



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 05:32 PM EDT

PDB ID : 3ZIF  
EMDB ID: : EMD-2273  
Title : Cryo-EM structures of two intermediates provide insight into adenovirus assembly and disassembly  
Authors : Cheng, L.; Huang, X.; Li, X.; Xiong, W.; Sun, W.; Yang, C.; Zhang, K.; Wang, Y.; Liu, H.; Ji, G.; Sun, F.; Zheng, C.; Zhu, P.  
Deposited on : unknown  
Resolution : 4.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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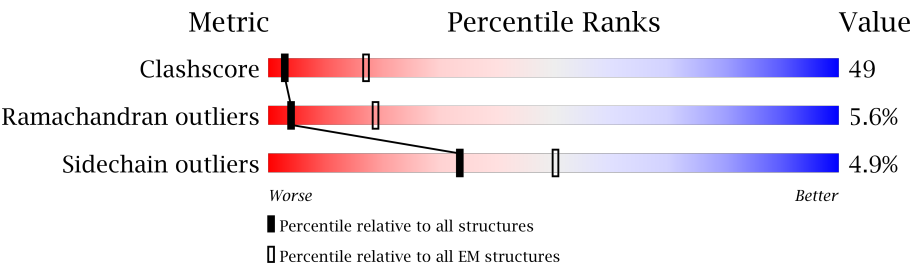
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 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 4.50 Å.

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






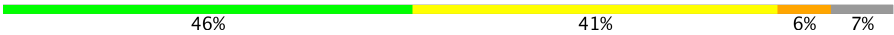





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	911	<div><div>42%</div><div>51%</div><div>5% ..</div></div>
1	B	911	<div><div>42%</div><div>51%</div><div>5% ..</div></div>
1	C	911	<div><div>44%</div><div>49%</div><div>5% ..</div></div>
1	D	911	<div><div>42%</div><div>50%</div><div>5% ..</div></div>
1	E	911	<div><div>42%</div><div>51%</div><div>5% ..</div></div>
1	F	911	<div><div>44%</div><div>50%</div><div>5% ..</div></div>
1	G	911	<div><div>41%</div><div>52%</div><div>5% ..</div></div>
1	H	911	<div><div>43%</div><div>51%</div><div>5% ..</div></div>
1	I	911	<div><div>44%</div><div>50%</div><div>5% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	J	911	 42%51%5% ..
1	K	911	 42%52%5% ..
1	L	911	 43%50%5% ..
2	M	482	 46%41%6%7%
3	N	125	 10%36%25%14%14%
3	O	125	 10%37%25%14%14%
3	P	125	 8%38%25%14%14%
3	Q	125	 10%37%25%14%14%
4	R	216	 15%27%5% •52%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 94377 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 HEXON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	B	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	C	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	D	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	E	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	F	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	G	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	H	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	I	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	J	904	Total 7223	C 4573	N 1266	O 1354	S 30	0	1
1	K	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0
1	L	903	Total 7222	C 4573	N 1265	O 1354	S 30	0	0

- Molecule 2 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	450	Total 3596	C 2275	N 621	O 688	S 12	0	0

- Molecule 3 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	107	Total	C	N	O	S	0	0
			826	507	155	161	3		
3	O	107	Total	C	N	O	S	0	0
			826	507	155	161	3		
3	P	107	Total	C	N	O	S	0	0
			826	507	155	161	3		
3	Q	107	Total	C	N	O	S	0	0
			826	507	155	161	3		

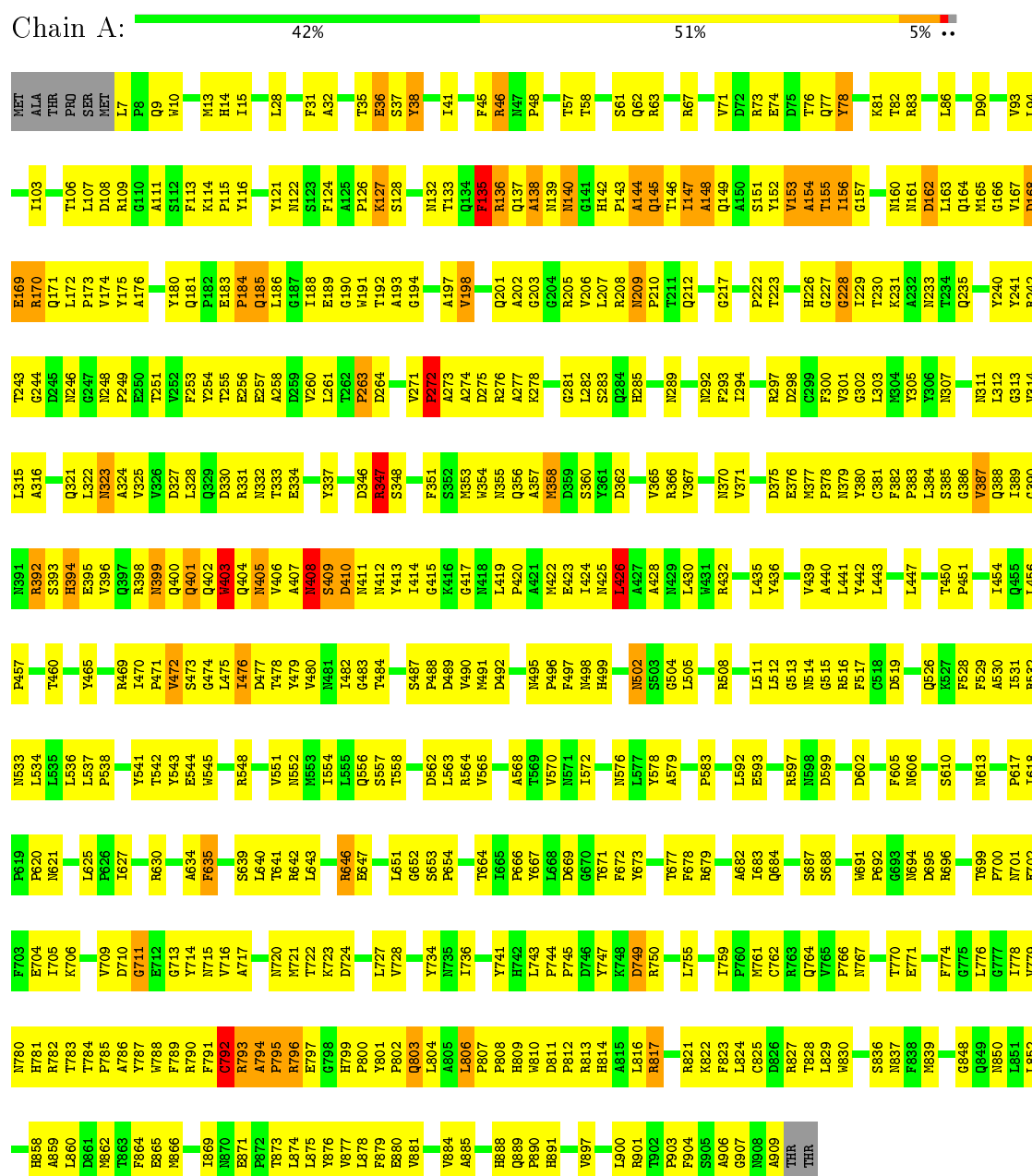
- Molecule 4 is a protein called PVIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	103	Total	C	N	O	S	0	0
			812	514	138	156	4		

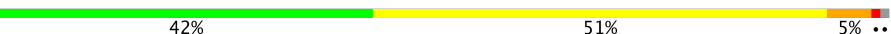
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

#### • Molecule 1: HEXON PROTEIN



#### • Molecule 1: HEXON PROTEIN

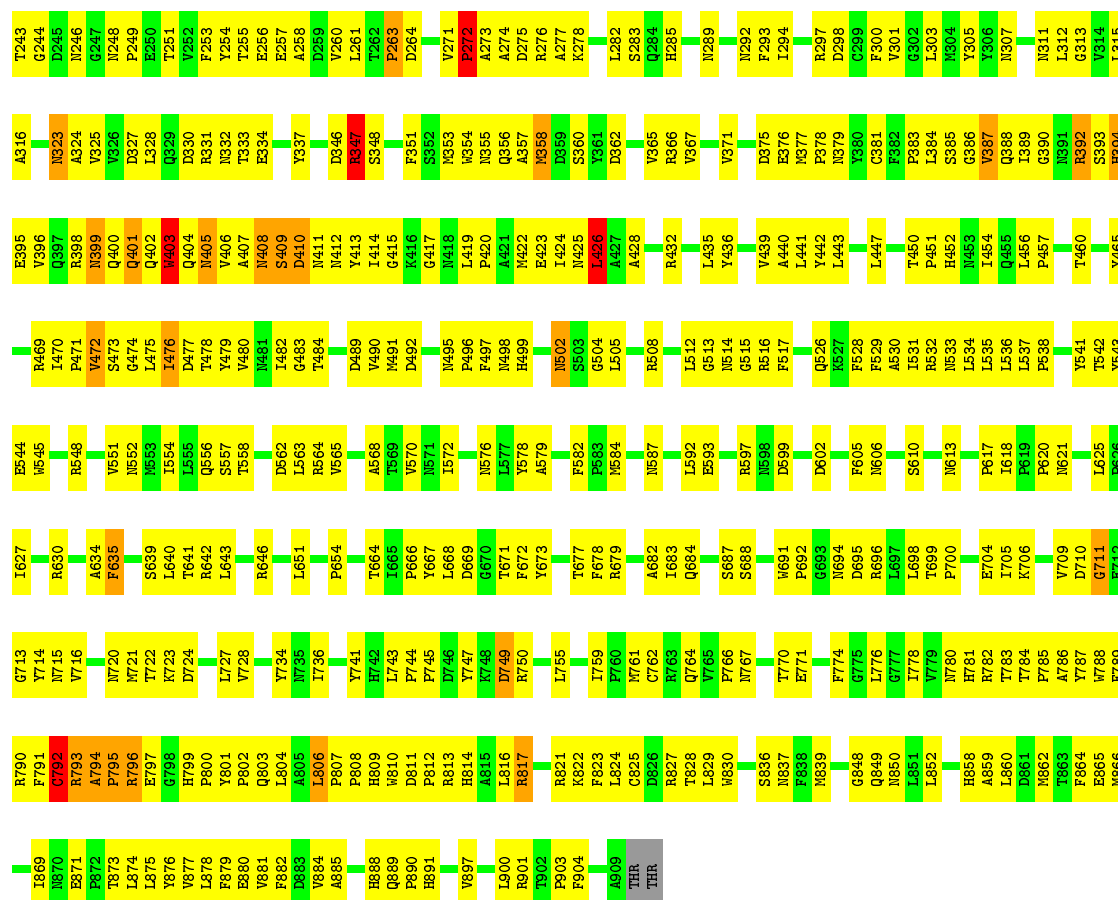
Chain B:  42% 51% 5% ..

MET	ALA	THR	PRO	SER	MET	L7	P8	Q9	W10	M13	I15	A20	S21	E22	L28	F31	A32	T35	E36	S37	Y38	I41	F45	R46	N47	P48	T57	T58	S61	Q62	R63	L64	Q65	L66	R67	V71	D72	R73	T76	Q77	Y78	K81	T82	R83	L86													
	V93			N96		D102	I103	R104	G105	T106	L107	D108	R109	G110	A111	F113	K114	P115	Y116		Y121	S122	F124	A125	P126	K127	S128		N132	T133	Q134	F135	R136	Q137	A138	N139	N140	G141	H142	P143	A144	Q145	T146	I147	A148	Q149	S151	Y152	V153	A154	T155	I156	G157	N160	N161	D162		
	L163	Q164	M165	G166	V167	D168	E169	A170	Q171	L172	P173	Y174	Y175	A176		Y180	Q181	P182	E183	P184	Q185	G187	L188	E189	G190	Y191	T192	S193	G194	A197	V198	Q201	A202	R205	V206	L207	R208	N209	P210	Q211	Q212		G217		N282	F293	L294	R297	D298	C299	F300	V301	G302	L303	A232	N233	L234	
	Q235	Y240	Y241	R242	T243	Q244	D245	I246	Q247	P248	E249	T250	T251	V252	F253	Y254	T255	E256	E257	A258	D259	V260	L261	T262	P263	D264		Y268		V271	T272	K273	A274	D275	R276	A277	K278	V279	L282	S283	Q284	H285		N289		N292	F293	L294	R297	D298	C299	F300	V301	G302	L303	A232	N233	L234
	Y306	N307	S308	G309	G310	N311	L312	G313	V314	A316		N323	A324	V325	V326	D327	L328	Q329	D330	R331	N332	T333		Y337	D346	R347	S348		F351	S352	K353	W354	N355	Q356	A357	N358	D359	S360	Y361	D362	V365	R366	V367		V371		D375	E376	P377	D378	N379	C299	F300	C381	F382	P383	L384	S385
	G386	V387	L388	G389	N391	R392	S393	E394	V395	V396	Q397	R398	N399	Q400	Q401	Q402	N403	Q404	N405	V406	A407	N408	G415	Q416	P417	L419	P420	A421	N422	E423	N425	L426	A428	R432	L435	Y436	V439	A440	L441	Y442	L443		L447	T450	P451	H452												
	N453	I454	Q455	L456	P457	T460	Y465	R469	P470	P471	N472	G473	G474	A475	I476	D477	T478	Y479	N480	V481	N482	L483	D484	N485	S487	P488	D489	V490	N491	D492	N495	P496	P497	N498	H499	N502	S503	G504	L505	R508	L511	G513	N514	G515	R516	F517	L518	D519	F520	H521	F605	N606						
	F528	F529	A530	L531	N532	N533	L534	L535	L536	L537	P538		T541	T542	T543	E544	N545	R548	V551	N552	L553	L554	L555	Q556	S557	T558	D562	L563	R564	V565	A568	T569	V570	N571	L572	N576	L577	Y578	F582	P583	N584	L592	E593	N597	D598	S599	D602	F605	N606									
	M613	P617	G618	P619	P620	M621	L625	P626	I627	R630	M631	M632	A633	A634	P635	S639	L640	T641	R642	L643	R646	L651	G652	S653	P654	T664	P665	Y667	L668	D669	G670	T671	P672	Y673	T677	P678	R679	A682	L683	Q684	P685	D686	S687	S688	V689	T690	N691	P692	G693									
	N694	D695	R696	L697	L698	T699	P700	E704	L705	K706	V709	D710	G711	E712	G713	Y714	N715	V716	N720	N721	N722	K723	D724	W725	F726	L727	K728	Q729	Y734	N735	I736	Y741	H742	L743	P744	P745	D746	Y747	K748	D749	R750	L755	I759	P760	M761	C762	R763	Q764	Y765	P766	N767	T770						
	E771	G777	L778	T779	N780	H781	R782	T783	T784	P785	V786	T787	T788	F789	R790	F791	G792	R793	F794	P795	R796	T797	G798	H799	P800	R801	Q803	L804	A805	P807	N808	N809	N810	D811	P812	R813	R814	A815	L816	R817	K821	R822	F823	L824	C825	S826	R827	T828	L829	N830	S836	N837	F838	N839				
	G848	Q849	N850	L851	L852	A857	H858	A859	L860	D861	N862	T863	F864	E865	N866	L869	N870	E871	P872	T873	L874	L875	Y876	N877	L878	F879	E880	V881	P882	L883	V884	A885	H888	Q889	P890	H891	V894	L895	E896	V897	L900	R901	T902	P903	F904	N908	A909	THR	THR									

• Molecule 1: HEXON PROTEIN

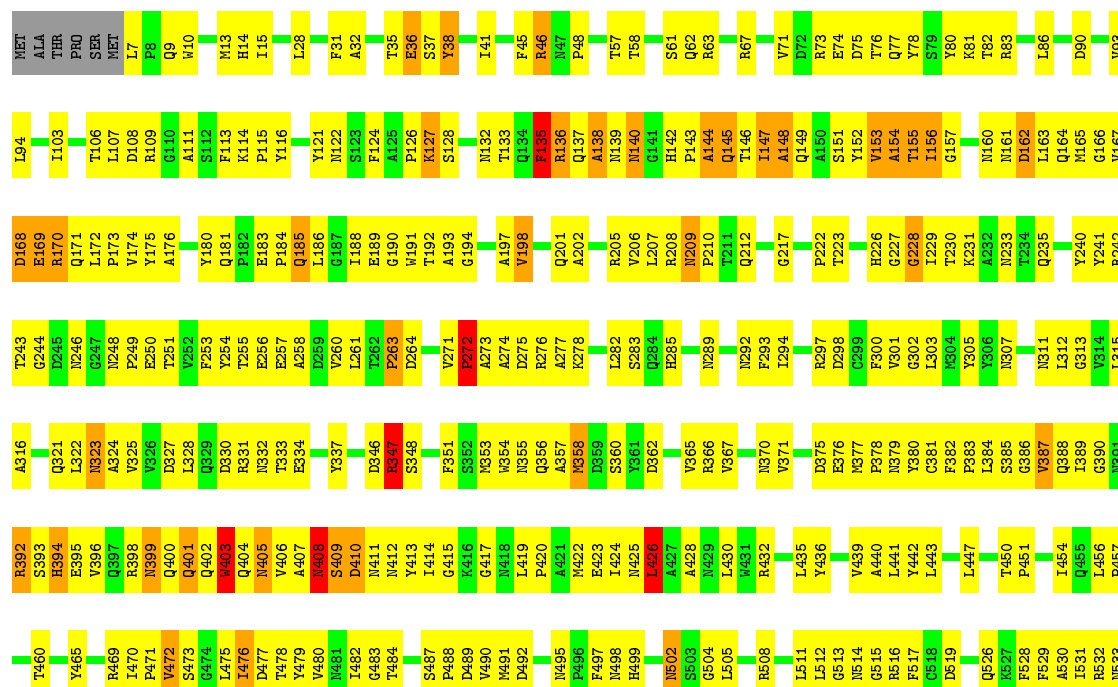
Chain C:  44% 49% 5% ..

										MET									
										ALA									
										THR									
										PRO									
										SER									
										MET									
										L7									
										P8									
										Q9									
										W10									
										M13									
										H14									
										I15									
										A20									
										S21									
										E22									
										L28									
										F31									
										A32									
										T35									
										E36									
										S37									
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										I41									
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										Q62									
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										K81									
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										L107									
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Q181																			
P182																			
E183																			
P184																			
Q185																			
L186																			
G187																			
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E189																			
G190																			
Y191																			
T192																			
A193																			
G194																			
V198																			
Q201																			
A202																			
R203																			
G204																			
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L207																			
R208																			
N209																			
P210																			
T211																			
Q212																			
G217																			
P222																			
H226																			
G227																			
G228																			
I229																			
T230																			
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R242																			

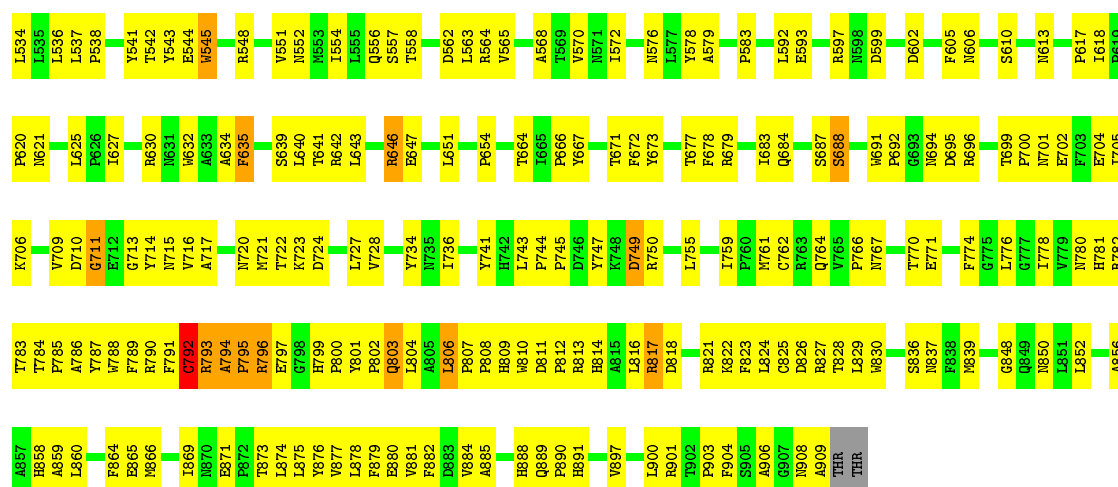


# Molecule 1: HEXON PROTEIN

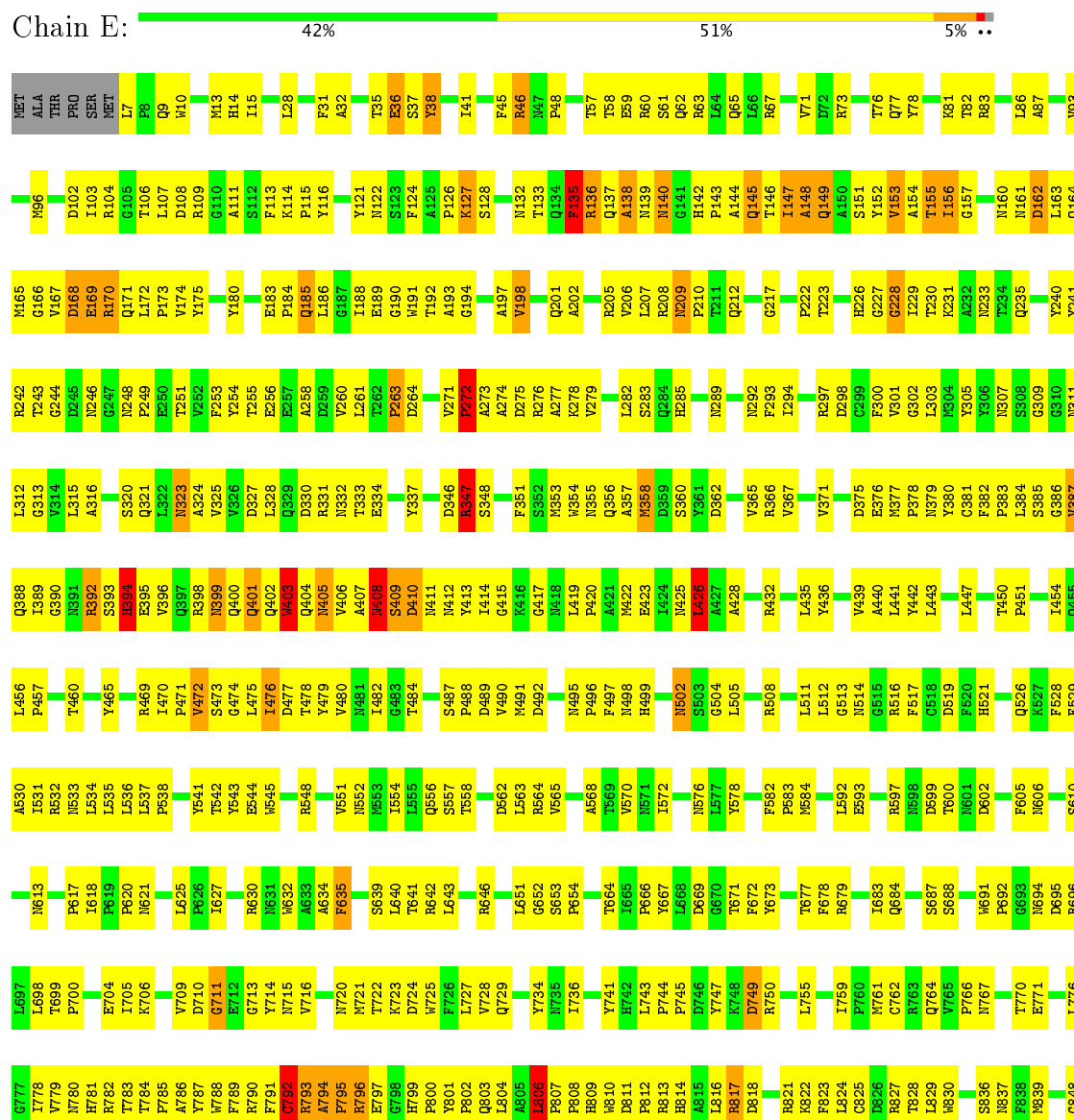
Chain D: 42% 50% 5% ..

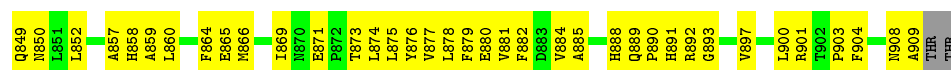






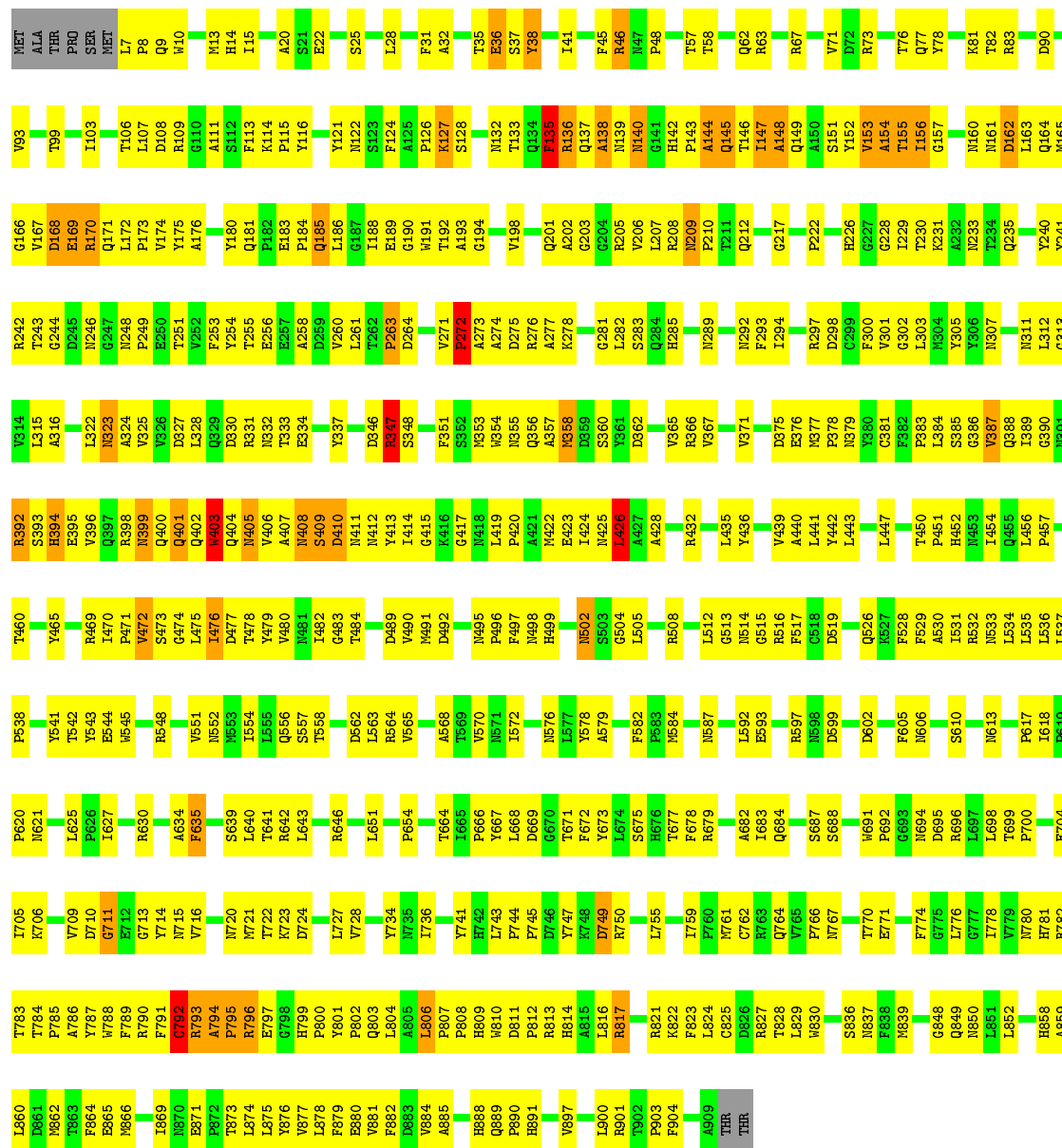
# Molecule 1: HEXON PROTEIN





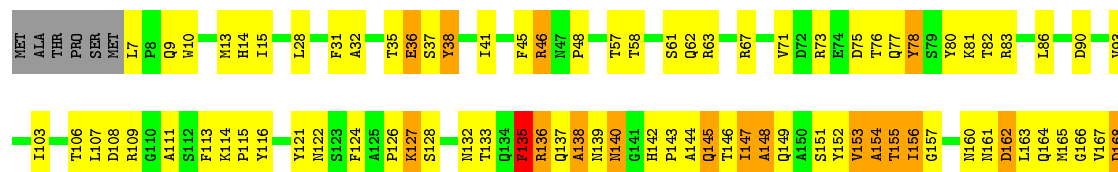
### • Molecule 1: HEXON PROTEIN

Chain F: 44% 50% 5% ..



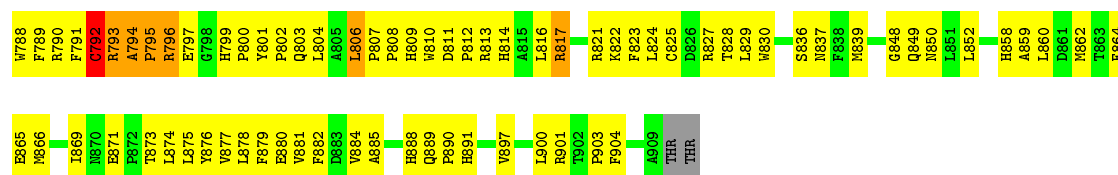
### • Molecule 1: HEXON PROTEIN

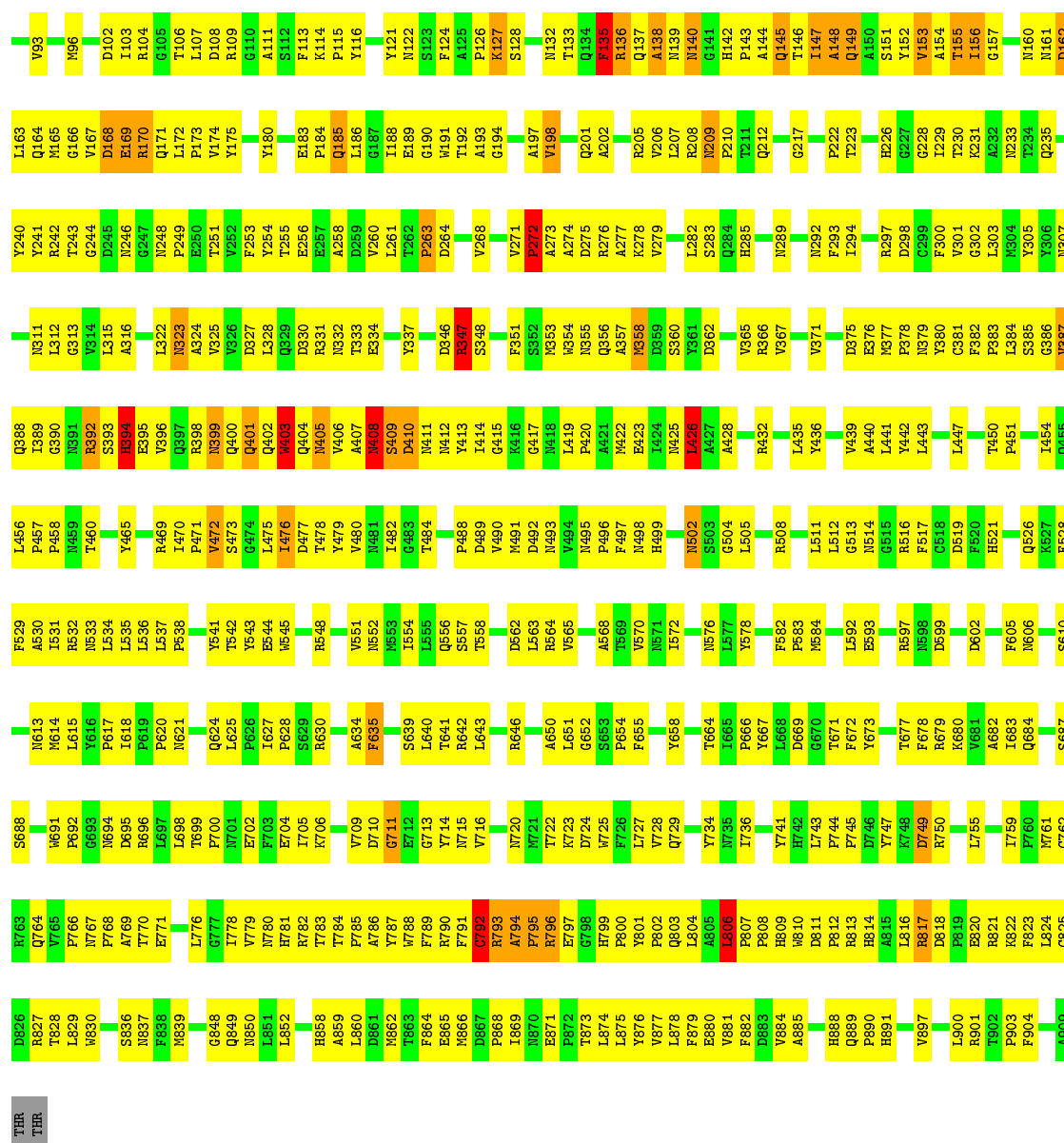
Chain G: 41% 52% 5% ..

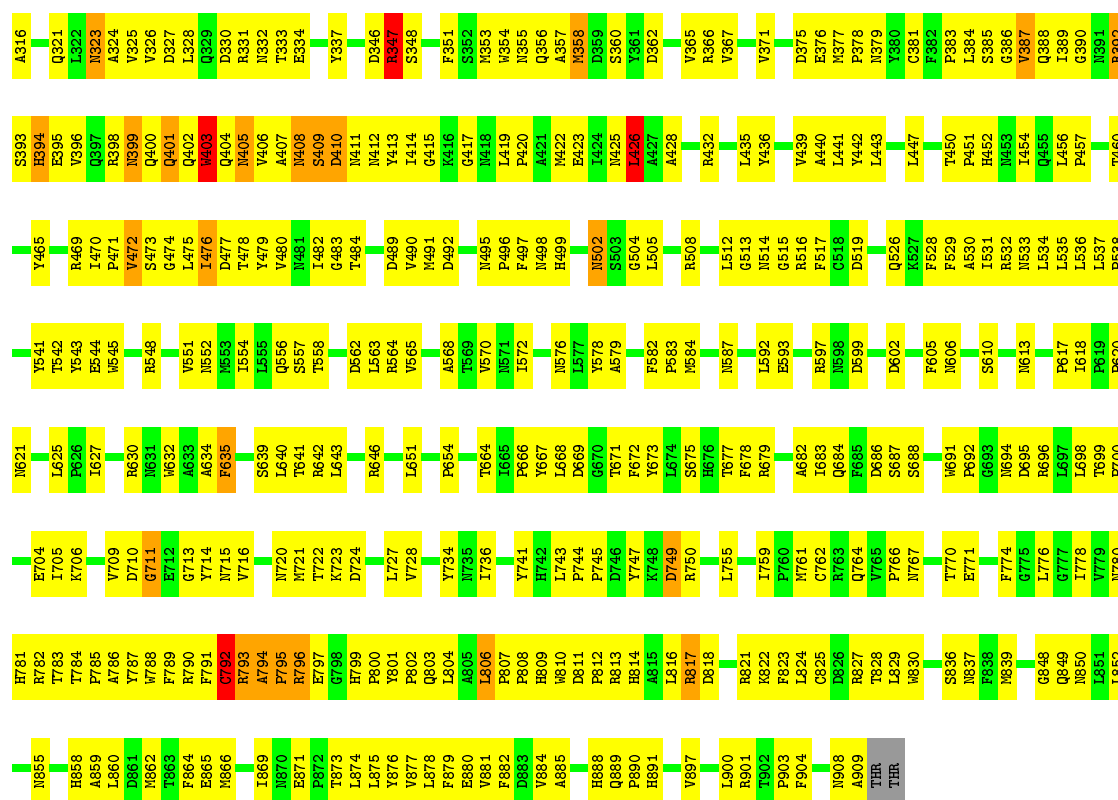






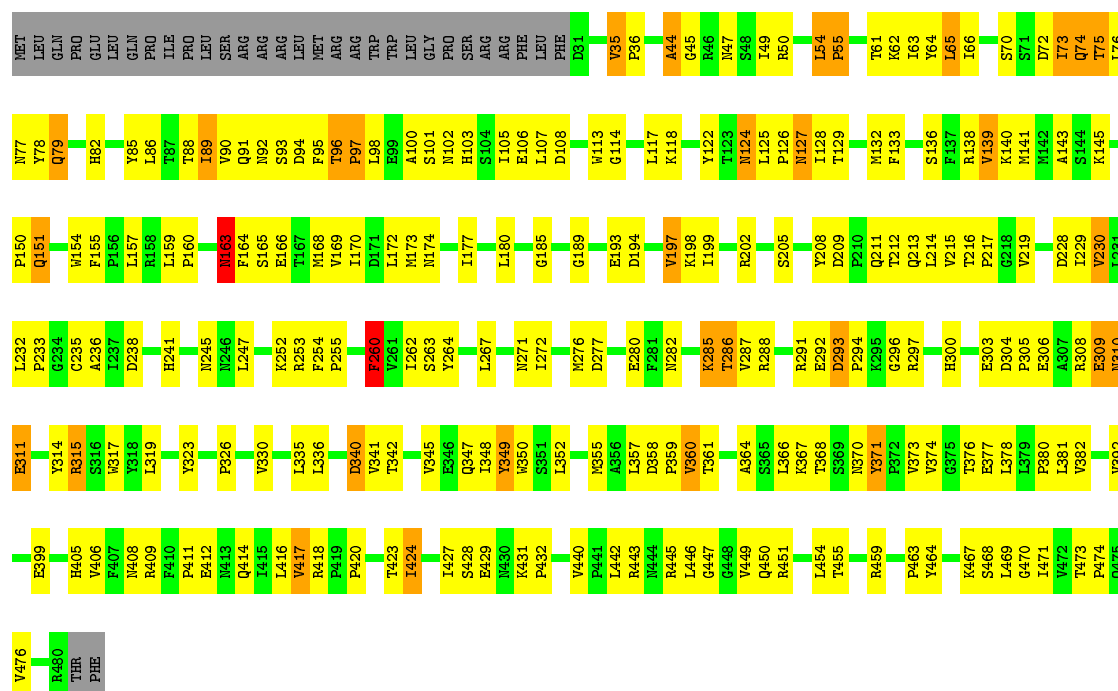






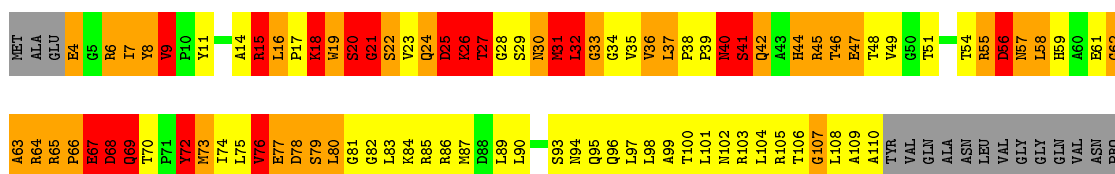
## • Molecule 2: PENTON PROTEIN

Chain M: 46% 41% 6% 7%



## • Molecule 3: PIX

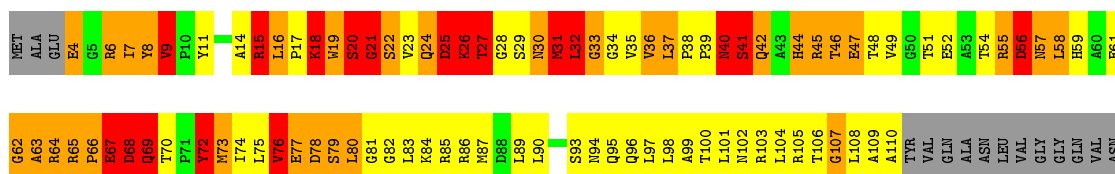
Chain N: 10% 36% 25% 14%



PHE  
VAL

- Molecule 3: PIX

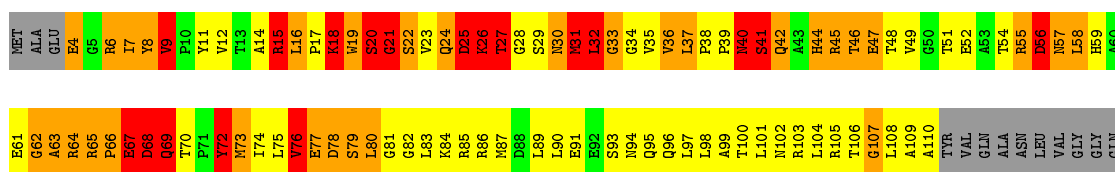
Chain O: 10% 37% 25% 14% 14%



PRO  
PHE  
VAL

- Molecule 3: PIX

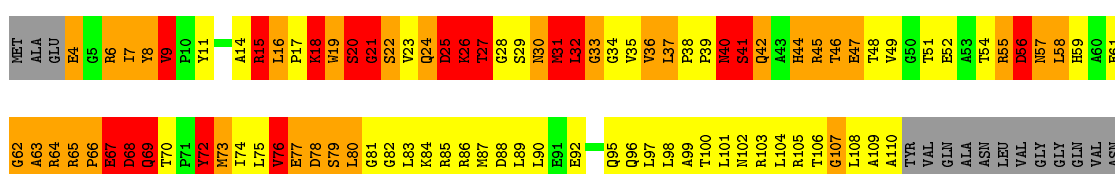
Chain P: 8% 38% 25% 14% 14%



VAL  
ASN  
PRO  
PHE  
VAL

- Molecule 3: PIX

Chain Q: 10% 37% 25% 14% 14%



PRO  
PHE  
VAL

- Molecule 4: PVIII

Chain R: 15% 27% 5% 52%



LEU	ASP	MET
THR	PRO	SER
ALA	ARG	LYS
SER	GLN	E4
CYS	TRP	I5
LEU	ALA	P6
ARG	ALA	T7
PRO	HIS	P8
ASP	LEU	Y9
GLY	ILE	V10
VAL	LYS	M11
PHE	GLN	T12
GLN	PRO	F13
LEU	VAL	Q14
GLY	VAL	P15
GLY	GLY	Q16
GLY	THR	M17
SER	THR	G18
ARG	HIS	
SER	VAL	A23
SER	GLU	S24
PHE	MET	Q25
ASN	PRO	D26
PRO	ARG	Y27
LEU	ASN	S28
GLN	GLU	T29
THR	VAL	R30
ASP	LEU	M31
PHE	GLU	N32
ALA	GLN	N33
PHE	HIS	F34
HIS	LEU	S35
ALA	THR	A36
LEU	SER	G37
PRO	HIS	P38
SER	GLY	D39
ARG	ALA	M40
PRO	GLN	I41
ARG	ILE	
HIS	ALA	V44
G170	GLY	M45
I172	GLY	
G173	ALA	A50
S174	ALA	Q51
R175	GLY	R52
Q176	ASP	E53
F177	TYR	I54
V178	PHE	L55
	LYS	
V182	SER	S59
P183	PRO	A60
A184	THR	I61
V185	SER	ALA
Y186	ALA	THR
I187	ARG	PRO
N188	THR	ARG
P189	LEU	ASN
Y190	ILE	LEU
S191	PRO	ILE

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11910	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL IMAGES	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125390	Depositor
Image detector	GENERIC GATAN	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	0.27	0/7431	0.48	0/10139
1	B	0.27	0/7431	0.48	0/10139
1	C	0.27	0/7431	0.48	0/10139
1	D	0.27	0/7431	0.48	0/10139
1	E	0.27	0/7431	0.47	0/10139
1	F	0.27	0/7431	0.48	0/10139
1	G	0.27	0/7431	0.47	0/10139
1	H	0.27	0/7431	0.47	0/10139
1	I	0.27	0/7431	0.48	0/10139
1	J	0.27	0/7432	0.47	0/10141
1	K	0.27	0/7431	0.47	0/10139
1	L	0.27	0/7431	0.48	0/10139
2	M	0.67	2/3682 (0.1%)	1.02	8/5013 (0.2%)
3	N	0.92	4/838 (0.5%)	1.94	34/1135 (3.0%)
3	O	0.92	4/838 (0.5%)	1.93	33/1135 (2.9%)
3	P	0.91	4/838 (0.5%)	1.93	34/1135 (3.0%)
3	Q	0.91	4/838 (0.5%)	1.94	34/1135 (3.0%)
4	R	0.27	0/837	0.42	0/1142
All	All	0.33	18/97044 (0.0%)	0.61	143/132365 (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
2	M	0	2
3	N	1	5
3	O	1	5
3	P	1	5
3	Q	1	5
All	All	4	22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	69	GLN	CB-CG	-8.32	1.30	1.52
3	N	69	GLN	CB-CG	-8.31	1.30	1.52
3	P	69	GLN	CB-CG	-8.30	1.30	1.52
3	Q	69	GLN	CB-CG	-8.29	1.30	1.52
2	M	65	LEU	C-N	-6.67	1.18	1.34

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	68	ASP	N-CA-C	21.04	167.81	111.00
3	P	68	ASP	N-CA-C	21.04	167.79	111.00
3	N	68	ASP	N-CA-C	21.02	167.77	111.00
3	O	68	ASP	N-CA-C	21.02	167.75	111.00
3	N	26	LYS	CA-C-N	-13.04	88.51	117.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	68	ASP	CA
3	O	68	ASP	CA
3	P	68	ASP	CA
3	Q	68	ASP	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	282	ASN	Peptide
2	M	371	TYR	Sidechain
3	N	26	LYS	Mainchain
3	N	67	GLU	Mainchain,Peptide
3	N	68	ASP	Mainchain

## 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	7222	0	6877	712	0
1	B	7222	0	6873	816	0
1	C	7222	0	6877	663	0
1	D	7222	0	6875	756	0
1	E	7222	0	6877	781	0
1	F	7222	0	6878	650	0
1	G	7222	0	6875	827	0
1	H	7222	0	6878	727	0
1	I	7222	0	6878	646	0
1	J	7223	0	6875	835	0
1	K	7222	0	6875	745	0
1	L	7222	0	6871	698	0
2	M	3596	0	3533	265	0
3	N	826	0	826	443	0
3	O	826	0	826	465	0
3	P	826	0	821	501	0
3	Q	826	0	828	308	0
4	R	812	0	744	192	0
All	All	94377	0	90087	8994	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 49.

The worst 5 of 8994 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:632:TRP:CD1	1:G:321:GLN:HB3	1.25	1.68
1:K:658:TYR:CZ	3:P:39:PRO:HD3	1.33	1.64
3:N:83:LEU:CD2	3:P:83:LEU:HD21	1.18	1.64
3:N:104:LEU:CD2	3:O:104:LEU:HD13	1.26	1.63
1:E:909:ALA:HB3	1:G:544:GLU:CB	1.25	1.62

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	901/911 (99%)	722 (80%)	132 (15%)	47 (5%)	2	27
1	B	901/911 (99%)	722 (80%)	133 (15%)	46 (5%)	2	28
1	C	901/911 (99%)	726 (81%)	131 (14%)	44 (5%)	2	29
1	D	901/911 (99%)	720 (80%)	134 (15%)	47 (5%)	2	27
1	E	901/911 (99%)	722 (80%)	132 (15%)	47 (5%)	2	27
1	F	901/911 (99%)	726 (81%)	131 (14%)	44 (5%)	2	29
1	G	901/911 (99%)	721 (80%)	133 (15%)	47 (5%)	2	27
1	H	901/911 (99%)	723 (80%)	131 (14%)	47 (5%)	2	27
1	I	901/911 (99%)	726 (81%)	131 (14%)	44 (5%)	2	29
1	J	902/911 (99%)	722 (80%)	133 (15%)	47 (5%)	2	27
1	K	901/911 (99%)	723 (80%)	131 (14%)	47 (5%)	2	27
1	L	901/911 (99%)	726 (81%)	131 (14%)	44 (5%)	2	29
2	M	448/482 (93%)	321 (72%)	90 (20%)	37 (8%)	1	17
3	N	105/125 (84%)	64 (61%)	26 (25%)	15 (14%)	0	5
3	O	105/125 (84%)	64 (61%)	26 (25%)	15 (14%)	0	5
3	P	105/125 (84%)	64 (61%)	26 (25%)	15 (14%)	0	5
3	Q	105/125 (84%)	64 (61%)	26 (25%)	15 (14%)	0	5
4	R	99/216 (46%)	80 (81%)	12 (12%)	7 (7%)	1	20
All	All	11780/12130 (97%)	9336 (79%)	1789 (15%)	655 (6%)	4	26

5 of 655 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ALA
1	A	140	ASN
1	A	162	ASP
1	A	169	GLU
1	A	170	ARG

### 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	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	B	779/786 (99%)	751 (96%)	28 (4%)	40	69
1	C	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	D	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	E	779/786 (99%)	751 (96%)	28 (4%)	40	69
1	F	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	G	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	H	779/786 (99%)	751 (96%)	28 (4%)	40	69
1	I	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	J	779/786 (99%)	752 (96%)	27 (4%)	41	70
1	K	779/786 (99%)	751 (96%)	28 (4%)	40	69
1	L	779/786 (99%)	752 (96%)	27 (4%)	41	70
2	M	401/432 (93%)	393 (98%)	8 (2%)	60	82
3	N	89/103 (86%)	51 (57%)	38 (43%)	0	0
3	O	89/103 (86%)	51 (57%)	38 (43%)	0	0
3	P	89/103 (86%)	51 (57%)	38 (43%)	0	0
3	Q	89/103 (86%)	51 (57%)	38 (43%)	0	0
4	R	87/179 (49%)	77 (88%)	10 (12%)	6	31
All	All	10192/10455 (98%)	9694 (95%)	498 (5%)	33	62

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	136	ARG
1	K	136	ARG
3	Q	26	LYS
1	I	392	ARG
1	J	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 420 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	684	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	233	ASN
1	L	684	GLN
1	G	62	GLN
1	G	502	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	65:LEU	C	66:ILE	N	1.18