



wwPDB EM Validation Summary Report ⓘ

Jun 11, 2025 – 11:05 am BST

PDB ID : 9GTP / pdb_00009gtp
EMDB ID : EMD-51564
Title : Cryo-EM structure of a contractile injection system in *Streptomyces coelicolor*, the baseplate complex in extended state applied 6-fold symmetry.
Authors : Casu, B.; Sallmen, J.W.; Haas, P.E.; Afanasyev, P.; Xu, J.; Schlimpert, S.; Pilhofer, M.
Deposited on : 2024-09-18
Resolution : 3.50 Å(reported)

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 ⓘ 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

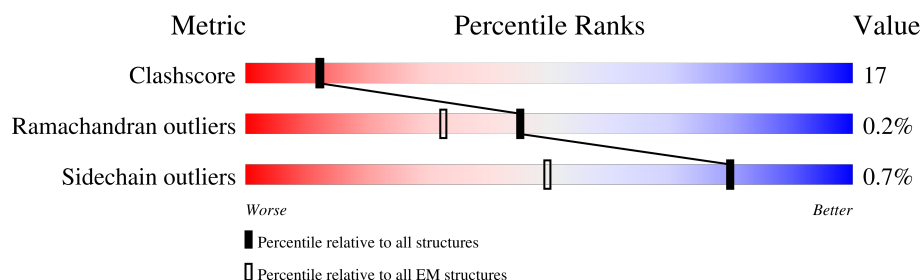
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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




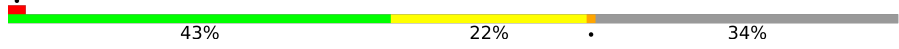
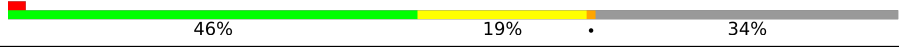
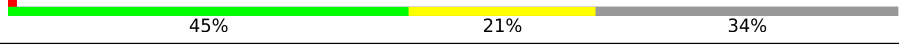



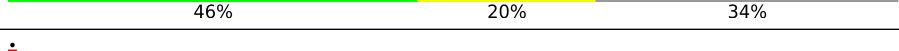
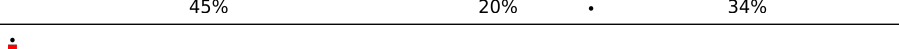
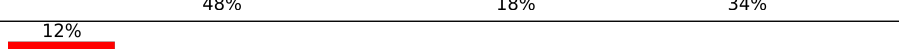

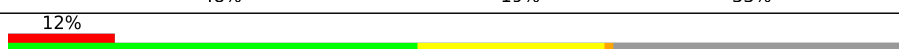
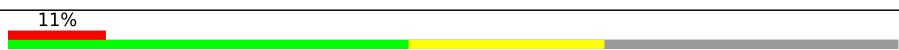
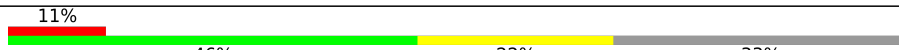
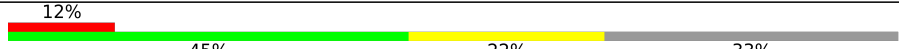





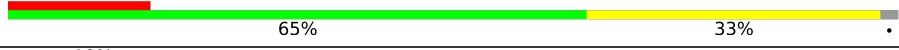
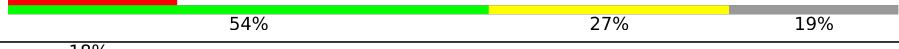



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	k	149	
1	l	149	
1	m	149	
1	n	149	
1	o	149	
1	p	149	
2	1e	534	
2	1f	534	

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Mol	Chain	Length	Quality of chain
2	1g	534	
2	1h	534	
2	1i	534	
2	1j	534	
2	2e	534	
2	2f	534	
2	2g	534	
2	2h	534	
2	2i	534	
2	2j	534	
2	3e	534	
2	3f	534	
2	3g	534	
2	3h	534	
2	3i	534	
2	3j	534	
3	1G	652	
3	1H	652	
3	1J	652	
3	1K	652	
3	1L	652	
3	1l	652	
3	2G	652	
3	2H	652	
3	2J	652	

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Mol	Chain	Length	Quality of chain
3	2K	652	
3	2L	652	
3	2I	652	
4	M	240	
4	N	240	
4	O	240	
4	P	240	
4	Q	240	
4	R	240	
5	A	190	
5	B	190	
5	C	190	
5	D	190	
5	E	190	
5	F	190	
6	S	150	
6	T	150	
6	U	150	
6	V	150	
6	W	150	
6	X	150	
7	a	140	
7	b	140	
7	c	140	
7	d	140	

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Mol	Chain	Length	Quality of chain
7	e	140	<div><div></div><div>69%</div><div>31%</div><div></div></div>
7	f	140	<div><div></div><div>63%</div><div>37%</div><div></div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 140250 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 Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
1	p	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
1	k	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
1	l	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
1	m	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		
1	n	149	Total	C	N	O	S	0	0
			1152	717	200	227	8		

- Molecule 2 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1h	350	Total	C	N	O	S	0	0
			2716	1723	481	505	7		
2	2i	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3i	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		
2	1i	351	Total	C	N	O	S	0	0
			2721	1726	482	506	7		
2	2j	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3j	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		
2	1j	351	Total	C	N	O	S	0	0
			2721	1726	482	506	7		
2	2e	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3e	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	1e	351	Total	C	N	O	S	0	0
			2721	1726	482	506	7		
2	2f	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3f	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		
2	1f	350	Total	C	N	O	S	0	0
			2714	1722	481	504	7		
2	2g	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3g	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		
2	1g	351	Total	C	N	O	S	0	0
			2721	1726	482	506	7		
2	2h	352	Total	C	N	O	S	0	0
			2725	1728	483	507	7		
2	3h	359	Total	C	N	O	S	0	0
			2787	1774	493	513	7		

- Molecule 3 is a protein called Baseplate protein J-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1K	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2K	528	Total	C	N	O	S	0	0
			4028	2504	740	774	10		
3	1L	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2L	528	Total	C	N	O	S	0	0
			4028	2504	740	774	10		
3	1G	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2G	528	Total	C	N	O	S	0	0
			4028	2504	740	774	10		
3	1H	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2H	528	Total	C	N	O	S	0	0
			4028	2504	740	774	10		
3	1I	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2I	528	Total	C	N	O	S	0	0
			4028	2504	740	774	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1J	639	Total	C	N	O	S	0	0
			4886	3043	896	937	10		
3	2J	528	Total	C	N	O	S	0	0
			4022	2501	737	774	10		

- Molecule 4 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		
4	Q	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		
4	R	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		
4	M	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		
4	N	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		
4	O	225	Total	C	N	O	S	0	0
			1704	1083	295	318	8		

- Molecule 5 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		
5	F	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		
5	A	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		
5	B	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		
5	C	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		
5	D	179	Total	C	N	O	S	0	0
			1338	849	238	247	4		

- Molecule 6 is a protein called IraD/Gp25-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	122	Total	C	N	O	S	0	0
			965	612	169	181	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	122	Total 965	C 612	N 169	O 181	S 3	0	0
6	X	122	Total 965	C 612	N 169	O 181	S 3	0	0
6	S	122	Total 965	C 612	N 169	O 181	S 3	0	0
6	T	122	Total 965	C 612	N 169	O 181	S 3	0	0
6	U	122	Total 965	C 612	N 169	O 181	S 3	0	0

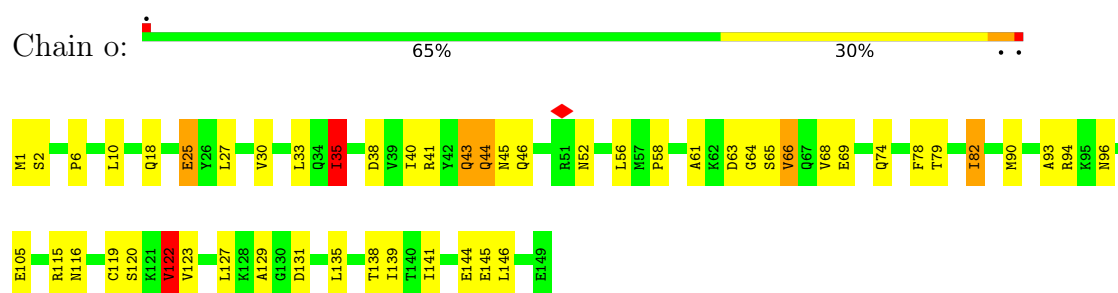
- Molecule 7 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	140	Total 1072	C 673	N 189	O 208	S 2	0	0
7	b	140	Total 1072	C 673	N 189	O 208	S 2	0	0
7	c	140	Total 1072	C 673	N 189	O 208	S 2	0	0
7	d	140	Total 1072	C 673	N 189	O 208	S 2	0	0
7	e	140	Total 1072	C 673	N 189	O 208	S 2	0	0
7	f	140	Total 1072	C 673	N 189	O 208	S 2	0	0

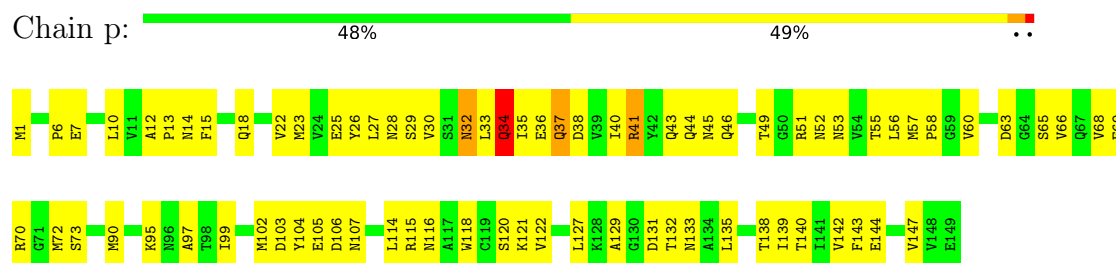
3 Residue-property plots [i](#)

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.

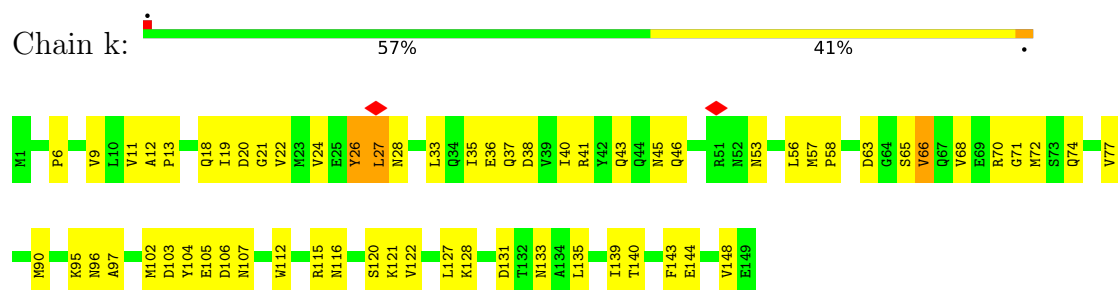
- Molecule 1: Phage tail protein



- Molecule 1: Phage tail protein



- Molecule 1: Phage tail protein

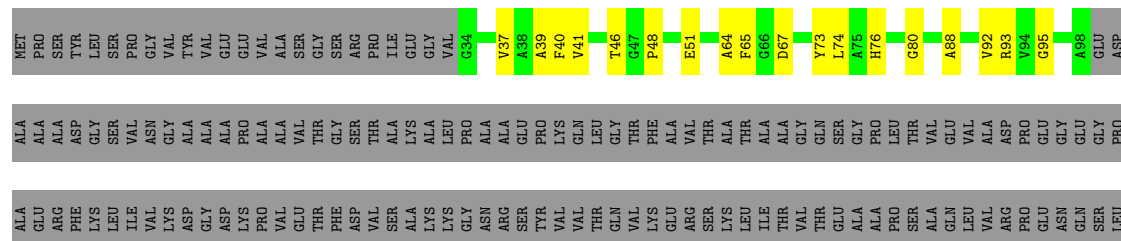


- Molecule 1: Phage tail protein



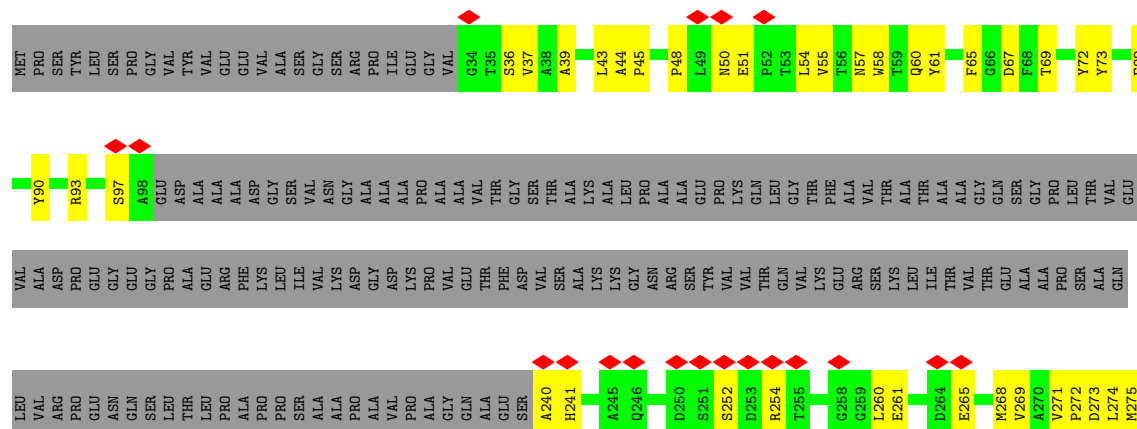
- Molecule 2: Phage tail sheath family protein

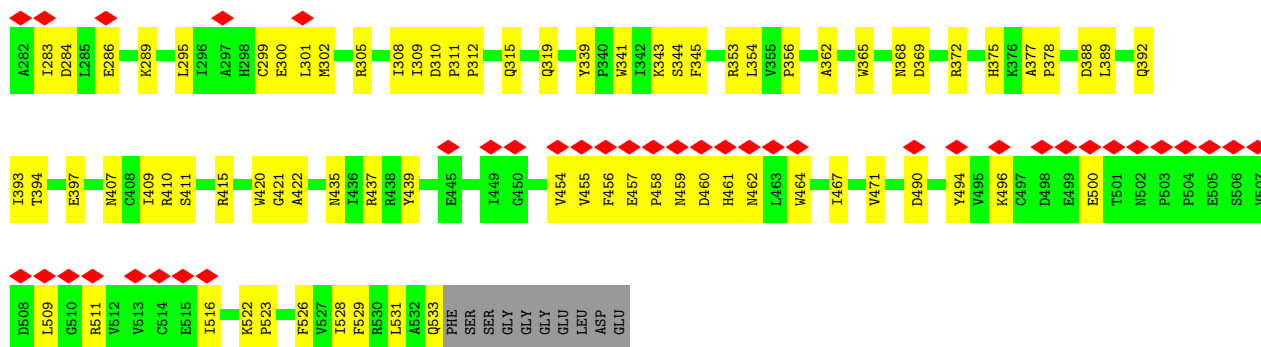
Chain 2i:



- Molecule 2: Phage tail sheath family protein

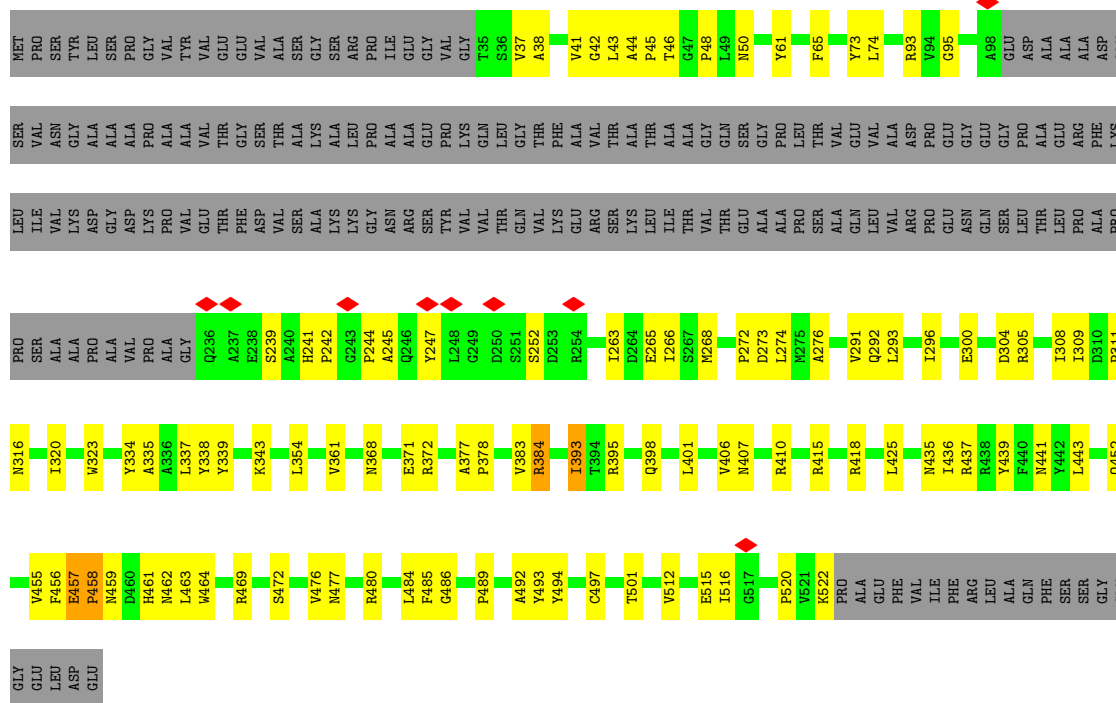
Chain 3i:





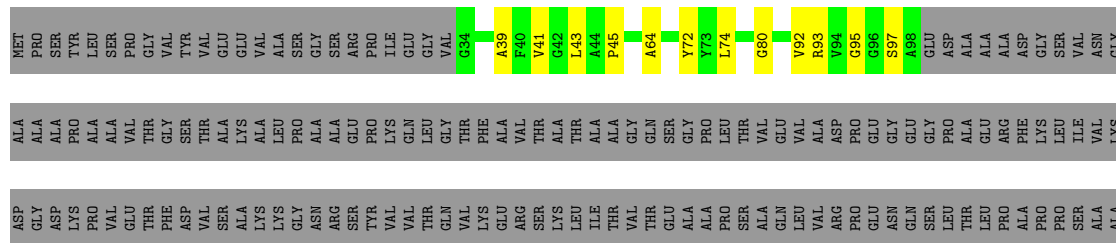
• Molecule 2: Phage tail sheath family protein

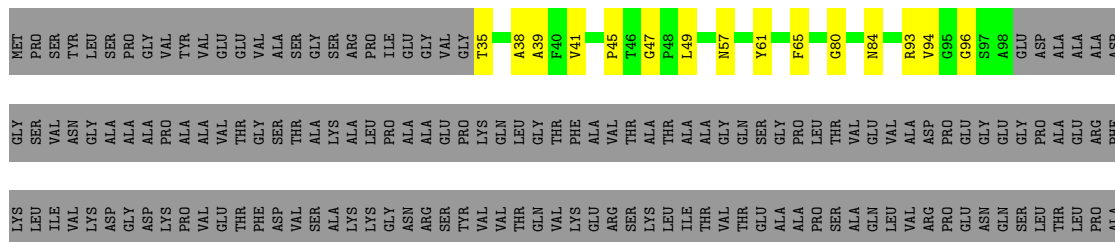
Chain 1i: 46% 19% 34%



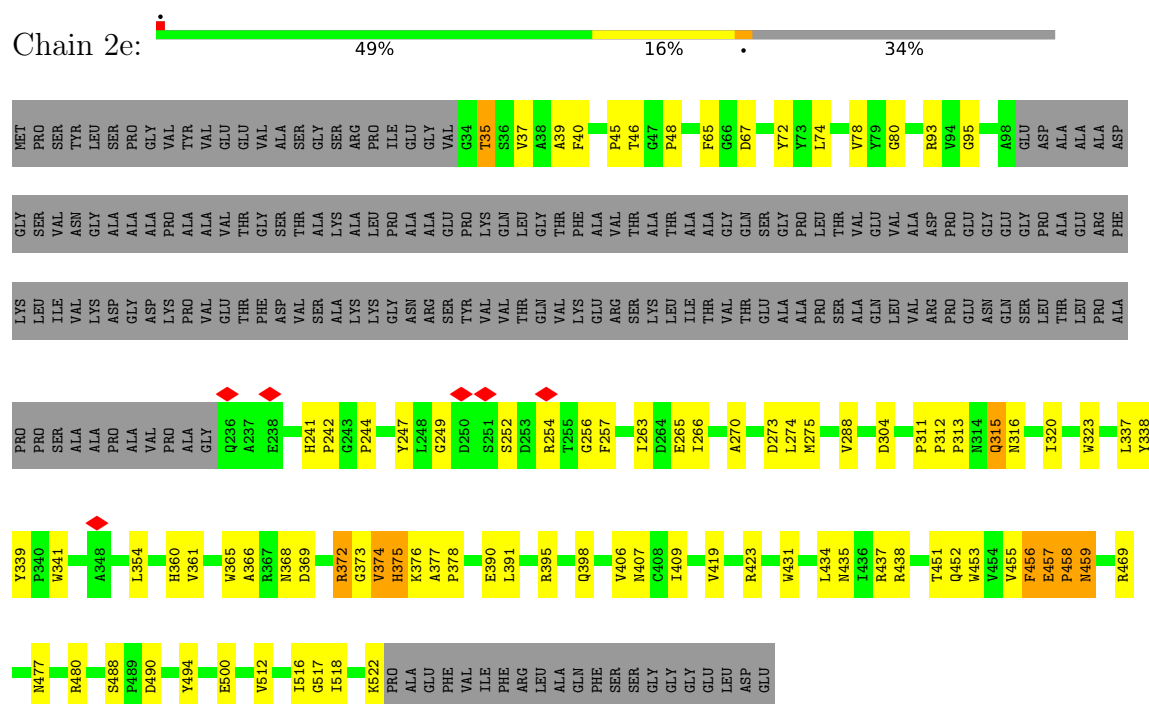
• Molecule 2: Phage tail sheath family protein

Chain 2j: 48% 18% 34%

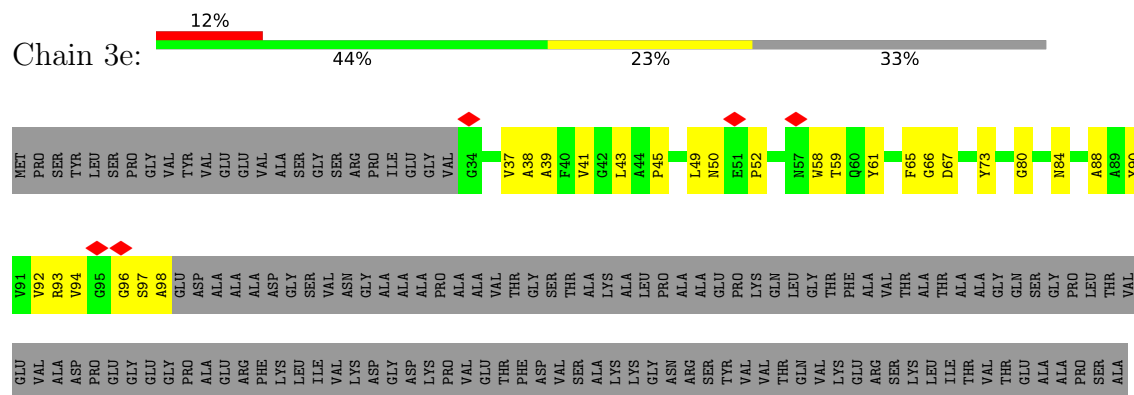


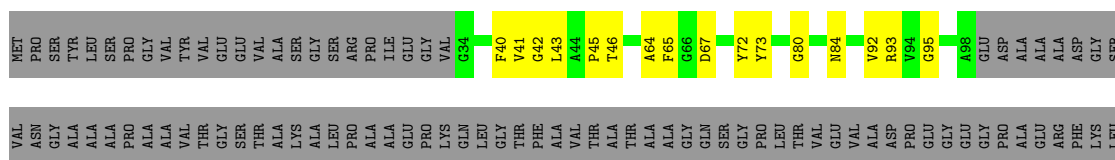


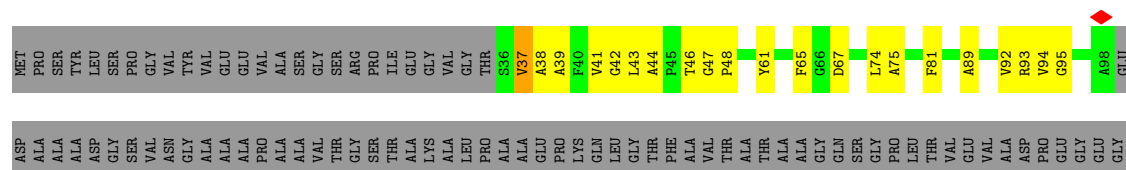
- Molecule 2: Phage tail sheath family protein

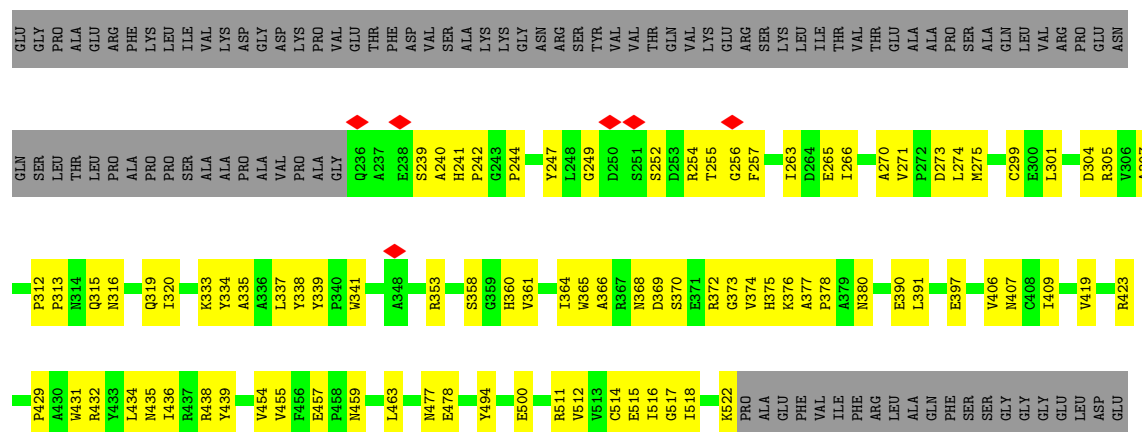


- Molecule 2: Phage tail sheath family protein

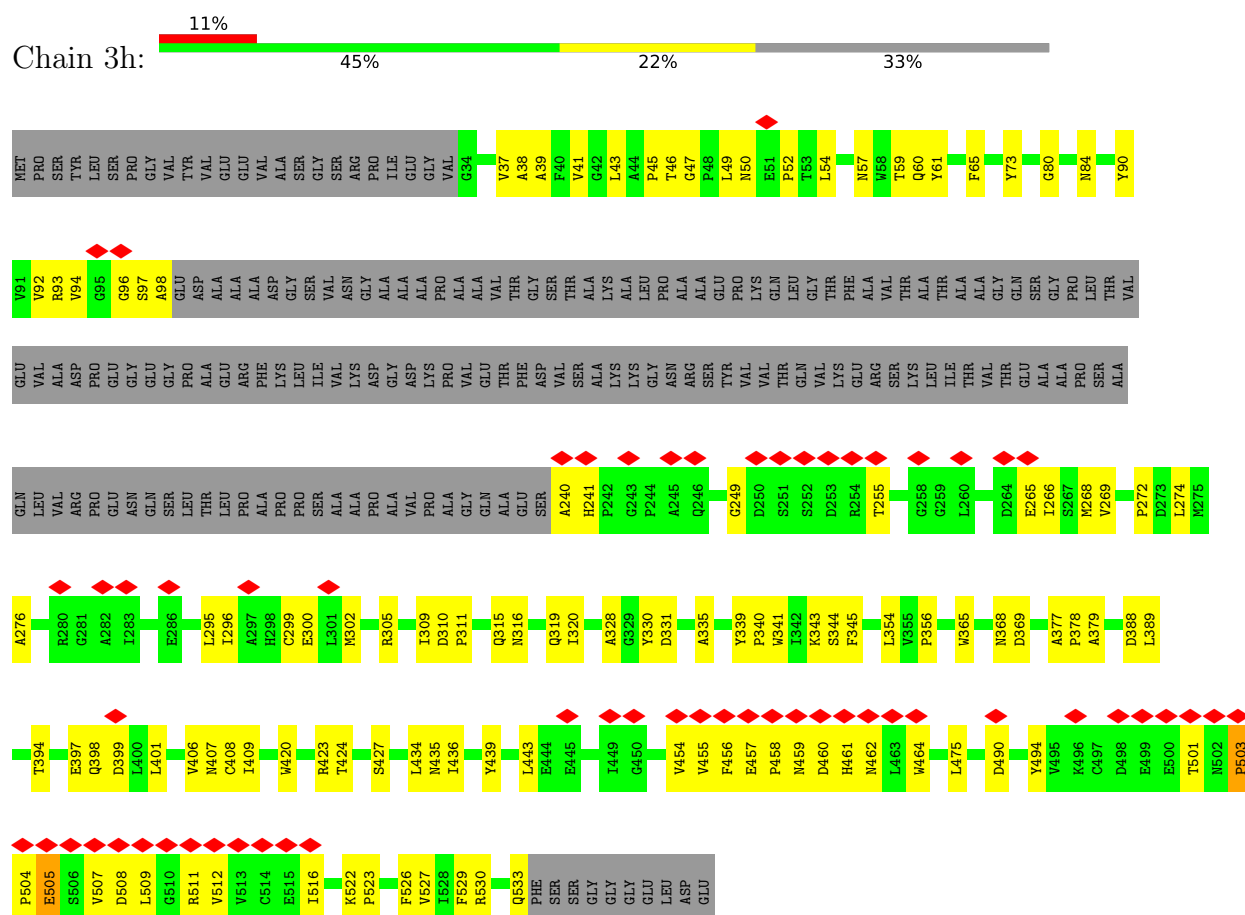




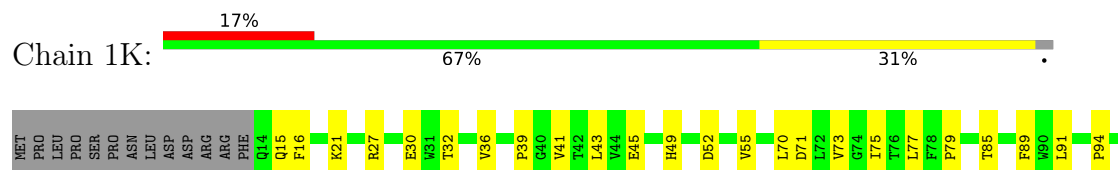


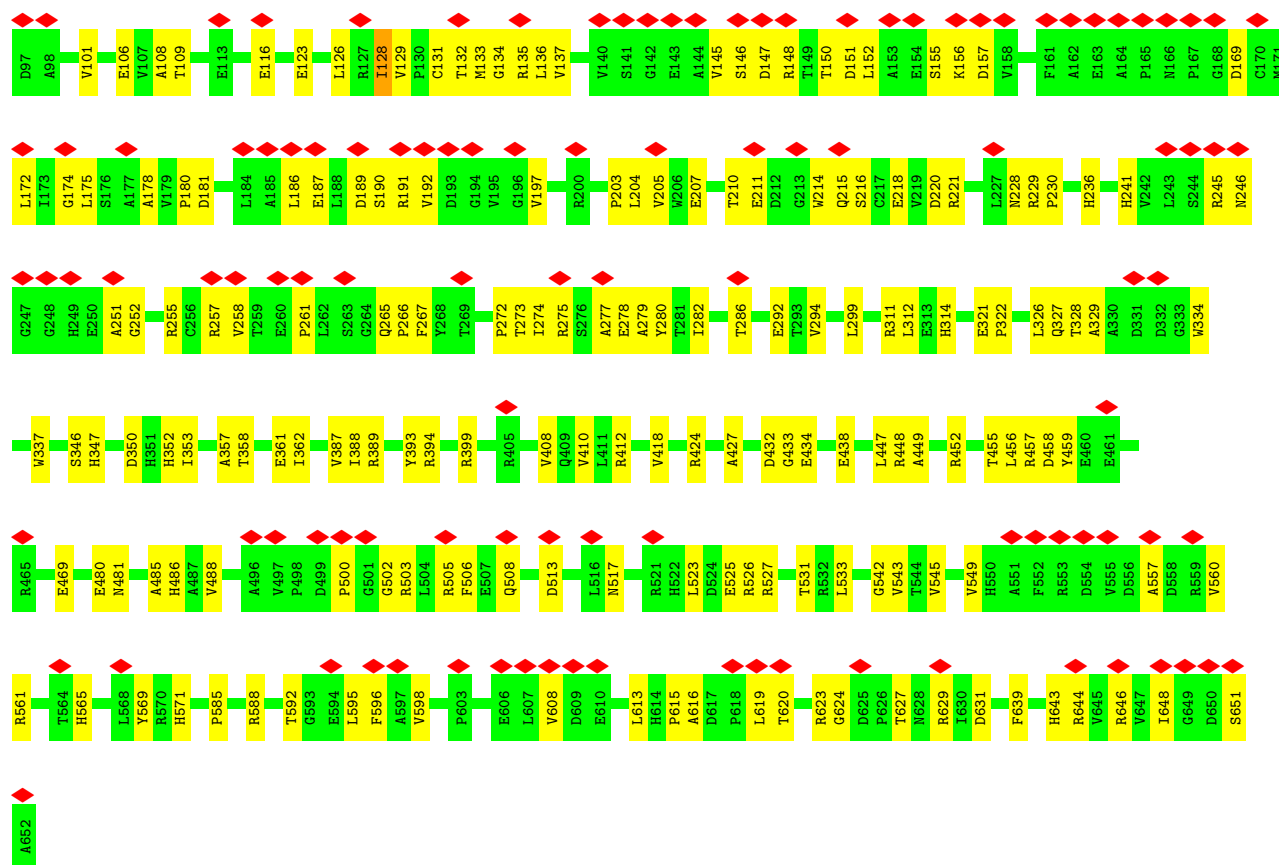


• Molecule 2: Phage tail sheath family protein

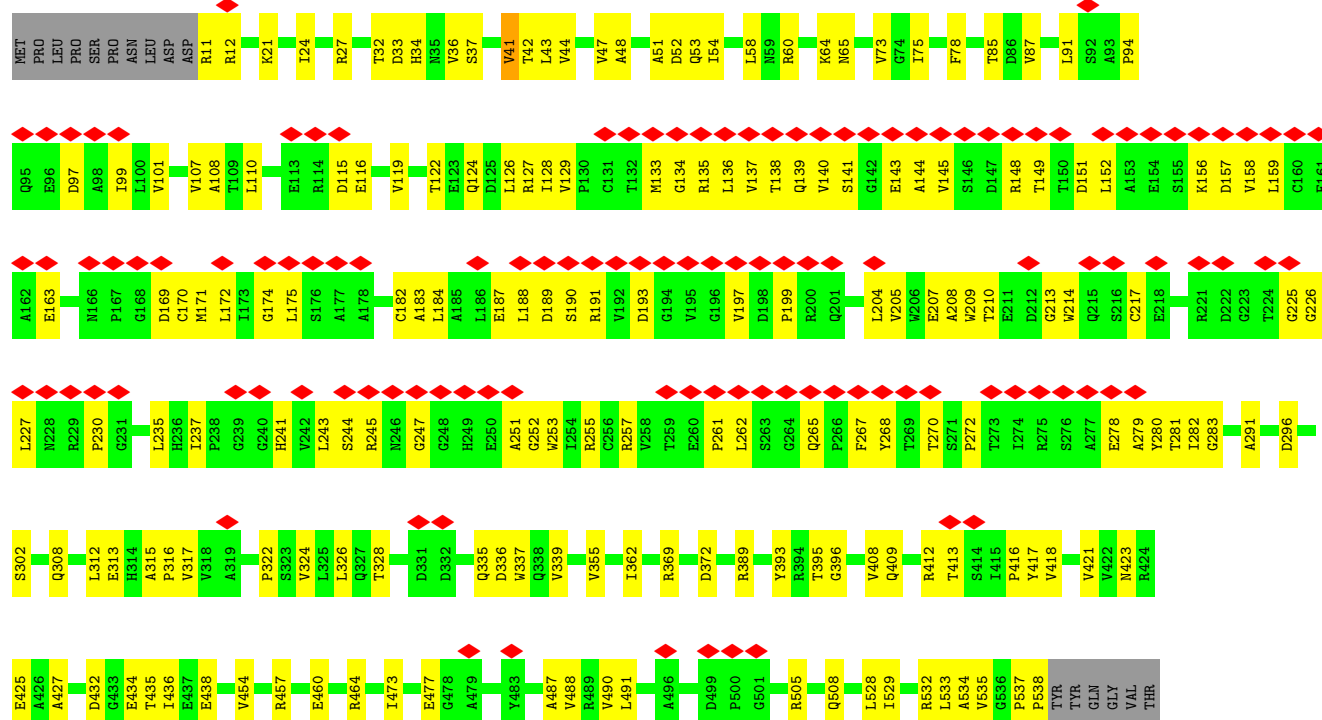


• Molecule 3: Baseplate protein J-like domain-containing protein

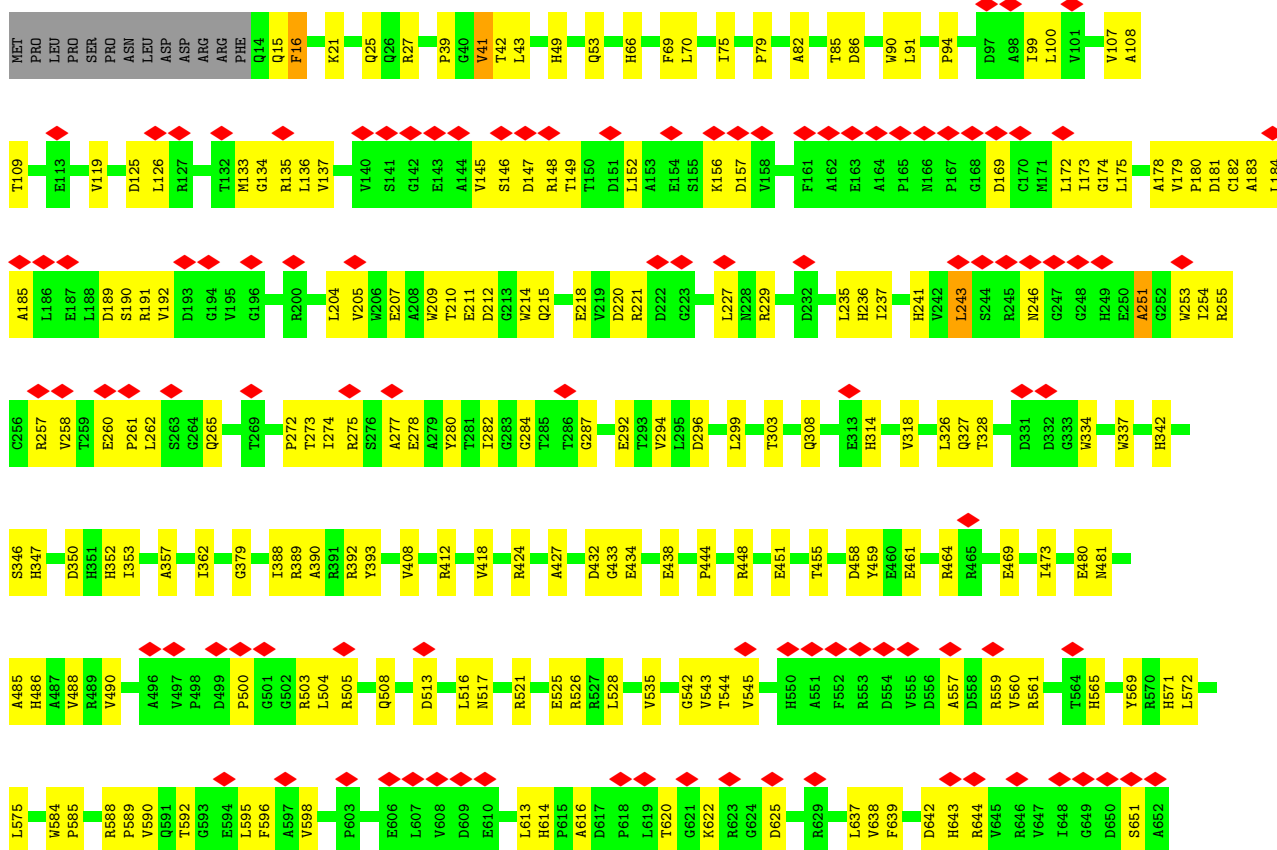




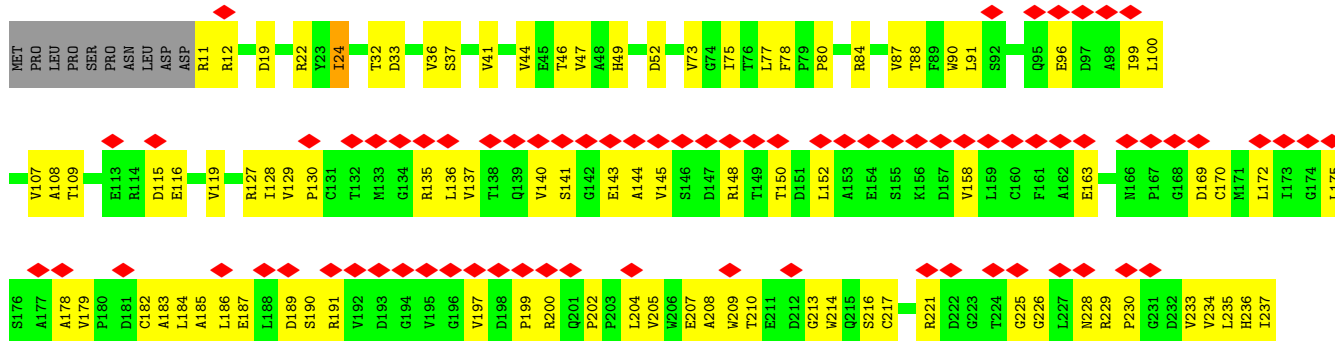
• Molecule 3: Baseplate protein J-like domain-containing protein



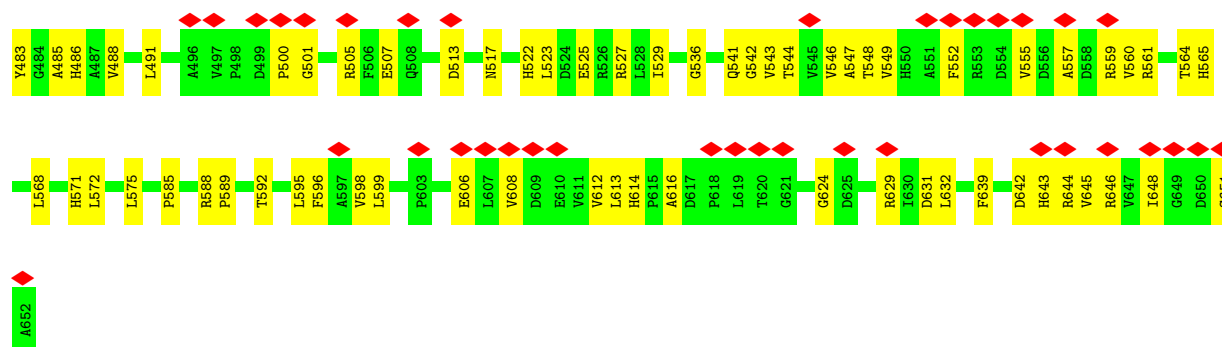
- Molecule 3: Baseplate protein J-like domain-containing protein



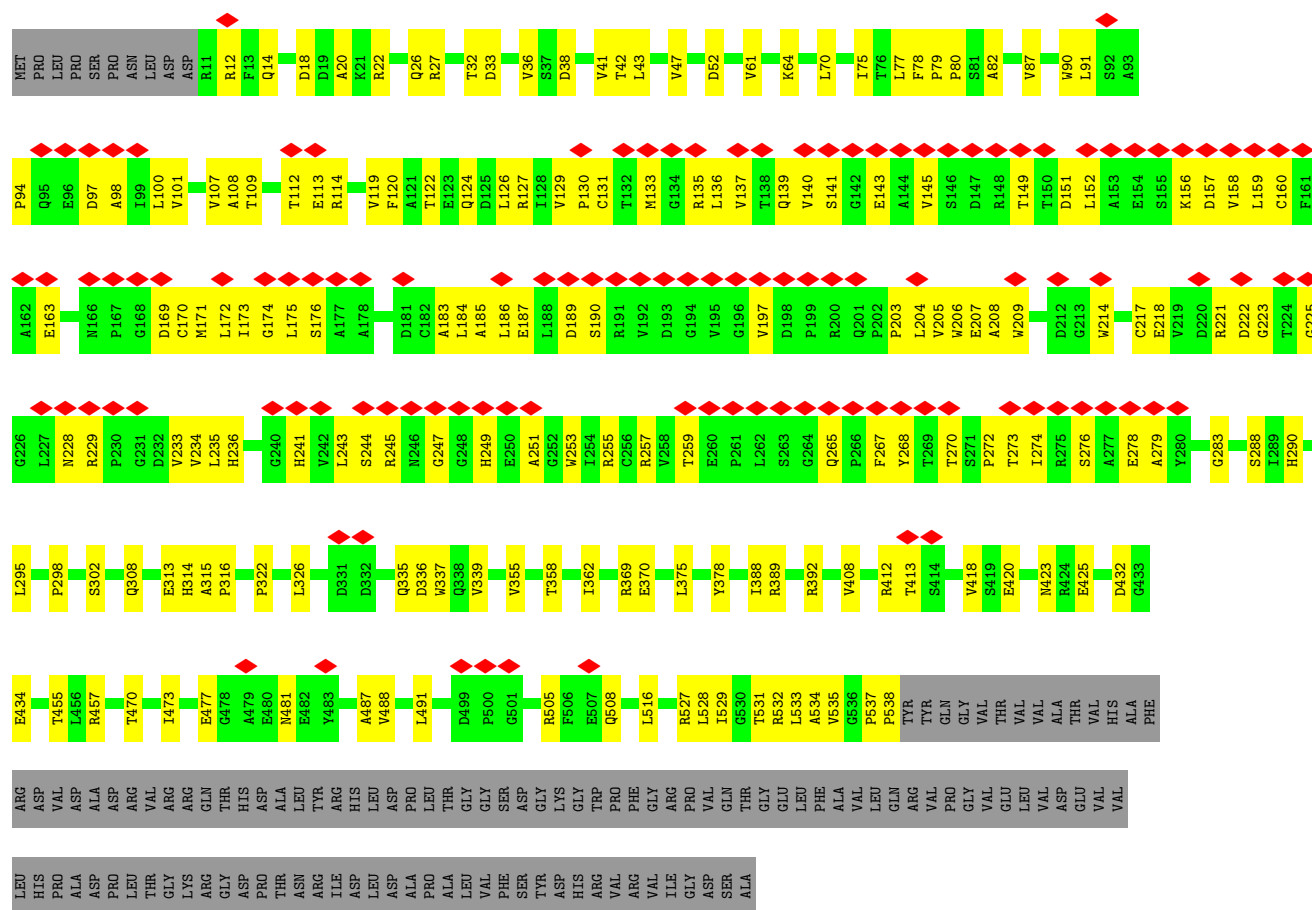
- Molecule 3: Baseplate protein J-like domain-containing protein





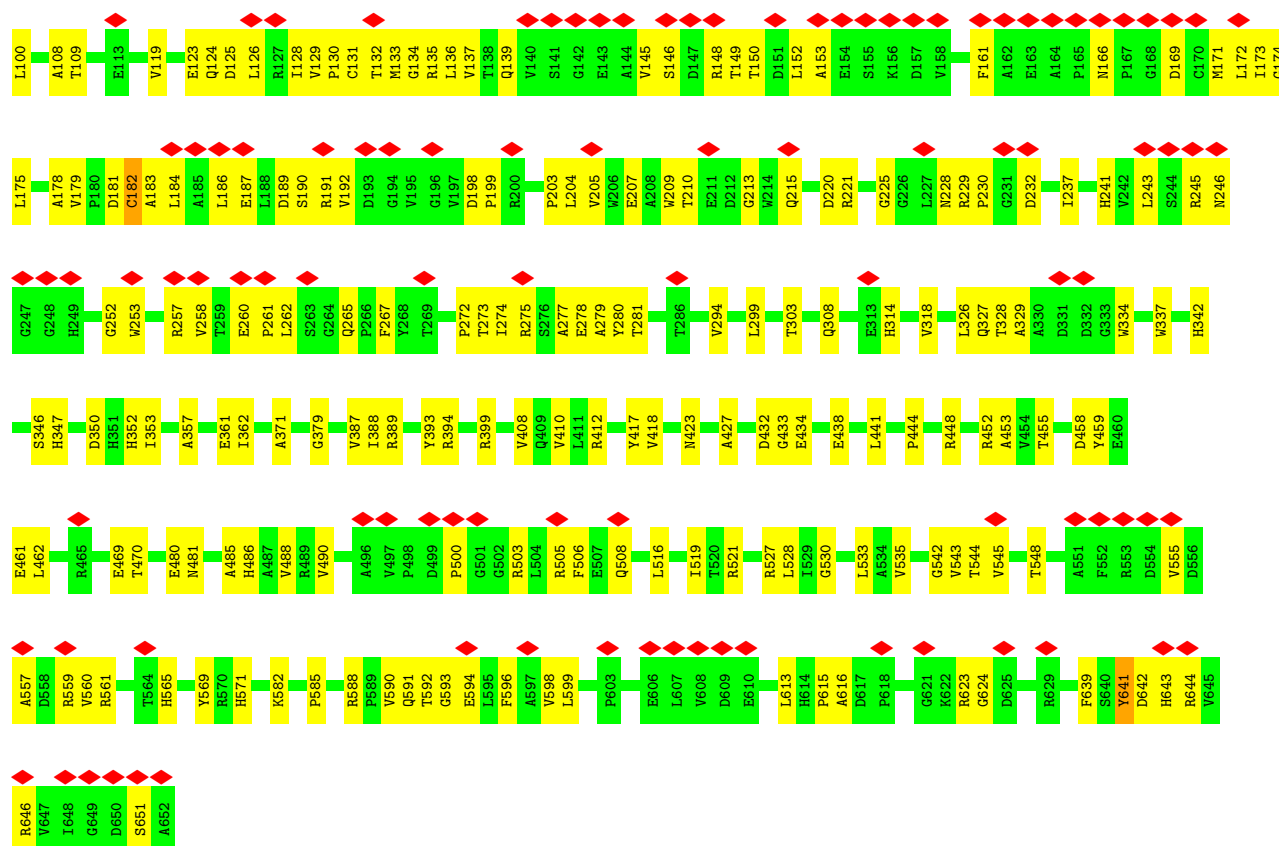


• Molecule 3: Baseplate protein J-like domain-containing protein

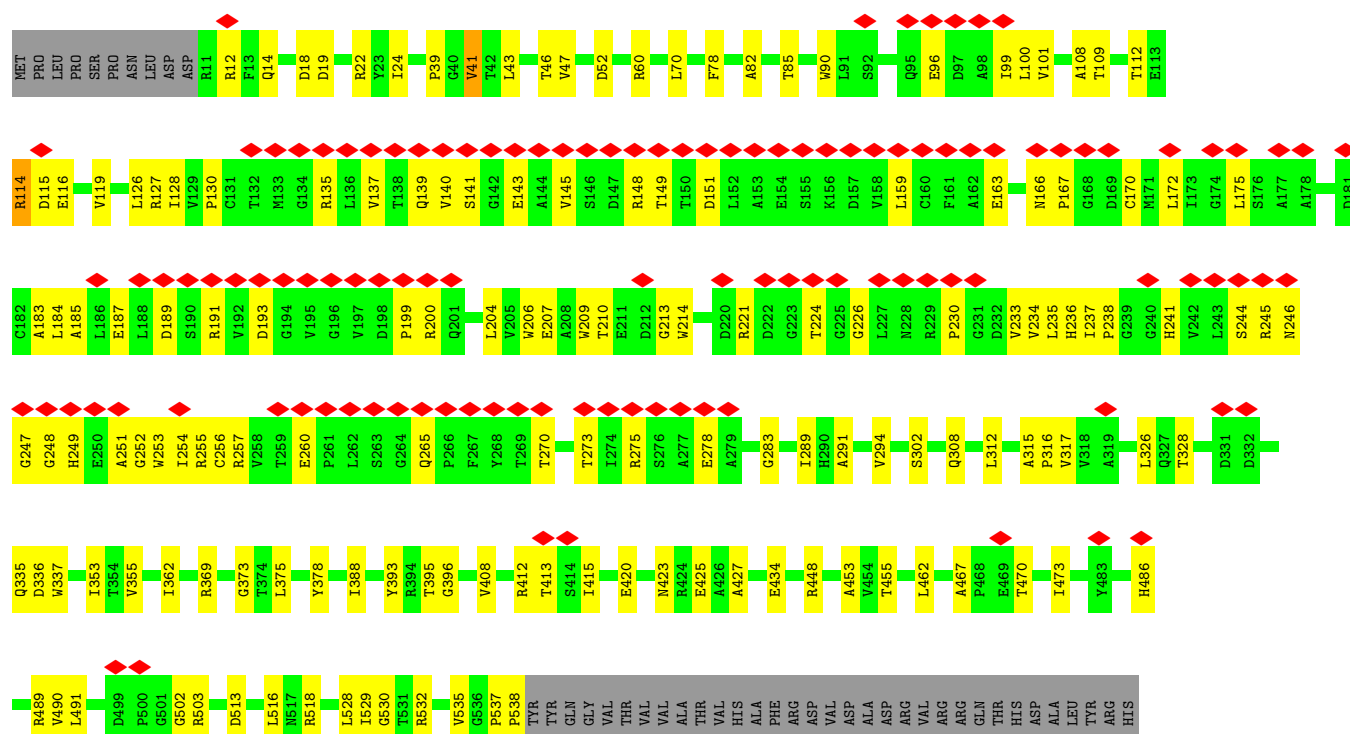


• Molecule 3: Baseplate protein J-like domain-containing protein

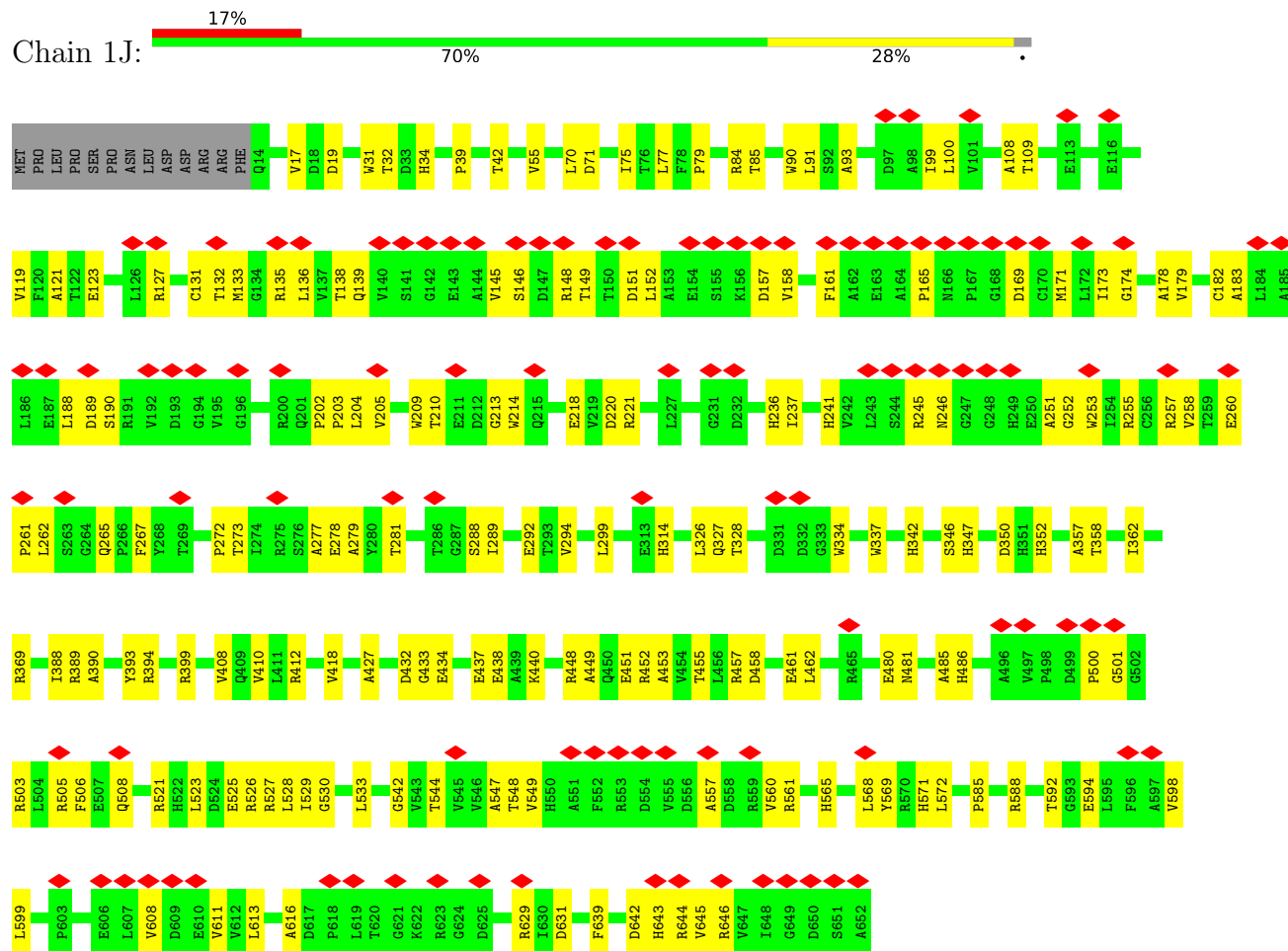




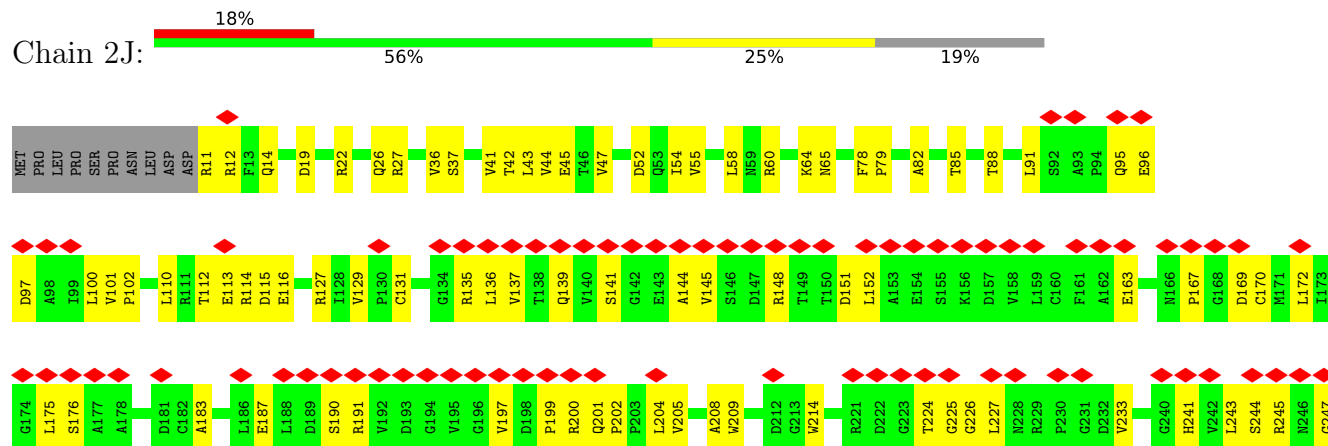
• Molecule 3: Baseplate protein J-like domain-containing protein

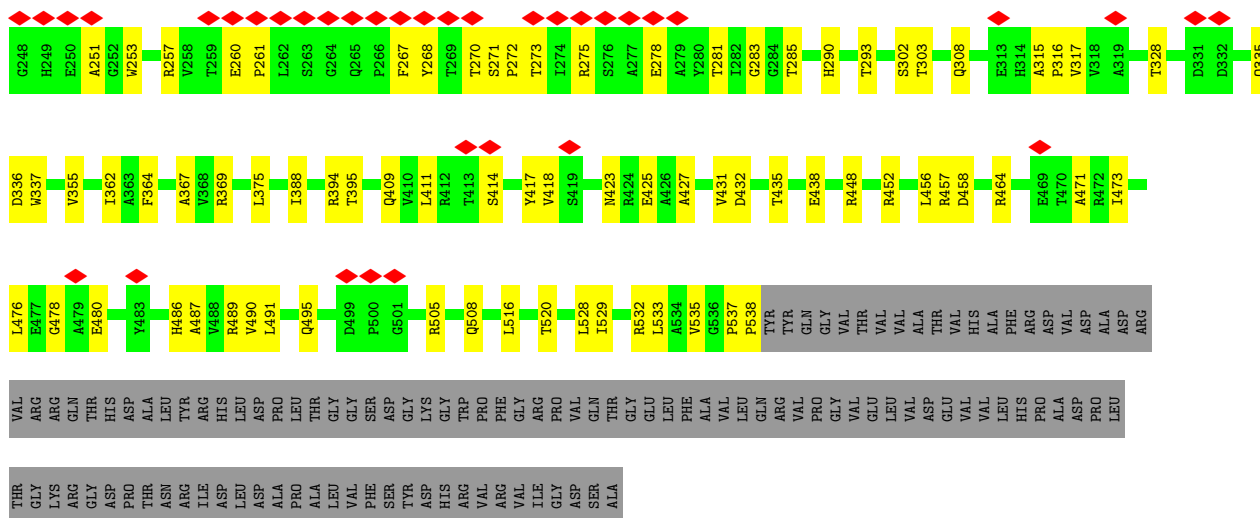


- Molecule 3: Baseplate protein J-like domain-containing protein



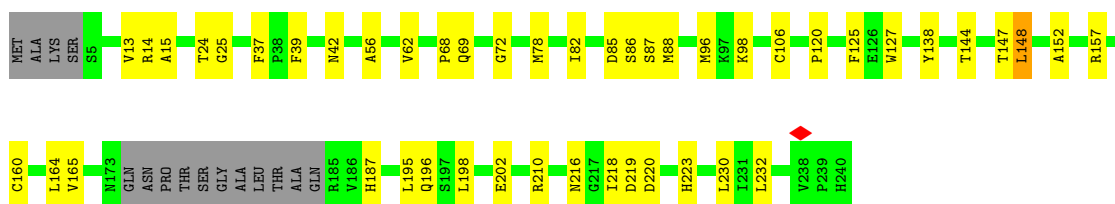
- Molecule 3: Baseplate protein J-like domain-containing protein





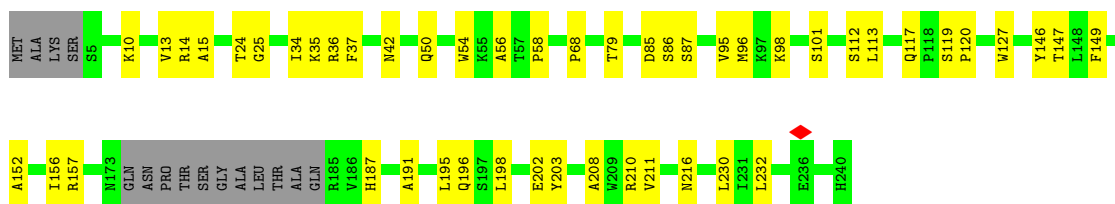
• Molecule 4: LysM domain-containing protein

Chain P: 74% 19% 6%



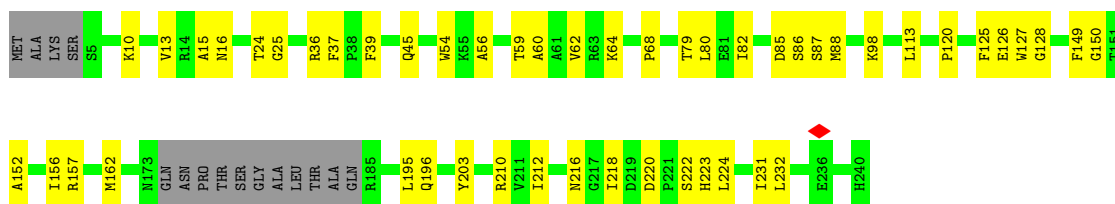
• Molecule 4: LysM domain-containing protein

Chain Q: 73% 20% 6%



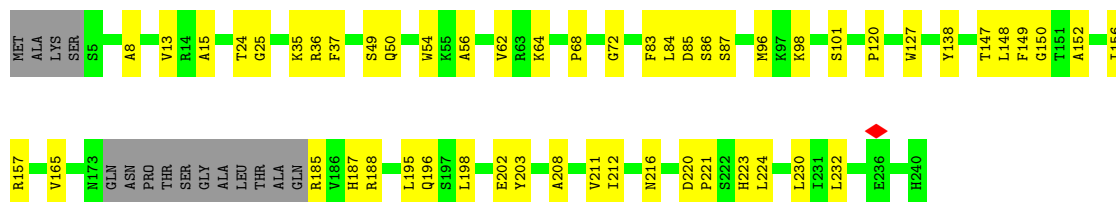
• Molecule 4: LysM domain-containing protein

Chain R: 73% 21% 6%



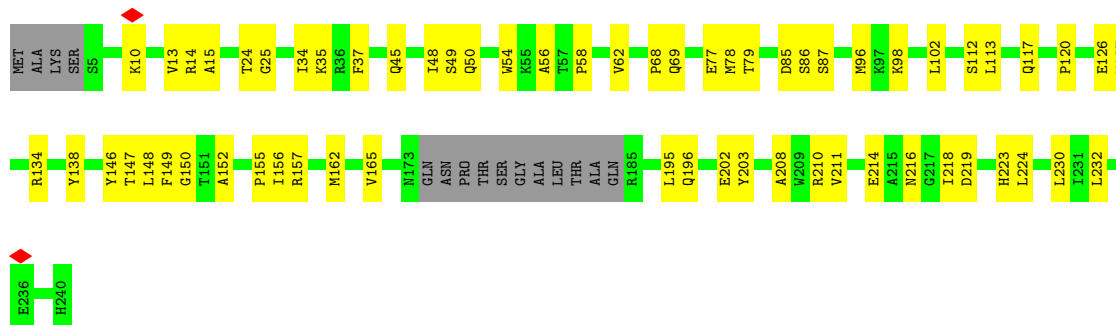
• Molecule 4: LysM domain-containing protein

Chain M:  72% 22% 6%



- Molecule 4: LysM domain-containing protein

Chain N:  68% 26% 6%



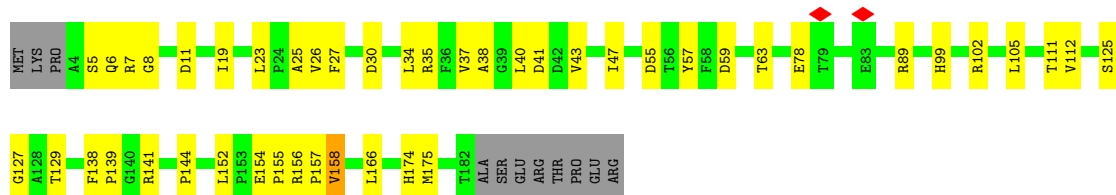
- Molecule 4: LysM domain-containing protein

Chain O:  73% 21% 6%



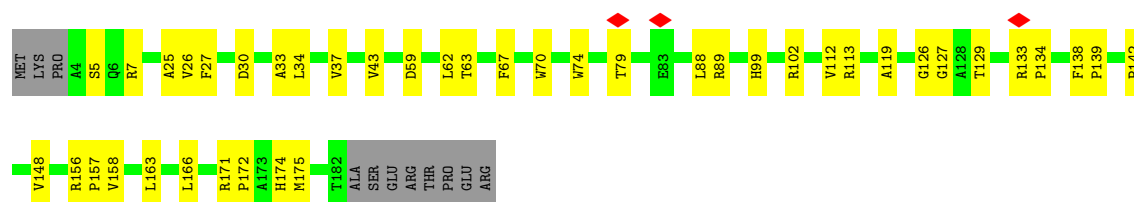
- Molecule 5: Secreted protein

Chain E:  70% 24% 6%

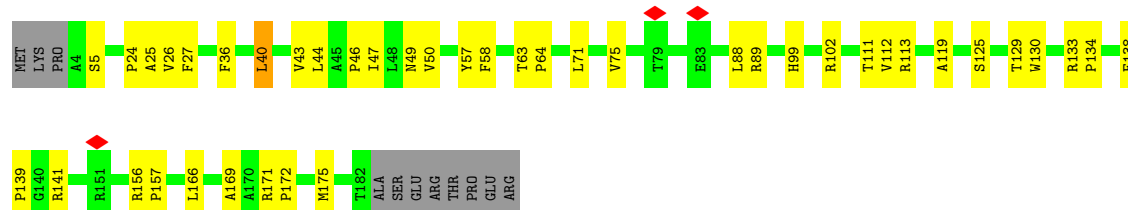


- Molecule 5: Secreted protein

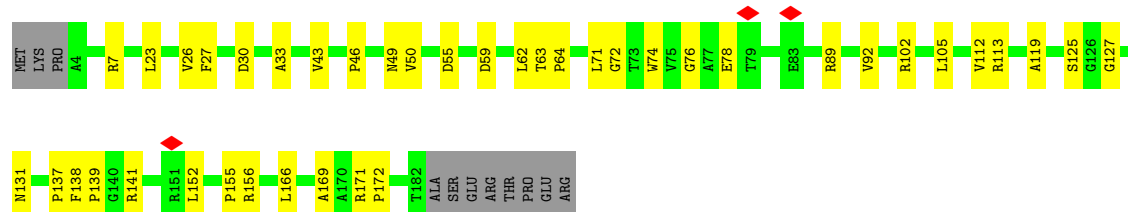
Chain F:  72% 22% 6%



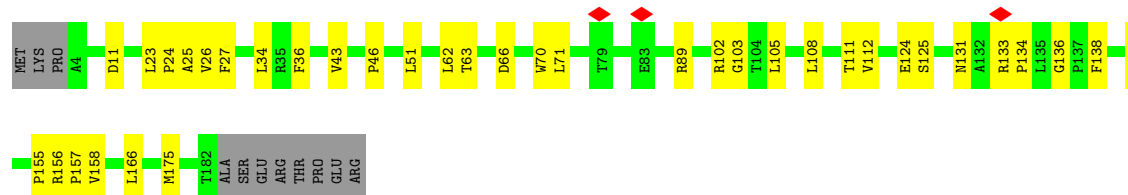
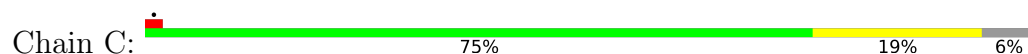
• Molecule 5: Secreted protein



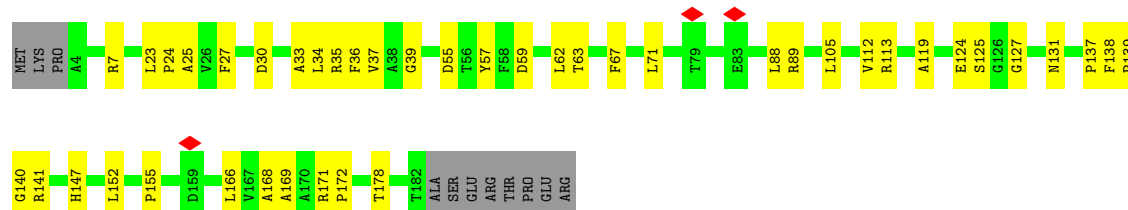
• Molecule 5: Secreted protein



• Molecule 5: Secreted protein

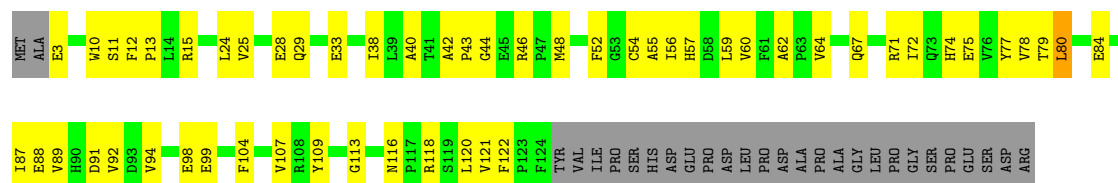


• Molecule 5: Secreted protein



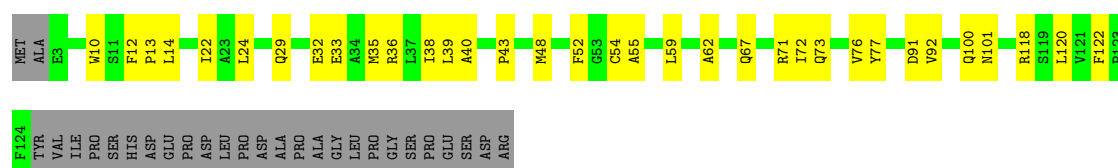
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain V: 



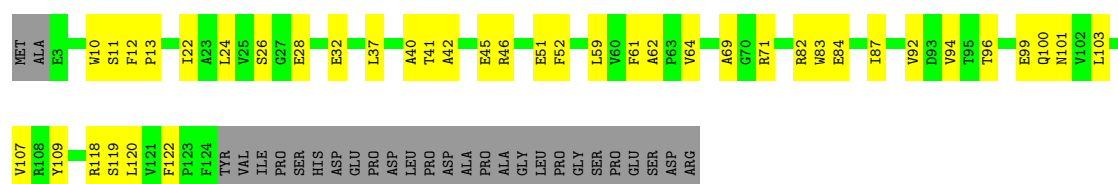
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain W: 



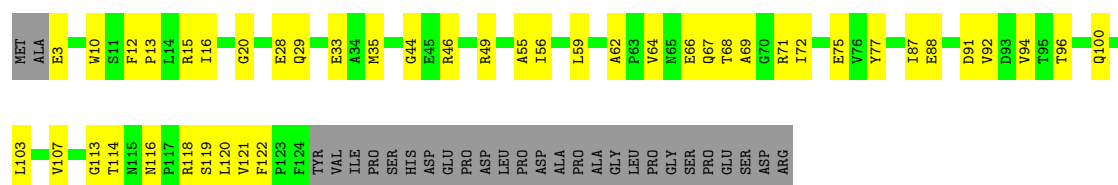
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain X: 



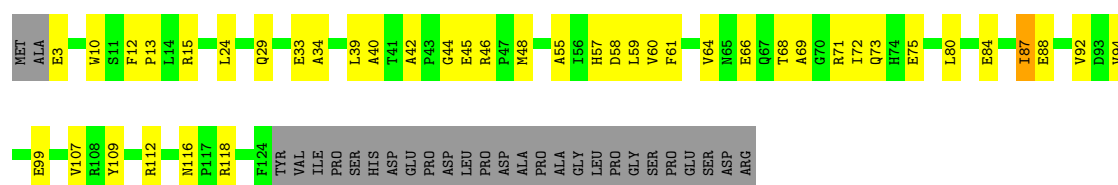
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain S: 



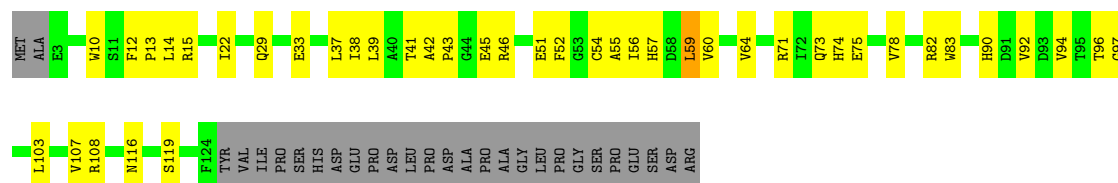
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain T: 



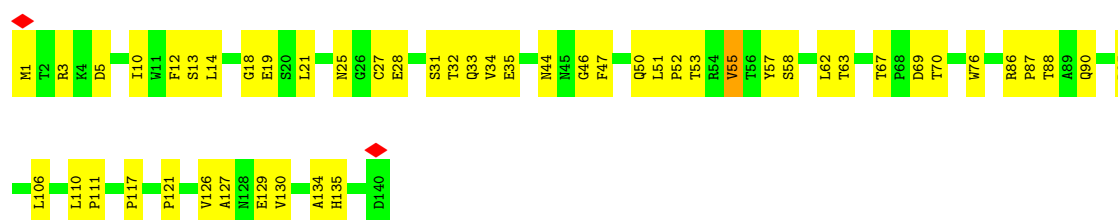
- Molecule 6: IraD/Gp25-like domain-containing protein

Chain U:  53% 27% 19%



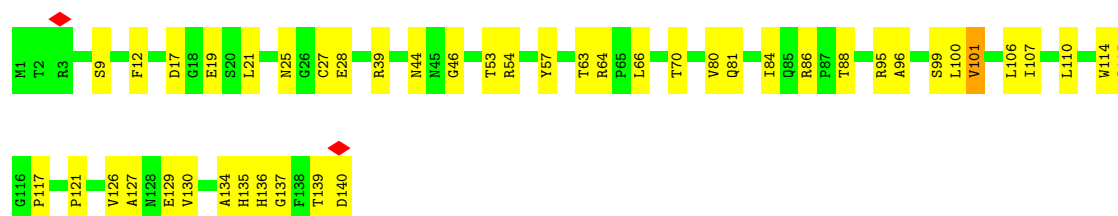
- Molecule 7: Phage tail protein

Chain a:  64% 35%



- Molecule 7: Phage tail protein

Chain b:  68% 31%



- Molecule 7: Phage tail protein

Chain c:  66% 34%



- Molecule 7: Phage tail protein

Chain d:  64% 36%

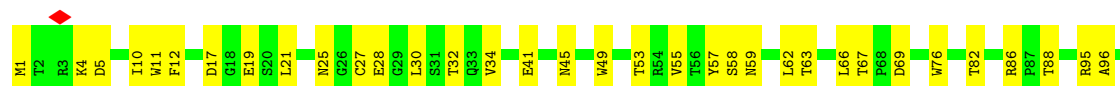




• Molecule 7: Phage tail protein



• Molecule 7: Phage tail protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22980	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.965	Depositor
Minimum map value	-1.225	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.122	Depositor
Recommended contour level	0.421	Depositor
Map size (Å)	447.30002, 447.30002, 447.30002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	k	0.31	0/1168	0.65	3/1586 (0.2%)
1	l	0.39	0/1168	0.66	2/1586 (0.1%)
1	m	0.25	0/1168	0.59	1/1586 (0.1%)
1	n	0.29	0/1168	0.68	4/1586 (0.3%)
1	o	0.45	0/1168	0.79	5/1586 (0.3%)
1	p	0.28	0/1168	0.58	1/1586 (0.1%)
2	1e	0.23	0/2793	0.41	2/3811 (0.1%)
2	1f	0.25	0/2786	0.42	0/3801
2	1g	0.31	0/2793	0.40	1/3811 (0.0%)
2	1h	0.23	0/2788	0.41	0/3804
2	1i	0.23	0/2793	0.40	0/3811
2	1j	0.24	0/2793	0.40	1/3811 (0.0%)
2	2e	0.28	0/2797	0.50	3/3816 (0.1%)
2	2f	0.28	0/2797	0.45	4/3816 (0.1%)
2	2g	0.30	1/2797 (0.0%)	0.48	2/3816 (0.1%)
2	2h	0.24	0/2797	0.40	0/3816
2	2i	0.26	0/2797	0.44	2/3816 (0.1%)
2	2j	0.22	0/2797	0.37	1/3816 (0.0%)
2	3e	0.17	0/2862	0.36	0/3905
2	3f	0.17	0/2862	0.37	0/3905
2	3g	0.20	0/2862	0.47	3/3905 (0.1%)
2	3h	0.16	0/2862	0.37	0/3905
2	3i	0.17	0/2862	0.36	0/3905
2	3j	0.17	0/2862	0.36	0/3905
3	1G	0.14	0/4994	0.34	0/6824
3	1H	0.14	0/4994	0.32	0/6824
3	1J	0.14	0/4994	0.31	0/6824
3	1K	0.15	0/4994	0.33	0/6824
3	1L	0.14	0/4994	0.35	1/6824 (0.0%)
3	1l	0.14	0/4994	0.32	0/6824
3	2G	0.14	0/4114	0.37	2/5620 (0.0%)
3	2H	0.15	0/4114	0.34	0/5620
3	2J	0.15	0/4108	0.36	0/5613
3	2K	0.14	0/4114	0.33	1/5620 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	2L	0.15	0/4114	0.35	0/5620
3	2I	0.14	0/4114	0.34	1/5620 (0.0%)
4	M	0.19	0/1748	0.33	0/2378
4	N	0.20	0/1748	0.31	0/2378
4	O	0.20	0/1748	0.34	0/2378
4	P	0.19	0/1748	0.33	0/2378
4	Q	0.19	0/1748	0.30	0/2378
4	R	0.19	0/1748	0.31	0/2378
5	A	0.15	0/1372	0.30	0/1883
5	B	0.17	0/1372	0.36	0/1883
5	C	0.14	0/1372	0.28	0/1883
5	D	0.14	0/1372	0.29	0/1883
5	E	0.16	0/1372	0.35	1/1883 (0.1%)
5	F	0.14	0/1372	0.28	0/1883
6	S	0.20	0/989	0.47	0/1347
6	T	0.23	0/989	0.46	0/1347
6	U	0.22	0/989	0.43	0/1347
6	V	0.20	0/989	0.46	0/1347
6	W	0.20	0/989	0.46	0/1347
6	X	0.21	0/989	0.38	0/1347
7	a	0.31	0/1097	0.46	0/1495
7	b	0.23	0/1097	0.36	0/1495
7	c	0.20	0/1097	0.32	0/1495
7	d	0.23	0/1097	0.36	0/1495
7	e	0.22	0/1097	0.34	0/1495
7	f	0.22	0/1097	0.34	0/1495
All	All	0.20	1/143586 (0.0%)	0.39	41/195966 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2g	452	GLN	CA-C	-5.26	1.50	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	66	VAL	N-CA-C	9.34	120.64	108.12
1	k	26	TYR	N-CA-C	8.06	120.06	111.28
3	2I	114	ARG	N-CA-C	7.99	119.77	111.14
2	3g	412	PHE	CA-C-N	7.33	129.00	119.84
2	3g	412	PHE	C-N-CA	7.33	129.00	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	k	1152	0	1150	117	0
1	l	1152	0	1150	103	0
1	m	1152	0	1150	105	0
1	n	1152	0	1150	91	0
1	o	1152	0	1150	74	0
1	p	1152	0	1150	118	0
2	1e	2721	0	2625	96	0
2	1f	2714	0	2618	117	0
2	1g	2721	0	2625	102	0
2	1h	2716	0	2620	125	0
2	1i	2721	0	2625	104	0
2	1j	2721	0	2625	104	0
2	2e	2725	0	2628	126	0
2	2f	2725	0	2628	125	0
2	2g	2725	0	2628	131	0
2	2h	2725	0	2628	108	0
2	2i	2725	0	2628	109	0
2	2j	2725	0	2628	98	0
2	3e	2787	0	2697	112	0
2	3f	2787	0	2697	88	0
2	3g	2787	0	2697	127	0
2	3h	2787	0	2697	99	0
2	3i	2787	0	2697	106	0
2	3j	2787	0	2697	107	0
3	1G	4886	0	4786	151	0
3	1H	4886	0	4786	152	0
3	1J	4886	0	4786	136	0
3	1K	4886	0	4786	149	0
3	1L	4886	0	4786	170	0
3	1l	4886	0	4786	165	0
3	2G	4028	0	3953	138	0
3	2H	4028	0	3953	145	0
3	2J	4022	0	3942	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2K	4028	0	3953	139	0
3	2L	4028	0	3953	135	0
3	2I	4028	0	3953	127	0
4	M	1704	0	1704	43	0
4	N	1704	0	1704	58	0
4	O	1704	0	1704	43	0
4	P	1704	0	1704	50	0
4	Q	1704	0	1704	41	0
4	R	1704	0	1704	45	0
5	A	1338	0	1330	40	0
5	B	1338	0	1330	41	0
5	C	1338	0	1330	33	0
5	D	1338	0	1330	37	0
5	E	1338	0	1330	41	0
5	F	1338	0	1330	36	0
6	S	965	0	934	48	0
6	T	965	0	934	47	0
6	U	965	0	934	39	0
6	V	965	0	934	49	0
6	W	965	0	934	32	0
6	X	965	0	934	31	0
7	a	1072	0	1048	64	0
7	b	1072	0	1048	45	0
7	c	1072	0	1048	40	0
7	d	1072	0	1048	52	0
7	e	1072	0	1048	41	0
7	f	1072	0	1048	66	0
All	All	140250	0	137107	4678	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 17.

The worst 5 of 4678 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)
3:2l:41:VAL:CG1	6:T:10:TRP:HB2	1.33	1.52
2:2f:457:GLU:HG3	2:2f:458:PRO:CD	1.50	1.37
2:2e:457:GLU:CB	2:2e:458:PRO:HD3	1.54	1.36
1:k:27:LEU:CB	1:k:68:VAL:HB	1.54	1.35
2:2e:457:GLU:HB3	2:2e:458:PRO:CD	1.58	1.31

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	k	147/149 (99%)	115 (78%)	32 (22%)	0	100	100
1	l	147/149 (99%)	112 (76%)	34 (23%)	1 (1%)	19	53
1	m	147/149 (99%)	117 (80%)	29 (20%)	1 (1%)	19	53
1	n	147/149 (99%)	115 (78%)	32 (22%)	0	100	100
1	o	147/149 (99%)	113 (77%)	32 (22%)	2 (1%)	9	40
1	p	147/149 (99%)	112 (76%)	33 (22%)	2 (1%)	9	40
2	1e	347/534 (65%)	307 (88%)	39 (11%)	1 (0%)	37	68
2	1f	346/534 (65%)	302 (87%)	40 (12%)	4 (1%)	11	43
2	1g	347/534 (65%)	304 (88%)	43 (12%)	0	100	100
2	1h	346/534 (65%)	307 (89%)	38 (11%)	1 (0%)	37	68
2	1i	347/534 (65%)	306 (88%)	39 (11%)	2 (1%)	22	56
2	1j	347/534 (65%)	308 (89%)	39 (11%)	0	100	100
2	2e	348/534 (65%)	311 (89%)	33 (10%)	4 (1%)	12	45
2	2f	348/534 (65%)	318 (91%)	28 (8%)	2 (1%)	22	56
2	2g	348/534 (65%)	317 (91%)	31 (9%)	0	100	100
2	2h	348/534 (65%)	315 (90%)	33 (10%)	0	100	100
2	2i	348/534 (65%)	321 (92%)	26 (8%)	1 (0%)	37	68
2	2j	348/534 (65%)	314 (90%)	34 (10%)	0	100	100
2	3e	355/534 (66%)	312 (88%)	42 (12%)	1 (0%)	37	68
2	3f	355/534 (66%)	319 (90%)	35 (10%)	1 (0%)	37	68
2	3g	355/534 (66%)	316 (89%)	37 (10%)	2 (1%)	22	56
2	3h	355/534 (66%)	323 (91%)	29 (8%)	3 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3i	355/534 (66%)	318 (90%)	36 (10%)	1 (0%)	37	68
2	3j	355/534 (66%)	326 (92%)	28 (8%)	1 (0%)	37	68
3	1G	637/652 (98%)	569 (89%)	68 (11%)	0	100	100
3	1H	637/652 (98%)	569 (89%)	68 (11%)	0	100	100
3	1J	637/652 (98%)	572 (90%)	65 (10%)	0	100	100
3	1K	637/652 (98%)	578 (91%)	59 (9%)	0	100	100
3	1L	637/652 (98%)	568 (89%)	69 (11%)	0	100	100
3	1l	637/652 (98%)	583 (92%)	54 (8%)	0	100	100
3	2G	526/652 (81%)	472 (90%)	54 (10%)	0	100	100
3	2H	526/652 (81%)	466 (89%)	60 (11%)	0	100	100
3	2J	526/652 (81%)	467 (89%)	59 (11%)	0	100	100
3	2K	526/652 (81%)	469 (89%)	57 (11%)	0	100	100
3	2L	526/652 (81%)	469 (89%)	57 (11%)	0	100	100
3	2l	526/652 (81%)	467 (89%)	58 (11%)	1 (0%)	44	75
4	M	221/240 (92%)	201 (91%)	20 (9%)	0	100	100
4	N	221/240 (92%)	203 (92%)	18 (8%)	0	100	100
4	O	221/240 (92%)	202 (91%)	19 (9%)	0	100	100
4	P	221/240 (92%)	198 (90%)	23 (10%)	0	100	100
4	Q	221/240 (92%)	202 (91%)	19 (9%)	0	100	100
4	R	221/240 (92%)	201 (91%)	20 (9%)	0	100	100
5	A	177/190 (93%)	162 (92%)	15 (8%)	0	100	100
5	B	177/190 (93%)	161 (91%)	16 (9%)	0	100	100
5	C	177/190 (93%)	163 (92%)	14 (8%)	0	100	100
5	D	177/190 (93%)	167 (94%)	10 (6%)	0	100	100
5	E	177/190 (93%)	161 (91%)	16 (9%)	0	100	100
5	F	177/190 (93%)	164 (93%)	13 (7%)	0	100	100
6	S	120/150 (80%)	106 (88%)	14 (12%)	0	100	100
6	T	120/150 (80%)	102 (85%)	18 (15%)	0	100	100
6	U	120/150 (80%)	106 (88%)	14 (12%)	0	100	100
6	V	120/150 (80%)	107 (89%)	13 (11%)	0	100	100
6	W	120/150 (80%)	106 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	X	120/150 (80%)	110 (92%)	10 (8%)	0	100	100
7	a	138/140 (99%)	124 (90%)	14 (10%)	0	100	100
7	b	138/140 (99%)	123 (89%)	15 (11%)	0	100	100
7	c	138/140 (99%)	120 (87%)	18 (13%)	0	100	100
7	d	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
7	e	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
7	f	138/140 (99%)	123 (89%)	15 (11%)	0	100	100
All	All	18094/22650 (80%)	16142 (89%)	1921 (11%)	31 (0%)	45	75

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1h	455	VAL
2	3j	459	ASN
2	2e	457	GLU
2	3e	459	ASN
2	2f	457	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	129/129 (100%)	128 (99%)	1 (1%)	79	88
1	l	129/129 (100%)	128 (99%)	1 (1%)	79	88
1	m	129/129 (100%)	128 (99%)	1 (1%)	79	88
1	n	129/129 (100%)	126 (98%)	3 (2%)	45	69
1	o	129/129 (100%)	124 (96%)	5 (4%)	27	56
1	p	129/129 (100%)	127 (98%)	2 (2%)	58	76
2	1e	279/414 (67%)	276 (99%)	3 (1%)	70	83
2	1f	278/414 (67%)	276 (99%)	2 (1%)	81	89
2	1g	279/414 (67%)	276 (99%)	3 (1%)	70	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1h	279/414 (67%)	275 (99%)	4 (1%)	62	79
2	1i	279/414 (67%)	277 (99%)	2 (1%)	81	89
2	1j	279/414 (67%)	279 (100%)	0	100	100
2	2e	279/414 (67%)	275 (99%)	4 (1%)	62	79
2	2f	279/414 (67%)	274 (98%)	5 (2%)	54	74
2	2g	279/414 (67%)	274 (98%)	5 (2%)	54	74
2	2h	279/414 (67%)	277 (99%)	2 (1%)	81	89
2	2i	279/414 (67%)	275 (99%)	4 (1%)	62	79
2	2j	279/414 (67%)	278 (100%)	1 (0%)	89	95
2	3e	285/414 (69%)	284 (100%)	1 (0%)	89	95
2	3f	285/414 (69%)	285 (100%)	0	100	100
2	3g	285/414 (69%)	282 (99%)	3 (1%)	70	83
2	3h	285/414 (69%)	284 (100%)	1 (0%)	89	95
2	3i	285/414 (69%)	284 (100%)	1 (0%)	89	95
2	3j	285/414 (69%)	284 (100%)	1 (0%)	89	95
3	1G	515/528 (98%)	513 (100%)	2 (0%)	89	95
3	1H	515/528 (98%)	513 (100%)	2 (0%)	89	95
3	1J	515/528 (98%)	514 (100%)	1 (0%)	92	97
3	1K	515/528 (98%)	512 (99%)	3 (1%)	84	91
3	1L	515/528 (98%)	511 (99%)	4 (1%)	79	88
3	1l	515/528 (98%)	511 (99%)	4 (1%)	79	88
3	2G	424/528 (80%)	423 (100%)	1 (0%)	92	97
3	2H	424/528 (80%)	422 (100%)	2 (0%)	86	93
3	2J	423/528 (80%)	418 (99%)	5 (1%)	67	82
3	2K	424/528 (80%)	421 (99%)	3 (1%)	81	89
3	2L	424/528 (80%)	421 (99%)	3 (1%)	81	89
3	2l	424/528 (80%)	424 (100%)	0	100	100
4	M	183/194 (94%)	182 (100%)	1 (0%)	86	93
4	N	183/194 (94%)	181 (99%)	2 (1%)	70	83
4	O	183/194 (94%)	183 (100%)	0	100	100
4	P	183/194 (94%)	180 (98%)	3 (2%)	58	76

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	183/194 (94%)	182 (100%)	1 (0%)	86	93
4	R	183/194 (94%)	183 (100%)	0	100	100
5	A	137/147 (93%)	136 (99%)	1 (1%)	81	89
5	B	137/147 (93%)	137 (100%)	0	100	100
5	C	137/147 (93%)	135 (98%)	2 (2%)	60	77
5	D	137/147 (93%)	137 (100%)	0	100	100
5	E	137/147 (93%)	137 (100%)	0	100	100
5	F	137/147 (93%)	137 (100%)	0	100	100
6	S	104/127 (82%)	104 (100%)	0	100	100
6	T	104/127 (82%)	103 (99%)	1 (1%)	73	84
6	U	104/127 (82%)	103 (99%)	1 (1%)	73	84
6	V	104/127 (82%)	103 (99%)	1 (1%)	73	84
6	W	104/127 (82%)	104 (100%)	0	100	100
6	X	104/127 (82%)	103 (99%)	1 (1%)	73	84
7	a	116/116 (100%)	115 (99%)	1 (1%)	75	86
7	b	116/116 (100%)	115 (99%)	1 (1%)	75	86
7	c	116/116 (100%)	116 (100%)	0	100	100
7	d	116/116 (100%)	115 (99%)	1 (1%)	75	86
7	e	116/116 (100%)	115 (99%)	1 (1%)	75	86
7	f	116/116 (100%)	116 (100%)	0	100	100
All	All	14704/18066 (81%)	14601 (99%)	103 (1%)	80	89

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	147	THR
3	1l	590	VAL
6	U	59	LEU
3	2H	375	LEU
2	2f	494	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
2	2g	368	ASN
2	3g	315	GLN
3	2J	517	ASN
2	2j	368	ASN
2	2j	319	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 oligosaccharides 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.

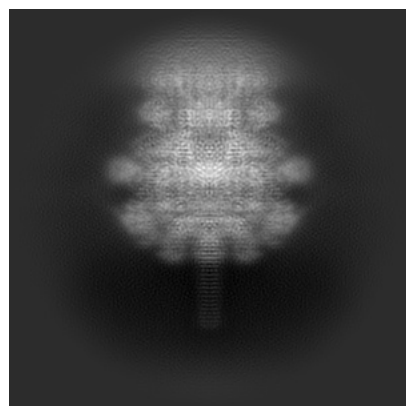
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51564. These allow visual inspection of the internal detail of the map and identification of artifacts.

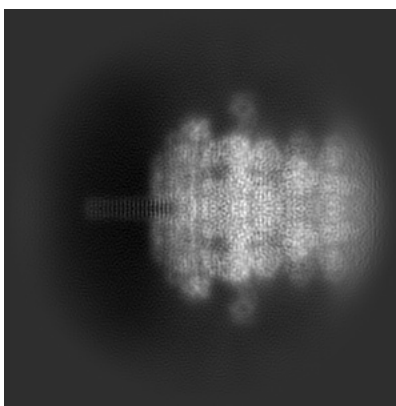
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

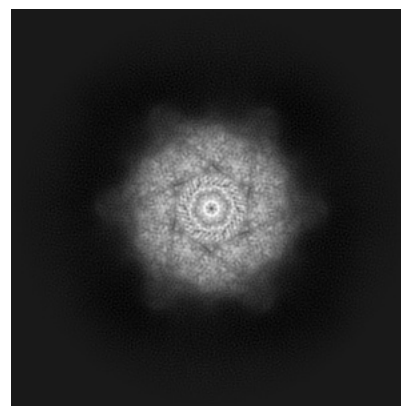
6.1.1 Primary map



X

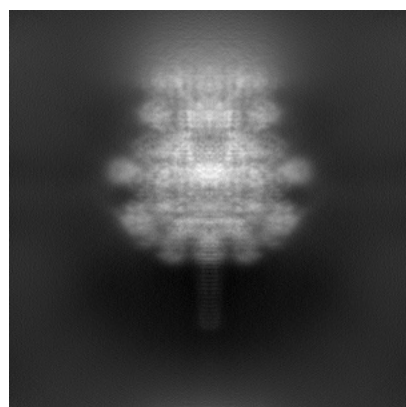


Y

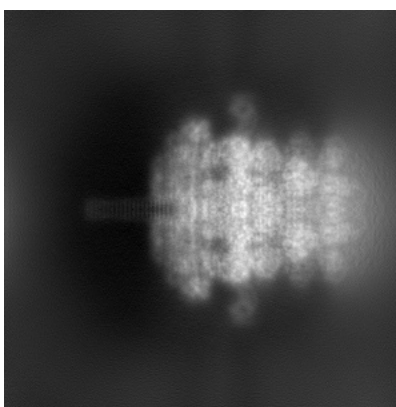


Z

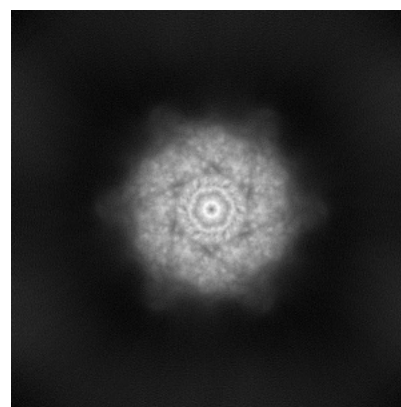
6.1.2 Raw map



X



Y

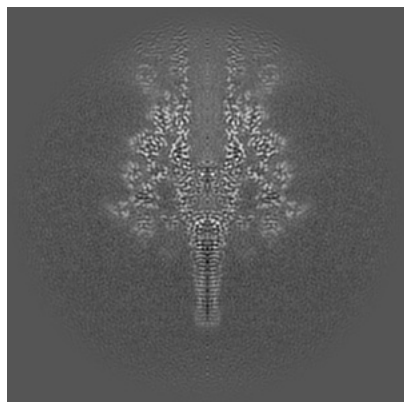


Z

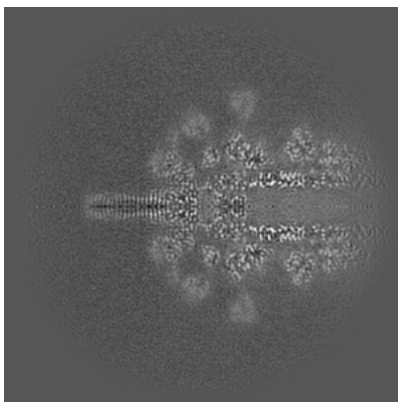
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

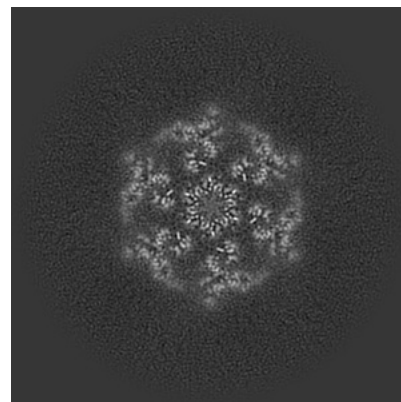
6.2.1 Primary map



X Index: 210

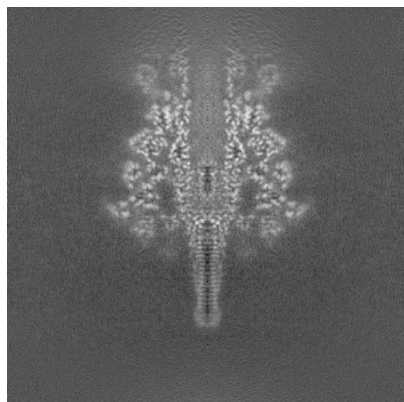


Y Index: 210

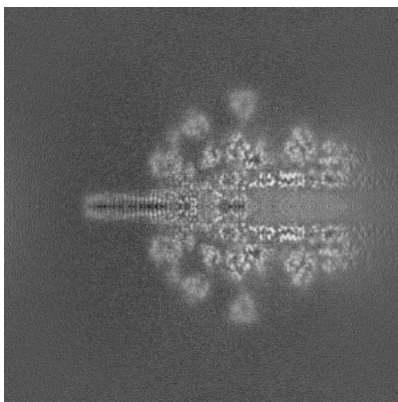


Z Index: 210

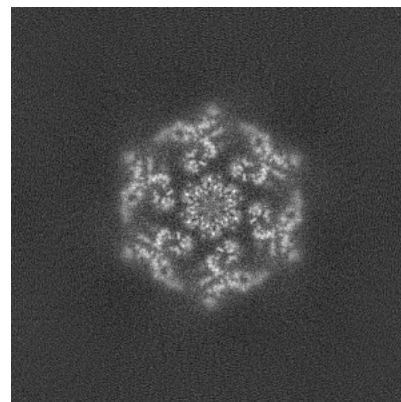
6.2.2 Raw map



X Index: 210



Y Index: 210

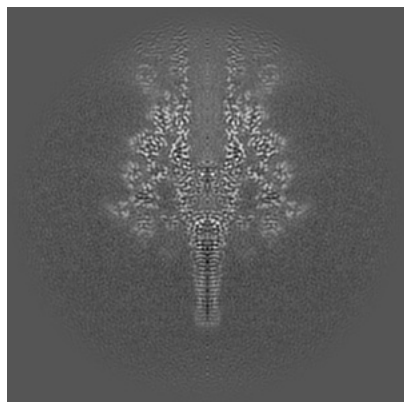


Z Index: 210

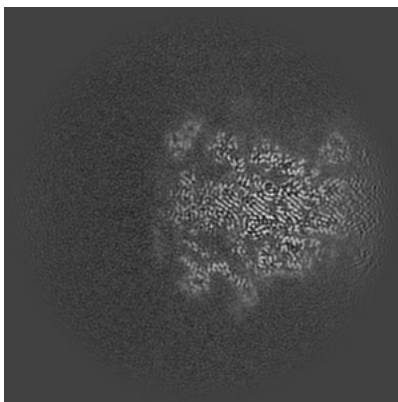
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

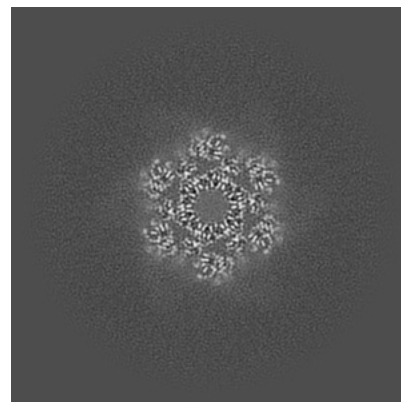
6.3.1 Primary map



X Index: 210

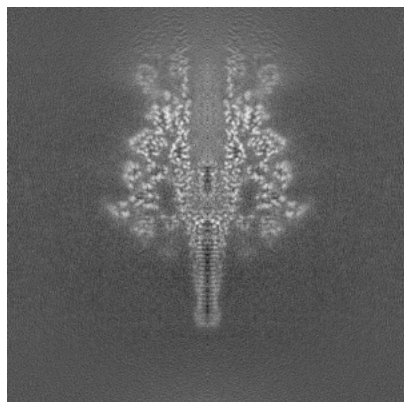


Y Index: 231

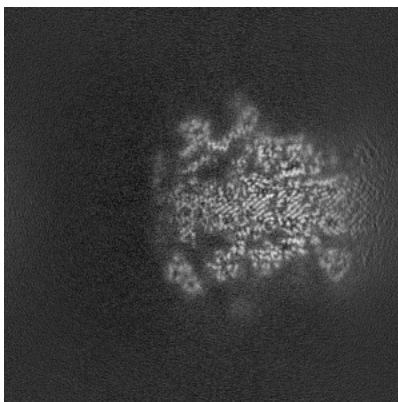


Z Index: 269

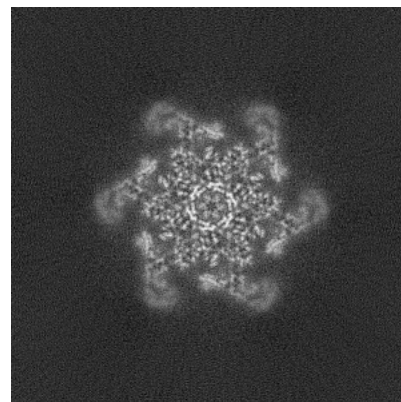
6.3.2 Raw map



X Index: 210



Y Index: 189

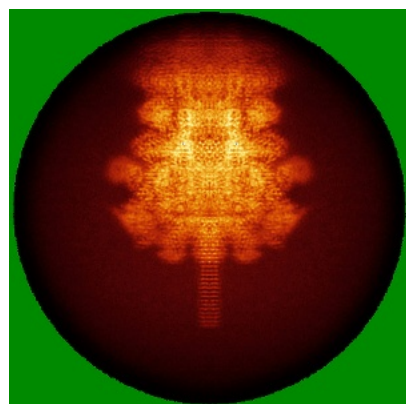


Z Index: 252

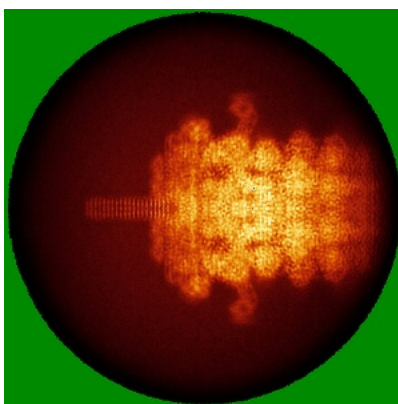
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

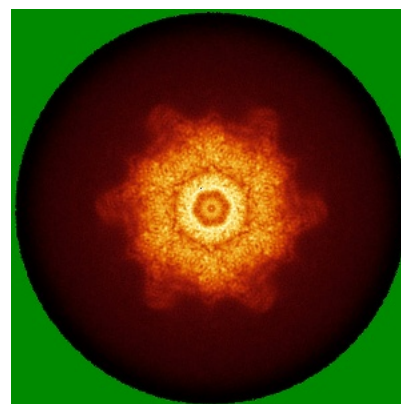
6.4.1 Primary map



X

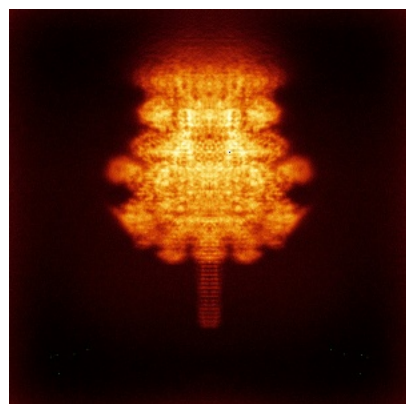


Y

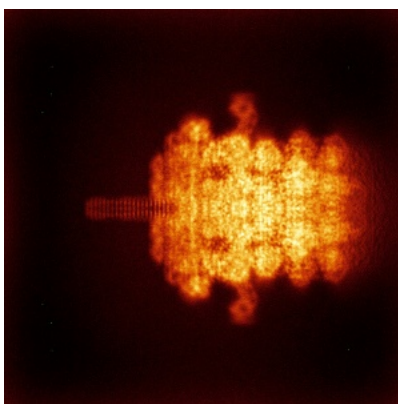


Z

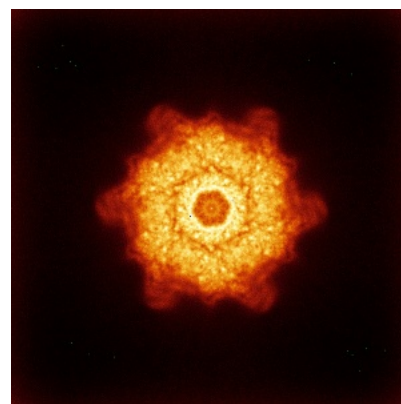
6.4.2 Raw map



X



Y

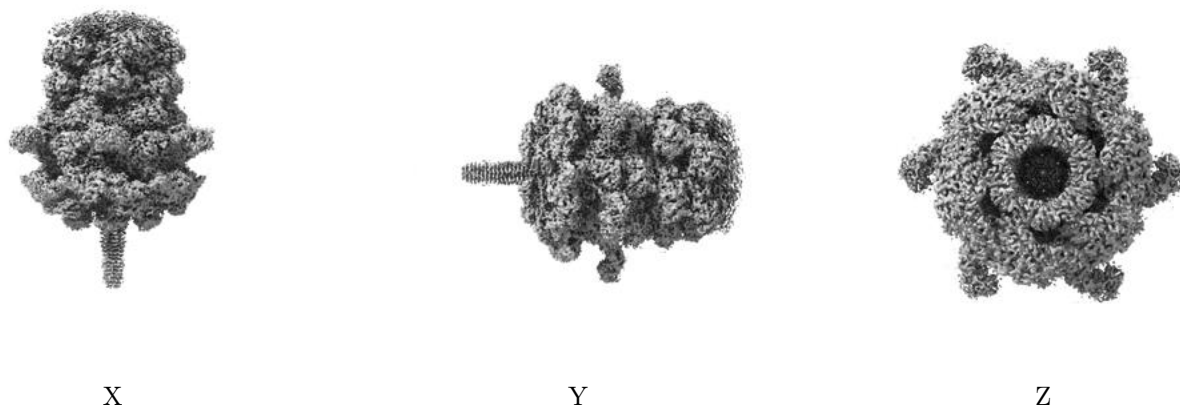


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

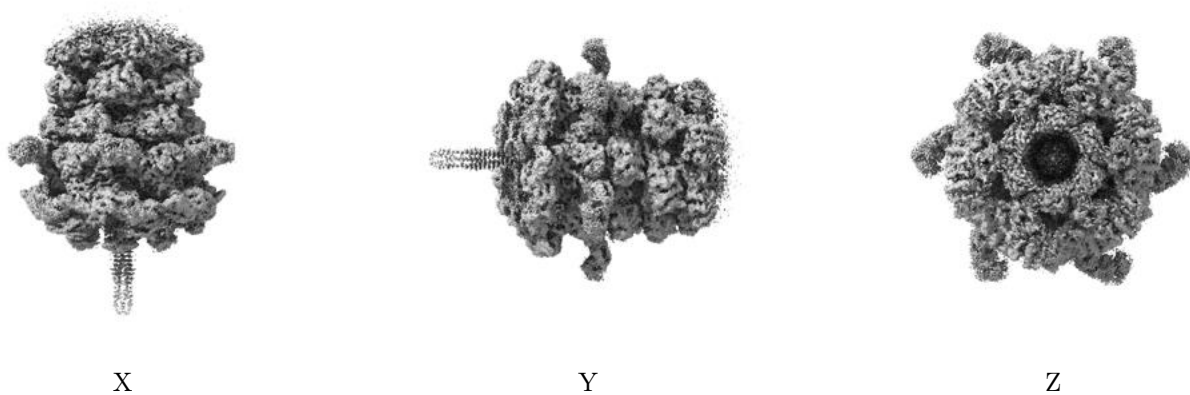
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.421. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

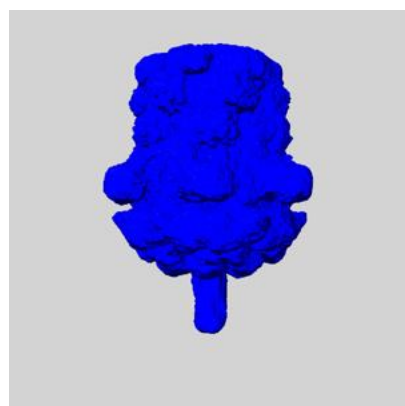
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

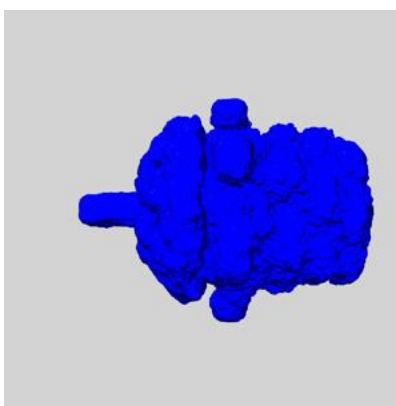
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

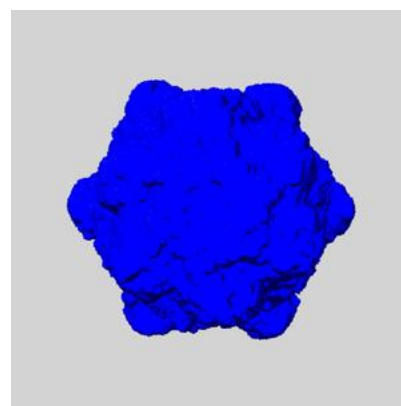
6.6.1 emd_51564_msk_1.map [i](#)



X



Y

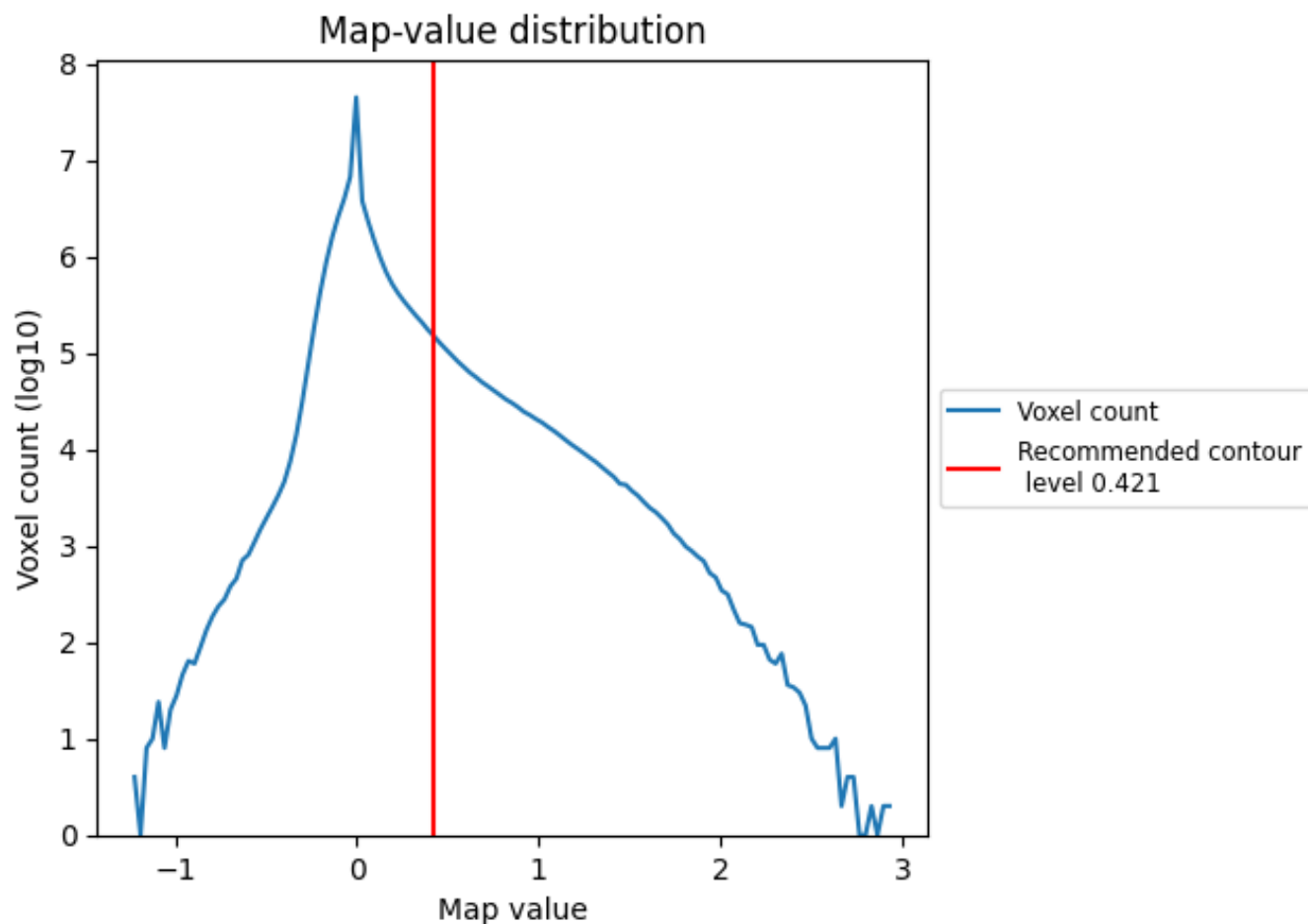


Z

7 Map analysis [i](#)

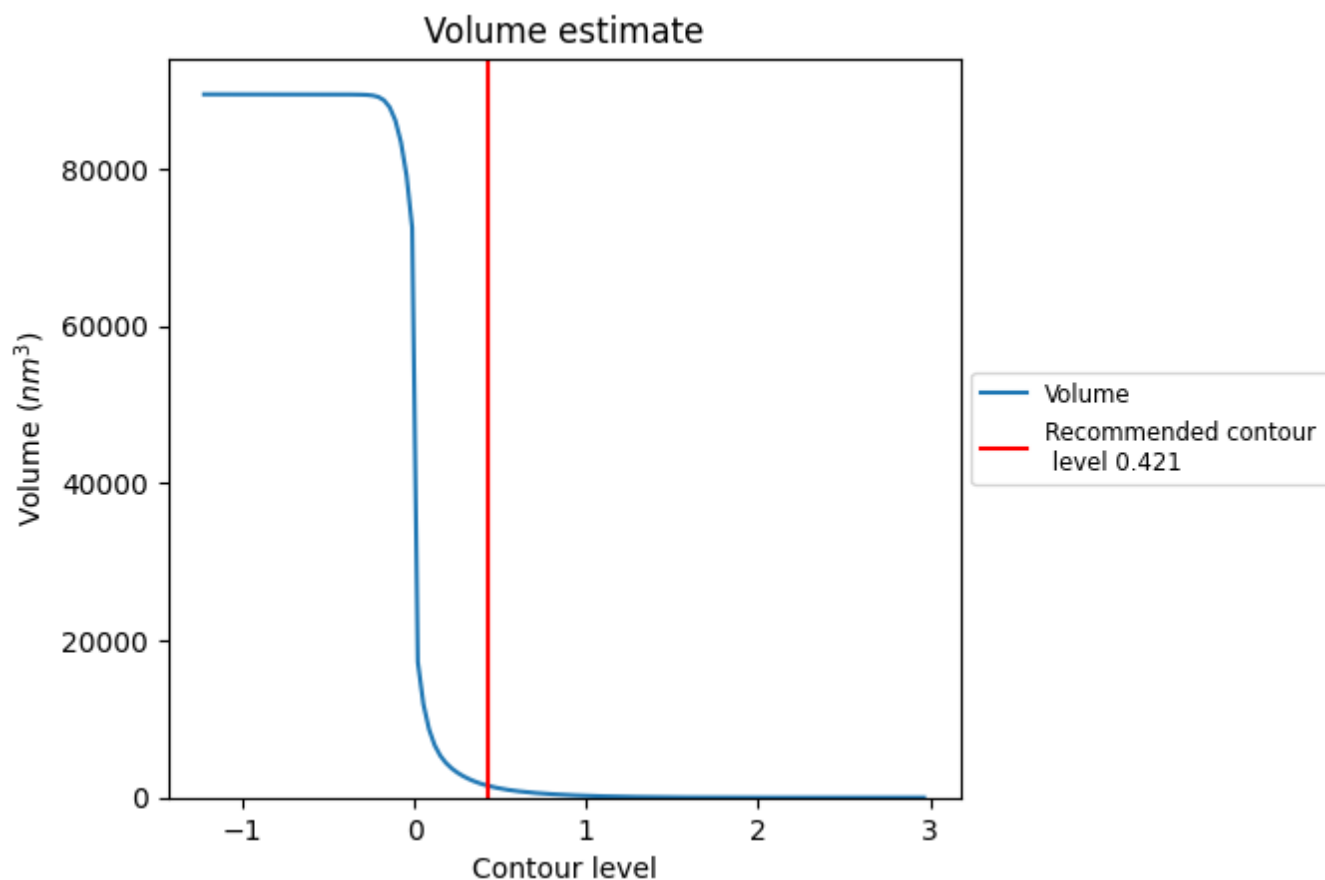
This section contains the results of statistical analysis of the map.

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.

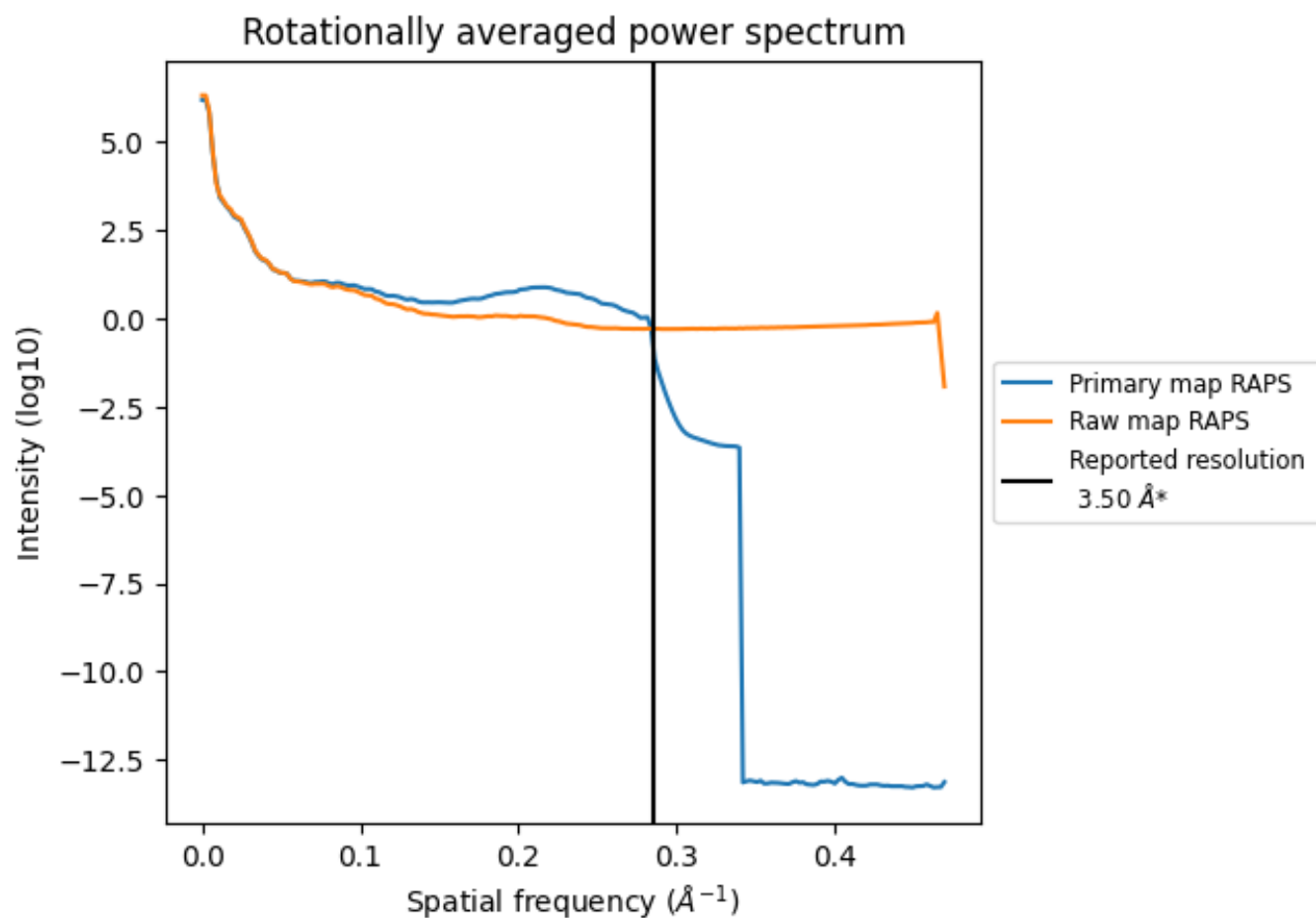
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1541 nm³; this corresponds to an approximate mass of 1392 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 ⓘ

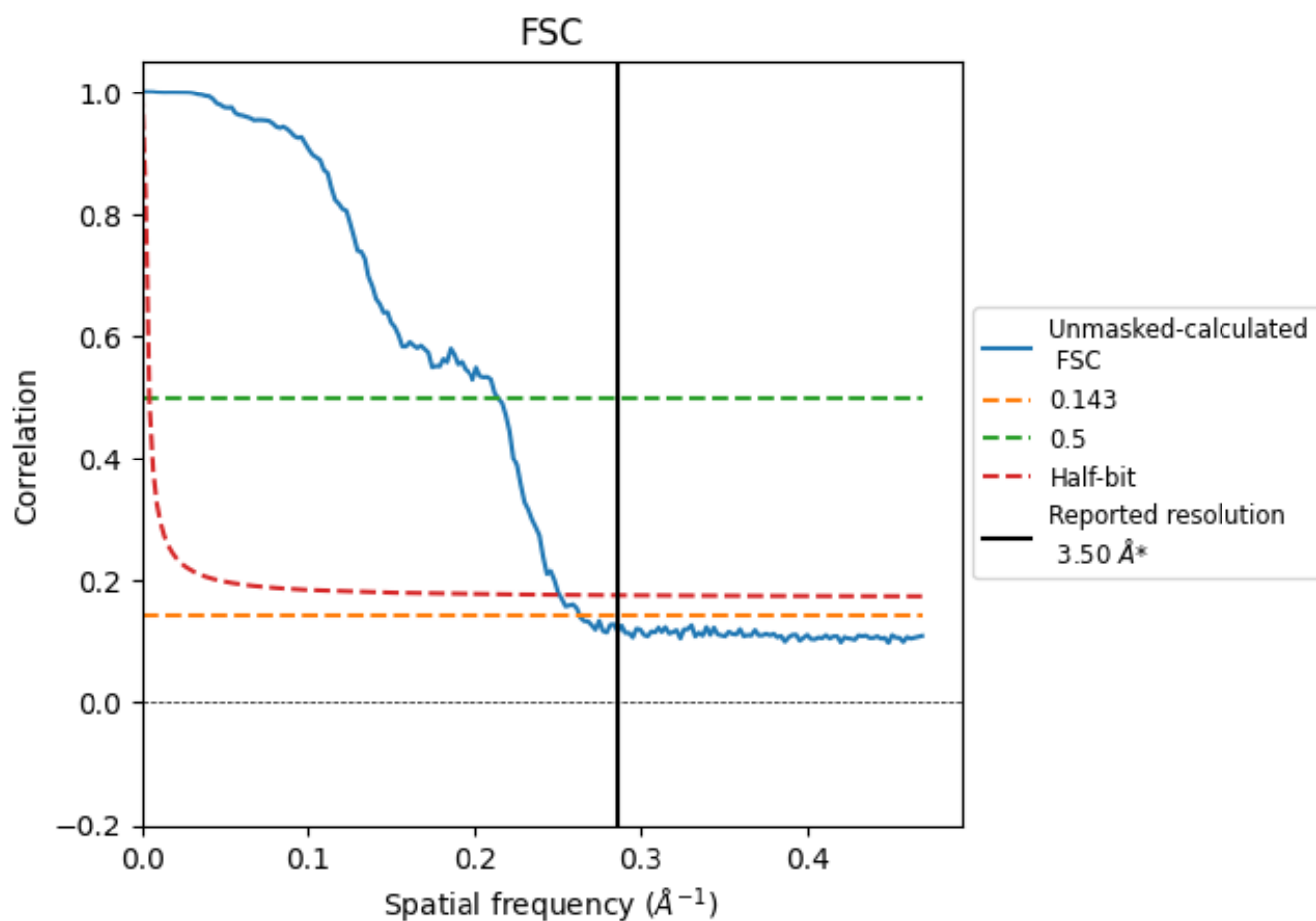


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

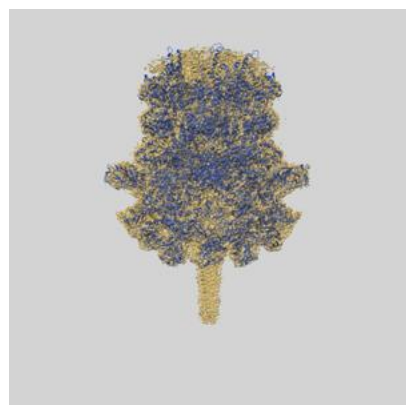
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.67	3.98

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

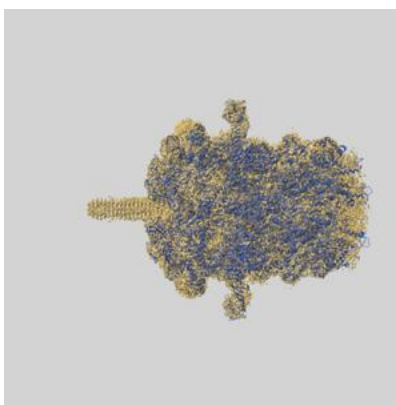
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51564 and PDB model 9GTP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

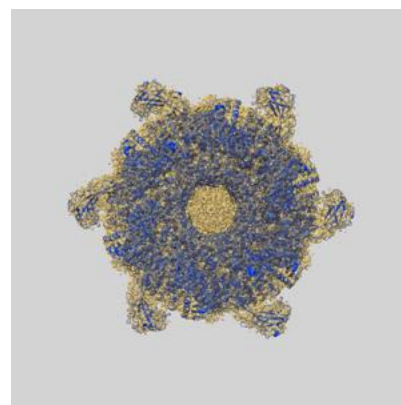
9.1 Map-model overlay [i](#)



X



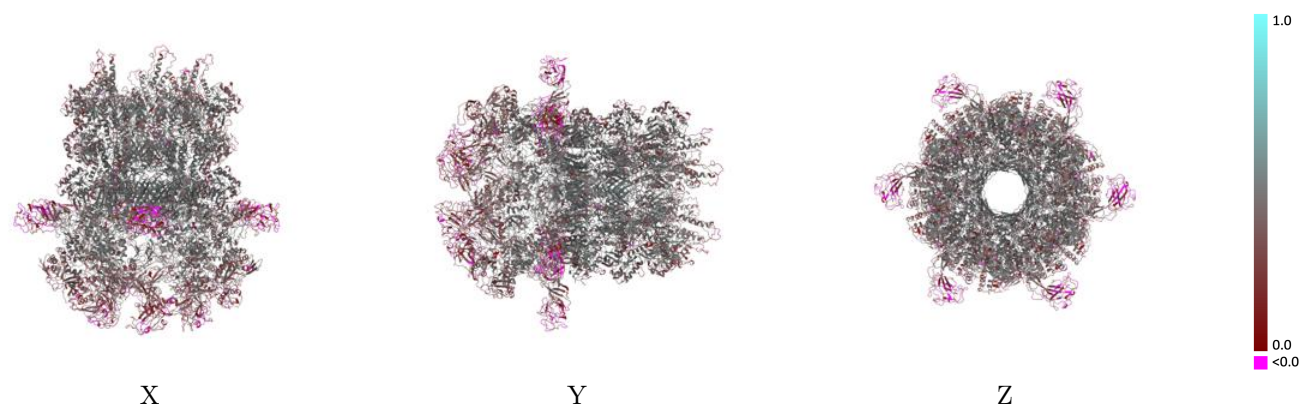
Y



Z

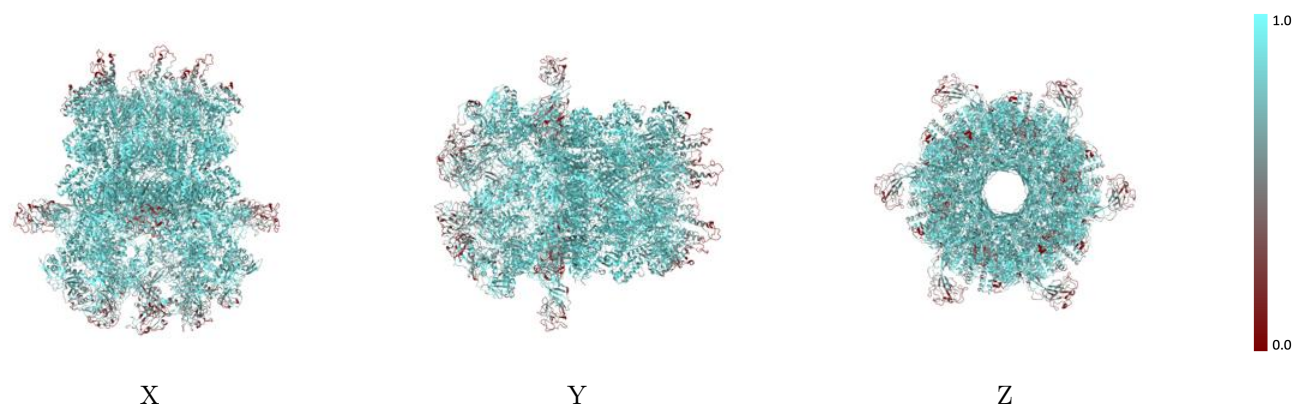
The images above show the 3D surface view of the map at the recommended contour level 0.421 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



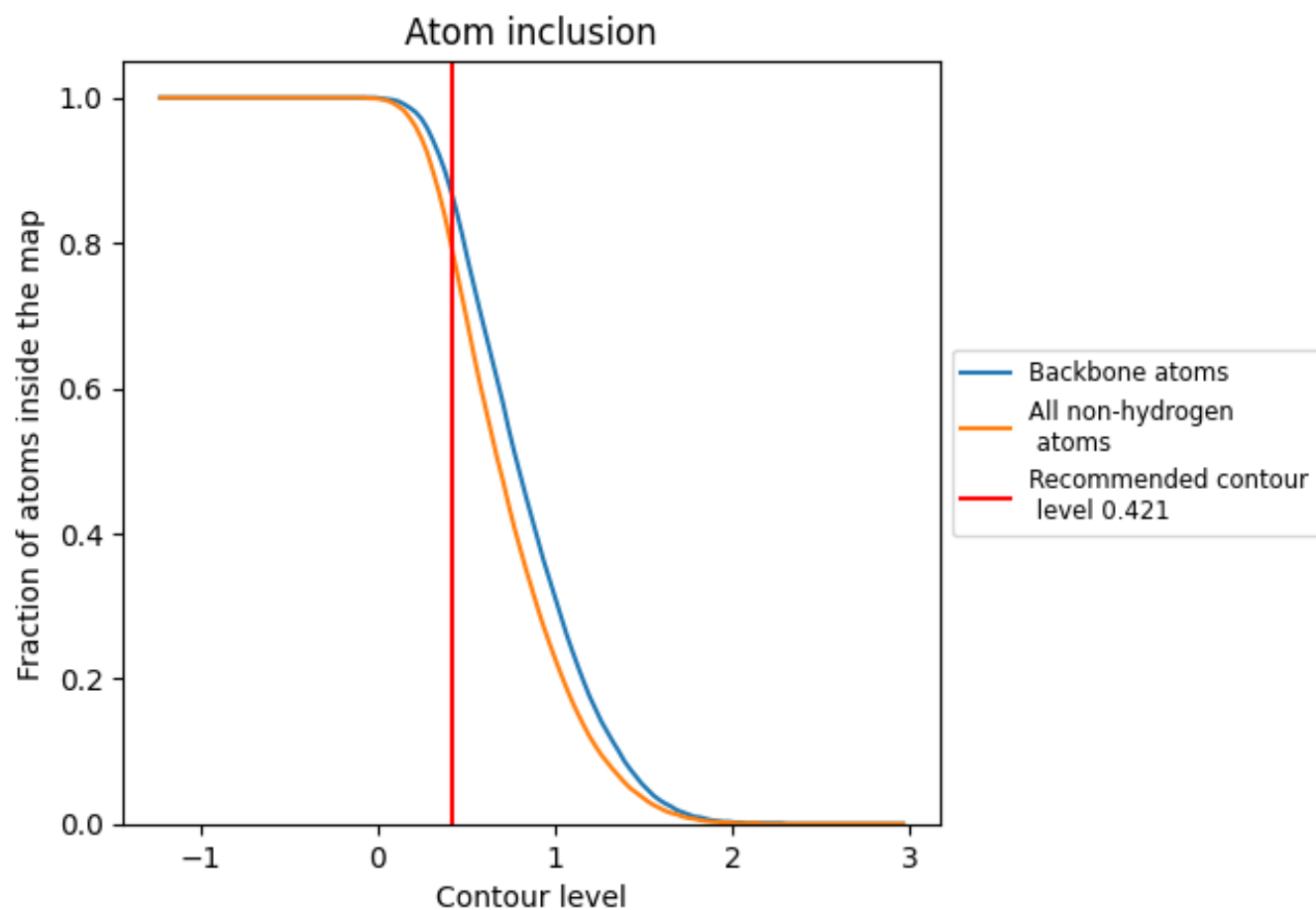
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.421).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.421) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.3810
1G	 0.6960	 0.3170
1H	 0.6950	 0.3210
1J	 0.6920	 0.3160
1K	 0.6940	 0.3170
1L	 0.6910	 0.3180
1e	 0.9060	 0.4360
1f	 0.8990	 0.4310
1g	 0.9050	 0.4310
1h	 0.9060	 0.4330
1i	 0.9030	 0.4330
1j	 0.9090	 0.4350
1l	 0.6930	 0.3170
2G	 0.6840	 0.2850
2H	 0.6820	 0.2840
2J	 0.6860	 0.2870
2K	 0.6890	 0.2860
2L	 0.6840	 0.2860
2e	 0.8810	 0.4110
2f	 0.8890	 0.4140
2g	 0.8760	 0.4100
2h	 0.8820	 0.4120
2i	 0.8790	 0.4110
2j	 0.8850	 0.4120
2l	 0.6810	 0.2880
3e	 0.6840	 0.3940
3f	 0.6850	 0.3910
3g	 0.6800	 0.3890
3h	 0.6880	 0.3930
3i	 0.6840	 0.3990
3j	 0.6810	 0.3950
A	 0.8530	 0.3940
B	 0.8550	 0.3950
C	 0.8550	 0.4000
D	 0.8490	 0.3920



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Chain	Atom inclusion	Q-score
E	 0.8600	 0.3910
F	 0.8610	 0.3970
M	 0.9090	 0.4740
N	 0.9070	 0.4770
O	 0.9160	 0.4760
P	 0.9160	 0.4800
Q	 0.9120	 0.4770
R	 0.9160	 0.4760
S	 0.9140	 0.4550
T	 0.9140	 0.4540
U	 0.9180	 0.4560
V	 0.9150	 0.4570
W	 0.9090	 0.4570
X	 0.9210	 0.4550
a	 0.9300	 0.4890
b	 0.9220	 0.4910
c	 0.9280	 0.4960
d	 0.9280	 0.4930
e	 0.9290	 0.4950
f	 0.9270	 0.4900
k	 0.8640	 0.4210
l	 0.8530	 0.4200
m	 0.8580	 0.4230
n	 0.8680	 0.4230
o	 0.8650	 0.4280
p	 0.8580	 0.4260