



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2025 – 06:06 PM EDT

PDB ID : 9MUV / pdb\_00009muv  
Title : Oxidized state of a turn-on thiol-disulfide redox biosensor with a fluorescence-lifetime readout  
Authors : Rosen, P.; Yellen, G.; Lim, D.C.  
Deposited on : 2025-01-14  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.43.1

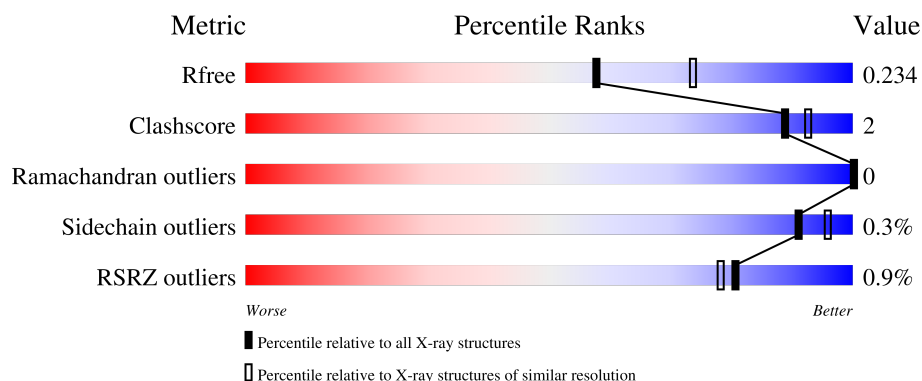
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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](#)

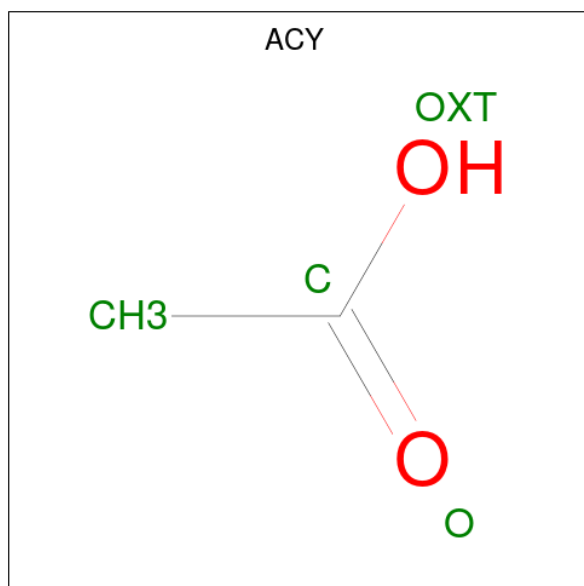
There are 6 unique types of molecules in this entry. The entry contains 7452 atoms, of which 3510 are hydrogens and 0 are deuteriums.

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	228	Total	C	H	N	O	S	0	4	0
			3569	1172	1738	309	344	6			
1	B	226	Total	C	H	N	O	S	0	1	0
			3519	1153	1710	306	344	6			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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 TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	120	Total	O	0	0
			120	120		

### 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: Fluorescent thiol-disulfide redox biosensor

Chain A: 



- Molecule 1: Fluorescent thiol-disulfide redox biosensor

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.55Å 140.43Å 130.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.11 – 2.20 35.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.11-2.20) 98.0 (35.11-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.189 , 0.234 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	23062 reflections (8.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality

### 5.1 Standard geometry

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

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	0/1858	0.25	0/2511
1	B	0.09	0/1830	0.26	0/2471
All	All	0.09	0/3688	0.26	0/4982

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	1831	1738	1783	6	0
1	B	1809	1710	1752	8	0
2	A	4	3	3	1	0
2	B	4	3	3	1	0
3	A	10	14	14	0	0
4	A	6	8	8	0	0
4	B	18	24	24	0	0
5	A	7	10	10	0	0
6	A	133	0	0	0	0
6	B	120	0	0	1	0
All	All	3942	3510	3597	13	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.

All (13) 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:70:ALA:HA	1:A:223[B]:VAL:HG13	1.76	0.68
1:B:179:ASP:OD2	2:B:304:ACY:H1	1.94	0.68
1:A:75:HIS:HB3	2:A:301:ACY:H3	1.89	0.54
1:B:70:ALA:HA	1:B:223:VAL:HG13	1.91	0.52
1:B:134:ILE:HD12	1:B:134:ILE:N	2.29	0.48
1:B:123:LEU:HD23	1:B:123:LEU:C	2.41	0.46
1:A:117:LEU:HD13	1:A:117:LEU:C	2.40	0.46
1:A:196:ASP:OD2	1:B:167:ARG:NH2	2.49	0.45
1:A:123:LEU:HD23	1:A:123:LEU:C	2.43	0.44
1:B:162:ALA:HB3	1:B:182:GLN:HB3	2.00	0.43
1:A:65:SWG:CE2	1:A:202:THR:HG21	2.50	0.42
1:B:17:GLU:HG3	6:B:425: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	226/251 (90%)	223 (99%)	3 (1%)	0	100	100
1	B	222/251 (88%)	218 (98%)	4 (2%)	0	100	100
All	All	448/502 (89%)	441 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	196/214 (92%)	195 (100%)	1 (0%)	86	93
1	B	194/214 (91%)	194 (100%)	0	100	100
All	All	390/428 (91%)	389 (100%)	1 (0%)	91	96

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

Mol	Chain	Res	Type
1	A	155	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	A	65	1	22,25,26	1.61	7 (31%)	27,35,37	2.16	9 (33%)
1	SWG	B	65	1	22,25,26	1.59	7 (31%)	27,35,37	2.20	9 (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
1	SWG	A	65	1	-	1/8/29/30	0/3/3/3
1	SWG	B	65	1	-	1/8/29/30	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	SWG	CB2-CA2	3.02	1.38	1.35
1	B	65	SWG	CB2-CA2	2.96	1.38	1.35
1	B	65	SWG	CG-CD2	2.89	1.47	1.41
1	A	65	SWG	CG-CD2	2.87	1.47	1.41
1	A	65	SWG	C1-N2	2.57	1.36	1.32
1	B	65	SWG	C1-N2	2.47	1.35	1.32
1	A	65	SWG	CA2-C2	-2.36	1.46	1.48
1	A	65	SWG	CA3-N3	-2.32	1.43	1.47
1	B	65	SWG	CA3-N3	-2.28	1.43	1.47
1	B	65	SWG	CA2-C2	-2.17	1.46	1.48
1	A	65	SWG	C2-N3	-2.07	1.35	1.40
1	B	65	SWG	C1-N3	-2.06	1.33	1.37
1	A	65	SWG	C1-N3	-2.05	1.33	1.37
1	B	65	SWG	C2-N3	-2.01	1.35	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SWG	C3-CA3-N3	5.17	124.20	112.43
1	B	65	SWG	C3-CA3-N3	5.17	124.20	112.43
1	B	65	SWG	CG-CB2-CA2	-4.48	122.22	130.86
1	A	65	SWG	C2-N3-C1	4.27	110.05	108.07
1	A	65	SWG	CG-CB2-CA2	-4.25	122.65	130.86
1	B	65	SWG	C2-N3-C1	4.22	110.02	108.07
1	B	65	SWG	CB2-CA2-C2	3.74	126.89	122.36
1	A	65	SWG	C2-CA2-N2	-3.43	106.49	108.95
1	A	65	SWG	CB2-CA2-C2	3.32	126.38	122.36
1	B	65	SWG	C2-CA2-N2	-3.25	106.62	108.95
1	A	65	SWG	CA2-C2-N3	2.51	105.61	103.50
1	B	65	SWG	CH2-CZ2-CE2	-2.46	116.73	120.09
1	A	65	SWG	CH2-CZ2-CE2	-2.43	116.77	120.09
1	B	65	SWG	CA2-C2-N3	2.30	105.43	103.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	SWG	CZ3-CH2-CZ2	2.25	123.41	120.40
1	A	65	SWG	CZ3-CH2-CZ2	2.19	123.34	120.40
1	B	65	SWG	CG-CD1-NE1	2.16	112.23	108.59
1	A	65	SWG	CG-CD1-NE1	2.13	112.19	108.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	SWG	N1-CA1-CB1-OG1
1	B	65	SWG	N1-CA1-CB1-OG1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	SWG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	GOL	A	303	-	5,5,5	0.96	0	5,5,5	1.00	0
2	ACY	A	301	-	3,3,3	0.75	0	3,3,3	0.58	0
4	GOL	B	301	-	5,5,5	0.94	0	5,5,5	1.06	0
2	ACY	B	304	-	3,3,3	0.94	0	3,3,3	0.54	0
5	PEG	A	304	-	6,6,6	0.12	0	5,5,5	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	302	-	5,5,5	0.96	0	5,5,5	1.04	0
3	PGE	A	302	-	9,9,9	0.32	0	8,8,8	0.28	0
4	GOL	B	303	-	5,5,5	0.96	0	5,5,5	1.03	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
4	GOL	A	303	-	-	4/4/4/4	-
4	GOL	B	301	-	-	2/4/4/4	-
5	PEG	A	304	-	-	2/4/4/4	-
4	GOL	B	302	-	-	2/4/4/4	-
3	PGE	A	302	-	-	5/7/7/7	-
4	GOL	B	303	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	GOL	C1-C2-C3-O3
4	B	301	GOL	O1-C1-C2-O2
4	B	301	GOL	O1-C1-C2-C3
4	A	303	GOL	O2-C2-C3-O3
4	B	303	GOL	O1-C1-C2-C3
3	A	302	PGE	O2-C3-C4-O3
5	A	304	PEG	O1-C1-C2-O2
3	A	302	PGE	O3-C5-C6-O4
4	B	302	GOL	O1-C1-C2-O2
4	B	302	GOL	O2-C2-C3-O3
5	A	304	PEG	C4-C3-O2-C2
3	A	302	PGE	C1-C2-O2-C3
3	A	302	PGE	C4-C3-O2-C2
4	A	303	GOL	O1-C1-C2-C3
3	A	302	PGE	C3-C4-O3-C5
4	A	303	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACY	1	0
2	B	304	ACY	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/251 (90%)	-0.07	3 (1%) 74 71	19, 36, 55, 82	4 (1%)
1	B	225/251 (89%)	-0.02	1 (0%) 89 87	22, 38, 59, 86	1 (0%)
All	All	452/502 (90%)	-0.04	4 (0%) 81 78	19, 37, 58, 86	5 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	LEU	4.8
1	A	172	ASP	3.0
1	B	228	ILE	2.3
1	A	229	THR	2.1

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SWG	A	65	23/24	0.94	0.09	23,28,30,35	0
1	SWG	B	65	23/24	0.94	0.09	21,29,36,37	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PGE	A	302	10/10	0.62	0.18	61,78,83,85	0
5	PEG	A	304	7/7	0.73	0.18	48,58,69,69	0
4	GOL	B	303	6/6	0.75	0.22	33,50,54,60	0
4	GOL	B	301	6/6	0.77	0.17	42,59,76,79	0
2	ACY	B	304	4/4	0.78	0.14	51,54,65,65	0
2	ACY	A	301	4/4	0.80	0.12	52,58,62,62	0
4	GOL	A	303	6/6	0.81	0.14	48,60,68,72	0
4	GOL	B	302	6/6	0.86	0.14	28,41,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.