W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 10:27 AM GMT

PDB ID	:	1A2L
Title	:	REDUCED DSBA AT 2.7 ANGSTROMS RESOLUTION
Authors	:	Martin, J.L.; Guddat, L.W.
Deposited on	:	1998-01-06
Resolution	:	2.70 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.8%
Sidechain outliers		3.9%

Worse ——————————————————————— *Better*

▮ Percentile relative to all X-ray structures

⧘ Percentile relative to X-ray structures of similar resolution
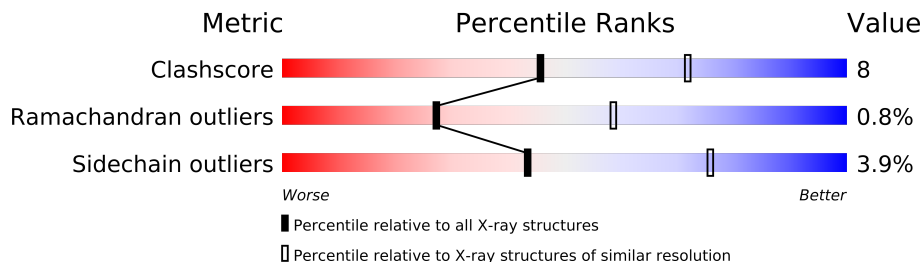
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	189	
1	B	189	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2816 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 DISULFIDE BOND FORMATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1403	897	229	269	8			
1	B	186	Total	C	N	O	S	0	0	0
			1397	898	225	266	8			

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	7	Total	O	0	0
			7	7		

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.

Note EDS was not executed.

• Molecule 1: DISULFIDE BOND FORMATION PROTEIN

Chain A:
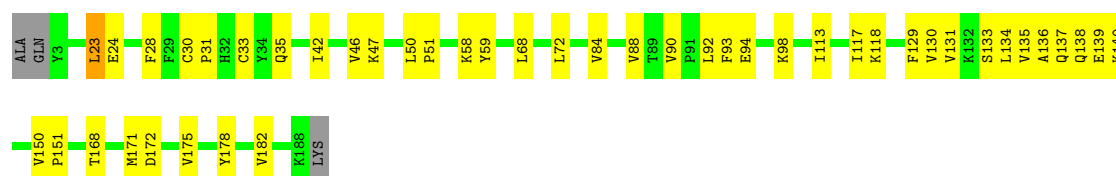
• Molecule 1: DISULFIDE BOND FORMATION PROTEIN

Chain B:

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.88Å　　83.36Å　　58.30Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　2.70	Depositor
% Data completeness (in resolution range)	71.9 (50.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.233　,　0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2816	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

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	0.30	0/1434	0.47	0/1952
1	B	0.30	0/1429	0.47	0/1948
All	All	0.30	0/2863	0.47	0/3900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1403	0	1308	24	0
1	B	1397	0	1298	22	0
2	A	9	0	0	0	0
2	B	7	0	0	0	0
All	All	2816	0	2606	45	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 8.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:VAL:HG21	1:A:117:ILE:HD11	1.66	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:VAL:O	1:B:135:VAL:HG23	2.03	0.59
1:A:24:GLU:HB3	1:A:58:LYS:HG2	1.84	0.57
1:B:46:VAL:O	1:B:50:LEU:HG	2.04	0.57
1:B:74:GLN:O	1:B:78:VAL:HG23	2.06	0.56

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	184/189 (97%)	173 (94%)	10 (5%)	1 (0%)	38	70
1	B	184/189 (97%)	172 (94%)	10 (5%)	2 (1%)	21	49
All	All	368/378 (97%)	345 (94%)	20 (5%)	3 (1%)	27	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	LYS
1	A	98	LYS
1	B	96	VAL

5.3.2 Protein sidechains ⓘ

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	141/159 (89%)	135 (96%)	6 (4%)	40	72
1	B	139/159 (87%)	134 (96%)	5 (4%)	47	79
All	All	280/318 (88%)	269 (96%)	11 (4%)	43	76

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	MET
1	A	172	ASP
1	B	62	ASN
1	A	168	THR
1	B	35	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	137	GLN
1	A	160	GLN
1	B	62	ASN
1	B	177	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

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6.4 Ligands ⓘ

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6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.