



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 11:52 PM EST

PDB ID : 6CGR
EMDB ID : EMD-7472
Title : CryoEM structure of herpes simplex virus 1 capsid with associated tegument protein complexes.
Authors : Dai, X.H.; Zhou, Z.H.
Deposited on : 2018-02-20
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

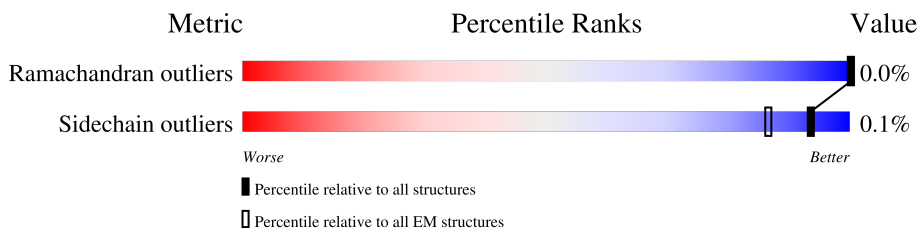
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.20 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)
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 $\leq 5\%$. 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	4	1374	
1	A	1374	
1	B	1374	
1	C	1374	
1	D	1374	
1	E	1374	
1	F	1374	
1	M	1374	
1	N	1374	

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Mol	Chain	Length	Quality of chain	
1	O	1374	13%	99%
1	S	1374	21%	98%
1	T	1374	21%	98%
1	U	1374	17%	99%
1	V	1374	18%	99%
1	W	1374	17%	99%
1	X	1374	21%	98%
2	0	112	55%	90%
2	1	112	48%	90%
2	2	112	54%	90%
2	3	112	53%	90%
2	G	112	47%	90%
2	H	112	40%	90%
2	I	112	46%	90%
2	J	112	38%	90%
2	K	112	48%	90%
2	L	112	41%	90%
2	P	112	36%	90%
2	Q	112	39%	90%
2	R	112	29%	90%
2	Y	112	62%	90%
2	Z	112	61%	90%
3	5	465	21%	76%
3	8	465	11%	77%
3	b	465	17%	78%

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Mol	Chain	Length	Quality of chain
3	e	465	15% 76% 24%
3	h	465	14% 75% 24%
4	6	318	31% 86% 13%
4	7	318	32% 96% ..
4	9	318	12% 86% 14%
4	a	318	14% 96% ..
4	c	318	14% 86% 14%
4	d	318	11% 95% ..
4	f	318	14% 85% 14%
4	g	318	20% 96% ..
4	i	318	16% 86% 13%
4	j	318	11% 96% ..
5	k	703	33% 78% 22%
6	l	580	10% 16% 84%
6	m	580	9% 13% 86%
7	n	3139	.. 99%
7	o	3139	.. 99%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 219702 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1362	10409	6575	1871	1909	54	0	0
1	B	1364	10423	6585	1873	1911	54	0	0
1	C	1364	10423	6585	1873	1911	54	0	0
1	D	1362	10409	6575	1871	1909	54	0	0
1	E	1366	10442	6595	1878	1915	54	0	0
1	F	1362	10409	6575	1871	1909	54	0	0
1	M	1362	10409	6575	1871	1909	54	0	0
1	N	1366	10442	6595	1878	1915	54	0	0
1	O	1364	10423	6585	1873	1911	54	0	0
1	S	1357	10365	6547	1864	1900	54	0	0
1	T	1357	10379	6553	1868	1904	54	0	0
1	U	1364	10423	6585	1873	1911	54	0	0
1	V	1362	10409	6575	1871	1909	54	0	0
1	W	1364	10423	6585	1873	1911	54	0	0
1	X	1348	10314	6516	1857	1888	53	0	0
1	4	1259	9648	6103	1726	1769	50	0	0

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	H	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	I	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	J	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	K	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	L	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	P	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Q	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	R	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Y	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Z	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	0	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	1	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	2	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	3	101	Total	C	N	O	S	0	0
			774	488	146	137	3		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	353	Total	C	N	O	S	0	0
			2724	1708	518	481	17		
3	8	363	Total	C	N	O	S	0	0
			2786	1741	531	496	18		
3	b	363	Total	C	N	O	S	0	0
			2786	1741	531	496	18		
3	e	352	Total	C	N	O	S	0	0
			2720	1706	517	480	17		
3	h	353	Total	C	N	O	S	0	0
			2724	1708	518	481	17		

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	276	Total	C	N	O	S	0	0
			2116	1354	375	380	7		
4	7	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	9	274	Total	C	N	O	S	0	0
			2091	1338	370	376	7		
4	a	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	c	274	Total	C	N	O	S	0	0
			2091	1338	370	376	7		
4	d	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	f	272	Total	C	N	O	S	0	0
			2089	1337	371	374	7		
4	g	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	i	276	Total	C	N	O	S	0	0
			2116	1354	375	380	7		
4	j	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		

- Molecule 5 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	550	Total	C	N	O	S	0	0
			4206	2674	764	747	21		

- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	94	Total	C	N	O	S	0	0
			766	486	138	138	4		
6	m	80	Total	C	N	O	S	0	0
			654	413	124	115	2		

- Molecule 7 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	47	Total	C	N	O	S	0	0
			384	237	84	61	2		
7	o	47	Total	C	N	O	S	0	0
			384	237	84	61	2		

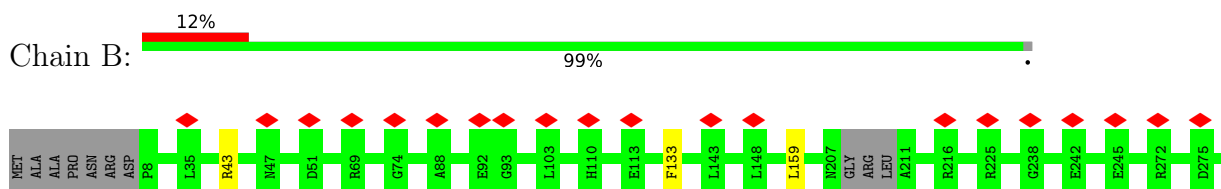
3 Residue-property plots [i](#)

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: Major capsid protein



- Molecule 1: Major capsid protein

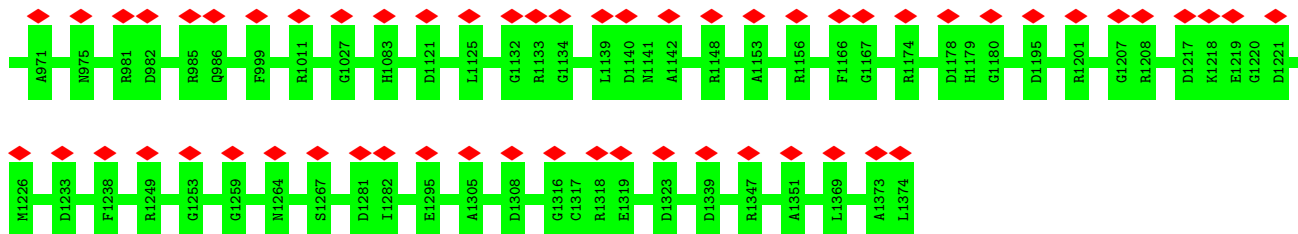




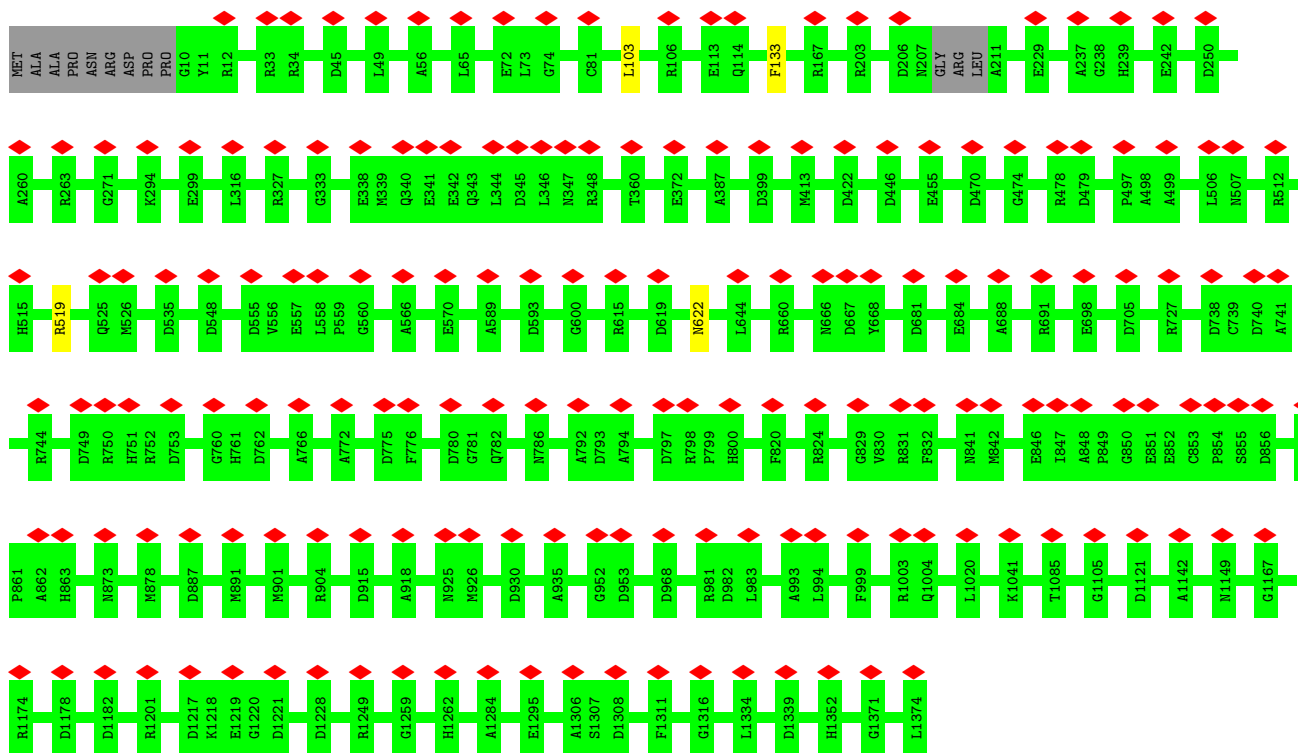
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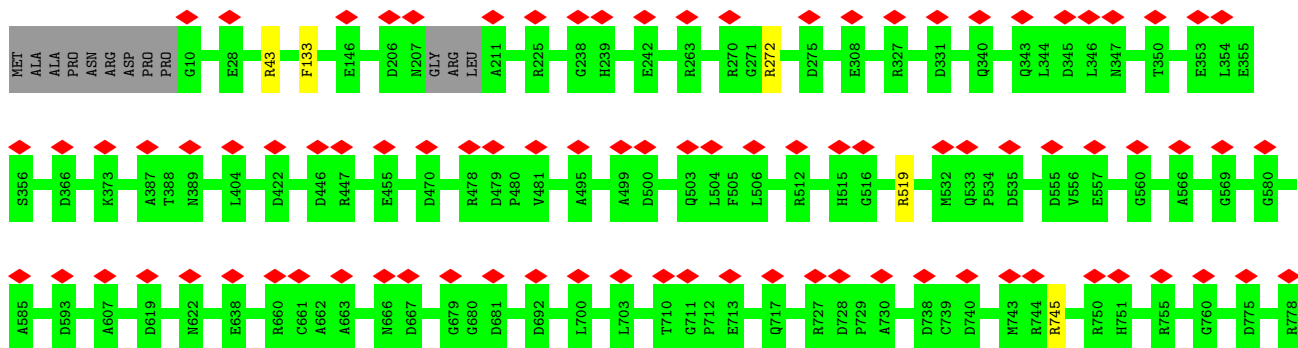
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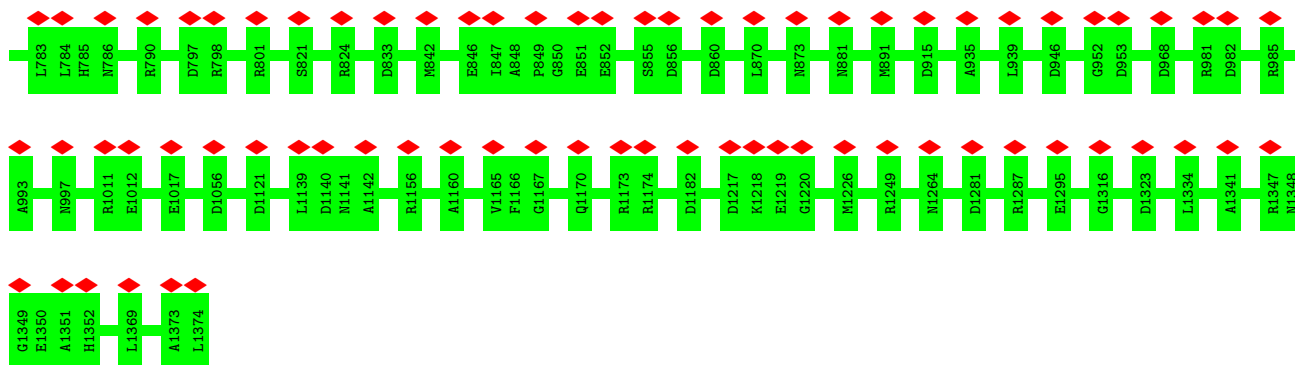


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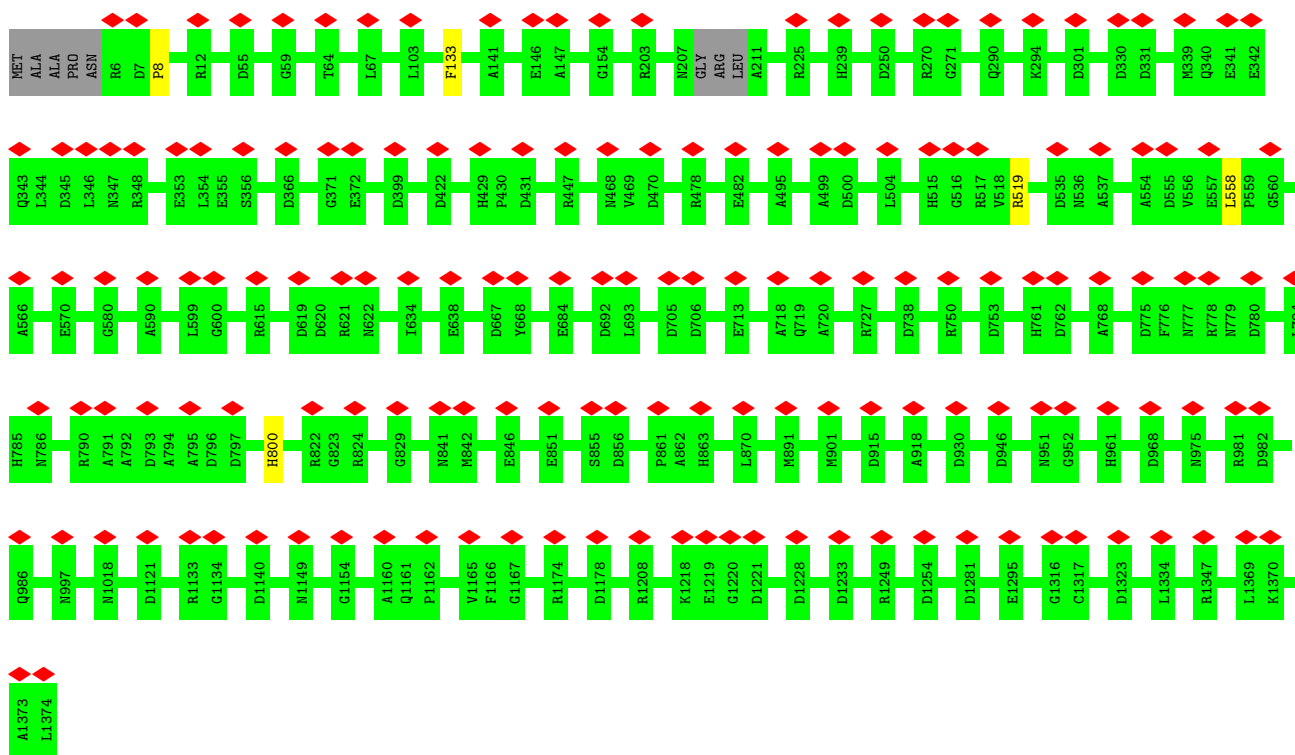


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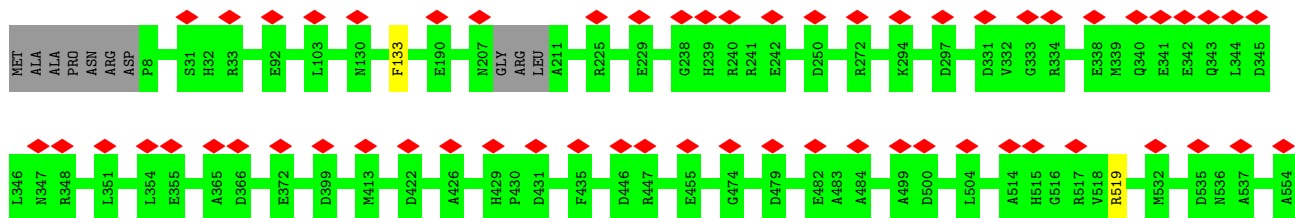


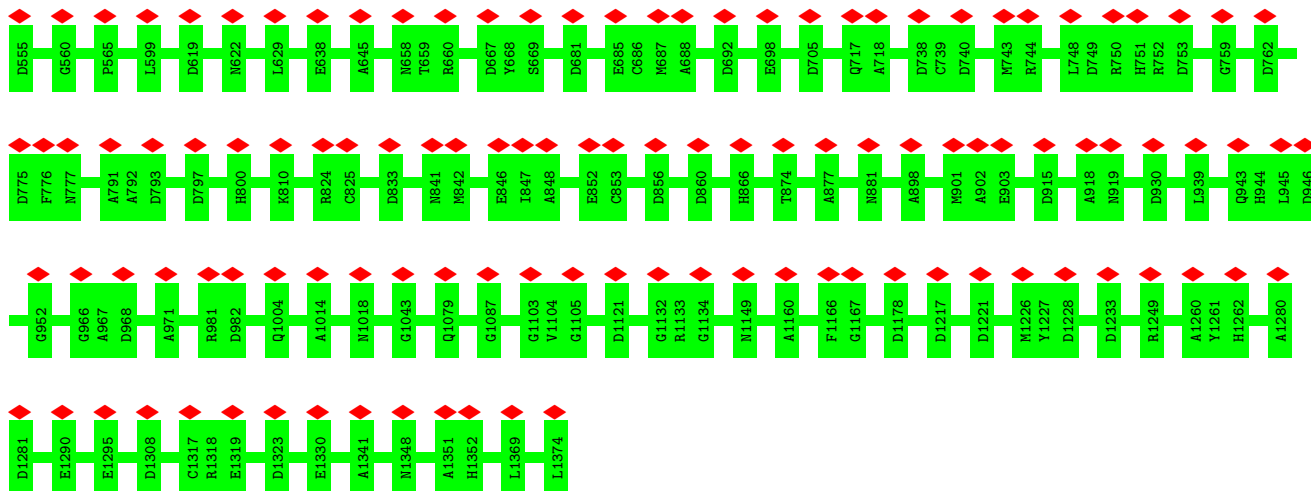


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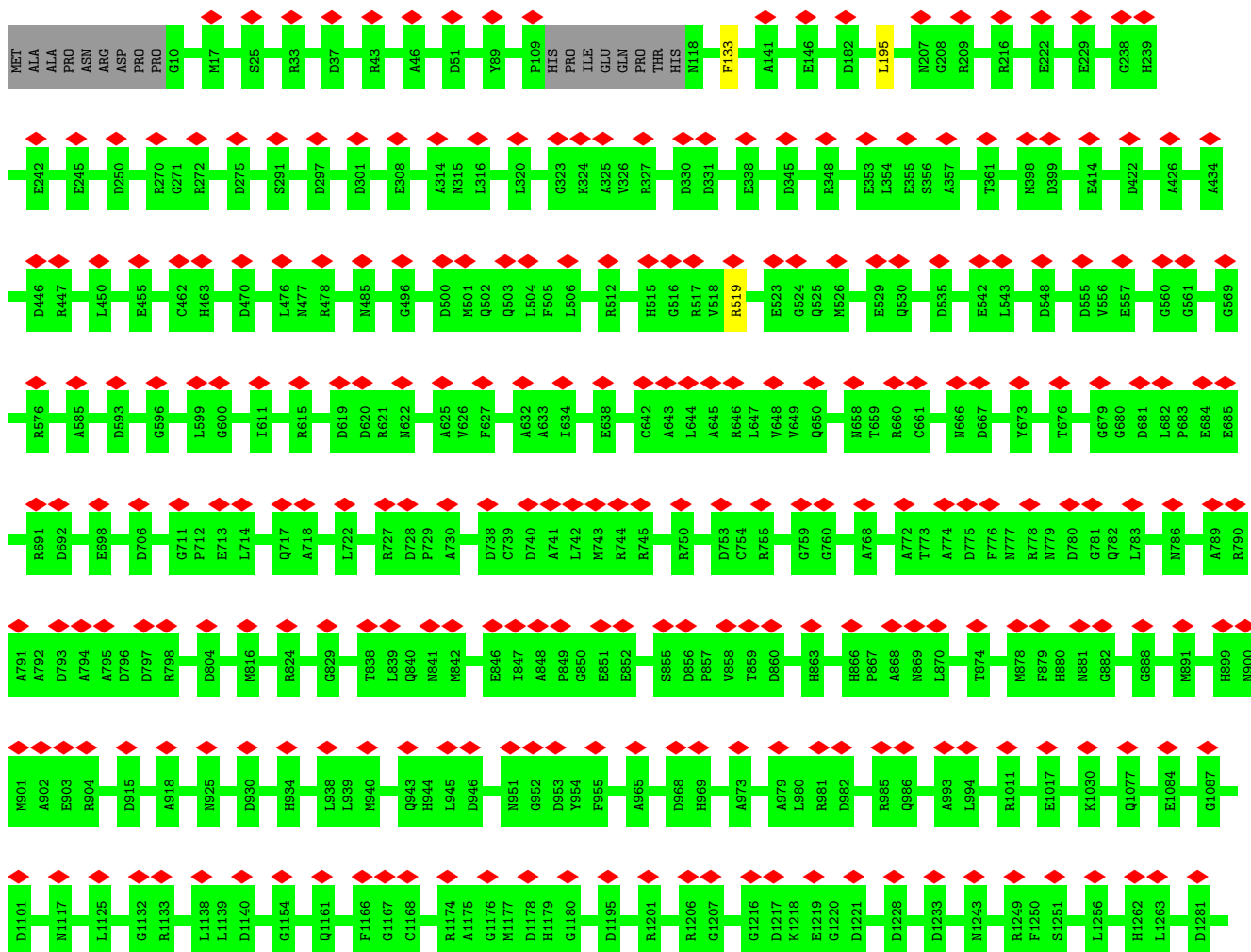


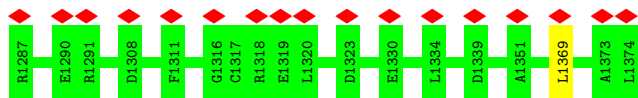
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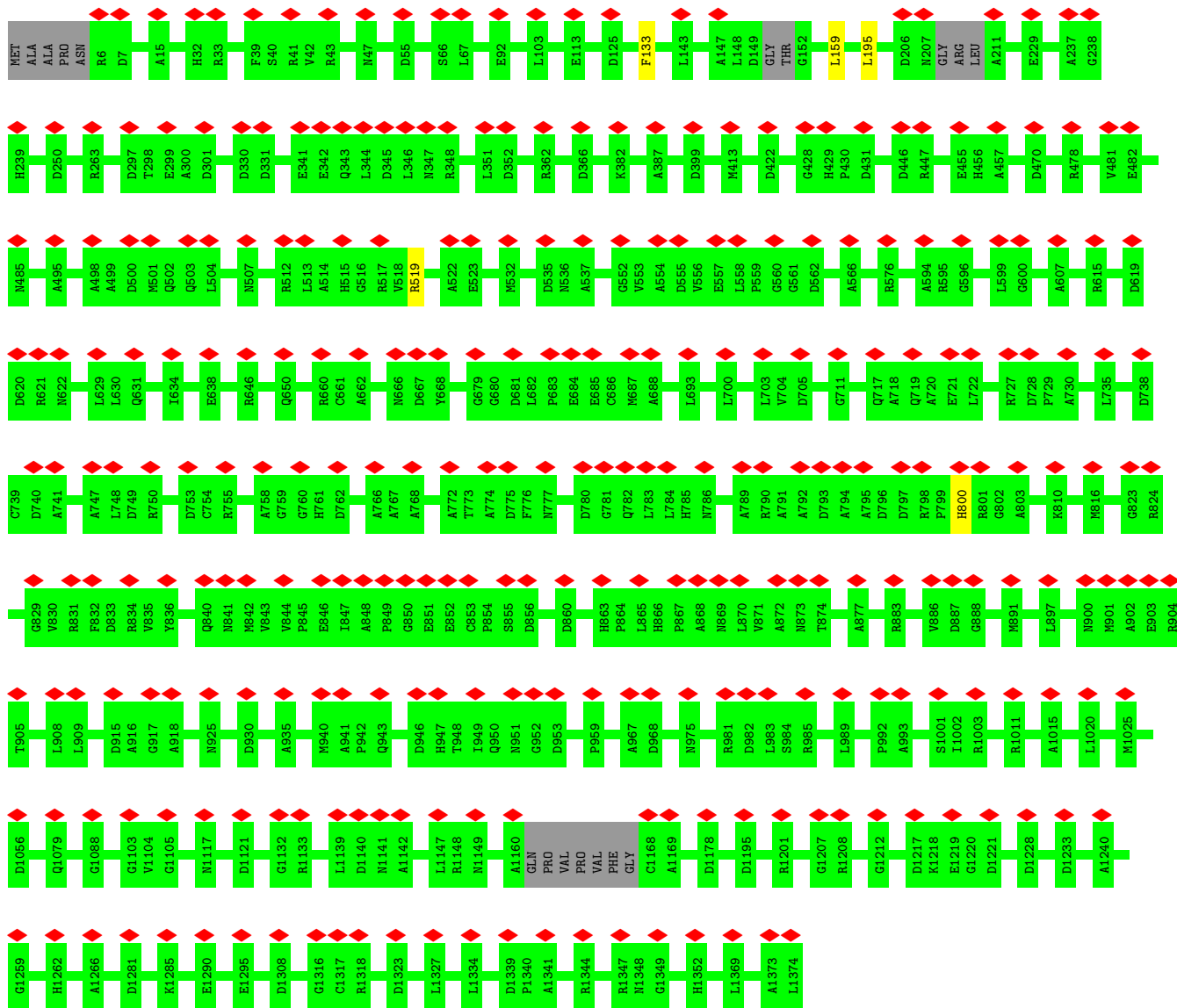


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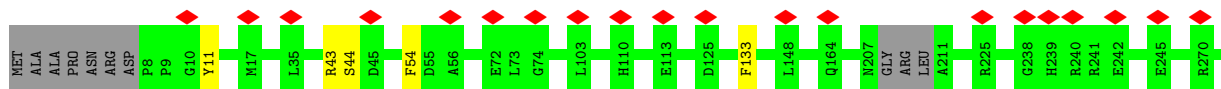


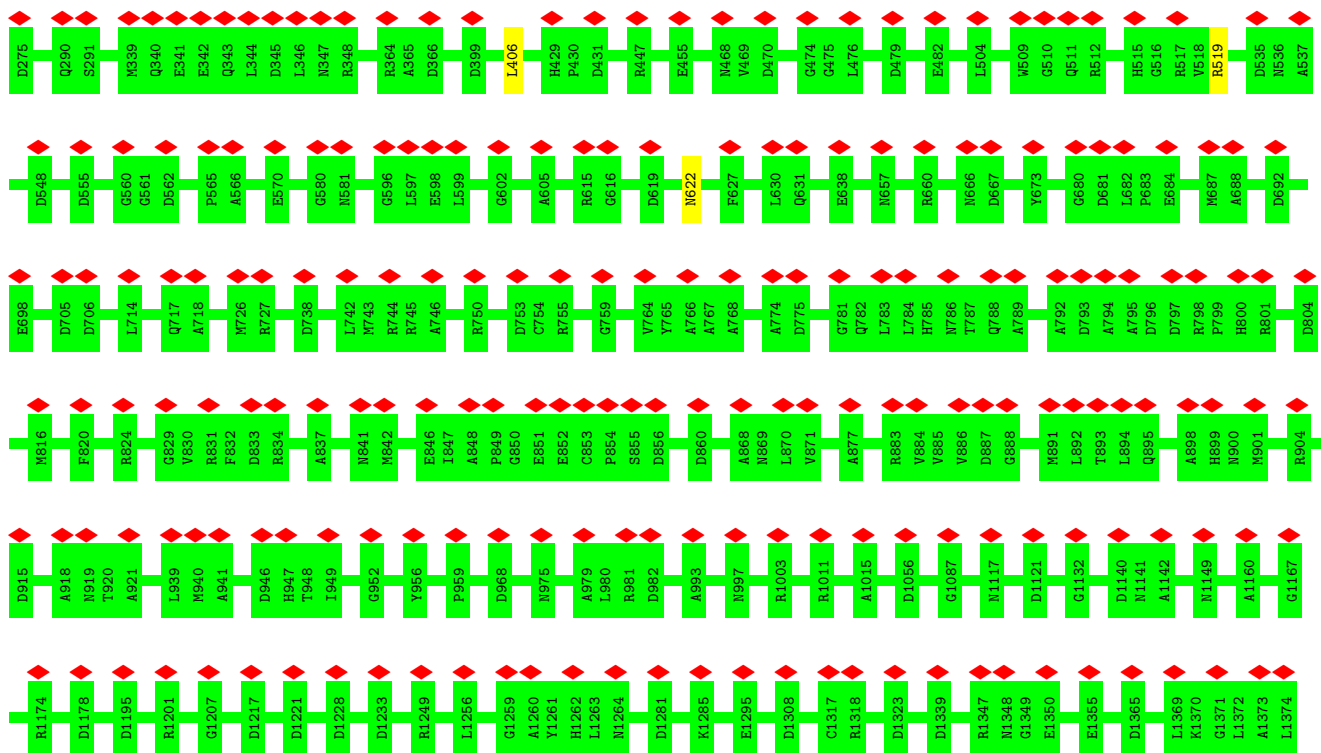


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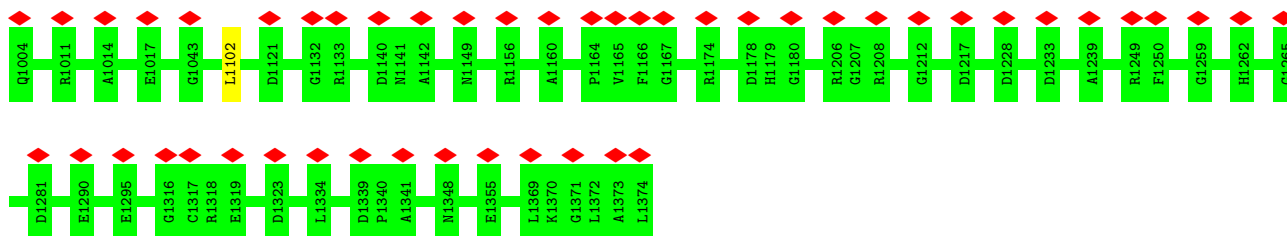
• Molecule 1: Major capsid protein



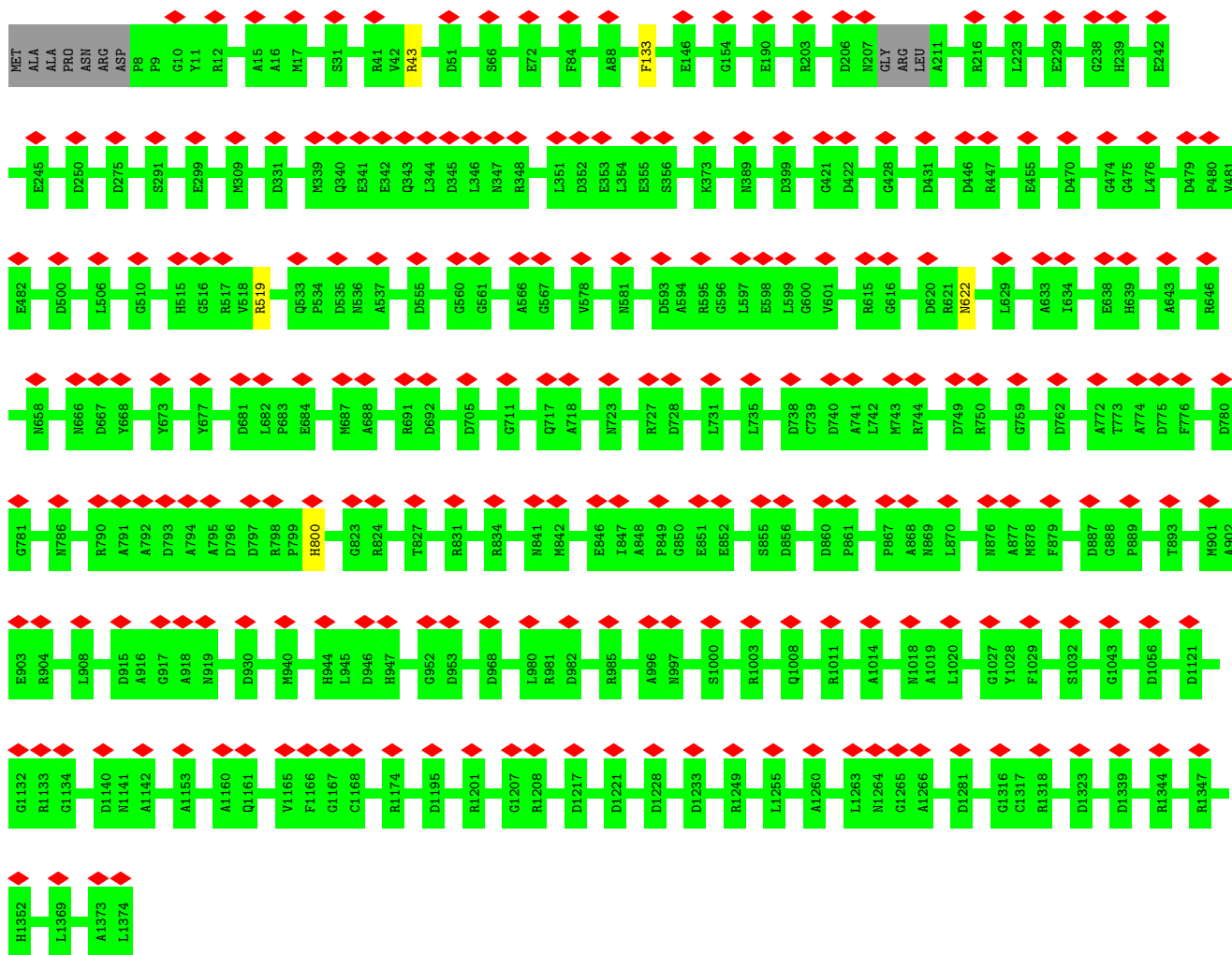


• Molecule 1: Major capsid protein

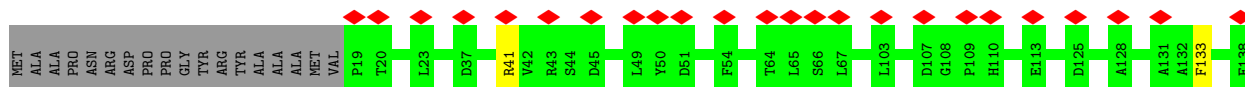


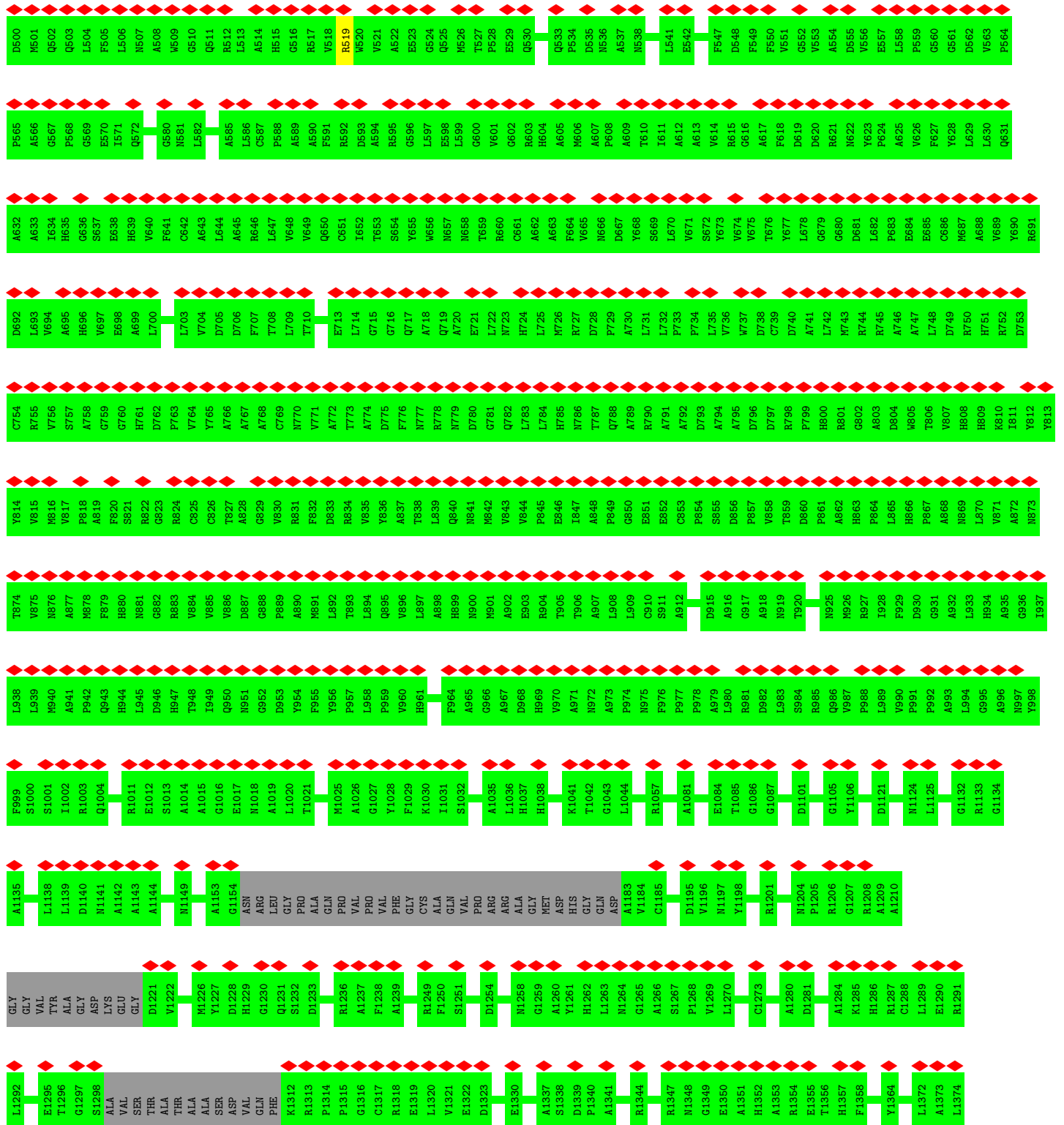


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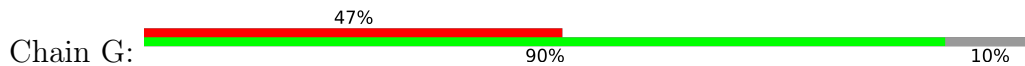


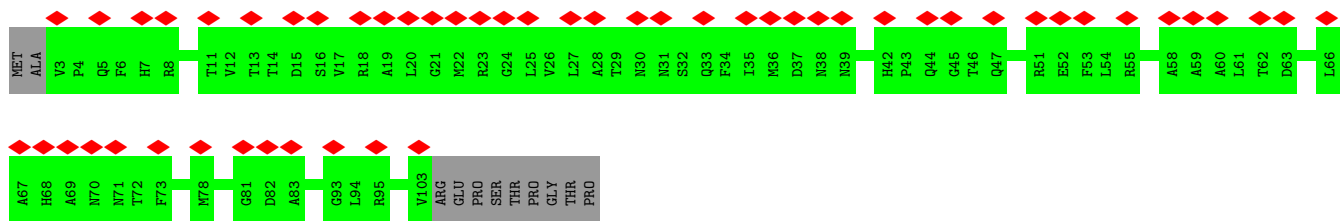
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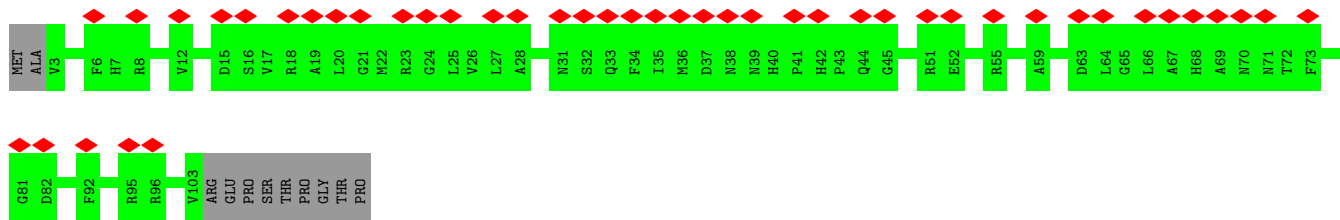
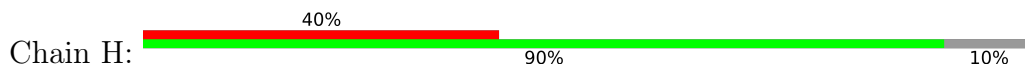


● Molecule 2: Small capsomere-interacting protein

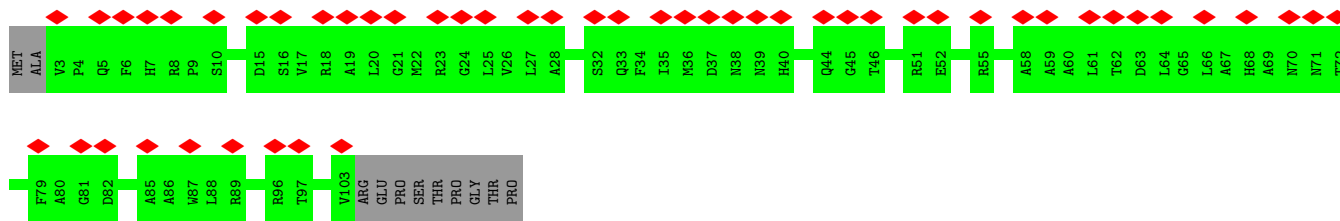
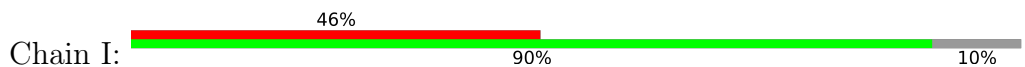




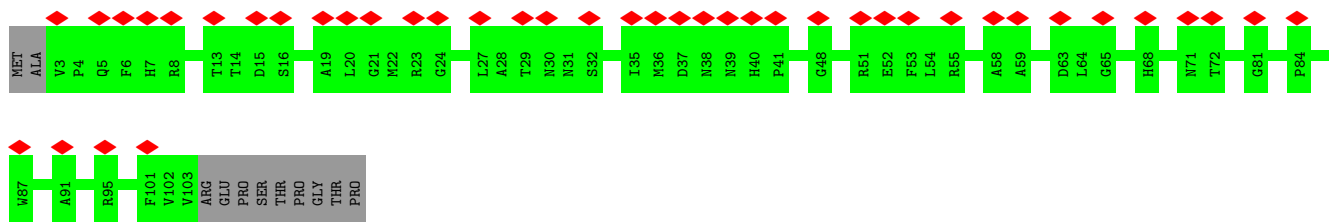
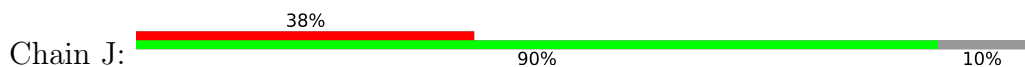
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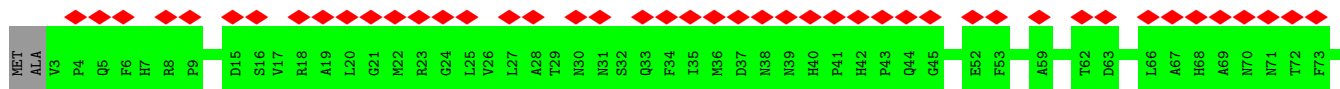
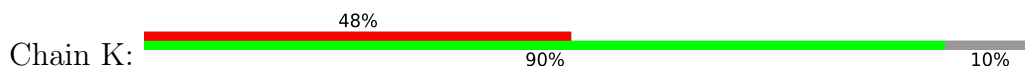
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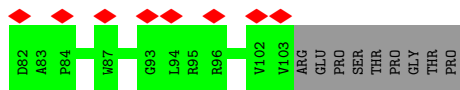


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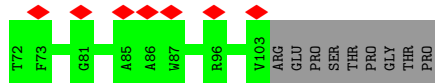
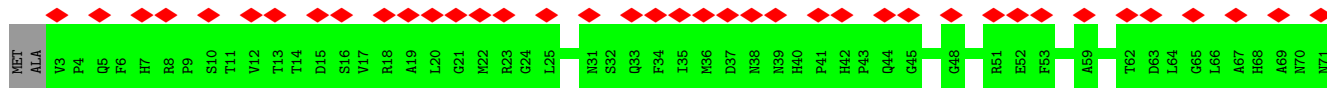
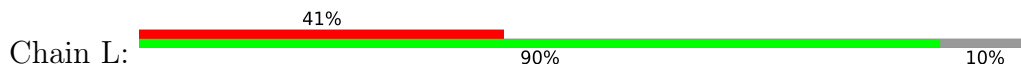


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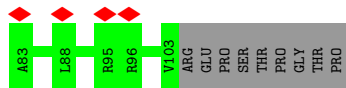
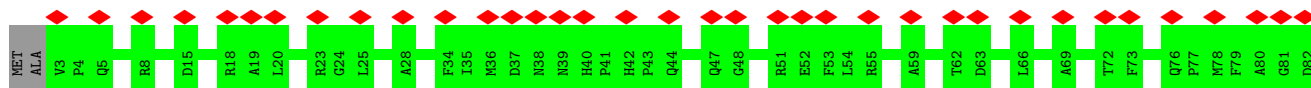
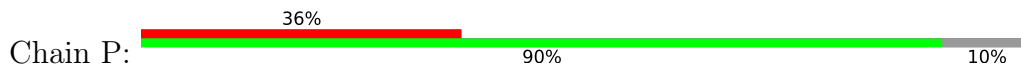




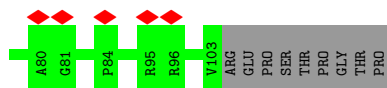
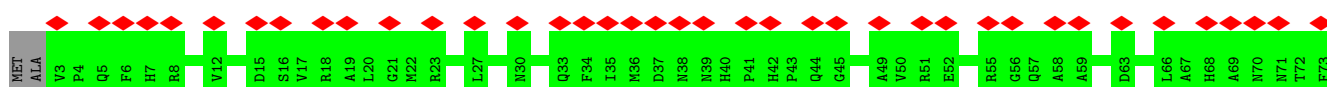
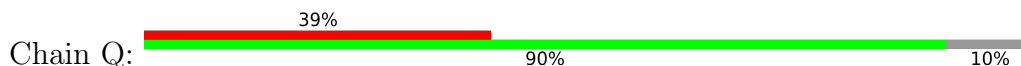
• Molecule 2: Small capsomere-interacting protein



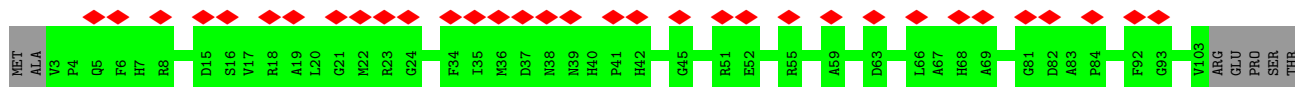
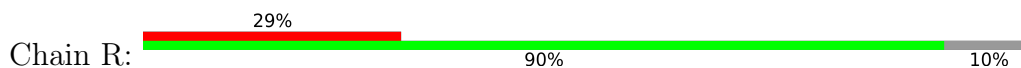
• Molecule 2: Small capsomere-interacting protein



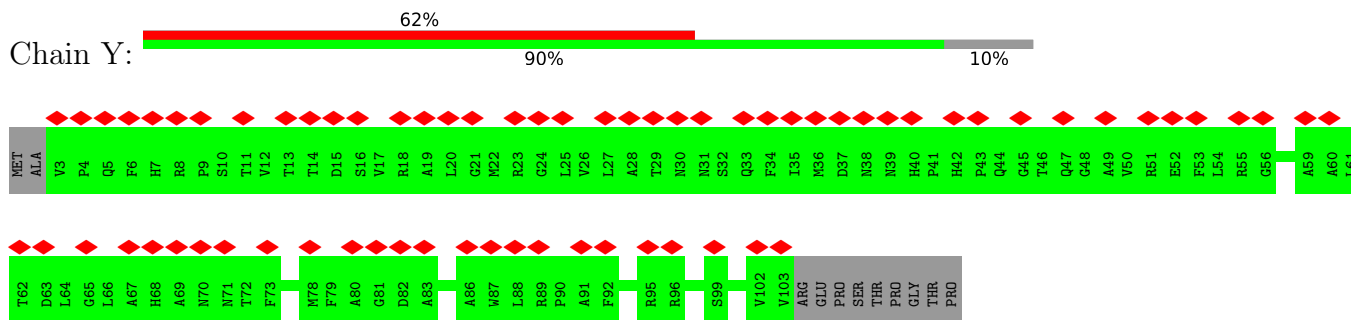
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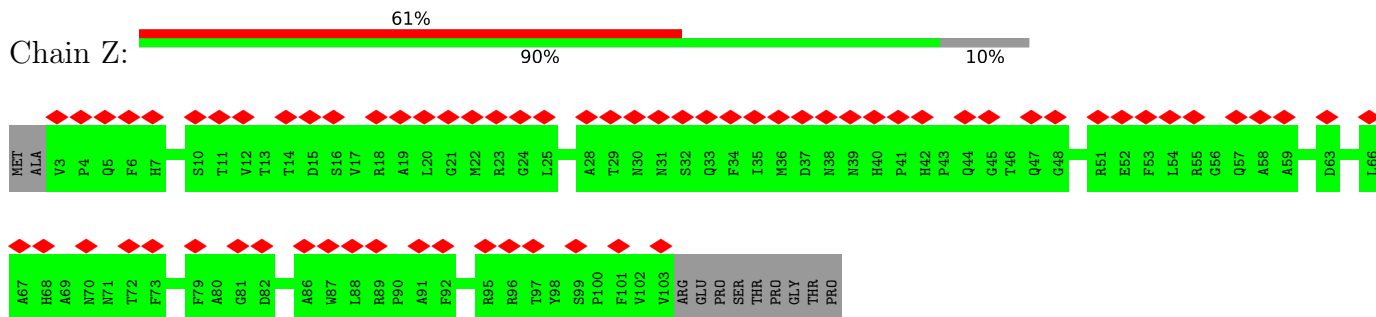
• Molecule 2: Small capsomere-interacting protein



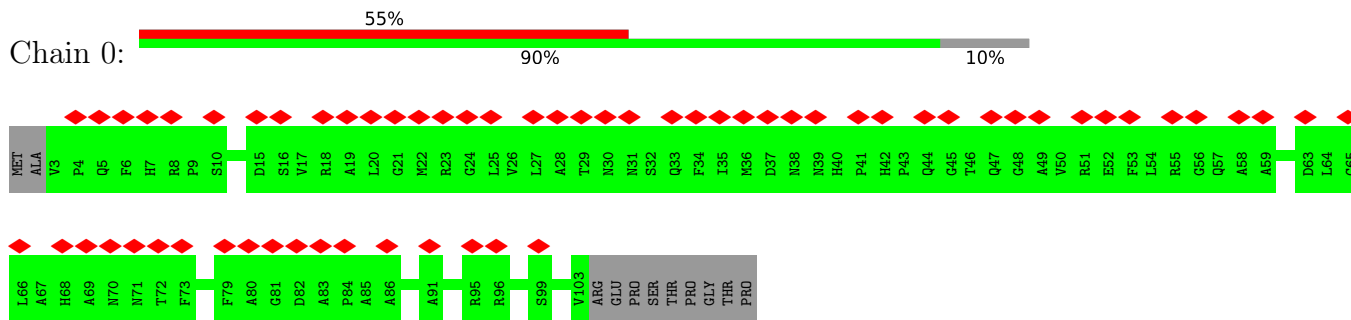
• Molecule 2: Small capsomere-interacting protein



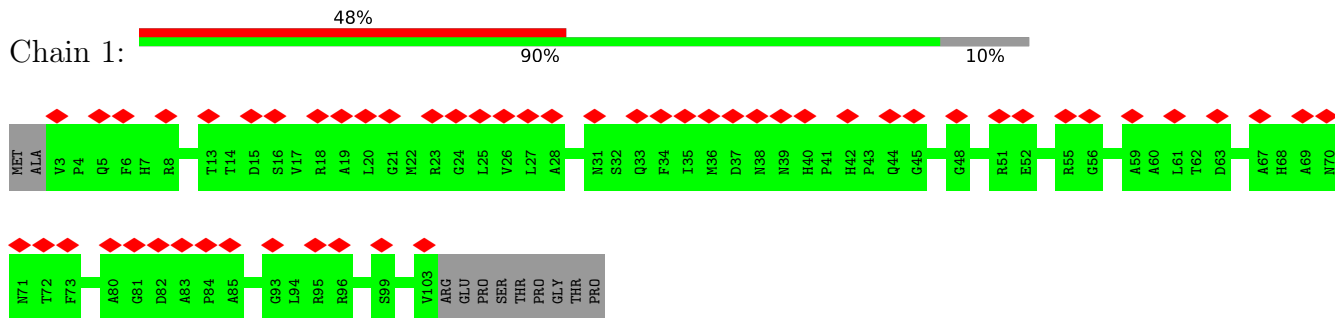
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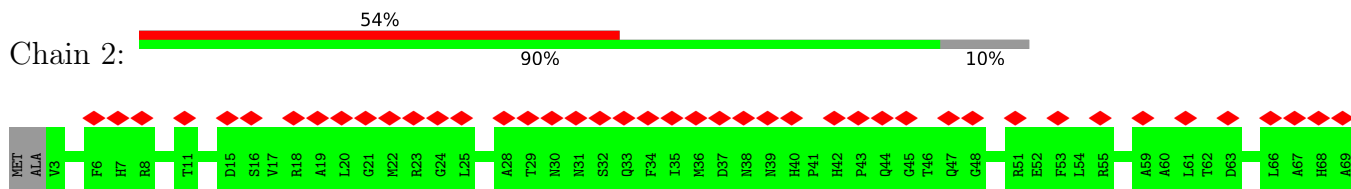
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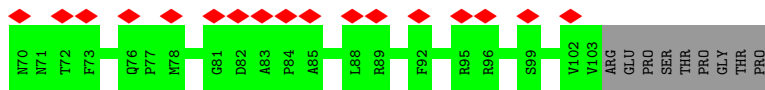


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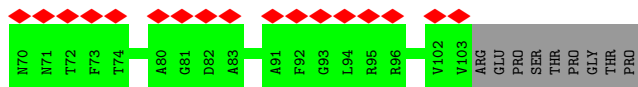
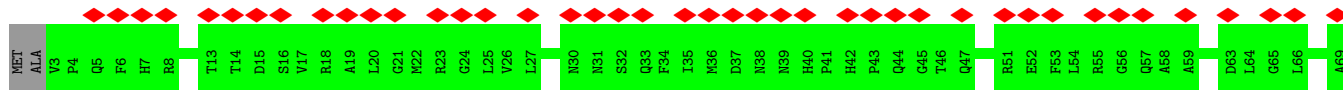
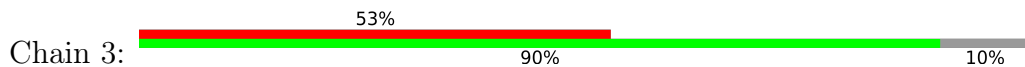


• Molecule 2: Small capsomere-interacting protein

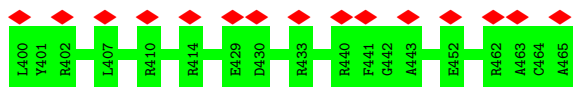
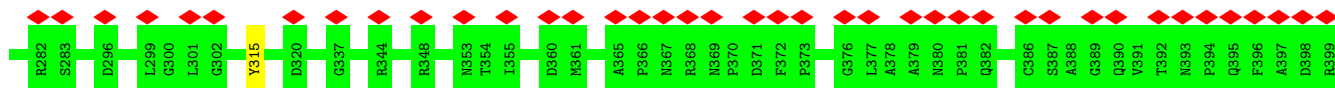
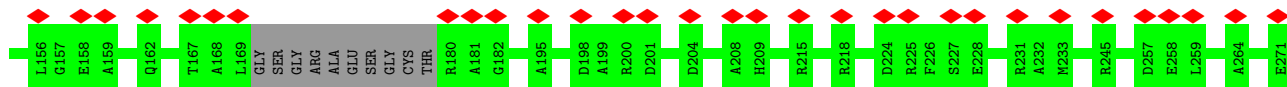
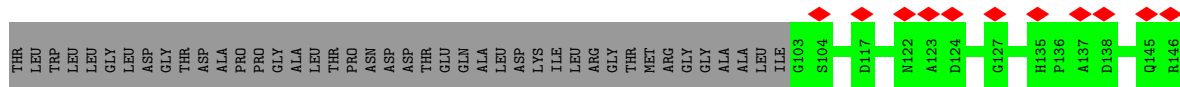
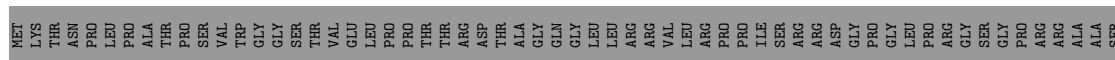
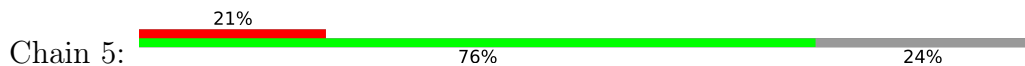




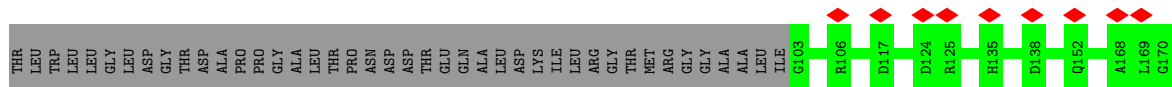
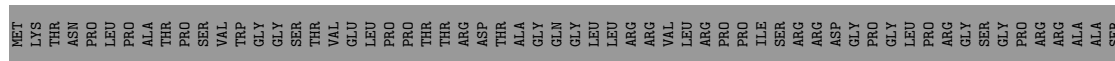
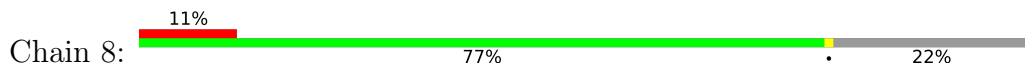
• Molecule 2: Small capsomere-interacting protein

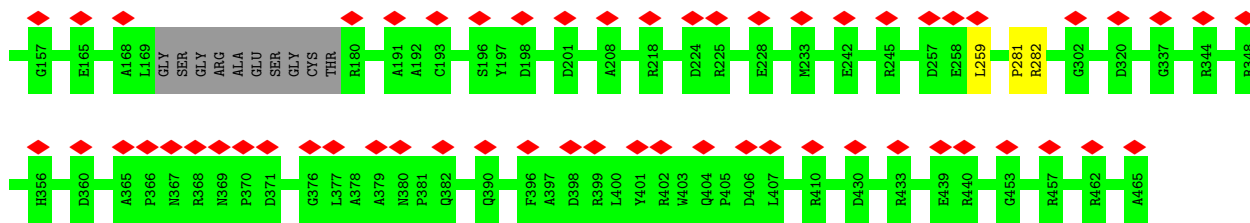


• Molecule 3: Triplex capsid protein 1

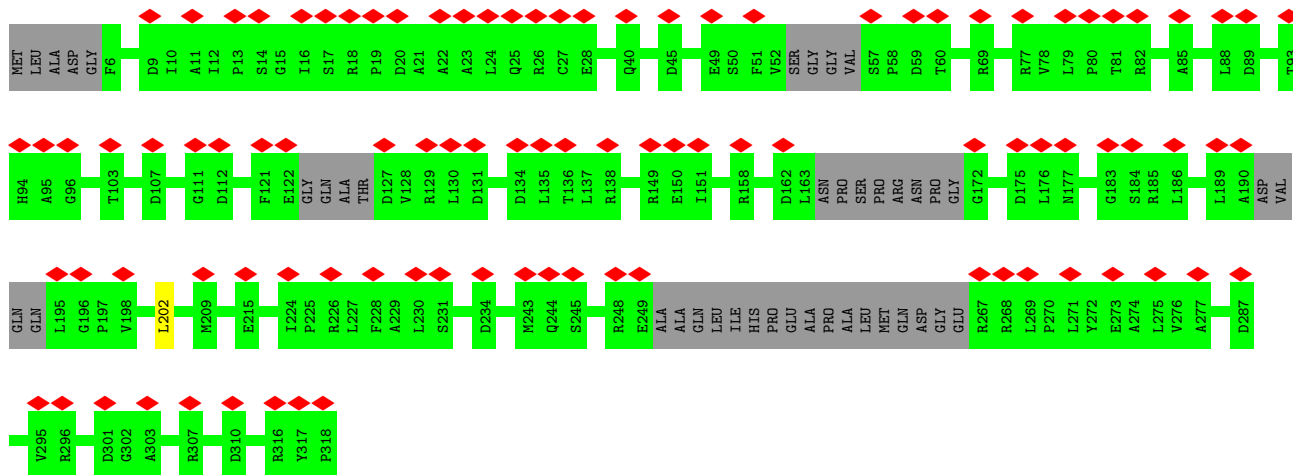
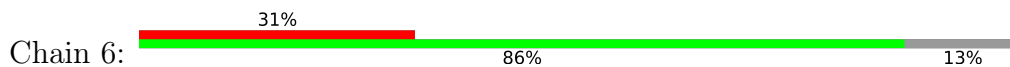


• Molecule 3: Triplex capsid protein 1

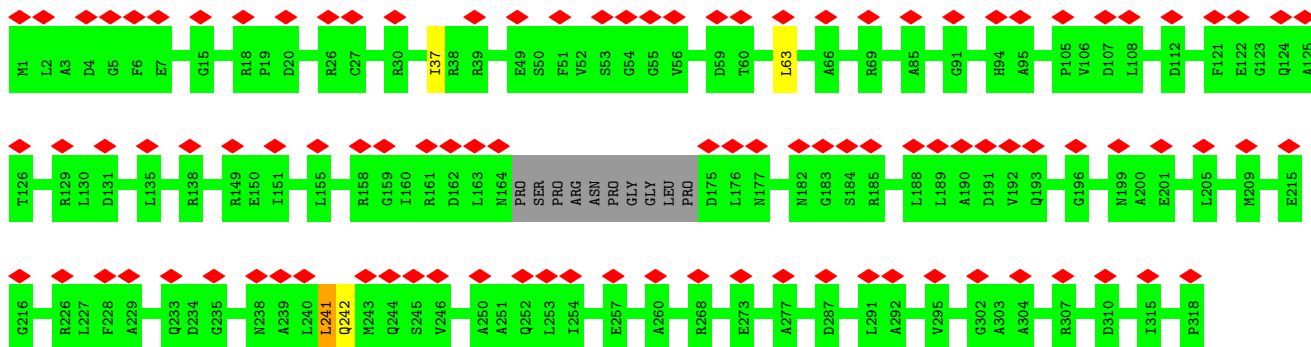




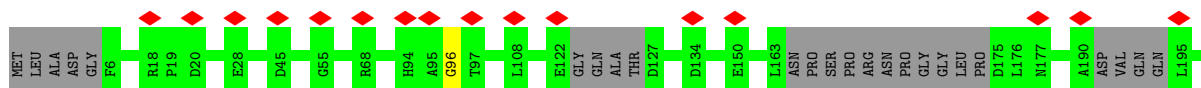
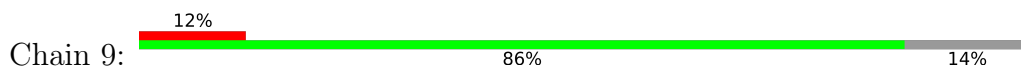
• Molecule 4: Triplex capsid protein 2

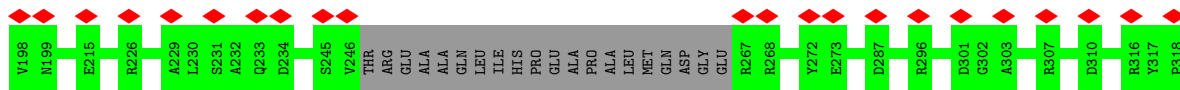


• Molecule 4: Triplex capsid protein 2

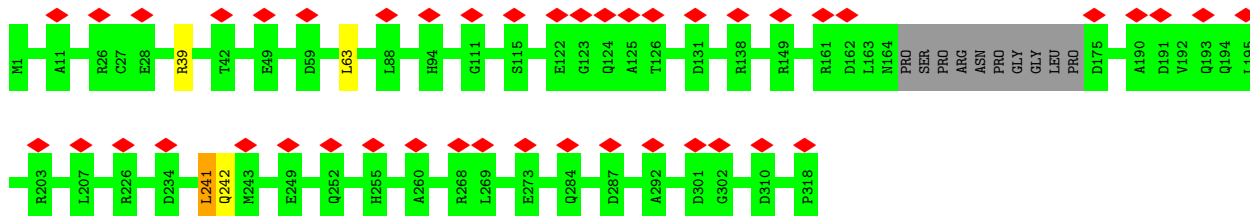


• Molecule 4: Triplex capsid protein 2

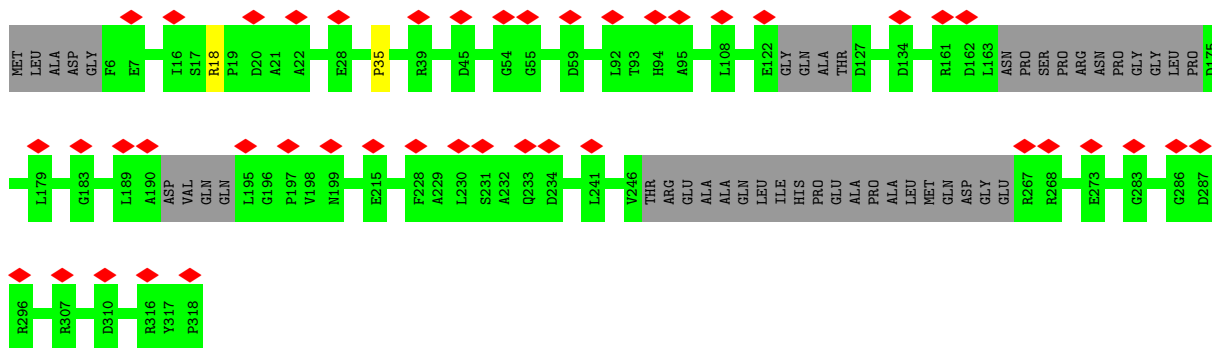
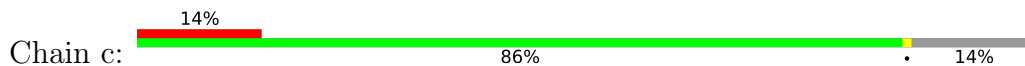




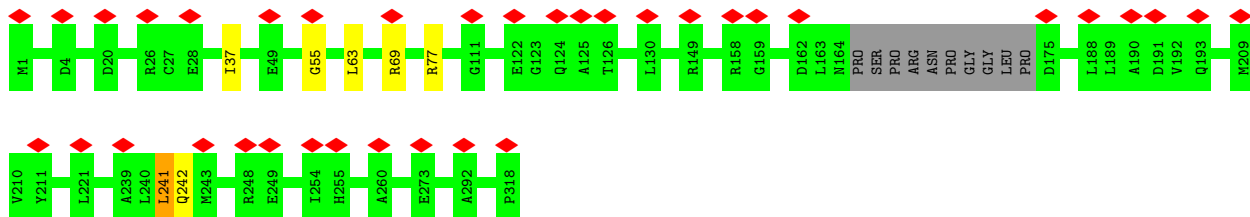
• Molecule 4: Triplex capsid protein 2



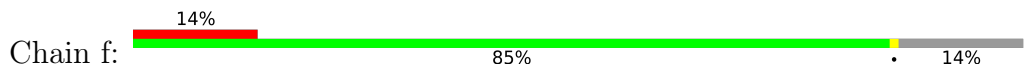
• Molecule 4: Triplex capsid protein 2

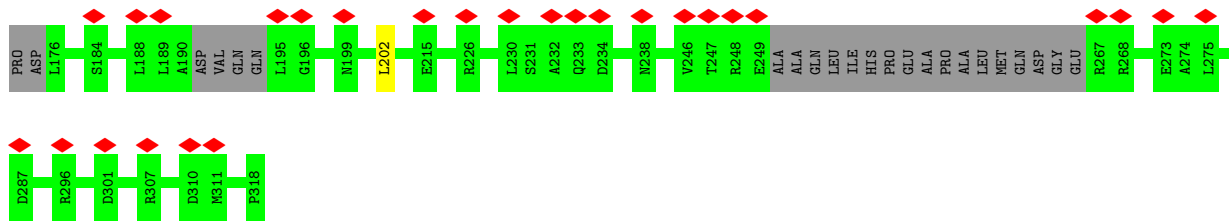


• Molecule 4: Triplex capsid protein 2

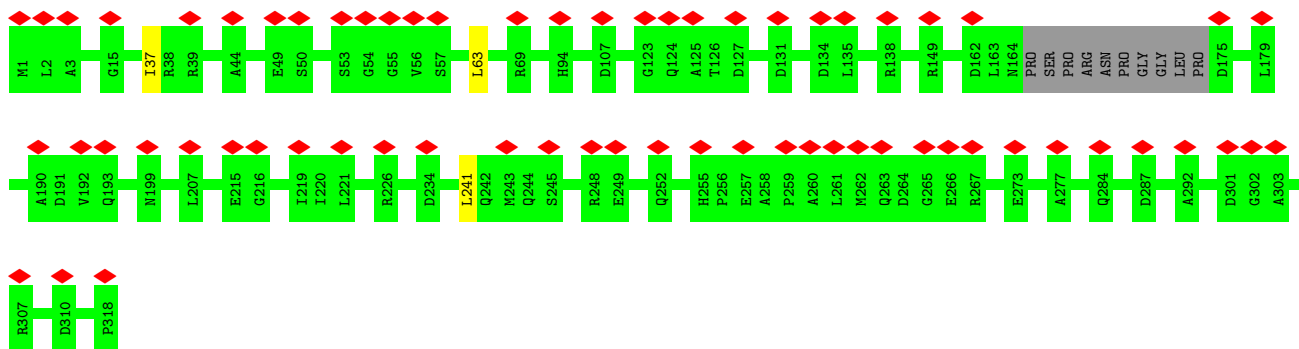


• Molecule 4: Triplex capsid protein 2

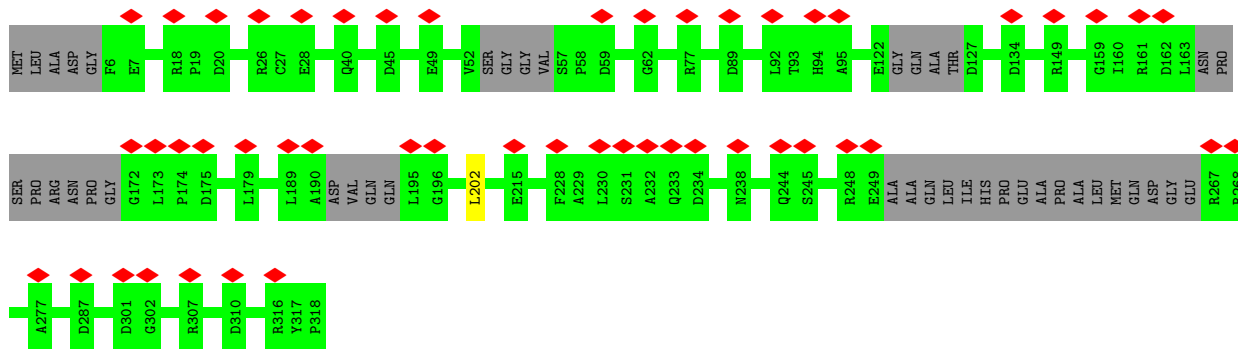
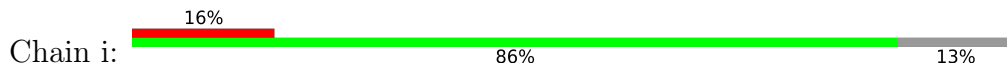




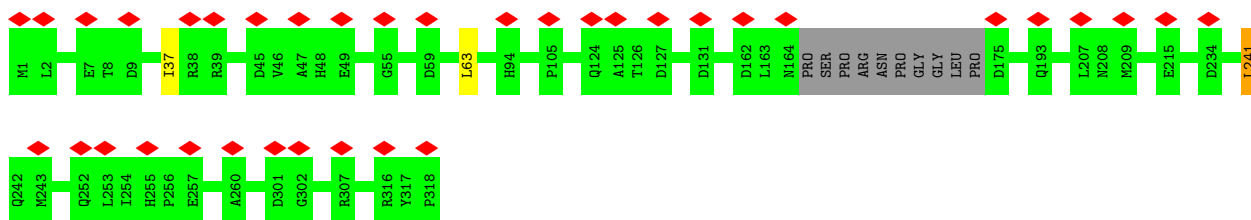
• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



• Molecule 5: Capsid vertex component 1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	28042	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.209	Depositor
Minimum map value	-10.389	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.999	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	1318.3999, 1318.3999, 1318.3999	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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 >5	RMSZ	# Z >5
1	4	0.34	0/9878	0.57	3/13478 (0.0%)
1	A	0.36	0/10664	0.58	3/14556 (0.0%)
1	B	0.37	0/10680	0.59	1/14579 (0.0%)
1	C	0.37	1/10680 (0.0%)	0.58	3/14579 (0.0%)
1	D	0.39	0/10664	0.60	3/14556 (0.0%)
1	E	0.39	0/10699	0.60	2/14605 (0.0%)
1	F	0.38	0/10664	0.59	1/14556 (0.0%)
1	M	0.38	0/10664	0.60	1/14556 (0.0%)
1	N	0.39	0/10699	0.59	0/14605
1	O	0.37	0/10680	0.58	0/14579
1	S	0.36	0/10616	0.58	2/14487 (0.0%)
1	T	0.38	0/10631	0.60	2/14507 (0.0%)
1	U	0.39	1/10680 (0.0%)	0.60	1/14579 (0.0%)
1	V	0.37	0/10664	0.59	3/14556 (0.0%)
1	W	0.37	0/10680	0.58	0/14579
1	X	0.37	0/10567	0.59	3/14423 (0.0%)
2	0	0.31	0/796	0.48	0/1087
2	1	0.31	0/796	0.48	0/1087
2	2	0.31	0/796	0.48	0/1087
2	3	0.31	0/796	0.48	0/1087
2	G	0.31	0/796	0.48	0/1087
2	H	0.31	0/796	0.48	0/1087
2	I	0.31	0/796	0.48	0/1087
2	J	0.31	0/796	0.48	0/1087
2	K	0.31	0/796	0.48	0/1087
2	L	0.31	0/796	0.48	0/1087
2	P	0.31	0/796	0.48	0/1087
2	Q	0.31	0/796	0.48	0/1087
2	R	0.31	0/796	0.48	0/1087
2	Y	0.31	0/796	0.48	0/1087
2	Z	0.31	0/796	0.48	0/1087
3	5	0.38	1/2795 (0.0%)	0.57	0/3810
3	8	0.37	0/2858	0.59	1/3895 (0.0%)
3	b	0.37	0/2858	0.58	0/3895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.35	0/2791	0.57	0/3805
3	h	0.35	0/2795	0.59	1/3810 (0.0%)
4	6	0.36	0/2152	0.62	1/2939 (0.0%)
4	7	0.36	0/2383	0.66	2/3259 (0.1%)
4	9	0.36	0/2127	0.62	0/2906
4	a	0.38	0/2383	0.68	3/3259 (0.1%)
4	c	0.36	0/2127	0.64	1/2906 (0.0%)
4	d	0.38	0/2383	0.67	3/3259 (0.1%)
4	f	0.36	0/2124	0.63	2/2900 (0.1%)
4	g	0.37	0/2383	0.63	2/3259 (0.1%)
4	i	0.35	0/2152	0.60	1/2939 (0.0%)
4	j	0.36	0/2383	0.65	2/3259 (0.1%)
5	k	0.33	0/4307	0.54	0/5866
6	l	0.33	0/786	0.52	0/1072
6	m	0.34	0/670	0.57	1/912 (0.1%)
7	n	0.22	0/388	0.40	0/521
7	o	0.22	0/388	0.40	0/521
All	All	0.37	3/224983 (0.0%)	0.59	48/307077 (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	4	0	2
1	A	0	2
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	M	0	2
1	N	0	2
1	O	0	1
1	S	0	1
1	T	0	2
1	U	0	5
1	V	0	3
1	W	0	4
1	X	0	1
3	8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	h	0	1
4	7	0	1
4	9	0	1
4	a	0	1
4	d	0	1
4	g	0	1
4	j	0	1
All	All	0	41

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	315	TYR	CD1-CE1	-6.41	1.29	1.39
1	C	954	TYR	CD1-CE1	-6.12	1.30	1.39
1	U	11	TYR	CD2-CE2	-5.88	1.30	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	159	LEU	CB-CG-CD1	-8.25	96.97	111.00
4	j	63	LEU	CA-CB-CG	7.91	133.48	115.30
4	a	63	LEU	CA-CB-CG	7.26	132.00	115.30
6	m	55	LEU	CA-CB-CG	7.17	131.79	115.30
4	7	63	LEU	CA-CB-CG	7.08	131.58	115.30
1	D	745	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	V	159	LEU	CA-CB-CG	-6.97	99.27	115.30
1	B	159	LEU	CA-CB-CG	-6.90	99.42	115.30
1	E	159	LEU	CB-CG-CD1	-6.77	99.48	111.00
3	h	259	LEU	CA-CB-CG	6.74	130.79	115.30
4	a	39	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	4	195	LEU	CA-CB-CG	6.62	130.52	115.30
1	C	159	LEU	CA-CB-CG	-6.58	100.17	115.30
4	d	69	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	159	LEU	CB-CG-CD1	-6.32	100.27	111.00
1	E	27	ILE	CG1-CB-CG2	-6.29	97.57	111.40
1	X	311	LEU	CA-CB-CG	5.94	128.96	115.30
4	d	63	LEU	CA-CB-CG	5.93	128.93	115.30
1	U	406	LEU	CA-CB-CG	5.80	128.64	115.30
4	6	202	LEU	CA-CB-CG	5.65	128.29	115.30
4	g	63	LEU	CA-CB-CG	5.60	128.19	115.30
4	d	37	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	V	103	LEU	CA-CB-CG	5.55	128.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8	259	LEU	CA-CB-CG	5.54	128.03	115.30
1	M	745	ARG	NE-CZ-NH1	-5.53	117.53	120.30
4	f	202	LEU	CA-CB-CG	5.53	128.01	115.30
1	X	195	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	1102	LEU	CA-CB-CG	5.48	127.91	115.30
1	T	195	LEU	CA-CB-CG	5.42	127.77	115.30
1	S	1369	LEU	CA-CB-CG	5.41	127.75	115.30
1	X	41	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	103	LEU	CA-CB-CG	5.34	127.58	115.30
1	S	195	LEU	CA-CB-CG	5.34	127.58	115.30
4	g	37	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	D	103	LEU	CA-CB-CG	5.28	127.44	115.30
1	V	1102	LEU	CA-CB-CG	5.27	127.42	115.30
4	7	37	ILE	CG1-CB-CG2	-5.27	99.81	111.40
1	A	406	LEU	CA-CB-CG	5.26	127.39	115.30
1	4	406	LEU	CA-CB-CG	5.22	127.31	115.30
4	f	18	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	4	344	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	103	LEU	CA-CB-CG	5.12	127.07	115.30
4	c	18	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	1102	LEU	CA-CB-CG	5.11	127.04	115.30
4	a	39	ARG	CG-CD-NE	-5.06	101.17	111.80
4	i	202	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	406	LEU	CA-CB-CG	5.00	126.81	115.30
4	j	37	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	112	ILE	Peptide
1	4	64	THR	Peptide
4	7	241	LEU	Peptide
3	8	281	PRO	Peptide
4	9	96	GLY	Peptide
1	A	133	PHE	Peptide
1	A	800	HIS	Peptide
1	B	133	PHE	Peptide
1	B	43	ARG	Peptide
1	C	133	PHE	Peptide
1	D	622	ASN	Peptide
1	D	800	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	E	133	PHE	Peptide
1	F	133	PHE	Peptide
1	F	622	ASN	Peptide
1	M	133	PHE	Peptide
1	M	43	ARG	Peptide
1	N	133	PHE	Peptide
1	N	800	HIS	Peptide
1	O	133	PHE	Peptide
1	S	133	PHE	Peptide
1	T	133	PHE	Peptide
1	T	800	HIS	Peptide
1	U	133	PHE	Peptide
1	U	43	ARG	Peptide
1	U	44	SER	Peptide
1	U	54	PHE	Peptide
1	U	622	ASN	Peptide
1	V	133	PHE	Peptide
1	V	159	LEU	Peptide
1	V	800	HIS	Peptide
1	W	133	PHE	Peptide
1	W	43	ARG	Peptide
1	W	622	ASN	Peptide
1	W	800	HIS	Peptide
1	X	133	PHE	Peptide
4	a	241	LEU	Peptide
4	d	241	LEU	Peptide
4	g	241	LEU	Peptide
3	h	281	PRO	Peptide
4	j	241	LEU	Peptide

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	4	1243/1374 (90%)	1169 (94%)	74 (6%)	0	100	100
1	A	1358/1374 (99%)	1262 (93%)	96 (7%)	0	100	100
1	B	1360/1374 (99%)	1258 (92%)	102 (8%)	0	100	100
1	C	1360/1374 (99%)	1265 (93%)	95 (7%)	0	100	100
1	D	1358/1374 (99%)	1246 (92%)	112 (8%)	0	100	100
1	E	1362/1374 (99%)	1254 (92%)	108 (8%)	0	100	100
1	F	1358/1374 (99%)	1244 (92%)	114 (8%)	0	100	100
1	M	1358/1374 (99%)	1244 (92%)	114 (8%)	0	100	100
1	N	1362/1374 (99%)	1253 (92%)	108 (8%)	1 (0%)	51	85
1	O	1360/1374 (99%)	1260 (93%)	100 (7%)	0	100	100
1	S	1353/1374 (98%)	1272 (94%)	81 (6%)	0	100	100
1	T	1349/1374 (98%)	1272 (94%)	77 (6%)	0	100	100
1	U	1360/1374 (99%)	1244 (92%)	116 (8%)	0	100	100
1	V	1358/1374 (99%)	1247 (92%)	111 (8%)	0	100	100
1	W	1360/1374 (99%)	1252 (92%)	108 (8%)	0	100	100
1	X	1344/1374 (98%)	1260 (94%)	84 (6%)	0	100	100
2	0	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	1	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	2	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	3	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	G	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	H	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	I	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	J	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	K	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	L	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	P	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	Q	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	R	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	Y	99/112 (88%)	94 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
3	5	349/465 (75%)	332 (95%)	17 (5%)	0	100	100
3	8	361/465 (78%)	340 (94%)	20 (6%)	1 (0%)	41	76
3	b	361/465 (78%)	341 (94%)	20 (6%)	0	100	100
3	e	348/465 (75%)	324 (93%)	24 (7%)	0	100	100
3	h	349/465 (75%)	326 (93%)	22 (6%)	1 (0%)	41	76
4	6	264/318 (83%)	249 (94%)	15 (6%)	0	100	100
4	7	304/318 (96%)	283 (93%)	19 (6%)	2 (1%)	22	62
4	9	264/318 (83%)	244 (92%)	20 (8%)	0	100	100
4	a	304/318 (96%)	277 (91%)	25 (8%)	2 (1%)	22	62
4	c	264/318 (83%)	246 (93%)	17 (6%)	1 (0%)	34	72
4	d	304/318 (96%)	274 (90%)	27 (9%)	3 (1%)	15	54
4	f	260/318 (82%)	238 (92%)	21 (8%)	1 (0%)	34	72
4	g	304/318 (96%)	276 (91%)	28 (9%)	0	100	100
4	i	264/318 (83%)	246 (93%)	18 (7%)	0	100	100
4	j	304/318 (96%)	273 (90%)	30 (10%)	1 (0%)	41	76
5	k	534/703 (76%)	514 (96%)	20 (4%)	0	100	100
6	l	92/580 (16%)	87 (95%)	5 (5%)	0	100	100
6	m	78/580 (13%)	77 (99%)	1 (1%)	0	100	100
7	n	45/3139 (1%)	45 (100%)	0	0	100	100
7	o	45/3139 (1%)	45 (100%)	0	0	100	100
All	All	28486/37310 (76%)	26449 (93%)	2024 (7%)	13 (0%)	100	100

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	8	282	ARG
4	7	241	LEU
4	d	241	LEU
4	d	242	GLN
3	h	282	ARG
1	N	8	PRO
4	7	242	GLN
4	a	241	LEU
4	a	242	GLN

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Mol	Chain	Res	Type
4	f	76	THR
4	j	241	LEU
4	d	55	GLY
4	c	35	PRO

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	4	1003/1085 (92%)	1002 (100%)	1 (0%)	93 97
1	A	1076/1085 (99%)	1075 (100%)	1 (0%)	93 97
1	B	1078/1085 (99%)	1077 (100%)	1 (0%)	93 97
1	C	1078/1085 (99%)	1077 (100%)	1 (0%)	93 97
1	D	1076/1085 (99%)	1075 (100%)	1 (0%)	93 97
1	E	1080/1085 (100%)	1079 (100%)	1 (0%)	93 97
1	F	1076/1085 (99%)	1075 (100%)	1 (0%)	93 97
1	M	1076/1085 (99%)	1074 (100%)	2 (0%)	93 96
1	N	1080/1085 (100%)	1078 (100%)	2 (0%)	93 96
1	O	1078/1085 (99%)	1077 (100%)	1 (0%)	93 97
1	S	1070/1085 (99%)	1069 (100%)	1 (0%)	93 97
1	T	1073/1085 (99%)	1072 (100%)	1 (0%)	93 97
1	U	1078/1085 (99%)	1077 (100%)	1 (0%)	93 97
1	V	1076/1085 (99%)	1075 (100%)	1 (0%)	93 97
1	W	1078/1085 (99%)	1077 (100%)	1 (0%)	93 97
1	X	1069/1085 (98%)	1067 (100%)	2 (0%)	93 96
2	0	80/89 (90%)	80 (100%)	0	100 100
2	1	80/89 (90%)	80 (100%)	0	100 100
2	2	80/89 (90%)	80 (100%)	0	100 100
2	3	80/89 (90%)	80 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	80/89 (90%)	80 (100%)	0	100	100
2	H	80/89 (90%)	80 (100%)	0	100	100
2	I	80/89 (90%)	80 (100%)	0	100	100
2	J	80/89 (90%)	80 (100%)	0	100	100
2	K	80/89 (90%)	80 (100%)	0	100	100
2	L	80/89 (90%)	80 (100%)	0	100	100
2	P	80/89 (90%)	80 (100%)	0	100	100
2	Q	80/89 (90%)	80 (100%)	0	100	100
2	R	80/89 (90%)	80 (100%)	0	100	100
2	Y	80/89 (90%)	80 (100%)	0	100	100
2	Z	80/89 (90%)	80 (100%)	0	100	100
3	5	279/364 (77%)	279 (100%)	0	100	100
3	8	285/364 (78%)	285 (100%)	0	100	100
3	b	285/364 (78%)	285 (100%)	0	100	100
3	e	279/364 (77%)	279 (100%)	0	100	100
3	h	279/364 (77%)	279 (100%)	0	100	100
4	6	234/264 (89%)	234 (100%)	0	100	100
4	7	256/264 (97%)	256 (100%)	0	100	100
4	9	231/264 (88%)	231 (100%)	0	100	100
4	a	256/264 (97%)	256 (100%)	0	100	100
4	c	231/264 (88%)	231 (100%)	0	100	100
4	d	256/264 (97%)	255 (100%)	1 (0%)	91	94
4	f	231/264 (88%)	231 (100%)	0	100	100
4	g	256/264 (97%)	256 (100%)	0	100	100
4	i	234/264 (89%)	234 (100%)	0	100	100
4	j	256/264 (97%)	256 (100%)	0	100	100
5	k	429/529 (81%)	428 (100%)	1 (0%)	93	96
6	l	80/448 (18%)	80 (100%)	0	100	100
6	m	67/448 (15%)	66 (98%)	1 (2%)	65	80
7	n	41/2430 (2%)	40 (98%)	1 (2%)	49	69
7	o	41/2430 (2%)	40 (98%)	1 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	22851/29440 (78%)	22827 (100%)	24 (0%)	93 97

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	519	ARG
1	B	519	ARG
1	C	519	ARG
1	D	519	ARG
1	E	519	ARG
1	F	519	ARG
1	M	272	ARG
1	M	519	ARG
1	N	519	ARG
1	N	558	LEU
1	O	519	ARG
1	S	519	ARG
1	T	519	ARG
1	U	519	ARG
1	V	519	ARG
1	W	519	ARG
1	X	451	ARG
1	X	519	ARG
1	4	519	ARG
4	d	77	ARG
5	k	103	ARG
6	m	82	ARG
7	n	3115	ARG
7	o	3115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (345) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	164	GLN
1	A	168	ASN
1	A	266	HIS
1	A	429	HIS
1	A	456	HIS
1	A	485	ASN
1	A	723	ASN

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Mol	Chain	Res	Type
1	A	777	ASN
1	A	808	HIS
1	A	863	HIS
1	A	895	GLN
1	A	961	HIS
1	A	969	HIS
1	A	1004	GLN
1	A	1037	HIS
1	A	1039	GLN
1	A	1127	GLN
1	A	1128	ASN
1	A	1248	GLN
1	B	63	ASN
1	B	91	ASN
1	B	164	GLN
1	B	168	ASN
1	B	266	HIS
1	B	429	HIS
1	B	456	HIS
1	B	502	GLN
1	B	717	GLN
1	B	723	ASN
1	B	782	GLN
1	B	808	HIS
1	B	863	HIS
1	B	866	HIS
1	B	961	HIS
1	B	969	HIS
1	B	1009	HIS
1	B	1037	HIS
1	B	1039	GLN
1	C	63	ASN
1	C	429	HIS
1	C	456	HIS
1	C	657	ASN
1	C	658	ASN
1	C	777	ASN
1	C	788	GLN
1	C	841	ASN
1	C	866	HIS
1	C	961	HIS
1	C	1009	HIS

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Mol	Chain	Res	Type
1	C	1037	HIS
1	C	1128	ASN
1	C	1248	GLN
1	C	1258	ASN
1	C	1286	HIS
1	D	91	ASN
1	D	164	GLN
1	D	168	ASN
1	D	266	HIS
1	D	315	ASN
1	D	429	HIS
1	D	456	HIS
1	D	502	GLN
1	D	503	GLN
1	D	604	HIS
1	D	696	HIS
1	D	723	ASN
1	D	724	HIS
1	D	777	ASN
1	D	788	GLN
1	D	808	HIS
1	D	841	ASN
1	D	863	HIS
1	D	969	HIS
1	D	972	ASN
1	D	1009	HIS
1	D	1039	GLN
1	D	1127	GLN
1	D	1248	GLN
1	D	1262	HIS
1	E	164	GLN
1	E	168	ASN
1	E	266	HIS
1	E	429	HIS
1	E	456	HIS
1	E	485	ASN
1	E	502	GLN
1	E	658	ASN
1	E	785	HIS
1	E	863	HIS
1	E	969	HIS
1	E	1009	HIS

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Mol	Chain	Res	Type
1	E	1037	HIS
1	E	1117	ASN
1	E	1127	GLN
1	E	1128	ASN
1	E	1248	GLN
1	F	47	ASN
1	F	63	ASN
1	F	118	ASN
1	F	456	HIS
1	F	723	ASN
1	F	863	HIS
1	F	961	HIS
1	F	1009	HIS
1	F	1039	GLN
1	F	1117	ASN
1	F	1127	GLN
1	F	1128	ASN
1	F	1248	GLN
2	J	57	GLN
1	M	32	HIS
1	M	266	HIS
1	M	429	HIS
1	M	456	HIS
1	M	485	ASN
1	M	658	ASN
1	M	723	ASN
1	M	785	HIS
1	M	841	ASN
1	M	863	HIS
1	M	961	HIS
1	M	969	HIS
1	M	1009	HIS
1	M	1037	HIS
1	M	1039	GLN
1	M	1083	HIS
1	M	1090	ASN
1	M	1127	GLN
1	M	1128	ASN
1	M	1248	GLN
1	N	32	HIS
1	N	63	ASN
1	N	164	GLN

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Mol	Chain	Res	Type
1	N	168	ASN
1	N	266	HIS
1	N	315	ASN
1	N	429	HIS
1	N	456	HIS
1	N	502	GLN
1	N	723	ASN
1	N	724	HIS
1	N	777	ASN
1	N	785	HIS
1	N	808	HIS
1	N	863	HIS
1	N	961	HIS
1	N	969	HIS
1	N	1037	HIS
1	N	1039	GLN
1	N	1083	HIS
1	N	1128	ASN
1	O	266	HIS
1	O	456	HIS
1	O	502	GLN
1	O	515	HIS
1	O	658	ASN
1	O	717	GLN
1	O	723	ASN
1	O	777	ASN
1	O	866	HIS
1	O	876	ASN
1	O	961	HIS
1	O	969	HIS
1	O	1004	GLN
1	O	1037	HIS
1	O	1039	GLN
1	O	1127	GLN
1	O	1248	GLN
1	S	100	HIS
1	S	130	ASN
1	S	156	HIS
1	S	164	GLN
1	S	168	ASN
1	S	186	HIS
1	S	266	HIS

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Mol	Chain	Res	Type
1	S	456	HIS
1	S	515	HIS
1	S	717	GLN
1	S	723	ASN
1	S	724	HIS
1	S	863	HIS
1	S	866	HIS
1	S	961	HIS
1	S	969	HIS
1	S	1004	GLN
1	S	1037	HIS
1	S	1039	GLN
1	S	1258	ASN
1	T	63	ASN
1	T	118	ASN
1	T	156	HIS
1	T	163	GLN
1	T	164	GLN
1	T	168	ASN
1	T	266	HIS
1	T	456	HIS
1	T	717	GLN
1	T	723	ASN
1	T	724	HIS
1	T	777	ASN
1	T	788	GLN
1	T	863	HIS
1	T	866	HIS
1	T	961	HIS
1	T	969	HIS
1	T	1004	GLN
1	T	1037	HIS
1	T	1039	GLN
1	T	1090	ASN
1	T	1128	ASN
1	U	63	ASN
1	U	163	GLN
1	U	164	GLN
1	U	168	ASN
1	U	429	HIS
1	U	456	HIS
1	U	639	HIS

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Mol	Chain	Res	Type
1	U	717	GLN
1	U	723	ASN
1	U	777	ASN
1	U	785	HIS
1	U	808	HIS
1	U	841	ASN
1	U	863	HIS
1	U	866	HIS
1	U	895	GLN
1	U	899	HIS
1	U	900	ASN
1	U	969	HIS
1	U	1037	HIS
1	U	1039	GLN
1	V	63	ASN
1	V	163	GLN
1	V	164	GLN
1	V	168	ASN
1	V	266	HIS
1	V	456	HIS
1	V	502	GLN
1	V	658	ASN
1	V	723	ASN
1	V	782	GLN
1	V	841	ASN
1	V	863	HIS
1	V	866	HIS
1	V	961	HIS
1	V	969	HIS
1	V	1004	GLN
1	V	1009	HIS
1	V	1037	HIS
1	V	1039	GLN
1	V	1127	GLN
1	V	1248	GLN
1	W	156	HIS
1	W	266	HIS
1	W	456	HIS
1	W	723	ASN
1	W	788	GLN
1	W	808	HIS
1	W	863	HIS

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Mol	Chain	Res	Type
1	W	866	HIS
1	W	961	HIS
1	W	969	HIS
1	W	1009	HIS
1	W	1037	HIS
1	W	1039	GLN
1	W	1127	GLN
1	X	266	HIS
1	X	429	HIS
1	X	456	HIS
1	X	658	ASN
1	X	717	GLN
1	X	723	ASN
1	X	724	HIS
1	X	777	ASN
1	X	863	HIS
1	X	866	HIS
1	X	961	HIS
1	X	969	HIS
1	X	1004	GLN
1	X	1037	HIS
1	X	1039	GLN
1	X	1117	ASN
1	X	1128	ASN
1	X	1262	HIS
2	Y	68	HIS
2	Z	68	HIS
2	1	68	HIS
1	4	100	HIS
1	4	117	HIS
1	4	186	HIS
1	4	266	HIS
1	4	340	GLN
1	4	456	HIS
1	4	515	HIS
1	4	658	ASN
1	4	717	GLN
1	4	724	HIS
1	4	785	HIS
1	4	961	HIS
1	4	969	HIS
1	4	1004	GLN

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Mol	Chain	Res	Type
1	4	1009	HIS
1	4	1037	HIS
1	4	1258	ASN
3	5	145	GLN
3	5	235	HIS
3	5	356	HIS
4	6	281	HIS
4	7	40	GLN
4	7	193	GLN
4	7	281	HIS
3	8	120	GLN
3	8	135	HIS
3	8	356	HIS
4	a	193	GLN
4	a	242	GLN
3	b	120	GLN
3	b	135	HIS
3	b	235	HIS
3	b	237	HIS
3	b	356	HIS
3	b	369	ASN
3	b	393	ASN
4	d	193	GLN
4	d	208	ASN
3	e	120	GLN
3	e	369	ASN
4	f	238	ASN
4	f	281	HIS
4	g	99	ASN
4	g	124	GLN
4	g	193	GLN
4	g	242	GLN
3	h	120	GLN
3	h	356	HIS
4	i	110	ASN
4	i	208	ASN
4	i	238	ASN
4	j	193	GLN
5	k	157	ASN
5	k	483	HIS
5	k	506	GLN
5	k	586	HIS

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Mol	Chain	Res	Type
6	m	15	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 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.

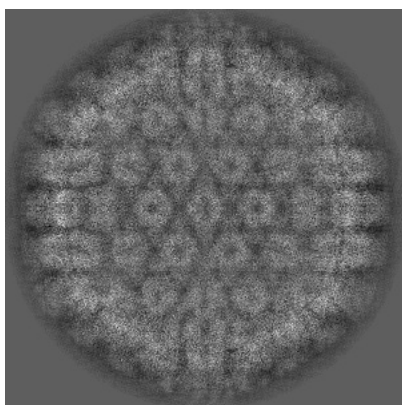
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7472. These allow visual inspection of the internal detail of the map and identification of artifacts.

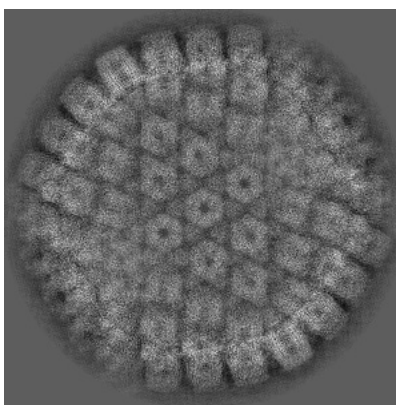
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

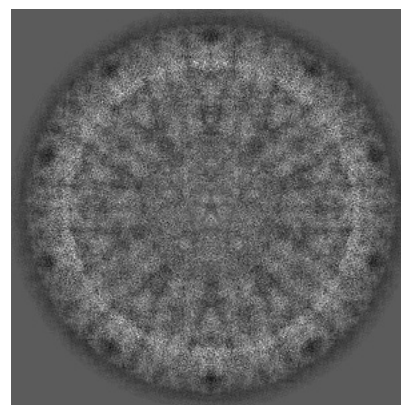
6.1.1 Primary map



X



Y

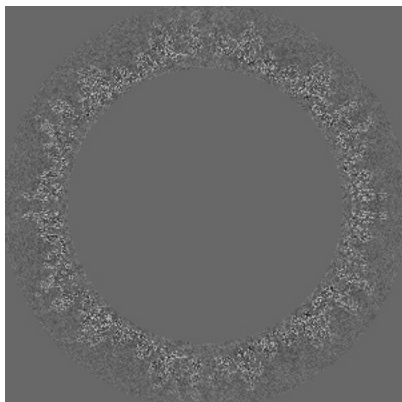


Z

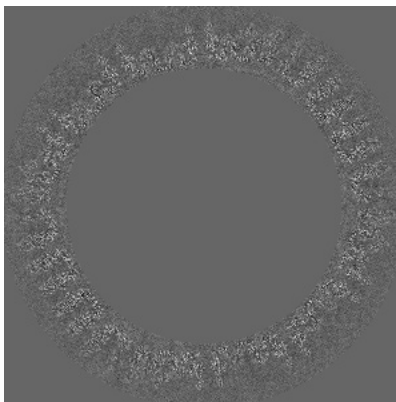
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

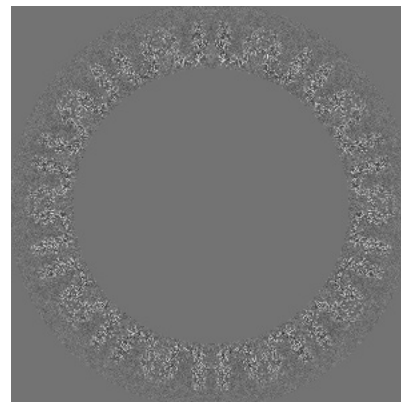
6.2.1 Primary map



X Index: 640



Y Index: 640

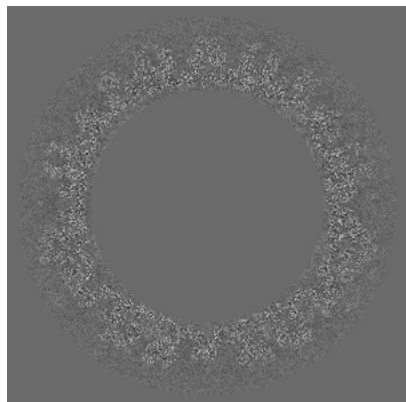


Z Index: 640

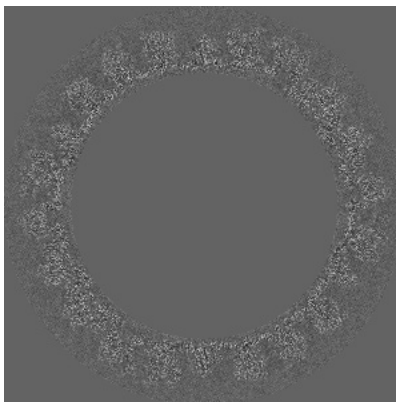
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

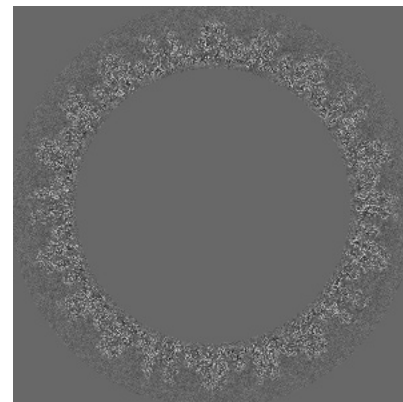
6.3.1 Primary map



X Index: 405



Y Index: 753

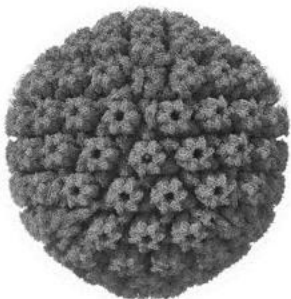


Z Index: 668

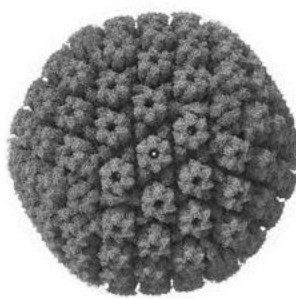
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

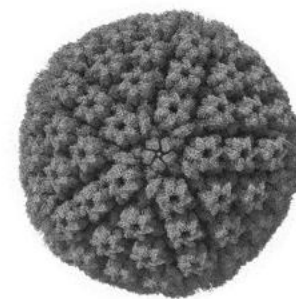
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

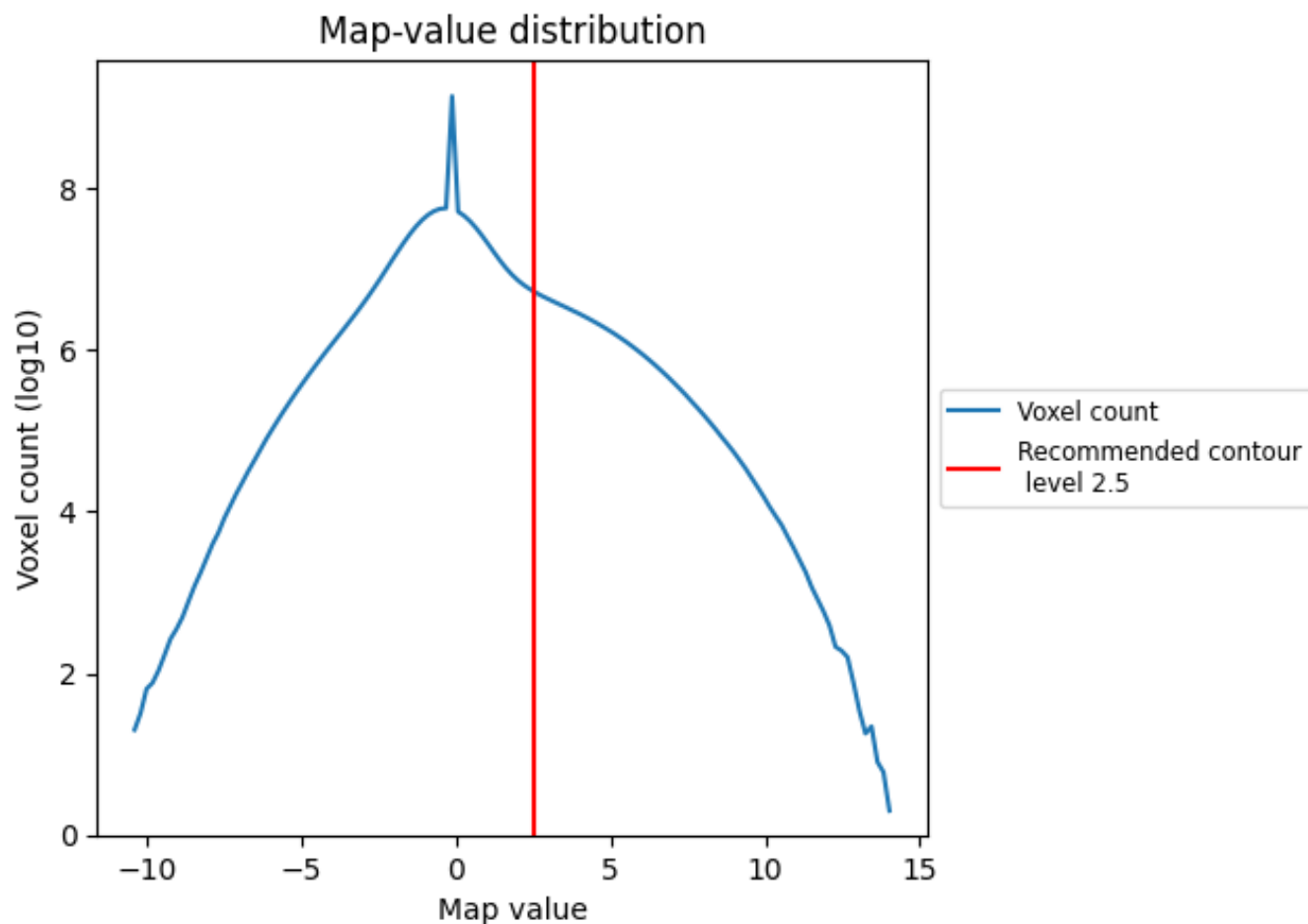
6.5 Mask visualisation

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

7 Map analysis [i](#)

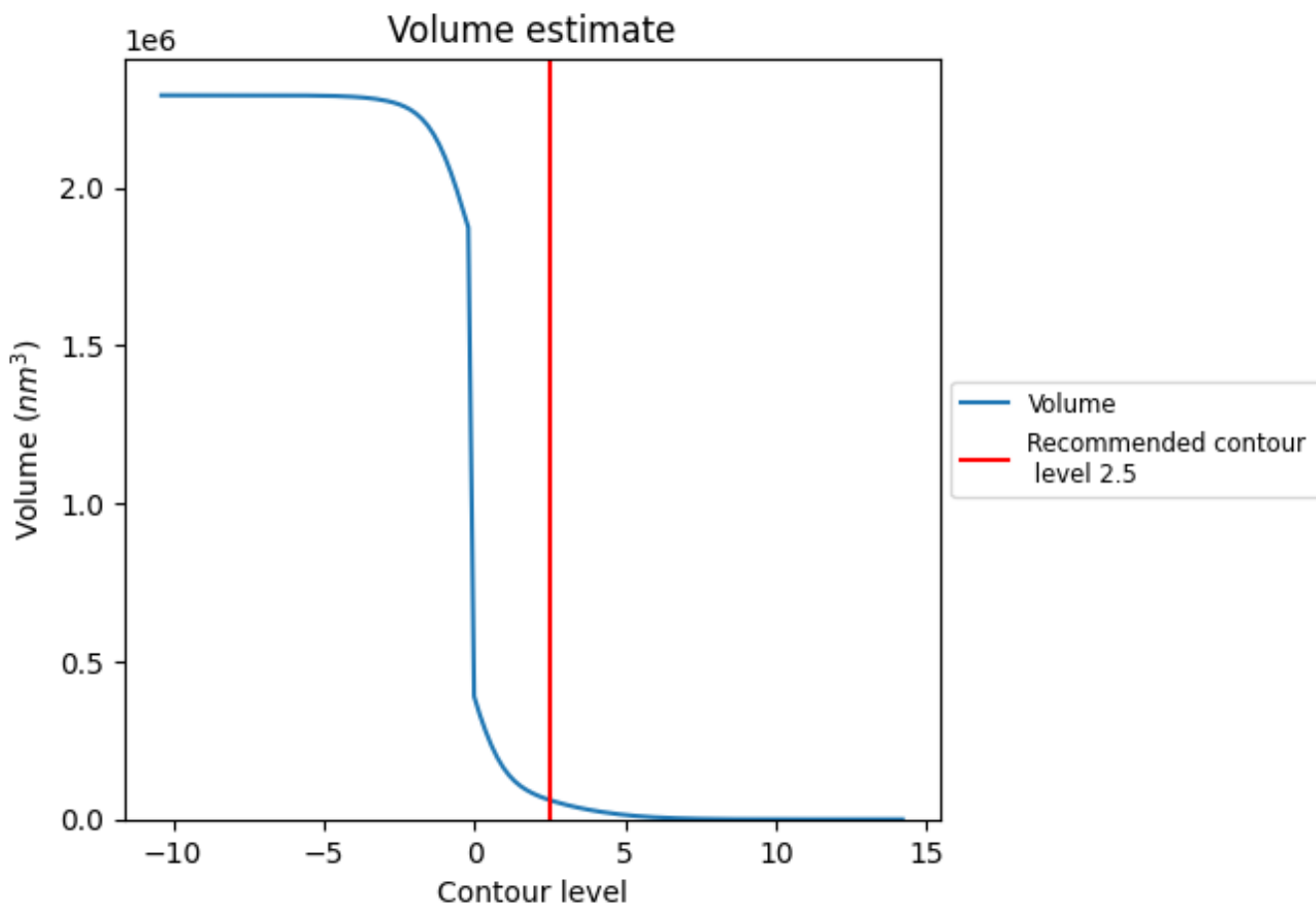
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

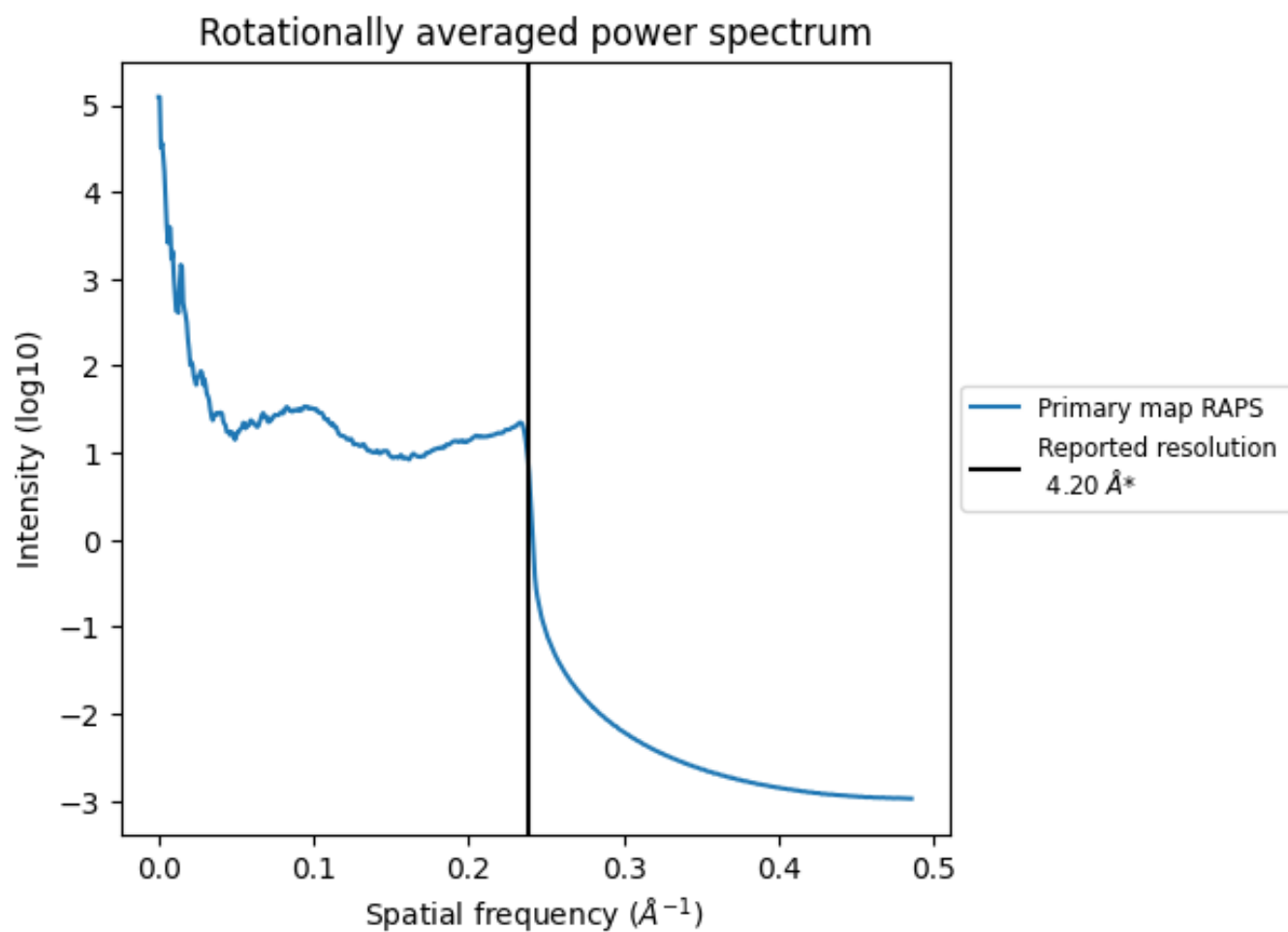
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60862 nm^3 ; this corresponds to an approximate mass of 54978 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 0.238\AA^{-1}

8 Fourier-Shell correlation

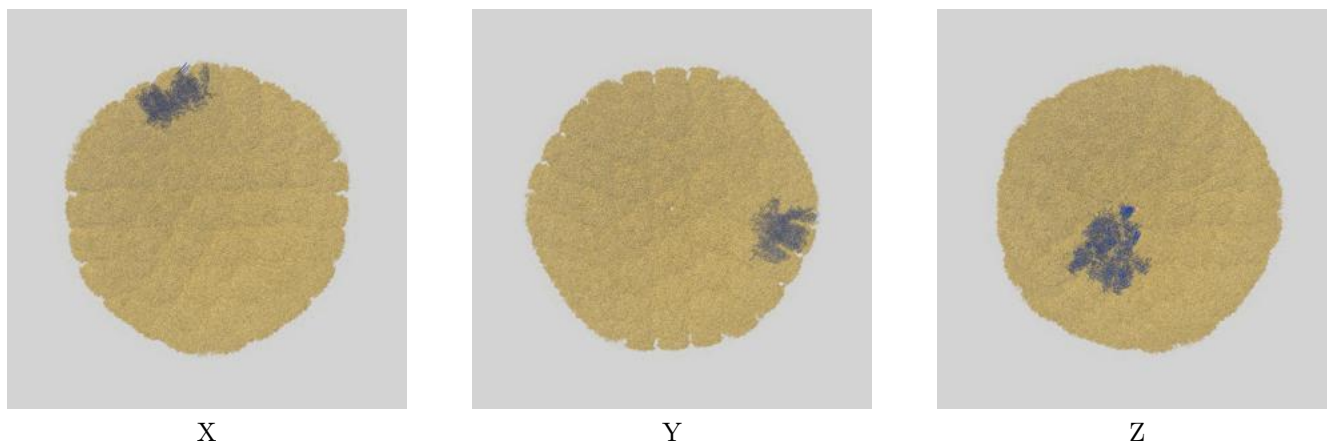
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

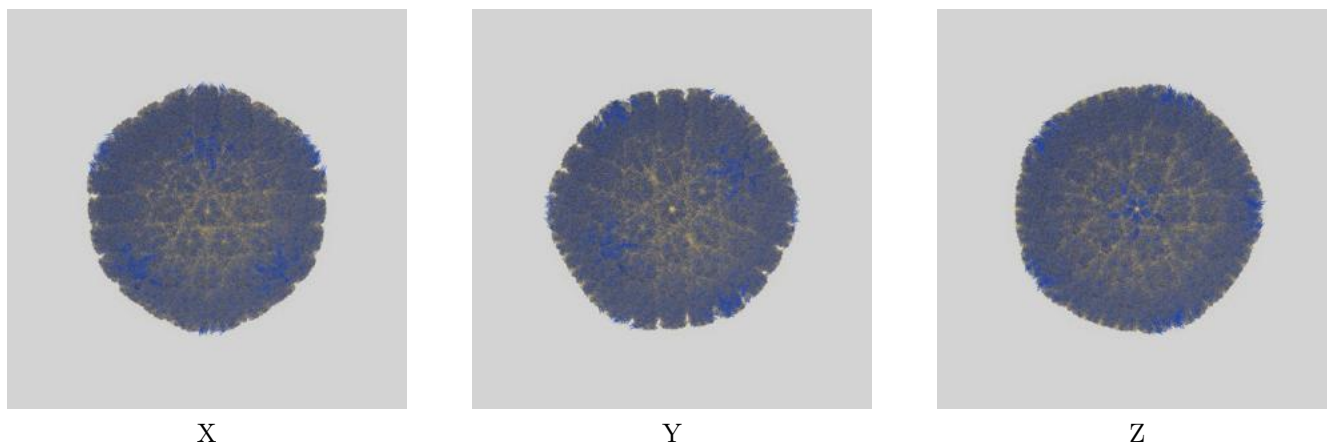
This section contains information regarding the fit between EMDB map EMD-7472 and PDB model 6CGR. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

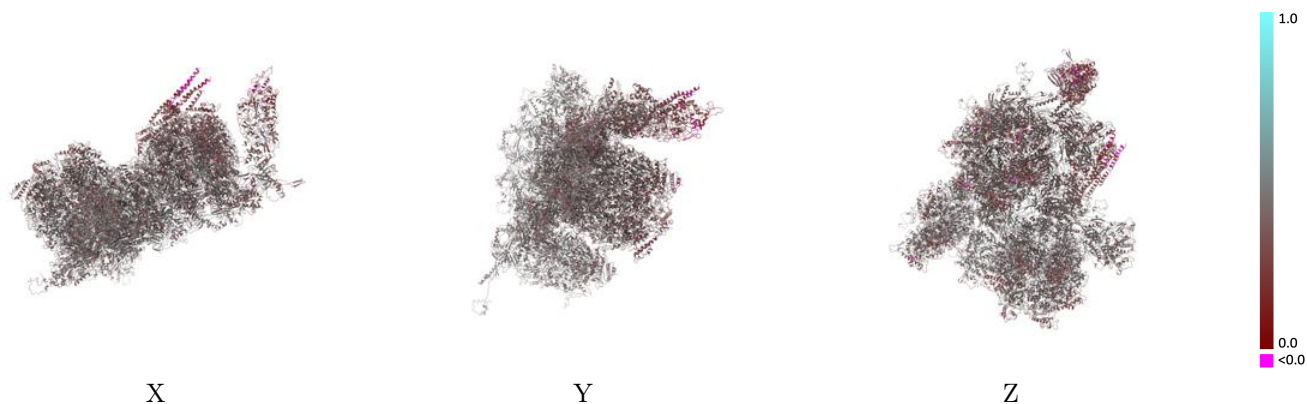


9.1.2 Map-model assembly overlay [i](#)



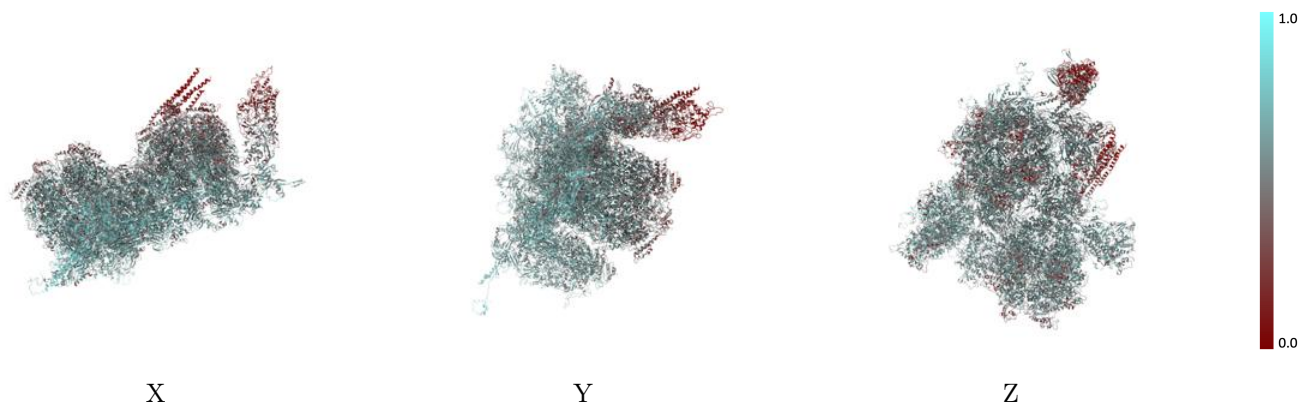
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



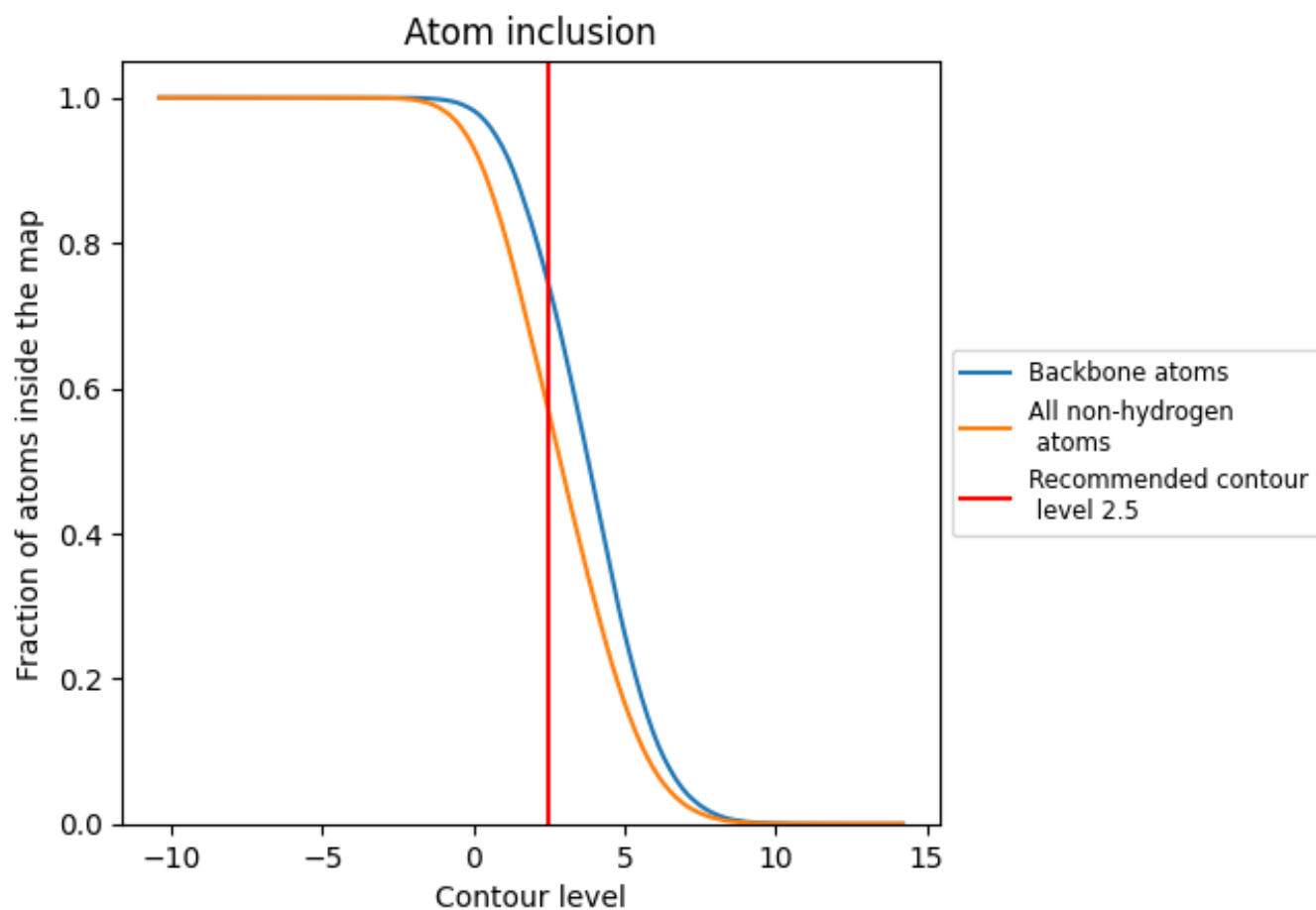
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 57% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5656	 0.3920
0	 0.3439	 0.3060
1	 0.3955	 0.3050
2	 0.3664	 0.2980
3	 0.3611	 0.3360
4	 0.3638	 0.3180
5	 0.5292	 0.3910
6	 0.4635	 0.3550
7	 0.4840	 0.3510
8	 0.6060	 0.4140
9	 0.6134	 0.4020
A	 0.6090	 0.4070
B	 0.6191	 0.4130
C	 0.6008	 0.4070
D	 0.6100	 0.4090
E	 0.5999	 0.4020
F	 0.6034	 0.4090
G	 0.4193	 0.3370
H	 0.4272	 0.3240
I	 0.4140	 0.3400
J	 0.4140	 0.3330
K	 0.3902	 0.2940
L	 0.3968	 0.3340
M	 0.6239	 0.4150
N	 0.6233	 0.4120
O	 0.6211	 0.4140
P	 0.4630	 0.3390
Q	 0.4550	 0.3590
R	 0.4907	 0.3630
S	 0.5516	 0.3880
T	 0.5605	 0.3780
U	 0.5929	 0.4070
V	 0.5955	 0.4050
W	 0.5802	 0.4020
X	 0.5511	 0.3820



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Chain	Atom inclusion	Q-score
Y	 0.3108	 0.3090
Z	 0.3267	 0.3010
a	 0.6107	 0.4070
b	 0.5830	 0.4050
c	 0.5903	 0.4000
d	 0.6168	 0.4090
e	 0.5695	 0.4090
f	 0.5806	 0.4000
g	 0.5712	 0.4010
h	 0.5925	 0.4080
i	 0.5880	 0.3950
j	 0.5949	 0.4030
k	 0.4474	 0.3600
l	 0.3136	 0.3060
m	 0.3386	 0.3010
n	 0.0899	 0.1410
o	 0.1526	 0.1920