Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2021 – 01:49 PM EST

PDB ID	:	3BJS
Title	:	Crystal structure of a member of enolase superfamily from Polaromonas sp. JS666
Authors	:	Patskovsky, Y.; Bonanno, J.B.; Ozyurt, S.; Dickey, M.; Sauder, J.M.; Reyes, C.; Groshong, C.; Gheyi, T.; Smith, D.; Wasserman, S.R.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-12-04
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ①) were used in the production of this report:

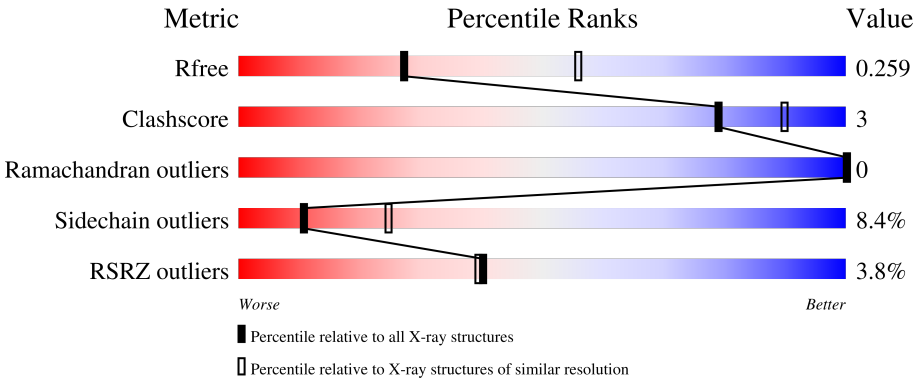
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 >=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 <=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	428	4% 77% 9% 14%
1	B	428	3% 75% 13% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5730 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	4	0
			2831	1793	501	521	16			
1	B	376	Total	C	N	O	S	0	4	0
			2870	1820	505	529	16			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q120Q7
A	0	SER	-	expression tag	UNP Q120Q7
A	1	LEU	-	expression tag	UNP Q120Q7
A	2	GLN	-	expression tag	UNP Q120Q7
A	3	TRP	-	expression tag	UNP Q120Q7
A	4	GLU	-	expression tag	UNP Q120Q7
A	5	CYS	-	expression tag	UNP Q120Q7
A	6	TRP	-	expression tag	UNP Q120Q7
A	7	PRO	-	expression tag	UNP Q120Q7
A	8	SER	-	expression tag	UNP Q120Q7
A	9	LEU	-	expression tag	UNP Q120Q7
A	10	PRO	-	expression tag	UNP Q120Q7
A	11	CYS	-	expression tag	UNP Q120Q7
A	12	TRP	-	expression tag	UNP Q120Q7
A	13	ARG	-	expression tag	UNP Q120Q7
A	14	CYS	-	expression tag	UNP Q120Q7
A	15	PHE	-	expression tag	UNP Q120Q7
A	16	ALA	-	expression tag	UNP Q120Q7
A	17	ALA	-	expression tag	UNP Q120Q7
A	18	SER	-	expression tag	UNP Q120Q7
A	19	GLY	-	expression tag	UNP Q120Q7
A	20	ARG	-	expression tag	UNP Q120Q7
A	21	ILE	-	expression tag	UNP Q120Q7
A	22	THR	-	expression tag	UNP Q120Q7
A	23	LEU	-	expression tag	UNP Q120Q7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q120Q7
A	25	ILE	-	expression tag	UNP Q120Q7
A	26	LYS	-	expression tag	UNP Q120Q7
A	27	ARG	-	expression tag	UNP Q120Q7
A	28	PHE	-	expression tag	UNP Q120Q7
A	29	THR	-	expression tag	UNP Q120Q7
A	30	GLN	-	expression tag	UNP Q120Q7
A	31	ASN	-	expression tag	UNP Q120Q7
A	32	SER	-	expression tag	UNP Q120Q7
A	33	ARG	-	expression tag	UNP Q120Q7
A	34	ARG	-	expression tag	UNP Q120Q7
A	35	HIS	-	expression tag	UNP Q120Q7
A	36	ASP	-	expression tag	UNP Q120Q7
A	419	GLU	-	expression tag	UNP Q120Q7
A	420	GLY	-	expression tag	UNP Q120Q7
A	421	HIS	-	expression tag	UNP Q120Q7
A	422	HIS	-	expression tag	UNP Q120Q7
A	423	HIS	-	expression tag	UNP Q120Q7
A	424	HIS	-	expression tag	UNP Q120Q7
A	425	HIS	-	expression tag	UNP Q120Q7
A	426	HIS	-	expression tag	UNP Q120Q7
B	-1	MET	-	expression tag	UNP Q120Q7
B	0	SER	-	expression tag	UNP Q120Q7
B	1	LEU	-	expression tag	UNP Q120Q7
B	2	GLN	-	expression tag	UNP Q120Q7
B	3	TRP	-	expression tag	UNP Q120Q7
B	4	GLU	-	expression tag	UNP Q120Q7
B	5	CYS	-	expression tag	UNP Q120Q7
B	6	TRP	-	expression tag	UNP Q120Q7
B	7	PRO	-	expression tag	UNP Q120Q7
B	8	SER	-	expression tag	UNP Q120Q7
B	9	LEU	-	expression tag	UNP Q120Q7
B	10	PRO	-	expression tag	UNP Q120Q7
B	11	CYS	-	expression tag	UNP Q120Q7
B	12	TRP	-	expression tag	UNP Q120Q7
B	13	ARG	-	expression tag	UNP Q120Q7
B	14	CYS	-	expression tag	UNP Q120Q7
B	15	PHE	-	expression tag	UNP Q120Q7
B	16	ALA	-	expression tag	UNP Q120Q7
B	17	ALA	-	expression tag	UNP Q120Q7
B	18	SER	-	expression tag	UNP Q120Q7
B	19	GLY	-	expression tag	UNP Q120Q7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ARG	-	expression tag	UNP Q120Q7
B	21	ILE	-	expression tag	UNP Q120Q7
B	22	THR	-	expression tag	UNP Q120Q7
B	23	LEU	-	expression tag	UNP Q120Q7
B	24	SER	-	expression tag	UNP Q120Q7
B	25	ILE	-	expression tag	UNP Q120Q7
B	26	LYS	-	expression tag	UNP Q120Q7
B	27	ARG	-	expression tag	UNP Q120Q7
B	28	PHE	-	expression tag	UNP Q120Q7
B	29	THR	-	expression tag	UNP Q120Q7
B	30	GLN	-	expression tag	UNP Q120Q7
B	31	ASN	-	expression tag	UNP Q120Q7
B	32	SER	-	expression tag	UNP Q120Q7
B	33	ARG	-	expression tag	UNP Q120Q7
B	34	ARG	-	expression tag	UNP Q120Q7
B	35	HIS	-	expression tag	UNP Q120Q7
B	36	ASP	-	expression tag	UNP Q120Q7
B	419	GLU	-	expression tag	UNP Q120Q7
B	420	GLY	-	expression tag	UNP Q120Q7
B	421	HIS	-	expression tag	UNP Q120Q7
B	422	HIS	-	expression tag	UNP Q120Q7
B	423	HIS	-	expression tag	UNP Q120Q7
B	424	HIS	-	expression tag	UNP Q120Q7
B	425	HIS	-	expression tag	UNP Q120Q7
B	426	HIS	-	expression tag	UNP Q120Q7

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is water.

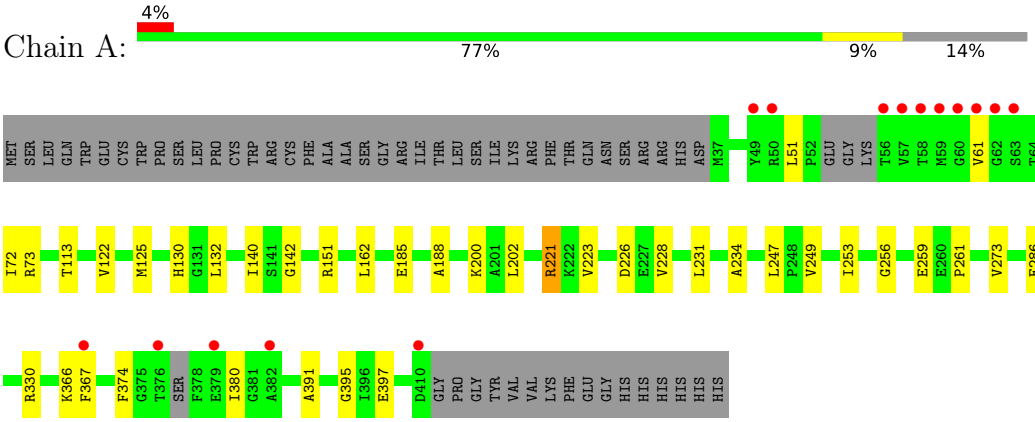
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	14	Total O 14 14	0	0

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.

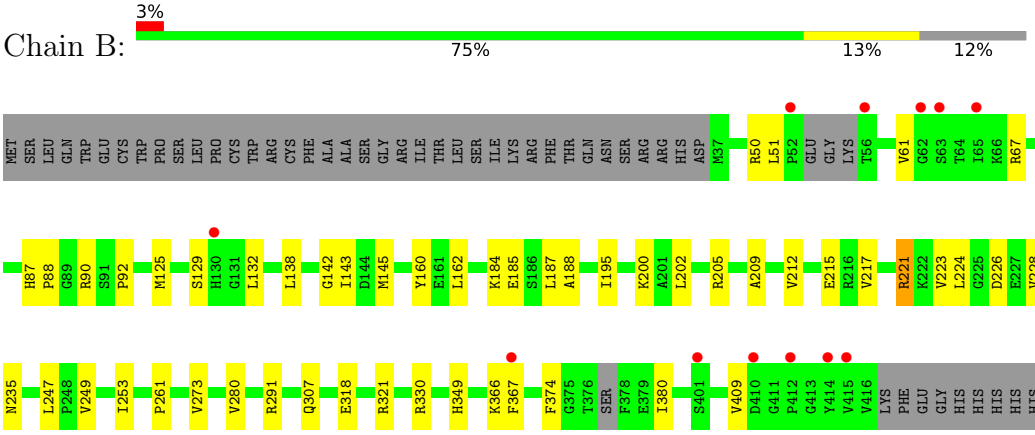
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain A:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	274.64Å 274.64Å 274.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 33.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.70) 99.8 (33.55-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.205 , 0.263 0.204 , 0.259	Depositor DCC
R_{free} test set	797 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.35	0/2901	0.57	0/3929
1	B	0.34	0/2942	0.56	0/3988
All	All	0.34	0/5843	0.56	0/7917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2831	0	2837	13	0
1	B	2870	0	2872	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	0	2	0
3	B	14	0	0	0	0
All	All	5730	0	5709	32	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 3.

All (32) 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:B:221:ARG:HG3	1:B:253:ILE:HB	1.55	0.89
1:A:221:ARG:HG3	1:A:253:ILE:HB	1.58	0.84
1:B:221:ARG:NH1	1:B:228:VAL:O	2.37	0.57
1:A:221:ARG:NH1	1:A:228:VAL:O	2.33	0.54
1:B:188:ALA:HB1	1:B:223:VAL:HG21	1.89	0.53
1:A:188:ALA:HB1	1:A:223:VAL:HG21	1.92	0.51
1:B:87:HIS:HB3	1:B:138:LEU:HD22	1.93	0.49
1:B:195:ILE:HD11	1:B:224:LEU:HD13	1.94	0.48
1:B:205:ARG:HH11	1:B:235:ASN:HD21	1.63	0.47
1:B:88:PRO:HB3	1:B:92:PRO:HB3	1.98	0.46
1:B:72:ILE:HD13	1:B:143:ILE:HG13	1.98	0.46
1:A:113:THR:HG22	1:A:151:ARG:HG2	1.98	0.45
1:A:259:GLU:HG3	1:A:307:GLN:HE22	1.82	0.45
1:A:130:HIS:HB2	1:B:90:ARG:HH11	1.81	0.45
1:A:122:VAL:HG21	1:A:140:ILE:HD13	1.98	0.44
1:B:318:GLU:OE1	1:B:321:ARG:NH2	2.51	0.44
1:A:391:ALA:HB3	1:A:395:GLY:HA2	1.99	0.44
1:B:72:ILE:HD12	1:B:142:GLY:HA3	2.00	0.44
1:A:286:GLU:HG3	3:A:605:HOH:O	2.18	0.43
1:B:209:ALA:HB3	1:B:212:VAL:HG22	2.00	0.42
1:B:205:ARG:HD2	1:B:235:ASN:HD21	1.84	0.42
1:B:184:LYS:HD3	1:B:215:GLU:HG2	2.02	0.42
1:B:50[B]:ARG:HE	1:B:409:VAL:HG11	1.84	0.42
1:B:87:HIS:HA	1:B:88:PRO:HD3	1.93	0.42
1:A:234:ALA:HB3	1:A:261:PRO:HA	2.01	0.42
1:B:221:ARG:HG2	1:B:230:ILE:HD12	2.01	0.42
1:A:231:LEU:HD23	1:A:256:GLY:HA3	2.01	0.41
1:A:72:ILE:HD12	1:A:142:GLY:HA3	2.03	0.41
1:B:234:ALA:HB3	1:B:261:PRO:HA	2.01	0.41
1:A:291:ARG:NH2	3:A:602:HOH:O	2.53	0.41
1:B:84:GLY:HA2	1:B:145:MET:HE2	2.03	0.41
1:B:160:TYR:H	1:B:349[B]:HIS:HD2	1.69	0.40

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	368/428 (86%)	353 (96%)	15 (4%)	0	100 100
1	B	374/428 (87%)	355 (95%)	19 (5%)	0	100 100
All	All	742/856 (87%)	708 (95%)	34 (5%)	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	287/334 (86%)	265 (92%)	22 (8%)	13 30
1	B	291/334 (87%)	264 (91%)	27 (9%)	9 21
All	All	578/668 (86%)	529 (92%)	49 (8%)	11 24

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	61	VAL
1	A	68	ASP
1	A	73	ARG
1	A	125	MET
1	A	132	LEU
1	A	162	LEU
1	A	185	GLU

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Mol	Chain	Res	Type
1	A	200	LYS
1	A	202	LEU
1	A	221	ARG
1	A	226	ASP
1	A	247	LEU
1	A	249	VAL
1	A	273	VAL
1	A	291	ARG
1	A	330	ARG
1	A	366	LYS
1	A	367	PHE
1	A	374	PHE
1	A	380	ILE
1	A	397	GLU
1	B	51	LEU
1	B	61	VAL
1	B	67	ARG
1	B	73	ARG
1	B	125	MET
1	B	129	SER
1	B	132	LEU
1	B	162	LEU
1	B	185	GLU
1	B	187	LEU
1	B	200	LYS
1	B	202	LEU
1	B	217	VAL
1	B	221	ARG
1	B	226	ASP
1	B	247	LEU
1	B	249	VAL
1	B	273	VAL
1	B	280	VAL
1	B	291	ARG
1	B	307[A]	GLN
1	B	307[B]	GLN
1	B	330	ARG
1	B	366	LYS
1	B	367	PHE
1	B	374	PHE
1	B	380	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	B	235	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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.

No monomer is involved in short contacts.

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^{th} 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	370/428 (86%)	-0.15	16 (4%)	35	33	34, 55, 97, 128	0
1	B	376/428 (87%)	-0.13	12 (3%)	47	48	30, 54, 97, 124	0
All	All	746/856 (87%)	-0.14	28 (3%)	40	39	30, 55, 97, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	THR	4.8
1	A	57	VAL	3.8
1	A	367	PHE	3.8
1	B	410	ASP	3.8
1	A	62	GLY	3.6
1	A	61	VAL	3.6
1	A	58	THR	3.6
1	A	60	GLY	3.5
1	A	410	ASP	3.4
1	B	414	TYR	3.3
1	B	56	THR	3.2
1	B	52	PRO	3.1
1	A	63	SER	3.0
1	A	59	MET	2.9
1	B	415	VAL	2.9
1	A	376	THR	2.7
1	B	412	PRO	2.6
1	A	65	ILE	2.5
1	B	65	ILE	2.5
1	A	50[A]	ARG	2.5
1	A	382	ALA	2.3
1	B	63	SER	2.3
1	A	49	TYR	2.3
1	B	62	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	130	HIS	2.2
1	B	401	SER	2.1
1	B	367	PHE	2.1
1	A	379	GLU	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 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^{th} 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(Å^2)	Q<0.9
2	MG	A	501	1/1	0.82	0.16	57,57,57,57	0
2	MG	B	501	1/1	0.82	0.41	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.