



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:56 am BST

PDB ID : 2W18  
Title : Crystal structure of the C-terminal WD40 domain of human PALB2  
Authors : Oliver, A.W.; Pearl, L.H.  
Deposited on : 2008-10-15  
Resolution : 1.90 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.

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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 : 2.11  
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) : 2.11

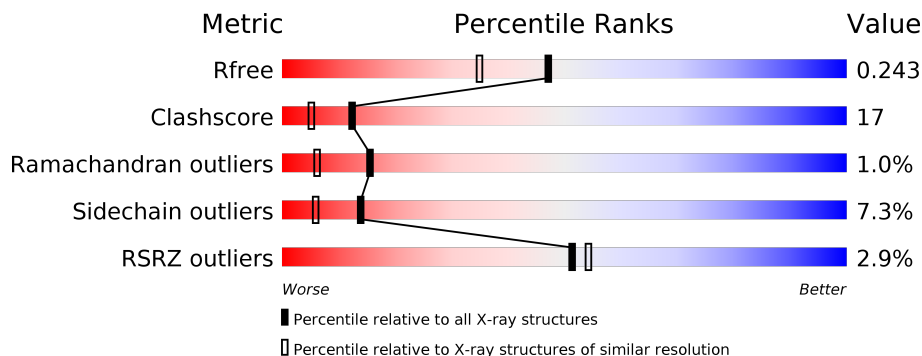
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	356	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2543 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 PARTNER AND LOCALIZER OF BRCA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2326	1510	371	427	18	0	2	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

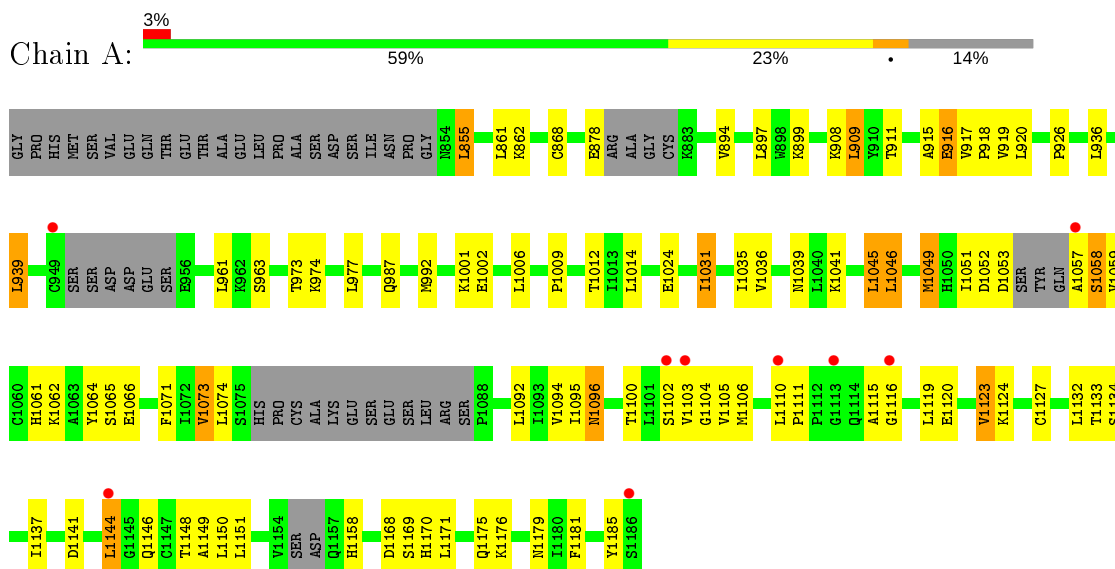
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	187	Total 187	O 187	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: PARTNER AND LOCALIZER OF BRCA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.78Å 64.65Å 77.25Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	49.27 – 1.90 49.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.27-1.90) 93.8 (49.26-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 1.90Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.209 , 0.246 0.204 , 0.243	Depositor DCC
$R_{free}$ test set	1405 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/2381	0.72	2/3243 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	861	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	1045	LEU	CA-CB-CG	5.26	127.40	115.30

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	2326	0	2293	76	0
2	A	30	0	40	6	0
3	A	187	0	0	8	0
All	All	2543	0	2333	79	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 17.

All (79) 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:1057:ALA:HA	1:A:1058:SER:HB2	1.30	1.04
1:A:1057:ALA:HA	1:A:1058:SER:CB	1.93	0.98
1:A:1014:LEU:HD21	1:A:1031:ILE:HG22	1.48	0.95
2:A:2188:GOL:H11	3:A:3182:HOH:O	1.66	0.92
1:A:1035:ILE:HG23	1:A:1051:ILE:HD11	1.53	0.91
1:A:1049:MET:HG3	1:A:1100:THR:HG23	1.55	0.88
2:A:2190:GOL:H12	3:A:3082:HOH:O	1.74	0.87
1:A:1057:ALA:CA	1:A:1058:SER:HB2	2.10	0.81
1:A:1062:LYS:HB3	1:A:1073:VAL:HG13	1.67	0.76
1:A:855:LEU:HD13	1:A:1185:TYR:HD2	1.56	0.70
1:A:1103:VAL:HB	3:A:3144:HOH:O	1.91	0.70
1:A:1141:ASP:HB3	1:A:1144:LEU:HB2	1.74	0.69
1:A:1175:GLN:HE21	1:A:1181:PHE:HE2	1.40	0.69
1:A:961:LEU:HD13	1:A:992:MET:HE1	1.77	0.66
1:A:961:LEU:HD13	1:A:992:MET:CE	2.25	0.66
2:A:2188:GOL:H12	3:A:3135:HOH:O	1.95	0.66
1:A:1124:LYS:HD3	2:A:2191:GOL:H11	1.78	0.66
1:A:1119:LEU:HD22	1:A:1133:THR:HA	1.79	0.65
1:A:1001:LYS:HG2	1:A:1002:GLU:HG2	1.77	0.65
1:A:1062:LYS:HE3	1:A:1064:TYR:CE1	2.33	0.62
1:A:868:CYS:SG	1:A:1176:LYS:HG2	2.40	0.62
1:A:1127:CYS:HB2	3:A:3187:HOH:O	1.99	0.62
1:A:862:LYS:HA	1:A:1179:ASN:OD1	2.00	0.61
1:A:1035:ILE:CG2	1:A:1051:ILE:HD11	2.31	0.59
1:A:1062:LYS:HG2	1:A:1064:TYR:CZ	2.37	0.59
1:A:919:VAL:HG22	1:A:936:LEU:CD2	2.33	0.59
1:A:1071:PHE:CD1	1:A:1094:VAL:HG22	2.39	0.58
1:A:1092:LEU:HB3	1:A:1106:MET:HB2	1.85	0.58
1:A:1035:ILE:HD11	1:A:1049:MET:HE2	1.86	0.57
1:A:894:VAL:CG2	1:A:911:THR:HG23	2.34	0.57
1:A:1168:ASP:CG	1:A:1170:HIS:HD1	2.09	0.55
1:A:1012:THR:HB	1:A:1031:ILE:HD12	1.88	0.55
1:A:1039:ASN:HB2	1:A:1046:LEU:HD11	1.87	0.54
1:A:1061:HIS:HB3	1:A:1123:VAL:HG13	1.89	0.54
1:A:899:LYS:HB2	1:A:909:LEU:HD22	1.90	0.54
1:A:908:LYS:HD3	1:A:911:THR:OG1	2.08	0.54
1:A:1095:ILE:HG12	1:A:1102:SER:CB	2.39	0.53
1:A:894:VAL:HG23	1:A:911:THR:HG23	1.91	0.52
1:A:1100:THR:O	1:A:1100:THR:HG22	2.10	0.52
1:A:1095:ILE:HG12	1:A:1102:SER:HB2	1.92	0.51
1:A:1111:PRO:HG2	1:A:1150:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LYS:HG2	1:A:1064:TYR:OH	2.11	0.50
1:A:1110:LEU:HD21	1:A:1132:LEU:HD11	1.92	0.50
1:A:1168:ASP:OD1	1:A:1170:HIS:ND1	2.31	0.50
1:A:1103:VAL:HG12	1:A:1104:GLY:O	2.13	0.48
1:A:915:ALA:O	1:A:916:GLU:CB	2.61	0.48
1:A:1169:SER:HA	2:A:2191:GOL:H12	1.96	0.48
1:A:1134:SER:O	1:A:1158:HIS:CE1	2.66	0.48
1:A:1137:ILE:HB	1:A:1151:LEU:HB3	1.95	0.48
1:A:868:CYS:SG	1:A:1176:LYS:HD3	2.54	0.48
1:A:973:THR:O	1:A:974:LYS:HB2	2.15	0.47
1:A:1144:LEU:HB3	1:A:1146:GLN:HG2	1.97	0.47
1:A:963:SER:HB3	2:A:2190:GOL:O3	2.13	0.47
1:A:1148:THR:O	1:A:1149:ALA:HB2	2.16	0.46
1:A:919:VAL:HG22	1:A:936:LEU:HD22	1.99	0.45
1:A:1024:GLU:HB2	1:A:1041:LYS:HE3	1.98	0.45
1:A:1119:LEU:HD13	1:A:1133:THR:HG22	1.99	0.44
1:A:926:PRO:HB2	1:A:973:THR:HA	2.00	0.44
1:A:1051:ILE:O	1:A:1052:ASP:C	2.54	0.44
1:A:987:GLN:OE1	1:A:1009:PRO:HD2	2.17	0.43
1:A:897:LEU:HD23	1:A:909:LEU:HB2	2.01	0.43
1:A:1041:LYS:HE3	3:A:3126:HOH:O	2.19	0.43
1:A:1062:LYS:CG	1:A:1064:TYR:CZ	3.01	0.43
1:A:1039:ASN:HB2	1:A:1046:LEU:CD1	2.48	0.43
1:A:1110:LEU:HD11	1:A:1132:LEU:HD13	2.01	0.43
1:A:1036:VAL:HB	1:A:1045:LEU:HD11	2.00	0.43
1:A:1065:SER:O	1:A:1066:GLU:HG3	2.19	0.42
1:A:1103:VAL:O	1:A:1105:VAL:HG23	2.20	0.42
1:A:961:LEU:HD13	1:A:992:MET:HE3	1.98	0.42
1:A:1175:GLN:NE2	1:A:1181:PHE:HE2	2.14	0.42
1:A:1105:VAL:O	1:A:1105:VAL:HG12	2.19	0.42
1:A:1127:CYS:CB	3:A:3187:HOH:O	2.65	0.41
1:A:1115:ALA:HA	1:A:1116:GLY:HA2	1.83	0.41
1:A:1096:ASN:ND2	3:A:3142:HOH:O	2.52	0.41
1:A:1119:LEU:HD12	1:A:1119:LEU:HA	1.78	0.41
1:A:1096:ASN:O	1:A:1100:THR:N	2.53	0.40
1:A:917:VAL:HA	1:A:918:PRO:HD3	1.80	0.40
1:A:1035:ILE:HG12	1:A:1049:MET:HB3	2.04	0.40
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.50	0.40

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	296/356 (83%)	280 (95%)	13 (4%)	3 (1%)	15   6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1058	SER
1	A	916	GLU
1	A	939	LEU

### 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	250/308 (81%)	232 (93%)	18 (7%)	14   6

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	855	LEU
1	A	878	GLU
1	A	909	LEU
1	A	920	LEU
1	A	939	LEU
1	A	977	LEU
1	A	1006	LEU
1	A	1031	ILE

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Mol	Chain	Res	Type
1	A	1046	LEU
1	A	1049	MET
1	A	1059	VAL
1	A	1073	VAL
1	A	1074	LEU
1	A	1096	ASN
1	A	1120	GLU
1	A	1123	VAL
1	A	1144	LEU
1	A	1171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1004	GLN
1	A	1044	GLN
1	A	1096	ASN
1	A	1114	GLN
1	A	1158	HIS
1	A	1175	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 carbohydrates 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 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	GOL	A	2191	-	5,5,5	0.34	0	5,5,5	0.47	0
2	GOL	A	2189	-	5,5,5	0.31	0	5,5,5	0.38	0
2	GOL	A	2190	-	5,5,5	0.47	0	5,5,5	0.54	0
2	GOL	A	2188	-	5,5,5	0.50	0	5,5,5	0.95	0
2	GOL	A	2187	-	5,5,5	0.39	0	5,5,5	0.70	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	GOL	A	2191	-	-	0/4/4/4	-
2	GOL	A	2189	-	-	4/4/4/4	-
2	GOL	A	2190	-	-	2/4/4/4	-
2	GOL	A	2188	-	-	4/4/4/4	-
2	GOL	A	2187	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2189	GOL	O1-C1-C2-C3
2	A	2190	GOL	O1-C1-C2-C3
2	A	2188	GOL	O1-C1-C2-C3
2	A	2189	GOL	O1-C1-C2-O2
2	A	2189	GOL	C1-C2-C3-O3
2	A	2189	GOL	O2-C2-C3-O3
2	A	2190	GOL	O1-C1-C2-O2
2	A	2188	GOL	O1-C1-C2-O2
2	A	2188	GOL	O2-C2-C3-O3
2	A	2188	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2191	GOL	2	0
2	A	2190	GOL	2	0
2	A	2188	GOL	2	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	306/356 (85%)	0.04	9 (2%) 51 54	18, 35, 56, 76	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1113	GLY	3.8
1	A	1144	LEU	3.3
1	A	1057	ALA	3.0
1	A	1103	VAL	2.8
1	A	1102	SER	2.8
1	A	1116	GLY	2.7
1	A	949	CYS	2.5
1	A	1110	LEU	2.2
1	A	1186	SER	2.1

### 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	2189	6/6	0.85	0.14	37,47,48,48	0
2	GOL	A	2191	6/6	0.86	0.37	42,51,55,58	0
2	GOL	A	2190	6/6	0.88	0.17	36,41,43,45	0
2	GOL	A	2187	6/6	0.92	0.10	37,39,43,47	0
2	GOL	A	2188	6/6	0.94	0.13	23,35,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.