



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:07 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : trunk26865

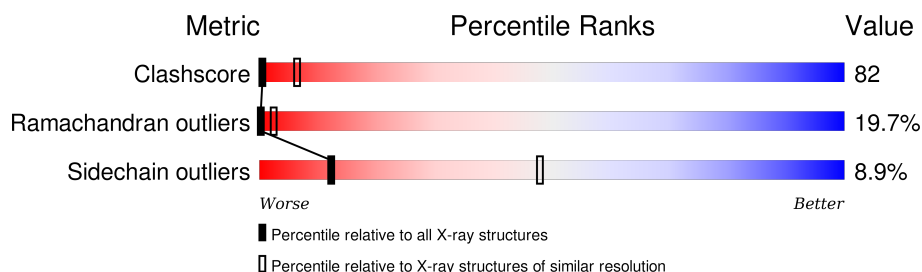
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	618	
1	C	618	
1	E	618	
1	G	618	
1	I	618	
1	K	618	
2	B	584	

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Mol	Chain	Length	Quality of chain
2	D	584	
2	F	584	
2	H	584	
2	J	584	
2	L	584	
3	M	423	
3	N	423	
3	O	423	
3	P	423	
3	R	423	
3	V	423	
4	Q	158	
4	S	158	
4	T	158	
4	U	158	
4	W	158	
4	X	158	

2 Entry composition

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

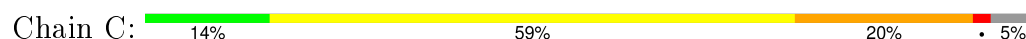
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

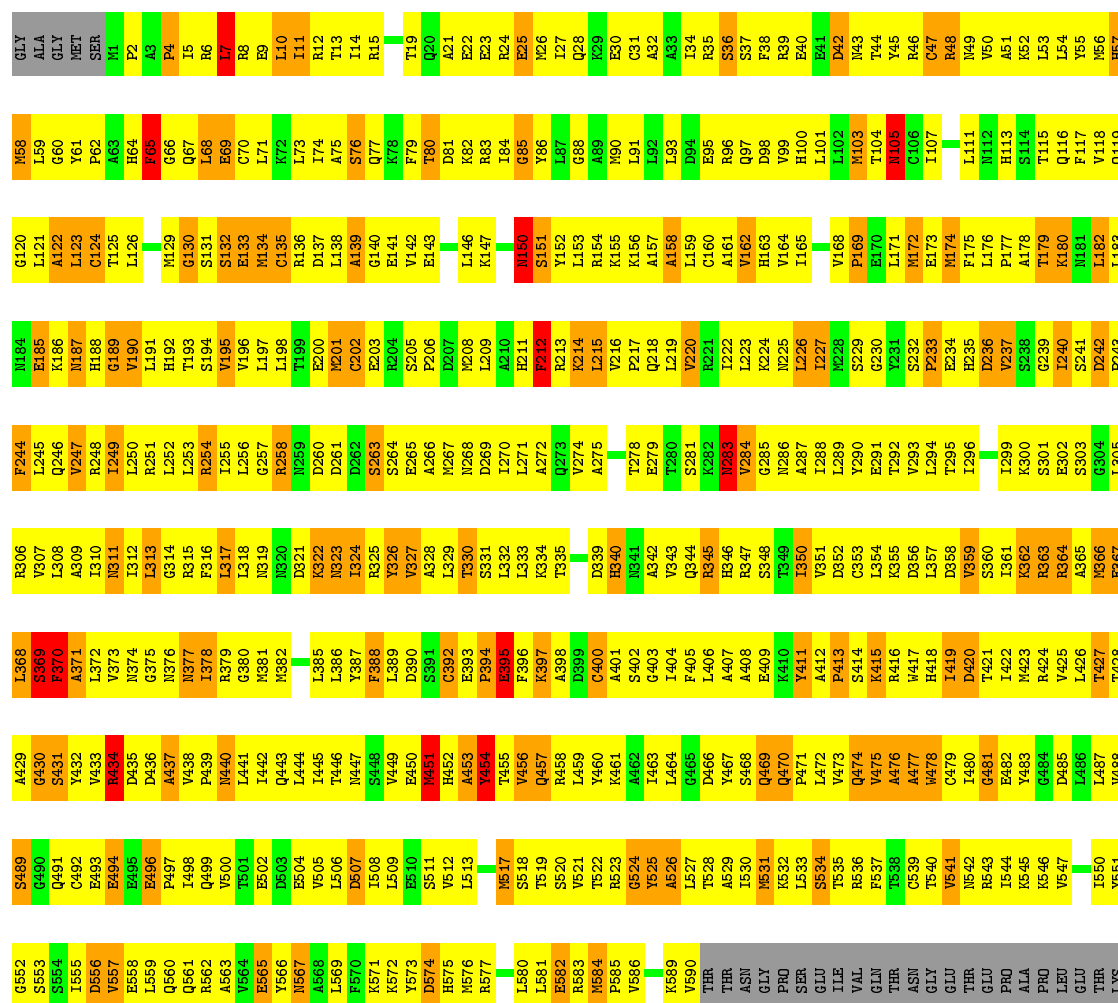
Note EDS was not executed.

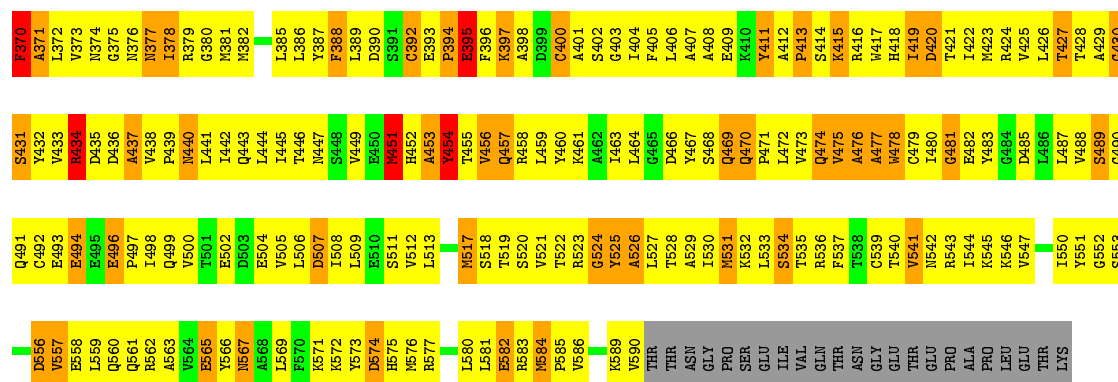
- Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT



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

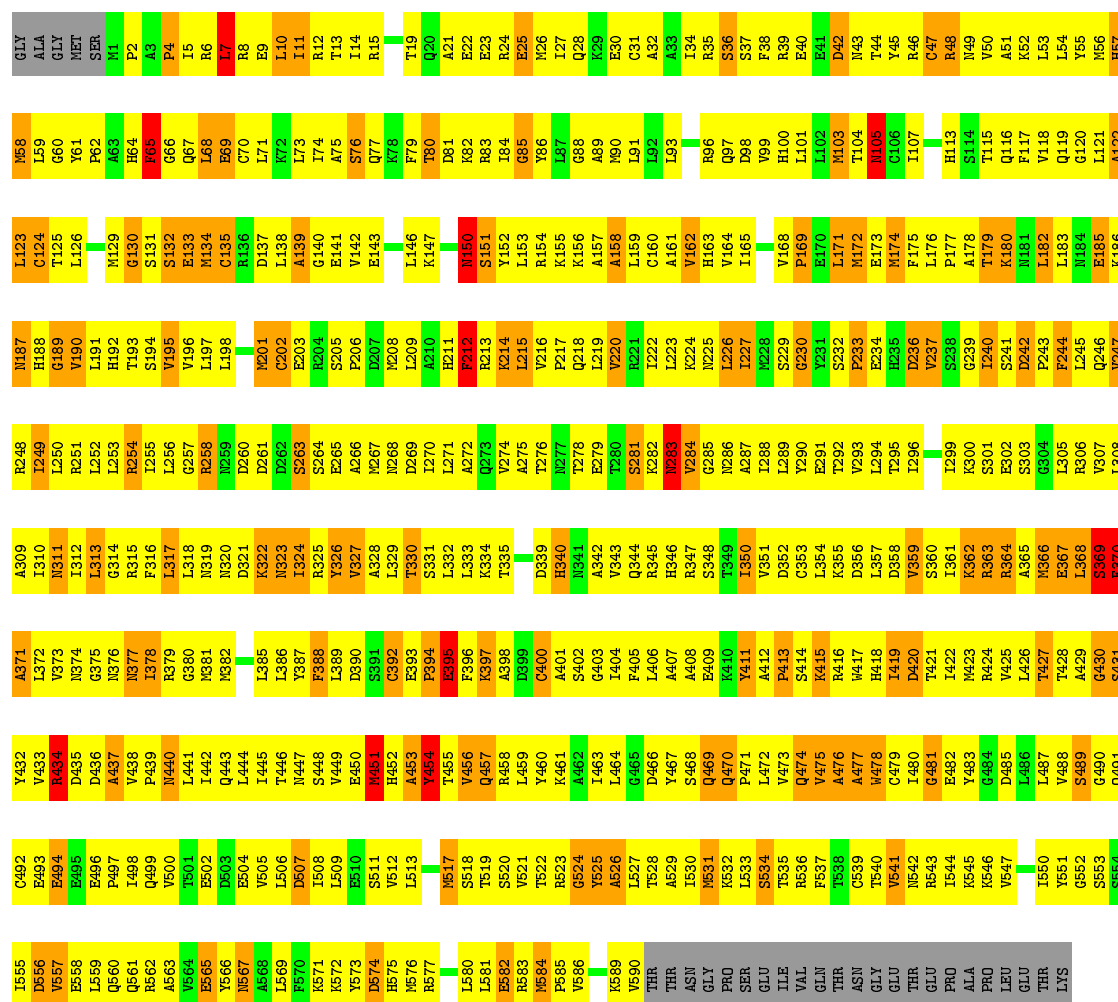






• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

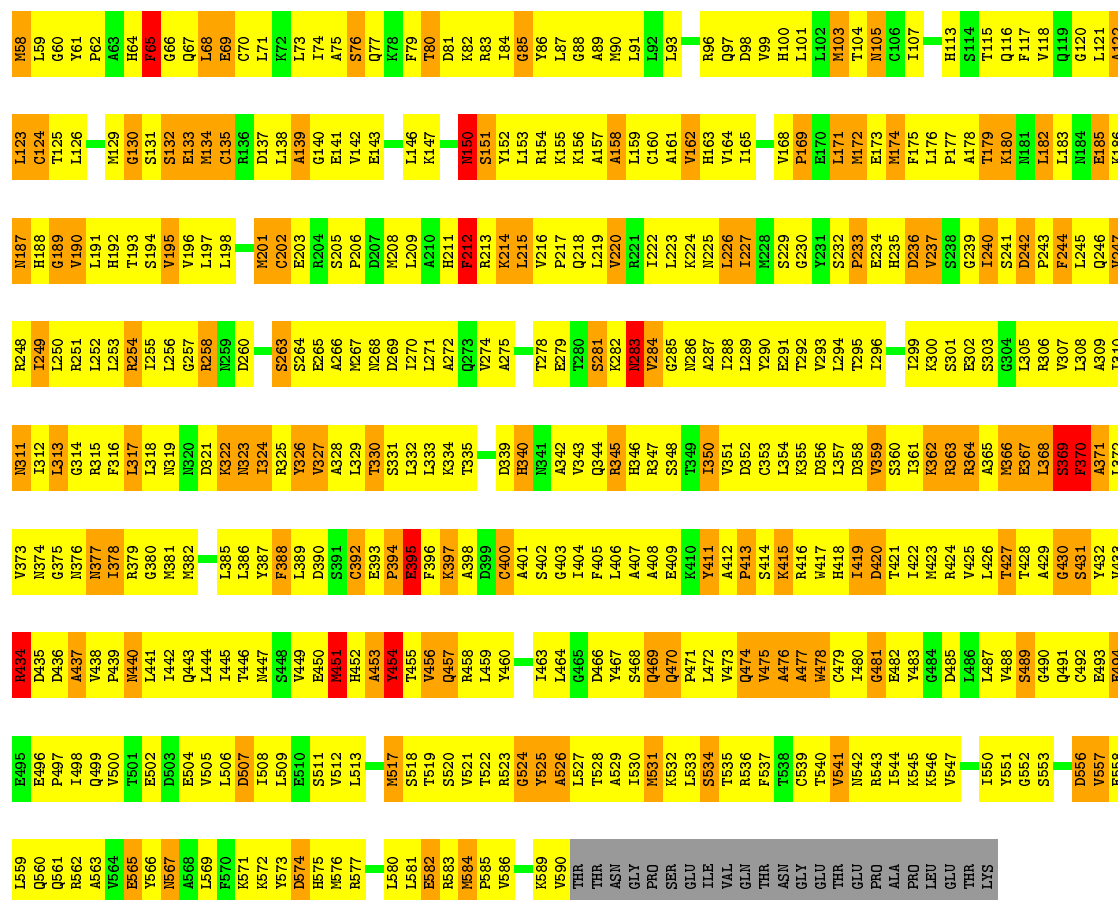
Chain G: 14% 59% 20% 5%



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

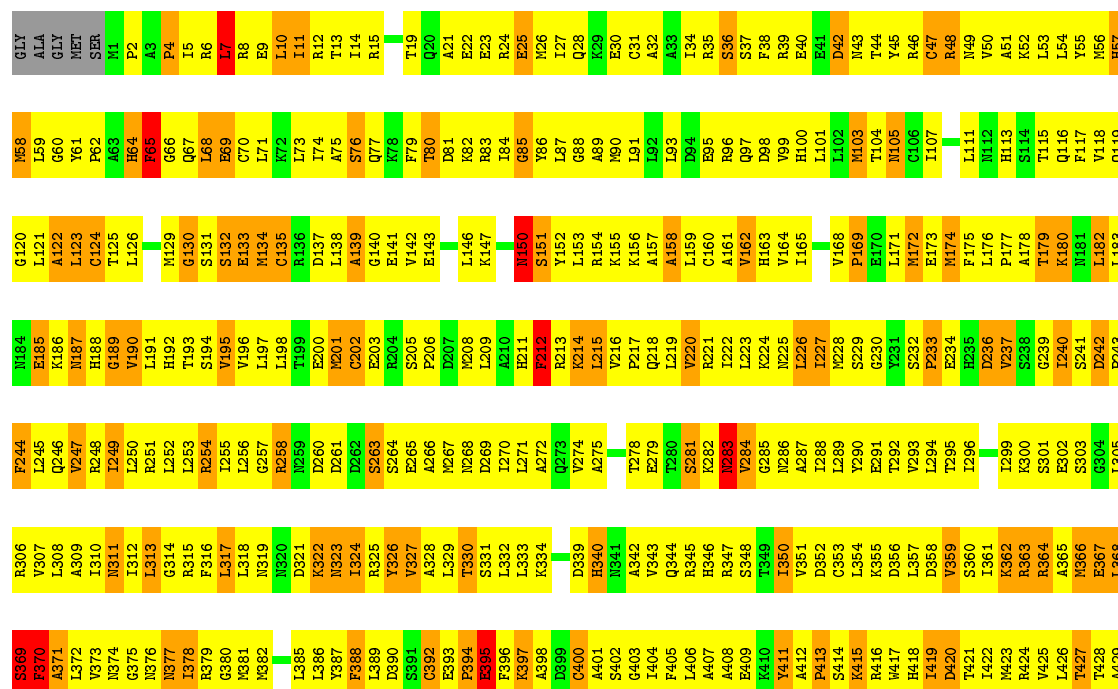
Chain I: 15% 59% 20% 5%

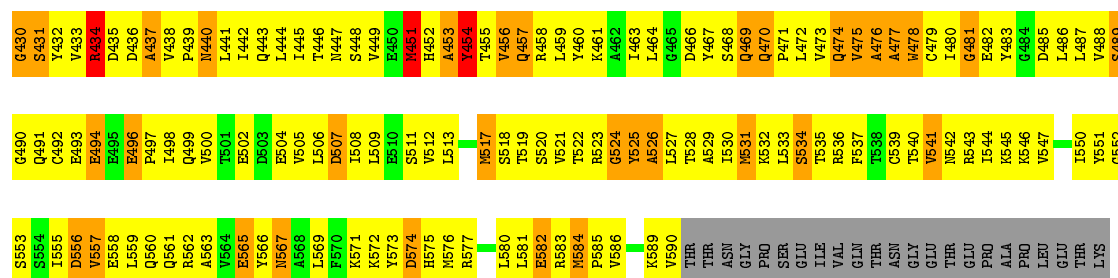




• Molecule 1: ADAPTER-RELATED PROTEIN COMPLEX 1 GAMMA 1 SUBUNIT

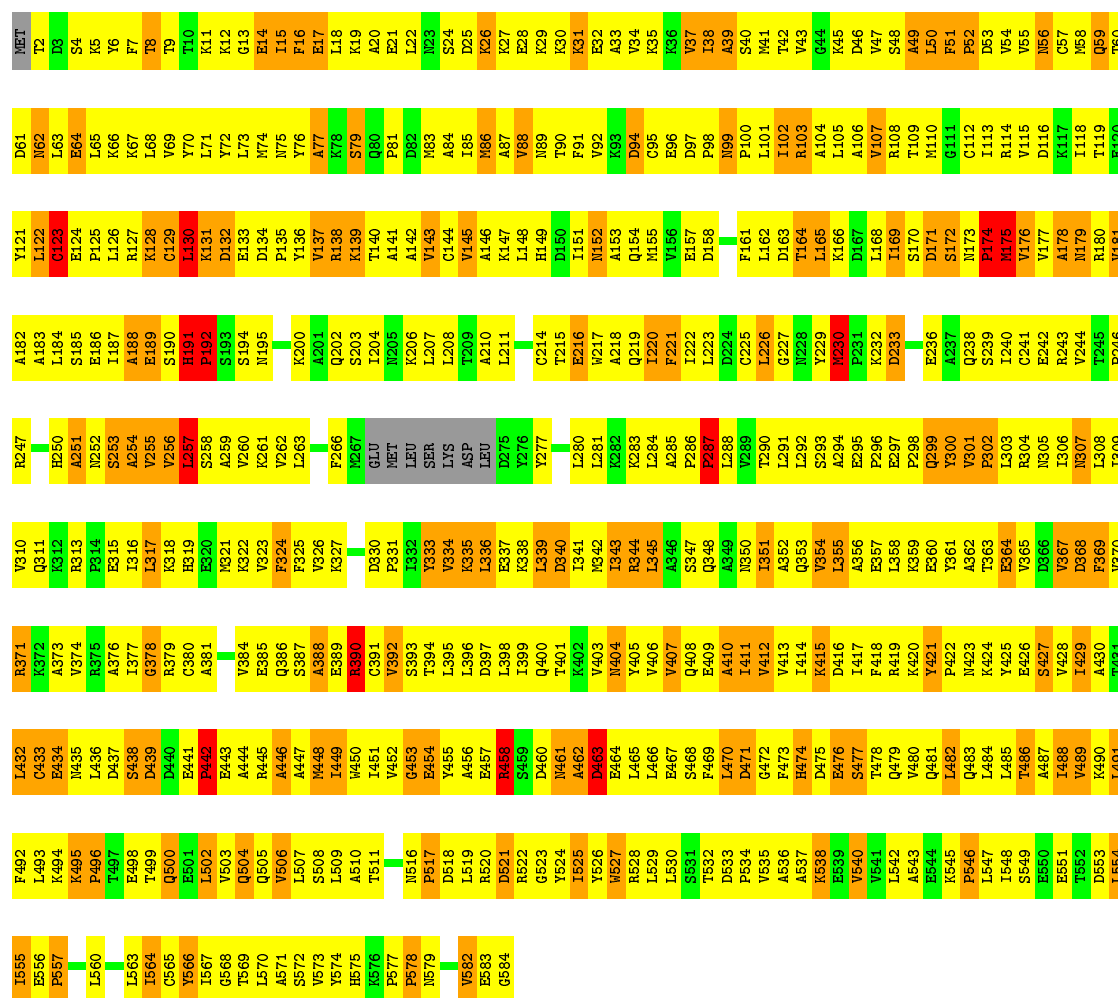
Chain K: 13% 60% 20% 5%





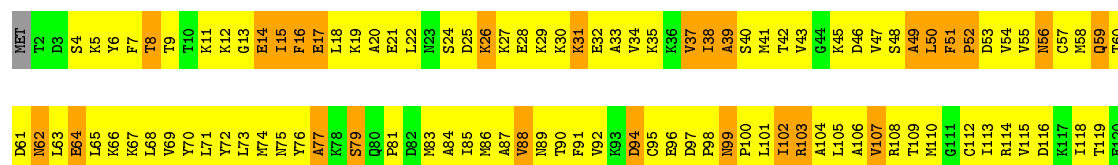
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain B: 14% 59% 23%

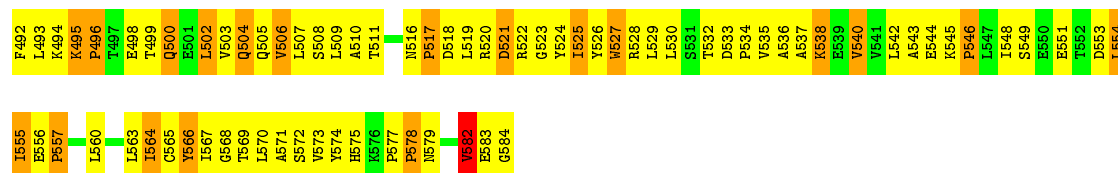


• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

Chain D: 14% 59% 23%

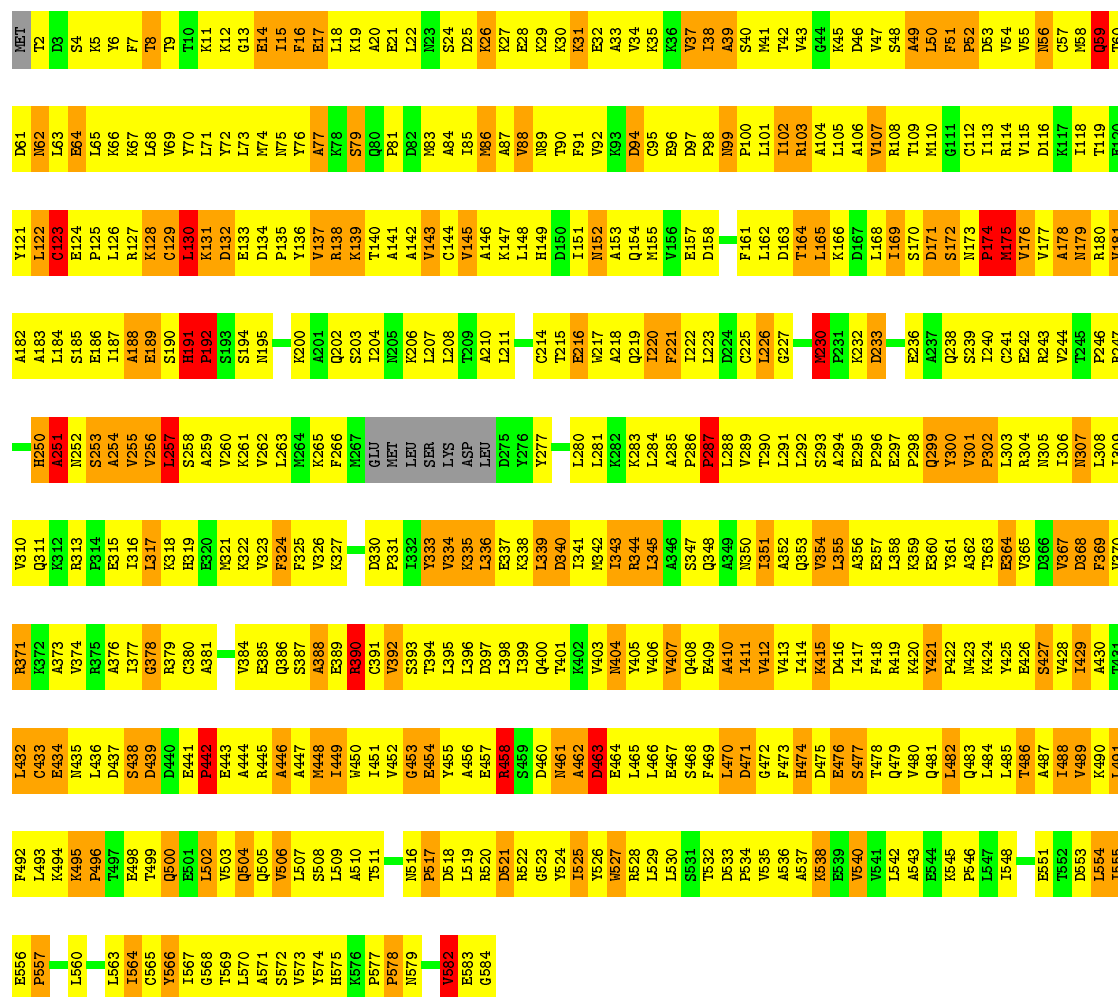






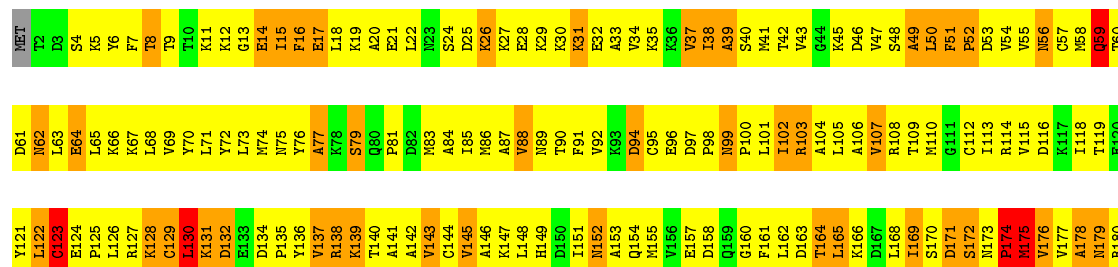
• Molecule 2: ADAPTER-RELATED PROTEIN COMPLEX 1 BETA 1 SUBUNIT

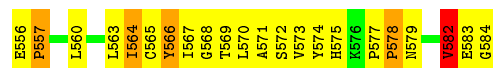
Chain H: 14% 59% 23% ..



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

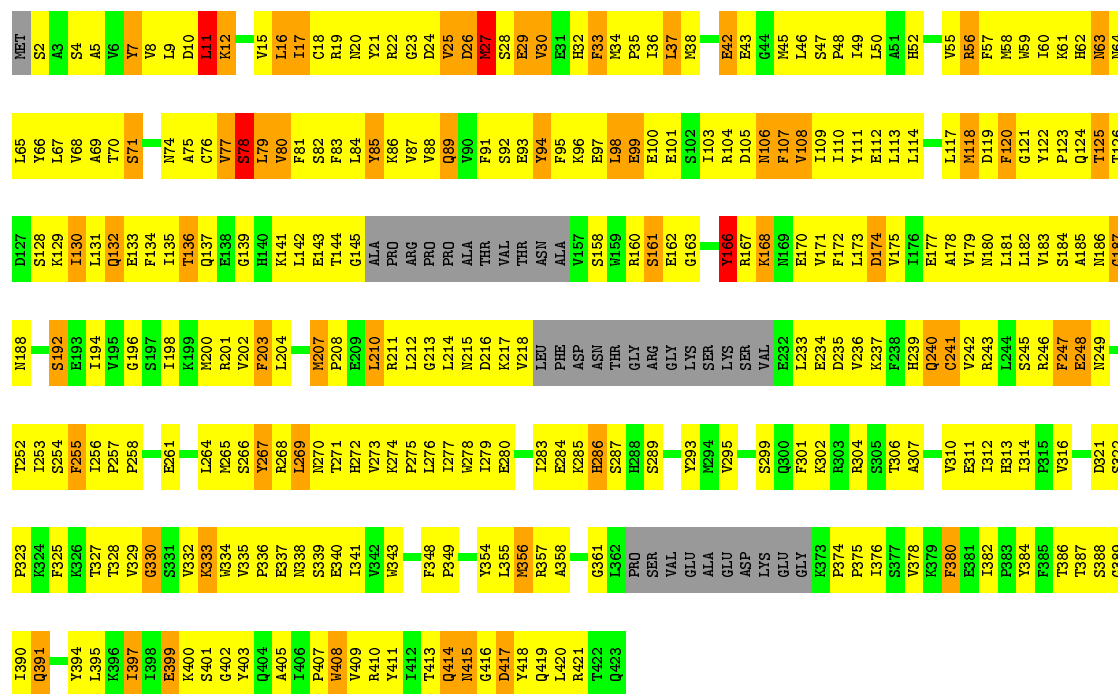
Chain J: 14% 59% 23% ..





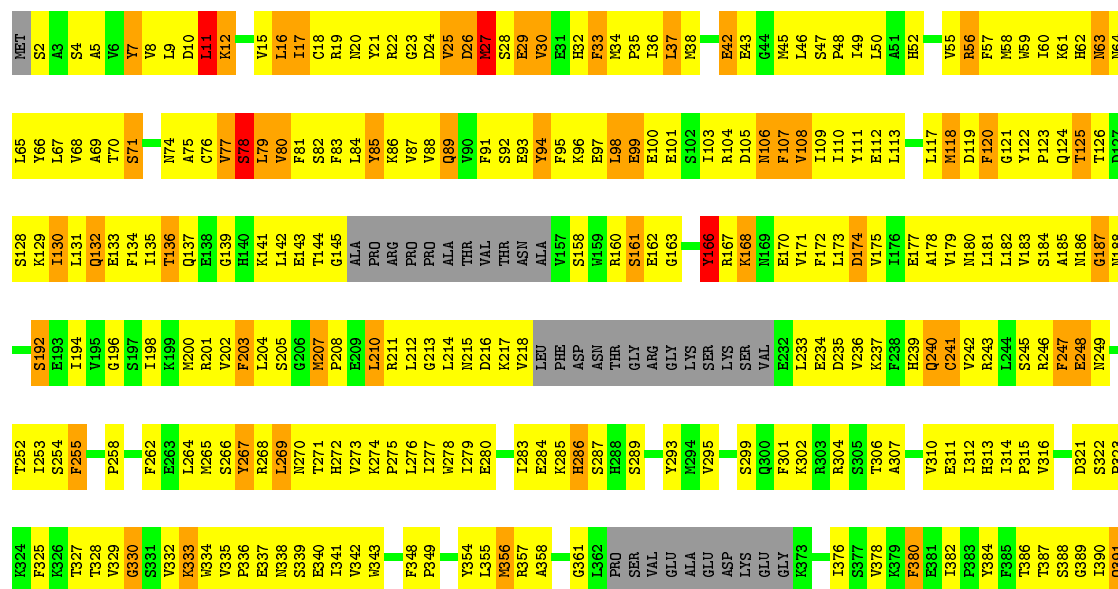
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

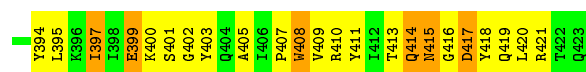
Chain M: 23% 54% 14% 8%



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

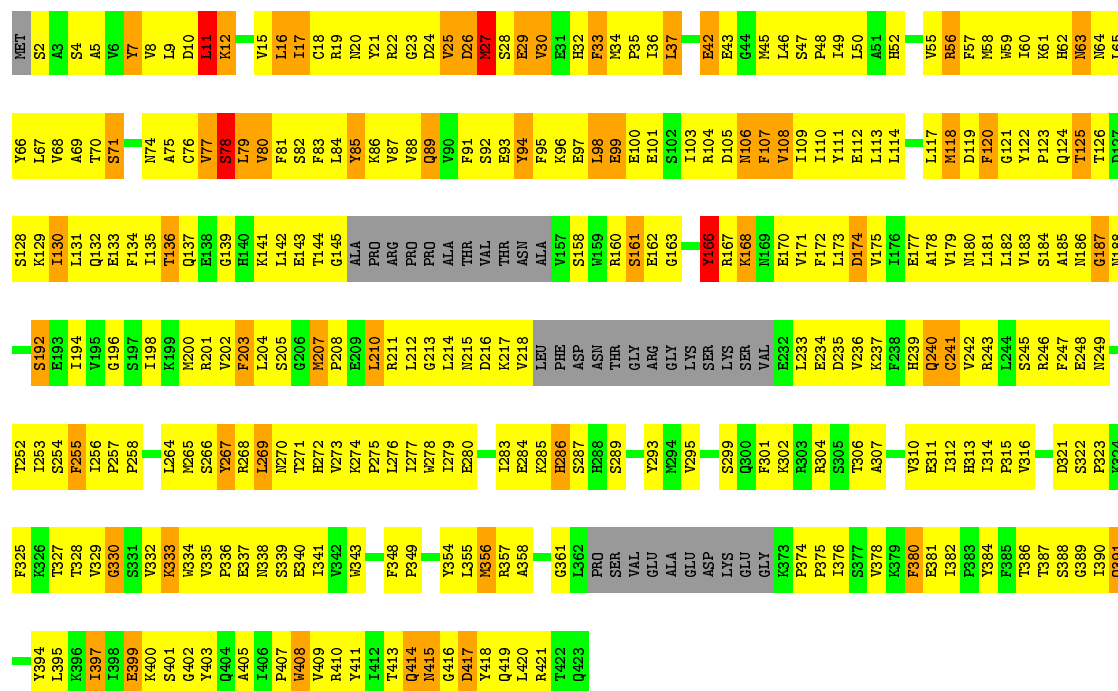
Chain N: 23% 54% 14% 8%





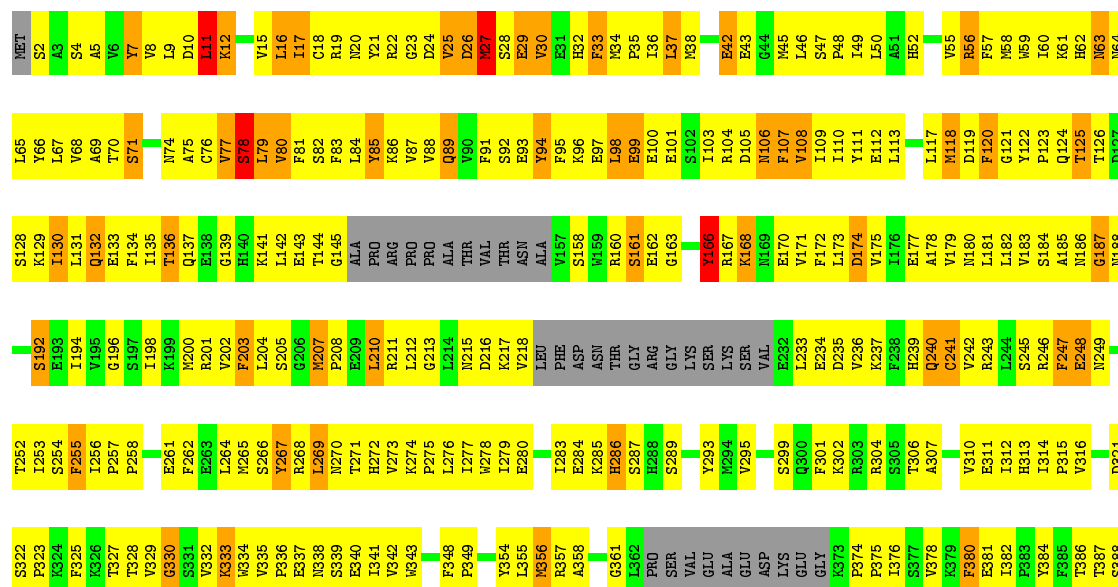
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

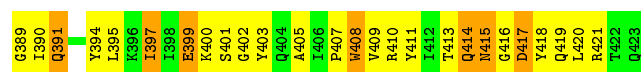
Chain O: 22% 55% 13% 8%



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

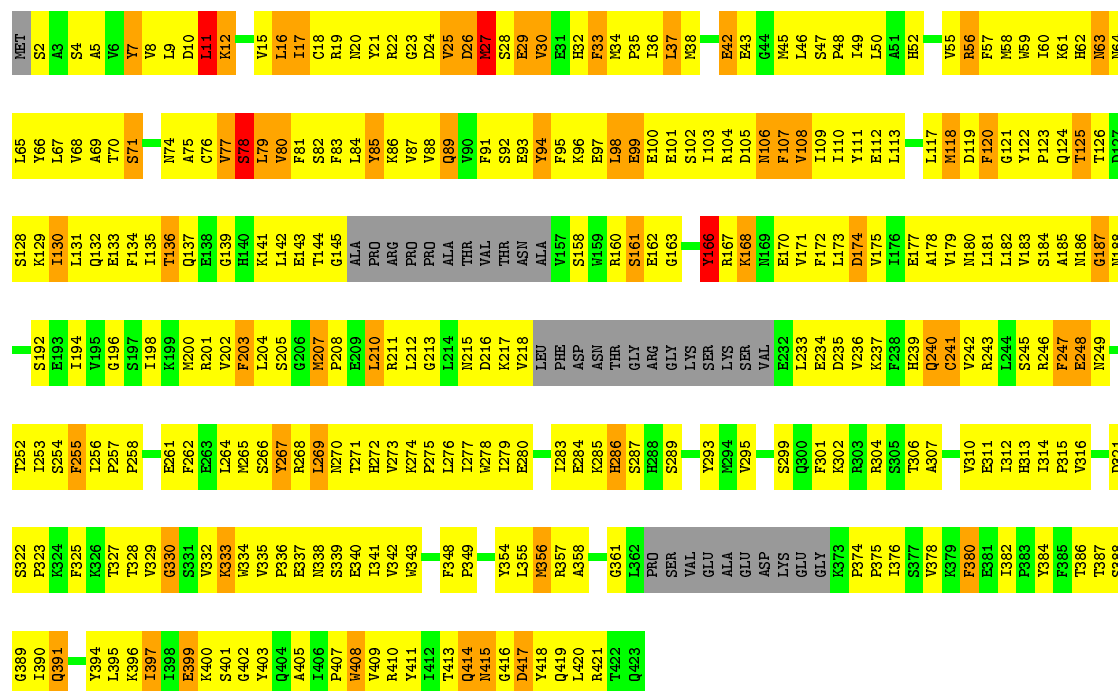
Chain P: 22% 55% 14% 8%





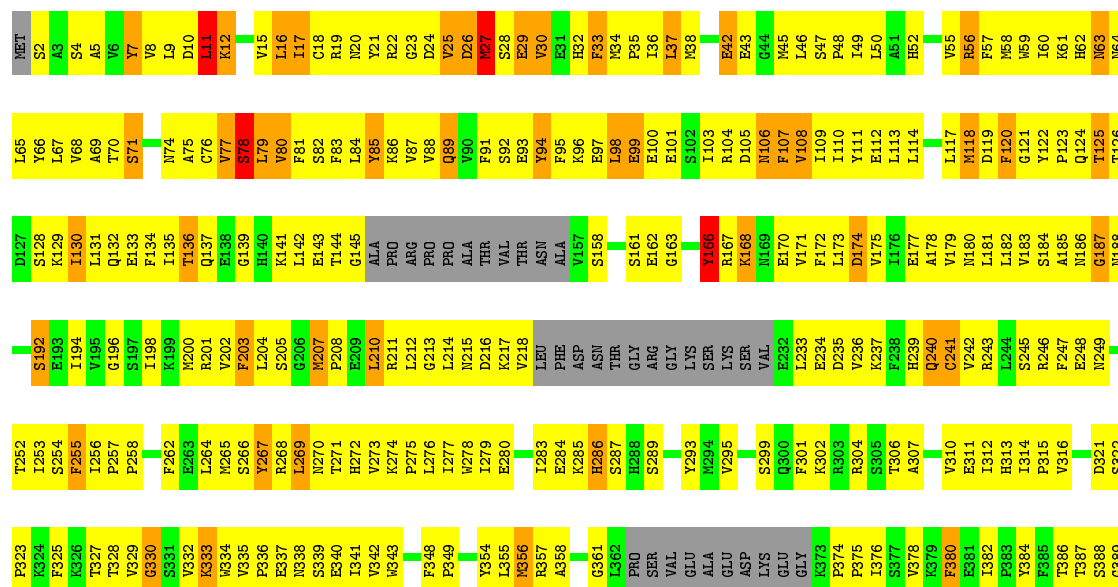
• Molecule 3: ADAPTOR-RELATED PROTEIN COMPLEX 1, MU 1 SUBUNIT

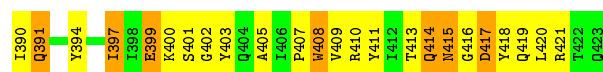
Chain R: 22% 56% 13% 8%



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

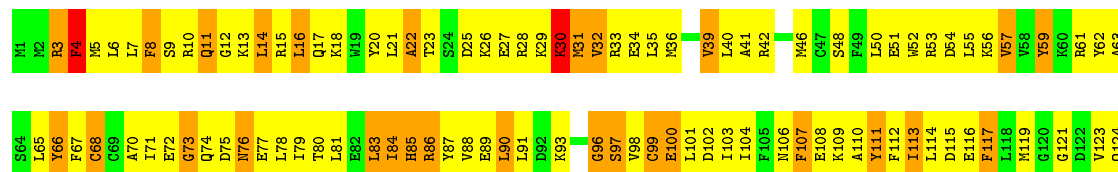
Chain V: 22% 56% 13% 8%





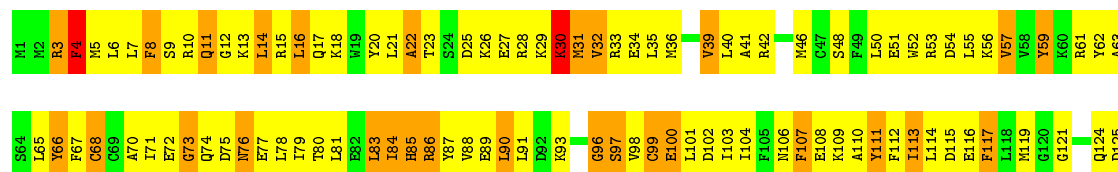
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain Q: 20% 54% 19% 6%



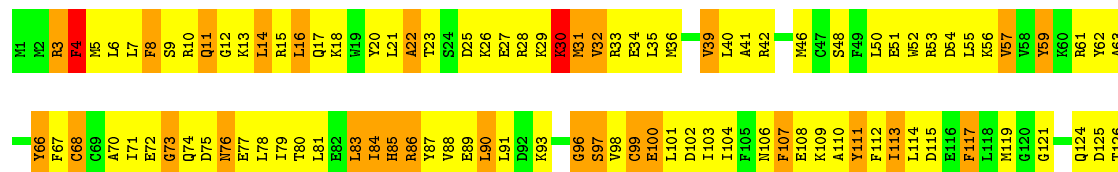
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain S: 22% 53% 18% 6%



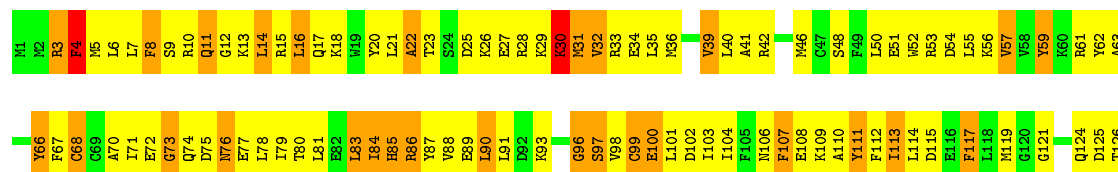
• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

Chain T: 22% 53% 18% 6%



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

Chain U: 22% 53% 18% 6%



S127	K128	K129	S130	V131	L132	K133	A134	I135	E136	Q142	S147	P148	R149	SER	VAL	LEU	GLU	GLU	GLU	MET	GLY	LEU	ALA
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• Molecule 4: ADAPTER-RELATED PROTEIN COMPLEX 1 SIGMA 1A SUBUNIT

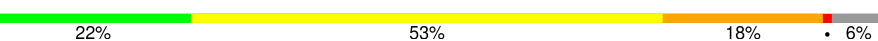
Chain W:  22% 53% 18% 6%

M1	M2	R3	F4	M5	L6	L7	F8	S9	R10	Q11	G12	K13	L14	R15	L16	Q17	K18	H19	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
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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	R92	D93	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
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T126	S127	K128	K129	S130	V131	L132	K133	A134	I135	E136	Q142	S147	P148	R149	SER	VAL	LEU	GLU	GLU	GLU	MET	GLY	LEU	ALA
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• 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	H19	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
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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	R92	D93	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
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T126	S127	K128	K129	S130	V131	L132	K133	A134	I135	E136	Q142	S147	P148	R149	SER	VAL	LEU	GLU	GLU	GLU	MET	GLY	LEU	ALA
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 ⓘ

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	0.61	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(°)	Ideal(°)
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

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:K:482:GLU:HB3	1:K:584:MET:SD	1.83	1.17
1:G:482:GLU:HB3	1:G: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:I:345:ARG:NE	2:L:457:GLU:OE2[5_445]	1.44	0.76
1:E:265:GLU:OE1	1:K:221:ARG:NH2[1_545]	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	2
1	C	588/618 (95%)	254 (43%)	210 (36%)	124 (21%)	0	2
1	E	588/618 (95%)	253 (43%)	211 (36%)	124 (21%)	0	2
1	G	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	2
1	I	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	2
1	K	588/618 (95%)	255 (43%)	209 (36%)	124 (21%)	0	2
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	8
3	N	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	8
3	O	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	8
3	P	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	8
3	R	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	8
3	V	380/423 (90%)	257 (68%)	76 (20%)	47 (12%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
4	S	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
4	T	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
4	U	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
4	W	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
4	X	147/158 (93%)	81 (55%)	47 (32%)	19 (13%)	0	7
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 ⓘ

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%)	13	50
1	C	523/546 (96%)	478 (91%)	45 (9%)	13	50
1	E	523/546 (96%)	479 (92%)	44 (8%)	14	51
1	G	523/546 (96%)	478 (91%)	45 (9%)	13	50
1	I	523/546 (96%)	479 (92%)	44 (8%)	14	51
1	K	523/546 (96%)	478 (91%)	45 (9%)	13	50
2	B	515/523 (98%)	475 (92%)	40 (8%)	16	54
2	D	515/523 (98%)	475 (92%)	40 (8%)	16	54
2	F	515/523 (98%)	475 (92%)	40 (8%)	16	54
2	H	515/523 (98%)	475 (92%)	40 (8%)	16	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	515/523 (98%)	475 (92%)	40 (8%)	16	54
2	L	515/523 (98%)	475 (92%)	40 (8%)	16	54
3	M	355/383 (93%)	322 (91%)	33 (9%)	11	46
3	N	355/383 (93%)	322 (91%)	33 (9%)	11	46
3	O	355/383 (93%)	322 (91%)	33 (9%)	11	46
3	P	355/383 (93%)	322 (91%)	33 (9%)	11	46
3	R	355/383 (93%)	322 (91%)	33 (9%)	11	46
3	V	355/383 (93%)	322 (91%)	33 (9%)	11	46
4	Q	136/144 (94%)	118 (87%)	18 (13%)	5	30
4	S	136/144 (94%)	118 (87%)	18 (13%)	5	30
4	T	136/144 (94%)	118 (87%)	18 (13%)	5	30
4	U	136/144 (94%)	118 (87%)	18 (13%)	5	30
4	W	136/144 (94%)	118 (87%)	18 (13%)	5	30
4	X	136/144 (94%)	118 (87%)	18 (13%)	5	30
All	All	9174/9576 (96%)	8360 (91%)	814 (9%)	12	48

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

Mol	Chain	Res	Type
1	I	420	ASP
1	K	435	ASP
3	V	46	LEU
1	I	534	SER
2	J	442	PRO

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

Mol	Chain	Res	Type
1	G	443	GLN
1	I	311	ASN
4	U	11	GLN
2	H	59	GLN
1	I	43	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.