wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 04:03 PM EST

PDB ID	:	7S78
EMDB ID	:	EMD-24881
Title	:	Structure of a cell-entry defective human adenovirus provides insights into precursor proteins and capsid maturation
Authors	:	Reddy, V.S.; Yu, X.
Deposited on	:	2021-09-15
Resolution	:	3.72 Å(reported)
Based on initial model	:	3IYN

This is a wwPDB EM 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/EMValidationReportHelp
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:

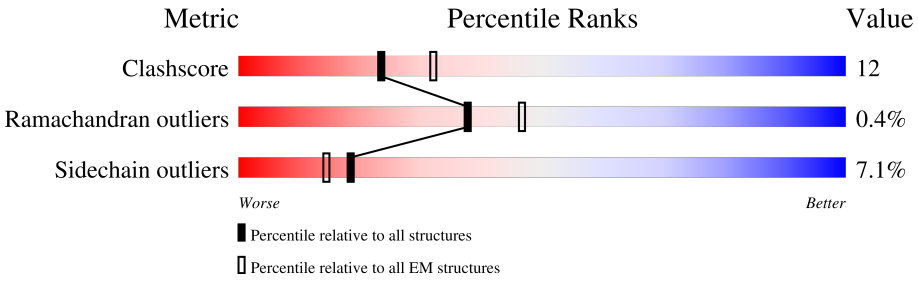
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.72 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	952	67% 28%
1	B	952	68% 26%
1	C	952	67% 28%
1	D	952	69% 26%
1	E	952	65% 29%
1	F	952	66% 28%
1	G	952	70% 25%
1	H	952	69% 27%

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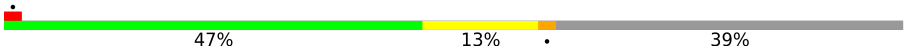
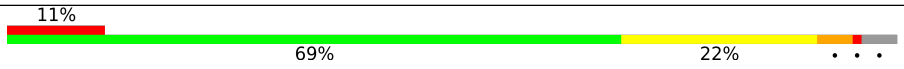
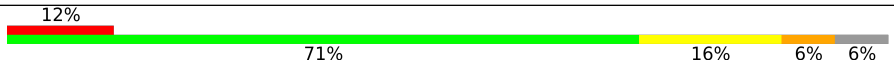
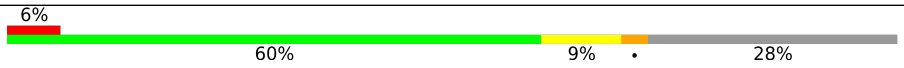
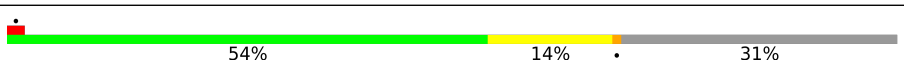
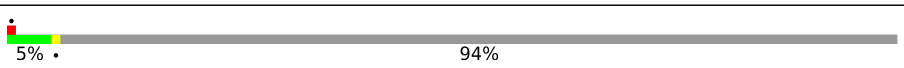
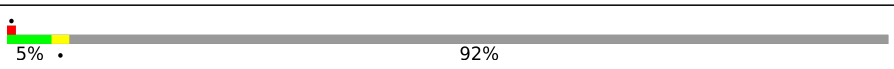
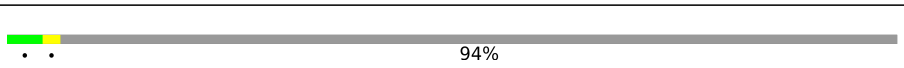
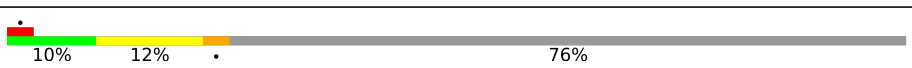
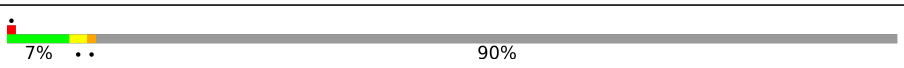
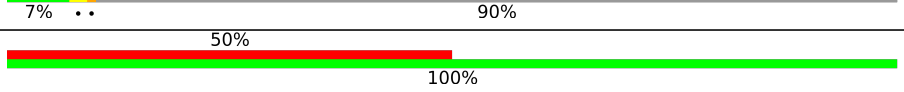
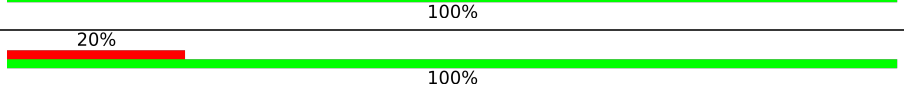
Mol	Chain	Length	Quality of chain
1	I	952	
1	J	952	
1	K	952	
1	L	952	
2	N	571	
3	M	585	
4	P	140	
4	Q	140	
4	R	140	
4	S	140	
5	U	227	
5	V	227	
6	0	250	
6	1	250	
6	2	250	
6	3	250	
6	4	250	
6	W	250	
6	X	250	
6	Y	250	
6	Z	250	
7	5	16	
8	6	10	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 104715 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	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		
1	B	929	Total	C	N	O	S	0	0
			7429	4719	1258	1416	36		
1	C	933	Total	C	N	O	S	0	0
			7456	4736	1262	1422	36		
1	D	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		
1	E	926	Total	C	N	O	S	0	0
			7408	4708	1255	1409	36		
1	F	929	Total	C	N	O	S	0	0
			7430	4721	1258	1415	36		
1	G	931	Total	C	N	O	S	0	0
			7441	4726	1260	1419	36		
1	H	933	Total	C	N	O	S	0	0
			7455	4736	1262	1420	37		
1	I	927	Total	C	N	O	S	0	0
			7417	4713	1256	1412	36		
1	J	928	Total	C	N	O	S	0	0
			7419	4713	1256	1414	36		
1	K	931	Total	C	N	O	S	0	0
			7442	4728	1260	1418	36		
1	L	929	Total	C	N	O	S	0	0
			7427	4718	1258	1415	36		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	466	Total	C	N	O	S	0	0
			3734	2365	646	711	12		

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	359	Total	C	N	O	S	0	0
			2813	1752	517	535	9		

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	134	Total	C	N	O	S	0	0
			972	600	171	199	2		
4	Q	131	Total	C	N	O	S	0	0
			952	587	168	195	2		
4	R	101	Total	C	N	O	S	0	0
			751	470	128	151	2		
4	S	97	Total	C	N	O	S	0	0
			727	448	128	149	2		

- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	165	Total	C	N	O	S	0	0
			1268	797	223	243	5		
5	V	184	Total	C	N	O	S	0	0
			1414	890	248	272	4		

- Molecule 6 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	35	Total	C	N	O	S	0	0
			262	165	48	47	2		
6	X	78	Total	C	N	O	S	0	0
			577	361	107	106	3		
6	Y	61	Total	C	N	O	S	0	0
			485	305	90	87	3		
6	Z	25	Total	C	N	O	S	0	0
			179	109	35	34	1		
6	0	16	Total	C	N	O	S	0	0
			114	68	23	22	1		
6	1	57	Total	C	N	O	S	0	0
			449	279	84	83	3		
6	2	19	Total	C	N	O	S	0	0
			133	81	26	25	1		
6	3	60	Total	C	N	O	S	0	0
			471	293	87	88	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	15	Total	C	N	O	S	0	0
			106	64	21	20	1		

- Molecule 7 is a protein called Unknown-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 8 is a protein called Unknown-2.

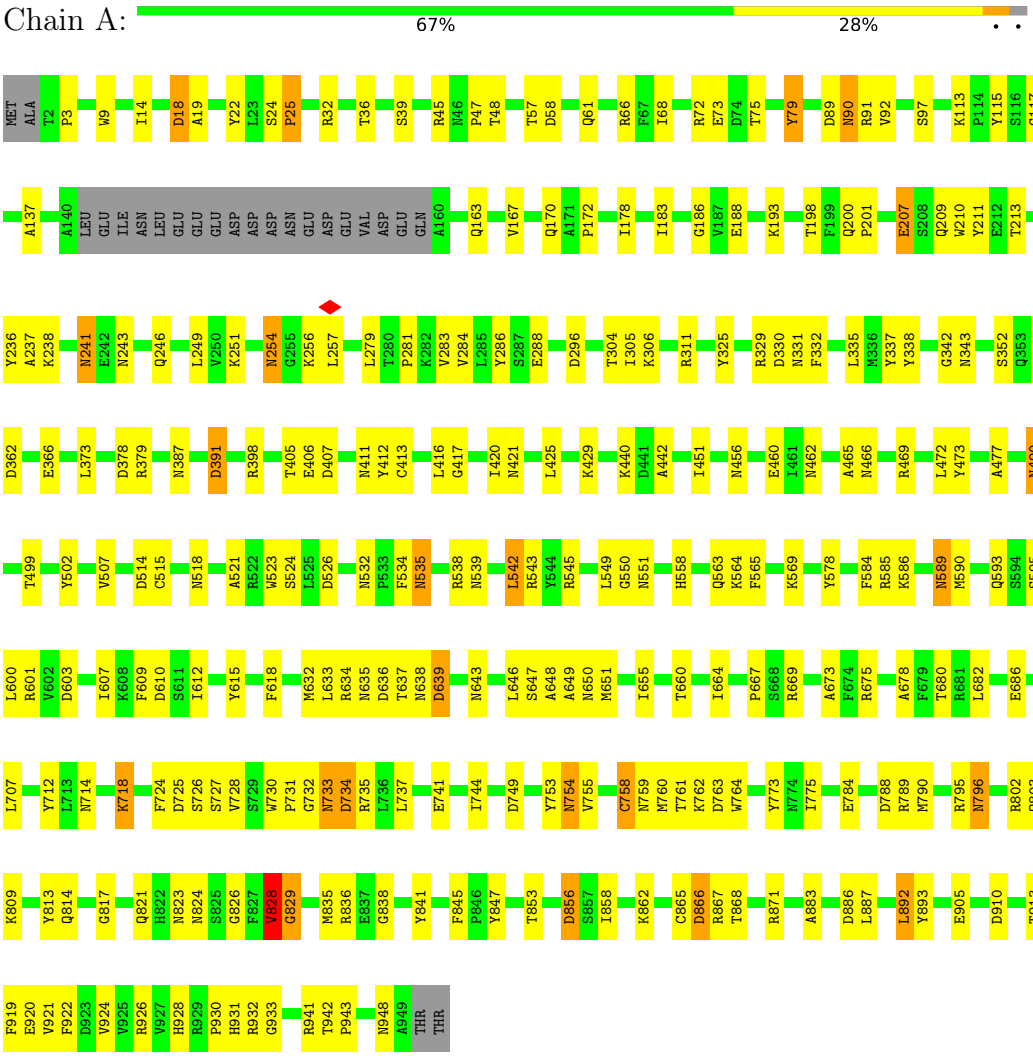
Mol	Chain	Residues	Atoms				AltConf	Trace
8	6	10	Total	C	N	O	0	0
			50	30	10	10		

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

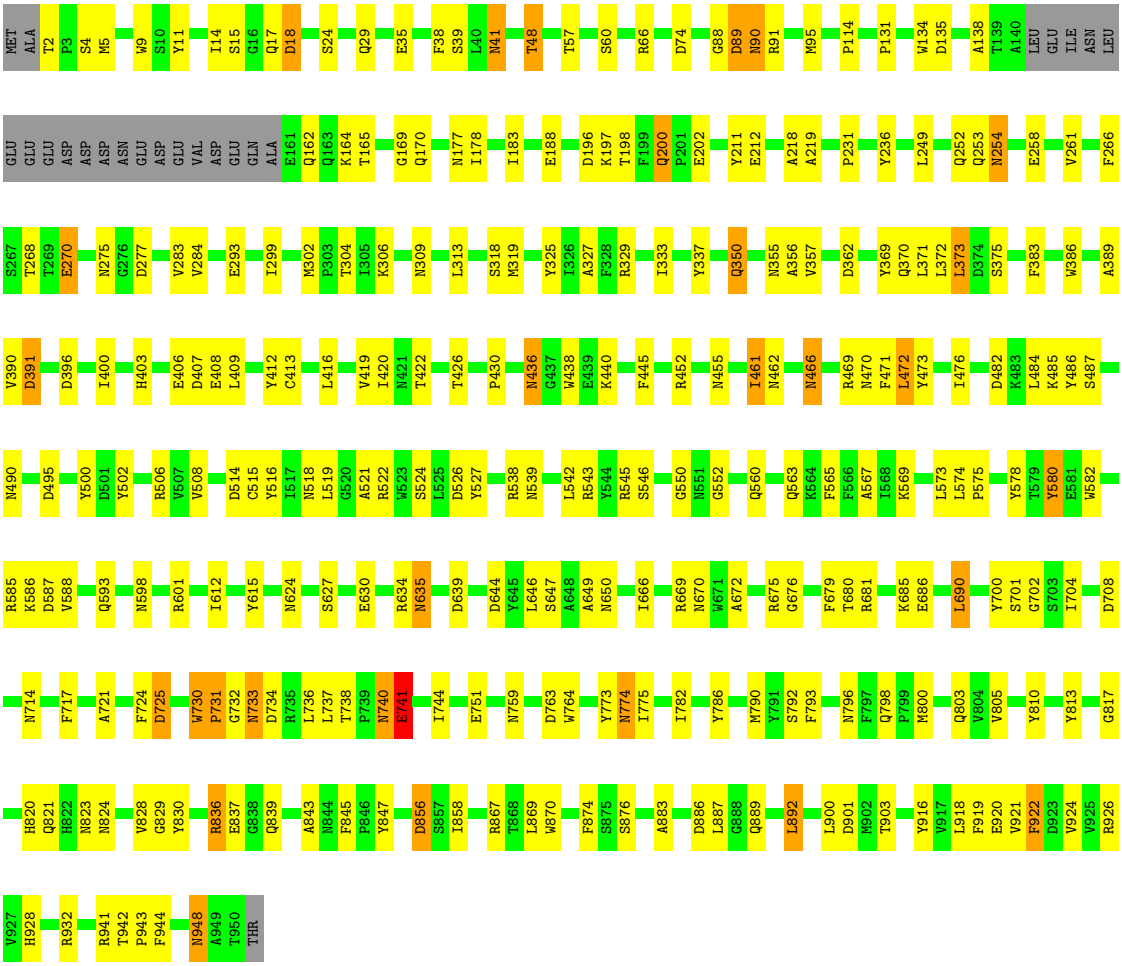
• Molecule 1: Hexon protein

Chain A:



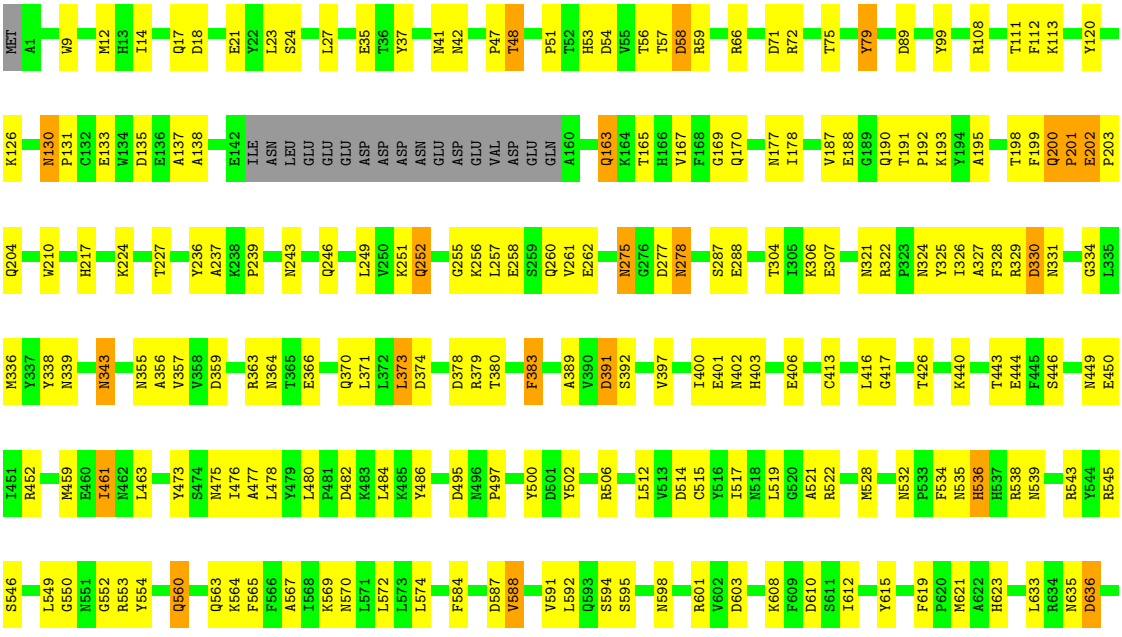
• Molecule 1: Hexon protein

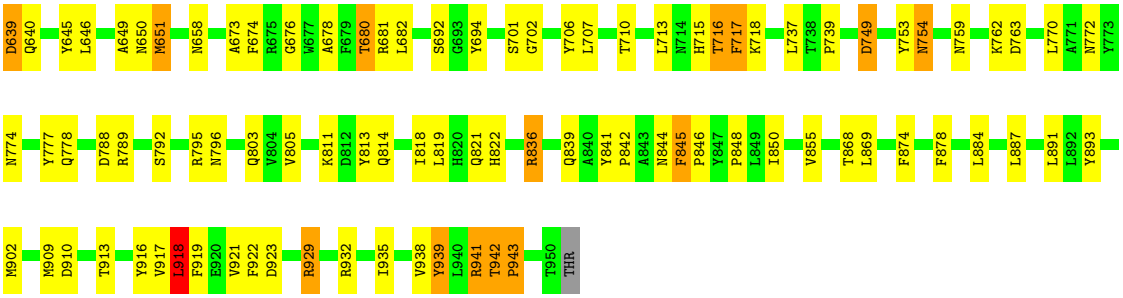
Chain B:



• Molecule 1: Hexon protein

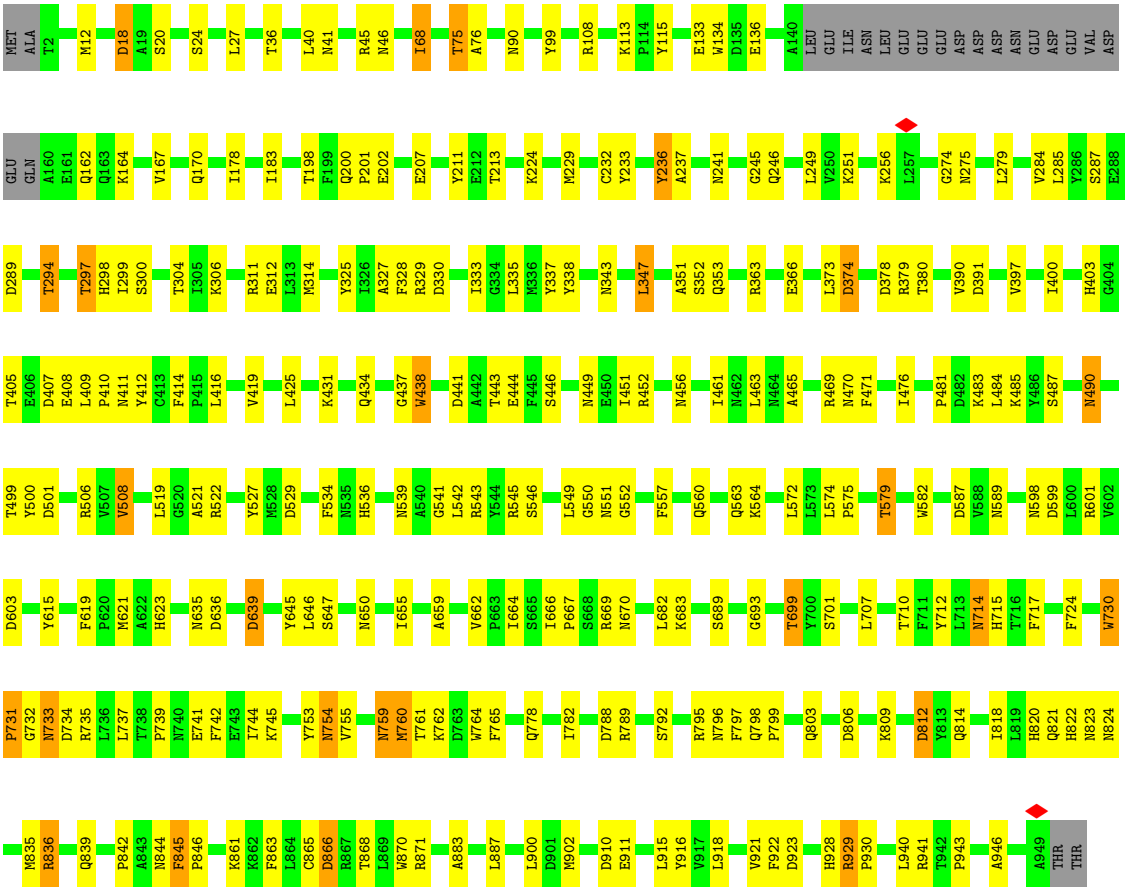
Chain C:





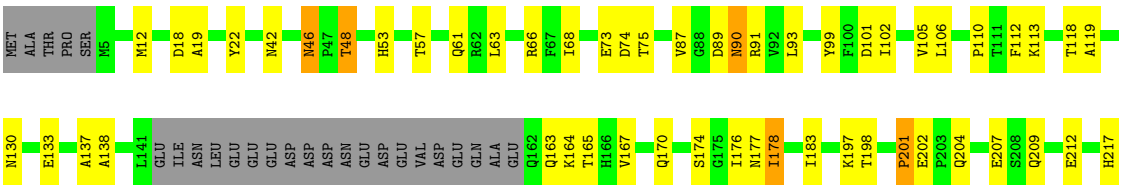
• Molecule 1: Hexon protein

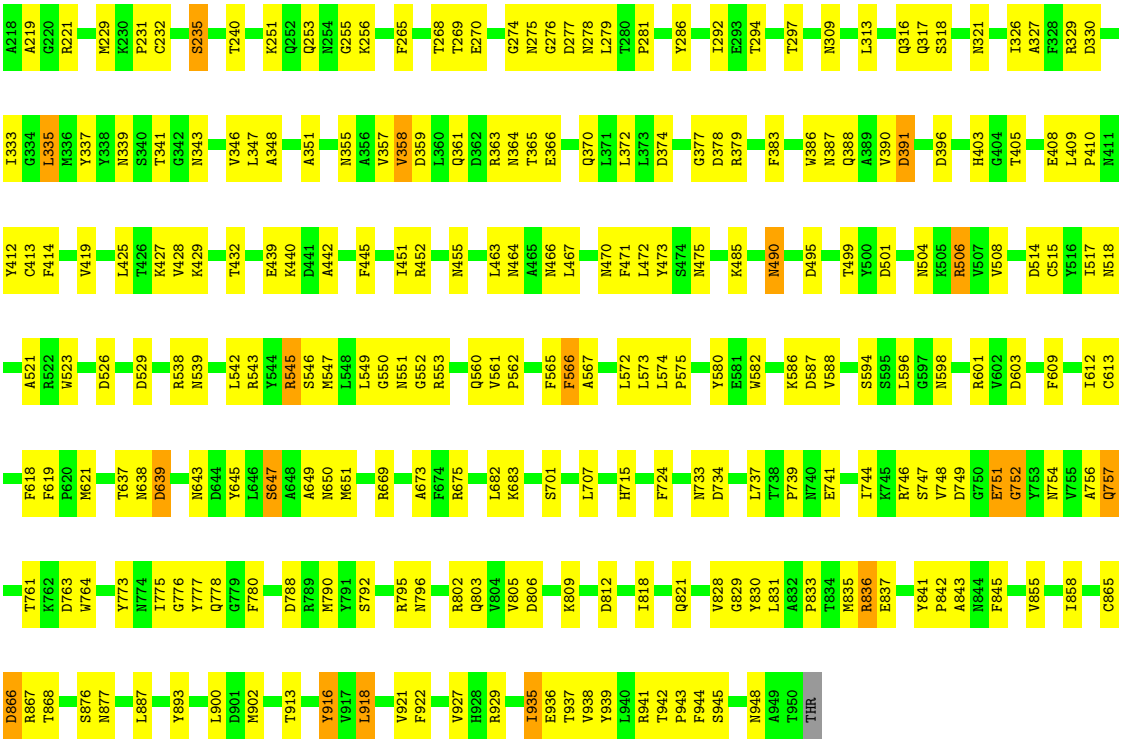
Chain D:



• Molecule 1: Hexon protein

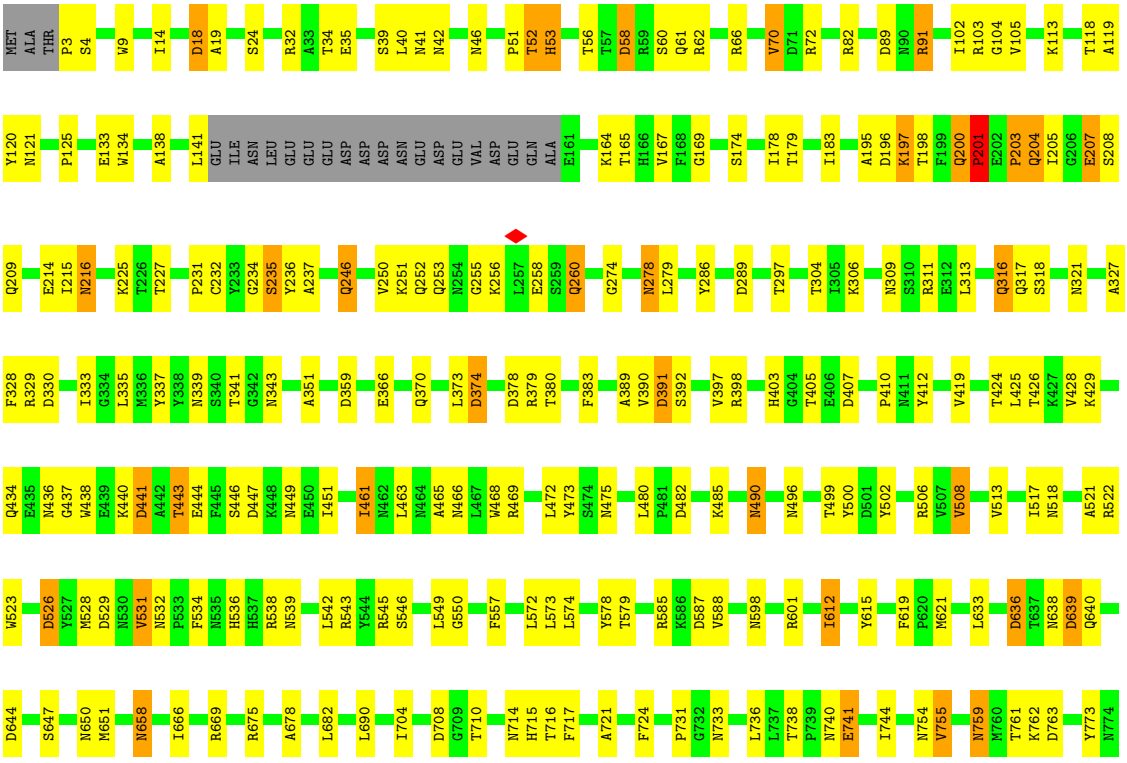
Chain E:

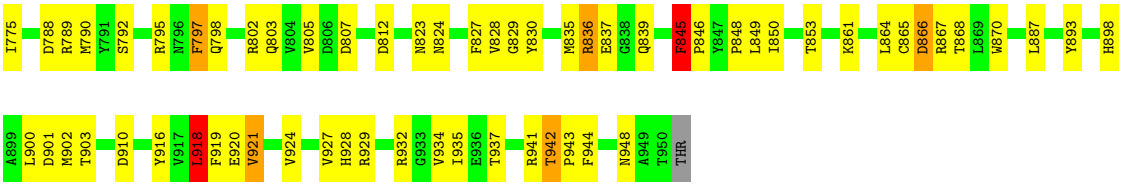




• Molecule 1: Hexon protein

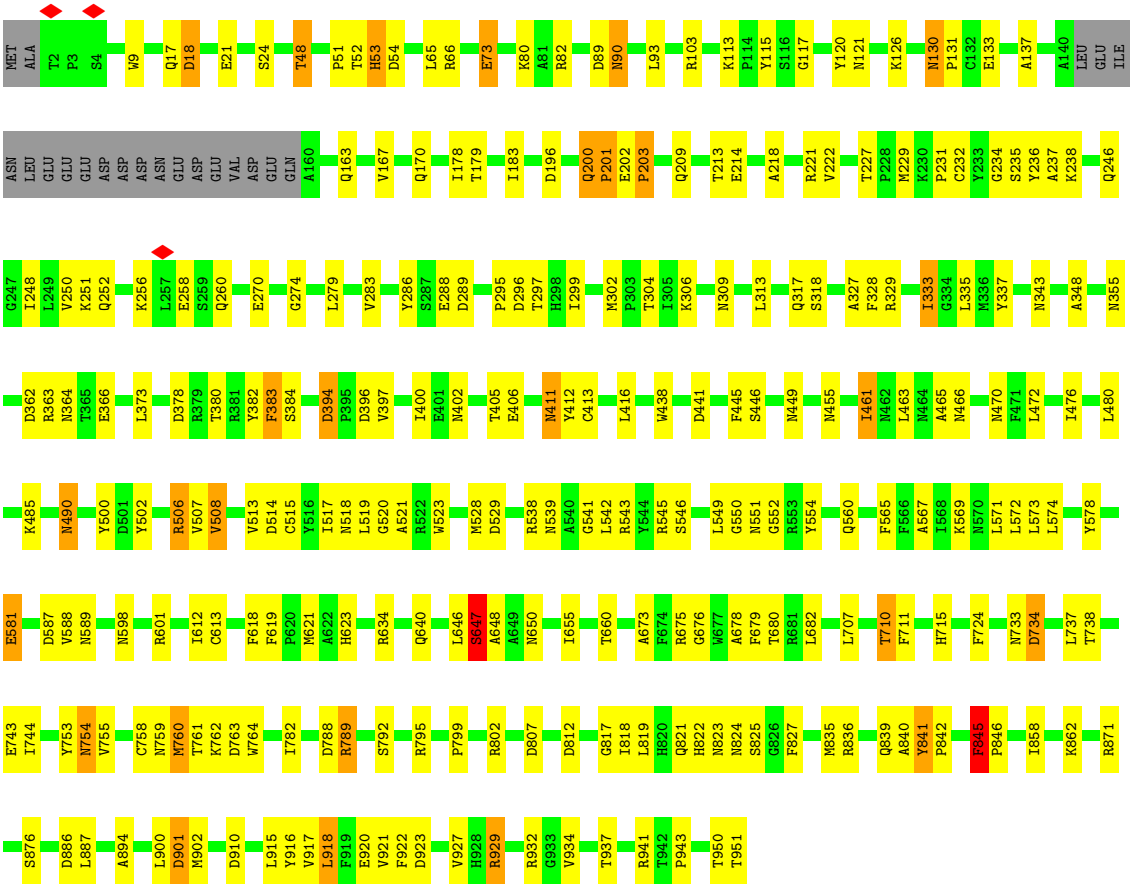
Chain F:





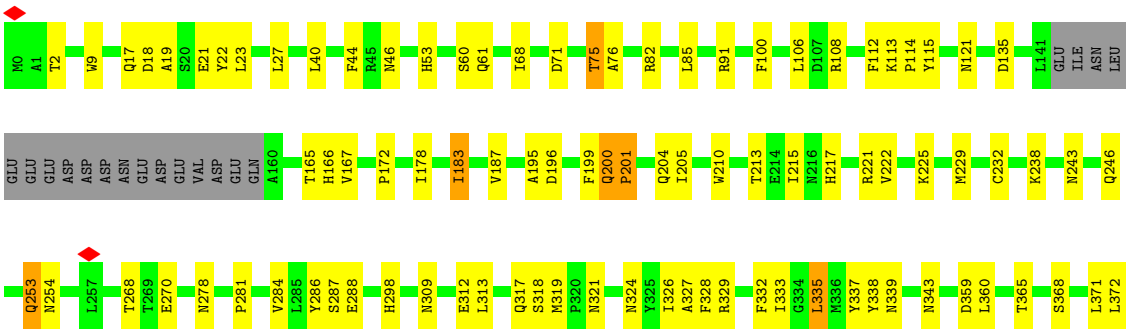
• Molecule 1: Hexon protein

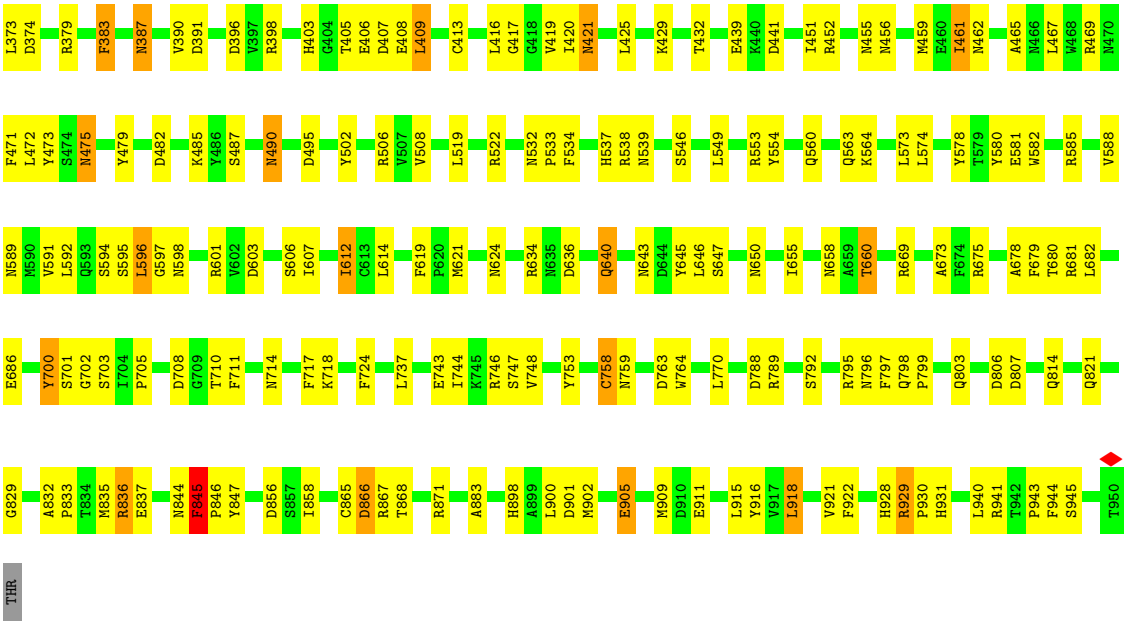
Chain G:



• Molecule 1: Hexon protein

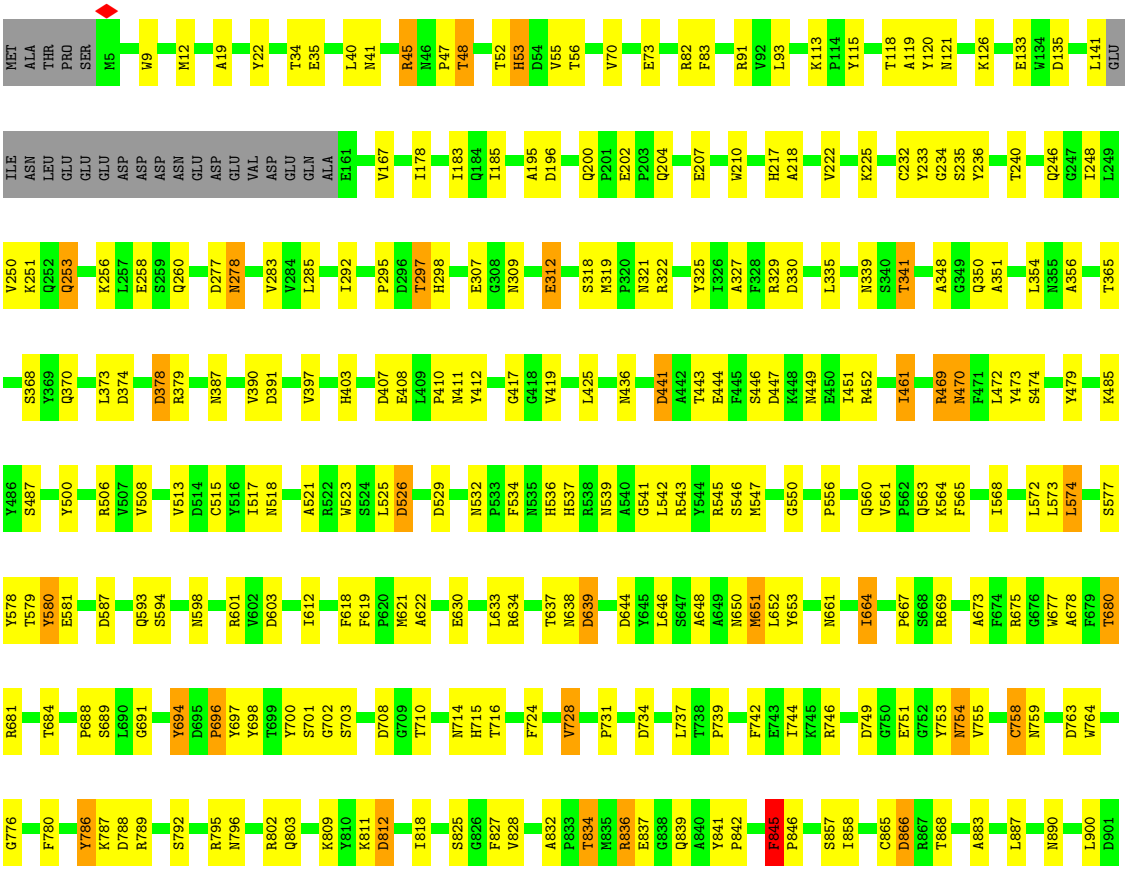
Chain H:





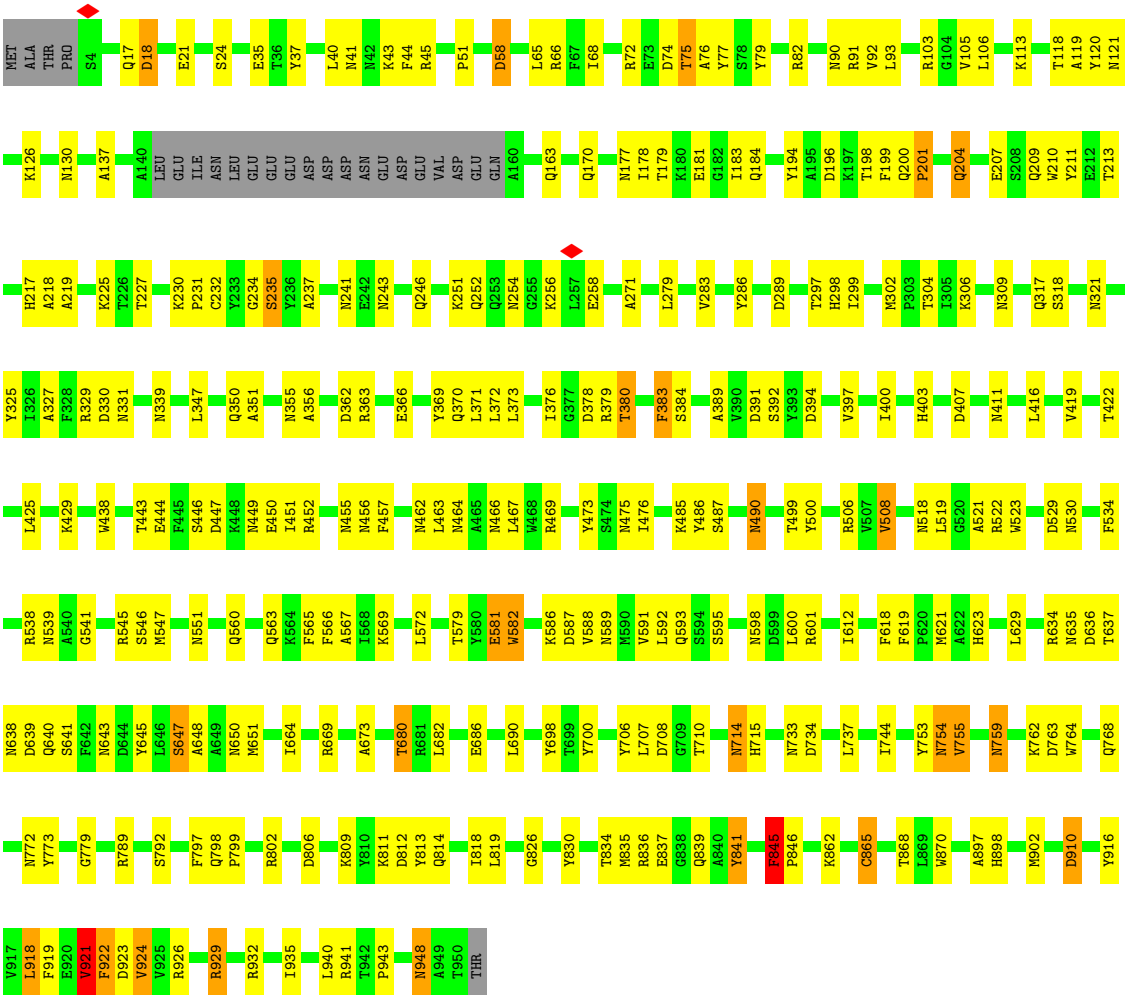
- Molecule 1: Hexon protein

Chain I:



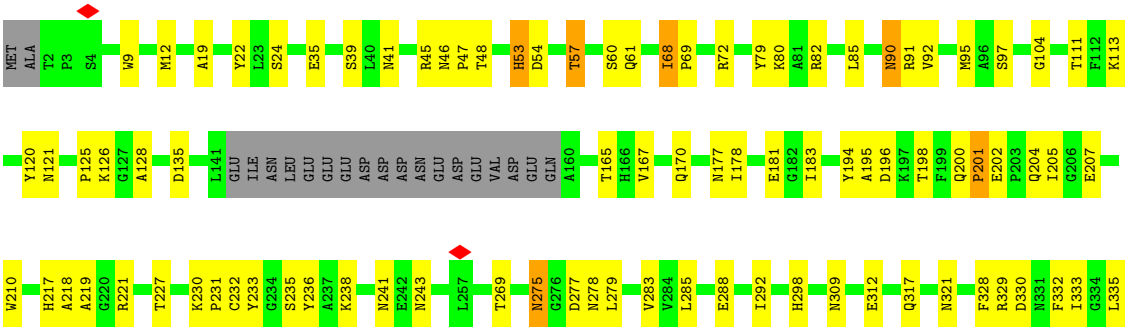
• Molecule 1: Hexon protein

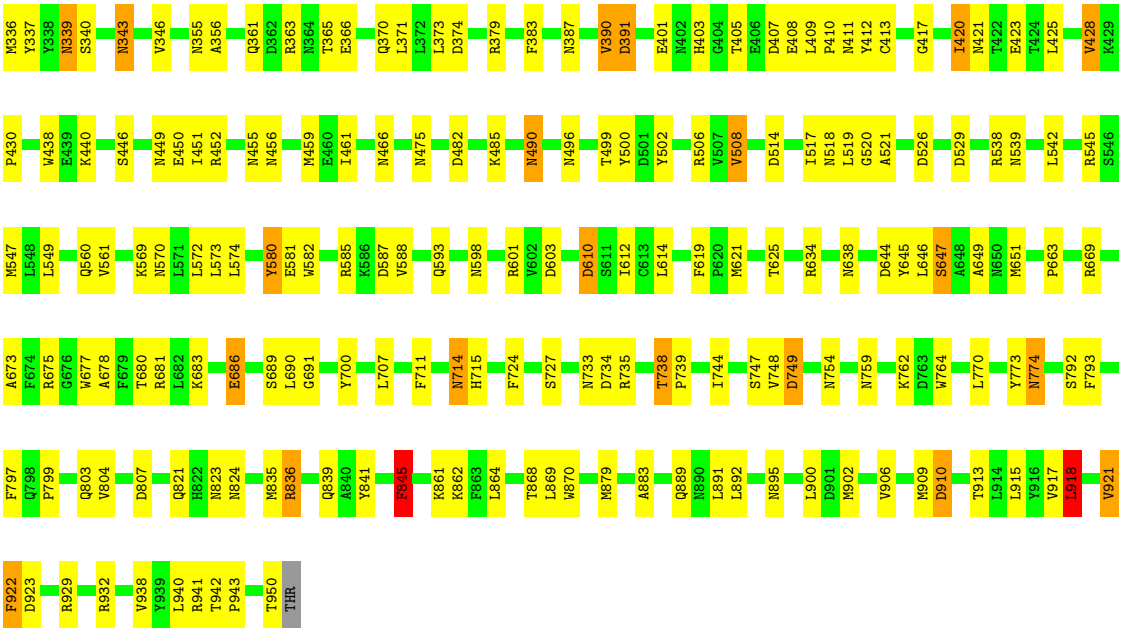
Chain J:



• Molecule 1: Hexon protein

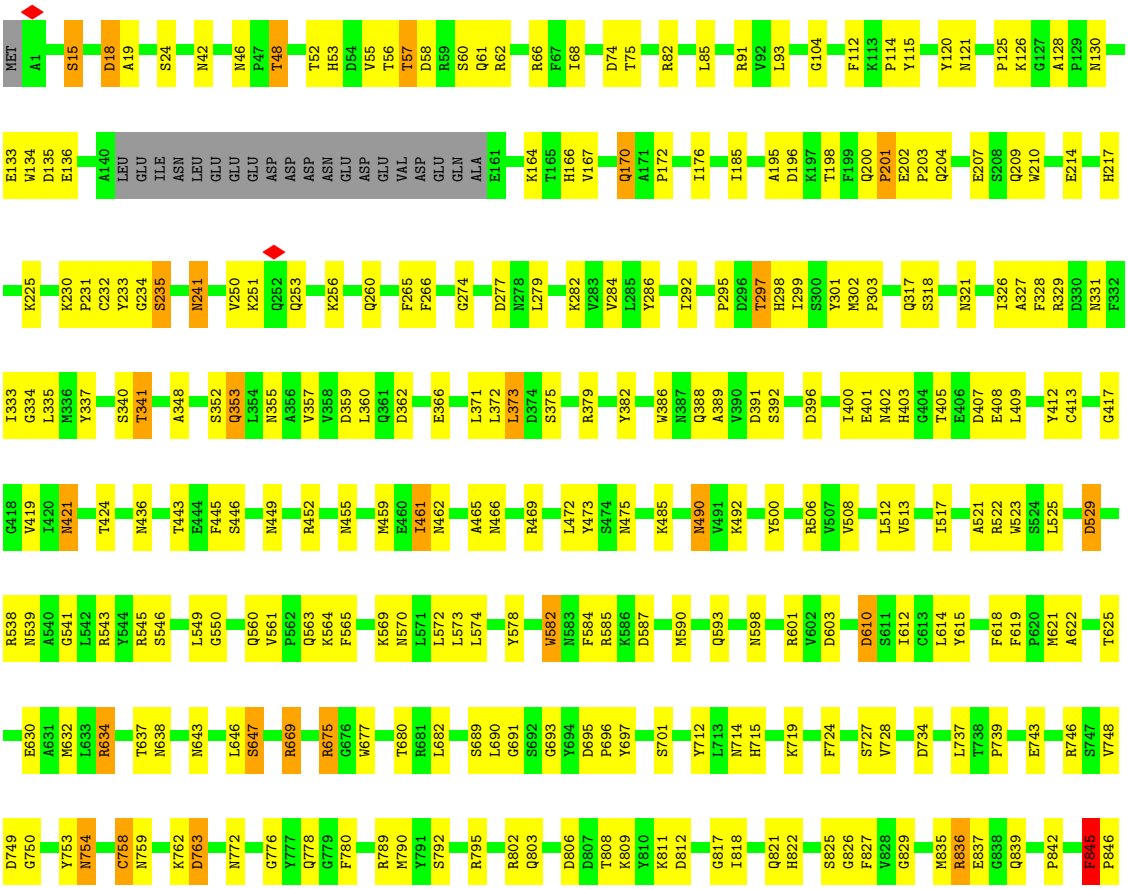
Chain K:

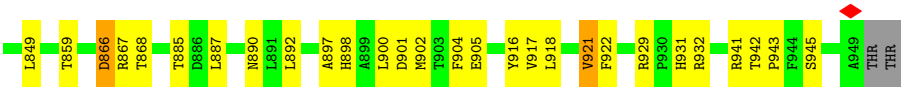




• Molecule 1: Hexon protein

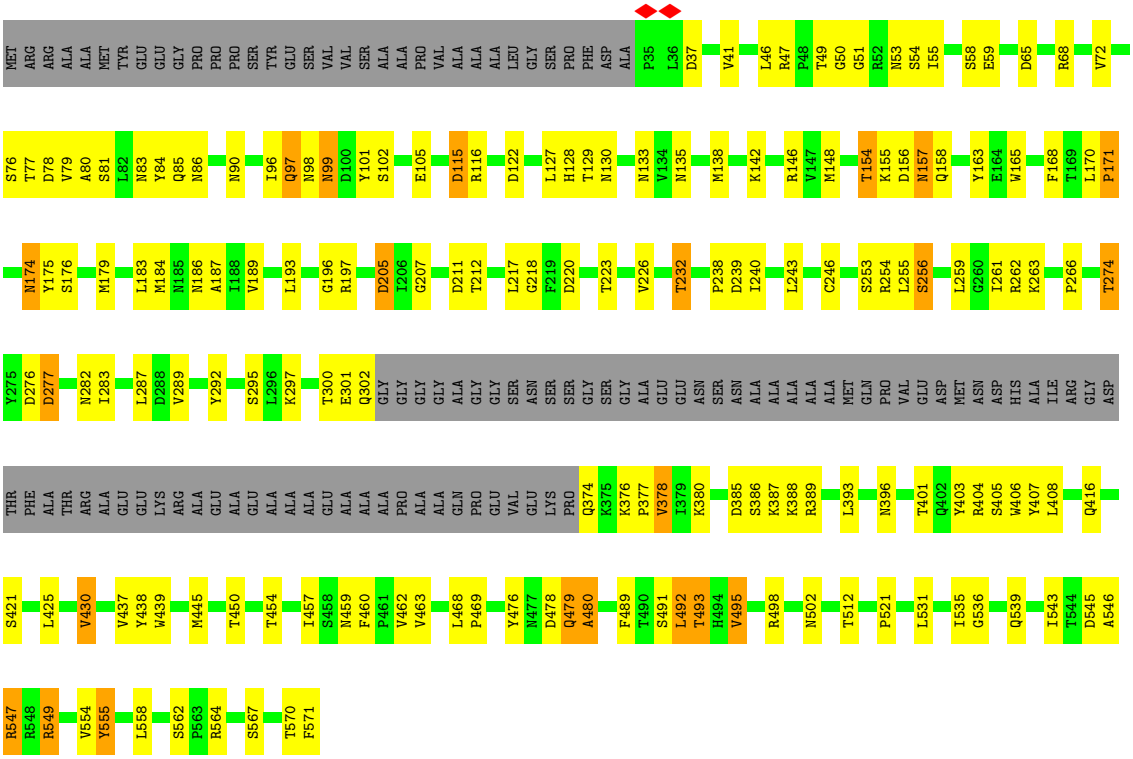
Chain L:





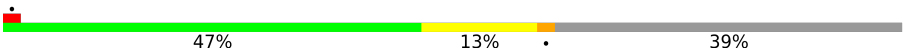
• Molecule 2: Penton protein

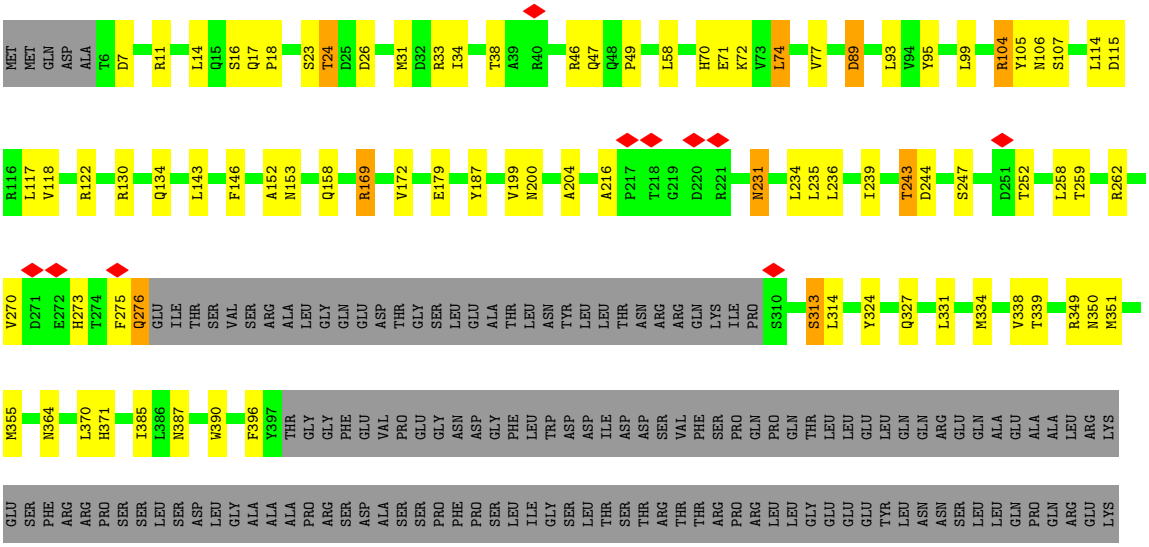
Chain N:



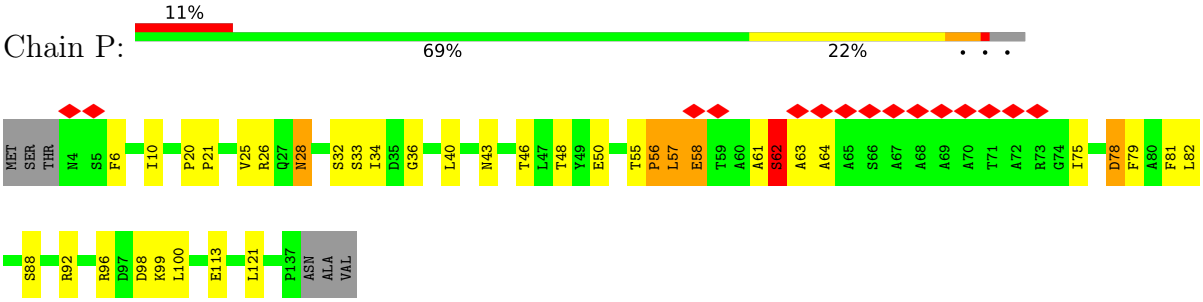
• Molecule 3: Pre-hexon-linking protein IIIa

Chain M:

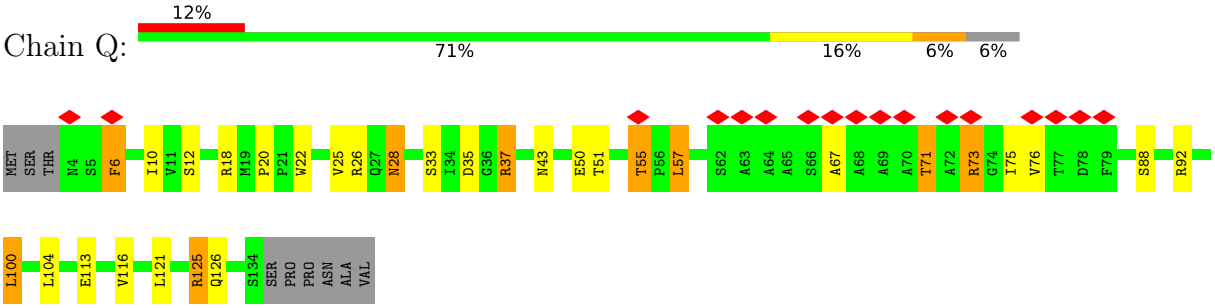




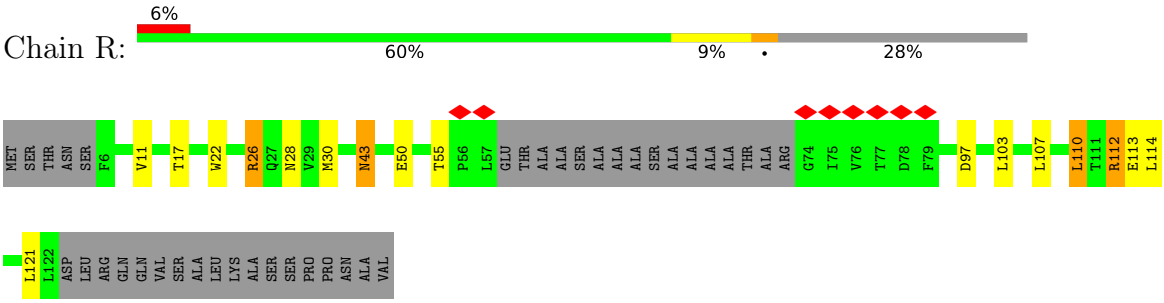
• Molecule 4: Hexon-interlacing protein



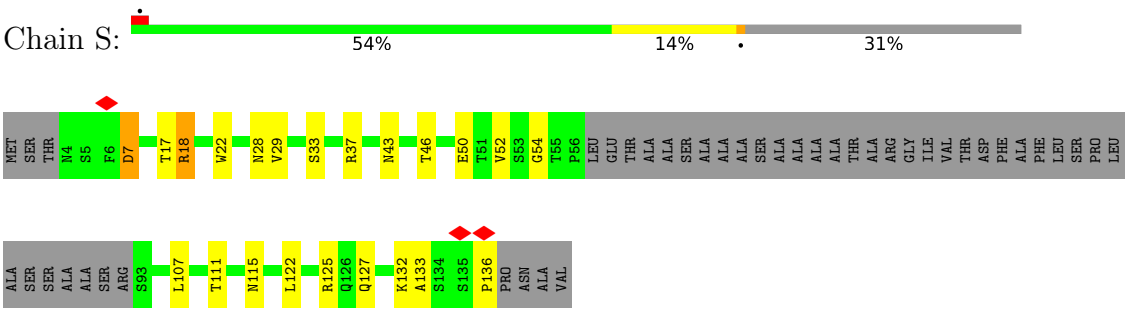
• Molecule 4: Hexon-interlacing protein



• Molecule 4: Hexon-interlacing protein

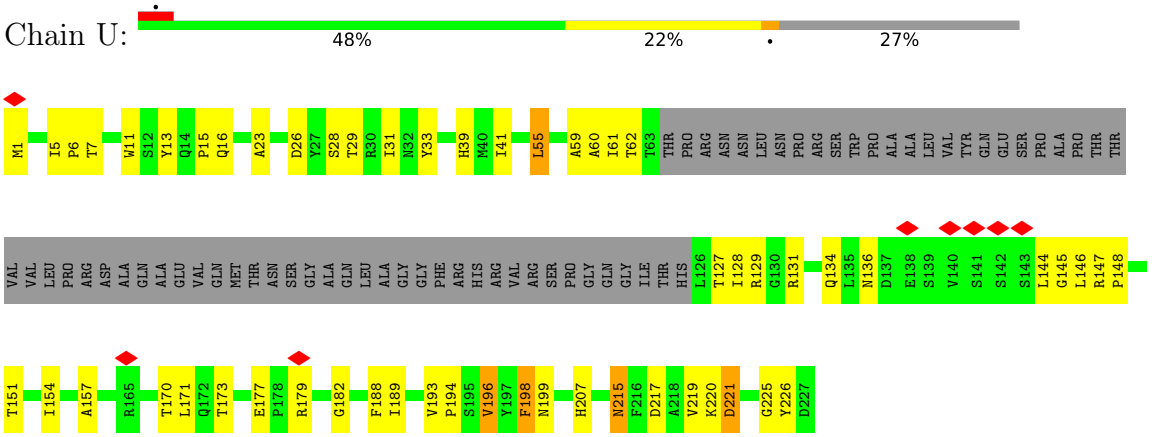


• Molecule 4: Hexon-interlacing protein



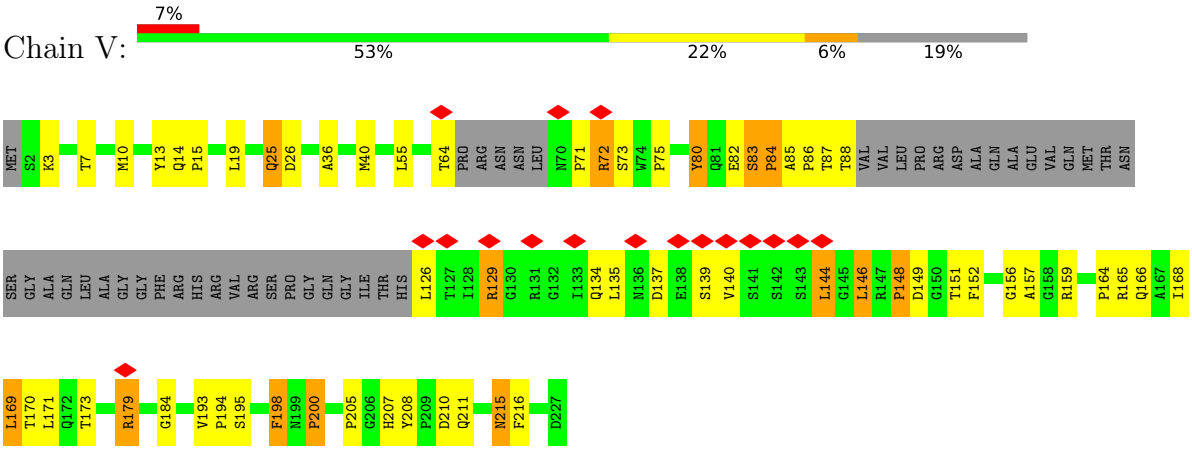
• Molecule 5: Pre-hexon-linking protein VIII

Chain U:



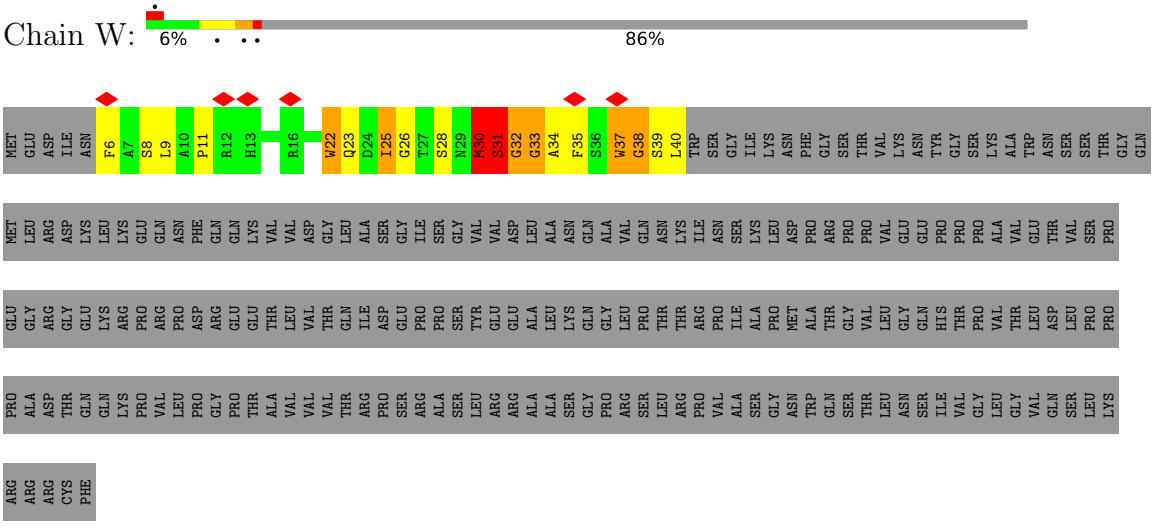
• Molecule 5: Pre-hexon-linking protein VIII

Chain V:



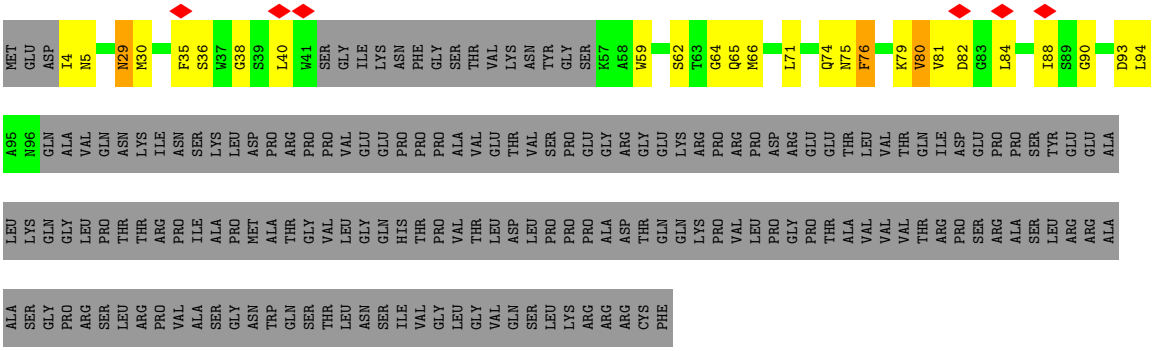
• Molecule 6: Pre-protein VI

Chain W:



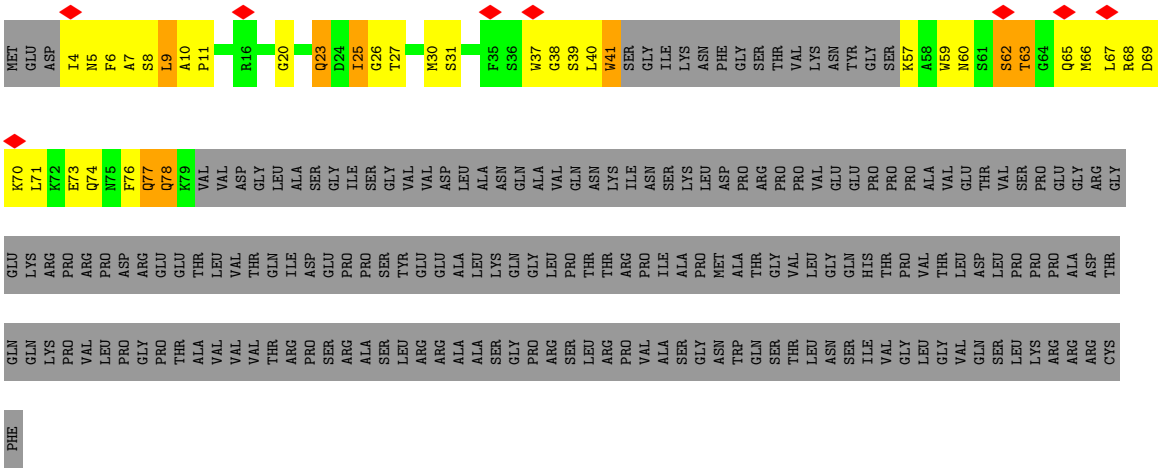
• Molecule 6: Pre-protein VI

Chain X:



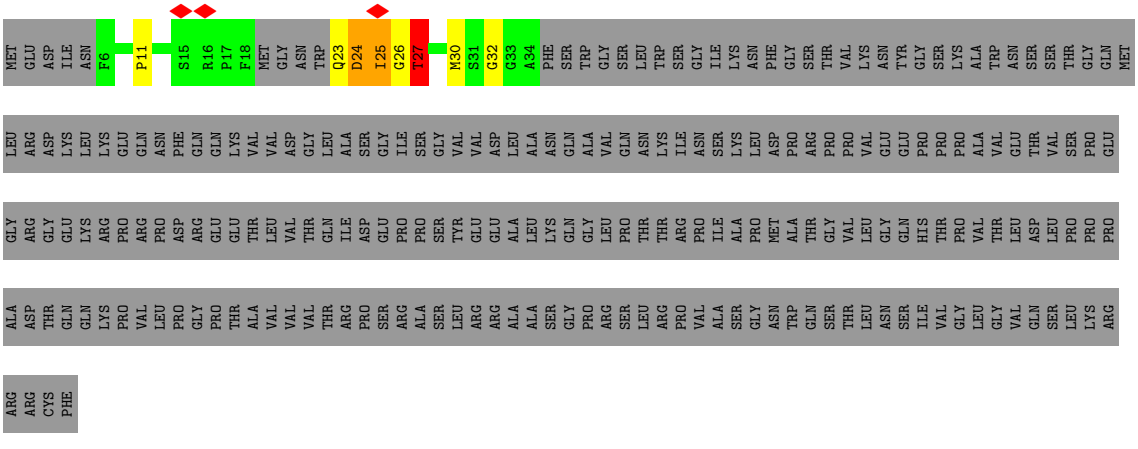
• Molecule 6: Pre-protein VI

Chain Y:



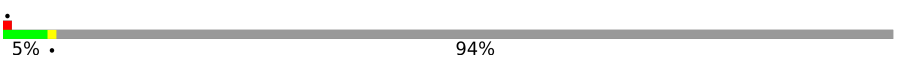
• Molecule 6: Pre-protein VI

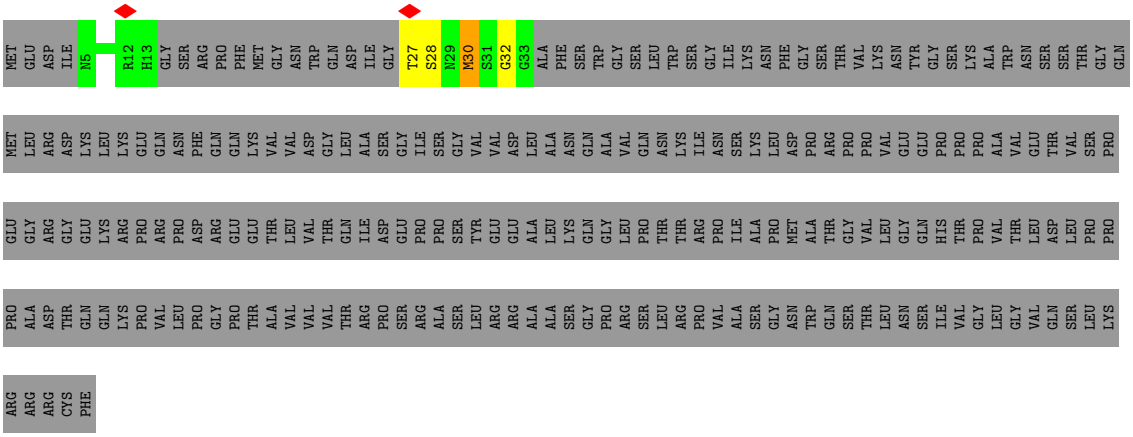
Chain Z:



• Molecule 6: Pre-protein VI

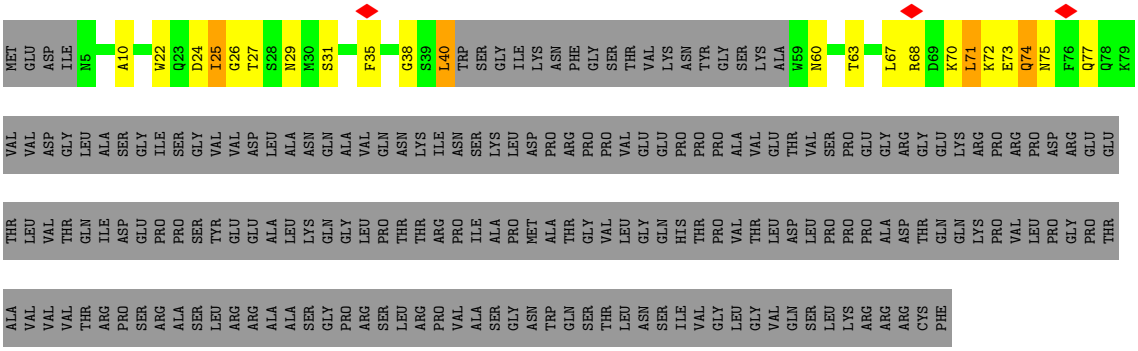
Chain 0:





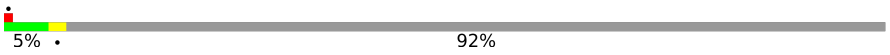
• Molecule 6: Pre-protein VI

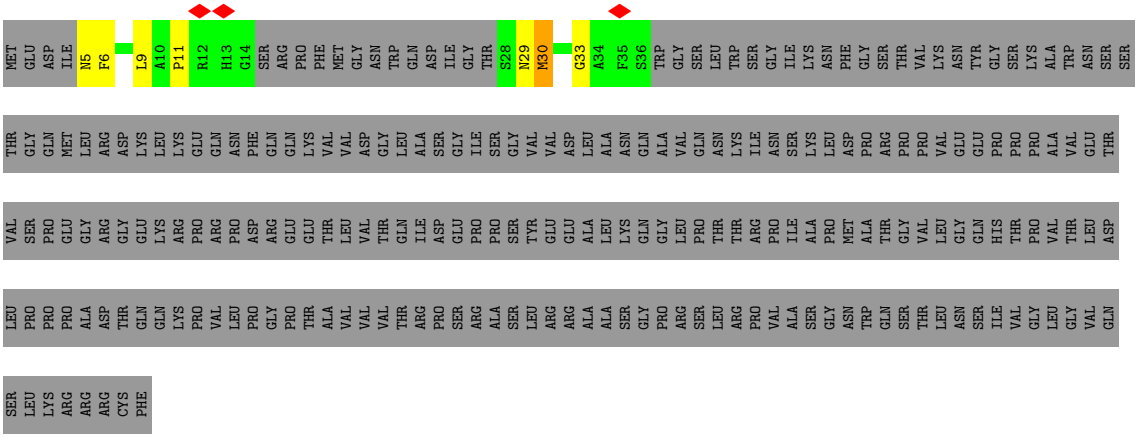
Chain 1:



• Molecule 6: Pre-protein VI

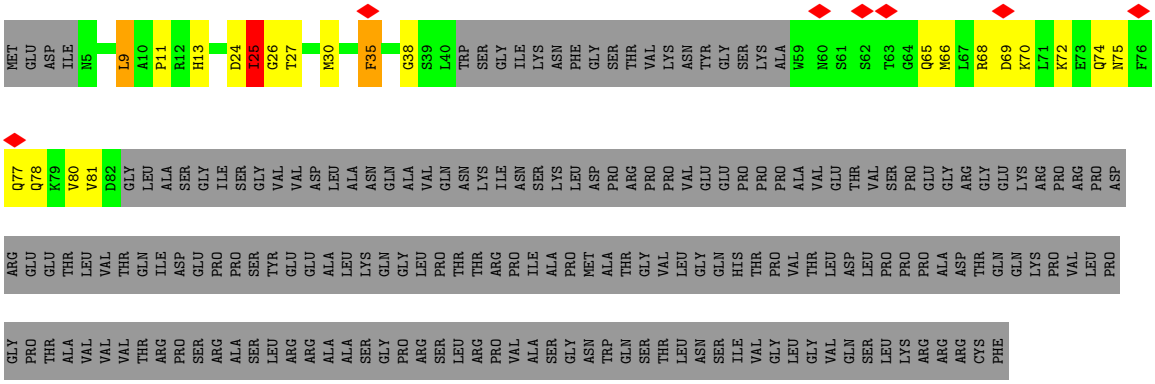
Chain 2:





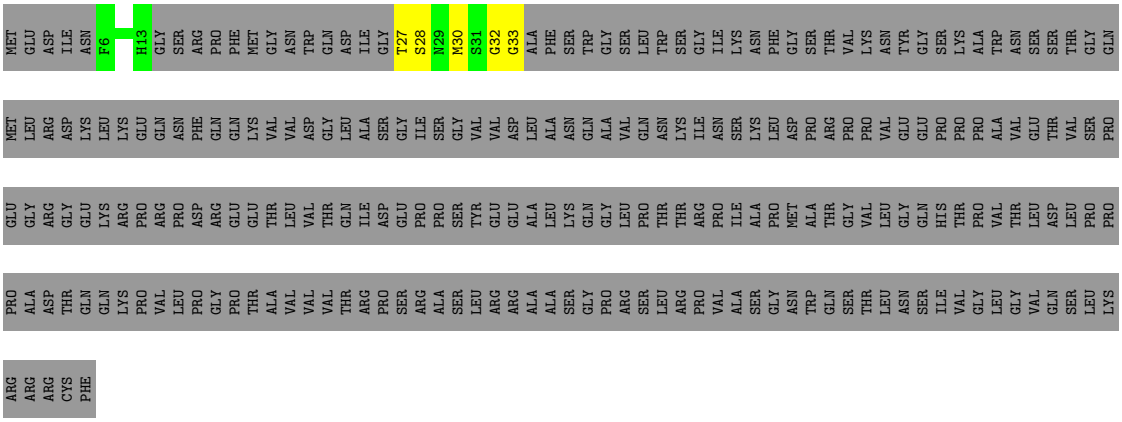
• Molecule 6: Pre-protein VI

Chain 3:



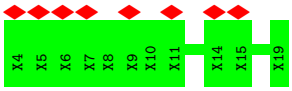
• Molecule 6: Pre-protein VI

Chain 4: 94%



• Molecule 7: Unknown-1

Chain 5: 50% 100%



• Molecule 8: Unknown-2

Chain 6: 20% 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	12	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	36.862	Depositor
Minimum map value	-27.573	Depositor
Average map value	-0.024	Depositor
Map value standard deviation	3.164	Depositor
Recommended contour level	3.15	Depositor
Map size (Å)	1089.9199, 1089.9199, 1089.9199	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

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	0.65	1/7626 (0.0%)	0.62	8/10371 (0.1%)
1	B	0.61	1/7628 (0.0%)	0.60	8/10374 (0.1%)
1	C	0.59	0/7655	0.60	8/10411 (0.1%)
1	D	0.67	2/7626 (0.0%)	0.62	9/10371 (0.1%)
1	E	0.63	0/7606	0.58	2/10343 (0.0%)
1	F	0.65	1/7629 (0.0%)	0.61	7/10374 (0.1%)
1	G	0.58	1/7640 (0.0%)	0.56	3/10391 (0.0%)
1	H	0.57	2/7654 (0.0%)	0.57	5/10409 (0.0%)
1	I	0.57	2/7615 (0.0%)	0.55	3/10355 (0.0%)
1	J	0.65	2/7617 (0.0%)	0.61	7/10357 (0.1%)
1	K	0.58	0/7641	0.58	5/10392 (0.0%)
1	L	0.62	2/7626 (0.0%)	0.60	6/10371 (0.1%)
2	N	0.83	0/3827	0.80	4/5215 (0.1%)
3	M	0.44	0/2869	0.51	1/3908 (0.0%)
4	P	0.61	2/986 (0.2%)	0.66	1/1347 (0.1%)
4	Q	0.40	0/964	0.50	0/1315
4	R	0.59	0/762	0.55	0/1039
4	S	0.31	0/736	0.44	0/1002
5	U	0.78	0/1300	0.66	0/1764
5	V	0.75	0/1452	0.77	6/1977 (0.3%)
6	0	0.65	0/115	0.82	0/152
6	1	1.05	0/460	1.23	5/615 (0.8%)
6	2	0.68	0/135	0.94	1/178 (0.6%)
6	3	0.55	0/482	0.95	2/646 (0.3%)
6	4	0.81	0/107	0.96	1/141 (0.7%)
6	W	1.08	1/271 (0.4%)	1.40	8/365 (2.2%)
6	X	0.72	0/590	0.92	3/794 (0.4%)
6	Y	1.01	0/498	1.27	4/667 (0.6%)
6	Z	1.09	0/182	1.20	1/242 (0.4%)
All	All	0.63	17/107299 (0.0%)	0.62	108/145886 (0.1%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	SER	CA-C	-5.97	1.37	1.52
1	F	201	PRO	CA-C	-5.85	1.41	1.52
1	I	694	TYR	CB-CG	-5.59	1.43	1.51
1	I	696	PRO	CA-C	-5.49	1.41	1.52
6	W	30	MET	CA-C	-5.36	1.39	1.52

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3	26	GLY	N-CA-C	14.88	150.30	113.10
6	1	26	GLY	N-CA-C	12.63	144.68	113.10
6	Y	26	GLY	N-CA-C	12.62	144.65	113.10
6	W	26	GLY	N-CA-C	9.94	137.94	113.10
1	A	45	ARG	N-CA-C	9.08	135.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	7427	0	7124	208	0
1	B	7429	0	7126	204	0
1	C	7456	0	7156	210	0
1	D	7427	0	7124	199	0
1	E	7408	0	7112	210	0
1	F	7430	0	7131	210	0
1	G	7441	0	7138	190	0
1	H	7455	0	7159	197	0
1	I	7417	0	7118	212	0
1	J	7419	0	7116	202	0
1	K	7442	0	7142	199	0
1	L	7427	0	7127	219	0
2	N	3734	0	3656	102	0
3	M	2813	0	2767	53	0
4	P	972	0	978	31	0
4	Q	952	0	959	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	751	0	757	14	0
4	S	727	0	732	11	0
5	U	1268	0	1227	42	0
5	V	1414	0	1360	39	0
6	0	114	0	104	2	0
6	1	449	0	419	15	0
6	2	133	0	119	3	0
6	3	471	0	441	13	0
6	4	106	0	98	3	0
6	W	262	0	238	20	0
6	X	577	0	526	24	0
6	Y	485	0	458	25	0
6	Z	179	0	166	10	0
7	5	80	0	19	0	0
8	6	50	0	12	0	0
All	All	104715	0	100609	2514	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 12.

The worst 5 of 2514 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:C:251:LYS:HG2	1:C:258:GLU:HB2	1.48	0.96
4:P:58:GLU:HA	4:P:61:ALA:HB3	1.52	0.92
2:N:51:GLY:HA2	2:N:116:ARG:NH2	1.87	0.90
1:B:635:ASN:HD22	3:M:18:PRO:HB3	1.37	0.87
1:H:432:THR:HB	1:H:439:GLU:HB2	1.57	0.86

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	925/952 (97%)	858 (93%)	65 (7%)	2 (0%)	47 78
1	B	925/952 (97%)	855 (92%)	69 (8%)	1 (0%)	51 83
1	C	929/952 (98%)	859 (92%)	69 (7%)	1 (0%)	51 83
1	D	925/952 (97%)	855 (92%)	69 (8%)	1 (0%)	51 83
1	E	922/952 (97%)	854 (93%)	63 (7%)	5 (0%)	29 65
1	F	925/952 (97%)	854 (92%)	66 (7%)	5 (0%)	29 65
1	G	927/952 (97%)	850 (92%)	76 (8%)	1 (0%)	51 83
1	H	929/952 (98%)	857 (92%)	71 (8%)	1 (0%)	51 83
1	I	923/952 (97%)	842 (91%)	78 (8%)	3 (0%)	41 74
1	J	924/952 (97%)	853 (92%)	66 (7%)	5 (0%)	29 65
1	K	927/952 (97%)	850 (92%)	75 (8%)	2 (0%)	47 78
1	L	925/952 (97%)	855 (92%)	67 (7%)	3 (0%)	41 74
2	N	462/571 (81%)	427 (92%)	31 (7%)	4 (1%)	17 53
3	M	355/585 (61%)	328 (92%)	26 (7%)	1 (0%)	41 74
4	P	132/140 (94%)	117 (89%)	14 (11%)	1 (1%)	19 56
4	Q	129/140 (92%)	112 (87%)	17 (13%)	0	100 100
4	R	97/140 (69%)	82 (84%)	15 (16%)	0	100 100
4	S	93/140 (66%)	87 (94%)	6 (6%)	0	100 100
5	U	161/227 (71%)	140 (87%)	21 (13%)	0	100 100
5	V	178/227 (78%)	148 (83%)	26 (15%)	4 (2%)	6 38
6	0	12/250 (5%)	11 (92%)	0	1 (8%)	1 11
6	1	53/250 (21%)	45 (85%)	8 (15%)	0	100 100
6	2	15/250 (6%)	10 (67%)	4 (27%)	1 (7%)	1 17
6	3	56/250 (22%)	52 (93%)	3 (5%)	1 (2%)	8 41
6	4	11/250 (4%)	6 (54%)	5 (46%)	0	100 100
6	W	33/250 (13%)	28 (85%)	4 (12%)	1 (3%)	4 32
6	X	74/250 (30%)	56 (76%)	15 (20%)	3 (4%)	3 26
6	Y	57/250 (23%)	46 (81%)	8 (14%)	3 (5%)	2 21
6	Z	21/250 (8%)	17 (81%)	1 (5%)	3 (14%)	0 3
All	All	13045/15844 (82%)	11954 (92%)	1038 (8%)	53 (0%)	38 69

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	733	ASN
1	D	733	ASN
1	F	197	LYS
1	F	203	PRO
2	N	495	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 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	806/829 (97%)	746 (93%)	60 (7%)	13	44
1	B	807/829 (97%)	753 (93%)	54 (7%)	16	47
1	C	809/829 (98%)	751 (93%)	58 (7%)	14	45
1	D	806/829 (97%)	765 (95%)	41 (5%)	24	55
1	E	804/829 (97%)	747 (93%)	57 (7%)	14	45
1	F	807/829 (97%)	746 (92%)	61 (8%)	13	43
1	G	808/829 (98%)	762 (94%)	46 (6%)	20	52
1	H	809/829 (98%)	761 (94%)	48 (6%)	19	51
1	I	805/829 (97%)	754 (94%)	51 (6%)	18	49
1	J	804/829 (97%)	758 (94%)	46 (6%)	20	52
1	K	808/829 (98%)	758 (94%)	50 (6%)	18	49
1	L	806/829 (97%)	750 (93%)	56 (7%)	15	46
2	N	423/489 (86%)	376 (89%)	47 (11%)	6	29
3	M	304/500 (61%)	283 (93%)	21 (7%)	15	46
4	P	107/112 (96%)	96 (90%)	11 (10%)	7	31
4	Q	104/112 (93%)	94 (90%)	10 (10%)	8	34
4	R	86/112 (77%)	77 (90%)	9 (10%)	7	30
4	S	85/112 (76%)	77 (91%)	8 (9%)	8	35
5	U	136/186 (73%)	121 (89%)	15 (11%)	6	29
5	V	152/186 (82%)	136 (90%)	16 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	0	12/210 (6%)	10 (83%)	2 (17%)	2 14
6	1	47/210 (22%)	39 (83%)	8 (17%)	2 13
6	2	13/210 (6%)	11 (85%)	2 (15%)	2 17
6	3	50/210 (24%)	43 (86%)	7 (14%)	3 20
6	4	11/210 (5%)	11 (100%)	0	100 100
6	W	26/210 (12%)	20 (77%)	6 (23%)	1 6
6	X	54/210 (26%)	48 (89%)	6 (11%)	6 29
6	Y	50/210 (24%)	38 (76%)	12 (24%)	0 5
6	Z	18/210 (9%)	16 (89%)	2 (11%)	6 29
All	All	11357/13647 (83%)	10547 (93%)	810 (7%)	18 45

5 of 810 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	700	TYR
1	L	18	ASP
6	1	71	LEU
1	J	18	ASP
1	I	689	SER

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

Mol	Chain	Res	Type
2	N	99	ASN
6	Y	13	HIS
2	N	174	ASN
3	M	276	GLN
6	Z	23	GLN

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 monosaccharides 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.

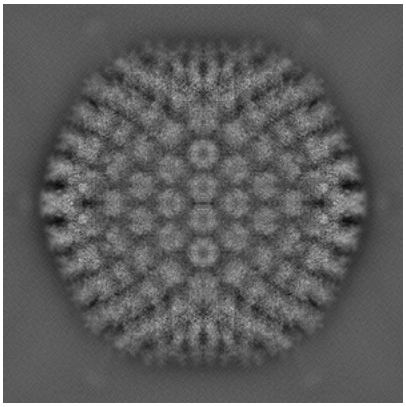
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24881. These allow visual inspection of the internal detail of the map and identification of artifacts.

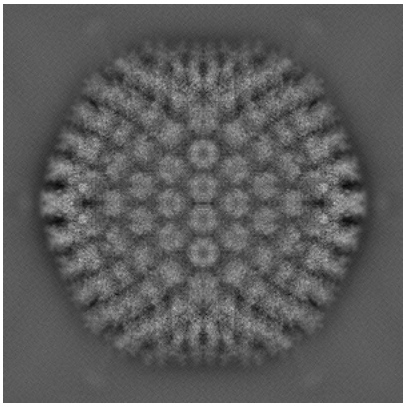
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

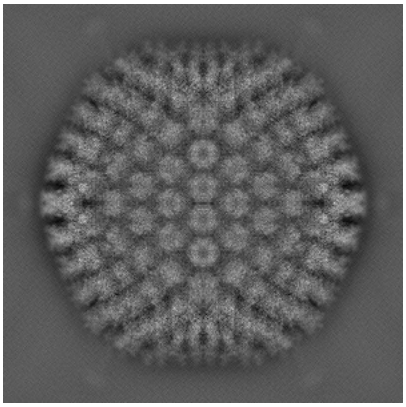
6.1.1 Primary map



X



Y

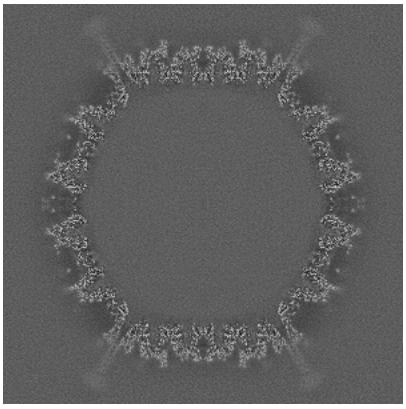


Z

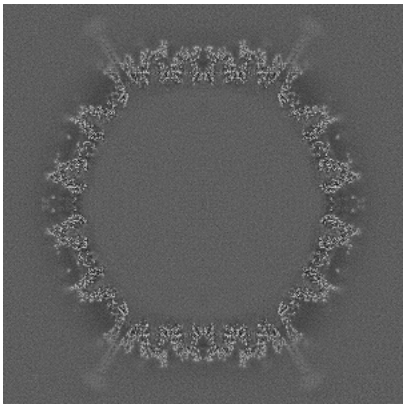
The images above show the map projected in three orthogonal directions.

6.2 Central slices

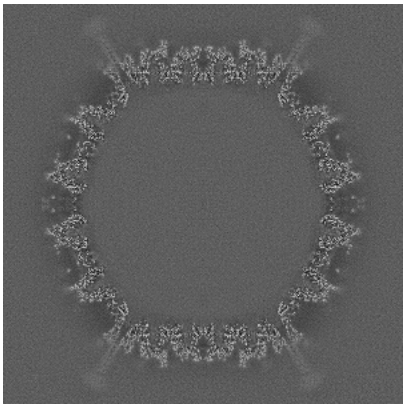
6.2.1 Primary map



X Index: 416



Y Index: 416

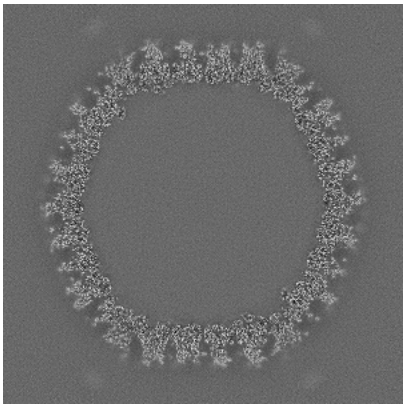


Z Index: 416

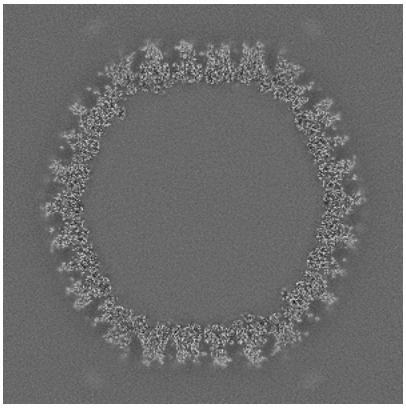
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

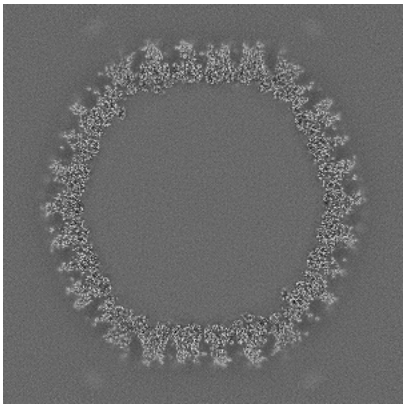
6.3.1 Primary map



X Index: 431



Y Index: 431

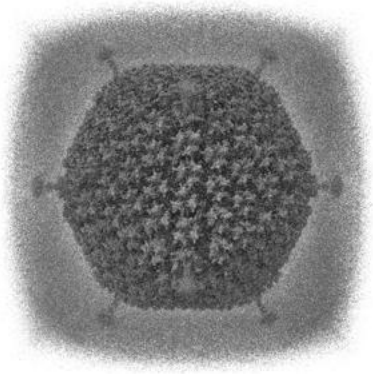


Z Index: 431

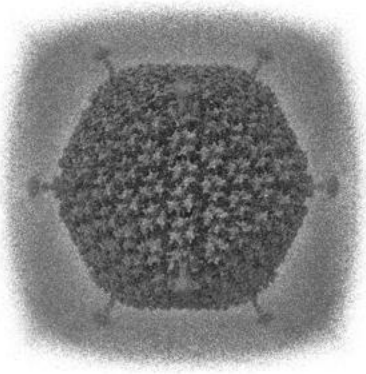
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

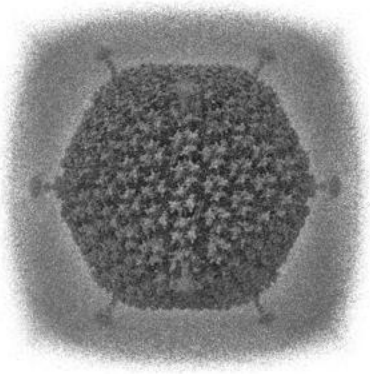
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

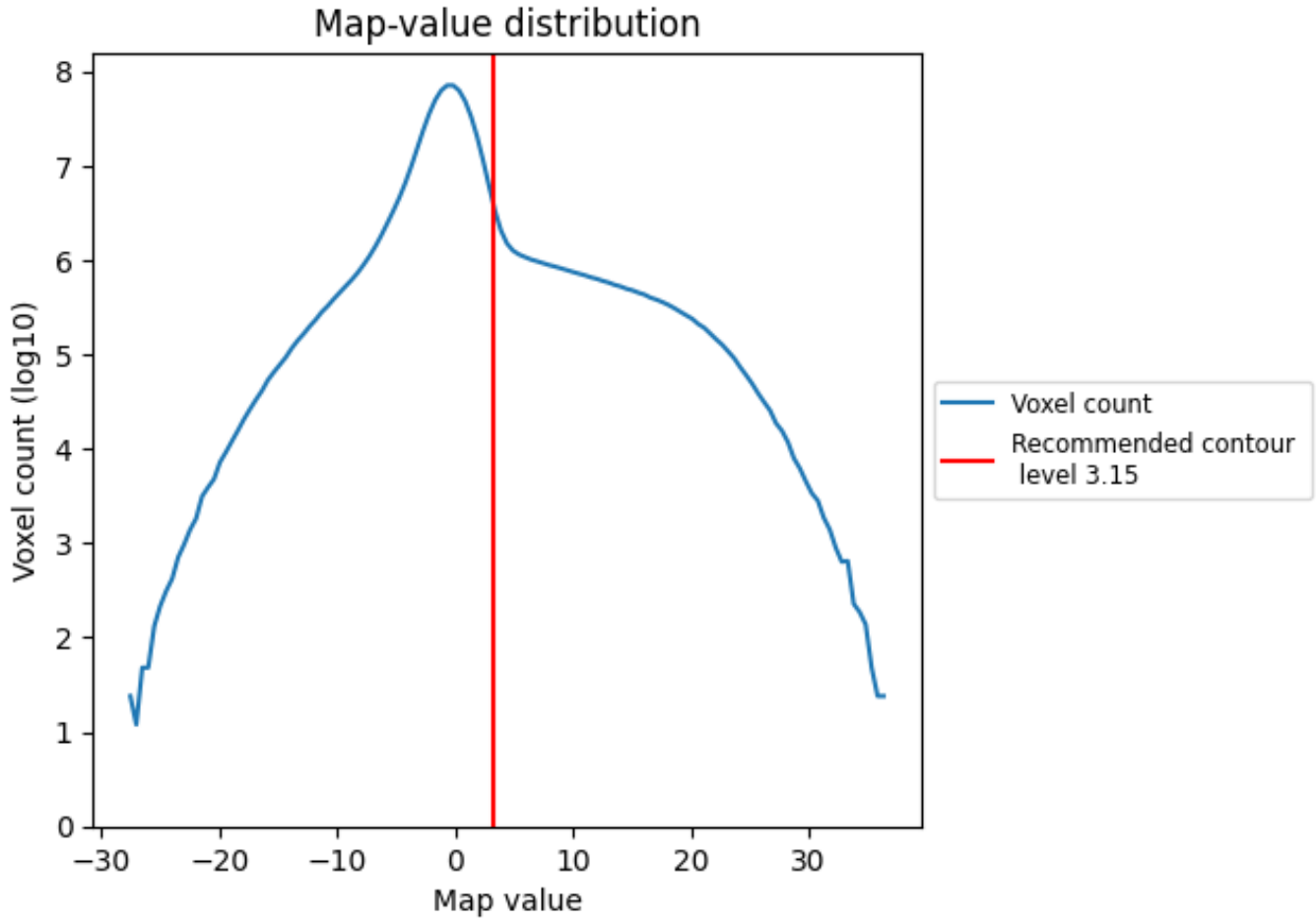
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

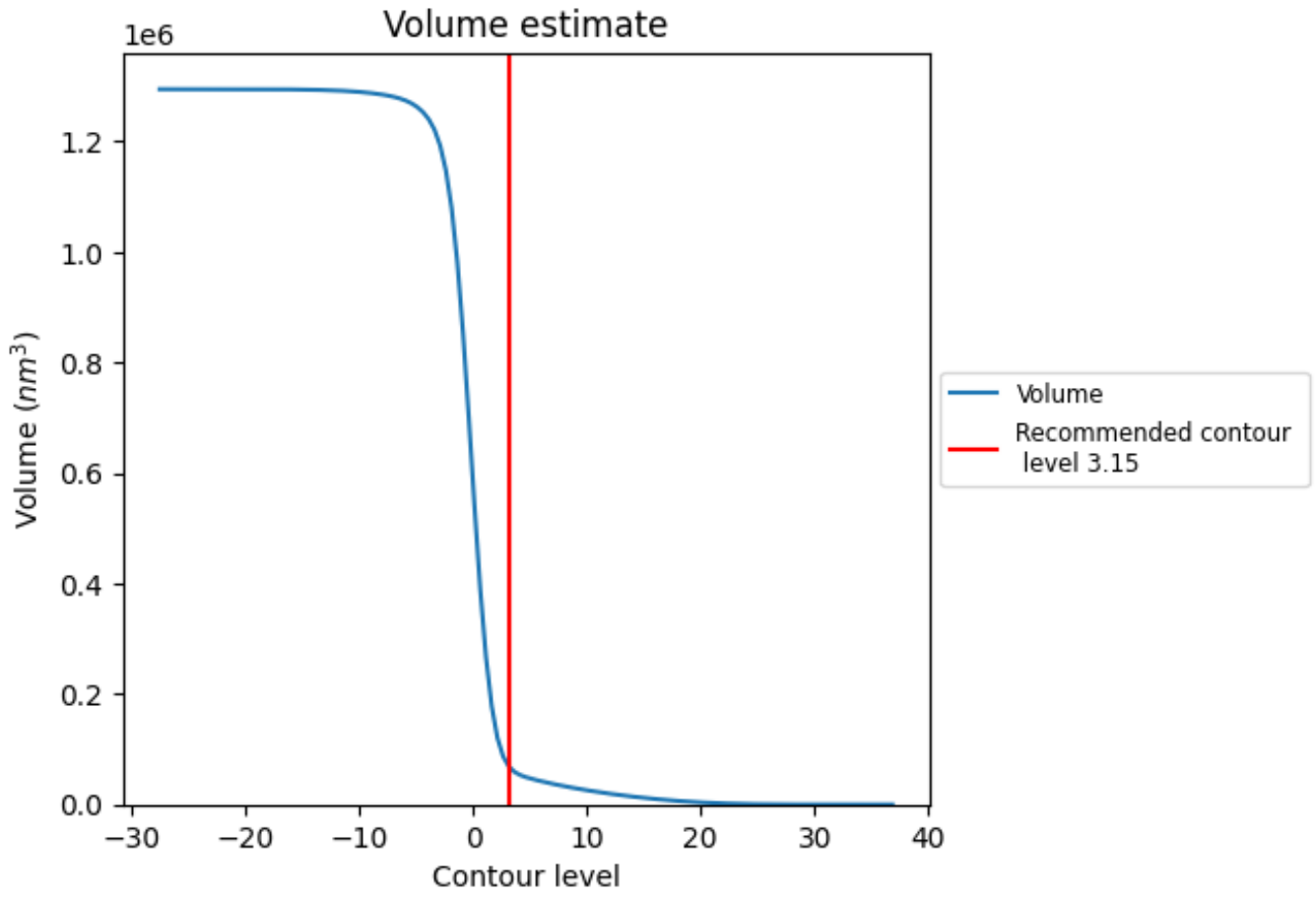
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

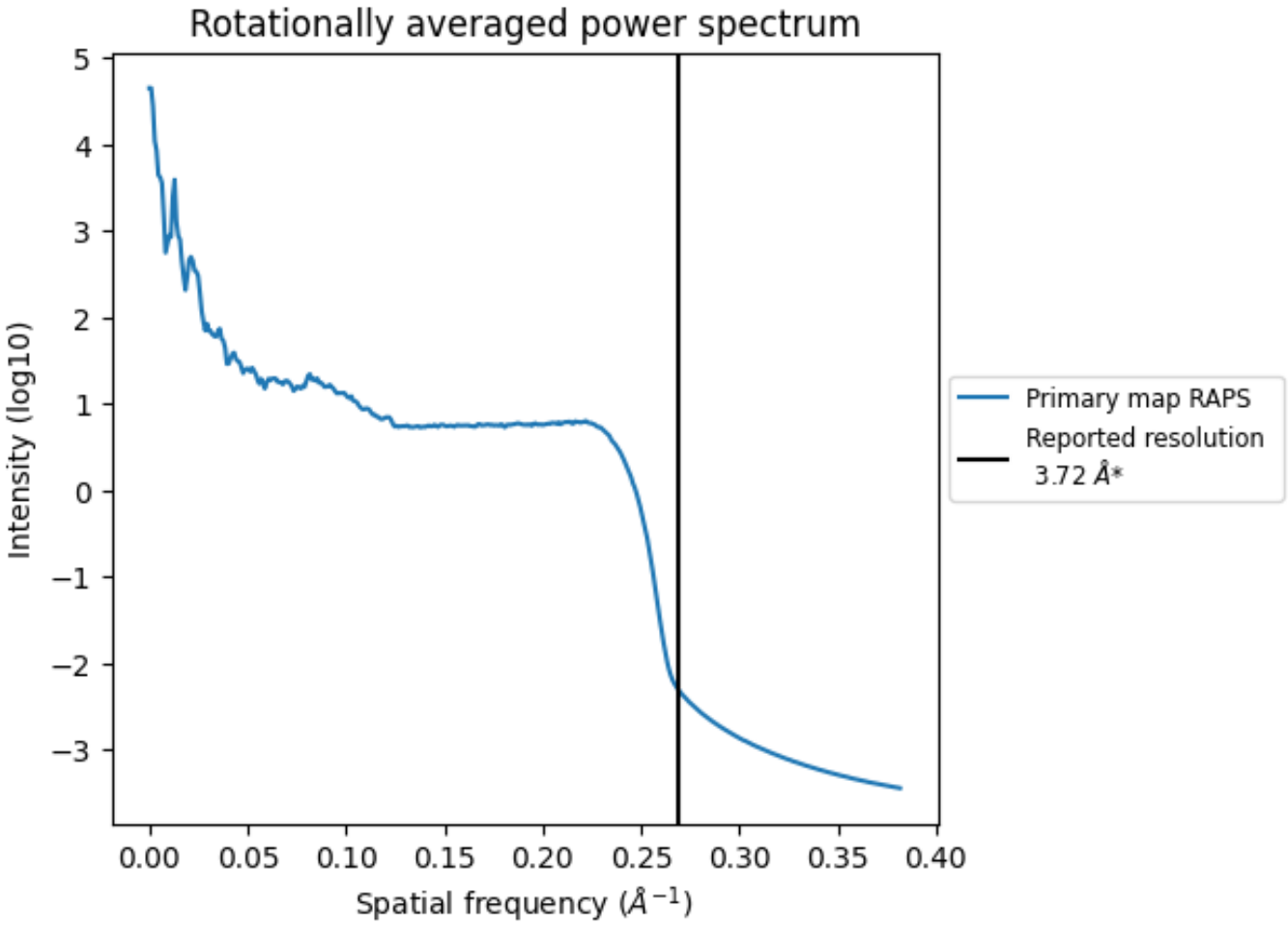
7.2 Volume estimate (i)



The volume at the recommended contour level is 68380 nm^3; this corresponds to an approximate mass of 61769 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

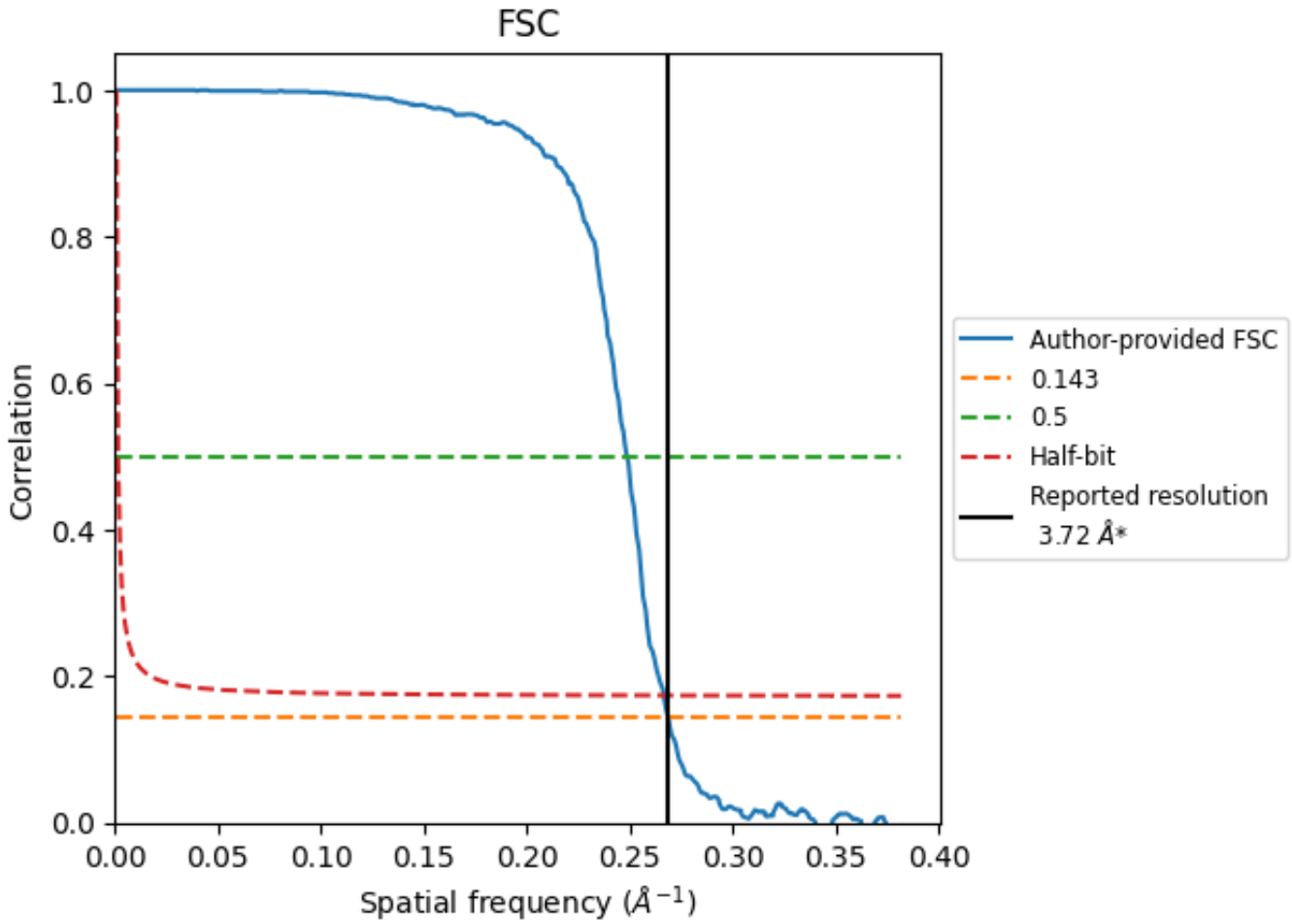


*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.72	4.02	3.75
Unmasked-calculated*	-	-	-

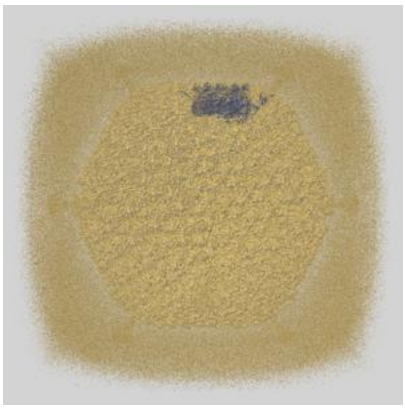
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

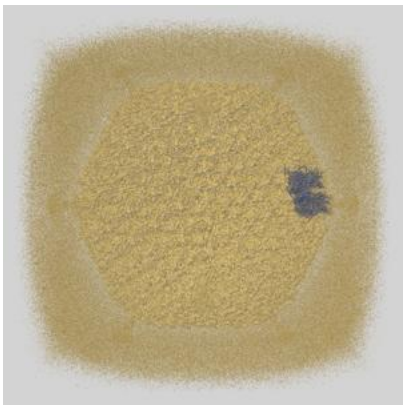
This section contains information regarding the fit between EMDB map EMD-24881 and PDB model 7S78. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

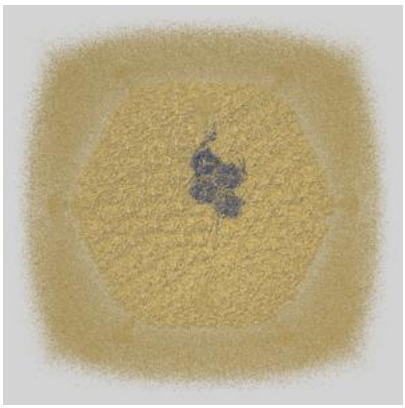
9.1.1 Map-model overlay



X

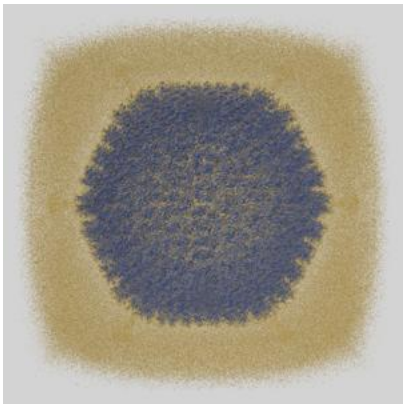


Y

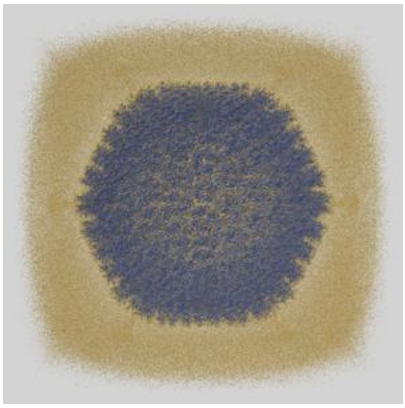


Z

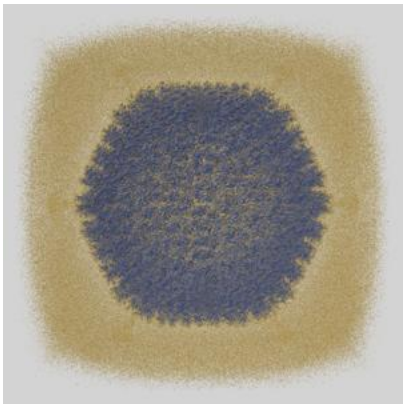
9.1.2 Map-model assembly overlay



X



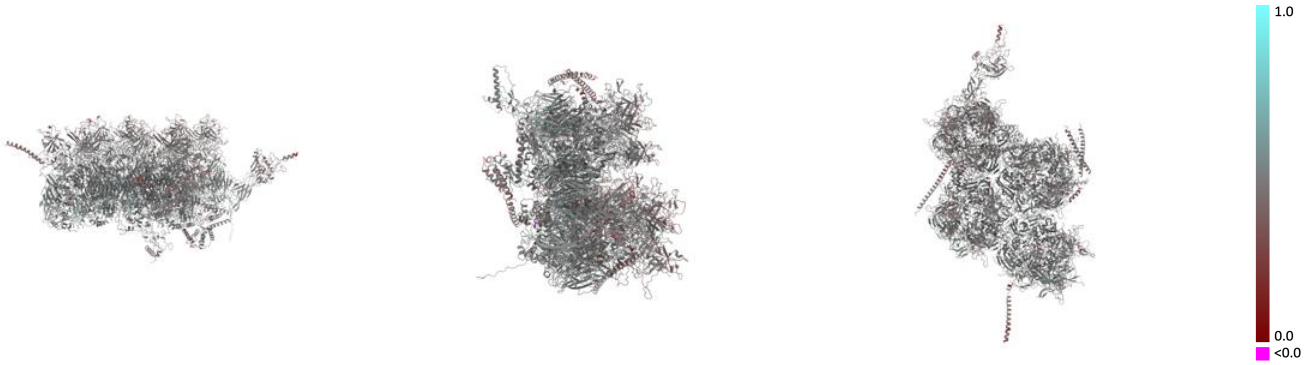
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

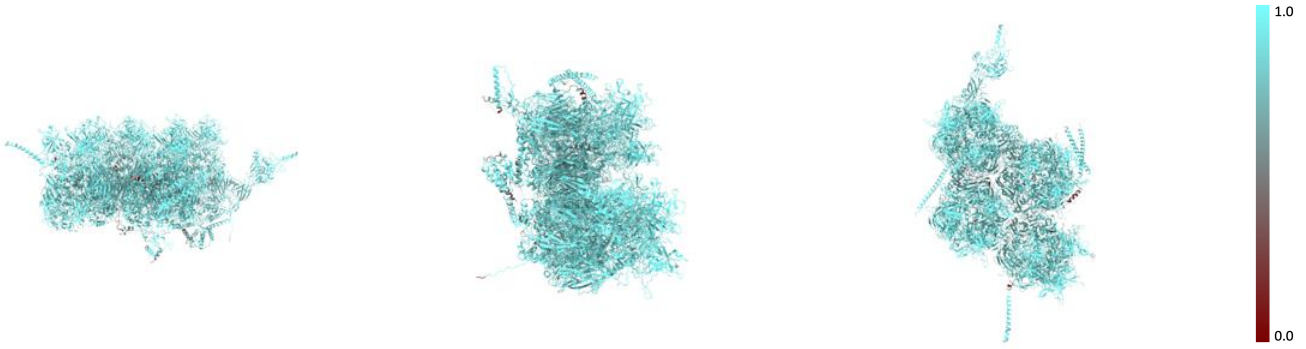
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

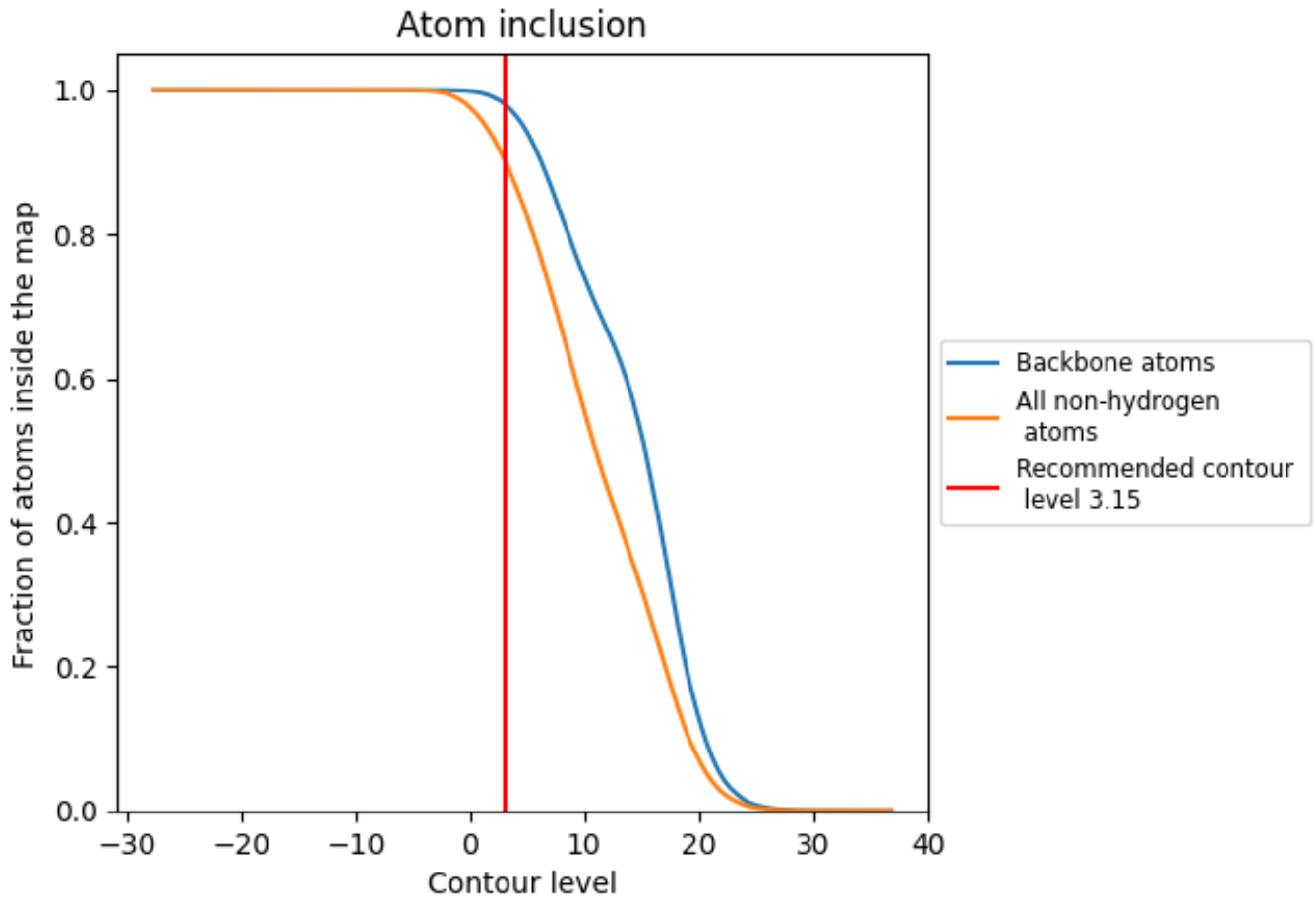
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.15).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8998	0.4710
0	0.7143	0.4920
1	0.7682	0.4890
2	0.6565	0.5190
3	0.7165	0.4610
4	0.6442	0.4730
5	0.5125	0.4670
6	0.6800	0.4480
A	0.9179	0.4710
B	0.9165	0.4650
C	0.9157	0.4680
D	0.9142	0.4770
E	0.9142	0.4770
F	0.9182	0.4790
G	0.9142	0.4810
H	0.9139	0.4810
I	0.9156	0.4790
J	0.9159	0.4770
K	0.9186	0.4740
L	0.9128	0.4770
M	0.8075	0.4370
N	0.8879	0.4510
P	0.7859	0.4080
Q	0.7964	0.4230
R	0.8274	0.4160
S	0.8736	0.4330
U	0.8344	0.4650
V	0.7899	0.4650
W	0.5586	0.4460
X	0.7531	0.4480
Y	0.6800	0.4580
Z	0.6857	0.4860