wwPDB EM Validation Summary Report (i)

Mar 5, 2026 – 07:41 AM UTC

PDB ID	:	9CZ2 / pdb_00009cz2
EMDB ID	:	EMD-46057
Title	:	Cryo-EM structure of a nautilus-like HflK/C assembly in complex with FtsH AAA protease
Authors	:	Ghanbarpour, A.; Sauer, R.T.; Davis, J.H.
Deposited on	:	2024-08-03
Resolution	:	4.40 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:

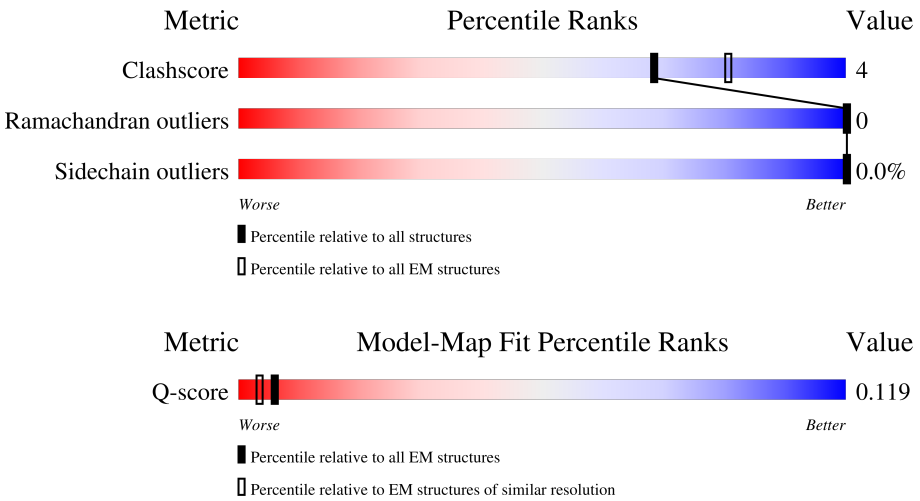
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	XA	419	61% 5% 34%
1	XC	419	61% 5% 34%
1	XE	419	61% 5% 34%
1	XG	419	61% 5% 34%

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Mol	Chain	Length	Quality of chain
1	XI	419	59% 7% 34%
1	XK	419	59% 7% 34%
1	XM	419	62% 34%
1	XO	419	61% 5% 34%
1	XQ	419	58% 8% 34%
1	XS	419	61% 5% 34%
1	XU	419	60% 6% 34%
1	XW	419	18% 79%
2	XB	334	81% 8% 10%
2	XD	334	81% 9% 10%
2	XF	334	84% 6% 10%
2	XH	334	81% 9% 10%
2	XJ	334	84% 6% 10%
2	XL	334	80% 10% 10%
2	XN	334	81% 9% 10%
2	XP	334	78% 11% 10%
2	XR	334	77% 13% 10%
2	XT	334	78% 11% 10%
2	XV	334	25% 71%
2	XX	334	28% 69%
3	A	644	9% 90%
3	B	644	10% 90%
3	C	644	9% 90%
3	D	644	10% 90%
3	E	644	9% 90%

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Mol	Chain	Length	Quality of chain
3	F	644	9% 90%
3	G	644	10% 90%
3	H	644	9% 90%
3	I	644	9% 90%
3	J	644	9% 90%
3	K	644	10% 90%
3	L	644	5% 9% 90%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 114310 atoms, of which 57401 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 Modulator of FtsH protease HflK.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	XA	277	4404	1379	2212	386	421	6	0	0
1	XC	277	4404	1379	2212	386	421	6	0	0
1	XE	277	4404	1379	2212	386	421	6	0	0
1	XG	277	4396	1379	2204	386	421	6	0	0
1	XI	277	4404	1379	2212	386	421	6	0	0
1	XK	277	4404	1379	2212	386	421	6	0	0
1	XM	277	4404	1379	2212	386	421	6	0	0
1	XO	277	4404	1379	2212	386	421	6	0	0
1	XQ	277	4404	1379	2212	386	421	6	0	0
1	XS	277	4404	1379	2212	386	421	6	0	0
1	XU	277	4404	1379	2212	386	421	6	0	0
1	XW	87	1402	434	712	124	130	2	0	0

- Molecule 2 is a protein called Modulator of FtsH protease HflC.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	XB	299	4828	1508	2431	429	450	10	0	0
2	XD	299	4828	1508	2431	429	450	10	0	0
2	XF	299	4828	1508	2431	429	450	10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	XH	299	4828	1508	2431	429	450	10	0	0
2	XJ	299	4828	1508	2431	429	450	10	0	0
2	XL	299	4828	1508	2431	429	450	10	0	0
2	XN	299	4828	1508	2431	429	450	10	0	0
2	XP	299	4828	1508	2431	429	450	10	0	0
2	XR	299	4828	1508	2431	429	450	10	0	0
2	XT	299	4828	1508	2431	429	450	10	0	0
2	XX	105	1645	517	802	160	161	5	0	0
2	XV	97	1515	480	737	142	152	4	0	0

- Molecule 3 is a protein called ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	A	67	1086	338	543	95	110	0	0
3	B	67	1086	338	543	95	110	0	0
3	C	67	1086	338	543	95	110	0	0
3	D	67	1086	338	543	95	110	0	0
3	E	67	1086	338	543	95	110	0	0
3	F	67	1086	338	543	95	110	0	0
3	G	67	1086	338	543	95	110	0	0
3	H	67	1086	338	543	95	110	0	0
3	I	67	1086	338	543	95	110	0	0
3	J	67	1086	338	543	95	110	0	0

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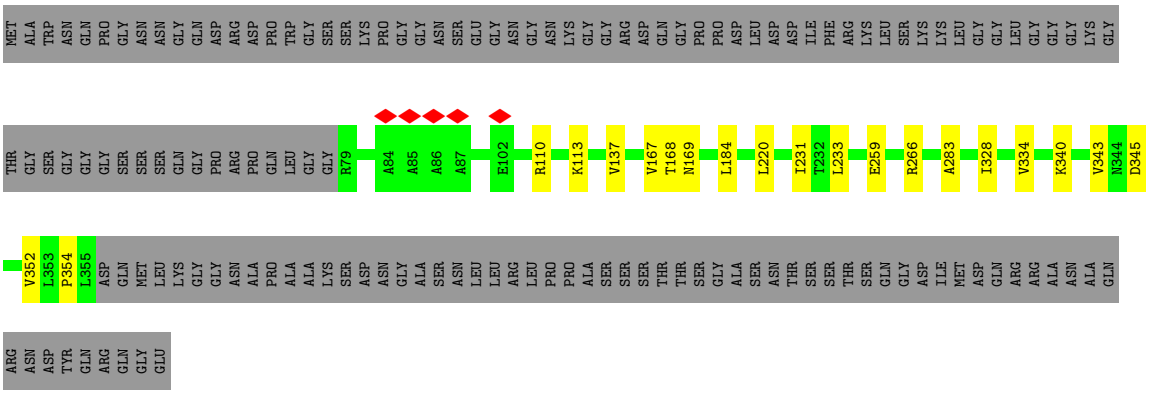
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	K	67	1086	338	543	95	110	0	0
			Total	C	H	N	O		
3	L	67	1086	338	543	95	110	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

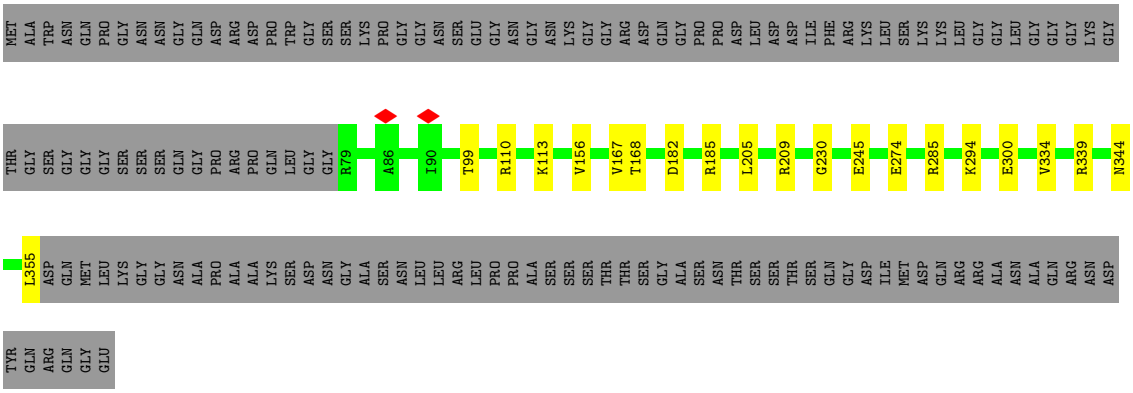
• Molecule 1: Modulator of FtsH protease HflK

Chain XA:



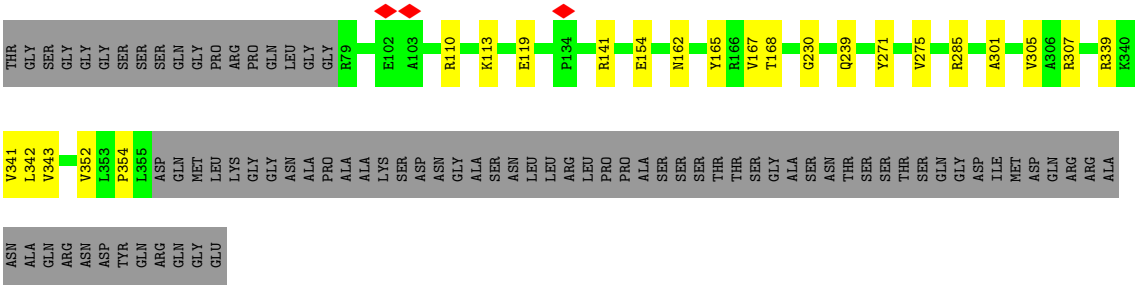
• Molecule 1: Modulator of FtsH protease HflK

Chain XC:



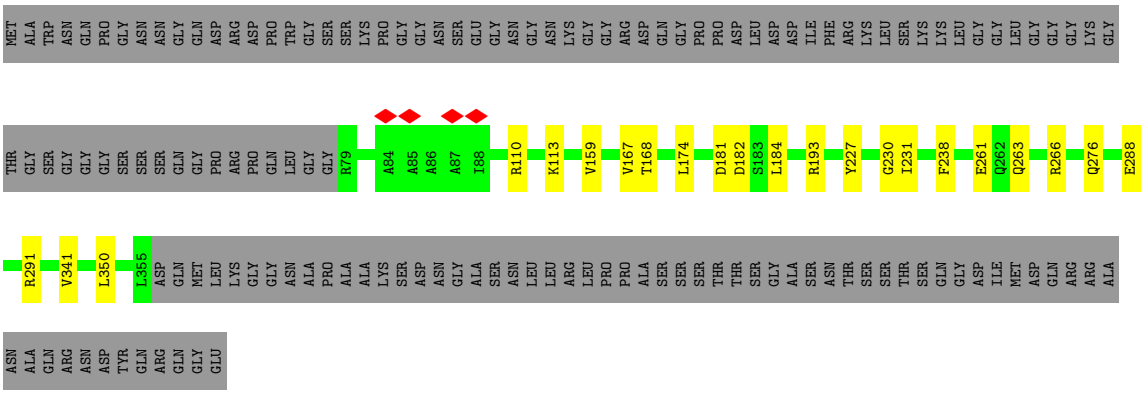
• Molecule 1: Modulator of FtsH protease HflK

Chain XE:



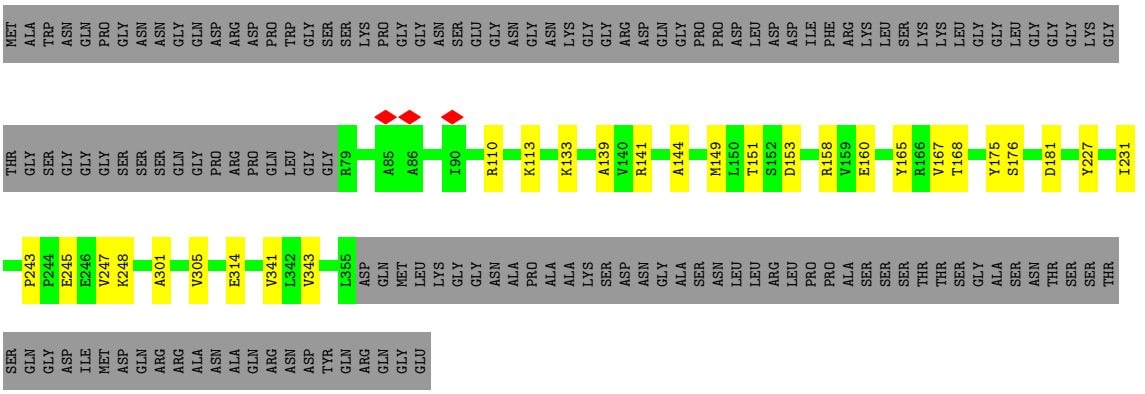
• Molecule 1: Modulator of FtsH protease HflK

Chain XG:



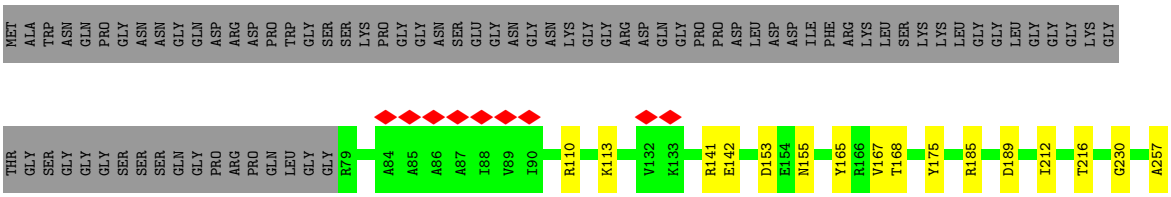
• Molecule 1: Modulator of FtsH protease HflK

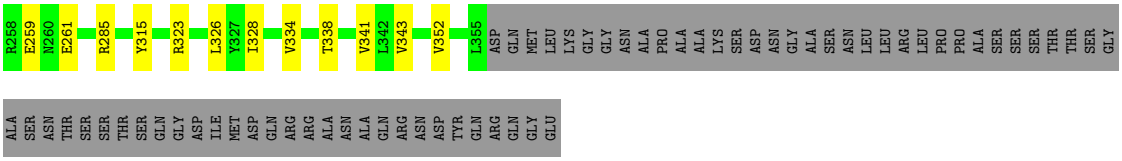
Chain XI:



• Molecule 1: Modulator of FtsH protease HflK

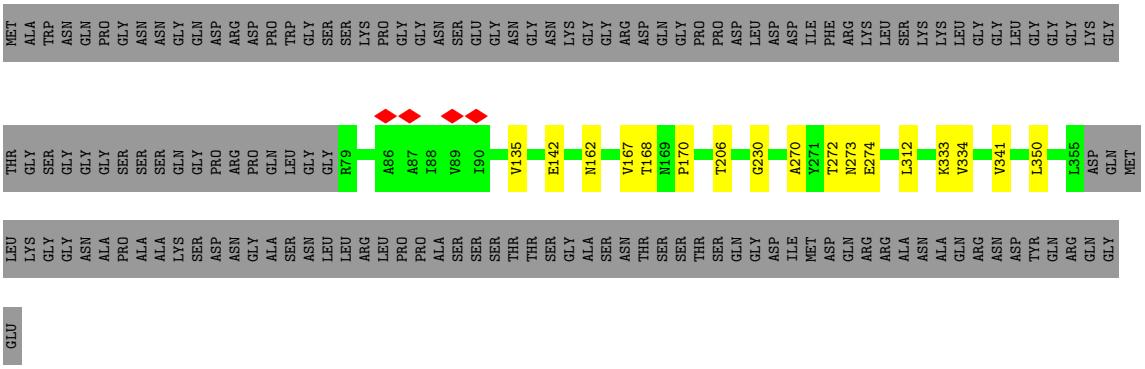
Chain XK:





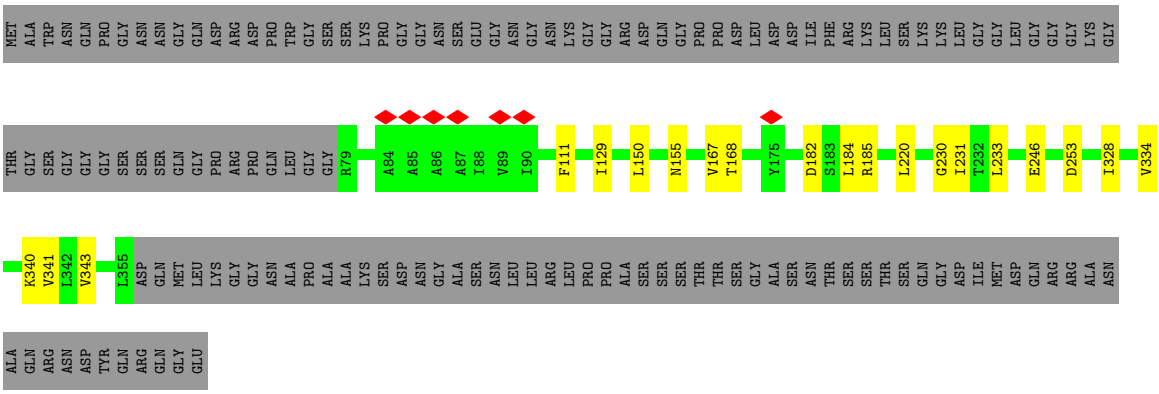
• Molecule 1: Modulator of FtsH protease HflK

Chain XM:



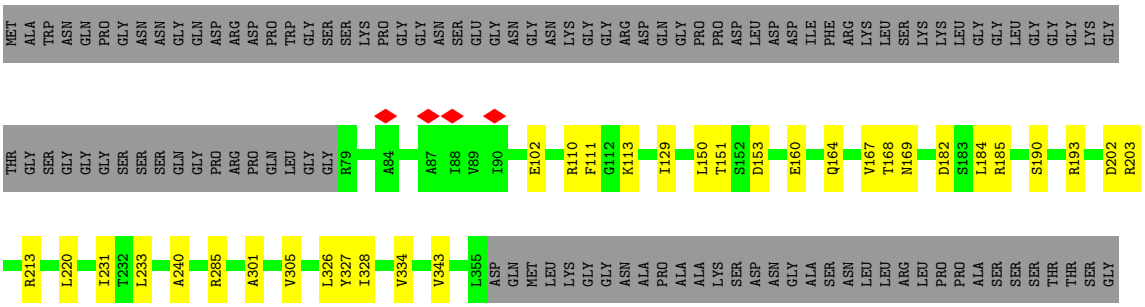
• Molecule 1: Modulator of FtsH protease HflK

Chain XO:



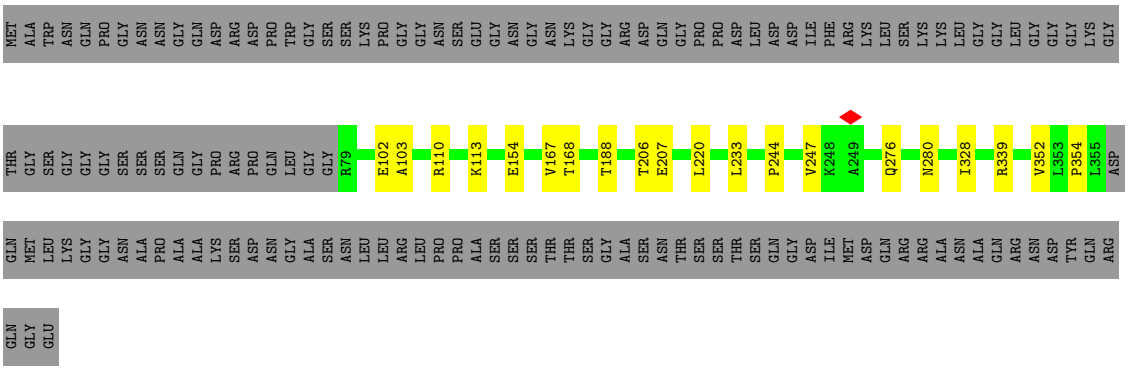
• Molecule 1: Modulator of FtsH protease HflK

Chain XQ:



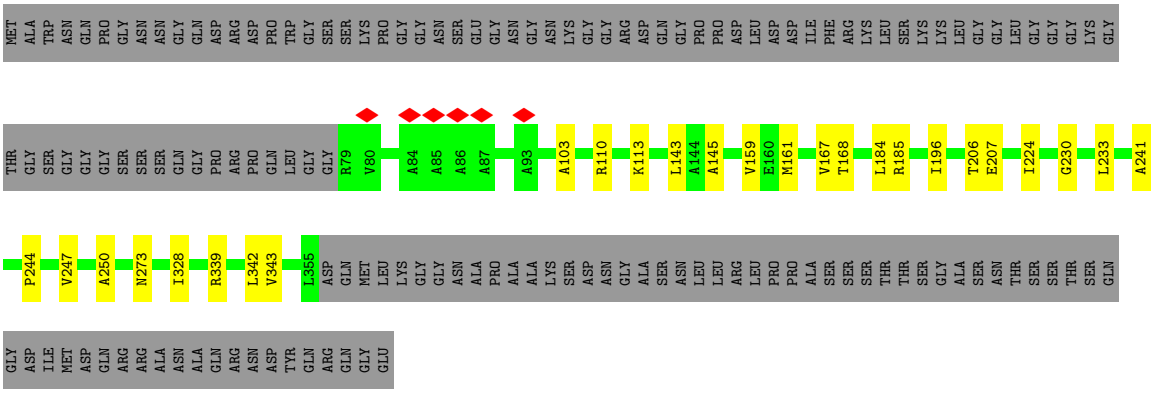
• Molecule 1: Modulator of FtsH protease HflK

Chain XS:



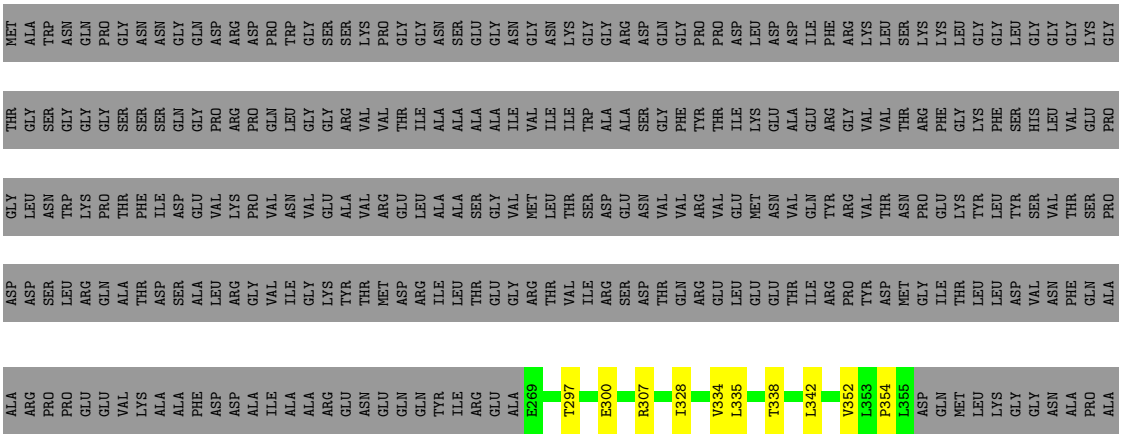
• Molecule 1: Modulator of FtsH protease HflK

Chain XU:



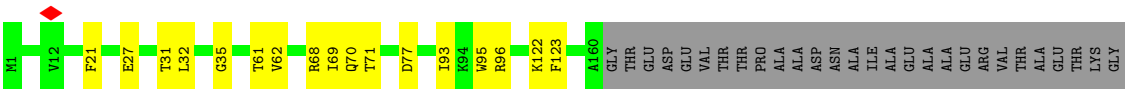
• Molecule 1: Modulator of FtsH protease HflK

Chain XW:



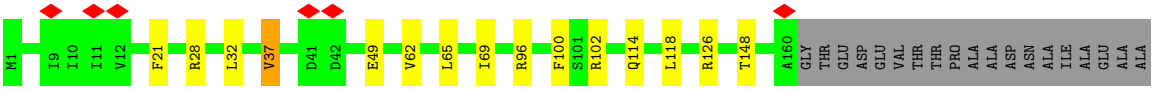
• Molecule 2: Modulator of FtsH protease HflC

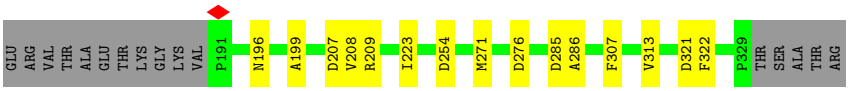
Chain XB:



• Molecule 2: Modulator of FtsH protease HflC

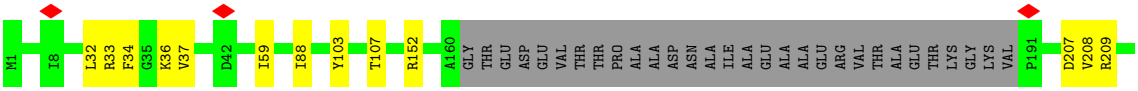
Chain XD:

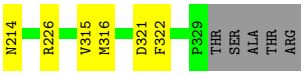




• Molecule 2: Modulator of FtsH protease HflC

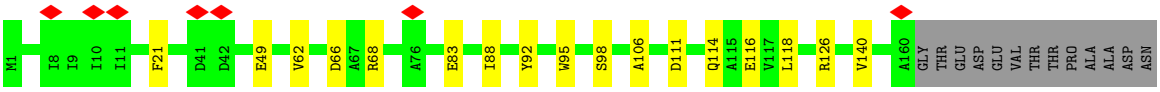
Chain XF:

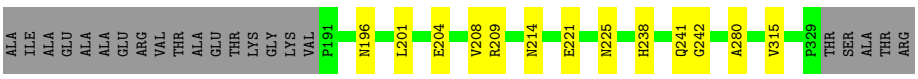




• Molecule 2: Modulator of FtsH protease HflC

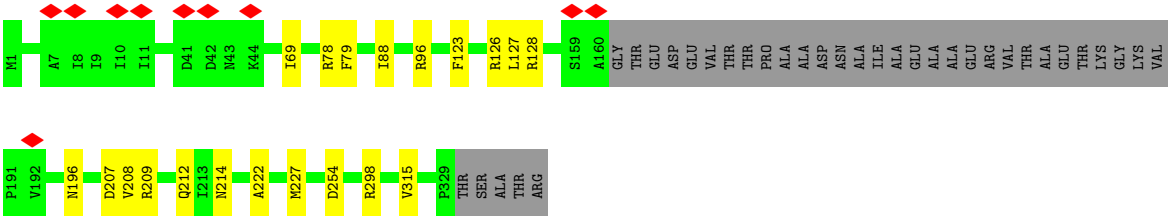
Chain XH:





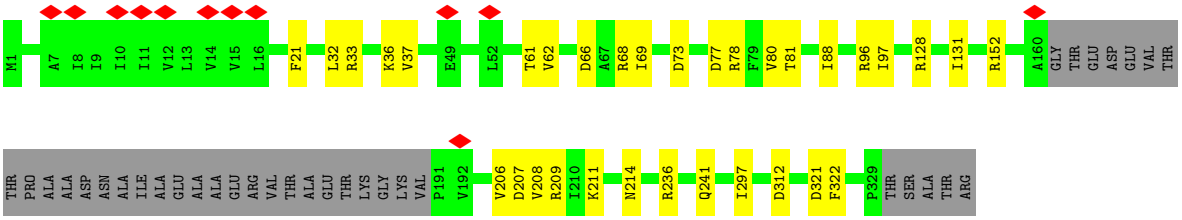
• Molecule 2: Modulator of FtsH protease HflC

Chain XJ:



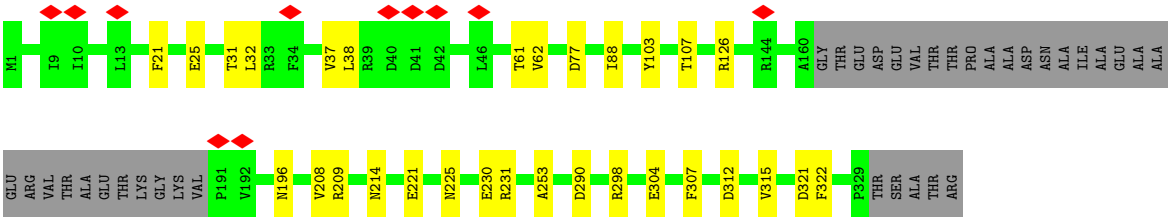
• Molecule 2: Modulator of FtsH protease HflC

Chain XL:



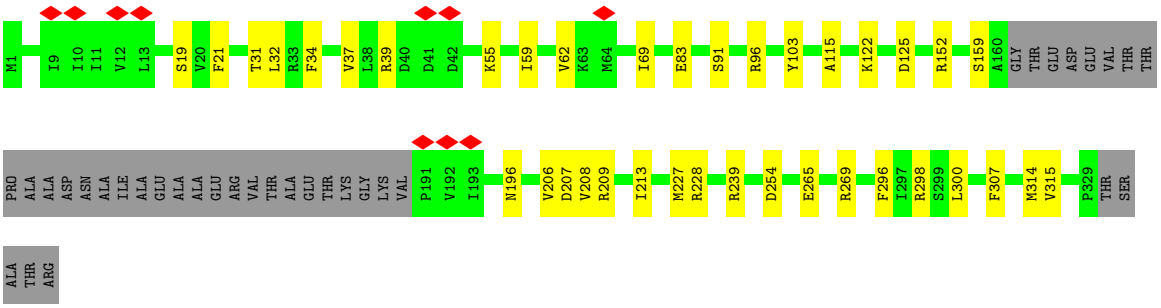
• Molecule 2: Modulator of FtsH protease HflC

Chain XN:



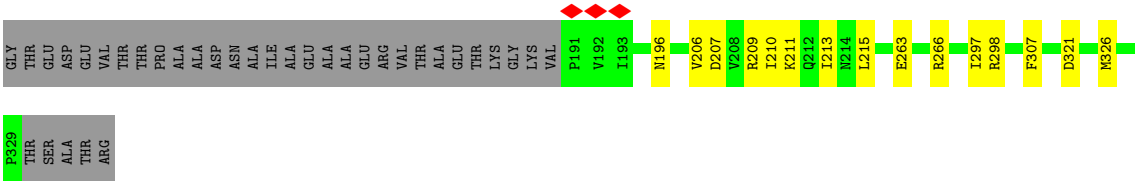
• Molecule 2: Modulator of FtsH protease HflC

Chain XP:



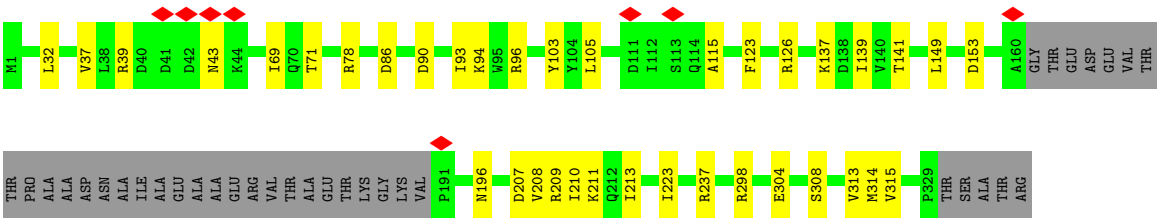
• Molecule 2: Modulator of FtsH protease HflC

Chain XR:



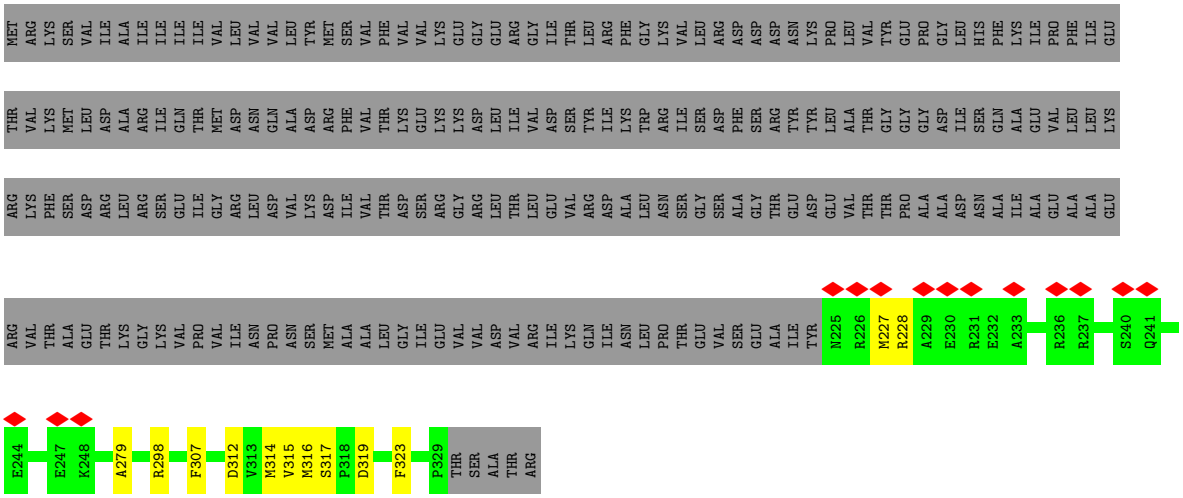
• Molecule 2: Modulator of FtsH protease HflC

Chain XT:



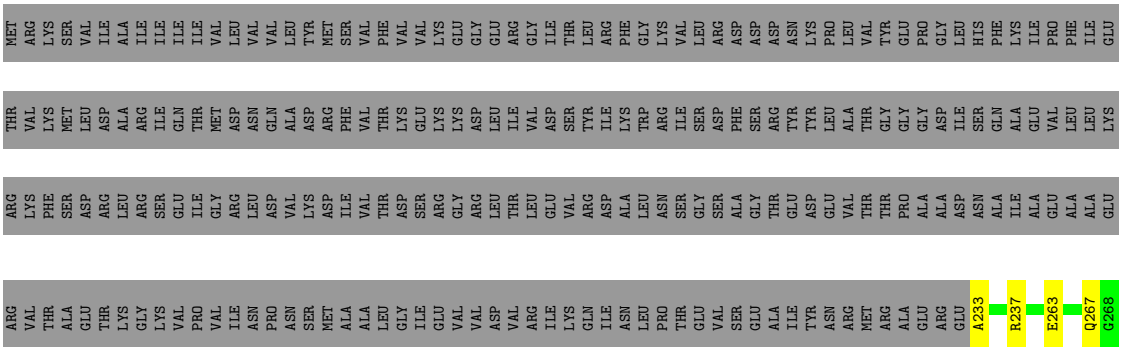
• Molecule 2: Modulator of FtsH protease HflC

Chain XX:



• Molecule 2: Modulator of FtsH protease HflC

Chain XV:

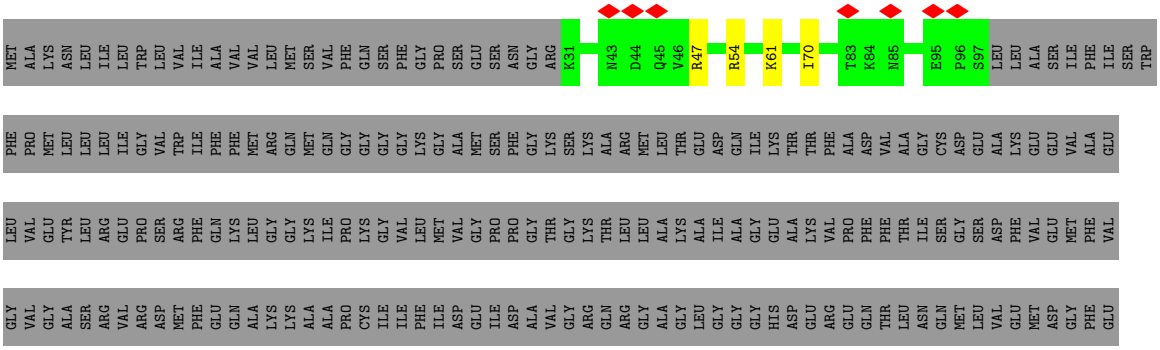


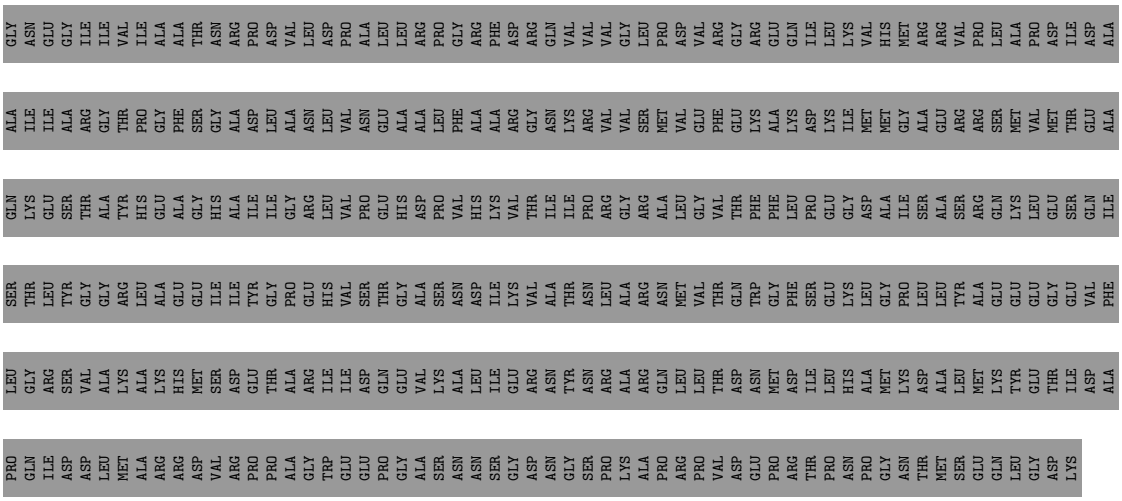
• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain A:

• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain B:



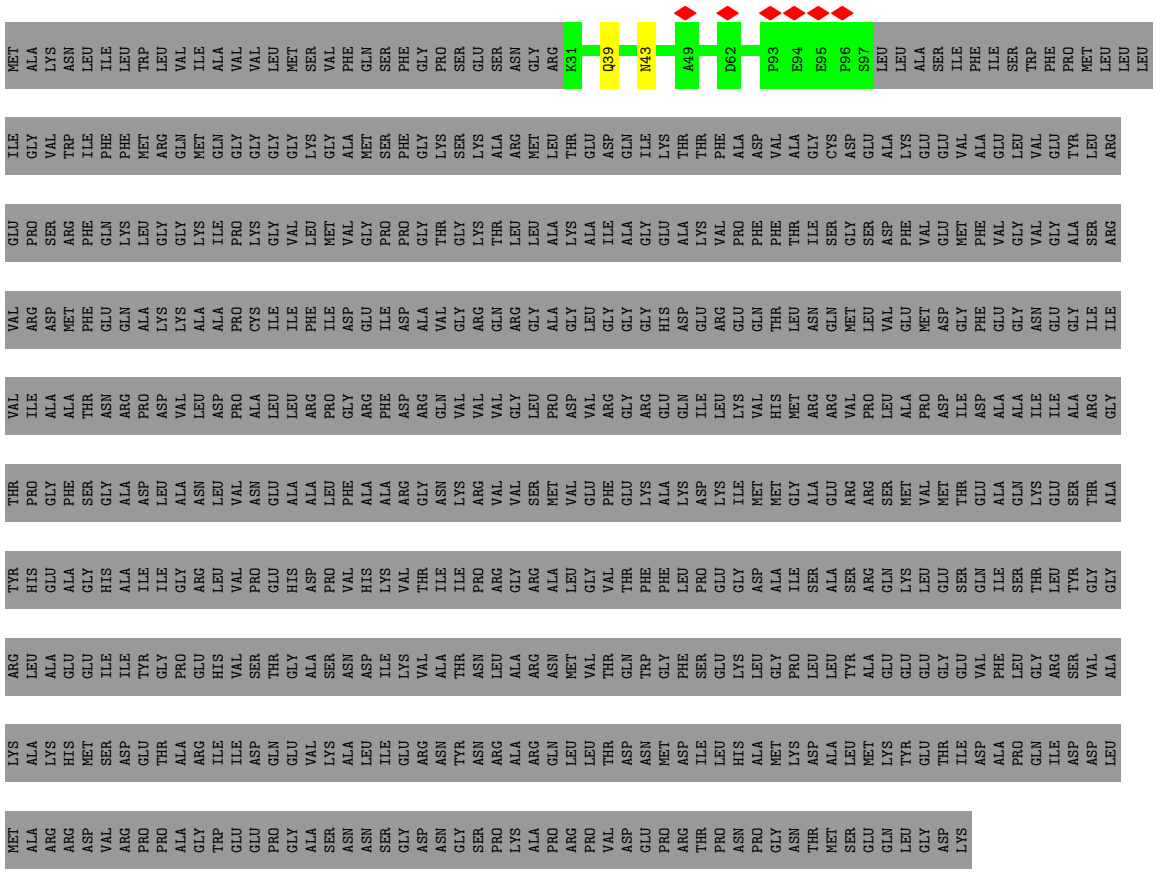


• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain C:

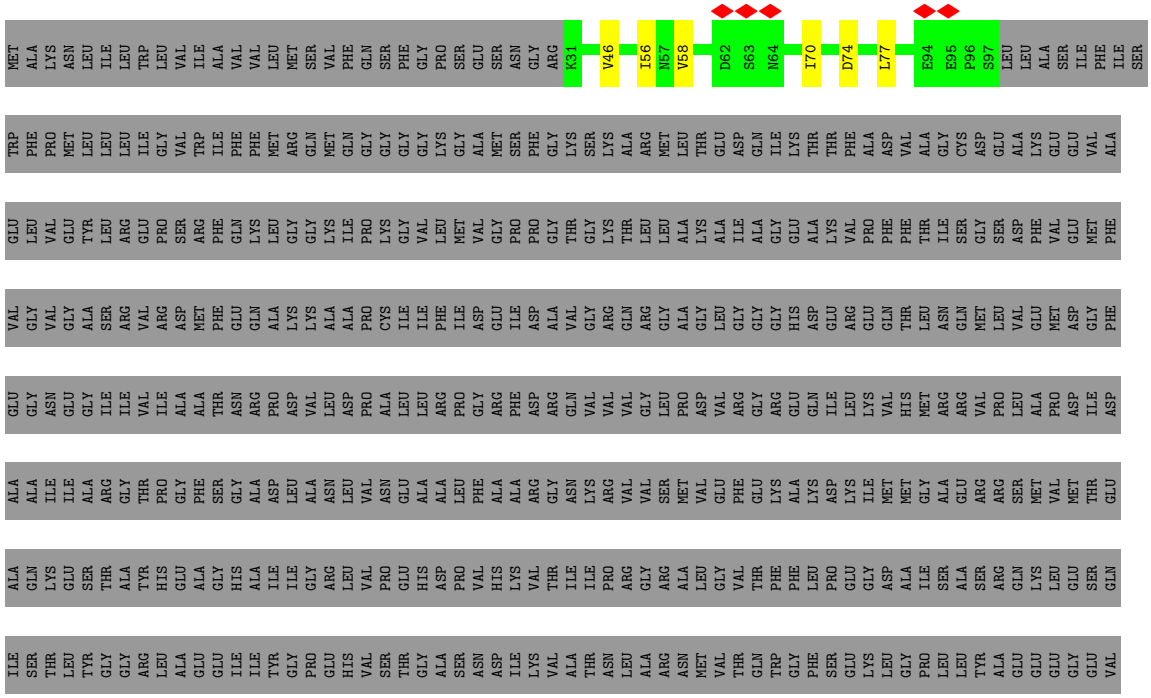
• Molecule 3: ATP-dependent zinc metalloprotease FtsH

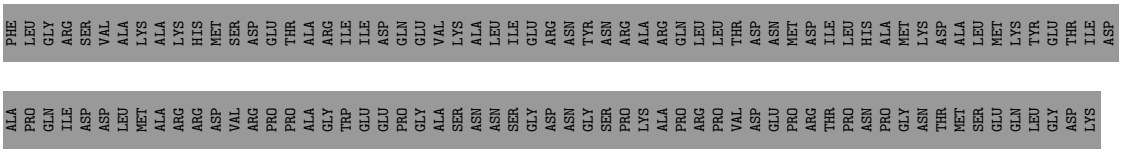
Chain D:



• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain E: 9% 90%



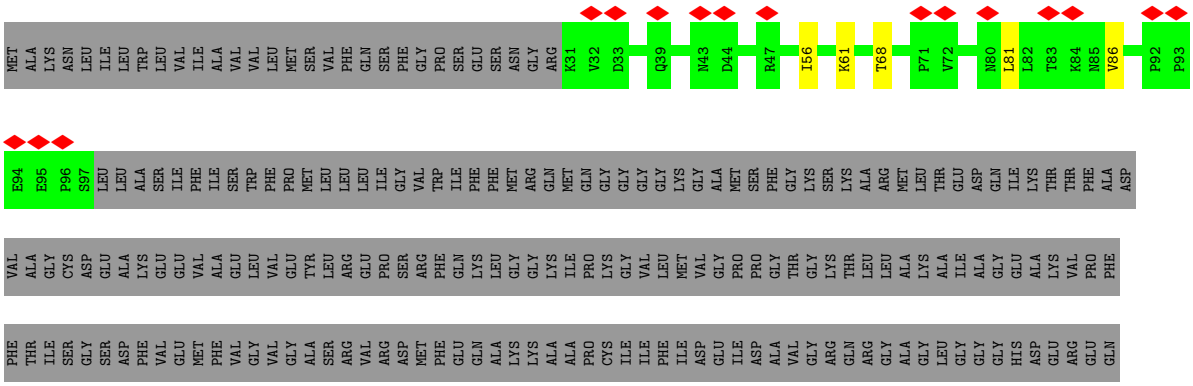


• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain F: 9% 90%

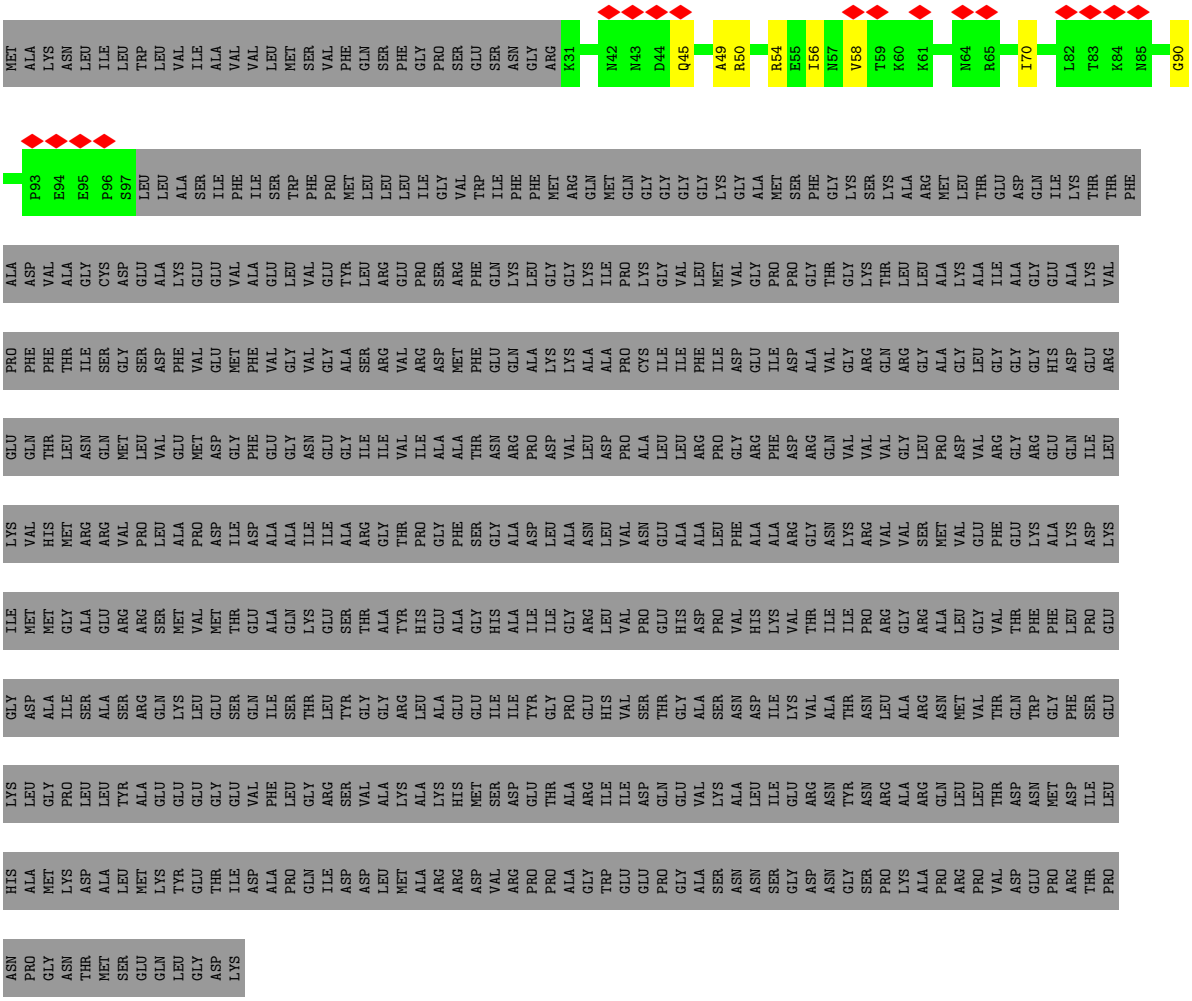
• Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain G: 10% 90%



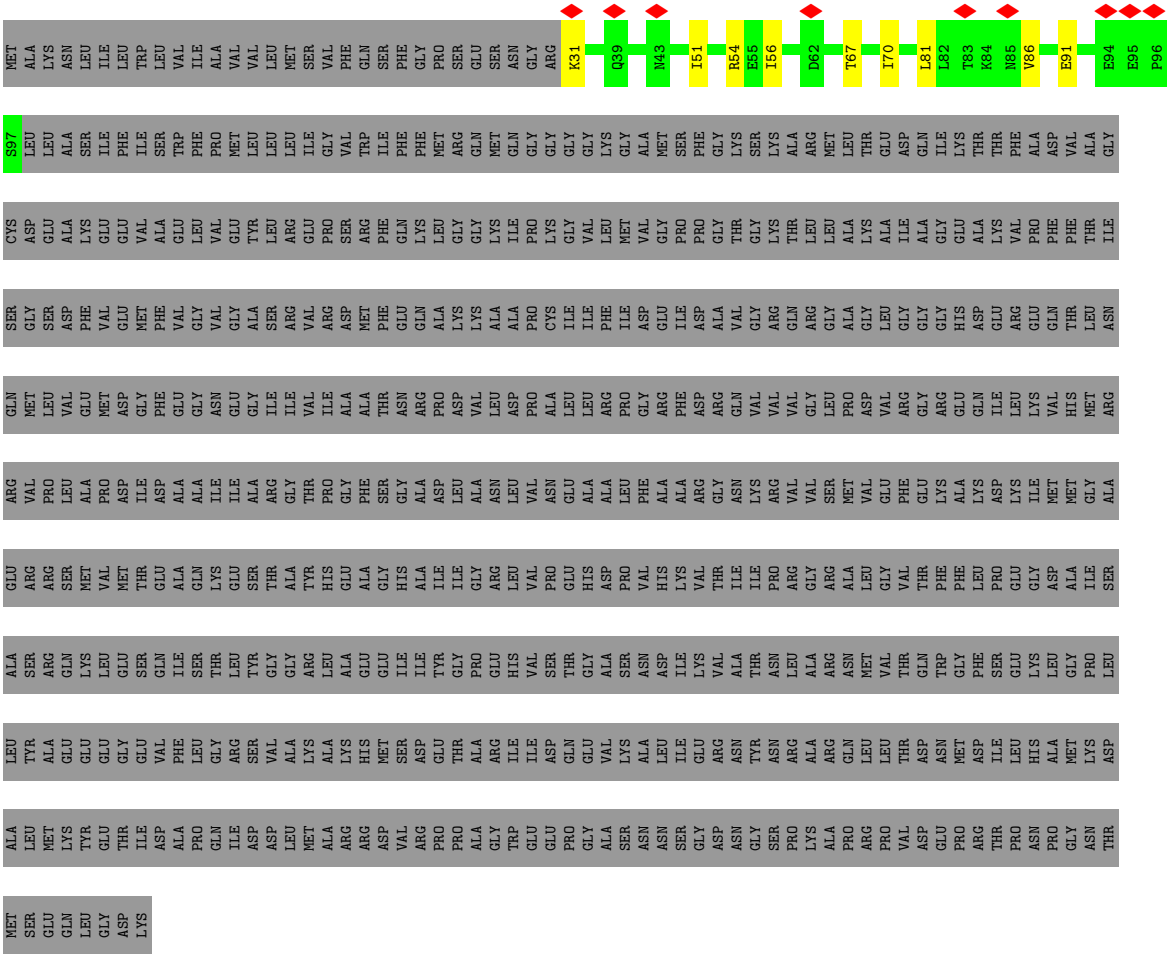
- Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain H:



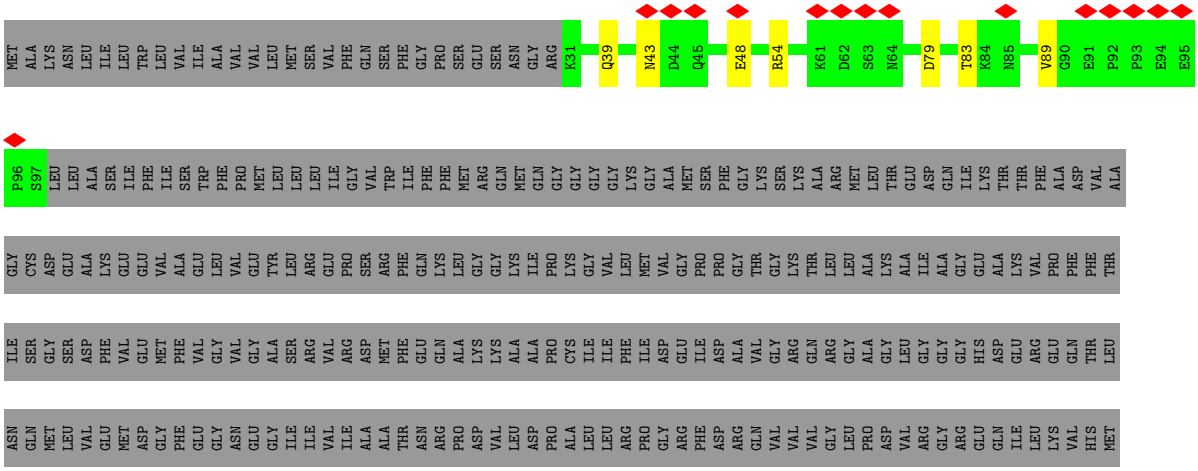
• Molecule 3: ATP-dependent zinc metalloprotease FtsH

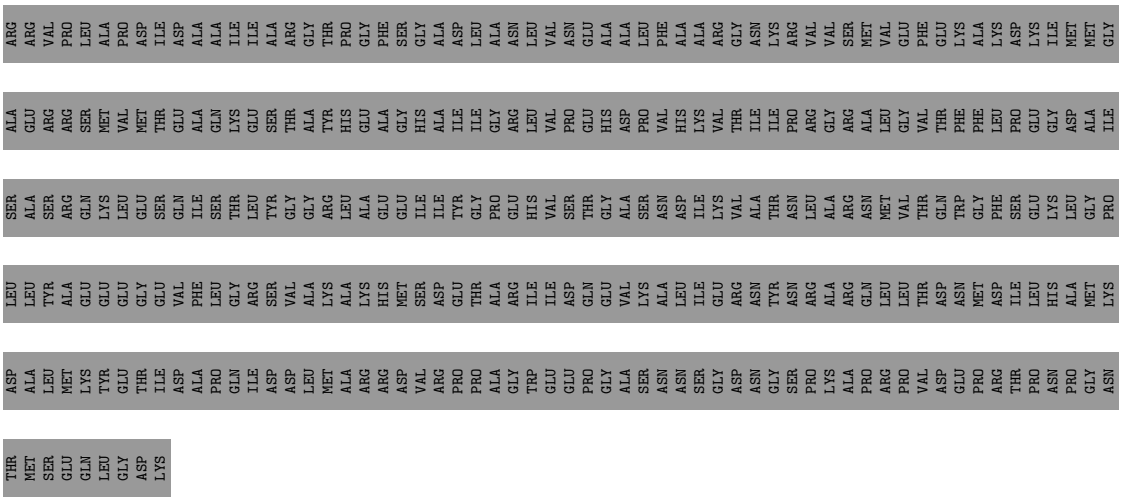
Chain I: 9% 90%



• Molecule 3: ATP-dependent zinc metalloprotease FtsH

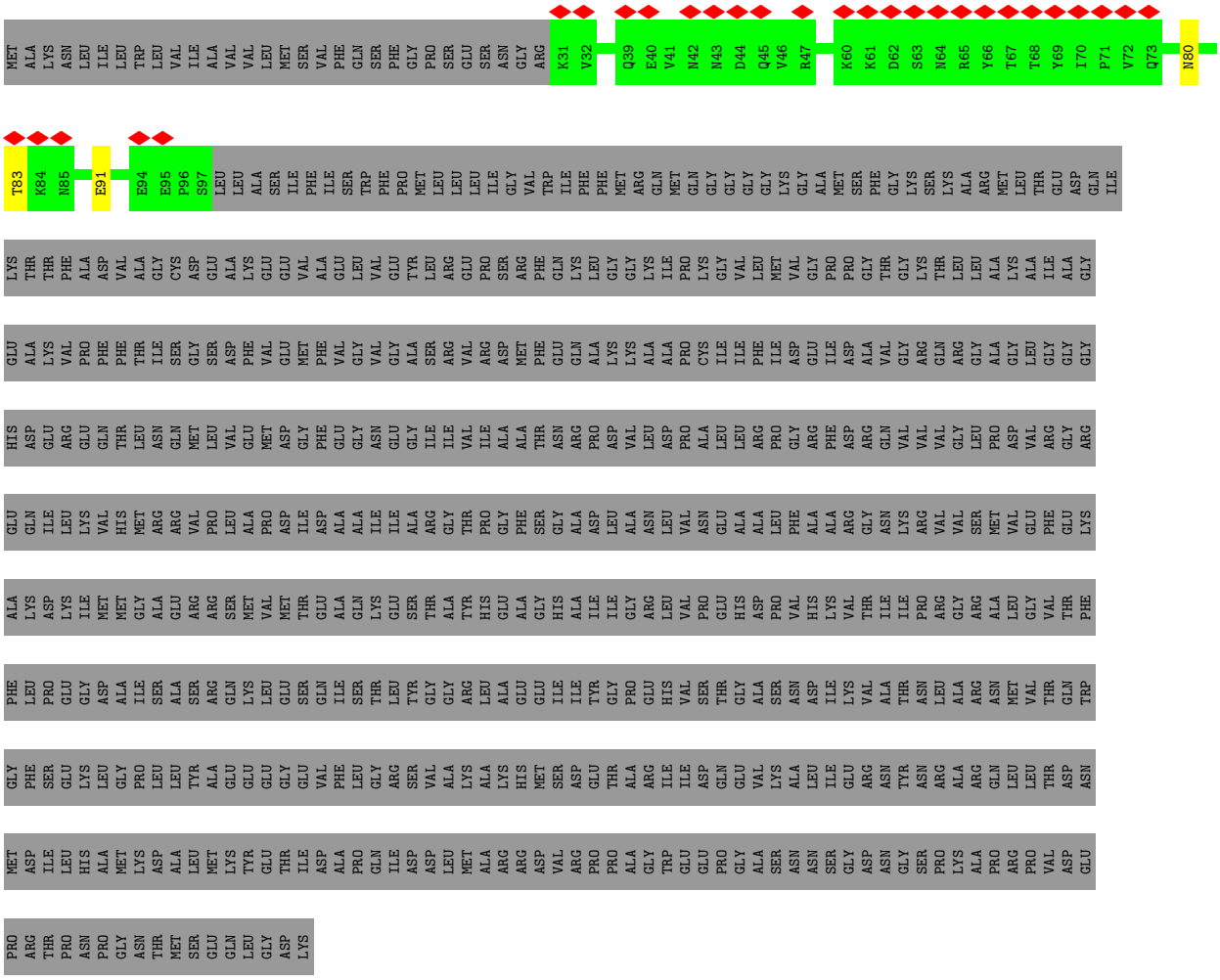
Chain J: 9% 90%





- Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain K:



- Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain L: 5% 9% 90%

MET ALA LYS ASN LEU ILE LEU TRP LEU VAL ILE ALA VAL VAL LEU MET SER VAL PHE GLN SER PHE GLY PRO SER GLU SER ASN GLY ARG K31 V32 D33 Y34 S35 T36 F37 L38 Q39 N42 N43 D44 Q45 R50 G53 R54 E55 I56 N57 V58 T59 K60 K61 D62 S63 N64 R65

Y66 T67 T68 Y69 I70 Q73 D74 P75 K76 T83 K84 N85 P92 P93 E94 E95 P96 S97 LEU LEU ALA SER ILE PHE ILE SER TRP PHE PRO MET LEU LEU LEU ILE GLY VAL TRP ILE PHE PHE MET ARG GLN MET GLN GLY GLY GLY LYS GLY ALA MET SER PHE GLY LYS

SER LYS ALA ARG MET LEU THR GLU ASP GLN ILE LYS THR THR PHE ALA ASP VAL ALA GLY CYS ASP GLU ALA LYS GLU GLU VAL ALA GLU LEU VAL GLU TYR LEU ARG GLU PRO SER ARG PHE GLN LYS LEU GLY GLY LYS ILE PRO LYS GLY VAL LEU MET VAL GLY PRO PRO GLY THR

GLY LYS THR LEU LEU ALA LYS ALA ILE ALA GLY GLU ALA LYS VAL PRO PHE PHE THR ILE SER GLY SER ASP PHE VAL GLU MET PHE VAL GLY VAL GLY ALA SER ARG VAL ARG ASP MET PHE GLU GLN ALA LYS LYS ALA ALA PRO CYS ILE ILE PHE ILE ASP GLU ILE ASP ALA VAL

GLY ARG GLN ARG GLY ALA GLY LEU GLY GLY GLY HIS ASP GLU ARG GLU GLN THR LEU ASN GLN MET LEU VAL GLU MET ASP GLY PHE GLU GLY ASN GLU GLY ILE ILE VAL ILE ILE ALA ALA THR ASN ARG PRO ASP VAL LEU ASP PRO ALA LEU LEU ARG PRO GLY ARG PHE ASP ARG GLN

VAL VAL VAL GLY LEU PRO ASP VAL ARG GLY ARG GLU GLN ILE LEU LYS VAL HIS MET ARG ARG VAL PRO LEU ALA PRO ASP ILE ASP ALA ALA ILE ILE ALA ARG GLY THR PRO GLY PHE SER GLY ALA ASP LEU ALA ASN LEU VAL ASN GLU ALA ALA LEU PHE ALA ALA ARG GLY ASN

LYS ARG VAL VAL SER MET VAL GLU PHE GLU LYS ALA LYS ASP LYS ILE MET MET MET GLY ALA GLU ARG ARG SER MET VAL MET THR GLU ALA GLN LYS GLU SER THR ALA TYR HIS GLU ALA GLY HIS ALA ILE ILE GLY ARG LEU VAL PRO GLU HIS ASP PRO VAL HIS LYS VAL THR ILE

ILE PRO ARG GLY ARG ALA LEU GLY VAL THR PHE PHE LEU PRO GLU GLY ASP ALA ILE SER ARG ALA SER ARG GLN LYS LEU GLU SER GLN ILE SER THR LEU TYR GLY GLY GLY ARG LEU ALA GLU GLU ILE ILE TYR GLY PRO GLU HIS VAL SER THR GLY ALA SER ASN ASP ILE LYS VAL ALA

THR ASN LEU ALA ARG ASN MET VAL THR GLN TRP GLY PHE SER GLU LYS LEU GLY PRO LEU LEU LEU TYR ALA GLU GLU GLU GLY GLU VAL PHE LEU GLY GLY ARG SER VAL ALA LYS ALA ALA LYS HIS MET SER ASP GLU THR ALA ARG ILE ILE ASP GLN GLU VAL LYS ALA LEU ILE GLU ARG ASN

TYR ASN ARG ALA ARG GLN LEU LEU THR ASP ASN MET ASP ILE LEU HIS ALA MET LYS ASP ALA LEU MET LYS TYR GLU THR ILE ASP ALA PRO GLN ILE ASP ASP LEU MET ALA ARG ARG ASP VAL ARG PRO PRO ALA GLY TRP GLU GLU PRO GLY ALA SER ASN ASN SER GLY ASP ASN

GLY SER PRO LYS ALA PRO ARG PRO VAL ASP GLU PRO ARG THR PRO ASN PRO GLY ASN THR MET SER GLU GLN LEU GLY ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Patch CTF estimation, cryoSPARC	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.1	Depositor
Minimum defocus (nm)	50	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.673	Depositor
Minimum map value	-0.212	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.053	Depositor
Map size (Å)	588.6, 588.6, 588.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.635, 1.635, 1.635	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	XA	0.20	0/2226	0.43	0/3018
1	XC	0.20	0/2226	0.44	0/3018
1	XE	0.19	0/2226	0.43	0/3018
1	XG	0.18	0/2226	0.41	0/3018
1	XI	0.19	0/2226	0.42	0/3018
1	XK	0.19	0/2226	0.43	0/3018
1	XM	0.19	0/2226	0.43	0/3018
1	XO	0.20	0/2226	0.43	0/3018
1	XQ	0.19	0/2226	0.43	0/3018
1	XS	0.19	0/2226	0.44	0/3018
1	XU	0.19	0/2226	0.46	0/3018
1	XW	0.19	0/698	0.41	0/941
2	XB	0.18	0/2432	0.43	0/3268
2	XD	0.18	0/2432	0.42	0/3268
2	XF	0.18	0/2432	0.40	0/3268
2	XH	0.18	0/2432	0.41	0/3268
2	XJ	0.19	0/2432	0.42	0/3268
2	XL	0.19	0/2432	0.43	0/3268
2	XN	0.18	0/2432	0.42	0/3268
2	XP	0.19	0/2432	0.41	0/3268
2	XR	0.18	0/2432	0.42	0/3268
2	XT	0.19	0/2432	0.45	0/3268
2	XV	0.17	0/792	0.42	0/1061
2	XX	0.19	0/857	0.45	0/1146
3	A	0.21	0/551	0.46	0/748
3	B	0.22	0/551	0.47	0/748
3	C	0.22	0/551	0.49	0/748
3	D	0.19	0/551	0.47	0/748
3	E	0.20	0/551	0.43	0/748
3	F	0.20	0/551	0.40	0/748
3	G	0.21	0/551	0.50	0/748
3	H	0.23	0/551	0.53	0/748
3	I	0.22	0/551	0.50	0/748
3	J	0.20	0/551	0.48	0/748

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	K	0.20	0/551	0.42	0/748
3	L	0.21	0/551	0.43	0/748
All	All	0.19	0/57765	0.43	0/78002

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 (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	XA	2192	2212	2212	15	0
1	XC	2192	2212	2212	17	0
1	XE	2192	2212	2212	20	0
1	XG	2192	2204	2212	22	0
1	XI	2192	2212	2212	18	0
1	XK	2192	2212	2212	22	0
1	XM	2192	2212	2212	13	0
1	XO	2192	2212	2212	15	0
1	XQ	2192	2212	2212	24	0
1	XS	2192	2212	2212	14	0
1	XU	2192	2212	2212	20	0
1	XW	690	712	712	10	0
2	XB	2397	2431	2431	20	0
2	XD	2397	2431	2431	21	0
2	XF	2397	2431	2431	14	0
2	XH	2397	2431	2431	26	0
2	XJ	2397	2431	2431	15	0
2	XL	2397	2431	2431	21	0
2	XN	2397	2431	2431	21	0
2	XP	2397	2431	2431	29	0
2	XR	2397	2431	2431	29	0
2	XT	2397	2431	2431	25	0
2	XV	778	737	737	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	XX	843	802	802	10	0
3	A	543	543	543	9	0
3	B	543	543	543	2	0
3	C	543	543	543	5	0
3	D	543	543	543	1	0
3	E	543	543	543	3	0
3	F	543	543	543	5	0
3	G	543	543	543	3	0
3	H	543	543	543	5	0
3	I	543	543	543	6	0
3	J	543	543	543	4	0
3	K	543	543	543	2	0
3	L	543	543	543	5	0
All	All	56909	57401	57409	396	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 4.

The worst 5 of 396 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:XG:261:GLU:HG3	2:XH:242:GLY:HA3	1.36	1.04
1:XQ:150:LEU:HD22	2:XR:215:LEU:HD12	1.57	0.84
1:XG:261:GLU:HG3	2:XH:242:GLY:CA	2.11	0.81
1:XQ:190:SER:OG	2:XR:210:ILE:O	2.03	0.76
1:XG:261:GLU:CD	2:XH:238:HIS:O	2.31	0.73

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	XA	275/419 (66%)	275 (100%)	0	0	100	100
1	XC	275/419 (66%)	275 (100%)	0	0	100	100
1	XE	275/419 (66%)	275 (100%)	0	0	100	100
1	XG	275/419 (66%)	275 (100%)	0	0	100	100
1	XI	275/419 (66%)	275 (100%)	0	0	100	100
1	XK	275/419 (66%)	275 (100%)	0	0	100	100
1	XM	275/419 (66%)	274 (100%)	1 (0%)	0	100	100
1	XO	275/419 (66%)	275 (100%)	0	0	100	100
1	XQ	275/419 (66%)	275 (100%)	0	0	100	100
1	XS	275/419 (66%)	275 (100%)	0	0	100	100
1	XU	275/419 (66%)	275 (100%)	0	0	100	100
1	XW	85/419 (20%)	85 (100%)	0	0	100	100
2	XB	295/334 (88%)	295 (100%)	0	0	100	100
2	XD	295/334 (88%)	295 (100%)	0	0	100	100
2	XF	295/334 (88%)	295 (100%)	0	0	100	100
2	XH	295/334 (88%)	295 (100%)	0	0	100	100
2	XJ	295/334 (88%)	295 (100%)	0	0	100	100
2	XL	295/334 (88%)	295 (100%)	0	0	100	100
2	XN	295/334 (88%)	295 (100%)	0	0	100	100
2	XP	295/334 (88%)	294 (100%)	1 (0%)	0	100	100
2	XR	295/334 (88%)	295 (100%)	0	0	100	100
2	XT	295/334 (88%)	295 (100%)	0	0	100	100
2	XV	95/334 (28%)	95 (100%)	0	0	100	100
2	XX	103/334 (31%)	103 (100%)	0	0	100	100
3	A	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
3	B	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
3	C	65/644 (10%)	65 (100%)	0	0	100	100
3	D	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
3	E	65/644 (10%)	65 (100%)	0	0	100	100
3	F	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
3	G	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
3	H	65/644 (10%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	65/644 (10%)	65 (100%)	0	0	100	100
3	J	65/644 (10%)	65 (100%)	0	0	100	100
3	K	65/644 (10%)	65 (100%)	0	0	100	100
3	L	65/644 (10%)	64 (98%)	1 (2%)	0	100	100
All	All	7038/16764 (42%)	7030 (100%)	8 (0%)	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	XA	232/336 (69%)	232 (100%)	0	100	100
1	XC	232/336 (69%)	232 (100%)	0	100	100
1	XE	232/336 (69%)	232 (100%)	0	100	100
1	XG	232/336 (69%)	232 (100%)	0	100	100
1	XI	232/336 (69%)	232 (100%)	0	100	100
1	XK	232/336 (69%)	232 (100%)	0	100	100
1	XM	232/336 (69%)	232 (100%)	0	100	100
1	XO	232/336 (69%)	232 (100%)	0	100	100
1	XQ	232/336 (69%)	232 (100%)	0	100	100
1	XS	232/336 (69%)	232 (100%)	0	100	100
1	XU	232/336 (69%)	232 (100%)	0	100	100
1	XW	71/336 (21%)	71 (100%)	0	100	100
2	XB	258/283 (91%)	258 (100%)	0	100	100
2	XD	258/283 (91%)	257 (100%)	1 (0%)	84	82
2	XF	258/283 (91%)	258 (100%)	0	100	100
2	XH	258/283 (91%)	258 (100%)	0	100	100
2	XJ	258/283 (91%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XL	258/283 (91%)	258 (100%)	0	100	100
2	XN	258/283 (91%)	258 (100%)	0	100	100
2	XP	258/283 (91%)	258 (100%)	0	100	100
2	XR	258/283 (91%)	258 (100%)	0	100	100
2	XT	258/283 (91%)	258 (100%)	0	100	100
2	XV	78/283 (28%)	78 (100%)	0	100	100
2	XX	83/283 (29%)	83 (100%)	0	100	100
3	A	64/527 (12%)	64 (100%)	0	100	100
3	B	64/527 (12%)	64 (100%)	0	100	100
3	C	64/527 (12%)	64 (100%)	0	100	100
3	D	64/527 (12%)	64 (100%)	0	100	100
3	E	64/527 (12%)	64 (100%)	0	100	100
3	F	64/527 (12%)	64 (100%)	0	100	100
3	G	64/527 (12%)	64 (100%)	0	100	100
3	H	64/527 (12%)	64 (100%)	0	100	100
3	I	64/527 (12%)	64 (100%)	0	100	100
3	J	64/527 (12%)	64 (100%)	0	100	100
3	K	64/527 (12%)	64 (100%)	0	100	100
3	L	64/527 (12%)	64 (100%)	0	100	100
All	All	6132/13752 (45%)	6131 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	XD	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	XP	74	ASN
2	XT	305	ASN
1	XS	123	ASN
1	XU	284	GLN
1	XG	284	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

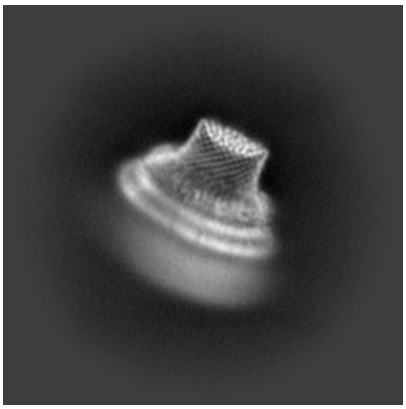
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-46057. These allow visual inspection of the internal detail of the map and identification of artifacts.

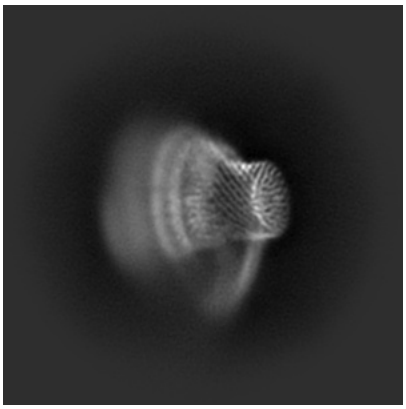
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

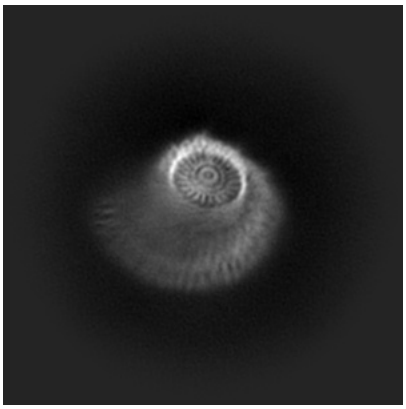
6.1.1 Primary map



X

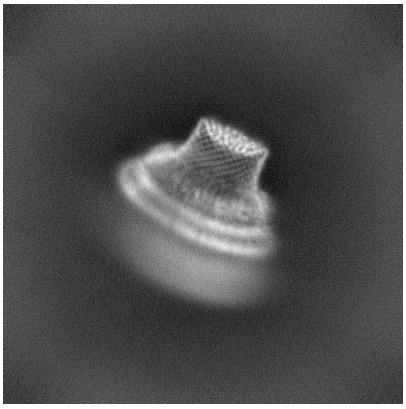


Y

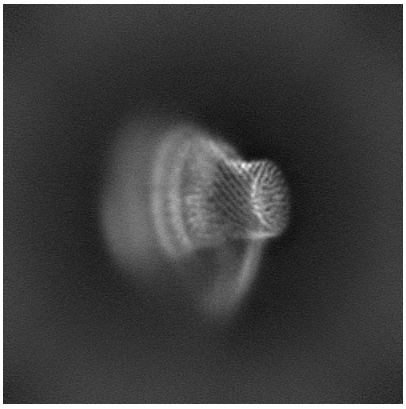


Z

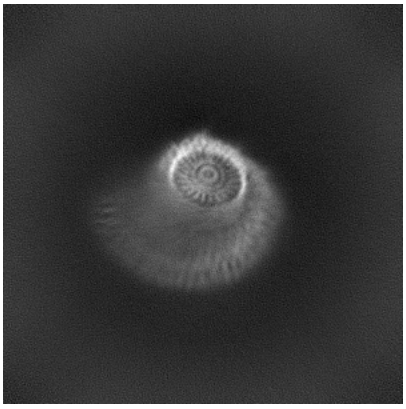
6.1.2 Raw map



X



Y

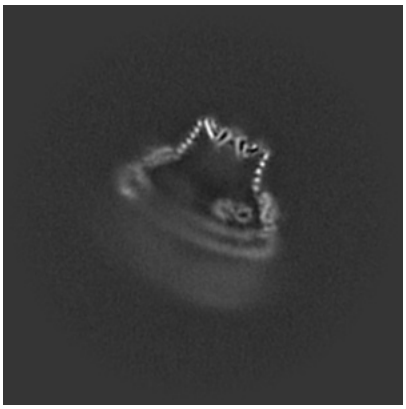


Z

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

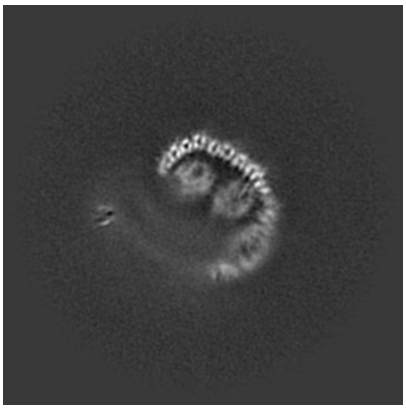
6.2 Central slices (i)

6.2.1 Primary map



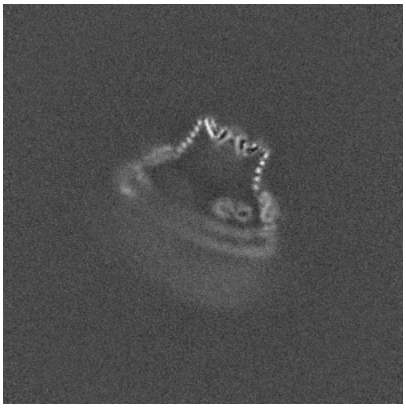
X Index: 180

Y Index: 180



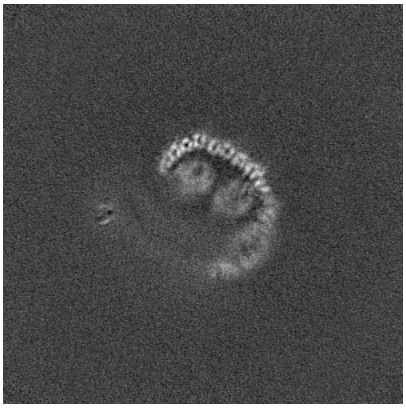
Z Index: 180

6.2.2 Raw map



X Index: 180

Y Index: 180

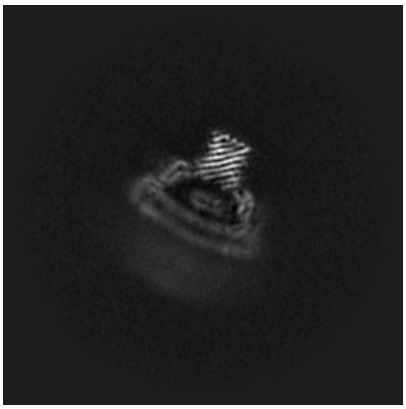


Z Index: 180

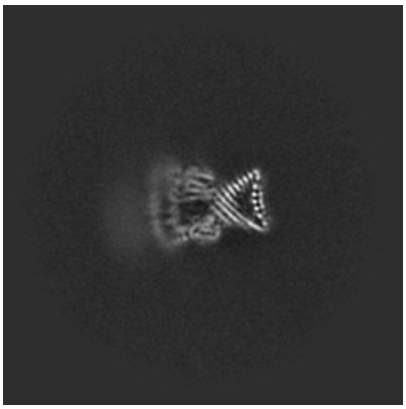
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

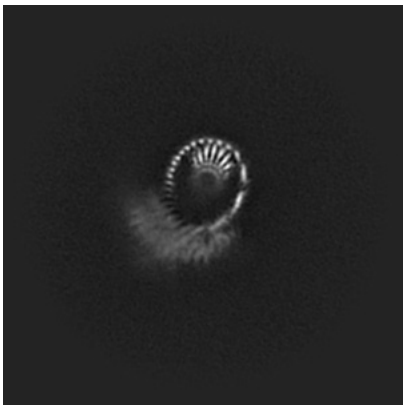
6.3.1 Primary map



X Index: 215

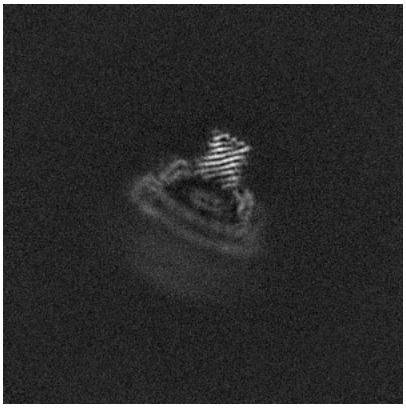


Y Index: 227

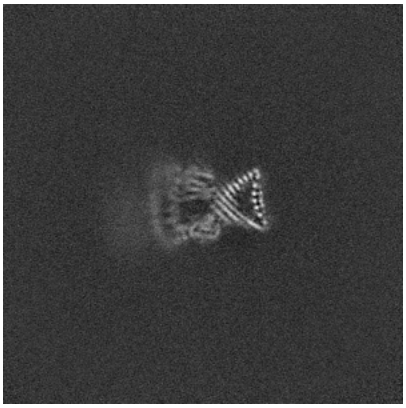


Z Index: 226

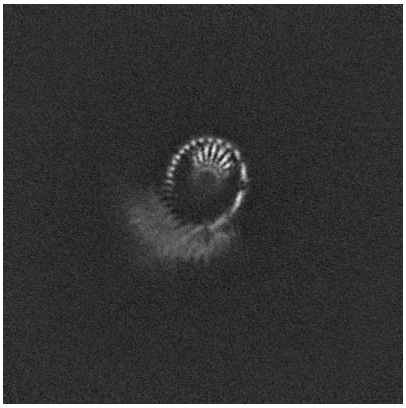
6.3.2 Raw map



X Index: 215



Y Index: 227

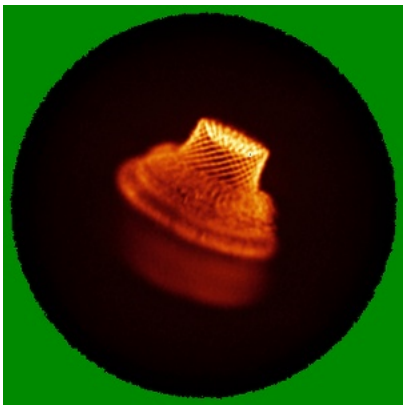


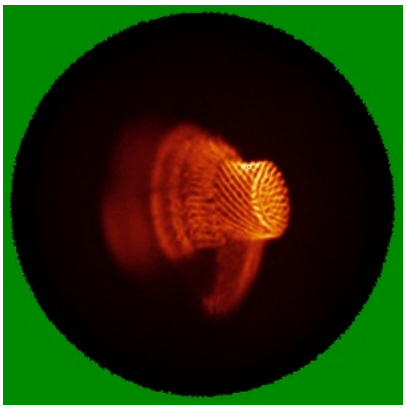
Z Index: 226

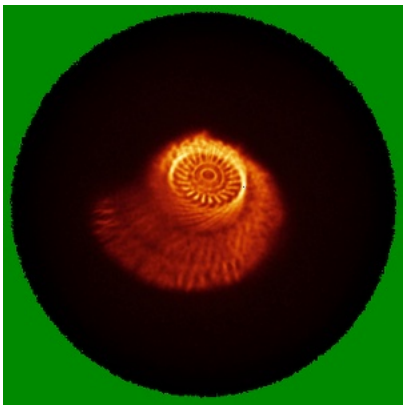
The images above show the largest variance slices of the map in three orthogonal directions.

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

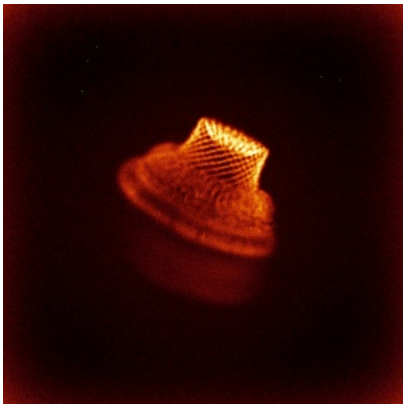
6.4.1 Primary map

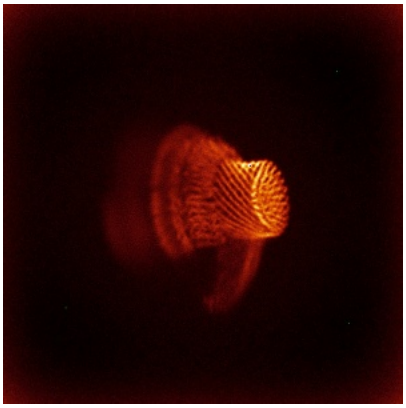

X

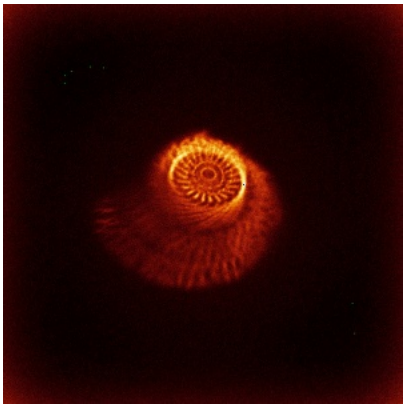

Y


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)

This section was not generated.

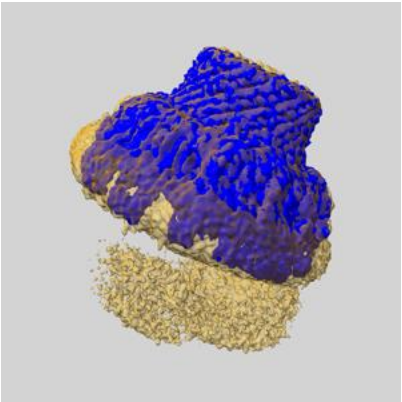
6.6 Mask visualisation (i)

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

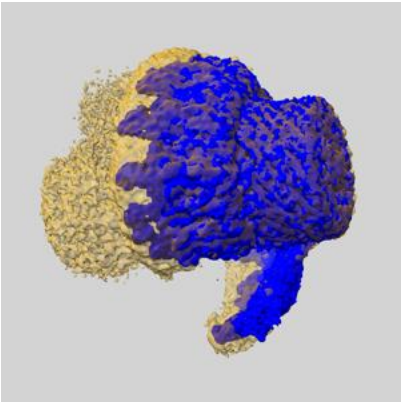
A mask typically either:

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

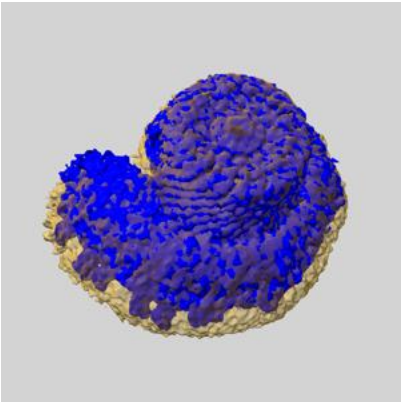
6.6.1 emd_46057_msk_1.map (i)



X



Y

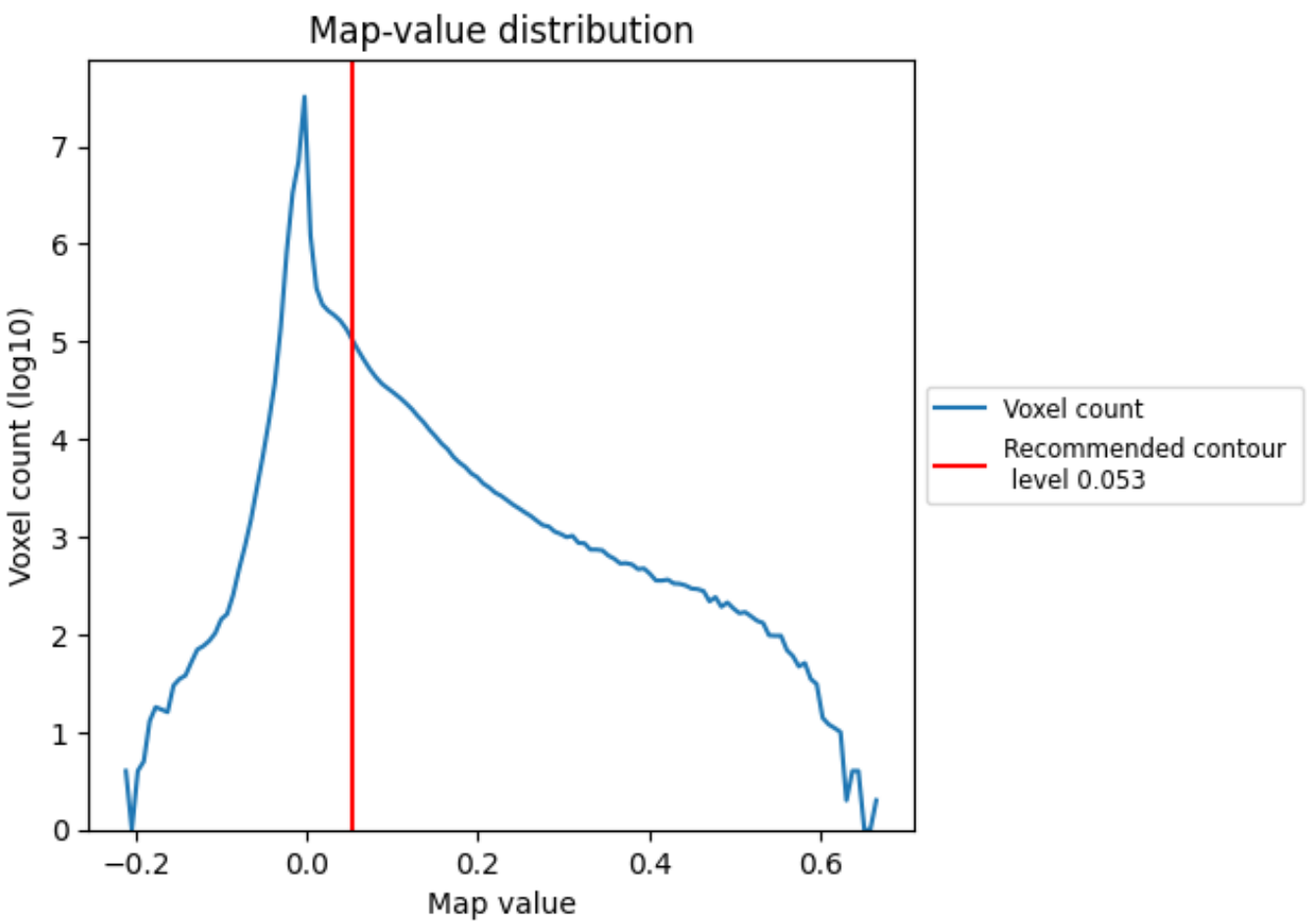


Z

7 Map analysis (i)

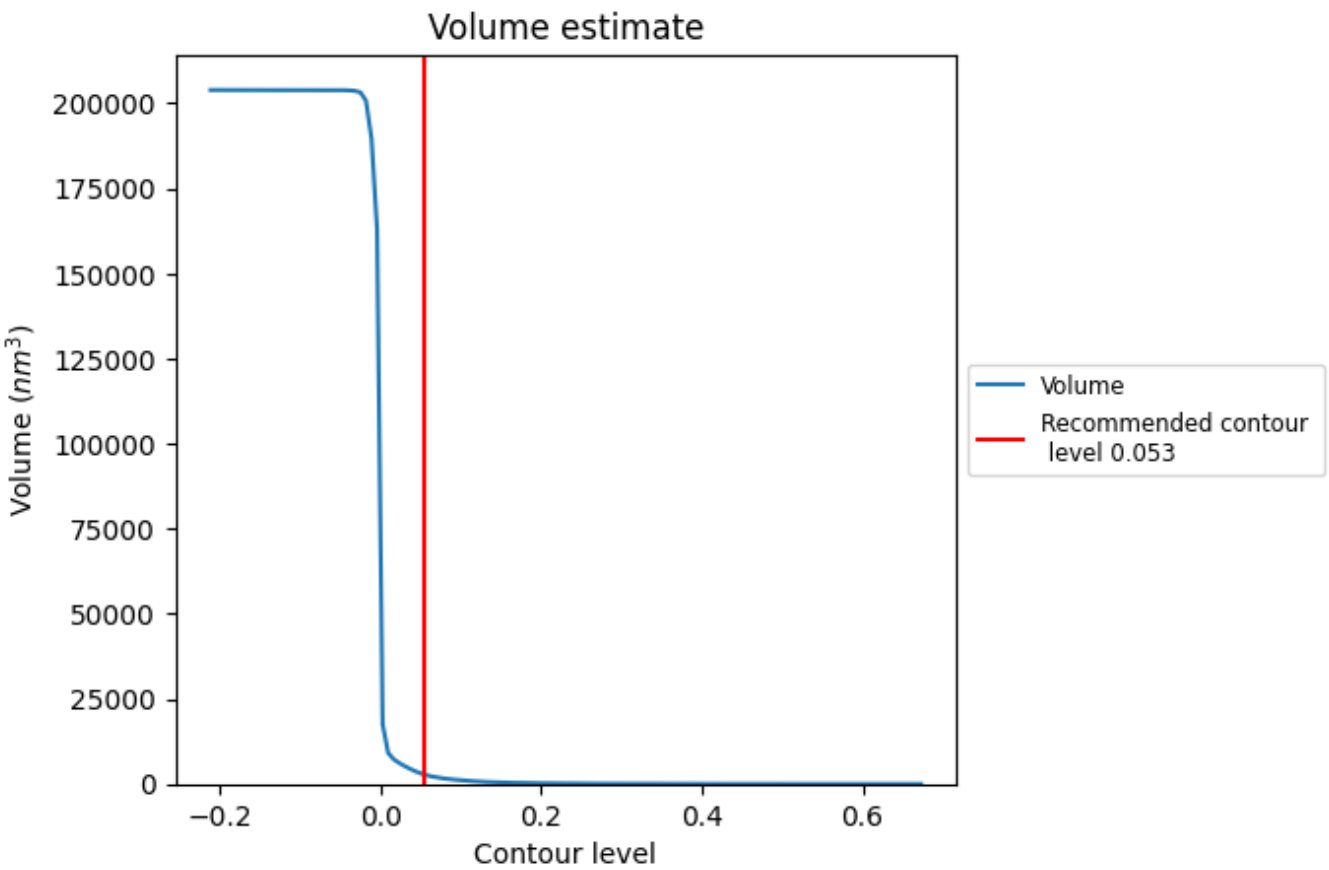
This section contains the results of statistical analysis of the map.

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.

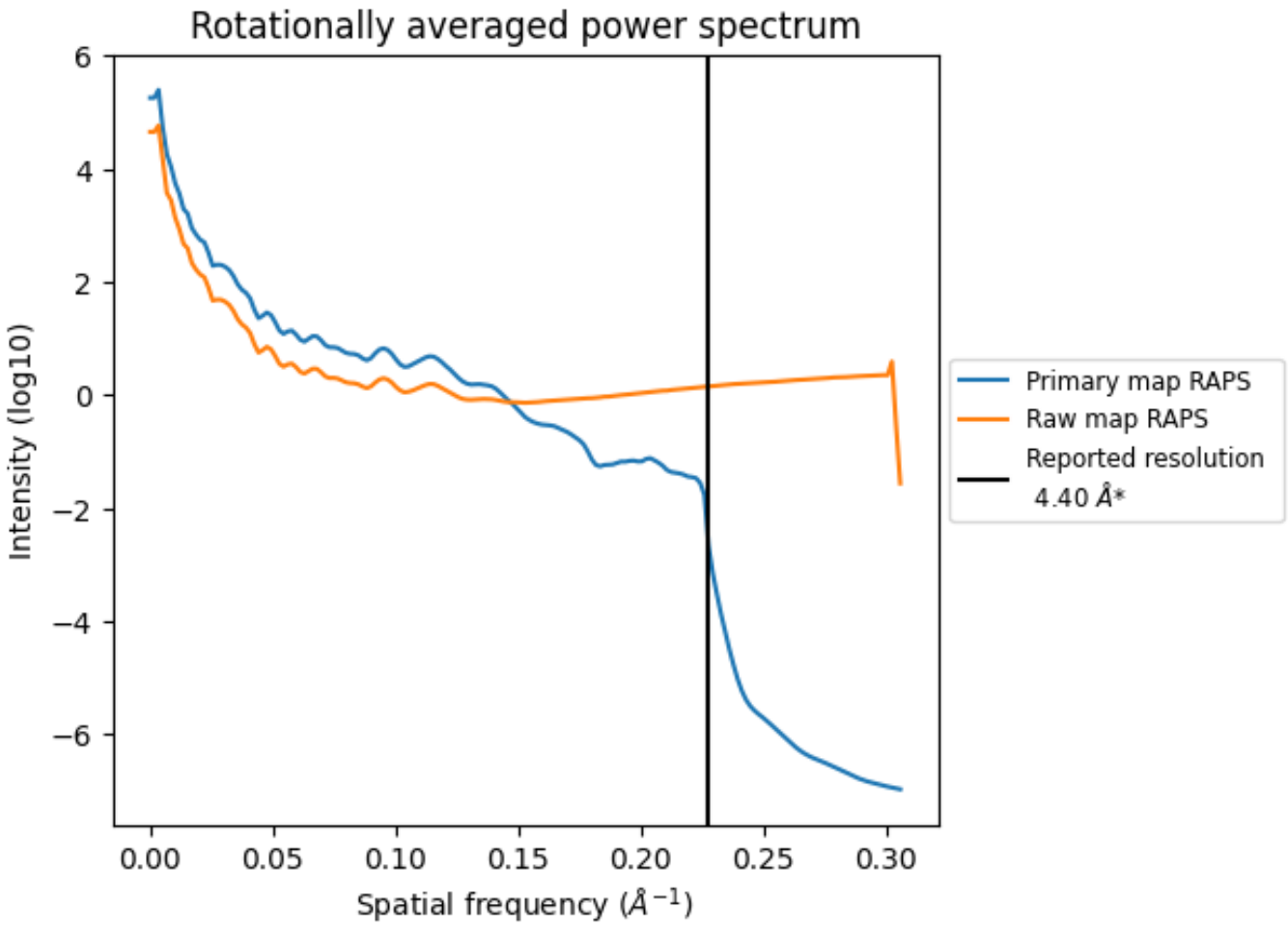
7.2 Volume estimate (i)



The volume at the recommended contour level is 2877 nm^3; this corresponds to an approximate mass of 2599 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)

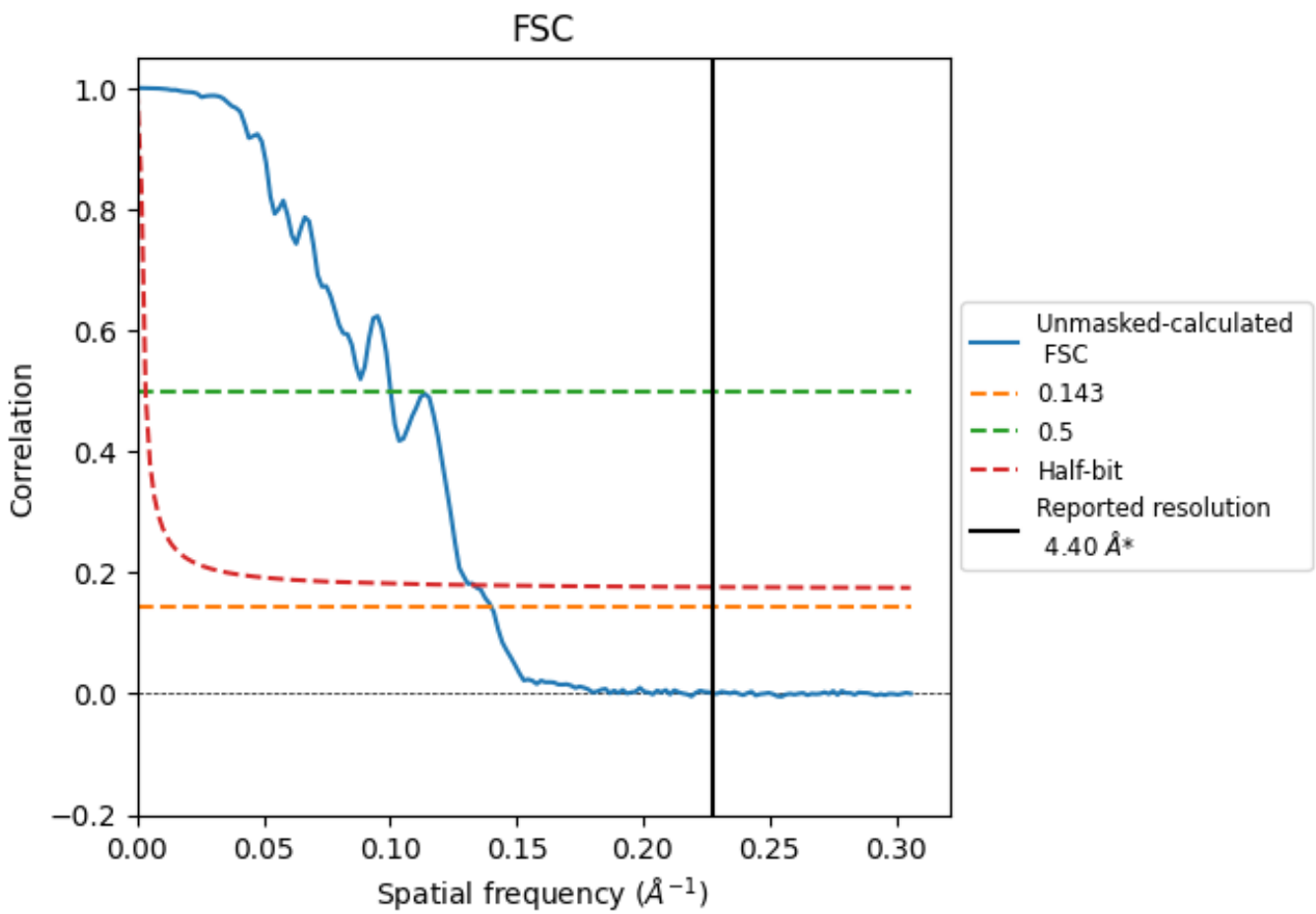


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

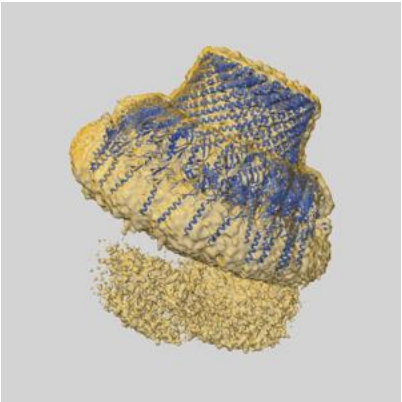
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.14	9.97	7.51

*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 7.14 differs from the reported value 4.4 by more than 10 %

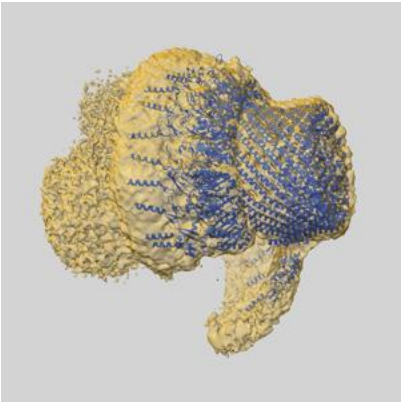
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-46057 and PDB model 9CZ2. Per-residue inclusion information can be found in section 3 on page 8.

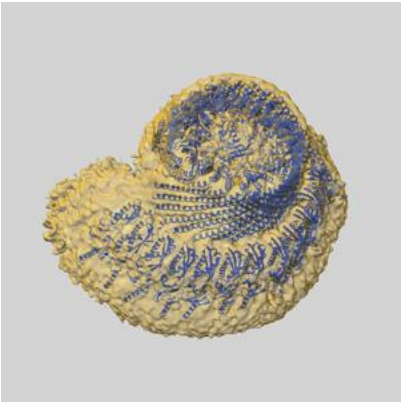
9.1 Map-model overlay (i)



X



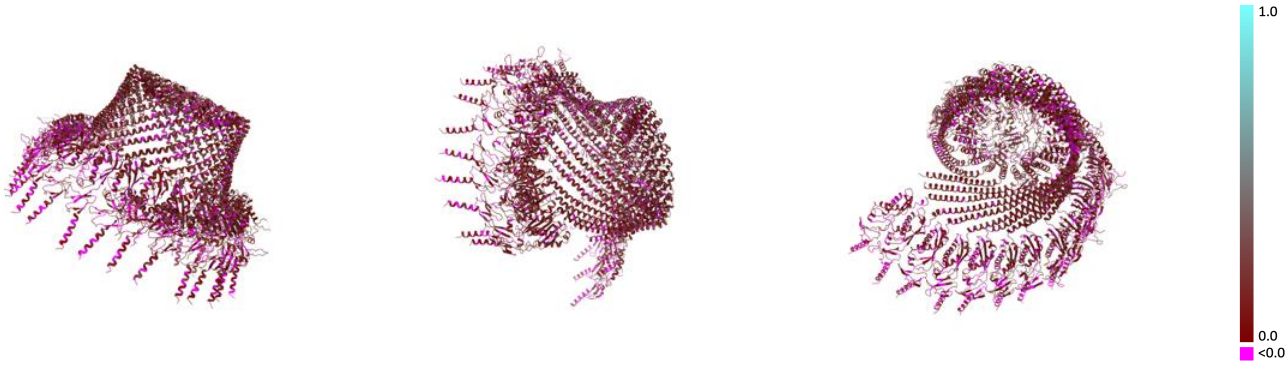
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.053 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.

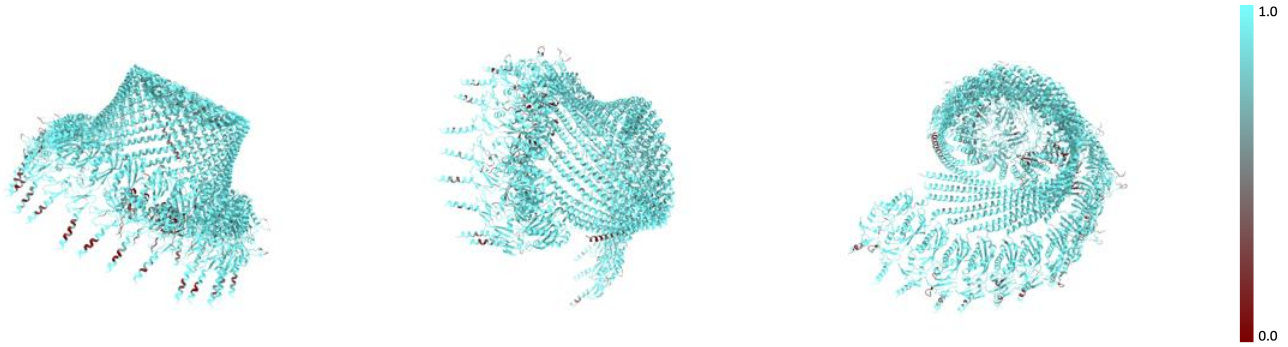
9.2 Q-score mapped to coordinate model (i)



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.

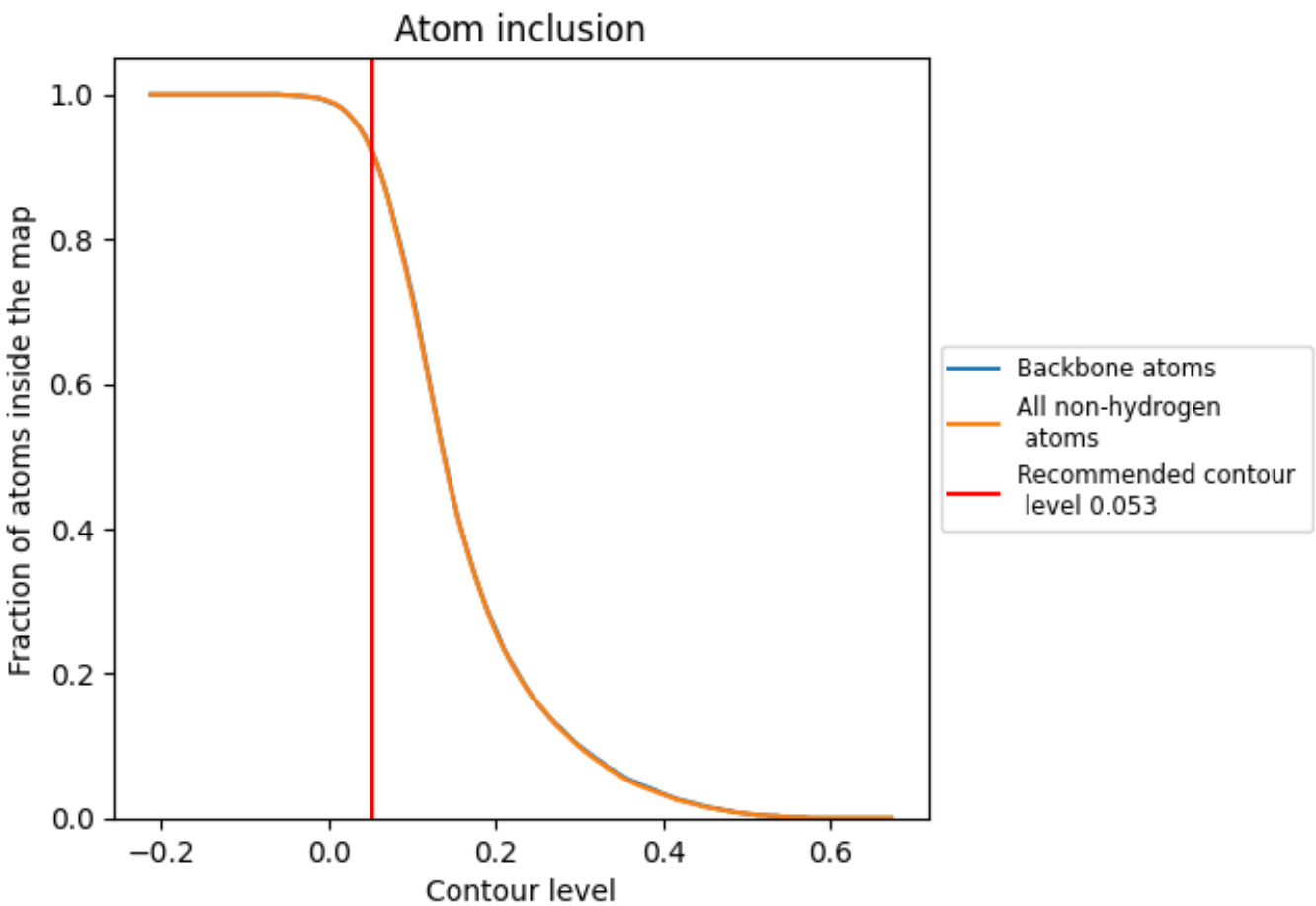
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.053).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.1190
A	0.8820	0.1300
B	0.8040	0.1070
C	0.8480	0.1380
D	0.8740	0.1250
E	0.8950	0.1100
F	0.9320	0.1030
G	0.6770	0.1020
H	0.6650	0.0800
I	0.8010	0.1040
J	0.7460	0.0810
K	0.5000	0.0640
L	0.5300	0.1000
XA	0.9500	0.1380
XB	0.9540	0.1360
XC	0.9540	0.1420
XD	0.9450	0.1430
XE	0.9360	0.1240
XF	0.9480	0.1370
XG	0.9500	0.1340
XH	0.9480	0.1320
XI	0.9480	0.1230
XJ	0.9210	0.1350
XK	0.9370	0.1150
XL	0.9240	0.1020
XM	0.9360	0.1140
XN	0.9220	0.1180
XO	0.9470	0.0960
XP	0.9410	0.1200
XQ	0.9530	0.0970
XR	0.9430	0.1050
XS	0.9680	0.0890
XT	0.9420	0.1070
XU	0.9520	0.0900
XV	0.9520	0.1860

Continued on next page...

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Chain	Atom inclusion	Q-score
XW	0.9380	0.1600
XX	0.7950	0.1430