



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:14 AM EDT

PDB ID : 5VOE
Title : DesGla-XaS195A Bound to Aptamer 11F7t
Authors : Gunaratne, R.; Kumar, S.; Frederiksen, J.W.; Stayrook, S.; Lohrmann, J.L.; Perry, K.; Chabata, C.V.; Thalji, N.K.; Ho, M.D.; Arepally, G.; Camire, R.M.; Krishnaswamy, S.K.; Sullenger, B.A.
Deposited on : 2017-05-02
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

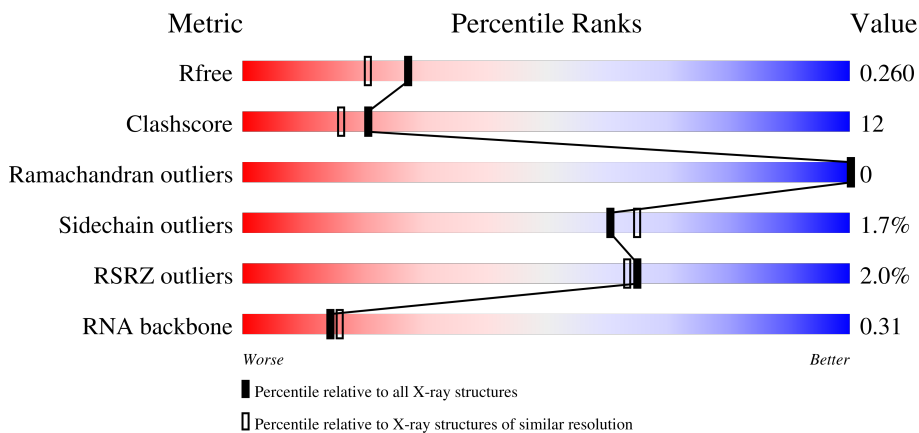
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

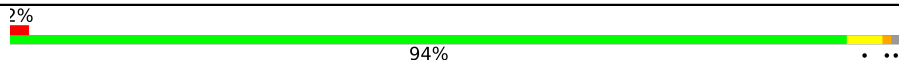
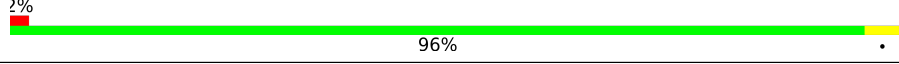

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

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	H	233	 2% 94%
2	L	51	 2% 96%
3	A	36	 19% 31% 42% 8%

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	CFL	A	28	-	-	X	-
3	CFL	A	29	-	-	X	-
3	CFL	A	32	-	-	X	-
3	UFT	A	33	-	-	X	-
3	CFL	A	6	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3129 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 protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	231	1831	1154	319	344	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	engineered mutation	UNP P00742

- Molecule 2 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	51	375	225	64	79	7	0	0	0

- Molecule 3 is a RNA chain called Aptamer 11F7t (36-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
3	A	36	760	341	19	135	230	35	0	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Mg 2	0	0

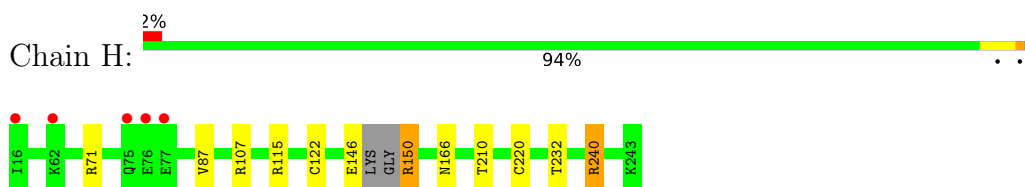
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	97	Total 97	O 97	0	0
7	L	26	Total 26	O 26	0	0
7	A	36	Total 36	O 36	0	0

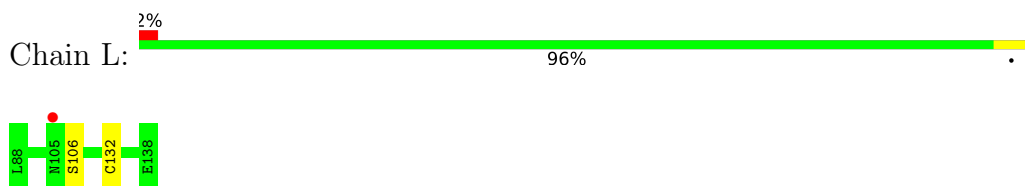
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

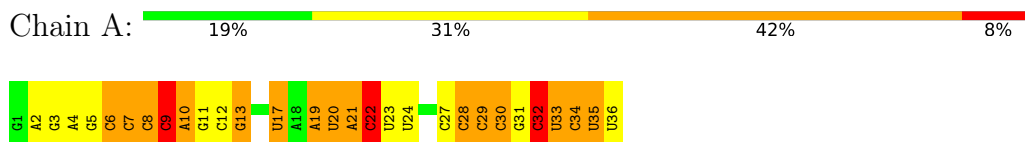
- Molecule 1: Coagulation factor X



- Molecule 2: Coagulation factor X



- Molecule 3: Aptamer 11F7t (36-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	55.92Å 164.60Å 124.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.30 – 2.00 48.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (82.30-2.00) 97.0 (48.73-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.248 0.221 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.509	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3129	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CFL, UFT, MG, NA

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	H	0.58	0/1868	0.81	6/2516 (0.2%)
2	L	0.58	0/381	0.75	0/516
3	A	2.16	2/430 (0.5%)	1.66	6/673 (0.9%)
All	All	1.01	2/2679 (0.1%)	1.01	12/3705 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	30	CFL	O3'-P	-42.55	1.10	1.61
3	A	9	CFL	O3'-P	5.50	1.67	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	30	CFL	P-O3'-C3'	19.03	142.53	119.70
3	A	12	CFL	P-O3'-C3'	-17.86	98.27	119.70
3	A	9	CFL	OP1-P-O3'	-16.68	68.50	105.20
3	A	9	CFL	OP2-P-O3'	15.43	139.15	105.20
3	A	12	CFL	OP2-P-O3'	11.01	129.42	105.20
3	A	12	CFL	OP1-P-O3'	-9.73	83.80	105.20
1	H	115	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	H	240	ARG	CG-CD-NE	5.87	124.12	111.80
1	H	240	ARG	CB-CG-CD	5.41	125.66	111.60
1	H	71	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	H	220	CYS	CA-CB-SG	5.07	123.13	114.00
1	H	107	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	H	1831	0	1784	12	0
2	L	375	0	336	1	0
3	A	760	0	376	54	0
4	H	1	0	0	0	0
5	H	1	0	0	0	0
6	A	2	0	0	1	0
7	A	36	0	0	2	1
7	H	97	0	0	2	0
7	L	26	0	0	0	0
All	All	3129	0	2496	63	1

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 12.

All (63) 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)
3:A:28:CFL:C3'	3:A:29:CFL:P	2.17	1.32
3:A:32:CFL:C3'	3:A:33:UFT:P	2.19	1.29
3:A:6:CFL:C3'	3:A:7:CFL:P	2.22	1.26
3:A:30:CFL:HO3'	3:A:31:G:P	1.13	1.21
3:A:6:CFL:HO3'	3:A:7:CFL:P	0.77	1.14
3:A:30:CFL:C3'	3:A:31:G:P	2.41	1.09
3:A:28:CFL:O3'	3:A:29:CFL:O2P	1.83	0.95
3:A:17:UFT:H5	3:A:19:A:N7	1.85	0.91
3:A:6:CFL:O3'	3:A:7:CFL:O1P	1.88	0.91
3:A:13:G:OP1	7:A:201:HOH:O	1.88	0.91
3:A:32:CFL:O3'	3:A:33:UFT:OP1	1.94	0.85
1:H:150:ARG:HG2	1:H:150:ARG:HH11	1.42	0.82
3:A:19:A:H4'	3:A:20:UFT:H5'	1.60	0.82
3:A:4:A:H2'	3:A:5:G:C8	2.15	0.81
3:A:32:CFL:O3'	3:A:33:UFT:O5'	1.98	0.80
3:A:32:CFL:H3'	3:A:33:UFT:P	2.21	0.80
3:A:32:CFL:HO3'	3:A:33:UFT:P	1.25	0.80
3:A:30:CFL:O3'	3:A:31:G:OP2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:28:CFL:O3'	3:A:29:CFL:O5'	1.99	0.79
3:A:28:CFL:H3'	3:A:29:CFL:P	2.22	0.77
3:A:10:A:H4'	3:A:11:G:OP2	1.89	0.73
3:A:6:CFL:H3'	3:A:7:CFL:P	2.29	0.73
3:A:10:A:OP2	6:A:102:MG:MG	1.33	0.71
3:A:28:CFL:HO3'	3:A:29:CFL:P	1.46	0.69
3:A:4:A:H2'	3:A:5:G:H8	1.56	0.67
1:H:150:ARG:HH11	1:H:150:ARG:CG	2.10	0.62
3:A:6:CFL:H6	3:A:6:CFL:O5'	2.01	0.60
3:A:19:A:H3'	3:A:19:A:OP1	2.00	0.60
3:A:32:CFL:F	3:A:33:UFT:O4'	2.11	0.57
3:A:19:A:C4'	3:A:20:UFT:H5'	2.34	0.57
1:H:146:GLU:C	1:H:150:ARG:HH21	2.08	0.56
1:H:146:GLU:C	1:H:150:ARG:NH2	2.60	0.55
3:A:31:G:H2'	3:A:32:CFL:H6	1.87	0.55
1:H:240:ARG:HD2	3:A:28:CFL:O2	2.07	0.55
3:A:3:G:C6	3:A:4:A:C6	2.97	0.52
3:A:10:A:C4	3:A:21:A:H5'	2.44	0.52
3:A:4:A:C2	3:A:34:CFL:N3	2.79	0.51
3:A:33:UFT:H2'	3:A:34:CFL:H6	1.93	0.51
3:A:2:A:H2'	3:A:3:G:C8	2.46	0.50
1:H:240:ARG:CD	3:A:28:CFL:O2	2.59	0.50
1:H:150:ARG:HG2	1:H:150:ARG:NH1	2.19	0.50
3:A:32:CFL:H6	3:A:32:CFL:O5'	2.11	0.49
3:A:29:CFL:O5'	3:A:29:CFL:H6	2.12	0.49
1:H:166:ASN:ND2	7:H:401:HOH:O	2.41	0.48
3:A:6:CFL:F	3:A:7:CFL:O4'	2.21	0.47
3:A:34:CFL:F	3:A:35:UFT:O4'	2.22	0.47
3:A:33:UFT:H2'	3:A:34:CFL:C6	2.45	0.46
3:A:30:CFL:H3'	3:A:31:G:OP2	2.14	0.46
3:A:20:UFT:F2'	3:A:21:A:OP2	2.24	0.45
3:A:6:CFL:HO3'	3:A:7:CFL:C5'	2.14	0.45
1:H:150:ARG:CG	1:H:150:ARG:NH1	2.73	0.44
1:H:240:ARG:HD3	3:A:29:CFL:H1'	1.99	0.44
1:H:232:THR:HG23	7:H:429:HOH:O	2.17	0.44
3:A:22:CFL:O1P	7:A:202:HOH:O	2.21	0.43
1:H:122:CYS:SG	2:L:132:CYS:C	2.96	0.43
3:A:33:UFT:O5'	3:A:33:UFT:H6	2.18	0.43
3:A:34:CFL:F	3:A:35:UFT:H6	2.10	0.42
3:A:10:A:C4'	3:A:11:G:OP2	2.56	0.41
3:A:3:G:C6	3:A:4:A:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:CFL:F	3:A:9:CFL:O4'	2.28	0.41
3:A:20:UFT:O2	3:A:20:UFT:C2'	2.69	0.41
3:A:31:G:H2'	3:A:32:CFL:C6	2.48	0.41
3:A:10:A:N3	3:A:21:A:H5'	2.36	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
7:A:213:HOH:O	7:A:213:HOH:O[3_454]	1.83	0.37

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	
1	H	227/233 (97%)	222 (98%)	5 (2%)	0	100	100
2	L	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
All	All	276/284 (97%)	269 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	H	196/197 (100%)	193 (98%)	3 (2%)	65	69
2	L	43/43 (100%)	42 (98%)	1 (2%)	50	53
All	All	239/240 (100%)	235 (98%)	4 (2%)	60	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	87	VAL
1	H	150	ARG
1	H	210	THR
2	L	106	SER

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

Mol	Chain	Res	Type
1	H	30	GLN
1	H	38	ASN
1	H	133	GLN
1	H	166	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	28/36 (77%)	7 (25%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	9	CFL
3	A	10	A
3	A	13	G
3	A	19	A
3	A	21	A
3	A	22	CFL
3	A	32	CFL

There are no RNA pucker outliers to report.

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

19 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	CFL	A	32	3	18,21,22	1.05	1 (5%)	26,30,33	1.66	4 (15%)
3	CFL	A	9	3	18,21,22	0.96	0	26,30,33	1.39	5 (19%)
3	CFL	A	30	3	18,21,22	1.10	2 (11%)	26,30,33	1.67	4 (15%)
3	CFL	A	6	3	18,21,22	1.26	2 (11%)	26,30,33	1.94	3 (11%)
3	CFL	A	8	3	18,21,22	1.01	1 (5%)	26,30,33	1.49	4 (15%)
3	UFT	A	23	3	18,21,22	1.36	3 (16%)	26,30,33	1.69	6 (23%)
3	UFT	A	33	3	18,21,22	1.49	3 (16%)	26,30,33	1.78	5 (19%)
3	UFT	A	17	3	18,21,22	1.47	3 (16%)	26,30,33	2.43	10 (38%)
3	UFT	A	35	3	18,21,22	1.39	3 (16%)	26,30,33	1.78	6 (23%)
3	CFL	A	27	3	18,21,22	1.32	2 (11%)	26,30,33	2.06	7 (26%)
3	CFL	A	34	3	18,21,22	1.08	1 (5%)	26,30,33	1.28	3 (11%)
3	UFT	A	24	3,6	18,21,22	1.34	1 (5%)	26,30,33	1.70	4 (15%)
3	CFL	A	29	3	18,21,22	1.09	2 (11%)	26,30,33	1.69	5 (19%)
3	CFL	A	22	3,6	18,21,22	1.04	2 (11%)	26,30,33	1.75	7 (26%)
3	CFL	A	28	3	18,21,22	1.07	1 (5%)	26,30,33	1.66	5 (19%)
3	UFT	A	36	3	18,21,22	1.29	2 (11%)	26,30,33	2.17	9 (34%)
3	UFT	A	20	3	18,21,22	1.57	3 (16%)	26,30,33	2.14	9 (34%)
3	CFL	A	12	3	18,21,22	1.00	1 (5%)	26,30,33	1.01	1 (3%)
3	CFL	A	7	3	18,21,22	1.18	2 (11%)	26,30,33	2.06	7 (26%)

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	CFL	A	32	3	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CFL	A	9	3	-	3/7/25/26	0/2/2/2
3	CFL	A	30	3	-	0/7/25/26	0/2/2/2
3	CFL	A	6	3	-	2/7/25/26	0/2/2/2
3	CFL	A	8	3	-	0/7/25/26	0/2/2/2
3	UFT	A	23	3	-	0/7/25/26	0/2/2/2
3	UFT	A	33	3	-	0/7/25/26	0/2/2/2
3	UFT	A	17	3	-	2/7/25/26	0/2/2/2
3	UFT	A	35	3	-	0/7/25/26	0/2/2/2
3	CFL	A	27	3	-	0/7/25/26	0/2/2/2
3	CFL	A	34	3	-	0/7/25/26	0/2/2/2
3	UFT	A	24	3,6	-	0/7/25/26	0/2/2/2
3	CFL	A	29	3	-	0/7/25/26	0/2/2/2
3	CFL	A	22	3,6	-	2/7/25/26	0/2/2/2
3	CFL	A	28	3	-	0/7/25/26	0/2/2/2
3	UFT	A	36	3	-	0/7/25/26	0/2/2/2
3	UFT	A	20	3	-	5/7/25/26	0/2/2/2
3	CFL	A	12	3	-	0/7/25/26	0/2/2/2
3	CFL	A	7	3	-	0/7/25/26	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	20	UFT	C4-N3	-3.86	1.31	1.38
3	A	27	CFL	F-C2'	-3.39	1.32	1.40
3	A	17	UFT	C2-N1	3.20	1.43	1.38
3	A	20	UFT	C2-N3	-3.13	1.32	1.38
3	A	33	UFT	C4-N3	-3.06	1.33	1.38
3	A	17	UFT	C4-N3	-2.97	1.33	1.38
3	A	35	UFT	C2-N1	2.93	1.43	1.38
3	A	7	CFL	F-C2'	-2.92	1.33	1.40
3	A	6	CFL	F-C2'	-2.75	1.34	1.40
3	A	36	UFT	C2-N1	2.73	1.42	1.38
3	A	23	UFT	C4-N3	-2.71	1.33	1.38
3	A	33	UFT	C2-N3	-2.69	1.33	1.38
3	A	7	CFL	C6-C5	2.66	1.41	1.35
3	A	24	UFT	C2-N1	2.62	1.42	1.38
3	A	20	UFT	C5-C4	-2.47	1.38	1.43
3	A	29	CFL	F-C2'	-2.43	1.35	1.40
3	A	23	UFT	C2-N3	-2.40	1.33	1.38
3	A	30	CFL	F-C2'	-2.38	1.35	1.40
3	A	32	CFL	F-C2'	-2.36	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	22	CFL	C6-C5	2.32	1.40	1.35
3	A	33	UFT	C5-C4	-2.32	1.38	1.43
3	A	28	CFL	F-C2'	-2.26	1.35	1.40
3	A	36	UFT	C5-C4	-2.26	1.38	1.43
3	A	6	CFL	C5-C4	-2.24	1.37	1.42
3	A	34	CFL	F-C2'	-2.23	1.35	1.40
3	A	23	UFT	C2-N1	2.21	1.42	1.38
3	A	22	CFL	F-C2'	-2.17	1.35	1.40
3	A	30	CFL	C5-C4	-2.14	1.38	1.42
3	A	35	UFT	C4-N3	-2.12	1.34	1.38
3	A	8	CFL	F-C2'	-2.08	1.35	1.40
3	A	35	UFT	C6-C5	2.05	1.39	1.35
3	A	12	CFL	C6-N1	-2.04	1.33	1.38
3	A	17	UFT	C6-C5	2.03	1.39	1.35
3	A	29	CFL	C5-C4	-2.02	1.38	1.42
3	A	27	CFL	O4'-C1'	2.01	1.46	1.42

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	6	CFL	C2'-C3'-C4'	-6.36	94.19	102.40
3	A	17	UFT	N3-C2-N1	5.83	122.63	114.89
3	A	27	CFL	O4'-C1'-C2'	-5.29	100.34	105.79
3	A	30	CFL	C2'-C3'-C4'	-5.17	95.72	102.40
3	A	7	CFL	O4'-C1'-C2'	-5.05	100.59	105.79
3	A	6	CFL	O4'-C1'-C2'	-4.91	100.73	105.79
3	A	17	UFT	C4-N3-C2	-4.89	120.13	126.58
3	A	20	UFT	N3-C2-N1	4.88	121.36	114.89
3	A	28	CFL	C2'-C3'-C4'	-4.70	96.33	102.40
3	A	29	CFL	C2'-C3'-C4'	-4.60	96.45	102.40
3	A	33	UFT	C4-N3-C2	-4.46	120.70	126.58
3	A	17	UFT	C2'-C1'-N1	-4.43	107.42	114.20
3	A	20	UFT	C4-N3-C2	-4.41	120.76	126.58
3	A	33	UFT	N3-C2-N1	4.38	120.70	114.89
3	A	36	UFT	C2'-C1'-N1	-4.34	107.57	114.20
3	A	27	CFL	O2-C2-N3	-4.31	115.32	122.33
3	A	7	CFL	C2'-C3'-C4'	-4.20	96.98	102.40
3	A	35	UFT	C4-N3-C2	-4.17	121.08	126.58
3	A	35	UFT	N3-C2-N1	4.15	120.40	114.89
3	A	36	UFT	O4-C4-C5	-4.09	117.97	125.16
3	A	32	CFL	C2'-C3'-C4'	-3.95	97.30	102.40
3	A	20	UFT	C5-C4-N3	3.94	120.74	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	22	CFL	F-C2'-C3'	3.92	117.42	109.22
3	A	36	UFT	C4-N3-C2	-3.91	121.42	126.58
3	A	23	UFT	C5-C4-N3	3.88	120.64	114.84
3	A	17	UFT	O4'-C1'-N1	3.79	117.03	108.36
3	A	36	UFT	N3-C2-N1	3.73	119.83	114.89
3	A	32	CFL	O4'-C1'-C2'	-3.65	102.03	105.79
3	A	17	UFT	C1'-N1-C2	3.62	124.12	117.57
3	A	24	UFT	C4-N3-C2	-3.61	121.81	126.58
3	A	24	UFT	O4-C4-C5	-3.59	118.86	125.16
3	A	33	UFT	C5-C4-N3	3.56	120.17	114.84
3	A	28	CFL	O4'-C1'-C2'	-3.49	102.20	105.79
3	A	7	CFL	F-C2'-C3'	3.47	116.50	109.22
3	A	23	UFT	C4-N3-C2	-3.47	122.01	126.58
3	A	27	CFL	C2'-C3'-C4'	-3.45	97.94	102.40
3	A	35	UFT	C5-C4-N3	3.41	119.95	114.84
3	A	24	UFT	C5-C4-N3	3.40	119.92	114.84
3	A	24	UFT	N3-C2-N1	3.39	119.39	114.89
3	A	23	UFT	N3-C2-N1	3.38	119.38	114.89
3	A	36	UFT	C5-C4-N3	3.38	119.90	114.84
3	A	22	CFL	O2-C2-N3	-3.37	116.84	122.33
3	A	35	UFT	O4-C4-C5	-3.35	119.27	125.16
3	A	20	UFT	F2'-C2'-C1'	3.32	116.00	109.08
3	A	34	CFL	C2'-C3'-C4'	-3.30	98.14	102.40
3	A	6	CFL	O3'-C3'-C4'	3.27	120.50	111.05
3	A	30	CFL	O4'-C1'-C2'	-3.23	102.46	105.79
3	A	8	CFL	C2'-C3'-C4'	-3.22	98.24	102.40
3	A	22	CFL	C2'-C3'-C4'	-3.18	98.30	102.40
3	A	17	UFT	O2-C2-N3	-3.17	115.59	121.50
3	A	29	CFL	O4'-C1'-C2'	-3.16	102.53	105.79
3	A	7	CFL	O2-C2-N3	-3.01	117.44	122.33
3	A	29	CFL	O2-C2-N3	-3.00	117.45	122.33
3	A	32	CFL	F-C2'-C3'	2.97	115.44	109.22
3	A	7	CFL	C6-N1-C2	-2.95	115.38	120.49
3	A	20	UFT	C1'-N1-C2	2.93	122.87	117.57
3	A	27	CFL	F-C2'-C1'	2.89	115.10	109.08
3	A	8	CFL	O2-C2-N3	-2.89	117.63	122.33
3	A	33	UFT	O4-C4-C5	-2.87	120.11	125.16
3	A	36	UFT	O4'-C1'-N1	2.85	114.88	108.36
3	A	17	UFT	C6-N1-C2	-2.84	117.36	120.99
3	A	8	CFL	O4'-C1'-C2'	-2.79	102.92	105.79
3	A	34	CFL	O2-C2-N3	-2.76	117.85	122.33
3	A	27	CFL	O2-C2-N1	2.76	124.58	118.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	20	UFT	O5'-C5'-C4'	2.74	118.32	108.99
3	A	28	CFL	O2-C2-N3	-2.70	117.95	122.33
3	A	9	CFL	O4'-C4'-C5'	2.68	118.18	109.37
3	A	30	CFL	O2-C2-N3	-2.67	117.99	122.33
3	A	17	UFT	C5-C4-N3	2.63	118.78	114.84
3	A	30	CFL	O3'-C3'-C4'	2.60	118.56	111.05
3	A	9	CFL	C2'-C3'-C4'	-2.60	99.05	102.40
3	A	29	CFL	F-C2'-C3'	2.54	114.53	109.22
3	A	20	UFT	O2-C2-N3	-2.51	116.82	121.50
3	A	9	CFL	F-C2'-C1'	2.48	114.24	109.08
3	A	23	UFT	F2'-C2'-C3'	2.46	114.37	109.22
3	A	27	CFL	O4'-C4'-C3'	-2.45	100.27	105.11
3	A	22	CFL	O4'-C1'-C2'	-2.44	103.28	105.79
3	A	22	CFL	O4'-C1'-N1	2.43	113.92	108.36
3	A	20	UFT	O4'-C1'-C2'	-2.42	103.29	105.79
3	A	22	CFL	N1-C2-N3	2.41	123.19	118.81
3	A	27	CFL	C1'-N1-C2	2.40	123.78	118.42
3	A	7	CFL	C3'-C2'-C1'	-2.37	100.26	103.13
3	A	36	UFT	C1'-N1-C2	2.35	121.82	117.57
3	A	34	CFL	O3'-C3'-C4'	2.34	117.82	111.05
3	A	32	CFL	O2-C2-N3	-2.33	118.53	122.33
3	A	35	UFT	O4'-C1'-N1	2.30	113.62	108.36
3	A	20	UFT	C6-N1-C2	-2.28	118.07	120.99
3	A	35	UFT	C6-N1-C2	-2.24	118.12	120.99
3	A	17	UFT	C3'-C2'-C1'	2.24	105.85	103.13
3	A	36	UFT	C3'-C2'-C1'	2.21	105.80	103.13
3	A	28	CFL	C2'-C1'-N1	-2.20	110.84	114.20
3	A	7	CFL	O4'-C1'-N1	2.20	113.39	108.36
3	A	17	UFT	O4-C4-C5	-2.18	121.33	125.16
3	A	8	CFL	O4'-C4'-C5'	2.16	116.49	109.37
3	A	33	UFT	F2'-C2'-C1'	-2.14	104.62	109.08
3	A	12	CFL	O2-C2-N3	-2.14	118.85	122.33
3	A	36	UFT	C6-N1-C2	-2.13	118.27	120.99
3	A	23	UFT	O4-C4-C5	-2.13	121.42	125.16
3	A	29	CFL	C3'-C2'-C1'	-2.12	100.56	103.13
3	A	22	CFL	C6-N1-C2	-2.08	116.89	120.49
3	A	23	UFT	C2'-C1'-N1	-2.07	111.04	114.20
3	A	9	CFL	C3'-C2'-C1'	-2.06	100.63	103.13
3	A	9	CFL	O4'-C4'-C3'	-2.05	101.06	105.11
3	A	28	CFL	O3'-C3'-C4'	2.04	116.94	111.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	9	CFL	O4'-C4'-C5'-O5'
3	A	9	CFL	C3'-C4'-C5'-O5'
3	A	17	UFT	O4'-C1'-N1-C6
3	A	17	UFT	O4'-C1'-N1-C2
3	A	20	UFT	C2'-C1'-N1-C6
3	A	20	UFT	C2'-C1'-N1-C2
3	A	32	CFL	O4'-C4'-C5'-O5'
3	A	20	UFT	O4'-C4'-C5'-O5'
3	A	22	CFL	O4'-C4'-C5'-O5'
3	A	32	CFL	C3'-C4'-C5'-O5'
3	A	20	UFT	C3'-C4'-C5'-O5'
3	A	22	CFL	C3'-C4'-C5'-O5'
3	A	6	CFL	O4'-C4'-C5'-O5'
3	A	6	CFL	C3'-C4'-C5'-O5'
3	A	20	UFT	C4'-C5'-O5'-P
3	A	9	CFL	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	32	CFL	9	0
3	A	9	CFL	1	0
3	A	30	CFL	4	0
3	A	6	CFL	7	0
3	A	8	CFL	1	0
3	A	33	UFT	9	0
3	A	17	UFT	1	0
3	A	35	UFT	2	0
3	A	34	CFL	5	0
3	A	29	CFL	7	0
3	A	22	CFL	1	0
3	A	28	CFL	7	0
3	A	20	UFT	4	0
3	A	7	CFL	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	31:G	O3'	32:CFL	P	1.33

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	H	231/233 (99%)	0.08	5 (2%) 62 60	28, 45, 83, 114	0
2	L	51/51 (100%)	0.28	1 (1%) 65 63	30, 42, 85, 99	0
3	A	17/36 (47%)	-0.07	0 100 100	52, 84, 112, 125	0
All	All	299/320 (93%)	0.11	6 (2%) 65 63	28, 46, 91, 125	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	75	GLN	3.3
1	H	76	GLU	2.5
2	L	105	ASN	2.5
1	H	16	ILE	2.3
1	H	62	LYS	2.2
1	H	77	GLU	2.2

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	UFT	A	17	20/21	0.82	0.22	105,116,126,132	0
3	CFL	A	6	20/21	0.83	0.18	61,74,93,95	0
3	UFT	A	36	20/21	0.83	0.27	74,92,112,120	0
3	UFT	A	20	20/21	0.86	0.18	92,104,116,131	0
3	CFL	A	28	20/21	0.88	0.13	54,61,70,71	0
3	UFT	A	24	20/21	0.88	0.22	74,83,87,89	0
3	UFT	A	23	20/21	0.89	0.20	82,87,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CFL	A	7	20/21	0.89	0.18	57,70,83,89	0
3	CFL	A	8	20/21	0.90	0.12	61,67,74,85	0
3	CFL	A	32	20/21	0.90	0.12	50,52,57,59	0
3	CFL	A	34	20/21	0.90	0.14	54,55,57,61	0
3	CFL	A	27	20/21	0.90	0.14	62,73,81,81	0
3	CFL	A	29	20/21	0.91	0.13	48,52,58,59	0
3	CFL	A	22	20/21	0.91	0.18	75,86,92,98	0
3	CFL	A	12	20/21	0.92	0.14	66,70,77,94	0
3	CFL	A	30	20/21	0.93	0.14	47,52,56,78	0
3	CFL	A	9	20/21	0.94	0.13	67,73,81,93	0
3	UFT	A	33	20/21	0.94	0.09	50,52,54,54	0
3	UFT	A	35	20/21	0.95	0.14	59,68,74,76	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
6	MG	A	102	1/1	0.69	0.22	49,49,49,49	0
4	NA	H	301	1/1	0.83	0.09	59,59,59,59	0
5	CA	H	302	1/1	0.92	0.10	93,93,93,93	0
6	MG	A	101	1/1	0.94	0.09	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.