



wwPDB X-ray Structure Validation Summary Report

Mar 10, 2021 – 05:07 pm GMT

PDB ID : 6YLI
Title : Crystal structure of human bcl-xL bound to trichoplax adhaerens trBak BH3
Authors : D Sa, J.; Banjara, S.; Kvensakul, M.
Deposited on : 2020-04-07
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references](#) ) 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 : 2.17.1
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) : 2.17.1

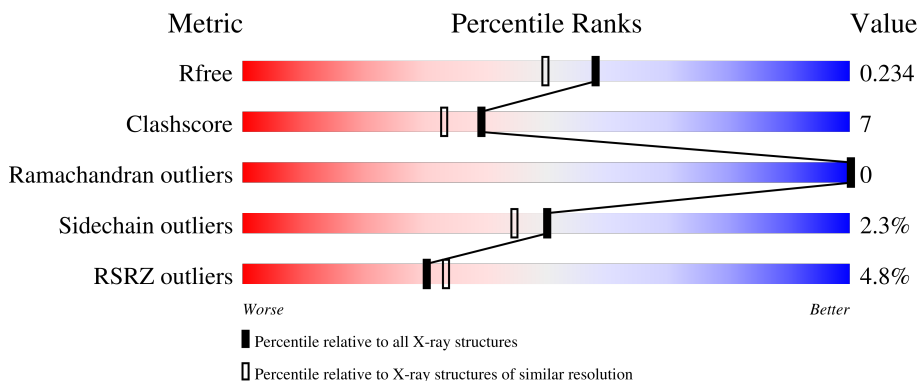
1 Overall quality at a glance

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}	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 $\leq 5\%$. 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	180	 5% 73% 11% • 14%
1	C	180	 3% 74% 11% • 15%
2	B	26	 8% 69% 19% • 8%
2	D	26	 77% 12% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5695 atoms, of which 2674 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	155	2411	788	1167	208	242	6	0	0	0
1	C	153	2400	784	1165	209	237	5	0	1	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q07817
A	-3	PRO	-	expression tag	UNP Q07817
A	-2	LEU	-	expression tag	UNP Q07817
A	-1	GLY	-	expression tag	UNP Q07817
A	0	SER	-	expression tag	UNP Q07817
A	1	MET	-	expression tag	UNP Q07817
A	2	SER	-	expression tag	UNP Q07817
A	3	MET	-	expression tag	UNP Q07817
A	4	ALA	-	expression tag	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	TRP	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ASP	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ARG	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	174	LEU	-	expression tag	UNP Q07817
A	175	GLU	-	expression tag	UNP Q07817
C	-4	GLY	-	expression tag	UNP Q07817
C	-3	PRO	-	expression tag	UNP Q07817
C	-2	LEU	-	expression tag	UNP Q07817
C	-1	GLY	-	expression tag	UNP Q07817
C	0	SER	-	expression tag	UNP Q07817
C	1	MET	-	expression tag	UNP Q07817
C	2	SER	-	expression tag	UNP Q07817
C	3	MET	-	expression tag	UNP Q07817
C	4	ALA	-	expression tag	UNP Q07817
C	?	-	MET	deletion	UNP Q07817
C	?	-	GLU	deletion	UNP Q07817
C	?	-	THR	deletion	UNP Q07817
C	?	-	PRO	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	?	-	ILE	deletion	UNP Q07817

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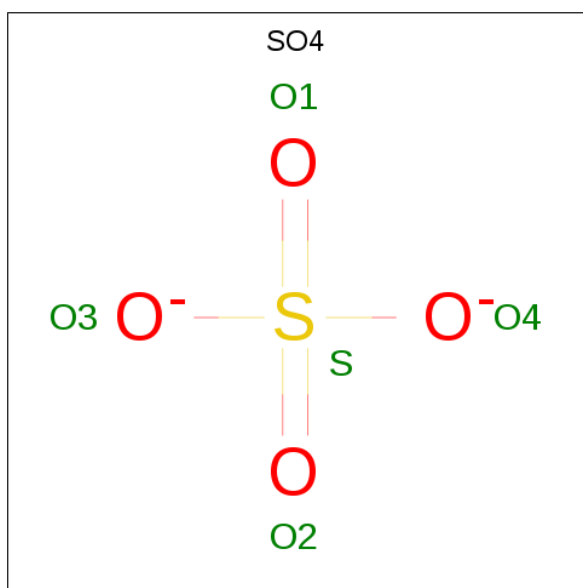
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP Q07817
C	?	-	GLY	deletion	UNP Q07817
C	?	-	ASN	deletion	UNP Q07817
C	?	-	PRO	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	TRP	deletion	UNP Q07817
C	?	-	HIS	deletion	UNP Q07817
C	?	-	LEU	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	?	-	ASP	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	PRO	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	?	-	VAL	deletion	UNP Q07817
C	?	-	ASN	deletion	UNP Q07817
C	?	-	GLY	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	?	-	THR	deletion	UNP Q07817
C	?	-	GLY	deletion	UNP Q07817
C	?	-	HIS	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	SER	deletion	UNP Q07817
C	?	-	LEU	deletion	UNP Q07817
C	?	-	ASP	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	?	-	ARG	deletion	UNP Q07817
C	?	-	GLU	deletion	UNP Q07817
C	?	-	VAL	deletion	UNP Q07817
C	?	-	ILE	deletion	UNP Q07817
C	?	-	PRO	deletion	UNP Q07817
C	?	-	MET	deletion	UNP Q07817
C	?	-	ALA	deletion	UNP Q07817
C	174	LEU	-	expression tag	UNP Q07817
C	175	GLU	-	expression tag	UNP Q07817

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	B	24	Total	C	H	N	O	0	0	0
			358	113	173	35	37			
2	D	23	Total	C	H	N	O	0	0	0
			348	110	169	34	35			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	63	Total O 63 63	0	0
4	D	6	Total O 6 6	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.14Å 63.80Å 69.76Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	39.02 – 1.90 47.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.02-1.90) 98.0 (47.01-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.199 , 0.236 0.197 , 0.234	Depositor DCC
R_{free} test set	1310 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.360	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5695	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% 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

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	0.43	1/1272 (0.1%)	0.70	5/1719 (0.3%)
1	C	0.35	0/1266	0.50	0/1711
2	B	1.29	4/188 (2.1%)	0.89	2/253 (0.8%)
2	D	0.34	0/182	0.45	0/244
All	All	0.50	5/2908 (0.2%)	0.62	7/3927 (0.2%)

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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	GLU	CD-OE1	-11.07	1.13	1.25
2	B	7	GLU	CB-CG	-8.04	1.36	1.52
2	B	7	GLU	CD-OE2	-7.55	1.17	1.25
1	A	66	ARG	CG-CD	-5.62	1.37	1.51
2	B	7	GLU	CG-CD	-5.32	1.44	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	A	3	MET	CA-CB-CG	-6.84	101.66	113.30
1	A	3	MET	CG-SD-CE	-6.79	89.34	100.20
2	B	7	GLU	OE1-CD-OE2	6.40	130.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	72	LEU	CA-CB-CG	5.51	127.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	MET	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	A	1244	1167	1169	25	2
1	C	1235	1165	1166	16	2
2	B	185	173	171	4	0
2	D	179	169	167	2	0
3	A	25	0	0	2	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
4	A	60	0	0	7	0
4	B	4	0	0	0	0
4	C	63	0	0	6	1
4	D	6	0	0	0	0
All	All	3021	2674	2673	41	3

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.

The worst 5 of 41 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:C:48:GLU:OE2	4:C:301:HOH:O	1.84	0.93
1:A:66:ARG:NH2	4:A:303:HOH:O	2.08	0.87
1:A:56:GLU:OE2	4:A:301:HOH:O	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:SO4:O2	4:A:302:HOH:O	2.06	0.74
1:C:10:ARG:NH1	4:C:304:HOH:O	2.21	0.73

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:303:HOH:O	4:C:339:HOH:O[1_455]	1.87	0.33
1:A:43:GLU:O	1:C:162:ASN:ND2[1_655]	2.07	0.13
1:A:46:GLU:OE1	1:C:49:ALA:O[1_655]	2.17	0.03

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	151/180 (84%)	148 (98%)	3 (2%)	0	100	100
1	C	150/180 (83%)	149 (99%)	1 (1%)	0	100	100
2	B	22/26 (85%)	22 (100%)	0	0	100	100
2	D	21/26 (81%)	21 (100%)	0	0	100	100
All	All	344/412 (84%)	340 (99%)	4 (1%)	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	131/151 (87%)	127 (97%)	4 (3%)	40	32
1	C	129/151 (85%)	127 (98%)	2 (2%)	62	60
2	B	20/23 (87%)	19 (95%)	1 (5%)	24	15
2	D	19/23 (83%)	19 (100%)	0	100	100
All	All	299/348 (86%)	292 (98%)	7 (2%)	50	45

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
2	B	22	ARG
1	C	47	SER
1	C	10	ARG
1	A	47	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	11	HIS
1	C	52	GLN
2	D	24	GLN

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](#)

9 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	$\# Z > 2$
3	SO4	A	205	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	C	201	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	A	201	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	A	203	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	B	101	-	4,4,4	0.19	0	6,6,6	0.30	0
3	SO4	A	202	-	4,4,4	0.17	0	6,6,6	0.08	0
3	SO4	D	101	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	C	202	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	A	204	-	4,4,4	0.15	0	6,6,6	0.13	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	SO4	1	0
3	A	203	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, 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	155/180 (86%)	0.26	9 (5%) 23 25	24, 38, 80, 113	0
1	C	153/180 (85%)	0.18	6 (3%) 39 42	22, 36, 65, 95	0
2	B	24/26 (92%)	0.41	2 (8%) 11 13	29, 40, 73, 98	0
2	D	23/26 (88%)	0.09	0 100 100	29, 35, 65, 68	0
All	All	355/412 (86%)	0.23	17 (4%) 30 33	22, 38, 72, 113	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	6.3
1	A	72	LEU	5.8
1	A	33	ASP	4.9
1	C	4	ALA	4.7
1	A	3	MET	4.3

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, 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(\AA^2)	Q<0.9
3	SO4	C	201	5/5	0.82	0.23	75,75,86,86	0
3	SO4	A	203	5/5	0.85	0.21	54,56,58,61	5
3	SO4	D	101	5/5	0.86	0.15	86,93,93,93	0
3	SO4	A	202	5/5	0.87	0.20	76,77,80,81	0
3	SO4	A	201	5/5	0.89	0.18	69,74,78,78	0
3	SO4	A	204	5/5	0.94	0.14	64,65,70,71	0
3	SO4	A	205	5/5	0.94	0.19	72,72,78,81	0
3	SO4	C	202	5/5	0.99	0.12	36,39,43,43	0
3	SO4	B	101	5/5	0.99	0.14	33,36,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.