Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 02:53 PM JST

PDB ID	:	7VBR
Title	:	Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI
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Deposited on	:	2021-09-01
Resolution	:	2.10 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:

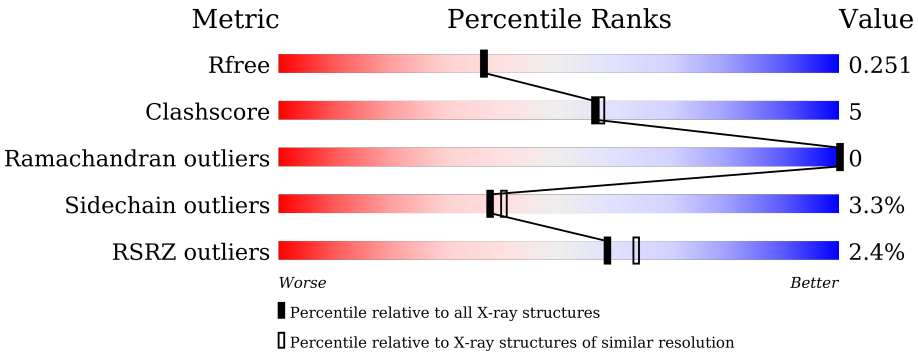
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	282	2% 71% 13% • 16%
1	B	282	2% 72% 11% 17%
1	C	282	2% 74% 11% 15%
1	D	282	2% 71% 12% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7770 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 Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	1	0
			1873	1199	320	347	7			
1	B	234	Total	C	N	O	S	0	0	0
			1801	1147	312	335	7			
1	D	236	Total	C	N	O	S	0	0	0
			1844	1178	318	341	7			
1	C	240	Total	C	N	O	S	0	0	0
			1876	1201	322	346	7			

- Molecule 2 is water.

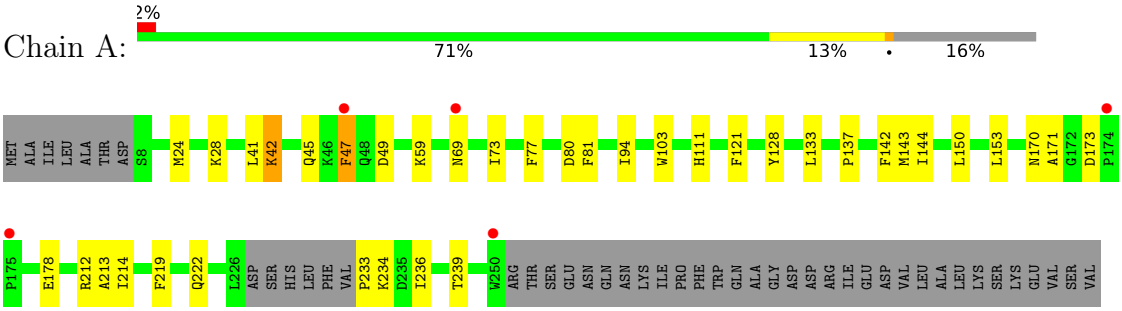
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	94	Total	O	0	0
			94	94		
2	D	83	Total	O	0	0
			83	83		
2	C	108	Total	O	0	0
			108	108		

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.

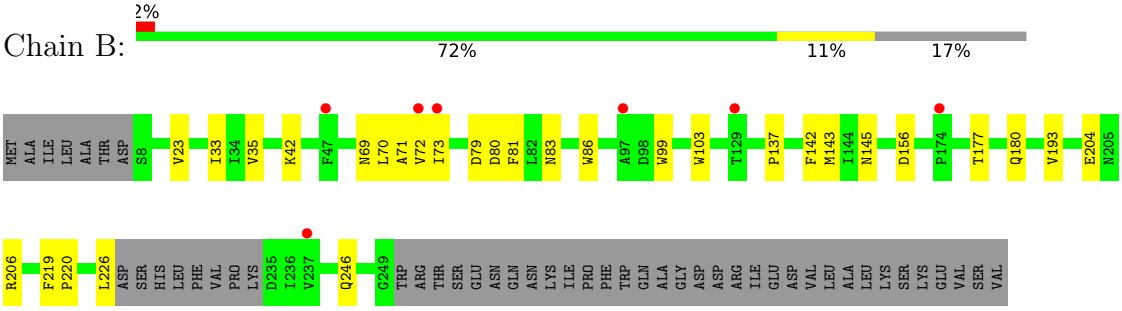
• Molecule 1: Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI

Chain A:



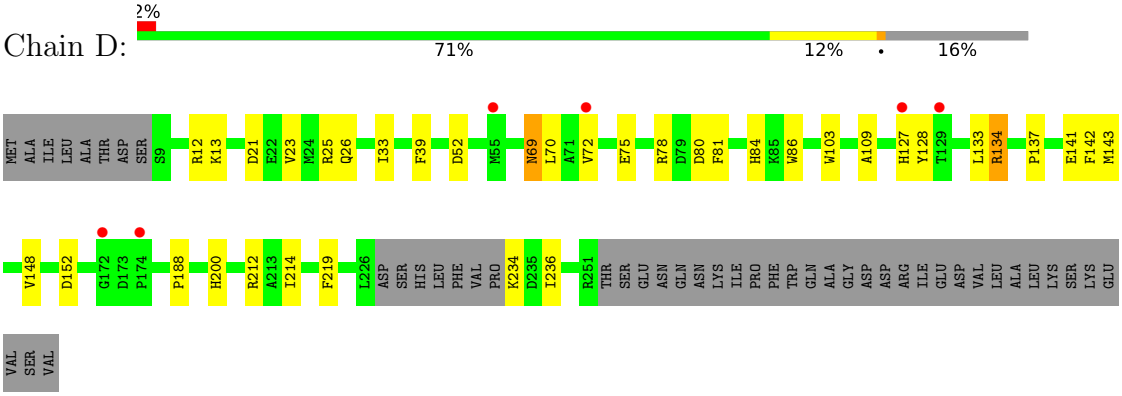
• Molecule 1: Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI

Chain B:



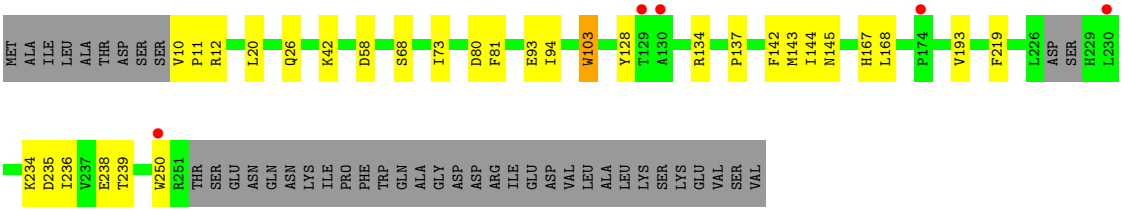
• Molecule 1: Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI

Chain D:



• Molecule 1: Fe(II)/(alpha)ketoglutarate-dependent dioxygenase TlxI

Chain C:


MET ALA ILE LEU ALA THR ASP SER SER V10 P11 R12 L20 Q26 K42 D58 S68 I73 D80 F81 E93 I94 W103 Y128 T129 A130 R134 P137 F142 M143 I144 N145 H167 L168 P174 V193 F219 L226 ASP SER H229 L230
K234 D235 I236 V237 E238 T239 W250 R251 THR SER GLU ASN GLN ASN LYS ILE PRO PHE TRP GLN ALA GLY ASP ASP ARG ILE GLU ASP VAL LEU ALA LEU LYS SER LYS GLU VAL SER VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.40Å 64.45Å 76.99Å 81.75° 73.70° 74.83°	Depositor
Resolution (Å)	49.32 – 2.10 49.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.32-2.10) 97.6 (49.32-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.209 , 0.254 0.208 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.01% 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	A	0.42	0/1920	0.61	0/2606
1	B	0.42	0/1843	0.59	0/2505
1	C	0.43	0/1922	0.59	0/2611
1	D	0.41	0/1888	0.59	0/2563
All	All	0.42	0/7573	0.60	0/10285

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	1873	0	1830	23	0
1	B	1801	0	1738	16	0
1	C	1876	0	1828	15	0
1	D	1844	0	1802	19	0
2	A	91	0	0	3	0
2	B	94	0	0	0	0
2	C	108	0	0	0	0
2	D	83	0	0	0	0
All	All	7770	0	7198	73	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 5.

All (73) 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:111:HIS:HE1	2:A:372:HOH:O	1.56	0.88
1:C:94:ILE:HD13	1:C:144:ILE:HD12	1.70	0.73
1:A:111:HIS:CE1	2:A:372:HOH:O	2.37	0.69
1:D:52:ASP:OD1	1:D:212:ARG:NH2	2.20	0.63
1:D:128:TYR:HB2	1:D:134:ARG:HB3	1.82	0.62
1:A:47[A]:PHE:CZ	1:A:77:PHE:HB2	2.34	0.61
1:D:109:ALA:HA	1:D:214:ILE:HD13	1.85	0.59
1:C:137:PRO:HA	1:C:142:PHE:CD2	2.37	0.59
1:A:142:PHE:CE1	1:A:143:MET:HG3	2.40	0.57
1:B:69:ASN:OD1	1:B:72:VAL:HG23	2.06	0.56
1:B:137:PRO:HA	1:B:142:PHE:CD2	2.41	0.55
1:A:222:GLN:OE1	1:A:222:GLN:N	2.34	0.55
1:A:94:ILE:HD13	1:A:144:ILE:HD12	1.89	0.54
1:B:70:LEU:HA	1:B:73:ILE:HG12	1.90	0.52
1:A:42:LYS:O	1:A:42:LYS:HD3	2.11	0.51
1:B:99:TRP:HB3	1:B:220:PRO:HB3	1.91	0.51
1:C:68:SER:HB3	1:C:73:ILE:HG21	1.94	0.50
1:D:21:ASP:O	1:D:25:ARG:HG3	2.13	0.49
1:A:233:PRO:HG2	1:A:236:ILE:HG12	1.94	0.49
1:C:234:LYS:O	1:C:238:GLU:HG2	2.12	0.48
1:A:133:LEU:HG	1:A:171:ALA:HB2	1.96	0.48
1:D:152:ASP:OD1	1:D:188:PRO:HD3	2.15	0.46
1:C:236:ILE:O	1:C:239:THR:HB	2.15	0.46
1:D:75:GLU:HG3	1:D:78:ARG:NH2	2.30	0.46
1:A:24:MET:HE3	1:A:28:LYS:HD2	1.98	0.45
1:B:177:THR:OG1	1:B:180:GLN:HG3	2.16	0.45
1:D:143:MET:HB2	1:D:143:MET:HE3	1.72	0.45
1:C:128:TYR:HB2	1:C:134:ARG:HB3	1.99	0.45
1:C:143:MET:HB2	1:C:143:MET:HE3	1.70	0.45
1:A:170:ASN:O	1:A:173:ASP:HB2	2.17	0.44
1:C:10:VAL:HA	1:C:11:PRO:C	2.37	0.44
1:B:42:LYS:HA	1:B:42:LYS:HD2	1.71	0.44
1:A:137:PRO:HA	1:A:142:PHE:CD2	2.52	0.44
1:C:142:PHE:HA	1:C:143:MET:HA	1.78	0.44
1:D:137:PRO:HA	1:D:142:PHE:CD1	2.53	0.44
1:B:70:LEU:HD23	1:B:73:ILE:HD11	2.00	0.44
1:D:12:ARG:HD3	1:D:26:GLN:OE1	2.18	0.44
1:A:150:LEU:HB2	1:A:212:ARG:HB2	2.00	0.44
1:D:234:LYS:HB2	1:D:236:ILE:H	1.83	0.43
1:A:69:ASN:O	1:A:73:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TRP:CD2	1:C:250:TRP:HD1	2.37	0.43
1:C:20:LEU:HD21	1:C:93:GLU:HG2	2.01	0.43
1:C:12:ARG:HD3	1:C:26:GLN:HG2	2.01	0.43
1:D:141:GLU:OE2	1:D:200:HIS:NE2	2.47	0.42
1:B:79:ASP:O	1:B:83:ASN:HB2	2.18	0.42
1:B:204:GLU:HG2	1:B:206:ARG:HG3	2.01	0.42
1:D:23:VAL:HG13	1:D:33:ILE:HD13	2.00	0.42
1:C:167:HIS:CE1	1:C:168:LEU:HG	2.54	0.42
1:D:69:ASN:O	1:D:72:VAL:HB	2.20	0.42
1:C:145:ASN:O	1:C:193:VAL:HA	2.19	0.42
1:A:47[A]:PHE:CE2	1:A:77:PHE:HB2	2.55	0.42
1:D:127:HIS:CE1	1:D:133:LEU:HD21	2.55	0.42
1:A:236:ILE:O	1:A:239:THR:OG1	2.20	0.42
1:D:84:HIS:CE1	1:D:86:TRP:HB3	2.55	0.42
1:A:142:PHE:HA	1:A:143:MET:HA	1.78	0.41
1:B:145:ASN:O	1:B:193:VAL:HA	2.20	0.41
1:A:59:LYS:HE2	2:A:386:HOH:O	2.20	0.41
1:B:156:ASP:OD1	1:B:206:ARG:NH2	2.50	0.41
1:D:70:LEU:HD11	1:D:214:ILE:HD12	2.01	0.41
1:B:69:ASN:O	1:B:73:ILE:HG23	2.21	0.41
1:D:142:PHE:HA	1:D:143:MET:HA	1.76	0.41
1:D:12:ARG:HG3	1:D:13:LYS:N	2.36	0.41
1:A:153:LEU:HD11	1:A:213:ALA:HB2	2.02	0.41
1:A:47[A]:PHE:CD1	1:A:214:ILE:HD11	2.56	0.41
1:D:39:PHE:HD2	1:D:148:VAL:HG11	1.86	0.41
1:A:41:LEU:HD13	1:A:41:LEU:HA	1.78	0.41
1:B:35:VAL:HG21	1:B:86:TRP:CH2	2.56	0.41
1:B:142:PHE:HA	1:B:143:MET:HA	1.83	0.40
1:A:45:GLN:NE2	1:A:49:ASP:OD1	2.54	0.40
1:A:121:PHE:CD1	1:A:178:GLU:HG2	2.56	0.40
1:B:69:ASN:OD1	1:B:71:ALA:HB3	2.22	0.40
1:C:235:ASP:HA	1:C:238:GLU:HG2	2.03	0.40
1:B:23:VAL:HG13	1:B:33:ILE:HD13	2.02	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	234/282 (83%)	227 (97%)	7 (3%)	0	100	100
1	B	230/282 (82%)	224 (97%)	6 (3%)	0	100	100
1	C	236/282 (84%)	229 (97%)	7 (3%)	0	100	100
1	D	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
All	All	932/1128 (83%)	906 (97%)	26 (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	202/243 (83%)	193 (96%)	9 (4%)	27	27
1	B	190/243 (78%)	184 (97%)	6 (3%)	39	41
1	C	200/243 (82%)	194 (97%)	6 (3%)	41	44
1	D	197/243 (81%)	191 (97%)	6 (3%)	41	44
All	All	789/972 (81%)	762 (97%)	27 (3%)	38	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	47[A]	PHE

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Mol	Chain	Res	Type
1	A	47[B]	PHE
1	A	80	ASP
1	A	81	PHE
1	A	103	TRP
1	A	128	TYR
1	A	219	PHE
1	A	234	LYS
1	B	80	ASP
1	B	81	PHE
1	B	103	TRP
1	B	219	PHE
1	B	226	LEU
1	B	246	GLN
1	D	69	ASN
1	D	80	ASP
1	D	81	PHE
1	D	103	TRP
1	D	134	ARG
1	D	219	PHE
1	C	42	LYS
1	C	58	ASP
1	C	80	ASP
1	C	81	PHE
1	C	103	TRP
1	C	219	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A	237/282 (84%)	0.27	5 (2%)	63	68	22, 35, 56, 68	0
1	B	234/282 (82%)	0.34	7 (2%)	50	56	20, 34, 57, 72	0
1	C	240/282 (85%)	0.35	5 (2%)	63	68	19, 33, 62, 88	0
1	D	236/282 (83%)	0.28	6 (2%)	57	62	19, 35, 61, 75	0
All	All	947/1128 (83%)	0.31	23 (2%)	59	64	19, 34, 60, 88	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	ALA	5.9
1	A	47[A]	PHE	3.8
1	B	97	ALA	3.1
1	D	172	GLY	3.1
1	C	174	PRO	3.0
1	D	55	MET	3.0
1	B	174	PRO	2.9
1	A	250	TRP	2.8
1	D	72	VAL	2.8
1	B	47	PHE	2.7
1	C	129	THR	2.6
1	A	175	PRO	2.6
1	B	129	THR	2.6
1	B	237	VAL	2.5
1	B	73	ILE	2.5
1	A	174	PRO	2.4
1	D	127	HIS	2.3
1	B	72	VAL	2.2
1	D	129	THR	2.2
1	D	174	PRO	2.2
1	C	230	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	250	TRP	2.1
1	A	69	ASN	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.