



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:53 AM UTC

PDB ID : 2LGS / pdb_00002lgs
Title : FEEDBACK INHIBITION OF FULLY UNADENYLYLATED GLUTAMINE SYNTHETASE FROM SALMONELLA TYPHIMURIUM BY GLYCINE, ALANINE, AND SERINE
Authors : Liaw, S.-H.; Eisenberg, D.
Deposited on : 1994-08-05
Resolution : 2.80 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 ⓘ 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

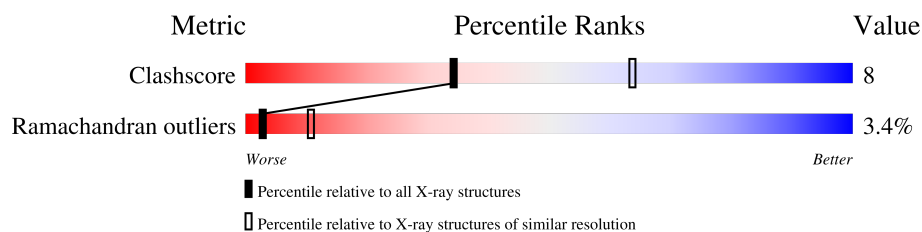
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	468	 63% 28% . . 5%
1	B	468	 63% 28% . . 5%
1	C	468	 61% 29% . . 5%
1	D	468	 62% 28% . . 5%
1	E	468	 63% 27% . . 5%
1	F	468	 62% 28% . . 5%
1	G	468	 63% 28% . . 5%
1	H	468	 62% 28% . . 5%
1	I	468	 63% 28% . . 5%

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Mol	Chain	Length	Quality of chain
1	J	468	62%28% 5%
1	K	468	61%29% 5%
1	L	468	62%28% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41604 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	B	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	C	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	D	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	E	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	F	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	G	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	H	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	I	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	J	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	K	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	L	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

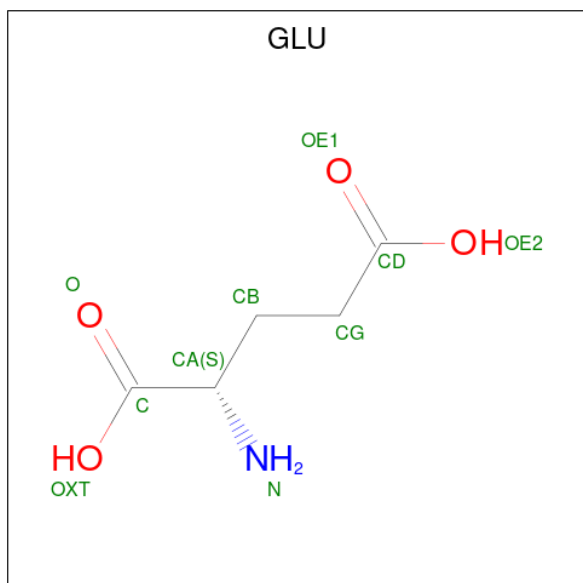
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0
2	H	2	Total 2	Mn 2	0	0
2	I	2	Total 2	Mn 2	0	0
2	J	2	Total 2	Mn 2	0	0
2	K	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 5	N 1	O 4	0	0

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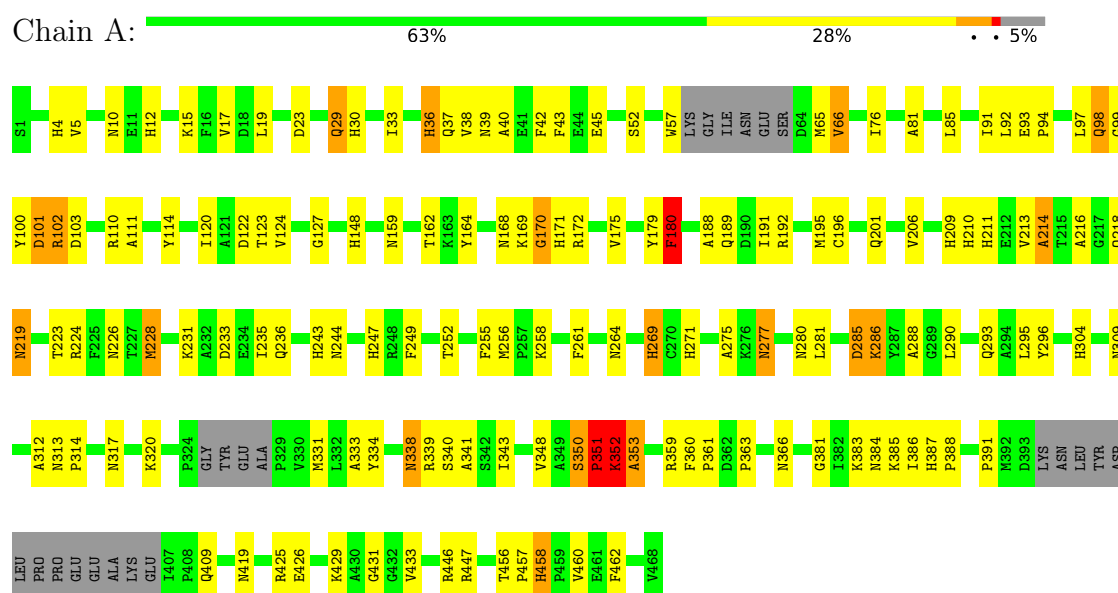
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		
3	F	1	Total	C	N	O	0	0
			10	5	1	4		
3	G	1	Total	C	N	O	0	0
			10	5	1	4		
3	H	1	Total	C	N	O	0	0
			10	5	1	4		
3	I	1	Total	C	N	O	0	0
			10	5	1	4		
3	J	1	Total	C	N	O	0	0
			10	5	1	4		
3	K	1	Total	C	N	O	0	0
			10	5	1	4		
3	L	1	Total	C	N	O	0	0
			10	5	1	4		

3 Residue-property plots

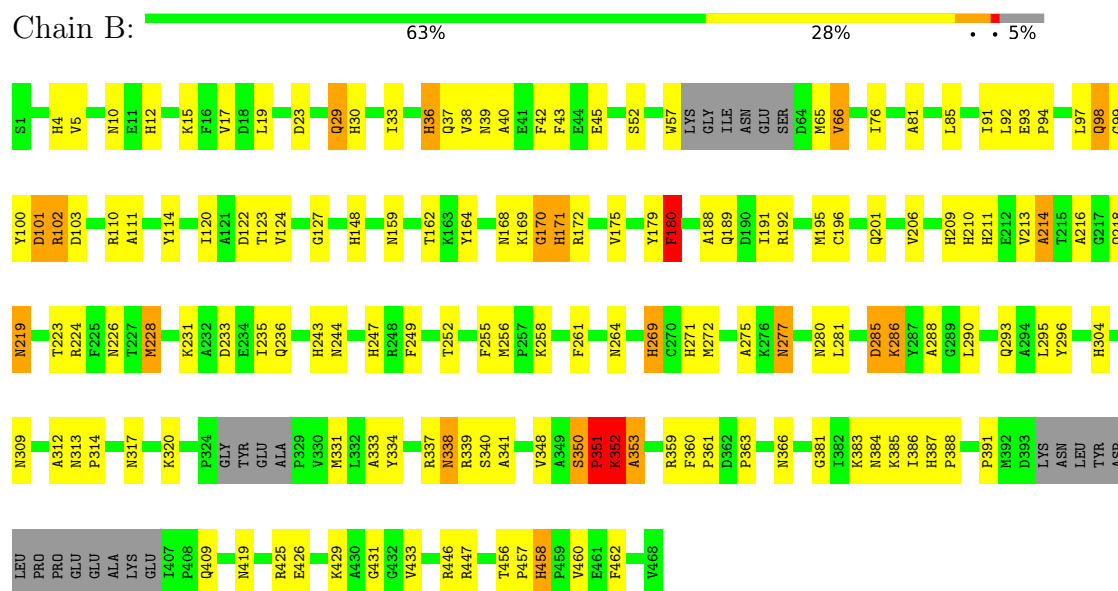
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: GLUTAMINE SYNTHETASE

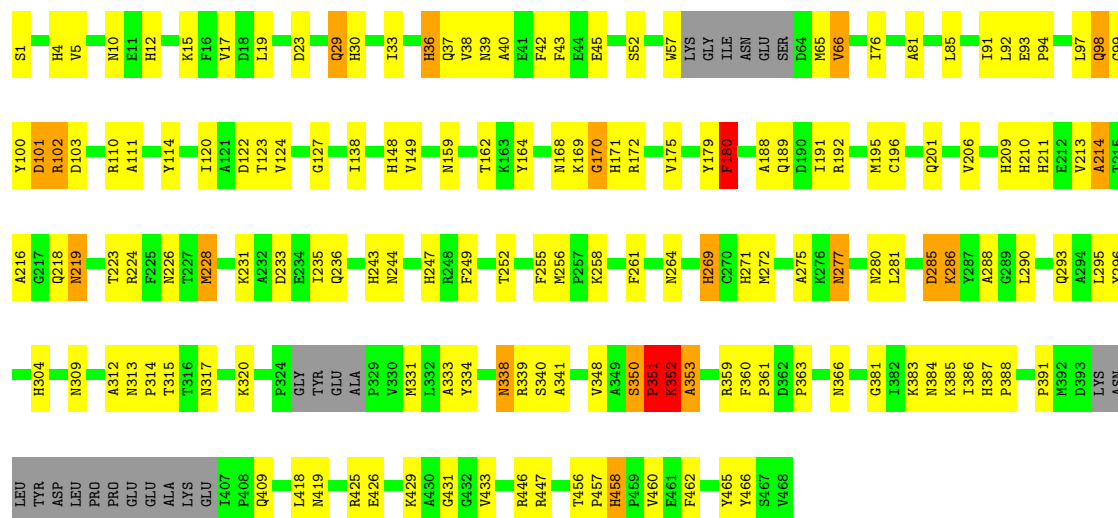


• Molecule 1: GLUTAMINE SYNTHETASE



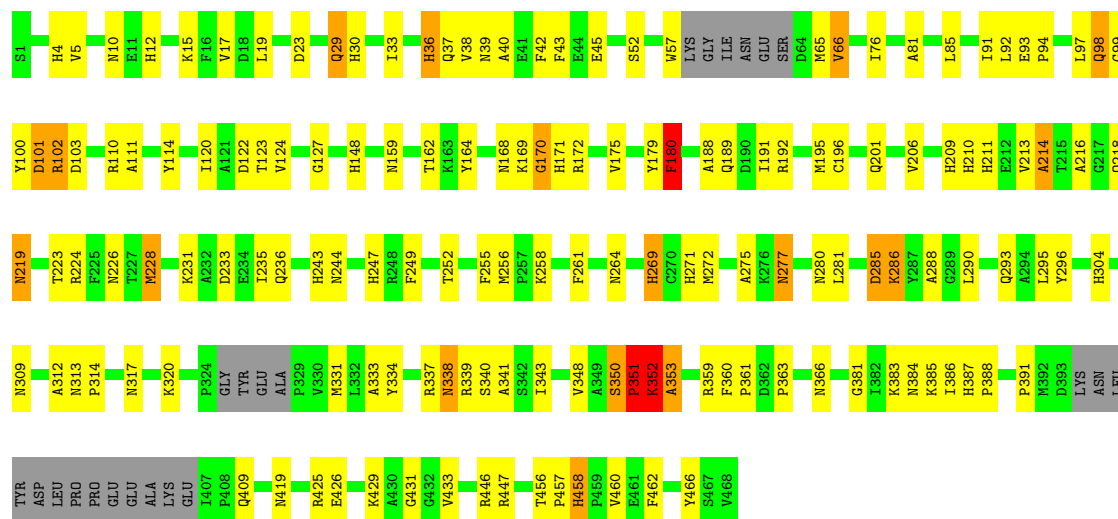
• Molecule 1: GLUTAMINE SYNTHETASE

Chain C:  61% 29% 5%



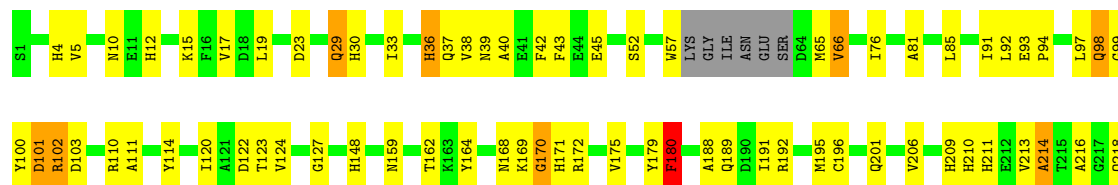
• Molecule 1: GLUTAMINE SYNTHETASE

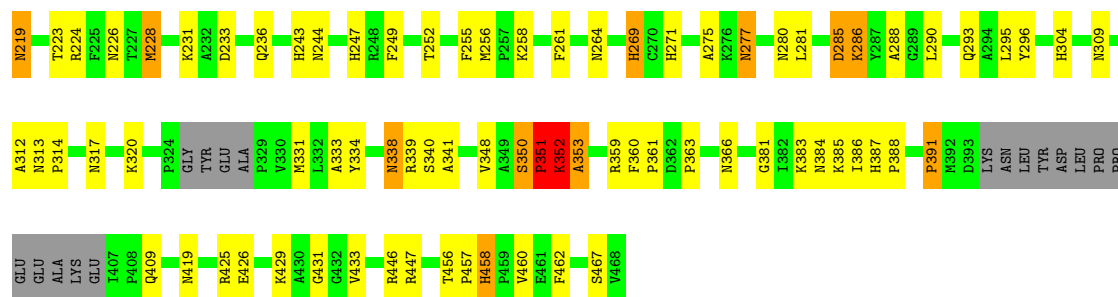
Chain D:  62% 28% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

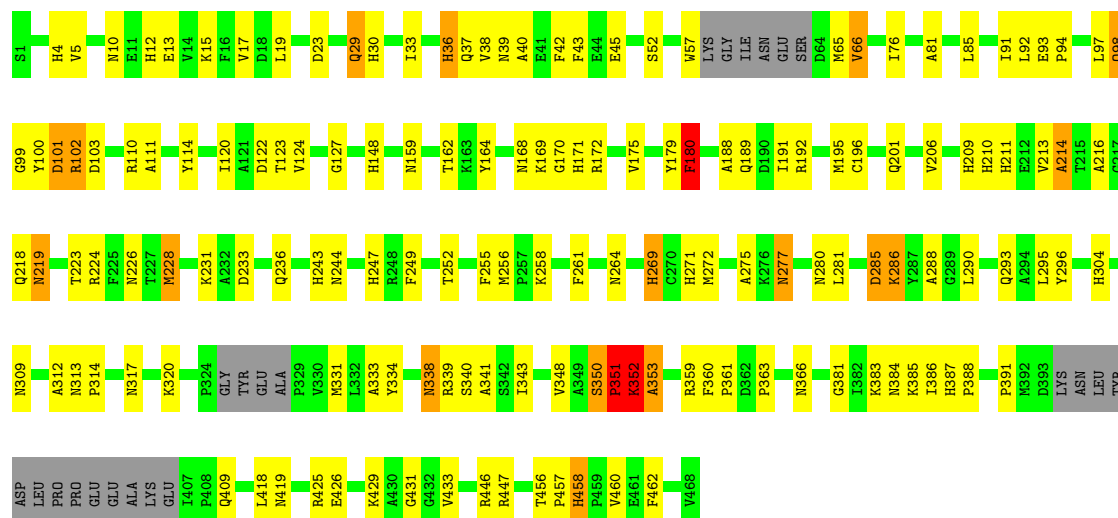
Chain E:  63% 27% 5%





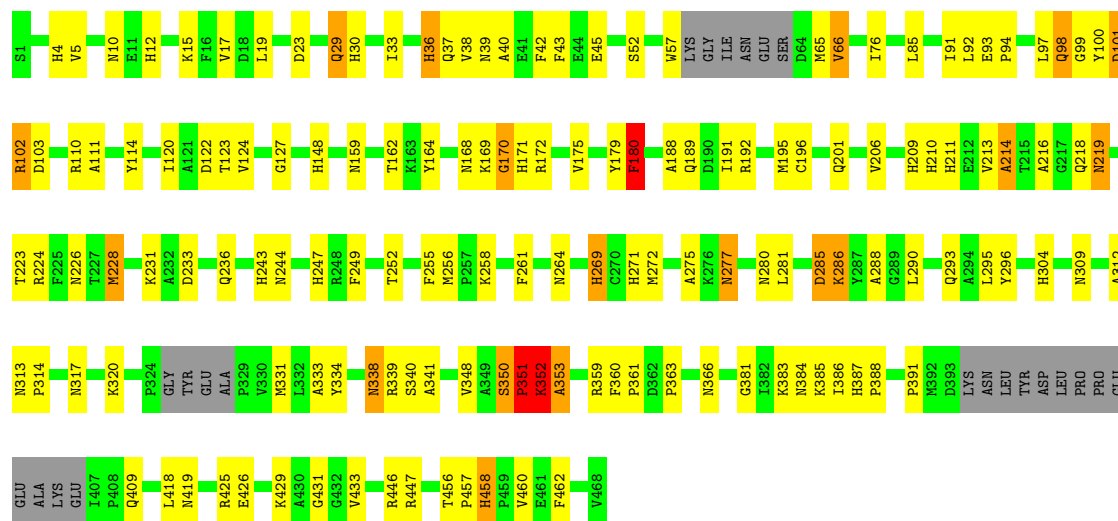
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F: 62% 28% 5%



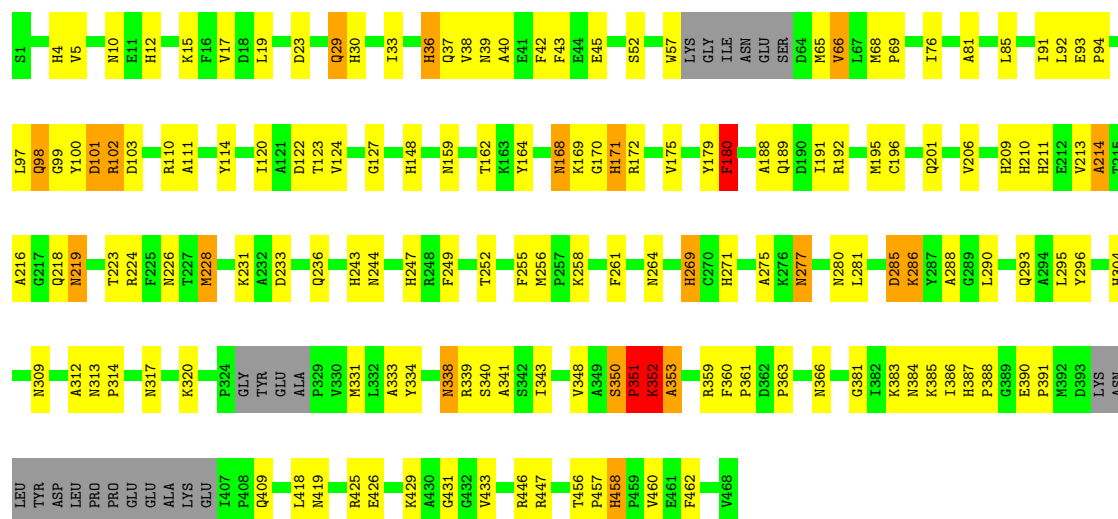
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G: 63% 28% 5%



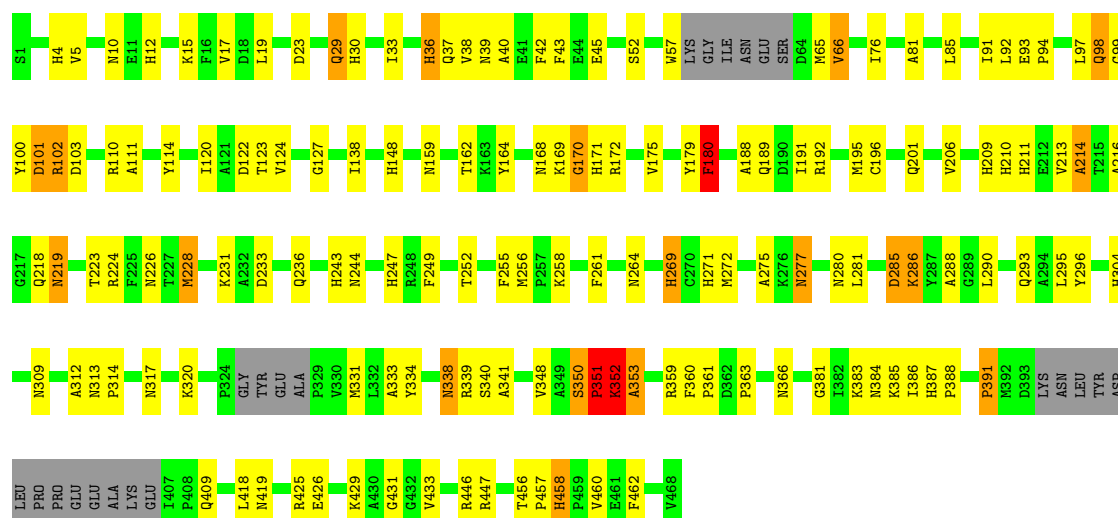
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:  62% 28% • • 5%



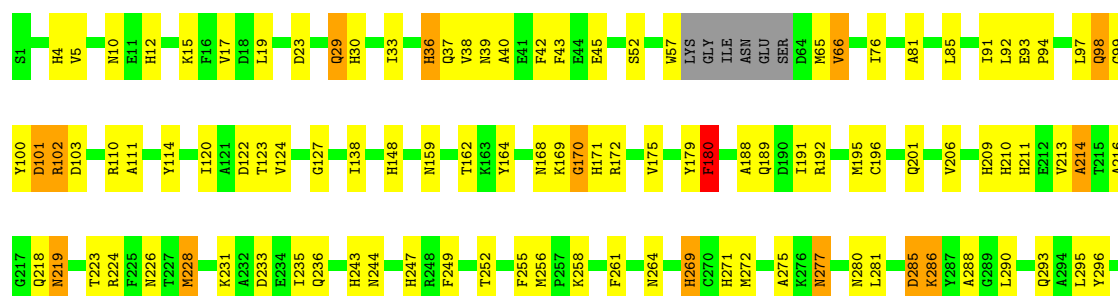
• Molecule 1: GLUTAMINE SYNTHETASE

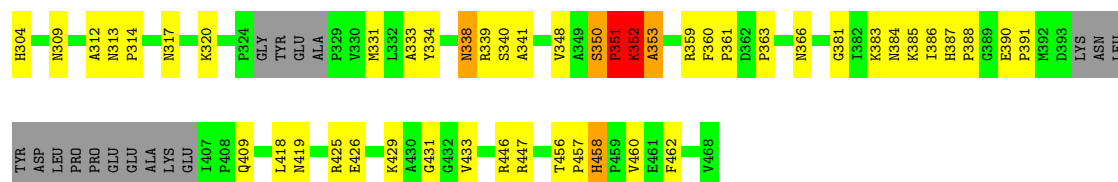
Chain I:  63% 28% • • 5%



• Molecule 1: GLUTAMINE SYNTHETASE

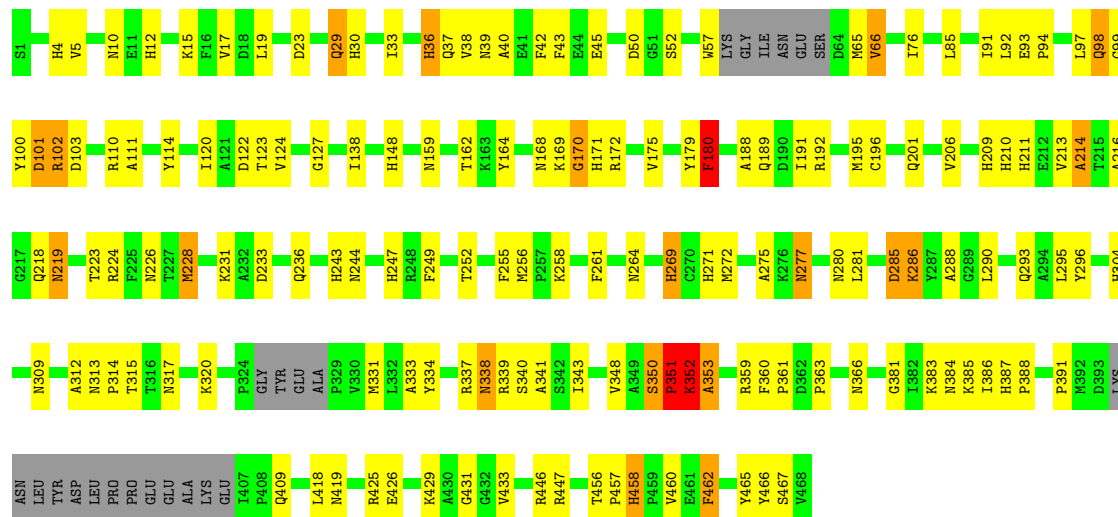
Chain J:  62% 28% • • 5%





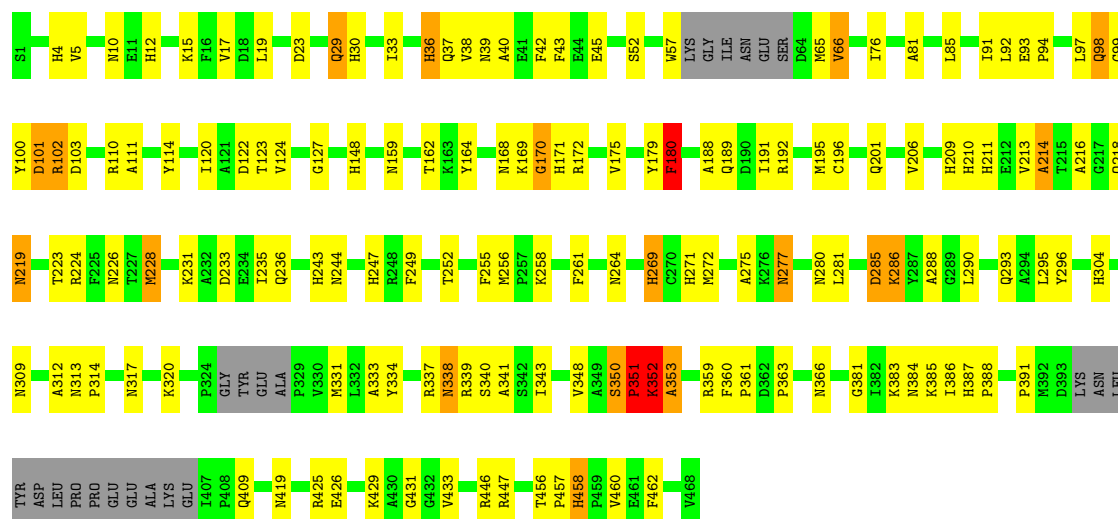
• Molecule 1: GLUTAMINE SYNTHETASE

Chain K: 61% 29% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 62% 28% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.50Å 134.50Å 200.10Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.235 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41604	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	B	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	C	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	D	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	E	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	F	0.96	19/3535 (0.5%)	1.88	99/4782 (2.1%)
1	G	0.96	18/3535 (0.5%)	1.88	99/4782 (2.1%)
1	H	0.96	18/3535 (0.5%)	1.88	99/4782 (2.1%)
1	I	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	J	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	K	0.96	19/3535 (0.5%)	1.88	100/4782 (2.1%)
1	L	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
All	All	0.96	218/42420 (0.5%)	1.88	1202/57384 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

The worst 5 of 218 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	HIS	CD2-NE2	-7.37	1.29	1.37
1	G	211	HIS	CD2-NE2	-7.36	1.29	1.37
1	J	211	HIS	CD2-NE2	-7.35	1.29	1.37
1	E	211	HIS	CD2-NE2	-7.34	1.29	1.37
1	H	211	HIS	CD2-NE2	-7.33	1.29	1.37

The worst 5 of 1202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	K	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	B	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	E	39	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	C	39	ASN	OD1-CG-ND2	-10.47	112.13	122.60

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	352	LYS	Peptide
1	B	224	ARG	Sidechain
1	B	352	LYS	Peptide
1	C	224	ARG	Sidechain

5.2 Too-close contacts

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	3455	0	3371	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3455	0	3371	55	0
1	C	3455	0	3371	61	2
1	D	3455	0	3371	56	0
1	E	3455	0	3371	54	0
1	F	3455	0	3371	54	2
1	G	3455	0	3371	53	0
1	H	3455	0	3371	58	0
1	I	3455	0	3371	56	0
1	J	3455	0	3371	59	0
1	K	3455	0	3371	63	0
1	L	3455	0	3371	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
3	E	10	0	5	1	0
3	F	10	0	5	1	0
3	G	10	0	5	1	0
3	H	10	0	5	1	0
3	I	10	0	5	1	0
3	J	10	0	5	1	0
3	K	10	0	5	1	0
3	L	10	0	5	1	0
All	All	41604	0	40512	622	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 622 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:K:258:LYS:HG2	1:K:320:LYS:HB3	1.79	0.65
1:C:258:LYS:HG2	1:C:320:LYS:HB3	1.79	0.65
1:E:258:LYS:HG2	1:E:320:LYS:HB3	1.79	0.65
1:G:258:LYS:HG2	1:G:320:LYS:HB3	1.79	0.65
1:F:258:LYS:HG2	1:F:320:LYS:HB3	1.79	0.65

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:SER:OG	1:F:13:GLU:OE2[4_454]	1.12	1.08
1:C:1:SER:OG	1:F:13:GLU:CD[4_454]	2.07	0.13

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	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	B	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11
1	C	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11
1	D	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	E	437/468 (93%)	392 (90%)	30 (7%)	15 (3%)	3	11
1	F	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	G	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	H	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	I	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	J	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11
1	K	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	L	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5244/5616 (93%)	4723 (90%)	341 (6%)	180 (3%)	3 11

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	B	180	PHE
1	C	180	PHE
1	D	180	PHE
1	E	180	PHE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLU	C	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.09	0
3	GLU	F	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	G	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	K	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.08	0
3	GLU	E	471	-	8,9,9	1.30	2 (25%)	8,11,11	1.09	0
3	GLU	A	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	B	473	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	H	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	J	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.08	0
3	GLU	D	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	I	471	-	8,9,9	1.30	2 (25%)	8,11,11	1.09	0
3	GLU	L	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	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	GLU	C	471	-	-	6/9/9/9	-
3	GLU	F	471	-	-	6/9/9/9	-
3	GLU	G	471	-	-	6/9/9/9	-
3	GLU	K	471	-	-	6/9/9/9	-
3	GLU	E	471	-	-	6/9/9/9	-
3	GLU	A	471	-	-	6/9/9/9	-
3	GLU	B	473	-	-	6/9/9/9	-
3	GLU	H	471	-	-	6/9/9/9	-
3	GLU	J	471	-	-	6/9/9/9	-
3	GLU	D	471	-	-	6/9/9/9	-
3	GLU	I	471	-	-	6/9/9/9	-
3	GLU	L	471	-	-	6/9/9/9	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	471	GLU	OE2-CD	-2.29	1.23	1.30
3	I	471	GLU	OE2-CD	-2.29	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	471	GLU	OE2-CD	-2.27	1.23	1.30
3	E	471	GLU	OE2-CD	-2.27	1.23	1.30
3	A	471	GLU	OE2-CD	-2.27	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	471	GLU	OXT-C-CA-CB
3	B	473	GLU	OXT-C-CA-CB
3	C	471	GLU	OXT-C-CA-CB
3	D	471	GLU	OXT-C-CA-CB
3	E	471	GLU	OXT-C-CA-CB

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	471	GLU	1	0
3	F	471	GLU	1	0
3	G	471	GLU	1	0
3	K	471	GLU	1	0
3	E	471	GLU	1	0
3	A	471	GLU	1	0
3	B	473	GLU	1	0
3	H	471	GLU	1	0
3	J	471	GLU	1	0
3	D	471	GLU	1	0
3	I	471	GLU	1	0
3	L	471	GLU	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.