



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:59 AM UTC

PDB ID : 1QYC / pdb_00001qyc
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

<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

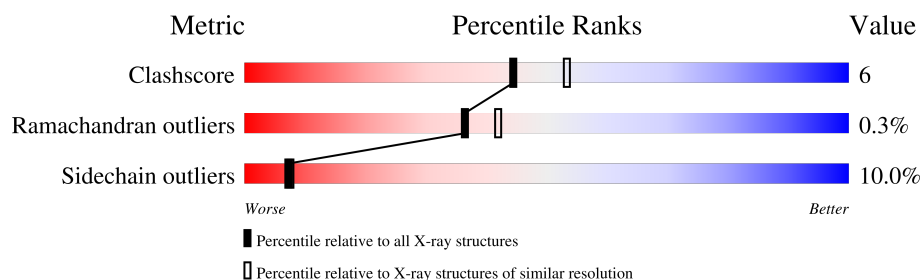
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	308	
1	B	308	

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.

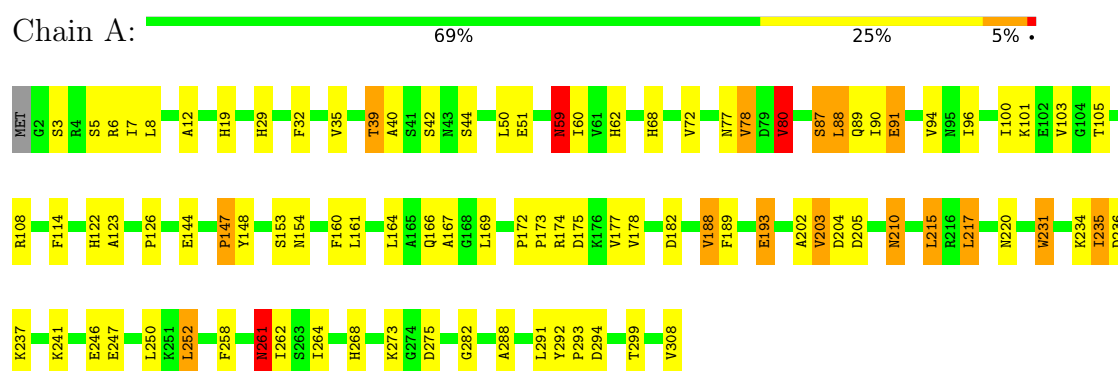
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total	O	0	0
			145	145		
2	B	146	Total	O	0	0
			146	146		

3 Residue-property plots [i](#)

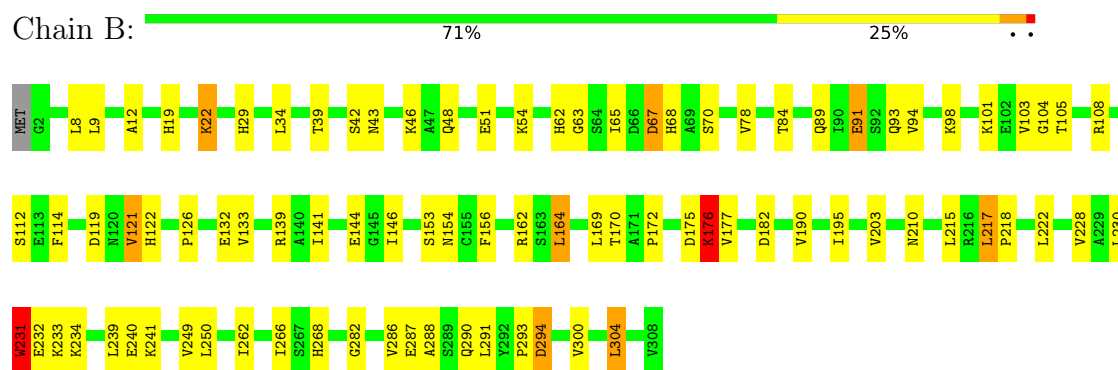
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 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 is therefore 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	0.92	11/2403 (0.5%)	1.78	51/3262 (1.6%)
1	B	0.96	7/2403 (0.3%)	1.76	44/3262 (1.3%)
All	All	0.94	18/4806 (0.4%)	1.77	95/6524 (1.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	80	VAL	CA-CB	6.73	1.63	1.54
1	B	268	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	29	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	62	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	29	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	68	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	19	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	122	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	19	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	68	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	188	VAL	CA-CB	5.82	1.62	1.54
1	A	122	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	39	THR	CA-CB	5.54	1.60	1.53
1	B	19	HIS	CG-ND1	-5.45	1.32	1.38
1	A	29	HIS	CG-ND1	-5.36	1.32	1.38
1	A	268	HIS	CG-ND1	-5.13	1.32	1.38

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LEU	N-CA-C	10.54	124.23	110.43
1	A	77	ASN	CA-CB-CG	9.85	122.45	112.60
1	A	182	ASP	CA-CB-CG	9.62	122.22	112.60
1	B	293	PRO	CA-C-N	9.56	133.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	PRO	C-N-CA	9.56	133.09	120.28
1	B	67	ASP	CA-CB-CG	9.27	121.87	112.60
1	A	44	SER	N-CA-C	8.93	120.70	110.97
1	B	294	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	105	THR	N-CA-C	8.15	121.19	111.33
1	B	288	ALA	N-CA-C	7.95	120.03	111.36
1	A	275	ASP	N-CA-C	7.93	122.39	112.87
1	B	182	ASP	CA-CB-CG	7.87	120.47	112.60
1	B	170	THR	N-CA-C	7.61	127.02	110.80
1	B	104	GLY	CA-C-N	7.61	130.80	120.38
1	B	104	GLY	C-N-CA	7.61	130.80	120.38
1	A	40	ALA	N-CA-C	7.46	121.49	112.38
1	A	203	VAL	N-CA-CB	-7.35	102.35	110.51
1	A	175	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	35	VAL	CA-C-O	7.25	128.33	120.43
1	A	203	VAL	N-CA-C	7.06	117.78	110.36
1	A	160	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	62	HIS	CA-CB-CG	6.76	120.56	113.80
1	B	144	GLU	CA-CB-CG	-6.66	100.78	114.10
1	B	175	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	60	ILE	N-CA-C	6.27	117.82	108.54
1	A	78	VAL	N-CA-C	6.27	119.30	108.95
1	B	121	VAL	N-CA-CB	-6.25	101.20	111.45
1	A	35	VAL	N-CA-C	6.10	117.07	108.17
1	B	91	GLU	CB-CG-CD	6.09	122.95	112.60
1	B	154	ASN	N-CA-C	6.04	118.28	108.08
1	B	286	VAL	N-CA-CB	-6.03	101.56	111.45
1	A	59	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	50	LEU	CA-C-N	5.87	128.42	120.38
1	A	50	LEU	C-N-CA	5.87	128.42	120.38
1	B	170	THR	CA-CB-OG1	-5.82	100.87	109.60
1	B	210	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	261	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	288	ALA	N-CA-C	5.77	119.58	112.54
1	A	217	LEU	CA-C-N	5.74	125.21	119.24
1	A	217	LEU	C-N-CA	5.74	125.21	119.24
1	B	12	ALA	N-CA-C	5.68	119.31	112.38
1	A	5	SER	N-CA-C	5.67	118.46	110.23
1	A	210	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	123	ALA	N-CA-C	5.67	118.50	110.50
1	A	292	TYR	CA-C-N	5.67	125.77	119.87
1	A	292	TYR	C-N-CA	5.67	125.77	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ALA	N-CA-C	5.65	119.27	112.38
1	A	147	PRO	CB-CA-C	5.62	118.26	111.46
1	B	195	ILE	N-CA-C	-5.62	105.05	110.72
1	A	202	ALA	CA-C-N	5.61	127.84	120.60
1	A	202	ALA	C-N-CA	5.61	127.84	120.60
1	B	169	LEU	CA-C-N	5.54	132.13	121.54
1	B	169	LEU	C-N-CA	5.54	132.13	121.54
1	A	205	ASP	CA-CB-CG	5.50	118.11	112.60
1	A	293	PRO	CA-C-N	5.48	128.64	120.31
1	A	293	PRO	C-N-CA	5.48	128.64	120.31
1	B	217	LEU	CA-C-N	5.47	124.66	118.97
1	B	217	LEU	C-N-CA	5.47	124.66	118.97
1	B	249	VAL	N-CA-C	-5.42	105.24	110.72
1	B	68	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	282	GLY	CA-C-N	5.40	125.04	119.05
1	A	282	GLY	C-N-CA	5.40	125.04	119.05
1	B	176	LYS	CA-CB-CG	5.39	124.89	114.10
1	A	51	GLU	CA-CB-CG	5.39	124.89	114.10
1	A	122	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	154	ASN	N-CA-C	5.32	117.08	108.08
1	B	231	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	B	132	GLU	N-CA-C	5.28	118.98	112.54
1	B	62	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	B	268	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	B	153	SER	N-CA-C	5.23	119.29	113.02
1	A	268	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	156	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	72	VAL	CA-C-N	5.21	127.22	120.44
1	A	72	VAL	C-N-CA	5.21	127.22	120.44
1	B	119	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	290	GLN	OE1-CD-NE2	-5.20	117.41	122.60
1	B	203	VAL	N-CA-C	5.19	119.30	112.04
1	B	282	GLY	CA-C-N	5.18	124.84	119.56
1	B	282	GLY	C-N-CA	5.18	124.84	119.56
1	B	29	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	204	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	266	ILE	O-C-N	-5.07	116.62	121.90
1	A	62	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	246	GLU	CA-C-N	5.06	127.06	120.28
1	A	246	GLU	C-N-CA	5.06	127.06	120.28
1	A	167	ALA	N-CA-C	5.06	121.58	110.80
1	A	68	HIS	CB-CG-CD2	-5.05	124.64	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	GLN	CB-CG-CD	5.05	121.18	112.60
1	B	122	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	A	114	PHE	N-CA-C	5.03	118.68	112.24
1	A	89	GLN	N-CA-C	5.03	118.44	111.71
1	A	19	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	48	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	B	286	VAL	CB-CA-C	5.02	119.39	110.71

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:NZ	1:B:22:LYS:HA	2.14	0.61
1:A:91:GLU:H	1:A:91:GLU:CD	2.08	0.60
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: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:B:22:LYS:HA	1:B:22:LYS:HZ1	1.75	0.51
1:A:103:VAL:HG12	1:A:105:THR:H	1.74	0.50
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:247:GLU:H	1:A:247:GLU:CD	2.20	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:B:91:GLU:H	1:B:91:GLU:CD	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	305/308 (99%)	285 (93%)	19 (6%)	1 (0%)	36	42
1	B	305/308 (99%)	289 (95%)	15 (5%)	1 (0%)	36	42
All	All	610/616 (99%)	574 (94%)	34 (6%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

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

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	209/260 (80%)	186 (89%)	23 (11%)	6	6
1	B	259/260 (100%)	235 (91%)	24 (9%)	8	9
All	All	468/520 (90%)	421 (90%)	47 (10%)	7	7

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	80	VAL
1	A	87	SER
1	A	88	LEU
1	A	91	GLU
1	A	94	VAL
1	A	108	ARG
1	A	144	GLU
1	A	161	LEU
1	A	164	LEU
1	A	177	VAL
1	A	188	VAL
1	A	193	GLU
1	A	215	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	291	LEU
1	A	294	ASP
1	B	9	LEU
1	B	22	LYS
1	B	34	LEU
1	B	46	LYS
1	B	65	ILE
1	B	67	ASP
1	B	89	GLN
1	B	94	VAL
1	B	98	LYS
1	B	101	LYS
1	B	103	VAL
1	B	108	ARG

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Mol	Chain	Res	Type
1	B	121	VAL
1	B	133	VAL
1	B	139	ARG
1	B	162	ARG
1	B	164	LEU
1	B	176	LYS
1	B	177	VAL
1	B	222	LEU
1	B	231	TRP
1	B	250	LEU
1	B	294	ASP
1	B	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	210	ASN
1	A	225	ASN
1	A	261	ASN
1	A	268	HIS
1	B	93	GLN
1	B	116	ASN
1	B	268	HIS

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

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.