



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:03 PM GMT

PDB ID : 4WJ3
Title : Crystal structure of the asparagine transamidosome from *Pseudomonas aeruginosa*
Authors : Suzuki, T.; Nakamura, A.; Kato, K.; Tanaka, I.; Yao, M.
Deposited on : 2014-09-29
Resolution : 3.71 Å(reported)

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

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

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

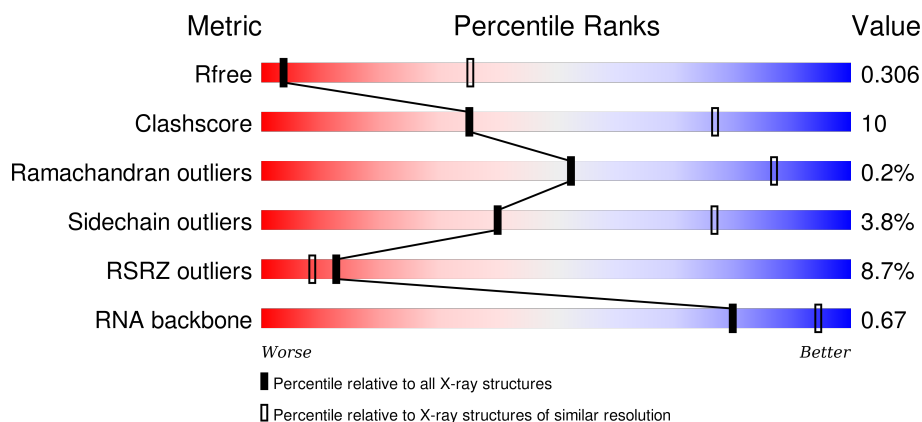
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	484	<div> <div>3%</div> <div>77%</div> <div>23%</div> </div>
1	D	484	<div> <div>2%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	G	484	<div> <div>28%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
1	J	484	<div> <div>36%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	481	
2	E	481	
2	H	481	
2	K	481	
3	C	104	
3	F	104	
3	I	104	
3	L	104	
4	M	599	
4	N	599	
4	O	599	
4	P	599	
5	Q	76	
5	R	76	
5	S	76	
5	T	76	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 56045 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	D	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	G	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	J	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	456	Total	C	N	O	S	0	0	0
			3372	2103	595	657	17			
2	E	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			
2	H	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			
2	K	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	F	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	I	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	L	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	expression tag	UNP Q9HVT9
C	-6	GLY	-	expression tag	UNP Q9HVT9
C	-5	HIS	-	expression tag	UNP Q9HVT9
C	-4	HIS	-	expression tag	UNP Q9HVT9
C	-3	HIS	-	expression tag	UNP Q9HVT9
C	-2	HIS	-	expression tag	UNP Q9HVT9
C	-1	HIS	-	expression tag	UNP Q9HVT9
C	0	HIS	-	expression tag	UNP Q9HVT9
F	-7	MET	-	expression tag	UNP Q9HVT9
F	-6	GLY	-	expression tag	UNP Q9HVT9
F	-5	HIS	-	expression tag	UNP Q9HVT9
F	-4	HIS	-	expression tag	UNP Q9HVT9
F	-3	HIS	-	expression tag	UNP Q9HVT9
F	-2	HIS	-	expression tag	UNP Q9HVT9
F	-1	HIS	-	expression tag	UNP Q9HVT9
F	0	HIS	-	expression tag	UNP Q9HVT9
I	-7	MET	-	expression tag	UNP Q9HVT9
I	-6	GLY	-	expression tag	UNP Q9HVT9
I	-5	HIS	-	expression tag	UNP Q9HVT9
I	-4	HIS	-	expression tag	UNP Q9HVT9
I	-3	HIS	-	expression tag	UNP Q9HVT9
I	-2	HIS	-	expression tag	UNP Q9HVT9
I	-1	HIS	-	expression tag	UNP Q9HVT9
I	0	HIS	-	expression tag	UNP Q9HVT9
L	-7	MET	-	expression tag	UNP Q9HVT9
L	-6	GLY	-	expression tag	UNP Q9HVT9
L	-5	HIS	-	expression tag	UNP Q9HVT9
L	-4	HIS	-	expression tag	UNP Q9HVT9
L	-3	HIS	-	expression tag	UNP Q9HVT9
L	-2	HIS	-	expression tag	UNP Q9HVT9
L	-1	HIS	-	expression tag	UNP Q9HVT9
L	0	HIS	-	expression tag	UNP Q9HVT9

- Molecule 4 is a protein called Aspartate--tRNA(Asp/Asn) ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			
4	N	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			
4	O	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	MET	-	expression tag	UNP Q51422
M	-6	GLY	-	expression tag	UNP Q51422
M	-5	HIS	-	expression tag	UNP Q51422
M	-4	HIS	-	expression tag	UNP Q51422
M	-3	HIS	-	expression tag	UNP Q51422
M	-2	HIS	-	expression tag	UNP Q51422
M	-1	HIS	-	expression tag	UNP Q51422
M	0	HIS	-	expression tag	UNP Q51422
N	-7	MET	-	expression tag	UNP Q51422
N	-6	GLY	-	expression tag	UNP Q51422
N	-5	HIS	-	expression tag	UNP Q51422
N	-4	HIS	-	expression tag	UNP Q51422
N	-3	HIS	-	expression tag	UNP Q51422
N	-2	HIS	-	expression tag	UNP Q51422
N	-1	HIS	-	expression tag	UNP Q51422
N	0	HIS	-	expression tag	UNP Q51422
O	-7	MET	-	expression tag	UNP Q51422
O	-6	GLY	-	expression tag	UNP Q51422
O	-5	HIS	-	expression tag	UNP Q51422
O	-4	HIS	-	expression tag	UNP Q51422
O	-3	HIS	-	expression tag	UNP Q51422
O	-2	HIS	-	expression tag	UNP Q51422
O	-1	HIS	-	expression tag	UNP Q51422
O	0	HIS	-	expression tag	UNP Q51422
P	-7	MET	-	expression tag	UNP Q51422
P	-6	GLY	-	expression tag	UNP Q51422
P	-5	HIS	-	expression tag	UNP Q51422
P	-4	HIS	-	expression tag	UNP Q51422
P	-3	HIS	-	expression tag	UNP Q51422
P	-2	HIS	-	expression tag	UNP Q51422
P	-1	HIS	-	expression tag	UNP Q51422
P	0	HIS	-	expression tag	UNP Q51422

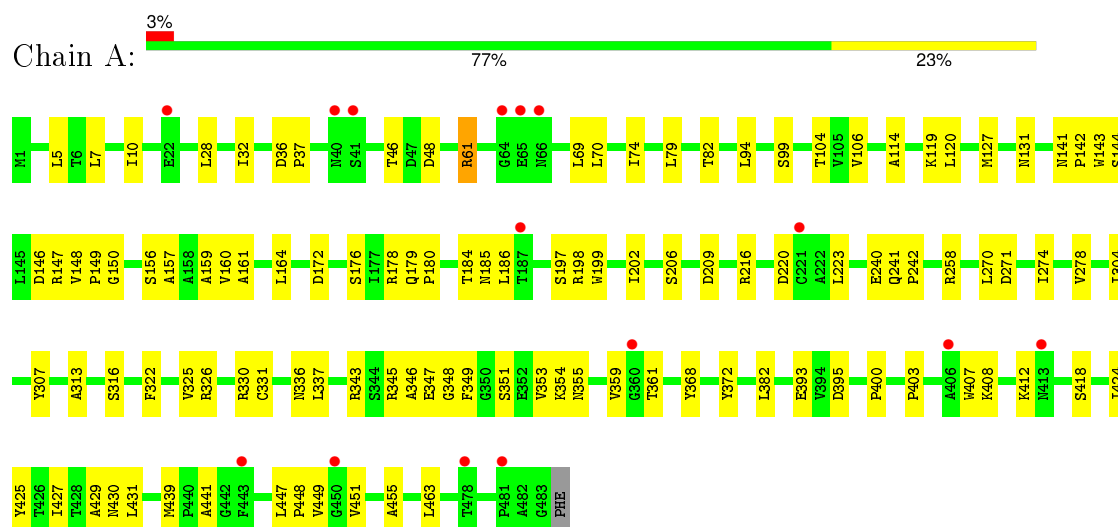
- Molecule 5 is a RNA chain called 76mer-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	76	Total 1622	C 723	N 288	O 535	P 76	0	0	0
5	R	76	Total 1622	C 723	N 288	O 535	P 76	0	0	0
5	S	76	Total 1622	C 723	N 288	O 535	P 76	0	0	0
5	T	76	Total 1622	C 723	N 288	O 535	P 76	0	0	0

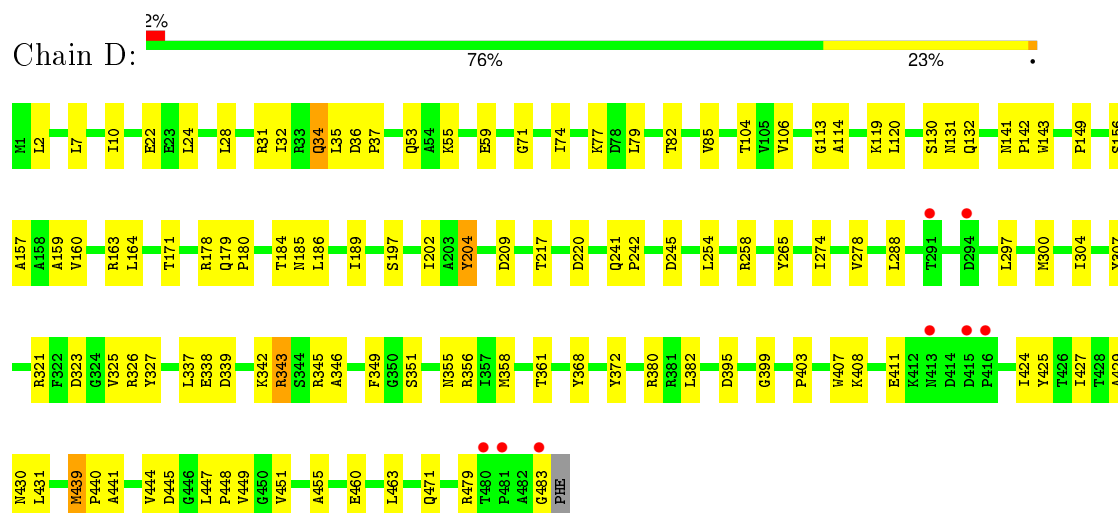
3 Residue-property plots

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

- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

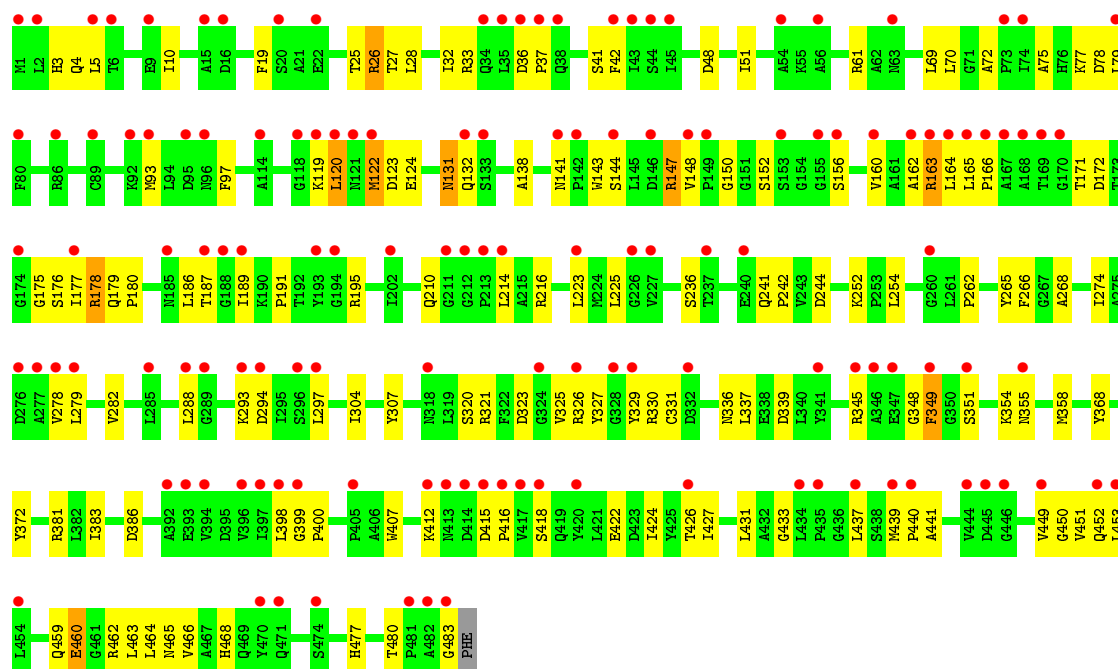


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

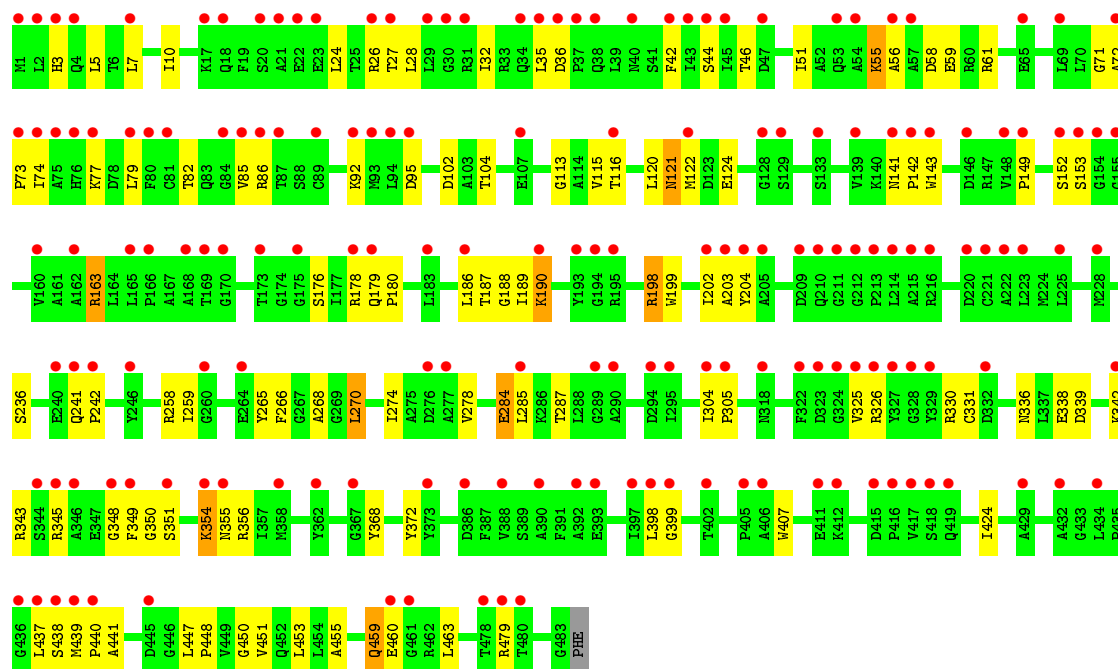
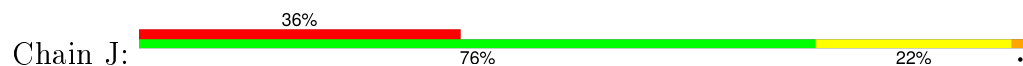


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

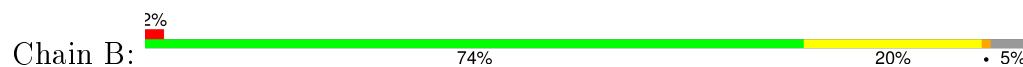


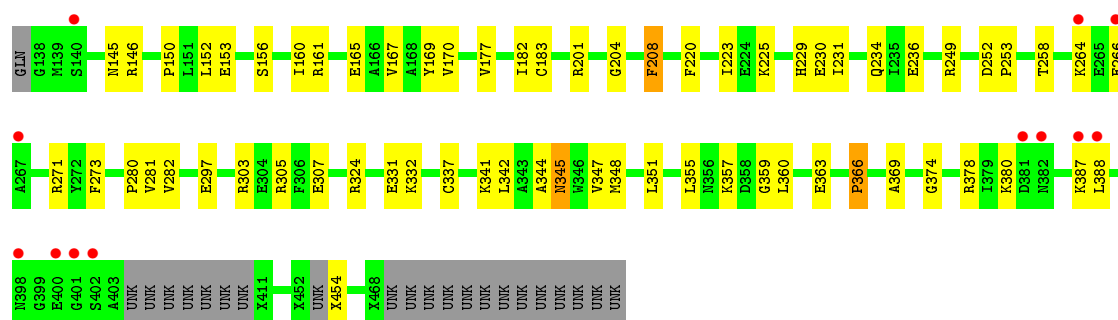


• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

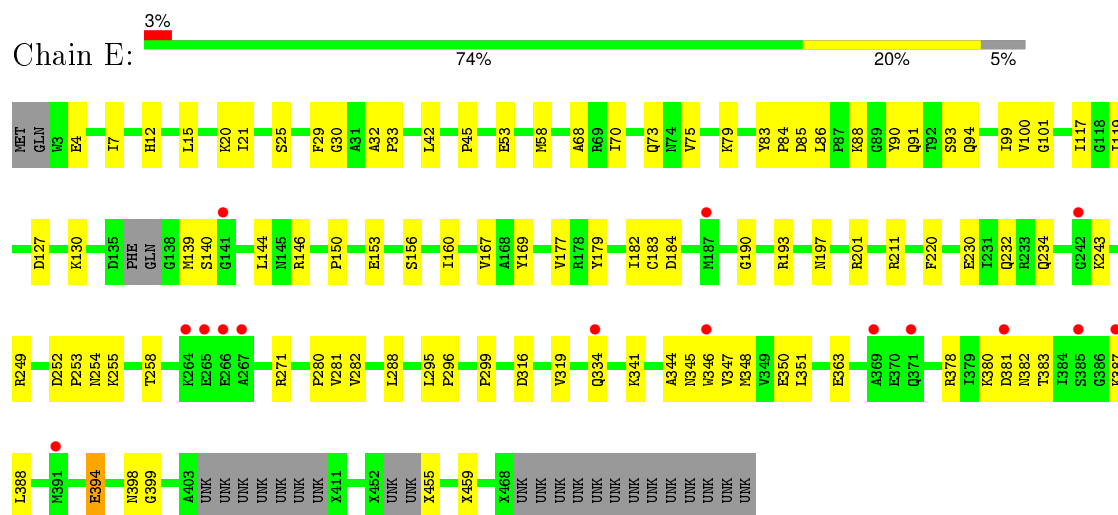


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

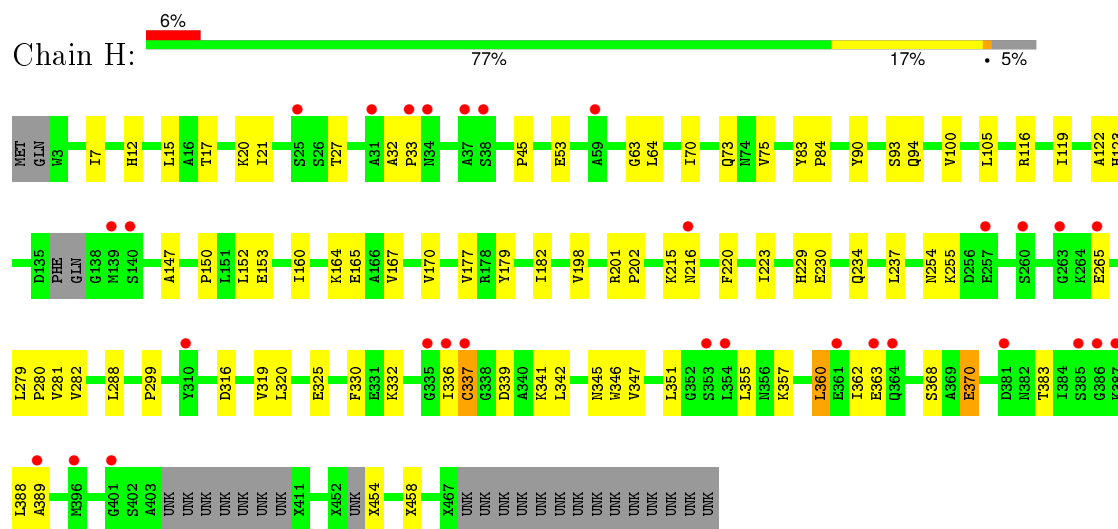




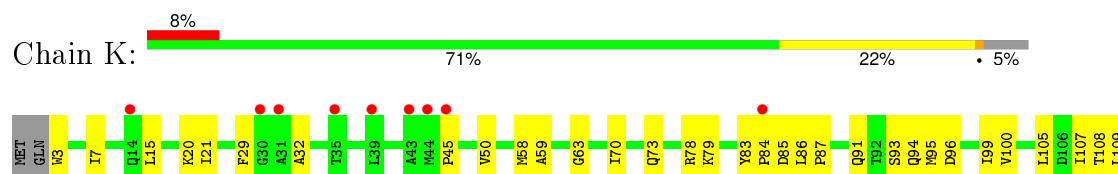
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

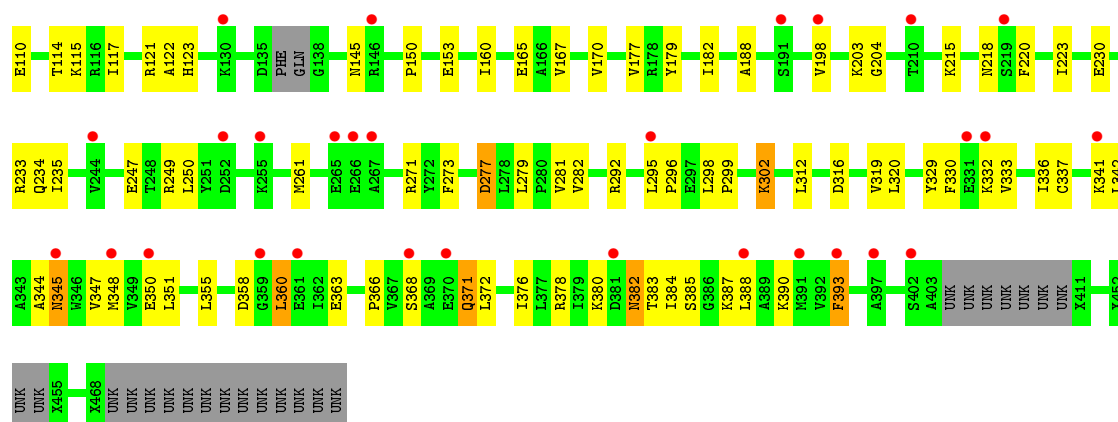


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

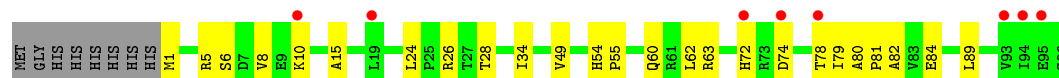


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



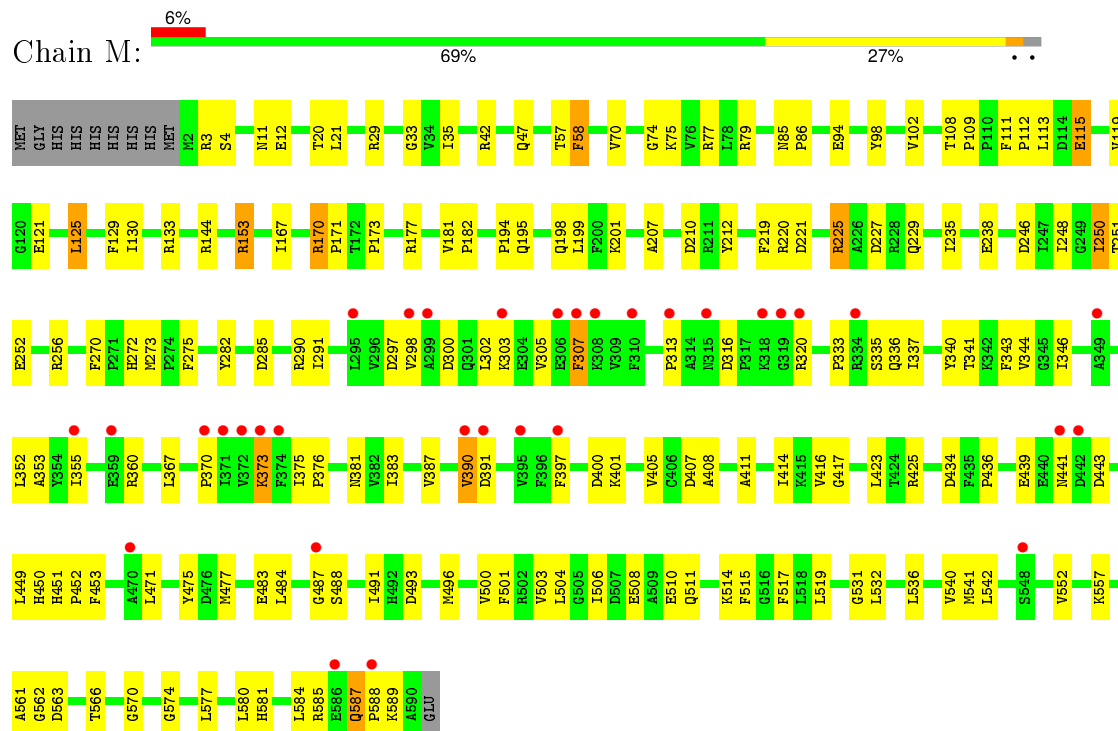
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



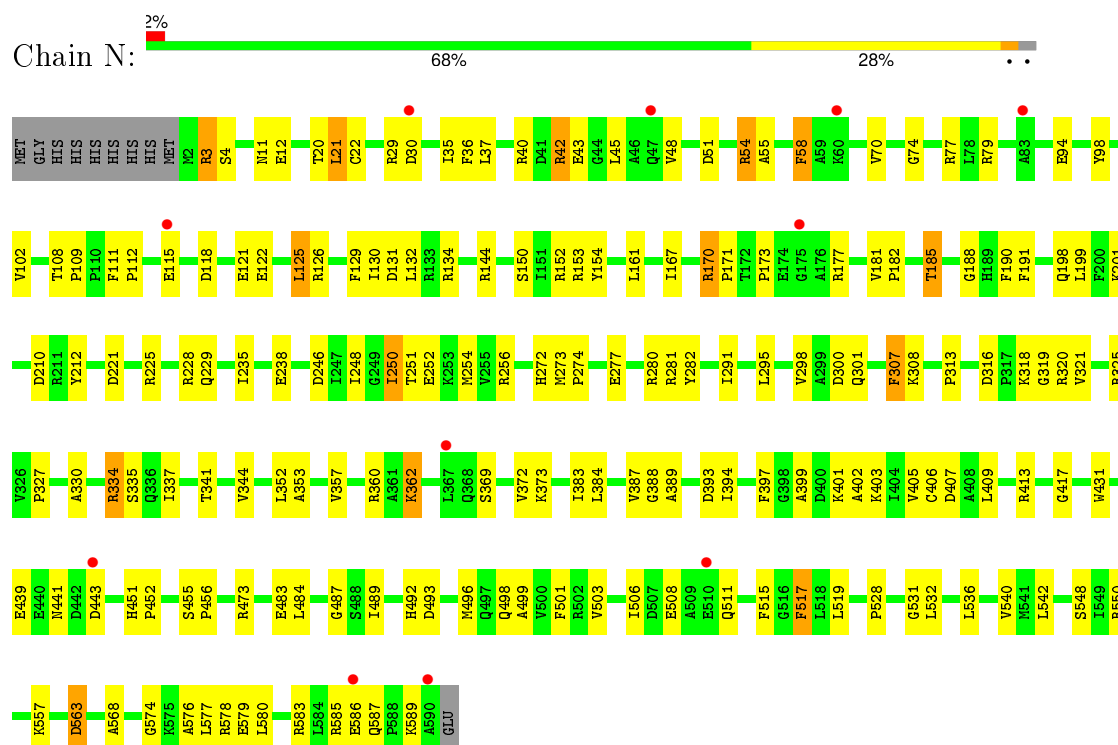
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

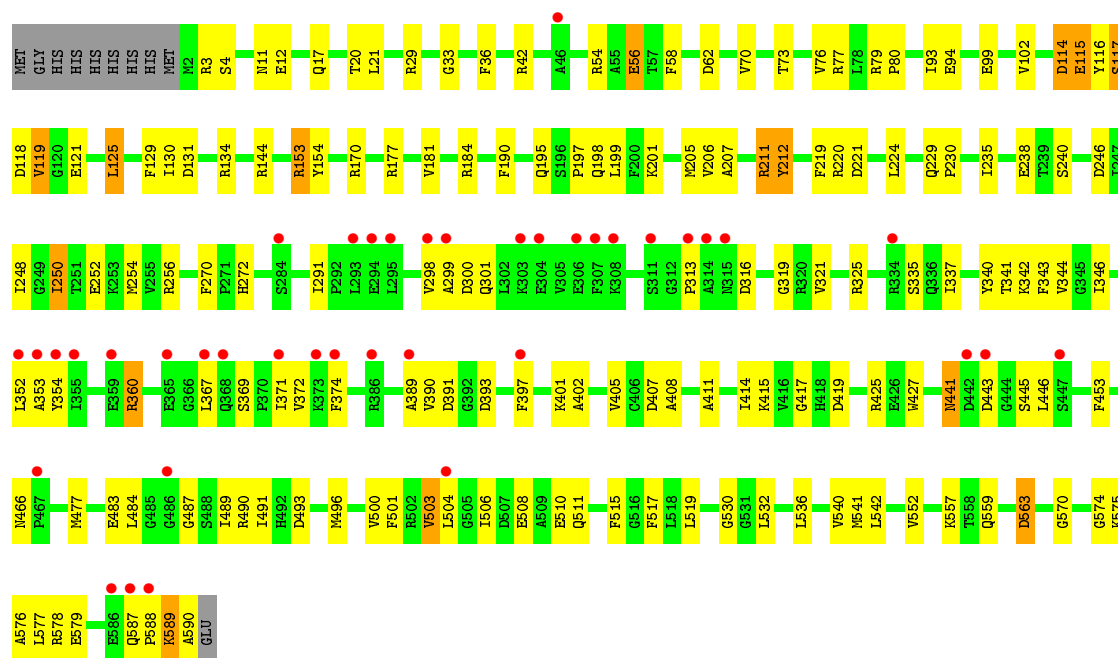


• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

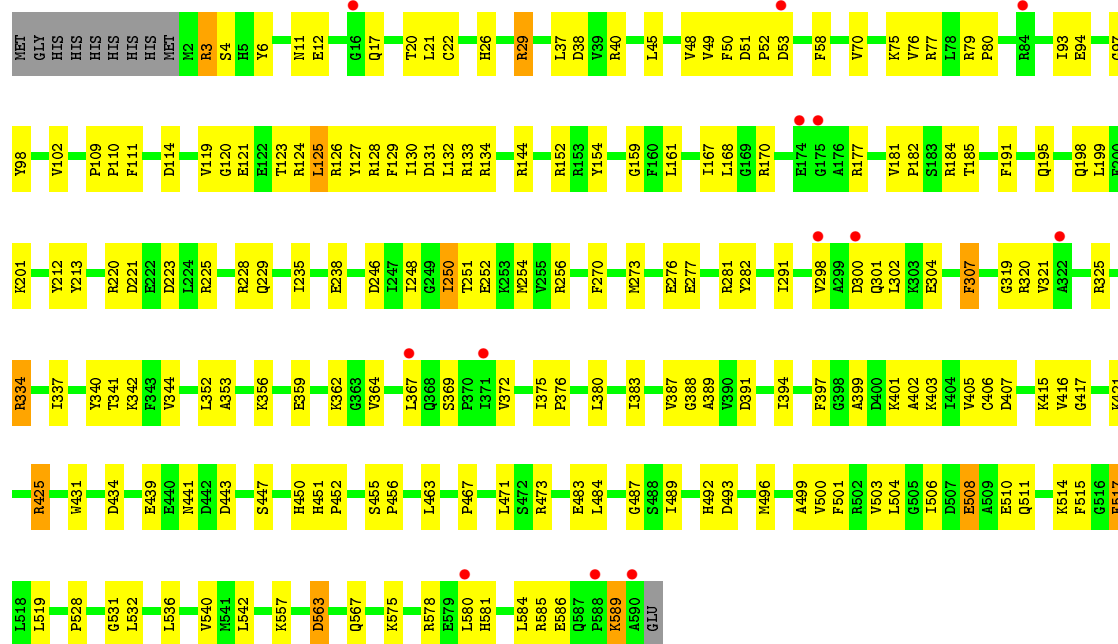


• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase





• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

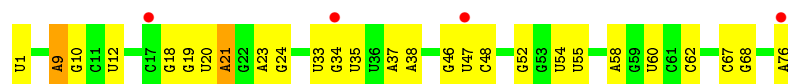


• Molecule 5: 76mer-tRNA



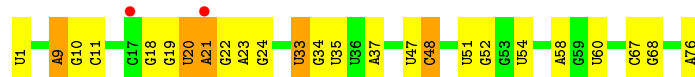
● Molecule 5: 76mer-tRNA

Chain R:  5% 64% 33%



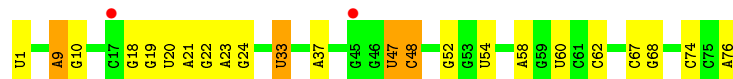
● Molecule 5: 76mer-tRNA

Chain S:  3% 67% 26% 7%



● Molecule 5: 76mer-tRNA

Chain T:  3% 70% 25% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.14Å 185.68Å 290.36Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	46.77 – 3.71 48.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.1 (46.77-3.71) 79.8 (48.12-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.292 , 0.329 0.287 , 0.306	Depositor DCC
R_{free} test set	4824 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.1	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 96489 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	56045	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4505e-03.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.21	0/3711	0.40	0/5044
1	D	0.21	0/3711	0.41	0/5044
1	G	0.22	0/3711	0.45	1/5044 (0.0%)
1	J	0.21	0/3711	0.44	0/5044
2	B	0.21	0/3137	0.42	0/4233
2	E	0.21	0/3137	0.42	0/4233
2	H	0.21	0/3137	0.42	0/4233
2	K	0.21	0/3137	0.42	0/4233
3	C	0.21	0/748	0.44	0/1020
3	F	0.21	0/748	0.45	0/1020
3	I	0.20	0/748	0.46	0/1020
3	L	0.20	0/748	0.45	0/1020
4	M	0.25	0/4743	0.55	1/6410 (0.0%)
4	N	0.25	0/4743	0.54	1/6410 (0.0%)
4	O	0.25	0/4743	0.54	1/6410 (0.0%)
4	P	0.25	0/4743	0.54	1/6410 (0.0%)
5	Q	0.28	1/1812 (0.1%)	0.69	1/2821 (0.0%)
5	R	0.28	1/1812 (0.1%)	0.67	0/2821
5	S	0.29	1/1812 (0.1%)	0.69	0/2821
5	T	0.28	1/1812 (0.1%)	0.68	0/2821
All	All	0.24	4/56604 (0.0%)	0.51	6/78112 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	O	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1	U	OP3-P	-10.66	1.48	1.61
5	Q	1	U	OP3-P	-10.60	1.48	1.61
5	R	1	U	OP3-P	-10.58	1.48	1.61
5	T	1	U	OP3-P	-10.53	1.48	1.61

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	250	ILE	CG1-CB-CG2	-6.66	96.76	111.40
4	M	250	ILE	CG1-CB-CG2	-6.63	96.82	111.40
5	Q	47	U	P-O3'-C3'	6.58	127.59	119.70
4	N	250	ILE	CG1-CB-CG2	-6.47	97.16	111.40
4	P	250	ILE	CG1-CB-CG2	-6.41	97.29	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	O	114	ASP	Peptide
4	O	117	SER	Peptide

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	3639	0	3612	67	0
1	D	3639	0	3612	75	0
1	G	3639	0	3612	98	1
1	J	3639	0	3612	73	1
2	B	3372	0	3129	55	0
2	E	3367	0	3128	61	0
2	H	3367	0	3129	54	0
2	K	3367	0	3128	72	0
3	C	738	0	741	17	0
3	F	738	0	741	24	0
3	I	738	0	741	17	0
3	L	738	0	741	19	0
4	M	4644	0	4618	115	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	4644	0	4618	131	0
4	O	4644	0	4618	111	1
4	P	4644	0	4618	126	0
5	Q	1622	0	819	12	0
5	R	1622	0	819	14	0
5	S	1622	0	819	14	0
5	T	1622	0	819	10	0
All	All	56045	0	51674	1052	2

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 10.

The worst 5 of 1052 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)
4:M:585:ARG:HH12	4:M:589:LYS:HB2	1.41	0.84
4:P:79:ARG:NH2	4:P:93:ILE:O	2.13	0.80
4:M:584:LEU:HD13	4:N:188:GLY:HA2	1.62	0.80
1:D:141:ASN:HD22	1:D:149:PRO:HA	1.50	0.77
1:G:178:ARG:NH1	1:G:426:THR:OG1	2.17	0.77

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:ALA:O	4:O:335:SER:OG[1_455]	2.12	0.08
1:J:268:ALA:O	4:M:335:SER:OG[1_455]	2.14	0.06

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	481/484 (99%)	446 (93%)	35 (7%)	0	100	100
1	D	481/484 (99%)	446 (93%)	35 (7%)	0	100	100
1	G	481/484 (99%)	447 (93%)	34 (7%)	0	100	100
1	J	481/484 (99%)	445 (92%)	36 (8%)	0	100	100
2	B	395/481 (82%)	358 (91%)	35 (9%)	2 (0%)	34	77
2	E	395/481 (82%)	362 (92%)	33 (8%)	0	100	100
2	H	395/481 (82%)	360 (91%)	34 (9%)	1 (0%)	46	83
2	K	395/481 (82%)	357 (90%)	37 (9%)	1 (0%)	46	83
3	C	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
3	F	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
3	I	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
3	L	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
4	M	587/599 (98%)	542 (92%)	43 (7%)	2 (0%)	46	83
4	N	587/599 (98%)	541 (92%)	44 (8%)	2 (0%)	46	83
4	O	587/599 (98%)	543 (92%)	43 (7%)	1 (0%)	52	87
4	P	587/599 (98%)	542 (92%)	43 (7%)	2 (0%)	46	83
All	All	6228/6672 (93%)	5752 (92%)	465 (8%)	11 (0%)	52	87

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	CYS
2	K	337	CYS
2	H	337	CYS
4	P	298	VAL
4	P	450	HIS

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	377/378 (100%)	367 (97%)	10 (3%)	52	83
1	D	377/378 (100%)	364 (97%)	13 (3%)	44	79
1	G	377/378 (100%)	361 (96%)	16 (4%)	36	75
1	J	377/378 (100%)	359 (95%)	18 (5%)	31	72
2	B	329/333 (99%)	319 (97%)	10 (3%)	48	81
2	E	329/333 (99%)	325 (99%)	4 (1%)	78	91
2	H	329/333 (99%)	324 (98%)	5 (2%)	72	90
2	K	329/333 (99%)	313 (95%)	16 (5%)	31	71
3	C	81/88 (92%)	79 (98%)	2 (2%)	55	84
3	F	81/88 (92%)	80 (99%)	1 (1%)	78	91
3	I	81/88 (92%)	75 (93%)	6 (7%)	17	58
3	L	81/88 (92%)	77 (95%)	4 (5%)	31	71
4	M	493/502 (98%)	472 (96%)	21 (4%)	35	74
4	N	493/502 (98%)	471 (96%)	22 (4%)	34	74
4	O	493/502 (98%)	468 (95%)	25 (5%)	29	70
4	P	493/502 (98%)	469 (95%)	24 (5%)	31	71
All	All	5120/5204 (98%)	4923 (96%)	197 (4%)	40	77

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	218	ASN
4	M	153	ARG
4	P	223	ASP
2	K	292	ARG
2	K	393	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	185	ASN
4	M	511	GLN
4	M	47	GLN
2	H	345	ASN
4	M	451	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	Q	75/76 (98%)	10 (13%)	1 (1%)
5	R	75/76 (98%)	10 (13%)	1 (1%)
5	S	75/76 (98%)	11 (14%)	0
5	T	75/76 (98%)	11 (14%)	1 (1%)
All	All	300/304 (98%)	42 (14%)	3 (1%)

5 of 42 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	Q	9	A
5	Q	18	G
5	Q	19	G
5	Q	20	U
5	Q	21	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	Q	47	U
5	R	47	U
5	T	47	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	483/484 (99%)	0.22	15 (3%) 52 37	45, 68, 100, 138	0
1	D	483/484 (99%)	0.09	8 (1%) 73 58	25, 51, 82, 110	0
1	G	483/484 (99%)	1.38	136 (28%) 1 1	85, 159, 207, 235	0
1	J	483/484 (99%)	1.69	173 (35%) 0 1	98, 173, 227, 253	0
2	B	399/481 (82%)	0.17	12 (3%) 54 37	37, 68, 135, 151	0
2	E	399/481 (82%)	0.19	15 (3%) 44 30	33, 69, 140, 156	0
2	H	399/481 (82%)	0.46	30 (7%) 17 11	58, 95, 164, 185	0
2	K	399/481 (82%)	0.64	38 (9%) 10 6	57, 115, 170, 202	0
3	C	96/104 (92%)	0.46	8 (8%) 14 9	49, 91, 131, 172	0
3	F	96/104 (92%)	0.05	3 (3%) 52 37	34, 73, 113, 152	0
3	I	96/104 (92%)	0.71	12 (12%) 5 5	84, 128, 163, 174	0
3	L	96/104 (92%)	0.82	13 (13%) 4 4	103, 137, 165, 169	0
4	M	589/599 (98%)	0.34	33 (5%) 28 18	39, 76, 173, 209	0
4	N	589/599 (98%)	0.10	11 (1%) 70 55	36, 69, 118, 140	0
4	O	589/599 (98%)	0.38	40 (6%) 20 12	39, 80, 196, 249	0
4	P	589/599 (98%)	0.10	13 (2%) 65 50	30, 69, 120, 159	0
5	Q	76/76 (100%)	0.45	3 (3%) 43 29	76, 126, 163, 182	0
5	R	76/76 (100%)	0.49	4 (5%) 30 20	65, 112, 149, 175	0
5	S	76/76 (100%)	0.23	2 (2%) 59 43	64, 94, 137, 188	0
5	T	76/76 (100%)	0.47	2 (2%) 59 43	84, 123, 160, 187	0
All	All	6572/6976 (94%)	0.47	571 (8%) 13 8	25, 85, 183, 253	0

The worst 5 of 571 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	27	THR	9.2
1	G	36	ASP	8.8
1	J	73	PRO	8.7
2	K	359	GLY	8.7
1	J	419	GLN	7.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.