wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Dec 6, 2016 – 11:54 AM EST

PDB ID	:	3ZBI
EMDB ID:	:	EMD-2233
Title	:	Fitting result in the O-layer of the subnanometer structure of the bacterial pKM101 type IV secretion system core complex digested with elastase
Authors	:	Rivera-Calzada, A.; Fronzes, R.; Savva, C.G.; Chandran, V.; Lian, P.W.; Laeremans, T.; Pardon, E.; Steyaert, J.; Remaut, H.; Waksman, G.; Orlova, E.V.
Deposited on	:	2012-11-10
Resolution	:	8.50 Å(reported)
Based on PDB ID	:	3JQO

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

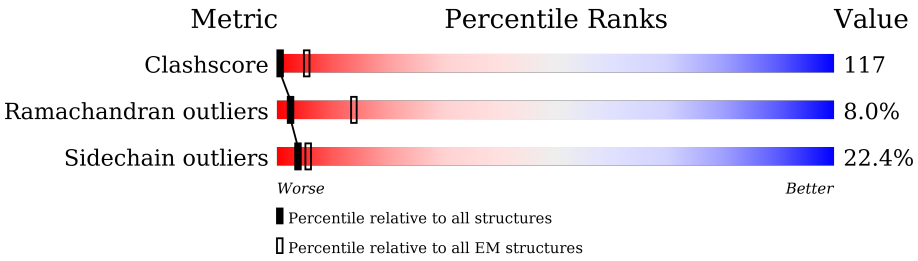
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	216	16% 55% 17% • 9%
1	D	216	15% 56% 17% • 9%
1	G	216	14% 56% 18% • 9%
1	J	216	14% 56% 17% • 9%
1	M	216	14% 56% 18% • 9%
1	P	216	14% 56% 18% • 9%
1	S	216	14% 56% 18% • 9%
1	V	216	15% 56% 17% • 9%
1	Y	216	18% 54% 16% • 9%

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Mol	Chain	Length	Quality of chain
1	b	216	69% 19% • 9%
1	e	216	69% 19% • 9%
1	h	216	69% 19% • 9%
1	k	216	69% 19% • 9%
1	n	216	69% 19% • 9%
2	B	130	18% 56% 25% •
2	E	130	18% 57% 24% •
2	H	130	18% 57% 24% •
2	K	130	18% 58% 24% •
2	N	130	18% 58% 24% •
2	Q	130	18% 57% 24% •
2	T	130	18% 57% 24% •
2	W	130	18% 57% 24% •
2	Z	130	18% 58% 23% •
2	c	130	68% 31% •
2	f	130	68% 31% •
2	i	130	68% 31% •
2	l	130	68% 31% •
2	o	130	68% 31% •
3	C	48	23% 29% 8% 40%
3	F	48	21% 31% 8% 40%
3	I	48	19% 33% 8% 40%
3	L	48	21% 31% 8% 40%
3	O	48	23% 29% 8% 40%
3	R	48	21% 31% 8% 40%

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Mol	Chain	Length	Quality of chain
3	U	48	19% 33% 8% 40%
3	X	48	21% 31% 8% 40%
3	a	48	48% 13% 40%
3	d	48	48% 13% 40%
3	g	48	48% 13% 40%
3	j	48	48% 13% 40%
3	m	48	48% 13% 40%
3	p	48	48% 13% 40%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TRAF PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	D	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	G	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	J	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	M	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	P	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	S	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	V	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	Y	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	b	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	e	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	h	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	k	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		
1	n	197	Total	C	N	O	S	0	1
			1459	903	256	293	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	846	ARG	ALA	CONFLICT	UNP Q46705
D	846	ARG	ALA	CONFLICT	UNP Q46705

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Chain	Residue	Modelled	Actual	Comment	Reference
G	846	ARG	ALA	CONFLICT	UNP Q46705
J	846	ARG	ALA	CONFLICT	UNP Q46705
M	846	ARG	ALA	CONFLICT	UNP Q46705
P	846	ARG	ALA	CONFLICT	UNP Q46705
S	846	ARG	ALA	CONFLICT	UNP Q46705
V	846	ARG	ALA	CONFLICT	UNP Q46705
Y	846	ARG	ALA	CONFLICT	UNP Q46705
b	846	ARG	ALA	CONFLICT	UNP Q46705
e	846	ARG	ALA	CONFLICT	UNP Q46705
h	846	ARG	ALA	CONFLICT	UNP Q46705
k	846	ARG	ALA	CONFLICT	UNP Q46705
n	846	ARG	ALA	CONFLICT	UNP Q46705

- Molecule 2 is a protein called TRAO PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	E	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	H	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	K	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	N	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	Q	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	T	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	W	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	Z	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	c	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	f	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	i	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		
2	l	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	o	130	Total	C	N	O	S	0	0
			1034	648	193	190	3		

- Molecule 3 is a protein called TRAN PROTEIN.

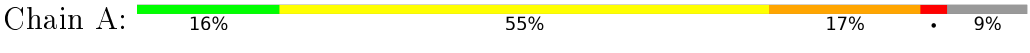
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	F	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	I	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	L	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	O	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	R	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	U	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	X	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	a	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	d	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	g	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	j	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	m	29	Total	C	N	O	S	0	1
			213	132	37	43	1		
3	p	29	Total	C	N	O	S	0	1
			213	132	37	43	1		

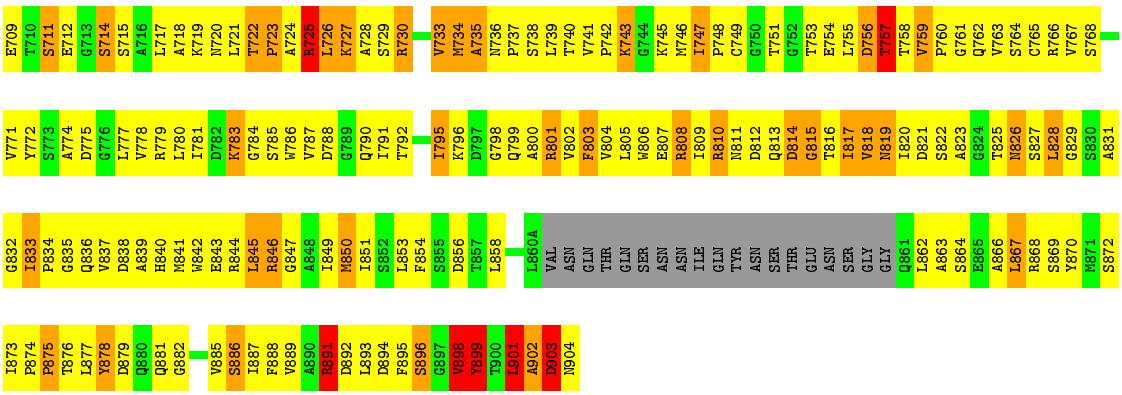
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: TRAF PROTEIN

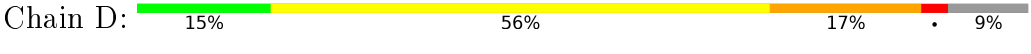
Chain A:

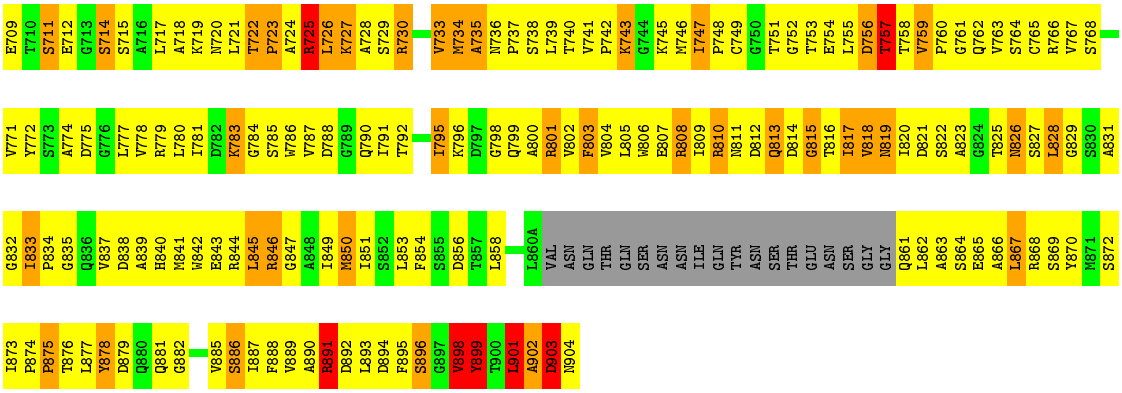




- Molecule 1: TRAF PROTEIN

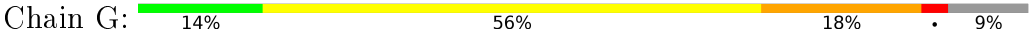
Chain D:

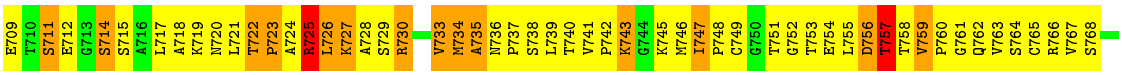


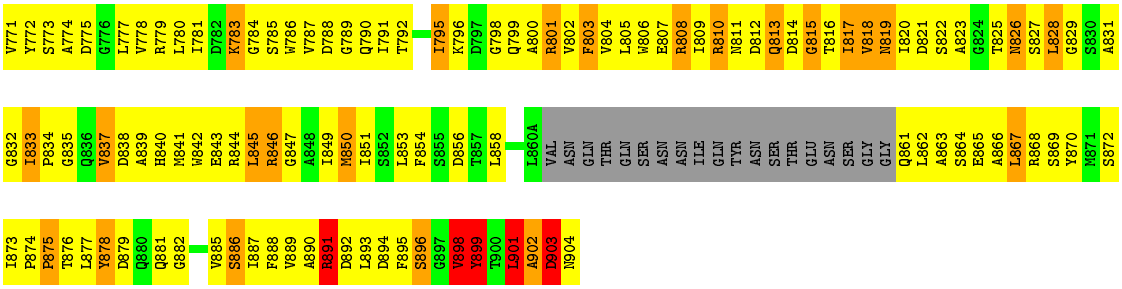


- Molecule 1: TRAF PROTEIN

Chain G:

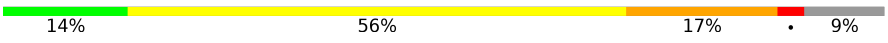


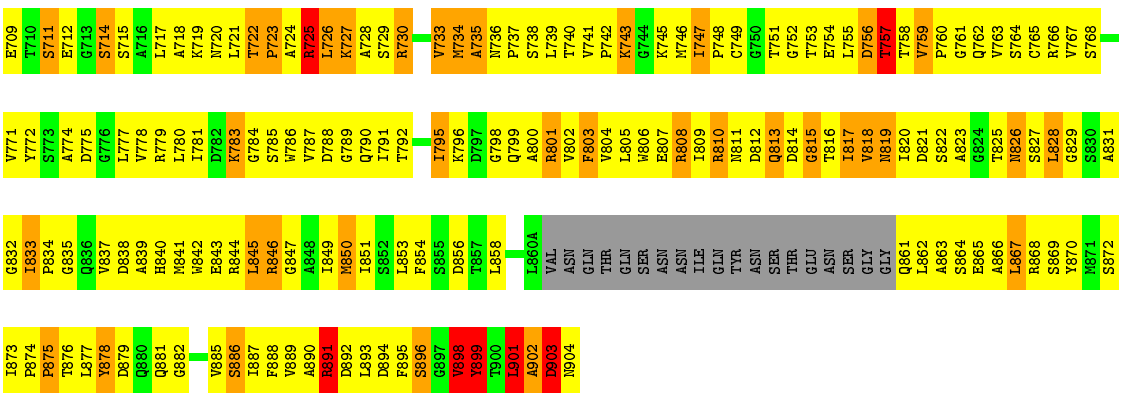




• Molecule 1: TRAF PROTEIN

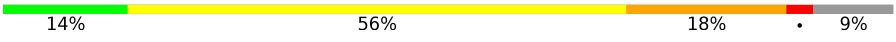
Chain J:

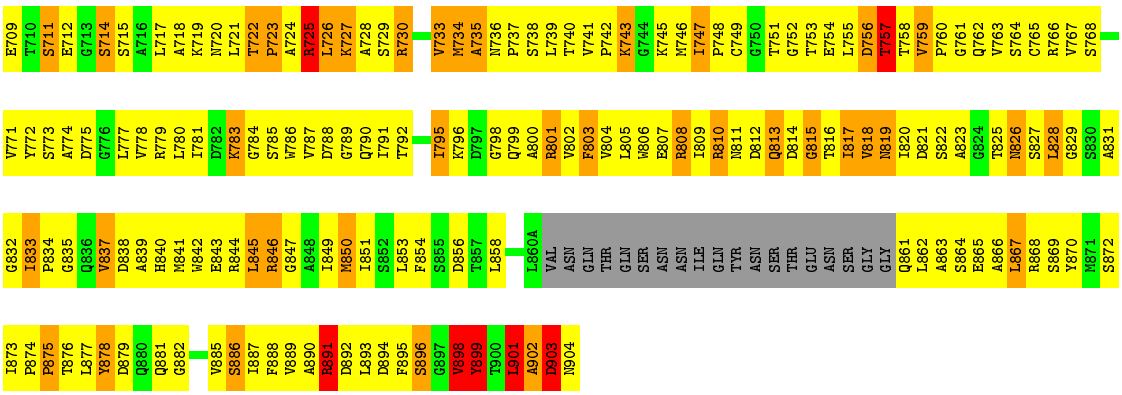




• Molecule 1: TRAF PROTEIN

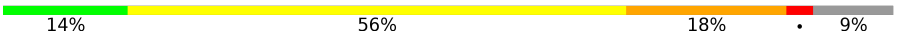
Chain M:

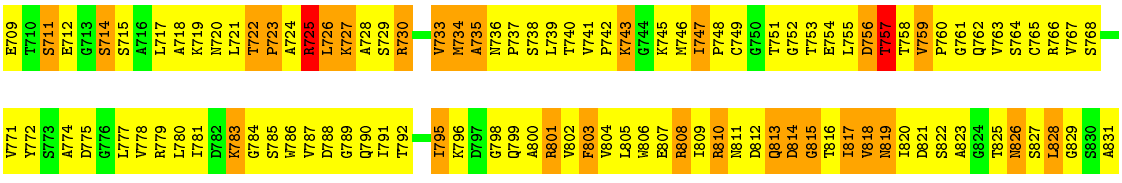


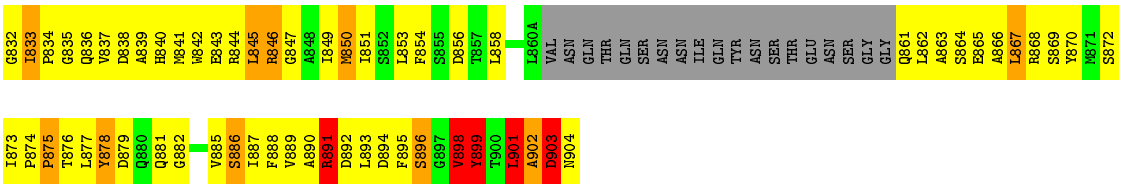


• Molecule 1: TRAF PROTEIN

Chain P:

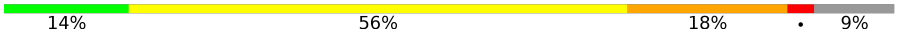


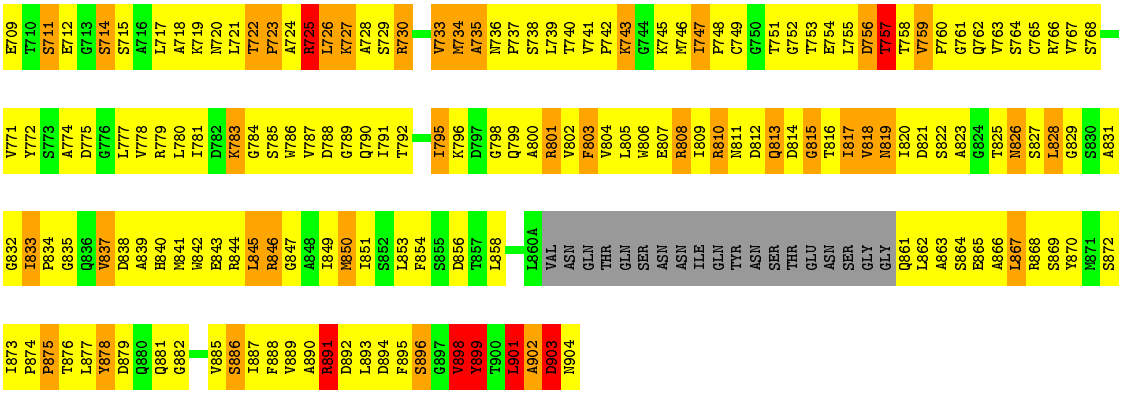




• Molecule 1: TRAF PROTEIN

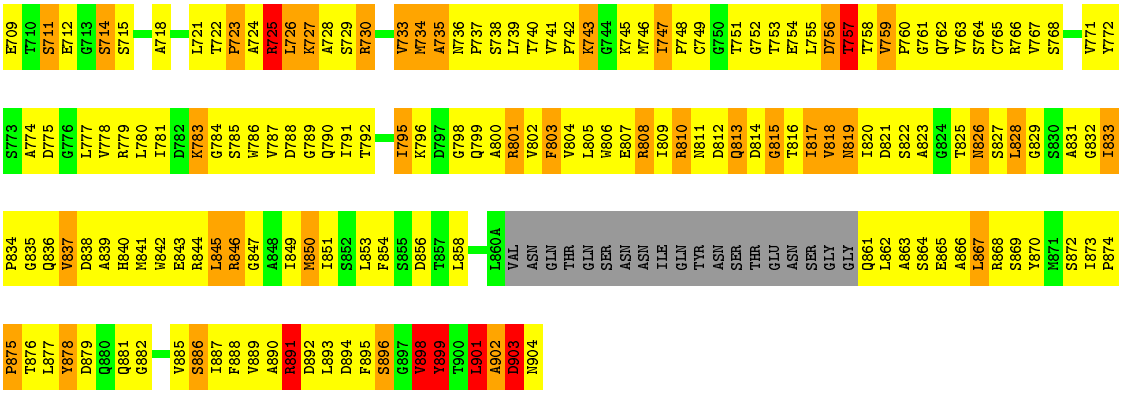
Chain S:





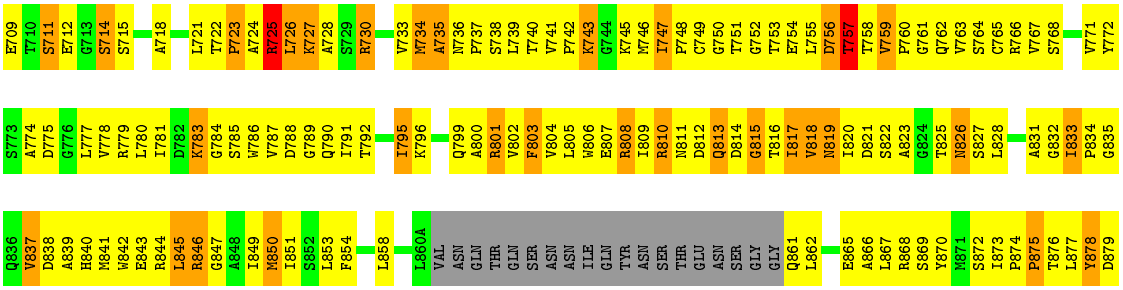
• Molecule 1: TRAF PROTEIN

Chain V:



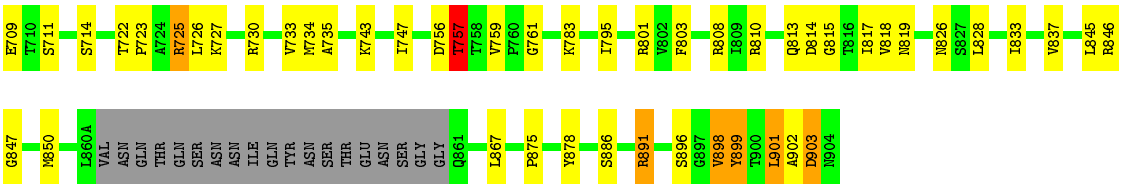
• Molecule 1: TRAF PROTEIN

Chain Y:



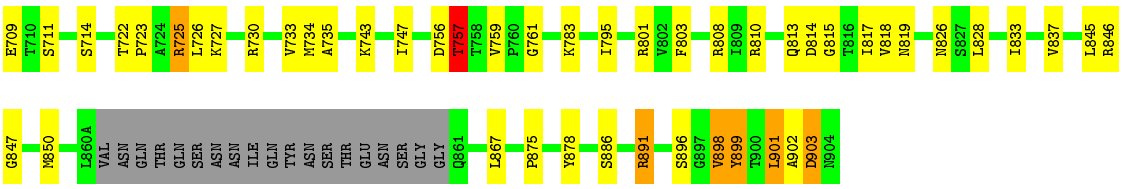
- Molecule 1: TRAF PROTEIN

Chain b:



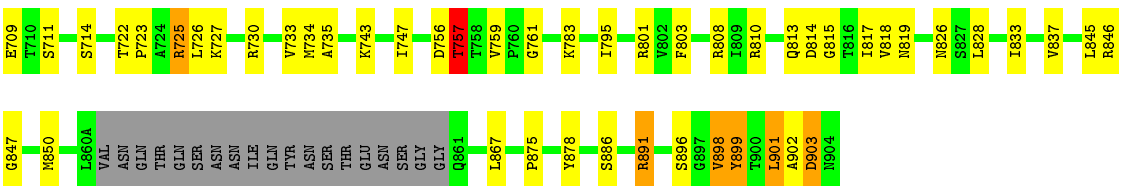
- Molecule 1: TRAF PROTEIN

Chain e:



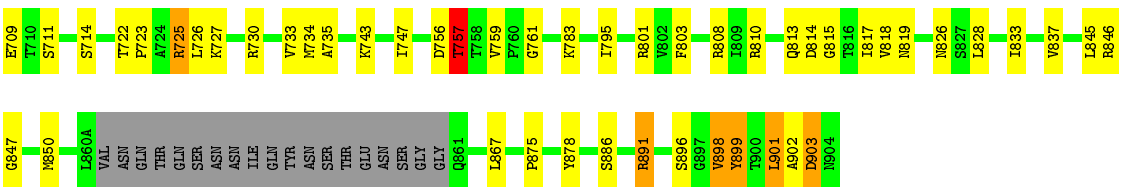
- Molecule 1: TRAF PROTEIN

Chain h:



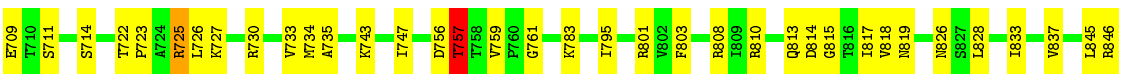
- Molecule 1: TRAF PROTEIN

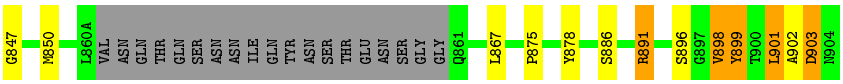
Chain k:



- Molecule 1: TRAF PROTEIN

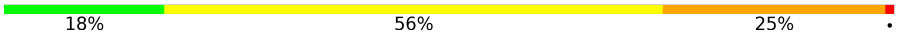
Chain n:

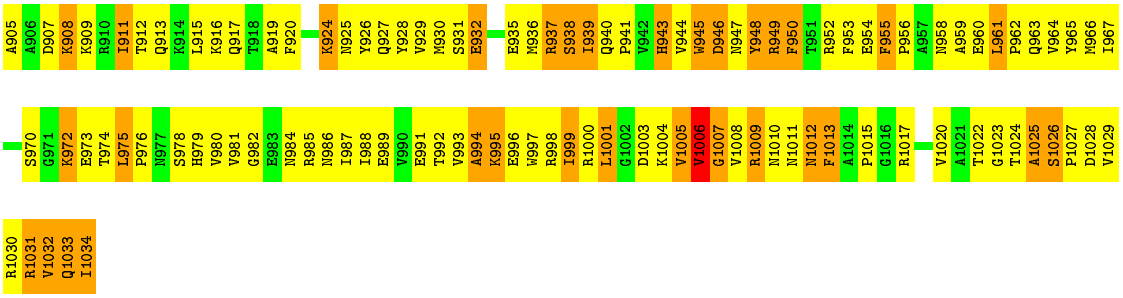




- Molecule 2: TRAO PROTEIN

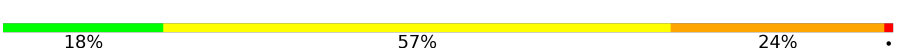
Chain B:

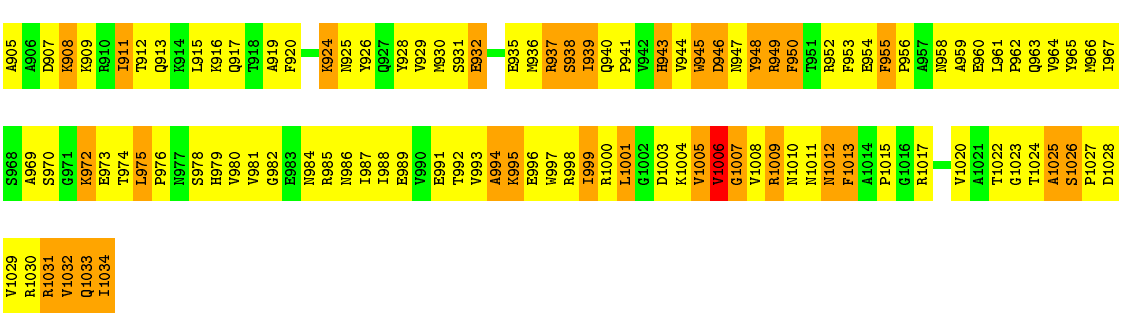




- Molecule 2: TRAO PROTEIN

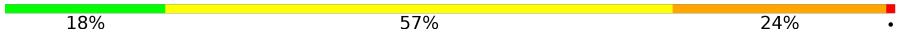
Chain E:

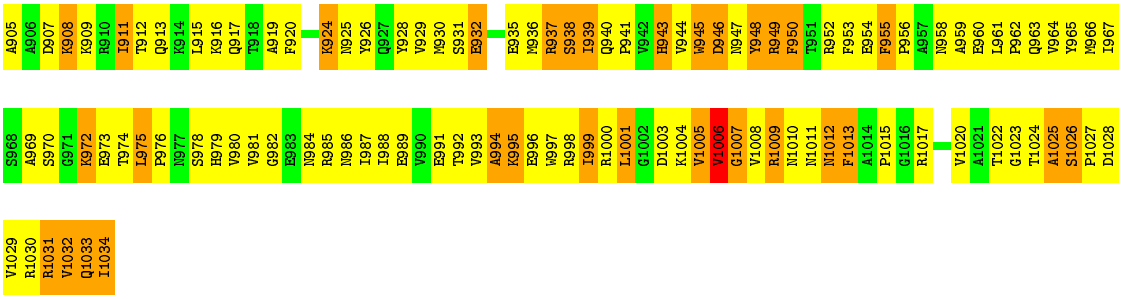




- Molecule 2: TRAO PROTEIN

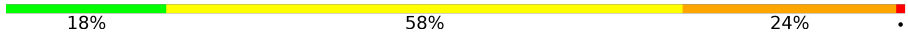
Chain H:

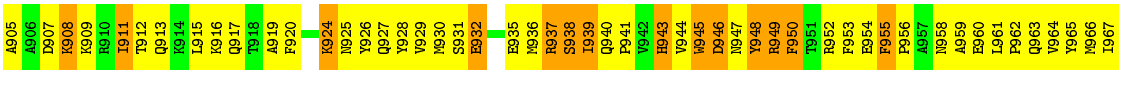


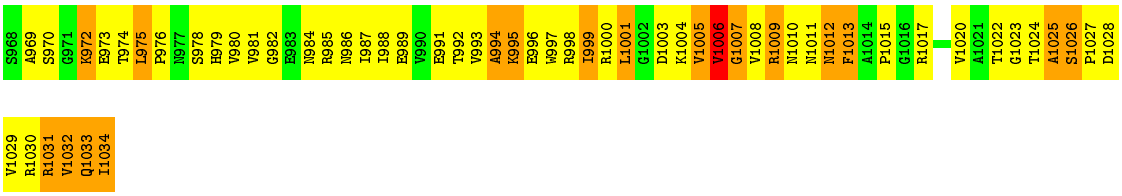


- Molecule 2: TRAO PROTEIN

Chain K:

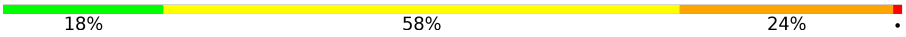


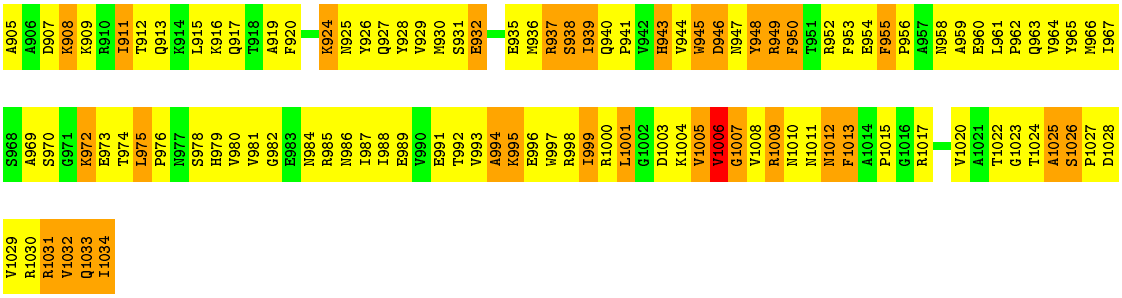




- Molecule 2: TRAO PROTEIN

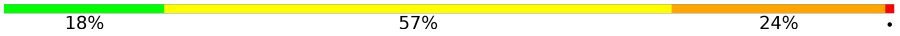
Chain N:

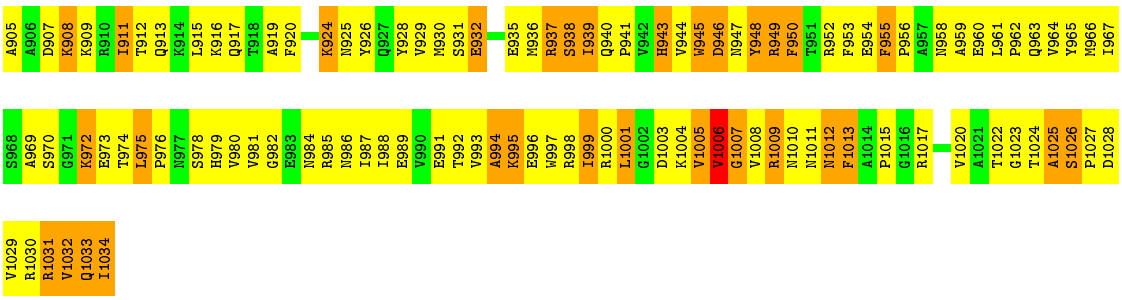




- Molecule 2: TRAO PROTEIN

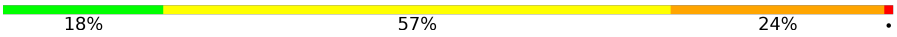
Chain Q:

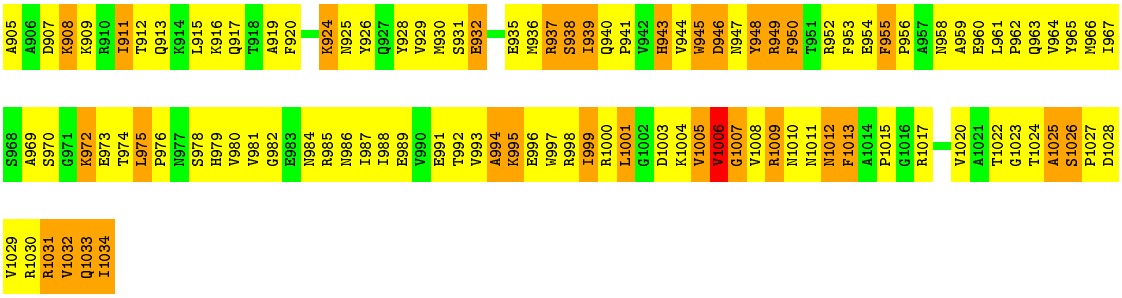




- Molecule 2: TRAO PROTEIN

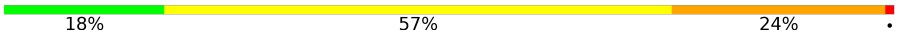
Chain T:

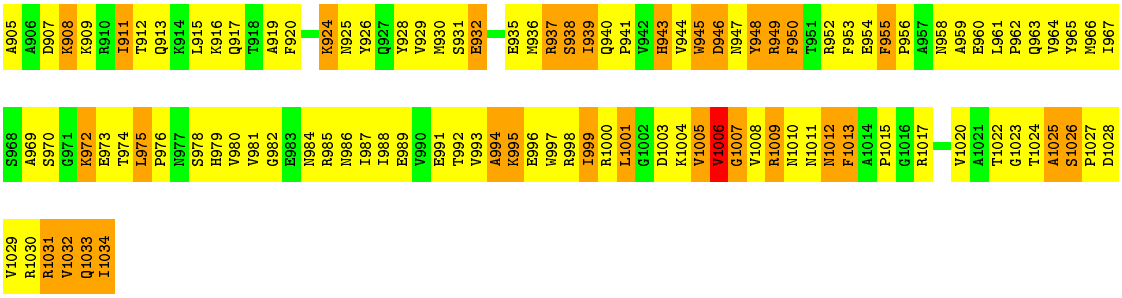




- Molecule 2: TRAO PROTEIN

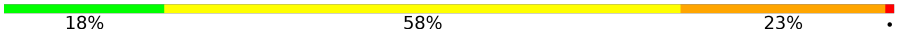
Chain W:

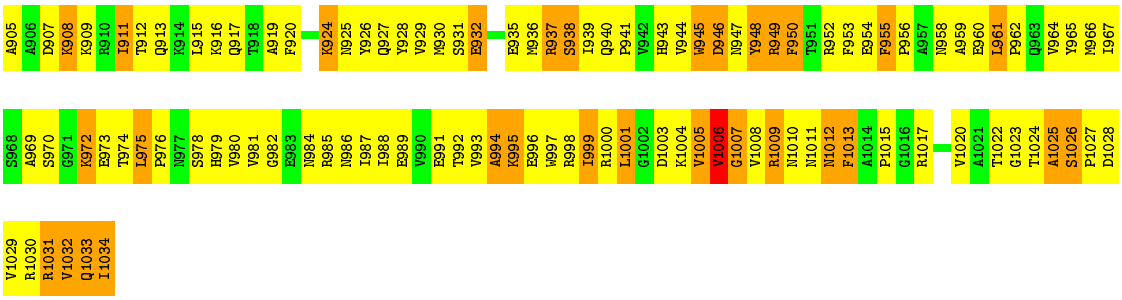




- Molecule 2: TRAO PROTEIN

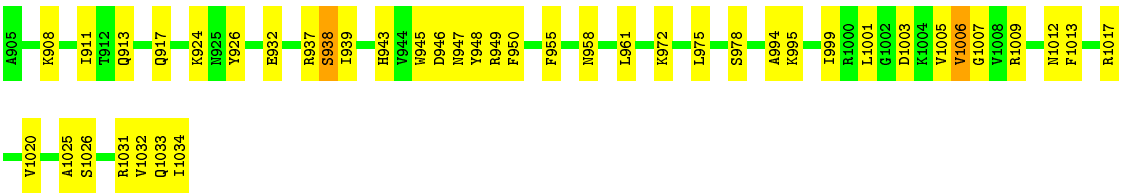
Chain Z:





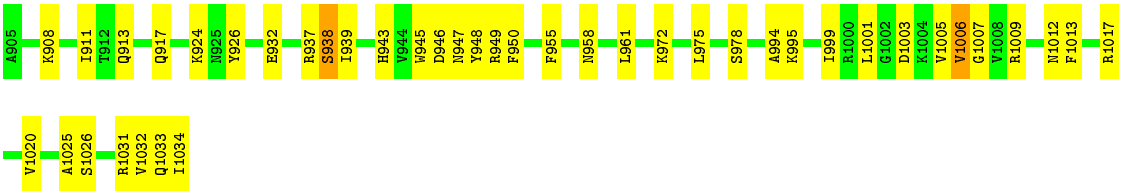
- Molecule 2: TRAO PROTEIN

Chain c:



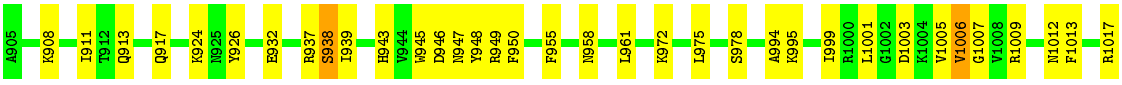
- Molecule 2: TRAO PROTEIN

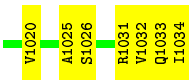
Chain f:



- Molecule 2: TRAO PROTEIN

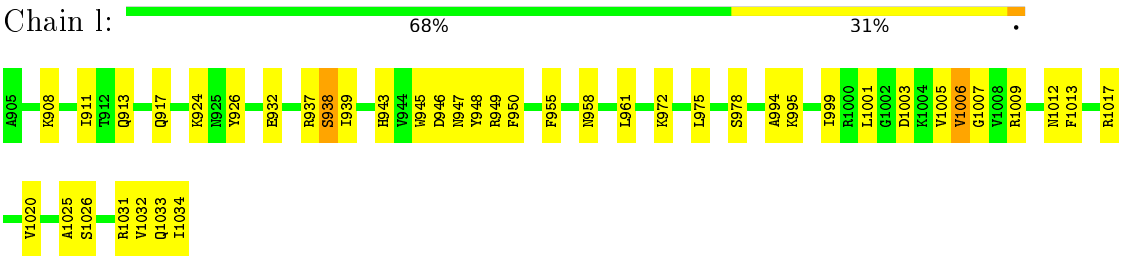
Chain i:





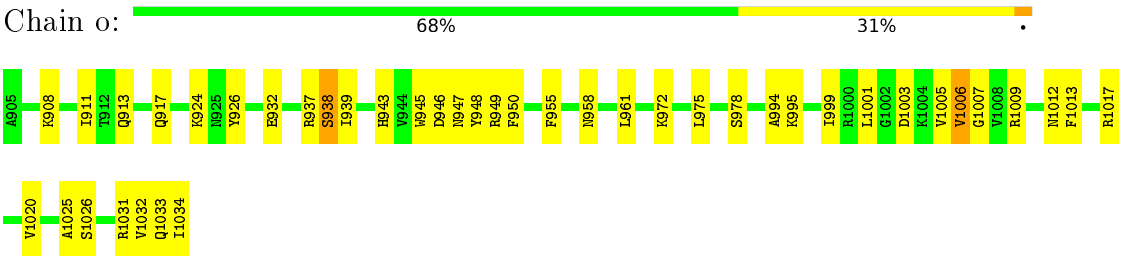
- Molecule 2: TRAO PROTEIN

Chain l:



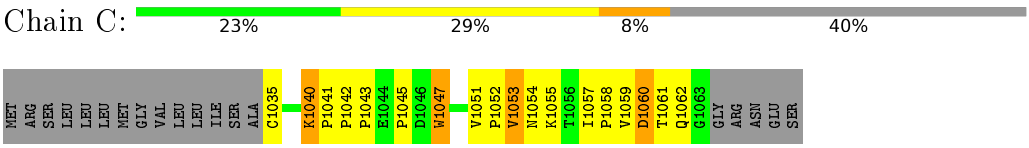
- Molecule 2: TRAO PROTEIN

Chain o:



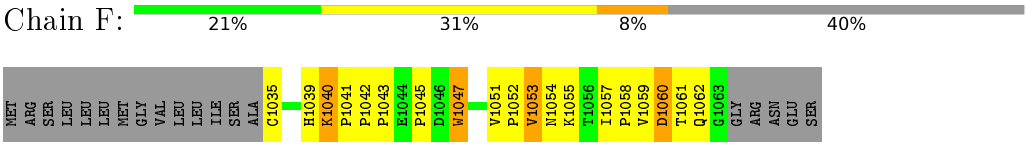
- Molecule 3: TRAN PROTEIN

Chain C:



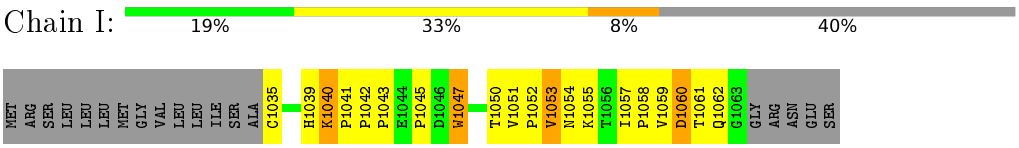
- Molecule 3: TRAN PROTEIN

Chain F:



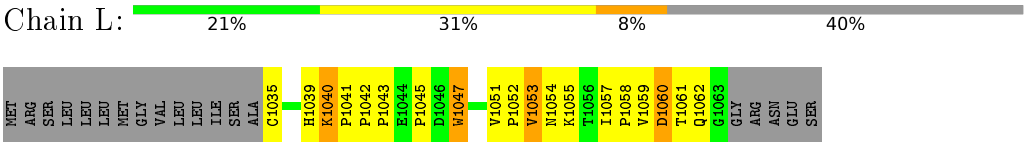
- Molecule 3: TRAN PROTEIN

Chain I:



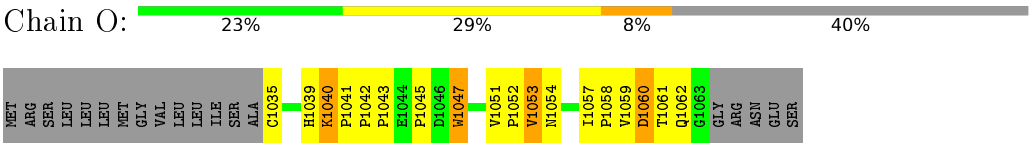
- Molecule 3: TRAN PROTEIN

Chain L:



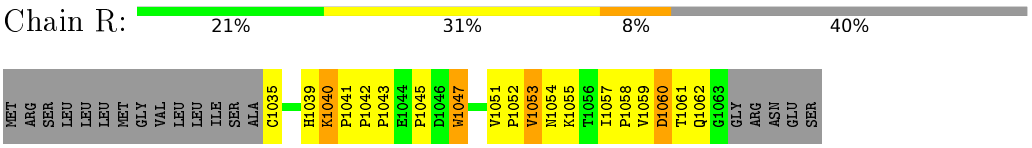
- Molecule 3: TRAN PROTEIN

Chain O:



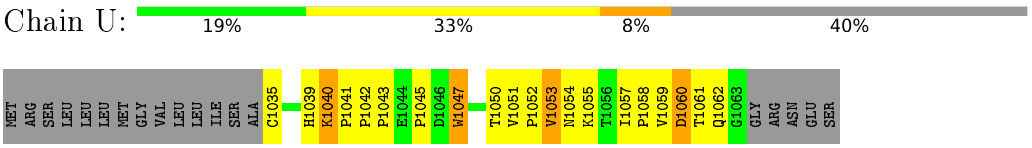
- Molecule 3: TRAN PROTEIN

Chain R:



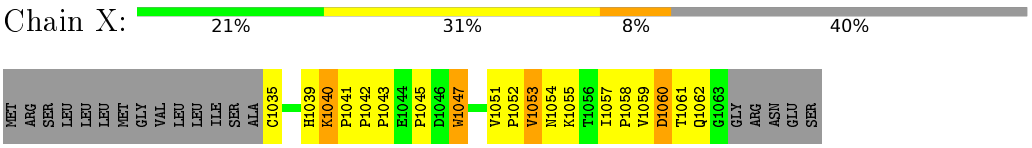
- Molecule 3: TRAN PROTEIN

Chain U:



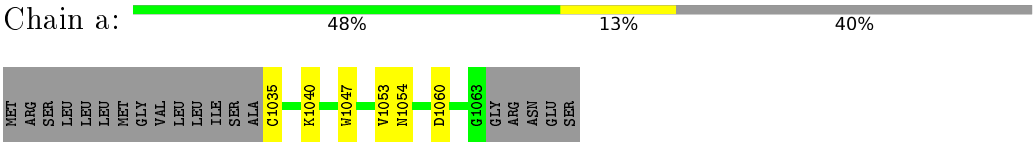
- Molecule 3: TRAN PROTEIN

Chain X:



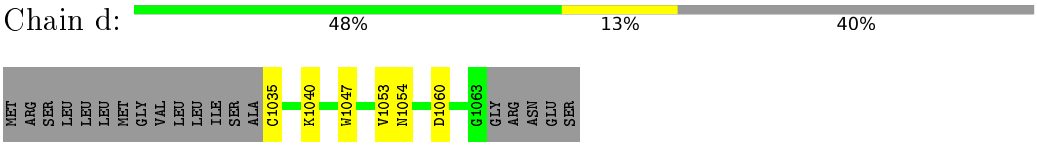
- Molecule 3: TRAN PROTEIN

Chain a:



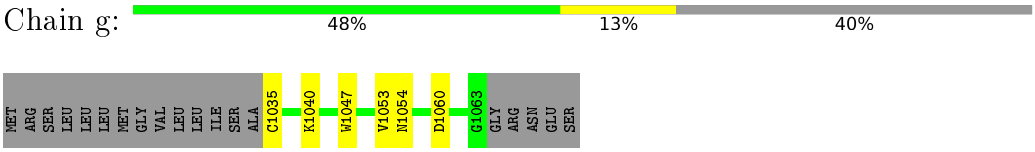
- Molecule 3: TRAN PROTEIN

Chain d:



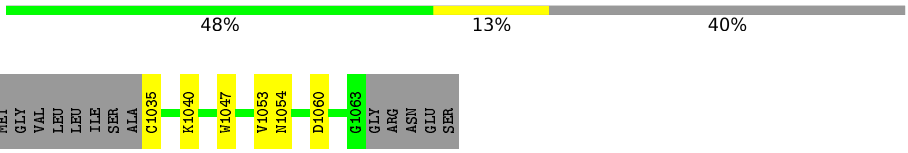
- Molecule 3: TRAN PROTEIN

Chain g:



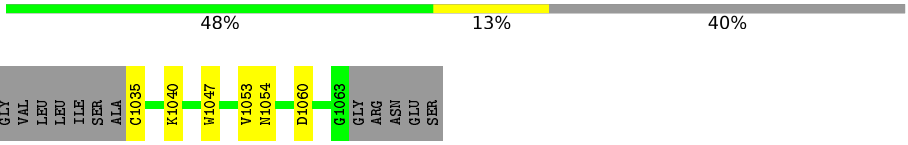
- Molecule 3: TRAN PROTEIN

Chain j:



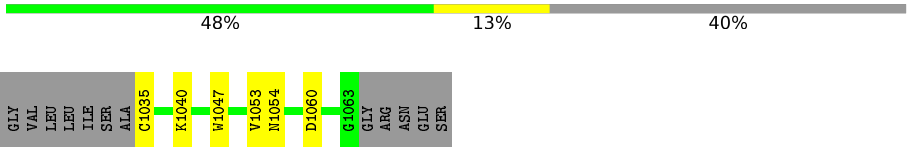
• Molecule 3: TRAN PROTEIN

Chain m:



• Molecule 3: TRAN PROTEIN

Chain p:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	5430	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	68100	Depositor
Image detector	GATAN CCD	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	1.06	0/1480	1.36	6/2007 (0.3%)
1	D	1.06	0/1480	1.36	6/2007 (0.3%)
1	G	1.06	0/1480	1.36	6/2007 (0.3%)
1	J	1.06	0/1480	1.36	6/2007 (0.3%)
1	M	1.06	0/1480	1.36	6/2007 (0.3%)
1	P	1.06	0/1480	1.36	6/2007 (0.3%)
1	S	1.06	0/1480	1.36	6/2007 (0.3%)
1	V	1.06	0/1480	1.36	6/2007 (0.3%)
1	Y	1.06	0/1480	1.36	6/2007 (0.3%)
1	b	1.06	0/1480	1.36	6/2007 (0.3%)
1	e	1.06	0/1480	1.36	6/2007 (0.3%)
1	h	1.06	0/1480	1.36	6/2007 (0.3%)
1	k	1.06	0/1480	1.36	6/2007 (0.3%)
1	n	1.06	0/1480	1.36	6/2007 (0.3%)
2	B	1.11	0/1055	1.37	3/1426 (0.2%)
2	E	1.11	0/1055	1.37	3/1426 (0.2%)
2	H	1.10	0/1055	1.37	3/1426 (0.2%)
2	K	1.11	0/1055	1.37	3/1426 (0.2%)
2	N	1.11	0/1055	1.37	3/1426 (0.2%)
2	Q	1.11	0/1055	1.37	3/1426 (0.2%)
2	T	1.11	0/1055	1.37	3/1426 (0.2%)
2	W	1.11	0/1055	1.37	3/1426 (0.2%)
2	Z	1.11	0/1055	1.37	3/1426 (0.2%)
2	c	1.10	0/1055	1.37	3/1426 (0.2%)
2	f	1.11	0/1055	1.37	3/1426 (0.2%)
2	i	1.11	0/1055	1.37	3/1426 (0.2%)
2	l	1.11	0/1055	1.37	3/1426 (0.2%)
2	o	1.11	0/1055	1.37	3/1426 (0.2%)
3	C	1.06	0/221	1.24	0/307
3	F	1.06	0/221	1.24	0/307
3	I	1.06	0/221	1.24	0/307
3	L	1.05	0/221	1.24	0/307
3	O	1.06	0/221	1.24	0/307
3	R	1.05	0/221	1.24	0/307

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
3	U	1.06	0/221	1.24	0/307
3	X	1.06	0/221	1.24	0/307
3	a	1.06	0/221	1.24	0/307
3	d	1.06	0/221	1.24	0/307
3	g	1.05	0/221	1.24	0/307
3	j	1.06	0/221	1.24	0/307
3	m	1.05	0/221	1.24	0/307
3	p	1.06	0/221	1.24	0/307
All	All	1.08	0/38584	1.36	126/52360 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	D	0	5
1	G	0	5
1	J	0	5
1	M	0	5
1	P	0	5
1	S	0	5
1	V	0	5
1	Y	0	5
1	b	0	5
1	e	0	5
1	h	0	5
1	k	0	5
1	n	0	5
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
2	N	0	1
2	Q	0	1
2	T	0	1
2	W	0	1
2	Z	0	1
2	c	0	1
2	f	0	1
2	i	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	l	0	1
2	o	0	1
All	All	0	84

There are no bond length outliers.

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	926	TYR	CB-CG-CD1	10.32	127.19	121.00
2	l	926	TYR	CB-CG-CD1	10.32	127.19	121.00
2	H	926	TYR	CB-CG-CD1	10.29	127.18	121.00
2	c	926	TYR	CB-CG-CD1	10.29	127.18	121.00
2	T	926	TYR	CB-CG-CD1	10.29	127.17	121.00

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	725	ARG	Peptide
1	A	757	THR	Peptide
1	A	761	GLY	Peptide
1	A	901	LEU	Peptide
1	A	903	ASP	Peptide

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	1459	0	1440	446	0
1	D	1459	0	1440	529	0
1	G	1459	0	1440	602	0
1	J	1459	0	1440	603	0
1	M	1459	0	1440	599	0
1	P	1459	0	1440	604	0
1	S	1459	0	1440	602	0
1	V	1459	0	1440	526	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1459	0	1440	458	0
1	b	1459	0	1440	0	0
1	e	1459	0	1440	0	0
1	h	1459	0	1440	0	0
1	k	1459	0	1440	0	0
1	n	1459	0	1440	0	0
2	B	1034	0	1032	205	0
2	E	1034	0	1032	206	0
2	H	1034	0	1032	202	0
2	K	1034	0	1032	204	0
2	N	1034	0	1032	203	0
2	Q	1034	0	1032	201	0
2	T	1034	0	1032	203	0
2	W	1034	0	1032	208	0
2	Z	1034	0	1032	181	0
2	c	1034	0	1032	0	0
2	f	1034	0	1032	0	0
2	i	1034	0	1032	0	0
2	l	1034	0	1032	0	0
2	o	1034	0	1032	0	0
3	C	213	0	200	35	0
3	F	213	0	200	34	0
3	I	213	0	200	36	0
3	L	213	0	200	36	0
3	O	213	0	200	34	0
3	R	213	0	200	34	0
3	U	213	0	200	37	0
3	X	213	0	200	35	0
3	a	213	0	200	0	0
3	d	213	0	200	0	0
3	g	213	0	200	0	0
3	j	213	0	200	0	0
3	m	213	0	200	0	0
3	p	213	0	200	0	0
All	All	37884	0	37408	5379	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 117.

The worst 5 of 5379 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:P:725:ARG:CZ	1:V:808:ARG:HG3	1.33	1.48
1:S:725:ARG:CZ	1:Y:808:ARG:HG3	1.33	1.46
1:S:725:ARG:NH1	1:Y:808:ARG:CG	1.77	1.46
1:D:721:LEU:HD23	1:J:805:LEU:CB	1.47	1.45
1:J:721:LEU:CD2	1:P:805:LEU:HA	0.98	1.45

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 PDB entries followed by that with respect to all EM entries.

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	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	D	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	G	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	J	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	M	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	P	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	S	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	V	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	Y	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	b	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	e	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	h	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	k	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
1	n	193/216 (89%)	147 (76%)	33 (17%)	13 (7%)	1 24
2	B	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0 11
2	E	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	K	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	N	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	Q	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	T	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	W	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	Z	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	c	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	f	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	i	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	l	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
2	o	128/130 (98%)	88 (69%)	26 (20%)	14 (11%)	0	11
3	C	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	F	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	I	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	L	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	O	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	R	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	U	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	X	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	a	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	d	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	g	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	j	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	m	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
3	p	27/48 (56%)	20 (74%)	6 (22%)	1 (4%)	4	38
All	All	4872/5516 (88%)	3570 (73%)	910 (19%)	392 (8%)	2	19

5 of 392 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	726	LEU
1	A	814	ASP

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Mol	Chain	Res	Type
1	A	878	TYR
1	A	899	TYR
1	A	902	ALA

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 PDB entries followed by that with respect to all EM entries.

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	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	D	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	G	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	J	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	M	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	P	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	S	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	V	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	Y	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	b	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	e	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	h	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	k	158/176 (90%)	124 (78%)	34 (22%)	1 9
1	n	158/176 (90%)	124 (78%)	34 (22%)	1 9
2	B	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	E	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	H	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	K	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	N	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	Q	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	T	109/109 (100%)	82 (75%)	27 (25%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	W	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	Z	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	c	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	f	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	i	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	l	109/109 (100%)	82 (75%)	27 (25%)	1 6
2	o	109/109 (100%)	82 (75%)	27 (25%)	1 6
3	C	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	F	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	I	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	L	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	O	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	R	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	U	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	X	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	a	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	d	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	g	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	j	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	m	27/43 (63%)	22 (82%)	5 (18%)	2 14
3	p	27/43 (63%)	22 (82%)	5 (18%)	2 14
All	All	4116/4592 (90%)	3192 (78%)	924 (22%)	4 9

5 of 924 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	819	ASN
2	W	1009	ARG
3	m	1035	CYS
2	T	908	LYS
1	V	733	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	861	GLN
2	W	963	GLN
3	m	1039	HIS
2	T	913	GLN
1	V	799	GLN

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 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.