



Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 04:11 AM JST

PDB ID : 7WI3
EMDB ID : EMD-32520
Title : Cryo-EM structure of E.Coli FtsH-HflkC AAA protease complex
Authors : Qiao, Z.; Gao, Y.G.
Deposited on : 2022-01-02
Resolution : 4.00 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

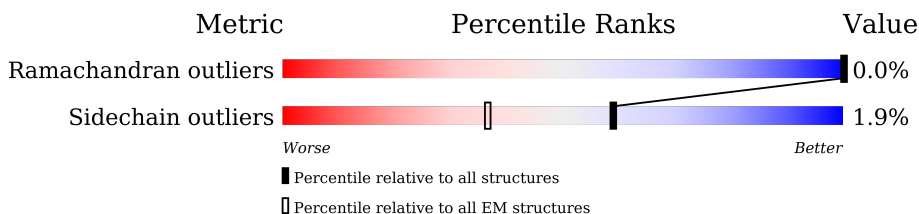
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	334	 86% 12%
1	C	334	 84% 14%
1	D	334	 86% 13%
1	M	334	 85% 12%
1	O	334	 84% 14%
1	P	334	 85% 13%
1	Y	334	 86% 12%
1	Z	334	 86% 12%
1	c	334	 84% 14%

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Mol	Chain	Length	Quality of chain	
1	d	334	84%	14%
1	e	334	86%	13%
1	f	334	84%	13%
2	B	419	63%	34%
2	F	419	63%	34%
2	G	419	64%	34%
2	N	419	64%	34%
2	R	419	63%	34%
2	S	419	63%	34%
2	a	419	63%	34%
2	b	419	62%	34%
2	i	419	63%	34%
2	j	419	63%	34%
2	k	419	63%	34%
2	l	419	64%	34%
3	E	644	13%	87%
3	H	644	12%	87%
3	I	644	12%	88%
3	J	644	12%	88%
3	K	644	12%	88%
3	L	644	12%	88%
3	Q	644	13%	87%
3	T	644	12%	87%
3	U	644	12%	88%
3	V	644	12%	88%

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Mol	Chain	Length	Quality of chain
3	W	644	 12% 88%
3	X	644	 12% 88%
3	g	644	 13% 87%
3	h	644	 12% 87%
3	m	644	 13% 87%
3	n	644	 12% 87%
3	o	644	 12% 88%
3	p	644	 12% 88%
3	q	644	 12% 88%
3	r	644	 12% 88%
3	s	644	 12% 88%
3	t	644	 12% 88%
3	u	644	 11% 88%
3	v	644	 12% 88%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 69304 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 Modulator of FtsH protease HflC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	293	2338	1472	419	437	10	0	0
1	C	287	2290	1444	411	426	9	0	0
1	D	290	2311	1457	414	430	10	0	0
1	Y	293	2338	1472	419	437	10	0	0
1	c	287	2290	1444	411	426	9	0	0
1	e	290	2311	1457	414	430	10	0	0
1	Z	293	2338	1472	419	437	10	0	0
1	d	287	2290	1444	411	426	9	0	0
1	f	290	2311	1457	414	430	10	0	0
1	M	293	2338	1472	419	437	10	0	0
1	O	287	2290	1444	411	426	9	0	0
1	P	290	2311	1457	414	430	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	275	2169	1362	383	418	6	0	0
2	F	275	2165	1360	383	416	6	0	0
2	G	275	2173	1364	384	419	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	i	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	k	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		
2	b	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	j	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	l	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		
2	N	275	Total	C	N	O	S	0	0
			2169	1362	383	418	6		
2	R	275	Total	C	N	O	S	0	0
			2165	1360	383	416	6		
2	S	275	Total	C	N	O	S	0	0
			2173	1364	384	419	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	H	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	I	79	Total	C	N	O		0	0
			643	408	111	124			
3	J	78	Total	C	N	O		0	0
			635	405	107	123			
3	K	79	Total	C	N	O		0	0
			643	408	111	124			
3	L	79	Total	C	N	O		0	0
			643	408	111	124			
3	g	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	m	81	Total	C	N	O	S	0	0
			658	418	113	126	1		
3	o	79	Total	C	N	O		0	0
			643	408	111	124			
3	q	78	Total	C	N	O		0	0
			635	405	107	123			

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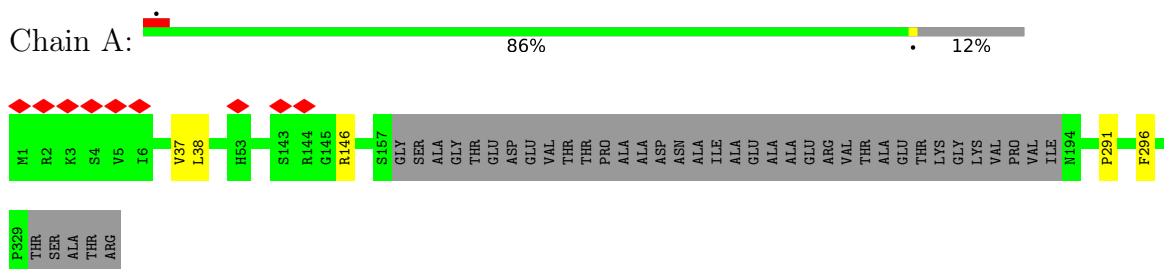
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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	s	79	Total 643	C 408	N 111	O 124	0	0	
3	u	79	Total 643	C 408	N 111	O 124	0	0	
3	h	81	Total 658	C 418	N 113	O 126	S 1	0	0
3	n	81	Total 658	C 418	N 113	O 126	S 1	0	0
3	p	79	Total 643	C 408	N 111	O 124		0	0
3	r	78	Total 635	C 405	N 107	O 123		0	0
3	t	79	Total 643	C 408	N 111	O 124		0	0
3	v	79	Total 643	C 408	N 111	O 124		0	0
3	Q	81	Total 658	C 418	N 113	O 126	S 1	0	0
3	T	81	Total 658	C 418	N 113	O 126	S 1	0	0
3	U	79	Total 643	C 408	N 111	O 124		0	0
3	V	78	Total 635	C 405	N 107	O 123		0	0
3	W	79	Total 643	C 408	N 111	O 124		0	0
3	X	79	Total 643	C 408	N 111	O 124		0	0

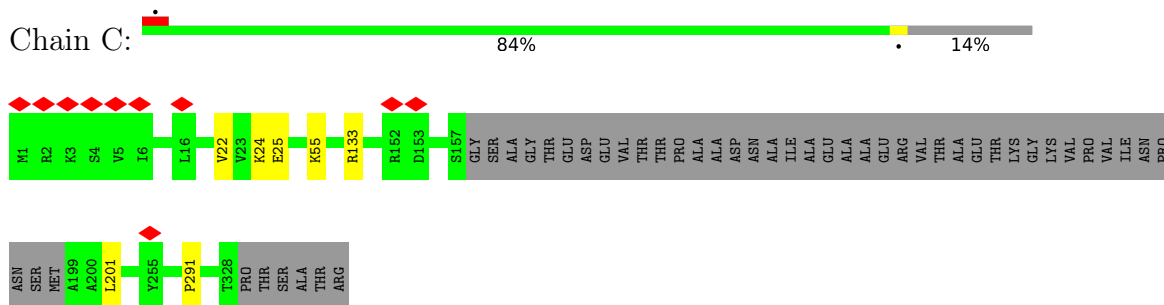
3 Residue-property plots [i](#)

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.

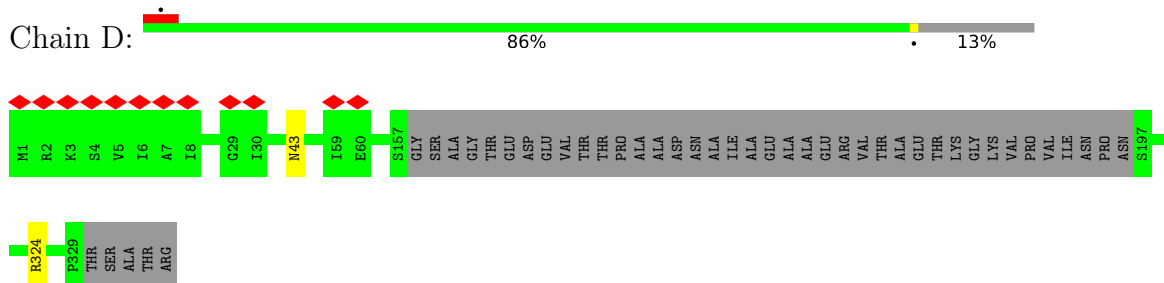
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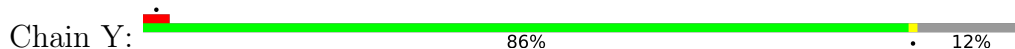
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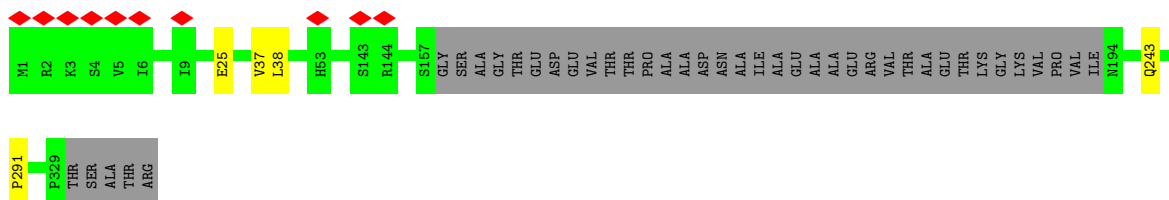


- Molecule 1: Modulator of FtsH protease HflC

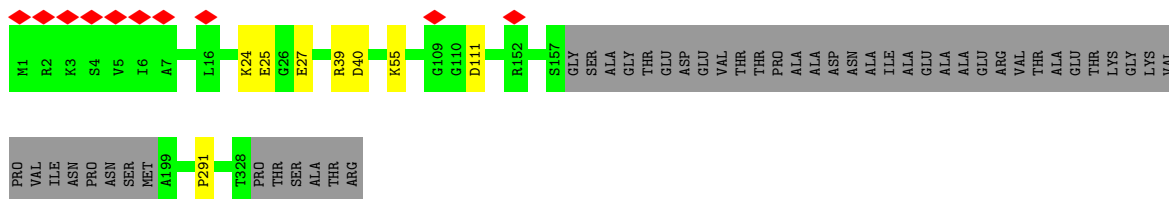
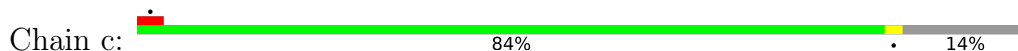


- Molecule 1: Modulator of FtsH protease HflC

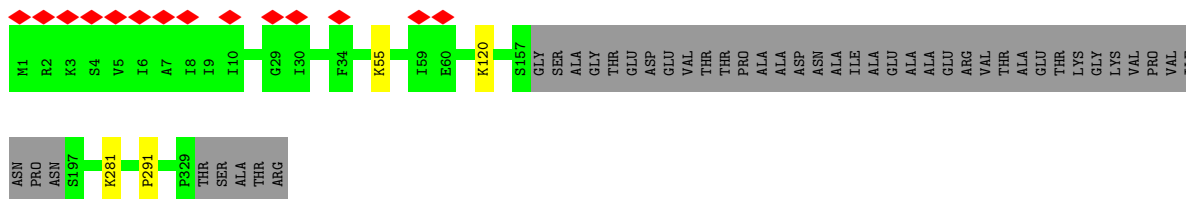
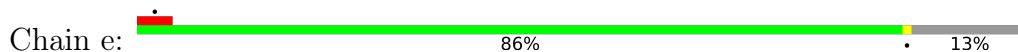




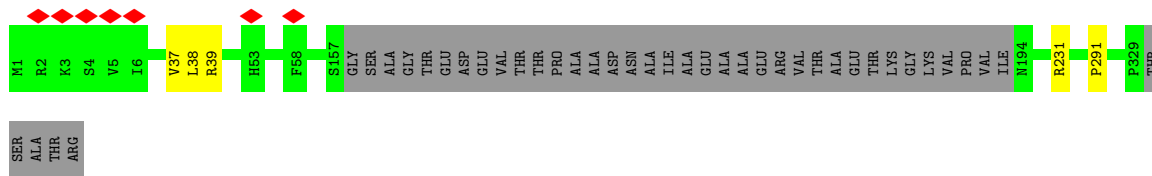
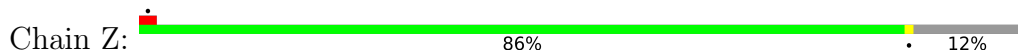
• Molecule 1: Modulator of FtsH protease HflC



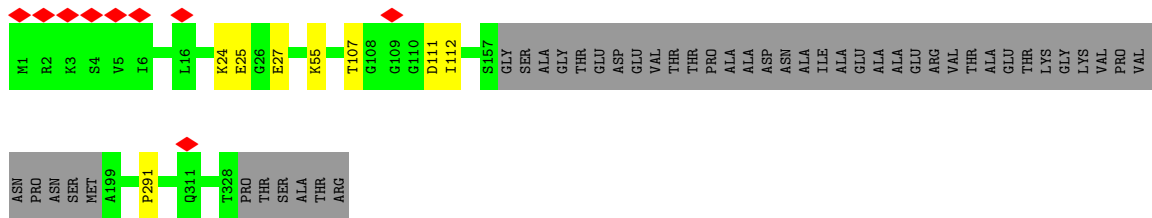
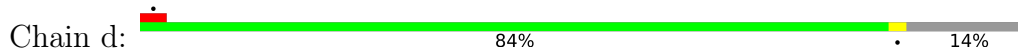
• Molecule 1: Modulator of FtsH protease HflC



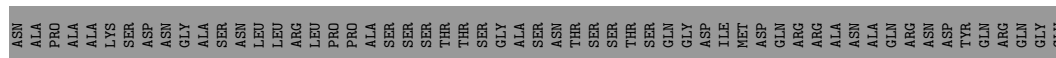
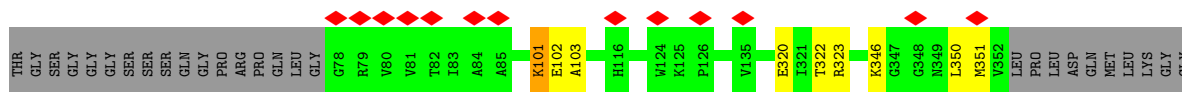
• Molecule 1: Modulator of FtsH protease HflC



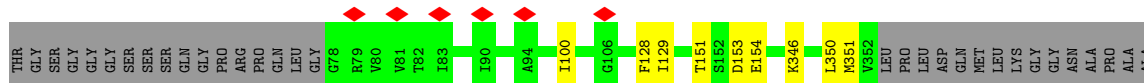
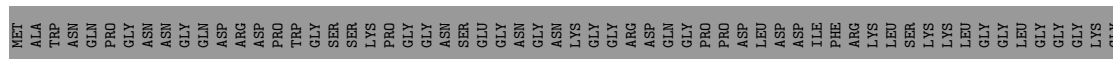
• Molecule 1: Modulator of FtsH protease HflC



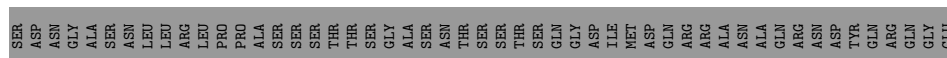
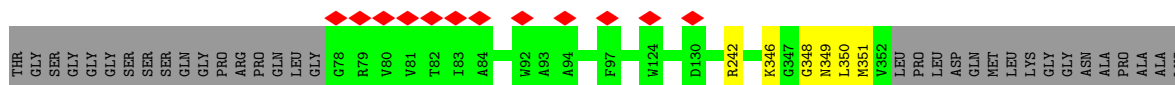
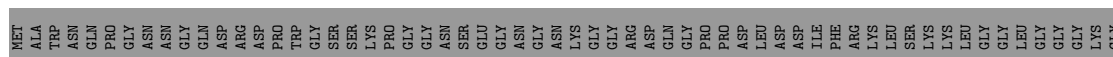
• Molecule 1: Modulator of FtsH protease HflC



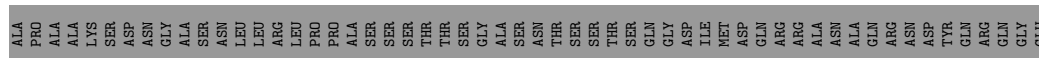
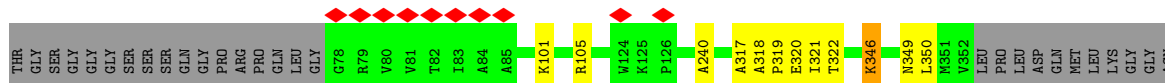
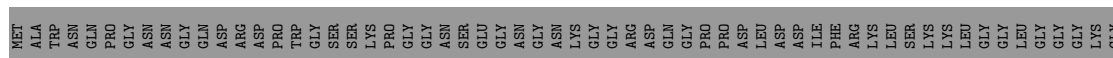
- Molecule 2: Modulator of FtsH protease HflK



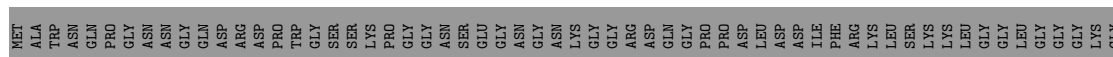
- Molecule 2: Modulator of FtsH protease HflK

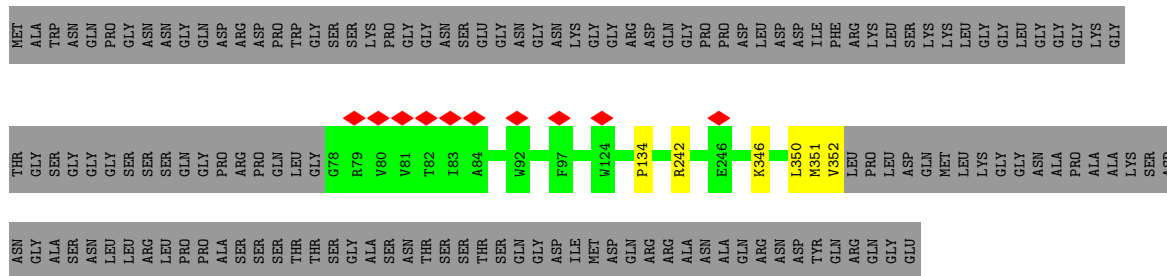


- Molecule 2: Modulator of FtsH protease HflK

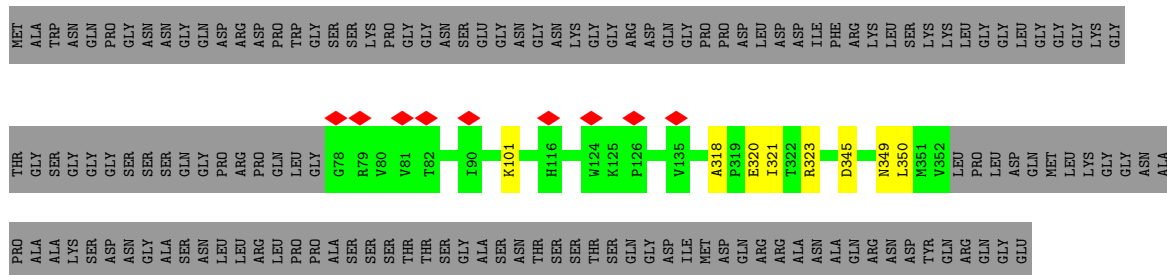


- Molecule 2: Modulator of FtsH protease HflK

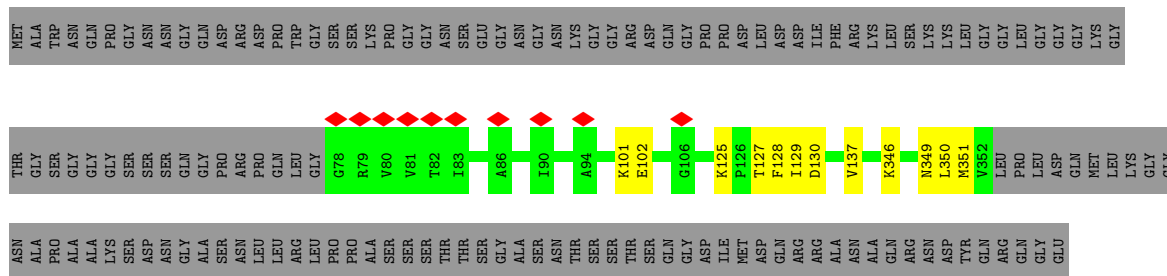




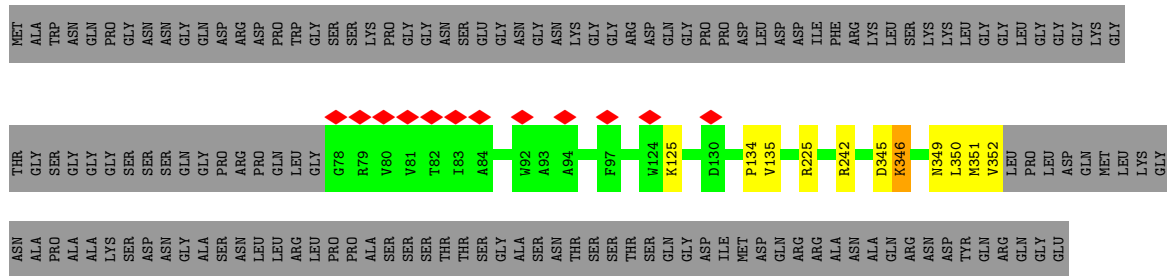
Molecule 2: Modulator of FtsH protease HflK



Molecule 2: Modulator of FtsH protease HflK

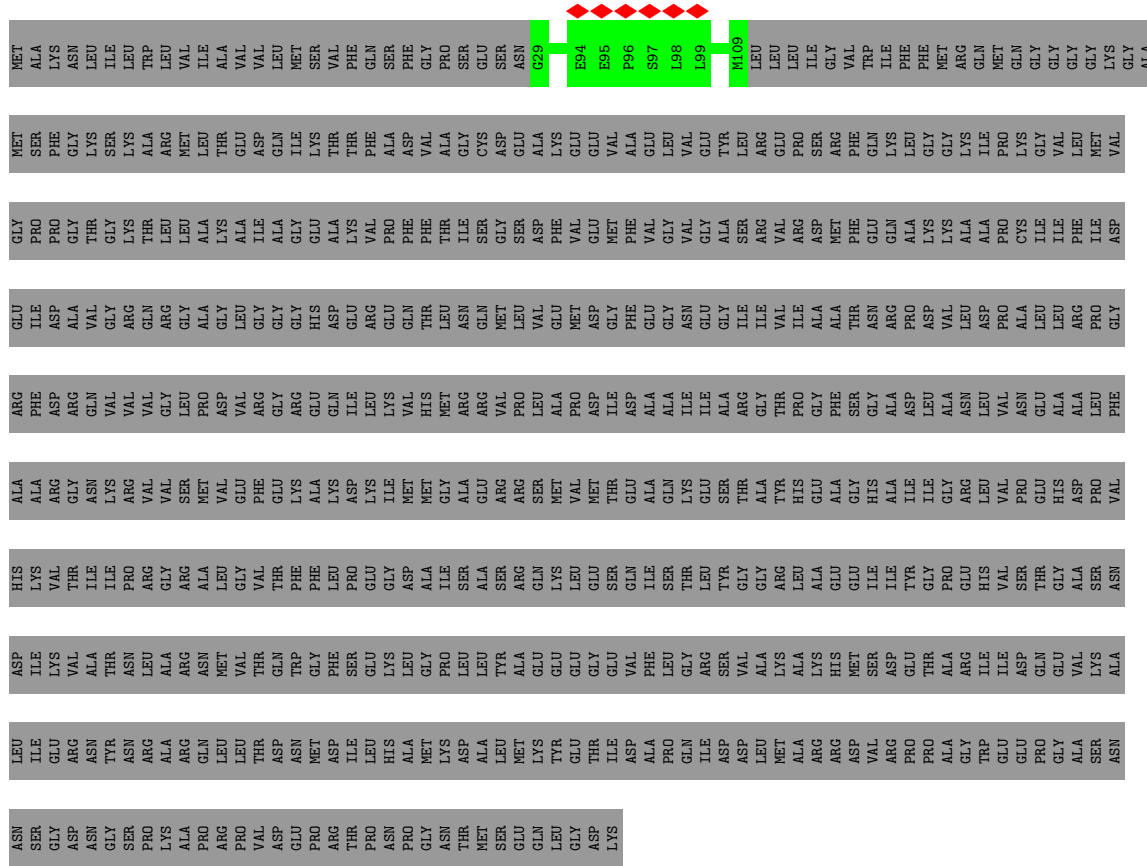


Molecule 2: Modulator of FtsH protease HflK



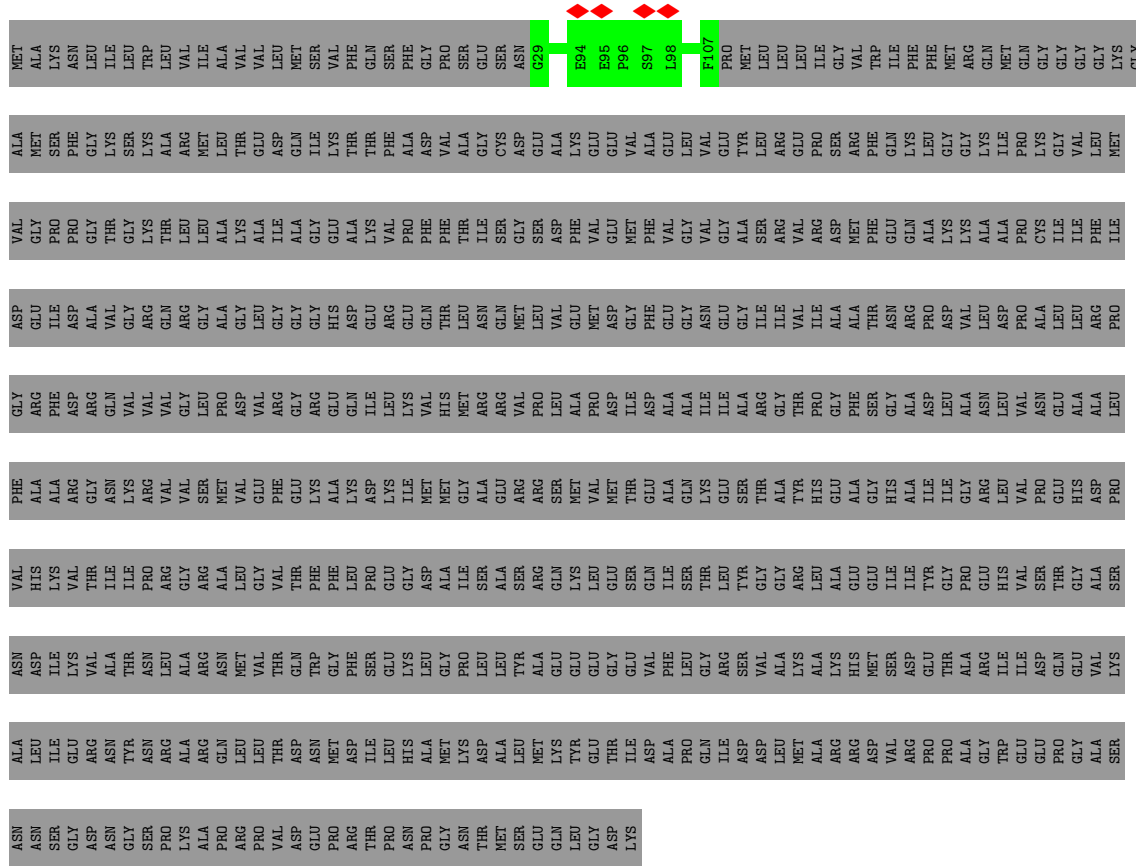
Molecule 3: ATP-dependent zinc metalloprotease FtsH





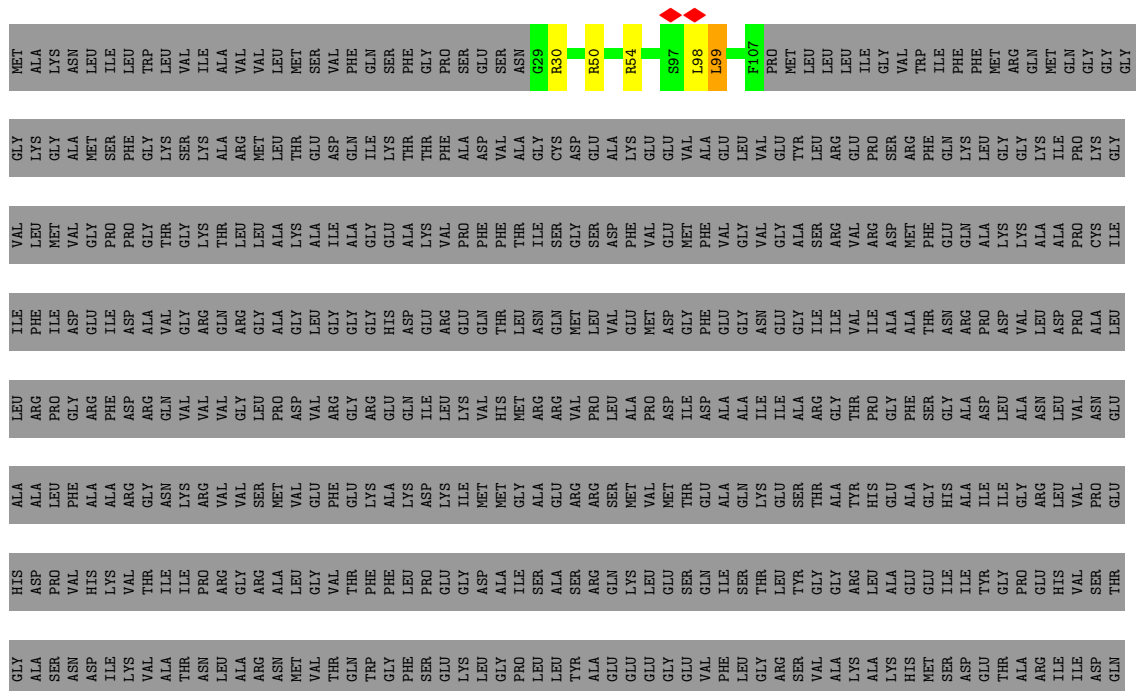
- Molecule 3: ATP-dependent zinc metalloprotease FtsH

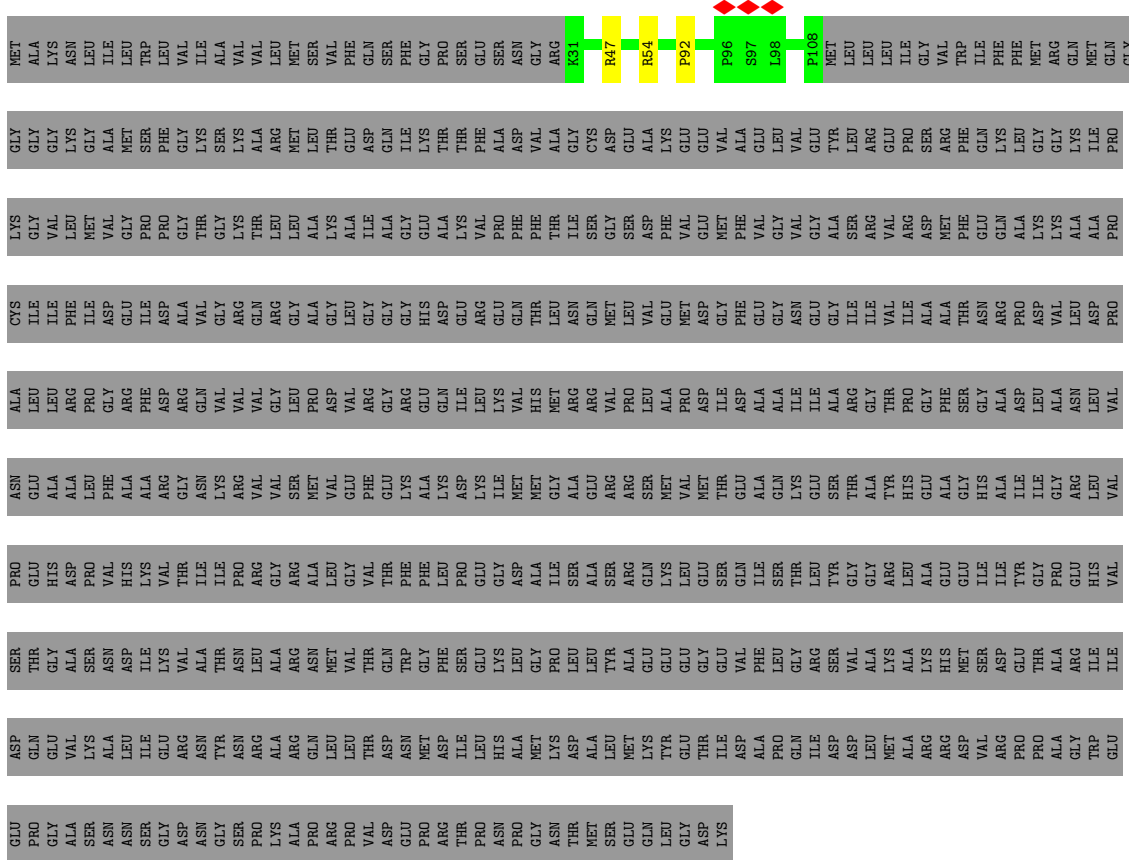




● Molecule 3: ATP-dependent zinc metalloprotease FtsH

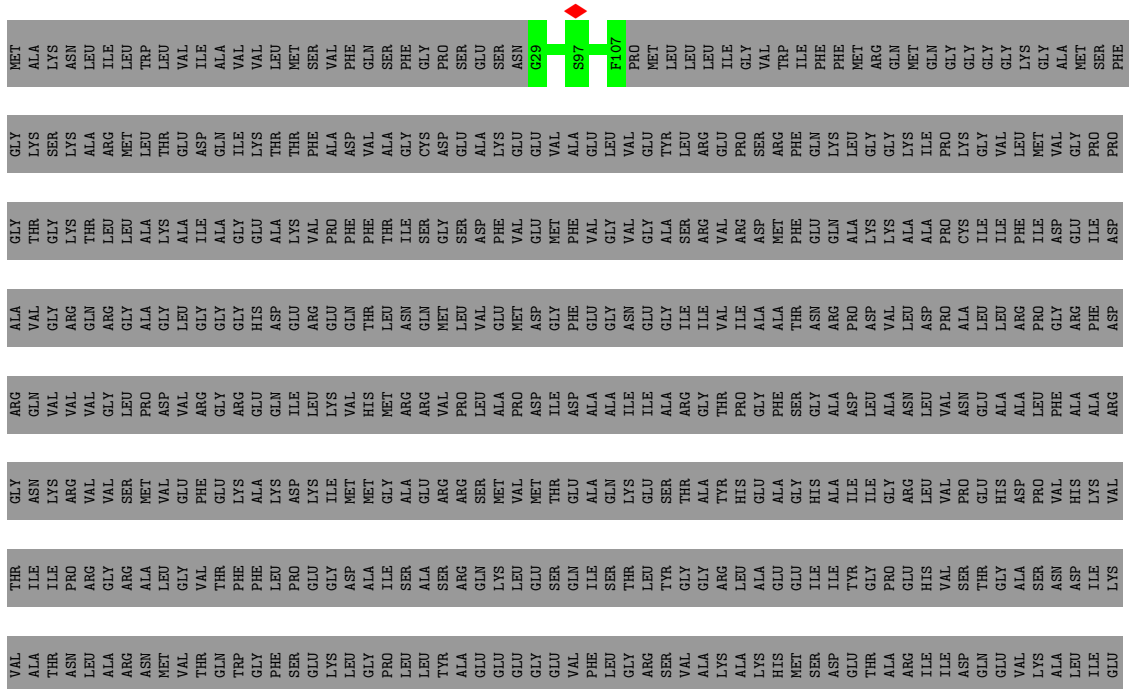
Chain u:  11% .  88%





- Molecule 3: ATP-dependent zinc metalloprotease FtsH

Chain t: 12% 88%



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

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

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

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

GLY ASP
ASN ASN
GLY GLY
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PRO PRO
LYS LYS
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PRO PRO
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PRO PRO
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PRO PRO
ARG ARG
THR THR
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PRO PRO
GLY GLY
THR THR
SER SER
LEU LEU
GLU GLU
GLN GLN
LEU LEU
GLY GLY
ASP ASP
LYS LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.032	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	384.384, 384.384, 384.384	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3728, 1.3728, 1.3728	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	A	0.31	0/2371	0.62	4/3187 (0.1%)
1	C	0.35	0/2321	0.61	3/3118 (0.1%)
1	D	0.32	0/2343	0.56	1/3148 (0.0%)
1	M	0.33	0/2371	0.61	4/3187 (0.1%)
1	O	0.33	0/2321	0.61	3/3118 (0.1%)
1	P	1.95	8/2343 (0.3%)	0.87	12/3148 (0.4%)
1	Y	0.31	0/2371	0.63	3/3187 (0.1%)
1	Z	0.31	0/2371	0.62	4/3187 (0.1%)
1	c	0.33	0/2321	0.53	1/3118 (0.0%)
1	d	0.34	0/2321	0.55	1/3118 (0.0%)
1	e	0.33	0/2343	0.56	1/3148 (0.0%)
1	f	0.36	0/2343	0.63	3/3148 (0.1%)
2	B	0.33	0/2202	0.74	6/2984 (0.2%)
2	F	0.33	0/2198	0.61	3/2979 (0.1%)
2	G	0.33	0/2206	0.59	3/2989 (0.1%)
2	N	0.34	0/2202	0.62	1/2984 (0.0%)
2	R	0.34	0/2198	0.64	3/2979 (0.1%)
2	S	0.33	0/2206	0.56	1/2989 (0.0%)
2	a	0.34	0/2202	0.67	4/2984 (0.1%)
2	b	0.36	0/2202	0.66	7/2984 (0.2%)
2	i	0.34	0/2198	0.74	7/2979 (0.2%)
2	j	0.36	0/2198	0.75	8/2979 (0.3%)
2	k	0.33	0/2206	0.60	3/2989 (0.1%)
2	l	0.34	0/2206	0.56	0/2989
3	E	0.30	0/671	0.49	0/911
3	H	0.32	0/671	0.52	1/911 (0.1%)
3	I	0.35	0/655	0.50	0/889
3	J	0.29	0/648	0.51	0/882
3	K	0.32	0/655	0.59	0/889
3	L	0.28	0/655	0.51	0/889
3	Q	0.29	0/671	0.52	0/911
3	T	0.32	0/671	0.55	1/911 (0.1%)
3	U	0.35	0/655	0.52	0/889
3	V	0.31	0/648	0.64	0/882

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.29	0/655	0.52	0/889
3	X	0.28	0/655	0.51	0/889
3	g	0.30	0/671	0.51	0/911
3	h	0.30	0/671	0.52	0/911
3	m	0.31	0/671	0.49	0/911
3	n	0.32	0/671	0.56	1/911 (0.1%)
3	o	0.34	0/655	0.54	1/889 (0.1%)
3	p	0.33	0/655	0.56	1/889 (0.1%)
3	q	0.38	0/648	0.69	3/882 (0.3%)
3	r	0.39	0/648	0.68	2/882 (0.2%)
3	s	0.39	0/655	0.54	0/889
3	t	0.28	0/655	0.50	0/889
3	u	0.32	0/655	0.75	3/889 (0.3%)
3	v	0.31	0/655	0.66	1/889 (0.1%)
All	All	0.48	8/70384 (0.0%)	0.62	100/95104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
1	c	0	2
2	R	0	1
2	S	0	2
2	a	0	1
2	b	0	1
2	j	0	1
2	k	0	2
2	l	0	1
3	h	0	1
3	q	0	1
All	All	0	14

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	PHE	CE1-CZ	43.58	2.20	1.37
1	P	34	PHE	CD2-CE2	40.31	2.19	1.39
1	P	34	PHE	CE2-CZ	40.10	2.13	1.37
1	P	34	PHE	CD1-CE1	39.01	2.17	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	PHE	CG-CD2	26.22	1.78	1.38
1	P	34	PHE	CG-CD1	25.85	1.77	1.38
1	P	39	ARG	CD-NE	21.40	1.82	1.46
1	P	39	ARG	NE-CZ	13.60	1.50	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	39	ARG	CD-NE-CZ	21.85	154.19	123.60
1	P	39	ARG	NE-CZ-NH1	21.70	131.15	120.30
2	i	101	LYS	CB-CA-C	-17.52	75.36	110.40
2	R	101	LYS	CB-CA-C	-17.05	76.29	110.40
2	j	101	LYS	CB-CA-C	-15.27	79.86	110.40
1	Y	37	VAL	N-CA-C	-14.89	70.80	111.00
2	B	102	GLU	N-CA-C	-14.55	71.72	111.00
1	A	37	VAL	N-CA-C	-14.29	72.42	111.00
1	Z	37	VAL	N-CA-C	-14.05	73.08	111.00
2	B	101	LYS	N-CA-C	13.95	148.66	111.00
2	a	346	LYS	N-CA-C	-13.42	74.75	111.00
1	C	201	LEU	N-CA-C	-13.34	74.98	111.00
2	j	139	ALA	N-CA-CB	12.96	128.25	110.10
1	O	24	LYS	N-CA-C	11.80	142.85	111.00
2	a	346	LYS	CB-CA-C	11.11	132.62	110.40
1	P	308	SER	N-CA-CB	10.27	125.91	110.50
1	M	38	LEU	N-CA-C	-9.92	84.21	111.00
2	F	100	ILE	CB-CA-C	9.65	130.91	111.60
2	j	129	ILE	CB-CA-C	9.47	130.53	111.60
1	Y	38	LEU	N-CA-CB	-9.31	91.79	110.40
1	M	39	ARG	N-CA-CB	9.23	127.22	110.60
1	A	38	LEU	N-CA-CB	-9.20	92.01	110.40
3	r	92	PRO	CA-N-CD	-9.11	98.74	111.50
1	M	39	ARG	N-CA-C	-9.09	86.47	111.00
2	j	101	LYS	N-CA-C	8.99	135.27	111.00
2	i	126	PRO	CB-CA-C	-8.76	90.11	112.00
2	B	103	ALA	N-CA-CB	8.63	122.19	110.10
2	b	250	ALA	N-CA-CB	8.50	122.00	110.10
2	G	348	GLY	N-CA-C	-8.37	92.17	113.10
2	i	126	PRO	N-CA-C	8.20	133.42	112.10
2	k	346	LYS	CB-CA-C	-8.13	94.14	110.40
2	j	139	ALA	N-CA-C	-7.96	89.50	111.00
3	q	50	ARG	CA-CB-CG	7.96	130.91	113.40
1	Z	38	LEU	N-CA-CB	-7.91	94.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	LEU	CB-CA-C	7.88	125.18	110.20
2	j	138	GLU	N-CA-C	-7.87	89.76	111.00
2	B	102	GLU	N-CA-CB	-7.79	96.58	110.60
1	P	39	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	b	320	GLU	CB-CA-C	-7.23	95.95	110.40
2	k	346	LYS	N-CA-C	7.22	130.50	111.00
1	P	39	ARG	CG-CD-NE	7.04	126.59	111.80
2	R	101	LYS	N-CA-C	7.00	129.89	111.00
1	O	25	GLU	N-CA-CB	6.95	123.10	110.60
2	F	129	ILE	N-CA-C	-6.93	92.28	111.00
2	S	346	LYS	CB-CA-C	-6.89	96.62	110.40
1	P	308	SER	N-CA-C	-6.80	92.63	111.00
2	B	101	LYS	CB-CA-C	-6.77	96.87	110.40
2	b	249	ALA	CB-CA-C	-6.67	100.09	110.10
1	P	39	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
1	f	57	PRO	CA-N-CD	-6.46	102.45	111.50
2	k	347	GLY	N-CA-C	6.46	129.24	113.10
2	i	101	LYS	N-CA-C	6.45	128.41	111.00
2	i	128	PHE	N-CA-C	-6.26	94.10	111.00
3	u	99	LEU	N-CA-C	6.26	127.90	111.00
1	f	308	SER	N-CA-CB	6.23	119.85	110.50
2	G	349	ASN	N-CA-C	-6.22	94.22	111.00
2	a	318	ALA	N-CA-CB	6.13	118.68	110.10
3	n	53	GLY	N-CA-C	-6.01	98.07	113.10
3	q	50	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	q	50	ARG	CD-NE-CZ	5.92	131.89	123.60
2	B	103	ALA	N-CA-C	-5.89	95.09	111.00
2	j	102	GLU	N-CA-C	5.88	126.86	111.00
3	u	54	ARG	CA-CB-CG	5.85	126.27	113.40
2	j	129	ILE	N-CA-C	-5.82	95.28	111.00
3	r	92	PRO	N-CD-CG	-5.82	94.48	103.20
2	i	323	ARG	CB-CA-C	-5.78	98.85	110.40
1	P	34	PHE	CB-CG-CD2	-5.75	116.78	120.80
3	u	98	LEU	CB-CA-C	5.69	121.01	110.20
1	Y	291	PRO	N-CA-CB	5.67	110.10	103.30
2	i	129	ILE	N-CA-C	-5.67	95.70	111.00
1	Z	291	PRO	N-CA-CB	5.66	110.09	103.30
1	M	291	PRO	N-CA-CB	5.65	110.08	103.30
2	a	317	ALA	CB-CA-C	-5.65	101.63	110.10
1	P	34	PHE	CD1-CG-CD2	5.62	125.60	118.30
3	H	53	GLY	N-CA-C	-5.59	99.13	113.10
2	b	321	ILE	N-CA-C	-5.58	95.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	PRO	N-CA-CB	5.57	109.99	103.30
2	G	349	ASN	N-CA-CB	-5.54	100.62	110.60
1	P	307	PHE	N-CA-C	-5.53	96.08	111.00
3	o	99	LEU	CA-CB-CG	5.46	127.87	115.30
2	b	320	GLU	O-C-N	-5.43	114.01	122.70
1	C	291	PRO	N-CA-CB	5.42	109.80	103.30
3	p	47	ARG	CB-CG-CD	5.40	125.65	111.60
1	c	291	PRO	N-CA-CB	5.39	109.77	103.30
1	O	291	PRO	N-CA-CB	5.39	109.77	103.30
2	N	318	ALA	N-CA-CB	5.38	117.63	110.10
1	e	291	PRO	N-CA-CB	5.37	109.75	103.30
1	f	291	PRO	N-CA-CB	5.36	109.73	103.30
1	D	291	PRO	N-CA-CB	5.36	109.73	103.30
1	P	291	PRO	N-CA-CB	5.33	109.70	103.30
1	d	291	PRO	N-CA-CB	5.32	109.69	103.30
2	F	128	PHE	N-CA-C	-5.31	96.67	111.00
3	v	47	ARG	CB-CG-CD	5.29	125.36	111.60
2	R	102	GLU	N-CA-C	5.25	125.17	111.00
3	T	53	GLY	N-CA-C	-5.15	100.24	113.10
1	Z	231	ARG	CB-CG-CD	-5.13	98.26	111.60
2	b	209	ARG	N-CA-CB	-5.08	101.45	110.60
1	A	296	PHE	CB-CA-C	-5.08	100.25	110.40
2	b	320	GLU	N-CA-C	5.04	124.60	111.00
1	P	39	ARG	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	40	ASP	Peptide
2	R	137	VAL	Peptide
2	S	134	PRO	Peptide
2	S	135	VAL	Peptide
2	a	240	ALA	Peptide
2	b	320	GLU	Mainchain
1	c	39	ARG	Peptide
1	c	40	ASP	Peptide
3	h	91	GLU	Peptide
2	j	243	PRO	Peptide
2	k	134	PRO	Peptide
2	k	135	VAL	Peptide
2	l	134	PRO	Peptide

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Mol	Chain	Res	Type	Group
3	q	57	ASN	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	289/334 (86%)	260 (90%)	29 (10%)	0	100	100
1	C	283/334 (85%)	264 (93%)	19 (7%)	0	100	100
1	D	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	M	289/334 (86%)	262 (91%)	27 (9%)	0	100	100
1	O	283/334 (85%)	259 (92%)	24 (8%)	0	100	100
1	P	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	Y	289/334 (86%)	266 (92%)	23 (8%)	0	100	100
1	Z	289/334 (86%)	262 (91%)	27 (9%)	0	100	100
1	c	283/334 (85%)	266 (94%)	17 (6%)	0	100	100
1	d	283/334 (85%)	268 (95%)	15 (5%)	0	100	100
1	e	286/334 (86%)	263 (92%)	23 (8%)	0	100	100
1	f	286/334 (86%)	259 (91%)	27 (9%)	0	100	100
2	B	273/419 (65%)	251 (92%)	22 (8%)	0	100	100
2	F	273/419 (65%)	246 (90%)	27 (10%)	0	100	100
2	G	273/419 (65%)	257 (94%)	16 (6%)	0	100	100
2	N	273/419 (65%)	254 (93%)	19 (7%)	0	100	100
2	R	273/419 (65%)	245 (90%)	28 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	273/419 (65%)	252 (92%)	21 (8%)	0	100	100
2	a	273/419 (65%)	254 (93%)	18 (7%)	1 (0%)	34	71
2	b	273/419 (65%)	256 (94%)	17 (6%)	0	100	100
2	i	273/419 (65%)	243 (89%)	30 (11%)	0	100	100
2	j	273/419 (65%)	245 (90%)	28 (10%)	0	100	100
2	k	273/419 (65%)	254 (93%)	19 (7%)	0	100	100
2	l	273/419 (65%)	256 (94%)	17 (6%)	0	100	100
3	E	79/644 (12%)	72 (91%)	7 (9%)	0	100	100
3	H	79/644 (12%)	71 (90%)	8 (10%)	0	100	100
3	I	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	J	76/644 (12%)	69 (91%)	7 (9%)	0	100	100
3	K	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	L	77/644 (12%)	73 (95%)	4 (5%)	0	100	100
3	Q	79/644 (12%)	74 (94%)	5 (6%)	0	100	100
3	T	79/644 (12%)	73 (92%)	6 (8%)	0	100	100
3	U	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	V	76/644 (12%)	69 (91%)	7 (9%)	0	100	100
3	W	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	X	77/644 (12%)	73 (95%)	4 (5%)	0	100	100
3	g	79/644 (12%)	73 (92%)	6 (8%)	0	100	100
3	h	79/644 (12%)	72 (91%)	7 (9%)	0	100	100
3	m	79/644 (12%)	72 (91%)	7 (9%)	0	100	100
3	n	79/644 (12%)	71 (90%)	8 (10%)	0	100	100
3	o	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	p	77/644 (12%)	72 (94%)	5 (6%)	0	100	100
3	q	76/644 (12%)	70 (92%)	6 (8%)	0	100	100
3	r	76/644 (12%)	70 (92%)	6 (8%)	0	100	100
3	s	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	t	77/644 (12%)	70 (91%)	7 (9%)	0	100	100
3	u	77/644 (12%)	71 (92%)	6 (8%)	0	100	100
3	v	77/644 (12%)	69 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8568/24492 (35%)	7876 (92%)	691 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	319	PRO

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	A	248/283 (88%)	247 (100%)	1 (0%)	91	94
1	C	241/283 (85%)	236 (98%)	5 (2%)	53	72
1	D	244/283 (86%)	242 (99%)	2 (1%)	81	89
1	M	248/283 (88%)	242 (98%)	6 (2%)	49	69
1	O	241/283 (85%)	237 (98%)	4 (2%)	60	78
1	P	244/283 (86%)	242 (99%)	2 (1%)	81	89
1	Y	248/283 (88%)	246 (99%)	2 (1%)	81	89
1	Z	248/283 (88%)	247 (100%)	1 (0%)	91	94
1	c	241/283 (85%)	236 (98%)	5 (2%)	53	72
1	d	241/283 (85%)	234 (97%)	7 (3%)	42	65
1	e	244/283 (86%)	241 (99%)	3 (1%)	71	84
1	f	244/283 (86%)	239 (98%)	5 (2%)	55	73
2	B	228/336 (68%)	221 (97%)	7 (3%)	40	63
2	F	227/336 (68%)	221 (97%)	6 (3%)	46	67
2	G	229/336 (68%)	225 (98%)	4 (2%)	60	78
2	N	228/336 (68%)	221 (97%)	7 (3%)	40	63
2	R	227/336 (68%)	218 (96%)	9 (4%)	31	57
2	S	229/336 (68%)	220 (96%)	9 (4%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	228/336 (68%)	220 (96%)	8 (4%)	36	61
2	b	228/336 (68%)	218 (96%)	10 (4%)	28	55
2	i	227/336 (68%)	222 (98%)	5 (2%)	52	71
2	j	227/336 (68%)	223 (98%)	4 (2%)	59	77
2	k	229/336 (68%)	222 (97%)	7 (3%)	40	63
2	l	229/336 (68%)	224 (98%)	5 (2%)	52	71
3	E	76/527 (14%)	76 (100%)	0	100	100
3	H	76/527 (14%)	76 (100%)	0	100	100
3	I	74/527 (14%)	70 (95%)	4 (5%)	22	50
3	J	74/527 (14%)	73 (99%)	1 (1%)	67	81
3	K	74/527 (14%)	74 (100%)	0	100	100
3	L	74/527 (14%)	74 (100%)	0	100	100
3	Q	76/527 (14%)	76 (100%)	0	100	100
3	T	76/527 (14%)	76 (100%)	0	100	100
3	U	74/527 (14%)	72 (97%)	2 (3%)	44	66
3	V	74/527 (14%)	73 (99%)	1 (1%)	67	81
3	W	74/527 (14%)	74 (100%)	0	100	100
3	X	74/527 (14%)	74 (100%)	0	100	100
3	g	76/527 (14%)	76 (100%)	0	100	100
3	h	76/527 (14%)	76 (100%)	0	100	100
3	m	76/527 (14%)	76 (100%)	0	100	100
3	n	76/527 (14%)	76 (100%)	0	100	100
3	o	74/527 (14%)	72 (97%)	2 (3%)	44	66
3	p	74/527 (14%)	74 (100%)	0	100	100
3	q	74/527 (14%)	73 (99%)	1 (1%)	67	81
3	r	74/527 (14%)	72 (97%)	2 (3%)	44	66
3	s	74/527 (14%)	74 (100%)	0	100	100
3	t	74/527 (14%)	74 (100%)	0	100	100
3	u	74/527 (14%)	71 (96%)	3 (4%)	30	57
3	v	74/527 (14%)	73 (99%)	1 (1%)	67	81
All	All	7460/20076 (37%)	7319 (98%)	141 (2%)	59	75

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
2	B	101	LYS
2	B	320	GLU
2	B	322	THR
2	B	323	ARG
2	B	346	LYS
2	B	350	LEU
2	B	351	MET
1	C	22	VAL
1	C	24	LYS
1	C	25	GLU
1	C	55	LYS
1	C	133	ARG
1	D	43	ASN
1	D	324	ARG
2	F	151	THR
2	F	153	ASP
2	F	154	GLU
2	F	346	LYS
2	F	350	LEU
2	F	351	MET
2	G	242	ARG
2	G	346	LYS
2	G	350	LEU
2	G	351	MET
3	I	47	ARG
3	I	50	ARG
3	I	61	LYS
3	I	87	LYS
3	J	50	ARG
1	Y	25	GLU
1	Y	243	GLN
2	a	101	LYS
2	a	105	ARG
2	a	320	GLU
2	a	321	ILE
2	a	322	THR
2	a	346	LYS
2	a	349	ASN
2	a	350	LEU
1	c	24	LYS
1	c	25	GLU

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Mol	Chain	Res	Type
1	c	27	GLU
1	c	55	LYS
1	c	111	ASP
1	e	55	LYS
1	e	120	LYS
1	e	281	LYS
2	i	102	GLU
2	i	127	THR
2	i	346	LYS
2	i	349	ASN
2	i	350	LEU
2	k	125	LYS
2	k	133	LYS
2	k	242	ARG
2	k	346	LYS
2	k	349	ASN
2	k	350	LEU
2	k	351	MET
3	o	94	GLU
3	o	95	GLU
3	q	50	ARG
3	u	30	ARG
3	u	50	ARG
3	u	99	LEU
1	Z	39	ARG
2	b	101	LYS
2	b	123	ASN
2	b	237	ASN
2	b	238	PHE
2	b	242	ARG
2	b	321	ILE
2	b	345	ASP
2	b	346	LYS
2	b	350	LEU
2	b	351	MET
1	d	24	LYS
1	d	25	GLU
1	d	27	GLU
1	d	55	LYS
1	d	107	THR
1	d	111	ASP
1	d	112	ILE

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Mol	Chain	Res	Type
1	f	33	ARG
1	f	55	LYS
1	f	126	ARG
1	f	281	LYS
1	f	310	ASN
2	j	127	THR
2	j	346	LYS
2	j	350	LEU
2	j	352	VAL
2	l	242	ARG
2	l	346	LYS
2	l	350	LEU
2	l	351	MET
2	l	352	VAL
3	r	47	ARG
3	r	54	ARG
3	v	50	ARG
1	M	24	LYS
1	M	37	VAL
1	M	39	ARG
1	M	40	ASP
1	M	41	ASP
1	M	133	ARG
2	N	101	LYS
2	N	320	GLU
2	N	321	ILE
2	N	323	ARG
2	N	345	ASP
2	N	349	ASN
2	N	350	LEU
1	O	24	LYS
1	O	25	GLU
1	O	27	GLU
1	O	55	LYS
1	P	281	LYS
1	P	308	SER
2	R	125	LYS
2	R	127	THR
2	R	128	PHE
2	R	129	ILE
2	R	130	ASP
2	R	346	LYS

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Mol	Chain	Res	Type
2	R	349	ASN
2	R	350	LEU
2	R	351	MET
2	S	125	LYS
2	S	225	ARG
2	S	242	ARG
2	S	345	ASP
2	S	346	LYS
2	S	349	ASN
2	S	350	LEU
2	S	351	MET
2	S	352	VAL
3	U	91	GLU
3	U	94	GLU
3	V	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	C	238	HIS
1	D	43	ASN
2	F	155	ASN
2	F	169	ASN
2	F	260	ASN
2	G	162	ASN
2	G	349	ASN
3	H	52	ASN
3	J	52	ASN
2	a	349	ASN
1	e	212	GLN
2	k	162	ASN
1	d	238	HIS
1	f	212	GLN
2	j	169	ASN
2	j	237	ASN
2	l	162	ASN
3	r	45	GLN
1	O	238	HIS
1	P	53	HIS
1	P	212	GLN
2	R	123	ASN

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Mol	Chain	Res	Type
2	S	162	ASN

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 monosaccharides 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.

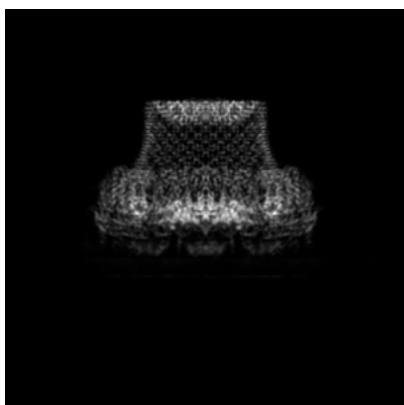
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32520. These allow visual inspection of the internal detail of the map and identification of artifacts.

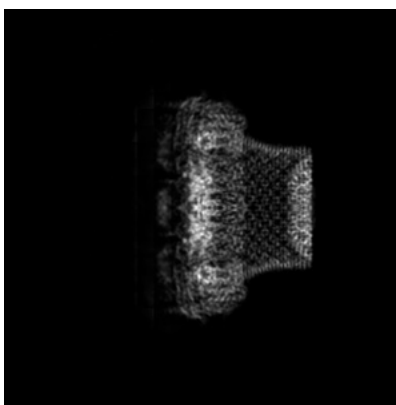
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

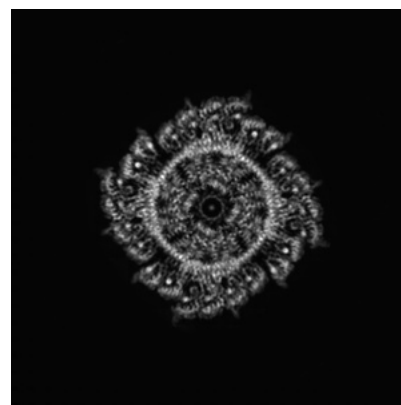
6.1.1 Primary map



X



Y

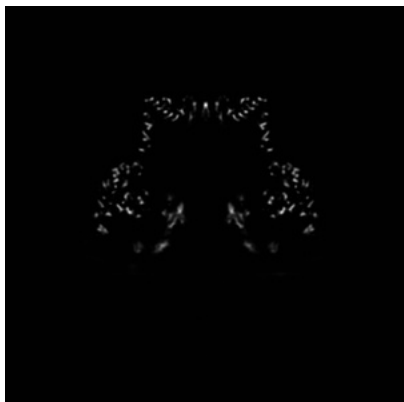


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

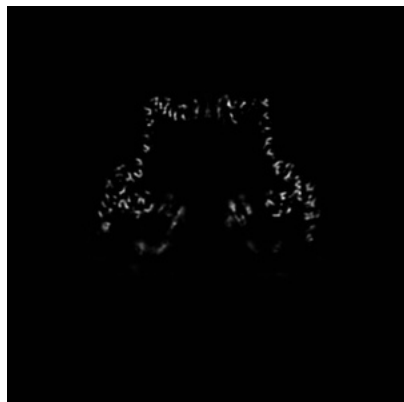


Z Index: 140

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: 142



Y Index: 142



Z Index: 139

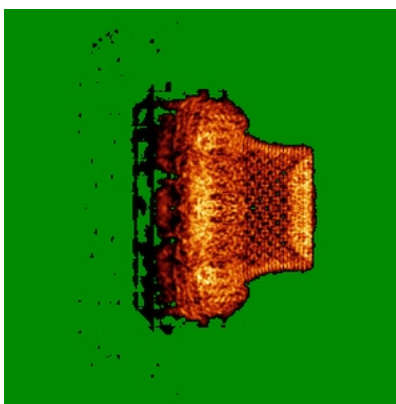
The images above show the largest variance slices of the map in three orthogonal directions.

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

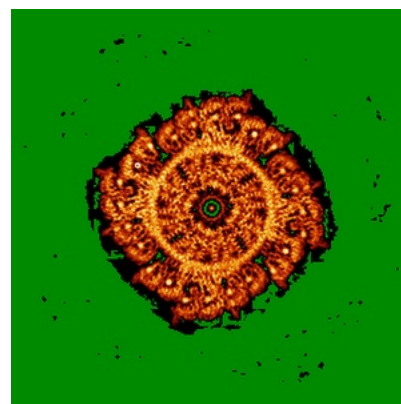
6.4.1 Primary map



X



Y

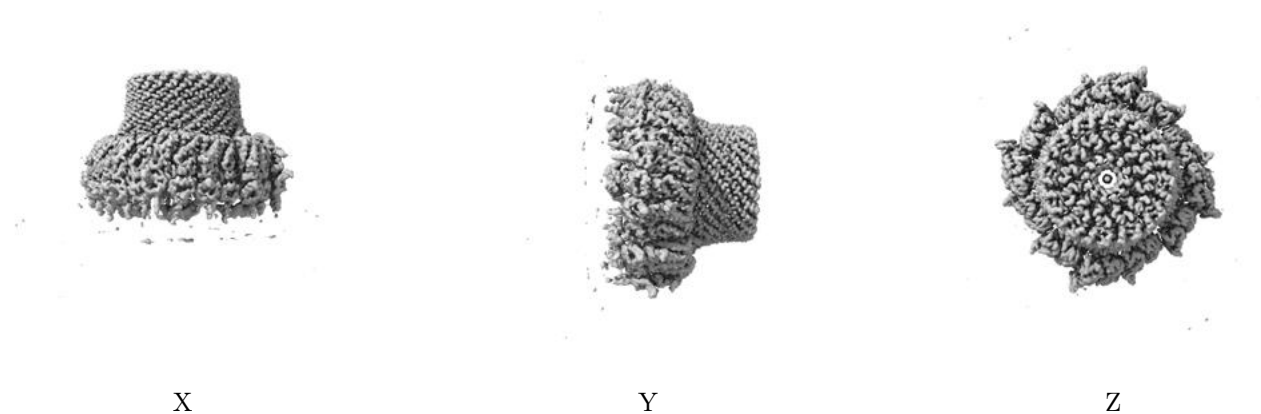


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

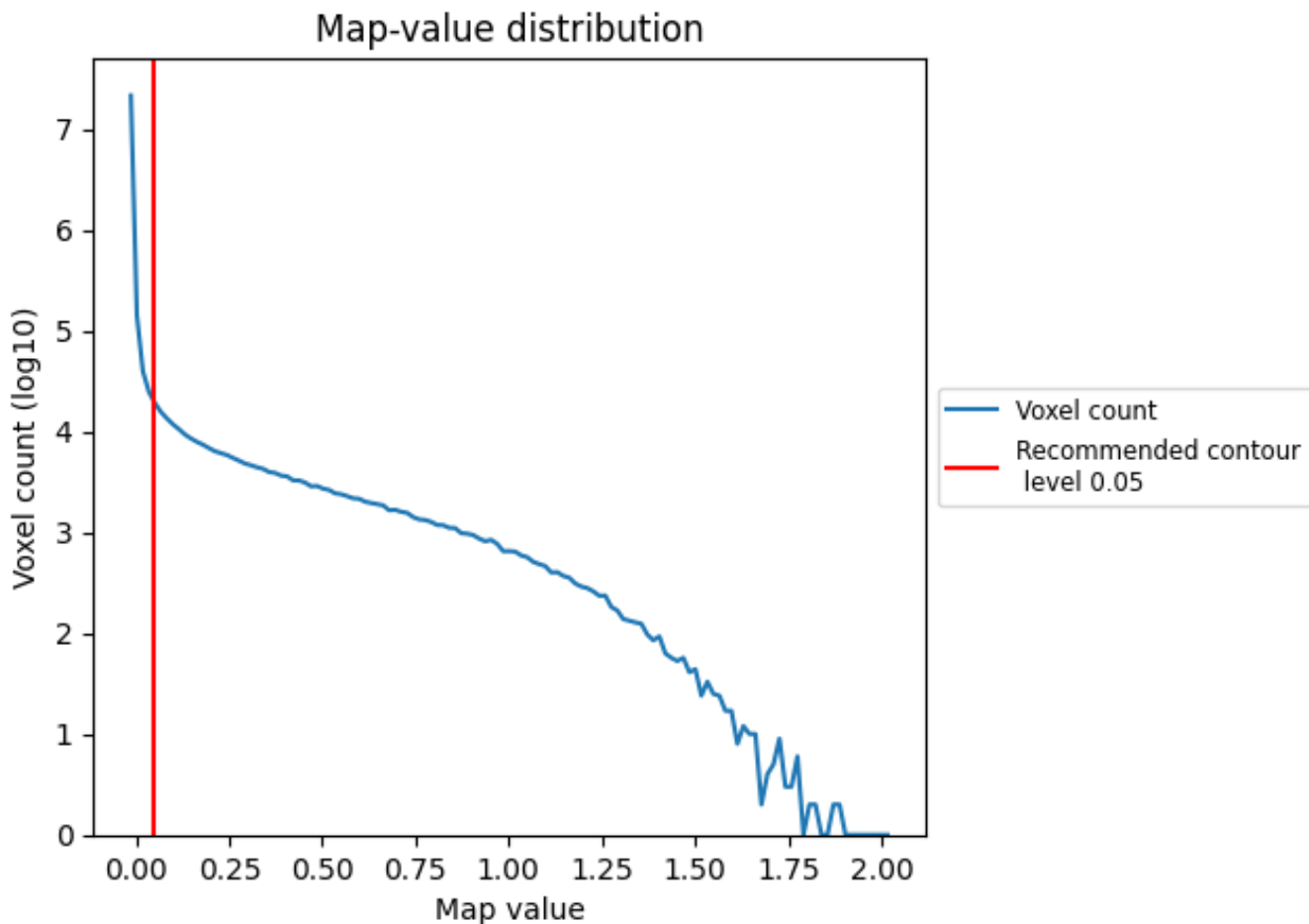
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

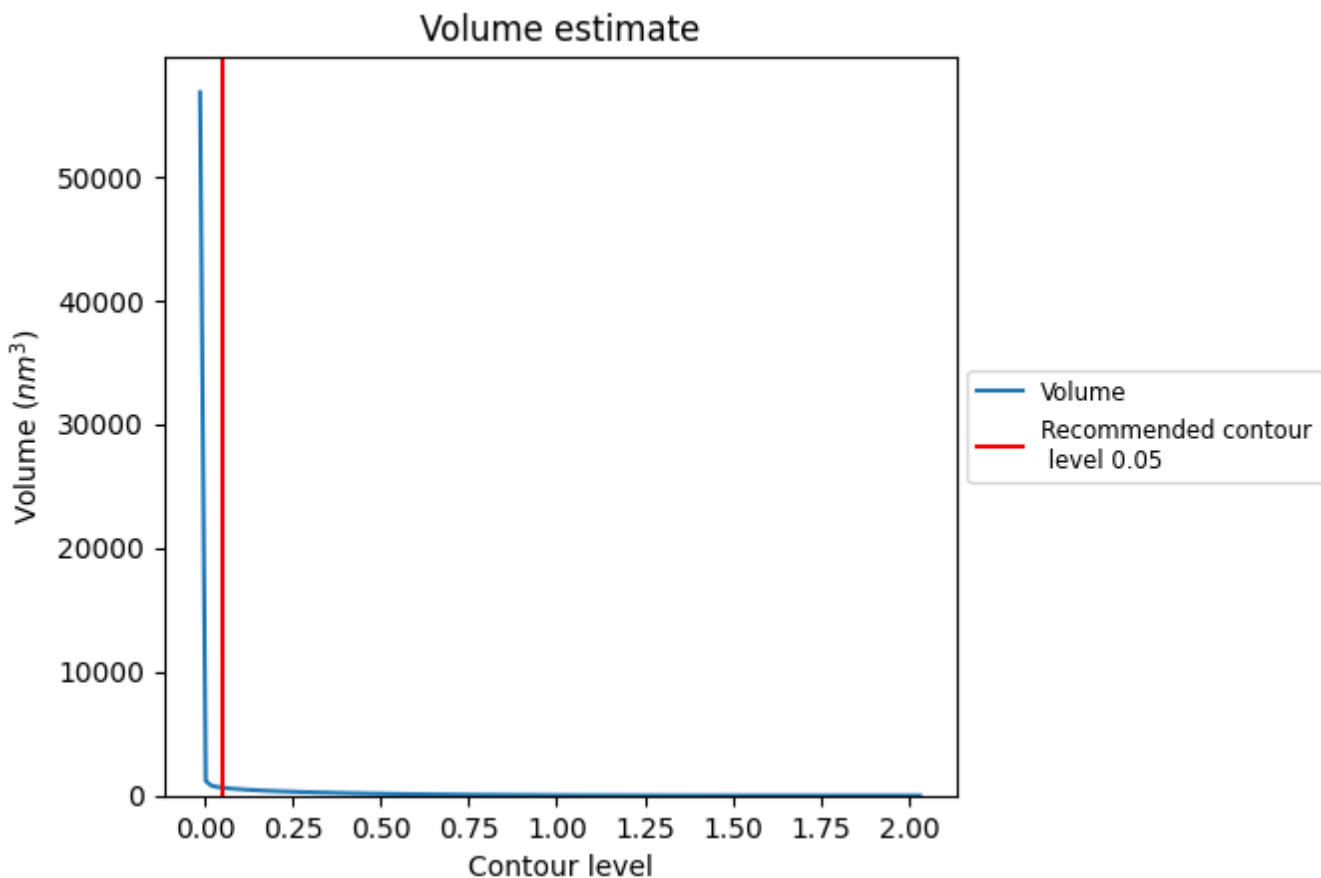
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

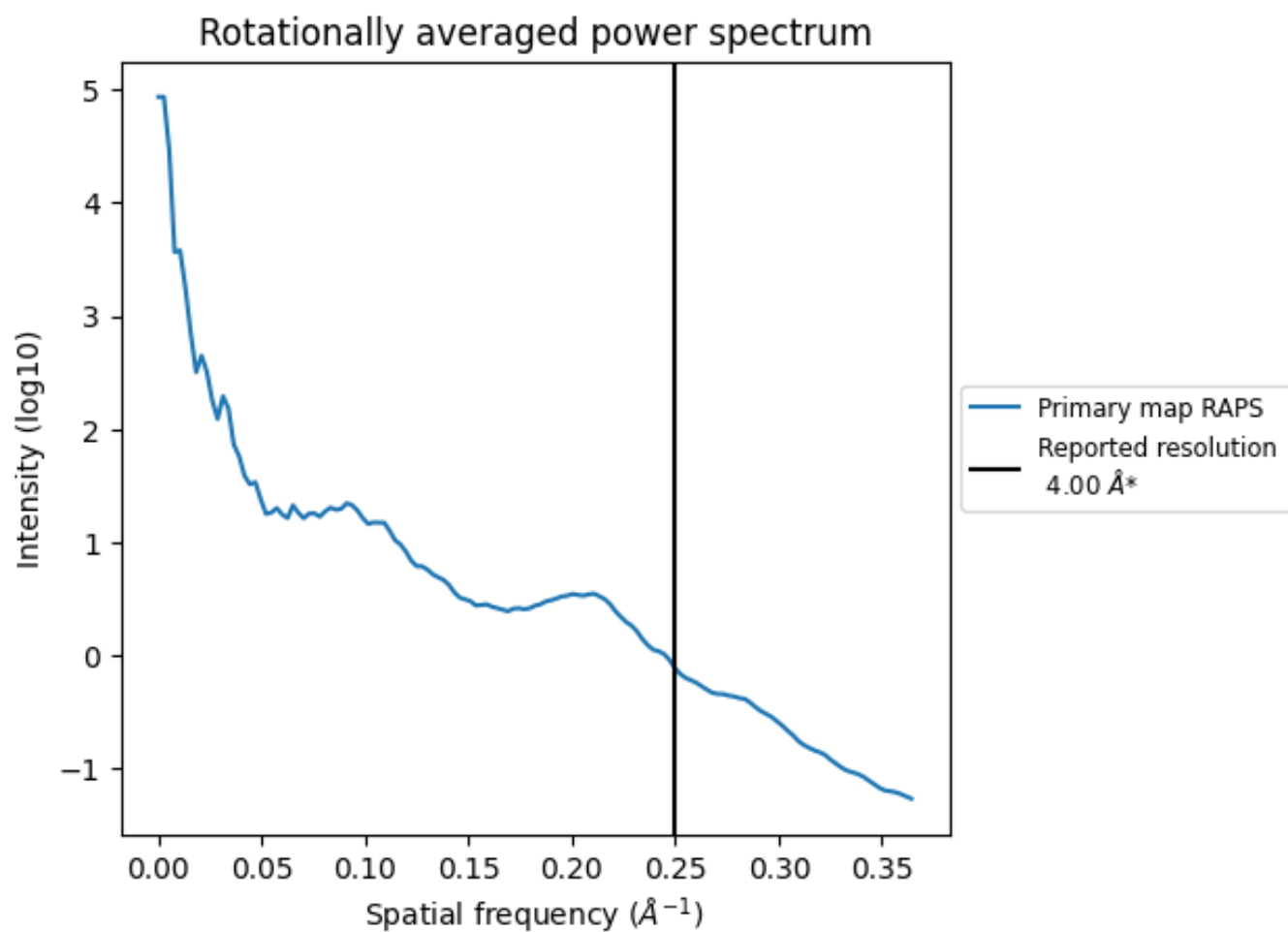
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 577 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 0.250 Å⁻¹

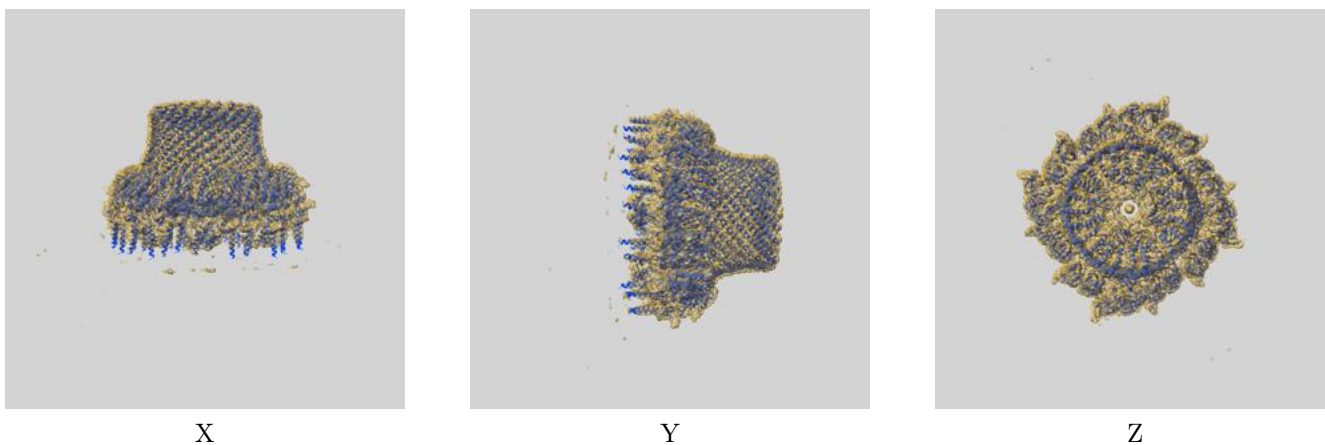
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

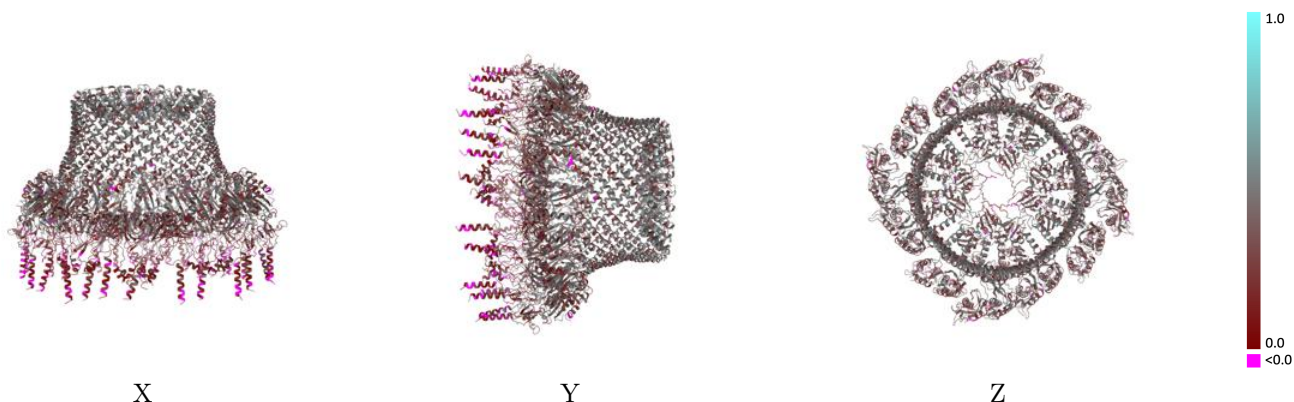
This section contains information regarding the fit between EMDB map EMD-32520 and PDB model 7WI3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



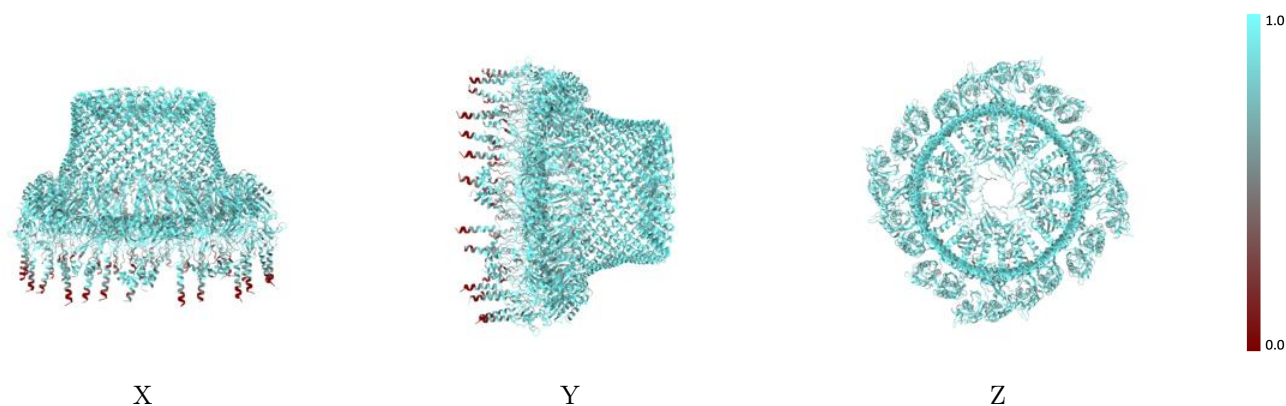
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



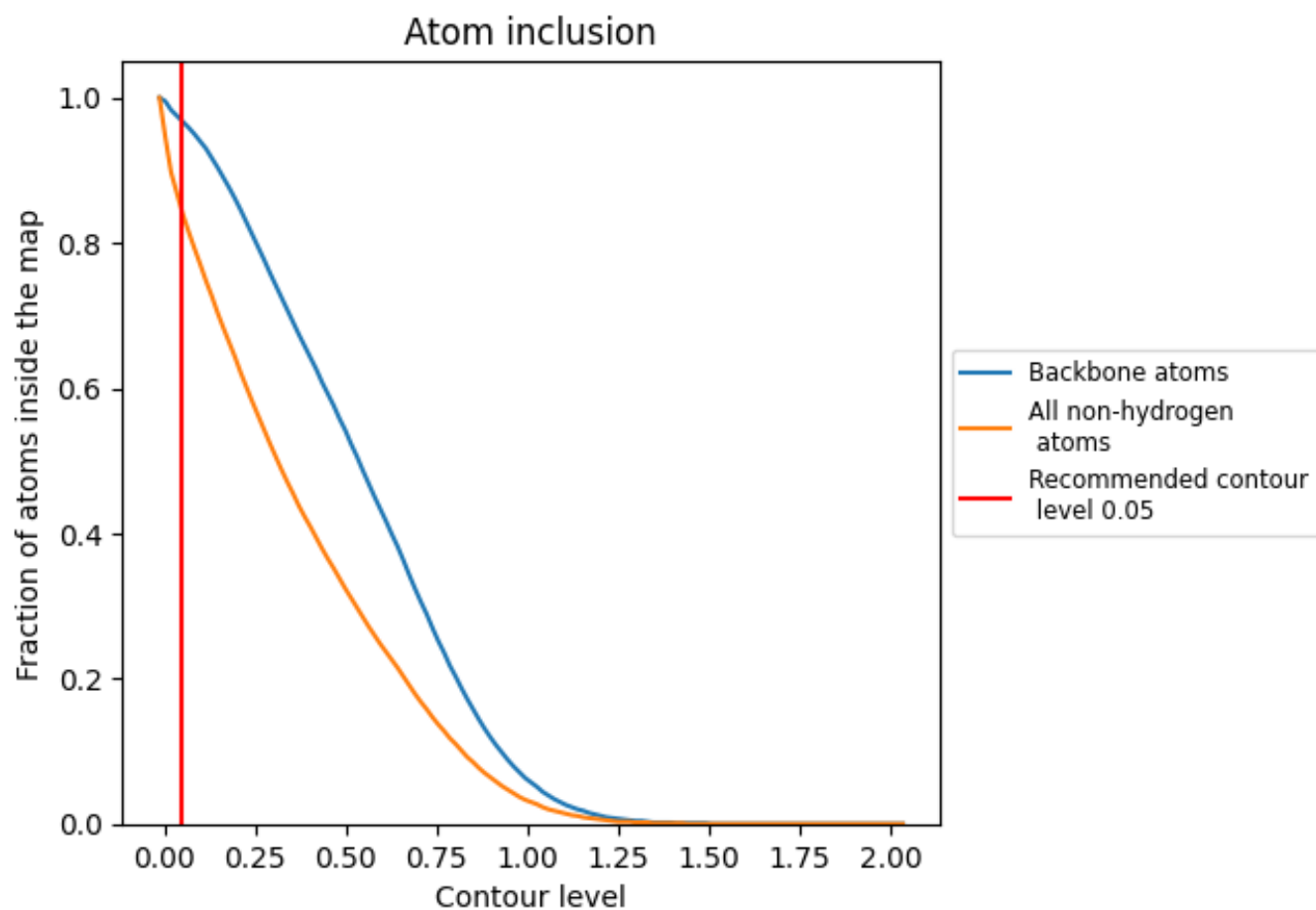
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.3350
A	 0.8590	 0.3640
B	 0.8360	 0.3420
C	 0.8300	 0.3410
D	 0.8280	 0.3310
E	 0.8250	 0.3270
F	 0.8700	 0.3760
G	 0.8430	 0.3500
H	 0.8370	 0.3540
I	 0.7900	 0.2600
J	 0.8520	 0.2250
K	 0.8300	 0.2860
L	 0.8630	 0.2260
M	 0.8580	 0.3600
N	 0.8540	 0.3470
O	 0.8360	 0.3410
P	 0.8270	 0.3310
Q	 0.8350	 0.3350
R	 0.8630	 0.3740
S	 0.8430	 0.3550
T	 0.8560	 0.3560
U	 0.7810	 0.2560
V	 0.8280	 0.2120
W	 0.8090	 0.2850
X	 0.8460	 0.2160
Y	 0.8540	 0.3620
Z	 0.8650	 0.3670
a	 0.8470	 0.3500
b	 0.8340	 0.3440
c	 0.8290	 0.3410
d	 0.8450	 0.3430
e	 0.8260	 0.3330
f	 0.8340	 0.3270
g	 0.8060	 0.3250
h	 0.8400	 0.3340



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Chain	Atom inclusion	Q-score
i	 0.8490	 0.3630
j	 0.8720	 0.3760
k	 0.8340	 0.3530
l	 0.8590	 0.3560
m	 0.8340	 0.3520
n	 0.8350	 0.3520
o	 0.8030	 0.2460
p	 0.7650	 0.2430
q	 0.8590	 0.2260
r	 0.8460	 0.2320
s	 0.8120	 0.2820
t	 0.8410	 0.2750
u	 0.8430	 0.2150
v	 0.8570	 0.2320