wwPDB EM Validation Summary Report (i)

Oct 26, 2026 – 04:13 PM JST

PDB ID	:	9XH6 / pdb_00009xh6
EMDB ID	:	EMD-66867
Title	:	The cryo-EM structure of F-PI2620 bound type1 amyloid beta 42 fibril
Authors	:	Zhao, Q.Y.; Cao, T.Y.; Liu, C.; Li, D.
Deposited on	:	2025-10-31
Resolution	:	3.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

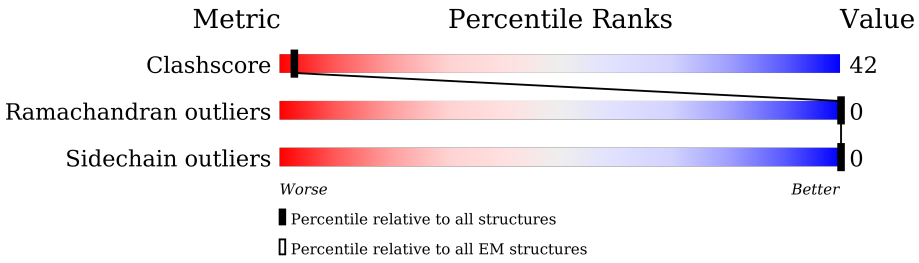
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

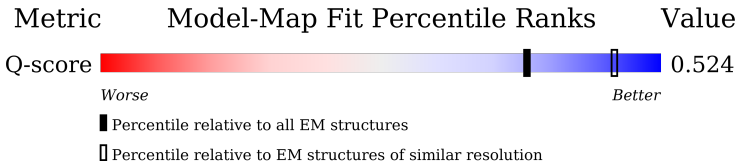
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	770	96%
1	D	770	96%
1	E	770	96%
1	F	770	96%

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Mol	Chain	Length	Quality of chain
1	G	770	96%
1	H	770	96%
1	K	770	96%
1	L	770	96%
1	M	770	96%
1	N	770	96%
1	O	770	96%
1	P	770	96%
1	S	770	96%
1	T	770	96%
1	U	770	96%
1	V	770	96%
1	W	770	96%
1	X	770	96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A1FCO	E	101	-	-	X	-
2	A1FCO	M	101	-	-	X	-
2	A1FCO	U	101	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4560 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 Amyloid-beta precursor protein.

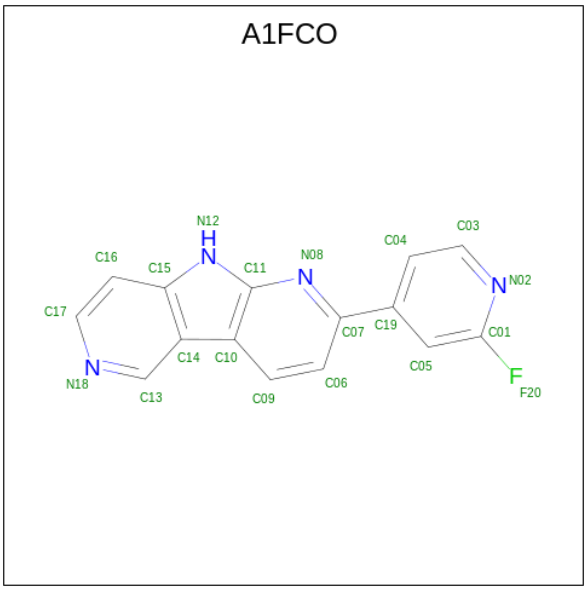
Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	D	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	E	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	F	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	G	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	H	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	K	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	L	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	M	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	N	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	O	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	P	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	S	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	T	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	U	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	V	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	W	34	Total	C	N	O	S	0	0
			250	163	42	44	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	34	Total	C	N	O	S	0	0
			250	163	42	44	1		

- Molecule 2 is Izaflortaucipir (CCD ID: A1FCO) (formula: $C_{15}H_9FN_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	F	N	0
			20	15	1	4	
2	M	1	Total	C	F	N	0
			20	15	1	4	
2	U	1	Total	C	F	N	0
			20	15	1	4	

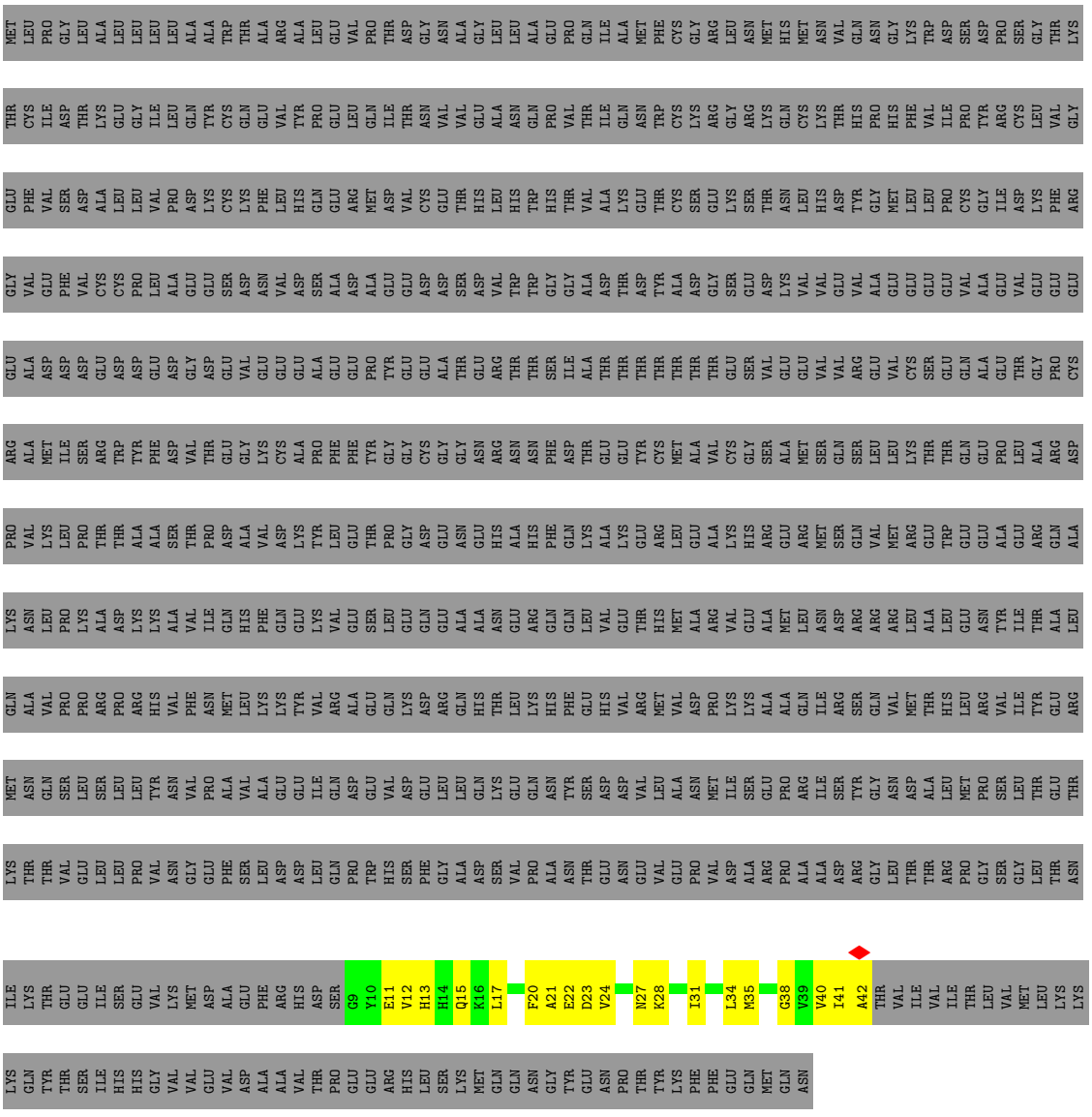
3 Residue-property plots (i)

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: Amyloid-beta precursor protein

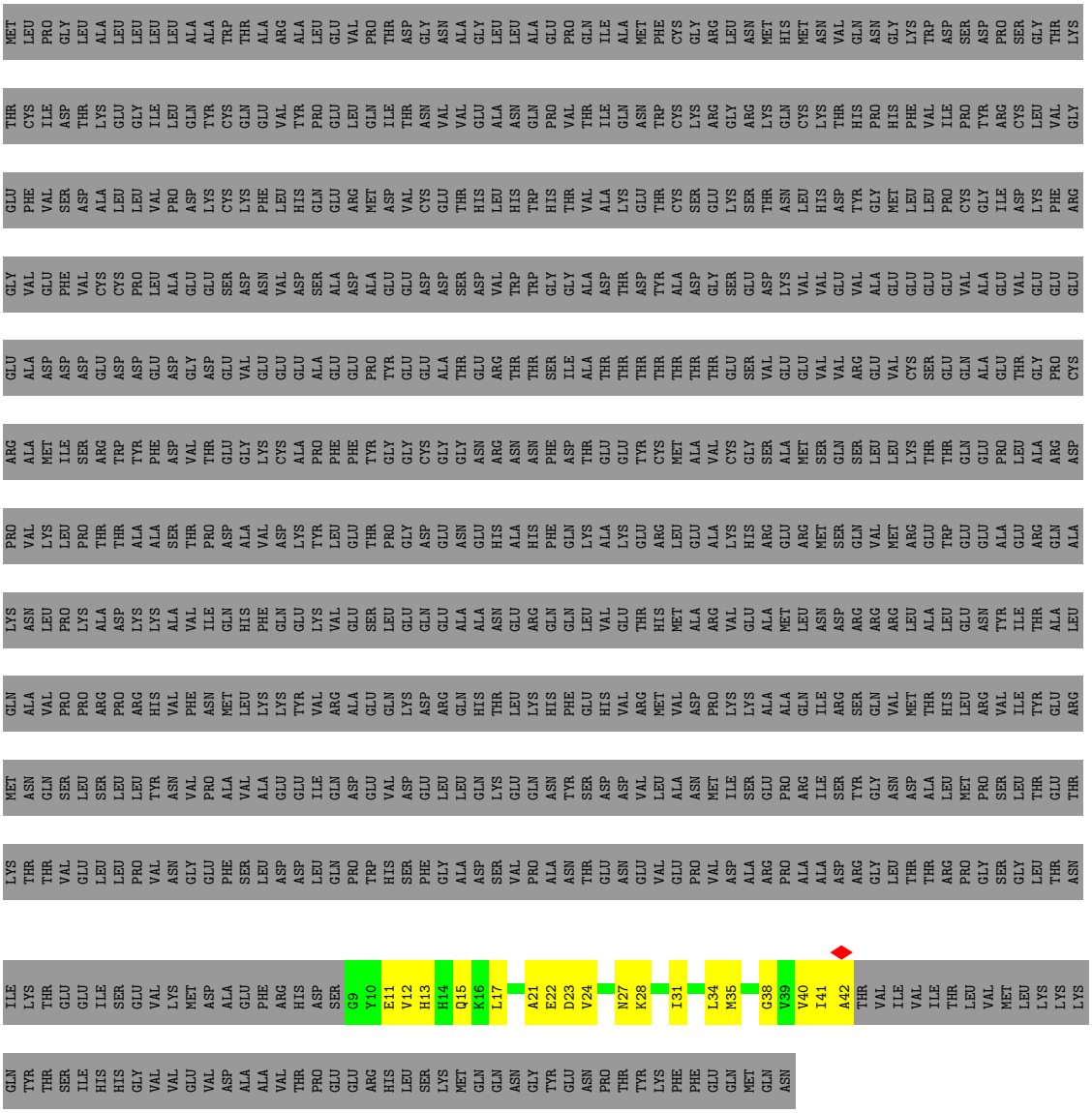
Chain C:





- Molecule 1: Amyloid-beta precursor protein

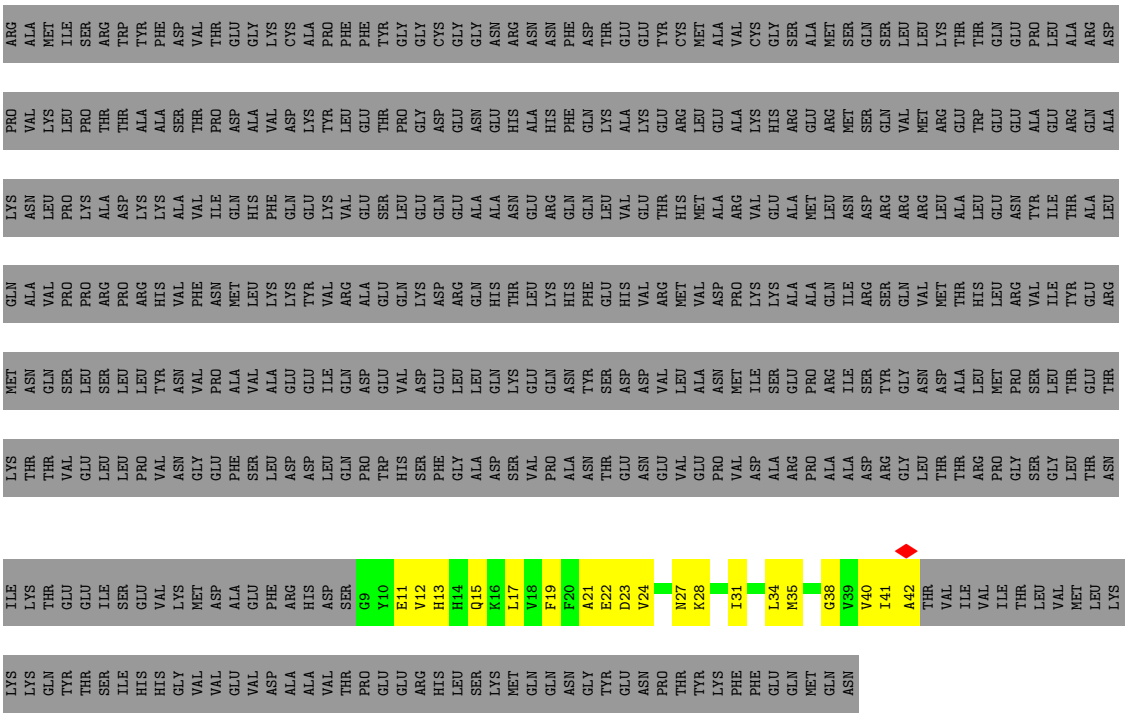
Chain D: 96%



• Molecule 1: Amyloid-beta precursor protein

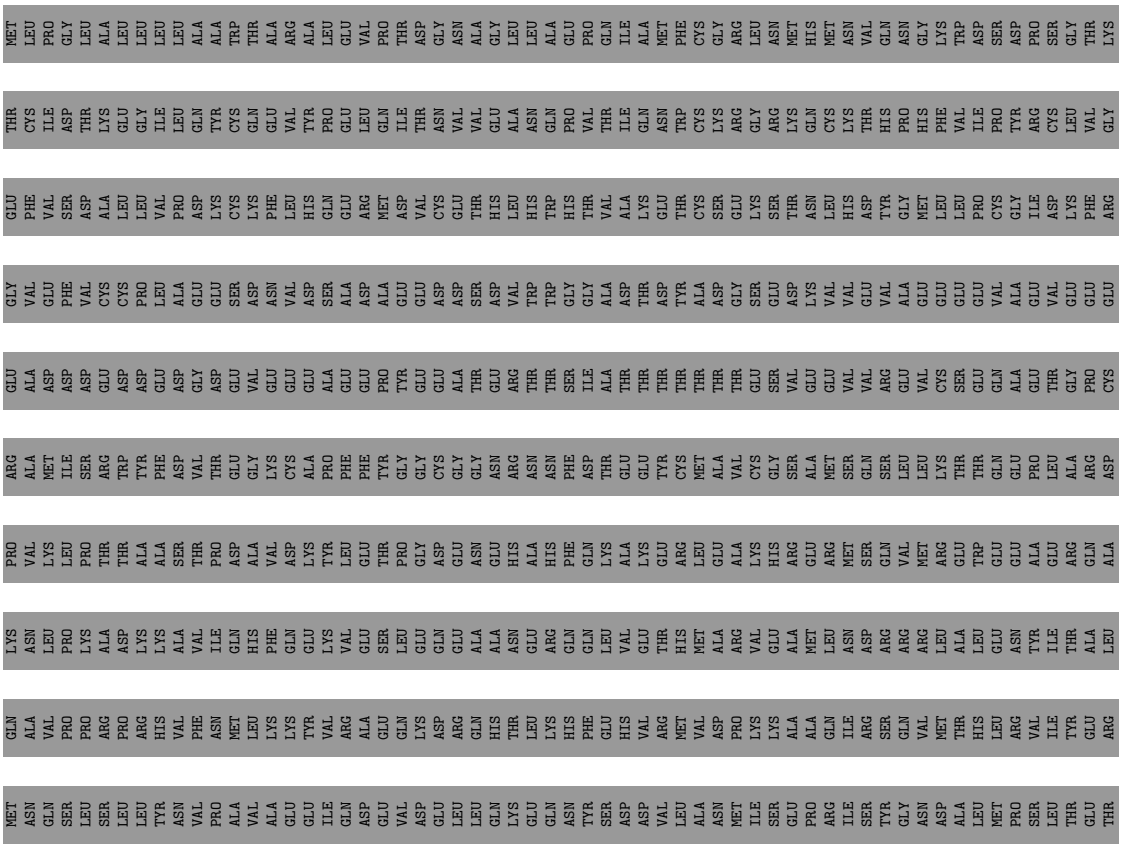
Chain E: 96%

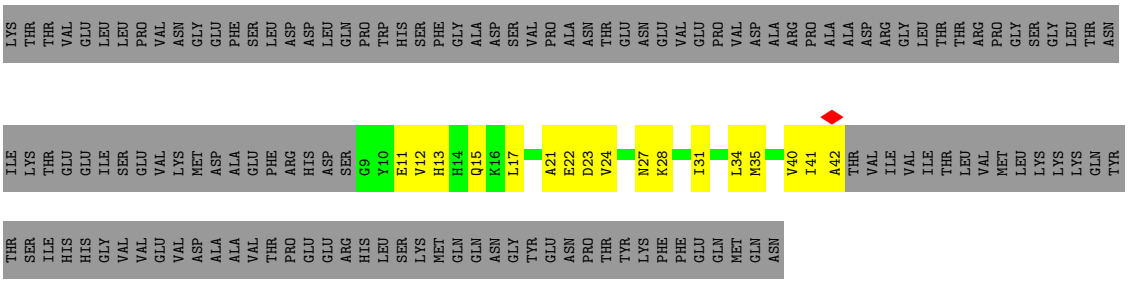




• Molecule 1: Amyloid-beta precursor protein

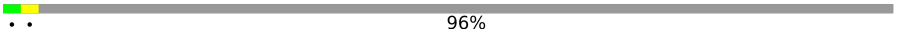
Chain F: 96%

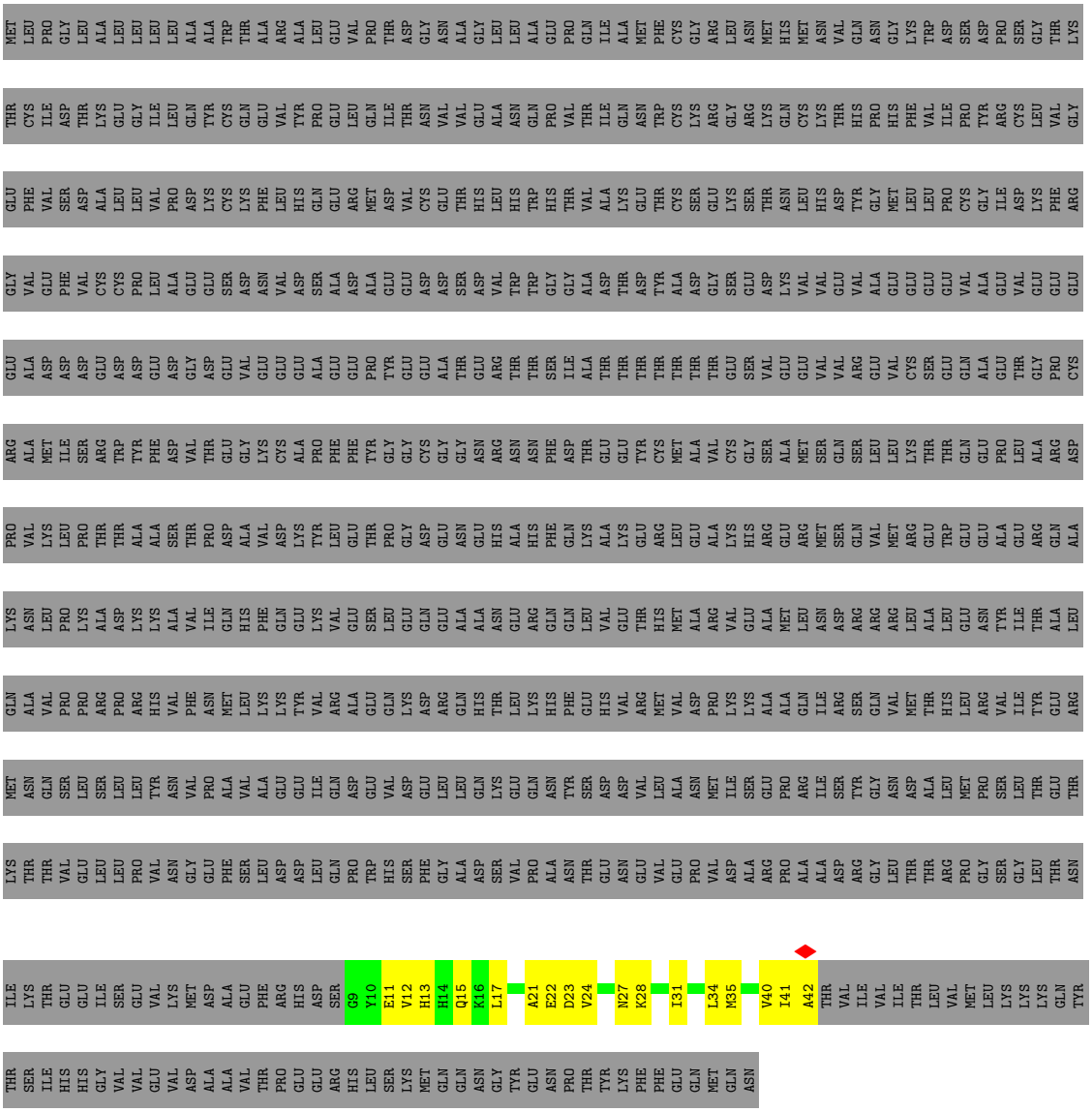




• Molecule 1: Amyloid-beta precursor protein

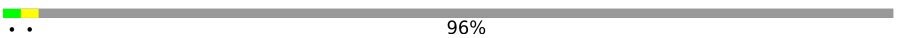
Chain G:

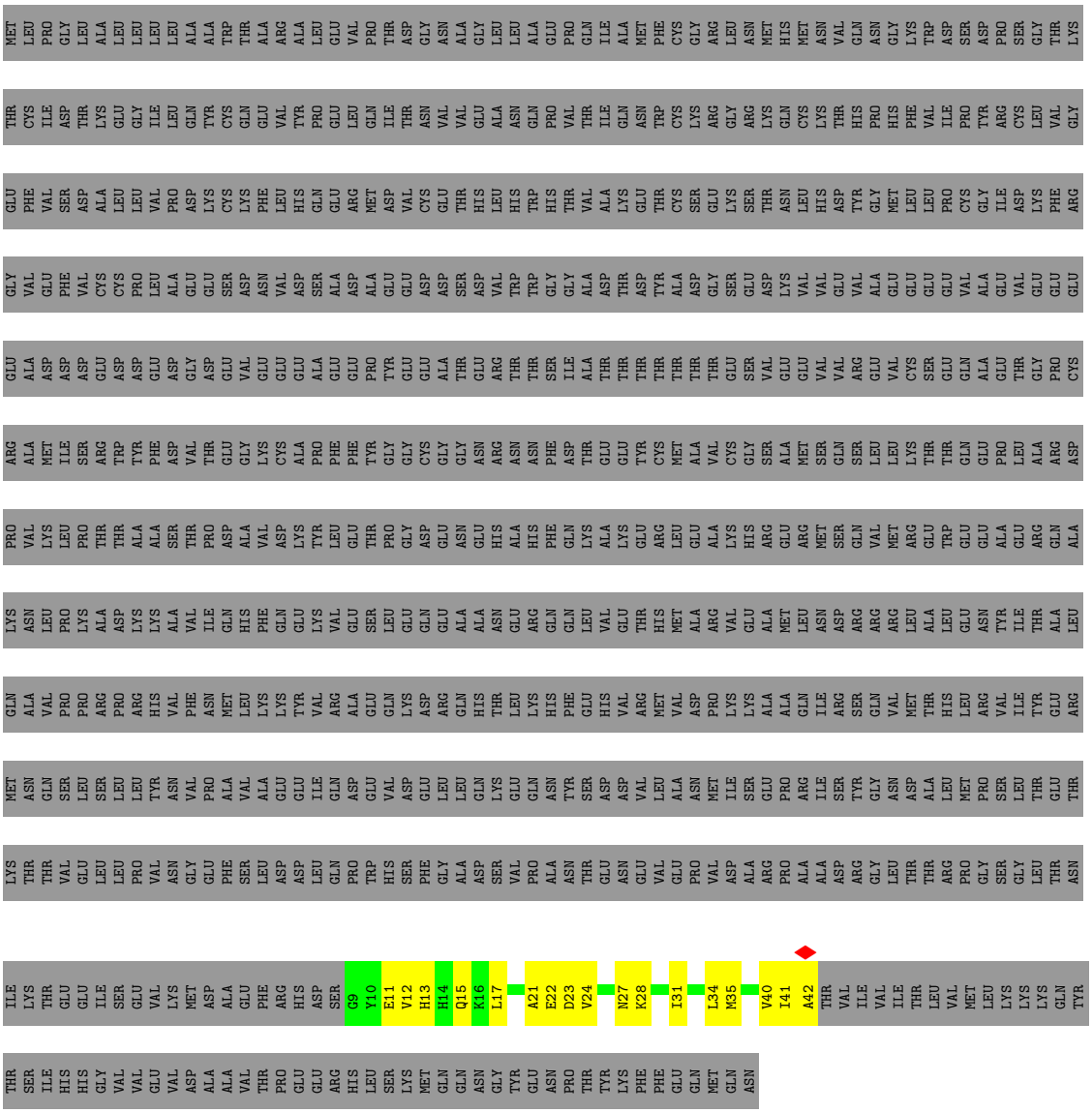




• Molecule 1: Amyloid-beta precursor protein

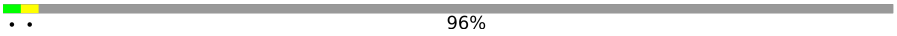
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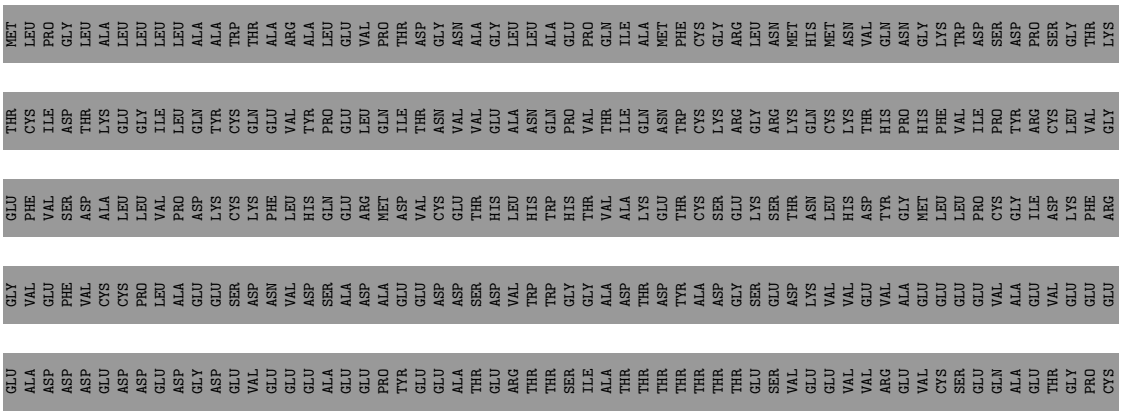


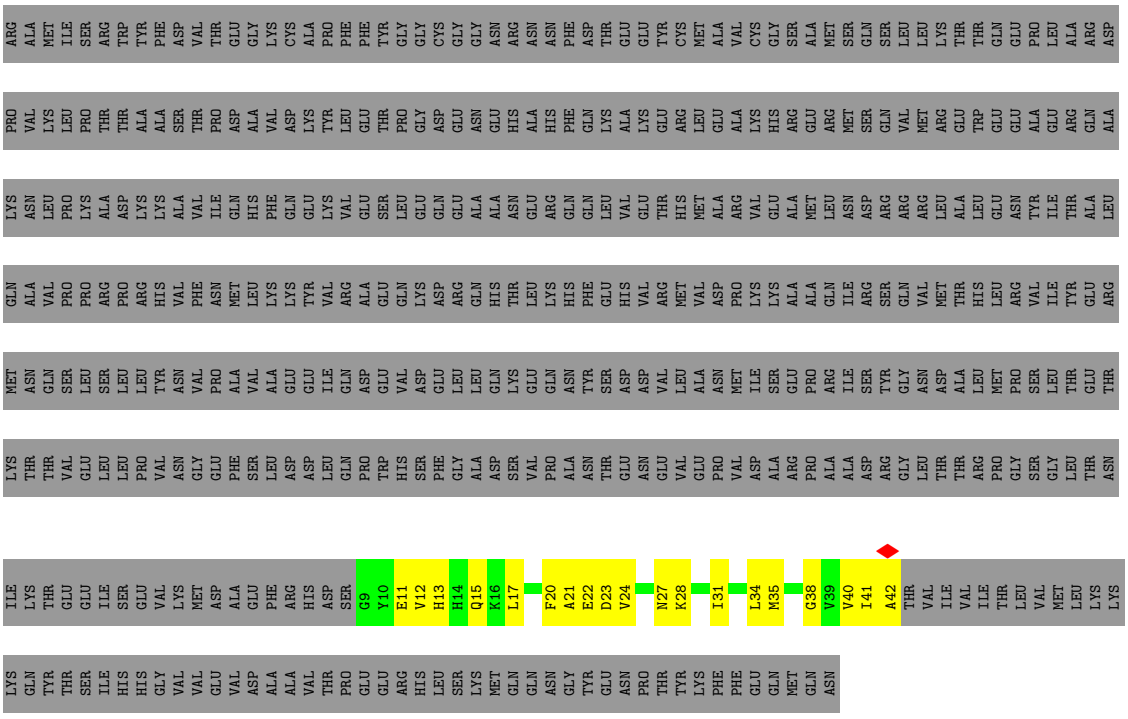


• Molecule 1: Amyloid-beta precursor protein

Chain K:

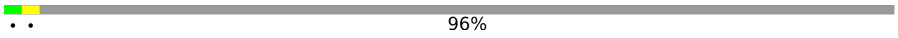


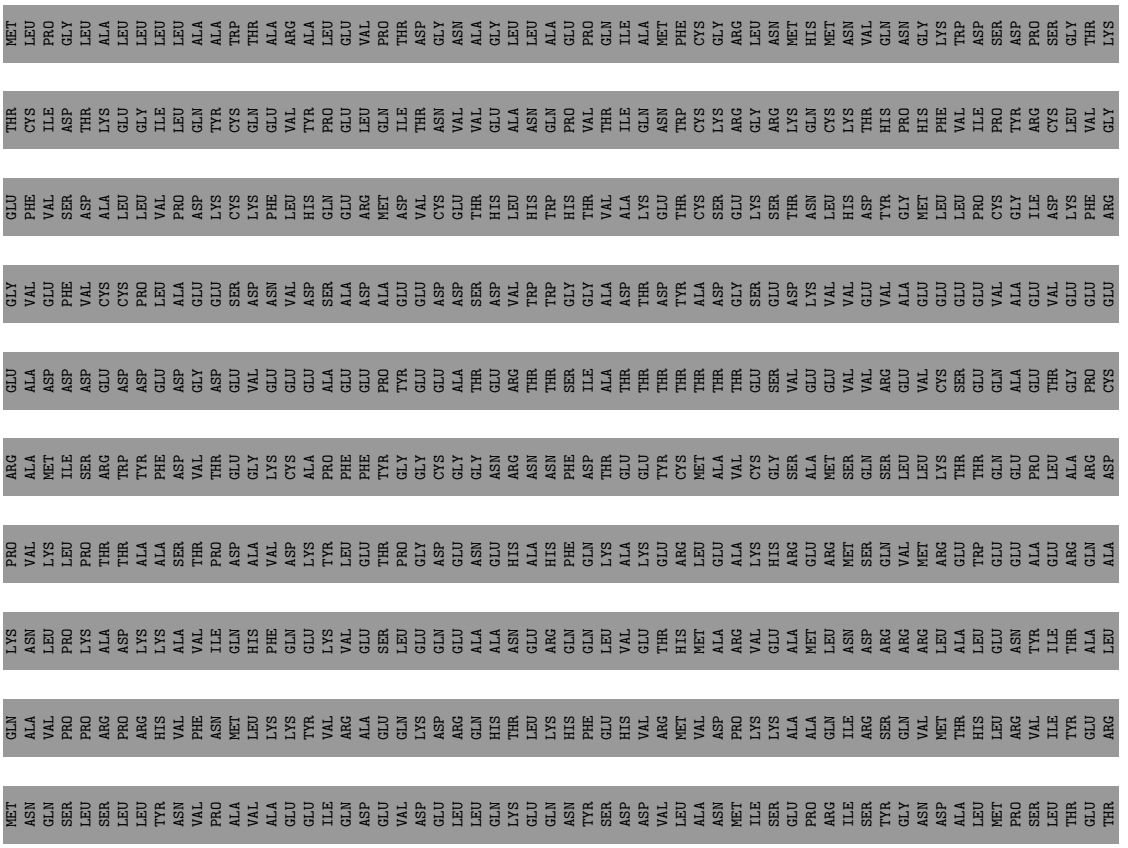


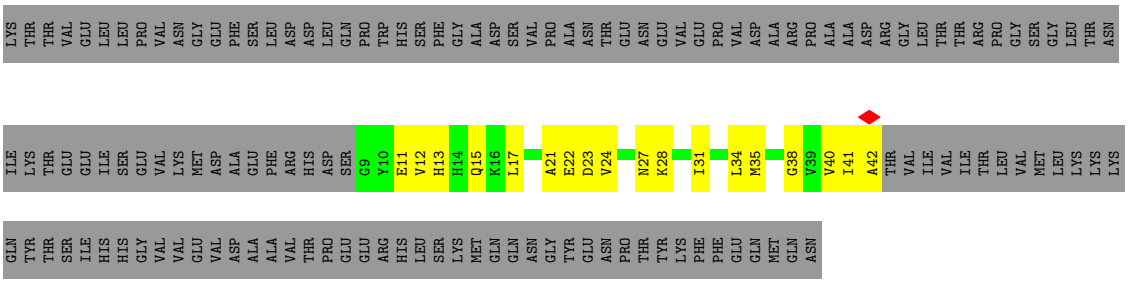


• Molecule 1: Amyloid-beta precursor protein

Chain L:

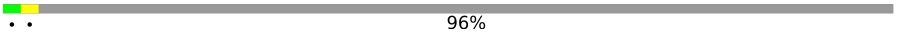


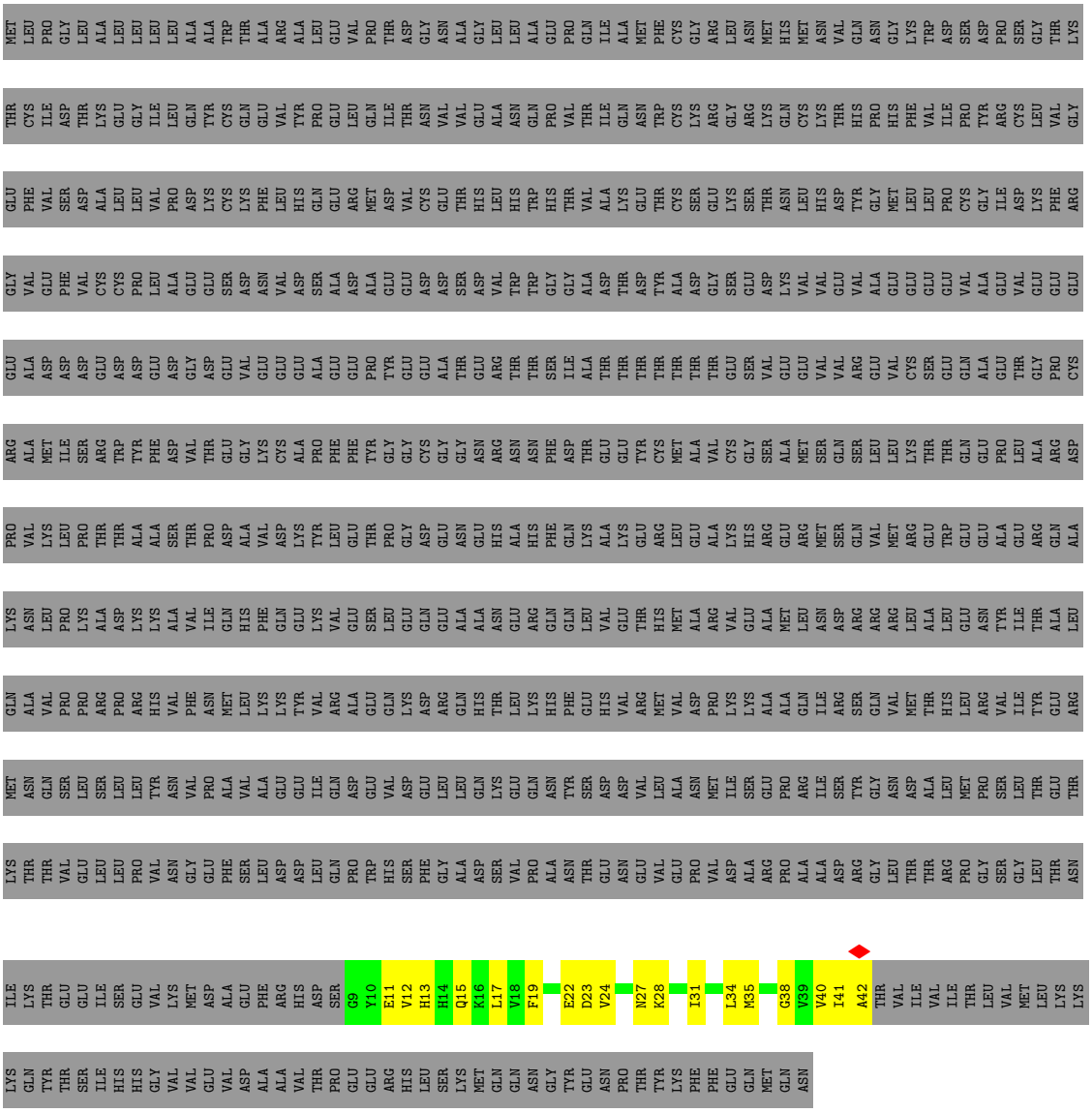




• Molecule 1: Amyloid-beta precursor protein

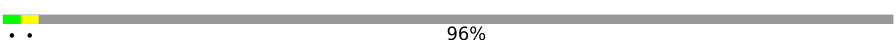
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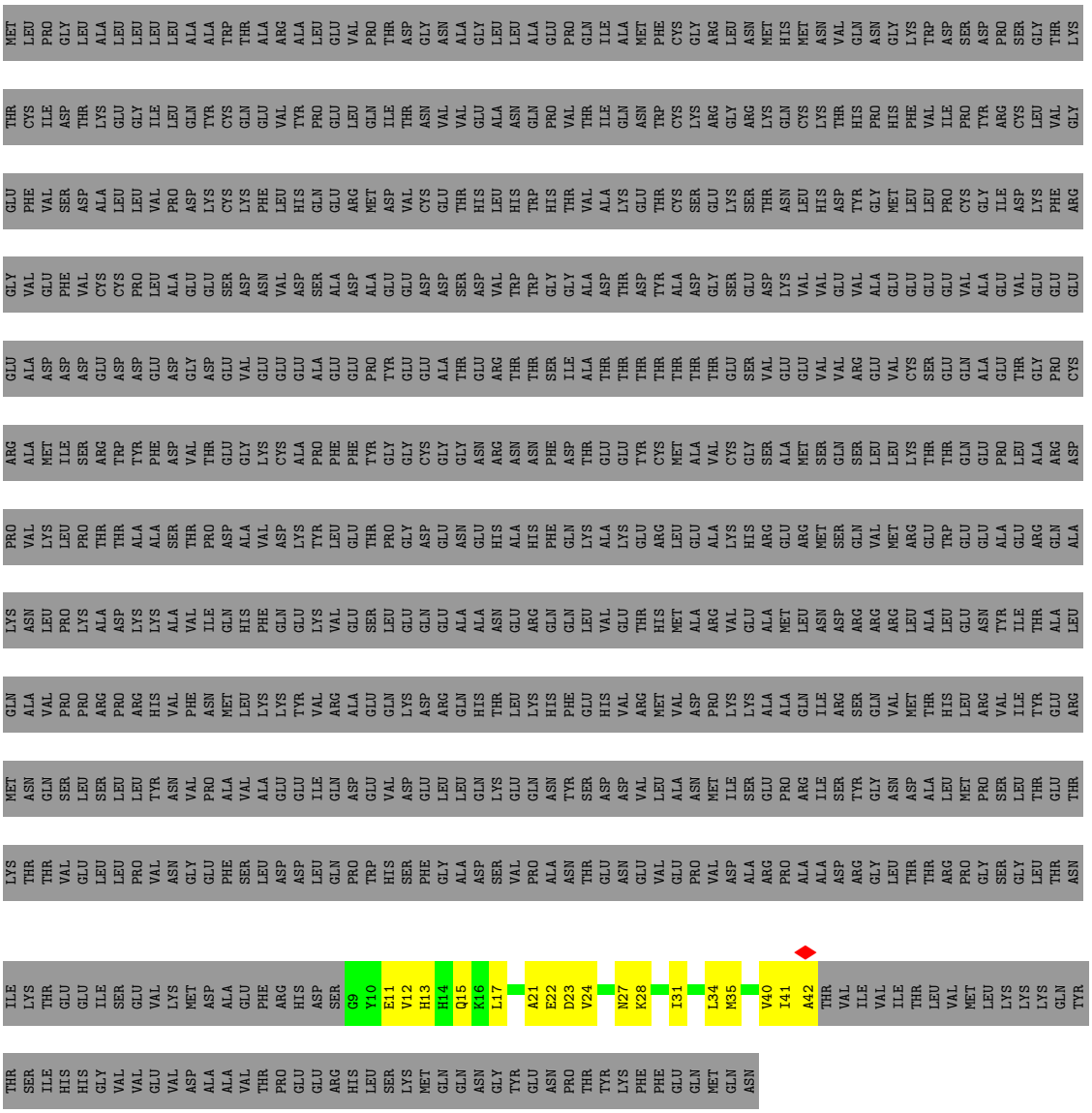




• Molecule 1: Amyloid-beta precursor protein

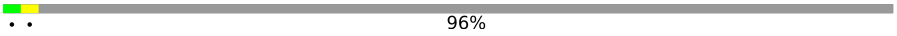
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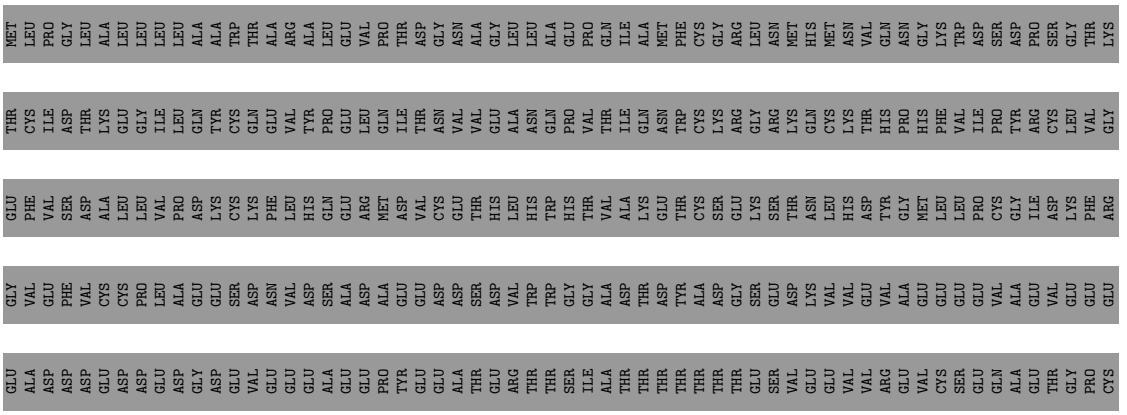


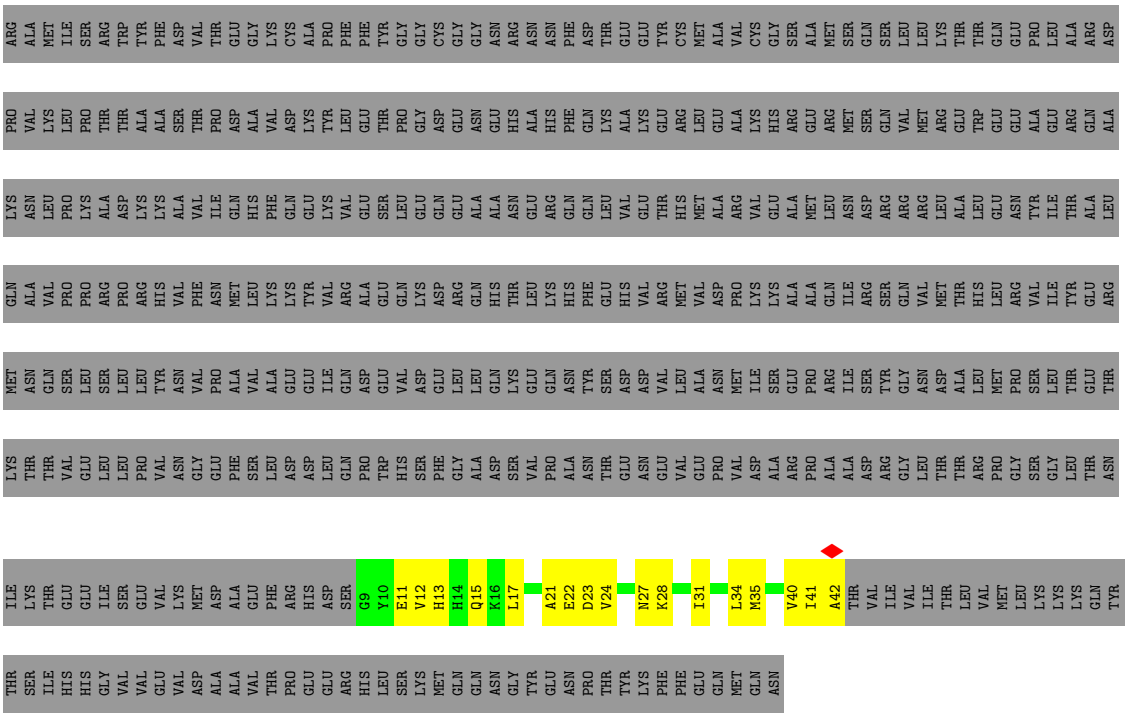


• Molecule 1: Amyloid-beta precursor protein

Chain O:

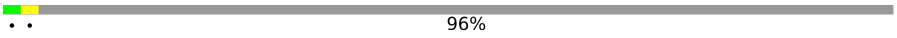


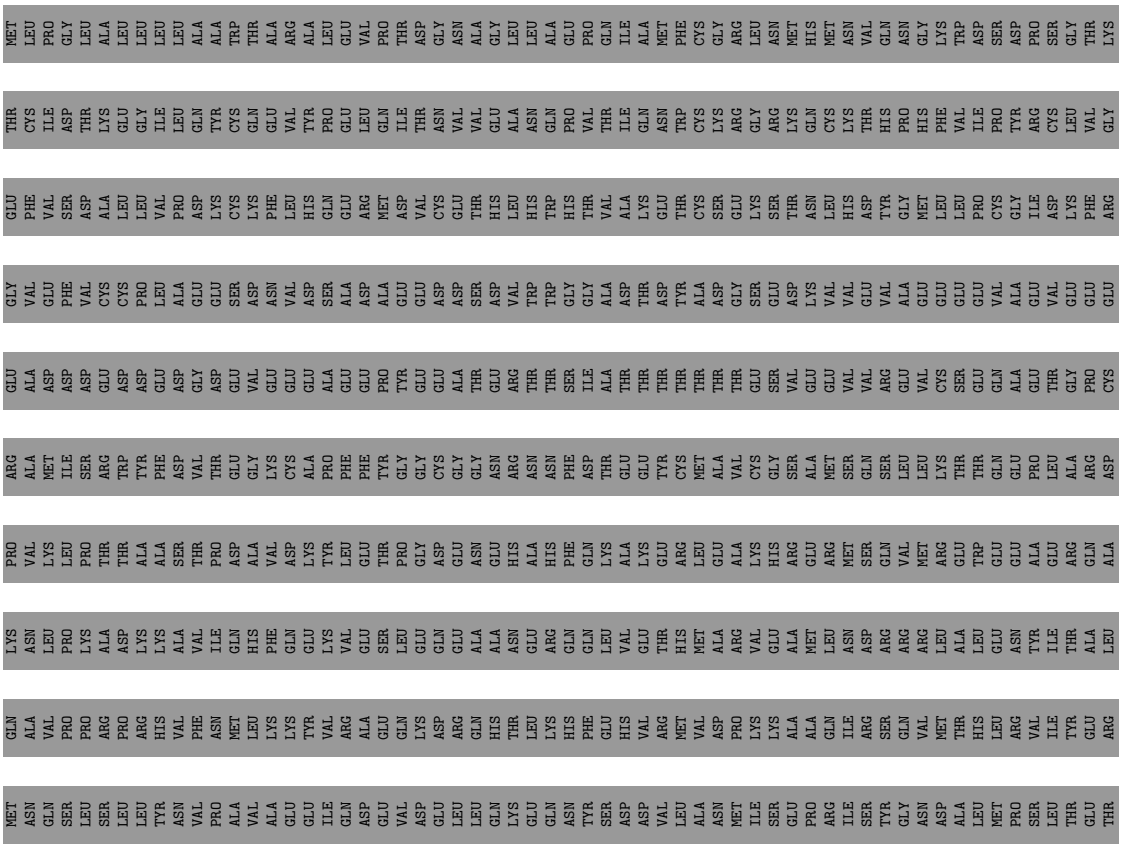


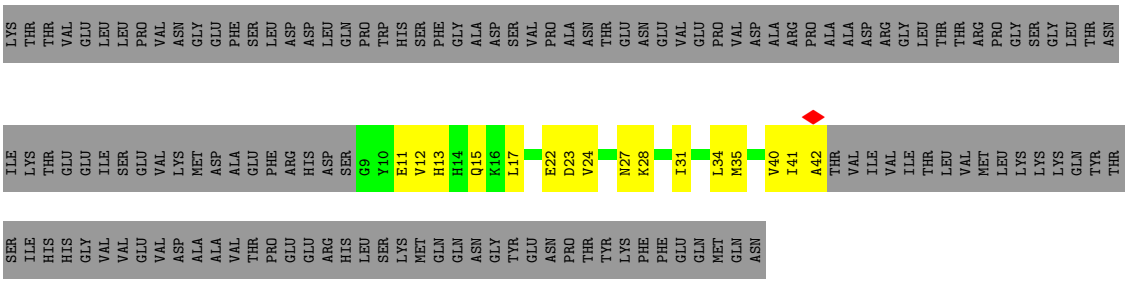


• Molecule 1: Amyloid-beta precursor protein

Chain P:

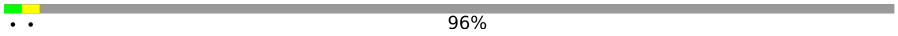


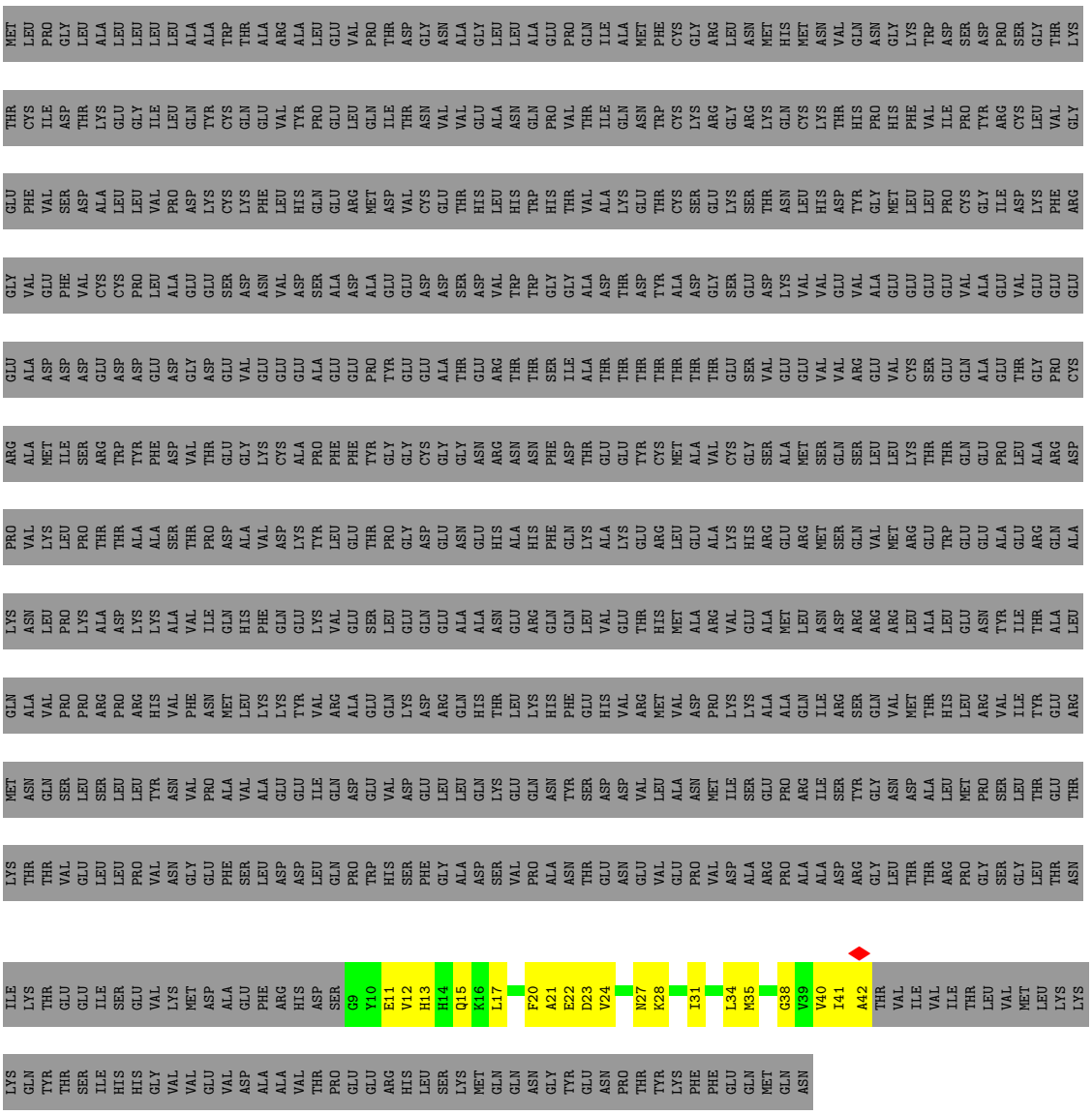




• Molecule 1: Amyloid-beta precursor protein

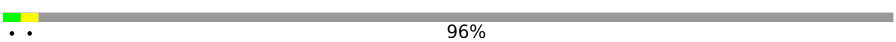
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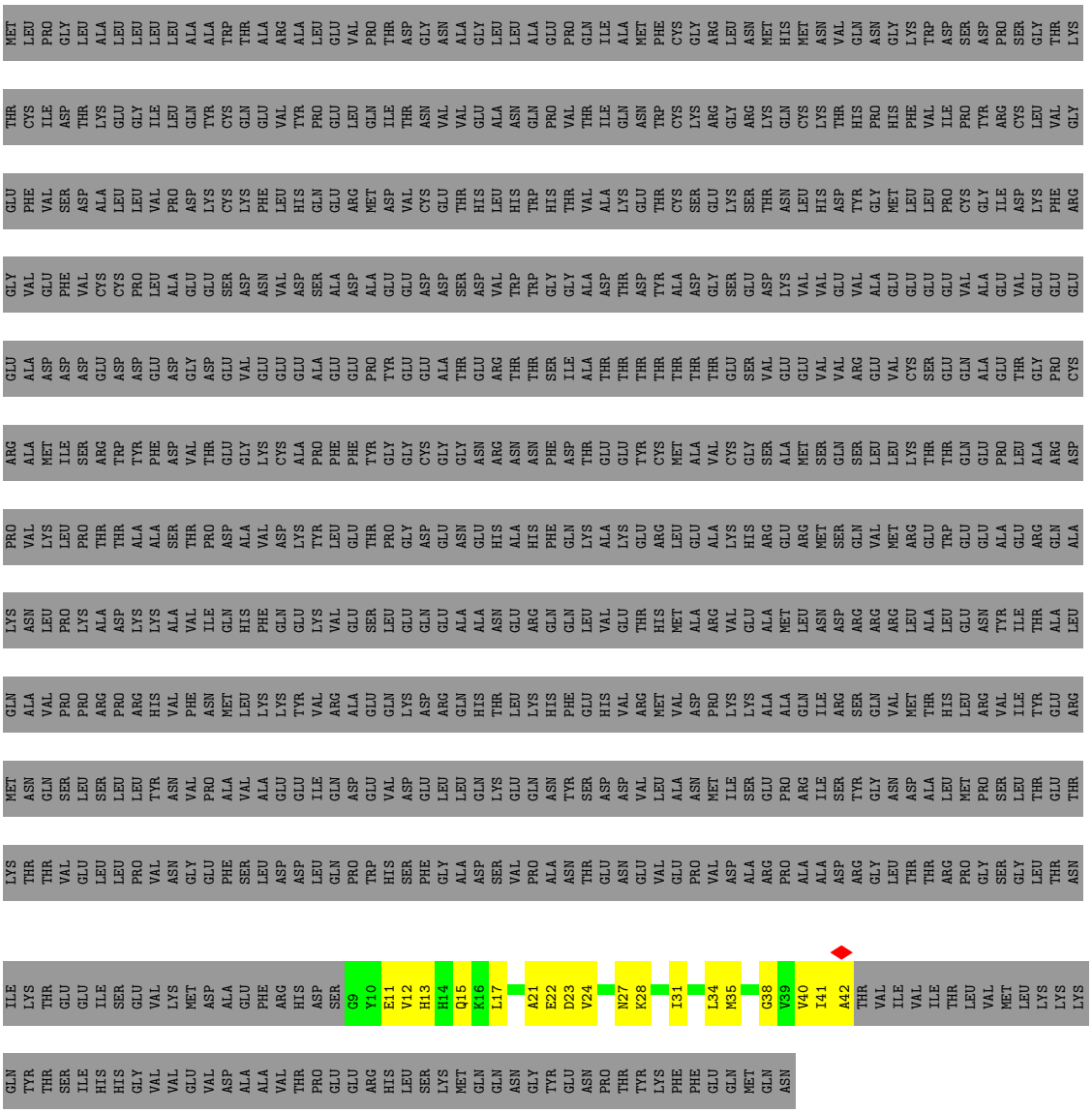




• Molecule 1: Amyloid-beta precursor protein

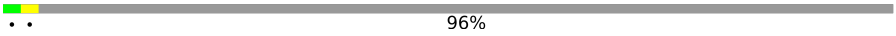
Chain T:

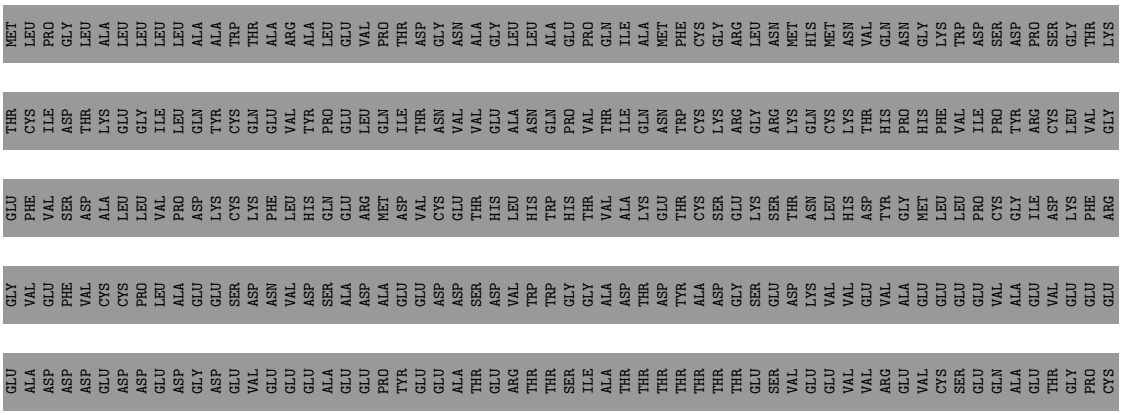


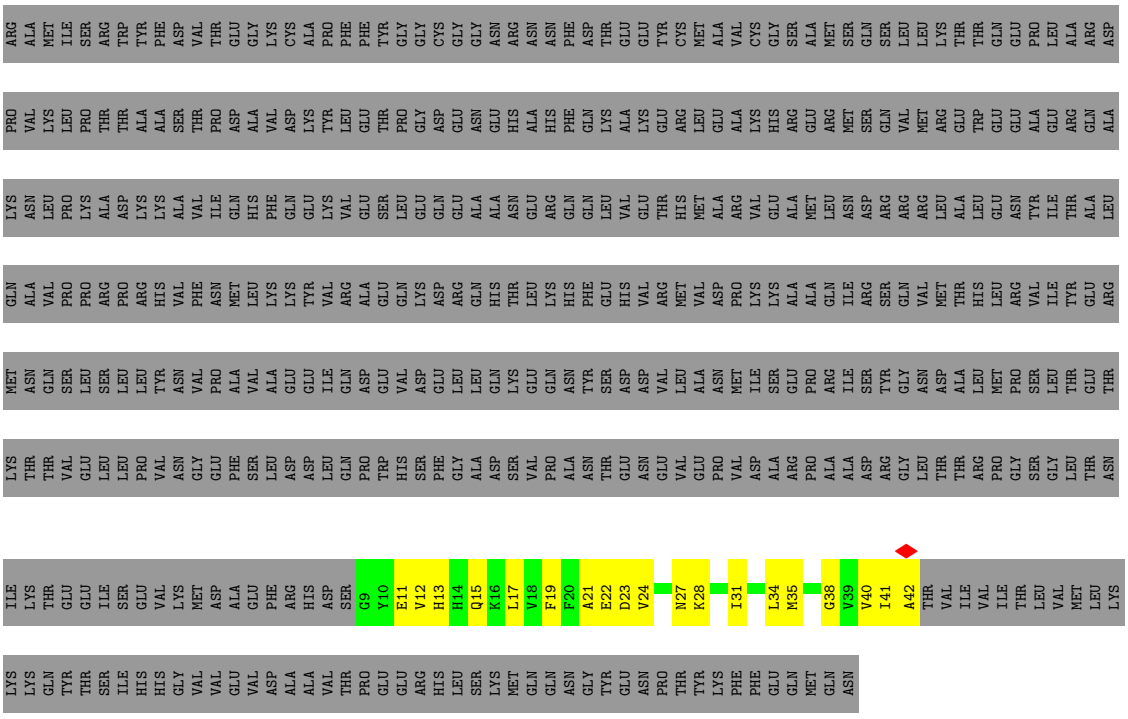


• Molecule 1: Amyloid-beta precursor protein

Chain U:

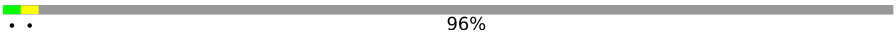


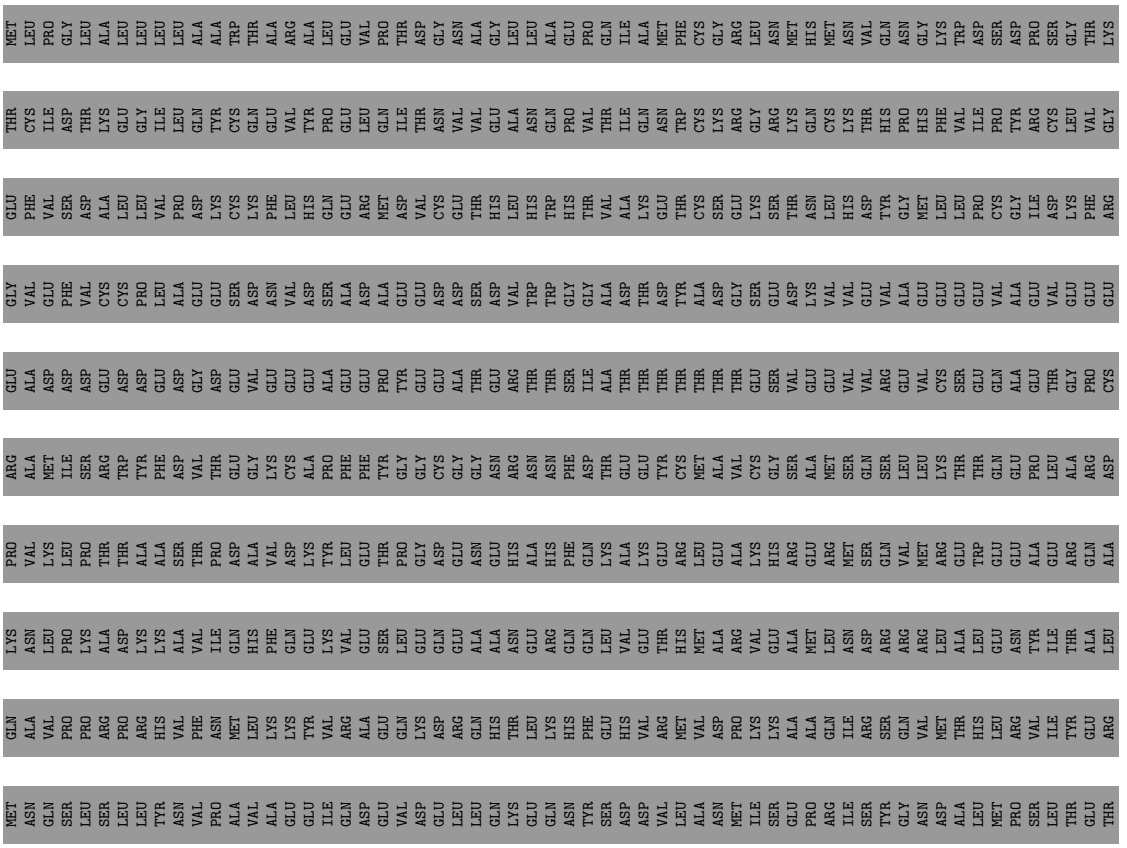


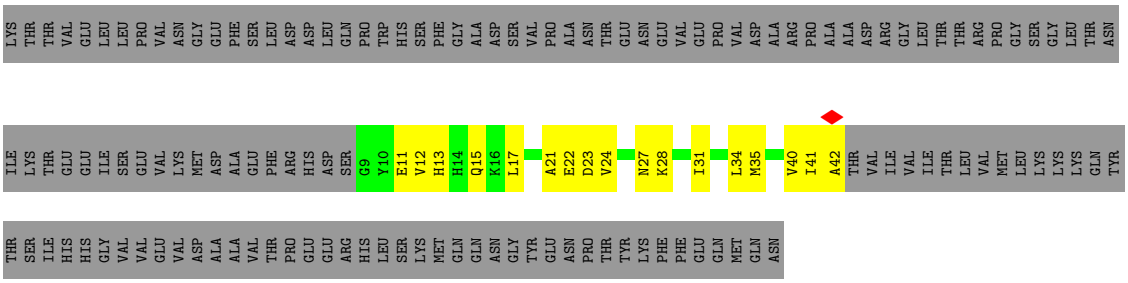


• Molecule 1: Amyloid-beta precursor protein

Chain V:

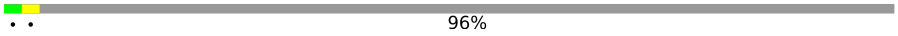


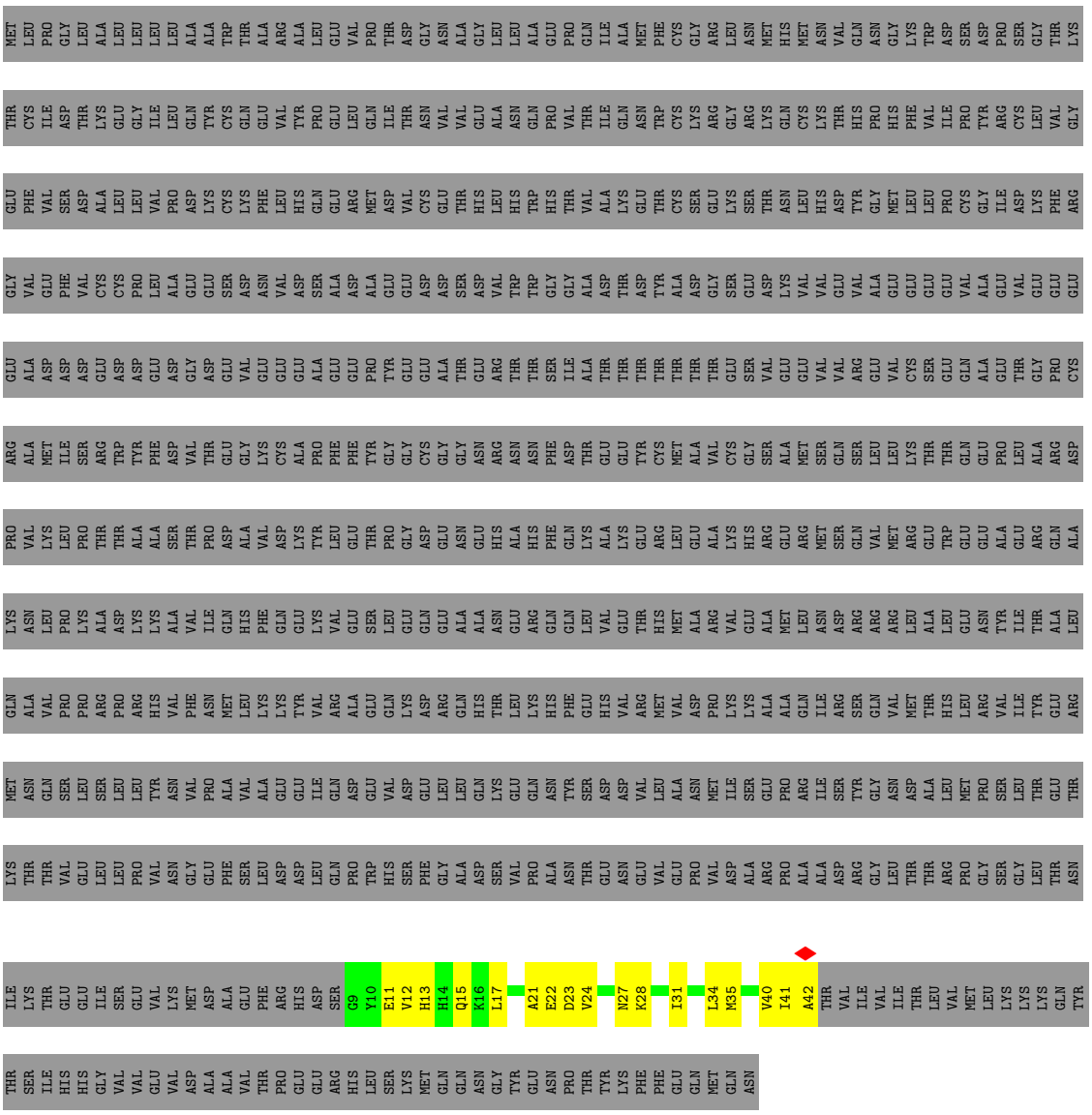




• Molecule 1: Amyloid-beta precursor protein

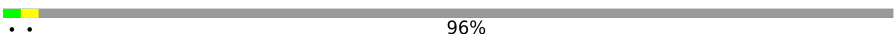
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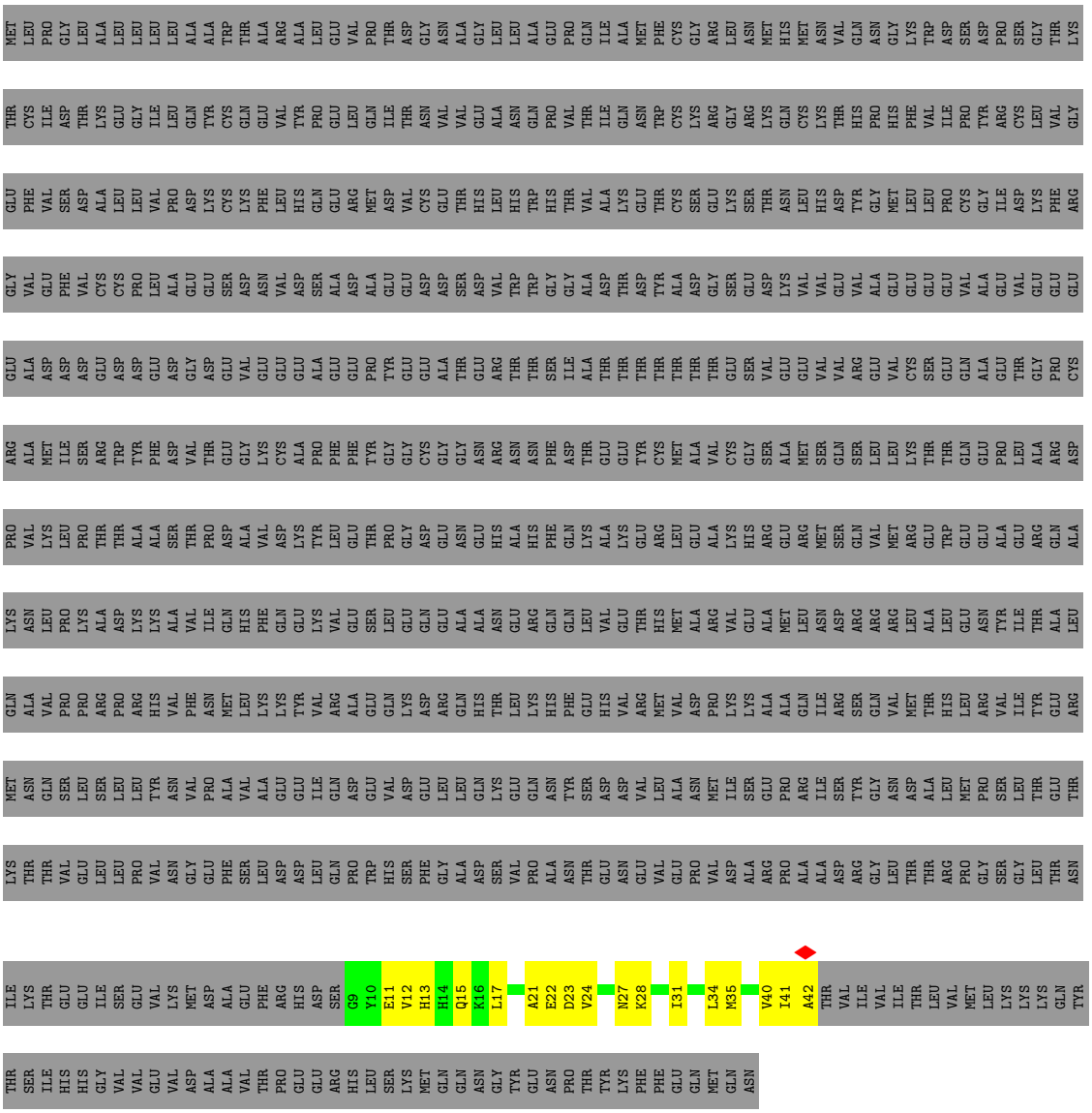




• Molecule 1: Amyloid-beta precursor protein

Chain X:




MET LEU PRO GLY LEU ALA LEU LEU LEU LEU ALA ALA ALA TRP THR ALA ARG ALA LEU GLU VAL PRO THR ASP GLY ASN ALA GLY LEU LEU ALA GLU PRO GLN ILE ALA MET PHE CYS GLY ARG LEU ASN MET HIS MET ASN VAL GLN ASN GLY LYS TRP ASP SER ASP PRO SER GLY THR LYS
THR CYS ILE ASP THR LYS GLU GLY ILE LEU GLN TYR CYS GLN GLU VAL TYR PRO GLU LEU GLN ILE THR ASN VAL VAL GLU ALA ASN GLN PRO VAL THR ILE GLN ASN TRP CYS LYS ARG GLY ARG LYS GLN CYS LYS THR HIS PRO HIS PHE VAL ILE PRO TYR ARG CYS LEU VAL GLY
GLU PHE VAL SER ASP ALA LEU LEU VAL PRO ASP LYS CYS LYS PHE LEU HIS GLN GLU ASP ARG MET ASP VAL CYS GLU THR HIS LEU HIS TRP HIS THR VAL ALA LYS GLU THR CYS SER GLU LYS SER THR ASN LEU HIS ASP TYR GLY MET LEU LEU PRO CYS GLY ILE ASP LYS PHE ARG
GLY VAL GLU PHE VAL CYS CYS PRO LEU ALA GLU GLU GLU SER ASP ASN VAL ASP SER ALA ASP ALA GLU GLU ASP ASP SER ASP VAL THR TRP TRP GLY GLY ALA ASP THR ASP TYR ALA ASP GLY SER GLU ASP LYS VAL VAL GLU VAL ALA GLU GLU VAL ALA GLU GLU GLU GLU
GLU ALA ASP ASP ASP GLU ASP GLU GLY ASP GLU GLU ALA GLU GLU PRO TYR GLU GLU ALA THR GLU ARG THR THR SER ILE ALA THR THR THR THR THR THR GLU SER VAL GLU GLU VAL GLU ARG GLU VAL CYS SER GLU GLN GLN ALA GLU THR GLY PRO CYS
ARG ALA MET ILE SER ARG TRP TYR PHE ASP VAL THR GLU GLY LYS CYS ALA PRO PHE PHE TYR GLY GLY CYS GLY GLY ASN ARG ASN ASN PHE ASP THR GLU GLU TYR CYS MET ALA VAL CYS GLY SER ALA MET SER GLN SER LEU LEU LYS THR THR GLN GLU PRO LEU ALA ARG ASP
PRO VAL LYS LEU PRO THR THR ALA ALA SER THR PRO ASP ALA VAL ASP LYS TYR LEU GLU THR PRO GLY ASP GLU ASN GLU HIS ALA HIS PHE GLN LYS ALA LYS GLU ARG LEU GLU ALA LYS HIS ARG GLU ARG MET SER GLN VAL MET ARG GLU TRP GLU GLU ALA GLU ARG GLN ALA
LYS ASN LEU PRO LYS ALA ASP LYS LYS ALA VAL ILE GLN HIS PHE GLN GLU LYS VAL GLU SER LEU GLU GLU GLN GLU ALA ALA ASN GLU ARG GLN GLN LEU VAL GLU THR HIS MET ALA ARG VAL GLU ALA MET LEU ASN ASP ARG ARG ARG LEU ALA LEU GLU ASN TYR ILE THR ALA LEU
GLN ALA VAL PRO PRO ARG PRO ARG HIS VAL PHE ASN MET LEU LYS LYS TYR VAL ARG ALA GLU GLN LYS ASP ARG GLN HIS THR LEU LYS HIS PHE GLU HIS VAL ARG MET VAL ASP PRO LYS LYS ALA ALA GLN ILE ARG SER GLN VAL MET THR HIS LEU ARG VAL ILE TYR GLU ARG
MET ASN GLN SER LEU SER LEU TYR ASN VAL PRO ALA VAL ALA GLU GLU ILE GLN ASP GLU VAL ASP GLU LEU LEU GLN LYS GLU GLN ASN TYR SER ASP ASP VAL LEU ALA ASN MET ILE SER GLU PRO ARG ILE SER TYR GLY ASN ASP ALA LEU MET PRO SER LEU THR GLU THR
LYS THR THR VAL GLU LEU LEU PRO VAL ASN GLY GLU PHE SER LEU ASP ASP LEU GLN PRO TRP HIS SER PHE GLY ALA ASP SER VAL PRO ALA ASN THR GLU ASN GLU VAL GLU PRO VAL ASP ALA ARG PRO ALA ALA ASP ARG GLY LEU THR THR ARG PRO GLY SER GLY LEU THR ASN
ILE LYS THR GLU GLU ILE SER GLU VAL LYS MET ASP ALA GLU PHE ARG HIS ASP SER G9 Y10 E11 V12 H13 H14 Q15 K16 L17 A21 E22 D23 V24 N27 K28 I31 L34 M35 V40 I41 A42 THR VAL ILE VAL ILE THR LEU VAL MET LEU LYS LYS LYS GLN TYR
THR SER ILE HIS HIS GLY VAL VAL GLU VAL ASP ALA ALA VAL THR PRO GLU GLU ARG HIS LEU SER LYS MET GLN GLN ASN PRO THR TYR LYS PHE PHE GLU GLN MET GLN ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=178.517°, rise=2.398 Å, axial sym=C1	Depositor
Number of segments used	11174	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1FCO

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	C	0.30	0/254	0.37	0/341
1	D	0.31	0/254	0.37	0/341
1	E	0.30	0/254	0.37	0/341
1	F	0.30	0/254	0.36	0/341
1	G	0.30	0/254	0.37	0/341
1	H	0.30	0/254	0.37	0/341
1	K	0.30	0/254	0.37	0/341
1	L	0.31	0/254	0.37	0/341
1	M	0.31	0/254	0.36	0/341
1	N	0.30	0/254	0.37	0/341
1	O	0.31	0/254	0.37	0/341
1	P	0.30	0/254	0.37	0/341
1	S	0.30	0/254	0.37	0/341
1	T	0.31	0/254	0.37	0/341
1	U	0.30	0/254	0.37	0/341
1	V	0.30	0/254	0.37	0/341
1	W	0.31	0/254	0.37	0/341
1	X	0.31	0/254	0.37	0/341
All	All	0.30	0/4572	0.37	0/6138

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	250	0	252	35	0
1	D	250	0	252	33	0
1	E	250	0	252	37	0
1	F	250	0	252	31	0
1	G	250	0	252	34	0
1	H	250	0	252	34	0
1	K	250	0	252	35	0
1	L	250	0	252	34	0
1	M	250	0	252	24	0
1	N	250	0	252	33	0
1	O	250	0	252	34	0
1	P	250	0	252	23	0
1	S	250	0	252	35	0
1	T	250	0	252	23	0
1	U	250	0	252	36	0
1	V	250	0	252	33	0
1	W	250	0	252	20	0
1	X	250	0	252	36	0
2	E	20	0	0	8	0
2	M	20	0	0	7	0
2	U	20	0	0	8	0
All	All	4560	0	4536	383	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 42.

The worst 5 of 383 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:GLY:H	2:M:101:A1FCO:C03	1.55	1.20
1:U:38:GLY:H	2:U:101:A1FCO:C03	1.55	1.19
1:E:38:GLY:H	2:E:101:A1FCO:C03	1.55	1.18
1:S:12:VAL:CG2	1:U:12:VAL:HG12	1.76	1.16
1:C:12:VAL:HG12	1:D:12:VAL:CG2	1.77	1.15

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	C	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	D	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	E	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	F	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	G	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	H	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	K	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	L	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	M	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	N	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	O	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	P	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	S	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	T	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	U	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	V	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	W	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
1	X	32/770 (4%)	31 (97%)	1 (3%)	0	100	100
All	All	576/13860 (4%)	558 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	25/669 (4%)	25 (100%)	0	100	100
1	D	25/669 (4%)	25 (100%)	0	100	100
1	E	25/669 (4%)	25 (100%)	0	100	100
1	F	25/669 (4%)	25 (100%)	0	100	100
1	G	25/669 (4%)	25 (100%)	0	100	100
1	H	25/669 (4%)	25 (100%)	0	100	100
1	K	25/669 (4%)	25 (100%)	0	100	100
1	L	25/669 (4%)	25 (100%)	0	100	100
1	M	25/669 (4%)	25 (100%)	0	100	100
1	N	25/669 (4%)	25 (100%)	0	100	100
1	O	25/669 (4%)	25 (100%)	0	100	100
1	P	25/669 (4%)	25 (100%)	0	100	100
1	S	25/669 (4%)	25 (100%)	0	100	100
1	T	25/669 (4%)	25 (100%)	0	100	100
1	U	25/669 (4%)	25 (100%)	0	100	100
1	V	25/669 (4%)	25 (100%)	0	100	100
1	W	25/669 (4%)	25 (100%)	0	100	100
1	X	25/669 (4%)	25 (100%)	0	100	100
All	All	450/12042 (4%)	450 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

3 ligands 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	$\#\|Z\| > 2$
2	A1FCO	E	101	-	23,23,23	1.25	3 (13%)	28,33,33	2.56	10 (35%)
2	A1FCO	U	101	-	23,23,23	1.25	3 (13%)	28,33,33	2.57	10 (35%)
2	A1FCO	M	101	-	23,23,23	1.25	3 (13%)	28,33,33	2.58	10 (35%)

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
2	A1FCO	E	101	-	-	0/4/4/4	0/4/4/4
2	A1FCO	U	101	-	-	0/4/4/4	0/4/4/4
2	A1FCO	M	101	-	-	0/4/4/4	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	101	A1FCO	C10-C11	-2.88	1.37	1.41
2	E	101	A1FCO	C10-C11	-2.85	1.37	1.41
2	U	101	A1FCO	C10-C11	-2.81	1.37	1.41
2	U	101	A1FCO	C19-C07	2.75	1.53	1.48
2	E	101	A1FCO	C19-C07	2.75	1.53	1.48

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	101	A1FCO	F20-C01-N02	6.97	119.48	114.95
2	M	101	A1FCO	F20-C01-N02	6.93	119.46	114.95
2	E	101	A1FCO	F20-C01-N02	6.87	119.41	114.95
2	M	101	A1FCO	C03-N02-C01	6.58	121.98	115.55
2	U	101	A1FCO	C03-N02-C01	6.54	121.94	115.55

There are no chirality outliers.

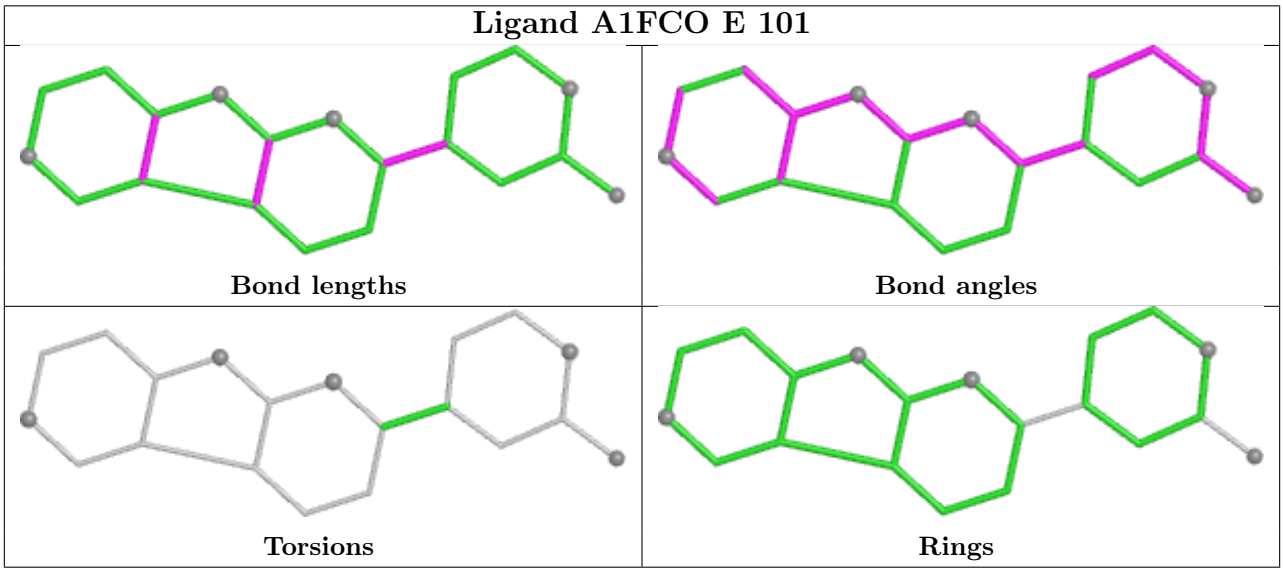
There are no torsion outliers.

There are no ring outliers.

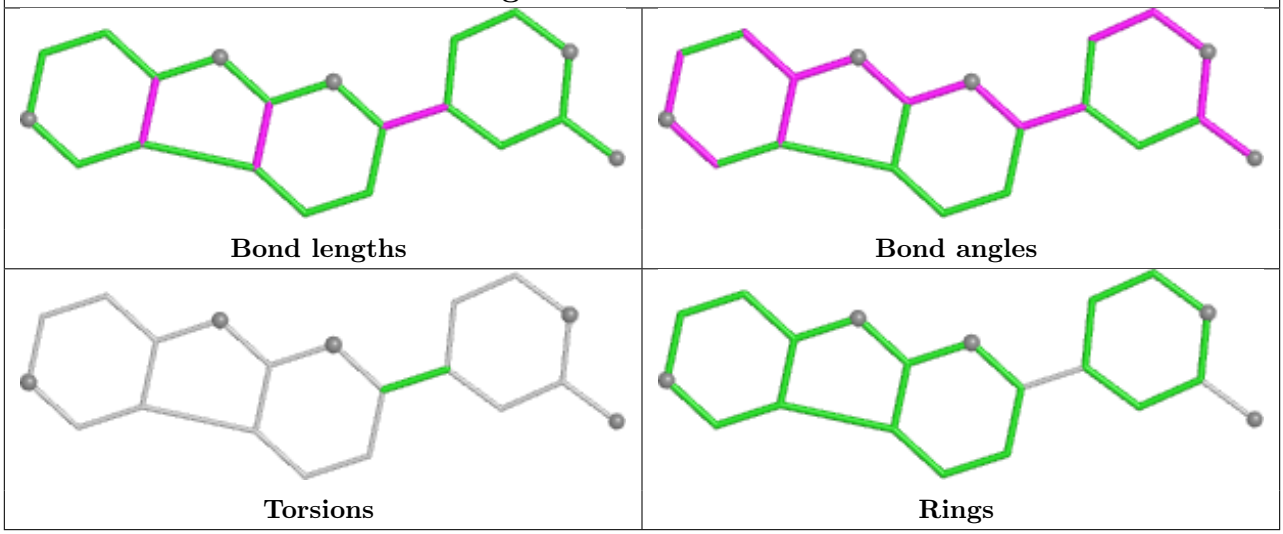
3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	101	A1FCO	8	0
2	U	101	A1FCO	8	0
2	M	101	A1FCO	7	0

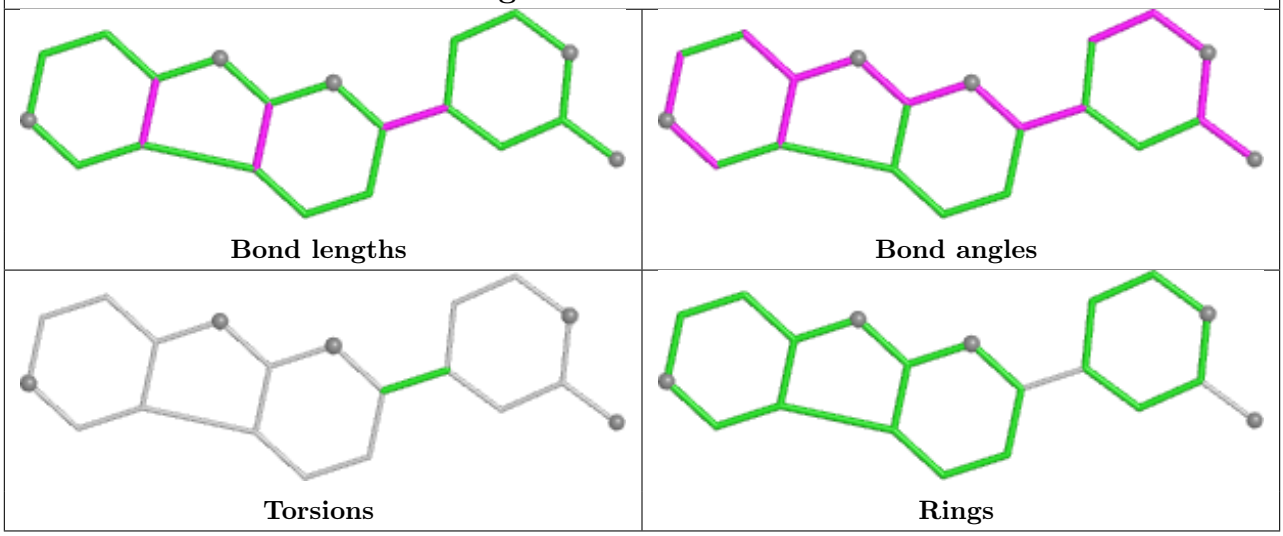
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand A1FCO U 101



Ligand A1FCO M 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

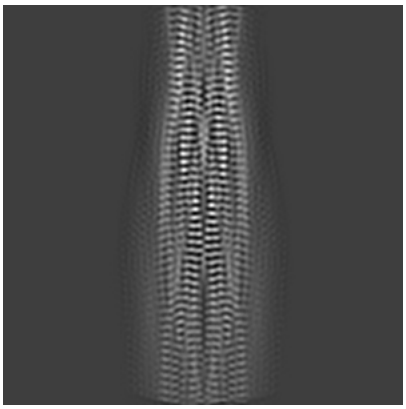
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66867. These allow visual inspection of the internal detail of the map and identification of artifacts.

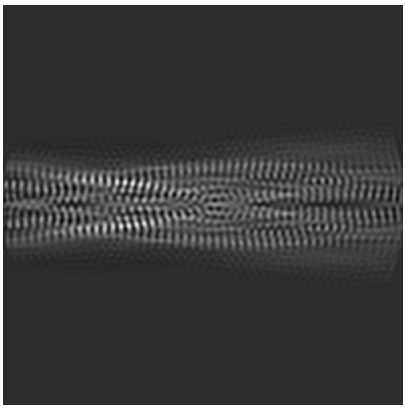
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

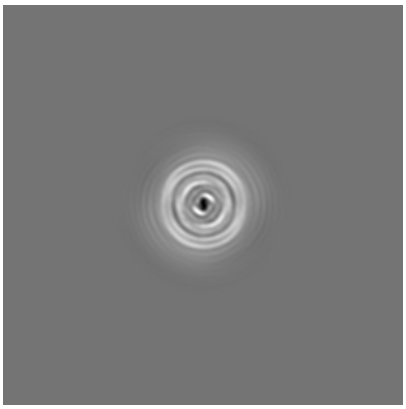
6.1.1 Primary map



X

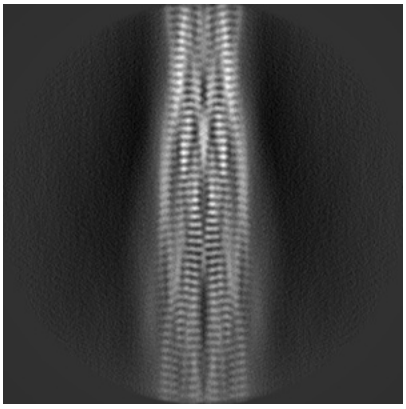


Y

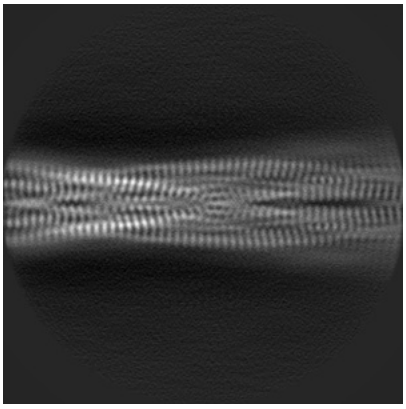


Z

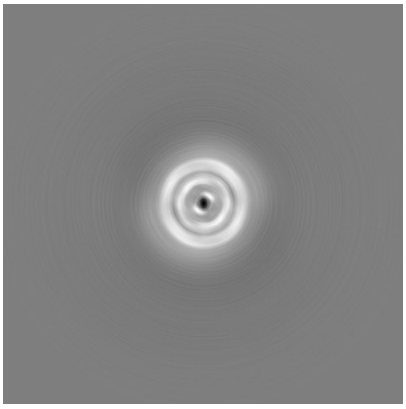
6.1.2 Raw map



X



Y

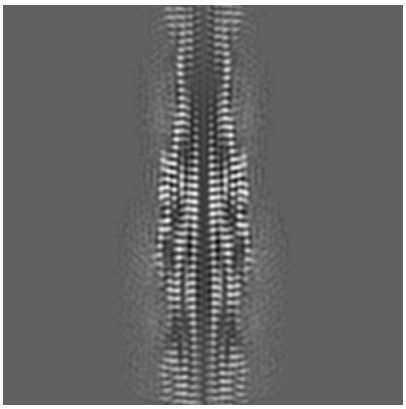


Z

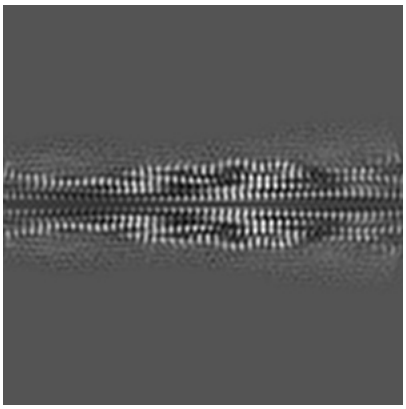
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

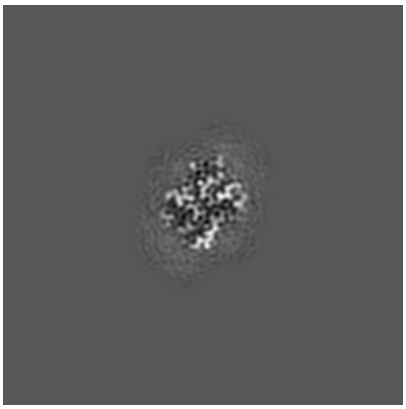
6.2.1 Primary map



X Index: 144

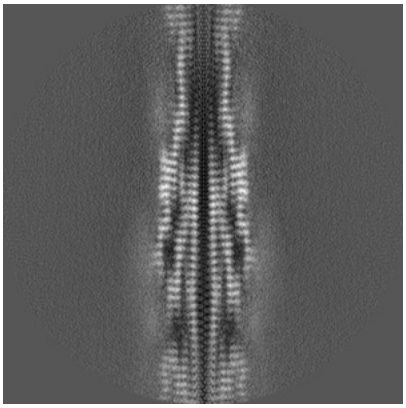


Y Index: 144

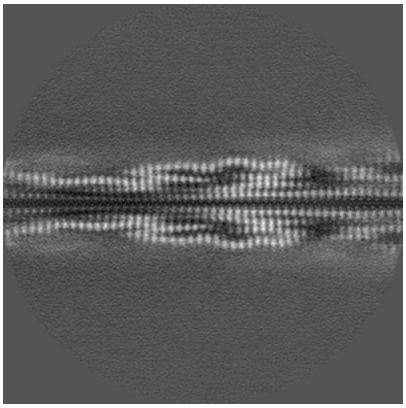


Z Index: 144

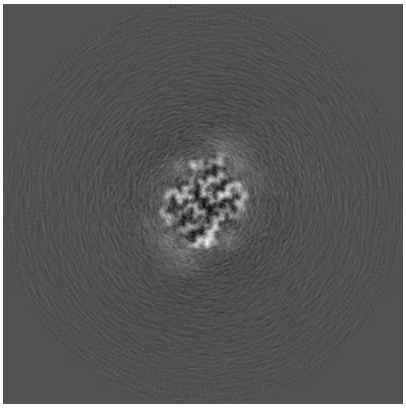
6.2.2 Raw map



X Index: 144



Y Index: 144

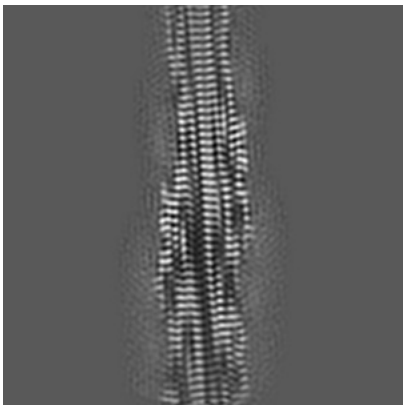


Z Index: 144

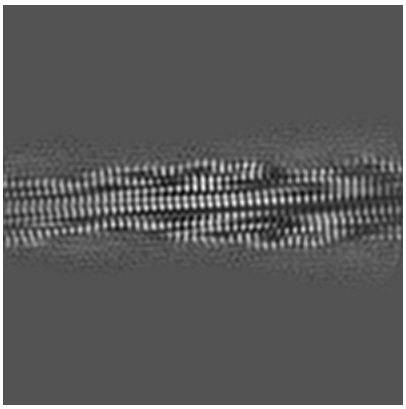
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

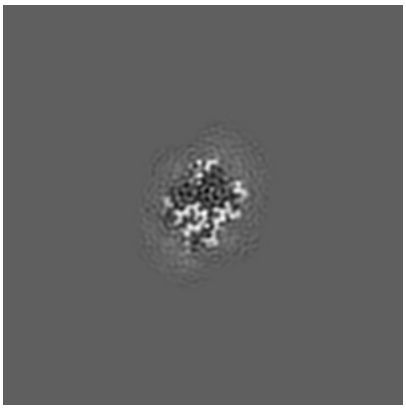
6.3.1 Primary map



X Index: 150

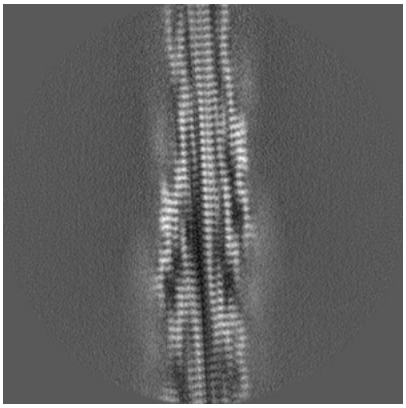


Y Index: 150

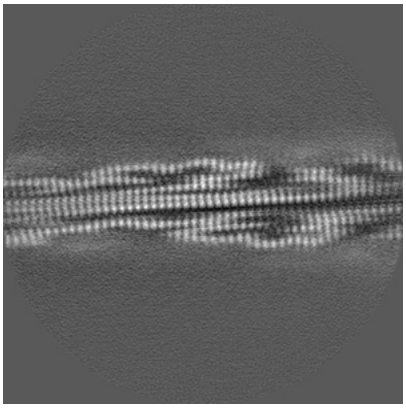


Z Index: 140

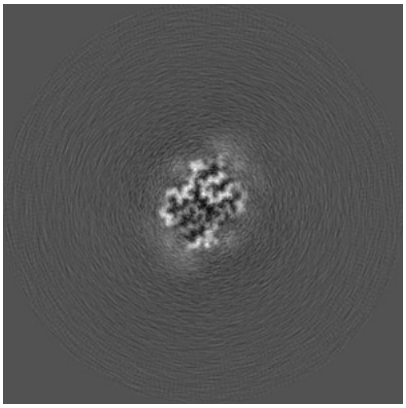
6.3.2 Raw map



X Index: 150



Y Index: 150

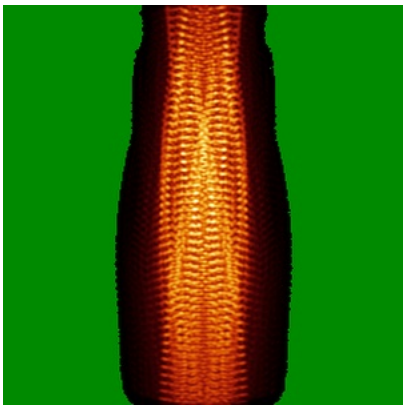


Z Index: 143

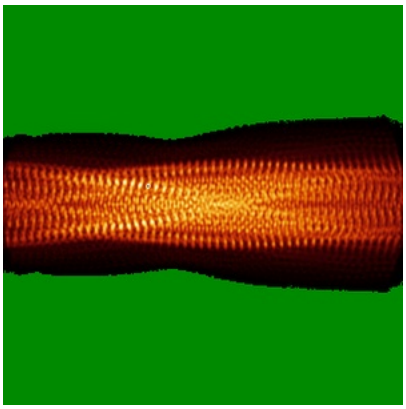
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

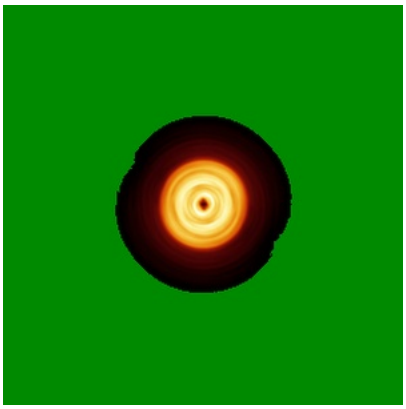
6.4.1 Primary map



X

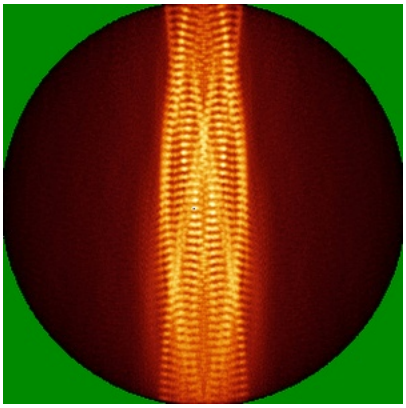


Y

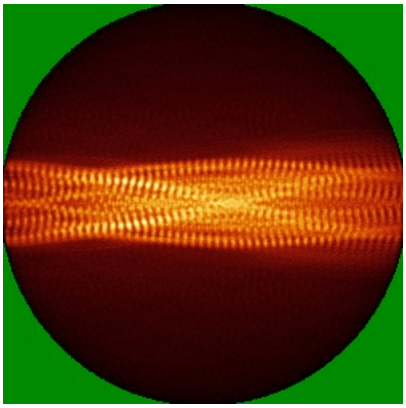


Z

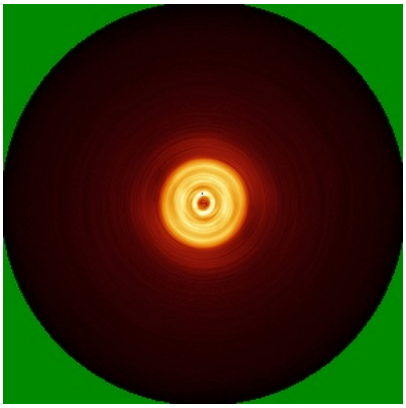
6.4.2 Raw map



X



Y

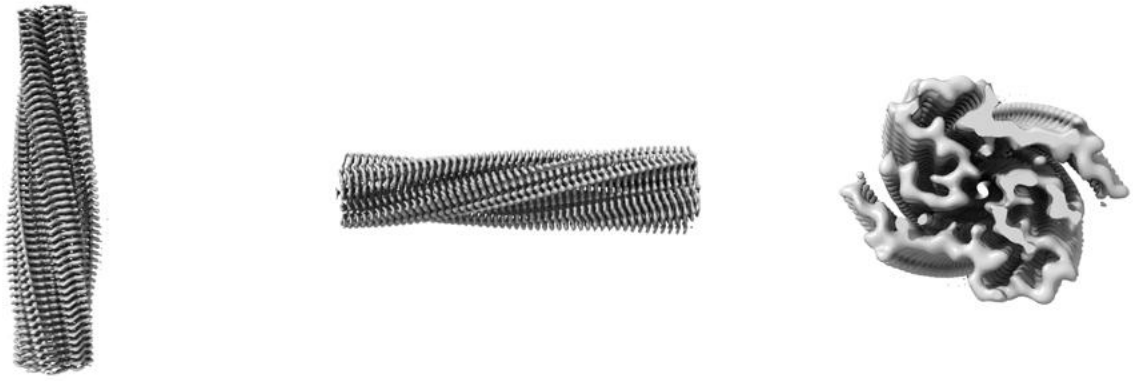


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. 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



X Y Z

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.

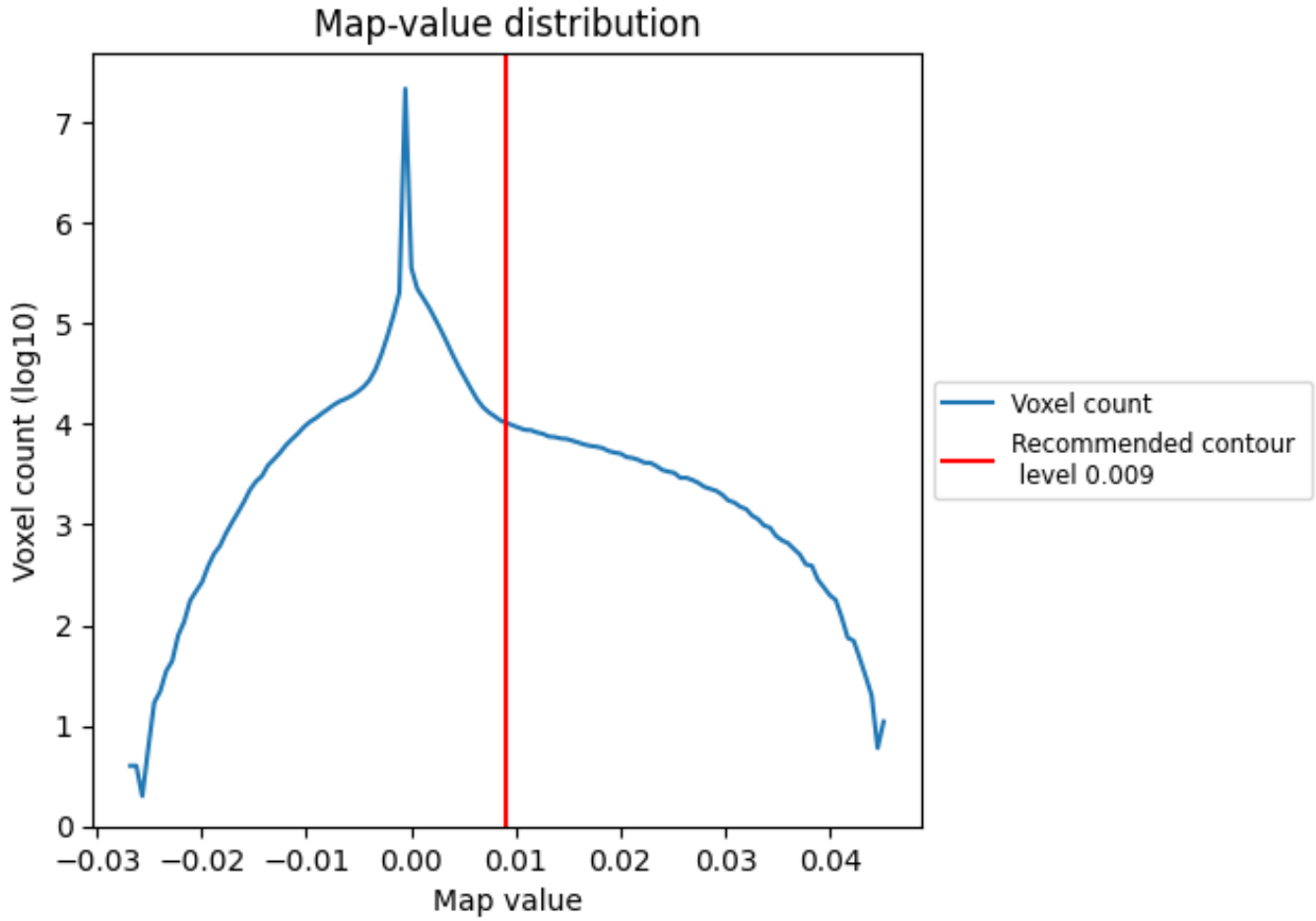
6.6 Mask visualisation (i)

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

7 Map analysis

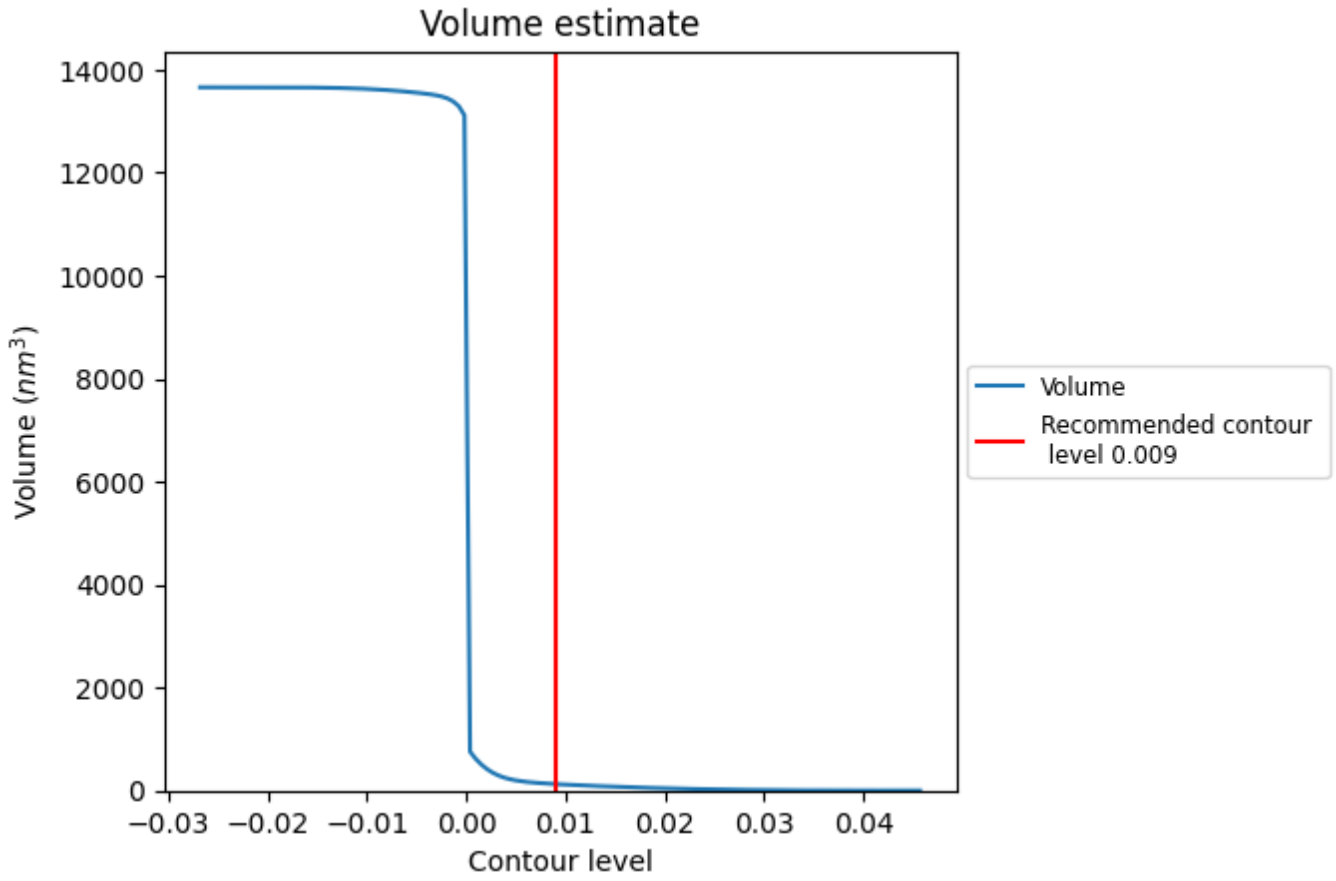
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

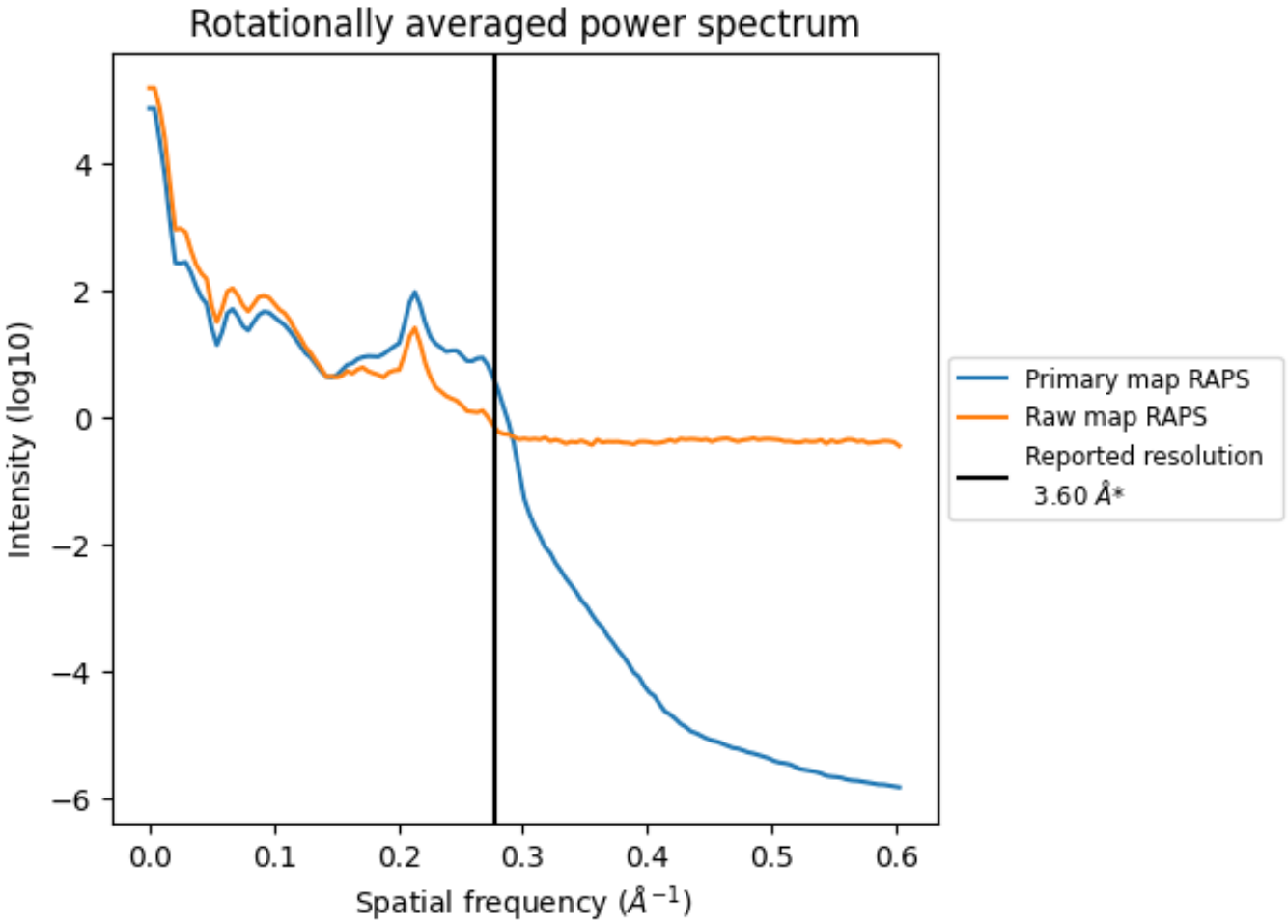
7.2 Volume estimate (i)



The volume at the recommended contour level is 126 nm^3; this corresponds to an approximate mass of 114 kDa.

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

7.3 Rotationally averaged power spectrum (i)

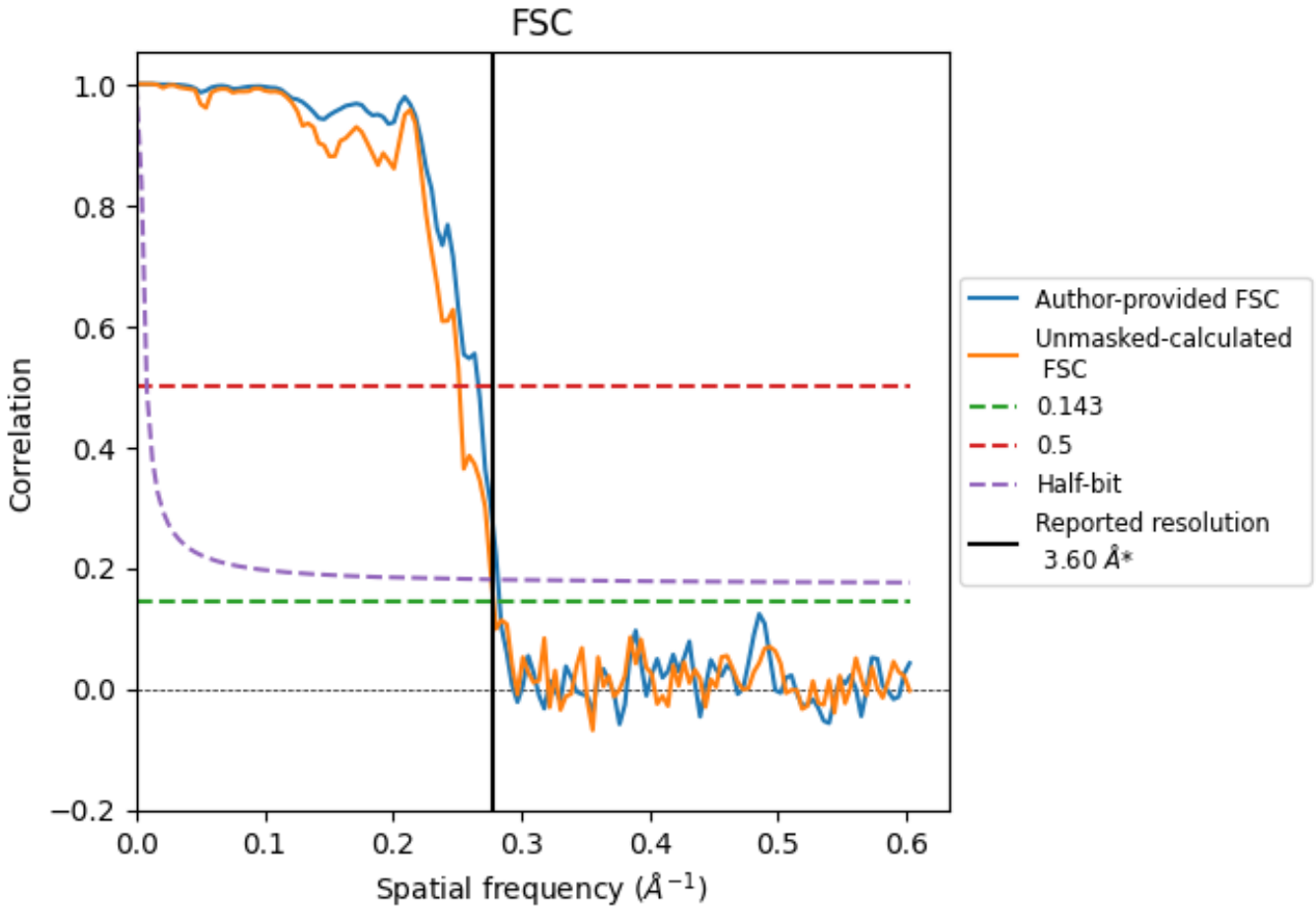


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

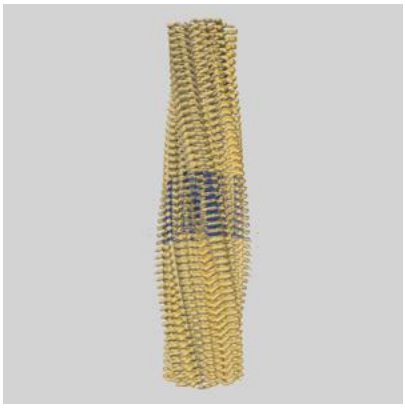
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	3.75	3.55
Unmasked-calculated*	3.59	3.97	3.61

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

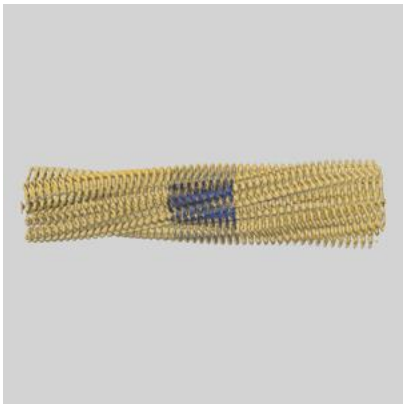
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66867 and PDB model 9XH6. Per-residue inclusion information can be found in section 3 on page 6.

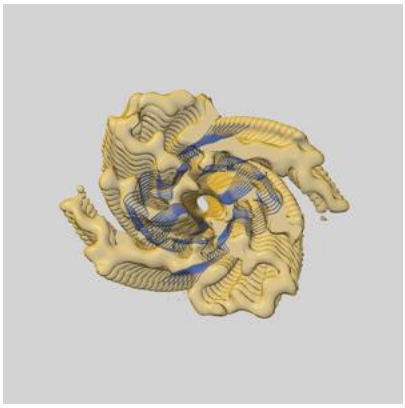
9.1 Map-model overlay



X



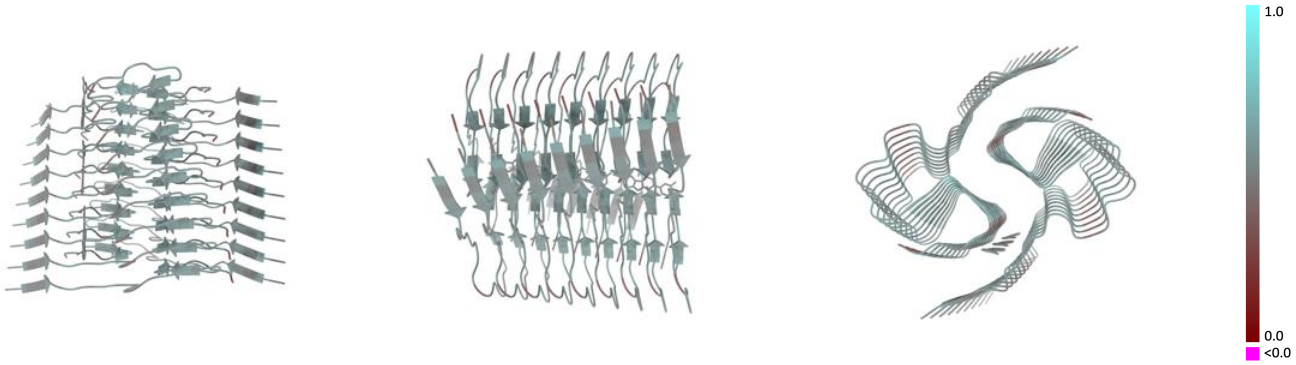
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

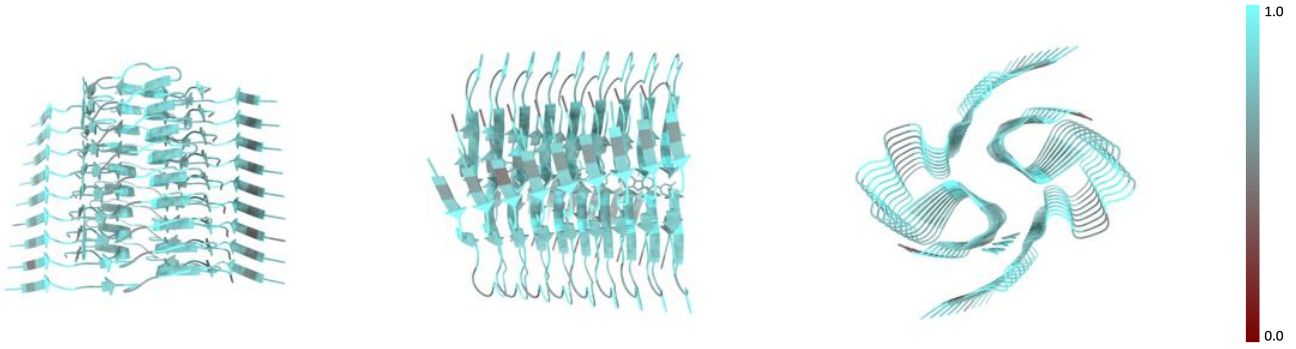
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

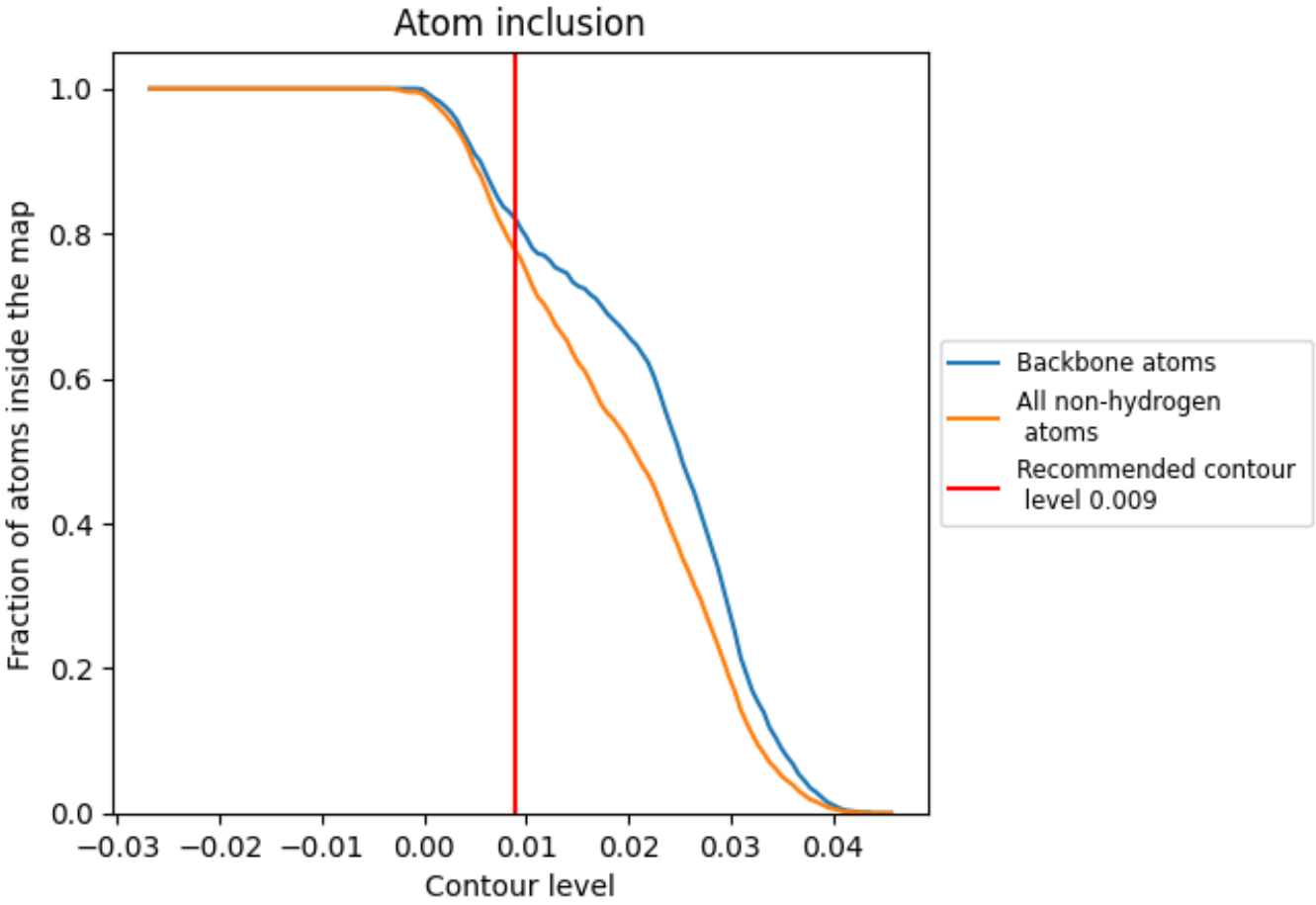
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.5240
C	0.7750	0.5270
D	0.7790	0.5260
E	0.7810	0.5230
F	0.7710	0.5240
G	0.7670	0.5240
H	0.7710	0.5220
K	0.7830	0.5260
L	0.7790	0.5240
M	0.7840	0.5230
N	0.7790	0.5250
O	0.7710	0.5240
P	0.7830	0.5220
S	0.7750	0.5250
T	0.7670	0.5230
U	0.7690	0.5220
V	0.7670	0.5230
W	0.7670	0.5220
X	0.7830	0.5250

