



## wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 10:37 am BST

PDB ID : 8AOX  
EMDB ID : EMD-15555  
Title : CryoEM structure of the Chikungunya virus nsP1 capping pores in complex with SAM  
Authors : Jones, R.; Hons, M.; Reguera, J.  
Deposited on : 2022-08-08  
Resolution : 2.80 Å(reported)  
Based on initial model : 6Z0V

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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

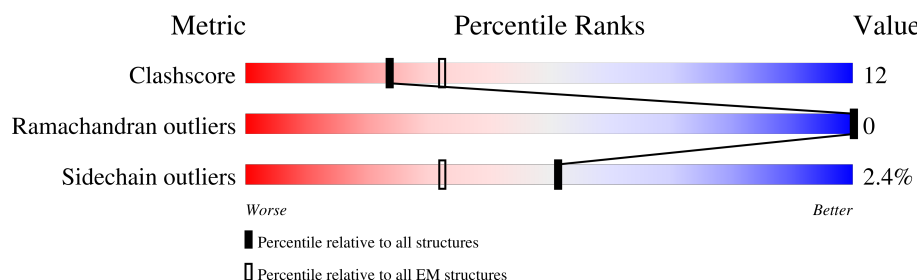
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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)
Clashscore	158937	4297
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  $\geq 3$ , 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	535	<div> <div>16%</div> <div>57%</div> <div>23%</div> <div>19%</div> </div>
1	BA	535	<div> <div>16%</div> <div>56%</div> <div>25%</div> <div>19%</div> </div>
1	C	535	<div> <div>15%</div> <div>58%</div> <div>22%</div> <div>19%</div> </div>
1	DA	535	<div> <div>15%</div> <div>59%</div> <div>22%</div> <div>19%</div> </div>
1	E	535	<div> <div>16%</div> <div>59%</div> <div>21%</div> <div>19%</div> </div>
1	FA	535	<div> <div>16%</div> <div>57%</div> <div>24%</div> <div>19%</div> </div>
1	G	535	<div> <div>16%</div> <div>59%</div> <div>21%</div> <div>19%</div> </div>
1	HA	535	<div> <div>15%</div> <div>58%</div> <div>23%</div> <div>19%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	I	535	
1	JA	535	
1	K	535	
1	LA	535	
1	M	535	
1	NA	535	
1	O	535	
1	PA	535	
1	Q	535	
1	RA	535	
1	S	535	
1	TA	535	
1	V	535	
1	VA	535	
1	X	535	
1	Z	535	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 87816 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 mRNA-capping enzyme nsP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	JA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	A	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	C	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	E	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	G	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	I	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	K	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	M	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	O	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	Q	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	S	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	V	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	X	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	Z	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	BA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	DA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	FA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	LA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	NA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	PA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	RA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	TA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		
1	VA	432	Total	C	N	O	S	9	0
			3429	2156	599	643	31		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

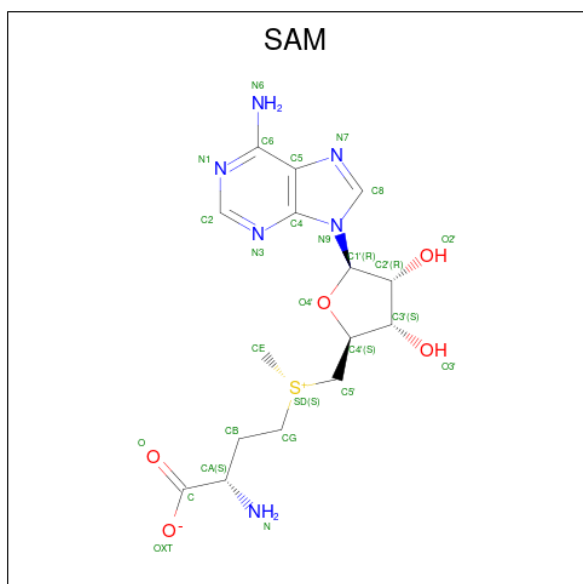
Mol	Chain	Residues	Atoms		AltConf
2	JA	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	E	1	Total	Zn	0
			1	1	
2	G	1	Total	Zn	0
			1	1	
2	I	1	Total	Zn	0
			1	1	
2	K	1	Total	Zn	0
			1	1	
2	M	1	Total	Zn	0
			1	1	
2	O	1	Total	Zn	0
			1	1	
2	Q	1	Total	Zn	0
			1	1	
2	S	1	Total	Zn	0
			1	1	
2	V	1	Total	Zn	0
			1	1	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
2	X	1	Total 1	Zn 1	0
2	Z	1	Total 1	Zn 1	0
2	BA	1	Total 1	Zn 1	0
2	DA	1	Total 1	Zn 1	0
2	FA	1	Total 1	Zn 1	0
2	HA	1	Total 1	Zn 1	0
2	LA	1	Total 1	Zn 1	0
2	NA	1	Total 1	Zn 1	0
2	PA	1	Total 1	Zn 1	0
2	RA	1	Total 1	Zn 1	0
2	TA	1	Total 1	Zn 1	0
2	VA	1	Total 1	Zn 1	0

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	JA	1	Total 27	C 15	N 6	O 5	S 1	0
3	A	1	Total 27	C 15	N 6	O 5	S 1	0
3	C	1	Total 27	C 15	N 6	O 5	S 1	0
3	E	1	Total 27	C 15	N 6	O 5	S 1	0
3	G	1	Total 27	C 15	N 6	O 5	S 1	0
3	I	1	Total 27	C 15	N 6	O 5	S 1	0
3	K	1	Total 27	C 15	N 6	O 5	S 1	0
3	M	1	Total 27	C 15	N 6	O 5	S 1	0
3	O	1	Total 27	C 15	N 6	O 5	S 1	0
3	Q	1	Total 27	C 15	N 6	O 5	S 1	0
3	S	1	Total 27	C 15	N 6	O 5	S 1	0
3	V	1	Total 27	C 15	N 6	O 5	S 1	0
3	X	1	Total 27	C 15	N 6	O 5	S 1	0
3	Z	1	Total 27	C 15	N 6	O 5	S 1	0
3	BA	1	Total 27	C 15	N 6	O 5	S 1	0
3	DA	1	Total 27	C 15	N 6	O 5	S 1	0
3	FA	1	Total 27	C 15	N 6	O 5	S 1	0
3	HA	1	Total 27	C 15	N 6	O 5	S 1	0
3	LA	1	Total 27	C 15	N 6	O 5	S 1	0
3	NA	1	Total 27	C 15	N 6	O 5	S 1	0
3	PA	1	Total 27	C 15	N 6	O 5	S 1	0
3	RA	1	Total 27	C 15	N 6	O 5	S 1	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
3	TA	1	Total	C	N	O	S	0
			27	15	6	5	1	
3	VA	1	Total	C	N	O	S	0
			27	15	6	5	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	JA	202	Total	O	0
			202	202	
4	A	199	Total	O	0
			199	199	
4	C	204	Total	O	0
			204	204	
4	E	204	Total	O	0
			204	204	
4	G	199	Total	O	0
			199	199	
4	I	204	Total	O	0
			204	204	
4	K	202	Total	O	0
			202	202	
4	M	202	Total	O	0
			202	202	
4	O	203	Total	O	0
			203	203	
4	Q	199	Total	O	0
			199	199	
4	S	202	Total	O	0
			202	202	
4	V	204	Total	O	0
			204	204	
4	X	203	Total	O	0
			203	203	
4	Z	199	Total	O	0
			199	199	
4	BA	202	Total	O	0
			202	202	
4	DA	203	Total	O	0
			203	203	
4	FA	202	Total	O	0
			202	202	

*Continued on next page...*



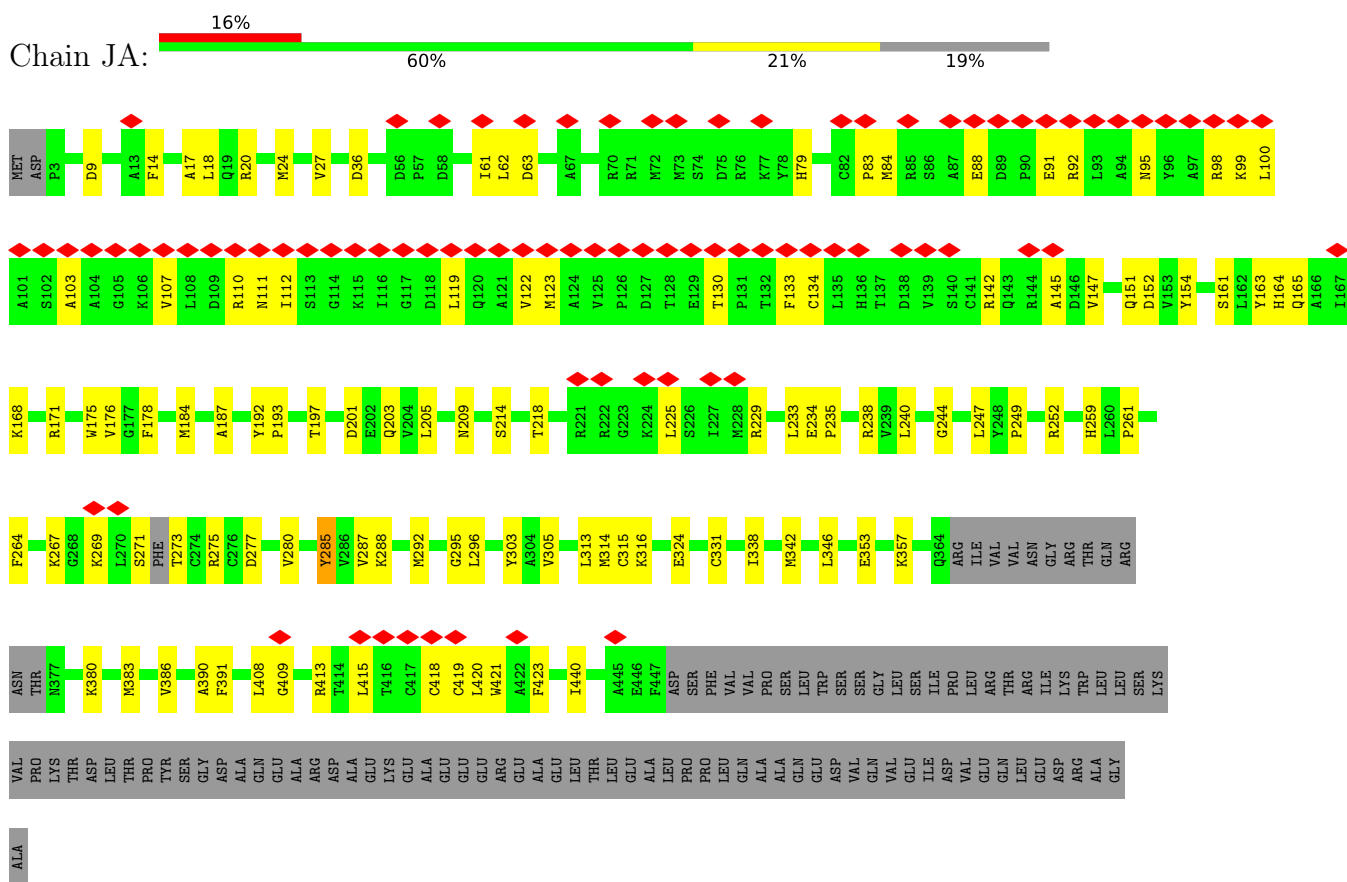
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
4	HA	203	Total 203	O 203	0
4	LA	203	Total 203	O 203	0
4	NA	200	Total 200	O 200	0
4	PA	203	Total 203	O 203	0
4	RA	203	Total 203	O 203	0
4	TA	201	Total 201	O 201	0
4	VA	202	Total 202	O 202	0

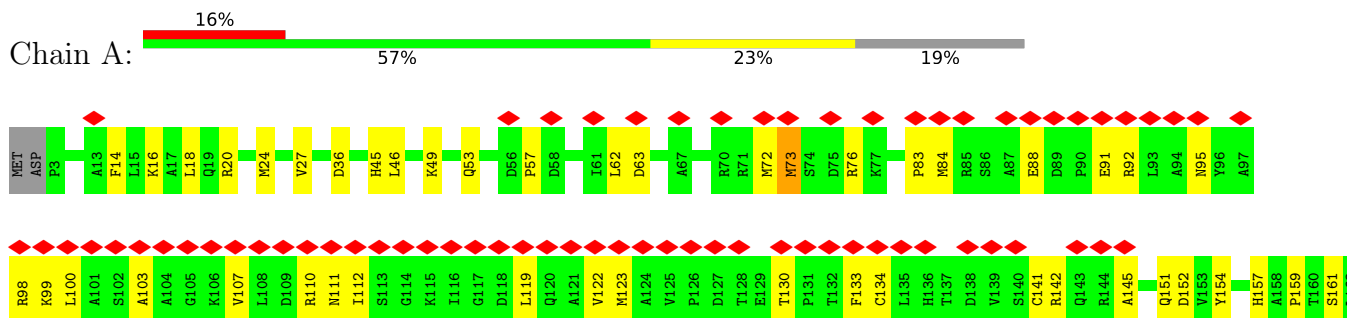
### 3 Residue-property plots

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.

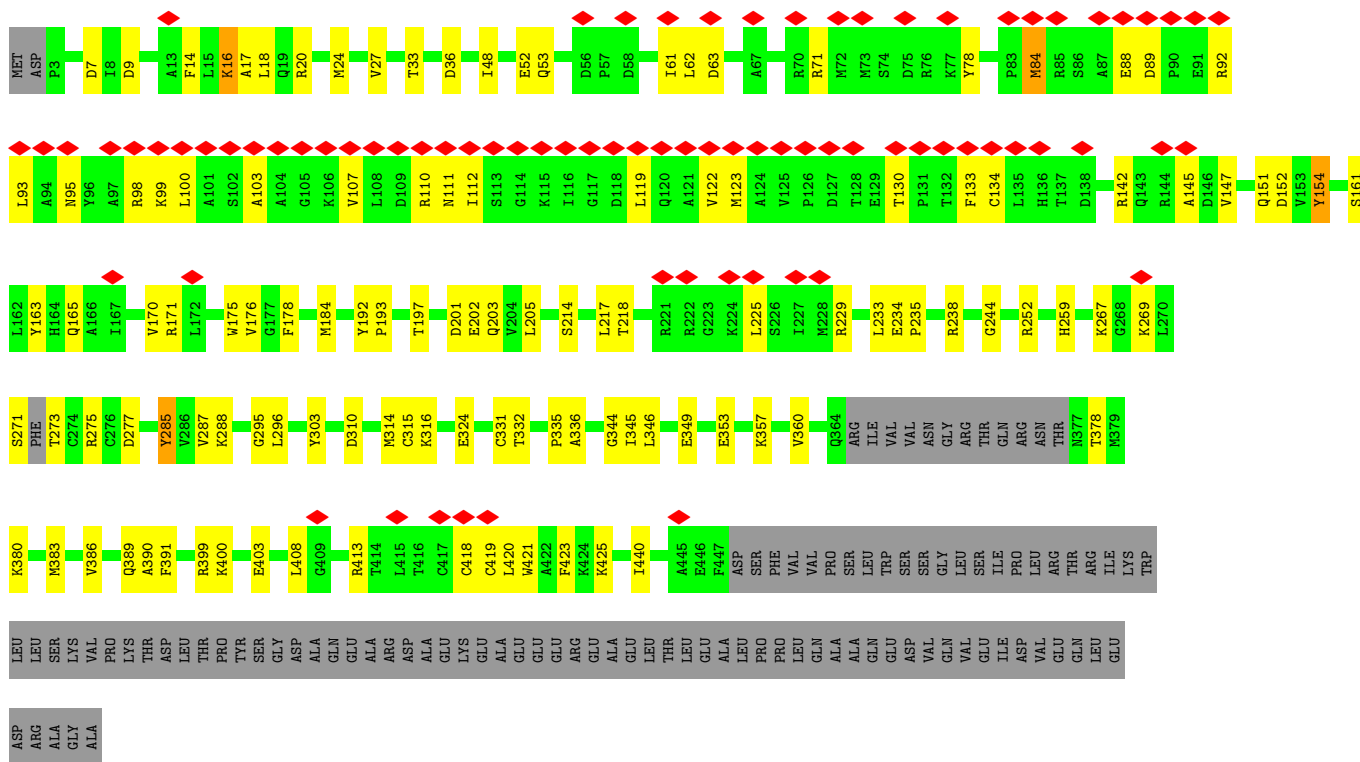
#### • Molecule 1: mRNA-capping enzyme nsP1



#### • Molecule 1: mRNA-capping enzyme nsP1

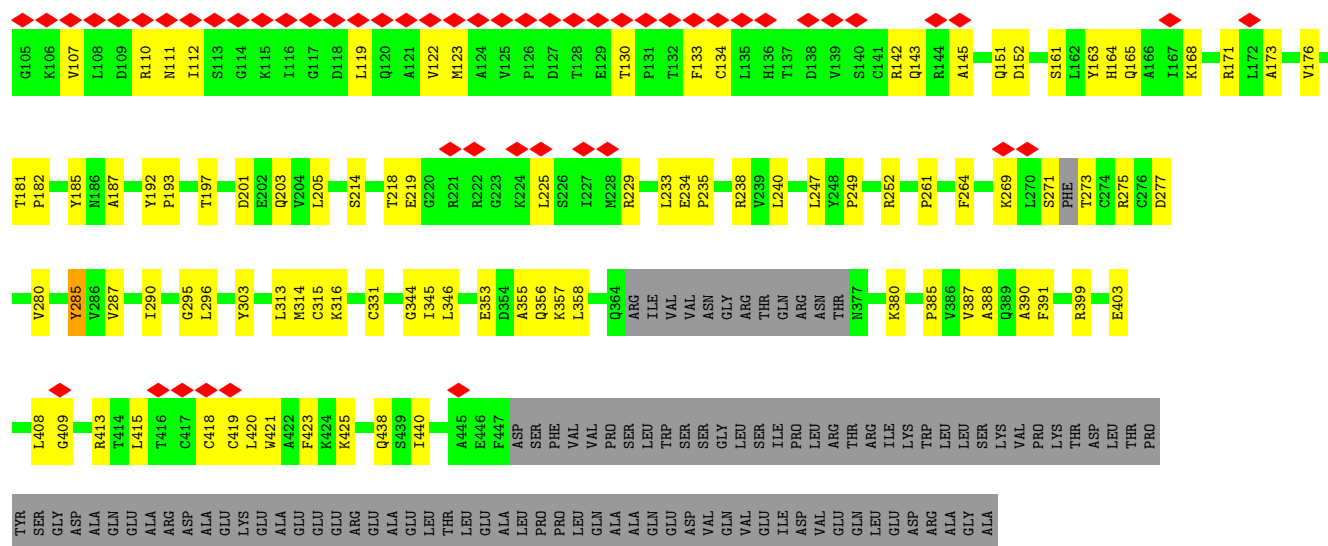


- Molecule 1: mRNA-capping enzyme nsP1

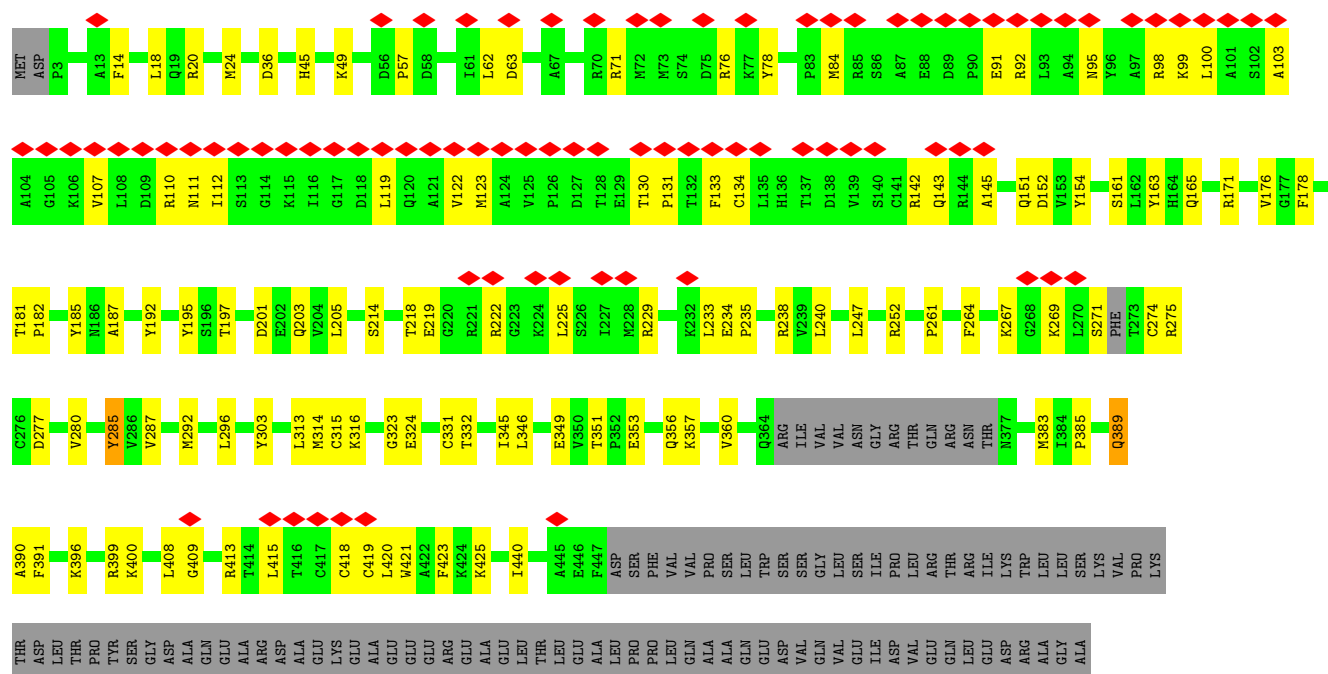


- Molecule 1: mRNA-capping enzyme nsP1

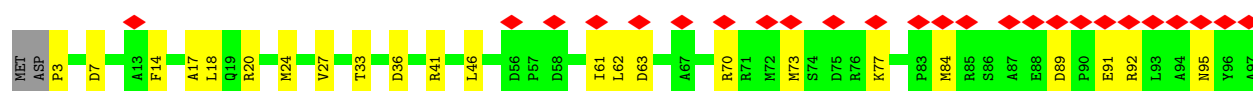


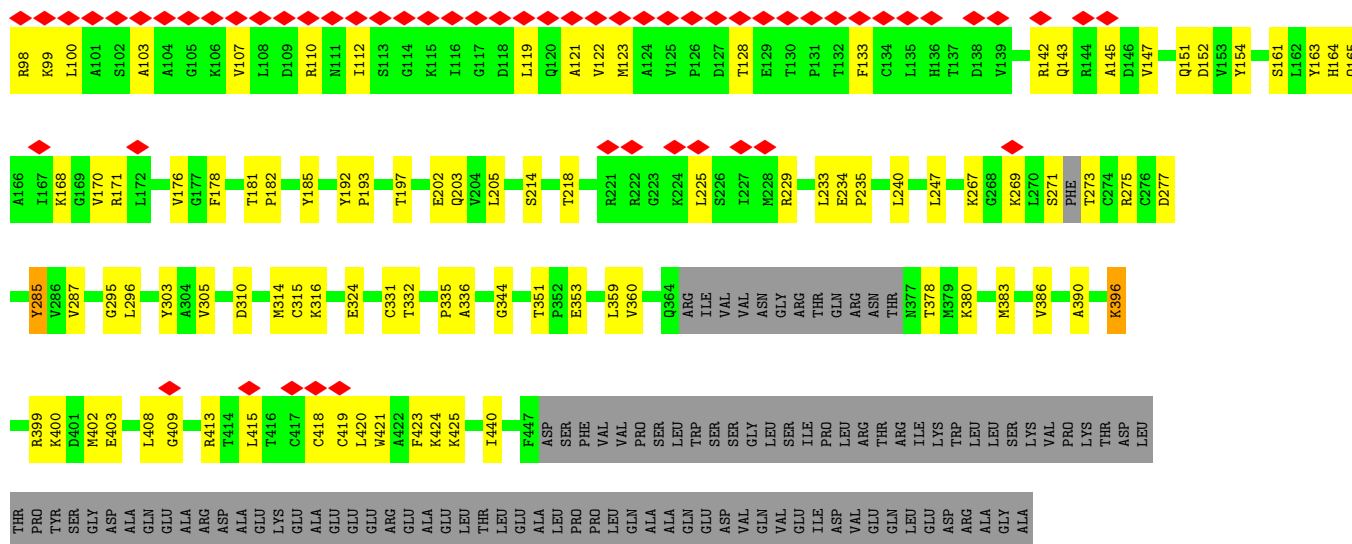


• Molecule 1: mRNA-capping enzyme nsP1

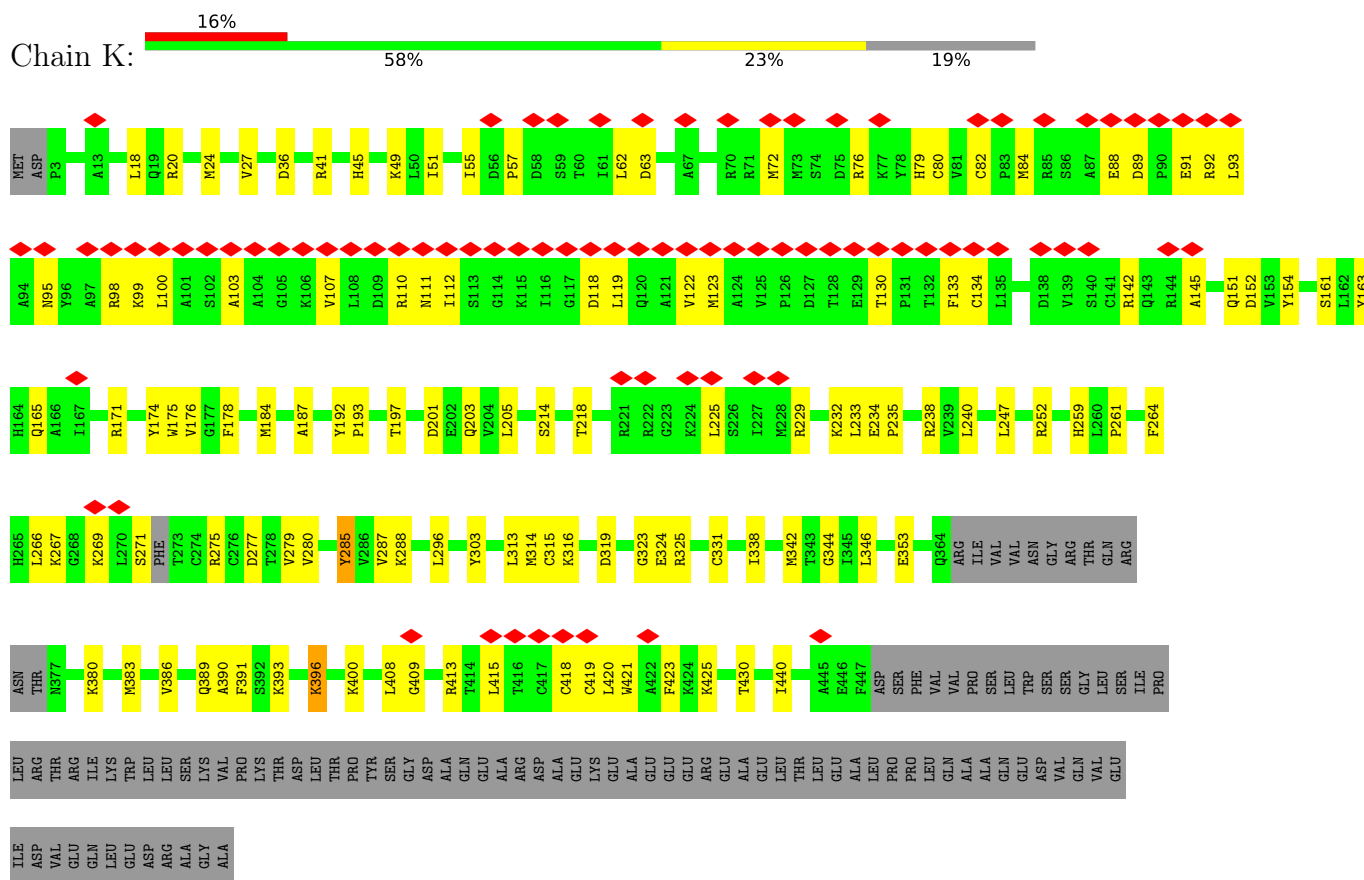


• Molecule 1: mRNA-capping enzyme nsP1

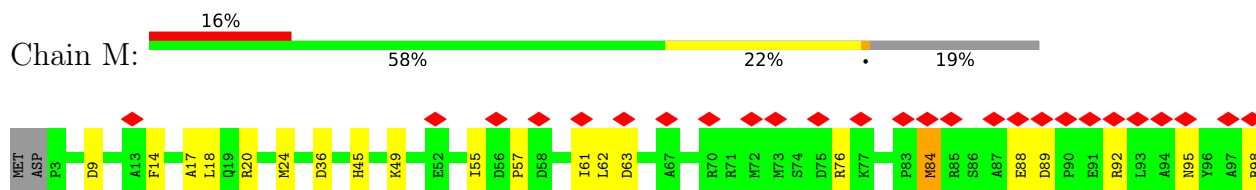


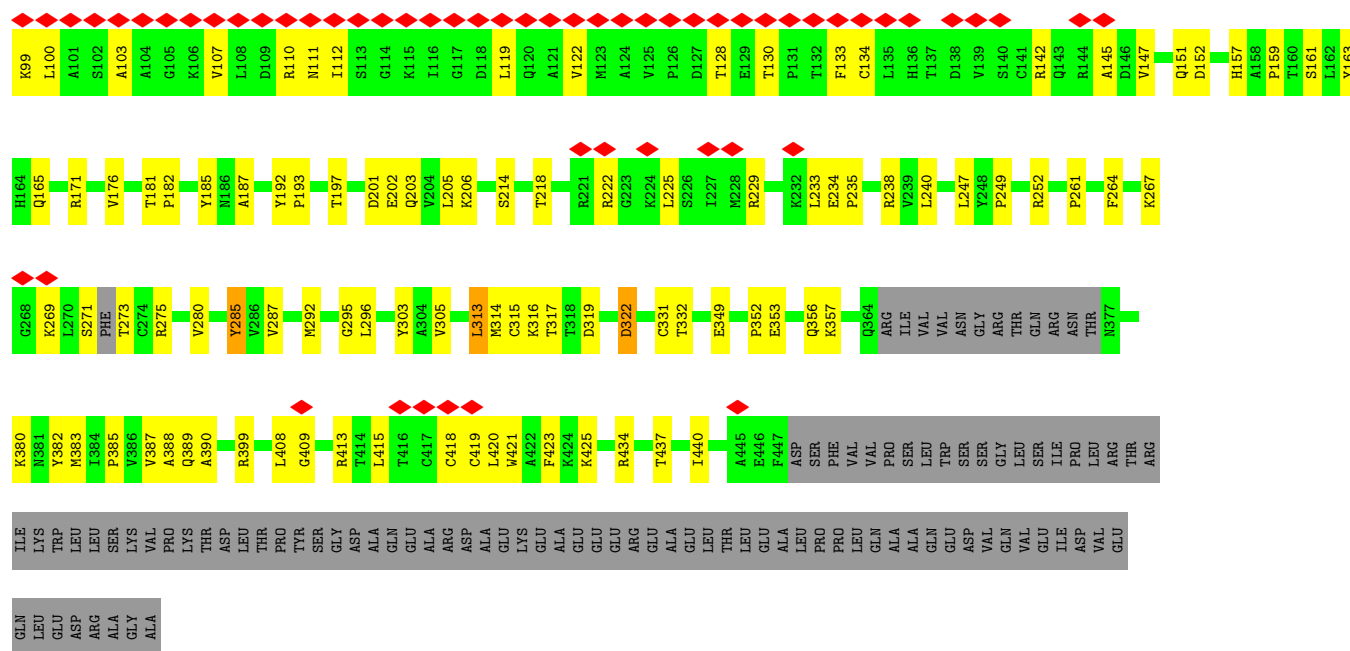


• Molecule 1: mRNA-capping enzyme nsP1



• Molecule 1: mRNA-capping enzyme nsP1

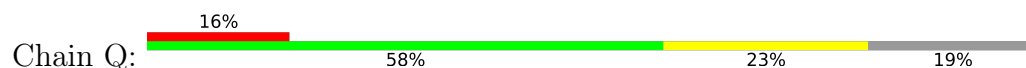


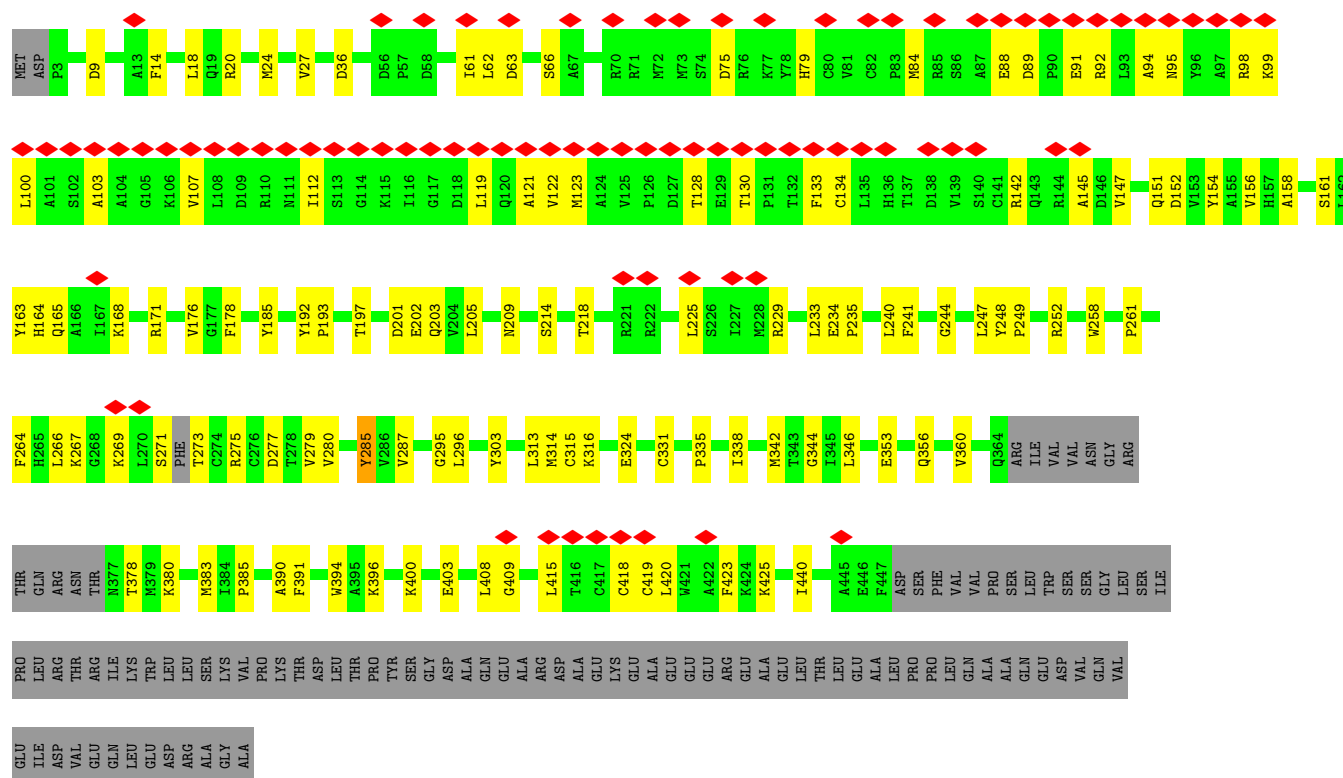


• Molecule 1: mRNA-capping enzyme nsP1

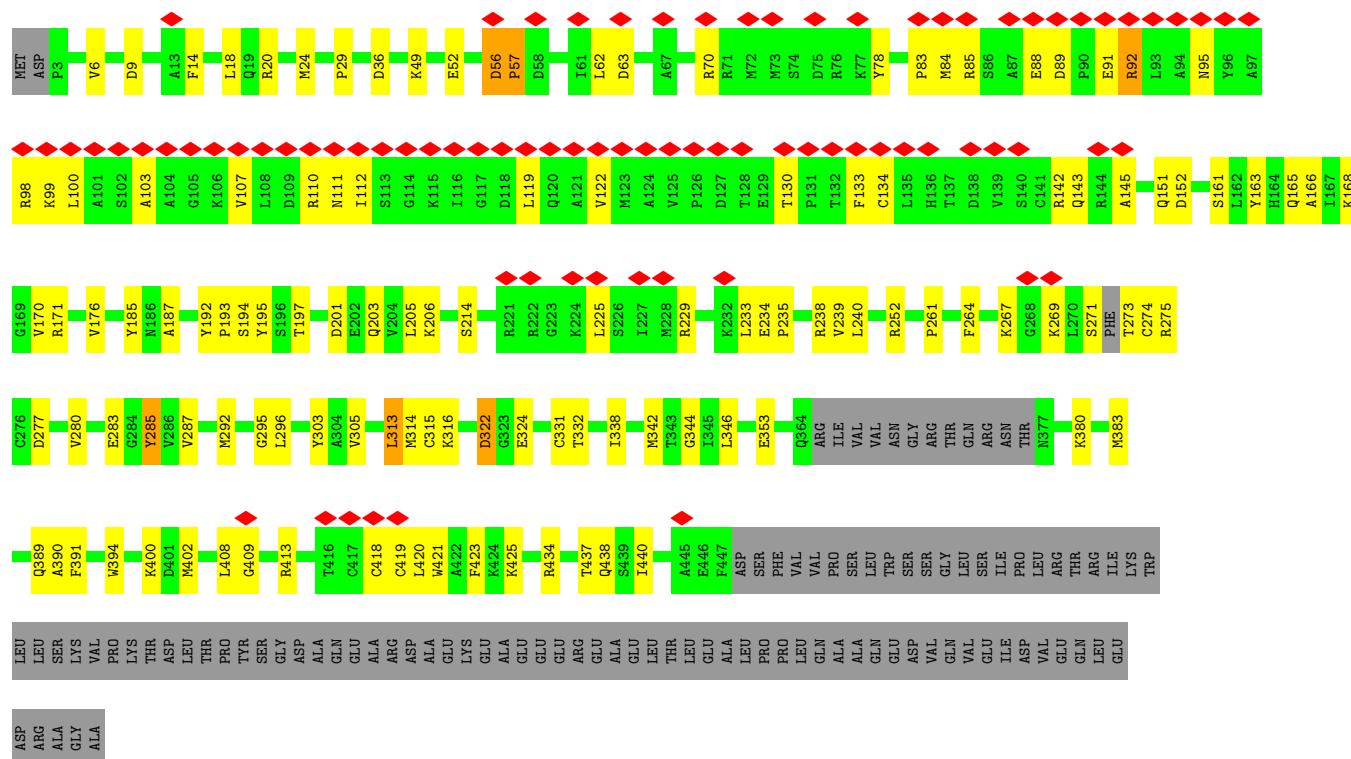


• Molecule 1: mRNA-capping enzyme nsP1

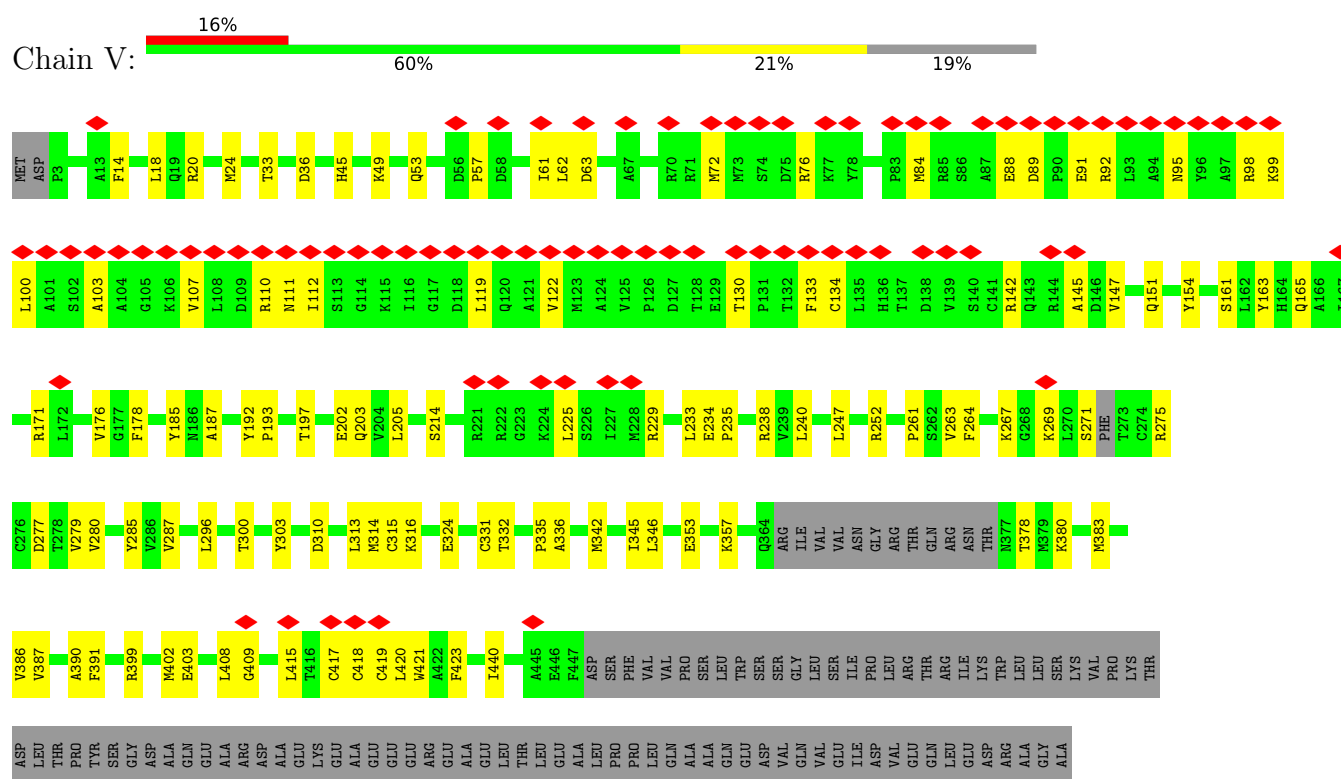




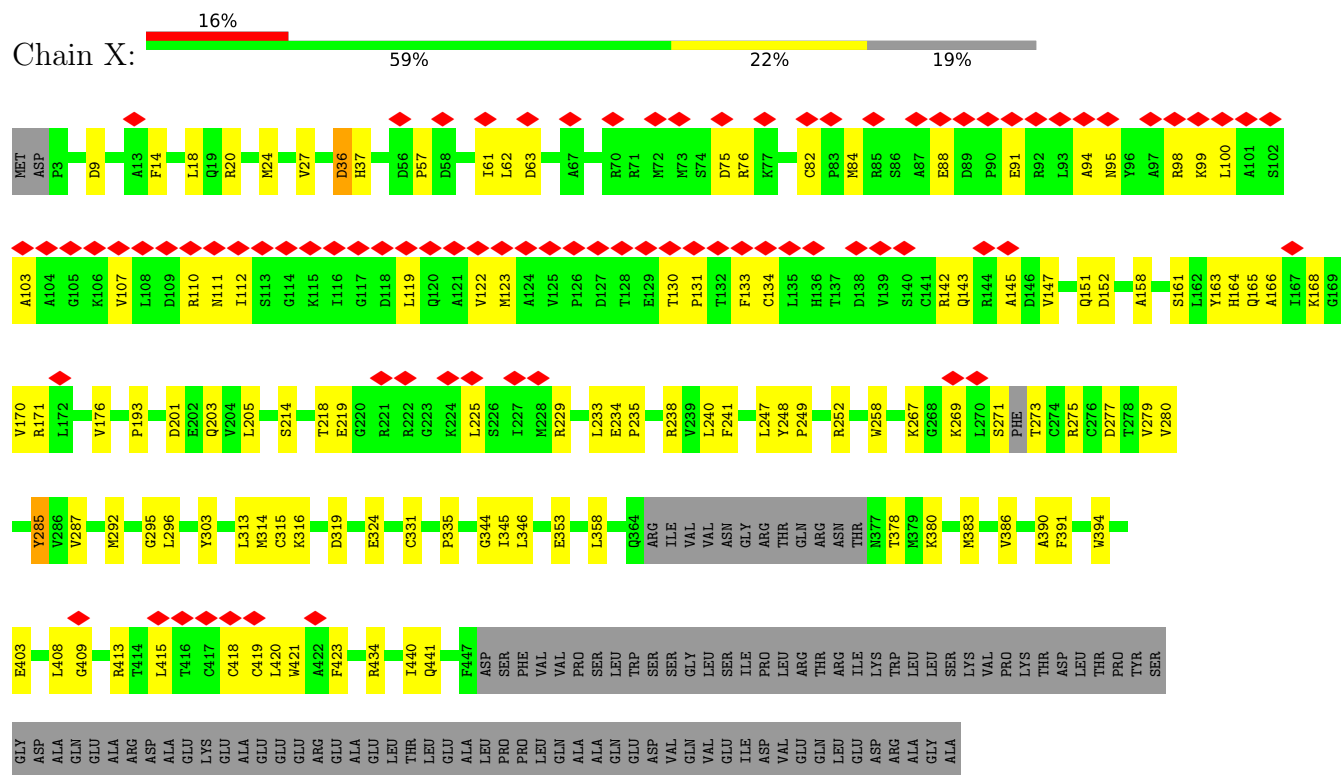
• Molecule 1: mRNA-capping enzyme nsP1



• Molecule 1: mRNA-capping enzyme nsP1



- Molecule 1: mRNA-capping enzyme nsP1

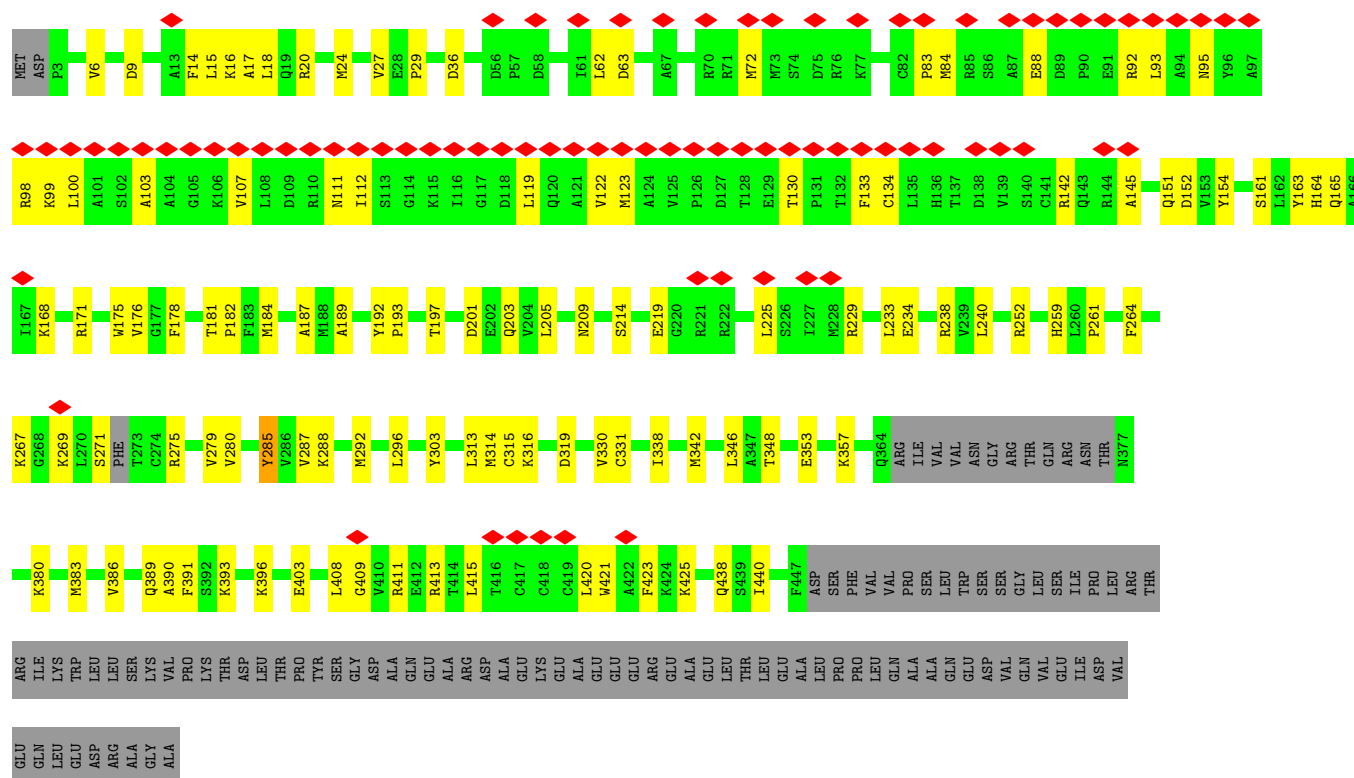


- Molecule 1: mRNA-capping enzyme nsP1

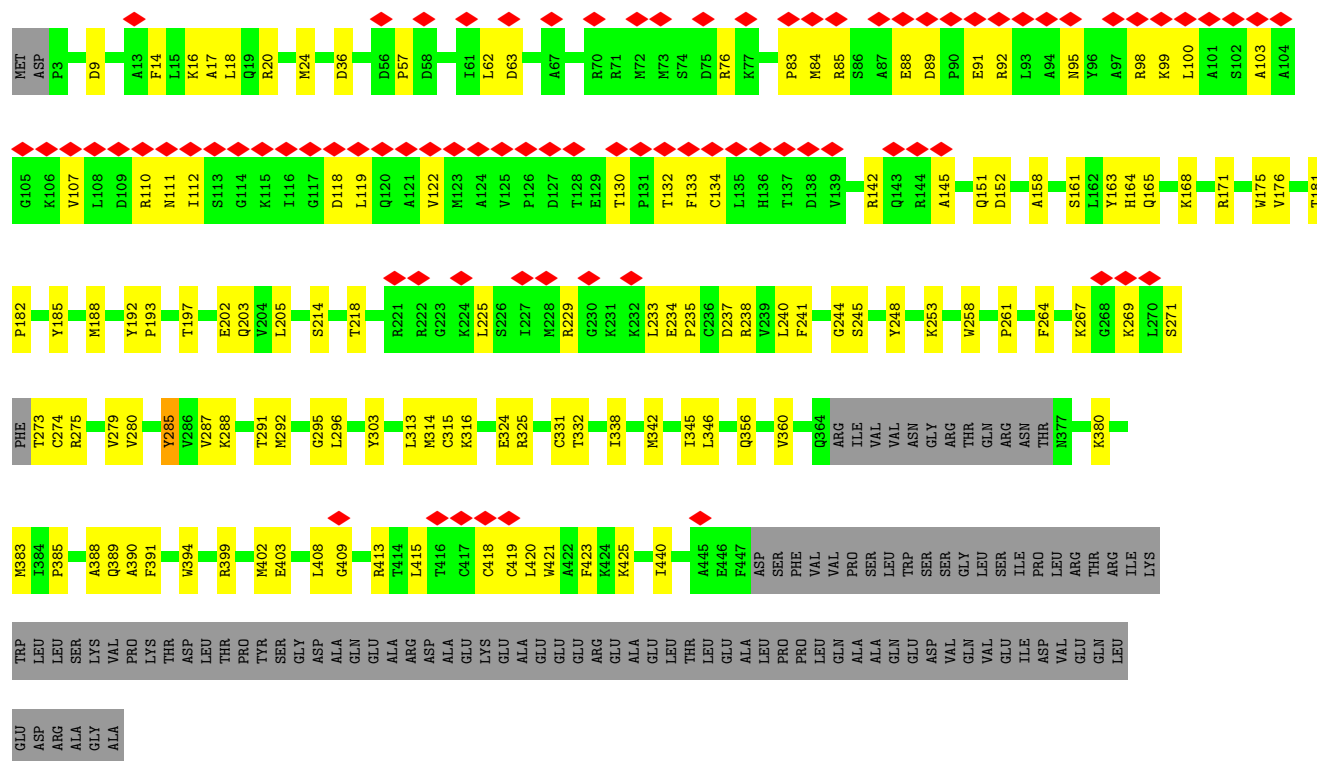




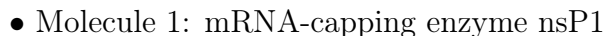




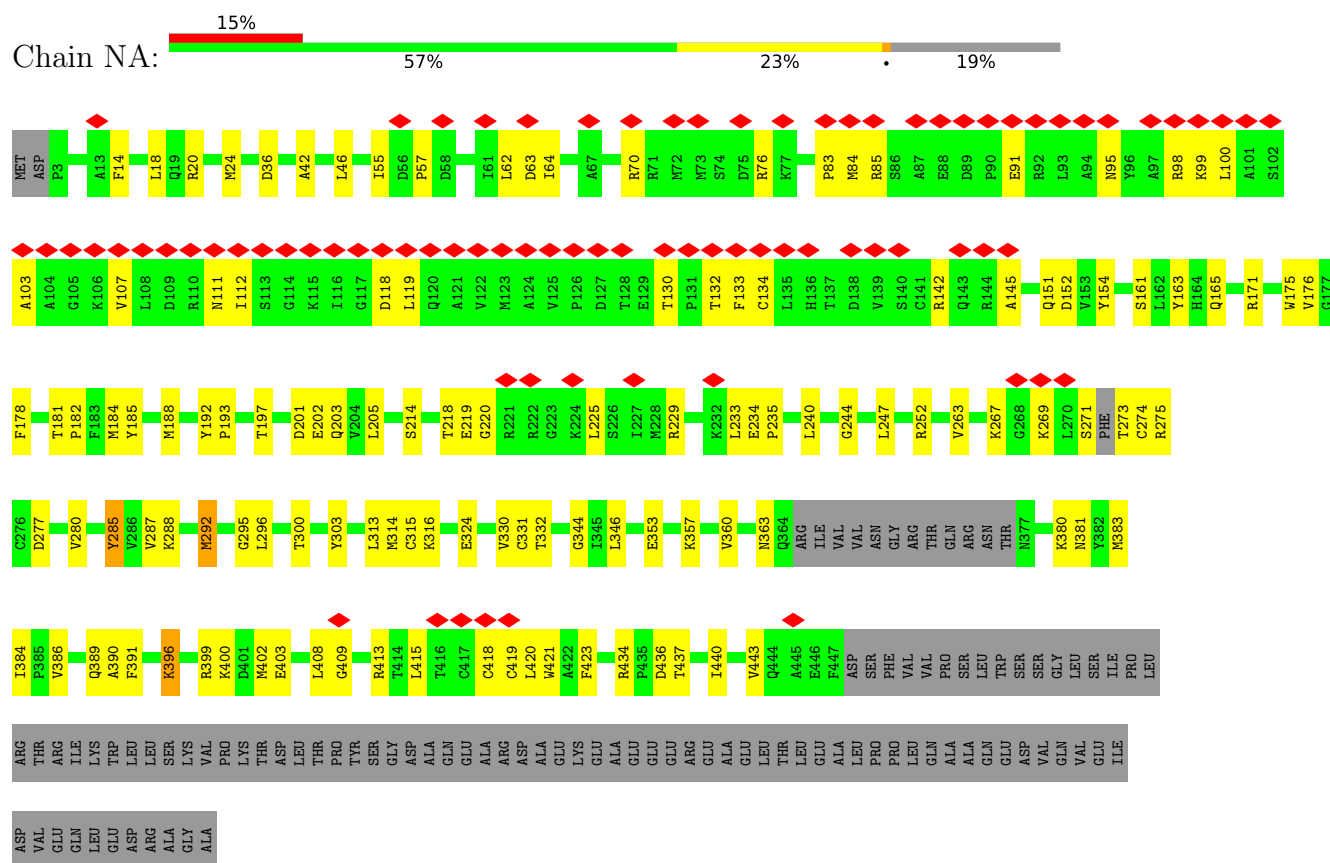
• Molecule 1: mRNA-capping enzyme nsP1



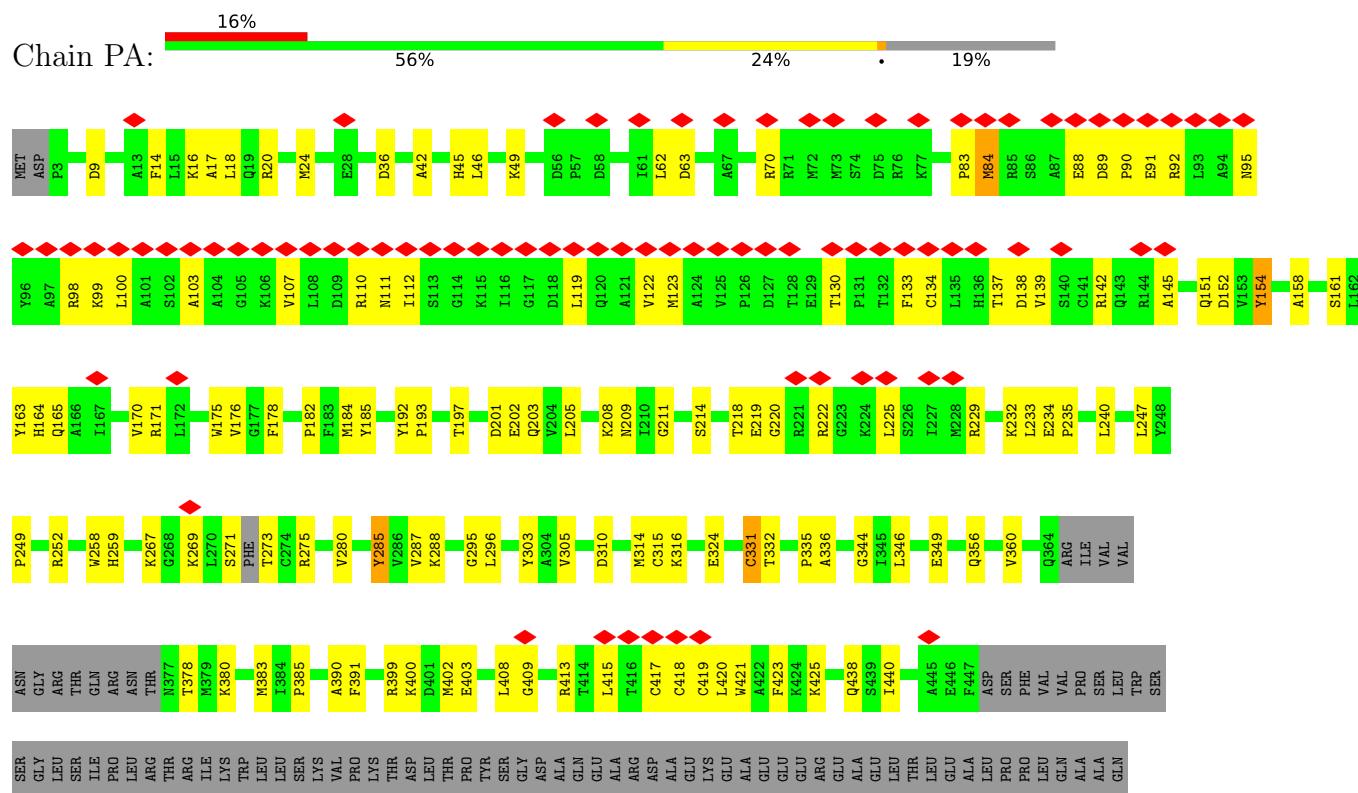
• Molecule 1: mRNA-capping enzyme nsP1



- Molecule 1: mRNA-capping enzyme nsP1



- Molecule 1: mRNA-capping enzyme nsP1





THR	PRO	TYR	SER	GLY	ASP	ALA	GLN	GLU	ALA	ARG	ASP	ALA	GLU	LYS	GLU	ALA	GLU	GLU	GLU	ARG	GLU	ALA	GLU	LEU	THR	LEU	GLU	ALA	LEU	PRO	PRO	LEU	GLN	ALA	ALA	GLN	GLU	ASP	VAL	GLN	VAL	GLU	GLN	LEU	GLU	ASP	ALA	GLY	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: mRNA-capping enzyme nsP1



MET	ASP	P3	D9	A13	F14	A17	L18	Q19	R20	M24	T33	D36	H45	K49	D56	P57	D58	I61	L62	D63	A67	R70	R71	M72	M73	S74	D75	R76	K77	P83	M84	R85	S86	A87	E88	D89	P90	E91	R92	L93	A94	N95	Y96	A97	R98	K99										
L100	A101	S102	A103	A104	G105	K106	V107	L108	D109	R110	N111	T112	S113	G114	K115	T116	G117	D118	L119	Q120	A121	V122	M123	A124	V125	P126	D127	T128	E129	T130	P131	T132	F133	C134	L135	H136	T137	D138	V139	R142	Q143	R144	A145	D146	V147	Q151	D152	V153	Y154	S161	L162	Y163	H164	Q165	A166	T167
K168	R171	L172	W175	V176	G177	F178	Y185	G295	L296	Y303	A304	V305	M314	C315	K316	E324	C331	T332	P335	M342	T343	G344	T345	L346	E349	E353	V360	Q364	ARG	ILE	VAL	VAL	ASN	GLY	ARG	THR	GLN	ARG	ASN	K267	G268	K269	L270	S271	PHE	T273	C274	R275	C276	D277						
V280	Y285	V286	V287	K288	M292	G295	L296	Y303	A304	V305	M314	C315	K316	E324	C331	T332	P335	M342	T343	G344	T345	L346	E349	E353	V360	Q364	ARG	ILE	VAL	VAL	ASN	GLY	ARG	THR	GLN	ARG	ASN	K267	G268	K269	L270	S271	PHE	T273	C274	R275	C276	D277								
V386	A390	F391	R399	M402	E403	L408	G409	R413	T414	L415	T416	C417	C418	C419	L420	F423	K424	K425	I440	F447	ASP	SER	PHE	VAL	VAL	PRO	SER	ALA	LEU	TRP	ASP	SER	GLY	VAL	LEU	SER	ILE	ASP	PRO	THR	GLN	ARG	ASN	ILE	LYS	TRP	LEU	LEU	ALA	GLY	ALA					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D12	Depositor
Number of particles used	69057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	248.1, 248.1, 248.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.25	0/3501	0.49	0/4742
1	BA	0.28	1/3501 (0.0%)	0.50	0/4742
1	C	0.26	0/3501	0.50	0/4742
1	DA	0.27	0/3501	0.50	0/4742
1	E	0.26	0/3501	0.50	0/4742
1	FA	0.26	0/3501	0.50	0/4742
1	G	0.26	0/3501	0.50	0/4742
1	HA	0.26	0/3501	0.50	0/4742
1	I	0.27	0/3501	0.50	0/4742
1	JA	0.26	0/3501	0.49	0/4742
1	K	0.27	0/3501	0.50	0/4742
1	LA	0.26	0/3501	0.49	0/4742
1	M	0.26	0/3501	0.49	0/4742
1	NA	0.26	0/3501	0.50	0/4742
1	O	0.25	0/3501	0.50	0/4742
1	PA	0.26	0/3501	0.50	0/4742
1	Q	0.26	0/3501	0.50	0/4742
1	RA	0.26	0/3501	0.50	0/4742
1	S	0.54	4/3501 (0.1%)	0.83	9/4742 (0.2%)
1	TA	0.26	0/3501	0.49	0/4742
1	V	0.26	0/3501	0.49	0/4742
1	VA	0.26	0/3501	0.49	0/4742
1	X	0.27	0/3501	0.50	0/4742
1	Z	0.26	0/3501	0.50	0/4742
All	All	0.28	5/84024 (0.0%)	0.52	9/113808 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	57	PRO	CG-CD	-18.52	0.89	1.50
1	S	57	PRO	CB-CG	17.50	2.37	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	57	PRO	CA-C	-5.82	1.41	1.52
1	S	56	ASP	C-O	-5.65	1.12	1.23
1	BA	91	GLU	CG-CD	-5.54	1.43	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	57	PRO	CB-CG-CD	-27.30	0.04	106.50
1	S	57	PRO	CA-N-CD	-20.07	83.40	111.50
1	S	57	PRO	N-CA-CB	-17.13	82.74	103.30
1	S	57	PRO	CA-CB-CG	-13.74	77.89	104.00
1	S	56	ASP	C-N-CD	13.01	155.73	128.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3429	0	3384	92	0
1	BA	3429	0	3384	111	0
1	C	3429	0	3384	91	0
1	DA	3429	0	3384	91	0
1	E	3429	0	3384	90	0
1	FA	3429	0	3384	98	0
1	G	3429	0	3384	90	0
1	HA	3429	0	3384	93	0
1	I	3429	0	3384	99	0
1	JA	3429	0	3384	83	0
1	K	3429	0	3384	105	0
1	LA	3429	0	3384	83	0
1	M	3429	0	3384	97	0
1	NA	3429	0	3384	103	0
1	O	3429	0	3384	95	0
1	PA	3429	0	3384	107	0
1	Q	3429	0	3384	95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	3429	0	3384	90	0
1	S	3429	0	3384	106	0
1	TA	3429	0	3384	84	0
1	V	3429	0	3384	81	0
1	VA	3429	0	3384	92	0
1	X	3429	0	3384	91	0
1	Z	3429	0	3384	98	0
2	A	1	0	0	0	0
2	BA	1	0	0	0	0
2	C	1	0	0	0	0
2	DA	1	0	0	0	0
2	E	1	0	0	0	0
2	FA	1	0	0	0	0
2	G	1	0	0	0	0
2	HA	1	0	0	0	0
2	I	1	0	0	0	0
2	JA	1	0	0	0	0
2	K	1	0	0	0	0
2	LA	1	0	0	0	0
2	M	1	0	0	0	0
2	NA	1	0	0	0	0
2	O	1	0	0	0	0
2	PA	1	0	0	0	0
2	Q	1	0	0	0	0
2	RA	1	0	0	0	0
2	S	1	0	0	0	0
2	TA	1	0	0	0	0
2	V	1	0	0	0	0
2	VA	1	0	0	0	0
2	X	1	0	0	0	0
2	Z	1	0	0	0	0
3	A	27	0	22	2	0
3	BA	27	0	22	5	0
3	C	27	0	22	5	0
3	DA	27	0	22	3	0
3	E	27	0	22	3	0
3	FA	27	0	22	6	0
3	G	27	0	22	3	0
3	HA	27	0	22	3	0
3	I	27	0	22	4	0
3	JA	27	0	22	3	0
3	K	27	0	22	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	LA	27	0	22	3	0
3	M	27	0	22	4	0
3	NA	27	0	22	5	0
3	O	27	0	22	3	0
3	PA	27	0	22	5	0
3	Q	27	0	22	3	0
3	RA	27	0	22	4	0
3	S	27	0	22	5	0
3	TA	27	0	22	3	0
3	V	27	0	22	3	0
3	VA	27	0	22	2	0
3	X	27	0	22	1	0
3	Z	27	0	22	1	0
4	A	199	0	0	8	0
4	BA	202	0	0	8	0
4	C	204	0	0	10	0
4	DA	203	0	0	7	0
4	E	204	0	0	9	0
4	FA	202	0	0	6	0
4	G	199	0	0	7	0
4	HA	203	0	0	8	0
4	I	204	0	0	7	0
4	JA	202	0	0	6	0
4	K	202	0	0	11	0
4	LA	203	0	0	7	0
4	M	202	0	0	8	0
4	NA	200	0	0	7	0
4	O	203	0	0	9	0
4	PA	203	0	0	7	0
4	Q	199	0	0	6	0
4	RA	203	0	0	5	0
4	S	202	0	0	11	0
4	TA	201	0	0	7	0
4	V	204	0	0	6	0
4	VA	202	0	0	9	0
4	X	203	0	0	11	0
4	Z	199	0	0	5	0
All	All	87816	0	81744	1993	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 12.

The worst 5 of 1993 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:57:PRO:CG	1:S:57:PRO:N	1.68	1.48
1:S:57:PRO:CD	1:S:57:PRO:HG3	1.66	1.17
1:X:20:ARG:NH1	4:X:1101:HOH:O	1.79	1.13
1:S:57:PRO:CD	1:S:57:PRO:HG2	1.66	1.08
1:S:57:PRO:CG	1:S:57:PRO:HD2	1.57	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/535 (81%)	430 (99%)	4 (1%)	0	100	100
1	BA	434/535 (81%)	430 (99%)	4 (1%)	0	100	100
1	C	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
1	DA	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
1	E	434/535 (81%)	432 (100%)	2 (0%)	0	100	100
1	FA	434/535 (81%)	426 (98%)	8 (2%)	0	100	100
1	G	434/535 (81%)	429 (99%)	5 (1%)	0	100	100
1	HA	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	I	434/535 (81%)	426 (98%)	8 (2%)	0	100	100
1	JA	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	K	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	LA	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	M	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
1	NA	434/535 (81%)	429 (99%)	5 (1%)	0	100	100
1	O	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
1	PA	434/535 (81%)	429 (99%)	5 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	434/535 (81%)	429 (99%)	5 (1%)	0	100	100
1	RA	434/535 (81%)	429 (99%)	5 (1%)	0	100	100
1	S	434/535 (81%)	425 (98%)	9 (2%)	0	100	100
1	TA	434/535 (81%)	424 (98%)	10 (2%)	0	100	100
1	V	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	VA	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	X	434/535 (81%)	428 (99%)	6 (1%)	0	100	100
1	Z	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
All	All	10416/12840 (81%)	10269 (99%)	147 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	372/460 (81%)	361 (97%)	11 (3%)	41	75
1	BA	372/460 (81%)	364 (98%)	8 (2%)	52	83
1	C	372/460 (81%)	362 (97%)	10 (3%)	44	78
1	DA	372/460 (81%)	362 (97%)	10 (3%)	44	78
1	E	372/460 (81%)	365 (98%)	7 (2%)	57	85
1	FA	372/460 (81%)	365 (98%)	7 (2%)	57	85
1	G	372/460 (81%)	364 (98%)	8 (2%)	52	83
1	HA	372/460 (81%)	361 (97%)	11 (3%)	41	75
1	I	372/460 (81%)	362 (97%)	10 (3%)	44	78
1	JA	372/460 (81%)	364 (98%)	8 (2%)	52	83
1	K	372/460 (81%)	364 (98%)	8 (2%)	52	83
1	LA	372/460 (81%)	363 (98%)	9 (2%)	49	81
1	M	372/460 (81%)	362 (97%)	10 (3%)	44	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NA	372/460 (81%)	363 (98%)	9 (2%)	49	81
1	O	372/460 (81%)	363 (98%)	9 (2%)	49	81
1	PA	372/460 (81%)	361 (97%)	11 (3%)	41	75
1	Q	372/460 (81%)	365 (98%)	7 (2%)	57	85
1	RA	372/460 (81%)	362 (97%)	10 (3%)	44	78
1	S	372/460 (81%)	361 (97%)	11 (3%)	41	75
1	TA	372/460 (81%)	363 (98%)	9 (2%)	49	81
1	V	372/460 (81%)	365 (98%)	7 (2%)	57	85
1	VA	372/460 (81%)	364 (98%)	8 (2%)	52	83
1	X	372/460 (81%)	366 (98%)	6 (2%)	62	88
1	Z	372/460 (81%)	365 (98%)	7 (2%)	57	85
All	All	8928/11040 (81%)	8717 (98%)	211 (2%)	51	81

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	73	MET
1	FA	389	GLN
1	TA	134	CYS
1	BA	24	MET
1	DA	72	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	FA	389	GLN
1	VA	209	ASN
1	I	143	GLN
1	M	389	GLN
1	V	111	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	SAM	DA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	A	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	K	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.58	4 (17%)
3	SAM	X	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	NA	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	TA	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	E	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	S	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.55	4 (17%)
3	SAM	M	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	LA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	Z	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.58	4 (17%)
3	SAM	Q	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.58	4 (17%)
3	SAM	RA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.58	4 (17%)
3	SAM	BA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	JA	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.58	4 (17%)
3	SAM	V	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	FA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.59	4 (17%)
3	SAM	PA	1002	-	24,29,29	1.20	3 (12%)	23,42,42	1.55	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SAM	VA	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.55	4 (17%)
3	SAM	G	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	I	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.56	4 (17%)
3	SAM	C	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	O	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.57	4 (17%)
3	SAM	HA	1002	-	24,29,29	1.21	3 (12%)	23,42,42	1.55	4 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	DA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	A	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	K	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	X	1002	-	-	4/12/33/33	0/3/3/3
3	SAM	NA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	TA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	E	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	S	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	M	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	LA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	Z	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	Q	1002	-	-	4/12/33/33	0/3/3/3
3	SAM	RA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	BA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	JA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	V	1002	-	-	5/12/33/33	0/3/3/3
3	SAM	FA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	PA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	VA	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	G	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	I	1002	-	-	3/12/33/33	0/3/3/3
3	SAM	C	1002	-	-	4/12/33/33	0/3/3/3
3	SAM	O	1002	-	-	4/12/33/33	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	HA	1002	-	-	3/12/33/33	0/3/3/3

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	NA	1002	SAM	C2-N3	3.92	1.38	1.32
3	A	1002	SAM	C2-N3	3.92	1.38	1.32
3	Z	1002	SAM	C2-N3	3.91	1.38	1.32
3	S	1002	SAM	C2-N3	3.91	1.38	1.32
3	G	1002	SAM	C2-N3	3.91	1.38	1.32

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1002	SAM	N3-C2-N1	-5.41	120.23	128.68
3	K	1002	SAM	N3-C2-N1	-5.40	120.24	128.68
3	RA	1002	SAM	N3-C2-N1	-5.39	120.25	128.68
3	M	1002	SAM	N3-C2-N1	-5.39	120.26	128.68
3	FA	1002	SAM	N3-C2-N1	-5.38	120.26	128.68

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	JA	1002	SAM	CA-CB-CG-SD
3	JA	1002	SAM	CB-CG-SD-CE
3	JA	1002	SAM	CB-CG-SD-C5'
3	A	1002	SAM	CA-CB-CG-SD
3	A	1002	SAM	CB-CG-SD-CE

There are no ring outliers.

24 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DA	1002	SAM	3	0
3	A	1002	SAM	2	0
3	K	1002	SAM	3	0
3	X	1002	SAM	1	0
3	NA	1002	SAM	5	0
3	TA	1002	SAM	3	0
3	E	1002	SAM	3	0

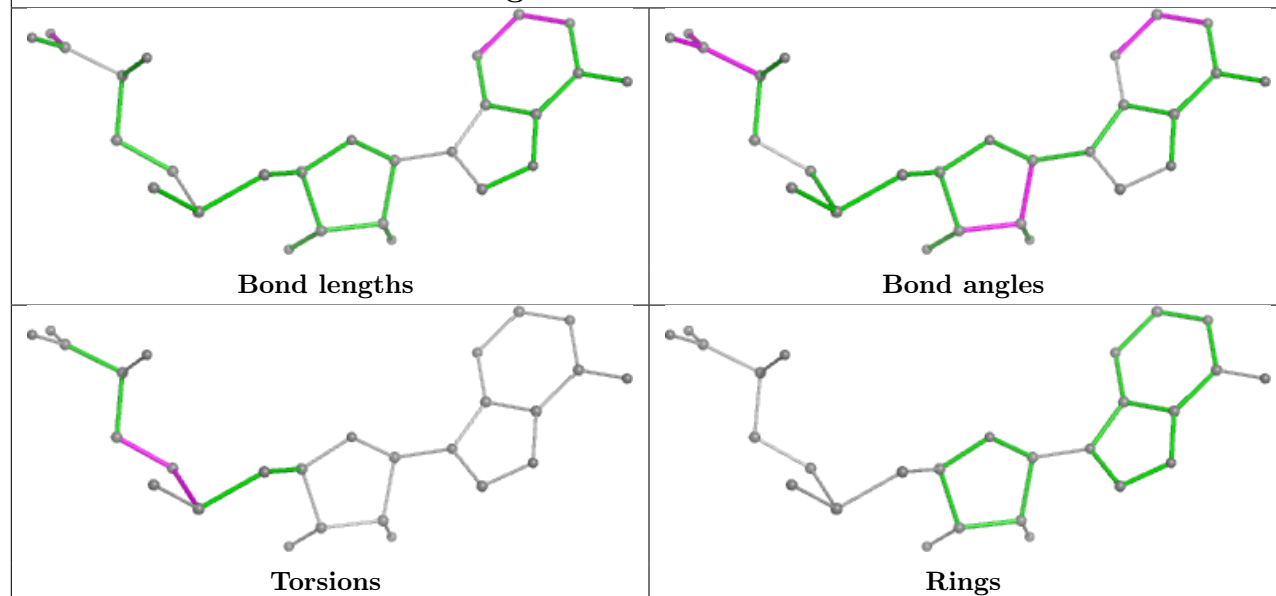
*Continued on next page...*

*Continued from previous page...*

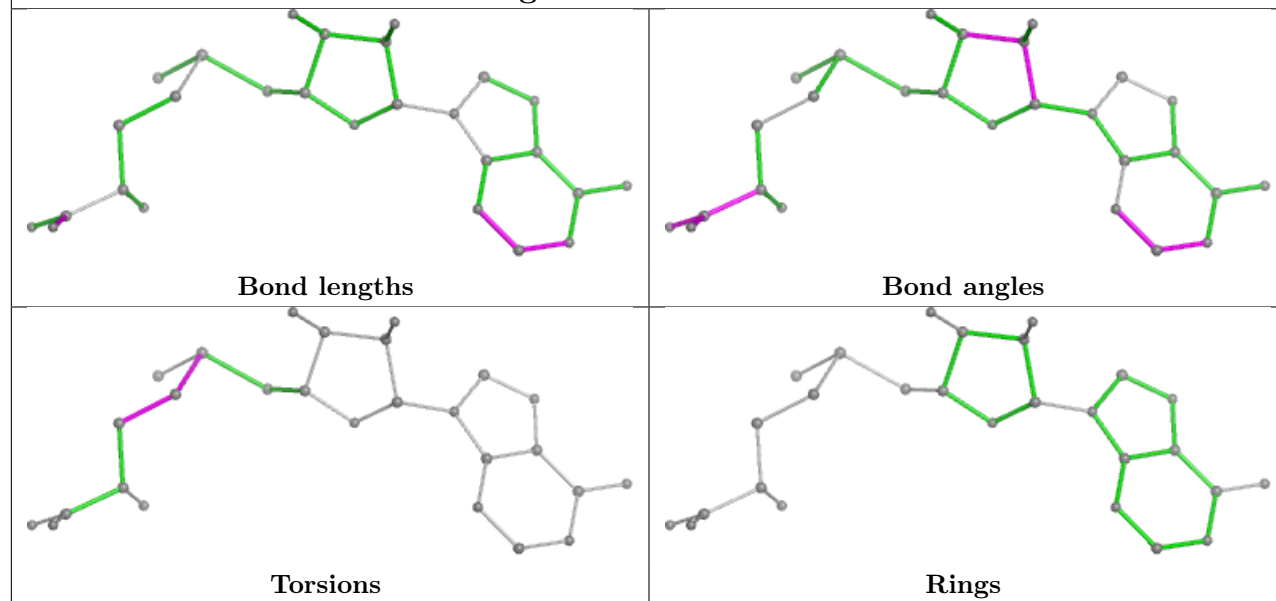
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1002	SAM	5	0
3	M	1002	SAM	4	0
3	LA	1002	SAM	3	0
3	Z	1002	SAM	1	0
3	Q	1002	SAM	3	0
3	RA	1002	SAM	4	0
3	BA	1002	SAM	5	0
3	JA	1002	SAM	3	0
3	V	1002	SAM	3	0
3	FA	1002	SAM	6	0
3	PA	1002	SAM	5	0
3	VA	1002	SAM	2	0
3	G	1002	SAM	3	0
3	I	1002	SAM	4	0
3	C	1002	SAM	5	0
3	O	1002	SAM	3	0
3	HA	1002	SAM	3	0

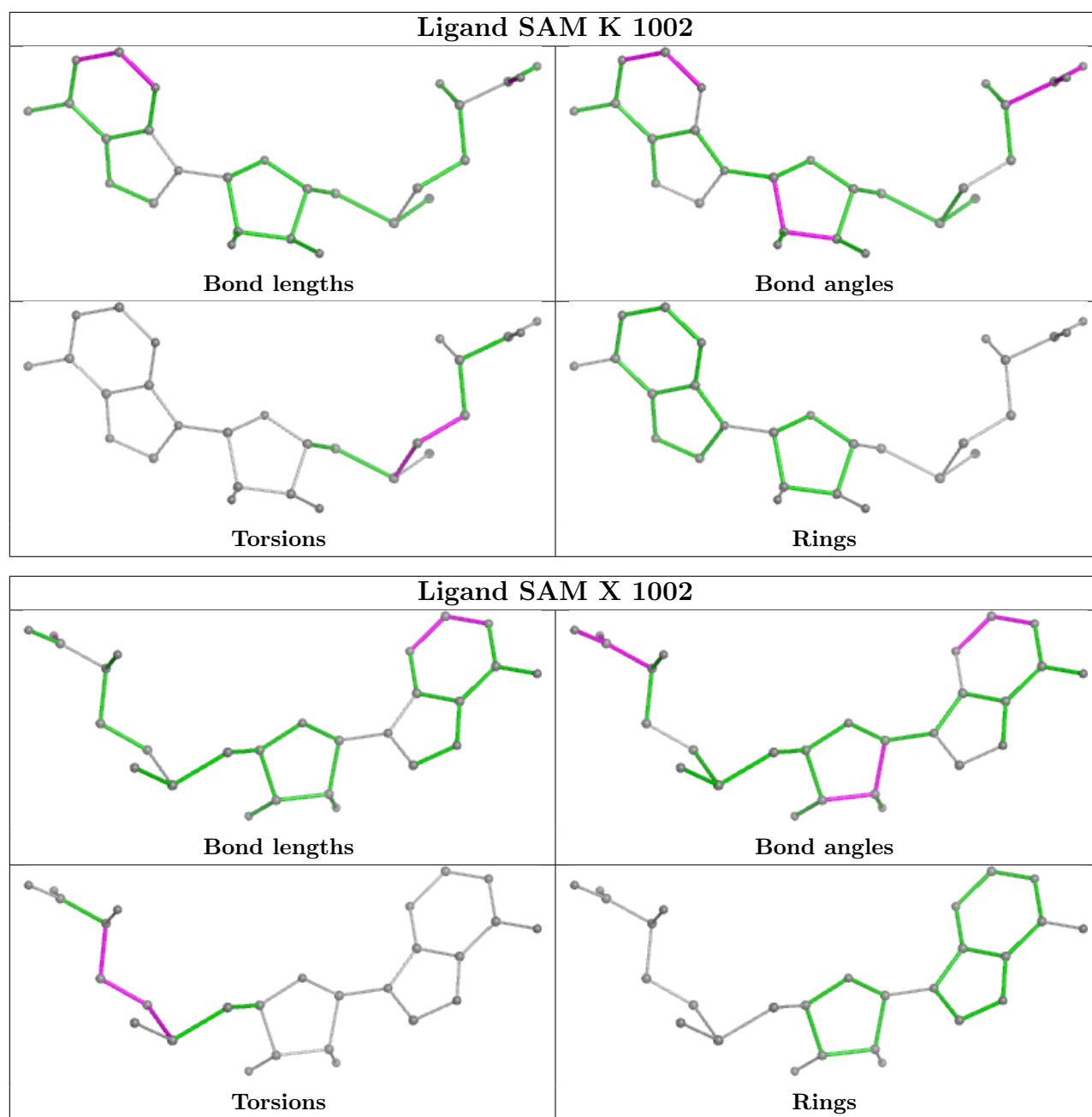
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

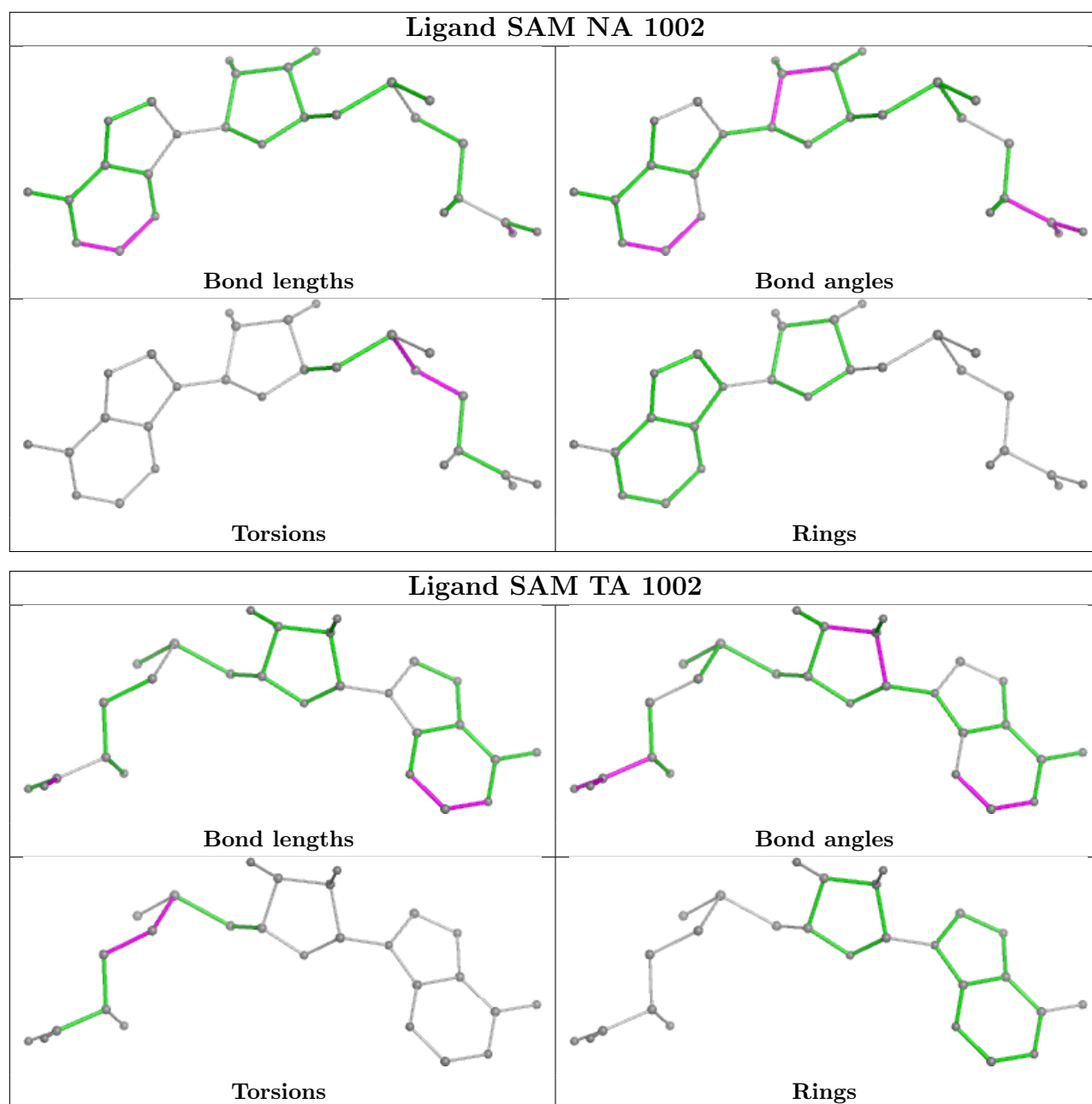
## Ligand SAM DA 1002

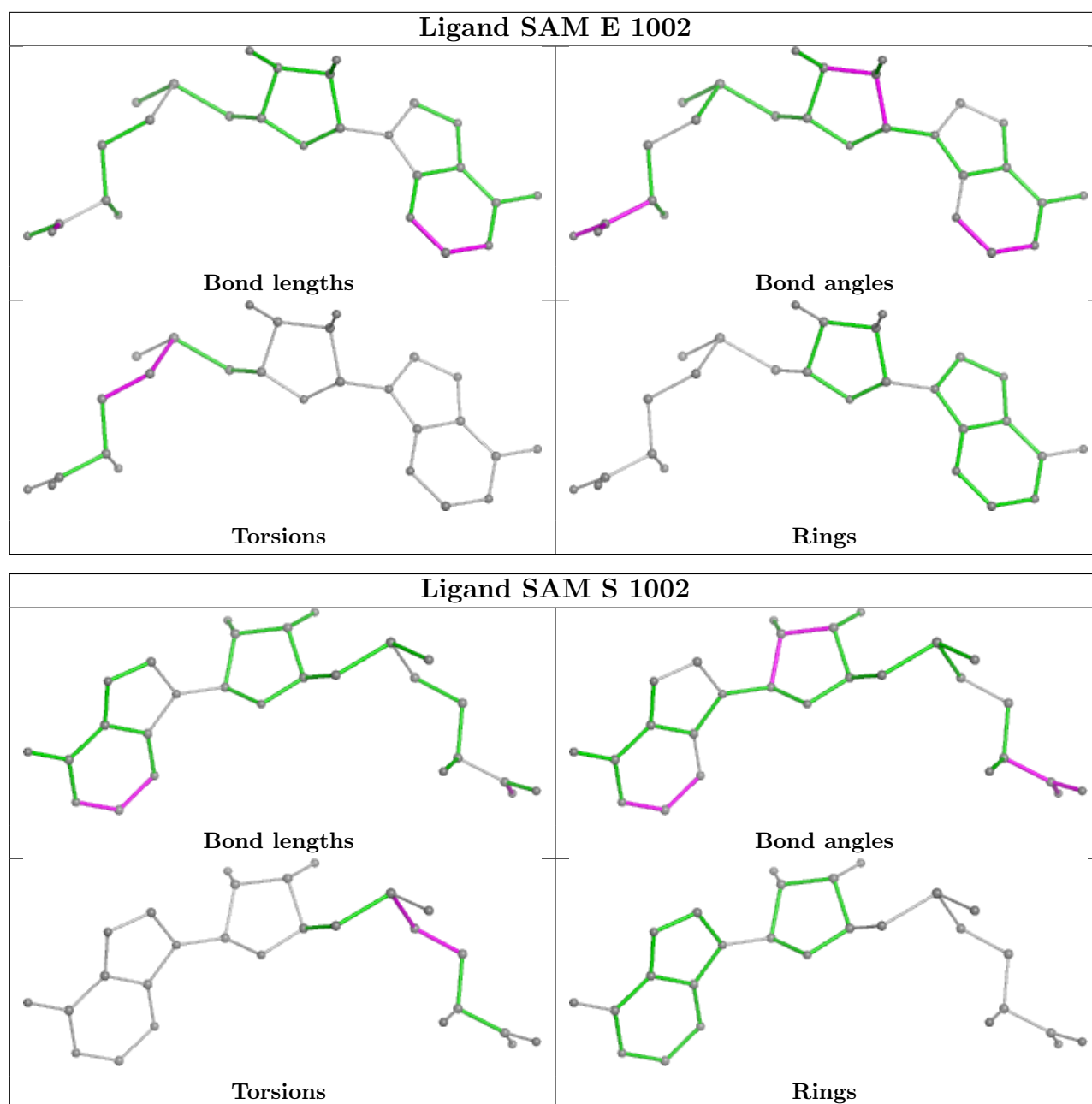


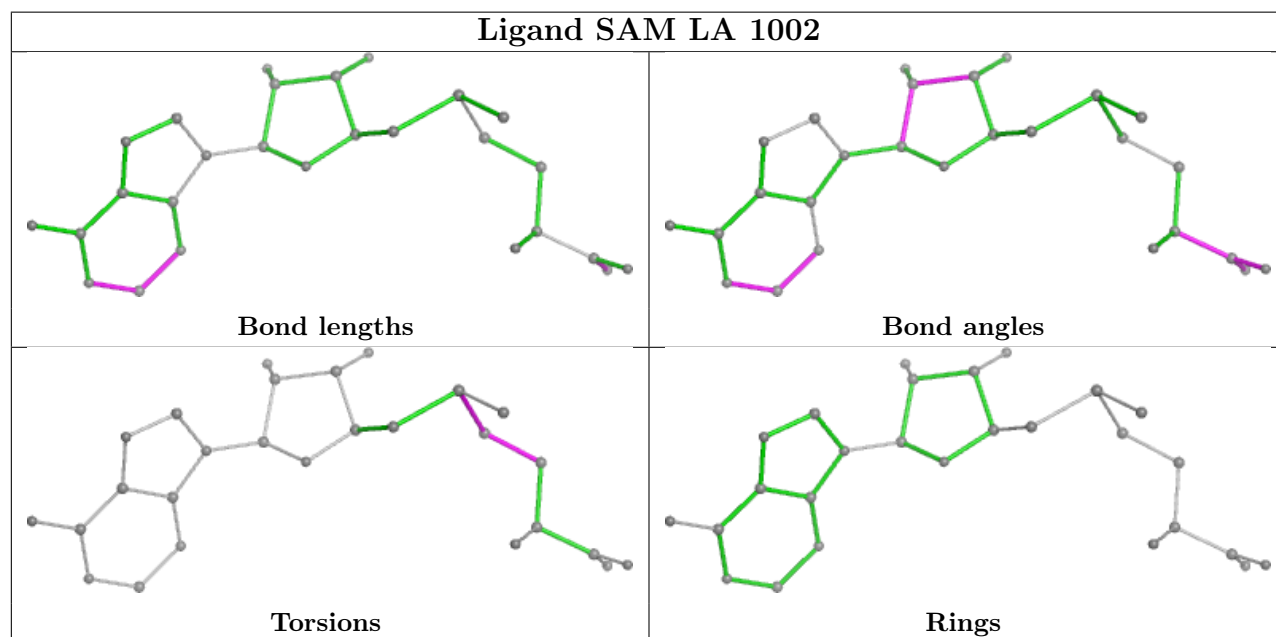
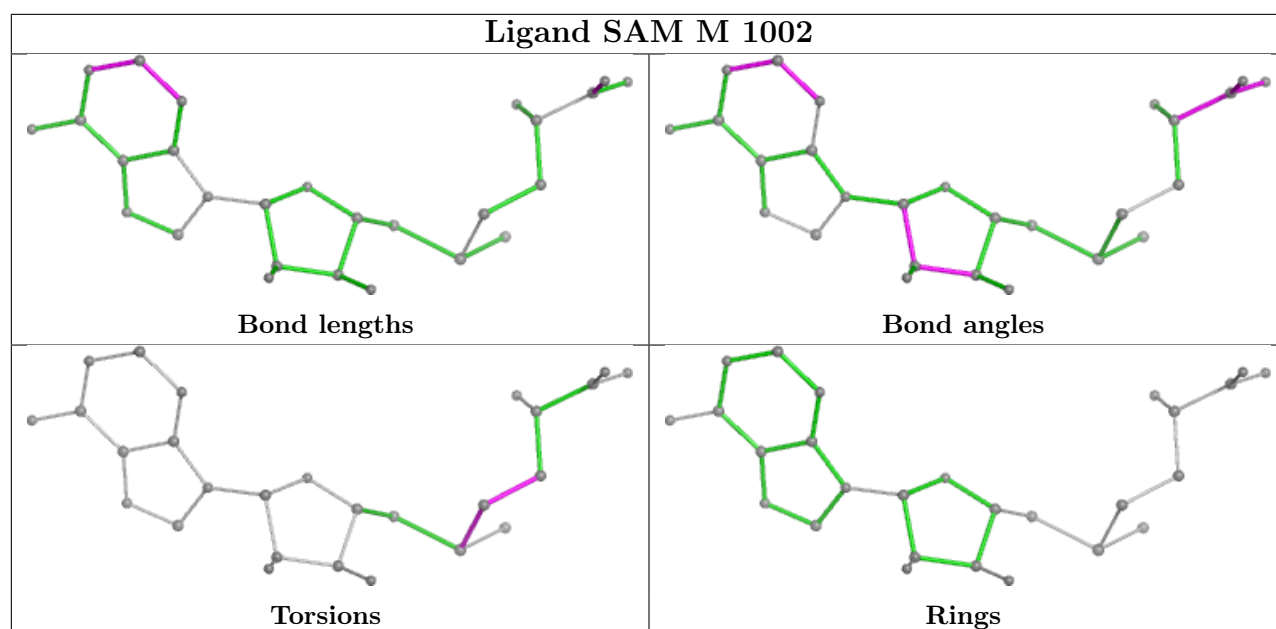
## Ligand SAM A 1002

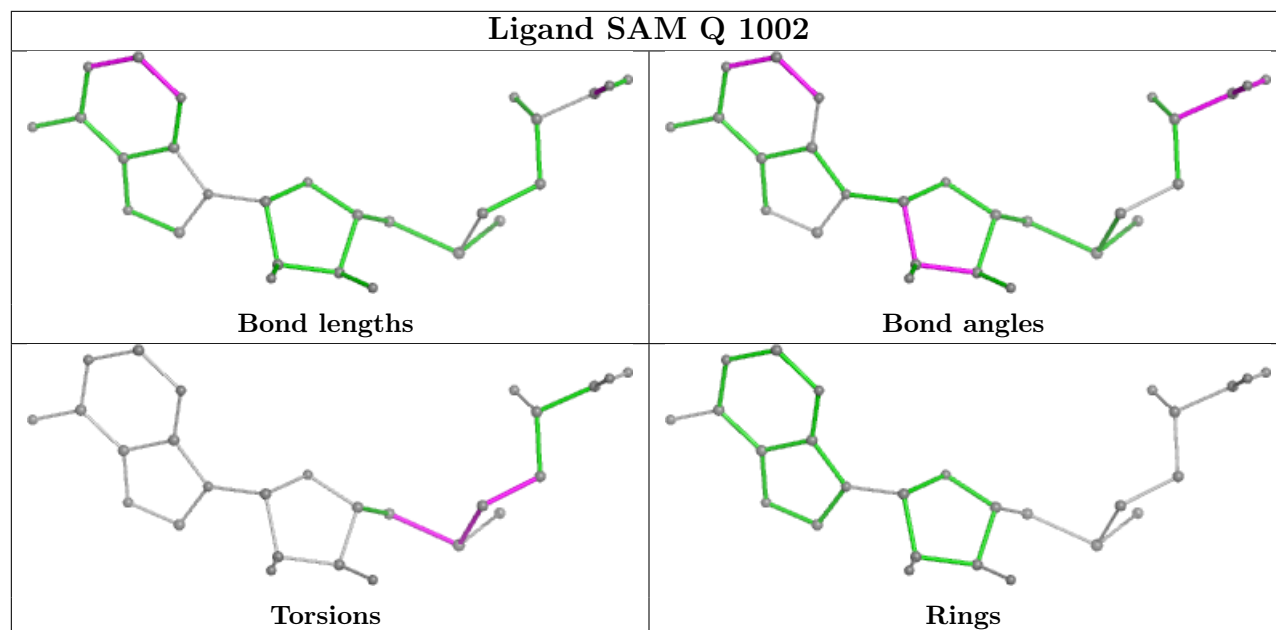
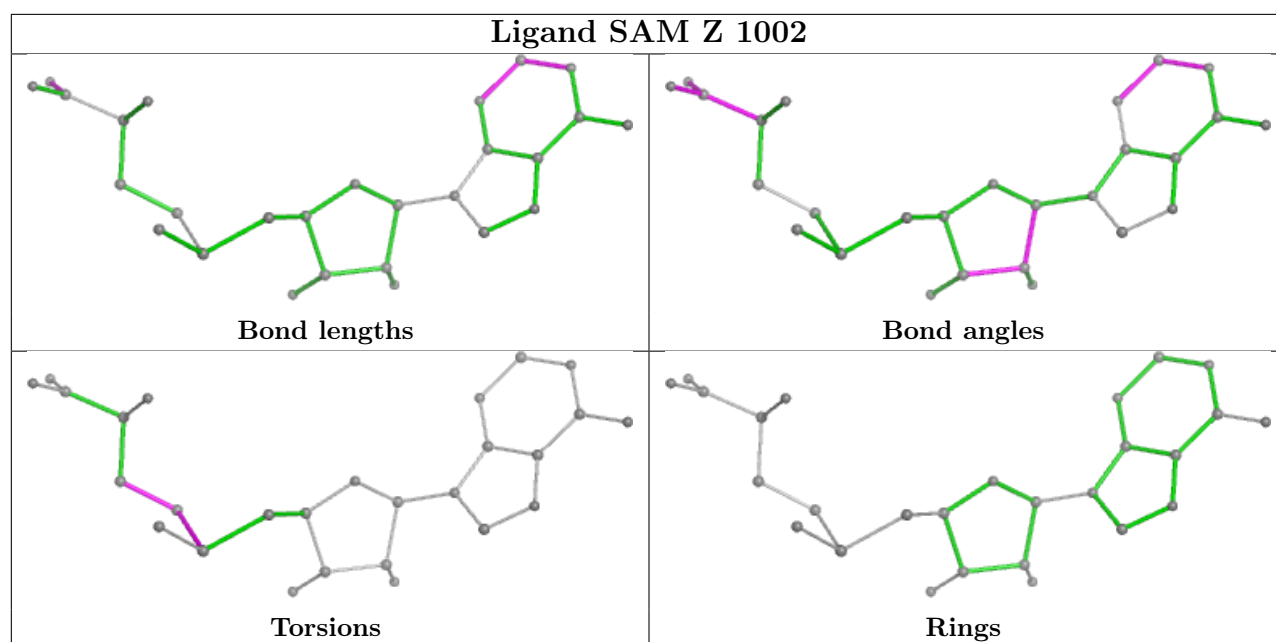




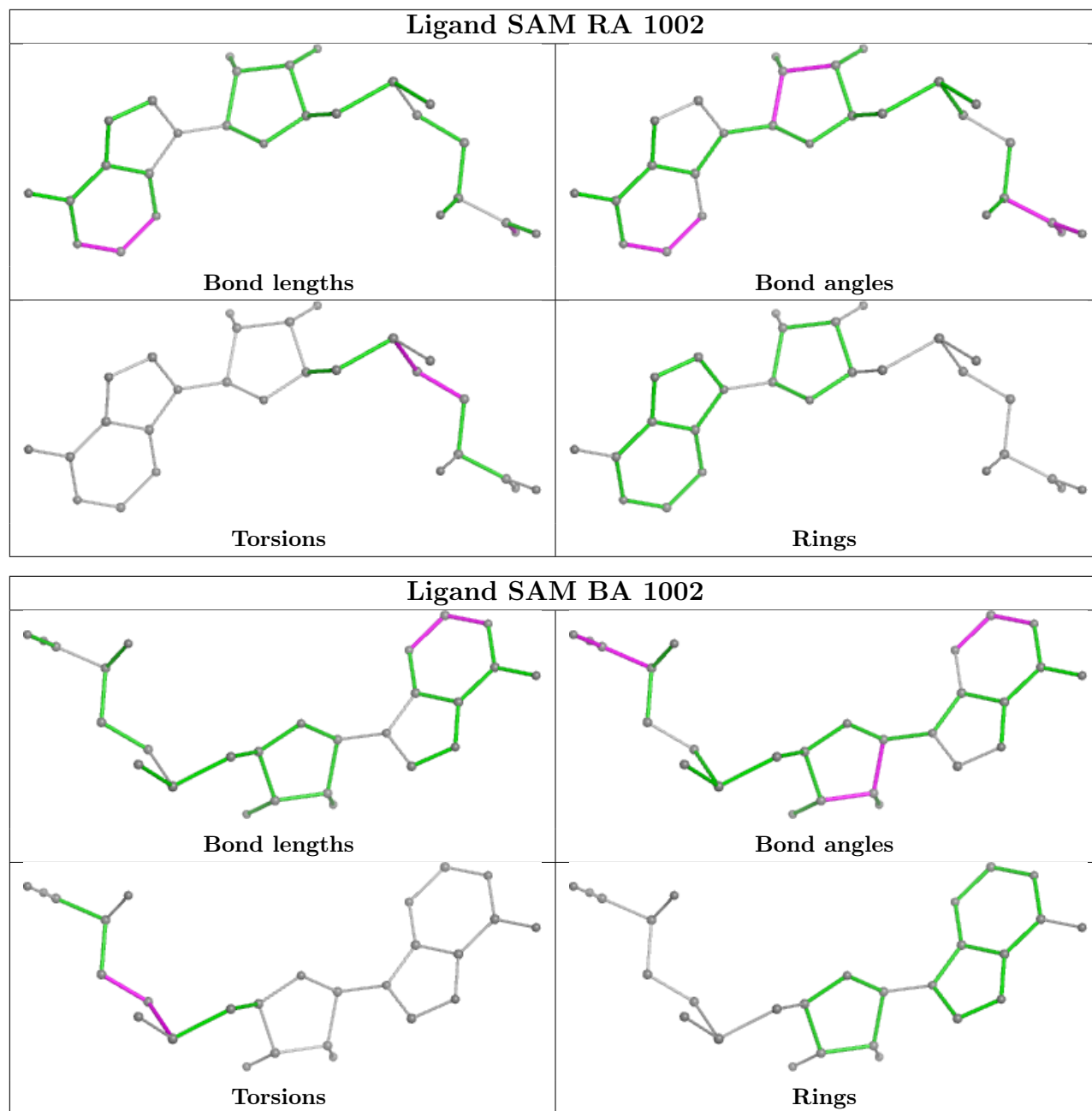


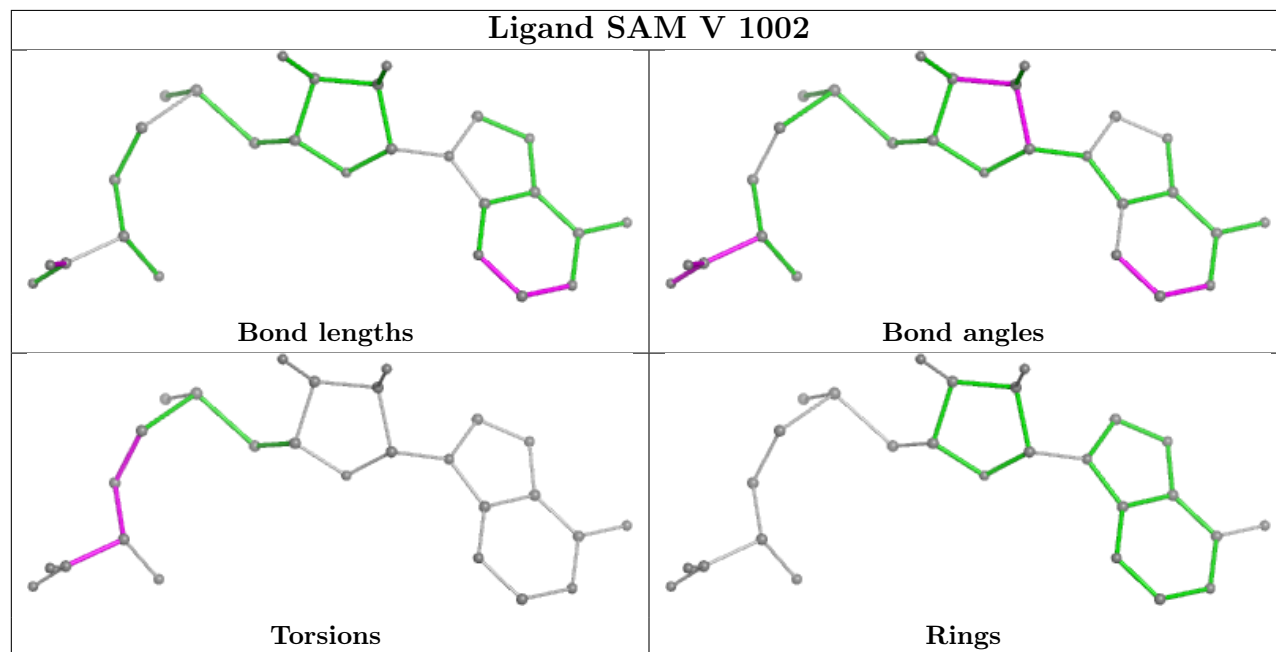
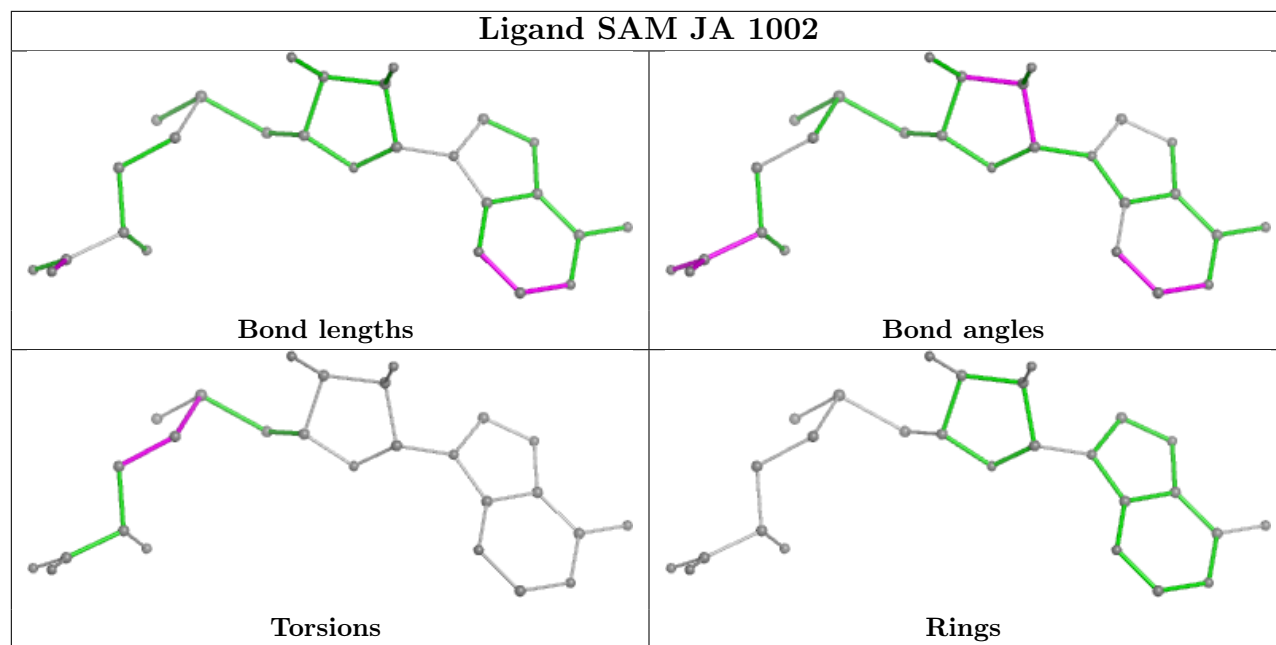


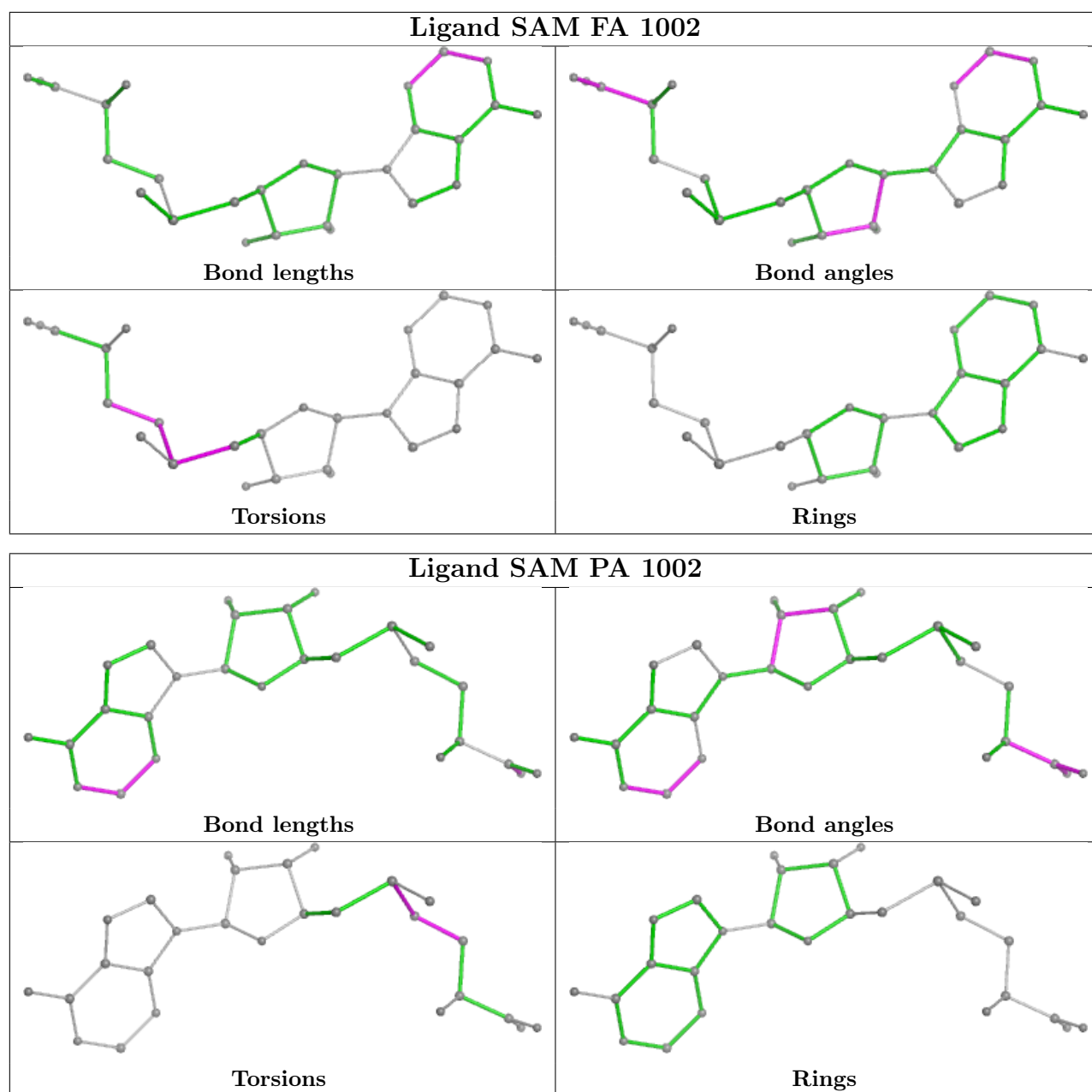


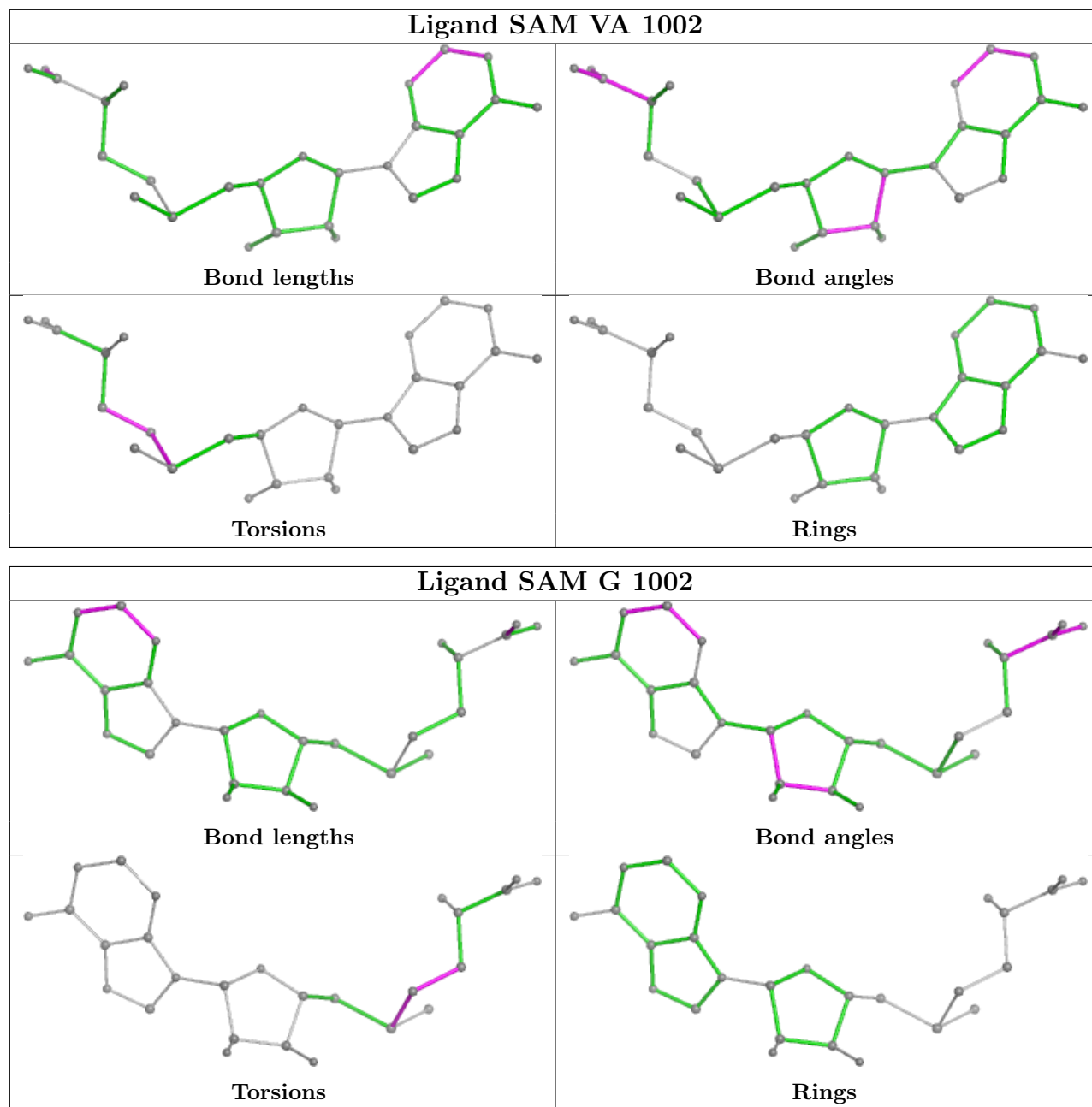


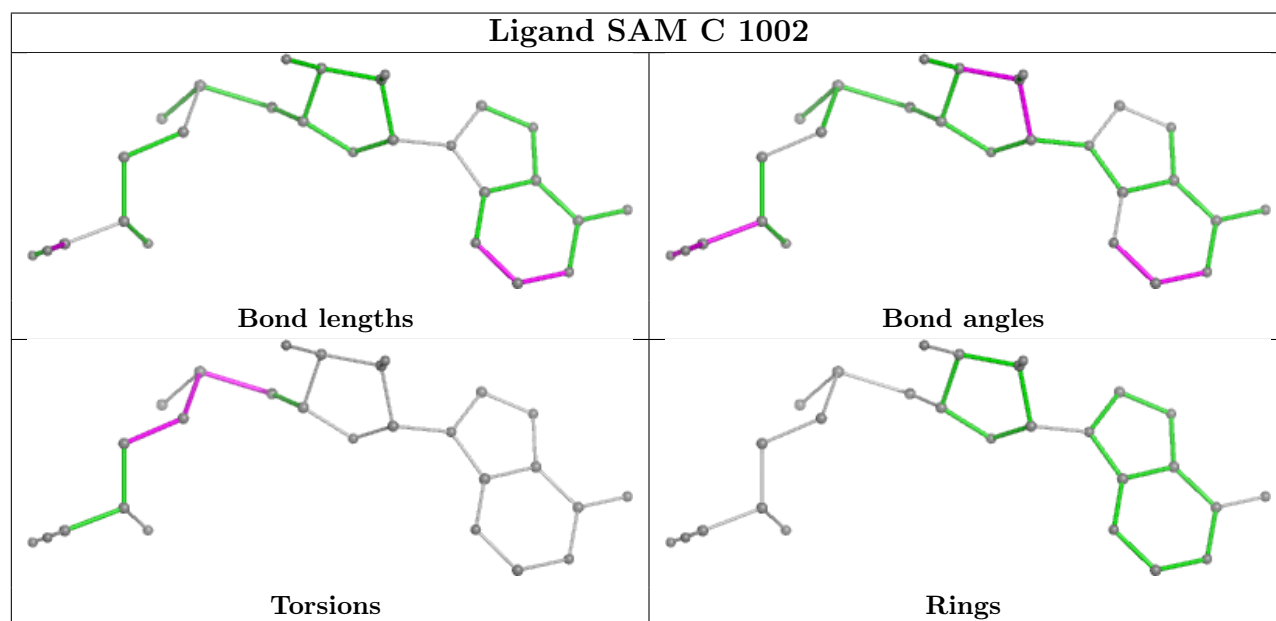
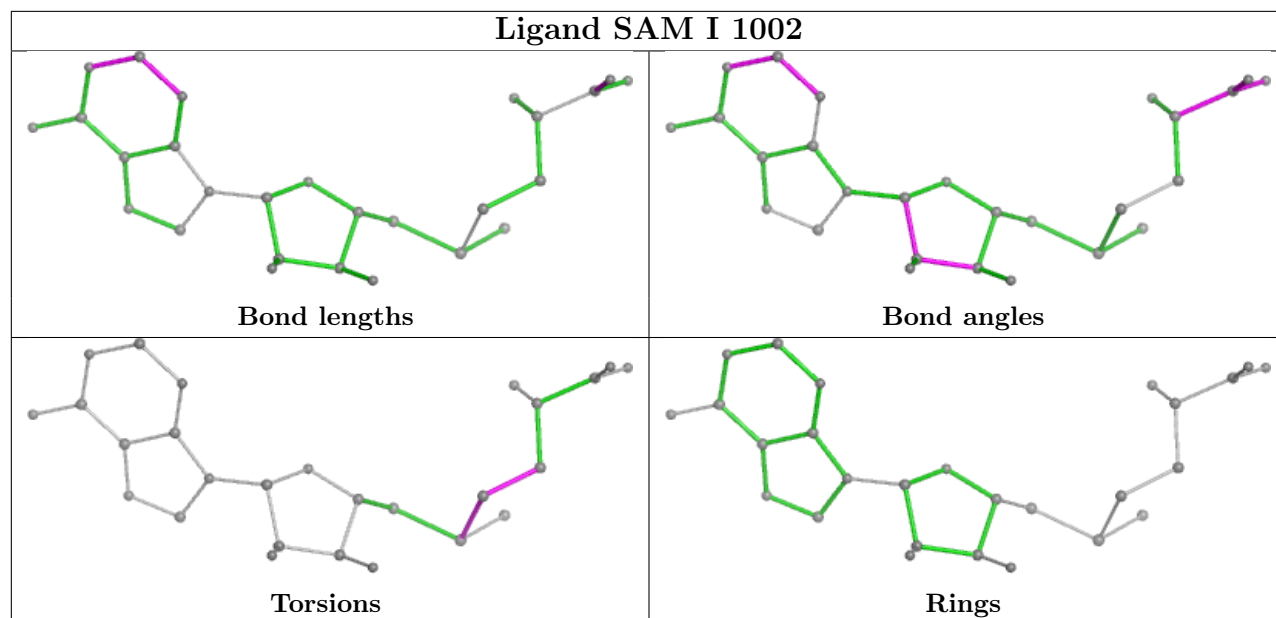


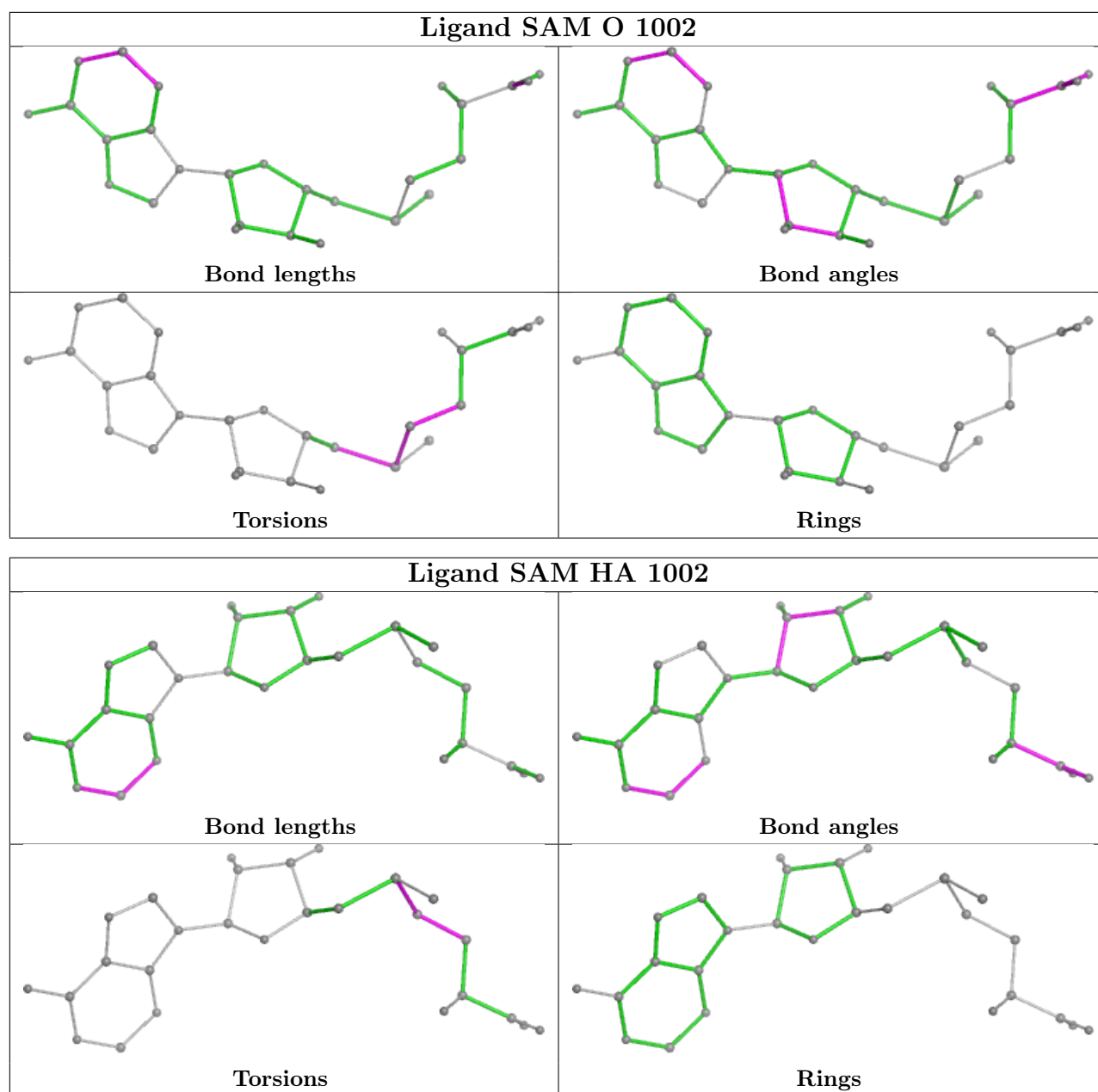












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

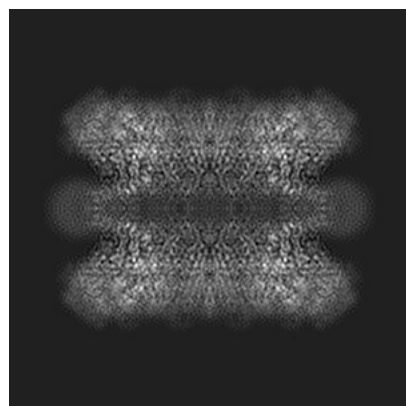
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15555. These allow visual inspection of the internal detail of the map and identification of artifacts.

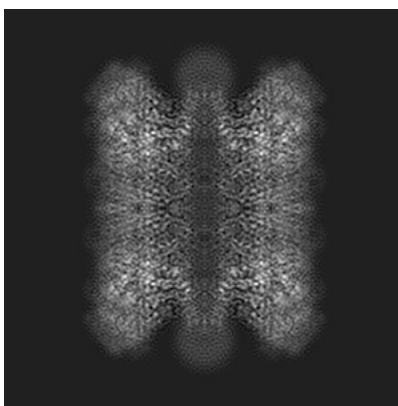
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

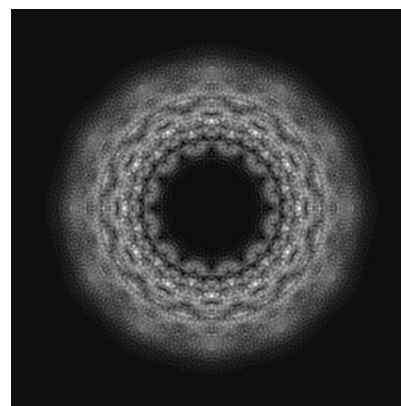
#### 6.1.1 Primary map



X

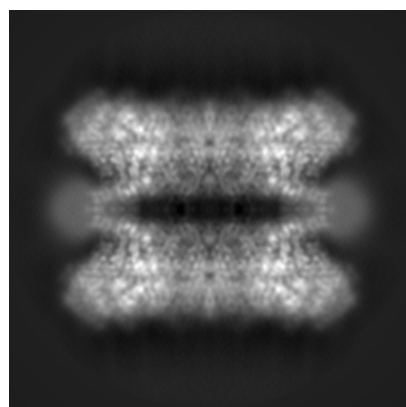


Y

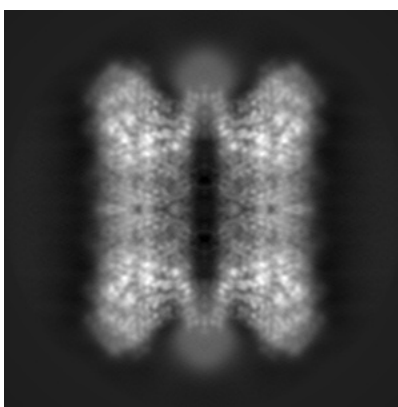


Z

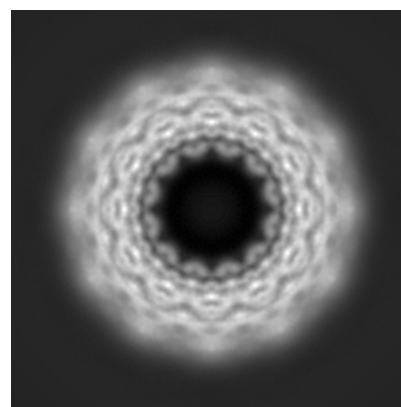
#### 6.1.2 Raw map



X



Y

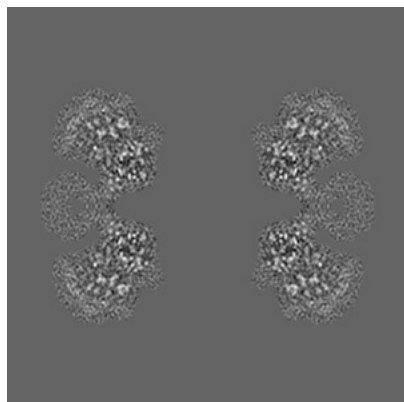


Z

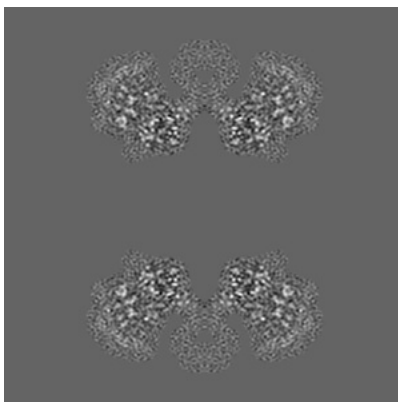
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

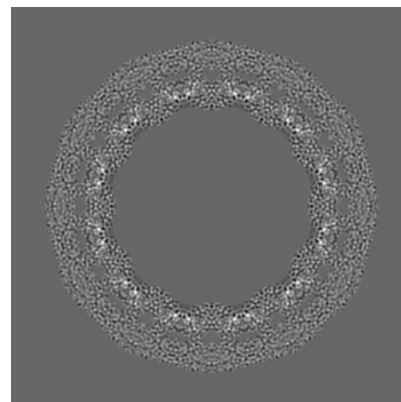
### 6.2.1 Primary map



X Index: 150

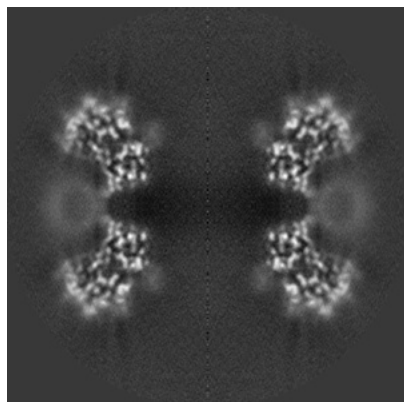


Y Index: 150

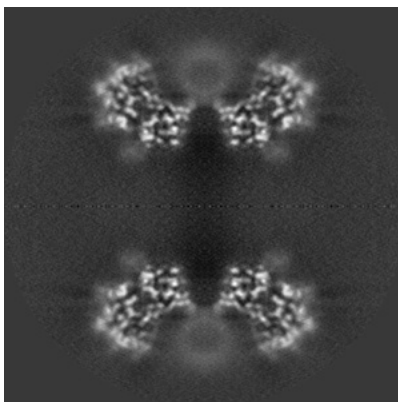


Z Index: 150

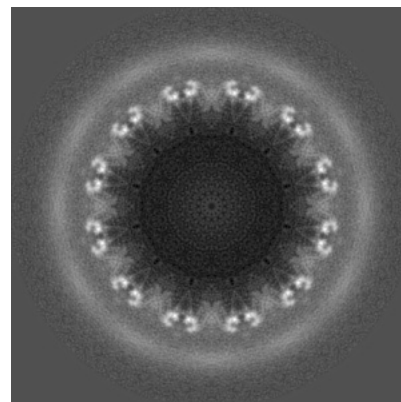
### 6.2.2 Raw map



X Index: 150



Y Index: 150



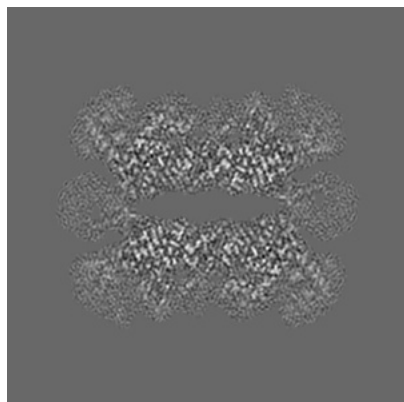
Z Index: 150

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

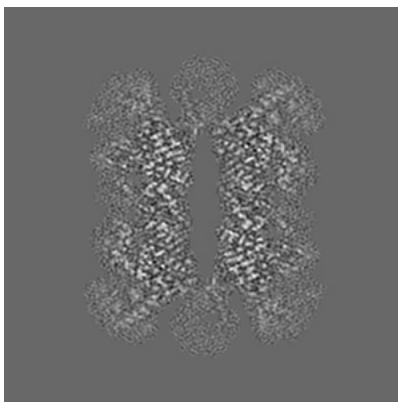


## 6.3 Largest variance slices [i](#)

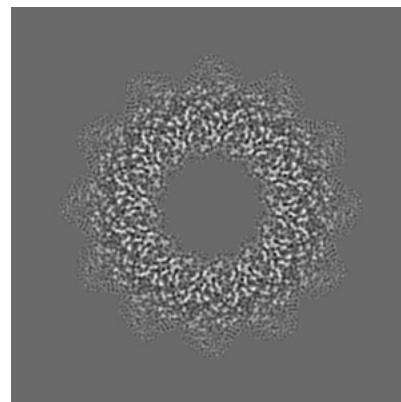
### 6.3.1 Primary map



X Index: 204

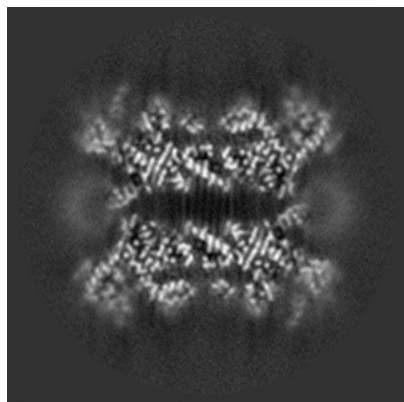


Y Index: 204

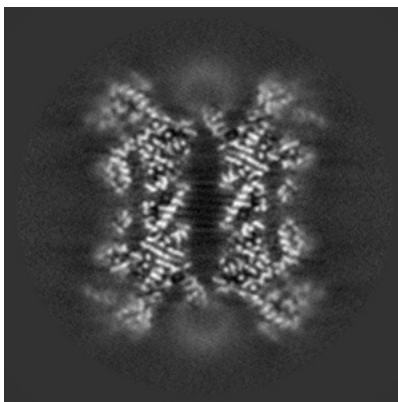


Z Index: 190

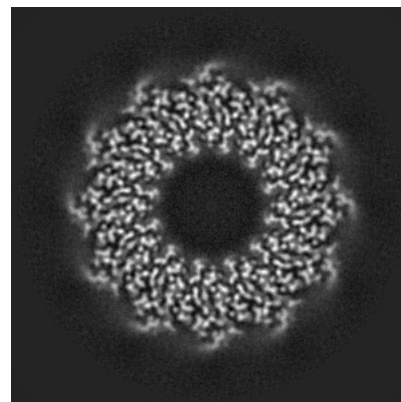
### 6.3.2 Raw map



X Index: 95



Y Index: 95

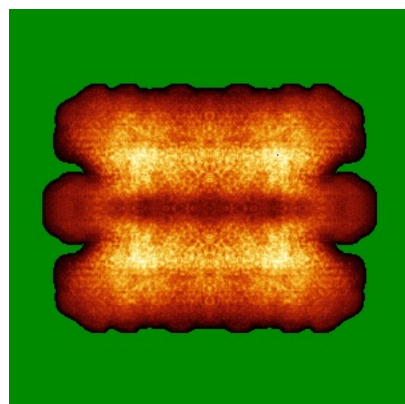


Z Index: 107

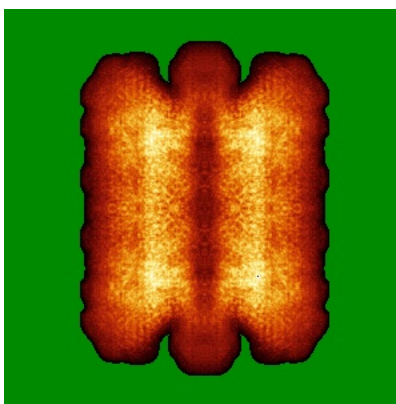
The images above show the largest variance slices of the map in three orthogonal directions.

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

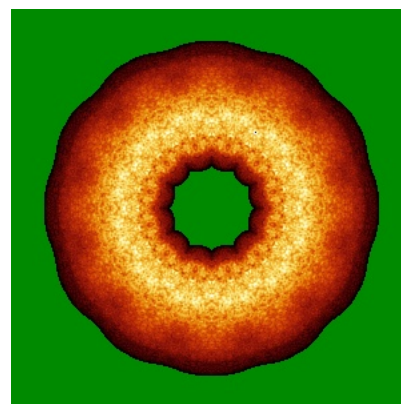
### 6.4.1 Primary map



X

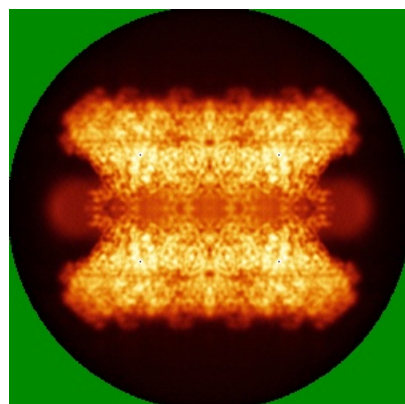


Y

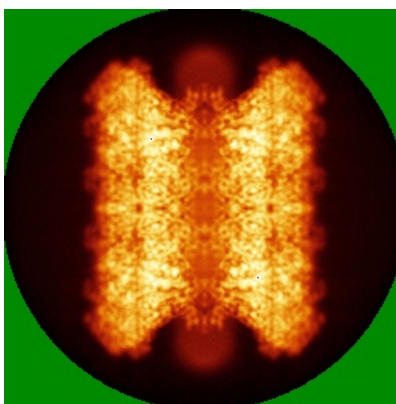


Z

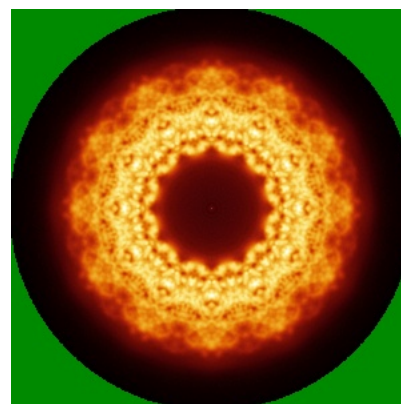
### 6.4.2 Raw map



X



Y

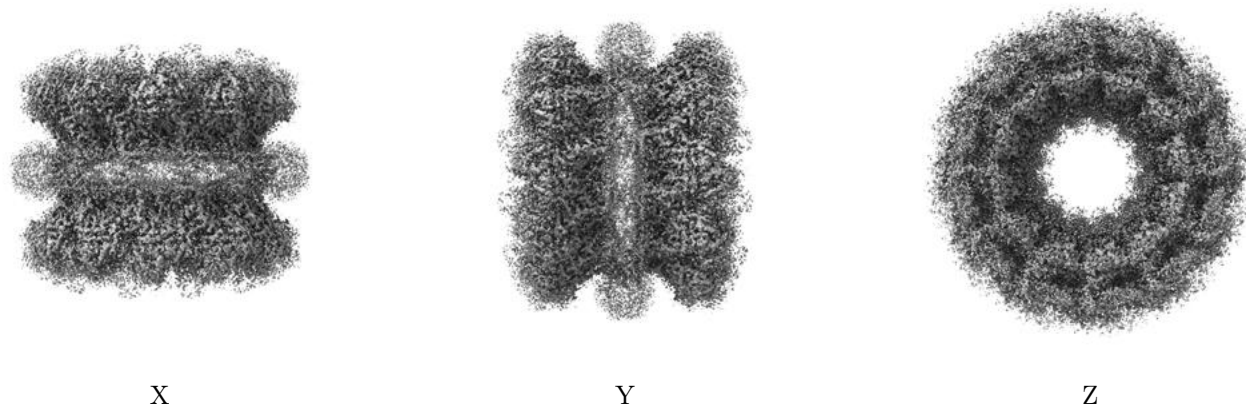


Z

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

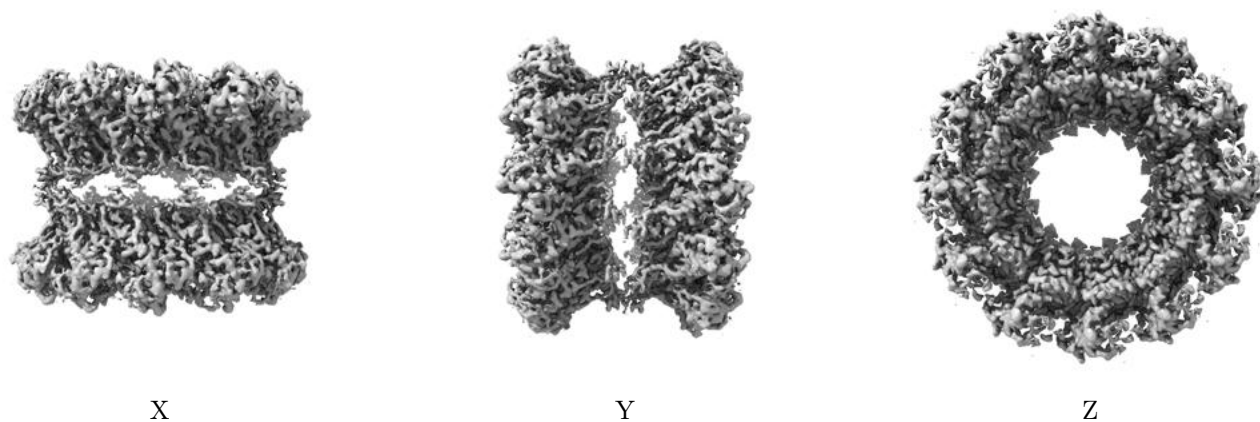
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

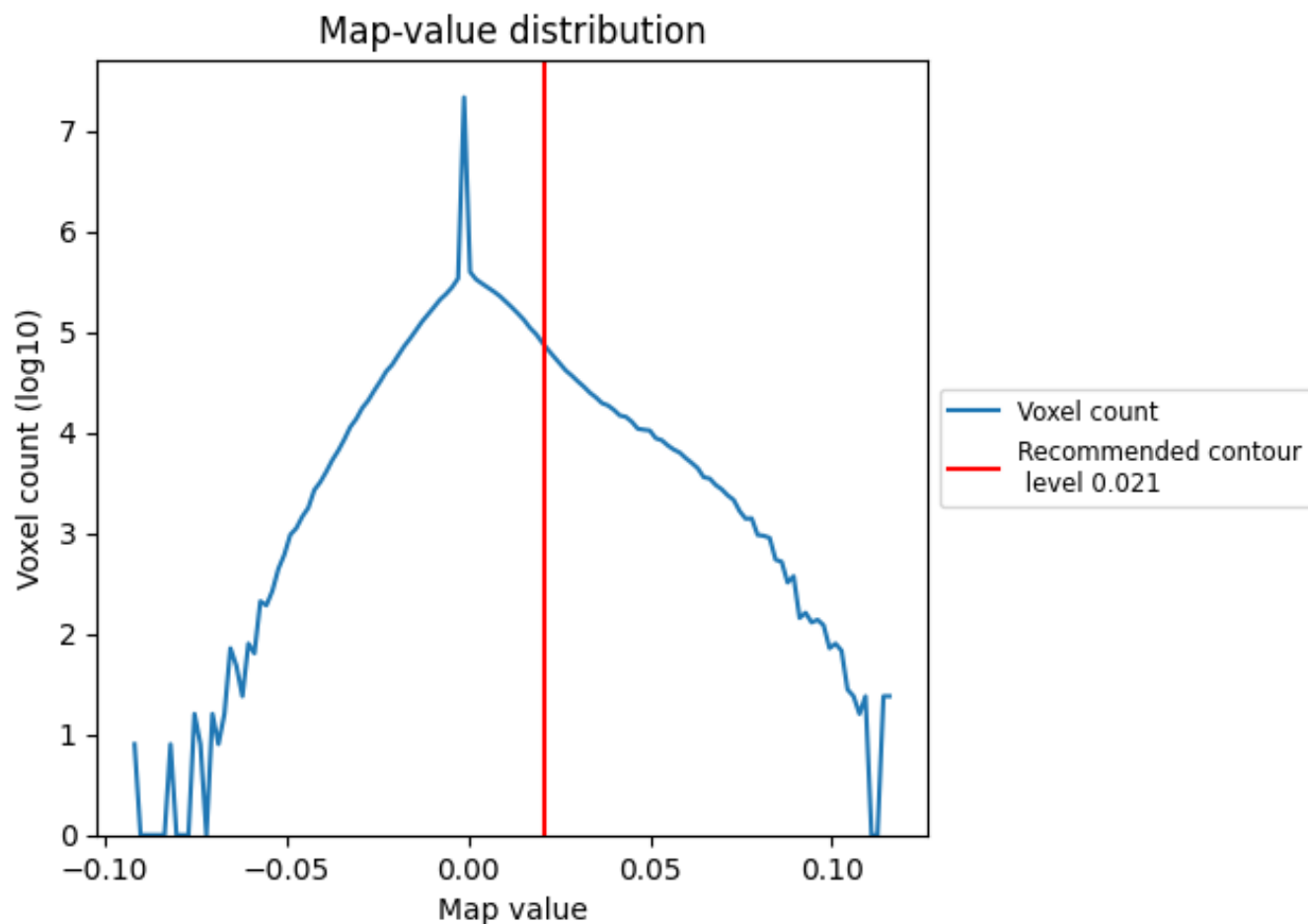
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

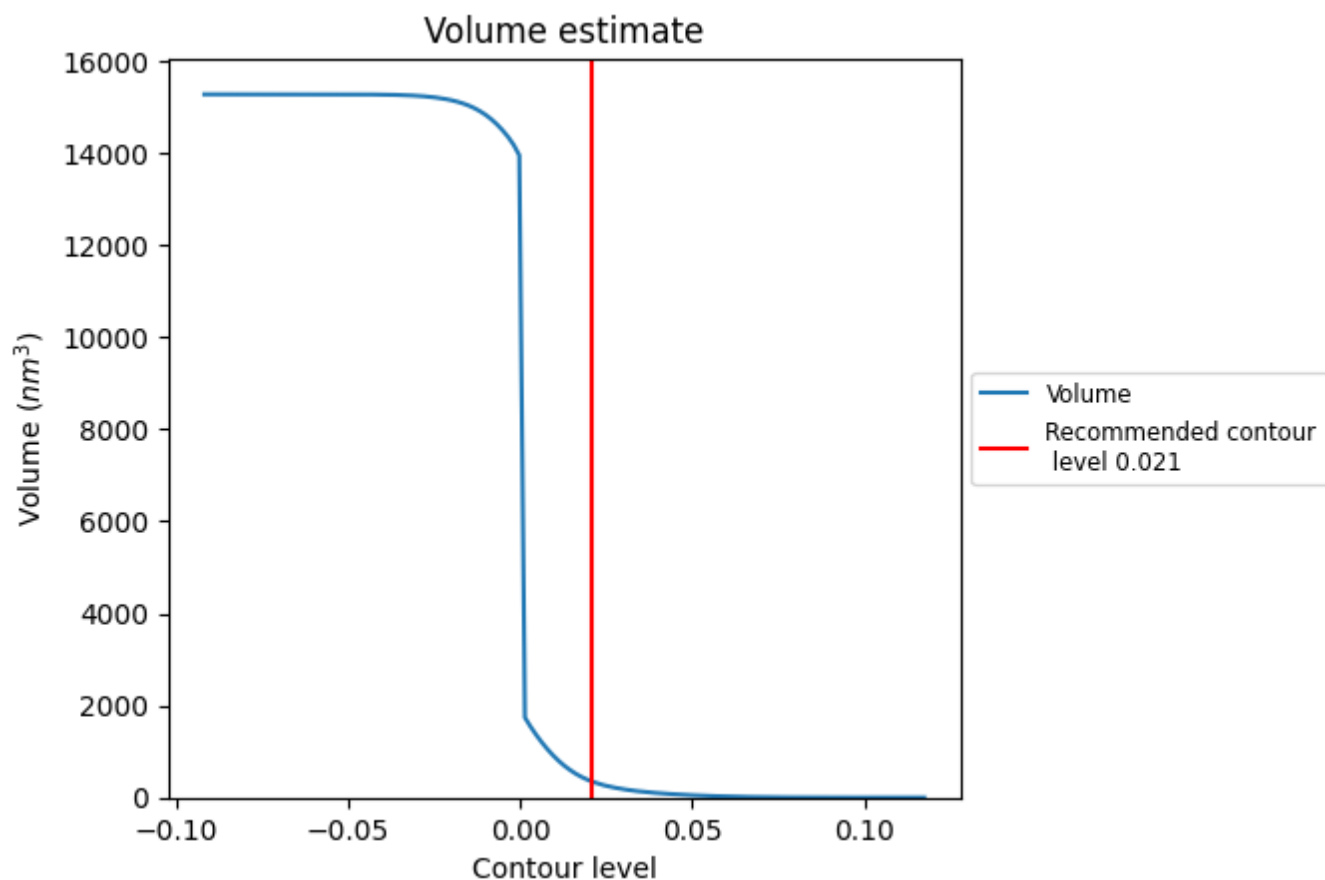
This section contains the results of statistical analysis of the map.

### 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.

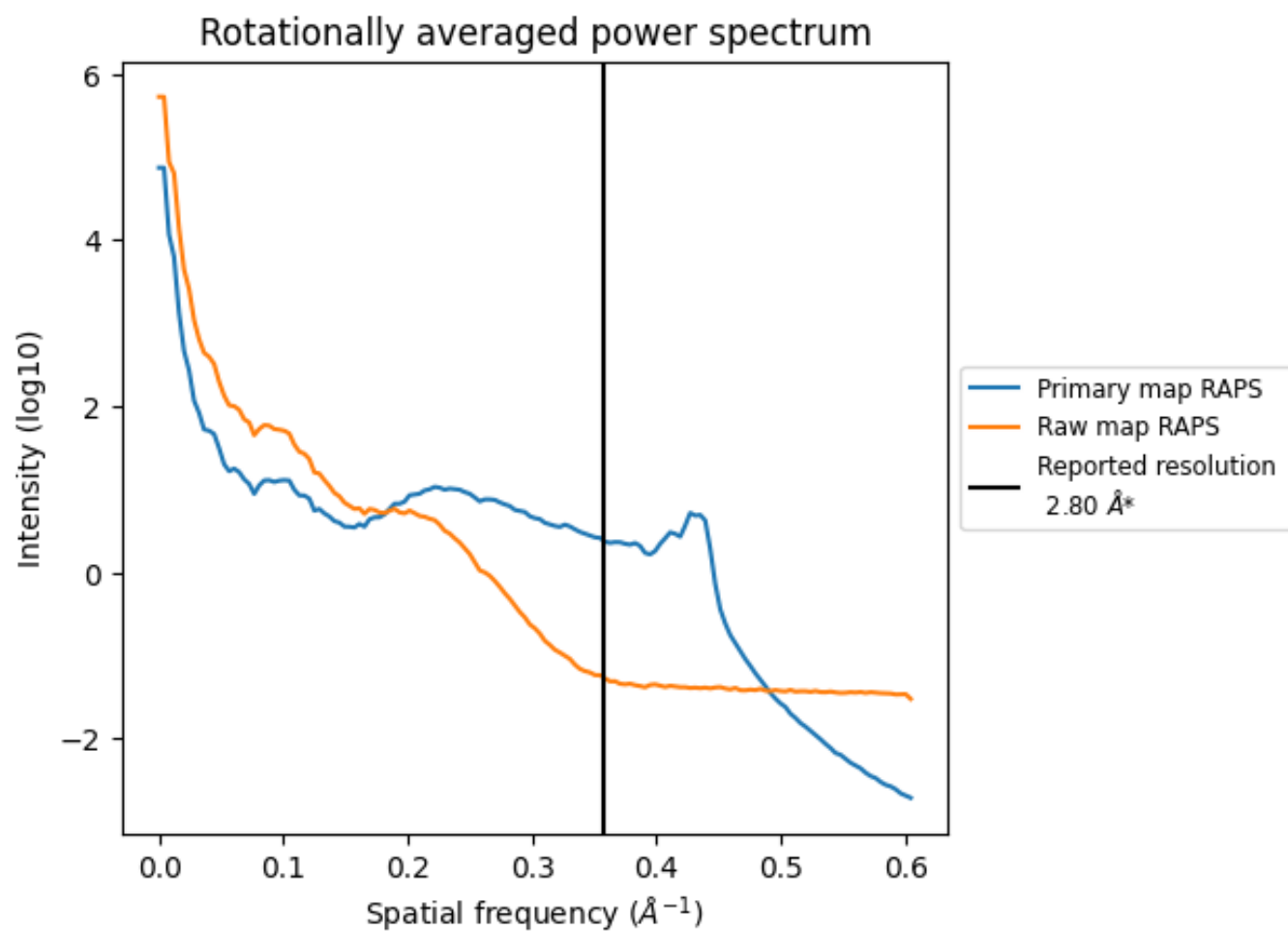
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 345 nm<sup>3</sup>; this corresponds to an approximate mass of 312 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 ⓘ

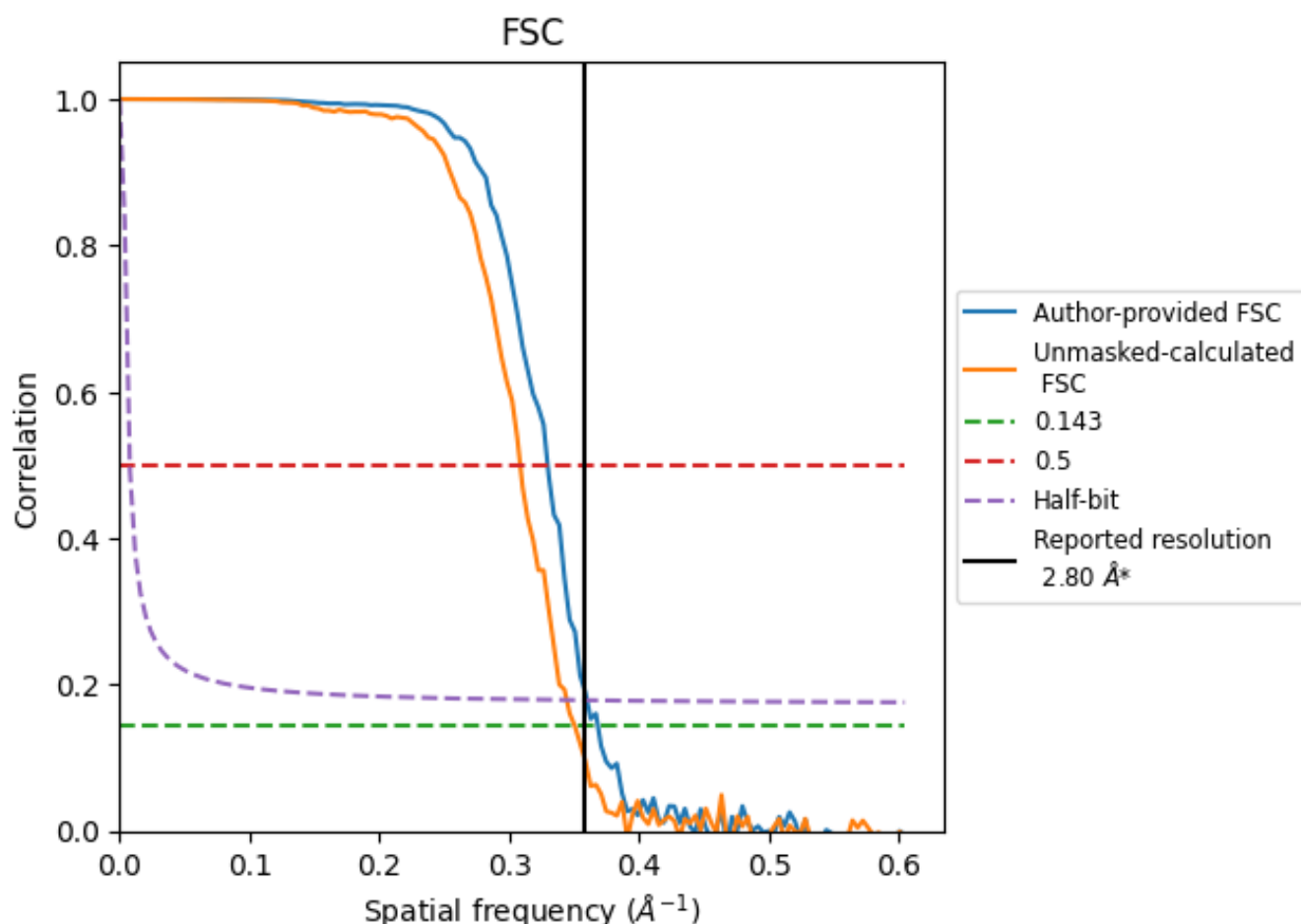


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.72	3.03	2.78
Unmasked-calculated*	2.85	3.24	2.90

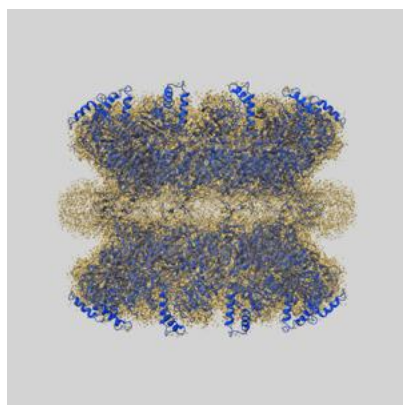
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



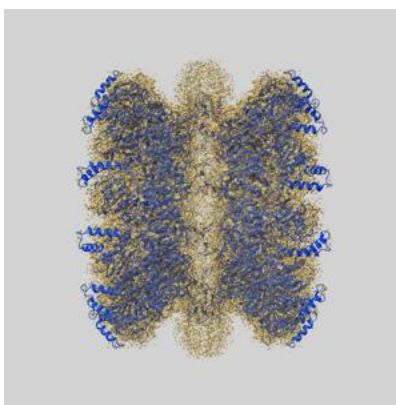
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15555 and PDB model 8AOX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

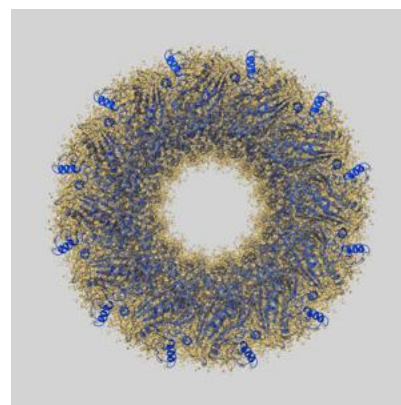
### 9.1 Map-model overlay [i](#)



X



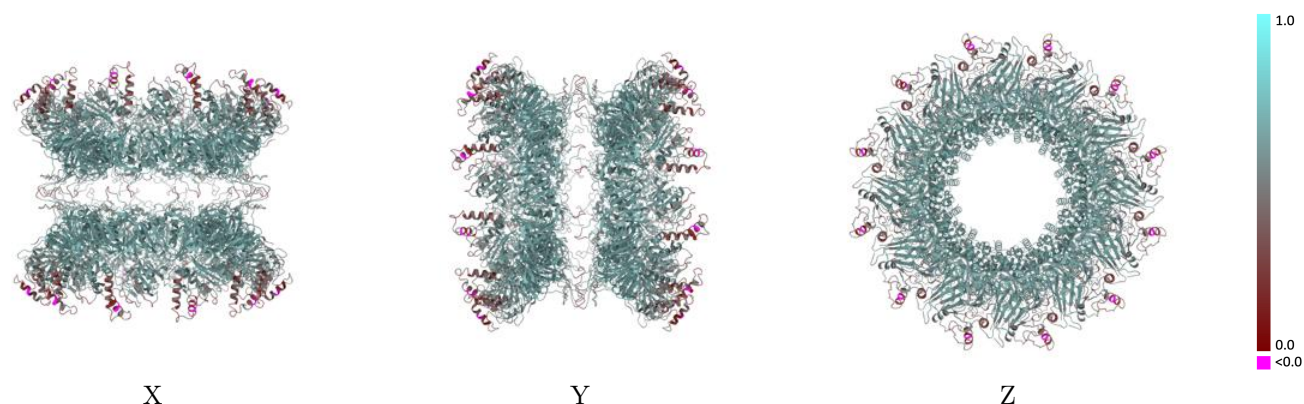
Y



Z

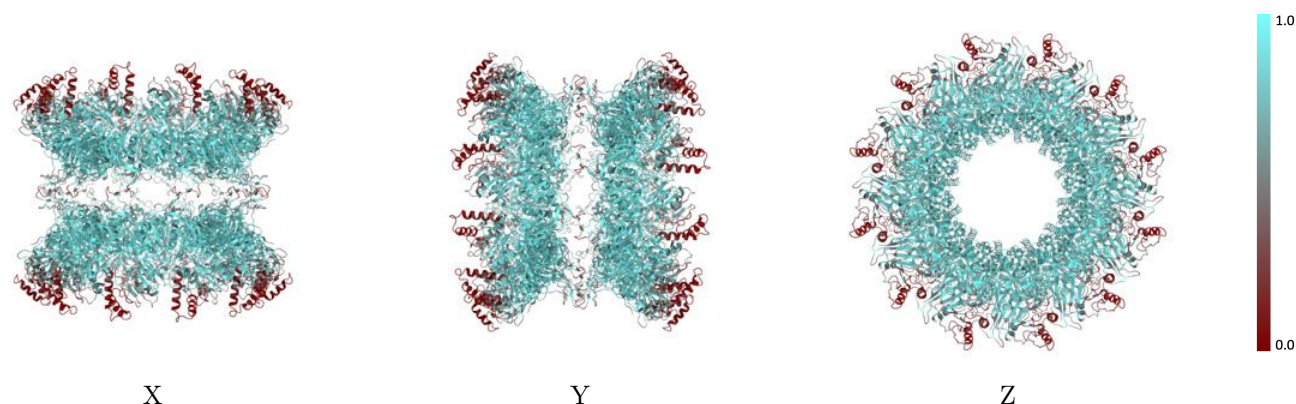
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



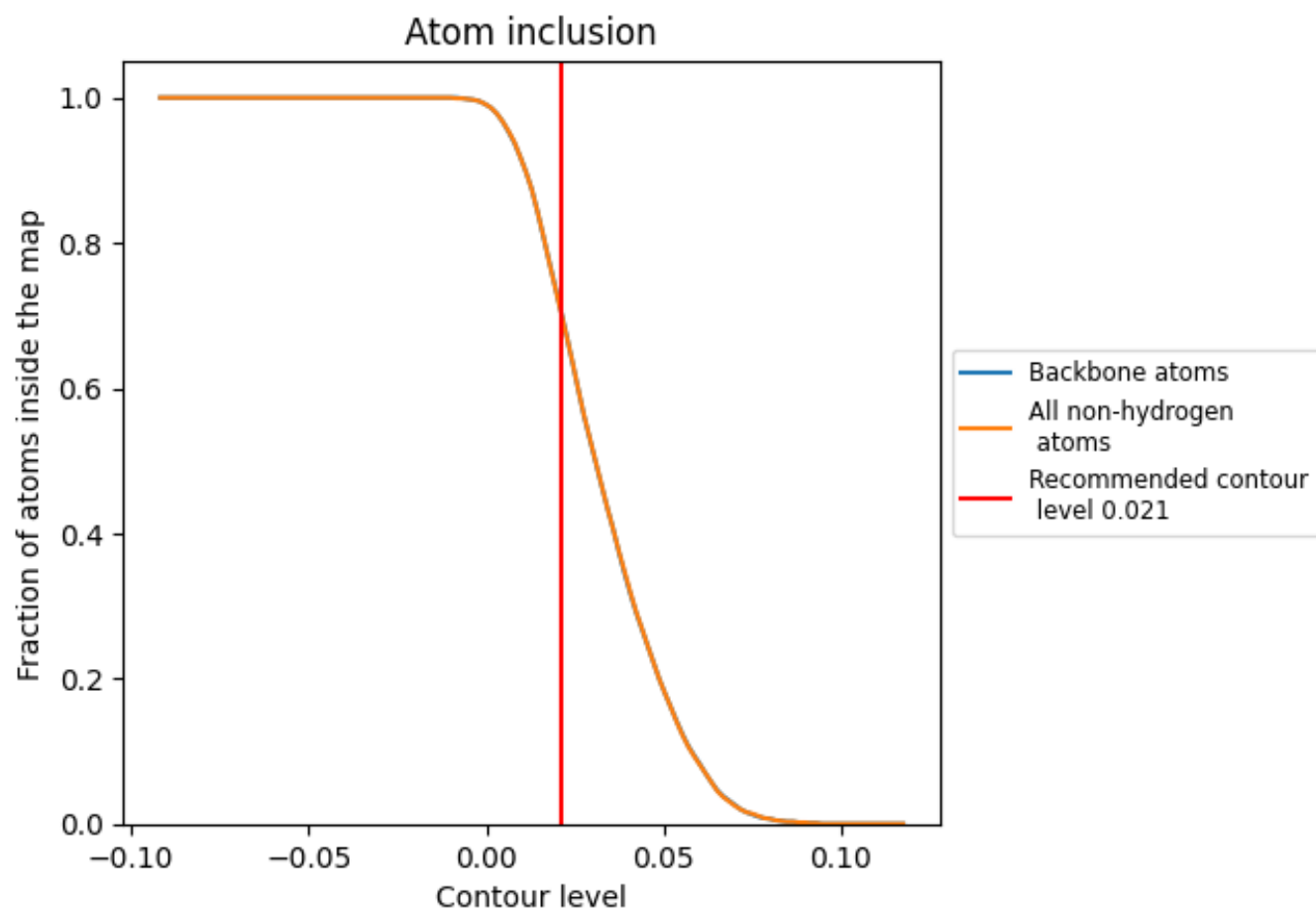
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 71% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.5740
A	 0.7120	 0.5730
BA	 0.7080	 0.5740
C	 0.7140	 0.5730
DA	 0.7130	 0.5740
E	 0.7140	 0.5760
FA	 0.7110	 0.5710
G	 0.7150	 0.5730
HA	 0.7090	 0.5740
I	 0.7110	 0.5750
JA	 0.7120	 0.5760
K	 0.7140	 0.5750
LA	 0.7110	 0.5750
M	 0.7140	 0.5730
NA	 0.7090	 0.5730
O	 0.7080	 0.5740
PA	 0.7110	 0.5730
Q	 0.7120	 0.5740
RA	 0.7130	 0.5730
S	 0.7120	 0.5730
TA	 0.7110	 0.5730
V	 0.7070	 0.5730
VA	 0.7120	 0.5760
X	 0.7120	 0.5750
Z	 0.7150	 0.5750

