wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:23 AM GMT

PDB ID	:	3L4G
Title	:	Crystal structure of Homo Sapiens cytoplasmic Phenylalanyl-tRNA synthetase
Authors	:	Finarov, I.; Moor, N.; Kessler, N.; Klipcan, L.; Safro, M.G.
Deposited on	:	2009-12-20
Resolution	:	3.30 Å(reported)

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

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

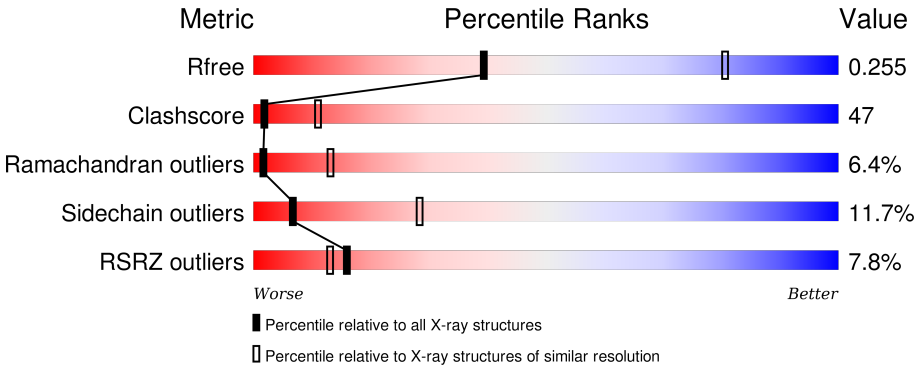
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	3% 22% 33% 7% • 37%
1	C	508	5% 37% 50% 12% •
1	E	508	3% 20% 31% 7% • 39%
1	G	508	3% 21% 31% 7% • 39%
1	I	508	2% 24% 31% 6% • 38%

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Mol	Chain	Length	Quality of chain
1	K	508	2% 29% 31% 7% 31%
1	M	508	6% 22% 31% 9% 37%
1	O	508	3% 22% 30% 8% 39%
2	B	589	3% 36% 53% 10%
2	D	589	12% 37% 53% 10%
2	F	589	6% 37% 53% 10%
2	H	589	11% 36% 52% 11%
2	J	589	2% 38% 51% 10%
2	L	589	13% 38% 52% 10%
2	N	589	13% 36% 52% 12%
2	P	589	15% 37% 51% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PHE	A	509	-	-	X	X
3	PHE	C	509	-	-	-	X
3	PHE	E	509	-	-	-	X
3	PHE	K	509	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 59395 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2589	1661	453	464	11			
1	C	508	Total	C	N	O	S	0	0	0
			4058	2571	724	747	16			
1	E	309	Total	C	N	O	S	0	0	0
			2517	1618	439	449	11			
1	G	309	Total	C	N	O	S	0	0	0
			2521	1620	440	450	11			
1	I	313	Total	C	N	O	S	0	0	0
			2551	1639	445	456	11			
1	K	349	Total	C	N	O	S	0	0	0
			2746	1755	482	498	11			
1	M	321	Total	C	N	O	S	0	0	0
			2582	1652	456	463	11			
1	O	309	Total	C	N	O	S	0	0	0
			2527	1623	443	450	11			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	D	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	F	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	H	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	J	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	L	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			

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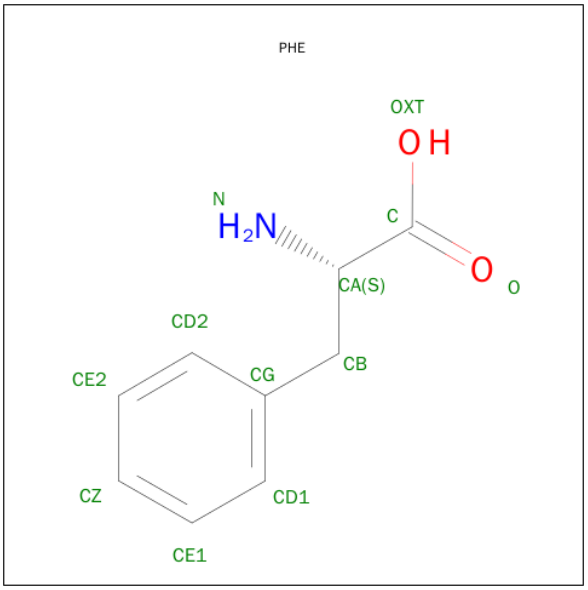
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			
2	P	589	Total	C	N	O	S	0	0	0
			4651	2981	781	866	23			

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



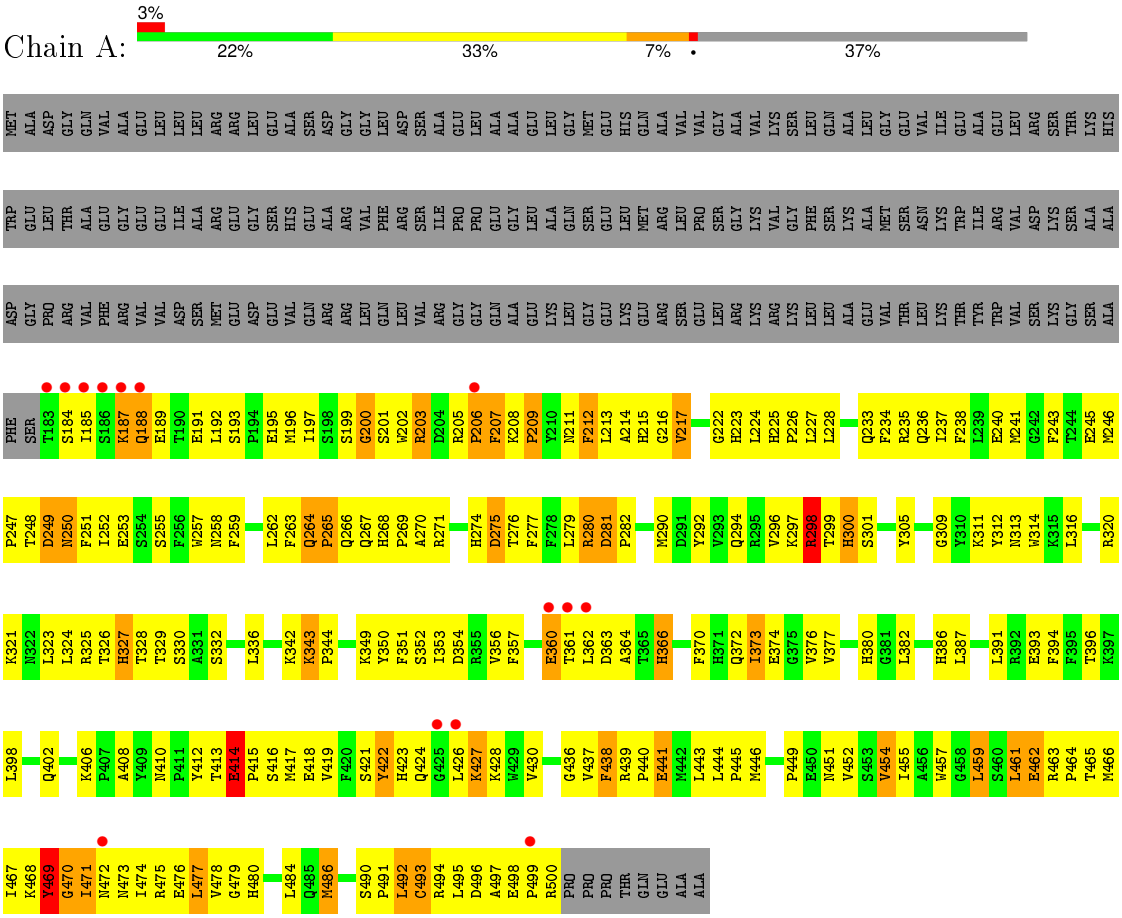
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	E	1	Total	C	N	O	0	0
			12	9	1	2		
3	G	1	Total	C	N	O	0	0
			12	9	1	2		
3	I	1	Total	C	N	O	0	0
			12	9	1	2		
3	K	1	Total	C	N	O	0	0
			12	9	1	2		
3	M	1	Total	C	N	O	0	0
			12	9	1	2		
3	O	1	Total	C	N	O	0	0
			12	9	1	2		

3 Residue-property plots (i)

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

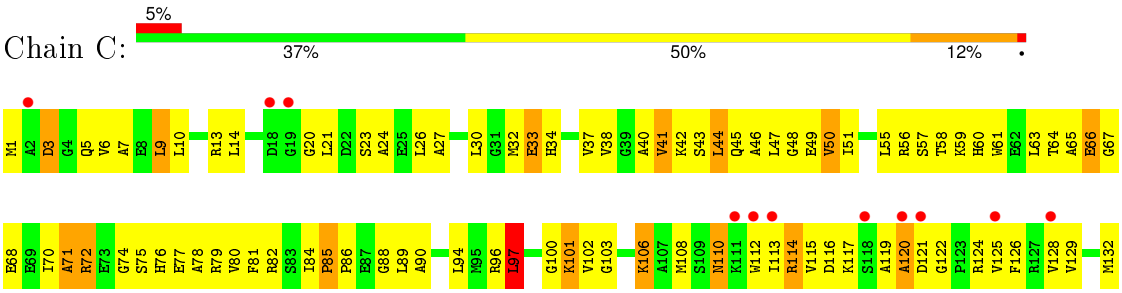
- Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

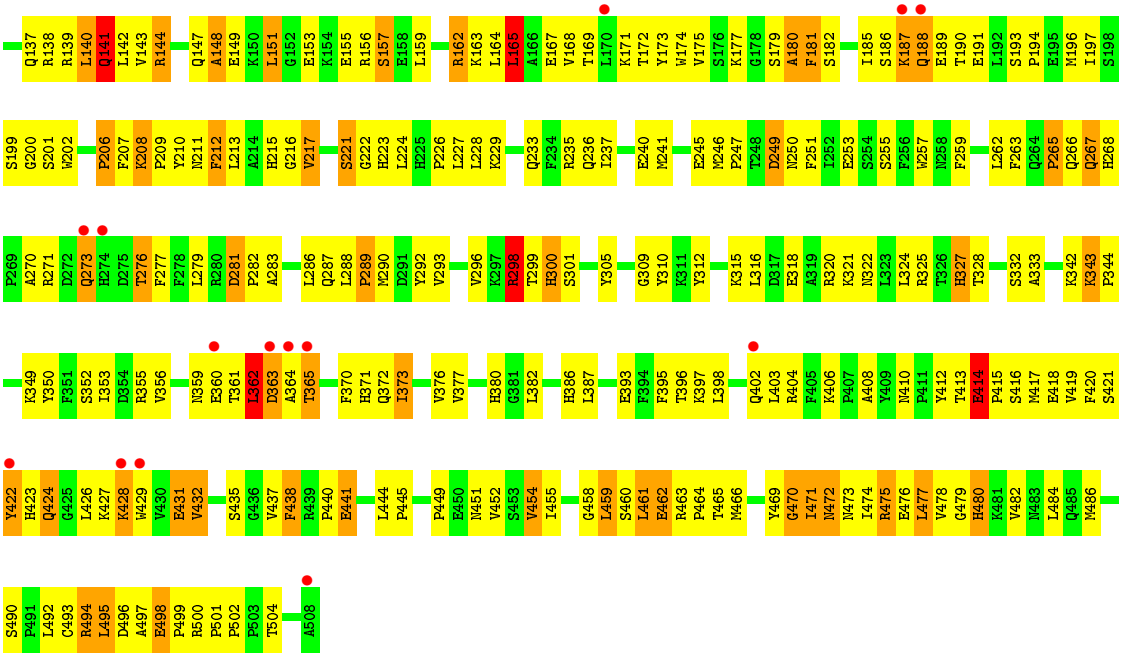
Chain A:



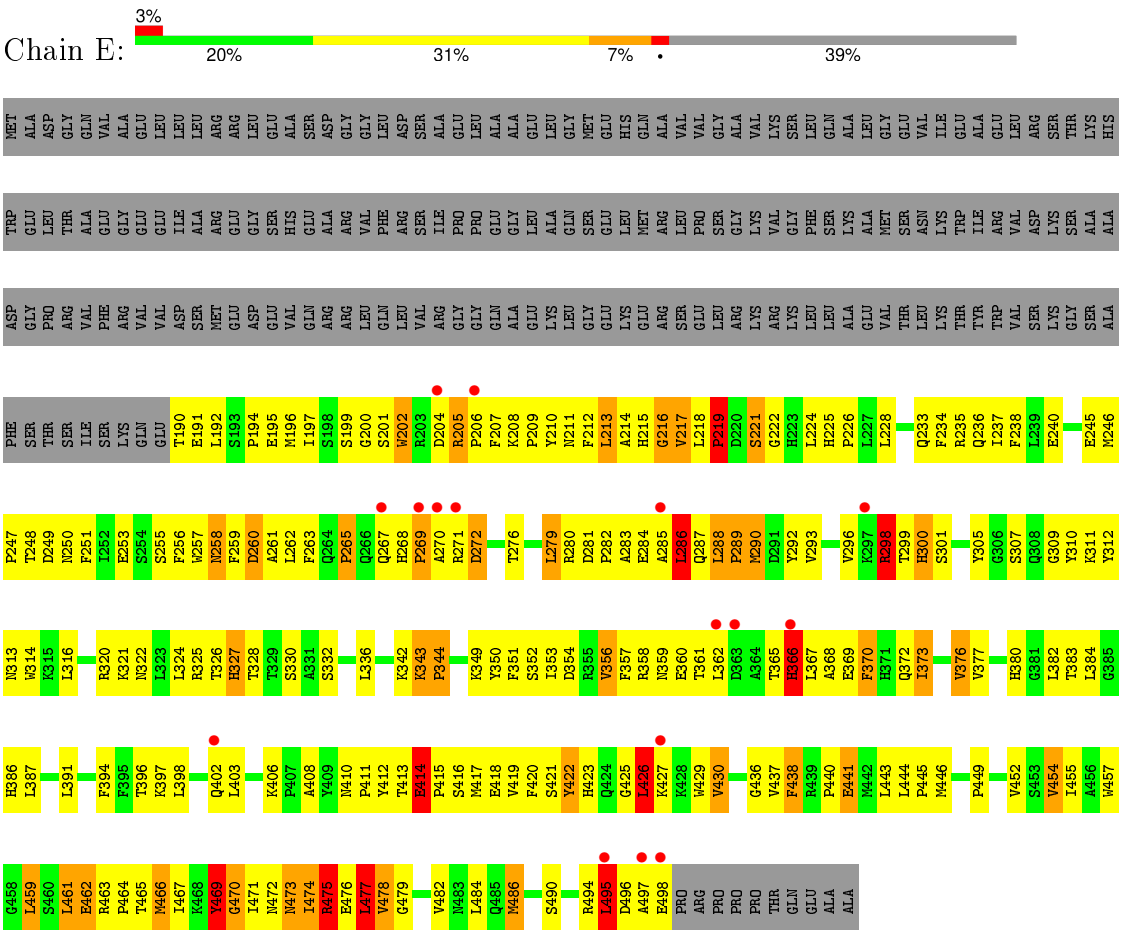
- Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

Chain C:

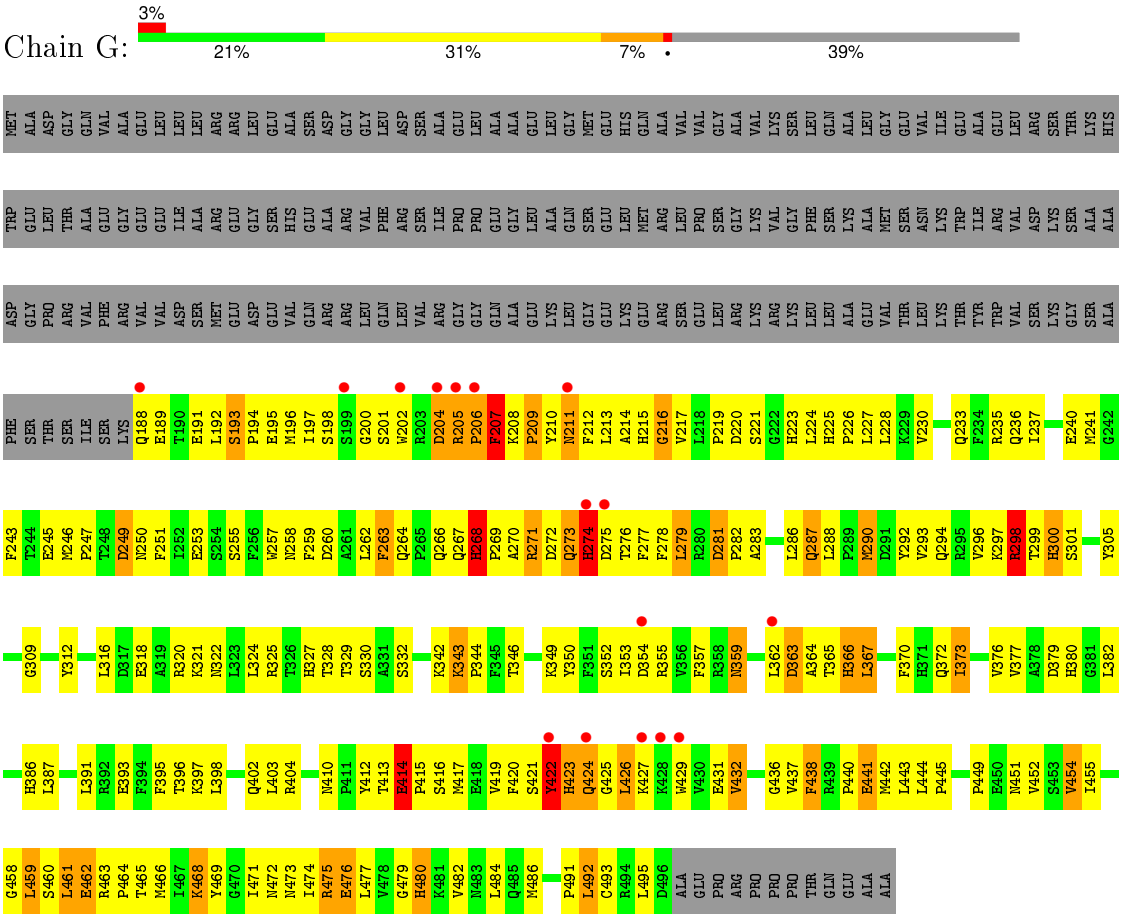




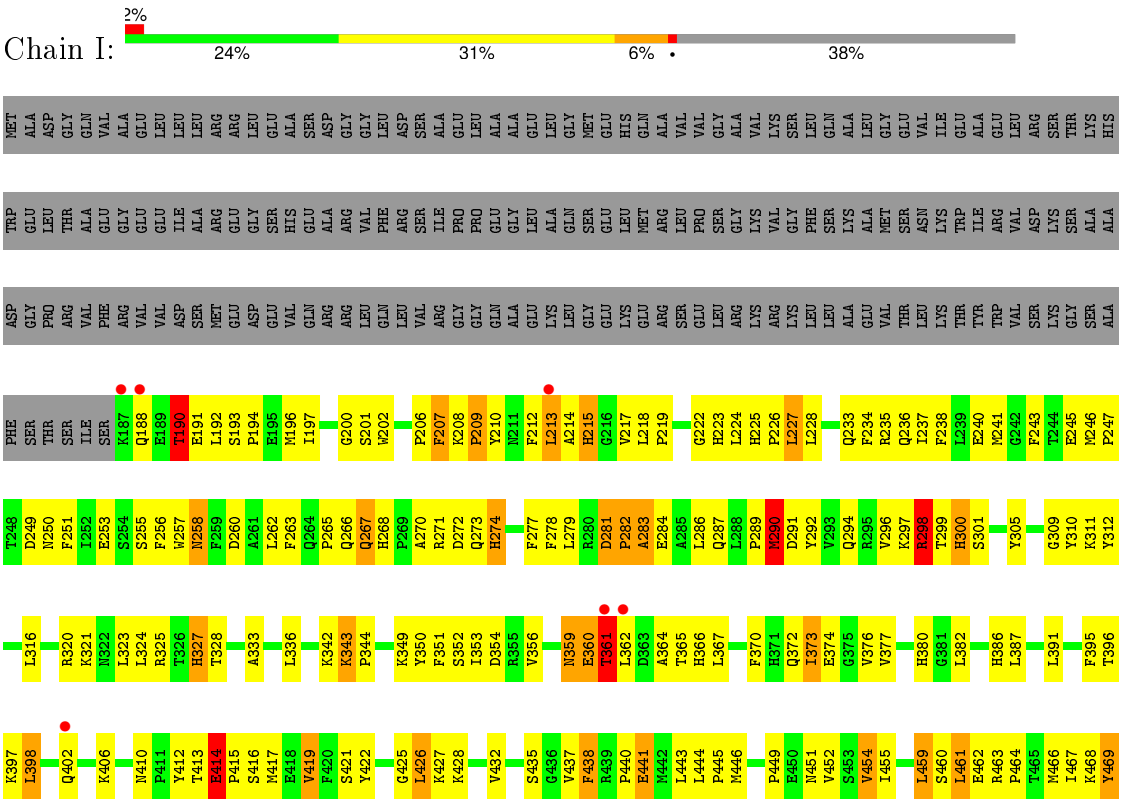
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

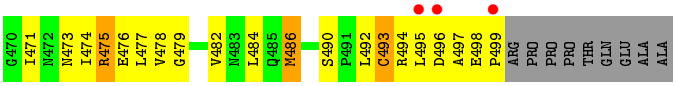


• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain



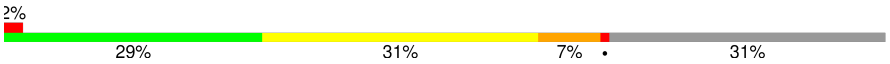
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

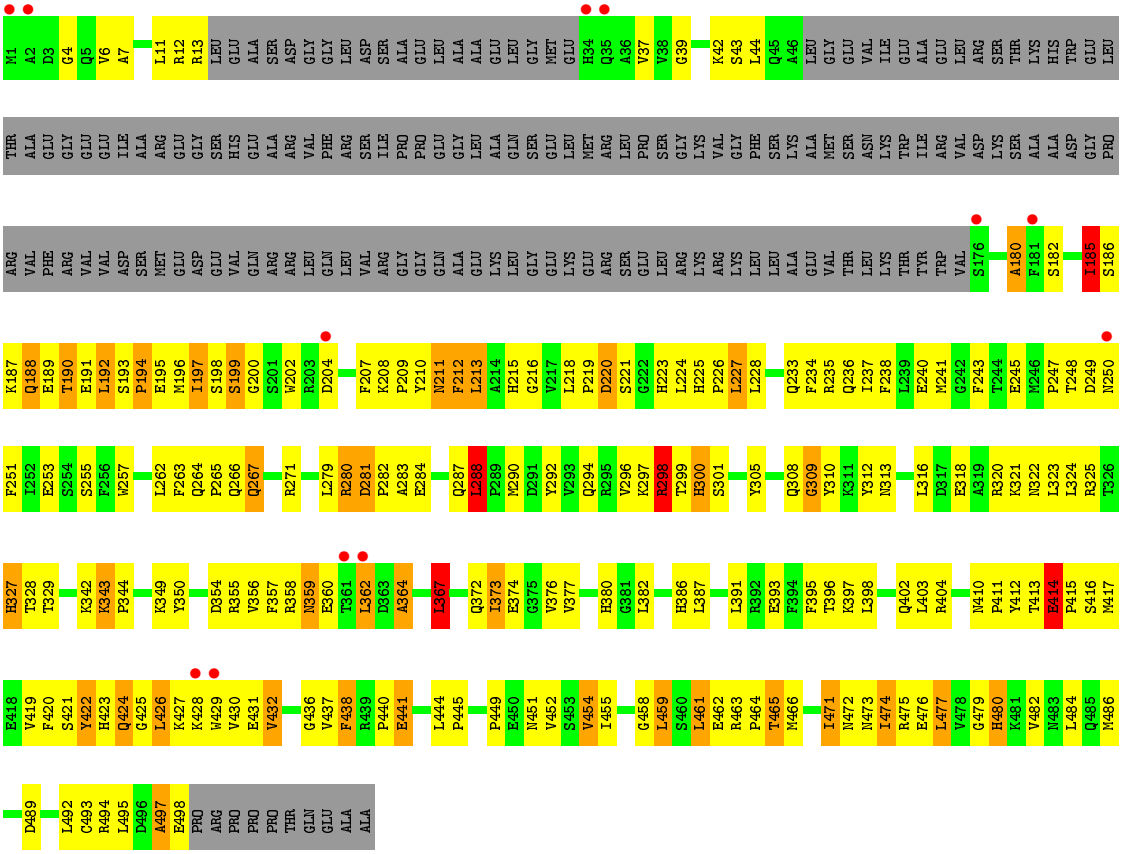




• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

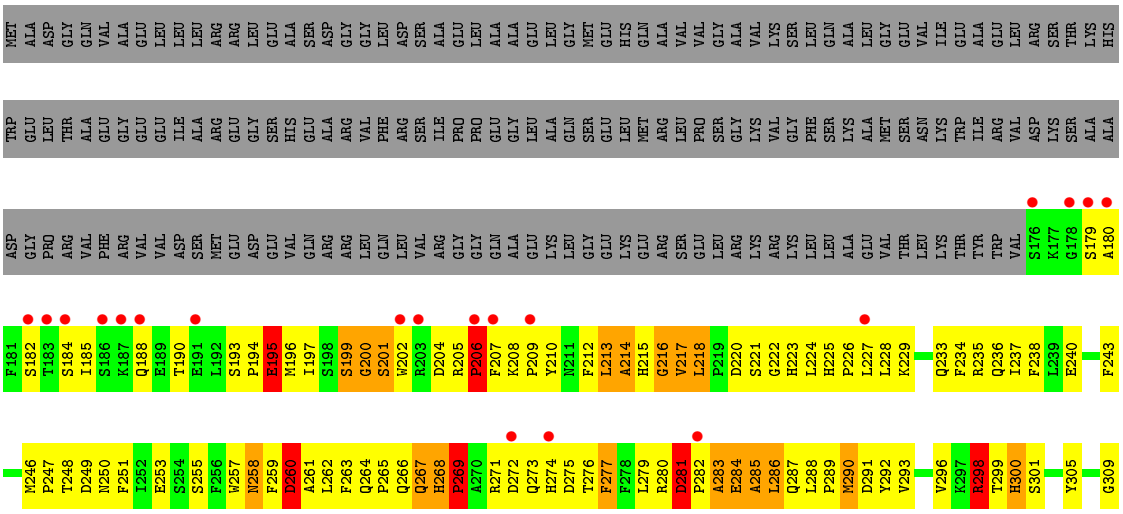
Chain K:

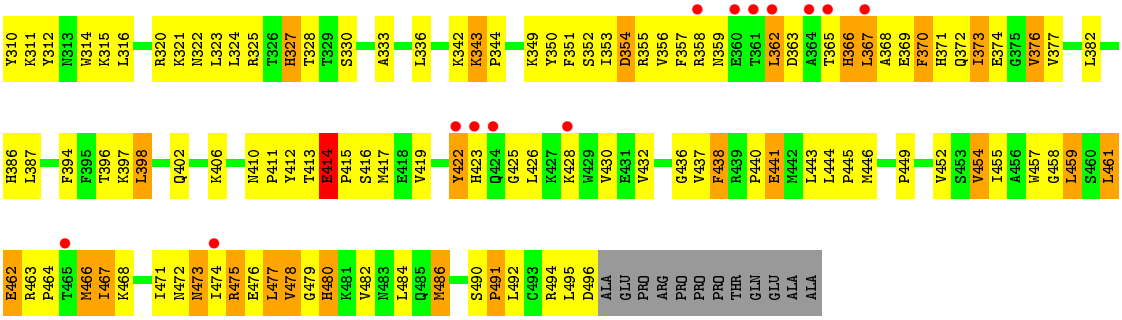




• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

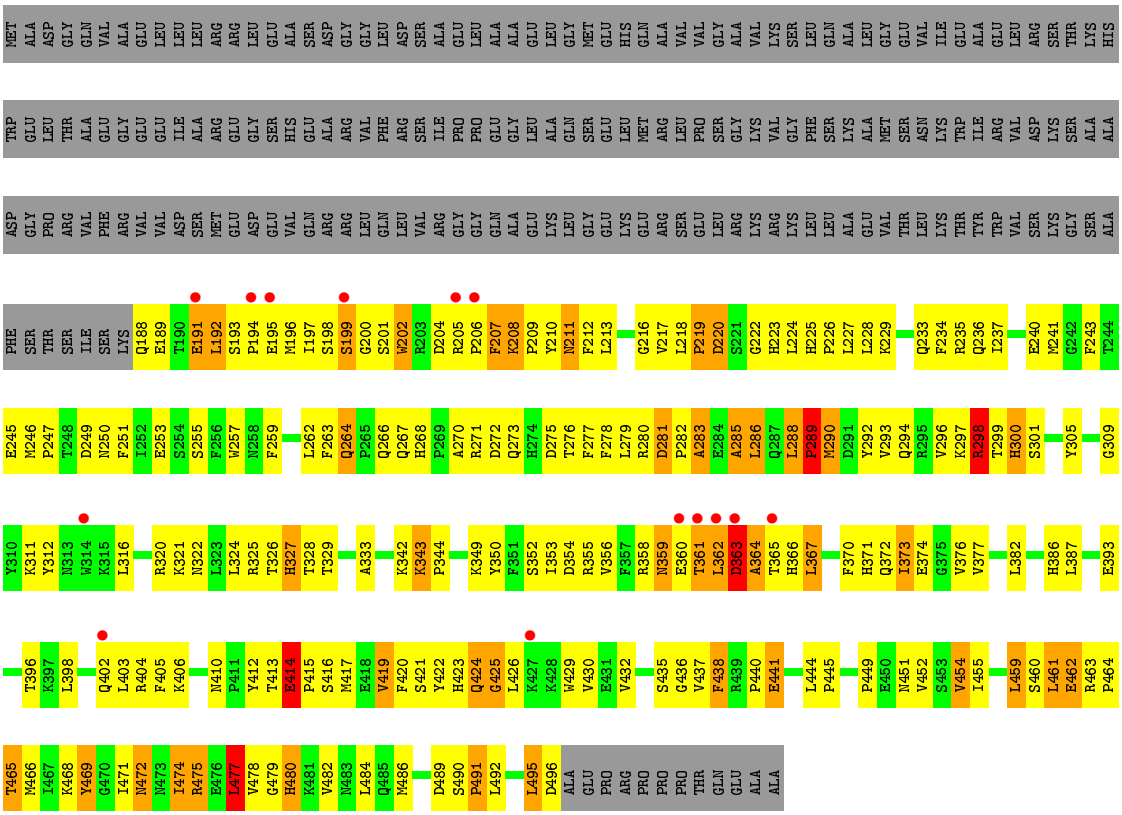
Chain M:





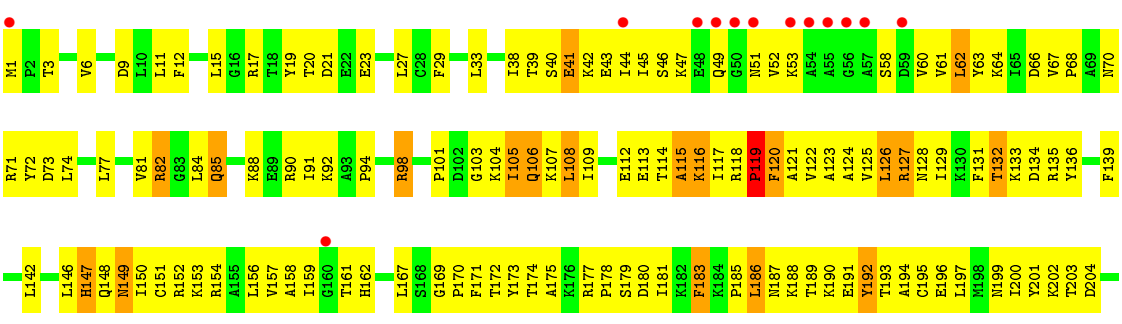
• Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

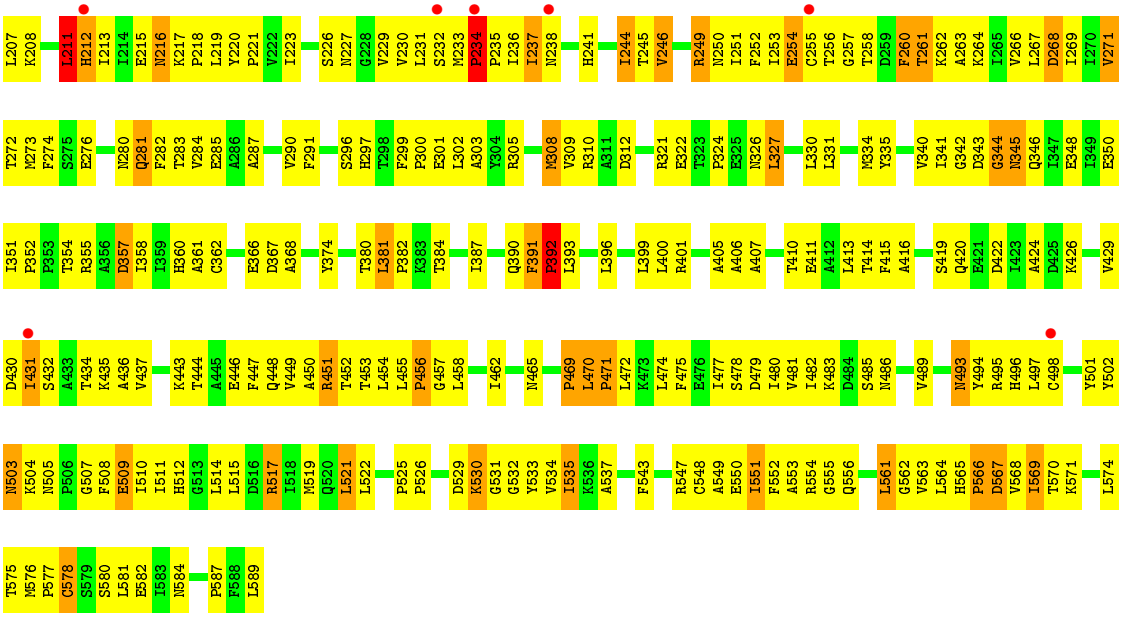
Chain O:



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

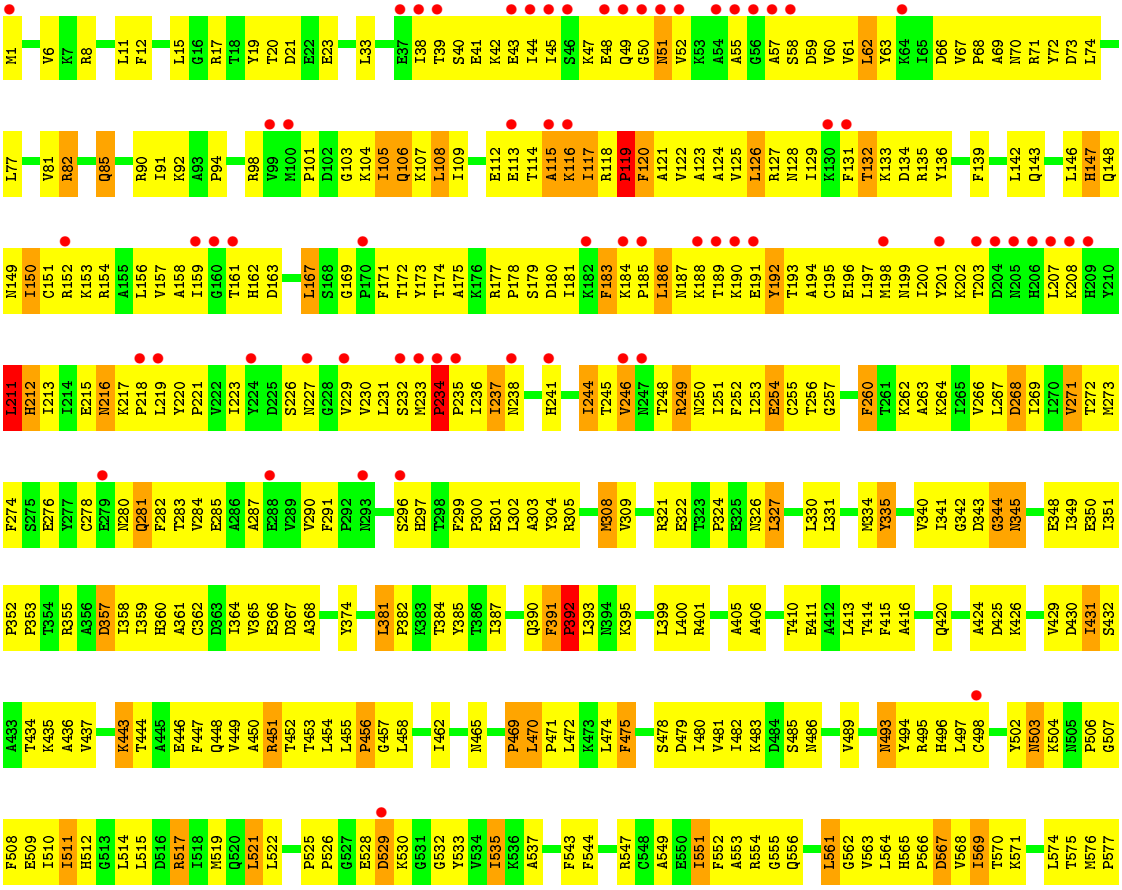
Chain B:

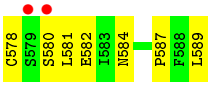




• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

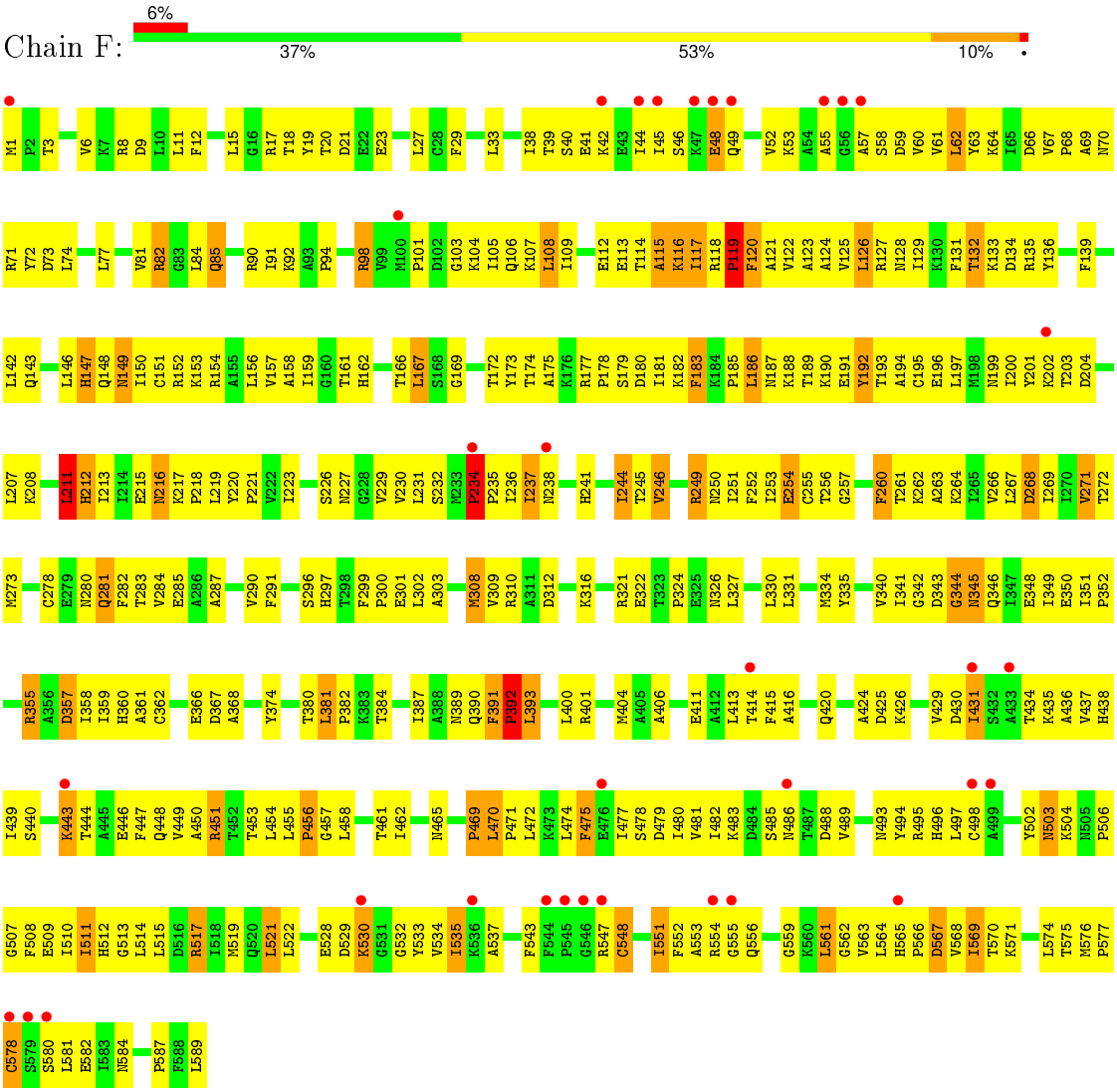
Chain D:





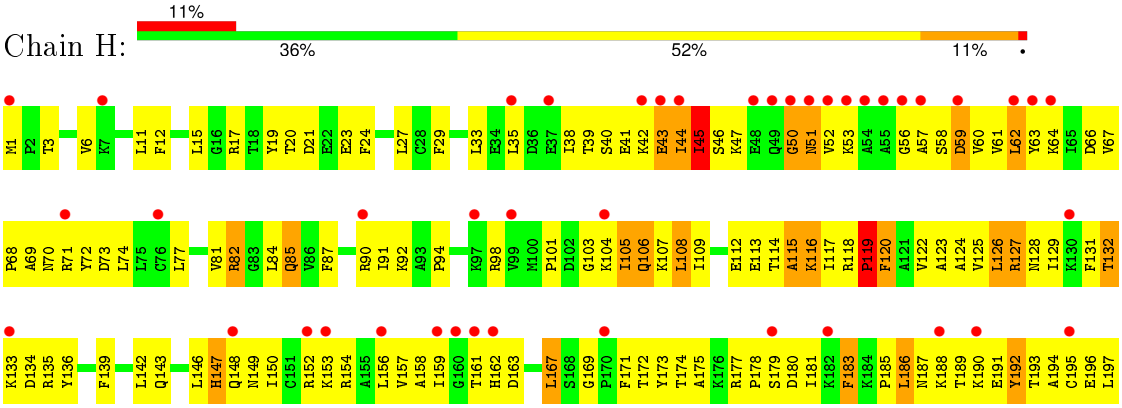
• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

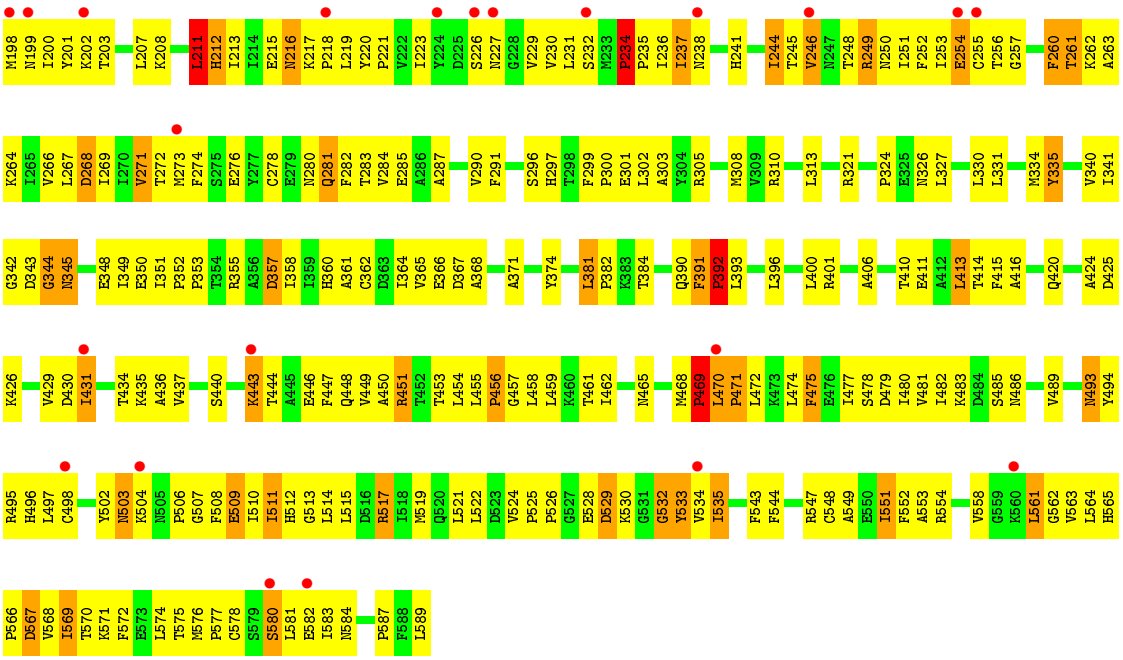
Chain F:



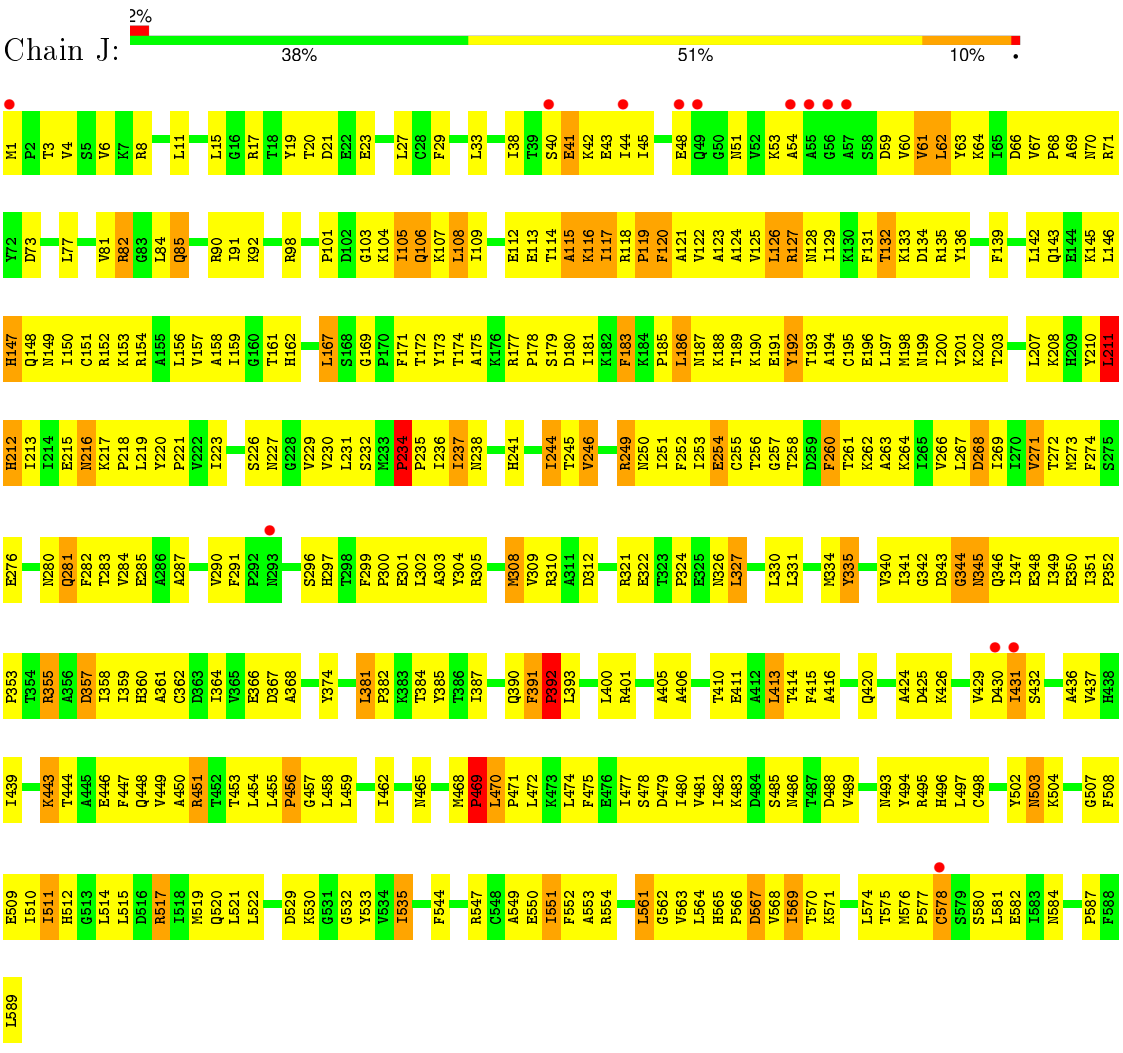
• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

Chain H:



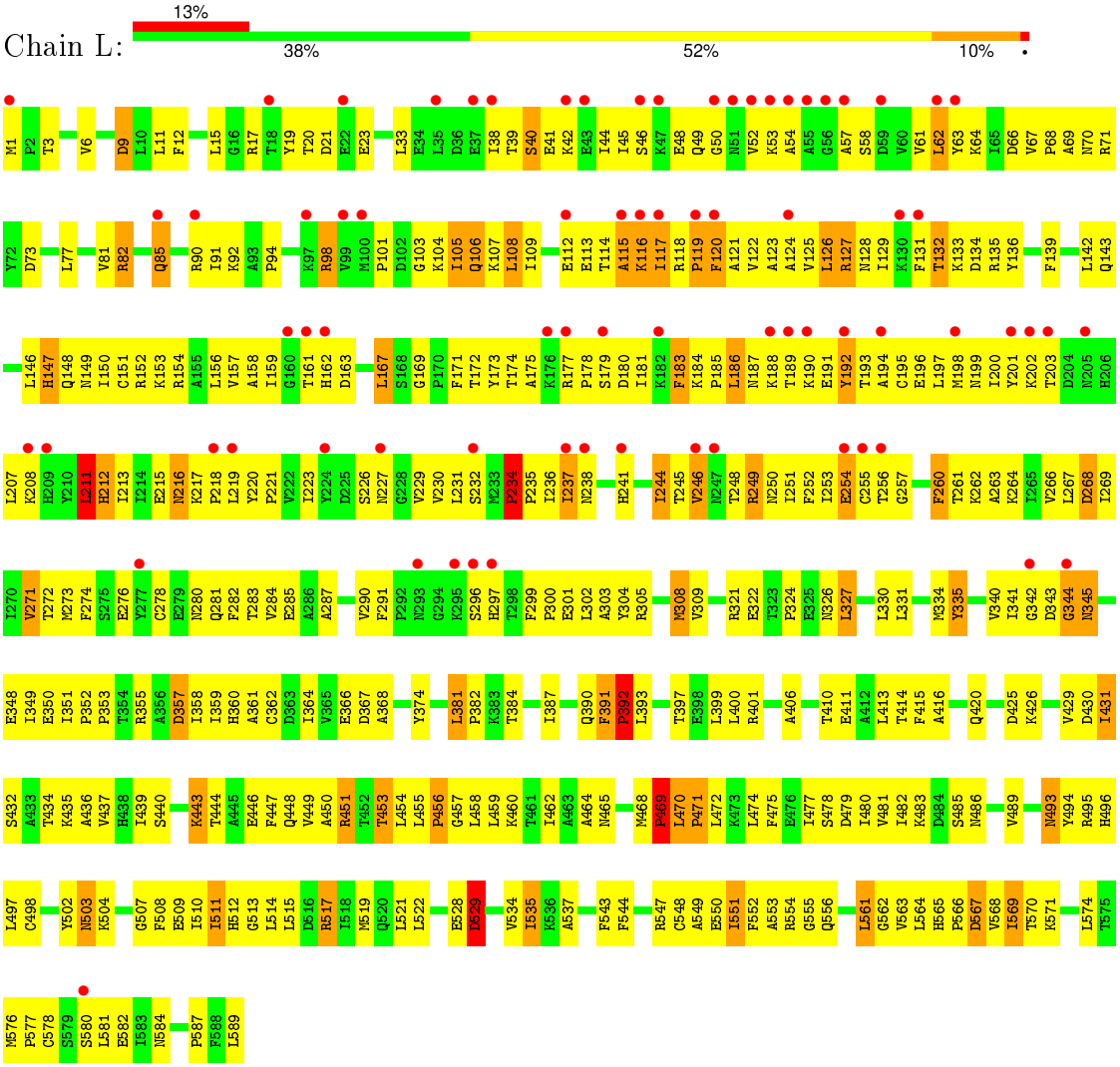


- Molecule 2: Phenylalanyl-tRNA synthetase beta chain



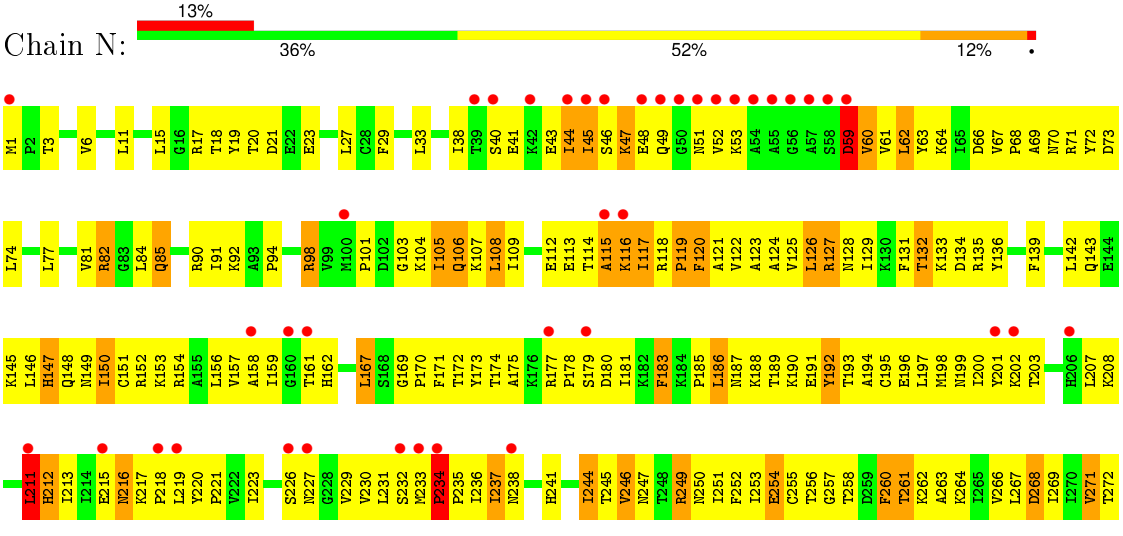
• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

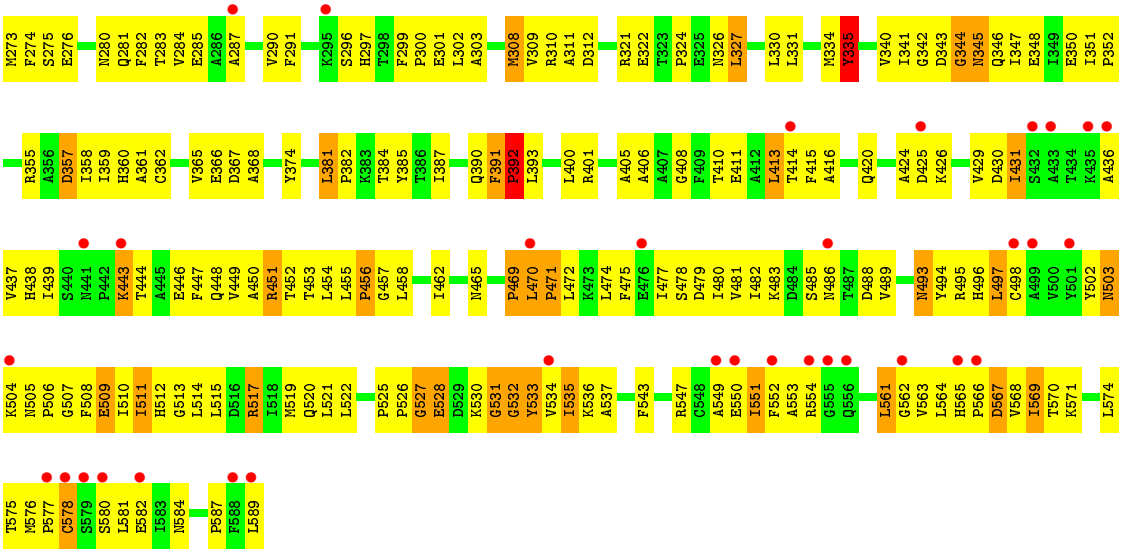
Chain L:



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

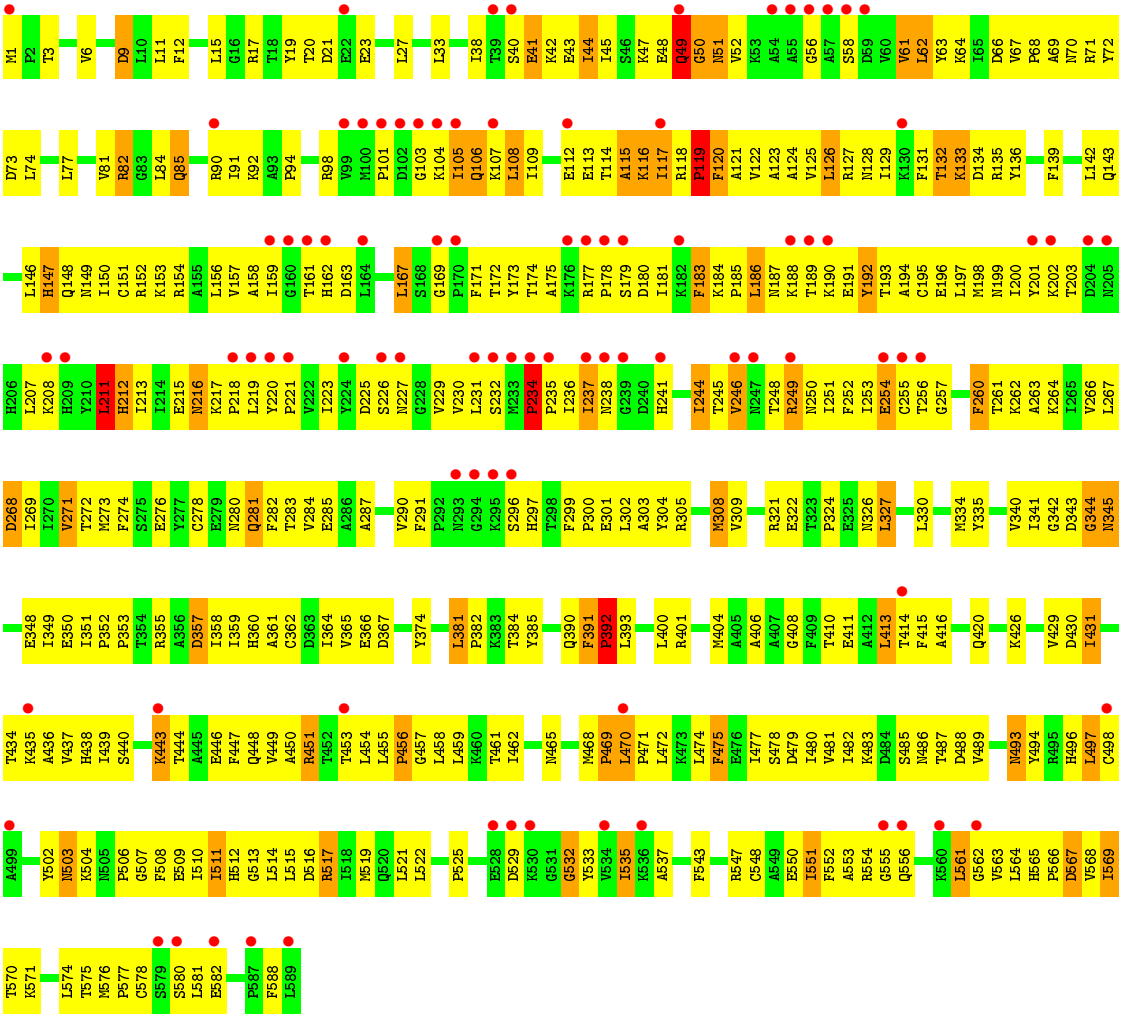
Chain N:





• Molecule 2: Phenylalanyl-tRNA synthetase beta chain

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	363.34Å 213.88Å 212.96Å 90.00° 125.20° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-3.30) 97.0 (29.99-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.287 0.251 , 0.255	Depositor DCC
R_{free} test set	9780 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 93.4	EDS
Estimated twinning fraction	0.009 for -h+k-l,-l,-k 0.002 for -h-k-l,l,k 0.000 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.000 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.000 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.000 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.019 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 193020 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	59395	wwPDB-VP

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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Property	Value	Source
Average B, all atoms ($Å^2$)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.50	0/2664	0.71	0/3609
1	C	0.44	0/4154	0.69	2/5611 (0.0%)
1	E	0.48	0/2591	0.71	1/3511 (0.0%)
1	G	0.46	0/2595	0.70	0/3516
1	I	0.46	0/2626	0.70	0/3558
1	K	0.46	0/2819	0.69	0/3818
1	M	0.42	0/2656	0.67	0/3592
1	O	0.41	0/2601	0.65	0/3523
2	B	0.46	0/4742	0.69	0/6420
2	D	0.40	0/4742	0.66	0/6420
2	F	0.45	0/4742	0.69	0/6420
2	H	0.40	0/4742	0.66	0/6420
2	J	0.44	0/4742	0.69	0/6420
2	L	0.39	0/4742	0.66	0/6420
2	N	0.42	0/4742	0.67	1/6420 (0.0%)
2	P	0.37	0/4742	0.65	1/6420 (0.0%)
All	All	0.43	0/60642	0.68	5/82098 (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
2	N	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	165	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	477	LEU	CA-CB-CG	5.10	127.03	115.30
2	N	497	LEU	N-CA-C	-5.06	97.33	111.00
2	P	497	LEU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	533	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	0	2537	259	0
1	C	4058	0	4030	447	0
1	E	2517	0	2462	283	0
1	G	2521	0	2465	300	0
1	I	2551	0	2496	232	0
1	K	2746	0	2632	276	0
1	M	2582	0	2506	316	0
1	O	2527	0	2476	279	0
2	B	4651	0	4751	471	0
2	D	4651	0	4751	452	0
2	F	4651	0	4751	496	0
2	H	4651	0	4751	445	0
2	J	4651	0	4751	452	0
2	L	4651	0	4751	449	0
2	N	4651	0	4751	487	0
2	P	4651	0	4751	453	0
3	A	12	0	8	6	0
3	C	12	0	8	2	0
3	E	12	0	8	1	0
3	G	12	0	8	2	0
3	I	12	0	8	2	0
3	K	12	0	8	7	0
3	M	12	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	12	0	8	5	0
All	All	59395	0	59676	5642	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 47.

The worst 5 of 5642 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)
2:N:49:GLN:HE21	2:N:52:VAL:HG11	1.06	1.13
2:N:381:LEU:HD23	2:N:382:PRO:HD2	1.30	1.12
2:J:381:LEU:HD23	2:J:382:PRO:HD2	1.26	1.11
2:N:117:ILE:HG23	2:N:217:LYS:HD2	1.33	1.11
1:O:188:GLN:HB2	1:O:206:PRO:HG2	1.33	1.10

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	316/508 (62%)	246 (78%)	42 (13%)	28 (9%)	1 6
1	C	506/508 (100%)	382 (76%)	84 (17%)	40 (8%)	1 8
1	E	307/508 (60%)	233 (76%)	42 (14%)	32 (10%)	1 4
1	G	307/508 (60%)	241 (78%)	34 (11%)	32 (10%)	1 4
1	I	311/508 (61%)	254 (82%)	38 (12%)	19 (6%)	2 14
1	K	343/508 (68%)	257 (75%)	58 (17%)	28 (8%)	1 8
1	M	319/508 (63%)	233 (73%)	46 (14%)	40 (12%)	0 2
1	O	307/508 (60%)	243 (79%)	36 (12%)	28 (9%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	587/589 (100%)	484 (82%)	77 (13%)	26 (4%)	3 22
2	D	587/589 (100%)	480 (82%)	77 (13%)	30 (5%)	2 19
2	F	587/589 (100%)	485 (83%)	78 (13%)	24 (4%)	3 24
2	H	587/589 (100%)	478 (81%)	74 (13%)	35 (6%)	2 15
2	J	587/589 (100%)	482 (82%)	78 (13%)	27 (5%)	3 21
2	L	587/589 (100%)	478 (81%)	82 (14%)	27 (5%)	3 21
2	N	587/589 (100%)	479 (82%)	75 (13%)	33 (6%)	2 16
2	P	587/589 (100%)	474 (81%)	84 (14%)	29 (5%)	3 19
All	All	7412/8776 (84%)	5929 (80%)	1005 (14%)	478 (6%)	2 13

5 of 478 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	GLY
1	A	203	ARG
1	A	206	PRO
1	A	215	HIS
1	A	265	PRO

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	281/434 (65%)	254 (90%)	27 (10%)	10 38
1	C	434/434 (100%)	382 (88%)	52 (12%)	6 27
1	E	272/434 (63%)	233 (86%)	39 (14%)	4 19
1	G	273/434 (63%)	241 (88%)	32 (12%)	7 28
1	I	276/434 (64%)	248 (90%)	28 (10%)	9 35
1	K	284/434 (65%)	247 (87%)	37 (13%)	5 22
1	M	276/434 (64%)	240 (87%)	36 (13%)	5 22
1	O	274/434 (63%)	235 (86%)	39 (14%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	513/513 (100%)	453 (88%)	60 (12%)	7	28
2	D	513/513 (100%)	456 (89%)	57 (11%)	8	31
2	F	513/513 (100%)	456 (89%)	57 (11%)	8	31
2	H	513/513 (100%)	455 (89%)	58 (11%)	7	30
2	J	513/513 (100%)	458 (89%)	55 (11%)	8	32
2	L	513/513 (100%)	455 (89%)	58 (11%)	7	30
2	N	513/513 (100%)	453 (88%)	60 (12%)	7	28
2	P	513/513 (100%)	454 (88%)	59 (12%)	7	29
All	All	6474/7576 (86%)	5720 (88%)	754 (12%)	7	29

5 of 754 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	192	TYR
2	J	127	ARG
2	P	21	ASP
2	H	271	VAL
1	I	190	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	480	HIS
1	I	372	GLN
1	O	308	GLN
2	H	187	ASN
2	H	448	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PHE	A	509	-	9,12,12	0.75	0	9,15,15	0.41	0
3	PHE	C	509	-	9,12,12	0.55	0	9,15,15	0.38	0
3	PHE	E	509	-	9,12,12	0.63	0	9,15,15	0.21	0
3	PHE	G	509	-	9,12,12	0.34	0	9,15,15	0.23	0
3	PHE	I	509	-	9,12,12	0.22	0	9,15,15	0.17	0
3	PHE	K	509	-	9,12,12	0.42	0	9,15,15	0.29	0
3	PHE	M	509	-	9,12,12	0.39	0	9,15,15	0.29	0
3	PHE	O	509	-	9,12,12	0.63	0	9,15,15	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PHE	A	509	-	-	0/4/8/8	0/1/1/1
3	PHE	C	509	-	-	0/4/8/8	0/1/1/1
3	PHE	E	509	-	-	0/4/8/8	0/1/1/1
3	PHE	G	509	-	-	0/4/8/8	0/1/1/1
3	PHE	I	509	-	-	0/4/8/8	0/1/1/1
3	PHE	K	509	-	-	0/4/8/8	0/1/1/1
3	PHE	M	509	-	-	0/4/8/8	0/1/1/1
3	PHE	O	509	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	PHE	6	0
3	C	509	PHE	2	0
3	E	509	PHE	1	0
3	G	509	PHE	2	0
3	I	509	PHE	2	0
3	K	509	PHE	7	0
3	M	509	PHE	4	0
3	O	509	PHE	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/508 (62%)	-0.03	14 (4%)	38	31	47, 84, 168, 200	0
1	C	508/508 (100%)	0.07	25 (4%)	33	27	50, 107, 181, 201	0
1	E	309/508 (60%)	0.09	16 (5%)	31	25	47, 103, 181, 201	0
1	G	309/508 (60%)	0.14	16 (5%)	31	25	54, 103, 179, 200	0
1	I	313/508 (61%)	-0.14	9 (2%)	55	49	42, 91, 164, 192	0
1	K	349/508 (68%)	0.05	12 (3%)	49	42	48, 101, 178, 201	0
1	M	321/508 (63%)	0.37	33 (10%)	9	7	51, 133, 189, 201	0
1	O	309/508 (60%)	0.19	14 (4%)	37	30	65, 112, 183, 201	0
2	B	589/589 (100%)	-0.10	20 (3%)	49	42	47, 93, 154, 201	0
2	D	589/589 (100%)	0.42	68 (11%)	6	5	56, 129, 199, 201	0
2	F	589/589 (100%)	0.11	34 (5%)	26	21	51, 104, 175, 201	0
2	H	589/589 (100%)	0.48	65 (11%)	7	6	63, 131, 188, 201	0
2	J	589/589 (100%)	-0.01	13 (2%)	65	59	57, 99, 158, 201	0
2	L	589/589 (100%)	0.51	75 (12%)	5	4	61, 139, 201, 201	0
2	N	589/589 (100%)	0.52	74 (12%)	5	4	58, 134, 192, 201	0
2	P	589/589 (100%)	0.63	91 (15%)	3	2	73, 153, 201, 201	0
All	All	7448/8776 (84%)	0.24	579 (7%)	16	13	42, 114, 190, 201	0

The worst 5 of 579 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	160	GLY	9.7
2	H	160	GLY	9.4
2	P	238	ASN	8.8
2	P	160	GLY	7.8
2	H	56	GLY	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PHE	C	509	12/12	0.87	0.44	4.98	81,83,172,174	0
3	PHE	E	509	12/12	0.92	0.41	4.83	68,71,201,201	0
3	PHE	A	509	12/12	0.94	0.33	3.67	90,92,129,130	0
3	PHE	K	509	12/12	0.95	0.34	2.17	82,83,189,189	0
3	PHE	O	509	12/12	0.95	0.38	1.56	82,84,201,201	0
3	PHE	G	509	12/12	0.95	0.33	1.14	81,86,201,201	0
3	PHE	I	509	12/12	0.96	0.24	0.78	64,69,201,201	0
3	PHE	M	509	12/12	0.91	0.27	0.10	96,99,201,201	0

6.5 Other polymers (i)

There are no such residues in this entry.