



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3J97
EMDB ID: : EMD-6207
Title : Structure of 20S supercomplex determined by single particle cryoelectron microscopy (State II)
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on : 2014-12-05
Resolution : 7.80 Å(reported)
Based on PDB ID : 1QCS, 1NSF, 1N7S

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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) : trunk27241

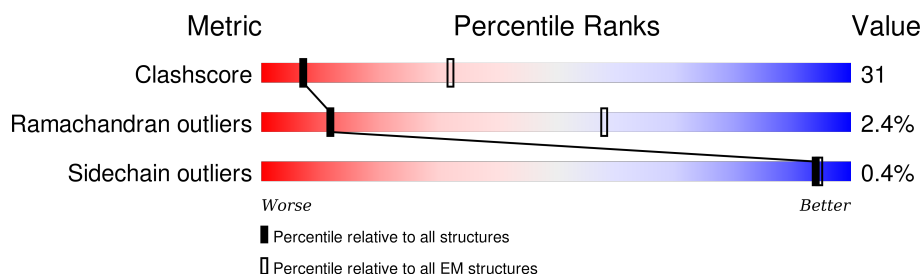
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	747	
1	B	747	
1	C	747	
1	D	747	
1	E	747	
1	F	747	
2	G	297	
2	H	297	
2	I	297	

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Mol	Chain	Length	Quality of chain
2	J	297	<div><div></div><div>53%</div><div>41%</div><div></div><div></div><div></div></div>
3	K	63	<div><div></div><div>32%</div><div>62%</div><div></div><div></div><div></div></div>
4	L	67	<div><div></div><div>39%</div><div>58%</div><div></div><div></div><div></div></div>
5	M	198	<div><div></div><div>26%</div><div>40%</div><div></div><div></div><div>34%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41095 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	678	Total	C	N	O	S	0	0
			5044	3201	874	946	23		
1	B	672	Total	C	N	O	S	0	0
			5015	3184	868	939	24		
1	C	676	Total	C	N	O	S	0	0
			5028	3189	869	947	23		
1	D	673	Total	C	N	O	S	0	0
			4986	3169	854	939	24		
1	E	670	Total	C	N	O	S	0	0
			5020	3185	871	940	24		
1	F	654	Total	C	N	O	S	0	0
			4932	3135	852	922	23		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P18708
A	-1	ALA	-	EXPRESSION TAG	UNP P18708
A	0	HIS	-	EXPRESSION TAG	UNP P18708
B	-2	GLY	-	EXPRESSION TAG	UNP P18708
B	-1	ALA	-	EXPRESSION TAG	UNP P18708
B	0	HIS	-	EXPRESSION TAG	UNP P18708
C	-2	GLY	-	EXPRESSION TAG	UNP P18708
C	-1	ALA	-	EXPRESSION TAG	UNP P18708
C	0	HIS	-	EXPRESSION TAG	UNP P18708
D	-2	GLY	-	EXPRESSION TAG	UNP P18708
D	-1	ALA	-	EXPRESSION TAG	UNP P18708
D	0	HIS	-	EXPRESSION TAG	UNP P18708
E	-2	GLY	-	EXPRESSION TAG	UNP P18708
E	-1	ALA	-	EXPRESSION TAG	UNP P18708
E	0	HIS	-	EXPRESSION TAG	UNP P18708
F	-2	GLY	-	EXPRESSION TAG	UNP P18708
F	-1	ALA	-	EXPRESSION TAG	UNP P18708
F	0	HIS	-	EXPRESSION TAG	UNP P18708

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		
2	I	286	Total	C	N	O	S	0	0
			2246	1416	373	441	16		
2	J	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		
2	G	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	EXPRESSION TAG	UNP P54921
H	0	SER	-	EXPRESSION TAG	UNP P54921
I	-1	GLY	-	EXPRESSION TAG	UNP P54921
I	0	SER	-	EXPRESSION TAG	UNP P54921
J	-1	GLY	-	EXPRESSION TAG	UNP P54921
J	0	SER	-	EXPRESSION TAG	UNP P54921
G	-1	GLY	-	EXPRESSION TAG	UNP P54921
G	0	SER	-	EXPRESSION TAG	UNP P54921

- Molecule 3 is a protein called Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	61	Total	C	N	O	S	0	0
			494	300	94	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	27	GLY	-	EXPRESSION TAG	UNP P63045

- Molecule 4 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	66	Total	C	N	O	S	0	0
			536	331	91	109	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	190	MET	-	EXPRESSION TAG	UNP P32851

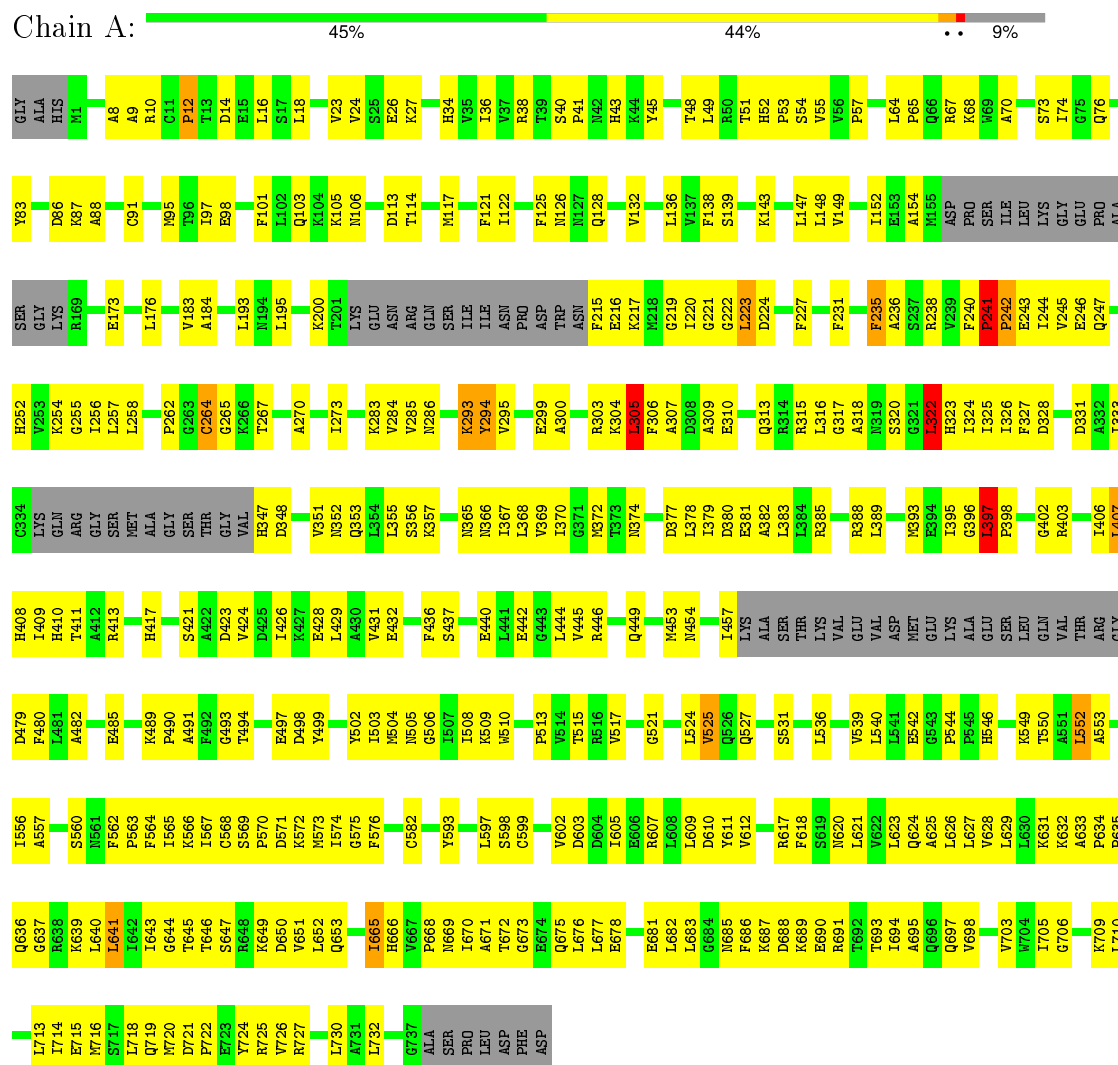
- Molecule 5 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1029	609	191	220	9		

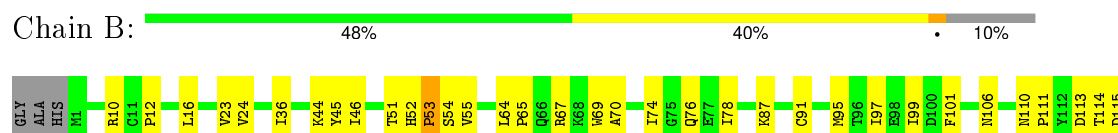
3 Residue-property plots

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. 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.

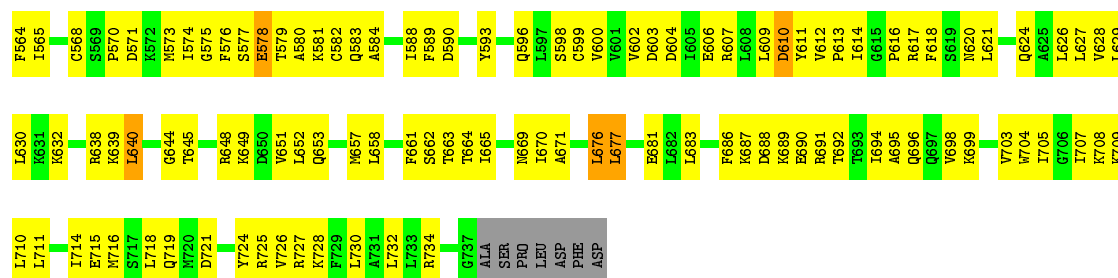
• Molecule 1: Vesicle-fusing ATPase



• Molecule 1: Vesicle-fusing ATPase

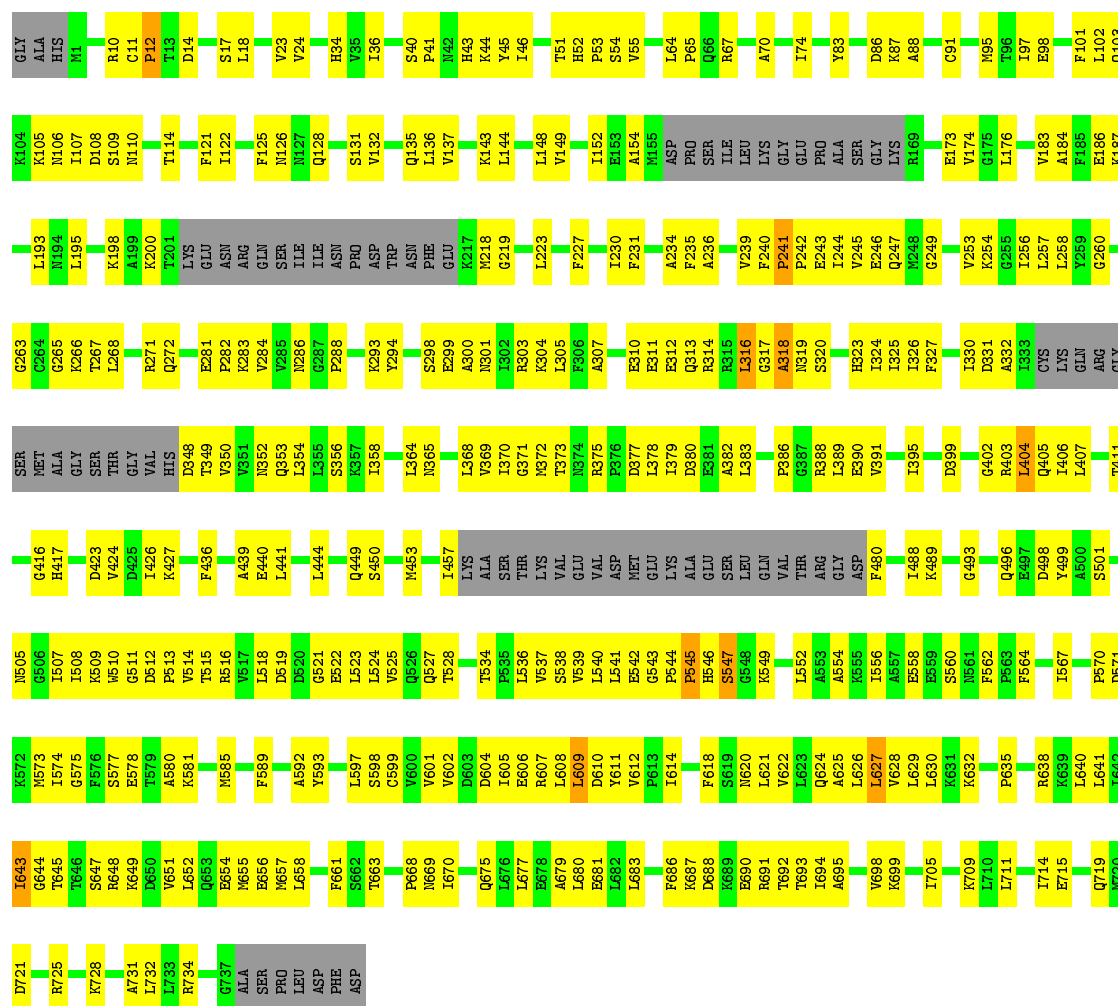






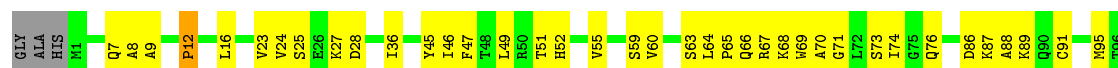
• Molecule 1: Vesicle-fusing ATPase

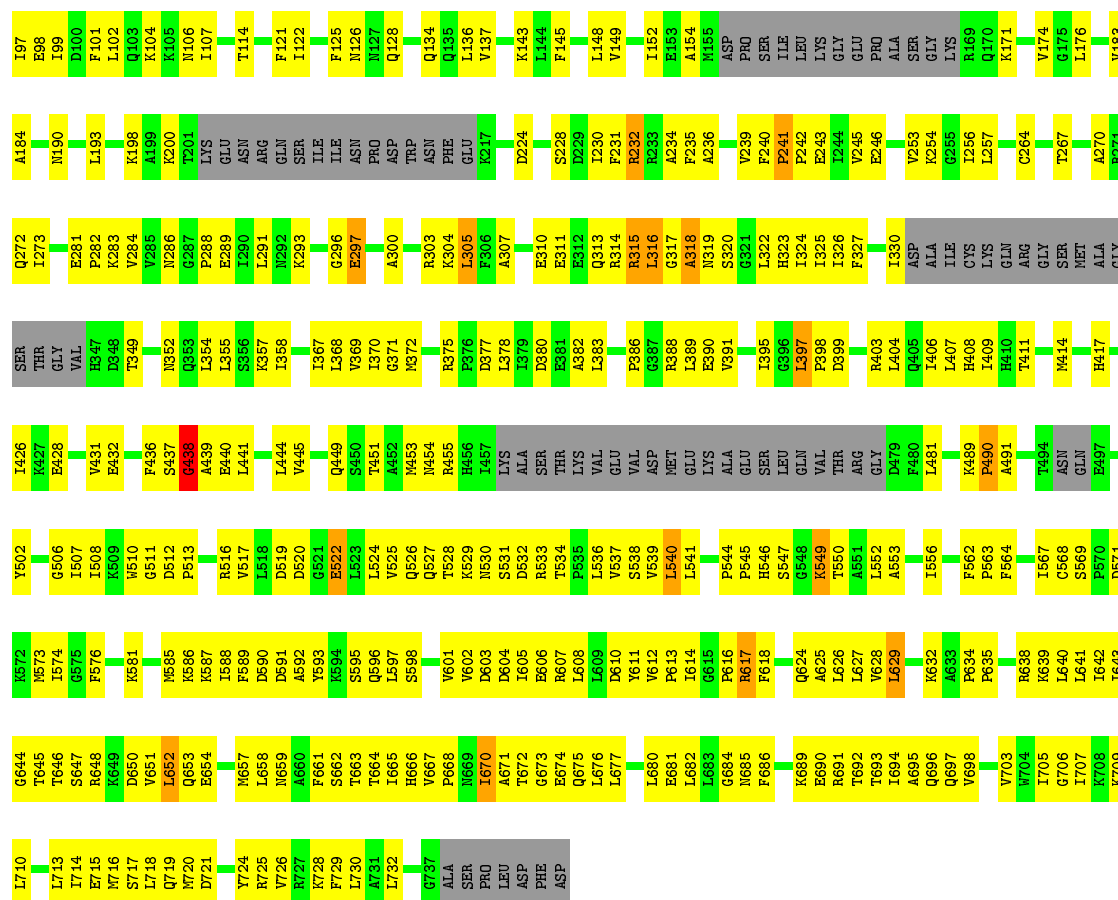
Chain D: 46% 43% • 10%



• Molecule 1: Vesicle-fusing ATPase

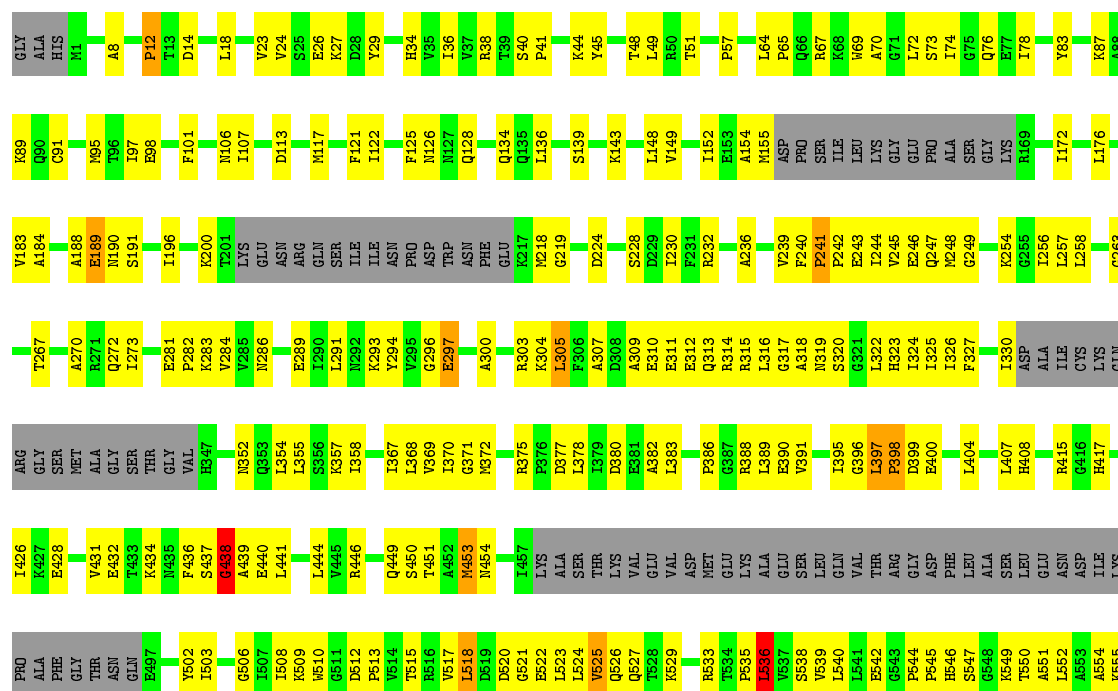
Chain E: 44% 44% • 10%

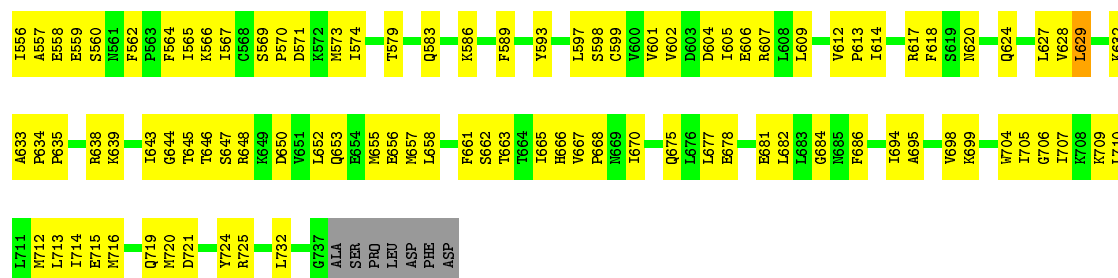




• Molecule 1: Vesicle-fusing ATPase

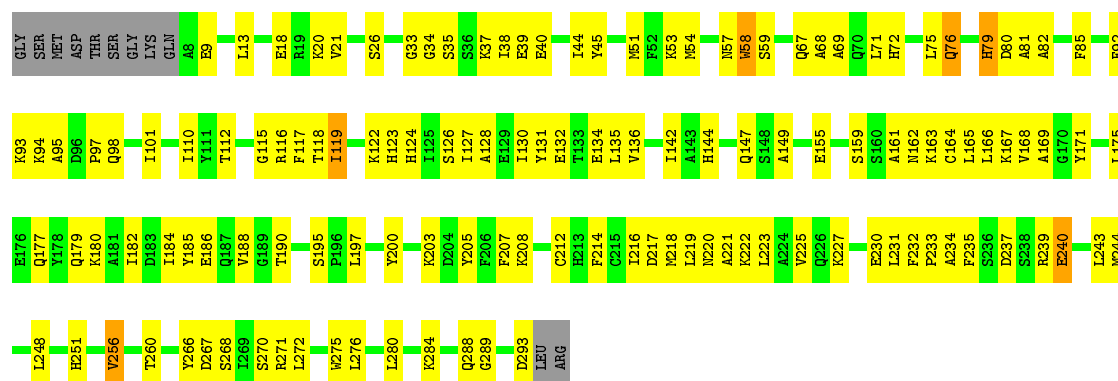
Chain F: 46% 40% 12%





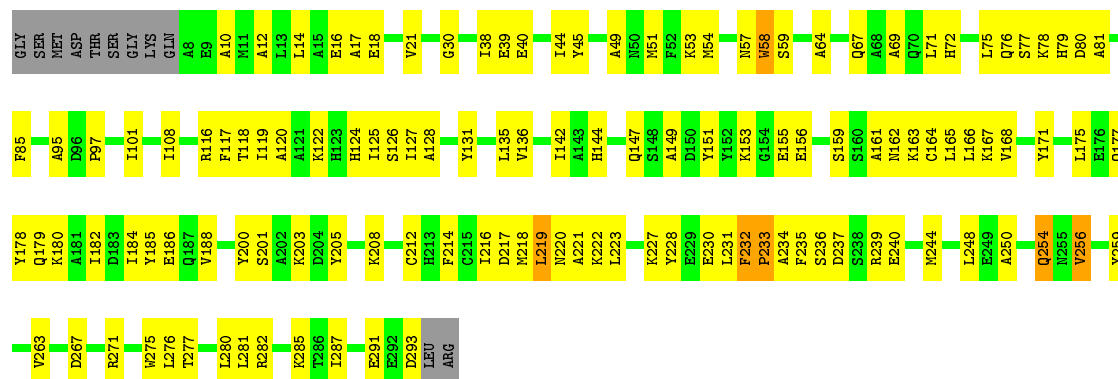
- Molecule 2: Alpha-soluble NSF attachment protein

Chain H: 52% 42%



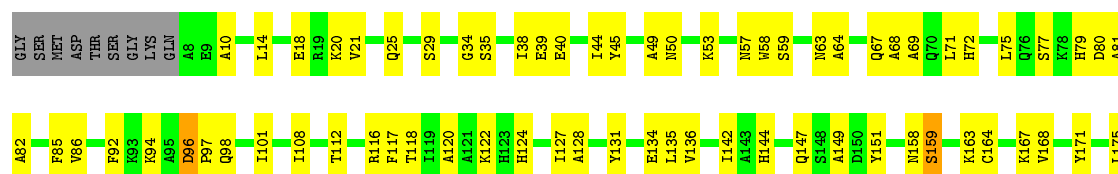
- Molecule 2: Alpha-soluble NSF attachment protein

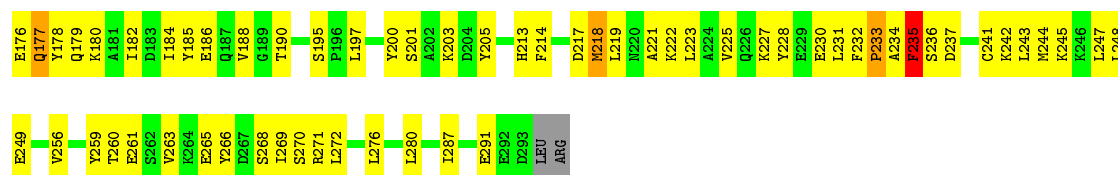
Chain I: 54% 40%



- Molecule 2: Alpha-soluble NSF attachment protein

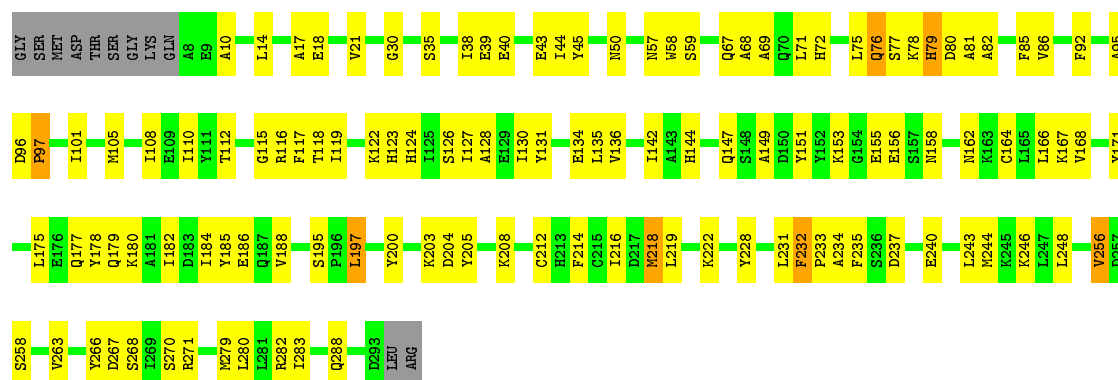
Chain J: 53% 41%





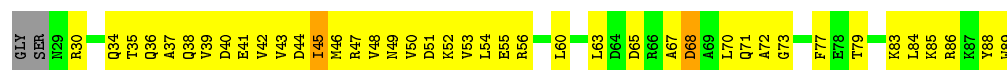
- Molecule 2: Alpha-soluble NSF attachment protein

Chain G: 56% 38%



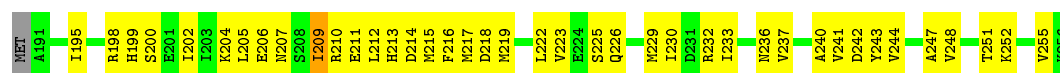
- Molecule 3: Vesicle-associated membrane protein 2

Chain K: 32% 62%



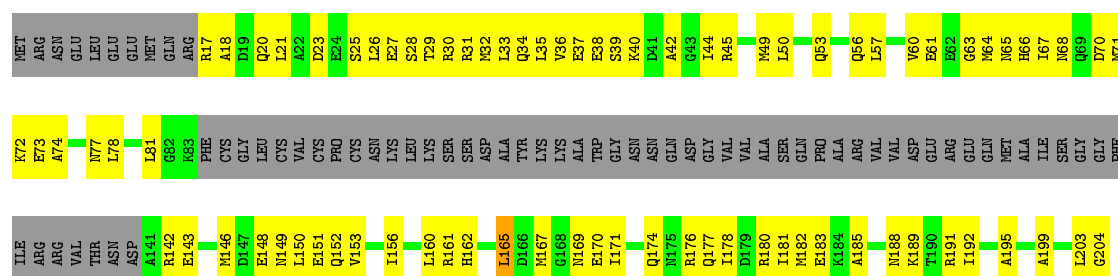
- Molecule 4: Syntaxin-1A

Chain L: 39% 58%



- Molecule 5: Synaptosomal-associated protein 25

Chain M: 26% 40% 34%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	21489	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.46	1/5120 (0.0%)	0.82	10/6930 (0.1%)
1	B	0.41	1/5091 (0.0%)	0.80	12/6887 (0.2%)
1	C	0.38	0/5104	0.72	5/6910 (0.1%)
1	D	0.43	0/5061	0.77	9/6854 (0.1%)
1	E	0.46	1/5095 (0.0%)	0.84	11/6890 (0.2%)
1	F	0.42	0/5007	0.78	10/6767 (0.1%)
2	G	0.33	0/2295	0.59	1/3086 (0.0%)
2	H	0.36	0/2295	0.63	1/3086 (0.0%)
2	I	0.33	0/2285	0.58	0/3074
2	J	0.34	0/2295	0.58	1/3086 (0.0%)
3	K	0.25	0/497	0.41	0/665
4	L	0.24	0/541	0.41	0/723
5	M	0.22	0/1029	0.45	0/1369
All	All	0.40	3/41715 (0.0%)	0.74	60/56327 (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
1	A	0	1
1	B	0	1
1	E	0	2
1	F	0	1
2	J	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	232	ARG	CB-CG	-6.33	1.35	1.52
1	B	547	SER	C-O	5.53	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	PHE	CB-CG	-5.23	1.42	1.51

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	LEU	CA-CB-CG	11.54	141.84	115.30
1	E	629	LEU	CB-CG-CD1	-9.86	94.24	111.00
1	F	518	LEU	CB-CG-CD1	-9.34	95.12	111.00
1	D	547	SER	C-N-CA	-8.76	103.92	122.30
1	F	629	LEU	CB-CG-CD1	-8.53	96.51	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	B	438	GLY	Peptide
1	E	315	ARG	Mainchain
1	E	438	GLY	Peptide
1	F	438	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5044	0	4963	347	0
1	B	5015	0	4953	300	0
1	C	5028	0	4939	343	0
1	D	4986	0	4905	341	0
1	E	5020	0	4974	390	0
1	F	4932	0	4914	335	0
2	G	2255	0	2199	126	0
2	H	2255	0	2199	138	0
2	I	2246	0	2185	109	0
2	J	2255	0	2199	132	0
3	K	494	0	488	80	0
4	L	536	0	527	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1029	0	996	143	0
All	All	41095	0	40441	2529	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 31.

The worst 5 of 2529 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:F:518:LEU:HD23	1:F:555:LYS:HG2	1.21	1.10
2:H:219:LEU:HB2	2:H:222:LYS:HB3	1.34	1.08
2:I:201:SER:HA	3:K:47:ARG:HH12	1.11	1.08
1:E:593:TYR:O	1:E:638:ARG:NH1	1.90	1.04
1:B:264:CYS:HA	1:B:437:SER:HB2	1.38	1.04

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	668/747 (89%)	613 (92%)	39 (6%)	16 (2%)	7	47
1	B	662/747 (89%)	589 (89%)	54 (8%)	19 (3%)	6	43
1	C	666/747 (89%)	616 (92%)	37 (6%)	13 (2%)	9	51
1	D	663/747 (89%)	601 (91%)	52 (8%)	10 (2%)	13	57
1	E	658/747 (88%)	603 (92%)	42 (6%)	13 (2%)	9	51
1	F	644/747 (86%)	585 (91%)	46 (7%)	13 (2%)	9	51
2	G	284/297 (96%)	227 (80%)	47 (16%)	10 (4%)	4	39
2	H	284/297 (96%)	230 (81%)	44 (16%)	10 (4%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	284/297 (96%)	229 (81%)	41 (14%)	14 (5%)	3	31
2	J	284/297 (96%)	229 (81%)	45 (16%)	10 (4%)	4	39
3	K	59/63 (94%)	56 (95%)	2 (3%)	1 (2%)	11	55
4	L	64/67 (96%)	58 (91%)	5 (8%)	1 (2%)	12	56
5	M	127/198 (64%)	119 (94%)	7 (6%)	1 (1%)	24	69
All	All	5347/5998 (89%)	4755 (89%)	461 (9%)	131 (2%)	12	47

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR
1	A	318	ALA
1	A	320	SER

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 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	514/638 (81%)	512 (100%)	2 (0%)	93	96
1	B	514/638 (81%)	510 (99%)	4 (1%)	86	94
1	C	513/638 (80%)	511 (100%)	2 (0%)	93	96
1	D	509/638 (80%)	507 (100%)	2 (0%)	93	96
1	E	518/638 (81%)	515 (99%)	3 (1%)	90	95
1	F	513/638 (80%)	510 (99%)	3 (1%)	90	95
2	G	235/244 (96%)	235 (100%)	0	100	100
2	H	235/244 (96%)	234 (100%)	1 (0%)	93	96
2	I	233/244 (96%)	233 (100%)	0	100	100
2	J	235/244 (96%)	235 (100%)	0	100	100
3	K	52/54 (96%)	50 (96%)	2 (4%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	60/61 (98%)	60 (100%)	0	100	100
5	M	111/171 (65%)	111 (100%)	0	100	100
All	All	4242/5090 (83%)	4223 (100%)	19 (0%)	94	96

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	305	LEU
1	E	305	LEU
1	F	536	LEU
1	C	676	LEU
2	H	251	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	527	GLN
1	F	527	GLN
5	M	53	GLN
1	E	659	ASN
1	E	666	HIS

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.