



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:22 PM GMT

PDB ID : 3TOP  
Title : Crystal Structure of the C-terminal Subunit of Human Maltase-Glucoamylase  
in Complex with Acarbose  
Authors : Shen, Y.; Qin, X.H.; Ren, L.M.  
Deposited on : 2011-09-06  
Resolution : 2.88 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.

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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 : 1.7 (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

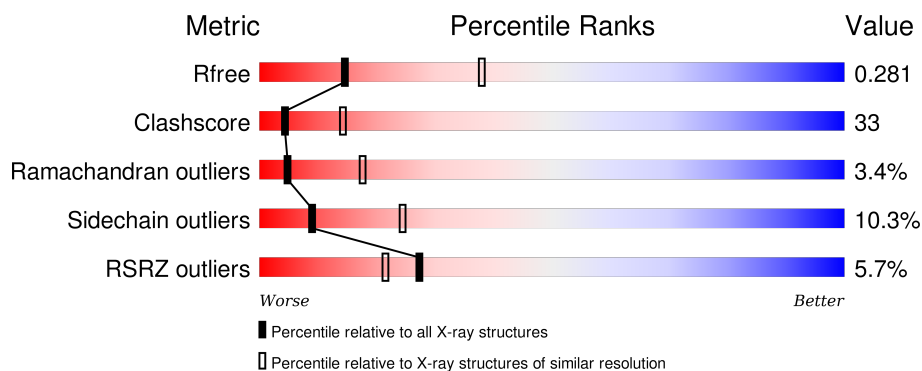
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	908	<div> <div>4%</div> <div>47%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>
1	B	908	<div> <div>7%</div> <div>47%</div> <div>43%</div> <div>8%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14388 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			
1	B	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			

There are 28 discrepancies between the modelled and reference sequences:

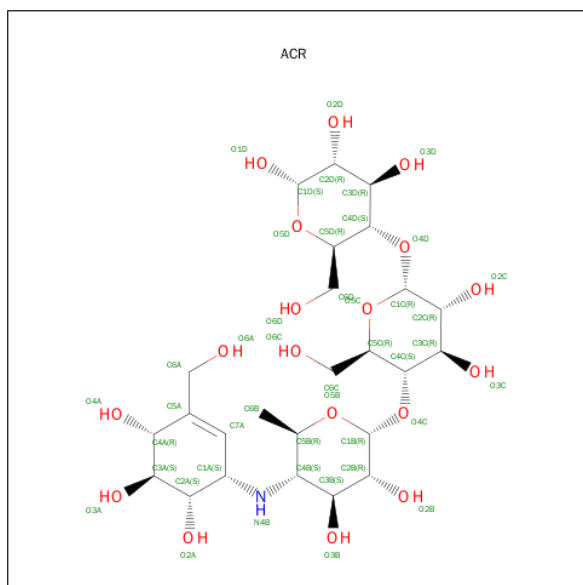
Chain	Residue	Modelled	Actual	Comment	Reference
A	952	TRP	-	EXPRESSION TAG	UNP O43451
A	953	SER	-	EXPRESSION TAG	UNP O43451
A	954	HIS	-	EXPRESSION TAG	UNP O43451
A	955	PRO	-	EXPRESSION TAG	UNP O43451
A	956	GLN	-	EXPRESSION TAG	UNP O43451
A	957	PHE	-	EXPRESSION TAG	UNP O43451
A	958	GLU	-	EXPRESSION TAG	UNP O43451
A	959	LYS	-	EXPRESSION TAG	UNP O43451
A	1854	HIS	-	EXPRESSION TAG	UNP O43451
A	1855	HIS	-	EXPRESSION TAG	UNP O43451
A	1856	HIS	-	EXPRESSION TAG	UNP O43451
A	1857	HIS	-	EXPRESSION TAG	UNP O43451
A	1858	HIS	-	EXPRESSION TAG	UNP O43451
A	1859	HIS	-	EXPRESSION TAG	UNP O43451
B	952	TRP	-	EXPRESSION TAG	UNP O43451
B	953	SER	-	EXPRESSION TAG	UNP O43451
B	954	HIS	-	EXPRESSION TAG	UNP O43451
B	955	PRO	-	EXPRESSION TAG	UNP O43451
B	956	GLN	-	EXPRESSION TAG	UNP O43451
B	957	PHE	-	EXPRESSION TAG	UNP O43451
B	958	GLU	-	EXPRESSION TAG	UNP O43451
B	959	LYS	-	EXPRESSION TAG	UNP O43451
B	1854	HIS	-	EXPRESSION TAG	UNP O43451
B	1855	HIS	-	EXPRESSION TAG	UNP O43451
B	1856	HIS	-	EXPRESSION TAG	UNP O43451

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1857	HIS	-	EXPRESSION TAG	UNP O43451
B	1858	HIS	-	EXPRESSION TAG	UNP O43451
B	1859	HIS	-	EXPRESSION TAG	UNP O43451

- Molecule 2 is SUGAR (ALPHA-ACARBOSE) (three-letter code: ACR) (formula: C<sub>25</sub>H<sub>43</sub>NO<sub>18</sub>).

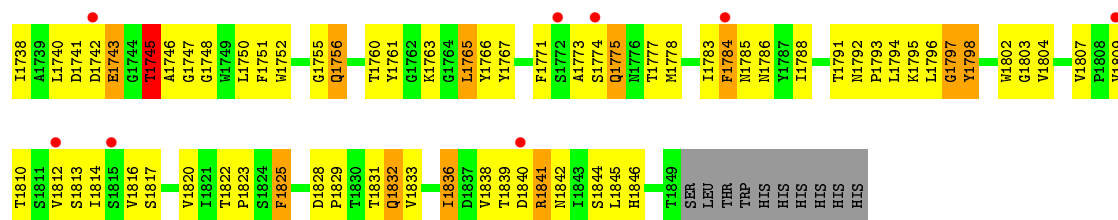


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	25	1	18		
2	B	1	Total	C	N	O	0	0
			44	25	1	18		

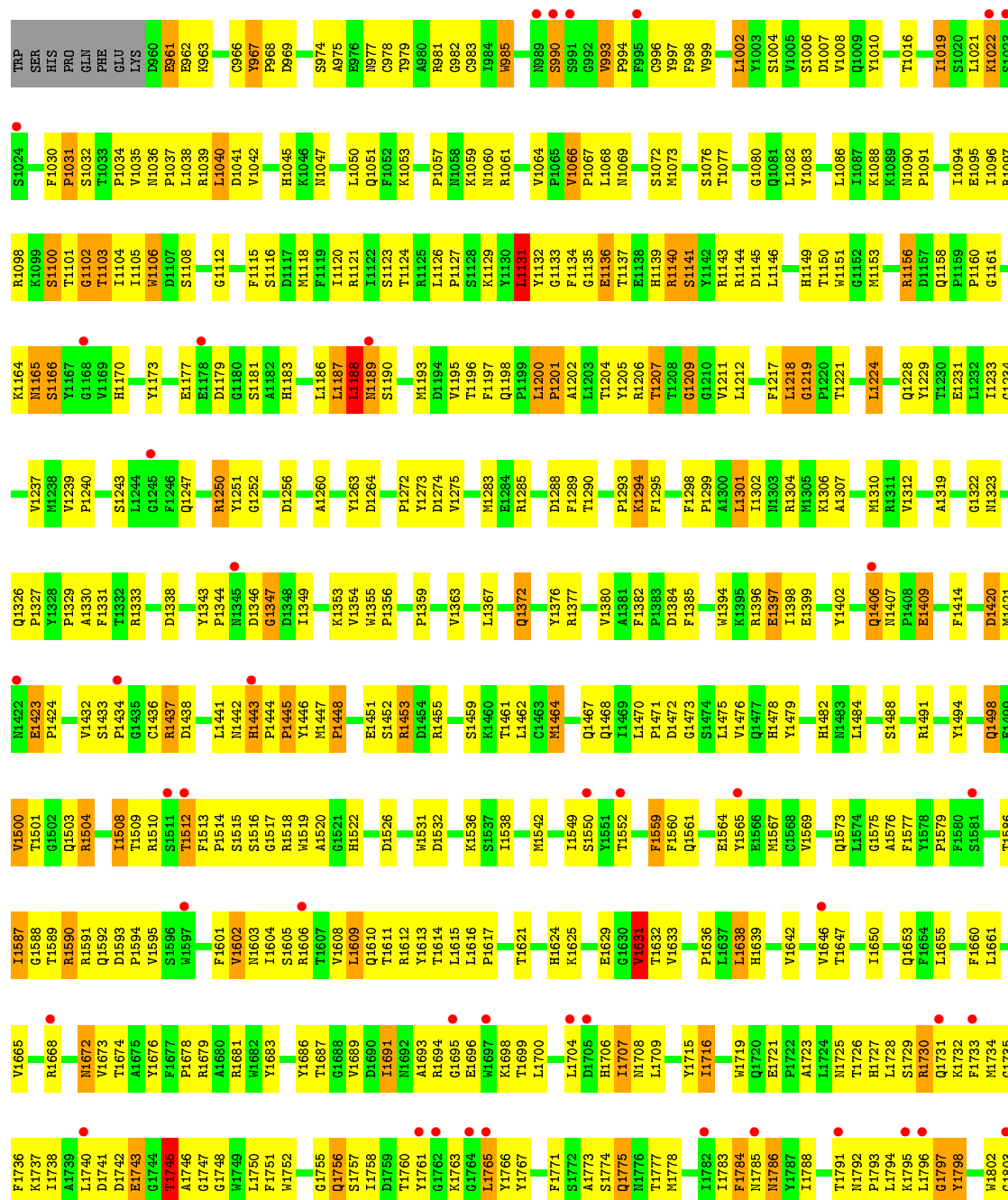
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	8	Total	O	0	0
			8	8		





• Molecule 1: Maltase-glucoamylase, intestinal



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.50 Å 105.50 Å 516.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.45 – 2.88 36.45 – 2.88	Depositor EDS
% Data completeness (in resolution range)	82.3 (36.45-2.88) 87.9 (36.45-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.90 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.218 , 0.284 0.222 , 0.281	Depositor DCC
$R_{free}$ test set	3014 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 59342 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.44	2/7350 (0.0%)	0.63	2/10031 (0.0%)
1	B	0.44	0/7350	0.63	2/10031 (0.0%)
All	All	0.44	2/14700 (0.0%)	0.63	4/20062 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1144	ARG	CB-CG	6.16	1.69	1.52
1	A	1323	ASN	CB-CG	5.42	1.63	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1219	GLY	N-CA-C	-6.06	97.95	113.10
1	A	1131	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	1219	GLY	N-CA-C	-5.73	98.77	113.10
1	B	1131	LEU	CA-CB-CG	5.69	128.38	115.30

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	7131	0	6766	463	0
1	B	7131	0	6766	454	0
2	A	44	0	43	10	0
2	B	44	0	43	1	0
3	A	30	0	0	1	0
3	B	8	0	0	1	0
All	All	14388	0	13618	919	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 33.

The worst 5 of 919 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:1734:MET:HE3	1:B:1794:LEU:HD21	1.29	1.10
1:A:1542:MET:HE1	1:A:1636:PRO:CB	1.81	1.10
1:B:967:TYR:CE2	1:B:1030:PHE:HZ	1.72	1.08
1:B:1542:MET:HE1	1:B:1636:PRO:HB3	1.09	1.06
1:B:1542:MET:HE1	1:B:1636:PRO:CB	1.85	1.06

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	888/908 (98%)	750 (84%)	109 (12%)	29 (3%)	5	18
1	B	888/908 (98%)	745 (84%)	111 (12%)	32 (4%)	4	16
All	All	1776/1816 (98%)	1495 (84%)	220 (12%)	61 (3%)	5	17

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PRO
1	A	1136	GLU
1	A	1347	GLY
1	A	1443	HIS
1	A	1445	PRO

### 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	773/800 (97%)	696 (90%)	77 (10%)	9	26
1	B	773/800 (97%)	690 (89%)	83 (11%)	8	22
All	All	1546/1600 (97%)	1386 (90%)	160 (10%)	9	24

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1810	THR
1	B	1068	LEU
1	B	1745	THR
1	A	1825	PHE
1	B	993	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1706	HIS
1	B	1058	ASN
1	B	1672	ASN
1	A	1792	ASN
1	B	1045	HIS

### 5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACR	A	1	-	46,47,47	1.63	12 (26%)	58,70,70	2.06	11 (18%)
2	ACR	B	1	-	46,47,47	1.55	9 (19%)	58,70,70	1.72	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACR	A	1	-	-	0/18/98/98	0/4/4/4
2	ACR	B	1	-	-	0/18/98/98	0/4/4/4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ACR	C3A-C4A	-4.31	1.47	1.53
2	A	1	ACR	O5C-C5C	-2.63	1.37	1.44
2	A	1	ACR	O2B-C2B	-2.54	1.36	1.43
2	A	1	ACR	C3B-C4B	-2.51	1.48	1.53
2	A	1	ACR	O3C-C3C	-2.39	1.37	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ACR	C1C-O4D-C4D	-4.49	106.26	118.01
2	B	1	ACR	C1B-O4C-C4C	-2.27	112.08	118.01
2	A	1	ACR	C3D-C4D-C5D	-2.21	105.85	110.84
2	A	1	ACR	C3B-C4B-C5B	-2.12	106.14	110.35
2	B	1	ACR	O6C-C6C-C5C	-2.12	104.34	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ACR	10	0
2	B	1	ACR	1	0

## 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	890/908 (98%)	0.21	34 (3%)	44	38	45, 81, 135, 207	0
1	B	890/908 (98%)	0.32	68 (7%)	17	11	50, 85, 141, 211	0
All	All	1780/1816 (98%)	0.26	102 (5%)	27	21	45, 83, 137, 211	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1443	HIS	7.4
1	B	1733	PHE	5.9
1	B	1821	ILE	5.8
1	B	991	SER	5.8
1	B	1815	SER	5.3

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACR	B	1	44/44	0.91	0.18	-0.42	54,88,110,121	0
2	ACR	A	1	44/44	0.92	0.18	-0.78	53,84,115,124	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.