



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 04:44 PM EDT

PDB ID : 2GDQ
Title : Crystal structure of mandelate racemase/muconate lactonizing enzyme from *Bacillus subtilis* at 1.8 Å resolution
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Schwinn, K.D.; Emtage, S.; Thompson, D.A.; Rutter, M.E.; Dickey, M.; Groshong, C.; Bain, K.T.; Adams, J.M.; Reyes, C.; Rooney, I.; Powell, A.; Boice, A.; Gheyi, T.; Ozyurt, S.; Atwell, S.; Wasserman, S.R.; Burley, S.K.; Sali, A.; Babbitt, P.; Pieper, U.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

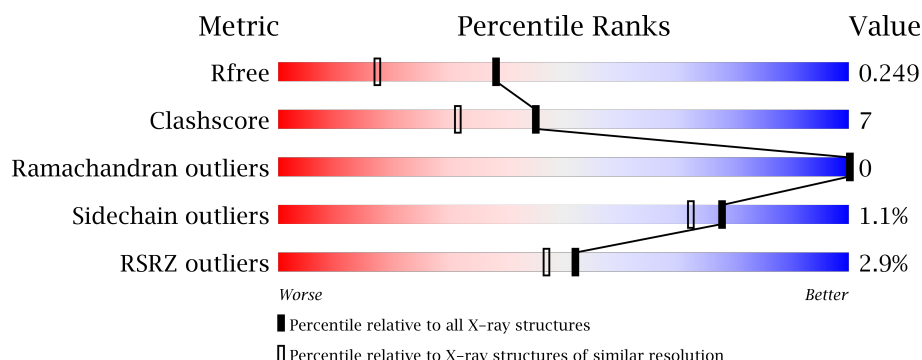
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 ≥ 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	382	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	382	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6705 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 yitF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2979	1907	516	540	16			
1	B	373	Total	C	N	O	S	0	1	0
			2985	1910	517	542	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP O06741
A	2	ALA	-	CLONING ARTIFACT	UNP O06741
A	3	LEU	-	CLONING ARTIFACT	UNP O06741
A	4	VAL	-	CLONING ARTIFACT	UNP O06741
A	375	GLU	-	CLONING ARTIFACT	UNP O06741
A	376	GLY	-	CLONING ARTIFACT	UNP O06741
A	377	HIS	-	EXPRESSION TAG	UNP O06741
A	378	HIS	-	EXPRESSION TAG	UNP O06741
A	379	HIS	-	EXPRESSION TAG	UNP O06741
A	380	HIS	-	EXPRESSION TAG	UNP O06741
A	381	HIS	-	EXPRESSION TAG	UNP O06741
A	382	HIS	-	EXPRESSION TAG	UNP O06741
B	1	MET	-	CLONING ARTIFACT	UNP O06741
B	2	ALA	-	CLONING ARTIFACT	UNP O06741
B	3	LEU	-	CLONING ARTIFACT	UNP O06741
B	4	VAL	-	CLONING ARTIFACT	UNP O06741
B	375	GLU	-	CLONING ARTIFACT	UNP O06741
B	376	GLY	-	CLONING ARTIFACT	UNP O06741
B	377	HIS	-	EXPRESSION TAG	UNP O06741
B	378	HIS	-	EXPRESSION TAG	UNP O06741
B	379	HIS	-	EXPRESSION TAG	UNP O06741
B	380	HIS	-	EXPRESSION TAG	UNP O06741
B	381	HIS	-	EXPRESSION TAG	UNP O06741
B	382	HIS	-	EXPRESSION TAG	UNP O06741

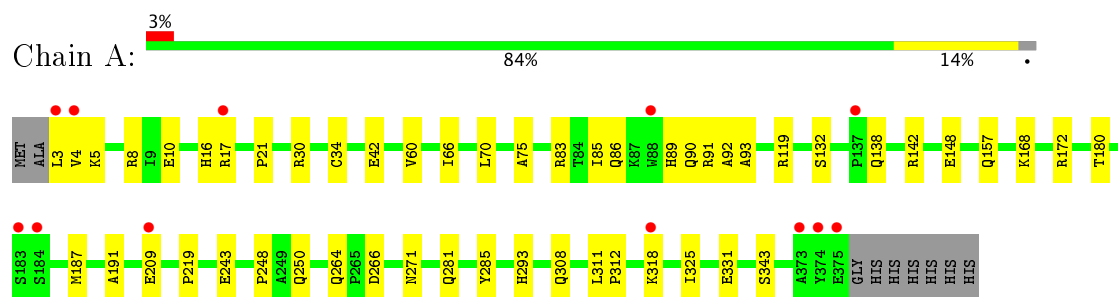
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	370	Total 370	O 370	0	0
2	B	371	Total 371	O 371	0	0

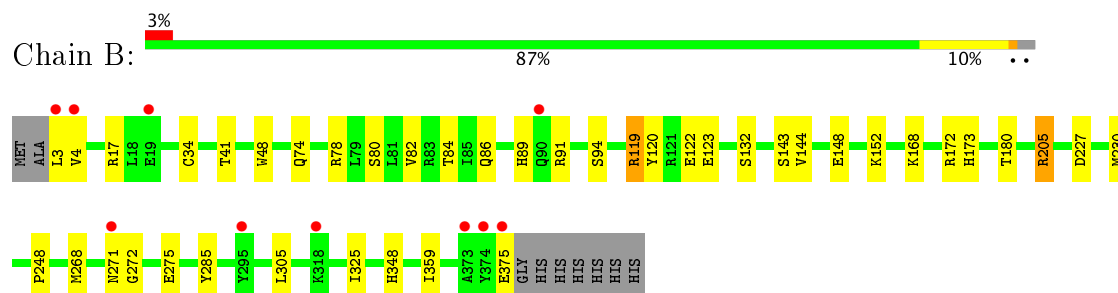
3 Residue-property plots [i](#)

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: yitF



• Molecule 1: yitF



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 113.25Å 168.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.46 – 1.80 27.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (27.46-1.80) 96.6 (27.46-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.252 0.196 , 0.249	Depositor DCC
R_{free} test set	3548 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.77	1/3058 (0.0%)	0.74	2/4145 (0.0%)
1	B	0.74	1/3064 (0.0%)	0.70	0/4153
All	All	0.76	2/6122 (0.0%)	0.72	2/8298 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	CYS	CB-SG	-7.49	1.69	1.82
1	B	34	CYS	CB-SG	-5.87	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	119	ARG	CG-CD-NE	-5.16	100.97	111.80

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	2979	0	2935	43	0
1	B	2985	0	2939	49	0
2	A	370	0	0	10	0
2	B	371	0	0	15	0
All	All	6705	0	5874	88	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 7.

All (88) 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:119:ARG:HG3	1:B:119:ARG:HH11	1.06	1.18
1:A:86:GLN:NE2	1:A:271:ASN:HB3	1.67	1.08
1:B:86:GLN:NE2	1:B:271:ASN:HB3	1.83	0.94
1:A:209:GLU:HB3	2:A:1036:HOH:O	1.78	0.83
1:B:132:SER:HB2	2:B:1165:HOH:O	1.79	0.82
1:A:271:ASN:OD1	2:A:1009:HOH:O	1.96	0.82
1:A:266:ASP:OD2	1:A:293:HIS:HD2	1.68	0.76
1:B:148:GLU:OE2	1:B:180:THR:HG21	1.85	0.75
1:B:119:ARG:HG3	1:B:119:ARG:NH1	1.84	0.74
1:B:172:ARG:HD2	2:B:1159:HOH:O	1.87	0.74
1:A:148:GLU:OE2	1:A:180:THR:HG21	1.87	0.74
1:A:4:VAL:HB	1:A:75:ALA:HB3	1.69	0.74
1:A:157:GLN:NE2	2:A:1000:HOH:O	2.21	0.72
1:A:86:GLN:CD	1:A:271:ASN:HB3	2.10	0.71
1:B:3:LEU:C	1:B:74:GLN:HE22	1.92	0.71
1:B:3:LEU:HA	1:B:74:GLN:HE22	1.55	0.70
1:A:3:LEU:N	2:A:1097:HOH:O	2.24	0.70
1:B:3:LEU:CA	1:B:74:GLN:HE22	2.04	0.70
1:B:3:LEU:HA	1:B:74:GLN:NE2	2.08	0.67
1:A:168:LYS:HE2	1:A:172:ARG:HH22	1.59	0.66
1:A:89:HIS:CE1	1:A:91:ARG:HB2	2.31	0.66
1:A:138:GLN:O	1:A:142:ARG:HG2	2.00	0.62
1:B:173:HIS:HD2	2:B:869:HOH:O	1.82	0.61
1:A:66:ILE:HD13	1:A:92:ALA:HB1	1.83	0.61
1:B:227:ASP:HA	1:B:230:MET:HE2	1.83	0.60
1:A:250:GLN:HG3	2:A:1130:HOH:O	2.02	0.58
1:B:80:SER:O	1:B:84:THR:HG23	2.04	0.58
1:A:132:SER:HB2	2:A:1160:HOH:O	2.04	0.56
1:A:90:GLN:CG	1:A:91:ARG:N	2.70	0.54
1:A:17:ARG:NH1	2:A:1154:HOH:O	2.41	0.54
1:A:83:ARG:HD2	1:B:120:TYR:HE1	1.72	0.53
1:A:66:ILE:HD13	1:A:92:ALA:CB	2.38	0.53
1:B:143:SER:OG	1:B:173:HIS:HE1	1.90	0.53
1:B:94:SER:HA	1:B:272:GLY:HA2	1.90	0.53
1:A:266:ASP:OD2	1:A:293:HIS:CD2	2.56	0.53
1:B:86:GLN:CD	1:B:271:ASN:HB3	2.30	0.53
1:A:70:LEU:HD21	1:A:85:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:OE2	1:B:180:THR:CG2	2.56	0.52
1:B:152:LYS:HE3	2:B:1127:HOH:O	2.10	0.52
1:B:119:ARG:NH2	1:B:122:GLU:HB3	2.25	0.52
1:B:271:ASN:HB2	1:B:275:GLU:CD	2.29	0.52
1:B:123:GLU:OE2	1:B:348:HIS:NE2	2.43	0.52
1:A:89:HIS:HE1	1:A:91:ARG:HB2	1.74	0.52
1:B:78:ARG:NH1	2:B:1062:HOH:O	2.42	0.52
1:A:21:PRO:HG2	1:A:30:ARG:HH11	1.75	0.51
1:B:268:MET:HB3	2:B:1170:HOH:O	2.11	0.51
1:B:4:VAL:HG12	1:B:41:THR:HB	1.93	0.50
1:A:311:LEU:HD12	1:A:312:PRO:HD2	1.93	0.50
1:A:86:GLN:NE2	1:A:271:ASN:CB	2.58	0.50
1:A:281:GLN:NE2	2:A:825:HOH:O	2.45	0.49
1:B:271:ASN:HB2	1:B:275:GLU:OE2	2.12	0.49
1:B:168:LYS:NZ	2:B:1141:HOH:O	2.44	0.49
1:B:86:GLN:HB3	2:B:1016:HOH:O	2.11	0.49
1:B:205:ARG:HD3	2:B:952:HOH:O	2.12	0.49
1:A:86:GLN:NE2	1:A:271:ASN:O	2.46	0.49
1:A:271:ASN:ND2	2:A:1155:HOH:O	2.46	0.48
1:B:119:ARG:CZ	1:B:122:GLU:HB3	2.44	0.48
1:A:83:ARG:HD2	1:B:120:TYR:CE1	2.49	0.48
1:B:3:LEU:CA	1:B:74:GLN:NE2	2.73	0.48
1:B:119:ARG:NH1	2:B:1087:HOH:O	2.47	0.47
1:B:144:VAL:O	1:B:148:GLU:HG3	2.14	0.47
1:B:305:LEU:HD23	1:B:325:ILE:HD12	1.94	0.47
1:A:90:GLN:HG3	1:A:91:ARG:N	2.29	0.46
1:B:271:ASN:ND2	1:B:275:GLU:OE2	2.47	0.46
1:B:123:GLU:OE2	1:B:348:HIS:CE1	2.69	0.46
1:B:74:GLN:NE2	2:B:965:HOH:O	2.49	0.45
1:B:143:SER:OG	1:B:173:HIS:CE1	2.69	0.45
1:A:91:ARG:NH1	2:A:1020:HOH:O	2.41	0.45
1:A:168:LYS:HE2	1:A:172:ARG:NH2	2.29	0.45
1:B:89:HIS:CE1	1:B:91:ARG:HB2	2.52	0.44
1:B:17:ARG:HD2	2:B:1137:HOH:O	2.17	0.44
1:B:119:ARG:HD3	2:B:1164:HOH:O	2.18	0.44
1:A:16:HIS:HE1	1:A:331:GLU:OE2	2.01	0.43
1:A:248:PRO:HG2	1:B:285:TYR:CZ	2.53	0.43
1:A:5:LYS:HB2	1:A:5:LYS:HE3	1.84	0.43
1:A:285:TYR:CZ	1:B:248:PRO:HG2	2.53	0.43
1:B:172:ARG:NH2	2:B:1141:HOH:O	2.51	0.42
1:A:308:GLN:HB2	1:A:325:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HD3	2:B:989:HOH:O	2.19	0.42
1:B:82:VAL:HG12	1:B:86:GLN:NE2	2.34	0.42
1:A:191:ALA:HB3	1:A:219:PRO:HA	2.02	0.42
1:A:243:GLU:HA	1:A:264:GLN:O	2.20	0.42
1:B:119:ARG:NE	1:B:122:GLU:HB3	2.34	0.42
1:A:148:GLU:OE2	1:A:180:THR:CG2	2.64	0.41
1:B:48:TRP:CD2	1:B:359:ILE:HG13	2.56	0.41
1:A:86:GLN:HG3	1:A:93:ALA:CB	2.51	0.41
1:A:8:ARG:NH1	1:A:10:GLU:OE2	2.51	0.40
1:A:5:LYS:HB3	1:A:42:GLU:HG3	2.03	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	371/382 (97%)	360 (97%)	11 (3%)	0	100	100
1	B	372/382 (97%)	362 (97%)	10 (3%)	0	100	100
All	All	743/764 (97%)	722 (97%)	21 (3%)	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	316/323 (98%)	312 (99%)	4 (1%)	73	66
1	B	317/323 (98%)	314 (99%)	3 (1%)	82	78
All	All	633/646 (98%)	626 (99%)	7 (1%)	78	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	187	MET
1	A	318	LYS
1	A	343	SER
1	B	119	ARG
1	B	205	ARG
1	B	375	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	86	GLN
1	A	131	GLN
1	A	226	GLN
1	A	244	ASN
1	A	271	ASN
1	A	281	GLN
1	A	293	HIS
1	A	348	HIS
1	A	365	ASN
1	B	16	HIS
1	B	74	GLN
1	B	86	GLN
1	B	131	GLN
1	B	173	HIS
1	B	224	GLN
1	B	226	GLN
1	B	244	ASN
1	B	281	GLN
1	B	365	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

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, 95th 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	373/382 (97%)	0.04	12 (3%) 48 43	16, 23, 35, 56	0
1	B	373/382 (97%)	0.08	10 (2%) 55 50	16, 24, 36, 58	0
All	All	746/764 (97%)	0.06	22 (2%) 52 47	16, 24, 35, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.8
1	A	3	LEU	5.3
1	B	375	GLU	5.2
1	A	375	GLU	4.6
1	B	373	ALA	4.4
1	B	4	VAL	4.0
1	B	374	TYR	4.0
1	A	373	ALA	3.5
1	A	88	TRP	3.0
1	B	271	ASN	3.0
1	A	209	GLU	2.8
1	B	90	GLN	2.8
1	A	374	TYR	2.8
1	A	137	PRO	2.7
1	B	19	GLU	2.7
1	A	183	SER	2.5
1	A	318	LYS	2.5
1	A	17	ARG	2.4
1	B	318	LYS	2.3
1	A	184	SER	2.3
1	B	295	TYR	2.0
1	A	4	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.