



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 01:56 AM BST

PDB ID : 6IWB  
Title : Crystal structure of a computationally designed protein (LD3) in complex with BCL-2  
Authors : Kim, S.; Kwak, M.J.; Oh, B.-H.; Correia, B.E.; Gainza, P.  
Deposited on : 2018-12-05  
Resolution : 2.50 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

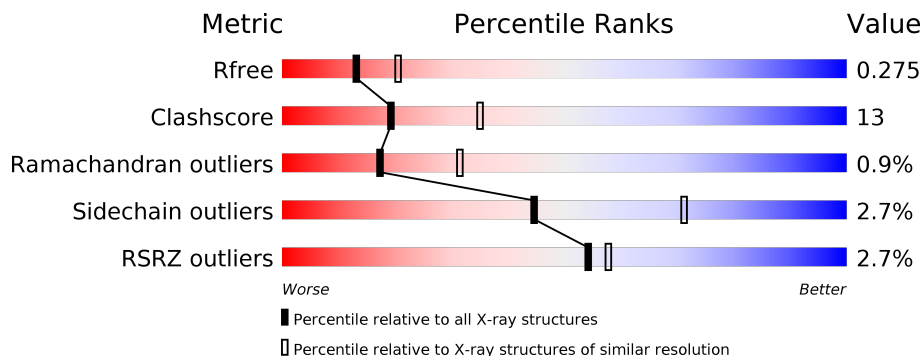
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	156	 2% (poor fit), 71% (0 outliers), 21% (1 outlier), 9% (2+ outliers)
1	C	156	 3% (poor fit), 67% (0 outliers), 22% (1 outlier), 8% (2+ outliers)
2	B	166	 % (poor fit), 64% (0 outliers), 17% (1 outlier), 16% (2+ outliers)
2	D	166	 3% (poor fit), 60% (0 outliers), 22% (1 outlier), 16% (2+ outliers)

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4463 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 Apolipoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	142	1123	702	199	218	4	0	0	0
1	C	143	1123	702	199	218	4	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P02649
A	2	HIS	-	expression tag	UNP P02649
A	3	HIS	-	expression tag	UNP P02649
A	4	HIS	-	expression tag	UNP P02649
A	5	HIS	-	expression tag	UNP P02649
A	6	HIS	-	expression tag	UNP P02649
A	7	HIS	-	expression tag	UNP P02649
A	8	GLY	-	expression tag	UNP P02649
A	9	SER	-	expression tag	UNP P02649
A	21	LEU	TRP	see sequence details	UNP P02649
A	22	GLU	ASP	see sequence details	UNP P02649
A	25	SER	ARG	see sequence details	UNP P02649
A	28	SER	GLN	see sequence details	UNP P02649
A	99	ARG	CYS	variant	UNP P02649
A	129	ILE	ARG	see sequence details	UNP P02649
A	130	ALA	LYS	see sequence details	UNP P02649
A	132	GLN	ARG	see sequence details	UNP P02649
A	133	LEU	LYS	see sequence details	UNP P02649
A	136	ILE	LEU	see sequence details	UNP P02649
A	137	GLY	ARG	see sequence details	UNP P02649
A	140	PHE	ASP	see sequence details	UNP P02649
A	154	ALA	ARG	see sequence details	UNP P02649
A	156	GLN	-	cloning artifact	UNP P02649
C	1	MET	-	initiating methionine	UNP P02649
C	2	HIS	-	expression tag	UNP P02649

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	HIS	-	expression tag	UNP P02649
C	4	HIS	-	expression tag	UNP P02649
C	5	HIS	-	expression tag	UNP P02649
C	6	HIS	-	expression tag	UNP P02649
C	7	HIS	-	expression tag	UNP P02649
C	8	GLY	-	expression tag	UNP P02649
C	9	SER	-	expression tag	UNP P02649
C	21	LEU	TRP	see sequence details	UNP P02649
C	22	GLU	ASP	see sequence details	UNP P02649
C	25	SER	ARG	see sequence details	UNP P02649
C	28	SER	GLN	see sequence details	UNP P02649
C	99	ARG	CYS	variant	UNP P02649
C	129	ILE	ARG	see sequence details	UNP P02649
C	130	ALA	LYS	see sequence details	UNP P02649
C	132	GLN	ARG	see sequence details	UNP P02649
C	133	LEU	LYS	see sequence details	UNP P02649
C	136	ILE	LEU	see sequence details	UNP P02649
C	137	GLY	ARG	see sequence details	UNP P02649
C	140	PHE	ASP	see sequence details	UNP P02649
C	154	ALA	ARG	see sequence details	UNP P02649
C	156	GLN	-	cloning artifact	UNP P02649

- Molecule 2 is a protein called Apoptosis regulator Bcl-2, Apoptosis regulator Bcl-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1102	707	189	201	5			
2	D	139	Total	C	N	O	S	0	0	0
			1096	702	185	203	6			

There are 32 discrepancies between the modelled and reference sequences:

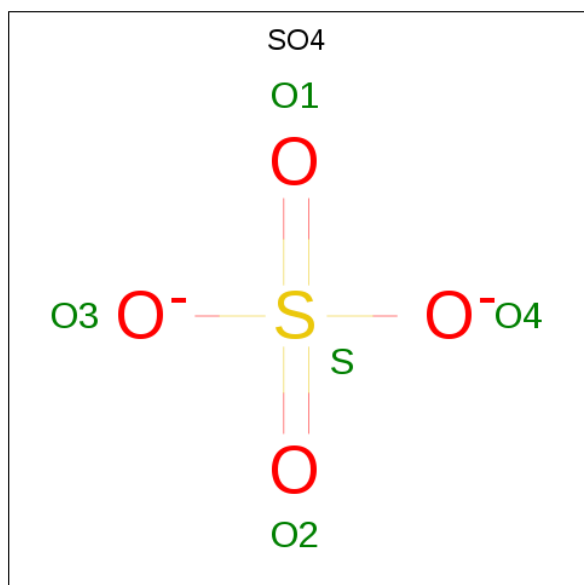
Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ASP	-	linker	UNP P10415
B	36	VAL	-	linker	UNP P10415
B	37	GLU	-	linker	UNP P10415
B	38	GLU	-	linker	UNP P10415
B	39	ASN	-	linker	UNP P10415
B	40	ARG	-	linker	UNP P10415
B	41	THR	-	linker	UNP P10415
B	42	GLU	-	linker	UNP P10415
B	43	ALA	-	linker	UNP P10415

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Chain	Residue	Modelled	Actual	Comment	Reference
B	44	PRO	-	linker	UNP P10415
B	45	GLU	-	linker	UNP P10415
B	46	GLY	-	linker	UNP P10415
B	47	THR	-	linker	UNP P10415
B	48	GLU	-	linker	UNP P10415
B	49	SER	-	linker	UNP P10415
B	50	GLU	-	linker	UNP P10415
D	35	ASP	-	linker	UNP P10415
D	36	VAL	-	linker	UNP P10415
D	37	GLU	-	linker	UNP P10415
D	38	GLU	-	linker	UNP P10415
D	39	ASN	-	linker	UNP P10415
D	40	ARG	-	linker	UNP P10415
D	41	THR	-	linker	UNP P10415
D	42	GLU	-	linker	UNP P10415
D	43	ALA	-	linker	UNP P10415
D	44	PRO	-	linker	UNP P10415
D	45	GLU	-	linker	UNP P10415
D	46	GLY	-	linker	UNP P10415
D	47	THR	-	linker	UNP P10415
D	48	GLU	-	linker	UNP P10415
D	49	SER	-	linker	UNP P10415
D	50	GLU	-	linker	UNP P10415

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

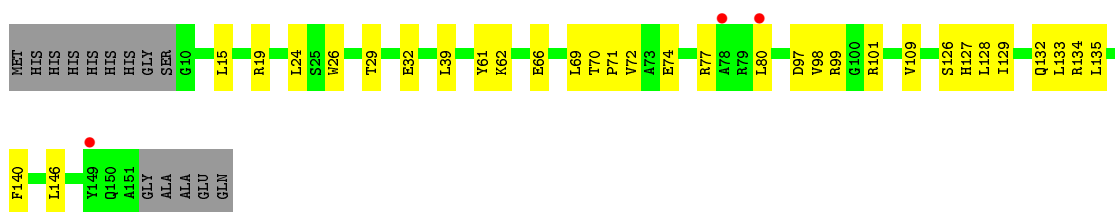
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	C	3	Total O 3 3	0	0
4	D	2	Total O 2 2	0	0

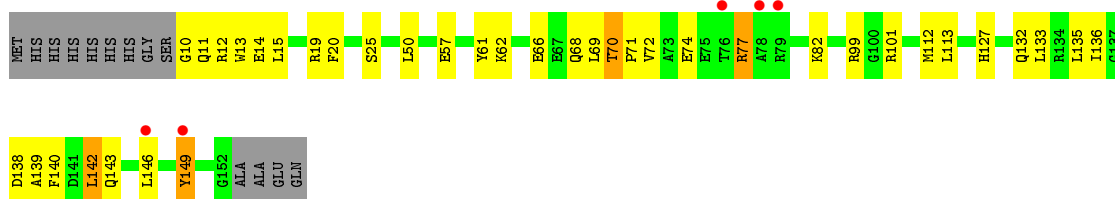
### 3 Residue-property plots [i](#)

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.

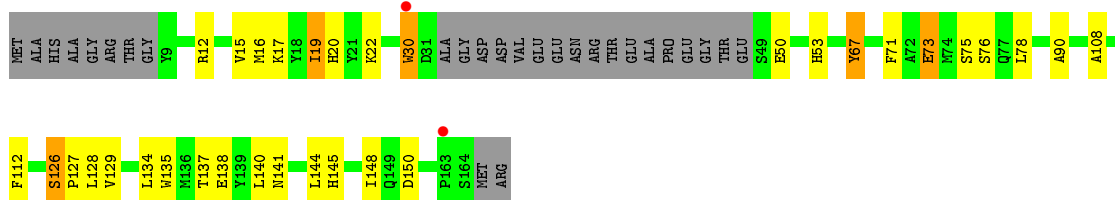
- Molecule 1: Apolipoprotein E



- Molecule 1: Apolipoprotein E

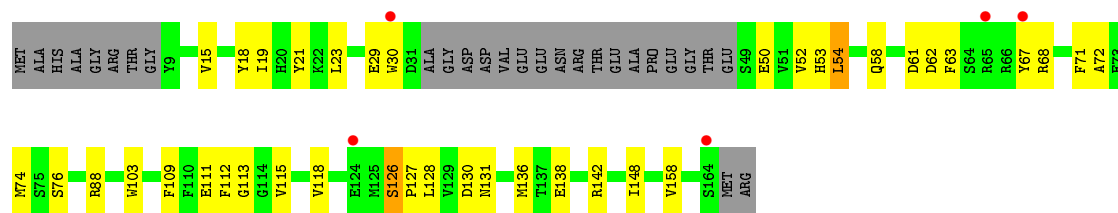


- Molecule 2: Apoptosis regulator Bcl-2, Apoptosis regulator Bcl-2



- Molecule 2: Apoptosis regulator Bcl-2, Apoptosis regulator Bcl-2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.72Å 129.72Å 80.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.02 – 2.50 46.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.1 (46.02-2.50) 85.7 (46.03-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.239 , 0.275 0.239 , 0.275	Depositor DCC
$R_{free}$ test set	1294 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 22.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.25	0/1134	0.44	0/1528
1	C	0.36	1/1134 (0.1%)	0.51	1/1528 (0.1%)
2	B	0.32	0/1132	0.51	1/1538 (0.1%)
2	D	0.27	0/1124	0.43	0/1526
All	All	0.30	1/4524 (0.0%)	0.47	2/6120 (0.0%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	LEU	CG-CD2	-6.23	1.28	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	LEU	CB-CG-CD1	8.07	124.72	111.00
2	B	19	ILE	CG1-CB-CG2	-6.96	96.09	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	70	THR	Peptide
1	C	77	ARG	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	1123	0	1126	21	0
1	C	1123	0	1123	45	0
2	B	1102	0	1000	31	0
2	D	1096	0	999	27	0
3	A	10	0	0	1	0
4	A	4	0	0	0	0
4	C	3	0	0	1	0
4	D	2	0	0	0	0
All	All	4463	0	4248	112	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 13.

The worst 5 of 112 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:C:142:LEU:H	1:C:142:LEU:HD23	1.24	1.02
2:B:138:GLU:OE1	2:B:138:GLU:N	1.94	1.00
1:C:142:LEU:N	1:C:142:LEU:HD23	1.82	0.90
2:B:140:LEU:HA	2:B:144:LEU:HB2	1.62	0.82
1:C:142:LEU:HG	1:C:143:GLN:N	1.96	0.81

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	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
1	C	141/156 (90%)	134 (95%)	6 (4%)	1 (1%)	22	39
2	B	135/166 (81%)	118 (87%)	14 (10%)	3 (2%)	6	10
2	D	135/166 (81%)	122 (90%)	12 (9%)	1 (1%)	22	39
All	All	551/644 (86%)	508 (92%)	38 (7%)	5 (1%)	17	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	GLU
2	B	126	SER
1	C	71	PRO
2	B	67	TYR
2	D	126	SER

### 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	116/130 (89%)	113 (97%)	3 (3%)	46	72
1	C	115/130 (88%)	113 (98%)	2 (2%)	60	82
2	B	109/141 (77%)	106 (97%)	3 (3%)	43	70
2	D	110/141 (78%)	106 (96%)	4 (4%)	35	61
All	All	450/542 (83%)	438 (97%)	12 (3%)	44	71

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	150	ASP
1	C	135	LEU

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Mol	Chain	Res	Type
2	D	76	SER
2	B	128	LEU
2	D	54	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	C	88	GLN
1	C	132	GLN
1	C	143	GLN
2	D	131	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](#)

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	$\# Z  > 2$
3	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.06	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	142/156 (91%)	0.07	3 (2%) 63 66	29, 53, 118, 140	0
1	C	143/156 (91%)	0.07	5 (3%) 44 47	31, 55, 116, 131	0
2	B	139/166 (83%)	0.10	2 (1%) 75 77	30, 64, 93, 111	0
2	D	139/166 (83%)	0.22	5 (3%) 42 46	28, 64, 93, 123	0
All	All	563/644 (87%)	0.11	15 (2%) 54 58	28, 60, 107, 140	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TYR	4.3
1	A	78	ALA	3.7
1	C	146	LEU	3.2
1	C	76	THR	3.1
2	D	67	TYR	2.9

### 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<sup>th</sup> 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	A	202	5/5	0.94	0.11	93,102,118,126	0
3	SO4	A	201	5/5	0.96	0.11	51,52,60,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.