

wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 11:07 AM JST

PDB ID : 7E6A

Title: Crystal structure of cysteine desulfurase SufS C361A from Bacillus subtilis

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Deposited on : 2021-02-22

Resolution : 1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

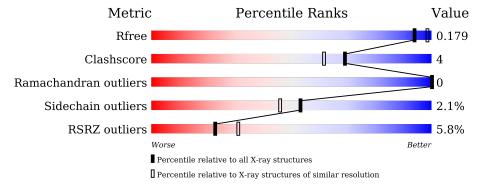
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 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	
			6%	
1	A	419	87%	10% ••



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3553 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 SufS.

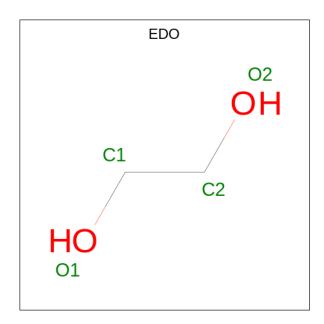
\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	412	Total 3269	C 2073	N 557	O 626	P 1	S 12	0	6	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP O32164
A	-1	GLY	-	expression tag	UNP O32164
A	0	HIS	-	expression tag	UNP O32164
A	361	ALA	CYS	engineered mutation	UNP O32164
A	407	VAL	-	expression tag	UNP O32164
A	408	ASP	-	expression tag	UNP O32164
A	409	LEU	-	expression tag	UNP O32164
A	410	GLU	-	expression tag	UNP O32164
A	411	HIS	-	expression tag	UNP O32164
A	412	HIS	-	expression tag	UNP O32164
A	413	HIS	-	expression tag	UNP O32164
A	414	HIS	_	expression tag	UNP O32164
A	415	HIS	-	expression tag	UNP O32164
A	416	HIS	-	expression tag	UNP O32164

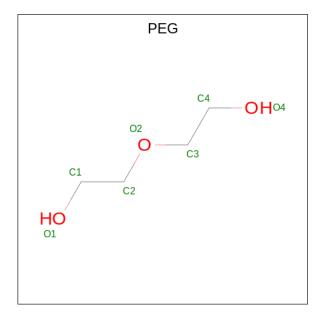
• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

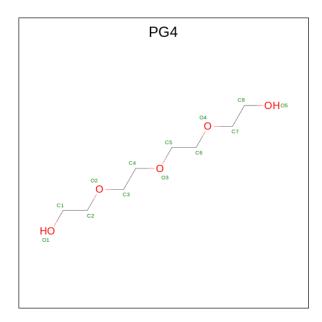
 $\bullet \ \ Molecule \ 3 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0

 \bullet Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\mathrm{C_8H_{18}O_5}).$



Mol	Chain	Residues	Atom	ıs	ZeroOcc	AltConf
4	A	1	Total C	5 5	0	0

• Molecule 5 is water.

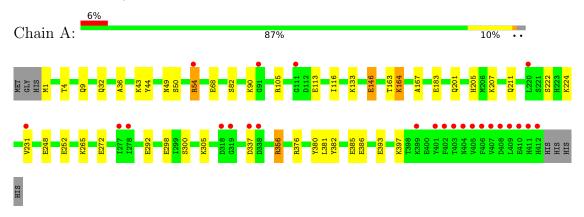
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0



3 Residue-property plots (i)

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 SufS





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	92.60Å 92.60Å 129.10Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	46.34 - 1.96	Depositor	
rtesolution (A)	46.30 - 1.96	EDS	
% Data completeness	99.8 (46.34-1.96)	Depositor	
(in resolution range)	99.8 (46.30-1.96)	EDS	
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.07 (at 1.97Å)	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
υ .	0.155 , 0.179	Depositor	
R, R_{free}	0.155 , 0.179	DCC	
R_{free} test set	2323 reflections (5.00%)	wwPDB-VP	
Wilson B-factor (Å ²)	37.0	Xtriage	
Anisotropy	0.026	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 54.9	EDS	
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	3553	wwPDB-VP	
Average B, all atoms (Å ²)	43.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, LLP, PG4, 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	Bo	nd lengths	Bo	nd angles
		Chain	RMSZ	# Z > 5	RMSZ	# Z >5
	1	A	1.02	$10/3330 \ (0.3\%)$	1.14	8/4519 (0.2%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
1	A	183	GLU	CD-OE1	11.07	1.37	1.25
1	A	386	GLU	CD-OE1	8.16	1.34	1.25
1	A	248	GLU	CD-OE2	-7.65	1.17	1.25
1	A	272	GLU	CD-OE1	7.29	1.33	1.25
1	A	50	SER	CA-CB	6.78	1.63	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	356	ARG	CG-CD-NE	9.23	131.19	111.80
1	A	356	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	105	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	248	GLU	CB-CA-C	-6.24	97.93	110.40
1	A	265	LYS	CB-CA-C	-6.21	97.98	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3269	0	3228	25	0
2	A	16	0	24	1	0
3	A	49	0	70	7	0
4	A	13	0	18	0	0
5	A	206	0	0	2	0
All	All	3553	0	3340	25	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.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$	
1:A:146:GLU:H	1:A:146:GLU:CD	1.81	0.81	
1:A:164:LYS:HE2	5:A:643:HOH:O	1.91	0.71	
1:A:43:LYS:NZ	3:A:509:PEG:H42	2.06	0.70	
1:A:397:LYS:HB3	3:A:510:PEG:H41	1.74	0.68	
1:A:54[B]:ARG:NH2	1:A:252:GLU:OE2	2.36	0.56	

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	415/419 (99%)	406 (98%)	9 (2%)	0	100 100		

There are no Ramachandran outliers to report.

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	347/347 (100%)	339 (98%)	8 (2%)	50 42	

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	TYR
1	A	380	TYR
1	A	146	GLU
1	A	133	LYS
1	A	164	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	191	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Typo	Chain	Pog	Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	1	LLP	A	224	1	23,24,25	1.06	2 (8%)	25,32,34	1.14	2 (8%)



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	224	1	-	1/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	224	LLP	C4-C5	-2.67	1.38	1.42
1	A	224	LLP	P-OP2	-2.39	1.45	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms Z		$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	224	LLP	C2'-C2-C3	2.19	123.59	120.89
1	A	224	LLP	C4-C4'-NZ	-2.08	114.74	124.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms
1	A	224	LLP	C4-C4'-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	Trino	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	507	-	6,6,6	0.19	0	5,5,5	0.30	0
2	EDO	A	504	-	3,3,3	0.13	0	2,2,2	0.34	0
2	EDO	A	502	-	3,3,3	0.41	0	2,2,2	0.59	0
4	PG4	A	512	-	12,12,12	0.29	0	11,11,11	0.52	0
3	PEG	A	509	-	6,6,6	0.09	0	5,5,5	0.23	0
2	EDO	A	501	-	3,3,3	0.19	0	2,2,2	0.65	0
3	PEG	A	510	-	6,6,6	0.16	0	5,5,5	0.14	0
3	PEG	A	508	-	6,6,6	0.57	0	5,5,5	0.44	0
2	EDO	A	503	-	3,3,3	0.31	0	2,2,2	0.25	0
3	PEG	A	506	-	6,6,6	0.21	0	5,5,5	0.16	0
3	PEG	A	505	-	6,6,6	0.41	0	5,5,5	0.23	0
3	PEG	A	511	-	6,6,6	0.23	0	5,5,5	0.15	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
3	PEG	A	507	-	-	2/4/4/4	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
4	PG4	A	512	-	-	1/10/10/10	-
3	PEG	A	509	-	-	4/4/4/4	-
2	EDO	A	501	-	-	1/1/1/1	-
3	PEG	A	510	-	-	0/4/4/4	-
3	PEG	A	508	-	-	3/4/4/4	-
2	EDO	A	503	-	-	1/1/1/1	-
3	PEG	A	506	-	-	2/4/4/4	-
3	PEG	A	505	-	-	1/4/4/4	-
3	PEG	A	511	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	507	PEG	O2-C3-C4-O4
3	A	507	PEG	O1-C1-C2-O2
3	A	506	PEG	O2-C3-C4-O4
2	A	501	EDO	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	PEG	1	0
2	A	504	EDO	1	0
3	A	509	PEG	3	0
3	A	510	PEG	2	0
3	A	505	PEG	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	$\# \mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9	
1	A	411/419 (98%)	0.26	24 (5%)	23	31	26, 39, 63, 129	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	PHE	10.3
1	A	409	LEU	9.9
1	A	407	VAL	9.4
1	A	405	VAL	7.7
1	A	411	HIS	7.7

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

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	LLP	A	224	24/25	0.99	0.13	26,33,38,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	PEG	A	511	7/7	0.52	0.22	85,92,99,108	0
3	PEG	A	508	7/7	0.79	0.18	45,56,74,74	0
3	PEG	A	510	7/7	0.83	0.37	75,80,86,87	0
2	EDO	A	504	4/4	0.83	0.13	64,67,68,70	0
3	PEG	A	509	7/7	0.85	0.16	70,76,91,92	0
3	PEG	A	506	7/7	0.86	0.15	60,66,75,85	0
2	EDO	A	502	4/4	0.89	0.10	54,60,65,68	0
2	EDO	A	501	4/4	0.90	0.11	57,58,60,63	0
4	PG4	A	512	13/13	0.90	0.15	48,58,83,86	0
2	EDO	A	503	4/4	0.91	0.10	56,62,65,66	0
3	PEG	A	505	7/7	0.93	0.16	45,52,63,68	0
3	PEG	A	507	7/7	0.95	0.11	59,63,76,77	0

6.5 Other polymers (i)

There are no such residues in this entry.

