Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 09:28 pm GMT

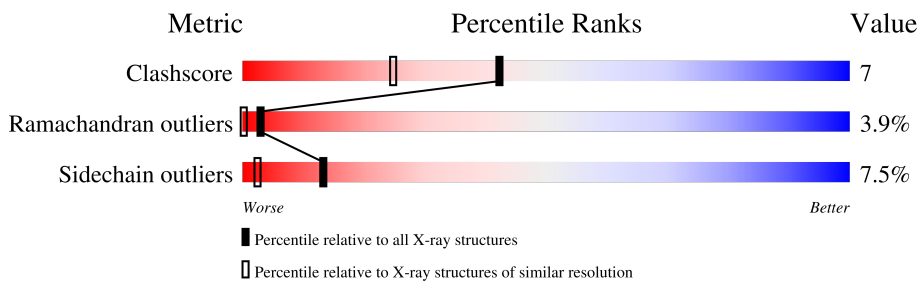|		
PDB ID	:	2BGK
Title	:	X-Ray structure of apo-Secoisolariciresinol Dehydrogenase
Authors	:	Youn, B.; Moinuddin, S.G.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on	:	2004-12-23
Resolution	:	1.60 Å(reported)

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		3.9%
Sidechain outliers		7.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	278	80% 13% • • •
1	B	278	69% 24% • • •

2 Entry composition (i)

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 SECOISOLARICIRESINOL 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		

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. 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.

Note EDS was not executed.

• Molecule 1: RHIZOME SECOISOLARICIRESINOL DEHYDROGENASE
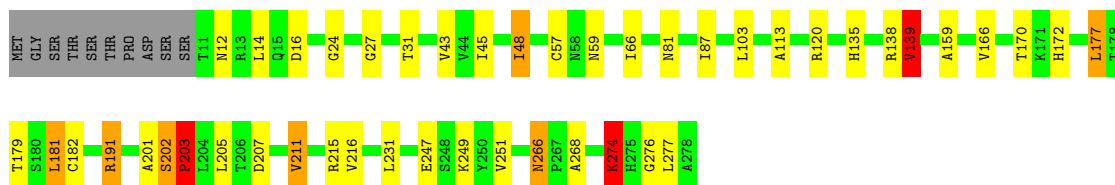
• Molecule 1: RHIZOME SECOISOLARICIRESINOL DEHYDROGENASE
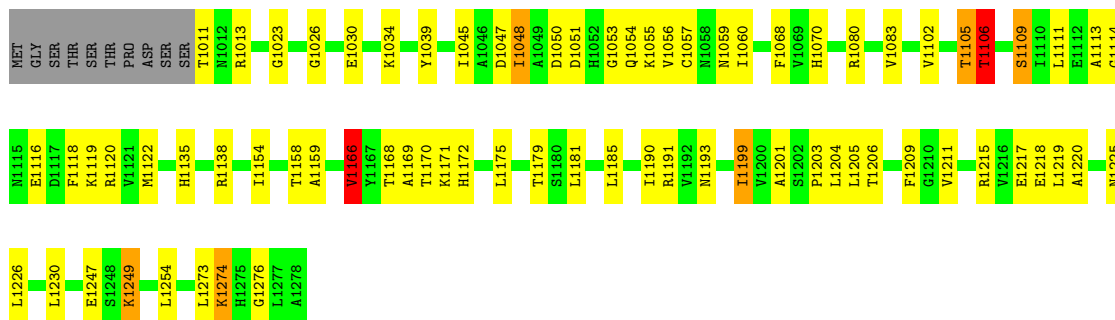
4 Data and refinement statistics (i)

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 (Å²)	25.0	wwPDB-VP

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	0/2018	1.19	6/2742 (0.2%)
1	B	0.66	0/2018	1.27	13/2742 (0.5%)
All	All	0.66	0/4036	1.23	19/5484 (0.3%)

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1166	VAL	CB-CA-C	-8.70	94.87	111.40
1	B	1166	VAL	CG1-CB-CG2	7.30	122.58	110.90
1	B	1109	SER	N-CA-CB	7.08	121.11	110.50
1	B	1106	THR	N-CA-CB	-6.84	97.30	110.30
1	A	113	ALA	CA-C-N	6.80	129.79	116.20
1	B	1225	ASN	N-CA-C	-6.01	94.78	111.00
1	A	191	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	1105	THR	N-CA-CB	-5.70	99.46	110.30
1	B	1120	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	1080	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	1191	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	1249	LYS	CA-CB-CG	5.47	125.42	113.40
1	A	139	VAL	N-CA-CB	-5.43	99.55	111.50
1	A	12	ASN	CA-C-N	-5.35	105.44	117.20
1	A	274	LYS	N-CA-C	5.32	125.37	111.00
1	B	1166	VAL	N-CA-CB	5.30	123.16	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	1080	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	1191	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	24	0
1	B	1986	0	1997	35	0
2	A	100	0	0	2	0
2	B	106	0	0	2	0
All	All	4178	0	3994	55	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 (55) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:266:ASN:HD22	1:A:266:ASN:C	2.12	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	1
1	B	266/278 (96%)	231 (87%)	20 (8%)	15 (6%)	2	0
All	All	532/556 (96%)	478 (90%)	33 (6%)	21 (4%)	3	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

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Mol	Chain	Res	Type
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 (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	213/222 (96%)	197 (92%)	16 (8%)	13	2
1	B	213/222 (96%)	197 (92%)	16 (8%)	13	2
All	All	426/444 (96%)	394 (92%)	32 (8%)	13	2

All (32) 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	81	ASN
1	A	103	LEU
1	A	139	VAL
1	A	177	LEU
1	A	181	LEU
1	A	182	CYS
1	A	203	PRO
1	A	207	ASP
1	A	231	LEU
1	A	247	GLU
1	A	251	VAL
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	277	LEU
1	B	1013	ARG
1	B	1048	ILE
1	B	1060	ILE
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	1215	ARG
1	B	1218	GLU
1	B	1219	LEU
1	B	1249	LYS
1	B	1274	LYS

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	15	GLN
1	A	115	ASN
1	A	135	HIS
1	A	172	HIS
1	A	225	ASN
1	A	266	ASN
1	B	1054	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 ⓘ

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.