

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 20, 2023 – 06:01 AM EDT

PDB ID	:	2H0H
Title	:	Crystal Structure of DsbG K113E mutant
Authors	:	Hiniker, A.; Heras, B.; Martin, J.L.; Stuckey, J.; Bardwell, J.C.A.
Deposited on	:	2006-05-15
Resolution	:	1.80  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:

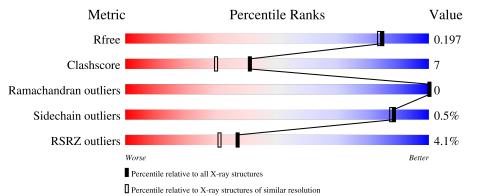
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	А	237	81%	16%	·
1	В	237	83%	14%	•



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4009 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	229	Total	С	Ν	0	$\mathbf{S}$	0	9	0
		229	1813	1159	300	343	11	0	ა	0
1	В	230	Total	С	Ν	0	S	0	2	0
	D	230	1815	1159	302	343	11	0	Δ	0

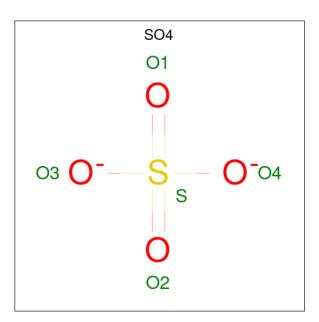
• Molecule 1 is a protein called Thiol:disulfide interchange protein dsbG.

113	OTI			
	GLU	LYS	engineered mutation	UNP P77202
232	HIS	-	expression tag	UNP P77202
233	HIS	-	expression tag	UNP P77202
234	HIS	-	expression tag	UNP P77202
235	HIS	-	expression tag	UNP P77202
236	HIS	-	expression tag	UNP P77202
237	HIS	-	expression tag	UNP P77202
113	GLU	LYS	engineered mutation	UNP P77202
232	HIS	-	expression tag	UNP P77202
233	HIS	-	expression tag	UNP P77202
234	HIS	-	expression tag	UNP P77202
235	HIS	-	expression tag	UNP P77202
236	HIS	-	expression tag	UNP P77202
237	HIS	-	expression tag	UNP P77202
	233         234         235         236         237         113         232         233         234         235         236	233         HIS           234         HIS           235         HIS           236         HIS           237         HIS           113         GLU           232         HIS           233         HIS           234         HIS           235         HIS           236         HIS	233       HIS       -         234       HIS       -         235       HIS       -         236       HIS       -         237       HIS       -         237       HIS       -         237       HIS       -         233       HIS       -         233       HIS       -         233       HIS       -         234       HIS       -         235       HIS       -         236       HIS       -	233HIS-expression tag234HIS-expression tag235HIS-expression tag236HIS-expression tag237HIS-expression tag237HIS-expression tag233HIS-expression tag233HIS-expression tag234HIS-expression tag235HIS-expression tag236HIS-expression tag236HIS-expression tag

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	192	Total O 192 192	0	0
3	В	164	Total O 164 164	0	0

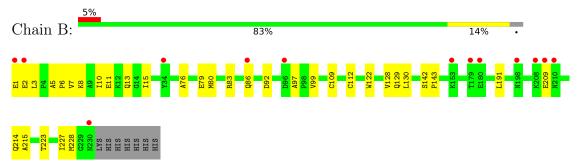


# 3 Residue-property plots (i)

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: Thiol:disulfide interchange protein dsbG

• Molecule 1: Thiol:disulfide interchange protein dsbG





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	117.11Å 56.98Å 85.00Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $94.84^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 1.80	Depositor
Resolution (A)	18.36 - 1.80	EDS
% Data completeness	97.1 (20.00-1.80)	Depositor
(in resolution range)	99.7 (18.36-1.80)	EDS
R <sub>merge</sub>	0.06	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.52 (at 1.80 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
D D	0.197 , $0.229$	Depositor
$R, R_{free}$	0.204 , $0.197$	DCC
$R_{free}$ test set	2653 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , $60.9$	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4009	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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:  $\mathrm{SO4}$ 

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		
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.32	0/1855	0.58	0/2515	
1	В	0.30	0/1857	0.57	0/2518	
All	All	0.31	0/3712	0.57	0/5033	

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 (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	А	1813	0	1810	26	0
1	В	1815	0	1814	28	0
2	А	10	0	0	0	0
2	В	15	0	0	0	0
3	А	192	0	0	0	0
3	В	164	0	0	0	0
All	All	4009	0	3624	51	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.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MET:HE1	1:B:83[B]:ARG:HD3	1.55	0.89
1:B:1:GLU:O	1:B:2:GLU:HB3	1.83	0.76
1:B:109:CYS:HG	1:B:112:CYS:HG	1.33	0.71
1:A:10:ILE:HG22	1:A:15:ILE:HD12	1.76	0.67
1:A:2:GLU:HG3	1:A:3:LEU:N	2.11	0.65

clash magnitude.

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	Favoured Allowed		Percentiles		
1	А	230/237~(97%)	226~(98%)	4 (2%)	0	100	100	
1	В	230/237~(97%)	225 (98%)	5 (2%)	0	100	100	
All	All	460/474~(97%)	451 (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	А	194/199~(98%)	194 (100%)	0	100 100		
1	В	194/199~(98%)	192 (99%)	2(1%)	76 71		

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Mol	Chain	Analysed Rotameric		Outliers	Percentiles		
All	All	388/398~(98%)	386 (100%)	2~(0%)	88 87		

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	191	LEU
1	В	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	198	ASN
1	В	210	ASN
1	В	225	ASN
1	А	221	GLN
1	В	13	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

5 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



Mol	Mol Type Chain Res	Chain	Dog	Link	B	ond leng	gths	B	ond ang	gles
		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	SO4	В	238	-	4,4,4	1.90	2 (50%)	6,6,6	0.90	0
2	SO4	А	239	-	4,4,4	1.86	2 (50%)	6,6,6	0.91	0
2	SO4	В	240	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	SO4	В	239	-	4,4,4	1.87	2 (50%)	6,6,6	0.90	0
2	SO4	А	238	-	4,4,4	1.86	2 (50%)	6,6,6	0.91	0

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).

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	238	SO4	O1-S	3.14	1.63	1.46
2	В	240	SO4	O1-S	3.10	1.62	1.46
2	А	239	SO4	O1-S	3.07	1.62	1.46
2	В	239	SO4	O1-S	3.06	1.62	1.46
2	А	238	SO4	O1-S	3.05	1.62	1.46

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 (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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	229/237~(96%)	-0.00	6 (2%) 56 5	1	13, 21, 38, 50	4 (1%)
1	В	230/237~(97%)	0.13	13 (5%) 23 1	19	13, 25, 41, 58	4 (1%)
All	All	459/474~(96%)	0.06	19 (4%) 37 3	31	13, 23, 40, 58	8 (1%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	2	GLU	4.9
1	В	1	GLU	3.7
1	А	230	ASN	3.3
1	В	209	GLU	3.1
1	А	34	TYR	3.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	А	239	5/5	0.86	0.34	80,80,82,82	0
2	SO4	В	239	5/5	0.86	0.24	71,71,74,75	0
2	SO4	В	240	5/5	0.88	0.18	85,87,87,88	0
2	SO4	В	238	5/5	0.93	0.21	$65,\!66,\!69,\!69$	0
2	SO4	А	238	5/5	0.94	0.20	72,72,74,74	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

