



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 08:02 PM EDT

PDB ID : 5WQN  
Title : Crystal structure of a carbonyl reductase from *Pseudomonas aeruginosa* PAO1 (condition II)  
Authors : Li, S.; Wang, Y.; Bartlam, M.  
Deposited on : unknown  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

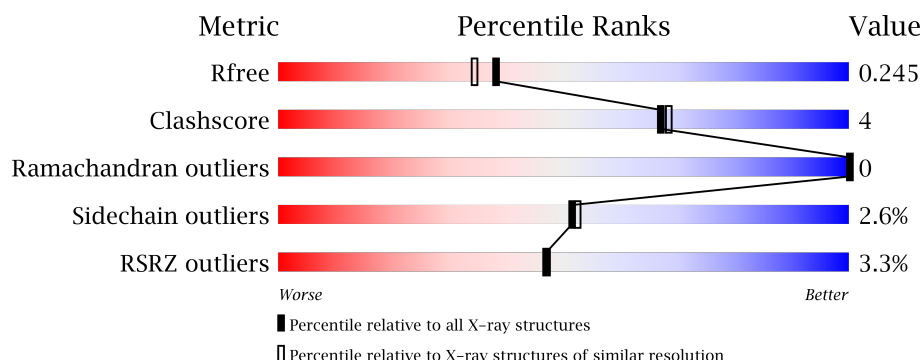
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	229	<div> <div>0.1%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
1	B	229	<div> <div>0.1%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	C	229	<div> <div>9%</div> <div>85%</div> <div>9%</div> <div>• •</div> </div>
1	D	229	<div> <div>0.1%</div> <div>87%</div> <div>11%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6985 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 Probable dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1619	1012	297	303	7			
1	B	217	Total	C	N	O	S	0	0	0
			1619	1012	297	303	7			
1	C	221	Total	C	N	O	S	0	0	0
			1652	1036	302	307	7			
1	D	226	Total	C	N	O	S	0	0	0
			1693	1059	310	316	8			

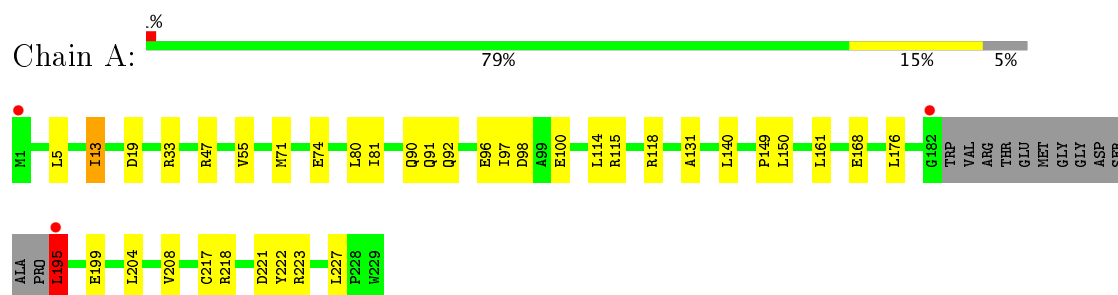
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	92	Total	O	0	0
			92	92		
2	C	90	Total	O	0	0
			90	90		
2	D	105	Total	O	0	0
			105	105		

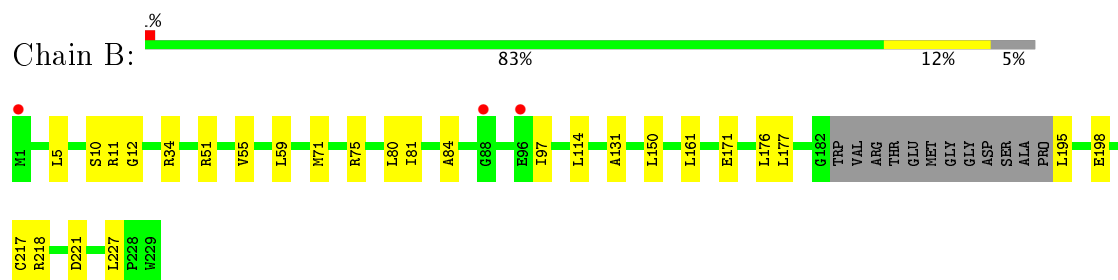
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

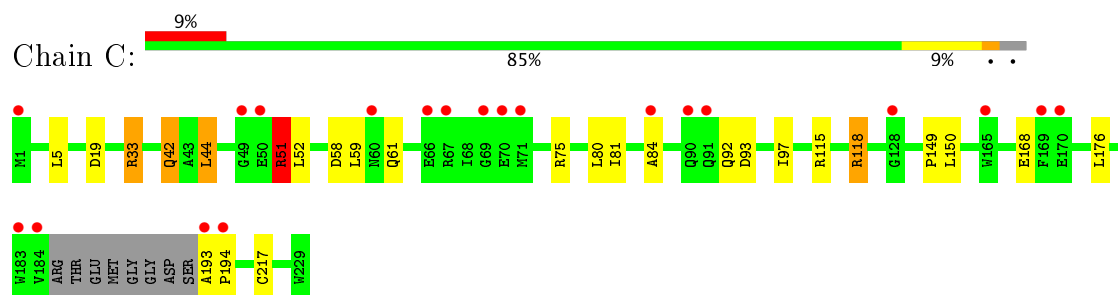
- Molecule 1: Probable dehydrogenase



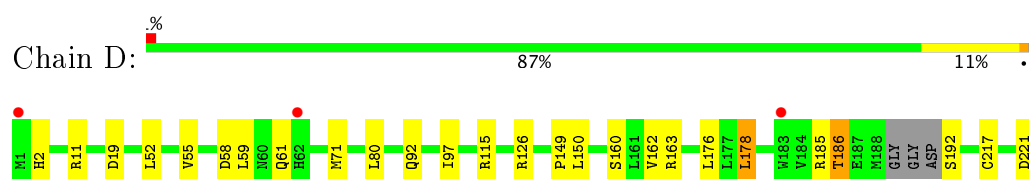
- Molecule 1: Probable dehydrogenase



- Molecule 1: Probable dehydrogenase



- Molecule 1: Probable dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.19Å 131.18Å 143.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 41.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.00) 99.7 (41.83-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.191 , 0.242 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	2000 reflections (4.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

### 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	0.78	0/1643	0.92	7/2223 (0.3%)
1	B	0.74	0/1643	0.89	2/2223 (0.1%)
1	C	0.70	0/1679	0.93	8/2275 (0.4%)
1	D	0.77	0/1720	0.91	4/2329 (0.2%)
All	All	0.75	0/6685	0.91	21/9050 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	51	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	42	GLN	CA-CB-CG	6.59	127.90	113.40
1	D	178	LEU	CB-CG-CD2	6.43	121.94	111.00
1	A	168	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	C	19	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	163	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	19	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	198	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	D	19	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	93	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	115	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	51	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	51	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	118	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	33	ARG	CG-CD-NE	5.12	122.55	111.80
1	C	115	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	218	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	80	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	195	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	C	33	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	1619	0	1626	19	0
1	B	1619	0	1626	14	0
1	C	1652	0	1657	13	0
1	D	1693	0	1697	16	0
2	A	115	0	0	3	0
2	B	92	0	0	2	0
2	C	90	0	0	0	0
2	D	105	0	0	3	0
All	All	6985	0	6606	59	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 4.

All (59) 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:D:185:ARG:O	1:D:186:THR:HB	1.78	0.80
1:D:58:ASP:O	1:D:61:GLN:HG2	1.82	0.80
1:A:90:GLN:OE1	2:A:301:HOH:O	2.07	0.71
1:C:118:ARG:NH2	1:C:168:GLU:OE2	2.22	0.67
1:A:55:VAL:HG22	1:A:71:MET:HG3	1.77	0.67
1:B:5:LEU:HD23	1:B:80:LEU:HD13	1.87	0.56
1:D:55:VAL:HG22	1:D:71:MET:HG2	1.88	0.56
1:C:44:LEU:HB3	1:C:52:LEU:HD22	1.86	0.56
1:C:5:LEU:HD23	1:C:80:LEU:HD13	1.88	0.55
1:A:195:LEU:HD12	1:B:12:GLY:HA2	1.88	0.55
1:C:59:LEU:HD23	1:C:84:ALA:HB2	1.89	0.55
1:A:5:LEU:HD23	1:A:80:LEU:HD13	1.89	0.54
1:C:59:LEU:CD2	1:C:84:ALA:HB2	2.38	0.54
1:D:192:SER:N	2:D:301:HOH:O	2.40	0.54
1:D:97:ILE:HD12	1:D:150:LEU:HD13	1.90	0.54
1:B:177:LEU:HD22	1:B:218:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NE	2:D:302:HOH:O	2.41	0.53
1:A:81:ILE:HD13	1:A:131:ALA:HB3	1.89	0.53
1:B:114:LEU:HD22	1:B:161:LEU:HB3	1.92	0.52
1:D:11:ARG:NH2	1:D:186:THR:HG23	2.25	0.51
1:C:193:ALA:N	1:C:194:PRO:CD	2.73	0.51
1:A:114:LEU:HD22	1:A:161:LEU:HB3	1.92	0.51
1:C:51:ARG:CD	1:C:51:ARG:N	2.75	0.49
1:D:185:ARG:O	1:D:186:THR:CB	2.55	0.49
1:D:221:ASP:HB3	1:D:227:LEU:HD11	1.94	0.49
1:A:13:ILE:HD11	1:A:204:LEU:HD12	1.95	0.49
1:A:98:ASP:OD1	1:A:100:GLU:HG2	2.13	0.48
1:A:91:GLN:HG2	1:A:96:GLU:OE1	2.14	0.48
1:C:97:ILE:HD12	1:C:150:LEU:HD13	1.95	0.48
1:B:221:ASP:HB3	1:B:227:LEU:HD11	1.97	0.46
1:B:75:ARG:HG2	2:B:352:HOH:O	2.15	0.46
1:A:223:ARG:NE	2:A:308:HOH:O	2.48	0.46
1:D:162:VAL:HG11	1:D:178:LEU:HD21	1.98	0.46
1:C:59:LEU:HD23	1:C:84:ALA:CB	2.46	0.45
1:A:195:LEU:CD1	1:B:12:GLY:HA2	2.45	0.45
1:B:55:VAL:HG22	1:B:71:MET:HG2	1.98	0.45
1:A:97:ILE:HD12	1:A:150:LEU:HD13	1.96	0.45
1:B:176:LEU:O	1:B:217:CYS:HA	2.17	0.45
1:A:176:LEU:O	1:A:217:CYS:HA	2.17	0.45
1:D:176:LEU:O	1:D:217:CYS:HA	2.18	0.44
1:C:176:LEU:O	1:C:217:CYS:HA	2.17	0.44
1:B:81:ILE:HD13	1:B:131:ALA:HB3	2.00	0.44
1:B:59:LEU:HD23	1:B:84:ALA:HB2	1.99	0.44
1:C:58:ASP:HB3	1:C:61:GLN:HG3	1.99	0.44
1:B:97:ILE:HD12	1:B:150:LEU:HD13	2.00	0.44
1:A:140:LEU:CD1	1:D:160:SER:HA	2.48	0.43
1:B:195:LEU:N	2:B:309:HOH:O	2.51	0.43
1:A:92:GLN:HB3	1:A:149:PRO:HD2	2.00	0.42
1:A:195:LEU:N	1:A:195:LEU:HD12	2.34	0.42
1:A:221:ASP:HB3	1:A:227:LEU:HD11	2.00	0.42
1:D:2:HIS:CG	2:D:345:HOH:O	2.72	0.42
1:A:47:ARG:NH2	2:A:307:HOH:O	2.47	0.42
1:B:10:SER:OG	1:B:11:ARG:NH1	2.53	0.41
1:C:92:GLN:HA	1:C:150:LEU:HD12	2.02	0.41
1:D:92:GLN:HA	1:D:150:LEU:HD12	2.01	0.41
1:C:92:GLN:HB3	1:C:149:PRO:HD2	2.02	0.41
1:D:92:GLN:HB3	1:D:149:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:HD11	1:A:208:VAL:HG21	2.04	0.40
1:D:11:ARG:HH22	1:D:186:THR:HG23	1.87	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	213/229 (93%)	209 (98%)	4 (2%)	0	100	100
1	B	213/229 (93%)	209 (98%)	4 (2%)	0	100	100
1	C	217/229 (95%)	211 (97%)	6 (3%)	0	100	100
1	D	222/229 (97%)	216 (97%)	6 (3%)	0	100	100
All	All	865/916 (94%)	845 (98%)	20 (2%)	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	162/171 (95%)	157 (97%)	5 (3%)	45	44
1	B	162/171 (95%)	160 (99%)	2 (1%)	75	80
1	C	165/171 (96%)	159 (96%)	6 (4%)	40	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	170/171 (99%)	166 (98%)	4 (2%)	54	56
All	All	659/684 (96%)	642 (97%)	17 (3%)	51	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	74	GLU
1	A	195	LEU
1	A	199	GLU
1	A	222	TYR
1	B	34	ARG
1	B	171	GLU
1	C	33	ARG
1	C	42	GLN
1	C	44	LEU
1	C	51	ARG
1	C	75	ARG
1	C	81	ILE
1	D	52	LEU
1	D	59	LEU
1	D	126	ARG
1	D	186	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	C	53	GLN

### 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 [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 ⓘ

### 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<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	217/229 (94%)	0.08	3 (1%) 75 75	13, 25, 45, 84	0
1	B	217/229 (94%)	0.23	3 (1%) 75 75	15, 29, 54, 79	0
1	C	221/229 (96%)	0.63	20 (9%) 10 10	18, 32, 65, 92	0
1	D	226/229 (98%)	0.12	3 (1%) 77 77	12, 27, 53, 75	0
All	All	881/916 (96%)	0.26	29 (3%) 47 47	12, 28, 57, 92	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	6.4
1	C	84	ALA	5.9
1	C	60	ASN	5.0
1	C	49	GLY	4.6
1	B	1	MET	4.1
1	C	165	TRP	3.8
1	C	128	GLY	3.6
1	C	183	TRP	3.6
1	D	1	MET	3.6
1	A	182	GLY	3.4
1	C	90	GLN	3.3
1	C	71	MET	3.2
1	D	62	HIS	3.1
1	D	183	TRP	3.0
1	C	169	PHE	2.9
1	B	88	GLY	2.7
1	C	170	GLU	2.7
1	C	193	ALA	2.7
1	A	1	MET	2.6
1	C	50	GLU	2.6
1	C	67	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	69	GLY	2.4
1	C	91	GLN	2.3
1	C	184	VAL	2.2
1	C	194	PRO	2.1
1	C	70	GLU	2.1
1	B	96	GLU	2.1
1	A	195	LEU	2.1
1	C	66	GLU	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 carbohydrates 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.