203:G:O4'[4_555]	1.41	0.79
2:B:203:G:N9	2:E:203:G:C8[4_555]	1.41	0.79
2:B:203:G:C5	2:E:203:G:N7[4_555]	1.41	0.79
2:B:203:G:C6	2:E:203:G:C5[4_555]	1.41	0.79
2:B:203:G:C2	2:E:203:G:N1[4_555]	1.41	0.79
2:B:203:G:C4	2:E:203:G:C5[4_555]	1.41	0.79
2:B:204:G:O4'	2:E:204:G:C1'[4_555]	1.41	0.79
2:B:204:G:N9	2:E:204:G:C4[4_555]	1.41	0.79
2:B:204:G:N7	2:E:204:G:C5[4_555]	1.41	0.79
2:B:205:C:C2	2:E:205:C:N3[4_555]	1.41	0.79
2:B:206:G:O5'	2:E:206:G:C5'[4_555]	1.41	0.79
2:B:206:G:O2'	2:E:206:G:C2'[4_555]	1.41	0.79
2:B:206:G:N7	2:E:206:G:C5[4_555]	1.41	0.79
2:B:206:G:C6	2:E:206:G:N1[4_555]	1.41	0.79
2:B:207:G:O2'	2:E:207:G:C2'[4_555]	1.41	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:207:G:C5	2:E:207:G:C6[4_555]	1.41	0.79
2:B:207:G:C5	2:E:207:G:C4[4_555]	1.41	0.79
2:B:207:G:C6	2:E:207:G:N1[4_555]	1.41	0.79
2:B:208:C:C1'	2:E:208:C:O4'[4_555]	1.41	0.79
2:B:208:C:C2	2:E:208:C:N1[4_555]	1.41	0.79
2:B:209:G:C5'	2:E:209:G:O5'[4_555]	1.41	0.79
2:B:209:G:C3'	2:E:209:G:C2'[4_555]	1.41	0.79
2:B:209:G:C5	2:E:209:G:C4[4_555]	1.41	0.79
2:B:209:G:C5	2:E:209:G:N7[4_555]	1.41	0.79
2:B:212:G:O4'	2:E:212:G:C1'[4_555]	1.41	0.79
2:B:212:G:C5	2:E:212:G:C6[4_555]	1.41	0.79
2:B:212:G:C2	2:E:212:G:N1[4_555]	1.41	0.79
2:B:212:G:N3	2:E:212:G:C4[4_555]	1.41	0.79
2:B:212:G:C4	2:E:212:G:N9[4_555]	1.41	0.79
2:B:213:G:C8	2:E:213:G:N9[4_555]	1.41	0.79
2:B:214:C:C4	2:E:214:C:N4[4_555]	1.41	0.79
2:B:214:C:C6	2:E:214:C:C5[4_555]	1.41	0.79
2:B:215:G:O5'	2:E:215:G:C5'[4_555]	1.41	0.79
2:B:216:G:C2'	2:E:216:G:O2'[4_555]	1.41	0.79
2:B:216:G:N7	2:E:216:G:C5[4_555]	1.41	0.79
2:B:216:G:C6	2:E:216:G:C5[4_555]	1.41	0.79
2:B:216:G:C6	2:E:216:G:N1[4_555]	1.41	0.79
2:B:217:C:O2'	2:E:217:C:C2'[4_555]	1.41	0.79
2:B:217:C:C1'	2:E:217:C:O4'[4_555]	1.41	0.79
2:B:218:G:OP1	2:E:218:G:P[4_555]	1.41	0.79
2:B:218:G:C8	2:E:218:G:N9[4_555]	1.41	0.79
2:B:219:C:O5'	2:E:219:C:C5'[4_555]	1.41	0.79
2:B:219:C:N3	2:E:219:C:C2[4_555]	1.41	0.79
2:B:202:C:O4'	2:E:202:C:C1'[4_555]	1.42	0.78
2:B:203:G:N1	2:E:203:G:C6[4_555]	1.42	0.78
2:B:206:G:C2'	2:E:206:G:O2'[4_555]	1.42	0.78
2:B:206:G:C6	2:E:206:G:C5[4_555]	1.42	0.78
2:B:207:G:C1'	2:E:207:G:O4'[4_555]	1.42	0.78
2:B:208:C:OP1	2:E:208:C:P[4_555]	1.42	0.78
2:B:208:C:C5'	2:E:208:C:O5'[4_555]	1.42	0.78
2:B:208:C:C5	2:E:208:C:C4[4_555]	1.42	0.78
2:B:209:G:O4'	2:E:209:G:C1'[4_555]	1.42	0.78
2:B:209:G:C1'	2:E:209:G:N9[4_555]	1.42	0.78
2:B:209:G:N1	2:E:209:G:C2[4_555]	1.42	0.78
2:B:209:G:C4	2:E:209:G:N9[4_555]	1.42	0.78
2:B:211:C:C5'	2:E:211:C:C4'[4_555]	1.42	0.78
2:B:211:C:C3'	2:E:211:C:C2'[4_555]	1.42	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:212:G:OP2	2:E:212:G:P[4_555]	1.42	0.78
2:B:212:G:C4	2:E:212:G:C5[4_555]	1.42	0.78
2:B:213:G:OP2	2:E:213:G:P[4_555]	1.42	0.78
2:B:213:G:C5'	2:E:213:G:C4'[4_555]	1.42	0.78
2:B:213:G:C1'	2:E:213:G:O4'[4_555]	1.42	0.78
2:B:214:C:C4	2:E:214:C:C5[4_555]	1.42	0.78
2:B:215:G:C3'	2:E:215:G:C4'[4_555]	1.42	0.78
2:B:216:G:O5'	2:E:216:G:C5'[4_555]	1.42	0.78
2:B:217:C:C5'	2:E:217:C:O5'[4_555]	1.42	0.78
2:B:218:G:C2'	2:E:218:G:C1'[4_555]	1.42	0.78
2:B:218:G:C1'	2:E:218:G:O4'[4_555]	1.42	0.78
2:B:218:G:C5	2:E:218:G:C4[4_555]	1.42	0.78
2:B:218:G:C6	2:E:218:G:N1[4_555]	1.42	0.78
2:B:218:G:N1	2:E:218:G:C2[4_555]	1.42	0.78
2:B:219:C:O4'	2:E:219:C:C1'[4_555]	1.42	0.78
2:B:219:C:C1'	2:E:219:C:N1[4_555]	1.42	0.78
2:B:219:C:C1'	2:E:219:C:O4'[4_555]	1.42	0.78
2:B:201[A]:G:C5'	2:E:201[A]:G:O5'[4_555]	1.43	0.77
2:B:202:C:C1'	2:E:202:C:O4'[4_555]	1.43	0.77
2:B:203:G:N9	2:E:203:G:C1'[4_555]	1.43	0.77
2:B:203:G:C5	2:E:203:G:C6[4_555]	1.43	0.77
2:B:206:G:OP1	2:E:206:G:P[4_555]	1.43	0.77
2:B:206:G:C3'	2:E:206:G:C4'[4_555]	1.43	0.77
2:B:207:G:C2'	2:E:207:G:O2'[4_555]	1.43	0.77
2:B:207:G:C6	2:E:207:G:C5[4_555]	1.43	0.77
2:B:209:G:C1'	2:E:209:G:O4'[4_555]	1.43	0.77
2:B:210:G:C3'	2:E:210:G:C4'[4_555]	1.43	0.77
2:B:212:G:N9	2:E:212:G:C8[4_555]	1.43	0.77
2:B:214:C:C3'	2:E:214:C:C4'[4_555]	1.43	0.77
2:B:214:C:N1	2:E:214:C:C1'[4_555]	1.43	0.77
2:B:214:C:N1	2:E:214:C:C2[4_555]	1.43	0.77
2:B:214:C:C2	2:E:214:C:N3[4_555]	1.43	0.77
2:B:216:G:C3'	2:E:216:G:C4'[4_555]	1.43	0.77
2:B:216:G:C2'	2:E:216:G:C1'[4_555]	1.43	0.77
2:B:216:G:O2'	2:E:216:G:C2'[4_555]	1.43	0.77
2:B:216:G:C5	2:E:216:G:C6[4_555]	1.43	0.77
2:B:217:C:OP1	2:E:217:C:P[4_555]	1.43	0.77
2:B:217:C:C2'	2:E:217:C:O2'[4_555]	1.43	0.77
2:B:217:C:C4	2:E:217:C:C5[4_555]	1.43	0.77
2:B:217:C:C5	2:E:217:C:C4[4_555]	1.43	0.77
2:B:218:G:O4'	2:E:218:G:C1'[4_555]	1.43	0.77
2:B:218:G:C1'	2:E:218:G:N9[4_555]	1.43	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:219:C:P	2:E:218:G:O3'[4_555]	1.43	0.77
2:B:201[A]:G:OP2	2:E:201[A]:G:P[4_555]	1.44	0.76
2:B:201[A]:G:C1'	2:E:201[A]:G:O4'[4_555]	1.44	0.76
2:B:201[B]:G:C1'	2:E:201[B]:G:O4'[4_555]	1.44	0.76
2:B:202:C:OP2	2:E:202:C:P[4_555]	1.44	0.76
2:B:202:C:N1	2:E:202:C:C1'[4_555]	1.44	0.76
2:B:202:C:C4	2:E:202:C:C5[4_555]	1.44	0.76
2:B:203:G:OP2	2:E:203:G:P[4_555]	1.44	0.76
2:B:203:G:O4'	2:E:203:G:C1'[4_555]	1.44	0.76
2:B:204:G:OP2	2:E:204:G:P[4_555]	1.44	0.76
2:B:204:G:C1'	2:E:204:G:O4'[4_555]	1.44	0.76
2:B:204:G:N9	2:E:204:G:C1'[4_555]	1.44	0.76
2:B:205:C:OP1	2:E:205:C:P[4_555]	1.44	0.76
2:B:205:C:N1	2:E:205:C:C1'[4_555]	1.44	0.76
2:B:206:G:C2'	2:E:206:G:C1'[4_555]	1.44	0.76
2:B:206:G:C5	2:E:206:G:C6[4_555]	1.44	0.76
2:B:207:G:OP1	2:E:207:G:P[4_555]	1.44	0.76
2:B:207:G:O4'	2:E:207:G:C1'[4_555]	1.44	0.76
2:B:207:G:C3'	2:E:207:G:C4'[4_555]	1.44	0.76
2:B:207:G:C2'	2:E:207:G:C1'[4_555]	1.44	0.76
2:B:208:C:O4'	2:E:208:C:C1'[4_555]	1.44	0.76
2:B:208:C:C2'	2:E:208:C:O2'[4_555]	1.44	0.76
2:B:208:C:C2'	2:E:208:C:C1'[4_555]	1.44	0.76
2:B:208:C:C1'	2:E:208:C:N1[4_555]	1.44	0.76
2:B:208:C:C4	2:E:208:C:C5[4_555]	1.44	0.76
2:B:209:G:P	2:E:209:G:OP2[4_555]	1.44	0.76
2:B:209:G:C2'	2:E:209:G:C1'[4_555]	1.44	0.76
2:B:210:G:O5'	2:E:210:G:C5'[4_555]	1.44	0.76
2:B:210:G:C5'	2:E:210:G:C4'[4_555]	1.44	0.76
2:B:211:C:N1	2:E:211:C:C6[4_555]	1.44	0.76
2:B:212:G:C5'	2:E:212:G:C4'[4_555]	1.44	0.76
2:B:212:G:C3'	2:E:212:G:O3'[4_555]	1.44	0.76
2:B:212:G:C1'	2:E:212:G:O4'[4_555]	1.44	0.76
2:B:212:G:N9	2:E:212:G:C1'[4_555]	1.44	0.76
2:B:212:G:C5	2:E:212:G:N7[4_555]	1.44	0.76
2:B:213:G:C3'	2:E:213:G:C2'[4_555]	1.44	0.76
2:B:213:G:N9	2:E:213:G:C4[4_555]	1.44	0.76
2:B:213:G:C6	2:E:213:G:N1[4_555]	1.44	0.76
2:B:214:C:O2'	2:E:214:C:C2'[4_555]	1.44	0.76
2:B:214:C:N1	2:E:214:C:C6[4_555]	1.44	0.76
2:B:214:C:C5	2:E:214:C:C4[4_555]	1.44	0.76
2:B:215:G:C2'	2:E:215:G:C1'[4_555]	1.44	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:215:G:O2'	2:E:215:G:C2'[4_555]	1.44	0.76
2:B:215:G:N9	2:E:215:G:C1'[4_555]	1.44	0.76
2:B:215:G:C5	2:E:215:G:C6[4_555]	1.44	0.76
2:B:216:G:OP1	2:E:216:G:P[4_555]	1.44	0.76
2:B:217:C:C3'	2:E:217:C:C4'[4_555]	1.44	0.76
2:B:217:C:C2'	2:E:217:C:C1'[4_555]	1.44	0.76
2:B:218:G:C5'	2:E:218:G:O5'[4_555]	1.44	0.76
2:B:218:G:C3'	2:E:218:G:C2'[4_555]	1.44	0.76
2:B:218:G:C6	2:E:218:G:C5[4_555]	1.44	0.76
2:B:219:C:C2'	2:E:219:C:O2'[4_555]	1.44	0.76
2:B:219:C:C2'	2:E:219:C:C1'[4_555]	1.44	0.76
2:B:219:C:C2	2:E:219:C:N1[4_555]	1.44	0.76
2:B:201[B]:G:OP3	2:E:201[B]:G:P[4_555]	1.45	0.75
2:B:201[B]:G:OP1	2:E:201[B]:G:P[4_555]	1.45	0.75
2:B:201[A]:G:O2'	2:E:201[A]:G:C2'[4_555]	1.45	0.75
2:B:201[B]:G:O2'	2:E:201[B]:G:C2'[4_555]	1.45	0.75
2:B:202:C:OP1	2:E:202:C:P[4_555]	1.45	0.75
2:B:202:C:C3'	2:E:202:C:O3'[4_555]	1.45	0.75
2:B:203:G:O2'	2:E:203:G:C2'[4_555]	1.45	0.75
2:B:204:G:C3'	2:E:204:G:C2'[4_555]	1.45	0.75
2:B:204:G:C5	2:E:204:G:C6[4_555]	1.45	0.75
2:B:205:C:O2'	2:E:205:C:C2'[4_555]	1.45	0.75
2:B:207:G:C1'	2:E:207:G:N9[4_555]	1.45	0.75
2:B:208:C:C3'	2:E:208:C:C4'[4_555]	1.45	0.75
2:B:209:G:O5'	2:E:209:G:C5'[4_555]	1.45	0.75
2:B:210:G:P	2:E:210:G:OP2[4_555]	1.45	0.75
2:B:212:G:OP1	2:E:212:G:P[4_555]	1.45	0.75
2:B:212:G:C3'	2:E:212:G:C2'[4_555]	1.45	0.75
2:B:212:G:C6	2:E:212:G:C5[4_555]	1.45	0.75
2:B:212:G:N1	2:E:212:G:C6[4_555]	1.45	0.75
2:B:213:G:N9	2:E:213:G:C1'[4_555]	1.45	0.75
2:B:213:G:N7	2:E:213:G:C5[4_555]	1.45	0.75
2:B:214:C:OP1	2:E:214:C:P[4_555]	1.45	0.75
2:B:214:C:OP2	2:E:214:C:P[4_555]	1.45	0.75
2:B:214:C:C3'	2:E:214:C:C2'[4_555]	1.45	0.75
2:B:215:G:OP2	2:E:215:G:P[4_555]	1.45	0.75
2:B:217:C:O4'	2:E:217:C:C1'[4_555]	1.45	0.75
2:B:218:G:O5'	2:E:218:G:C5'[4_555]	1.45	0.75
2:B:218:G:C3'	2:E:218:G:C4'[4_555]	1.45	0.75
2:B:218:G:O2'	2:E:218:G:C2'[4_555]	1.45	0.75
2:B:201[B]:G:P	2:E:201[B]:G:OP2[4_555]	1.46	0.74
2:B:201[A]:G:O5'	2:E:201[A]:G:C5'[4_555]	1.46	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:201[A]:G:C3'	2:E:201[A]:G:O3'[4_555]	1.46	0.74
2:B:201[B]:G:C3'	2:E:201[B]:G:O3'[4_555]	1.46	0.74
2:B:202:C:O2'	2:E:202:C:C2'[4_555]	1.46	0.74
2:B:203:G:OP1	2:E:203:G:P[4_555]	1.46	0.74
2:B:203:G:C3'	2:E:203:G:O3'[4_555]	1.46	0.74
2:B:203:G:C3'	2:E:203:G:C4'[4_555]	1.46	0.74
2:B:204:G:C5'	2:E:204:G:C4'[4_555]	1.46	0.74
2:B:204:G:O2'	2:E:204:G:C2'[4_555]	1.46	0.74
2:B:205:C:OP2	2:E:205:C:P[4_555]	1.46	0.74
2:B:205:C:N1	2:E:205:C:C2[4_555]	1.46	0.74
2:B:206:G:P	2:E:205:C:O3'[4_555]	1.46	0.74
2:B:206:G:C1'	2:E:206:G:N9[4_555]	1.46	0.74
2:B:208:C:O5'	2:E:208:C:C5'[4_555]	1.46	0.74
2:B:209:G:C6	2:E:209:G:C5[4_555]	1.46	0.74
2:B:211:C:O2'	2:E:211:C:C2'[4_555]	1.46	0.74
2:B:211:C:C1'	2:E:211:C:O4'[4_555]	1.46	0.74
2:B:211:C:N1	2:E:211:C:C1'[4_555]	1.46	0.74
2:B:211:C:C2	2:E:211:C:N1[4_555]	1.46	0.74
2:B:213:G:O2'	2:E:213:G:C2'[4_555]	1.46	0.74
2:B:215:G:P	2:E:214:C:O3'[4_555]	1.46	0.74
2:B:215:G:OP1	2:E:215:G:P[4_555]	1.46	0.74
2:B:216:G:C5'	2:E:216:G:O5'[4_555]	1.46	0.74
2:B:216:G:O4'	2:E:216:G:C1'[4_555]	1.46	0.74
2:B:216:G:C1'	2:E:216:G:N9[4_555]	1.46	0.74
2:B:216:G:N9	2:E:216:G:C1'[4_555]	1.46	0.74
2:B:217:C:O5'	2:E:217:C:C5'[4_555]	1.46	0.74
2:B:217:C:C1'	2:E:217:C:N1[4_555]	1.46	0.74
2:B:219:C:OP1	2:E:219:C:P[4_555]	1.46	0.74
2:B:219:C:C5'	2:E:219:C:O5'[4_555]	1.46	0.74
2:B:201[A]:G:P	2:E:201[A]:G:OP1[4_555]	1.47	0.73
2:B:201[A]:G:C5'	2:E:201[A]:G:C4'[4_555]	1.47	0.73
2:B:201[B]:G:C5'	2:E:201[B]:G:C4'[4_555]	1.47	0.73
2:B:201[B]:G:C5'	2:E:201[B]:G:O5'[4_555]	1.47	0.73
2:B:201[A]:G:C3'	2:E:201[A]:G:C2'[4_555]	1.47	0.73
2:B:201[B]:G:C3'	2:E:201[B]:G:C2'[4_555]	1.47	0.73
2:B:202:C:C5'	2:E:202:C:C4'[4_555]	1.47	0.73
2:B:202:C:C3'	2:E:202:C:C4'[4_555]	1.47	0.73
2:B:202:C:C3'	2:E:202:C:C2'[4_555]	1.47	0.73
2:B:203:G:C5'	2:E:203:G:O5'[4_555]	1.47	0.73
2:B:203:G:C2'	2:E:203:G:C1'[4_555]	1.47	0.73
2:B:204:G:OP1	2:E:204:G:P[4_555]	1.47	0.73
2:B:204:G:C2'	2:E:204:G:C1'[4_555]	1.47	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:205:C:C5	2:E:205:C:C4[4_555]	1.47	0.73
2:B:206:G:OP2	2:E:206:G:P[4_555]	1.47	0.73
2:B:206:G:C5'	2:E:206:G:O5'[4_555]	1.47	0.73
2:B:206:G:O4'	2:E:206:G:C1'[4_555]	1.47	0.73
2:B:206:G:N9	2:E:206:G:C1'[4_555]	1.47	0.73
2:B:209:G:C5'	2:E:209:G:C4'[4_555]	1.47	0.73
2:B:209:G:C3'	2:E:209:G:C4'[4_555]	1.47	0.73
2:B:210:G:O4'	2:E:210:G:C4'[4_555]	1.47	0.73
2:B:210:G:N7	2:E:210:G:C4[4_555]	1.47	0.73
2:B:211:C:C3'	2:E:211:C:O3'[4_555]	1.47	0.73
2:B:213:G:C3'	2:E:213:G:O3'[4_555]	1.47	0.73
2:B:213:G:C5	2:E:213:G:C6[4_555]	1.47	0.73
2:B:215:G:C5'	2:E:215:G:O5'[4_555]	1.47	0.73
2:B:215:G:O4'	2:E:215:G:C1'[4_555]	1.47	0.73
2:B:217:C:OP2	2:E:217:C:P[4_555]	1.47	0.73
2:B:219:C:C3'	2:E:219:C:C4'[4_555]	1.47	0.73
2:B:219:C:C4	2:E:219:C:C5[4_555]	1.47	0.73
2:B:202:C:C2'	2:E:202:C:C1'[4_555]	1.48	0.72
2:B:203:G:C3'	2:E:203:G:C2'[4_555]	1.48	0.72
2:B:204:G:C3'	2:E:204:G:C4'[4_555]	1.48	0.72
2:B:207:G:OP2	2:E:207:G:P[4_555]	1.48	0.72
2:B:207:G:C3'	2:E:207:G:C2'[4_555]	1.48	0.72
2:B:208:C:P	2:E:207:G:O3'[4_555]	1.48	0.72
2:B:208:C:P	2:E:208:C:OP2[4_555]	1.48	0.72
2:B:211:C:C1'	2:E:211:C:N1[4_555]	1.48	0.72
2:B:212:G:C5'	2:E:212:G:O5'[4_555]	1.48	0.72
2:B:212:G:C3'	2:E:212:G:C4'[4_555]	1.48	0.72
2:B:212:G:O2'	2:E:212:G:C2'[4_555]	1.48	0.72
2:B:213:G:OP1	2:E:213:G:P[4_555]	1.48	0.72
2:B:213:G:C3'	2:E:213:G:C4'[4_555]	1.48	0.72
2:B:213:G:C2'	2:E:213:G:C1'[4_555]	1.48	0.72
2:B:215:G:C1'	2:E:215:G:N9[4_555]	1.48	0.72
2:B:216:G:OP2	2:E:216:G:P[4_555]	1.48	0.72
2:B:218:G:P	2:E:218:G:OP2[4_555]	1.48	0.72
2:B:219:C:C3'	2:E:219:C:C2'[4_555]	1.48	0.72
2:B:201[A]:G:OP3	2:E:201[A]:G:P[4_555]	1.49	0.71
2:B:201[A]:G:OP1	2:E:201[A]:G:P[4_555]	1.49	0.71
2:B:202:C:C5'	2:E:202:C:O5'[4_555]	1.49	0.71
2:B:203:G:C5'	2:E:203:G:C4'[4_555]	1.49	0.71
2:B:203:G:C1'	2:E:203:G:N9[4_555]	1.49	0.71
2:B:204:G:P	2:E:204:G:OP1[4_555]	1.49	0.71
2:B:204:G:O5'	2:E:204:G:C5'[4_555]	1.49	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:204:G:C3'	2:E:204:G:O3'[4_555]	1.49	0.71
2:B:204:G:C1'	2:E:204:G:N9[4_555]	1.49	0.71
2:B:206:G:C4'	2:E:206:G:C5'[4_555]	1.49	0.71
2:B:207:G:N9	2:E:207:G:C1'[4_555]	1.49	0.71
2:B:208:C:C3'	2:E:208:C:C2'[4_555]	1.49	0.71
2:B:209:G:C3'	2:E:209:G:O3'[4_555]	1.49	0.71
2:B:210:G:OP2	2:E:210:G:P[4_555]	1.49	0.71
2:B:211:C:OP2	2:E:211:C:P[4_555]	1.49	0.71
2:B:211:C:C5'	2:E:211:C:O5'[4_555]	1.49	0.71
2:B:211:C:C2'	2:E:211:C:C1'[4_555]	1.49	0.71
2:B:211:C:C4	2:E:211:C:C5[4_555]	1.49	0.71
2:B:212:G:C2'	2:E:212:G:C1'[4_555]	1.49	0.71
2:B:212:G:C1'	2:E:212:G:N9[4_555]	1.49	0.71
2:B:213:G:C1'	2:E:213:G:N9[4_555]	1.49	0.71
2:B:214:C:O4'	2:E:214:C:C1'[4_555]	1.49	0.71
2:B:217:C:C3'	2:E:217:C:C2'[4_555]	1.49	0.71
2:B:218:G:OP2	2:E:218:G:P[4_555]	1.49	0.71
2:B:218:G:C5'	2:E:218:G:C4'[4_555]	1.49	0.71
2:B:219:C:C5'	2:E:219:C:C4'[4_555]	1.49	0.71
2:B:201[A]:G:P	2:E:201[A]:G:OP3[4_555]	1.50	0.70
2:B:201[A]:G:C3'	2:E:201[A]:G:C4'[4_555]	1.50	0.70
2:B:201[B]:G:C3'	2:E:201[B]:G:C4'[4_555]	1.50	0.70
2:B:201[A]:G:C2'	2:E:201[A]:G:C1'[4_555]	1.50	0.70
2:B:201[B]:G:C2'	2:E:201[B]:G:C1'[4_555]	1.50	0.70
2:B:202:C:C1'	2:E:202:C:N1[4_555]	1.50	0.70
2:B:205:C:C4'	2:E:205:C:C5'[4_555]	1.50	0.70
2:B:205:C:C3'	2:E:205:C:C2'[4_555]	1.50	0.70
2:B:207:G:C5'	2:E:207:G:C4'[4_555]	1.50	0.70
2:B:207:G:C3'	2:E:207:G:O3'[4_555]	1.50	0.70
2:B:208:C:OP2	2:E:208:C:P[4_555]	1.50	0.70
2:B:208:C:C4'	2:E:208:C:C5'[4_555]	1.50	0.70
2:B:209:G:N9	2:E:209:G:C1'[4_555]	1.50	0.70
2:B:210:G:C4'	2:E:210:G:O4'[4_555]	1.50	0.70
2:B:211:C:P	2:E:211:C:OP2[4_555]	1.50	0.70
2:B:211:C:C3'	2:E:211:C:C4'[4_555]	1.50	0.70
2:B:214:C:C5'	2:E:214:C:O5'[4_555]	1.50	0.70
2:B:214:C:C5'	2:E:214:C:C4'[4_555]	1.50	0.70
2:B:214:C:C3'	2:E:214:C:O3'[4_555]	1.50	0.70
2:B:215:G:C4'	2:E:215:G:C5'[4_555]	1.50	0.70
2:B:215:G:C3'	2:E:215:G:O3'[4_555]	1.50	0.70
2:B:215:G:C3'	2:E:215:G:C2'[4_555]	1.50	0.70
2:B:216:G:P	2:E:216:G:OP2[4_555]	1.50	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:216:G:C4'	2:E:216:G:C5'[4_555]	1.50	0.70
2:B:216:G:C3'	2:E:216:G:C2'[4_555]	1.50	0.70
2:B:217:C:N1	2:E:217:C:C1'[4_555]	1.50	0.70
2:B:218:G:N9	2:E:218:G:C1'[4_555]	1.50	0.70
2:B:201[B]:G:O4'	2:E:201[B]:G:C4'[4_555]	1.51	0.69
2:B:202:C:O4'	2:E:202:C:C4'[4_555]	1.51	0.69
2:B:203:G:P	2:E:203:G:OP1[4_555]	1.51	0.69
2:B:203:G:O4'	2:E:203:G:C4'[4_555]	1.51	0.69
2:B:204:G:P	2:E:203:G:O3'[4_555]	1.51	0.69
2:B:206:G:C3'	2:E:206:G:O3'[4_555]	1.51	0.69
2:B:207:G:P	2:E:207:G:OP2[4_555]	1.51	0.69
2:B:207:G:P	2:E:206:G:O3'[4_555]	1.51	0.69
2:B:208:C:C5'	2:E:208:C:C4'[4_555]	1.51	0.69
2:B:208:C:C3'	2:E:208:C:O3'[4_555]	1.51	0.69
2:B:208:C:N1	2:E:208:C:C1'[4_555]	1.51	0.69
2:B:210:G:C3'	2:E:210:G:C2'[4_555]	1.51	0.69
2:B:212:G:O4'	2:E:212:G:C4'[4_555]	1.51	0.69
2:B:213:G:P	2:E:213:G:OP1[4_555]	1.51	0.69
2:B:214:C:P	2:E:214:C:OP1[4_555]	1.51	0.69
2:B:215:G:C5'	2:E:215:G:C4'[4_555]	1.51	0.69
2:B:216:G:P	2:E:215:G:O3'[4_555]	1.51	0.69
2:B:217:C:P	2:E:217:C:OP2[4_555]	1.51	0.69
2:B:217:C:C5'	2:E:217:C:C4'[4_555]	1.51	0.69
2:B:217:C:C4'	2:E:217:C:C5'[4_555]	1.51	0.69
2:B:201[A]:G:P	2:E:201[A]:G:OP2[4_555]	1.52	0.68
2:B:201[B]:G:P	2:E:201[B]:G:OP1[4_555]	1.52	0.68
2:B:201[B]:G:OP2	2:E:201[B]:G:P[4_555]	1.52	0.68
2:B:201[A]:G:O4'	2:E:201[A]:G:C4'[4_555]	1.52	0.68
2:B:202:C:P	2:E:202:C:OP2[4_555]	1.52	0.68
2:B:202:C:P	2:E:202:C:OP1[4_555]	1.52	0.68
2:B:205:C:P	2:E:204:G:O3'[4_555]	1.52	0.68
2:B:205:C:P	2:E:205:C:OP2[4_555]	1.52	0.68
2:B:205:C:C5'	2:E:205:C:O5'[4_555]	1.52	0.68
2:B:206:G:C3'	2:E:206:G:C2'[4_555]	1.52	0.68
2:B:207:G:O5'	2:E:207:G:C5'[4_555]	1.52	0.68
2:B:209:G:OP2	2:E:209:G:P[4_555]	1.52	0.68
2:B:211:C:O4'	2:E:211:C:C4'[4_555]	1.52	0.68
2:B:212:G:P	2:E:212:G:OP2[4_555]	1.52	0.68
2:B:213:G:O4'	2:E:213:G:C4'[4_555]	1.52	0.68
2:B:215:G:O4'	2:E:215:G:C4'[4_555]	1.52	0.68
2:B:216:G:C5'	2:E:216:G:C4'[4_555]	1.52	0.68
2:B:216:G:C3'	2:E:216:G:O3'[4_555]	1.52	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:217:C:C3'	2:E:217:C:O3'[4_555]	1.52	0.68
2:B:218:G:P	2:E:217:C:O3'[4_555]	1.52	0.68
2:B:218:G:C3'	2:E:218:G:O3'[4_555]	1.52	0.68
2:B:219:C:C4'	2:E:219:C:C5'[4_555]	1.52	0.68
2:B:219:C:C3'	2:E:219:C:O3'[4_555]	1.52	0.68
2:B:201[B]:G:P	2:E:201[B]:G:OP3[4_555]	1.53	0.67
2:B:203:G:P	2:E:203:G:OP2[4_555]	1.53	0.67
2:B:203:G:P	2:E:202:C:O3'[4_555]	1.53	0.67
2:B:204:G:O4'	2:E:204:G:C4'[4_555]	1.53	0.67
2:B:205:C:C5'	2:E:205:C:C4'[4_555]	1.53	0.67
2:B:206:G:P	2:E:206:G:OP2[4_555]	1.53	0.67
2:B:206:G:C5'	2:E:206:G:C4'[4_555]	1.53	0.67
2:B:206:G:O4'	2:E:206:G:C4'[4_555]	1.53	0.67
2:B:207:G:C4'	2:E:207:G:C5'[4_555]	1.53	0.67
2:B:209:G:C4'	2:E:209:G:C5'[4_555]	1.53	0.67
2:B:210:G:P	2:E:210:G:O5'[4_555]	1.53	0.67
2:B:210:G:O4'	2:E:210:G:C1'[4_555]	1.53	0.67
2:B:210:G:C3'	2:E:210:G:O3'[4_555]	1.53	0.67
2:B:211:C:P	2:E:210:G:O3'[4_555]	1.53	0.67
2:B:211:C:P	2:E:211:C:O5'[4_555]	1.53	0.67
2:B:212:G:P	2:E:212:G:OP1[4_555]	1.53	0.67
2:B:212:G:P	2:E:212:G:O5'[4_555]	1.53	0.67
2:B:213:G:P	2:E:212:G:O3'[4_555]	1.53	0.67
2:B:213:G:P	2:E:213:G:O5'[4_555]	1.53	0.67
2:B:214:C:C4'	2:E:214:C:C5'[4_555]	1.53	0.67
2:B:214:C:O4'	2:E:214:C:C4'[4_555]	1.53	0.67
2:B:215:G:P	2:E:215:G:OP1[4_555]	1.53	0.67
2:B:216:G:P	2:E:216:G:OP1[4_555]	1.53	0.67
2:B:216:G:O4'	2:E:216:G:C4'[4_555]	1.53	0.67
2:B:219:C:N1	2:E:219:C:C1'[4_555]	1.53	0.67
2:B:201[A]:G:C4'	2:E:201[A]:G:C3'[4_555]	1.54	0.66
2:B:203:G:C4'	2:E:203:G:C5'[4_555]	1.54	0.66
2:B:204:G:P	2:E:204:G:OP2[4_555]	1.54	0.66
2:B:205:C:P	2:E:205:C:OP1[4_555]	1.54	0.66
2:B:205:C:C3'	2:E:205:C:O3'[4_555]	1.54	0.66
2:B:205:C:C1'	2:E:205:C:N1[4_555]	1.54	0.66
2:B:206:G:C2'	2:E:206:G:C3'[4_555]	1.54	0.66
2:B:207:G:P	2:E:207:G:OP1[4_555]	1.54	0.66
2:B:208:C:O4'	2:E:208:C:C4'[4_555]	1.54	0.66
2:B:209:G:P	2:E:208:C:O3'[4_555]	1.54	0.66
2:B:209:G:O4'	2:E:209:G:C4'[4_555]	1.54	0.66
2:B:209:G:O2'	2:E:209:G:C2'[4_555]	1.54	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:211:C:C4'	2:E:211:C:C3'[4_555]	1.54	0.66
2:B:214:C:C1'	2:E:214:C:N1[4_555]	1.54	0.66
2:B:215:G:P	2:E:215:G:OP2[4_555]	1.54	0.66
2:B:217:C:P	2:E:216:G:O3'[4_555]	1.54	0.66
2:B:217:C:O4'	2:E:217:C:C4'[4_555]	1.54	0.66
2:B:218:G:C4'	2:E:218:G:C5'[4_555]	1.54	0.66
2:B:201[A]:G:P	2:E:201[A]:G:O5'[4_555]	1.55	0.65
2:B:201[B]:G:P	2:E:201[B]:G:O5'[4_555]	1.55	0.65
2:B:201[B]:G:C4'	2:E:201[B]:G:C3'[4_555]	1.55	0.65
2:B:202:C:P	2:E:202:C:O5'[4_555]	1.55	0.65
2:B:202:C:C4'	2:E:202:C:C5'[4_555]	1.55	0.65
2:B:205:C:O4'	2:E:205:C:C1'[4_555]	1.55	0.65
2:B:206:G:P	2:E:206:G:OP1[4_555]	1.55	0.65
2:B:207:G:O4'	2:E:207:G:C4'[4_555]	1.55	0.65
2:B:208:C:C2'	2:E:208:C:C3'[4_555]	1.55	0.65
2:B:210:G:C2'	2:E:210:G:C3'[4_555]	1.55	0.65
2:B:212:G:P	2:E:211:C:O3'[4_555]	1.55	0.65
2:B:212:G:C4'	2:E:212:G:C3'[4_555]	1.55	0.65
2:B:213:G:C4'	2:E:213:G:C3'[4_555]	1.55	0.65
2:B:214:C:P	2:E:213:G:O3'[4_555]	1.55	0.65
2:B:214:C:P	2:E:214:C:O5'[4_555]	1.55	0.65
2:B:217:C:P	2:E:217:C:OP1[4_555]	1.55	0.65
2:B:218:G:O4'	2:E:218:G:C4'[4_555]	1.55	0.65
2:B:219:C:P	2:E:219:C:OP1[4_555]	1.55	0.65
2:B:219:C:O4'	2:E:219:C:C4'[4_555]	1.55	0.65
2:B:201[A]:G:C4'	2:E:201[A]:G:C5'[4_555]	1.56	0.64
2:B:201[B]:G:C4'	2:E:201[B]:G:C5'[4_555]	1.56	0.64
2:B:201[A]:G:C1'	2:E:201[A]:G:C2'[4_555]	1.56	0.64
2:B:202:C:P	2:E:201[A]:G:O3'[4_555]	1.56	0.64
2:B:202:C:P	2:E:201[B]:G:O3'[4_555]	1.56	0.64
2:B:204:G:C4'	2:E:204:G:C5'[4_555]	1.56	0.64
2:B:208:C:P	2:E:208:C:OP1[4_555]	1.56	0.64
2:B:209:G:C4'	2:E:209:G:C3'[4_555]	1.56	0.64
2:B:212:G:C4'	2:E:212:G:C5'[4_555]	1.56	0.64
2:B:213:G:C4'	2:E:213:G:C5'[4_555]	1.56	0.64
2:B:214:C:P	2:E:214:C:OP2[4_555]	1.56	0.64
2:B:215:G:C2'	2:E:215:G:C3'[4_555]	1.56	0.64
2:B:216:G:O5'	2:E:216:G:P[4_555]	1.56	0.64
2:B:216:G:C2'	2:E:216:G:C3'[4_555]	1.56	0.64
2:B:218:G:P	2:E:218:G:OP1[4_555]	1.56	0.64
2:B:201[B]:G:C1'	2:E:201[B]:G:C2'[4_555]	1.57	0.63
2:B:202:C:C4'	2:E:202:C:C3'[4_555]	1.57	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:202:C:C2'	2:E:202:C:C3'[4_555]	1.57	0.63
2:B:202:C:C1'	2:E:202:C:C2'[4_555]	1.57	0.63
2:B:203:G:P	2:E:203:G:O5'[4_555]	1.57	0.63
2:B:203:G:C2'	2:E:203:G:C3'[4_555]	1.57	0.63
2:B:204:G:C4'	2:E:204:G:C3'[4_555]	1.57	0.63
2:B:205:C:C2'	2:E:205:C:C3'[4_555]	1.57	0.63
2:B:206:G:O5'	2:E:206:G:P[4_555]	1.57	0.63
2:B:207:G:O5'	2:E:207:G:P[4_555]	1.57	0.63
2:B:207:G:C2'	2:E:207:G:C3'[4_555]	1.57	0.63
2:B:210:G:P	2:E:210:G:OP1[4_555]	1.57	0.63
2:B:210:G:P	2:E:209:G:O3'[4_555]	1.57	0.63
2:B:211:C:C1'	2:E:211:C:C2'[4_555]	1.57	0.63
2:B:212:G:C1'	2:E:212:G:C2'[4_555]	1.57	0.63
2:B:217:C:C2'	2:E:217:C:C3'[4_555]	1.57	0.63
2:B:219:C:C2'	2:E:219:C:C3'[4_555]	1.57	0.63
2:B:201[B]:G:C2'	2:E:201[B]:G:C3'[4_555]	1.58	0.62
2:B:205:C:P	2:E:205:C:O5'[4_555]	1.58	0.62
2:B:208:C:O5'	2:E:208:C:P[4_555]	1.58	0.62
2:B:209:G:P	2:E:209:G:OP1[4_555]	1.58	0.62
2:B:211:C:C4'	2:E:211:C:C5'[4_555]	1.58	0.62
2:B:213:G:P	2:E:213:G:OP2[4_555]	1.58	0.62
2:B:215:G:O5'	2:E:215:G:P[4_555]	1.58	0.62
2:B:219:C:O5'	2:E:219:C:P[4_555]	1.58	0.62
2:B:219:C:C4'	2:E:219:C:C3'[4_555]	1.58	0.62
2:B:201[A]:G:C2'	2:E:201[A]:G:C3'[4_555]	1.59	0.61
2:B:203:G:C4'	2:E:203:G:C3'[4_555]	1.59	0.61
2:B:203:G:C1'	2:E:203:G:C2'[4_555]	1.59	0.61
2:B:204:G:O5'	2:E:204:G:P[4_555]	1.59	0.61
2:B:204:G:C2'	2:E:204:G:C3'[4_555]	1.59	0.61
2:B:204:G:C1'	2:E:204:G:C2'[4_555]	1.59	0.61
2:B:205:C:O4'	2:E:205:C:C4'[4_555]	1.59	0.61
2:B:207:G:C4'	2:E:207:G:C3'[4_555]	1.59	0.61
2:B:208:C:C4'	2:E:208:C:C3'[4_555]	1.59	0.61
2:B:210:G:C4'	2:E:210:G:C5'[4_555]	1.59	0.61
2:B:210:G:C4'	2:E:210:G:C3'[4_555]	1.59	0.61
2:B:211:C:P	2:E:211:C:OP1[4_555]	1.59	0.61
2:B:213:G:C1'	2:E:213:G:C2'[4_555]	1.59	0.61
2:B:214:C:C2'	2:E:214:C:C3'[4_555]	1.59	0.61
2:B:217:C:O5'	2:E:217:C:P[4_555]	1.59	0.61
2:B:204:G:P	2:E:204:G:O5'[4_555]	1.60	0.60
2:B:209:G:P	2:E:209:G:O5'[4_555]	1.60	0.60
2:B:209:G:O5'	2:E:209:G:P[4_555]	1.60	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:G:N1	2:E:210:G:N7[4_555]	1.60	0.60
2:B:212:G:C2'	2:E:212:G:C3'[4_555]	1.60	0.60
2:B:213:G:C2'	2:E:213:G:C3'[4_555]	1.60	0.60
2:B:217:C:P	2:E:217:C:O5'[4_555]	1.60	0.60
2:B:217:C:C4'	2:E:217:C:C3'[4_555]	1.60	0.60
2:B:218:G:P	2:E:218:G:O5'[4_555]	1.60	0.60
2:B:218:G:O5'	2:E:218:G:P[4_555]	1.60	0.60
2:B:219:C:P	2:E:219:C:OP2[4_555]	1.60	0.60
2:B:205:C:O5'	2:E:205:C:P[4_555]	1.61	0.59
2:B:211:C:C2'	2:E:211:C:C3'[4_555]	1.61	0.59
2:B:215:G:P	2:E:215:G:O5'[4_555]	1.61	0.59
2:B:218:G:C4'	2:E:218:G:C3'[4_555]	1.61	0.59
2:B:218:G:C2'	2:E:218:G:C3'[4_555]	1.61	0.59
2:B:219:C:P	2:E:219:C:O5'[4_555]	1.61	0.59
2:B:203:G:O5'	2:E:203:G:P[4_555]	1.62	0.58
2:B:206:G:C4'	2:E:206:G:C3'[4_555]	1.62	0.58
2:B:208:C:P	2:E:208:C:O5'[4_555]	1.62	0.58
2:B:209:G:O3'	2:E:210:G:P[4_555]	1.62	0.58
2:B:214:C:C4'	2:E:214:C:C3'[4_555]	1.62	0.58
2:B:215:G:C4'	2:E:215:G:C3'[4_555]	1.62	0.58
2:B:215:G:C1'	2:E:215:G:C2'[4_555]	1.62	0.58
2:B:216:G:C4'	2:E:216:G:C3'[4_555]	1.62	0.58
2:B:201[A]:G:O5'	2:E:201[A]:G:P[4_555]	1.63	0.57
2:B:206:G:P	2:E:206:G:O5'[4_555]	1.63	0.57
2:B:206:G:C1'	2:E:206:G:C2'[4_555]	1.63	0.57
2:B:207:G:P	2:E:207:G:O5'[4_555]	1.63	0.57
2:B:207:G:C1'	2:E:207:G:C2'[4_555]	1.63	0.57
2:B:208:C:C1'	2:E:208:C:C2'[4_555]	1.63	0.57
2:B:214:C:O5'	2:E:214:C:P[4_555]	1.63	0.57
2:B:216:G:C1'	2:E:216:G:C2'[4_555]	1.63	0.57
2:B:217:C:C1'	2:E:217:C:C2'[4_555]	1.63	0.57
2:B:219:C:C1'	2:E:219:C:C2'[4_555]	1.63	0.57
2:B:201[B]:G:O5'	2:E:201[B]:G:P[4_555]	1.64	0.56
2:B:209:G:C1'	2:E:209:G:C2'[4_555]	1.64	0.56
2:B:210:G:N9	2:E:210:G:C1'[4_555]	1.64	0.56
2:B:213:G:O5'	2:E:213:G:P[4_555]	1.64	0.56
2:B:216:G:P	2:E:216:G:O5'[4_555]	1.64	0.56
2:B:218:G:C1'	2:E:218:G:C2'[4_555]	1.64	0.56
2:B:201[A]:G:O3'	2:E:202:C:P[4_555]	1.65	0.55
2:B:201[B]:G:O3'	2:E:202:C:P[4_555]	1.65	0.55
2:B:202:C:O5'	2:E:202:C:P[4_555]	1.65	0.55
2:B:209:G:C2'	2:E:209:G:C3'[4_555]	1.65	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:G:O5'	2:E:210:G:P[4_555]	1.65	0.55
2:B:212:G:O5'	2:E:212:G:P[4_555]	1.65	0.55
2:B:202:C:O3'	2:E:203:G:P[4_555]	1.66	0.54
2:B:211:C:O5'	2:E:211:C:P[4_555]	1.66	0.54
2:B:211:C:O3'	2:E:212:G:P[4_555]	1.66	0.54
2:B:214:C:C1'	2:E:214:C:C2'[4_555]	1.66	0.54
2:B:207:G:O3'	2:E:208:C:P[4_555]	1.67	0.53
2:B:203:G:O3'	2:E:204:G:P[4_555]	1.68	0.52
2:B:208:C:O3'	2:E:209:G:P[4_555]	1.68	0.52
2:B:210:G:O3'	2:E:211:C:P[4_555]	1.68	0.52
2:B:210:G:N9	2:E:210:G:N3[4_555]	1.68	0.52
2:B:212:G:O3'	2:E:213:G:P[4_555]	1.69	0.51
2:B:204:G:O3'	2:E:205:C:P[4_555]	1.70	0.50
2:B:205:C:C4'	2:E:205:C:C3'[4_555]	1.70	0.50
2:B:205:C:C1'	2:E:205:C:C2'[4_555]	1.70	0.50
2:B:210:G:C2'	2:E:210:G:O2'[4_555]	1.70	0.50
2:B:210:G:C8	2:E:210:G:C2[4_555]	1.70	0.50
2:B:213:G:O3'	2:E:214:C:P[4_555]	1.70	0.50
2:B:217:C:O3'	2:E:218:G:P[4_555]	1.70	0.50
2:B:206:G:O3'	2:E:207:G:P[4_555]	1.72	0.48
2:B:214:C:O3'	2:E:215:G:P[4_555]	1.72	0.48
2:B:215:G:O3'	2:E:216:G:P[4_555]	1.73	0.47
2:B:216:G:O3'	2:E:217:C:P[4_555]	1.74	0.46
2:B:210:G:C1'	2:E:210:G:C2'[4_555]	1.75	0.45
2:B:210:G:C5	2:E:210:G:N1[4_555]	1.76	0.44
2:E:201[B]:G:OP1	4:B:314:HOH:O[4_555]	1.77	0.43
2:B:205:C:O3'	2:E:206:G:P[4_555]	1.78	0.42
2:B:210:G:N3	2:E:210:G:N9[4_555]	1.79	0.41
2:B:218:G:O3'	2:E:219:C:P[4_555]	1.83	0.37
2:B:210:G:N1	2:E:210:G:O6[4_555]	1.88	0.32
2:B:210:G:C2	2:E:210:G:C8[4_555]	1.88	0.32
2:B:210:G:N3	2:E:210:G:C5[4_555]	1.89	0.31
2:B:210:G:N1	2:E:210:G:C5[4_555]	1.90	0.30
2:B:210:G:N7	2:E:210:G:C5[4_555]	1.96	0.24
2:B:210:G:C5	2:E:210:G:N7[4_555]	2.00	0.20
2:E:201[B]:G:OP3	4:A:744:HOH:O[4_555]	2.00	0.20
2:B:210:G:N9	2:E:210:G:O4'[4_555]	2.01	0.19
2:B:210:G:N7	2:E:210:G:C6[4_555]	2.01	0.19
2:B:210:G:O6	2:E:210:G:N1[4_555]	2.01	0.19
2:B:210:G:C5	2:E:210:G:N3[4_555]	2.03	0.17
2:B:210:G:N1	2:E:210:G:C6[4_555]	2.03	0.17
2:B:210:G:C6	2:E:210:G:N1[4_555]	2.04	0.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:213:G:C5	2:E:213:G:C8[4_555]	2.07	0.13
2:B:204:G:C5	2:E:204:G:C8[4_555]	2.10	0.10
2:B:209:G:C8	2:E:209:G:C5[4_555]	2.10	0.10
2:B:210:G:N9	2:E:210:G:C8[4_555]	2.10	0.10
2:B:212:G:C8	2:E:212:G:C5[4_555]	2.10	0.10
2:B:210:G:C5	2:E:210:G:C2[4_555]	2.11	0.09
2:B:210:G:C2	2:E:210:G:C5[4_555]	2.11	0.09
2:B:215:G:C5	2:E:215:G:C8[4_555]	2.11	0.09
2:B:218:G:C8	2:E:218:G:C5[4_555]	2.11	0.09
2:B:203:G:C5	2:E:203:G:C8[4_555]	2.12	0.08
2:B:206:G:C5	2:E:206:G:C8[4_555]	2.12	0.08
2:B:210:G:N7	2:E:210:G:N2[4_555]	2.12	0.08
2:B:216:G:C5	2:E:216:G:C8[4_555]	2.12	0.08
2:B:207:G:C8	2:E:207:G:C5[4_555]	2.13	0.07
2:B:207:G:C5	2:E:207:G:C8[4_555]	2.13	0.07
2:B:203:G:C8	2:E:203:G:C5[4_555]	2.14	0.06
2:B:206:G:C8	2:E:206:G:C5[4_555]	2.15	0.05
2:B:209:G:N9	2:E:209:G:C5[4_555]	2.15	0.05
2:B:212:G:C8	2:E:212:G:C4[4_555]	2.15	0.05
2:B:213:G:C2	2:E:213:G:C4[4_555]	2.15	0.05
2:B:213:G:C4	2:E:213:G:C8[4_555]	2.15	0.05
2:B:215:G:C8	2:E:215:G:C5[4_555]	2.15	0.05
2:B:216:G:C8	2:E:216:G:C5[4_555]	2.15	0.05
2:B:218:G:C5	2:E:218:G:C8[4_555]	2.15	0.05
2:B:204:G:C8	2:E:204:G:C5[4_555]	2.16	0.04
2:B:204:G:C5	2:E:204:G:N9[4_555]	2.16	0.04
2:B:205:C:C3'	2:E:205:C:O4'[4_555]	2.16	0.04
2:B:210:G:C8	2:E:210:G:N9[4_555]	2.16	0.04
2:B:210:G:C6	2:E:210:G:N7[4_555]	2.16	0.04
2:B:210:G:N2	2:E:210:G:N7[4_555]	2.16	0.04
2:B:212:G:C5	2:E:212:G:C8[4_555]	2.16	0.04
2:B:213:G:C5	2:E:213:G:N9[4_555]	2.16	0.04
2:B:215:G:C5	2:E:215:G:N9[4_555]	2.16	0.04
2:B:218:G:N9	2:E:218:G:C5[4_555]	2.16	0.04
2:B:203:G:C5	2:E:203:G:N9[4_555]	2.17	0.03
2:B:209:G:C5	2:E:209:G:C8[4_555]	2.17	0.03
2:B:210:G:C3'	2:E:210:G:O4'[4_555]	2.17	0.03
2:B:210:G:C2'	2:E:210:G:N9[4_555]	2.17	0.03
2:B:204:G:C4	2:E:204:G:C8[4_555]	2.18	0.02
2:B:207:G:O3'	2:E:207:G:C4'[4_555]	2.18	0.02
2:B:207:G:N9	2:E:207:G:C5[4_555]	2.18	0.02
2:B:209:G:C8	2:E:209:G:C4[4_555]	2.18	0.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:212:G:C4	2:E:212:G:C2[4_555]	2.18	0.02
2:B:203:G:C8	2:E:203:G:C4[4_555]	2.19	0.01
2:B:204:G:C2	2:E:204:G:C4[4_555]	2.19	0.01
2:B:206:G:C5	2:E:206:G:N9[4_555]	2.19	0.01
2:B:206:G:C4	2:E:206:G:C8[4_555]	2.19	0.01
2:B:209:G:C4	2:E:209:G:C2[4_555]	2.19	0.01
2:B:212:G:C5	2:E:212:G:N9[4_555]	2.19	0.01
2:B:213:G:C8	2:E:213:G:C5[4_555]	2.19	0.01
2:B:216:G:C5	2:E:216:G:N9[4_555]	2.19	0.01
2:B:216:G:C4	2:E:216:G:C8[4_555]	2.19	0.01
2:B:218:G:C4	2:E:218:G:C8[4_555]	2.19	0.01
2:B:206:G:N9	2:E:206:G:C5[4_555]	2.20	0.00
2:B:207:G:C4	2:E:207:G:C8[4_555]	2.20	0.00
2:B:210:G:N9	2:E:210:G:C5[4_555]	2.20	0.00
2:B:211:C:N1	2:E:211:C:O2[4_555]	2.20	0.00
2:B:212:G:N9	2:E:212:G:C5[4_555]	2.20	0.00
2:B:215:G:C4	2:E:215:G:C8[4_555]	2.20	0.00
2:B:216:G:N9	2:E:216:G:C5[4_555]	2.20	0.00
2:B:216:G:C2	2:E:216:G:C4[4_555]	2.20	0.00

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	
1	A	122/127 (96%)	119 (98%)	2 (2%)	1 (1%)	27	12

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP

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	
1	A	111/111 (100%)	108 (97%)	3 (3%)	57	46

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	65	LEU
1	A	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	24	ASN
1	A	31	GLN
1	A	85	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	18/19 (94%)	3 (16%)	0
2	E	18/19 (94%)	3 (16%)	0
All	All	36/38 (94%)	6 (16%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	207	G
2	B	210	G
2	B	213	G
2	E	207	G
2	E	210	G
2	E	213	G

There are no RNA pucker outliers to report.

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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SO4	A	601	-	4,4,4	1.43	1 (25%)	6,6,6	1.16	1 (16%)
3	SO4	A	602	-	4,4,4	0.64	0	6,6,6	0.72	0
3	SO4	A	603	-	4,4,4	0.43	0	6,6,6	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	SO4	O3-S	-2.61	1.37	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	SO4	O4-S-O3	2.09	117.79	109.05

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	121/127 (95%)	0.47	7 (5%)	22	22	28, 36, 65, 88	0
2	B	19/19 (100%)	0.70	2 (10%)	7	6	44, 63, 80, 81	19 (100%)
2	E	19/19 (100%)	0.69	2 (10%)	7	6	44, 62, 83, 84	19 (100%)
All	All	159/165 (96%)	0.53	11 (6%)	17	16	28, 40, 76, 88	38 (23%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	6.6
1	A	82	GLY	4.8
1	A	99	ILE	2.9
2	B	218	G	2.8
2	E	218	G	2.7
2	E	217	C	2.5
2	B	217	C	2.4
1	A	31	GLN	2.4
1	A	127	PRO	2.3
1	A	101	VAL	2.2
1	A	126	ALA	2.0

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

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

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
3	SO4	A	602	5/5	0.30	15.01	31,36,40,41	5
3	SO4	A	601	5/5	0.28	4.20	26,28,30,31	5
3	SO4	A	603	5/5	0.30	2.67	41,52,60,64	5

6.5 Other polymers ⓘ

There are no such residues in this entry.