



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2021 – 04:03 pm BST

PDB ID : 7BM5  
Title : Crystal structure of Fab1, the Fab fragment of the anti-BamA monoclonal antibody MAB1  
Authors : White, P.; Storek, K.M.; Rutherford, S.T.; Radford, S.E.  
Deposited on : 2021-01-19  
Resolution : 2.95 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  
Xtrriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

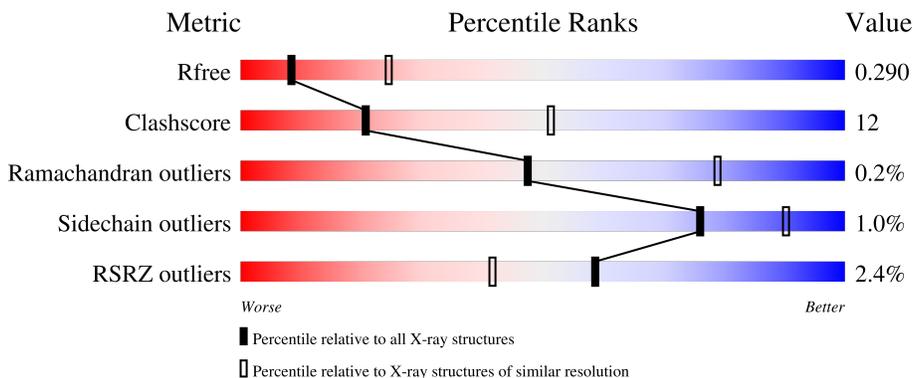
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	215	 72% 27%
1	C	215	 71% 23% 6%
1	E	215	 66% 22% 12%
1	G	215	 70% 20% 9%
1	J	215	 74% 24%

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Mol	Chain	Length	Quality of chain
1	L	215	<p>73% 24% 2% 1%</p>
2	B	228	<p>71% 24% 2% 3%</p>
2	D	228	<p>71% 20% 9% 2%</p>
2	F	228	<p>68% 21% 11% 4%</p>
2	H	228	<p>75% 22% 2% 1%</p>
2	I	228	<p>56% 11% 33% 2%</p>
2	K	228	<p>72% 22% 5%</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18443 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 Fab1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	212	Total 1643	C 1030	N 278	O 330	S 5	0	0	0
1	A	212	Total 1633	C 1024	N 274	O 330	S 5	0	0	0
1	C	203	Total 1547	C 967	N 260	O 315	S 5	0	0	0
1	E	190	Total 1446	C 905	N 242	O 293	S 6	0	0	0
1	J	212	Total 1631	C 1021	N 275	O 330	S 5	0	0	0
1	G	196	Total 1489	C 935	N 247	O 303	S 4	0	0	0

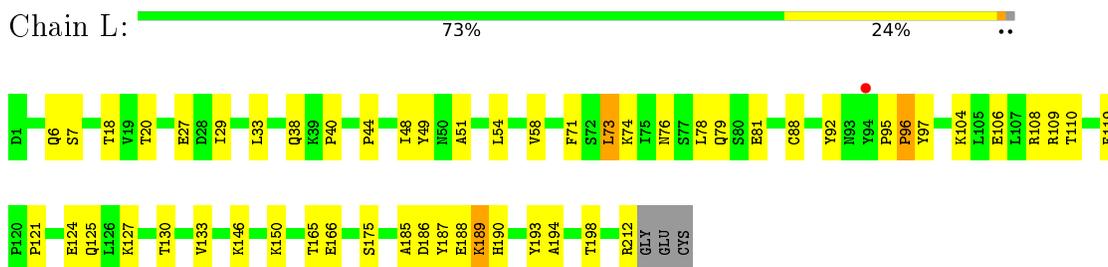
- Molecule 2 is a protein called Fab1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	Total 1658	C 1052	N 280	O 319	S 7	0	0	0
2	B	216	Total 1631	C 1037	N 274	O 313	S 7	0	0	0
2	D	208	Total 1545	C 979	N 259	O 300	S 7	0	0	0
2	F	204	Total 1503	C 950	N 253	O 293	S 7	0	0	0
2	K	216	Total 1605	C 1023	N 269	O 306	S 7	0	0	0
2	I	153	Total 1112	C 706	N 188	O 212	S 6	0	0	0

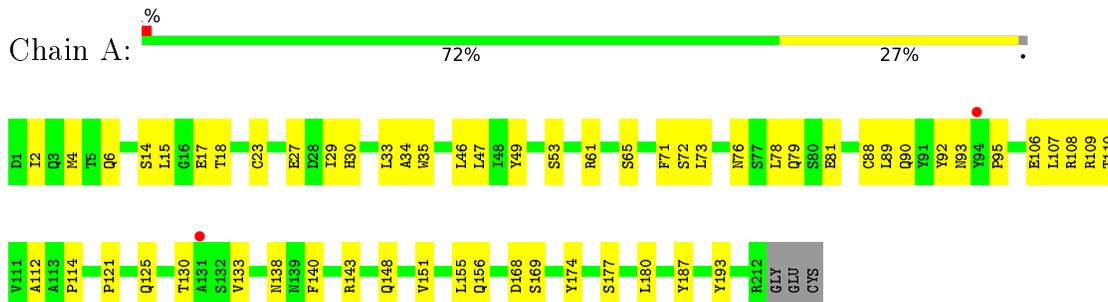
### 3 Residue-property plots [i](#)

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.

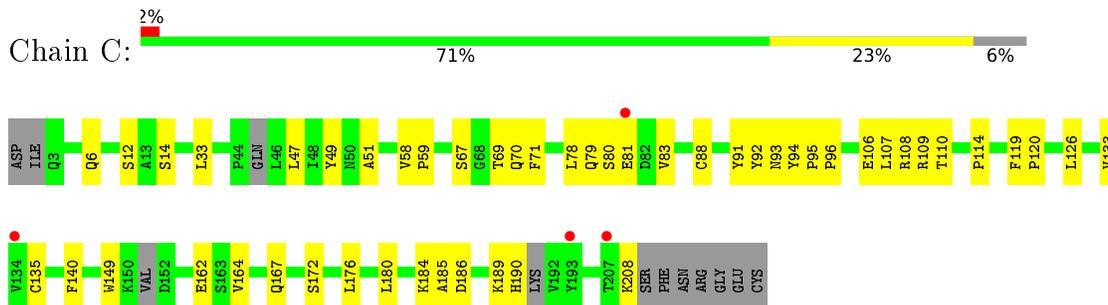
- Molecule 1: Fab1 light chain



- Molecule 1: Fab1 light chain



- Molecule 1: Fab1 light chain



- Molecule 1: Fab1 light chain

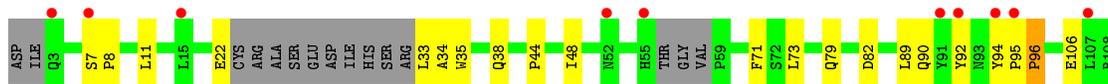




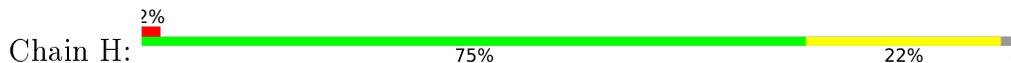
● Molecule 1: Fab1 light chain



● Molecule 1: Fab1 light chain



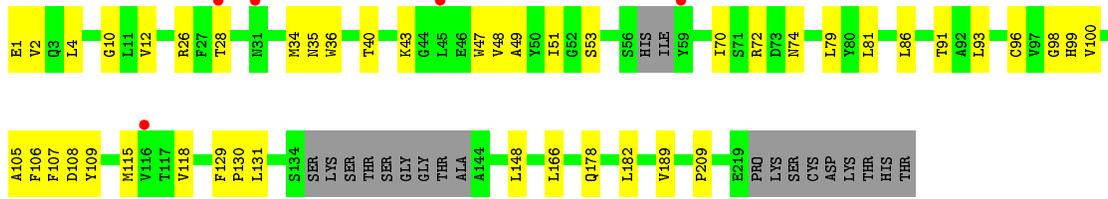
● Molecule 2: Fab1 heavy chain



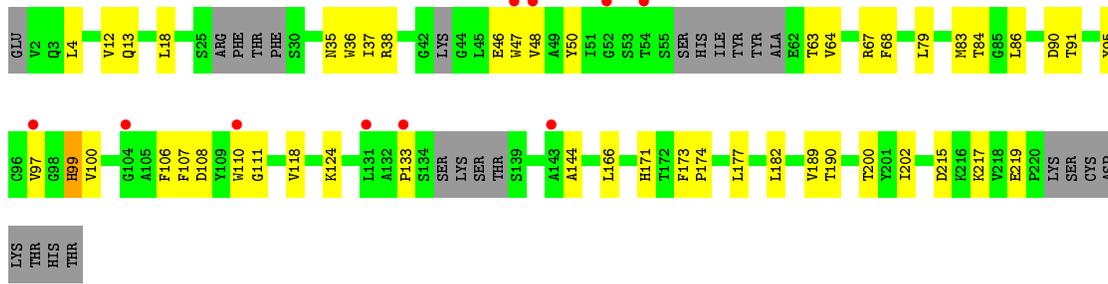
● Molecule 2: Fab1 heavy chain



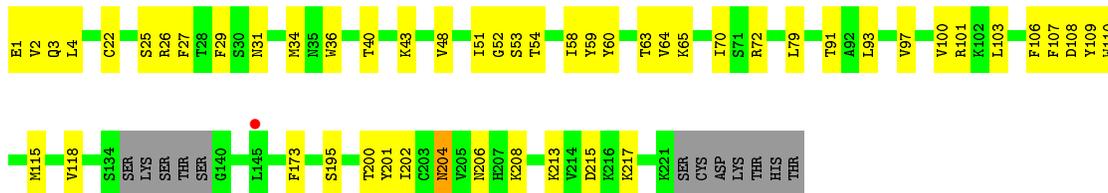
• Molecule 2: Fab1 heavy chain



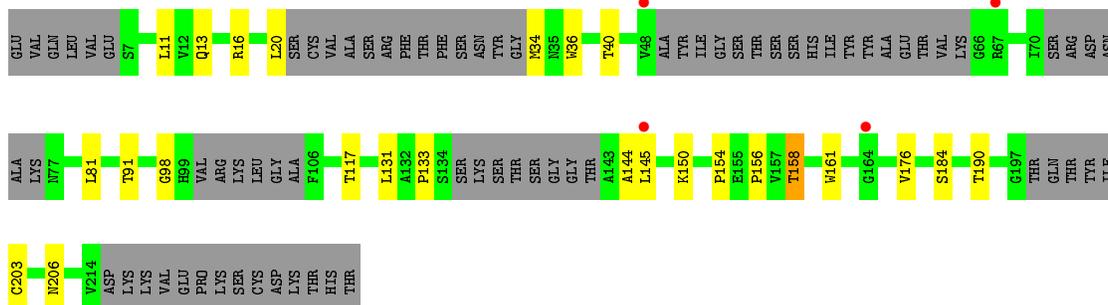
• Molecule 2: Fab1 heavy chain



• Molecule 2: Fab1 heavy chain



• Molecule 2: Fab1 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.01Å 130.14Å 138.92Å 90.00° 106.06° 90.00°	Depositor
Resolution (Å)	88.42 – 2.95 88.42 – 2.95	Depositor EDS
% Data completeness (in resolution range)	46.1 (88.42-2.95) 46.1 (88.42-2.95)	Depositor EDS
$R_{merge}$	0.42	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.257 , 0.290 0.262 , 0.290	Depositor DCC
$R_{free}$ test set	1494 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , -0.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	18443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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	0.32	0/1670	0.50	0/2270
1	C	0.33	0/1579	0.50	0/2145
1	E	0.33	0/1471	0.51	0/1990
1	G	0.31	0/1521	0.52	0/2068
1	J	0.32	0/1668	0.50	0/2269
1	L	0.33	0/1680	0.51	0/2281
2	B	0.27	0/1671	0.53	0/2275
2	D	0.29	0/1579	0.49	0/2150
2	F	0.34	0/1535	0.53	0/2089
2	H	0.28	0/1699	0.53	0/2313
2	I	0.27	0/1134	0.45	0/1541
2	K	0.31	0/1645	0.55	0/2243
All	All	0.31	0/18852	0.51	0/25634

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 [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	1633	0	1570	43	1
1	C	1547	0	1468	45	0
1	E	1446	0	1391	40	0
1	G	1489	0	1416	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1631	0	1559	37	1
1	L	1643	0	1592	43	0
2	B	1631	0	1598	45	0
2	D	1545	0	1494	31	0
2	F	1503	0	1453	42	0
2	H	1658	0	1626	40	0
2	I	1112	0	1075	16	0
2	K	1605	0	1558	61	0
All	All	18443	0	17800	445	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 12.

The worst 5 of 445 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:95:PRO:HG2	1:G:96:PRO:HD3	1.20	1.16
2:B:51:ILE:HD13	2:B:72:ARG:HG2	1.37	1.02
1:L:6:GLN:NE2	1:L:88:CYS:SG	2.33	1.02
1:G:95:PRO:CG	1:G:96:PRO:HD3	1.98	0.93
1:C:58:VAL:HG22	1:C:59:PRO:HD2	1.52	0.92

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)
1:A:53:SER:OG	1:J:189:LYS:NZ[1_455]	2.06	0.14

## 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	210/215 (98%)	202 (96%)	7 (3%)	1 (0%)	29	64
1	C	195/215 (91%)	189 (97%)	6 (3%)	0	100	100
1	E	180/215 (84%)	178 (99%)	2 (1%)	0	100	100
1	G	190/215 (88%)	181 (95%)	8 (4%)	1 (0%)	29	64
1	J	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
1	L	210/215 (98%)	203 (97%)	6 (3%)	1 (0%)	29	64
2	B	212/228 (93%)	205 (97%)	7 (3%)	0	100	100
2	D	202/228 (89%)	195 (96%)	7 (4%)	0	100	100
2	F	194/228 (85%)	187 (96%)	7 (4%)	0	100	100
2	H	219/228 (96%)	214 (98%)	5 (2%)	0	100	100
2	I	139/228 (61%)	130 (94%)	8 (6%)	1 (1%)	22	56
2	K	212/228 (93%)	202 (95%)	10 (5%)	0	100	100
All	All	2373/2658 (89%)	2288 (96%)	81 (3%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	PRO
1	A	95	PRO
1	G	96	PRO
2	I	156	PRO

### 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	184/188 (98%)	183 (100%)	1 (0%)	88	95
1	C	173/188 (92%)	173 (100%)	0	100	100
1	E	162/188 (86%)	161 (99%)	1 (1%)	86	94
1	G	166/188 (88%)	165 (99%)	1 (1%)	86	94
1	J	183/188 (97%)	180 (98%)	3 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	186/188 (99%)	182 (98%)	4 (2%)	52	79
2	B	181/193 (94%)	177 (98%)	4 (2%)	52	79
2	D	169/193 (88%)	169 (100%)	0	100	100
2	F	165/193 (86%)	163 (99%)	2 (1%)	71	88
2	H	184/193 (95%)	184 (100%)	0	100	100
2	I	122/193 (63%)	120 (98%)	2 (2%)	62	84
2	K	174/193 (90%)	172 (99%)	2 (1%)	73	89
All	All	2049/2286 (90%)	2029 (99%)	20 (1%)	76	90

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	99	HIS
2	K	204	ASN
2	I	158	THR
2	I	40	THR
1	J	7	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	90	GLN
2	F	171	HIS
1	G	125	GLN
2	K	3	GLN
2	F	35	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 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	212/215 (98%)	-0.06	2 (0%) 84 71	17, 29, 50, 59	0
1	C	203/215 (94%)	0.31	4 (1%) 65 48	27, 44, 69, 74	0
1	E	190/215 (88%)	0.39	13 (6%) 17 10	30, 54, 81, 94	0
1	G	196/215 (91%)	0.29	10 (5%) 28 17	35, 52, 83, 95	0
1	J	212/215 (98%)	-0.17	1 (0%) 91 81	21, 29, 42, 66	0
1	L	212/215 (98%)	-0.03	1 (0%) 91 81	18, 31, 56, 66	0
2	B	216/228 (94%)	-0.01	4 (1%) 66 49	17, 28, 53, 75	0
2	D	208/228 (91%)	0.19	5 (2%) 59 42	29, 46, 58, 72	0
2	F	204/228 (89%)	0.24	10 (4%) 29 18	24, 53, 76, 91	0
2	H	221/228 (96%)	0.10	4 (1%) 68 51	18, 32, 62, 91	0
2	I	153/228 (67%)	0.22	4 (2%) 56 39	31, 46, 71, 90	0
2	K	216/228 (94%)	0.00	1 (0%) 91 81	19, 32, 53, 77	0
All	All	2443/2658 (91%)	0.12	59 (2%) 59 42	17, 39, 71, 95	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	CYS	4.6
1	G	3	GLN	4.2
2	F	54	THR	4.1
1	E	89	LEU	4.1
1	E	33	LEU	4.0

### 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 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.