wwPDB EM Map/Model Validation Report (i)

Oct 18, 2016 – 12:02 PM EDT

PDB ID	:	5HX2
EMDB ID:	:	EMD-8064
Title	:	In vitro assembled star-shaped hubless T4 baseplate
Authors	:	Yap, M.L.; Klose, T.; Fokine, A.; Rossmann, M.G.
Deposited on	:	2016-01-29
Resolution	:	3.80 Å(reported)
Based on PDB ID	:	1N80, 3H2T, 2FKK

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

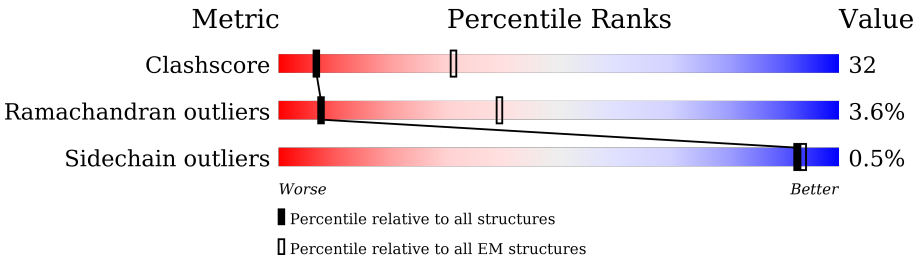
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1032	55% 42% ·
2	B	334	46% 47% 6% ·
2	C	334	52% 47% ··
3	D	660	54% 41% · ·
3	E	660	63% 30% · ·
4	F	196	50% 46% · ·
5	G	602	39% 16% · 44%
5	H	602	41% 14% · 44%
5	I	602	40% 15% · 44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28612 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 Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0
			7511	4844	1265	1383	19		

- Molecule 2 is a protein called Baseplate wedge protein gp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	334	Total	C	N	O	S	0	0
			2521	1598	423	485	15		
2	C	332	Total	C	N	O	S	0	0
			2585	1650	428	491	16		

- Molecule 3 is a protein called Baseplate wedge protein gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	647	Total	C	N	O	S	0	0
			4845	3072	811	953	9		
3	E	634	Total	C	N	O	S	0	0
			4660	2966	784	902	8		

- Molecule 4 is a protein called Baseplate wedge protein gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	192	Total	C	N	O	S	0	0
			1495	972	239	278	6		

- Molecule 5 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	340	Total	C	N	O	0	0
			1665	985	340	340		
5	H	340	Total	C	N	O	0	0
			1665	985	340	340		

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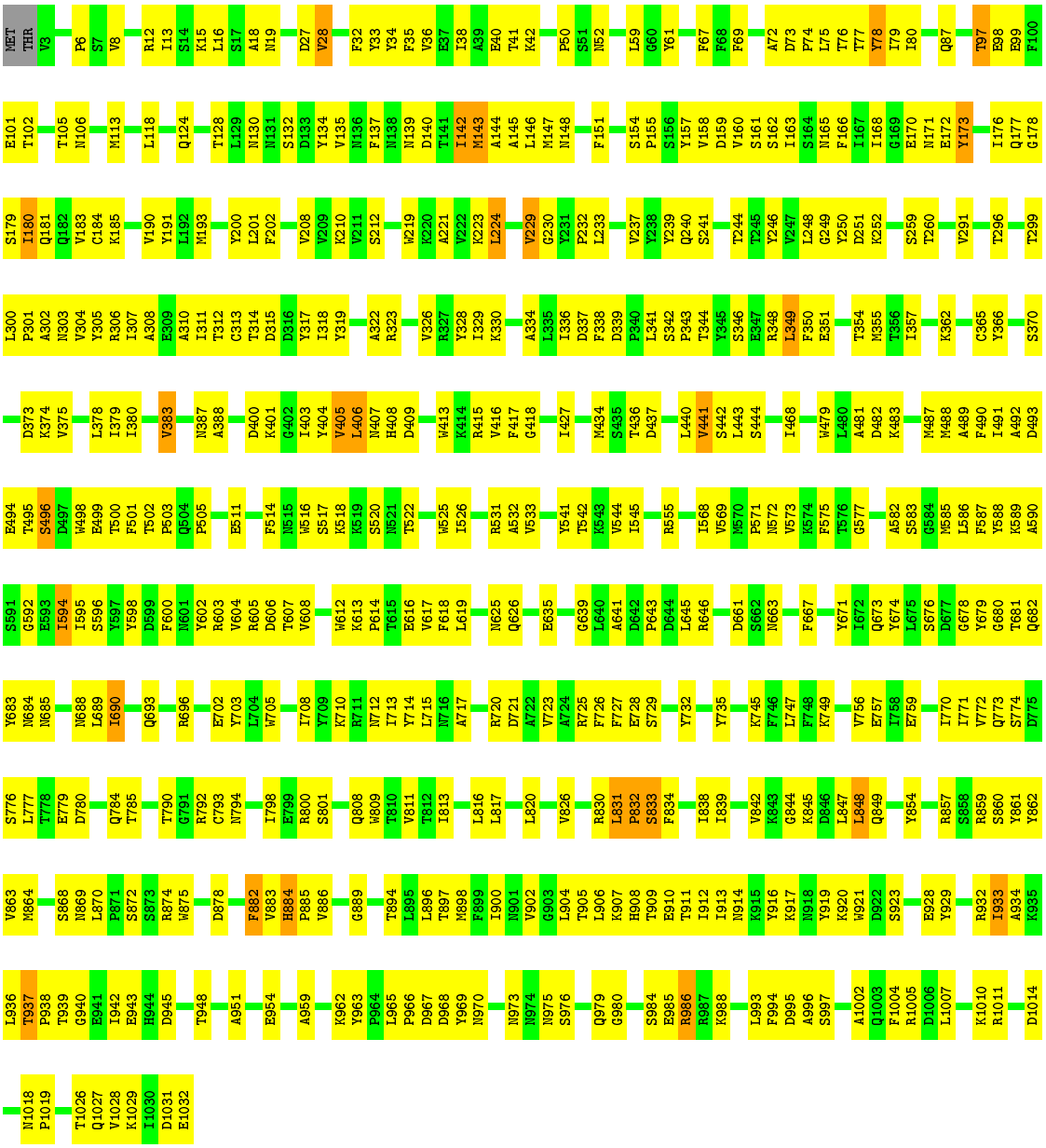
Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	340	Total	C	N	O	0	0
			1665	985	340	340		

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.

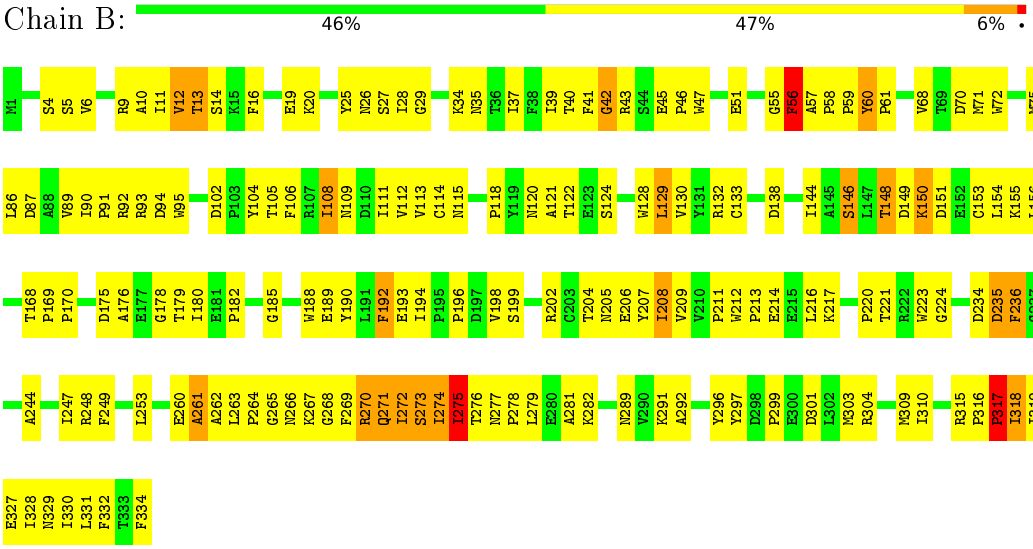
- Molecule 1: Baseplate wedge protein gp7

Chain A:



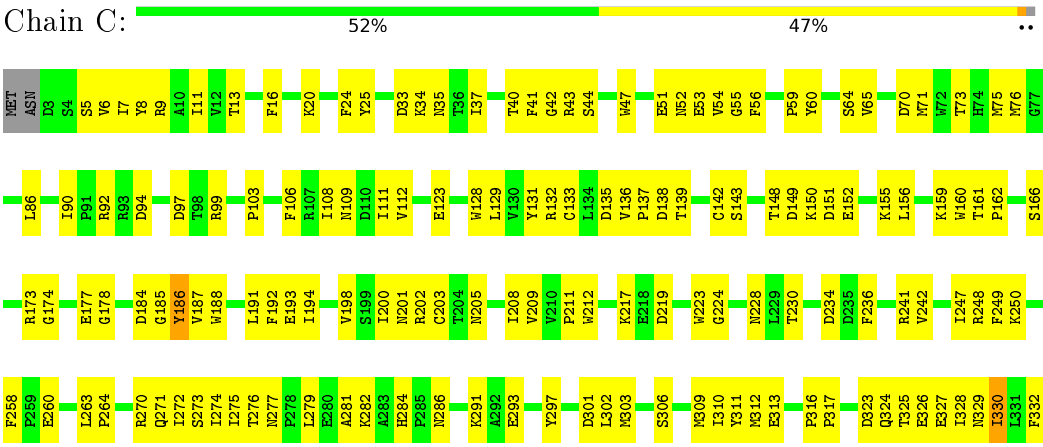
- Molecule 2: Baseplate wedge protein gp8

Chain B:



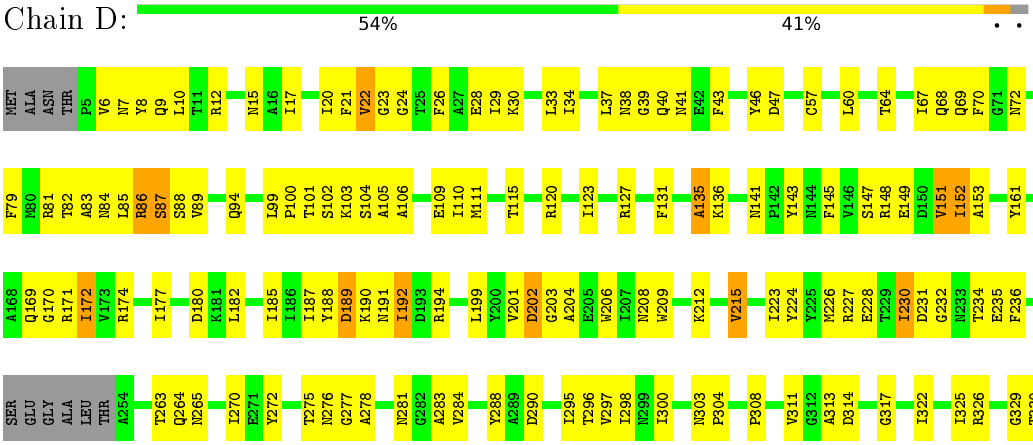
- Molecule 2: Baseplate wedge protein gp8

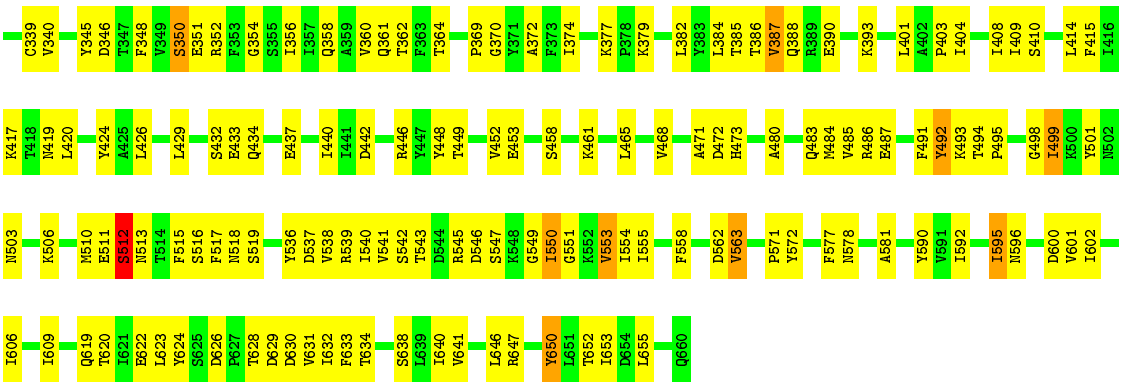
Chain C:



- Molecule 3: Baseplate wedge protein gp6

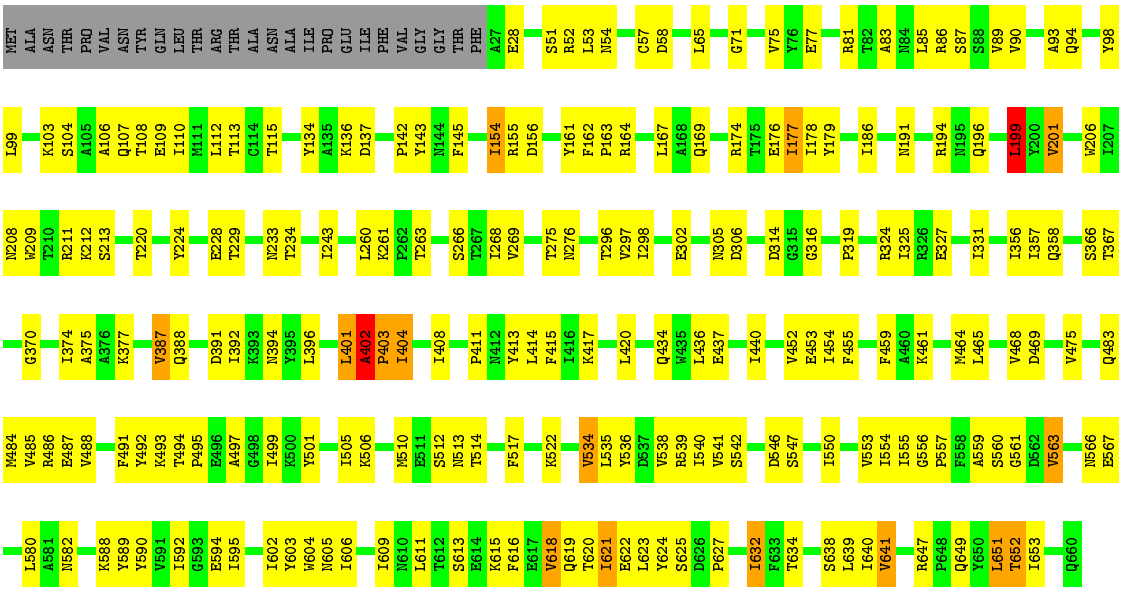
Chain D:





• Molecule 3: Baseplate wedge protein gp6

Chain E:

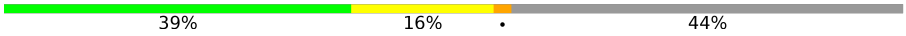


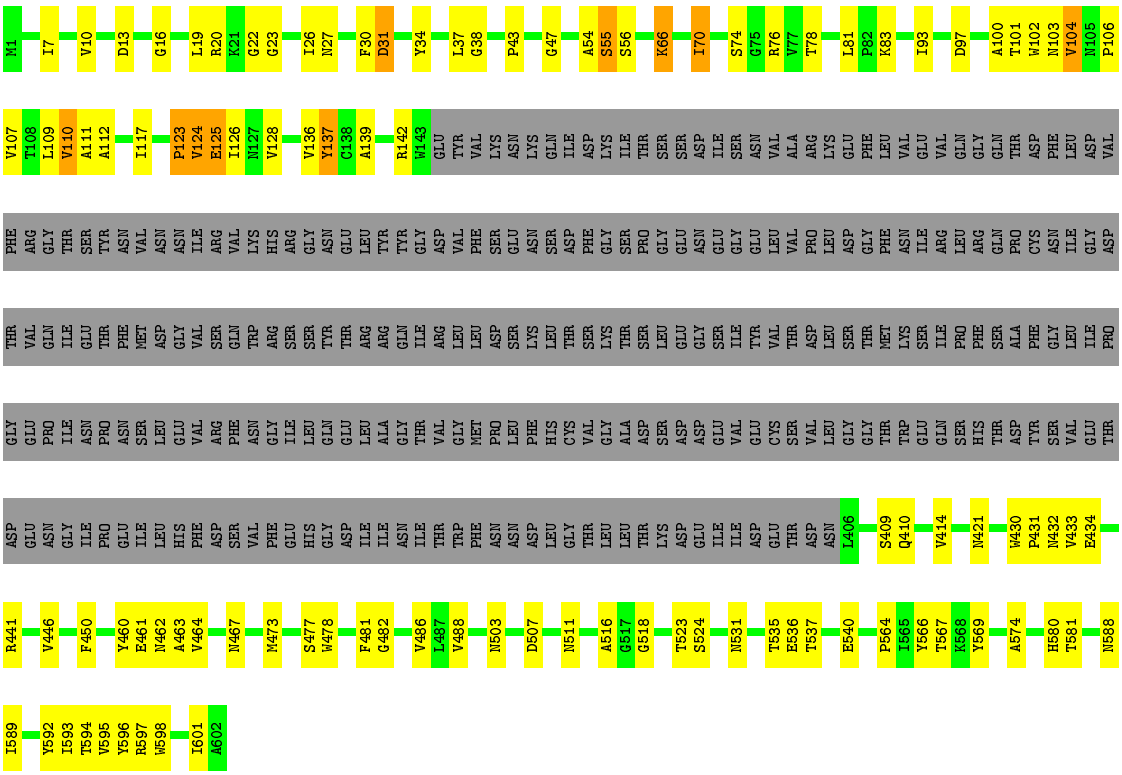
• Molecule 4: Baseplate wedge protein gp53

Chain F:

• Molecule 5: Baseplate wedge protein gp10

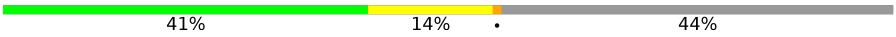
Chain G:

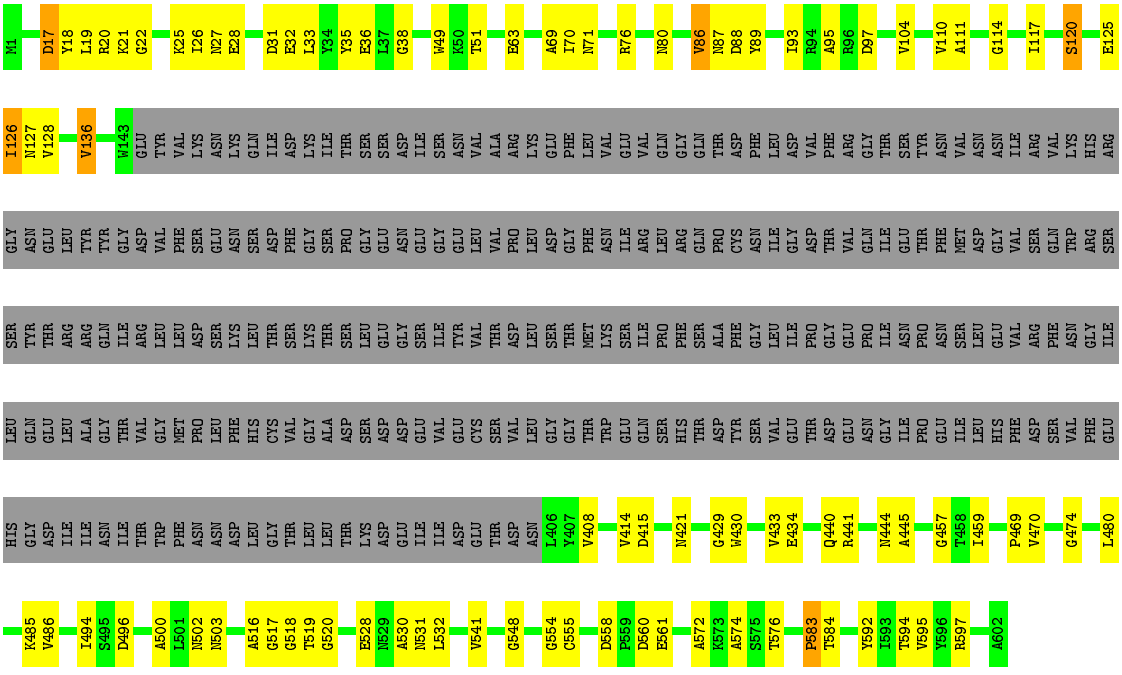




• Molecule 5: Baseplate wedge protein gp10

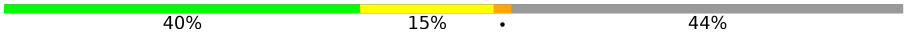
Chain H:

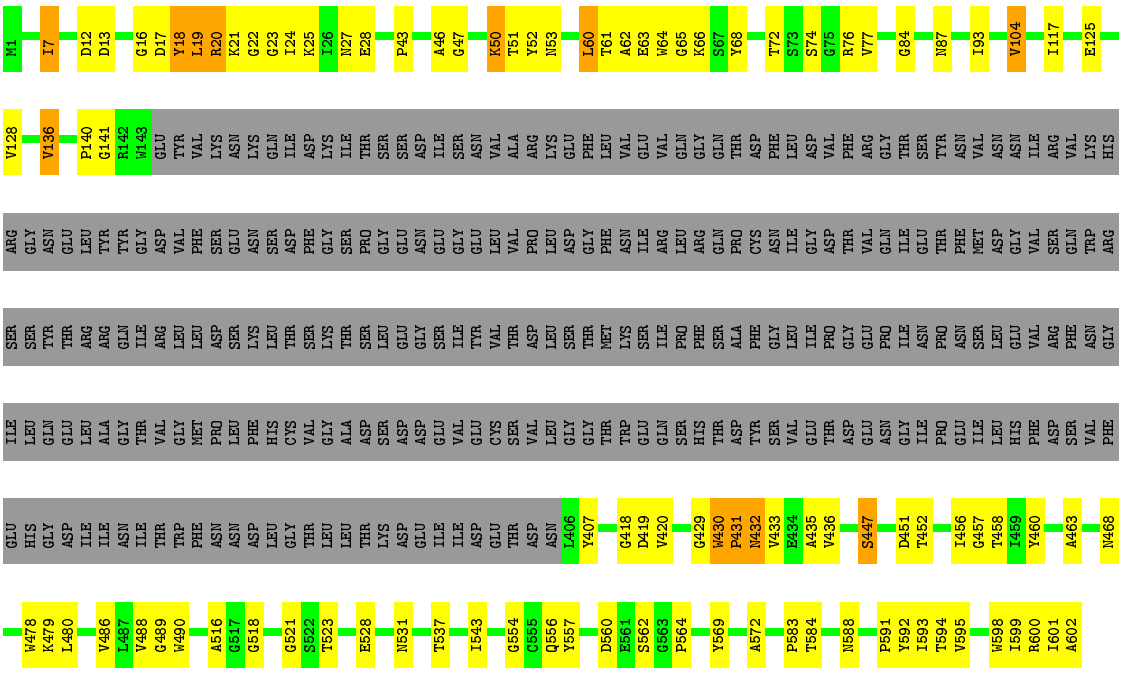




• Molecule 5: Baseplate wedge protein gp10

Chain I:




M1 I7 D12 D13 G16 D17 Y18 L19 R20 K21 G22 G23 I24 K25 I26 N27 E28 P43 A46 G47 K50 T51 Y52 N53 L60 T61 A62 E63 W64 G65 K66 S67 Y68 T72 S73 S74 G75 R76 Y77 G84 N87 I93 V104 I117 E125
V128 V136 P140 G141 R142 W143 GLU TYR VAL LYS ASN LYS GLN ILE ASP LYS ILE THR SER SER ASP ILE SER ASN VAL ALA ARG LYS GLU PHE LEU VAL GLU VAL GLN GLY GLN THR ASP PHE LEU ASP VAL PHE ARG GLY THR SER TYR ASN VAL ASN ASN ILE ARG VAL LYS HIS
ARG GLY ASN GLU LEU TYR TYR GLY ASP VAL PHE SER GLU ASN SER ASP PHE GLY SER PRO GLY GLU ASN GLU GLY GLU LEU VAL PRO LEU ASP GLY PHE ASN ILE ARG LEU GLN PRO CYS ASN ILE GLY ASP THR VAL GLN ILE GLU THR PHE MET ASP GLY VAL SER GLN TRP ARG
SER SER TYR THR ARG ARG GLN ILE ARG LEU LEU ASP SER LYS LEU THR SER LYS THR SER LEU GLU GLY SER ILE TYR VAL THR ASP LEU SER THR MET LYS SER ILE PRO PHE SER ALA PHE GLY LEU ILE PRO GLY GLU PRO ILE ASN PRO ASN SER LEU GLU VAL ARG PHE ASN GLY
ILE LEU GLN GLU LEU ALA GLY THR VAL GLY MET PRO LEU PHE HIS CYS VAL GLY ALA ASP SER ASP ASP GLU VAL GLU CYS SER VAL LEU GLY GLY THR TRP GLU GLN SER HIS THR ASP TYR SER VAL GLU THR ASP GLU ASN GLY ILE PRO GLU ILE LEU LEU HIS PHE ASP SER VAL PHE
GLU HIS GLY ASP ILE ILE ASN ILE THR TRP PHE ASN ASN ASP LEU GLY THR LEU LEU THR LYS ASP GLU ILE ILE ASP GLU THR ASP ASN L406 Y407 G418 D419 V420 G429 W430 P431 N432 V433 E434 A435 V436 S447 D451 T452 I456 G457 T458 I459 Y460 A463 N468
W478 K479 L480 V486 L487 V488 G489 W490 A516 G517 G518 G521 S522 T523 E528 N531 T537 I543 G554 C555 Q556 Y557 D560 E561 S562 G563 P564 Y569 A572 P583 T584 N588 P591 Y592 I593 T594 V595 W598 I599 R600 I601 A602

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of particles used	45607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	Not provided	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	0.37	0/7697	0.62	2/10550 (0.0%)
2	B	0.51	0/2591	0.72	2/3546 (0.1%)
2	C	0.55	0/2662	0.65	0/3640
3	D	0.30	0/4935	0.61	0/6735
3	E	0.28	0/4750	0.56	0/6485
4	F	0.52	0/1536	0.64	0/2095
5	G	0.33	0/1663	0.68	0/2304
5	H	0.34	0/1663	0.72	0/2304
5	I	0.35	0/1663	0.68	0/2304
All	All	0.39	0/29160	0.64	4/39963 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	3
2	C	0	2
3	D	0	9
3	E	0	5
4	F	0	1
5	G	0	9
5	H	0	10
5	I	0	11
All	All	0	55

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	848	LEU	CA-CB-CG	5.42	127.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	274	ILE	N-CA-C	-5.34	96.59	111.00
2	B	42	GLY	N-CA-C	5.29	126.31	113.10
1	A	349	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	496	SER	Peptide
1	A	831	LEU	Peptide
1	A	832	PRO	Peptide
1	A	917	LYS	Peptide
1	A	97	THR	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	7511	0	6716	677	0
2	B	2521	0	2282	345	0
2	C	2585	0	2410	232	0
3	D	4845	0	4477	346	0
3	E	4660	0	4258	182	0
4	F	1495	0	1361	121	0
5	G	1665	0	764	81	0
5	H	1665	0	764	81	0
5	I	1665	0	764	86	0
All	All	28612	0	23796	1674	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 32.

The worst 5 of 1674 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TRP:CZ2	2:B:59:PRO:HD2	1.18	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:VAL:HG21	2:B:16:PHE:CE2	1.20	1.67
1:A:685:ASN:ND2	3:D:21:PHE:CE1	1.68	1.58
1:A:663:ASN:CB	3:D:46:TYR:HA	1.11	1.57
1:A:898:MET:HE3	2:C:272:ILE:CD1	1.33	1.56

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	1028/1032 (100%)	803 (78%)	198 (19%)	27 (3%)	7 48
2	B	332/334 (99%)	266 (80%)	47 (14%)	19 (6%)	2 28
2	C	330/334 (99%)	286 (87%)	41 (12%)	3 (1%)	21 68
3	D	643/660 (97%)	454 (71%)	162 (25%)	27 (4%)	3 36
3	E	632/660 (96%)	483 (76%)	131 (21%)	18 (3%)	6 47
4	F	190/196 (97%)	151 (80%)	32 (17%)	7 (4%)	4 40
5	G	336/602 (56%)	250 (74%)	69 (20%)	17 (5%)	2 31
5	H	336/602 (56%)	253 (75%)	71 (21%)	12 (4%)	4 41
5	I	336/602 (56%)	254 (76%)	64 (19%)	18 (5%)	2 30
All	All	4163/5022 (83%)	3200 (77%)	815 (20%)	148 (4%)	7 41

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	383	VAL
1	A	468	ILE
1	A	690	ILE
1	A	833	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	683/921 (74%)	681 (100%)	2 (0%)	94 98
2	B	252/295 (85%)	245 (97%)	7 (3%)	51 81
2	C	272/295 (92%)	272 (100%)	0	100 100
3	D	479/578 (83%)	477 (100%)	2 (0%)	93 97
3	E	440/578 (76%)	439 (100%)	1 (0%)	95 98
4	F	140/169 (83%)	140 (100%)	0	100 100
All	All	2266/2836 (80%)	2254 (100%)	12 (0%)	92 97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	238	LEU
2	B	239	ILE
3	D	86	ARG
2	B	146	SER
2	B	275	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	B	305	HIS
3	E	582	ASN
2	B	205	ASN
2	B	233	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.