

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

#### Jan 20, 2024 - 01:31 pm GMT

PDB ID	:	7NIT
Title	:	X-ray structure of a multidomain BbgIII from Bifidobacterium bifidum
Authors	:	Moroz, O.V.; Blagova, E.; Lebedev, A.A.; Sanchez Rodriguez, F.; Rigden,
		D.J.; Tams, J.W.; Wilting, R.; Vester, J.K.; Longhin, E.; Krogh, K.B.R.;
		Pache, R.A.; Davies, G.J.; Wilson, K.S.
Deposited on	:	2021-02-14
Resolution	:	2.89 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* 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 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 2.89 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${igsimular resolution} \ (\# { m Entries, resolution range}({ m \AA}))$		
R <sub>free</sub>	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 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		
			6%		
1	А	1304	84%	10%	• 5%
			7%		
1	В	1304	82%	12%	• 5%
			9%		
1	С	1304	83%	11%	• 5%
			8%		
1	D	1304	84%	11%	• •
			20%		
1	Ε	1304	83%	11%	• 5%



Continued from previous page...

Mol	Chain	Length	Quality of chain		
			27%		
1	F	1304	83%	11%	• 5%

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	GOL	В	2302	-	-	Х	-
3	GOL	F	2302	-	-	Х	-



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 55867 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		Α	toms			ZeroOcc	AltConf	Trace
1	Δ	1930	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	Л	1239	9306	5807	1585	1897	17	0	0	0
1	В	1935	Total	С	Ν	Ο	S	0	0	0
	D	1235	9246	5768	1574	1888	16	0	0	U
1	С	19/3	Total	С	Ν	Ο	S	0	0	0
	U	1240	9326	5818	1585	1906	17	0	0	0
1	Л	1953	Total	С	Ν	Ο	S	0	0	0
	D	1200	9390	5856	1601	1916	17	0	0	0
1	F	1935	Total	С	Ν	Ο	S	0	0	0
	Ľ	1235	9195	5733	1567	1879	16	0	0	0
1	Б	1944	Total	С	Ν	Ο	S	0	0	0
	Г	1244	9324	5816	1586	1905	17		0	0

• Molecule 1 is a protein called Beta-galactosidase.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1165	GLU	ASP	conflict	UNP A0A415C3Q2
В	1165	GLU	ASP	conflict	UNP A0A415C3Q2
С	1165	GLU	ASP	conflict	UNP A0A415C3Q2
D	1165	GLU	ASP	conflict	UNP A0A415C3Q2
Е	1165	GLU	ASP	conflict	UNP A0A415C3Q2
F	1165	GLU	ASP	conflict	UNP A0A415C3Q2

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	F	1	$\begin{array}{c cc} Total & C & O \\ \hline 6 & 3 & 3 \end{array}$	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0
4	С	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	Ε	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total O 1 1	0	0
5	В	1	Total O 1 1	0	0
5	С	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	Total O 1 1	0	0
5	F	1	Total O 1 1	0	0



## 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: Beta-galactosidase











L102 K106 R106 R106 R110 C113 C113 C113 C113 C114 C114 C126 C128 C128 C128 C128 C133 C133 C133 C133 C133 C133 C133 C13	N205
M208 M208 M219 K213 K214 K213 K215 K227 K228 K228 K228 K228 K228 K228 K228	E317 K318
N319           V324           V324           V324           V324           V324           V325           V326           V336           V336           V361           V362           V361           V362	W421
T429           T429           T429           T440           M441           M441           M442           M443           E440           M443           E445           E445           E445           E455           E456           F455           F456           F526           F526           F526           F526           F526           F526           F526	G550
L558 T559 T559 T559 T559 C667 W577 W577 W566 W568 W566 W568 W568 W581 F584 F584 F594 F594 F594 F594 F594 F594 F594 F59	L652 P653 A654
W655           V660           V665           V665           V665           V665           V665           V665           V665           K661           K662           K663           K664           K665           K665           K667           K673           K674           K673           K679           K681           K682           K683           K684           K689           K689           K681           K682           K683           K684           K684           K691           K692           K693           K701           K701           K701           K702           K703           K704	A735 E736 G737
T738           1739           1739           1739           1739           1739           1745           1746           1746           1746           1746           1746           1761           1765           1766           1774           1773           1774           1773           1790           1790           1790           1790           1790           1800	K 839 G 843
K844 K844 L845 L845 L845 K853 F855 K853 F855 K853 K863 A865 A865 A865 A865 A865 A865 A865 A865	Y915 S916
1932           1932           1933           1933           1933           1935           1935           1935           1935           1935           1935           1935           1935           1935           1935           1935           1935           1935           1945           1945           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1955           1956           1955           1956           1957           1958           1956           1957           1958           1958           1958           1958           1958           1958           1958	A996 N997 F998
A999 A1000 D1000 V1000 V1000 V1000 V1000 V1000 V1016 V1016 V1016 V1016 V1016 V1016 P1009 P1019 P1028 P1028 P1028 P1028 P1028 P1028 P1028 P1028 P1038 P1008 P1008 P1008 P1008 P1008 P1008 P1008 P1008 P1008 P1008 P1008 P	E1105
Billis           Cillis           Ci	LEU THR VAL
LU ASN REG GLY VAL SER VAL SER ASP VAL VAL VAL VAL ASP ASP ASP ASP ASP ASP ASP VAL ANA ASP ASP ASP ASP ASP VAL ANA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	ASP SER ASP



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	116.95Å 130.04Å 200.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$86.99^{\circ}$ $84.83^{\circ}$ $83.79^{\circ}$	Depositor
$Bosolution(\AA)$	199.58 - 2.89	Depositor
Resolution (A)	199.58 - 2.89	EDS
% Data completeness	96.2 (199.58-2.89)	Depositor
(in resolution range)	96.2(199.58-2.89)	EDS
$R_{merge}$	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.13 (at 2.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.214 , $0.247$	Depositor
$n, n_{free}$	0.214 , $0.247$	DCC
$R_{free}$ test set	12571  reflections  (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	88.8	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 69.6	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	55867	wwPDB-VP
Average B, all atoms $(Å^2)$	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.81% 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: GOL, SO4, CA

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	0.36	0/9503	0.71	0/12962
1	В	0.39	0/9443	0.73	0/12889
1	С	0.37	0/9523	0.71	0/12990
1	D	0.36	0/9589	0.71	0/13082
1	Е	0.36	0/9390	0.70	0/12825
1	F	0.33	0/9521	0.68	0/12990
All	All	0.36	0/56969	0.70	0/77738

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	9306	0	8880	70	0
1	В	9246	0	8784	92	0
1	С	9326	0	8895	93	0
1	D	9390	0	8946	82	0
1	Е	9195	0	8696	73	0
1	F	9324	0	8877	74	0
2	А	5	0	0	0	0



(NIT
------

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	А	12	0	16	0	0
3	В	6	0	8	5	0
3	С	6	0	8	0	0
3	D	12	0	16	0	0
3	Ε	6	0	8	1	0
3	F	6	0	8	9	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
4	Ε	1	0	0	0	0
4	F	1	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
5	Е	1	0	0	0	0
5	F	1	0	0	0	0
All	All	55867	0	53142	474	0

Continued from previous page...

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 474 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:F:879:VAL:HB	1:F:882:THR:HG23	1.33	1.06
1:C:1023:THR:HG22	1:C:1028:GLU:HG3	1.52	0.91
1:C:959:ILE:HG21	1:C:962:ILE:HD11	1.59	0.85
1:B:1014:GLY:O	1:B:1037:VAL:HG22	1.79	0.82
1:E:1155:THR:HG22	1:F:704:THR:HA	1.65	0.79

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	ntiles
1	А	1233/1304~(95%)	1180 (96%)	52 (4%)	1 (0%)	51	82
1	В	1229/1304~(94%)	1180 (96%)	47 (4%)	2(0%)	47	78
1	С	1237/1304~(95%)	1186 (96%)	50 (4%)	1 (0%)	51	82
1	D	1249/1304~(96%)	1193 (96%)	53~(4%)	3~(0%)	47	78
1	Е	1229/1304~(94%)	1179 (96%)	46 (4%)	4 (0%)	41	71
1	F	1238/1304~(95%)	1186 (96%)	49 (4%)	3~(0%)	47	78
All	All	7415/7824~(95%)	7104 (96%)	297 (4%)	14 (0%)	47	78

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1267	HIS
1	F	9	SER
1	В	663	GLY
1	D	1270	VAL
1	Е	663	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	Perce	ntiles
1	А	982/1056~(93%)	938~(96%)	44 (4%)	27	61
1	В	972/1056~(92%)	927~(95%)	45 (5%)	27	60
1	С	986/1056~(93%)	943 (96%)	43 (4%)	28	61



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	989/1056~(94%)	944~(95%)	45~(5%)	27	60
1	Ε	960/1056~(91%)	911 (95%)	49 (5%)	24	56
1	F	983/1056~(93%)	936~(95%)	47 (5%)	25	58
All	All	5872/6336~(93%)	5599~(95%)	273 (5%)	27	60

Continued from previous page...

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	F	100	ARG
1	F	297	THR
1	F	971	SER
1	С	237	THR
1	С	185	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	896	ASN
1	С	896	ASN
1	Е	327	HIS
1	Е	711	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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.



 $7\mathrm{NIT}$ 

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	Tiple	B	ond leng	$\operatorname{gths}$	E	Bond ang	gles
	ivioi Type Cham	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
3	GOL	F	2302	-	$5,\!5,\!5$	0.08	0	$5,\!5,\!5$	0.43	0
3	GOL	А	2303	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.61	0
3	GOL	В	2302	-	$5,\!5,\!5$	0.17	0	$5,\!5,\!5$	0.53	0
2	SO4	С	2301	-	4,4,4	0.35	0	$6,\!6,\!6$	0.13	0
3	GOL	Е	2302	-	$5,\!5,\!5$	0.23	0	$5,\!5,\!5$	0.38	0
3	GOL	D	2303	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.60	0
2	SO4	А	2301	-	4,4,4	0.17	0	$6,\!6,\!6$	0.31	0
3	GOL	С	2302	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.46	0
3	GOL	D	2302	-	$5,\!5,\!5$	0.15	0	$5,\!5,\!5$	0.48	0
2	SO4	F	2301	-	4,4,4	0.32	0	$6,\!6,\!6$	0.07	0
2	SO4	D	2301	-	4,4,4	0.33	0	6,6,6	0.23	0
3	GOL	А	2302	-	$5,\!5,\!5$	0.18	0	$5,\!5,\!5$	0.59	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	GOL	F	2302	-	-	0/4/4/4	-
3	GOL	А	2303	-	-	2/4/4/4	-
3	GOL	В	2302	-	-	0/4/4/4	-
3	GOL	Е	2302	-	-	2/4/4/4	-
3	GOL	D	2303	-	-	0/4/4/4	-
3	GOL	С	2302	-	-	2/4/4/4	-
3	GOL	D	2302	-	-	0/4/4/4	-
3	GOL	А	2302	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	А	2302	GOL	C1-C2-C3-O3
3	А	2303	GOL	C1-C2-C3-O3
3	А	2303	GOL	O2-C2-C3-O3
3	А	2302	GOL	O1-C1-C2-C3
3	С	2302	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2302	GOL	9	0
3	В	2302	GOL	5	0
3	Е	2302	GOL	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	< <b>RSRZ</b> >	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	1239/1304~(95%)	0.67	73 (5%) 22	18	55, 88, 167, 221	0
1	В	1235/1304~(94%)	0.80	96 (7%) 13	10	48, 84, 169, 243	0
1	С	1243/1304~(95%)	0.79	117 (9%) 8	6	59, 96, 188, 248	0
1	D	1253/1304~(96%)	0.68	98 (7%) 13	10	57, 98, 155, 227	0
1	Е	1235/1304 (94%)	1.31	257 (20%) 1	. 0	59, 106, 248, 332	0
1	F	1244/1304~(95%)	1.43	356 (28%) 0	0	80, 148, 219, 297	0
All	All	7449/7824~(95%)	0.95	997 (13%) 3	2	48, 102, 203, 332	0

The worst 5 of 997 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	1191	THR	12.6
1	F	1029	PHE	12.3
1	F	998	PHE	12.2
1	F	1024	VAL	12.0
1	Е	1094	TRP	11.9

### 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,  $95^{th}$  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
2	SO4	F	2301	5/5	0.71	0.25	174,178,185,188	0
3	GOL	А	2303	6/6	0.78	0.26	76,103,120,133	0
4	CA	Е	2304	1/1	0.83	0.10	279,279,279,279	0
3	GOL	D	2303	6/6	0.85	0.20	92,111,124,130	0
3	GOL	F	2302	6/6	0.86	0.27	106,134,150,151	0
4	CA	F	2304	1/1	0.87	0.09	216,216,216,216	0
3	GOL	Е	2302	6/6	0.88	0.40	77,100,124,196	0
4	CA	А	2304	1/1	0.91	0.08	116,116,116,116	0
3	GOL	А	2302	6/6	0.92	0.38	48,76,85,93	0
4	CA	В	2304	1/1	0.92	0.10	140,140,140,140	0
3	GOL	В	2302	6/6	0.92	0.19	71,72,77,89	0
3	GOL	D	2302	6/6	0.92	0.37	86,92,100,104	0
4	CA	D	2304	1/1	0.94	0.06	146,146,146,146	0
3	GOL	С	2302	6/6	0.95	0.29	63,76,85,99	0
2	SO4	D	2301	5/5	0.97	0.21	78,107,131,132	0
2	SO4	С	2301	5/5	0.98	0.22	81,93,105,108	0
2	SO4	А	2301	5/5	0.98	0.25	54,72,83,111	0
4	CA	С	2304	1/1	0.99	0.04	138,138,138,138	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

