



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:28 pm BST

PDB ID : 5W6V  
Title : The Structure of human Argonaute-1 in complex with the hook motif of human GW182  
Authors : Elkayam, E.; Faehnle, C.R.; Joshua-Tor, L.  
Deposited on : 2017-06-17  
Resolution : 2.83 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](mailto: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 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	:	2.11
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)	:	2.11

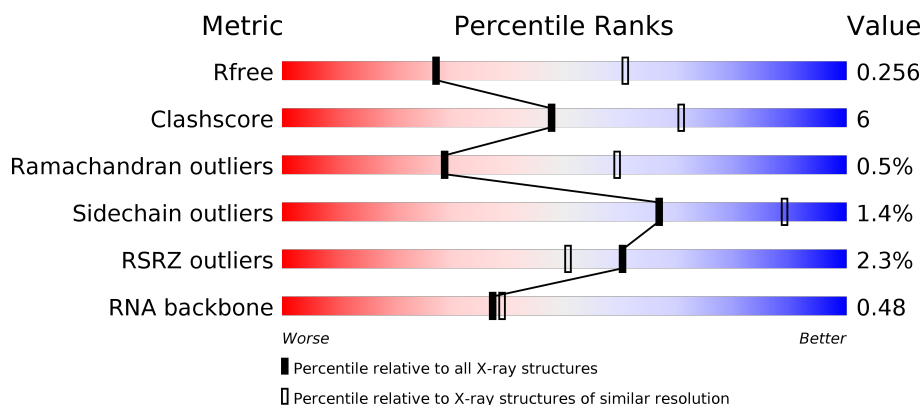
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)
RNA backbone	3102	1103 (3.10-2.54)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	859	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
2	R	20	<div> <div>5%</div> <div> <div></div> <div>30%</div> <div>20%</div> <div>50%</div> </div> </div>
3	B	24	<div> <div>21%</div> <div> <div></div> <div>42%</div> <div>25%</div> <div>• 29%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6752 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 Protein argonaute-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6412	4108	1139	1127	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UL18
A	0	ALA	-	expression tag	UNP Q9UL18

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*UP\*AP\*UP\*UP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	10	Total	C	N	O	P	0	0	0
			215	97	41	67	10			

- Molecule 3 is a protein called Trinucleotide repeat-containing gene 6A protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	17	Total	C	N	O	0	0	0
			121	76	21	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	818	GLY	-	expression tag	UNP Q8NDV7
B	819	ALA	-	expression tag	UNP Q8NDV7

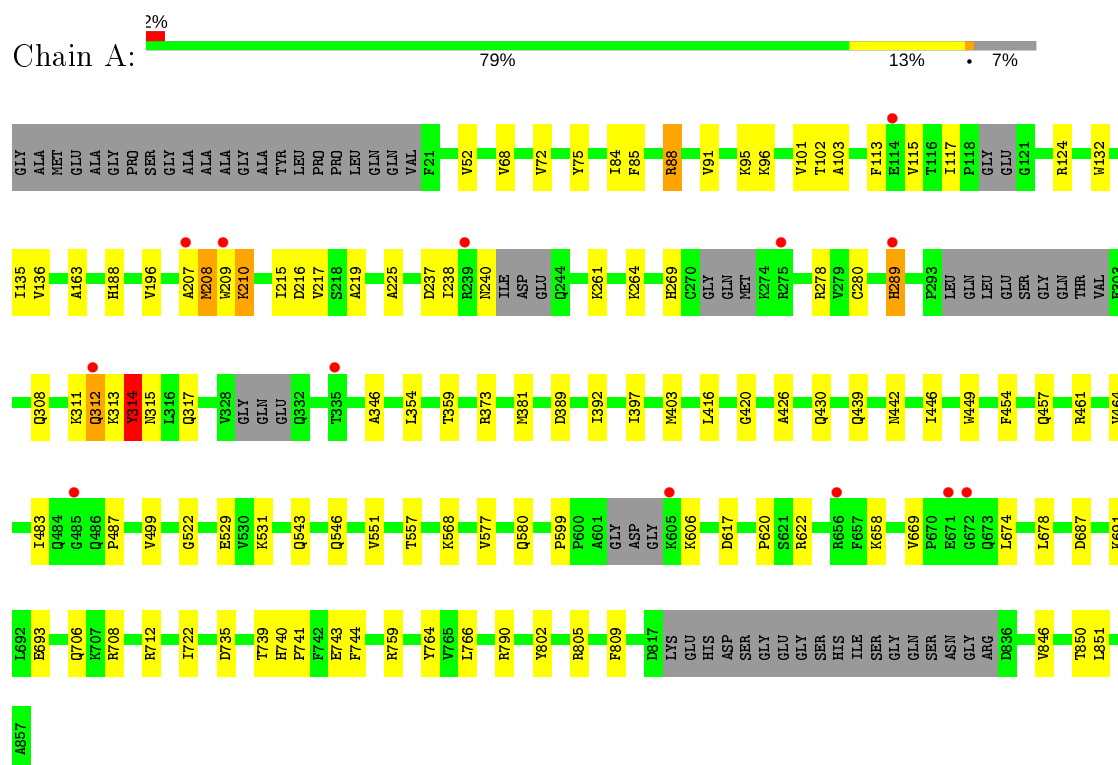
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	R	2	Total 2	O 2	0	0

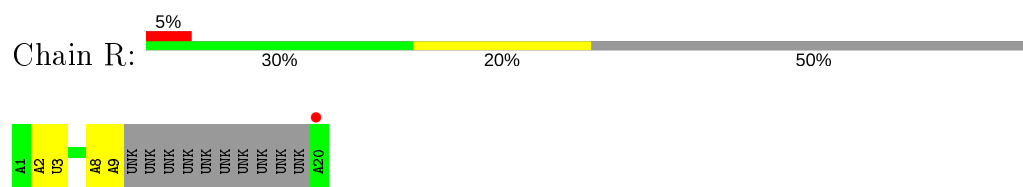
### 3 Residue-property plots [i](#)

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.

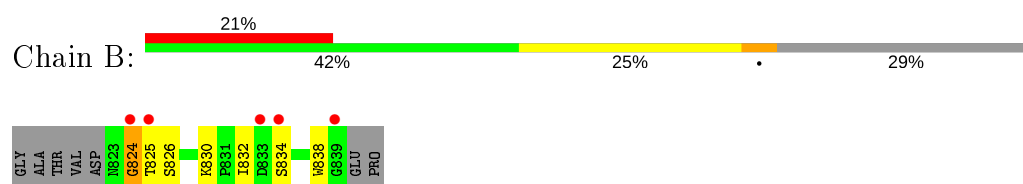
#### • Molecule 1: Protein argonaute-1



#### • Molecule 2: RNA (5'-R(P\*AP\*AP\*UP\*AP\*UP\*UP\*AP\*AP\*AP\*A)-3')



#### • Molecule 3: Trinucleotide repeat-containing gene 6A protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.75Å 136.86Å 86.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.34 – 2.83 77.34 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.7 (77.34-2.83) 99.7 (77.34-2.83)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.200 , 0.245 0.213 , 0.256	Depositor DCC
$R_{free}$ test set	1393 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.26	0/6566	0.44	0/8893
2	R	0.18	0/240	0.73	0/367
3	B	0.31	0/126	0.61	0/172
All	All	0.26	0/6932	0.46	0/9432

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 [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	6412	0	6496	78	0
2	R	215	0	109	5	0
3	B	121	0	106	6	0
4	A	2	0	0	0	0
4	R	2	0	0	0	0
All	All	6752	0	6711	82	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 (82) 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:209:TRP:O	1:A:210:LYS:HG3	1.09	1.21
1:A:209:TRP:O	1:A:210:LYS:CG	1.93	1.17
1:A:313:LYS:O	1:A:315:ASN:N	1.79	1.13
1:A:207:ALA:O	1:A:209:TRP:N	2.07	0.87
1:A:313:LYS:C	1:A:315:ASN:H	1.75	0.86
1:A:658:LYS:NZ	1:A:693:GLU:OE2	2.22	0.71
1:A:543:GLN:OE1	1:A:568:LYS:NZ	2.24	0.70
1:A:88:ARG:NH2	1:A:103:ALA:O	2.24	0.70
1:A:687:ASP:OD2	1:A:691:LYS:NZ	2.25	0.69
1:A:759:ARG:NH2	2:R:8:A:OP2	2.26	0.69
1:A:743:GLU:OE1	1:A:764:TYR:OH	2.10	0.68
1:A:209:TRP:O	1:A:210:LYS:CB	2.43	0.65
1:A:392:ILE:HG23	1:A:397:ILE:HB	1.79	0.65
1:A:208:MET:HA	1:A:741:PRO:HA	1.78	0.64
1:A:225:ALA:HB2	1:A:346:ALA:HB2	1.81	0.62
1:A:85:PHE:O	1:A:88:ARG:HD3	2.02	0.58
3:B:832:ILE:HG22	3:B:834:SER:H	1.70	0.57
1:A:790:ARG:NH2	2:R:3:U:OP1	2.29	0.57
1:A:264:LYS:HG2	1:A:278:ARG:HG2	1.86	0.56
1:A:420:GLY:HA3	1:A:439:GLN:HB2	1.89	0.55
1:A:269:HIS:CD2	1:A:314:TYR:CE1	2.95	0.54
1:A:72:VAL:HA	1:A:117:ILE:HD11	1.89	0.54
1:A:84:ILE:HD12	1:A:113:PHE:HZ	1.73	0.52
1:A:674:LEU:HD21	1:A:766:LEU:HD21	1.92	0.52
1:A:207:ALA:O	1:A:208:MET:C	2.48	0.51
1:A:669:VAL:O	1:A:706:GLN:NE2	2.39	0.51
1:A:264:LYS:HE2	1:A:278:ARG:HE	1.76	0.51
1:A:308:GLN:O	1:A:312:GLN:HB2	2.11	0.50
1:A:599:PRO:HB3	1:A:606:LYS:HB2	1.93	0.50
3:B:824:GLY:C	3:B:826:SER:H	2.15	0.50
1:A:446:ILE:HD12	1:A:483:ILE:HG12	1.95	0.49
1:A:52:VAL:HG23	1:A:136:VAL:HB	1.94	0.49
1:A:708:ARG:HG2	2:R:9:A:N6	2.28	0.48
1:A:311:LYS:HE2	1:A:317:GLN:HG2	1.96	0.48
1:A:84:ILE:HG22	1:A:85:PHE:H	1.79	0.48
1:A:617:ASP:HA	3:B:825:THR:HG23	1.96	0.48
1:A:693:GLU:HG3	3:B:838:TRP:HE1	1.77	0.48
1:A:75:TYR:CD1	1:A:115:VAL:HG13	2.49	0.48
1:A:846:VAL:HG12	1:A:850:THR:HB	1.94	0.47
1:A:219:ALA:O	2:R:8:A:H5'	2.14	0.47
1:A:457:GLN:O	1:A:461:ARG:HG2	2.14	0.47
1:A:454:PHE:CZ	1:A:499:VAL:HG12	2.50	0.47

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HB2	1:A:426:ALA:HB3	1.97	0.47
1:A:389:ASP:HB3	1:A:392:ILE:HB	1.97	0.47
1:A:269:HIS:HD2	1:A:314:TYR:CE1	2.33	0.46
1:A:289:HIS:ND1	1:A:289:HIS:O	2.49	0.46
1:A:313:LYS:HB3	1:A:313:LYS:HE3	1.38	0.46
1:A:68:VAL:O	1:A:72:VAL:HG23	2.16	0.46
1:A:237:ASP:C	1:A:238:ILE:HG13	2.36	0.46
3:B:824:GLY:O	3:B:825:THR:HB	2.15	0.45
1:A:740:HIS:CG	1:A:741:PRO:HD2	2.52	0.45
1:A:522:GLY:HA2	1:A:546:GLN:HE21	1.82	0.45
1:A:617:ASP:OD1	1:A:620:PRO:HA	2.17	0.45
1:A:735:ASP:HA	1:A:739:THR:HG21	1.99	0.45
1:A:101:VAL:HG13	1:A:102:THR:HG23	1.99	0.44
1:A:373:ARG:NH1	1:A:712:ARG:HE	2.14	0.44
1:A:313:LYS:HE2	1:A:314:TYR:CZ	2.53	0.44
1:A:678:LEU:HD22	1:A:766:LEU:HB3	2.00	0.44
1:A:261:LYS:HE2	1:A:280:CYS:O	2.18	0.43
1:A:354:LEU:HB2	1:A:359:THR:HG23	2.00	0.43
1:A:522:GLY:HA2	1:A:546:GLN:NE2	2.33	0.43
1:A:499:VAL:CG2	1:A:529:GLU:HG3	2.49	0.43
1:A:403:MET:HE2	1:A:403:MET:HB3	1.69	0.43
1:A:442:ASN:HD22	1:A:442:ASN:HA	1.69	0.43
1:A:449:TRP:CH2	1:A:487:PRO:HG3	2.53	0.43
1:A:708:ARG:HE	1:A:708:ARG:HB3	1.58	0.42
1:A:499:VAL:HG21	1:A:529:GLU:HG3	2.01	0.42
1:A:188:HIS:HB2	1:A:196:VAL:HB	2.01	0.42
1:A:430:GLN:OE1	1:A:722:ILE:HD13	2.19	0.42
1:A:132:TRP:HH2	1:A:135:ILE:HG13	1.85	0.42
1:A:91:VAL:HG11	1:A:163:ALA:HA	2.02	0.41
1:A:216:ASP:OD1	1:A:217:VAL:N	2.53	0.41
1:A:577:VAL:O	1:A:580:GLN:HG2	2.21	0.41
1:A:95:LYS:HG3	1:A:96:LYS:HG3	2.01	0.41
1:A:531:LYS:HD3	1:A:531:LYS:HA	1.83	0.41
1:A:805:ARG:O	1:A:809:PHE:HD1	2.02	0.41
1:A:557:THR:HG23	2:R:2:A:N9	2.35	0.41
1:A:846:VAL:HB	1:A:851:LEU:HD23	2.03	0.41
1:A:215:ILE:HG13	1:A:381:MET:SD	2.60	0.41
1:A:464:VAL:HG21	1:A:551:VAL:HA	2.03	0.41
1:A:313:LYS:C	1:A:315:ASN:N	2.47	0.40
3:B:824:GLY:C	3:B:826:SER:N	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	780/859 (91%)	755 (97%)	22 (3%)	3 (0%)	34	64
3	B	15/24 (62%)	8 (53%)	6 (40%)	1 (7%)	1	3
All	All	795/883 (90%)	763 (96%)	28 (4%)	4 (0%)	29	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	MET
1	A	210	LYS
1	A	314	TYR
3	B	824	GLY

### 5.3.2 Protein sidechains

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	703/746 (94%)	694 (99%)	9 (1%)	69	90
3	B	12/17 (71%)	11 (92%)	1 (8%)	11	31
All	All	715/763 (94%)	705 (99%)	10 (1%)	67	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	124	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	240	ASN
1	A	289	HIS
1	A	312	GLN
1	A	314	TYR
1	A	622	ARG
1	A	744	PHE
1	A	802	TYR
3	B	830	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/20 (40%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	796/859 (92%)	0.10	13 (1%) 72 65	27, 53, 100, 141	0
2	R	10/20 (50%)	0.87	1 (10%) 7 4	50, 62, 151, 153	0
3	B	17/24 (70%)	1.68	5 (29%) 0 0	70, 103, 137, 154	0
All	All	823/903 (91%)	0.15	19 (2%) 60 50	27, 54, 105, 154	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	825	THR	5.5
3	B	834	SER	3.6
3	B	833	ASP	3.6
1	A	209	TRP	3.5
1	A	114	GLU	3.2
2	R	20	A	3.0
1	A	312	GLN	2.8
1	A	275	ARG	2.7
1	A	289	HIS	2.7
1	A	239	ARG	2.5
1	A	485	GLY	2.3
1	A	605	LYS	2.2
3	B	839	GLY	2.2
1	A	656	ARG	2.2
1	A	671	GLU	2.2
1	A	672	GLY	2.1
3	B	824	GLY	2.1
1	A	207	ALA	2.0
1	A	335	THR	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.