



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:07 pm GMT

PDB ID : 4FQB  
Title : crystal structure of toxic effector Tse1 in complex with immune protein Tsi1  
Authors : Wang, T.; Li, L.; Zhang, W.  
Deposited on : 2012-06-25  
Resolution : 2.69 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

<http://wwpdb.org/validation/2016/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:

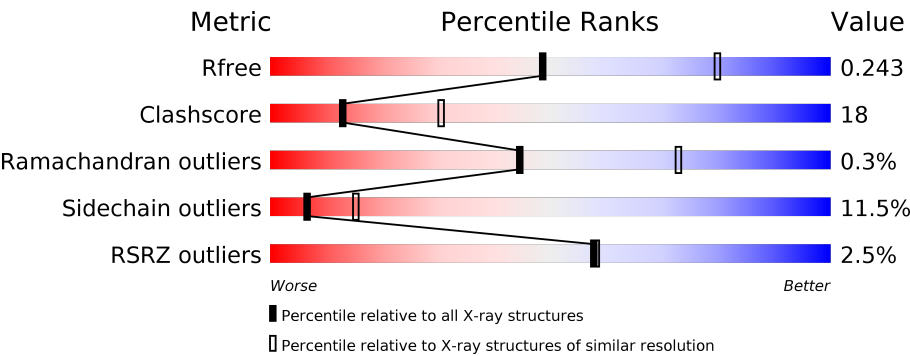
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

# 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 2.69 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	162	<div><div></div><div><div></div><div>69%</div><div>19%</div><div>••</div><div>10%</div></div></div>
1	C	162	<div><div>3%</div><div><div></div><div>59%</div><div>26%</div><div>6%</div><div>10%</div></div></div>
1	E	162	<div><div>2%</div><div><div></div><div>57%</div><div>25%</div><div>6%</div><div>•</div><div>10%</div></div></div>
1	G	162	<div><div>7%</div><div><div></div><div>64%</div><div>20%</div><div>6%</div><div>10%</div></div></div>
2	B	162	<div><div></div><div><div></div><div>62%</div><div>25%</div><div>•</div><div>9%</div></div></div>
2	D	162	<div><div></div><div><div></div><div>69%</div><div>19%</div><div>•</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	162	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>18%</div><div>6%</div><div>9%</div></div></div>
2	H	162	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>69%</div><div>19%</div><div>• •</div><div>9%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9004 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 toxic effector Tse1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	1	0	0
			1091	682	195	205	9			
1	C	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			
1	E	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			
1	G	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
A	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
A	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
C	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
C	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
E	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
E	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
G	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
G	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

- Molecule 2 is a protein called immune protein Tsi1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	D	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	F	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	H	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
B	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
B	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
B	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
D	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
D	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
D	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0

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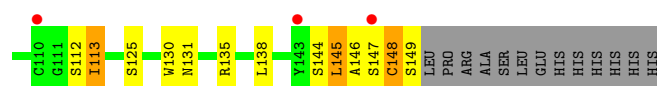
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Chain	Residue	Modelled	Actual	Comment	Reference
D	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
F	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
F	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
F	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
H	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
H	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
H	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	17	Total O 17 17	0	0
3	C	5	Total O 5 5	0	0
3	D	15	Total O 15 15	0	0
3	E	2	Total O 2 2	0	0
3	F	14	Total O 14 14	0	0
3	G	1	Total O 1 1	0	0
3	H	9	Total O 9 9	0	0

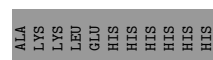




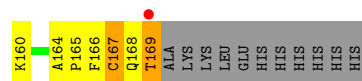
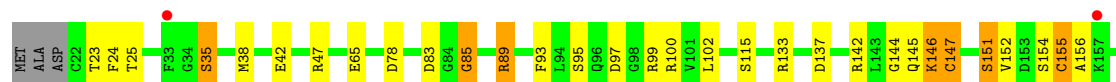
• Molecule 2: immune protein Ts1



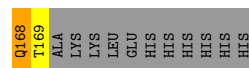
• Molecule 2: immune protein Ts1



• Molecule 2: immune protein Ts1



• Molecule 2: immune protein Ts1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.71Å 97.71Å 293.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.69 29.77 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.69) 93.7 (29.77-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.245 0.207 , 0.243	Depositor DCC
$R_{free}$ test set	2201 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

### 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	0.83	3/1113 (0.3%)	0.87	2/1508 (0.1%)
1	C	0.79	2/1113 (0.2%)	0.86	3/1508 (0.2%)
1	E	0.79	3/1113 (0.3%)	0.80	1/1508 (0.1%)
1	G	0.70	1/1113 (0.1%)	0.75	0/1508
2	B	1.03	3/1166 (0.3%)	1.06	4/1575 (0.3%)
2	D	1.02	1/1166 (0.1%)	0.94	1/1575 (0.1%)
2	F	0.90	0/1166	0.96	4/1575 (0.3%)
2	H	0.92	2/1166 (0.2%)	1.12	6/1575 (0.4%)
All	All	0.88	15/9116 (0.2%)	0.93	21/12332 (0.2%)

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
2	B	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	134	TRP	CD2-CE2	6.98	1.49	1.41
2	B	28	GLU	CD-OE1	6.85	1.33	1.25
1	C	16	TRP	CD2-CE2	5.68	1.48	1.41
2	H	118	SER	CB-OG	-5.37	1.35	1.42
1	A	16	TRP	CD2-CE2	5.37	1.47	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	GLN	CB-CA-C	-19.52	71.35	110.40
2	H	146	LYS	N-CA-C	-11.42	80.15	111.00
1	C	148	CYS	N-CA-CB	-10.22	92.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	GLN	N-CA-C	9.14	135.69	111.00
2	B	85	GLY	N-CA-C	-8.87	90.92	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	90	GLY	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	1091	0	1069	34	0
1	C	1091	0	1069	57	0
1	E	1091	0	1069	62	0
1	G	1091	0	1069	50	0
2	B	1142	0	1061	35	0
2	D	1142	0	1061	23	1
2	F	1142	0	1061	41	0
2	H	1142	0	1061	27	0
3	A	9	0	0	0	0
3	B	17	0	0	2	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	2	0	0	0	0
3	F	14	0	0	3	0
3	G	1	0	0	0	0
3	H	9	0	0	1	0
All	All	9004	0	8520	321	1

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 18.

The worst 5 of 321 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:G:144:SER:C	1:G:145:LEU:HD12	1.38	1.44
1:E:45:MET:CE	1:E:46:PRO:HD2	1.58	1.32
1:E:45:MET:HA	1:E:45:MET:CE	1.67	1.24
2:F:152:VAL:HG12	3:F:213:HOH:O	1.45	1.15
1:E:45:MET:HE1	1:E:46:PRO:HD2	1.21	1.13

All (1) 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)
2:D:33:PHE:O	2:D:35:SER:OG[4_555]	2.12	0.08

## 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	144/162 (89%)	133 (92%)	11 (8%)	0	100	100
1	C	144/162 (89%)	134 (93%)	10 (7%)	0	100	100
1	E	144/162 (89%)	134 (93%)	8 (6%)	2 (1%)	13	33
1	G	144/162 (89%)	128 (89%)	16 (11%)	0	100	100
2	B	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
2	D	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
2	F	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
2	H	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	25	53
All	All	1160/1296 (90%)	1089 (94%)	68 (6%)	3 (0%)	44	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	7	CYS

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Mol	Chain	Res	Type
1	E	8	ILE
2	H	146	LYS

### 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	113/128 (88%)	102 (90%)	11 (10%)	9	22
1	C	113/128 (88%)	95 (84%)	18 (16%)	3	7
1	E	113/128 (88%)	94 (83%)	19 (17%)	2	6
1	G	113/128 (88%)	100 (88%)	13 (12%)	6	15
2	B	127/139 (91%)	114 (90%)	13 (10%)	8	20
2	D	127/139 (91%)	113 (89%)	14 (11%)	7	17
2	F	127/139 (91%)	118 (93%)	9 (7%)	17	39
2	H	127/139 (91%)	114 (90%)	13 (10%)	8	20
All	All	960/1068 (90%)	850 (88%)	110 (12%)	6	15

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	137	ASP
1	E	31	SER
2	H	137	ASP
2	D	151	SER
2	D	169	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	132	GLN
2	D	168	GLN
1	G	10	ASN

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Mol	Chain	Res	Type
1	C	14	ASN
1	E	6	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 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	146/162 (90%)	-0.12	2 (1%) 75 76	46, 80, 124, 149	1 (0%)
1	C	146/162 (90%)	0.02	5 (3%) 46 45	55, 91, 139, 168	0
1	E	146/162 (90%)	-0.06	4 (2%) 55 55	57, 97, 140, 175	0
1	G	146/162 (90%)	0.21	11 (7%) 15 12	63, 102, 149, 175	0
2	B	148/162 (91%)	-0.31	1 (0%) 87 88	42, 63, 98, 160	0
2	D	148/162 (91%)	-0.36	0 100 100	43, 63, 92, 153	0
2	F	148/162 (91%)	-0.13	3 (2%) 65 66	45, 69, 121, 146	0
2	H	148/162 (91%)	-0.13	3 (2%) 65 66	44, 68, 134, 168	0
All	All	1176/1296 (90%)	-0.11	29 (2%) 58 58	42, 78, 137, 175	1 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	SER	5.4
1	E	23	GLY	4.9
1	C	4	LEU	4.1
1	C	147	SER	4.0
2	H	156	ALA	3.7

### 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.