



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:16 pm BST

PDB ID : 5UW8  
Title : Structure of E. coli MCE protein MlaD, core MCE domain  
Authors : Bhabha, G.; Ekiert, D.C.  
Deposited on : 2017-02-20  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

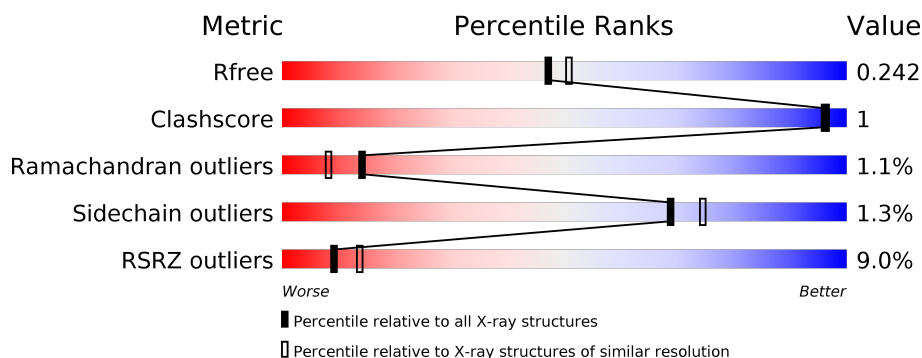
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	122	<div> <div>4%</div> <div>86%</div> <div>14%</div> </div>
1	B	122	<div> <div>8%</div> <div>78%</div> <div>20%</div> </div>
1	C	122	<div> <div>5%</div> <div>77%</div> <div>6%</div> <div>17%</div> </div>
1	D	122	<div> <div>8%</div> <div>80%</div> <div>16%</div> </div>
1	E	122	<div> <div>9%</div> <div>81%</div> <div>6%</div> <div>13%</div> </div>
1	F	122	<div> <div>11%</div> <div>79%</div> <div>6%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	122	<div><div></div><div>8%</div><div>80%</div><div>7%</div><div>13%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5728 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 Probable phospholipid ABC transporter-binding protein MlaD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	0	3	0
			820	516	135	169			
1	B	98	Total	C	N	O	0	0	0
			751	475	125	151			
1	C	101	Total	C	N	O	0	1	0
			776	488	129	159			
1	D	102	Total	C	N	O	0	1	0
			787	495	133	159			
1	E	106	Total	C	N	O	0	1	0
			822	516	140	166			
1	F	103	Total	C	N	O	0	2	0
			802	505	135	162			
1	G	106	Total	C	N	O	0	4	0
			845	529	144	172			

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P64605
A	20	HIS	-	expression tag	UNP P64605
A	21	HIS	-	expression tag	UNP P64605
A	22	HIS	-	expression tag	UNP P64605
A	23	HIS	-	expression tag	UNP P64605
A	24	HIS	-	expression tag	UNP P64605
A	25	HIS	-	expression tag	UNP P64605
A	26	GLU	-	expression tag	UNP P64605
A	27	ASN	-	expression tag	UNP P64605
A	28	LEU	-	expression tag	UNP P64605
A	29	TYR	-	expression tag	UNP P64605
A	30	PHE	-	expression tag	UNP P64605
A	31	GLN	-	expression tag	UNP P64605
B	19	MET	-	initiating methionine	UNP P64605
B	20	HIS	-	expression tag	UNP P64605

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	HIS	-	expression tag	UNP P64605
B	22	HIS	-	expression tag	UNP P64605
B	23	HIS	-	expression tag	UNP P64605
B	24	HIS	-	expression tag	UNP P64605
B	25	HIS	-	expression tag	UNP P64605
B	26	GLU	-	expression tag	UNP P64605
B	27	ASN	-	expression tag	UNP P64605
B	28	LEU	-	expression tag	UNP P64605
B	29	TYR	-	expression tag	UNP P64605
B	30	PHE	-	expression tag	UNP P64605
B	31	GLN	-	expression tag	UNP P64605
C	19	MET	-	initiating methionine	UNP P64605
C	20	HIS	-	expression tag	UNP P64605
C	21	HIS	-	expression tag	UNP P64605
C	22	HIS	-	expression tag	UNP P64605
C	23	HIS	-	expression tag	UNP P64605
C	24	HIS	-	expression tag	UNP P64605
C	25	HIS	-	expression tag	UNP P64605
C	26	GLU	-	expression tag	UNP P64605
C	27	ASN	-	expression tag	UNP P64605
C	28	LEU	-	expression tag	UNP P64605
C	29	TYR	-	expression tag	UNP P64605
C	30	PHE	-	expression tag	UNP P64605
C	31	GLN	-	expression tag	UNP P64605
D	19	MET	-	initiating methionine	UNP P64605
D	20	HIS	-	expression tag	UNP P64605
D	21	HIS	-	expression tag	UNP P64605
D	22	HIS	-	expression tag	UNP P64605
D	23	HIS	-	expression tag	UNP P64605
D	24	HIS	-	expression tag	UNP P64605
D	25	HIS	-	expression tag	UNP P64605
D	26	GLU	-	expression tag	UNP P64605
D	27	ASN	-	expression tag	UNP P64605
D	28	LEU	-	expression tag	UNP P64605
D	29	TYR	-	expression tag	UNP P64605
D	30	PHE	-	expression tag	UNP P64605
D	31	GLN	-	expression tag	UNP P64605
E	19	MET	-	initiating methionine	UNP P64605
E	20	HIS	-	expression tag	UNP P64605
E	21	HIS	-	expression tag	UNP P64605
E	22	HIS	-	expression tag	UNP P64605
E	23	HIS	-	expression tag	UNP P64605

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Chain	Residue	Modelled	Actual	Comment	Reference
E	24	HIS	-	expression tag	UNP P64605
E	25	HIS	-	expression tag	UNP P64605
E	26	GLU	-	expression tag	UNP P64605
E	27	ASN	-	expression tag	UNP P64605
E	28	LEU	-	expression tag	UNP P64605
E	29	TYR	-	expression tag	UNP P64605
E	30	PHE	-	expression tag	UNP P64605
E	31	GLN	-	expression tag	UNP P64605
F	19	MET	-	initiating methionine	UNP P64605
F	20	HIS	-	expression tag	UNP P64605
F	21	HIS	-	expression tag	UNP P64605
F	22	HIS	-	expression tag	UNP P64605
F	23	HIS	-	expression tag	UNP P64605
F	24	HIS	-	expression tag	UNP P64605
F	25	HIS	-	expression tag	UNP P64605
F	26	GLU	-	expression tag	UNP P64605
F	27	ASN	-	expression tag	UNP P64605
F	28	LEU	-	expression tag	UNP P64605
F	29	TYR	-	expression tag	UNP P64605
F	30	PHE	-	expression tag	UNP P64605
F	31	GLN	-	expression tag	UNP P64605
G	19	MET	-	initiating methionine	UNP P64605
G	20	HIS	-	expression tag	UNP P64605
G	21	HIS	-	expression tag	UNP P64605
G	22	HIS	-	expression tag	UNP P64605
G	23	HIS	-	expression tag	UNP P64605
G	24	HIS	-	expression tag	UNP P64605
G	25	HIS	-	expression tag	UNP P64605
G	26	GLU	-	expression tag	UNP P64605
G	27	ASN	-	expression tag	UNP P64605
G	28	LEU	-	expression tag	UNP P64605
G	29	TYR	-	expression tag	UNP P64605
G	30	PHE	-	expression tag	UNP P64605
G	31	GLN	-	expression tag	UNP P64605

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	9	Total O 9 9	0	0

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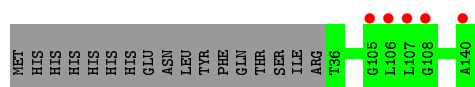
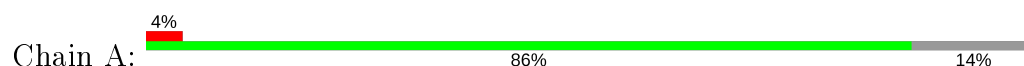
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	21	Total 21	O 21	0	0
2	D	20	Total 20	O 20	0	0
2	E	20	Total 20	O 20	0	0
2	F	17	Total 17	O 17	0	0
2	G	18	Total 18	O 18	0	0

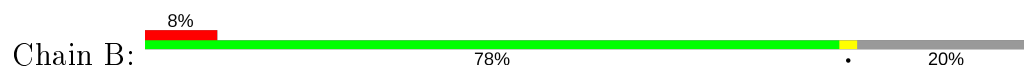
### 3 Residue-property plots [i](#)

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.

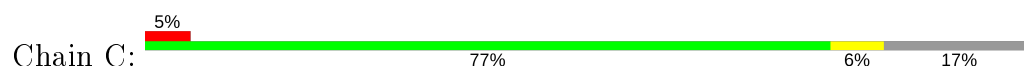
- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD



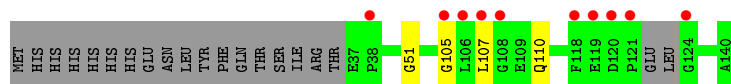
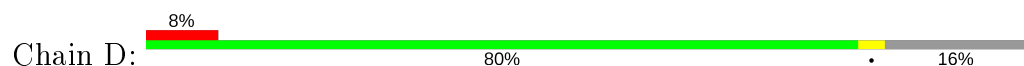
- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD



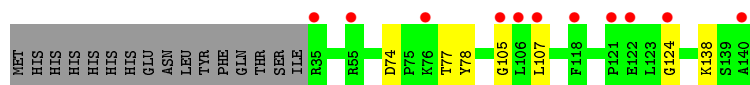
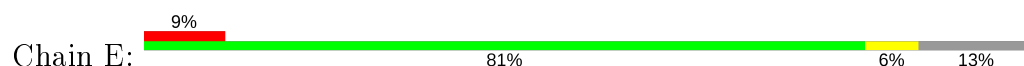
- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD



- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD

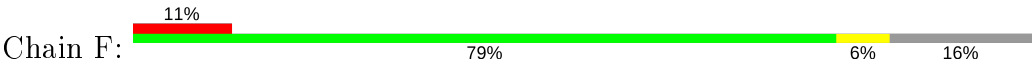


- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD

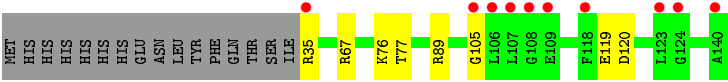
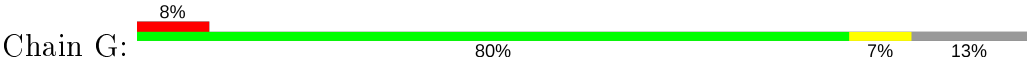


- Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD





● Molecule 1: Probable phospholipid ABC transporter-binding protein MlaD



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.66Å 103.82Å 77.21Å 90.00° 111.03° 90.00°	Depositor
Resolution (Å)	42.12 – 2.15 42.12 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.3 (42.12-2.15) 88.8 (42.12-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.204 , 0.244 0.208 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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	0.23	0/833	0.52	0/1135
1	B	0.21	0/762	0.46	0/1036
1	C	0.22	0/788	0.47	0/1073
1	D	0.23	0/799	0.49	0/1085
1	E	0.26	0/835	0.51	0/1135
1	F	0.31	0/816	0.50	0/1110
1	G	0.23	0/858	0.51	0/1167
All	All	0.24	0/5691	0.50	0/7741

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	820	0	818	0	0
1	B	751	0	756	1	0
1	C	776	0	766	3	0
1	D	787	0	787	1	0
1	E	822	0	825	2	0
1	F	802	0	799	2	1
1	G	845	0	841	2	0
2	A	20	0	0	0	0
2	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	21	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
2	F	17	0	0	1	0
2	G	18	0	0	1	0
All	All	5728	0	5592	11	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 1.

All (11) 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:55:ARG:O	1:C:67:ARG:NH1	2.35	0.59
1:E:74:ASP:O	1:E:78:TYR:N	2.33	0.54
1:F:47:ASP:OD2	2:F:201:HOH:O	2.21	0.45
1:C:47:ASP:OD1	1:C:48:ASN:N	2.50	0.45
1:G:76:LYS:HG3	1:G:77:THR:HG23	1.99	0.45
1:E:77:THR:O	1:E:78:TYR:HB2	2.17	0.44
1:G:89:ARG:NH2	2:G:203:HOH:O	2.51	0.43
1:C:69:ALA:HB2	1:C:85:GLU:HG2	2.02	0.42
1:F:49:ILE:HD13	1:F:71:ILE:HG21	2.02	0.41
1:B:55:ARG:O	1:B:67:ARG:NH1	2.53	0.41
1:D:51:GLY:N	1:D:110:GLN:OE1	2.47	0.41

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:F:121:PRO:CG	1:F:121:PRO:CG[2_556]	1.95	0.25

## 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	106/122 (87%)	103 (97%)	3 (3%)	0	100	100
1	B	94/122 (77%)	92 (98%)	2 (2%)	0	100	100
1	C	98/122 (80%)	97 (99%)	0	1 (1%)	15	9
1	D	99/122 (81%)	96 (97%)	2 (2%)	1 (1%)	15	9
1	E	105/122 (86%)	102 (97%)	1 (1%)	2 (2%)	8	2
1	F	103/122 (84%)	100 (97%)	1 (1%)	2 (2%)	8	2
1	G	108/122 (88%)	105 (97%)	1 (1%)	2 (2%)	8	2
All	All	713/854 (84%)	695 (98%)	10 (1%)	8 (1%)	14	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	105	GLY
1	G	105	GLY
1	D	105	GLY
1	F	105	GLY
1	F	124	GLY
1	G	120	ASP
1	C	124	GLY
1	E	124	GLY

### 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	92/106 (87%)	92 (100%)	0	100	100
1	B	84/106 (79%)	83 (99%)	1 (1%)	71	76
1	C	86/106 (81%)	86 (100%)	0	100	100
1	D	87/106 (82%)	86 (99%)	1 (1%)	73	78
1	E	91/106 (86%)	89 (98%)	2 (2%)	52	55
1	F	89/106 (84%)	88 (99%)	1 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	94/106 (89%)	90 (96%)	4 (4%)	29	27
All	All	623/742 (84%)	614 (99%)	9 (1%)	69	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ARG
1	D	107	LEU
1	E	107	LEU
1	E	138	LYS
1	F	85	GLU
1	G	35	ARG
1	G	67[A]	ARG
1	G	67[B]	ARG
1	G	119	GLU

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

Mol	Chain	Res	Type
1	E	115	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	105/122 (86%)	0.41	5 (4%) 30 39	37, 54, 118, 161	0
1	B	98/122 (80%)	0.66	10 (10%) 6 10	46, 81, 126, 154	0
1	C	101/122 (82%)	0.35	6 (5%) 22 30	40, 59, 125, 161	0
1	D	102/122 (83%)	0.55	10 (9%) 7 11	43, 60, 135, 169	0
1	E	106/122 (86%)	0.45	11 (10%) 6 9	43, 61, 126, 156	0
1	F	103/122 (84%)	0.80	13 (12%) 3 5	44, 71, 179, 236	0
1	G	106/122 (86%)	0.64	10 (9%) 8 12	41, 53, 136, 175	0
All	All	721/854 (84%)	0.55	65 (9%) 9 14	37, 63, 136, 236	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	106	LEU	14.1
1	G	107	LEU	12.5
1	F	118	PHE	11.6
1	F	123	LEU	11.4
1	A	106	LEU	11.2
1	F	106	LEU	10.8
1	B	106	LEU	9.3
1	G	140	ALA	8.6
1	D	121	PRO	7.9
1	D	106	LEU	7.9
1	A	107	LEU	7.0
1	F	107	LEU	6.8
1	B	118	PHE	6.8
1	B	107	LEU	6.2
1	E	121	PRO	5.9
1	D	118	PHE	5.7
1	E	106	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	5.5
1	G	108	GLY	5.5
1	F	122	GLU	5.1
1	D	124	GLY	4.9
1	F	121	PRO	4.7
1	F	120	ASP	4.6
1	A	108	GLY	4.6
1	F	108	GLY	4.5
1	E	124	GLY	4.2
1	E	105	GLY	4.1
1	D	105	GLY	3.9
1	F	124	GLY	3.6
1	G	105	GLY	3.5
1	B	139	SER	3.5
1	D	120	ASP	3.5
1	D	107	LEU	3.3
1	C	123	LEU	3.2
1	E	35	ARG	3.2
1	E	107	LEU	3.1
1	C	124	GLY	3.0
1	D	119	GLU	3.0
1	B	125	THR	3.0
1	D	38	PRO	3.0
1	B	55	ARG	2.9
1	C	118	PHE	2.9
1	A	140	ALA	2.8
1	B	105	GLY	2.8
1	F	109	GLU	2.8
1	G	123	LEU	2.8
1	C	140	ALA	2.7
1	G	109	GLU	2.7
1	G	124	GLY	2.6
1	B	138	LYS	2.5
1	G	118	PHE	2.5
1	B	119	GLU	2.5
1	E	76	LYS	2.4
1	F	119	GLU	2.4
1	B	95	ASP	2.4
1	F	38	PRO	2.3
1	D	108	GLY	2.3
1	E	55	ARG	2.2
1	F	105	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	109	GLU	2.1
1	E	122	GLU	2.1
1	E	140	ALA	2.1
1	C	36	THR	2.1
1	E	118	PHE	2.0
1	G	35	ARG	2.0

## 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 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.