



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 09:08 AM JST

PDB ID : 6A82  
Title : Crystal structure of the C-terminal periplasmic domain of EcEptC from Escherichia coli  
Authors : Zhao, Y.Q.; Gu, Y.J.; Cheng, W.  
Deposited on : 2018-07-06  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

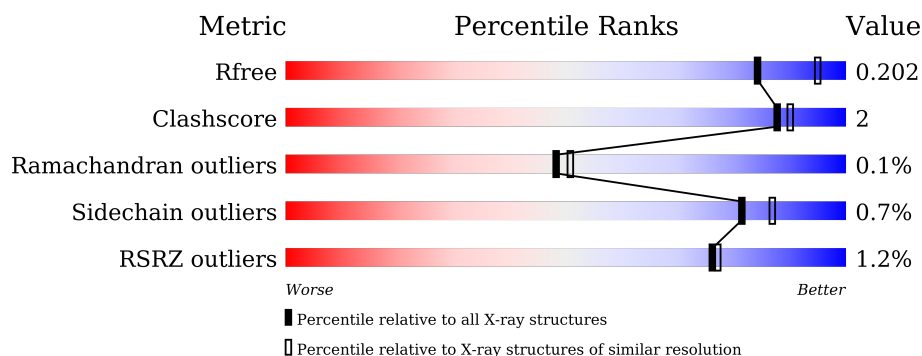
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	394	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">85%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">10%</span> </div> </div>
1	B	394	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">2%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">85%</span> </div> <div style="width: 6%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">6%</span> </div> <div style="width: 9%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">9%</span> </div> </div>
1	C	394	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">%</span> </div> <div style="width: 84%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">84%</span> </div> <div style="width: 5%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">5%</span> </div> <div style="width: 10%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; right: 0; top: -10px;">10%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9321 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 Phosphoethanolamine transferase EptC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	Se	0	0	0
			2882	1827	490	557	8			
1	B	357	Total	C	N	O	Se	0	0	0
			2912	1843	498	564	7			
1	C	353	Total	C	N	O	Se	0	0	0
			2882	1827	490	557	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	MSE	-	initiating methionine	UNP P0CB39
A	185	GLY	-	expression tag	UNP P0CB39
A	186	SER	-	expression tag	UNP P0CB39
A	187	SER	-	expression tag	UNP P0CB39
A	188	HIS	-	expression tag	UNP P0CB39
A	189	HIS	-	expression tag	UNP P0CB39
A	190	HIS	-	expression tag	UNP P0CB39
A	191	HIS	-	expression tag	UNP P0CB39
A	192	HIS	-	expression tag	UNP P0CB39
A	193	HIS	-	expression tag	UNP P0CB39
A	194	SER	-	expression tag	UNP P0CB39
A	195	SER	-	expression tag	UNP P0CB39
A	196	GLY	-	expression tag	UNP P0CB39
A	197	LEU	-	expression tag	UNP P0CB39
A	198	VAL	-	expression tag	UNP P0CB39
A	199	PRO	-	expression tag	UNP P0CB39
A	200	ARG	-	expression tag	UNP P0CB39
A	201	GLY	-	expression tag	UNP P0CB39
A	202	SER	-	expression tag	UNP P0CB39
A	203	HIS	-	expression tag	UNP P0CB39
A	204	MSE	-	expression tag	UNP P0CB39
B	184	MSE	-	initiating methionine	UNP P0CB39
B	185	GLY	-	expression tag	UNP P0CB39

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Chain	Residue	Modelled	Actual	Comment	Reference
B	186	SER	-	expression tag	UNP P0CB39
B	187	SER	-	expression tag	UNP P0CB39
B	188	HIS	-	expression tag	UNP P0CB39
B	189	HIS	-	expression tag	UNP P0CB39
B	190	HIS	-	expression tag	UNP P0CB39
B	191	HIS	-	expression tag	UNP P0CB39
B	192	HIS	-	expression tag	UNP P0CB39
B	193	HIS	-	expression tag	UNP P0CB39
B	194	SER	-	expression tag	UNP P0CB39
B	195	SER	-	expression tag	UNP P0CB39
B	196	GLY	-	expression tag	UNP P0CB39
B	197	LEU	-	expression tag	UNP P0CB39
B	198	VAL	-	expression tag	UNP P0CB39
B	199	PRO	-	expression tag	UNP P0CB39
B	200	ARG	-	expression tag	UNP P0CB39
B	201	GLY	-	expression tag	UNP P0CB39
B	202	SER	-	expression tag	UNP P0CB39
B	203	HIS	-	expression tag	UNP P0CB39
B	204	MSE	-	expression tag	UNP P0CB39
C	184	MSE	-	initiating methionine	UNP P0CB39
C	185	GLY	-	expression tag	UNP P0CB39
C	186	SER	-	expression tag	UNP P0CB39
C	187	SER	-	expression tag	UNP P0CB39
C	188	HIS	-	expression tag	UNP P0CB39
C	189	HIS	-	expression tag	UNP P0CB39
C	190	HIS	-	expression tag	UNP P0CB39
C	191	HIS	-	expression tag	UNP P0CB39
C	192	HIS	-	expression tag	UNP P0CB39
C	193	HIS	-	expression tag	UNP P0CB39
C	194	SER	-	expression tag	UNP P0CB39
C	195	SER	-	expression tag	UNP P0CB39
C	196	GLY	-	expression tag	UNP P0CB39
C	197	LEU	-	expression tag	UNP P0CB39
C	198	VAL	-	expression tag	UNP P0CB39
C	199	PRO	-	expression tag	UNP P0CB39
C	200	ARG	-	expression tag	UNP P0CB39
C	201	GLY	-	expression tag	UNP P0CB39
C	202	SER	-	expression tag	UNP P0CB39
C	203	HIS	-	expression tag	UNP P0CB39
C	204	MSE	-	expression tag	UNP P0CB39

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

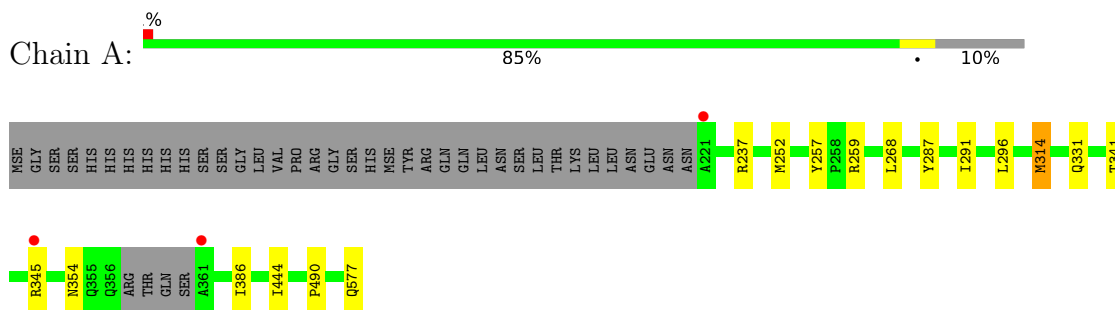
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0
3	B	196	Total O 196 196	0	0
3	C	233	Total O 233 233	0	0

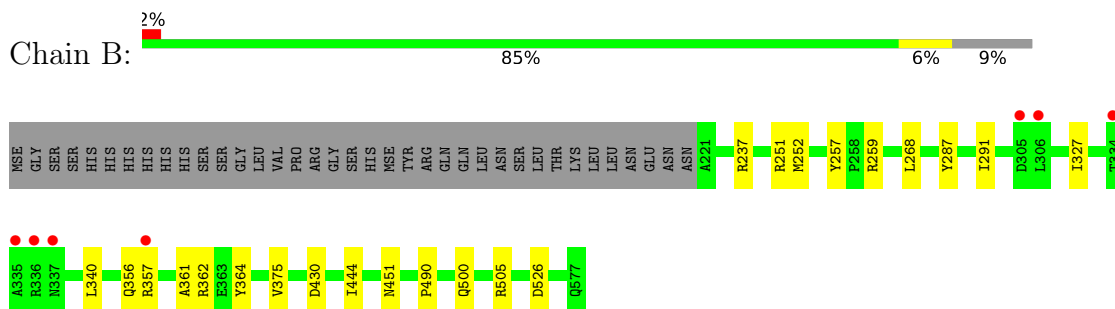
### 3 Residue-property plots [i](#)

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.

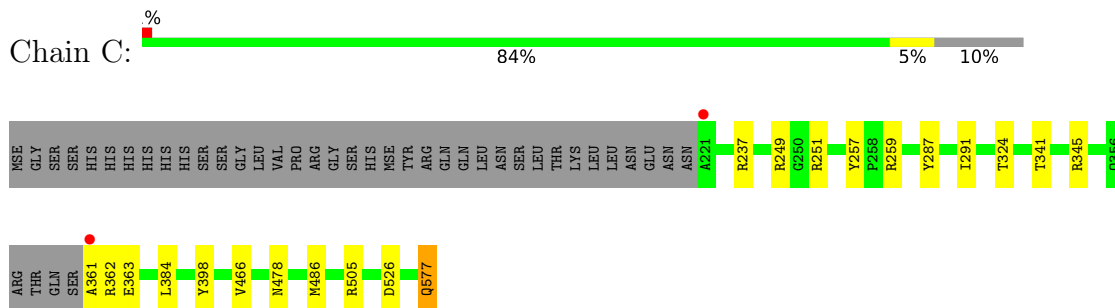
- Molecule 1: Phosphoethanolamine transferase EptC



- Molecule 1: Phosphoethanolamine transferase EptC



- Molecule 1: Phosphoethanolamine transferase EptC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.06Å 85.06Å 121.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.83 – 2.10 46.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.83-2.10) 98.7 (46.83-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.175 , 0.202 0.175 , 0.202	Depositor DCC
$R_{free}$ test set	2825 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.029 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
NA

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	0.25	0/2953	0.45	0/4011
1	B	0.26	0/2984	0.47	0/4055
1	C	0.25	0/2953	0.46	0/4011
All	All	0.25	0/8890	0.46	0/12077

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	2882	0	2757	10	0
1	B	2912	0	2784	11	0
1	C	2882	0	2757	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	213	0	0	0	0
3	B	196	0	0	0	0
3	C	233	0	0	0	0
All	All	9321	0	8298	32	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 2.

All (32) 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:B:356:GLN:HE22	1:B:361:ALA:HB3	1.32	0.95
1:C:251:ARG:NH2	1:C:466:VAL:O	2.28	0.66
1:C:362:ARG:NH2	1:C:363:GLU:OE2	2.34	0.60
1:B:251:ARG:NH1	1:B:430:ASP:OD1	2.36	0.59
1:B:362:ARG:HD3	1:B:364:TYR:OH	2.05	0.56
1:B:268:LEU:HD21	1:B:444:ILE:HG21	1.88	0.54
1:C:505:ARG:HH22	1:C:526:ASP:CG	2.12	0.52
1:A:331:GLN:HG2	1:A:354:ASN:O	2.11	0.51
1:A:296:LEU:HD22	1:A:314:MSE:HE1	1.91	0.51
1:C:324:THR:HG22	1:C:384:LEU:HB3	1.94	0.49
1:A:257:TYR:CE2	1:A:259:ARG:HB2	2.48	0.49
1:A:314:MSE:HE2	1:A:386:ILE:HD13	1.93	0.49
1:B:257:TYR:CE2	1:B:259:ARG:HB2	2.48	0.48
1:C:251:ARG:NH2	1:C:466:VAL:HB	2.27	0.48
1:B:500:GLN:HE22	1:B:505:ARG:H	1.61	0.48
1:B:287:TYR:O	1:B:291:ILE:HG22	2.15	0.47
1:B:340:LEU:HD12	1:B:340:LEU:HA	1.78	0.46
1:B:505:ARG:HH22	1:B:526:ASP:CG	2.19	0.46
1:C:287:TYR:O	1:C:291:ILE:HG22	2.14	0.46
1:A:296:LEU:HD13	1:A:314:MSE:HE1	1.97	0.46
1:A:268:LEU:HD21	1:A:444:ILE:HG21	1.98	0.45
1:A:287:TYR:O	1:A:291:ILE:HG22	2.17	0.45
1:A:341:THR:O	1:A:345:ARG:HG3	2.17	0.44
1:C:257:TYR:CE2	1:C:259:ARG:HB2	2.51	0.44
1:C:478:ASN:H	1:C:486:MSE:SE	2.51	0.44
1:C:341:THR:O	1:C:345:ARG:HG3	2.18	0.44
1:B:327:ILE:HD11	1:B:375:VAL:HG21	1.99	0.43
1:C:361:ALA:HB3	1:C:398:TYR:HB3	2.00	0.43
1:A:252:MSE:SE	1:A:490:PRO:HB3	2.69	0.42
1:C:249:ARG:NH2	1:C:577:GLN:O	2.48	0.42
1:A:331:GLN:HA	1:A:354:ASN:O	2.21	0.41
1:B:252:MSE:SE	1:B:490:PRO:HB3	2.71	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	349/394 (89%)	340 (97%)	9 (3%)	0	100	100
1	B	355/394 (90%)	345 (97%)	9 (2%)	1 (0%)	37	37
1	C	349/394 (89%)	341 (98%)	8 (2%)	0	100	100
All	All	1053/1182 (89%)	1026 (97%)	26 (2%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	ARG

### 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	318/346 (92%)	315 (99%)	3 (1%)	75	82
1	B	321/346 (93%)	319 (99%)	2 (1%)	84	89
1	C	318/346 (92%)	316 (99%)	2 (1%)	84	89
All	All	957/1038 (92%)	950 (99%)	7 (1%)	81	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	A	314	MSE

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Mol	Chain	Res	Type
1	A	577	GLN
1	B	237	ARG
1	B	451	ASN
1	C	237	ARG
1	C	577	GLN

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

Mol	Chain	Res	Type
1	B	356	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	345/394 (87%)	-0.34	3 (0%) 81 82	17, 26, 39, 58	0
1	B	349/394 (88%)	-0.26	7 (2%) 64 66	17, 25, 40, 69	0
1	C	345/394 (87%)	-0.33	2 (0%) 85 86	18, 25, 40, 64	0
All	All	1039/1182 (87%)	-0.31	12 (1%) 76 77	17, 25, 40, 69	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	361	ALA	5.0
1	B	357	ARG	4.9
1	C	361	ALA	3.8
1	C	221	ALA	3.6
1	A	221	ALA	3.0
1	B	305	ASP	3.0
1	B	334	THR	2.8
1	B	337	ASN	2.5
1	B	335	ALA	2.4
1	B	336	ARG	2.4
1	A	345	ARG	2.2
1	B	306	LEU	2.1

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	C	601	1/1	0.95	0.07	21,21,21,21	0
2	NA	A	601	1/1	0.97	0.08	23,23,23,23	0
2	NA	B	601	1/1	0.99	0.04	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.