



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:11 pm BST

PDB ID : 4YU5  
Title : Crystal structure of selenomethionine variant of Bacillus anthracis immune inhibitor A2 peptidase zymogen  
Authors : Arolas, J.L.; Goulas, T.; Gomis-Ruth, F.X.  
Deposited on : 2015-03-18  
Resolution : 2.90 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.

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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 : 2.11  
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

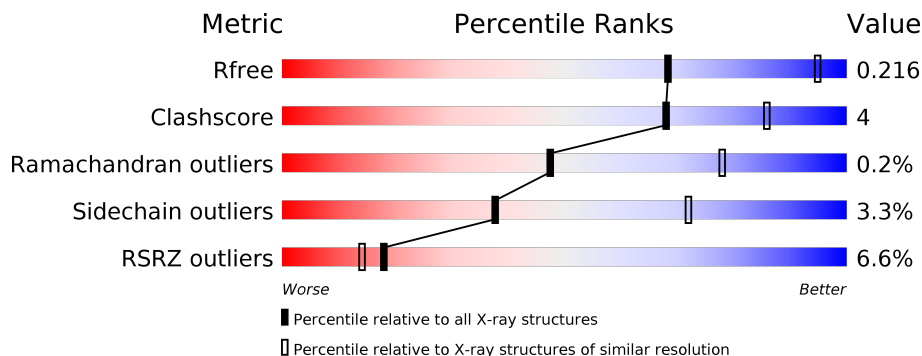
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	756	 4% 82% 9% • 8%
1	B	756	 7% 83% 8% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	KH2	A	1006	-	-	X	-
4	KH2	A	1007	-	-	X	-
5	GOL	A	1008	-	-	-	X
5	GOL	A	1013	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10942 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 Immune inhibitor A, metalloprotease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	695	5406	3409	916	1071	1	9	0	0	0
1	B	689	5357	3381	905	1061	1	9	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	HIS	TYR	conflict	UNP D8H130
A	380	ALA	GLU	engineered mutation	UNP D8H130
A	630	LEU	VAL	conflict	UNP D8H130
A	746	ASN	LYS	conflict	UNP D8H130
A	776	LYS	ASN	conflict	UNP D8H130
A	901	HIS	-	expression tag	UNP D8H130
A	902	HIS	-	expression tag	UNP D8H130
A	903	HIS	-	expression tag	UNP D8H130
A	904	HIS	-	expression tag	UNP D8H130
A	905	HIS	-	expression tag	UNP D8H130
A	906	HIS	-	expression tag	UNP D8H130
B	275	HIS	TYR	conflict	UNP D8H130
B	380	ALA	GLU	engineered mutation	UNP D8H130
B	630	LEU	VAL	conflict	UNP D8H130
B	746	ASN	LYS	conflict	UNP D8H130
B	776	LYS	ASN	conflict	UNP D8H130
B	901	HIS	-	expression tag	UNP D8H130
B	902	HIS	-	expression tag	UNP D8H130
B	903	HIS	-	expression tag	UNP D8H130
B	904	HIS	-	expression tag	UNP D8H130
B	905	HIS	-	expression tag	UNP D8H130
B	906	HIS	-	expression tag	UNP D8H130

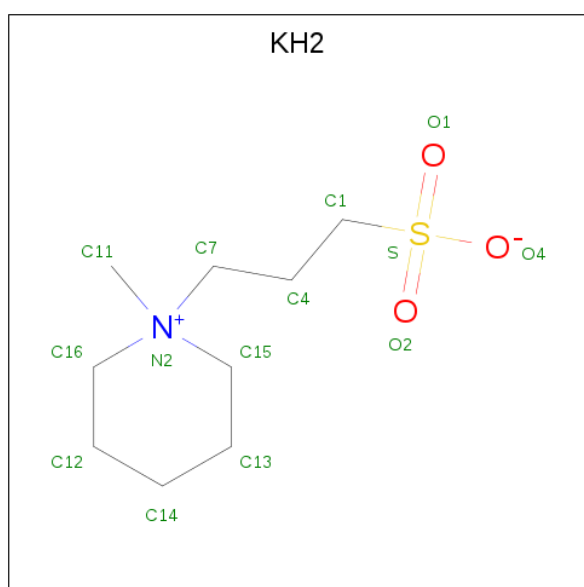
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Ca 4 4	0	0
3	A	4	Total Ca 4 4	0	0

- Molecule 4 is 3-(1-methylpiperidinium-1-yl)propane-1-sulfonate (three-letter code: KH2) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 14 9 1 3 1	0	0
4	A	1	Total C N O S 14 9 1 3 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0

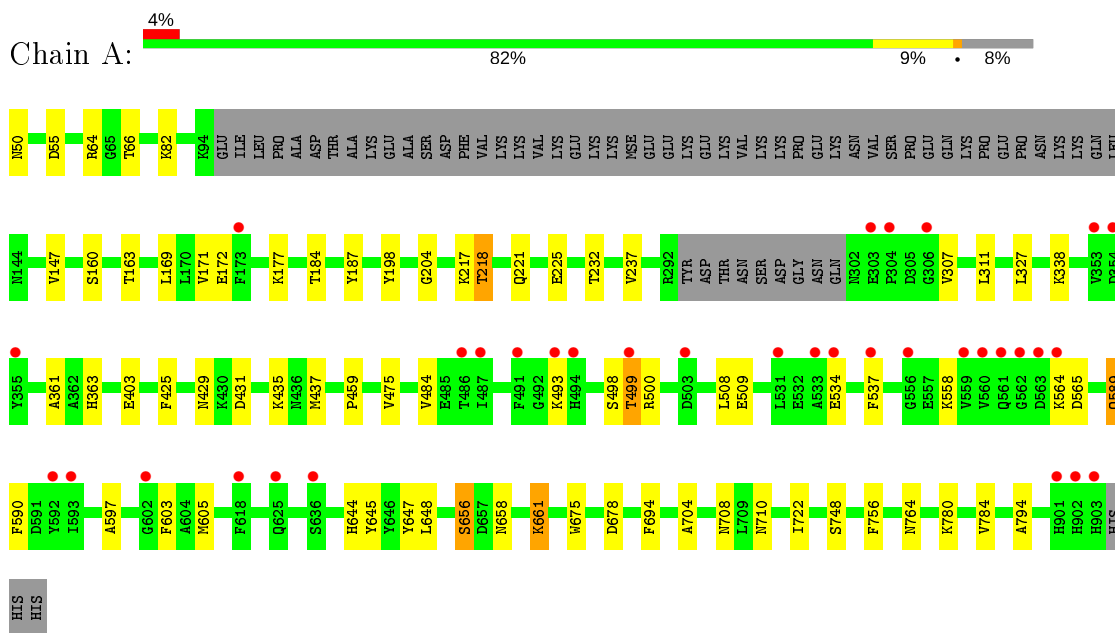
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	72	Total O 72 72	0	0
7	B	32	Total O 32 32	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: Immune inhibitor A, metalloprotease







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.61Å 102.41Å 242.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.46 – 2.90 48.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.46-2.90) 99.9 (48.80-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.91Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.182 , 0.207 0.188 , 0.216	Depositor DCC
$R_{free}$ test set	706 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtrriage
Anisotropy	0.721	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: K, GOL, ZN, CA, KH2

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	0.51	0/5526	0.69	0/7458
1	B	0.51	0/5476	0.69	1/7391 (0.0%)
All	All	0.51	0/11002	0.69	1/14849 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ASN	N-CA-CB	-5.31	101.05	110.60

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	5406	0	5160	42	0
1	B	5357	0	5117	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	28	0	38	16	0
5	A	36	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	72	0	0	1	0
7	B	32	0	0	1	0
All	All	10942	0	10363	80	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 4.

The worst 5 of 80 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:A:218:THR:HG22	1:A:221:GLN:H	1.24	1.02
1:B:218:THR:HG22	1:B:221:GLN:H	1.34	0.90
1:A:431:ASP:OD1	1:A:435:LYS:HE3	1.76	0.85
1:A:204:GLY:O	1:A:218:THR:HG21	1.82	0.79
1:B:204:GLY:O	1:B:218:THR:HG21	1.83	0.78

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	689/756 (91%)	662 (96%)	25 (4%)	2 (0%)	41 71
1	B	683/756 (90%)	652 (96%)	30 (4%)	1 (0%)	51 82
All	All	1372/1512 (91%)	1314 (96%)	55 (4%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	597	ALA

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Mol	Chain	Res	Type
1	A	597	ALA
1	A	499	THR

### 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	570/617 (92%)	552 (97%)	18 (3%)	39 73
1	B	565/617 (92%)	546 (97%)	19 (3%)	37 71
All	All	1135/1234 (92%)	1098 (97%)	37 (3%)	38 72

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	710	ASN
1	B	77	LYS
1	B	708	ASN
1	A	748	SER
1	B	50	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	199	GLN
1	B	50	ASN
1	B	199	GLN
1	B	669	ASN

### 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](#)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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
5	GOL	A	1010	-	5,5,5	0.07	0	5,5,5	0.37	0
5	GOL	A	1008	-	5,5,5	0.21	0	5,5,5	0.36	0
5	GOL	A	1011	-	5,5,5	0.06	0	5,5,5	0.16	0
5	GOL	A	1012	-	5,5,5	0.15	0	5,5,5	0.35	0
5	GOL	A	1009	-	5,5,5	0.14	0	5,5,5	0.39	0
4	KH2	A	1006	-	14,14,14	1.64	3 (21%)	19,20,20	3.04	9 (47%)
5	GOL	A	1013	-	5,5,5	0.35	0	5,5,5	0.44	0
4	KH2	A	1007	-	14,14,14	1.70	3 (21%)	19,20,20	2.47	8 (42%)

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
5	GOL	A	1010	-	-	4/4/4/4	-
5	GOL	A	1008	-	-	2/4/4/4	-
5	GOL	A	1011	-	-	2/4/4/4	-
5	GOL	A	1012	-	-	0/4/4/4	-
5	GOL	A	1009	-	-	0/4/4/4	-
4	KH2	A	1006	-	-	7/8/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1013	-	-	1/4/4/4	-
4	KH2	A	1007	-	-	5/8/18/18	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1006	KH2	O1-S	4.17	1.57	1.45
4	A	1007	KH2	O1-S	3.75	1.56	1.45
4	A	1007	KH2	C1-S	3.57	1.82	1.77
4	A	1007	KH2	O2-S	2.53	1.52	1.45
4	A	1006	KH2	O2-S	2.33	1.51	1.45

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1006	KH2	C4-C1-S	-7.54	101.69	113.25
4	A	1007	KH2	C11-N2-C16	-5.08	93.61	110.06
4	A	1006	KH2	C11-N2-C7	-4.63	94.04	109.34
4	A	1007	KH2	O4-S-C1	4.54	113.10	105.77
4	A	1006	KH2	C13-C15-N2	4.42	118.17	112.58

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1008	GOL	O1-C1-C2-C3
5	A	1010	GOL	O1-C1-C2-C3
4	A	1006	KH2	C4-C1-S-O1
4	A	1006	KH2	C4-C7-N2-C11
4	A	1006	KH2	C1-C4-C7-N2

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	GOL	1	0
4	A	1006	KH2	14	0
4	A	1007	KH2	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	686/756 (90%)	0.22	34 (4%) 28 25	34, 62, 102, 143	0
1	B	680/756 (89%)	0.48	56 (8%) 11 9	36, 74, 120, 147	0
All	All	1366/1512 (90%)	0.35	90 (6%) 18 14	34, 67, 116, 147	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	561	GLN	9.8
1	B	303	GLU	6.3
1	B	250	TYR	5.7
1	B	302	ASN	5.6
1	A	560	VAL	4.5

### 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. 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
5	GOL	A	1008	6/6	0.50	0.48	102,103,105,105	0
5	GOL	A	1013	6/6	0.60	0.42	79,85,88,89	0
6	K	B	1006	1/1	0.78	0.18	78,78,78,78	0
5	GOL	A	1009	6/6	0.78	0.17	101,102,105,106	0
3	CA	B	1005	1/1	0.79	0.06	130,130,130,130	0
5	GOL	A	1012	6/6	0.80	0.33	94,97,99,101	0
5	GOL	A	1011	6/6	0.90	0.20	88,90,95,98	0
5	GOL	A	1010	6/6	0.92	0.24	69,73,75,77	0
4	KH2	A	1006	14/14	0.92	0.26	32,45,80,81	0
4	KH2	A	1007	14/14	0.93	0.26	39,52,89,90	0
3	CA	B	1003	1/1	0.94	0.16	112,112,112,112	0
3	CA	A	1005	1/1	0.95	0.06	115,115,115,115	0
3	CA	B	1004	1/1	0.98	0.06	103,103,103,103	0
3	CA	A	1002	1/1	0.98	0.18	52,52,52,52	0
3	CA	A	1003	1/1	0.98	0.10	87,87,87,87	0
3	CA	B	1002	1/1	0.98	0.24	61,61,61,61	0
2	ZN	B	1001	1/1	0.98	0.25	72,72,72,72	0
2	ZN	A	1001	1/1	0.99	0.20	54,54,54,54	0
3	CA	A	1004	1/1	0.99	0.07	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.