



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:09 AM GMT

PDB ID : 1ZX2
Title : Crystal Structure of Yeast UBP3-associated Protein BRE5
Authors : Li, K.; Zhao, K.; Ossareh-Nazari, B.; Da, G.; Dargemont, C.; Marmorstein, R.
Deposited on : 2005-06-06
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
<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
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

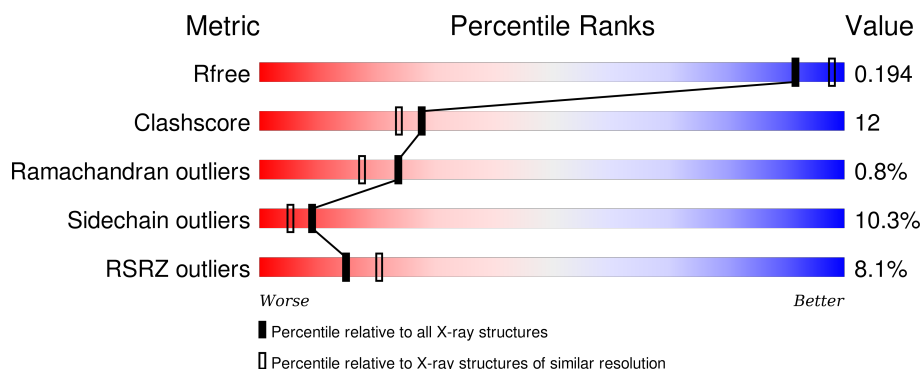
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 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	147	<div> <div>11%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>6% •</div> <div>12%</div> </div> </div>
1	B	147	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>7% •</div> <div>12%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2248 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 UBP3-associated protein BRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1052	681	171	194	6			
1	B	130	Total	C	N	O	S	0	1	0
			1050	679	171	194	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P53741
B	0	SER	-	CLONING ARTIFACT	UNP P53741

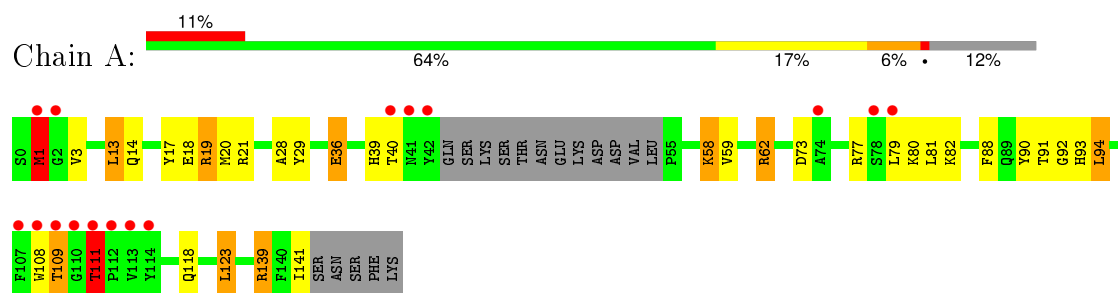
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	88	Total	O	0	0
			88	88		

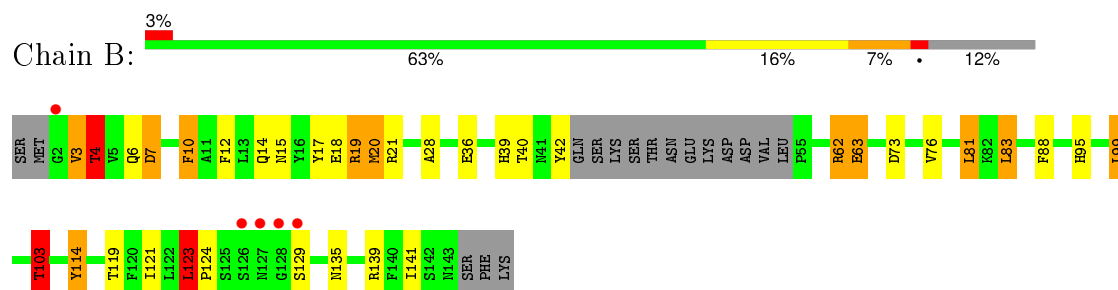
3 Residue-property plots [i](#)

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: UBP3-associated protein BRE5



- Molecule 1: UBP3-associated protein BRE5



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.91Å 90.91Å 194.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.06 – 2.10 39.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (79.06-2.10) 97.6 (39.36-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.213 0.198 , 0.194	Depositor DCC
R_{free} test set	2822 reflections (11.20%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28529 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2248	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, 0.375 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	1.26	11/1077 (1.0%)	1.60	15/1456 (1.0%)
1	B	1.44	11/1080 (1.0%)	1.48	19/1461 (1.3%)
All	All	1.35	22/2157 (1.0%)	1.54	34/2917 (1.2%)

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	A	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	MET	SD-CE	-8.74	1.28	1.77
1	A	139	ARG	CD-NE	-7.83	1.33	1.46
1	B	62	ARG	CD-NE	-7.65	1.33	1.46
1	A	59	VAL	CB-CG2	-7.22	1.37	1.52
1	B	103	THR	CB-CG2	-6.85	1.29	1.52
1	B	20	MET	CG-SD	6.79	1.98	1.81
1	A	62	ARG	CD-NE	-6.73	1.35	1.46
1	B	36	GLU	CD-OE1	6.71	1.33	1.25
1	A	36	GLU	CD-OE2	6.57	1.32	1.25
1	B	4	THR	CB-CG2	-6.52	1.30	1.52
1	B	10	PHE	CE2-CZ	6.26	1.49	1.37
1	A	36	GLU	CD-OE1	6.00	1.32	1.25
1	A	58	LYS	CD-CE	5.48	1.65	1.51
1	B	17	TYR	CZ-OH	5.45	1.47	1.37
1	B	36	GLU	CD-OE2	5.38	1.31	1.25
1	B	3	VAL	CB-CG2	-5.33	1.41	1.52
1	A	20	MET	SD-CE	-5.32	1.48	1.77
1	A	58	LYS	CE-NZ	5.26	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ARG	NE-CZ	-5.11	1.26	1.33
1	B	12	PHE	CE2-CZ	5.11	1.47	1.37
1	A	139	ARG	NE-CZ	-5.07	1.26	1.33
1	A	90	TYR	CD1-CE1	5.00	1.46	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-25.45	107.57	120.30
1	A	62	ARG	NE-CZ-NH2	-21.89	109.36	120.30
1	B	62	ARG	NE-CZ-NH2	-18.86	110.87	120.30
1	A	62	ARG	NE-CZ-NH1	18.24	129.42	120.30
1	B	62	ARG	NE-CZ-NH1	15.95	128.27	120.30
1	A	139	ARG	NE-CZ-NH1	15.87	128.23	120.30
1	B	139	ARG	NE-CZ-NH2	-11.53	114.54	120.30
1	B	20	MET	CG-SD-CE	-11.50	81.81	100.20
1	B	81	LEU	CA-CB-CG	8.99	135.97	115.30
1	A	62	ARG	CD-NE-CZ	8.92	136.09	123.60
1	A	123	LEU	CB-CG-CD2	8.81	125.97	111.00
1	A	139	ARG	CG-CD-NE	-7.98	95.04	111.80
1	A	36	GLU	OE1-CD-OE2	7.67	132.51	123.30
1	B	19	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	99	LEU	CB-CG-CD2	7.45	123.67	111.00
1	B	123	LEU	CB-CG-CD1	6.96	122.84	111.00
1	A	19	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	36	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	B	62	ARG	CD-NE-CZ	6.57	132.80	123.60
1	B	4	THR	N-CA-CB	-6.40	98.14	110.30
1	B	123	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	103	THR	N-CA-CB	-6.13	98.65	110.30
1	A	73	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	139	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	19	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	103	THR	CA-CB-CG2	5.36	119.91	112.40
1	B	73	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	29	TYR	CA-CB-CG	-5.20	103.53	113.40
1	A	62	ARG	CG-CD-NE	-5.11	101.06	111.80
1	B	83	LEU	CA-CB-CG	5.09	127.00	115.30
1	B	119	THR	OG1-CB-CG2	-5.08	98.32	110.00
1	B	19	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	7	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	13	LEU	CB-CG-CD1	5.02	119.54	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	111	THR	Peptide

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	1052	0	1037	25	0
1	B	1050	0	1028	29	4
2	A	58	0	0	5	0
2	B	88	0	0	13	0
All	All	2248	0	2065	49	4

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 12.

All (49) 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:91:THR:HG23	1:B:135:ASN:ND2	1.84	0.91
1:B:4:THR:HG21	2:B:203:HOH:O	1.73	0.87
1:A:91:THR:HG23	1:B:135:ASN:HD21	1.39	0.87
1:B:4:THR:HG22	1:B:7:ASP:H	1.41	0.86
1:B:15:ASN:HB2	2:B:232:HOH:O	1.82	0.79
1:B:63:GLU:OE1	2:B:231:HOH:O	2.02	0.78
1:A:28:ALA:O	1:A:62:ARG:HD2	1.90	0.72
1:A:91:THR:HG22	1:A:92:GLY:H	1.55	0.70
1:A:91:THR:HG22	1:A:92:GLY:N	2.06	0.70
1:B:103:THR:HG23	2:B:205:HOH:O	1.93	0.69
1:A:36:GLU:CG	2:A:204:HOH:O	2.40	0.69
1:B:39:HIS:HD2	1:B:40:THR:O	1.75	0.68
1:A:93:HIS:HD2	2:B:233:HOH:O	1.78	0.67
1:B:95:HIS:CE1	2:B:230:HOH:O	2.50	0.65
1:B:39:HIS:HE1	2:B:212:HOH:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:CD	2:A:204:HOH:O	2.39	0.61
1:B:95:HIS:ND1	2:B:230:HOH:O	2.32	0.57
1:B:20:MET:HE1	2:B:212:HOH:O	2.03	0.57
1:A:28:ALA:O	1:A:62:ARG:CD	2.54	0.56
1:B:103:THR:CG2	2:B:205:HOH:O	2.54	0.54
1:A:36:GLU:HG2	2:A:204:HOH:O	2.03	0.54
1:A:79:LEU:HD12	1:A:108:TRP:NE1	2.25	0.52
1:A:17:TYR:OH	1:A:118:GLN:NE2	2.43	0.52
1:A:39:HIS:ND1	2:A:195:HOH:O	2.34	0.52
1:B:28:ALA:O	1:B:62:ARG:HD2	2.09	0.52
1:A:79:LEU:CD1	1:A:108:TRP:NE1	2.76	0.49
1:B:28:ALA:HB1	1:B:62:ARG:HG3	1.95	0.48
1:B:15:ASN:CG	2:B:232:HOH:O	2.52	0.48
1:A:91:THR:HG21	1:B:121:ILE:HD13	1.96	0.47
1:B:15:ASN:CB	2:B:232:HOH:O	2.50	0.47
1:B:3:VAL:HG22	1:B:7:ASP:HB2	1.96	0.46
1:B:123:LEU:HD22	1:B:124:PRO:HD2	1.97	0.46
1:A:139:ARG:HD2	2:A:179:HOH:O	2.16	0.46
1:A:39:HIS:CD2	1:A:40:THR:H	2.34	0.46
1:A:18:GLU:OE2	1:A:21:ARG:NH1	2.49	0.46
1:A:36:GLU:OE2	1:A:58:LYS:NZ	2.45	0.45
1:A:91:THR:HG21	1:B:121:ILE:CD1	2.47	0.45
1:B:19:ARG:HA	1:B:19:ARG:HD3	1.79	0.44
1:A:93:HIS:CE1	1:A:94:LEU:HD22	2.53	0.43
1:A:28:ALA:HB1	1:A:62:ARG:HG3	1.99	0.43
1:B:28:ALA:O	1:B:62:ARG:CD	2.67	0.43
1:B:4:THR:HG23	1:B:6:GLN:H	1.84	0.43
1:B:14:GLN:NE2	2:B:234:HOH:O	2.33	0.43
1:B:18:GLU:OE1	1:B:21:ARG:NH1	2.51	0.43
1:A:1:MET:HG2	1:A:3:VAL:HG12	2.02	0.42
1:B:42:TYR:CZ	1:B:76:VAL:HG22	2.55	0.42
1:B:114:TYR:HB3	1:B:141:ILE:O	2.19	0.41
1:A:39:HIS:CG	1:A:40:THR:H	2.37	0.41
1:A:91:THR:CG2	1:B:135:ASN:ND2	2.70	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PHE:CE2	1:B:10:PHE:CE2[10_665]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:NH2	1:B:21:ARG:NH2[10_665]	1.85	0.35
1:B:10:PHE:CE2	1:B:10:PHE:CZ[10_665]	1.94	0.26
1:B:10:PHE:CD2	1:B:10:PHE:CZ[10_665]	2.09	0.11

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	126/147 (86%)	121 (96%)	3 (2%)	2 (2%)	12	6
1	B	127/147 (86%)	125 (98%)	2 (2%)	0	100	100
All	All	253/294 (86%)	246 (97%)	5 (2%)	2 (1%)	24	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	111	THR

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	117/135 (87%)	103 (88%)	14 (12%)	6	3
1	B	117/135 (87%)	107 (92%)	10 (8%)	13	9
All	All	234/270 (87%)	210 (90%)	24 (10%)	9	5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	LEU
1	A	14	GLN
1	A	19	ARG
1	A	77	ARG
1	A	80	LYS
1	A	81	LEU
1	A	82	LYS
1	A	88	PHE
1	A	94	LEU
1	A	109	THR
1	A	111	THR
1	A	123	LEU
1	A	141	ILE
1	B	4	THR
1	B	63	GLU
1	B	81	LEU
1	B	83	LEU
1	B	88	PHE
1	B	99	LEU
1	B	103	THR
1	B	114	TYR
1	B	123	LEU
1	B	129	SER

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

Mol	Chain	Res	Type
1	A	39	HIS
1	A	93	HIS
1	A	118	GLN
1	A	135	ASN
1	B	39	HIS
1	B	66	ASN
1	B	118	GLN
1	B	135	ASN
1	B	143	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	130/147 (88%)	0.56	16 (12%) 5 7	17, 30, 60, 83	0
1	B	130/147 (88%)	0.01	5 (3%) 44 53	15, 25, 46, 61	0
All	All	260/294 (88%)	0.29	21 (8%) 15 20	15, 28, 57, 83	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	THR	9.7
1	A	108	TRP	9.6
1	A	109	THR	8.7
1	A	110	GLY	7.2
1	A	107	PHE	5.8
1	B	126	SER	5.4
1	A	2	GLY	5.2
1	B	129	SER	4.1
1	A	79	LEU	3.8
1	A	40	THR	3.7
1	A	113	VAL	3.6
1	B	2	GLY	3.3
1	A	78	SER	3.3
1	A	42	TYR	3.2
1	A	112	PRO	3.2
1	B	128	GLY	2.9
1	A	114	TYR	2.8
1	A	74	ALA	2.6
1	A	41	ASN	2.6
1	A	1	MET	2.1
1	B	127	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 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.