



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2023 – 05:59 AM EDT

PDB ID : 3FKY  
Title : Crystal structure of the glutamine synthetase Gln1deltaN18 from the yeast *Saccharomyces cerevisiae*  
Authors : He, Y.X.; Gui, L.; Liu, Y.Z.; Du, Y.; Zhou, Y.Y.; Li, P.; Zhou, C.Z.  
Deposited on : 2008-12-18  
Resolution : 2.95 Å (reported)

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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>.

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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 : 2.36  
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) : 2.36

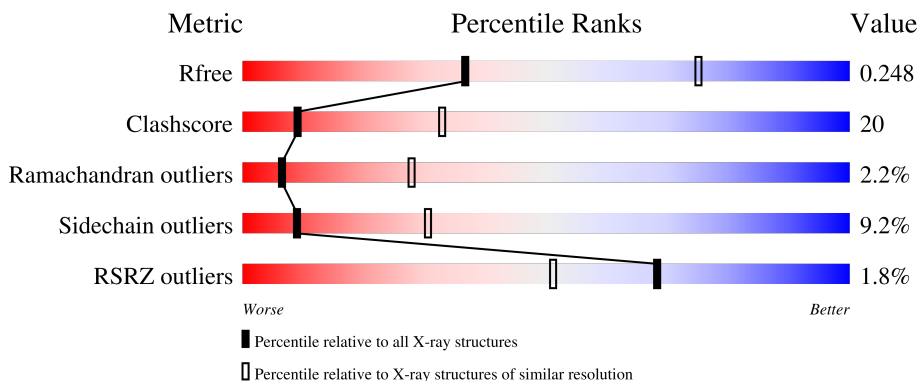
# 1 Overall quality at a glance i

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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\geq 3$ , 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	370	
1	B	370	
1	C	370	
1	D	370	
1	E	370	

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Mol	Chain	Length	Quality of chain			
1	F	370				
1	G	370				
1	H	370				
1	I	370				
1	J	370				
1	K	370				
1	L	370				
1	M	370				
1	N	370				
1	O	370				
1	P	370				
1	Q	370				
1	R	370				
1	S	370				
1	T	370				

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
2	FLC	C	371	-	-	X	-
2	FLC	D	371	-	-	X	-
2	FLC	E	371	-	-	X	-
2	FLC	I	371	-	-	X	-
2	FLC	K	371	-	-	X	-
2	FLC	O	371	-	-	X	-
2	FLC	R	371	-	-	X	-
2	FLC	S	371	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 53518 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
			Total	C	N	O	S			
1	A	336	2661	1683	465	496	17	0	0	0
1	B	336	2661	1683	465	496	17	0	0	0
1	C	342	2699	1705	471	506	17	0	0	0
1	D	336	2661	1683	465	496	17	0	0	0
1	E	336	2661	1683	465	496	17	0	0	0
1	F	336	2661	1683	465	496	17	0	0	0
1	G	336	2661	1683	465	496	17	0	0	0
1	H	336	2661	1683	465	496	17	0	0	0
1	I	336	2661	1683	465	496	17	0	0	0
1	J	336	2661	1683	465	496	17	0	0	0
1	K	336	2661	1683	465	496	17	0	0	0
1	L	336	2661	1683	465	496	17	0	0	0
1	M	336	2661	1683	465	496	17	0	0	0
1	N	336	2661	1683	465	496	17	0	0	0
1	O	336	2661	1683	465	496	17	0	0	0
1	P	336	2661	1683	465	496	17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	336	2661	1683	465	496	17	0	0	0
1	R	336	2661	1683	465	496	17	0	0	0
1	S	336	2661	1683	465	496	17	0	0	0
1	T	336	2661	1683	465	496	17	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

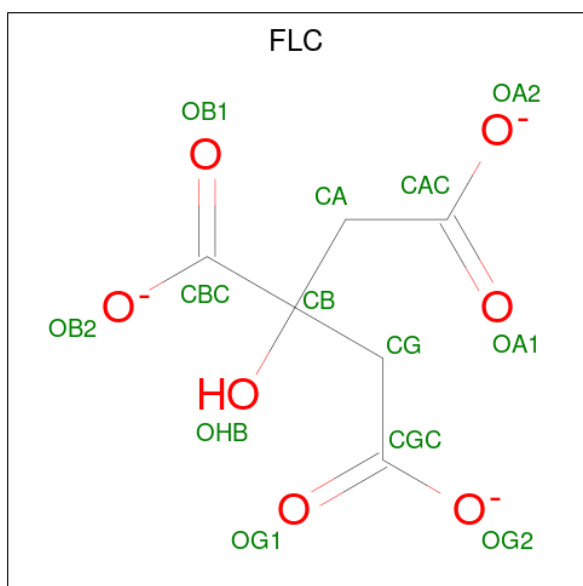
Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	THR	SEE REMARK 999	UNP P32288
A	264	THR	MET	SEE REMARK 999	UNP P32288
B	251	ALA	THR	SEE REMARK 999	UNP P32288
B	264	THR	MET	SEE REMARK 999	UNP P32288
C	251	ALA	THR	SEE REMARK 999	UNP P32288
C	264	THR	MET	SEE REMARK 999	UNP P32288
D	251	ALA	THR	SEE REMARK 999	UNP P32288
D	264	THR	MET	SEE REMARK 999	UNP P32288
E	251	ALA	THR	SEE REMARK 999	UNP P32288
E	264	THR	MET	SEE REMARK 999	UNP P32288
F	251	ALA	THR	SEE REMARK 999	UNP P32288
F	264	THR	MET	SEE REMARK 999	UNP P32288
G	251	ALA	THR	SEE REMARK 999	UNP P32288
G	264	THR	MET	SEE REMARK 999	UNP P32288
H	251	ALA	THR	SEE REMARK 999	UNP P32288
H	264	THR	MET	SEE REMARK 999	UNP P32288
I	251	ALA	THR	SEE REMARK 999	UNP P32288
I	264	THR	MET	SEE REMARK 999	UNP P32288
J	251	ALA	THR	SEE REMARK 999	UNP P32288
J	264	THR	MET	SEE REMARK 999	UNP P32288
K	251	ALA	THR	SEE REMARK 999	UNP P32288
K	264	THR	MET	SEE REMARK 999	UNP P32288
L	251	ALA	THR	SEE REMARK 999	UNP P32288
L	264	THR	MET	SEE REMARK 999	UNP P32288
M	251	ALA	THR	SEE REMARK 999	UNP P32288
M	264	THR	MET	SEE REMARK 999	UNP P32288
N	251	ALA	THR	SEE REMARK 999	UNP P32288
N	264	THR	MET	SEE REMARK 999	UNP P32288
O	251	ALA	THR	SEE REMARK 999	UNP P32288
O	264	THR	MET	SEE REMARK 999	UNP P32288
P	251	ALA	THR	SEE REMARK 999	UNP P32288

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Chain	Residue	Modelled	Actual	Comment	Reference
P	264	THR	MET	SEE REMARK 999	UNP P32288
Q	251	ALA	THR	SEE REMARK 999	UNP P32288
Q	264	THR	MET	SEE REMARK 999	UNP P32288
R	251	ALA	THR	SEE REMARK 999	UNP P32288
R	264	THR	MET	SEE REMARK 999	UNP P32288
S	251	ALA	THR	SEE REMARK 999	UNP P32288
S	264	THR	MET	SEE REMARK 999	UNP P32288
T	251	ALA	THR	SEE REMARK 999	UNP P32288
T	264	THR	MET	SEE REMARK 999	UNP P32288

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0

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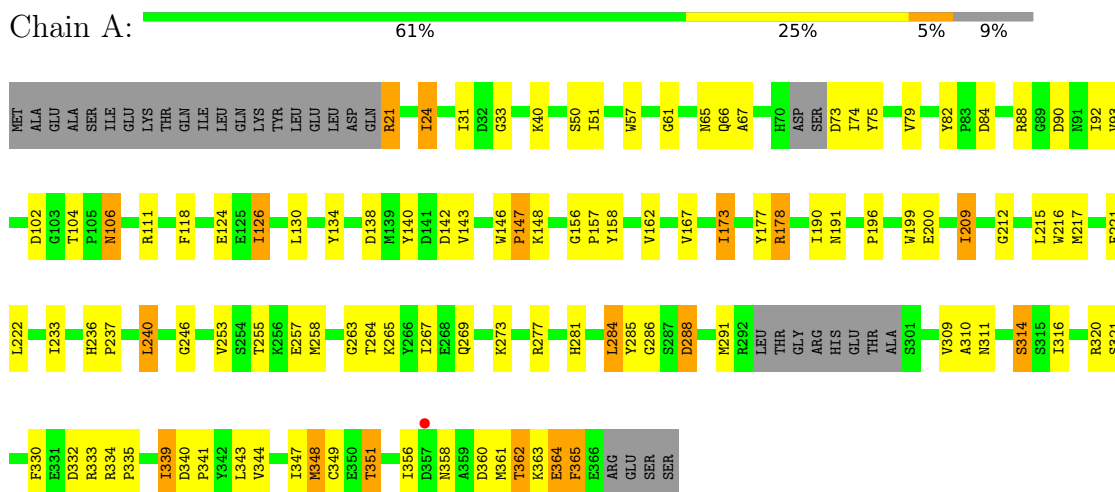
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		
2	M	1	Total	C	O	0	0
			13	6	7		
2	N	1	Total	C	O	0	0
			13	6	7		
2	O	1	Total	C	O	0	0
			13	6	7		
2	P	1	Total	C	O	0	0
			13	6	7		
2	Q	1	Total	C	O	0	0
			13	6	7		
2	R	1	Total	C	O	0	0
			13	6	7		
2	S	1	Total	C	O	0	0
			13	6	7		
2	T	1	Total	C	O	0	0
			13	6	7		

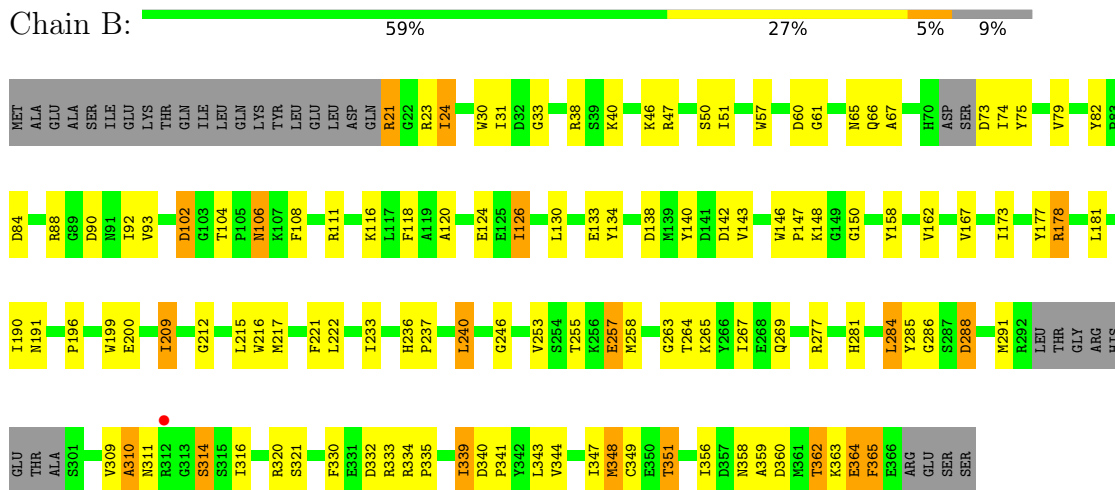
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamine synthetase



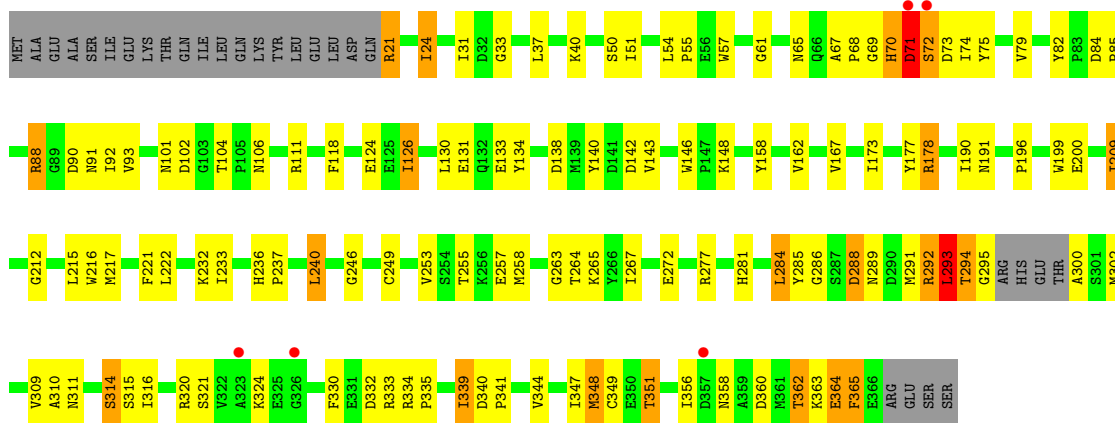
- Molecule 1: Glutamine synthetase



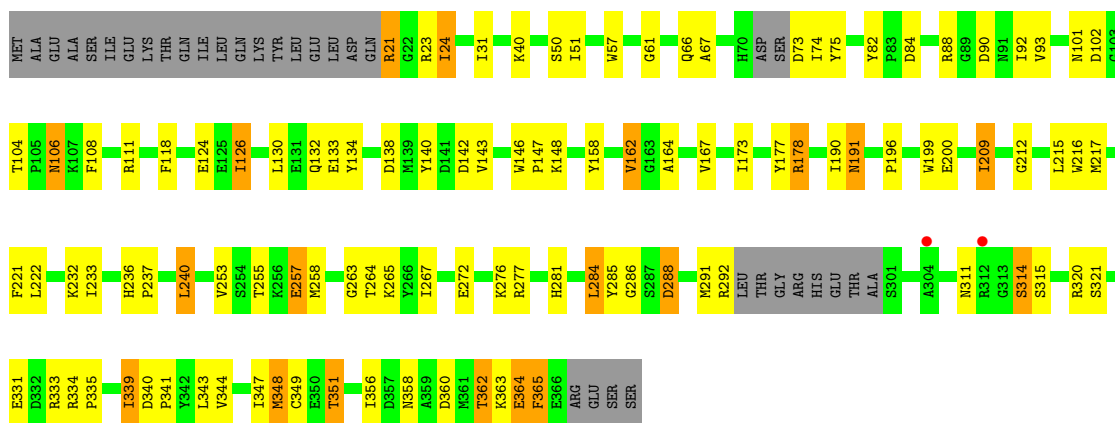
- Molecule 1: Glutamine synthetase



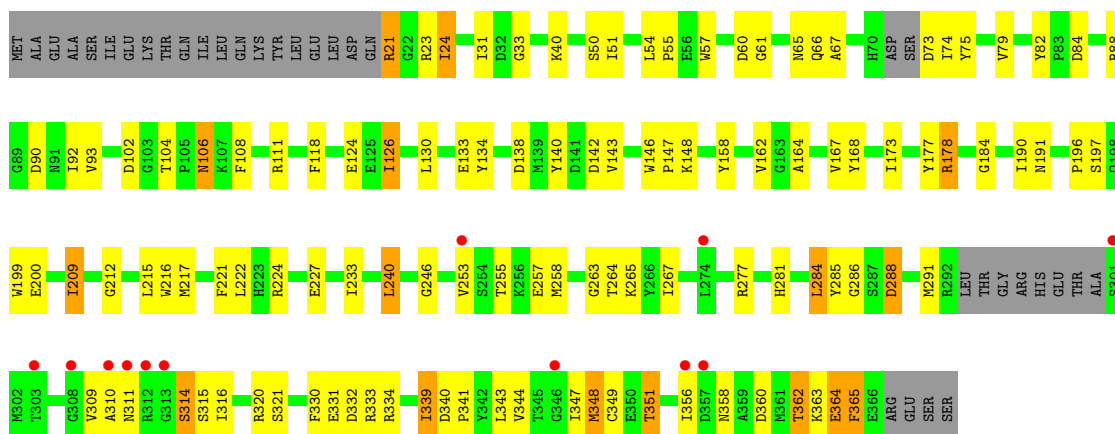




• Molecule 1: Glutamine synthetase

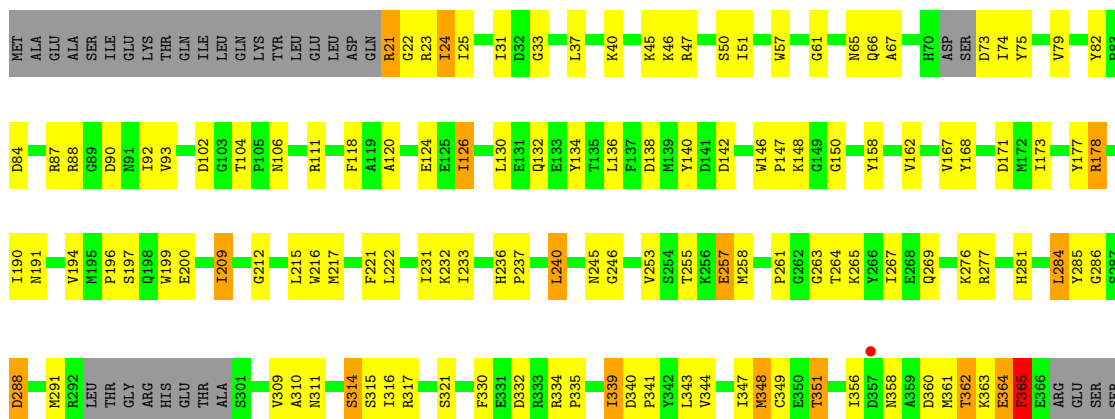


• Molecule 1: Glutamine synthetase



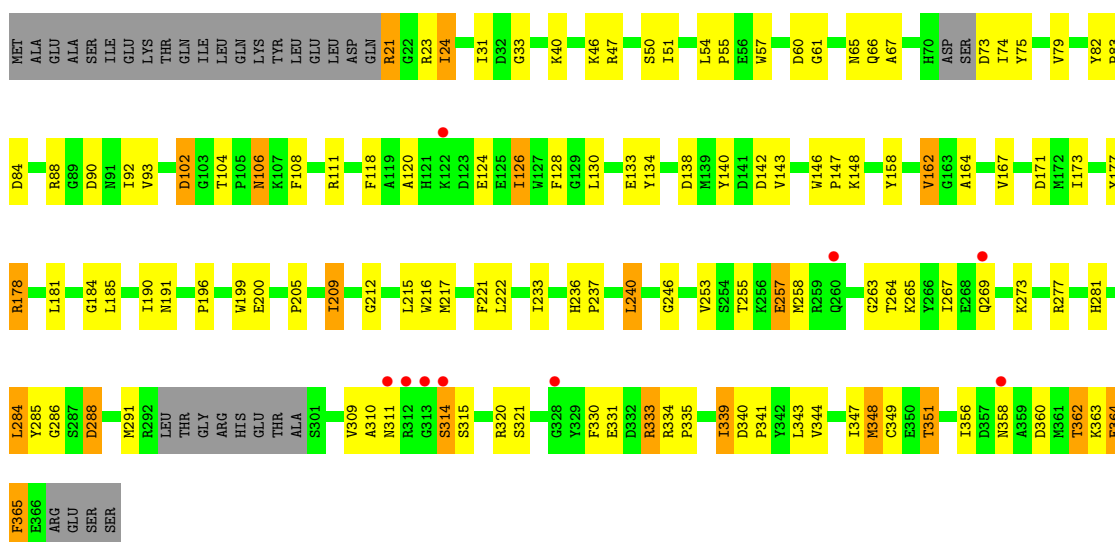
• Molecule 1: Glutamine synthetase

Chain F:  57% 30% 9%



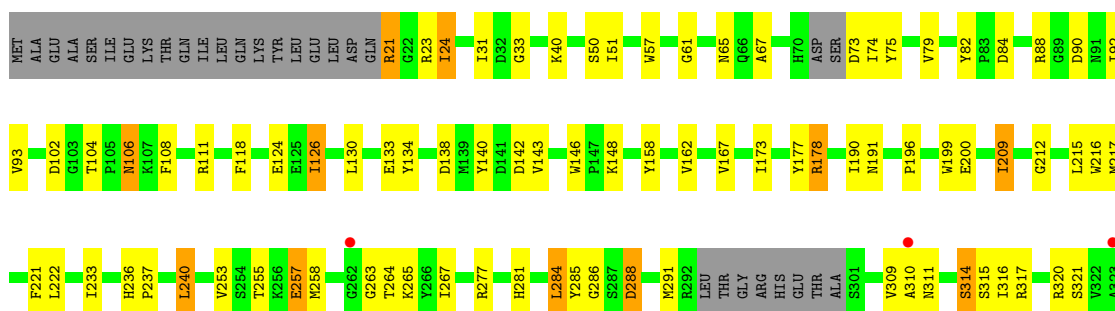
• Molecule 1: Glutamine synthetase

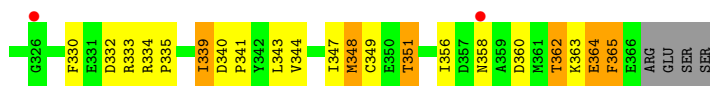
Chain G:  2% 58% 28% 5% 9%



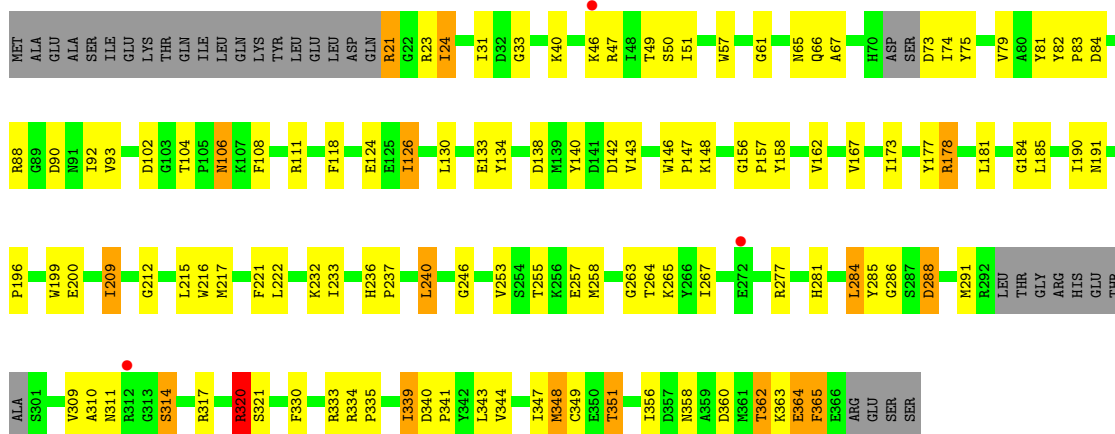
• Molecule 1: Glutamine synthetase

Chain H:  62% 24% 5% 9%

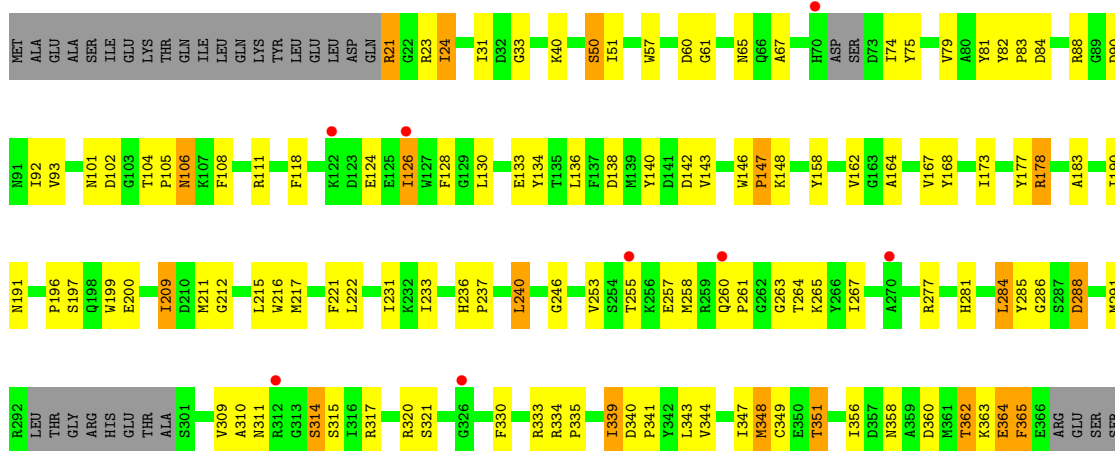




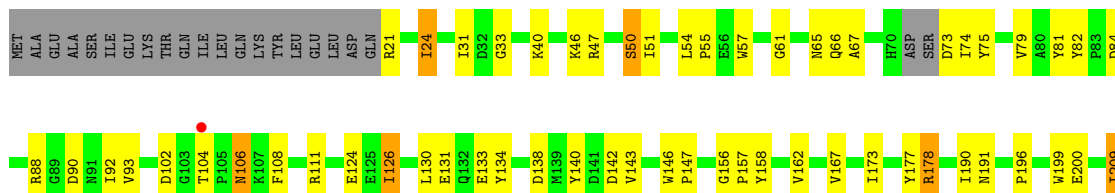
- Molecule 1: Glutamine synthetase

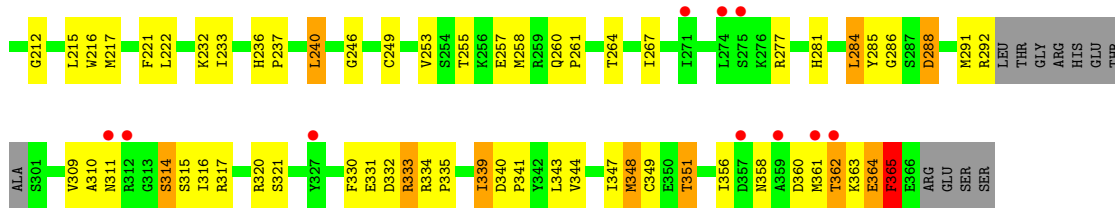


- Molecule 1: Glutamine synthetase

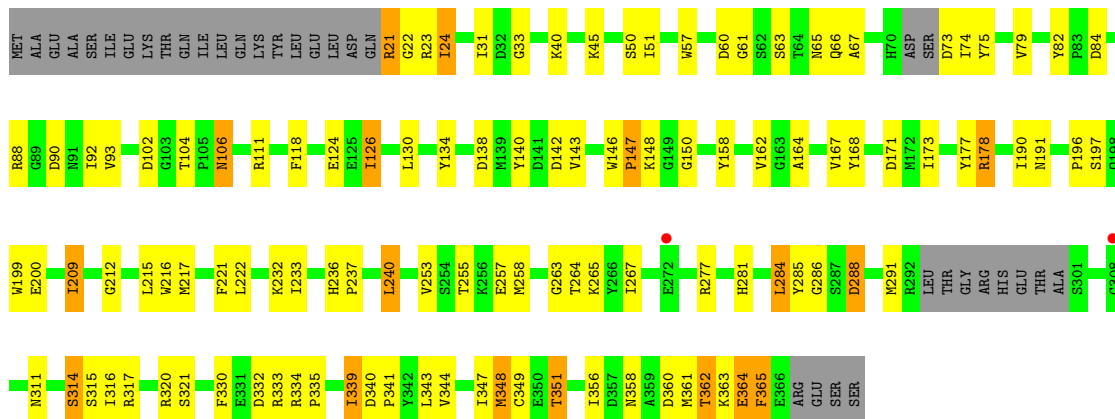


- Molecule 1: Glutamine synthetase

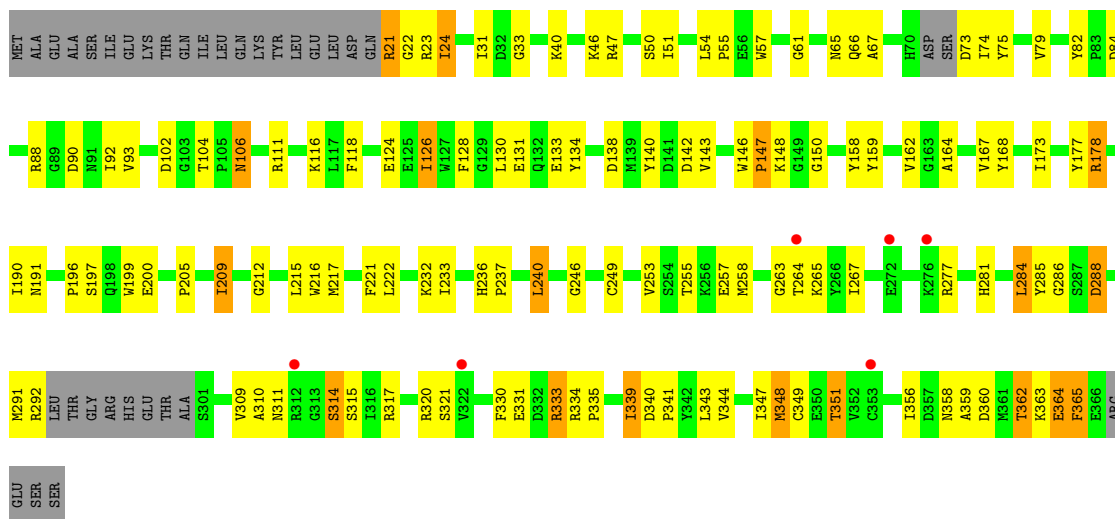




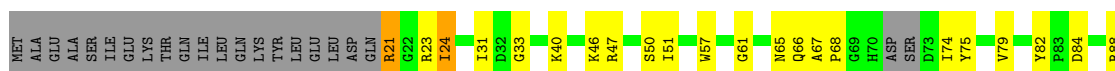
• Molecule 1: Glutamine synthetase

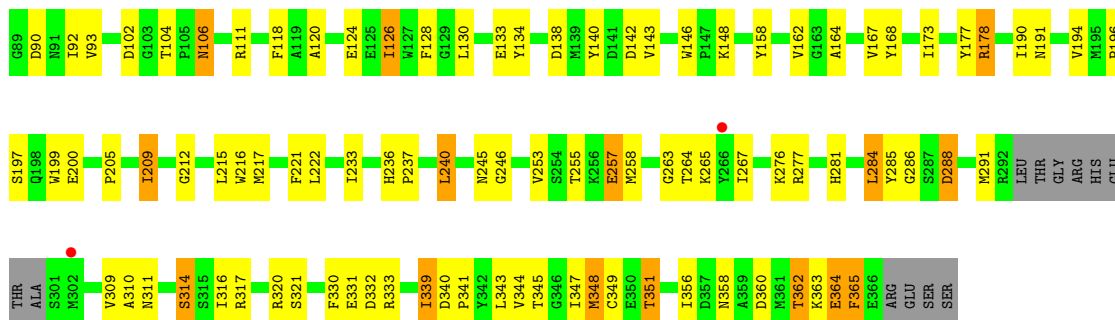


• Molecule 1: Glutamine synthetase

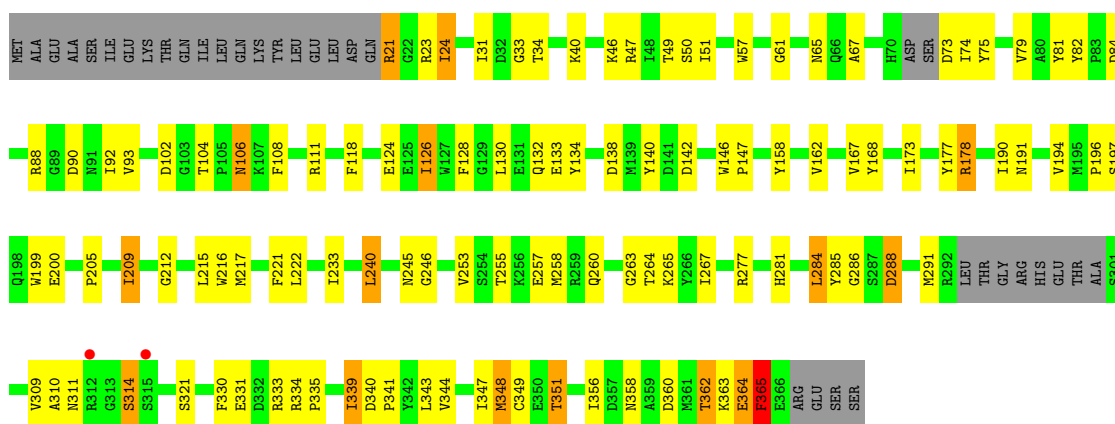


• Molecule 1: Glutamine synthetase

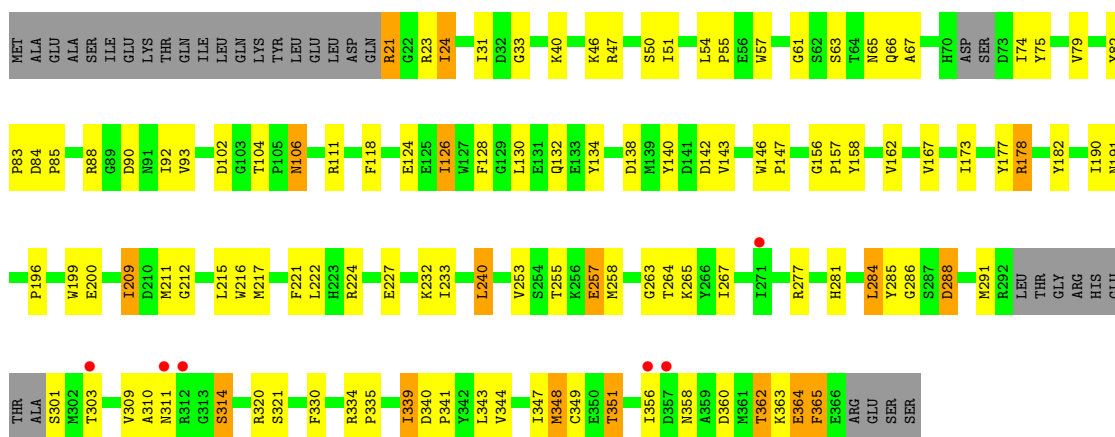




● Molecule 1: Glutamine synthetase

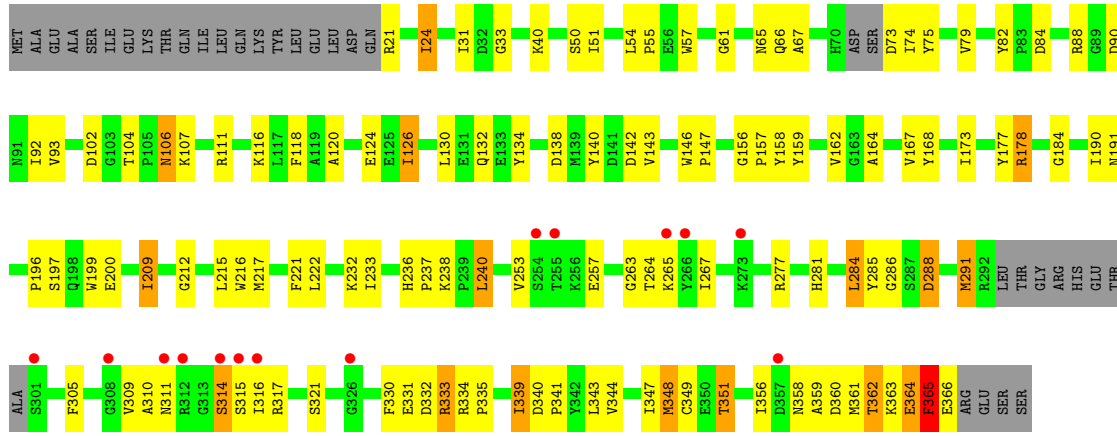


● Molecule 1: Glutamine synthetase

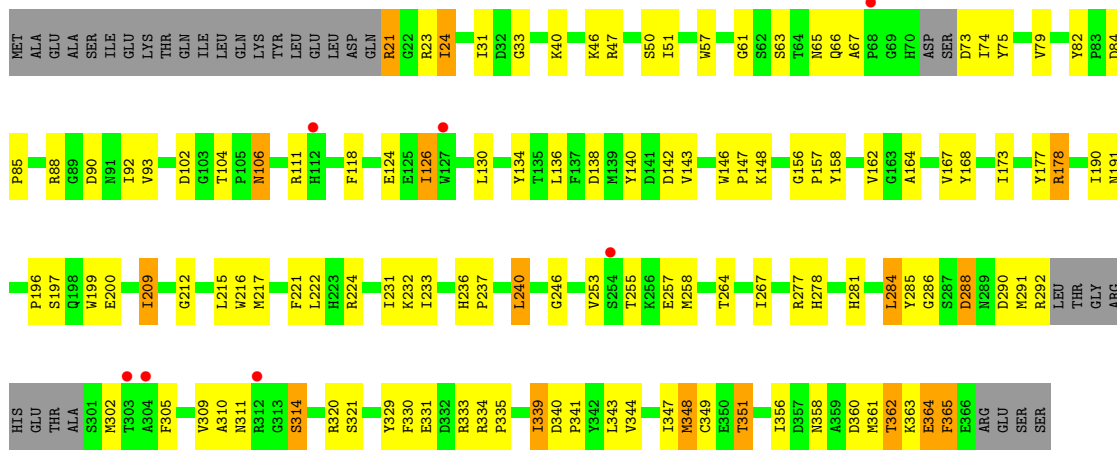


● Molecule 1: Glutamine synthetase

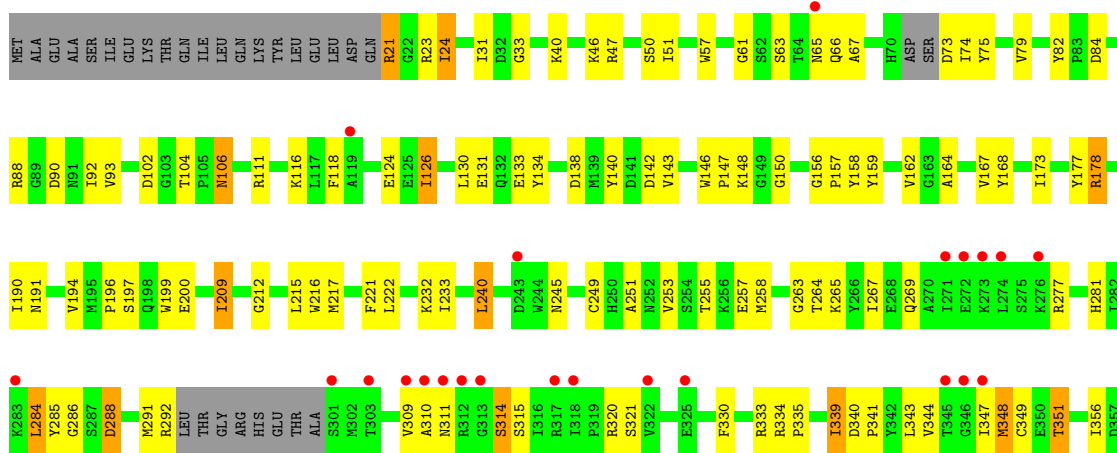


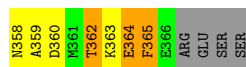


• Molecule 1: Glutamine synthetase



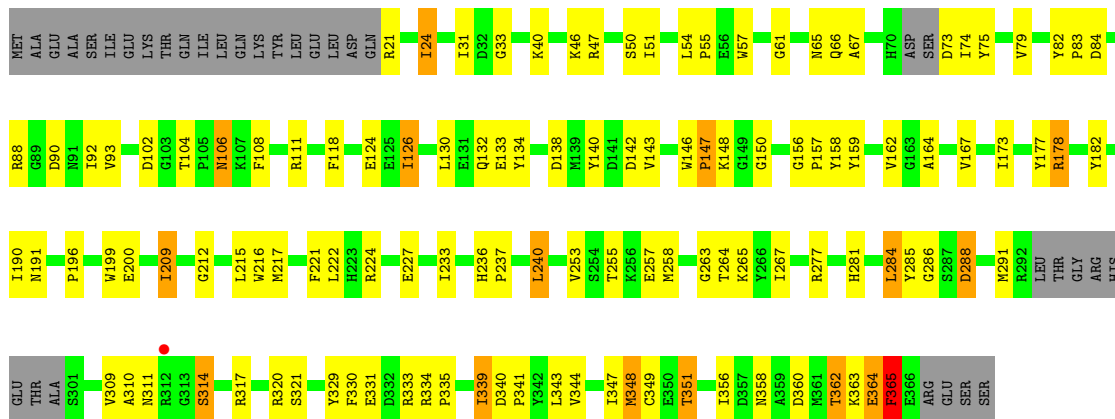
• Molecule 1: Glutamine synthetase





- Molecule 1: Glutamine synthetase

Chain T: 58% 28% 9%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.65Å 129.94Å 135.61Å 93.46° 104.61° 104.01°	Depositor
Resolution (Å)	65.22 – 2.95 65.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.1 (65.22-2.95) 95.1 (65.22-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.225 , 0.258 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	3299 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.238	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.008 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	53518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.52	0/2733	0.62	0/3695
1	B	0.52	0/2733	0.62	0/3695
1	C	0.54	0/2772	0.65	1/3750 (0.0%)
1	D	0.51	0/2733	0.61	0/3695
1	E	0.48	0/2733	0.62	0/3695
1	F	0.53	0/2733	0.63	0/3695
1	G	0.50	0/2733	0.61	0/3695
1	H	0.52	0/2733	0.63	0/3695
1	I	0.50	0/2733	0.80	3/3695 (0.1%)
1	J	0.49	0/2733	0.61	0/3695
1	K	0.47	0/2733	0.61	0/3695
1	L	0.48	0/2733	0.61	0/3695
1	M	0.48	0/2733	0.61	0/3695
1	N	0.49	0/2733	0.62	0/3695
1	O	0.49	0/2733	0.61	0/3695
1	P	0.49	0/2733	0.61	0/3695
1	Q	0.51	0/2733	0.62	0/3695
1	R	0.51	0/2733	0.62	0/3695
1	S	0.49	0/2733	0.61	0/3695
1	T	0.48	0/2733	0.61	0/3695
All	All	0.50	0/54699	0.63	4/73955 (0.0%)

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	I	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	320	ARG	NE-CZ-NH1	-24.86	107.87	120.30
1	I	320	ARG	NE-CZ-NH2	14.53	127.57	120.30
1	I	320	ARG	CD-NE-CZ	13.77	142.88	123.60
1	C	292	ARG	O-C-N	-5.31	114.20	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	320	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2661	0	2530	103	0
1	B	2661	0	2530	105	0
1	C	2699	0	2566	125	2
1	D	2661	0	2530	98	2
1	E	2661	0	2530	103	0
1	F	2661	0	2530	125	2
1	G	2661	0	2530	121	0
1	H	2661	0	2530	108	0
1	I	2661	0	2530	104	0
1	J	2661	0	2530	123	0
1	K	2661	0	2530	121	0
1	L	2661	0	2530	115	0
1	M	2661	0	2530	125	0
1	N	2661	0	2530	104	0
1	O	2661	0	2530	100	0
1	P	2661	0	2530	96	2
1	Q	2661	0	2530	102	0
1	R	2661	0	2530	109	0
1	S	2661	0	2530	119	0
1	T	2661	0	2530	110	0
2	A	13	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	3	0
2	C	13	0	5	8	0
2	D	13	0	5	5	0
2	E	13	0	5	4	0
2	F	13	0	5	1	0
2	G	13	0	5	3	0
2	H	13	0	5	3	0
2	I	13	0	5	6	0
2	J	13	0	5	3	0
2	K	13	0	5	4	0
2	L	13	0	5	0	0
2	M	13	0	5	3	0
2	N	13	0	5	3	0
2	O	13	0	5	5	0
2	P	13	0	5	1	0
2	Q	13	0	5	2	0
2	R	13	0	5	4	0
2	S	13	0	5	5	0
2	T	13	0	5	2	0
All	All	53518	0	50736	2093	4

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 20.

The worst 5 of 2093 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:D:178:ARG:HG3	1:D:178:ARG:HH11	1.13	1.14
1:C:70:HIS:O	1:C:72:SER:N	1.82	1.11
1:H:222:LEU:HG	1:H:233:ILE:HD13	1.33	1.10
1:J:260:GLN:HG2	1:K:260:GLN:HG2	1.24	1.10
1:J:222:LEU:HG	1:J:233:ILE:HD13	1.33	1.09

All (4) 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:D:272:GLU:OE1	1:P:301:SER:OG[1_656]	1.97	0.23
1:C:324:LYS:O	1:F:276:LYS:NZ[1_655]	2.06	0.14
1:D:272:GLU:OE1	1:P:303:THR:OG1[1_656]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLU:OE2	1:F:356:ILE:CG2[1_655]	2.15	0.05

## 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	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	B	330/370 (89%)	301 (91%)	21 (6%)	8 (2%)	6	26
1	C	338/370 (91%)	305 (90%)	23 (7%)	10 (3%)	4	20
1	D	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	E	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	F	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	G	330/370 (89%)	302 (92%)	21 (6%)	7 (2%)	7	29
1	H	330/370 (89%)	306 (93%)	18 (6%)	6 (2%)	8	33
1	I	330/370 (89%)	306 (93%)	17 (5%)	7 (2%)	7	29
1	J	330/370 (89%)	301 (91%)	22 (7%)	7 (2%)	7	29
1	K	330/370 (89%)	302 (92%)	20 (6%)	8 (2%)	6	26
1	L	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	M	330/370 (89%)	302 (92%)	21 (6%)	7 (2%)	7	29
1	N	330/370 (89%)	305 (92%)	19 (6%)	6 (2%)	8	33
1	O	330/370 (89%)	303 (92%)	19 (6%)	8 (2%)	6	26
1	P	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	Q	330/370 (89%)	303 (92%)	19 (6%)	8 (2%)	6	26
1	R	330/370 (89%)	303 (92%)	20 (6%)	7 (2%)	7	29
1	S	330/370 (89%)	302 (92%)	22 (7%)	6 (2%)	8	33
1	T	330/370 (89%)	302 (92%)	20 (6%)	8 (2%)	6	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6608/7400 (89%)	6061 (92%)	402 (6%)	145 (2%)	6	28

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	TYR
1	A	364	GLU
1	B	285	TYR
1	B	364	GLU
1	C	70	HIS

### 5.3.2 Protein sidechains [i](#)

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	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	B	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	C	277/304 (91%)	248 (90%)	29 (10%)	7	24
1	D	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	E	273/304 (90%)	249 (91%)	24 (9%)	10	33
1	F	273/304 (90%)	249 (91%)	24 (9%)	10	33
1	G	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	H	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	I	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	J	273/304 (90%)	247 (90%)	26 (10%)	8	29
1	K	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	L	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	M	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	N	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	O	273/304 (90%)	248 (91%)	25 (9%)	9	30
1	P	273/304 (90%)	249 (91%)	24 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	273/304 (90%)	248 (91%)	25 (9%)	9 30
1	R	273/304 (90%)	249 (91%)	24 (9%)	10 33
1	S	273/304 (90%)	248 (91%)	25 (9%)	9 30
1	T	273/304 (90%)	249 (91%)	24 (9%)	10 33
All	All	5464/6080 (90%)	4959 (91%)	505 (9%)	9 30

5 of 505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	365	PHE
1	R	191	ASN
1	L	51	ILE
1	R	126	ILE
1	S	314	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	36	ASN
1	R	110	HIS
1	L	106	ASN
1	R	106	ASN
1	T	36	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FLC	L	371	-	12,12,12	0.98	0	17,17,17	1.95	4 (23%)
2	FLC	O	371	-	12,12,12	0.97	0	17,17,17	1.74	4 (23%)
2	FLC	I	371	-	12,12,12	0.96	0	17,17,17	1.64	3 (17%)
2	FLC	P	371	-	12,12,12	1.07	0	17,17,17	2.19	3 (17%)
2	FLC	K	371	-	12,12,12	0.92	0	17,17,17	1.46	2 (11%)
2	FLC	H	371	-	12,12,12	1.01	0	17,17,17	2.16	4 (23%)
2	FLC	S	371	-	12,12,12	1.02	0	17,17,17	1.53	2 (11%)
2	FLC	A	371	-	12,12,12	1.07	0	17,17,17	1.75	3 (17%)
2	FLC	N	371	-	12,12,12	0.88	0	17,17,17	2.06	6 (35%)
2	FLC	M	371	-	12,12,12	0.84	0	17,17,17	1.54	4 (23%)
2	FLC	R	371	-	12,12,12	1.01	0	17,17,17	1.56	5 (29%)
2	FLC	D	371	-	12,12,12	1.00	0	17,17,17	2.68	5 (29%)
2	FLC	Q	371	-	12,12,12	1.00	0	17,17,17	1.67	4 (23%)
2	FLC	E	371	-	12,12,12	1.03	0	17,17,17	2.32	4 (23%)
2	FLC	B	371	-	12,12,12	1.01	0	17,17,17	2.24	3 (17%)
2	FLC	F	371	-	12,12,12	0.99	0	17,17,17	1.79	3 (17%)
2	FLC	J	371	-	12,12,12	0.90	0	17,17,17	1.64	2 (11%)
2	FLC	G	371	-	12,12,12	0.85	0	17,17,17	1.91	4 (23%)
2	FLC	C	371	-	12,12,12	0.98	0	17,17,17	1.89	5 (29%)
2	FLC	T	371	-	12,12,12	0.94	0	17,17,17	1.63	3 (17%)

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
2	FLC	L	371	-	-	5/16/16/16	-
2	FLC	O	371	-	-	9/16/16/16	-
2	FLC	I	371	-	-	3/16/16/16	-
2	FLC	P	371	-	-	4/16/16/16	-
2	FLC	K	371	-	-	8/16/16/16	-
2	FLC	H	371	-	-	6/16/16/16	-
2	FLC	S	371	-	-	10/16/16/16	-
2	FLC	A	371	-	-	7/16/16/16	-
2	FLC	N	371	-	-	4/16/16/16	-
2	FLC	M	371	-	-	6/16/16/16	-
2	FLC	R	371	-	-	5/16/16/16	-
2	FLC	D	371	-	-	6/16/16/16	-
2	FLC	Q	371	-	-	10/16/16/16	-
2	FLC	E	371	-	-	8/16/16/16	-
2	FLC	B	371	-	-	6/16/16/16	-
2	FLC	F	371	-	-	9/16/16/16	-
2	FLC	J	371	-	-	6/16/16/16	-
2	FLC	G	371	-	-	6/16/16/16	-
2	FLC	C	371	-	-	8/16/16/16	-
2	FLC	T	371	-	-	4/16/16/16	-

There are no bond length outliers.

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	371	FLC	OHB-CB-CBC	6.34	117.77	108.86
2	D	371	FLC	OB2-CBC-CB	6.31	124.01	113.05
2	B	371	FLC	OHB-CB-CBC	5.34	116.36	108.86
2	P	371	FLC	OB2-CBC-CB	5.09	121.89	113.05
2	H	371	FLC	OB2-CBC-CB	5.05	121.83	113.05

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	371	FLC	CG-CB-CBC-OB1
2	A	371	FLC	CG-CB-CBC-OB2
2	A	371	FLC	OHB-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
2	B	371	FLC	CAC-CA-CB-CBC
2	B	371	FLC	CAC-CA-CB-CG

There are no ring outliers.

19 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	371	FLC	5	0
2	I	371	FLC	6	0
2	P	371	FLC	1	0
2	K	371	FLC	4	0
2	H	371	FLC	3	0
2	S	371	FLC	5	0
2	A	371	FLC	3	0
2	N	371	FLC	3	0
2	M	371	FLC	3	0
2	R	371	FLC	4	0
2	D	371	FLC	5	0
2	Q	371	FLC	2	0
2	E	371	FLC	4	0
2	B	371	FLC	3	0
2	F	371	FLC	1	0
2	J	371	FLC	3	0
2	G	371	FLC	3	0
2	C	371	FLC	8	0
2	T	371	FLC	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	336/370 (90%)	0.06	1 (0%) 94 87	27, 43, 69, 96	0
1	B	336/370 (90%)	0.06	1 (0%) 94 87	25, 42, 71, 98	0
1	C	342/370 (92%)	0.16	5 (1%) 73 57	26, 42, 70, 96	0
1	D	336/370 (90%)	0.05	2 (0%) 89 78	26, 43, 69, 97	0
1	E	336/370 (90%)	0.25	12 (3%) 42 28	28, 44, 71, 97	0
1	F	336/370 (90%)	0.04	1 (0%) 94 87	28, 43, 70, 90	0
1	G	336/370 (90%)	0.26	9 (2%) 54 38	26, 45, 72, 94	0
1	H	336/370 (90%)	0.14	5 (1%) 73 57	28, 43, 70, 92	0
1	I	336/370 (90%)	0.01	3 (0%) 84 71	28, 44, 73, 96	0
1	J	336/370 (90%)	0.14	8 (2%) 59 42	28, 44, 72, 94	0
1	K	336/370 (90%)	0.28	11 (3%) 46 30	29, 45, 74, 95	0
1	L	336/370 (90%)	0.12	2 (0%) 89 78	28, 46, 72, 93	0
1	M	336/370 (90%)	0.15	6 (1%) 68 51	30, 46, 74, 95	0
1	N	336/370 (90%)	0.05	2 (0%) 89 78	29, 44, 69, 88	0
1	O	336/370 (90%)	0.03	2 (0%) 89 78	29, 45, 74, 94	0
1	P	336/370 (90%)	0.11	6 (1%) 68 51	28, 46, 73, 99	0
1	Q	336/370 (90%)	0.35	14 (4%) 36 23	31, 48, 76, 97	0
1	R	336/370 (90%)	0.22	7 (2%) 63 46	31, 48, 75, 98	0
1	S	336/370 (90%)	0.43	23 (6%) 17 10	29, 47, 73, 94	0
1	T	336/370 (90%)	-0.02	1 (0%) 94 87	28, 45, 70, 98	0
All	All	6726/7400 (90%)	0.15	121 (1%) 68 51	25, 45, 72, 99	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	GLY	4.4
1	P	303	THR	4.3
1	B	312	ARG	4.1
1	A	357	ASP	3.9
1	K	104	THR	3.9

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	FLC	N	371	13/13	0.85	0.21	47,66,105,118	0
2	FLC	F	371	13/13	0.87	0.18	35,54,78,79	0
2	FLC	E	371	13/13	0.87	0.21	29,54,76,79	0
2	FLC	Q	371	13/13	0.88	0.19	46,53,80,86	0
2	FLC	R	371	13/13	0.89	0.17	52,66,89,94	0
2	FLC	A	371	13/13	0.90	0.13	37,46,61,70	0
2	FLC	P	371	13/13	0.90	0.18	39,54,65,75	0
2	FLC	B	371	13/13	0.90	0.17	29,52,69,76	0
2	FLC	L	371	13/13	0.90	0.21	46,61,83,88	0
2	FLC	S	371	13/13	0.91	0.20	51,68,84,89	0
2	FLC	T	371	13/13	0.91	0.16	35,51,61,62	0
2	FLC	J	371	13/13	0.92	0.15	41,53,67,77	0
2	FLC	K	371	13/13	0.92	0.17	35,56,68,72	0
2	FLC	H	371	13/13	0.92	0.17	36,50,74,78	0
2	FLC	M	371	13/13	0.92	0.19	58,70,83,87	0
2	FLC	I	371	13/13	0.92	0.20	41,57,75,85	0
2	FLC	O	371	13/13	0.93	0.13	37,50,67,69	0
2	FLC	G	371	13/13	0.93	0.17	37,54,61,63	0
2	FLC	D	371	13/13	0.94	0.14	31,50,58,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FLC	C	371	13/13	0.95	0.13	26,39,48,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.