



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 02:43 PM EDT

PDB ID : 7RBP  
Title : Medicago truncatula D-1-piperidine-2-carboxylic acid reductase  
Authors : Torrens-spence, M.P.; Weng, J.K.  
Deposited on : 2021-07-06  
Resolution : 2.10 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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

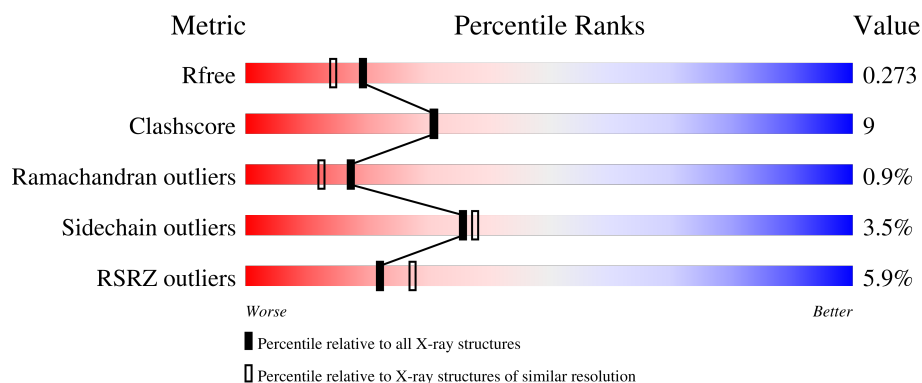
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	B	336	<div> <div>8%</div> <div>59%</div> <div>18%</div> <div>•</div> <div>21%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4601 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 Ornithine cyclodeaminase/mu-crystallin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2509	1587	423	490	9			
1	B	265	Total	C	N	O	S	0	0	0
			2020	1276	343	393	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LYS	ARG	conflict	UNP B7FJU0
A	181	ILE	LYS	conflict	UNP B7FJU0
A	182	ASN	THR	conflict	UNP B7FJU0
B	169	LYS	ARG	conflict	UNP B7FJU0
B	181	ILE	LYS	conflict	UNP B7FJU0
B	182	ASN	THR	conflict	UNP B7FJU0

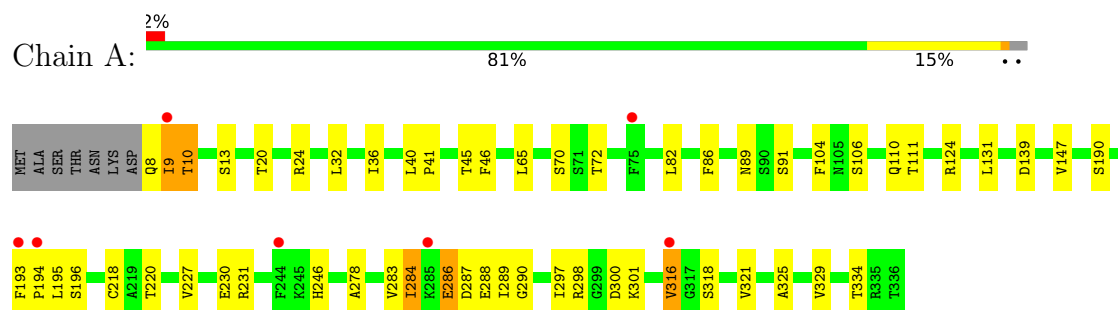
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	14	Total	O	0	0
			14	14		

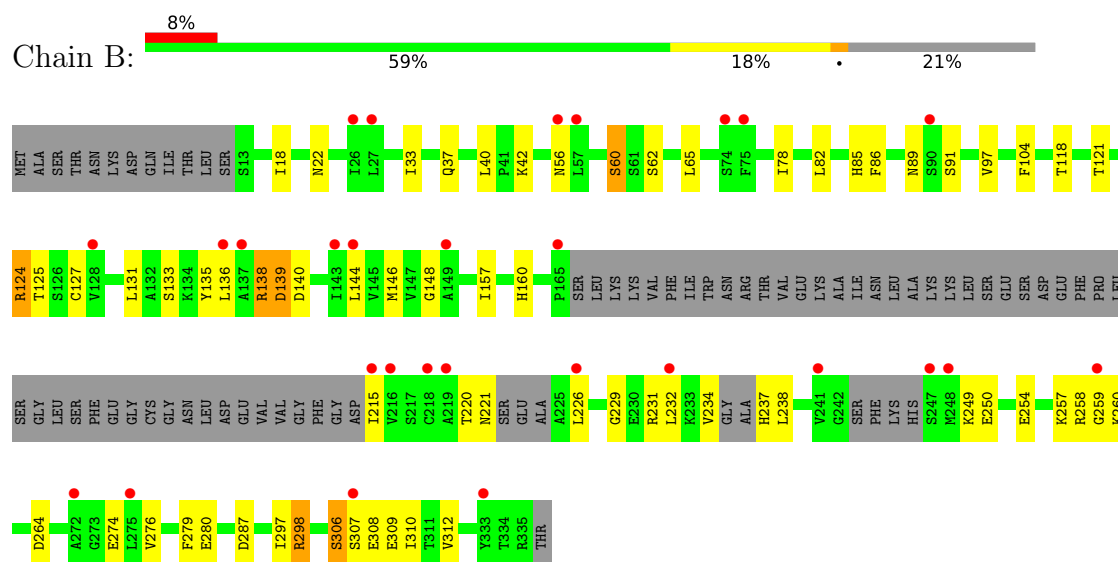
### 3 Residue-property plots [i](#)

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 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.

- Molecule 1: Ornithine cyclodeaminase/mu-crystallin



- Molecule 1: Ornithine cyclodeaminase/mu-crystallin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.14Å 83.67Å 113.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.41 – 2.10 67.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (67.41-2.10) 98.8 (67.41-2.10)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.252 , 0.272 0.252 , 0.273	Depositor DCC
$R_{free}$ test set	1987 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.42	0/2554	0.57	1/3459 (0.0%)
1	B	0.29	0/2052	0.52	0/2777
All	All	0.37	0/4606	0.55	1/6236 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	VAL	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2509	0	2520	35	0
1	B	2020	0	2032	50	0
2	A	58	0	0	0	0
2	B	14	0	0	0	0
All	All	4601	0	4552	83	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 9.

All (83) 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:215:ILE:HG22	1:B:237:HIS:HB3	1.40	0.97
1:A:9:ILE:HD12	1:A:10:THR:HG23	1.63	0.79
1:A:290:GLY:O	1:A:301:LYS:HE3	1.83	0.78
1:B:258:ARG:HB3	1:B:310:ILE:HG12	1.65	0.78
1:B:254:GLU:HB2	1:B:257:LYS:HB2	1.66	0.75
1:B:298:ARG:C	1:B:298:ARG:HD3	2.06	0.74
1:B:258:ARG:HB2	1:B:310:ILE:HG21	1.72	0.71
1:A:284:ILE:HG22	1:A:288:GLU:OE2	1.91	0.71
1:A:40:LEU:N	1:A:41:PRO:HD2	2.08	0.69
1:B:306:SER:OG	1:B:307:SER:N	2.22	0.68
1:A:46:PHE:HE1	1:B:287:ASP:HB3	1.59	0.68
1:B:238:LEU:HB3	1:B:312:VAL:HG12	1.76	0.66
1:B:144:LEU:HD23	1:B:215:ILE:HG13	1.78	0.66
1:B:259:GLY:HA3	1:B:310:ILE:HB	1.78	0.65
1:A:46:PHE:CE2	1:A:72:THR:HG21	2.31	0.64
1:A:286:GLU:HA	1:A:289:ILE:HD13	1.79	0.64
1:B:56:ASN:OD1	1:B:62:SER:HB3	1.99	0.62
1:A:193:PHE:CD2	1:A:194:PRO:HD3	2.35	0.61
1:B:276:VAL:O	1:B:280:GLU:HG2	2.00	0.61
1:A:13:SER:HA	1:A:110:GLN:HE22	1.65	0.61
1:A:13:SER:HA	1:A:110:GLN:NE2	2.17	0.60
1:B:131:LEU:HD21	1:B:297:ILE:HD11	1.83	0.59
1:B:56:ASN:HA	1:B:62:SER:HA	1.84	0.58
1:A:65:LEU:HD22	1:A:82:LEU:HD22	1.85	0.58
1:A:104:PHE:CE2	1:A:111:THR:HG22	2.38	0.58
1:A:46:PHE:CD2	1:A:72:THR:HG21	2.39	0.57
1:B:306:SER:HB3	1:B:309:GLU:HG3	1.85	0.57
1:A:46:PHE:CE1	1:B:287:ASP:HB3	2.39	0.57
1:B:238:LEU:O	1:B:312:VAL:HA	2.05	0.57
1:A:13:SER:C	1:A:110:GLN:NE2	2.59	0.56
1:B:276:VAL:HA	1:B:279:PHE:CD2	2.41	0.55
1:B:62:SER:OG	1:B:85:HIS:HB2	2.05	0.55
1:B:121:THR:O	1:B:125:THR:HG23	2.06	0.55
1:B:65:LEU:HD22	1:B:82:LEU:HD22	1.87	0.55
1:B:226:LEU:HD13	1:B:249:LYS:HB2	1.88	0.54
1:A:40:LEU:N	1:A:41:PRO:CD	2.70	0.54
1:B:306:SER:HG	1:B:307:SER:H	1.53	0.54
1:B:309:GLU:HG2	1:B:310:ILE:H	1.72	0.54
1:B:33:ILE:HG13	1:B:127:CYS:HB3	1.89	0.53
1:B:135:TYR:CZ	1:B:297:ILE:HA	2.43	0.53
1:A:32:LEU:O	1:A:36:ILE:HG12	2.09	0.53
1:B:298:ARG:HD3	1:B:298:ARG:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HG23	1:B:22:ASN:HB3	1.91	0.53
1:B:86:PHE:O	1:B:89:ASN:HB2	2.08	0.52
1:B:229:GLY:HA2	1:B:232:LEU:HD12	1.91	0.52
1:A:20:THR:O	1:A:24:ARG:HG3	2.10	0.52
1:B:148:GLY:HA3	1:B:220:THR:HB	1.91	0.52
1:A:325:ALA:O	1:A:329:VAL:HG23	2.11	0.51
1:A:318:SER:OG	1:A:321:VAL:HG23	2.10	0.50
1:A:45:THR:HG22	1:A:46:PHE:CD1	2.46	0.50
1:B:124:ARG:HH11	1:B:125:THR:HG22	1.76	0.49
1:A:9:ILE:HG13	1:A:334:THR:O	2.13	0.49
1:B:146:MET:CE	1:B:157:ILE:HG13	2.43	0.49
1:A:8:GLN:HG2	1:A:9:ILE:HG23	1.95	0.48
1:B:60:SER:O	1:B:60:SER:OG	2.29	0.48
1:B:144:LEU:CD2	1:B:215:ILE:HG13	2.44	0.48
1:B:78:ILE:HB	1:B:104:PHE:HB2	1.97	0.47
1:B:234:VAL:HB	1:B:308:GLU:HB3	1.97	0.47
1:B:250:GLU:HB2	1:B:274:GLU:OE2	2.15	0.47
1:A:124:ARG:HG3	1:A:321:VAL:HG12	1.96	0.47
1:B:146:MET:HE3	1:B:157:ILE:HG13	1.98	0.46
1:B:42:LYS:H	1:B:42:LYS:HZ3	1.64	0.46
1:A:13:SER:CA	1:A:110:GLN:HE22	2.30	0.45
1:A:40:LEU:HD23	1:A:297:ILE:HD12	1.99	0.45
1:B:133:SER:HG	1:B:160:HIS:CE1	2.34	0.45
1:B:306:SER:HB3	1:B:309:GLU:HB2	1.97	0.45
1:B:91:SER:O	1:B:91:SER:OG	2.28	0.45
1:A:131:LEU:HD21	1:A:297:ILE:HD11	1.99	0.44
1:B:37:GLN:HB2	1:B:131:LEU:HD13	1.98	0.44
1:B:221:ASN:ND2	1:B:250:GLU:HG3	2.31	0.44
1:A:298:ARG:HG3	1:A:300:ASP:OD2	2.18	0.44
1:A:230:GLU:OE2	1:A:231:ARG:HG2	2.17	0.44
1:A:278:ALA:HB1	1:A:284:ILE:HG13	1.98	0.44
1:B:97:VAL:O	1:B:118:THR:HG21	2.18	0.44
1:B:40:LEU:HD23	1:B:297:ILE:HD12	2.00	0.44
1:A:86:PHE:O	1:A:89:ASN:HB2	2.18	0.43
1:A:13:SER:CA	1:A:110:GLN:NE2	2.79	0.43
1:A:218:CYS:SG	1:A:227:VAL:HG21	2.58	0.43
1:A:147:VAL:HG12	1:A:220:THR:HG21	2.01	0.42
1:A:194:PRO:O	1:A:195:LEU:HD23	2.21	0.41
1:B:264:ASP:N	1:B:264:ASP:OD1	2.53	0.41
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.80	0.40
1:B:138:ARG:O	1:B:140:ASP:N	2.55	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	327/336 (97%)	313 (96%)	10 (3%)	4 (1%)	13	8
1	B	255/336 (76%)	240 (94%)	14 (6%)	1 (0%)	34	32
All	All	582/672 (87%)	553 (95%)	24 (4%)	5 (1%)	17	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	316	VAL
1	B	139	ASP
1	A	286	GLU
1	A	9	ILE

### 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	282/288 (98%)	272 (96%)	10 (4%)	36	38
1	B	228/288 (79%)	220 (96%)	8 (4%)	36	38
All	All	510/576 (88%)	492 (96%)	18 (4%)	36	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	91	SER
1	A	106	SER
1	A	139	ASP
1	A	190	SER
1	A	196	SER
1	A	246	HIS
1	A	283	VAL
1	A	284	ILE
1	A	287	ASP
1	B	60	SER
1	B	124	ARG
1	B	138	ARG
1	B	139	ASP
1	B	231	ARG
1	B	260	LYS
1	B	298	ARG
1	B	306	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	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 monosaccharides 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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	329/336 (97%)	0.42	7 (2%) 63 68	49, 70, 118, 167	0
1	B	265/336 (78%)	0.77	28 (10%) 6 7	56, 96, 144, 174	0
All	All	594/672 (88%)	0.58	35 (5%) 22 27	49, 81, 139, 174	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	PHE	8.2
1	B	26	ILE	5.7
1	B	75	PHE	5.3
1	B	232	LEU	5.1
1	A	194	PRO	5.0
1	B	144	LEU	4.6
1	B	149	ALA	4.4
1	B	218	CYS	3.8
1	B	216	VAL	3.7
1	B	74	SER	3.3
1	B	56	ASN	3.3
1	A	244	PHE	3.3
1	B	219	ALA	3.2
1	B	90	SER	3.1
1	B	272	ALA	2.9
1	A	75	PHE	2.8
1	B	143	ILE	2.7
1	B	27	LEU	2.7
1	B	215	ILE	2.6
1	B	275	LEU	2.6
1	B	137	ALA	2.5
1	B	259	GLY	2.5
1	A	316	VAL	2.5
1	A	9	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	165	PRO	2.3
1	A	285	LYS	2.3
1	B	333	TYR	2.2
1	B	307	SER	2.2
1	B	241	VAL	2.2
1	B	57	LEU	2.1
1	B	248	MET	2.1
1	B	226	LEU	2.0
1	B	128	VAL	2.0
1	B	247	SER	2.0
1	B	136	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.