



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8XR3 / pdb_00008xr3
Title : Crystal structure of AKRtyl-apo2
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Deposited on : 2024-01-06
Resolution : 2.31 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

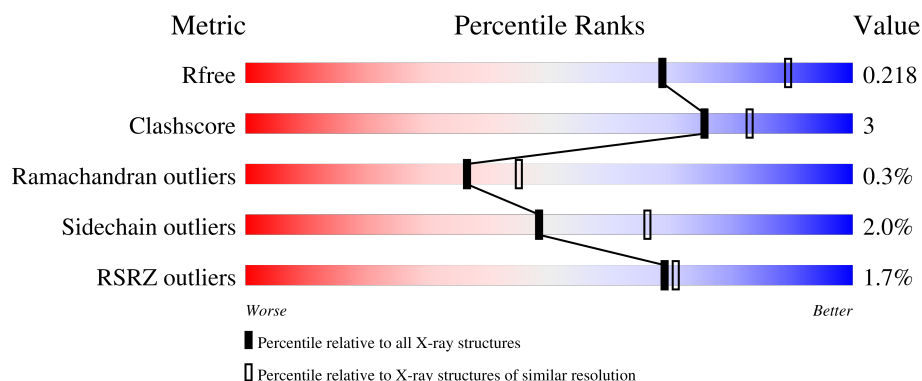
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	331	
1	C	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5244 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 Aldo/keto reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	320	Total	C	N	O	S	0	0	0
			2478	1560	442	468	8			
1	A	319	Total	C	N	O	S	0	0	0
			2469	1555	440	466	8			

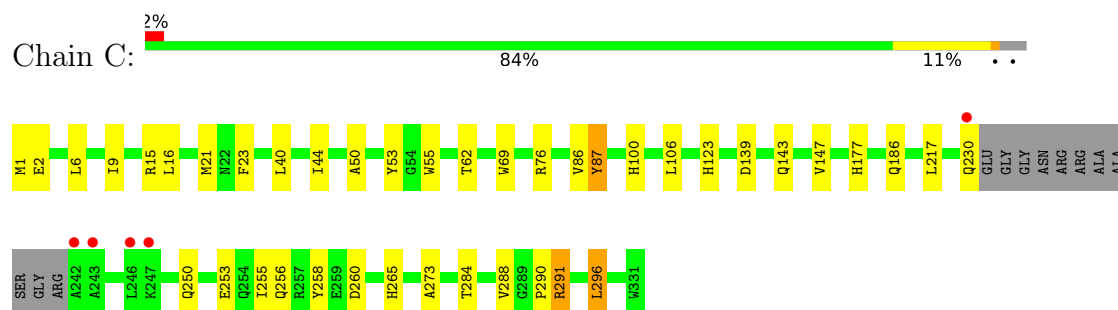
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	156	Total	O	0	0
			156	156		
2	A	141	Total	O	0	0
			141	141		

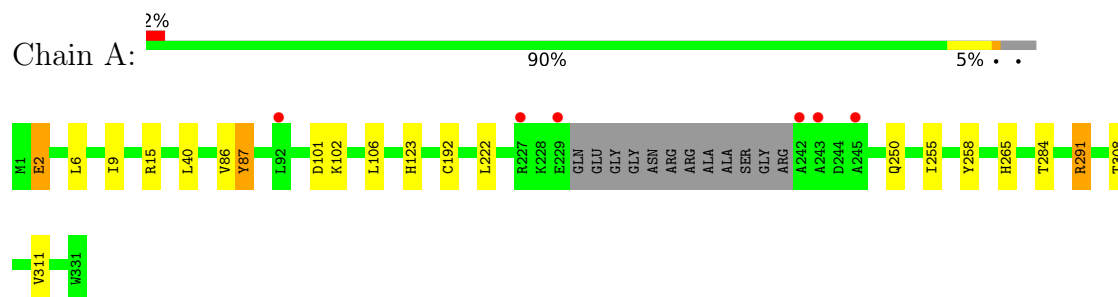
3 Residue-property plots

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 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.

- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	109.33Å 109.33Å 140.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.65 – 2.31 38.65 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.65-2.31) 100.0 (38.65-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.173 , 0.219 0.174 , 0.218	Depositor DCC
R_{free} test set	1950 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.040 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.67	2/2524 (0.1%)	1.02	1/3429 (0.0%)
1	C	0.68	4/2533 (0.2%)	1.02	3/3441 (0.1%)
All	All	0.67	6/5057 (0.1%)	1.02	4/6870 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	HIS	CE1-NE2	7.71	1.40	1.32
1	C	265	HIS	CE1-NE2	5.65	1.38	1.32
1	C	100	HIS	CE1-NE2	5.62	1.38	1.32
1	A	265	HIS	CE1-NE2	5.39	1.38	1.32
1	C	177	HIS	CE1-NE2	5.10	1.37	1.32
1	C	123	HIS	CE1-NE2	5.04	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	ARG	N-CA-C	-7.97	103.77	113.97
1	A	291	ARG	N-CA-C	-6.67	105.05	113.72
1	C	186	GLN	CB-CA-C	5.74	120.14	110.79
1	C	139	ASP	CA-CB-CG	5.16	117.75	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2469	0	2410	10	0
1	C	2478	0	2418	19	0
2	A	141	0	0	0	0
2	C	156	0	0	1	0
All	All	5244	0	4828	29	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 (29) 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:C:1:MET:HE1	1:C:16:LEU:HD12	1.76	0.68
1:C:44:ILE:HD12	1:C:296:LEU:HD21	1.79	0.63
1:C:256:GLN:HE21	1:C:260:ASP:CG	2.11	0.58
1:C:256:GLN:NE2	1:C:260:ASP:OD1	2.37	0.58
1:C:15:ARG:HD2	1:C:284:THR:O	2.04	0.57
1:C:21:MET:HE3	1:C:55:TRP:HZ2	1.76	0.51
1:A:15:ARG:HD2	1:A:284:THR:O	2.11	0.51
1:C:1:MET:N	2:C:404:HOH:O	2.46	0.49
1:C:21:MET:CE	1:C:55:TRP:HZ2	2.25	0.48
1:C:6:LEU:O	1:C:9:ILE:HG12	2.14	0.47
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.29	0.47
1:A:192:CYS:SG	1:A:222:LEU:HD21	2.55	0.47
1:A:255:ILE:O	1:A:258:TYR:HB3	2.16	0.46
1:C:106:LEU:HD23	1:C:106:LEU:C	2.42	0.45
1:A:6:LEU:O	1:A:9:ILE:HG12	2.17	0.45
1:C:217:LEU:CD2	1:C:273:ALA:HB3	2.49	0.43
1:C:143:GLN:O	1:C:147:VAL:HG23	2.20	0.42
1:A:2:GLU:HB3	1:A:15:ARG:HG3	2.02	0.41
1:C:69:TRP:CE2	1:C:76:ARG:HD3	2.56	0.41
1:C:23:PHE:HB2	1:C:62:THR:HG23	2.03	0.41
1:C:50:ALA:HB3	1:C:53:TYR:CD1	2.56	0.41
1:C:288:VAL:O	1:C:290:PRO:HD3	2.21	0.41
1:A:106:LEU:C	1:A:106:LEU:HD23	2.46	0.41
1:A:308:THR:OG1	1:A:311:VAL:HG23	2.21	0.41
1:C:86:VAL:O	1:C:87:TYR:HB2	2.20	0.40
1:A:86:VAL:O	1:A:87:TYR:HB2	2.21	0.40
1:A:101:ASP:O	1:A:102:LYS:HB2	2.21	0.40
1:C:255:ILE:O	1:C:258:TYR:HB3	2.21	0.40
1:C:86:VAL:O	1:C:87:TYR:CB	2.70	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	315/331 (95%)	304 (96%)	10 (3%)	1 (0%)	36	45
1	C	316/331 (96%)	304 (96%)	11 (4%)	1 (0%)	36	45
All	All	631/662 (95%)	608 (96%)	21 (3%)	2 (0%)	36	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	TYR
1	A	87	TYR

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	251/258 (97%)	248 (99%)	3 (1%)	63	78
1	C	252/258 (98%)	245 (97%)	7 (3%)	38	55
All	All	503/516 (98%)	493 (98%)	10 (2%)	48	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	GLU

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Mol	Chain	Res	Type
1	C	40	LEU
1	C	230	GLN
1	C	250	GLN
1	C	253	GLU
1	C	291	ARG
1	C	296	LEU
1	A	2	GLU
1	A	40	LEU
1	A	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	128	GLN
1	C	161	ASN
1	C	169	GLN
1	C	177	HIS
1	C	256	GLN
1	A	22	ASN
1	A	107	ASN
1	A	151	GLN
1	A	186	GLN
1	A	250	GLN
1	A	254	GLN
1	A	256	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

6.1 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, 95th 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>2	OWAB(Å ²)	Q<0.9
1	A	319/331 (96%)	-0.13	6 (1%) 66 68	24, 35, 72, 99	0
1	C	320/331 (96%)	-0.17	5 (1%) 70 72	24, 34, 68, 99	0
All	All	639/662 (96%)	-0.15	11 (1%) 69 71	24, 34, 71, 99	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ALA	5.6
1	C	243	ALA	4.2
1	A	243	ALA	3.9
1	C	242	ALA	3.5
1	A	227	ARG	3.3
1	A	92	LEU	3.2
1	C	230	GLN	2.8
1	A	229	GLU	2.2
1	C	246	LEU	2.2
1	C	247	LYS	2.2
1	A	245	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.