



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 06:09 PM JST

PDB ID : 7EVT  
Title : Crystal structure of the N-terminal degtron-truncated human glutamine synthetase  
Authors : Chek, M.F.; Kim, S.Y.; Mori, T.; Hakoshima, T.  
Deposited on : 2021-05-22  
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

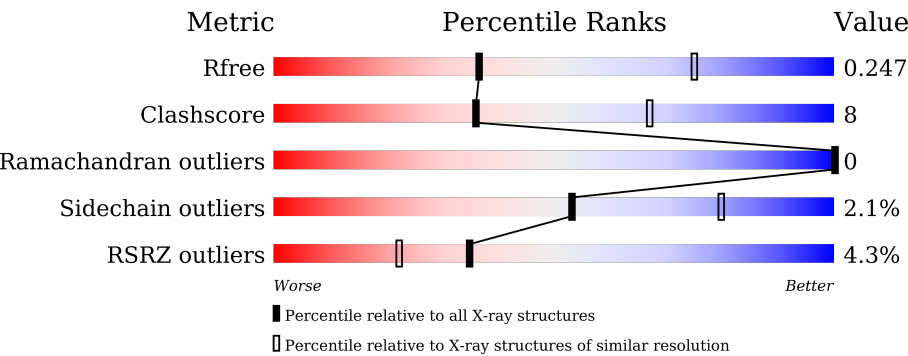
# 1 Overall quality at a glance i

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	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>75%17%8%</div></div>
1	B	370	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>74%18%7%</div></div>
1	C	370	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>76%16%8%</div></div>
1	D	370	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%21%9%</div></div>
1	E	370	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>69%16%15%</div></div>
1	F	370	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>72%20%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	370	<div><div><div></div><div></div><div></div></div><div>2%75%16%8%</div></div>
1	H	370	<div><div><div></div><div></div><div></div></div><div>%79%14%6%</div></div>
1	I	370	<div><div><div></div><div></div><div></div></div><div>5%78%14%8%</div></div>
1	J	370	<div><div><div></div><div></div><div></div></div><div>4%70%22%7%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25797 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	341	Total	C	N	O	S	0	0	0
			2476	1554	433	468	21			
1	B	344	Total	C	N	O	S	0	0	0
			2624	1644	464	495	21			
1	C	341	Total	C	N	O	S	0	0	0
			2670	1678	471	500	21			
1	D	335	Total	C	N	O	S	0	0	0
			2503	1568	438	476	21			
1	E	316	Total	C	N	O	S	0	0	0
			2226	1396	384	427	19			
1	F	340	Total	C	N	O	S	0	0	0
			2620	1645	462	492	21			
1	G	342	Total	C	N	O	S	0	0	0
			2655	1671	464	499	21			
1	H	348	Total	C	N	O	S	0	0	0
			2746	1724	488	513	21			
1	I	342	Total	C	N	O	S	0	0	0
			2647	1660	467	499	21			
1	J	343	Total	C	N	O	S	0	0	0
			2630	1657	461	491	21			

There are 190 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15104
A	5	ALA	-	expression tag	UNP P15104
A	6	HIS	-	expression tag	UNP P15104
A	7	HIS	-	expression tag	UNP P15104
A	8	HIS	-	expression tag	UNP P15104
A	9	HIS	-	expression tag	UNP P15104
A	10	HIS	-	expression tag	UNP P15104
A	11	HIS	-	expression tag	UNP P15104
A	12	SER	-	expression tag	UNP P15104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	-	expression tag	UNP P15104
A	14	ALA	-	expression tag	UNP P15104
A	15	LEU	-	expression tag	UNP P15104
A	16	GLU	-	expression tag	UNP P15104
A	17	VAL	-	expression tag	UNP P15104
A	18	LEU	-	expression tag	UNP P15104
A	19	PHE	-	expression tag	UNP P15104
A	20	GLN	-	expression tag	UNP P15104
A	21	GLY	-	expression tag	UNP P15104
A	22	PRO	-	expression tag	UNP P15104
B	4	MET	-	initiating methionine	UNP P15104
B	5	ALA	-	expression tag	UNP P15104
B	6	HIS	-	expression tag	UNP P15104
B	7	HIS	-	expression tag	UNP P15104
B	8	HIS	-	expression tag	UNP P15104
B	9	HIS	-	expression tag	UNP P15104
B	10	HIS	-	expression tag	UNP P15104
B	11	HIS	-	expression tag	UNP P15104
B	12	SER	-	expression tag	UNP P15104
B	13	ALA	-	expression tag	UNP P15104
B	14	ALA	-	expression tag	UNP P15104
B	15	LEU	-	expression tag	UNP P15104
B	16	GLU	-	expression tag	UNP P15104
B	17	VAL	-	expression tag	UNP P15104
B	18	LEU	-	expression tag	UNP P15104
B	19	PHE	-	expression tag	UNP P15104
B	20	GLN	-	expression tag	UNP P15104
B	21	GLY	-	expression tag	UNP P15104
B	22	PRO	-	expression tag	UNP P15104
C	4	MET	-	initiating methionine	UNP P15104
C	5	ALA	-	expression tag	UNP P15104
C	6	HIS	-	expression tag	UNP P15104
C	7	HIS	-	expression tag	UNP P15104
C	8	HIS	-	expression tag	UNP P15104
C	9	HIS	-	expression tag	UNP P15104
C	10	HIS	-	expression tag	UNP P15104
C	11	HIS	-	expression tag	UNP P15104
C	12	SER	-	expression tag	UNP P15104
C	13	ALA	-	expression tag	UNP P15104
C	14	ALA	-	expression tag	UNP P15104
C	15	LEU	-	expression tag	UNP P15104
C	16	GLU	-	expression tag	UNP P15104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	VAL	-	expression tag	UNP P15104
C	18	LEU	-	expression tag	UNP P15104
C	19	PHE	-	expression tag	UNP P15104
C	20	GLN	-	expression tag	UNP P15104
C	21	GLY	-	expression tag	UNP P15104
C	22	PRO	-	expression tag	UNP P15104
D	4	MET	-	initiating methionine	UNP P15104
D	5	ALA	-	expression tag	UNP P15104
D	6	HIS	-	expression tag	UNP P15104
D	7	HIS	-	expression tag	UNP P15104
D	8	HIS	-	expression tag	UNP P15104
D	9	HIS	-	expression tag	UNP P15104
D	10	HIS	-	expression tag	UNP P15104
D	11	HIS	-	expression tag	UNP P15104
D	12	SER	-	expression tag	UNP P15104
D	13	ALA	-	expression tag	UNP P15104
D	14	ALA	-	expression tag	UNP P15104
D	15	LEU	-	expression tag	UNP P15104
D	16	GLU	-	expression tag	UNP P15104
D	17	VAL	-	expression tag	UNP P15104
D	18	LEU	-	expression tag	UNP P15104
D	19	PHE	-	expression tag	UNP P15104
D	20	GLN	-	expression tag	UNP P15104
D	21	GLY	-	expression tag	UNP P15104
D	22	PRO	-	expression tag	UNP P15104
E	4	MET	-	initiating methionine	UNP P15104
E	5	ALA	-	expression tag	UNP P15104
E	6	HIS	-	expression tag	UNP P15104
E	7	HIS	-	expression tag	UNP P15104
E	8	HIS	-	expression tag	UNP P15104
E	9	HIS	-	expression tag	UNP P15104
E	10	HIS	-	expression tag	UNP P15104
E	11	HIS	-	expression tag	UNP P15104
E	12	SER	-	expression tag	UNP P15104
E	13	ALA	-	expression tag	UNP P15104
E	14	ALA	-	expression tag	UNP P15104
E	15	LEU	-	expression tag	UNP P15104
E	16	GLU	-	expression tag	UNP P15104
E	17	VAL	-	expression tag	UNP P15104
E	18	LEU	-	expression tag	UNP P15104
E	19	PHE	-	expression tag	UNP P15104
E	20	GLN	-	expression tag	UNP P15104

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Chain	Residue	Modelled	Actual	Comment	Reference
E	21	GLY	-	expression tag	UNP P15104
E	22	PRO	-	expression tag	UNP P15104
F	4	MET	-	initiating methionine	UNP P15104
F	5	ALA	-	expression tag	UNP P15104
F	6	HIS	-	expression tag	UNP P15104
F	7	HIS	-	expression tag	UNP P15104
F	8	HIS	-	expression tag	UNP P15104
F	9	HIS	-	expression tag	UNP P15104
F	10	HIS	-	expression tag	UNP P15104
F	11	HIS	-	expression tag	UNP P15104
F	12	SER	-	expression tag	UNP P15104
F	13	ALA	-	expression tag	UNP P15104
F	14	ALA	-	expression tag	UNP P15104
F	15	LEU	-	expression tag	UNP P15104
F	16	GLU	-	expression tag	UNP P15104
F	17	VAL	-	expression tag	UNP P15104
F	18	LEU	-	expression tag	UNP P15104
F	19	PHE	-	expression tag	UNP P15104
F	20	GLN	-	expression tag	UNP P15104
F	21	GLY	-	expression tag	UNP P15104
F	22	PRO	-	expression tag	UNP P15104
G	4	MET	-	initiating methionine	UNP P15104
G	5	ALA	-	expression tag	UNP P15104
G	6	HIS	-	expression tag	UNP P15104
G	7	HIS	-	expression tag	UNP P15104
G	8	HIS	-	expression tag	UNP P15104
G	9	HIS	-	expression tag	UNP P15104
G	10	HIS	-	expression tag	UNP P15104
G	11	HIS	-	expression tag	UNP P15104
G	12	SER	-	expression tag	UNP P15104
G	13	ALA	-	expression tag	UNP P15104
G	14	ALA	-	expression tag	UNP P15104
G	15	LEU	-	expression tag	UNP P15104
G	16	GLU	-	expression tag	UNP P15104
G	17	VAL	-	expression tag	UNP P15104
G	18	LEU	-	expression tag	UNP P15104
G	19	PHE	-	expression tag	UNP P15104
G	20	GLN	-	expression tag	UNP P15104
G	21	GLY	-	expression tag	UNP P15104
G	22	PRO	-	expression tag	UNP P15104
H	4	MET	-	initiating methionine	UNP P15104
H	5	ALA	-	expression tag	UNP P15104

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Chain	Residue	Modelled	Actual	Comment	Reference
H	6	HIS	-	expression tag	UNP P15104
H	7	HIS	-	expression tag	UNP P15104
H	8	HIS	-	expression tag	UNP P15104
H	9	HIS	-	expression tag	UNP P15104
H	10	HIS	-	expression tag	UNP P15104
H	11	HIS	-	expression tag	UNP P15104
H	12	SER	-	expression tag	UNP P15104
H	13	ALA	-	expression tag	UNP P15104
H	14	ALA	-	expression tag	UNP P15104
H	15	LEU	-	expression tag	UNP P15104
H	16	GLU	-	expression tag	UNP P15104
H	17	VAL	-	expression tag	UNP P15104
H	18	LEU	-	expression tag	UNP P15104
H	19	PHE	-	expression tag	UNP P15104
H	20	GLN	-	expression tag	UNP P15104
H	21	GLY	-	expression tag	UNP P15104
H	22	PRO	-	expression tag	UNP P15104
I	4	MET	-	initiating methionine	UNP P15104
I	5	ALA	-	expression tag	UNP P15104
I	6	HIS	-	expression tag	UNP P15104
I	7	HIS	-	expression tag	UNP P15104
I	8	HIS	-	expression tag	UNP P15104
I	9	HIS	-	expression tag	UNP P15104
I	10	HIS	-	expression tag	UNP P15104
I	11	HIS	-	expression tag	UNP P15104
I	12	SER	-	expression tag	UNP P15104
I	13	ALA	-	expression tag	UNP P15104
I	14	ALA	-	expression tag	UNP P15104
I	15	LEU	-	expression tag	UNP P15104
I	16	GLU	-	expression tag	UNP P15104
I	17	VAL	-	expression tag	UNP P15104
I	18	LEU	-	expression tag	UNP P15104
I	19	PHE	-	expression tag	UNP P15104
I	20	GLN	-	expression tag	UNP P15104
I	21	GLY	-	expression tag	UNP P15104
I	22	PRO	-	expression tag	UNP P15104
J	4	MET	-	initiating methionine	UNP P15104
J	5	ALA	-	expression tag	UNP P15104
J	6	HIS	-	expression tag	UNP P15104
J	7	HIS	-	expression tag	UNP P15104
J	8	HIS	-	expression tag	UNP P15104
J	9	HIS	-	expression tag	UNP P15104

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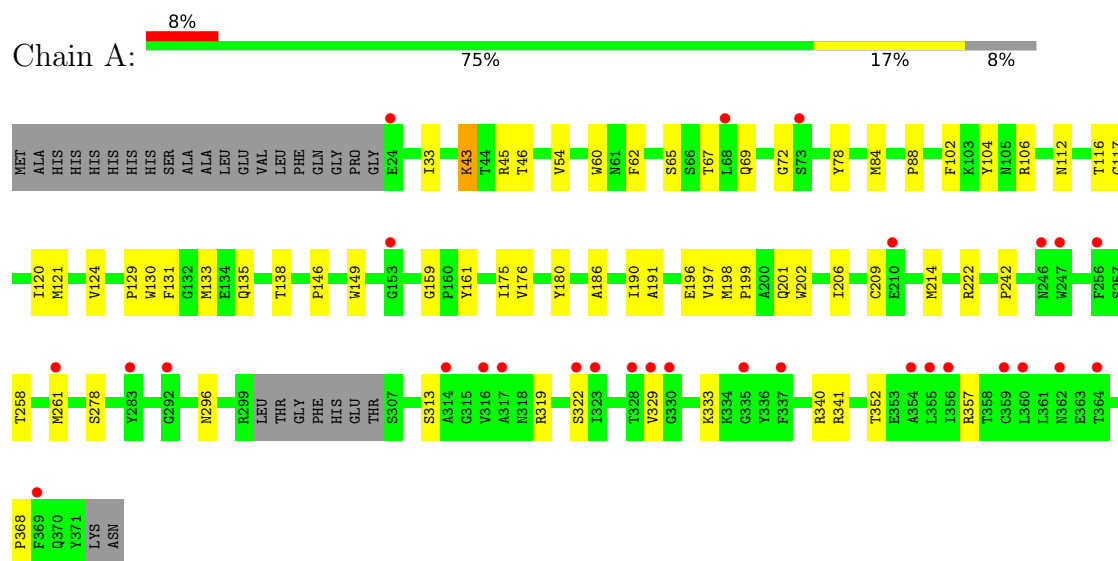
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Chain	Residue	Modelled	Actual	Comment	Reference
J	10	HIS	-	expression tag	UNP P15104
J	11	HIS	-	expression tag	UNP P15104
J	12	SER	-	expression tag	UNP P15104
J	13	ALA	-	expression tag	UNP P15104
J	14	ALA	-	expression tag	UNP P15104
J	15	LEU	-	expression tag	UNP P15104
J	16	GLU	-	expression tag	UNP P15104
J	17	VAL	-	expression tag	UNP P15104
J	18	LEU	-	expression tag	UNP P15104
J	19	PHE	-	expression tag	UNP P15104
J	20	GLN	-	expression tag	UNP P15104
J	21	GLY	-	expression tag	UNP P15104
J	22	PRO	-	expression tag	UNP P15104

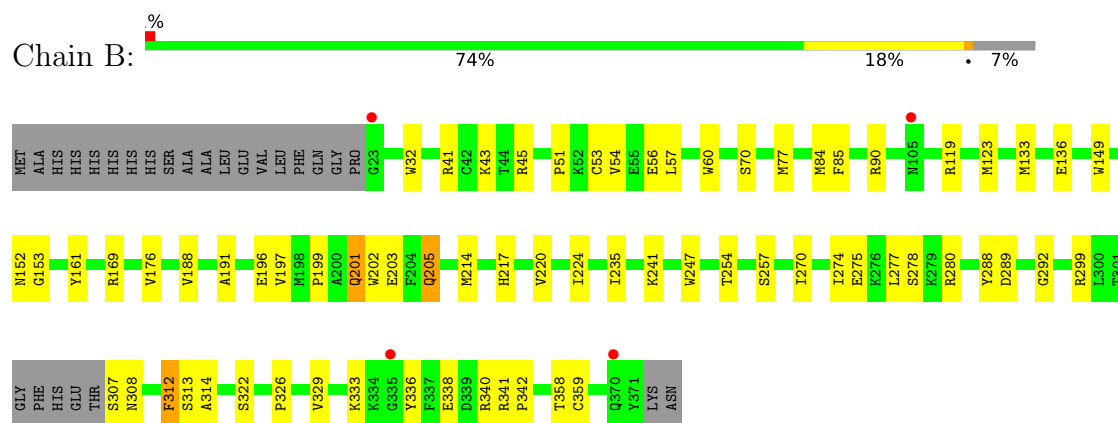
### 3 Residue-property plots [i](#)

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.

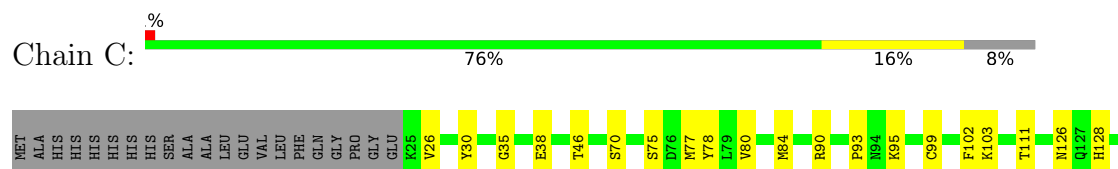
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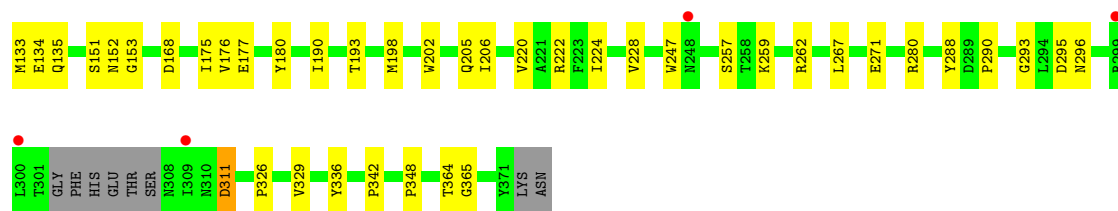


#### • Molecule 1: Glutamine synthetase

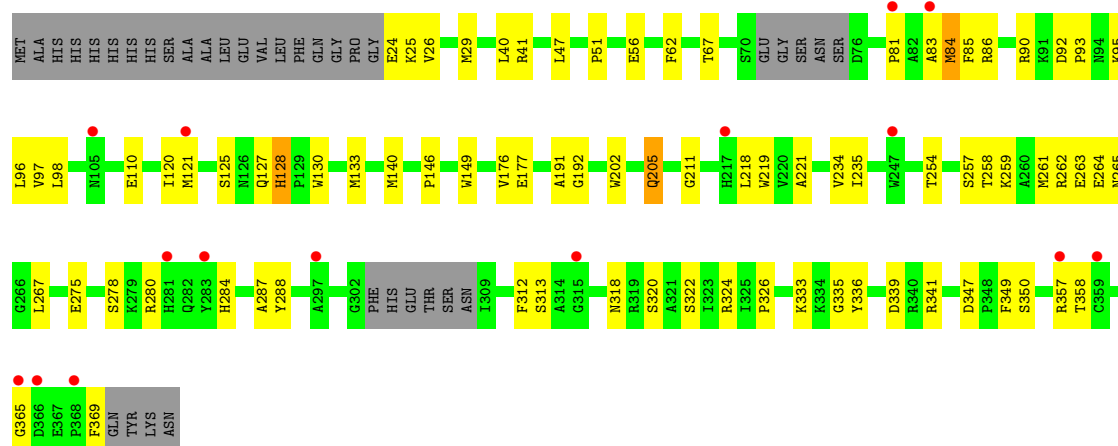


#### • Molecule 1: Glutamine synthetase

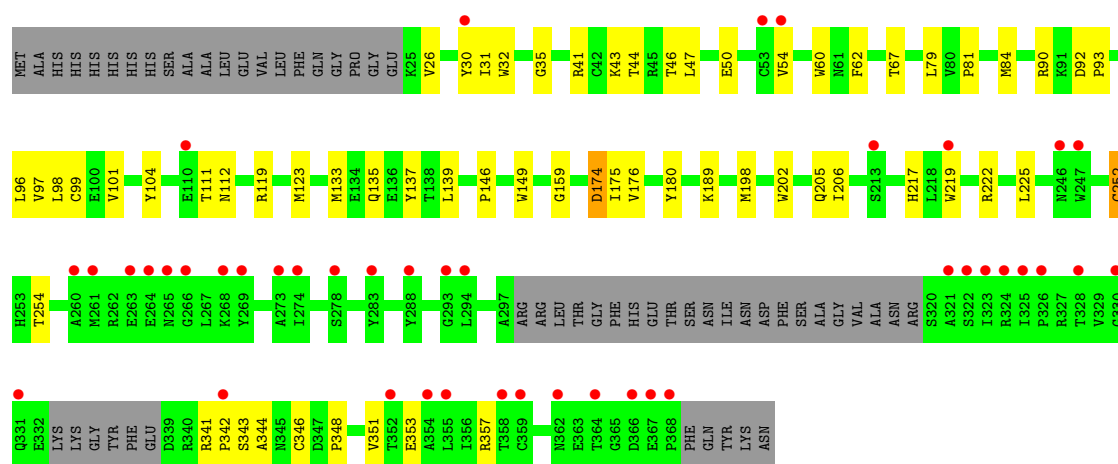




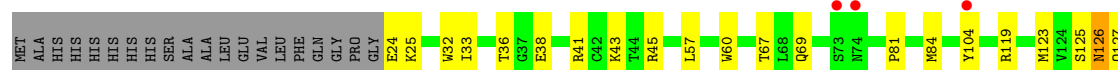
• Molecule 1: Glutamine synthetase

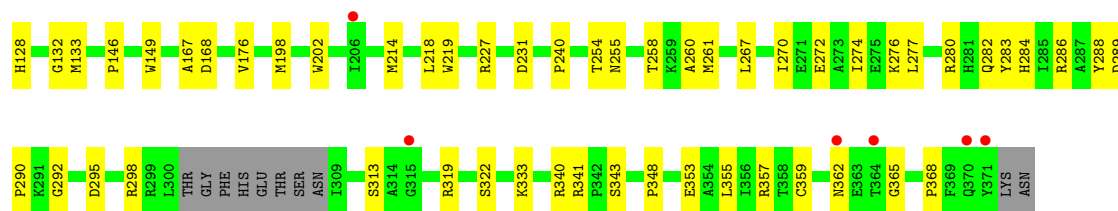


• Molecule 1: Glutamine synthetase

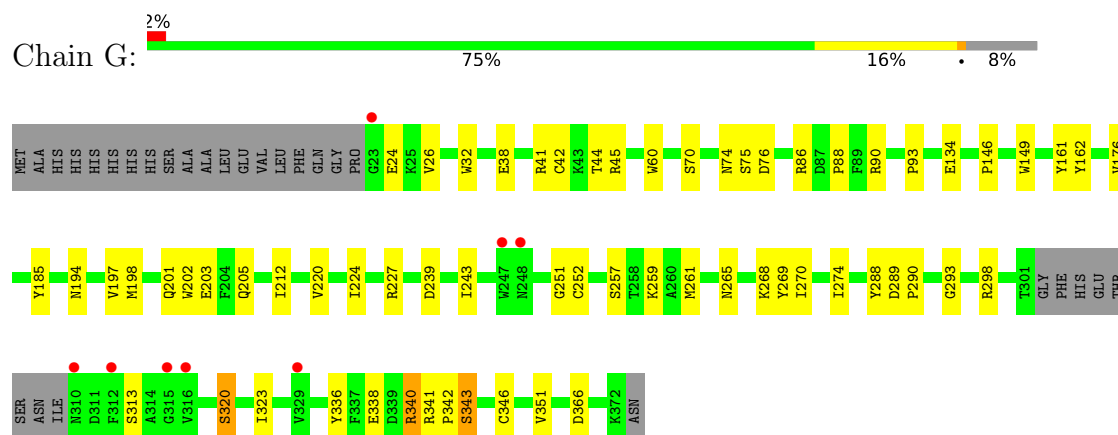


• Molecule 1: Glutamine synthetase

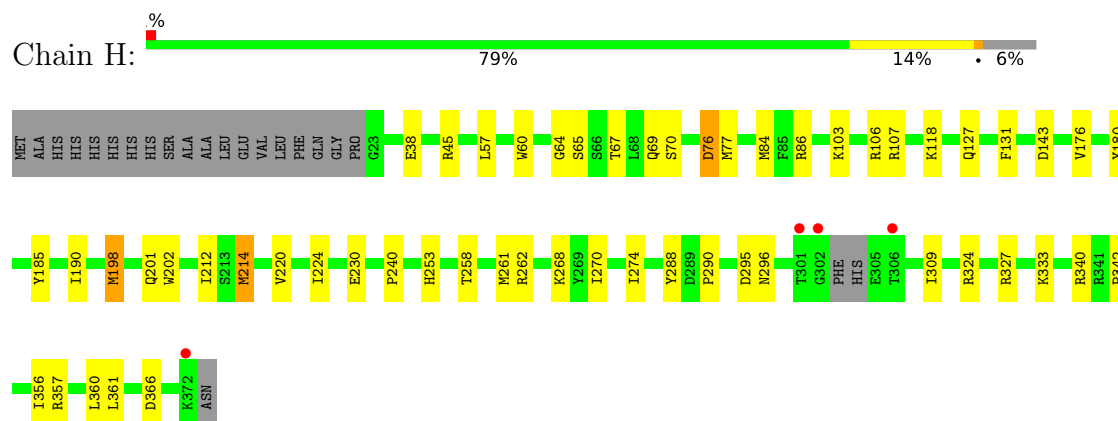




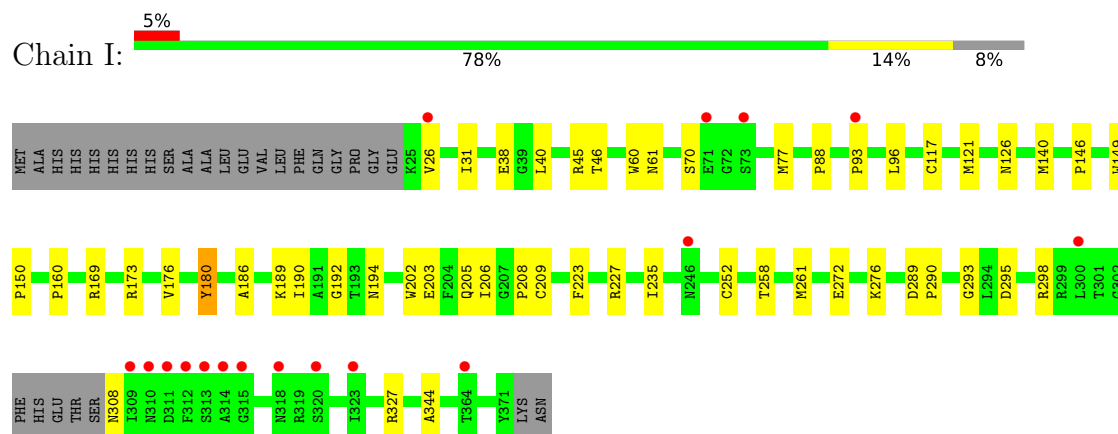
• Molecule 1: Glutamine synthetase



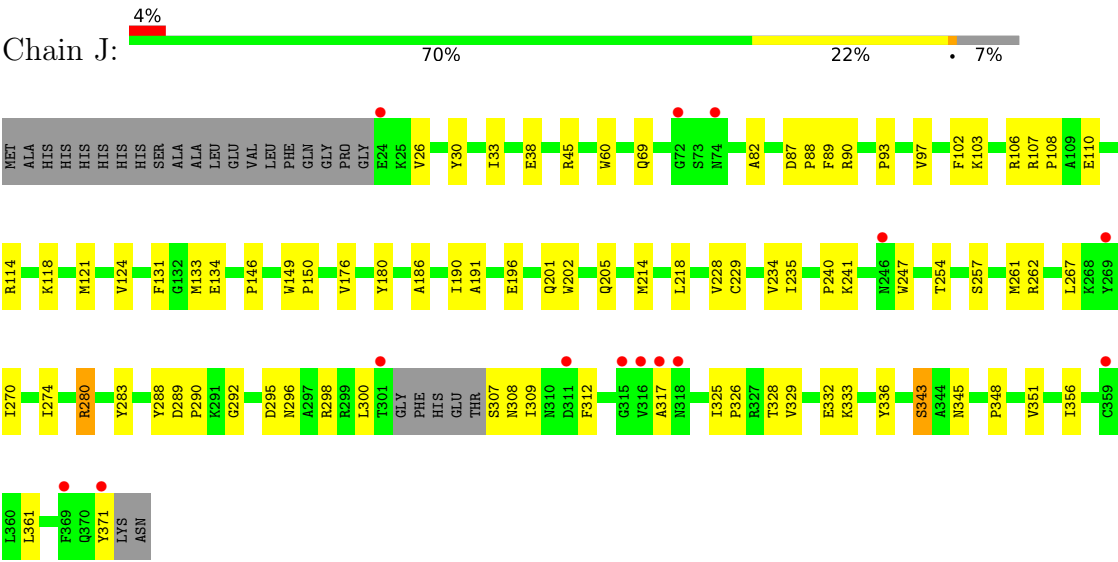
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



● Molecule 1: Glutamine synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.92Å 158.87Å 118.91Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	44.43 – 2.95 44.43 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.43-2.95) 99.7 (44.43-2.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.19.4092	Depositor
R, $R_{free}$	0.219 , 0.250 0.218 , 0.247	Depositor DCC
$R_{free}$ test set	4592 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.015 for h,-k,-l 0.002 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.25	0/2542	0.50	0/3471
1	B	0.26	0/2695	0.50	0/3666
1	C	0.26	0/2743	0.51	0/3719
1	D	0.36	2/2570 (0.1%)	0.52	0/3500
1	E	0.26	0/2286	0.49	0/3134
1	F	0.25	0/2692	0.50	0/3657
1	G	0.27	0/2728	0.49	0/3701
1	H	0.26	0/2819	0.49	0/3815
1	I	0.26	0/2719	0.50	0/3694
1	J	0.25	0/2703	0.49	0/3676
All	All	0.27	2/26497 (0.0%)	0.50	0/36033

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	TRP	CE3-CZ3	-7.31	1.26	1.38
1	D	130	TRP	CZ3-CH2	5.56	1.49	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2476	0	2170	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2624	0	2397	44	0
1	C	2670	0	2501	38	0
1	D	2503	0	2241	53	0
1	E	2226	0	1895	40	0
1	F	2620	0	2405	46	0
1	G	2655	0	2472	42	0
1	H	2746	0	2607	35	0
1	I	2647	0	2451	30	0
1	J	2630	0	2412	48	0
All	All	25797	0	23551	396	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 8.

All (396) 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:138:THR:HG22	1:A:201:GLN:HG3	1.53	0.90
1:G:338:GLU:OE1	1:G:340:ARG:NH1	2.05	0.89
1:F:261:MET:HG2	1:F:270:ILE:HG13	1.63	0.80
1:A:313:SER:HB2	1:A:322:SER:H	1.48	0.77
1:D:280:ARG:NH2	1:D:365:GLY:O	2.18	0.77
1:H:261:MET:HG2	1:H:270:ILE:HG13	1.68	0.73
1:C:133:MET:HE1	1:C:348:PRO:HB3	1.70	0.72
1:F:282:GLN:HB3	1:F:286:ARG:HH12	1.54	0.72
1:E:44:THR:HG21	1:E:90:ARG:HH22	1.55	0.72
1:G:162:TYR:HB2	1:G:197:VAL:HG22	1.71	0.71
1:J:296:ASN:HD22	1:J:343:SER:HB3	1.55	0.71
1:D:133:MET:HG2	1:D:254:THR:HG23	1.74	0.69
1:D:41:ARG:NH2	1:E:159:GLY:O	2.25	0.69
1:J:267:LEU:HD12	1:J:333:LYS:HA	1.76	0.68
1:C:134:GLU:HG3	1:C:205:GLN:HG3	1.76	0.67
1:F:280:ARG:NH1	1:F:365:GLY:O	2.27	0.67
1:G:38:GLU:HG2	1:G:290:PRO:HG2	1.77	0.67
1:C:84:MET:CE	1:C:95:LYS:HD2	2.25	0.67
1:F:267:LEU:HD12	1:F:333:LYS:HA	1.76	0.66
1:D:62:PHE:HE2	1:D:67:THR:HG21	1.60	0.66
1:D:263:GLU:HG2	1:D:264:GLU:HG2	1.78	0.66
1:F:319:ARG:O	1:F:340:ARG:NH1	2.29	0.66
1:G:341:ARG:N	1:G:342:PRO:HD3	2.10	0.65
1:E:189:LYS:H	1:E:217:HIS:CE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:CYS:N	1:E:343:SER:O	2.30	0.64
1:D:339:ASP:OD1	1:D:341:ARG:HD2	1.98	0.64
1:I:31:ILE:HD11	1:I:96:LEU:HD22	1.80	0.64
1:I:70:SER:HB3	1:I:77:MET:HE2	1.79	0.64
1:A:33:ILE:O	1:A:69:GLN:NE2	2.31	0.64
1:B:257:SER:HB3	1:B:336:TYR:HB3	1.80	0.63
1:J:88:PRO:HG3	1:J:186:ALA:HB2	1.80	0.63
1:A:131:PHE:CD1	1:A:352:THR:HG22	2.33	0.63
1:I:88:PRO:HG3	1:I:186:ALA:HB2	1.79	0.63
1:A:62:PHE:HE2	1:A:67:THR:HG21	1.64	0.63
1:H:57:LEU:HD11	1:H:84:MET:HG3	1.81	0.63
1:F:276:LYS:NZ	1:F:362:ASN:OD1	2.32	0.63
1:A:43:LYS:HD2	1:A:60:TRP:CH2	2.34	0.62
1:A:138:THR:HG21	1:A:242:PRO:HG3	1.80	0.62
1:J:38:GLU:HG2	1:J:290:PRO:HG2	1.80	0.62
1:J:261:MET:HG2	1:J:270:ILE:HG13	1.82	0.62
1:C:80:VAL:HG11	1:C:102:PHE:HE2	1.64	0.61
1:A:159:GLY:O	1:E:41:ARG:NH2	2.33	0.61
1:F:41:ARG:NH1	1:G:162:TYR:O	2.34	0.61
1:C:38:GLU:HG2	1:C:290:PRO:HG2	1.83	0.60
1:C:90:ARG:NH2	1:D:177:GLU:OE2	2.33	0.60
1:E:174:ASP:N	1:E:174:ASP:OD1	2.32	0.60
1:C:84:MET:HE3	1:C:95:LYS:HD2	1.83	0.60
1:C:128:HIS:O	1:C:262:ARG:NH2	2.34	0.60
1:A:196:GLU:HB3	1:A:201:GLN:HE21	1.66	0.60
1:D:287:ALA:O	1:D:350:SER:OG	2.20	0.59
1:B:196:GLU:HG3	1:B:197:VAL:H	1.67	0.59
1:D:26:VAL:HG12	1:D:47:LEU:HB2	1.85	0.59
1:E:101:VAL:O	1:E:112:ASN:ND2	2.34	0.59
1:D:127:GLN:O	1:D:258:THR:OG1	2.21	0.59
1:G:257:SER:HB3	1:G:336:TYR:HB3	1.84	0.59
1:D:288:TYR:HE2	1:D:341:ARG:HD3	1.68	0.58
1:A:190:ILE:HA	1:A:206:ILE:HG22	1.84	0.58
1:J:257:SER:OG	1:J:262:ARG:NH1	2.36	0.58
1:F:127:GLN:O	1:F:258:THR:OG1	2.20	0.58
1:J:343:SER:OG	1:J:345:ASN:OD1	2.22	0.58
1:J:26:VAL:HG12	1:J:93:PRO:HG2	1.87	0.57
1:F:133:MET:HG2	1:F:254:THR:HG23	1.87	0.57
1:G:320:SER:O	1:G:320:SER:OG	2.23	0.57
1:J:257:SER:HB3	1:J:336:TYR:HB3	1.86	0.57
1:G:26:VAL:HG22	1:G:93:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ARG:HH12	1:D:369:PHE:HB2	1.70	0.56
1:F:45:ARG:HB3	1:F:60:TRP:CH2	2.41	0.56
1:D:93:PRO:O	1:D:95:LYS:HE2	2.05	0.56
1:I:26:VAL:HG22	1:I:93:PRO:HG2	1.87	0.56
1:A:54:VAL:HG22	1:A:84:MET:HB2	1.87	0.56
1:E:341:ARG:N	1:E:342:PRO:HD3	2.20	0.56
1:J:103:LYS:NZ	1:J:110:GLU:OE2	2.39	0.56
1:D:192:GLY:C	1:D:205:GLN:HE21	2.08	0.56
1:I:227:ARG:HG3	1:I:227:ARG:HH11	1.71	0.56
1:J:133:MET:HG2	1:J:254:THR:HG23	1.88	0.56
1:H:69:GLN:HB3	1:H:77:MET:SD	2.46	0.55
1:A:319:ARG:O	1:A:340:ARG:NH1	2.40	0.55
1:G:366:ASP:OD1	1:G:366:ASP:N	2.40	0.55
1:B:70:SER:HB3	1:B:77:MET:HE2	1.88	0.55
1:F:67:THR:OG1	1:F:69:GLN:OE1	2.24	0.55
1:F:270:ILE:O	1:F:274:ILE:HG13	2.07	0.55
1:G:341:ARG:H	1:G:342:PRO:HD3	1.70	0.55
1:H:127:GLN:O	1:H:258:THR:OG1	2.23	0.54
1:B:288:TYR:HB3	1:B:342:PRO:HA	1.89	0.54
1:H:86:ARG:NH1	1:H:185:TYR:O	2.41	0.54
1:A:88:PRO:HG3	1:A:186:ALA:HB2	1.89	0.54
1:F:36:THR:HG23	1:F:38:GLU:H	1.72	0.54
1:D:85:PHE:HB2	1:D:96:LEU:HD11	1.90	0.54
1:F:295:ASP:OD1	1:F:298:ARG:NH2	2.42	0.53
1:C:26:VAL:HG22	1:C:93:PRO:HG2	1.89	0.53
1:F:240:PRO:HB3	1:F:343:SER:HB2	1.89	0.53
1:B:280:ARG:NH2	1:B:358:THR:OG1	2.41	0.53
1:D:140:MET:HB2	1:D:235:ILE:HB	1.90	0.53
1:D:258:THR:H	1:D:261:MET:HE1	1.73	0.53
1:B:188:VAL:O	1:B:217:HIS:ND1	2.27	0.53
1:F:353:GLU:O	1:F:357:ARG:HG3	2.09	0.53
1:C:77:MET:HE2	1:C:103:LYS:HA	1.89	0.53
1:F:176:VAL:HG21	1:F:202:TRP:CD2	2.44	0.53
1:J:270:ILE:O	1:J:274:ILE:HG12	2.09	0.53
1:C:84:MET:HE2	1:C:95:LYS:HD2	1.91	0.53
1:D:29:MET:O	1:D:97:VAL:N	2.38	0.52
1:I:176:VAL:HG21	1:I:202:TRP:CD2	2.43	0.52
1:G:88:PRO:HG3	1:G:224:ILE:HD13	1.91	0.52
1:C:257:SER:HB3	1:C:336:TYR:HB3	1.91	0.52
1:B:275:GLU:O	1:B:278:SER:OG	2.23	0.52
1:E:44:THR:HG21	1:E:90:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:O	1:C:271:GLU:HG3	2.10	0.51
1:E:81:PRO:HB3	1:E:97:VAL:HG21	1.92	0.51
1:A:130:TRP:C	1:A:131:PHE:HD2	2.14	0.51
1:E:139:LEU:HD21	1:E:175:ILE:HG21	1.90	0.51
1:J:240:PRO:HB3	1:J:343:SER:HB2	1.91	0.51
1:F:57:LEU:HD11	1:F:84:MET:HG3	1.92	0.51
1:I:189:LYS:NZ	1:I:208:PRO:O	2.43	0.51
1:J:134:GLU:HG2	1:J:205:GLN:HG2	1.91	0.51
1:H:198:MET:HE3	1:H:201:GLN:HB2	1.92	0.51
1:A:45:ARG:HB3	1:A:60:TRP:CH2	2.46	0.51
1:D:218:LEU:HD12	1:D:221:ALA:HB3	1.93	0.51
1:I:289:ASP:OD1	1:I:293:GLY:N	2.44	0.51
1:E:254:THR:HG23	1:E:342:PRO:HG2	1.93	0.50
1:F:313:SER:O	1:F:322:SER:N	2.43	0.50
1:H:38:GLU:HG2	1:H:290:PRO:HG2	1.93	0.50
1:E:353:GLU:OE2	1:E:357:ARG:NH1	2.45	0.50
1:H:176:VAL:HG21	1:H:202:TRP:CD2	2.46	0.50
1:D:259:LYS:N	1:D:262:ARG:HH11	2.09	0.50
1:G:198:MET:HE3	1:G:201:GLN:HB2	1.93	0.50
1:J:307:SER:OG	1:J:308:ASN:N	2.42	0.50
1:E:62:PHE:HE2	1:E:67:THR:HG21	1.77	0.50
1:E:119:ARG:O	1:E:123:MET:HG3	2.12	0.50
1:A:117:CYS:O	1:A:121:MET:HG2	2.12	0.50
1:B:220:VAL:O	1:B:224:ILE:HG13	2.12	0.50
1:J:33:ILE:O	1:J:69:GLN:NE2	2.44	0.50
1:C:176:VAL:HG21	1:C:202:TRP:CD2	2.47	0.49
1:G:227:ARG:HG3	1:G:227:ARG:HH11	1.77	0.49
1:I:180:TYR:OH	1:I:192:GLY:HA2	2.12	0.49
1:I:227:ARG:HG3	1:I:227:ARG:NH1	2.27	0.49
1:C:259:LYS:HD3	1:C:262:ARG:NH1	2.28	0.49
1:F:168:ASP:HB3	1:J:235:ILE:HD11	1.94	0.49
1:J:241:LYS:NZ	1:J:247:TRP:O	2.45	0.49
1:B:277:LEU:HD21	1:B:359:CYS:SG	2.52	0.49
1:C:280:ARG:NH2	1:C:365:GLY:O	2.42	0.49
1:F:125:SER:O	1:F:128:HIS:ND1	2.46	0.49
1:A:258:THR:HB	1:A:261:MET:HG3	1.95	0.49
1:C:35:GLY:HA2	1:C:111:THR:HG21	1.95	0.49
1:D:263:GLU:HG2	1:D:264:GLU:H	1.78	0.49
1:I:194:ASN:ND2	1:I:203:GLU:OE2	2.44	0.49
1:J:317:ALA:N	1:J:325:ILE:O	2.41	0.49
1:B:235:ILE:HD11	1:C:168:ASP:CG	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HD2	1:B:60:TRP:CH2	2.47	0.48
1:D:120:ILE:HD11	1:D:357:ARG:NH2	2.28	0.48
1:E:43:LYS:HD2	1:E:60:TRP:CH2	2.48	0.48
1:J:121:MET:HE1	1:J:131:PHE:HE2	1.78	0.48
1:G:76:ASP:OD2	1:H:324:ARG:NH2	2.47	0.48
1:G:239:ASP:OD2	1:G:298:ARG:NH2	2.46	0.48
1:D:326:PRO:HG2	1:D:336:TYR:CZ	2.48	0.48
1:D:347:ASP:OD1	1:D:349:PHE:HD2	1.97	0.48
1:I:252:CYS:HB2	1:I:344:ALA:HA	1.96	0.48
1:D:83:ALA:HB3	1:D:98:LEU:HB3	1.96	0.48
1:G:134:GLU:O	1:G:252:CYS:HA	2.14	0.48
1:D:312:PHE:HE2	1:D:341:ARG:NH2	2.12	0.48
1:A:129:PRO:HB2	1:A:131:PHE:HE2	1.79	0.48
1:E:137:TYR:CD1	1:E:225:LEU:HD21	2.48	0.48
1:J:328:THR:O	1:J:332:GLU:HG3	2.14	0.48
1:E:343:SER:OG	1:E:344:ALA:N	2.45	0.48
1:G:176:VAL:HG21	1:G:202:TRP:CD2	2.49	0.48
1:H:220:VAL:O	1:H:224:ILE:HG13	2.14	0.47
1:H:274:ILE:HD12	1:H:274:ILE:H	1.79	0.47
1:J:124:VAL:HG21	1:J:356:ILE:HD12	1.96	0.47
1:E:35:GLY:HA2	1:E:111:THR:HG21	1.96	0.47
1:F:119:ARG:O	1:F:123:MET:HG3	2.14	0.47
1:G:289:ASP:OD1	1:G:293:GLY:N	2.39	0.47
1:J:289:ASP:OD1	1:J:292:GLY:N	2.47	0.47
1:D:51:PRO:HG2	1:D:84:MET:CE	2.43	0.47
1:E:135:GLN:OE1	1:E:222:ARG:NH2	2.40	0.47
1:E:254:THR:HG21	1:E:351:VAL:HG11	1.95	0.47
1:G:74:ASN:HB3	1:H:327:ARG:HH12	1.79	0.47
1:H:65:SER:HA	1:H:70:SER:O	2.15	0.47
1:B:133:MET:H	1:B:214:MET:HE1	1.80	0.47
1:B:241:LYS:NZ	1:B:247:TRP:O	2.44	0.47
1:I:38:GLU:HG2	1:I:290:PRO:HG2	1.96	0.47
1:B:136:GLU:HG3	1:B:203:GLU:HG3	1.97	0.47
1:G:194:ASN:ND2	1:G:203:GLU:OE1	2.46	0.47
1:H:261:MET:HG2	1:H:270:ILE:CG1	2.41	0.47
1:J:103:LYS:HG3	1:J:107:ARG:O	2.14	0.47
1:C:198:MET:HG3	1:C:247:TRP:HE3	1.80	0.47
1:A:116:THR:O	1:A:120:ILE:HG12	2.15	0.47
1:A:120:ILE:HG13	1:A:357:ARG:HE	1.80	0.47
1:A:329:VAL:O	1:A:333:LYS:N	2.48	0.47
1:I:40:LEU:HD13	1:I:223:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HG3	1:A:214:MET:SD	2.56	0.46
1:E:342:PRO:O	1:E:346:CYS:HB3	2.15	0.46
1:F:277:LEU:HD21	1:F:359:CYS:SG	2.55	0.46
1:J:361:LEU:HD12	1:J:371:TYR:OH	2.14	0.46
1:D:357:ARG:NH1	1:D:369:PHE:H	2.14	0.46
1:H:143:ASP:OD1	1:H:143:ASP:N	2.48	0.46
1:J:196:GLU:HB2	1:J:201:GLN:HG2	1.98	0.46
1:I:258:THR:H	1:I:261:MET:HE3	1.80	0.46
1:B:54:VAL:HG22	1:B:84:MET:HB3	1.98	0.46
1:G:268:LYS:HG3	1:G:269:TYR:N	2.31	0.46
1:H:296:ASN:HB3	1:H:309:ILE:HD12	1.97	0.46
1:I:295:ASP:OD1	1:I:298:ARG:NH1	2.49	0.46
1:J:45:ARG:HB3	1:J:60:TRP:CH2	2.50	0.46
1:D:257:SER:OG	1:D:336:TYR:HA	2.16	0.46
1:J:87:ASP:HB3	1:J:90:ARG:O	2.15	0.46
1:J:180:TYR:CD1	1:J:190:ILE:HD13	2.51	0.46
1:J:218:LEU:HD23	1:J:348:PRO:HB3	1.98	0.46
1:J:229:CYS:HB3	1:J:234:VAL:O	2.16	0.46
1:A:161:TYR:CD2	1:A:199:PRO:HD3	2.51	0.46
1:B:45:ARG:HB3	1:B:60:TRP:CH2	2.50	0.46
1:B:338:GLU:OE1	1:B:340:ARG:NH1	2.49	0.46
1:C:151:SER:OG	1:C:152:ASN:N	2.48	0.46
1:H:77:MET:HE2	1:H:103:LYS:HA	1.98	0.46
1:I:46:THR:N	1:J:191:ALA:O	2.48	0.46
1:J:176:VAL:HG11	1:J:202:TRP:CD2	2.51	0.46
1:A:146:PRO:HB2	1:A:149:TRP:CG	2.51	0.46
1:D:51:PRO:HB3	1:D:56:GLU:OE1	2.16	0.46
1:F:133:MET:HE2	1:F:218:LEU:HD22	1.97	0.46
1:F:289:ASP:OD1	1:F:292:GLY:N	2.48	0.46
1:D:125:SER:O	1:D:128:HIS:ND1	2.49	0.46
1:H:258:THR:O	1:H:262:ARG:HG3	2.15	0.46
1:E:30:TYR:HE2	1:E:60:TRP:HB2	1.79	0.45
1:F:313:SER:H	1:F:322:SER:HB3	1.82	0.45
1:H:76:ASP:OD1	1:I:327:ARG:NH1	2.50	0.45
1:H:131:PHE:HB2	1:H:214:MET:HG2	1.97	0.45
1:F:258:THR:HG23	1:F:260:ALA:H	1.81	0.45
1:F:272:GLU:O	1:F:276:LYS:HG3	2.15	0.45
1:I:272:GLU:O	1:I:276:LYS:HG3	2.16	0.45
1:B:90:ARG:NH2	1:C:177:GLU:OE2	2.50	0.45
1:B:149:TRP:HE1	1:B:199:PRO:HB2	1.82	0.45
1:D:86:ARG:NH2	1:D:92:ASP:OD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:PRO:O	1:G:346:CYS:HB3	2.17	0.45
1:B:153:GLY:HA3	1:J:150:PRO:HG2	1.98	0.45
1:D:176:VAL:HG21	1:D:202:TRP:CD2	2.51	0.45
1:F:288:TYR:HE2	1:F:341:ARG:HE	1.65	0.45
1:A:78:TYR:HB2	1:A:102:PHE:HB2	1.97	0.45
1:C:326:PRO:O	1:C:329:VAL:HG12	2.17	0.45
1:B:270:ILE:O	1:B:274:ILE:HG13	2.17	0.45
1:E:133:MET:HE3	1:E:348:PRO:HB3	1.99	0.45
1:F:284:HIS:HE1	1:F:355:LEU:HD23	1.81	0.45
1:G:220:VAL:O	1:G:224:ILE:HG13	2.17	0.45
1:G:227:ARG:HG3	1:G:227:ARG:NH1	2.31	0.45
1:H:64:GLY:HA3	1:H:77:MET:HG3	1.99	0.45
1:B:196:GLU:HB3	1:B:201:GLN:HB3	1.99	0.45
1:C:70:SER:OG	1:C:75:SER:HA	2.17	0.45
1:J:102:PHE:HD1	1:J:108:PRO:HA	1.82	0.45
1:E:133:MET:SD	1:E:254:THR:HG22	2.57	0.45
1:J:296:ASN:ND2	1:J:343:SER:HB3	2.28	0.45
1:A:124:VAL:HG22	1:A:124:VAL:O	2.16	0.44
1:C:198:MET:HG3	1:C:247:TRP:CE3	2.51	0.44
1:E:341:ARG:N	1:E:342:PRO:CD	2.80	0.44
1:D:275:GLU:HA	1:D:278:SER:HB3	1.99	0.44
1:B:51:PRO:HG3	1:B:57:LEU:HD21	1.98	0.44
1:A:191:ALA:O	1:E:46:THR:N	2.38	0.44
1:C:293:GLY:C	1:C:295:ASP:H	2.20	0.44
1:G:341:ARG:N	1:G:342:PRO:CD	2.79	0.44
1:I:45:ARG:HB3	1:I:60:TRP:CH2	2.53	0.44
1:A:131:PHE:HE1	1:A:352:THR:HA	1.82	0.44
1:B:161:TYR:CE2	1:B:199:PRO:HG3	2.52	0.44
1:F:24:GLU:HG3	1:F:25:LYS:H	1.83	0.44
1:F:176:VAL:HG21	1:F:202:TRP:CE3	2.53	0.44
1:G:212:ILE:HD12	1:G:212:ILE:HA	1.88	0.44
1:H:118:LYS:HA	1:H:212:ILE:HD13	1.99	0.44
1:H:253:HIS:CD2	1:H:340:ARG:HE	2.36	0.44
1:I:146:PRO:HB2	1:I:149:TRP:CD1	2.52	0.44
1:E:32:TRP:HB3	1:E:79:LEU:HD21	1.99	0.44
1:D:121:MET:SD	1:D:211:GLY:HA2	2.58	0.44
1:E:146:PRO:HB2	1:E:149:TRP:CG	2.52	0.44
1:F:57:LEU:HB2	1:F:81:PRO:HG2	1.98	0.44
1:G:146:PRO:HB2	1:G:149:TRP:CD1	2.52	0.44
1:B:278:SER:HA	1:B:312:PHE:CE1	2.52	0.44
1:B:326:PRO:HB2	1:B:329:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:TYR:CD2	1:C:193:THR:HG23	2.52	0.44
1:I:160:PRO:HB2	1:I:169:ARG:HD2	1.99	0.44
1:A:296:ASN:ND2	1:A:341:ARG:O	2.50	0.43
1:F:227:ARG:NH1	1:F:231:ASP:OD1	2.51	0.43
1:J:295:ASP:OD1	1:J:298:ARG:NH2	2.51	0.43
1:C:78:TYR:HB2	1:C:102:PHE:HB2	2.00	0.43
1:D:259:LYS:HA	1:D:262:ARG:HD3	1.99	0.43
1:F:146:PRO:HB2	1:F:149:TRP:CG	2.53	0.43
1:G:24:GLU:N	1:G:24:GLU:OE1	2.52	0.43
1:G:76:ASP:HB2	1:H:327:ARG:NH2	2.33	0.43
1:B:241:LYS:HA	1:B:241:LYS:HD3	1.75	0.43
1:B:312:PHE:HE2	1:B:314:ALA:HB2	1.82	0.43
1:J:133:MET:HG3	1:J:214:MET:CE	2.48	0.43
1:E:98:LEU:HD12	1:E:99:CYS:H	1.84	0.43
1:E:219:TRP:CZ2	1:E:348:PRO:HD2	2.54	0.43
1:H:288:TYR:HB3	1:H:342:PRO:HA	1.99	0.43
1:J:82:ALA:HB1	1:J:114:ARG:CZ	2.49	0.43
1:E:252:CYS:HB3	1:E:343:SER:O	2.19	0.43
1:C:128:HIS:CD2	1:C:259:LYS:HE2	2.53	0.43
1:C:175:ILE:HG23	1:C:228:VAL:HG12	2.00	0.43
1:D:263:GLU:HG2	1:D:264:GLU:N	2.33	0.43
1:F:38:GLU:HG2	1:F:290:PRO:HG2	2.01	0.43
1:F:133:MET:HE1	1:F:348:PRO:HB3	2.01	0.43
1:H:106:ARG:HH11	1:H:106:ARG:HG2	1.83	0.43
1:I:146:PRO:HB2	1:I:149:TRP:CG	2.53	0.43
1:I:117:CYS:O	1:I:121:MET:HG2	2.18	0.43
1:A:146:PRO:HB2	1:A:149:TRP:CD1	2.54	0.43
1:B:289:ASP:OD1	1:B:292:GLY:N	2.52	0.43
1:F:167:ALA:HB3	1:J:235:ILE:HG13	2.00	0.43
1:G:32:TRP:CE2	1:G:41:ARG:HB2	2.54	0.43
1:D:257:SER:OG	1:D:335:GLY:O	2.21	0.43
1:E:205:GLN:N	1:E:205:GLN:OE1	2.52	0.43
1:B:32:TRP:CE2	1:B:41:ARG:HB2	2.54	0.42
1:F:126:ASN:N	1:F:126:ASN:OD1	2.52	0.42
1:G:288:TYR:CD1	1:G:351:VAL:HG22	2.53	0.42
1:H:240:PRO:HG3	1:H:295:ASP:HB3	2.01	0.42
1:H:357:ARG:HA	1:H:361:LEU:HD23	2.01	0.42
1:B:299:ARG:NH2	1:B:341:ARG:O	2.51	0.42
1:D:110:GLU:H	1:D:110:GLU:CD	2.22	0.42
1:G:161:TYR:HB2	1:G:197:VAL:O	2.19	0.42
1:J:326:PRO:HB2	1:J:329:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:O	1:B:123:MET:HG3	2.19	0.42
1:D:146:PRO:HB2	1:D:149:TRP:CD1	2.54	0.42
1:D:284:HIS:HB3	1:D:288:TYR:CE2	2.53	0.42
1:E:137:TYR:CE1	1:E:225:LEU:HD21	2.54	0.42
1:A:196:GLU:HG3	1:A:197:VAL:H	1.85	0.42
1:B:85:PHE:CE1	1:B:220:VAL:HG21	2.55	0.42
1:E:54:VAL:HG23	1:E:84:MET:HB2	2.01	0.42
1:H:356:ILE:HD13	1:H:360:LEU:HD12	2.02	0.42
1:J:89:PHE:HE1	1:J:228:VAL:HG12	1.85	0.42
1:J:146:PRO:HB2	1:J:149:TRP:CD1	2.55	0.42
1:C:288:TYR:HB3	1:C:342:PRO:HA	2.01	0.42
1:I:189:LYS:HZ1	1:I:209:CYS:HA	1.85	0.42
1:B:307:SER:OG	1:B:308:ASN:N	2.53	0.42
1:E:206:ILE:HD13	1:E:206:ILE:HA	1.86	0.42
1:G:44:THR:HG21	1:G:90:ARG:HH12	1.84	0.42
1:G:261:MET:HB3	1:G:270:ILE:HG13	2.01	0.42
1:G:274:ILE:HG12	1:G:323:ILE:HG21	2.00	0.42
1:J:280:ARG:HB2	1:J:283:TYR:HB3	2.02	0.42
1:A:176:VAL:HG11	1:A:202:TRP:CD2	2.55	0.42
1:B:176:VAL:HG11	1:B:202:TRP:CD2	2.55	0.42
1:B:329:VAL:O	1:B:333:LYS:N	2.53	0.42
1:D:51:PRO:HG2	1:D:84:MET:HE1	2.01	0.42
1:H:180:TYR:CE1	1:H:190:ILE:HG12	2.55	0.42
1:A:65:SER:HB2	1:A:72:GLY:HA2	2.02	0.42
1:C:135:GLN:OE1	1:C:222:ARG:NE	2.44	0.42
1:D:318:ASN:OD1	1:D:320:SER:OG	2.27	0.42
1:G:251:GLY:HA2	1:G:343:SER:HA	2.00	0.42
1:D:40:LEU:HD21	1:D:219:TRP:CE3	2.55	0.42
1:D:312:PHE:HE2	1:D:341:ARG:HH21	1.67	0.42
1:E:92:ASP:N	1:E:93:PRO:HD2	2.35	0.42
1:F:133:MET:CE	1:F:218:LEU:HD22	2.50	0.42
1:J:300:LEU:HD12	1:J:309:ILE:HA	2.01	0.41
1:A:175:ILE:HD12	1:A:175:ILE:H	1.85	0.41
1:C:311:ASP:OD1	1:C:311:ASP:N	2.52	0.41
1:D:267:LEU:HD12	1:D:333:LYS:HA	2.02	0.41
1:D:280:ARG:HD3	1:D:358:THR:OG1	2.20	0.41
1:H:230:GLU:OE2	1:I:173:ARG:NE	2.46	0.41
1:B:53:CYS:SG	1:B:56:GLU:HG3	2.60	0.41
1:B:161:TYR:HB2	1:B:197:VAL:O	2.20	0.41
1:H:131:PHE:CB	1:H:214:MET:HG2	2.50	0.41
1:H:366:ASP:OD1	1:H:366:ASP:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:TYR:HA	1:J:97:VAL:HG13	2.01	0.41
1:A:209:CYS:HB2	1:A:214:MET:HB2	2.01	0.41
1:B:149:TRP:NE1	1:B:199:PRO:HB2	2.35	0.41
1:B:152:ASN:OD1	1:B:152:ASN:N	2.52	0.41
1:B:313:SER:H	1:B:322:SER:HB2	1.86	0.41
1:H:45:ARG:HB3	1:H:60:TRP:CH2	2.54	0.41
1:A:357:ARG:NH1	1:A:368:PRO:HB2	2.35	0.41
1:C:220:VAL:O	1:C:224:ILE:HG13	2.21	0.41
1:E:31:ILE:HD11	1:E:96:LEU:HD22	2.02	0.41
1:F:133:MET:HG3	1:F:214:MET:HE2	2.03	0.41
1:F:261:MET:CG	1:F:270:ILE:HG13	2.43	0.41
1:G:45:ARG:HB3	1:G:60:TRP:CH2	2.55	0.41
1:A:46:THR:N	1:B:191:ALA:O	2.45	0.41
1:C:126:ASN:H	1:C:126:ASN:ND2	2.18	0.41
1:E:176:VAL:HG11	1:E:202:TRP:CD2	2.56	0.41
1:G:146:PRO:HB2	1:G:149:TRP:CG	2.56	0.41
1:I:190:ILE:HA	1:I:206:ILE:HD13	2.03	0.41
1:D:234:VAL:C	1:D:235:ILE:HD13	2.41	0.41
1:I:140:MET:HB2	1:I:235:ILE:HB	2.02	0.41
1:C:46:THR:N	1:D:191:ALA:O	2.47	0.41
1:E:26:VAL:HG12	1:E:47:LEU:HB2	2.03	0.41
1:A:209:CYS:HB2	1:A:214:MET:CB	2.51	0.41
1:G:86:ARG:NH1	1:G:185:TYR:O	2.54	0.41
1:H:67:THR:OG1	1:H:69:GLN:OE1	2.34	0.41
1:C:153:GLY:HA3	1:I:150:PRO:HG2	2.02	0.40
1:D:81:PRO:HB3	1:D:97:VAL:HG11	2.03	0.40
1:G:257:SER:HA	1:G:261:MET:CE	2.51	0.40
1:J:296:ASN:OD1	1:J:300:LEU:HG	2.20	0.40
1:B:133:MET:HA	1:B:254:THR:HA	2.02	0.40
1:B:205:GLN:HE21	1:B:205:GLN:HB2	1.76	0.40
1:F:132:GLY:O	1:F:255:ASN:N	2.38	0.40
1:G:70:SER:OG	1:G:75:SER:HA	2.21	0.40
1:A:135:GLN:OE1	1:A:222:ARG:NH2	2.49	0.40
1:D:313:SER:OG	1:D:322:SER:N	2.50	0.40
1:F:283:TYR:OH	1:F:368:PRO:HG3	2.22	0.40
1:G:146:PRO:HG3	1:G:243:ILE:HD11	2.04	0.40
1:I:126:ASN:OD1	1:I:126:ASN:N	2.54	0.40
1:J:288:TYR:CD1	1:J:351:VAL:HG22	2.57	0.40
1:C:30:TYR:HD2	1:C:99:CYS:HG	1.69	0.40
1:F:32:TRP:CE2	1:F:41:ARG:HB2	2.57	0.40
1:C:190:ILE:HA	1:C:206:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLU:HG3	1:D:25:LYS:H	1.87	0.40
1:D:357:ARG:NH1	1:D:369:PHE:HB2	2.34	0.40
1:F:33:ILE:HD11	1:F:219:TRP:CE2	2.57	0.40

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	337/370 (91%)	324 (96%)	13 (4%)	0	100	100
1	B	340/370 (92%)	329 (97%)	11 (3%)	0	100	100
1	C	337/370 (91%)	323 (96%)	14 (4%)	0	100	100
1	D	329/370 (89%)	312 (95%)	17 (5%)	0	100	100
1	E	310/370 (84%)	295 (95%)	15 (5%)	0	100	100
1	F	336/370 (91%)	323 (96%)	13 (4%)	0	100	100
1	G	338/370 (91%)	327 (97%)	11 (3%)	0	100	100
1	H	344/370 (93%)	332 (96%)	12 (4%)	0	100	100
1	I	338/370 (91%)	324 (96%)	14 (4%)	0	100	100
1	J	339/370 (92%)	324 (96%)	15 (4%)	0	100	100
All	All	3348/3700 (90%)	3213 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	230/309 (74%)	223 (97%)	7 (3%)	41	72
1	B	263/309 (85%)	259 (98%)	4 (2%)	65	85
1	C	276/309 (89%)	273 (99%)	3 (1%)	73	89
1	D	244/309 (79%)	238 (98%)	6 (2%)	47	76
1	E	201/309 (65%)	195 (97%)	6 (3%)	41	72
1	F	263/309 (85%)	259 (98%)	4 (2%)	65	85
1	G	272/309 (88%)	264 (97%)	8 (3%)	42	73
1	H	287/309 (93%)	281 (98%)	6 (2%)	53	80
1	I	271/309 (88%)	267 (98%)	4 (2%)	65	85
1	J	263/309 (85%)	258 (98%)	5 (2%)	57	81
All	All	2570/3090 (83%)	2517 (98%)	53 (2%)	53	80

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	104	TYR
1	A	106	ARG
1	A	112	ASN
1	A	180	TYR
1	A	198	MET
1	A	278	SER
1	B	169	ARG
1	B	201	GLN
1	B	205	GLN
1	B	312	PHE
1	C	296	ASN
1	C	311	ASP
1	C	364	THR
1	D	84	MET
1	D	90	ARG
1	D	128	HIS
1	D	205	GLN
1	D	265	ASN
1	D	324	ARG
1	E	50	GLU
1	E	104	TYR

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Mol	Chain	Res	Type
1	E	174	ASP
1	E	180	TYR
1	E	198	MET
1	E	252	CYS
1	F	43	LYS
1	F	104	TYR
1	F	126	ASN
1	F	198	MET
1	G	42	CYS
1	G	205	GLN
1	G	259	LYS
1	G	265	ASN
1	G	313	SER
1	G	320	SER
1	G	340	ARG
1	G	343	SER
1	H	76	ASP
1	H	107	ARG
1	H	198	MET
1	H	214	MET
1	H	268	LYS
1	H	333	LYS
1	I	61	ASN
1	I	180	TYR
1	I	205	GLN
1	I	308	ASN
1	J	106	ARG
1	J	118	LYS
1	J	280	ARG
1	J	312	PHE
1	J	343	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	201	GLN
1	B	318	ASN
1	C	126	ASN
1	D	205	GLN
1	F	127	GLN
1	I	205	GLN

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Mol	Chain	Res	Type
1	I	248	ASN
1	J	296	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 [i](#)

There are no ligands in this entry.

### 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

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	341/370 (92%)	0.50	29 (8%) 10 6	69, 102, 140, 187	0
1	B	344/370 (92%)	0.10	4 (1%) 79 63	58, 86, 120, 130	0
1	C	341/370 (92%)	0.09	4 (1%) 79 63	48, 79, 113, 132	0
1	D	335/370 (90%)	0.43	15 (4%) 33 21	65, 115, 140, 192	0
1	E	316/370 (85%)	0.72	43 (13%) 3 1	79, 118, 147, 159	0
1	F	340/370 (91%)	0.34	9 (2%) 56 39	62, 90, 122, 136	0
1	G	342/370 (92%)	0.20	8 (2%) 60 43	55, 79, 116, 141	0
1	H	348/370 (94%)	0.11	4 (1%) 80 65	56, 76, 105, 140	0
1	I	342/370 (92%)	0.32	17 (4%) 28 18	58, 87, 115, 134	0
1	J	343/370 (92%)	0.26	14 (4%) 37 24	64, 93, 120, 134	0
All	All	3392/3700 (91%)	0.30	147 (4%) 35 22	48, 92, 133, 192	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	317	ALA	5.9
1	E	359	CYS	4.6
1	E	265	ASN	4.4
1	I	315	GLY	4.4
1	A	354	ALA	4.4
1	G	23	GLY	4.2
1	E	260	ALA	4.1
1	J	318	ASN	4.0
1	E	266	GLY	3.9
1	G	316	VAL	3.8
1	J	315	GLY	3.8
1	B	335	GLY	3.7
1	D	105	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	310	ASN	3.5
1	E	268	LYS	3.5
1	D	366	ASP	3.5
1	E	294	LEU	3.4
1	F	315	GLY	3.4
1	E	274	ILE	3.4
1	A	247	TRP	3.4
1	A	316	VAL	3.4
1	A	330	GLY	3.3
1	E	366	ASP	3.3
1	A	246	ASN	3.2
1	A	362	ASN	3.2
1	I	311	ASP	3.2
1	J	371	TYR	3.2
1	A	24	GLU	3.2
1	C	300	LEU	3.2
1	F	364	THR	3.1
1	E	331	GLN	3.1
1	I	71	GLU	3.1
1	D	368	PRO	3.1
1	A	283	TYR	3.0
1	I	314	ALA	3.0
1	E	367	GLU	3.0
1	E	354	ALA	3.0
1	H	302	GLY	2.9
1	G	247	TRP	2.9
1	F	371	TYR	2.9
1	J	72	GLY	2.9
1	E	328	THR	2.8
1	E	273	ALA	2.8
1	A	292	GLY	2.8
1	E	283	TYR	2.8
1	G	312	PHE	2.8
1	A	314	ALA	2.8
1	J	246	ASN	2.8
1	E	278	SER	2.8
1	E	323	ILE	2.7
1	J	359	CYS	2.7
1	A	337	PHE	2.7
1	E	362	ASN	2.7
1	I	246	ASN	2.7
1	D	83	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	73	SER	2.7
1	I	93	PRO	2.7
1	H	372	LYS	2.6
1	A	359	CYS	2.6
1	E	263	GLU	2.6
1	I	313	SER	2.6
1	A	317	ALA	2.6
1	D	283	TYR	2.6
1	I	73	SER	2.6
1	I	320	SER	2.6
1	E	364	THR	2.5
1	B	370	GLN	2.5
1	A	329	VAL	2.5
1	C	309	ILE	2.5
1	E	326	PRO	2.5
1	G	329	VAL	2.5
1	E	324	ARG	2.5
1	A	335	GLY	2.5
1	I	312	PHE	2.4
1	E	322	SER	2.4
1	G	248	ASN	2.4
1	I	309	ILE	2.4
1	E	30	TYR	2.4
1	H	301	THR	2.4
1	C	248	ASN	2.4
1	A	356	ILE	2.4
1	E	261	MET	2.4
1	D	365	GLY	2.4
1	F	362	ASN	2.4
1	D	217	HIS	2.4
1	A	210	GLU	2.4
1	E	264	GLU	2.4
1	J	269	TYR	2.4
1	A	328	THR	2.4
1	E	246	ASN	2.4
1	I	364	THR	2.3
1	E	325	ILE	2.3
1	F	206	ILE	2.3
1	D	315	GLY	2.3
1	G	315	GLY	2.3
1	E	54	VAL	2.3
1	E	269	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	213	SER	2.3
1	E	247	TRP	2.3
1	E	330	GLY	2.3
1	H	306	THR	2.3
1	I	26	VAL	2.3
1	D	359	CYS	2.3
1	F	104	TYR	2.3
1	A	364	THR	2.3
1	D	121	MET	2.3
1	E	355	LEU	2.3
1	A	369	PHE	2.3
1	J	369	PHE	2.3
1	F	370	GLN	2.3
1	E	219	TRP	2.2
1	A	153	GLY	2.2
1	F	74	ASN	2.2
1	A	73	SER	2.2
1	J	316	VAL	2.2
1	I	318	ASN	2.2
1	J	301	THR	2.2
1	A	323	ILE	2.2
1	A	322	SER	2.2
1	I	300	LEU	2.2
1	D	81	PRO	2.2
1	A	360	LEU	2.2
1	A	256	PHE	2.2
1	B	105	ASN	2.2
1	A	261	MET	2.2
1	D	357	ARG	2.2
1	E	53	CYS	2.2
1	E	352	THR	2.2
1	G	310	ASN	2.1
1	I	323	ILE	2.1
1	E	368	PRO	2.1
1	B	23	GLY	2.1
1	E	358	THR	2.1
1	E	288	TYR	2.1
1	J	311	ASP	2.1
1	J	74	ASN	2.1
1	C	299	ARG	2.1
1	D	247	TRP	2.1
1	J	24	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	297	ALA	2.0
1	E	293	GLY	2.0
1	A	355	LEU	2.0
1	E	342	PRO	2.0
1	A	68	LEU	2.0
1	E	110	GLU	2.0
1	E	321	ALA	2.0
1	D	281	HIS	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.