



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:06 pm BST

PDB ID : 5WTB  
Title : Complex Structure of Staphylococcus aureus SdrE with human complement factor H  
Authors : Wu, M.; Zhang, Y.; Hang, T.; Wang, C.; Yang, Y.; Zang, J.; Zhang, M.; Zhang, X.  
Deposited on : 2016-12-10  
Resolution : 3.30 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	:	2.11
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

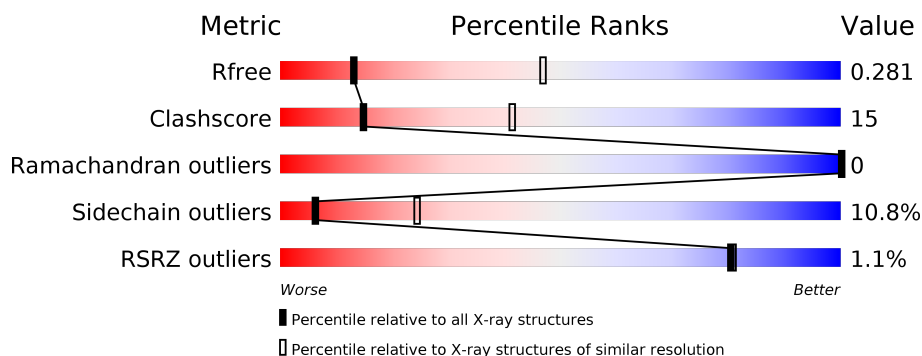
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	338	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	338	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	338	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	338	<div> <div></div> <div> <div></div> <div>66%</div> <div>25%</div> <div>•</div> <div>7%</div> </div> </div>
2	E	21	<div> <div></div> <div> <div>19%</div> <div>43%</div> <div>19%</div> <div>19%</div> </div> </div>
2	F	21	<div> <div></div> <div> <div>14%</div> <div>43%</div> <div>10%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	21	<div><div></div><div></div><div></div><div></div><div></div><div>29%</div><div>14%</div><div>19%</div><div>5%</div><div>33%</div></div>
2	H	21	<div><div></div><div></div><div></div><div></div><div></div><div>48%</div><div>19%</div><div>14%</div><div>19%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10427 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 Serine-aspartate repeat-containing protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	313	Total	C	N	O	S	0	0	0
			2447	1524	397	522	4			
1	A	313	Total	C	N	O	S	0	0	0
			2447	1524	397	522	4			
1	B	319	Total	C	N	O	S	0	0	0
			2491	1549	405	533	4			
1	C	323	Total	C	N	O	S	0	0	0
			2528	1575	410	539	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	489	MET	ILE	engineered mutation	UNP Q932F7
D	600	LEU	-	expression tag	UNP Q932F7
D	601	GLU	-	expression tag	UNP Q932F7
D	602	HIS	-	expression tag	UNP Q932F7
D	603	HIS	-	expression tag	UNP Q932F7
D	604	HIS	-	expression tag	UNP Q932F7
D	605	HIS	-	expression tag	UNP Q932F7
D	606	HIS	-	expression tag	UNP Q932F7
D	607	HIS	-	expression tag	UNP Q932F7
A	489	MET	ILE	engineered mutation	UNP Q932F7
A	600	LEU	-	expression tag	UNP Q932F7
A	601	GLU	-	expression tag	UNP Q932F7
A	602	HIS	-	expression tag	UNP Q932F7
A	603	HIS	-	expression tag	UNP Q932F7
A	604	HIS	-	expression tag	UNP Q932F7
A	605	HIS	-	expression tag	UNP Q932F7
A	606	HIS	-	expression tag	UNP Q932F7
A	607	HIS	-	expression tag	UNP Q932F7
B	489	MET	ILE	engineered mutation	UNP Q932F7
B	600	LEU	-	expression tag	UNP Q932F7
B	601	GLU	-	expression tag	UNP Q932F7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	602	HIS	-	expression tag	UNP Q932F7
B	603	HIS	-	expression tag	UNP Q932F7
B	604	HIS	-	expression tag	UNP Q932F7
B	605	HIS	-	expression tag	UNP Q932F7
B	606	HIS	-	expression tag	UNP Q932F7
B	607	HIS	-	expression tag	UNP Q932F7
C	489	MET	ILE	engineered mutation	UNP Q932F7
C	600	LEU	-	expression tag	UNP Q932F7
C	601	GLU	-	expression tag	UNP Q932F7
C	602	HIS	-	expression tag	UNP Q932F7
C	603	HIS	-	expression tag	UNP Q932F7
C	604	HIS	-	expression tag	UNP Q932F7
C	605	HIS	-	expression tag	UNP Q932F7
C	606	HIS	-	expression tag	UNP Q932F7
C	607	HIS	-	expression tag	UNP Q932F7

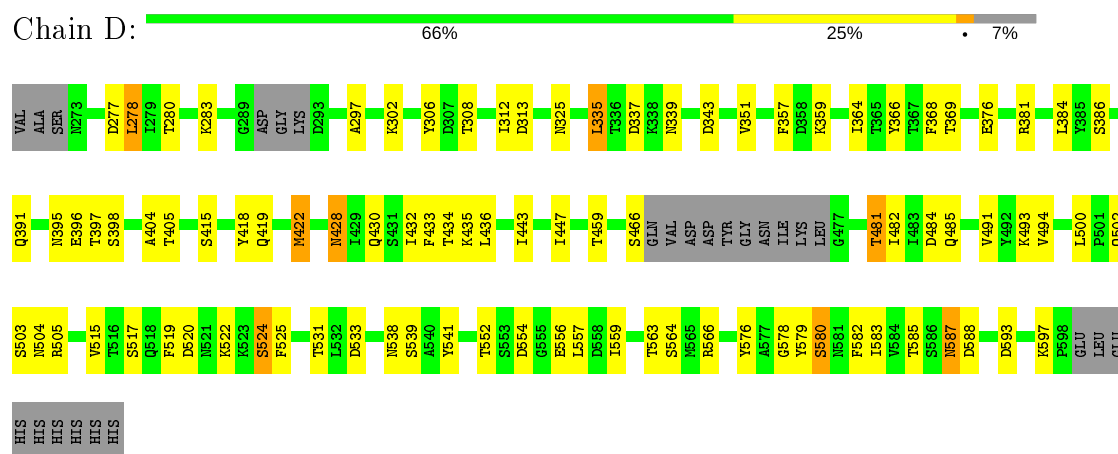
- Molecule 2 is a protein called Peptide from Complement factor H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	S	0	0	0
			139	83	30	25	1			
2	F	14	Total	C	N	O	S	0	0	0
			118	71	26	20	1			
2	G	14	Total	C	N	O	S	0	0	0
			118	71	26	20	1			
2	H	17	Total	C	N	O	S	0	0	0
			139	83	30	25	1			

### 3 Residue-property plots

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: Serine-aspartate repeat-containing protein E

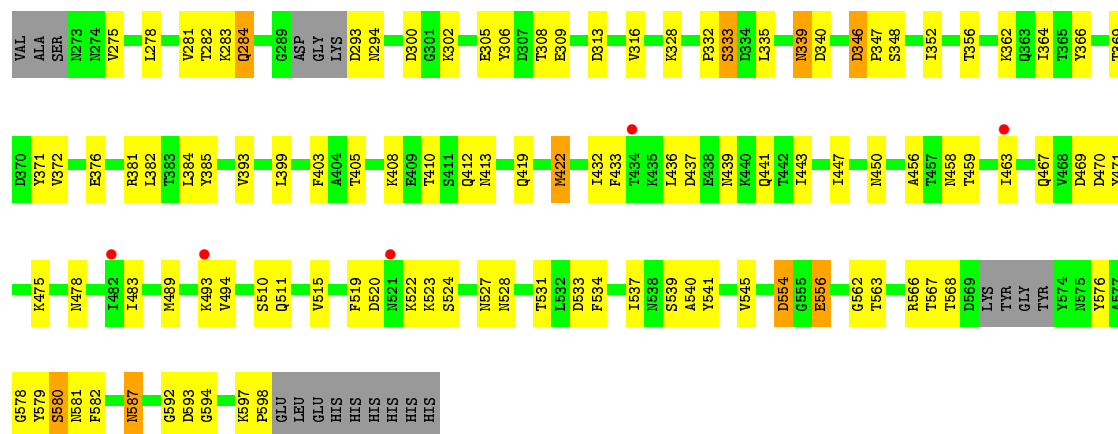


- Molecule 1: Serine-aspartate repeat-containing protein E

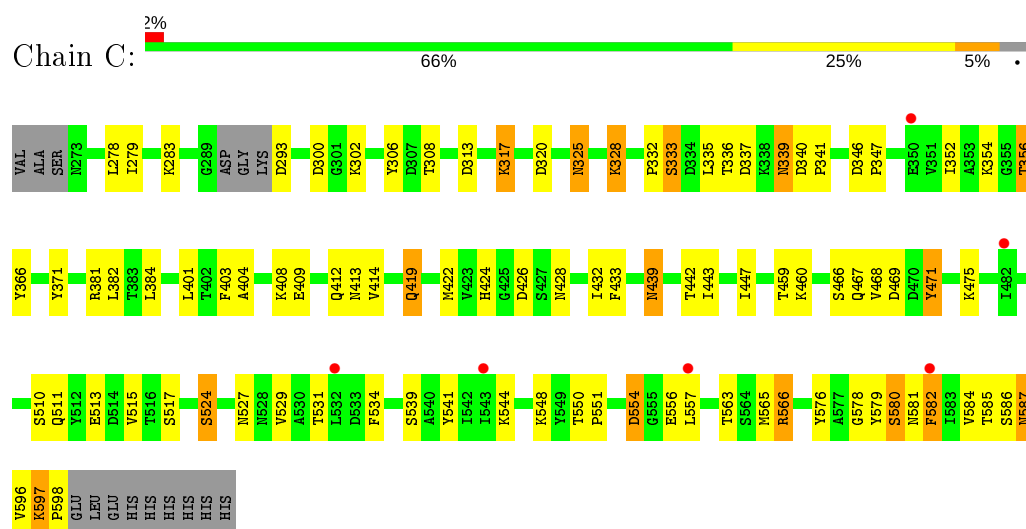


- Molecule 1: Serine-aspartate repeat-containing protein E

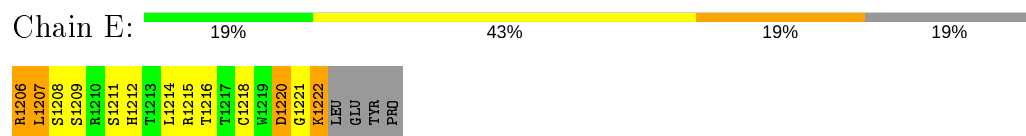




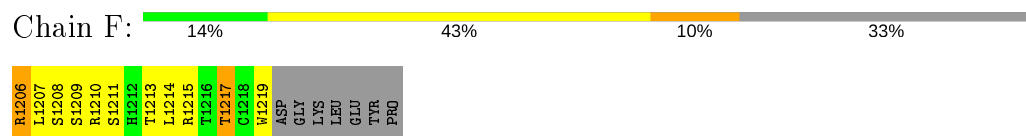
• Molecule 1: Serine-aspartate repeat-containing protein E



• Molecule 2: Peptide from Complement factor H

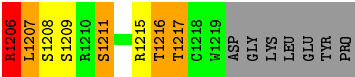


• Molecule 2: Peptide from Complement factor H

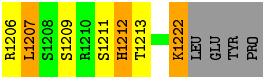


• Molecule 2: Peptide from Complement factor H





● Molecule 2: Peptide from Complement factor H





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.50Å 117.50Å 154.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.30 49.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.79-3.30) 95.2 (49.75-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.222 , 0.281 0.223 , 0.281	Depositor DCC
$R_{free}$ test set	1580 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.418 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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	0.53	0/2485	0.71	1/3372 (0.0%)
1	B	0.50	0/2528	0.70	0/3431
1	C	0.51	0/2568	0.69	0/3486
1	D	0.54	0/2485	0.73	0/3372
2	E	0.54	0/141	0.92	0/188
2	F	0.62	0/120	0.93	0/161
2	G	0.62	0/120	1.02	1/161 (0.6%)
2	H	0.67	0/141	0.89	0/188
All	All	0.53	0/10588	0.72	2/14359 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ASP	CB-CG-OD2	5.19	122.97	118.30
2	G	1206	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	2447	0	2356	75	0
1	B	2491	0	2400	89	0
1	C	2528	0	2435	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2447	0	2356	65	0
2	E	139	0	138	24	0
2	F	118	0	118	17	0
2	G	118	0	118	13	0
2	H	139	0	138	13	0
All	All	10427	0	10059	312	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 15.

The worst 5 of 312 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:C:493:LYS:HG2	1:C:541:TYR:CE1	1.68	1.28
1:B:493:LYS:HG2	1:B:541:TYR:CE1	1.68	1.26
1:D:493:LYS:HG2	1:D:541:TYR:CE2	1.82	1.13
1:C:493:LYS:HG2	1:C:541:TYR:HE1	0.97	1.10
1:B:493:LYS:HG2	1:B:541:TYR:HE1	1.18	0.98

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	307/338 (91%)	278 (91%)	29 (9%)	0	100	100
1	B	313/338 (93%)	285 (91%)	28 (9%)	0	100	100
1	C	319/338 (94%)	287 (90%)	32 (10%)	0	100	100
1	D	307/338 (91%)	275 (90%)	32 (10%)	0	100	100
2	E	15/21 (71%)	14 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	12/21 (57%)	10 (83%)	2 (17%)	0	100	100
2	G	12/21 (57%)	11 (92%)	1 (8%)	0	100	100
2	H	15/21 (71%)	15 (100%)	0	0	100	100
All	All	1300/1436 (90%)	1175 (90%)	125 (10%)	0	100	100

There are no Ramachandran outliers to report.

### 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	279/301 (93%)	248 (89%)	31 (11%)	6	23
1	B	285/301 (95%)	262 (92%)	23 (8%)	11	36
1	C	288/301 (96%)	255 (88%)	33 (12%)	5	22
1	D	279/301 (93%)	257 (92%)	22 (8%)	12	37
2	E	16/20 (80%)	9 (56%)	7 (44%)	0	0
2	F	14/20 (70%)	9 (64%)	5 (36%)	0	0
2	G	14/20 (70%)	9 (64%)	5 (36%)	0	0
2	H	16/20 (80%)	13 (81%)	3 (19%)	1	6
All	All	1191/1284 (93%)	1062 (89%)	129 (11%)	6	24

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	340	ASP
1	B	556	GLU
2	F	1213	THR
1	B	348	SER
1	B	422	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	424	HIS
1	B	504	ASN
1	C	467	GLN
1	B	419	GLN
1	C	478	ASN

### 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	313/338 (92%)	0.17	3 (0%) 82 82	62, 85, 109, 128	18 (5%)
1	B	319/338 (94%)	0.19	5 (1%) 72 70	63, 92, 128, 154	19 (5%)
1	C	323/338 (95%)	0.18	6 (1%) 66 65	63, 93, 122, 132	25 (7%)
1	D	313/338 (92%)	0.20	0 100 100	62, 85, 106, 126	20 (6%)
2	E	17/21 (80%)	0.04	0 100 100	66, 82, 98, 98	1 (5%)
2	F	14/21 (66%)	0.32	0 100 100	71, 87, 108, 120	2 (14%)
2	G	14/21 (66%)	0.23	0 100 100	67, 83, 92, 93	3 (21%)
2	H	17/21 (80%)	0.09	0 100 100	67, 81, 99, 104	1 (5%)
All	All	1330/1436 (92%)	0.18	14 (1%) 80 81	62, 88, 120, 154	89 (6%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	LEU	2.8
1	A	446	GLN	2.8
1	C	532	LEU	2.7
1	B	434	THR	2.6
1	A	436	LEU	2.6

### 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.