



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 11:34 PM GMT

PDB ID : 2PMQ  
Title : Crystal structure of a mandelate racemase/muconate lactonizing enzyme from *Roseovarius* sp. HTCC2601  
Authors : Bonanno, J.B.; Rutter, M.; Bain, K.T.; Lau, C.; Sridhar, V.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-04-23  
Resolution : 1.72 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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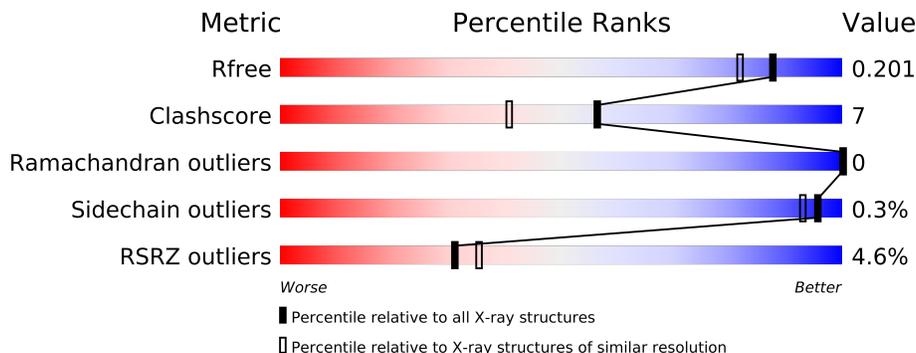
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.72 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))
$R_{free}$	66092	2979 (1.74-1.70)
Clashscore	79885	3506 (1.74-1.70)
Ramachandran outliers	78287	3449 (1.74-1.70)
Sidechain outliers	78261	3449 (1.74-1.70)
RSRZ outliers	66119	2979 (1.74-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	901	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6407 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	367	2827	1791	493	526	9	8	0	7	0
1	B	374	2888	1830	512	530	8	8	0	8	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	CLONING ARTIFACT	UNP Q0FPQ4
A	0	SER	-	CLONING ARTIFACT	UNP Q0FPQ4
A	1	LEU	-	CLONING ARTIFACT	UNP Q0FPQ4
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	217	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	240	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	264	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	275	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	316	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
A	368	GLU	-	CLONING ARTIFACT	UNP Q0FPQ4
A	369	GLY	-	CLONING ARTIFACT	UNP Q0FPQ4
A	370	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
A	371	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
A	372	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
A	373	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
A	374	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
A	375	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	-1	MSE	-	CLONING ARTIFACT	UNP Q0FPQ4
B	0	SER	-	CLONING ARTIFACT	UNP Q0FPQ4
B	1	LEU	-	CLONING ARTIFACT	UNP Q0FPQ4
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	217	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	240	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	275	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	316	MSE	MET	MODIFIED RESIDUE	UNP Q0FPQ4
B	368	GLU	-	CLONING ARTIFACT	UNP Q0FPQ4
B	369	GLY	-	CLONING ARTIFACT	UNP Q0FPQ4
B	370	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	371	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	372	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	373	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	374	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4
B	375	HIS	-	CLONING ARTIFACT	UNP Q0FPQ4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is water.

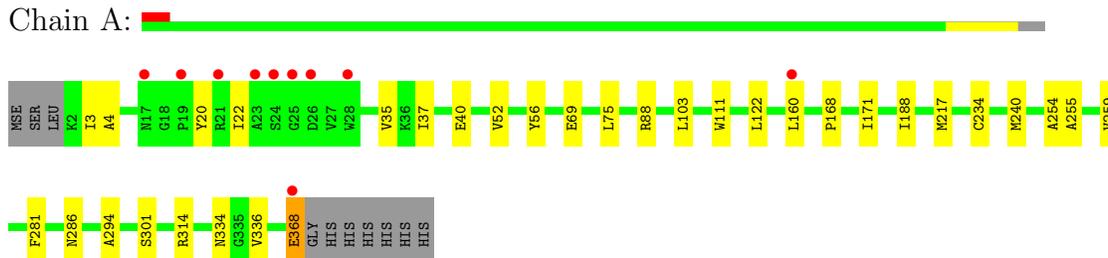
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	364	Total O 364 364	0	0
3	B	323	Total O 323 323	0	0

### 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 errors 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.

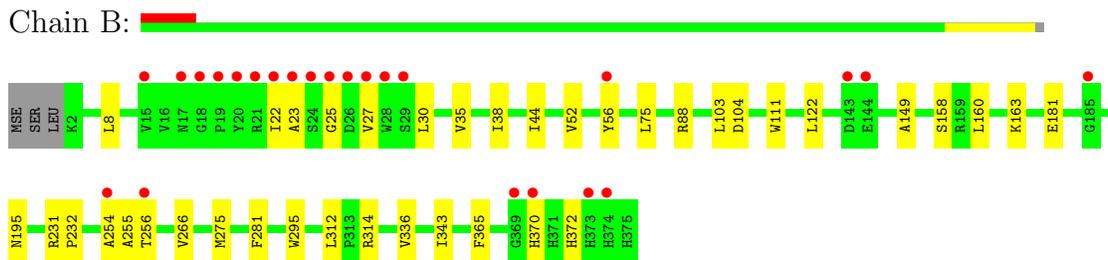
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain A:



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain B:



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.38Å 136.38Å 80.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.72 24.67 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.72) 99.7 (24.67-1.72)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.72Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.165 , 0.191 0.176 , 0.201	Depositor DCC
$R_{free}$ test set	4062 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 81048 reflections	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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

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	0.59	0/2906	0.70	0/3945
1	B	0.57	0/2977	0.68	0/4041
All	All	0.58	0/5883	0.69	0/7986

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	TYR	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2827	0	2785	30	1
1	B	2888	0	2851	44	1
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	364	0	0	5	0
3	B	323	0	0	6	0
All	All	6407	0	5636	74	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:ALA:CB	1:A:281[A]:PHE:HZ	1.25	1.49
1:B:254:ALA:CB	1:B:281[B]:PHE:HZ	1.25	1.46
1:B:254:ALA:CB	1:B:281[B]:PHE:CZ	2.12	1.33
1:A:254:ALA:CB	1:A:281[A]:PHE:CZ	2.11	1.31
1:A:254:ALA:HB3	1:A:281[A]:PHE:HZ	1.06	1.14
1:B:254:ALA:HB3	1:B:281[B]:PHE:HZ	0.95	1.08
1:B:254:ALA:HB3	1:B:281[B]:PHE:CZ	1.80	1.06
1:A:254:ALA:HB2	1:A:281[A]:PHE:HZ	1.17	1.03
1:A:254:ALA:HB2	1:A:281[A]:PHE:CZ	1.90	1.00
1:A:254:ALA:HB3	1:A:281[A]:PHE:CZ	1.86	0.98
1:B:254:ALA:HB2	1:B:281[B]:PHE:CZ	1.97	0.96
1:B:254:ALA:HB2	1:B:281[B]:PHE:HZ	1.28	0.92
1:B:22:ILE:HG13	1:B:163:LYS:HZ3	1.37	0.87
1:A:301:SER:HB3	1:A:336[A]:VAL:CG2	2.06	0.85
1:A:301:SER:HB3	1:A:336[A]:VAL:HG21	1.63	0.79
1:B:22:ILE:HG21	1:B:56:TYR:CE1	2.18	0.77
1:B:22:ILE:CG1	1:B:163:LYS:HZ3	2.00	0.75
1:B:22:ILE:HG21	1:B:56:TYR:HE1	1.51	0.73
1:B:22:ILE:CG1	1:B:163:LYS:NZ	2.54	0.70
1:A:75:LEU:HD23	1:A:88:ARG:HG2	1.75	0.69
1:B:75:LEU:HD23	1:B:88:ARG:HG2	1.76	0.68
1:B:22:ILE:HG13	1:B:163:LYS:NZ	2.08	0.67
1:B:254:ALA:HB1	1:B:281[B]:PHE:CZ	2.28	0.66
1:B:256:THR:HA	3:B:1131:HOH:O	1.96	0.64
1:A:22:ILE:HG21	1:A:56[B]:TYR:CE2	2.32	0.64
1:B:22:ILE:HG23	1:B:163:LYS:HZ1	1.62	0.63
1:B:22:ILE:HG23	1:B:163:LYS:NZ	2.14	0.62
1:A:254:ALA:HB1	1:A:281[A]:PHE:CZ	2.28	0.60
1:B:254:ALA:HB2	1:B:281[B]:PHE:CE2	2.37	0.60
1:A:254:ALA:HA	3:A:1139:HOH:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:ALA:O	1:A:368:GLU:HB3	2.02	0.59
1:B:254:ALA:HA	3:B:1057:HOH:O	2.04	0.58
1:A:254:ALA:HB2	1:A:281[A]:PHE:CE2	2.36	0.57
1:B:370[A]:HIS:CD2	3:B:1124:HOH:O	2.57	0.57
1:B:27:VAL:HG11	1:B:52:VAL:HG12	1.87	0.56
1:B:23:ALA:HB3	1:B:195:ASN:HB2	1.87	0.56
1:B:266:VAL:HG22	1:B:275:MSE:HG3	1.88	0.56
1:B:8:LEU:CD2	1:B:35[A]:VAL:HG12	2.36	0.55
1:A:52:VAL:HG23	1:A:294:ALA:HB1	1.88	0.55
1:A:40:GLU:OE1	3:A:1213:HOH:O	2.18	0.55
1:A:22:ILE:HG21	1:A:56[B]:TYR:HE2	1.70	0.54
1:B:370[A]:HIS:HD2	3:B:1124:HOH:O	1.90	0.54
1:B:312:LEU:HG	1:B:314:ARG:HG2	1.91	0.53
1:A:301:SER:CB	1:A:336[A]:VAL:CG2	2.82	0.53
1:B:22:ILE:HD13	1:B:25:GLY:O	2.09	0.52
1:B:336[A]:VAL:HG13	1:B:343:ILE:HG23	1.90	0.52
1:B:30:LEU:HD12	1:B:295:TRP:CE2	2.45	0.51
1:A:35:VAL:HG11	1:A:103:LEU:HD23	1.92	0.51
1:B:231:ARG:HB3	1:B:232:PRO:HD3	1.93	0.51
1:B:22:ILE:CG2	1:B:163:LYS:HZ1	2.25	0.50
1:B:158:SER:OG	3:B:1210:HOH:O	2.19	0.50
1:B:22:ILE:HG23	1:B:163:LYS:CE	2.42	0.49
1:A:160:LEU:HD12	1:A:188:ILE:HD13	1.95	0.48
1:B:23:ALA:HB3	1:B:195:ASN:CB	2.42	0.48
1:A:334:ASN:ND2	3:A:1266:HOH:O	2.45	0.48
1:B:181:GLU:HG2	3:B:1070:HOH:O	2.14	0.48
1:B:30:LEU:HD13	1:B:295:TRP:CG	2.49	0.48
1:B:163:LYS:HE3	1:B:195:ASN:HD21	1.79	0.47
1:B:111:TRP:CE3	1:B:122:LEU:HD13	2.49	0.47
1:A:254:ALA:HB3	1:A:281[A]:PHE:CE1	2.46	0.45
1:B:38:ILE:HG12	1:B:44:ILE:HG22	1.99	0.45
1:A:240:MSE:HB2	1:A:259:VAL:HG11	1.99	0.45
1:B:22:ILE:HG21	1:B:56:TYR:CD1	2.52	0.45
1:B:149:ALA:CB	1:B:160:LEU:HD21	2.48	0.43
1:A:217[B]:MSE:SE	1:A:234[B]:CYS:SG	3.27	0.42
1:A:69:GLU:OE1	3:A:1134:HOH:O	2.21	0.42
1:A:168:PRO:HD2	1:A:171:ILE:HD12	2.02	0.42
1:A:56[B]:TYR:HD2	3:A:1263:HOH:O	2.04	0.41
1:B:30:LEU:CD1	1:B:295:TRP:CE2	3.03	0.41
1:B:365:PHE:CZ	1:B:372:HIS:HB2	2.56	0.41
1:B:35[B]:VAL:HG11	1:B:103:LEU:HD23	2.03	0.41
1:A:3:ILE:HG23	1:A:37:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:TRP:CE3	1:A:122:LEU:HD13	2.55	0.40
1:A:286:ASN:OD1	1:A:314:ARG:NH1	2.48	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:255:ALA:CB	1:B:255:ALA:CB[4_555]	1.98	0.22

## 5.3 Torsion angles

### 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	372/377 (99%)	368 (99%)	4 (1%)	0	100	100
1	B	380/377 (101%)	377 (99%)	3 (1%)	0	100	100
All	All	752/754 (100%)	745 (99%)	7 (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	293/287 (102%)	292 (100%)	1 (0%)	96	93
1	B	300/287 (104%)	299 (100%)	1 (0%)	96	93
All	All	593/574 (103%)	591 (100%)	2 (0%)	96	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	B	104	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	B	195	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	367/377 (97%)	-0.01	10 (2%) 52 58	11, 18, 29, 38	0
1	B	374/377 (99%)	0.27	24 (6%) 19 22	11, 18, 36, 50	0
All	All	741/754 (98%)	0.13	34 (4%) 31 35	11, 18, 32, 50	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	TRP	10.4
1	B	23	ALA	10.4
1	B	27	VAL	9.7
1	B	22	ILE	7.1
1	B	26	ASP	6.9
1	A	28[A]	TRP	5.6
1	B	18	GLY	5.1
1	B	21	ARG	5.1
1	A	23	ALA	4.9
1	B	20	TYR	4.6
1	B	25	GLY	4.2
1	B	19	PRO	4.1
1	B	24	SER	4.0
1	B	56	TYR	3.5
1	A	24	SER	3.5
1	B	143	ASP	3.4
1	B	144	GLU	3.2
1	A	25	GLY	3.2
1	B	29	SER	3.1
1	A	368	GLU	3.1
1	B	17	ASN	3.0
1	A	26	ASP	2.6
1	B	254	ALA	2.6
1	A	17	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	369	GLY	2.5
1	B	370[A]	HIS	2.3
1	A	19	PRO	2.3
1	B	15	VAL	2.3
1	A	21	ARG	2.2
1	B	256	THR	2.2
1	B	374	HIS	2.1
1	B	185	GLY	2.1
1	B	373	HIS	2.0
1	A	160	LEU	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 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	MG	A	901	1/1	0.20	2.81	31,31,31,31	0
2	MG	B	904	1/1	0.05	-1.28	19,19,19,19	0
2	MG	A	902	1/1	0.05	-1.83	18,18,18,18	0
2	MG	B	905	1/1	0.08	-	14,14,14,14	1
2	MG	A	903	1/1	0.05	-	12,12,12,12	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.