



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:45 AM UTC

PDB ID : 9IUE / pdb_00009iue
EMDB ID : EMD-60898
Title : cryo-EM structure of FtsE/X and ZipA complex in filament
Authors : Zhu, K.F.; Li, J.W.; Luo, M.
Deposited on : 2024-07-20
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

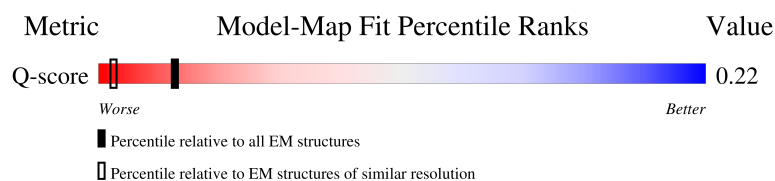
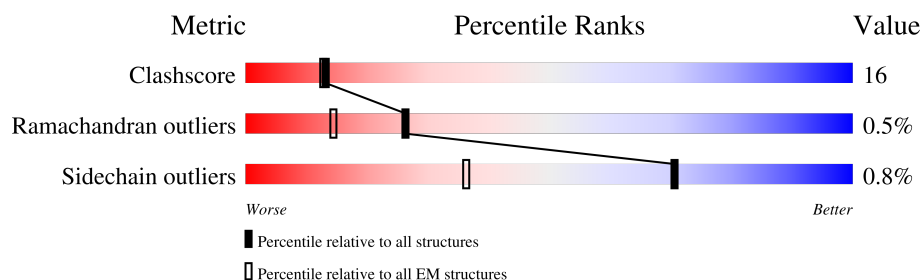
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



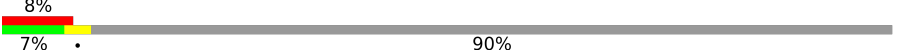
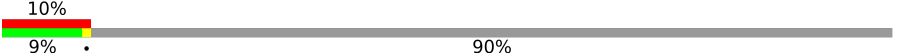
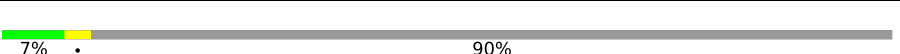
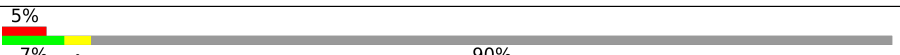
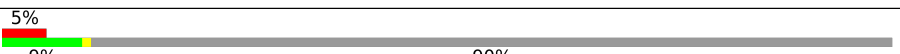
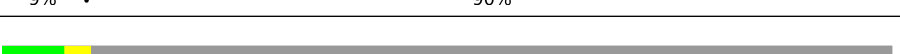
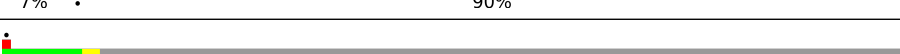
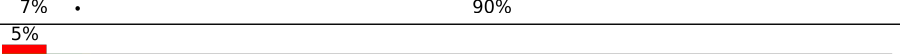
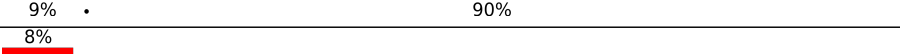
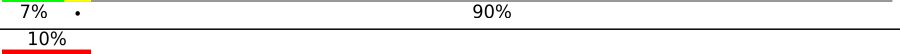
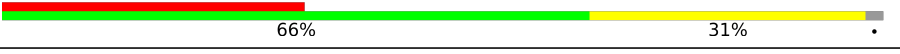
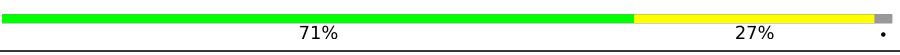
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1	328	6% . 90%
1	2	328	9% . 90%
1	E	328	5% 7% . 90%
1	F	328	5% 9% . 90%

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Mol	Chain	Length	Quality of chain
1	K	328	
1	L	328	
1	Q	328	
1	R	328	
1	W	328	
1	X	328	
1	c	328	
1	d	328	
1	i	328	
1	j	328	
1	o	328	
1	p	328	
1	u	328	
1	v	328	
2	5	226	
2	6	226	
2	G	226	
2	H	226	
2	M	226	
2	N	226	
2	S	226	
2	T	226	
2	Y	226	
2	Z	226	
2	e	226	

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Mol	Chain	Length	Quality of chain
2	f	226	
2	k	226	
2	l	226	
2	q	226	
2	r	226	
2	w	226	
2	x	226	
3	A	352	
3	B	352	
3	C	352	
3	D	352	
3	I	352	
3	J	352	
3	O	352	
3	P	352	
3	U	352	
3	V	352	
3	a	352	
3	b	352	
3	g	352	
3	h	352	
3	m	352	
3	n	352	
3	s	352	
3	t	352	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 75492 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 Cell division protein ZipA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	2	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	E	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	F	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	K	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	L	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	Q	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	R	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	W	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	X	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	c	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	d	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	i	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	j	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	o	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	p	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	u	33	Total	C	N	O	S	0	0
			263	175	46	41	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	33	Total	C	N	O	S	0	0
			263	175	46	41	1		

- Molecule 2 is a protein called Cell division ATP-binding protein FtsE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	6	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	G	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	H	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	M	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	N	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	S	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	T	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	Y	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	Z	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	e	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	f	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	k	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	l	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	q	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	r	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	w	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	x	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	-3	SER	-	expression tag	UNP W1F1D8
5	0	VAL	THR	conflict	UNP W1F1D8
6	-3	SER	-	expression tag	UNP W1F1D8
6	0	VAL	THR	conflict	UNP W1F1D8
G	-3	SER	-	expression tag	UNP W1F1D8
G	0	VAL	THR	conflict	UNP W1F1D8
H	-3	SER	-	expression tag	UNP W1F1D8
H	0	VAL	THR	conflict	UNP W1F1D8
M	-3	SER	-	expression tag	UNP W1F1D8
M	0	VAL	THR	conflict	UNP W1F1D8
N	-3	SER	-	expression tag	UNP W1F1D8
N	0	VAL	THR	conflict	UNP W1F1D8
S	-3	SER	-	expression tag	UNP W1F1D8
S	0	VAL	THR	conflict	UNP W1F1D8
T	-3	SER	-	expression tag	UNP W1F1D8
T	0	VAL	THR	conflict	UNP W1F1D8
Y	-3	SER	-	expression tag	UNP W1F1D8
Y	0	VAL	THR	conflict	UNP W1F1D8
Z	-3	SER	-	expression tag	UNP W1F1D8
Z	0	VAL	THR	conflict	UNP W1F1D8
e	-3	SER	-	expression tag	UNP W1F1D8
e	0	VAL	THR	conflict	UNP W1F1D8
f	-3	SER	-	expression tag	UNP W1F1D8
f	0	VAL	THR	conflict	UNP W1F1D8
k	-3	SER	-	expression tag	UNP W1F1D8
k	0	VAL	THR	conflict	UNP W1F1D8
l	-3	SER	-	expression tag	UNP W1F1D8
l	0	VAL	THR	conflict	UNP W1F1D8
q	-3	SER	-	expression tag	UNP W1F1D8
q	0	VAL	THR	conflict	UNP W1F1D8
r	-3	SER	-	expression tag	UNP W1F1D8
r	0	VAL	THR	conflict	UNP W1F1D8
w	-3	SER	-	expression tag	UNP W1F1D8
w	0	VAL	THR	conflict	UNP W1F1D8
x	-3	SER	-	expression tag	UNP W1F1D8
x	0	VAL	THR	conflict	UNP W1F1D8

- Molecule 3 is a protein called Cell division protein FtsX.

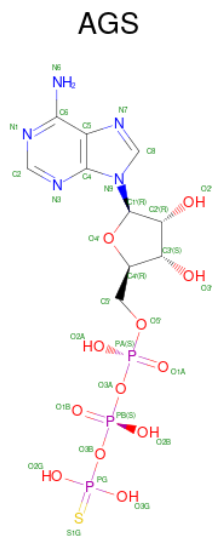
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	C	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	D	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	I	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	J	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	O	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	P	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	U	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	V	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	a	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	b	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	g	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	h	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	m	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	n	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	s	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	t	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



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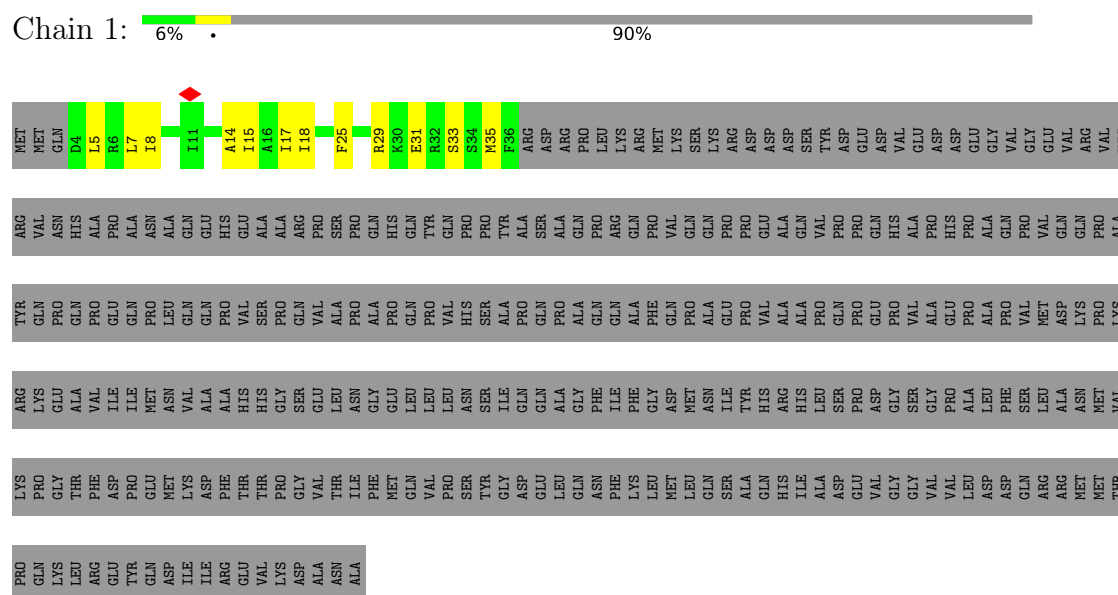
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Mol	Chain	Residues	Atoms						AltConf
4	q	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	r	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	w	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	x	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

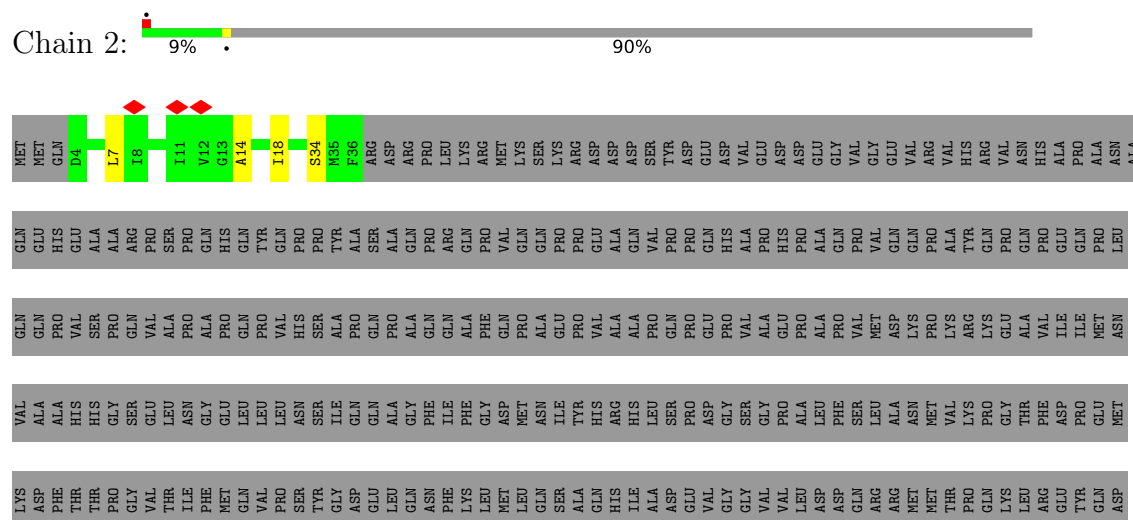
3 Residue-property plots [i](#)

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: Cell division protein ZipA



• Molecule 1: Cell division protein ZipA





- Molecule 1: Cell division protein ZipA

[illegible]

- Molecule 1: Cell division protein ZipA

[illegible]

- Molecule 1: Cell division protein ZipA

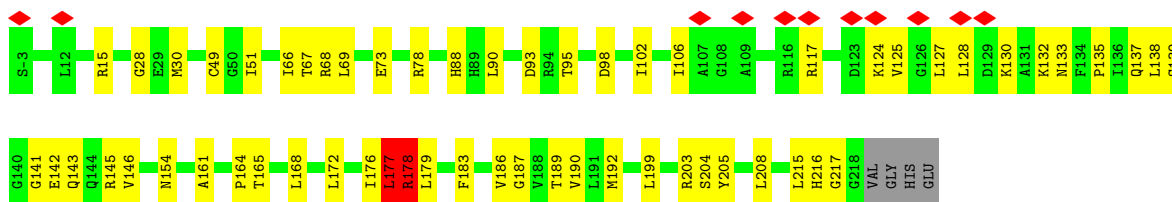


LYS	GLY	GLU	PRO	ASN	MET
LEU	THR	ALA	GLN	HIS	MET
ARG	PHE	VAL	PRO	ALA	GLN
GLU	ASP	ILE	GLU	PRO	D4
TYR	GLU	MET	PRO	ALA	
GLN	MET	ASN	LEU	ASN	T8
ASP	GLN	VAL	GLN	ALA	L9
ILE	ASP	ALA	GLN	GLU	I10
ARG	PHE	ALA	PRO	HIS	I11
GLU	THR	HIS	VAL	GLU	V12
VAL	THR	HIS	SER	ALA	G13
LYS	PRO	GLY	PRO	ALA	
ASP	GLY	SER	GLN	ARG	A14
ALA	VAL	GLU	VAL	PRO	I15
ASN	THR	LEU	ALA	SER	A16
ALA	ILE	ASN	PRO	PRO	I17
	PHE	GLY	ALA	GLN	
	MET	GLU	PRO	HIS	I18
	GLN	LEU	GLN	GLN	A19
	VAL	LEU	PRO	TYR	L20
	PRO	LEU	VAL	GLN	L21
	SER	ASN	HIS	PRO	
	TYR	SER	SER	PRO	R32
	GLY	ILE	ALA	TYR	S33
	ASP	GLN	PRO	ALA	
	GLU	GLN	GLN	SER	S34
	LEU	ALA	PRO	ALA	H35
	ASN	GLY	ALA	GLN	F36
	GLN	PHE	GLN	ARG	ARG
	PHE	ILE	ALA	GLN	ASP
	LYS	GLY	PHE	PRO	ARG
	LEU	GLY	GLN	VAL	PRO
	MET	ASP	GLN	PRO	LEU
	LEU	MET	PRO	GLN	LYS
	GLN	ASN	ALA	GLN	ARG
	ASN	GLY	ALA	ALA	MET
	GLN	THR	VAL	GLU	LYS
	ILE	HIS	ARG	ALA	SER
	ALA	LEU	PRO	VAL	LYS
	ASP	LEU	PRO	VAL	ARG
	VAL	ASP	PRO	GLN	ASP
	GLY	GLY	GLU	GLN	ASP
	GLY	SER	VAL	HIS	SER
	VAL	GLY	ALA	ALA	TYR
	VAL	PRO	GLU	HIS	ASP
	LEU	LEU	PRO	PRO	GLU
	ASP	LEU	ALA	ALA	VAL
	ASP	PHE	PRO	GLN	GLU
	GLN	SER	VAL	PRO	ASP
	ARG	LEU	MET	VAL	GLY
	GLN	ARG	ASP	GLN	GLY
	THR	ASN	LYS	GLN	VAL
	MET	ASN	PRO	PRO	VAL
	THR	MET	PRO	GLY	GLY
	PRO	LYS	ARG	TYR	GLU
	GLN	PRO	LYS	GLN	VAL
			LYS		ARG
					VAL
					HIS
					ARG

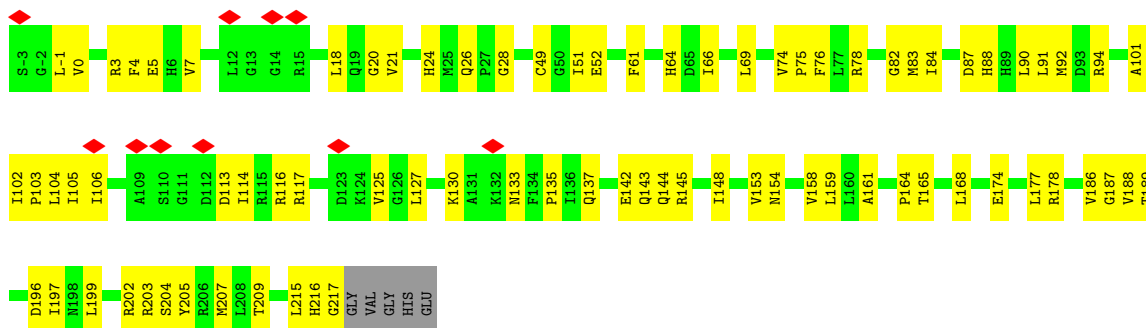
- Molecule 1: Cell division protein ZipA



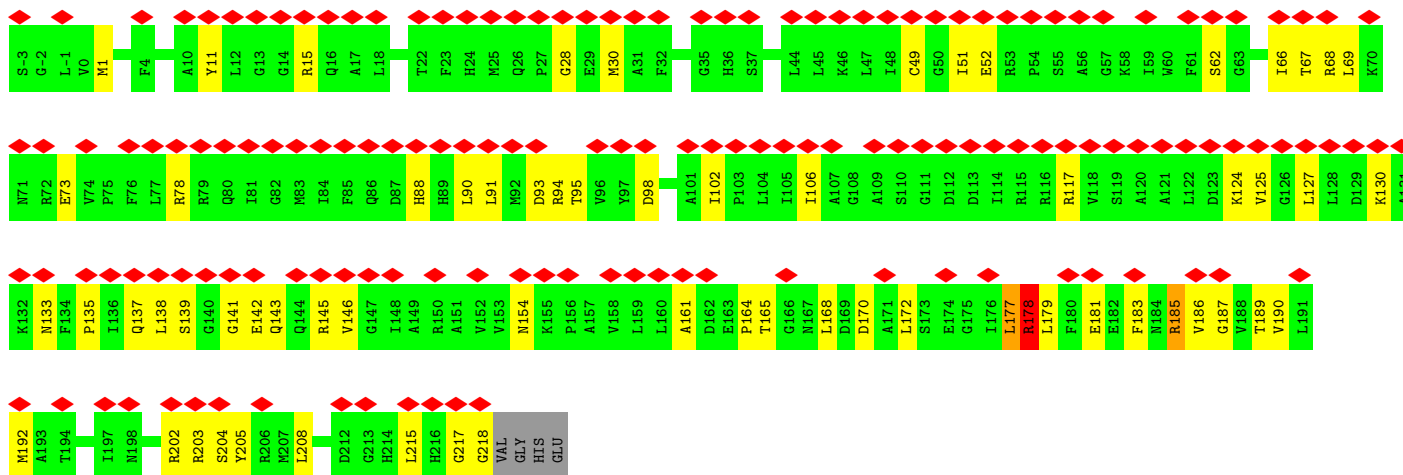
SER	VAL	PRO	GLY	MET
LEU	MET	VAL	GLU	MET
ALA	ASP	GLN	VAL	GLN
ASN	LYS	GLN	ARG	D4
MET	LYS	PRO	ARG	L5
VAL	ARG	ALA	HIS	R6
LYS	GLY	TYR	ARG	L7
PRO	ARG	GLN	VAL	I8
THR	GLU	PRO	ASN	L9
PHE	ALA	GLN	HIS	I10
ASP	VAL	PRO	ALA	I11
PRO	ILE	GLU	PRO	V12
GLU	MET	PRO	ASN	G13
MET	ASN	LEU	ALA	A14
LYS	VAL	GLN	GLN	I15
ASP	ALA	GLN	GLU	A16
PHE	ALA	PRO	HIS	I17
THR	HIS	VAL	ALA	I18
PRO	GLY	SER	ALA	A19
THR	SER	PRO	ARG	L20
GLY	GLU	GLN	PRO	L21
VAL	LEU	PRO	HIS	V22
PRO	LEU	PRO	TYR	F25
ASN	ASN	VAL	GLN	R29
TYR	ASN	HIS	PRO	K30
GLY	ILE	SER	TYR	E31
ASP	ILE	ALA	ALA	R32
GLU	GLN	GLN	SER	S33
LEU	ALA	PRO	ALA	S34
GLN	PHE	ALA	GLN	M35
ASN	ILE	GLN	ARG	F36
LYS	PHE	ALA	GLN	ASP
LEU	GLY	PHE	PRO	ARG
MET	GLY	GLY	VAL	ARG
MET	ASP	GLN	VAL	PRO
GLN	MET	PRO	GLN	LEU
SER	ILE	GLU	PRO	LYS
ALA	TYR	PRO	PRO	ARG
GLN	HIS	VAL	GLU	ARG
HIS	ARG	ALA	ALA	MET
ILE	HIS	ALA	GLN	LYS
ALA	LEU	PRO	VAL	SER
ALA	SER	GLN	PRO	LYS
ASP	PRO	PRO	PRO	ARG
GLU	ASP	GLU	GLN	ASP
VAL	GLY	PRO	HIS	ASP
GLY	SER	VAL	ALA	SER
VAL	GLY	ALA	PRO	TYR
VAL	PRO	GLU	HIS	ASP
LEU	ALA	PRO	PRO	GLU
ASP	LEU	ALA	ALA	ASP
ASP	PHE	PRO	GLN	VAL



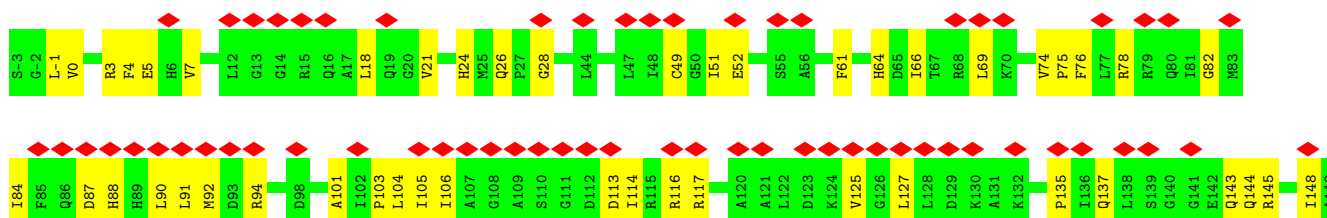
• Molecule 2: Cell division ATP-binding protein FtsE

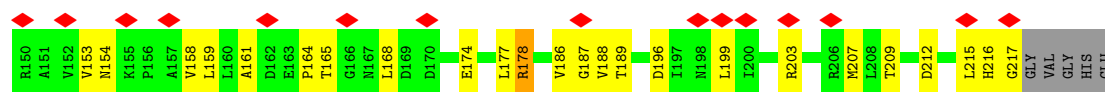


• Molecule 2: Cell division ATP-binding protein FtsE



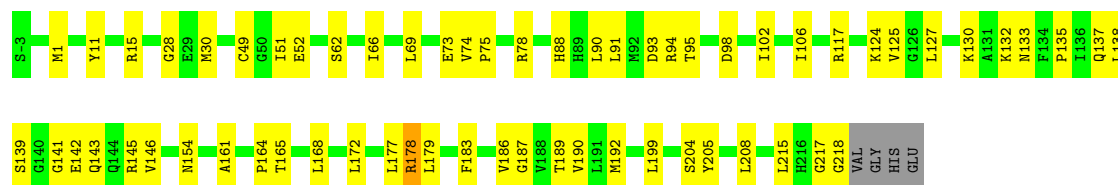
• Molecule 2: Cell division ATP-binding protein FtsE





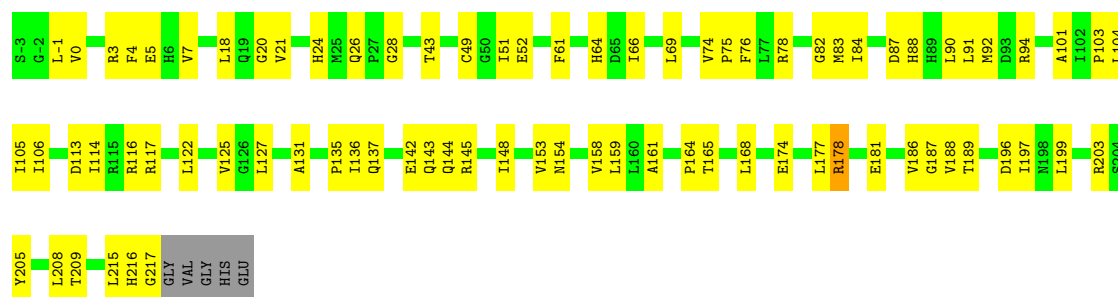
• Molecule 2: Cell division ATP-binding protein FtsE

Chain S: 71% 27%



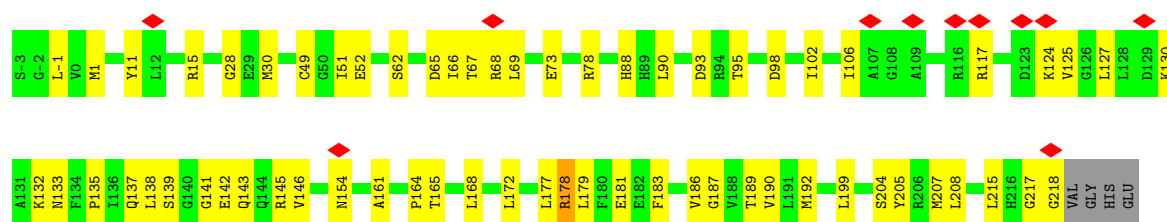
• Molecule 2: Cell division ATP-binding protein FtsE

Chain T: 62% 35%



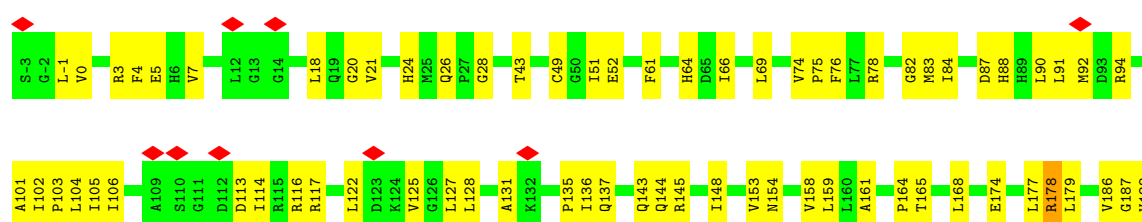
• Molecule 2: Cell division ATP-binding protein FtsE

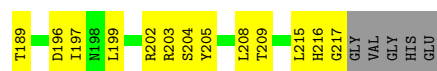
Chain Y: 5% 70% 28%



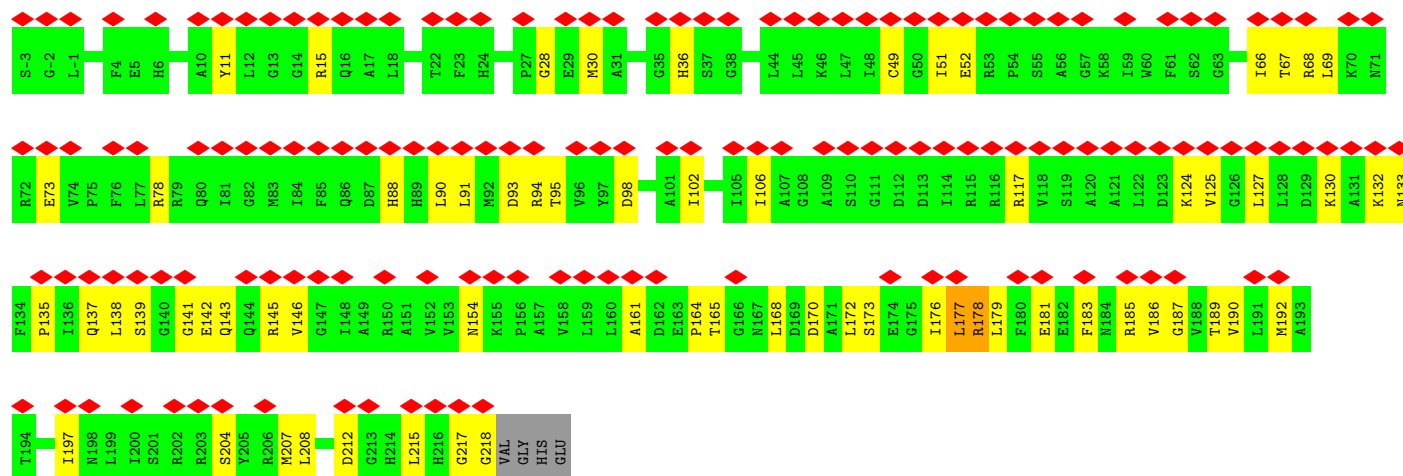
• Molecule 2: Cell division ATP-binding protein FtsE

Chain Z: 61% 36%

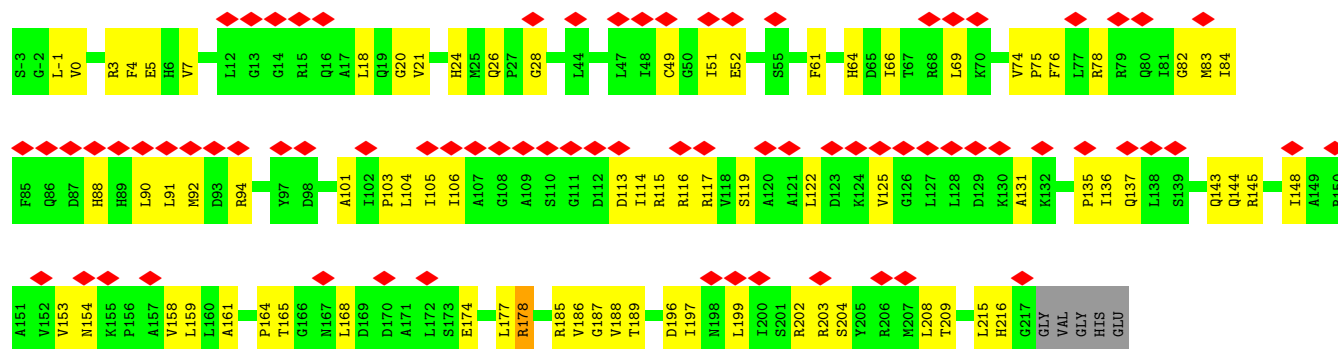




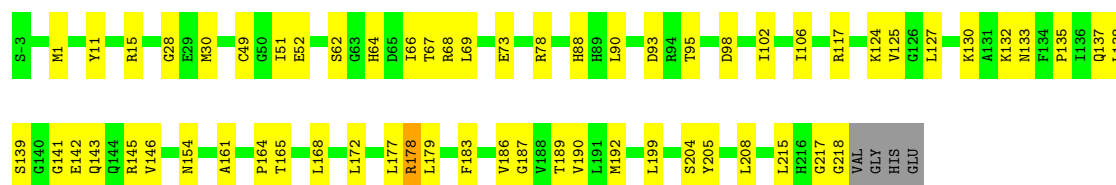
• Molecule 2: Cell division ATP-binding protein FtsE



• Molecule 2: Cell division ATP-binding protein FtsE

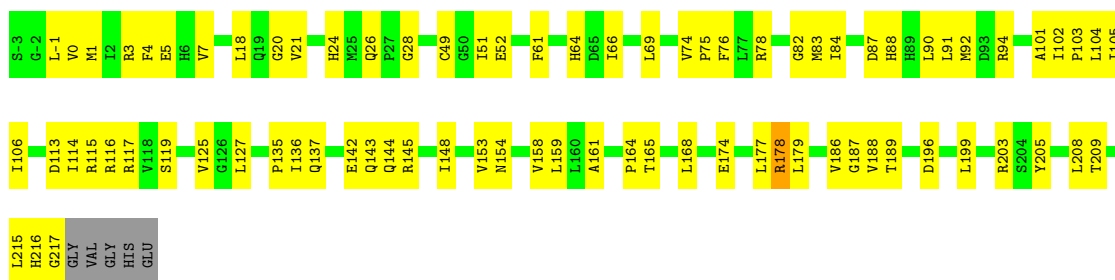


• Molecule 2: Cell division ATP-binding protein FtsE



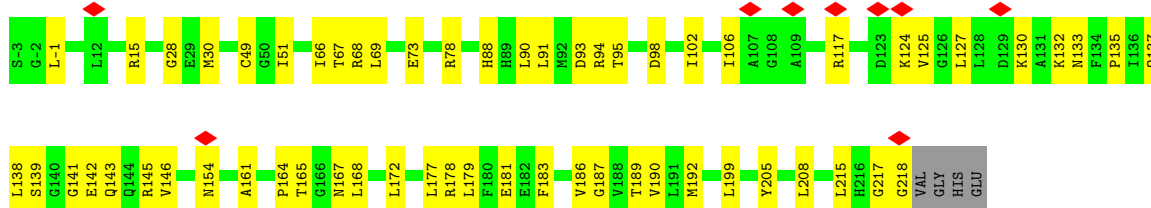
• Molecule 2: Cell division ATP-binding protein FtsE





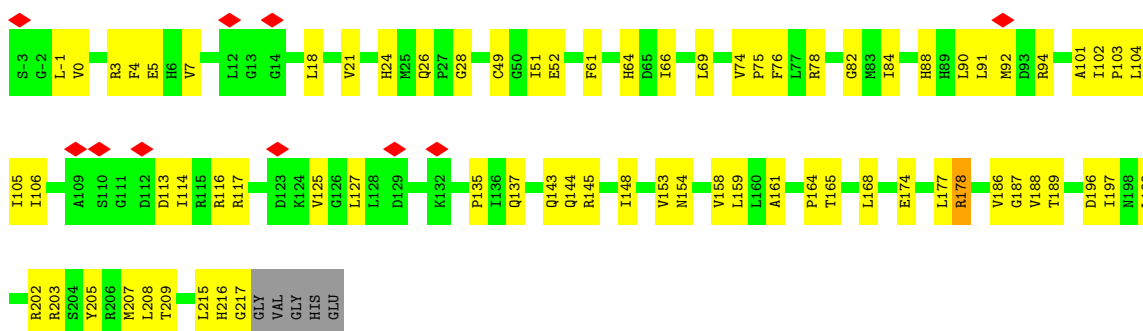
• Molecule 2: Cell division ATP-binding protein FtsE

Chain q: 72% 27% .



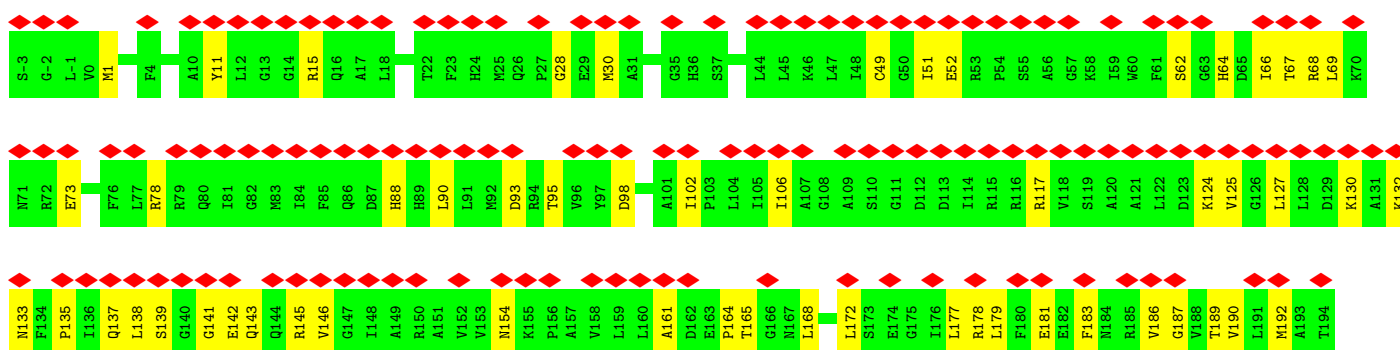
• Molecule 2: Cell division ATP-binding protein FtsE

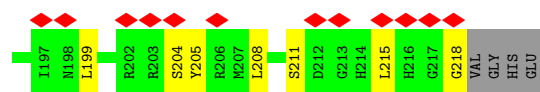
Chain r: 65% 32% .



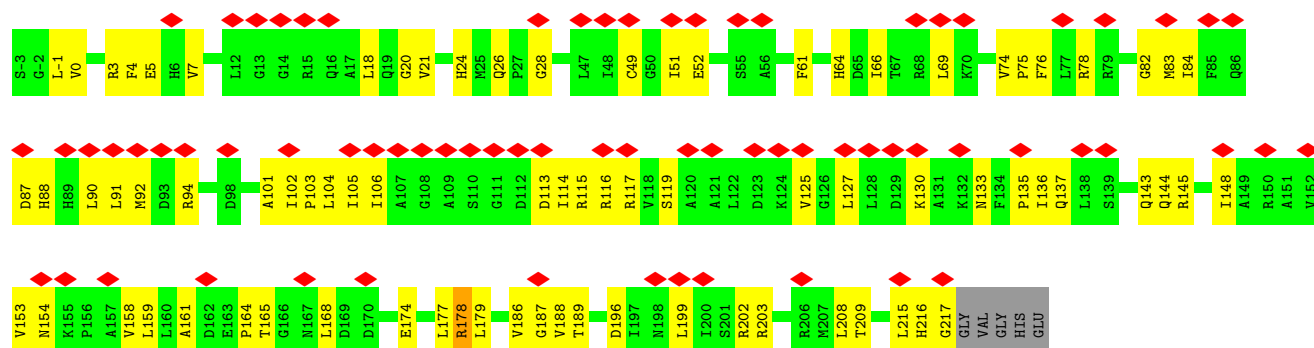
• Molecule 2: Cell division ATP-binding protein FtsE

Chain w: 66% 27% .

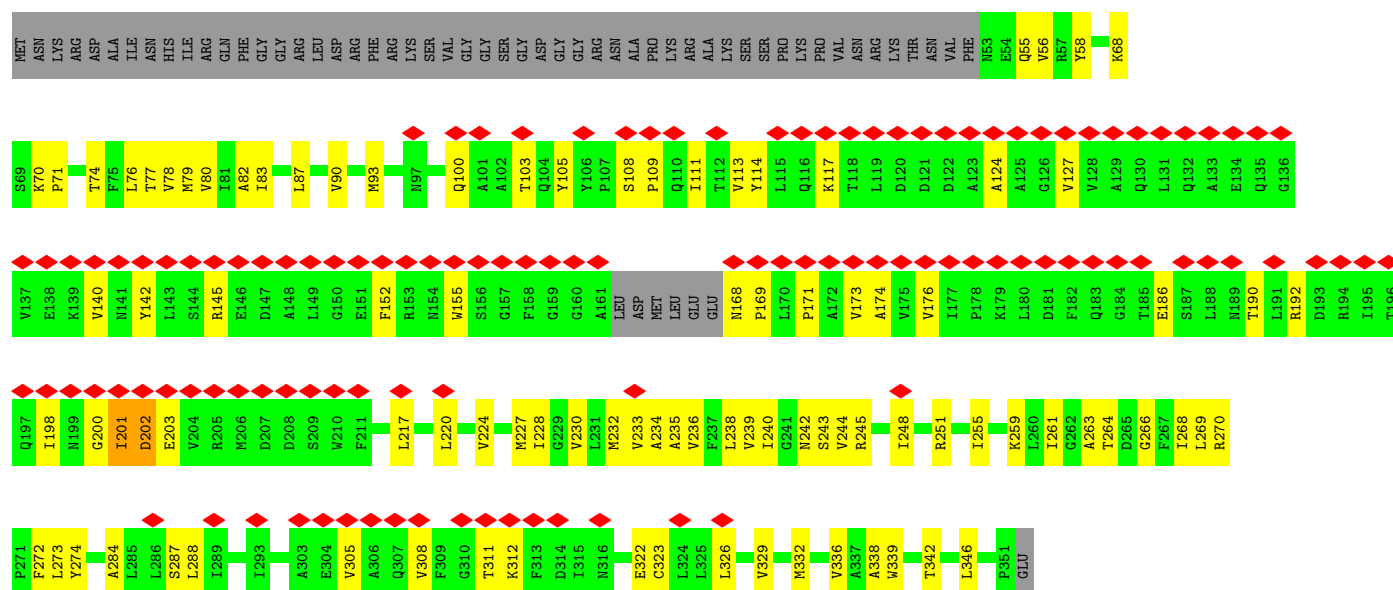




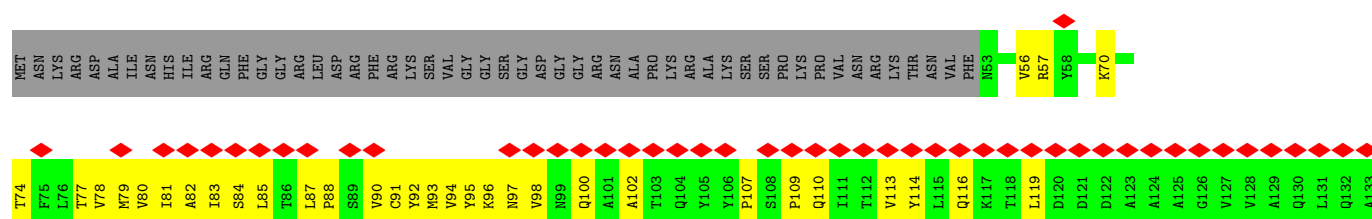
• Molecule 2: Cell division ATP-binding protein FtsE

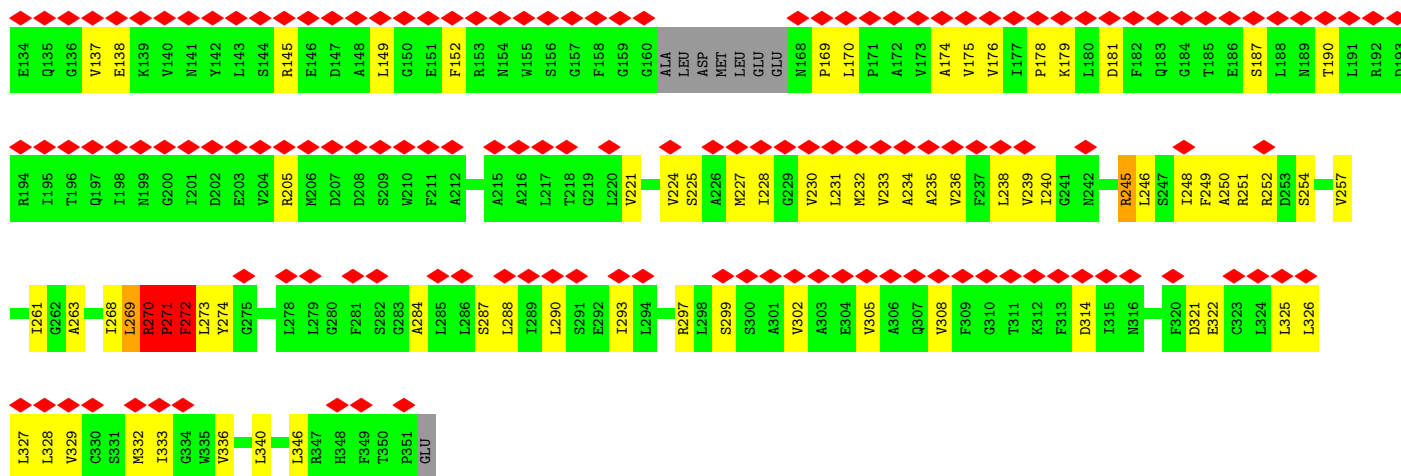


• Molecule 3: Cell division protein FtsX

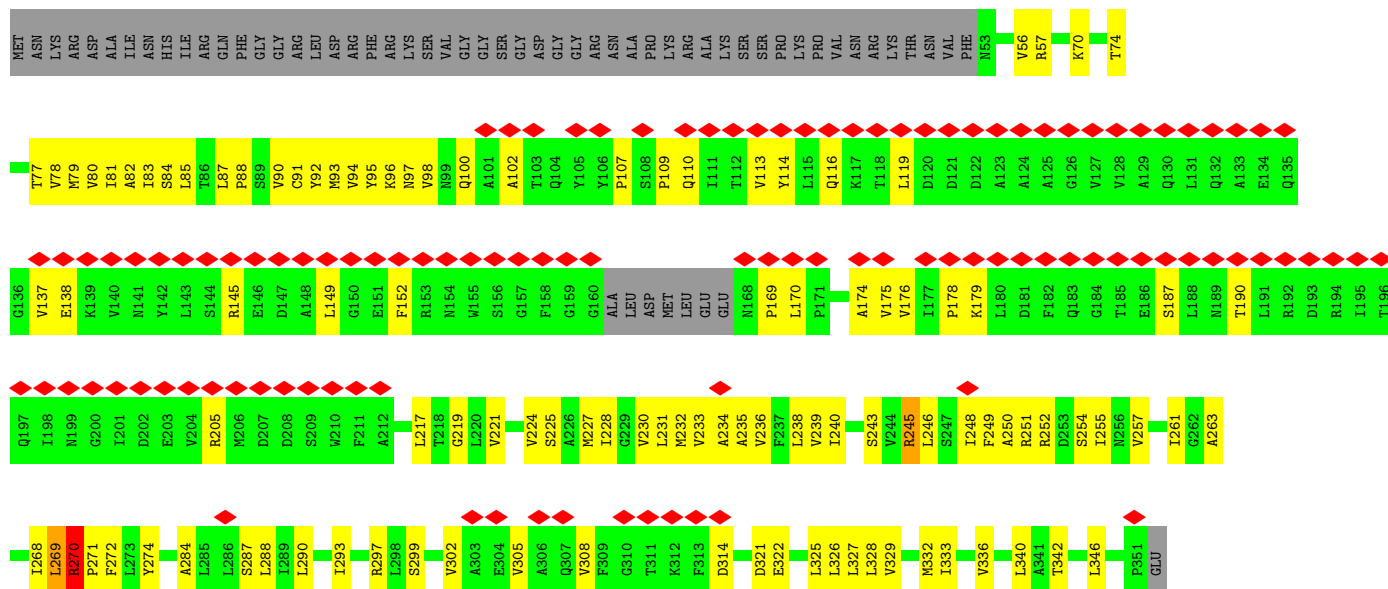


• Molecule 3: Cell division protein FtsX

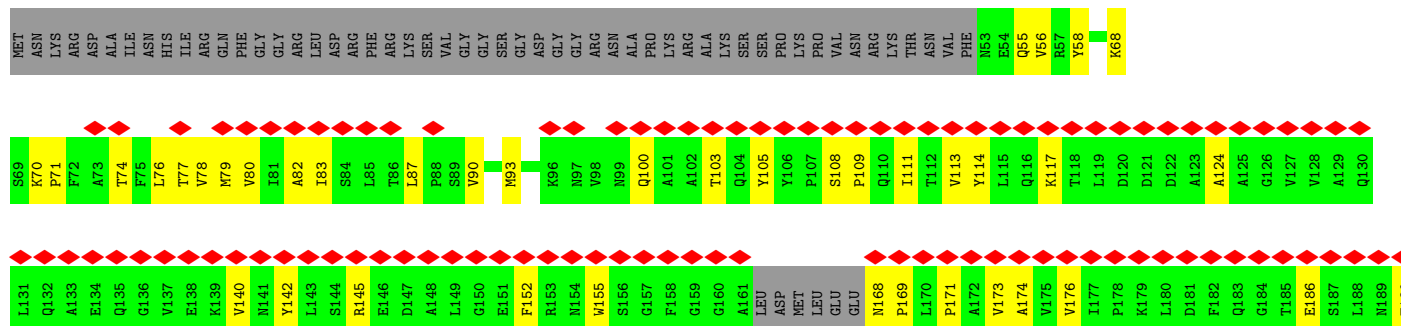


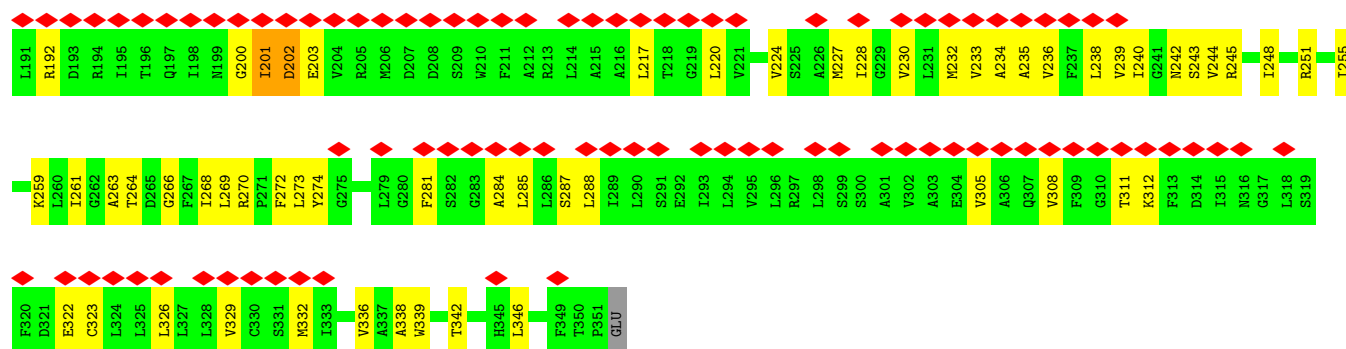


• Molecule 3: Cell division protein FtsX

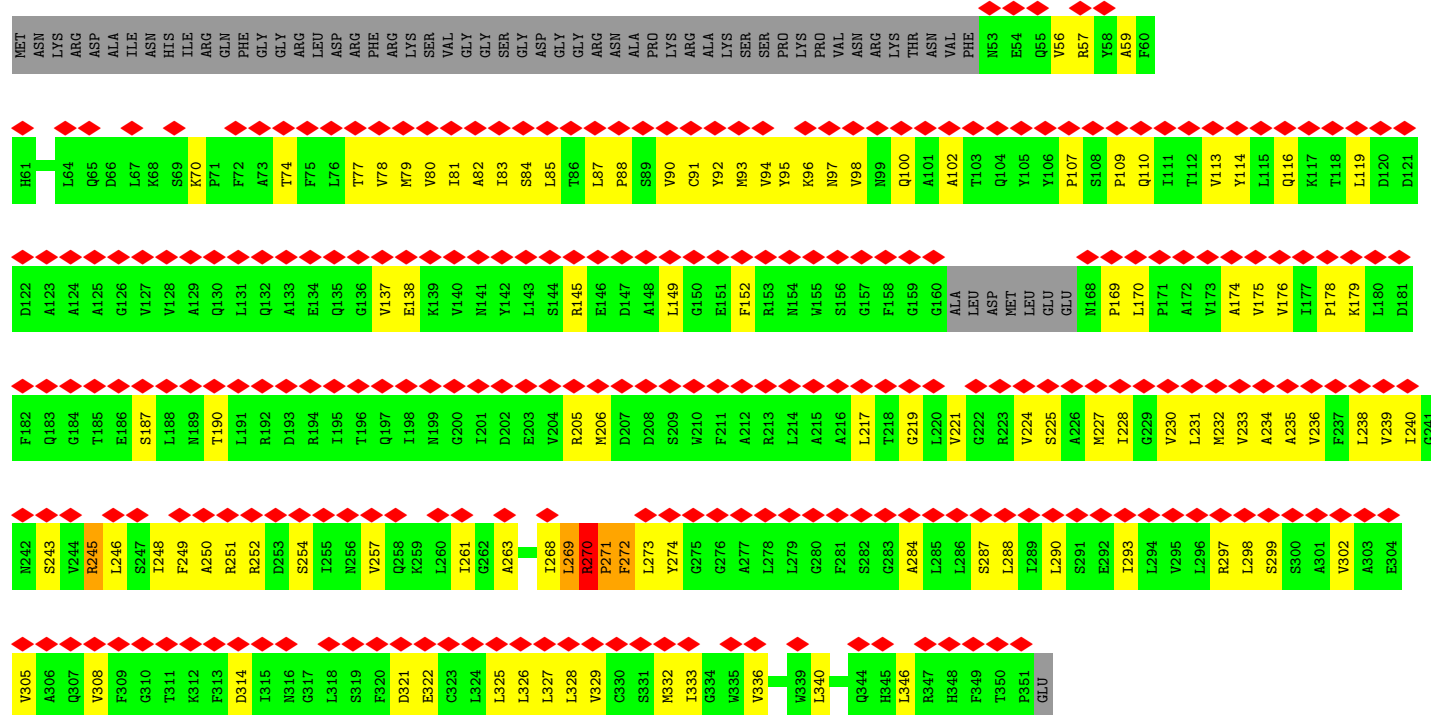


• Molecule 3: Cell division protein FtsX

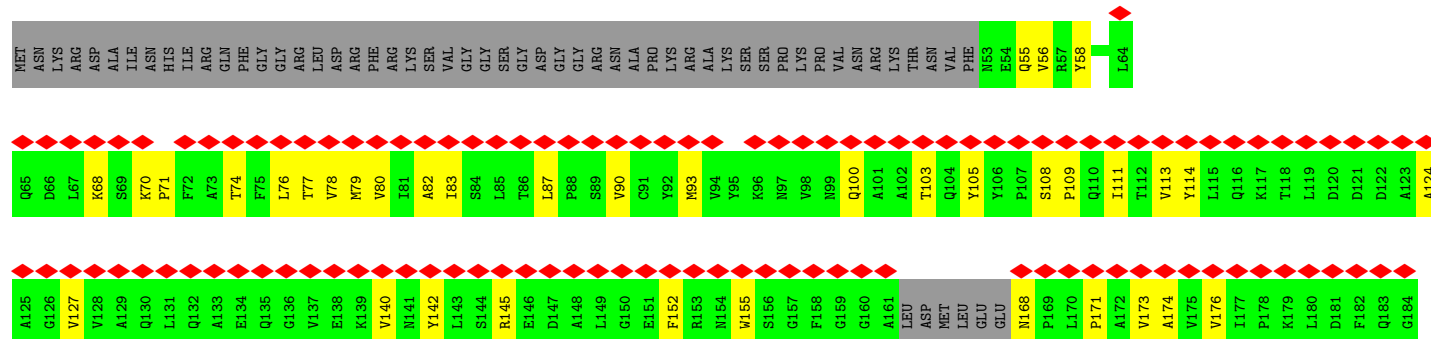


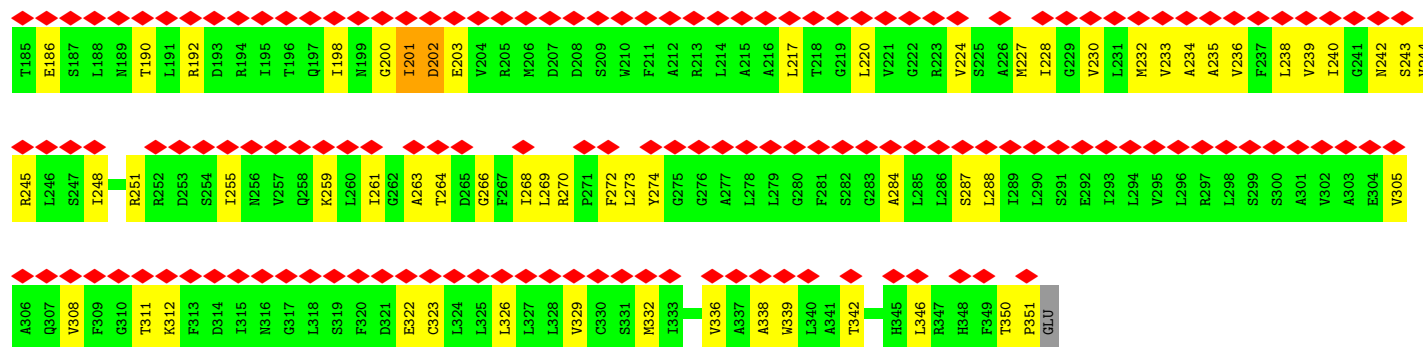


• Molecule 3: Cell division protein FtsX

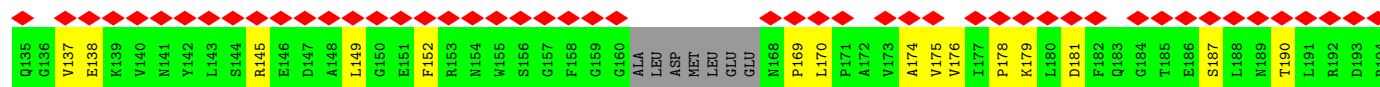
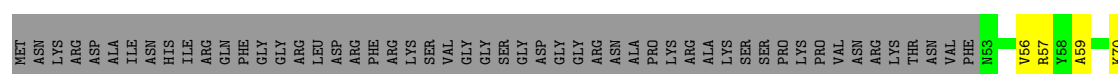


• Molecule 3: Cell division protein FtsX

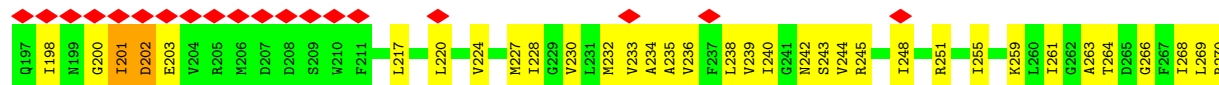
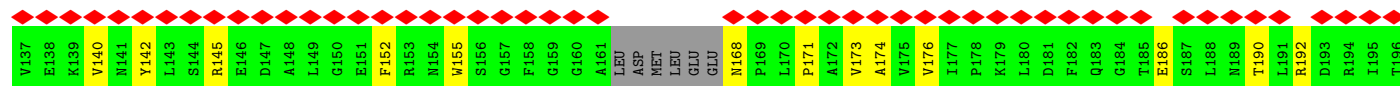
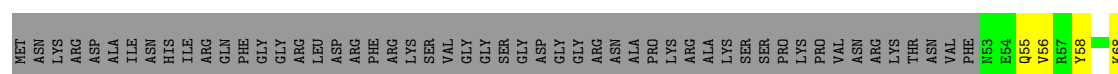




• Molecule 3: Cell division protein FtsX

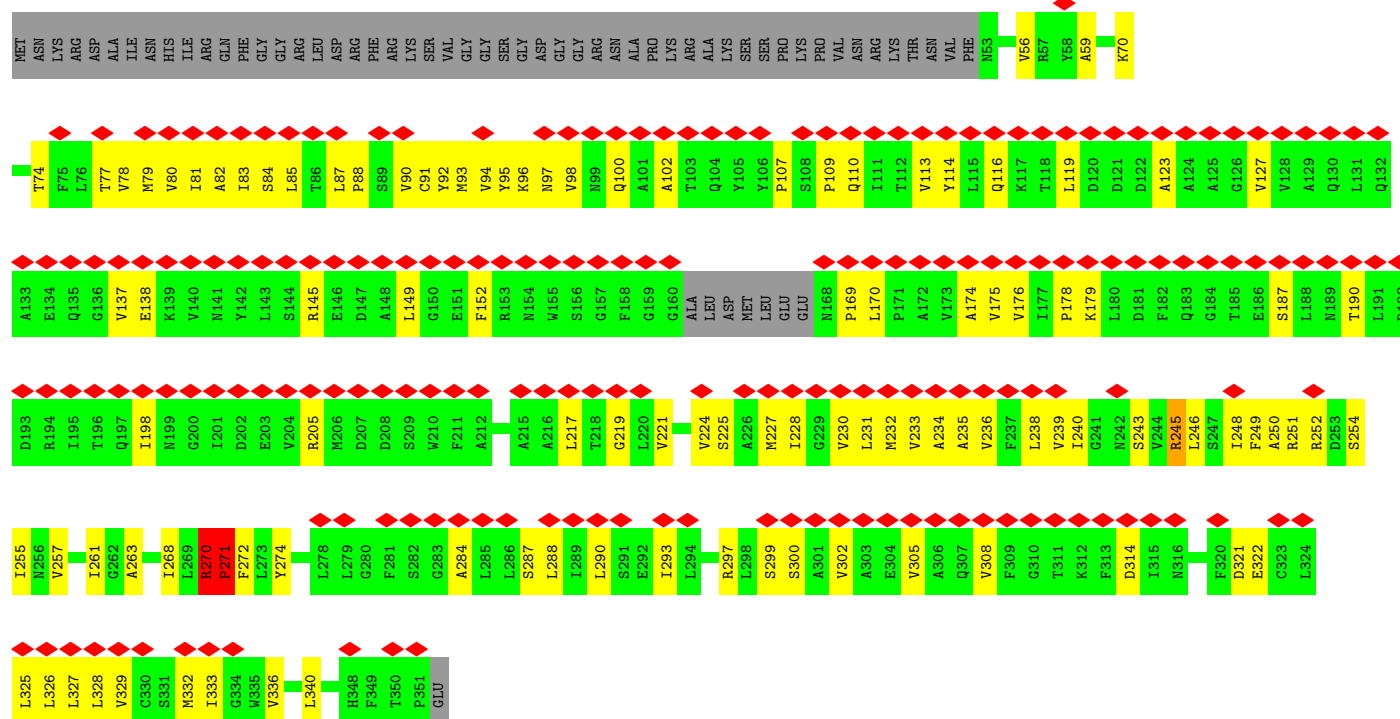


• Molecule 3: Cell division protein FtsX

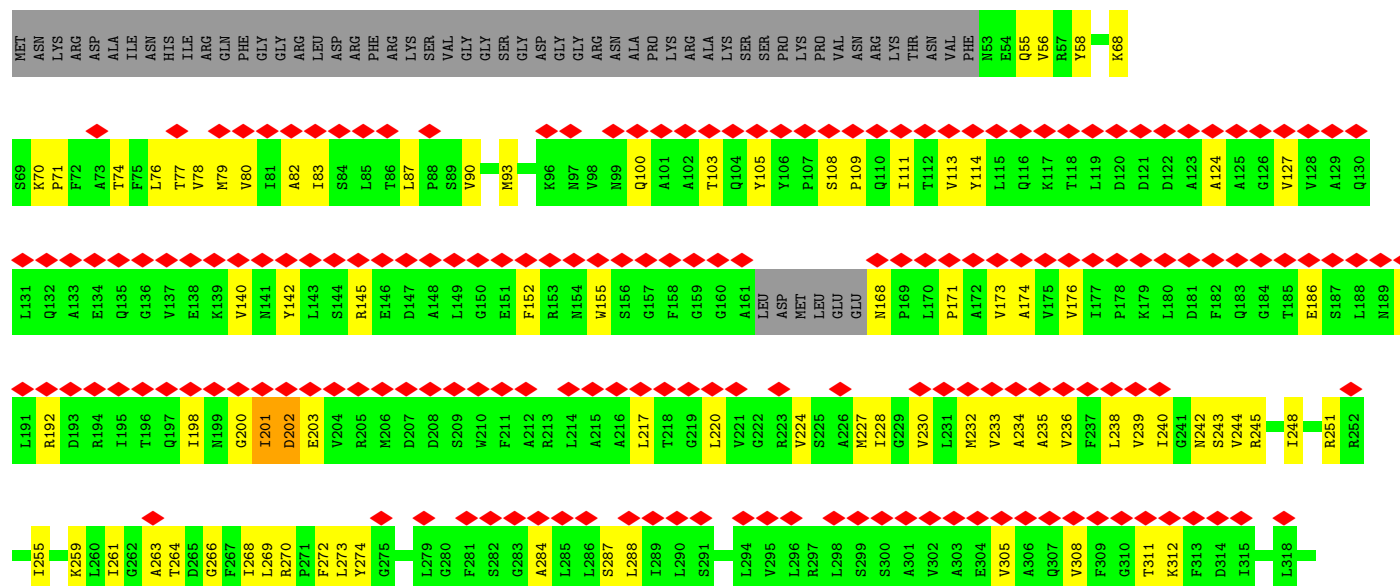


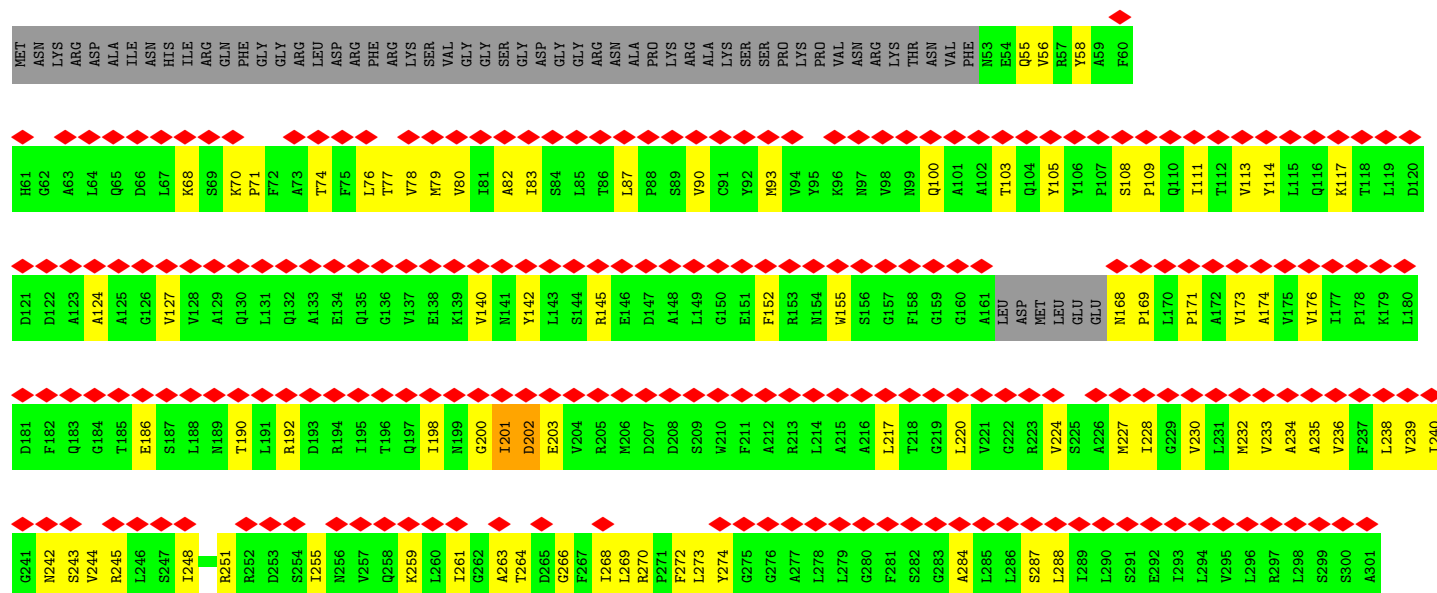
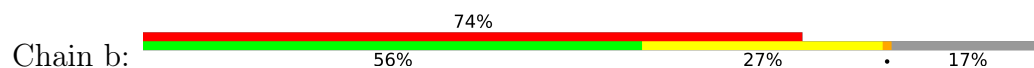
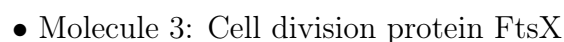
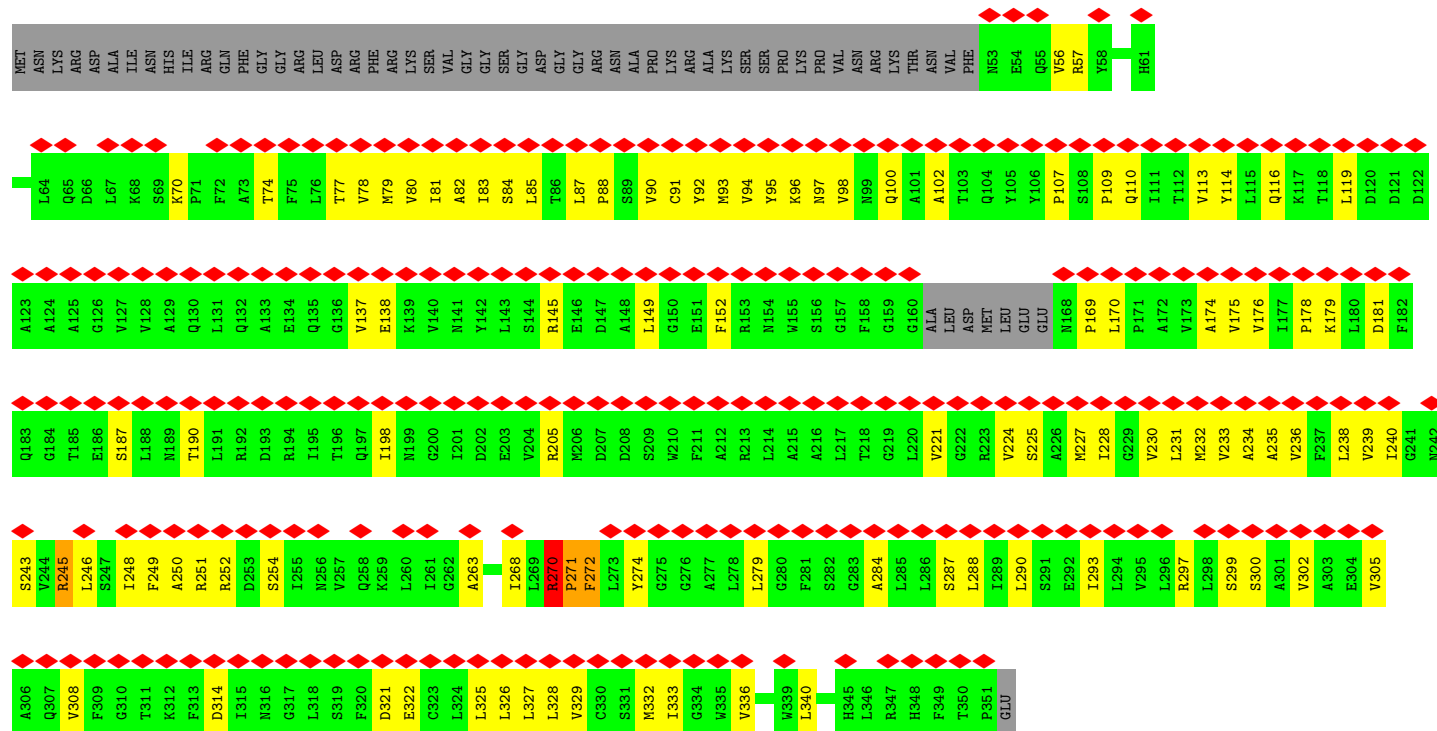
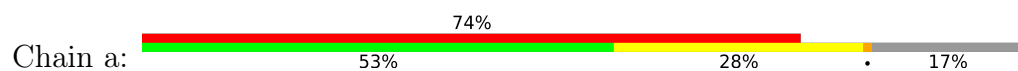
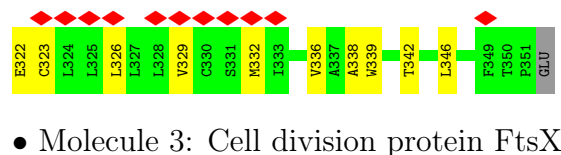


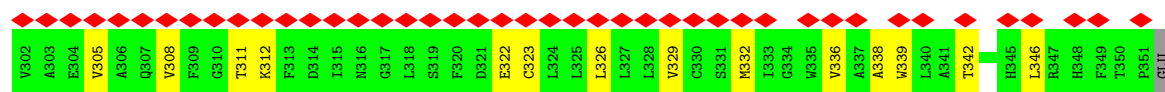
• Molecule 3: Cell division protein FtsX



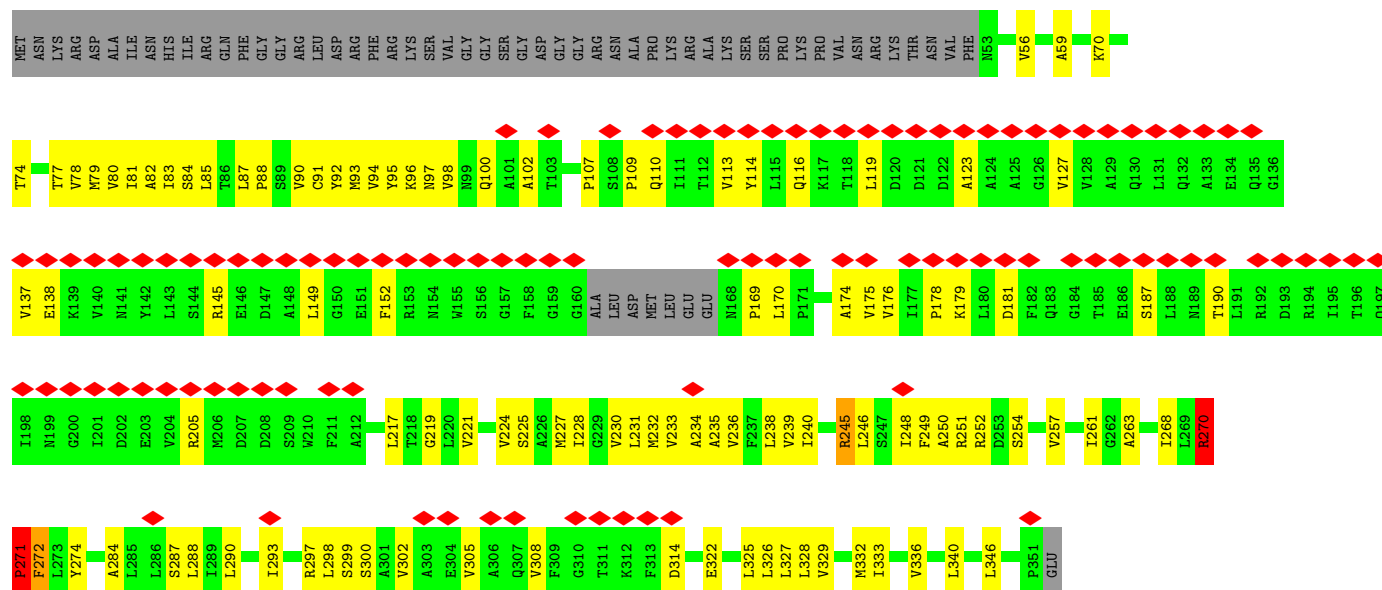
• Molecule 3: Cell division protein FtsX



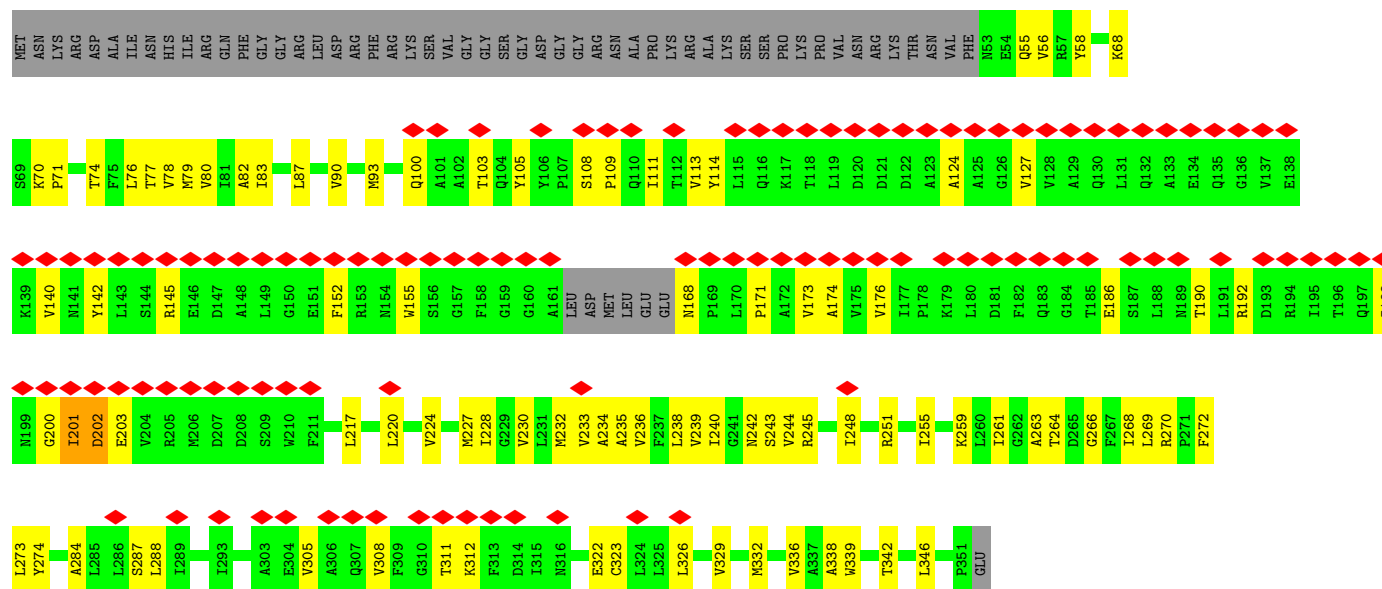




• Molecule 3: Cell division protein FtsX

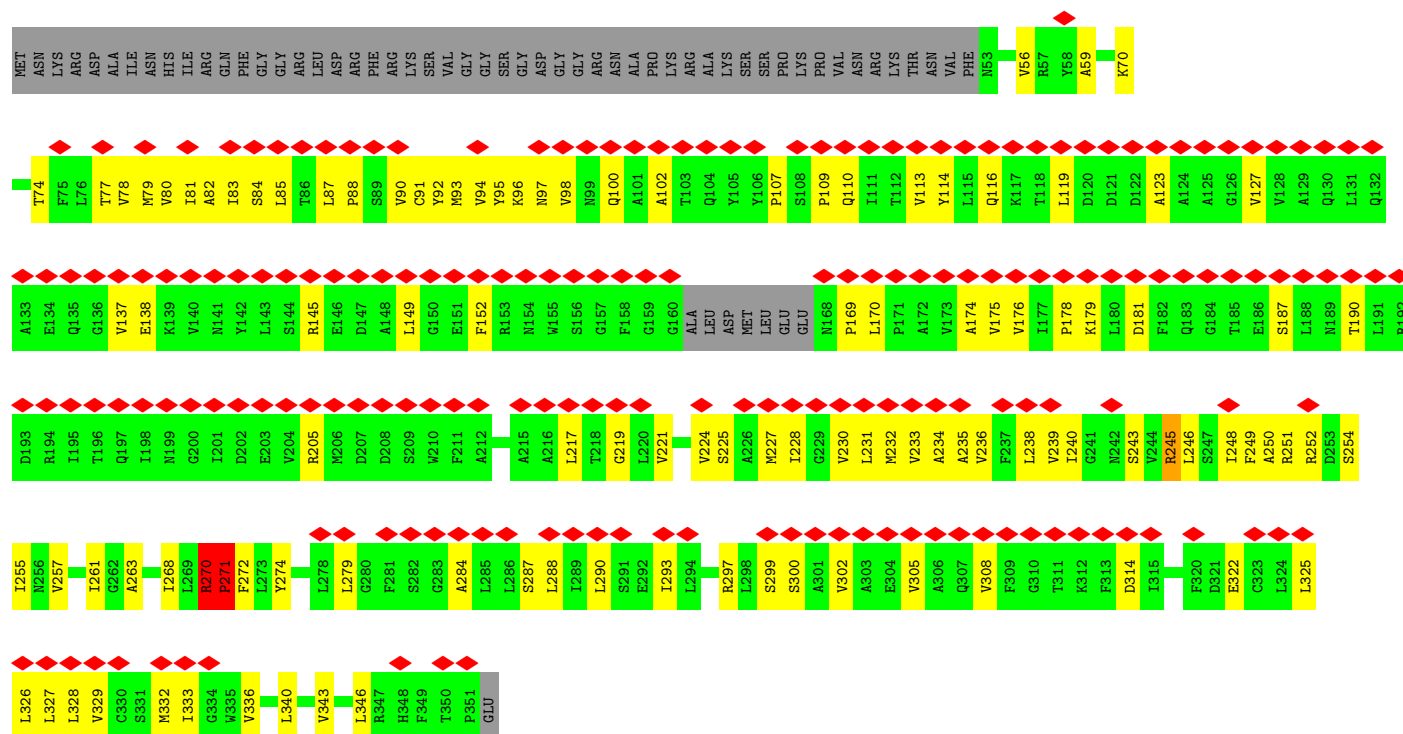


• Molecule 3: Cell division protein FtsX

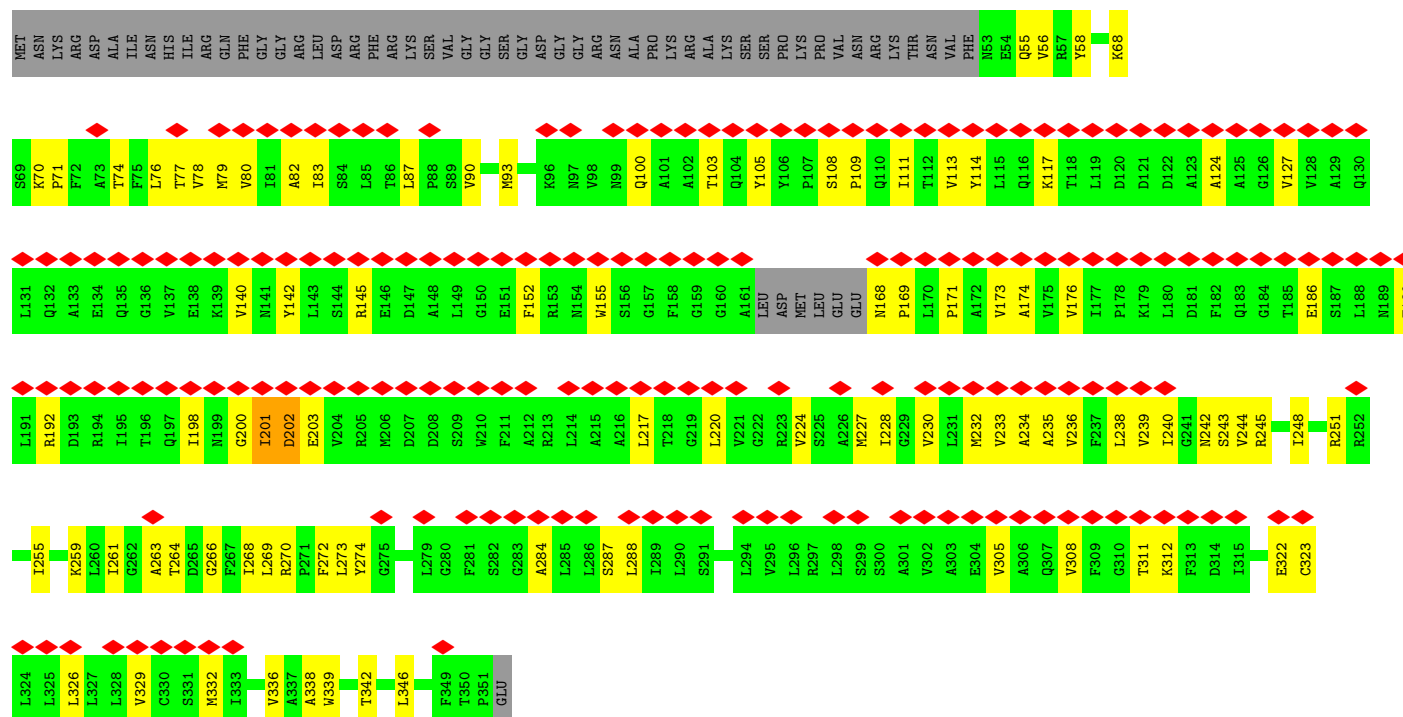


• Molecule 3: Cell division protein FtsX



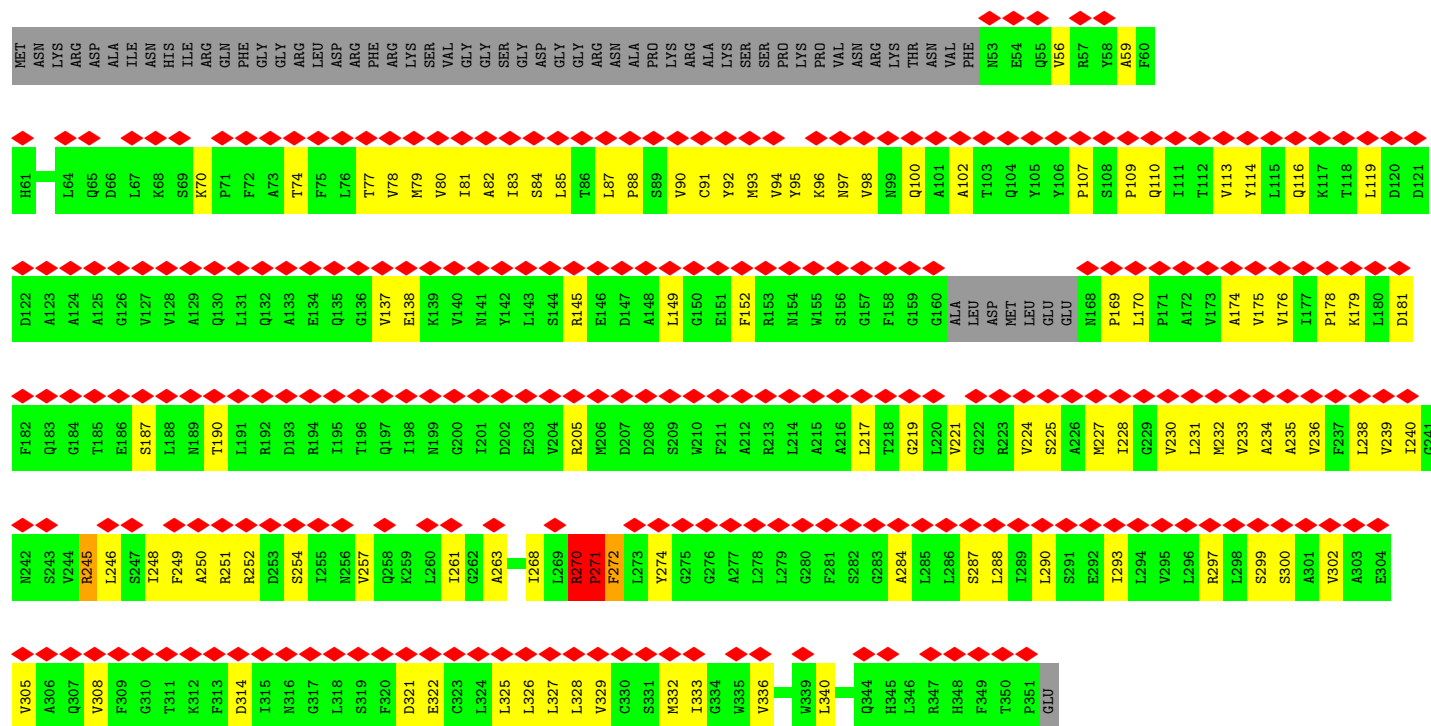


• Molecule 3: Cell division protein FtsX

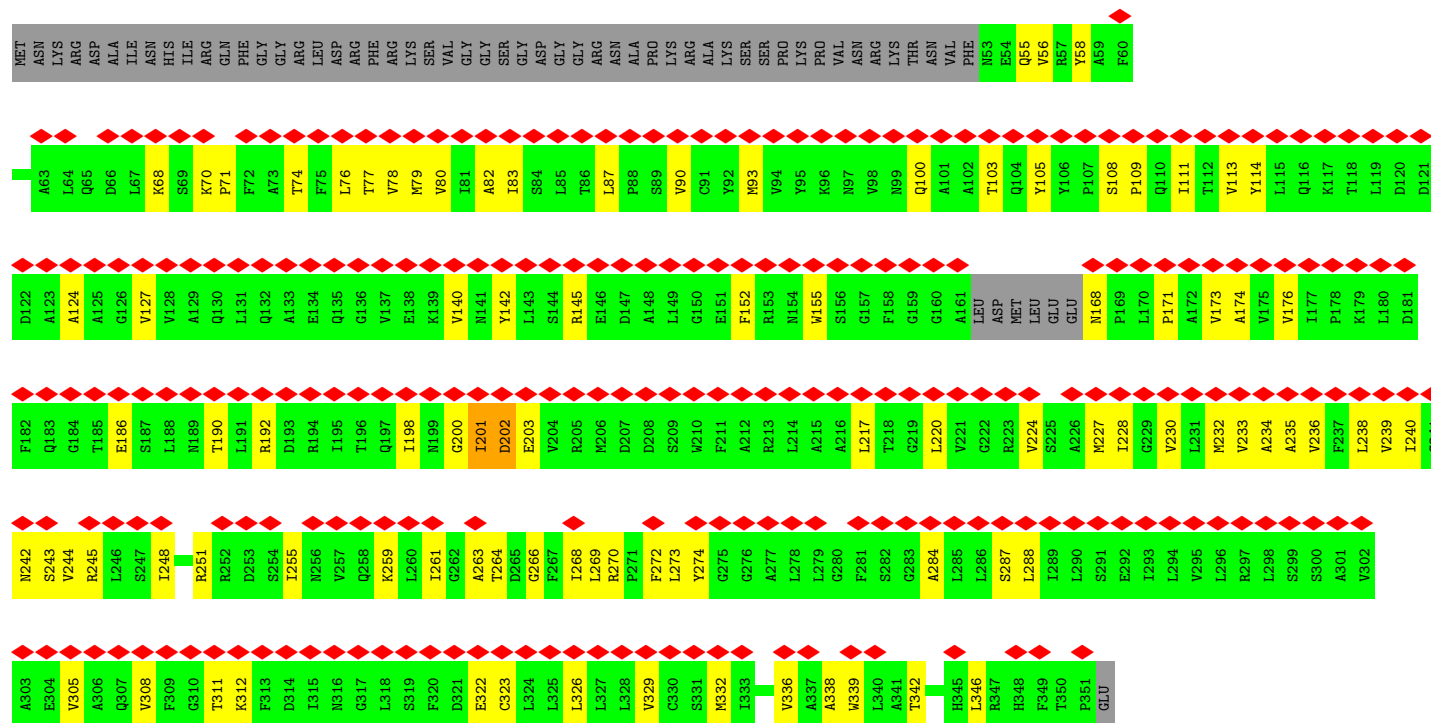


• Molecule 3: Cell division protein FtsX





• Molecule 3: Cell division protein FtsX



Property	Value	Source
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF,	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00, 36.65, 36.65	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor

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Property	Value	Source
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.764	Depositor
Minimum map value	-0.847	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.10	0/267	0.29	0/359
1	2	0.12	0/267	0.32	0/359
1	E	0.11	0/267	0.29	0/359
1	F	0.12	0/267	0.32	0/359
1	K	0.11	0/267	0.29	0/359
1	L	0.13	0/267	0.33	0/359
1	Q	0.11	0/267	0.29	0/359
1	R	0.13	0/267	0.32	0/359
1	W	0.11	0/267	0.30	0/359
1	X	0.13	0/267	0.33	0/359
1	c	0.11	0/267	0.30	0/359
1	d	0.12	0/267	0.32	0/359
1	i	0.11	0/267	0.30	0/359
1	j	0.12	0/267	0.32	0/359
1	o	0.11	0/267	0.30	0/359
1	p	0.12	0/267	0.32	0/359
1	u	0.11	0/267	0.30	0/359
1	v	0.13	0/267	0.32	0/359
2	5	0.23	0/1742	0.44	0/2346
2	6	0.21	0/1738	0.44	0/2341
2	G	0.26	0/1742	0.50	1/2346 (0.0%)
2	H	0.21	0/1738	0.42	0/2341
2	M	0.29	0/1742	0.50	0/2346
2	N	0.22	0/1738	0.40	0/2341
2	S	0.23	0/1742	0.44	0/2346
2	T	0.21	0/1738	0.43	1/2341 (0.0%)
2	Y	0.23	0/1742	0.45	0/2346
2	Z	0.23	0/1738	0.44	0/2341
2	e	0.30	0/1742	0.49	0/2346
2	f	0.25	0/1738	0.42	0/2341
2	k	0.23	0/1742	0.44	0/2346
2	l	0.21	0/1738	0.43	0/2341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q	0.23	0/1742	0.45	0/2346
2	r	0.21	0/1738	0.43	0/2341
2	w	0.23	0/1742	0.44	0/2346
2	x	0.22	0/1738	0.40	0/2341
3	A	0.18	0/2214	0.44	0/3021
3	B	0.25	0/2244	0.66	4/3056 (0.1%)
3	C	0.20	0/2244	0.50	0/3056
3	D	0.18	0/2214	0.43	0/3021
3	I	0.21	0/2244	0.53	1/3056 (0.0%)
3	J	0.18	0/2214	0.43	0/3021
3	O	0.18	0/2244	0.54	2/3056 (0.1%)
3	P	0.18	0/2214	0.44	0/3021
3	U	0.18	0/2244	0.54	3/3056 (0.1%)
3	V	0.18	0/2214	0.43	0/3021
3	a	0.20	0/2244	0.54	1/3056 (0.0%)
3	b	0.18	0/2214	0.44	0/3021
3	g	0.20	0/2244	0.55	1/3056 (0.0%)
3	h	0.18	0/2214	0.44	0/3021
3	m	0.18	0/2244	0.54	3/3056 (0.1%)
3	n	0.18	0/2214	0.44	0/3021
3	s	0.20	0/2244	0.54	2/3056 (0.1%)
3	t	0.18	0/2214	0.44	0/3021
All	All	0.21	0/76248	0.47	19/103338 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	1
2	6	0	1
2	G	0	1
2	H	0	1
2	M	0	2
2	N	0	1
2	S	0	1
2	T	0	1
2	Y	0	1
2	Z	0	1
2	e	0	1
2	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	k	0	1
2	l	0	1
2	q	0	1
2	r	0	1
2	w	0	1
2	x	0	1
3	B	0	1
3	C	0	1
3	I	0	1
3	O	0	1
3	U	0	1
3	a	0	1
3	g	0	1
3	m	0	1
3	s	0	1
All	All	0	29

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	272	PHE	CA-C-N	-14.65	100.76	120.54
3	B	272	PHE	C-N-CA	-14.65	100.76	120.54
3	B	271	PRO	N-CA-C	-7.54	96.93	112.47
3	U	271	PRO	CB-CA-C	6.52	122.32	111.56
3	g	270	ARG	CB-CA-C	6.50	122.98	110.17

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	5	178	ARG	Sidechain
2	6	178	ARG	Sidechain
3	B	270	ARG	Sidechain
3	C	270	ARG	Sidechain
2	G	178	ARG	Sidechain

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	1	263	0	287	11	0
1	2	263	0	287	3	0
1	E	263	0	287	9	0
1	F	263	0	287	3	0
1	K	263	0	287	10	0
1	L	263	0	287	3	0
1	Q	263	0	287	9	0
1	R	263	0	287	2	0
1	W	263	0	287	10	0
1	X	263	0	287	3	0
1	c	263	0	287	10	0
1	d	263	0	287	2	0
1	i	263	0	287	9	0
1	j	263	0	287	4	0
1	o	263	0	287	8	0
1	p	263	0	287	2	0
1	u	263	0	287	9	0
1	v	263	0	287	4	0
2	5	1713	0	1756	58	0
2	6	1709	0	1753	52	0
2	G	1713	0	1756	52	0
2	H	1709	0	1753	61	0
2	M	1713	0	1756	62	0
2	N	1709	0	1753	51	0
2	S	1713	0	1756	52	0
2	T	1709	0	1753	57	0
2	Y	1713	0	1756	60	0
2	Z	1709	0	1753	61	0
2	e	1713	0	1756	57	0
2	f	1709	0	1753	55	0
2	k	1713	0	1756	55	0
2	l	1709	0	1753	58	0
2	q	1713	0	1756	52	0
2	r	1709	0	1753	55	0
2	w	1713	0	1756	54	0
2	x	1709	0	1753	59	0
3	A	2174	0	2173	78	0
3	B	2204	0	2224	107	0
3	C	2204	0	2224	95	0
3	D	2174	0	2173	77	0
3	I	2204	0	2224	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2174	0	2173	77	0
3	O	2204	0	2224	98	0
3	P	2174	0	2173	72	0
3	U	2204	0	2224	102	0
3	V	2174	0	2173	76	0
3	a	2204	0	2224	99	0
3	b	2174	0	2173	75	0
3	g	2204	0	2224	100	0
3	h	2174	0	2173	79	0
3	m	2204	0	2224	101	0
3	n	2174	0	2173	79	0
3	s	2204	0	2224	97	0
3	t	2174	0	2173	77	0
4	5	31	0	12	0	0
4	6	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
4	M	31	0	12	0	0
4	N	31	0	12	0	0
4	S	31	0	12	0	0
4	T	31	0	12	1	0
4	Y	31	0	12	0	0
4	Z	31	0	12	1	0
4	e	31	0	12	0	0
4	f	31	0	12	0	0
4	k	31	0	12	0	0
4	l	31	0	12	0	0
4	q	31	0	12	0	0
4	r	31	0	12	0	0
4	w	31	0	12	0	0
4	x	31	0	12	0	0
All	All	75492	0	76536	2476	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 16.

The worst 5 of 2476 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:204:SER:O	2:Y:218:GLY:HA3	1.28	1.31
2:M:218:GLY:HA3	2:w:204:SER:O	1.37	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:204:SER:O	2:q:218:GLY:HA3	1.31	1.24
2:5:218:GLY:HA3	2:k:204:SER:O	1.35	1.23
2:S:204:SER:O	2:k:218:GLY:HA3	1.39	1.22

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	1	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	2	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	E	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	F	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	K	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	L	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	Q	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	R	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	W	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	X	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	c	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	d	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	i	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	j	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	o	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	p	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	u	31/328 (10%)	30 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
2	5	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	6	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	G	220/226 (97%)	205 (93%)	15 (7%)	0	100	100
2	H	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	M	220/226 (97%)	208 (94%)	12 (6%)	0	100	100
2	N	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	S	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	T	219/226 (97%)	208 (95%)	11 (5%)	0	100	100
2	Y	220/226 (97%)	208 (94%)	12 (6%)	0	100	100
2	Z	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	e	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	f	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	k	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	l	219/226 (97%)	208 (95%)	11 (5%)	0	100	100
2	q	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	r	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	w	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	x	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
3	A	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	B	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	12	40
3	C	288/352 (82%)	265 (92%)	21 (7%)	2 (1%)	18	49
3	D	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	I	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	33
3	J	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	O	288/352 (82%)	264 (92%)	21 (7%)	3 (1%)	12	40
3	P	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	U	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	12	40
3	V	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	a	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	33
3	b	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	33
3	h	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	m	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	12	40
3	n	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
3	s	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	33
3	t	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	18	49
All	All	9702/16308 (60%)	9118 (94%)	536 (6%)	48 (0%)	26	55

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	201	ILE
3	B	272	PHE
3	D	201	ILE
3	I	270	ARG
3	I	271	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	28/279 (10%)	28 (100%)	0	100	100
1	2	28/279 (10%)	28 (100%)	0	100	100
1	E	28/279 (10%)	28 (100%)	0	100	100
1	F	28/279 (10%)	28 (100%)	0	100	100
1	K	28/279 (10%)	28 (100%)	0	100	100
1	L	28/279 (10%)	28 (100%)	0	100	100
1	Q	28/279 (10%)	28 (100%)	0	100	100
1	R	28/279 (10%)	28 (100%)	0	100	100
1	W	28/279 (10%)	28 (100%)	0	100	100
1	X	28/279 (10%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	28/279 (10%)	28 (100%)	0	100	100
1	d	28/279 (10%)	28 (100%)	0	100	100
1	i	28/279 (10%)	28 (100%)	0	100	100
1	j	28/279 (10%)	28 (100%)	0	100	100
1	o	28/279 (10%)	28 (100%)	0	100	100
1	p	28/279 (10%)	27 (96%)	1 (4%)	31	58
1	u	28/279 (10%)	28 (100%)	0	100	100
1	v	28/279 (10%)	28 (100%)	0	100	100
2	5	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	6	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	G	181/184 (98%)	178 (98%)	3 (2%)	53	71
2	H	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	M	181/184 (98%)	178 (98%)	3 (2%)	53	71
2	N	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	S	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	T	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	Y	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	Z	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	e	181/184 (98%)	178 (98%)	3 (2%)	53	71
2	f	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	k	181/184 (98%)	180 (99%)	1 (1%)	78	81
2	l	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	q	181/184 (98%)	181 (100%)	0	100	100
2	r	181/184 (98%)	179 (99%)	2 (1%)	65	76
2	w	181/184 (98%)	181 (100%)	0	100	100
2	x	181/184 (98%)	179 (99%)	2 (1%)	65	76
3	A	222/289 (77%)	222 (100%)	0	100	100
3	B	231/289 (80%)	228 (99%)	3 (1%)	61	74
3	C	231/289 (80%)	228 (99%)	3 (1%)	61	74
3	D	222/289 (77%)	222 (100%)	0	100	100
3	I	231/289 (80%)	226 (98%)	5 (2%)	45	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	222/289 (77%)	222 (100%)	0	100	100
3	O	231/289 (80%)	227 (98%)	4 (2%)	53	71
3	P	222/289 (77%)	222 (100%)	0	100	100
3	U	231/289 (80%)	228 (99%)	3 (1%)	61	74
3	V	222/289 (77%)	222 (100%)	0	100	100
3	a	231/289 (80%)	228 (99%)	3 (1%)	61	74
3	b	222/289 (77%)	222 (100%)	0	100	100
3	g	231/289 (80%)	228 (99%)	3 (1%)	61	74
3	h	222/289 (77%)	222 (100%)	0	100	100
3	m	231/289 (80%)	227 (98%)	4 (2%)	53	71
3	n	222/289 (77%)	222 (100%)	0	100	100
3	s	231/289 (80%)	229 (99%)	2 (1%)	70	78
3	t	222/289 (77%)	222 (100%)	0	100	100
All	All	7839/13536 (58%)	7779 (99%)	60 (1%)	70	79

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	188	VAL
2	r	188	VAL
3	a	232	MET
2	r	178	ARG
2	x	188	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	26	GLN
2	x	216	HIS
2	f	216	HIS
2	x	214	HIS
2	r	216	HIS

5.3.3 RNA ⓘ

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](#)

18 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	$\# Z > 2$
4	AGS	N	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	k	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.69	1 (2%)
4	AGS	S	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	Z	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	5	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	H	301	-	32,33,33	0.58	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	e	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	x	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	T	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	G	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	Y	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.69	1 (2%)
4	AGS	f	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	6	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	l	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	w	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.69	1 (2%)
4	AGS	r	301	-	32,33,33	0.59	1 (3%)	45,52,52	0.67	1 (2%)
4	AGS	q	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.69	1 (2%)
4	AGS	M	301	-	32,33,33	0.60	1 (3%)	45,52,52	0.69	1 (2%)

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
4	AGS	N	301	-	-	3/21/38/38	0/3/3/3
4	AGS	k	301	-	-	6/21/38/38	0/3/3/3
4	AGS	S	301	-	-	6/21/38/38	0/3/3/3
4	AGS	Z	301	-	-	3/21/38/38	0/3/3/3
4	AGS	5	301	-	-	6/21/38/38	0/3/3/3
4	AGS	H	301	-	-	3/21/38/38	0/3/3/3
4	AGS	e	301	-	-	6/21/38/38	0/3/3/3
4	AGS	x	301	-	-	3/21/38/38	0/3/3/3
4	AGS	T	301	-	-	3/21/38/38	0/3/3/3
4	AGS	G	301	-	-	6/21/38/38	0/3/3/3
4	AGS	Y	301	-	-	6/21/38/38	0/3/3/3
4	AGS	f	301	-	-	3/21/38/38	0/3/3/3
4	AGS	6	301	-	-	3/21/38/38	0/3/3/3
4	AGS	l	301	-	-	3/21/38/38	0/3/3/3
4	AGS	w	301	-	-	6/21/38/38	0/3/3/3
4	AGS	r	301	-	-	3/21/38/38	0/3/3/3
4	AGS	q	301	-	-	6/21/38/38	0/3/3/3
4	AGS	M	301	-	-	6/21/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	301	AGS	PG-S1G	2.11	1.95	1.90
4	G	301	AGS	PG-S1G	2.09	1.95	1.90
4	Z	301	AGS	PG-S1G	2.08	1.95	1.90
4	q	301	AGS	PG-S1G	2.08	1.95	1.90
4	6	301	AGS	PG-S1G	2.07	1.95	1.90

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	q	301	AGS	PB-O3B-PG	-3.91	118.86	133.17
4	M	301	AGS	PB-O3B-PG	-3.91	118.87	133.17
4	Y	301	AGS	PB-O3B-PG	-3.91	118.87	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	k	301	AGS	PB-O3B-PG	-3.91	118.88	133.17
4	w	301	AGS	PB-O3B-PG	-3.90	118.89	133.17

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

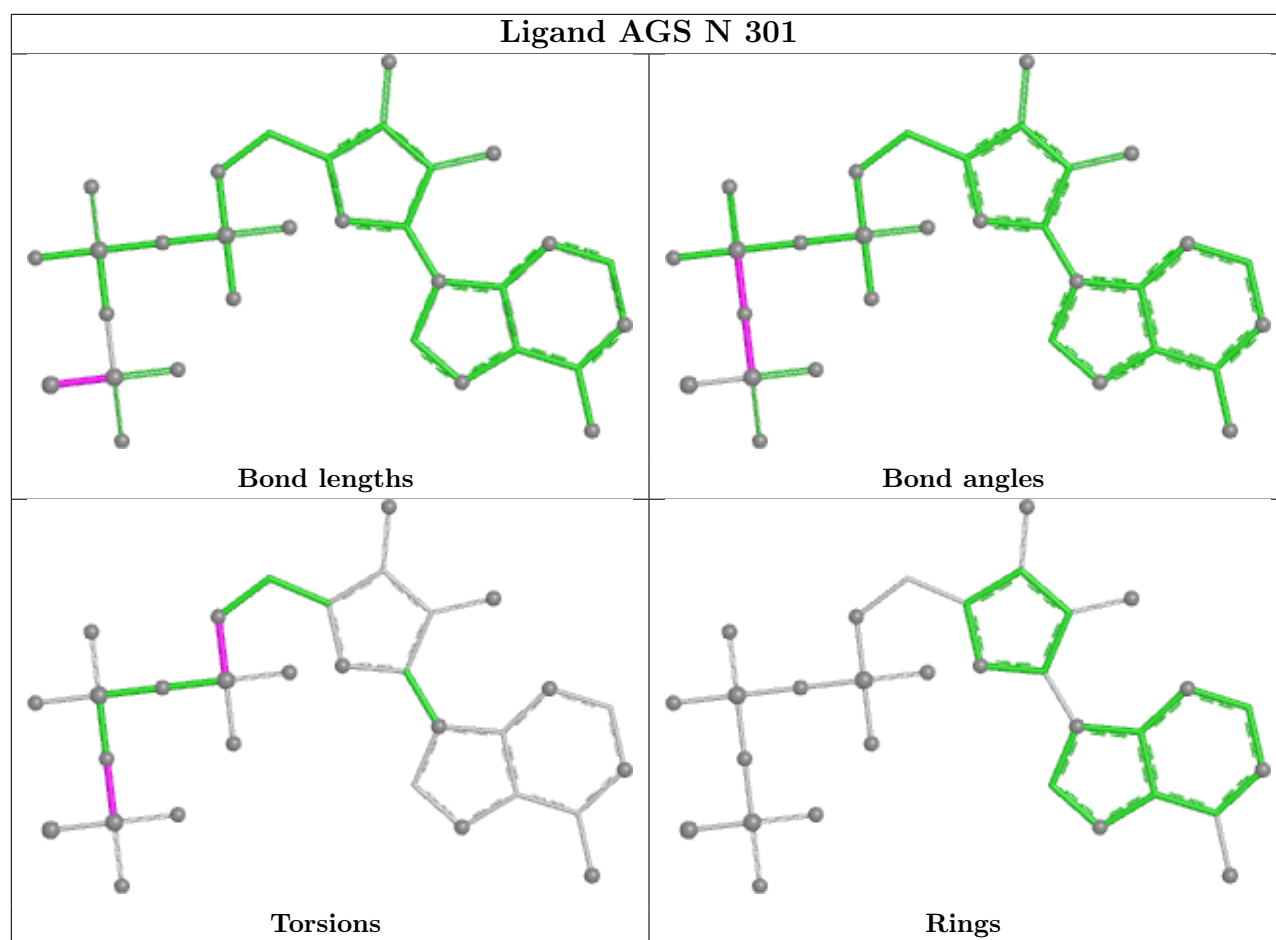
Mol	Chain	Res	Type	Atoms
4	5	301	AGS	PB-O3B-PG-O2G
4	5	301	AGS	PB-O3B-PG-O3G
4	5	301	AGS	C5'-O5'-PA-O1A
4	5	301	AGS	O4'-C4'-C5'-O5'
4	6	301	AGS	PB-O3B-PG-O2G

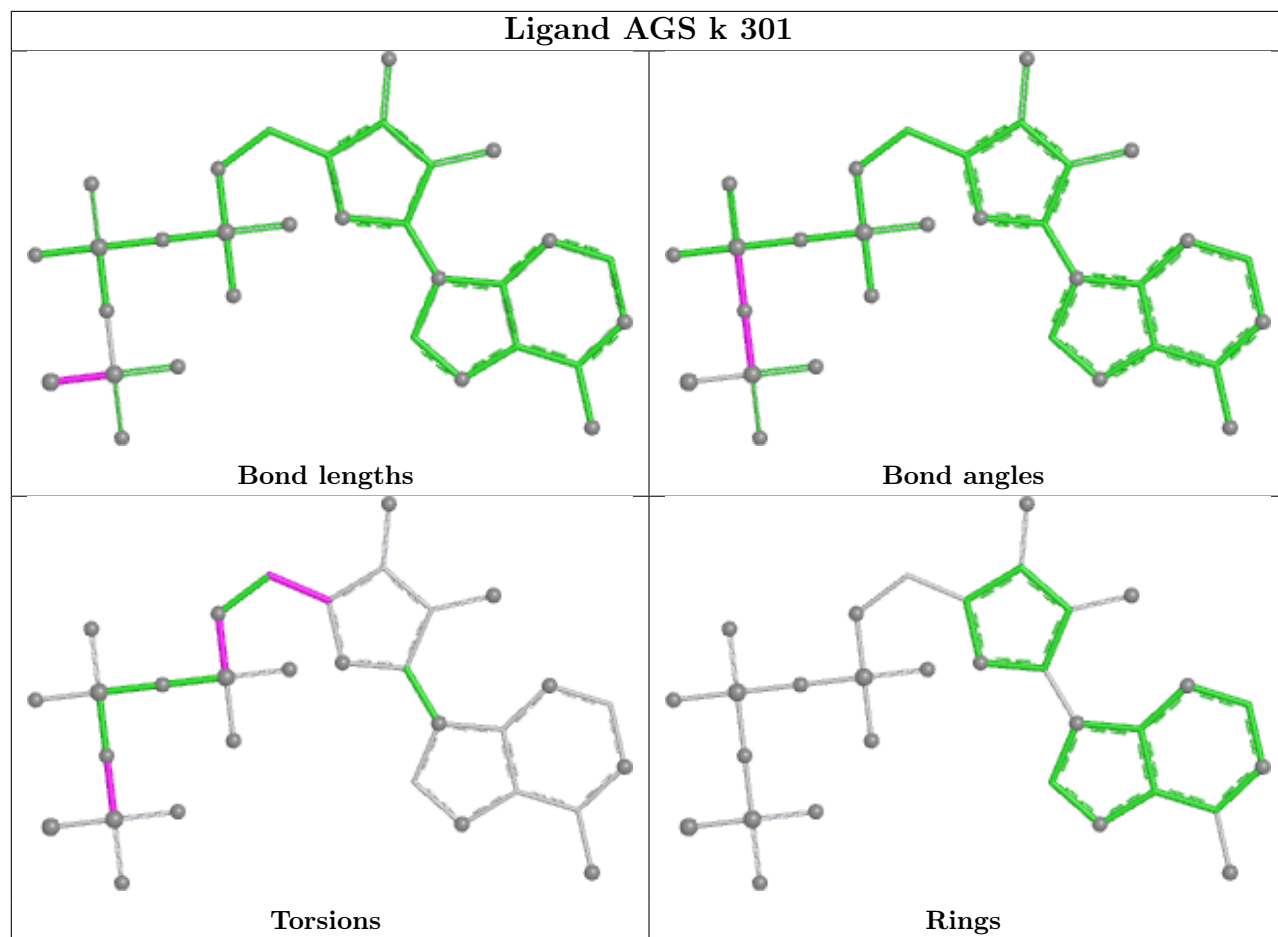
There are no ring outliers.

2 monomers are involved in 2 short contacts:

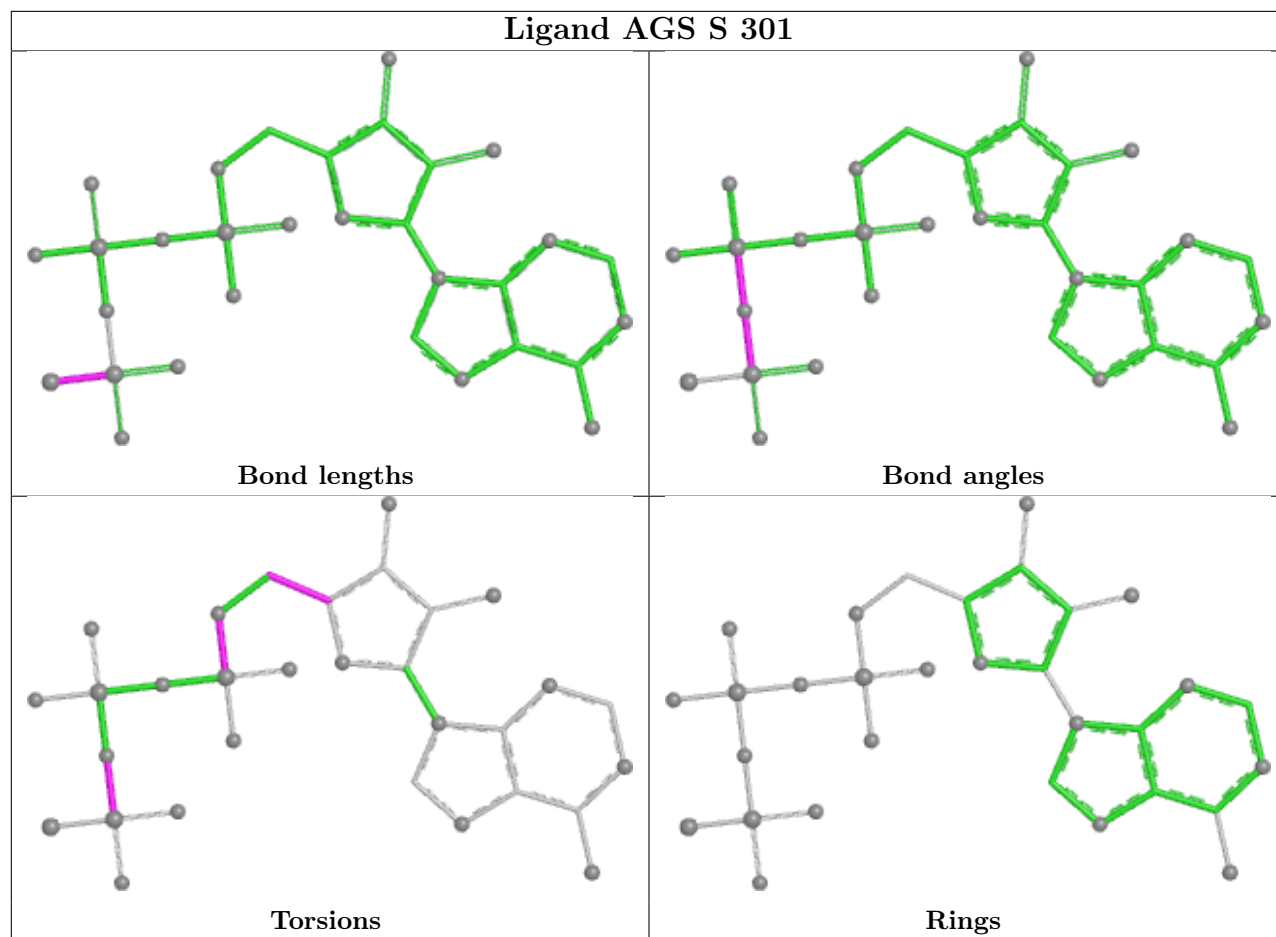
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	301	AGS	1	0
4	T	301	AGS	1	0

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 than 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.

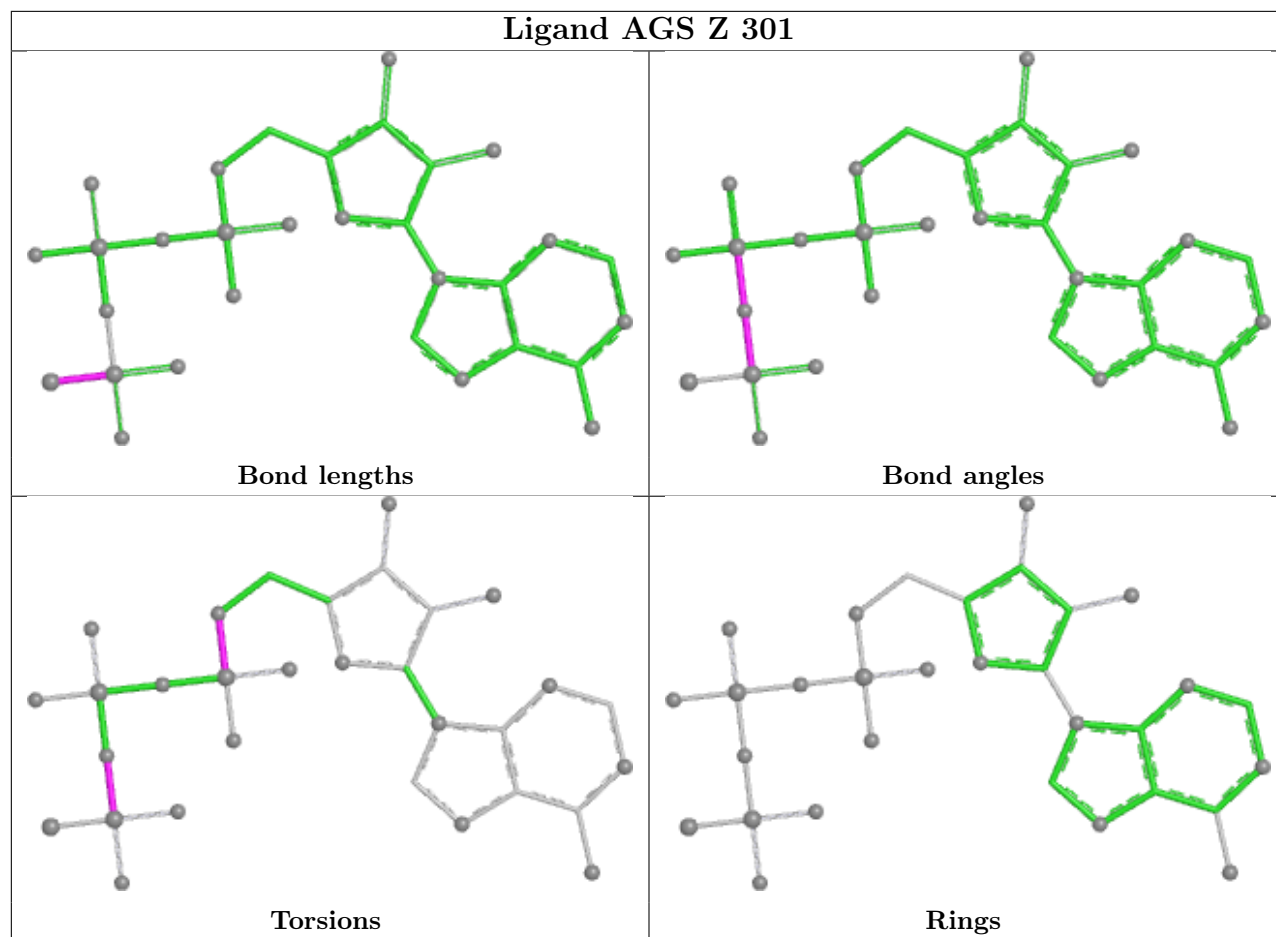


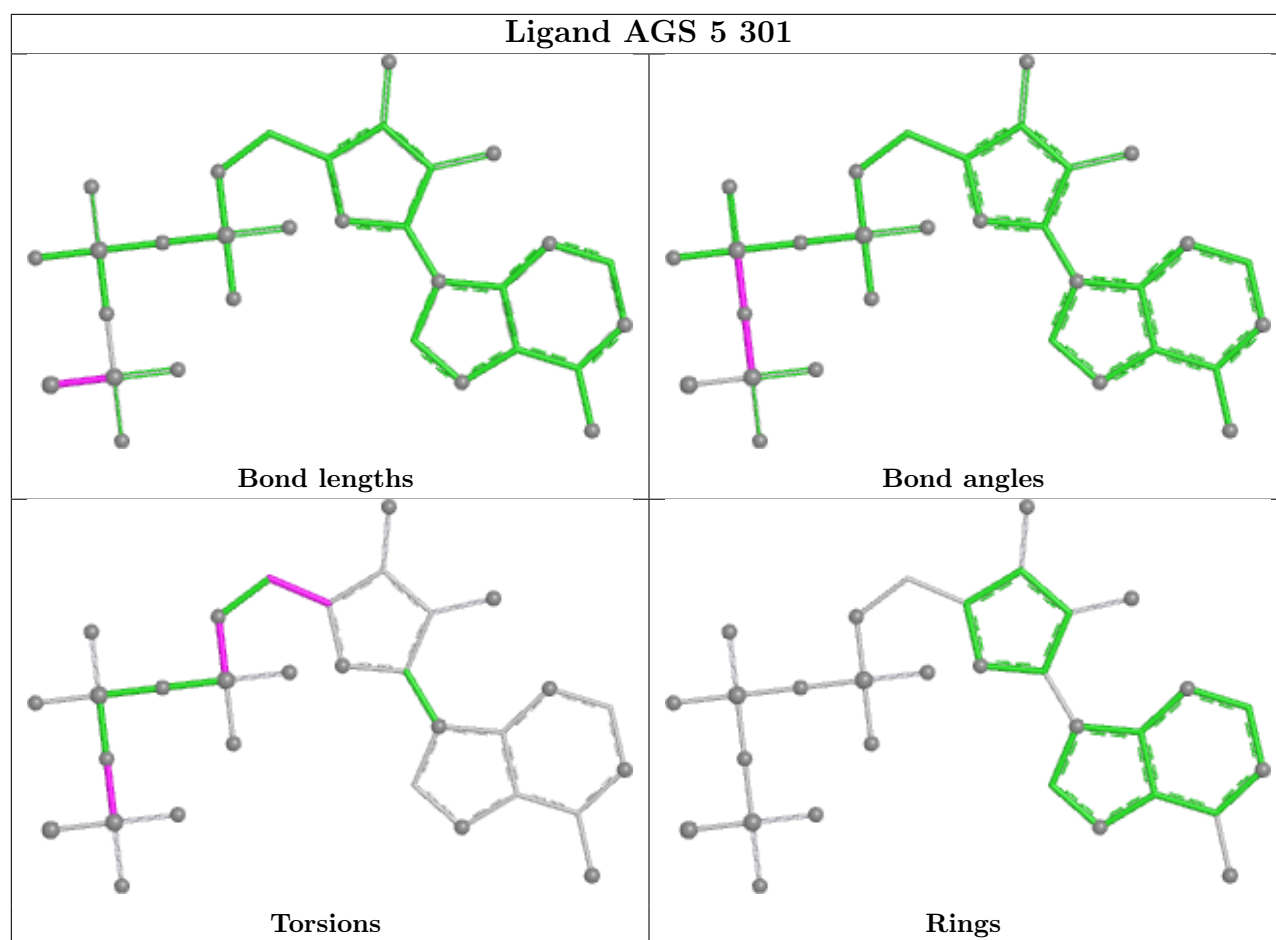


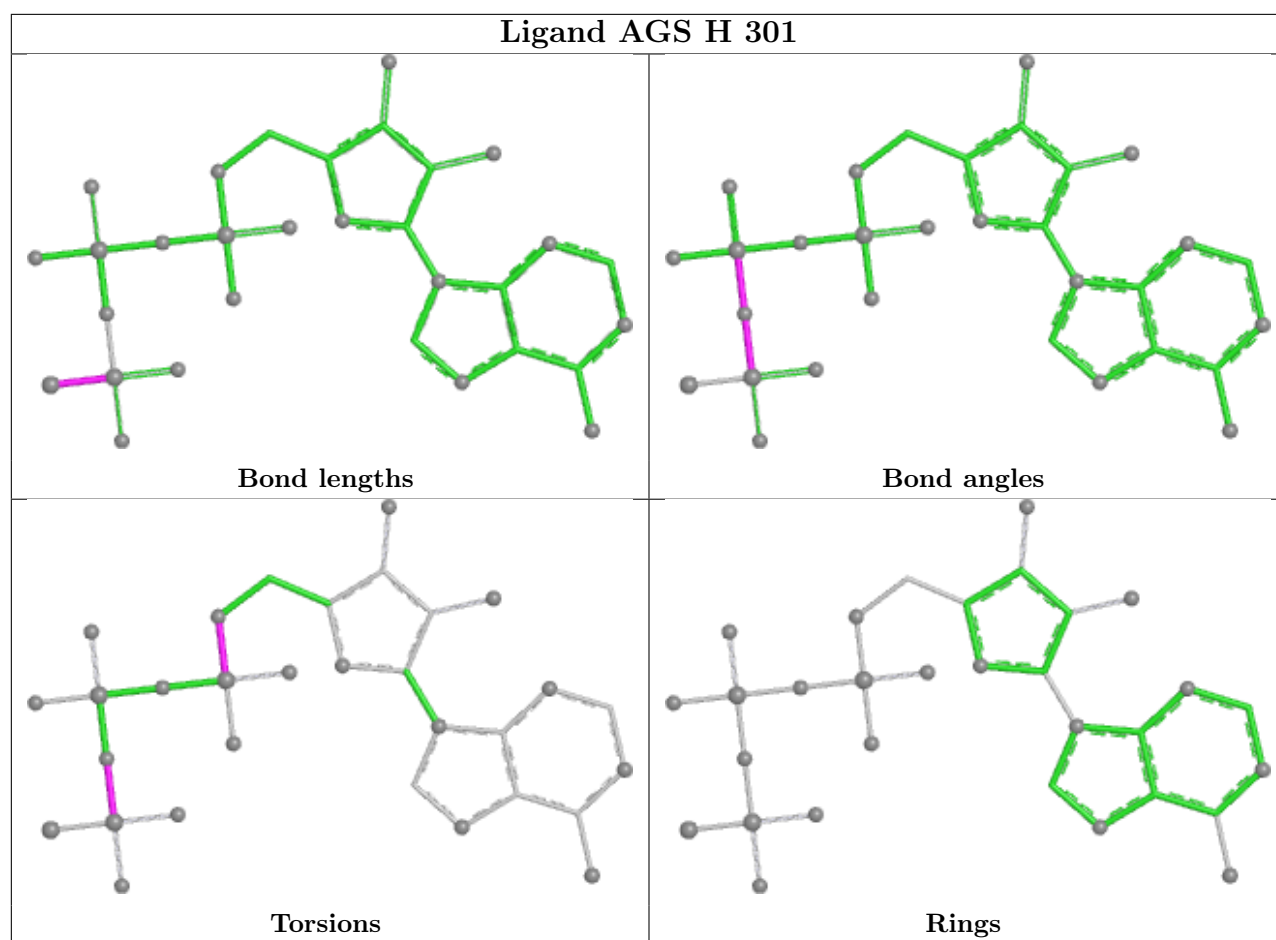
Ligand AGS S 301

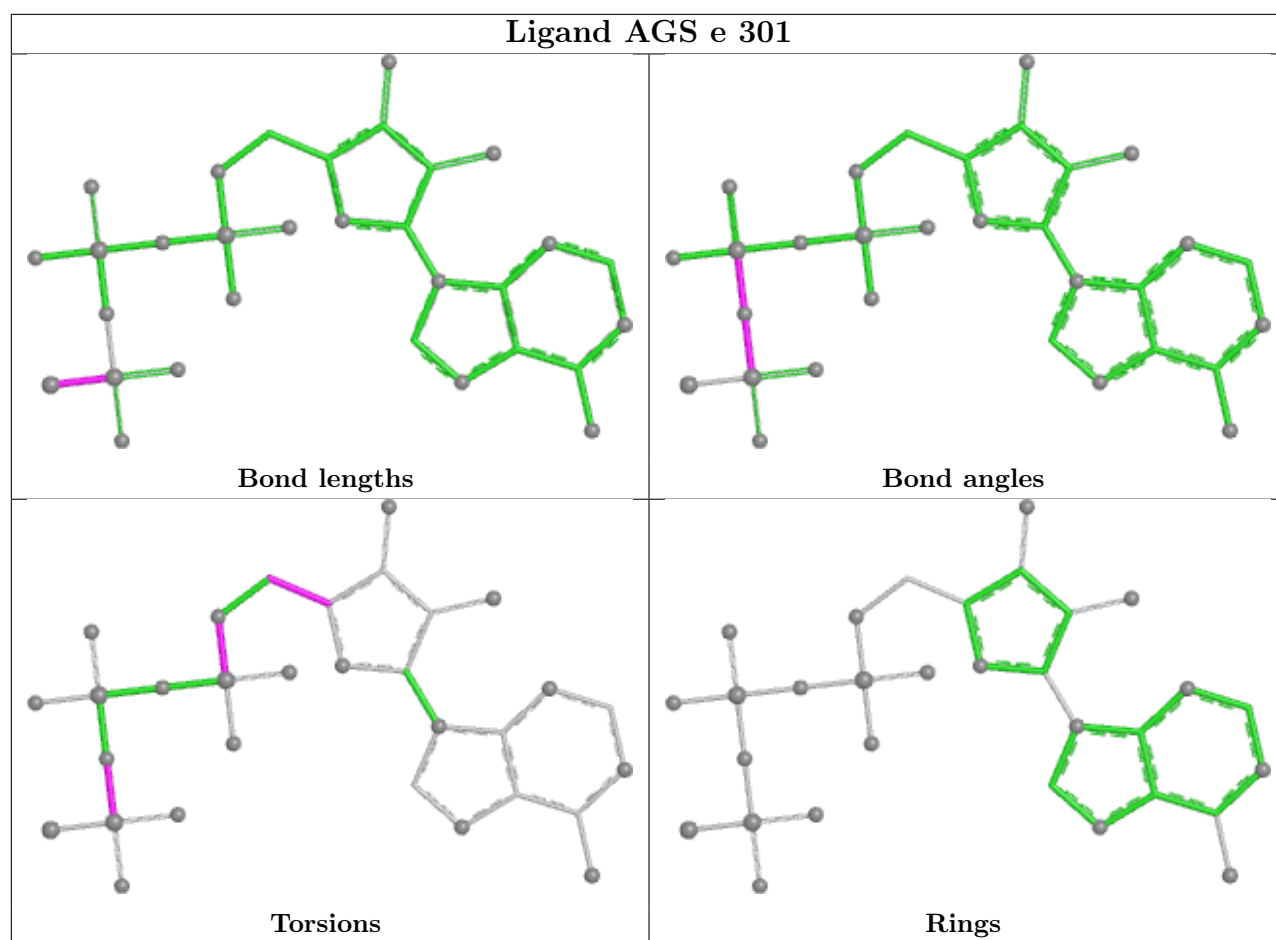


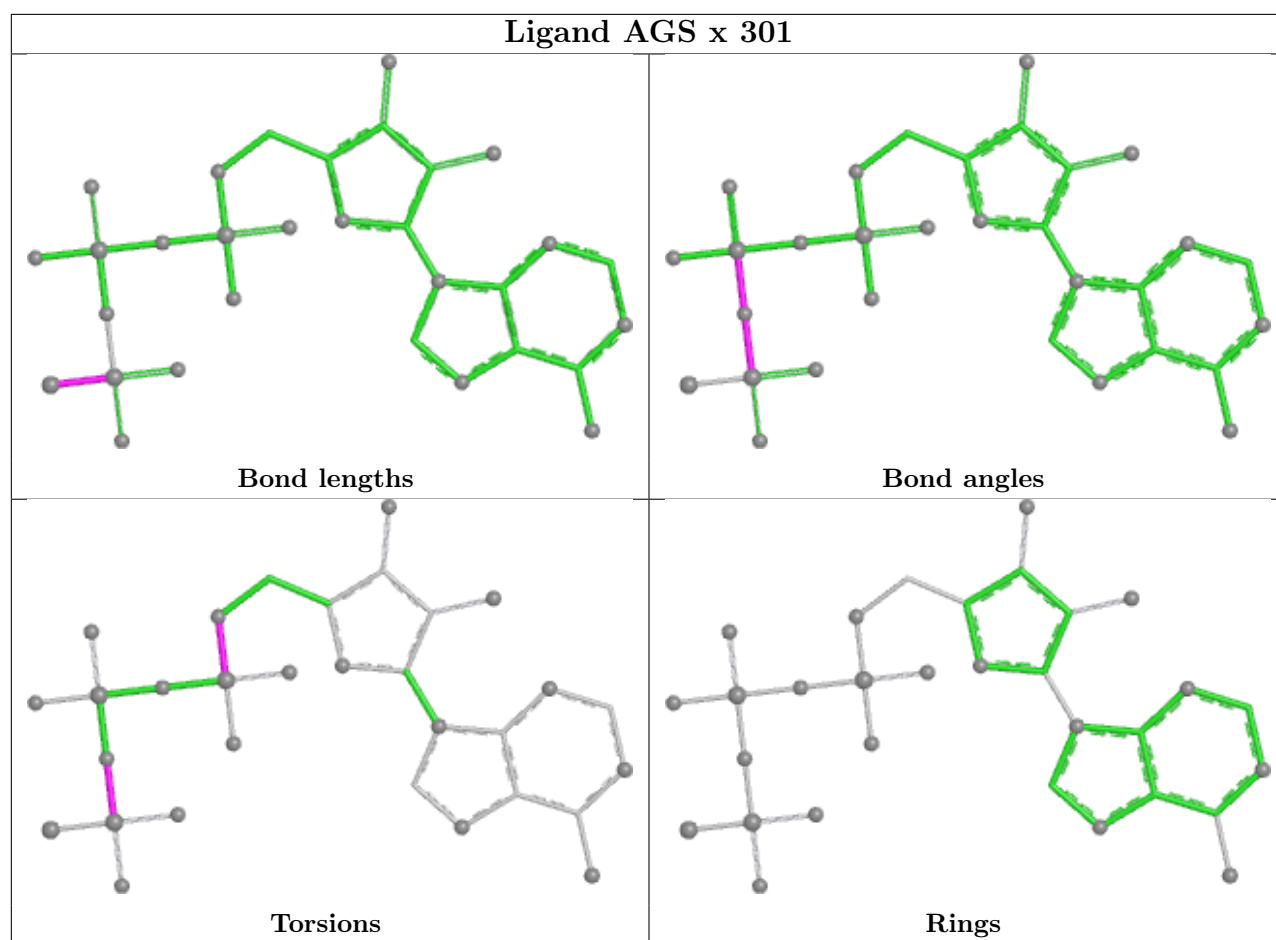
Ligand AGS Z 301



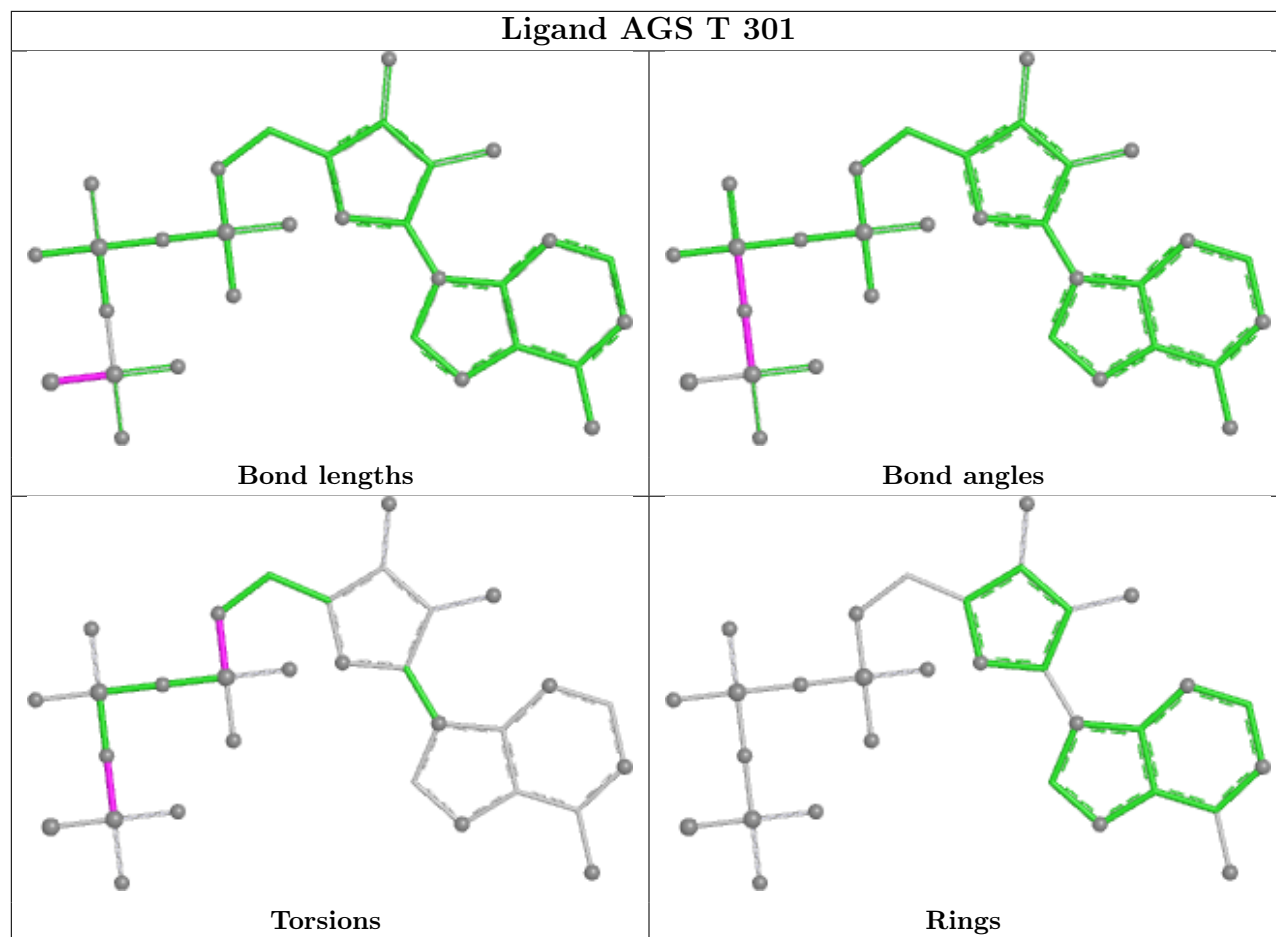


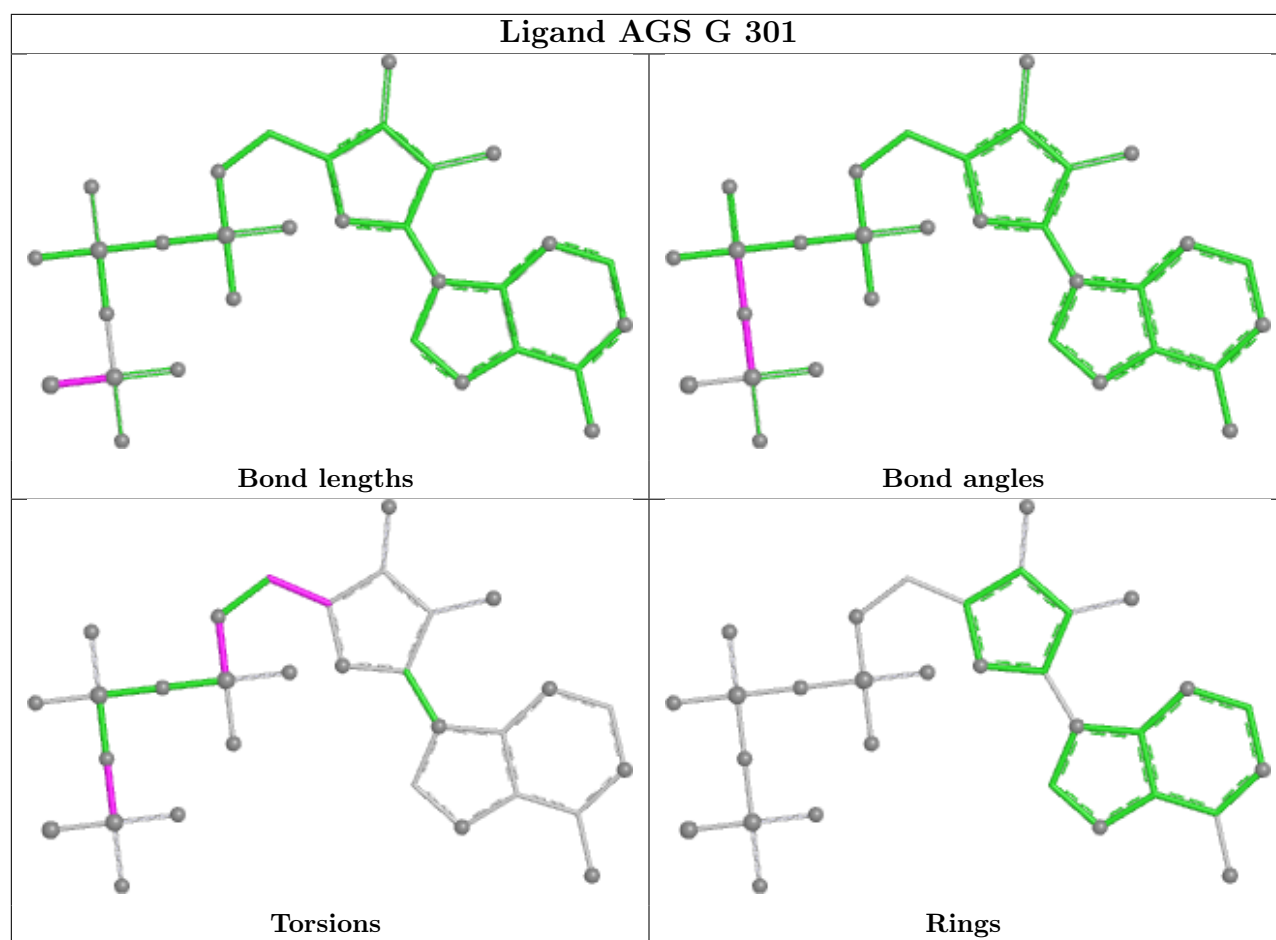


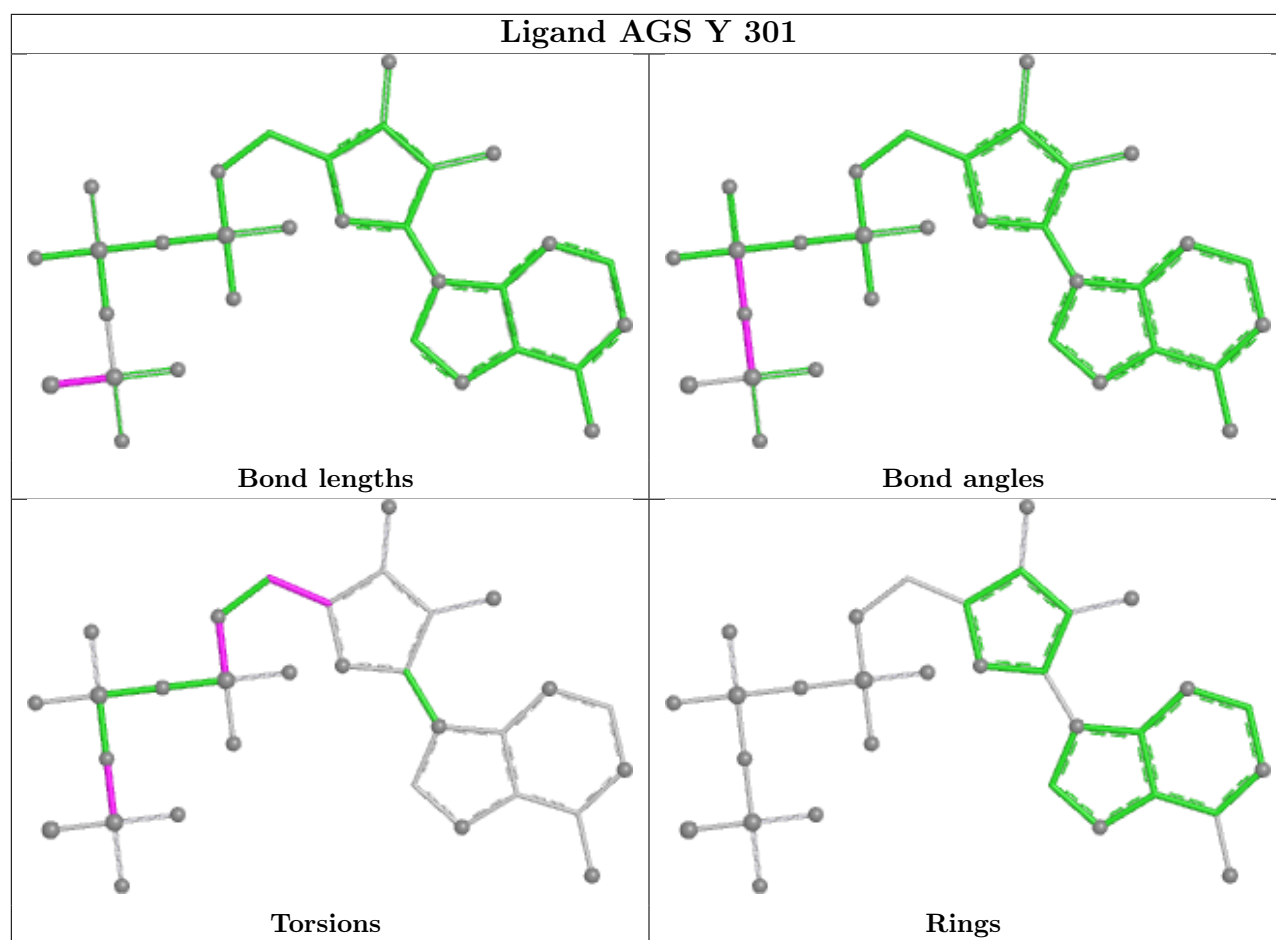


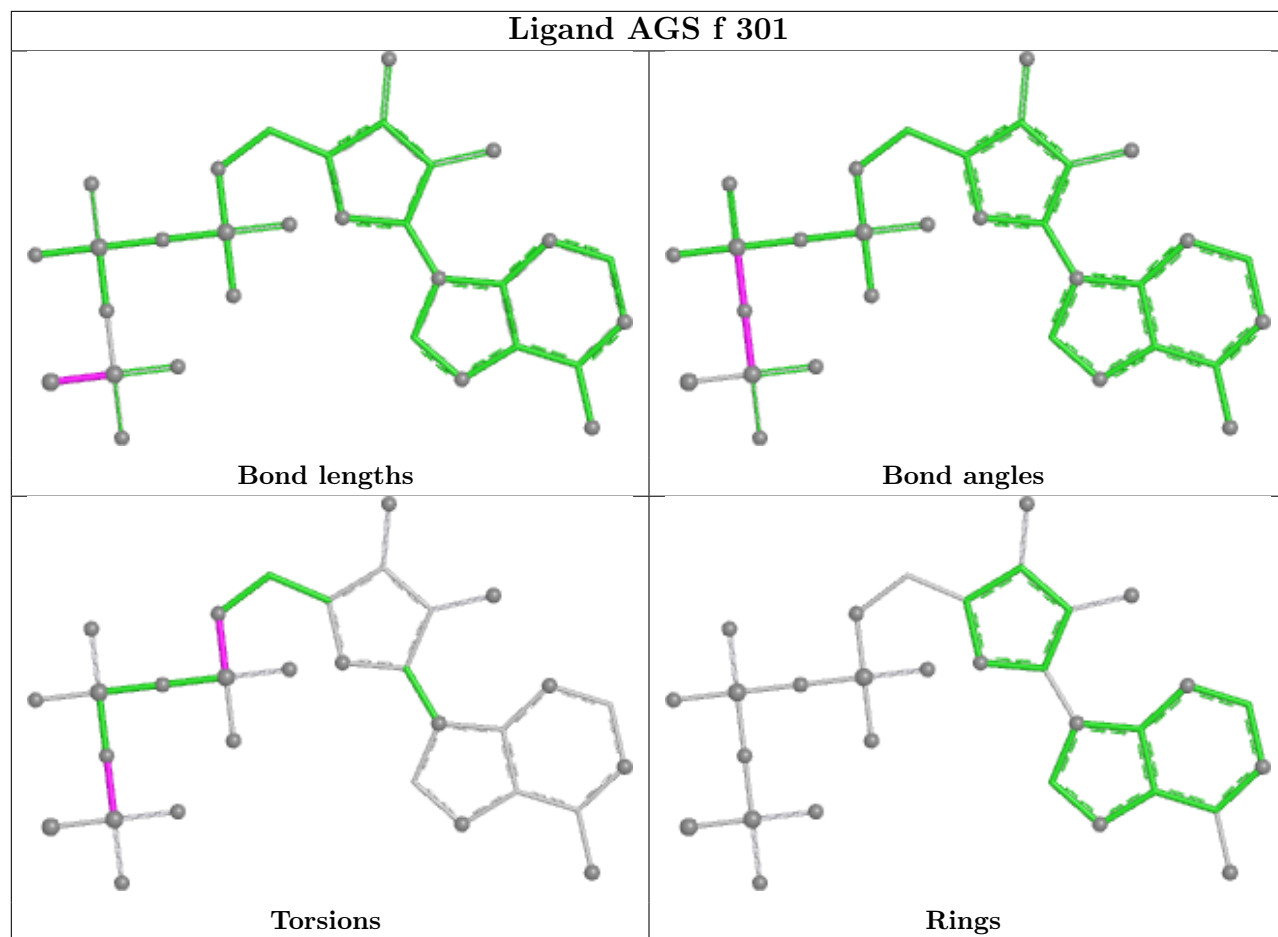


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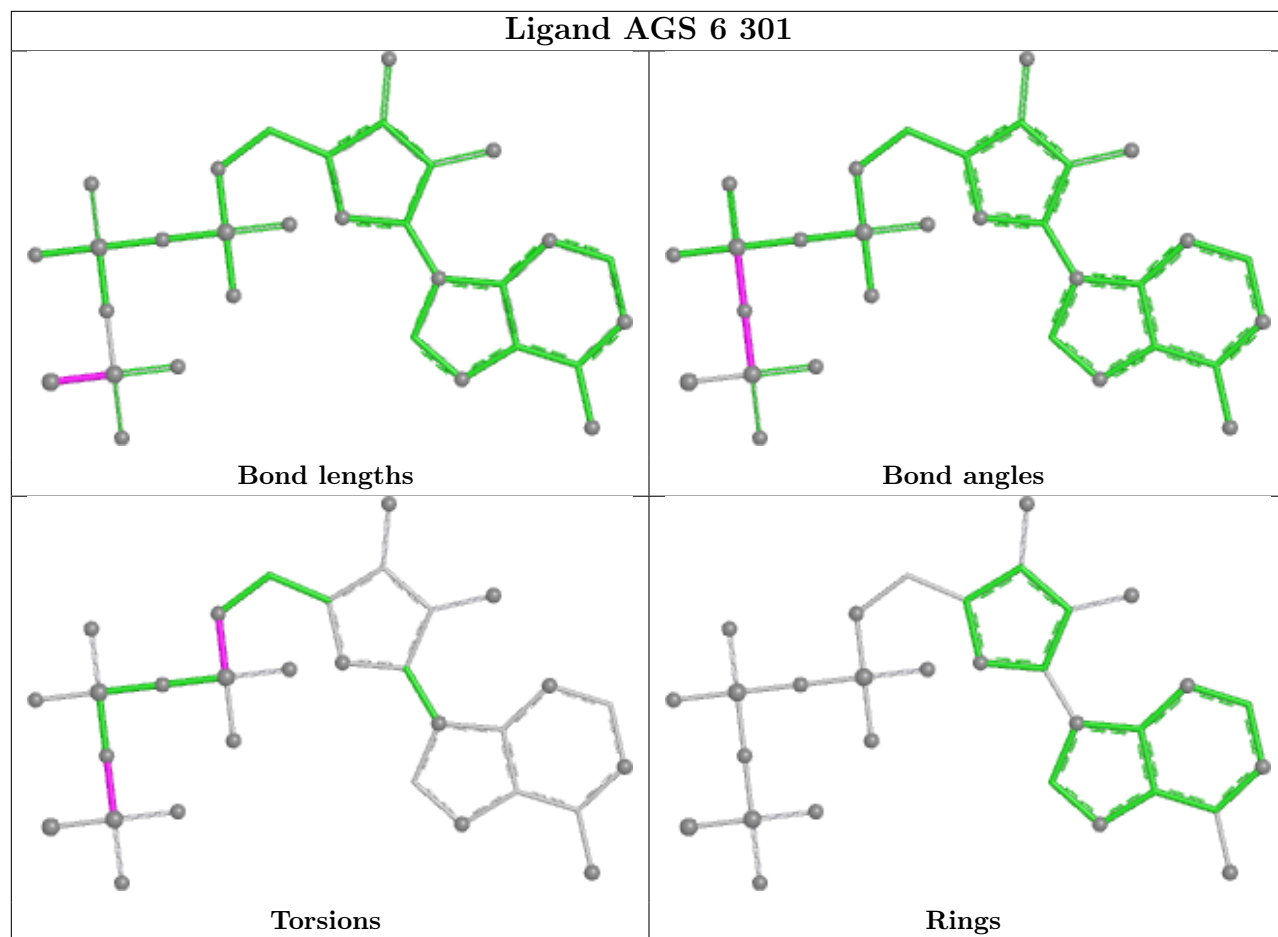


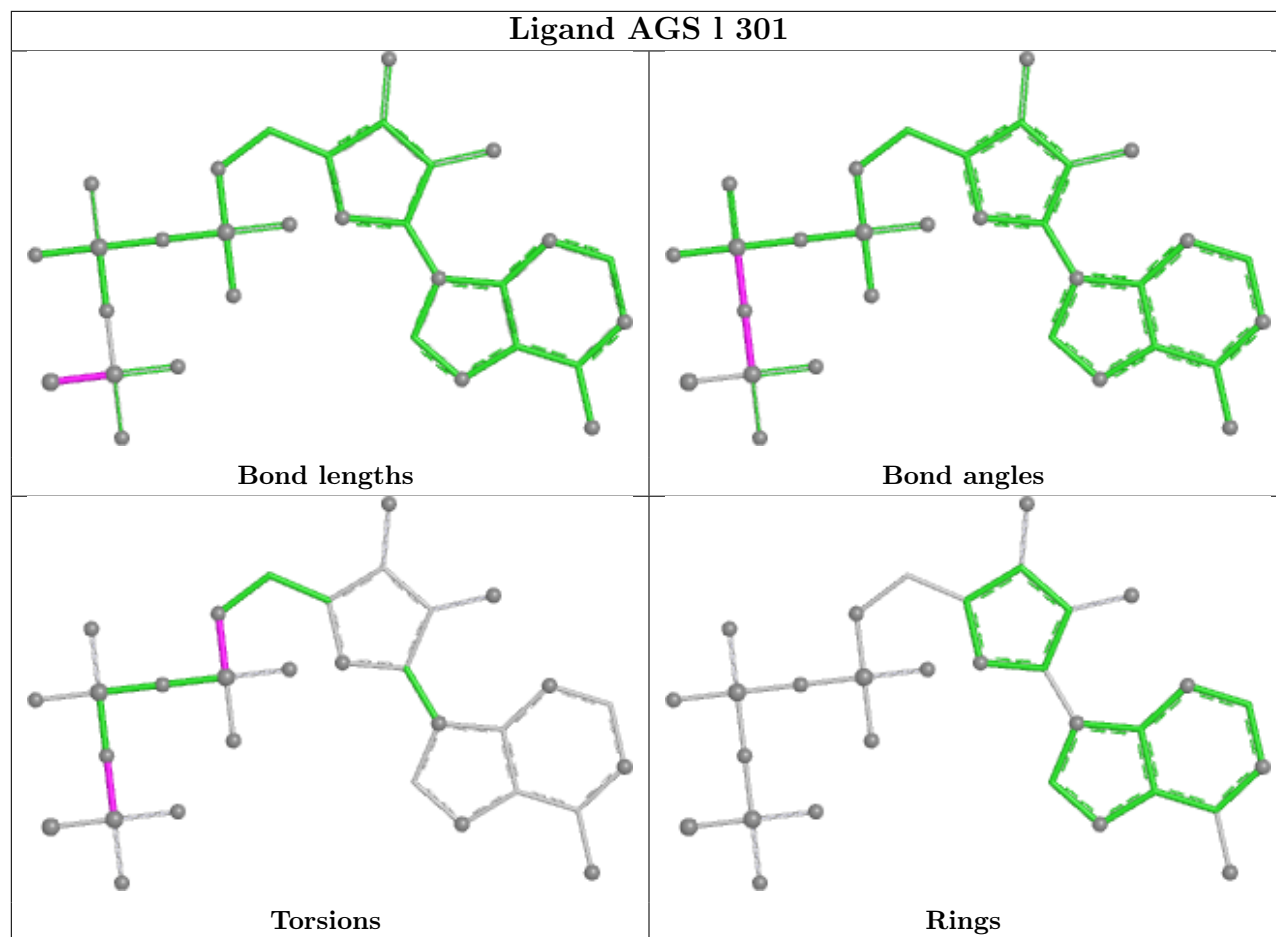


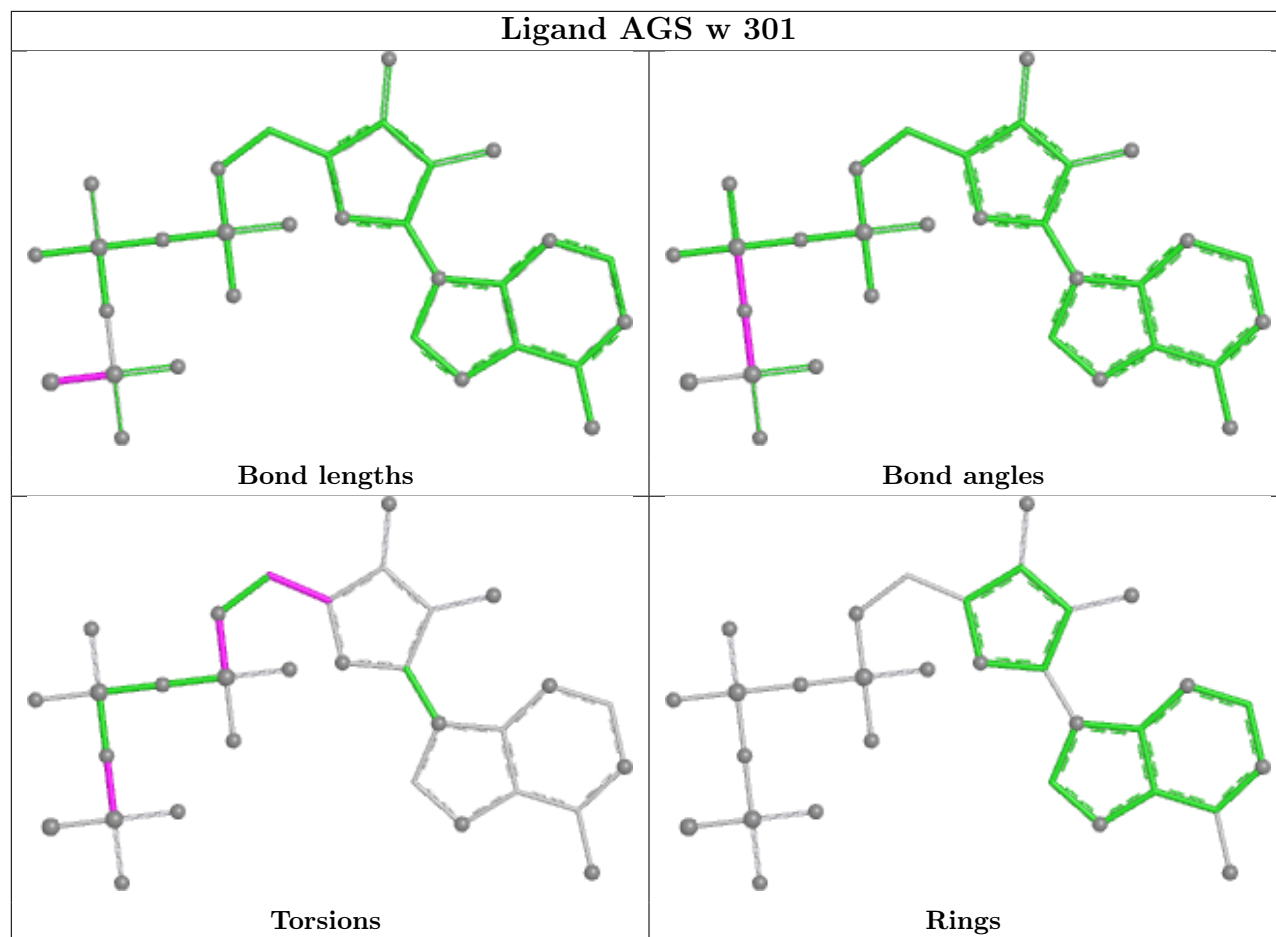




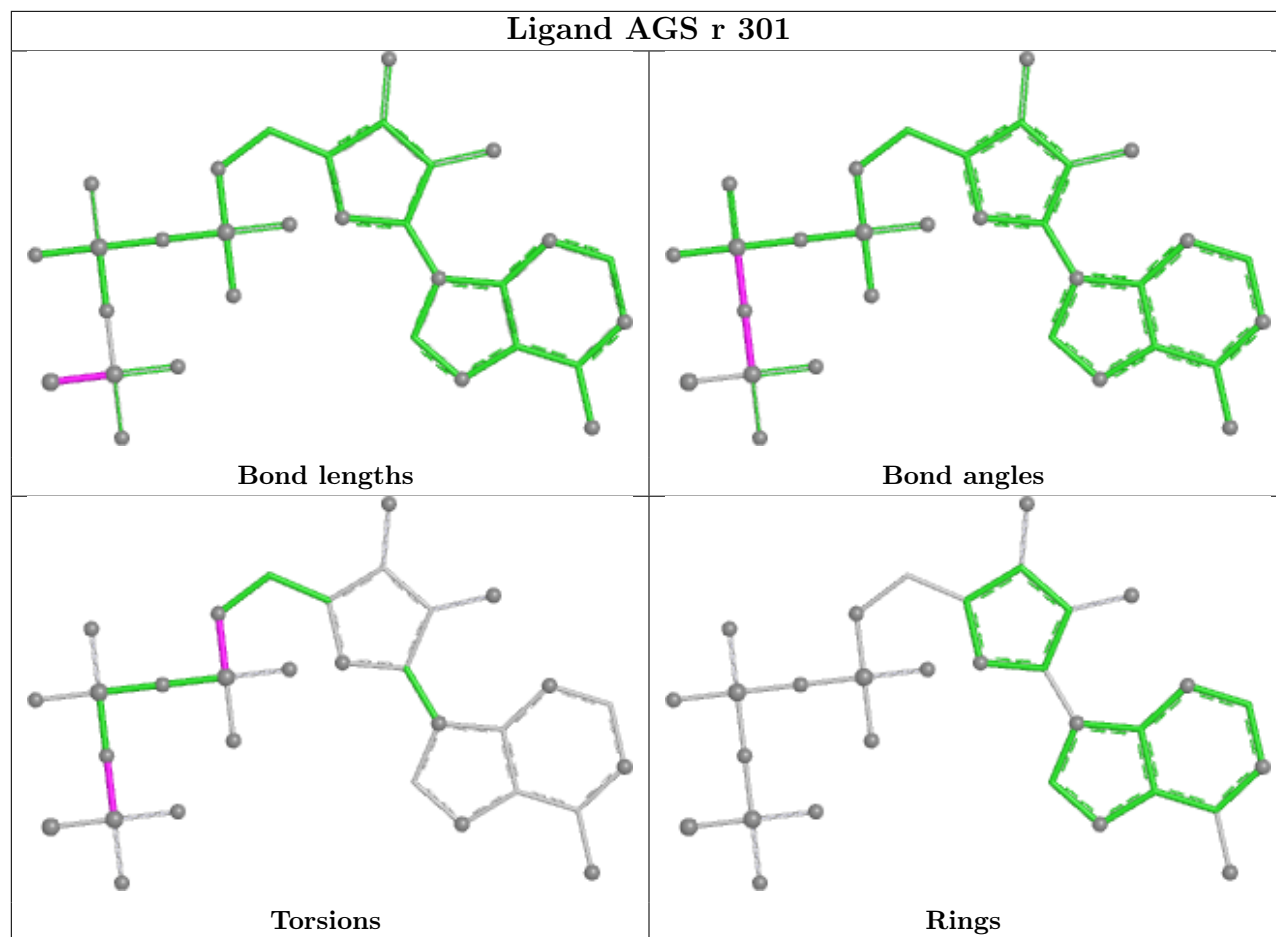
Ligand AGS 6 301

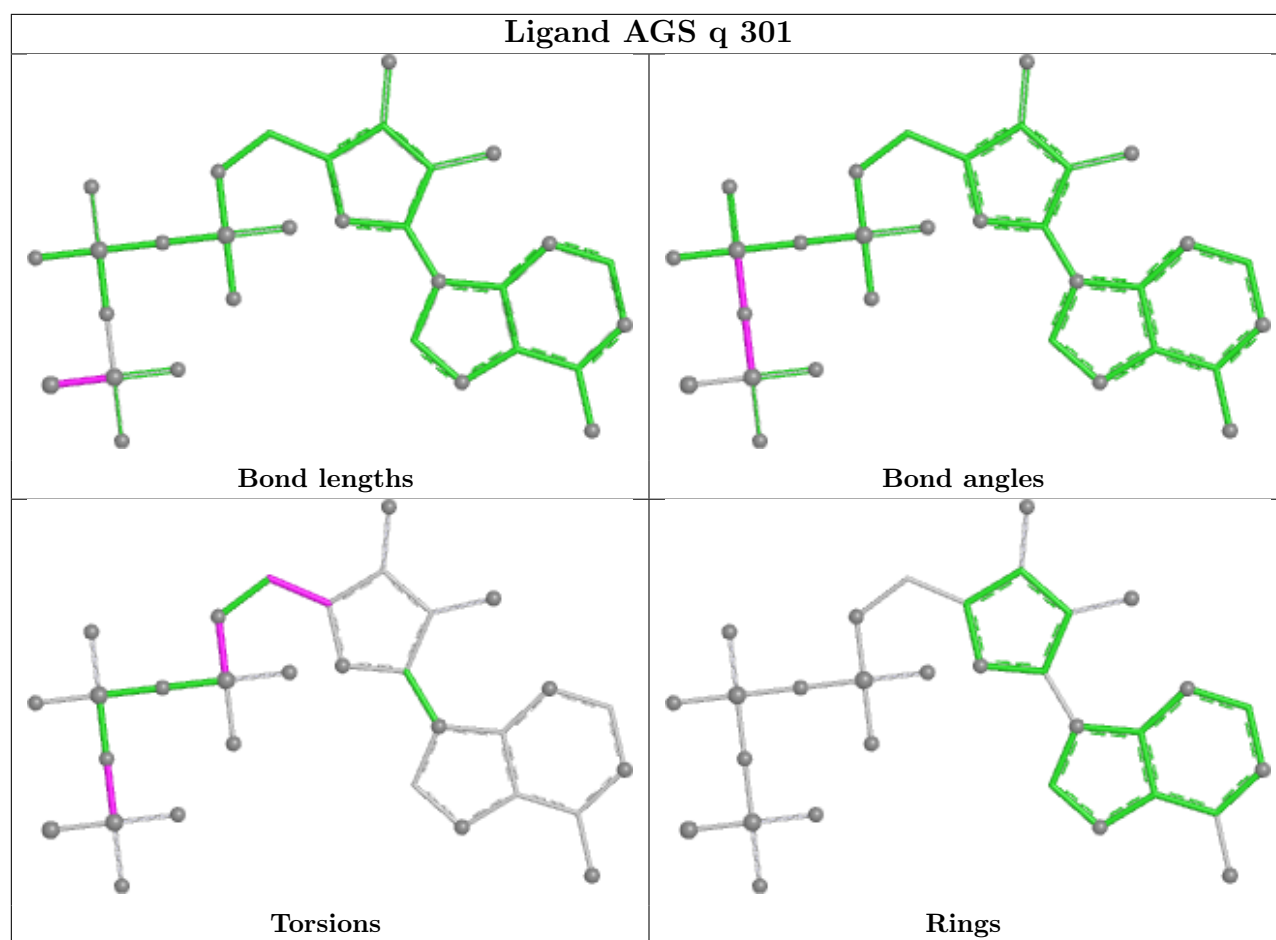


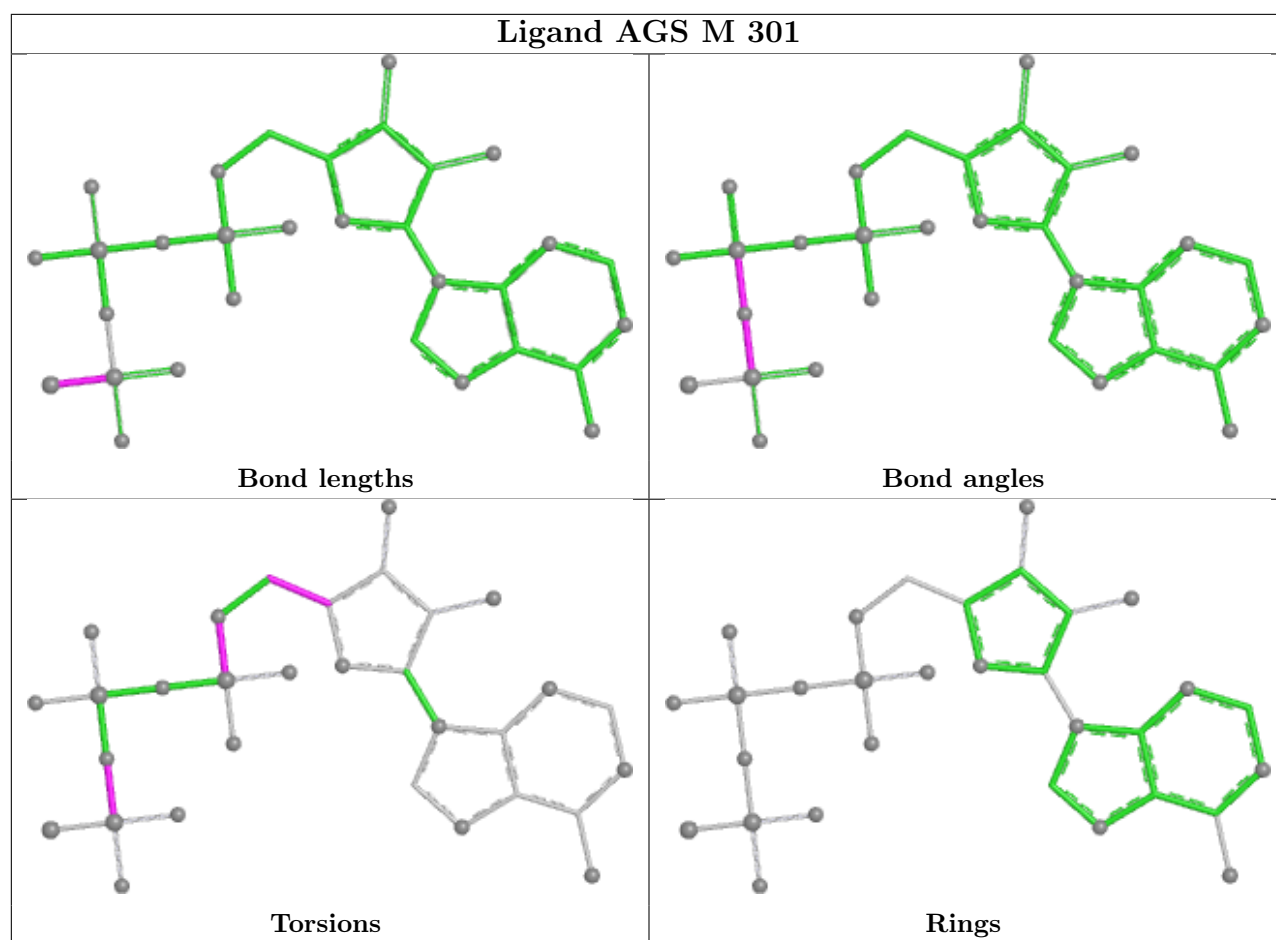




Ligand AGS r 301







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.

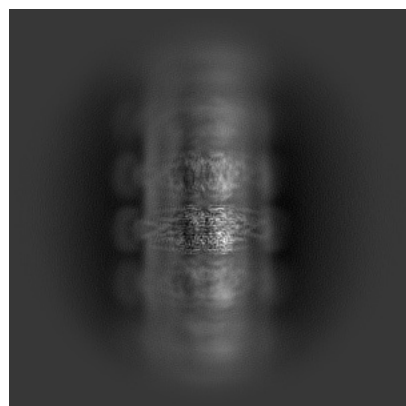
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60898. These allow visual inspection of the internal detail of the map and identification of artifacts.

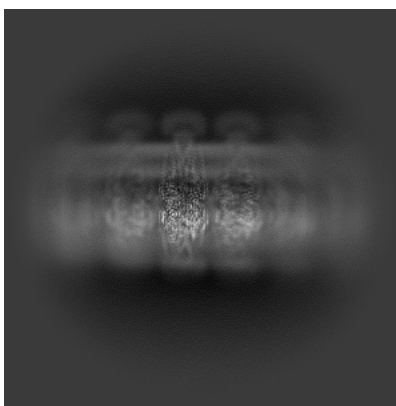
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

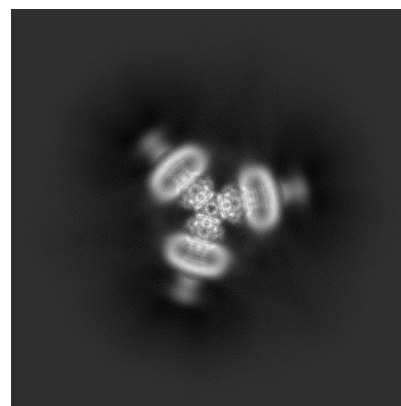
6.1.1 Primary map



X

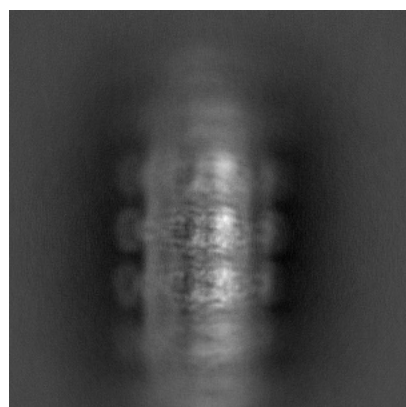


Y

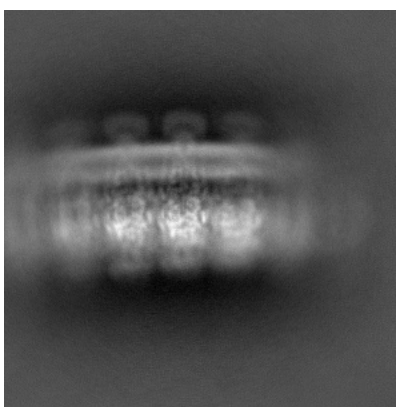


Z

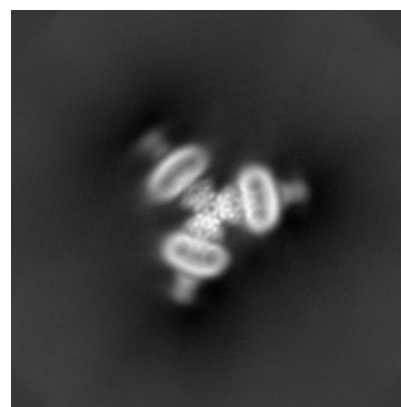
6.1.2 Raw map



X



Y

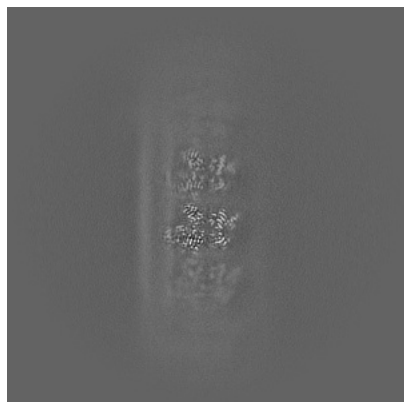


Z

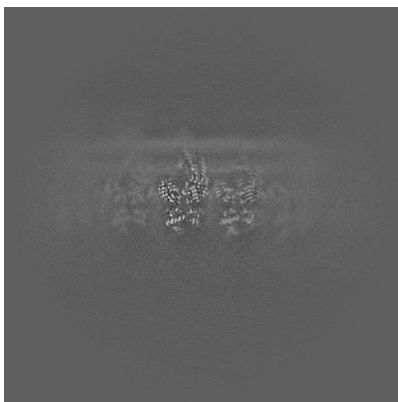
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

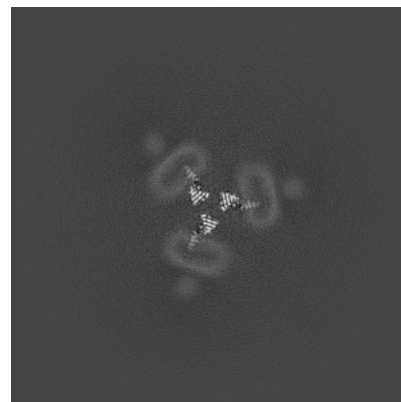
6.2.1 Primary map



X Index: 256

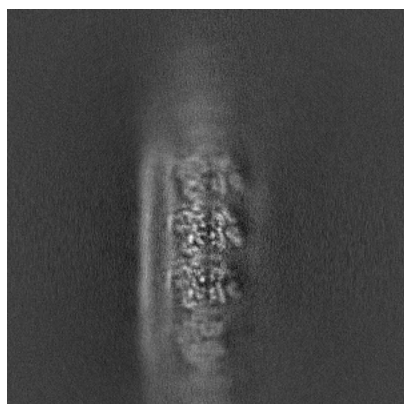


Y Index: 256

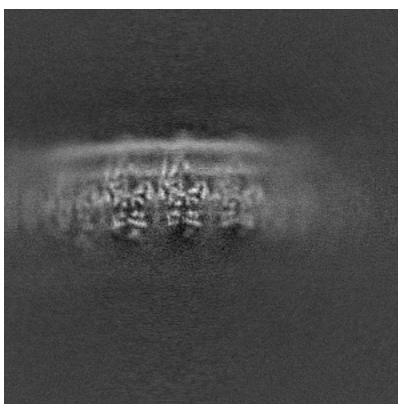


Z Index: 256

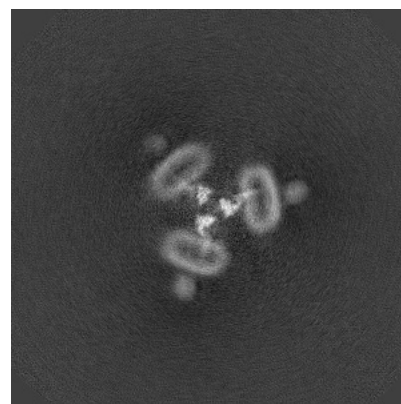
6.2.2 Raw map



X Index: 256



Y Index: 256

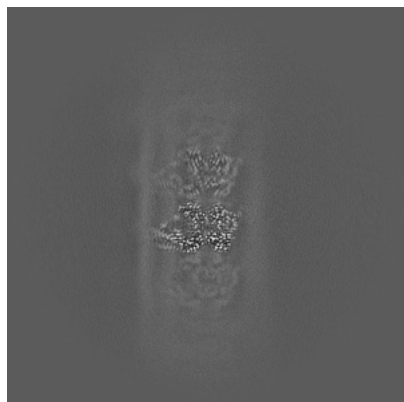


Z Index: 256

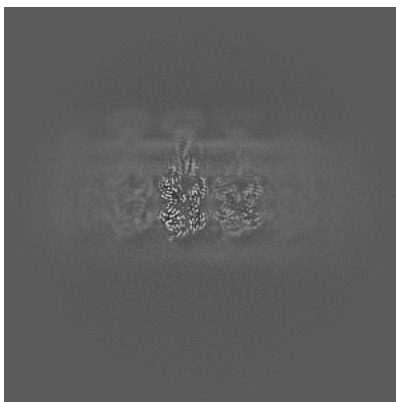
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

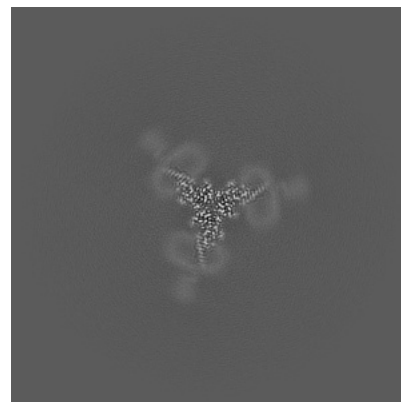
6.3.1 Primary map



X Index: 248

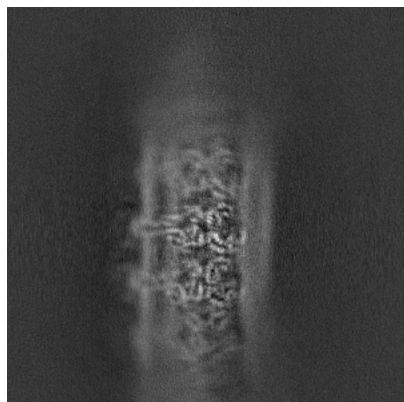


Y Index: 266

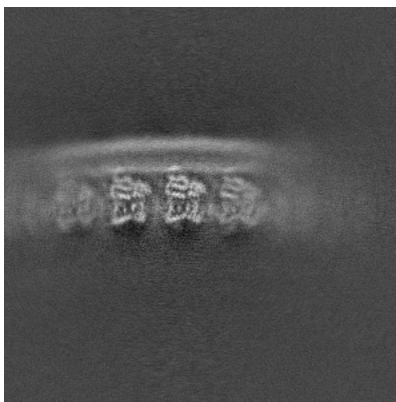


Z Index: 215

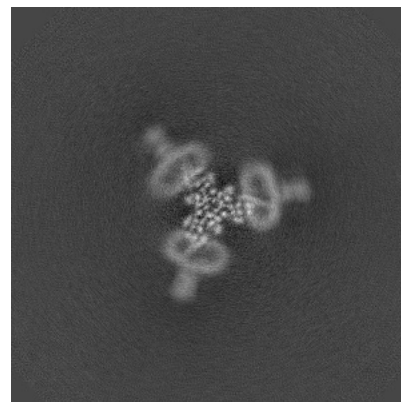
6.3.2 Raw map



X Index: 239



Y Index: 248

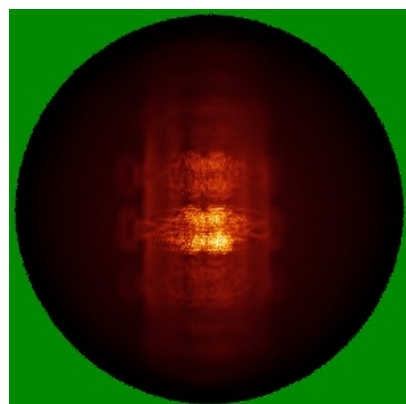


Z Index: 216

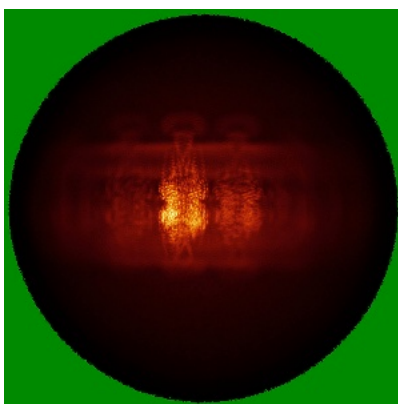
The images above show the largest variance slices of the map in three orthogonal directions.

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

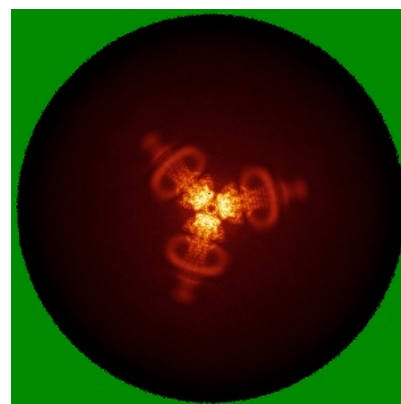
6.4.1 Primary map



X

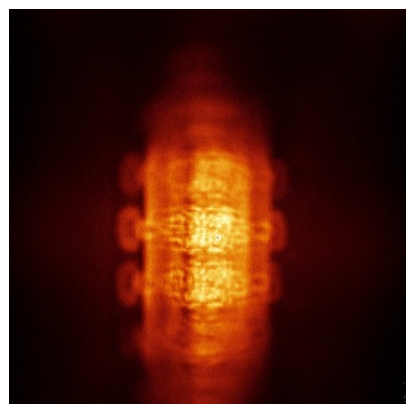


Y

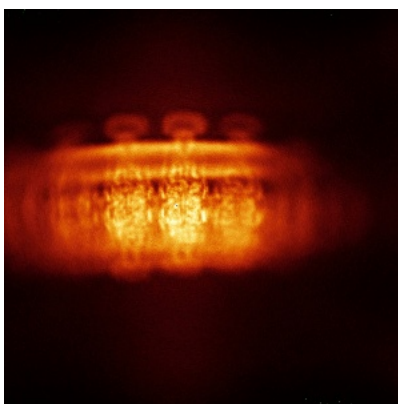


Z

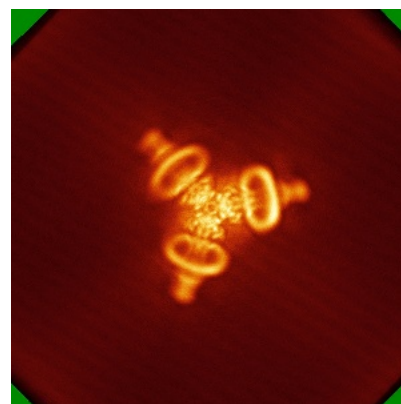
6.4.2 Raw map



X



Y

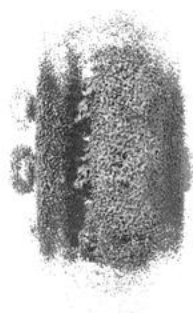


Z

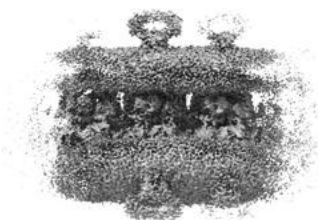
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



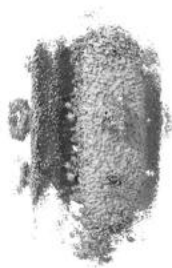
Y



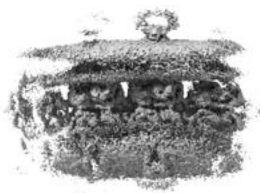
Z

The images above show the 3D surface view of the map at the recommended contour level 0.123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

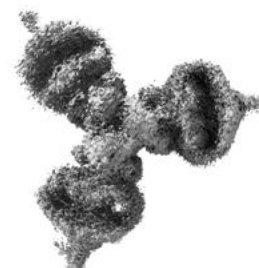
6.5.2 Raw map



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.

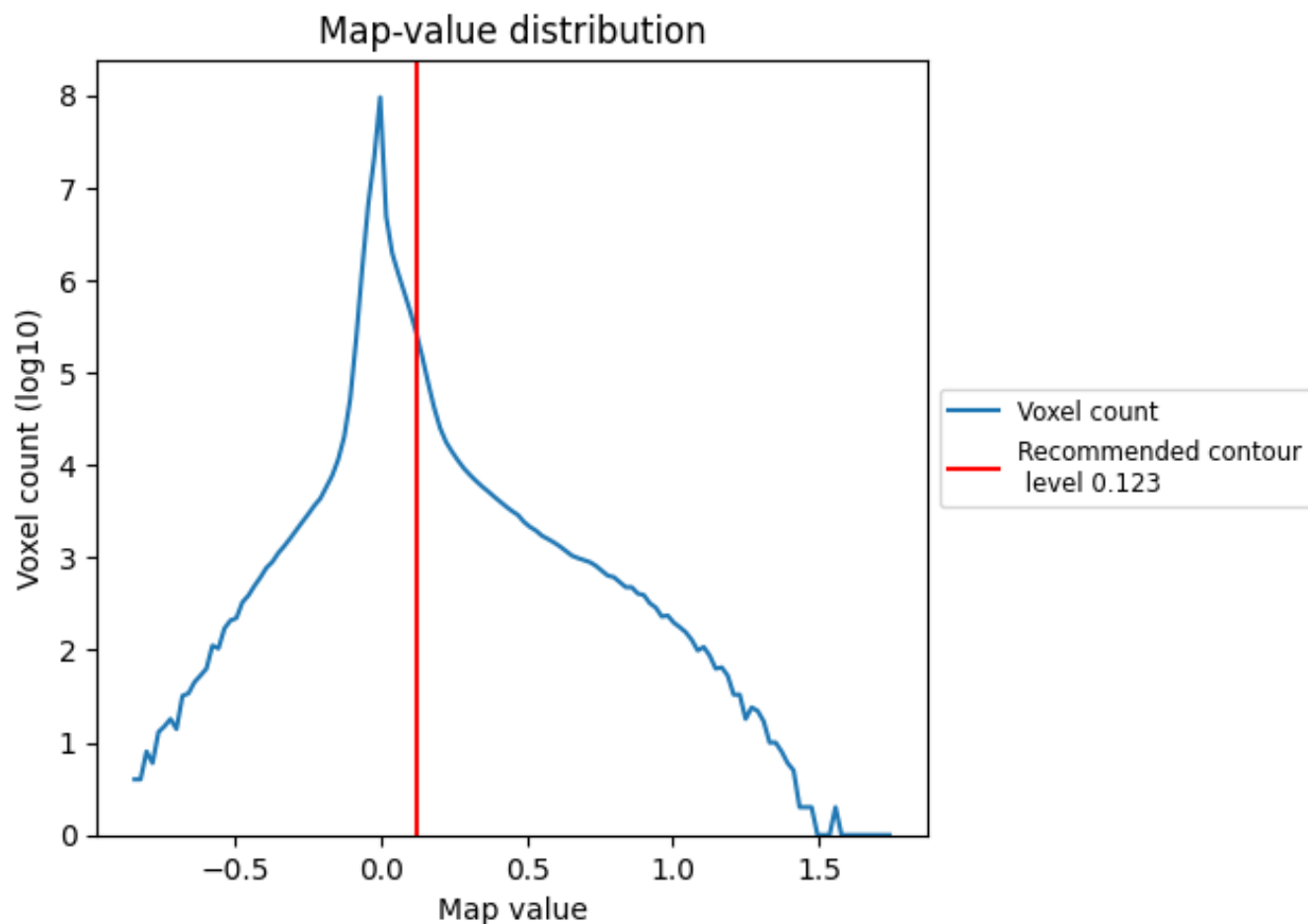
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

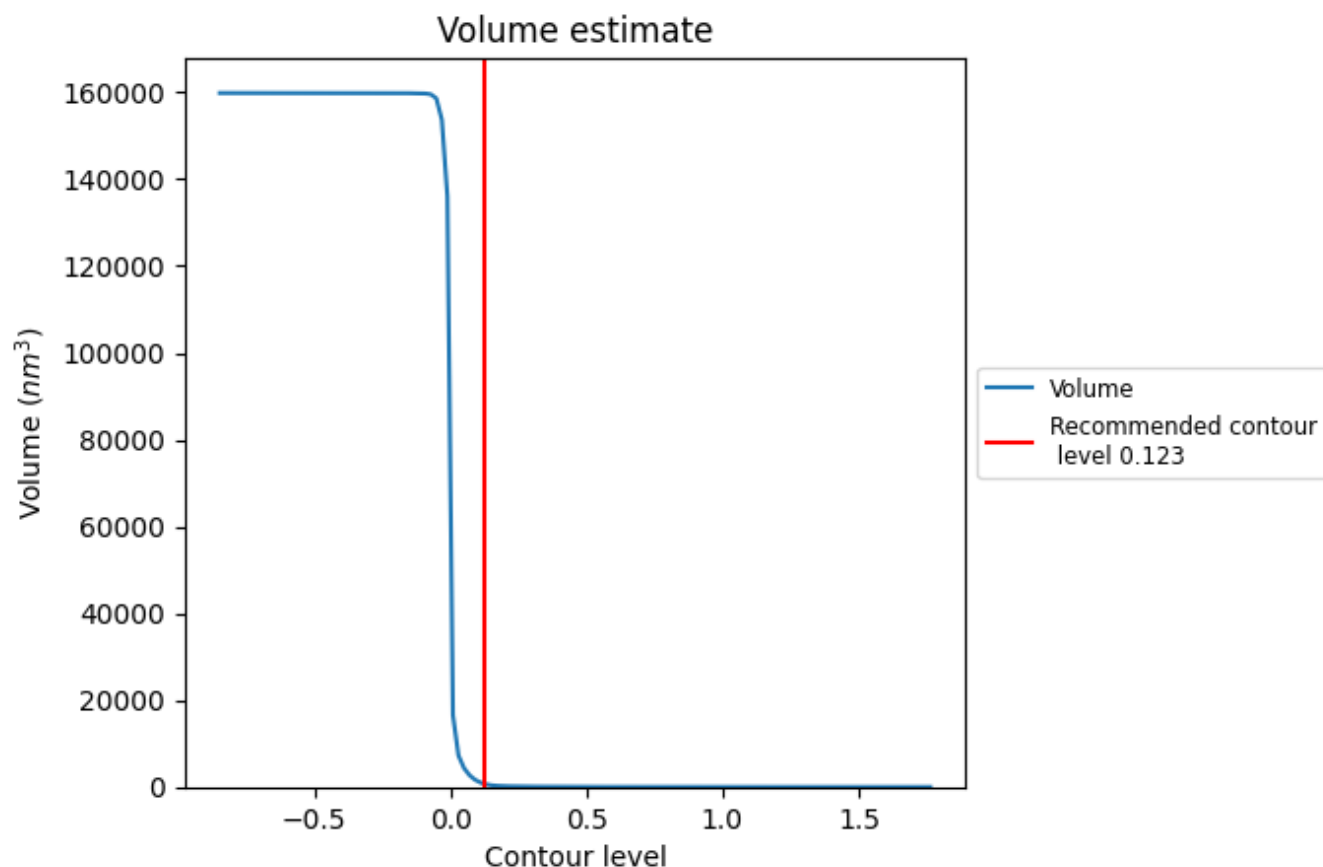
This section contains the results of statistical analysis of the map.

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.

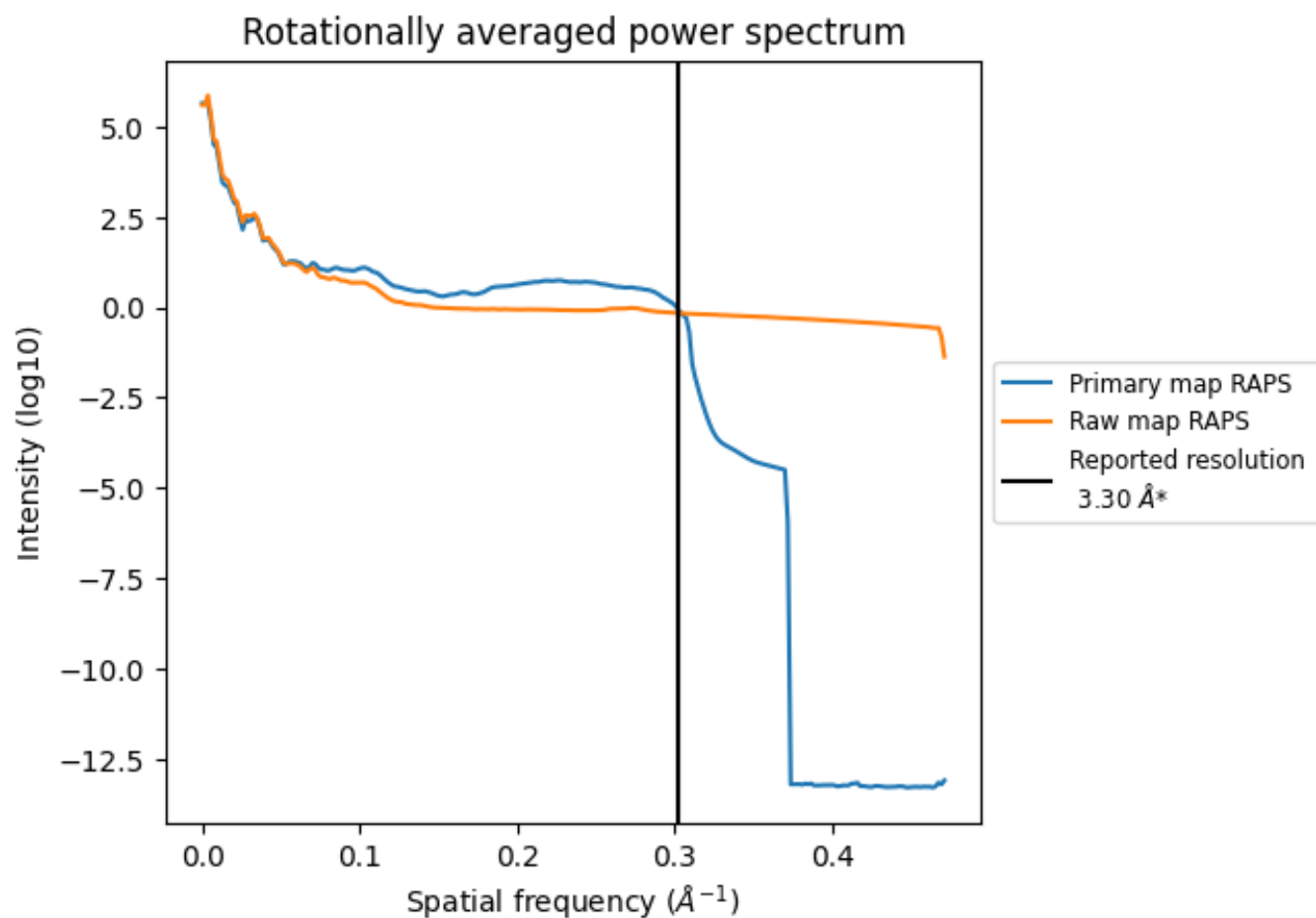
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 777 nm³; this corresponds to an approximate mass of 701 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

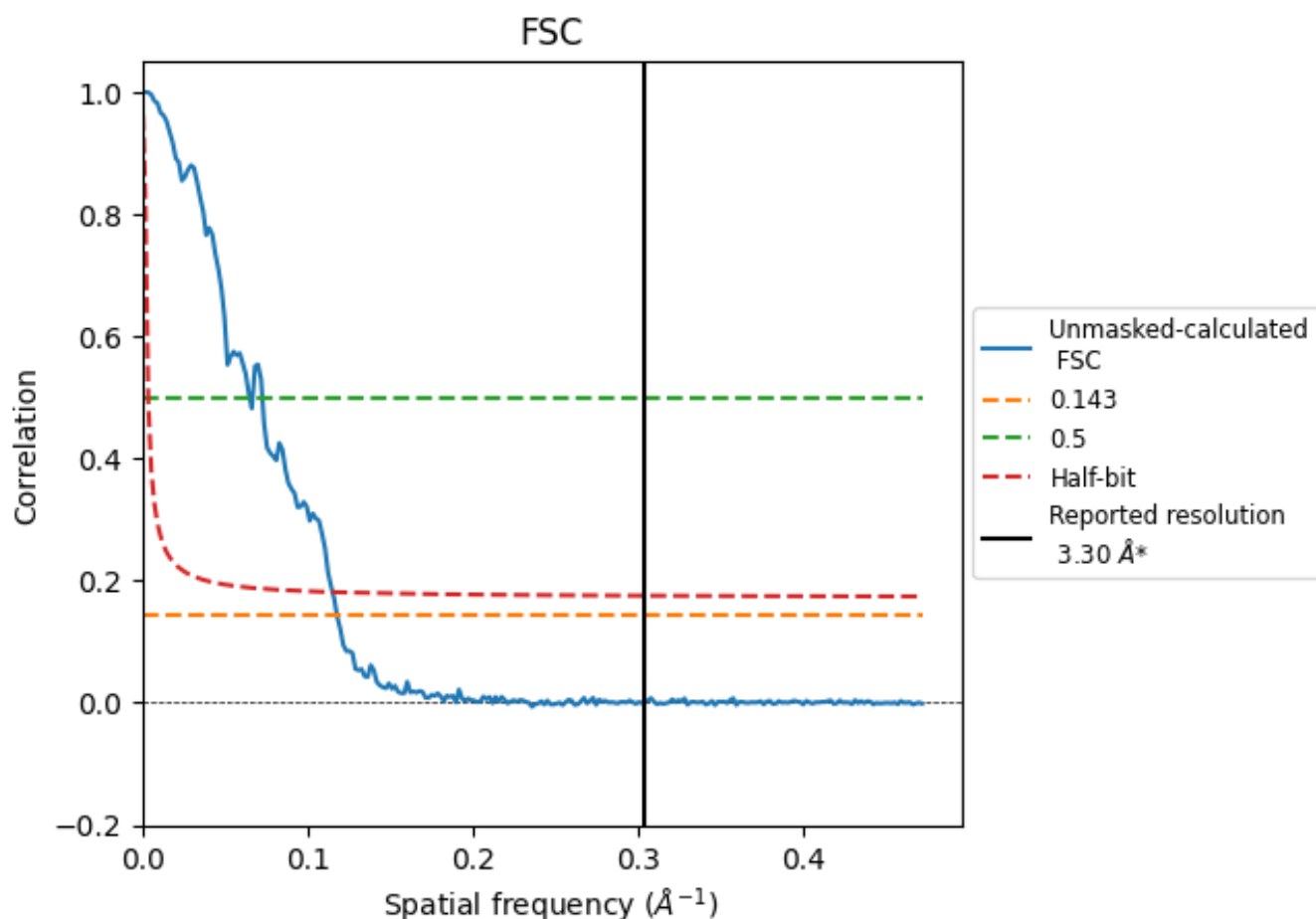


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

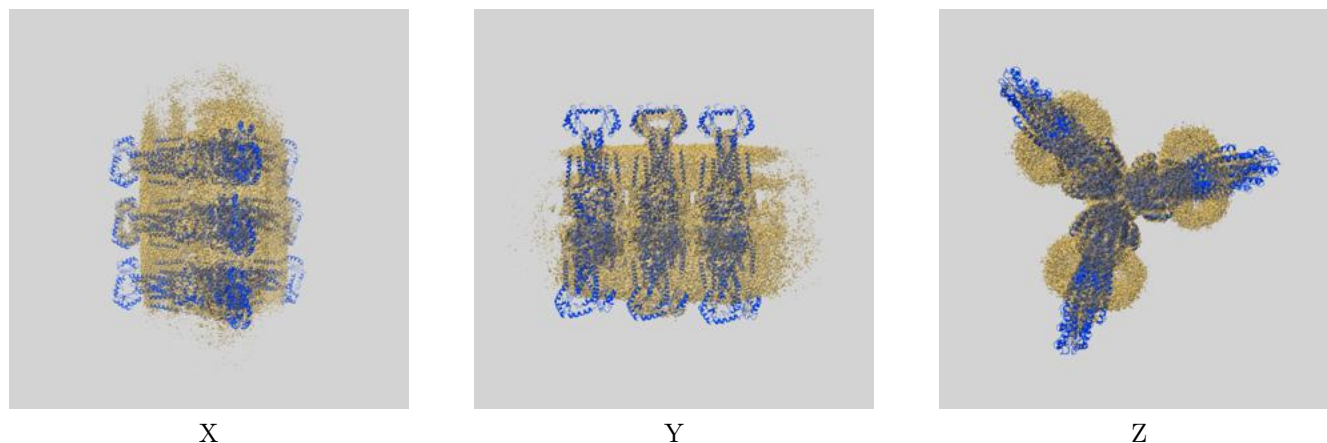
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.49	15.41	8.69

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

9 Map-model fit [i](#)

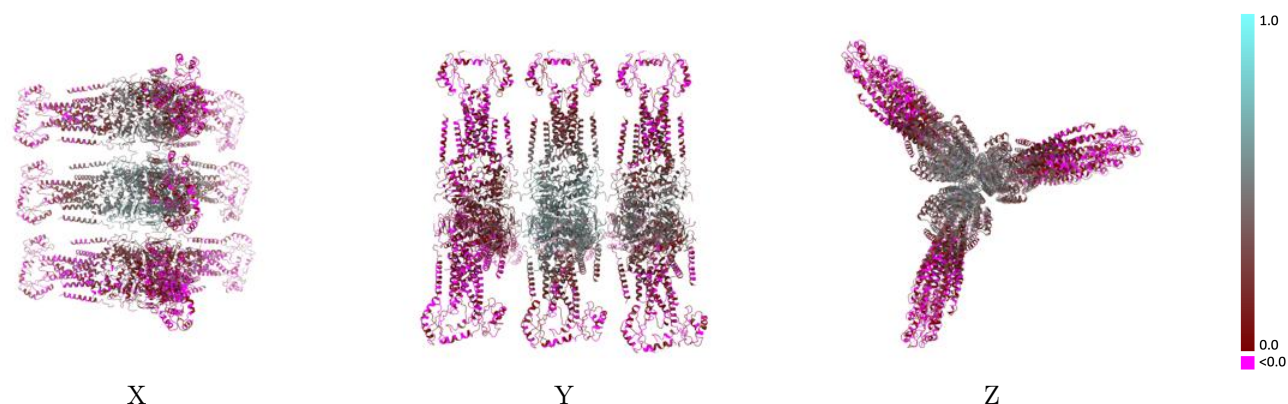
This section contains information regarding the fit between EMDB map EMD-60898 and PDB model 9IUE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



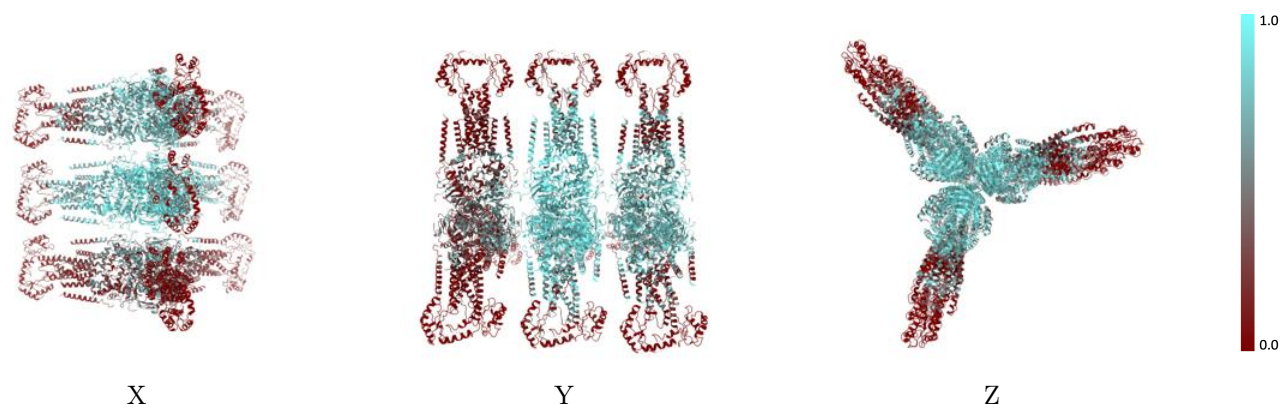
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



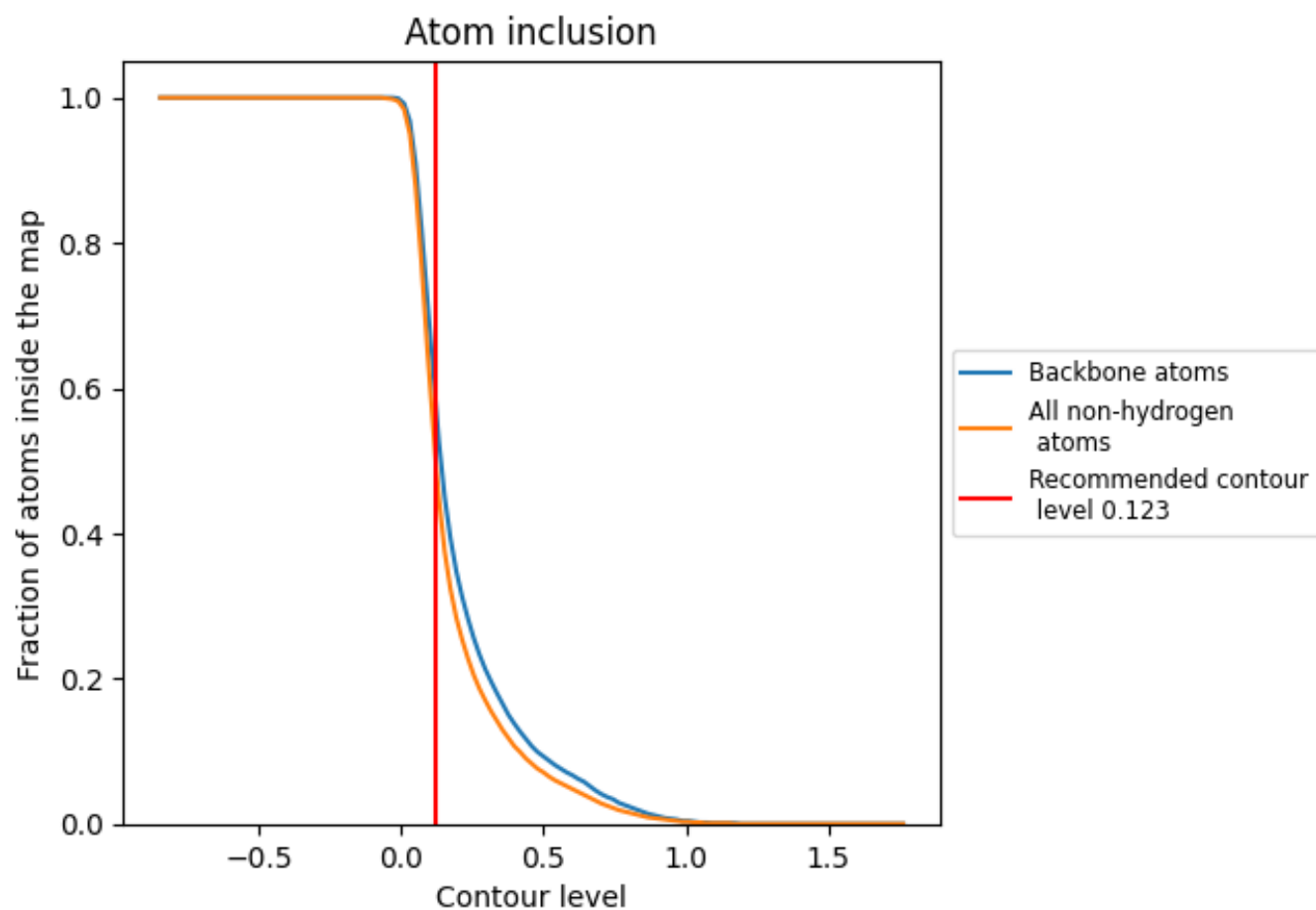
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% 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 (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2200
1	 0.7770	 0.3660
2	 0.7930	 0.3450
5	 0.9450	 0.5500
6	 0.9360	 0.5370
A	 0.5160	 0.2080
B	 0.2940	 0.0820
C	 0.5440	 0.2250
D	 0.2910	 0.0910
E	 0.4060	 0.1280
F	 0.4530	 0.1310
G	 0.7720	 0.3700
H	 0.7850	 0.3790
I	 0.1120	 0.0350
J	 0.1240	 0.0470
K	 0.2540	 0.0700
L	 0.1090	 0.0390
M	 0.3230	 0.1160
N	 0.5030	 0.1950
O	 0.5430	 0.2260
P	 0.5140	 0.2090
Q	 0.7770	 0.3630
R	 0.7970	 0.3480
S	 0.9440	 0.5470
T	 0.9340	 0.5330
U	 0.2930	 0.0820
V	 0.2930	 0.0890
W	 0.4100	 0.1220
X	 0.4490	 0.1330
Y	 0.7850	 0.3810
Z	 0.7860	 0.3810
a	 0.1120	 0.0310
b	 0.1280	 0.0510
c	 0.2660	 0.0710
d	 0.1090	 0.0220



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Chain	Atom inclusion	Q-score
e	 0.3230	 0.1170
f	 0.4990	 0.1920
g	 0.5480	 0.2250
h	 0.5190	 0.2100
i	 0.7850	 0.3630
j	 0.7810	 0.3430
k	 0.9430	 0.5470
l	 0.9330	 0.5330
m	 0.2970	 0.0820
n	 0.2940	 0.0920
o	 0.4180	 0.1270
p	 0.4410	 0.1340
q	 0.7840	 0.3810
r	 0.7920	 0.3840
s	 0.1130	 0.0340
t	 0.1330	 0.0520
u	 0.2500	 0.0760
v	 0.0980	 0.0330
w	 0.3260	 0.1160
x	 0.5080	 0.1980