Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:48 AM GMT

PDB ID	:	2YFK
Title	:	Crystal structure of a putative transcarbamoylase from Enterococcus faecalis
Authors	:	Polo, L.M.; Fita, I.; Rubio, V.
Deposited on	:	2011-04-06
Resolution	:	2.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

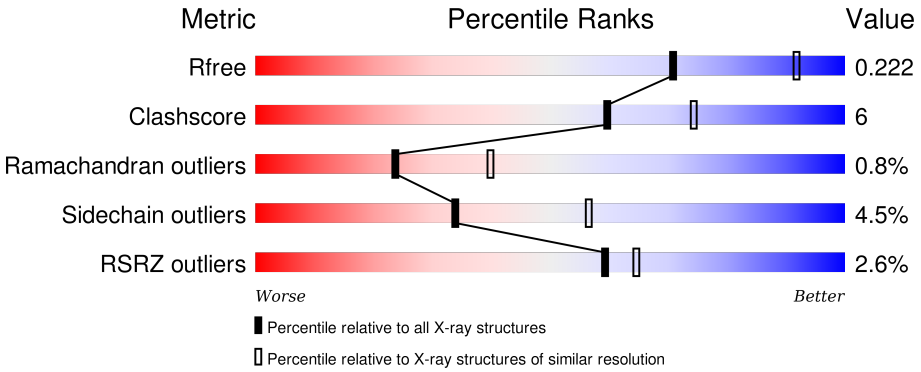
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 <=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	418	2% 79% 12% • 8%
1	B	418	2% 83% 8% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6056 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 ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2994	1897	488	590	19			
1	B	386	Total	C	N	O	S	0	0	0
			2999	1901	488	591	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ASP	-	EXPRESSION TAG	UNP C7YCV8
A	399	PRO	-	EXPRESSION TAG	UNP C7YCV8
A	400	ASN	-	EXPRESSION TAG	UNP C7YCV8
A	401	SER	-	EXPRESSION TAG	UNP C7YCV8
A	402	SER	-	EXPRESSION TAG	UNP C7YCV8
A	403	SER	-	EXPRESSION TAG	UNP C7YCV8
A	404	VAL	-	EXPRESSION TAG	UNP C7YCV8
A	405	ASP	-	EXPRESSION TAG	UNP C7YCV8
A	406	LYS	-	EXPRESSION TAG	UNP C7YCV8
A	407	LEU	-	EXPRESSION TAG	UNP C7YCV8
A	408	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	409	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	410	ALA	-	EXPRESSION TAG	UNP C7YCV8
A	411	LEU	-	EXPRESSION TAG	UNP C7YCV8
A	412	GLU	-	EXPRESSION TAG	UNP C7YCV8
A	413	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	414	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	415	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	416	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	417	HIS	-	EXPRESSION TAG	UNP C7YCV8
A	418	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	398	ASP	-	EXPRESSION TAG	UNP C7YCV8
B	399	PRO	-	EXPRESSION TAG	UNP C7YCV8
B	400	ASN	-	EXPRESSION TAG	UNP C7YCV8
B	401	SER	-	EXPRESSION TAG	UNP C7YCV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	402	SER	-	EXPRESSION TAG	UNP C7YCV8
B	403	SER	-	EXPRESSION TAG	UNP C7YCV8
B	404	VAL	-	EXPRESSION TAG	UNP C7YCV8
B	405	ASP	-	EXPRESSION TAG	UNP C7YCV8
B	406	LYS	-	EXPRESSION TAG	UNP C7YCV8
B	407	LEU	-	EXPRESSION TAG	UNP C7YCV8
B	408	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	409	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	410	ALA	-	EXPRESSION TAG	UNP C7YCV8
B	411	LEU	-	EXPRESSION TAG	UNP C7YCV8
B	412	GLU	-	EXPRESSION TAG	UNP C7YCV8
B	413	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	414	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	415	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	416	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	417	HIS	-	EXPRESSION TAG	UNP C7YCV8
B	418	HIS	-	EXPRESSION TAG	UNP C7YCV8

- Molecule 2 is water.

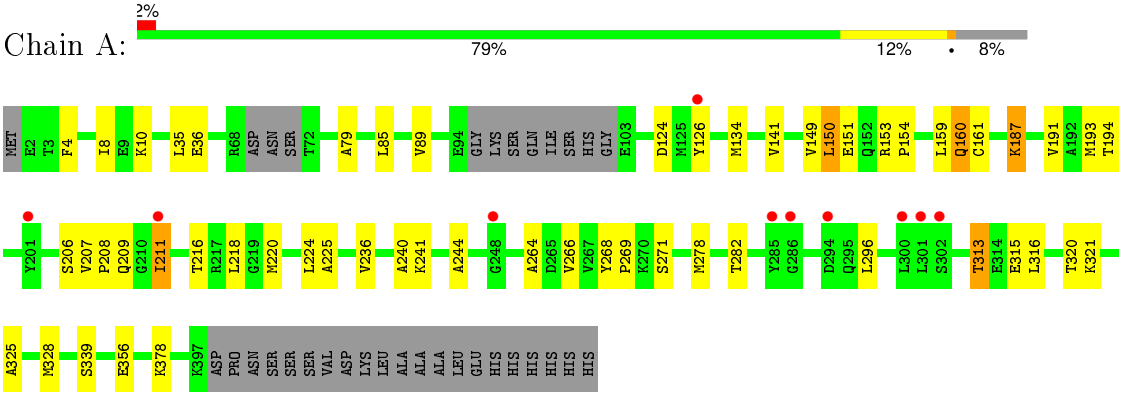
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	35	Total O 35 35	0	0

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 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.

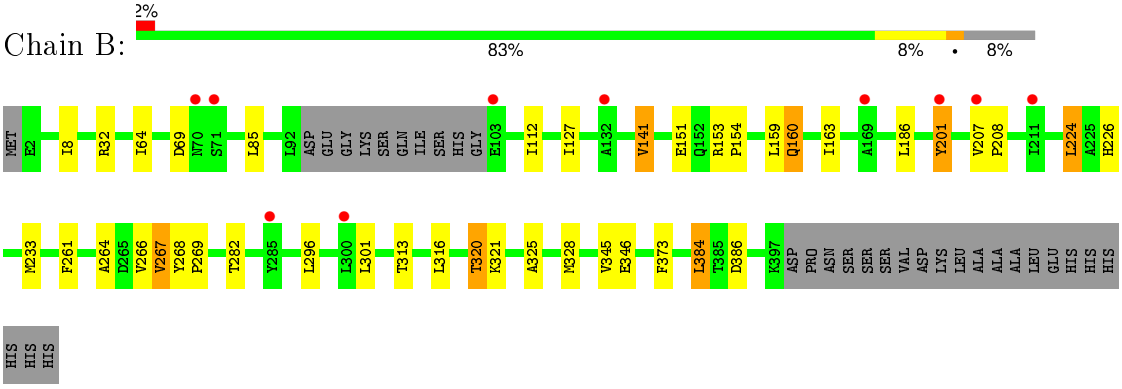
- Molecule 1: ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE

Chain A:



- Molecule 1: ASPARTATE/ORNITHINE CARBAMOYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	117.37Å 117.37Å 120.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.55) 99.8 (29.52-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0112	Depositor
R, R_{free}	0.169 , 0.202 0.187 , 0.222	Depositor DCC
R_{free} test set	1540 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.1	EDS
Estimated twinning fraction	0.551 for H, K, L 0.449 for K, H, -L 0.115 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.551 for H, K, L 0.449 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 30624 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6056	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	1/3050 (0.0%)	0.49	0/4121
1	B	0.38	1/3057 (0.0%)	0.49	0/4136
All	All	0.38	2/6107 (0.0%)	0.49	0/8257

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	GLU	CD-OE2	6.80	1.33	1.25
1	A	151	GLU	CD-OE2	6.53	1.32	1.25

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	2994	0	2881	41	0
1	B	2999	0	2878	26	0
2	A	28	0	0	2	0
2	B	35	0	0	0	0
All	All	6056	0	5759	67	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 6.

All (67) 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:320:THR:CG2	1:A:325:ALA:HB2	1.84	1.07
1:A:320:THR:HG21	1:A:325:ALA:CB	1.87	1.04
1:A:320:THR:HG21	1:A:325:ALA:HB2	1.39	1.00
1:A:149:VAL:HG12	1:A:150:LEU:HD13	1.57	0.84
1:A:266:VAL:HG11	1:A:328:MET:HE1	1.63	0.81
1:B:320:THR:HG21	1:B:325:ALA:H	1.46	0.80
1:A:141:VAL:HG13	1:A:154:PRO:HD2	1.63	0.80
1:B:141:VAL:HG13	1:B:154:PRO:HD2	1.66	0.77
1:B:320:THR:CG2	1:B:325:ALA:HB2	2.17	0.74
1:B:320:THR:HG21	1:B:325:ALA:CB	2.20	0.71
1:A:320:THR:HG23	1:A:325:ALA:HB2	1.74	0.69
1:B:320:THR:HG21	1:B:325:ALA:HB2	1.74	0.69
1:A:266:VAL:HG11	1:A:328:MET:CE	2.24	0.67
1:A:264:ALA:O	1:A:320:THR:HG23	1.95	0.67
1:A:216:THR:HG21	1:A:240:ALA:O	1.96	0.66
1:B:261:PHE:CE2	1:B:267:VAL:HG21	2.32	0.64
1:A:79:ALA:HA	1:A:89:VAL:HG21	1.80	0.63
1:A:356:GLU:OE1	2:A:2026:HOH:O	2.16	0.62
1:A:266:VAL:CG1	1:A:328:MET:CE	2.79	0.61
1:A:10:LYS:NZ	1:A:36:GLU:OE2	2.33	0.60
1:A:266:VAL:CG1	1:A:328:MET:HE2	2.31	0.60
1:B:313:THR:HG23	1:B:316:LEU:H	1.66	0.59
1:B:320:THR:HG21	1:B:325:ALA:N	2.15	0.58
1:A:320:THR:HG22	1:A:321:LYS:N	2.18	0.58
1:A:320:THR:HG21	1:A:325:ALA:HB3	1.81	0.58
1:B:320:THR:HG23	1:B:325:ALA:HB2	1.86	0.56
1:B:64:ILE:HG21	1:B:112:ILE:HD12	1.86	0.56
1:A:4:PHE:CZ	1:A:8:ILE:HD11	2.40	0.56
1:A:141:VAL:CG1	1:A:154:PRO:HD2	2.35	0.56
1:B:201:TYR:HA	1:B:301:LEU:HD11	1.89	0.54
1:A:320:THR:CG2	1:A:321:LYS:N	2.70	0.53
1:B:163:ILE:HG23	1:B:233:MET:HE3	1.90	0.53
1:A:191:VAL:CG2	1:A:220:MET:CE	2.86	0.52
1:B:320:THR:CG2	1:B:321:LYS:N	2.73	0.52
1:A:207:VAL:HB	1:A:208:PRO:HD3	1.91	0.52
1:B:127:ILE:N	1:B:282:THR:HG21	2.26	0.51
1:B:159:LEU:O	1:B:160:GLN:HB2	2.12	0.50
1:A:313:THR:HG23	1:A:315:GLU:H	1.77	0.50
1:A:296:LEU:O	1:A:296:LEU:HD23	2.12	0.49
1:B:264:ALA:O	1:B:320:THR:HG23	2.13	0.49
1:A:191:VAL:HG22	1:A:220:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:HG23	1:A:315:GLU:N	2.28	0.49
1:A:149:VAL:HG12	1:A:150:LEU:CD1	2.37	0.47
1:A:313:THR:HG22	1:A:316:LEU:H	1.79	0.47
1:B:224:LEU:HD22	1:B:226:HIS:HD2	1.79	0.47
1:B:345:VAL:HG22	1:B:346:GLU:O	2.15	0.46
1:A:191:VAL:CG2	1:A:220:MET:HE2	2.45	0.46
1:A:191:VAL:HG22	1:A:220:MET:HE1	1.99	0.45
1:B:261:PHE:CZ	1:B:267:VAL:HG21	2.51	0.45
1:B:373:PHE:CZ	1:B:384:LEU:HD13	2.51	0.45
1:A:159:LEU:O	1:A:160:GLN:HB2	2.17	0.44
1:A:320:THR:HG21	1:A:325:ALA:H	1.81	0.43
1:A:124:ASP:HB3	1:A:160:GLN:HG2	2.00	0.43
1:A:134:MET:HE3	1:A:161:CYS:HB3	2.00	0.43
1:A:193:MET:HB2	1:A:211:ILE:HD11	2.00	0.43
1:A:126:TYR:HB3	1:A:282:THR:HG22	2.00	0.43
1:B:266:VAL:HG11	1:B:328:MET:HE1	2.00	0.43
1:B:207:VAL:HB	1:B:208:PRO:HD3	2.01	0.43
1:B:320:THR:CG2	1:B:325:ALA:H	2.25	0.42
1:B:320:THR:HG23	1:B:321:LYS:N	2.34	0.42
1:A:194:THR:HG22	1:A:225:ALA:HB3	2.01	0.42
1:B:296:LEU:C	1:B:296:LEU:HD23	2.40	0.42
1:A:313:THR:CG2	1:A:316:LEU:H	2.33	0.42
1:A:209:GLN:HB3	1:A:236:VAL:HG11	2.02	0.41
1:A:187:LYS:NZ	2:A:2017:HOH:O	2.53	0.41
1:B:163:ILE:HG23	1:B:233:MET:CE	2.52	0.40
1:A:216:THR:HG23	1:A:244:ALA:HB2	2.04	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	379/418 (91%)	363 (96%)	14 (4%)	2 (0%)	34 54
1	B	382/418 (91%)	367 (96%)	11 (3%)	4 (1%)	19 33
All	All	761/836 (91%)	730 (96%)	25 (3%)	6 (1%)	24 40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	B	160	GLN
1	A	269	PRO
1	B	201	TYR
1	B	69	ASP
1	B	269	PRO

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	314/358 (88%)	298 (95%)	16 (5%)	29 50
1	B	315/358 (88%)	303 (96%)	12 (4%)	40 65
All	All	629/716 (88%)	601 (96%)	28 (4%)	34 56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	85	LEU
1	A	150	LEU
1	A	153	ARG
1	A	187	LYS
1	A	206	SER
1	A	211	ILE
1	A	218	LEU
1	A	224	LEU
1	A	241	LYS

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Mol	Chain	Res	Type
1	A	268	TYR
1	A	271	SER
1	A	278	MET
1	A	313	THR
1	A	339	SER
1	A	378	LYS
1	B	8	ILE
1	B	32	ARG
1	B	85	LEU
1	B	141	VAL
1	B	153	ARG
1	B	186	LEU
1	B	224	LEU
1	B	267	VAL
1	B	268	TYR
1	B	320	THR
1	B	384	LEU
1	B	386	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	250	ASN
1	A	287	ASN
1	A	290	GLN
1	B	142	GLN
1	B	158	ASN
1	B	287	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	385/418 (92%)	0.04	10 (2%) 59 64	21, 34, 60, 72	0
1	B	386/418 (92%)	0.02	10 (2%) 59 64	19, 33, 54, 72	0
All	All	771/836 (92%)	0.03	20 (2%) 59 64	19, 33, 55, 72	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ASN	5.0
1	B	201	TYR	4.1
1	A	126	TYR	3.7
1	B	71	SER	3.0
1	B	103	GLU	2.8
1	A	201	TYR	2.8
1	A	285	TYR	2.7
1	B	285	TYR	2.7
1	A	301	LEU	2.5
1	A	211	ILE	2.4
1	B	132	ALA	2.3
1	B	207	VAL	2.2
1	B	211	ILE	2.2
1	A	300	LEU	2.2
1	B	300	LEU	2.2
1	A	302	SER	2.2
1	A	248	GLY	2.1
1	B	169	ALA	2.1
1	A	286	GLY	2.1
1	A	294	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.