



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 03:46 AM EDT

PDB ID : 3D8K  
Title : Crystal structure of a phosphatase from a toxoplasma gondii  
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Deposited on : 2008-05-23  
Resolution : 2.71 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

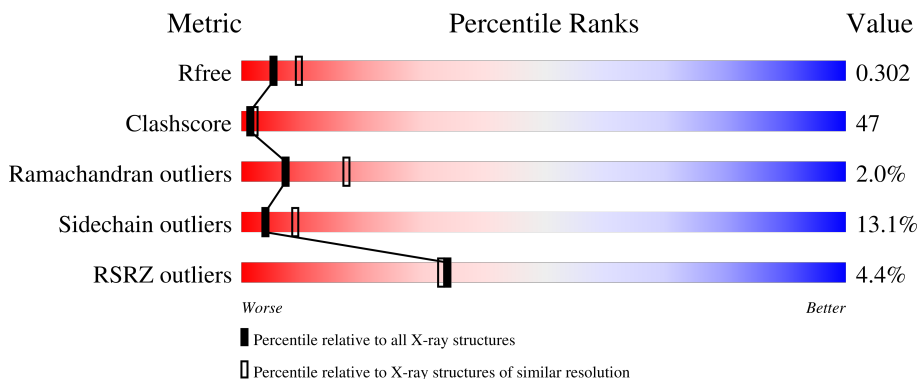
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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  $\geq 3$ , 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	377	
1	B	377	
1	C	377	
1	D	377	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10892 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 Protein phosphatase 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2664	1656	498	497	2	11			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2679	1662	499	505	2	11			
1	C	351	Total	C	N	O	S	Se	0	0	0
			2696	1674	503	507	2	10			
1	D	346	Total	C	N	O	S	Se	0	0	0
			2652	1645	496	499	2	10			

There are 44 discrepancies between the modelled and reference sequences:

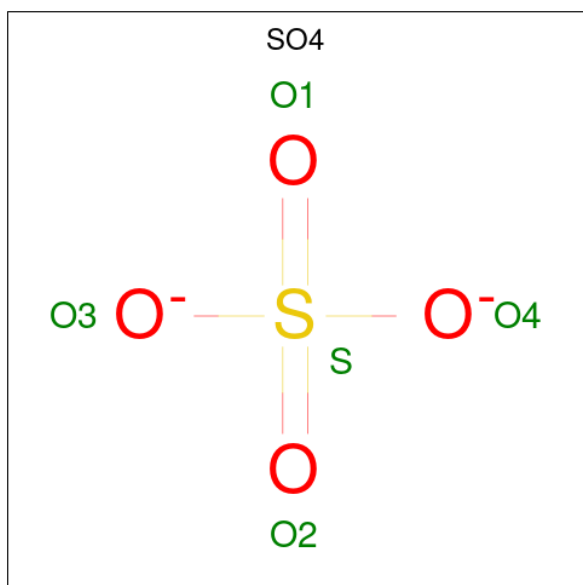
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MSE	-	expression tag	UNP A4GX63
A	77	SER	-	expression tag	UNP A4GX63
A	78	LEU	-	expression tag	UNP A4GX63
A	445	GLU	-	expression tag	UNP A4GX63
A	446	GLY	-	expression tag	UNP A4GX63
A	447	HIS	-	expression tag	UNP A4GX63
A	448	HIS	-	expression tag	UNP A4GX63
A	449	HIS	-	expression tag	UNP A4GX63
A	450	HIS	-	expression tag	UNP A4GX63
A	451	HIS	-	expression tag	UNP A4GX63
A	452	HIS	-	expression tag	UNP A4GX63
B	76	MSE	-	expression tag	UNP A4GX63
B	77	SER	-	expression tag	UNP A4GX63
B	78	LEU	-	expression tag	UNP A4GX63
B	445	GLU	-	expression tag	UNP A4GX63
B	446	GLY	-	expression tag	UNP A4GX63
B	447	HIS	-	expression tag	UNP A4GX63
B	448	HIS	-	expression tag	UNP A4GX63
B	449	HIS	-	expression tag	UNP A4GX63
B	450	HIS	-	expression tag	UNP A4GX63
B	451	HIS	-	expression tag	UNP A4GX63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	HIS	-	expression tag	UNP A4GX63
C	76	MSE	-	expression tag	UNP A4GX63
C	77	SER	-	expression tag	UNP A4GX63
C	78	LEU	-	expression tag	UNP A4GX63
C	445	GLU	-	expression tag	UNP A4GX63
C	446	GLY	-	expression tag	UNP A4GX63
C	447	HIS	-	expression tag	UNP A4GX63
C	448	HIS	-	expression tag	UNP A4GX63
C	449	HIS	-	expression tag	UNP A4GX63
C	450	HIS	-	expression tag	UNP A4GX63
C	451	HIS	-	expression tag	UNP A4GX63
C	452	HIS	-	expression tag	UNP A4GX63
D	76	MSE	-	expression tag	UNP A4GX63
D	77	SER	-	expression tag	UNP A4GX63
D	78	LEU	-	expression tag	UNP A4GX63
D	445	GLU	-	expression tag	UNP A4GX63
D	446	GLY	-	expression tag	UNP A4GX63
D	447	HIS	-	expression tag	UNP A4GX63
D	448	HIS	-	expression tag	UNP A4GX63
D	449	HIS	-	expression tag	UNP A4GX63
D	450	HIS	-	expression tag	UNP A4GX63
D	451	HIS	-	expression tag	UNP A4GX63
D	452	HIS	-	expression tag	UNP A4GX63

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).

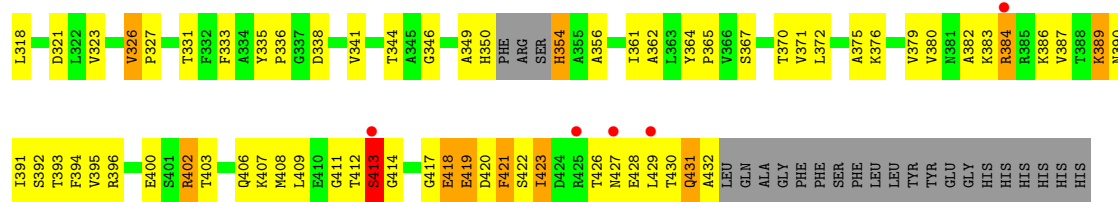


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

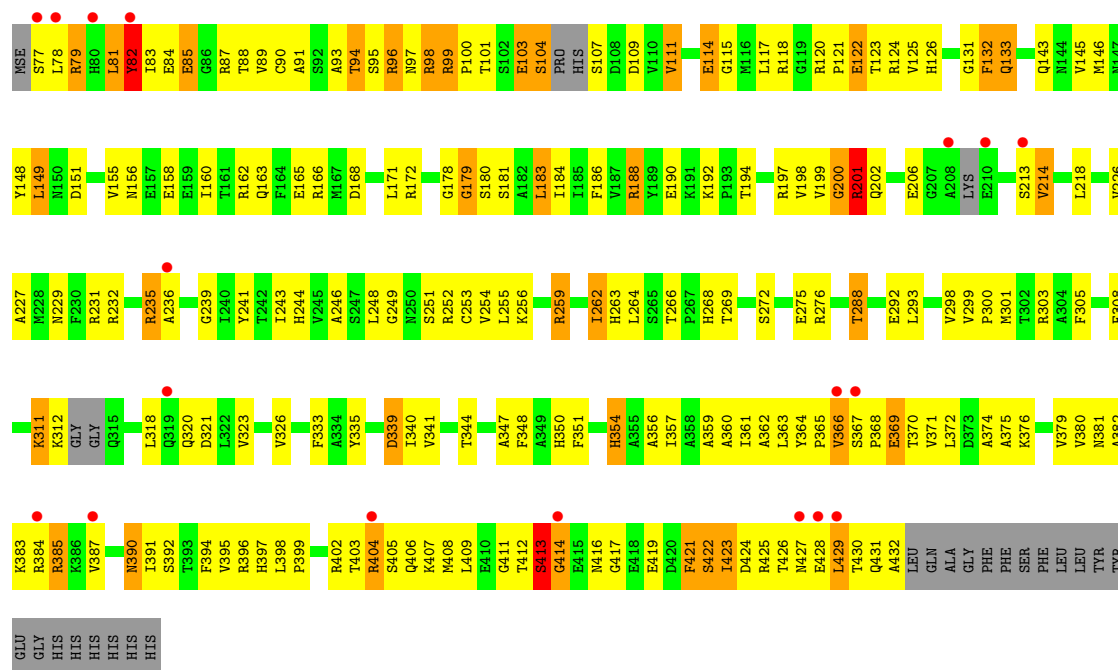
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	42	Total	O	0	0
			42	42		
3	C	50	Total	O	0	0
			50	50		
3	D	39	Total	O	0	0
			39	39		

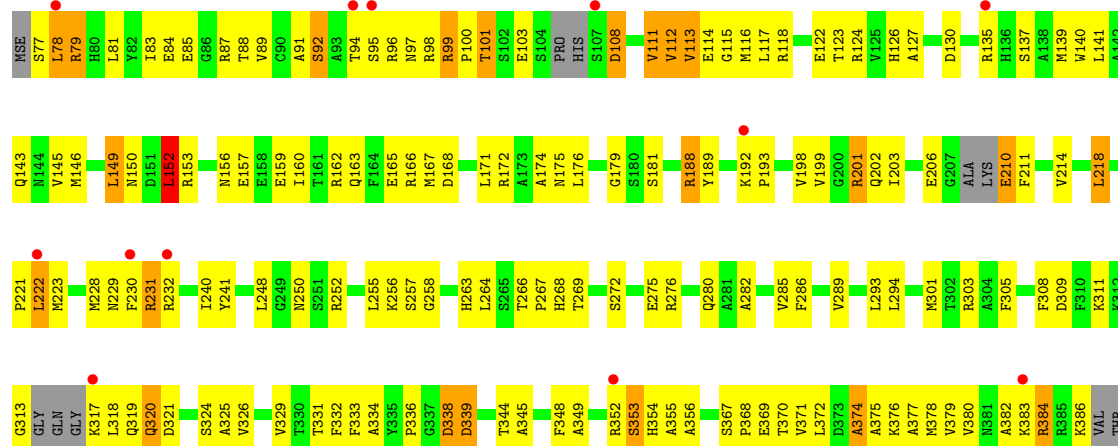
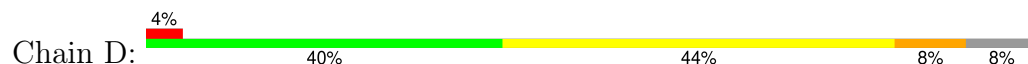


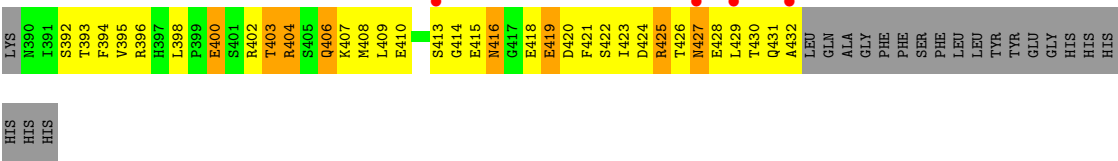


• Molecule 1: Protein phosphatase 2C



• Molecule 1: Protein phosphatase 2C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.88Å 169.05Å 87.01Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	46.71 – 2.71 46.84 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.6 (46.71-2.71) 91.8 (46.84-2.59)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.251 , 0.304 0.250 , 0.302	Depositor DCC
$R_{free}$ test set	1052 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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	0.48	0/2700	0.84	6/3628 (0.2%)
1	B	0.44	0/2714	0.74	2/3646 (0.1%)
1	C	0.45	0/2732	0.80	6/3671 (0.2%)
1	D	0.43	0/2686	0.80	5/3607 (0.1%)
All	All	0.45	0/10832	0.79	19/14552 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	GLY	N-CA-C	-10.70	86.35	113.10
1	A	389	LYS	N-CA-C	-10.67	82.19	111.00
1	D	414	GLY	N-CA-C	-10.16	87.70	113.10
1	A	385	ARG	N-CA-C	-8.97	86.77	111.00
1	B	414	GLY	N-CA-C	-8.52	91.80	113.10

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	2664	0	2646	280	0
1	B	2679	0	2663	239	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2696	0	2680	270	0
1	D	2652	0	2630	240	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
3	A	50	0	0	2	0
3	B	42	0	0	6	0
3	C	50	0	0	7	0
3	D	39	0	0	4	0
All	All	10892	0	10619	999	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 47.

The worst 5 of 999 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:87:ARG:HH11	1:D:84:GLU:HG2	1.05	1.16
1:D:222:LEU:O	1:D:223:MSE:HE2	1.45	1.15
1:D:371:VAL:HG23	1:D:427:ASN:HD22	0.96	1.13
1:B:98:ARG:HG2	1:B:146:MSE:HG3	1.26	1.12
1:D:221:PRO:HB2	1:D:223:MSE:HE3	1.31	1.12

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	340/377 (90%)	302 (89%)	30 (9%)	8 (2%)	6	13
1	B	342/377 (91%)	299 (87%)	36 (10%)	7 (2%)	7	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	343/377 (91%)	298 (87%)	38 (11%)	7 (2%)	7	17
1	D	336/377 (89%)	296 (88%)	35 (10%)	5 (2%)	10	24
All	All	1361/1508 (90%)	1195 (88%)	139 (10%)	27 (2%)	7	17

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	220	GLY
1	A	413	SER
1	C	214	VAL
1	D	78	LEU

### 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	280/295 (95%)	243 (87%)	37 (13%)	4	8
1	B	283/295 (96%)	246 (87%)	37 (13%)	4	9
1	C	285/295 (97%)	246 (86%)	39 (14%)	3	8
1	D	280/295 (95%)	245 (88%)	35 (12%)	4	10
All	All	1128/1180 (96%)	980 (87%)	148 (13%)	4	9

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	ARG
1	D	416	ASN
1	D	113	VAL
1	D	231	ARG
1	B	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	147	ASN
1	D	431	GLN
1	D	163	GLN
1	D	320	GLN
1	B	156	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](#)

4 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	SO4	C	453	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	C	454	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	B	453	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	A	453	-	4,4,4	0.18	0	6,6,6	0.14	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
2	C	453	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	337/377 (89%)	0.24	13 (3%) 39 39	13, 32, 56, 75	0
1	B	339/377 (89%)	0.22	13 (3%) 40 40	9, 33, 51, 82	0
1	C	341/377 (90%)	0.24	18 (5%) 26 25	10, 29, 55, 65	0
1	D	336/377 (89%)	0.28	16 (4%) 30 29	14, 33, 58, 74	0
All	All	1353/1508 (89%)	0.24	60 (4%) 34 33	9, 32, 56, 82	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	ALA	5.1
1	C	78	LEU	4.9
1	D	95	SER	4.2
1	C	414	GLY	4.1
1	A	77	SER	4.0

### 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<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
2	SO4	C	453	5/5	0.89	0.18	82,82,82,83	0
2	SO4	B	453	5/5	0.94	0.18	60,61,62,63	0
2	SO4	C	454	5/5	0.94	0.17	61,62,62,63	0
2	SO4	A	453	5/5	0.97	0.16	38,39,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.