



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 01:11 pm BST

PDB ID : 8BCQ / pdb_00008bcq
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

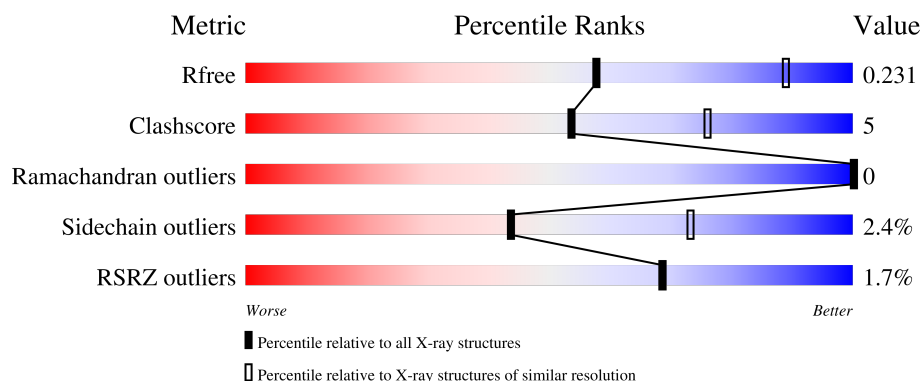
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	<div> <div>0%</div> <div>70% 8% 21%</div> </div>
1	B	249	<div> <div>0%</div> <div>71% 11% 18%</div> </div>
1	C	249	<div> <div>2%</div> <div>65% 14% 20%</div> </div>
1	D	249	<div> <div>0%</div> <div>66% 13% 21%</div> </div>
1	E	249	<div> <div>2%</div> <div>62% 13% 23%</div> </div>

2 Entry composition

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.

- Molecule 1 is a protein called Glutamate-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1687	1104	279	300	4			
1	B	203	Total	C	N	O	S	0	0	0
			1738	1134	290	310	4			
1	C	198	Total	C	N	O	S	0	0	0
			1699	1111	284	300	4			
1	D	196	Total	C	N	O	S	0	0	0
			1680	1101	277	298	4			
1	E	191	Total	C	N	O	S	0	0	0
			1629	1068	268	289	4			

There are 120 discrepancies between the modelled and reference sequences:

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

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

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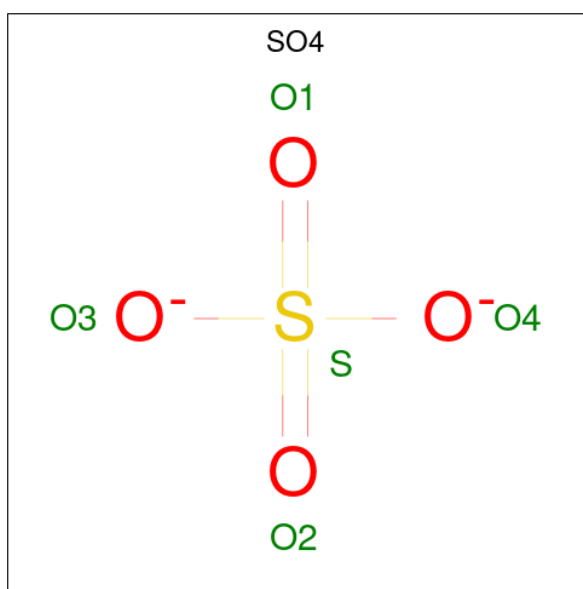
Chain	Residue	Modelled	Actual	Comment	Reference
C	239	PRO	-	expression tag	UNP A0A509AR09
C	240	ARG	-	expression tag	UNP A0A509AR09
C	241	GLY	-	expression tag	UNP A0A509AR09
C	242	SER	-	expression tag	UNP A0A509AR09
C	243	SER	-	expression tag	UNP A0A509AR09
C	244	HIS	-	expression tag	UNP A0A509AR09
C	245	HIS	-	expression tag	UNP A0A509AR09
C	246	HIS	-	expression tag	UNP A0A509AR09
C	247	HIS	-	expression tag	UNP A0A509AR09
C	248	HIS	-	expression tag	UNP A0A509AR09
C	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
E	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
E	232	GLY	-	expression tag	UNP A0A509AR09

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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



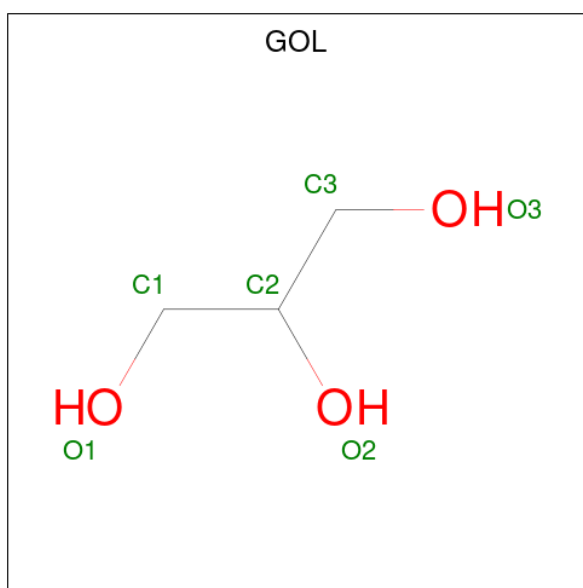
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

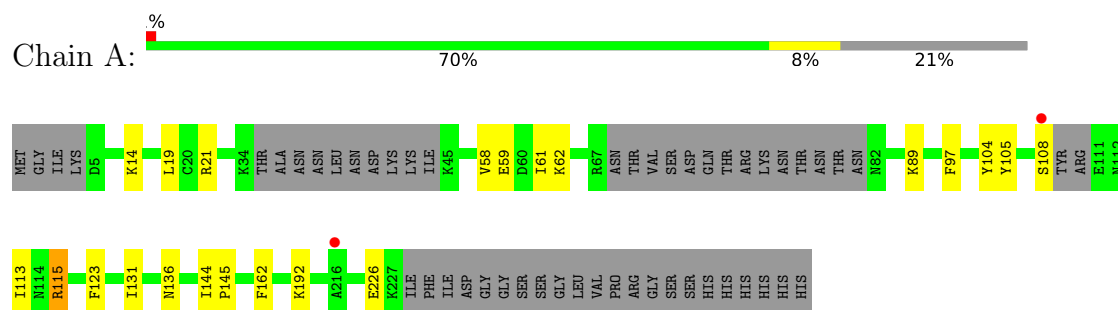
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	4	Total	O	0	0
			4	4		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

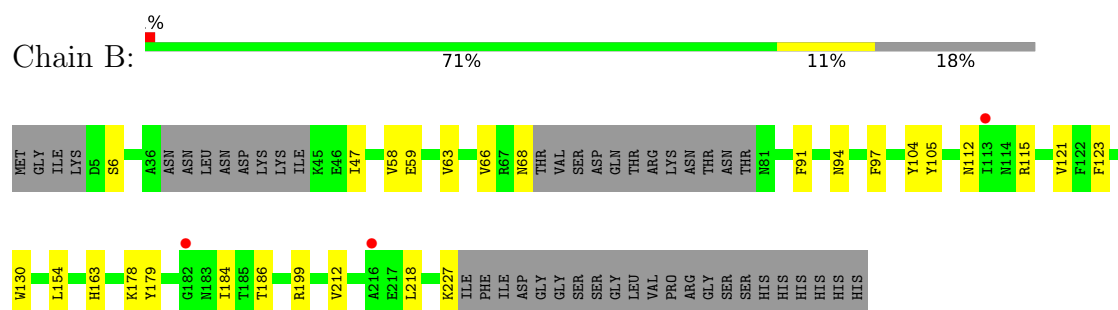
3 Residue-property plots [i](#)

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.

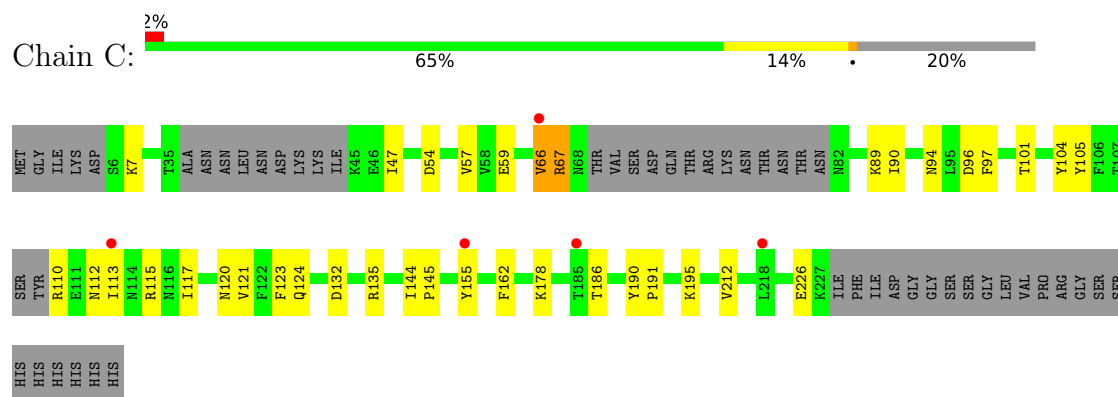
• Molecule 1: Glutamate-tRNA ligase



• Molecule 1: Glutamate-tRNA ligase

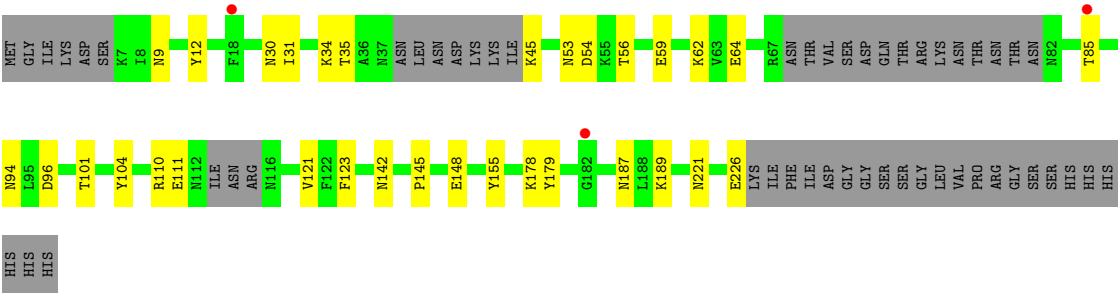


• Molecule 1: Glutamate-tRNA ligase

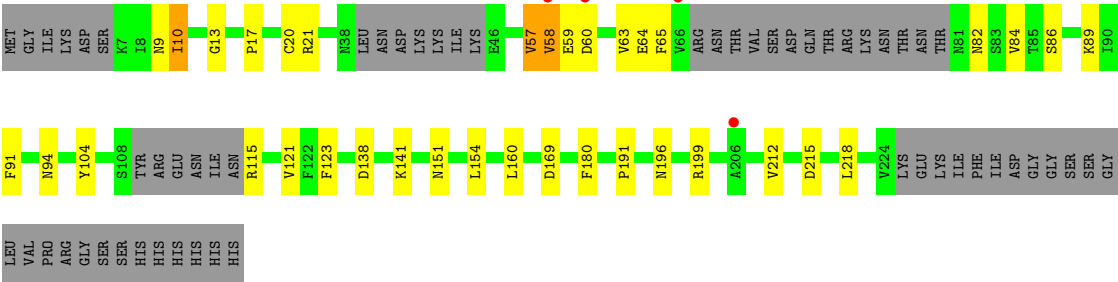


• Molecule 1: Glutamate-tRNA ligase





• Molecule 1: Glutamate-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.98Å 88.68Å 169.28Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	47.16 – 2.70 47.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.16-2.70) 93.2 (47.16-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 2.69Å)	Xtriage
Refinement program	PHENIX dev_4701	Depositor
R, R_{free}	0.199 , 0.234 0.199 , 0.231	Depositor DCC
R_{free} test set	2545 reflections (4.99%)	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 , 88.2	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.*

¹Intensities estimated from amplitudes.

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.

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, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1725	0.23	0/2327
1	B	0.09	0/1778	0.25	0/2401
1	C	0.07	0/1737	0.21	0/2343
1	D	0.07	0/1719	0.22	0/2321
1	E	0.07	0/1667	0.21	0/2254
All	All	0.08	0/8626	0.22	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	A	1687	0	1688	15	0
1	B	1738	0	1735	16	0
1	C	1699	0	1705	21	0
1	D	1680	0	1676	17	0
1	E	1629	0	1622	19	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	64	3	0
3	B	42	0	56	2	0
3	C	18	0	24	0	0
3	D	6	0	8	0	0
4	A	10	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8603	0	8578	82	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 (82) 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: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:D:54:ASP:OD1	1:D:56:THR:OG1	2.23	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:HA	1:D:123:PHE:HE2	1.76	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASP:HB3	1:C:57:VAL:HG22	2.01	0.42
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: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:D:142:ASN:C	1:D:145:PRO:HD2	2.46	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
1:C:120:ASN:HD22	1:C:120:ASN:C	2.29	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	A	189/249 (76%)	183 (97%)	6 (3%)	0	100	100
1	B	197/249 (79%)	183 (93%)	14 (7%)	0	100	100
1	C	190/249 (76%)	184 (97%)	6 (3%)	0	100	100
1	D	188/249 (76%)	183 (97%)	5 (3%)	0	100	100
1	E	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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/236 (80%)	186 (98%)	4 (2%)	48	76
1	B	195/236 (83%)	195 (100%)	0	100	100
1	C	191/236 (81%)	184 (96%)	7 (4%)	29	58
1	D	188/236 (80%)	182 (97%)	6 (3%)	34	63
1	E	183/236 (78%)	177 (97%)	6 (3%)	33	62
All	All	947/1180 (80%)	924 (98%)	23 (2%)	44	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	113	ILE
1	A	115	ARG
1	A	226	GLU
1	C	47	ILE
1	C	66	VAL
1	C	67	ARG
1	C	113	ILE
1	C	155	TYR
1	C	186	THR
1	C	212	VAL
1	D	45	LYS
1	D	59	GLU
1	D	148	GLU
1	D	189	LYS
1	D	221	ASN
1	D	226	GLU
1	E	10	ILE
1	E	57	VAL
1	E	58	VAL
1	E	82	ASN
1	E	89	LYS
1	E	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	221	ASN
1	B	112	ASN
1	B	142	ASN
1	C	142	ASN
1	D	112	ASN
1	D	163	HIS
1	E	38	ASN
1	E	82	ASN
1	E	126	GLN
1	E	163	HIS

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 oligosaccharides 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	302	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	310	-	5,5,5	0.31	0	5,5,5	0.40	0
2	SO4	C	301	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	303	-	4,4,4	0.10	0	6,6,6	0.09	0
3	GOL	C	303	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	A	304	-	5,5,5	0.32	0	5,5,5	0.41	0
3	GOL	B	306	-	5,5,5	0.33	0	5,5,5	0.38	0
3	GOL	A	309	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	C	304	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	B	311	-	5,5,5	0.32	0	5,5,5	0.39	0
3	GOL	B	308	-	5,5,5	0.31	0	5,5,5	0.36	0
3	GOL	A	307	-	5,5,5	0.33	0	5,5,5	0.36	0
2	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.08	0
3	GOL	B	307	-	5,5,5	0.33	0	5,5,5	0.35	0
3	GOL	A	310	-	5,5,5	0.33	0	5,5,5	0.39	0
2	SO4	B	301	-	4,4,4	0.13	0	6,6,6	0.09	0
3	GOL	A	311	-	5,5,5	0.33	0	5,5,5	0.37	0
3	GOL	A	305	-	5,5,5	0.33	0	5,5,5	0.37	0
3	GOL	A	306	-	5,5,5	0.33	0	5,5,5	0.37	0
3	GOL	C	302	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	D	301	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	B	305	-	5,5,5	0.32	0	5,5,5	0.33	0
3	GOL	A	308	-	5,5,5	0.32	0	5,5,5	0.38	0
3	GOL	B	309	-	5,5,5	0.34	0	5,5,5	0.37	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	B	310	-	-	2/4/4/4	-
3	GOL	C	303	-	-	0/4/4/4	-
3	GOL	A	304	-	-	1/4/4/4	-
3	GOL	B	306	-	-	0/4/4/4	-
3	GOL	A	309	-	-	2/4/4/4	-
3	GOL	C	304	-	-	0/4/4/4	-
3	GOL	B	311	-	-	0/4/4/4	-
3	GOL	B	308	-	-	3/4/4/4	-
3	GOL	A	307	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	307	-	-	0/4/4/4	-
3	GOL	A	310	-	-	0/4/4/4	-
3	GOL	A	311	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
3	GOL	D	301	-	-	0/4/4/4	-
3	GOL	B	305	-	-	2/4/4/4	-
3	GOL	A	308	-	-	0/4/4/4	-
3	GOL	B	309	-	-	1/4/4/4	-

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	A	305	GOL	C1-C2-C3-O3
3	A	309	GOL	O1-C1-C2-O2
3	A	309	GOL	O1-C1-C2-C3
3	A	311	GOL	C1-C2-C3-O3
3	B	305	GOL	O1-C1-C2-C3
3	B	308	GOL	O1-C1-C2-C3
3	B	310	GOL	O1-C1-C2-C3
3	B	308	GOL	O1-C1-C2-O2
3	A	304	GOL	O1-C1-C2-C3
3	B	308	GOL	C1-C2-C3-O3
3	A	305	GOL	O2-C2-C3-O3
3	A	311	GOL	O2-C2-C3-O3
3	B	305	GOL	O1-C1-C2-O2
3	B	310	GOL	O1-C1-C2-O2
3	B	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	B	310	GOL	1	0
3	A	307	GOL	1	0
3	A	305	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	GOL	1	0
3	B	309	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	A	197/249 (79%)	-0.17	2 (1%) 79 79	58, 74, 129, 176	0
1	B	203/249 (81%)	-0.04	3 (1%) 71 71	62, 86, 152, 241	0
1	C	198/249 (79%)	0.12	5 (2%) 58 57	71, 107, 169, 226	0
1	D	196/249 (78%)	0.23	3 (1%) 71 71	101, 149, 193, 219	0
1	E	191/249 (76%)	0.27	4 (2%) 63 63	127, 170, 207, 238	0
All	All	985/1245 (79%)	0.08	17 (1%) 69 68	58, 116, 194, 241	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	ILE	3.8
1	C	113	ILE	3.1
1	B	216	ALA	2.9
1	C	185	THR	2.8
1	B	182	GLY	2.7
1	C	66	VAL	2.6
1	A	108	SER	2.5
1	C	155	TYR	2.4
1	C	218	LEU	2.4
1	D	18	PHE	2.4
1	E	206	ALA	2.3
1	A	216	ALA	2.1
1	E	60	ASP	2.1
1	D	182	GLY	2.1
1	D	85	THR	2.0
1	E	66	VAL	2.0
1	E	58	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 oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
2	SO4	C	301	5/5	0.52	0.12	114,120,158,160	0
2	SO4	A	303	5/5	0.58	0.18	110,136,167,237	0
3	GOL	A	306	6/6	0.64	0.18	113,134,152,162	0
3	GOL	A	311	6/6	0.64	0.14	123,134,141,150	0
3	GOL	C	304	6/6	0.64	0.12	127,144,151,154	0
3	GOL	B	305	6/6	0.65	0.26	86,99,100,102	0
2	SO4	B	303	5/5	0.69	0.08	166,183,203,215	0
2	SO4	A	301	5/5	0.75	0.13	100,105,135,145	0
3	GOL	C	302	6/6	0.76	0.13	118,123,130,136	0
3	GOL	A	305	6/6	0.81	0.12	83,102,115,125	0
3	GOL	A	304	6/6	0.82	0.20	83,99,107,108	0
2	SO4	A	302	5/5	0.83	0.09	114,144,147,153	0
3	GOL	B	311	6/6	0.84	0.17	89,92,105,112	0
3	GOL	A	307	6/6	0.85	0.10	91,116,117,129	0
3	GOL	A	310	6/6	0.87	0.21	92,104,109,129	0
2	SO4	B	304	5/5	0.87	0.12	105,116,138,148	0
2	SO4	B	302	5/5	0.87	0.09	86,109,128,131	0
3	GOL	A	309	6/6	0.88	0.13	101,118,121,125	0
3	GOL	A	308	6/6	0.89	0.17	83,108,111,118	0
3	GOL	B	308	6/6	0.89	0.14	87,101,106,118	0
3	GOL	C	303	6/6	0.89	0.24	96,99,114,120	0
3	GOL	B	310	6/6	0.89	0.13	82,85,94,100	0
3	GOL	D	301	6/6	0.89	0.09	131,139,141,151	0
3	GOL	B	307	6/6	0.90	0.18	91,110,122,127	0
3	GOL	B	306	6/6	0.91	0.09	91,104,109,111	0
2	SO4	B	301	5/5	0.92	0.10	152,156,196,279	0
3	GOL	B	309	6/6	0.92	0.12	105,107,115,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.