



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:29 PM GMT

PDB ID : 1B15
Title : ALCOHOL DEHYDROGENASE FROM DROSOPHILA LEBANONENSIS
TERNARY COMPLEX WITH NAD-ACETONE
Authors : Benach, J.; Atrian, S.; Gonzalez-Duarte, R.; Ladenstein, R.
Deposited on : 1998-11-25
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

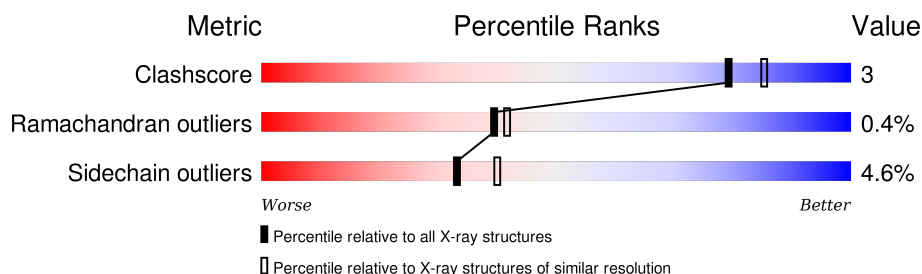
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	 83% 15% •
1	B	254	 84% 14% •

2 Entry composition [i](#)

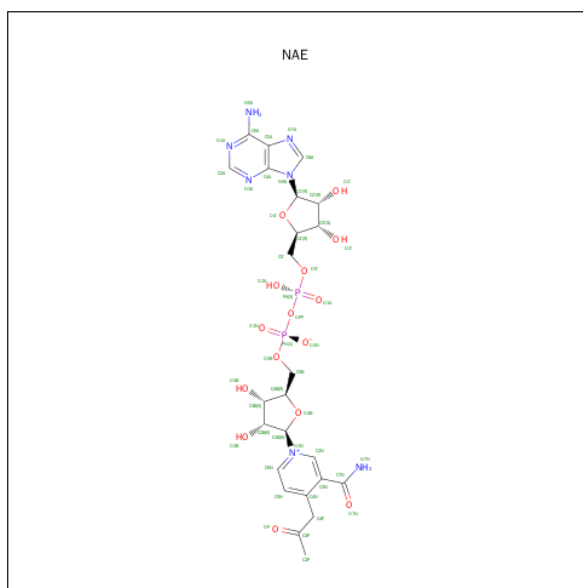
There are 3 unique types of molecules in this entry. The entry contains 4150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1962	1259	336	364	3			
1	B	254	Total	C	N	O	S	0	0	0
			1962	1259	336	364	3			

- Molecule 2 is NICOTINAMIDE ADENINE DINUCLEOTIDE ACETONE ADDUCT (three-letter code: NAE) (formula: $C_{24}H_{31}N_7O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
2	B	1	Total	C	N	O	P	0	0
			48	24	7	15	2		

- Molecule 3 is water.

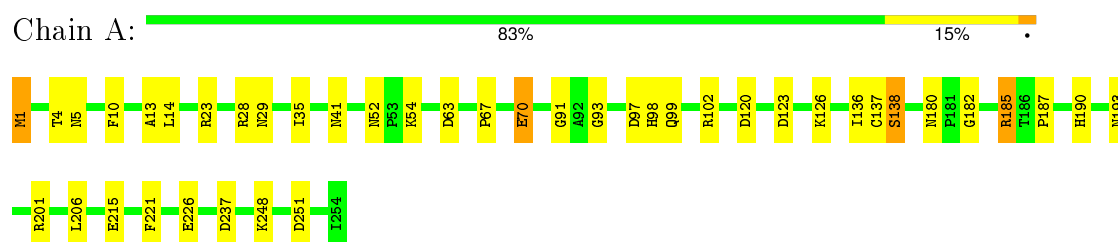
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total 71	O 71	0	0
3	B	59	Total 59	O 59	0	0

3 Residue-property plots

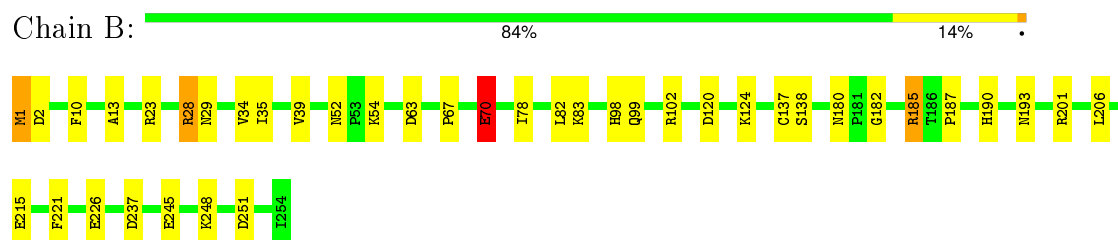
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.70 Å 53.50 Å 70.70 Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: NAE

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	0.54	0/2001	1.17	14/2727 (0.5%)
1	B	0.55	0/2001	1.17	10/2727 (0.4%)
All	All	0.54	0/4002	1.17	24/5454 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	B	70	GLU	CG-CD-OE1	10.96	140.23	118.30
1	B	70	GLU	CG-CD-OE2	-9.81	98.67	118.30
1	A	201	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	70	GLU	CG-CD-OE1	9.62	137.54	118.30
1	A	185	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	B	201	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	70	GLU	CG-CD-OE2	-8.84	100.62	118.30
1	B	63	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	251	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	123	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	201	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	2	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	251	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	63	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	23	ARG	CD-NE-CZ	6.00	132.01	123.60
1	A	185	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	23	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	123	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	28	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	A	97	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	70	GLU	CA-CB-CG	-5.33	101.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	A	63	ASP	CB-CG-OD1	5.01	122.81	118.30

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	A	1962	0	2013	15	0
1	B	1962	0	2013	13	0
2	A	48	0	29	1	0
2	B	48	0	29	0	0
3	A	71	0	0	0	0
3	B	59	0	0	1	0
All	All	4150	0	4084	28	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 3.

All (28) 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:93:GLY:HA3	2:A:255:NAE:H3B	1.81	0.60
1:B:137:CYS:HB2	1:B:180:ASN:OD1	2.11	0.51
1:B:1:MET:N	1:B:226:GLU:O	2.45	0.50
1:B:185:ARG:NH2	3:B:299:HOH:O	2.45	0.50
1:A:99:GLN:OE1	1:A:102:ARG:HD3	2.13	0.49
1:A:67:PRO:HD2	1:A:70:GLU:OE1	2.11	0.49
1:B:98:HIS:CD2	1:B:193:ASN:HB3	2.47	0.48
1:B:13:ALA:HB3	1:B:35:ILE:HG23	1.96	0.48
1:B:182:GLY:HA3	1:B:237:ASP:OD1	2.14	0.47
1:B:99:GLN:OE1	1:B:102:ARG:HD3	2.14	0.47
1:B:34:VAL:HG11	1:B:78:ILE:HD13	1.97	0.47
1:B:52:ASN:OD1	1:B:54:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:O	1:B:29:ASN:HB2	2.14	0.46
1:B:187:PRO:HA	1:B:190:HIS:CD2	2.50	0.46
1:A:137:CYS:HB2	1:A:180:ASN:OD1	2.16	0.46
1:B:67:PRO:HD2	1:B:70:GLU:OE1	2.15	0.45
1:A:52:ASN:OD1	1:A:54:LYS:HB2	2.17	0.45
1:A:13:ALA:HB3	1:A:35:ILE:HG23	1.99	0.44
1:A:98:HIS:CD2	1:A:193:ASN:HB3	2.53	0.44
1:A:4:THR:O	1:A:5:ASN:HB2	2.18	0.44
1:A:28:ARG:O	1:A:29:ASN:HB2	2.18	0.43
1:A:187:PRO:HA	1:A:190:HIS:CD2	2.53	0.43
1:B:82:LEU:O	1:B:83:LYS:HB2	2.19	0.42
1:A:14:LEU:HD13	1:A:41:ASN:HB3	2.01	0.41
1:A:91:GLY:HA3	1:A:136:ILE:HD12	2.02	0.41
1:A:137:CYS:O	1:A:138:SER:HB2	2.21	0.40
1:A:182:GLY:HA3	1:A:237:ASP:OD1	2.21	0.40
1:A:1:MET:N	1:A:226:GLU:O	2.55	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	252/254 (99%)	241 (96%)	10 (4%)	1 (0%)	39	42
1	B	252/254 (99%)	240 (95%)	11 (4%)	1 (0%)	39	42
All	All	504/508 (99%)	481 (95%)	21 (4%)	2 (0%)	39	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	SER
1	A	138	SER

5.3.2 Protein sidechains ⓘ

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	216/216 (100%)	207 (96%)	9 (4%)	36	44
1	B	216/216 (100%)	205 (95%)	11 (5%)	29	34
All	All	432/432 (100%)	412 (95%)	20 (5%)	33	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	PHE
1	A	120	ASP
1	A	126	LYS
1	A	185	ARG
1	A	206	LEU
1	A	215	GLU
1	A	221	PHE
1	A	248	LYS
1	B	1	MET
1	B	10	PHE
1	B	39	VAL
1	B	70	GLU
1	B	120	ASP
1	B	124	LYS
1	B	185	ARG
1	B	206	LEU
1	B	215	GLU
1	B	221	PHE
1	B	248	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	190	HIS
1	A	228	ASN
1	B	5	ASN
1	B	81	GLN
1	B	190	HIS
1	B	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

2 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	NAE	A	255	-	42,52,52	2.64	13 (30%)	52,79,79	2.17	18 (34%)
2	NAE	B	256	-	42,52,52	2.62	13 (30%)	52,79,79	2.42	15 (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
2	NAE	A	255	-	-	0/26/66/66	0/5/5/5
2	NAE	B	256	-	-	0/26/66/66	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	255	NAE	O4'-C1'	-6.57	1.32	1.41
2	B	256	NAE	O4'-C1'	-6.54	1.32	1.41
2	B	256	NAE	O3B-C3B	-2.81	1.36	1.43
2	A	255	NAE	O2B-C2B	-2.61	1.36	1.43
2	A	255	NAE	O3B-C3B	-2.37	1.37	1.43
2	B	256	NAE	O2'-C2'	-2.21	1.37	1.43
2	B	256	NAE	PN-O1N	-2.08	1.43	1.51
2	B	256	NAE	C3N-C4N	2.21	1.43	1.40
2	A	255	NAE	O3'-C3'	2.26	1.48	1.43
2	A	255	NAE	C7N-N7N	2.29	1.37	1.33
2	A	255	NAE	C3'-C4'	2.38	1.59	1.53
2	B	256	NAE	C3B-C4B	2.48	1.59	1.53
2	B	256	NAE	C7N-N7N	2.90	1.38	1.33
2	B	256	NAE	C4P-C4N	3.09	1.56	1.51
2	A	255	NAE	C3B-C4B	3.23	1.61	1.53
2	A	255	NAE	C4P-C4N	3.37	1.56	1.51
2	A	255	NAE	OP-C3P	3.50	1.34	1.21
2	A	255	NAE	C5N-C4N	3.54	1.45	1.39
2	B	256	NAE	C5N-C4N	3.65	1.46	1.39
2	B	256	NAE	OP-C3P	3.82	1.35	1.21
2	A	255	NAE	C4A-N3A	4.07	1.41	1.35
2	B	256	NAE	C4A-N3A	4.68	1.42	1.35
2	B	256	NAE	C2A-N3A	5.33	1.41	1.32
2	A	255	NAE	C2A-N3A	5.79	1.42	1.32
2	B	256	NAE	C3N-C7N	9.50	1.61	1.50
2	A	255	NAE	C3N-C7N	9.93	1.61	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	NAE	C5N-C4N-C3N	-6.88	110.07	118.48
2	B	256	NAE	N3A-C2A-N1A	-6.54	123.88	128.89
2	B	256	NAE	C4P-C4N-C5N	-6.31	109.28	120.12
2	B	256	NAE	C2'-C1'-N9A	-5.56	105.80	114.29
2	B	256	NAE	C4P-C4N-C3N	-5.55	112.55	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	255	NAE	C4P-C4N-C5N	-4.63	112.17	120.12
2	A	255	NAE	C5N-C4N-C3N	-4.63	112.83	118.48
2	A	255	NAE	C3N-C2N-N1N	-4.24	114.20	121.96
2	A	255	NAE	O7N-C7N-C3N	-4.21	115.07	120.29
2	A	255	NAE	C4P-C4N-C3N	-4.09	115.41	123.40
2	A	255	NAE	N3A-C2A-N1A	-4.03	125.81	128.89
2	A	255	NAE	C2'-C1'-N9A	-3.78	108.52	114.29
2	B	256	NAE	C3N-C2N-N1N	-3.30	115.92	121.96
2	B	256	NAE	C4A-C5A-N7A	-2.85	106.86	109.48
2	B	256	NAE	C2N-C3N-C7N	-2.58	111.21	120.80
2	A	255	NAE	C2N-C3N-C7N	-2.42	111.80	120.80
2	A	255	NAE	O5'-C5'-C4'	-2.40	100.28	109.12
2	A	255	NAE	O5B-PN-O1N	-2.22	100.99	109.62
2	A	255	NAE	O3B-C3B-C4B	-2.07	104.84	111.05
2	B	256	NAE	O4B-C4B-C3B	-2.05	101.01	105.15
2	B	256	NAE	C4'-O4'-C1'	-2.03	107.48	109.72
2	B	256	NAE	O7N-C7N-C3N	-2.01	117.80	120.29
2	B	256	NAE	O2A-PA-O1A	2.07	123.76	112.53
2	A	255	NAE	O4'-C1'-N9A	2.13	112.55	108.10
2	A	255	NAE	O2N-PN-O1N	2.18	124.33	112.53
2	A	255	NAE	PN-OPP-PA	2.57	139.94	132.73
2	A	255	NAE	N6A-C6A-N1A	2.59	124.77	119.20
2	A	255	NAE	O2'-C2'-C3'	2.75	120.76	111.83
2	B	256	NAE	O2'-C2'-C3'	2.80	120.93	111.83
2	B	256	NAE	O4'-C1'-N9A	3.12	114.63	108.10
2	A	255	NAE	C2A-N1A-C6A	3.38	124.81	118.77
2	B	256	NAE	C2A-N1A-C6A	4.01	125.93	118.77
2	A	255	NAE	C3N-C7N-N7N	4.17	124.22	118.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	255	NAE	1	0

5.7 Other polymers

There are no such residues in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.