wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 03:38 AM EST

PDB ID	:	1J0E
Title	:	ACC deaminase mutant reacton intermediate
Authors	:	Ose, T.; Fujino, A.; Yao, M.; Honma, M.; Tanaka, I.
Deposited on	:	2002-11-12
Resolution	:	2.45 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
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:

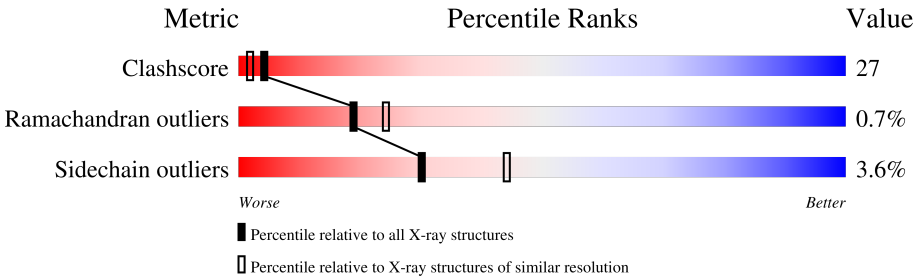
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.45 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))
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	341	57% 41% .
1	B	341	55% 42% .
1	C	341	65% 32% .
1	D	341	65% 32% .

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
1	LLP	A	51	-	-	X	-
1	LLP	B	51	-	-	X	-
2	1AC	A	1001	-	-	X	-
2	1AC	B	2001	-	-	X	-
2	1AC	C	3001	-	-	X	-
2	1AC	D	4001	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11447 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.

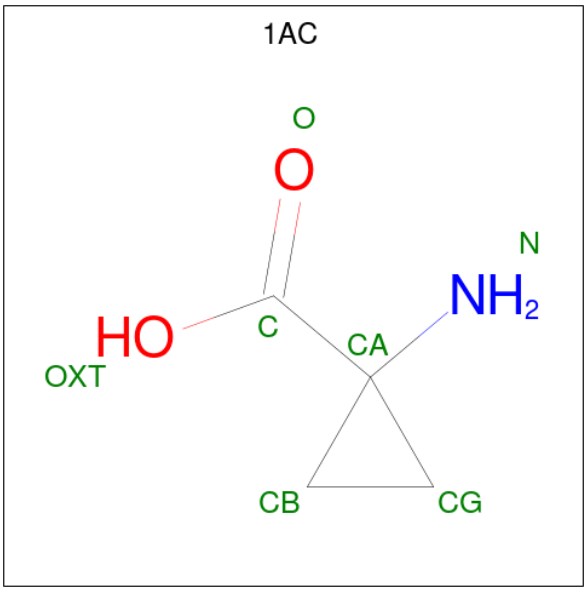
- Molecule 1 is a protein called 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	P	S	0	0	0
			2620	1663	442	502	1	12			
1	B	341	Total	C	N	O	P	S	0	0	0
			2620	1663	442	502	1	12			
1	C	341	Total	C	N	O	P	S	0	0	0
			2620	1663	442	502	1	12			
1	D	341	Total	C	N	O	P	S	0	0	0
			2620	1663	442	502	1	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	SER	engineered mutation	UNP Q7M523
A	295	PHE	TYR	engineered mutation	UNP Q7M523
B	1	ALA	SER	engineered mutation	UNP Q7M523
B	295	PHE	TYR	engineered mutation	UNP Q7M523
C	1	ALA	SER	engineered mutation	UNP Q7M523
C	295	PHE	TYR	engineered mutation	UNP Q7M523
D	1	ALA	SER	engineered mutation	UNP Q7M523
D	295	PHE	TYR	engineered mutation	UNP Q7M523

- Molecule 2 is 1-AMINOCYCLOPROPANECARBOXYLIC ACID (three-letter code: 1AC) (formula: $C_4H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 7 4 1 2	0	0
2	B	1	Total C N O 7 4 1 2	0	0
2	C	1	Total C N O 7 4 1 2	0	0
2	D	1	Total C N O 7 4 1 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	129	Total O 129 129	0	0
3	B	124	Total O 124 124	0	0
3	C	372	Total O 372 372	0	0
3	D	314	Total O 314 314	0	0

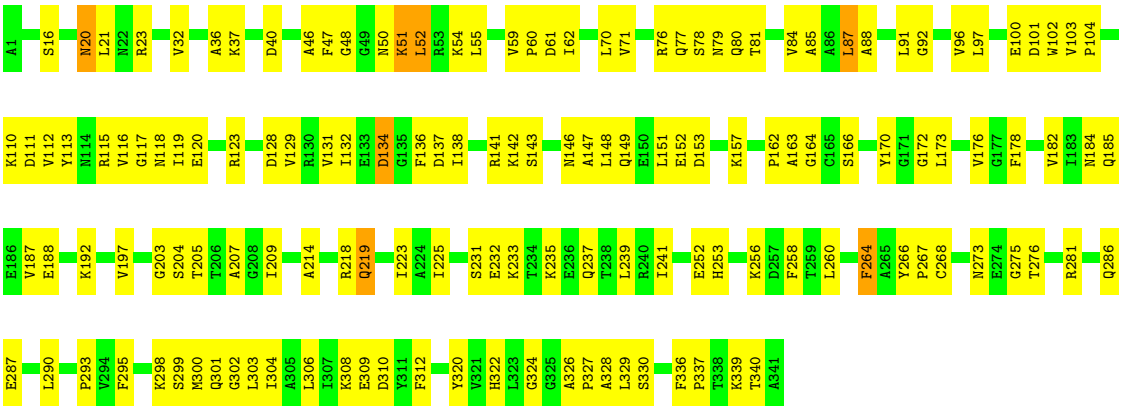
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

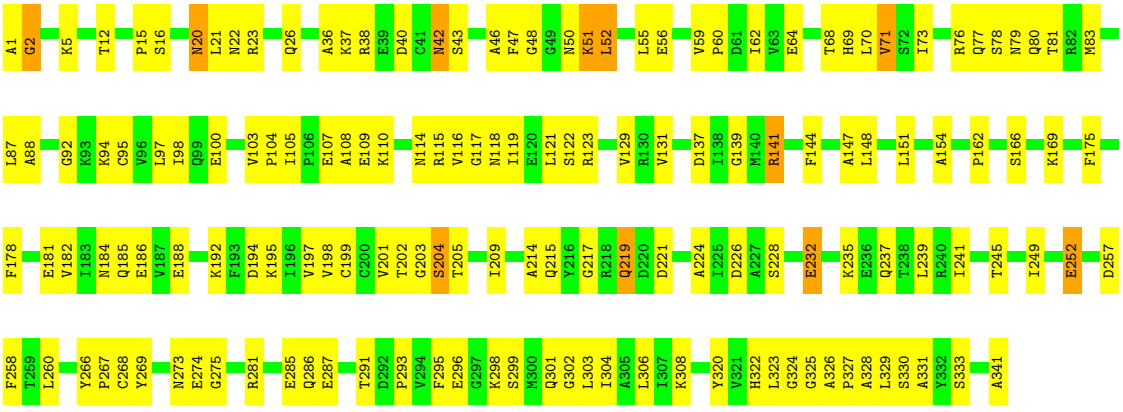
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain A:



• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain B:



• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain C:

• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain D:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	65.40Å 269.59Å 186.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45	Depositor
% Data completeness (in resolution range)	99.4 (10.00-2.45)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11447	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, 1AC

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	0.30	0/2646	0.56	1/3578 (0.0%)
1	B	0.32	0/2646	0.57	0/3578
1	C	0.38	0/2646	0.63	0/3578
1	D	0.39	0/2646	0.63	1/3578 (0.0%)
All	All	0.35	0/10584	0.60	2/14312 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	203	GLY	N-CA-C	6.10	128.35	113.10
1	A	203	GLY	N-CA-C	5.70	127.36	113.10

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	A	2620	0	2600	167	0
1	B	2620	0	2600	177	0
1	C	2620	0	2600	120	0
1	D	2620	0	2600	114	0
2	A	7	0	6	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	6	23	0
2	C	7	0	6	15	0
2	D	7	0	6	18	0
3	A	129	0	0	17	0
3	B	124	0	0	15	1
3	C	372	0	0	23	1
3	D	314	0	0	17	0
All	All	11447	0	10424	558	2

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 27.

The worst 5 of 558 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:A:51:LLP:C4'	1:A:51:LLP:NZ	1.68	1.50
1:C:51:LLP:H4'1	2:C:3001:1AC:N	1.36	1.36
1:D:51:LLP:H4'1	2:D:4001:1AC:N	1.46	1.29
1:A:51:LLP:H4'1	2:A:1001:1AC:N	1.51	1.25
1:B:51:LLP:H4'1	2:B:2001:1AC:N	1.52	1.23

All (2) 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)
3:B:2052:HOH:O	3:B:2052:HOH:O[3_655]	2.05	0.15
3:C:3212:HOH:O	3:C:3212:HOH:O[3_655]	2.05	0.15

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	338/341 (99%)	302 (89%)	34 (10%)	2 (1%)	22	28
1	B	338/341 (99%)	302 (89%)	33 (10%)	3 (1%)	14	18
1	C	338/341 (99%)	313 (93%)	23 (7%)	2 (1%)	22	28
1	D	338/341 (99%)	318 (94%)	17 (5%)	3 (1%)	14	18
All	All	1352/1364 (99%)	1235 (91%)	107 (8%)	10 (1%)	19	24

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	A	113	TYR
1	D	66	ASP
1	B	108	ALA
1	C	231	SER

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	274/274 (100%)	267 (97%)	7 (3%)	41	57
1	B	274/274 (100%)	265 (97%)	9 (3%)	33	47
1	C	274/274 (100%)	264 (96%)	10 (4%)	30	44
1	D	274/274 (100%)	261 (95%)	13 (5%)	22	32
All	All	1096/1096 (100%)	1057 (96%)	39 (4%)	30	44

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	LEU
1	D	273	ASN
1	D	70	LEU
1	D	220	ASP
1	D	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	273	ASN
1	D	273	ASN
1	C	301	GLN
1	D	69	HIS
1	D	322	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	LLP	D	51	1	23,24,25	1.57	3 (13%)	25,32,34	2.78	4 (16%)
1	LLP	C	51	1	23,24,25	2.25	4 (17%)	25,32,34	2.32	6 (24%)
1	LLP	A	51	1	23,24,25	2.96	5 (21%)	25,32,34	2.56	7 (28%)
1	LLP	B	51	1	23,24,25	2.36	6 (26%)	25,32,34	3.27	7 (28%)

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	LLP	D	51	1	-	4/16/17/19	0/1/1/1
1	LLP	C	51	1	-	5/16/17/19	0/1/1/1
1	LLP	A	51	1	-	9/16/17/19	0/1/1/1
1	LLP	B	51	1	-	6/16/17/19	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	LLP	C4'-NZ	12.28	1.68	1.27
1	B	51	LLP	C4'-NZ	8.61	1.56	1.27
1	C	51	LLP	C4'-NZ	8.09	1.54	1.27
1	D	51	LLP	C4-C4'	4.67	1.56	1.46
1	C	51	LLP	C4-C4'	4.34	1.55	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	51	LLP	CE-NZ-C4'	13.57	162.17	118.72
1	D	51	LLP	CE-NZ-C4'	10.52	152.40	118.72
1	A	51	LLP	CE-NZ-C4'	9.54	149.28	118.72
1	C	51	LLP	CE-NZ-C4'	-6.87	96.73	118.72
1	D	51	LLP	OP4-C5'-C5	6.49	121.52	109.36

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	51	LLP	C5'-OP4-P-OP2
1	A	51	LLP	C5'-OP4-P-OP3
1	A	51	LLP	CG-CD-CE-NZ
1	A	51	LLP	CD-CE-NZ-C4'
1	B	51	LLP	C4-C4'-NZ-CE

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	51	LLP	8	0
1	C	51	LLP	8	0
1	A	51	LLP	12	0
1	B	51	LLP	9	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	1AC	D	4001	-	5,7,7	4.57	2 (40%)	6,11,11	2.08	2 (33%)
2	1AC	C	3001	-	5,7,7	4.62	2 (40%)	6,11,11	2.07	2 (33%)
2	1AC	B	2001	-	5,7,7	4.63	2 (40%)	6,11,11	2.07	2 (33%)
2	1AC	A	1001	-	5,7,7	4.56	2 (40%)	6,11,11	2.05	2 (33%)

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
2	1AC	D	4001	-	-	0/4/10/10	0/1/1/1
2	1AC	C	3001	-	-	0/4/10/10	0/1/1/1
2	1AC	B	2001	-	-	0/4/10/10	0/1/1/1
2	1AC	A	1001	-	-	0/4/10/10	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	1AC	CG-CA	7.64	1.59	1.51
2	B	2001	1AC	CG-CA	7.59	1.59	1.51
2	A	1001	1AC	CG-CA	7.51	1.58	1.51
2	D	4001	1AC	CG-CA	7.46	1.58	1.51
2	B	2001	1AC	CB-CA	6.75	1.58	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4001	1AC	CG-CA-CB	-3.42	57.56	59.24
2	B	2001	1AC	CG-CA-CB	-3.38	57.59	59.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3001	1AC	CG-CA-CB	-3.36	57.60	59.24
2	A	1001	1AC	CG-CA-CB	-3.33	57.61	59.24
2	C	3001	1AC	CG-CB-CA	2.81	61.52	60.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4001	1AC	18	0
2	C	3001	1AC	15	0
2	B	2001	1AC	23	0
2	A	1001	1AC	21	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.