



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1QYC
Title : Crystal structures of pinoresinol-lariciresinol and phenylcoumaran benzylic ether reductases, and their relationship to isoflavone reductases
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Deposited on : 2003-09-10
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

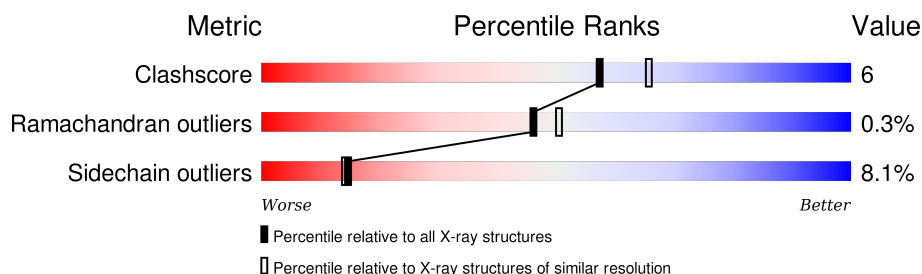
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	 78% 18% . .
1	B	308	 81% 17% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5011 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 phenylcoumaran benzylic ether reductase PT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2360	1507	397	455	1			
1	B	307	Total	C	N	O	S	0	0	0
			2360	1507	397	455	1			

- Molecule 2 is water.

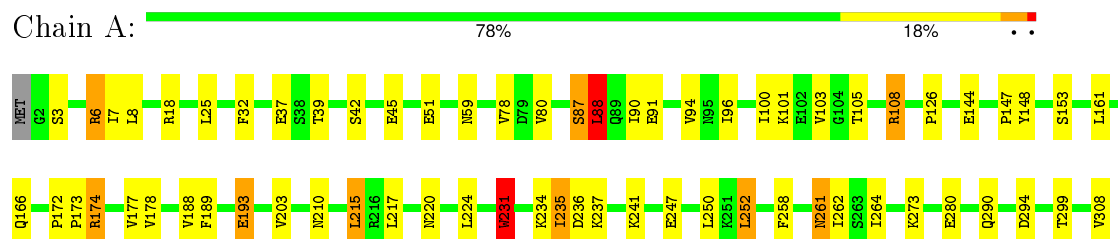
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total	O	0	0
			145	145		
2	B	146	Total	O	0	0
			146	146		

3 Residue-property plots

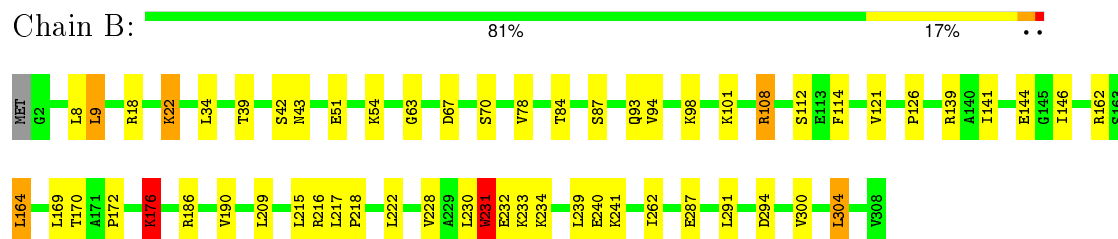
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: phenylcoumaran benzylic ether reductase PT1



- Molecule 1: phenylcoumaran benzylic ether reductase PT1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.19Å 67.94Å 75.02Å 90.00° 115.08° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5011	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	0.72	0/2403	1.34	10/3262 (0.3%)
1	B	0.74	0/2403	1.36	15/3262 (0.5%)
All	All	0.73	0/4806	1.35	25/6524 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	B	108	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	88	LEU	CA-CB-CG	7.87	133.40	115.30
1	B	108	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	186	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	231	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	231	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	A	231	TRP	CD1-CG-CD2	6.64	111.61	106.30
1	A	108	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	216	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	170	THR	N-CA-C	5.93	127.02	111.00
1	B	144	GLU	CA-CB-CG	-5.74	100.78	113.40
1	A	174	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	169	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	174	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	18	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	18	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	209	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	176	LYS	CA-CB-CG	5.22	124.89	113.40
1	A	51	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	231	TRP	NE1-CE2-CZ2	-5.13	124.75	130.40
1	B	18	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	216	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	6	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	9	LEU	CB-CG-CD1	-5.10	102.34	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2360	0	2393	33	0
1	B	2360	0	2393	24	0
2	A	145	0	0	3	0
2	B	146	0	0	2	0
All	All	5011	0	4786	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 6.

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:93:GLN:HE22	1:B:112:SER:H	1.18	0.88
1:A:147:PRO:HA	1:A:210:ASN:HD21	1.41	0.84
1:B:51:GLU:HA	1:B:54:LYS:HE3	1.64	0.78
1:A:80:VAL:HG11	1:A:203:VAL:HG13	1.69	0.74
1:A:88:LEU:H	1:A:88:LEU:HD13	1.59	0.68
1:A:166:GLN:HE22	1:A:178:VAL:H	1.45	0.64
1:A:148:TYR:H	1:A:210:ASN:ND2	1.97	0.62
1:A:235:ILE:HG23	1:A:237:LYS:HG2	1.80	0.62
1:B:141:ILE:HG23	1:B:146:ILE:HB	1.81	0.61
1:B:22:LYS:HA	1:B:22:LYS:NZ	2.14	0.61
1:A:87:SER:HA	1:A:90:ILE:HG12	1.84	0.58
1:B:190:VAL:HG11	1:B:215:LEU:HD23	1.86	0.56
1:A:91:GLU:H	1:A:91:GLU:CD	2.08	0.56
1:A:234:LYS:HD3	1:A:308:VAL:HG21	1.88	0.55
1:A:88:LEU:HB3	2:B:433:HOH:O	2.07	0.54
1:A:174:ARG:HE	1:A:235:ILE:HD11	1.73	0.54
1:B:39:THR:HG21	2:B:405:HOH:O	2.08	0.53
1:B:232:GLU:HG2	1:B:239:LEU:HD13	1.90	0.53
1:A:103:VAL:HG12	1:A:105:THR:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:NE2	1:A:178:VAL:H	2.10	0.50
1:B:176:LYS:HB3	1:B:240:GLU:HB2	1.94	0.50
1:B:228:VAL:O	1:B:232:GLU:HG3	2.12	0.49
1:A:153:SER:HA	1:A:215:LEU:HG	1.94	0.49
1:A:189:PHE:O	1:A:220:ASN:HB3	2.14	0.48
1:B:63:GLY:HA3	1:B:70:SER:HB2	1.96	0.47
1:A:173:PRO:O	1:A:231:TRP:HZ3	1.98	0.46
1:A:217:LEU:HB2	1:A:220:ASN:HB2	1.97	0.46
1:B:231:TRP:CD1	1:B:304:LEU:HG	2.50	0.46
1:A:6:ARG:HH11	1:A:78:VAL:HA	1.81	0.45
1:A:7:ILE:HG12	1:A:80:VAL:HG22	1.98	0.45
1:B:39:THR:HG21	1:B:43:ASN:H	1.81	0.45
1:A:8:LEU:HB2	1:A:78:VAL:HG11	1.98	0.45
1:B:287:GLU:O	1:B:291:LEU:HB2	2.17	0.45
1:A:126:PRO:HG2	1:A:262:ILE:HA	1.99	0.44
1:A:96:ILE:O	1:A:100:ILE:HG13	2.17	0.44
1:A:247:GLU:H	1:A:247:GLU:CD	2.20	0.44
1:B:230:LEU:O	1:B:234:LYS:HG2	2.18	0.44
1:B:233:LYS:HB2	1:B:233:LYS:HE3	1.80	0.43
1:B:300:VAL:O	1:B:304:LEU:HB2	2.17	0.43
1:B:228:VAL:HG11	1:B:241:LYS:HE3	2.00	0.43
1:B:217:LEU:HA	1:B:218:PRO:HD3	1.83	0.43
1:B:22:LYS:HA	1:B:22:LYS:HZ2	1.84	0.43
1:A:39:THR:HG23	1:A:42:SER:HB3	2.01	0.42
1:A:258:PHE:HA	1:A:261:ASN:ND2	2.34	0.42
1:A:193:GLU:HG3	2:A:316:HOH:O	2.18	0.42
1:A:252:LEU:HD22	1:A:264:ILE:HD13	2.00	0.42
1:B:8:LEU:HB2	1:B:78:VAL:HG11	2.01	0.42
1:A:32:PHE:HA	1:A:59:ASN:O	2.19	0.42
1:B:164:LEU:HD13	1:B:172:PRO:HB3	2.02	0.41
1:B:22:LYS:HZ1	1:B:22:LYS:HA	1.85	0.41
1:B:126:PRO:HG2	1:B:262:ILE:HA	2.02	0.41
1:A:6:ARG:HH11	1:A:6:ARG:HB2	1.86	0.41
1:A:273:LYS:HE3	2:A:332:HOH:O	2.21	0.41
1:A:101:LYS:HD2	2:A:309:HOH:O	2.20	0.41
1:A:220:ASN:OD1	1:A:299:THR:HA	2.21	0.40
1:A:172:PRO:HB2	1:A:231:TRP:CH2	2.56	0.40
1:B:84:THR:HG22	1:B:114:PHE:CE1	2.56	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	305/308 (99%)	285 (93%)	19 (6%)	1 (0%)	46	50
1	B	305/308 (99%)	289 (95%)	15 (5%)	1 (0%)	46	50
All	All	610/616 (99%)	574 (94%)	34 (6%)	2 (0%)	46	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	SER
1	A	3	SER

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	259/260 (100%)	235 (91%)	24 (9%)	11	10
1	B	259/260 (100%)	241 (93%)	18 (7%)	19	20
All	All	518/520 (100%)	476 (92%)	42 (8%)	15	14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	37	GLU
1	A	45	GLU
1	A	87	SER

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	94	VAL
1	A	108	ARG
1	A	144	GLU
1	A	161	LEU
1	A	177	VAL
1	A	188	VAL
1	A	193	GLU
1	A	215	LEU
1	A	224	LEU
1	A	231	TRP
1	A	235	ILE
1	A	236	ASP
1	A	241	LYS
1	A	250	LEU
1	A	252	LEU
1	A	261	ASN
1	A	280	GLU
1	A	290	GLN
1	A	294	ASP
1	B	9	LEU
1	B	22	LYS
1	B	34	LEU
1	B	67	ASP
1	B	87	SER
1	B	94	VAL
1	B	98	LYS
1	B	101	LYS
1	B	108	ARG
1	B	121	VAL
1	B	139	ARG
1	B	162	ARG
1	B	164	LEU
1	B	176	LYS
1	B	222	LEU
1	B	231	TRP
1	B	294	ASP
1	B	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	166	GLN
1	A	210	ASN
1	A	225	ASN
1	A	261	ASN
1	A	268	HIS
1	B	48	GLN
1	B	77	ASN
1	B	89	GLN
1	B	93	GLN
1	B	116	ASN
1	B	120	ASN
1	B	268	HIS

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.