



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 05:58 PM BST

PDB ID : 4LNF  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-Q  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 2.95 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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) : 2.14.4.dev1

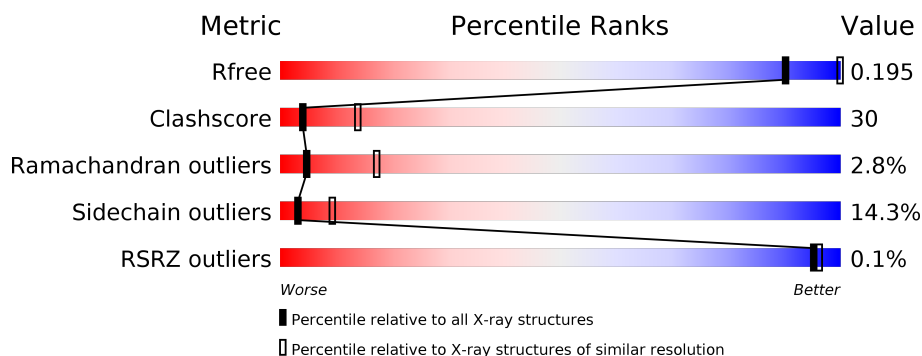
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	443	<div> <div>53%</div> <div>39%</div> <div>9%</div> </div>
1	B	443	<div> <div>48%</div> <div>45%</div> <div>7%</div> </div>
1	C	443	<div> <div>48%</div> <div>43%</div> <div>9%</div> </div>
1	D	443	<div> <div>51%</div> <div>40%</div> <div>8%</div> </div>
1	E	443	<div> <div>54%</div> <div>38%</div> <div>7%</div> </div>
1	F	443	<div> <div>46%</div> <div>43%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	443	
1	H	443	
1	I	443	
1	J	443	
1	K	443	
1	L	443	

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
4	PO4	A	504	-	-	X	-
4	PO4	C	504	-	-	X	-
4	PO4	G	504	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42824 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	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	G	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	H	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	I	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	J	441	Total	C	N	O	S	0	0	0
			3521	2250	587	668	16			
1	K	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	L	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

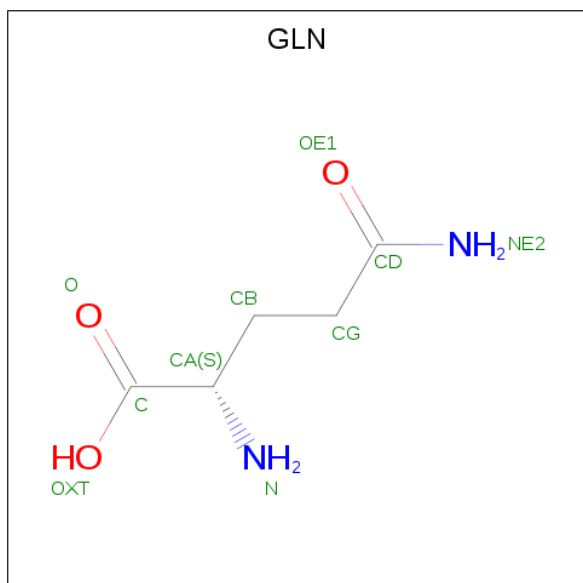
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mg	0	0
			3	3		
2	J	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total 3	Mg 3	0	0
2	K	3	Total 3	Mg 3	0	0
2	E	3	Total 3	Mg 3	0	0
2	H	3	Total 3	Mg 3	0	0
2	B	3	Total 3	Mg 3	0	0
2	I	3	Total 3	Mg 3	0	0
2	C	3	Total 3	Mg 3	0	0
2	A	3	Total 3	Mg 3	0	0
2	L	3	Total 3	Mg 3	0	0
2	F	3	Total 3	Mg 3	0	0

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula:  $C_5H_{10}N_2O_3$ ).



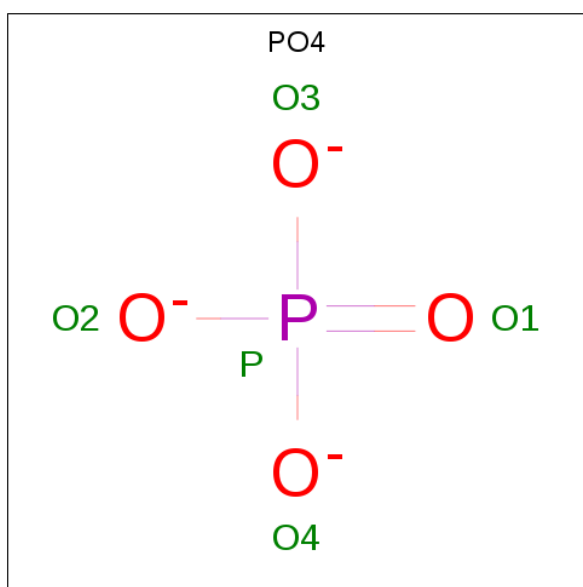
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 5	N 2	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	0
			9	5	2	2		
3	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	E	1	Total	C	N	O	0	0
			9	5	2	2		
3	F	1	Total	C	N	O	0	0
			9	5	2	2		
3	G	1	Total	C	N	O	0	0
			9	5	2	2		
3	H	1	Total	C	N	O	0	0
			9	5	2	2		
3	I	1	Total	C	N	O	0	0
			9	5	2	2		
3	J	1	Total	C	N	O	0	0
			9	5	2	2		
3	K	1	Total	C	N	O	0	0
			9	5	2	2		
3	L	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

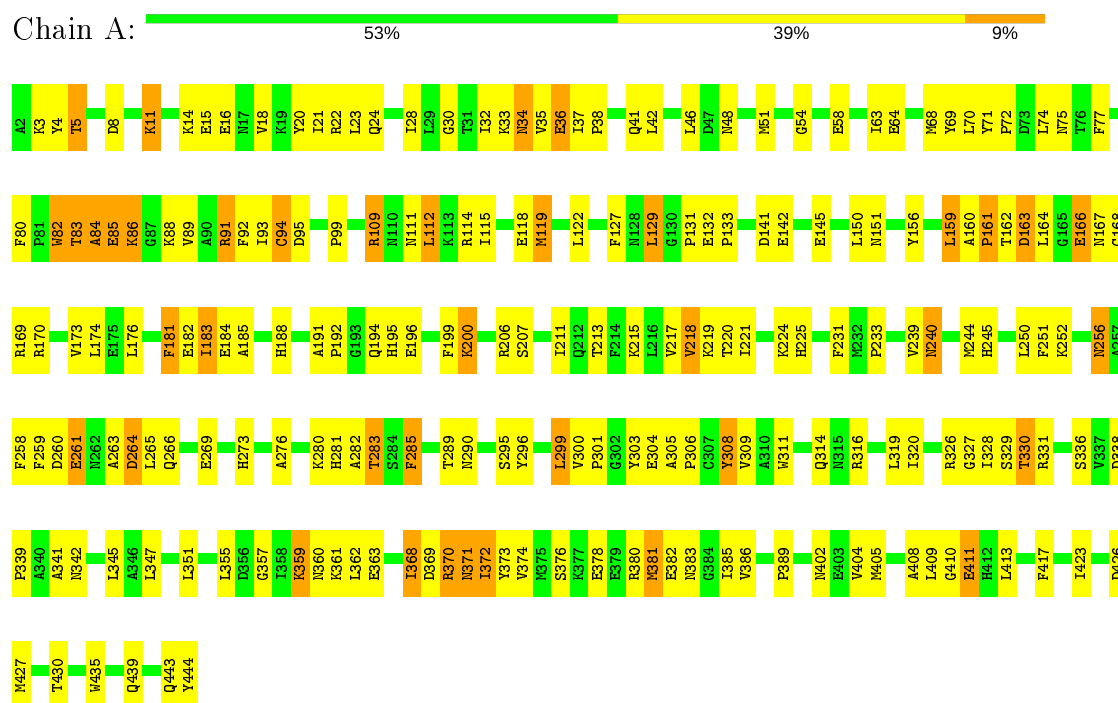
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	20	Total O 20 20	0	0
5	C	18	Total O 18 18	0	0
5	D	29	Total O 29 29	0	0
5	E	18	Total O 18 18	0	0
5	F	19	Total O 19 19	0	0
5	G	14	Total O 14 14	0	0
5	H	21	Total O 21 21	0	0
5	I	21	Total O 21 21	0	0
5	J	27	Total O 27 27	0	0
5	K	27	Total O 27 27	0	0
5	L	23	Total O 23 23	0	0

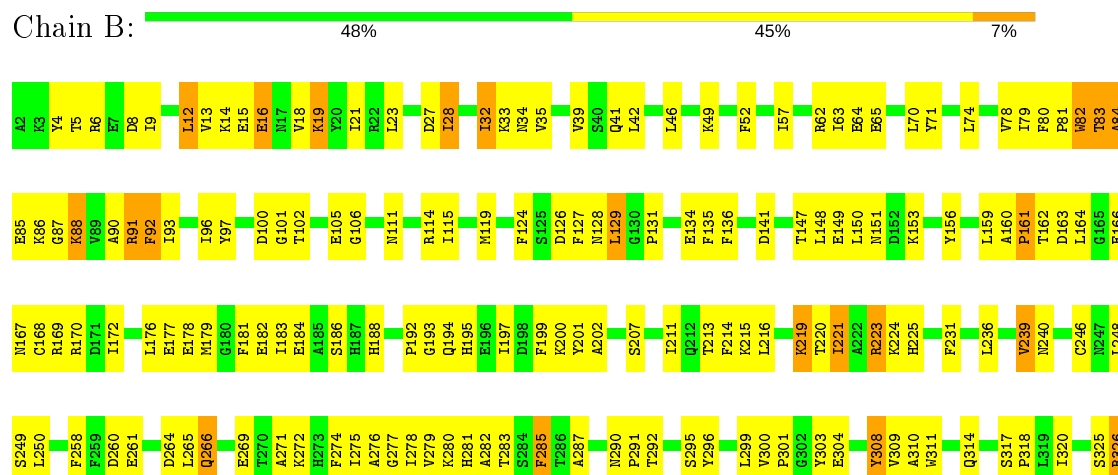
### 3 Residue-property plots

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 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.

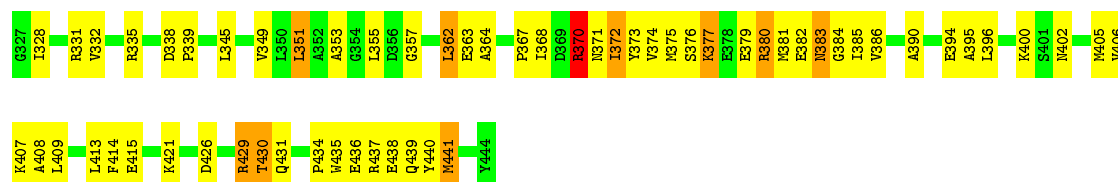
#### • Molecule 1: Glutamine synthetase



#### • Molecule 1: Glutamine synthetase

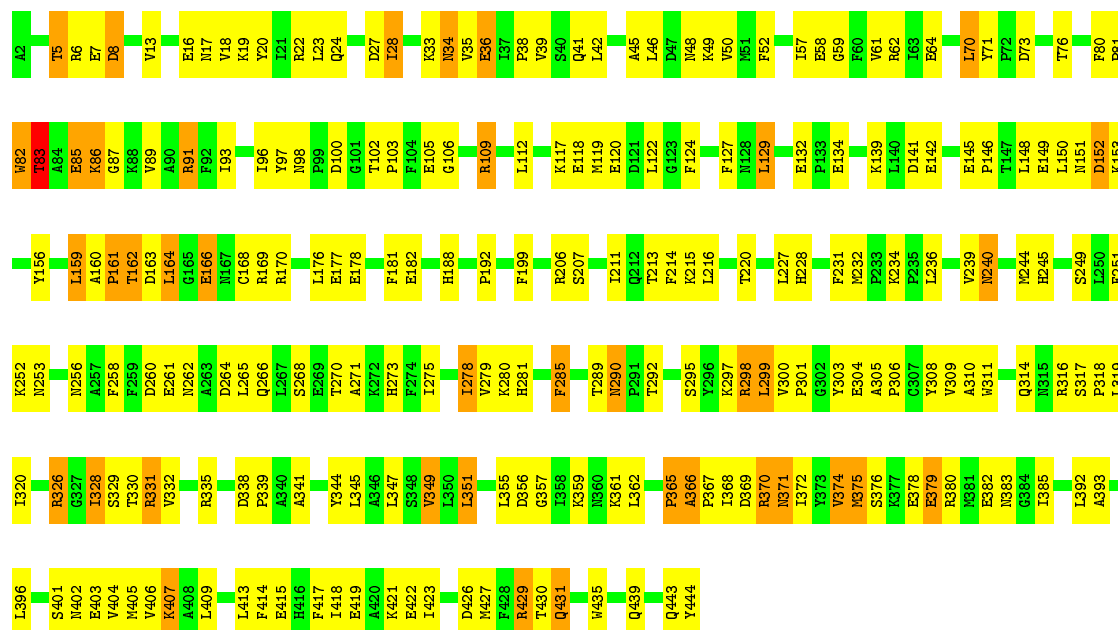






• Molecule 1: Glutamine synthetase

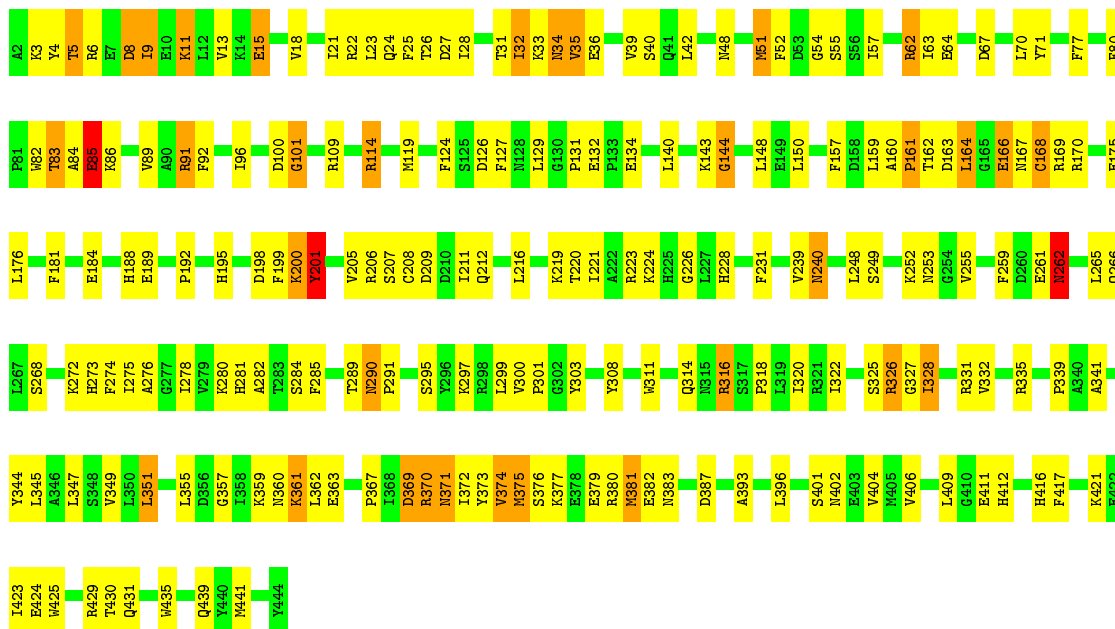
Chain C: 48% 43% 9%





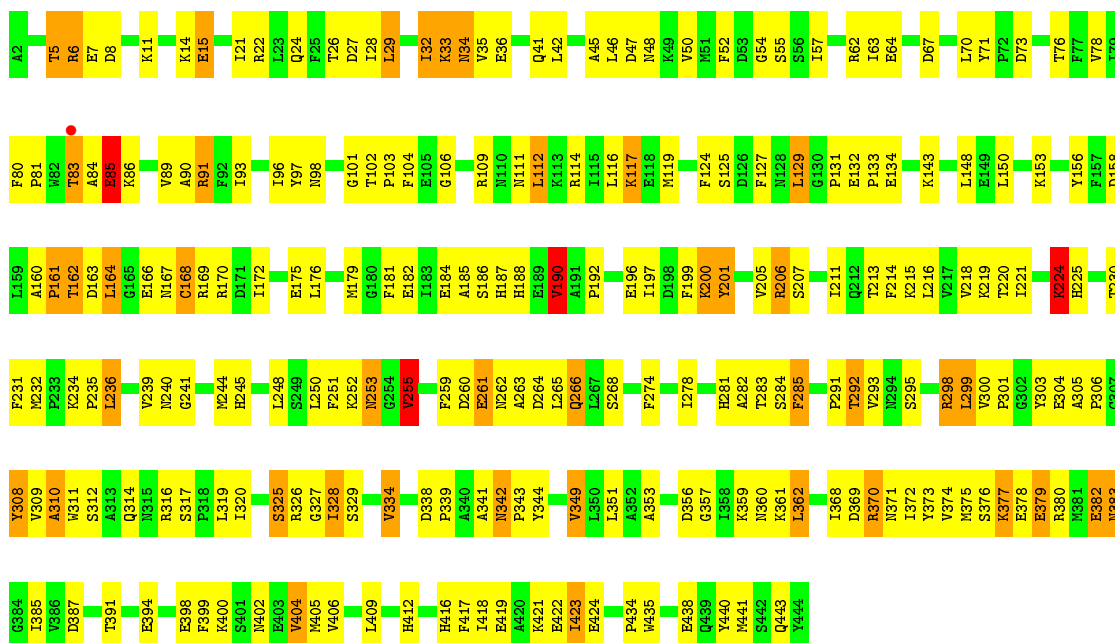
• Molecule 1: Glutamine synthetase

Chain E: 54% 38% 7% •

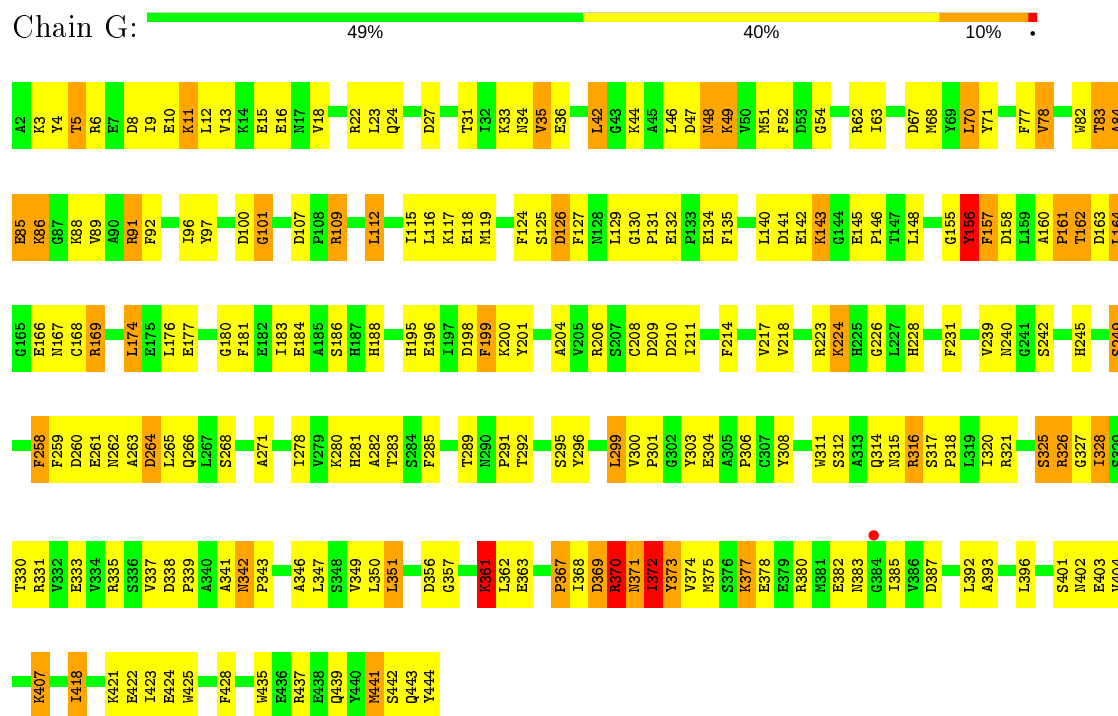


• Molecule 1: Glutamine synthetase

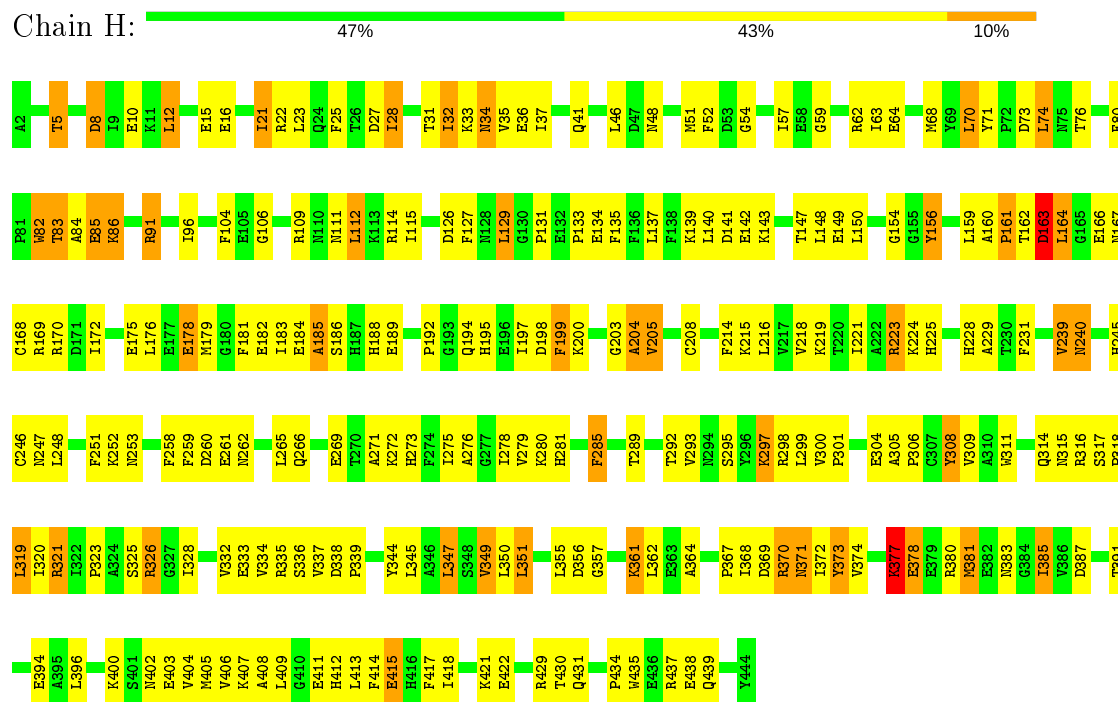
Chain F: 46% 43% 9% •



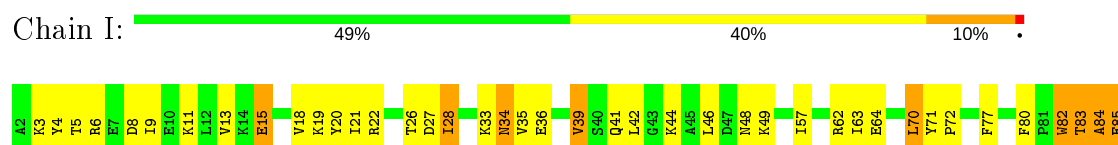
• Molecule 1: Glutamine synthetase

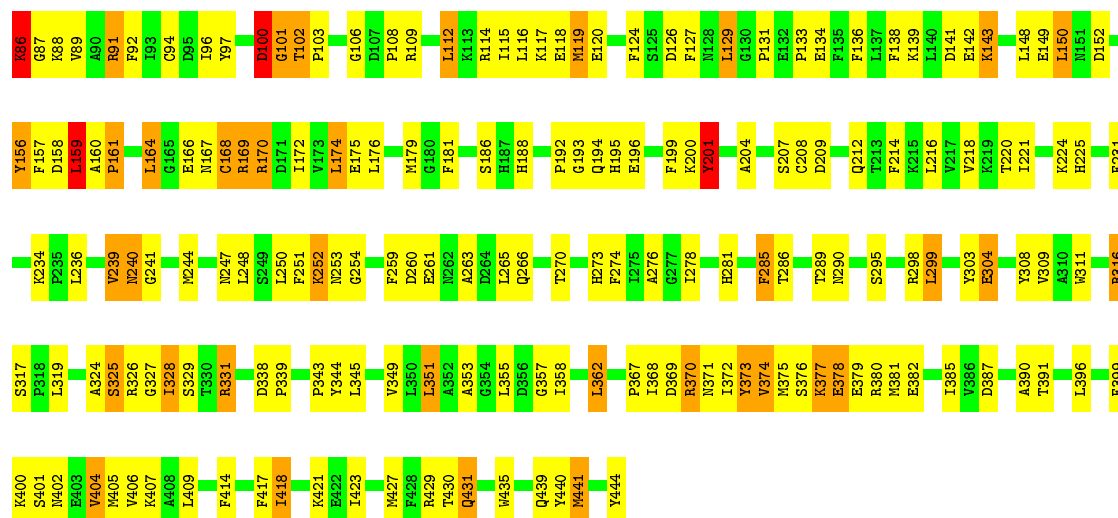


• Molecule 1: Glutamine synthetase

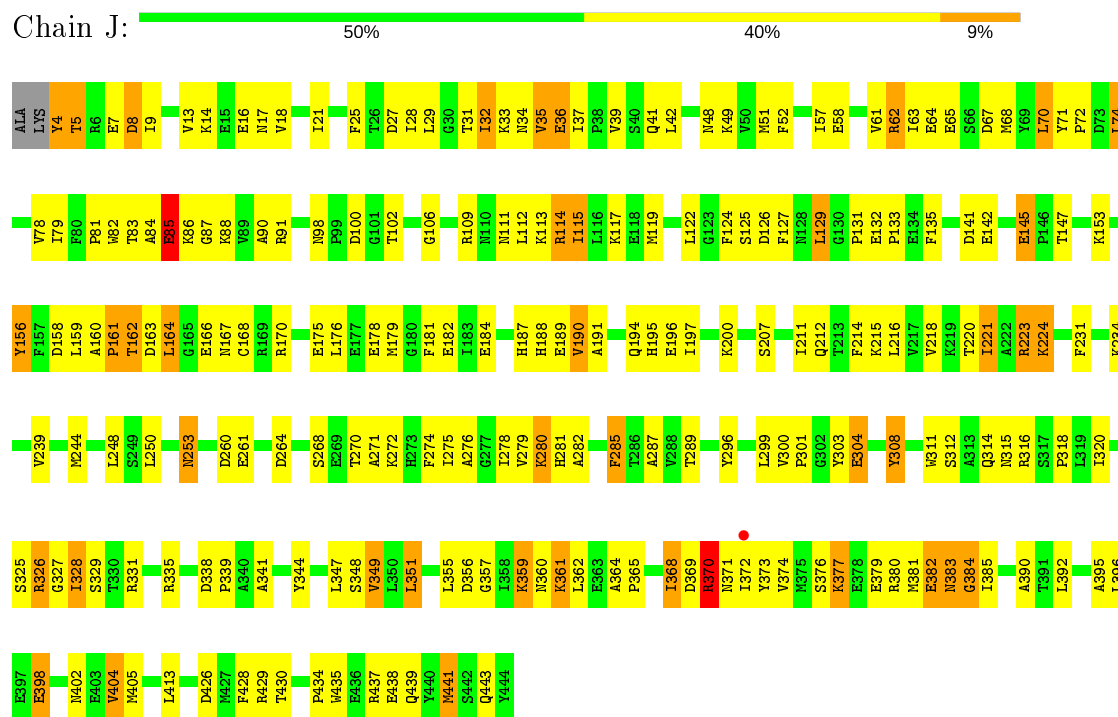


• Molecule 1: Glutamine synthetase

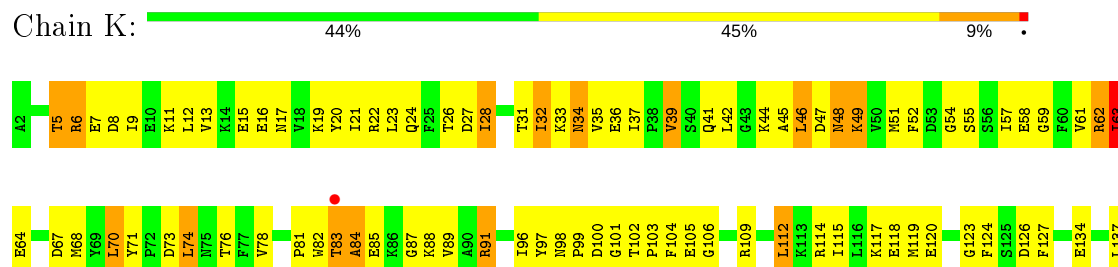


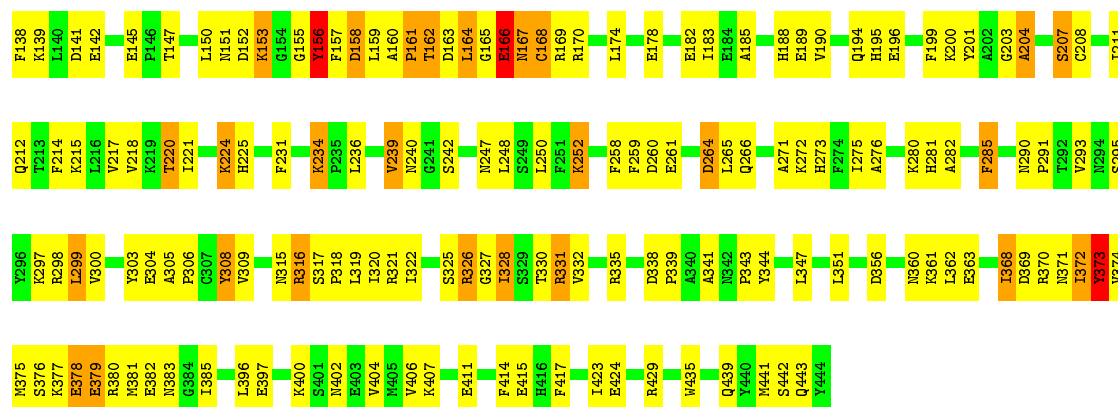


• Molecule 1: Glutamine synthetase

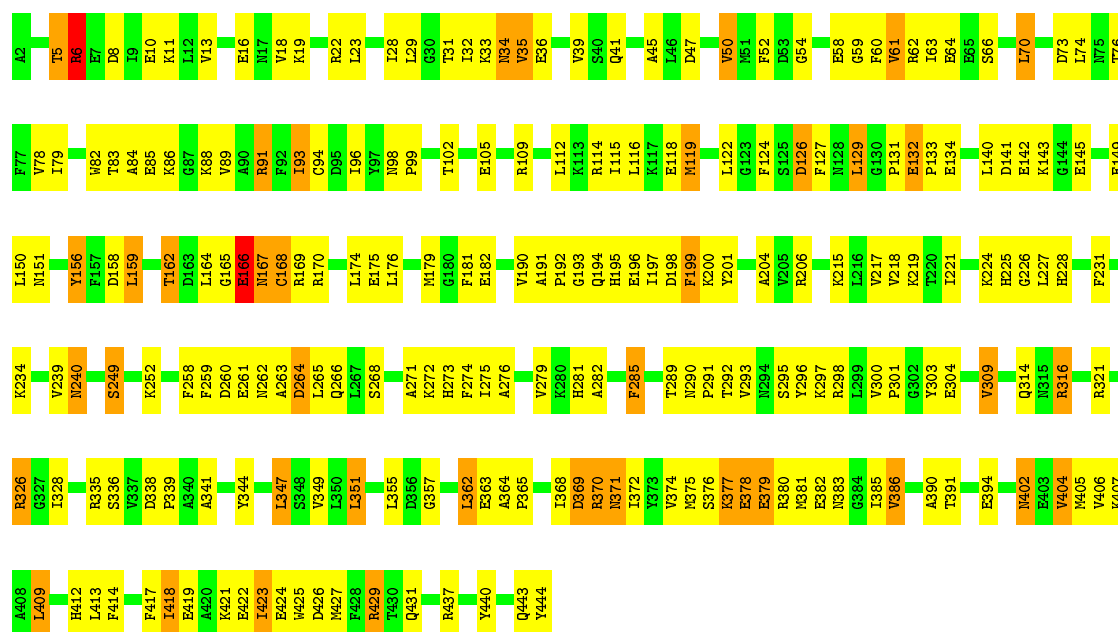


• Molecule 1: Glutamine synthetase





• Molecule 1: Glutamine synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 137.50Å 137.70Å 119.80° 90.30° 93.40°	Depositor
Resolution (Å)	119.01 – 2.95 119.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (119.01-2.95) 94.2 (119.01-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.194 , 0.259 0.188 , 0.195	Depositor DCC
$R_{free}$ test set	11503 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 19.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.357 for -h,-k-l,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	42824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	0.43	0/3618	0.56	0/4895
1	B	0.44	0/3618	0.56	0/4895
1	C	0.44	0/3618	0.58	0/4895
1	D	0.45	1/3618 (0.0%)	0.58	0/4895
1	E	0.46	1/3618 (0.0%)	0.58	0/4895
1	F	0.45	0/3618	0.58	0/4895
1	G	0.44	0/3618	0.59	0/4895
1	H	0.43	0/3618	0.57	0/4895
1	I	0.44	0/3618	0.58	0/4895
1	J	0.45	0/3604	0.57	0/4877
1	K	0.46	0/3618	0.59	0/4895
1	L	0.44	0/3618	0.58	0/4895
All	All	0.45	2/43402 (0.0%)	0.58	0/58722

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	CD-OE2	5.29	1.31	1.25
1	E	168	CYS	CB-SG	-5.09	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3535	0	3466	222	0
1	B	3535	0	3466	238	0
1	C	3535	0	3466	210	0
1	D	3535	0	3466	216	0
1	E	3535	0	3466	218	0
1	F	3535	0	3466	251	0
1	G	3535	0	3466	211	0
1	H	3535	0	3466	228	0
1	I	3535	0	3466	232	0
1	J	3521	0	3448	212	0
1	K	3535	0	3466	261	0
1	L	3535	0	3466	207	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	9	0	7	0	0
3	B	9	0	7	1	0
3	C	9	0	7	3	0
3	D	9	0	7	1	0
3	E	9	0	7	2	0
3	F	9	0	7	1	0
3	G	9	0	7	0	0
3	H	9	0	7	5	0
3	I	9	0	7	1	0
3	J	9	0	7	1	0
3	K	9	0	7	1	0
3	L	10	0	7	0	0
4	A	5	0	0	3	0
4	C	5	0	0	3	0
4	G	5	0	0	2	0
4	H	5	0	0	1	0
5	A	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	0	1	0
5	C	18	0	0	0	0
5	D	29	0	0	4	0
5	E	18	0	0	2	0
5	F	19	0	0	4	0
5	G	14	0	0	0	0
5	H	21	0	0	2	0
5	I	21	0	0	0	0
5	J	27	0	0	1	0
5	K	27	0	0	2	0
5	L	23	0	0	0	0
All	All	42824	0	41658	2533	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 30.

The worst 5 of 2533 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:160:ALA:HB1	1:K:161:PRO:HD2	1.20	1.10
1:G:84:ALA:HB2	1:G:88:LYS:HD3	1.30	1.10
1:H:357:GLY:HA2	1:H:362:LEU:HD23	1.21	1.09
1:K:316:ARG:HD3	1:K:316:ARG:N	1.66	1.09
1:A:357:GLY:HA2	1:A:362:LEU:HD12	1.11	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	441/443 (100%)	383 (87%)	46 (10%)	12 (3%)	5 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	441/443 (100%)	390 (88%)	46 (10%)	5 (1%)	14	40
1	C	441/443 (100%)	392 (89%)	38 (9%)	11 (2%)	5	19
1	D	441/443 (100%)	391 (89%)	38 (9%)	12 (3%)	5	18
1	E	441/443 (100%)	385 (87%)	42 (10%)	14 (3%)	4	14
1	F	441/443 (100%)	385 (87%)	44 (10%)	12 (3%)	5	18
1	G	441/443 (100%)	372 (84%)	52 (12%)	17 (4%)	3	10
1	H	441/443 (100%)	395 (90%)	33 (8%)	13 (3%)	4	16
1	I	441/443 (100%)	385 (87%)	40 (9%)	16 (4%)	3	12
1	J	439/443 (99%)	392 (89%)	36 (8%)	11 (2%)	5	19
1	K	441/443 (100%)	381 (86%)	43 (10%)	17 (4%)	3	10
1	L	441/443 (100%)	382 (87%)	50 (11%)	9 (2%)	7	25
All	All	5290/5316 (100%)	4633 (88%)	508 (10%)	149 (3%)	5	17

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	161	PRO
1	A	166	GLU
1	A	371	ASN
1	A	411	GLU

### 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	382/382 (100%)	333 (87%)	49 (13%)	4	12
1	B	382/382 (100%)	330 (86%)	52 (14%)	3	10
1	C	382/382 (100%)	326 (85%)	56 (15%)	3	9
1	D	382/382 (100%)	328 (86%)	54 (14%)	3	10
1	E	382/382 (100%)	332 (87%)	50 (13%)	4	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	382/382 (100%)	327 (86%)	55 (14%)	3	9
1	G	382/382 (100%)	324 (85%)	58 (15%)	3	8
1	H	382/382 (100%)	330 (86%)	52 (14%)	3	10
1	I	382/382 (100%)	329 (86%)	53 (14%)	3	10
1	J	381/382 (100%)	319 (84%)	62 (16%)	2	6
1	K	382/382 (100%)	330 (86%)	52 (14%)	3	10
1	L	382/382 (100%)	324 (85%)	58 (15%)	3	8
All	All	4583/4584 (100%)	3932 (86%)	651 (14%)	3	9

5 of 651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	292	THR
1	G	372	ILE
1	L	70	LEU
1	F	342	ASN
1	G	91	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	290	ASN
1	G	342	ASN
1	L	128	ASN
1	F	314	GLN
1	G	167	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 52 ligands modelled in this entry, 36 are monoatomic - leaving 16 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	GLN	F	503	-	7,8,9	0.47	0	4,9,11	0.11	0
3	GLN	D	503	2	7,8,9	0.47	0	4,9,11	0.46	0
3	GLN	E	501	2	7,8,9	0.88	0	4,9,11	0.26	0
3	GLN	J	503	2	7,8,9	0.50	0	4,9,11	0.09	0
4	PO4	H	504	2	4,4,4	0.92	0	6,6,6	0.66	0
3	GLN	I	503	-	7,8,9	0.67	0	4,9,11	0.14	0
3	GLN	K	503	-	7,8,9	0.45	0	4,9,11	0.24	0
3	GLN	B	503	2	7,8,9	0.79	0	4,9,11	0.32	0
4	PO4	C	504	2	4,4,4	0.89	0	6,6,6	0.62	0
3	GLN	A	503	2	7,8,9	0.41	0	4,9,11	0.02	0
4	PO4	G	504	2	4,4,4	0.84	0	6,6,6	0.70	0
3	GLN	G	503	2	7,8,9	0.54	0	4,9,11	0.04	0
3	GLN	C	502	2	7,8,9	0.54	0	4,9,11	0.14	0
3	GLN	H	503	2	7,8,9	0.55	0	4,9,11	0.10	0
4	PO4	A	504	2	4,4,4	0.77	0	6,6,6	0.93	0
3	GLN	L	503	2	5,9,9	0.31	0	5,11,11	0.55	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	GLN	F	503	-	-	2/6/7/9	-
3	GLN	D	503	2	-	1/6/7/9	-
3	GLN	E	501	2	-	3/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLN	J	503	2	-	3/6/7/9	-
3	GLN	K	503	-	-	2/6/7/9	-
3	GLN	I	503	-	-	4/6/7/9	-
3	GLN	B	503	2	-	2/6/7/9	-
3	GLN	A	503	2	-	0/6/7/9	-
3	GLN	G	503	2	-	2/6/7/9	-
3	GLN	C	502	2	-	4/6/7/9	-
3	GLN	H	503	2	-	4/6/7/9	-
3	GLN	L	503	2	-	2/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GLN	N-CA-CB-CG
3	B	503	GLN	C-CA-CB-CG
3	I	503	GLN	O-C-CA-CB
3	I	503	GLN	N-CA-CB-CG
3	I	503	GLN	C-CA-CB-CG

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	503	GLN	1	0
3	D	503	GLN	1	0
3	E	501	GLN	2	0
3	J	503	GLN	1	0
4	H	504	PO4	1	0
3	I	503	GLN	1	0
3	K	503	GLN	1	0
3	B	503	GLN	1	0
4	C	504	PO4	3	0
4	G	504	PO4	2	0
3	C	502	GLN	3	0
3	H	503	GLN	5	0
4	A	504	PO4	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	443/443 (100%)	-0.66	0	100	100	24, 38, 70, 96	0
1	B	443/443 (100%)	-0.67	0	100	100	24, 37, 71, 98	0
1	C	443/443 (100%)	-0.68	0	100	100	20, 36, 65, 98	0
1	D	443/443 (100%)	-0.70	0	100	100	22, 34, 68, 92	0
1	E	443/443 (100%)	-0.64	0	100	100	21, 35, 69, 99	0
1	F	443/443 (100%)	-0.62	1 (0%)	95	95	20, 36, 70, 102	0
1	G	443/443 (100%)	-0.66	1 (0%)	95	95	24, 37, 68, 100	0
1	H	443/443 (100%)	-0.63	0	100	100	24, 36, 68, 104	0
1	I	443/443 (100%)	-0.66	0	100	100	20, 35, 67, 97	0
1	J	441/443 (99%)	-0.68	1 (0%)	95	95	21, 34, 67, 98	0
1	K	443/443 (100%)	-0.64	1 (0%)	95	95	22, 36, 70, 106	0
1	L	443/443 (100%)	-0.69	0	100	100	23, 36, 68, 101	0
All	All	5314/5316 (99%)	-0.66	4 (0%)	95	96	20, 36, 70, 106	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	384	GLY	2.9
1	K	83	THR	2.7
1	F	83	THR	2.6
1	J	372	ILE	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PO4	G	504	5/5	0.77	0.39	81,82,94,97	0
4	PO4	H	504	5/5	0.82	0.32	91,92,112,116	0
4	PO4	A	504	5/5	0.86	0.25	80,81,89,94	0
2	MG	I	504	1/1	0.87	0.12	28,28,28,28	0
2	MG	I	501	1/1	0.88	0.15	19,19,19,19	0
3	GLN	K	503	9/10	0.88	0.19	26,33,39,40	0
2	MG	K	501	1/1	0.88	0.19	19,19,19,19	0
2	MG	L	501	1/1	0.89	0.17	22,22,22,22	0
2	MG	C	505	1/1	0.89	0.16	32,32,32,32	0
3	GLN	J	503	9/10	0.90	0.16	25,32,37,41	0
2	MG	B	504	1/1	0.91	0.12	39,39,39,39	0
2	MG	H	501	1/1	0.92	0.17	32,32,32,32	0
2	MG	G	502	1/1	0.92	0.18	35,35,35,35	0
2	MG	H	502	1/1	0.92	0.06	50,50,50,50	0
3	GLN	E	501	9/10	0.92	0.17	22,26,33,36	0
2	MG	J	502	1/1	0.93	0.17	23,23,23,23	0
2	MG	E	502	1/1	0.93	0.12	28,28,28,28	0
2	MG	F	504	1/1	0.93	0.14	25,25,25,25	0
2	MG	G	501	1/1	0.93	0.07	45,45,45,45	0
2	MG	E	503	1/1	0.94	0.08	25,25,25,25	0
3	GLN	G	503	9/10	0.94	0.15	35,39,44,45	0
2	MG	A	505	1/1	0.94	0.12	31,31,31,31	0
2	MG	L	504	1/1	0.94	0.12	28,28,28,28	0
4	PO4	C	504	5/5	0.94	0.12	35,44,67,68	0
2	MG	J	504	1/1	0.94	0.12	21,21,21,21	0
3	GLN	H	503	9/10	0.94	0.15	32,37,47,47	0
2	MG	D	501	1/1	0.94	0.17	23,23,23,23	0
3	GLN	C	502	9/10	0.94	0.14	31,34,37,39	0
3	GLN	I	503	9/10	0.95	0.15	26,29,34,35	0
3	GLN	F	503	9/10	0.95	0.21	29,32,35,36	0
2	MG	E	504	1/1	0.95	0.08	30,30,30,30	0
2	MG	F	501	1/1	0.95	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	502	1/1	0.95	0.19	35,35,35,35	0
2	MG	F	502	1/1	0.95	0.09	29,29,29,29	0
2	MG	A	501	1/1	0.96	0.11	31,31,31,31	0
3	GLN	L	503	10/10	0.96	0.15	31,33,41,44	0
3	GLN	A	503	9/10	0.96	0.14	37,41,50,57	0
2	MG	H	505	1/1	0.96	0.14	21,21,21,21	0
3	GLN	D	503	9/10	0.96	0.15	23,29,33,35	0
2	MG	C	503	1/1	0.96	0.17	33,33,33,33	0
2	MG	K	504	1/1	0.96	0.08	21,21,21,21	0
3	GLN	B	503	9/10	0.96	0.14	28,34,37,38	0
2	MG	B	501	1/1	0.97	0.15	24,24,24,24	0
2	MG	C	501	1/1	0.97	0.07	29,29,29,29	0
2	MG	L	502	1/1	0.97	0.11	26,26,26,26	0
2	MG	B	502	1/1	0.98	0.12	29,29,29,29	0
2	MG	J	501	1/1	0.98	0.11	28,28,28,28	0
2	MG	G	505	1/1	0.98	0.15	31,31,31,31	0
2	MG	D	504	1/1	0.98	0.04	20,20,20,20	0
2	MG	A	502	1/1	0.98	0.06	45,45,45,45	0
2	MG	I	502	1/1	0.99	0.12	28,28,28,28	0
2	MG	K	502	1/1	0.99	0.14	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.