



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2025 – 03:05 PM EDT

PDB ID : 9MUS / pdb_00009mus
Title : Reduced state of a turn-off thiol-disulfide redox biosensor with a fluorescence-lifetime readout
Authors : Rosen, P.; Yellen, G.; Lim, D.C.
Deposited on : 2025-01-14
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

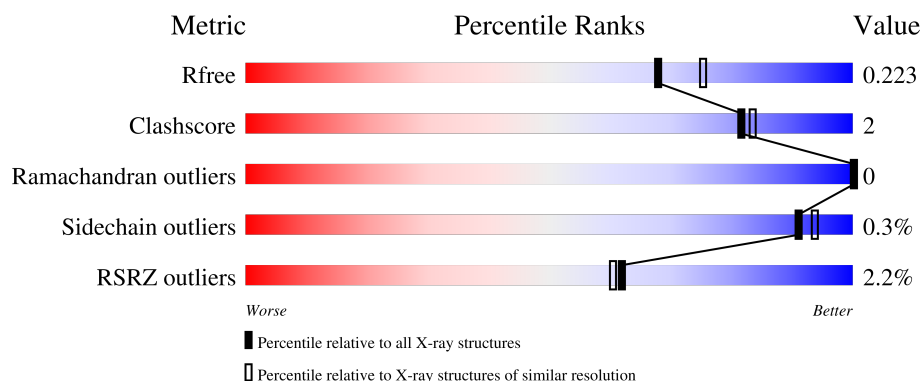
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. 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	251	
1	B	251	

2 Entry composition [i](#)

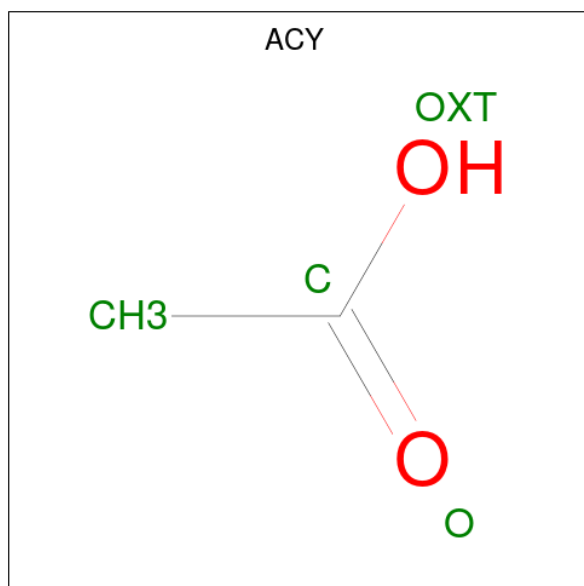
There are 5 unique types of molecules in this entry. The entry contains 7481 atoms, of which 3541 are hydrogens and 0 are deuteriums.

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 Fluorescent thiol-disulfide redox biosensor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	H	N	O	S	0	5	0
			3581	1161	1760	307	345	8			
1	B	226	Total	C	H	N	O	S	0	5	0
			3552	1155	1745	308	338	6			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



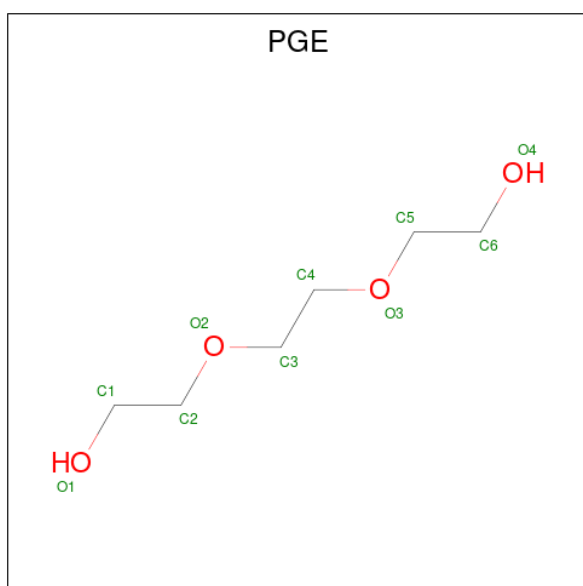
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total 139	O 139	0	0
5	B	143	Total 143	O 143	0	0

- Molecule 1: Fluorescent thiol-disulfide redox biosensor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	52.80Å 140.18Å 130.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.85 – 2.00 30.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.85-2.00) 98.3 (30.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.225 0.187 , 0.223	Depositor DCC
R_{free} test set	31085 reflections (6.11%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7481	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8964e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SWG, GOL, PGE, ACY

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	0.09	0/1849	0.25	0/2494
1	B	0.08	0/1838	0.24	0/2482
All	All	0.09	0/3687	0.25	0/4976

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	1821	1760	1779	8	0
1	B	1807	1745	1767	10	0
2	A	4	3	3	0	0
2	B	4	3	3	0	0
3	B	12	16	16	0	0
4	B	10	14	14	0	0
5	A	139	0	0	0	0
5	B	143	0	0	2	0
All	All	3940	3541	3582	17	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 2.

The worst 5 of 17 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:66:SWG:HE3	1:A:66:SWG:N2	2.07	0.69
1:B:66:SWG:N2	1:B:66:SWG:HE3	2.13	0.64
1:A:72:ALA:HA	1:A:225[B]:VAL:HG13	1.79	0.64
1:B:72:ALA:HA	1:B:225[A]:VAL:HG13	1.79	0.63
1:B:107:LYS:NZ	5:B:402:HOH:O	2.31	0.62

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	226/251 (90%)	222 (98%)	4 (2%)	0	100	100
1	B	226/251 (90%)	222 (98%)	4 (2%)	0	100	100
All	All	452/502 (90%)	444 (98%)	8 (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	197/214 (92%)	196 (100%)	1 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	193/214 (90%)	193 (100%)	0	100	100
All	All	390/428 (91%)	389 (100%)	1 (0%)	91	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	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	150	ASN
1	A	185	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SWG	B	66	1	22,25,26	3.07	10 (45%)	27,35,37	2.68	9 (33%)
1	SWG	A	66	1	22,25,26	3.08	11 (50%)	27,35,37	2.62	11 (40%)

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	SWG	B	66	1	-	5/8/29/30	0/3/3/3
1	SWG	A	66	1	-	4/8/29/30	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	SWG	CA2-C2	-9.61	1.38	1.48
1	A	66	SWG	CA2-C2	-9.59	1.38	1.48
1	A	66	SWG	OG1-CB1	-5.63	1.18	1.42
1	B	66	SWG	OG1-CB1	-5.58	1.19	1.42
1	A	66	SWG	C2-N3	-3.99	1.30	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	SWG	O2-C2-CA2	-7.44	126.27	131.02
1	A	66	SWG	O2-C2-CA2	-6.87	126.64	131.02
1	B	66	SWG	CZ3-CE3-CD2	-5.24	113.84	120.91
1	A	66	SWG	CZ3-CE3-CD2	-5.10	114.03	120.91
1	B	66	SWG	CE3-CD2-CE2	4.80	124.53	118.17

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	SWG	C2-CA2-CB2-CG
1	A	66	SWG	N1-CA1-CB1-OG1
1	B	66	SWG	N2-CA2-CB2-CG
1	B	66	SWG	C2-CA2-CB2-CG
1	B	66	SWG	N1-CA1-CB1-OG1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	SWG	1	0
1	A	66	SWG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 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	$\# Z > 2$
4	PGE	B	302	-	9,9,9	0.32	0	8,8,8	0.30	0
3	GOL	B	303	-	5,5,5	0.95	0	5,5,5	1.02	0
3	GOL	B	301	-	5,5,5	0.98	0	5,5,5	1.10	0
2	ACY	B	304	-	3,3,3	1.42	0	3,3,3	1.73	1 (33%)
2	ACY	A	301	-	3,3,3	1.48	0	3,3,3	1.69	1 (33%)

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	GOL	B	301	-	-	0/4/4/4	-
4	PGE	B	302	-	-	4/7/7/7	-
3	GOL	B	303	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	ACY	O-C-CH3	-2.36	112.84	122.53
2	A	301	ACY	O-C-CH3	-2.31	113.06	122.53

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	GOL	O1-C1-C2-O2
4	B	302	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	B	303	GOL	O1-C1-C2-C3
4	B	302	PGE	C1-C2-O2-C3
4	B	302	PGE	O2-C3-C4-O3

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, 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	225/251 (89%)	-0.16	6 (2%) 56 54	17, 32, 58, 80	5 (2%)
1	B	225/251 (89%)	-0.04	4 (1%) 67 66	18, 36, 63, 84	5 (2%)
All	All	450/502 (89%)	-0.10	10 (2%) 62 60	17, 34, 60, 84	10 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	GLY	3.3
1	A	174	ASP	3.2
1	A	47	ILE	2.9
1	B	146	GLY	2.7
1	A	3	LYS	2.5

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, 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	SWG	B	66	23/24	0.92	0.09	21,27,38,42	0
1	SWG	A	66	23/24	0.94	0.07	19,24,31,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
4	PGE	B	302	10/10	0.68	0.16	40,55,67,71	0
3	GOL	B	301	6/6	0.79	0.16	27,42,51,52	0
3	GOL	B	303	6/6	0.86	0.10	52,66,82,82	0
2	ACY	A	301	4/4	0.89	0.10	29,37,39,42	0
2	ACY	B	304	4/4	0.93	0.10	26,30,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.