



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 04:06 AM GMT

PDB ID : 2GER  
Title : Crystal Structure and Oxidative Mechanism of Human Pyrroline-5-carboxylate Reductase  
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.  
Deposited on : 2006-03-20  
Resolution : 3.10 Å (reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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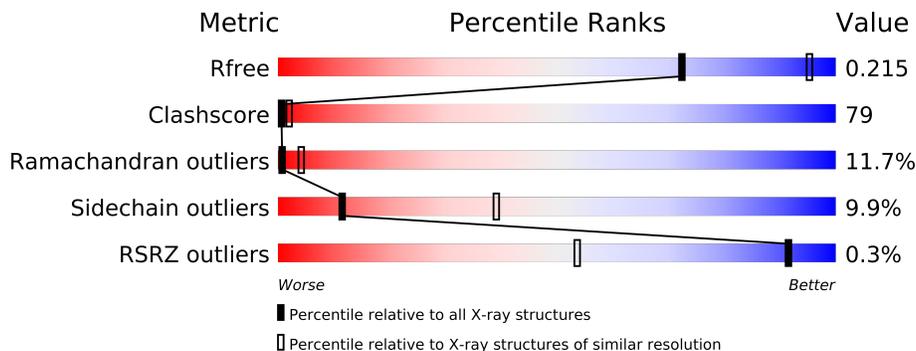
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10768 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pyrroline-5-carboxylatereductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2038	1279	363	383	13	0	0	0
1	B	276	2025	1271	359	382	13	0	0	0
1	C	277	2032	1276	360	383	13	0	0	0
1	D	277	2038	1279	363	383	13	0	0	0
1	E	277	2038	1279	363	383	13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P32322
A	0	ALA	-	CLONING ARTIFACT	UNP P32322
B	-1	ARG	-	CLONING ARTIFACT	UNP P32322
B	0	ALA	-	CLONING ARTIFACT	UNP P32322
C	-1	ARG	-	CLONING ARTIFACT	UNP P32322
C	0	ALA	-	CLONING ARTIFACT	UNP P32322
D	-1	ARG	-	CLONING ARTIFACT	UNP P32322
D	0	ALA	-	CLONING ARTIFACT	UNP P32322
E	-1	ARG	-	CLONING ARTIFACT	UNP P32322
E	0	ALA	-	CLONING ARTIFACT	UNP P32322

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	118	Total	O	0	0
			118	118		

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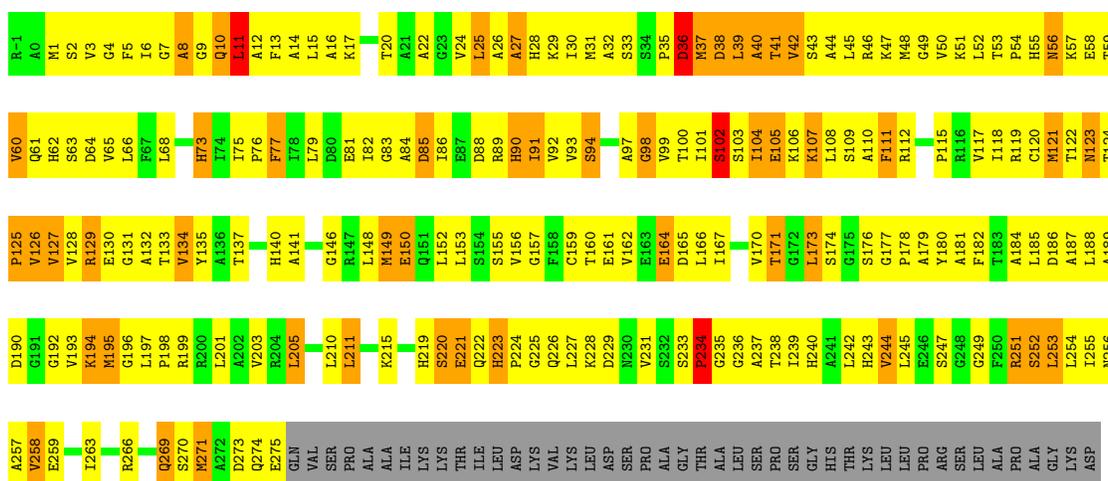
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

### 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.

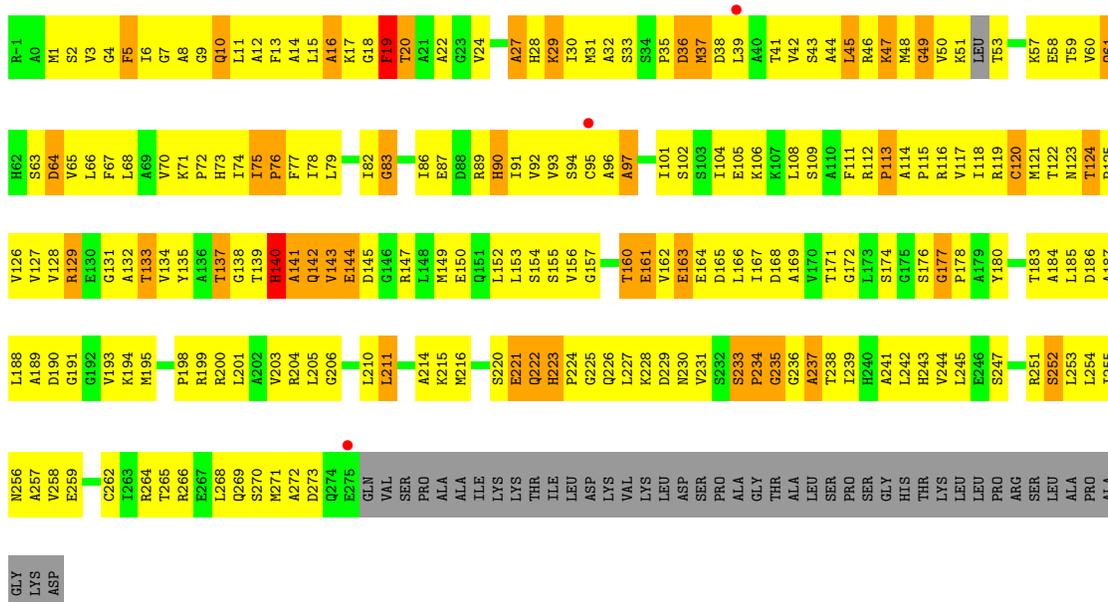
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain A:



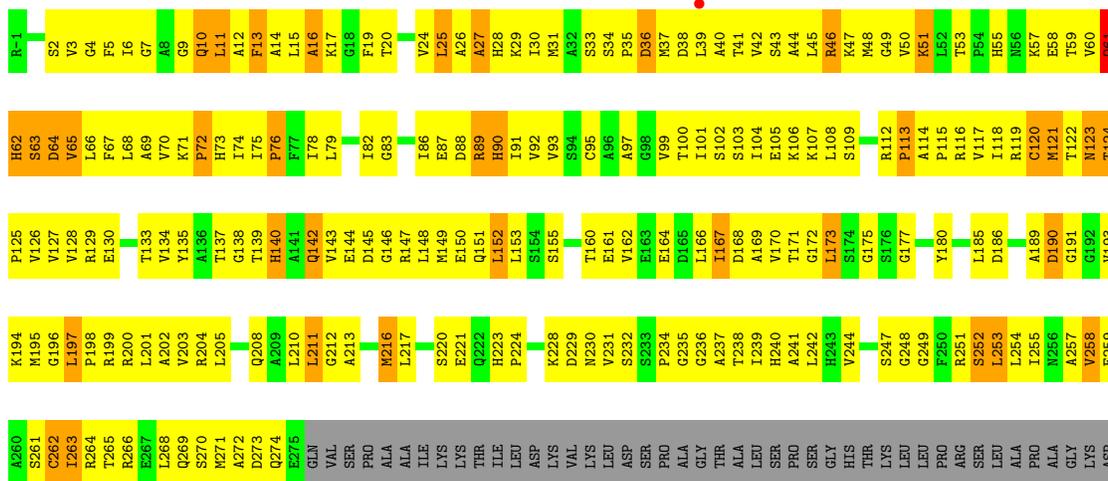
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain B:



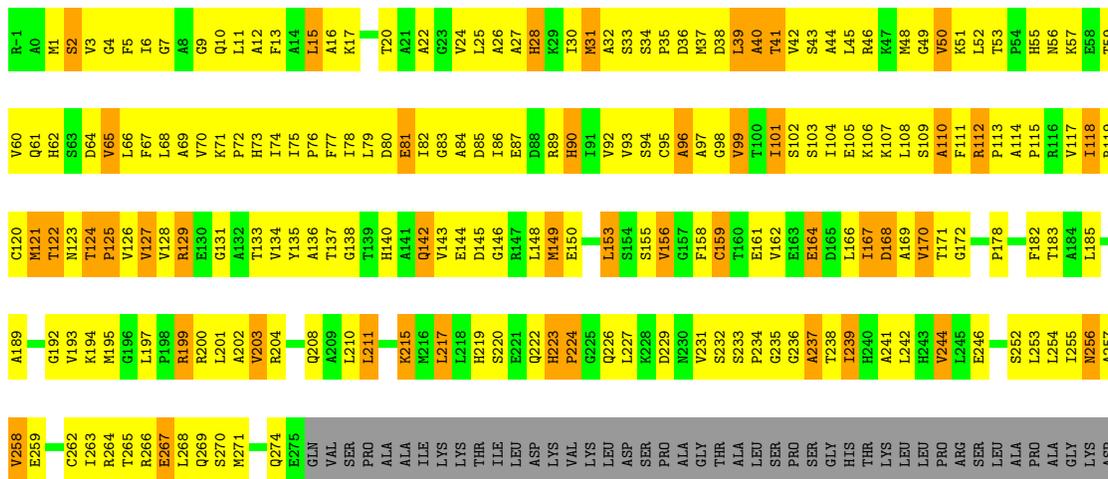
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain C:



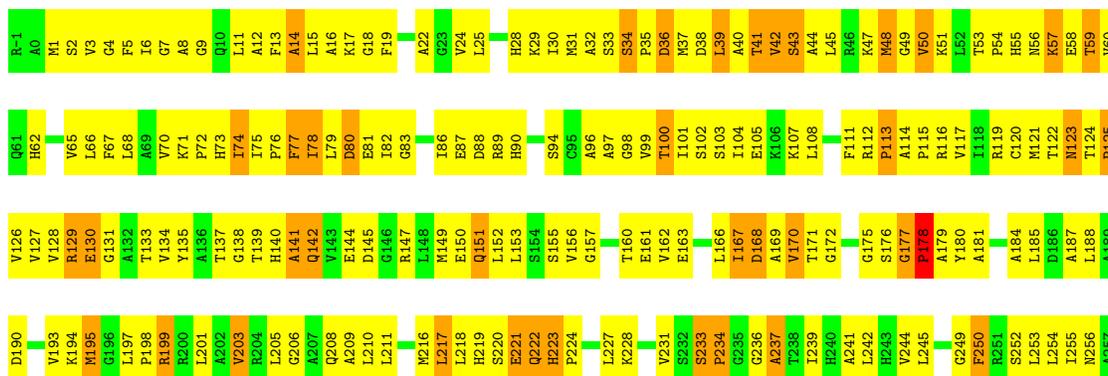
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain D:



- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain E:



Y258	S261	I263	R264	T265	R266	E267	L268	Q269	S270	Q274	E275	GLN	VAL	SER	PRO	ALA	ALA	ILE	LYS	LYS	THR	THR	ILE	LEU	ASP	LYS	VAL	VAL	LYS	LYS	LEU	ASP	SER	PRO	PRO	ALA	GLY	GLY	THR	THR	ALA	LEU	SER	PRO	PRO	SER	GLY	HIS	THR	THR	LYS	LYS	LEU	LEU	PRO	PRO	ARG	SER	SER	LEU	LEU	ALA	ALA	PRO	PRO	ALA	ALA	GLY	LYS	LYS	ASP
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## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.61Å 123.81Å 120.79Å 90.00° 121.76° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 28.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 98.7 (28.79-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 3.11Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.233 , 0.261 0.222 , 0.215	Depositor DCC
$R_{free}$ test set	2326 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 88.4	EDS
Estimated twinning fraction	0.028 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.036 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 47010 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.68	0/2069	0.90	0/2800
1	B	0.58	0/2055	0.85	2/2781 (0.1%)
1	C	0.62	0/2063	0.86	2/2793 (0.1%)
1	D	0.68	0/2069	0.88	0/2800
1	E	0.65	0/2069	0.89	1/2800 (0.0%)
All	All	0.64	0/10325	0.88	5/13974 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLY	N-CA-C	-6.07	97.94	113.10
1	C	120	CYS	CA-CB-SG	5.82	124.48	114.00
1	B	45	LEU	CA-CB-CG	5.27	127.43	115.30
1	E	39	LEU	N-CA-C	-5.04	97.39	111.00
1	B	49	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2082	320	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2025	0	2063	352	0
1	C	2032	0	2071	359	0
1	D	2038	0	2082	291	0
1	E	2038	0	2082	311	0
2	A	106	0	0	48	0
2	B	118	0	0	54	0
2	C	119	0	0	55	0
2	D	126	0	0	49	0
2	E	128	0	0	60	0
All	All	10768	0	10380	1614	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 79.

The worst 5 of 1614 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:239:ILE:H	1:D:239:ILE:HD12	1.08	1.16
1:C:75:ILE:HD12	1:C:99:VAL:HG21	1.27	1.16
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.22	1.14
1:E:101:ILE:HD11	1:E:138:GLY:HA2	1.28	1.14
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.34	1.09

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	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	1 4
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0 2
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	1 4
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	1 9
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	1 4

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	GLN
1	A	11	LEU
1	A	36	ASP
1	A	37	MET

### 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	215/250 (86%)	185 (86%)	30 (14%)	5 21
1	B	213/250 (85%)	197 (92%)	16 (8%)	19 58
1	C	214/250 (86%)	196 (92%)	18 (8%)	16 52
1	D	215/250 (86%)	185 (86%)	30 (14%)	5 21
1	E	215/250 (86%)	203 (94%)	12 (6%)	30 70
All	All	1072/1250 (86%)	966 (90%)	106 (10%)	11 39

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	LYS
1	C	211	LEU
1	E	120	CYS
1	C	89	ARG
1	C	123	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	HIS
1	C	90	HIS
1	D	140	HIS
1	B	240	HIS
1	D	240	HIS

### 5.3.3 RNA [i](#)

There are no RNA chains 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

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	277/321 (86%)	-0.30	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	27, 79, 115, 154	0
1	B	276/321 (85%)	-0.08	3 (1%) <span style="border: 1px solid blue; padding: 2px;">77</span> <span style="border: 1px solid red; padding: 2px;">22</span>	26, 120, 172, 187	0
1	C	277/321 (86%)	-0.06	1 (0%) <span style="border: 1px solid blue; padding: 2px;">90</span> <span style="border: 1px solid gray; padding: 2px;">45</span>	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.34	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.32	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.22	4 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid gray; padding: 2px;">53</span>	23, 82, 160, 187	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	2.2
1	B	275	GLU	2.1
1	C	39	LEU	2.1
1	B	95	CYS	2.1

### 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 carbohydrates in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.