

Full wwPDB X-ray Structure Validation Report (i)

Jan 18, 2023 - 12:32 pm GMT

PDB ID	:	8BCQ
Title	:	N-terminal domain of Plasmodium berghei glutamyl-tRNA synthetase (native
		crystal structure)
Authors	:	Benas, P.; Jaramillo Ponce, J.R.; Frugier, M.; Sauter, C.
Deposited on	:	2022-10-17
Resolution	:	2.70 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

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 2.70 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	2808 (2.70-2.70)	
Clashscore	141614	3122 (2.70-2.70)	
Ramachandran outliers	138981	3069 (2.70-2.70)	
Sidechain outliers	138945	3069 (2.70-2.70)	
RSRZ outliers	127900	2737 (2.70-2.70)	

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					
			2%					
1	А	249	7	0%	9%	21%		
			6%					
1	В	249	7	0%	12%	18%		
			12%					
1	С	249	65%	5	13% •	20%		
			25%					
1	D	249	66%	6	12%	21%		
			26%					
1	Ε	249	61%	1	.4% •	23%		



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	А	306	-	-	-	Х
3	GOL	С	303	-	-	-	Х
3	GOL	С	304	-	-	-	Х



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8603 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		Ate	oms		ZeroOcc	AltConf	Trace	
1	1 1	107	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	A	197	1687	1104	279	300	4	0	0	0
1	В	203	Total	С	Ν	Ο	S	0	0	0
1	D	203	1738	1134	290	310	4		0	0
1	С	198	Total	С	Ν	Ο	S	0	0	0
1			1699	1111	284	300	4	0	0	0
1	Л	106	Total	С	Ν	Ο	S	0	0	0
1	D	190	1680	1101	277	298	4	0	0	0
1	F	101	Total	С	Ν	Ο	S	0	0	0
	Ľ	191	1629	1068	268	289	4	0	U	0

• Molecule 1 is a protein called Glutamate–tRNA ligase.

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP A0A509AR09
А	2	GLY	-	expression tag	UNP A0A509AR09
А	228	ILE	-	expression tag	UNP A0A509AR09
А	229	PHE	-	expression tag	UNP A0A509AR09
А	230	ILE	-	expression tag	UNP A0A509AR09
А	231	ASP	-	expression tag	UNP A0A509AR09
А	232	GLY	-	expression tag	UNP A0A509AR09
А	233	GLY	-	expression tag	UNP A0A509AR09
А	234	SER	-	expression tag	UNP A0A509AR09
А	235	SER	-	expression tag	UNP A0A509AR09
А	236	GLY	-	expression tag	UNP A0A509AR09
А	237	LEU	-	expression tag	UNP A0A509AR09
А	238	VAL	-	expression tag	UNP A0A509AR09
А	239	PRO	-	expression tag	UNP A0A509AR09
А	240	ARG	-	expression tag	UNP A0A509AR09
А	241	GLY	-	expression tag	UNP A0A509AR09
A	242	SER	-	expression tag	UNP A0A509AR09
A	243	SER	-	expression tag	UNP A0A509AR09
А	244	HIS	-	expression tag	UNP A0A509AR09



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Chain	Residue	Modelled	Actual	Comment	Reference
А	245	HIS	-	expression tag	UNP A0A509AR09
А	246	HIS	-	expression tag	UNP A0A509AR09
А	247	HIS	-	expression tag	UNP A0A509AR09
А	248	HIS	-	expression tag	UNP A0A509AR09
А	249	HIS	-	expression tag	UNP A0A509AR09
В	1	MET	-	initiating methionine	UNP A0A509AR09
В	2	GLY	_	expression tag	UNP A0A509AR09
В	228	ILE	-	expression tag	UNP A0A509AR09
В	229	PHE	-	expression tag	UNP A0A509AR09
В	230	ILE	-	expression tag	UNP A0A509AR09
В	231	ASP	-	expression tag	UNP A0A509AR09
В	232	GLY	-	expression tag	UNP A0A509AR09
В	233	GLY	-	expression tag	UNP A0A509AR09
В	234	SER	-	expression tag	UNP A0A509AR09
В	235	SER	-	expression tag	UNP A0A509AR09
В	236	GLY	-	expression tag	UNP A0A509AR09
В	237	LEU	-	expression tag	UNP A0A509AR09
В	238	VAL	-	expression tag	UNP A0A509AR09
В	239	PRO	-	expression tag	UNP A0A509AR09
В	240	ARG	-	expression tag	UNP A0A509AR09
В	241	GLY	-	expression tag	UNP A0A509AR09
В	242	SER	-	expression tag	UNP A0A509AR09
В	243	SER	-	expression tag	UNP A0A509AR09
В	244	HIS	-	expression tag	UNP A0A509AR09
В	245	HIS	-	expression tag	UNP A0A509AR09
В	246	HIS	-	expression tag	UNP A0A509AR09
В	247	HIS	-	expression tag	UNP A0A509AR09
В	248	HIS	-	expression tag	UNP A0A509AR09
В	249	HIS	-	expression tag	UNP A0A509AR09
С	1	MET	-	initiating methionine	UNP A0A509AR09
С	2	GLY	-	expression tag	UNP A0A509AR09
С	228	ILE	-	expression tag	UNP A0A509AR09
С	229	PHE	-	expression tag	UNP A0A509AR09
С	230	ILE	-	expression tag	UNP A0A509AR09
С	231	ASP	-	expression tag	UNP A0A509AR09
C	232	GLY	_	expression tag	UNP A0A509AR09
C	233	GLY	_	expression tag	UNP A0A509AR09
С	234	SER	-	expression tag	UNP A0A509AR09
C	235	SER	_	expression tag	UNP A0A509AR09
С	236	GLY	-	expression tag	UNP A0A509AR09
C	237	LEU	_	expression tag	UNP A0A509AR09
С	238	VAL	-	expression tag	UNP A0A509AR09



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Chain	Residue	Modelled	Actual	Comment	Reference
С	239	PRO	-	expression tag	UNP A0A509AR09
C	240	ARG	_	expression tag	UNP A0A509AR09
С	241	GLY	_	expression tag	UNP A0A509AR09
С	242	SER	_	expression tag	UNP A0A509AR09
С	243	SER	-	expression tag	UNP A0A509AR09
С	244	HIS	-	expression tag	UNP A0A509AR09
С	245	HIS	-	expression tag	UNP A0A509AR09
С	246	HIS	-	expression tag	UNP A0A509AR09
С	247	HIS	-	expression tag	UNP A0A509AR09
С	248	HIS	-	expression tag	UNP A0A509AR09
С	249	HIS	-	expression tag	UNP A0A509AR09
D	1	MET	-	initiating methionine	UNP A0A509AR09
D	2	GLY	-	expression tag	UNP A0A509AR09
D	228	ILE	-	expression tag	UNP A0A509AR09
D	229	PHE	-	expression tag	UNP A0A509AR09
D	230	ILE	-	expression tag	UNP A0A509AR09
D	231	ASP	-	expression tag	UNP A0A509AR09
D	232	GLY	-	expression tag	UNP A0A509AR09
D	233	GLY	-	expression tag	UNP A0A509AR09
D	234	SER	-	expression tag	UNP A0A509AR09
D	235	SER	-	expression tag	UNP A0A509AR09
D	236	GLY	-	expression tag	UNP A0A509AR09
D	237	LEU	-	expression tag	UNP A0A509AR09
D	238	VAL	-	expression tag	UNP A0A509AR09
D	239	PRO	-	expression tag	UNP A0A509AR09
D	240	ARG	-	expression tag	UNP A0A509AR09
D	241	GLY	-	expression tag	UNP A0A509AR09
D	242	SER	-	expression tag	UNP A0A509AR09
D	243	SER	-	expression tag	UNP A0A509AR09
D	244	HIS	-	expression tag	UNP A0A509AR09
D	245	HIS	-	expression tag	UNP A0A509AR09
D	246	HIS	-	expression tag	UNP A0A509AR09
D	247	HIS	-	expression tag	UNP A0A509AR09
D	248	HIS	-	expression tag	UNP A0A509AR09
D	249	HIS	-	expression tag	UNP A0A509AR09
Е	1	MET	-	initiating methionine	UNP A0A509AR09
E	2	GLY	-	expression tag	UNP A0A509AR09
E	228	ILE	-	expression tag	UNP A0A509AR09
E	229	PHE	-	expression tag	UNP A0A509AR09
E	230	ILE	-	expression tag	UNP A0A509AR09
E	231	ASP	-	expression tag	UNP A0A509AR09
Е	232	GLY	-	expression tag	UNP A0A509AR09



Chain	Residue	Modelled	Actual	Comment	Reference
Е	233	GLY	-	expression tag	UNP A0A509AR09
Е	234	SER	-	expression tag	UNP A0A509AR09
Е	235	SER	-	expression tag	UNP A0A509AR09
Е	236	GLY	-	expression tag	UNP A0A509AR09
E	237	LEU	-	expression tag	UNP A0A509AR09
E	238	VAL	-	expression tag	UNP A0A509AR09
Е	239	PRO	-	expression tag	UNP A0A509AR09
E	240	ARG	-	expression tag	UNP A0A509AR09
E	241	GLY	-	expression tag	UNP A0A509AR09
E	242	SER	-	expression tag	UNP A0A509AR09
Е	243	SER	-	expression tag	UNP A0A509AR09
Е	244	HIS	-	expression tag	UNP A0A509AR09
E	245	HIS	-	expression tag	UNP A0A509AR09
Е	246	HIS	-	expression tag	UNP A0A509AR09
E	247	HIS	-	expression tag	UNP A0A509AR09
E	248	HIS	-	expression tag	UNP A0A509AR09
Е	249	HIS	-	expression tag	UNP A0A509AR09

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{c cc} Total & O & S \\ 5 & 4 & 1 \end{array}$	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



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

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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	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	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



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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	В	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	В	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	В	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	С	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	$\begin{array}{c cc} Total & C & O \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	10	Total O 10 10	0	0
4	В	4	Total O 4 4	0	0
4	С	1	Total O 1 1	0	0
4	D	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: Glutamate–tRNA ligase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	129.98Å 88.68Å 169.28Å	Depositor
a, b, c, α , β , γ	90.00° 106.13° 90.00°	Depositor
Resolution(A)	47.16 - 2.70	Depositor
Resolution (A)	47.17 - 2.70	EDS
% Data completeness	99.7 (47.16-2.70)	Depositor
(in resolution range)	93.3 (47.17-2.70)	EDS
R _{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.85 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_4701	Depositor
P. P.	0.199 , 0.234	Depositor
n, n_{free}	0.196 , 0.226	DCC
R_{free} test set	2535 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	76.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 83.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8603	wwPDB-VP
Average B, all atoms $(Å^2)$	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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, $\mathrm{SO4}$

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/1725	0.41	0/2327
1	В	0.24	0/1778	0.42	0/2401
1	С	0.24	0/1737	0.41	0/2343
1	D	0.24	0/1719	0.41	0/2321
1	Е	0.24	0/1667	0.39	0/2254
All	All	0.24	0/8626	0.41	0/11646

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	1687	0	1688	15	0
1	В	1738	0	1735	16	0
1	С	1699	0	1705	20	0
1	D	1680	0	1676	16	0
1	Е	1629	0	1622	19	0
2	А	15	0	0	0	0
2	В	20	0	0	0	0
2	С	5	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
3	А	48	0	64	3	0		
3	В	42	0	56	2	0		
3	С	18	0	24	0	0		
3	D	6	0	8	0	0		
4	А	10	0	0	0	0		
4	В	4	0	0	0	0		
4	С	1	0	0	0	0		
4	D	1	0	0	0	0		
All	All	8603	0	8578	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 5.

All (80) 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	distance (Å)	overlap (Å)
1:C:123:PHE:HB2	1:C:162:PHE:HE2	1.51	0.75
1:B:163:HIS:HB3	3:B:310:GOL:H32	1.71	0.72
1:A:21:ARG:HH22	3:A:307:GOL:H2	1.55	0.71
1:C:132:ASP:OD1	1:C:135:ARG:NH2	2.26	0.69
1:D:30:ASN:HB3	1:D:34:LYS:HE2	1.76	0.66
1:D:94:ASN:HB3	1:E:121:VAL:HG13	1.78	0.64
1:D:12:TYR:O	1:D:53:ASN:ND2	2.29	0.61
1:B:94:ASN:HB3	1:C:121:VAL:HG13	1.81	0.61
1:C:67:ARG:HD2	1:C:67:ARG:H	1.67	0.59
1:A:104:TYR:HA	1:A:123:PHE:HE2	1.67	0.59
1:B:104:TYR:HA	1:B:123:PHE:HE2	1.69	0.58
1:D:62:LYS:HE2	1:D:85:THR:HG22	1.88	0.56
1:B:6:SER:HB2	1:B:47:ILE:HG12	1.87	0.56
1:C:112:ASN:HB2	1:C:115:ARG:HB2	1.87	0.56
1:D:121:VAL:HG13	1:E:94:ASN:HB3	1.88	0.55
1:A:97:PHE:HB2	1:A:105:TYR:CE2	2.42	0.55
1:C:144:ILE:HB	1:C:145:PRO:HD3	1.89	0.53
1:B:97:PHE:HB2	1:B:105:TYR:CE2	2.45	0.52
1:E:17:PRO:HB2	1:E:20:CYS:HB2	1.91	0.52
1:D:96:ASP:OD1	1:D:101:THR:OG1	2.27	0.51
1:D:110:ARG:HG2	1:D:111:GLU:H	1.74	0.51
1:B:58:VAL:HG12	1:B:59:GLU:HG3	1.92	0.51
1:B:184:ILE:HG22	1:B:186:THR:HG22	1.92	0.51
1:E:104:TYR:HA	1:E:123:PHE:HE2	1.76	0.51
1:D:104:TYR:HA	1:D:123:PHE:HE2	1.76	0.51



	io ae page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:58:VAL:HG12	1:A:59:GLU:HG3	1.93	0.50
1:A:89:LYS:HD2	1:A:131:ILE:HD12	1.92	0.50
1:E:21:ARG:HH21	1:E:215:ASP:HB2	1.77	0.50
1:B:178:LYS:HE3	1:B:179:TYR:CZ	2.48	0.49
1:D:31:ILE:O	1:D:35:THR:OG1	2.22	0.49
1:E:60:ASP:HB2	1:E:86:SER:O	2.13	0.49
1:B:66:VAL:HG12	1:B:68:ASN:H	1.78	0.49
1:A:136:ASN:H	3:A:305:GOL:H11	1.78	0.49
1:C:104:TYR:HA	1:C:123:PHE:HE2	1.78	0.49
1:A:108:SER:HB3	1:A:115:ARG:HG2	1.96	0.48
1:A:62:LYS:HG2	3:A:308:GOL:H11	1.96	0.47
1:A:123:PHE:HB2	1:A:162:PHE:HE2	1.79	0.47
1:E:58:VAL:HG13	1:E:59:GLU:H	1.79	0.47
1:E:138:ASP:HB3	1:E:141:LYS:HB3	1.97	0.47
1:E:10:ILE:HG23	1:E:63:VAL:HG22	1.96	0.47
1:C:178:LYS:HG3	1:C:226:GLU:HG2	1.97	0.47
1:B:121:VAL:HG13	1:C:94:ASN:HB3	1.97	0.46
1:E:160:LEU:HD12	1:E:169:ASP:HA	1.96	0.46
1:E:65:PHE:HE1	1:E:84:VAL:HG22	1.80	0.46
1:D:178:LYS:HE3	1:D:179:TYR:CZ	2.51	0.46
1:D:12:TYR:CE2	1:D:53:ASN:HB2	2.50	0.46
1:B:154:LEU:O	1:B:199:ARG:NH2	2.49	0.45
1:A:123:PHE:HB2	1:A:162:PHE:CE2	2.52	0.45
1:C:96:ASP:OD1	1:C:101:THR:OG1	2.29	0.45
1:C:97:PHE:HB2	1:C:105:TYR:CE1	2.51	0.45
1:D:178:LYS:O	1:D:187:ASN:ND2	2.40	0.45
1:C:110:ARG:HE	1:C:117:ILE:HG13	1.82	0.45
1:D:9:ASN:HB2	1:D:64:GLU:HB3	1.98	0.45
1:E:13:GLY:HA3	1:E:57:VAL:HG22	1.99	0.45
1:E:60:ASP:OD1	1:E:60:ASP:N	2.34	0.45
1:C:89:LYS:HG3	1:C:90:ILE:HG12	1.99	0.44
1:A:19:LEU:HD23	1:A:89:LYS:HA	1.99	0.44
1:B:63:VAL:HG11	1:B:91:PHE:CZ	2.53	0.44
1:E:180:PHE:HA	1:E:191:PRO:HG3	1.99	0.44
1:B:212:VAL:HG13	1:B:218:LEU:HD22	2.00	0.43
1:C:190:TYR:HB2	1:C:191:PRO:HD3	1.99	0.43
1:B:227:LYS:HE2	1:B:227:LYS:HB2	1.86	0.43
1:C:7:LYS:HB3	1:C:66:VAL:HG23	2.01	0.42
1:E:9:ASN:HB2	1:E:64:GLU:HB3	2.01	0.42
1:E:212:VAL:HB	1:E:218:LEU:HD22	2.01	0.42
1:C:54:ASP:HB3	1:C:57:VAL:HG22	2.01	0.42



Atom-1	Atom-2	Interatomic	Clash	
		distance (A)	overlap (A)	
1:A:14:LYS:HB3	1:A:58:VAL:O	2.20	0.42	
1:B:130:TRP:CE2	3:B:309:GOL:H31	2.54	0.42	
1:D:54:ASP:OD1	1:D:56:THR:OG1	2.23	0.42	
1:A:192:LYS:HE2	1:A:192:LYS:HB3	1.92	0.41	
1:A:144:ILE:HB	1:A:145:PRO:HD3	2.01	0.41	
1:B:112:ASN:HB2	1:B:115:ARG:HB2	2.02	0.41	
1:C:195:LYS:HD3	1:D:155:TYR:HE1	1.85	0.41	
1:E:151:ASN:OD1	1:E:196:ASN:HB2	2.20	0.41	
1:A:115:ARG:HD3	1:A:115:ARG:HA	1.70	0.41	
1:C:120:ASN:O	1:C:124:GLN:HG3	2.20	0.41	
1:E:154:LEU:O	1:E:199:ARG:NH2	2.54	0.41	
1:C:195:LYS:HD3	1:D:155:TYR:CE1	2.56	0.41	
1:E:63:VAL:HG11	1:E:91:PHE:CZ	2.56	0.41	
1:C:59:GLU:N	1:C:59:GLU:OE1	2.53	0.40	

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	А	189/249~(76%)	183~(97%)	6 (3%)	0	100 100
1	В	197/249~(79%)	183~(93%)	14 (7%)	0	100 100
1	С	190/249~(76%)	184 (97%)	6 (3%)	0	100 100
1	D	188/249~(76%)	183 (97%)	5(3%)	0	100 100
1	Ε	183/249~(74%)	178 (97%)	5(3%)	0	100 100
All	All	947/1245~(76%)	911 (96%)	36 (4%)	0	100 100

There are no Ramachandran outliers to report.



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	190/236~(80%)	185~(97%)	5(3%)	46 75
1	В	195/236~(83%)	193~(99%)	2(1%)	76 91
1	С	191/236~(81%)	184 (96%)	7 (4%)	34 63
1	D	188/236~(80%)	181~(96%)	7 (4%)	34 63
1	Ε	183/236~(78%)	176~(96%)	7 (4%)	33 62
All	All	947/1180 (80%)	919~(97%)	28~(3%)	41 70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	61	ILE
1	А	115	ARG
1	А	120	ASN
1	А	155	TYR
1	А	226	GLU
1	В	120	ASN
1	В	141	LYS
1	С	47	ILE
1	С	66	VAL
1	С	67	ARG
1	С	120	ASN
1	С	155	TYR
1	С	186	THR
1	С	212	VAL
1	D	59	GLU
1	D	89	LYS
1	D	120	ASN
1	D	148	GLU
1	D	189	LYS
1	D	221	ASN
1	D	226	GLU
1	Е	57	VAL
1	Е	58	VAL



Continued from previous page...

Mol	Chain	Res	Type
1	Ε	82	ASN
1	Е	89	LYS
1	Ε	115	ARG
1	Е	120	ASN
1	Е	155	TYR

Sometimes 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)

27 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).

Mol Type Chain		Dec	Link	B	Bond lengths			Bond angles		
MOI	Type	Unain	in nes	nes Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	GOL	A	307	-	5,5,5	0.33	0	$5,\!5,\!5$	0.36	0
3	GOL	А	311	-	5,5,5	0.33	0	$5,\!5,\!5$	0.37	0
3	GOL	В	309	-	5,5,5	0.34	0	$5,\!5,\!5$	0.37	0
3	GOL	С	304	-	5,5,5	0.33	0	$5,\!5,\!5$	0.36	0
3	GOL	С	302	-	5,5,5	0.34	0	$5,\!5,\!5$	0.37	0
3	GOL	В	308	-	5,5,5	0.31	0	$5,\!5,\!5$	0.36	0



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	E	Bond angle	
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	А	302	-	4,4,4	0.13	0	$6,\!6,\!6$	0.09	0
3	GOL	А	309	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.36	0
3	GOL	А	304	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.41	0
3	GOL	А	305	-	5,5,5	0.33	0	$5,\!5,\!5$	0.37	0
3	GOL	В	307	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.35	0
2	SO4	А	303	-	4,4,4	0.10	0	$6,\!6,\!6$	0.09	0
2	SO4	В	303	-	4,4,4	0.14	0	6,6,6	0.09	0
3	GOL	В	311	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.39	0
2	SO4	В	304	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	В	302	-	4,4,4	0.14	0	$6,\!6,\!6$	0.08	0
3	GOL	А	306	-	5,5,5	0.33	0	$5,\!5,\!5$	0.37	0
3	GOL	С	303	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.36	0
3	GOL	D	301	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.38	0
3	GOL	В	310	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.40	0
3	GOL	В	305	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.33	0
2	SO4	С	301	-	4,4,4	0.16	0	$6,\!6,\!6$	0.08	0
2	SO4	В	301	-	4,4,4	0.13	0	$6,\!6,\!6$	0.09	0
2	SO4	A	301	-	4,4,4	0.15	0	$6,\!6,\!6$	0.08	0
3	GOL	A	310	-	5,5,5	0.33	0	5,5,5	0.39	0
3	GOL	A	308	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.38	0
3	GOL	В	306	-	5,5,5	0.33	0	$\overline{5,5,5}$	0.38	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	\mathbf{Res}	Link	Chirals	Torsions	Rings
3	GOL	А	307	-	-	0/4/4/4	-
3	GOL	А	311	-	-	2/4/4/4	-
3	GOL	В	309	-	-	1/4/4/4	-
3	GOL	С	304	-	-	0/4/4/4	-
3	GOL	С	302	-	-	0/4/4/4	-
3	GOL	В	308	-	-	3/4/4/4	-
3	GOL	А	309	-	-	2/4/4/4	-
3	GOL	А	304	-	-	1/4/4/4	-
3	GOL	А	305	-	-	2/4/4/4	-
3	GOL	В	307	-	-	0/4/4/4	-
3	GOL	В	311	-	-	0/4/4/4	-
3	GOL	А	306	-	-	0/4/4/4	-
3	GOL	С	303	-	-	0/4/4/4	-
3	GOL	D	301	-	-	0/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	В	310	-	-	2/4/4/4	-
3	GOL	В	305	-	-	2/4/4/4	-
3	GOL	А	310	-	-	0/4/4/4	-
3	GOL	А	308	-	-	0/4/4/4	-
3	GOL	В	306	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	305	GOL	C1-C2-C3-O3
3	А	309	GOL	O1-C1-C2-O2
3	А	309	GOL	O1-C1-C2-C3
3	А	311	GOL	C1-C2-C3-O3
3	В	305	GOL	O1-C1-C2-C3
3	В	308	GOL	O1-C1-C2-C3
3	В	310	GOL	O1-C1-C2-C3
3	В	308	GOL	O1-C1-C2-O2
3	А	304	GOL	O1-C1-C2-C3
3	В	308	GOL	C1-C2-C3-O3
3	А	305	GOL	O2-C2-C3-O3
3	А	311	GOL	O2-C2-C3-O3
3	В	305	GOL	O1-C1-C2-O2
3	В	310	GOL	O1-C1-C2-O2
3	В	309	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	307	GOL	1	0
3	В	309	GOL	1	0
3	А	305	GOL	1	0
3	В	310	GOL	1	0
3	А	308	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	<RSRZ $>$	#RSRZ>2	2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	197/249~(79%)	0.36	5 (2%) 57	59	58, 74, 129, 176	0
1	В	203/249~(81%)	0.70	14 (6%) 16	15	62, 86, 152, 241	0
1	C	198/249~(79%)	0.96	29 (14%) 2	1	71, 107, 169, 226	0
1	D	196/249~(78%)	1.65	63 (32%) 0	0	101, 149, 193, 219	0
1	E	191/249~(76%)	1.86	65~(34%) 0	0	127, 170, 207, 238	0
All	All	985/1245~(79%)	1.10	176~(17%) 1	1	58, 116, 194, 241	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	109	TYR	9.1	
1	D	52	ILE	8.5	
1	Е	35	THR	8.0	
1	1 E 17		TYR	7.3	
1	Ε	186	THR	7.2	
1	Е	190	TYR	7.0	
1	Е	18	PHE	7.0	
1	D	D 194 TYR		6.9	
1	Е	185	THR	6.8	
1	Е	184	ILE	6.6	
1	Е	187	ASN	6.6	
1	Ε	58	VAL	6.5	
1	D	8	ILE	6.3	
1	Ε	192	LYS	6.3	
1	С	113	ILE	6.2	
1	С	184	ILE	6.0	
1	D	187	ASN	6.0	
1	Е	195	LYS	5.9	
1	D	223	LYS	5.9	
1	E	181	SER	5.5	



Mol	Chain	Res	Type	RSRZ	
1	Е	162	PHE	5.4	
1	Е	60	ASP	5.4	
1	Е	194	TYR	5.3	
1	D	51	PHE	5.3	
1	В	68	ASN	5.2	
1	D	11	TYR	5.1	
1	D	18	PHE	5.0	
1	Е	155	TYR	5.0	
1	D	57	VAL	4.9	
1	Е	53	ASN	4.9	
1	D	225	LYS	4.9	
1	Е	55	LYS	4.9	
1	D	186	THR	4.8	
1	В	35	THR	4.8	
1	Е	52	ILE	4.7	
1	Е	188	LEU	4.6	
1	Е	212	VAL	4.6	
1	Е	34	LYS	4.6	
1	D	32	LYS	4.6	
1	D	35	THR	4.6	
1	D	188	LEU	4.4	
1	С	45	LYS	4.4	
1	С	185	THR	4.3	
1	С	6	SER	4.3	
1	С	34	LYS	4.2	
1	D	14	LYS	4.2	
1	D	10	ILE	4.2	
1	В	36	ALA	4.2	
1	А	34	LYS	4.2	
1	С	114	ASN	4.1	
1	С	111	GLU	4.1	
1	D	34	LYS	4.1	
1	Е	180	PHE	4.1	
1	D	222	LEU	4.0	
1	Е	177	HIS	4.0	
1	С	225	LYS	4.0	
1	Е	54	ASP	3.9	
1	С	35	THR	3.9	
1	D	47	ILE	3.8	
1	E	12	TYR	3.8	
1	D	7	LYS	3.8	
1	Е	37	ASN	3.8	



Mol	Chain	Res	Type	RSRZ
1	D	12	TYR	3.7
1	D	185	THR	3.7
1	В	34	LYS	3.7
1	Е	59	GLU	3.7
1	С	183	33 ASN 3	
1	А	5	ASP	3.6
1	D	139	ILE	3.6
1	D	37	ASN	3.5
1	D	54	ASP	3.5
1	Е	16	TYR	3.4
1	Е	182	GLY	3.4
1	Е	144	ILE	3.4
1	Е	178	LYS	3.4
1	Е	81	ASN	3.4
1	Е	36	ALA	3.3
1	С	68	ASN	3.3
1	D	9	ASN	3.3
1	D	216	ALA	3.3
1	С	218	LEU	3.3
1	D	67	ARG	3.3
1	В	184	ILE	3.2
1	D	65	PHE	3.2
1	D	226	GLU	3.2
1	D	190	TYR	3.2
1	Е	32	LYS	3.1
1	D	112	ASN	3.1
1	Е	176	MET	3.1
1	Е	146	ILE	3.1
1	D	36	ALA	3.1
1	С	58	VAL	3.1
1	Ε	221	ASN	3.1
1	А	45	LYS	3.0
1	Е	31	ILE	3.0
1	C	46	GLU	3.0
1	D	180	PHE	3.0
1	Е	224	VAL	3.0
1	C	7	LYS	3.0
1	В	190	TYR	2.9
1	D	66	VAL	2.9
1	D	82	ASN	2.9
1	D	224	VAL	2.9
1	Е	139	ILE	2.9



Mol	Chain	Res	Type	RSRZ	
1	Е	183	ASN	2.9	
1	В	113	ILE	2.9	
1	Е	209	HIS	2.8	
1	Е	14	LYS	2.8	
1	Е	214	THR	2.8	
1	Е	223	LYS	2.8	
1	С	155	TYR	2.8	
1	Е	7	LYS	2.8	
1	D	59	GLU	2.8	
1	С	33	LYS	2.8	
1	С	47	ILE	2.8	
1	D	55	LYS	2.7	
1	С	112	ASN	2.7	
1	C	187	ASN	2.7	
1	Е	122	PHE	2.7	
1	Е	200	TRP	2.7	
1	С	223	LYS	2.7	
1	D	45	LYS	2.7	
1	Е	189	LYS	2.7	
1	Ε	213	ALA	2.6	
1	D	141	LYS	2.6	
1	D	155	TYR	2.6	
1	D	98	LEU	2.6	
1	С	226	GLU	2.6	
1	D	144	ILE	2.5	
1	D	191	PRO	2.5	
1	В	45	LYS	2.5	
1	Е	11	TYR	2.5	
1	D	178	LYS	2.4	
1	С	224	VAL	2.4	
1	D	64	GLU	2.4	
1	E	142	ASN	2.4	
1	D	184	ILE	2.4	
1	С	140	GLU	2.4	
1	E	174	TYR	2.3	
1	D	192	LYS	2.3	
1	D	49	VAL	2.3	
1	D	109	TYR	2.3	
1	E	10	ILE	2.3	
1	C	115	ARG	2.3	
1	В	166	THR	2.3	
1	D	56	THR	2.2	



8BCQ

Mol	Chain	Res	Type	RSRZ
1	D	219	ILE	2.2
1	D	179	TYR	2.2
1	D	62	LYS	2.2
1	Е	141	LYS	2.2
1	В	168	SER	2.2
1	В	187	ASN	2.2
1	Е	17	PRO	2.2
1	Е	218	LEU	2.2
1	D	200	TRP	2.2
1	Е	219	ILE	2.1
1	Е	138	ASP	2.1
1	D	27	TYR	2.1
1	D	53	ASN	2.1
1	Е	215	ASP	2.1
1	D	46	GLU	2.1
1	Е	151	ASN	2.1
1	D	177	HIS	2.1
1	D	193	GLN	2.1
1	Е	216	ALA	2.1
1	Е	38	ASN	2.1
1	С	227	LYS	2.1
1	D	128	ASN	2.1
1	В	183	ASN	2.0
1	A	185	THR	2.0
1	Е	163	HIS	2.0
1	A	27	TYR	2.0
1	С	55	LYS	2.0
1	С	123	PHE	2.0
1	В	110	ARG	2.0
1	D	212	VAL	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^{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	$B-factors(A^2)$	Q<0.9
3	GOL	А	306	6/6	0.42	0.63	113,134,152,162	0
3	GOL	А	311	6/6	0.61	0.32	123,134,141,150	0
3	GOL	С	303	6/6	0.61	0.54	96,99,114,120	0
3	GOL	В	305	6/6	0.70	0.26	86,99,100,102	0
3	GOL	С	304	6/6	0.71	0.40	127,144,151,154	0
3	GOL	В	308	6/6	0.74	0.32	87,101,106,118	0
3	GOL	А	304	6/6	0.77	0.33	83,99,107,108	0
3	GOL	А	305	6/6	0.77	0.28	83,102,115,125	0
3	GOL	D	301	6/6	0.78	0.28	131,139,141,151	0
3	GOL	В	307	6/6	0.81	0.36	91,110,122,127	0
3	GOL	А	310	6/6	0.82	0.52	92,104,109,129	0
2	SO4	В	303	5/5	0.82	0.27	166,183,203,215	0
3	GOL	А	307	6/6	0.84	0.39	91,116,117,129	0
3	GOL	С	302	6/6	0.85	0.20	118,123,130,136	0
3	GOL	В	310	6/6	0.85	0.27	82,85,94,100	0
3	GOL	В	311	6/6	0.86	0.43	89,92,105,112	0
3	GOL	А	308	6/6	0.88	0.26	83,108,111,118	0
2	SO4	А	303	5/5	0.88	0.79	110,136,167,237	0
2	SO4	С	301	5/5	0.88	0.21	114,120,158,160	0
3	GOL	А	309	6/6	0.89	0.25	101,118,121,125	0
3	GOL	В	306	6/6	0.89	0.28	91,104,109,111	0
2	SO4	В	304	5/5	0.91	0.36	105,116,138,148	0
3	GOL	В	309	6/6	0.91	0.17	105,107,115,117	0
2	SO4	В	301	5/5	0.93	0.20	152,156,196,279	0
2	SO4	A	301	5/5	0.94	0.15	100,105,135,145	0
2	SO4	А	302	5/5	0.94	0.27	114,144,147,153	0
2	SO4	В	302	5/5	0.96	0.08	86,109,128,131	0

6.5 Other polymers (i)

There are no such residues in this entry.

