



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:09 PM UTC

PDB ID : 2R1Z / pdb_00002r1z
Title : Crystal Structure of the BARD1 BRCT Repeat
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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

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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

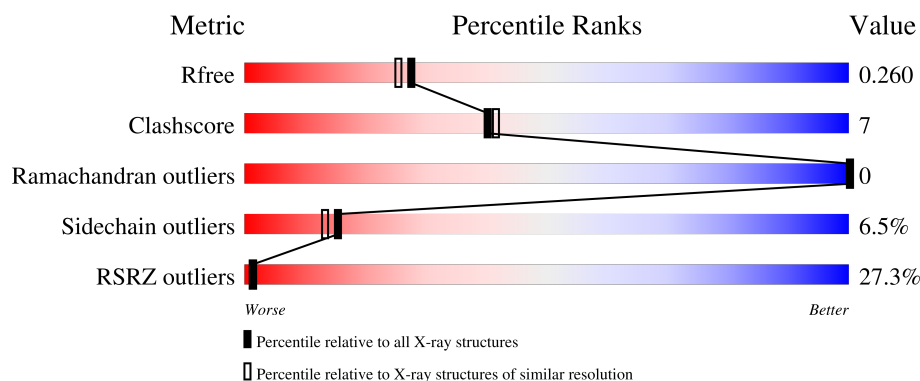
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	209	39% 81%12%••
1	B	209	15% 83%14%•

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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

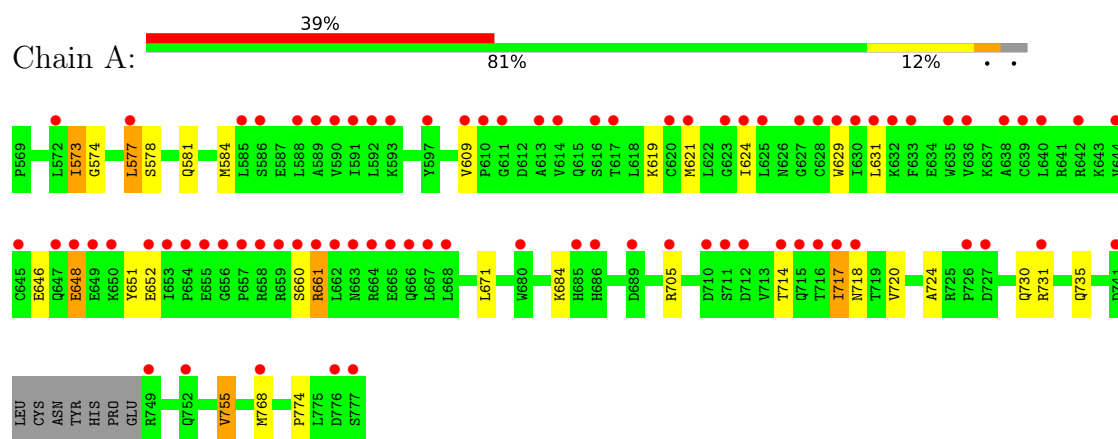
- Molecule 3 is water.

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

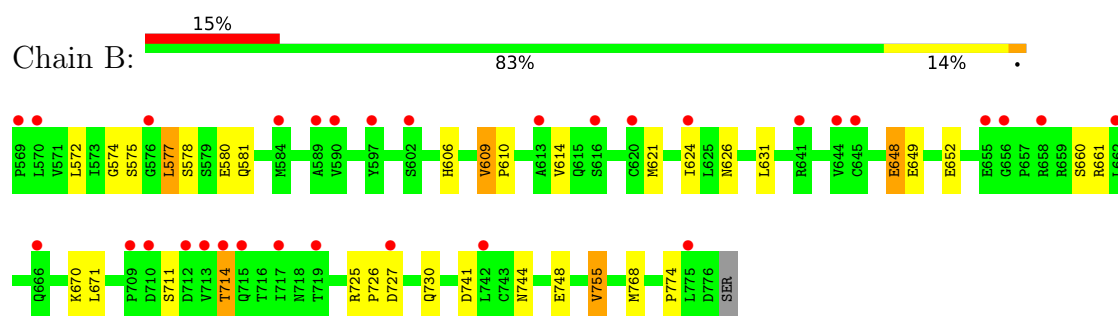
3 Residue-property plots

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: 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, α , β , γ	56.82Å 75.55Å 117.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.10 29.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.49-2.10) 94.9 (29.49-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.262 0.221 , 0.260	Depositor DCC
R_{free} test set	1445 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3439	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [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	0.62	0/1673	0.85	1/2259 (0.0%)
1	B	0.56	0/1724	0.84	2/2333 (0.1%)
All	All	0.59	0/3397	0.84	3/4592 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	741	ASP	N-CA-C	-6.14	100.00	109.76
1	A	755	VAL	N-CA-C	6.02	116.54	107.75
1	B	755	VAL	N-CA-C	5.20	115.46	108.17

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	23	0
1	B	1682	0	1696	21	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	44	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.

All (44) 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	1.44	0.96
1:A:621:MET:HG2	1:A:768:MET:HE3	1.56	0.88
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:768:MET:HA	1:A:768:MET:HE2	1.70	0.72
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:A:578:SER:H	1:A:581:GLN:HE21	1.46	0.64
1:B:730:GLN:HE22	1:B:774:PRO:HA	1.63	0.64
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:A:621:MET:HG2	1:A:768:MET:CE	2.29	0.60
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:B:621:MET:CG	1:B:768:MET:HE3	2.28	0.55
1:B:574:GLY:HA3	1:B:577:LEU:HD22	1.92	0.51
1:B:670:LYS:HE3	2:B:802:GOL:C1	2.41	0.51
1:B:768:MET:HA	1:B:768:MET:HE2	1.94	0.50
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:581:GLN:HA	1:A:584:MET:HE3	1.95	0.49
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:646:GLU:HG3	1:A:651:TYR:HE1	1.82	0.45
1:A:730:GLN:NE2	1:A:774:PRO:HA	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:ILE:O	1:B:660:SER:OG	2.35	0.43
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:A:573:ILE:HD12	1:A:619:LYS:HD3	2.02	0.41
1:B:614:VAL:HG21	1:B:624:ILE:HD11	2.02	0.41
1:A:624:ILE:O	1:A:660:SER:OG	2.36	0.41
1:A:629:TRP:CE2	1:A:648:GLU:HG3	2.56	0.41
1:B:621:MET:HG2	1:B:768:MET:HE1	1.95	0.40
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%)	15	13
1	B	188/189 (100%)	176 (94%)	12 (6%)	16	14
All	All	371/378 (98%)	347 (94%)	24 (6%)	15	13

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	648	GLU
1	A	661	ARG
1	A	671	LEU
1	A	684	LYS
1	A	705	ARG
1	A	717	ILE
1	A	718	ASN
1	A	720	VAL
1	A	755	VAL
1	B	577	LEU
1	B	580	GLU
1	B	609	VAL
1	B	626	ASN
1	B	648	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	GLN
1	A	615	GLN
1	A	626	ASN
1	A	663	ASN
1	A	690	ASN
1	A	718	ASN

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Mol	Chain	Res	Type
1	A	730	GLN
1	A	752	GLN
1	B	581	GLN
1	B	626	ASN
1	B	690	ASN
1	B	730	GLN
1	B	744	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.33	0	5,5,5	0.38	0
2	GOL	B	802	-	5,5,5	0.31	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	-
2	GOL	B	802	-	-	0/4/4/4	-

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, 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	202/209 (96%)	1.80	81 (40%)	0 1	37, 46, 61, 70	1 (0%)
1	B	208/209 (99%)	1.19	31 (14%)	5 5	37, 46, 56, 65	0
All	All	410/418 (98%)	1.49	112 (27%)	1 1	37, 46, 60, 70	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	668	LEU	7.3
1	A	777	SER	5.9
1	A	656	GLY	5.2
1	A	657	PRO	5.2
1	A	591	ILE	5.0
1	A	660	SER	4.9
1	A	716	THR	4.8
1	A	629	TRP	4.8
1	B	570	LEU	4.8
1	B	742	LEU	4.8
1	A	624	ILE	4.7
1	A	590	VAL	4.5
1	A	654	PRO	4.3
1	A	712	ASP	4.3
1	A	655	GLU	4.2
1	A	717	ILE	4.2
1	A	661	ARG	4.1
1	A	663	ASN	4.0
1	A	662	LEU	4.0
1	A	666	GLN	4.0
1	B	569	PRO	3.9
1	A	664	ARG	3.9
1	A	667	LEU	3.9
1	A	649	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	589	ALA	3.7
1	A	627	GLY	3.7
1	A	609	VAL	3.7
1	B	645	CYS	3.6
1	B	613	ALA	3.6
1	A	644	VAL	3.5
1	A	653	ILE	3.4
1	A	625	LEU	3.4
1	A	726	PRO	3.3
1	A	647	GLN	3.3
1	A	714	THR	3.3
1	A	640	LEU	3.3
1	A	592	LEU	3.2
1	B	602	SER	3.2
1	B	710	ASP	3.1
1	B	714	THR	3.1
1	A	635	TRP	3.1
1	A	727	ASP	3.1
1	A	586	SER	3.0
1	B	709	PRO	3.0
1	B	712	ASP	3.0
1	A	633	PHE	3.0
1	A	645	CYS	2.9
1	A	710	ASP	2.9
1	A	659	ARG	2.9
1	B	775	LEU	2.8
1	A	623	GLY	2.8
1	A	628	CYS	2.8
1	A	650	LYS	2.8
1	A	577	LEU	2.8
1	A	588	LEU	2.8
1	A	632	LYS	2.7
1	A	705	ARG	2.7
1	B	662	LEU	2.6
1	A	610	PRO	2.6
1	A	585	LEU	2.6
1	A	711	SER	2.6
1	A	741	ASP	2.6
1	A	642	ARG	2.6
1	B	620	CYS	2.6
1	B	715	GLN	2.6
1	A	680	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	624	ILE	2.5
1	A	621	MET	2.5
1	B	713	VAL	2.5
1	A	718	ASN	2.5
1	A	611	GLY	2.5
1	B	576	GLY	2.5
1	A	620[A]	CYS	2.4
1	B	589	ALA	2.4
1	A	631	LEU	2.4
1	A	658	ARG	2.4
1	B	656	GLY	2.4
1	A	652	GLU	2.4
1	A	715	GLN	2.4
1	B	644	VAL	2.4
1	A	638	ALA	2.4
1	A	648	GLU	2.4
1	A	639	CYS	2.4
1	A	597	TYR	2.3
1	B	655	GLU	2.3
1	A	776	ASP	2.3
1	A	752	GLN	2.3
1	A	613	ALA	2.3
1	A	749	ARG	2.3
1	A	614	VAL	2.3
1	B	717	ILE	2.2
1	A	689	ASP	2.2
1	A	665	GLU	2.2
1	B	666	GLN	2.2
1	B	597	TYR	2.2
1	A	630	ILE	2.2
1	A	685	HIS	2.2
1	A	572	LEU	2.2
1	B	584	MET	2.2
1	B	727	ASP	2.2
1	B	641	ARG	2.1
1	B	658	ARG	2.1
1	A	593	LYS	2.1
1	A	616	SER	2.1
1	A	768	MET	2.1
1	B	590	VAL	2.1
1	A	617	THR	2.1
1	A	636	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	616	SER	2.1
1	A	686	HIS	2.0
1	A	731	ARG	2.0
1	B	719	THR	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 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	802	6/6	0.69	0.22	46,47,48,48	6
2	GOL	A	801	6/6	0.83	0.25	48,48,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.