Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 08:03 AM EST

PDB ID	:	3LWT
Title	:	Crystal structure of the Yeast Sac1: Implications for its phosphoinositide phosphatase function
Authors	:	Mao, Y.; Manford, A.; Xia, T.; Saxena, A.K.; Stefan, C.; Hu, F.; Emr, S.D.
Deposited on	:	2010-02-24
Resolution	:	1.96 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

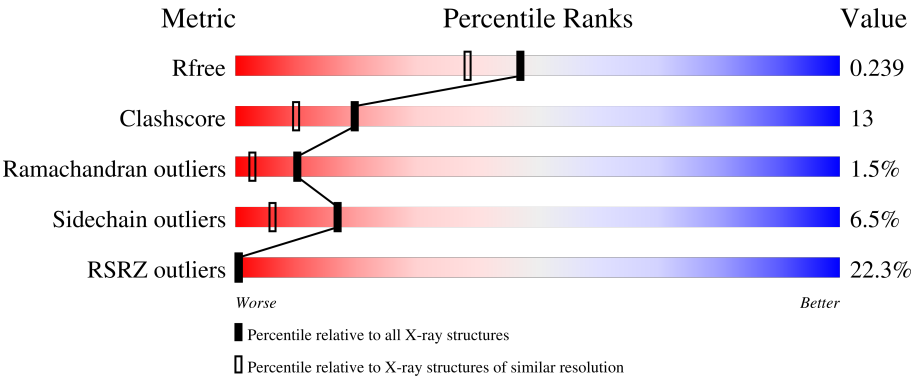
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	X	505	20% 65% 21% • • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3851 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 Phosphoinositide phosphatase SAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	457	Total	C	N	O	S	0	0	0
			3683	2344	637	695	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	0	SER	-	expression tag	UNP P32368

- Molecule 2 is water.

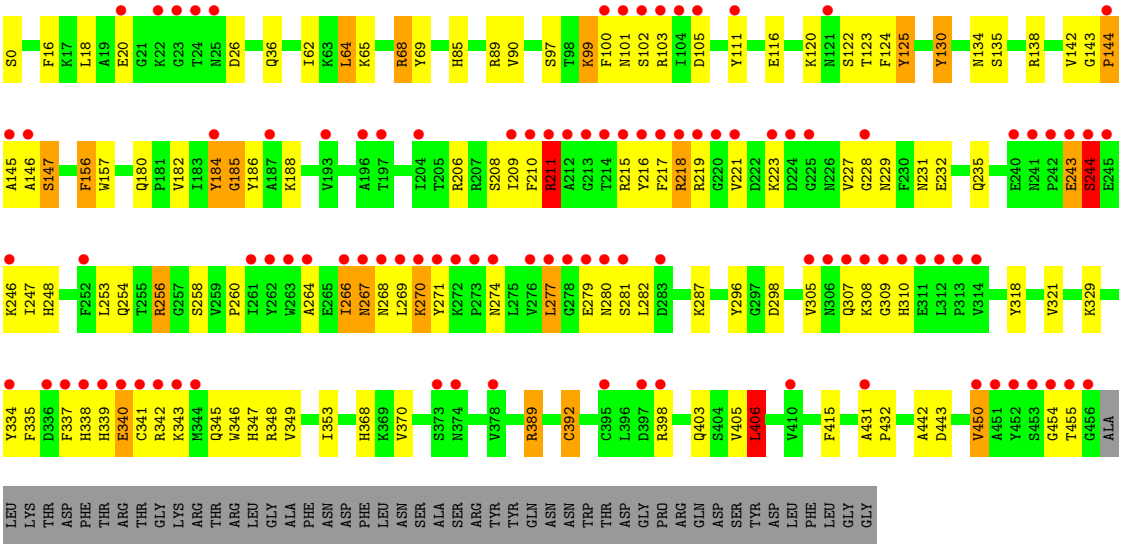
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	168	Total	O	0	0
			168	168		

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: Phosphoinositide phosphatase SAC1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	86.16Å 94.73Å 155.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.18 – 1.96 33.18 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.18-1.96) 99.2 (33.18-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.199 , 0.243 0.196 , 0.239	Depositor DCC
R_{free} test set	2327 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3851	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

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	X	1.29	17/3768 (0.5%)	1.06	12/5113 (0.2%)

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	X	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	392	CYS	CB-SG	-12.77	1.60	1.82
1	X	389	ARG	CG-CD	-8.38	1.31	1.51
1	X	16	PHE	CE2-CZ	6.81	1.50	1.37
1	X	130	TYR	CD2-CE2	6.70	1.49	1.39
1	X	156	PHE	N-CA	6.40	1.59	1.46
1	X	329	LYS	CD-CE	6.23	1.66	1.51
1	X	135	SER	CB-OG	6.10	1.50	1.42
1	X	90	VAL	CB-CG1	5.67	1.64	1.52
1	X	182	VAL	CB-CG1	-5.64	1.41	1.52
1	X	296	TYR	CD2-CE2	5.62	1.47	1.39
1	X	184	TYR	C-N	-5.61	1.23	1.33
1	X	182	VAL	CB-CG2	5.38	1.64	1.52
1	X	415	PHE	CE2-CZ	5.38	1.47	1.37
1	X	442	ALA	CA-CB	5.29	1.63	1.52
1	X	130	TYR	CD1-CE1	5.22	1.47	1.39
1	X	125	TYR	CD2-CE2	5.14	1.47	1.39
1	X	180	GLN	CB-CG	5.00	1.66	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	256	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	X	206	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	X	147	SER	N-CA-CB	-7.50	99.25	110.50
1	X	406	LEU	CA-CB-CG	7.45	132.42	115.30
1	X	89	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	X	185	GLY	N-CA-C	6.25	128.73	113.10
1	X	89	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	X	68	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	X	184	TYR	CB-CA-C	5.45	121.29	110.40
1	X	156	PHE	N-CA-CB	-5.42	100.84	110.60
1	X	184	TYR	O-C-N	-5.27	114.24	123.20
1	X	99	LYS	CD-CE-NZ	-5.25	99.61	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	389	ARG	Sidechain

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	X	3683	0	3582	92	0
2	X	168	0	0	9	0
All	All	3851	0	3582	92	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 13.

All (92) 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:X:185:GLY:N	2:X:660:HOH:O	1.62	1.22
1:X:123:THR:O	1:X:184:TYR:O	1.67	1.10
1:X:146:ALA:HB1	1:X:147:SER:HA	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:209:ILE:HG23	2:X:642:HOH:O	1.65	0.97
1:X:338:HIS:HB2	1:X:348:ARG:NH1	1.80	0.95
1:X:64:LEU:HD11	1:X:111:TYR:CE2	2.04	0.92
1:X:62:ILE:HD11	1:X:111:TYR:OH	1.70	0.91
1:X:208:SER:O	2:X:661:HOH:O	1.90	0.88
1:X:36:GLN:HE21	1:X:68:ARG:H	1.23	0.86
1:X:267:ASN:O	1:X:267:ASN:ND2	2.16	0.78
1:X:210:PHE:HB2	1:X:211:ARG:HB2	1.63	0.78
1:X:266:ILE:HD12	1:X:266:ILE:H	1.49	0.77
1:X:134:ASN:HD22	1:X:138:ARG:HE	1.32	0.77
1:X:184:TYR:CA	2:X:660:HOH:O	2.33	0.77
1:X:431:ALA:HB3	1:X:432:PRO:HD3	1.70	0.74
1:X:146:ALA:HB1	1:X:147:SER:CA	2.18	0.73
1:X:353:ILE:HG12	1:X:406:LEU:HD13	1.72	0.72
1:X:0:SER:HB2	2:X:599:HOH:O	1.90	0.71
1:X:64:LEU:CD1	1:X:111:TYR:CE2	2.76	0.69
1:X:116:GLU:OE2	1:X:120:LYS:HE3	1.93	0.69
1:X:184:TYR:C	2:X:660:HOH:O	2.10	0.68
1:X:143:GLY:HA2	2:X:651:HOH:O	1.93	0.68
1:X:338:HIS:HB2	1:X:348:ARG:HH12	1.56	0.67
1:X:20:GLU:HG3	2:X:624:HOH:O	1.96	0.65
1:X:146:ALA:CB	1:X:147:SER:HA	2.19	0.64
1:X:64:LEU:HG	1:X:111:TYR:CD2	2.32	0.64
1:X:337:PHE:CE1	1:X:349:VAL:HG23	2.33	0.63
1:X:270:LYS:HG3	1:X:271:TYR:HD1	1.62	0.63
1:X:62:ILE:HD11	1:X:111:TYR:HH	1.64	0.63
1:X:247:ILE:HD12	1:X:247:ILE:N	2.14	0.62
1:X:210:PHE:HB3	1:X:228:GLY:HA2	1.81	0.61
1:X:337:PHE:CE1	1:X:345:GLN:HG2	2.34	0.61
1:X:246:LYS:HZ2	1:X:370:VAL:HG11	1.66	0.60
1:X:338:HIS:CB	1:X:348:ARG:NH1	2.60	0.60
1:X:243:GLU:O	1:X:244:SER:HB3	2.02	0.59
1:X:341:CYS:HA	1:X:345:GLN:HB2	1.85	0.59
1:X:157:TRP:HA	1:X:209:ILE:HG13	1.84	0.59
1:X:99:LYS:CB	1:X:102:SER:HB2	2.32	0.59
1:X:282:LEU:HD23	1:X:321:VAL:HG13	1.85	0.58
1:X:143:GLY:O	1:X:145:ALA:N	2.33	0.57
1:X:218:ARG:HG3	1:X:219:ARG:N	2.20	0.57
1:X:248:HIS:HD2	1:X:368:HIS:NE2	2.01	0.57
1:X:307:GLN:HG2	1:X:309:GLY:H	1.70	0.56
1:X:142:VAL:O	1:X:144:PRO:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:99:LYS:HB3	1:X:102:SER:HB2	1.89	0.54
1:X:36:GLN:NE2	1:X:68:ARG:H	2.00	0.53
1:X:270:LYS:HG3	1:X:271:TYR:CD1	2.44	0.53
1:X:269:LEU:HD23	1:X:270:LYS:HE3	1.91	0.53
1:X:338:HIS:CB	1:X:348:ARG:HH12	2.21	0.53
1:X:210:PHE:CB	1:X:211:ARG:HB2	2.37	0.52
1:X:337:PHE:CE1	1:X:349:VAL:CG2	2.92	0.52
1:X:211:ARG:O	1:X:216:TYR:HE1	1.91	0.52
1:X:122:SER:HB2	1:X:124:PHE:CZ	2.45	0.52
1:X:65:LYS:HE2	1:X:105:ASP:OD2	2.11	0.51
1:X:339:HIS:HB2	1:X:340:GLU:HA	1.92	0.51
1:X:254:GLN:HE22	1:X:403:GLN:HA	1.75	0.51
1:X:229:ASN:ND2	1:X:392:CYS:SG	2.85	0.50
1:X:146:ALA:CB	1:X:147:SER:CA	2.86	0.50
1:X:343:LYS:N	2:X:659:HOH:O	2.44	0.50
1:X:335:PHE:CZ	1:X:348:ARG:O	2.66	0.48
1:X:221:VAL:HB	1:X:227:VAL:HG12	1.96	0.48
1:X:100:PHE:CG	1:X:101:ASN:N	2.81	0.48
1:X:218:ARG:NH1	1:X:258:SER:OG	2.47	0.48
1:X:346:TRP:O	1:X:347:HIS:C	2.51	0.47
1:X:260:PRO:HD2	1:X:318:TYR:CE1	2.50	0.47
1:X:337:PHE:HE1	1:X:349:VAL:HG23	1.77	0.46
1:X:307:GLN:HG2	1:X:308:LYS:N	2.30	0.46
1:X:279:GLU:O	1:X:279:GLU:HG2	2.16	0.46
1:X:243:GLU:O	1:X:244:SER:CB	2.65	0.45
1:X:307:GLN:HG3	1:X:310:HIS:O	2.16	0.45
1:X:143:GLY:C	1:X:145:ALA:H	2.19	0.44
1:X:232:GLU:HB3	1:X:253:LEU:HD11	1.99	0.44
1:X:85:HIS:CG	1:X:130:TYR:HB2	2.53	0.44
1:X:266:ILE:H	1:X:266:ILE:CD1	2.23	0.44
1:X:122:SER:HB2	1:X:124:PHE:CE2	2.53	0.43
1:X:62:ILE:CD1	1:X:111:TYR:OH	2.56	0.43
1:X:231:ASN:HD22	1:X:256:ARG:HH21	1.65	0.43
1:X:246:LYS:NZ	1:X:370:VAL:HG11	2.31	0.43
1:X:341:CYS:HA	1:X:345:GLN:CB	2.48	0.43
1:X:215:ARG:HH22	1:X:223:LYS:HD2	1.85	0.42
1:X:188:LYS:HE3	1:X:188:LYS:HB2	1.81	0.42
1:X:335:PHE:HZ	1:X:348:ARG:O	2.02	0.42
1:X:341:CYS:HB2	1:X:345:GLN:CD	2.40	0.41
1:X:277:LEU:HB3	1:X:281:SER:HB2	2.02	0.41
1:X:211:ARG:O	1:X:216:TYR:CE1	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:243:GLU:H	1:X:243:GLU:HG3	1.62	0.41
1:X:337:PHE:CZ	1:X:345:GLN:HG2	2.55	0.41
1:X:125:TYR:CE2	1:X:186:TYR:HA	2.56	0.41
1:X:349:VAL:HG11	1:X:405:VAL:HB	2.02	0.40
1:X:454:GLY:HA3	1:X:455:THR:HA	1.94	0.40
1:X:64:LEU:CG	1:X:111:TYR:CD2	3.02	0.40
1:X:69:TYR:CE1	1:X:97:SER:HB3	2.57	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	X	455/505 (90%)	425 (93%)	23 (5%)	7 (2%)	10 3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	144	PRO
1	X	244	SER
1	X	450	VAL
1	X	217	PHE
1	X	264	ALA
1	X	305	VAL
1	X	211	ARG

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	X	400/441 (91%)	374 (94%)	26 (6%)	17 6

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	18	LEU
1	X	26	ASP
1	X	64	LEU
1	X	103	ARG
1	X	156	PHE
1	X	211	ARG
1	X	218	ARG
1	X	235	GLN
1	X	243	GLU
1	X	244	SER
1	X	266	ILE
1	X	267	ASN
1	X	268	ASN
1	X	270	LYS
1	X	274	ASN
1	X	277	LEU
1	X	280	ASN
1	X	287	LYS
1	X	298	ASP
1	X	334	TYR
1	X	340	GLU
1	X	342	ARG
1	X	398	ARG
1	X	406	LEU
1	X	443	ASP
1	X	450	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	36	GLN
1	X	67	ASN
1	X	134	ASN
1	X	229	ASN

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Mol	Chain	Res	Type
1	X	248	HIS
1	X	254	GLN
1	X	280	ASN
1	X	391	ASN
1	X	408	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 monosaccharides 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, 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	X	457/505 (90%)	1.55	102 (22%)	0	0	23, 45, 105, 145	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	271	TYR	23.0
1	X	341	CYS	18.3
1	X	456	GLY	17.6
1	X	455	THR	16.9
1	X	273	PRO	15.1
1	X	212	ALA	11.5
1	X	216	TYR	11.2
1	X	309	GLY	10.8
1	X	272	LYS	10.7
1	X	214	THR	10.5
1	X	266	ILE	9.7
1	X	24	THR	9.6
1	X	308	LYS	9.4
1	X	267	ASN	8.3
1	X	452	TYR	8.1
1	X	211	ARG	8.1
1	X	310	HIS	8.0
1	X	100	PHE	7.8
1	X	337	PHE	7.7
1	X	312	LEU	7.7
1	X	311	GLU	7.6
1	X	103	ARG	7.5
1	X	217	PHE	7.3
1	X	263	TRP	7.1
1	X	453	SER	7.0
1	X	213	GLY	6.9
1	X	270	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
1	X	215	ARG	6.7
1	X	305	VAL	6.3
1	X	342	ARG	6.2
1	X	274	ASN	6.2
1	X	307	GLN	6.0
1	X	269	LEU	6.0
1	X	306	ASN	6.0
1	X	334	TYR	5.8
1	X	276	VAL	5.3
1	X	210	PHE	5.2
1	X	243	GLU	5.1
1	X	196	ALA	5.0
1	X	339	HIS	4.9
1	X	22	LYS	4.9
1	X	101	ASN	4.9
1	X	268	ASN	4.7
1	X	246	LYS	4.6
1	X	111	TYR	4.5
1	X	245	GLU	4.5
1	X	145	ALA	4.4
1	X	451	ALA	4.4
1	X	242	PRO	4.3
1	X	25	ASN	4.3
1	X	373	SER	4.3
1	X	244	SER	4.2
1	X	23	GLY	4.1
1	X	102	SER	4.1
1	X	281	SER	4.1
1	X	314	VAL	3.9
1	X	221	VAL	3.8
1	X	218	ARG	3.6
1	X	450	VAL	3.6
1	X	209	ILE	3.6
1	X	283	ASP	3.5
1	X	223	LYS	3.5
1	X	262	TYR	3.5
1	X	228	GLY	3.5
1	X	280	ASN	3.5
1	X	224	ASP	3.3
1	X	340	GLU	3.3
1	X	279	GLU	3.2
1	X	338	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	X	264	ALA	3.0
1	X	146	ALA	3.0
1	X	454	GLY	3.0
1	X	193	VAL	2.9
1	X	104	ILE	2.9
1	X	313	PRO	2.8
1	X	240	GLU	2.7
1	X	241	ASN	2.7
1	X	219	ARG	2.7
1	X	20	GLU	2.6
1	X	204	ILE	2.6
1	X	252	PHE	2.5
1	X	431	ALA	2.5
1	X	144	PRO	2.5
1	X	374	ASN	2.5
1	X	261	ILE	2.4
1	X	197	THR	2.4
1	X	410	VAL	2.4
1	X	395	CYS	2.3
1	X	336	ASP	2.3
1	X	343	LYS	2.3
1	X	121	ASN	2.3
1	X	277	LEU	2.2
1	X	187	ALA	2.2
1	X	378	VAL	2.2
1	X	220	GLY	2.1
1	X	184	TYR	2.1
1	X	225	GLY	2.1
1	X	278	GLY	2.0
1	X	397	ASP	2.0
1	X	105	ASP	2.0
1	X	344	MET	2.0
1	X	398	ARG	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.