



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 11:33 pm GMT

PDB ID : 1D8C  
Title : MALATE SYNTHASE G COMPLEXED WITH MAGNESIUM AND GLY-  
OXYLATE  
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Deposited on : 1999-10-22  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

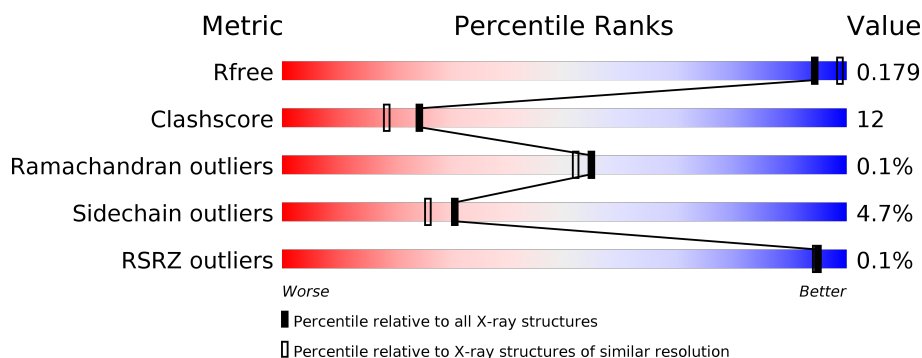
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	723	 66% 28% . . .

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
2	SOR	A	4000	-	-	-	X
4	SO4	A	5000	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	8000	-	-	-	X
4	SO4	A	9000	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5719 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.

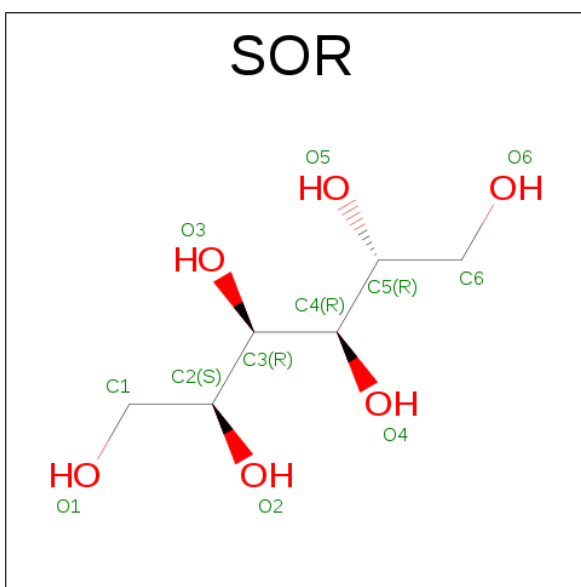
- Molecule 1 is a protein called MALATE SYNTHASE G.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	Se	0	0	0
			5331	3365	930	1009	6	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CONFLICT	UNP P37330
A	2	ALA	SER	ENGINEERED	UNP P37330
A	122	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	154	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	294	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	302	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	344	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	366	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	393	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	412	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	415	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	422	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	425	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	461	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	465	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	470	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	476	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	508	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	511	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	515	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	518	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	629	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	663	MSE	MET	MODIFIED RESIDUE	UNP P37330
A	680	MSE	MET	MODIFIED RESIDUE	UNP P37330

- Molecule 2 is D-SORBITOL (three-letter code: SOR) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>).

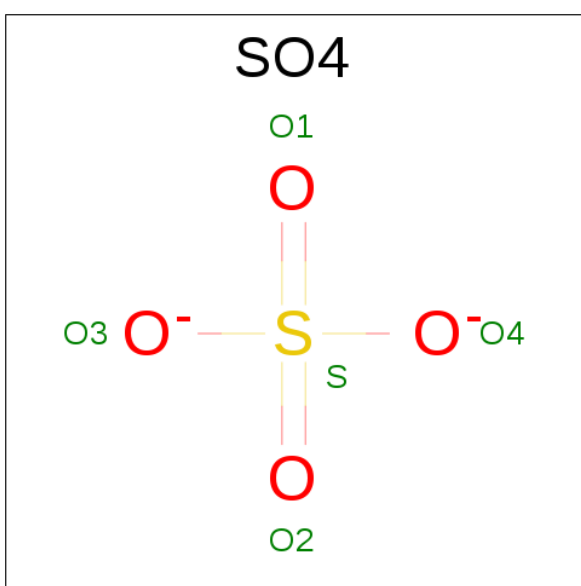


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

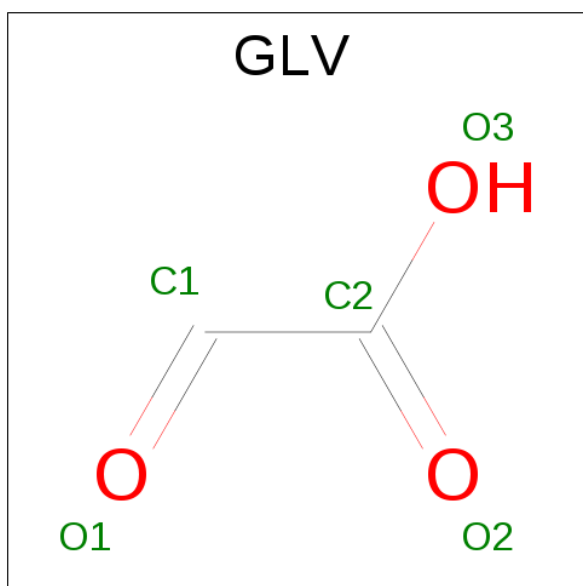
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 5 is GLYOXYLIC ACID (three-letter code: GLV) (formula:  $C_2H_2O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 5 2 3	0	0

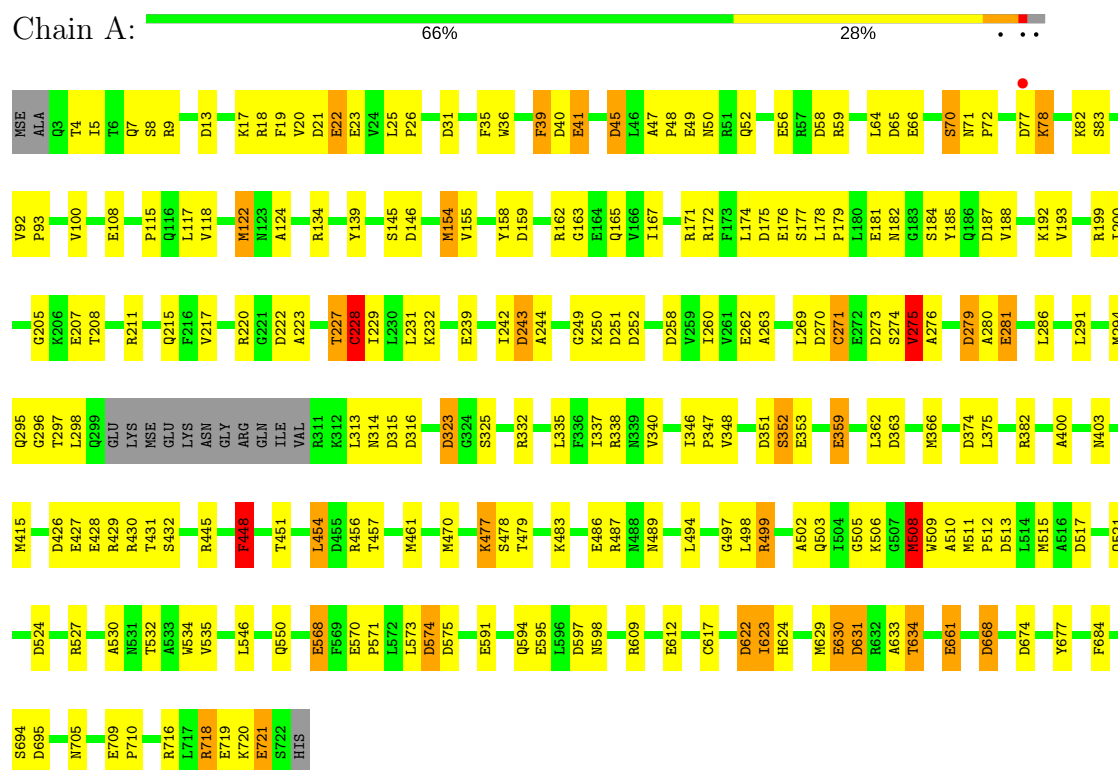
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	345	Total O 345 345	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: MALATE SYNTHASE G



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.80Å 88.70Å 109.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.00) 99.5 (19.90-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.01Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.174 , 0.179	Depositor DCC
$R_{free}$ test set	2520 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 114.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MG, SOR, SO4, GLV

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	1.02	24/5416 (0.4%)	1.51	101/7345 (1.4%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CD-OE2	8.08	1.34	1.25
1	A	262	GLU	CD-OE2	7.75	1.34	1.25
1	A	630	GLU	CD-OE2	7.45	1.33	1.25
1	A	486	GLU	CD-OE2	6.82	1.33	1.25
1	A	41	GLU	CD-OE2	6.63	1.32	1.25

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	A	382	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	382	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	243	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	A	175	ASP	CB-CG-OD1	9.12	126.51	118.30

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	5331	0	5096	130	0
2	A	12	0	14	0	0
3	A	1	0	0	0	0
4	A	25	0	0	1	0
5	A	5	0	1	0	0
6	A	345	0	0	9	0
All	All	5719	0	5111	130	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 12.

The worst 5 of 130 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:346:ILE:HG13	1:A:347:PRO:HD2	1.40	1.03
1:A:122:MSE:HE2	1:A:276:ALA:H	1.23	1.00
1:A:508:MSE:HG3	1:A:534:TRP:HB3	1.51	0.91
1:A:7:GLN:HG2	1:A:36:TRP:HB3	1.53	0.91
1:A:508:MSE:HG3	1:A:534:TRP:CB	2.07	0.85

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	705/723 (98%)	684 (97%)	20 (3%)	1 (0%)	<a href="#">55</a> <a href="#">52</a>

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL

### 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	531/576 (92%)	506 (95%)	25 (5%)	30	26

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	CYS
1	A	275	VAL
1	A	694	SER
1	A	260	ILE
1	A	281	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	ASN
1	A	705	ASN
1	A	441	GLN
1	A	165	GLN
1	A	521	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
5	GLV	A	2000	3	1,4,4	0.67	0	0,4,4	0.00	-
2	SOR	A	4000	-	11,11,11	0.39	0	14,14,14	1.09	0
4	SO4	A	5000	-	4,4,4	0.95	0	6,6,6	0.21	0
4	SO4	A	6000	-	4,4,4	1.00	0	6,6,6	0.37	0
4	SO4	A	7000	-	4,4,4	1.77	1 (25%)	6,6,6	0.32	0
4	SO4	A	8000	-	4,4,4	1.16	0	6,6,6	0.37	0
4	SO4	A	9000	-	4,4,4	0.93	0	6,6,6	0.15	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
5	GLV	A	2000	3	-	0/0/2/2	0/0/0/0
2	SOR	A	4000	-	-	0/16/16/16	0/0/0/0
4	SO4	A	5000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	6000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	7000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	8000	-	-	0/0/0/0	0/0/0/0
4	SO4	A	9000	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7000	SO4	O1-S	2.80	1.60	1.45

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
4	A	6000	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	688/723 (95%)	-0.39	1 (0%) 95 94	17, 29, 53, 71	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	ASP	2.1

### 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	8000	5/5	0.84	0.20	5.31	98,98,100,100	0
2	SOR	A	4000	12/12	0.92	0.16	5.28	24,38,97,100	0
4	SO4	A	9000	5/5	0.87	0.19	4.59	95,95,100,100	0
4	SO4	A	5000	5/5	0.92	0.20	4.13	88,88,89,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GLV	A	2000	5/5	0.97	0.09	0.94	21,23,33,33	0
3	MG	A	3001	1/1	0.99	0.02	-3.82	23,23,23,23	0
4	SO4	A	7000	5/5	0.69	0.37	-	100,100,100,100	0
4	SO4	A	6000	5/5	0.90	0.21	-	77,81,82,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.