Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 06:52 pm GMT

PDB ID	:	6R6T
Title	:	Crystal structure of mouse cis-aconitate decarboxylase
Authors	:	Lukat, P.; Chen, F.; Saile, K.; Buessow, K.; Pessler, F.; Blankenfeldt, W.
Deposited on	:	2019-03-28
Resolution	:	2.54 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:

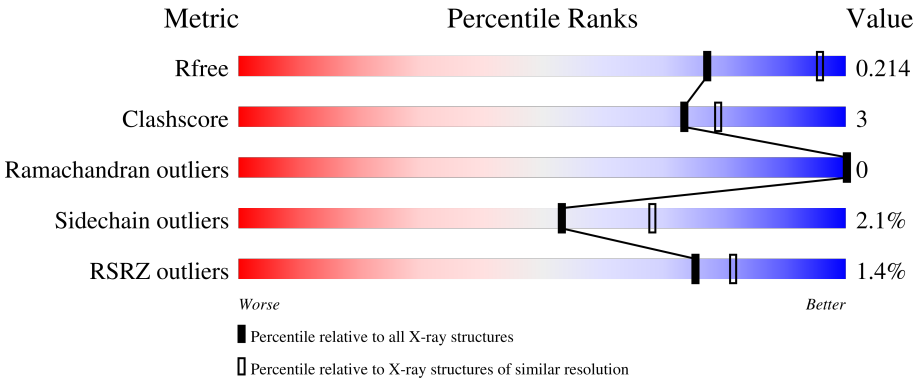
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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% 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	530	2% 78% 6% 15%
1	B	530	% 77% 8% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13849 atoms, of which 6851 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 Cis-aconitate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	450	Total	C	H	N	O	S	0	1	0
			6906	2217	3427	608	642	12			
1	B	451	Total	C	H	N	O	S	0	0	0
			6896	2216	3424	605	638	13			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	GLY	-	expression tag	UNP A0A0R4J027
A	490	THR	-	expression tag	UNP A0A0R4J027
A	491	LEU	-	expression tag	UNP A0A0R4J027
A	492	VAL	-	expression tag	UNP A0A0R4J027
A	493	PRO	-	expression tag	UNP A0A0R4J027
A	494	ARG	-	expression tag	UNP A0A0R4J027
A	495	GLY	-	expression tag	UNP A0A0R4J027
A	496	SER	-	expression tag	UNP A0A0R4J027
A	497	ALA	-	expression tag	UNP A0A0R4J027
A	498	ALA	-	expression tag	UNP A0A0R4J027
A	499	GLY	-	expression tag	UNP A0A0R4J027
A	500	LYS	-	expression tag	UNP A0A0R4J027
A	501	GLY	-	expression tag	UNP A0A0R4J027
A	502	SER	-	expression tag	UNP A0A0R4J027
A	503	ALA	-	expression tag	UNP A0A0R4J027
A	504	TRP	-	expression tag	UNP A0A0R4J027
A	505	SER	-	expression tag	UNP A0A0R4J027
A	506	HIS	-	expression tag	UNP A0A0R4J027
A	507	PRO	-	expression tag	UNP A0A0R4J027
A	508	GLN	-	expression tag	UNP A0A0R4J027
A	509	PHE	-	expression tag	UNP A0A0R4J027
A	510	GLU	-	expression tag	UNP A0A0R4J027
A	511	LYS	-	expression tag	UNP A0A0R4J027
A	512	GLY	-	expression tag	UNP A0A0R4J027
A	513	GLY	-	expression tag	UNP A0A0R4J027

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Chain	Residue	Modelled	Actual	Comment	Reference
A	514	GLY	-	expression tag	UNP A0A0R4J027
A	515	SER	-	expression tag	UNP A0A0R4J027
A	516	GLY	-	expression tag	UNP A0A0R4J027
A	517	GLY	-	expression tag	UNP A0A0R4J027
A	518	GLY	-	expression tag	UNP A0A0R4J027
A	519	SER	-	expression tag	UNP A0A0R4J027
A	520	GLY	-	expression tag	UNP A0A0R4J027
A	521	GLY	-	expression tag	UNP A0A0R4J027
A	522	SER	-	expression tag	UNP A0A0R4J027
A	523	ALA	-	expression tag	UNP A0A0R4J027
A	524	TRP	-	expression tag	UNP A0A0R4J027
A	525	SER	-	expression tag	UNP A0A0R4J027
A	526	HIS	-	expression tag	UNP A0A0R4J027
A	527	PRO	-	expression tag	UNP A0A0R4J027
A	528	GLN	-	expression tag	UNP A0A0R4J027
A	529	PHE	-	expression tag	UNP A0A0R4J027
A	530	GLU	-	expression tag	UNP A0A0R4J027
A	531	LYS	-	expression tag	UNP A0A0R4J027
B	489	GLY	-	expression tag	UNP A0A0R4J027
B	490	THR	-	expression tag	UNP A0A0R4J027
B	491	LEU	-	expression tag	UNP A0A0R4J027
B	492	VAL	-	expression tag	UNP A0A0R4J027
B	493	PRO	-	expression tag	UNP A0A0R4J027
B	494	ARG	-	expression tag	UNP A0A0R4J027
B	495	GLY	-	expression tag	UNP A0A0R4J027
B	496	SER	-	expression tag	UNP A0A0R4J027
B	497	ALA	-	expression tag	UNP A0A0R4J027
B	498	ALA	-	expression tag	UNP A0A0R4J027
B	499	GLY	-	expression tag	UNP A0A0R4J027
B	500	LYS	-	expression tag	UNP A0A0R4J027
B	501	GLY	-	expression tag	UNP A0A0R4J027
B	502	SER	-	expression tag	UNP A0A0R4J027
B	503	ALA	-	expression tag	UNP A0A0R4J027
B	504	TRP	-	expression tag	UNP A0A0R4J027
B	505	SER	-	expression tag	UNP A0A0R4J027
B	506	HIS	-	expression tag	UNP A0A0R4J027
B	507	PRO	-	expression tag	UNP A0A0R4J027
B	508	GLN	-	expression tag	UNP A0A0R4J027
B	509	PHE	-	expression tag	UNP A0A0R4J027
B	510	GLU	-	expression tag	UNP A0A0R4J027
B	511	LYS	-	expression tag	UNP A0A0R4J027
B	512	GLY	-	expression tag	UNP A0A0R4J027

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Chain	Residue	Modelled	Actual	Comment	Reference
B	513	GLY	-	expression tag	UNP A0A0R4J027
B	514	GLY	-	expression tag	UNP A0A0R4J027
B	515	SER	-	expression tag	UNP A0A0R4J027
B	516	GLY	-	expression tag	UNP A0A0R4J027
B	517	GLY	-	expression tag	UNP A0A0R4J027
B	518	GLY	-	expression tag	UNP A0A0R4J027
B	519	SER	-	expression tag	UNP A0A0R4J027
B	520	GLY	-	expression tag	UNP A0A0R4J027
B	521	GLY	-	expression tag	UNP A0A0R4J027
B	522	SER	-	expression tag	UNP A0A0R4J027
B	523	ALA	-	expression tag	UNP A0A0R4J027
B	524	TRP	-	expression tag	UNP A0A0R4J027
B	525	SER	-	expression tag	UNP A0A0R4J027
B	526	HIS	-	expression tag	UNP A0A0R4J027
B	527	PRO	-	expression tag	UNP A0A0R4J027
B	528	GLN	-	expression tag	UNP A0A0R4J027
B	529	PHE	-	expression tag	UNP A0A0R4J027
B	530	GLU	-	expression tag	UNP A0A0R4J027
B	531	LYS	-	expression tag	UNP A0A0R4J027

- Molecule 2 is water.

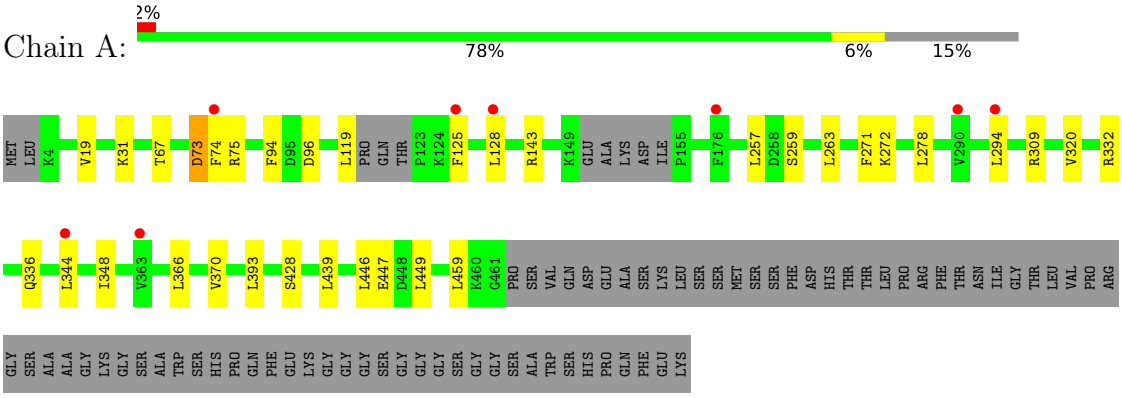
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0
2	B	26	Total O 26 26	0	0

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.

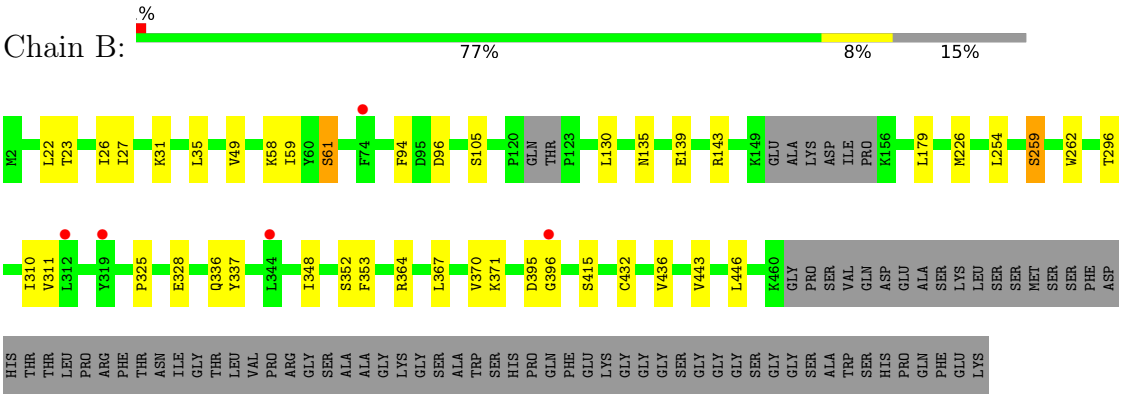
• Molecule 1: Cis-aconitate decarboxylase

Chain A:



• Molecule 1: Cis-aconitate decarboxylase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.07Å 174.07Å 71.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.85 – 2.54 123.09 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.3 (77.85-2.54) 97.3 (123.09-2.53)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.55Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.247 0.211 , 0.214	Depositor DCC
R_{free} test set	1869 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13849	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.25	0/3570	0.41	0/4854
1	B	0.25	0/3560	0.41	0/4843
All	All	0.25	0/7130	0.41	0/9697

There are no bond length outliers.

There are no bond angle outliers.

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	3479	3427	3430	18	0
1	B	3472	3424	3421	27	0
2	A	21	0	0	1	0
2	B	26	0	0	1	0
All	All	6998	6851	6851	45	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 3.

All (45) 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:A:31:LYS:NZ	1:A:447:GLU:OE2	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PRO:O	1:B:364:ARG:NH1	2.28	0.67
1:B:26:ILE:HD11	1:B:262:TRP:HB2	1.78	0.66
1:B:143:ARG:HD3	1:B:254:LEU:HD22	1.78	0.66
1:B:26:ILE:HD11	1:B:262:TRP:CB	2.27	0.65
1:A:344:LEU:HD13	1:A:366:LEU:HD12	1.79	0.64
1:B:49:VAL:HG23	2:B:616:HOH:O	1.99	0.62
1:B:23:THR:O	1:B:27:ILE:HD12	2.00	0.61
1:B:58:LYS:O	1:B:61:SER:OG	2.19	0.60
1:B:432:CYS:O	1:B:436:VAL:HG23	2.05	0.56
1:B:27:ILE:HG22	1:B:31:LYS:HE2	1.91	0.53
1:B:139:GLU:OE1	1:B:143:ARG:NE	2.38	0.51
1:B:179:LEU:HD11	1:B:226:MET:SD	2.50	0.51
1:B:259:SER:O	1:B:259:SER:OG	2.28	0.50
1:A:439:LEU:HD21	1:A:459:LEU:HD23	1.95	0.49
1:A:446:LEU:CD1	1:A:449:LEU:HD22	2.42	0.49
1:A:294:LEU:HD22	1:A:393:LEU:HD21	1.96	0.48
1:B:26:ILE:CD1	1:B:262:TRP:CG	2.96	0.48
1:B:310:ILE:O	1:B:370:VAL:HA	2.14	0.48
1:B:348:ILE:HG23	1:B:348:ILE:O	2.13	0.48
1:A:67:THR:OG1	1:A:75:ARG:NH2	2.43	0.48
1:B:130:LEU:O	1:B:130:LEU:HD23	2.14	0.47
1:B:22:LEU:HB3	1:B:27:ILE:HD11	1.97	0.47
1:A:348:ILE:HG23	1:A:348:ILE:O	2.15	0.46
1:B:96:ASP:OD2	1:B:105:SER:OG	2.22	0.46
1:A:119:LEU:HD11	1:A:125:PHE:HE2	1.81	0.46
1:A:128:LEU:O	1:A:128:LEU:HD23	2.16	0.46
1:B:328:GLU:HG3	1:B:353:PHE:O	2.16	0.45
1:A:446:LEU:HD12	1:A:449:LEU:HD22	1.97	0.45
1:A:320:VAL:HG12	1:A:320:VAL:O	2.15	0.45
1:A:73:ASP:OD1	1:A:73:ASP:N	2.48	0.45
1:B:367:LEU:O	1:B:370:VAL:HG12	2.17	0.44
1:A:336:GLN:HG3	1:A:370:VAL:HG11	1.99	0.44
1:B:26:ILE:HD11	1:B:262:TRP:CG	2.51	0.44
1:B:26:ILE:HG23	1:B:135:ASN:OD1	2.17	0.44
1:B:395:ASP:OD1	1:B:396:GLY:N	2.50	0.44
1:B:336:GLN:OE1	1:B:336:GLN:N	2.44	0.44
1:A:19:VAL:CG1	1:A:128:LEU:HD22	2.48	0.43
1:A:96[B]:ASP:OD1	1:A:271:PHE:CE1	2.71	0.43
1:B:311:VAL:HA	1:B:371:LYS:O	2.17	0.43
1:B:35:LEU:HB2	1:B:443:VAL:HG11	1.99	0.43
1:B:337:TYR:OH	1:B:352:SER:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HD3	1:A:263:LEU:HD11	2.02	0.42
1:A:272:LYS:NZ	2:A:603:HOH:O	2.54	0.41

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	445/530 (84%)	428 (96%)	17 (4%)	0	100	100
1	B	445/530 (84%)	431 (97%)	14 (3%)	0	100	100
All	All	890/1060 (84%)	859 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	376/442 (85%)	367 (98%)	9 (2%)	49	64
1	B	374/442 (85%)	367 (98%)	7 (2%)	57	72
All	All	750/884 (85%)	734 (98%)	16 (2%)	53	68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	74	PHE
1	A	94	PHE
1	A	257	LEU
1	A	259	SER
1	A	278	LEU
1	A	309	ARG
1	A	332	ARG
1	A	428	SER
1	B	59	ILE
1	B	61	SER
1	B	94	PHE
1	B	259	SER
1	B	296	THR
1	B	415	SER
1	B	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	450/530 (84%)	0.31	8 (1%)	68	74	38, 60, 86, 112	0
1	B	451/530 (85%)	0.26	5 (1%)	80	85	37, 60, 89, 116	0
All	All	901/1060 (85%)	0.29	13 (1%)	75	81	37, 60, 88, 116	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	TYR	2.9
1	A	74	PHE	2.6
1	B	312	LEU	2.5
1	A	125	PHE	2.5
1	A	294	LEU	2.5
1	B	396	GLY	2.4
1	A	176	PHE	2.4
1	B	74	PHE	2.3
1	B	344	LEU	2.2
1	A	290	VAL	2.1
1	A	128	LEU	2.1
1	A	344	LEU	2.1
1	A	363	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.