



Full wwPDB X-ray Structure Validation Report ⓘ

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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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

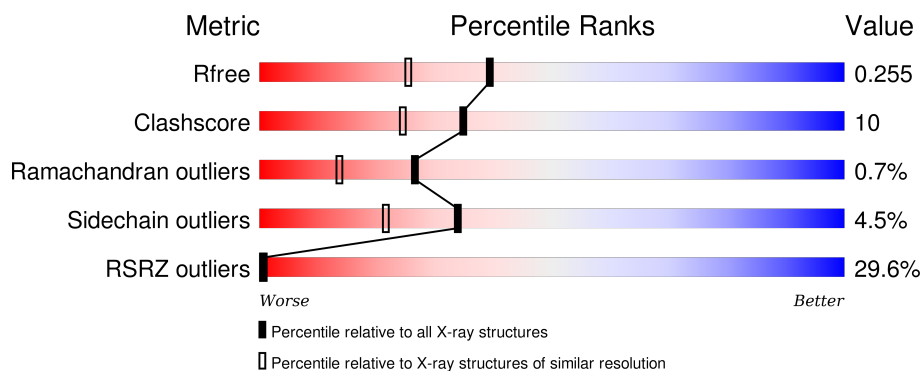
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 ≥ 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	210	<div> <div>27%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	210	<div> <div>32%</div> <div>80%</div> <div>17%</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
3	CL	B	305	-	-	X	-
4	EDO	A	309	-	-	-	X
4	EDO	A	310	-	-	-	X
4	EDO	B	308	-	-	-	X

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	A	210	Total	C	N	O	S	0	0	0
			1693	1086	290	306	11			
1	B	209	Total	C	N	O	S	0	0	0
			1689	1084	289	305	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

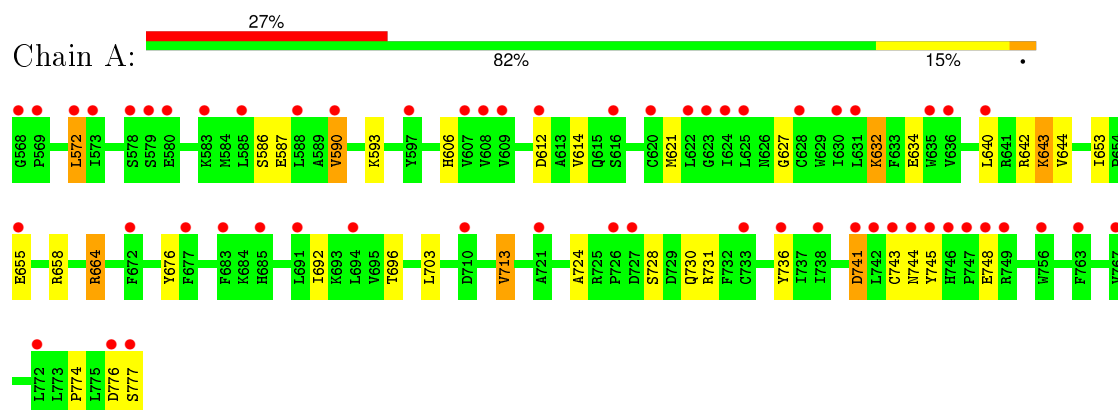
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	133	Total O 133 133	0	2
5	B	105	Total O 105 105	0	0

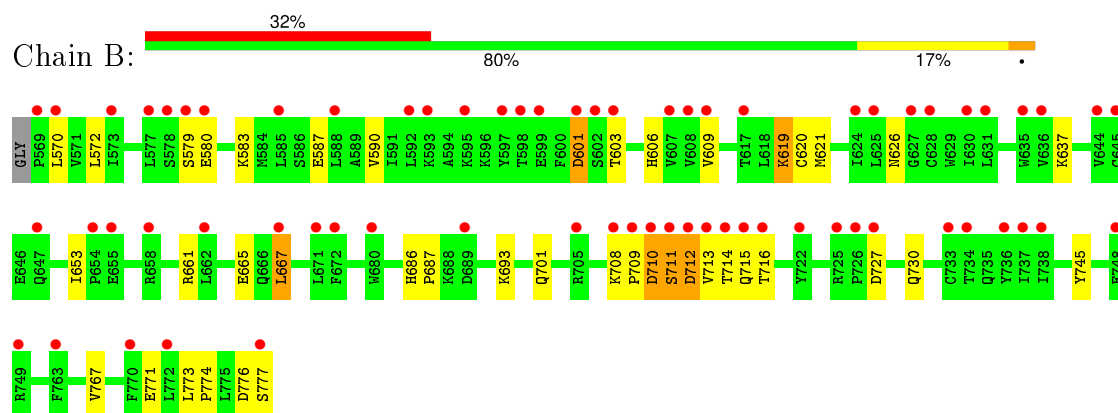
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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	57.44Å 75.80Å 116.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 1.90 19.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.87-1.90) 93.8 (19.86-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.247 0.200 , 0.255	Depositor DCC
R_{free} test set	1910 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38311 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, SO4

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	1.09	3/1735 (0.2%)	0.97	4/2347 (0.2%)
1	B	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	B	0	1

All (4) bond length outliers are listed below:

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

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	741	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	658	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	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	B	776	ASP	Peptide

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	1693	0	1703	31	0
1	B	1689	0	1701	36	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	1	0	0	0	0
3	B	2	0	0	2	0
4	A	12	0	18	4	0
4	B	8	0	12	3	0
5	A	133	0	0	3	0
5	B	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 distance (Å)	Clash 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:NH1	1:A:664:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:708:LYS:H	1:B:714:THR:HG21	1.69	0.58
1:A:743:CYS:SG	1:A:745:TYR:HB3	2.42	0.58
1:B:570:LEU:HD22	1:B:606:HIS:HE1	1.68	0.57
1:A:692:ILE:O	1:A:696:THR:HG23	2.04	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:B:711:SER:O	1:B:713:VAL:N	2.46	0.48
1:A:621:MET:CE	4:A:310:EDO:H12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LYS:N	1:B:714:THR:HG21	2.32	0.43
1:B:693:LYS:CE	5:B:144:HOH:O	2.66	0.43
1:A:748:GLU:CD	1:A:748:GLU:H	2.22	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:HD12	1:B:667:LEU:N	2.36	0.40

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	208/210 (99%)	204 (98%)	3 (1%)	1 (0%)	34	21
1	B	207/210 (99%)	202 (98%)	3 (1%)	2 (1%)	19	7
All	All	415/420 (99%)	406 (98%)	6 (1%)	3 (1%)	26	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	710	ASP
1	B	712	ASP
1	A	655	GLU

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	189/189 (100%)	180 (95%)	9 (5%)	31	19
1	B	189/189 (100%)	181 (96%)	8 (4%)	36	24
All	All	378/378 (100%)	361 (96%)	17 (4%)	34	21

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

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

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

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

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Mol	Chain	Res	Type
1	B	663	ASN
1	B	701	GLN
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](#)

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	302	-	4,4,4	0.46	0	6,6,6	0.95	1 (16%)
4	EDO	A	307	-	3,3,3	0.30	0	2,2,2	0.11	0
4	EDO	A	309	-	3,3,3	1.16	0	2,2,2	1.53	0
4	EDO	A	310	-	3,3,3	0.53	0	2,2,2	0.84	0
2	SO4	B	301	1	4,4,4	0.29	0	6,6,6	0.83	0
4	EDO	B	308	-	3,3,3	0.58	0	2,2,2	1.32	0
4	EDO	B	311	-	3,3,3	1.11	0	2,2,2	0.12	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	SO4	A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	A	307	-	-	0/1/1/1	0/0/0/0
4	EDO	A	309	-	-	0/1/1/1	0/0/0/0
4	EDO	A	310	-	-	0/1/1/1	0/0/0/0
2	SO4	B	301	1	-	0/0/0/0	0/0/0/0
4	EDO	B	308	-	-	0/1/1/1	0/0/0/0
4	EDO	B	311	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	SO4	O4-S-O3	2.17	117.80	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	307	EDO	1	0
4	A	309	EDO	1	0
4	A	310	EDO	2	0
2	B	301	SO4	1	0
4	B	308	EDO	3	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	210/210 (100%)	1.65	57 (27%)  	41, 50, 66, 78	0
1	B	209/210 (99%)	1.57	67 (32%)  	36, 50, 61, 66	0
All	All	419/420 (99%)	1.61	124 (29%)  	36, 50, 63, 78	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	743	CYS	17.0
1	A	744	ASN	13.2
1	A	742	LEU	11.6
1	B	712	ASP	9.0
1	A	777	SER	8.8
1	A	569	PRO	7.0
1	A	726	PRO	6.7
1	B	569	PRO	6.5
1	B	608	VAL	6.2
1	B	579	SER	5.9
1	A	608	VAL	5.9
1	A	585	LEU	5.8
1	B	713	VAL	5.7
1	B	777	SER	5.5
1	A	745	TYR	5.4
1	A	631	LEU	5.3
1	B	607	VAL	5.3
1	B	710	ASP	5.0
1	B	636	VAL	5.0
1	A	630	ILE	4.9
1	B	598	THR	4.8
1	A	609	VAL	4.8
1	B	578	SER	4.7
1	A	727	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	572	LEU	4.7
1	B	599	GLU	4.6
1	B	711	SER	4.6
1	A	685	HIS	4.6
1	B	709	PRO	4.5
1	A	607	VAL	4.5
1	A	580	GLU	4.4
1	A	568	GLY	4.4
1	B	602	SER	4.2
1	A	636	VAL	4.1
1	B	726	PRO	3.9
1	B	585	LEU	3.8
1	A	741	ASP	3.8
1	A	767	VAL	3.7
1	B	580	GLU	3.7
1	A	748	GLU	3.7
1	B	630	ILE	3.6
1	B	737	ILE	3.6
1	A	588	LEU	3.6
1	B	588	LEU	3.5
1	A	746	HIS	3.5
1	A	625	LEU	3.5
1	A	624	ILE	3.4
1	B	738	ILE	3.4
1	B	625	LEU	3.3
1	B	631	LEU	3.3
1	A	597	TYR	3.3
1	A	747	PRO	3.2
1	A	776	ASP	3.2
1	B	635	TRP	3.1
1	B	645	CYS	3.1
1	B	736	TYR	3.1
1	A	620	CYS	3.1
1	B	597	TYR	3.0
1	A	583	LYS	3.0
1	B	671	LEU	3.0
1	B	577	LEU	2.9
1	B	603	THR	2.9
1	A	623	GLY	2.9
1	A	772	LEU	2.9
1	A	655	GLU	2.8
1	B	689	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	592	LEU	2.8
1	B	749	ARG	2.8
1	B	570	LEU	2.8
1	B	658	ARG	2.8
1	A	738	ILE	2.6
1	B	672	PHE	2.6
1	B	624	ILE	2.6
1	B	595	LYS	2.6
1	A	763	PHE	2.6
1	B	705	ARG	2.5
1	A	694	LEU	2.5
1	A	672	PHE	2.5
1	B	708	LYS	2.5
1	A	749	ARG	2.5
1	A	590	VAL	2.5
1	B	734	THR	2.5
1	A	691	LEU	2.5
1	B	772	LEU	2.5
1	B	601	ASP	2.4
1	A	578	SER	2.4
1	A	683	PHE	2.4
1	B	644	VAL	2.4
1	A	628	CYS	2.4
1	A	733	CYS	2.4
1	B	725	ARG	2.4
1	B	748	GLU	2.4
1	B	667	LEU	2.4
1	A	635	TRP	2.4
1	B	727	ASP	2.4
1	A	736	TYR	2.3
1	A	640	LEU	2.3
1	B	647	GLN	2.3
1	B	714	THR	2.3
1	B	716	THR	2.3
1	A	573	ILE	2.3
1	A	756	TRP	2.3
1	B	628	CYS	2.3
1	A	612	ASP	2.3
1	A	710	ASP	2.2
1	B	609	VAL	2.2
1	B	573	ILE	2.2
1	A	579	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	655	GLU	2.2
1	B	662	LEU	2.2
1	B	733	CYS	2.2
1	B	722	TYR	2.2
1	A	616	SER	2.2
1	B	617	THR	2.2
1	B	654	PRO	2.1
1	B	763	PHE	2.1
1	B	715	GLN	2.1
1	A	677	PHE	2.1
1	B	627	GLY	2.1
1	B	770	PHE	2.1
1	A	622	LEU	2.0
1	B	680	TRP	2.0
1	A	721	ALA	2.0
1	B	593	LYS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	B	308	4/4	0.65	0.48	10.87	61,66,66,66	0
4	EDO	A	309	4/4	0.74	0.29	4.76	41,50,51,57	0
4	EDO	A	310	4/4	0.71	0.26	2.13	57,58,60,61	0
2	SO4	B	301	5/5	0.94	0.24	0.98	64,66,68,70	0
4	EDO	A	307	4/4	0.97	0.13	-0.48	47,47,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	304	1/1	0.84	0.09	-1.20	63,63,63,63	0
3	CL	B	305	1/1	0.90	0.09	-2.00	90,90,90,90	0
4	EDO	B	311	4/4	0.84	0.15	-	48,48,49,50	0
2	SO4	A	302	5/5	0.91	0.32	-	61,62,66,69	0
3	CL	B	306	1/1	0.92	0.06	-	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.