



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 06:51 PM BST

PDB ID : 4S0R
Title : Structure of GS-ThrA 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

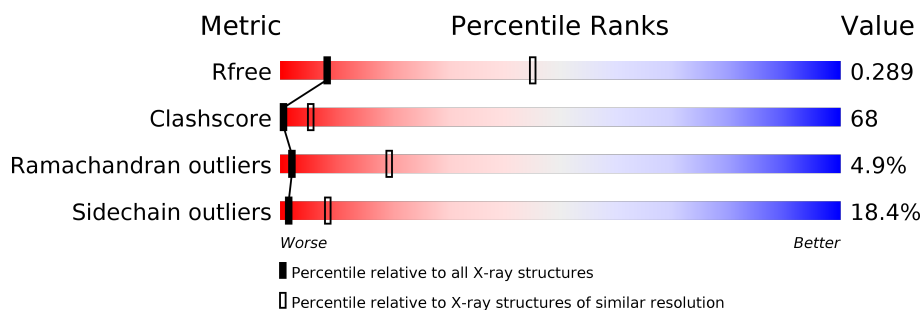
1 Overall quality at a glance

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.





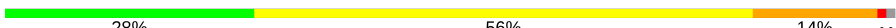
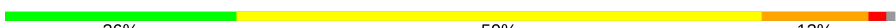
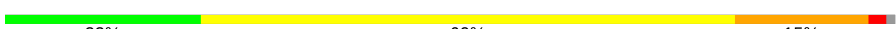
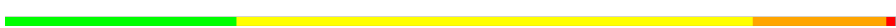













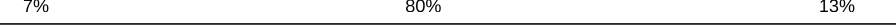

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	447	<div> <div>25%</div> <div>60%</div> <div>13%</div> <div>..</div> </div>
1	B	447	<div> <div>23%</div> <div>59%</div> <div>16%</div> <div>..</div> </div>
1	C	447	<div> <div>22%</div> <div>61%</div> <div>15%</div> <div>..</div> </div>
1	D	447	<div> <div>24%</div> <div>58%</div> <div>17%</div> <div>.</div> </div>
1	E	447	<div> <div>21%</div> <div>61%</div> <div>16%</div> <div>..</div> </div>
1	F	447	<div> <div>23%</div> <div>62%</div> <div>13%</div> <div>..</div> </div>
1	G	447	<div> <div>23%</div> <div>59%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
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	-

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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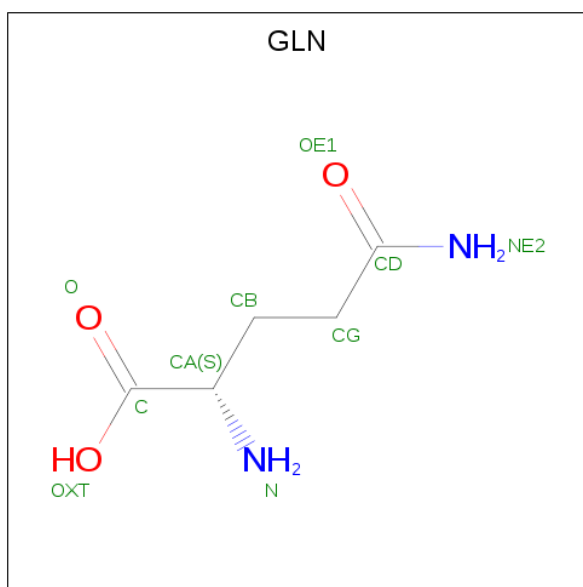
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P12425
A	0	HIS	-	EXPRESSION TAG	UNP P12425
B	-2	GLY	-	EXPRESSION TAG	UNP P12425
B	-1	SER	-	EXPRESSION TAG	UNP P12425
B	0	HIS	-	EXPRESSION TAG	UNP P12425
C	-2	GLY	-	EXPRESSION 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 133	C 82	N 28	O 22	S 1	0	0	0
2	P	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	Q	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	R	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	S	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	T	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	U	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	V	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	W	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	X	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	Y	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	Z	15	Total 133	C 82	N 28	O 22	S 1	0	0	0
2	1	15	Total 132	C 82	N 28	O 21	S 1	0	0	0
2	2	15	Total 133	C 82	N 28	O 22	S 1	0	0	0

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



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

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

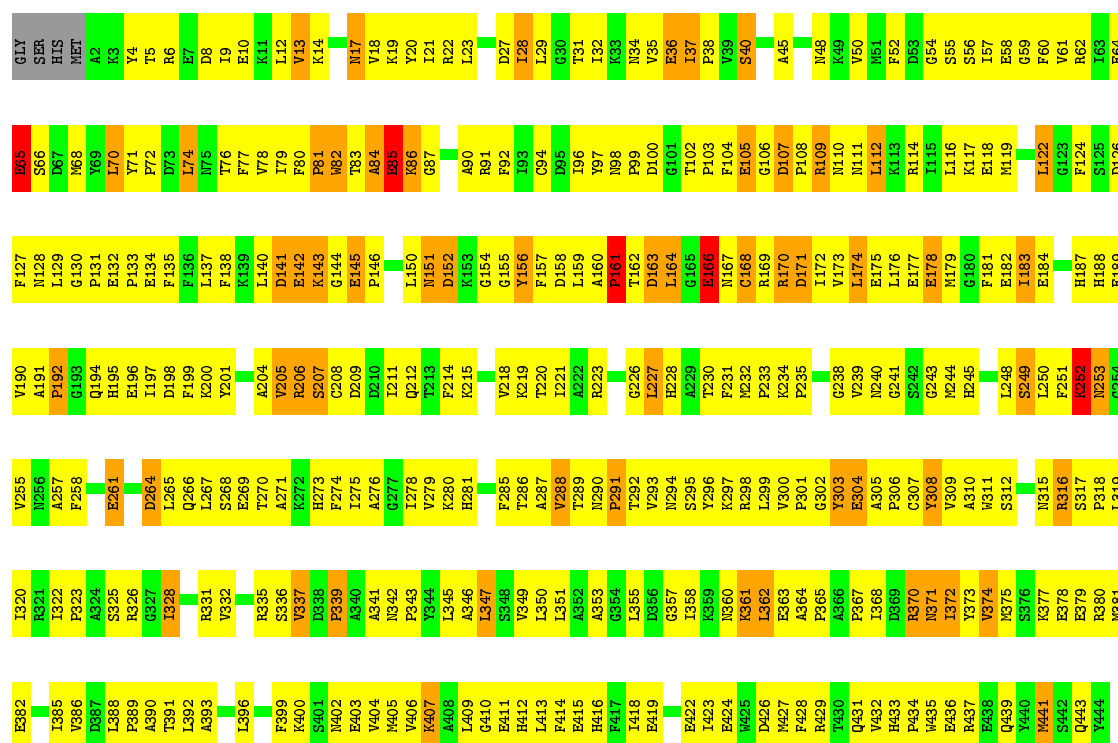
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	J	3	Total 3	Mg 3	0	0
4	D	8	Total 8	Mg 8	0	0
4	K	3	Total 3	Mg 3	0	0
4	E	2	Total 2	Mg 2	0	0
4	H	3	Total 3	Mg 3	0	0
4	B	3	Total 3	Mg 3	0	0
4	I	2	Total 2	Mg 2	0	0
4	C	7	Total 7	Mg 7	0	0
4	A	4	Total 4	Mg 4	0	0
4	N	2	Total 2	Mg 2	0	0
4	L	3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

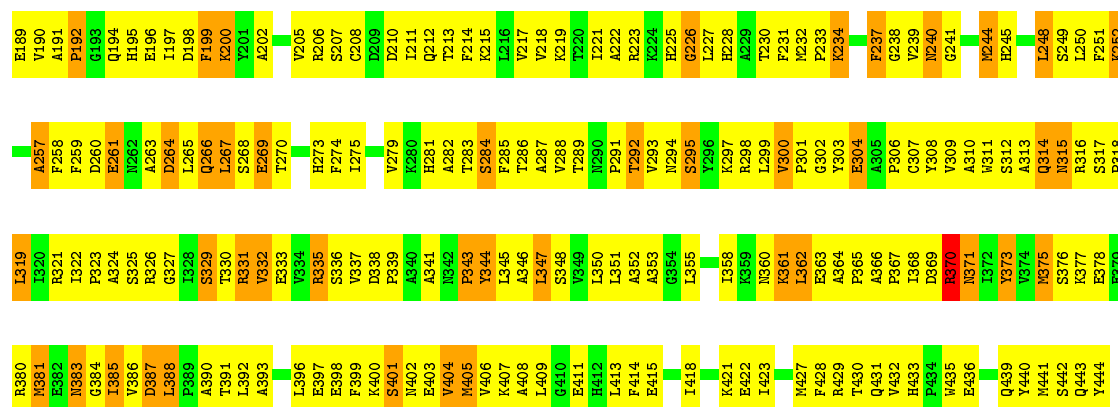
3 Residue-property plots

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. 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. 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

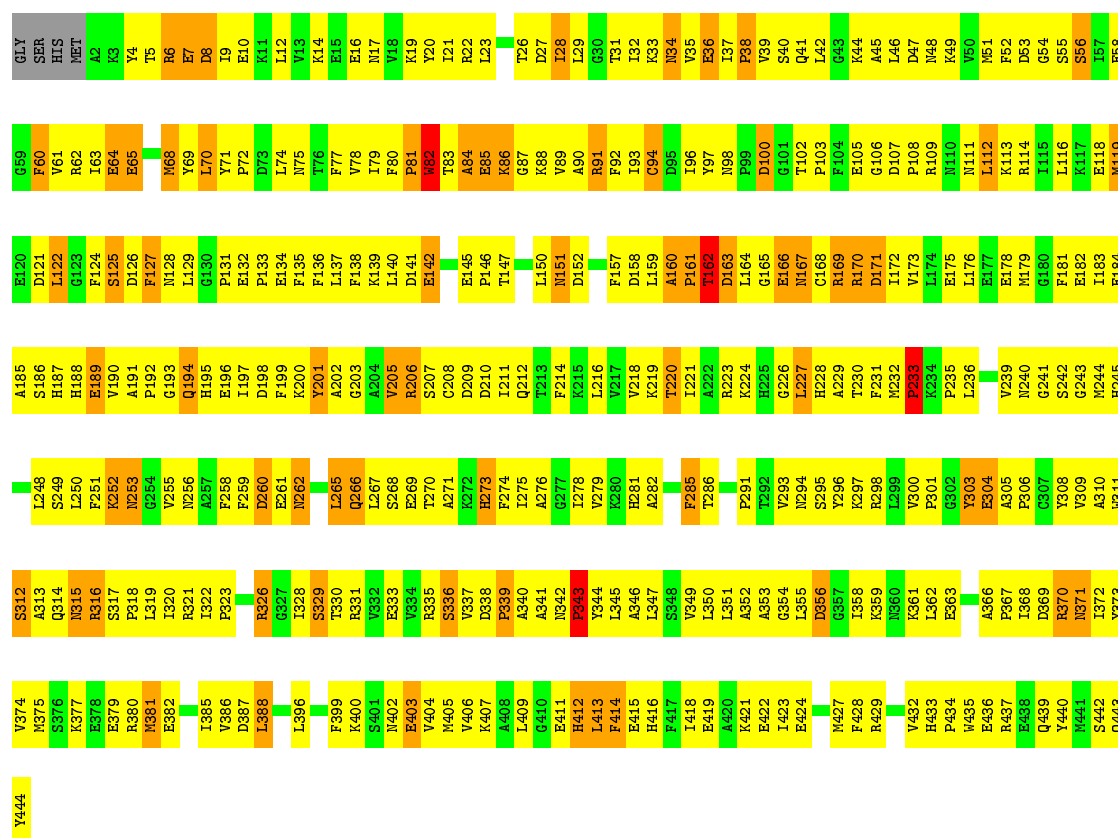
Chain A: 





• Molecule 1: Glutamine synthetase

Chain C: 22% 61% 15% ..

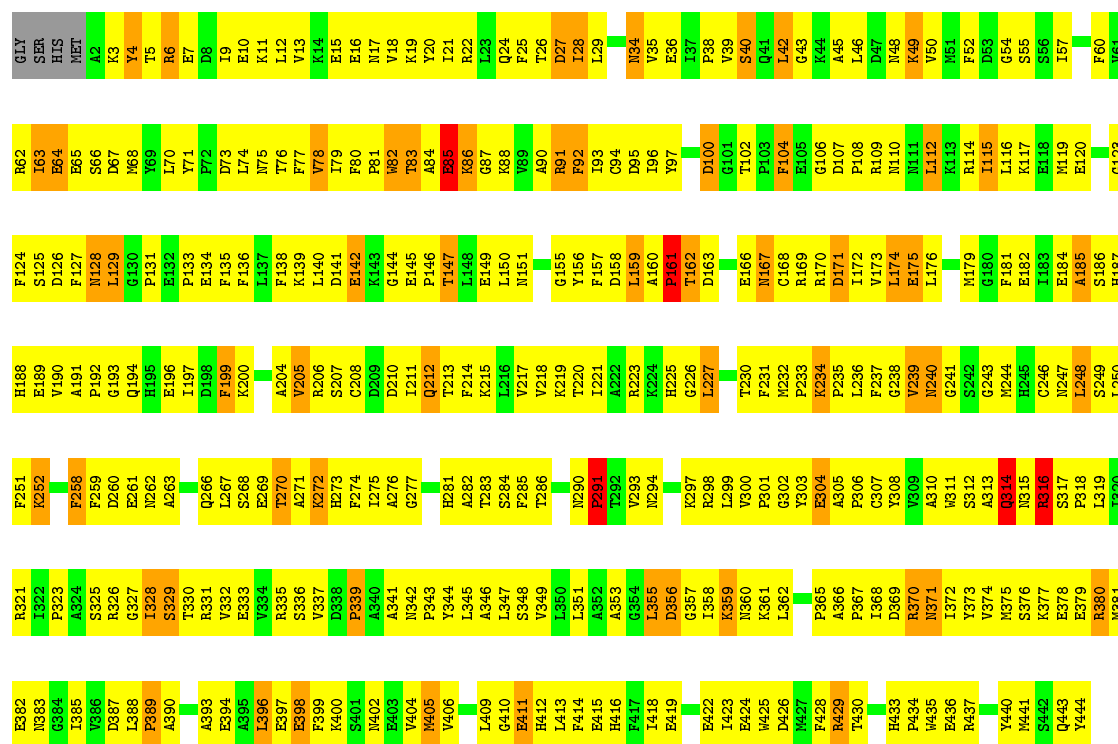


• Molecule 1: Glutamine synthetase

Chain D: 24% 58% 17% .

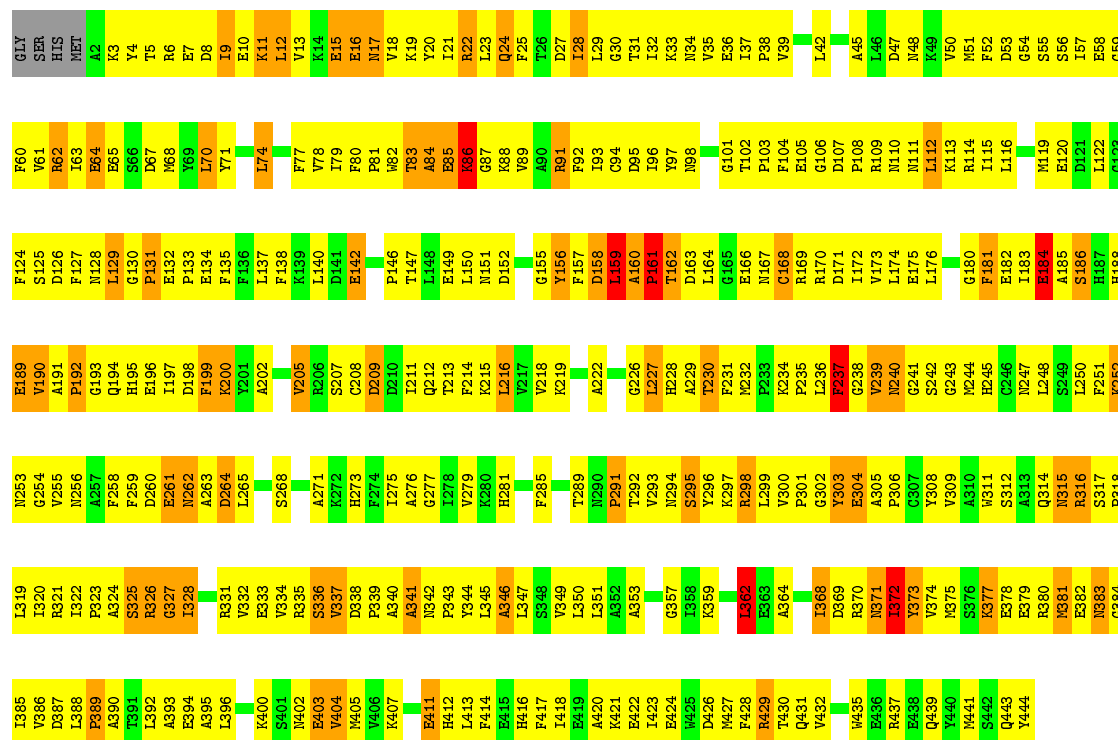


Chain F:  23% 62% 13% ..



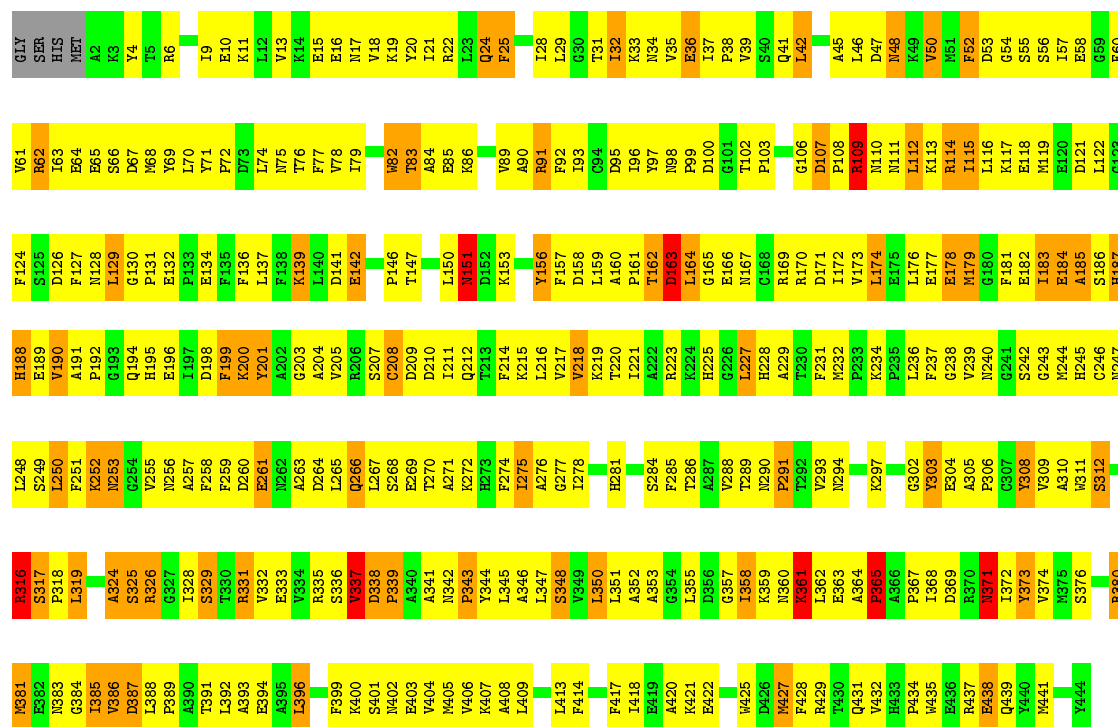
• Molecule 1: Glutamine synthetase

Chain G:  23% 59% 16% ..



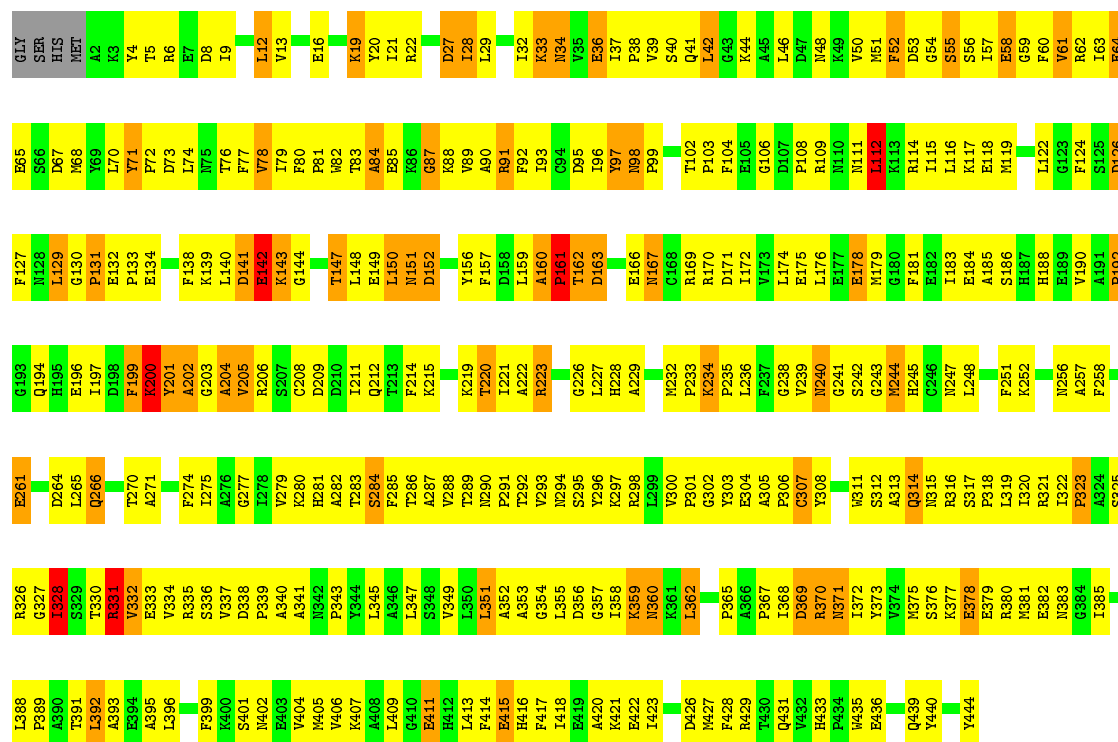
- Molecule 1: Glutamine synthetase

Chain H: 



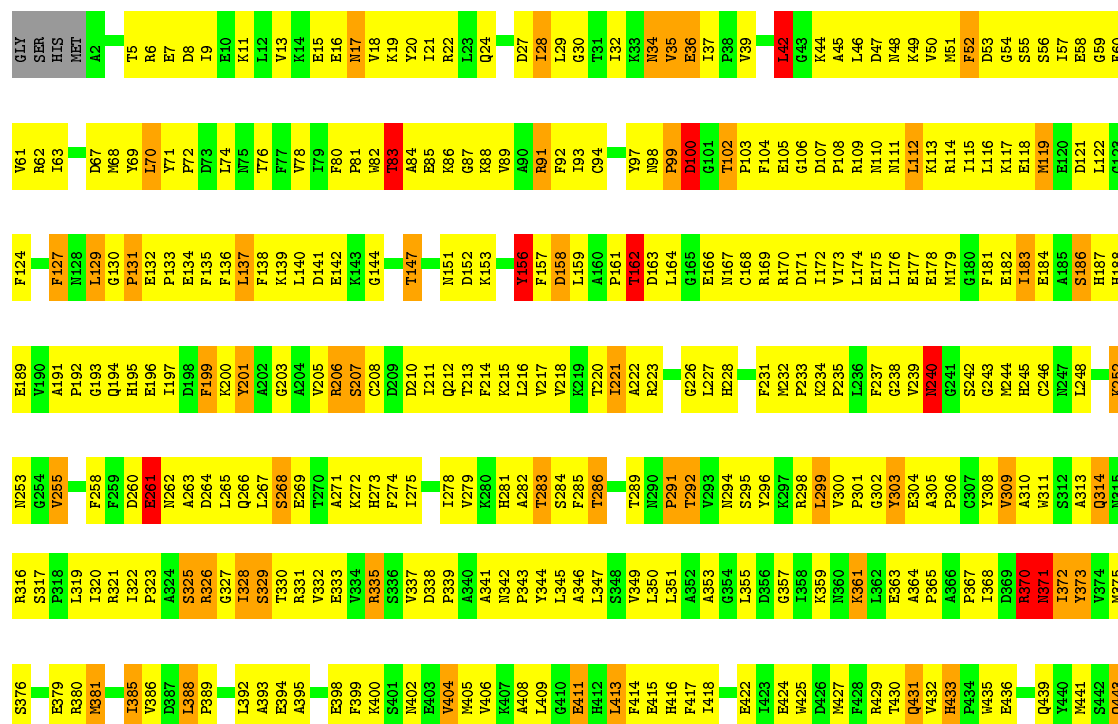
- Molecule 1: Glutamine synthetase

Chain J:  28% 56% 14% ..



- Molecule 1: Glutamine synthetase

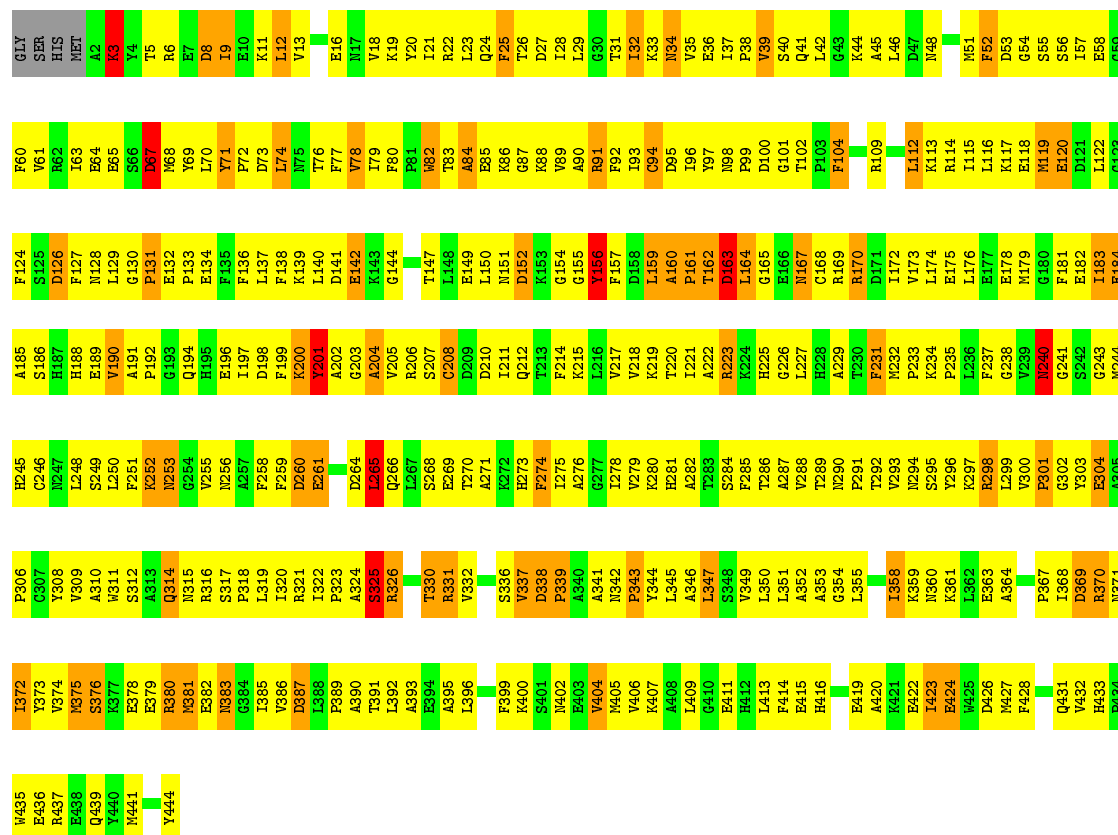
Chain K:  26% 59% 12% ..



Y444

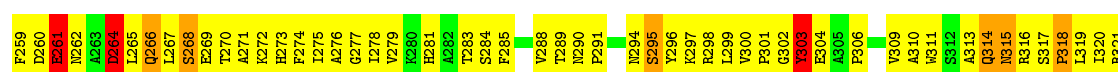
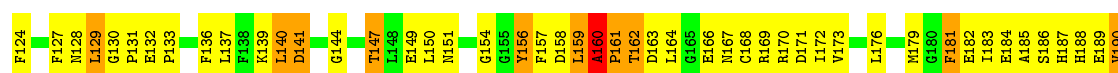
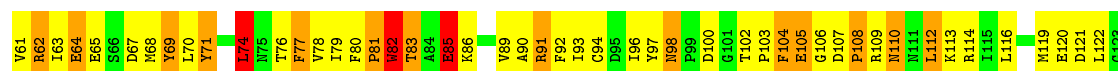
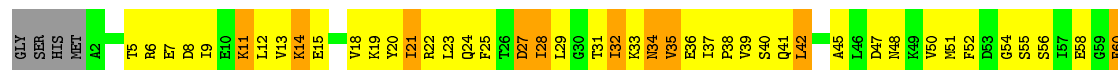
• Molecule 1: Glutamine synthetase

Chain L:  22% 60% 15% ..

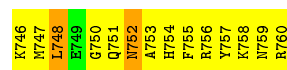




• Molecule 1: Glutamine synthetase



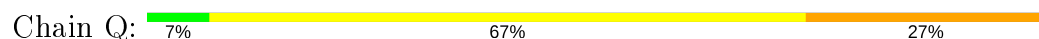
• Molecule 2: ThrA peptide



• Molecule 2: ThrA peptide



• Molecule 2: ThrA peptide





- Molecule 2: ThrA peptide



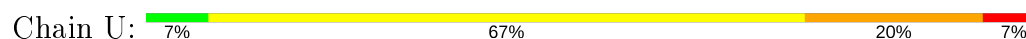
- Molecule 2: ThrA peptide



- Molecule 2: ThrA peptide



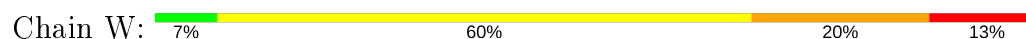
- Molecule 2: ThrA peptide



- Molecule 2: ThrA peptide



- Molecule 2: ThrA peptide



- Molecule 2: ThrA peptide




- Molecule 2: ThrA peptide

Chain Y:  7% 53% 40%


K746	K747	L748	E749	G750	Q751	N752	A753	H754	F755	R756	Y757	K758	N759	R760
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 2: TnrA peptide

Chain Z:  80% 20%

K746	K747	L748	E749	G750	Q751	N752	A753	H754	F755	R756	Y757	K758	N759	R760
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 2: TnrA peptide

Chain 1:  67% 27% 7%

K746	K747	L748	E749	G750	Q751	N752	A753	H754	F755	R756	Y757	K758	N759	R760
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 2: TnrA peptide

Chain 2:  73% 27%

K746	K747	L748	E749	G750	Q751	N752	A753	H754	F755	R756	Y757	K758	N759	R760
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.284 0.258 , 0.289	Depositor DCC
R_{free} test set	14819 reflections (12.09%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.380 for -h,-k,l 0.387 for h,-h-k,-l 0.387 for -k,-h,-l	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 ⓘ

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:O	2:W:758:LYS:HD2	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/447 (99%)	330 (75%)	96 (22%)	15 (3%)	3	28
1	B	441/447 (99%)	338 (77%)	80 (18%)	23 (5%)	2	18
1	C	441/447 (99%)	325 (74%)	91 (21%)	25 (6%)	1	16
1	D	445/447 (100%)	333 (75%)	84 (19%)	28 (6%)	1	14
1	E	441/447 (99%)	331 (75%)	93 (21%)	17 (4%)	3	25
1	F	441/447 (99%)	335 (76%)	92 (21%)	14 (3%)	4	29
1	G	441/447 (99%)	327 (74%)	83 (19%)	31 (7%)	1	12
1	H	441/447 (99%)	335 (76%)	83 (19%)	23 (5%)	2	18
1	I	441/447 (99%)	333 (76%)	78 (18%)	30 (7%)	1	13
1	J	441/447 (99%)	338 (77%)	83 (19%)	20 (4%)	2	21
1	K	441/447 (99%)	339 (77%)	85 (19%)	17 (4%)	3	25
1	L	441/447 (99%)	340 (77%)	83 (19%)	18 (4%)	3	23
1	M	441/447 (99%)	336 (76%)	89 (20%)	16 (4%)	3	26
1	N	441/447 (99%)	317 (72%)	94 (21%)	30 (7%)	1	13
2	1	13/15 (87%)	12 (92%)	0	1 (8%)	1	10
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	10
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	10

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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%)	2	19

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 ⓘ

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%)	2	15
1	B	382/385 (99%)	313 (82%)	69 (18%)	1	9
1	C	382/385 (99%)	313 (82%)	69 (18%)	1	9
1	D	385/385 (100%)	310 (80%)	75 (20%)	1	7
1	E	382/385 (99%)	300 (78%)	82 (22%)	1	5
1	F	382/385 (99%)	314 (82%)	68 (18%)	2	10
1	G	382/385 (99%)	312 (82%)	70 (18%)	1	8
1	H	382/385 (99%)	303 (79%)	79 (21%)	1	6
1	I	382/385 (99%)	314 (82%)	68 (18%)	2	10
1	J	382/385 (99%)	317 (83%)	65 (17%)	2	12
1	K	382/385 (99%)	316 (83%)	66 (17%)	2	11
1	L	382/385 (99%)	307 (80%)	75 (20%)	1	7
1	M	382/385 (99%)	313 (82%)	69 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	382/385 (99%)	321 (84%)	61 (16%)	2 14
2	1	13/13 (100%)	11 (85%)	2 (15%)	2 16
2	2	13/13 (100%)	10 (77%)	3 (23%)	1 4
2	O	13/13 (100%)	11 (85%)	2 (15%)	2 16
2	P	13/13 (100%)	12 (92%)	1 (8%)	13 42
2	Q	13/13 (100%)	9 (69%)	4 (31%)	0 2
2	R	13/13 (100%)	8 (62%)	5 (38%)	0 1
2	S	13/13 (100%)	11 (85%)	2 (15%)	2 16
2	T	13/13 (100%)	10 (77%)	3 (23%)	1 4
2	U	13/13 (100%)	9 (69%)	4 (31%)	0 2
2	V	13/13 (100%)	11 (85%)	2 (15%)	2 16
2	W	13/13 (100%)	9 (69%)	4 (31%)	0 2
2	X	13/13 (100%)	12 (92%)	1 (8%)	13 42
2	Y	13/13 (100%)	8 (62%)	5 (38%)	0 1
2	Z	13/13 (100%)	11 (85%)	2 (15%)	2 16
All	All	5533/5572 (99%)	4517 (82%)	1016 (18%)	1 8

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 monosaccharides 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	N	501	4	7,8,9	0.45	0	4,9,11	0.18	0
3	GLN	H	501	4	7,8,9	0.52	0	4,9,11	0.08	0
3	GLN	J	501	-	7,8,9	0.51	0	4,9,11	0.21	0
3	GLN	G	501	-	7,8,9	0.52	0	4,9,11	0.18	0
3	GLN	A	501	4	7,8,9	0.79	0	4,9,11	0.20	0
3	GLN	I	501	4	7,8,9	0.48	0	4,9,11	0.12	0
3	GLN	K	501	4	7,8,9	0.69	0	4,9,11	0.45	0
3	GLN	E	501	-	7,8,9	0.48	0	4,9,11	0.12	0
3	GLN	D	501	-	7,8,9	0.51	0	4,9,11	0.07	0
3	GLN	C	503	-	5,9,9	0.49	0	5,11,11	0.18	0
3	GLN	F	501	-	7,8,9	0.73	0	4,9,11	0.26	0
3	GLN	B	501	4	7,8,9	0.67	0	4,9,11	0.14	0
3	GLN	M	503	-	5,9,9	0.30	0	5,11,11	0.26	0
3	GLN	L	501	4	5,9,9	0.34	0	5,11,11	0.11	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	N	501	4	-	2/6/7/9	-
3	GLN	H	501	4	-	2/6/7/9	-
3	GLN	J	501	-	-	1/6/7/9	-
3	GLN	G	501	-	-	0/6/7/9	-
3	GLN	A	501	4	-	1/6/7/9	-
3	GLN	I	501	4	-	3/6/7/9	-
3	GLN	K	501	4	-	0/6/7/9	-
3	GLN	E	501	-	-	0/6/7/9	-
3	GLN	D	501	-	-	2/6/7/9	-
3	GLN	C	503	-	-	4/5/9/9	-
3	GLN	F	501	-	-	2/6/7/9	-
3	GLN	B	501	4	-	3/6/7/9	-
3	GLN	M	503	-	-	0/5/9/9	-
3	GLN	L	501	4	-	1/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	GLN	N-CA-CB-CG
3	D	501	GLN	C-CA-CB-CG
3	C	503	GLN	N-CA-CB-CG
3	C	503	GLN	C-CA-CB-CG
3	H	501	GLN	N-CA-CB-CG

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	501	GLN	1	0
3	H	501	GLN	1	0
3	J	501	GLN	3	0
3	G	501	GLN	2	0
3	A	501	GLN	5	0
3	I	501	GLN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	GLN	2	0
3	D	501	GLN	3	0
3	C	503	GLN	3	0
3	F	501	GLN	5	0
3	B	501	GLN	6	0
3	L	501	GLN	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.