



# Full wwPDB X-ray Structure Validation Report

Aug 21, 2020 – 01:40 PM BST

PDB ID : 6NVX  
Title : Crystal structure of penicillin G acylase from Bacillus sp. FJAT-27231  
Authors : Blankenfeldt, W.  
Deposited on : 2019-02-05  
Resolution : 1.36 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.

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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 : 2.13.1  
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) : 2.13.1

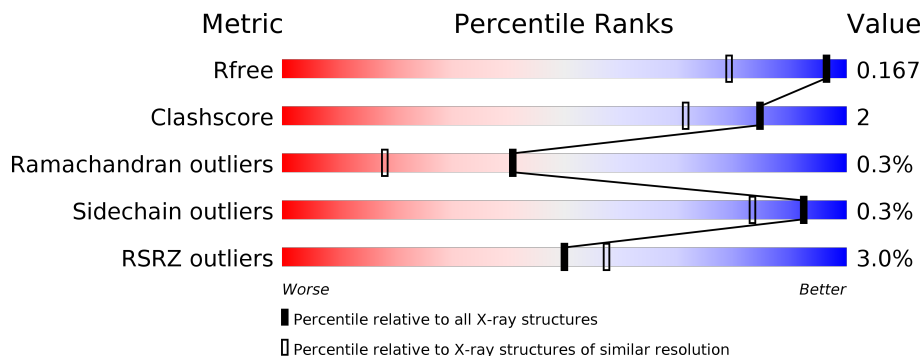
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	212	
2	B	538	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13118 atoms, of which 6021 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.

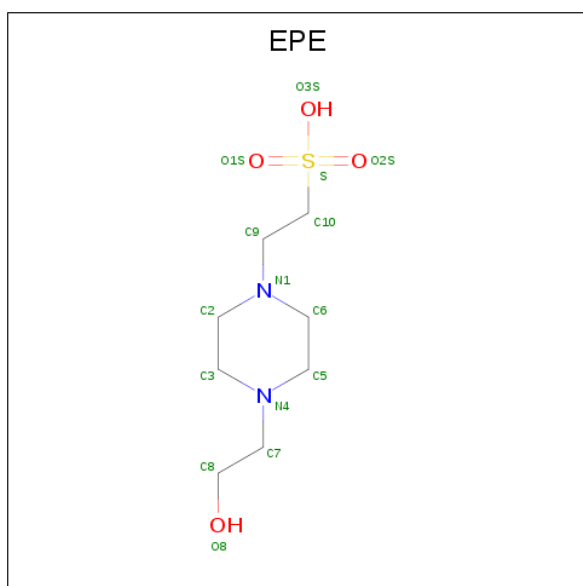
- Molecule 1 is a protein called penicillin G acylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	203	3439	1096	1711	289	336	7	0	11	0

- Molecule 2 is a protein called penicillin G acylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	527	8562	2786	4231	730	805	10	0	11	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	A	1	32	8	17	2	4	1	0	0
3	B	1	32	8	17	2	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		

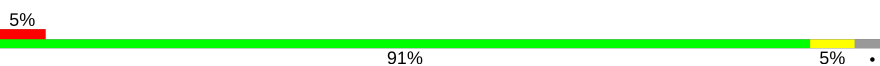
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	272	Total	O	0	0
			272	272		
6	B	698	Total	O	0	0
			698	698		

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

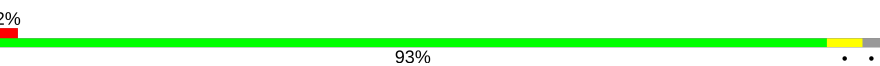
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

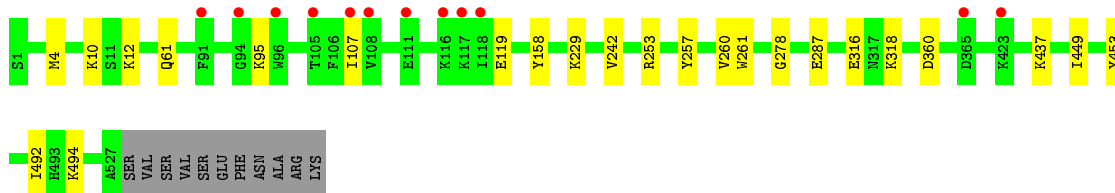
- Molecule 1: penicillin G acylase, alpha-subunit

Chain A: 



- Molecule 2: penicillin G acylase, beta-subunit

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.37Å 77.69Å 210.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.15 – 1.36 46.15 – 1.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.15-1.36) 100.0 (46.15-1.36)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.36Å)	Xtrriage
Refinement program	PHENIX dev_3386	Depositor
R, $R_{free}$	0.149 , 0.167 0.149 , 0.167	Depositor DCC
$R_{free}$ test set	9839 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	13118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: GOL, CA, EPE

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	0.55	0/1793	0.70	0/2408
2	B	0.57	0/4488	0.72	0/6051
All	All	0.56	0/6281	0.71	0/8459

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 [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	1728	1711	1710	9	0
2	B	4331	4231	4214	21	1
3	A	15	17	17	2	0
3	B	15	17	18	0	1
4	A	18	24	24	0	0
4	B	18	21	24	2	0
5	B	2	0	0	0	0
6	A	272	0	0	5	3
6	B	698	0	0	11	4
All	All	7097	6021	6007	28	5

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 (28) 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)
2:B:287[B]:GLU:OE2	6:B:701:HOH:O	1.98	0.82
1:A:124:ASP:OD2	2:B:453:TYR:OH	2.00	0.79
2:B:360:ASP:OD2	6:B:702:HOH:O	2.04	0.75
1:A:53:GLU:OE1	6:A:401:HOH:O	2.09	0.70
1:A:7:GLU:OE2	6:A:402:HOH:O	2.10	0.69
2:B:437[B]:LYS:HD2	6:B:1059:HOH:O	1.95	0.66
2:B:12[B]:LYS:CE	6:B:712:HOH:O	2.43	0.65
2:B:316:GLU:OE2	6:B:703:HOH:O	2.13	0.65
2:B:453:TYR:HD2	2:B:492:ILE:HD12	1.66	0.61
4:B:604:GOL:H32	6:B:738:HOH:O	2.00	0.60
2:B:95:LYS:NZ	6:B:710:HOH:O	2.36	0.58
3:A:301:EPE:O1S	2:B:229:LYS:NZ	2.32	0.58
1:A:65:VAL:O	1:A:69[B]:GLU:HG3	2.08	0.53
1:A:130:ARG:NH1	6:A:409:HOH:O	2.44	0.50
2:B:260:VAL:HG23	2:B:261:TRP:CD1	2.47	0.50
2:B:318:LYS:HD3	6:B:817:HOH:O	2.13	0.49
2:B:437[A]:LYS:HE2	6:B:1182:HOH:O	2.14	0.48
1:A:67[A]:LYS:HG2	2:B:449:ILE:HD11	1.96	0.47
2:B:119:GLU:OE2	6:B:704:HOH:O	2.21	0.46
2:B:4:MET:HG2	2:B:242:VAL:HG12	1.97	0.46
1:A:67[B]:LYS:NZ	6:A:403:HOH:O	2.33	0.43
2:B:253:ARG:O	4:B:604:GOL:H2	2.18	0.43
2:B:61:GLN:NE2	2:B:61:GLN:O	2.47	0.42
1:A:58[B]:GLU:HG2	2:B:107:ILE:O	2.19	0.42
2:B:12[B]:LYS:NZ	6:B:712:HOH:O	2.40	0.42
3:A:301:EPE:O1S	2:B:229:LYS:CE	2.68	0.41
1:A:27:LYS:HE3	6:A:599:HOH:O	2.20	0.41
2:B:10:LYS:O	2:B:10:LYS:HG3	2.21	0.41

All (5) 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)
6:A:556:HOH:O	6:B:720:HOH:O[1_655]	1.84	0.36
6:B:1003:HOH:O	6:B:1307:HOH:O[1_655]	1.97	0.23
6:A:631:HOH:O	6:B:1144:HOH:O[1_565]	2.09	0.11
2:B:494:LYS:NZ	3:B:601:EPE:O2S[1_655]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:608:HOH:O	6:B:999:HOH:O[1_655]	2.14	0.06

### 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	212/212 (100%)	207 (98%)	4 (2%)	1 (0%)	29 8
2	B	536/538 (100%)	522 (97%)	12 (2%)	2 (0%)	34 12
All	All	748/750 (100%)	729 (98%)	16 (2%)	3 (0%)	41 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
2	B	278[A]	GLY
2	B	278[B]	GLY

#### 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	189/189 (100%)	189 (100%)	0	100 100
2	B	457/457 (100%)	455 (100%)	2 (0%)	91 81
All	All	646/646 (100%)	644 (100%)	2 (0%)	92 83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	158	TYR
2	B	257	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 10 ligands modelled in this entry, 2 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$
4	GOL	B	604	-	5,5,5	1.26	0	5,5,5	1.27	1 (20%)
3	EPE	B	601	-	15,15,15	0.48	0	18,20,20	2.84	9 (50%)
4	GOL	B	603	-	5,5,5	0.94	0	5,5,5	0.99	0
3	EPE	A	301	-	15,15,15	0.85	1 (6%)	18,20,20	2.14	5 (27%)
4	GOL	A	302	-	5,5,5	0.63	0	5,5,5	0.71	0
4	GOL	A	304	-	5,5,5	0.87	0	5,5,5	0.73	0
4	GOL	A	303	-	5,5,5	0.67	0	5,5,5	0.96	0
4	GOL	B	602	-	5,5,5	0.74	0	5,5,5	1.01	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
4	GOL	B	604	-	-	3/4/4/4	-
3	EPE	B	601	-	-	2/9/19/19	0/1/1/1
4	GOL	B	603	-	-	0/4/4/4	-
3	EPE	A	301	-	-	8/9/19/19	0/1/1/1
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	A	304	-	-	3/4/4/4	-
4	GOL	A	303	-	-	0/4/4/4	-
4	GOL	B	602	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	EPE	C10-S	3.01	1.81	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EPE	C5-N4-C3	5.50	121.20	108.83
3	B	601	EPE	C6-N1-C2	5.48	121.17	108.83
3	A	301	EPE	C5-N4-C3	4.67	119.35	108.83
3	B	601	EPE	O2S-S-C10	4.41	112.23	106.92
3	A	301	EPE	O2S-S-C10	3.89	111.60	106.92
3	A	301	EPE	C7-N4-C3	3.78	120.90	111.23
3	B	601	EPE	C9-N1-C6	3.47	120.11	111.23
3	B	601	EPE	C7-N4-C3	3.31	119.70	111.23
3	B	601	EPE	O1S-S-C10	3.30	110.89	106.92
3	A	301	EPE	C7-N4-C5	3.27	119.60	111.23
3	B	601	EPE	C7-N4-C5	3.06	119.07	111.23
3	A	301	EPE	O3S-S-C10	2.87	110.40	105.77
3	B	601	EPE	C2-C3-N4	2.43	115.63	110.64
4	B	604	GOL	C3-C2-C1	-2.19	103.17	111.70
3	B	601	EPE	O2S-S-O1S	-2.12	106.60	113.95

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	EPE	C10-C9-N1-C6
3	A	301	EPE	C8-C7-N4-C3
4	B	604	GOL	C1-C2-C3-O3
3	B	601	EPE	C8-C7-N4-C5
3	A	301	EPE	C10-C9-N1-C6
3	A	301	EPE	C9-C10-S-O3S
4	A	304	GOL	O2-C2-C3-O3
4	A	302	GOL	O1-C1-C2-C3
3	A	301	EPE	C9-C10-S-O1S
3	A	301	EPE	C9-C10-S-O2S
3	A	301	EPE	N4-C7-C8-O8
3	A	301	EPE	C10-C9-N1-C2
4	A	304	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
3	A	301	EPE	C8-C7-N4-C5
4	B	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O2-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	2	0
3	B	601	EPE	0	1
3	A	301	EPE	2	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

### 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	203/212 (95%)	-0.23	10 (4%) 29 33	11, 18, 47, 86	0
2	B	527/538 (97%)	-0.23	12 (2%) 60 66	9, 16, 38, 60	0
All	All	730/750 (97%)	-0.23	22 (3%) 50 57	9, 17, 39, 86	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	GLU	7.2
2	B	107	ILE	3.7
1	A	5	LYS	3.6
2	B	94	GLY	3.5
2	B	118	ILE	3.3
1	A	204	GLY	3.3
1	A	201	LYS	3.2
2	B	108	VAL	3.2
1	A	6	VAL	3.1
1	A	202	LYS	3.0
2	B	96	TRP	3.0
1	A	198	THR	2.7
1	A	62	GLU	2.6
2	B	117	LYS	2.6
1	A	200	ILE	2.5
2	B	365	ASP	2.4
2	B	423	LYS	2.3
2	B	116	LYS	2.2
2	B	91	PHE	2.2
2	B	111	GLU	2.1
2	B	105	THR	2.1
1	A	199	ASP	2.0

## 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
4	GOL	B	603	6/6	0.75	0.14	33,64,82,85	0
3	EPE	A	301	15/15	0.78	0.18	64,77,85,89	0
4	GOL	A	303	6/6	0.79	0.10	43,55,67,69	0
4	GOL	A	304	6/6	0.84	0.36	38,78,94,109	0
4	GOL	A	302	6/6	0.90	0.11	26,63,72,75	0
4	GOL	B	604	6/6	0.90	0.14	24,54,67,67	0
3	EPE	B	601	15/15	0.96	0.14	21,48,80,88	0
4	GOL	B	602	6/6	0.97	0.16	20,29,35,38	0
5	CA	B	605	1/1	0.98	0.04	19,19,19,19	0
5	CA	B	606	1/1	0.99	0.06	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.