



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:41 pm GMT

PDB ID : 4Z6Y  
Title : Structure of the TBC1D7-TSC1 complex  
Authors : Gai, Z.; Wu, G.  
Deposited on : 2015-04-06  
Resolution : 2.81 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:

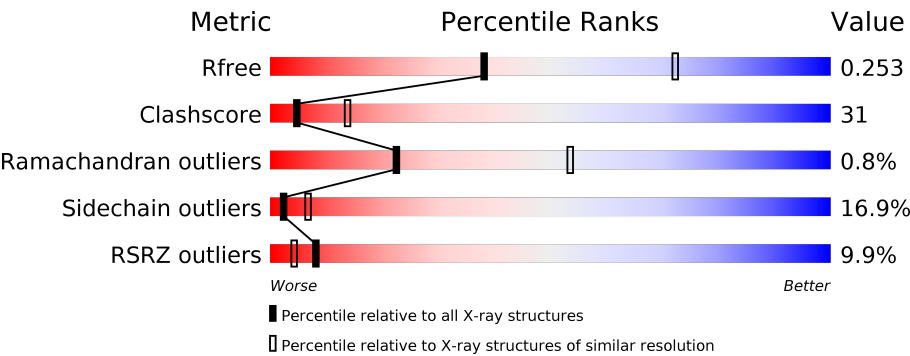
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
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 2.81 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	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

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	273	<div><div>3%</div><div><div></div><div>67%</div><div>26%</div><div>7%</div></div></div>
1	B	273	<div><div>2%</div><div><div></div><div>67%</div><div>25%</div><div>7%</div></div></div>
1	E	273	<div><div>3%</div><div><div></div><div>63%</div><div>30%</div><div>6%</div></div></div>
1	G	273	<div><div>2%</div><div><div></div><div>65%</div><div>27%</div><div>7%</div><div></div></div></div>
2	C	56	<div><div>50%</div><div><div></div><div>32%</div><div>45%</div><div>18%</div><div>5%</div></div></div>
2	D	56	<div><div>43%</div><div><div></div><div>43%</div><div>41%</div><div>11%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	56	<div><div><div></div><div></div><div></div><div></div></div><div>34%45%38%14%•</div></div>
2	H	56	<div><div><div></div><div></div><div></div><div></div></div><div>57%39%30%27%••</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10471 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 TBC1 domain family member 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	272	Total	C	N	O	S	0	1	0
			2200	1424	368	393	15			
1	G	272	Total	C	N	O	S	0	1	0
			2206	1427	371	393	15			
1	E	272	Total	C	N	O	S	0	1	0
			2206	1427	371	393	15			
1	A	273	Total	C	N	O	S	0	1	0
			2212	1430	372	395	15			

- Molecule 2 is a protein called Hamartin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	53	Total	C	N	O	0	0	0
			402	252	69	81			
2	H	55	Total	C	N	O	0	0	0
			415	259	71	85			
2	F	54	Total	C	N	O	0	0	0
			407	255	70	82			
2	D	53	Total	C	N	O	0	0	0
			402	252	69	81			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		
3	G	6	Total	O	0	0
			6	6		
3	H	2	Total	O	0	0
			2	2		

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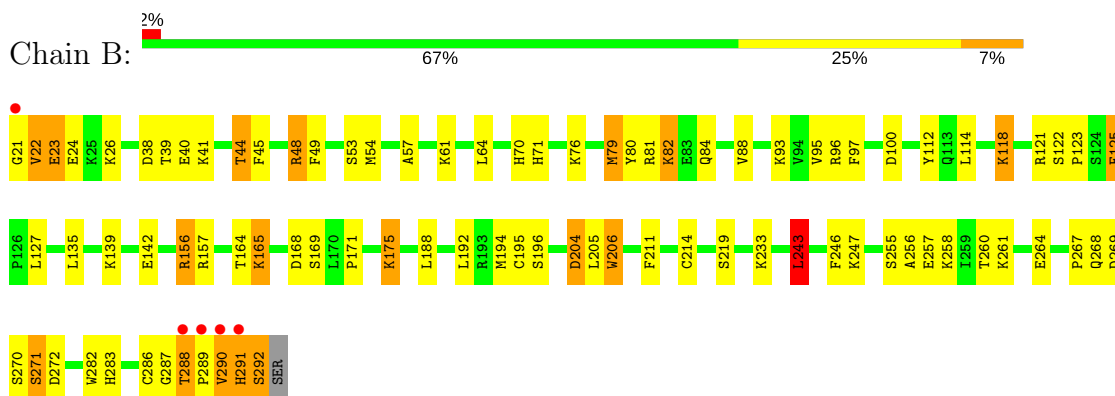
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	A	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	0	0

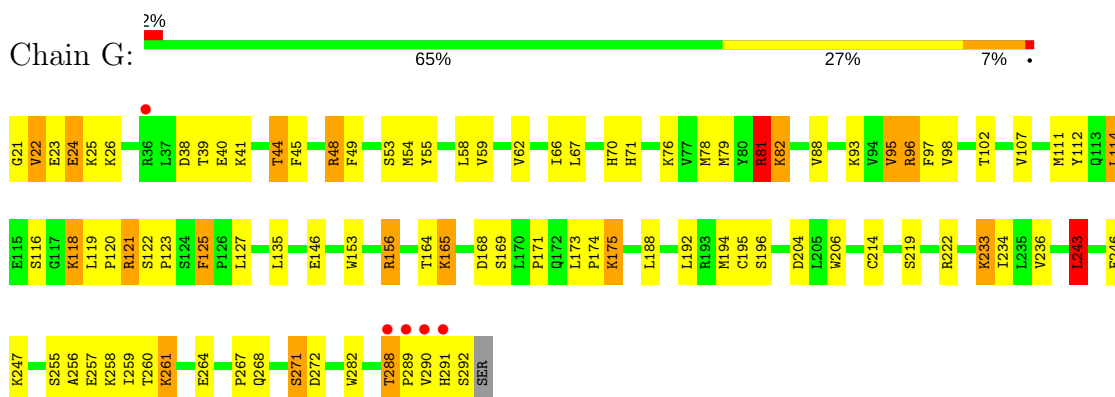
### 3 Residue-property plots [i](#)

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.

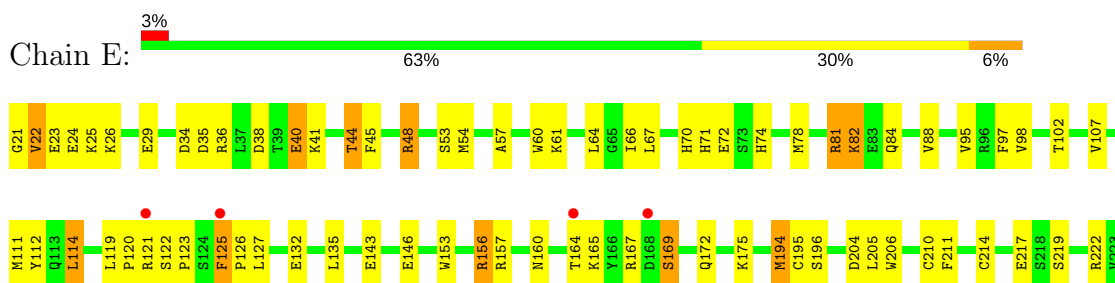
- Molecule 1: TBC1 domain family member 7



- Molecule 1: TBC1 domain family member 7

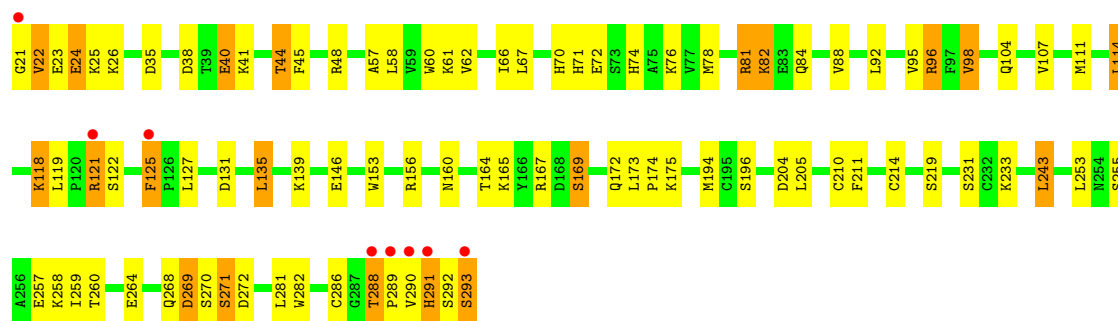


- Molecule 1: TBC1 domain family member 7





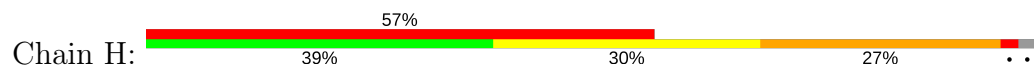
• Molecule 1: TBC1 domain family member 7



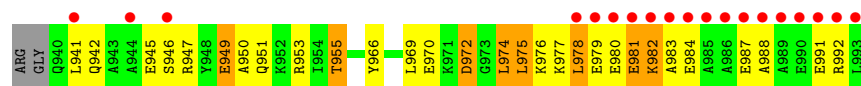
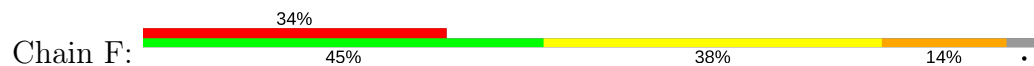
• Molecule 2: Hamartin



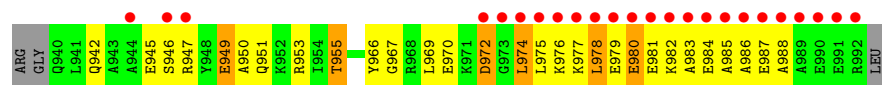
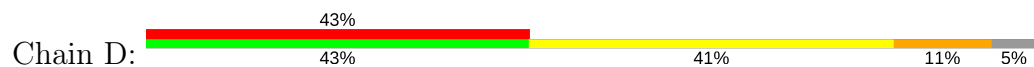
• Molecule 2: Hamartin



• Molecule 2: Hamartin



• Molecule 2: Hamartin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.99Å 145.69Å 114.76Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 44.89 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.81) 97.3 (44.89-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.206 , 0.255 0.206 , 0.253	Depositor DCC
$R_{free}$ test set	2260 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 7.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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	0.78	2/2269 (0.1%)	0.86	2/3073 (0.1%)
1	B	0.78	2/2257 (0.1%)	0.88	1/3058 (0.0%)
1	E	0.79	3/2263 (0.1%)	0.88	0/3065
1	G	0.77	3/2263 (0.1%)	0.88	3/3065 (0.1%)
2	C	0.56	0/404	0.72	1/543 (0.2%)
2	D	0.59	0/404	0.72	0/543
2	F	0.58	0/409	0.75	0/550
2	H	0.54	0/417	0.72	0/560
All	All	0.75	10/10686 (0.1%)	0.85	7/14457 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	TRP	CD2-CE2	5.96	1.48	1.41
1	B	282	TRP	CD2-CE2	5.82	1.48	1.41
1	G	282	TRP	CD2-CE2	5.73	1.48	1.41
1	G	206	TRP	CD2-CE2	5.53	1.48	1.41
1	A	282	TRP	CD2-CE2	5.43	1.47	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	LEU	CA-CB-CG	-7.63	97.75	115.30
1	G	243	LEU	CA-CB-CG	-6.56	100.21	115.30
1	G	81	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	243	LEU	CA-CB-CG	-5.71	102.16	115.30
1	G	81	ARG	NE-CZ-NH2	5.70	123.15	120.30

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	2212	0	2253	103	1
1	B	2200	0	2237	58	1
1	E	2206	0	2248	71	2
1	G	2206	0	2248	100	2
2	C	402	0	382	64	0
2	D	402	0	383	87	0
2	F	407	0	385	81	0
2	H	415	0	392	92	0
3	A	1	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	6	0	0	0	0
3	H	2	0	0	0	0
All	All	10471	0	10528	644	3

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 31.

The worst 5 of 644 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:121:ARG:HD2	1:A:125:PHE:CE2	1.20	1.73
1:A:121:ARG:CD	1:A:125:PHE:CE2	1.89	1.54
2:D:975:LEU:HA	2:D:978:LEU:CD1	1.29	1.53
2:D:975:LEU:CA	2:D:978:LEU:HD11	1.05	1.51
2:D:975:LEU:CA	2:D:978:LEU:CD1	1.86	1.50

All (3) 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:G:24:GLU:OE1	1:E:290:VAL:N[1_655]	1.80	0.40
1:G:23:GLU:O	1:E:288:THR:O[1_655]	1.88	0.32
1:B:290:VAL:CG2	1:A:40:GLU:OE2[1_655]	2.18	0.02

## 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	272/273 (100%)	253 (93%)	18 (7%)	1 (0%)	38	70
1	B	271/273 (99%)	254 (94%)	16 (6%)	1 (0%)	38	70
1	E	271/273 (99%)	254 (94%)	17 (6%)	0	100	100
1	G	271/273 (99%)	255 (94%)	16 (6%)	0	100	100
2	C	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	11
2	D	51/56 (91%)	39 (76%)	11 (22%)	1 (2%)	9	27
2	F	52/56 (93%)	48 (92%)	3 (6%)	1 (2%)	9	29
2	H	53/56 (95%)	47 (89%)	2 (4%)	4 (8%)	1	2
All	All	1292/1316 (98%)	1193 (92%)	89 (7%)	10 (1%)	22	53

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	981	GLU
2	H	991	GLU
2	F	982	LYS
2	D	980	GLU
1	B	23	GLU

### 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	249/249 (100%)	209 (84%)	40 (16%)	3	8
1	B	247/249 (99%)	212 (86%)	35 (14%)	4	11
1	E	248/249 (100%)	208 (84%)	40 (16%)	3	8
1	G	248/249 (100%)	207 (84%)	41 (16%)	2	7
2	C	36/45 (80%)	26 (72%)	10 (28%)	0	1
2	D	36/45 (80%)	30 (83%)	6 (17%)	2	7
2	F	36/45 (80%)	27 (75%)	9 (25%)	1	2
2	H	37/45 (82%)	24 (65%)	13 (35%)	0	0
All	All	1137/1176 (97%)	943 (83%)	194 (17%)	2	6

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	941	LEU
1	E	72	GLU
1	A	243	LEU
2	H	946	SER
2	H	981	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	942	GLN
1	E	84	GLN
1	A	84	GLN
1	G	291	HIS
2	F	942	GLN

### 5.3.3 RNA ⓘ

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	273/273 (100%)	-0.24	8 (2%) 52 41	38, 59, 109, 198	0
1	B	272/273 (99%)	-0.36	5 (1%) 69 60	39, 60, 99, 165	0
1	E	272/273 (99%)	-0.26	8 (2%) 52 41	39, 59, 105, 185	0
1	G	272/273 (99%)	-0.27	5 (1%) 69 60	40, 60, 103, 170	0
2	C	53/56 (94%)	3.00	28 (52%) 0 0	36, 72, 150, 155	21 (39%)
2	D	53/56 (94%)	2.30	24 (45%) 0 0	34, 71, 125, 160	25 (47%)
2	F	54/56 (96%)	1.78	19 (35%) 0 0	51, 70, 126, 149	21 (38%)
2	H	55/56 (98%)	3.27	32 (58%) 0 0	38, 75, 195, 213	22 (40%)
All	All	1304/1316 (99%)	0.19	129 (9%) 8 4	34, 61, 121, 213	89 (6%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	985	ALA	12.6
2	C	985	ALA	11.6
1	A	290	VAL	10.5
2	F	989	ALA	9.8
2	C	980	GLU	9.7

### 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.