wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:44 AM GMT

PDB ID	:	3C1P
Title	:	Crystal Structure of an alternating D-Alanyl, L-Homoalanyl PNA
Authors	:	Cuesta-Seijo, J.A.; Sheldrick, G.M.; Zhang, J.; Diederichsen, U.
Deposited on	:	2008-01-23
Resolution	:	1.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk26765
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 Å.

There are no percentiles available for this entry.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 814 atoms, of which 263 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 an unknown type called Peptide Nucleic Acid DLY-HGL-AGD-LHC-AGD-LHC-CUD-LYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
1	A	8	Total	C	H	N	O	0	2
			172	56	70	33	13		
1	B	8	Total	C	H	N	O	0	0
			166	54	66	33	13		
1	C	8	Total	C	H	N	O	0	0
			166	54	66	33	13		
1	D	8	Total	C	H	N	O	0	4
			170	59	61	35	15		

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	29	Total	O	0	0
			29	29		
2	C	34	Total	O	0	0
			34	34		
2	D	33	Total	O	0	0
			33	33		

3 Residue-property plots

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	26.31Å 30.73Å 33.55Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	40.00 – 1.00 33.09 – 1.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.00) 99.5 (33.09-1.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.150 , 0.202 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 28562 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	814	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

MolProbity failed to run properly - this section will therefore be empty.

5.2 Too-close contacts

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA

MolProbity failed to run properly - this section will therefore be empty.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

Of 37 such residues modelled in this entry, 3 are modelled with single atom - leaving 34 for Mogul analysis.

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	DLY	A	11	1	7,8,9	0.58	0	6,8,10	1.29	1 (16%)
1	HGL	A	12	1	14,18,19	1.25	1 (7%)	9,25,27	3.53	3 (33%)
1	AGD	A	13	1	13,17,18	1.42	2 (15%)	8,24,26	2.85	4 (50%)
1	LHC	A	14	1	10,14,15	1.12	1 (10%)	10,18,20	1.46	1 (10%)
1	AGD	A	15	1	13,17,18	1.55	3 (23%)	8,24,26	2.74	2 (25%)
1	LHC	A	16	1	10,14,15	1.14	1 (10%)	10,18,20	1.66	1 (10%)
1	CUD	A	17[A]	1	9,13,14	1.26	0	9,17,19	1.52	3 (33%)
1	CUD	A	17[B]	-	8,12,14	1.24	0	8,16,19	1.40	2 (25%)
1	DLY	B	21	1	7,8,9	0.51	0	6,8,10	1.27	0
1	HGL	B	22	1	14,18,19	2.29	6 (42%)	9,25,27	2.16	3 (33%)
1	AGD	B	23	1	13,17,18	1.80	4 (30%)	8,24,26	2.75	2 (25%)
1	LHC	B	24	1	10,14,15	1.27	1 (10%)	10,18,20	1.93	3 (30%)
1	AGD	B	25	1	13,17,18	1.38	1 (7%)	8,24,26	5.09	4 (50%)
1	LHC	B	26	1	10,14,15	1.30	1 (10%)	10,18,20	2.08	3 (30%)
1	CUD	B	27	1	9,13,14	0.80	0	9,17,19	1.38	2 (22%)
1	DLY	C	31	1	7,8,9	0.91	0	6,8,10	1.70	2 (33%)
1	HGL	C	32	1	14,18,19	1.45	2 (14%)	9,25,27	2.84	2 (22%)
1	AGD	C	33	1	13,17,18	1.35	3 (23%)	8,24,26	2.49	2 (25%)
1	LHC	C	34	1	10,14,15	1.03	1 (10%)	10,18,20	1.34	1 (10%)
1	AGD	C	35	1	13,17,18	1.55	2 (15%)	8,24,26	3.19	1 (12%)
1	LHC	C	36	1	10,14,15	1.23	2 (20%)	10,18,20	1.13	2 (20%)
1	CUD	C	37	1	9,13,14	1.30	1 (11%)	9,17,19	1.65	3 (33%)
1	DLY	D	41[A]	1	3,4,9	0.61	0	0,4,10	0.00	-
1	DLY	D	41[B]	1	3,4,9	0.55	0	0,4,10	0.00	-
1	HGL	D	42[A]	1	14,18,19	1.27	2 (14%)	9,25,27	3.18	1 (11%)
1	HGL	D	42[B]	1	14,18,19	1.58	3 (21%)	9,25,27	3.27	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	AGD	D	43	1	13,17,18	1.45	3 (23%)	8,24,26	2.86	3 (37%)
1	LHC	D	44	1	10,14,15	0.87	0	10,18,20	1.08	1 (10%)
1	AGD	D	45	1	13,17,18	1.69	4 (30%)	8,24,26	3.29	2 (25%)
1	LHC	D	46	1	10,14,15	0.95	0	10,18,20	1.26	1 (10%)
1	CUD	D	47[A]	1	9,13,14	1.70	2 (22%)	9,17,19	2.07	4 (44%)
1	CUD	D	47[B]	1	9,13,14	1.63	2 (22%)	9,17,19	2.01	3 (33%)
1	LYS	D	48[A]	1	0,1,9	0.00	-	0,0,10	0.00	-
1	LYS	D	48[B]	1	0,1,9	0.00	-	0,0,10	0.00	-

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	DLY	A	11	1	-	0/5/7/9	0/0/0/0
1	HGL	A	12	1	-	0/5/7/9	0/2/2/2
1	AGD	A	13	1	-	0/1/6/8	0/2/2/2
1	LHC	A	14	1	-	0/5/7/9	0/1/1/1
1	AGD	A	15	1	-	0/1/6/8	0/2/2/2
1	LHC	A	16	1	-	0/5/7/9	0/1/1/1
1	CUD	A	17[A]	1	-	0/3/6/8	0/1/1/1
1	CUD	A	17[B]	-	-	0/4/4/8	0/1/1/1
1	DLY	B	21	1	-	0/5/7/9	0/0/0/0
1	HGL	B	22	1	-	0/5/7/9	0/2/2/2
1	AGD	B	23	1	-	0/1/6/8	0/2/2/2
1	LHC	B	24	1	-	0/5/7/9	0/1/1/1
1	AGD	B	25	1	-	0/1/6/8	0/2/2/2
1	LHC	B	26	1	-	0/5/7/9	0/1/1/1
1	CUD	B	27	1	-	0/3/6/8	0/1/1/1
1	DLY	C	31	1	-	0/5/7/9	0/0/0/0
1	HGL	C	32	1	-	0/5/7/9	0/2/2/2
1	AGD	C	33	1	-	0/1/6/8	0/2/2/2
1	LHC	C	34	1	-	0/5/7/9	0/1/1/1
1	AGD	C	35	1	-	0/1/6/8	0/2/2/2
1	LHC	C	36	1	-	0/5/7/9	0/1/1/1
1	CUD	C	37	1	-	0/3/6/8	0/1/1/1
1	DLY	D	41[A]	1	-	0/0/2/9	0/0/0/0
1	DLY	D	41[B]	1	-	0/0/2/9	0/0/0/0
1	HGL	D	42[A]	1	-	0/5/7/9	0/2/2/2
1	HGL	D	42[B]	1	-	0/5/7/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGD	D	43	1	-	0/1/6/8	0/2/2/2
1	LHC	D	44	1	-	0/5/7/9	0/1/1/1
1	AGD	D	45	1	-	0/1/6/8	0/2/2/2
1	LHC	D	46	1	-	0/5/7/9	0/1/1/1
1	CUD	D	47[A]	1	-	0/3/6/8	0/1/1/1
1	CUD	D	47[B]	1	-	0/3/6/8	0/1/1/1
1	LYS	D	48[A]	1	-	0/0/0/9	0/0/0/0
1	LYS	D	48[B]	1	-	0/0/0/9	0/0/0/0

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	AGD	CB-N9	-3.74	1.44	1.48
1	D	42[B]	HGL	CB-CA	-3.62	1.50	1.53
1	B	25	AGD	CB-N9	-3.58	1.44	1.48
1	D	45	AGD	C8-N7	-3.39	1.28	1.34
1	D	45	AGD	CB-N9	-3.27	1.45	1.48

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	22	HGL	N2-C2-N1	-4.10	113.32	117.80
1	B	25	AGD	N2-C2-N1	-3.56	113.91	117.80
1	C	37	CUD	O-C-CA	-3.28	116.94	125.49
1	C	31	DLY	O-C-CA	-3.23	117.08	125.49
1	D	43	AGD	N2-C2-N1	-3.03	114.49	117.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

There are no RSRZ outliers to report within protein, DNA, RNA chains in this entry.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.