



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 05:40 AM EDT

PDB ID : 3DZG
Title : Crystal structure of human CD38 extracellular domain, ara-F-ribose-5'-phosphate/nicotinamide complex
Authors : Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.
Deposited on : 2008-07-29
Resolution : 1.65 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)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

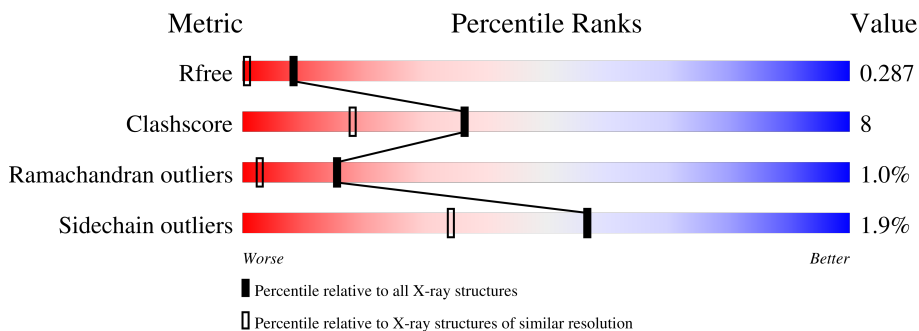
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	262	 78% 17% . .
1	B	262	 81% 15% .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4612 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.

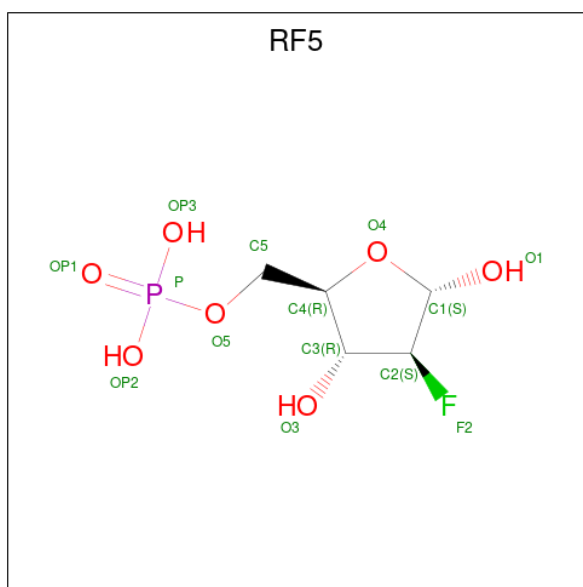
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	2050	1290	358	386	16	0	0	0
1	B	252	2050	1290	358	386	16	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

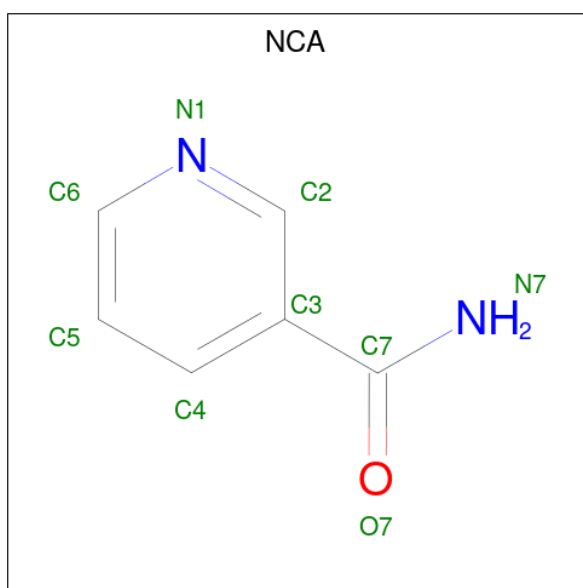
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	expression tag	UNP P28907
A	40	ARG	-	expression tag	UNP P28907
A	41	GLU	-	expression tag	UNP P28907
A	42	ALA	-	expression tag	UNP P28907
A	43	GLU	-	expression tag	UNP P28907
A	44	ALA	-	expression tag	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	39	LYS	-	expression tag	UNP P28907
B	40	ARG	-	expression tag	UNP P28907
B	41	GLU	-	expression tag	UNP P28907
B	42	ALA	-	expression tag	UNP P28907
B	43	GLU	-	expression tag	UNP P28907
B	44	ALA	-	expression tag	UNP P28907
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907

- Molecule 2 is 2-deoxy-2-fluoro-5-O-phosphono-alpha-D-arabinofuranose (three-letter code: RF5) (formula: C₅H₁₀FO₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	O			P
2	A	1	13	5	1	6	1	0	0
2	B	1	13	5	1	6	1	0	0

- Molecule 3 is NICOTINAMIDE (three-letter code: NCA) (formula: $C_6H_6N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	9	6	2	1	0	0
3	B	1	9	6	2	1	0	0


- Molecule 4 is water.

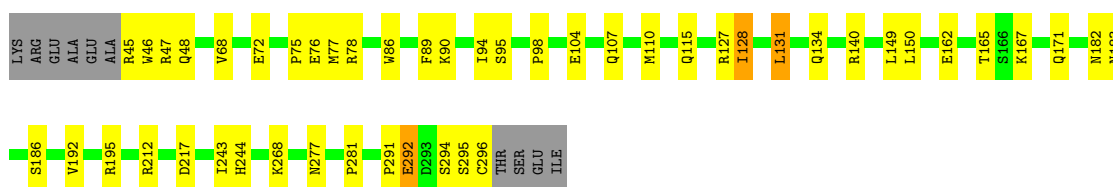
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	236	Total 236	O 236	0	0
4	B	232	Total 232	O 232	0	0

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. 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. 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.

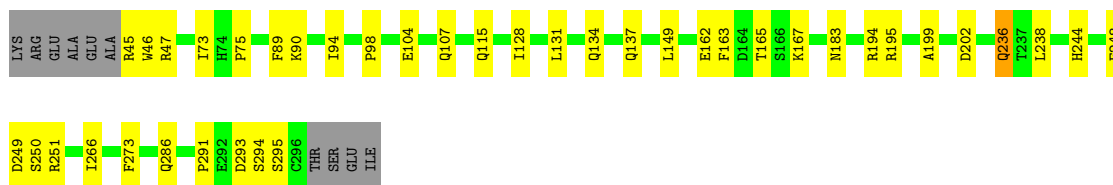
- Molecule 1: ADP-ribosyl cyclase 1

Chain A:  78% 17%



- Molecule 1: ADP-ribosyl cyclase 1

Chain B:  81% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.69Å 52.81Å 65.38Å 106.06° 91.95° 95.12°	Depositor
Resolution (Å)	20.00 – 1.65 30.12 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.65) 95.9 (30.12-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 1.64Å)	Xtrriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.174 , 0.211 0.262 , 0.287	Depositor DCC
R_{free} test set	3139 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: RF5, NCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.72	3/2101 (0.1%)	0.77	2/2846 (0.1%)
1	B	0.59	0/2101	0.67	0/2846
All	All	0.66	3/4202 (0.1%)	0.72	2/5692 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	GLU	CD-OE2	13.79	1.40	1.25
1	A	68	VAL	CA-CB	5.68	1.66	1.54
1	A	72	GLU	CD-OE1	5.51	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	VAL	CA-CB-CG1	-7.06	100.31	110.90
1	A	131	LEU	CB-CG-CD2	5.37	120.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2050	0	1976	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2050	0	1976	34	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
3	A	9	0	6	0	0
3	B	9	0	6	0	0
4	A	236	0	0	6	0
4	B	232	0	0	10	0
All	All	4612	0	3976	64	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 8.

All (64) 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:B:194:ARG:HD2	4:B:541:HOH:O	1.67	0.94
1:B:115:GLN:HE22	1:B:149:LEU:H	1.18	0.92
1:A:115:GLN:HE22	1:A:149:LEU:H	1.18	0.90
1:A:165:THR:HG23	1:A:167:LYS:H	1.36	0.88
1:B:165:THR:HG23	1:B:167:LYS:H	1.35	0.87
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.60	0.82
1:B:202:ASP:HB3	4:B:503:HOH:O	1.80	0.80
1:A:75:PRO:HA	1:A:78:ARG:HG3	1.67	0.77
1:A:195:ARG:HD3	4:A:531:HOH:O	1.84	0.75
1:B:90:LYS:HG3	1:B:94:ILE:HG13	1.70	0.73
1:B:236:GLN:NE2	4:B:630:HOH:O	2.27	0.68
1:A:127:ARG:NH1	1:A:217:ASP:OD2	2.21	0.67
1:A:294:SER:O	1:A:296:CYS:N	2.28	0.67
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.25	0.65
1:A:183:ASN:ND2	1:A:186:SER:H	1.95	0.65
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.32	0.65
1:A:140:ARG:NH2	4:A:431:HOH:O	2.29	0.64
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.79	0.64
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.80	0.63
1:A:182:ASN:HB2	4:A:413:HOH:O	1.99	0.62
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.35	0.61
1:A:110:MET:HE1	1:A:150:LEU:HD13	1.82	0.61
1:B:137:GLN:HG2	4:B:627:HOH:O	2.02	0.60
1:A:127:ARG:HB3	1:A:212:ARG:HE	1.66	0.60
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.66	0.58
1:B:115:GLN:NE2	1:B:149:LEU:H	1.96	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.88	0.56
1:A:46:TRP:HE1	1:A:47:ARG:NH2	2.04	0.56
1:B:244:HIS:HD2	1:B:250:SER:HB3	1.70	0.55
1:A:48:GLN:NE2	1:A:171:GLN:HB3	2.22	0.55
1:B:195:ARG:HB2	4:B:528:HOH:O	2.07	0.54
1:B:45:ARG:HG3	1:B:46:TRP:N	2.23	0.54
1:A:78:ARG:NH1	4:A:395:HOH:O	2.41	0.53
1:B:194:ARG:NH1	4:B:634:HOH:O	2.41	0.53
1:B:195:ARG:HG3	4:B:527:HOH:O	2.09	0.52
1:B:293:ASP:CG	1:B:294:SER:H	2.13	0.52
1:B:47:ARG:NH2	4:B:639:HOH:O	2.41	0.52
1:B:244:HIS:CD2	1:B:250:SER:HB3	2.44	0.52
1:B:266:ILE:HD11	1:B:273:PHE:CA	2.40	0.52
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.94	0.50
1:A:183:ASN:HD21	1:A:186:SER:H	1.58	0.49
1:A:243:ILE:HG23	1:A:281:PRO:HG3	1.95	0.49
1:B:90:LYS:CG	1:B:94:ILE:HG13	2.39	0.49
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.95	0.47
1:A:134:GLN:CD	4:A:444:HOH:O	2.53	0.47
1:A:76:GLU:HG2	1:A:77:MET:HG2	1.97	0.46
1:B:98:PRO:O	1:B:183:ASN:HA	2.15	0.46
1:B:45:ARG:HG3	1:B:47:ARG:H	1.81	0.46
1:B:195:ARG:HD3	4:B:528:HOH:O	2.14	0.46
1:B:248:GLU:HG3	1:B:249:ASP:H	1.81	0.45
1:A:115:GLN:NE2	1:A:149:LEU:H	1.99	0.45
1:A:98:PRO:O	1:A:183:ASN:HA	2.18	0.44
1:B:134:GLN:O	1:B:137:GLN:HB2	2.18	0.43
1:A:104:GLU:HA	1:A:107:GLN:HG2	2.00	0.43
1:A:291:PRO:O	1:A:292:GLU:HB3	2.18	0.43
1:B:199:ALA:HB3	4:B:591:HOH:O	2.19	0.42
1:B:162:GLU:HB2	1:B:165:THR:CG2	2.47	0.42
1:A:94:ILE:O	1:A:95:SER:HB2	2.20	0.42
1:A:128:ILE:HG13	4:A:418:HOH:O	2.19	0.42
1:A:243:ILE:CG2	1:A:281:PRO:HG3	2.49	0.41
1:B:73:ILE:O	1:B:75:PRO:HD3	2.21	0.41
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.85	0.41
1:A:110:MET:HE1	1:A:192:VAL:HG12	2.02	0.41
1:A:78:ARG:HE	1:A:78:ARG:HB2	1.70	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	
1	A	250/262 (95%)	240 (96%)	8 (3%)	2 (1%)	19	5
1	B	250/262 (95%)	239 (96%)	8 (3%)	3 (1%)	13	2
All	All	500/524 (95%)	479 (96%)	16 (3%)	5 (1%)	15	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	B	291	PRO
1	B	295	SER
1	A	128	ILE
1	B	128	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	
1	A	233/241 (97%)	229 (98%)	4 (2%)	60	39
1	B	233/241 (97%)	228 (98%)	5 (2%)	53	29
All	All	466/482 (97%)	457 (98%)	9 (2%)	57	34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89	PHE
1	A	131	LEU
1	A	292	GLU
1	B	89	PHE
1	B	131	LEU
1	B	236	GLN
1	B	251	ARG
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	183	ASN
1	A	244	HIS
1	B	115	GLN
1	B	134	GLN
1	B	229	ASN
1	B	244	HIS
1	B	270	ASN
1	B	286	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	NCA	A	302	-	9,9,9	0.58	0	11,11,11	2.06	4 (36%)
2	RF5	A	301	-	13,13,14	0.80	0	17,19,21	1.56	4 (23%)
3	NCA	B	302	-	9,9,9	0.42	0	11,11,11	1.67	4 (36%)
2	RF5	B	301	-	13,13,14	0.82	1 (7%)	17,19,21	1.34	2 (11%)

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	NCA	A	302	-	-	0/4/4/4	0/1/1/1
2	RF5	A	301	-	-	2/6/19/22	0/1/1/1
3	NCA	B	302	-	-	0/4/4/4	0/1/1/1
2	RF5	B	301	-	-	1/6/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RF5	F2-C2	-2.12	1.35	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RF5	O4-C4-C3	-4.07	101.10	104.70
3	A	302	NCA	C3-C2-N1	-3.31	118.59	123.49
3	A	302	NCA	O7-C7-C3	-3.18	115.82	119.63
3	A	302	NCA	C4-C3-C2	2.92	120.94	117.63
3	A	302	NCA	C6-N1-C2	2.88	121.84	116.85
3	B	302	NCA	C6-N1-C2	2.81	121.71	116.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	NCA	C3-C2-N1	-2.80	119.35	123.49
2	B	301	RF5	O4-C4-C3	-2.42	102.57	104.70
3	B	302	NCA	C3-C7-N7	2.40	120.62	117.75
2	B	301	RF5	P-O5-C5	2.21	124.38	118.30
3	B	302	NCA	O7-C7-C3	-2.20	117.00	119.63
2	A	301	RF5	OP2-P-O5	-2.16	100.98	106.73
2	A	301	RF5	O3-C3-C4	2.10	117.12	111.05
2	A	301	RF5	C1-O4-C4	2.05	112.94	108.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	RF5	C3-C4-C5-O5
2	B	301	RF5	C3-C4-C5-O5
2	A	301	RF5	C4-C5-O5-P

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.