



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:50 PM GMT

PDB ID : 4MX8  
Title : Crystal Structure of TroA-like Periplasmic Binding Protein Peripla\_BP\_2 from Xylanimonas cellulosilytica  
Authors : Kim, Y.; Wu, R.; Endres, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2013-09-26  
Resolution : 2.91 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

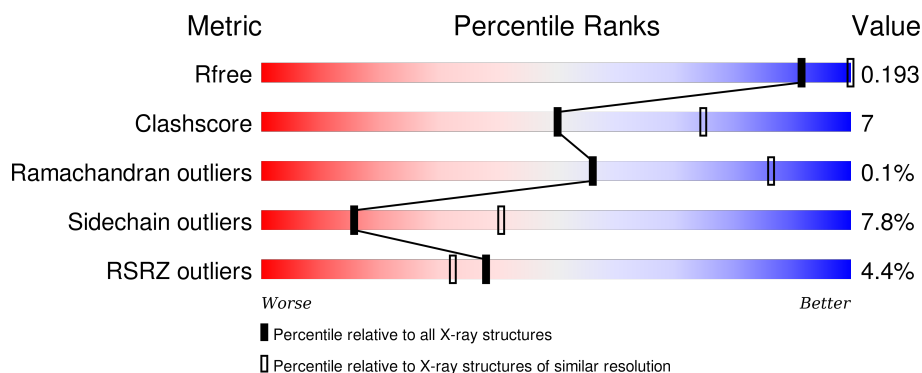
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	315	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	315	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	315	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	315	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	E	315	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	315	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '5%', a large green segment labeled '71%', a yellow segment labeled '22%', and a small grey segment at the end. Two small black dots are visible at the far right end of the bar.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13799 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 Periplasmic binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	Se	0	2	0
			2273	1434	367	469	3			
1	B	302	Total	C	N	O	Se	0	2	0
			2272	1430	370	469	3			
1	C	301	Total	C	N	O	Se	0	0	0
			2246	1415	364	464	3			
1	D	302	Total	C	N	O	Se	0	1	0
			2264	1429	366	466	3			
1	E	301	Total	C	N	O	Se	0	1	0
			2255	1420	365	467	3			
1	F	301	Total	C	N	O	Se	0	1	0
			2255	1420	366	466	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
A	0	ASN	-	EXPRESSION TAG	UNP D1BRG9
A	1	ALA	-	EXPRESSION TAG	UNP D1BRG9
B	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
B	0	ASN	-	EXPRESSION TAG	UNP D1BRG9
B	1	ALA	-	EXPRESSION TAG	UNP D1BRG9
C	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
C	0	ASN	-	EXPRESSION TAG	UNP D1BRG9
C	1	ALA	-	EXPRESSION TAG	UNP D1BRG9
D	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
D	0	ASN	-	EXPRESSION TAG	UNP D1BRG9
D	1	ALA	-	EXPRESSION TAG	UNP D1BRG9
E	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
E	0	ASN	-	EXPRESSION TAG	UNP D1BRG9
E	1	ALA	-	EXPRESSION TAG	UNP D1BRG9
F	-1	SER	-	EXPRESSION TAG	UNP D1BRG9
F	0	ASN	-	EXPRESSION TAG	UNP D1BRG9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ALA	-	EXPRESSION TAG	UNP D1BRG9

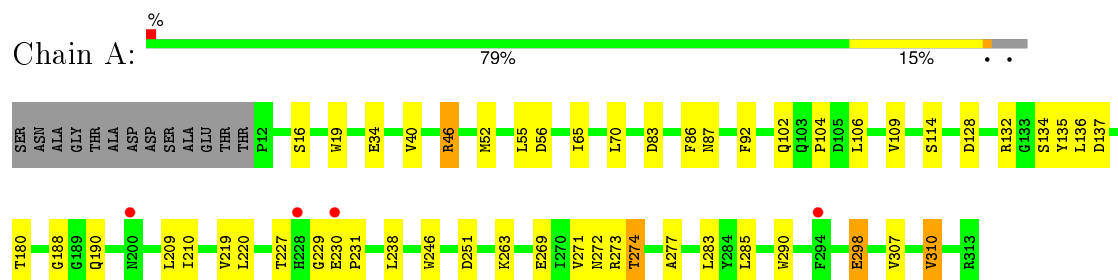
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	56	Total O 56 56	0	0
2	C	18	Total O 18 18	0	0
2	D	56	Total O 56 56	0	0
2	E	18	Total O 18 18	0	0
2	F	13	Total O 13 13	0	0

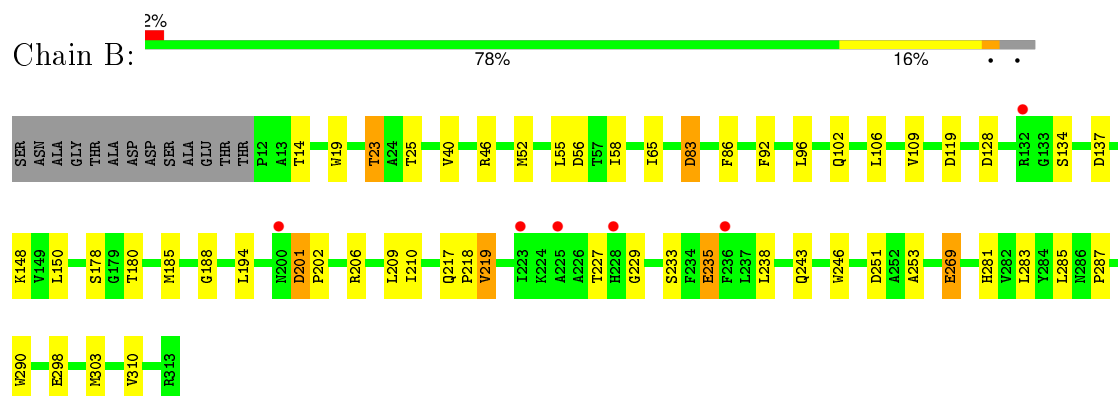
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

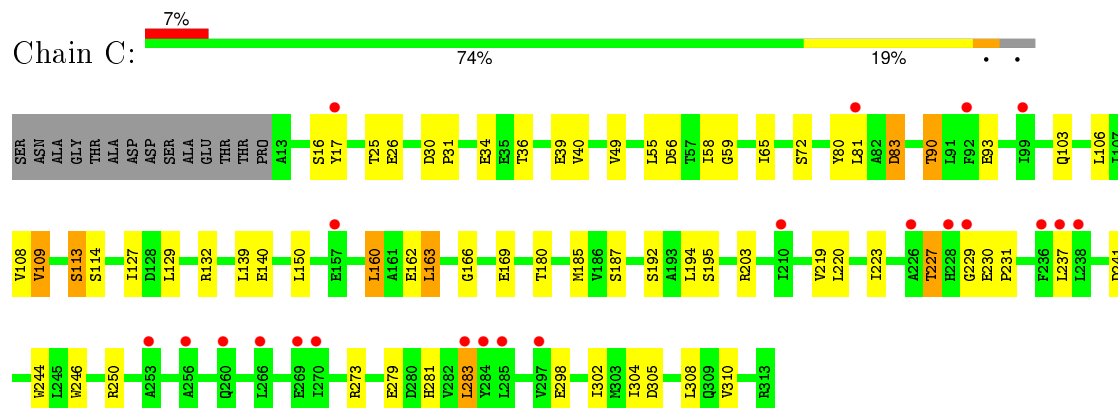
- Molecule 1: Periplasmic binding protein



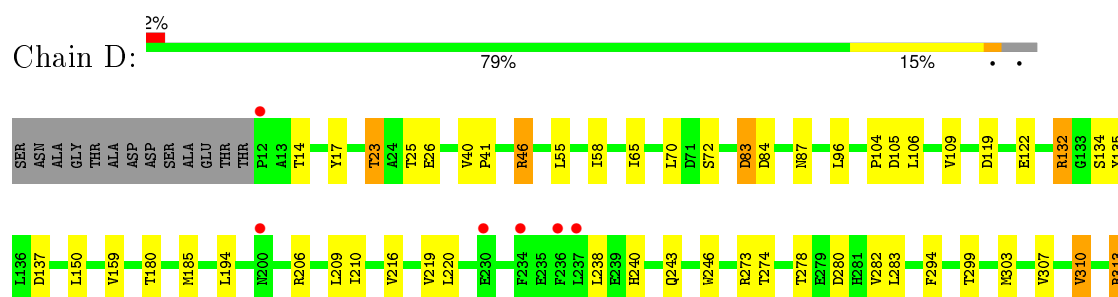
- Molecule 1: Periplasmic binding protein



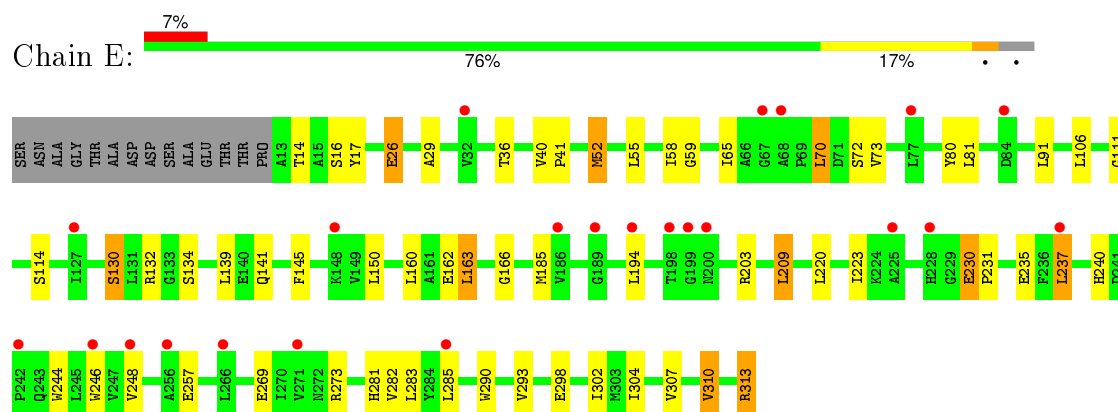
- Molecule 1: Periplasmic binding protein



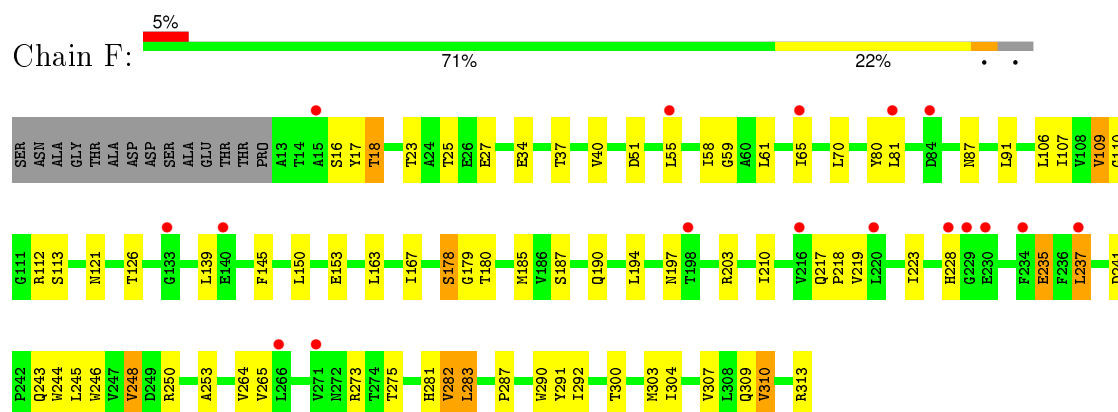
- Molecule 1: Periplasmic binding protein



- Molecule 1: Periplasmic binding protein



- Molecule 1: Periplasmic binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.66Å 116.55Å 177.16Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	49.37 – 2.91 50.19 – 2.91	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.37-2.91) 96.3 (50.19-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1367)	Depositor
R, $R_{free}$	0.159 , 0.196 0.151 , 0.193	Depositor DCC
$R_{free}$ test set	4016 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.467 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.468 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 80532 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/2313	0.61	0/3161
1	B	0.46	0/2311	0.61	0/3158
1	C	0.38	0/2284	0.54	0/3122
1	D	0.46	0/2304	0.62	0/3149
1	E	0.37	0/2293	0.54	0/3134
1	F	0.37	0/2293	0.53	0/3134
All	All	0.42	0/13798	0.58	0/18858

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

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	2273	0	2185	30	0
1	B	2272	0	2187	35	0
1	C	2246	0	2164	34	0
1	D	2264	0	2180	30	0
1	E	2255	0	2169	32	0
1	F	2255	0	2171	39	0
2	A	73	0	0	3	0
2	B	56	0	0	2	0
2	C	18	0	0	1	0
2	D	56	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	18	0	0	1	0
2	F	13	0	0	1	0
All	All	13799	0	13056	186	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 7.

The worst 5 of 186 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:E:111:GLY:H	1:E:130:SER:HB3	1.44	0.82
1:C:230:GLU:HG3	1:C:231:PRO:HD2	1.62	0.82
1:C:55:LEU:HG	1:C:65:ILE:HG13	1.66	0.77
1:B:134:SER:HB2	1:B:137:ASP:H	1.51	0.74
1:E:52:MSE:HE2	1:E:91:LEU:HD21	1.70	0.74

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	302/315 (96%)	291 (96%)	11 (4%)	0	100	100
1	B	302/315 (96%)	294 (97%)	7 (2%)	1 (0%)	46	78
1	C	299/315 (95%)	289 (97%)	10 (3%)	0	100	100
1	D	301/315 (96%)	292 (97%)	9 (3%)	0	100	100
1	E	300/315 (95%)	285 (95%)	15 (5%)	0	100	100
1	F	300/315 (95%)	285 (95%)	14 (5%)	1 (0%)	46	78
All	All	1804/1890 (95%)	1736 (96%)	66 (4%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	178	SER
1	B	178	SER

### 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	234/238 (98%)	221 (94%)	13 (6%)	26	59
1	B	234/238 (98%)	221 (94%)	13 (6%)	26	59
1	C	231/238 (97%)	208 (90%)	23 (10%)	9	28
1	D	233/238 (98%)	220 (94%)	13 (6%)	26	59
1	E	232/238 (98%)	208 (90%)	24 (10%)	9	26
1	F	232/238 (98%)	207 (89%)	25 (11%)	8	23
All	All	1396/1428 (98%)	1285 (92%)	111 (8%)	16	39

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	THR
1	E	14	THR
1	F	237	LEU
1	D	25	THR
1	D	109	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	272	ASN
1	F	141	GLN
1	D	281	HIS
1	B	217	GLN
1	D	240	HIS

### 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 ⓘ

### 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	299/315 (94%)	0.71	4 (1%) 79 78	23, 42, 78, 143	0
1	B	299/315 (94%)	0.68	6 (2%) 68 64	22, 42, 76, 138	0
1	C	298/315 (94%)	0.80	22 (7%) 17 12	47, 68, 109, 155	0
1	D	299/315 (94%)	0.63	6 (2%) 68 64	26, 42, 75, 153	0
1	E	298/315 (94%)	0.82	23 (7%) 16 11	46, 69, 106, 154	0
1	F	298/315 (94%)	0.73	17 (5%) 27 22	45, 69, 108, 150	0
All	All	1791/1890 (94%)	0.73	78 (4%) 38 32	22, 59, 99, 155	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	200	ASN	7.4
1	F	228	HIS	4.4
1	F	81	LEU	4.2
1	C	269	GLU	4.1
1	F	266	LEU	4.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.