

# Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2020 – 09:28 AM BST

PDB ID	:	6Z9L
$\operatorname{Title}$	:	Enterococcal PrgA
Authors	:	Berntsson, R.P.A.; Schmitt, A.
Deposited on	:	2020-06-04
Resolution	:	3.06  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

## 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 3.06 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 >=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 <=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	А	787	80%	14%	• 5%
2	F	9	100%		
2	G	9	11%		

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:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	А	908	-	-	-	Х
3	SO4	А	911	-	-	-	Х
3	SO4	А	912	-	-	-	Х
3	SO4	А	913	-	-	-	Х



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11803 atoms, of which 5855 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 PrgA.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Λ	744	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	л	144	11555	3532	5767	1013	1235	8	0	0	0

• Molecule 2 is a protein called Poly-alanine peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	Б	0	Total	С	Η	Ν	Ο	0	0	0
	Г	9	89	27	44	9	9	0	0	0
9	C	0	Total	С	Η	Ν	Ο	0	0	0
	G	9	89	27	44	9	9	U	U	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 5	0 4	${ m S}$ 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	А	1	Total O S	0	0	
			5 4 1			
3	А	1	Total O S	0	0	
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ \hline \\ \hline \\ \end{array}$			
3	А	1	$\begin{bmatrix} 10tal & 0 & 5 \\ 5 & 4 & 1 \end{bmatrix}$	0	0	
			$\begin{array}{ccc} \mathbf{J} & 4 & \mathbf{I} \\ \hline \mathbf{Total} & \mathbf{O} & \mathbf{S} \end{array}$			
3	А	1	5 4 1	0	0	
			Total O S			
3	А	1	5 4 1	0	0	
			Total O S			
3	А	1	5 4 1	0	0	
	Α	-1	Total O S	0	0	
3	А		5 4 1	0	0	
2	Δ	1	Total O S	0	0	
0	A	L	5 4 1	0	0	
3	Δ	1	Total O S	0	Ο	
5	11	I	5 4 1	0	0	
3	А	1	Total O S	0	Ο	
		-	5 4 1	0	0	
3	А	1	Total O S	0	0	
		-	5 $4$ $1$			
3	А	1	Iotal O S	0	0	
3	А	1	Total O S	0	0	
		<b>*</b>	5 4 1		-	



## 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: PrgA



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants	126.36Å $126.36$ Å $293.91$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Baselution} \left( \overset{\circ}{\mathbf{A}} \right)$	49.11 - 3.06	Depositor
	49.11 - 3.06	EDS
$\% { m Data \ completeness}$	99.5(49.11-3.06)	Depositor
(in resolution range $)$	99.5(49.11 - 3.06)	EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.09 (at 3.07 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
D D .	0.286 , $0.318$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.287 , $0.318$	DCC
$R_{free}$ test set	2100 reflections $(4.62%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	102.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , $87.5$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11803	wwPDB-VP
Average B, all atoms $(Å^2)$	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



 $<sup>^{1} \</sup>mathrm{Intensities}$  estimated from amplitudes.

## 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: SO4

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).

Mal	Chain	Bond	lengths	Bond angles		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.26	0/5828	0.43	0/7840	
2	F	0.26	0/44	0.33	0/60	
2	G	0.27	0/44	0.29	0/60	
All	All	0.26	0/5916	0.43	0/7960	

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	А	5788	5767	5767	53	2
2	F	45	44	44	0	0
2	G	45	44	44	0	0
3	А	70	0	0	1	0
All	All	5948	5855	5855	53	2

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.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:341:PHE:HB3	1:A:342:PRO:CD	2.16	0.76
1:A:771:VAL:O	1:A:774:ASP:N	2.27	0.67
1:A:311:PRO:HB2	1:A:312:PRO:HD2	1.83	0.61
1:A:358:GLN:NE2	1:A:495:GLY:O	2.35	0.59
1:A:311:PRO:HB2	1:A:312:PRO:CD	2.36	0.55
1:A:451:SER:O	1:A:454:THR:OG1	2.21	0.54
1:A:475:TYR:O	1:A:479:HIS:ND1	2.39	0.53
1:A:501:SER:N	1:A:502:PRO:HD3	2.25	0.52
1:A:341:PHE:HB3	1:A:342:PRO:HD3	1.91	0.52
1:A:309:ASN:O	1:A:338:ASN:ND2	2.43	0.51
1:A:754:ALA:O	1:A:758:LEU:HD23	2.11	0.50
1:A:594:ALA:O	1:A:598:THR:HG23	2.11	0.50
1:A:94:GLN:O	1:A:98:VAL:HG23	2.12	0.50
1:A:95:GLN:O	1:A:98:VAL:HB	2.11	0.49
1:A:367:GLU:OE1	1:A:452:LYS:NZ	2.29	0.49
1:A:341:PHE:HB3	1:A:342:PRO:HD2	1.94	0.47
1:A:122:ALA:HA	1:A:125:VAL:HG12	1.95	0.47
1:A:401:ILE:HD12	1:A:507:ILE:HD12	1.96	0.47
1:A:87:ILE:HD11	1:A:747:ALA:HB1	1.96	0.46
1:A:489:LEU:HD13	1:A:490:GLY:N	2.31	0.46
1:A:463:LEU:O	1:A:467:LEU:HD22	2.16	0.46
1:A:118:VAL:O	1:A:121:GLU:HB3	2.17	0.45
1:A:310:LEU:HD21	1:A:382:LYS:HD3	1.98	0.45
1:A:290:GLN:O	1:A:294:THR:HG23	2.16	0.45
1:A:221:LYS:HZ2	1:A:618:THR:CG2	2.29	0.45
1:A:113:THR:O	1:A:116:GLN:HB3	2.17	0.44
1:A:73:LYS:HA	1:A:76:VAL:HG22	1.99	0.44
1:A:355:TRP:CE3	1:A:355:TRP:HA	2.53	0.44
1:A:307:GLY:O	1:A:460:ARG:NH2	2.51	0.43
1:A:661:GLN:O	1:A:665:LYS:HG2	2.18	0.43
1:A:706:GLN:HB2	1:A:707:PRO:HD3	2.01	0.43
1:A:768:TYR:N	1:A:768:TYR:CD1	2.85	0.43
1:A:80:ALA:HB2	1:A:758:LEU:HD21	2.01	0.43
1:A:402:ALA:HB2	1:A:492:SER:CB	2.49	0.43
1:A:162:VAL:O	1:A:166:GLN:HB2	2.20	0.42
1:A:698:SER:O	1:A:701:ARG:HB3	2.18	0.42
1:A:83:GLU:OE1	1:A:83:GLU:N	2.52	0.42
1:A:624:THR:O	1:A:627:GLU:HB3	2.20	0.42
1:A:302:LEU:O	1:A:305:HIS:HB2	2.19	0.42
1:A:83:GLU:O	1:A:87:ILE:HD13	2.19	0.42
1:A:666:ALA:O	1:A:670:THR:HG23	2.20	0.42
1:A:436:GLU:HB2	1:A:507:ILE:HD13	2.02	0.42



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:ND2	3:A:908:SO4:O3	2.52	0.41
1:A:134:ILE:O	1:A:138:LYS:HG3	2.20	0.41
1:A:748:THR:O	1:A:751:TYR:HB3	2.20	0.41
1:A:91:VAL:HG13	1:A:92:LYS:N	2.36	0.41
1:A:402:ALA:HB2	1:A:492:SER:HB2	2.02	0.41
1:A:768:TYR:N	1:A:768:TYR:HD1	2.18	0.41
1:A:311:PRO:HG2	1:A:330:LEU:CD1	2.50	0.41
1:A:366:LYS:O	1:A:370:VAL:HG23	2.20	0.41
1:A:398:ALA:HB1	1:A:492:SER:OG	2.21	0.41
1:A:778:GLN:HA	1:A:781:GLU:HB2	2.02	0.41
1:A:380:ARG:NH2	1:A:483:GLN:O	2.40	0.40

Continued from previous page...

All (2) 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:404:TYR:O	1:A:419:LYS:NZ[8_665]	2.06	0.14
1:A:404:TYR:O	1:A:419:LYS:HZ1[8_665]	1.57	0.03

### 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	Perce	$\mathbf{ntiles}$
1	А	742/787~(94%)	711~(96%)	27~(4%)	4 (0%)	29	60
2	F	7/9~(78%)	7 (100%)	0	0	100	100
2	G	7/9~(78%)	7 (100%)	0	0	100	100
All	All	756/805~(94%)	725~(96%)	27~(4%)	4 (0%)	29	60

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	131	PRO
1	А	341	PHE
1	А	498	ASN
1	А	311	PRO

#### 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	Analysed Rotameric Out		Percentiles
1	А	622/659~(94%)	585~(94%)	37~(6%)	19 47

All (37) residues with a non-rotameric sidechain are listed below:

$\mathbf{Mol}$	Chain	Res	Type
1	А	58	GLU
1	А	69	ILE
1	А	83	GLU
1	А	107	GLN
1	А	128	GLU
1	А	161	ASP
1	А	225	LEU
1	А	292	GLN
1	А	308	ILE
1	А	335	LEU
1	А	341	PHE
1	А	355	TRP
1	А	368	LEU
1	А	375	LEU
1	А	438	LEU
1	А	463	LEU
1	А	467	LEU
1	А	489	LEU
1	А	492	SER
1	А	500	ILE
1	А	514	LEU
1	A	534	LEU
1	A	559	ARG



Mol	Chain	Res	Type
1	А	580	LEU
1	А	605	VAL
1	А	615	LEU
1	А	622	LEU
1	А	629	ILE
1	А	636	LEU
1	А	659	GLU
1	А	670	THR
1	А	671	LEU
1	А	673	SER
1	А	709	TYR
1	A	746	VAL
1	А	763	LEU
1	A	773	ARG

Continued from previous page...

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)

14 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).



Mal	Tune	Chain	Dog	BoxLinkBond lengthsBox		Bond ang	gles			
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	SO4	A	904	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	А	903	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	А	912	-	4,4,4	0.14	0	$^{6,6,6}$	0.06	0
3	SO4	А	908	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	A	901	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	A	911	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	А	905	-	4,4,4	0.14	0	$^{6,6,6}$	0.04	0
3	SO4	A	910	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	А	902	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	A	909	-	4,4,4	0.14	0	$^{6,6,6}$	0.04	0
3	SO4	А	906	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	A	907	-	4,4,4	0.14	0	$^{6,6,6}$	0.05	0
3	SO4	А	913	-	4,4,4	0.15	0	$6,\!6,\!6$	0.04	0
3	SO4	А	914	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	908	SO4	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,  $95^{th}$  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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	744/787~(94%)	0.93	90~(12%)	4 1	50,  96,  246,  455	0
2	F	9/9~(100%)	0.46	0 100	100	174, 196, 211, 213	0
2	G	9/9~(100%)	1.01	1 (11%)	5 2	163, 204, 224, 230	0
All	All	762/805~(94%)	0.93	91 (11%)	4 1	50, 97, 246, 455	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	99	ASP	7.2
1	А	89	GLN	6.1
1	А	737	LEU	6.1
1	А	88	ASP	5.8
1	А	71	ASP	5.4
1	А	755	GLN	5.2
1	А	64	THR	5.1
1	А	94	GLN	5.1
1	А	769	GLN	4.9
1	А	746	VAL	4.9
1	А	98	VAL	4.7
1	А	744	GLN	4.7
1	А	101	ASN	4.7
1	А	776	GLU	4.6
1	А	516	ASP	4.3
1	А	57	THR	4.3
1	А	751	TYR	4.2
1	А	75	GLN	4.2
1	A	759	SER	4.2
1	A	90	SER	4.1
1	A	100	GLN	4.1
1	A	743	GLN	4.0
1	A	757	ASP	4.0



6Z9L

Mol	Chain	Res	Type	RSRZ
1	А	73	LYS	3.9
1	А	742	GLU	3.9
1	A	740	LEU	3.9
1	A	739	GLU	3.7
1	A	729	ALA	3.6
1	A	85	ASP	3.6
1	A	80	ALA	3.6
1	A	722	ALA	3.6
1	A	779	GLN	3.5
1	A	758	LEU	3.4
1	A	719	ALA	3.4
1	A	770	GLY	3.3
1	A	735	LYS	3.3
1	A	774	ASP	3.3
1	A	760	ASN	3.2
1	A	107	GLN	3.1
1	A	93	ASP	3.1
1	A	70	VAL	3.0
1	A	771	VAL	3.0
1	A	60	GLN	3.0
1	A	77	ALA	2.9
1	A	767	GLN	2.9
1	A	733	SER	2.9
1	A	754	ALA	2.9
1	A	114	ASP	2.9
1	A	752	ALA	2.9
1	A	67	GLN	2.8
1	A	108	SER	2.8
1	A	753	GLN	2.8
1	A	724	VAL	2.8
1	A	83	GLU	2.8
1	A	110	GLN	2.7
1	A	777	ALA	2.7
1	A	119	VAL	2.6
1	A	79	THR	2.6
1	A	747	ALA	2.5
1	A	78	ASP	2.5
1	A	72	GLN	2.5
1	A	84	LYS	2.5
1	A	723	VAL	2.5
1	А	727	GLN	2.5
1	А	728	GLU	2.5

Continued from previous page...



6Z9L
------

Mol	Chain	Res	Type	RSRZ
1	А	761	ALA	2.4
1	А	82	LYS	2.4
1	А	749	LEU	2.4
1	А	92	LYS	2.4
1	А	745	ALA	2.4
1	А	58	GLU	2.4
1	А	63	VAL	2.4
1	А	74	GLN	2.4
1	А	721	ALA	2.4
1	А	748	THR	2.3
1	А	59	LYS	2.3
1	А	798	ARG	2.3
1	А	756	GLU	2.2
1	А	738	GLU	2.2
1	А	750	ALA	2.2
1	А	709	TYR	2.2
1	А	768	TYR	2.2
1	А	355	TRP	2.2
1	А	795	GLU	2.2
1	А	65	GLU	2.2
1	A	111	ALA	2.1
1	A	763	LEU	2.1
2	G	16	ALA	2.1
1	A	109	GLN	2.0
1	A	387	GLN	2.0
1	A	407	THR	2.0

#### Continued from previous page...

#### 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,  $95^{th}$  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	${f B}$ -factors( ${f A}^2$ )	Q<0.9
3	SO4	А	914	5/5	0.44	0.37	176,233,261,263	0
3	SO4	А	904	5/5	0.45	0.27	$168,\!186,\!196,\!207$	0
3	SO4	А	901	5/5	0.56	0.26	$169,\!175,\!181,\!182$	0
3	SO4	А	911	5/5	0.61	0.50	137,147,176,193	0
3	SO4	А	909	5/5	0.68	0.31	$143,\!146,\!155,\!175$	0
3	SO4	A	912	5/5	0.68	0.46	$143,\!148,\!151,\!156$	0
3	SO4	А	905	5/5	0.72	0.35	132,134,138,158	0
3	SO4	А	907	5/5	0.74	0.23	185,188,218,222	0
3	SO4	А	903	5/5	0.74	0.22	165,172,182,183	0
3	SO4	А	910	5/5	0.76	0.34	174,178,189,217	0
3	SO4	А	908	5/5	0.77	0.44	117,119,131,153	0
3	SO4	А	902	5/5	0.78	0.24	$126,\!135,\!138,\!162$	0
3	SO4	A	913	5/5	0.79	0.43	107,134,158,174	0
3	SO4	A	906	5/5	0.86	0.40	102,120,147,200	0

### 6.5 Other polymers (i)

There are no such residues in this entry.



