

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 02:39 pm GMT

PDB ID : 5AC2

Title: human aldehyde dehydrogenase 1A1 with duocarmycin analog

Authors: Koch, M.F.; Harteis, S.; Blank, I.D.; Pestel, G.; Tietze, L.F.; Ochsenfeld, C.;

Schneider, S.; Sieber, S.A.

Deposited on : 2015-08-11

Resolution : 1.85 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.orgA 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

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)

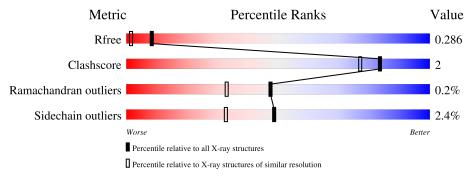
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Mol	Chain	Length	Quality of chain	
1	A	501	91%	7% •

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	\mathbf{Type}	Chain	Res	Chirality	Geometry	Clashes	Electron density	
4	TXE	A	1504	X	-	-	-	



2 Entry composition (i)

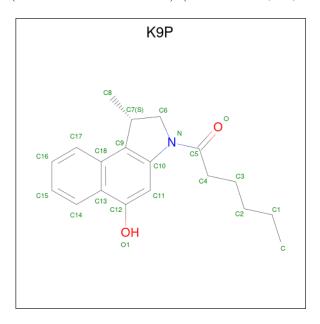
There are 5 unique types of molecules in this entry. The entry contains 4076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINAL DEHYDROGENASE 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	494	Total 3840	C 2449	N 647	O 724	S 20	0	4	0

• Molecule 2 is 1-[(1S)-1-methyl-5-oxidanyl-1,2-dihydrobenzo[e]indol-3-yl]hexan-1-one (three-letter code: K9P) (formula: $C_{19}H_{23}NO_2$).



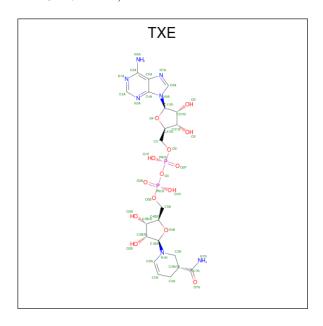
M	[ol	Chain	Residues	Atoms				ZeroOcc	AltConf
:	2	A	1	Total 22	C 19	N 1	O 2	0	0

• Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Yb 3 3	0	0



• Molecule 4 is [[(2R,3S,4R,5R)-5-[(3R)-3-aminocarbonyl-3,4-dihydro-2H-pyridin-1-yl]-3,4-b is(oxidanyl)oxolan-2-yl]methoxy-oxidanidyl-ph osphoryl] [(2R,3S,4R,5R)-5-(6-aminopuri n-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphate (three-letter code: TXE) (formula: $C_{21}H_{31}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

• Molecule 5 is water.

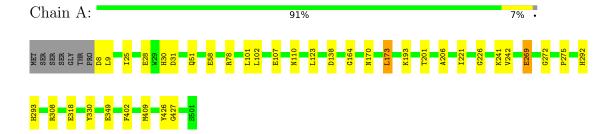
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	167	Total O 167 167	0	0



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.

• Molecule 1: RETINAL DEHYDROGENASE 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants	109.12Å 109.12Å 83.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 - 1.85	Depositor
rtesolution (A)	48.80 - 1.85	EDS
% Data completeness	99.8 (48.80-1.85)	Depositor
(in resolution range)	99.8 (48.80-1.85)	EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.19 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
P. P.	0.199 , 0.251	Depositor
R, R_{free}	0.247 , 0.286	DCC
R_{free} test set	2182 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 34.7	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4076	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TXE, YB, K9P

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	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.96	4/3928 (0.1%)	0.89	4/5316 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\textup{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	9	LEU	C-N	-14.68	1.06	1.34
1	A	101	LEU	C-N	-10.61	1.09	1.34
1	A	8	ASP	C-N	-9.71	1.11	1.34
1	A	269	GLU	CD-OE2	-5.14	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	78	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	9	LEU	O-C-N	-5.61	110.44	121.10
1	A	138	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	31	ASP	CB-CG-OD1	5.35	123.11	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	102	LEU	Mainchain

5.2 Too-close contacts (i)

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	3840	0	3833	15	0
2	A	22	0	20	3	0
3	A	3	0	0	1	0
4	A	44	0	28	3	0
5	A	167	0	0	2	0
All	All	4076	0	3881	19	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 2.

The worst 5 of 19 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:206:ALA:HB2	1:A:221:ILE:HD12	1.72	0.69
3:A:1507:YB:YB	5:A:2164:HOH:O	1.89	0.64
1:A:170:ASN:HD21	4:A:1504:TXE:HN7N	1.49	0.60
1:A:349:GLU:OE2	5:A:2123:HOH:O	2.18	0.56
1:A:292:HIS:NE2	1:A:330:TYR:OH	2.38	0.54

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	496/501 (99%)	481 (97%)	14 (3%)	1 (0%)	47 33	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	GLY

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	413/415 (100%)	403 (98%)	10 (2%)	49 33	

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	GLU
1	A	402	PHE
1	A	409	MET
1	A	173	LEU
1	A	193	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	383	GLN
1	A	474	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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).

Mal	Mol Type Chain Res		Res Link		В	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	K9P	A	1502	1	24,24,24	1.95	8 (33%)	31,34,34	1.22	4 (12%)	
4	TXE	A	1504	3	41,48,48	2.29	10 (24%)	44,73,73	2.00	9 (20%)	

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.

\mathbf{N}	/Iol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	K9P	A	1502	1	-	2/9/21/21	0/3/3/3
	4	TXE	A	1504	3	1/1/13/15	5/26/72/72	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(\mathring{A})$	Ideal(Å)
4	A	1504	TXE	C2N-C3N	-9.48	1.38	1.53
4	A	1504	TXE	C2N-N1N	-5.50	1.37	1.47
2	A	1502	K9P	C9-C7	-4.42	1.46	1.51
4	A	1504	TXE	C4N-C5N	-4.37	1.40	1.49
4	A	1504	TXE	C4N-C3N	-3.71	1.39	1.52



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
4	A	1504	TXE	O4B-C1B-N1N	5.63	116.95	109.35
4	A	1504	TXE	C5'-C4'-C3'	-4.76	97.35	115.18
4	A	1504	TXE	C2N-C3N-C7N	4.62	118.74	110.07
4	A	1504	TXE	N3A-C2A-N1A	-3.39	123.38	128.68
4	A	1504	TXE	O1N-PN-O2N	3.12	127.66	112.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1504	TXE	C3N

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1504	TXE	O4B-C1B-N1N-C2N
2	A	1502	K9P	C1-C2-C3-C4
4	A	1504	TXE	C4N-C3N-C7N-N7N
4	A	1504	TXE	C5'-O5'-PA-O3
4	A	1504	TXE	C5'-O5'-PA-O1P

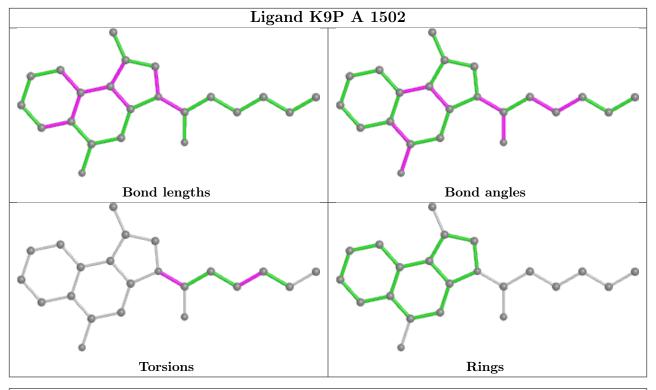
There are no ring outliers.

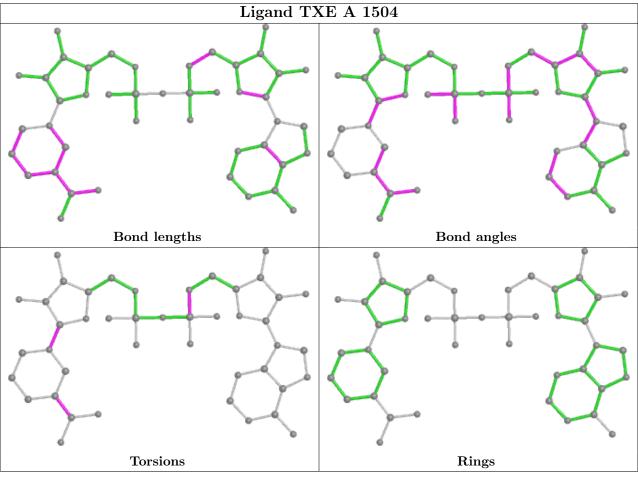
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1502	K9P	3	0
4	A	1504	TXE	3	0

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	8:ASP	С	9:LEU	N	1.11
1	A	101:LEU	С	102:LEU	N	1.09
1	A	9:LEU	С	10:PRO	N	1.06



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

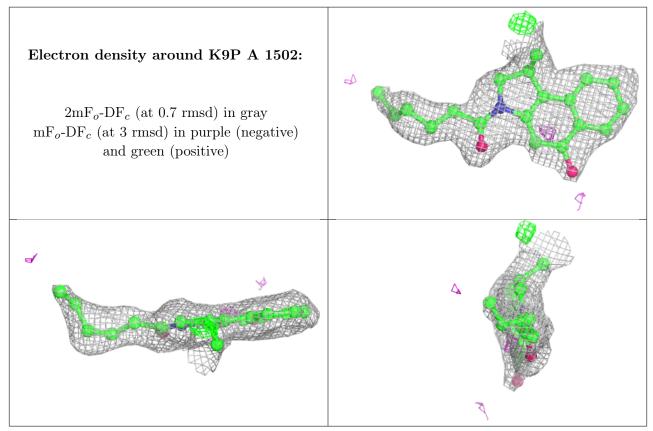
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

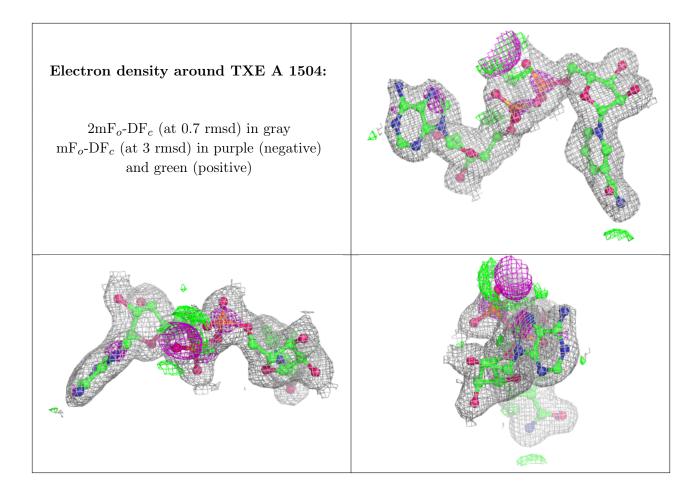
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

