



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 22, 2021 – 10:43 AM EST

PDB ID : 6WWA  
Title : Crystal structure of human SHLD2-SHLD3-REV7 complex  
Authors : Xie, W.; Patel, D.J.  
Deposited on : 2020-05-08  
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 2.17.1  
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) : 2.17.1

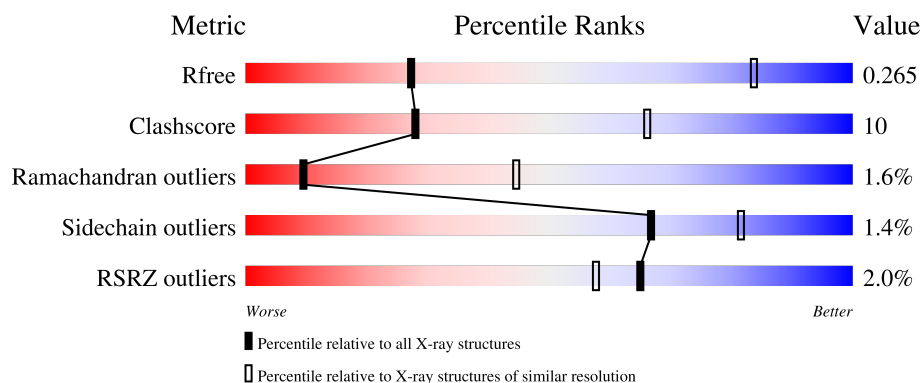
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 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	211	<div> <div>2%</div> <div>76%</div> <div>15%</div> <div>9%</div> </div>
1	B	211	<div> <div>%</div> <div>51%</div> <div>18%</div> <div>29%</div> </div>
1	C	211	<div> <div>%</div> <div>61%</div> <div>12%</div> <div>26%</div> </div>
1	D	211	<div> <div>71%</div> <div>19%</div> <div>9%</div> </div>
2	X	99	<div> <div>2%</div> <div>49%</div> <div>17%</div> <div>6%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Y	99	<div><div></div><div>4%</div><div>45%</div><div>23%</div><div>5%</div><div>26%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6776 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 Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1563	1011	265	277	10			
1	D	192	Total	C	N	O	S	0	0	0
			1563	1011	265	277	10			
1	C	157	Total	C	N	O	S	0	0	0
			1268	818	214	228	8			
1	B	149	Total	C	N	O	S	0	0	0
			1209	782	207	213	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9UI95
D	1	SER	-	expression tag	UNP Q9UI95
C	1	SER	-	expression tag	UNP Q9UI95
B	1	SER	-	expression tag	UNP Q9UI95

- Molecule 2 is a protein called Shieldin complex subunit 2,Shieldin complex subunit 3 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	73	Total	C	N	O	S	0	0	0
			592	387	104	100	1			
2	X	72	Total	C	N	O	S	0	0	0
			581	381	100	99	1			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	MET	-	initiating methionine	UNP Q86V20
Y	17	GLY	-	linker	UNP Q86V20
Y	18	SER	-	linker	UNP Q86V20
Y	19	GLY	-	linker	UNP Q86V20

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	20	SER	-	linker	UNP Q86V20
Y	21	GLY	-	linker	UNP Q86V20
Y	22	SER	-	linker	UNP Q86V20
Y	23	GLY	-	linker	UNP Q86V20
Y	24	SER	-	linker	UNP Q86V20
Y	25	GLY	-	linker	UNP Q86V20
Y	26	SER	-	linker	UNP Q86V20
Y	27	GLY	-	linker	UNP Q86V20
Y	28	SER	-	linker	UNP Q86V20
Y	29	GLY	-	linker	UNP Q86V20
Y	30	SER	-	linker	UNP Q86V20
Y	31	GLY	-	linker	UNP Q86V20
Y	32	SER	-	linker	UNP Q86V20
Y	90	ALA	-	expression tag	UNP Q6ZNX1
Y	91	SER	-	expression tag	UNP Q6ZNX1
Y	92	ARG	-	expression tag	UNP Q6ZNX1
Y	93	GLU	-	expression tag	UNP Q6ZNX1
Y	94	GLU	-	expression tag	UNP Q6ZNX1
Y	95	ILE	-	expression tag	UNP Q6ZNX1
Y	96	MET	-	expression tag	UNP Q6ZNX1
Y	97	ALA	-	expression tag	UNP Q6ZNX1
Y	98	THR	-	expression tag	UNP Q6ZNX1
Y	99	LEU	-	expression tag	UNP Q6ZNX1
X	1	MET	-	initiating methionine	UNP Q86V20
X	17	GLY	-	linker	UNP Q86V20
X	18	SER	-	linker	UNP Q86V20
X	19	GLY	-	linker	UNP Q86V20
X	20	SER	-	linker	UNP Q86V20
X	21	GLY	-	linker	UNP Q86V20
X	22	SER	-	linker	UNP Q86V20
X	23	GLY	-	linker	UNP Q86V20
X	24	SER	-	linker	UNP Q86V20
X	25	GLY	-	linker	UNP Q86V20
X	26	SER	-	linker	UNP Q86V20
X	27	GLY	-	linker	UNP Q86V20
X	28	SER	-	linker	UNP Q86V20
X	29	GLY	-	linker	UNP Q86V20
X	30	SER	-	linker	UNP Q86V20
X	31	GLY	-	linker	UNP Q86V20
X	32	SER	-	linker	UNP Q86V20
X	90	ALA	-	expression tag	UNP Q6ZNX1
X	91	SER	-	expression tag	UNP Q6ZNX1

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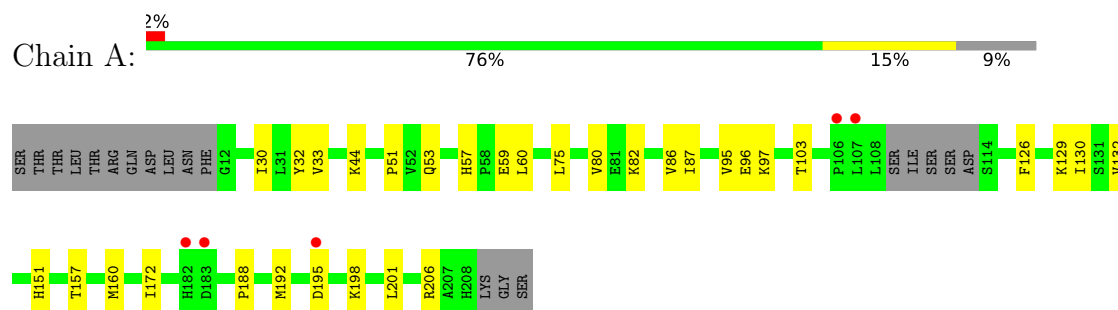
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Chain	Residue	Modelled	Actual	Comment	Reference
X	92	ARG	-	expression tag	UNP Q6ZNX1
X	93	GLU	-	expression tag	UNP Q6ZNX1
X	94	GLU	-	expression tag	UNP Q6ZNX1
X	95	ILE	-	expression tag	UNP Q6ZNX1
X	96	MET	-	expression tag	UNP Q6ZNX1
X	97	ALA	-	expression tag	UNP Q6ZNX1
X	98	THR	-	expression tag	UNP Q6ZNX1
X	99	LEU	-	expression tag	UNP Q6ZNX1

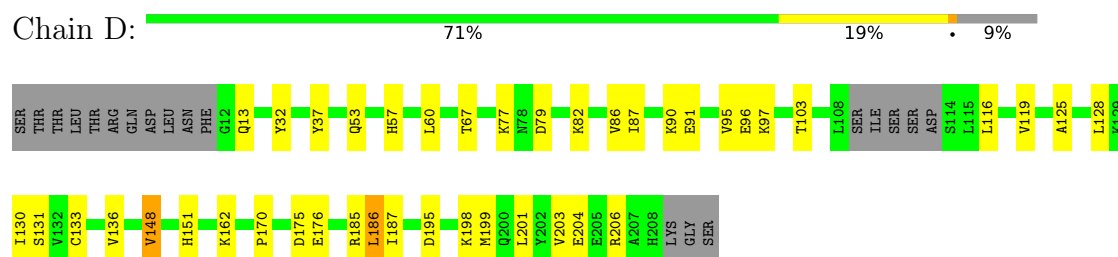
### 3 Residue-property plots [i](#)

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.

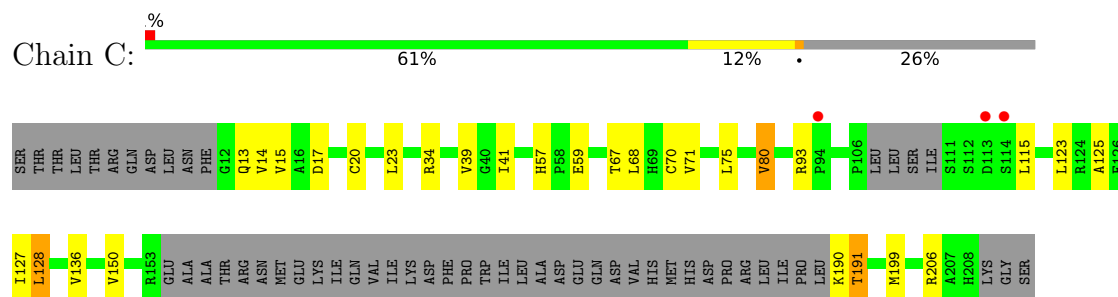
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



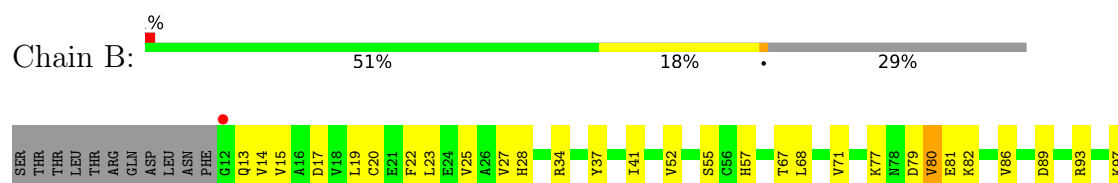
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B

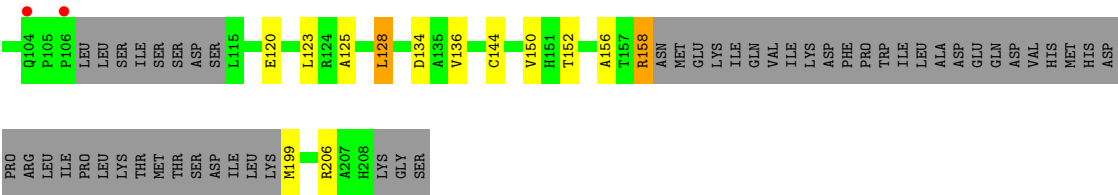


- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B

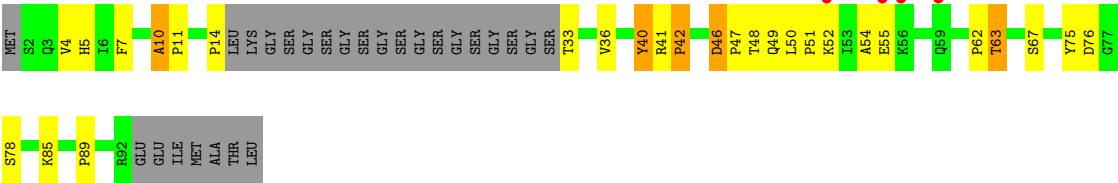


- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B

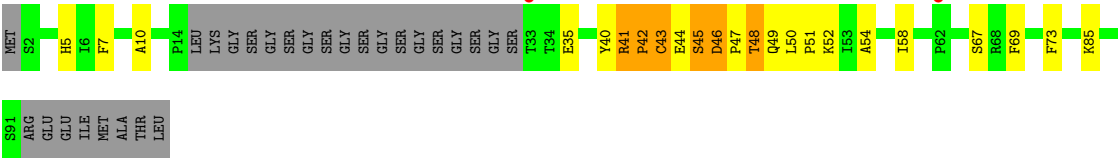




● Molecule 2: Shieldin complex subunit 2,Shieldin complex subunit 3 chimera



● Molecule 2: Shieldin complex subunit 2,Shieldin complex subunit 3 chimera



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	331.84Å 331.84Å 331.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.66 – 3.80 39.66 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.66-3.80) 99.9 (39.66-3.80)	Depositor EDS
$R_{merge}$	0.40	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, $R_{free}$	0.239 , 0.266 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	1551 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	155.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 164.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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	0.24	0/1597	0.41	0/2170
1	B	0.24	0/1234	0.44	0/1676
1	C	0.23	0/1293	0.46	0/1754
1	D	0.24	0/1597	0.44	1/2170 (0.0%)
2	X	0.29	0/604	0.50	0/827
2	Y	0.29	0/615	0.56	0/841
All	All	0.25	0/6940	0.46	1/9438 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	LEU	CA-CB-CG	5.91	128.89	115.30

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	1563	0	1606	20	0
1	B	1209	0	1237	29	0
1	C	1268	0	1300	24	0
1	D	1563	0	1606	30	0
2	X	581	0	581	28	0
2	Y	592	0	594	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6776	0	6924	135	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 10.

The worst 5 of 135 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:Y:46:ASP:H	2:Y:47:PRO:HD3	1.29	0.94
2:Y:46:ASP:H	2:Y:47:PRO:CD	1.97	0.77
1:A:82:LYS:HG2	1:A:151:HIS:HB2	1.67	0.76
1:D:130:ILE:HD11	1:D:201:LEU:HD21	1.71	0.72
1:A:87:ILE:HD11	1:A:96:GLU:HB2	1.73	0.71

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	188/211 (89%)	184 (98%)	4 (2%)	0	100	100
1	B	143/211 (68%)	133 (93%)	10 (7%)	0	100	100
1	C	151/211 (72%)	139 (92%)	11 (7%)	1 (1%)	22	60
1	D	188/211 (89%)	182 (97%)	6 (3%)	0	100	100
2	X	68/99 (69%)	55 (81%)	6 (9%)	7 (10%)	0	9
2	Y	69/99 (70%)	55 (80%)	9 (13%)	5 (7%)	1	17
All	All	807/1042 (77%)	748 (93%)	46 (6%)	13 (2%)	9	44

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	THR
2	Y	42	PRO
2	Y	46	ASP
2	X	46	ASP
2	X	42	PRO

### 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	181/199 (91%)	181 (100%)	0	100	100
1	B	139/199 (70%)	135 (97%)	4 (3%)	42	67
1	C	149/199 (75%)	146 (98%)	3 (2%)	55	75
1	D	181/199 (91%)	178 (98%)	3 (2%)	60	78
2	X	65/83 (78%)	65 (100%)	0	100	100
2	Y	66/83 (80%)	65 (98%)	1 (2%)	65	81
All	All	781/962 (81%)	770 (99%)	11 (1%)	67	81

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	VAL
1	B	128	LEU
2	Y	63	THR
1	B	158	ARG
1	C	115	LEU

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

Mol	Chain	Res	Type
1	C	62	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 [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	192/211 (90%)	-0.03	5 (2%)	56	47	134, 188, 269, 312	0
1	B	149/211 (70%)	-0.13	3 (2%)	65	58	122, 203, 278, 355	0
1	C	157/211 (74%)	-0.18	3 (1%)	66	59	119, 184, 266, 336	0
1	D	192/211 (90%)	-0.33	0	100	100	102, 145, 222, 334	0
2	X	72/99 (72%)	-0.06	2 (2%)	53	43	130, 200, 310, 333	0
2	Y	73/99 (73%)	0.05	4 (5%)	25	21	115, 197, 314, 371	0
All	All	835/1042 (80%)	-0.14	17 (2%)	65	58	102, 182, 275, 371	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	PRO	5.1
2	X	33	THR	4.0
1	A	107	LEU	3.6
1	C	113	ASP	3.1
1	B	104	GLN	2.9

### 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.