



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 09:21 AM UTC

PDB ID : 9PGG / pdb_00009pgg
EMDB ID : EMD-71631
Title : Cryo-EM structure of bacteriophage P22 gp1-gp5-gp4 complex at 2.76 angstrom
Authors : Yu, H.; Liu, J.; Molienux, I.J.
Deposited on : 2025-07-07
Resolution : 2.76 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:

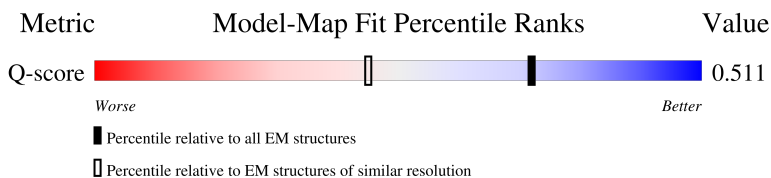
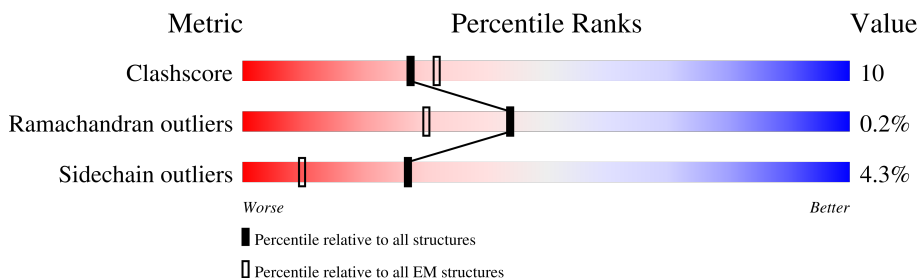
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.76 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.



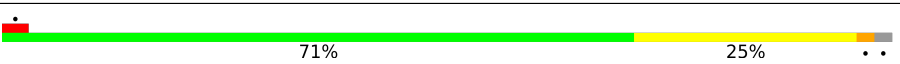
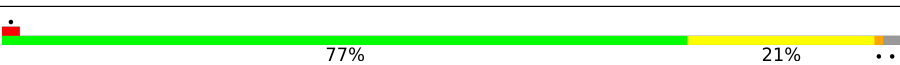
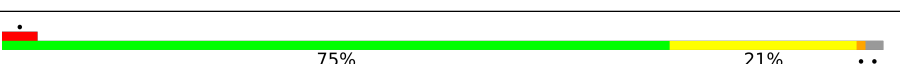
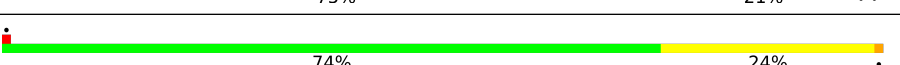
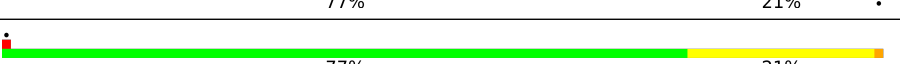
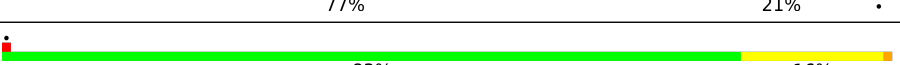
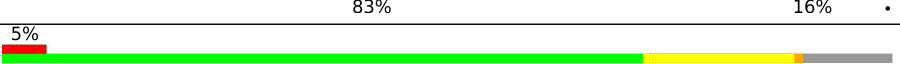
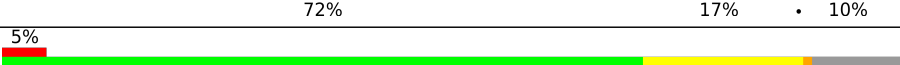
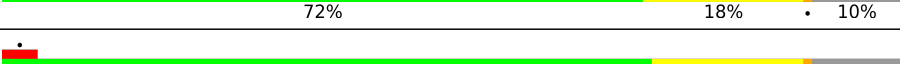
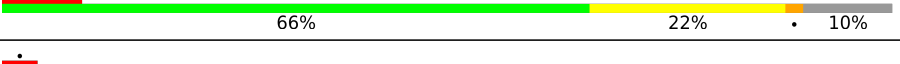
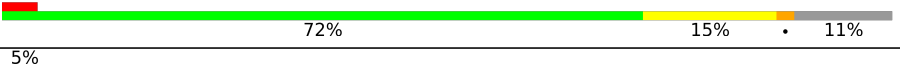
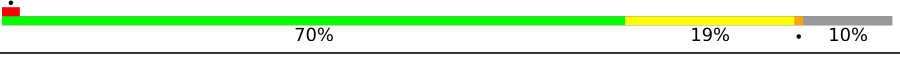
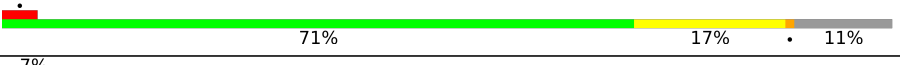
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10642 (2.26 - 3.26)

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	Aa	430	
1	Ab	430	
1	Ac	430	
1	Ad	430	

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Mol	Chain	Length	Quality of chain
1	Ae	430	
1	Af	430	
1	Ag	430	
1	Ah	430	
1	Ai	430	
1	Aj	430	
1	Ak	430	
1	Al	430	
1	Am	430	
1	An	430	
1	Ao	430	
2	Ap	166	
2	Aq	166	
2	Ar	166	
2	As	166	
2	At	166	
2	Au	166	
2	Av	166	
2	Aw	166	
2	Ax	166	
2	Ay	166	
2	Az	166	
2	Ba	166	
3	Bb	725	
3	Bd	725	

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Mol	Chain	Length	Quality of chain
3	Bf	725	
3	Bh	725	
3	Bj	725	
3	Bl	725	
3	Bn	725	
3	Bp	725	
3	Br	725	
3	Bt	725	
3	Bv	725	
3	Bx	725	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 120038 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
1	Aa	429	Total	C	N	O	S	0	0
			3275	2051	568	643	13		
1	Ab	422	Total	C	N	O	S	0	0
			3226	2022	559	632	13		
1	Ac	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
1	Ad	429	Total	C	N	O	S	0	0
			3275	2051	568	643	13		
1	Ae	429	Total	C	N	O	S	0	0
			3275	2051	568	643	13		
1	Af	429	Total	C	N	O	S	0	0
			3275	2051	568	643	13		
1	Ag	429	Total	C	N	O	S	0	0
			3275	2051	568	643	13		
1	Ah	420	Total	C	N	O	S	0	0
			3212	2013	557	629	13		
1	Ai	423	Total	C	N	O	S	0	0
			3234	2028	560	633	13		
1	Aj	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
1	Ak	422	Total	C	N	O	S	0	0
			3226	2022	559	632	13		
1	Al	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
1	Am	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
1	An	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
1	Ao	428	Total	C	N	O	S	0	0
			3272	2050	567	642	13		

- Molecule 2 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ap	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	Aq	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	Ar	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	As	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	At	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	Au	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	Av	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	Aw	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	Ax	148	Total	C	N	O	S	0	0
			1136	714	195	222	5		
2	Ay	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	Az	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	Ba	148	Total	C	N	O	S	0	0
			1136	714	195	222	5		

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Bb	590	Total	C	N	O	S	0	0
			4774	3008	819	926	21		
3	Bd	592	Total	C	N	O	S	0	0
			4791	3017	822	931	21		
3	Bf	591	Total	C	N	O	S	0	0
			4782	3012	821	928	21		
3	Bh	592	Total	C	N	O	S	0	0
			4791	3017	822	931	21		
3	Bj	591	Total	C	N	O	S	0	0
			4783	3013	820	929	21		
3	Bl	592	Total	C	N	O	S	0	0
			4791	3017	822	931	21		
3	Bn	593	Total	C	N	O	S	0	0
			4799	3021	823	934	21		
3	Bp	590	Total	C	N	O	S	0	0
			4774	3008	819	926	21		

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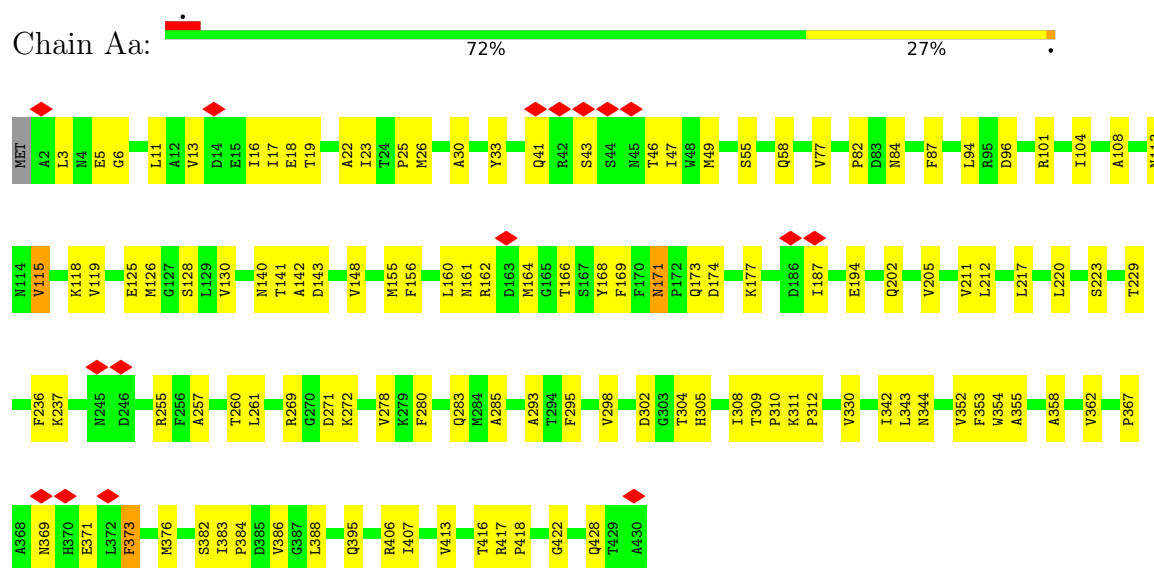
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Br	591	Total	C	N	O	S	0	0
			4782	3012	821	928	21		
3	Bt	591	Total	C	N	O	S	0	0
			4783	3013	820	929	21		
3	Bv	591	Total	C	N	O	S	0	0
			4783	3013	820	929	21		
3	Bx	594	Total	C	N	O	S	0	0
			4807	3025	825	936	21		

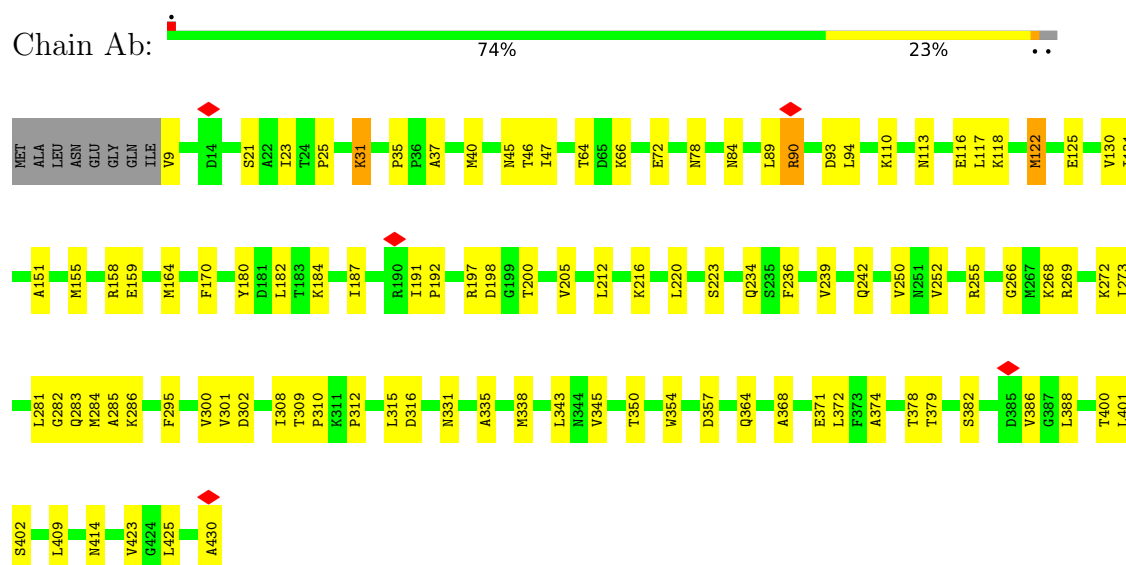
3 Residue-property plots

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.

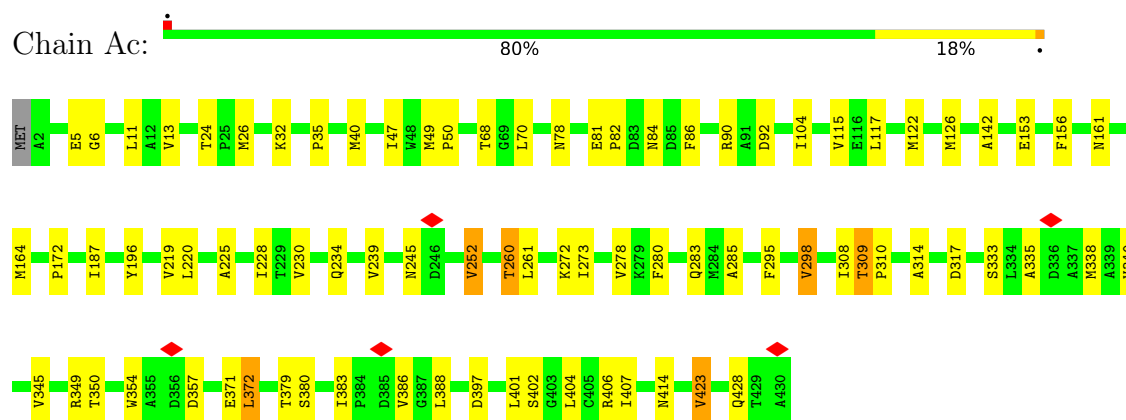
- Molecule 1: Major capsid protein



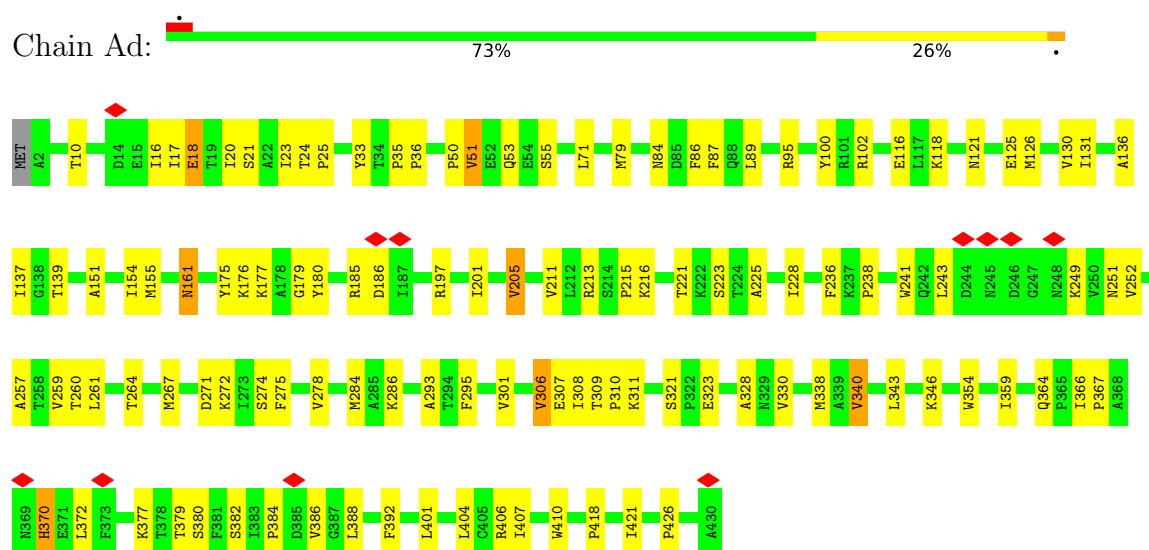
- Molecule 1: Major capsid protein



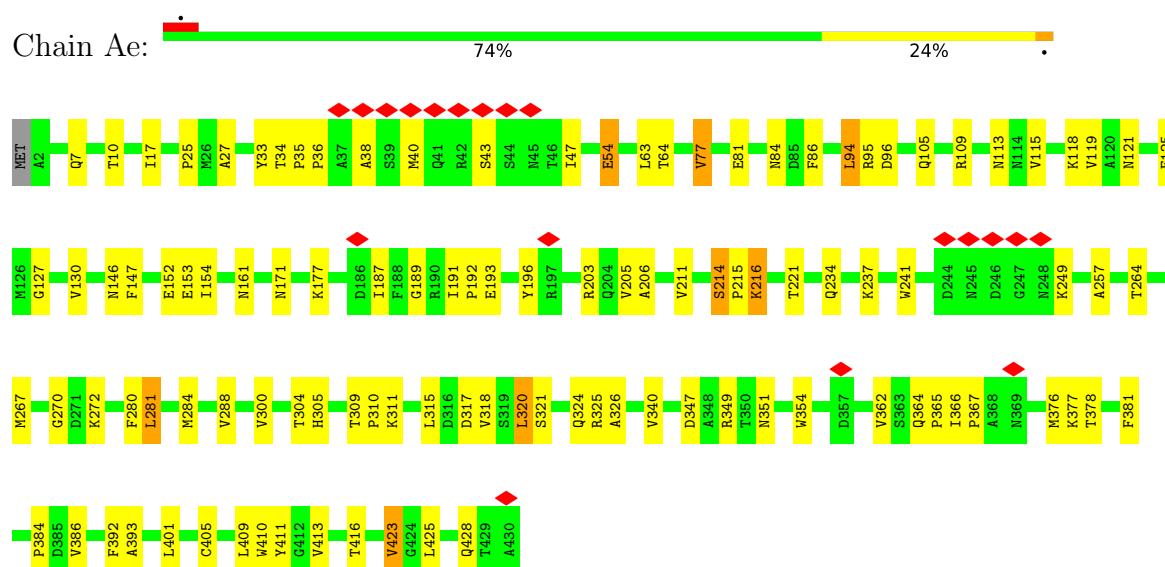
- Molecule 1: Major capsid protein



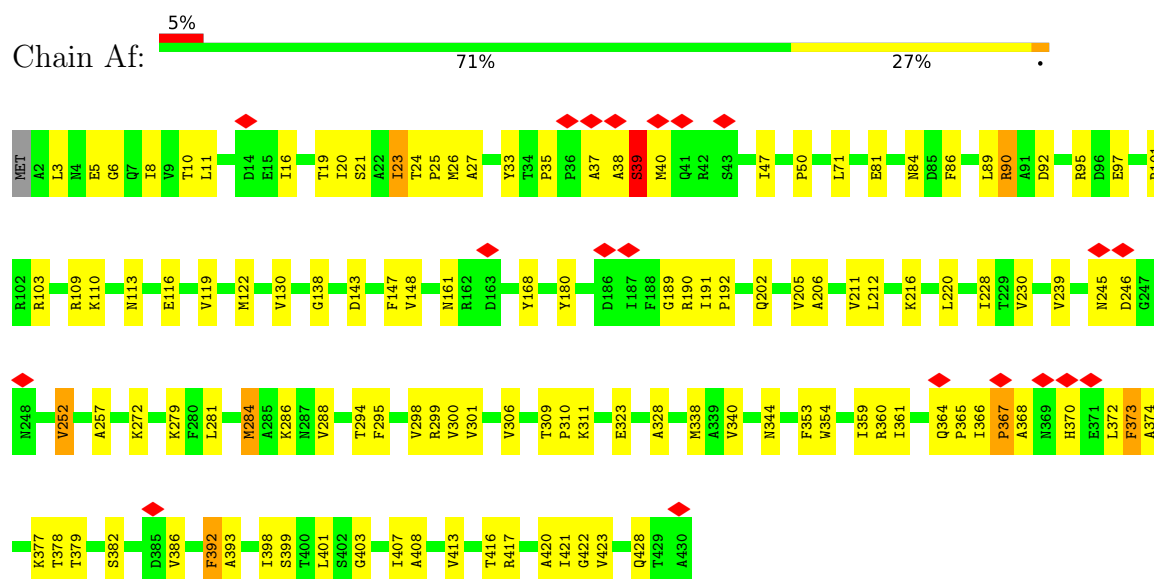
- Molecule 1: Major capsid protein



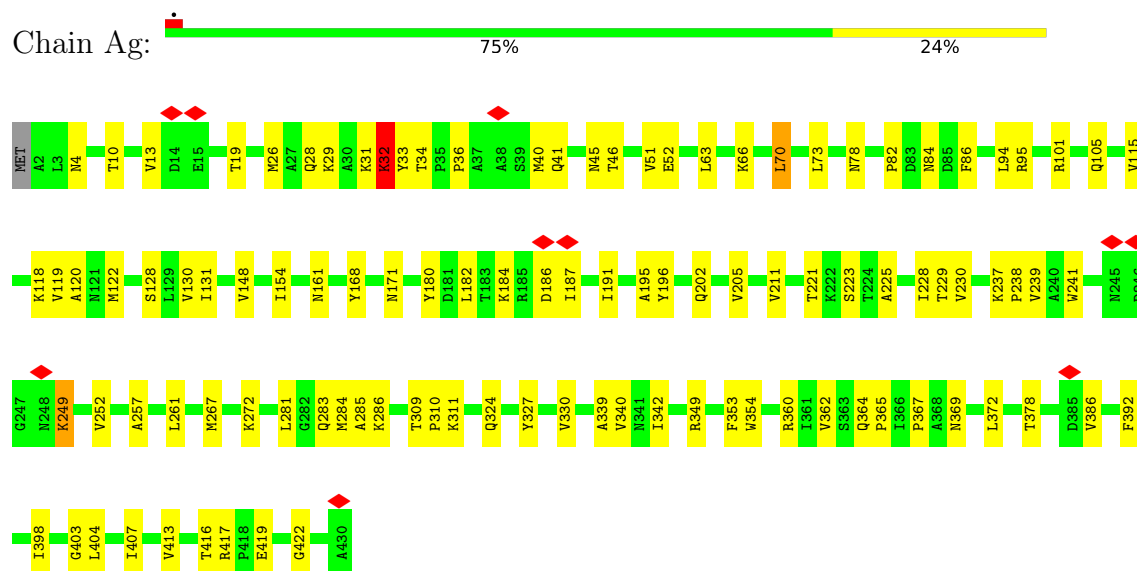
- Molecule 1: Major capsid protein



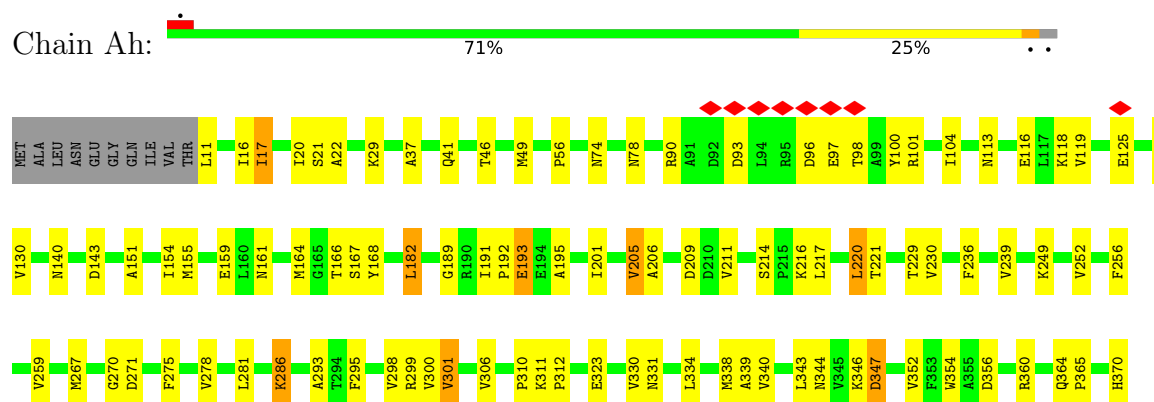
- Molecule 1: Major capsid protein

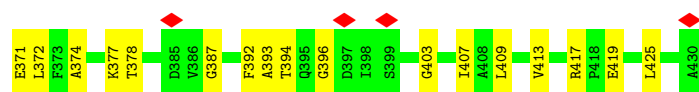


• Molecule 1: Major capsid protein



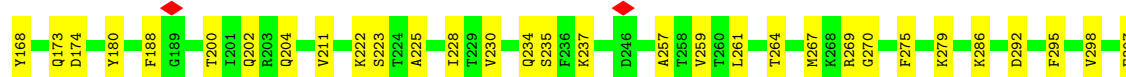
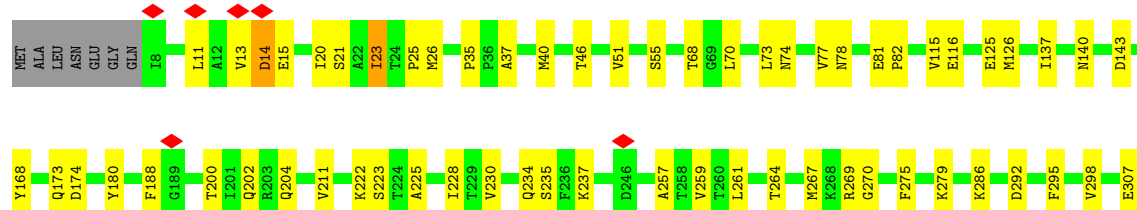
• Molecule 1: Major capsid protein





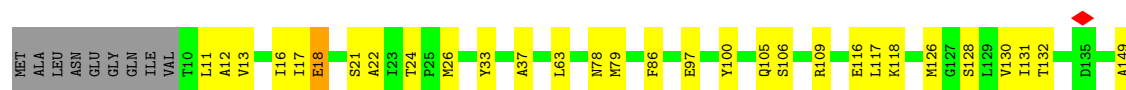
- Molecule 1: Major capsid protein

Chain Ai: 77% 21% ..



- Molecule 1: Major capsid protein

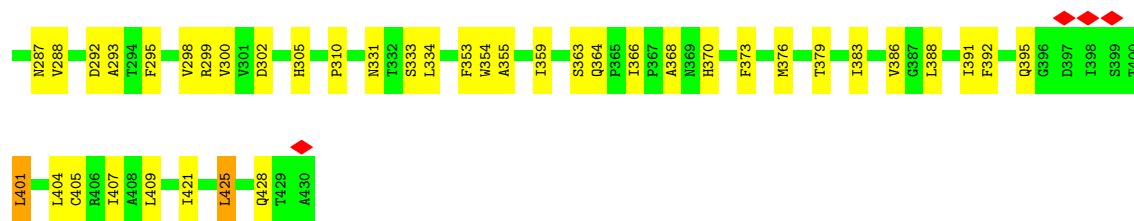
Chain Aj: 74% 23% ..



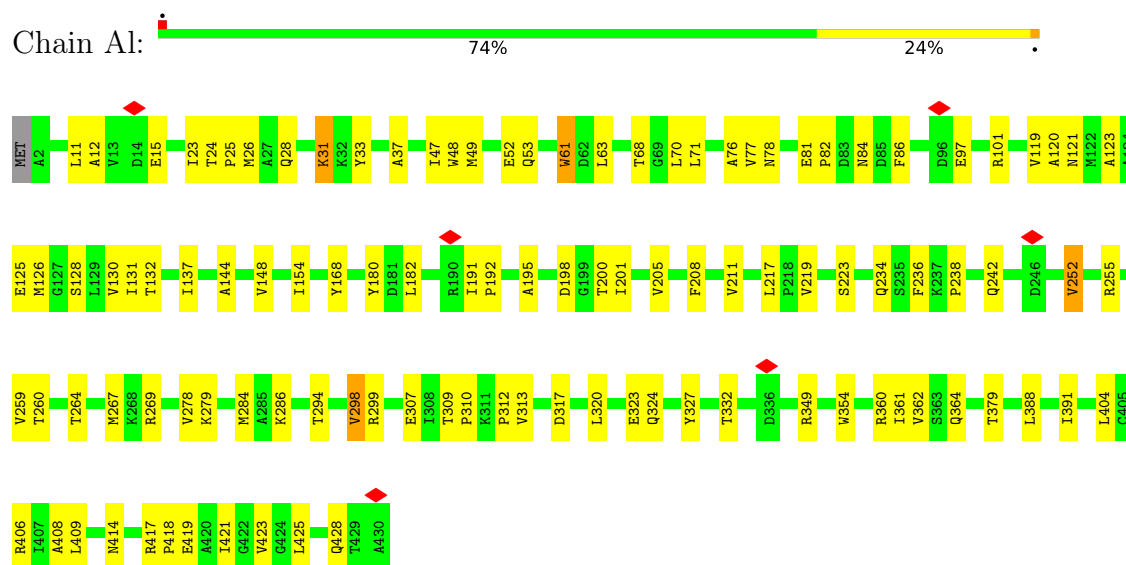
- Molecule 1: Major capsid protein

Chain Ak: 75% 21% ..

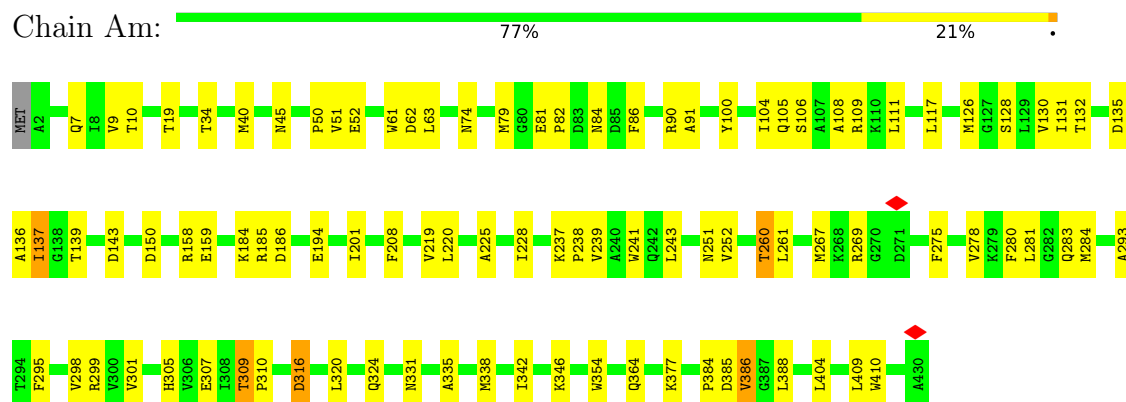




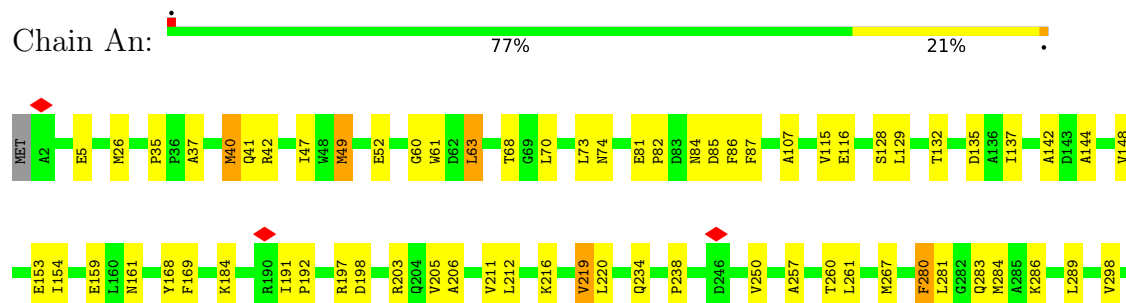
- Molecule 1: Major capsid protein



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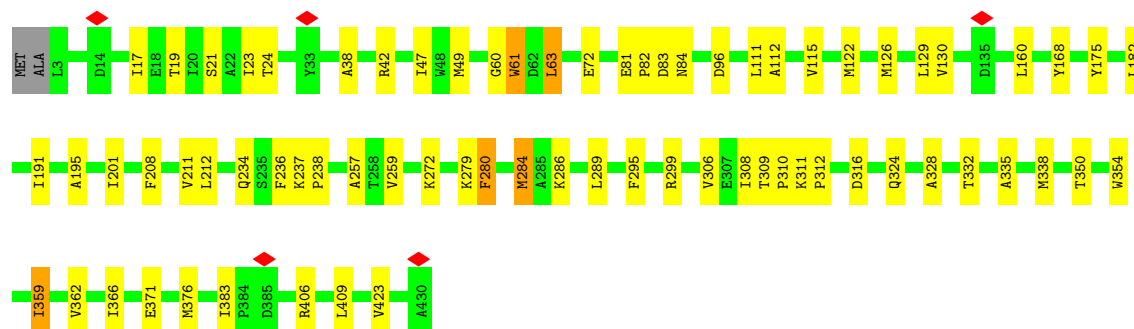
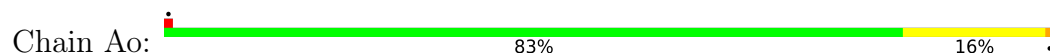


- Molecule 1: Major capsid protein

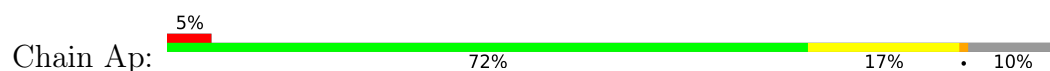




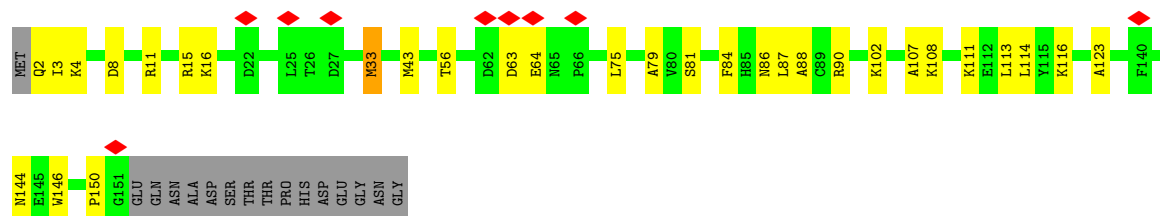
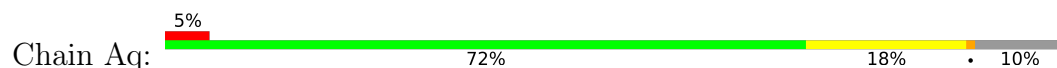
- Molecule 1: Major capsid protein



- Molecule 2: Peptidoglycan hydrolase gp4

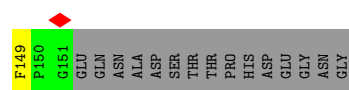


- Molecule 2: Peptidoglycan hydrolase gp4



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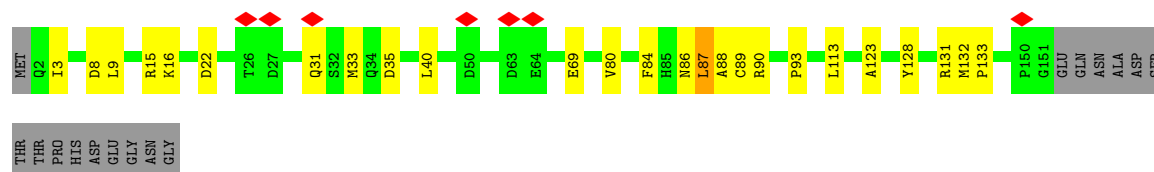
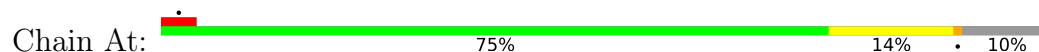




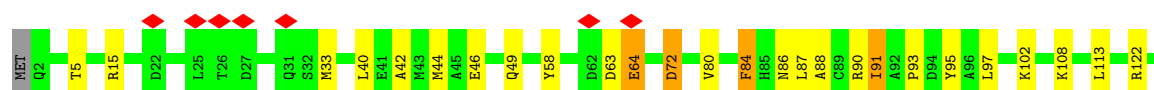
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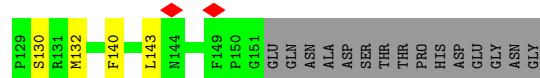
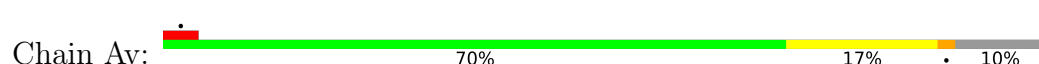
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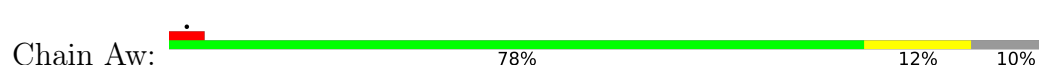
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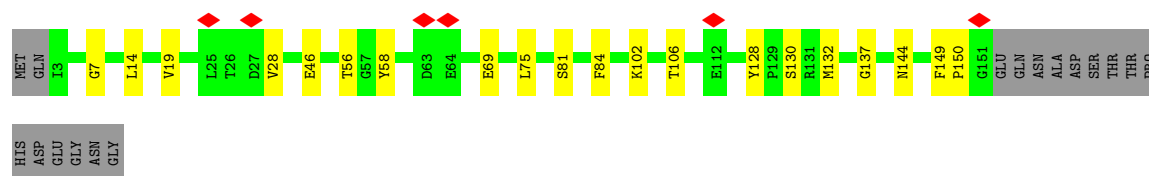


- Molecule 2: Peptidoglycan hydrolase gp4

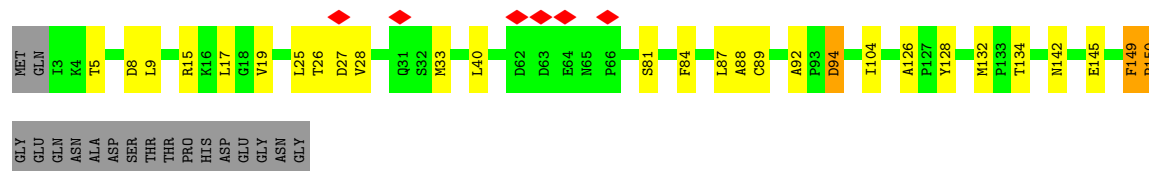


- Molecule 2: Peptidoglycan hydrolase gp4

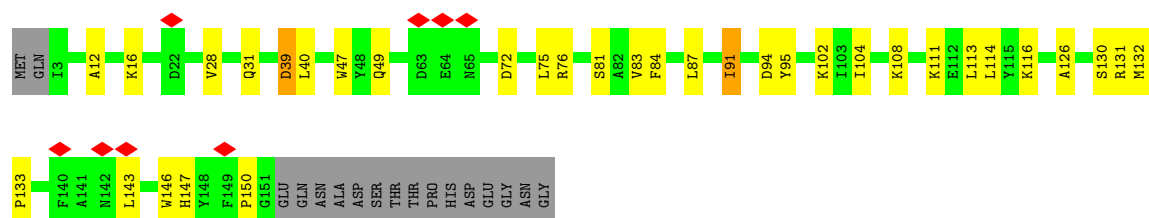




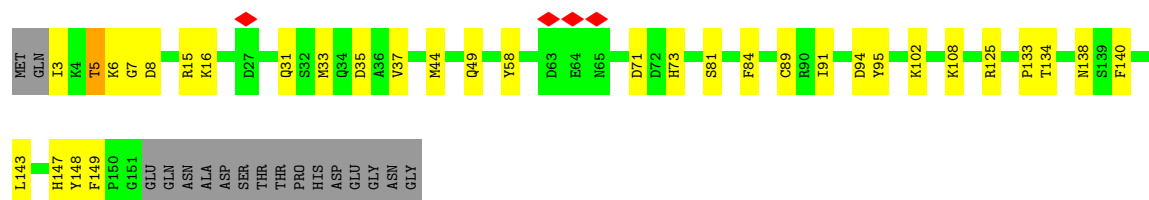
• Molecule 2: Peptidoglycan hydrolase gp4



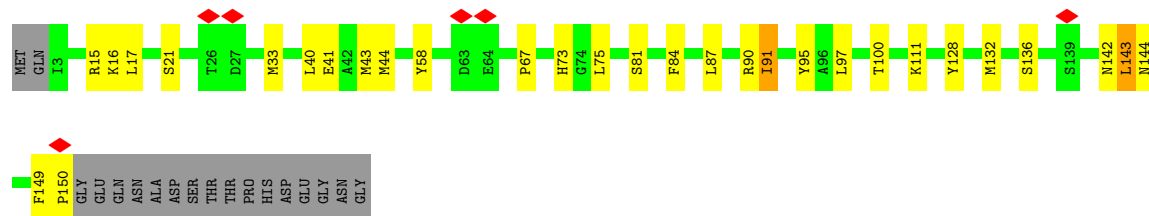
• Molecule 2: Peptidoglycan hydrolase gp4



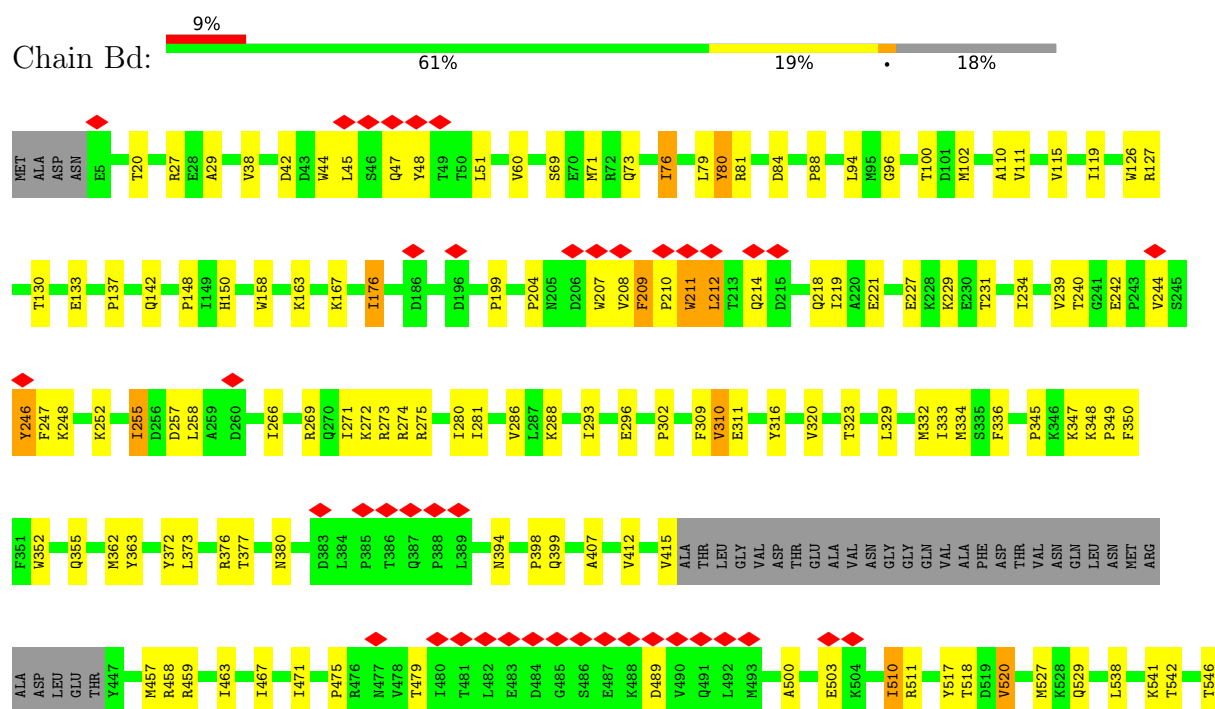
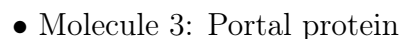
• Molecule 2: Peptidoglycan hydrolase gp4

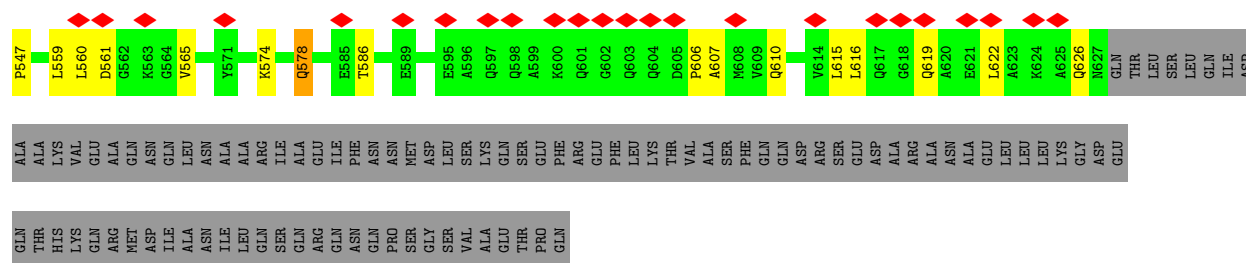


• Molecule 2: Peptidoglycan hydrolase gp4

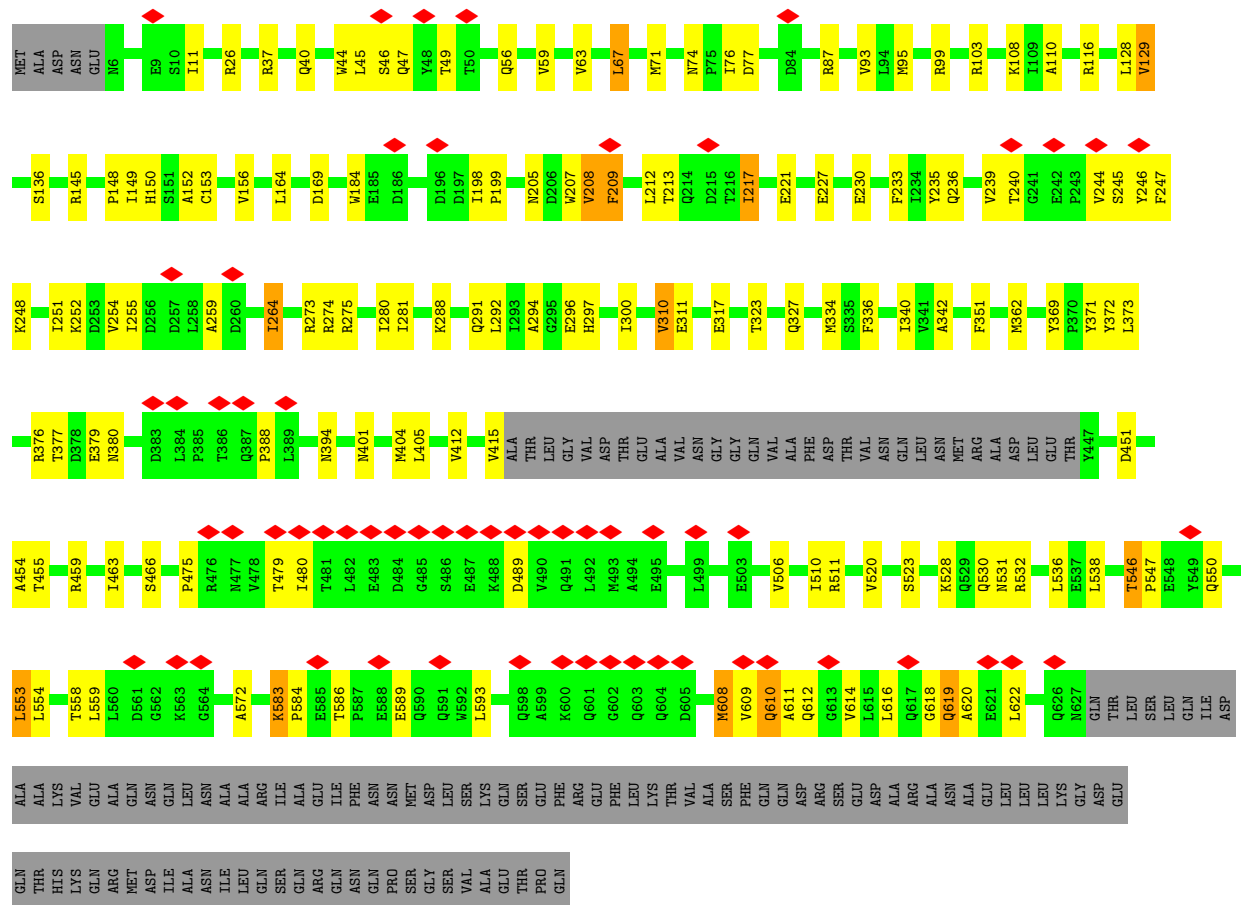


• Molecule 3: Portal protein

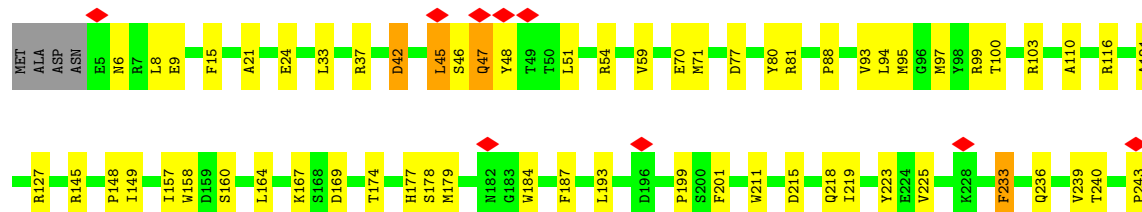


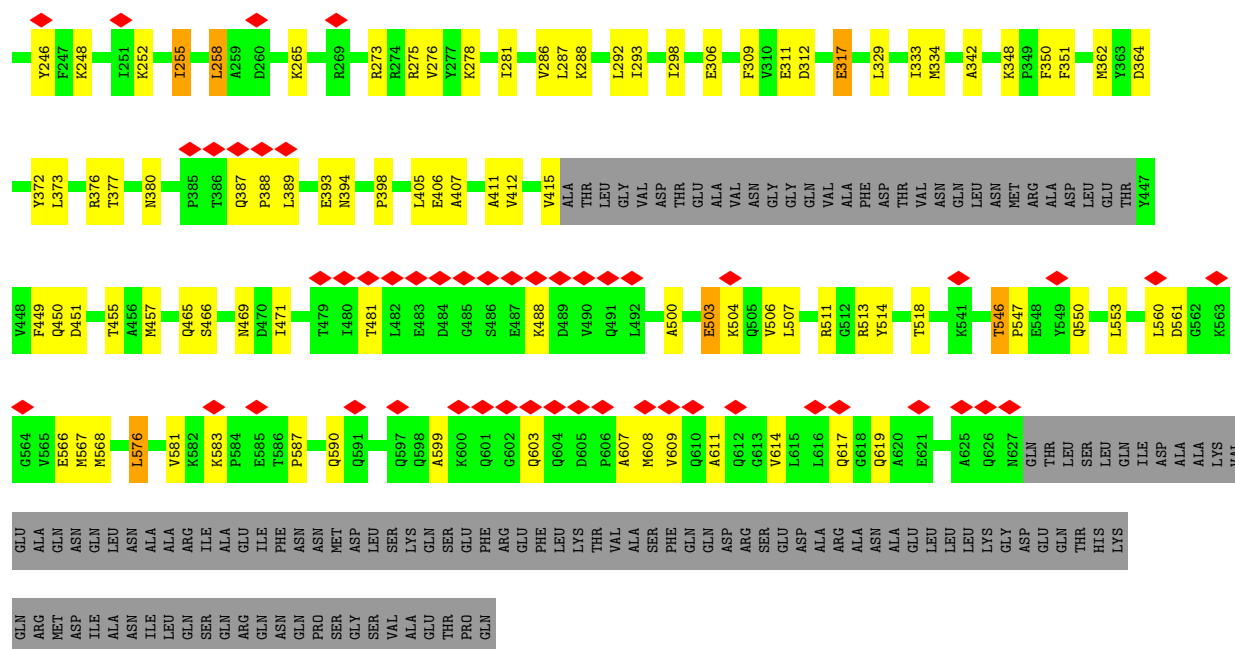


• Molecule 3: Portal protein

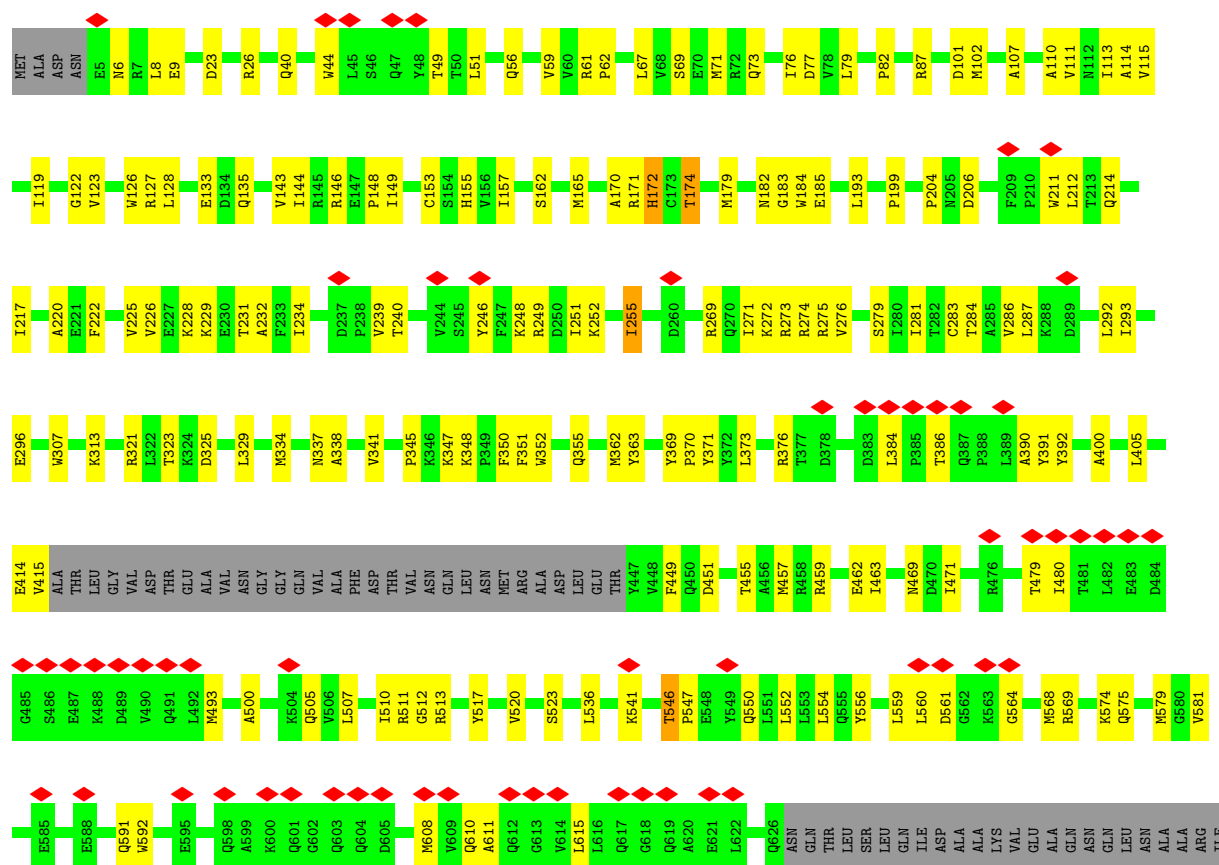


• Molecule 3: Portal protein

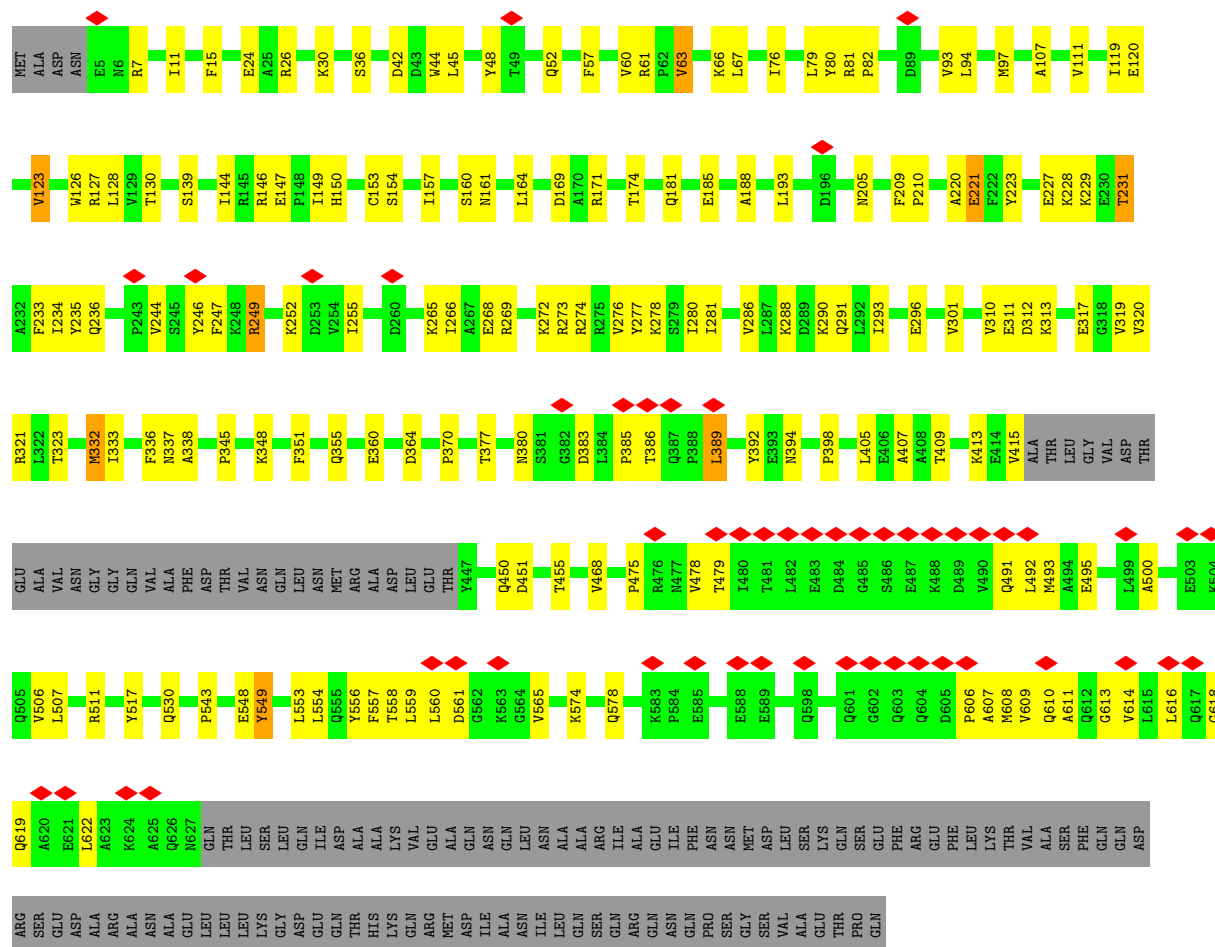




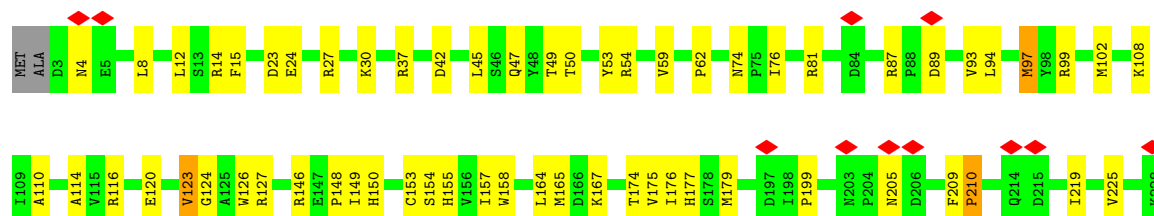
• Molecule 3: Portal protein

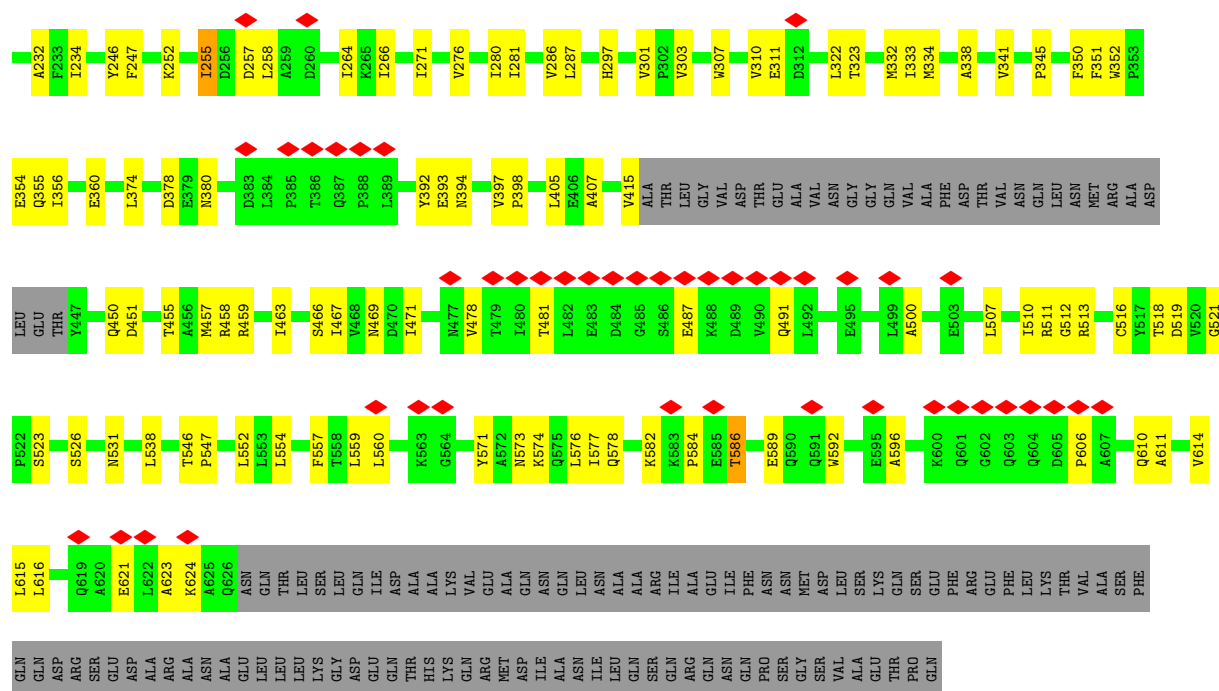


- Molecule 3: Portal protein

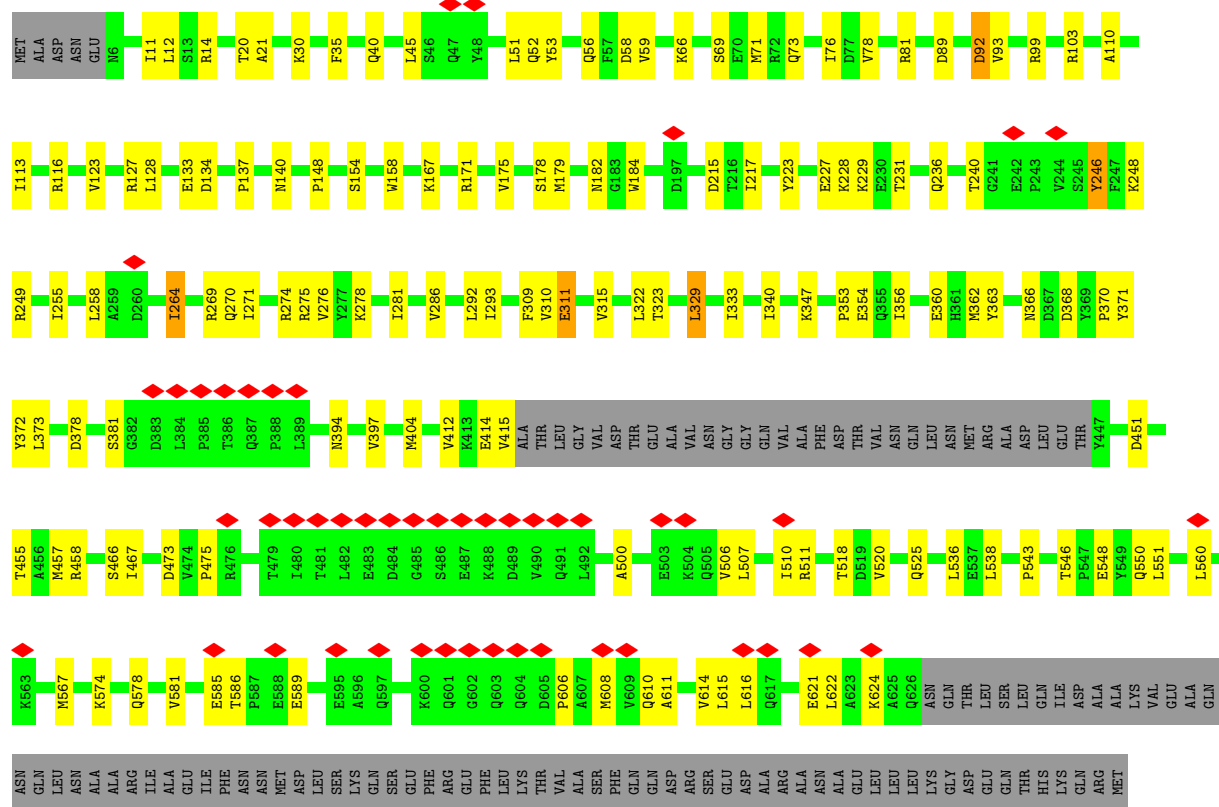


- Molecule 3: Portal protein



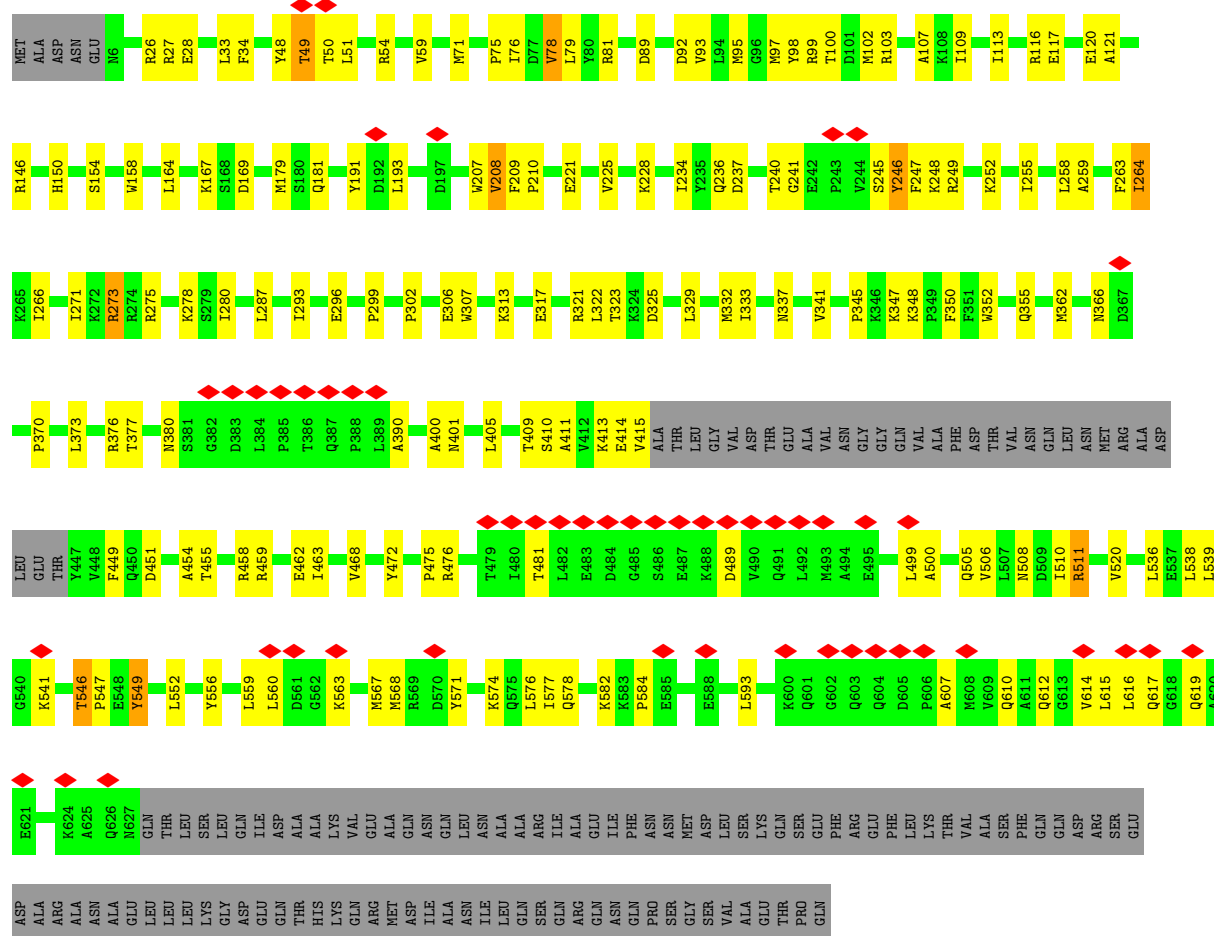


• Molecule 3: Portal protein

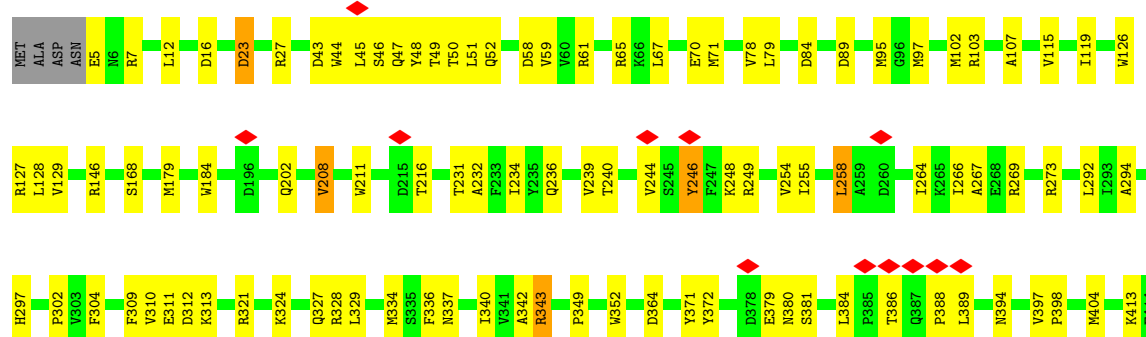


ASP
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SER
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ARG
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VAL
ALA
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THR
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GLN

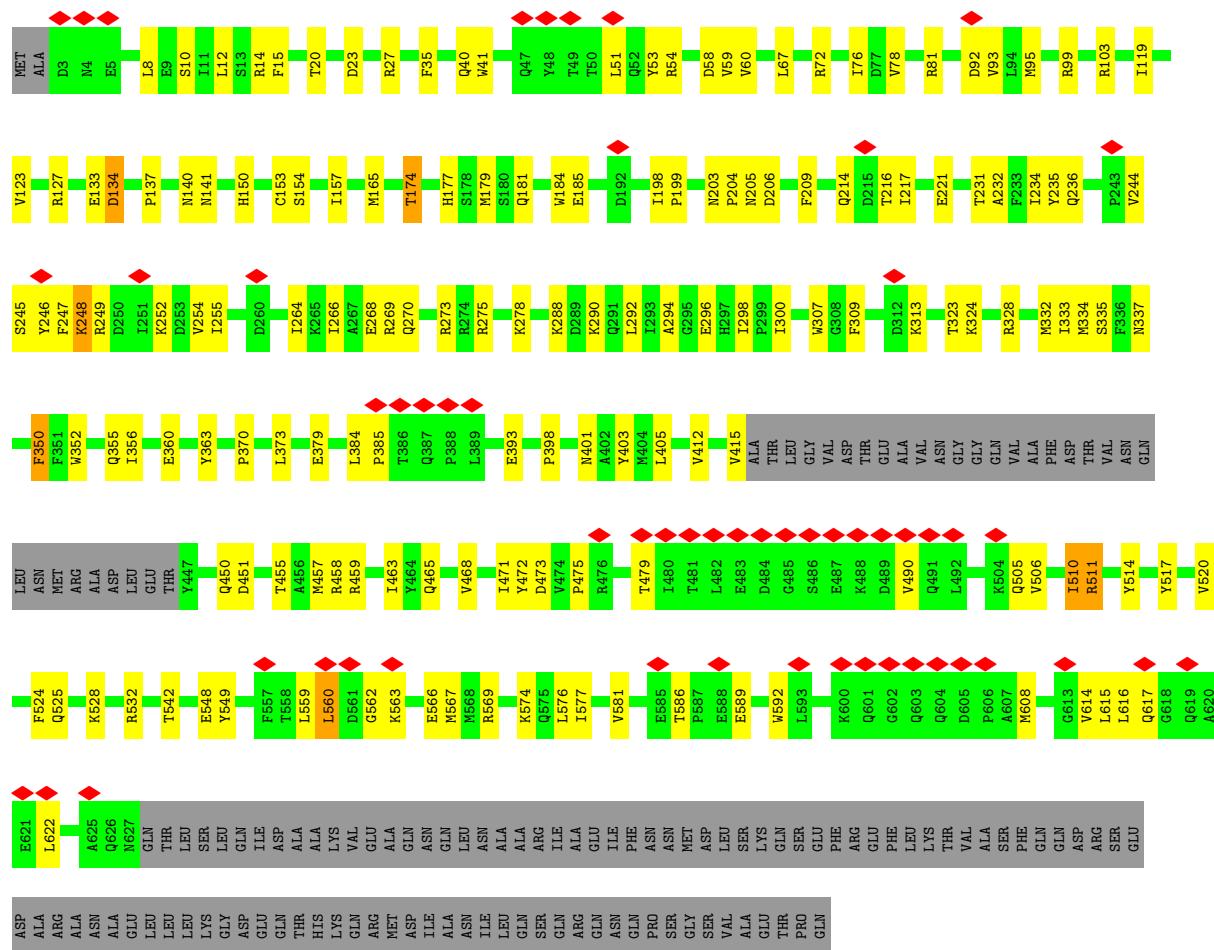
• Molecule 3: Portal protein



• Molecule 3: Portal protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.916	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.13	0/3332	0.33	1/4530 (0.0%)
1	Ab	0.14	0/3284	0.36	0/4466
1	Ac	0.15	0/3335	0.36	0/4535
1	Ad	0.13	0/3332	0.35	1/4530 (0.0%)
1	Ae	0.14	0/3332	0.35	1/4530 (0.0%)
1	Af	0.15	0/3332	0.46	3/4530 (0.1%)
1	Ag	0.14	0/3332	0.36	1/4530 (0.0%)
1	Ah	0.14	0/3270	0.35	0/4446
1	Ai	0.14	0/3292	0.35	0/4477
1	Aj	0.14	0/3277	0.33	0/4456
1	Ak	0.14	0/3284	0.35	0/4466
1	Al	0.13	0/3335	0.33	0/4535
1	Am	0.14	0/3335	0.38	0/4535
1	An	0.14	0/3335	0.35	0/4535
1	Ao	0.15	0/3330	0.36	0/4528
2	Ap	0.15	0/1174	0.35	0/1592
2	Aq	0.14	0/1174	0.33	0/1592
2	Ar	0.13	0/1174	0.33	0/1592
2	As	0.14	0/1174	0.38	0/1592
2	At	0.14	0/1174	0.36	0/1592
2	Au	0.15	0/1174	0.42	0/1592
2	Av	0.14	0/1165	0.34	0/1580
2	Aw	0.14	0/1165	0.35	0/1580
2	Ax	0.15	0/1161	0.37	0/1575
2	Ay	0.14	0/1165	0.32	0/1580
2	Az	0.15	0/1165	0.36	0/1580
2	Ba	0.14	0/1161	0.36	0/1575
3	Bb	0.15	0/4875	0.36	1/6610 (0.0%)
3	Bd	0.14	0/4892	0.35	0/6633
3	Bf	0.14	0/4883	0.39	0/6621
3	Bh	0.14	0/4892	0.37	0/6633
3	Bj	0.15	0/4884	0.37	0/6622
3	Bl	0.14	0/4892	0.36	0/6633
3	Bn	0.15	0/4900	0.39	1/6644 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Bp	0.14	0/4875	0.35	0/6610
3	Br	0.14	0/4883	0.36	1/6621 (0.0%)
3	Bt	0.14	0/4884	0.36	0/6622
3	Bv	0.14	0/4884	0.35	1/6622 (0.0%)
3	Bx	0.14	0/4908	0.39	0/6655
All	All	0.14	0/122415	0.36	11/166177 (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	Ag	0	1
3	Bf	0	1
3	Bl	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Af	367	PRO	N-CA-CB	12.62	111.23	102.65
1	Ad	367	PRO	N-CA-CB	8.01	110.32	103.35
1	Aa	367	PRO	N-CA-CB	7.93	110.70	103.33
1	Ag	367	PRO	N-CA-CB	7.45	109.97	103.27
3	Bn	59	VAL	N-CA-C	-6.94	107.12	113.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ag	32	LYS	Peptide
3	Bf	208	VAL	Peptide
3	Bl	57	PHE	Peptide

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	Aa	3275	0	3241	77	0
1	Ab	3226	0	3197	65	0
1	Ac	3277	0	3247	53	0
1	Ad	3275	0	3241	75	0
1	Ae	3275	0	3241	78	0
1	Af	3275	0	3241	93	0
1	Ag	3275	0	3241	81	0
1	Ah	3212	0	3181	77	0
1	Ai	3234	0	3208	55	0
1	Aj	3219	0	3188	61	0
1	Ak	3226	0	3197	71	0
1	Al	3277	0	3247	69	0
1	Am	3277	0	3247	59	0
1	An	3277	0	3247	62	0
1	Ao	3272	0	3242	43	0
2	Ap	1149	0	1115	17	0
2	Aq	1149	0	1115	24	0
2	Ar	1149	0	1115	23	0
2	As	1149	0	1115	27	0
2	At	1149	0	1115	19	0
2	Au	1149	0	1115	41	0
2	Av	1140	0	1107	24	0
2	Aw	1140	0	1107	12	0
2	Ax	1136	0	1104	30	0
2	Ay	1140	0	1107	26	0
2	Az	1140	0	1107	25	0
2	Ba	1136	0	1104	24	0
3	Bb	4774	0	4636	135	0
3	Bd	4791	0	4648	123	0
3	Bf	4782	0	4642	128	0
3	Bh	4791	0	4648	120	0
3	Bj	4783	0	4642	146	0
3	Bl	4791	0	4648	129	0
3	Bn	4799	0	4652	139	0
3	Bp	4774	0	4636	118	0
3	Br	4782	0	4642	130	0
3	Bt	4783	0	4642	119	0
3	Bv	4783	0	4642	144	0
3	Bx	4807	0	4658	133	0
All	All	120038	0	117468	2313	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 10.

The worst 5 of 2313 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:Bd:255:ILE:HD12	3:Bh:506:VAL:HB	1.44	0.99
3:Bn:334:MET:HE3	3:Bn:405:LEU:HD11	1.52	0.92
3:Bf:40:GLN:HE22	3:Bf:327:GLN:HE21	1.16	0.88
2:Aw:144:ASN:HB3	3:Bl:44:TRP:HE1	1.38	0.88
2:Ap:40:LEU:HD13	2:Ap:87:LEU:HD22	1.57	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	427/430 (99%)	411 (96%)	15 (4%)	1 (0%)	43	64
1	Ab	420/430 (98%)	400 (95%)	20 (5%)	0	100	100
1	Ac	427/430 (99%)	417 (98%)	10 (2%)	0	100	100
1	Ad	427/430 (99%)	409 (96%)	17 (4%)	1 (0%)	43	64
1	Ae	427/430 (99%)	406 (95%)	20 (5%)	1 (0%)	43	64
1	Af	427/430 (99%)	398 (93%)	28 (7%)	1 (0%)	43	64
1	Ag	427/430 (99%)	405 (95%)	22 (5%)	0	100	100
1	Ah	418/430 (97%)	396 (95%)	22 (5%)	0	100	100
1	Ai	421/430 (98%)	405 (96%)	16 (4%)	0	100	100
1	Aj	419/430 (97%)	406 (97%)	13 (3%)	0	100	100
1	Ak	420/430 (98%)	394 (94%)	26 (6%)	0	100	100
1	Al	427/430 (99%)	414 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Am	427/430 (99%)	407 (95%)	19 (4%)	1 (0%)	43	64
1	An	427/430 (99%)	408 (96%)	19 (4%)	0	100	100
1	Ao	426/430 (99%)	407 (96%)	19 (4%)	0	100	100
2	Ap	148/166 (89%)	141 (95%)	7 (5%)	0	100	100
2	Aq	148/166 (89%)	140 (95%)	8 (5%)	0	100	100
2	Ar	148/166 (89%)	139 (94%)	9 (6%)	0	100	100
2	As	148/166 (89%)	139 (94%)	8 (5%)	1 (1%)	18	34
2	At	148/166 (89%)	136 (92%)	12 (8%)	0	100	100
2	Au	148/166 (89%)	131 (88%)	17 (12%)	0	100	100
2	Av	147/166 (89%)	141 (96%)	6 (4%)	0	100	100
2	Aw	147/166 (89%)	141 (96%)	6 (4%)	0	100	100
2	Ax	146/166 (88%)	139 (95%)	7 (5%)	0	100	100
2	Ay	147/166 (89%)	144 (98%)	3 (2%)	0	100	100
2	Az	147/166 (89%)	142 (97%)	5 (3%)	0	100	100
2	Ba	146/166 (88%)	138 (94%)	8 (6%)	0	100	100
3	Bb	586/725 (81%)	544 (93%)	40 (7%)	2 (0%)	36	56
3	Bd	588/725 (81%)	535 (91%)	49 (8%)	4 (1%)	18	34
3	Bf	587/725 (81%)	529 (90%)	57 (10%)	1 (0%)	43	64
3	Bh	588/725 (81%)	544 (92%)	43 (7%)	1 (0%)	43	64
3	Bj	587/725 (81%)	539 (92%)	47 (8%)	1 (0%)	43	64
3	Bl	588/725 (81%)	531 (90%)	56 (10%)	1 (0%)	43	64
3	Bn	589/725 (81%)	524 (89%)	64 (11%)	1 (0%)	43	64
3	Bp	586/725 (81%)	530 (90%)	55 (9%)	1 (0%)	43	64
3	Br	587/725 (81%)	544 (93%)	42 (7%)	1 (0%)	43	64
3	Bt	587/725 (81%)	543 (92%)	41 (7%)	3 (0%)	24	43
3	Bv	587/725 (81%)	552 (94%)	34 (6%)	1 (0%)	43	64
3	Bx	590/725 (81%)	549 (93%)	40 (7%)	1 (0%)	43	64
All	All	15185/17142 (89%)	14218 (94%)	943 (6%)	24 (0%)	44	64

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	As	124	LYS

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Mol	Chain	Res	Type
3	Bl	389	LEU
3	Br	208	VAL
3	Bt	23	ASP
1	Af	39	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	350/352 (99%)	335 (96%)	15 (4%)	26	47
1	Ab	346/352 (98%)	329 (95%)	17 (5%)	22	43
1	Ac	351/352 (100%)	337 (96%)	14 (4%)	28	50
1	Ad	350/352 (99%)	329 (94%)	21 (6%)	17	32
1	Ae	350/352 (99%)	333 (95%)	17 (5%)	22	43
1	Af	350/352 (99%)	336 (96%)	14 (4%)	28	50
1	Ag	350/352 (99%)	339 (97%)	11 (3%)	35	59
1	Ah	344/352 (98%)	327 (95%)	17 (5%)	22	43
1	Ai	347/352 (99%)	332 (96%)	15 (4%)	26	47
1	Aj	345/352 (98%)	328 (95%)	17 (5%)	22	43
1	Ak	346/352 (98%)	327 (94%)	19 (6%)	19	37
1	Al	351/352 (100%)	338 (96%)	13 (4%)	30	54
1	Am	351/352 (100%)	335 (95%)	16 (5%)	24	45
1	An	351/352 (100%)	331 (94%)	20 (6%)	18	35
1	Ao	351/352 (100%)	334 (95%)	17 (5%)	23	44
2	Ap	118/131 (90%)	115 (98%)	3 (2%)	42	64
2	Aq	118/131 (90%)	117 (99%)	1 (1%)	73	84
2	Ar	118/131 (90%)	115 (98%)	3 (2%)	42	64
2	As	118/131 (90%)	109 (92%)	9 (8%)	12	23
2	At	118/131 (90%)	114 (97%)	4 (3%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Au	118/131 (90%)	113 (96%)	5 (4%)	26	49
2	Av	117/131 (89%)	112 (96%)	5 (4%)	26	47
2	Aw	117/131 (89%)	115 (98%)	2 (2%)	53	71
2	Ax	117/131 (89%)	113 (97%)	4 (3%)	32	57
2	Ay	117/131 (89%)	111 (95%)	6 (5%)	21	40
2	Az	117/131 (89%)	115 (98%)	2 (2%)	53	71
2	Ba	117/131 (89%)	113 (97%)	4 (3%)	32	57
3	Bb	517/630 (82%)	494 (96%)	23 (4%)	25	47
3	Bd	519/630 (82%)	495 (95%)	24 (5%)	24	45
3	Bf	518/630 (82%)	499 (96%)	19 (4%)	30	54
3	Bh	519/630 (82%)	495 (95%)	24 (5%)	24	45
3	Bj	518/630 (82%)	499 (96%)	19 (4%)	30	54
3	Bl	519/630 (82%)	496 (96%)	23 (4%)	25	47
3	Bn	520/630 (82%)	502 (96%)	18 (4%)	32	56
3	Bp	517/630 (82%)	493 (95%)	24 (5%)	24	45
3	Br	518/630 (82%)	494 (95%)	24 (5%)	24	45
3	Bt	518/630 (82%)	499 (96%)	19 (4%)	30	54
3	Bv	518/630 (82%)	498 (96%)	20 (4%)	28	51
3	Bx	521/630 (83%)	495 (95%)	26 (5%)	22	42
All	All	12865/14412 (89%)	12311 (96%)	554 (4%)	27	47

5 of 554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Bp	536	LEU
3	Br	264	ILE
3	Bp	520	VAL
3	Bv	455	THR
1	Am	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
3	Bn	598	GLN

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Mol	Chain	Res	Type
3	Bv	469	ASN
3	Bp	270	GLN
3	Br	366	ASN
3	Bx	135	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.

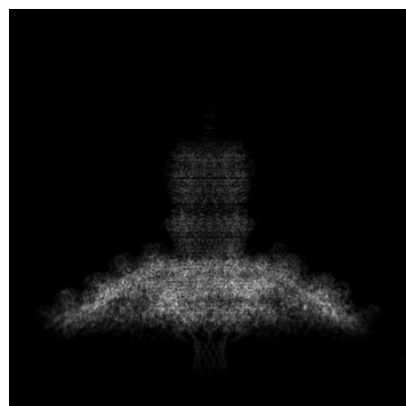
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71631. These allow visual inspection of the internal detail of the map and identification of artifacts.

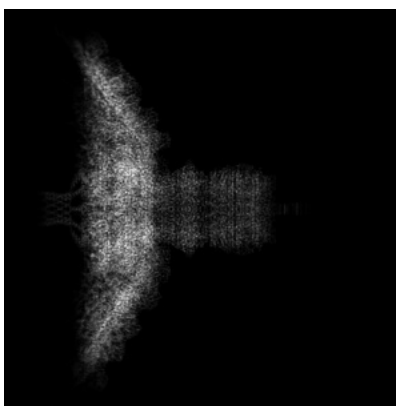
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

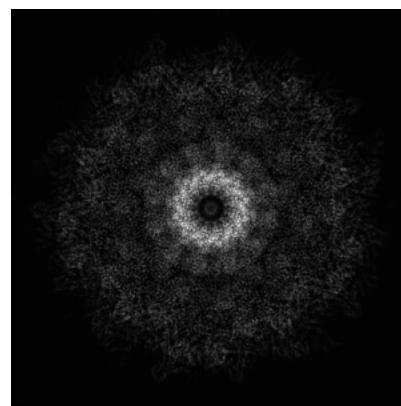
6.1.1 Primary map



X

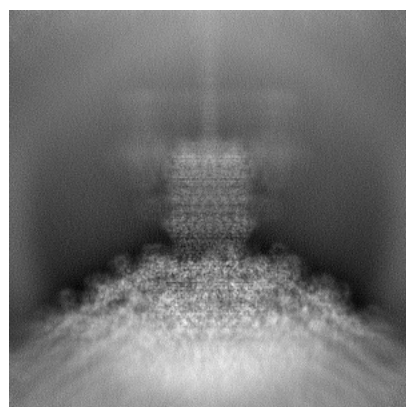


Y

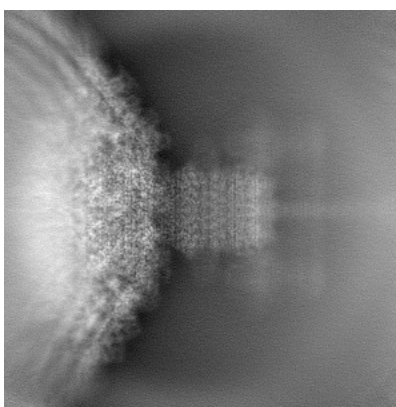


Z

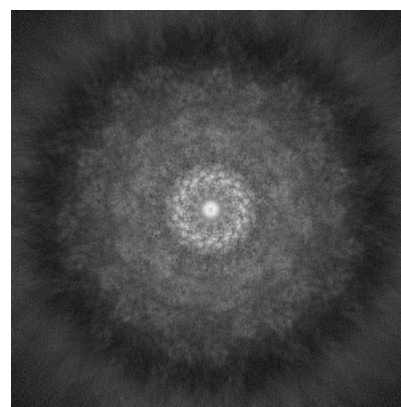
6.1.2 Raw map



X



Y

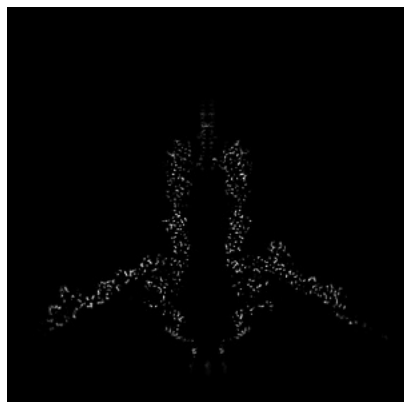


Z

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

6.2 Central slices [i](#)

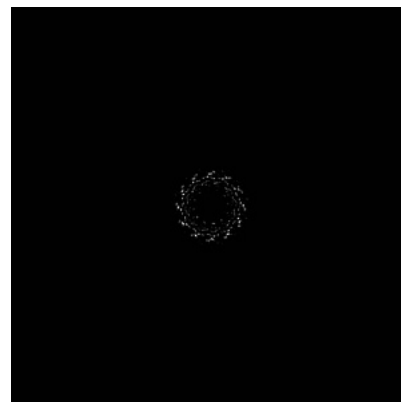
6.2.1 Primary map



X Index: 224

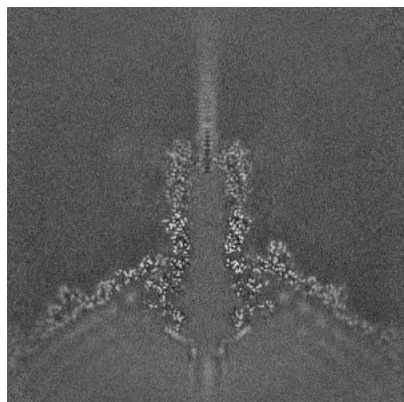


Y Index: 224

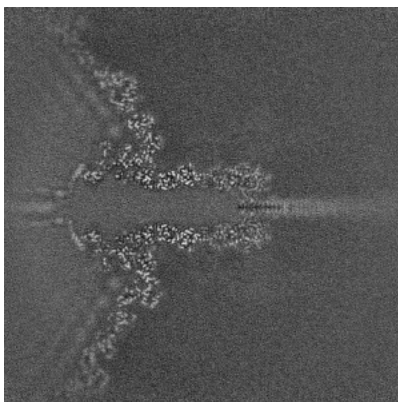


Z Index: 224

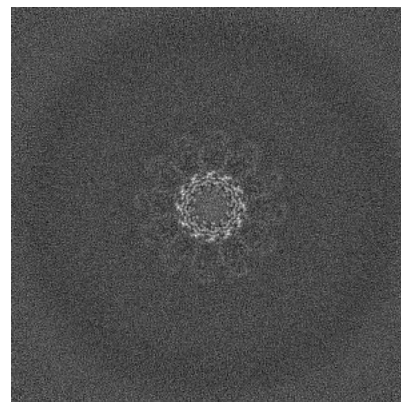
6.2.2 Raw map



X Index: 224



Y Index: 224

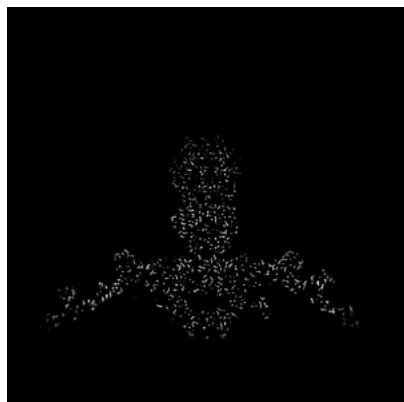


Z Index: 224

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

6.3 Largest variance slices [i](#)

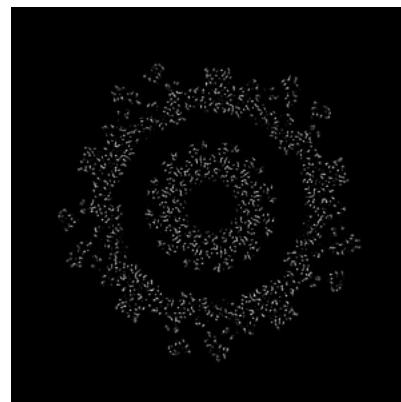
6.3.1 Primary map



X Index: 192

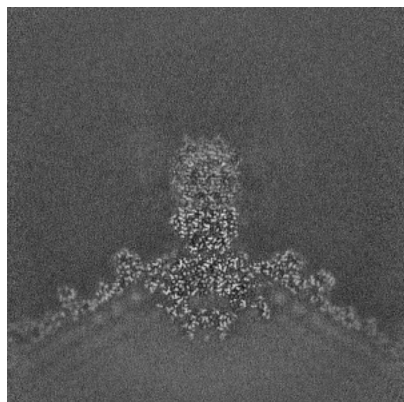


Y Index: 253

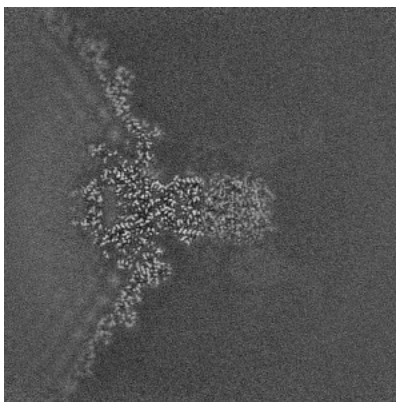


Z Index: 128

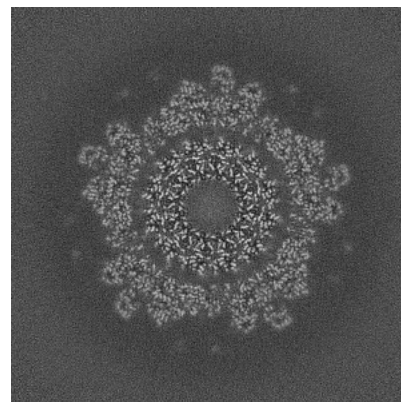
6.3.2 Raw map



X Index: 193



Y Index: 253

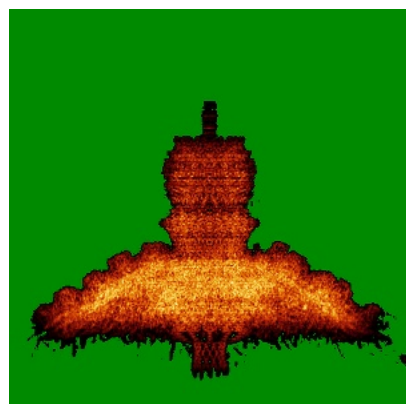


Z Index: 137

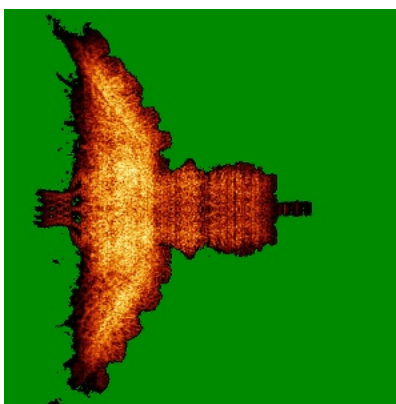
The images above show the largest variance slices of the map in three orthogonal directions.

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

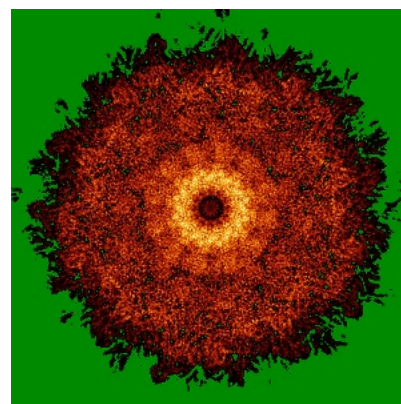
6.4.1 Primary map



X

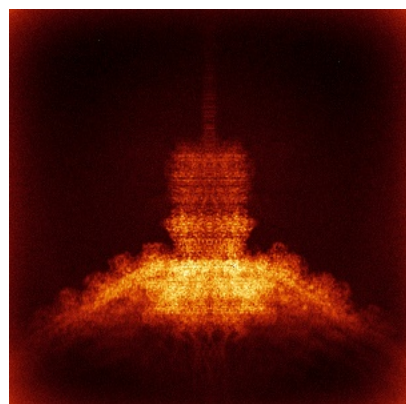


Y

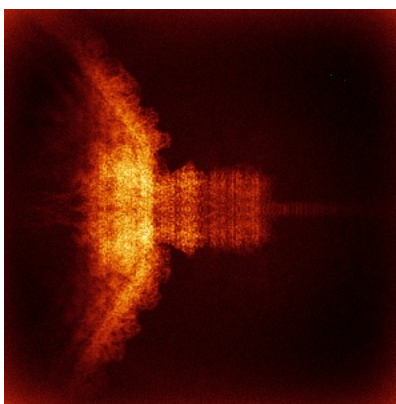


Z

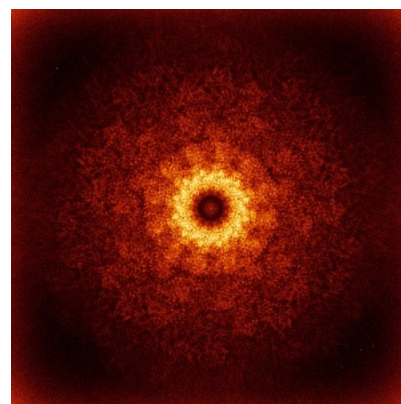
6.4.2 Raw map



X



Y

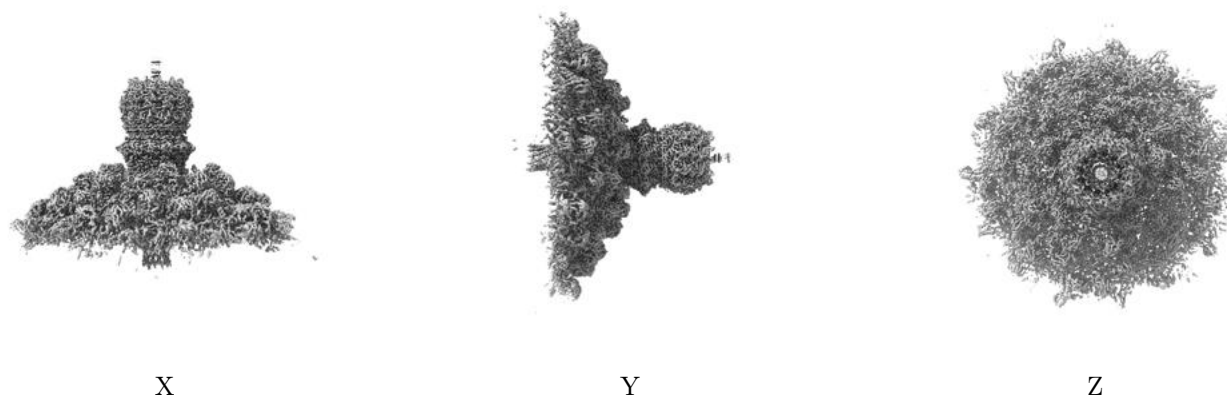


Z

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.

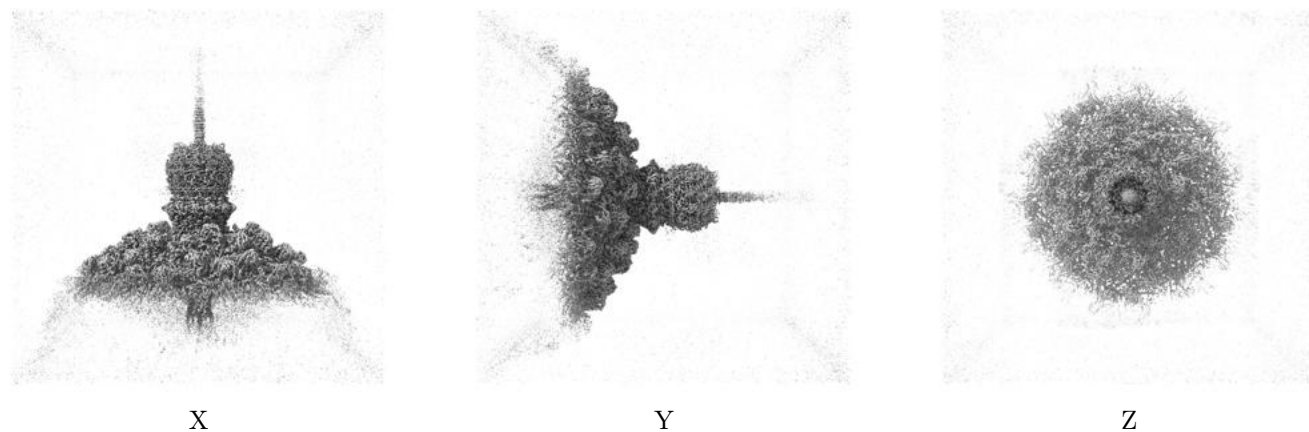
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

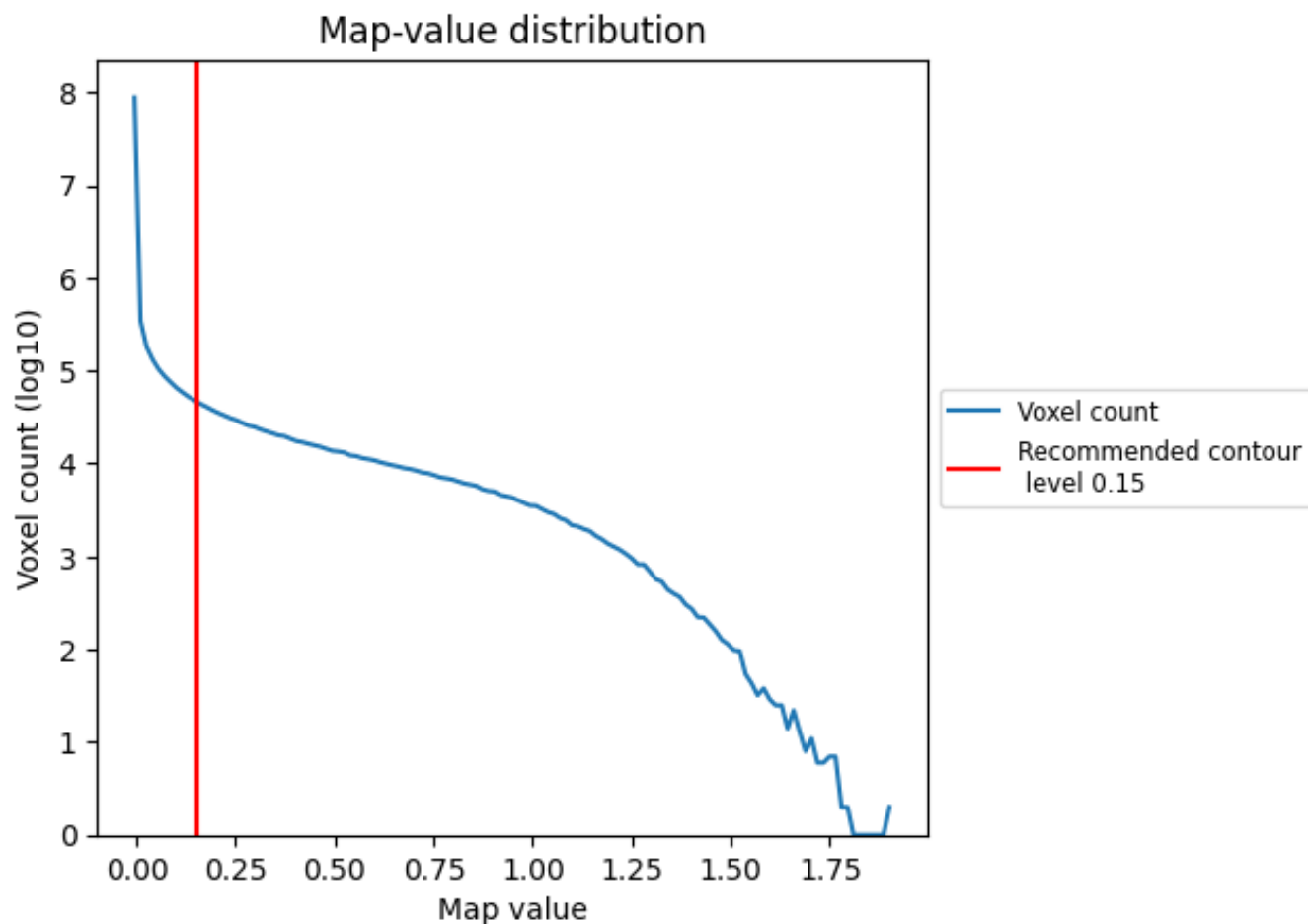
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

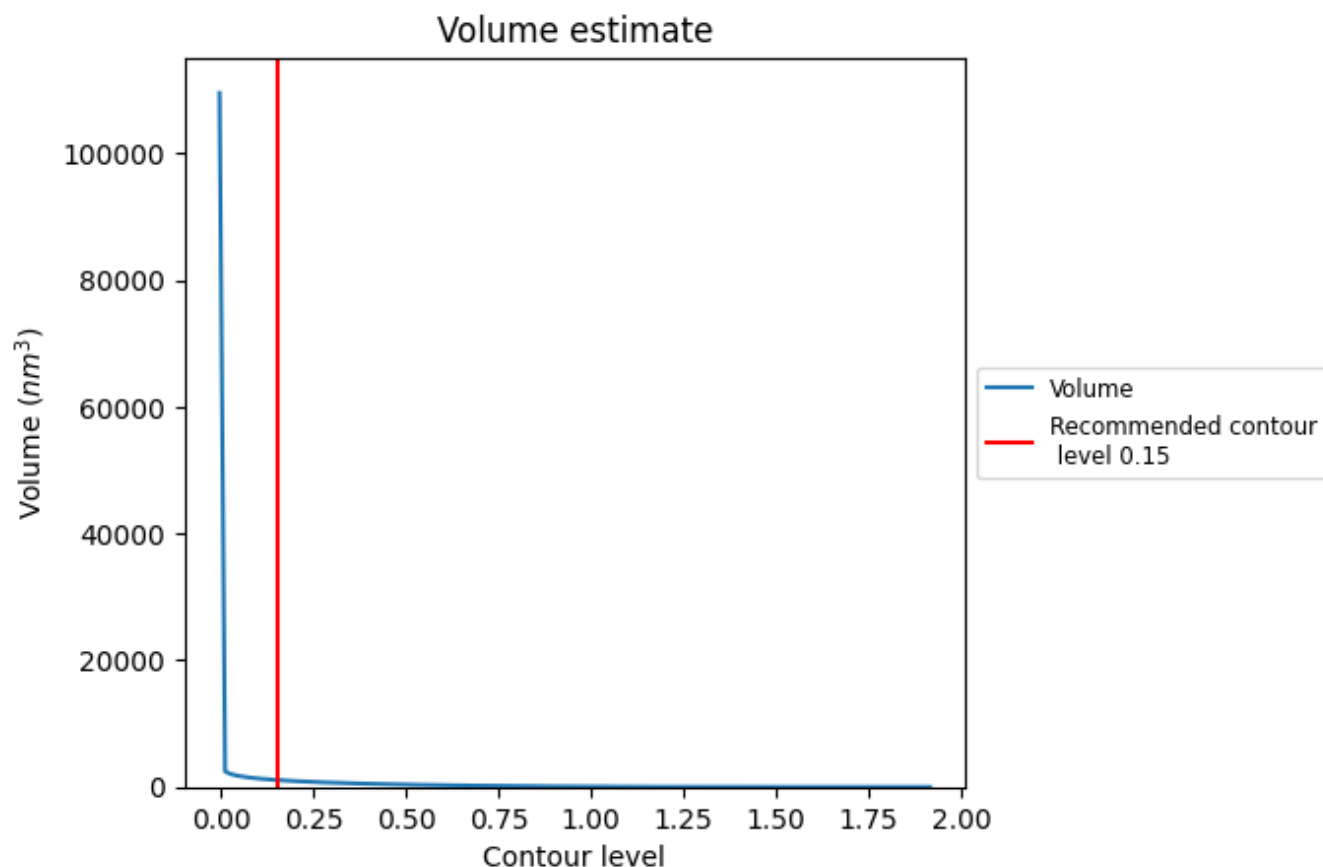
This section contains the results of statistical analysis of the map.

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.

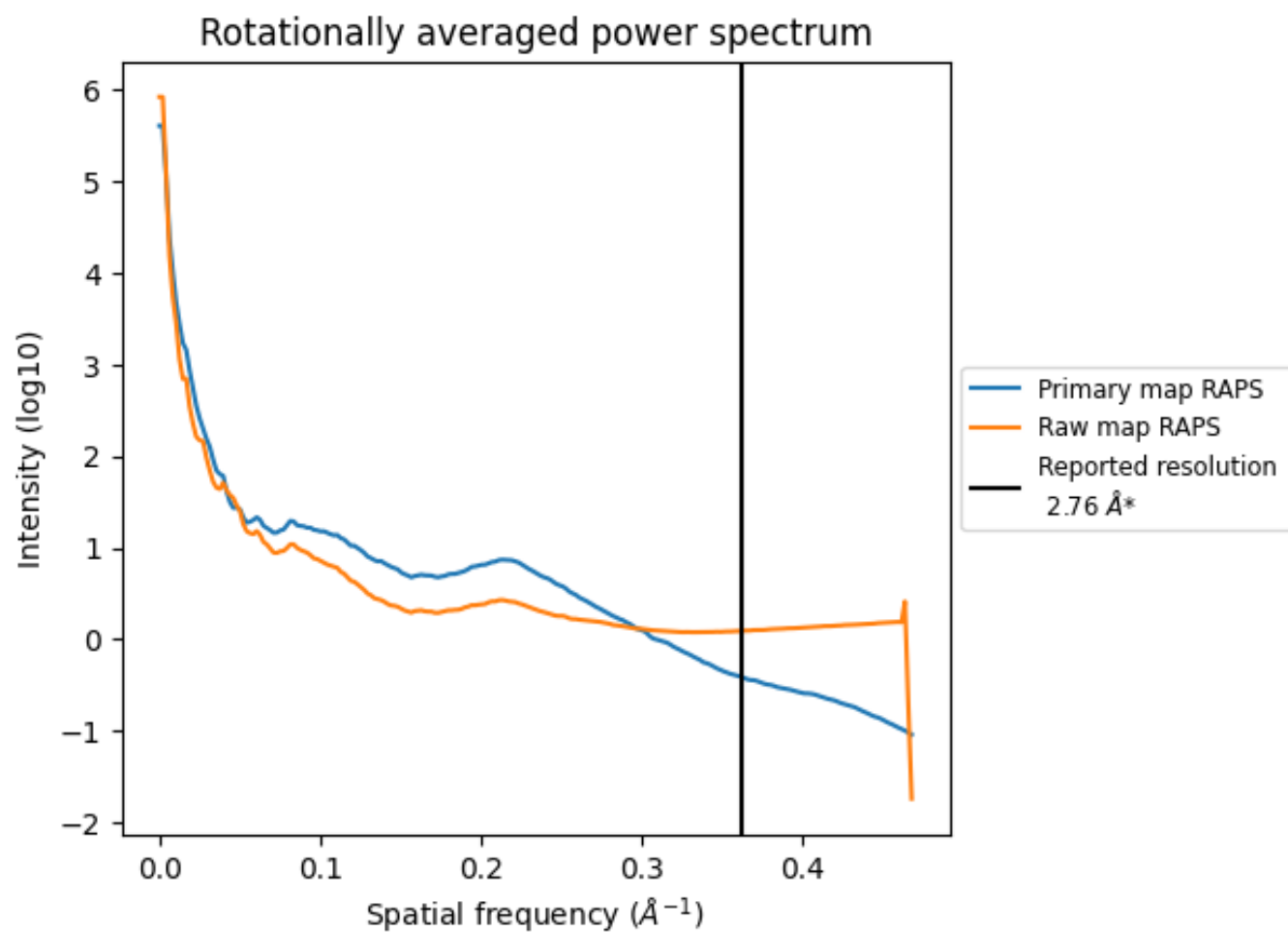
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1095 nm^3 ; this corresponds to an approximate mass of 989 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 ⓘ

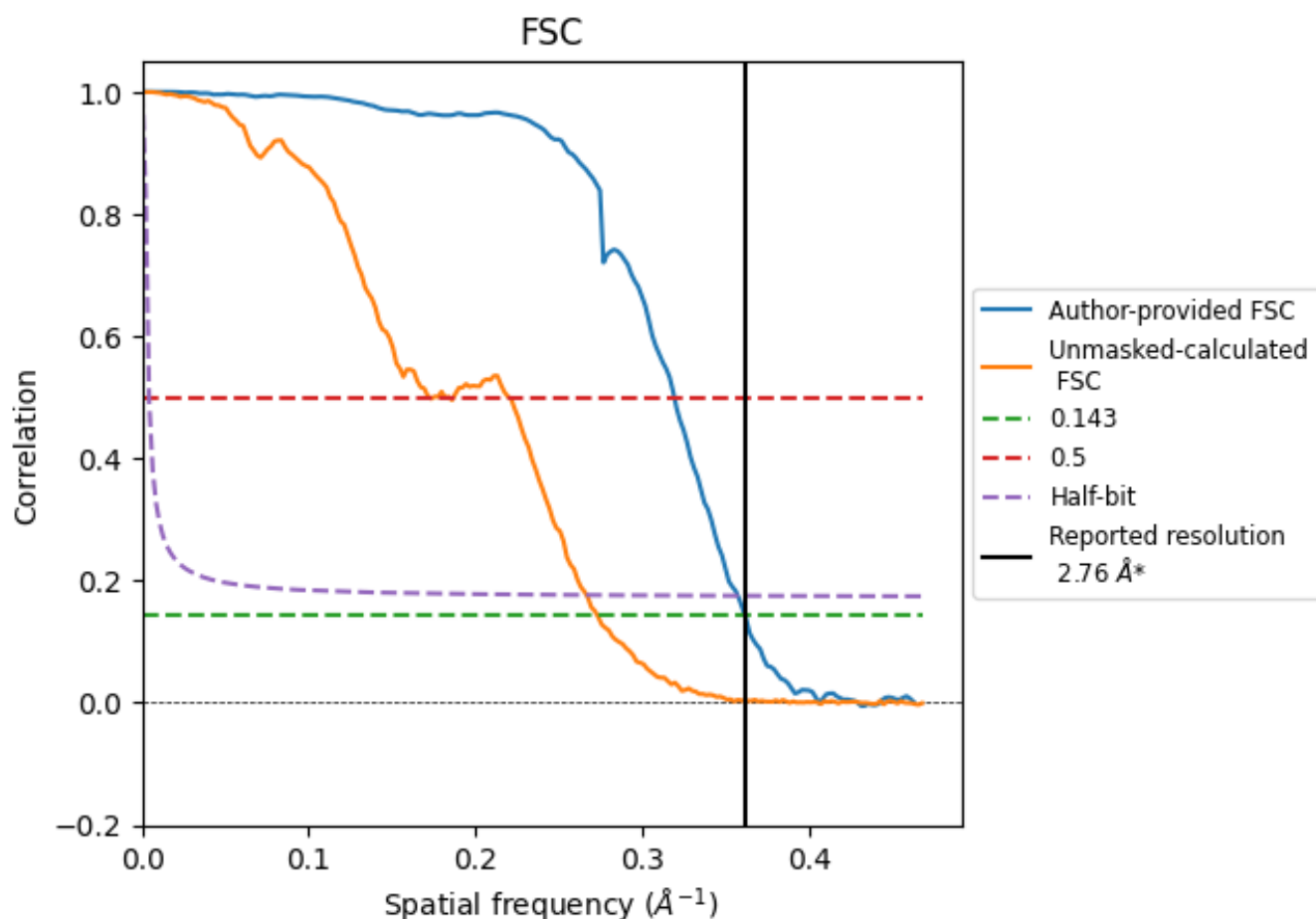


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

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 $0.362 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

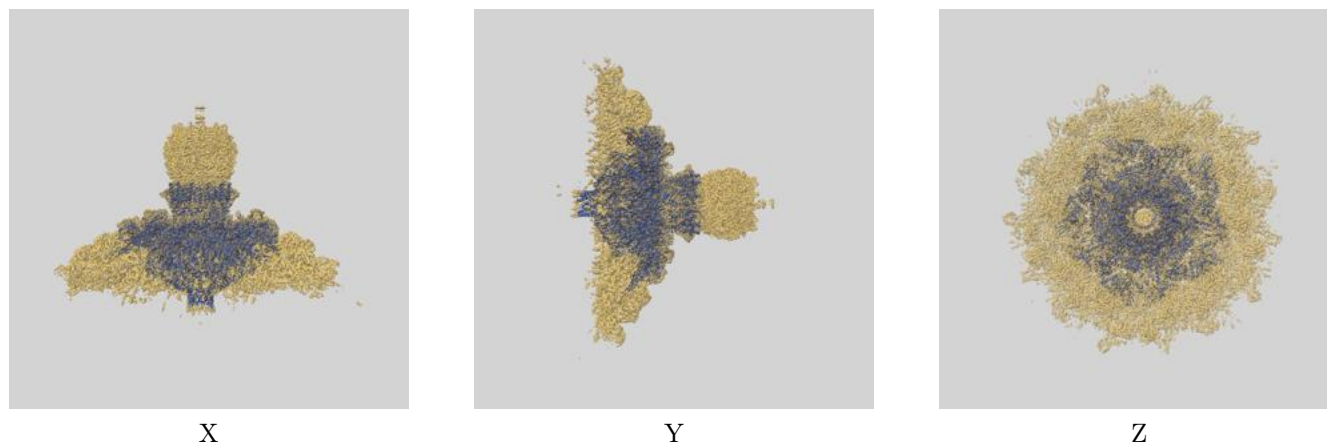
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.13	2.80
Unmasked-calculated*	3.66	5.80	3.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

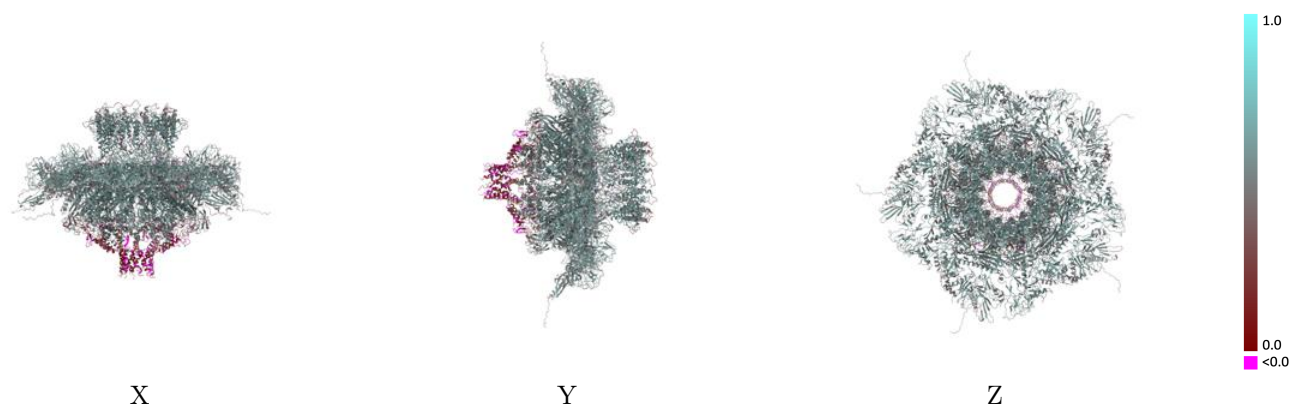
This section contains information regarding the fit between EMDB map EMD-71631 and PDB model 9PGG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



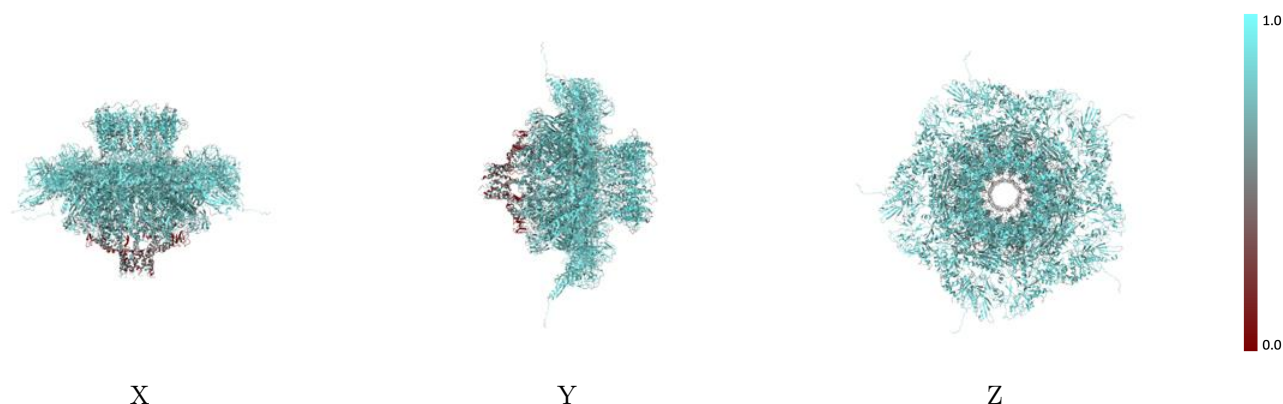
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



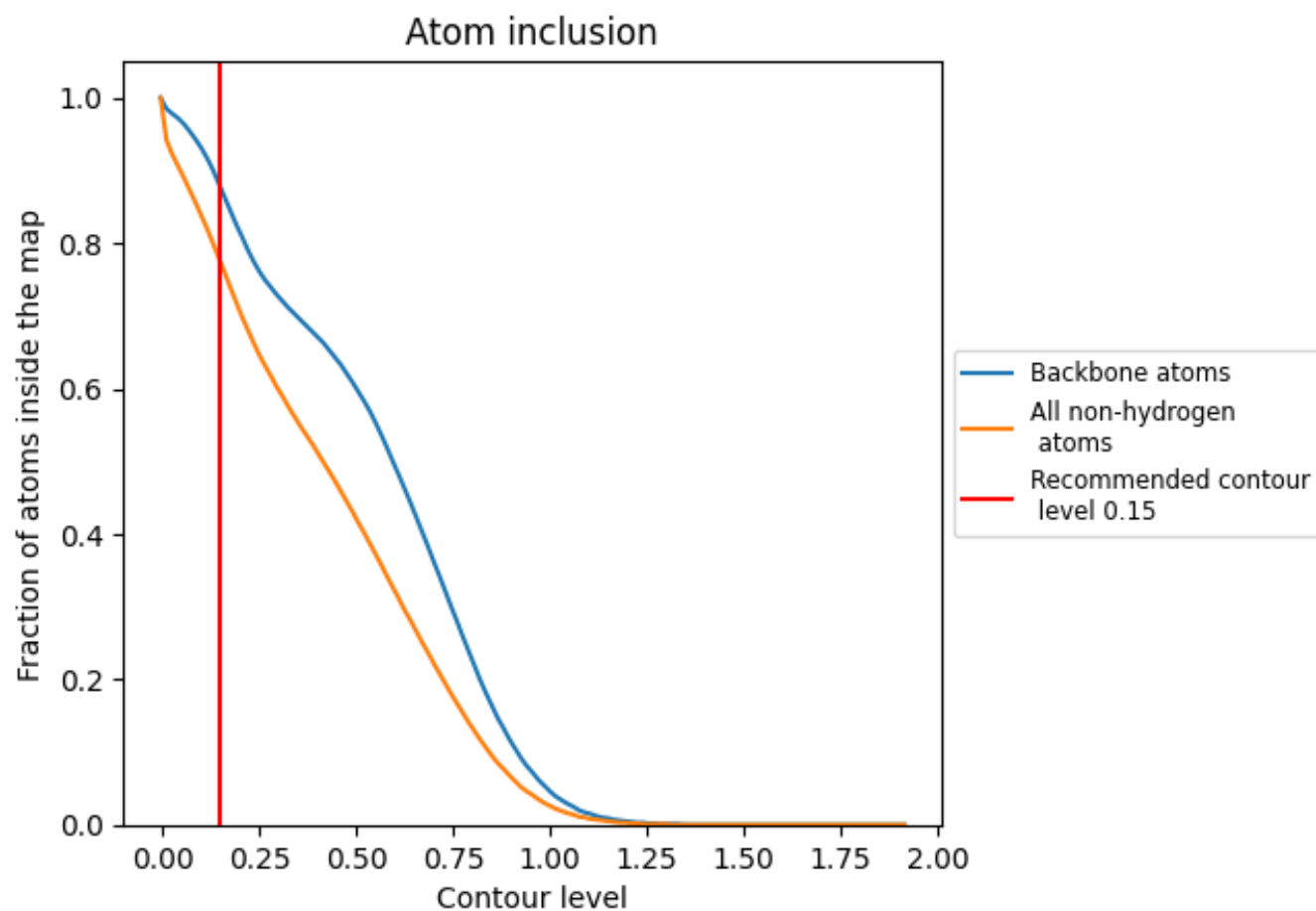
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5110
Aa	 0.7910	 0.5330
Ab	 0.8080	 0.5460
Ac	 0.7970	 0.5270
Ad	 0.8090	 0.5610
Ae	 0.7960	 0.5280
Af	 0.7910	 0.5380
Ag	 0.8010	 0.5380
Ah	 0.7890	 0.5170
Ai	 0.8050	 0.5320
Aj	 0.8020	 0.5410
Ak	 0.7770	 0.5130
Al	 0.7800	 0.5140
Am	 0.7990	 0.5340
An	 0.7960	 0.5260
Ao	 0.7880	 0.5110
Ap	 0.7960	 0.5280
Aq	 0.7870	 0.5180
Ar	 0.8050	 0.5180
As	 0.7740	 0.5090
At	 0.8020	 0.5180
Au	 0.7540	 0.4810
Av	 0.8220	 0.5350
Aw	 0.8210	 0.5300
Ax	 0.8200	 0.5220
Ay	 0.8100	 0.5280
Az	 0.8230	 0.5290
Ba	 0.8080	 0.5190
Bb	 0.7500	 0.4890
Bd	 0.7320	 0.4850
Bf	 0.7360	 0.4840
Bh	 0.7490	 0.4940
Bj	 0.7360	 0.4810
Bl	 0.7520	 0.4990
Bn	 0.7450	 0.4830



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Chain	Atom inclusion	Q-score
Bp	 0.7550	 0.4990
Br	 0.7500	 0.5010
Bt	 0.7570	 0.5040
Bv	 0.7460	 0.4930
Bx	 0.7490	 0.4950