



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 06:22 PM UTC

PDB ID : 6MU5 / pdb_00006mu5
Title : Bst DNA polymerase I TNA/DNA binary complex
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Deposited on : 2018-10-22
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

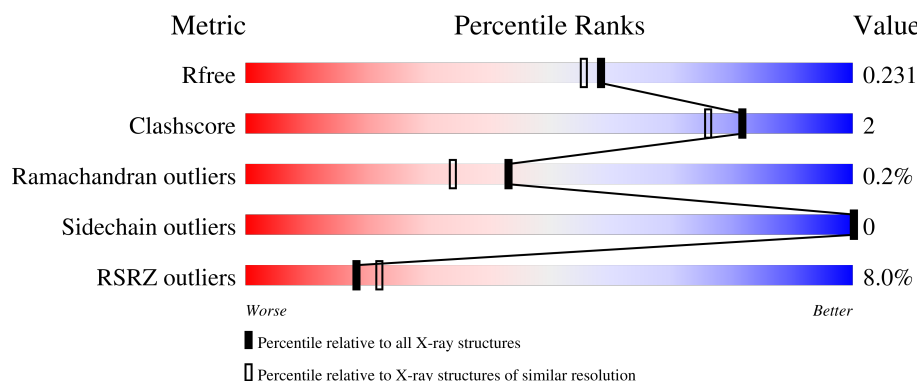
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	10	20% 70% 30%
2	A	580	8% 94% 6%
3	T	13	54% 46%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TC	T	15	-	-	-	X
3	FA2	T	16	-	-	-	X
3	FA2	T	6	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA chain called DNA (5'-D(P*GP*CP*GP*AP*TP*CP*AP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			

- Molecule 2 is a protein called DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	578	Total	C	N	O	S	0	0	0
			4644	2951	808	868	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	THR	SER	conflict	UNP E1C9K5

- Molecule 3 is a DNA chain called TNA (5'-D(P*(TG)P*(TFT)P*(FA2)P*(TC)P*(TG)P*(TFT)P*(TG)P*(FA2)P*(TFT)P*(TC)P*(TG)P*(TC)P*(FA2))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	13	Total	C	N	O	P	0	0	0
			255	114	50	78	13			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

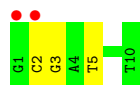
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	14	Total	O	0	0
			14	14		
5	A	259	Total	O	0	0
			259	259		
5	T	25	Total	O	0	0
			25	25		

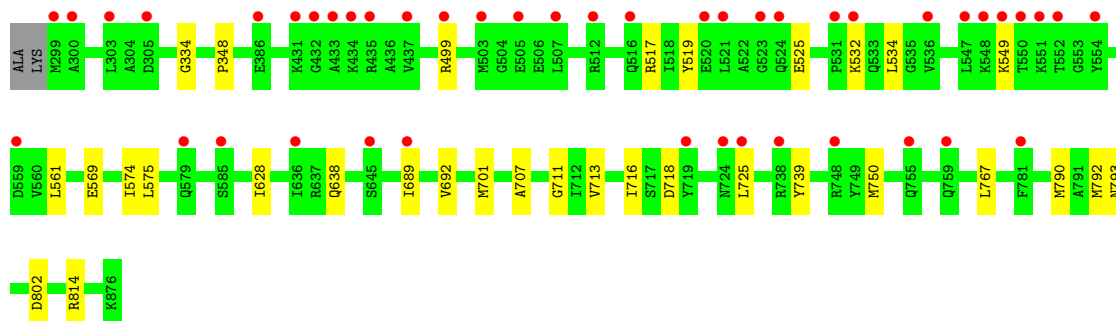
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: DNA (5'-D(P*GP*CP*GP*AP*TP*CP*AP*CP*GP*T)-3')



- Molecule 2: DNA polymerase I



- Molecule 3: TNA (5'-D(P*(TG)P*(TFT)P*(FA2)P*(TC)P*(TG)P*(TFT)P*(TG)P*(FA2)P*(TFT)P*(TC)P*(TG)P*(TC)P*(FA2))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.39Å 93.28Å 103.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.84 – 1.91 66.84 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (66.84-1.91) 91.8 (66.84-1.91)	Depositor EDS
R_{merge}	0.72	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.91Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.191 , 0.225 0.197 , 0.231	Depositor DCC
R_{free} test set	2011 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5437	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TG, SO4, TFT, TC, FA2

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	P	0.33	0/229	0.55	0/351
2	A	0.35	1/4727 (0.0%)	0.48	0/6388
All	All	0.35	1/4956 (0.0%)	0.49	0/6739

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	718	ASP	C-O	-6.44	1.16	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	205	0	113	3	0
2	A	4644	0	4699	17	0
3	T	255	0	57	8	0
4	A	30	0	0	0	0
4	P	5	0	0	0	0
5	A	259	0	0	0	0
5	P	14	0	0	0	0
5	T	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5437	0	4869	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:2:DC:H2'	1:P:3:DG:C8	2.26	0.70
2:A:692:VAL:HG21	2:A:701:MET:HE1	1.85	0.59
2:A:517:ARG:NH2	2:A:569:GLU:OE1	2.37	0.57
2:A:750:MET:SD	2:A:792:MET:HB3	2.44	0.57
2:A:689:ILE:HD11	2:A:739:TYR:HA	1.89	0.55
1:P:5:DT:H3	3:T:11:FA2:C2	2.22	0.52
2:A:519:TYR:CD2	2:A:525:GLU:HG2	2.46	0.50
3:T:11:FA2:H8	3:T:11:FA2:O3'	2.12	0.49
3:T:9:TFT:O3T	3:T:9:TFT:H6	2.13	0.49
2:A:790:MET:HE1	3:T:6:FA2:H4'1	1.95	0.48
2:A:549:LYS:N	2:A:549:LYS:HD3	2.30	0.46
2:A:814:ARG:HA	2:A:814:ARG:HD2	1.78	0.46
2:A:532:LYS:HE2	3:T:14:TG:C4'	2.45	0.46
2:A:711:GLY:HA2	2:A:716:ILE:HG12	1.97	0.46
2:A:534:LEU:HD11	2:A:574:ILE:HD13	1.98	0.46
2:A:499:ARG:NH2	2:A:638:GLN:OE1	2.34	0.44
3:T:5:TFT:H6	3:T:5:TFT:O3T	2.18	0.44
1:P:5:DT:H3	3:T:11:FA2:H2	1.82	0.43
2:A:713:VAL:O	2:A:793:ASN:ND2	2.49	0.43
2:A:707:ALA:CB	2:A:725:LEU:HD21	2.48	0.42
3:T:12:TFT:H6	3:T:12:TFT:O3T	2.19	0.42
2:A:561:LEU:HB2	2:A:575:LEU:HD21	2.02	0.41
2:A:334:GLY:HA2	2:A:348:PRO:HD3	2.04	0.40
2:A:767:LEU:HD12	2:A:802:ASP:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	576/580 (99%)	560 (97%)	15 (3%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	628	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	495/496 (100%)	495 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
2	A	516	GLN
2	A	704	GLN
2	A	724	ASN
2	A	812	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TFT	T	5	3	17,20,21	4.45	12 (70%)	23,29,32	2.62	12 (52%)
3	TG	T	14	3,1	20,23,24	4.53	13 (65%)	28,34,37	2.38	12 (42%)
3	TFT	T	9	3,1	17,20,21	4.36	11 (64%)	23,29,32	2.45	10 (43%)
3	TFT	T	12	3,1	17,20,21	4.58	11 (64%)	23,29,32	2.84	10 (43%)
3	TC	T	13	3,1	16,19,20	4.49	8 (50%)	21,27,30	1.40	4 (19%)
3	TC	T	15	3,1	16,19,20	4.44	8 (50%)	21,27,30	1.57	4 (19%)
3	TG	T	8	3,1	20,23,24	4.16	13 (65%)	28,34,37	2.38	12 (42%)
3	FA2	T	6	3,1	19,22,23	5.55	14 (73%)	26,32,35	4.33	16 (61%)
3	FA2	T	16	3	19,22,23	5.91	15 (78%)	26,32,35	4.55	13 (50%)
3	TC	T	7	3,1	16,19,20	4.24	8 (50%)	21,27,30	1.57	4 (19%)
3	TG	T	10	3,1	20,23,24	4.43	14 (70%)	28,34,37	2.33	11 (39%)
3	FA2	T	11	3,1	19,22,23	5.93	15 (78%)	26,32,35	4.55	13 (50%)
3	TG	T	4	3	20,23,24	4.60	14 (70%)	28,34,37	2.36	11 (39%)

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	TFT	T	5	3	-	3/5/21/22	0/2/2/2
3	TG	T	14	3,1	-	3/5/21/22	0/3/3/3
3	TFT	T	9	3,1	-	2/5/21/22	0/2/2/2
3	TFT	T	12	3,1	-	2/5/21/22	0/2/2/2
3	TC	T	13	3,1	-	4/5/21/22	0/2/2/2
3	TC	T	15	3,1	-	5/5/21/22	0/2/2/2
3	TG	T	8	3,1	-	0/5/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FA2	T	6	3,1	-	3/5/21/22	0/3/3/3
3	FA2	T	16	3	-	3/5/21/22	0/3/3/3
3	TC	T	7	3,1	-	5/5/21/22	0/2/2/2
3	TG	T	10	3,1	-	0/5/21/22	0/3/3/3
3	FA2	T	11	3,1	-	0/5/21/22	0/3/3/3
3	TG	T	4	3	-	0/5/21/22	0/3/3/3

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	11	FA2	C2-N3	11.68	1.54	1.33
3	T	16	FA2	C2-N3	11.66	1.54	1.33
3	T	6	FA2	C2-N3	10.68	1.52	1.33
3	T	11	FA2	O2'-C2'	-9.72	1.18	1.43
3	T	16	FA2	O2'-C2'	-9.70	1.18	1.43
3	T	4	TG	O2'-C2'	-9.64	1.19	1.43
3	T	13	TC	O2'-C2'	-9.48	1.19	1.43
3	T	15	TC	O2'-C2'	-9.38	1.19	1.43
3	T	14	TG	O2'-C2'	-9.20	1.20	1.43
3	T	14	TG	C5-N7	9.03	1.57	1.39
3	T	4	TG	C5-N7	8.93	1.57	1.39
3	T	11	FA2	C4-N3	8.93	1.51	1.34
3	T	16	FA2	C4-N3	8.91	1.51	1.34
3	T	10	TG	O2'-C2'	-8.89	1.20	1.43
3	T	10	TG	O6-C6	8.89	1.40	1.23
3	T	10	TG	C5-N7	8.88	1.56	1.39
3	T	14	TG	O6-C6	8.88	1.40	1.23
3	T	13	TC	O2-C2	8.86	1.40	1.23
3	T	15	TC	O2-C2	8.85	1.40	1.23
3	T	4	TG	O6-C6	8.80	1.40	1.23
3	T	6	FA2	O2'-C2'	-8.71	1.21	1.43
3	T	7	TC	O2'-C2'	-8.70	1.21	1.43
3	T	12	TFT	O2T-C2T	-8.69	1.21	1.43
3	T	8	TG	C5-N7	8.56	1.56	1.39
3	T	16	FA2	C5-C6	-8.49	1.17	1.41
3	T	11	FA2	C5-C6	-8.48	1.17	1.41
3	T	7	TC	O4'-C1'	8.42	1.54	1.42
3	T	9	TFT	O2T-C2T	-8.34	1.22	1.43
3	T	5	TFT	O2T-C2T	-8.17	1.22	1.43
3	T	8	TG	O6-C6	8.11	1.38	1.23
3	T	8	TG	O2'-C2'	-8.07	1.23	1.43
3	T	7	TC	O2-C2	8.05	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	6	FA2	C4-N3	7.98	1.49	1.34
3	T	6	FA2	C6-N1	-7.93	1.13	1.35
3	T	6	FA2	C5-C4	7.92	1.53	1.39
3	T	13	TC	O4'-C1'	7.87	1.53	1.42
3	T	15	TC	O4'-C1'	7.86	1.53	1.42
3	T	11	FA2	C5-C4	7.55	1.52	1.39
3	T	6	FA2	C5-C6	-7.55	1.20	1.41
3	T	16	FA2	C5-C4	7.51	1.52	1.39
3	T	11	FA2	C8-N9	-7.42	1.24	1.37
3	T	16	FA2	C8-N9	-7.41	1.24	1.37
3	T	16	FA2	C6-N1	-7.34	1.15	1.35
3	T	11	FA2	C6-N1	-7.32	1.15	1.35
3	T	12	TFT	C6-N1	7.25	1.50	1.38
3	T	9	TFT	O4T-C4T	6.94	1.58	1.43
3	T	9	TFT	C6-N1	6.71	1.49	1.38
3	T	6	FA2	C8-N9	-6.63	1.26	1.37
3	T	5	TFT	C2-N1	6.61	1.48	1.38
3	T	5	TFT	O4T-C4T	6.57	1.58	1.43
3	T	5	TFT	C6-N1	6.48	1.49	1.38
3	T	12	TFT	C2-N1	6.41	1.48	1.38
3	T	12	TFT	O4T-C4T	6.39	1.57	1.43
3	T	5	TFT	C4-C5	6.08	1.54	1.44
3	T	12	TFT	C4-C5	6.05	1.54	1.44
3	T	9	TFT	C2-N1	5.82	1.47	1.38
3	T	12	TFT	C2T-C3T	-5.72	1.38	1.53
3	T	5	TFT	C2T-C3T	-5.69	1.38	1.53
3	T	9	TFT	C4-C5	5.57	1.53	1.44
3	T	9	TFT	C2T-C3T	-5.54	1.38	1.53
3	T	4	TG	C4-N9	-5.51	1.24	1.38
3	T	12	TFT	O4T-C1T	5.47	1.50	1.42
3	T	4	TG	C8-N9	-5.45	1.25	1.37
3	T	10	TG	C8-N9	-5.41	1.25	1.37
3	T	14	TG	C8-N9	-5.41	1.25	1.37
3	T	8	TG	C8-N9	-5.28	1.25	1.37
3	T	14	TG	C4-N9	-5.20	1.24	1.38
3	T	10	TG	C4-N9	-5.19	1.24	1.38
3	T	11	FA2	C8-N7	-5.13	1.21	1.31
3	T	16	FA2	C8-N7	-5.08	1.21	1.31
3	T	5	TFT	O4T-C1T	5.02	1.49	1.42
3	T	8	TG	C4-N9	-4.98	1.25	1.38
3	T	14	TG	C2-N2	4.95	1.45	1.34
3	T	4	TG	C2-N2	4.94	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	15	TC	C4-N4	4.90	1.45	1.33
3	T	13	TC	C4-N4	4.81	1.45	1.33
3	T	16	FA2	C6-N6	4.80	1.46	1.34
3	T	9	TFT	O4T-C1T	4.79	1.49	1.42
3	T	11	FA2	C6-N6	4.78	1.46	1.34
3	T	8	TG	C2-N2	4.60	1.44	1.34
3	T	6	FA2	C6-N6	4.52	1.45	1.34
3	T	11	FA2	O4'-C1'	4.51	1.48	1.42
3	T	13	TC	C2'-C3'	-4.47	1.41	1.53
3	T	10	TG	C2-N2	4.31	1.44	1.34
3	T	7	TC	C4-N4	4.31	1.44	1.33
3	T	16	FA2	O4'-C1'	4.31	1.48	1.42
3	T	6	FA2	O4'-C4'	4.21	1.52	1.43
3	T	15	TC	C2'-C3'	-4.07	1.42	1.53
3	T	11	FA2	O4'-C4'	4.05	1.52	1.43
3	T	6	FA2	O4'-C1'	4.03	1.48	1.42
3	T	16	FA2	O4'-C4'	4.02	1.52	1.43
3	T	15	TC	C2-N3	3.96	1.44	1.36
3	T	4	TG	O4'-C1'	3.93	1.47	1.42
3	T	13	TC	C2-N3	3.93	1.44	1.36
3	T	6	FA2	C8-N7	-3.89	1.24	1.31
3	T	6	FA2	C5-N7	3.85	1.46	1.39
3	T	13	TC	O4'-C4'	3.83	1.52	1.43
3	T	14	TG	C4-N3	3.74	1.42	1.34
3	T	7	TC	O4'-C4'	3.72	1.51	1.43
3	T	7	TC	C2'-C3'	-3.71	1.43	1.53
3	T	14	TG	O4'-C1'	3.65	1.47	1.42
3	T	10	TG	O4'-C1'	3.65	1.47	1.42
3	T	7	TC	C2-N3	3.64	1.43	1.36
3	T	4	TG	O4'-C4'	3.59	1.51	1.43
3	T	15	TC	O4'-C4'	3.57	1.51	1.43
3	T	10	TG	O4'-C4'	3.57	1.51	1.43
3	T	12	TFT	C2-N3	3.53	1.44	1.38
3	T	8	TG	O4'-C4'	3.51	1.51	1.43
3	T	4	TG	C4-N3	3.50	1.42	1.34
3	T	11	FA2	C2'-C3'	-3.49	1.44	1.53
3	T	5	TFT	C2-N3	3.39	1.43	1.38
3	T	16	FA2	C2'-C3'	-3.39	1.44	1.53
3	T	14	TG	O4'-C4'	3.30	1.51	1.43
3	T	14	TG	C2-N3	3.25	1.41	1.33
3	T	6	FA2	C2'-C3'	-3.20	1.44	1.53
3	T	9	TFT	C2-N3	3.17	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	8	TG	O4'-C1'	3.16	1.46	1.42
3	T	4	TG	C2'-C3'	-3.14	1.45	1.53
3	T	10	TG	C5-C4	3.07	1.47	1.38
3	T	12	TFT	C4T-C3T	3.07	1.58	1.52
3	T	11	FA2	C5-N7	3.07	1.44	1.39
3	T	4	TG	C2-N3	3.06	1.40	1.33
3	T	16	FA2	C5-N7	3.06	1.44	1.39
3	T	5	TFT	C4T-C3T	3.00	1.58	1.52
3	T	4	TG	C2-N1	2.99	1.44	1.37
3	T	14	TG	C2'-C3'	-2.99	1.45	1.53
3	T	10	TG	C4-N3	2.98	1.41	1.34
3	T	9	TFT	C4T-C3T	2.96	1.58	1.52
3	T	14	TG	C5-C4	2.96	1.46	1.38
3	T	10	TG	C2-N3	2.96	1.40	1.33
3	T	4	TG	C5-C4	2.93	1.46	1.38
3	T	10	TG	C2'-C3'	-2.91	1.45	1.53
3	T	8	TG	C2'-C3'	-2.86	1.45	1.53
3	T	8	TG	C4-N3	2.84	1.40	1.34
3	T	8	TG	C5-C4	2.81	1.46	1.38
3	T	14	TG	C2-N1	2.78	1.44	1.37
3	T	8	TG	C2-N1	2.75	1.44	1.37
3	T	12	TFT	C2T-C1T	-2.67	1.45	1.53
3	T	5	TFT	C5M-C5	2.67	1.57	1.50
3	T	8	TG	C2-N3	2.54	1.39	1.33
3	T	12	TFT	C5M-C5	2.51	1.56	1.50
3	T	10	TG	C2-N1	2.51	1.43	1.37
3	T	9	TFT	C5M-C5	2.46	1.56	1.50
3	T	5	TFT	C2T-C1T	-2.46	1.45	1.53
3	T	9	TFT	C2T-C1T	-2.41	1.45	1.53
3	T	16	FA2	C4-N9	2.39	1.42	1.37
3	T	7	TC	C6-C5	2.38	1.40	1.35
3	T	11	FA2	C4-N9	2.37	1.42	1.37
3	T	15	TC	C6-C5	2.33	1.40	1.35
3	T	13	TC	C6-C5	2.28	1.40	1.35
3	T	6	FA2	C4-N9	2.21	1.42	1.37
3	T	4	TG	C2'-C1'	-2.08	1.47	1.53
3	T	5	TFT	C4-N3	2.07	1.42	1.38
3	T	10	TG	C6-N1	-2.06	1.35	1.38
3	T	11	FA2	C2'-C1'	-2.04	1.47	1.53
3	T	16	FA2	C2'-C1'	-2.02	1.47	1.53

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	11	FA2	N3-C4-N9	10.48	144.99	127.17
3	T	16	FA2	N3-C4-N9	10.44	144.92	127.17
3	T	6	FA2	C4-C5-N7	-10.01	99.14	110.58
3	T	11	FA2	C4-N9-C8	9.53	115.75	105.74
3	T	16	FA2	C4-N9-C8	9.48	115.69	105.74
3	T	6	FA2	N3-C4-N9	8.62	141.83	127.17
3	T	16	FA2	C4-C5-N7	-7.66	101.82	110.58
3	T	6	FA2	C5-C4-N3	-7.65	116.18	126.72
3	T	11	FA2	C4-C5-N7	-7.64	101.85	110.58
3	T	6	FA2	C4-N9-C8	7.62	113.74	105.74
3	T	16	FA2	C5-C4-N3	-7.37	116.57	126.72
3	T	11	FA2	C5-C4-N3	-7.36	116.58	126.72
3	T	6	FA2	C5-N7-C8	6.97	114.40	103.45
3	T	11	FA2	C5-C4-N9	-6.77	98.43	105.81
3	T	16	FA2	C5-C4-N9	-6.70	98.51	105.81
3	T	14	TG	C8-N9-C4	6.59	118.37	106.03
3	T	11	FA2	C2-N1-C6	6.54	129.47	118.73
3	T	16	FA2	C2-N1-C6	6.53	129.46	118.73
3	T	4	TG	C8-N9-C4	6.51	118.23	106.03
3	T	6	FA2	C2-N1-C6	6.21	128.92	118.73
3	T	16	FA2	C5-N7-C8	6.11	113.06	103.45
3	T	11	FA2	C5-N7-C8	6.08	113.01	103.45
3	T	16	FA2	C6-C5-C4	5.84	125.15	117.18
3	T	10	TG	C8-N9-C4	5.83	116.96	106.03
3	T	11	FA2	C6-C5-C4	5.82	125.13	117.18
3	T	12	TFT	C5-C4-N3	5.78	120.35	115.32
3	T	12	TFT	C4-N3-C2	-5.68	119.89	127.34
3	T	6	FA2	C6-C5-C4	5.58	124.79	117.18
3	T	12	TFT	O4T-C1T-N1	-5.57	101.83	108.90
3	T	8	TG	C8-N9-C4	5.53	116.39	106.03
3	T	5	TFT	C4-N3-C2	-5.30	120.39	127.34
3	T	16	FA2	N1-C2-N3	-5.20	120.71	128.58
3	T	11	FA2	N1-C2-N3	-5.18	120.74	128.58
3	T	9	TFT	C5-C4-N3	5.10	119.76	115.32
3	T	9	TFT	C4-N3-C2	-5.00	120.78	127.34
3	T	5	TFT	O4T-C4T-C3T	-4.73	96.23	104.42
3	T	7	TC	O4'-C1'-N1	-4.71	102.92	108.90
3	T	5	TFT	C5-C4-N3	4.53	119.26	115.32
3	T	5	TFT	N3-C2-N1	4.32	120.51	114.89
3	T	12	TFT	O4-C4-C5	-4.29	120.00	124.92
3	T	8	TG	C5-C4-N3	-4.29	121.56	128.39
3	T	4	TG	C8-N7-C5	-4.20	96.77	104.26
3	T	12	TFT	N3-C2-N1	4.18	120.34	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	14	TG	N9-C4-N3	4.13	134.22	125.95
3	T	10	TG	C4-C5-N7	-4.05	104.26	110.67
3	T	14	TG	C8-N7-C5	-4.04	97.07	104.26
3	T	15	TC	C4'-O4'-C1'	-4.02	96.62	107.53
3	T	9	TFT	O4-C4-C5	-3.96	120.39	124.92
3	T	10	TG	C5-C4-N3	-3.92	122.16	128.39
3	T	6	FA2	N1-C2-N3	-3.91	122.66	128.58
3	T	4	TG	N9-C4-N3	3.89	133.74	125.95
3	T	8	TG	C4-C5-N7	-3.87	104.55	110.67
3	T	10	TG	C6-C5-N7	3.80	137.21	130.29
3	T	8	TG	C2-N1-C6	-3.70	118.39	125.11
3	T	9	TFT	N3-C2-N1	3.69	119.70	114.89
3	T	12	TFT	C3T-C2T-C1T	3.65	107.94	99.91
3	T	14	TG	C5-C4-N3	-3.63	122.61	128.39
3	T	8	TG	C6-C5-N7	3.60	136.84	130.29
3	T	6	FA2	C4-N9-C1'	-3.58	118.27	126.63
3	T	8	TG	N9-C4-N3	3.54	133.03	125.95
3	T	6	FA2	C5-C4-N9	-3.52	101.97	105.81
3	T	5	TFT	O4-C4-C5	-3.41	121.01	124.92
3	T	9	TFT	O4T-C4T-C3T	-3.37	98.59	104.42
3	T	4	TG	C5-C4-N3	-3.35	123.06	128.39
3	T	10	TG	C8-N7-C5	-3.32	98.35	104.26
3	T	8	TG	C8-N7-C5	-3.25	98.46	104.26
3	T	10	TG	N9-C4-N3	3.24	132.42	125.95
3	T	10	TG	C2-N1-C6	-3.22	119.27	125.11
3	T	13	TC	C3'-C2'-C1'	3.18	106.92	99.91
3	T	15	TC	O4'-C1'-N1	3.11	112.85	108.90
3	T	16	FA2	C3'-C2'-C1'	3.10	106.73	99.91
3	T	9	TFT	C3T-C2T-C1T	3.03	106.59	99.91
3	T	5	TFT	C5M-C5-C6	-2.98	118.82	122.85
3	T	14	TG	C6-C5-N7	2.96	135.67	130.29
3	T	11	FA2	C3'-C2'-C1'	2.94	106.40	99.91
3	T	4	TG	C6-C5-N7	2.94	135.65	130.29
3	T	9	TFT	C5-C6-N1	-2.93	120.14	123.31
3	T	4	TG	C2-N1-C6	-2.90	119.85	125.11
3	T	14	TG	C4-C5-N7	-2.89	106.09	110.67
3	T	4	TG	C4-C5-N7	-2.88	106.11	110.67
3	T	12	TFT	C5-C6-N1	-2.86	120.21	123.31
3	T	14	TG	C2-N1-C6	-2.85	119.93	125.11
3	T	14	TG	C3'-C2'-C1'	2.83	106.14	99.91
3	T	8	TG	C5-C6-N1	2.82	120.44	113.25
3	T	14	TG	C5-C6-N1	2.69	120.11	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	TFT	C6-C5-C4	2.68	120.23	118.02
3	T	13	TC	C4'-O4'-C1'	-2.67	100.29	107.53
3	T	4	TG	C5-C6-N1	2.59	119.84	113.25
3	T	4	TG	O6-C6-C5	-2.54	119.83	126.53
3	T	10	TG	C3'-C2'-C1'	2.53	105.49	99.91
3	T	5	TFT	C6-N1-C2	-2.53	118.78	121.30
3	T	12	TFT	O4T-C4T-C3T	-2.51	100.08	104.42
3	T	10	TG	C5-C6-N1	2.50	119.63	113.25
3	T	10	TG	O4'-C4'-C3'	-2.50	100.09	104.42
3	T	5	TFT	C4T-O4T-C1T	-2.50	100.75	107.53
3	T	7	TC	O2-C2-N3	-2.49	118.40	122.33
3	T	15	TC	C3'-C2'-C1'	2.48	105.38	99.91
3	T	14	TG	O6-C6-C5	-2.45	120.06	126.53
3	T	5	TFT	C3T-C2T-C1T	2.40	105.19	99.91
3	T	10	TG	C1'-N9-C4	-2.37	119.47	126.49
3	T	6	FA2	C2-N3-C4	-2.36	106.08	111.83
3	T	6	FA2	N6-C6-N1	-2.33	113.20	118.38
3	T	8	TG	O4'-C4'-C3'	-2.30	100.43	104.42
3	T	11	FA2	C2-N3-C4	-2.30	106.21	111.83
3	T	5	TFT	C5-C6-N1	-2.30	120.81	123.31
3	T	16	FA2	C2-N3-C4	-2.30	106.22	111.83
3	T	9	TFT	O4T-C1T-N1	-2.30	105.98	108.90
3	T	7	TC	C3'-C2'-C1'	2.29	104.95	99.91
3	T	11	FA2	C1'-N9-C8	-2.28	122.04	127.09
3	T	6	FA2	C3'-C2'-C1'	2.27	104.92	99.91
3	T	12	TFT	O2T-C2T-C3T	-2.26	104.58	111.08
3	T	6	FA2	N9-C8-N7	-2.25	110.75	113.94
3	T	9	TFT	C6-C5-C4	2.22	119.85	118.02
3	T	8	TG	O4'-C1'-N9	-2.21	106.09	108.90
3	T	12	TFT	C6-C5-C4	2.21	119.84	118.02
3	T	14	TG	C1'-N9-C4	-2.21	119.96	126.49
3	T	14	TG	O3'-C3'-C4'	-2.21	105.93	113.24
3	T	4	TG	C3'-C2'-C1'	2.21	104.77	99.91
3	T	7	TC	C4'-O4'-C1'	-2.18	101.60	107.53
3	T	16	FA2	C1'-N9-C8	-2.17	122.28	127.09
3	T	4	TG	C1'-N9-C4	-2.14	120.17	126.49
3	T	16	FA2	N9-C8-N7	-2.13	110.92	113.94
3	T	13	TC	O4'-C1'-N1	-2.12	106.20	108.90
3	T	15	TC	O3'-C3'-C4'	-2.12	106.22	113.24
3	T	9	TFT	C4T-O4T-C1T	-2.10	101.82	107.53
3	T	11	FA2	N9-C8-N7	-2.10	110.96	113.94
3	T	13	TC	O4'-C4'-C3'	2.10	108.06	104.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	6	FA2	O3'-C3'-C4'	-2.09	106.32	113.24
3	T	6	FA2	C6-C5-N7	2.06	136.06	132.09
3	T	8	TG	C1'-N9-C4	-2.06	120.40	126.49
3	T	5	TFT	C5M-C5-C4	2.03	120.95	118.78
3	T	8	TG	O6-C6-C5	-2.01	121.22	126.53

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	13	TC	C2'-C1'-N1-C2
3	T	13	TC	C2'-C1'-N1-C6
3	T	14	TG	C2'-C3'-O3'-P
3	T	15	TC	C2'-C1'-N1-C2
3	T	15	TC	C2'-C1'-N1-C6
3	T	15	TC	C2'-C3'-O3'-P
3	T	16	FA2	C2'-C3'-O3'-P
3	T	16	FA2	C2'-C1'-N9-C8
3	T	16	FA2	C2'-C1'-N9-C4
3	T	15	TC	O4'-C1'-N1-C6
3	T	6	FA2	C2'-C1'-N9-C8
3	T	15	TC	O4'-C1'-N1-C2
3	T	5	TFT	O4T-C1T-N1-C6
3	T	5	TFT	C2T-C1T-N1-C6
3	T	6	FA2	C2'-C1'-N9-C4
3	T	13	TC	O4'-C1'-N1-C6
3	T	7	TC	O4'-C1'-N1-C6
3	T	5	TFT	O4T-C1T-N1-C2
3	T	9	TFT	O4T-C1T-N1-C6
3	T	7	TC	C2'-C1'-N1-C6
3	T	14	TG	C2'-C1'-N9-C8
3	T	7	TC	O4'-C1'-N1-C2
3	T	13	TC	O4'-C1'-N1-C2
3	T	7	TC	C2'-C3'-O3'-P
3	T	12	TFT	O4T-C1T-N1-C6
3	T	6	FA2	O4'-C1'-N9-C8
3	T	14	TG	C2'-C1'-N9-C4
3	T	12	TFT	O4T-C1T-N1-C2
3	T	9	TFT	C2T-C1T-N1-C6
3	T	7	TC	C2'-C1'-N1-C2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	TFT	1	0
3	T	14	TG	1	0
3	T	9	TFT	1	0
3	T	12	TFT	1	0
3	T	6	FA2	1	0
3	T	11	FA2	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	SO4	A	901	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	904	-	4,4,4	0.23	0	6,6,6	0.18	0
4	SO4	P	101	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	902	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	A	903	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	A	906	-	4,4,4	0.22	0	6,6,6	0.04	0
4	SO4	A	905	-	4,4,4	0.22	0	6,6,6	0.11	0

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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(Å ²)	Q<0.9
1	P	10/10 (100%)	2.12	2 (20%) 3 3	31, 42, 64, 86	2 (20%)
2	A	578/580 (99%)	0.59	45 (7%) 19 22	24, 39, 66, 101	0
3	T	0/13	-	-	-	-
All	All	588/603 (97%)	0.61	47 (7%) 18 22	24, 39, 66, 101	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	1	DG	8.9
1	P	2	DC	8.1
2	A	299	MET	5.0
2	A	431	LYS	4.7
2	A	512	ARG	4.3
2	A	554	TYR	4.2
2	A	300	ALA	4.1
2	A	719	TYR	4.0
2	A	523	GLY	4.0
2	A	433	ALA	3.9
2	A	645	SER	3.5
2	A	531	PRO	3.3
2	A	724	ASN	3.1
2	A	781	PHE	3.1
2	A	547	LEU	3.1
2	A	432	GLY	3.1
2	A	689	ILE	3.0
2	A	505	GLU	3.0
2	A	434	LYS	2.9
2	A	551	LYS	2.9
2	A	532	LYS	2.9
2	A	549	LYS	2.9
2	A	524	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	550	THR	2.8
2	A	725	LEU	2.7
2	A	559	ASP	2.6
2	A	521	LEU	2.5
2	A	305	ASP	2.5
2	A	507	LEU	2.5
2	A	499	ARG	2.5
2	A	548	LYS	2.4
2	A	386	GLU	2.3
2	A	636	ILE	2.3
2	A	536	VAL	2.3
2	A	435	ARG	2.3
2	A	516	GLN	2.3
2	A	759	GLN	2.2
2	A	503	MET	2.2
2	A	437	VAL	2.2
2	A	755	GLN	2.2
2	A	585	SER	2.2
2	A	520	GLU	2.2
2	A	579	GLN	2.1
2	A	303	LEU	2.1
2	A	738	ARG	2.1
2	A	552	THR	2.0
2	A	748	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FA2	T	16	20/21	0.30	0.45	100,106,135,136	20
3	TC	T	15	18/19	0.42	0.45	96,113,121,123	18
3	TG	T	4	21/22	0.79	0.18	67,83,91,91	0
3	TG	T	14	21/22	0.80	0.20	63,76,102,108	0
3	TFT	T	12	19/20	0.91	0.12	44,49,62,63	0
3	FA2	T	11	20/21	0.91	0.13	39,46,63,89	0
3	TC	T	13	18/19	0.92	0.12	44,54,70,76	0
3	TFT	T	5	19/20	0.93	0.13	33,43,53,54	0
3	TG	T	10	21/22	0.95	0.08	30,37,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TFT	T	9	19/20	0.97	0.08	28,34,40,43	0
3	TC	T	7	18/19	0.97	0.09	25,30,34,35	0
3	FA2	T	6	20/21	0.98	0.07	26,31,33,34	0
3	TG	T	8	21/22	0.98	0.05	25,29,34,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	901	5/5	0.74	0.13	77,81,91,92	0
4	SO4	A	906	5/5	0.77	0.14	106,110,112,114	0
4	SO4	A	903	5/5	0.82	0.14	87,93,96,100	0
4	SO4	A	905	5/5	0.83	0.11	87,89,92,97	0
4	SO4	P	101	5/5	0.83	0.14	91,93,95,99	0
4	SO4	A	904	5/5	0.85	0.11	88,89,93,94	0
4	SO4	A	902	5/5	0.96	0.11	39,39,41,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.