



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 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 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) : **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

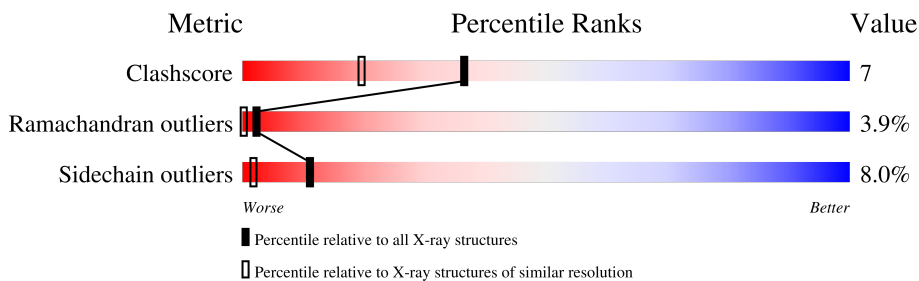
1 Overall quality at a glance

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	 74% 17% . . .
1	B	278	 66% 23% 6% . .

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

Xtriage (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.	Xtriage
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

All (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
1	A	69	VAL	CA-CB	6.70	1.63	1.54
1	A	275	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	1090	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	1052	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	221	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	52	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	1070	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	1165	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	165	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	1275	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	90	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	1141	ILE	CA-CB	5.92	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1221	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	172	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	1172	HIS	CD2-NE2	-5.45	1.31	1.37
1	B	1168	THR	CA-CB	5.31	1.62	1.53
1	A	16	ASP	CA-CB	5.15	1.60	1.54
1	B	1199	ILE	CA-CB	5.14	1.60	1.53

All (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
1	B	1105	THR	N-CA-CB	-7.45	99.46	110.49
1	B	1106	THR	N-CA-CB	-7.34	97.30	110.37
1	A	64	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	81	ASN	CA-CB-CG	7.19	119.79	112.60
1	B	1206	THR	N-CA-C	7.03	120.41	110.50
1	A	113	ALA	O-C-N	-6.85	114.86	122.12
1	A	274	LYS	N-CA-C	6.84	125.37	110.80
1	B	1209	PHE	CA-CB-CG	6.82	120.61	113.80
1	B	1108	TYR	N-CA-C	-6.61	99.25	109.76
1	A	250	TYR	CA-C-N	-6.33	115.34	123.19
1	A	250	TYR	C-N-CA	-6.33	115.34	123.19
1	B	1057	CYS	N-CA-C	6.32	118.70	111.11
1	B	1109	SER	N-CA-CB	6.29	121.11	110.49
1	B	1064	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	1052	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	B	1085	THR	CA-CB-OG1	-6.05	100.53	109.60
1	A	135	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	A	113	ALA	N-CA-C	6.00	118.59	111.33
1	A	62	SER	CA-C-N	5.82	125.50	119.56
1	A	62	SER	C-N-CA	5.82	125.50	119.56
1	A	123	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	275	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	B	1113	ALA	CA-C-N	5.75	127.21	120.71
1	B	1113	ALA	C-N-CA	5.75	127.21	120.71
1	A	139	VAL	N-CA-CB	-5.73	99.55	111.24
1	B	1249	LYS	CA-CB-CG	5.66	125.42	114.10
1	A	206	THR	CA-C-N	5.62	127.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	THR	C-N-CA	5.62	127.81	120.28
1	B	1102	VAL	N-CA-CB	-5.61	103.05	112.47
1	B	1135	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	B	1070	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	A	12	ASN	CA-C-N	5.54	128.73	120.31
1	A	12	ASN	C-N-CA	5.54	128.73	120.31
1	B	1275	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	B	1048	ILE	CB-CA-C	-5.47	104.67	112.22
1	A	232	ARG	CA-CB-CG	-5.37	103.36	114.10
1	B	1011	THR	N-CA-CB	-5.37	102.38	111.50
1	B	1011	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	90	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	B	1166	VAL	CG1-CB-CG2	5.36	122.58	110.80
1	A	50	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	50	ASP	N-CA-C	5.32	116.94	111.03
1	A	249	LYS	N-CA-C	5.25	119.17	112.87
1	B	1109	SER	N-CA-C	-5.24	99.64	110.80
1	B	1106	THR	CB-CA-C	5.22	120.46	110.17
1	A	203	PRO	N-CA-C	5.21	123.20	112.47
1	A	48	ILE	CB-CA-C	-5.17	103.73	112.16
1	A	200	VAL	O-C-N	5.16	129.24	122.94
1	B	1085	THR	CA-CB-CG2	5.16	119.27	110.50
1	A	269	PHE	CA-C-N	5.14	125.18	119.32
1	A	269	PHE	C-N-CA	5.14	125.18	119.32
1	B	1089	LYS	N-CA-C	5.11	116.66	111.14
1	A	200	VAL	CA-C-N	5.04	131.16	121.54
1	A	200	VAL	C-N-CA	5.04	131.16	121.54
1	A	202	SER	CA-C-N	5.03	126.13	119.84
1	A	202	SER	C-N-CA	5.03	126.13	119.84

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

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.

All (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
1:B:1106:THR:CG2	1:B:1114:GLY:H	2.01	0.73
1:A:135:HIS:HD2	1:A:138:ARG:HH21	1.43	0.67
1:B:1050:ASP:HA	1:B:1068:PHE:CZ	2.30	0.67
1:B:1193:ASN:HD22	1:B:1254:LEU:H	1.42	0.65
1:A:203:PRO:HB2	1:A:216:VAL:HG11	1.80	0.64
1:B:1135:HIS:CD2	1:B:1138:ARG:HH21	2.15	0.64
1:A:249:LYS:HA	1:A:249:LYS:HE2	1.79	0.64
1:A:122:MET:HE1	1:B:1126:VAL:HG11	1.81	0.62
1:B:1193:ASN:ND2	1:B:1254:LEU:H	2.00	0.59
1:A:177:LEU:HD13	1:B:1169:ALA:HB2	1.87	0.57
1:A:266:ASN:HD22	1:A:266:ASN:C	2.12	0.57
1:A:172:HIS:HE1	2:B:2067:HOH:O	1.88	0.57
1:B:1199:ILE:HD13	1:B:1220:ALA:HB2	1.86	0.56
1:A:57:CYS:SG	1:A:66:ILE:HG12	2.46	0.55
1:A:24:GLY:HA3	1:A:45:ILE:CG2	2.37	0.54
1:B:1154:ILE:O	1:B:1158:THR:HG22	2.08	0.54
1:B:1217:GLU:O	1:B:1230:LEU:HD11	2.07	0.54
1:B:1247:GLU:HG2	2:B:2089:HOH:O	2.07	0.53
1:A:48:ILE:H	1:A:48:ILE:HD13	1.74	0.52
2:A:2065:HOH:O	1:B:1172:HIS:HE1	1.91	0.52
1:B:1166:VAL:O	1:B:1170:THR:HG23	2.09	0.52
1:A:266:ASN:ND2	1:A:268:ALA:H	2.08	0.52
1:A:135:HIS:CD2	1:A:138:ARG:HH21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG22	1:B:1159:ALA:HB2	1.94	0.50
1:B:1048:ILE:HG22	1:B:1070:HIS:CE1	2.46	0.50
1:B:1122:MET:SD	1:B:1170:THR:HG22	2.53	0.49
1:A:120:ARG:HD3	2:A:2047:HOH:O	2.12	0.48
1:A:159:ALA:HB2	1:B:1179:THR:HG22	1.96	0.48
1:B:1106:THR:HG21	1:B:1114:GLY:N	2.11	0.48
1:B:1118:PHE:CD1	1:B:1166:VAL:HG13	2.50	0.46
1:A:43:VAL:HG23	1:A:66:ILE:HG13	1.97	0.45
1:B:1045:ILE:HB	1:B:1057:CYS:SG	2.57	0.45
1:A:166:VAL:O	1:A:170:THR:HG23	2.16	0.45
1:A:205:LEU:HB2	1:A:211:VAL:HG13	1.99	0.45
1:A:27:GLY:O	1:A:31:THR:HG23	2.16	0.44
1:A:126:VAL:HG11	1:B:1122:MET:HE3	1.98	0.44
1:B:1055:LYS:HA	1:B:1059:ASN:HB2	1.99	0.44
1:B:1106:THR:HG23	1:B:1113:ALA:HA	1.99	0.44
1:A:177:LEU:O	1:A:181:LEU:HB2	2.17	0.44
1:A:191:ARG:HE	1:A:249:LYS:HE2	1.83	0.44
1:B:1206:THR:HA	1:B:1211:VAL:CG2	2.49	0.43
1:B:1135:HIS:HD2	1:B:1138:ARG:NH2	2.10	0.43
1:B:1171:LYS:HA	1:B:1171:LYS:HD3	1.79	0.42
1:B:1023:GLY:O	1:B:1047:ASP:HB3	2.19	0.42
1:A:87:ILE:HD11	1:A:139:VAL:HG13	2.02	0.42
1:B:1083:VAL:HG21	1:B:1135:HIS:HB3	2.01	0.42
1:A:138:ARG:HA	1:B:1111:LEU:HD21	2.02	0.42
1:A:274:LYS:HE3	1:A:276:GLY:H	1.85	0.42
1:B:1030:GLU:HG2	1:B:1034:LYS:HE2	2.02	0.41
1:B:1116:GLU:HA	1:B:1119:LYS:NZ	2.35	0.41
1:B:1185:LEU:HB3	1:B:1190:ILE:HB	2.03	0.41
1:B:1206:THR:HA	1:B:1211:VAL:HG23	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

All (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
1	A	59	ASN
1	A	211	VAL
1	B	1053	GLY
1	B	1205	LEU
1	B	1209	PHE
1	B	1273	LEU
1	B	1276	GLY
1	A	202	SER
1	B	1051	ASP
1	B	1054	GLN
1	B	1026	GLY
1	B	1203	PRO
1	B	1226	LEU
1	B	1274	LYS
1	B	1204	LEU
1	B	1056	VAL

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	426/444 (96%)	392 (92%)	34 (8%)	11 2

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	16	ASP
1	A	48	ILE
1	A	69	VAL
1	A	77	GLU
1	A	81	ASN
1	A	103	LEU
1	A	139	VAL
1	A	177	LEU
1	A	181	LEU
1	A	203	PRO
1	A	207	ASP
1	A	211	VAL
1	A	231	LEU
1	A	247	GLU
1	A	251	VAL
1	A	266	ASN
1	B	1013	ARG
1	B	1048	ILE
1	B	1060	ILE
1	B	1085	THR
1	B	1102	VAL
1	B	1105	THR
1	B	1106	THR
1	B	1166	VAL
1	B	1168	THR
1	B	1175	LEU
1	B	1181	LEU
1	B	1199	ILE
1	B	1211	VAL
1	B	1215	ARG
1	B	1218	GLU
1	B	1219	LEU
1	B	1274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	115	ASN
1	A	135	HIS
1	A	172	HIS
1	A	222	GLN
1	A	266	ASN
1	B	1115	ASN
1	B	1135	HIS
1	B	1172	HIS
1	B	1193	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 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.