

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 03:12 pm GMT

PDB ID	:	2CLP
Title	:	Crystal structure of human aflatoxin B1 aldehyde reductase member 3
Authors	:	Debreczeni, J.E.; Marsden, B.D.; Johansson, C.; Kavanagh, K.; Guo, K.; Smee,
		C.; Gileadi, O.; Turnbull, A.; Papagrigoriou, E.; von Delft, F.; Edwards, A.;
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Deposited on	:	2006-04-28
Resolution	:	3.00 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 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	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.00 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.



Motrio	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	2092 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27441 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	303	Total	С	Ν	0	S	0	0	0
1	Л	525	2445	1566	419	444	16	0	0	0
1	В	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	525	2445	1566	418	445	16	0	0	0
1	С	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U	525	2443	1565	417	445	16	0	0	0
1	п	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	525	2444	1568	416	444	16	0	0	0
1	F	303	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L	Ľ	525	2445	1568	417	444	16	0	Ū	0
1	F	303	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	525	2451	1569	420	446	16	0	0	0
1	G	393	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	u	525	2455	1569	424	446	16	0	0	0
1	н	393	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	11	525	2439	1564	417	442	16	0	0	0
1	т	399	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	T	022	2427	1556	412	443	16	0	0	0
1	Т	323	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	5	020	2443	1565	417	445	16	0	0	0
1	K	323	Total	\mathbf{C}	Ν	Ο	S	0	0	0
1	17	020	2460	1573	424	447	16	U		

• Molecule 1 is a protein called AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 3.

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	244	ASP	ASN	variant	UNP O95154
В	244	ASP	ASN	variant	UNP O95154
С	244	ASP	ASN	variant	UNP O95154
D	244	ASP	ASN	variant	UNP O95154
Е	244	ASP	ASN	variant	UNP O95154
F	244	ASP	ASN	variant	UNP O95154
G	244	ASP	ASN	variant	UNP O95154

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Chain	Residue	Modelled	Actual	Comment	Reference
Н	244	ASP	ASN	variant	UNP O95154
Ι	244	ASP	ASN	variant	UNP O95154
J	244	ASP	ASN	variant	UNP O95154
K	244	ASP	ASN	variant	UNP 095154

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• Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf										
0	Λ	1	Total	С	Ν	Ο	Р	0	0										
	A	1	48	21	7	17	3	0	0										
0	В	1	Total	С	Ν	Ο	Р	0	0										
	D	1	48	21	7	17	3	0	0										
2	С	1	Total	С	Ν	Ο	Р	0	0										
	U	1	48	21	7	17	3	0	0										
0	D	1	Total	С	Ν	Ο	Р	0	0										
		D	D		D	D	D	D	D	D	D	D	1	48	21	7	17	3	0
0	Е	Е	1	Total	С	Ν	Ο	Р	0	0									
			Ľ		Ľ	Ľ	Ľ	T	48	21	7	17	3	0	0				
2	F	F	F	F	F	F	F	F	F	Б	1	Total	С	Ν	Ο	Р	0	0	
										1	48	21	7	17	3	0	0		
2	С	1	Total	С	Ν	Ο	Р	0	0										
	G	1	48	21	7	17	3	0	0										
2	- п	TT 1	1	Total	С	Ν	Ο	Р	0	0									
	11	1	48	21	7	17	3	0	0										
2	T	1	Total	С	Ν	0	Р	0	0										
2	L	L	48	21	7	17	3	0											

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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
0	J	1	Total	С	Ν	Ο	Р	0	0
			48	21	7	17	3	0	0
0	К	1	Total	С	Ν	Ο	Р	0	0
2		K J	L	48	21	7	17	3	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ca 1 1	0	0
3	С	1	Total Ca 1 1	0	0
3	Ε	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total O 2 2	0	0
4	В	2	Total O 2 2	0	0
4	D	1	Total O 1 1	0	0
4	Ε	2	Total O 2 2	0	0
4	F	2	Total O 2 2	0	0
4	G	1	Total O 1 1	0	0
4	Н	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	126.96Å 126.96 Å 490.50 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	164.40 - 3.00	Depositor
Resolution (A)	59.18 - 3.00	EDS
% Data completeness	99.8 (164.40-3.00)	Depositor
(in resolution range)	99.7(59.18-3.00)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.34 (at 3.01 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.239 , 0.253	Depositor
Λ, Λ_{free}	0.243 , 0.255	DCC
R_{free} test set	4628 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.25, 19.7	EDS
L-test for twinning ²	$< L > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27441	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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



	True Chain Des Lin		T 1.	Bo	ond leng	ths	Bond angles			
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	F	1361	-	45,52,52	1.52	4 (8%)	53,80,80	1.38	7 (13%)
2	NDP	G	1361	-	45,52,52	1.54	5 (11%)	53,80,80	1.54	6 (11%)
2	NDP	Н	1361	-	45,52,52	1.60	5 (11%)	53,80,80	1.39	<mark>6 (11%)</mark>
2	NDP	J	1361	-	45,52,52	1.60	4 (8%)	53,80,80	1.29	5 (9%)
2	NDP	Е	1361	-	45,52,52	1.59	4 (8%)	53,80,80	1.18	3 (5%)
2	NDP	K	1361	-	45,52,52	1.62	4 (8%)	53,80,80	1.32	3 (5%)
2	NDP	Ι	1361	-	45,52,52	1.60	4 (8%)	53,80,80	1.24	2 (3%)
2	NDP	В	1361	-	45,52,52	1.64	4 (8%)	53,80,80	1.31	7 (13%)
2	NDP	А	1361	-	45,52,52	1.58	4 (8%)	53,80,80	1.17	5 (9%)
2	NDP	С	1361	-	45,52,52	1.49	4 (8%)	53,80,80	1.22	5 (9%)
2	NDP	D	1361	-	45,52,52	1.59	4 (8%)	53,80,80	1.14	2 (3%)

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).

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	NDP	F	1361	-	-	5/30/77/77	0/5/5/5
2	NDP	G	1361	-	-	7/30/77/77	0/5/5/5
2	NDP	Н	1361	-	-	5/30/77/77	0/5/5/5
2	NDP	J	1361	-	-	8/30/77/77	0/5/5/5
2	NDP	Е	1361	-	-	3/30/77/77	0/5/5/5
2	NDP	К	1361	-	-	4/30/77/77	0/5/5/5
2	NDP	Ι	1361	-	-	7/30/77/77	0/5/5/5
2	NDP	В	1361	-	-	4/30/77/77	0/5/5/5
2	NDP	А	1361	-	-	11/30/77/77	0/5/5/5
2	NDP	С	1361	-	-	8/30/77/77	0/5/5/5
2	NDP	D	1361	-	-	2/30/77/77	0/5/5/5

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1361	NDP	O7N-C7N	7.14	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	Ε	1361	NDP	O7N-C7N	7.13	1.41	1.24
2	Κ	1361	NDP	O7N-C7N	7.06	1.41	1.24
2	В	1361	NDP	O7N-C7N	7.04	1.41	1.24
2	Н	1361	NDP	O7N-C7N	7.03	1.41	1.24

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The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ι	1361	NDP	N3A-C2A-N1A	-6.07	119.20	128.68
2	J	1361	NDP	N3A-C2A-N1A	-5.63	119.88	128.68
2	Е	1361	NDP	N3A-C2A-N1A	-5.53	120.04	128.68
2	С	1361	NDP	N3A-C2A-N1A	-5.47	120.13	128.68
2	F	1361	NDP	N3A-C2A-N1A	-5.47	120.13	128.68

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	А	1361	NDP	C2B-O2B-P2B-O2X
2	А	1361	NDP	C2N-C3N-C7N-N7N
2	В	1361	NDP	PN-O3-PA-O5B
2	С	1361	NDP	C2N-C3N-C7N-N7N
2	F	1361	NDP	C2B-O2B-P2B-O2X

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















































4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	323/347~(93%)	-0.29	0 100 100	50, 56, 60, 66	0
1	В	323/347~(93%)	-0.17	1 (0%) 94 84	47, 56, 61, 64	0
1	С	323/347~(93%)	-0.26	1 (0%) 94 84	48,56,61,65	0
1	D	323/347~(93%)	-0.27	0 100 100	47, 55, 61, 66	0
1	Ε	323/347~(93%)	-0.31	0 100 100	48,55,61,66	0
1	F	323/347~(93%)	-0.28	0 100 100	47, 56, 60, 63	0
1	G	323/347~(93%)	-0.22	0 100 100	48,56,60,69	0
1	Н	323/347~(93%)	-0.06	3 (0%) 84 63	48, 56, 61, 63	0
1	Ι	322/347~(92%)	0.30	19 (5%) 22 7	51,56,59,61	0
1	J	323/347~(93%)	0.22	12 (3%) 41 17	51, 56, 60, 61	0
1	K	323/347~(93%)	-0.26	0 100 100	47, 56, 62, 66	0
All	All	3552/3817~(93%)	-0.14	36 (1%) 82 59	47, 56, 61, 69	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	284	ALA	3.9
1	Ι	316	LEU	3.7
1	J	190	GLY	3.4
1	Ι	300	MET	3.4
1	В	97	SER	3.4

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

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



5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	NDP	Ι	1361	48/48	0.91	0.28	63,71,88,88	0
3	CA	С	1362	1/1	0.92	0.19	41,41,41,41	0
2	NDP	J	1361	48/48	0.94	0.23	67,70,82,83	0
2	NDP	Н	1361	48/48	0.94	0.15	52,57,67,68	0
2	NDP	В	1361	48/48	0.96	0.15	$35,\!45,\!56,\!57$	0
2	NDP	С	1361	48/48	0.96	0.14	27,40,55,57	0
2	NDP	А	1361	48/48	0.96	0.15	24,31,56,57	0
2	NDP	D	1361	48/48	0.97	0.14	28,40,54,55	0
2	NDP	Е	1361	48/48	0.97	0.21	33,41,50,50	0
2	NDP	F	1361	48/48	0.97	0.12	27,35,44,45	0
2	NDP	K	1361	48/48	0.97	0.14	30,38,44,45	0
3	CA	А	1362	1/1	0.97	0.19	37,37,37,37	0
2	NDP	G	1361	48/48	0.97	0.12	26,34,44,44	0
3	CA	Е	1362	1/1	0.97	0.13	35,35,35,35	0
3	CA	G	1362	1/1	0.97	0.18	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

























5.5 Other polymers (i)

There are no such residues in this entry.

