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Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 03:39 AM EST

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 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 (i) 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 (i)) were used in the production of this report:

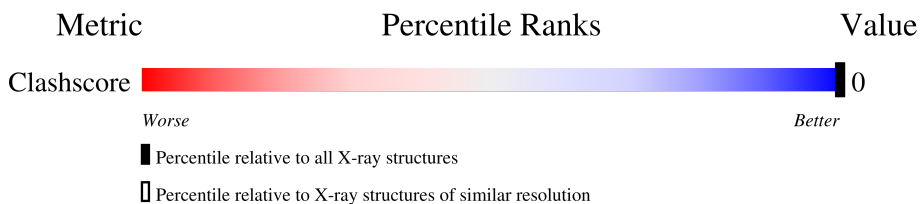|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.00 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	Percentile Ranks	Value
Clashscore		0

Worse ⟵　　　⟶ *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1117 (1.06-0.94)

ENTRY-COMPOSITION INFOmissingINFO

2 Residue-property plots (i)

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

3 Data and refinement statistics ⓘ

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.	wwPDB-VP
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
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AGD, DLY, LHC, HGL, CUD

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	D	0.33	0/2	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	102	70	65	0	0
1	B	100	66	64	0	0
1	C	100	66	65	0	0
1	D	109	61	56	0	0
2	A	44	0	0	0	0
2	B	29	0	0	0	0
2	C	34	0	0	0	0
2	D	33	0	0	0	0
All	All	551	263	250	0	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 0.

There are no clashes within the asymmetric unit.

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There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

4.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

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	AGD	A	13	1	12,17,18	1.77	2 (16%)	9,24,26	1.21	1 (11%)
1	CUD	C	37	1	12,13,14	0.83	0	11,17,19	1.60	3 (27%)
1	LHC	B	26	1	13,14,15	0.91	0	12,18,20	1.24	1 (8%)
1	AGD	C	33	1	12,17,18	1.59	3 (25%)	9,24,26	1.22	1 (11%)
1	AGD	C	35	1	12,17,18	1.76	3 (25%)	9,24,26	1.44	1 (11%)
1	CUD	D	47[A]	1	12,13,14	1.01	1 (8%)	11,17,19	1.10	1 (9%)
1	HGL	A	12	1	13,18,19	1.54	3 (23%)	10,25,27	1.16	1 (10%)
1	AGD	B	25	1	12,17,18	1.61	3 (25%)	9,24,26	1.70	2 (22%)
1	LHC	A	14	1	13,14,15	0.78	0	12,18,20	0.60	0
1	HGL	C	32	1	13,18,19	1.63	3 (23%)	10,25,27	1.05	0
1	LHC	C	34	1	13,14,15	1.25	1 (7%)	12,18,20	1.19	2 (16%)
1	LHC	D	44	1	13,14,15	0.74	0	12,18,20	0.86	1 (8%)
1	LHC	B	24	1	13,14,15	1.05	1 (7%)	12,18,20	0.47	0
1	CUD	A	17[B]	-	12,12,14	3.69	3 (25%)	11,16,19	0.87	0
1	LHC	C	36	1	13,14,15	0.93	0	12,18,20	0.81	0
1	AGD	B	23	1	12,17,18	1.89	3 (25%)	9,24,26	1.03	1 (11%)
1	LHC	D	46	1	13,14,15	1.17	1 (7%)	12,18,20	1.16	1 (8%)
1	HGL	D	42[B]	1	13,18,19	1.63	3 (23%)	10,25,27	0.82	1 (10%)
1	AGD	D	43	1	12,17,18	1.58	4 (33%)	9,24,26	1.15	1 (11%)
1	CUD	D	47[B]	1	12,13,14	0.90	0	11,17,19	1.10	1 (9%)
1	CUD	A	17[A]	1	12,13,14	1.18	1 (8%)	11,17,19	0.87	0
1	LHC	A	16	1	13,14,15	1.15	1 (7%)	12,18,20	1.71	3 (25%)
1	AGD	D	45	1	12,17,18	1.91	3 (25%)	9,24,26	0.73	0
1	HGL	B	22	1	13,18,19	2.21	5 (38%)	10,25,27	1.55	1 (10%)
1	HGL	D	42[A]	1	13,18,19	1.43	2 (15%)	10,25,27	0.82	1 (10%)
1	AGD	A	15	1	12,17,18	1.68	2 (16%)	9,24,26	1.50	2 (22%)
1	CUD	B	27	1	12,13,14	0.41	0	11,17,19	1.68	2 (18%)

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	AGD	A	13	1	-	0/1/6/8	0/2/2/2
1	CUD	C	37	1	-	0/3/6/8	0/1/1/1
1	LHC	B	26	1	-	0/6/7/9	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGD	C	33	1	-	0/1/6/8	0/2/2/2
1	AGD	C	35	1	-	0/1/6/8	0/2/2/2
1	CUD	D	47[A]	1	-	0/3/6/8	0/1/1/1
1	HGL	A	12	1	-	0/6/7/9	0/2/2/2
1	AGD	B	25	1	-	0/1/6/8	0/2/2/2
1	LHC	A	14	1	-	0/6/7/9	0/1/1/1
1	HGL	C	32	1	-	0/6/7/9	0/2/2/2
1	LHC	C	34	1	-	0/6/7/9	0/1/1/1
1	LHC	D	44	1	-	0/6/7/9	0/1/1/1
1	LHC	B	24	1	-	0/6/7/9	0/1/1/1
1	CUD	A	17[B]	-	-	1/3/4/8	0/1/1/1
1	LHC	C	36	1	-	0/6/7/9	0/1/1/1
1	AGD	B	23	1	-	0/1/6/8	0/2/2/2
1	LHC	D	46	1	-	0/6/7/9	0/1/1/1
1	HGL	D	42[B]	1	-	0/6/7/9	0/2/2/2
1	AGD	D	43	1	-	0/1/6/8	0/2/2/2
1	CUD	D	47[B]	1	-	0/3/6/8	0/1/1/1
1	CUD	A	17[A]	1	-	0/3/6/8	0/1/1/1
1	LHC	A	16	1	-	0/6/7/9	0/1/1/1
1	AGD	D	45	1	-	0/1/6/8	0/2/2/2
1	HGL	B	22	1	-	0/6/7/9	0/2/2/2
1	HGL	D	42[A]	1	-	0/6/7/9	0/2/2/2
1	AGD	A	15	1	-	0/1/6/8	0/2/2/2
1	CUD	B	27	1	-	1/3/6/8	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17[B]	CUD	O-C	12.02	1.67	1.19
1	A	13	AGD	C5-C6	-4.18	1.38	1.47
1	D	45	AGD	C8-N7	-4.06	1.28	1.35
1	B	22	HGL	C6-N1	3.87	1.43	1.37
1	B	22	HGL	C8-N7	-3.87	1.28	1.35
1	C	35	AGD	C5-C6	-3.70	1.39	1.47
1	A	15	AGD	C5-C6	-3.68	1.39	1.47
1	B	23	AGD	C5-C6	-3.50	1.40	1.47
1	C	32	HGL	C5-C6	-3.45	1.40	1.47
1	C	34	LHC	C2-N1	-3.44	1.35	1.40
1	C	35	AGD	CB-N9	-3.39	1.44	1.48
1	B	25	AGD	CB-N9	-3.23	1.44	1.48
1	B	22	HGL	C5-C4	-3.21	1.34	1.43
1	B	23	AGD	C8-N7	-3.20	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	HGL	C5-C6	-3.14	1.41	1.47
1	D	42[A]	HGL	C5-C6	-3.13	1.41	1.47
1	D	42[B]	HGL	C5-C6	-3.13	1.41	1.47
1	D	43	AGD	C8-N7	-3.07	1.29	1.35
1	D	45	AGD	C5-C6	-3.03	1.41	1.47
1	D	45	AGD	CB-N9	-2.93	1.45	1.48
1	B	23	AGD	C6-N1	2.93	1.42	1.37
1	C	33	AGD	C5-C6	-2.87	1.41	1.47
1	D	42[A]	HGL	C8-N7	-2.86	1.30	1.35
1	D	42[B]	HGL	C8-N7	-2.86	1.30	1.35
1	C	33	AGD	C8-N7	-2.80	1.30	1.35
1	B	22	HGL	C5-C6	-2.76	1.41	1.47
1	C	32	HGL	C8-N7	-2.70	1.30	1.35
1	A	13	AGD	C8-N7	-2.63	1.30	1.35
1	A	12	HGL	C5-C4	-2.63	1.36	1.43
1	B	22	HGL	CG-N9	-2.60	1.44	1.48
1	C	35	AGD	C6-N1	2.53	1.41	1.37
1	D	43	AGD	CB-N9	-2.51	1.45	1.48
1	D	42[B]	HGL	CB-CA	-2.50	1.50	1.53
1	A	17[B]	CUD	CB-CA	2.42	1.56	1.53
1	B	25	AGD	C8-N7	-2.39	1.31	1.35
1	B	24	LHC	CB-CG	-2.39	1.47	1.52
1	A	15	AGD	C6-N1	2.38	1.41	1.37
1	D	43	AGD	C5-C6	-2.37	1.42	1.47
1	D	46	LHC	C2-N1	-2.31	1.37	1.40
1	A	16	LHC	C2-N1	-2.28	1.37	1.40
1	D	47[A]	CUD	CB-CA	2.19	1.55	1.53
1	C	33	AGD	CB-N9	-2.18	1.45	1.48
1	A	17[A]	CUD	C2-N1	-2.10	1.37	1.40
1	A	17[B]	CUD	C2-N1	-2.10	1.37	1.40
1	C	32	HGL	C5-C4	-2.10	1.37	1.43
1	A	12	HGL	CG-N9	-2.09	1.44	1.48
1	D	43	AGD	C5-C4	-2.04	1.37	1.43
1	B	25	AGD	C5-C6	-2.01	1.43	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	CUD	C6-N1-C2	3.82	122.80	120.23
1	A	16	LHC	C6-N1-C2	3.78	122.77	120.23
1	C	37	CUD	N1-C2-N3	3.48	121.97	118.45
1	B	25	AGD	O6-C6-N1	3.47	124.74	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	LHC	C6-N1-C2	-3.02	118.19	120.23
1	B	22	HGL	O6-C6-C5	3.00	130.22	124.37
1	A	16	LHC	C5-C6-N1	-2.99	119.64	122.44
1	C	35	AGD	O6-C6-C5	2.93	130.10	124.37
1	A	15	AGD	O6-C6-C5	2.91	130.06	124.37
1	D	46	LHC	C5-C6-N1	-2.90	119.72	122.44
1	A	12	HGL	O6-C6-C5	2.75	129.75	124.37
1	A	15	AGD	O6-C6-N1	-2.50	117.70	120.65
1	D	47[A]	CUD	C6-N1-C2	-2.48	118.56	120.23
1	D	47[B]	CUD	C6-N1-C2	-2.48	118.56	120.23
1	C	37	CUD	C6-N1-C2	-2.38	118.62	120.23
1	B	25	AGD	C5-C6-N1	-2.38	109.75	113.95
1	D	43	AGD	O6-C6-C5	2.22	128.72	124.37
1	B	23	AGD	O6-C6-C5	2.19	128.64	124.37
1	C	33	AGD	O6-C6-C5	2.16	128.60	124.37
1	C	34	LHC	N1-C2-N3	2.15	120.62	118.45
1	C	34	LHC	C5-C6-N1	-2.14	120.44	122.44
1	A	13	AGD	O6-C6-C5	2.09	128.45	124.37
1	A	16	LHC	CG-N1-C2	-2.09	116.85	119.05
1	C	37	CUD	O2-C2-N3	-2.06	118.97	122.33
1	D	44	LHC	C5-C6-N1	-2.06	120.51	122.44
1	B	27	CUD	C5-C4-N3	2.05	124.82	121.33
1	D	42[A]	HGL	O6-C6-C5	2.01	128.31	124.37
1	D	42[B]	HGL	O6-C6-C5	2.01	128.31	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	27	CUD	CA-CB-N1-C2
1	A	17[B]	CUD	C-CA-CB-N1

There are no ring outliers.

No monomer is involved in short contacts.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

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

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

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 Ligands ⓘ

There are no ligands in this entry.

5.5 Other polymers ⓘ

There are no such residues in this entry.