Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 04:31 am BST

PDB ID	:	2F9S
Title	:	2nd Crystal Structure Of A Soluble Domain Of ResA In The Oxidised Form
Authors	:	Colbert, C.L.; Wu, Q.; Erbel, P.J.A.; Gardner, K.H.; Deisenhofer, J.
Deposited on	:	2005-12-06
Resolution	:	1.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

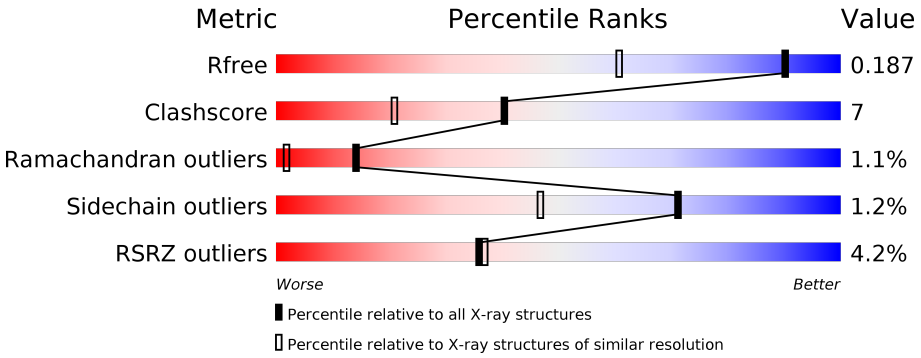
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 >=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	151	4% 80% 9% • 9%
1	B	151	3% 81% 7% •• 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2522 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 Thiol-disulfide oxidoreductase resA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	Se	41	20	0
			1167	757	184	215	3	8			
1	B	136	Total	C	N	O	S	Se	37	26	0
			1184	769	189	218	3	5			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MSE	MET	MODIFIED RESIDUE	UNP P35160
A	114	MSE	MET	MODIFIED RESIDUE	UNP P35160
A	160	MSE	MET	MODIFIED RESIDUE	UNP P35160
A	164	MSE	MET	MODIFIED RESIDUE	UNP P35160
A	169	MSE	MET	MODIFIED RESIDUE	UNP P35160
A	180	LEU	-	EXPRESSION TAG	UNP P35160
A	181	GLU	-	EXPRESSION TAG	UNP P35160
A	182	HIS	-	EXPRESSION TAG	UNP P35160
A	183	HIS	-	EXPRESSION TAG	UNP P35160
A	184	HIS	-	EXPRESSION TAG	UNP P35160
A	185	HIS	-	EXPRESSION TAG	UNP P35160
A	186	HIS	-	EXPRESSION TAG	UNP P35160
A	187	HIS	-	EXPRESSION TAG	UNP P35160
B	84	MSE	MET	MODIFIED RESIDUE	UNP P35160
B	114	MSE	MET	MODIFIED RESIDUE	UNP P35160
B	160	MSE	MET	MODIFIED RESIDUE	UNP P35160
B	164	MSE	MET	MODIFIED RESIDUE	UNP P35160
B	169	MSE	MET	MODIFIED RESIDUE	UNP P35160
B	180	LEU	-	EXPRESSION TAG	UNP P35160
B	181	GLU	-	EXPRESSION TAG	UNP P35160
B	182	HIS	-	EXPRESSION TAG	UNP P35160
B	183	HIS	-	EXPRESSION TAG	UNP P35160
B	184	HIS	-	EXPRESSION TAG	UNP P35160
B	185	HIS	-	EXPRESSION TAG	UNP P35160
B	186	HIS	-	EXPRESSION TAG	UNP P35160

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Chain	Residue	Modelled	Actual	Comment	Reference
B	187	HIS	-	EXPRESSION TAG	UNP P35160

- Molecule 2 is water.

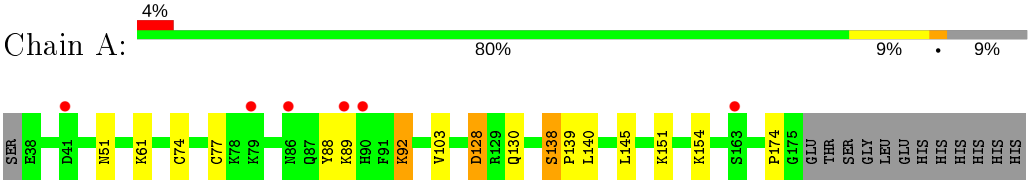
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	86	Total O 86 86	0	0
2	B	85	Total O 85 85	0	0

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.

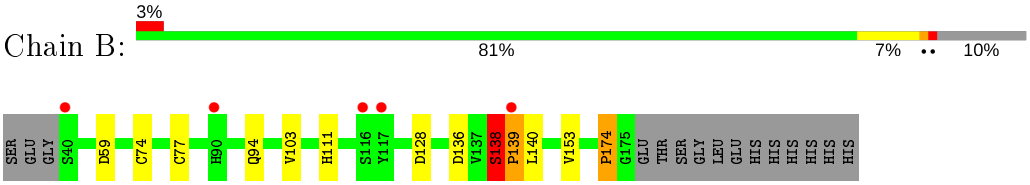
- Molecule 1: Thiol-disulfide oxidoreductase resA

Chain A:



- Molecule 1: Thiol-disulfide oxidoreductase resA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	61.19Å 61.19Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.70 – 1.40 38.38 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.70-1.40) 99.9 (38.38-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.162 , 0.175 0.187 , 0.187	Depositor DCC
R_{free} test set	3509 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2522	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	1.30	4/1275 (0.3%)	0.99	6/1714 (0.4%)
1	B	0.70	1/1315 (0.1%)	0.81	6/1774 (0.3%)
All	All	1.04	5/2590 (0.2%)	0.91	12/3488 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	C-N	-36.26	0.67	1.33
1	B	174	PRO	C-N	-17.11	1.02	1.33
1	A	151[A]	LYS	CD-CE	-15.82	1.11	1.51
1	A	151[B]	LYS	CD-CE	-15.82	1.11	1.51
1	A	89	LYS	CD-CE	-6.81	1.34	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	PRO	C-N-CA	17.68	159.44	122.30
1	A	151[A]	LYS	CG-CD-CE	13.48	152.33	111.90
1	A	151[B]	LYS	CG-CD-CE	13.48	152.33	111.90
1	B	174	PRO	CA-C-N	8.96	134.12	116.20
1	A	174	PRO	O-C-N	7.11	135.28	123.20
1	B	174	PRO	O-C-N	-6.77	111.70	123.20
1	B	59	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	136[A]	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	136[B]	ASP	CB-CG-OD2	5.17	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	128[A]	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	128[B]	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	138[B]	SER	Peptide
1	B	174	PRO	Mainchain

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	1167	0	1171	16	0
1	B	1184	0	1155	21	0
2	A	86	0	0	1	0
2	B	85	0	0	0	0
All	All	2522	0	2326	31	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 7.

All (31) 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:138[B]:SER:HB3	1:B:139[B]:PRO:CG	1.61	1.29
1:B:138[B]:SER:CB	1:B:139[B]:PRO:HG2	1.81	1.09
1:B:138[B]:SER:HB3	1:B:139[B]:PRO:HG2	0.93	0.92
1:B:138[B]:SER:OG	1:B:139[B]:PRO:HD2	1.67	0.91
1:B:138[B]:SER:CB	1:B:139[B]:PRO:CG	2.47	0.87
1:A:51:ASN:C	1:B:111[A]:HIS:HD1	1.81	0.82
1:A:128[A]:ASP:OD1	2:A:260:HOH:O	2.00	0.79
1:B:138[B]:SER:CB	1:B:139[B]:PRO:CD	2.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74[A]:CYS:HG	1:B:77:CYS:HG	1.27	0.75
1:B:138[B]:SER:HB3	1:B:139[B]:PRO:CD	2.24	0.68
1:A:51:ASN:C	1:B:111[A]:HIS:ND1	2.48	0.66
1:B:103[A]:VAL:HG21	1:B:140:LEU:HD11	1.78	0.64
1:B:138[B]:SER:OG	1:B:139[B]:PRO:CD	2.44	0.64
1:A:51:ASN:HA	1:B:111[A]:HIS:ND1	2.14	0.63
1:A:103[A]:VAL:HG21	1:A:140:LEU:HD11	1.81	0.63
1:B:138[B]:SER:CB	1:B:139[B]:PRO:HD2	2.33	0.57
1:A:51:ASN:CA	1:B:111[A]:HIS:HD1	2.22	0.53
1:A:51:ASN:CA	1:B:111[A]:HIS:ND1	2.73	0.51
1:A:51:ASN:O	1:B:111[A]:HIS:ND1	2.39	0.49
1:A:128[A]:ASP:OD1	1:A:130:GLN:HG2	2.13	0.48
1:B:74[B]:CYS:CB	1:B:77:CYS:HG	2.27	0.48
1:A:88:TYR:O	1:A:92[A]:LYS:HG2	2.14	0.47
1:A:138[B]:SER:HB3	1:A:139:PRO:CD	2.47	0.45
1:B:138[B]:SER:HB3	1:B:139[B]:PRO:CB	2.44	0.44
1:A:74[B]:CYS:CB	1:A:77:CYS:HG	2.31	0.43
1:A:138[A]:SER:HB2	1:A:139:PRO:CD	2.48	0.42
1:A:145:LEU:HD12	1:A:154:LYS:HB3	2.02	0.40
1:A:88:TYR:O	1:A:92[A]:LYS:CG	2.69	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	156/151 (103%)	154 (99%)	0	2 (1%)	12 1
1	B	160/151 (106%)	156 (98%)	0	4 (2%)	5 0
All	All	316/302 (105%)	310 (98%)	0	6 (2%)	14 0

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138[A]	SER
1	B	138[B]	SER
1	B	139[A]	PRO
1	B	139[B]	PRO
1	A	138[A]	SER
1	A	138[B]	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	142/129 (110%)	138 (97%)	4 (3%)	43	11
1	B	147/129 (114%)	145 (99%)	2 (1%)	67	40
All	All	289/258 (112%)	283 (98%)	6 (2%)	71	21

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	LYS
1	A	61[B]	LYS
1	A	92[A]	LYS
1	A	92[B]	LYS
1	B	153[A]	VAL
1	B	153[B]	VAL

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

Mol	Chain	Res	Type
1	A	68	ASN

5.3.3 RNA (i)

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 carbohydrates 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	174:PRO	C	175:GLY	N	1.02
1	A	174:PRO	C	175:GLY	N	0.67

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	132/151 (87%)	0.44	6 (4%)	33	33	9, 14, 22, 29	5 (3%)
1	B	130/151 (86%)	0.32	5 (3%)	40	40	9, 13, 21, 28	1 (0%)
All	All	262/302 (86%)	0.38	11 (4%)	36	37	9, 13, 21, 29	6 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86[A]	ASN	3.5
1	A	90	HIS	3.4
1	A	41	ASP	2.9
1	B	90[A]	HIS	2.9
1	B	117	TYR	2.6
1	A	79[A]	LYS	2.5
1	A	163[A]	SER	2.3
1	A	89	LYS	2.2
1	B	139[A]	PRO	2.1
1	B	116[A]	SER	2.1
1	B	40	SER	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 carbohydrates 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.