



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:11 AM UTC

PDB ID : 9MMY / pdb_00009mmy
EMDB ID : EMD-48407
Title : E. coli GroEL bound with ATP and PBZ1587 inhibitor
Authors : Johnson, S.M.; Chen, Q.
Deposited on : 2024-12-20
Resolution : 2.70 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:

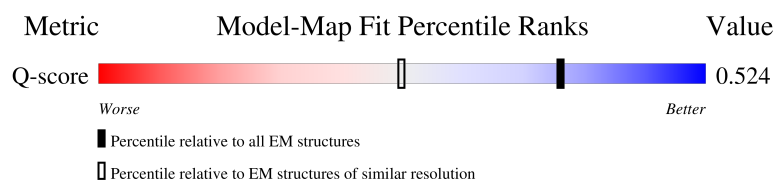
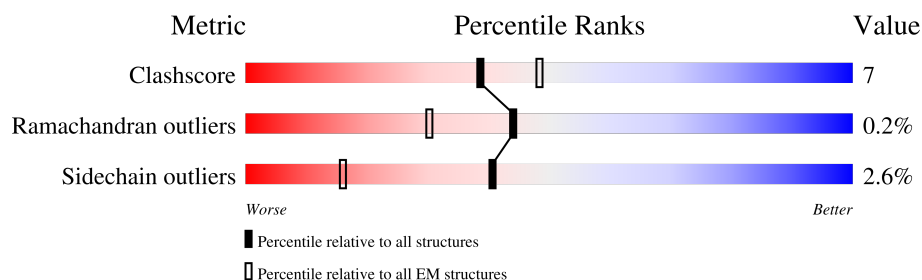
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	

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Mol	Chain	Length	Quality of chain
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 54831 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	B	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	C	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	D	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	E	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	F	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	G	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	H	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	I	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	J	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	K	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	L	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	M	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	N	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

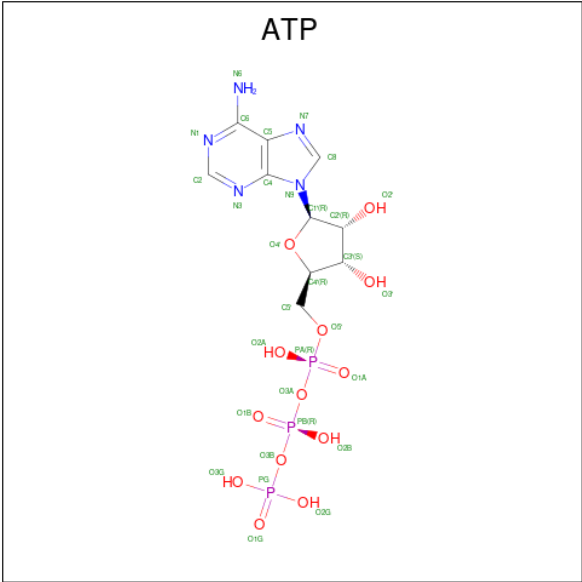
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total 1	Mg 1	0
2	C	1	Total 1	Mg 1	0
2	D	1	Total 1	Mg 1	0
2	E	1	Total 1	Mg 1	0
2	F	1	Total 1	Mg 1	0
2	G	1	Total 1	Mg 1	0
2	H	1	Total 1	Mg 1	0
2	I	1	Total 1	Mg 1	0
2	J	1	Total 1	Mg 1	0
2	K	1	Total 1	Mg 1	0
2	L	1	Total 1	Mg 1	0
2	M	1	Total 1	Mg 1	0
2	N	1	Total 1	Mg 1	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

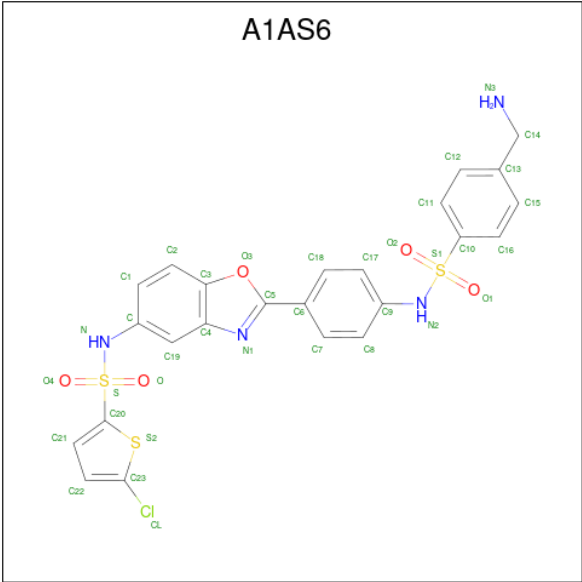


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	N	1	Total	C	N	O	P	0
			31	10	5	13	3	

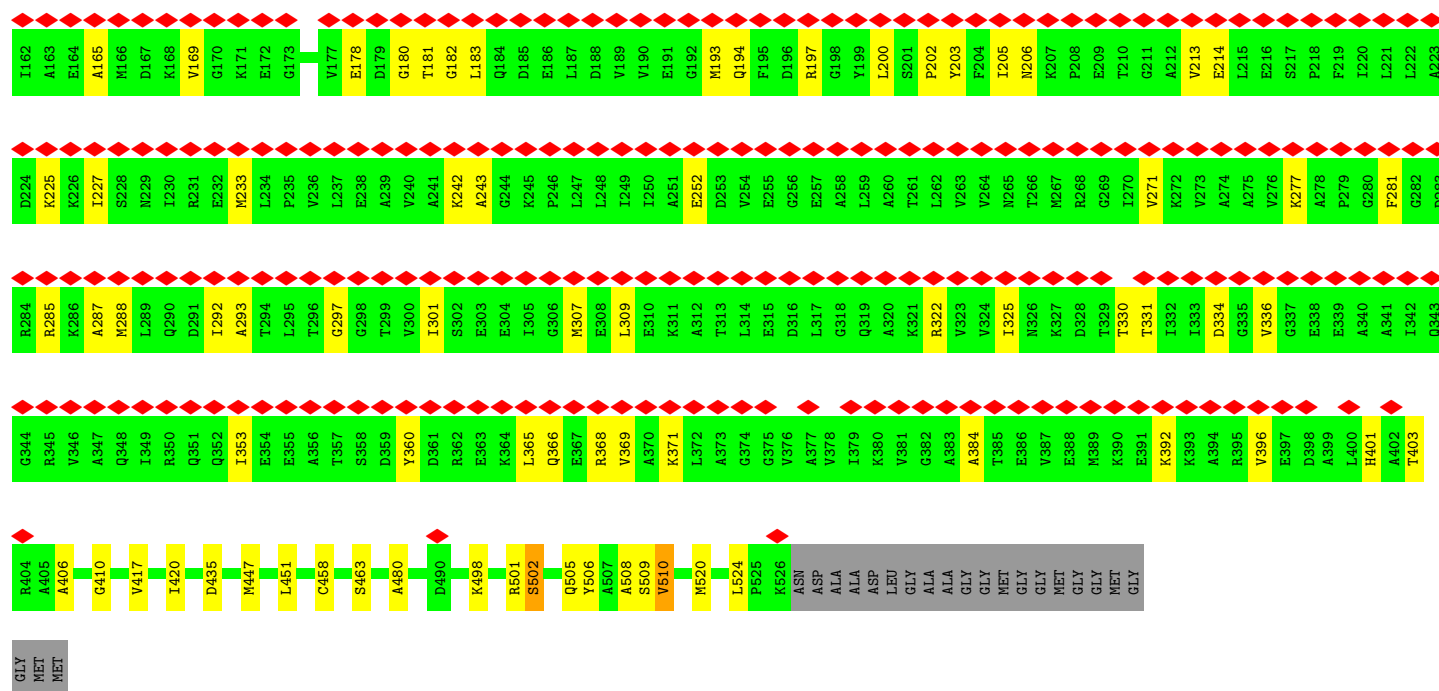
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	K 2	0
4	B	2	Total 2	K 2	0
4	C	2	Total 2	K 2	0
4	D	2	Total 2	K 2	0
4	E	2	Total 2	K 2	0
4	F	2	Total 2	K 2	0
4	G	2	Total 2	K 2	0
4	H	2	Total 2	K 2	0
4	I	2	Total 2	K 2	0
4	J	2	Total 2	K 2	0
4	K	2	Total 2	K 2	0
4	L	2	Total 2	K 2	0
4	M	2	Total 2	K 2	0
4	N	2	Total 2	K 2	0

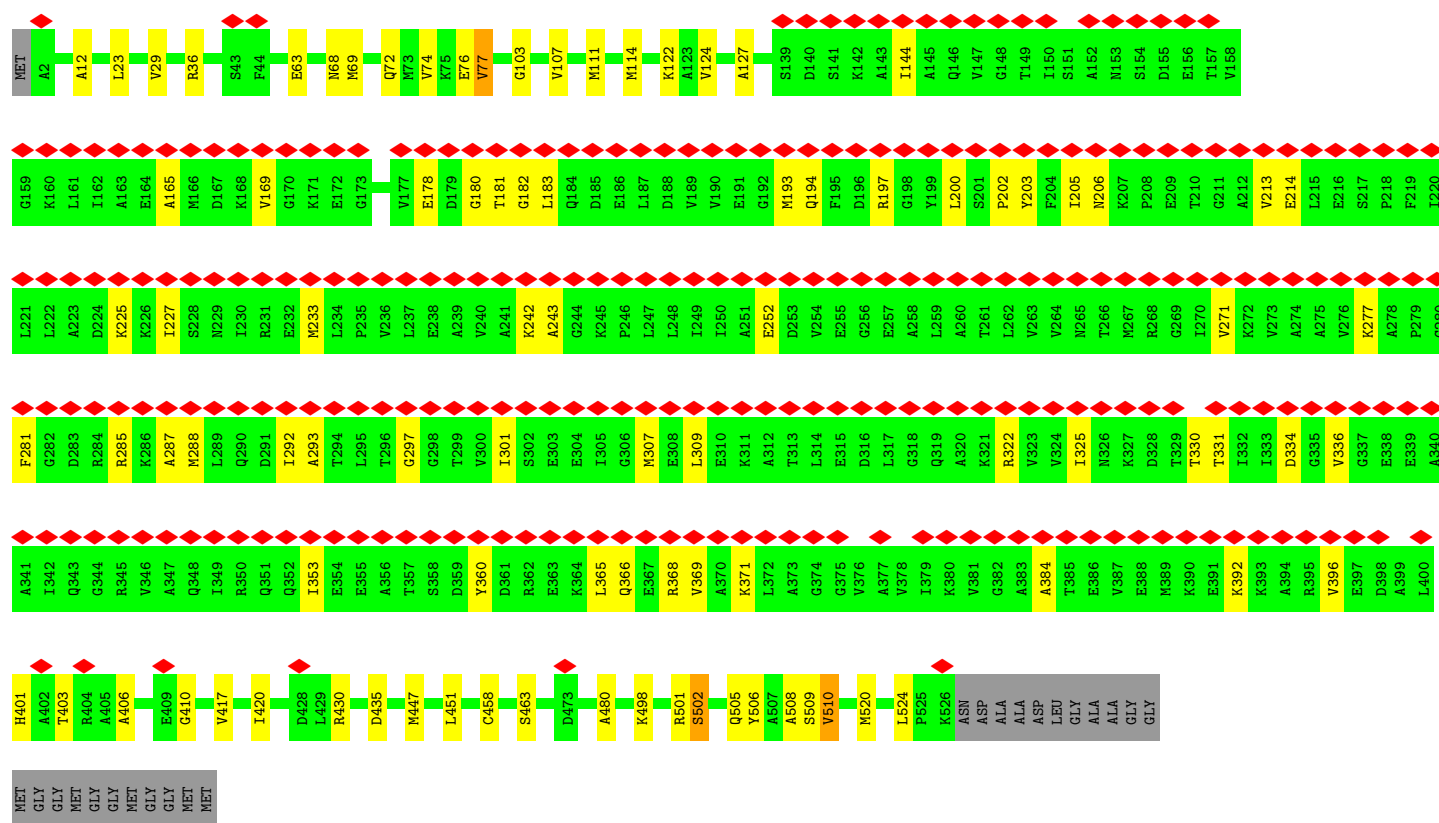
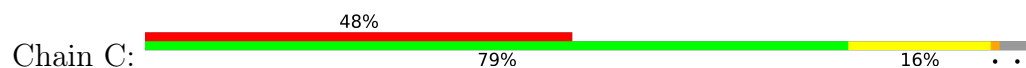
- Molecule 5 is N-(2-{4-[4-(aminomethyl)benzene-1-sulfonamido]phenyl}-1,3-benzoxazol-5-yl)-5-chlorothiophene-2-sulfonamide (CCD ID: A1AS6) (formula: C₂₄H₁₉ClN₄O₅S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	B	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	C	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	D	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	E	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	F	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	
5	G	1	Total	C	Cl	N	O	S	0
			37	24	1	4	5	3	

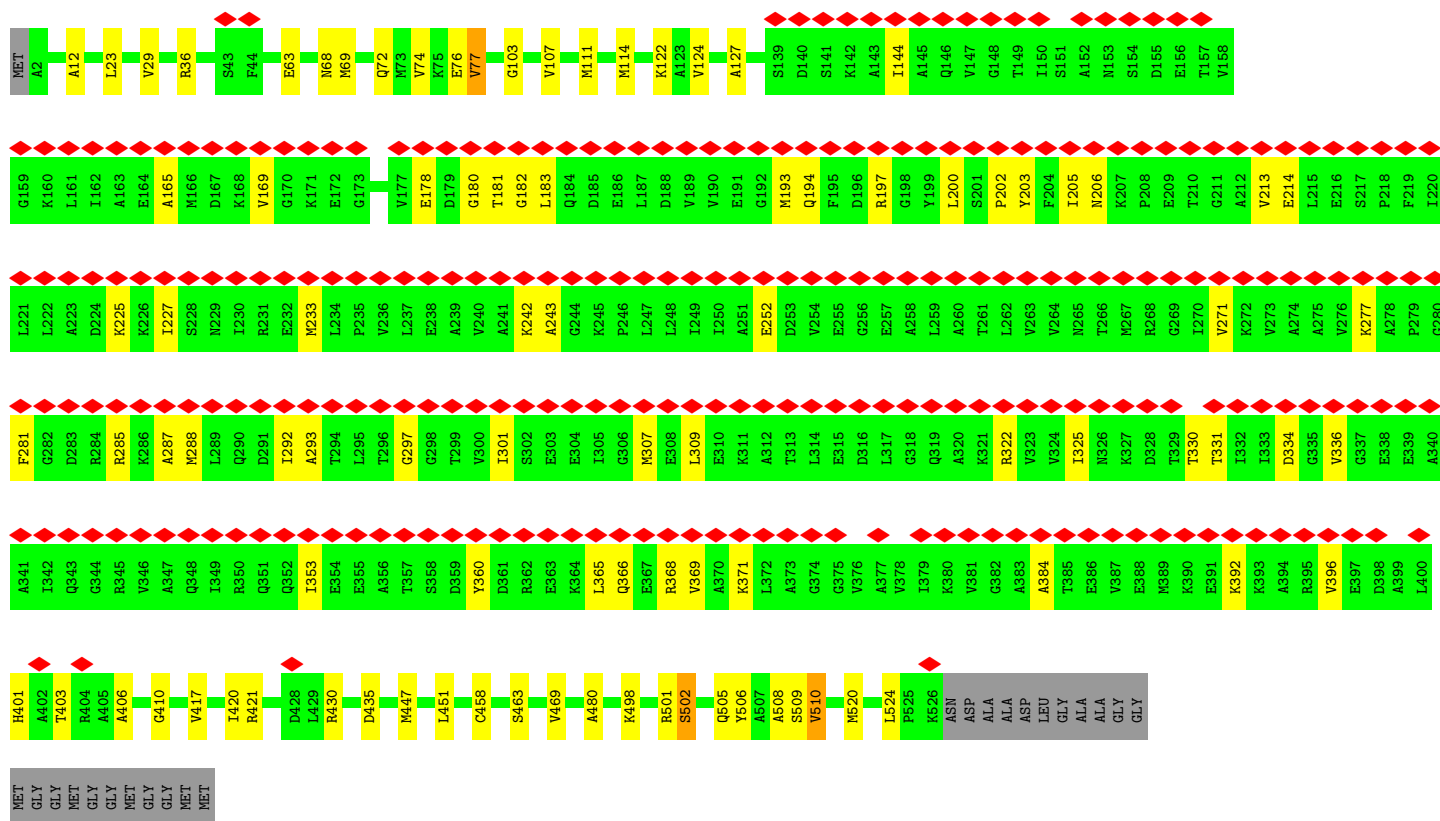


• Molecule 1: 60 kDa chaperonin



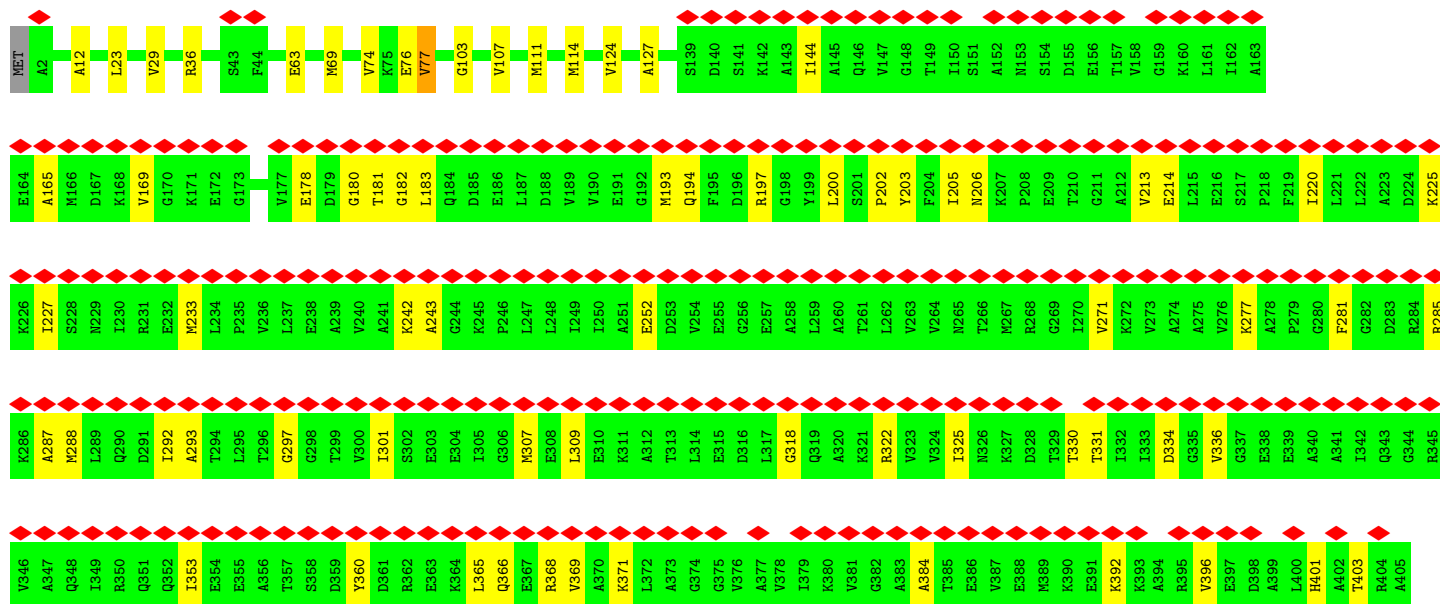
• Molecule 1: 60 kDa chaperonin

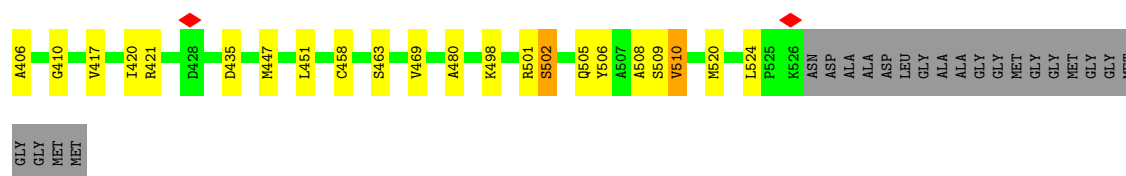
Chain D: 



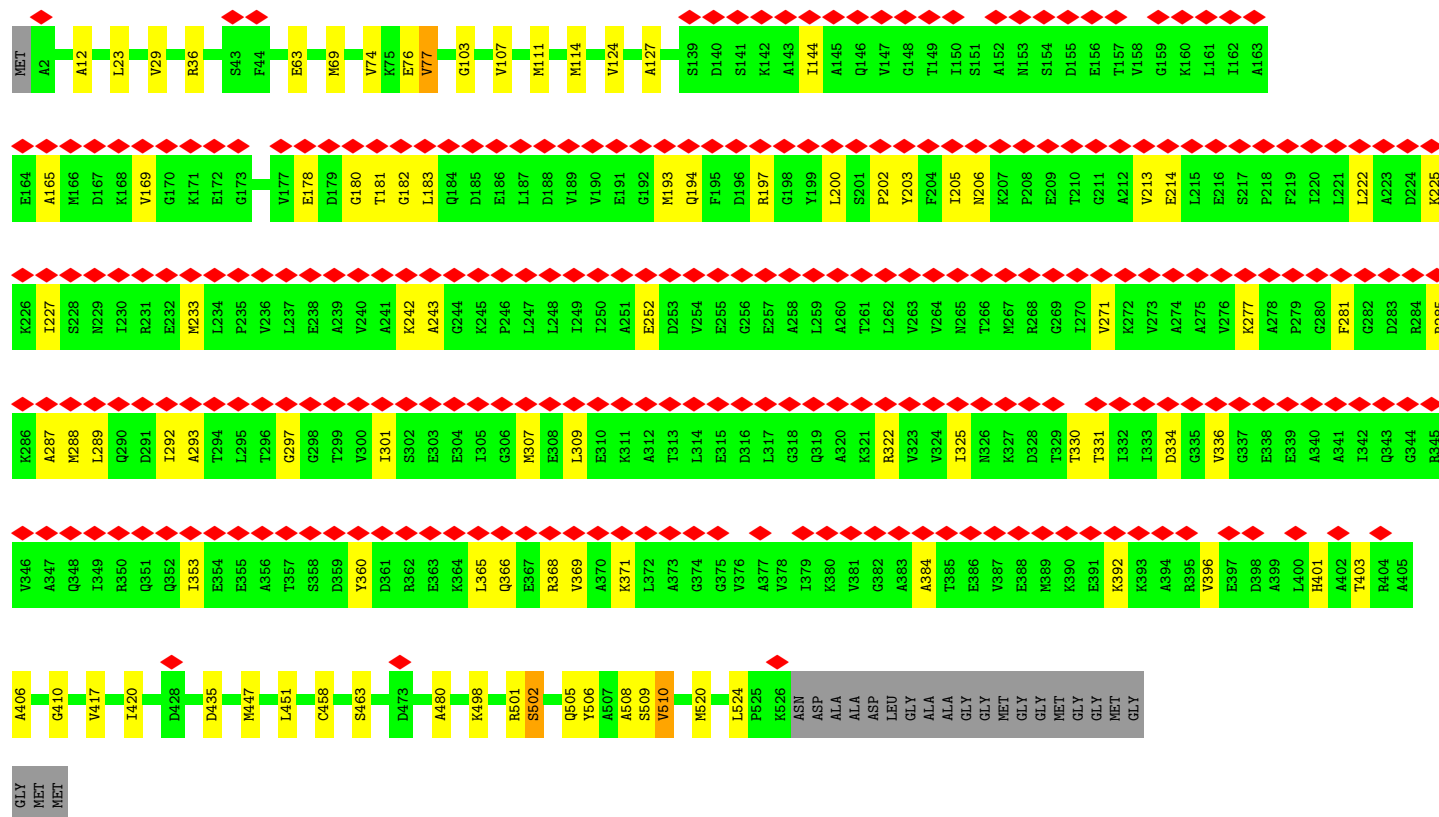
• Molecule 1: 60 kDa chaperonin

Chain E: 

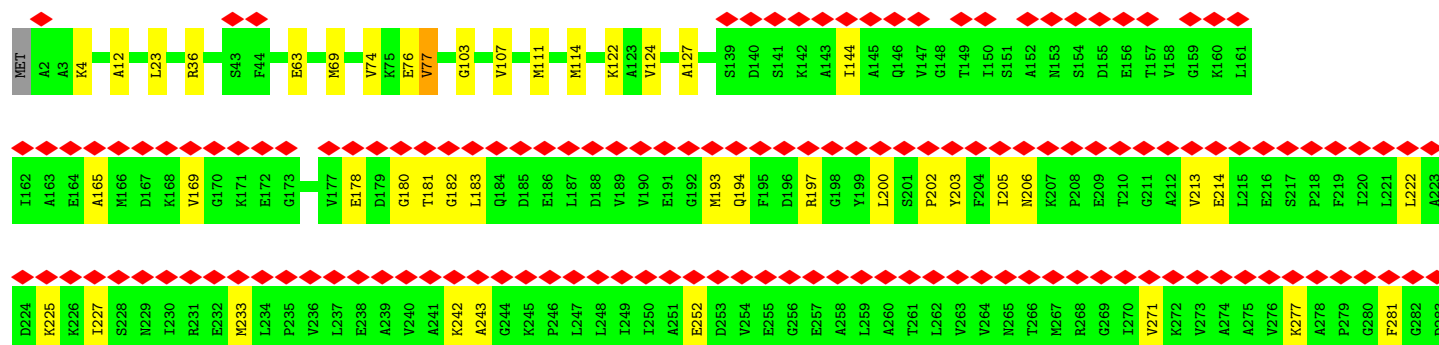


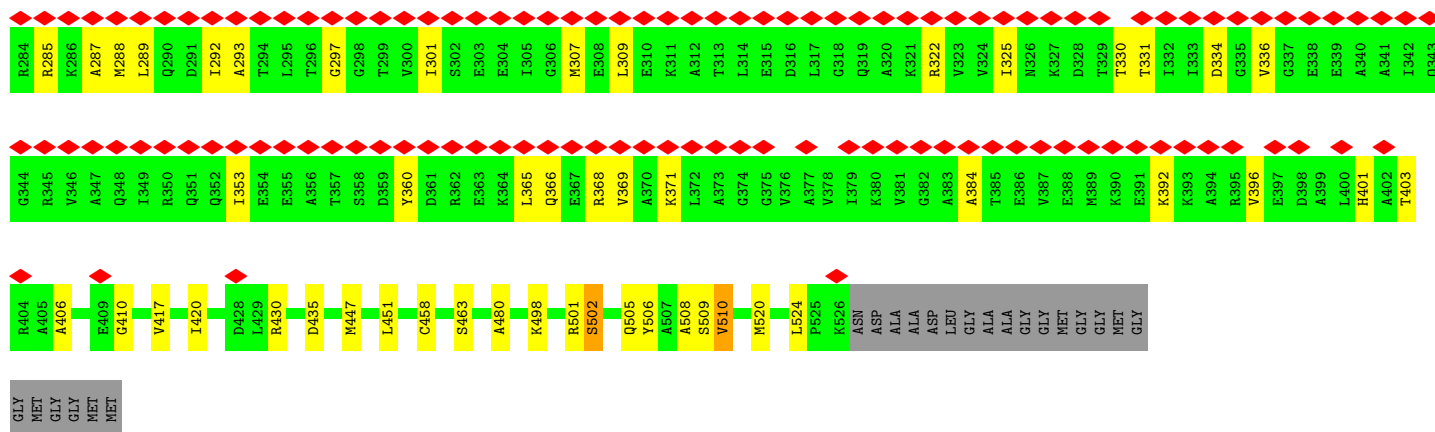


- Molecule 1: 60 kDa chaperonin

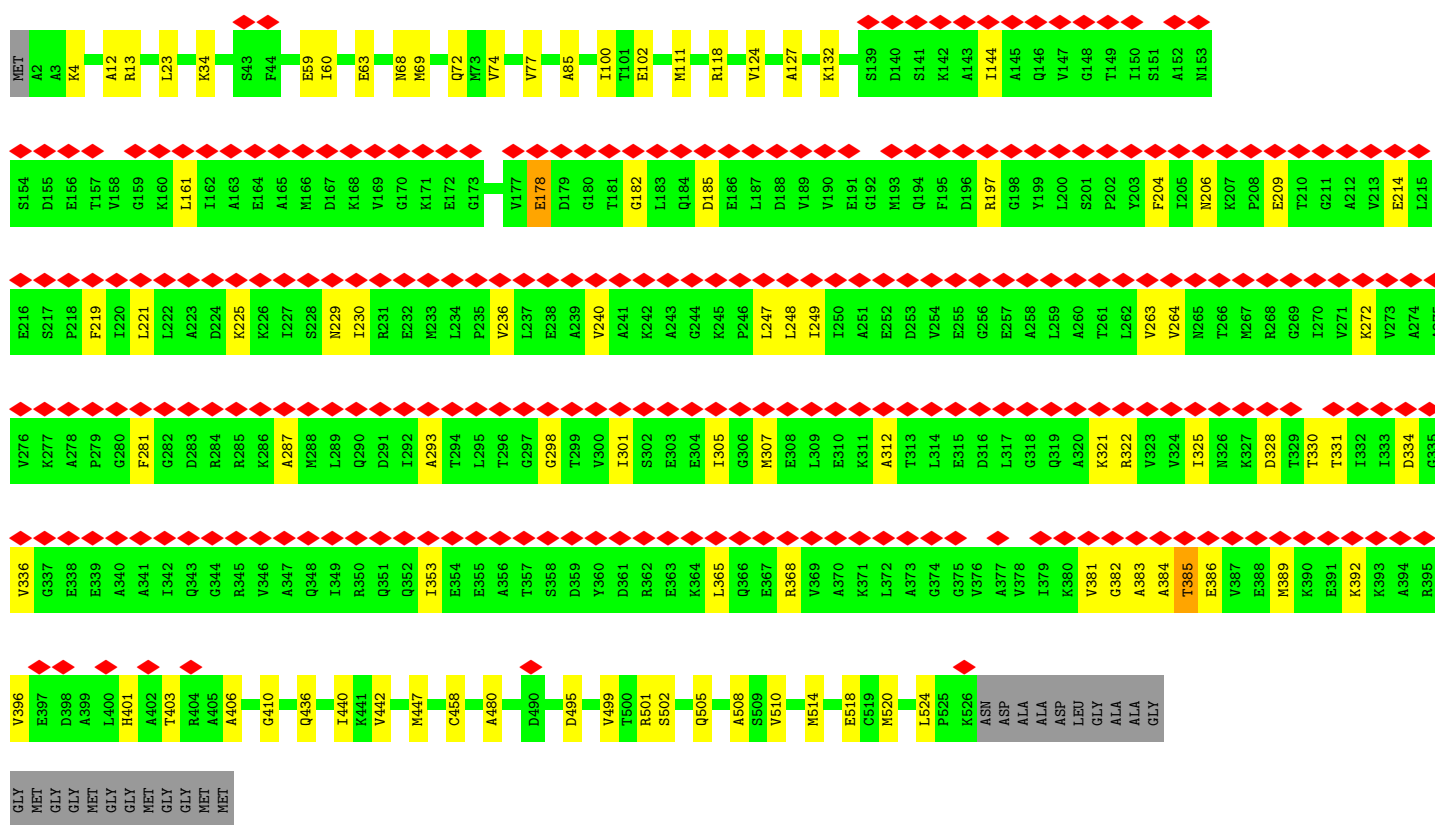
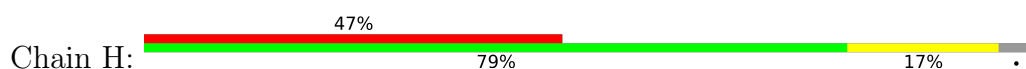


- Molecule 1: 60 kDa chaperonin

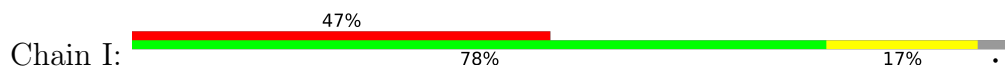


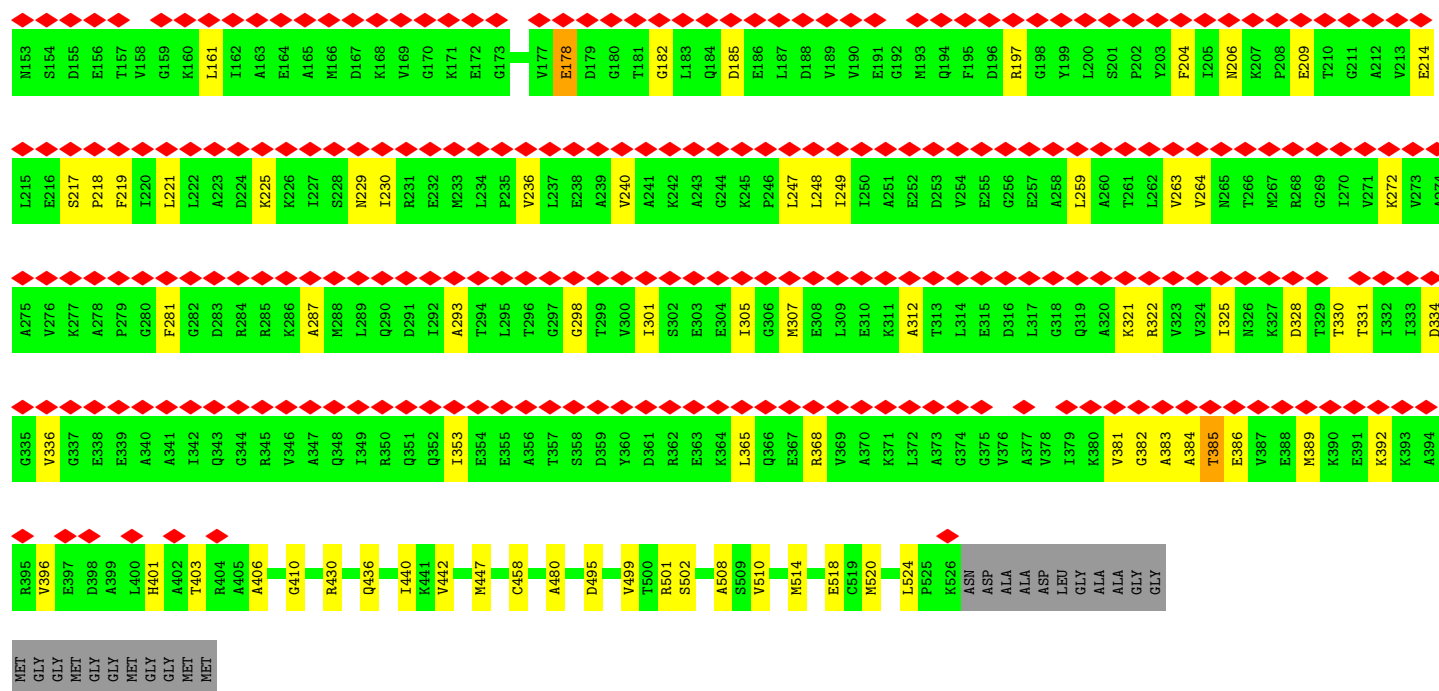


• Molecule 1: 60 kDa chaperonin

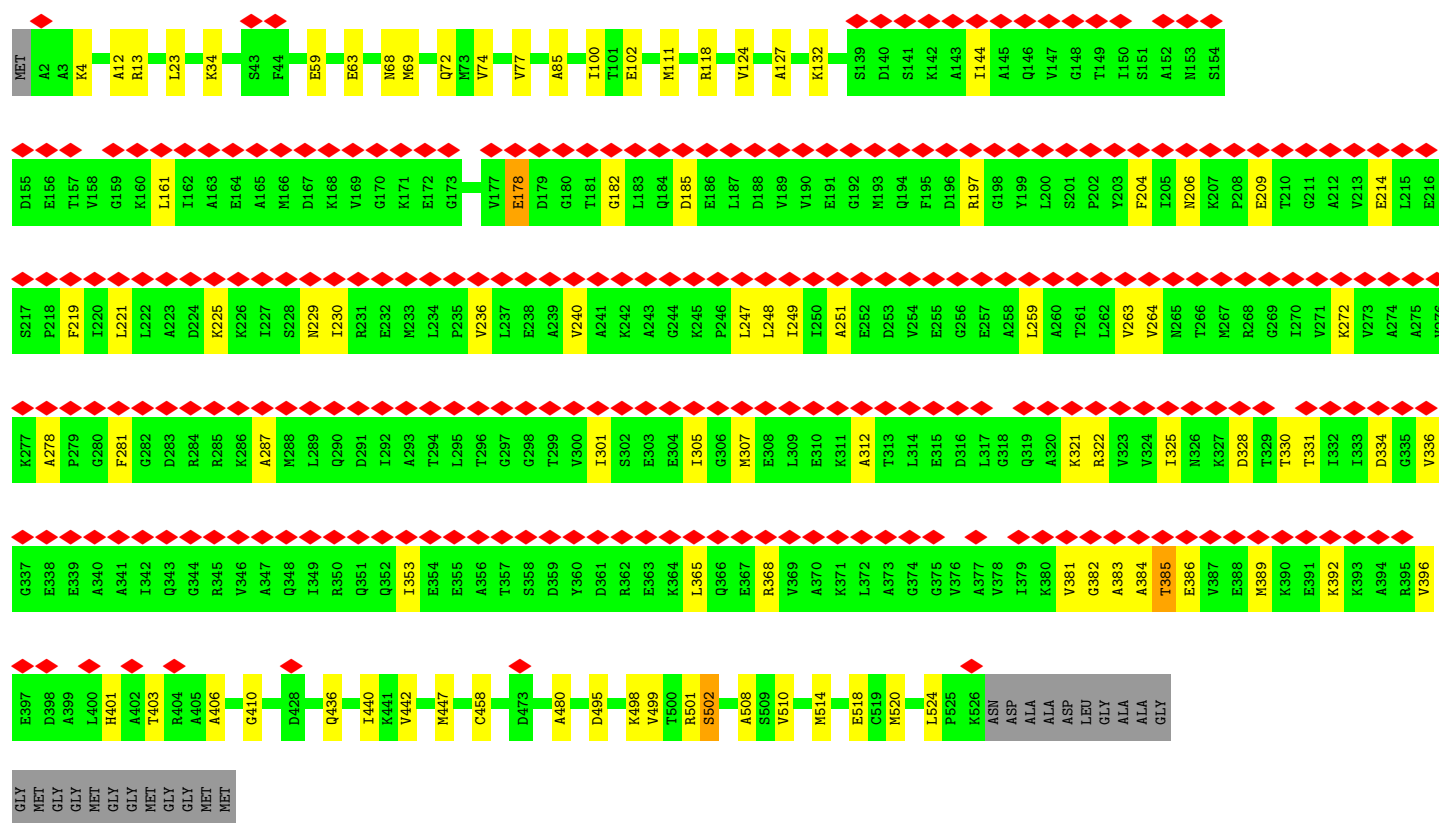
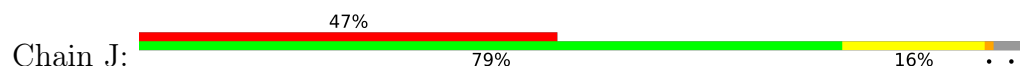


• Molecule 1: 60 kDa chaperonin



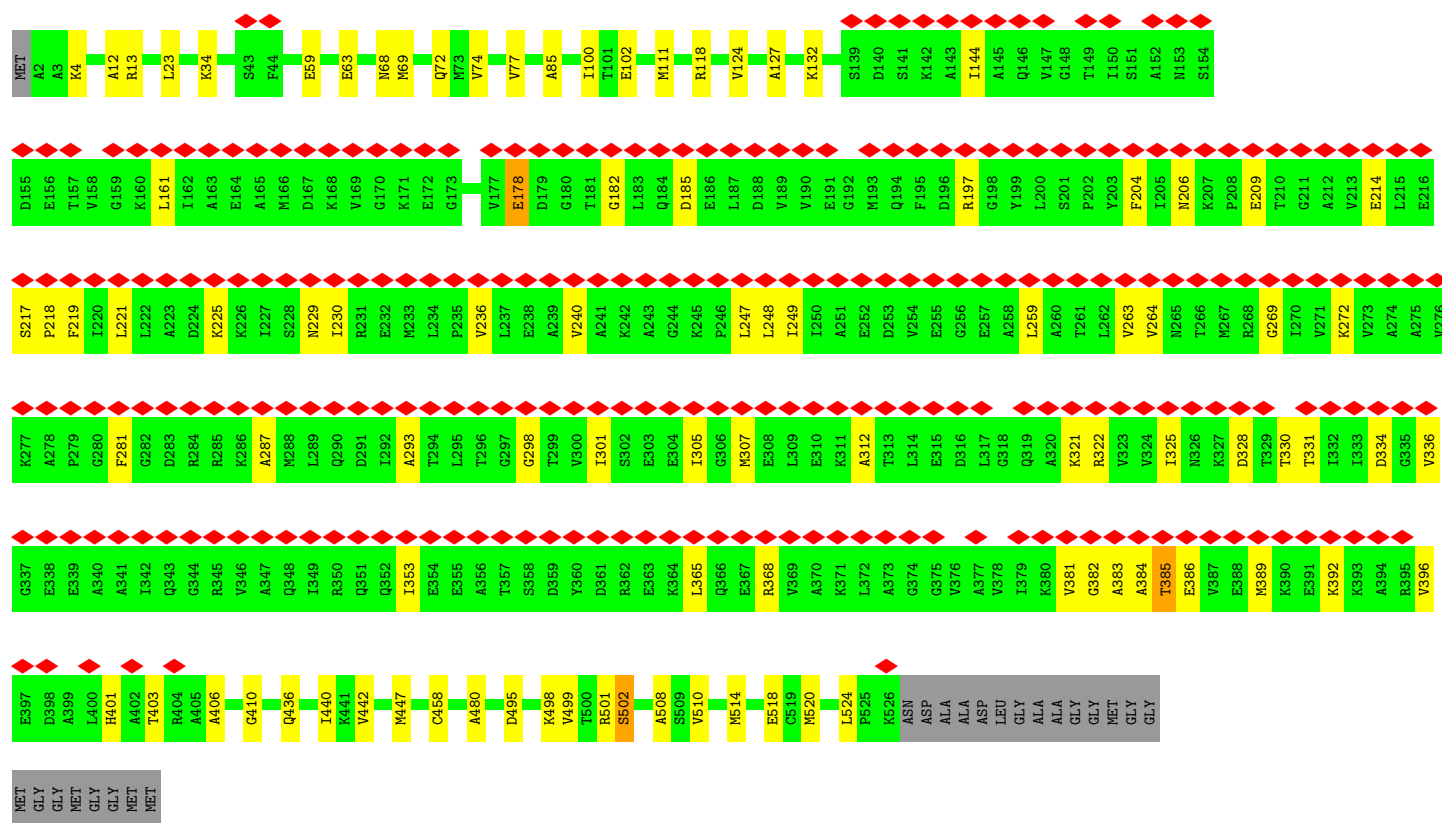


• Molecule 1: 60 kDa chaperonin



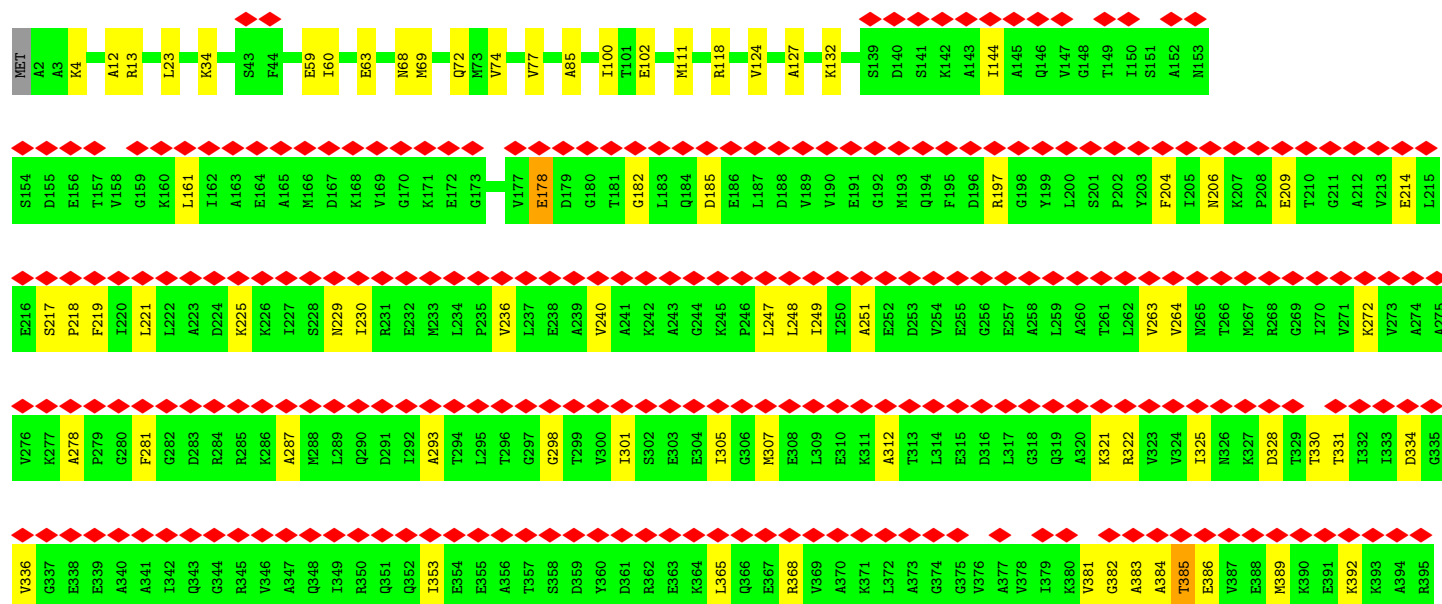
• Molecule 1: 60 kDa chaperonin

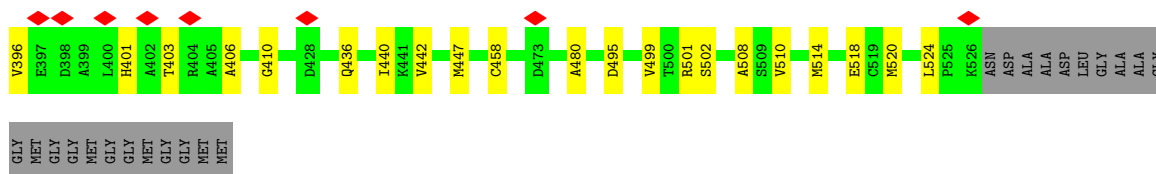
Chain K: 



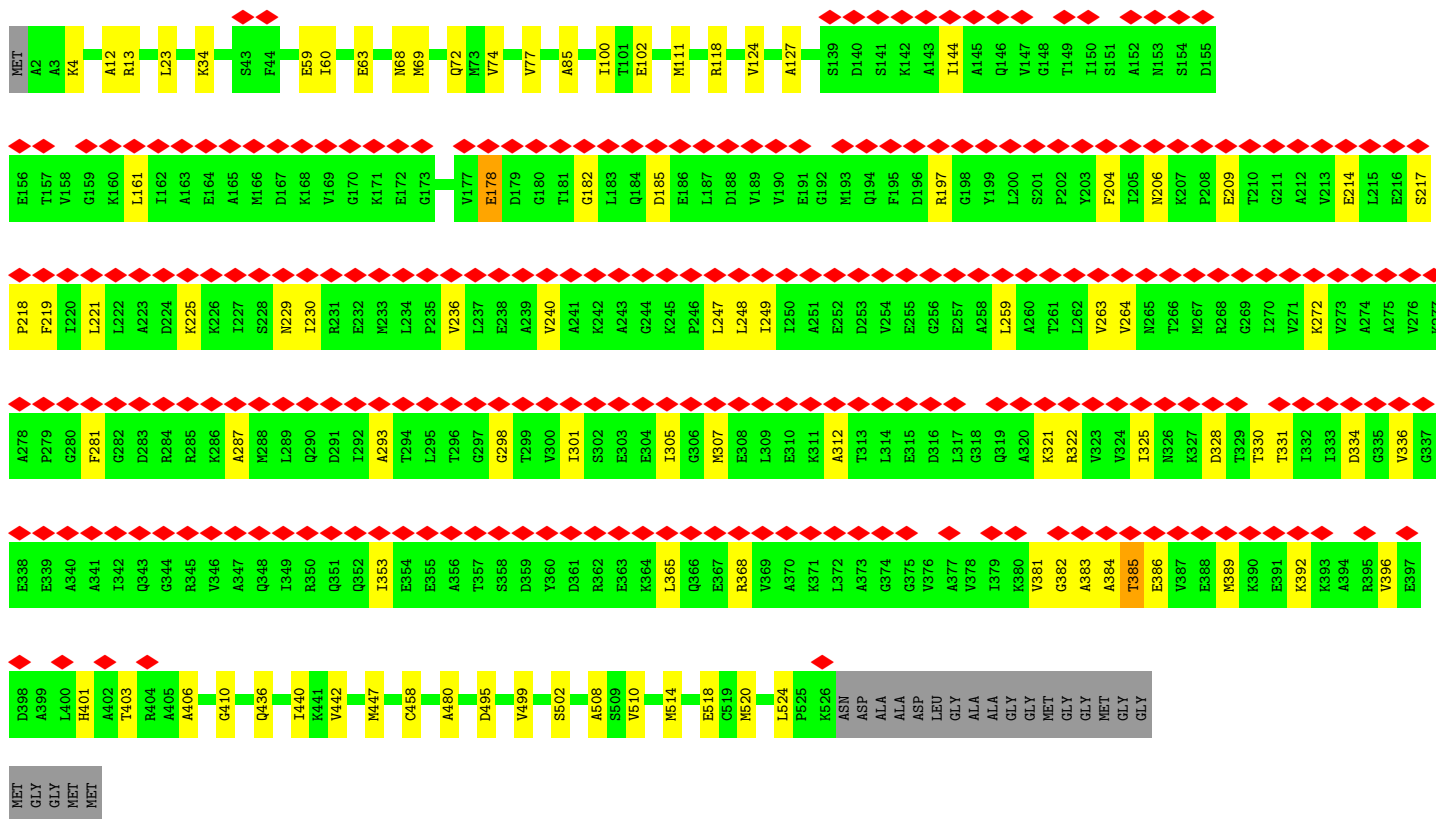
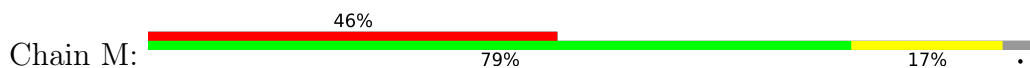
• Molecule 1: 60 kDa chaperonin

Chain L: 

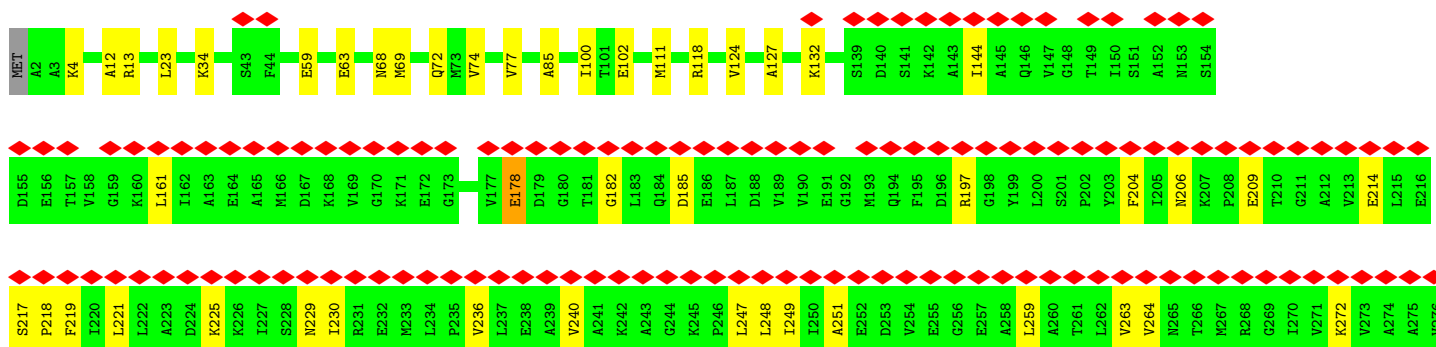
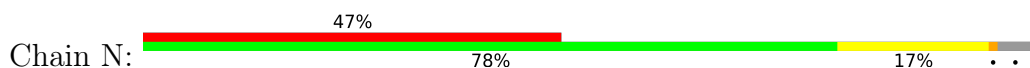




• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



GLY	E397	G337	K277
GLY	D398	E338	A278
MET	A399	E339	P279
GLY	L400	A340	G280
MET	H401	A341	F281
GLY	T402	I342	G282
GLY	T403	Q343	D283
MET	R404	G344	R284
MET	A405	R346	R285
MET		V346	K286
	G410	A347	A287
	Q436	Q348	M288
	L440	I349	L289
GLY	K441	R350	Q290
GLY	V442	Q351	D291
	M447	Q352	I292
		I353	A293
	C458	E354	T294
	A480	E355	L295
	D495	A356	T296
	K498	T357	G297
V499	T500	S358	G298
R501	F509	D359	T299
S502	F509	Y360	V300
Q505	R502	D361	I301
		R362	S302
		E363	E303
		K364	E304
	A508	L365	I305
S509	V510	Q366	G306
		E367	M307
	M514	R368	E308
E518		V369	L309
S519		A370	E310
M520		K371	K311
	L524	L372	A312
P525		A373	T313
K526		G374	L314
ASN		Q375	E315
ASP		V376	D316
ALA		A377	L317
ALA		V378	G318
ASP		I379	Q319
LEU		K380	A320
GLY		V381	K321
ALA		G382	R322
GLY		A383	G323
GLY		A384	V324
MET		T385	I325
		E386	N326
		V387	K327
		E388	D328
		M389	T329
		K390	T330
		E391	T331
		K392	I332
		K393	I333
		A394	D334
		R395	G335
		V396	V336

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.781	Depositor
Minimum map value	-1.480	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.468	Depositor
Map size ($\text{\AA}$)	379.44, 379.44, 379.44	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AS6, ATP, MG, K

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	0.18	0/3892	0.34	1/5254 (0.0%)
1	B	0.18	0/3892	0.34	1/5254 (0.0%)
1	C	0.18	0/3892	0.34	1/5254 (0.0%)
1	D	0.18	0/3892	0.34	1/5254 (0.0%)
1	E	0.18	0/3892	0.34	1/5254 (0.0%)
1	F	0.18	0/3892	0.34	1/5254 (0.0%)
1	G	0.18	0/3892	0.34	1/5254 (0.0%)
1	H	0.14	0/3892	0.29	0/5254
1	I	0.14	0/3892	0.29	0/5254
1	J	0.14	0/3892	0.29	0/5254
1	K	0.14	0/3892	0.29	0/5254
1	L	0.14	0/3892	0.29	0/5254
1	M	0.14	0/3892	0.29	0/5254
1	N	0.14	0/3892	0.29	0/5254
All	All	0.16	0/54488	0.31	7/73556 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	435	ASP	N-CA-C	-6.31	105.89	113.97
1	D	435	ASP	N-CA-C	-6.30	105.91	113.97
1	E	435	ASP	N-CA-C	-6.29	105.92	113.97
1	A	435	ASP	N-CA-C	-6.28	105.93	113.97
1	B	435	ASP	N-CA-C	-6.28	105.94	113.97

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	3864	0	3988	68	0
1	B	3864	0	3988	65	0
1	C	3864	0	3988	65	0
1	D	3864	0	3988	67	0
1	E	3864	0	3988	65	0
1	F	3864	0	3988	65	0
1	G	3864	0	3988	66	0
1	H	3864	0	3989	74	0
1	I	3864	0	3989	75	0
1	J	3864	0	3989	74	0
1	K	3864	0	3989	76	0
1	L	3864	0	3989	76	0
1	M	3864	0	3989	76	0
1	N	3864	0	3989	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	0	0
3	H	31	0	12	0	0
3	I	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	31	0	12	0	0
3	K	31	0	12	0	0
3	L	31	0	12	0	0
3	M	31	0	12	0	0
3	N	31	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
5	A	37	0	0	1	0
5	B	37	0	0	1	0
5	C	37	0	0	1	0
5	D	37	0	0	1	0
5	E	37	0	0	1	0
5	F	37	0	0	1	0
5	G	37	0	0	1	0
All	All	54831	0	56007	804	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 7.

The worst 5 of 804 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:H:383:ALA:CB	1:J:281:PHE:CZ	2.23	1.22
1:H:281:PHE:CZ	1:I:383:ALA:CB	2.23	1.22
1:J:383:ALA:CB	1:K:281:PHE:CZ	2.23	1.22
1:I:281:PHE:CZ	1:N:383:ALA:CB	2.23	1.22
1:K:383:ALA:CB	1:L:281:PHE:CZ	2.23	1.21

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	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	B	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	C	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	D	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	E	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	F	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	G	523/548 (95%)	508 (97%)	14 (3%)	1 (0%)	43	68
1	H	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	I	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	J	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	K	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	L	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	M	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
1	N	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	43	68
All	All	7322/7672 (95%)	7119 (97%)	189 (3%)	14 (0%)	44	68

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	385	THR
1	I	385	THR
1	J	385	THR
1	K	385	THR
1	L	385	THR

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	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	B	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	C	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	D	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	E	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	F	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	G	405/415 (98%)	393 (97%)	12 (3%)	36	66
1	H	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	I	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	J	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	K	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	L	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	M	405/415 (98%)	396 (98%)	9 (2%)	45	74
1	N	405/415 (98%)	396 (98%)	9 (2%)	45	74
All	All	5670/5810 (98%)	5523 (97%)	147 (3%)	41	70

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	264	VAL
1	N	331	THR
1	K	502	SER
1	M	178	GLU
1	E	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	72	GLN

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Mol	Chain	Res	Type
1	H	475	ASN
1	N	319	GLN
1	G	436	GLN
1	H	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 42 are monoatomic - leaving 21 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$
5	A1AS6	E	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.64	18 (30%)
3	ATP	J	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
3	ATP	L	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
3	ATP	I	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
5	A1AS6	B	605	-	41,41,41	5.67	13 (31%)	60,61,61	2.64	18 (30%)
3	ATP	N	602	4,2	32,33,33	0.42	0	48,52,52	0.68	0
3	ATP	F	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0
3	ATP	K	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
3	ATP	G	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1AS6	C	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.65	18 (30%)
5	A1AS6	G	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.65	18 (30%)
3	ATP	A	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0
3	ATP	E	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0
3	ATP	M	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
5	A1AS6	A	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.64	18 (30%)
3	ATP	D	602	4,2	32,33,33	0.44	0	48,52,52	0.67	0
5	A1AS6	D	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.65	18 (30%)
3	ATP	B	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0
5	A1AS6	F	605	-	41,41,41	5.66	13 (31%)	60,61,61	2.64	18 (30%)
3	ATP	H	602	4,2	32,33,33	0.43	0	48,52,52	0.68	0
3	ATP	C	602	4,2	32,33,33	0.45	0	48,52,52	0.67	0

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
5	A1AS6	E	605	-	-	6/28/28/28	0/5/5/5
3	ATP	J	602	4,2	-	5/22/38/38	0/3/3/3
3	ATP	L	602	4,2	-	5/22/38/38	0/3/3/3
3	ATP	I	602	4,2	-	5/22/38/38	0/3/3/3
5	A1AS6	B	605	-	-	6/28/28/28	0/5/5/5
3	ATP	N	602	4,2	-	5/22/38/38	0/3/3/3
3	ATP	F	602	4,2	-	4/22/38/38	0/3/3/3
3	ATP	K	602	4,2	-	5/22/38/38	0/3/3/3
3	ATP	G	602	4,2	-	4/22/38/38	0/3/3/3
5	A1AS6	C	605	-	-	6/28/28/28	0/5/5/5
5	A1AS6	G	605	-	-	6/28/28/28	0/5/5/5
3	ATP	A	602	4,2	-	4/22/38/38	0/3/3/3
3	ATP	E	602	4,2	-	4/22/38/38	0/3/3/3
3	ATP	M	602	4,2	-	5/22/38/38	0/3/3/3
5	A1AS6	A	605	-	-	6/28/28/28	0/5/5/5
3	ATP	D	602	4,2	-	4/22/38/38	0/3/3/3
5	A1AS6	D	605	-	-	6/28/28/28	0/5/5/5
3	ATP	B	602	4,2	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1AS6	F	605	-	-	6/28/28/28	0/5/5/5
3	ATP	H	602	4,2	-	5/22/38/38	0/3/3/3
3	ATP	C	602	4,2	-	4/22/38/38	0/3/3/3

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	605	A1AS6	O2-S1	18.91	1.65	1.43
5	B	605	A1AS6	O1-S1	18.89	1.65	1.43
5	G	605	A1AS6	O2-S1	18.88	1.65	1.43
5	F	605	A1AS6	O2-S1	18.87	1.65	1.43
5	C	605	A1AS6	O2-S1	18.86	1.65	1.43

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	605	A1AS6	O2-S1-O1	-8.71	108.94	119.52
5	D	605	A1AS6	O2-S1-O1	-8.70	108.95	119.52
5	A	605	A1AS6	O2-S1-O1	-8.70	108.96	119.52
5	B	605	A1AS6	O2-S1-O1	-8.70	108.96	119.52
5	E	605	A1AS6	O2-S1-O1	-8.69	108.96	119.52

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ATP	PB-O3B-PG-O3G
3	B	602	ATP	PB-O3B-PG-O3G
3	C	602	ATP	PB-O3B-PG-O3G
3	D	602	ATP	PB-O3B-PG-O3G
3	E	602	ATP	PB-O3B-PG-O3G

There are no ring outliers.

7 monomers are involved in 7 short contacts:

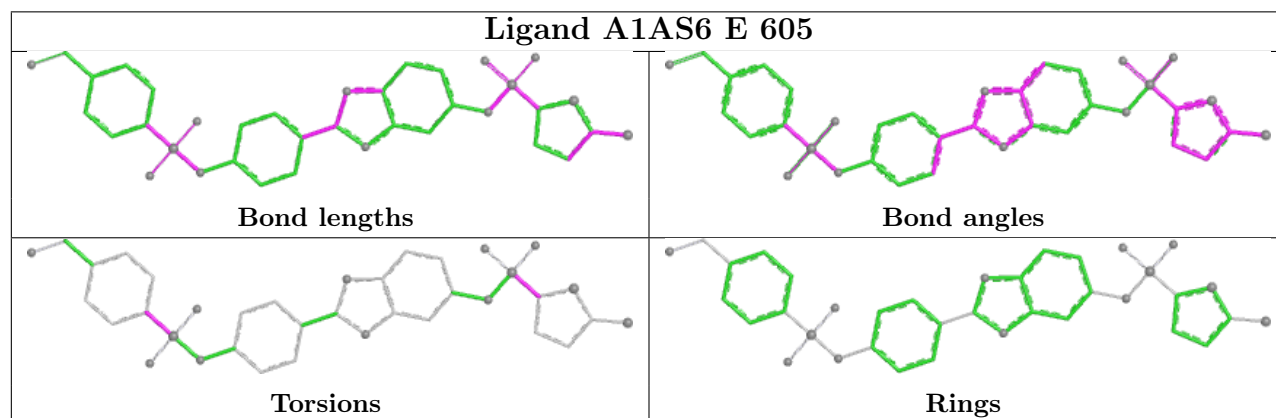
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	605	A1AS6	1	0
5	B	605	A1AS6	1	0
5	C	605	A1AS6	1	0
5	G	605	A1AS6	1	0

Continued on next page...

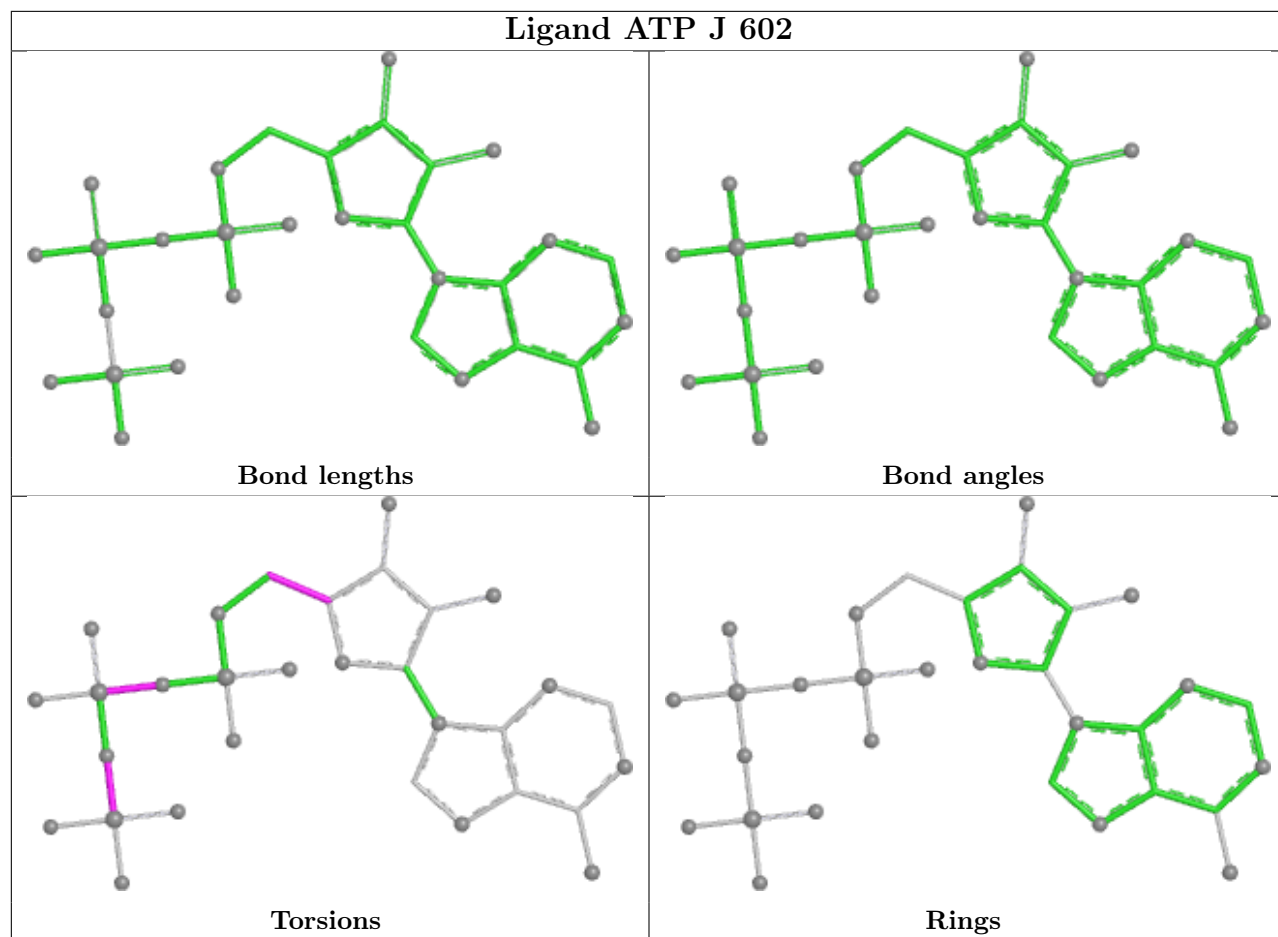
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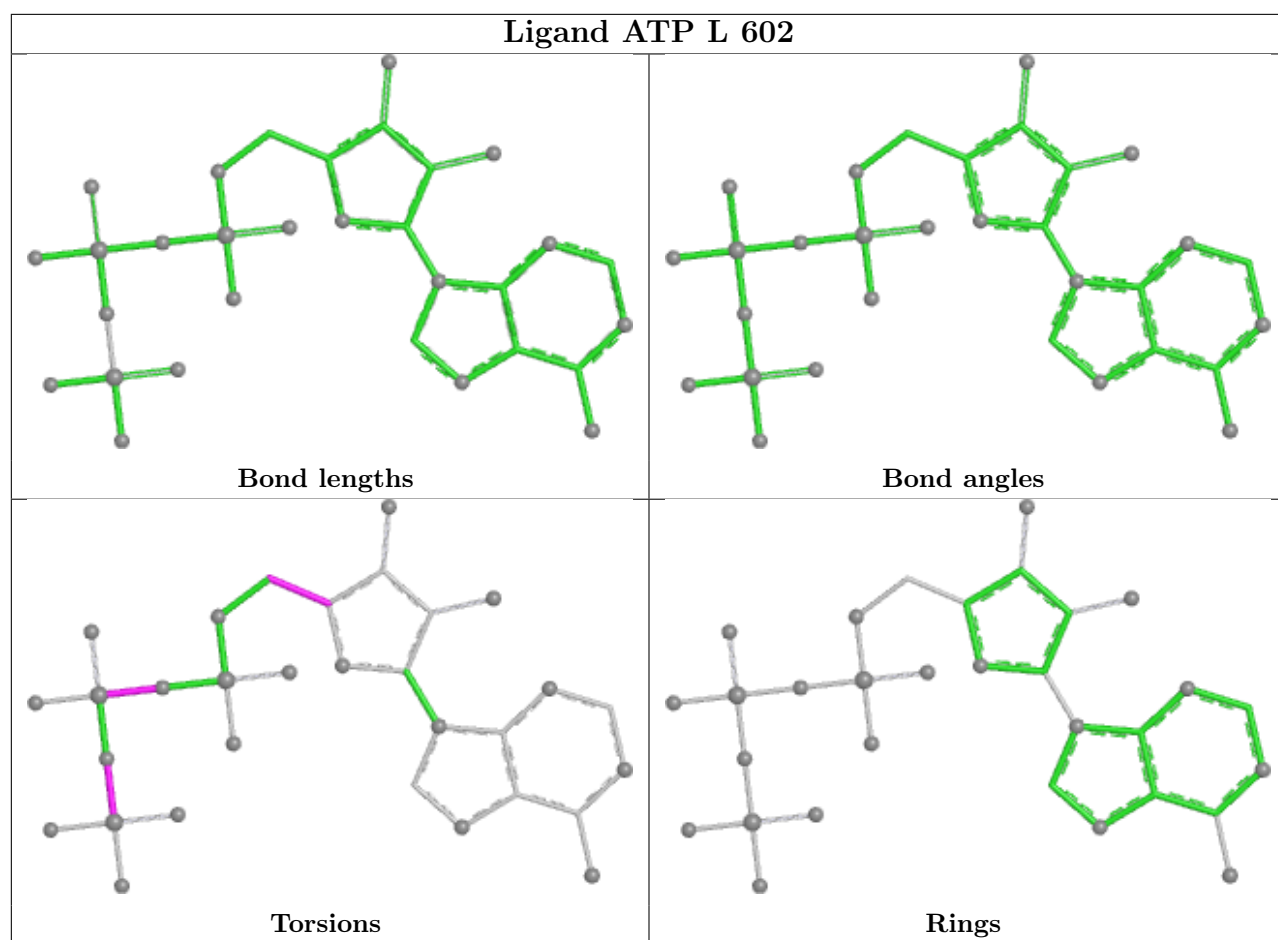
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	A1AS6	1	0
5	D	605	A1AS6	1	0
5	F	605	A1AS6	1	0

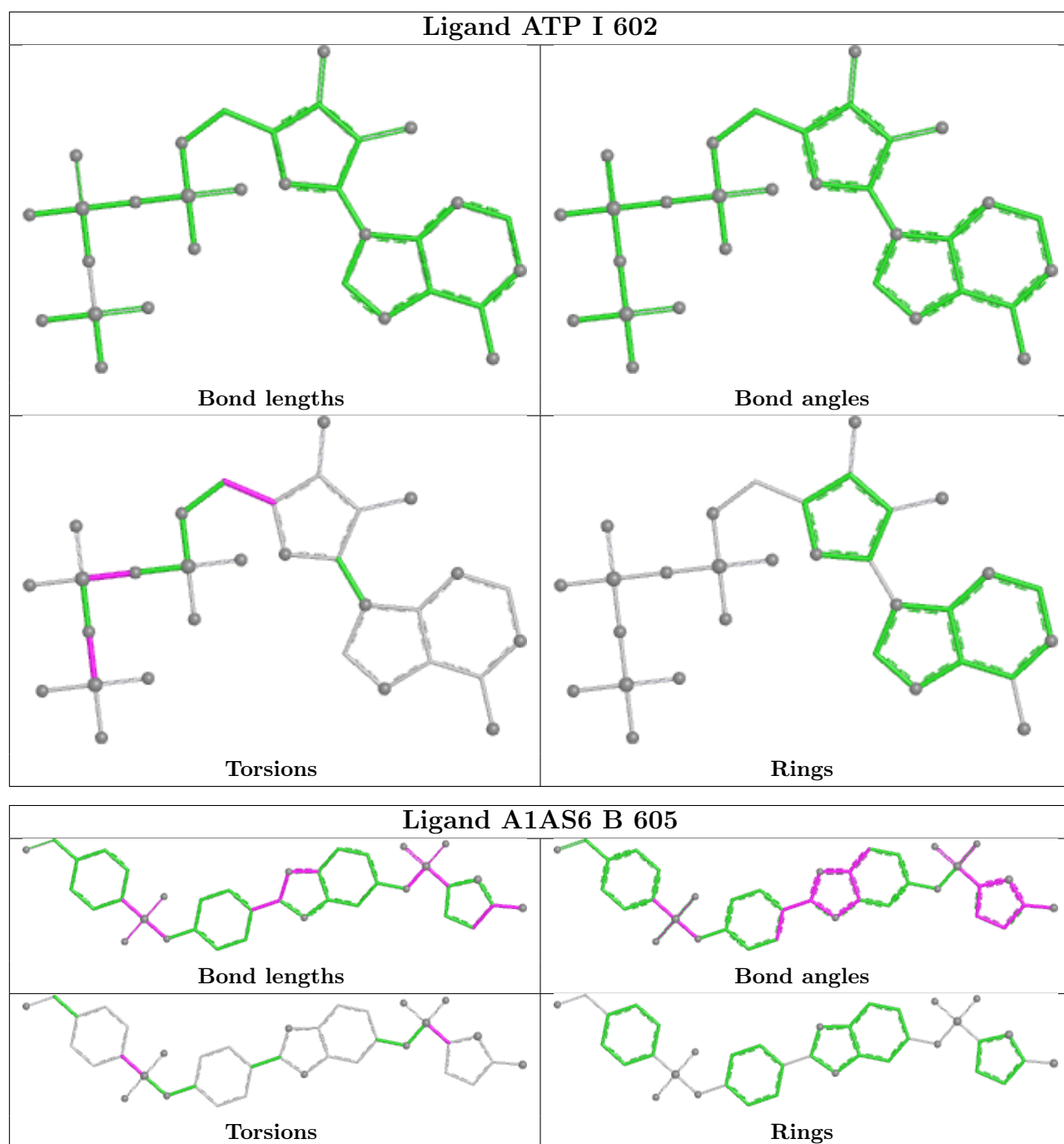
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

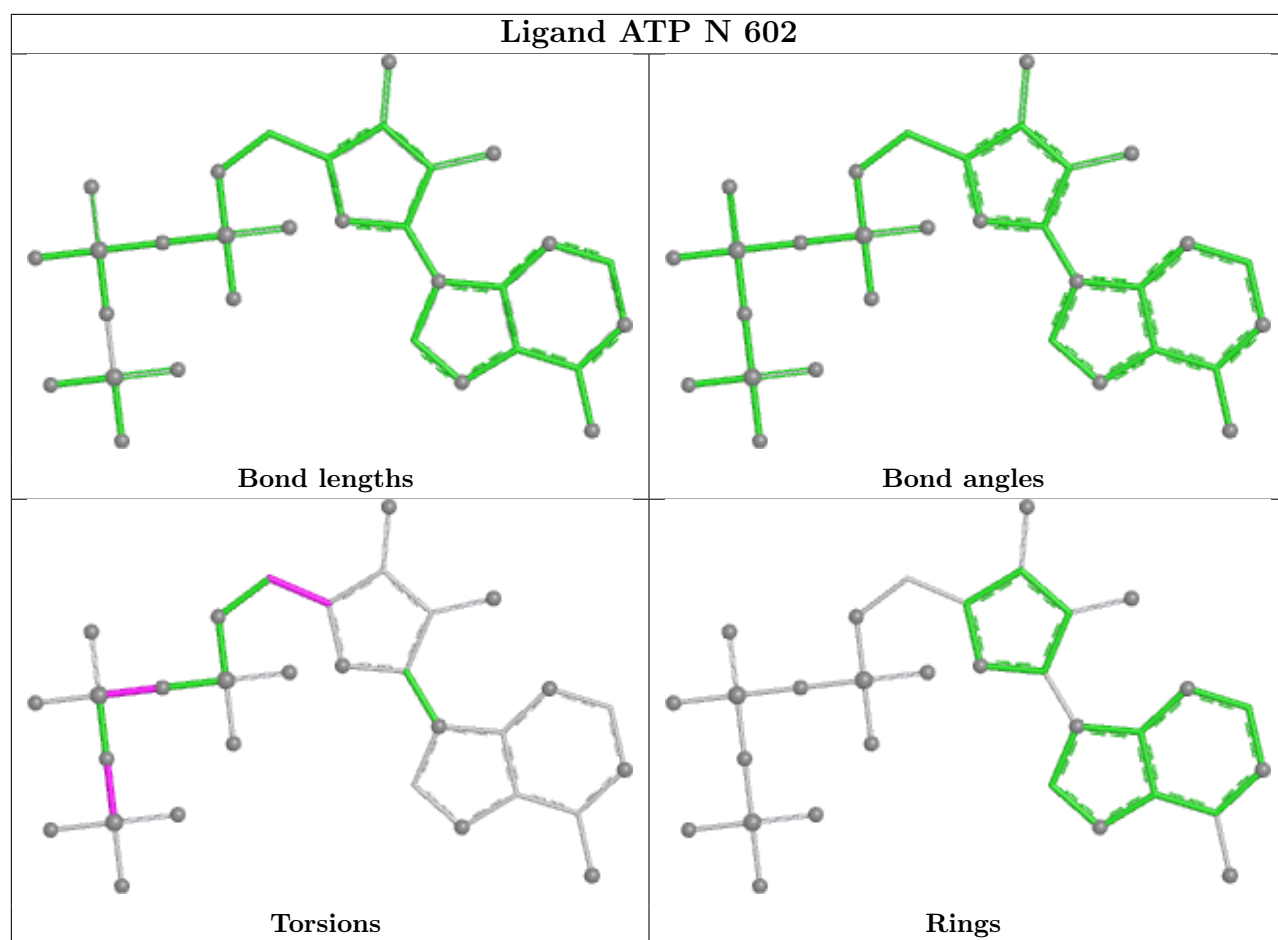


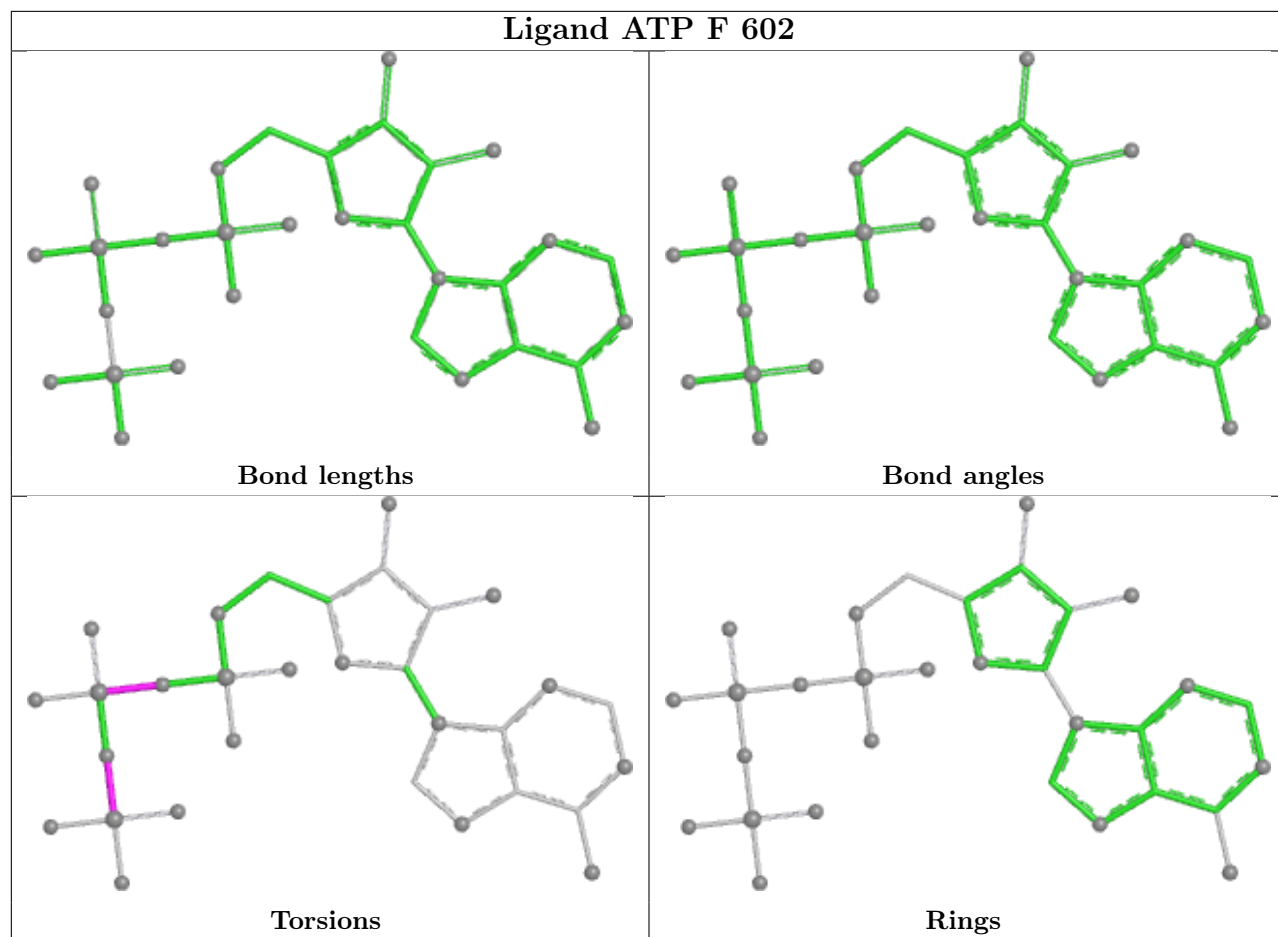
Ligand ATP J 602

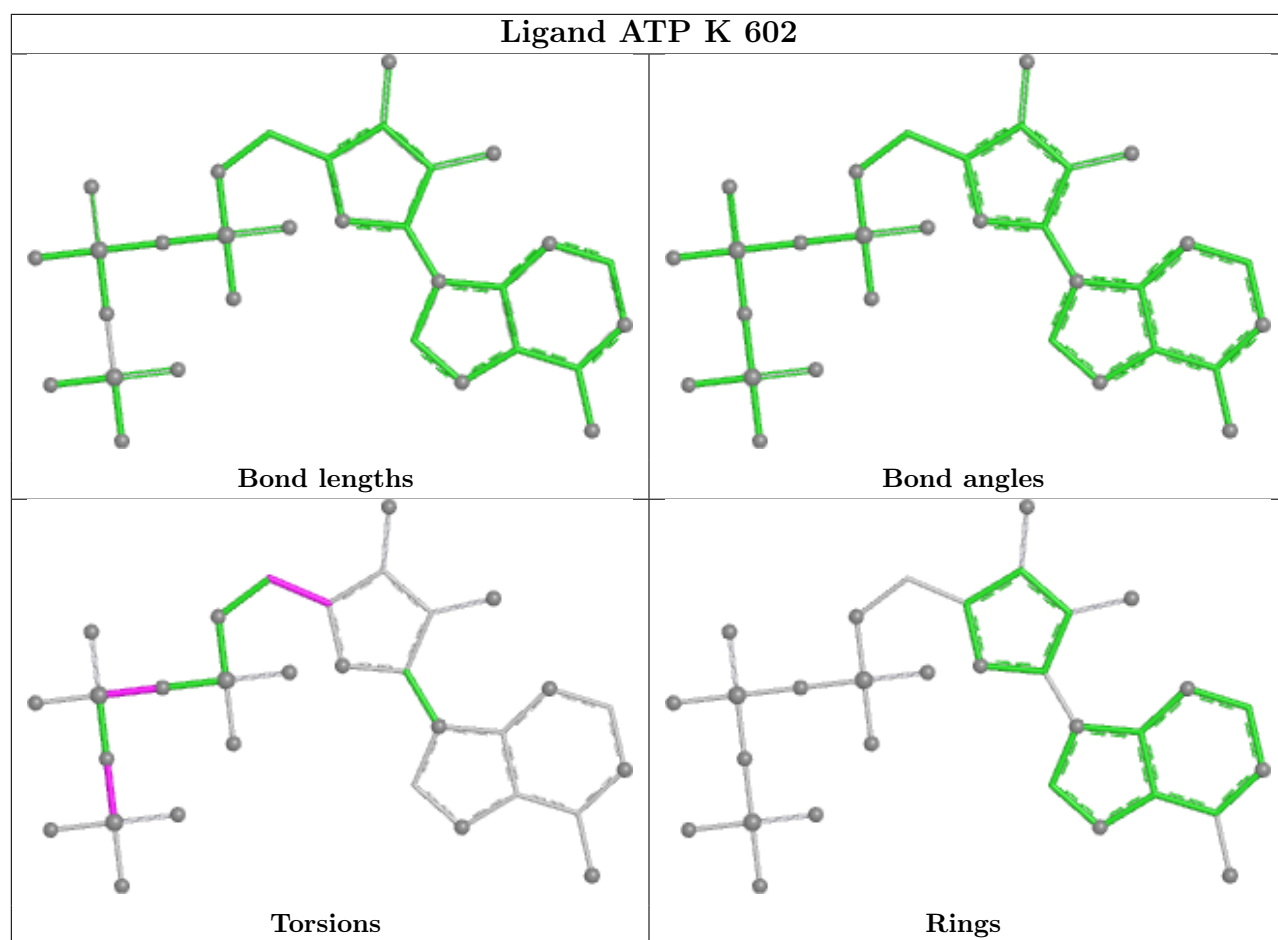


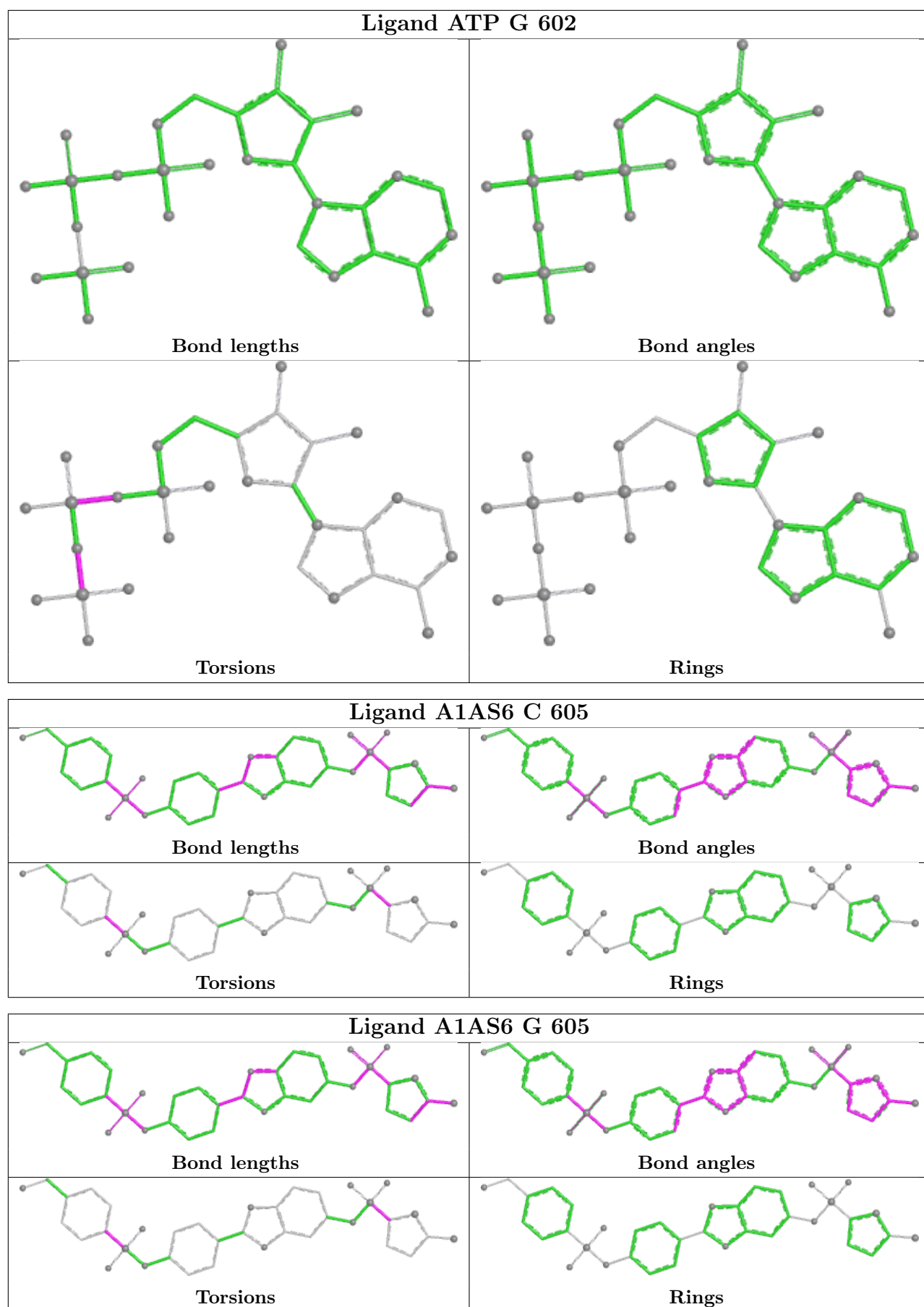


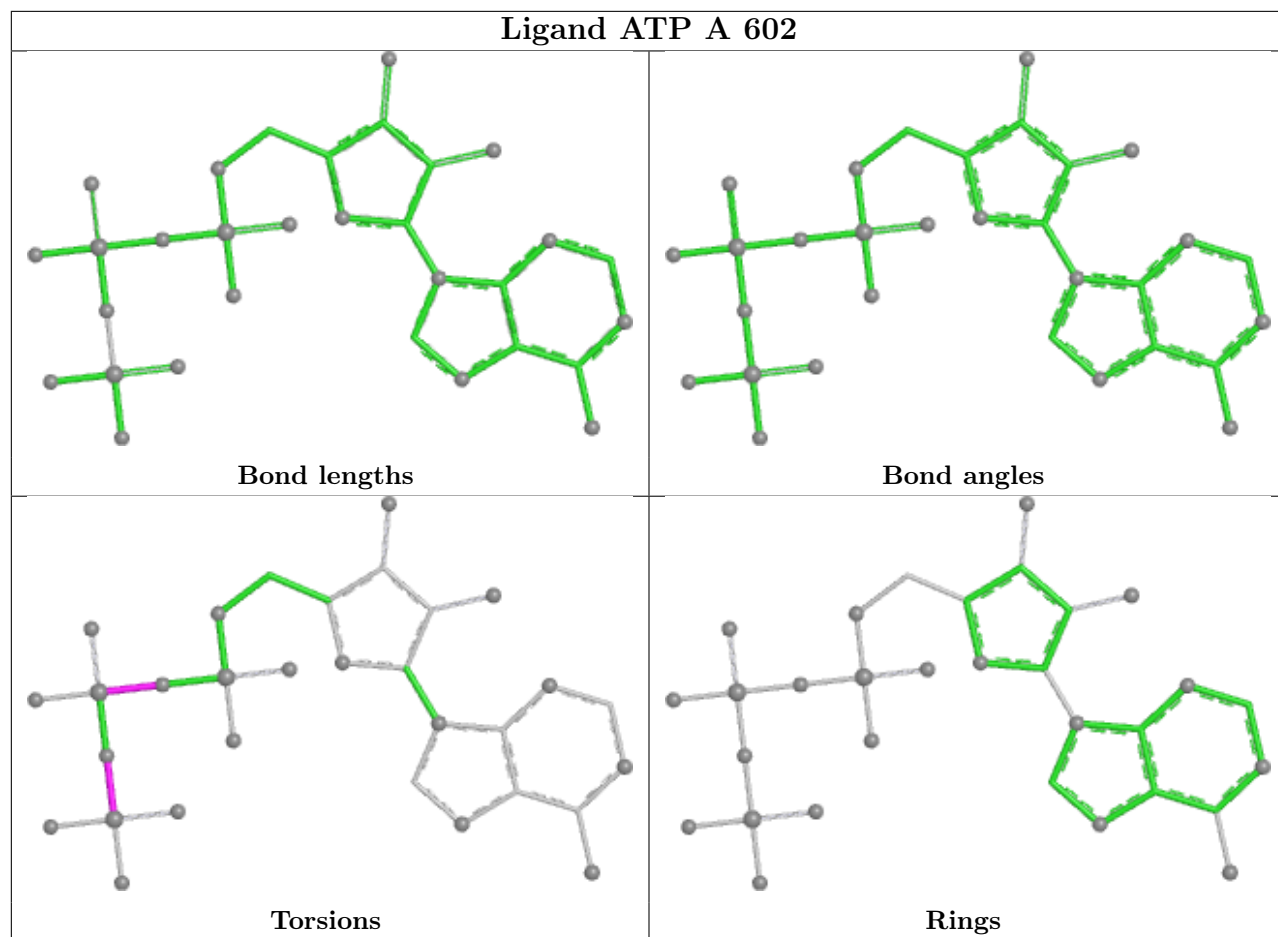


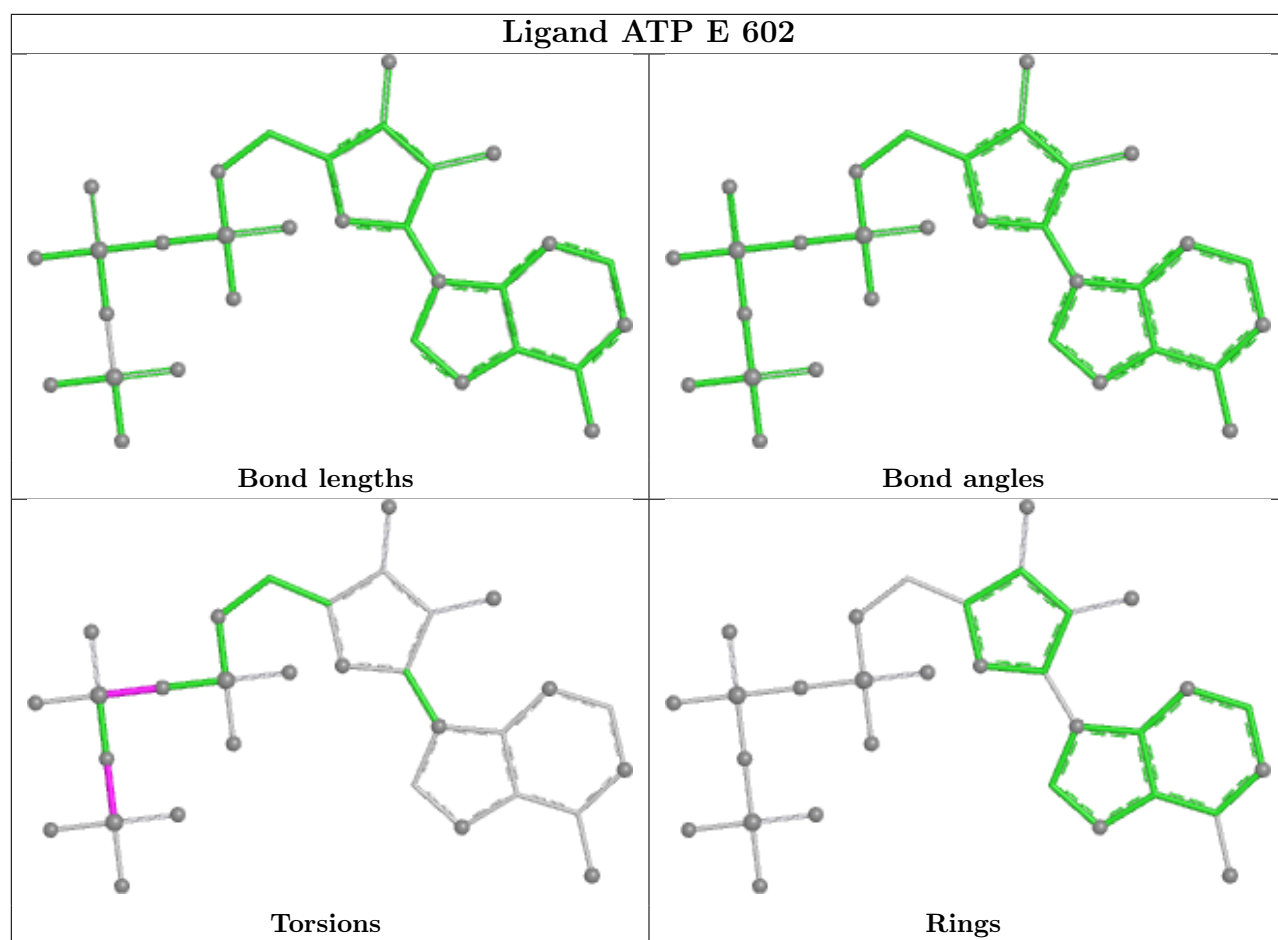


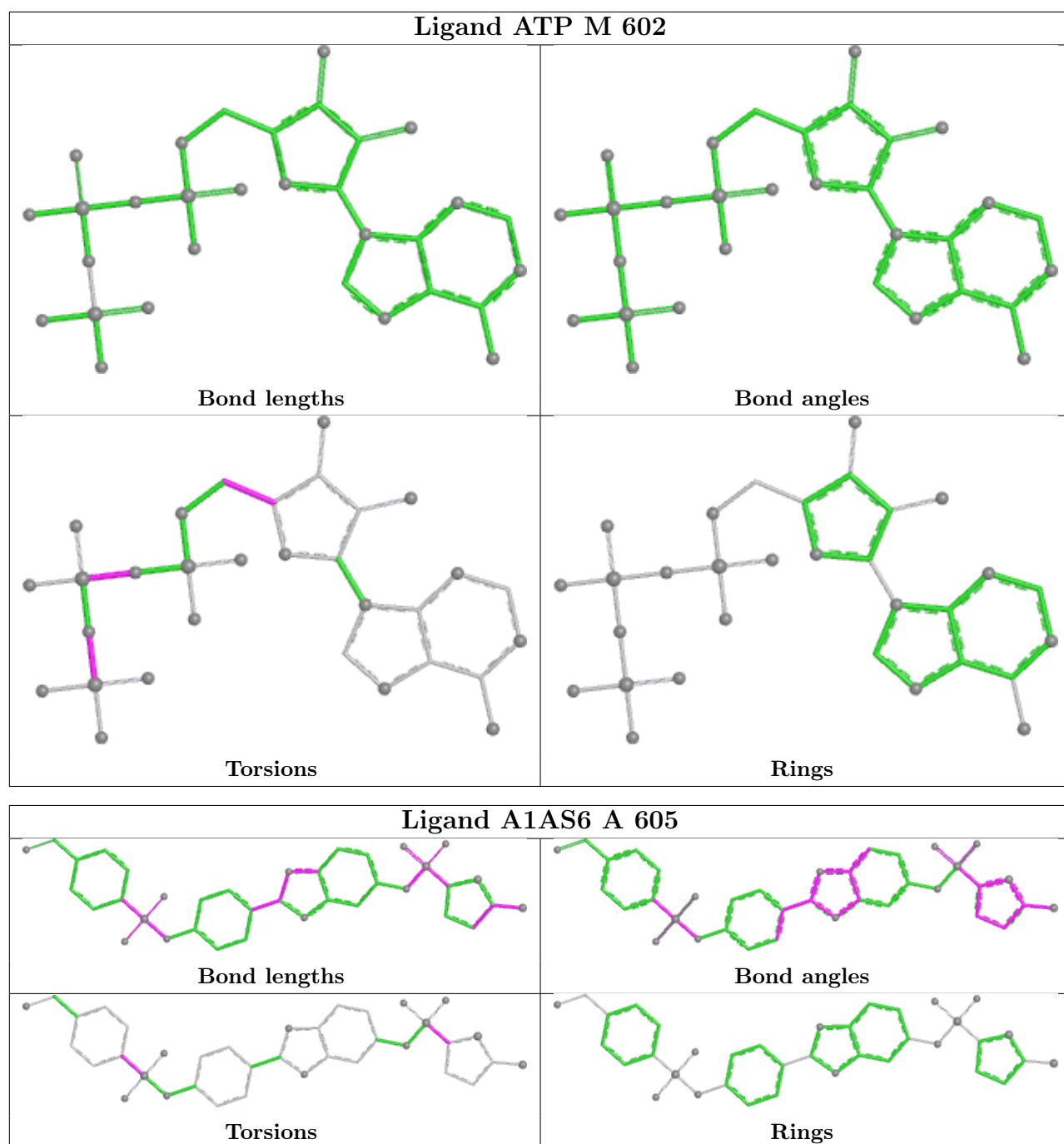


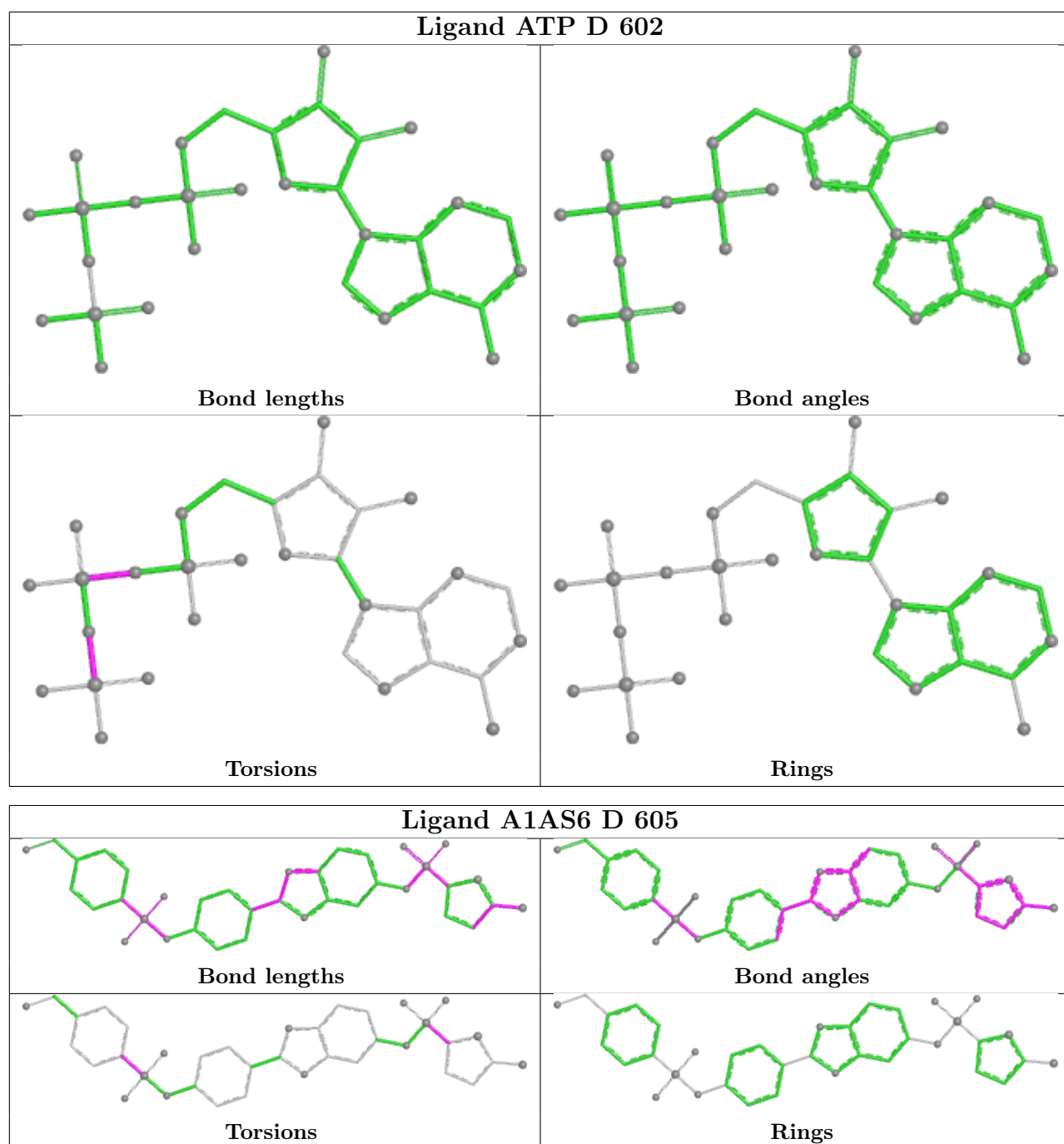


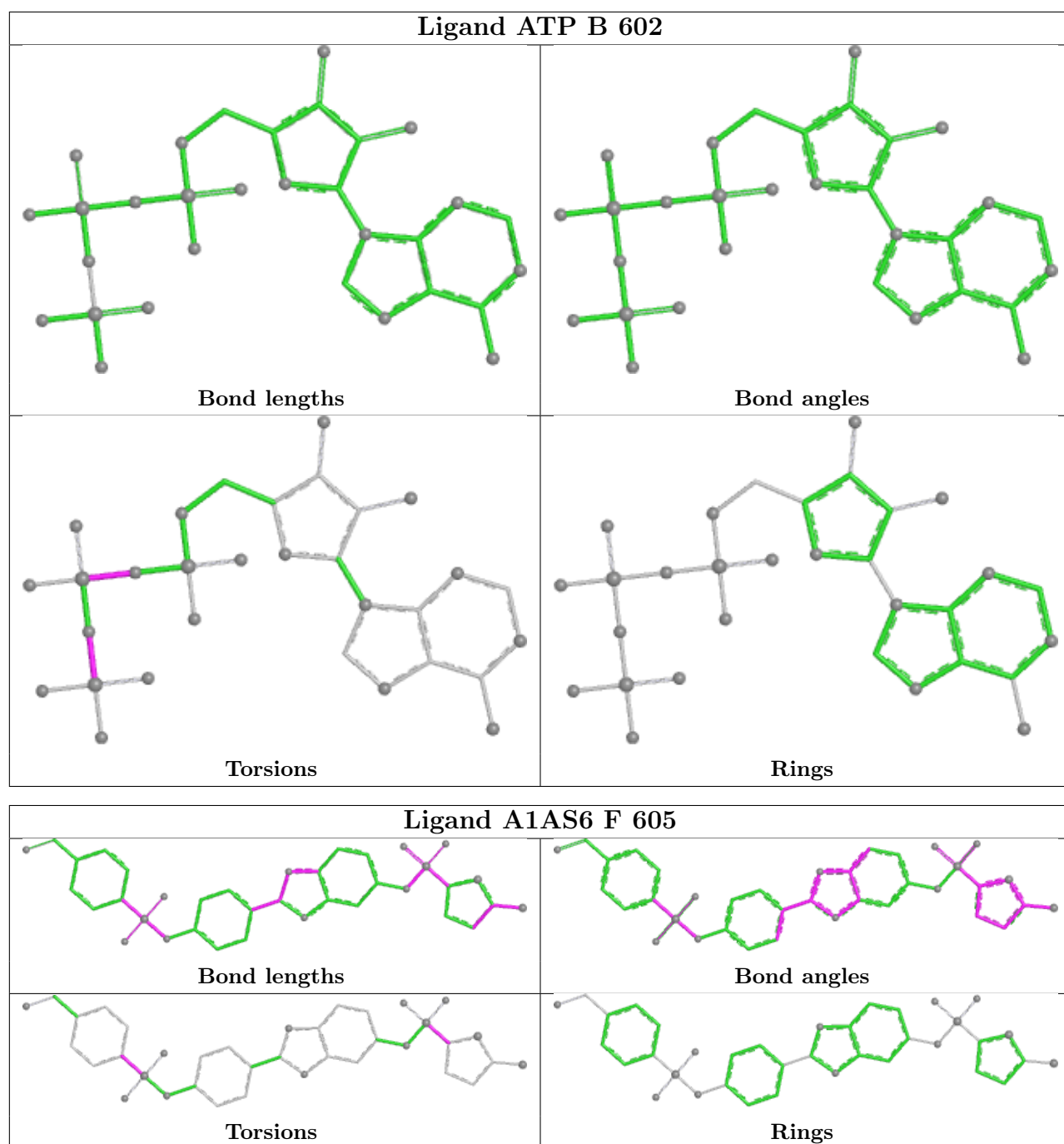


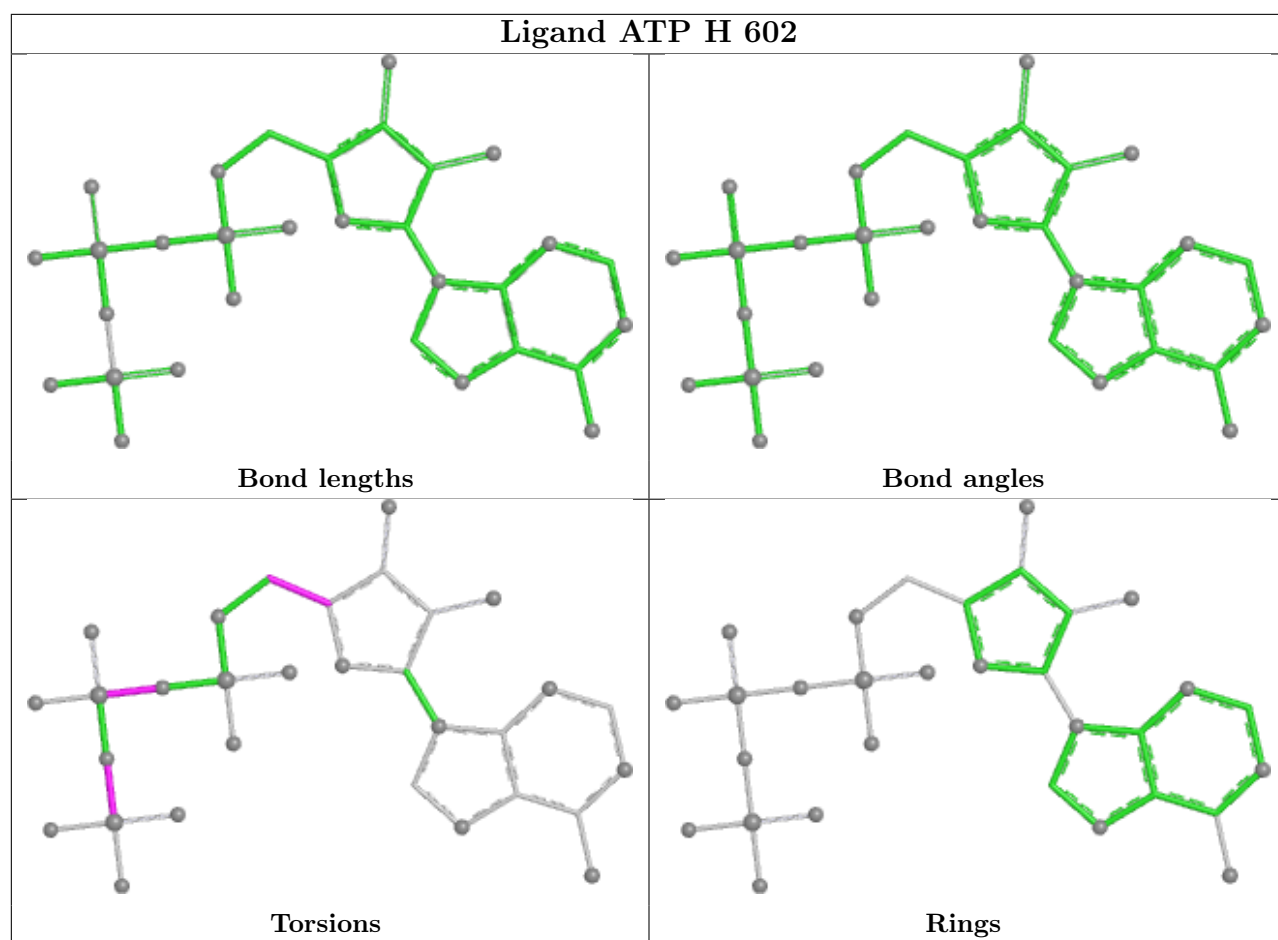


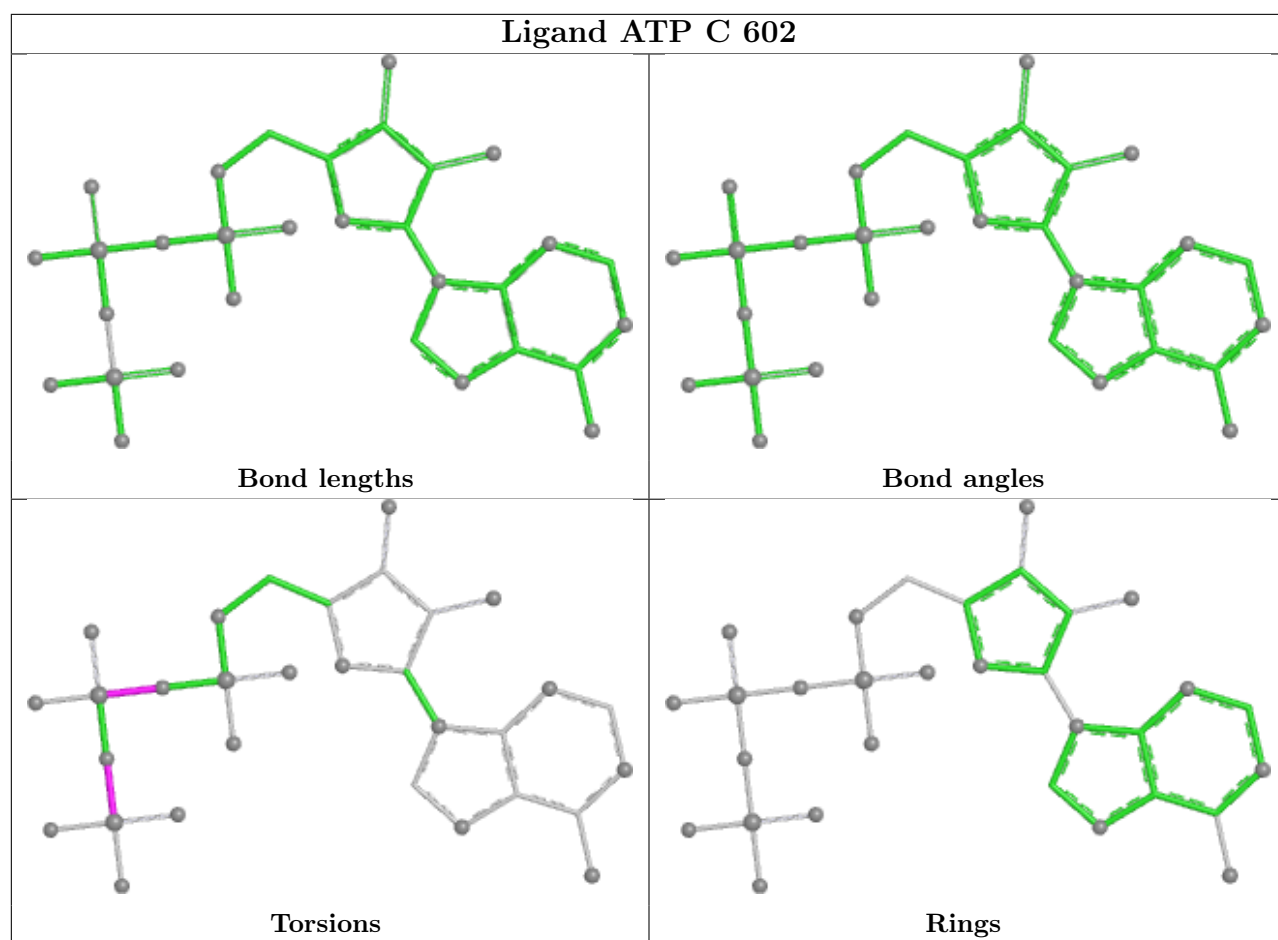












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

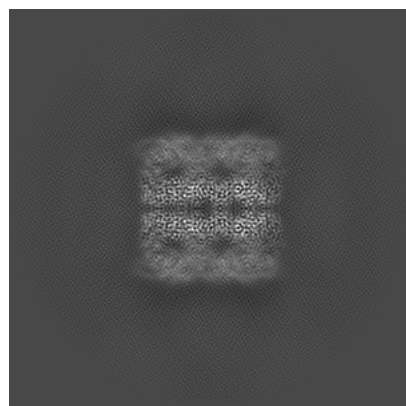
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48407. These allow visual inspection of the internal detail of the map and identification of artifacts.

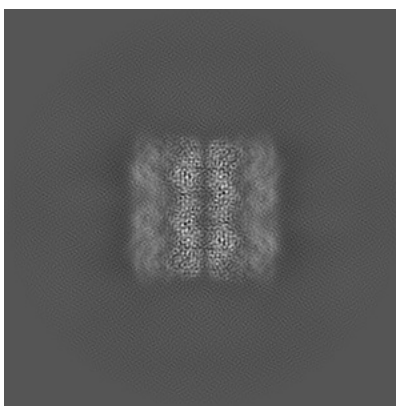
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

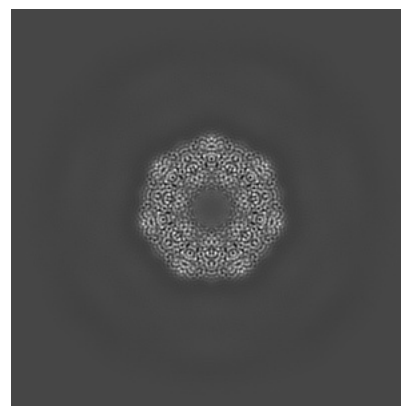
6.1.1 Primary map



X

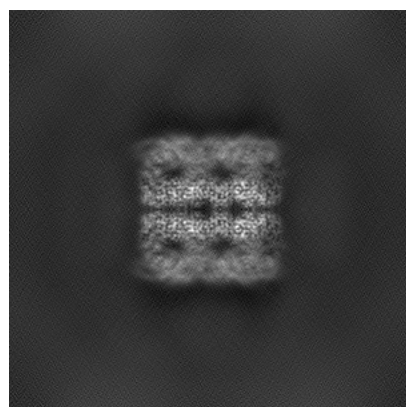


Y

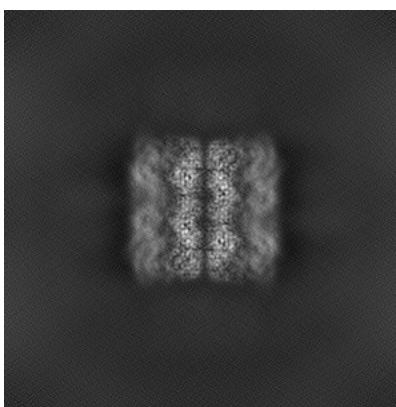


Z

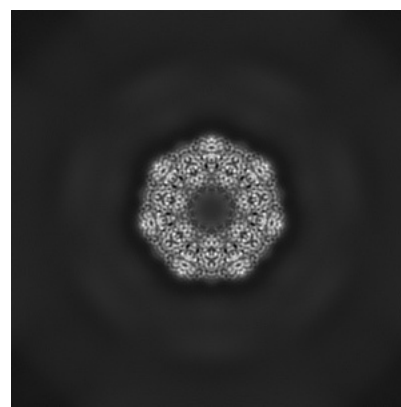
6.1.2 Raw map



X



Y

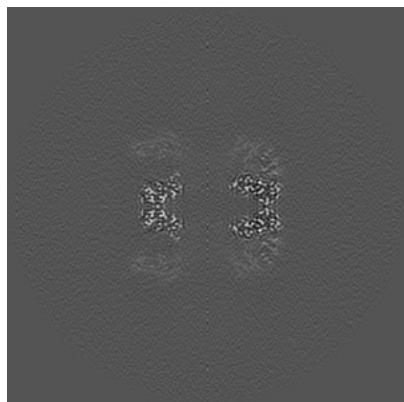


Z

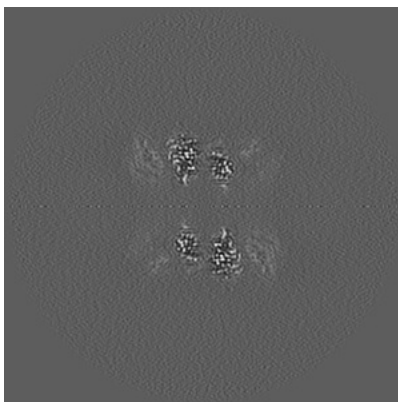
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

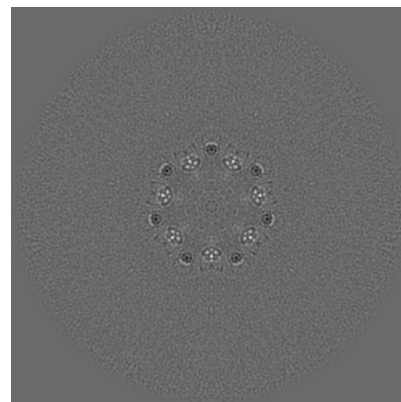
6.2.1 Primary map



X Index: 180

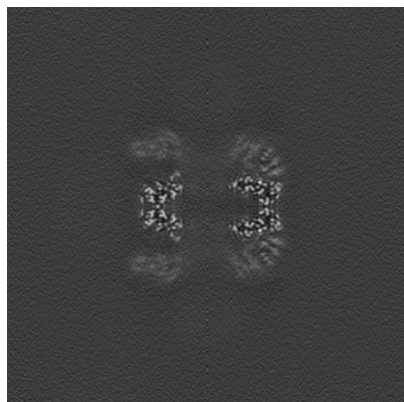


Y Index: 180

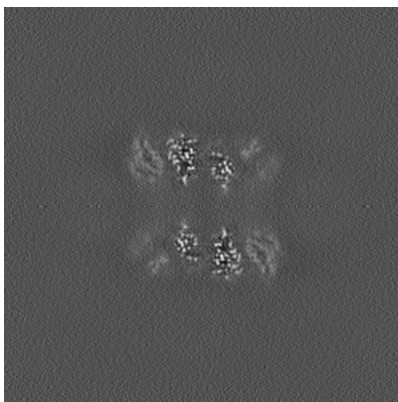


Z Index: 180

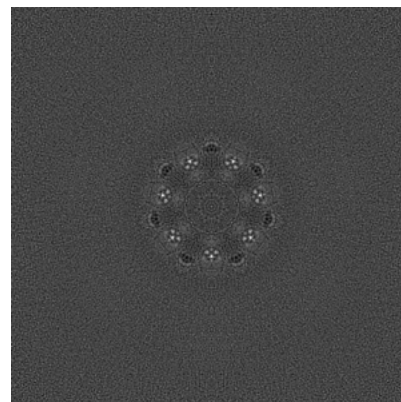
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

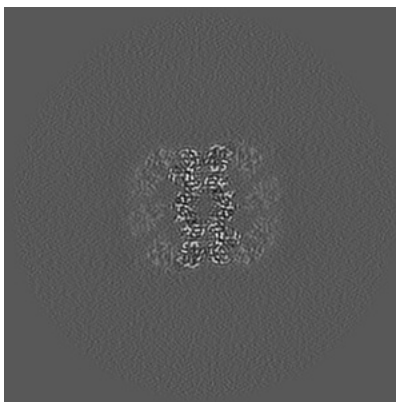
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

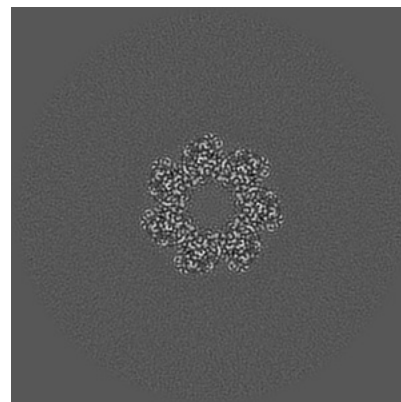
6.3.1 Primary map



X Index: 156

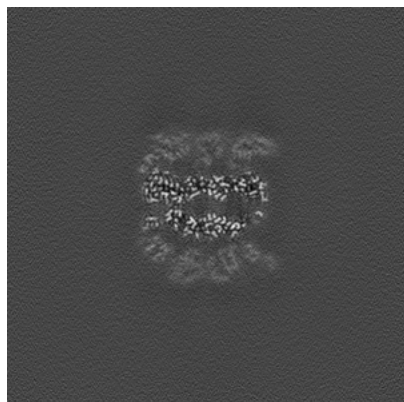


Y Index: 215

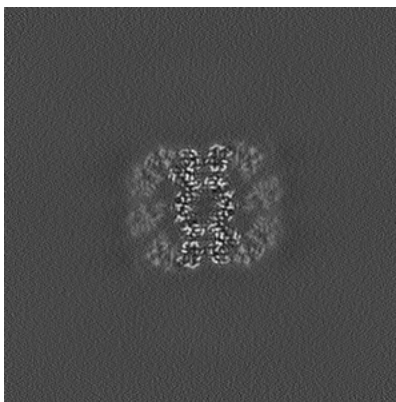


Z Index: 165

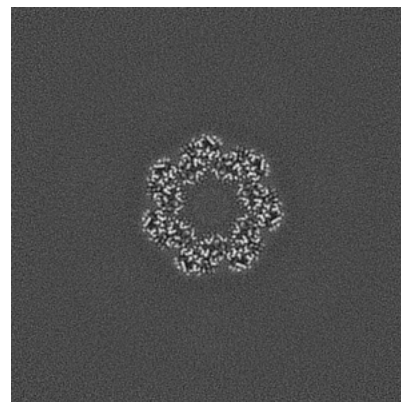
6.3.2 Raw map



X Index: 149



Y Index: 215

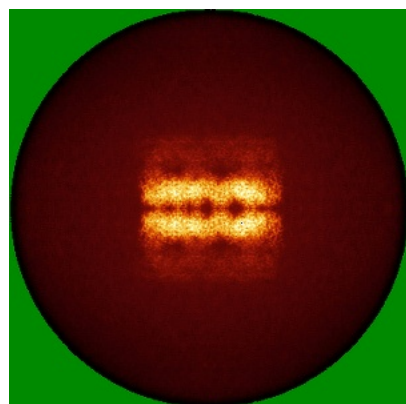


Z Index: 168

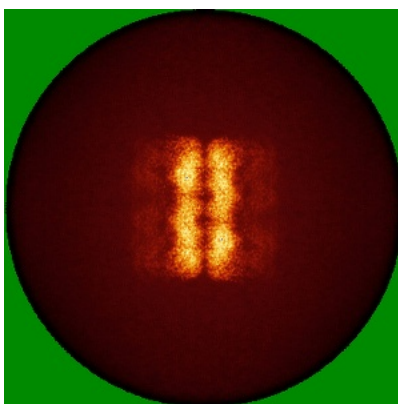
The images above show the largest variance slices of the map in three orthogonal directions.

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

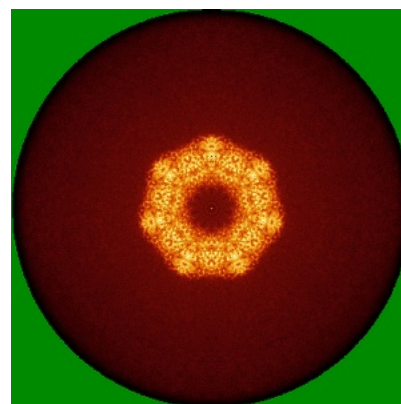
6.4.1 Primary map



X

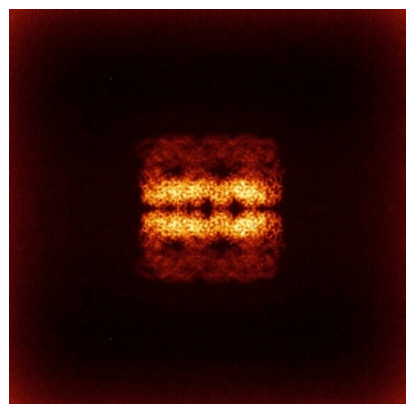


Y

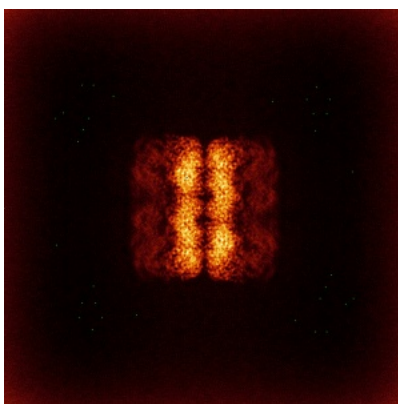


Z

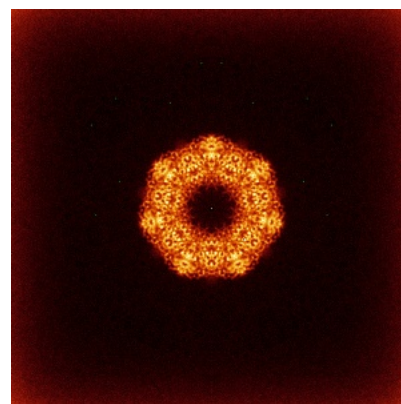
6.4.2 Raw map



X



Y

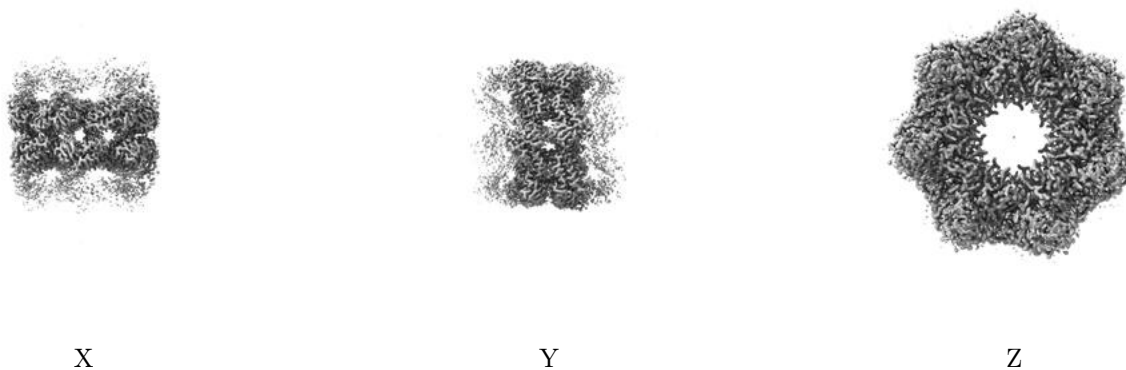


Z

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 0.468. 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.

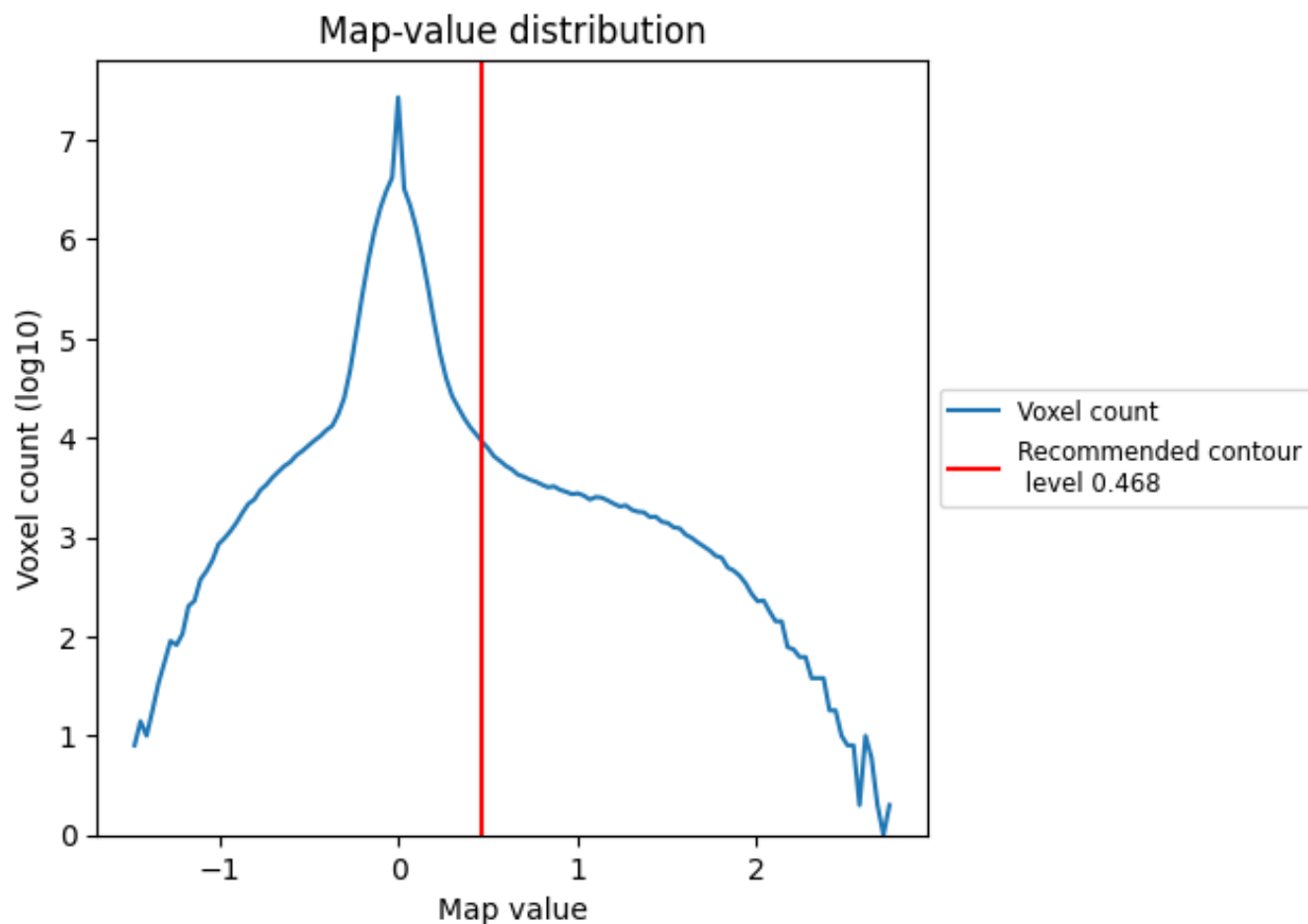
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

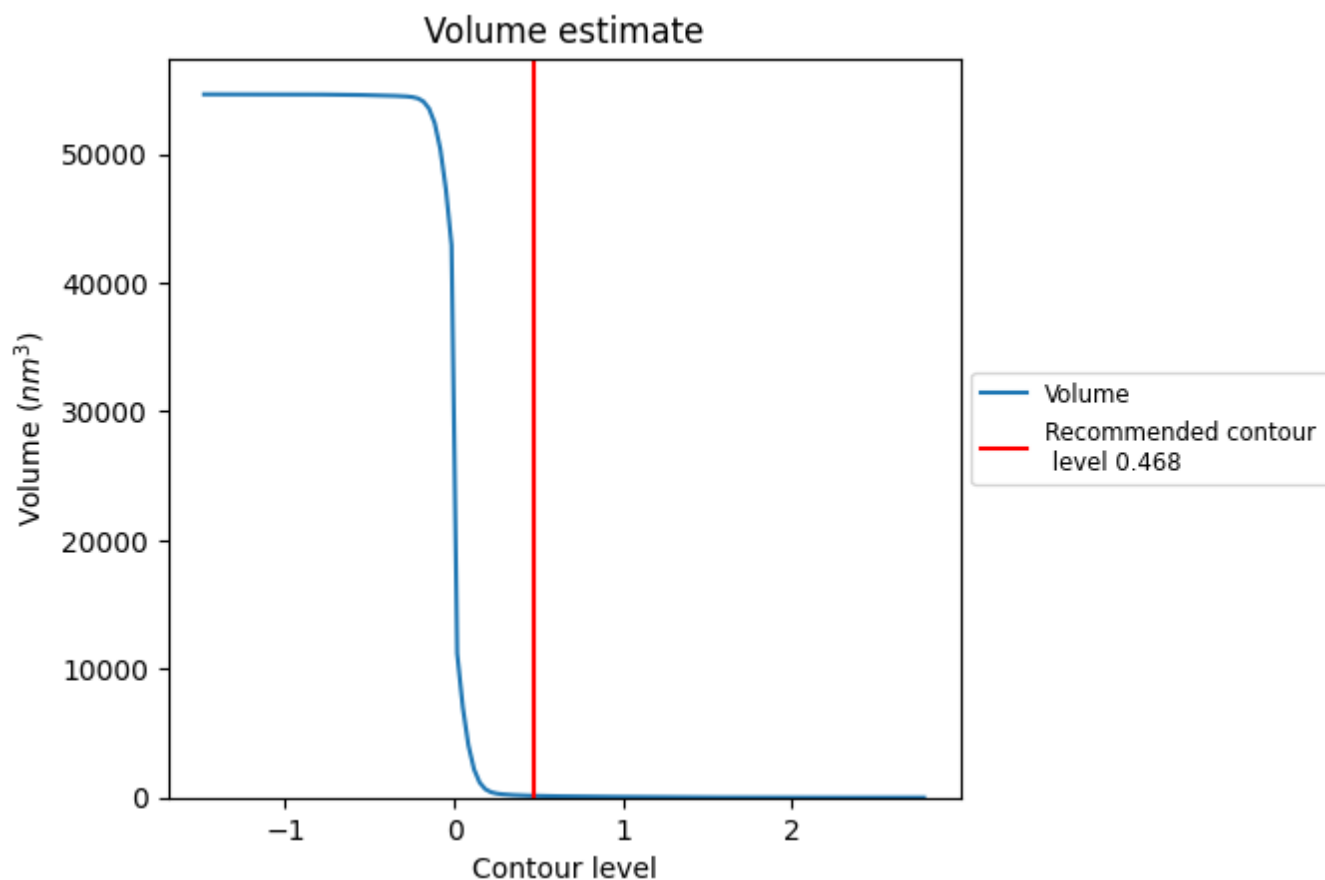
This section contains the results of statistical analysis of the map.

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.

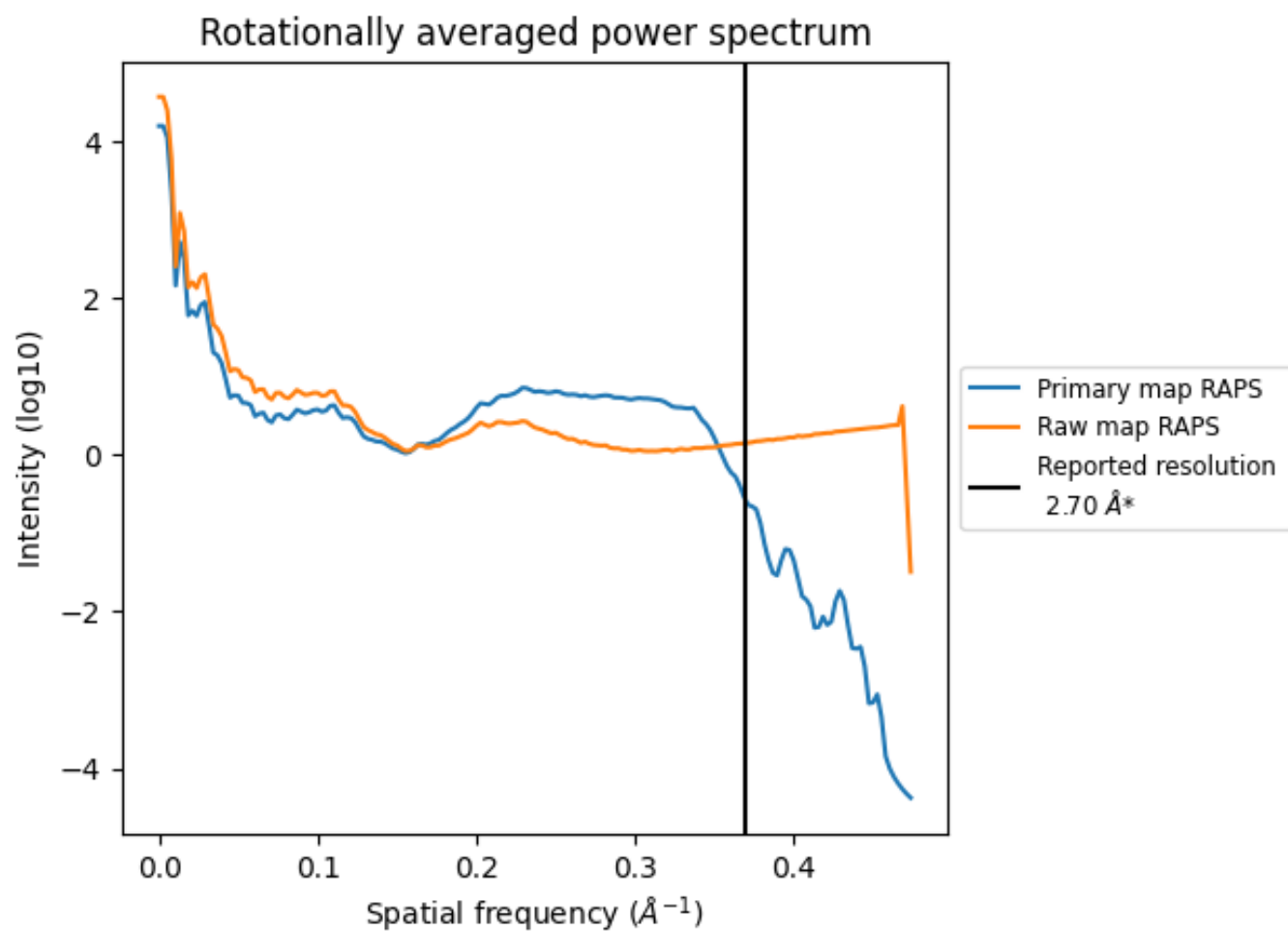
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 124 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 ⓘ

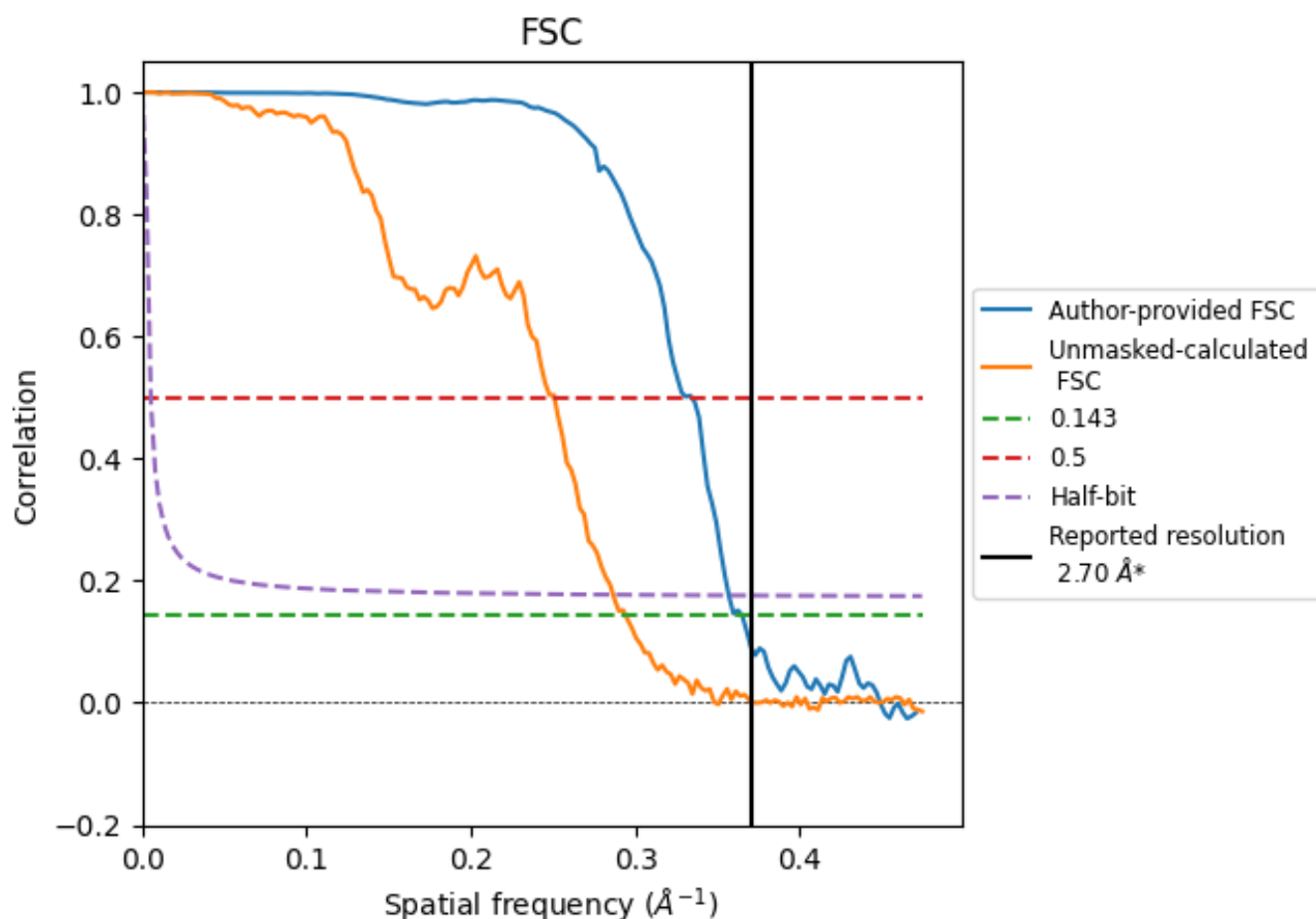


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

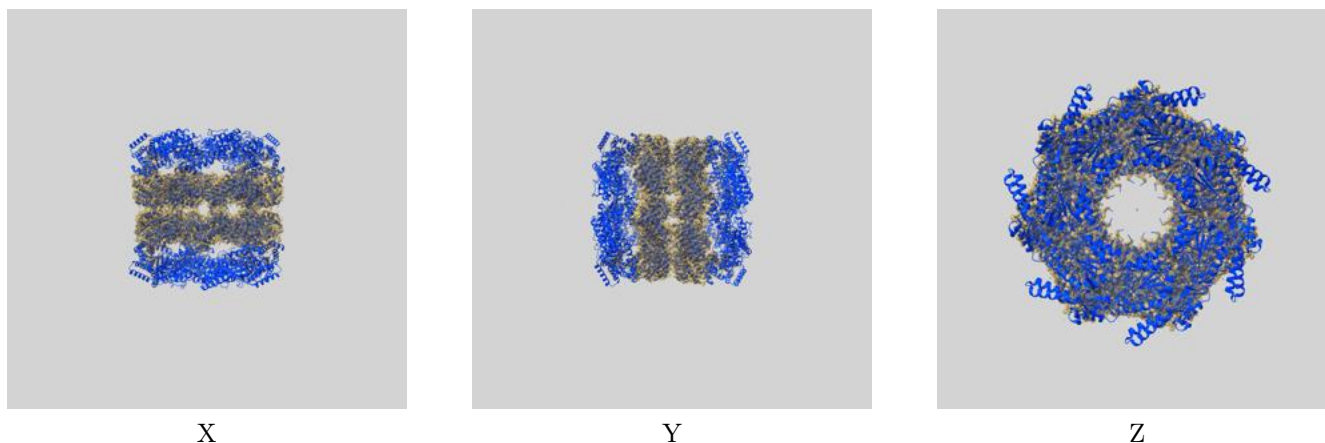
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.74	2.99	2.80
Unmasked-calculated*	3.40	3.99	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

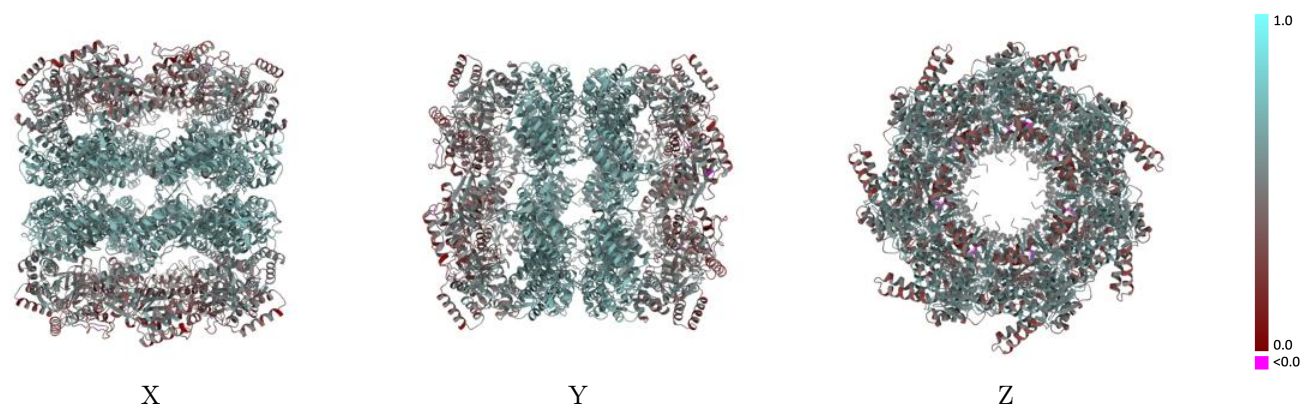
This section contains information regarding the fit between EMDB map EMD-48407 and PDB model 9MMY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



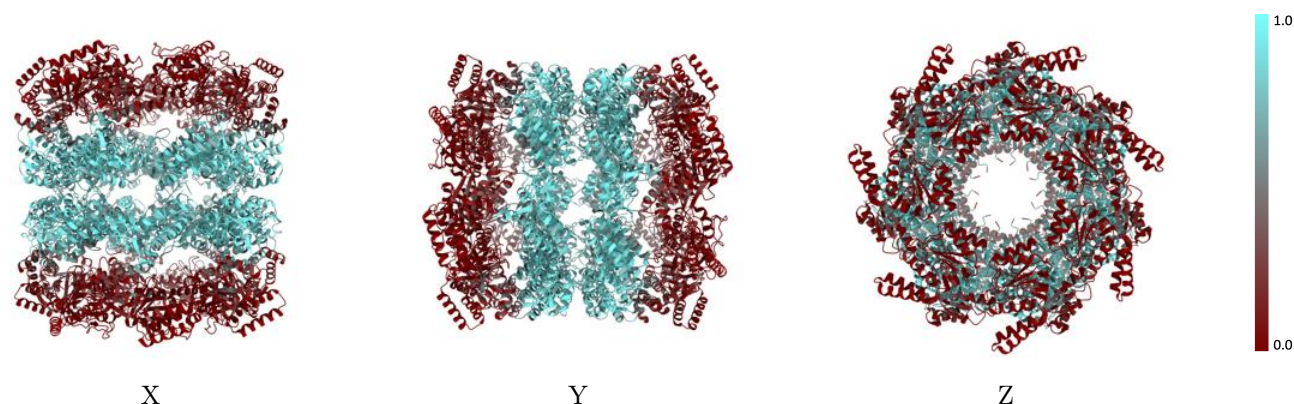
The images above show the 3D surface view of the map at the recommended contour level 0.468 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



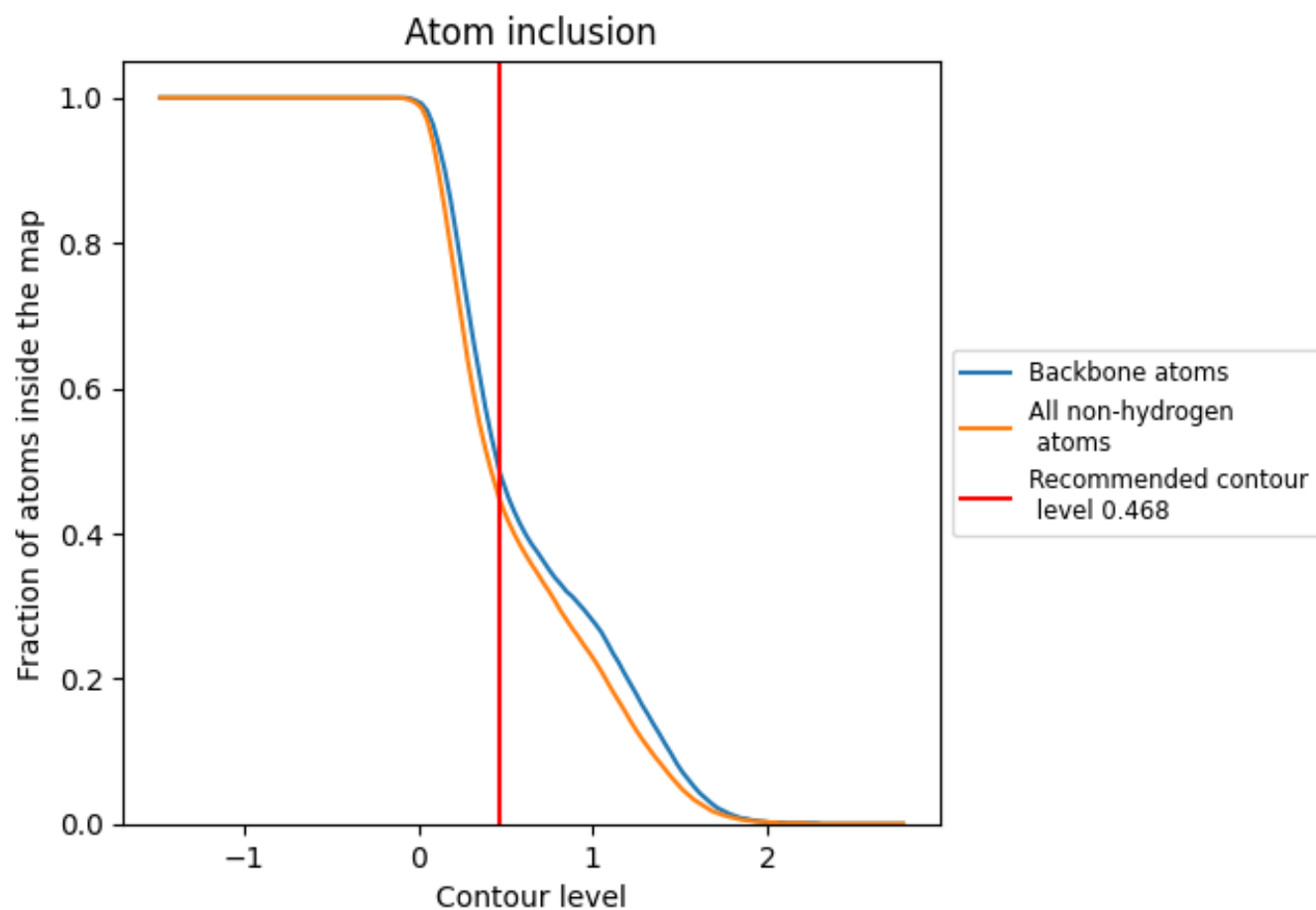
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.468).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 44% 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 (0.468) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4450	0.5240
A	0.4490	0.5270
B	0.4480	0.5250
C	0.4460	0.5260
D	0.4470	0.5260
E	0.4470	0.5250
F	0.4480	0.5250
G	0.4470	0.5240
H	0.4410	0.5210
I	0.4470	0.5240
J	0.4430	0.5200
K	0.4420	0.5220
L	0.4420	0.5220
M	0.4440	0.5220
N	0.4420	0.5220

1.0

0.0

<0.0