



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:11 AM UTC

PDB ID : 2BGK / pdb_00002bgk
Title : X-Ray structure of apo-Secoisolariciresinol Dehydrogenase
Authors : Youn, B.; Moinuddin, S.G.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on : 2004-12-23
Resolution : 1.60 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 ⓘ 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

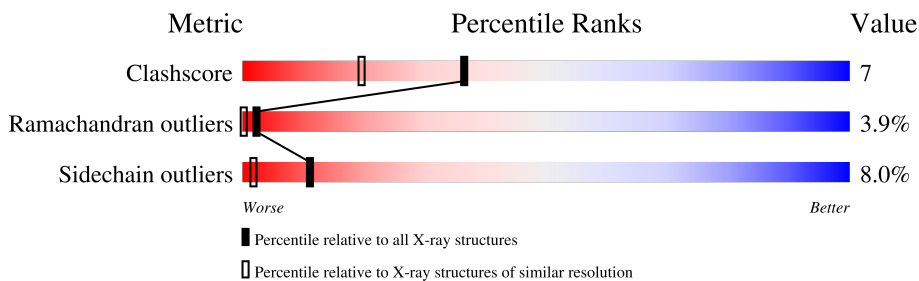
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	278	
1	B	278	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4178 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 RHIZOME SECOISOLARICIRE SINOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	1
			1986	1254	340	385	7			
1	B	268	Total	C	N	O	S	0	0	1
			1986	1254	340	385	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	106	Total	O	0	0
			106	106		

4 Data and refinement statistics

Xtrriage (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	107.34Å 133.56Å 69.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	99.7 (10.00-1.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.95	12/2018 (0.6%)	1.58	32/2742 (1.2%)
1	B	0.91	12/2018 (0.6%)	1.63	29/2742 (1.1%)
All	All	0.93	24/4036 (0.6%)	1.60	61/5484 (1.1%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	VAL	CA-CB	8.68	1.64	1.54
1	A	135	HIS	CD2-NE2	-7.04	1.30	1.37
1	B	1277	LEU	C-N	-6.88	1.23	1.33
1	B	1135	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	277	LEU	C-N	-6.79	1.23	1.33

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1166	VAL	CB-CA-C	-13.36	94.87	111.97
1	B	1060	ILE	N-CA-C	-11.61	100.64	111.67
1	A	16	ASP	CA-CB-CG	10.95	123.55	112.60
1	B	1166	VAL	N-CA-CB	10.78	123.16	110.55
1	B	1225	ASN	N-CA-C	-9.04	94.78	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	SER	Peptide

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	1986	0	1997	26	0
1	B	1986	0	1997	37	0
2	A	100	0	0	2	0
2	B	106	0	0	2	0
All	All	4178	0	3994	57	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 7.

The worst 5 of 57 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:B:1106:THR:HG21	1:B:1114:GLY:H	1.26	0.99
1:A:24:GLY:HA3	1:A:45:ILE:HG23	1.63	0.79
1:B:1011:THR:HA	1:B:1039:TYR:HA	1.67	0.75
1:B:1057:CYS:SG	1:B:1068:PHE:HB2	2.27	0.75
1:B:1135:HIS:HD2	1:B:1138:ARG:HH21	1.36	0.74

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	266/278 (96%)	247 (93%)	13 (5%)	6 (2%)	5	0
1	B	266/278 (96%)	231 (87%)	20 (8%)	15 (6%)	1	0
All	All	532/556 (96%)	478 (90%)	33 (6%)	21 (4%)	2	0

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ALA
1	A	203	PRO
1	A	274	LYS
1	B	1109	SER
1	B	1201	ALA

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	213/222 (96%)	196 (92%)	17 (8%)	11	2
1	B	213/222 (96%)	196 (92%)	17 (8%)	11	2
All	All	426/444 (96%)	392 (92%)	34 (8%)	11	2

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1199	ILE
1	B	1211	VAL
1	B	1219	LEU
1	A	211	VAL
1	A	207	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1135	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1172	HIS
1	B	1193	ASN
1	A	172	HIS
1	A	222	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.