



# wwPDB X-ray Structure Validation Summary Report

Jun 25, 2024 – 02:04 AM EDT

PDB ID : 6CKB  
Title : Crystal structure of an extended beta3 integrin P33  
Authors : Zhou, D.; Zhu, J.  
Deposited on : 2018-02-27  
Resolution : 2.80 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.

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 : 2.37.1  
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) : 2.37.1

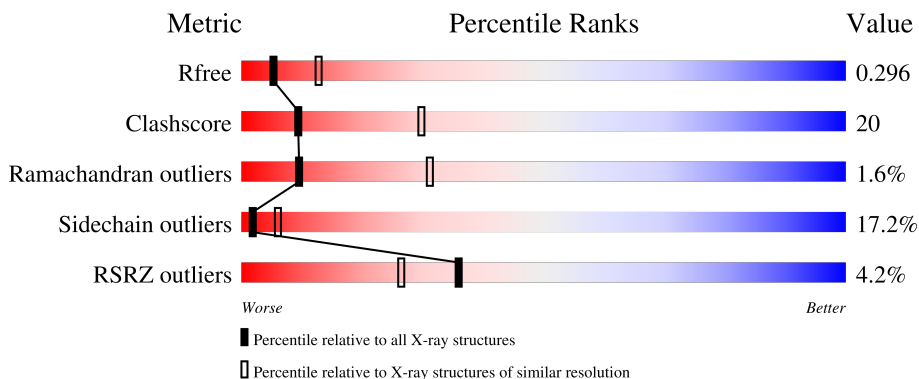
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	466	
1	B	466	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7299 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 Chimera protein of Integrin beta-3 and Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3606	2247	613	714	32	0	0	0
1	B	465	3617	2256	614	715	32	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	PRO	LEU	conflict	UNP P05106
A	171	TRP	ARG	conflict	UNP P20701
A	460	THR	-	expression tag	UNP P05106
A	461	ARG	-	expression tag	UNP P05106
A	462	GLU	-	expression tag	UNP P05106
A	463	LEU	-	expression tag	UNP P05106
A	464	TYR	-	expression tag	UNP P05106
A	465	PHE	-	expression tag	UNP P05106
A	466	GLN	-	expression tag	UNP P05106
B	33	PRO	LEU	conflict	UNP P05106
B	171	TRP	ARG	conflict	UNP P20701
B	460	THR	-	expression tag	UNP P05106
B	461	ARG	-	expression tag	UNP P05106
B	462	GLU	-	expression tag	UNP P05106
B	463	LEU	-	expression tag	UNP P05106
B	464	TYR	-	expression tag	UNP P05106
B	465	PHE	-	expression tag	UNP P05106
B	466	GLN	-	expression tag	UNP P05106

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

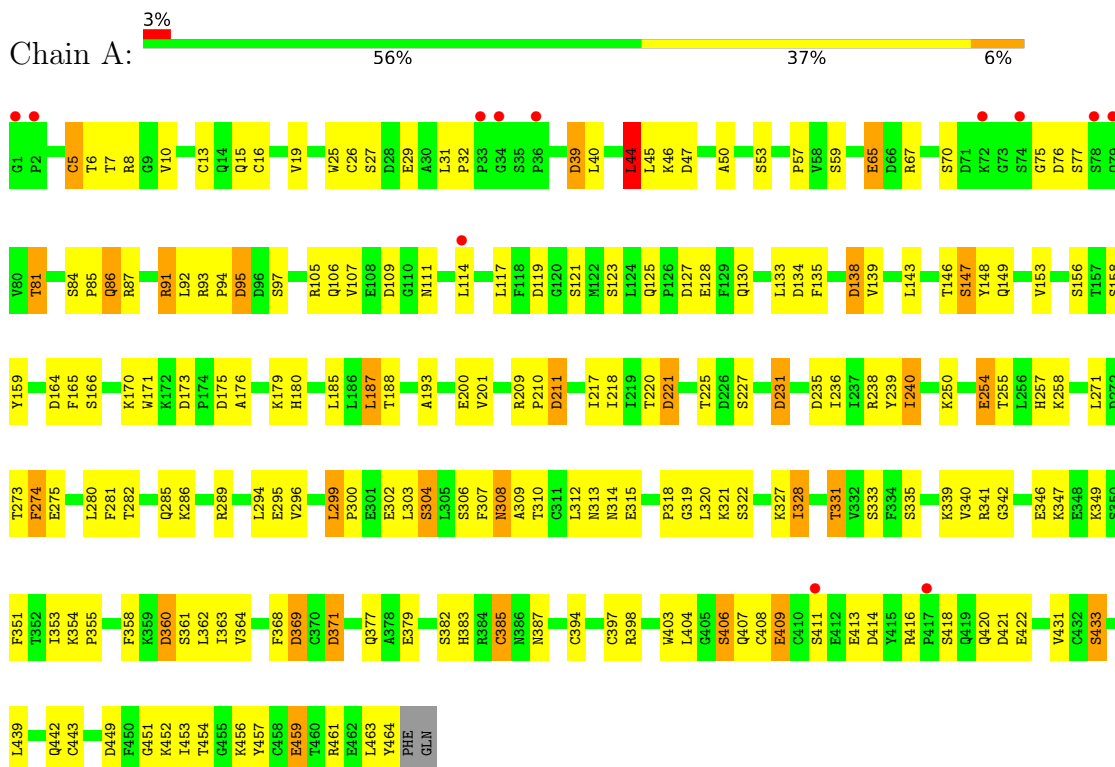
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		

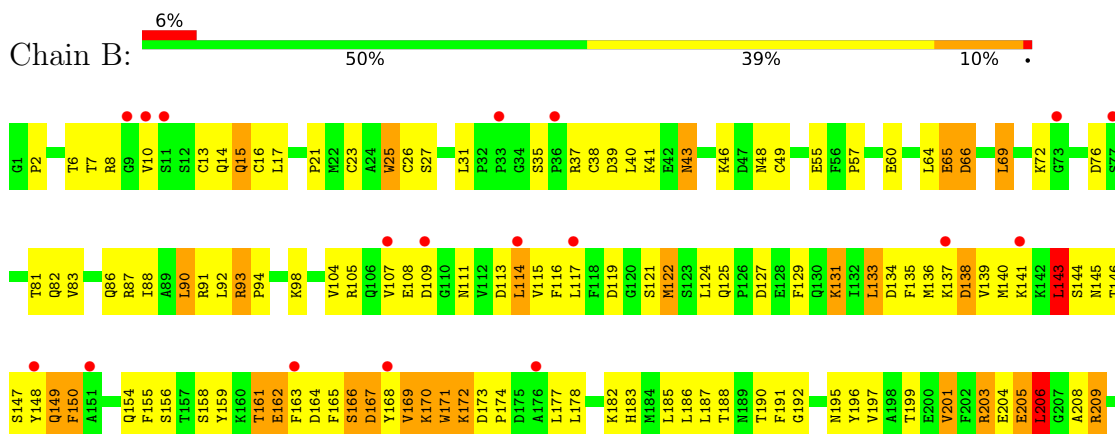
### 3 Residue-property plots [i](#)

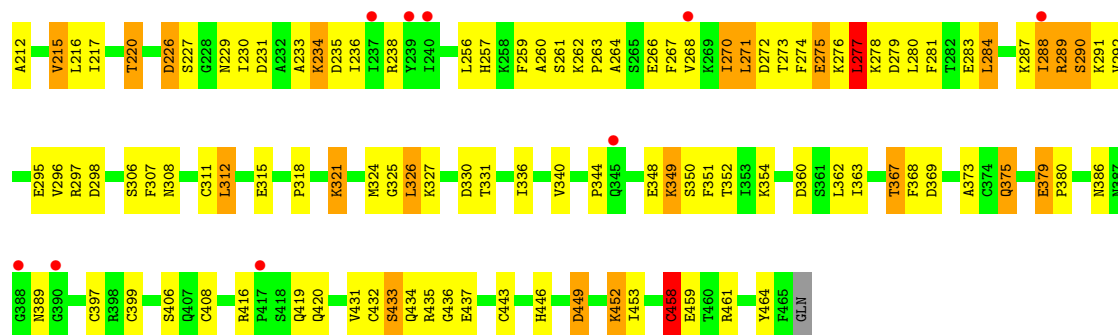
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chimera protein of Integrin beta-3 and Integrin alpha-L



- Molecule 1: Chimera protein of Integrin beta-3 and Integrin alpha-L





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.08Å 80.91Å 126.72Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	58.70 – 2.80 58.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.70-2.80) 99.8 (58.72-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.239 , 0.296 0.239 , 0.296	Depositor DCC
$R_{free}$ test set	1479 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.1	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 99.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, MG

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	0.34	0/3672	0.54	1/4955 (0.0%)
1	B	0.36	1/3684 (0.0%)	0.59	5/4971 (0.1%)
All	All	0.35	1/7356 (0.0%)	0.57	6/9926 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	CYS	CB-SG	-5.23	1.73	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LEU	CA-CB-CG	6.02	129.15	115.30
1	B	170	LYS	CA-C-N	-5.83	104.37	117.20
1	B	206	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	143	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	277	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	206	LEU	Peptide
1	B	279	ASP	Peptide

## 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	3606	0	3504	118	1
1	B	3617	0	3511	165	1
2	A	1	0	0	0	0
3	A	28	0	26	1	0
3	B	42	0	39	0	0
4	B	1	0	0	0	0
5	A	4	0	0	1	0
All	All	7299	0	7080	283	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 20.

The worst 5 of 283 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:119:ASP:HB2	1:B:220:THR:HA	1.57	0.86
1:A:67:ARG:HD3	1:A:86:GLN:HE22	1.42	0.84
1:A:306:SER:HB2	3:A:503:NAG:H81	1.64	0.80
1:B:449:ASP:OD1	1:B:449:ASP:N	2.13	0.79
1:A:121:SER:OG	1:A:123:SER:OG	2.03	0.76

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:327:LYS:NZ	1:B:386:ASN:OD1[2_458]	2.19	0.01

## 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	462/466 (99%)	407 (88%)	47 (10%)	8 (2%)	9 29
1	B	463/466 (99%)	403 (87%)	53 (11%)	7 (2%)	10 33
All	All	925/932 (99%)	810 (88%)	100 (11%)	15 (2%)	9 31

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	406	SER
1	B	433	SER
1	B	458	CYS
1	A	76	ASP

### 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	412/414 (100%)	353 (86%)	59 (14%)	3 10
1	B	413/414 (100%)	330 (80%)	83 (20%)	1 4
All	All	825/828 (100%)	683 (83%)	142 (17%)	2 6

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	278	LYS

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Mol	Chain	Res	Type
1	B	289	ARG
1	B	362	LEU
1	A	409	GLU
1	A	404	LEU

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

Mol	Chain	Res	Type
1	A	86	GLN

### 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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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
3	NAG	B	502	1	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	A	502	1	14,14,15	0.50	0	17,19,21	0.50	0
3	NAG	B	501	1	14,14,15	1.12	1 (7%)	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	503	1	14,14,15	0.71	0	17,19,21	0.78	1 (5%)
3	NAG	B	503	1	14,14,15	0.42	0	17,19,21	0.41	0

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
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	503	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAG	O5-C1	-3.54	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	NAG	C1-O5-C5	2.51	115.59	112.19
3	B	501	NAG	C1-O5-C5	-2.28	109.11	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	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	464/466 (99%)	0.22	12 (2%) 56 46	63, 137, 212, 290	0
1	B	465/466 (99%)	0.32	27 (5%) 23 15	87, 144, 224, 301	0
All	All	929/932 (99%)	0.27	39 (4%) 36 26	63, 142, 220, 301	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	6.3
1	B	148	TYR	5.5
1	B	114	LEU	5.2
1	A	79	GLN	5.1
1	B	151	ALA	4.9

### 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	502	14/15	0.81	0.28	180,212,238,256	0
3	NAG	B	503	14/15	0.83	0.21	122,143,175,179	0
2	MG	A	501	1/1	0.85	0.20	130,130,130,130	0
3	NAG	A	502	14/15	0.85	0.38	142,193,258,263	0
4	CA	B	504	1/1	0.90	0.18	191,191,191,191	0
3	NAG	A	503	14/15	0.91	0.31	164,244,289,303	0
3	NAG	B	501	14/15	0.95	0.21	62,90,112,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.