Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 05:07 PM EST

PDB ID	:	8D8S
Title	:	SufS from Staphylococcus aureus
Authors	:	Morrison, C.N.; Boncella, A.E.; Lunin, V.
Deposited on	:	2022-06-08
Resolution	:	1.39 Å(reported)

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

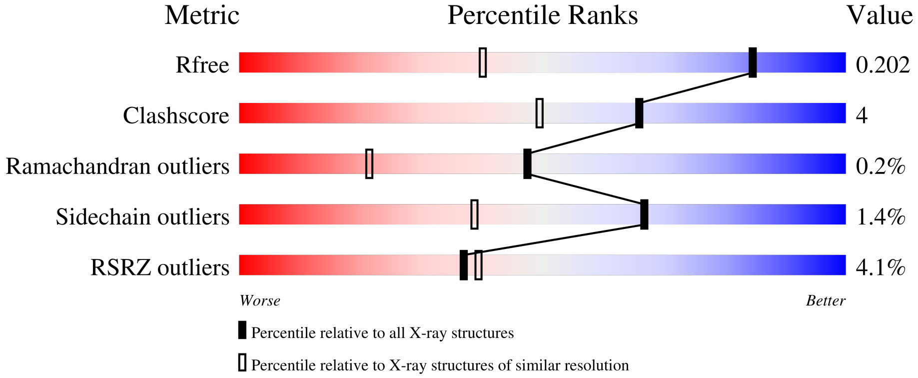
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

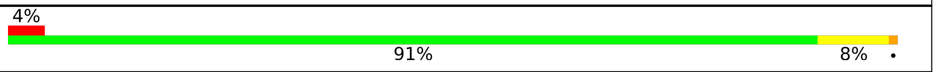
The reported resolution of this entry is 1.39 Å.

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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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% 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	414	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3759 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.

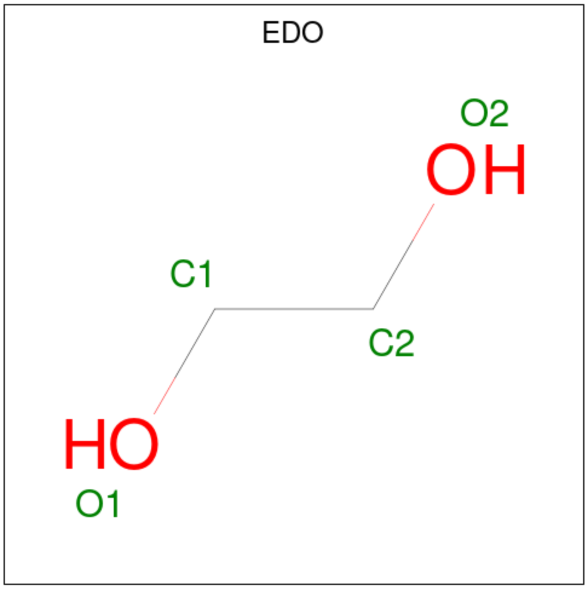
- Molecule 1 is a protein called Cysteine desulfurase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	414	3378	2136	574	654	1	13	22	13	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP X5E2K8
A	19	HIS	-	expression tag	UNP X5E2K8
A	20	MET	-	expression tag	UNP X5E2K8
A	21	ALA	-	expression tag	UNP X5E2K8
A	22	SER	-	expression tag	UNP X5E2K8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

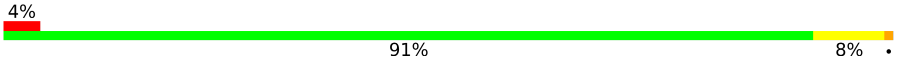
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	369	Total O 369 369	0	0

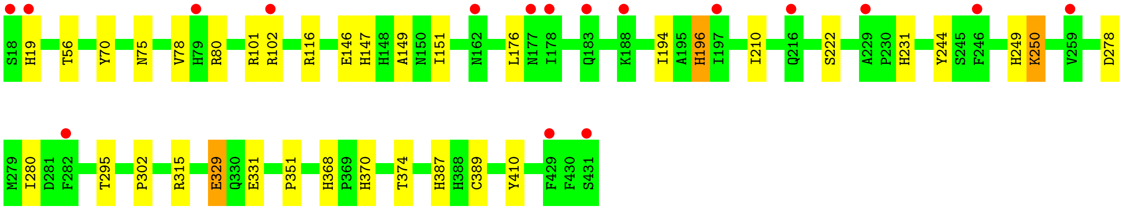
3 Residue-property plots ⓘ

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 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: Cysteine desulfurase

Chain A:





4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.85Å 93.85Å 101.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.74 – 1.39 31.72 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.74-1.39) 99.9 (31.72-1.39)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.191 0.178 , 0.202	Depositor DCC
R_{free} test set	2054 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3759	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, EDO

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	0.86	2/3421 (0.1%)	0.98	4/4636 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CD-OE2	-5.63	1.19	1.25
1	A	222	SER	CB-OG	5.02	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	A	116	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	A	116	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	101	ARG	NE-CZ-NH2	5.25	122.92	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	3378	0	3291	27	0
2	A	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	369	0	0	4	0
All	All	3759	0	3309	27	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 (27) 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:147:HIS:HD2	1:A:149:ALA:H	1.24	0.85
1:A:368:HIS:HE1	1:A:370:HIS:HD2	1.29	0.80
1:A:231:HIS:HD2	1:A:329:GLU:OE2	1.71	0.73
1:A:368:HIS:CE1	1:A:370:HIS:HD2	2.06	0.73
1:A:387:HIS:HD2	1:A:389:CYS:H	1.44	0.64
1:A:78:VAL:HG21	1:A:302:PRO:HG2	1.83	0.60
1:A:196:HIS:HD2	1:A:244:TYR:OH	1.87	0.58
1:A:387:HIS:CD2	1:A:389:CYS:H	2.22	0.56
1:A:368:HIS:HE1	1:A:370:HIS:CD2	2.17	0.55
1:A:249:HIS:HE1	1:A:250:LLP:OP2	1.91	0.54
1:A:78:VAL:CG2	1:A:302:PRO:HG2	2.38	0.53
1:A:387:HIS:HD2	1:A:389:CYS:N	2.07	0.51
1:A:56:THR:OG1	1:A:249:HIS:HD2	1.93	0.51
1:A:231:HIS:CD2	1:A:329:GLU:OE2	2.59	0.50
1:A:231:HIS:HE1	3:A:604:HOH:O	1.96	0.48
1:A:280:ILE:HD12	1:A:280:ILE:C	2.33	0.48
1:A:19:HIS:HE1	1:A:331:GLU:OE1	1.96	0.48
1:A:368:HIS:CE1	1:A:370:HIS:CD2	2.95	0.48
1:A:374[B]:THR:HG23	3:A:797:HOH:O	2.13	0.48
1:A:194:ILE:HD13	1:A:210:ILE:HD13	1.96	0.46
1:A:146:GLU:HB2	1:A:151[A]:ILE:CG1	2.46	0.46
1:A:102:ARG:CD	3:A:934:HOH:O	2.66	0.44
1:A:146:GLU:HB2	1:A:151[A]:ILE:HG13	2.00	0.42
1:A:147:HIS:CD2	1:A:149:ALA:H	2.16	0.42
1:A:176:LEU:CD1	1:A:194:ILE:HD11	2.49	0.42
1:A:70:TYR:CZ	1:A:75:ASN:HA	2.55	0.41
1:A:102:ARG:HD3	3:A:934:HOH:O	2.21	0.41

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	424/414 (102%)	412 (97%)	11 (3%)	1 (0%)	47	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ASP

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	358/345 (104%)	352 (98%)	6 (2%)	60	30

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

Mol	Chain	Res	Type
1	A	80	ARG
1	A	196	HIS
1	A	295[A]	THR
1	A	295[B]	THR
1	A	351	PRO
1	A	410	TYR

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

Mol	Chain	Res	Type
1	A	19	HIS
1	A	147	HIS
1	A	196	HIS
1	A	231	HIS
1	A	249	HIS
1	A	370	HIS
1	A	387	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	A	250	1	23,24,25	1.12	3 (13%)	25,32,34	2.98	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	250	1	-	2/16/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	LLP	P-OP4	3.16	1.70	1.60
1	A	250	LLP	P-OP1	-2.58	1.42	1.50
1	A	250	LLP	P-OP2	-2.27	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	LLP	OP4-P-OP1	-9.72	79.22	106.47
1	A	250	LLP	OP2-P-OP4	-6.60	89.17	106.73
1	A	250	LLP	OP3-P-OP4	-5.82	91.25	106.73
1	A	250	LLP	OP4-C5'-C5	3.97	116.91	109.35
1	A	250	LLP	OP2-P-OP1	3.23	123.34	110.68
1	A	250	LLP	OP3-P-OP2	2.23	116.14	107.64
1	A	250	LLP	OP3-P-OP1	2.21	119.34	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	250	LLP	C4-C4'-NZ-CE
1	A	250	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	250	LLP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	502	-	3,3,3	0.25	0	2,2,2	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	503	-	3,3,3	0.29	0	2,2,2	0.11	0
2	EDO	A	501	-	3,3,3	0.57	0	2,2,2	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	410/414 (99%)	0.43	17 (4%)	37	39	11, 17, 29, 41	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	PHE	5.0
1	A	79	HIS	4.5
1	A	431	SER	3.5
1	A	18	SER	3.4
1	A	162	ASN	3.1
1	A	197	ILE	2.9
1	A	19	HIS	2.8
1	A	216	GLN	2.8
1	A	429	PHE	2.7
1	A	259	VAL	2.6
1	A	183	GLN	2.5
1	A	102	ARG	2.5
1	A	246	PHE	2.3
1	A	178	ILE	2.3
1	A	177	ASN	2.2
1	A	188	LYS	2.1
1	A	229	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled '$Q < 0.9$' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	LLP	A	250	24/25	0.95	0.19	10,18,28,33	15

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	EDO	A	501	4/4	0.86	0.13	29,31,32,32	0
2	EDO	A	502	4/4	0.90	0.16	29,32,36,39	0
2	EDO	A	503	4/4	0.93	0.10	21,30,33,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.