



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 PM UTC

PDB ID : 3P4B / pdb_00003p4b
Title : Alternatingly modified 2'Fluoro RNA octamer f/rA2U2-P3
Authors : Pallan, P.S.; Greene, E.M.; Jicman, P.A.; Pandey, R.K.; Manoharan, M.;
Rozners, E.; Egli, M.
Deposited on : 2010-10-06
Resolution : 1.45 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

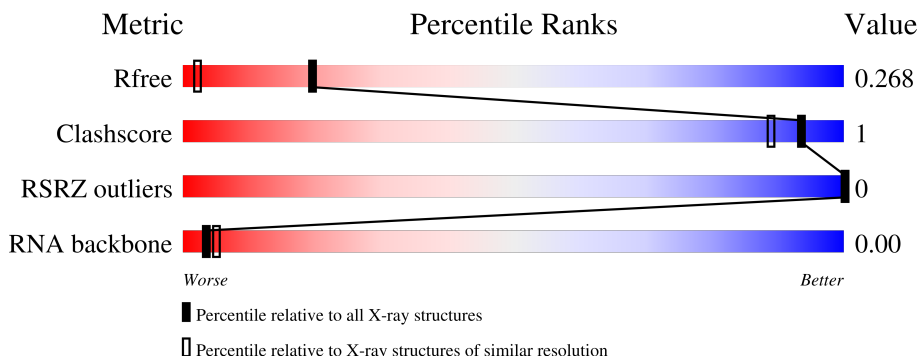
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

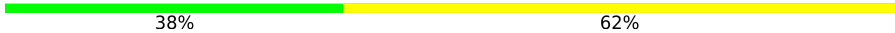
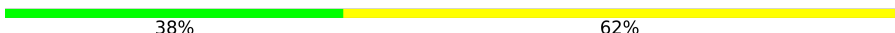
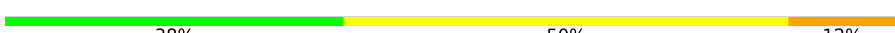
The reported resolution of this entry is 1.45 Å.

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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)
RNA backbone	3983	1019 (2.10-0.86)

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	A	8	 38% 62%
1	B	8	 50% 50%
1	C	8	 38% 62%
1	D	8	 38% 62%
1	E	8	 38% 50% 12%
1	F	8	 38% 50% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1145 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 RNA chain called 5'-R*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	8	Total	C	F	N	O	P	0	0	0
			167	76	4	30	50	7			
1	B	8	Total	C	F	N	O	P	0	0	0
			167	76	4	30	50	7			
1	C	8	Total	C	F	N	O	P	0	0	0
			167	76	4	30	50	7			
1	D	8	Total	C	F	N	O	P	0	0	0
			167	76	4	30	50	7			
1	E	8	Total	C	F	N	O	P	7	0	0
			167	76	4	30	50	7			
1	F	8	Total	C	F	N	O	P	7	0	0
			167	76	4	30	50	7			

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ba	0	0
			1	1		
2	D	1	Total	Ba	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	27	Total	O	0	0
			27	27		
3	C	30	Total	O	0	0
			30	30		
3	D	20	Total	O	0	0
			20	20		

Continued on next page...

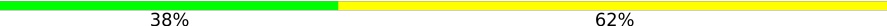
Continued from previous page...

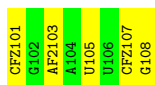
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	21	Total	O	0	0
			21	21		
3	F	19	Total	O	0	0
			19	19		

3 Residue-property plots

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.

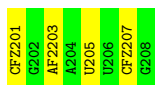
- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain A: 

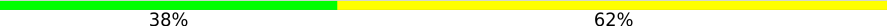


- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain B: 



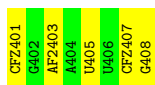
- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain C: 



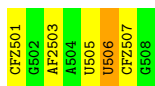
- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain D: 



- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain E: 



- Molecule 1: 5'-R(*(CFZ)P*GP*(AF2)P*AP*(UFT)P*UP*(CFZ)P*G)-3'

Chain F: 

CFZ601
G602
AF2603
A604
U605
U606
CFZ607
G608

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	43.38Å 43.38Å 60.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.69 – 1.45 21.69 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (21.69-1.45) 98.5 (21.69-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.251 0.215 , 0.268	Depositor DCC
R_{free} test set	1141 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.468 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1145	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.33% 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: CFZ, AF2, BA, UFT

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	1.30	1/96 (1.0%)	1.11	0/143
1	B	1.41	1/96 (1.0%)	0.88	0/143
1	C	1.49	2/96 (2.1%)	0.98	0/143
1	D	1.33	1/96 (1.0%)	1.08	0/143
1	E	1.58	3/96 (3.1%)	1.43	2/143 (1.4%)
1	F	2.71	2/96 (2.1%)	1.24	1/143 (0.7%)
All	All	1.71	10/576 (1.7%)	1.13	3/858 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	606	U	O5'-C5'	-21.59	1.10	1.42
1	F	606	U	C3'-O3'	9.62	1.56	1.42
1	C	305	UFT	O3'-P	8.72	1.65	1.56
1	E	506	U	O5'-C5'	-7.38	1.31	1.42
1	B	205	UFT	O3'-P	6.57	1.62	1.56
1	A	105	UFT	O3'-P	5.88	1.62	1.56
1	E	505	UFT	O3'-P	5.61	1.61	1.56
1	E	506	U	C3'-O3'	-5.57	1.33	1.42
1	D	405	UFT	O3'-P	5.36	1.61	1.56
1	C	306	U	C2'-C1'	-5.04	1.45	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	506	U	P-O5'-C5'	8.00	132.90	120.90
1	F	606	U	P-O5'-C5'	7.41	132.02	120.90
1	E	506	U	C4'-C3'-C2'	-5.38	97.22	102.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	506	U	Sidechain
1	F	606	U	Sidechain

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	A	167	0	83	1	0
1	B	167	0	83	0	0
1	C	167	0	83	0	0
1	D	167	0	83	1	0
1	E	167	0	83	0	0
1	F	167	0	83	0	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	0	1	0
3	B	27	0	0	0	0
3	C	30	0	0	0	0
3	D	20	0	0	1	0
3	E	21	0	0	0	0
3	F	19	0	0	0	0
All	All	1145	0	498	2	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 1.

All (2) 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:D:408:G:O3'	3:D:780:HOH:O	2.15	0.64
1:A:108:G:O3'	3:A:826:HOH:O	2.14	0.53

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/8	-	-
1	B	0/8	-	-
1	C	0/8	-	-
1	D	0/8	-	-
1	E	0/8	-	-
1	F	0/8	-	-
All	All	0/48	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	AF2	D	403	1	21,24,25	1.44	4 (19%)	30,35,38	1.90	9 (30%)
1	CFZ	B	207	1	18,21,22	1.26	2 (11%)	25,30,33	0.95	1 (4%)
1	CFZ	F	607	1	18,21,22	1.15	2 (11%)	25,30,33	0.89	2 (8%)
1	AF2	F	603	1	21,24,25	1.24	3 (14%)	30,35,38	2.11	9 (30%)
1	UFT	A	105	2,1	18,21,22	1.44	3 (16%)	25,30,33	1.92	6 (24%)
1	CFZ	B	201	1	18,18,22	1.00	2 (11%)	26,26,33	0.75	0
1	AF2	B	203	1	21,24,25	1.03	1 (4%)	30,35,38	2.22	10 (33%)
1	UFT	C	305	1	18,21,22	1.79	4 (22%)	25,30,33	1.92	4 (16%)
1	AF2	C	303	1	21,24,25	0.90	1 (4%)	30,35,38	2.19	10 (33%)
1	CFZ	C	301	1	18,18,22	1.01	1 (5%)	26,26,33	0.86	0
1	UFT	B	205	1	18,21,22	1.64	4 (22%)	25,30,33	1.84	4 (16%)
1	CFZ	D	401	1	18,18,22	0.81	0	26,26,33	1.08	2 (7%)
1	UFT	E	505	1	18,21,22	1.93	4 (22%)	25,30,33	1.92	5 (20%)
1	CFZ	E	501	1	18,18,22	1.31	1 (5%)	26,26,33	0.83	1 (3%)
1	UFT	D	405	2,1	18,21,22	1.24	1 (5%)	25,30,33	1.71	6 (24%)
1	CFZ	E	507	1	18,21,22	1.57	4 (22%)	25,30,33	1.02	1 (4%)
1	CFZ	F	601	1	18,18,22	1.19	2 (11%)	26,26,33	0.96	1 (3%)
1	UFT	F	605	1	18,21,22	1.99	4 (22%)	25,30,33	1.93	6 (24%)
1	CFZ	A	101	1	18,18,22	1.02	1 (5%)	26,26,33	0.96	2 (7%)
1	CFZ	A	107	1	18,21,22	0.94	0	25,30,33	1.26	3 (12%)
1	AF2	A	103	1	21,24,25	1.50	3 (14%)	30,35,38	1.93	8 (26%)
1	CFZ	D	407	1	18,21,22	0.77	0	25,30,33	1.13	2 (8%)
1	AF2	E	503	1	21,24,25	1.26	2 (9%)	30,35,38	2.05	8 (26%)
1	CFZ	C	307	1	18,21,22	1.16	1 (5%)	25,30,33	1.07	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AF2	D	403	1	-	0/7/25/26	0/3/3/3
1	CFZ	B	207	1	-	0/7/25/26	0/2/2/2
1	CFZ	F	607	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AF2	F	603	1	-	0/7/25/26	0/3/3/3
1	UFT	A	105	2,1	-	0/7/25/26	0/2/2/2
1	CFZ	B	201	1	-	2/6/22/26	0/2/2/2
1	AF2	B	203	1	-	0/7/25/26	0/3/3/3
1	UFT	C	305	1	-	0/7/25/26	0/2/2/2
1	AF2	C	303	1	-	0/7/25/26	0/3/3/3
1	CFZ	C	301	1	-	0/6/22/26	0/2/2/2
1	UFT	B	205	1	-	0/7/25/26	0/2/2/2
1	CFZ	D	401	1	-	0/6/22/26	0/2/2/2
1	UFT	E	505	1	-	0/7/25/26	0/2/2/2
1	CFZ	E	501	1	-	0/6/22/26	0/2/2/2
1	UFT	D	405	2,1	-	0/7/25/26	0/2/2/2
1	CFZ	E	507	1	-	0/7/25/26	0/2/2/2
1	CFZ	F	601	1	-	0/6/22/26	0/2/2/2
1	UFT	F	605	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	101	1	-	0/6/22/26	0/2/2/2
1	CFZ	A	107	1	-	0/7/25/26	0/2/2/2
1	AF2	A	103	1	-	0/7/25/26	0/3/3/3
1	CFZ	D	407	1	-	0/7/25/26	0/2/2/2
1	AF2	E	503	1	-	0/7/25/26	0/3/3/3
1	CFZ	C	307	1	-	0/7/25/26	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	505	UFT	O4-C4	5.59	1.35	1.24
1	F	605	UFT	O4-C4	5.39	1.35	1.24
1	C	305	UFT	C2'-C1'	-4.87	1.47	1.53
1	A	105	UFT	O4-C4	4.03	1.32	1.24
1	B	205	UFT	C2'-C1'	-4.01	1.48	1.53
1	A	103	AF2	C2'-C1'	-3.87	1.48	1.53
1	E	501	CFZ	C2'-C1'	-3.85	1.48	1.53
1	C	307	CFZ	O3'-C3'	3.77	1.52	1.43
1	B	207	CFZ	O3'-C3'	3.69	1.52	1.43
1	E	507	CFZ	O3'-C3'	3.52	1.51	1.43
1	F	605	UFT	C2'-C3'	-3.45	1.48	1.52
1	F	605	UFT	C2-N3	-3.34	1.32	1.38
1	B	205	UFT	O4-C4	3.26	1.30	1.24
1	F	601	CFZ	C2'-C1'	-3.23	1.49	1.53
1	C	305	UFT	O4-C4	3.11	1.30	1.24
1	D	403	AF2	C2'-C1'	-3.10	1.49	1.53
1	D	403	AF2	C5-N7	-2.92	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	505	UFT	C2'-C3'	-2.91	1.48	1.52
1	D	405	UFT	O4-C4	2.89	1.30	1.24
1	E	507	CFZ	O5'-C5'	-2.89	1.35	1.44
1	E	505	UFT	O2-C2	2.87	1.28	1.23
1	F	605	UFT	C4-N3	-2.83	1.33	1.38
1	F	607	CFZ	C2'-C1'	-2.82	1.49	1.53
1	E	505	UFT	C2-N3	-2.74	1.33	1.38
1	E	503	AF2	C4-N9	-2.74	1.32	1.37
1	B	205	UFT	C2'-C3'	-2.60	1.49	1.52
1	B	207	CFZ	O2-C2	2.50	1.28	1.23
1	A	103	AF2	C2-N3	2.46	1.38	1.33
1	E	503	AF2	C8-N7	2.45	1.36	1.31
1	F	603	AF2	C4-N9	-2.40	1.32	1.37
1	C	303	AF2	C8-N7	2.39	1.36	1.31
1	E	507	CFZ	C2'-C1'	-2.37	1.50	1.53
1	B	203	AF2	C8-N7	2.36	1.36	1.31
1	B	205	UFT	C6-C5	2.31	1.40	1.35
1	C	305	UFT	C2'-C3'	-2.29	1.49	1.52
1	D	403	AF2	O4'-C1'	2.26	1.47	1.42
1	F	603	AF2	C8-N7	2.23	1.36	1.31
1	C	301	CFZ	C1'-N1	2.20	1.53	1.47
1	A	105	UFT	C6-C5	2.19	1.40	1.35
1	B	201	CFZ	C1'-N1	2.19	1.53	1.47
1	A	103	AF2	C5-N7	-2.11	1.35	1.39
1	A	101	CFZ	C2-N1	2.10	1.44	1.40
1	A	105	UFT	F2'-C2'	-2.10	1.36	1.40
1	F	607	CFZ	O3'-C3'	2.10	1.48	1.43
1	C	305	UFT	C6-C5	2.06	1.39	1.35
1	B	201	CFZ	C2-N1	2.06	1.44	1.40
1	E	507	CFZ	C5-C4	2.06	1.47	1.42
1	F	603	AF2	F-C2'	2.06	1.44	1.40
1	D	403	AF2	C2-N3	2.04	1.37	1.33
1	F	601	CFZ	F2'-C2'	-2.01	1.36	1.40

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	603	AF2	N3-C2-N1	-5.64	120.05	128.58
1	E	503	AF2	N3-C2-N1	-5.63	120.06	128.58
1	A	103	AF2	N3-C2-N1	-5.47	120.30	128.58
1	B	203	AF2	N3-C2-N1	-5.43	120.36	128.58
1	C	303	AF2	N3-C2-N1	-5.12	120.83	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	UFT	C4-N3-C2	-4.93	120.49	126.61
1	B	205	UFT	C4-N3-C2	-4.85	120.59	126.61
1	D	403	AF2	N3-C2-N1	-4.81	121.30	128.58
1	B	203	AF2	C5-C4-N3	-4.67	120.28	126.72
1	E	505	UFT	C4-N3-C2	-4.66	120.83	126.61
1	C	303	AF2	C5-C4-N3	-4.65	120.31	126.72
1	A	105	UFT	N3-C2-N1	4.65	120.95	114.89
1	C	305	UFT	N3-C2-N1	4.62	120.91	114.89
1	B	203	AF2	N9-C8-N7	-4.54	107.49	113.94
1	C	305	UFT	C5-C4-N3	4.40	120.97	114.80
1	B	205	UFT	C5-C4-N3	4.35	120.89	114.80
1	F	605	UFT	C5-C4-N3	4.33	120.87	114.80
1	D	403	AF2	C5-C4-N3	-4.33	120.76	126.72
1	B	205	UFT	N3-C2-N1	4.32	120.52	114.89
1	F	605	UFT	C4-N3-C2	-4.30	121.28	126.61
1	A	105	UFT	C4-N3-C2	-4.28	121.30	126.61
1	C	303	AF2	N9-C8-N7	-4.27	107.87	113.94
1	E	503	AF2	N9-C8-N7	-4.21	107.97	113.94
1	F	605	UFT	N3-C2-N1	4.20	120.36	114.89
1	F	603	AF2	N9-C8-N7	-4.15	108.05	113.94
1	E	505	UFT	C5-C4-N3	4.11	120.56	114.80
1	D	405	UFT	C4-N3-C2	-3.99	121.66	126.61
1	E	505	UFT	N3-C2-N1	3.94	120.03	114.89
1	F	603	AF2	C5-C4-N3	-3.93	121.31	126.72
1	D	405	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	105	UFT	C2'-C1'-N1	-3.60	108.73	114.27
1	A	107	CFZ	C2'-C1'-N1	-3.58	108.77	114.27
1	A	103	AF2	N9-C8-N7	-3.57	108.87	113.94
1	E	505	UFT	O4-C4-C5	-3.56	119.03	125.16
1	E	505	UFT	C2'-C1'-N1	-3.51	108.88	114.27
1	A	103	AF2	C5-C4-N3	-3.49	121.90	126.72
1	B	203	AF2	C2'-C1'-N9	-3.47	107.71	113.92
1	F	605	UFT	O4-C4-C5	-3.47	119.18	125.16
1	B	203	AF2	C2-N3-C4	3.44	120.23	111.83
1	F	603	AF2	C4-N9-C8	3.44	109.35	105.74
1	E	503	AF2	C4-N9-C8	3.43	109.34	105.74
1	E	503	AF2	C5-C4-N3	-3.43	122.00	126.72
1	A	105	UFT	O2-C2-N1	-3.39	118.38	122.80
1	A	105	UFT	C5-C4-N3	3.39	119.55	114.80
1	D	401	CFZ	C3'-C2'-C1'	-3.31	99.26	103.10
1	C	303	AF2	C2'-C1'-N9	-3.29	108.02	113.92
1	E	507	CFZ	C2'-C3'-C4'	-3.26	98.13	102.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	603	AF2	C2-N3-C4	3.24	119.75	111.83
1	D	405	UFT	C5-C4-N3	3.23	119.32	114.80
1	C	303	AF2	C2-N3-C4	3.20	119.64	111.83
1	E	503	AF2	C2-N3-C4	3.13	119.46	111.83
1	D	405	UFT	C2'-C1'-N1	-3.11	109.50	114.27
1	D	403	AF2	N9-C8-N7	-3.11	109.53	113.94
1	F	603	AF2	C4-C5-N7	-3.07	107.08	110.58
1	B	203	AF2	C4-N9-C8	3.06	108.95	105.74
1	D	403	AF2	N3-C4-N9	3.00	132.28	127.17
1	F	605	UFT	C2'-C1'-N1	-2.99	109.67	114.27
1	D	407	CFZ	C2'-C1'-N1	-2.97	109.71	114.27
1	A	103	AF2	C2-N3-C4	2.97	119.07	111.83
1	E	503	AF2	C4-C5-N7	-2.96	107.19	110.58
1	A	107	CFZ	C3'-C2'-C1'	-2.93	99.70	103.10
1	D	407	CFZ	C3'-C2'-C1'	-2.92	99.71	103.10
1	C	303	AF2	C5-N7-C8	2.91	108.03	103.45
1	A	105	UFT	O4-C4-C5	-2.88	120.19	125.16
1	B	203	AF2	N3-C4-N9	2.88	132.06	127.17
1	D	401	CFZ	C2'-C3'-C4'	-2.85	98.67	102.43
1	C	303	AF2	C4-N9-C8	2.84	108.72	105.74
1	F	603	AF2	C5-N7-C8	2.82	107.88	103.45
1	C	303	AF2	C2'-C3'-C4'	-2.81	98.73	102.43
1	C	303	AF2	C4-C5-N7	-2.79	107.39	110.58
1	B	203	AF2	C5-N7-C8	2.77	107.80	103.45
1	D	405	UFT	O2-C2-N1	-2.75	119.21	122.80
1	F	601	CFZ	C3'-C2'-C1'	-2.75	99.90	103.10
1	B	207	CFZ	C2'-C3'-C4'	-2.75	98.81	102.43
1	D	403	AF2	C5-N7-C8	2.74	107.76	103.45
1	D	403	AF2	C2-N3-C4	2.71	118.45	111.83
1	C	305	UFT	O4-C4-C5	-2.69	120.53	125.16
1	B	203	AF2	C2'-C3'-C4'	-2.69	98.89	102.43
1	A	101	CFZ	C3'-C2'-C1'	-2.68	99.98	103.10
1	C	303	AF2	N3-C4-N9	2.68	131.72	127.17
1	A	103	AF2	C5-N7-C8	2.67	107.65	103.45
1	F	607	CFZ	C2'-C3'-C4'	-2.63	98.97	102.43
1	D	405	UFT	O4-C4-C5	-2.63	120.64	125.16
1	E	503	AF2	C5-N7-C8	2.60	107.54	103.45
1	B	205	UFT	O4-C4-C5	-2.59	120.69	125.16
1	C	307	CFZ	C3'-C2'-C1'	-2.56	100.13	103.10
1	D	403	AF2	C2-N1-C6	2.44	122.73	118.73
1	E	501	CFZ	C3'-C2'-C1'	-2.40	100.31	103.10
1	A	103	AF2	C4-N9-C8	2.39	108.24	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	AF2	N3-C4-N9	2.37	131.20	127.17
1	A	101	CFZ	C2'-C3'-C4'	-2.34	99.35	102.43
1	F	603	AF2	C2-N1-C6	2.33	122.55	118.73
1	F	603	AF2	N3-C4-N9	2.28	131.04	127.17
1	D	403	AF2	C3'-C2'-C1'	-2.28	100.45	103.10
1	A	103	AF2	C2-N1-C6	2.27	122.47	118.73
1	F	605	UFT	C2'-C3'-C4'	-2.20	99.53	102.43
1	B	203	AF2	C4-C5-N7	-2.20	108.07	110.58
1	A	107	CFZ	C2'-C3'-C4'	-2.20	99.54	102.43
1	E	503	AF2	C2-N1-C6	2.17	122.29	118.73
1	C	307	CFZ	C2'-C3'-C4'	-2.15	99.60	102.43
1	D	403	AF2	C4-C5-N7	-2.11	108.17	110.58
1	F	607	CFZ	F2'-C2'-C1'	-2.01	104.84	108.88

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	201	CFZ	O4'-C4'-C5'-O5'
1	B	201	CFZ	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	4/8 (50%)	-1.01	0 100 100	15, 16, 18, 20	0
1	B	4/8 (50%)	-1.08	0 100 100	13, 15, 17, 20	0
1	C	4/8 (50%)	-1.08	0 100 100	13, 15, 17, 19	0
1	D	4/8 (50%)	-1.01	0 100 100	15, 15, 17, 20	0
1	E	4/8 (50%)	-0.89	0 100 100	17, 17, 18, 23	1 (25%)
1	F	4/8 (50%)	-0.89	0 100 100	17, 17, 17, 23	1 (25%)
All	All	24/48 (50%)	-0.99	0 100 100	13, 17, 20, 23	2 (8%)

There are no RSRZ outliers to report.

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
1	CFZ	E	507	20/21	0.97	0.06	16,21,32,34	0
1	UFT	A	105	20/21	0.98	0.04	12,18,20,20	0
1	CFZ	B	201	17/21	0.98	0.04	15,20,27,30	0
1	CFZ	C	301	17/21	0.98	0.04	15,20,25,29	0
1	CFZ	D	401	17/21	0.98	0.04	13,17,22,22	0
1	AF2	D	403	22/23	0.98	0.04	13,15,19,20	0
1	UFT	D	405	20/21	0.98	0.04	12,18,20,20	0
1	CFZ	E	501	17/21	0.98	0.05	14,17,19,21	0
1	AF2	E	503	22/23	0.98	0.05	17,19,26,29	0
1	CFZ	A	101	17/21	0.98	0.04	12,17,21,23	0
1	CFZ	F	601	17/21	0.98	0.04	14,16,19,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	AF2	F	603	22/23	0.98	0.05	17,20,26,28	0
1	UFT	F	605	20/21	0.98	0.05	15,21,27,27	0
1	CFZ	F	607	20/21	0.98	0.05	15,20,32,36	0
1	UFT	B	205	20/21	0.99	0.03	11,13,16,16	0
1	CFZ	D	407	20/21	0.99	0.04	13,16,19,20	0
1	CFZ	B	207	20/21	0.99	0.04	12,13,21,23	0
1	CFZ	A	107	20/21	0.99	0.04	13,16,19,19	0
1	UFT	E	505	20/21	0.99	0.04	15,21,27,27	0
1	AF2	C	303	22/23	0.99	0.04	13,17,21,23	0
1	UFT	C	305	20/21	0.99	0.04	11,13,16,16	0
1	CFZ	C	307	20/21	0.99	0.04	11,14,20,24	0
1	AF2	A	103	22/23	0.99	0.03	12,16,19,21	0
1	AF2	B	203	22/23	0.99	0.04	13,17,20,24	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
2	BA	D	702	1/1	0.98	0.33	45,45,45,45	0
2	BA	A	701	1/1	0.99	0.28	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.