



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 7EVT / pdb_00007evt
Title : Crystal structure of the N-terminal degron-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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

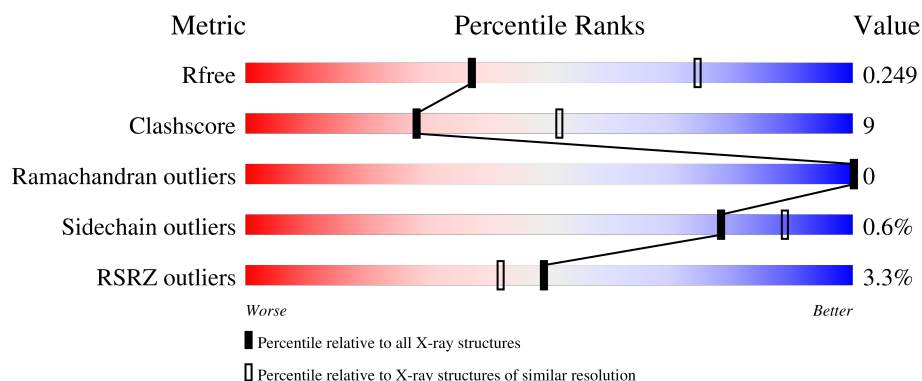
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	9% 75% 17% 8%
1	B	370	% 74% 19% 7%
1	C	370	% 74% 18% 8%
1	D	370	6% 67% 23% 9%
1	E	370	7% 68% 17% • 15%

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Mol	Chain	Length	Quality of chain
1	F	370	% 72%19%8%
1	G	370	2% 75%17%8%
1	H	370	80%14%6%
1	I	370	% 76%16%8%
1	J	370	2% 69%23%7%

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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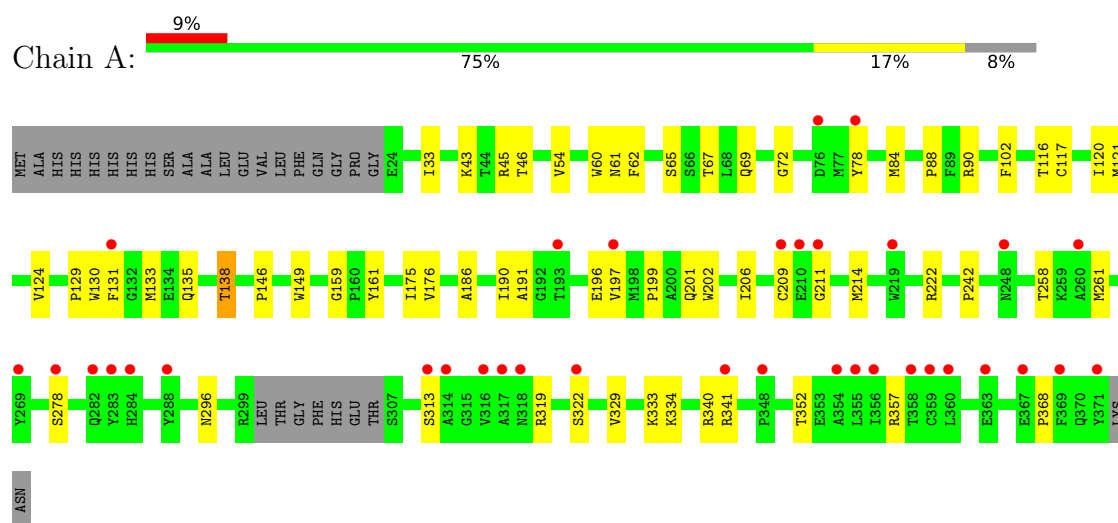
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Chain	Residue	Modelled	Actual	Comment	Reference
J	10	HIS	-	expression tag	UNP P15104
J	11	HIS	-	expression tag	UNP P15104
J	12	SER	-	expression tag	UNP P15104
J	13	ALA	-	expression tag	UNP P15104
J	14	ALA	-	expression tag	UNP P15104
J	15	LEU	-	expression 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

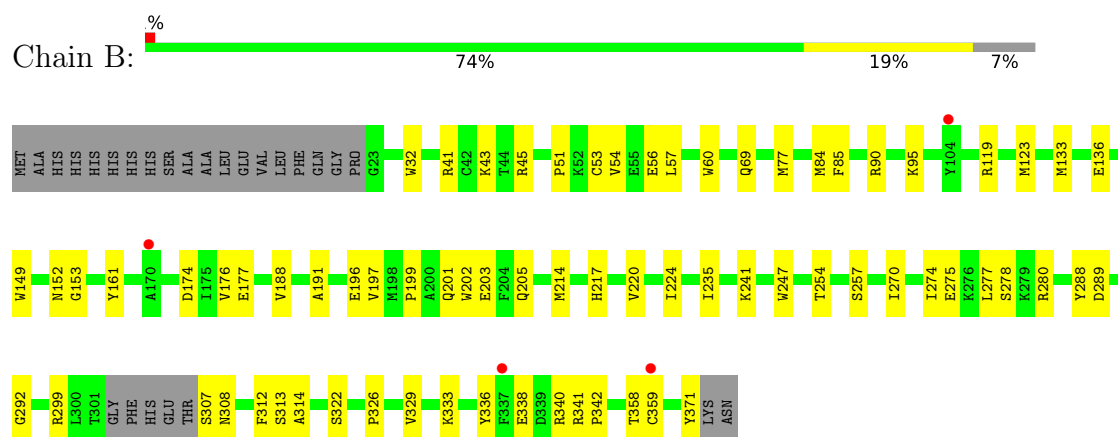
3 Residue-property plots [i](#)

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.

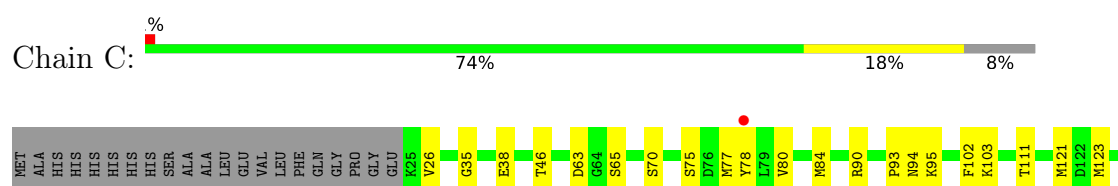
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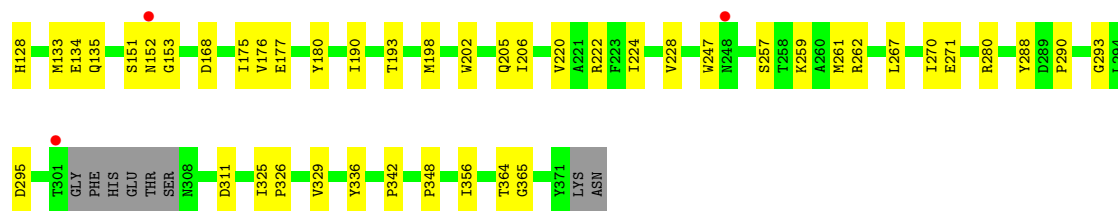


• Molecule 1: Glutamine synthetase

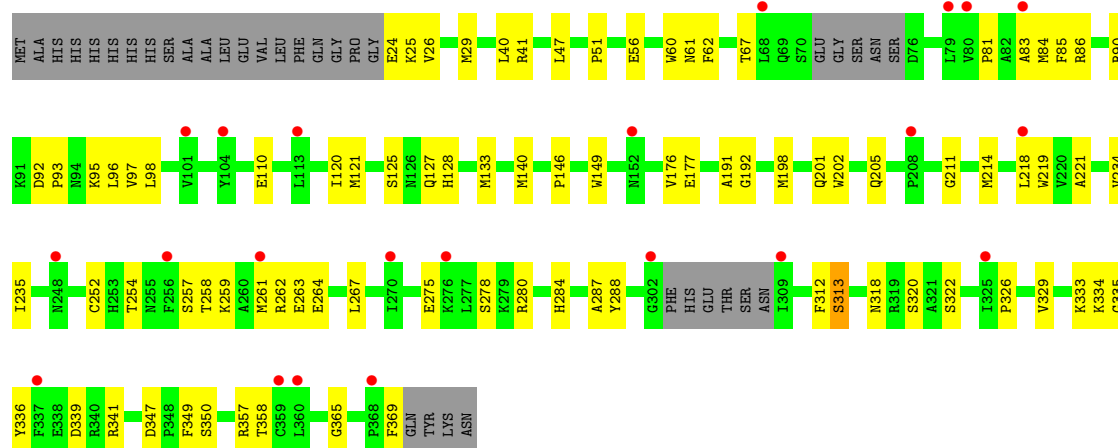


• Molecule 1: Glutamine synthetase

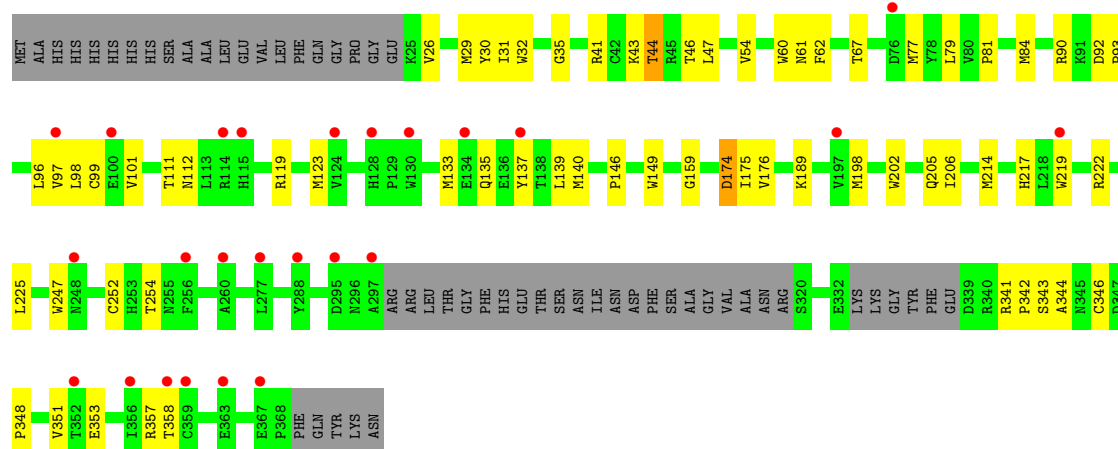




• Molecule 1: Glutamine synthetase

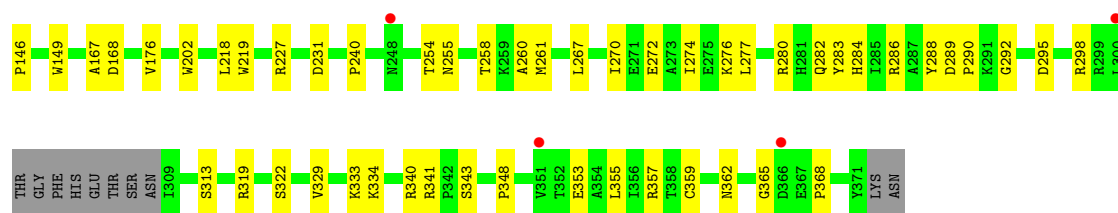


• Molecule 1: Glutamine synthetase

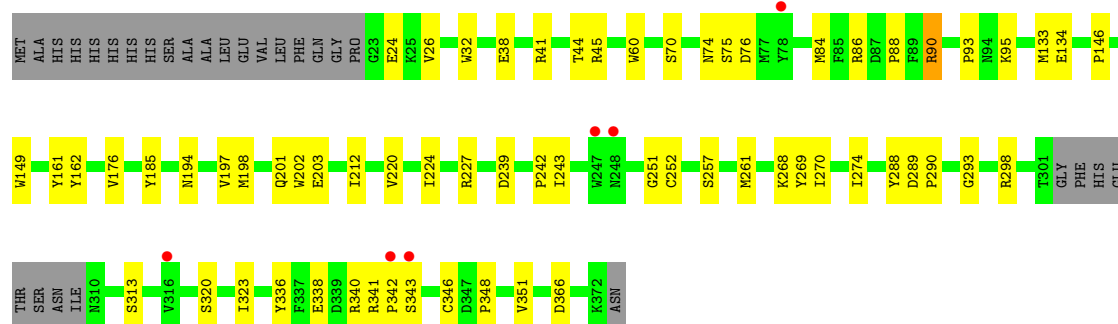
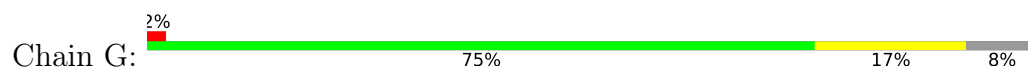


• Molecule 1: Glutamine synthetase

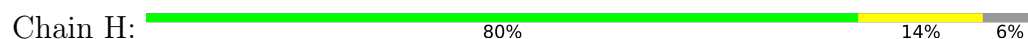




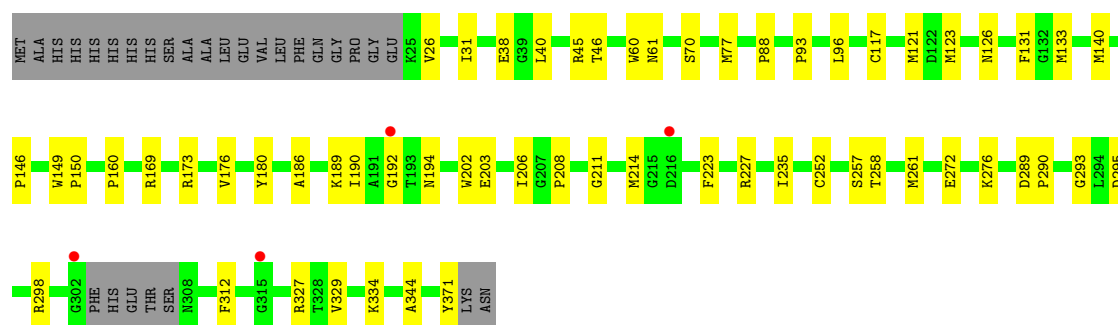
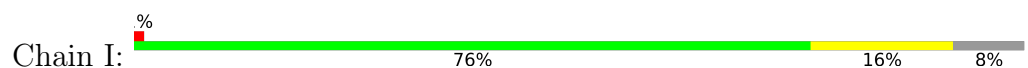
● Molecule 1: Glutamine synthetase



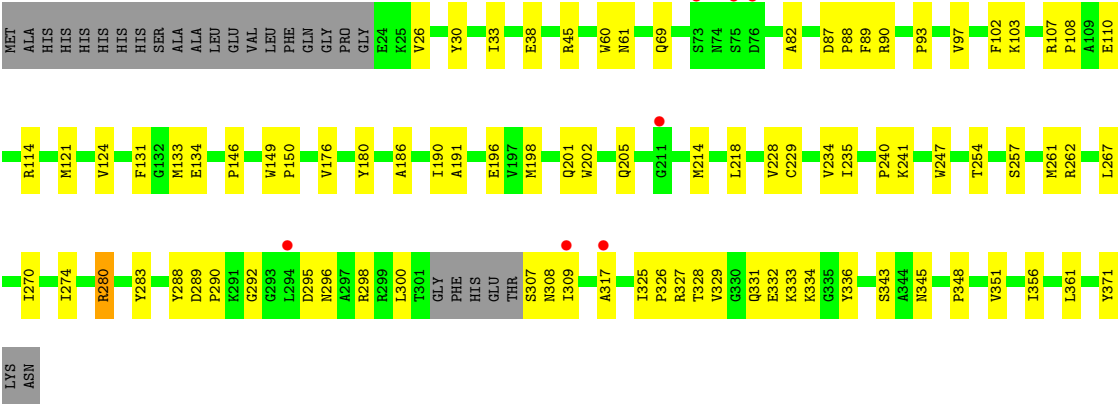
● Molecule 1: Glutamine synthetase



● Molecule 1: Glutamine synthetase



● Molecule 1: Glutamine synthetase



LYS
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.8 (44.43-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.19.4092	Depositor
R, R_{free}	0.219 , 0.250 0.220 , 0.249	Depositor DCC
R_{free} test set	4595 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/2542	0.31	0/3471
1	B	0.13	0/2695	0.29	0/3666
1	C	0.13	0/2743	0.32	0/3719
1	D	0.23	0/2570	0.36	0/3500
1	E	0.13	0/2286	0.35	0/3134
1	F	0.11	0/2692	0.28	0/3657
1	G	0.14	0/2728	0.31	0/3701
1	H	0.12	0/2819	0.27	0/3815
1	I	0.12	0/2719	0.29	0/3694
1	J	0.11	0/2703	0.29	0/3676
All	All	0.14	0/26497	0.31	0/36033

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2476	0	2170	47	0
1	B	2624	0	2397	48	0
1	C	2670	0	2501	40	0
1	D	2503	0	2241	59	0
1	E	2226	0	1895	47	0
1	F	2620	0	2405	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2655	0	2472	45	0
1	H	2746	0	2607	36	0
1	I	2647	0	2451	37	0
1	J	2630	0	2412	53	0
All	All	25797	0	23551	441	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 9.

All (441) 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:C:84:MET:HE2	1:C:95:LYS:HD2	1.56	0.87
1:F:261:MET:HG2	1:F:270:ILE:HG13	1.63	0.80
1:F:258:THR:HG22	1:F:261:MET:HE3	1.62	0.80
1:D:133:MET:HG3	1:D:214:MET:HE2	1.66	0.78
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:C:133:MET:HE1	1:C:348:PRO:HB3	1.69	0.75
1:H:261:MET:HG2	1:H:270:ILE:HG13	1.68	0.73
1:F:282:GLN:HB3	1:F:286:ARG:HH12	1.54	0.72
1:D:51:PRO:HG2	1:D:84:MET:HE1	1.72	0.72
1:E:44:THR:HG21	1:E:90:ARG:HH22	1.55	0.72
1:H:258:THR:HG22	1:H:261:MET:HE3	1.71	0.71
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:B:133:MET:HG3	1:B:214:MET:HE2	1.76	0.68
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:C:77:MET:HE3	1:C:103:LYS:HA	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:133:MET:HG3	1:I:214:MET:HE2	1.80	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:I:70:SER:HB3	1:I:77:MET:HE2	1.80	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:G:84:MET:HE3	1:G:95:LYS:HD2	1.82	0.61
1:F:41:ARG:NH1	1:G:162:TYR:O	2.34	0.61
1:E:133:MET:HE3	1:E:214:MET:HE1	1.80	0.61
1:E:198:MET:HE2	1:E:247:TRP:HB3	1.83	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:D:192:GLY:C	1:D:205:GLN:HE21	2.08	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:A:131:PHE:HB2	1:A:214:MET:HE2	1.83	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:133:MET:HG3	1:J:214:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:257:SER:HB3	1:J:336:TYR:HB3	1.86	0.57
1:F:69:GLN:HB3	1:F:77:MET:HE2	1.87	0.57
1:G:26:VAL:HG22	1:G:93:PRO:HG2	1.86	0.57
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: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:A:130:TRP:C	1:A:131:PHE:HD2	2.14	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:I:121:MET:HE3	1:I:211:GLY:HA2	1.90	0.53
1:B:235:ILE:HD11	1:C:168:ASP:CG	2.32	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HE1	1:B:371:TYR:HE2	1.75	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:H:198:MET:HE3	1:H:201:GLN:HB2	1.91	0.52
1:B:69:GLN:HB3	1:B:77:MET:HE3	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
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: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:I:60:TRP:CD1	1:I:61:ASN:H	2.29	0.51
1:J:134:GLU:HG2	1:J:205:GLN:HG2	1.91	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: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:E:60:TRP:CD1	1:E:61:ASN:H	2.30	0.49
1:J:307:SER:OG	1:J:308:ASN:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:198:MET:HE3	1:J:247:TRP:HB3	1.95	0.49
1:C:293:GLY:C	1:C:295:ASP:H	2.20	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:43:LYS:HD2	1:B:60:TRP:CH2	2.47	0.48
1:B:84:MET:HE3	1:B:95:LYS:HD2	1.95	0.48
1:A:133:MET:HE3	1:A:214:MET:HE1	1.94	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: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:G:198:MET:HE3	1:G:201:GLN:HB2	1.95	0.47
1:C:261:MET:HE2	1:C:270:ILE:HA	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:D:110:GLU:CD	1:D:110:GLU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:SER:HA	1:H:70:SER:O	2.15	0.47
1:I:123:MET:HE1	1:I:371:TYR:CE2	2.49	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:A:131:PHE:CB	1:A:214:MET:HE2	2.43	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:E:214:MET:C	1:E:214:MET:HE3	2.40	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:121:MET:HE3	1:A:211:GLY:HA2	1.95	0.47
1:A:329:VAL:O	1:A:333:LYS:N	2.48	0.47
1:E:29:MET:HE3	1:E:44:THR:CG2	2.44	0.47
1:F:133:MET:HE2	1:F:218:LEU:HD22	1.96	0.47
1:I:40:LEU:HD13	1:I:223:PHE:HB2	1.97	0.47
1:J:60:TRP:CD1	1:J:61:ASN:H	2.33	0.47
1:I:121:MET:HE1	1:I:131:PHE:CE1	2.50	0.46
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:B:54:VAL:HG22	1:B:84:MET:HB3	1.98	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:D:234:VAL:C	1:D:235:ILE:HD13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:133:MET:HE3	1:H:214:MET:HG3	1.97	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:J:121:MET:HE1	1:J:131:PHE:HE2	1.82	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
1:G:342:PRO:O	1:G:346:CYS:HB3	2.17	0.45
1:A:258:THR:OG1	1:A:261:MET:HE3	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:G:268:LYS:HG3	1:G:269:TYR:N	2.31	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:D:257:SER:HA	1:D:261:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:133:MET:CG	1:B:214:MET:HE2	2.45	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:J:327:ARG:C	1:J:331:GLN:HE21	2.24	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:D:198:MET:HE2	1:D:201:GLN:HB2	2.00	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:133:MET:HE1	1:G:348:PRO:HA	2.00	0.44
1:G:146:PRO:HB2	1:G:149:TRP:CD1	2.52	0.44
1:A:90:ARG:HH21	1:B:177:GLU:CD	2.26	0.44
1:B:278:SER:HA	1:B:312:PHE:CE1	2.52	0.44
1:A:329:VAL:HG23	1:A:334:LYS:C	2.43	0.44
1:B:326:PRO:HB2	1:B:329:VAL:HG12	1.98	0.44
1:C:180:TYR:CD2	1:C:193:THR:HG23	2.52	0.44
1:E:140:MET:HE3	1:E:140:MET:HB3	1.78	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:H:67:THR:OG1	1:H:69:GLN:OE1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:MET:HE3	1:E:44:THR:HG22	2.01	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:G:320:SER:O	1:G:320:SER:OG	2.23	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:D:133:MET:HE3	1:D:252:CYS:SG	2.59	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:G:242:PRO:C	1:G:243:ILE:HD12	2.44	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: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
1:A:60:TRP:CD1	1:A:61:ASN:H	2.36	0.42
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:D:329:VAL:HG23	1:D:334:LYS:C	2.44	0.42
1:E:137:TYR:CE1	1:E:225:LEU:HD21	2.54	0.42
1:F:133:MET:HE1	1:F:348:PRO:HB3	2.01	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:D:60:TRP:CD1	1:D:61:ASN:H	2.38	0.42
1:E:54:VAL:HG23	1:E:84:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:ASP:OD2	1:C:65:SER:OG	2.33	0.42
1:C:288:TYR:HB3	1:C:342:PRO:HA	2.01	0.42
1:B:307:SER:OG	1:B:308:ASN:N	2.53	0.42
1:C:121:MET:HE1	1:C:356:ILE:HG13	2.02	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:E:77:MET:HE3	1:E:77:MET:HB3	1.84	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:H:180:TYR:CE1	1:H:190:ILE:HG12	2.55	0.42
1:J:329:VAL:HG23	1:J:334:LYS:C	2.45	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:F:329:VAL:HG23	1:F:334:LYS:C	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:SER:H	1:B:322:SER:HB2	1.86	0.41
1:F:84:MET:HE2	1:F:84:MET:HB3	1.83	0.41
1:H:45:ARG:HB3	1:H:60:TRP:CH2	2.54	0.41
1:I:257:SER:HA	1:I:261:MET:HE3	2.03	0.41
1:C:94:ASN:C	1:C:95:LYS:HG2	2.46	0.41
1:D:258:THR:HG22	1:D:261:MET:HE1	2.03	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: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: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:I:258:THR:H	1:I:261:MET:HE3	1.86	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:C:123:MET:HE3	1:C:123:MET:HB3	1.93	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: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:I:312:PHE:C	1:I:312:PHE:CD1	2.99	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:F:32:TRP:CE2	1:F:41:ARG:HB2	2.57	0.40
1:I:329:VAL:HG23	1:I:334:LYS:C	2.47	0.40
1:C:190:ILE:HA	1:C:206:ILE:HD13	2.03	0.40
1:D:24:GLU:HG3	1:D:25:LYS:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	228 (99%)	2 (1%)	70	83
1	B	263/309 (85%)	262 (100%)	1 (0%)	84	92
1	C	276/309 (89%)	274 (99%)	2 (1%)	76	87
1	D	244/309 (79%)	242 (99%)	2 (1%)	73	85
1	E	201/309 (65%)	198 (98%)	3 (2%)	57	76
1	F	263/309 (85%)	262 (100%)	1 (0%)	84	92
1	G	272/309 (88%)	270 (99%)	2 (1%)	76	87
1	H	287/309 (93%)	286 (100%)	1 (0%)	86	92
1	I	271/309 (88%)	271 (100%)	0	100	100
1	J	263/309 (85%)	262 (100%)	1 (0%)	84	92
All	All	2570/3090 (83%)	2555 (99%)	15 (1%)	78	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	278	SER
1	B	174	ASP
1	C	325	ILE
1	C	364	THR
1	D	90	ARG
1	D	313	SER
1	E	44	THR
1	E	174	ASP
1	E	358	THR
1	F	127	GLN
1	G	90	ARG
1	G	313	SER
1	H	277	LEU
1	J	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	B	318	ASN

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Mol	Chain	Res	Type
1	C	126	ASN
1	D	61	ASN
1	D	205	GLN
1	D	248	ASN
1	E	27	GLN
1	E	179	HIS
1	F	179	HIS
1	F	282	GLN
1	G	145	HIS
1	G	158	GLN
1	G	205	GLN
1	G	248	ASN
1	H	27	GLN
1	H	115	HIS
1	H	255	ASN
1	I	61	ASN
1	I	205	GLN
1	I	226	HIS
1	I	248	ASN
1	I	255	ASN
1	J	61	ASN
1	J	128	HIS
1	J	179	HIS
1	J	194	ASN
1	J	226	HIS
1	J	296	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/370 (92%)	0.81	35 (10%) 12 11	69, 102, 140, 187	0
1	B	344/370 (92%)	0.23	4 (1%) 76 71	58, 86, 120, 130	0
1	C	341/370 (92%)	0.18	4 (1%) 76 71	48, 79, 113, 132	0
1	D	335/370 (90%)	0.69	22 (6%) 24 21	65, 115, 140, 192	0
1	E	316/370 (85%)	0.84	25 (7%) 18 16	79, 118, 147, 159	0
1	F	340/370 (91%)	0.26	4 (1%) 76 71	62, 90, 122, 136	0
1	G	342/370 (92%)	0.16	6 (1%) 67 59	55, 79, 116, 141	0
1	H	348/370 (94%)	-0.01	1 (0%) 90 88	56, 76, 105, 140	0
1	I	342/370 (92%)	0.27	4 (1%) 76 71	58, 87, 115, 134	0
1	J	343/370 (92%)	0.38	7 (2%) 65 57	64, 93, 120, 134	0
All	All	3392/3700 (91%)	0.37	112 (3%) 49 42	48, 92, 133, 192	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	76	ASP	4.2
1	A	288	TYR	4.2
1	A	284	HIS	3.9
1	A	356	ILE	3.8
1	C	248	ASN	3.5
1	A	354	ALA	3.4
1	H	306	THR	3.4
1	A	371	TYR	3.4
1	A	318	ASN	3.3
1	E	100	GLU	3.2
1	I	302	GLY	3.1
1	E	297	ALA	3.1
1	D	337	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	104	TYR	3.1
1	E	359	CYS	3.1
1	E	248	ASN	3.1
1	G	248	ASN	3.0
1	F	300	LEU	3.0
1	A	317	ALA	3.0
1	J	317	ALA	3.0
1	E	256	PHE	3.0
1	A	322	SER	3.0
1	A	348	PRO	2.9
1	E	260	ALA	2.9
1	A	355	LEU	2.9
1	D	302	GLY	2.9
1	D	104	TYR	2.8
1	D	218	LEU	2.8
1	E	363	GLU	2.8
1	A	260	ALA	2.8
1	J	211	GLY	2.8
1	A	359	CYS	2.7
1	E	219	TRP	2.7
1	A	269	TYR	2.7
1	A	341	ARG	2.7
1	D	325	ILE	2.7
1	D	248	ASN	2.7
1	D	360	LEU	2.7
1	A	78	TYR	2.7
1	A	369	PHE	2.6
1	D	83	ALA	2.6
1	I	192	GLY	2.6
1	A	76	ASP	2.6
1	A	282	GLN	2.6
1	A	316	VAL	2.6
1	A	363	GLU	2.6
1	A	131	PHE	2.6
1	D	309	ILE	2.6
1	A	197	VAL	2.6
1	A	193	THR	2.5
1	G	342	PRO	2.5
1	A	248	ASN	2.5
1	E	115	HIS	2.5
1	D	261	MET	2.5
1	D	68	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	367	GLU	2.4
1	C	78	TYR	2.4
1	F	248	ASN	2.4
1	D	359	CYS	2.4
1	D	368	PRO	2.4
1	I	216	ASP	2.4
1	D	256	PHE	2.4
1	C	301	THR	2.4
1	A	210	GLU	2.4
1	E	367	GLU	2.4
1	A	209	CYS	2.3
1	A	219	TRP	2.3
1	E	130	TRP	2.3
1	D	79	LEU	2.3
1	E	128	HIS	2.3
1	D	270	ILE	2.3
1	J	309	ILE	2.3
1	A	360	LEU	2.3
1	E	356	ILE	2.3
1	I	315	GLY	2.2
1	E	295	ASP	2.2
1	A	313	SER	2.2
1	J	75	SER	2.2
1	A	211	GLY	2.2
1	D	113	LEU	2.2
1	F	366	ASP	2.2
1	D	80	VAL	2.2
1	E	197	VAL	2.2
1	F	351	VAL	2.2
1	D	152	ASN	2.2
1	A	283	TYR	2.2
1	B	359	CYS	2.2
1	G	316	VAL	2.1
1	J	73	SER	2.1
1	E	134	GLU	2.1
1	A	358	THR	2.1
1	E	358	THR	2.1
1	E	288	TYR	2.1
1	E	76	ASP	2.1
1	J	294	LEU	2.1
1	B	337	PHE	2.1
1	E	352	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	78	TYR	2.1
1	E	124	VAL	2.1
1	E	137	TYR	2.1
1	D	208	PRO	2.0
1	C	152	ASN	2.0
1	A	314	ALA	2.0
1	B	170	ALA	2.0
1	G	247	TRP	2.0
1	A	278	SER	2.0
1	D	101	VAL	2.0
1	E	97	VAL	2.0
1	G	343	SER	2.0
1	E	277	LEU	2.0
1	E	114	ARG	2.0
1	D	276	LYS	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 oligosaccharides 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.