



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 4A9F / pdb_00004a9f
Title : N-TERMINAL BROMODOMAIN OF HUMAN BRD2 WITH 1-METHYLPYRROLIDIN-2-ONE
Authors : Chung, C.W.; Bamborough, P.
Deposited on : 2011-11-26
Resolution : 1.73 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

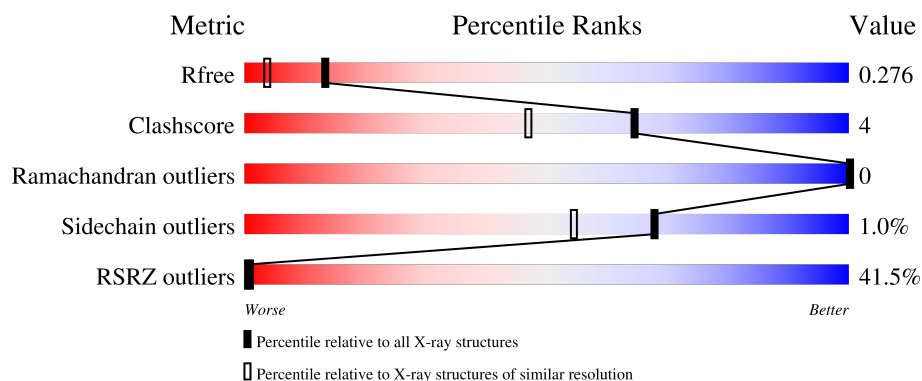
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	154	19% 62% 8% 30%
1	B	154	19% 68% . 29%
1	C	154	49% 62% 8% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3278 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 BROMODOMAIN-CONTAINING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	3	0
			928	603	155	161	9			
1	B	110	Total	C	N	O	S	0	3	0
			940	613	157	160	10			
1	C	107	Total	C	N	O	S	0	3	0
			921	598	155	159	9			

There are 60 discrepancies between the modelled and reference sequences:

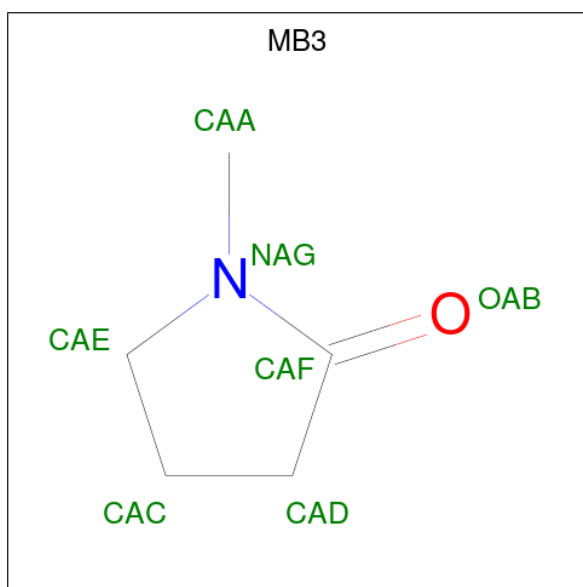
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP P25440
A	48	SER	-	expression tag	UNP P25440
A	49	SER	-	expression tag	UNP P25440
A	50	HIS	-	expression tag	UNP P25440
A	51	HIS	-	expression tag	UNP P25440
A	52	HIS	-	expression tag	UNP P25440
A	53	HIS	-	expression tag	UNP P25440
A	54	HIS	-	expression tag	UNP P25440
A	55	HIS	-	expression tag	UNP P25440
A	56	SER	-	expression tag	UNP P25440
A	57	SER	-	expression tag	UNP P25440
A	58	GLY	-	expression tag	UNP P25440
A	59	LEU	-	expression tag	UNP P25440
A	60	VAL	-	expression tag	UNP P25440
A	61	PRO	-	expression tag	UNP P25440
A	62	ARG	-	expression tag	UNP P25440
A	63	GLY	-	expression tag	UNP P25440
A	64	SER	-	expression tag	UNP P25440
A	65	HIS	-	expression tag	UNP P25440
A	66	MET	-	expression tag	UNP P25440
B	47	GLY	-	expression tag	UNP P25440
B	48	SER	-	expression tag	UNP P25440
B	49	SER	-	expression tag	UNP P25440

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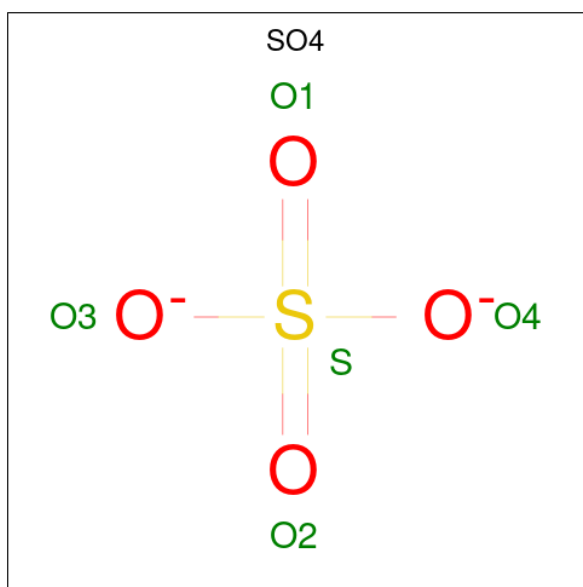
Chain	Residue	Modelled	Actual	Comment	Reference
B	50	HIS	-	expression tag	UNP P25440
B	51	HIS	-	expression tag	UNP P25440
B	52	HIS	-	expression tag	UNP P25440
B	53	HIS	-	expression tag	UNP P25440
B	54	HIS	-	expression tag	UNP P25440
B	55	HIS	-	expression tag	UNP P25440
B	56	SER	-	expression tag	UNP P25440
B	57	SER	-	expression tag	UNP P25440
B	58	GLY	-	expression tag	UNP P25440
B	59	LEU	-	expression tag	UNP P25440
B	60	VAL	-	expression tag	UNP P25440
B	61	PRO	-	expression tag	UNP P25440
B	62	ARG	-	expression tag	UNP P25440
B	63	GLY	-	expression tag	UNP P25440
B	64	SER	-	expression tag	UNP P25440
B	65	HIS	-	expression tag	UNP P25440
B	66	MET	-	expression tag	UNP P25440
C	47	GLY	-	expression tag	UNP P25440
C	48	SER	-	expression tag	UNP P25440
C	49	SER	-	expression tag	UNP P25440
C	50	HIS	-	expression tag	UNP P25440
C	51	HIS	-	expression tag	UNP P25440
C	52	HIS	-	expression tag	UNP P25440
C	53	HIS	-	expression tag	UNP P25440
C	54	HIS	-	expression tag	UNP P25440
C	55	HIS	-	expression tag	UNP P25440
C	56	SER	-	expression tag	UNP P25440
C	57	SER	-	expression tag	UNP P25440
C	58	GLY	-	expression tag	UNP P25440
C	59	LEU	-	expression tag	UNP P25440
C	60	VAL	-	expression tag	UNP P25440
C	61	PRO	-	expression tag	UNP P25440
C	62	ARG	-	expression tag	UNP P25440
C	63	GLY	-	expression tag	UNP P25440
C	64	SER	-	expression tag	UNP P25440
C	65	HIS	-	expression tag	UNP P25440
C	66	MET	-	expression tag	UNP P25440

- Molecule 2 is 1-methylpyrrolidin-2-one (CCD ID: MB3) (formula: C₅H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



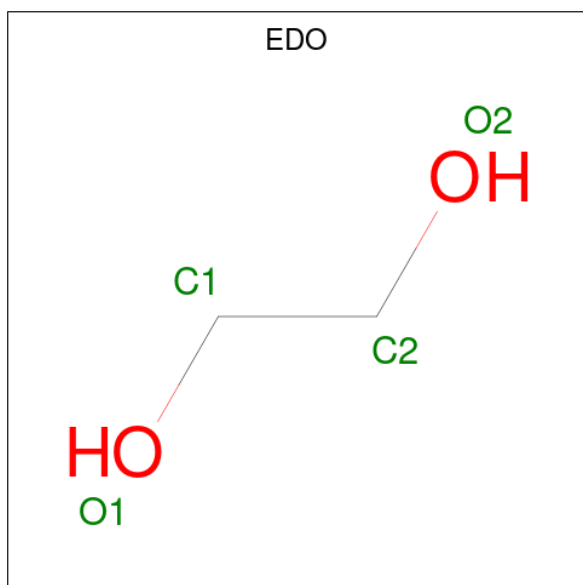
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		
5	B	127	Total	O	0	0
			127	127		
5	C	120	Total	O	0	0
			120	120		

● Molecule 1: BROMODOMAIN-CONTAINING PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.23Å 55.53Å 67.97Å 90.00° 94.85° 90.00°	Depositor
Resolution (Å)	23.60 – 1.73 23.60 – 1.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.60-1.73) 96.4 (23.60-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.214 0.243 , 0.276	Depositor DCC
R_{free} test set	2160 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3278	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: SO4, EDO, MB3

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	0.47	0/953	0.70	0/1291
1	B	0.44	0/967	0.66	0/1310
1	C	0.43	0/945	0.67	0/1277
All	All	0.44	0/2865	0.68	0/3878

There are no bond length outliers.

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	928	0	927	13	0
1	B	940	0	928	4	0
1	C	921	0	920	7	0
2	A	7	0	9	1	0
2	B	7	0	9	0	0
2	C	7	0	9	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	202	0	0	0	0
5	B	127	0	0	0	0
5	C	120	0	0	0	0
All	All	3278	0	2808	22	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 4.

All (22) 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:96:ALA:HB1	1:A:123:MET:HE1	1.57	0.86
1:A:75:VAL:HG13	1:A:80:GLN:HE21	1.44	0.81
1:A:75:VAL:HG13	1:A:80:GLN:NE2	2.07	0.69
1:C:96:ALA:HB1	1:C:123:MET:HE1	1.75	0.67
1:C:139:SER:O	1:C:143[A]:GLN:HG2	2.02	0.59
1:A:108:LEU:HD13	2:A:1183:MB3:HAC	1.84	0.59
1:A:139:SER:O	1:A:143:GLN:HG2	2.07	0.55
1:A:174:LEU:CD1	1:B:146:ASN:HB2	2.40	0.51
1:A:75:VAL:CG1	1:A:80:GLN:HE21	2.19	0.50
1:C:143[B]:GLN:NE2	1:C:143[B]:GLN:HA	2.27	0.50
1:C:96:ALA:HB1	1:C:123:MET:CE	2.42	0.49
1:B:139:SER:O	1:B:143:GLN:HG2	2.13	0.49
1:A:174:LEU:HD11	1:B:146:ASN:HB2	1.96	0.47
1:A:142:MET:SD	1:A:180:MET:HE1	2.54	0.47
1:B:91:TRP:HA	1:B:123[A]:MET:HE1	1.98	0.46
1:C:78:GLN:HB3	1:C:138:ALA:HB2	1.98	0.45
1:A:99:PHE:HB2	1:A:123:MET:HE2	1.98	0.45
1:A:75:VAL:CG1	1:A:80:GLN:NE2	2.79	0.43
1:C:97:TRP:CG	1:C:98:PRO:HD3	2.54	0.42
1:C:182[B]:GLN:O	1:C:182[B]:GLN:OE1	2.38	0.42
1:A:177:VAL:HG13	1:A:180:MET:HE2	2.01	0.42
1:A:96:ALA:CB	1:A:123:MET:HE1	2.40	0.41

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	109/154 (71%)	109 (100%)	0	0	100	100
1	B	111/154 (72%)	110 (99%)	1 (1%)	0	100	100
1	C	107/154 (70%)	107 (100%)	0	0	100	100
All	All	327/462 (71%)	326 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	102/139 (73%)	102 (100%)	0	100	100
1	B	101/139 (73%)	101 (100%)	0	100	100
1	C	101/139 (73%)	98 (97%)	3 (3%)	36	12
All	All	304/417 (73%)	301 (99%)	3 (1%)	68	54

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	118	LYS
1	C	136	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	B	101	GLN
1	B	156	ASN
1	C	80	GLN
1	C	119	GLN
1	C	146	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	MB3	C	1183	-	7,7,7	0.65	0	9,9,9	0.53	0
2	MB3	A	1183	-	7,7,7	0.59	0	9,9,9	0.52	0
2	MB3	B	1187	-	7,7,7	0.55	0	9,9,9	0.52	0
3	SO4	C	1184	-	4,4,4	0.25	0	6,6,6	0.14	0
4	EDO	B	1186	-	3,3,3	0.41	0	2,2,2	0.34	0
3	SO4	B	1188	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	1184	-	4,4,4	0.22	0	6,6,6	0.11	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	B	1186	-	-	1/1/1/1	-
2	MB3	C	1183	-	-	-	0/1/1/1
2	MB3	A	1183	-	-	-	0/1/1/1
2	MB3	B	1187	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1186	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1183	MB3	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 ⓘ

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	108/154 (70%)	1.44	29 (26%) 1 2	14, 34, 51, 60	3 (2%)
1	B	110/154 (71%)	1.53	30 (27%) 1 1	14, 36, 54, 71	3 (2%)
1	C	107/154 (69%)	2.57	76 (71%) 0 0	16, 39, 55, 70	3 (2%)
All	All	325/462 (70%)	1.84	135 (41%) 0 1	14, 36, 54, 71	9 (2%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164[A]	LEU	6.0
1	C	76	THR	5.6
1	B	136[A]	TRP	5.4
1	C	136	TRP	5.2
1	B	183	GLU	4.9
1	C	159	THR	4.7
1	C	154	ILE	4.7
1	C	116	ILE	4.7
1	B	181	PRO	4.6
1	C	137	ALA	4.4
1	A	111	PRO	4.3
1	A	75	VAL	4.2
1	A	106	VAL	4.2
1	A	77	ASN	4.1
1	B	182	GLN	4.1
1	C	85	VAL	4.0
1	C	79	LEU	3.8
1	C	163	VAL	3.8
1	B	111	PRO	3.8
1	C	166	ALA	3.7
1	C	134	TYR	3.7
1	B	184	GLU	3.7
1	C	117	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	150	THR	3.6
1	C	152	CYS	3.6
1	C	182[A]	GLN	3.6
1	C	97	TRP	3.5
1	A	110	LEU	3.5
1	C	179	SER	3.5
1	C	89	ALA	3.5
1	C	143[A]	GLN	3.5
1	C	103	VAL	3.5
1	C	147	THR	3.5
1	A	134	TYR	3.5
1	C	153	TYR	3.4
1	A	116	ILE	3.3
1	C	169	LEU	3.3
1	C	86	VAL	3.3
1	B	77	ASN	3.3
1	A	177	VAL	3.3
1	B	164[A]	LEU	3.2
1	C	175	GLN	3.2
1	B	76	THR	3.2
1	C	126	ILE	3.2
1	C	162	ILE	3.2
1	C	146	ASN	3.2
1	B	185	GLN	3.2
1	C	141	CYS	3.1
1	A	105	ALA	3.1
1	C	178	ALA	3.1
1	C	177	VAL	3.1
1	B	79	LEU	3.1
1	C	119	GLN	3.0
1	C	167	GLN	2.9
1	A	80	GLN	2.9
1	C	168	THR	2.9
1	C	155	TYR	2.9
1	C	81	TYR	2.9
1	C	158	PRO	2.9
1	B	80	GLN	2.8
1	C	113	TYR	2.8
1	A	76	THR	2.8
1	A	164[A]	LEU	2.8
1	A	182	GLN	2.7
1	A	79	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	2.7
1	C	138	ALA	2.7
1	C	98	PRO	2.7
1	A	85	VAL	2.7
1	C	149	PHE	2.7
1	A	159	THR	2.7
1	C	106	VAL	2.7
1	C	142	MET	2.7
1	C	174	LEU	2.6
1	C	77	ASN	2.6
1	B	110	LEU	2.6
1	C	176	LYS	2.5
1	C	172	ILE	2.5
1	C	108	LEU	2.5
1	A	155	TYR	2.5
1	C	80	GLN	2.5
1	C	111	PRO	2.5
1	A	133	ASN	2.5
1	C	95	PHE	2.5
1	C	88	LYS	2.4
1	C	110	LEU	2.4
1	C	118	LYS	2.4
1	C	135	TYR	2.4
1	B	85	VAL	2.4
1	B	106	VAL	2.4
1	C	161	ASP	2.4
1	A	175	GLN	2.4
1	A	117	ILE	2.4
1	C	145	PHE	2.3
1	C	165	MET	2.3
1	A	136	TRP	2.3
1	C	144	ASP	2.3
1	A	178	ALA	2.3
1	B	104	ASP	2.3
1	B	159	THR	2.3
1	A	109	GLY	2.3
1	C	93	HIS	2.2
1	C	151	ASN	2.2
1	B	130	LEU	2.2
1	B	81	TYR	2.2
1	A	166	ALA	2.2
1	A	139	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	82	LEU	2.2
1	C	121	MET	2.2
1	C	170	GLU	2.2
1	A	154	ILE	2.2
1	B	87	MET	2.1
1	C	171	LYS	2.1
1	C	139	SER	2.1
1	C	99	PHE	2.1
1	C	140	GLU	2.1
1	B	116	ILE	2.1
1	C	96	ALA	2.1
1	C	84	LYS	2.1
1	A	130	LEU	2.1
1	C	130	LEU	2.1
1	C	102	PRO	2.1
1	B	83	HIS	2.1
1	B	105	ALA	2.1
1	A	132	ASN	2.1
1	C	156	ASN	2.1
1	B	78	GLN	2.1
1	B	112	ASP	2.1
1	B	108	LEU	2.1
1	B	89	ALA	2.0
1	A	103	VAL	2.0
1	B	160	ASP	2.0
1	B	162	ILE	2.0
1	C	173	PHE	2.0
1	B	107	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 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
3	SO4	B	1188	5/5	0.40	0.15	133,133,133,133	0
4	EDO	B	1186	4/4	0.79	0.17	58,59,59,60	0
3	SO4	A	1184	5/5	0.85	0.13	66,67,67,68	0
2	MB3	C	1183	7/7	0.88	0.13	35,36,38,38	0
3	SO4	C	1184	5/5	0.91	0.14	52,54,55,56	0
2	MB3	A	1183	7/7	0.91	0.10	28,34,36,37	0
2	MB3	B	1187	7/7	0.93	0.10	31,32,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.