



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 AM GMT

PDB ID : 2R1Z  
Title : Crystal Structure of the BARD1 BRCT Repeat  
Authors : Lee, M.S.; Edwards, R.A.; Williams, R.S.; Glover, M.J.N.  
Deposited on : 2007-08-23  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

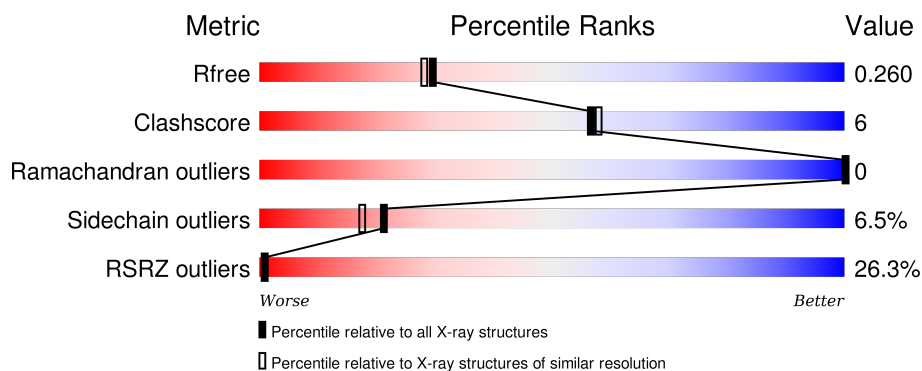
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	209	<div> <div>26%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>
1	B	209	<div> <div>26%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	801	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3439 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 BRCA1-associated RING domain protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	1	0
			1630	1046	279	294	11			
1	B	208	Total	C	N	O	S	0	0	0
			1682	1081	288	302	11			

- 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

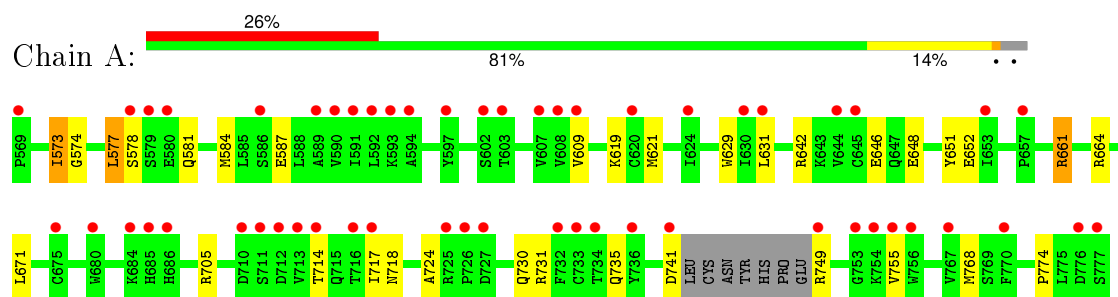
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	58	Total 58	O 58	0	0

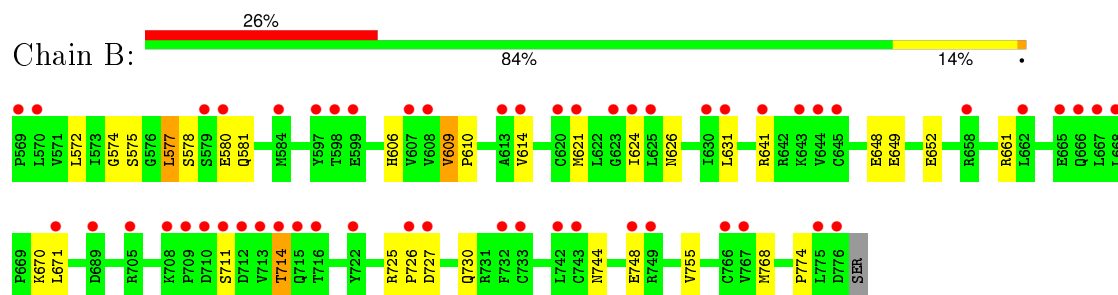
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: BRCA1-associated RING domain protein 1



- Molecule 1: BRCA1-associated RING domain protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.82Å 75.55Å 117.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.10 27.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.49-2.10) 95.0 (27.76-2.10)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.222 , 0.262 0.220 , 0.260	Depositor DCC
$R_{free}$ test set	1445 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28782 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	3/1673 (0.2%)	0.60	0/2259
1	B	0.43	0/1724	0.59	0/2333
All	All	0.48	3/3397 (0.1%)	0.60	0/4592

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	GLU	CD-OE2	6.76	1.33	1.25
1	A	587	GLU	CD-OE1	6.38	1.32	1.25
1	A	587	GLU	CG-CD	5.90	1.60	1.51

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	A	1630	0	1650	22	0
1	B	1682	0	1696	19	0
2	A	6	0	8	0	0
2	B	6	0	8	2	0
3	A	57	0	0	0	0
3	B	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3439	0	3362	41	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 6.

All (41) 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:B:621:MET:HG2	1:B:768:MET:HE3	1.56	0.87
1:B:621:MET:HG2	1:B:768:MET:CE	2.04	0.86
1:A:730:GLN:HE22	1:A:774:PRO:HA	1.54	0.73
1:A:714:THR:HG23	1:A:735:GLN:OE1	1.97	0.65
1:B:578:SER:H	1:B:581:GLN:HE21	1.46	0.64
1:B:730:GLN:HE22	1:B:774:PRO:HA	1.63	0.64
1:A:578:SER:H	1:A:581:GLN:HE21	1.46	0.64
1:A:621:MET:HG2	1:A:768:MET:CE	2.29	0.62
1:B:575:SER:O	1:B:610:PRO:HD3	1.98	0.62
1:B:670:LYS:HE3	2:B:802:GOL:H11	1.81	0.61
1:B:621:MET:HG2	1:B:768:MET:HE1	1.82	0.61
1:A:724:ALA:HB3	1:A:731:ARG:HD2	1.83	0.59
1:B:711:SER:HB3	1:B:714:THR:HG23	1.85	0.59
1:A:621:MET:HG2	1:A:768:MET:HE1	1.90	0.53
1:B:574:GLY:HA3	1:B:577:LEU:HD22	1.92	0.51
1:A:621:MET:HG2	1:A:768:MET:HE3	1.91	0.51
1:B:670:LYS:HE3	2:B:802:GOL:C1	2.41	0.51
1:B:730:GLN:NE2	1:B:774:PRO:HA	2.27	0.50
1:B:572:LEU:HD23	1:B:606:HIS:HB2	1.94	0.50
1:A:652:GLU:OE2	1:A:661:ARG:HD3	2.13	0.49
1:A:629:TRP:CZ3	1:A:661:ARG:HD2	2.48	0.48
1:A:574:GLY:HA3	1:A:577:LEU:HD22	1.94	0.48
1:A:646:GLU:HG3	1:A:651:TYR:CE1	2.49	0.47
1:B:578:SER:H	1:B:581:GLN:NE2	2.12	0.47
1:B:631:LEU:HD21	1:B:648:GLU:HB2	1.97	0.47
1:A:646:GLU:CG	1:A:651:TYR:CE1	2.98	0.46
1:B:609:VAL:HG13	3:B:43:HOH:O	2.16	0.45
1:A:646:GLU:HG2	1:A:651:TYR:CZ	2.51	0.45
1:A:717:ILE:HD13	1:A:717:ILE:HA	1.81	0.45
1:A:730:GLN:NE2	1:A:774:PRO:HA	2.25	0.45
1:A:646:GLU:HG3	1:A:651:TYR:HE1	1.82	0.45
1:A:581:GLN:HA	1:A:584:MET:HE3	1.98	0.44
1:B:768:MET:HA	1:B:768:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:TRP:CD2	1:A:648:GLU:HG3	2.54	0.43
1:A:631:LEU:HD21	1:A:648:GLU:HB2	2.01	0.43
1:B:725:ARG:HA	1:B:726:PRO:HD3	1.88	0.43
1:B:614:VAL:HG21	1:B:624:ILE:HD11	2.02	0.41
1:A:573:ILE:HD12	1:A:619:LYS:HD3	2.02	0.41
1:A:629:TRP:CE2	1:A:648:GLU:HG3	2.56	0.41
1:A:577:LEU:HG	1:A:581:GLN:HB3	2.03	0.40
1:B:652:GLU:OE2	1:B:661:ARG:HD3	2.22	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	199/209 (95%)	195 (98%)	4 (2%)	0	100	100
1	B	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
All	All	405/418 (97%)	393 (97%)	12 (3%)	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	183/189 (97%)	171 (93%)	12 (7%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	188/189 (100%)	176 (94%)	12 (6%)	22	18
All	All	371/378 (98%)	347 (94%)	24 (6%)	21	17

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	ILE
1	A	577	LEU
1	A	609	VAL
1	A	642	ARG
1	A	661	ARG
1	A	664	ARG
1	A	671	LEU
1	A	705	ARG
1	A	718	ASN
1	A	741	ASP
1	A	749	ARG
1	A	755	VAL
1	B	577	LEU
1	B	580	GLU
1	B	609	VAL
1	B	626	ASN
1	B	641	ARG
1	B	649	GLU
1	B	671	LEU
1	B	714	THR
1	B	727	ASP
1	B	744	ASN
1	B	748	GLU
1	B	755	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	GLN
1	A	626	ASN
1	A	663	ASN
1	A	690	ASN
1	A	718	ASN
1	A	730	GLN
1	A	752	GLN

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Mol	Chain	Res	Type
1	B	581	GLN
1	B	690	ASN
1	B	730	GLN
1	B	744	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](#)

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](#)

2 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	801	-	5,5,5	0.32	0	5,5,5	0.35	0
2	GOL	B	802	-	5,5,5	0.27	0	5,5,5	0.25	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	801	-	-	0/4/4/4	0/0/0/0
2	GOL	B	802	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	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

### 6.1 Protein, DNA and RNA chains

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	202/209 (96%)	1.42	54 (26%)  	37, 46, 61, 70	0
1	B	208/209 (99%)	1.48	54 (25%)  	37, 46, 56, 65	0
All	All	410/418 (98%)	1.45	108 (26%)  	37, 46, 60, 70	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	SER	9.4
1	B	712	ASP	8.3
1	B	710	ASP	6.4
1	B	709	PRO	5.2
1	B	667	LEU	5.2
1	B	607	VAL	4.9
1	B	624	ILE	4.9
1	B	644	VAL	4.8
1	A	685	HIS	4.6
1	B	625	LEU	4.6
1	A	727	ASP	4.6
1	A	716	THR	4.6
1	A	591	ILE	4.5
1	A	712	ASP	4.5
1	A	644	VAL	4.4
1	A	630	ILE	4.3
1	B	713	VAL	4.2
1	B	569	PRO	4.2
1	B	630	ILE	4.1
1	B	570	LEU	4.1
1	B	579	SER	3.9
1	A	741	ASP	3.8
1	A	578	SER	3.7
1	B	767	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	716	THR	3.7
1	B	614	VAL	3.6
1	B	598	THR	3.6
1	A	579	SER	3.6
1	A	569	PRO	3.5
1	B	711	SER	3.5
1	A	726	PRO	3.5
1	A	733	CYS	3.5
1	B	665	GLU	3.5
1	B	705	ARG	3.4
1	B	645	CYS	3.4
1	B	597	TYR	3.4
1	B	722	TYR	3.4
1	B	620	CYS	3.4
1	A	590	VAL	3.4
1	B	666	GLN	3.4
1	A	586	SER	3.3
1	A	717	ILE	3.3
1	B	776	ASP	3.3
1	A	602	SER	3.2
1	A	749	ARG	3.1
1	B	580	GLU	3.1
1	A	645	CYS	3.1
1	A	710	ASP	3.1
1	A	594	ALA	3.0
1	A	684	LYS	3.0
1	B	643	LYS	3.0
1	B	608	VAL	3.0
1	B	733	CYS	2.9
1	A	732	PHE	2.9
1	A	755	VAL	2.9
1	A	736	TYR	2.9
1	A	597	TYR	2.9
1	B	599	GLU	2.9
1	A	776	ASP	2.9
1	B	668	LEU	2.9
1	B	715	GLN	2.8
1	B	708	LYS	2.8
1	A	653	ILE	2.8
1	B	662	LEU	2.8
1	A	631	LEU	2.7
1	A	713	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	743	CYS	2.6
1	A	603	THR	2.5
1	B	749	ARG	2.5
1	A	592	LEU	2.5
1	B	742	LEU	2.5
1	A	711	SER	2.5
1	A	657	PRO	2.5
1	B	689	ASP	2.5
1	B	621	MET	2.5
1	B	631	LEU	2.5
1	A	767	VAL	2.5
1	A	725	ARG	2.5
1	B	584	MET	2.4
1	A	754	LYS	2.4
1	A	620[A]	CYS	2.4
1	B	658	ARG	2.4
1	B	732	PHE	2.4
1	A	580	GLU	2.4
1	A	753	GLY	2.4
1	A	756	TRP	2.4
1	A	608	VAL	2.3
1	B	613	ALA	2.3
1	B	775	LEU	2.3
1	B	727	ASP	2.3
1	A	686	HIS	2.3
1	B	714	THR	2.3
1	A	593	LYS	2.3
1	B	641	ARG	2.2
1	B	726	PRO	2.2
1	A	624	ILE	2.2
1	A	589	ALA	2.2
1	A	714	THR	2.2
1	B	766	CYS	2.1
1	B	671	LEU	2.1
1	A	675	CYS	2.1
1	A	680	TRP	2.1
1	A	609	VAL	2.1
1	A	734	THR	2.0
1	A	770	PHE	2.0
1	A	607	VAL	2.0
1	B	623	GLY	2.0
1	B	748	GLU	2.0



## 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	801	6/6	0.95	0.27	2.03	48,48,49,51	0
2	GOL	B	802	6/6	0.69	0.34	1.56	46,47,48,48	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.