



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 02:19 AM UTC

PDB ID : 6YL3 / pdb_00006yl3
EMDB ID : EMD-10835
Title : High resolution cryo-EM structure of urease from the pathogen *Yersinia enterocolitica*
Authors : Righetto, R.D.; Anton, L.; Adaixo, R.; Jakob, R.; Zivanov, J.; Mahi, M.A.; Ringler, P.; Schwede, T.; Maier, T.; Stahlberg, H.
Deposited on : 2020-04-06
Resolution : 1.98 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:

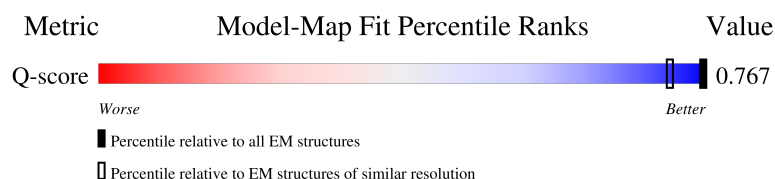
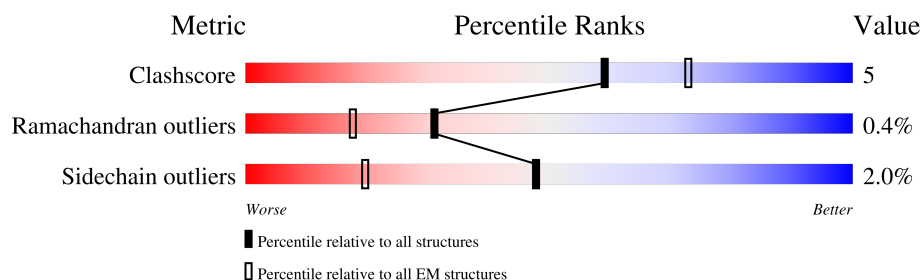
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 1.98 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.



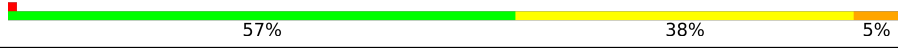
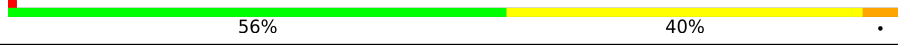
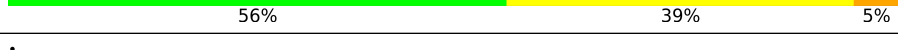
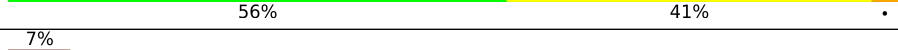
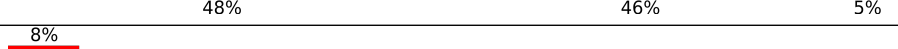
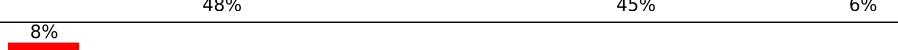
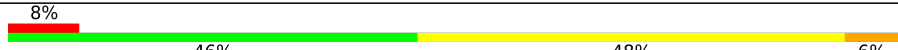
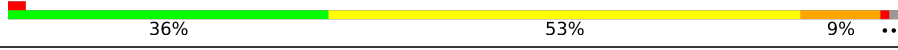
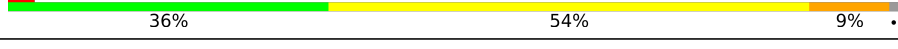
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1383 (1.50 - 2.48)

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	2	100	
1	5	100	
1	8	100	
1	A	100	

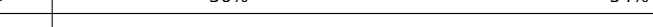
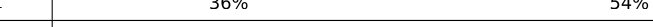
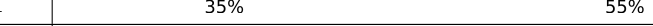
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Mol	Chain	Length	Quality of chain
1	D	100	
1	G	100	
1	J	100	
1	M	100	
1	P	100	
1	S	100	
1	W	100	
1	Z	100	
2	0	132	
2	3	132	
2	6	132	
2	9	132	
2	B	132	
2	E	132	
2	H	132	
2	K	132	
2	N	132	
2	Q	132	
2	T	132	
2	X	132	
3	1	571	
3	4	571	
3	7	571	
3	C	571	
3	F	571	

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Mol	Chain	Length	Quality of chain
3	I	571	 36%54%8% ..
3	L	571	 36%54%9% .
3	O	571	 35%55%8% ..
3	R	571	 35%54%9% .
3	U	571	 36%55%8% ..
3	V	571	 36%55%8% .
3	Y	571	 36%55%8% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 150276 atoms, of which 73164 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	D	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	G	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	J	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	M	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	P	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	S	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	W	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	Z	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	2	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	5	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	8	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	E	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	H	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	N	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	Q	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	T	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	X	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	0	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	3	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	6	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	9	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	F	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	I	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	L	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	O	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	R	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	V	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	Y	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	1	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	4	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	7	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	U	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	Ni	0
			2	2	
4	F	2	Total	Ni	0
			2	2	
4	I	2	Total	Ni	0
			2	2	
4	L	2	Total	Ni	0
			2	2	
4	O	2	Total	Ni	0
			2	2	
4	R	2	Total	Ni	0
			2	2	
4	V	2	Total	Ni	0
			2	2	
4	Y	2	Total	Ni	0
			2	2	
4	1	2	Total	Ni	0
			2	2	
4	4	2	Total	Ni	0
			2	2	
4	7	2	Total	Ni	0
			2	2	
4	U	2	Total	Ni	0
			2	2	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	25	Total	O	0
			25	25	
5	B	59	Total	O	0
			59	59	
5	C	224	Total	O	0
			224	224	

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Mol	Chain	Residues	Atoms		AltConf
5	D	25	Total 25	O 25	0
5	E	59	Total 59	O 59	0
5	F	225	Total 225	O 225	0
5	G	27	Total 27	O 27	0
5	H	58	Total 58	O 58	0
5	I	227	Total 227	O 227	0
5	J	25	Total 25	O 25	0
5	K	59	Total 59	O 59	0
5	L	227	Total 227	O 227	0
5	M	25	Total 25	O 25	0
5	N	57	Total 57	O 57	0
5	O	222	Total 222	O 222	0
5	P	25	Total 25	O 25	0
5	Q	57	Total 57	O 57	0
5	R	216	Total 216	O 216	0
5	S	25	Total 25	O 25	0
5	T	58	Total 58	O 58	0
5	V	227	Total 227	O 227	0
5	W	25	Total 25	O 25	0
5	X	58	Total 58	O 58	0
5	Y	226	Total 226	O 226	0

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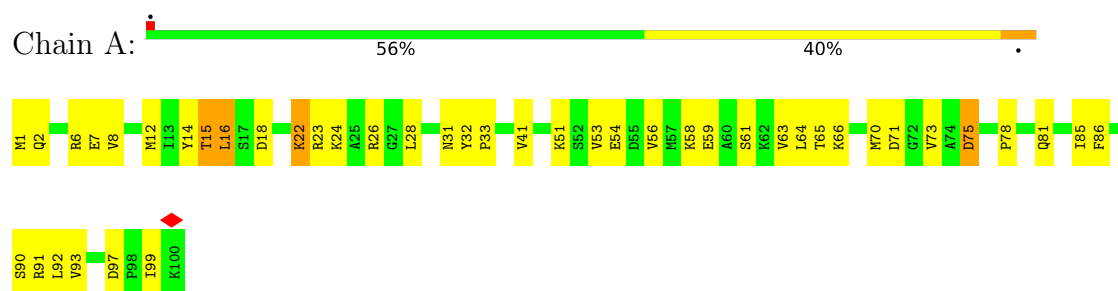
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Mol	Chain	Residues	Atoms		AltConf
5	Z	26	Total 26	O 26	0
5	0	57	Total 57	O 57	0
5	1	224	Total 224	O 224	0
5	2	25	Total 25	O 25	0
5	3	57	Total 57	O 57	0
5	4	216	Total 216	O 216	0
5	5	25	Total 25	O 25	0
5	6	57	Total 57	O 57	0
5	7	220	Total 220	O 220	0
5	8	25	Total 25	O 25	0
5	9	56	Total 56	O 56	0
5	U	223	Total 223	O 223	0

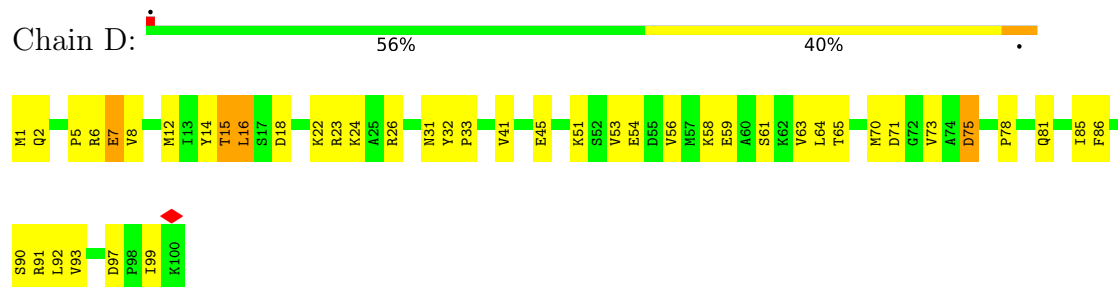
3 Residue-property plots [i](#)

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.

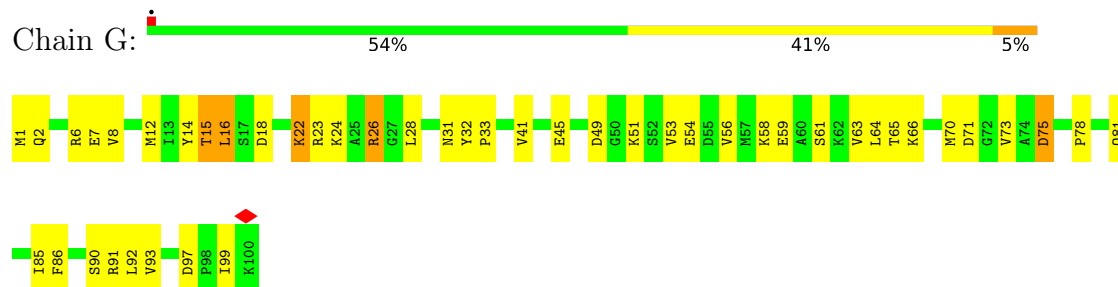
- Molecule 1: Urease subunit gamma



- Molecule 1: Urease subunit gamma

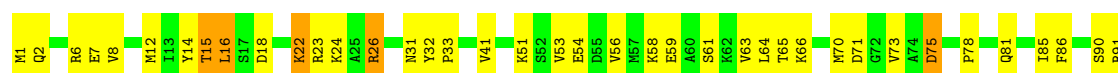


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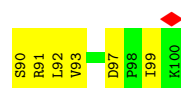
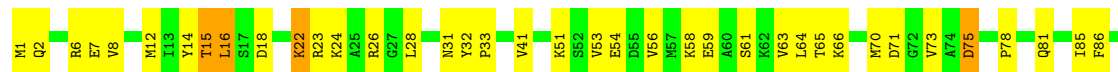


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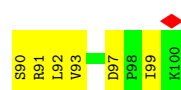




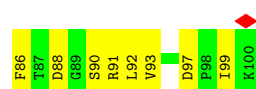
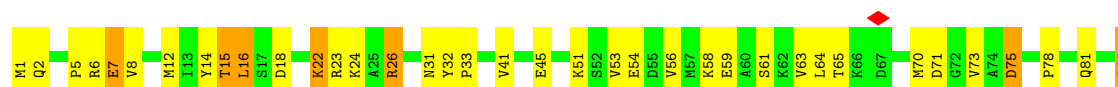
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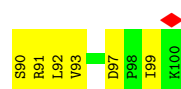
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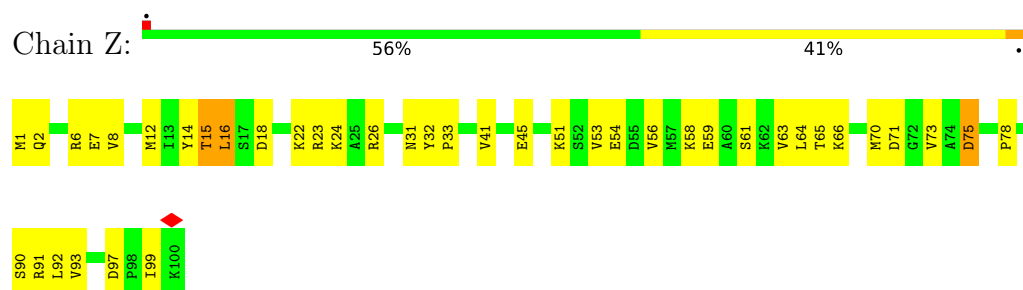
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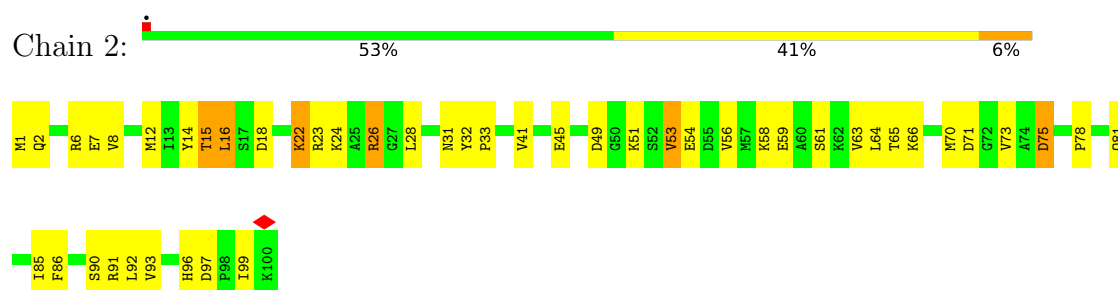
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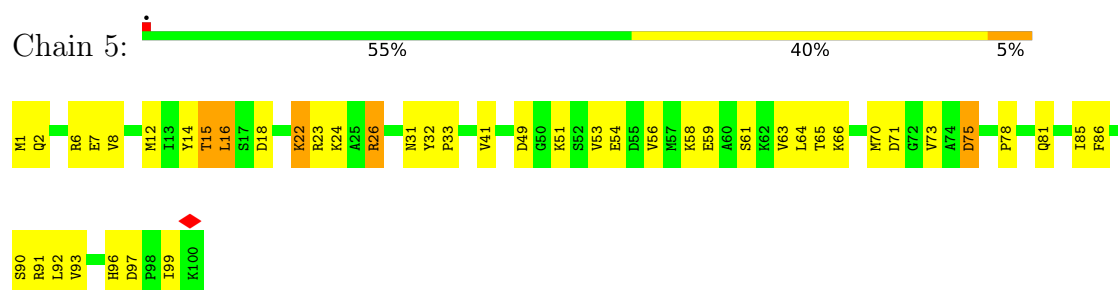
- Molecule 1: Urease subunit gamma



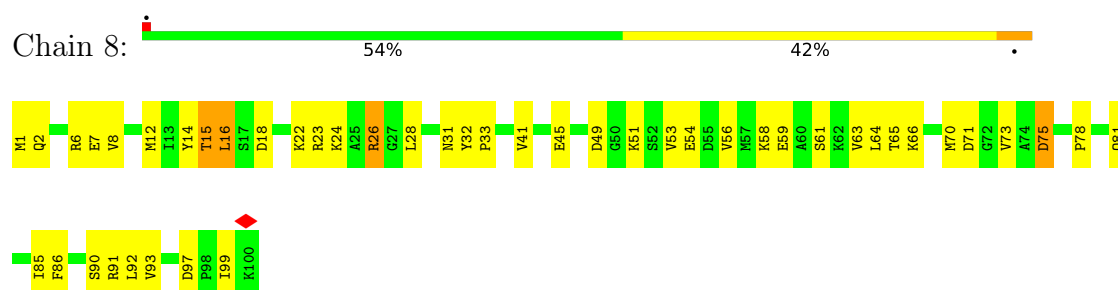
- Molecule 1: Urease subunit gamma



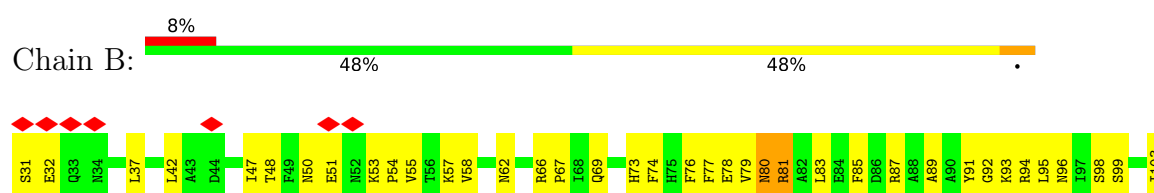
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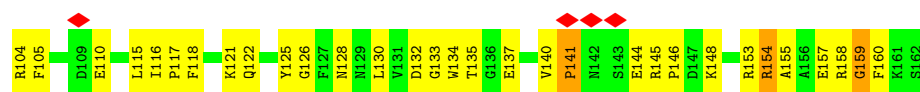


- Molecule 1: Urease subunit gamma

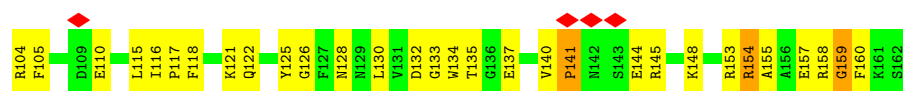


- Molecule 2: Urease subunit beta

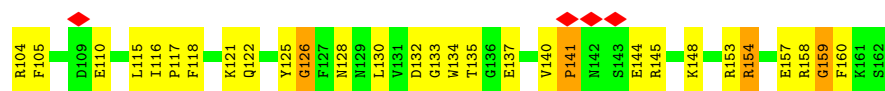
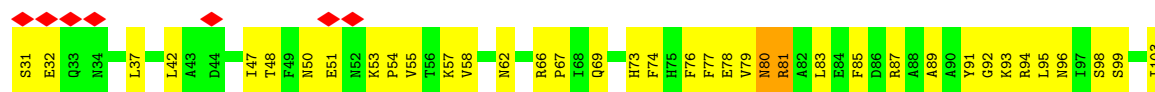




• Molecule 2: Urease subunit beta



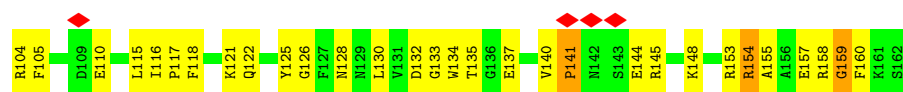
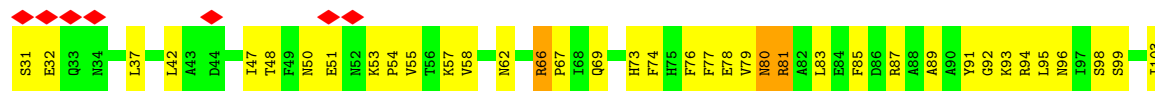
• Molecule 2: Urease subunit beta



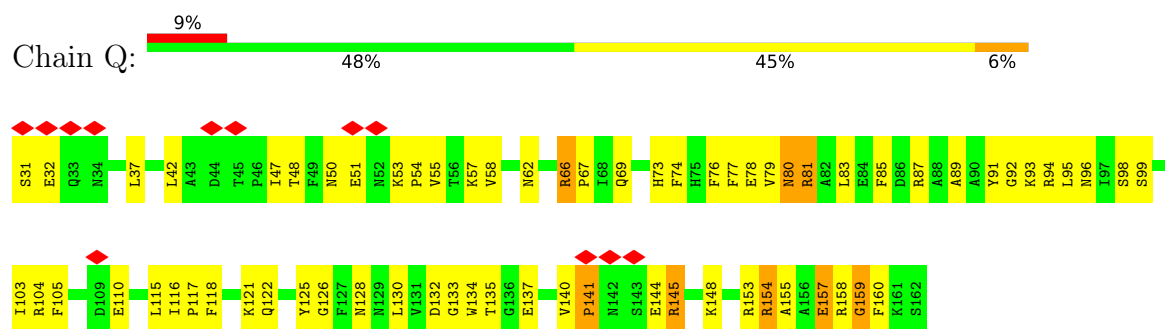
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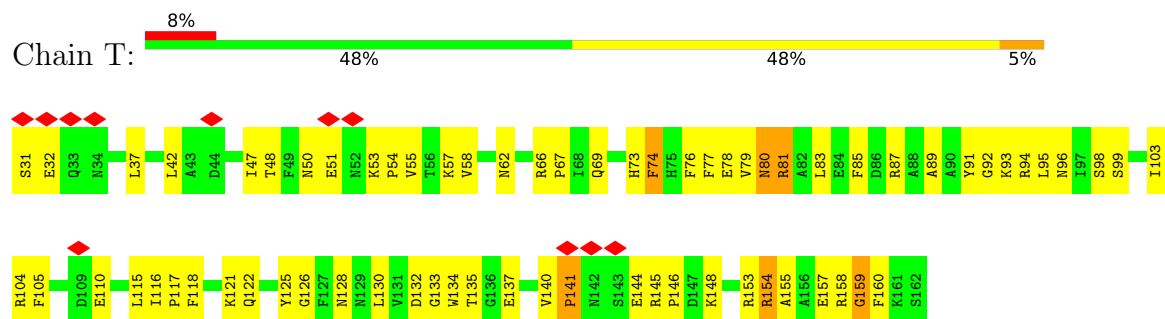
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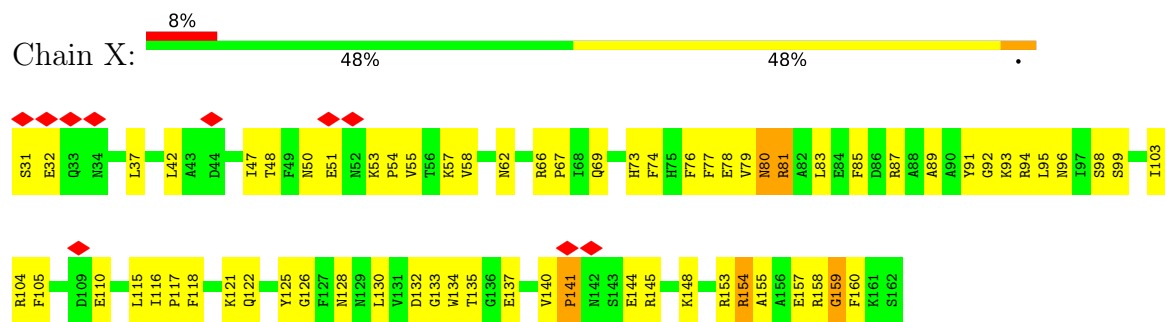
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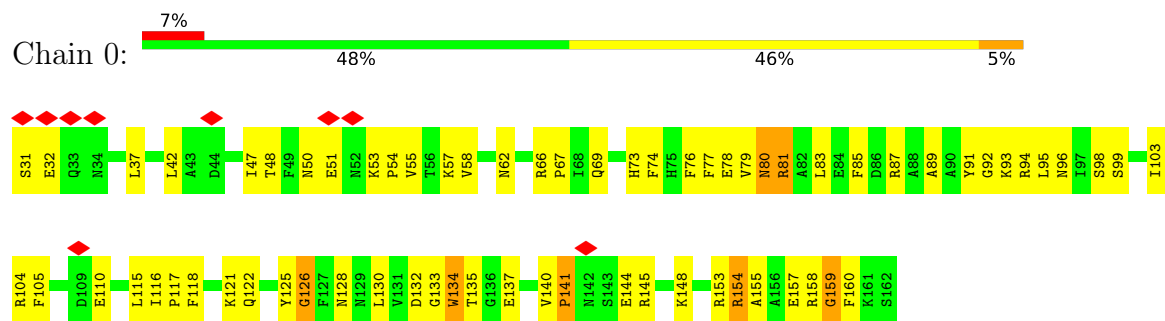
• Molecule 2: Urease subunit beta



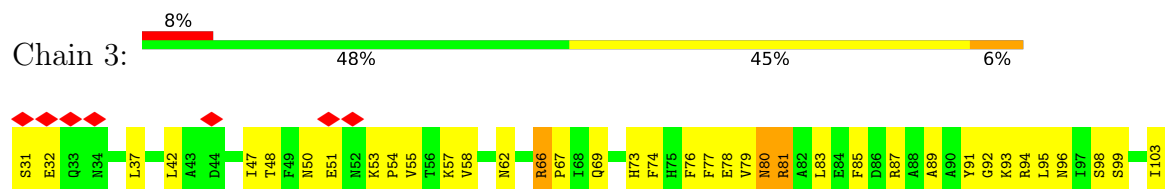
• Molecule 2: Urease subunit beta

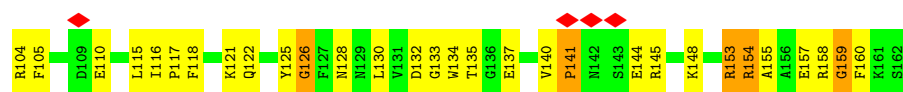


• Molecule 2: Urease subunit beta

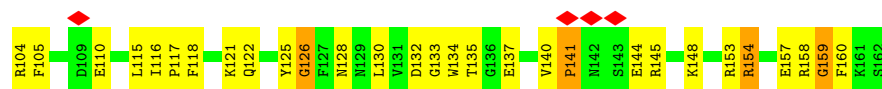
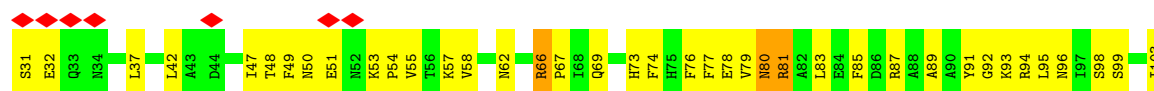


• Molecule 2: Urease subunit beta

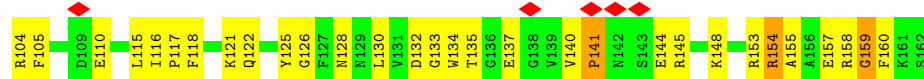
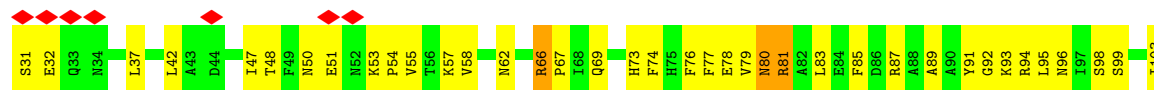




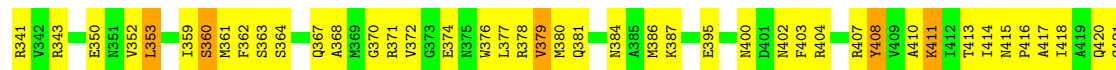
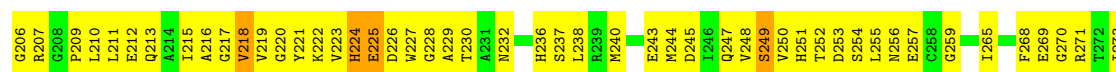
• Molecule 2: Urease subunit beta



• Molecule 2: Urease subunit beta

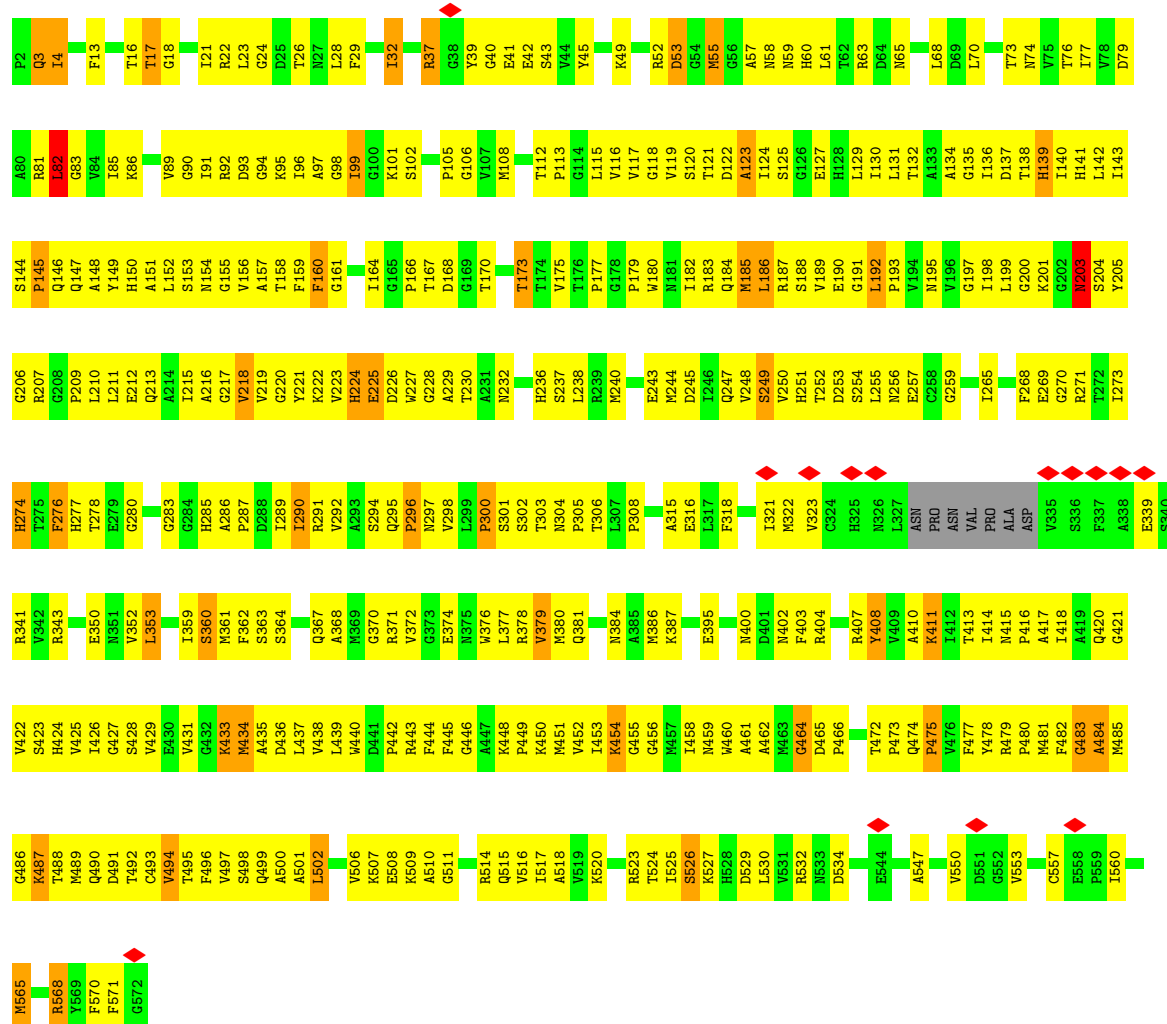


• Molecule 3: Urease subunit alpha



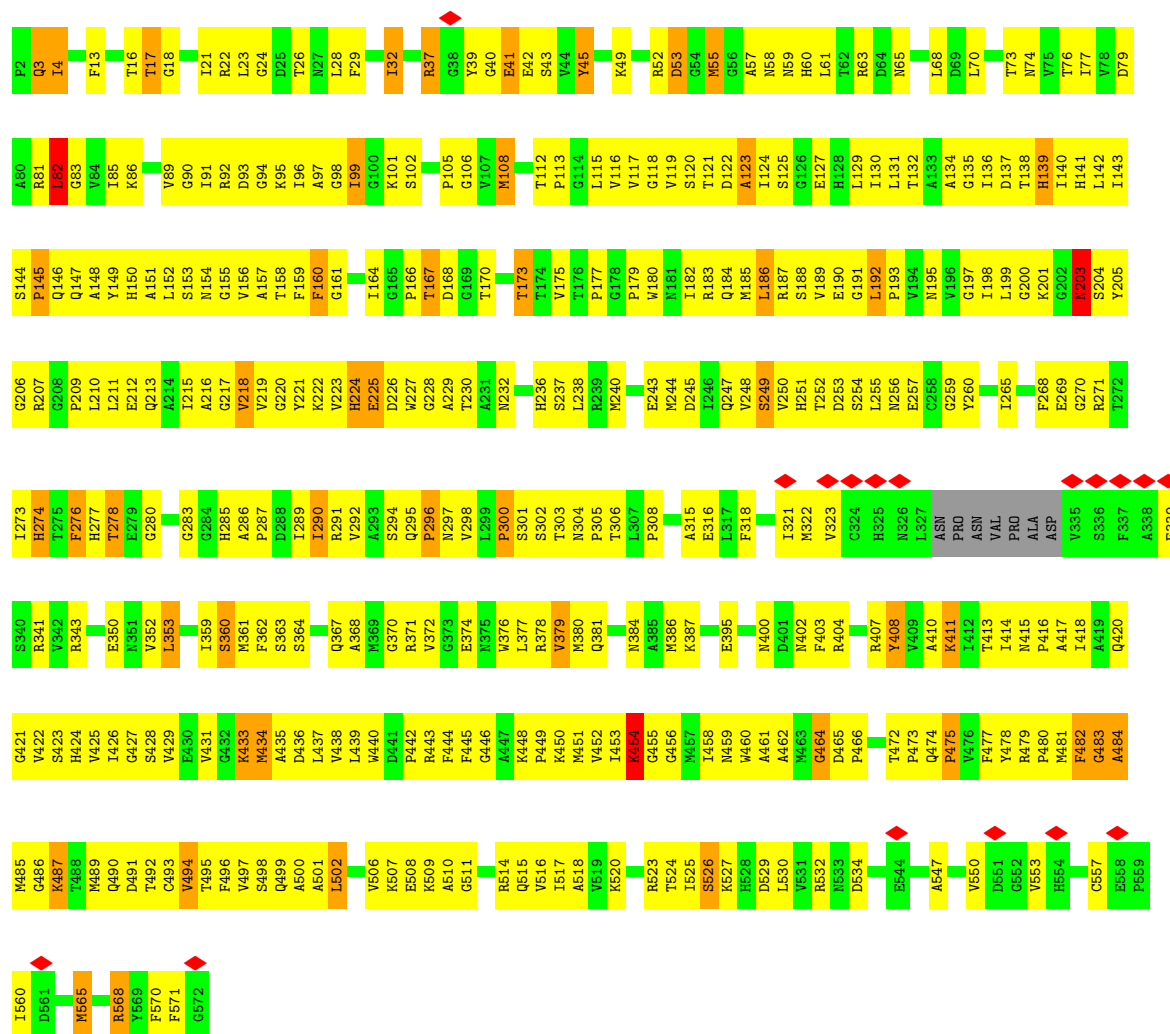


• Molecule 3: Urease subunit alpha

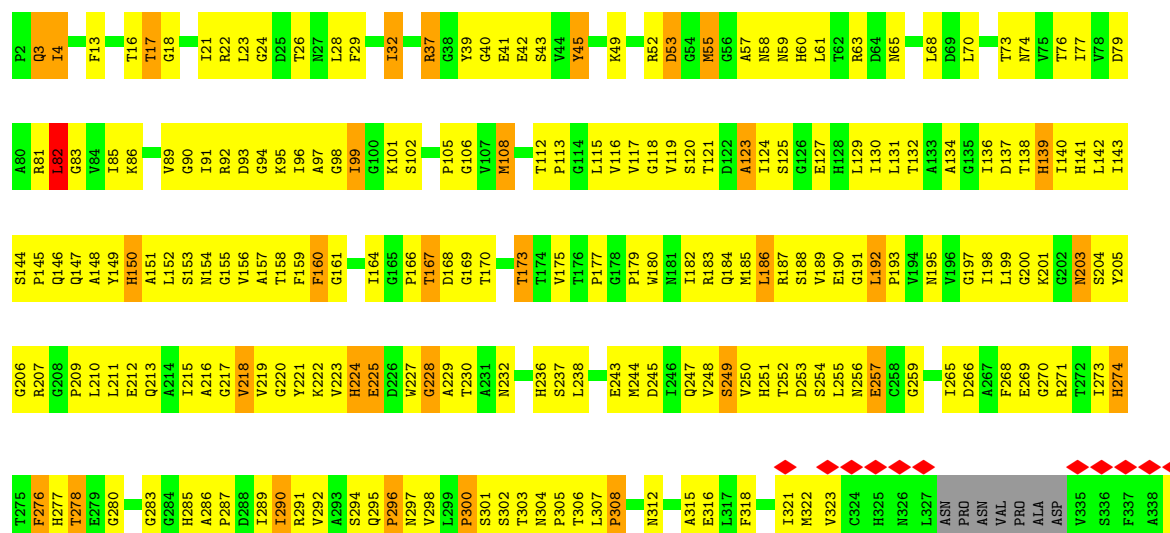


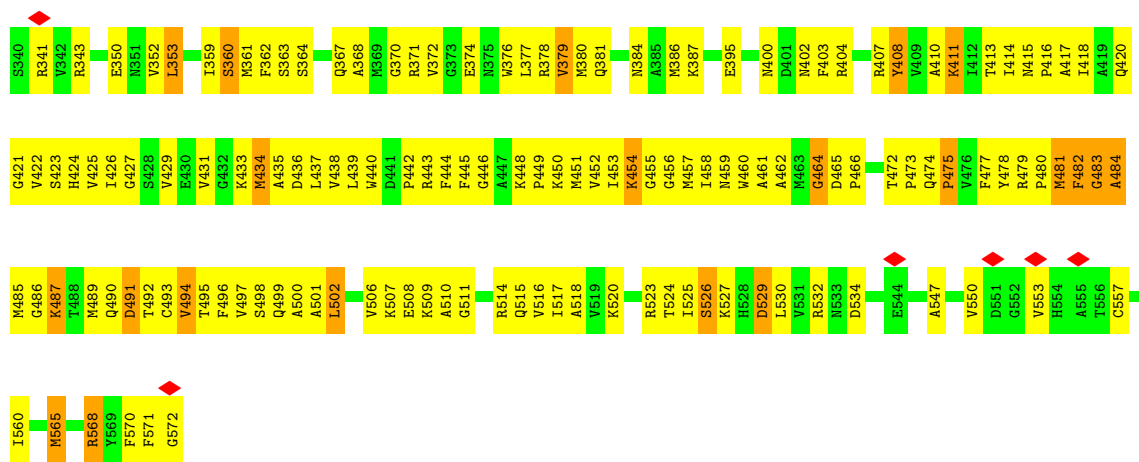
• Molecule 3: Urease subunit alpha



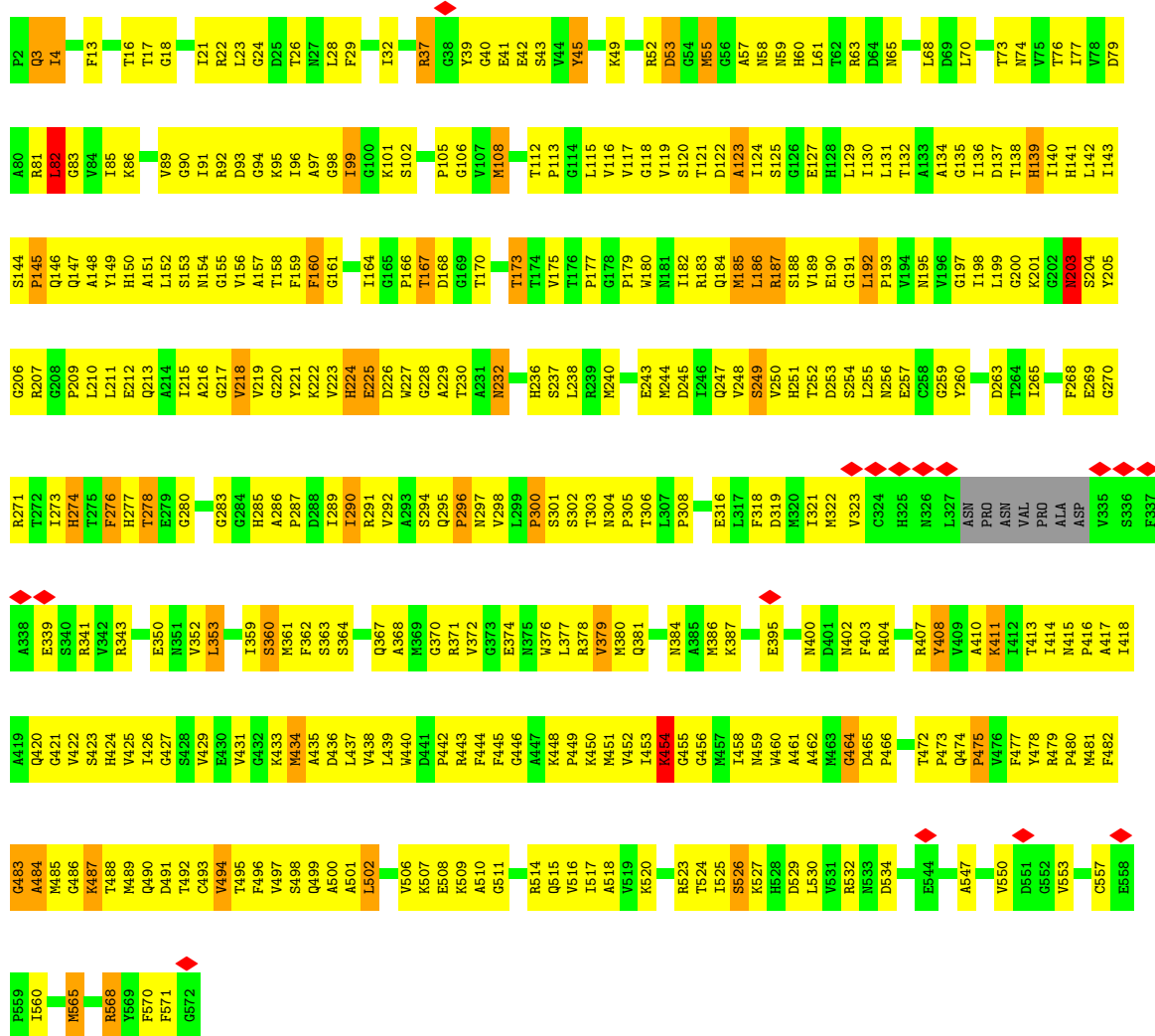


• Molecule 3: Urease subunit alpha



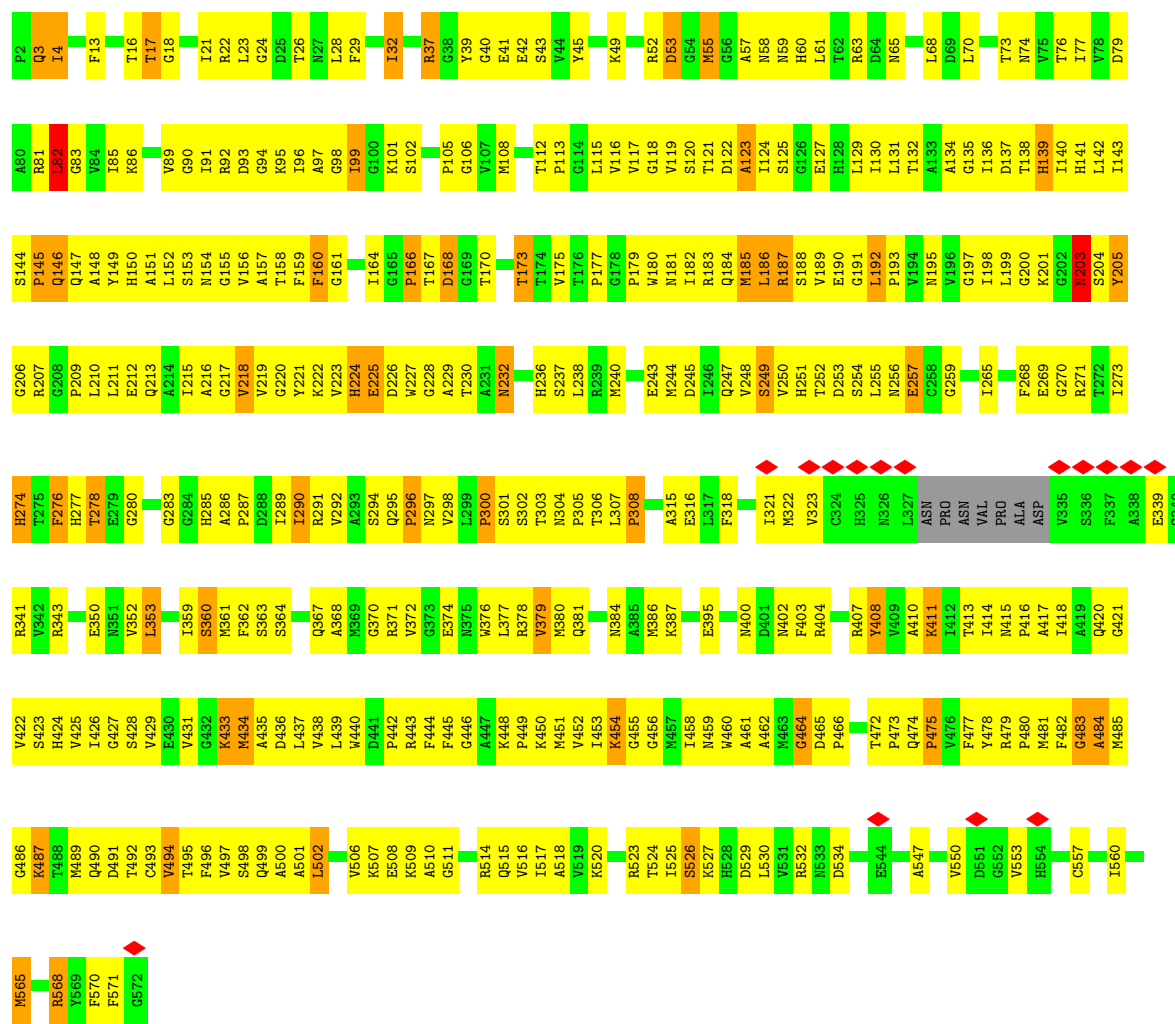


• Molecule 3: Urease subunit alpha



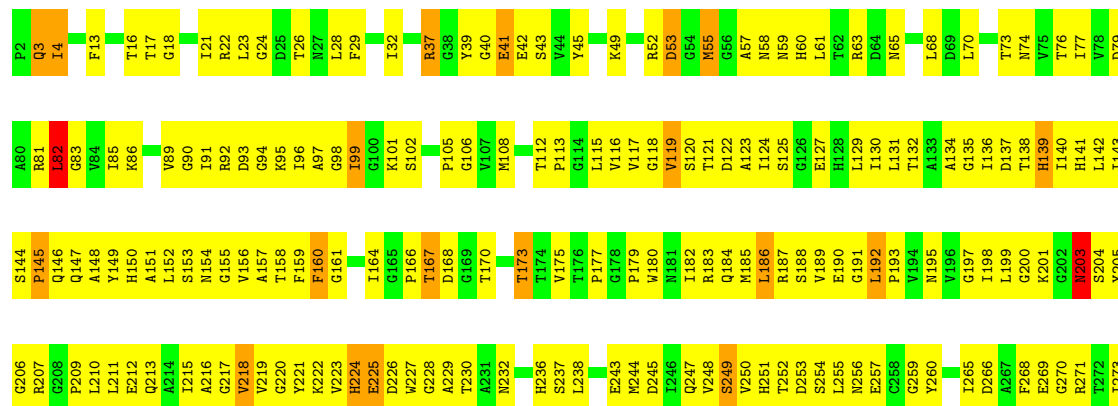
• Molecule 3: Urease subunit alpha

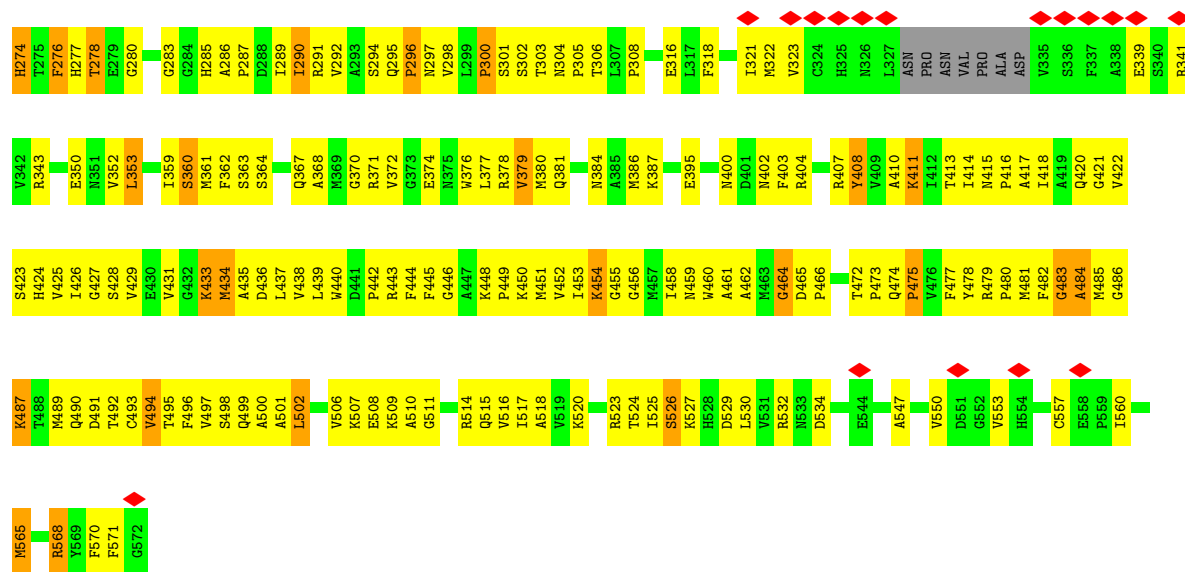
Chain R:  35% 54% 9%



• Molecule 3: Urease subunit alpha

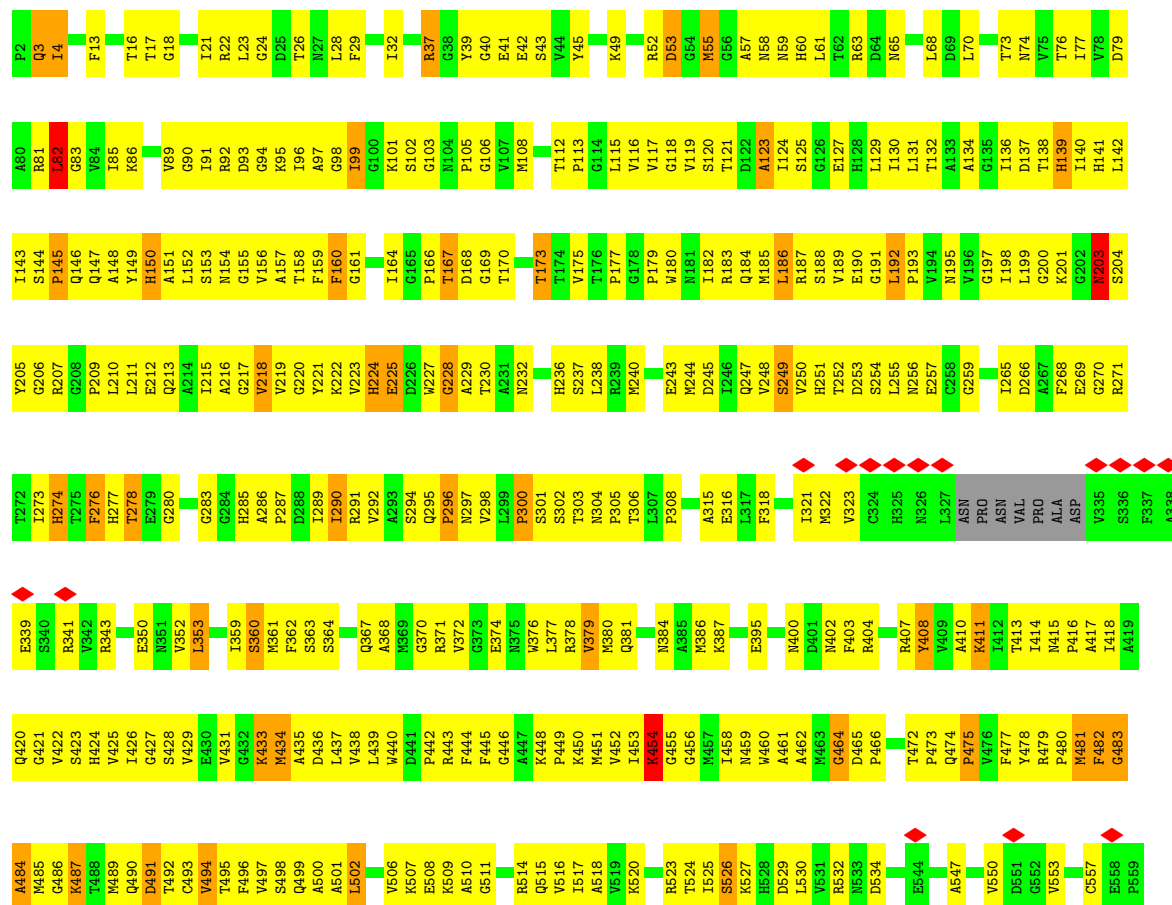
Chain V:  36% 55% 8%

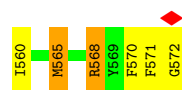




• Molecule 3: Urease subunit alpha

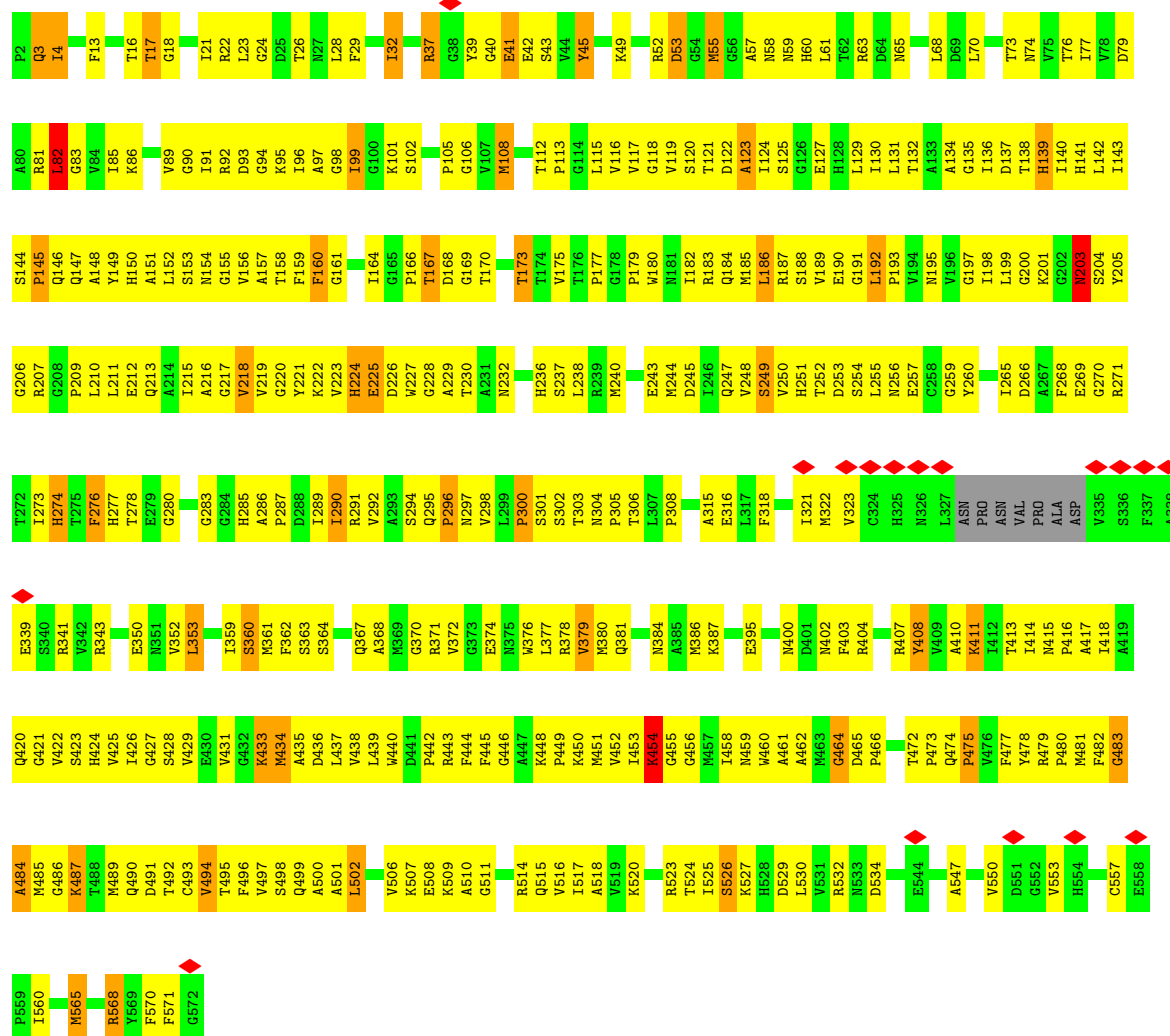
Chain Y: 36% 55% 8% ..





• Molecule 3: Urease subunit alpha

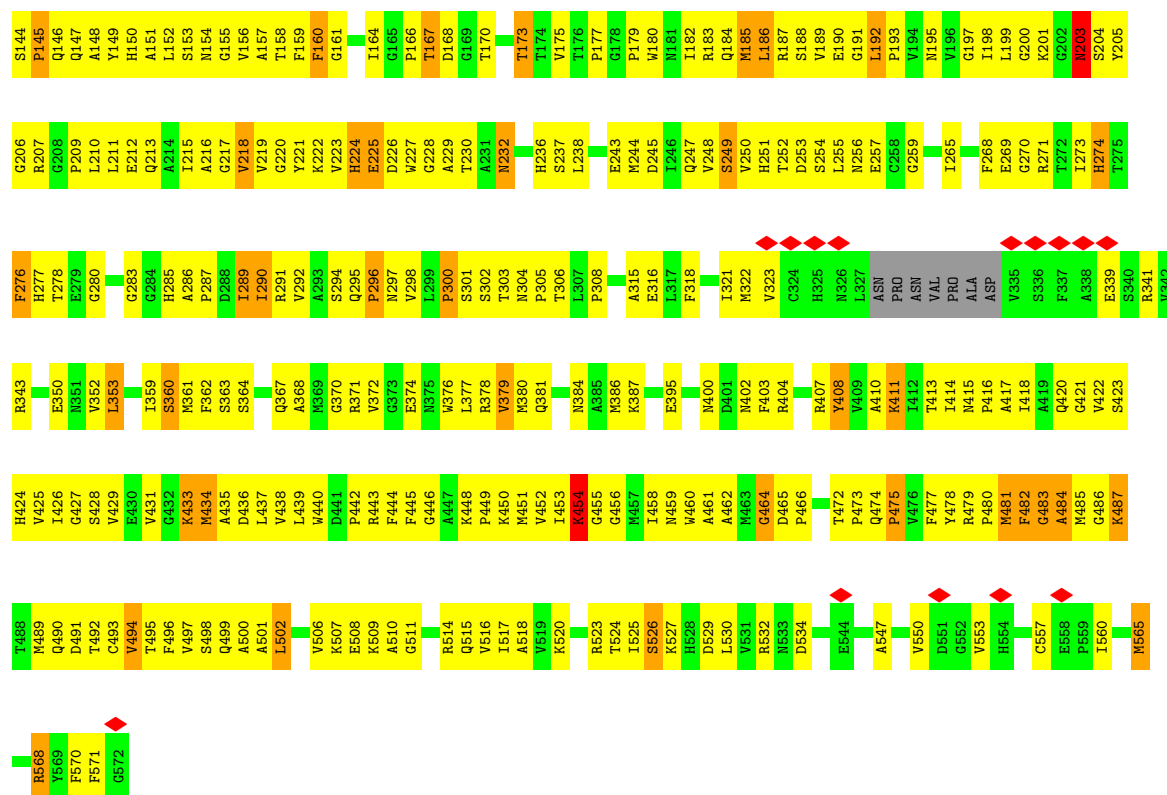
Chain 1: 35% 55% 8% ..



• Molecule 3: Urease subunit alpha

Chain 4: 36% 53% 9% ..

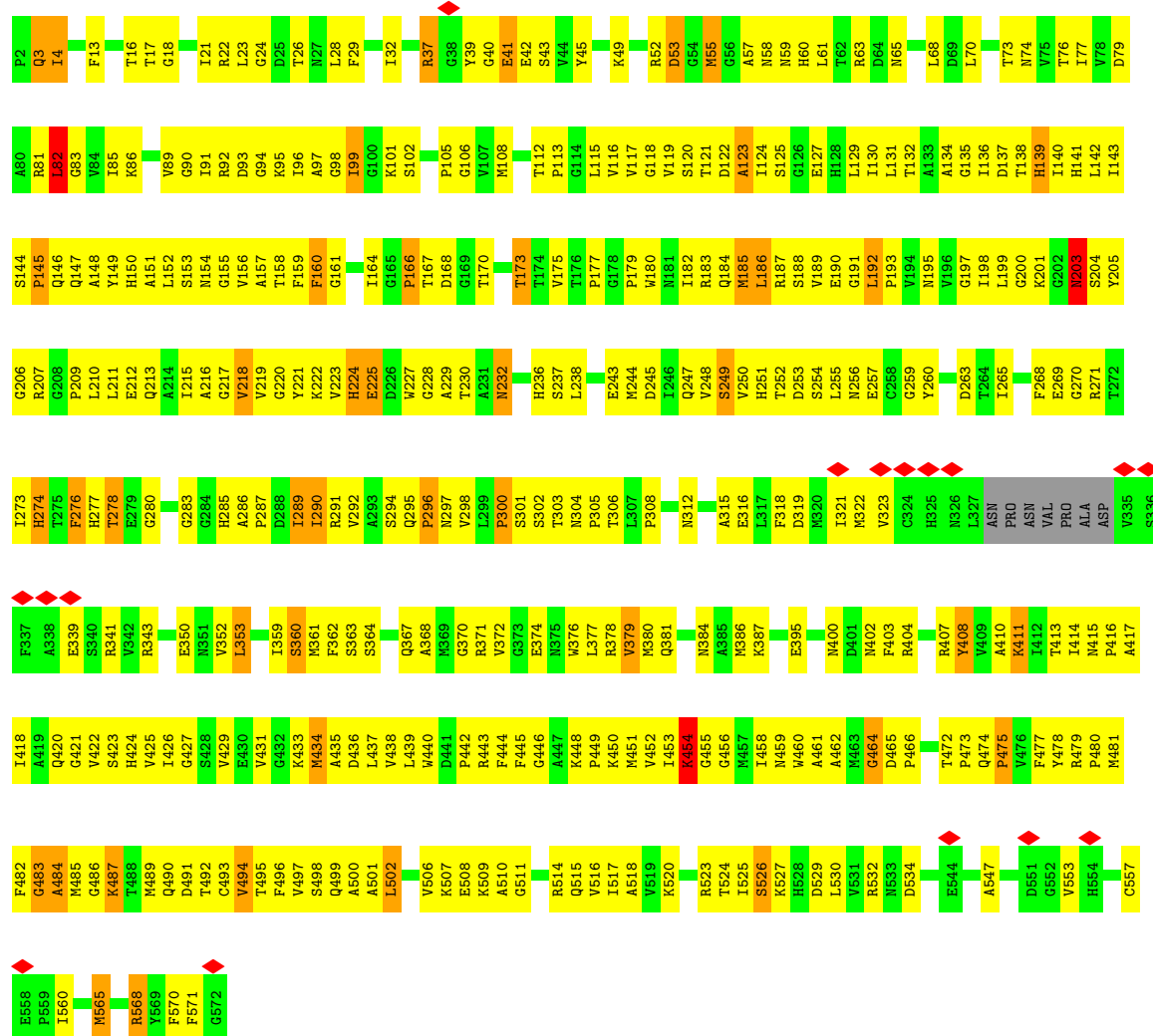






• Molecule 3: Urease subunit alpha

Chain U: 36% 55% 8% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	97627	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.248	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	327.168, 327.168, 327.168	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.639, 0.639, 0.639	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, KCX

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	2	2.65	50/844 (5.9%)	2.08	24/1135 (2.1%)
1	5	2.65	50/844 (5.9%)	2.08	24/1135 (2.1%)
1	8	2.65	50/844 (5.9%)	2.07	23/1135 (2.0%)
1	A	2.65	50/844 (5.9%)	2.07	24/1135 (2.1%)
1	D	2.65	48/844 (5.7%)	2.07	23/1135 (2.0%)
1	G	2.65	50/844 (5.9%)	2.07	24/1135 (2.1%)
1	J	2.65	50/844 (5.9%)	2.08	24/1135 (2.1%)
1	M	2.65	49/844 (5.8%)	2.07	24/1135 (2.1%)
1	P	2.65	49/844 (5.8%)	2.07	24/1135 (2.1%)
1	S	2.65	47/844 (5.6%)	2.07	24/1135 (2.1%)
1	W	2.65	50/844 (5.9%)	2.07	24/1135 (2.1%)
1	Z	2.65	50/844 (5.9%)	2.07	23/1135 (2.0%)
2	0	2.84	76/1076 (7.1%)	2.21	47/1455 (3.2%)
2	3	2.83	77/1076 (7.2%)	2.21	47/1455 (3.2%)
2	6	2.83	77/1076 (7.2%)	2.21	47/1455 (3.2%)
2	9	2.83	76/1076 (7.1%)	2.21	47/1455 (3.2%)
2	B	2.83	76/1076 (7.1%)	2.21	47/1455 (3.2%)
2	E	2.83	76/1076 (7.1%)	2.21	47/1455 (3.2%)
2	H	2.84	76/1076 (7.1%)	2.21	47/1455 (3.2%)
2	K	2.83	78/1076 (7.2%)	2.21	47/1455 (3.2%)
2	N	2.83	77/1076 (7.2%)	2.21	47/1455 (3.2%)
2	Q	2.84	77/1076 (7.2%)	2.21	47/1455 (3.2%)
2	T	2.84	77/1076 (7.2%)	2.21	47/1455 (3.2%)
2	X	2.84	77/1076 (7.2%)	2.21	47/1455 (3.2%)
3	1	3.14	445/4377 (10.2%)	2.42	319/5934 (5.4%)
3	4	3.14	447/4377 (10.2%)	2.42	318/5934 (5.4%)
3	7	3.14	447/4377 (10.2%)	2.43	321/5934 (5.4%)
3	C	3.14	448/4377 (10.2%)	2.44	324/5934 (5.5%)
3	F	3.14	446/4377 (10.2%)	2.42	320/5934 (5.4%)
3	I	3.14	445/4377 (10.2%)	2.42	319/5934 (5.4%)
3	L	3.14	445/4377 (10.2%)	2.42	316/5934 (5.3%)
3	O	3.14	448/4377 (10.2%)	2.43	321/5934 (5.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	R	3.14	447/4377 (10.2%)	2.43	322/5934 (5.4%)
3	U	3.14	448/4377 (10.2%)	2.42	316/5934 (5.3%)
3	V	3.14	446/4377 (10.2%)	2.42	317/5934 (5.3%)
3	Y	3.14	448/4377 (10.2%)	2.43	316/5934 (5.3%)
All	All	3.03	6873/75564 (9.1%)	2.35	4678/102288 (4.6%)

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	2	0	2
1	5	0	2
1	8	0	2
1	A	0	2
1	D	0	2
1	G	0	2
1	J	0	2
1	M	0	2
1	P	0	2
1	S	0	2
1	W	0	2
1	Z	0	2
3	1	0	1
3	4	0	1
3	7	0	1
3	C	0	1
3	F	0	1
3	I	0	1
3	L	0	1
3	O	0	1
3	R	0	1
3	U	0	1
3	V	0	1
3	Y	0	1
All	All	0	36

The worst 5 of 6873 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	141	PRO	N-CA	19.13	1.70	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	141	PRO	N-CA	19.12	1.70	1.47
2	3	141	PRO	N-CA	19.08	1.70	1.47
2	B	141	PRO	N-CA	19.07	1.70	1.47
2	T	141	PRO	N-CA	19.07	1.70	1.47

The worst 5 of 4678 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	140	VAL	CA-C-N	14.47	135.46	119.83
2	E	140	VAL	C-N-CA	14.47	135.46	119.83
2	6	140	VAL	CA-C-N	14.46	135.44	119.83
2	6	140	VAL	C-N-CA	14.46	135.44	119.83
2	Q	140	VAL	CA-C-N	14.45	135.44	119.83

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	THR	Mainchain
3	C	287	PRO	Peptide
1	D	15	THR	Mainchain
3	F	287	PRO	Peptide
1	G	15	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	805	856	819	8	0
1	5	805	856	819	5	0
1	8	805	856	819	6	0
1	A	805	856	819	3	0
1	D	805	856	819	5	0
1	G	805	856	819	6	0
1	J	805	856	819	3	0
1	M	805	856	819	3	0
1	P	805	856	819	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	805	856	819	10	0
1	W	805	856	819	4	0
1	Z	805	856	819	3	0
2	0	1042	1019	1008	9	0
2	3	1042	1019	1008	11	0
2	6	1042	1019	1008	8	0
2	9	1042	1019	1008	7	0
2	B	1042	1019	1008	7	0
2	E	1042	1019	1008	6	0
2	H	1042	1019	1008	7	0
2	K	1042	1019	1008	14	0
2	N	1042	1019	1008	7	0
2	Q	1042	1019	1008	11	0
2	T	1042	1019	1008	8	0
2	X	1042	1019	1008	6	0
3	1	4271	4222	4173	51	0
3	4	4271	4222	4173	52	0
3	7	4271	4222	4173	53	0
3	C	4271	4222	4173	53	0
3	F	4271	4222	4173	44	0
3	I	4271	4222	4173	50	0
3	L	4271	4222	4173	65	0
3	O	4271	4222	4173	55	0
3	R	4271	4222	4173	61	0
3	U	4271	4222	4173	51	0
3	V	4271	4222	4173	47	0
3	Y	4271	4222	4173	53	0
4	1	2	0	0	0	0
4	4	2	0	0	0	0
4	7	2	0	0	0	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
4	I	2	0	0	0	0
4	L	2	0	0	0	0
4	O	2	0	0	0	0
4	R	2	0	0	0	0
4	U	2	0	0	0	0
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
5	0	57	0	0	2	0
5	1	224	0	0	8	0
5	2	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	3	57	0	0	2	0
5	4	216	0	0	6	0
5	5	25	0	0	0	0
5	6	57	0	0	3	0
5	7	220	0	0	8	0
5	8	25	0	0	0	0
5	9	56	0	0	2	0
5	A	25	0	0	0	0
5	B	59	0	0	2	0
5	C	224	0	0	8	0
5	D	25	0	0	0	0
5	E	59	0	0	2	0
5	F	225	0	0	6	0
5	G	27	0	0	0	0
5	H	58	0	0	3	0
5	I	227	0	0	9	0
5	J	25	0	0	0	0
5	K	59	0	0	2	0
5	L	227	0	0	12	0
5	M	25	0	0	0	0
5	N	57	0	0	6	0
5	O	222	0	0	9	0
5	P	25	0	0	0	0
5	Q	57	0	0	2	0
5	R	216	0	0	8	0
5	S	25	0	0	0	0
5	T	58	0	0	2	0
5	U	223	0	0	10	0
5	V	227	0	0	8	0
5	W	25	0	0	0	0
5	X	58	0	0	2	0
5	Y	226	0	0	8	0
5	Z	26	0	0	0	0
All	All	77112	73164	72000	671	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 5.

The worst 5 of 671 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)
2:9:141:PRO:N	2:9:141:PRO:CA	1.70	1.48
2:E:141:PRO:N	2:E:141:PRO:CA	1.70	1.47
2:6:141:PRO:N	2:6:141:PRO:CA	1.70	1.46
2:N:141:PRO:N	2:N:141:PRO:CA	1.70	1.45
2:X:141:PRO:N	2:X:141:PRO:CA	1.70	1.44

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	5	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	8	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	A	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	D	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	G	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	J	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	M	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	P	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	S	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	W	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	Z	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
2	0	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	3	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	6	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	9	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	E	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	H	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	K	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	N	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	Q	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	T	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	X	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
3	1	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	4	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	7	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	C	569/571 (100%)	538 (95%)	31 (5%)	0	100	100
3	F	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	I	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	L	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	O	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	R	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	U	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	V	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	Y	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
All	All	9684/9636 (100%)	9117 (94%)	531 (6%)	36 (0%)	31	20

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	GLU
2	E	32	GLU
2	H	32	GLU
2	K	32	GLU
2	N	32	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	2	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	5	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	8	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	A	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	D	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	G	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	J	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	M	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	P	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	S	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	W	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	Z	95/87 (109%)	92 (97%)	3 (3%)	34	24
2	0	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	3	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	6	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	9	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	B	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	E	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	H	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	K	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	N	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	Q	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	T	112/110 (102%)	108 (96%)	4 (4%)	31	20
2	X	112/110 (102%)	108 (96%)	4 (4%)	31	20
3	1	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	4	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	7	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	C	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	F	458/456 (100%)	450 (98%)	8 (2%)	53	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	L	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	O	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	R	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	U	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	V	458/456 (100%)	450 (98%)	8 (2%)	53	48
3	Y	458/456 (100%)	450 (98%)	8 (2%)	53	48
All	All	7980/7836 (102%)	7800 (98%)	180 (2%)	48	37

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Y	82	LEU
3	4	4	ILE
3	Y	454	LYS
3	1	82	LEU
1	5	16[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	142	ASN
3	Y	528	HIS
2	9	52	ASN
3	V	420	GLN
2	X	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KCX	Y	222	3,4	10,11,12	1.68	2 (20%)	6,12,14	2.46	1 (16%)
3	KCX	C	222	3,4	10,11,12	1.69	3 (30%)	6,12,14	2.46	1 (16%)
3	KCX	1	222	3,4	10,11,12	1.70	3 (30%)	6,12,14	2.47	1 (16%)
3	KCX	F	222	3,4	10,11,12	1.42	1 (10%)	6,12,14	1.04	0
3	KCX	7	222	3,4	10,11,12	1.42	2 (20%)	6,12,14	1.05	0
3	KCX	U	222	3,4	10,11,12	1.69	3 (30%)	6,12,14	2.45	1 (16%)
3	KCX	I	222	3,4	10,11,12	1.69	3 (30%)	6,12,14	2.46	1 (16%)
3	KCX	V	222	3,4	10,11,12	1.43	2 (20%)	6,12,14	1.05	0
3	KCX	R	222	3,4	10,11,12	1.68	2 (20%)	6,12,14	2.46	1 (16%)
3	KCX	O	222	3,4	10,11,12	1.68	3 (30%)	6,12,14	2.47	1 (16%)
3	KCX	L	222	3,4	10,11,12	1.67	2 (20%)	6,12,14	2.47	1 (16%)
3	KCX	4	222	3,4	10,11,12	1.68	3 (30%)	6,12,14	2.47	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KCX	Y	222	3,4	-	0/9/10/12	-
3	KCX	C	222	3,4	-	0/9/10/12	-
3	KCX	1	222	3,4	-	0/9/10/12	-
3	KCX	F	222	3,4	-	0/9/10/12	-
3	KCX	7	222	3,4	-	0/9/10/12	-
3	KCX	U	222	3,4	-	0/9/10/12	-
3	KCX	I	222	3,4	-	0/9/10/12	-
3	KCX	V	222	3,4	-	0/9/10/12	-
3	KCX	R	222	3,4	-	0/9/10/12	-
3	KCX	O	222	3,4	-	0/9/10/12	-
3	KCX	L	222	3,4	-	0/9/10/12	-
3	KCX	4	222	3,4	-	0/9/10/12	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	222	KCX	OQ1-CX	2.99	1.27	1.21
3	C	222	KCX	OQ1-CX	2.96	1.27	1.21
3	I	222	KCX	OQ1-CX	2.96	1.27	1.21
3	4	222	KCX	OQ1-CX	2.95	1.27	1.21
3	L	222	KCX	OQ1-CX	2.95	1.27	1.21

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	222	KCX	OQ1-CX-NZ	-5.62	116.39	124.92
3	4	222	KCX	OQ1-CX-NZ	-5.62	116.39	124.92
3	O	222	KCX	OQ1-CX-NZ	-5.61	116.39	124.92
3	1	222	KCX	OQ1-CX-NZ	-5.61	116.40	124.92
3	Y	222	KCX	OQ1-CX-NZ	-5.60	116.41	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	I	7
3	O	7
3	V	7
3	1	7
3	U	7
3	7	6
3	C	6
3	F	6
3	L	6
3	R	6
3	Y	6
3	4	6
2	B	3
2	E	3
2	H	3
2	K	3
2	N	3
2	Q	3
2	T	3
2	X	3
2	0	3
2	3	3
2	6	3
2	9	3

The worst 5 of 113 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	156:VAL	C	157:ALA	N	1.20
1	O	156:VAL	C	157:ALA	N	1.20
1	V	156:VAL	C	157:ALA	N	1.20
1	1	156:VAL	C	157:ALA	N	1.20
1	U	156:VAL	C	157:ALA	N	1.20

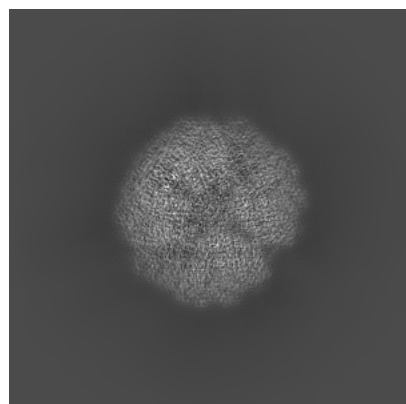
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10835. These allow visual inspection of the internal detail of the map and identification of artifacts.

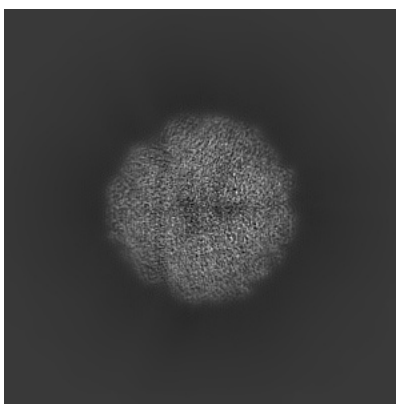
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

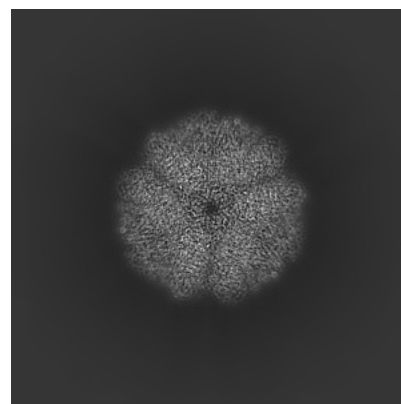
6.1.1 Primary map



X

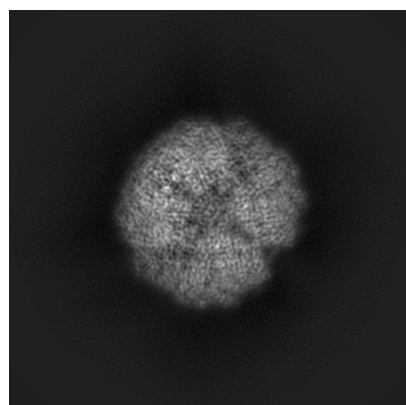


Y

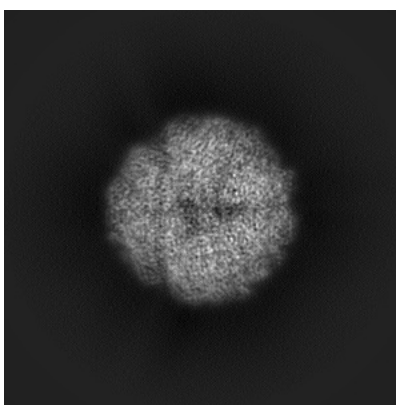


Z

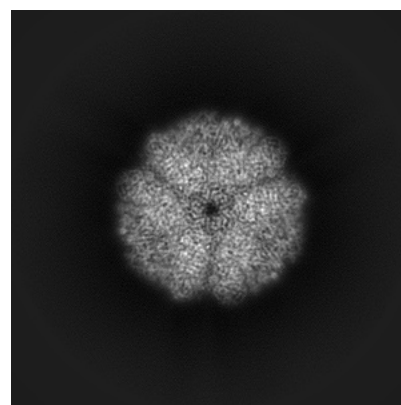
6.1.2 Raw map



X



Y

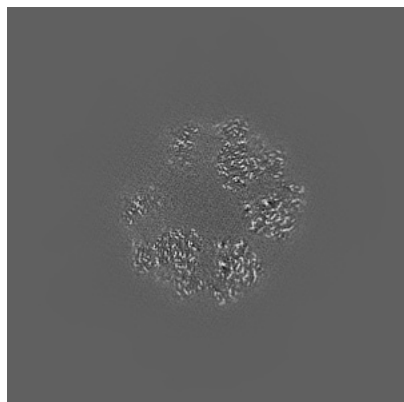


Z

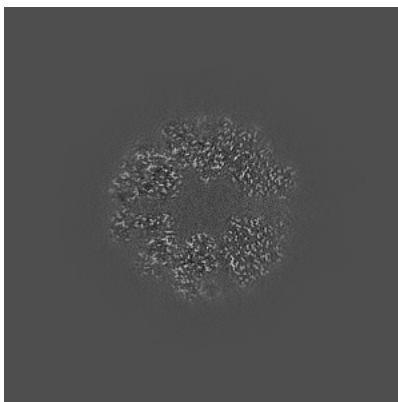
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

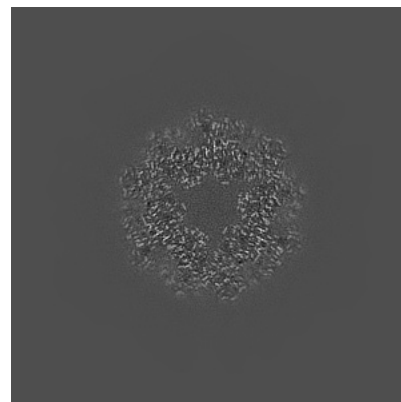
6.2.1 Primary map



X Index: 256

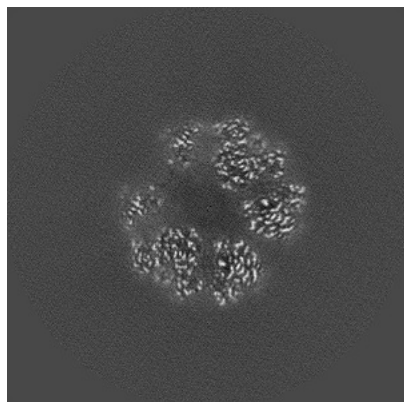


Y Index: 256

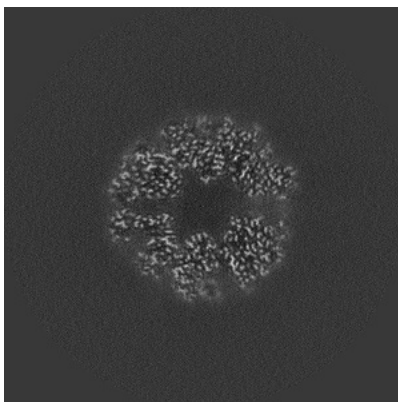


Z Index: 256

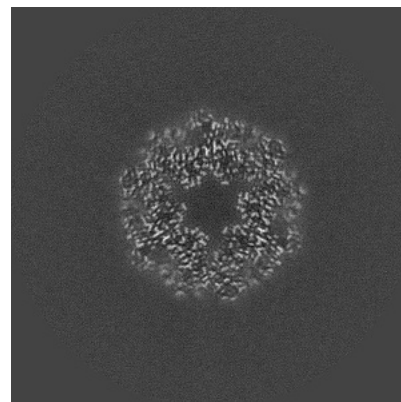
6.2.2 Raw map



X Index: 256



Y Index: 256

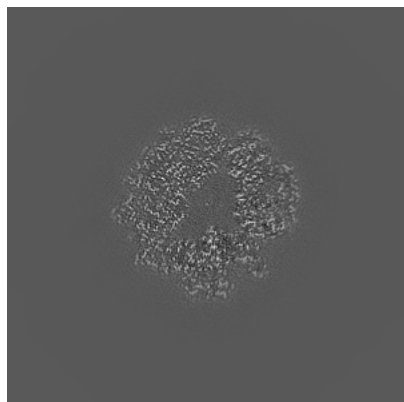


Z Index: 256

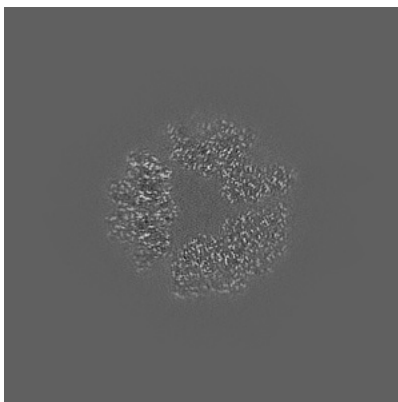
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

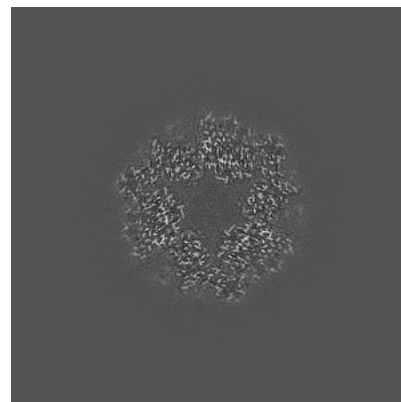
6.3.1 Primary map



X Index: 288

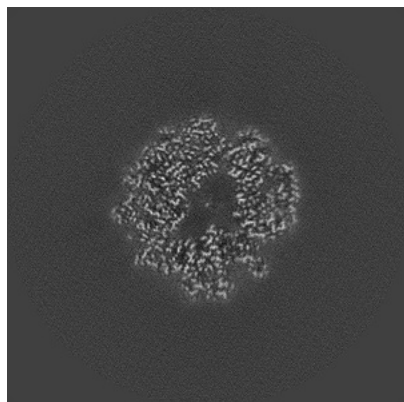


Y Index: 243

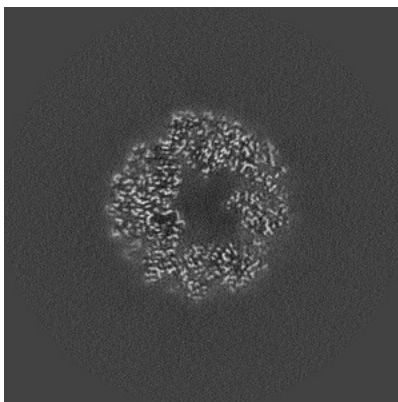


Z Index: 250

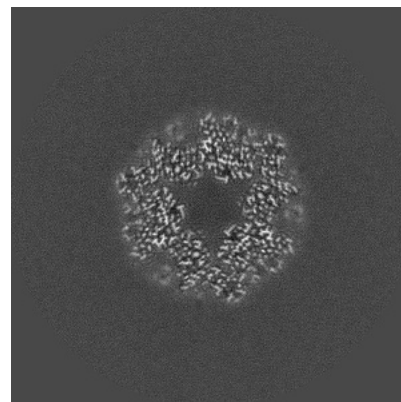
6.3.2 Raw map



X Index: 288



Y Index: 273

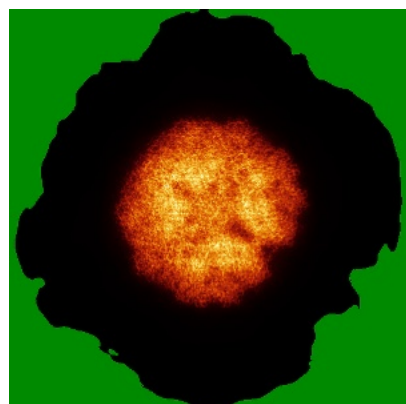


Z Index: 250

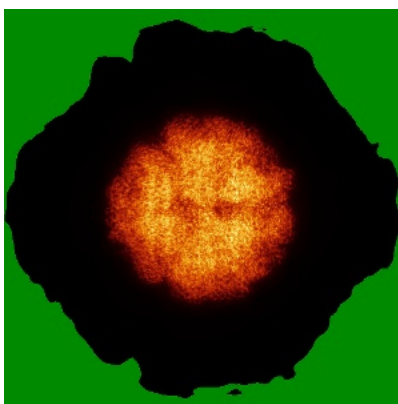
The images above show the largest variance slices of the map in three orthogonal directions.

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

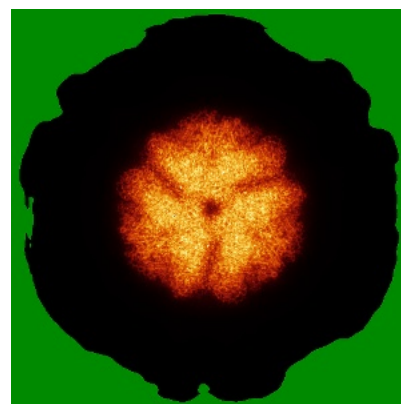
6.4.1 Primary map



X

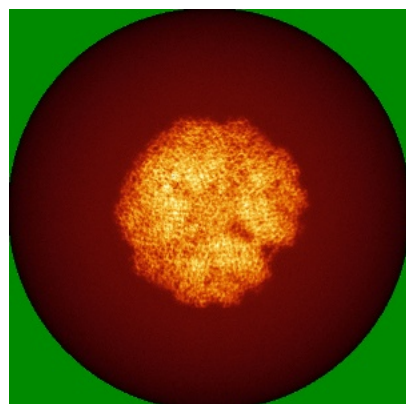


Y

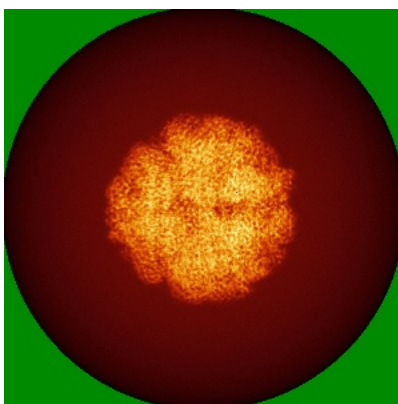


Z

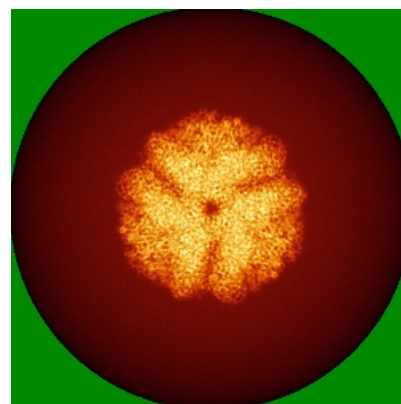
6.4.2 Raw map



X



Y

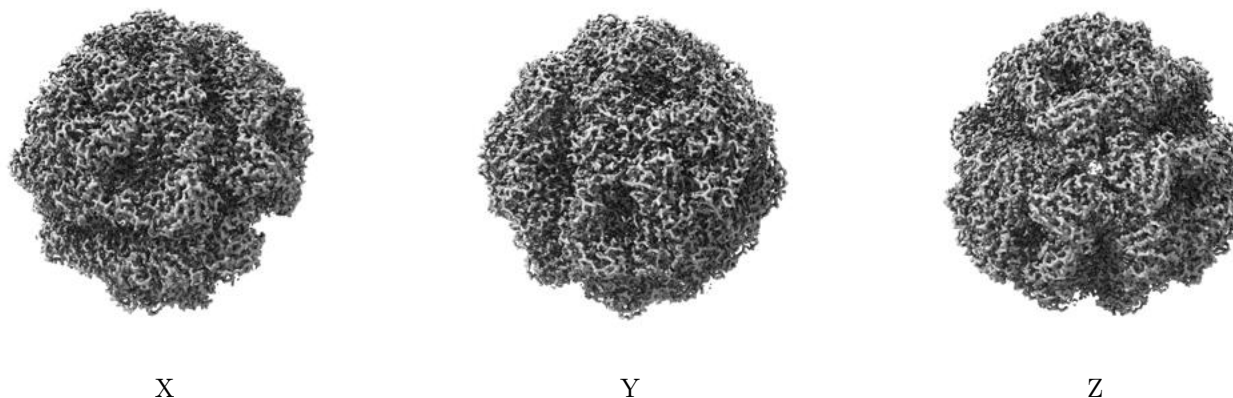


Z

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.

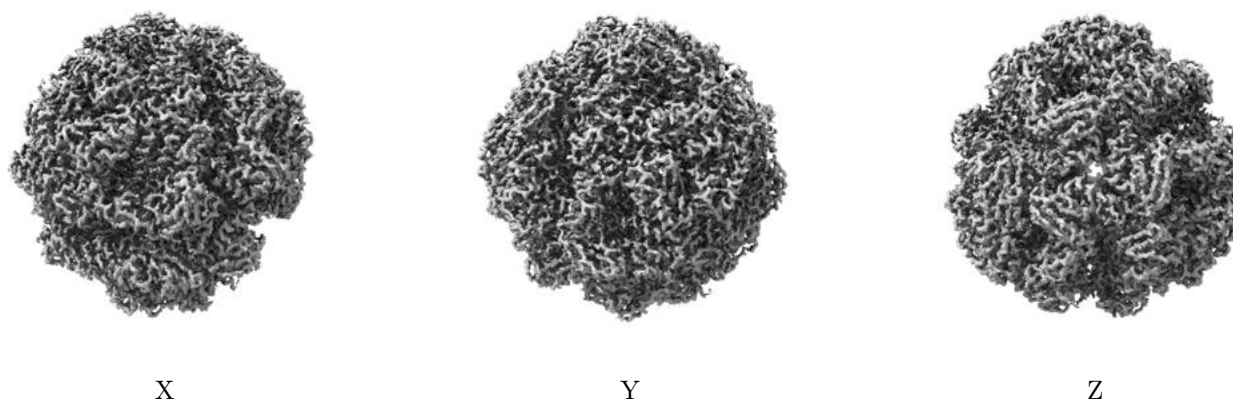
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

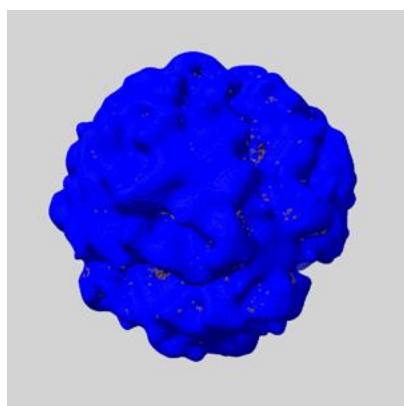
6.6 Mask visualisation [i](#)

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

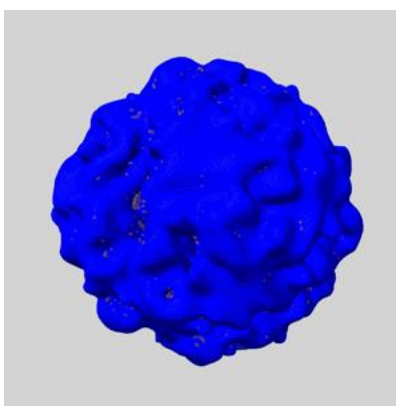
A mask typically either:

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

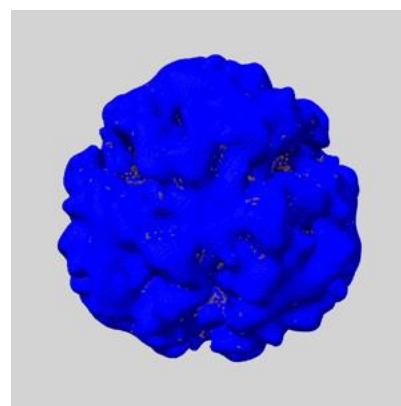
6.6.1 emd_10835_msk_1.map [i](#)



X



Y

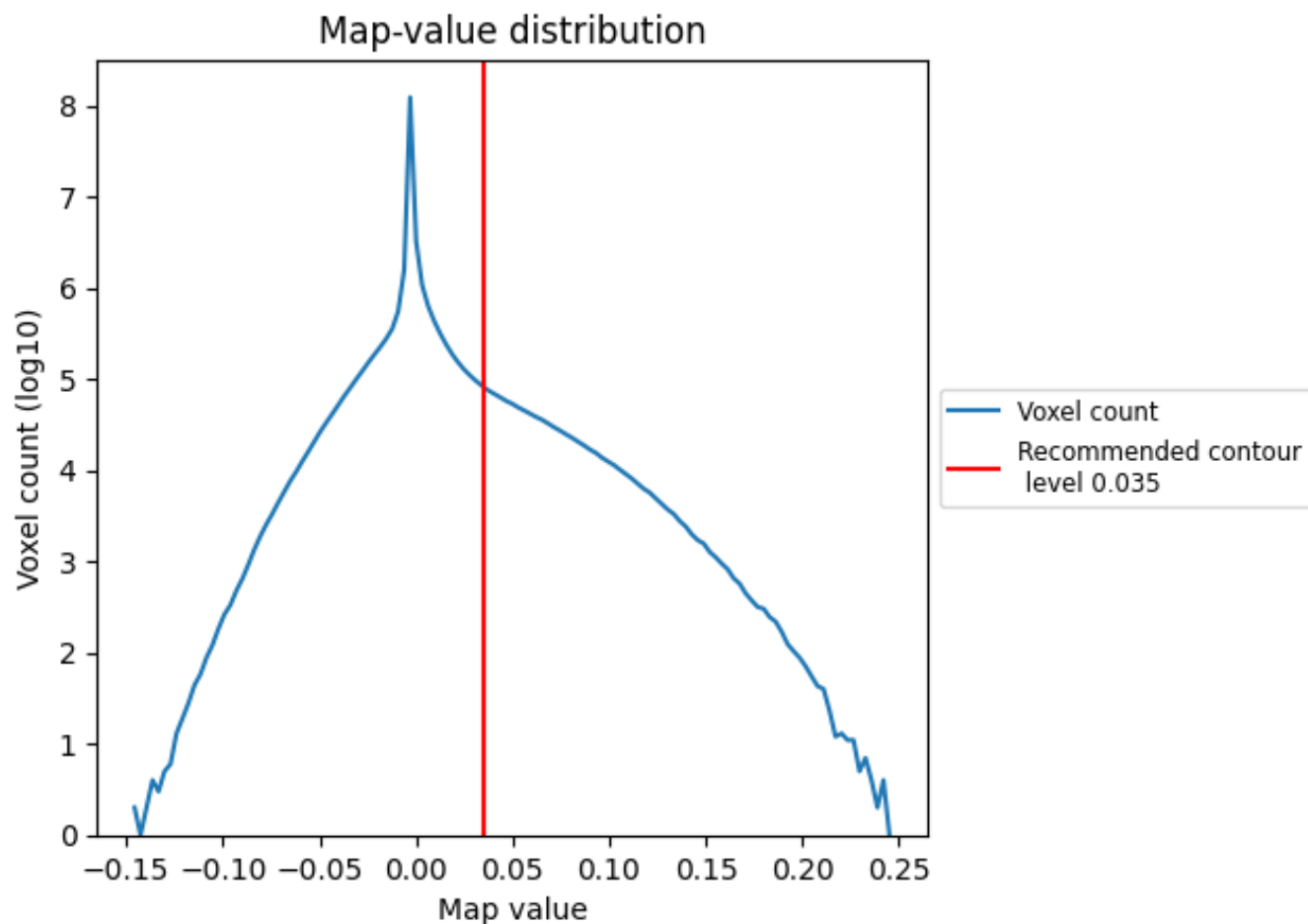


Z

7 Map analysis [i](#)

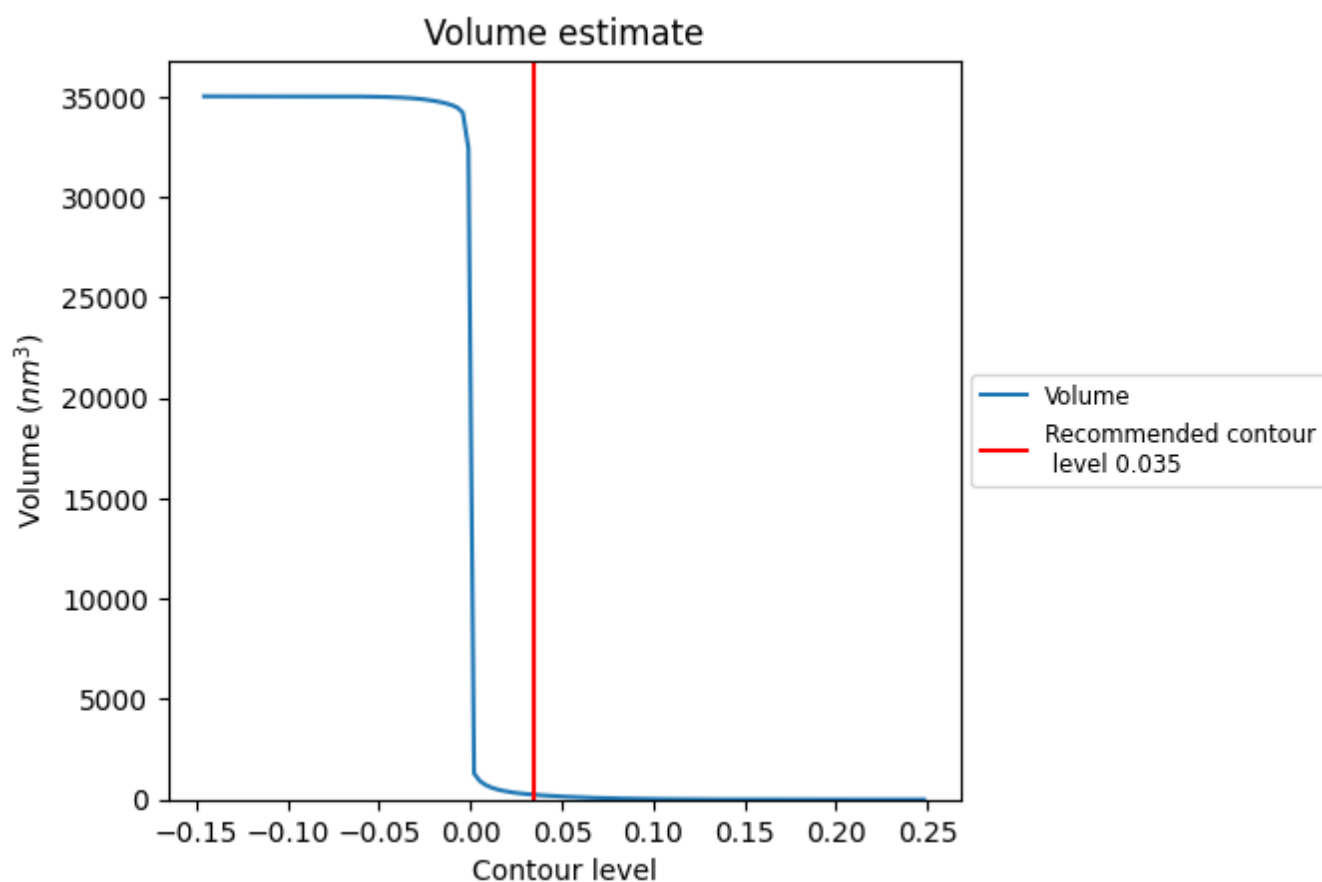
This section contains the results of statistical analysis of the map.

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.

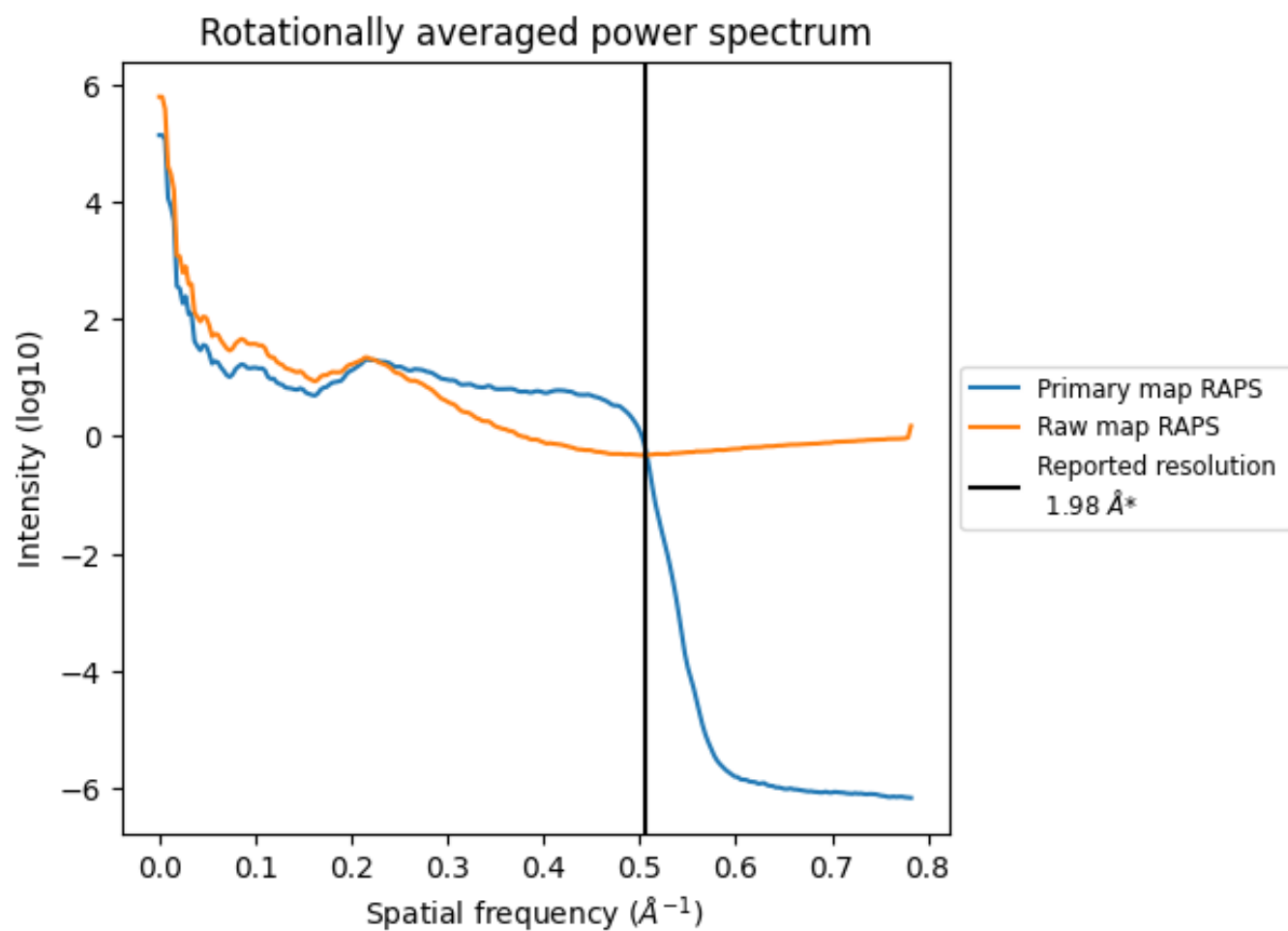
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 217 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 ⓘ

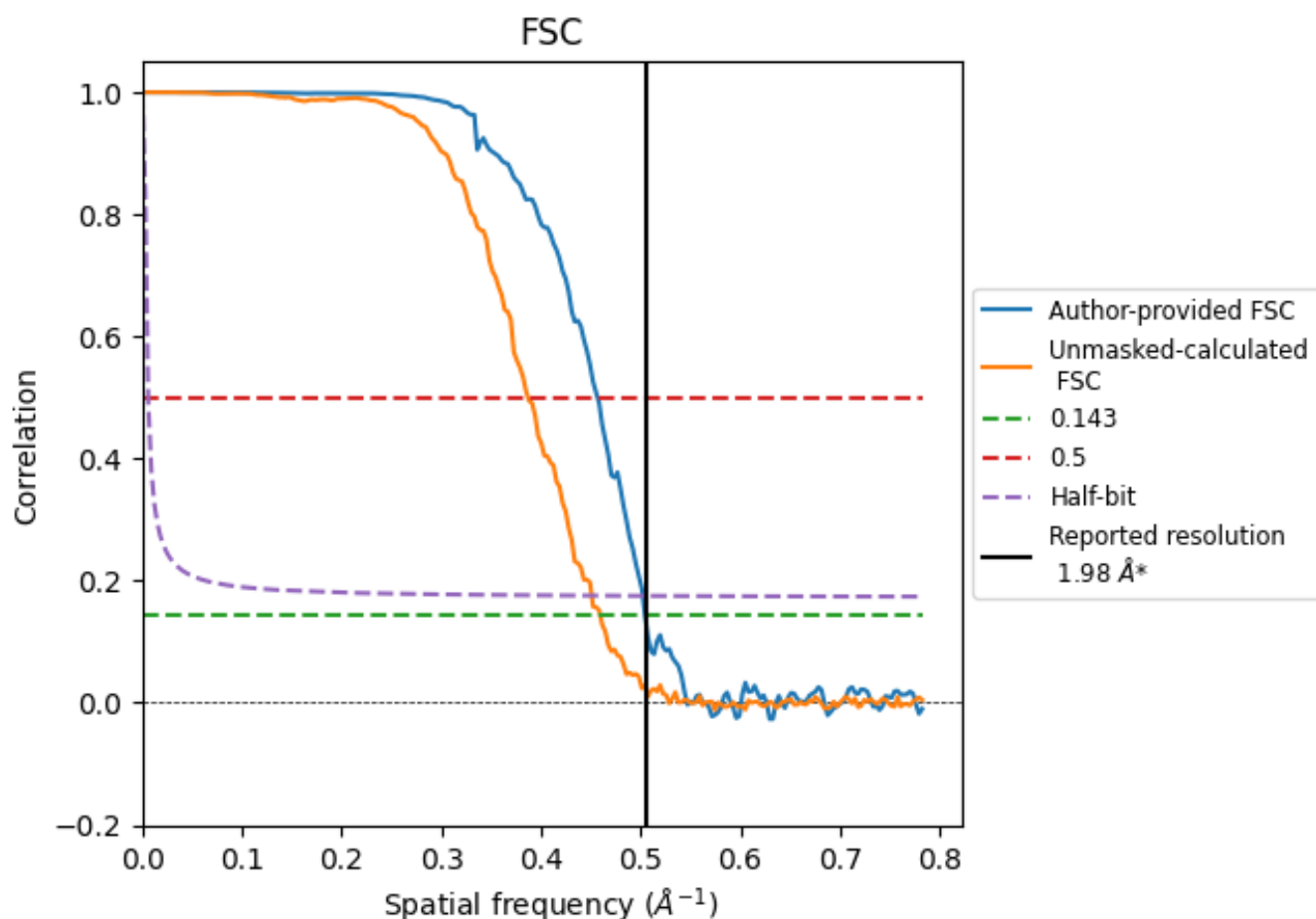


*Reported resolution corresponds to spatial frequency of 0.505 Å⁻¹

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 $0.505 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

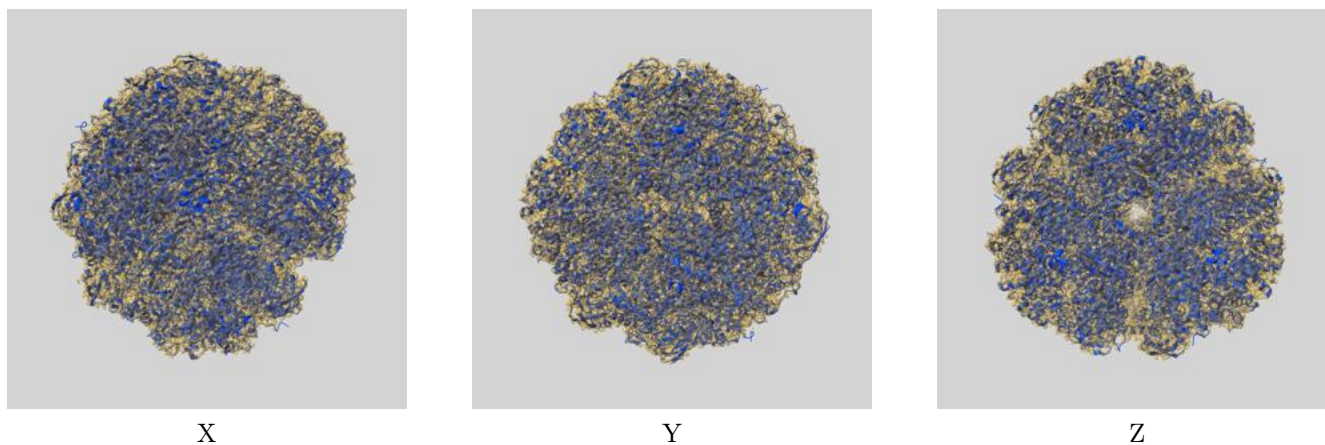
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.98	-	-
Author-provided FSC curve	1.98	2.19	1.99
Unmasked-calculated*	2.18	2.58	2.22

*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 2.18 differs from the reported value 1.98 by more than 10 %

9 Map-model fit [i](#)

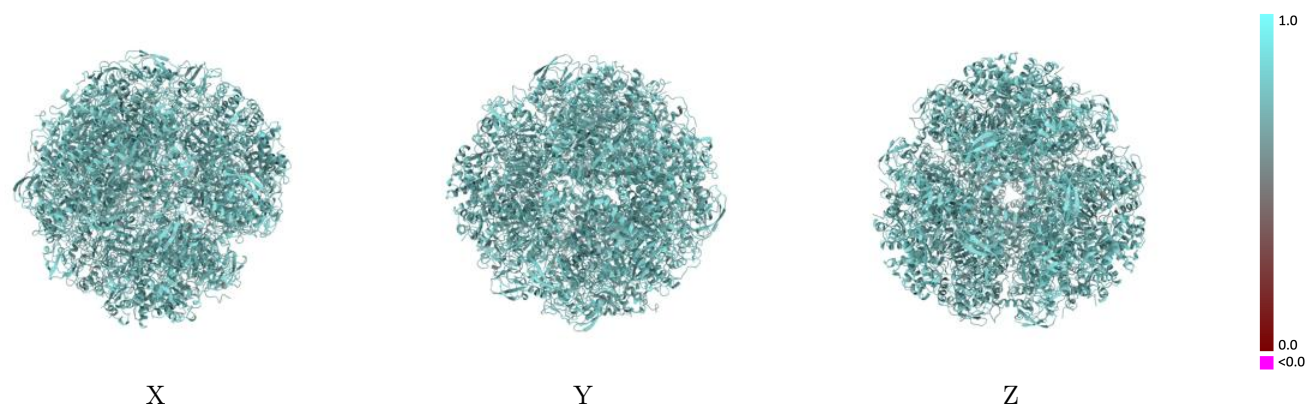
This section contains information regarding the fit between EMDB map EMD-10835 and PDB model 6YL3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



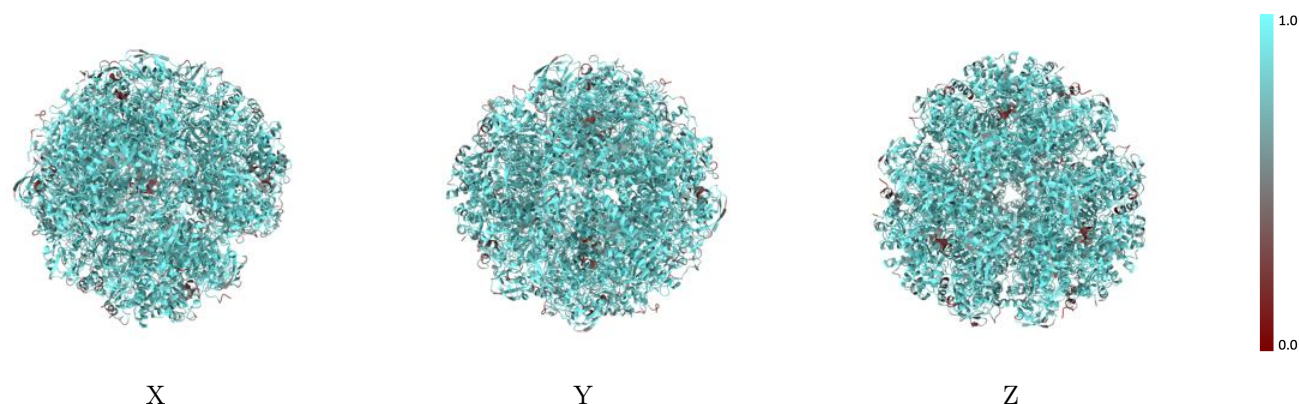
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



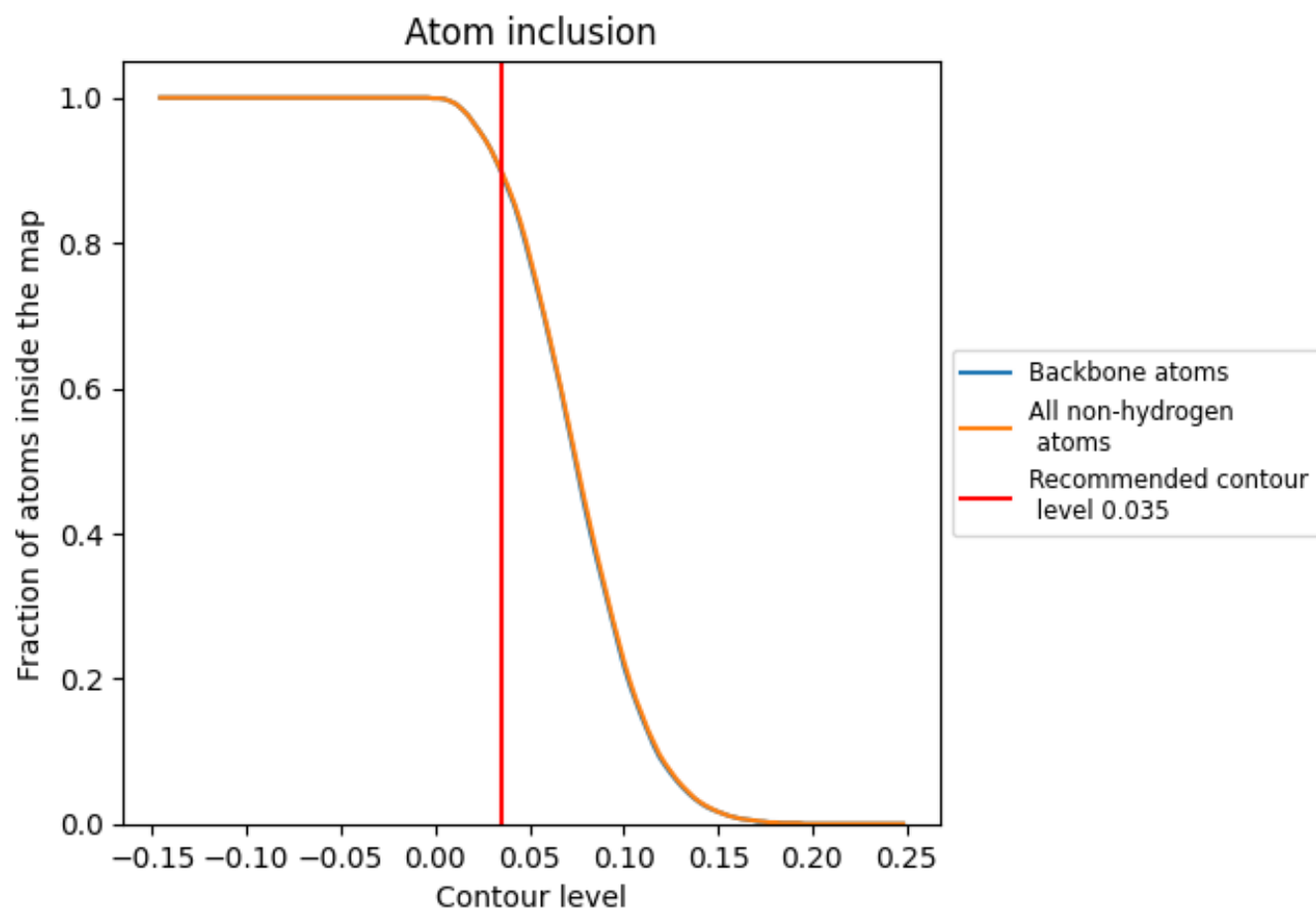
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.7670
0	 0.8400	 0.7590
1	 0.9230	 0.7790
2	 0.8770	 0.7620
3	 0.8310	 0.7530
4	 0.9210	 0.7720
5	 0.8810	 0.7610
6	 0.8330	 0.7460
7	 0.9220	 0.7760
8	 0.8770	 0.7570
9	 0.8260	 0.7350
A	 0.8790	 0.7670
B	 0.8420	 0.7630
C	 0.9260	 0.7840
D	 0.8800	 0.7660
E	 0.8340	 0.7590
F	 0.9250	 0.7800
G	 0.8750	 0.7600
H	 0.8390	 0.7560
I	 0.9200	 0.7740
J	 0.8770	 0.7660
K	 0.8250	 0.7360
L	 0.9120	 0.7490
M	 0.8750	 0.7660
N	 0.8340	 0.7560
O	 0.9210	 0.7730
P	 0.8800	 0.7650
Q	 0.8340	 0.7410
R	 0.9200	 0.7700
S	 0.8790	 0.7670
T	 0.8240	 0.7380
U	 0.9140	 0.7600
V	 0.9190	 0.7660
W	 0.8770	 0.7620
X	 0.8380	 0.7580



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.9230	 0.7760
Z	 0.8830	 0.7640