

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

#### Aug 16, 2023 – 10:10 AM EDT

PDB ID	:	1ZRO
Title	:	Crystal structure of EBA-175 Region II (RII) crystallized in the presence of (
		alpha)2,3-sialyllactose
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Deposited on	:	2005-05-19
Resolution	:	2.25  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.35
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35
	:::::::::::::::::::::::::::::::::::::::

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.25 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 >=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	602	89%	9%	·		
1	В	602	89%	8%	·		



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10862 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	599	Total	С	Ν	0	$\mathbf{S}$	0	22	0
I A	000	5069	3210	877	944	38	0	22		
1	Р	599	Total	С	Ν	0	S	0	22	0
I D	500	5069	3210	877	944	38	0		0	

• Molecule 1 is a protein called erythrocyte binding antigen region II.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	3	GLN	ASN	engineered mutation	UNP Q25735
А	50	ALA	SER	engineered mutation	UNP Q25735
А	195	ALA	SER	engineered mutation	UNP Q25735
А	206	ALA	THR	engineered mutation	UNP Q25735
В	3	GLN	ASN	engineered mutation	UNP Q25735
В	50	ALA	SER	engineered mutation	UNP Q25735
В	195	ALA	SER	engineered mutation	UNP Q25735
В	206	ALA	THR	engineered mutation	UNP Q25735

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).







Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	Total         O         S           10         8         2	0	1
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	Total         O         S           10         8         2	0	1
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	Total         O         S           10         8         2	0	1
2	В	1	Total         O         S           10         8         2	0	1
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	Total         O         S           10         8         2	0	1
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total         O         S           10         8         2	0	1
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Cl 2 2	0	0
3	В	2	Total Cl 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	301	Total O 307 307	0	6
4	В	298	Total O 303 303	0	5



# 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: erythrocyte binding antigen region II





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	145.75Å 146.21Å 214.74Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.62 - 2.25	Depositor
Resolution (A)	46.22 - 2.25	EDS
% Data completeness	95.5 (47.62-2.25)	Depositor
(in resolution range)	94.7(46.22-2.25)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.81 (at 2.24 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.216 , $0.232$	Depositor
$\Pi, \Pi_{free}$	0.233 , $0.244$	DCC
$R_{free}$ test set	5468 reflections $(5.05\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $28.5$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.460 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10862	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% 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>&</sup>lt;sup>1</sup>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: CL,  $\mathrm{SO4}$ 

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).

Mol	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.50	0/5270	0.57	0/7058	
1	В	0.50	0/5270	0.56	0/7058	
All	All	0.50	0/10540	0.57	0/14116	

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	5069	0	4993	27	0
1	В	5069	0	4993	25	0
2	А	55	0	0	0	0
2	В	55	0	0	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
4	А	307	0	0	3	0
4	В	303	0	0	2	0
All	All	10862	0	9986	44	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 2.



A + a 1	A + ama 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:31[C]:ARG:NH2	1:B:415[C]:TYR:CE2	2.33	0.95
1:A:415[C]:TYR:CE2	1:B:31[C]:ARG:NH2	2.35	0.93
1:A:31[C]:ARG:NH2	1:B:415[C]:TYR:HE2	1.80	0.78
1:A:415[C]:TYR:HE2	1:B:31[C]:ARG:NH2	1.82	0.77
1:B:216:ILE:O	1:B:220:MET:HG2	2.08	0.55
1:B:467:ASP:HB3	1:B:470:VAL:HG23	1.89	0.54
1:A:31[C]:ARG:CZ	1:B:415[C]:TYR:CE2	2.91	0.53
1:B:49:LEU:HD12	1:B:63:HIS:HB3	1.90	0.53
1:A:467:ASP:HB3	1:A:470:VAL:HG23	1.90	0.52
1:A:49:LEU:HD12	1:A:63:HIS:HB3	1.92	0.52
1:A:216:ILE:O	1:A:220:MET:HG2	2.09	0.52
1:B:337:LYS:CE	4:B:842:HOH:O	2.58	0.51
1:A:415[C]:TYR:CE2	1:B:31[C]:ARG:CZ	2.92	0.51
1:B:210:ALA:HA	1:B:215:CYS:SG	2.54	0.48
1:A:102:ALA:O	1:A:140:ARG:HD2	2.14	0.47
1:B:102:ALA:O	1:B:140:ARG:HD2	2.14	0.47
1:A:29[B]:ASN:OD1	1:A:31[B]:ARG:HB2	2.14	0.47
1:A:494:CYS:SG	1:A:577:LEU:HD22	2.55	0.47
1:A:210:ALA:HA	1:A:215:CYS:SG	2.56	0.46
1:B:297:ASN:ND2	1:B:299:ASN:OD1	2.48	0.46
1:B:494:CYS:SG	1:B:577:LEU:HD22	2.56	0.46
1:B:328:LYS:HG3	1:B:351:GLU:HG3	1.98	0.46
1:A:337:LYS:CE	4:A:810:HOH:O	2.64	0.46
1:A:297:ASN:ND2	1:A:299:ASN:OD1	2.49	0.45
1:B:29[A]:ASN:OD1	1:B:31[A]:ARG:HB2	2.16	0.45
1:A:29[A]:ASN:OD1	1:A:31[A]:ARG:HB2	2.16	0.44
1:A:401:LYS:NZ	4:A:956:HOH:O	2.49	0.44
1:A:133:GLU:HG3	4:A:808:HOH:O	2.17	0.44
1:A:242:THR:HG23	1:B:549:GLY:HA2	2.00	0.43
1:A:328:LYS:HG3	1:A:351:GLU:HG3	2.00	0.43
1:A:556:SER:HA	1:A:559:LYS:HD3	2.00	0.43
1:B:48:ASN:HB2	1:B:52:ILE:HD12	1.99	0.43
1:B:556:SER:HA	1:B:559:LYS:HD3	2.01	0.43
1:A:48:ASN:HB2	1:A:52:ILE:HD12	2.00	0.43
1:B:29[B]:ASN:OD1	1:B:31[B]:ARG:HB2	2.18	0.43
1:B:245:VAL:HB	1:B:246:PRO:CD	2.50	0.42
1:A:245:VAL:HB	1:A:246:PRO:CD	2.50	0.42
1:A:538:LYS:NZ	1:A:542[A]:GLN:NE2	2.67	0.42
1:B:538:LYS:NZ	1:B:542[A]:GLN:NE2	2.67	0.42
1:B:49:LEU:O	1:B:119:LYS:HD2	2.21	0.41

All (44) 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:49:LEU:O	1:A:119:LYS:HD2	2.21	0.41
1:A:549:GLY:HA2	1:B:242:THR:HG23	2.02	0.41
1:B:337:LYS:HE2	4:B:842:HOH:O	2.21	0.41
1:A:529:ILE:HD12	1:A:588:HIS:CE1	2.56	0.41

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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	Perce	entiles
1	А	606/602~(101%)	585~(96%)	17 (3%)	4 (1%)	22	21
1	В	606/602~(101%)	586 (97%)	16 (3%)	4 (1%)	22	21
All	All	1212/1204~(101%)	1171 (97%)	33 (3%)	8 (1%)	22	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	167	LYS
1	А	599	PRO
1	В	167	LYS
1	В	599	PRO
1	А	517	ASN
1	В	517	ASN
1	А	161	ASN
1	В	161	ASN

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed Rotameric Outliers		Percentiles		
1	А	580/569~(102%)	560~(97%)	20 (3%)	37 45	
1	В	580/569~(102%)	560~(97%)	20 (3%)	37 45	
All	All	1160/1138~(102%)	1120 (97%)	40 (3%)	37 45	

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	18	ARG
1	А	24	ASP
1	А	49	LEU
1	А	133	GLU
1	А	166	CYS
1	А	220	MET
1	А	241	GLU
1	А	261	LYS
1	А	327	THR
1	А	338	LEU
1	А	340[A]	THR
1	А	340[B]	THR
1	А	393	LYS
1	А	444	LEU
1	А	455	LYS
1	А	463	TRP
1	А	466	LYS
1	А	469	THR
1	А	513	CYS
1	А	598	CYS
1	В	18	ARG
1	В	24	ASP
1	В	49	LEU
1	В	133	GLU
1	В	166	CYS
1	В	220	MET
1	В	241	GLU
1	В	261	LYS
1	В	327	THR
1	В	338	LEU
1	В	340[A]	THR
1	В	340[B]	THR
1	В	393	LYS



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Mol	Chain	Res	Type
1	В	444	LEU
1	В	455	LYS
1	В	463	TRP
1	В	466	LYS
1	В	469	THR
1	В	513	CYS
1	В	598	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	73	GLN
1	А	105	ASN
1	А	162	ASN
1	А	249	ASN
1	А	271	ASN
1	В	73	GLN
1	В	105	ASN
1	В	162	ASN
1	В	249	ASN
1	В	271	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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).

Mal	Turne	Chain	Dec	Tink	B	Bond lengths		Bond angles		
	Type	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	А	707[A]	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	В	717[B]	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	А	708	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	В	713	-	4,4,4	0.24	0	$6,\!6,\!6$	0.28	0
2	SO4	В	715[A]	-	4,4,4	0.12	0	6,6,6	0.20	0
2	SO4	А	707[B]	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	А	711[A]	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	В	701[A]	-	4,4,4	0.16	0	6,6,6	0.29	0
2	SO4	В	718	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	А	703	-	4,4,4	0.22	0	6,6,6	0.30	0
2	SO4	В	715[B]	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	А	705[A]	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	В	716	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	А	711[B]	-	4,4,4	0.12	0	$6,\!6,\!6$	0.19	0
2	SO4	В	701[B]	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	А	705[B]	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	В	714	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	В	717[A]	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	А	702	-	4,4,4	0.23	0	$6,\!6,\!6$	0.28	0
2	SO4	A	704	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	В	712	-	4,4,4	0.24	0	6,6,6	0.32	0
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.16	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.

No monomer is involved in short contacts.



## 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	$OWAB(Å^2)$	Q<0.9
1	А	588/602~(97%)	0.55	27 (4%) 32 35	36, 52, 80, 103	0
1	В	588/602~(97%)	0.55	30 (5%) 28 30	36, 52, 80, 103	0
All	All	1176/1204~(97%)	0.55	57 (4%) 30 33	36, 52, 80, 103	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	245	VAL	7.7
1	А	259	GLU	6.0
1	В	245	VAL	5.8
1	А	516	ASP	5.5
1	В	516	ASP	5.5
1	В	259	GLU	4.9
1	В	167	LYS	3.8
1	А	597	MET	3.7
1	А	167	LYS	3.6
1	А	261	LYS	3.6
1	А	599	PRO	3.5
1	В	597	MET	3.2
1	В	520	ARG	3.1
1	В	268	LEU	2.9
1	А	600	GLU	2.8
1	В	601	VAL	2.8
1	В	261	LYS	2.8
1	В	599	PRO	2.7
1	А	153	GLU	2.7
1	A	192	ASP	2.7
1	A	520	ARG	2.6
1	В	519	LYS	2.6
1	В	160	LYS	2.6
1	А	545[A]	GLU	2.5



Mol	Chain	Res	Type	RSRZ	
1	А	502	GLU	2.5	
1	В	327	THR	2.5	
1	А	256	LYS	2.5	
1	А	590	ASP	2.4	
1	В	166	CYS	2.4	
1	В	600	GLU	2.4	
1	А	82	LYS	2.4	
1	А	327	THR	2.4	
1	А	601	VAL	2.4	
1	А	474	ASP	2.4	
1	В	73	GLN	2.4	
1	В	474	ASP	2.3	
1	В	502	GLU	2.3	
1	В	153	GLU	2.3	
1	В	548	LYS	2.3	
1	А	514	GLU	2.3	
1	В	594	LYS	2.2	
1	В	514	GLU	2.2	
1	В	545[A]	GLU	2.2	
1	В	550[A]	ASN	2.2	
1	А	280	TYR	2.2	
1	А	247	LYS	2.2	
1	В	469	THR	2.1	
1	A	73	GLN	2.1	
1	В	86	LYS	2.1	
1	В	517	ASN	2.1	
1	A	258	SER	2.1	
1	А	8	ASN	2.1	
1	В	158	GLU	2.0	
1	В	82	LYS	2.0	
1	A	268	LEU	2.0	
1	В	260	ASN	2.0	
1	А	519	LYS	2.0	

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### 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	$B-factors(Å^2)$	Q<0.9
3	CL	В	720	1/1	0.75	0.18	85,85,85,85	0
3	CL	А	710	1/1	0.85	0.10	85,85,85,85	0
2	SO4	А	708	5/5	0.87	0.18	101,101,101,102	0
2	SO4	В	718	5/5	0.88	0.15	101,101,101,102	0
2	SO4	В	716	5/5	0.91	0.12	88,89,90,91	0
2	SO4	А	706	5/5	0.91	0.13	88,89,90,91	0
3	CL	В	719	1/1	0.93	0.10	75,75,75,75	0
2	SO4	А	707[A]	5/5	0.95	0.12	84,84,84,85	5
2	SO4	А	707[B]	5/5	0.95	0.12	100,100,100,100	5
2	SO4	В	717[A]	5/5	0.95	0.13	84,84,84,85	5
2	SO4	В	717[B]	5/5	0.95	0.13	100,100,100,100	5
2	SO4	В	715[B]	5/5	0.96	0.18	83,83,84,84	5
2	SO4	А	703	5/5	0.96	0.11	65,66,67,67	0
2	SO4	В	713	5/5	0.96	0.09	65,66,67,67	0
2	SO4	В	715[A]	5/5	0.96	0.18	63,64,64,64	5
3	CL	А	709	1/1	0.97	0.10	75,75,75,75	0
2	SO4	В	712	5/5	0.98	0.12	47,47,50,52	0
2	SO4	А	705[A]	5/5	0.98	0.16	63,64,64,64	5
2	SO4	А	705[B]	5/5	0.98	0.16	83,83,84,84	5
2	SO4	А	702	5/5	0.98	0.12	46,47,50,51	0
2	SO4	А	711[A]	5/5	0.99	0.14	47,47,48,48	5
2	SO4	В	714	5/5	0.99	0.12	$63,\!65,\!65,\!65$	0
2	SO4	А	711[B]	5/5	0.99	0.14	43,43,44,44	5
2	SO4	В	701[A]	5/5	0.99	0.16	47,47,48,49	5
2	SO4	В	701[B]	5/5	0.99	0.16	43,43,44,44	5
2	SO4	А	704	5/5	0.99	0.11	63,65,65,65	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

