



Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B3S
Title : structure of the DSBA mutant (P31G-C33A)
Authors : Vives, C.; Royant, A.; Serre, L.
Deposited on : 2005-09-21
Resolution : 1.96 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

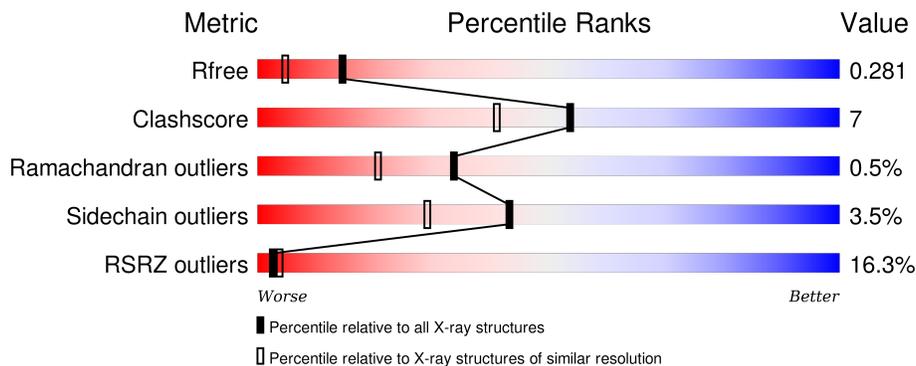
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	189	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">17% 82% 16% ..</p>
1	B	189	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">15% 81% 16% ..</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3158 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 interchange protein dsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	1469	940	241	281	7	0	0	0
1	B	187	1469	940	241	281	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	PRO	ENGINEERED	UNP P0AEG4
A	33	ALA	CYS	ENGINEERED	UNP P0AEG4
B	31	GLY	PRO	ENGINEERED	UNP P0AEG4
B	33	ALA	CYS	ENGINEERED	UNP P0AEG4

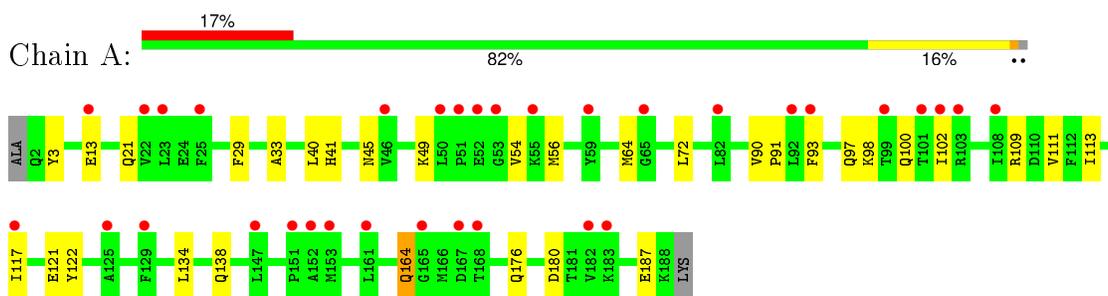
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	120	Total	O	0	0
			120	120		

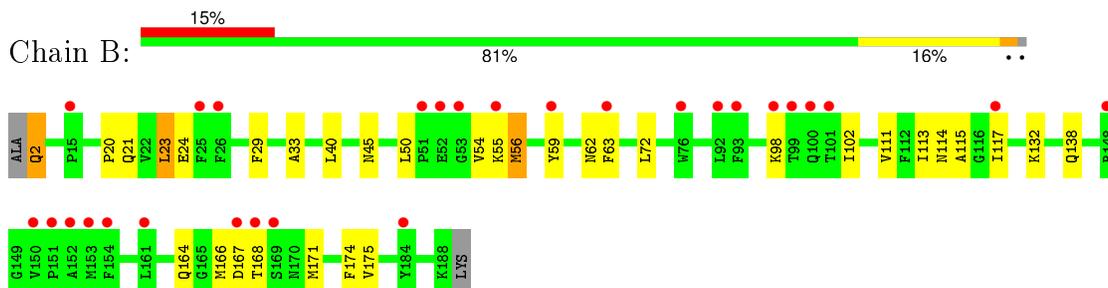
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Thiol:disulfide interchange protein dsbA



- Molecule 1: Thiol:disulfide interchange protein dsbA



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	56.31Å 56.31Å 108.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.82 – 1.96 23.79 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.0 (14.82-1.96) 94.8 (23.79-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.214 , 0.257 0.254 , 0.281	Depositor DCC
R_{free} test set	1130 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.063 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22528 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3158	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	0/1500	0.62	0/2027
1	B	0.60	0/1500	0.63	0/2027
All	All	0.59	0/3000	0.63	0/4054

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	GLN	Peptide

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	1469	0	1438	21	0
1	B	1469	0	1438	20	0
2	A	100	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	120	0	0	2	0
All	All	3158	0	2876	38	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 (38) 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:121:GLU:OE1	2:A:198:HOH:O	1.97	0.80
1:A:164:GLN:HG2	1:B:98:LYS:HA	1.65	0.79
1:A:21:GLN:NE2	1:A:54:VAL:HG22	2.08	0.69
1:A:21:GLN:HE22	1:A:54:VAL:HG22	1.59	0.65
1:A:33:ALA:HA	1:A:97:GLN:HE22	1.62	0.63
1:A:164:GLN:CG	1:B:98:LYS:HA	2.29	0.61
1:A:49:LYS:HZ3	1:A:176:GLN:HA	1.67	0.58
1:A:98:LYS:HA	1:B:164:GLN:HG3	1.89	0.55
1:B:24:GLU:OE1	1:B:56:MET:HE1	2.07	0.55
1:B:113:ILE:HA	1:B:117:ILE:O	2.09	0.53
1:A:90:VAL:HA	1:A:93:PHE:CD2	2.43	0.52
1:B:50:LEU:HD11	1:B:56:MET:HG3	1.90	0.52
1:A:41:HIS:CE1	1:A:45:ASN:OD1	2.64	0.50
1:B:164:GLN:HG2	2:B:288:HOH:O	2.12	0.49
1:B:20:PRO:HG2	1:B:23:LEU:HG	1.95	0.48
1:A:100:GLN:NE2	2:A:275:HOH:O	2.46	0.48
1:B:62:ASN:OD1	1:B:63:PHE:N	2.47	0.47
1:B:33:ALA:HB1	1:B:98:LYS:HE2	1.96	0.47
1:A:90:VAL:HG13	1:A:93:PHE:CE2	2.50	0.47
1:B:113:ILE:C	1:B:115:ALA:H	2.18	0.46
1:A:3:TYR:OH	1:A:180:ASP:HB3	2.15	0.46
1:A:102:ILE:HD11	1:A:111:VAL:HG21	1.97	0.46
1:B:171:MET:O	1:B:175:VAL:HG23	2.16	0.46
1:B:21:GLN:HE22	1:B:54:VAL:HG22	1.82	0.45
1:A:93:PHE:O	1:A:97:GLN:N	2.26	0.45
2:A:287:HOH:O	1:B:168:THR:HG21	2.16	0.45
1:B:132:LYS:HE3	2:B:304:HOH:O	2.16	0.44
1:A:29:PHE:HZ	1:A:72:LEU:HD12	1.81	0.44
1:B:167:ASP:O	1:B:174:PHE:HB2	2.18	0.44
1:A:90:VAL:HB	1:A:91:PRO:HD3	1.99	0.43
1:A:98:LYS:HB3	2:A:228:HOH:O	2.18	0.43
1:A:109:ARG:HG3	1:A:122:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:O	1:A:138:GLN:HG3	2.20	0.42
1:A:113:ILE:HA	1:A:117:ILE:O	2.19	0.42
1:B:29:PHE:HZ	1:B:72:LEU:HD12	1.85	0.41
1:B:102:ILE:HD11	1:B:111:VAL:HG21	2.03	0.41
1:B:164:GLN:C	1:B:166:MET:H	2.23	0.41
1:B:59:TYR:CG	1:B:138:GLN:HG2	2.56	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	185/189 (98%)	180 (97%)	4 (2%)	1 (0%)	34	21
1	B	185/189 (98%)	177 (96%)	7 (4%)	1 (0%)	34	21
All	All	370/378 (98%)	357 (96%)	11 (3%)	2 (0%)	34	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	B	114	ASN

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	156/157 (99%)	151 (97%)	5 (3%)	46	33
1	B	156/157 (99%)	150 (96%)	6 (4%)	40	25
All	All	312/314 (99%)	301 (96%)	11 (4%)	43	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	40	LEU
1	A	56	MET
1	A	64	MET
1	A	164	GLN
1	B	2	GLN
1	B	23	LEU
1	B	40	LEU
1	B	45	ASN
1	B	55	LYS
1	B	56	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	41	HIS
1	A	97	GLN
1	A	137	GLN
1	B	45	ASN
1	B	97	GLN
1	B	137	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 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, 95th 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	187/189 (98%)	1.16	33 (17%) 2 3	20, 36, 50, 55	0
1	B	187/189 (98%)	1.05	28 (14%) 3 5	18, 32, 47, 53	0
All	All	374/378 (98%)	1.10	61 (16%) 2 4	18, 34, 49, 55	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	GLY	7.1
1	B	161	LEU	5.4
1	B	15	PRO	4.5
1	A	93	PHE	4.4
1	A	161	LEU	4.0
1	B	169	SER	3.9
1	A	52	GLU	3.9
1	B	168	THR	3.7
1	A	50	LEU	3.5
1	B	152	ALA	3.5
1	B	93	PHE	3.4
1	A	129	PHE	3.2
1	B	25	PHE	3.2
1	B	154	PHE	3.2
1	B	51	PRO	3.1
1	A	59	TYR	3.0
1	B	117	ILE	3.0
1	A	153	MET	3.0
1	A	51	PRO	2.9
1	A	99	THR	2.9
1	B	53	GLY	2.9
1	B	52	GLU	2.8
1	B	76	TRP	2.7
1	B	101	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	150	VAL	2.6
1	A	23	LEU	2.6
1	A	151	PRO	2.5
1	A	167	ASP	2.5
1	B	98	LYS	2.5
1	B	99	THR	2.5
1	B	59	TYR	2.5
1	B	26	PHE	2.5
1	B	148	ARG	2.4
1	A	182	VAL	2.4
1	B	153	MET	2.4
1	A	82	LEU	2.4
1	A	22	VAL	2.4
1	A	108	ILE	2.4
1	A	101	THR	2.3
1	B	184	TYR	2.3
1	B	167	ASP	2.2
1	A	183	LYS	2.2
1	A	25	PHE	2.2
1	A	13	GLU	2.2
1	A	92	LEU	2.2
1	A	117	ILE	2.2
1	B	55	LYS	2.1
1	B	92	LEU	2.1
1	B	151	PRO	2.1
1	A	168	THR	2.1
1	B	63	PHE	2.1
1	A	147	LEU	2.1
1	A	125	ALA	2.1
1	A	102	ILE	2.1
1	B	100	GLN	2.1
1	A	103	ARG	2.1
1	A	55	LYS	2.0
1	A	165	GLY	2.0
1	A	152	ALA	2.0
1	A	65	GLY	2.0
1	A	46	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 [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.