

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2NTE
Title	:	Crystal Structure of the BARD1 BRCT Domains
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Deposited on	:	2006-11-07
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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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))		
Rfree	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 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 <=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		
			27%		
1	А	210	82%	15%	•
			29%		
1	В	210	80%	17%	•

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
3	CL	В	305	-	-	Х	-
4	EDO	В	308	-	-	-	Х



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3653 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	Δ	210	Total	С	Ν	0	\mathbf{S}	0	0	0
1		210	1693	1086	290	306	11	0		
1	В	200	Total	С	Ν	0	S	0	0	0
	D	209	1689	1084	289	305	11	0	0	0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0
3	В	2	Total Cl 2 2	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	133	Total O 133 133	0	2
5	В	105	Total O 105 105	0	0



3 Residue-property plots (i)

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





L772 L773 P774 L775 L775 D776 S777



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	57.44Å 75.80Å 116.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	19.87 - 1.90	Depositor
	19.86 - 1.90	EDS
% Data completeness	93.8 (19.87-1.90)	Depositor
(in resolution range)	93.8 (19.86-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$4.57 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.196 , 0.247	Depositor
II, II, <i>free</i>	0.200 , 0.255	DCC
R_{free} test set	1910 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	32.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.34 , 53.7	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3653	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: EDO, SO4, CL

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		Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.09	3/1735~(0.2%)	0.97	4/2347~(0.2%)	
1	В	1.01	1/1731~(0.1%)	0.87	0/2341	
All	All	1.05	4/3466~(0.1%)	0.92	4/4688~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	620	CYS	CB-SG	-6.61	1.71	1.82
1	А	728	SER	CB-OG	5.52	1.49	1.42
1	А	676	TYR	CD1-CE1	-5.17	1.31	1.39
1	А	736	TYR	CE1-CZ	-5.14	1.31	1.38

All (4) bond length outliers are listed below:

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	А	612	ASP	CB-CG-OD1	6.16	123.84	118.30
1	А	741	ASP	CB-CG-OD2	6.00	123.70	118.30
1	А	658	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	А	658	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	776	ASP	Peptide

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	А	1693	0	1703	31	0
1	В	1689	0	1701	36	0
2	А	5	0	0	0	0
2	В	5	0	0	1	0
3	А	1	0	0	0	0
3	В	2	0	0	2	0
4	А	12	0	18	4	0
4	В	8	0	12	3	0
5	А	133	0	0	3	0
5	В	105	0	0	6	0
All	All	3653	0	3434	67	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 10.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:614:VAL:HG23	1:A:653:ILE:HG21	1.32	1.10
1:B:701:GLN:HE21	4:B:308:EDO:H11	0.93	1.10
1:B:714:THR:HG22	5:B:214:HOH:O	1.60	1.00
1:B:701:GLN:NE2	4:B:308:EDO:H11	1.79	0.96
1:B:701:GLN:HE21	4:B:308:EDO:C1	1.83	0.88
1:A:587:GLU:O	1:A:590:VAL:HG23	1.79	0.81
1:B:609:VAL:HG21	1:B:653:ILE:HD11	1.71	0.72
1:A:730:GLN:HE22	1:A:774:PRO:HA	1.57	0.69
1:B:711:SER:O	1:B:712:ASP:C	2.34	0.66
1:A:664:ARG:HG3	1:A:664:ARG:NH1	2.12	0.64
1:B:712:ASP:O	1:B:716:THR:HG23	1.99	0.63
1:B:587:GLU:O	1:B:590:VAL:HG22	1.99	0.62
1:A:724:ALA:HB3	1:A:731:ARG:HD2	1.82	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:572:LEU:HD12	1:A:606:HIS:HB2	1.84	0.59
1:B:771:GLU:HG2	1:B:773:LEU:HD23	1.84	0.59
1:A:664:ARG:HH11	1:A:664:ARG:CG	2.16	0.59
1:B:609:VAL:HG21	1:B:653:ILE:CD1	2.32	0.58
1:B:609:VAL:CG2	1:B:653:ILE:HD11	2.33	0.58
1:A:587:GLU:O	1:A:590:VAL:CG2	2.51	0.58
1:A:743:CYS:SG	1:A:745:TYR:HB3	2.42	0.58
1:B:708:LYS:H	1:B:714:THR:HG21	1.69	0.58
1:A:692:ILE:O	1:A:696:THR:HG23	2.04	0.57
1:B:570:LEU:HD22	1:B:606:HIS:HE1	1.68	0.57
1:A:664:ARG:HG3	1:A:664:ARG:HH11	1.69	0.57
1:A:590:VAL:HG23	5:A:54:HOH:O	2.05	0.56
1:A:776:ASP:OD1	1:A:777:SER:OG	2.23	0.56
1:A:642:ARG:HB2	1:A:644:VAL:HG12	1.89	0.55
1:B:570:LEU:HD22	1:B:606:HIS:CE1	2.42	0.54
1:B:709:PRO:O	1:B:710:ASP:OD1	2.26	0.53
1:B:667:LEU:CD1	1:B:667:LEU:N	2.71	0.52
1:A:664:ARG:NH1	1:A:664:ARG:CG	2.73	0.51
1:A:627:GLY:HA3	1:A:664:ARG:HG2	1.93	0.51
1:B:693:LYS:NZ	5:B:144:HOH:O	2.31	0.51
1:B:626:ASN:HB2	5:B:56:HOH:O	2.11	0.51
1:B:619:LYS:NZ	2:B:301:SO4:O1	2.44	0.50
1:B:621:MET:HE3	1:B:767:VAL:HB	1.93	0.50
1:A:634:GLU:HG3	5:A:53:HOH:O	2.11	0.50
1:A:614:VAL:CG2	1:A:653:ILE:HG21	2.23	0.49
1:A:640:LEU:O	1:A:643:LYS:NZ	2.28	0.49
1:A:621:MET:CE	4:A:310:EDO:H12	2.43	0.48
1:B:711:SER:O	1:B:713:VAL:N	2.46	0.48
1:B:579:SER:O	1:B:583:LYS:HG3	2.14	0.48
1:B:710:ASP:HA	3:B:305:CL:CL	2.52	0.46
1:B:730:GLN:HE22	1:B:774:PRO:HA	1.80	0.46
1:B:661:ARG:O	1:B:665:GLU:HG3	2.16	0.46
1:A:632:LYS:HD3	1:A:634:GLU:CD	2.36	0.45
1:B:715:GLN:HB2	3:B:305:CL:CL	2.52	0.45
1:B:745:TYR:OH	5:B:111:HOH:O	2.20	0.45
1:B:621:MET:HE3	1:B:767:VAL:CG1	2.47	0.45
1:A:730:GLN:NE2	1:A:774:PRO:HA	2.27	0.45
1:A:703:LEU:HD22	4:A:309:EDO:H22	1.99	0.44
1:A:590:VAL:CG2	5:A:54:HOH:O	2.63	0.43
1:A:621:MET:HE1	4:A:310:EDO:H12	1.99	0.43
1:A:587:GLU:HG2	1:A:640:LEU:HD21	2.00	0.43



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLU:H	1:A:748:GLU:CD	2.22	0.43
1:B:693:LYS:CE	5:B:144:HOH:O	2.66	0.43
1:B:708:LYS:N	1:B:714:THR:HG21	2.32	0.43
1:B:665:GLU:O	1:B:667:LEU:HD13	2.19	0.42
1:B:621:MET:HE3	1:B:767:VAL:HG11	2.02	0.42
1:A:632:LYS:HD3	1:A:634:GLU:OE1	2.19	0.42
1:B:601:ASP:HB3	1:B:603:THR:H	1.85	0.42
1:A:586:SER:O	1:A:590:VAL:HG22	2.19	0.41
1:A:713:VAL:HG22	4:A:307:EDO:O2	2.20	0.41
1:B:686:HIS:O	1:B:687:PRO:C	2.59	0.41
1:A:587:GLU:HG2	1:A:640:LEU:CD2	2.51	0.41
1:B:777:SER:HB3	5:B:116:HOH:O	2.20	0.41
1:B:667:LEU:N	1:B:667:LEU:HD12	2.36	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	А	208/210~(99%)	204 (98%)	3~(1%)	1 (0%)	29 18
1	В	207/210~(99%)	202~(98%)	3~(1%)	2(1%)	15 6
All	All	415/420 (99%)	406 (98%)	6 (1%)	3 (1%)	22 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	710	ASP
1	В	712	ASP
1	А	655	GLU



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	189/189~(100%)	180~(95%)	9~(5%)	25 16
1	В	189/189~(100%)	181 (96%)	8 (4%)	30 20
All	All	378/378~(100%)	361~(96%)	17 (4%)	27 18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	572	LEU
1	А	590	VAL
1	А	593	LYS
1	А	632	LYS
1	А	643	LYS
1	А	664	ARG
1	А	713	VAL
1	А	741	ASP
1	А	744	ASN
1	В	572	LEU
1	В	580	GLU
1	В	601	ASP
1	В	619	LYS
1	В	637	LYS
1	В	667	LEU
1	В	711	SER
1	В	727	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	663	ASN
1	А	686	HIS
1	А	690	ASN
1	А	730	GLN
1	А	744	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	В	663	ASN
1	В	701	GLN
1	В	730	GLN
1	В	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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).

Mal	Type	Chain	Dog	Tink	B	ond leng	$_{ m gths}$	E	Bond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	А	307	-	3,3,3	0.29	0	2,2,2	0.19	0
4	EDO	В	308	-	3,3,3	0.58	0	2,2,2	1.23	0
4	EDO	А	309	-	3,3,3	1.19	0	2,2,2	1.61	0
4	EDO	А	310	-	3,3,3	0.52	0	2,2,2	0.77	0
2	SO4	А	302	-	4,4,4	0.25	0	6,6,6	0.98	1 (16%)
2	SO4	В	301	1	4,4,4	0.22	0	$6,\!6,\!6$	1.09	0
4	EDO	В	311	-	3,3,3	1.14	0	2,2,2	0.18	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	EDO	А	307	-	-	0/1/1/1	-
4	EDO	В	308	-	-	1/1/1/1	-
4	EDO	А	309	-	-	0/1/1/1	-
4	EDO	А	310	-	-	1/1/1/1	-
4	EDO	В	311	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	302	SO4	O4-S-O3	2.05	117.80	109.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	308	EDO	O1-C1-C2-O2
4	А	310	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	307	EDO	1	0
4	В	308	EDO	3	0
4	А	309	EDO	1	0
4	А	310	EDO	2	0
2	В	301	SO4	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^{th} 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	$\langle RSRZ \rangle$	# RSRZ	Z>2	2	$OWAB(Å^2)$	Q<0.9
1	А	210/210~(100%)	1.57	56 (26%)	0	0	41, 50, 66, 78	0
1	В	209/210~(99%)	1.50	61 (29%)	0	0	36, 50, 61, 66	0
All	All	419/420 (99%)	1.53	117 (27%)	0	0	36, 50, 63, 78	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	743	CYS	16.1
1	А	744	ASN	13.3
1	А	742	LEU	11.2
1	А	777	SER	8.5
1	В	712	ASP	8.4
1	А	726	PRO	6.5
1	А	569	PRO	6.4
1	В	569	PRO	6.0
1	А	585	LEU	5.9
1	В	608	VAL	5.8
1	А	608	VAL	5.7
1	В	777	SER	5.7
1	В	579	SER	5.6
1	В	713	VAL	5.4
1	А	745	TYR	5.3
1	В	607	VAL	5.2
1	В	710	ASP	5.0
1	А	631	LEU	5.0
1	А	630	ILE	4.9
1	В	636	VAL	4.9
1	В	578	SER	4.8
1	A	685	HIS	4.6
1	A	609	VAL	4.6
1	Α	572	LEU	4.6



Mol	Chain	Res	Type	RSRZ
1	В	599	GLU	4.4
1	В	711	SER	4.4
1	А	727	ASP	4.4
1	А	580	GLU	4.4
1	А	607	VAL	4.4
1	В	709	PRO	4.3
1	В	598	THR	4.3
1	А	568	GLY	4.1
1	В	602	SER	3.9
1	А	636	VAL	3.8
1	В	580	GLU	3.8
1	А	741	ASP	3.7
1	А	748	GLU	3.7
1	В	585	LEU	3.6
1	В	726	PRO	3.6
1	В	630	ILE	3.6
1	В	737	ILE	3.6
1	А	588	LEU	3.6
1	А	767	VAL	3.4
1	В	625	LEU	3.4
1	А	625	LEU	3.4
1	В	738	ILE	3.3
1	В	588	LEU	3.3
1	А	597	TYR	3.3
1	А	776	ASP	3.3
1	А	746	HIS	3.2
1	В	631	LEU	3.2
1	А	624	ILE	3.2
1	В	736	TYR	3.2
1	А	747	PRO	3.2
1	В	577	LEU	3.1
1	А	583	LYS	3.1
1	В	635	TRP	3.0
1	В	570	LEU	3.0
1	A	623	GLY	2.9
1	А	620	CYS	2.9
1	А	655	GLU	2.9
1	В	597	TYR	2.9
1	A	772	LEU	2.9
1	В	671	LEU	2.9
1	В	645	CYS	2.8
1	В	749	ARG	2.7



Mol	Chain	Res	Type	RSRZ
1	В	592	LEU	2.7
1	В	658	ARG	2.7
1	В	603	THR	2.7
1	В	689	ASP	2.7
1	В	672	PHE	2.6
1	А	672	PHE	2.6
1	А	749	ARG	2.6
1	А	763	PHE	2.5
1	А	738	ILE	2.5
1	В	624	ILE	2.5
1	А	691	LEU	2.5
1	В	705	ARG	2.5
1	В	734	THR	2.4
1	В	715	GLN	2.4
1	В	595	LYS	2.4
1	А	635	TRP	2.4
1	А	628	CYS	2.4
1	А	733	CYS	2.4
1	В	772	LEU	2.4
1	В	714	THR	2.3
1	В	662	LEU	2.3
1	А	683	PHE	2.3
1	В	644	VAL	2.3
1	В	727	ASP	2.3
1	А	694	LEU	2.2
1	В	667	LEU	2.2
1	А	579	SER	2.2
1	В	654	PRO	2.2
1	А	590	VAL	2.2
1	A	736	TYR	2.2
1	В	647	GLN	2.2
1	В	601	ASP	2.2
1	А	573	ILE	2.2
1	В	748	GLU	2.2
1	A	578	SER	2.1
1	B	716	THR	2.1
1	А	710	ASP	2.1
1	A	616	SER	2.1
1	В	628	CYS	2.1
1	В	725	ARG	2.1
1	A	756	TRP	2.1
1	В	733	CYS	2.1



Mol	Chain	Res	Type	RSRZ
1	А	612	ASP	2.1
1	А	622	LEU	2.1
1	В	655	GLU	2.1
1	В	573	ILE	2.1
1	А	640	LEU	2.1
1	В	708	LYS	2.1
1	В	609	VAL	2.0
1	В	617	THR	2.0
1	А	677	PHE	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 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^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	EDO	В	308	4/4	0.62	0.49	$61,\!66,\!66,\!66$	0
4	EDO	А	310	4/4	0.72	0.25	$57,\!58,\!60,\!61$	0
4	EDO	А	309	4/4	0.76	0.30	41,50,51,57	0
3	CL	А	304	1/1	0.84	0.10	$63,\!63,\!63,\!63$	0
4	EDO	В	311	4/4	0.86	0.14	48,48,49,50	0
2	SO4	А	302	5/5	0.90	0.33	$61,\!62,\!66,\!69$	0
3	CL	В	305	1/1	0.91	0.09	90,90,90,90	0
3	CL	В	306	1/1	0.93	0.05	70,70,70,70	0
2	SO4	В	301	5/5	0.94	0.25	64,66,68,70	0
4	EDO	А	307	4/4	0.97	0.14	47,47,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.

