



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:25 AM GMT

PDB ID : 3IF8  
Title : Crystal Structure of ZWILCH, a member of the RZZ kinetochore complex  
Authors : Wehenkel, A.; Civril, F.; Musacchio, A.  
Deposited on : 2009-07-24  
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](mailto: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

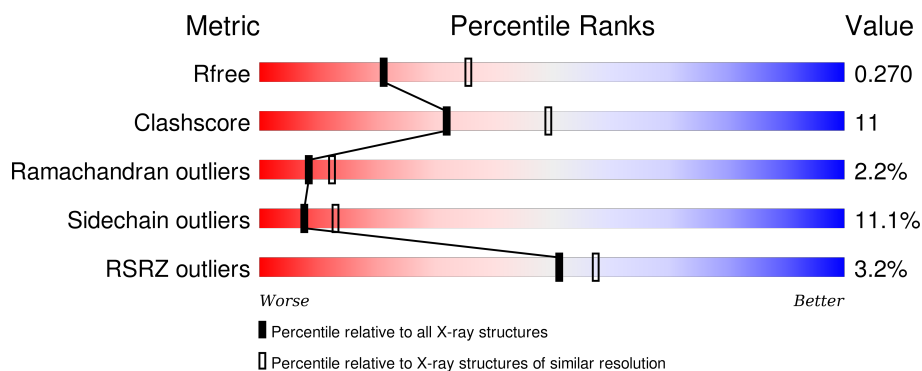
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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  $\geq 3$ , 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	339	
2	B	257	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4006 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 zwilch homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2055	1325	341	382	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9H900
A	-3	PRO	-	EXPRESSION TAG	UNP Q9H900
A	-2	LEU	-	EXPRESSION TAG	UNP Q9H900
A	-1	GLY	-	EXPRESSION TAG	UNP Q9H900
A	0	SER	-	EXPRESSION TAG	UNP Q9H900

- Molecule 2 is a protein called Protein zwilch homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1914	1244	314	346	10			

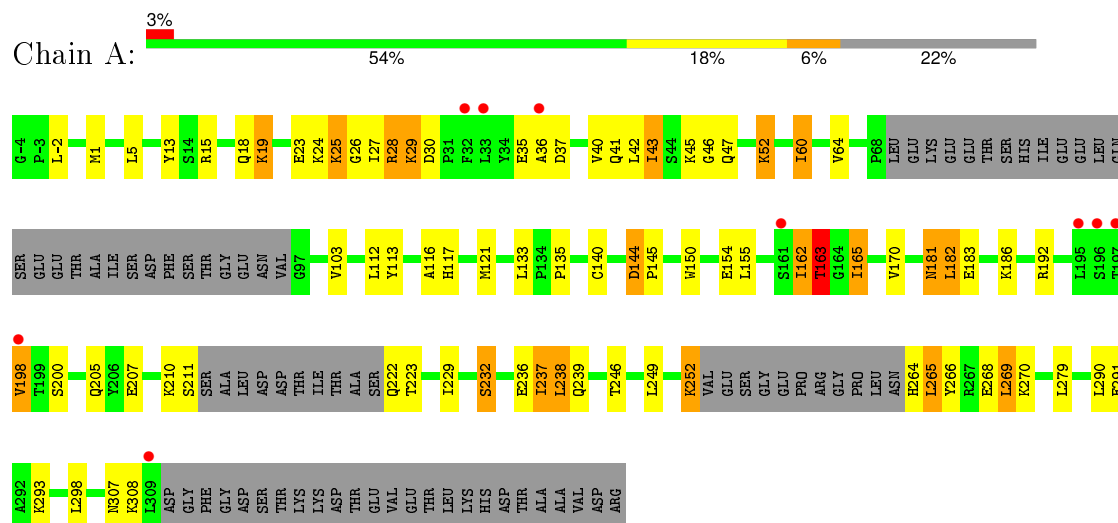
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	16	Total	O	0	0
			16	16		

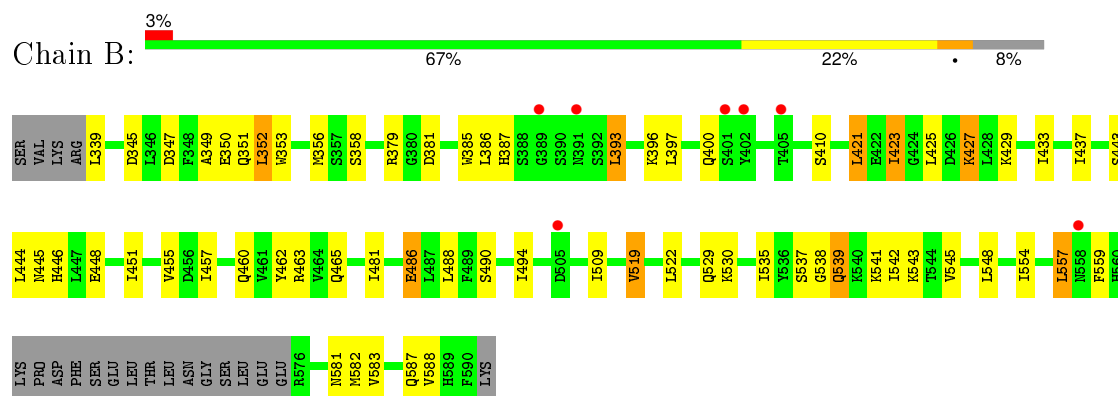
### 3 Residue-property plots [i](#)

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: Protein zwilch homolog



#### • Molecule 2: Protein zwilch homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.60Å 86.60Å 166.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.68 – 2.55 44.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.68-2.55) 99.5 (44.68-2.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.229 , 0.274 0.226 , 0.270	Depositor DCC
$R_{free}$ test set	1228 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.1	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24132 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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.*

<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, 0.375 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	0.50	0/2098	0.68	0/2859
2	B	0.50	0/1959	0.64	0/2653
All	All	0.50	0/4057	0.66	0/5512

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	2055	0	2054	51	0
2	B	1914	0	1911	43	0
3	A	21	0	0	0	0
3	B	16	0	0	0	0
All	All	4006	0	3965	84	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 11.

All (84) 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)
2:B:379:ARG:HD2	2:B:381:ASP:OD2	1.70	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG22	1:A:163:THR:H	1.45	0.81
1:A:165:ILE:HD12	2:B:588:VAL:HB	1.67	0.76
2:B:352:LEU:HD13	2:B:356:MET:HE3	1.68	0.75
1:A:13:TYR:HB2	1:A:116:ALA:HB1	1.69	0.75
1:A:207:GLU:H	2:B:529:GLN:HE21	1.35	0.74
2:B:539:GLN:HE22	2:B:587:GLN:NE2	1.91	0.69
1:A:291:GLU:HG2	1:A:298:LEU:HD11	1.73	0.69
1:A:162:ILE:HG22	1:A:163:THR:N	2.08	0.68
1:A:23:GLU:C	1:A:25:LYS:H	1.98	0.67
2:B:353:TRP:HB2	2:B:423:ILE:CG2	2.25	0.67
1:A:135:PRO:HG3	1:A:154:GLU:HG3	1.78	0.66
1:A:28:ARG:O	1:A:30:ASP:N	2.26	0.65
2:B:539:GLN:HE22	2:B:587:GLN:HE22	1.45	0.64
1:A:162:ILE:CG2	1:A:163:THR:H	2.12	0.63
1:A:113:TYR:O	1:A:117:HIS:HD2	1.82	0.62
2:B:443:SER:H	2:B:446:HIS:CD2	2.18	0.61
2:B:519:VAL:HG22	2:B:522:LEU:HD12	1.83	0.61
2:B:347:ASP:OD1	2:B:350:GLU:HG3	2.02	0.59
1:A:155:LEU:HD23	1:A:165:ILE:HG23	1.84	0.58
1:A:165:ILE:CD1	2:B:588:VAL:HB	2.34	0.58
1:A:236:GLU:HB3	1:A:239:GLN:HB2	1.86	0.57
1:A:35:GLU:O	1:A:37:ASP:N	2.27	0.57
1:A:268:GLU:OE1	2:B:427:LYS:HE2	2.05	0.55
2:B:462:TYR:HA	2:B:465:GLN:HE21	1.73	0.54
2:B:539:GLN:HB3	2:B:542:ILE:HG12	1.92	0.52
1:A:210:LYS:O	1:A:211:SER:HB3	2.09	0.52
2:B:445:ASN:O	2:B:448:GLU:HG2	2.10	0.51
1:A:27:ILE:O	1:A:27:ILE:HG22	2.10	0.51
1:A:23:GLU:HA	1:A:26:GLY:O	2.11	0.50
1:A:237:ILE:O	1:A:238:LEU:HB2	2.10	0.50
1:A:23:GLU:C	1:A:25:LYS:N	2.64	0.50
1:A:182:LEU:HD22	1:A:186:LYS:HD2	1.92	0.50
1:A:205:GLN:HB3	2:B:530:LYS:HG2	1.93	0.50
1:A:13:TYR:HB2	1:A:116:ALA:CB	2.41	0.50
2:B:455:VAL:HG11	2:B:463:ARG:NH2	2.27	0.49
2:B:554:ILE:HB	2:B:557:LEU:HB2	1.95	0.49
1:A:265:LEU:HD12	1:A:270:LYS:HB2	1.95	0.48
2:B:530:LYS:HA	2:B:548:LEU:O	2.14	0.48
1:A:181:ASN:HD22	1:A:183:GLU:H	1.61	0.48
2:B:353:TRP:HB2	2:B:423:ILE:HG23	1.97	0.47
1:A:222:GLN:O	1:A:223:THR:OG1	2.26	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG22	1:A:64:VAL:HG22	1.97	0.47
2:B:353:TRP:CD1	2:B:427:LYS:HG2	2.50	0.47
2:B:349:ALA:HB1	2:B:423:ILE:HG13	1.97	0.47
1:A:181:ASN:ND2	1:A:183:GLU:H	2.13	0.46
1:A:265:LEU:CD1	1:A:270:LYS:HB2	2.46	0.46
1:A:150:TRP:HB2	1:A:170:VAL:HB	1.96	0.46
2:B:393:LEU:O	2:B:397:LEU:HG	2.16	0.46
2:B:537:SER:O	2:B:539:GLN:N	2.49	0.46
2:B:481:ILE:HD11	2:B:488:LEU:HD23	1.98	0.46
1:A:19:LYS:N	1:A:19:LYS:HE3	2.30	0.46
2:B:421:LEU:HD13	2:B:457:ILE:HG12	1.97	0.46
1:A:18:GLN:HB2	1:A:19:LYS:NZ	2.31	0.45
1:A:144:ASP:O	1:A:145:PRO:C	2.54	0.45
1:A:43:ILE:HA	1:A:47:GLN:OE1	2.16	0.45
1:A:252:LYS:HD3	2:B:509:ILE:HG12	1.98	0.45
2:B:345:ASP:O	2:B:387:HIS:CE1	2.70	0.44
2:B:443:SER:H	2:B:446:HIS:HD2	1.64	0.44
2:B:455:VAL:HG23	2:B:460:GLN:HG2	2.00	0.43
1:A:198:VAL:HG13	2:B:535:ILE:HG23	2.01	0.43
1:A:307:ASN:OD1	2:B:381:ASP:HB3	2.19	0.43
2:B:545:VAL:HB	2:B:583:VAL:HB	2.00	0.43
2:B:396:LYS:HG2	2:B:400:GLN:NE2	2.34	0.43
1:A:265:LEU:HD22	1:A:269:LEU:HD13	2.00	0.43
2:B:486:GLU:H	2:B:486:GLU:CD	2.23	0.43
1:A:52:LYS:HA	1:A:52:LYS:HD2	1.79	0.43
1:A:60:ILE:H	1:A:60:ILE:HG12	1.56	0.42
1:A:103:VAL:HG22	1:A:140:CYS:HB3	2.00	0.42
1:A:45:LYS:HB3	1:A:46:GLY:H	1.45	0.42
2:B:433:ILE:HG23	2:B:437:ILE:HD13	2.02	0.42
1:A:41:GLN:HE21	1:A:42:LEU:H	1.67	0.42
1:A:170:VAL:HA	2:B:582:MET:O	2.20	0.42
2:B:352:LEU:HD13	2:B:356:MET:CE	2.43	0.41
1:A:266:TYR:CZ	1:A:269:LEU:HB2	2.55	0.41
1:A:210:LYS:HB3	1:A:211:SER:H	1.52	0.41
2:B:353:TRP:HB2	2:B:423:ILE:HG22	2.02	0.41
1:A:27:ILE:O	1:A:29:LYS:N	2.54	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.68	0.41
2:B:347:ASP:O	2:B:351:GLN:HG3	2.21	0.40
1:A:198:VAL:HA	2:B:537:SER:HB2	2.02	0.40
2:B:557:LEU:HD13	2:B:559:PHE:CE2	2.56	0.40
2:B:425:LEU:O	2:B:429:LYS:HG3	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:O	1:A:232:SER:OG	2.32	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	257/339 (76%)	234 (91%)	15 (6%)	8 (3%)	5	6
2	B	233/257 (91%)	215 (92%)	15 (6%)	3 (1%)	15	25
All	All	490/596 (82%)	449 (92%)	30 (6%)	11 (2%)	8	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	29	LYS
1	A	24	LYS
1	A	162	ILE
1	A	163	THR
1	A	308	LYS
2	B	539	GLN
1	A	25	LYS
1	A	36	ALA
2	B	538	GLY
2	B	410	SER

### 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	225/300 (75%)	195 (87%)	30 (13%)	5	8
2	B	218/245 (89%)	199 (91%)	19 (9%)	13	22
All	All	443/545 (81%)	394 (89%)	49 (11%)	8	13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	LEU
1	A	1	MET
1	A	5	LEU
1	A	15	ARG
1	A	19	LYS
1	A	43	ILE
1	A	52	LYS
1	A	60	ILE
1	A	112	LEU
1	A	121	MET
1	A	133	LEU
1	A	144	ASP
1	A	163	THR
1	A	165	ILE
1	A	181	ASN
1	A	182	LEU
1	A	192	ARG
1	A	198	VAL
1	A	229	ILE
1	A	232	SER
1	A	237	ILE
1	A	238	LEU
1	A	246	THR
1	A	252	LYS
1	A	264	HIS
1	A	265	LEU
1	A	269	LEU
1	A	279	LEU
1	A	290	LEU
1	A	293	LYS
2	B	339	LEU
2	B	352	LEU
2	B	358	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	385	TRP
2	B	386	LEU
2	B	393	LEU
2	B	421	LEU
2	B	423	ILE
2	B	427	LYS
2	B	444	LEU
2	B	451	ILE
2	B	486	GLU
2	B	490	SER
2	B	494	ILE
2	B	519	VAL
2	B	541	LYS
2	B	543	LYS
2	B	557	LEU
2	B	581	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	117	HIS
1	A	181	ASN
2	B	387	HIS
2	B	400	GLN
2	B	446	HIS
2	B	460	GLN
2	B	465	GLN
2	B	469	HIS
2	B	529	GLN
2	B	587	GLN

### 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	265/339 (78%)	0.35	9 (3%) 49 55	31, 48, 69, 77	0
2	B	237/257 (92%)	0.29	7 (2%) 54 60	30, 47, 68, 82	0
All	All	502/596 (84%)	0.32	16 (3%) 51 57	30, 47, 69, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	SER	3.8
1	A	309	LEU	3.7
1	A	33	LEU	2.9
2	B	402	TYR	2.8
2	B	401	SER	2.8
2	B	391	ASN	2.5
2	B	405	THR	2.4
2	B	389	GLY	2.3
2	B	558	ASN	2.3
1	A	36	ALA	2.2
2	B	505	ASP	2.2
1	A	161	SER	2.1
1	A	195	LEU	2.1
1	A	197	THR	2.1
1	A	32	PHE	2.0
1	A	198	VAL	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.