WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 11:45 PM EDT

PDB ID	:	1VRS
Title	:	Crystal structure of the disulfide-linked complex between the N-terminal and C-terminal domain of the electron transfer catalyst DsbD
Authors	:	Rozhkova, A.; Stirnimann, C.U.; Frei, P.; Grauschopf, U.; Brunisholz, R.; Gruetter, M.G.; Capitani, G.; Glockshuber, R.
Deposited on	:	2005-06-17
Resolution	:	2.85 Å(reported)

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

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 2.85 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		20
Ramachandran outliers		0.9%
Sidechain outliers		6.8%

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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	65% 19% • 15%
1	B	143	65% 19% • 13%
1	C	143	45% 31% • 21%
2	D	134	52% 33% • 12%
2	E	134	48% 36% • 12%
2	F	134	54% 30% • 12%

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5954 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 dsbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			971	623	161	186	1			
1	B	125	Total	C	N	O	S	0	0	0
			999	639	168	191	1			
1	C	113	Total	C	N	O	S	0	0	0
			914	585	152	176	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	SER	CYS	engineered mutation	UNP P36655
B	103	SER	CYS	engineered mutation	UNP P36655
C	103	SER	CYS	engineered mutation	UNP P36655

- Molecule 2 is a protein called Thiol:disulfide interchange protein dsbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	118	Total	C	N	O	S	0	0	0
			930	591	158	178	3			
2	E	118	Total	C	N	O	S	0	0	0
			926	589	155	179	3			
2	F	118	Total	C	N	O	S	0	0	0
			930	591	158	178	3			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	464	SER	CYS	engineered mutation	UNP P36655
D	547	HIS	-	expression tag	UNP P36655
D	548	HIS	-	expression tag	UNP P36655
D	549	HIS	-	expression tag	UNP P36655
D	550	HIS	-	expression tag	UNP P36655

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Chain	Residue	Modelled	Actual	Comment	Reference
D	551	HIS	-	expression tag	UNP P36655
D	552	HIS	-	expression tag	UNP P36655
E	464	SER	CYS	engineered mutation	UNP P36655
E	547	HIS	-	expression tag	UNP P36655
E	548	HIS	-	expression tag	UNP P36655
E	549	HIS	-	expression tag	UNP P36655
E	550	HIS	-	expression tag	UNP P36655
E	551	HIS	-	expression tag	UNP P36655
E	552	HIS	-	expression tag	UNP P36655
F	464	SER	CYS	engineered mutation	UNP P36655
F	547	HIS	-	expression tag	UNP P36655
F	548	HIS	-	expression tag	UNP P36655
F	549	HIS	-	expression tag	UNP P36655
F	550	HIS	-	expression tag	UNP P36655
F	551	HIS	-	expression tag	UNP P36655
F	552	HIS	-	expression tag	UNP P36655

- Molecule 3 is water.

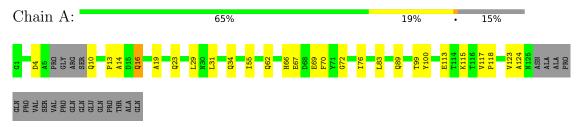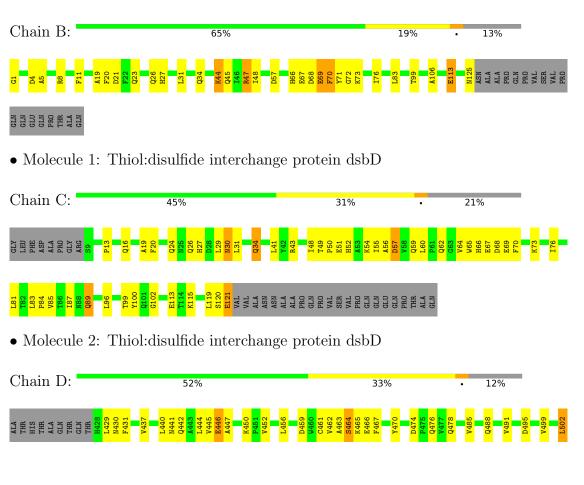| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total 93	O 93	0	0
3	D	31	Total 31	O 31	0	0
3	B	75	Total 75	O 75	0	0
3	E	34	Total 34	O 34	0	0
3	C	25	Total 25	O 25	0	0
3	F	26	Total 26	O 26	0	0

3 Residue-property plots ⓘ

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. 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. 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: Thiol:disulfide interchange protein dsbD

Chain A:

- Molecule 1: Thiol:disulfide interchange protein dsbD

Chain B:

- Molecule 1: Thiol:disulfide interchange protein dsbD

Chain C:

- Molecule 2: Thiol:disulfide interchange protein dsbD

Chain D:

K503 H504 L505 N506 V507 P511 T512 F516 D517 G518 Q519 G520 Q521 E522 H523 P524 Q525 A526 R527 E535 Q545 PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: Thiol:disulfide interchange protein dsbD

Chain E:

	48%	36%	•	12%

ALA THR HIS THR ALA GLN THR Q426 L429 N430 F431 I434 V437 Q442 A443 L444 V445 E446 A447 V452 L456 Y457 A458 D459 W460 C461 V462 A463 S464 K465 E466 F467 E468 K469 Y470 T471 D474 P475 Q476 V477 Q478 K479 A480 V485 Q488 L501 H504 L505 N506

T512 I513 L514 F515 F516 Q519 G520 Q521 E522 H523 P524 Q525 A526 R527 A534 F537 S538 L541 R542 D543 ARG GLN PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: Thiol:disulfide interchange protein dsbD

Chain F:

	54%	30%	•	12%

ALA THR HIS THR ALA GLN THR GLN THR H428 L429 T436 E439 L440 N441 L444 V445 E446 A447 K448 P451 L456 Y457 A458 D459 W460 C461 V462 A463 S464 K465 E466 F467 D474 P475 Q476 V477 Q478 K479 T484 N490 V491 T492 A493 N494 D495 A496 Q497 D498 V499 L505

N506 V507 L508 P511 F516 Q521 E522 H523 P524 Q525 A526 F531 L541 R544 Q545 PRO HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	188.46Å 52.60Å 107.92Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5954	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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	0.47	0/997	0.61	0/1359
1	B	0.46	0/1027	0.62	0/1401
1	C	0.42	0/940	0.64	0/1282
2	D	0.39	0/948	0.60	0/1287
2	E	0.40	0/944	0.61	0/1283
2	F	0.38	0/948	0.60	0/1287
All	All	0.42	0/5804	0.62	0/7899

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	971	0	923	23	0
1	B	999	0	952	35	0
1	C	914	0	865	46	0
2	D	930	0	912	46	0
2	E	926	0	906	48	0
2	F	930	0	912	37	0
3	A	93	0	0	3	0
3	B	75	0	0	4	0
3	C	25	0	0	1	0
3	D	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	34	0	0	2	0
3	F	26	0	0	0	0
All	All	5954	0	5470	222	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 20.

The worst 5 of 222 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)
2:E:452:VAL:HG12	2:E:485:VAL:HB	1.33	1.06
2:D:452:VAL:HG12	2:D:485:VAL:HB	1.41	1.02
2:E:452:VAL:HG23	2:E:516:PHE:HB2	1.40	1.01
1:C:50:PRO:HG3	1:C:55:ILE:HD12	1.55	0.88
2:F:458:ALA:HA	2:F:492:THR:HG22	1.56	0.86

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	117/143 (82%)	106 (91%)	10 (8%)	1 (1%)	17	43
1	B	123/143 (86%)	113 (92%)	9 (7%)	1 (1%)	19	46
1	C	111/143 (78%)	103 (93%)	8 (7%)	0	100	100
2	D	116/134 (87%)	107 (92%)	8 (7%)	1 (1%)	17	43
2	E	116/134 (87%)	108 (93%)	6 (5%)	2 (2%)	9	27
2	F	116/134 (87%)	111 (96%)	4 (3%)	1 (1%)	17	43
All	All	699/831 (84%)	648 (93%)	45 (6%)	6 (1%)	17	43

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	PHE
2	D	518	GLY
1	A	124	ALA
2	F	448	LYS
2	E	542	ARG

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	102/120 (85%)	97 (95%)	5 (5%)	25	54
1	B	105/120 (88%)	98 (93%)	7 (7%)	16	39
1	C	97/120 (81%)	87 (90%)	10 (10%)	7	19
2	D	100/114 (88%)	93 (93%)	7 (7%)	15	37
2	E	100/114 (88%)	93 (93%)	7 (7%)	15	37
2	F	100/114 (88%)	95 (95%)	5 (5%)	24	53
All	All	604/702 (86%)	563 (93%)	41 (7%)	16	38

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	THR
1	C	121	GLU
1	C	57	ASP
1	C	68	ASP
2	F	467	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	101	GLN
2	F	441	ASN

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Mol	Chain	Res	Type
2	F	497	GLN
1	B	59	GLN
1	B	45	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 ⓘ

There are no monosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.