



# wwPDB X-ray Structure Validation Summary Report

Sep 16, 2014 – 02:54 PM EDT

PDB ID : 4IS4  
Title : The glutamine synthetase from the dicotyledonous plant *M. truncatula* is a decamer  
Authors : Seabra, A.R.; Carvalho, H.; Pereira, P.J.B.  
Deposited on : 2013-01-16  
Resolution : 2.35 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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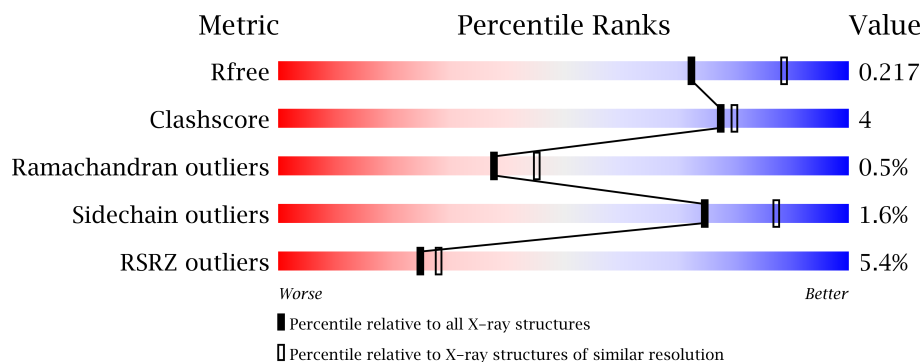
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	378	
1	B	378	
1	C	378	
1	D	378	
1	E	378	
1	F	378	
1	G	378	
1	H	378	
1	I	378	
1	J	378	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24909 atoms, of which 0 are hydrogen and 0 are deuterium.

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	339	Total	C	N	O	S	0	0	0
			2636	1680	446	501	9			
1	B	306	Total	C	N	O	S	0	0	0
			2378	1520	397	452	9			
1	C	311	Total	C	N	O	S	0	0	0
			2424	1551	405	459	9			
1	D	304	Total	C	N	O	S	0	0	0
			2360	1514	388	449	9			
1	E	293	Total	C	N	O	S	0	0	0
			2276	1462	373	432	9			
1	F	307	Total	C	N	O	S	0	0	0
			2389	1530	397	453	9			
1	G	311	Total	C	N	O	S	0	0	0
			2419	1547	404	459	9			
1	H	302	Total	C	N	O	S	0	0	0
			2354	1509	389	447	9			
1	I	303	Total	C	N	O	S	0	0	0
			2356	1512	387	448	9			
1	J	302	Total	C	N	O	S	0	0	0
			2348	1505	387	447	9			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP O04998
A	-20	GLY	-	EXPRESSION TAG	UNP O04998
A	-19	SER	-	EXPRESSION TAG	UNP O04998
A	-18	SER	-	EXPRESSION TAG	UNP O04998
A	-17	HIS	-	EXPRESSION TAG	UNP O04998
A	-16	HIS	-	EXPRESSION TAG	UNP O04998
A	-15	HIS	-	EXPRESSION TAG	UNP O04998
A	-14	HIS	-	EXPRESSION TAG	UNP O04998
A	-13	HIS	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	EXPRESSION TAG	UNP O04998
A	-11	SER	-	EXPRESSION TAG	UNP O04998
A	-10	SER	-	EXPRESSION TAG	UNP O04998
A	-9	GLY	-	EXPRESSION TAG	UNP O04998
A	-8	LEU	-	EXPRESSION TAG	UNP O04998
A	-7	VAL	-	EXPRESSION TAG	UNP O04998
A	-6	PRO	-	EXPRESSION TAG	UNP O04998
A	-5	ARG	-	EXPRESSION TAG	UNP O04998
A	-4	GLY	-	EXPRESSION TAG	UNP O04998
A	-3	SER	-	EXPRESSION TAG	UNP O04998
A	-2	HIS	-	EXPRESSION TAG	UNP O04998
A	-1	ALA	-	EXPRESSION TAG	UNP O04998
A	0	SER	-	EXPRESSION TAG	UNP O04998
B	-21	MET	-	EXPRESSION TAG	UNP O04998
B	-20	GLY	-	EXPRESSION TAG	UNP O04998
B	-19	SER	-	EXPRESSION TAG	UNP O04998
B	-18	SER	-	EXPRESSION TAG	UNP O04998
B	-17	HIS	-	EXPRESSION TAG	UNP O04998
B	-16	HIS	-	EXPRESSION TAG	UNP O04998
B	-15	HIS	-	EXPRESSION TAG	UNP O04998
B	-14	HIS	-	EXPRESSION TAG	UNP O04998
B	-13	HIS	-	EXPRESSION TAG	UNP O04998
B	-12	HIS	-	EXPRESSION TAG	UNP O04998
B	-11	SER	-	EXPRESSION TAG	UNP O04998
B	-10	SER	-	EXPRESSION TAG	UNP O04998
B	-9	GLY	-	EXPRESSION TAG	UNP O04998
B	-8	LEU	-	EXPRESSION TAG	UNP O04998
B	-7	VAL	-	EXPRESSION TAG	UNP O04998
B	-6	PRO	-	EXPRESSION TAG	UNP O04998
B	-5	ARG	-	EXPRESSION TAG	UNP O04998
B	-4	GLY	-	EXPRESSION TAG	UNP O04998
B	-3	SER	-	EXPRESSION TAG	UNP O04998
B	-2	HIS	-	EXPRESSION TAG	UNP O04998
B	-1	ALA	-	EXPRESSION TAG	UNP O04998
B	0	SER	-	EXPRESSION TAG	UNP O04998
C	-21	MET	-	EXPRESSION TAG	UNP O04998
C	-20	GLY	-	EXPRESSION TAG	UNP O04998
C	-19	SER	-	EXPRESSION TAG	UNP O04998
C	-18	SER	-	EXPRESSION TAG	UNP O04998
C	-17	HIS	-	EXPRESSION TAG	UNP O04998
C	-16	HIS	-	EXPRESSION TAG	UNP O04998
C	-15	HIS	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP O04998
C	-13	HIS	-	EXPRESSION TAG	UNP O04998
C	-12	HIS	-	EXPRESSION TAG	UNP O04998
C	-11	SER	-	EXPRESSION TAG	UNP O04998
C	-10	SER	-	EXPRESSION TAG	UNP O04998
C	-9	GLY	-	EXPRESSION TAG	UNP O04998
C	-8	LEU	-	EXPRESSION TAG	UNP O04998
C	-7	VAL	-	EXPRESSION TAG	UNP O04998
C	-6	PRO	-	EXPRESSION TAG	UNP O04998
C	-5	ARG	-	EXPRESSION TAG	UNP O04998
C	-4	GLY	-	EXPRESSION TAG	UNP O04998
C	-3	SER	-	EXPRESSION TAG	UNP O04998
C	-2	HIS	-	EXPRESSION TAG	UNP O04998
C	-1	ALA	-	EXPRESSION TAG	UNP O04998
C	0	SER	-	EXPRESSION TAG	UNP O04998
D	-21	MET	-	EXPRESSION TAG	UNP O04998
D	-20	GLY	-	EXPRESSION TAG	UNP O04998
D	-19	SER	-	EXPRESSION TAG	UNP O04998
D	-18	SER	-	EXPRESSION TAG	UNP O04998
D	-17	HIS	-	EXPRESSION TAG	UNP O04998
D	-16	HIS	-	EXPRESSION TAG	UNP O04998
D	-15	HIS	-	EXPRESSION TAG	UNP O04998
D	-14	HIS	-	EXPRESSION TAG	UNP O04998
D	-13	HIS	-	EXPRESSION TAG	UNP O04998
D	-12	HIS	-	EXPRESSION TAG	UNP O04998
D	-11	SER	-	EXPRESSION TAG	UNP O04998
D	-10	SER	-	EXPRESSION TAG	UNP O04998
D	-9	GLY	-	EXPRESSION TAG	UNP O04998
D	-8	LEU	-	EXPRESSION TAG	UNP O04998
D	-7	VAL	-	EXPRESSION TAG	UNP O04998
D	-6	PRO	-	EXPRESSION TAG	UNP O04998
D	-5	ARG	-	EXPRESSION TAG	UNP O04998
D	-4	GLY	-	EXPRESSION TAG	UNP O04998
D	-3	SER	-	EXPRESSION TAG	UNP O04998
D	-2	HIS	-	EXPRESSION TAG	UNP O04998
D	-1	ALA	-	EXPRESSION TAG	UNP O04998
D	0	SER	-	EXPRESSION TAG	UNP O04998
E	-21	MET	-	EXPRESSION TAG	UNP O04998
E	-20	GLY	-	EXPRESSION TAG	UNP O04998
E	-19	SER	-	EXPRESSION TAG	UNP O04998
E	-18	SER	-	EXPRESSION TAG	UNP O04998
E	-17	HIS	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	EXPRESSION TAG	UNP O04998
E	-15	HIS	-	EXPRESSION TAG	UNP O04998
E	-14	HIS	-	EXPRESSION TAG	UNP O04998
E	-13	HIS	-	EXPRESSION TAG	UNP O04998
E	-12	HIS	-	EXPRESSION TAG	UNP O04998
E	-11	SER	-	EXPRESSION TAG	UNP O04998
E	-10	SER	-	EXPRESSION TAG	UNP O04998
E	-9	GLY	-	EXPRESSION TAG	UNP O04998
E	-8	LEU	-	EXPRESSION TAG	UNP O04998
E	-7	VAL	-	EXPRESSION TAG	UNP O04998
E	-6	PRO	-	EXPRESSION TAG	UNP O04998
E	-5	ARG	-	EXPRESSION TAG	UNP O04998
E	-4	GLY	-	EXPRESSION TAG	UNP O04998
E	-3	SER	-	EXPRESSION TAG	UNP O04998
E	-2	HIS	-	EXPRESSION TAG	UNP O04998
E	-1	ALA	-	EXPRESSION TAG	UNP O04998
E	0	SER	-	EXPRESSION TAG	UNP O04998
F	-21	MET	-	EXPRESSION TAG	UNP O04998
F	-20	GLY	-	EXPRESSION TAG	UNP O04998
F	-19	SER	-	EXPRESSION TAG	UNP O04998
F	-18	SER	-	EXPRESSION TAG	UNP O04998
F	-17	HIS	-	EXPRESSION TAG	UNP O04998
F	-16	HIS	-	EXPRESSION TAG	UNP O04998
F	-15	HIS	-	EXPRESSION TAG	UNP O04998
F	-14	HIS	-	EXPRESSION TAG	UNP O04998
F	-13	HIS	-	EXPRESSION TAG	UNP O04998
F	-12	HIS	-	EXPRESSION TAG	UNP O04998
F	-11	SER	-	EXPRESSION TAG	UNP O04998
F	-10	SER	-	EXPRESSION TAG	UNP O04998
F	-9	GLY	-	EXPRESSION TAG	UNP O04998
F	-8	LEU	-	EXPRESSION TAG	UNP O04998
F	-7	VAL	-	EXPRESSION TAG	UNP O04998
F	-6	PRO	-	EXPRESSION TAG	UNP O04998
F	-5	ARG	-	EXPRESSION TAG	UNP O04998
F	-4	GLY	-	EXPRESSION TAG	UNP O04998
F	-3	SER	-	EXPRESSION TAG	UNP O04998
F	-2	HIS	-	EXPRESSION TAG	UNP O04998
F	-1	ALA	-	EXPRESSION TAG	UNP O04998
F	0	SER	-	EXPRESSION TAG	UNP O04998
G	-21	MET	-	EXPRESSION TAG	UNP O04998
G	-20	GLY	-	EXPRESSION TAG	UNP O04998
G	-19	SER	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	SER	-	EXPRESSION TAG	UNP O04998
G	-17	HIS	-	EXPRESSION TAG	UNP O04998
G	-16	HIS	-	EXPRESSION TAG	UNP O04998
G	-15	HIS	-	EXPRESSION TAG	UNP O04998
G	-14	HIS	-	EXPRESSION TAG	UNP O04998
G	-13	HIS	-	EXPRESSION TAG	UNP O04998
G	-12	HIS	-	EXPRESSION TAG	UNP O04998
G	-11	SER	-	EXPRESSION TAG	UNP O04998
G	-10	SER	-	EXPRESSION TAG	UNP O04998
G	-9	GLY	-	EXPRESSION TAG	UNP O04998
G	-8	LEU	-	EXPRESSION TAG	UNP O04998
G	-7	VAL	-	EXPRESSION TAG	UNP O04998
G	-6	PRO	-	EXPRESSION TAG	UNP O04998
G	-5	ARG	-	EXPRESSION TAG	UNP O04998
G	-4	GLY	-	EXPRESSION TAG	UNP O04998
G	-3	SER	-	EXPRESSION TAG	UNP O04998
G	-2	HIS	-	EXPRESSION TAG	UNP O04998
G	-1	ALA	-	EXPRESSION TAG	UNP O04998
G	0	SER	-	EXPRESSION TAG	UNP O04998
H	-21	MET	-	EXPRESSION TAG	UNP O04998
H	-20	GLY	-	EXPRESSION TAG	UNP O04998
H	-19	SER	-	EXPRESSION TAG	UNP O04998
H	-18	SER	-	EXPRESSION TAG	UNP O04998
H	-17	HIS	-	EXPRESSION TAG	UNP O04998
H	-16	HIS	-	EXPRESSION TAG	UNP O04998
H	-15	HIS	-	EXPRESSION TAG	UNP O04998
H	-14	HIS	-	EXPRESSION TAG	UNP O04998
H	-13	HIS	-	EXPRESSION TAG	UNP O04998
H	-12	HIS	-	EXPRESSION TAG	UNP O04998
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H	-10	SER	-	EXPRESSION TAG	UNP O04998
H	-9	GLY	-	EXPRESSION TAG	UNP O04998
H	-8	LEU	-	EXPRESSION TAG	UNP O04998
H	-7	VAL	-	EXPRESSION TAG	UNP O04998
H	-6	PRO	-	EXPRESSION TAG	UNP O04998
H	-5	ARG	-	EXPRESSION TAG	UNP O04998
H	-4	GLY	-	EXPRESSION TAG	UNP O04998
H	-3	SER	-	EXPRESSION TAG	UNP O04998
H	-2	HIS	-	EXPRESSION TAG	UNP O04998
H	-1	ALA	-	EXPRESSION TAG	UNP O04998
H	0	SER	-	EXPRESSION TAG	UNP O04998
I	-21	MET	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-20	GLY	-	EXPRESSION TAG	UNP O04998
I	-19	SER	-	EXPRESSION TAG	UNP O04998
I	-18	SER	-	EXPRESSION TAG	UNP O04998
I	-17	HIS	-	EXPRESSION TAG	UNP O04998
I	-16	HIS	-	EXPRESSION TAG	UNP O04998
I	-15	HIS	-	EXPRESSION TAG	UNP O04998
I	-14	HIS	-	EXPRESSION TAG	UNP O04998
I	-13	HIS	-	EXPRESSION TAG	UNP O04998
I	-12	HIS	-	EXPRESSION TAG	UNP O04998
I	-11	SER	-	EXPRESSION TAG	UNP O04998
I	-10	SER	-	EXPRESSION TAG	UNP O04998
I	-9	GLY	-	EXPRESSION TAG	UNP O04998
I	-8	LEU	-	EXPRESSION TAG	UNP O04998
I	-7	VAL	-	EXPRESSION TAG	UNP O04998
I	-6	PRO	-	EXPRESSION TAG	UNP O04998
I	-5	ARG	-	EXPRESSION TAG	UNP O04998
I	-4	GLY	-	EXPRESSION TAG	UNP O04998
I	-3	SER	-	EXPRESSION TAG	UNP O04998
I	-2	HIS	-	EXPRESSION TAG	UNP O04998
I	-1	ALA	-	EXPRESSION TAG	UNP O04998
I	0	SER	-	EXPRESSION TAG	UNP O04998
J	-21	MET	-	EXPRESSION TAG	UNP O04998
J	-20	GLY	-	EXPRESSION TAG	UNP O04998
J	-19	SER	-	EXPRESSION TAG	UNP O04998
J	-18	SER	-	EXPRESSION TAG	UNP O04998
J	-17	HIS	-	EXPRESSION TAG	UNP O04998
J	-16	HIS	-	EXPRESSION TAG	UNP O04998
J	-15	HIS	-	EXPRESSION TAG	UNP O04998
J	-14	HIS	-	EXPRESSION TAG	UNP O04998
J	-13	HIS	-	EXPRESSION TAG	UNP O04998
J	-12	HIS	-	EXPRESSION TAG	UNP O04998
J	-11	SER	-	EXPRESSION TAG	UNP O04998
J	-10	SER	-	EXPRESSION TAG	UNP O04998
J	-9	GLY	-	EXPRESSION TAG	UNP O04998
J	-8	LEU	-	EXPRESSION TAG	UNP O04998
J	-7	VAL	-	EXPRESSION TAG	UNP O04998
J	-6	PRO	-	EXPRESSION TAG	UNP O04998
J	-5	ARG	-	EXPRESSION TAG	UNP O04998
J	-4	GLY	-	EXPRESSION TAG	UNP O04998
J	-3	SER	-	EXPRESSION TAG	UNP O04998
J	-2	HIS	-	EXPRESSION TAG	UNP O04998
J	-1	ALA	-	EXPRESSION TAG	UNP O04998

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	EXPRESSION TAG	UNP O04998

- Molecule 2 is water.

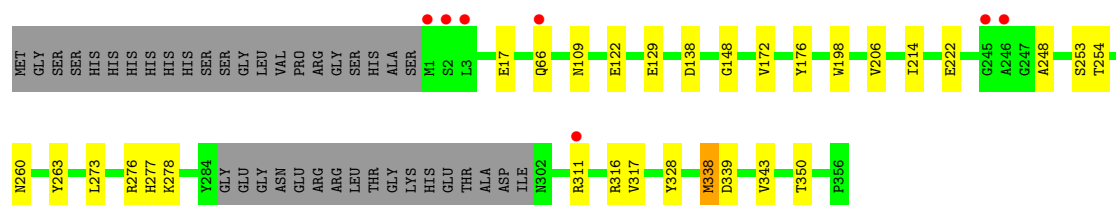
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total 122	O 122	0	0
2	B	66	Total 66	O 66	0	0
2	C	98	Total 98	O 98	0	0
2	D	83	Total 83	O 83	0	0
2	E	111	Total 111	O 111	0	0
2	F	76	Total 76	O 76	0	0
2	G	103	Total 103	O 103	0	0
2	H	80	Total 80	O 80	0	0
2	I	109	Total 109	O 109	0	0
2	J	121	Total 121	O 121	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

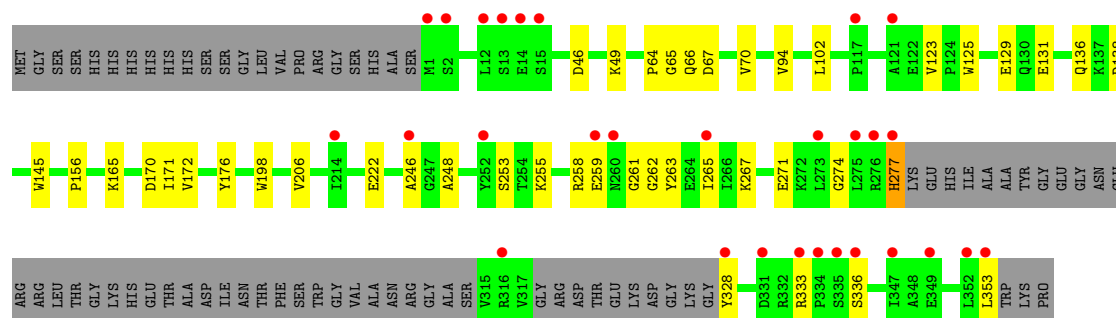
- Molecule 1: Glutamine synthetase

Chain A: 



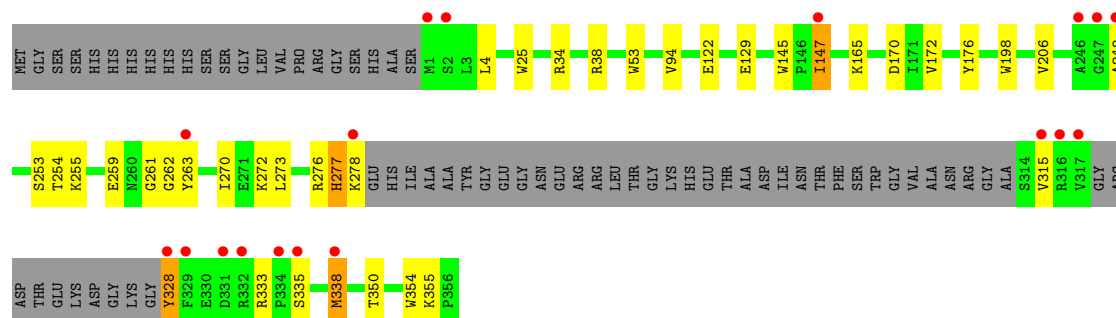
- Molecule 1: Glutamine synthetase

Chain B: 



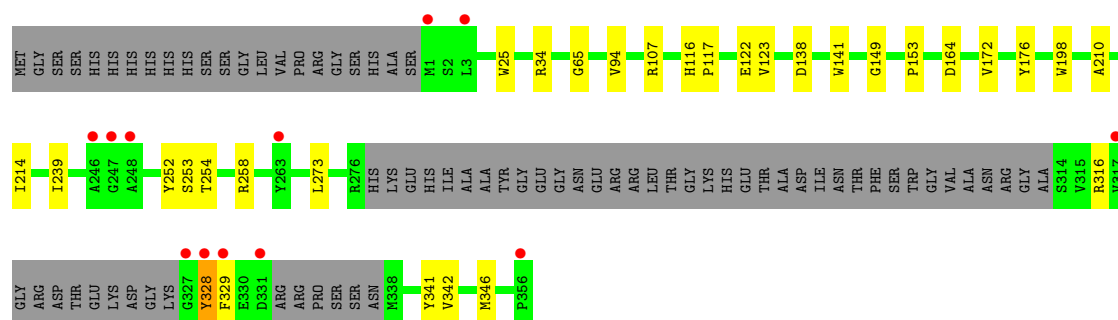
- Molecule 1: Glutamine synthetase

Chain C: 



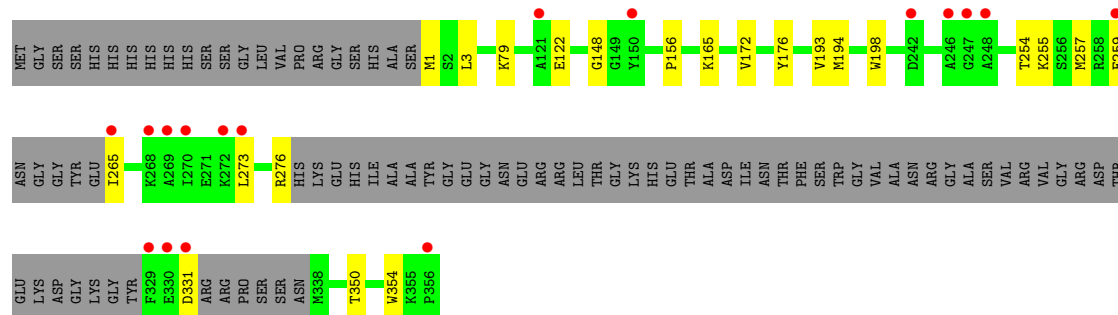
- Molecule 1: Glutamine synthetase

Chain D: 



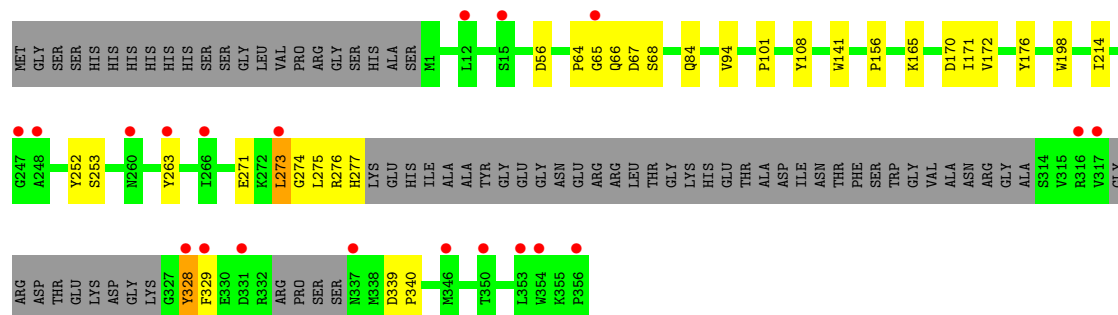
• Molecule 1: Glutamine synthetase

Chain E:



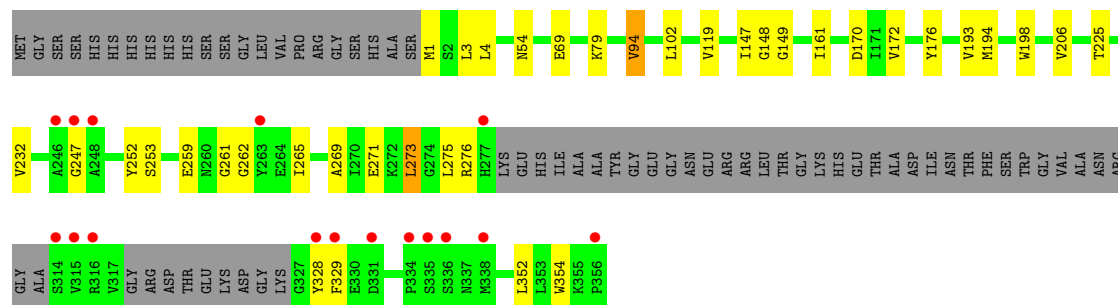
• Molecule 1: Glutamine synthetase

Chain F:

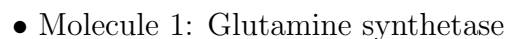


• Molecule 1: Glutamine synthetase

Chain G:



• Molecule 1: Glutamine synthetase



Age Group	Percentage
18-24	10%
25-34	85%
35-44	5%
45-54	1%
55-64	5%
65-74	2%
75-84	2%
85+	2%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.33Å 101.67Å 188.08Å 90.00° 103.69° 90.00°	Depositor
Resolution (Å)	96.51 – 2.35 96.51 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (96.51-2.35) 98.7 (96.51-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.175 , 0.217 0.174 , 0.217	Depositor DCC
$R_{free}$ test set	7517 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.7	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 149512 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.44	0/2710	0.60	0/3687
1	B	0.39	0/2443	0.58	0/3327
1	C	0.43	0/2492	0.58	0/3392
1	D	0.43	0/2425	0.57	0/3301
1	E	0.45	0/2339	0.58	0/3185
1	F	0.41	0/2455	0.56	1/3341 (0.0%)
1	G	0.41	0/2487	0.59	1/3386 (0.0%)
1	H	0.40	0/2421	0.57	0/3297
1	I	0.43	0/2421	0.58	0/3296
1	J	0.44	0/2414	0.57	0/3287
All	All	0.42	0/24607	0.58	2/33499 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	GLY	N-CA-C	5.55	126.99	113.10
1	F	273	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2557	20	0
1	B	2378	0	2315	25	0
1	C	2424	0	2363	20	1
1	D	2360	0	2296	19	0
1	E	2276	0	2221	11	0
1	F	2389	0	2322	17	0
1	G	2419	0	2353	22	0
1	H	2354	0	2284	16	1
1	I	2356	0	2293	21	0
1	J	2348	0	2280	12	0
2	A	122	0	0	3	0
2	B	66	0	0	0	0
2	C	98	0	0	0	0
2	D	83	0	0	2	0
2	E	111	0	0	0	0
2	F	76	0	0	1	0
2	G	103	0	0	2	0
2	H	80	0	0	1	0
2	I	109	0	0	1	0
2	J	121	0	0	0	0
All	All	24909	0	23284	173	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 173 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:122:GLU:HG3	1:C:254:THR:HB	1.61	0.82
1:B:65:GLY:O	1:B:67:ASP:N	2.13	0.82
1:A:122:GLU:HG3	1:A:254:THR:HB	1.64	0.80
1:A:338:MET:HG3	1:A:343:VAL:HG21	1.68	0.75
1:A:311:ARG:HG3	1:A:316:ARG:HH22	1.52	0.74

All (1) 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	Distance(Å)	Clash(Å)
1:C:355:LYS:O	1:H:268:LYS:NZ[2.555]	2.09	0.11



## 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	335/378 (89%)	323 (96%)	11 (3%)	1 (0%)	50	62
1	B	300/378 (79%)	289 (96%)	8 (3%)	3 (1%)	22	24
1	C	305/378 (81%)	294 (96%)	9 (3%)	2 (1%)	30	34
1	D	296/378 (78%)	288 (97%)	8 (3%)	0	100	100
1	E	285/378 (75%)	276 (97%)	9 (3%)	0	100	100
1	F	299/378 (79%)	288 (96%)	9 (3%)	2 (1%)	30	34
1	G	305/378 (81%)	296 (97%)	8 (3%)	1 (0%)	50	62
1	H	296/378 (78%)	287 (97%)	7 (2%)	2 (1%)	30	34
1	I	295/378 (78%)	284 (96%)	7 (2%)	4 (1%)	16	15
1	J	296/378 (78%)	287 (97%)	8 (3%)	1 (0%)	50	62
All	All	3012/3780 (80%)	2912 (97%)	84 (3%)	16 (0%)	38	45

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	HIS
1	B	66	GLN
1	B	262	GLY
1	C	262	GLY
1	F	66	GLN

### 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	277/308 (90%)	273 (99%)	4 (1%)	78	90
1	B	253/308 (82%)	250 (99%)	3 (1%)	82	92
1	C	258/308 (84%)	251 (97%)	7 (3%)	57	74
1	D	250/308 (81%)	246 (98%)	4 (2%)	75	87
1	E	242/308 (79%)	240 (99%)	2 (1%)	89	95
1	F	253/308 (82%)	249 (98%)	4 (2%)	75	87
1	G	257/308 (83%)	254 (99%)	3 (1%)	82	92
1	H	249/308 (81%)	243 (98%)	6 (2%)	61	78
1	I	250/308 (81%)	247 (99%)	3 (1%)	82	92
1	J	248/308 (80%)	243 (98%)	5 (2%)	68	83
All	All	2537/3080 (82%)	2496 (98%)	41 (2%)	75	87

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	176	TYR
1	F	276	ARG
1	J	140	ASN
1	E	331	ASP
1	F	176	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	339/378 (89%)	0.12	7 (2%) 60 63	17, 35, 76, 139	0
1	B	306/378 (80%)	0.45	29 (9%) 8 10	17, 46, 111, 166	0
1	C	311/378 (82%)	0.21	18 (5%) 22 25	19, 36, 92, 176	0
1	D	304/378 (80%)	0.36	12 (3%) 37 41	20, 43, 87, 135	0
1	E	293/378 (77%)	0.19	17 (5%) 22 25	17, 32, 101, 182	0
1	F	307/378 (81%)	0.30	20 (6%) 18 21	18, 42, 106, 219	0
1	G	311/378 (82%)	0.32	16 (5%) 27 30	17, 38, 111, 166	0
1	H	302/378 (79%)	0.42	16 (5%) 25 29	20, 43, 105, 212	0
1	I	303/378 (80%)	0.25	16 (5%) 25 29	18, 36, 104, 190	0
1	J	302/378 (79%)	0.35	14 (4%) 31 35	19, 34, 93, 224	0
All	All	3078/3780 (81%)	0.30	165 (5%) 25 28	17, 38, 100, 224	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	247	GLY	22.1
1	H	248	ALA	17.7
1	J	248	ALA	13.2
1	D	248	ALA	12.7
1	H	247	GLY	12.4

### 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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.