WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2023 – 05:51 AM EDT

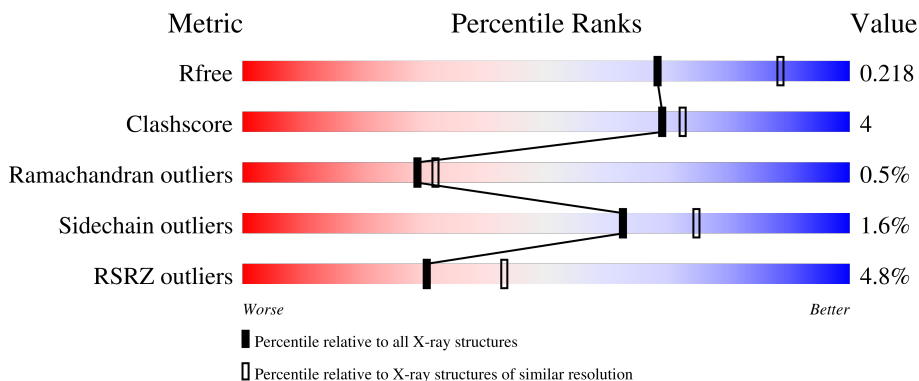|		
PDB ID	:	4IS4
Title	:	The glutamine synthetase from the dicotyledonous plant M. truncatula is a decamer
Authors	:	Seabra, A.R.; Carvalho, H.; Pereira, P.J.B.
Deposited on	:	2013-01-16
Resolution	:	2.35 Å(reported)

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 2.35 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.
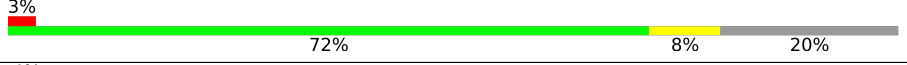
Metric	Percentile Ranks	Value
Rfree		0.218
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		1.6%
RSRZ outliers		4.8%

Worse — *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	378	2% / 82% / 8% / 10%
1	B	378	5% / 70% / 11% / 19%
1	C	378	4% / 72% / 9% / · / 18%
1	D	378	3% / 72% / 8% / 20%
1	E	378	4% / 72% / 6% / 22%

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Mol	Chain	Length	Quality of chain
1	F	378	6%　73%　8%　·　19%
1	G	378	4%　72%　10%　·　18%
1	H	378	3%　72%　8%　20%
1	I	378	4%　70%　9%　·　20%
1	J	378	3%　73%　7%　20%

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 24909 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	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
H	-11	SER	-	expression tag	UNP O04998
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, 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
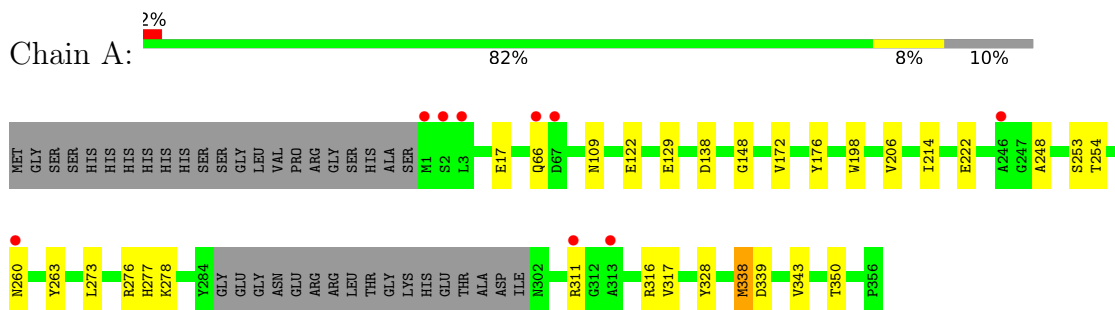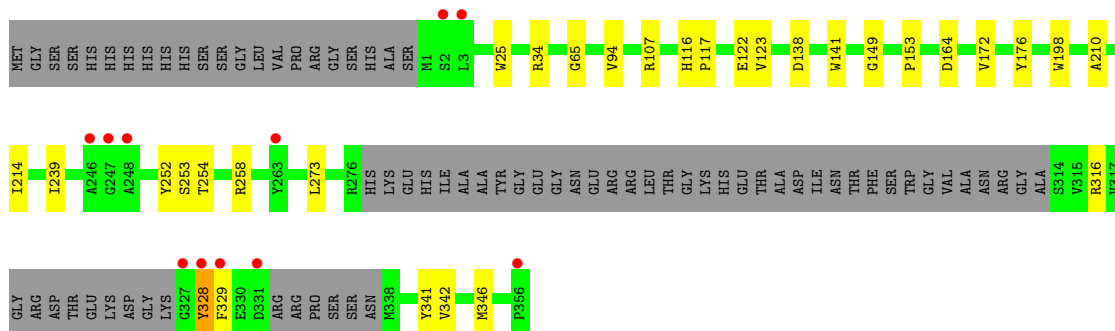
Chain A:

- Molecule 1: Glutamine synthetase
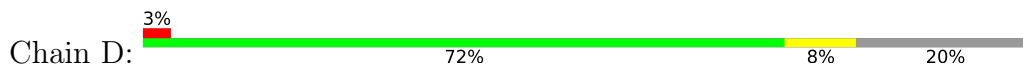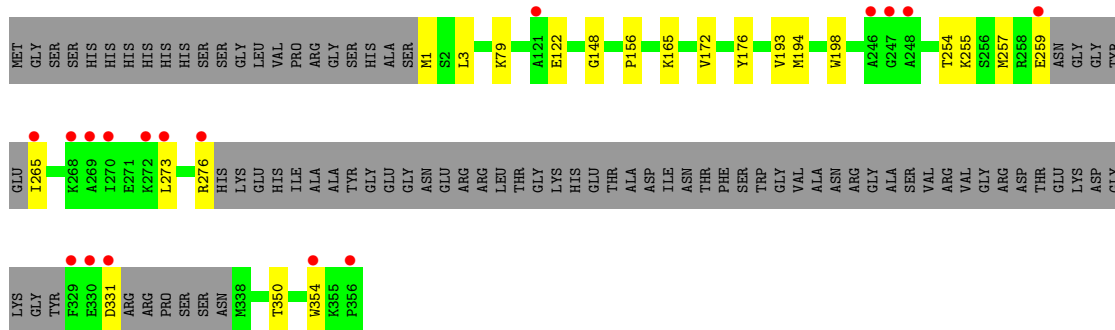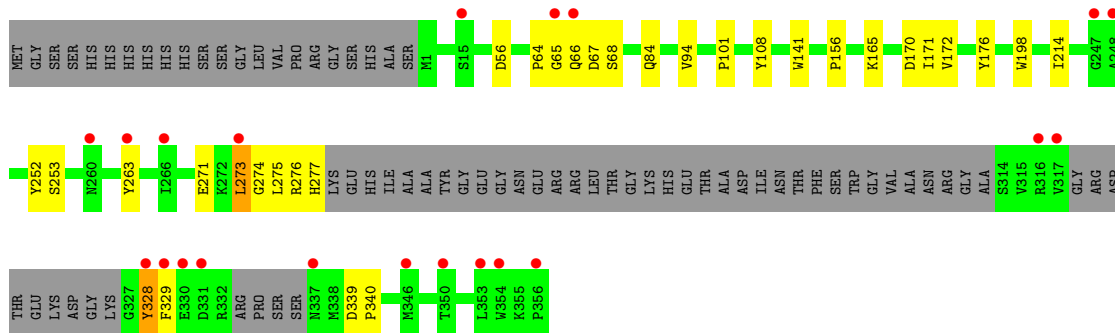
Chain B:

- Molecule 1: Glutamine synthetase

Chain C:

• Molecule 1: Glutamine synthetase

Chain D:
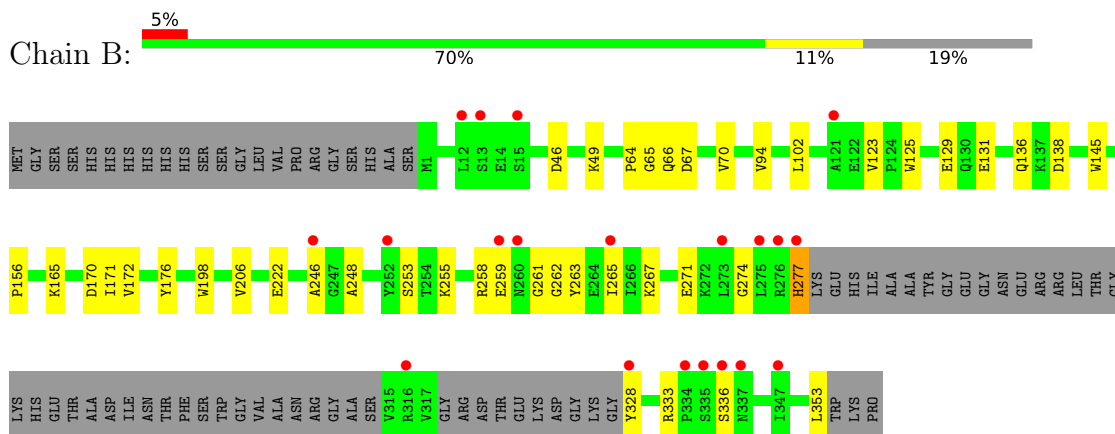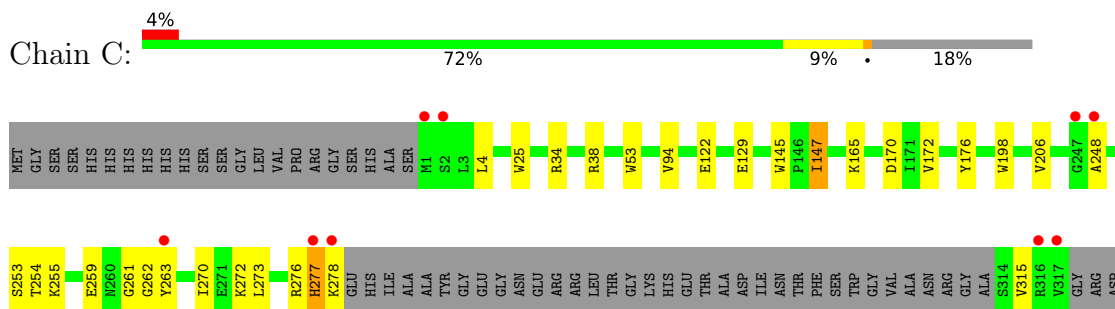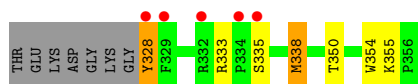
• Molecule 1: Glutamine synthetase

Chain E:

• Molecule 1: Glutamine synthetase

Chain F:

• Molecule 1: Glutamine synthetase
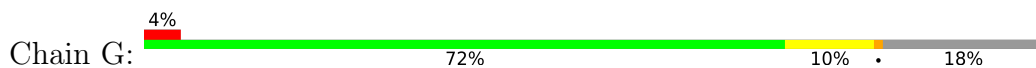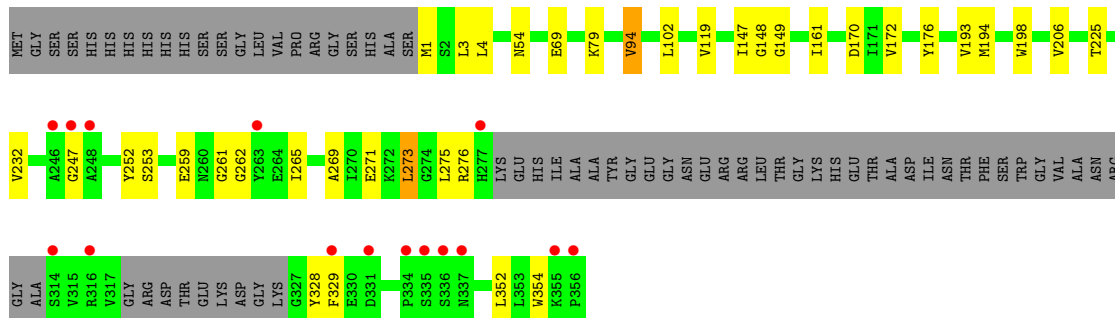
Chain G:

- Molecule 1: Glutamine synthetase
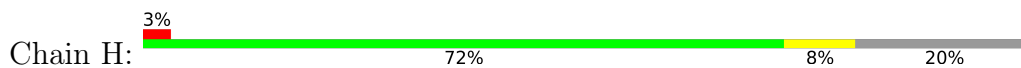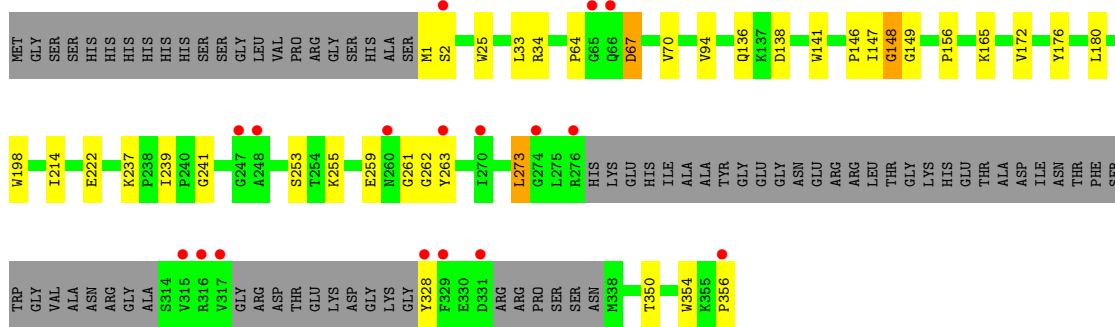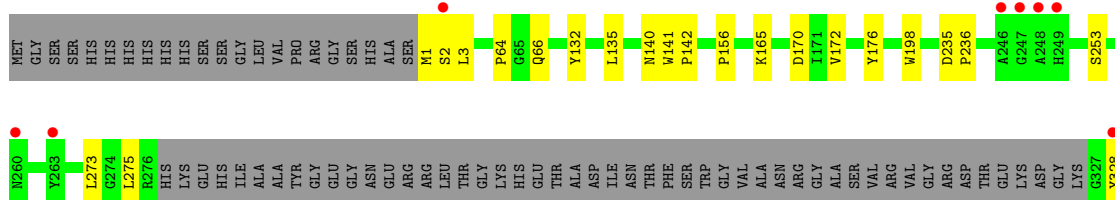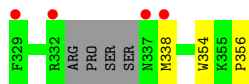
Chain H:

- Molecule 1: Glutamine synthetase

Chain I:

- Molecule 1: Glutamine synthetase

Chain J:
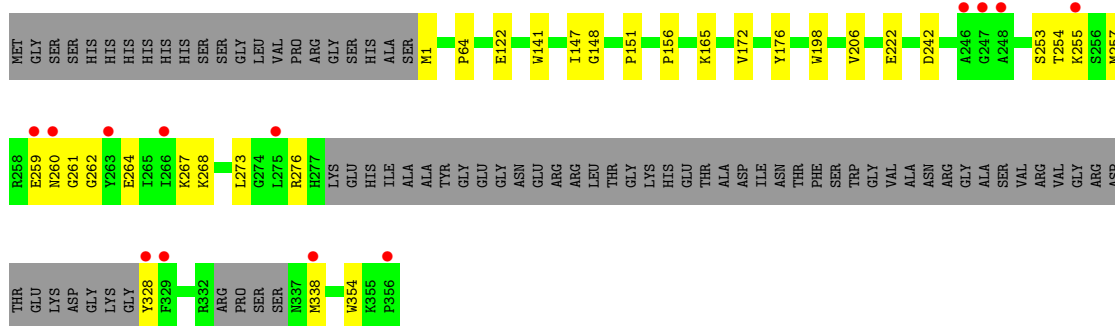
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.14 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.175 , 0.217 0.176 , 0.218	Depositor DCC
R_{free} test set	7520 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24909	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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 ⓘ

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(^{o})	Ideal(^{o})
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   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	2636	0	2557	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 4.

The worst 5 of 173 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: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	Interatomic distance (Å)	Clash overlap (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%)	41	47
1	B	300/378 (79%)	289 (96%)	8 (3%)	3 (1%)	15	15
1	C	305/378 (81%)	294 (96%)	9 (3%)	2 (1%)	22	23
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%)	22	23
1	G	305/378 (81%)	296 (97%)	8 (3%)	1 (0%)	41	47
1	H	296/378 (78%)	287 (97%)	7 (2%)	2 (1%)	22	23
1	I	295/378 (78%)	284 (96%)	7 (2%)	4 (1%)	11	9
1	J	296/378 (78%)	287 (97%)	8 (3%)	1 (0%)	41	47
All	All	3012/3780 (80%)	2912 (97%)	84 (3%)	16 (0%)	29	32

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%)	67	78
1	B	253/308 (82%)	250 (99%)	3 (1%)	71	82
1	C	258/308 (84%)	251 (97%)	7 (3%)	44	55
1	D	250/308 (81%)	246 (98%)	4 (2%)	62	75
1	E	242/308 (79%)	240 (99%)	2 (1%)	81	89
1	F	253/308 (82%)	249 (98%)	4 (2%)	62	75
1	G	257/308 (83%)	254 (99%)	3 (1%)	71	82
1	H	249/308 (81%)	243 (98%)	6 (2%)	49	59
1	I	250/308 (81%)	247 (99%)	3 (1%)	71	82
1	J	248/308 (80%)	243 (98%)	5 (2%)	55	66
All	All	2537/3080 (82%)	2496 (98%)	41 (2%)	62	75

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

Mol	Chain	Res	Type
1	H	176	TYR
1	I	273	LEU
1	H	206	VAL
1	H	338	MET
1	J	140	ASN

Sometimes 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 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 ⓘ

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, 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	339/378 (89%)	0.06	9 (2%)	54	64	17, 35, 76, 139	0
1	B	306/378 (80%)	0.38	20 (6%)	18	27	17, 46, 111, 166	0
1	C	311/378 (82%)	0.12	14 (4%)	33	46	19, 36, 92, 176	0
1	D	304/378 (80%)	0.25	11 (3%)	42	55	20, 43, 87, 135	0
1	E	293/378 (77%)	0.16	17 (5%)	23	33	17, 32, 101, 182	0
1	F	307/378 (81%)	0.20	21 (6%)	17	25	18, 42, 106, 219	0
1	G	311/378 (82%)	0.24	15 (4%)	30	43	17, 38, 111, 166	0
1	H	302/378 (79%)	0.27	13 (4%)	35	47	20, 43, 105, 212	0
1	I	303/378 (80%)	0.20	17 (5%)	24	35	18, 36, 104, 190	0
1	J	302/378 (79%)	0.22	12 (3%)	38	51	19, 34, 93, 224	0
All	All	3078/3780 (81%)	0.21	149 (4%)	30	43	17, 38, 100, 224	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	247	GLY	15.2
1	D	248	ALA	11.8
1	H	248	ALA	11.7
1	J	248	ALA	10.6
1	G	335	SER	8.5

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 ⓘ

There are no ligands in this entry.

6.5　Other polymers ⓘ

There are no such residues in this entry.