wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2023 – 01:42 pm GMT

PDB ID	:	1W63
Title	:	AP1 clathrin adaptor core
Authors	:	Heldwein, E.; Macia, E.; Wang, J.; Yin, H.L.; Kirchhausen, T.; Harrison, S.C.
Deposited on	:	2004-08-12
Resolution	:	4.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

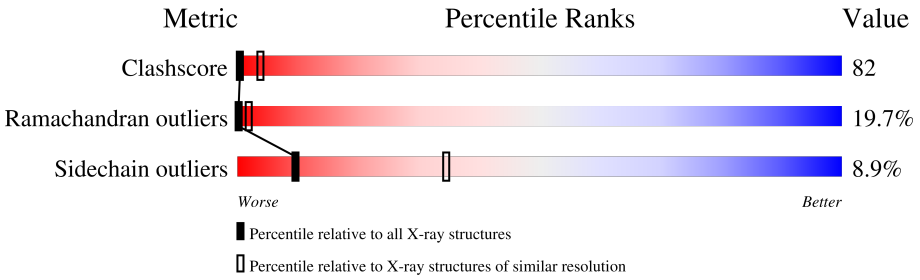
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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))
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	618	14% 59% 21% • 5%
1	C	618	14% 59% 20% • 5%
1	E	618	14% 59% 20% • 5%
1	G	618	14% 59% 20% • 5%
1	I	618	15% 59% 20% • 5%
1	K	618	13% 60% 20% • 5%
2	B	584	14% 59% 23% ••
2	D	584	14% 59% 23% ••

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Mol	Chain	Length	Quality of chain
2	F	584	14% 59% 23%
2	H	584	14% 59% 23%
2	J	584	14% 59% 23%
2	L	584	14% 59% 23%
3	M	423	23% 54% 14% 8%
3	N	423	23% 54% 14% 8%
3	O	423	22% 55% 13% 8%
3	P	423	22% 55% 14% 8%
3	R	423	22% 56% 13% 8%
3	V	423	22% 56% 13% 8%
4	Q	158	20% 54% 19% 6%
4	S	158	22% 53% 18% 6%
4	T	158	22% 53% 18% 6%
4	U	158	22% 53% 18% 6%
4	W	158	22% 53% 18% 6%
4	X	158	22% 53% 18% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 81744 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 ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	C	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	E	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	G	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	I	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			
1	K	590	Total	C	N	O	S	0	0	1
			4663	2933	821	869	40			

- Molecule 2 is a protein called ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	D	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	F	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	H	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	J	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			
2	L	576	Total	C	N	O	S	0	0	1
			4558	2907	750	874	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	MET	LEU	conflict	UNP P52303
B	439	ASP	LEU	conflict	UNP P52303
B	459	SER	ILE	conflict	UNP P52303
D	155	MET	LEU	conflict	UNP P52303
D	439	ASP	LEU	conflict	UNP P52303
D	459	SER	ILE	conflict	UNP P52303
F	155	MET	LEU	conflict	UNP P52303
F	439	ASP	LEU	conflict	UNP P52303
F	459	SER	ILE	conflict	UNP P52303
H	155	MET	LEU	conflict	UNP P52303
H	439	ASP	LEU	conflict	UNP P52303
H	459	SER	ILE	conflict	UNP P52303
J	155	MET	LEU	conflict	UNP P52303
J	439	ASP	LEU	conflict	UNP P52303
J	459	SER	ILE	conflict	UNP P52303
L	155	MET	LEU	conflict	UNP P52303
L	439	ASP	LEU	conflict	UNP P52303
L	459	SER	ILE	conflict	UNP P52303

- Molecule 3 is a protein called ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	N	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	O	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	P	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	R	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			
3	V	388	Total	C	N	O	S	0	0	0
			3166	2042	531	579	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	134	PHE	TYR	conflict	UNP P35585
M	406	ILE	LEU	conflict	UNP P35585
N	134	PHE	TYR	conflict	UNP P35585
N	406	ILE	LEU	conflict	UNP P35585

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Chain	Residue	Modelled	Actual	Comment	Reference
O	134	PHE	TYR	conflict	UNP P35585
O	406	ILE	LEU	conflict	UNP P35585
P	134	PHE	TYR	conflict	UNP P35585
P	406	ILE	LEU	conflict	UNP P35585
R	134	PHE	TYR	conflict	UNP P35585
R	406	ILE	LEU	conflict	UNP P35585
V	134	PHE	TYR	conflict	UNP P35585
V	406	ILE	LEU	conflict	UNP P35585

- Molecule 4 is a protein called ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	S	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	T	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	U	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	W	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			
4	X	149	Total	C	N	O	S	0	0	1
			1237	800	203	223	11			

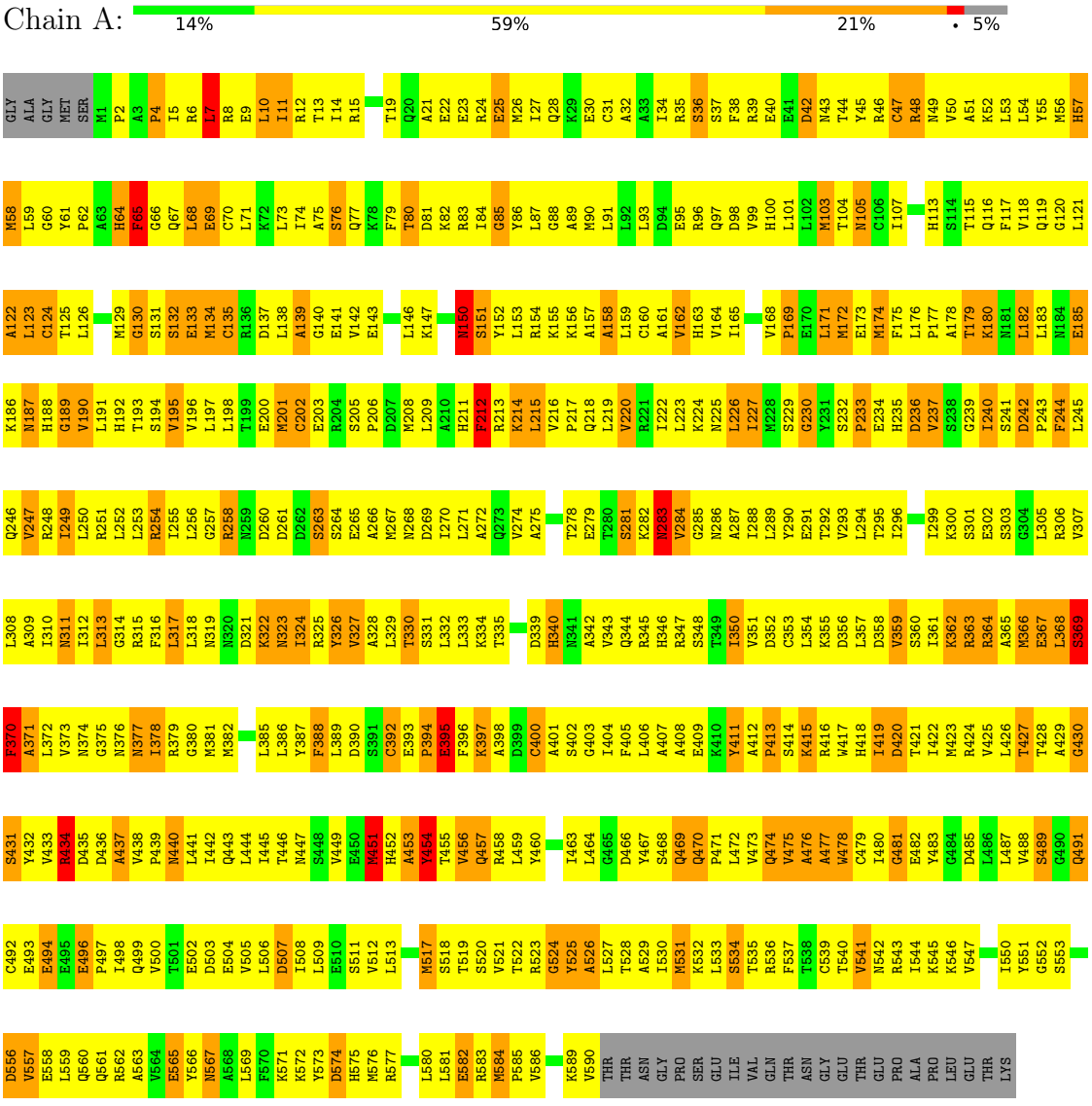
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

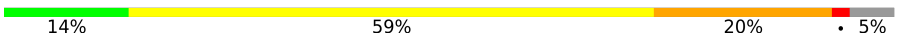
• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

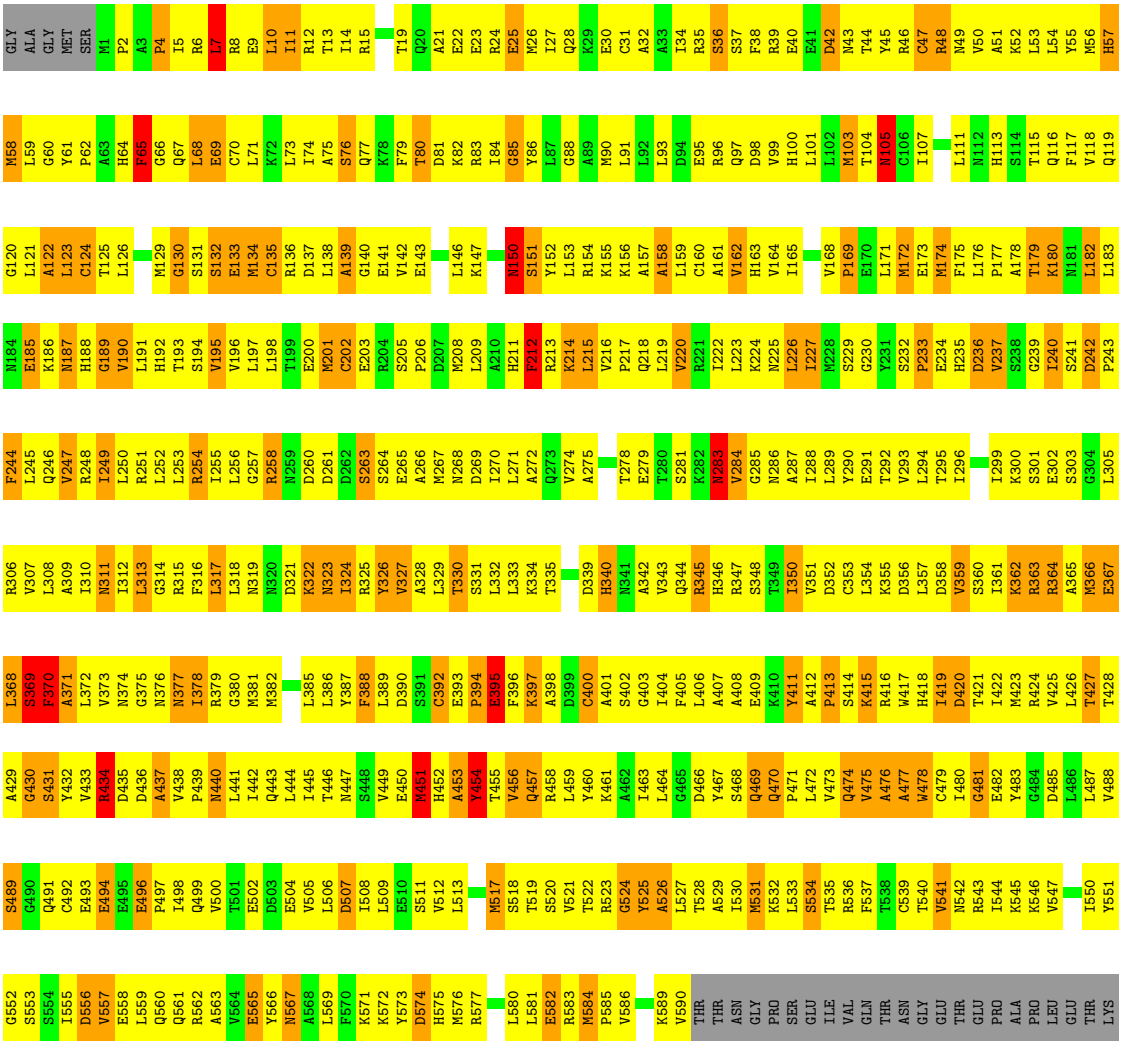
Chain A:



• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

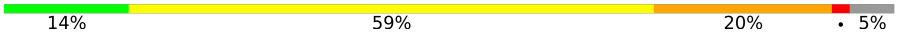
Chain C:

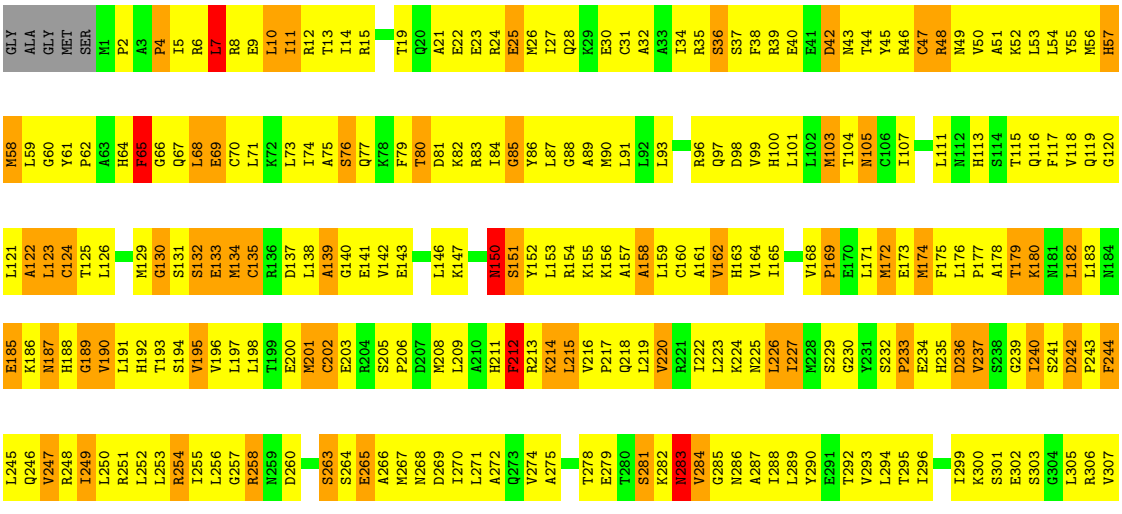


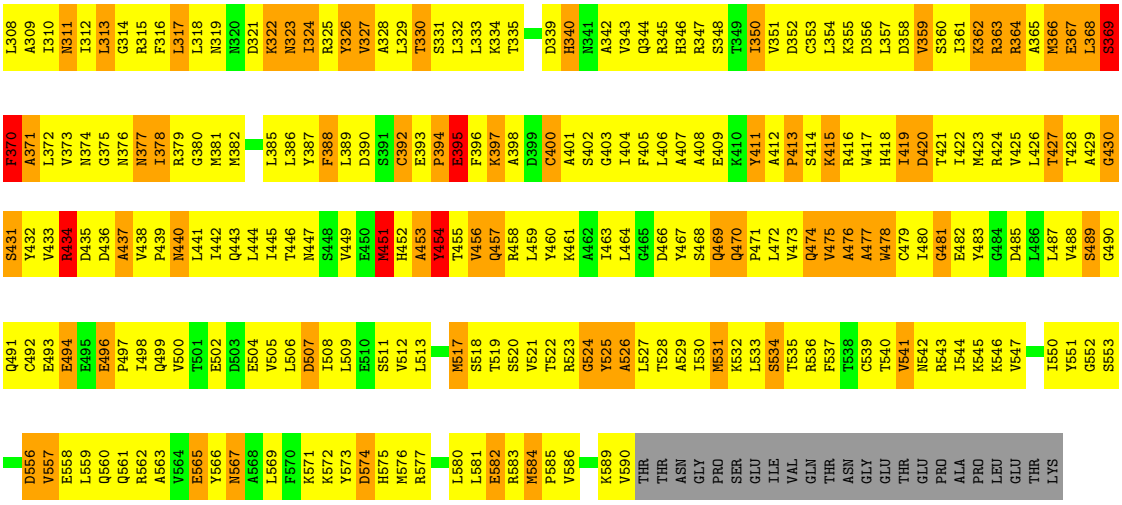


• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

Chain E:

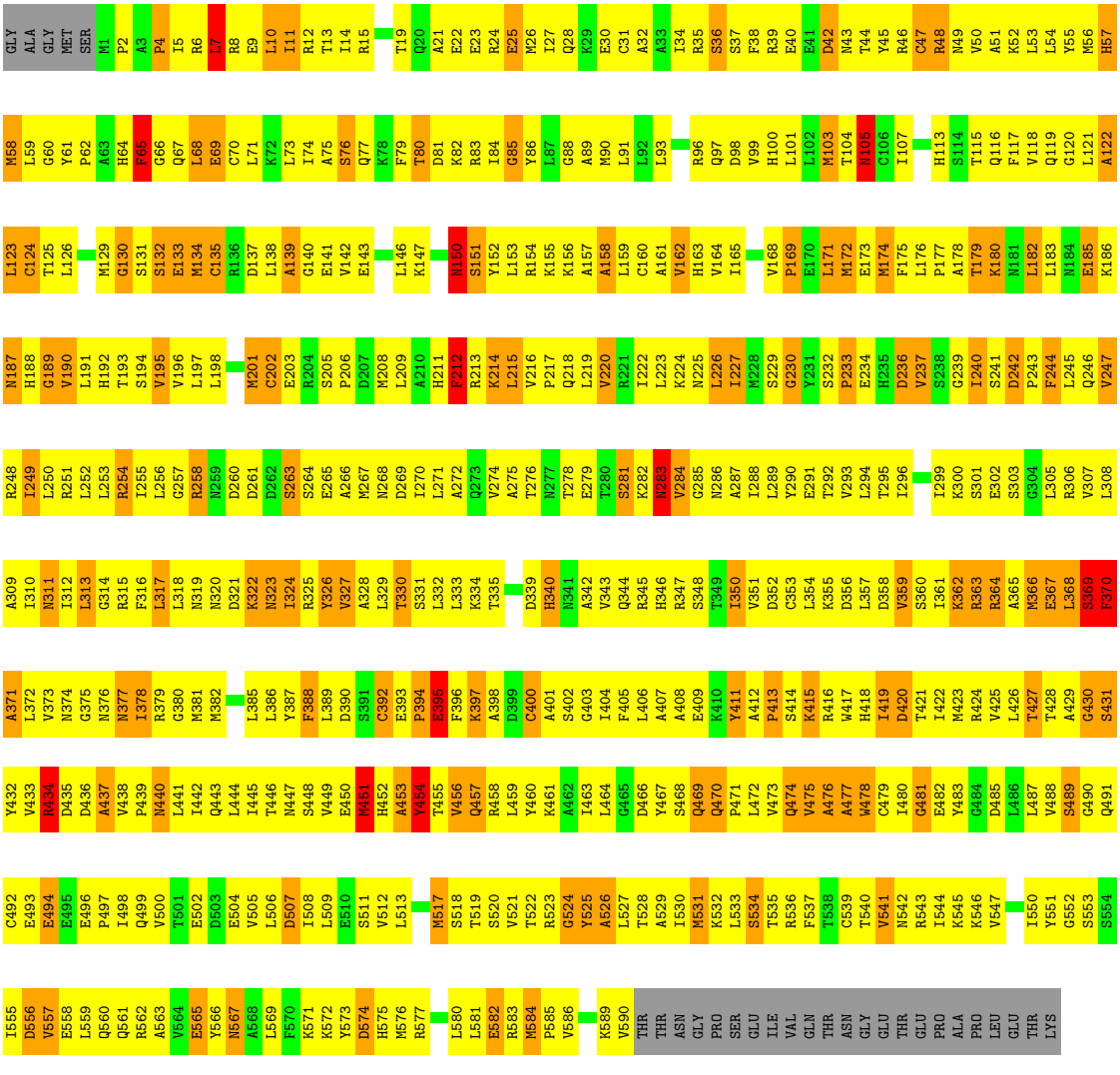






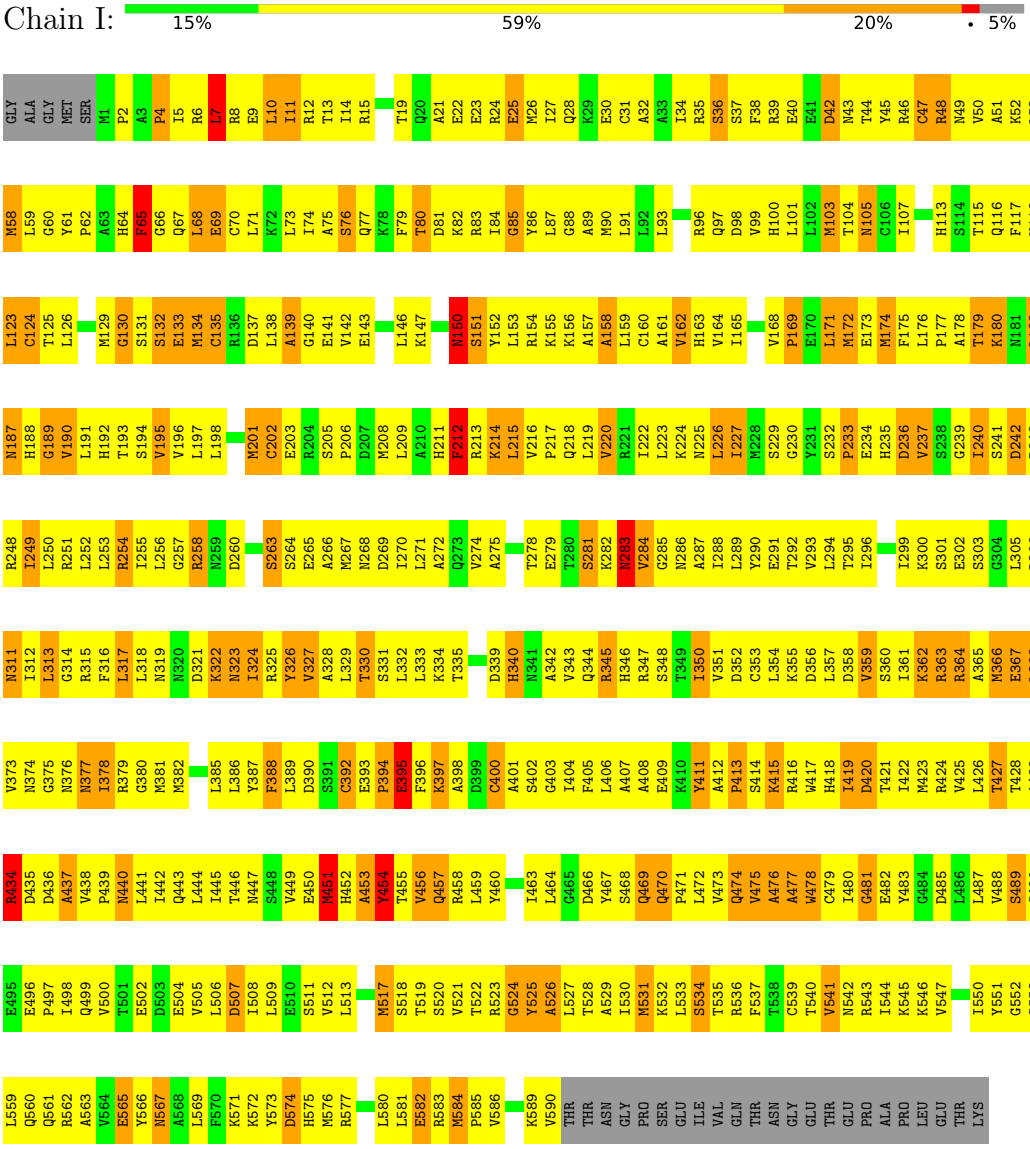
• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

Chain G:



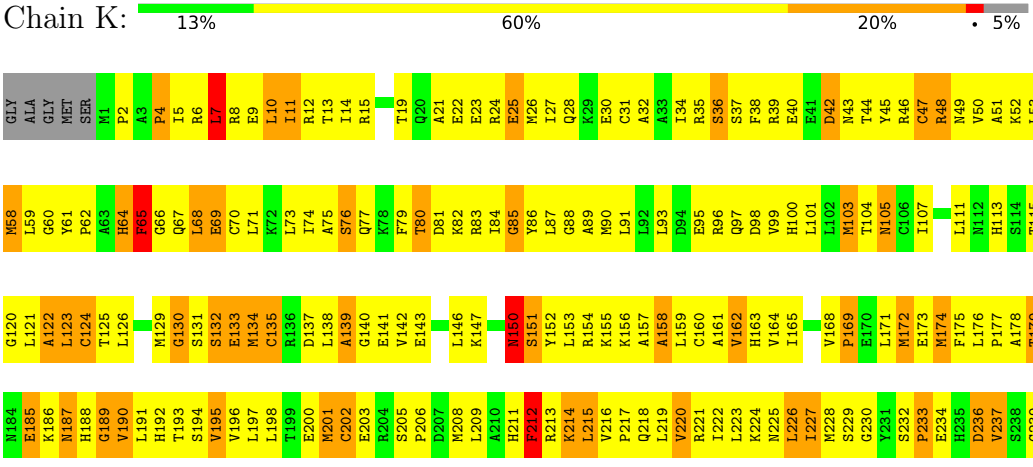
• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

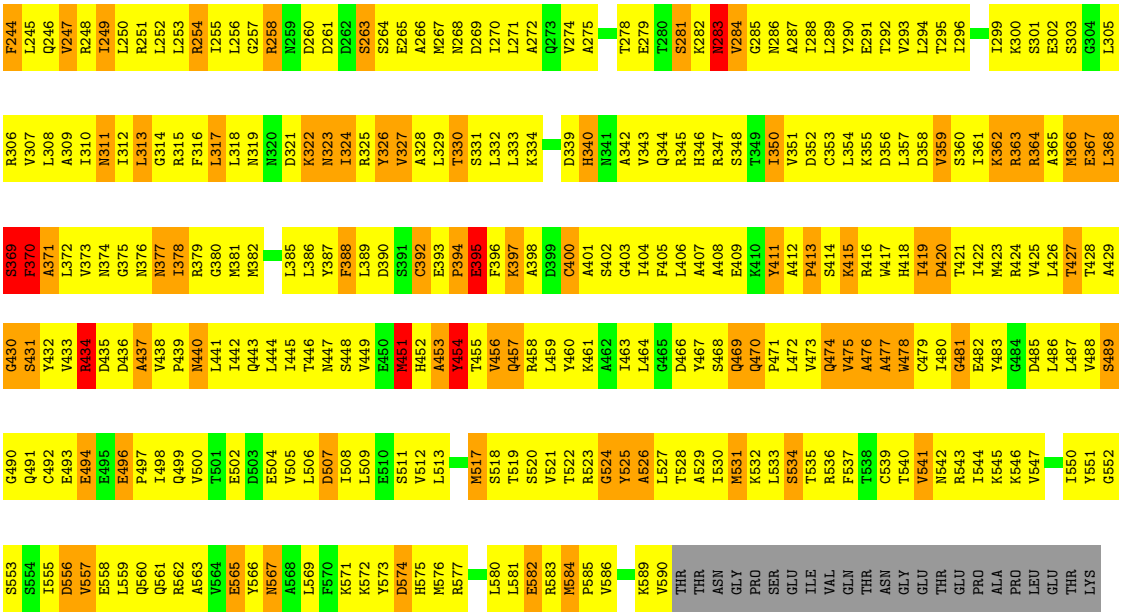
Chain I:



• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

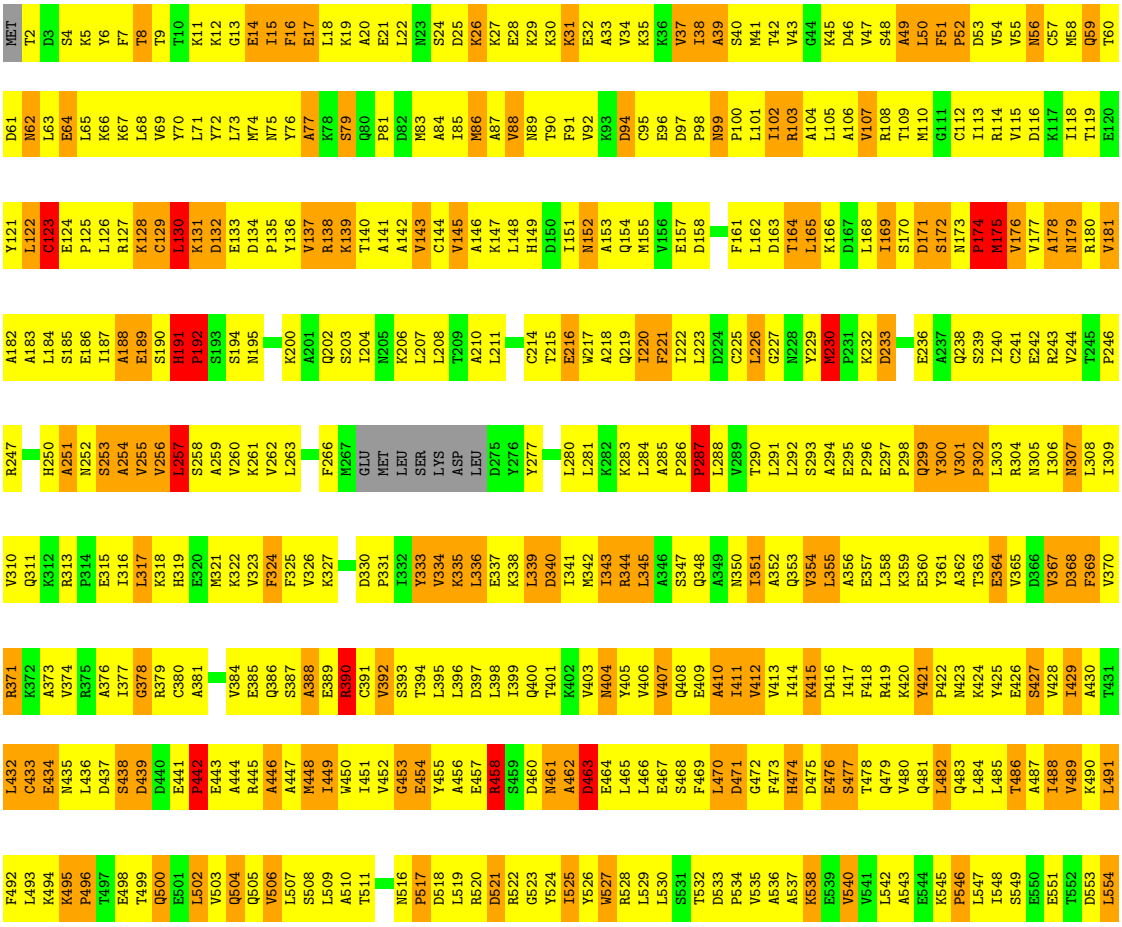
Chain K:

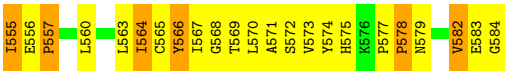




• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

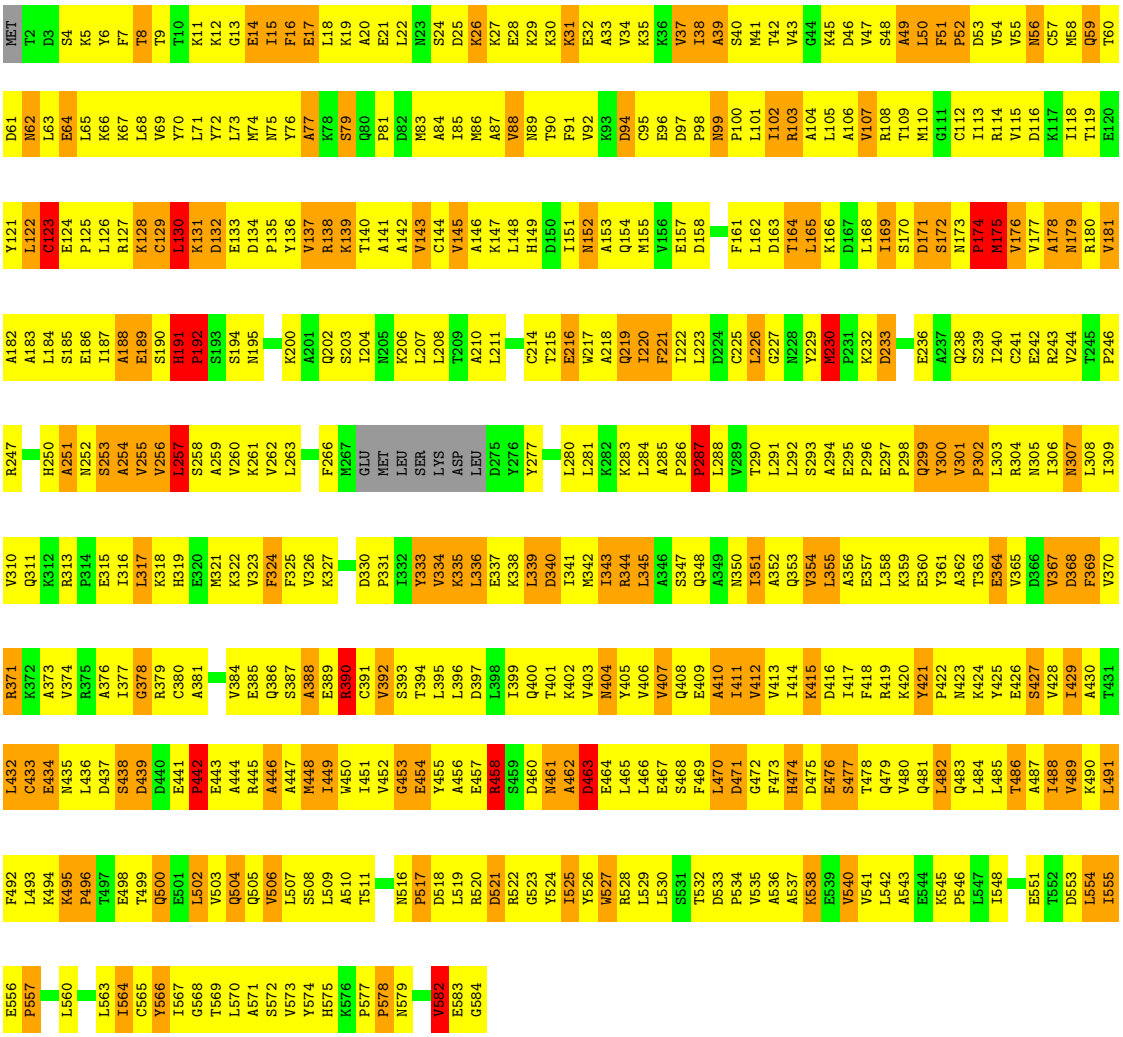
Chain B:





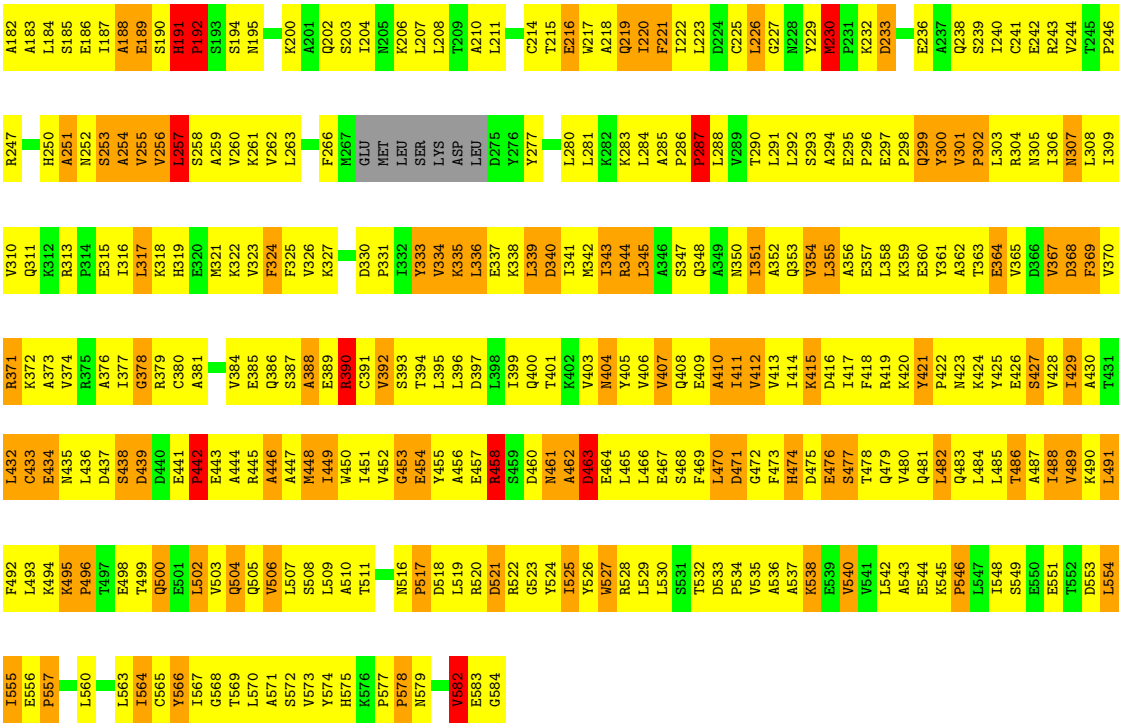
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain D:



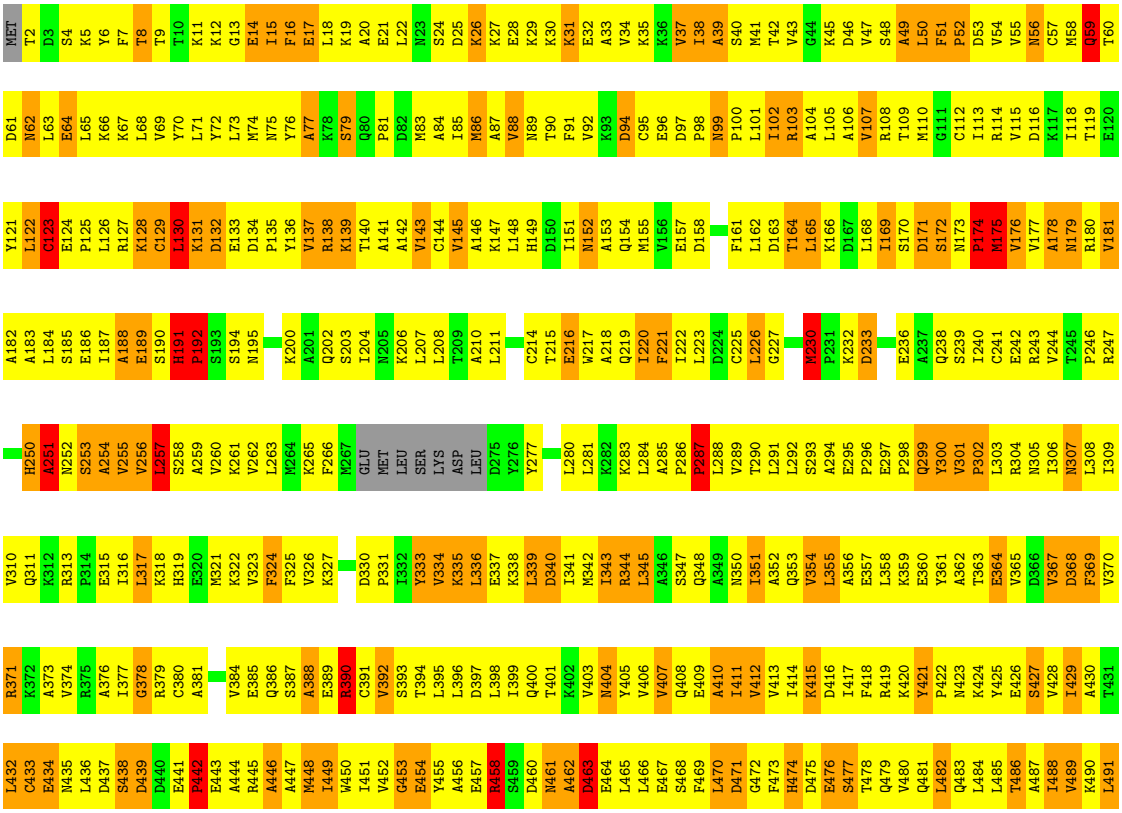
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain F:



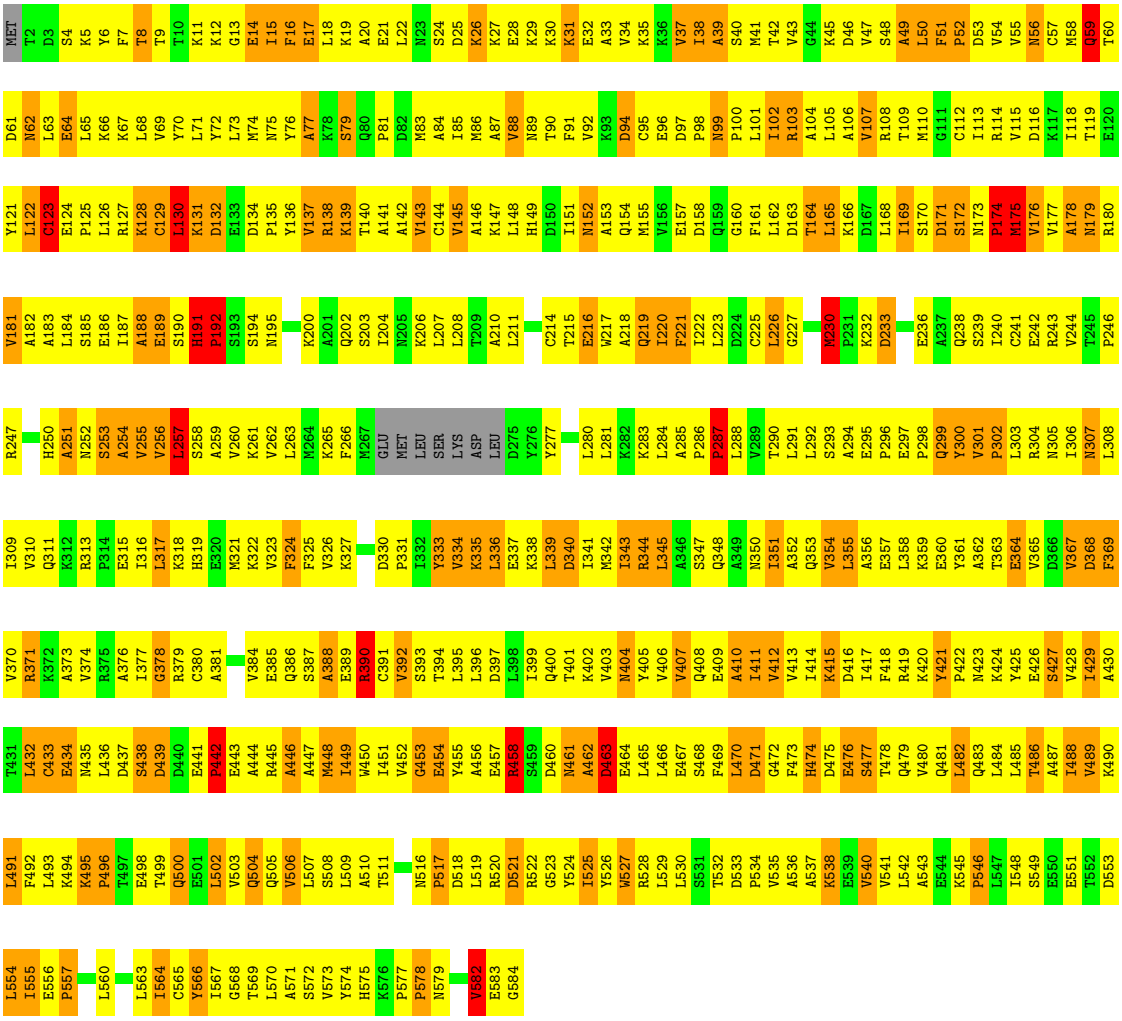
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain H:



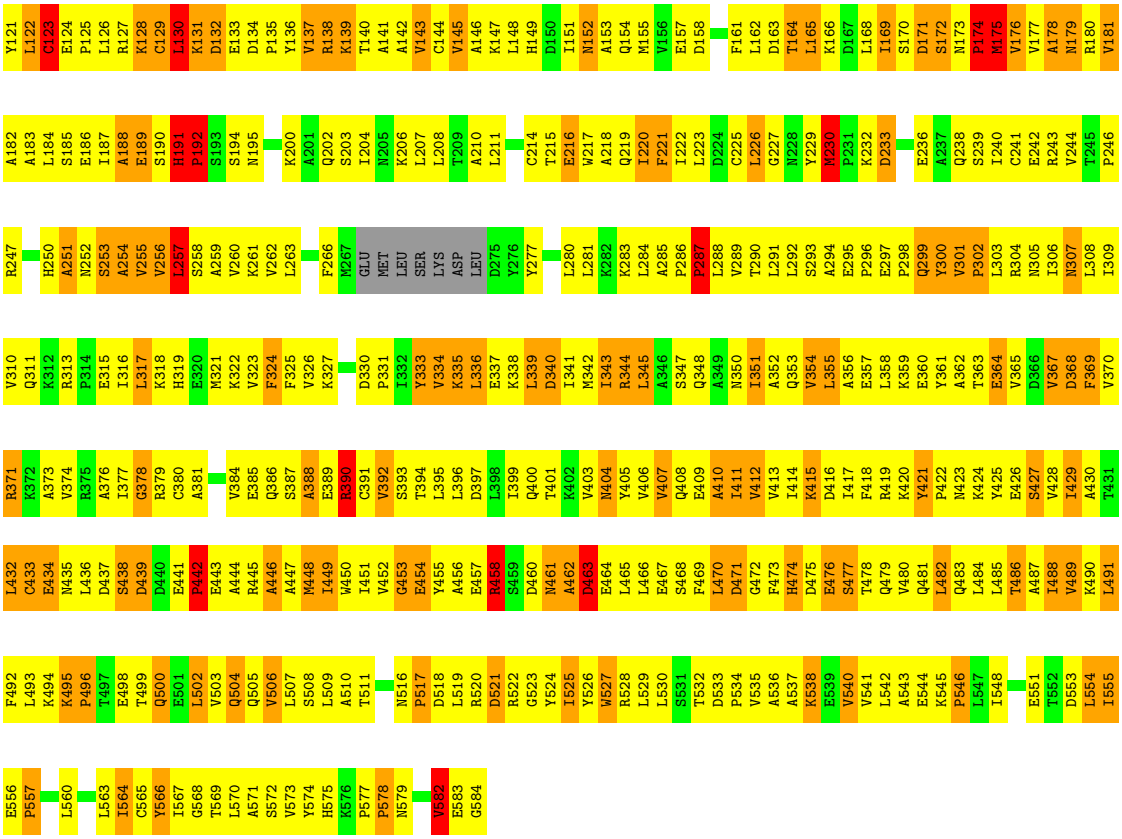
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain J:



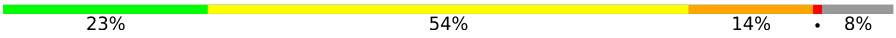
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

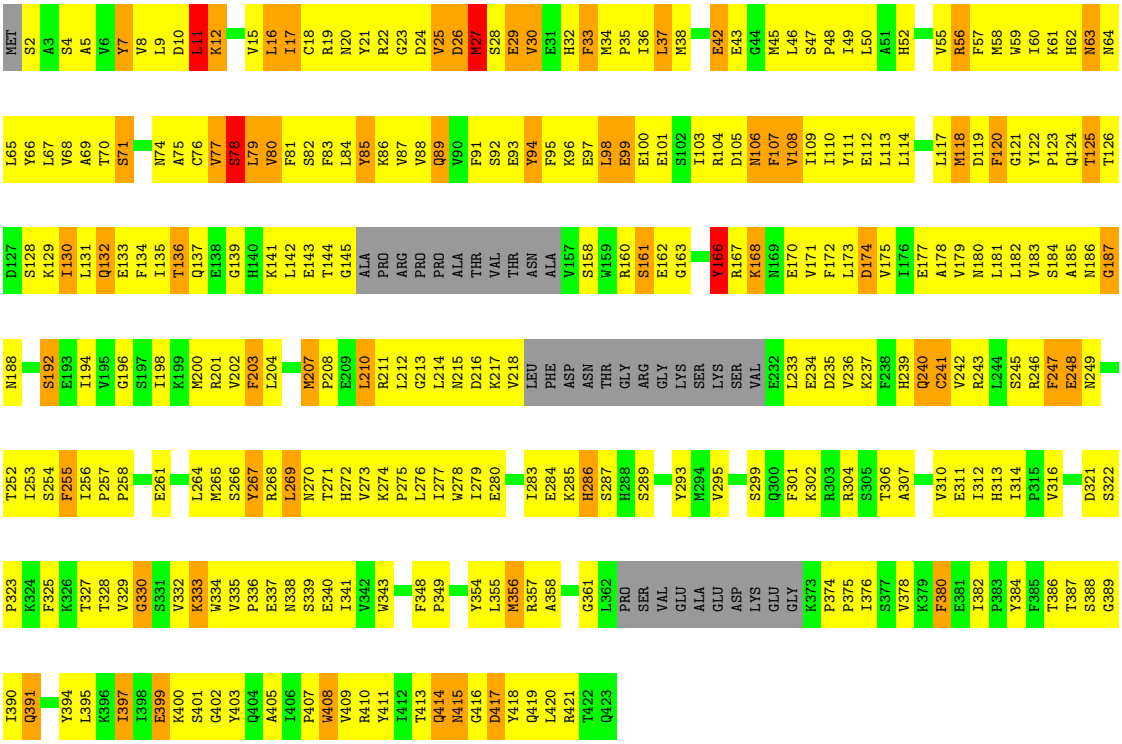
Chain L:



• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

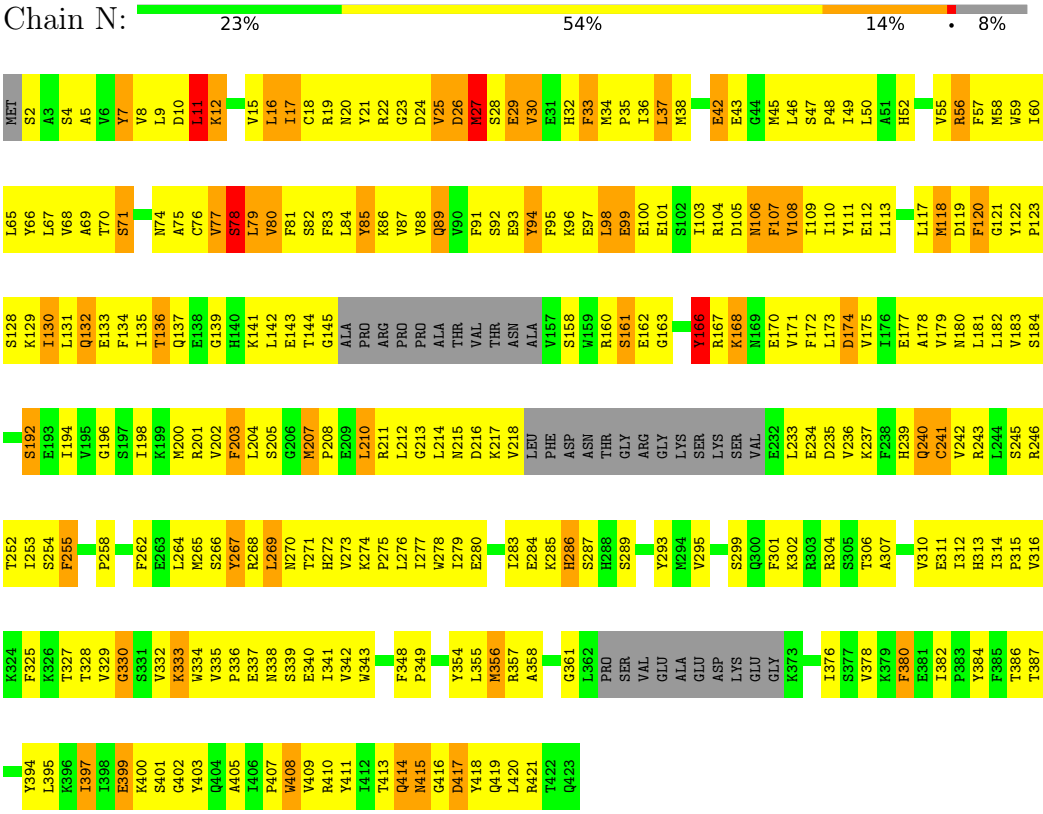
Chain M:





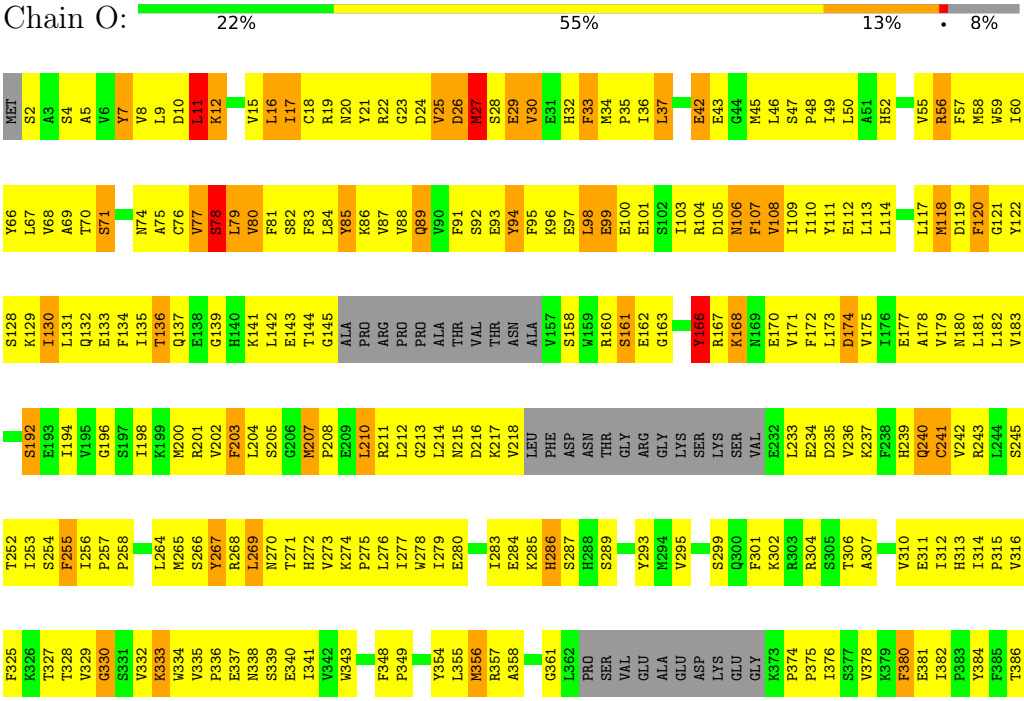
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

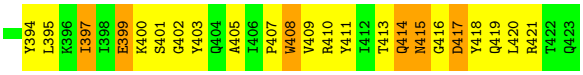
Chain N:



• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

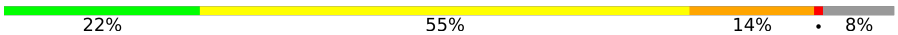
Chain O:

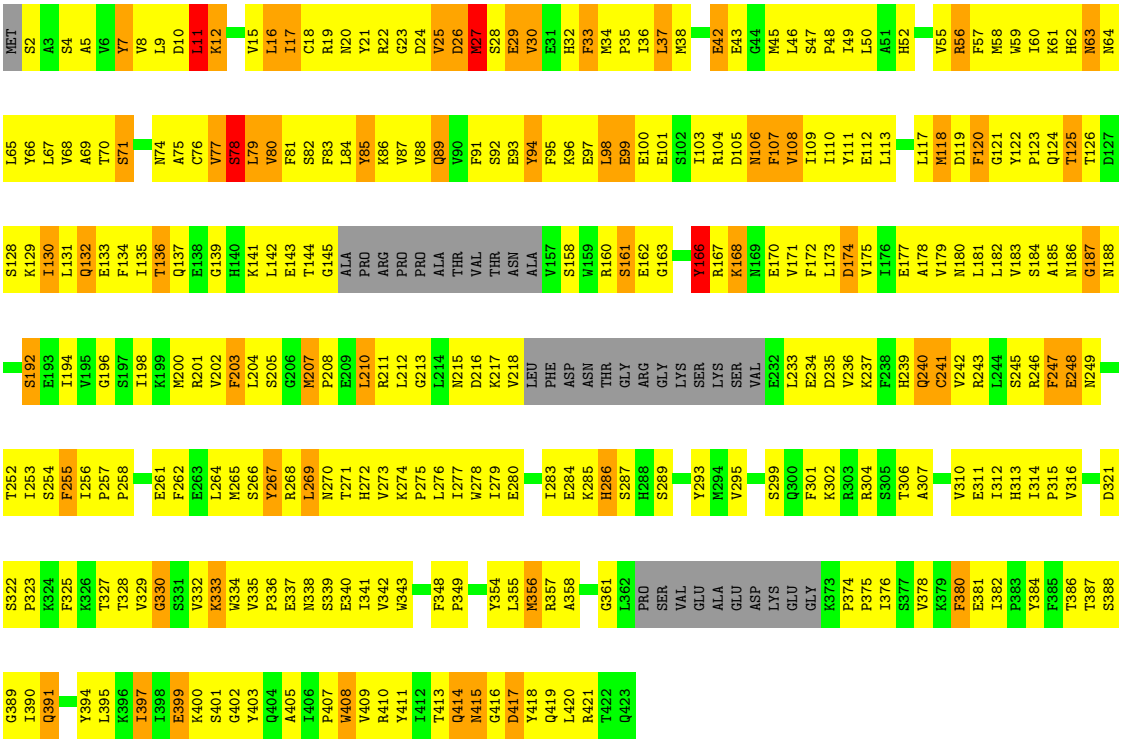




• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

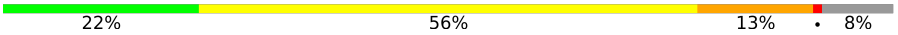
Chain P:

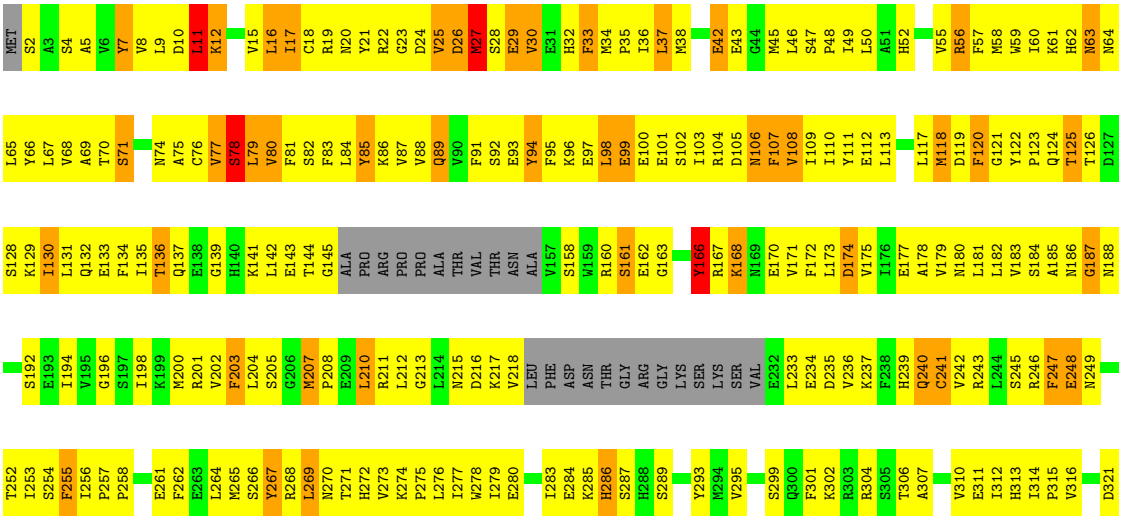


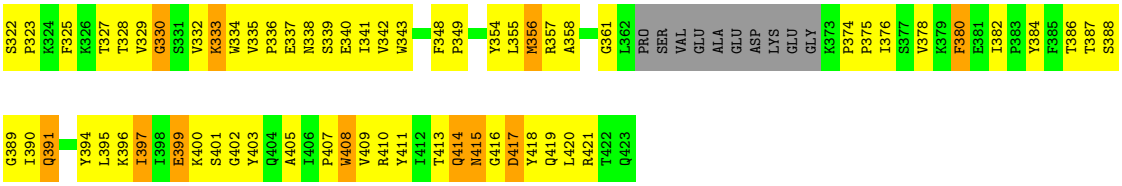


• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

Chain R:

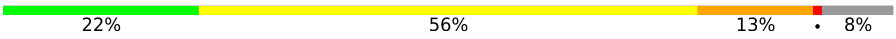


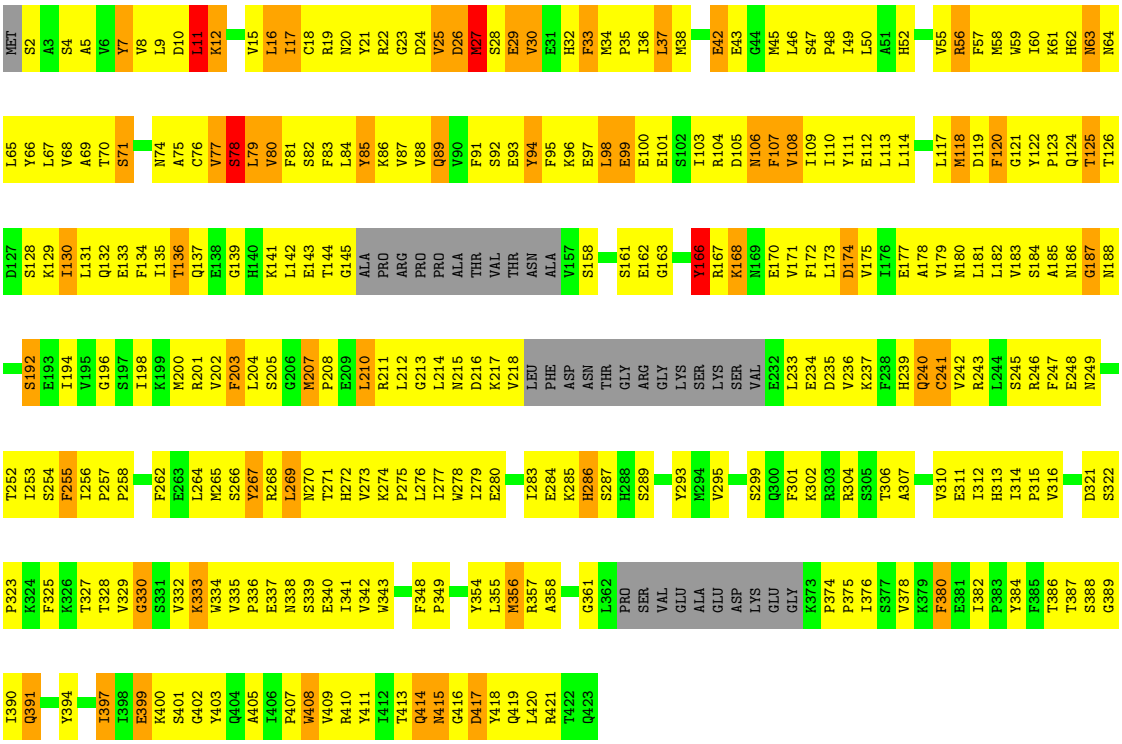




• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

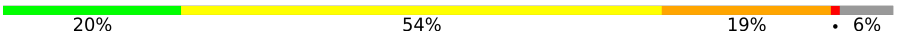
Chain V:

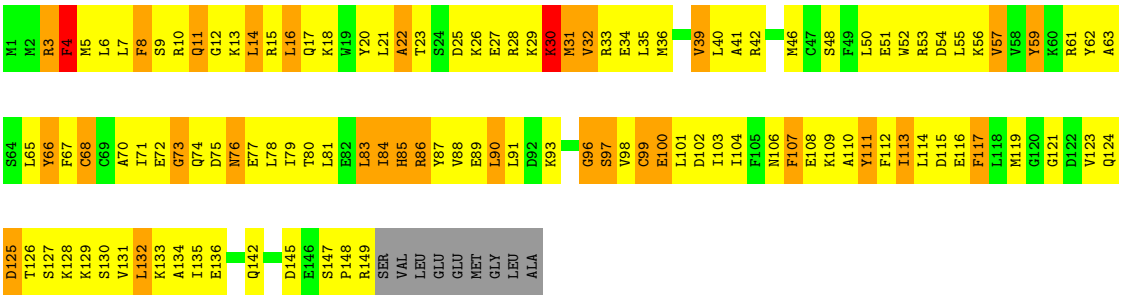




• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

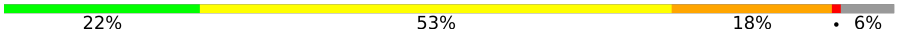
Chain Q:

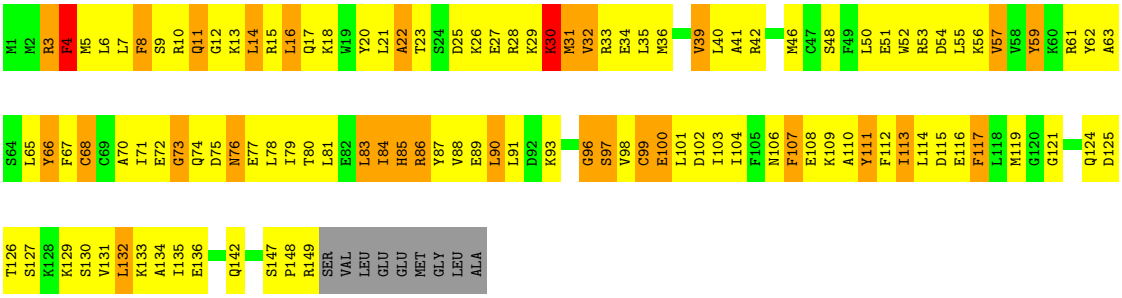




• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

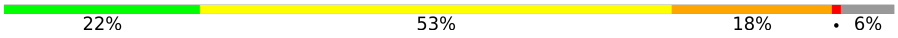
Chain S:

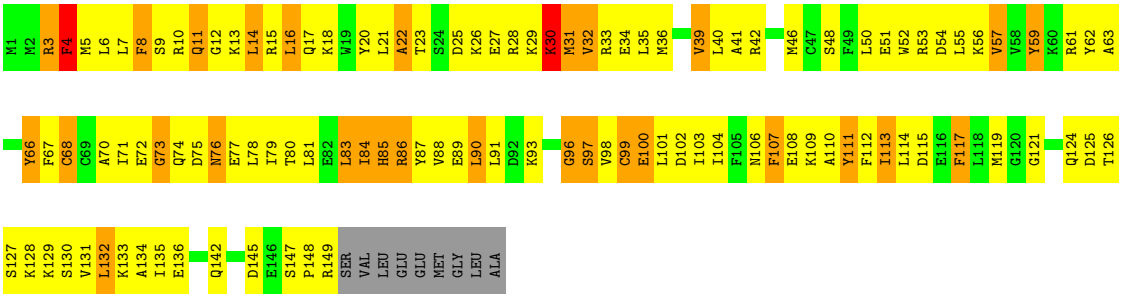




• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

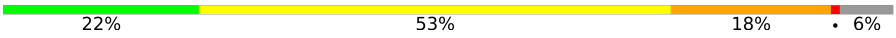
Chain T:

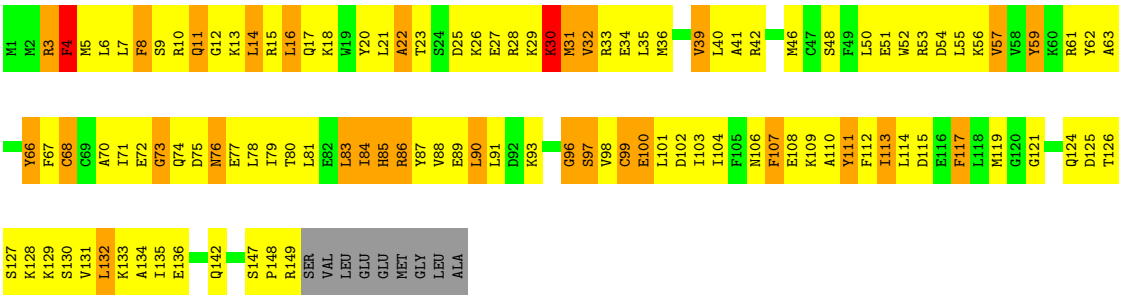




• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

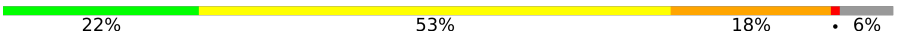
Chain U:

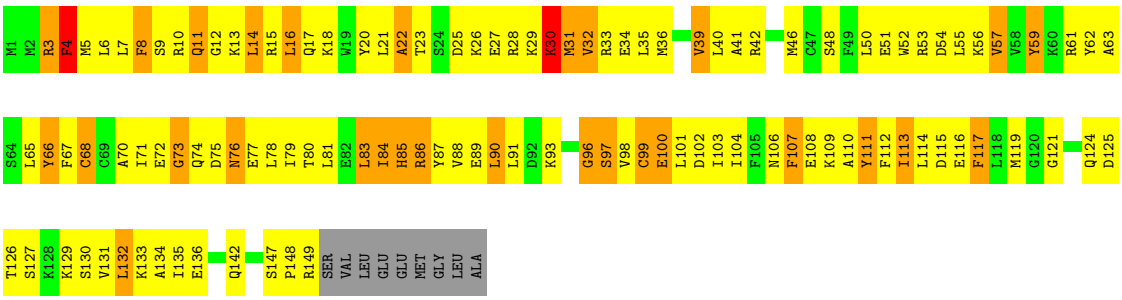




• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

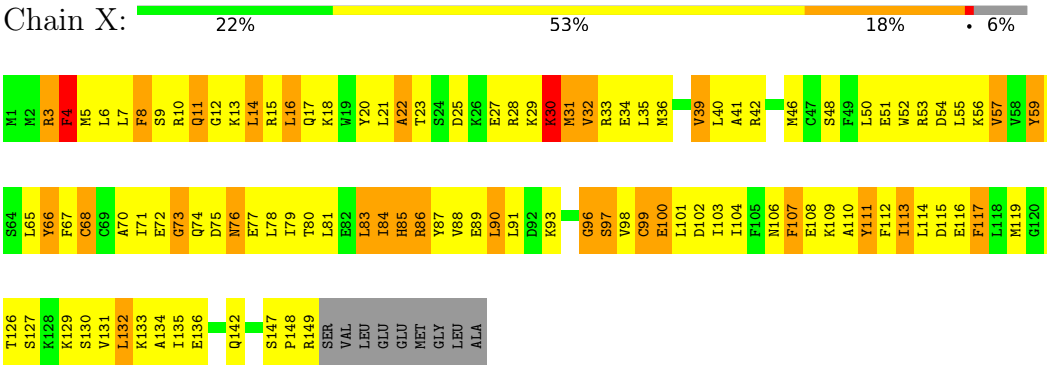
Chain W:





• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain X:


22%
53%
18%
6%
M1 M2 R3 F4 M5 L6 L7 F8 S9 R10 Q11 G12 K13 L14 R15 L16 Q17 K18 W19 Y20 L21 A22 T23 S24 D25 K26 E27 R28 K29 K30 M31 V32 R33 E34 L35 M36 V39 L40 A41 R42 M46 C47 S48 F49 L50 E51 W52 R53 D54 L55 K56 V57 V58 Y59 K60 R61 Y62 A63
S64 L65 Y66 F67 C68 C69 A70 I71 E72 G73 Q74 D75 N76 E77 L78 I79 T80 L81 E82 L83 I84 H85 R86 Y87 V88 E89 L90 L91 D92 K93 G96 S97 V98 C99 E100 L101 D102 I103 I104 F105 N106 F107 E108 K109 A110 Y111 F112 I113 L114 D115 E116 F117 L118 M119 G120 G121 Q124 D125
T126 S127 K128 K129 S130 V131 L132 K133 A134 I135 E136 Q142 S147 P148 R149 SER VAL LEU GLU GLU MET GLY LEU ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	178.14Å 178.14Å 1134.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 4.00	Depositor
% Data completeness (in resolution range)	78.8 (40.00-4.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.297 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	81744	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

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	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
1	C	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
1	E	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
1	G	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
1	I	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
1	K	0.61	1/4728 (0.0%)	0.83	4/6381 (0.1%)
2	B	0.62	0/4630	0.90	11/6278 (0.2%)
2	D	0.63	0/4630	0.90	12/6278 (0.2%)
2	F	0.63	0/4630	0.90	12/6278 (0.2%)
2	H	0.62	0/4630	0.90	12/6278 (0.2%)
2	J	0.62	0/4630	0.90	12/6278 (0.2%)
2	L	0.62	0/4630	0.90	12/6278 (0.2%)
3	M	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
3	N	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
3	O	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
3	P	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
3	R	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
3	V	0.73	1/3237 (0.0%)	0.93	3/4366 (0.1%)
4	Q	0.64	1/1259 (0.1%)	0.75	0/1686
4	S	0.64	1/1259 (0.1%)	0.75	0/1686
4	T	0.64	1/1259 (0.1%)	0.75	0/1686
4	U	0.64	1/1259 (0.1%)	0.75	0/1686
4	W	0.64	1/1259 (0.1%)	0.75	0/1686
4	X	0.64	1/1259 (0.1%)	0.75	0/1686
All	All	0.65	18/83124 (0.0%)	0.87	113/112266 (0.1%)

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
3	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	2
3	O	0	2
3	P	0	2
3	R	0	2
3	V	0	2
All	All	0	12

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	68	CYS	CB-SG	-5.94	1.72	1.81
4	Q	68	CYS	CB-SG	-5.92	1.72	1.81
4	W	68	CYS	CB-SG	-5.90	1.72	1.81
4	S	68	CYS	CB-SG	-5.89	1.72	1.81
4	U	68	CYS	CB-SG	-5.87	1.72	1.81

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	174	PRO	CA-N-CD	-11.26	95.73	111.50
2	B	174	PRO	CA-N-CD	-11.24	95.77	111.50
2	L	174	PRO	CA-N-CD	-11.23	95.78	111.50
2	F	174	PRO	CA-N-CD	-11.22	95.78	111.50
2	J	174	PRO	CA-N-CD	-11.22	95.79	111.50

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	166	TYR	Sidechain
3	M	85	TYR	Sidechain
3	N	166	TYR	Sidechain
3	N	85	TYR	Sidechain
3	O	85	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	4663	0	4792	832	0
1	C	4663	0	4792	817	6
1	E	4663	0	4792	826	12
1	G	4663	0	4792	824	0
1	I	4663	0	4792	816	7
1	K	4663	0	4792	819	12
2	B	4558	0	4674	867	0
2	D	4558	0	4674	877	0
2	F	4558	0	4674	874	3
2	H	4558	0	4674	876	0
2	J	4558	0	4674	876	0
2	L	4558	0	4674	861	4
3	M	3166	0	3178	431	0
3	N	3166	0	3178	432	0
3	O	3166	0	3178	422	0
3	P	3166	0	3178	436	0
3	R	3166	0	3178	434	0
3	V	3166	0	3178	419	0
4	Q	1237	0	1261	227	0
4	S	1237	0	1261	217	0
4	T	1237	0	1261	221	0
4	U	1237	0	1261	216	0
4	W	1237	0	1261	225	0
4	X	1237	0	1261	221	0
All	All	81744	0	83430	13624	22

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 82.

The worst 5 of 13624 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:E:488:VAL:HA	1:E:500:VAL:HG11	1.20	1.19
1:A:482:GLU:HB3	1:A:584:MET:SD	1.83	1.18
1:E:482:GLU:HB3	1:E:584:MET:SD	1.83	1.18
1:G:482:GLU:HB3	1:G:584:MET:SD	1.83	1.17
1:K:482:GLU:HB3	1:K:584:MET:SD	1.83	1.17

The worst 5 of 22 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:E:265:GLU:OE2	1:K:221:ARG:NH1[1_545]	1.07	1.13
1:E:265:GLU:OE1	1:K:221:ARG:CZ[1_545]	1.30	0.90
1:E:265:GLU:CD	1:K:221:ARG:NH2[1_545]	1.42	0.78
1:E:265:GLU:OE1	1:K:221:ARG:NH2[1_545]	1.44	0.76
1:I:345:ARG:NE	2:L:457:GLU:OE2[5_445]	1.44	0.76

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	588/618 (95%)	254 (43%)	210 (36%)	124 (21%)	0	1
1	C	588/618 (95%)	254 (43%)	210 (36%)	124 (21%)	0	1
1	E	588/618 (95%)	253 (43%)	211 (36%)	124 (21%)	0	1
1	G	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
1	I	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
1	K	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	1
2	B	572/584 (98%)	239 (42%)	192 (34%)	141 (25%)	0	1
2	D	572/584 (98%)	239 (42%)	191 (33%)	142 (25%)	0	1
2	F	572/584 (98%)	240 (42%)	190 (33%)	142 (25%)	0	1
2	H	572/584 (98%)	238 (42%)	193 (34%)	141 (25%)	0	1
2	J	572/584 (98%)	239 (42%)	191 (33%)	142 (25%)	0	1
2	L	572/584 (98%)	239 (42%)	192 (34%)	141 (25%)	0	1
3	M	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5
3	N	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5
3	O	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5
3	P	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5
3	R	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5
3	V	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	Q	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
4	S	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
4	T	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
4	U	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
4	W	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
4	X	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0 4
All	All	10122/10698 (95%)	4988 (49%)	3145 (31%)	1989 (20%)	0 2

5 of 1989 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	58	MET
1	A	76	SER
1	A	132	SER
1	A	162	VAL

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	523/546 (96%)	478 (91%)	45 (9%)	10 37
1	C	523/546 (96%)	478 (91%)	45 (9%)	10 37
1	E	523/546 (96%)	479 (92%)	44 (8%)	11 37
1	G	523/546 (96%)	478 (91%)	45 (9%)	10 37
1	I	523/546 (96%)	479 (92%)	44 (8%)	11 37
1	K	523/546 (96%)	478 (91%)	45 (9%)	10 37
2	B	515/523 (98%)	475 (92%)	40 (8%)	12 39
2	D	515/523 (98%)	475 (92%)	40 (8%)	12 39
2	F	515/523 (98%)	475 (92%)	40 (8%)	12 39
2	H	515/523 (98%)	475 (92%)	40 (8%)	12 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	515/523 (98%)	475 (92%)	40 (8%)	12 39
2	L	515/523 (98%)	475 (92%)	40 (8%)	12 39
3	M	355/383 (93%)	322 (91%)	33 (9%)	9 32
3	N	355/383 (93%)	322 (91%)	33 (9%)	9 32
3	O	355/383 (93%)	322 (91%)	33 (9%)	9 32
3	P	355/383 (93%)	322 (91%)	33 (9%)	9 32
3	R	355/383 (93%)	322 (91%)	33 (9%)	9 32
3	V	355/383 (93%)	322 (91%)	33 (9%)	9 32
4	Q	136/144 (94%)	118 (87%)	18 (13%)	4 21
4	S	136/144 (94%)	118 (87%)	18 (13%)	4 21
4	T	136/144 (94%)	118 (87%)	18 (13%)	4 21
4	U	136/144 (94%)	118 (87%)	18 (13%)	4 21
4	W	136/144 (94%)	118 (87%)	18 (13%)	4 21
4	X	136/144 (94%)	118 (87%)	18 (13%)	4 21
All	All	9174/9576 (96%)	8360 (91%)	814 (9%)	9 34

5 of 814 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	531	MET
3	N	414	GLN
4	X	11	GLN
2	L	138	ARG
1	K	518	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 215 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	163	HIS
1	K	163	HIS
4	U	76	ASN
1	I	235	HIS
2	J	152	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 monosaccharides 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.