wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:38 PM GMT

PDB ID	:	4S0R
Title	:	Structure of GS-TnrA complex
Authors	:	Schumacher, M.A.; Chinnam, N.G.; Cuthbert, B.; Tonthat, N.K.
Deposited on	:	2015-01-04
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

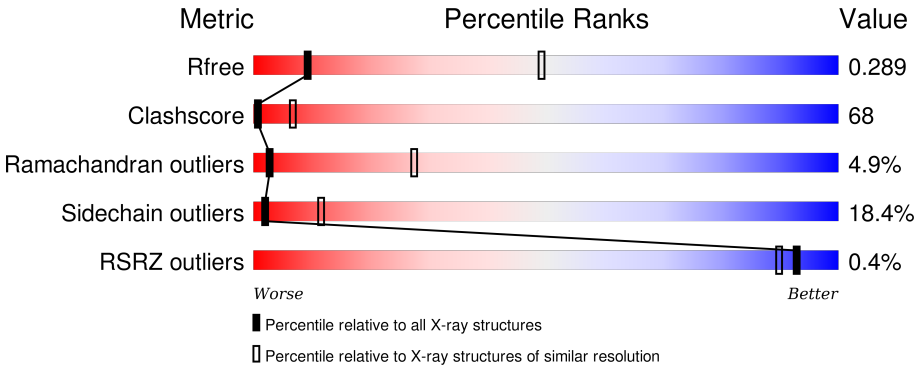
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	447	25% 60% 13%
1	B	447	23% 59% 16%
1	C	447	22% 61% 15%
1	D	447	24% 58% 17%
1	E	447	21% 61% 16%

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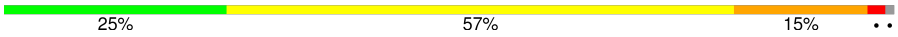
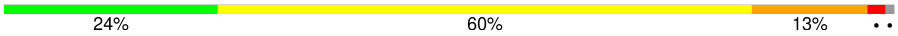
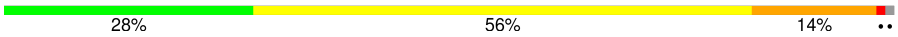
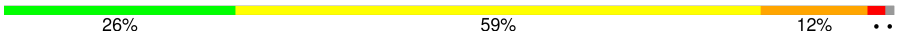
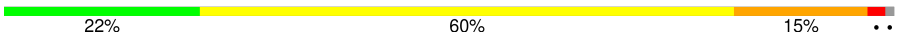
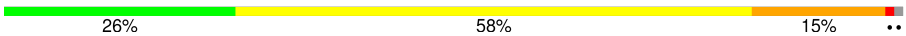
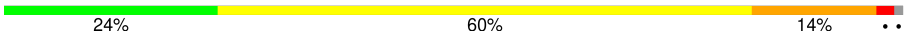
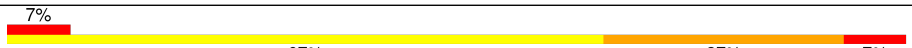
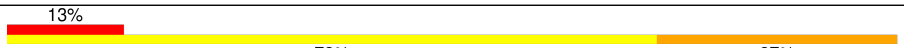
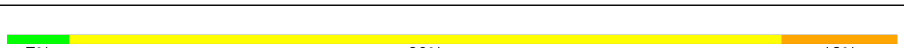
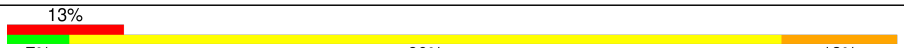
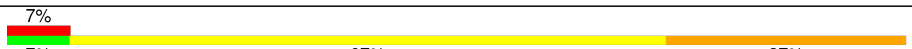
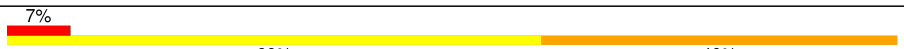
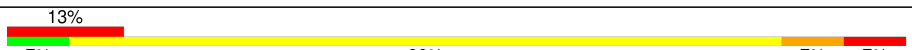
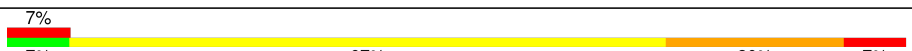
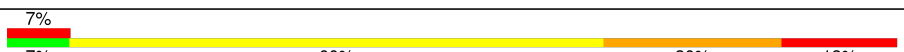
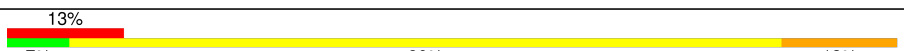
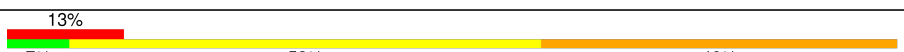
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	
1	I	447	
1	J	447	
1	K	447	
1	L	447	
1	M	447	
1	N	447	
2	1	15	
2	2	15	
2	O	15	
2	P	15	
2	Q	15	
2	R	15	
2	S	15	
2	T	15	
2	U	15	
2	V	15	
2	W	15	
2	X	15	
2	Y	15	
2	Z	15	

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
3	GLN	B	501	-	-	X	-
3	GLN	C	503	-	-	-	X
3	GLN	H	501	-	-	-	X
3	GLN	M	503	-	-	-	X
4	MG	C	504	-	-	-	X
4	MG	F	504	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51555 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	447	Total	C	N	O	S	0	0	0
			3563	2275	596	675	17			
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	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	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			
1	M	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	N	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P12425

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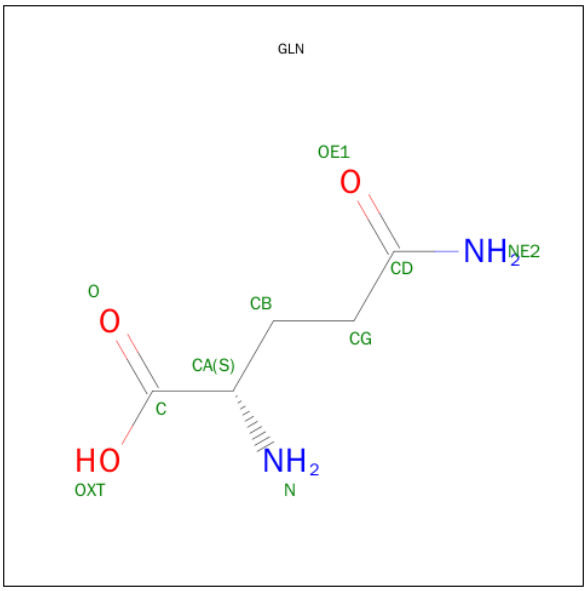
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P12425
A	0	HIS	-	EXPRESSION TAG	UNP P12425
B	-2	GLY	-	EXPRESSION TAG	UNP P12425
B	-1	SER	-	EXPRESSION TAG	UNP P12425
B	0	HIS	-	EXPRESSION TAG	UNP P12425
C	-2	GLY	-	EXPRESSION TAG	UNP P12425
C	-1	SER	-	EXPRESSION TAG	UNP P12425
C	0	HIS	-	EXPRESSION TAG	UNP P12425
D	-2	GLY	-	EXPRESSION TAG	UNP P12425
D	-1	SER	-	EXPRESSION TAG	UNP P12425
D	0	HIS	-	EXPRESSION TAG	UNP P12425
E	-2	GLY	-	EXPRESSION TAG	UNP P12425
E	-1	SER	-	EXPRESSION TAG	UNP P12425
E	0	HIS	-	EXPRESSION TAG	UNP P12425
F	-2	GLY	-	EXPRESSION TAG	UNP P12425
F	-1	SER	-	EXPRESSION TAG	UNP P12425
F	0	HIS	-	EXPRESSION TAG	UNP P12425
G	-2	GLY	-	EXPRESSION TAG	UNP P12425
G	-1	SER	-	EXPRESSION TAG	UNP P12425
G	0	HIS	-	EXPRESSION TAG	UNP P12425
H	-2	GLY	-	EXPRESSION TAG	UNP P12425
H	-1	SER	-	EXPRESSION TAG	UNP P12425
H	0	HIS	-	EXPRESSION TAG	UNP P12425
I	-2	GLY	-	EXPRESSION TAG	UNP P12425
I	-1	SER	-	EXPRESSION TAG	UNP P12425
I	0	HIS	-	EXPRESSION TAG	UNP P12425
J	-2	GLY	-	EXPRESSION TAG	UNP P12425
J	-1	SER	-	EXPRESSION TAG	UNP P12425
J	0	HIS	-	EXPRESSION TAG	UNP P12425
K	-2	GLY	-	EXPRESSION TAG	UNP P12425
K	-1	SER	-	EXPRESSION TAG	UNP P12425
K	0	HIS	-	EXPRESSION TAG	UNP P12425
L	-2	GLY	-	EXPRESSION TAG	UNP P12425
L	-1	SER	-	EXPRESSION TAG	UNP P12425
L	0	HIS	-	EXPRESSION TAG	UNP P12425
M	-2	GLY	-	EXPRESSION TAG	UNP P12425
M	-1	SER	-	EXPRESSION TAG	UNP P12425
M	0	HIS	-	EXPRESSION TAG	UNP P12425
N	-2	GLY	-	EXPRESSION TAG	UNP P12425
N	-1	SER	-	EXPRESSION TAG	UNP P12425
N	0	HIS	-	EXPRESSION TAG	UNP P12425

- Molecule 2 is a protein called TnrA peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	P	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	Q	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	R	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	S	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	T	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	U	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	V	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	W	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	X	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	Y	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	Z	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			
2	1	15	Total	C	N	O	S	0	0	0
			132	82	28	21	1			
2	2	15	Total	C	N	O	S	0	0	0
			133	82	28	22	1			

- 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 C N O 9 5 2 2	0	0
3	B	1	Total C N O 9 5 2 2	0	0
3	C	1	Total C N O 10 5 2 3	0	0
3	D	1	Total C N O 9 5 2 2	0	0
3	E	1	Total C N O 9 5 2 2	0	0
3	F	1	Total C N O 9 5 2 2	0	0
3	G	1	Total C N O 9 5 2 2	0	0
3	H	1	Total C N O 9 5 2 2	0	0
3	I	1	Total C N O 9 5 2 2	0	0
3	J	1	Total C N O 9 5 2 2	0	0
3	K	1	Total C N O 9 5 2 2	0	0
3	L	1	Total C N O 10 5 2 3	0	0
3	M	1	Total C N O 10 5 2 3	0	0
3	N	1	Total C N O 9 5 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

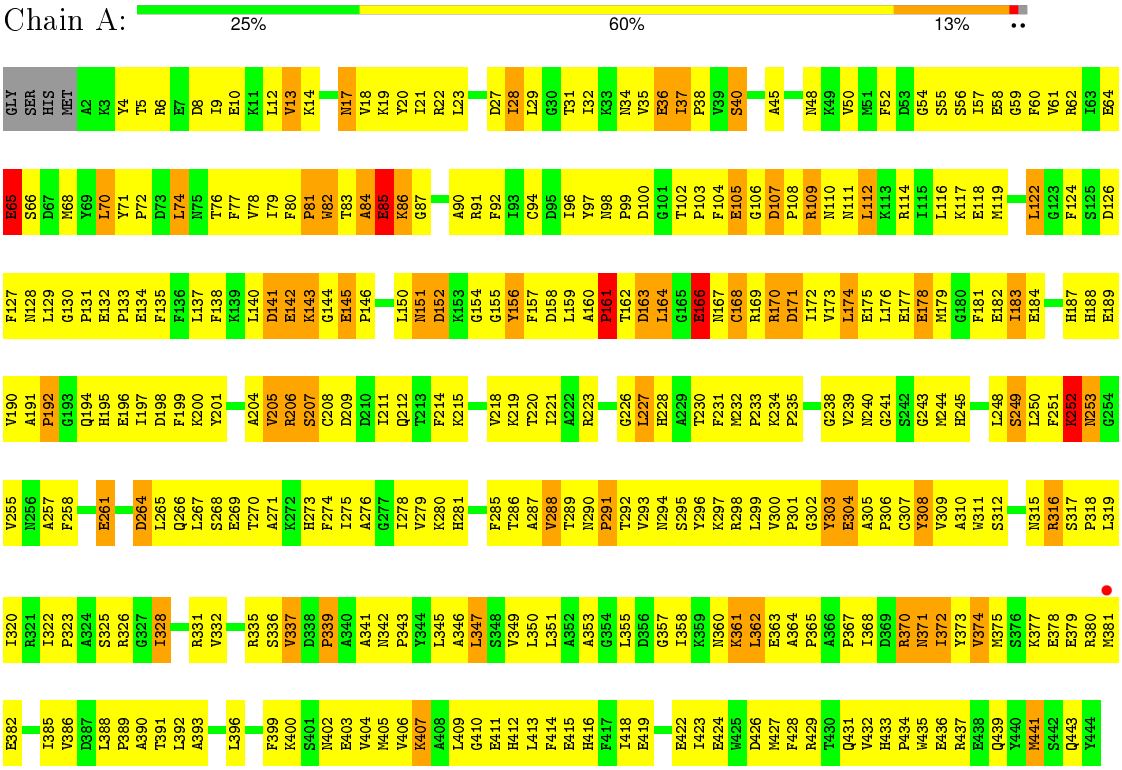
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	3	Total Mg 3 3	0	0
4	D	8	Total Mg 8 8	0	0
4	K	3	Total Mg 3 3	0	0
4	E	2	Total Mg 2 2	0	0
4	H	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0
4	I	2	Total Mg 2 2	0	0
4	C	7	Total Mg 7 7	0	0
4	A	4	Total Mg 4 4	0	0
4	N	2	Total Mg 2 2	0	0
4	L	3	Total Mg 3 3	0	0
4	F	3	Total Mg 3 3	0	0
4	M	3	Total Mg 3 3	0	0

3 Residue-property plots (i)

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.

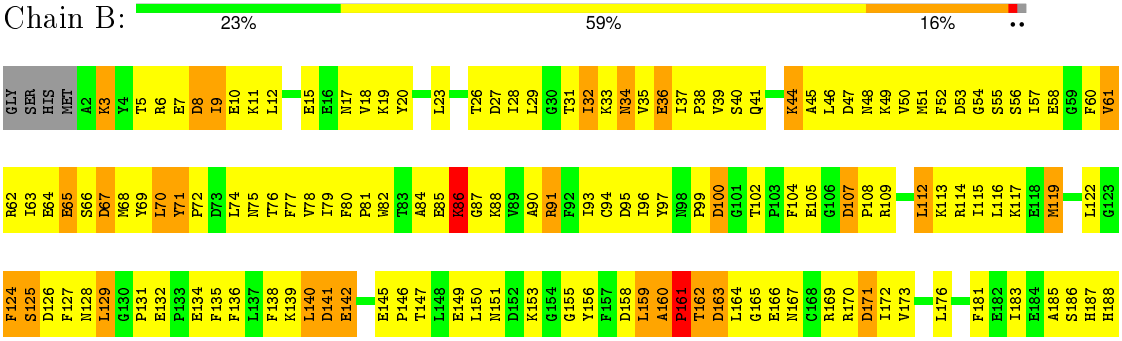
- Molecule 1: Glutamine synthetase

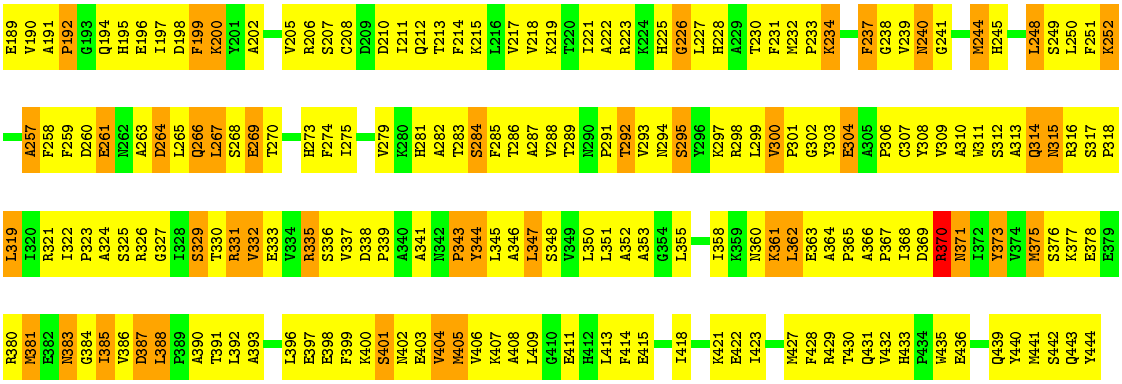
Chain A:



- Molecule 1: Glutamine synthetase

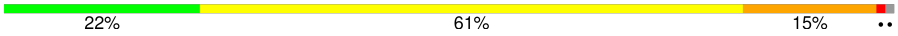
Chain B:

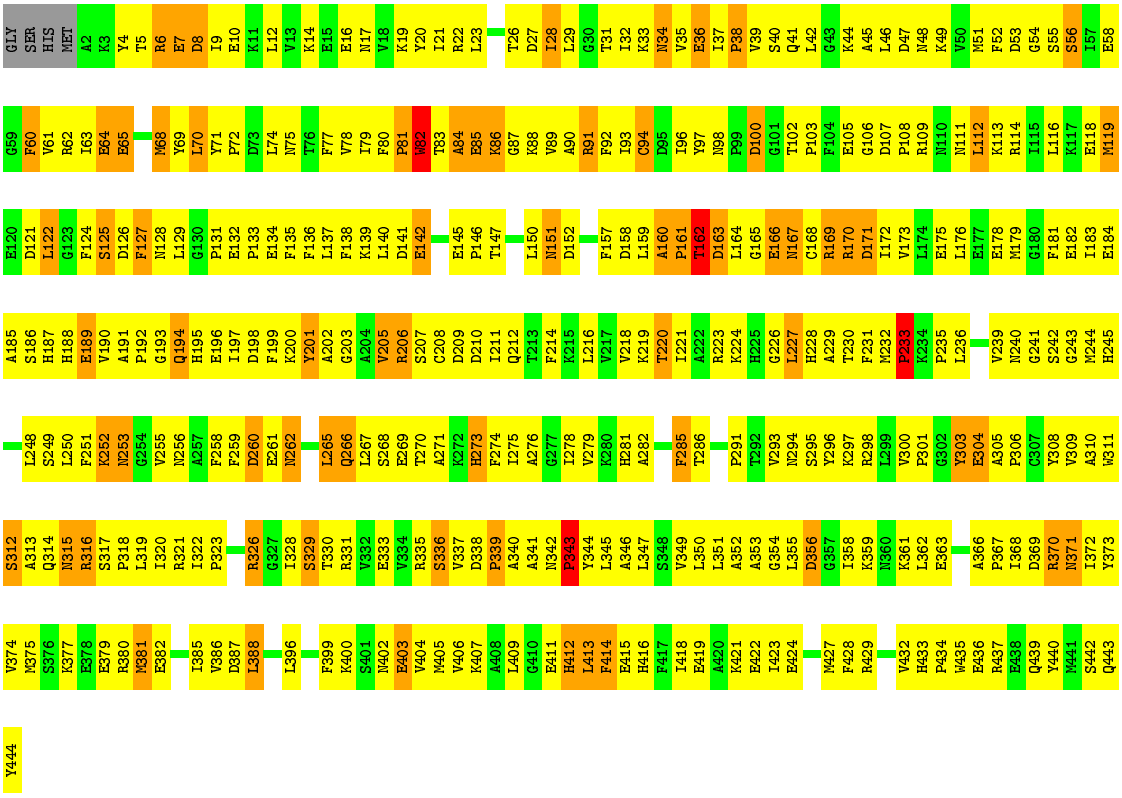




- Molecule 1: Glutamine synthetase

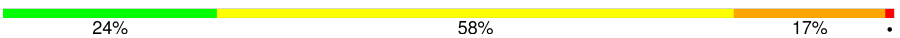
Chain C:

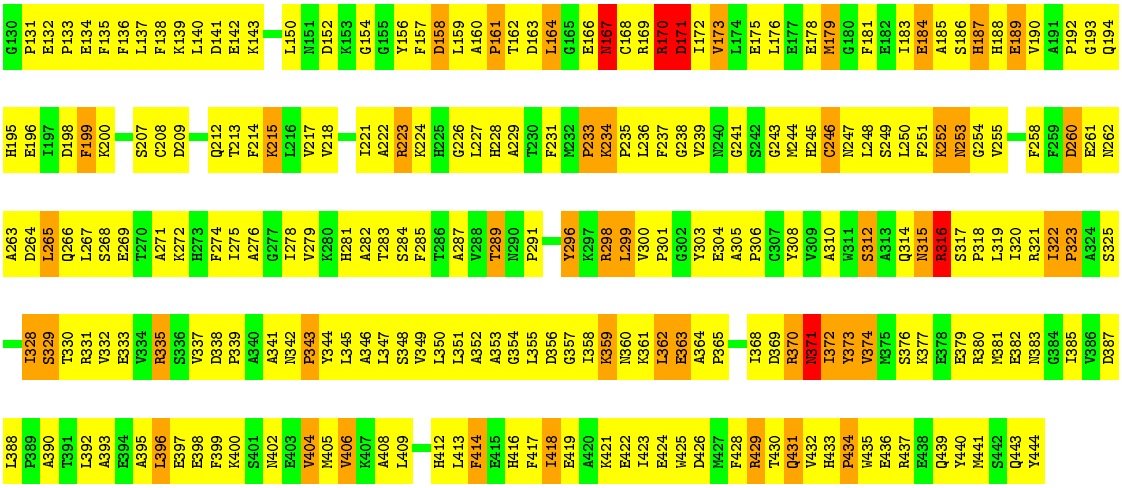




- Molecule 1: Glutamine synthetase

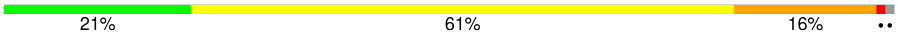
Chain D:

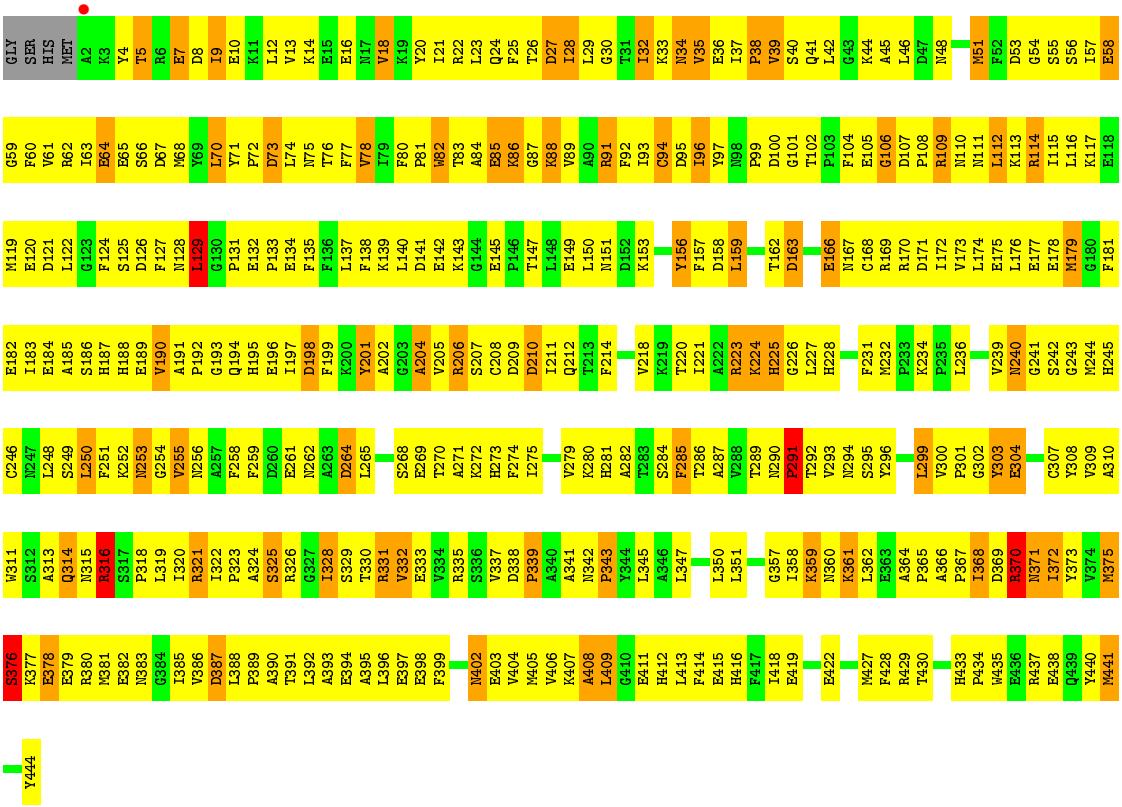




- Molecule 1: Glutamine synthetase

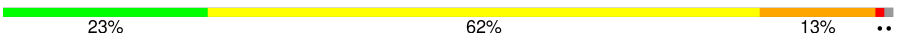
Chain E:

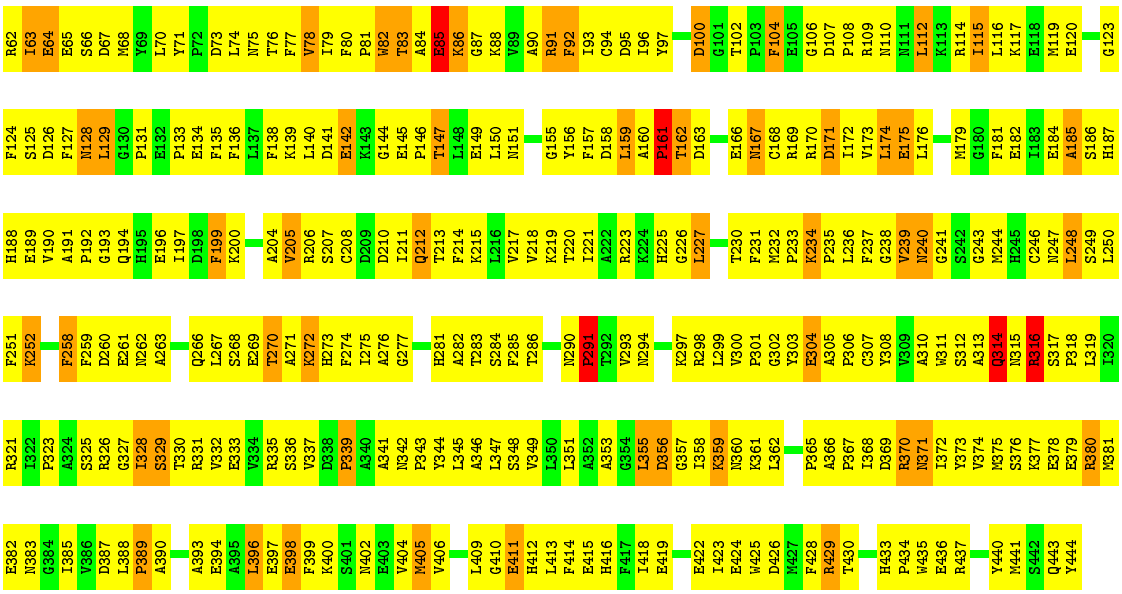




- Molecule 1: Glutamine synthetase

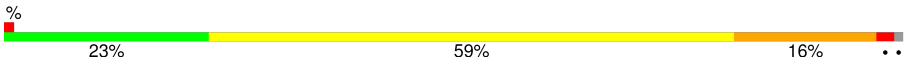
Chain F:

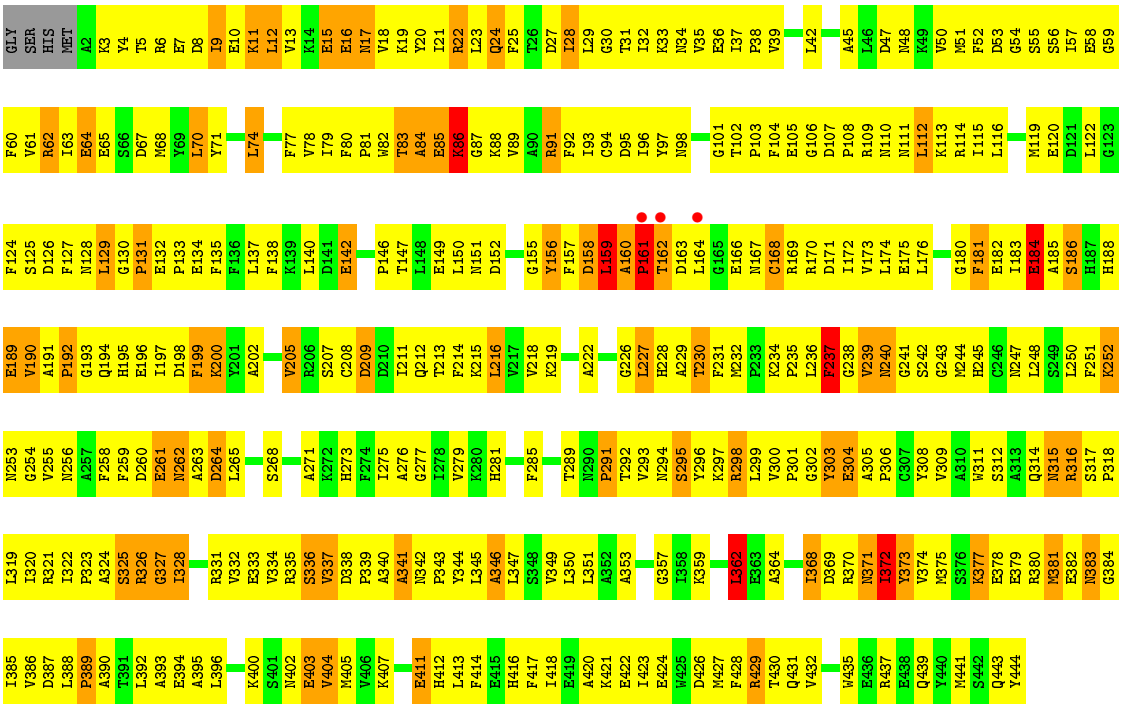




• Molecule 1: Glutamine synthetase

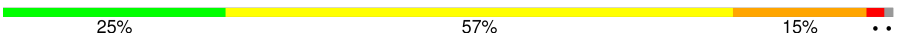
Chain G:

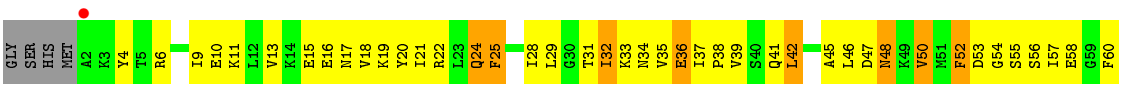


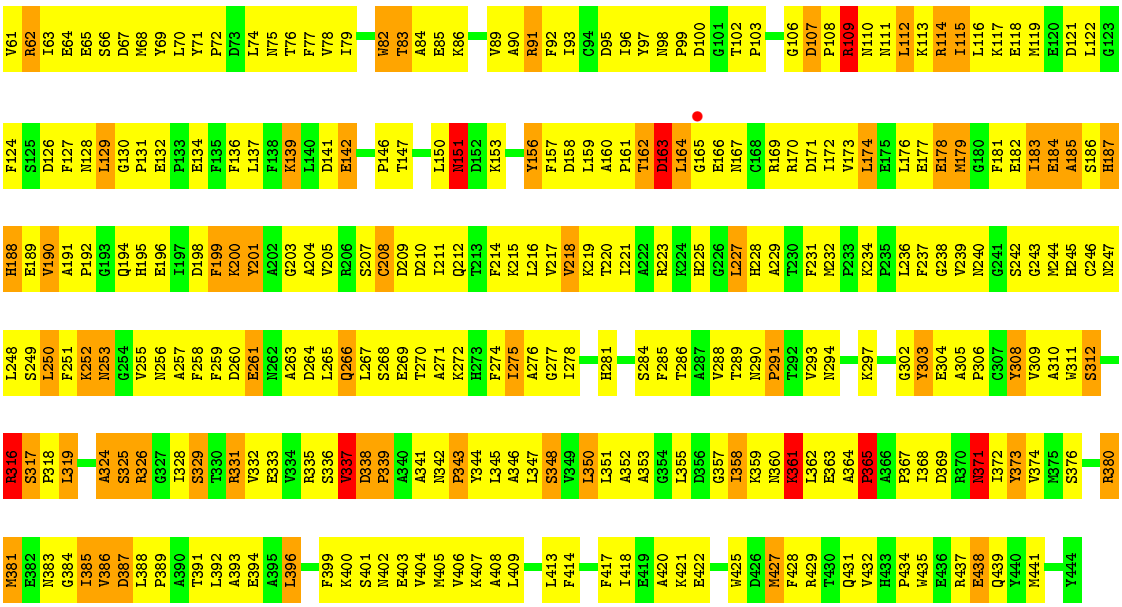


• Molecule 1: Glutamine synthetase

Chain H:

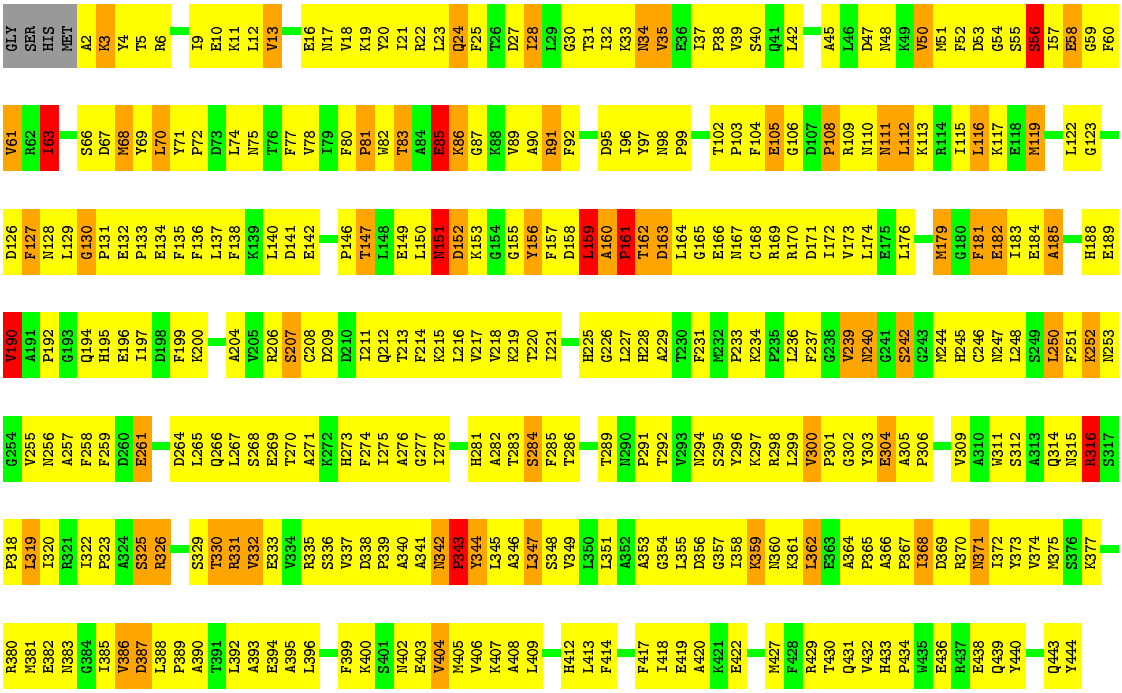






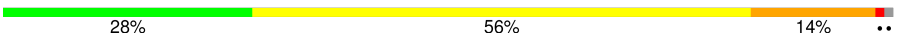
• Molecule 1: Glutamine synthetase

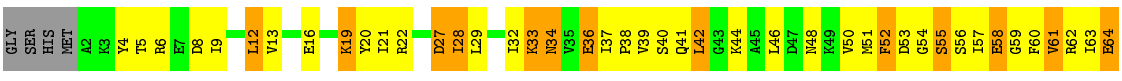
Chain I:

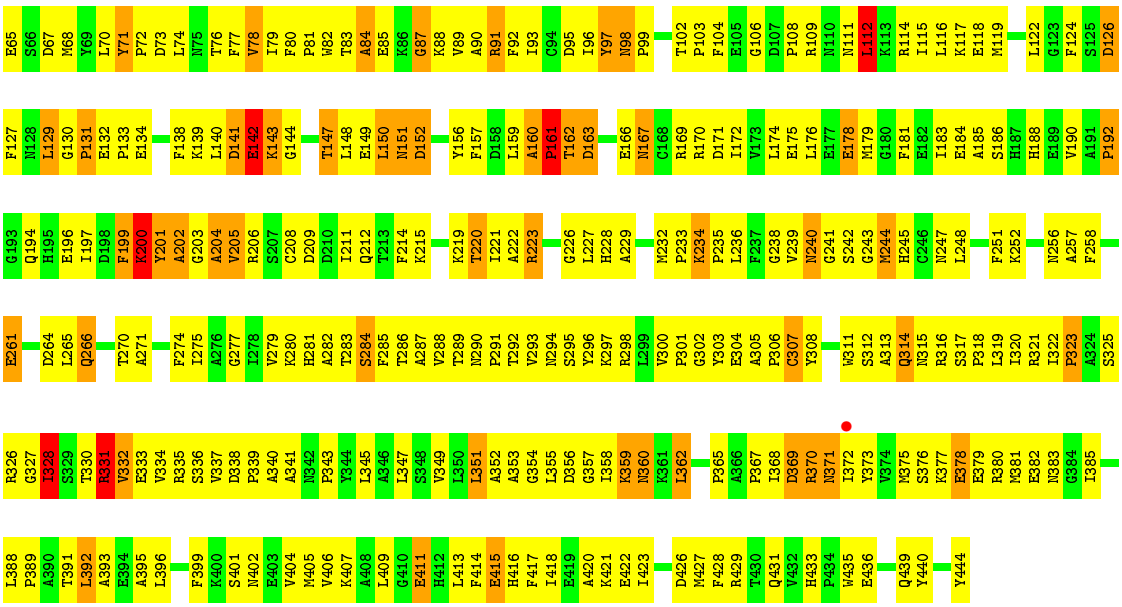


• Molecule 1: Glutamine synthetase

Chain J:

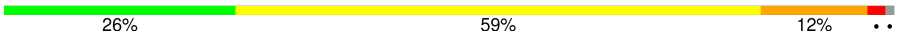


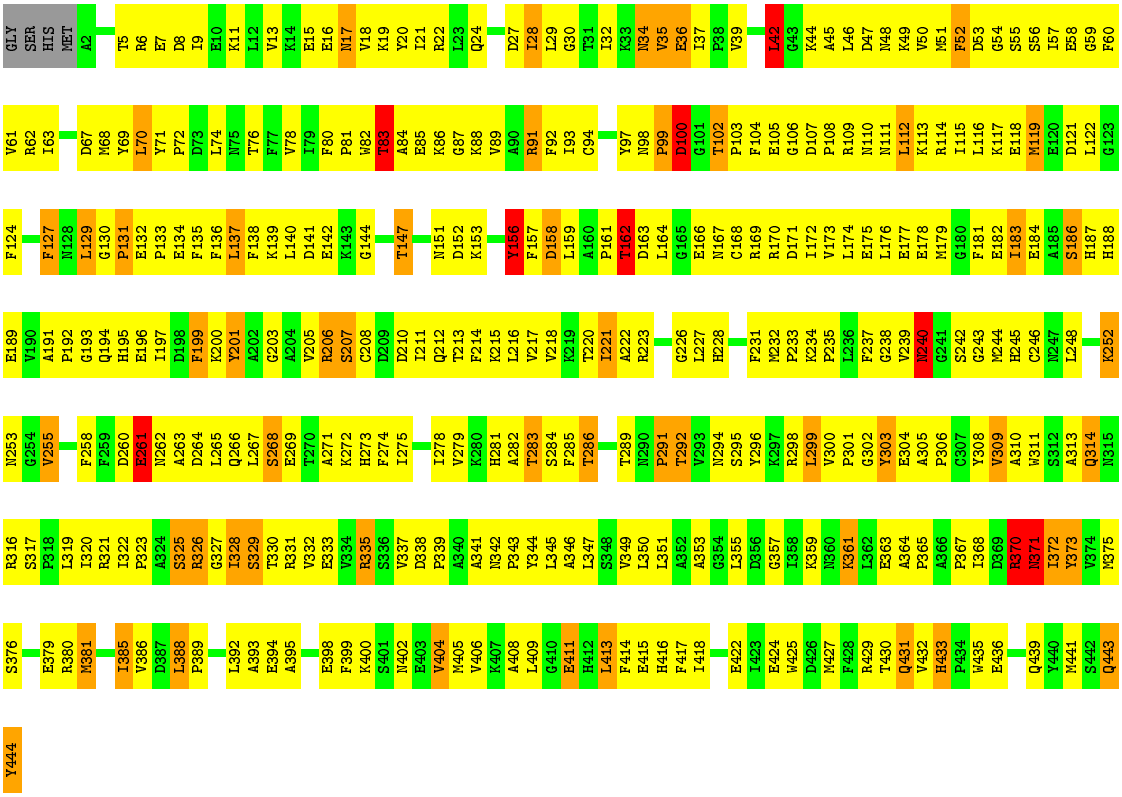




• Molecule 1: Glutamine synthetase

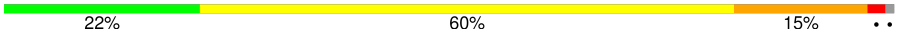
Chain K:

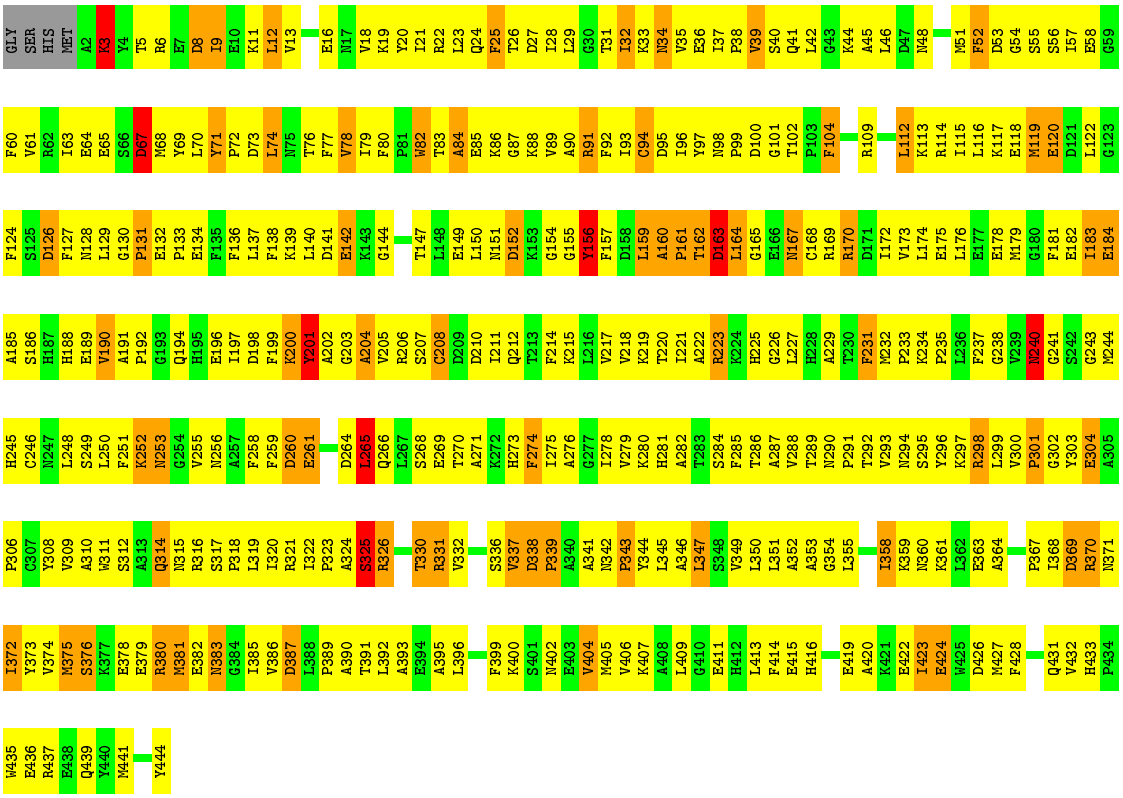




• Molecule 1: Glutamine synthetase

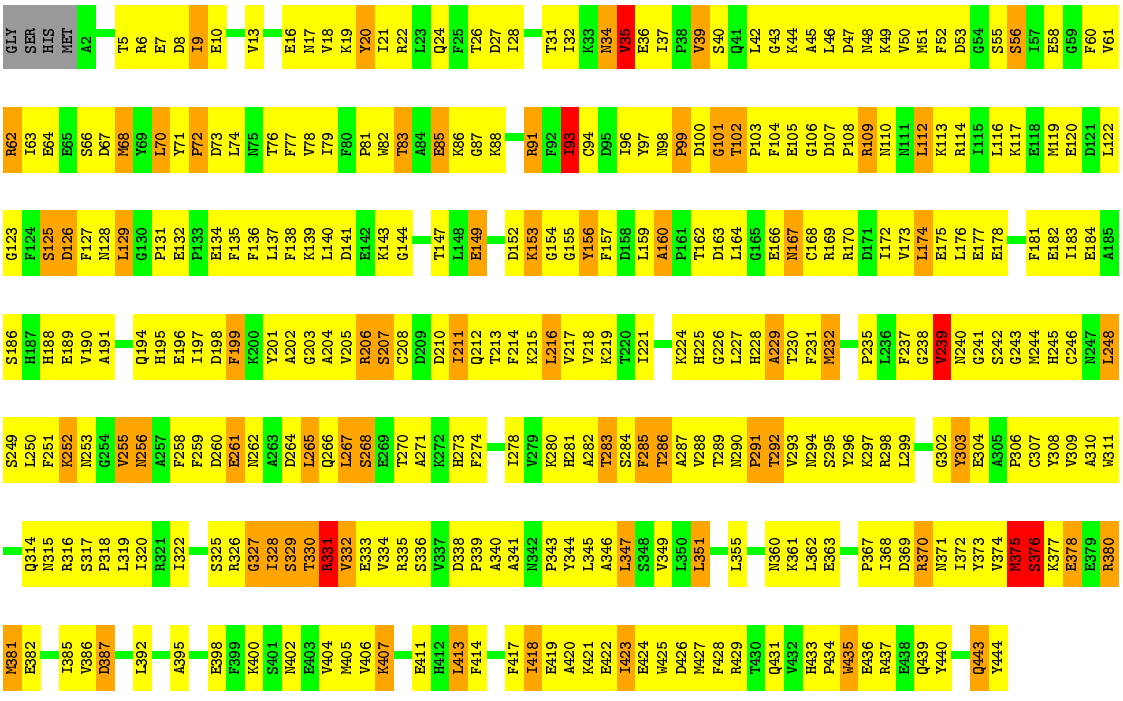
Chain L:





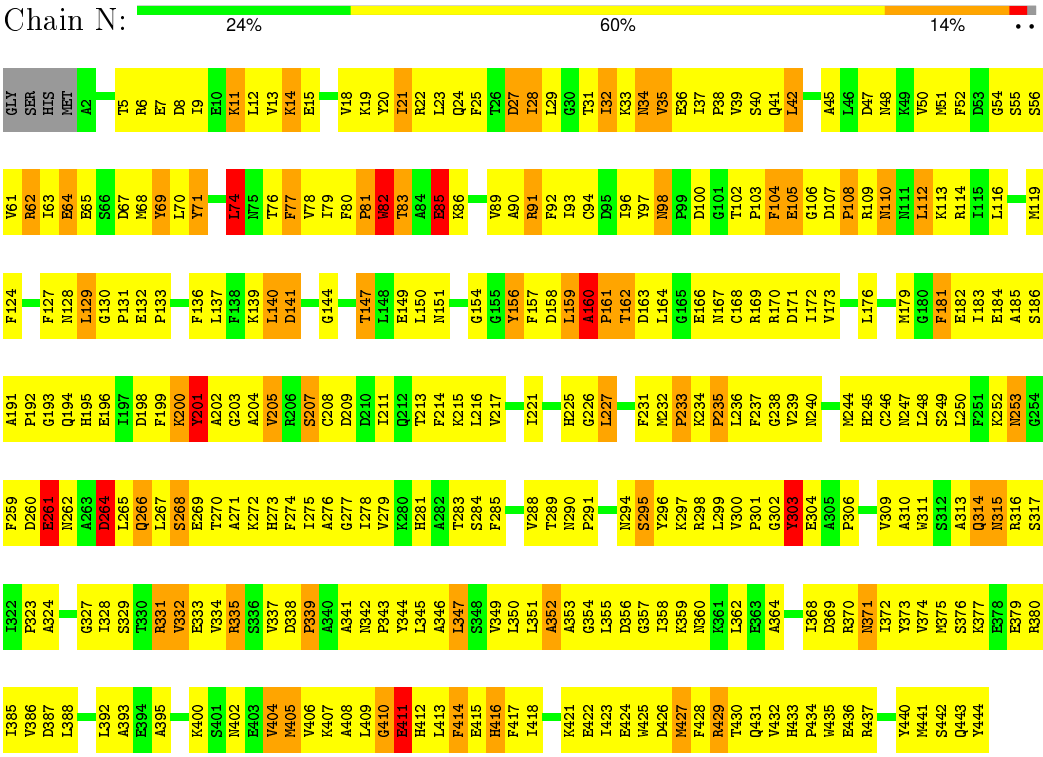
• Molecule 1: Glutamine synthetase

Chain M:



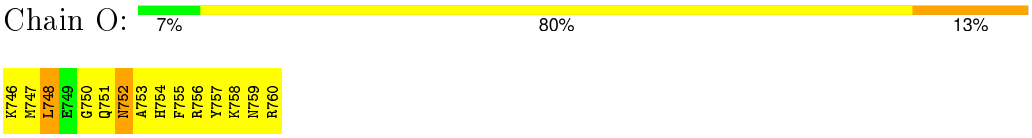
• Molecule 1: Glutamine synthetase

Chain N:



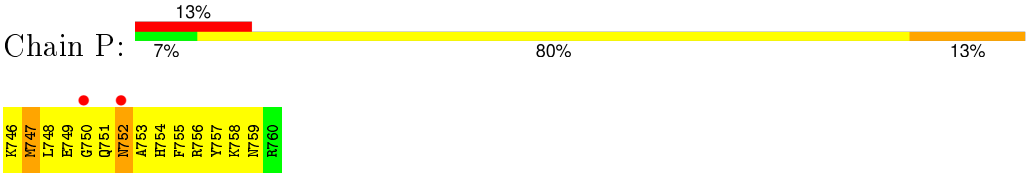
- Molecule 2: TnrA peptide

Chain O:



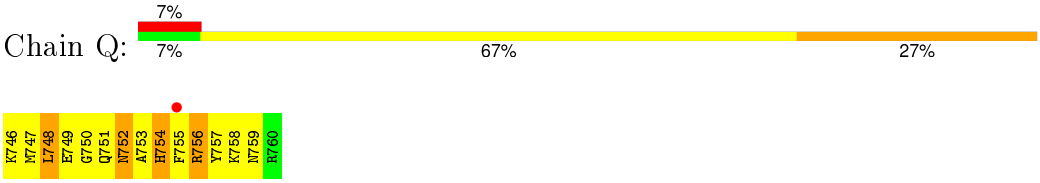
- Molecule 2: TnrA peptide

Chain P:



- Molecule 2: TnrA peptide

Chain Q:

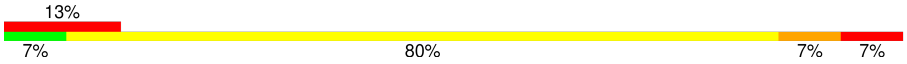


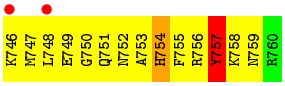
- Molecule 2: TnrA peptide

Chain R:

- Molecule 2: TnrA peptide

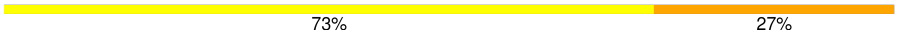
Chain S:





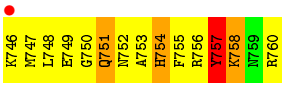
- Molecule 2: TnrA peptide

Chain T:



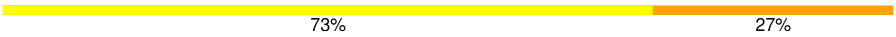
- Molecule 2: TnrA peptide

Chain U:



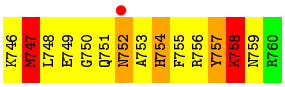
- Molecule 2: TnrA peptide

Chain V:



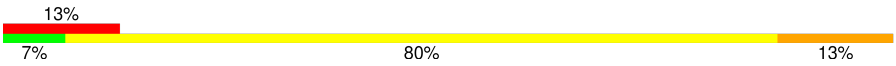
- Molecule 2: TnrA peptide

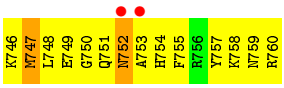
Chain W:



- Molecule 2: TnrA peptide

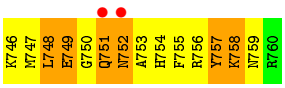
Chain X:





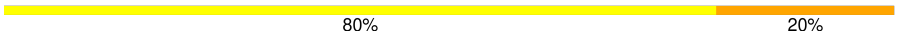
- Molecule 2: TnrA peptide

Chain Y:



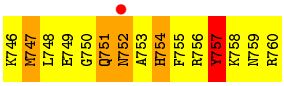
- Molecule 2: TnrA peptide

Chain Z:



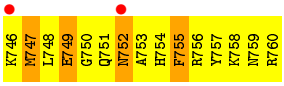
- Molecule 2: TnrA peptide

Chain 1:



- Molecule 2: TnrA peptide

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	295.80Å 295.80Å 103.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	147.90 – 3.50 147.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (147.90-3.50) 95.8 (147.90-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.49Å)	Xtriage
Refinement program	CNS.1.2	Depositor
R, R_{free}	0.243 , 0.284 0.258 , 0.289	Depositor DCC
R_{free} test set	14817 reflections (12.09%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.380 for -h,-k,l 0.387 for h,-h-k,-l 0.387 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 122569 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	51555	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.59	0/3618	0.97	9/4895 (0.2%)
1	B	0.58	0/3618	0.98	6/4895 (0.1%)
1	C	0.56	0/3618	0.94	4/4895 (0.1%)
1	D	0.59	0/3647	0.97	4/4933 (0.1%)
1	E	0.58	1/3618 (0.0%)	0.91	5/4895 (0.1%)
1	F	0.58	0/3618	0.91	3/4895 (0.1%)
1	G	0.56	0/3618	0.94	8/4895 (0.2%)
1	H	0.56	1/3618 (0.0%)	0.92	3/4895 (0.1%)
1	I	0.57	0/3618	0.95	6/4895 (0.1%)
1	J	0.55	0/3618	0.96	9/4895 (0.2%)
1	K	0.53	0/3618	0.91	5/4895 (0.1%)
1	L	0.57	1/3618 (0.0%)	0.94	5/4895 (0.1%)
1	M	0.60	1/3618 (0.0%)	0.99	15/4895 (0.3%)
1	N	0.59	0/3618	0.98	6/4895 (0.1%)
2	1	0.63	0/134	1.37	3/175 (1.7%)
2	2	0.67	0/135	1.07	1/175 (0.6%)
2	O	0.55	0/135	0.84	0/175
2	P	0.55	0/135	1.01	0/175
2	Q	0.72	0/135	1.09	0/175
2	R	0.68	0/135	1.27	1/175 (0.6%)
2	S	0.72	0/135	1.15	1/175 (0.6%)
2	T	0.60	0/135	1.12	1/175 (0.6%)
2	U	0.61	0/135	1.19	1/175 (0.6%)
2	V	1.06	1/135 (0.7%)	1.32	2/175 (1.1%)
2	W	0.81	0/135	1.39	3/175 (1.7%)
2	X	0.63	0/135	1.19	1/175 (0.6%)
2	Y	0.89	0/135	1.27	1/175 (0.6%)
2	Z	0.75	0/135	1.06	1/175 (0.6%)
All	All	0.58	5/52570 (0.0%)	0.96	104/71018 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	D	0	1
1	F	0	1
1	J	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	408	ALA	CA-CB	8.77	1.70	1.52
2	V	760	ARG	C-O	8.06	1.38	1.23
1	H	208	CYS	CB-SG	-5.99	1.72	1.81
1	M	435	TRP	CB-CG	-5.13	1.41	1.50
1	L	201	TYR	CB-CG	-5.10	1.44	1.51

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	747	MET	N-CA-C	-10.28	83.24	111.00
1	J	331	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	J	331	ARG	NE-CZ-NH2	-9.24	115.68	120.30
2	W	747	MET	N-CA-C	-7.96	89.52	111.00
2	1	747	MET	N-CA-C	-7.57	90.55	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	TYR	Sidechain
1	A	296	TYR	Sidechain
1	A	4	TYR	Sidechain
1	B	303	TYR	Sidechain
1	D	296	TYR	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	3535	0	3466	464	0
1	B	3535	0	3466	483	0
1	C	3535	0	3466	473	0
1	D	3563	0	3493	527	0
1	E	3535	0	3466	567	0
1	F	3535	0	3466	506	0
1	G	3535	0	3466	526	0
1	H	3535	0	3466	484	0
1	I	3535	0	3466	444	0
1	J	3535	0	3466	445	0
1	K	3535	0	3466	479	0
1	L	3535	0	3466	521	0
1	M	3535	0	3466	494	0
1	N	3535	0	3466	525	0
2	1	132	0	130	51	0
2	2	133	0	130	49	0
2	O	133	0	130	45	0
2	P	133	0	130	46	0
2	Q	133	0	130	49	0
2	R	133	0	130	36	0
2	S	133	0	130	55	0
2	T	133	0	130	56	0
2	U	133	0	130	46	0
2	V	133	0	130	47	0
2	W	133	0	130	73	0
2	X	133	0	130	41	0
2	Y	133	0	130	60	0
2	Z	133	0	130	65	0
3	A	9	0	7	5	0
3	B	9	0	7	6	0
3	C	10	0	7	3	0
3	D	9	0	7	3	0
3	E	9	0	7	2	0
3	F	9	0	7	5	0
3	G	9	0	7	2	0
3	H	9	0	7	1	0
3	I	9	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	9	0	7	3	0
3	K	9	0	7	0	0
3	L	10	0	7	4	0
3	M	10	0	7	0	0
3	N	9	0	7	1	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	7	0	0	0	0
4	D	8	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	I	2	0	0	0	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
4	M	3	0	0	0	0
4	N	2	0	0	0	0
All	All	51555	0	50469	6970	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 68.

The worst 5 of 6970 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:A:163:ASP:HA	1:A:170:ARG:NH2	1.36	1.38
2:W:758:LYS:HD2	2:W:758:LYS:O	1.23	1.26
1:C:113:LYS:HA	1:C:116:LEU:HD12	1.22	1.19
1:A:163:ASP:CA	1:A:170:ARG:HH22	1.56	1.18
1:M:329:SER:O	1:M:331:ARG:HD3	1.42	1.15

There are no symmetry-related clashes.

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	441/447 (99%)	330 (75%)	96 (22%)	15 (3%)	5 39
1	B	441/447 (99%)	338 (77%)	80 (18%)	23 (5%)	2 25
1	C	441/447 (99%)	325 (74%)	91 (21%)	25 (6%)	2 23
1	D	445/447 (100%)	333 (75%)	84 (19%)	28 (6%)	2 21
1	E	441/447 (99%)	331 (75%)	93 (21%)	17 (4%)	4 34
1	F	441/447 (99%)	335 (76%)	92 (21%)	14 (3%)	5 40
1	G	441/447 (99%)	327 (74%)	83 (19%)	31 (7%)	1 18
1	H	441/447 (99%)	335 (76%)	83 (19%)	23 (5%)	2 25
1	I	441/447 (99%)	333 (76%)	78 (18%)	30 (7%)	1 19
1	J	441/447 (99%)	338 (77%)	83 (19%)	20 (4%)	3 30
1	K	441/447 (99%)	339 (77%)	85 (19%)	17 (4%)	4 34
1	L	441/447 (99%)	340 (77%)	83 (19%)	18 (4%)	3 33
1	M	441/447 (99%)	336 (76%)	89 (20%)	16 (4%)	4 37
1	N	441/447 (99%)	317 (72%)	94 (21%)	30 (7%)	1 19
2	1	13/15 (87%)	12 (92%)	0	1 (8%)	1 14
2	2	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
2	O	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
2	P	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1 14
2	Q	13/15 (87%)	10 (77%)	3 (23%)	0	100 100
2	R	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
2	S	13/15 (87%)	10 (77%)	3 (23%)	0	100 100
2	T	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
2	U	13/15 (87%)	8 (62%)	5 (38%)	0	100 100
2	V	13/15 (87%)	11 (85%)	2 (15%)	0	100 100
2	W	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	X	13/15 (87%)	8 (62%)	5 (38%)	0	100 100
2	Y	13/15 (87%)	9 (69%)	4 (31%)	0	100 100
2	Z	13/15 (87%)	13 (100%)	0	0	100 100
All	All	6360/6468 (98%)	4808 (76%)	1242 (20%)	310 (5%)	3 27

5 of 310 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	A	371	ASN
1	B	86	LYS
1	B	161	PRO
1	B	162	THR

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	382/385 (99%)	322 (84%)	60 (16%)	3 19
1	B	382/385 (99%)	313 (82%)	69 (18%)	2 12
1	C	382/385 (99%)	313 (82%)	69 (18%)	2 12
1	D	385/385 (100%)	310 (80%)	75 (20%)	2 10
1	E	382/385 (99%)	300 (78%)	82 (22%)	1 7
1	F	382/385 (99%)	314 (82%)	68 (18%)	2 13
1	G	382/385 (99%)	312 (82%)	70 (18%)	2 12
1	H	382/385 (99%)	303 (79%)	79 (21%)	1 8
1	I	382/385 (99%)	314 (82%)	68 (18%)	2 13
1	J	382/385 (99%)	317 (83%)	65 (17%)	2 15
1	K	382/385 (99%)	316 (83%)	66 (17%)	2 14
1	L	382/385 (99%)	307 (80%)	75 (20%)	1 9
1	M	382/385 (99%)	313 (82%)	69 (18%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	382/385 (99%)	321 (84%)	61 (16%)	3 18
2	1	13/13 (100%)	11 (85%)	2 (15%)	3 20
2	2	13/13 (100%)	10 (77%)	3 (23%)	1 5
2	O	13/13 (100%)	11 (85%)	2 (15%)	3 20
2	P	13/13 (100%)	12 (92%)	1 (8%)	16 54
2	Q	13/13 (100%)	9 (69%)	4 (31%)	0 3
2	R	13/13 (100%)	8 (62%)	5 (38%)	0 1
2	S	13/13 (100%)	11 (85%)	2 (15%)	3 20
2	T	13/13 (100%)	10 (77%)	3 (23%)	1 5
2	U	13/13 (100%)	9 (69%)	4 (31%)	0 3
2	V	13/13 (100%)	11 (85%)	2 (15%)	3 20
2	W	13/13 (100%)	9 (69%)	4 (31%)	0 3
2	X	13/13 (100%)	12 (92%)	1 (8%)	16 54
2	Y	13/13 (100%)	8 (62%)	5 (38%)	0 1
2	Z	13/13 (100%)	11 (85%)	2 (15%)	3 20
All	All	5533/5572 (99%)	4517 (82%)	1016 (18%)	2 11

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	205	VAL
1	H	391	THR
1	N	110	ASN
1	G	326	ARG
1	H	151	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	128	ASN
1	J	194	GLN
2	T	759	ASN
1	H	187	HIS
1	I	111	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 61 ligands modelled in this entry, 47 are monoatomic - leaving 14 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	A	501	4	7,8,9	0.81	0	6,9,11	0.59	0
3	GLN	B	501	4	7,8,9	0.67	0	6,9,11	0.70	0
3	GLN	C	503	-	6,9,9	0.27	0	5,11,11	0.20	0
3	GLN	D	501	-	7,8,9	0.54	0	6,9,11	0.72	0
3	GLN	E	501	-	7,8,9	0.49	0	6,9,11	0.84	1 (16%)
3	GLN	F	501	-	7,8,9	0.73	0	6,9,11	0.80	0
3	GLN	G	501	-	7,8,9	0.46	0	6,9,11	0.74	0
3	GLN	H	501	4	7,8,9	0.53	0	6,9,11	0.80	0
3	GLN	I	501	4	7,8,9	0.42	0	6,9,11	0.66	0
3	GLN	J	501	-	7,8,9	0.47	0	6,9,11	0.79	0
3	GLN	K	501	4	7,8,9	0.67	0	6,9,11	0.66	0
3	GLN	L	501	4	6,9,9	0.35	0	5,11,11	0.18	0
3	GLN	M	503	-	6,9,9	0.34	0	5,11,11	0.20	0
3	GLN	N	501	4	7,8,9	0.42	0	6,9,11	0.69	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	A	501	4	-	0/5/7/9	0/0/0/0
3	GLN	B	501	4	-	0/5/7/9	0/0/0/0
3	GLN	C	503	-	-	0/5/9/9	0/0/0/0
3	GLN	D	501	-	-	0/5/7/9	0/0/0/0
3	GLN	E	501	-	-	0/5/7/9	0/0/0/0
3	GLN	F	501	-	-	0/5/7/9	0/0/0/0
3	GLN	G	501	-	-	0/5/7/9	0/0/0/0
3	GLN	H	501	4	-	0/5/7/9	0/0/0/0
3	GLN	I	501	4	-	0/5/7/9	0/0/0/0
3	GLN	J	501	-	-	0/5/7/9	0/0/0/0
3	GLN	K	501	4	-	0/5/7/9	0/0/0/0
3	GLN	L	501	4	-	0/5/9/9	0/0/0/0
3	GLN	M	503	-	-	0/5/9/9	0/0/0/0
3	GLN	N	501	4	-	0/5/7/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	GLN	O-C-CA	-2.05	120.15	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GLN	5	0
3	B	501	GLN	6	0
3	C	503	GLN	3	0
3	D	501	GLN	3	0
3	E	501	GLN	2	0
3	F	501	GLN	5	0
3	G	501	GLN	2	0
3	H	501	GLN	1	0
3	I	501	GLN	2	0
3	J	501	GLN	3	0
3	L	501	GLN	4	0
3	N	501	GLN	1	0

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^{th} 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	443/447 (99%)	-0.14	1 (0%) 95 93	21, 48, 89, 114	0
1	B	443/447 (99%)	-0.14	0 100 100	16, 47, 93, 118	0
1	C	443/447 (99%)	-0.14	0 100 100	19, 47, 90, 118	0
1	D	447/447 (100%)	-0.14	0 100 100	19, 49, 89, 117	0
1	E	443/447 (99%)	-0.14	1 (0%) 95 93	17, 50, 88, 122	0
1	F	443/447 (99%)	-0.14	0 100 100	19, 52, 91, 121	0
1	G	443/447 (99%)	-0.14	3 (0%) 89 82	21, 50, 97, 123	0
1	H	443/447 (99%)	-0.09	2 (0%) 91 88	19, 51, 93, 128	0
1	I	443/447 (99%)	-0.14	0 100 100	18, 50, 90, 125	0
1	J	443/447 (99%)	-0.05	1 (0%) 95 93	25, 58, 97, 119	0
1	K	443/447 (99%)	-0.05	0 100 100	27, 60, 96, 122	0
1	L	443/447 (99%)	-0.09	0 100 100	26, 59, 92, 113	0
1	M	443/447 (99%)	-0.09	0 100 100	24, 61, 95, 118	0
1	N	443/447 (99%)	-0.10	0 100 100	21, 51, 96, 125	0
2	1	15/15 (100%)	0.74	1 (6%) 21 16	68, 75, 89, 94	0
2	2	15/15 (100%)	0.91	2 (13%) 4 5	60, 77, 89, 91	0
2	O	15/15 (100%)	0.62	0 100 100	73, 87, 93, 97	0
2	P	15/15 (100%)	1.11	2 (13%) 4 5	73, 88, 94, 95	0
2	Q	15/15 (100%)	0.67	1 (6%) 21 16	79, 92, 95, 96	0
2	R	15/15 (100%)	0.62	1 (6%) 21 16	74, 81, 87, 91	0
2	S	15/15 (100%)	0.94	2 (13%) 4 5	56, 78, 88, 88	0
2	T	15/15 (100%)	0.47	0 100 100	56, 83, 92, 95	0
2	U	15/15 (100%)	0.89	1 (6%) 21 16	66, 85, 91, 92	0
2	V	15/15 (100%)	0.54	0 100 100	68, 81, 96, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	W	15/15 (100%)	0.50	1 (6%) 21 16	65, 86, 91, 94	0
2	X	15/15 (100%)	0.70	2 (13%) 4 5	67, 83, 91, 91	0
2	Y	15/15 (100%)	0.80	2 (13%) 4 5	61, 84, 92, 92	0
2	Z	15/15 (100%)	0.24	0 100 100	66, 78, 91, 97	0
All	All	6416/6468 (99%)	-0.09	23 (0%) 93 90	16, 54, 94, 128	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ALA	4.3
2	S	746	LYS	3.1
1	G	161	PRO	3.1
2	P	750	GLY	2.9
2	U	746	LYS	2.8

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
4	MG	F	504	1/1	0.21	1.03	11.21	86,86,86,86	0
4	MG	C	504	1/1	0.91	0.77	9.59	73,73,73,73	0
3	GLN	C	503	10/10	0.97	0.35	3.39	31,57,81,83	0
3	GLN	M	503	10/10	0.92	0.38	2.37	81,91,96,96	0
3	GLN	H	501	9/10	0.97	0.34	2.24	37,48,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GLN	E	501	9/10	0.99	0.30	1.46	27,33,47,47	0
3	GLN	K	501	9/10	0.95	0.32	1.34	46,53,60,66	0
3	GLN	L	501	10/10	0.95	0.31	1.03	59,65,70,70	0
3	GLN	G	501	9/10	0.96	0.27	0.98	30,39,59,66	0
3	GLN	N	501	9/10	0.98	0.24	0.69	24,32,44,46	0
3	GLN	J	501	9/10	0.96	0.21	-0.41	52,62,68,76	0
3	GLN	F	501	9/10	0.98	0.23	-0.53	29,45,60,63	0
3	GLN	I	501	9/10	0.99	0.21	-0.75	33,42,47,52	0
4	MG	H	504	1/1	0.93	0.25	-0.79	38,38,38,38	0
3	GLN	B	501	9/10	0.96	0.20	-1.03	45,52,60,61	0
3	GLN	D	501	9/10	0.98	0.19	-1.05	31,33,41,44	0
3	GLN	A	501	9/10	0.98	0.18	-1.09	32,36,40,40	0
4	MG	N	502	1/1	0.98	0.17	-1.23	12,12,12,12	0
4	MG	I	502	1/1	0.98	0.19	-1.27	24,24,24,24	0
4	MG	H	502	1/1	0.88	0.15	-1.38	36,36,36,36	0
4	MG	N	503	1/1	0.93	0.16	-1.52	17,17,17,17	0
4	MG	B	503	1/1	0.93	0.17	-2.06	24,24,24,24	0
4	MG	L	502	1/1	0.98	0.11	-2.11	31,31,31,31	0
4	MG	D	505	1/1	0.98	0.13	-2.36	14,14,14,14	0
4	MG	D	503	1/1	0.99	0.17	-2.96	16,16,16,16	0
4	MG	F	502	1/1	0.98	0.11	-3.13	26,26,26,26	0
4	MG	C	508	1/1	0.92	0.08	-3.35	24,24,24,24	0
4	MG	E	502	1/1	0.92	0.12	-3.50	30,30,30,30	0
4	MG	J	502	1/1	0.98	0.10	-3.71	28,28,28,28	0
4	MG	M	501	1/1	0.98	0.09	-3.80	10,10,10,10	0
4	MG	A	503	1/1	0.98	0.13	-3.83	19,19,19,19	0
4	MG	H	503	1/1	0.98	0.07	-3.92	25,25,25,25	0
4	MG	K	503	1/1	0.97	0.13	-4.34	24,24,24,24	0
4	MG	G	502	1/1	0.97	0.10	-4.93	31,31,31,31	0
4	MG	C	502	1/1	0.97	0.09	-5.20	23,23,23,23	0
4	MG	A	502	1/1	0.94	0.11	-5.24	37,37,37,37	0
4	MG	D	502	1/1	0.95	0.12	-5.44	32,32,32,32	0
4	MG	L	503	1/1	0.95	0.09	-5.51	23,23,23,23	0
4	MG	J	503	1/1	0.97	0.08	-5.66	16,16,16,16	0
4	MG	C	501	1/1	0.94	0.13	-5.87	22,22,22,22	0
4	MG	K	502	1/1	0.98	0.07	-6.52	20,20,20,20	0
4	MG	B	502	1/1	0.88	0.09	-6.63	30,30,30,30	0
4	MG	D	504	1/1	0.85	0.17	-7.28	33,33,33,33	0
4	MG	E	503	1/1	0.95	0.11	-	59,59,59,59	0
4	MG	L	504	1/1	0.92	0.31	-	40,40,40,40	0
4	MG	K	504	1/1	0.15	0.89	-	87,87,87,87	0
4	MG	A	504	1/1	0.97	0.10	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	M	502	1/1	0.98	0.08	-	55,55,55,55	0
4	MG	D	508	1/1	0.97	0.10	-	14,14,14,14	0
4	MG	C	506	1/1	0.97	0.12	-	16,16,16,16	0
4	MG	D	509	1/1	0.90	0.13	-	32,32,32,32	0
4	MG	A	505	1/1	0.89	0.17	-	14,14,14,14	0
4	MG	J	504	1/1	0.26	0.89	-	80,80,80,80	0
4	MG	B	504	1/1	0.97	0.12	-	11,11,11,11	0
4	MG	F	503	1/1	0.98	0.18	-	18,18,18,18	0
4	MG	C	507	1/1	0.98	0.06	-	14,14,14,14	0
4	MG	D	507	1/1	0.58	0.48	-	76,76,76,76	0
4	MG	M	504	1/1	0.85	0.67	-	84,84,84,84	0
4	MG	I	503	1/1	0.99	0.15	-	21,21,21,21	0
4	MG	C	505	1/1	0.84	0.20	-	28,28,28,28	0
4	MG	D	506	1/1	0.92	0.15	-	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.