



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:34 AM UTC

PDB ID : 6LT4 / pdb_00006lt4
EMDB ID : EMD-0967
Title : AAA+ ATPase, ClpL from *Streptococcus pneumoniae*: ATP_rS-bound
Authors : Kim, G.; Lee, S.G.; Han, S.; Jung, J.; Jeong, H.S.; Hyun, J.K.; Rhee, D.K.;
Kim, H.M.; Lee, S.
Deposited on : 2020-01-21
Resolution : 4.50 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:

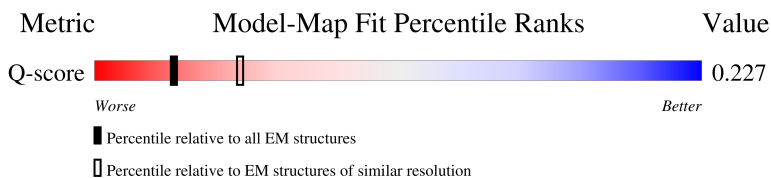
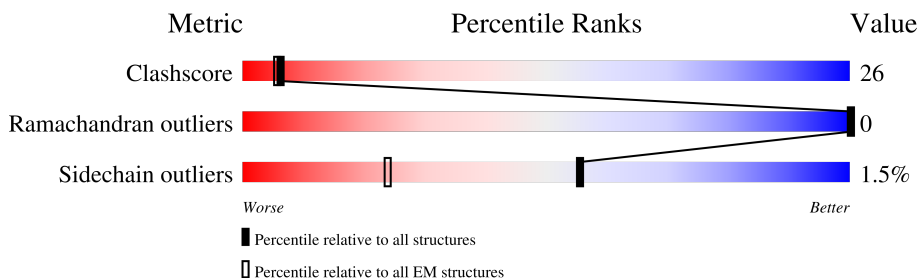
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	701	<p>39% (Upper red bar), 50% (Red), 37% (Yellow), 11% (Grey)</p>
1	B	701	<p>41% (Upper red bar), 50% (Red), 38% (Yellow), 11% (Grey)</p>
1	C	701	<p>39% (Upper red bar), 51% (Red), 37% (Yellow), 11% (Grey)</p>
1	D	701	<p>41% (Upper red bar), 51% (Red), 37% (Yellow), 11% (Grey)</p>

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Mol	Chain	Length	Quality of chain
1	E	701	<p>39% 50% 38% • 11%</p>
1	F	701	<p>39% 52% 36% • 11%</p>
1	G	701	<p>39% 51% 37% • 11%</p>
1	H	701	<p>42% 51% 37% • 11%</p>
1	I	701	<p>44% 51% 37% • 11%</p>
1	J	701	<p>43% 51% 37% • 11%</p>
1	K	701	<p>40% 51% 37% • 11%</p>
1	L	701	<p>40% 51% 37% • 11%</p>
1	M	701	<p>42% 51% 36% • 11%</p>
1	N	701	<p>42% 50% 38% • 11%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 68432 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 ATP-dependent Clp protease, ATP-binding subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	623	4824	3005	850	958	11	0	0
1	B	623	4824	3005	850	958	11	0	0
1	C	623	4824	3005	850	958	11	0	0
1	D	623	4824	3005	850	958	11	0	0
1	E	623	4824	3005	850	958	11	0	0
1	F	623	4824	3005	850	958	11	0	0
1	G	623	4824	3005	850	958	11	0	0
1	H	623	4824	3005	850	958	11	0	0
1	I	623	4824	3005	850	958	11	0	0
1	J	623	4824	3005	850	958	11	0	0
1	K	623	4824	3005	850	958	11	0	0
1	L	623	4824	3005	850	958	11	0	0
1	M	623	4824	3005	850	958	11	0	0
1	N	623	4824	3005	850	958	11	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
A	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
B	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
C	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
C	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
D	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
D	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
E	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
E	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
F	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
F	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
G	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
G	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
H	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
H	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
I	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
I	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
J	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
J	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
K	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
K	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
L	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
L	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
M	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
M	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
N	193	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9
N	526	ALA	GLU	engineered mutation	UNP A0A0H2ZMB9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

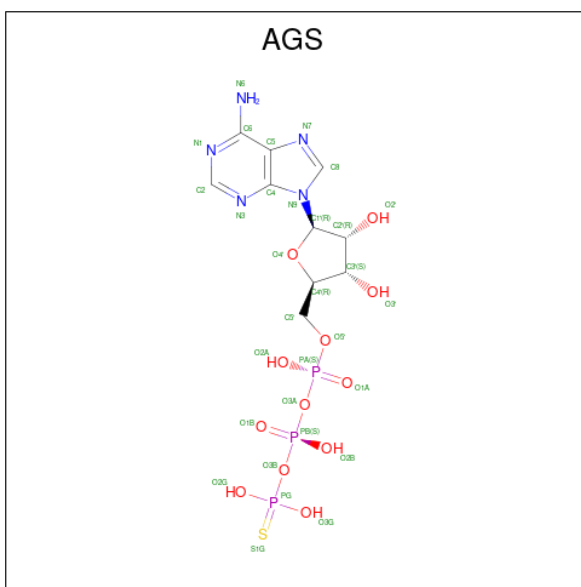
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0
2	B	2	Total Mg 2 2	0
2	C	2	Total Mg 2 2	0
2	D	2	Total Mg 2 2	0
2	E	2	Total Mg 2 2	0
2	F	2	Total Mg 2 2	0

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Mol	Chain	Residues	Atoms		AltConf
2	G	2	Total	Mg	0
			2	2	
2	H	2	Total	Mg	0
			2	2	
2	I	2	Total	Mg	0
			2	2	
2	J	2	Total	Mg	0
			2	2	
2	K	2	Total	Mg	0
			2	2	
2	L	2	Total	Mg	0
			2	2	
2	M	2	Total	Mg	0
			2	2	
2	N	2	Total	Mg	0
			2	2	

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

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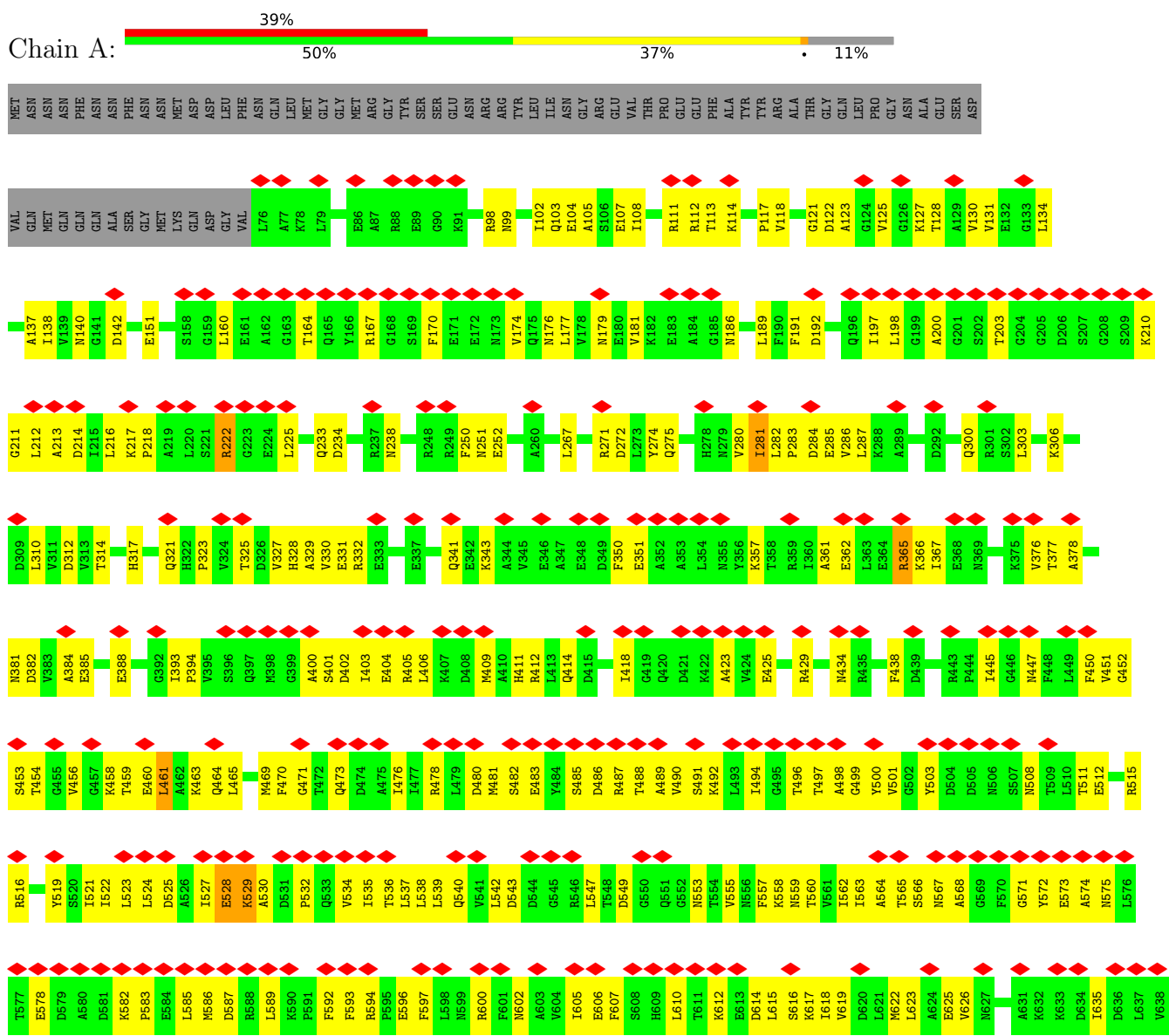
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Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	M	1	Total 31	10	5	12	3	1	0
3	M	1	Total 31	10	5	12	3	1	0
3	N	1	Total 31	10	5	12	3	1	0
3	N	1	Total 31	10	5	12	3	1	0

3 Residue-property plots

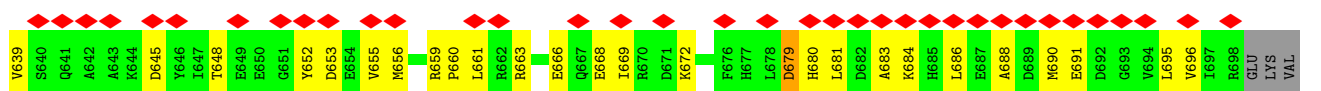
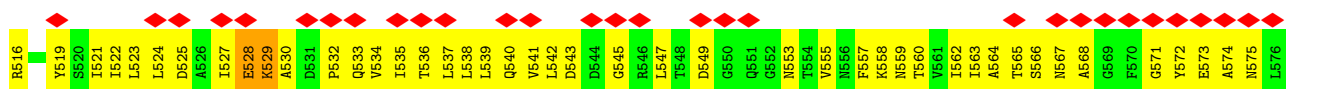
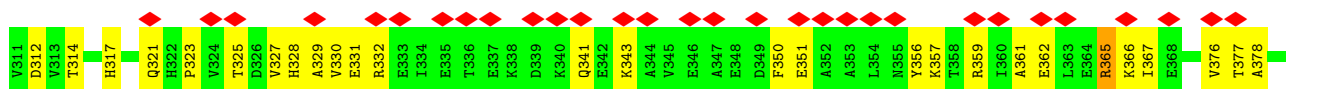
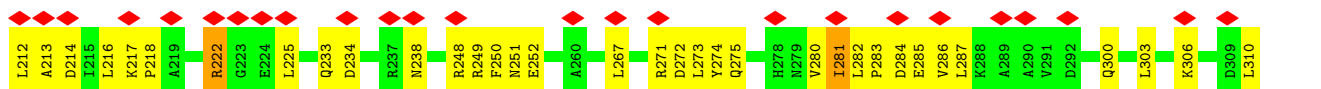
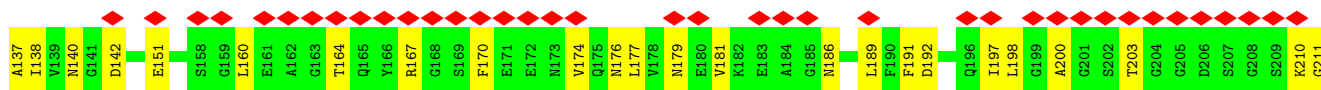
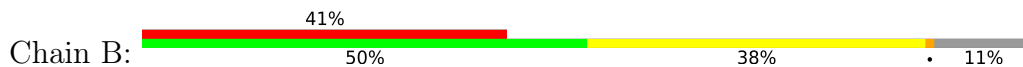
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-dependent Clp protease, ATP-binding subunit

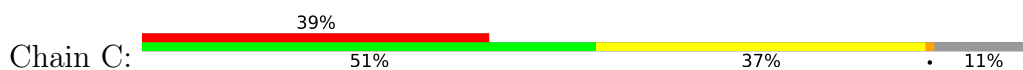


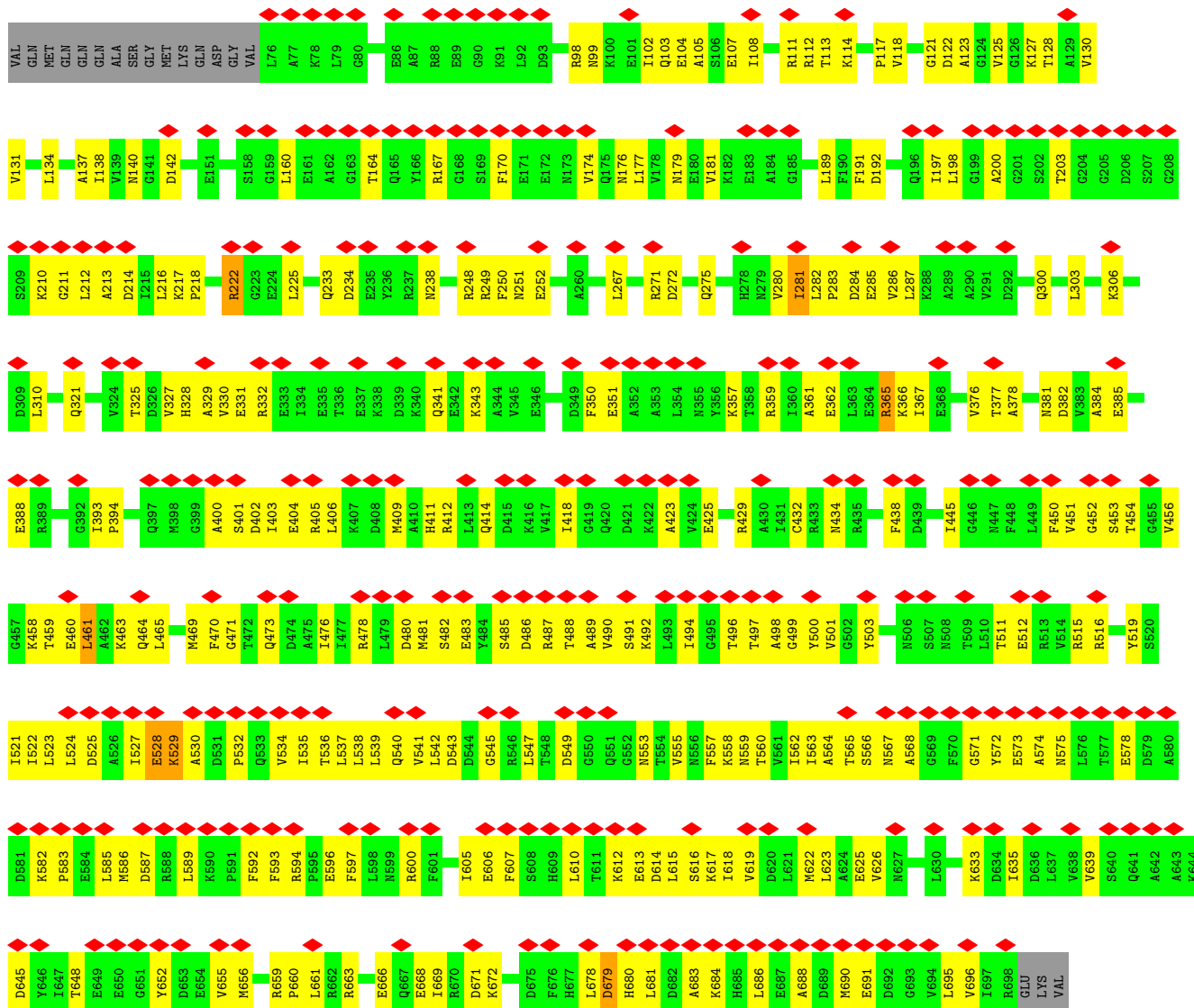


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

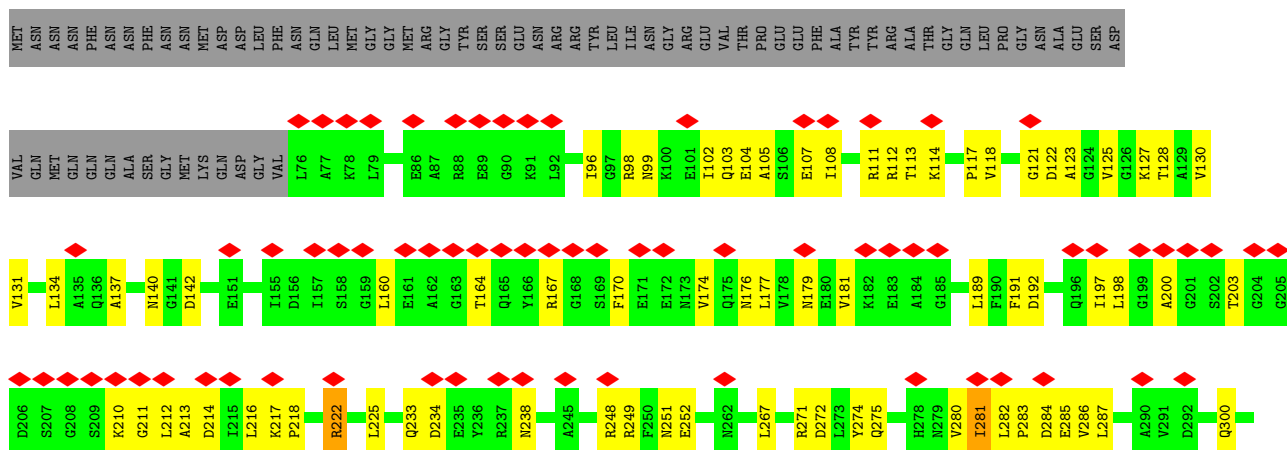
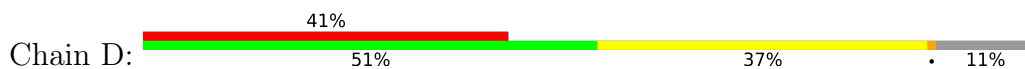


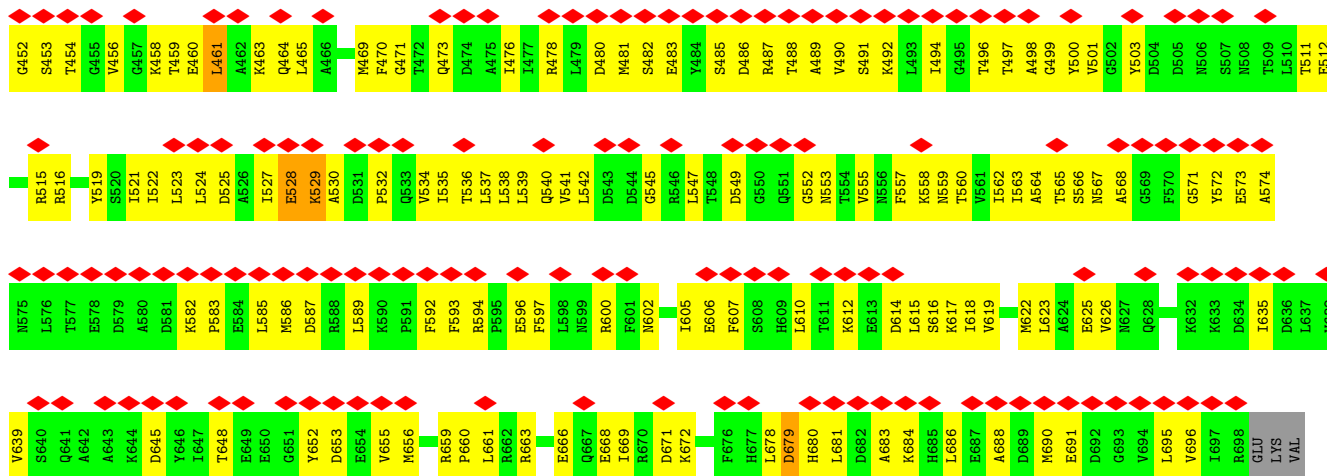
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



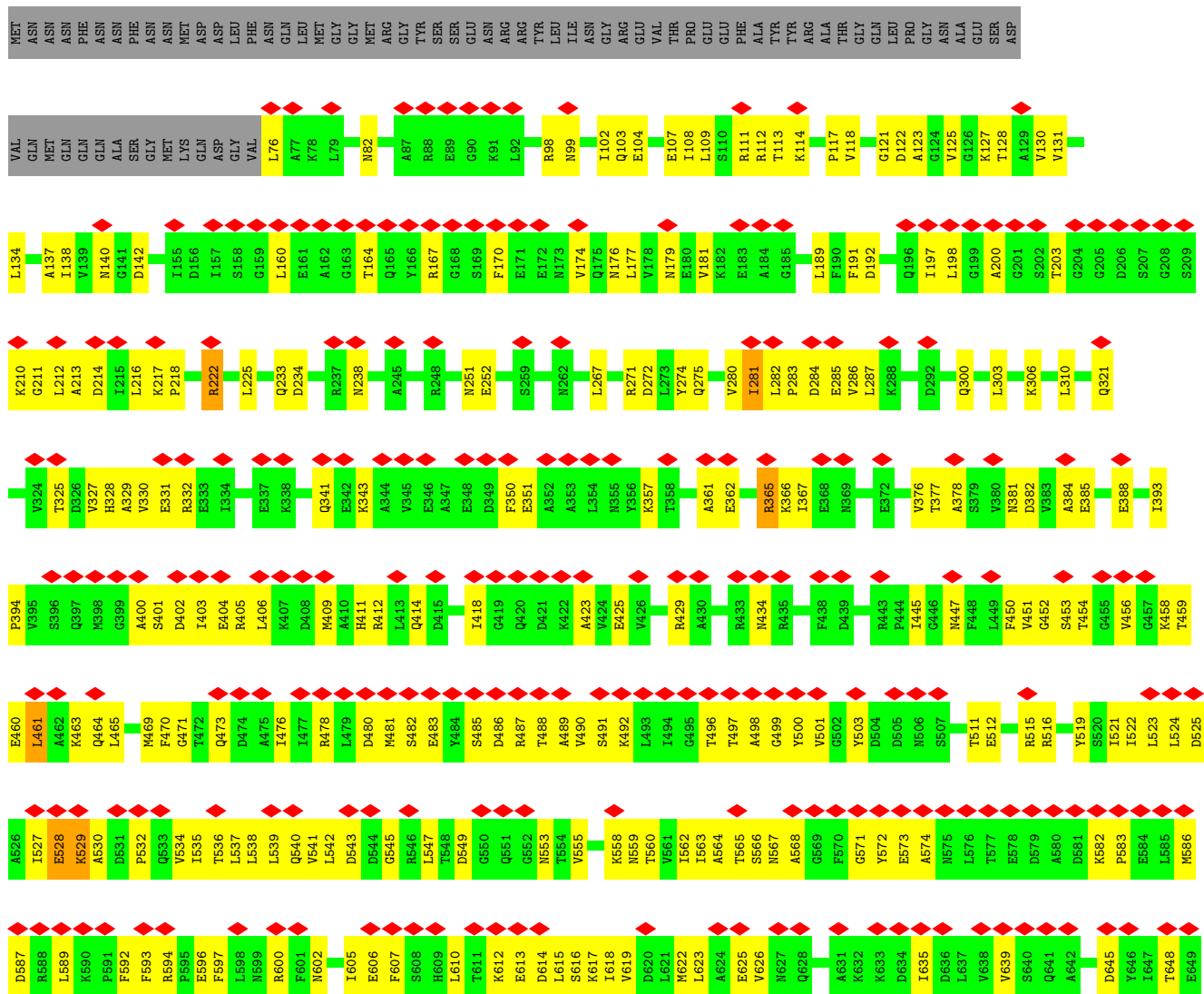


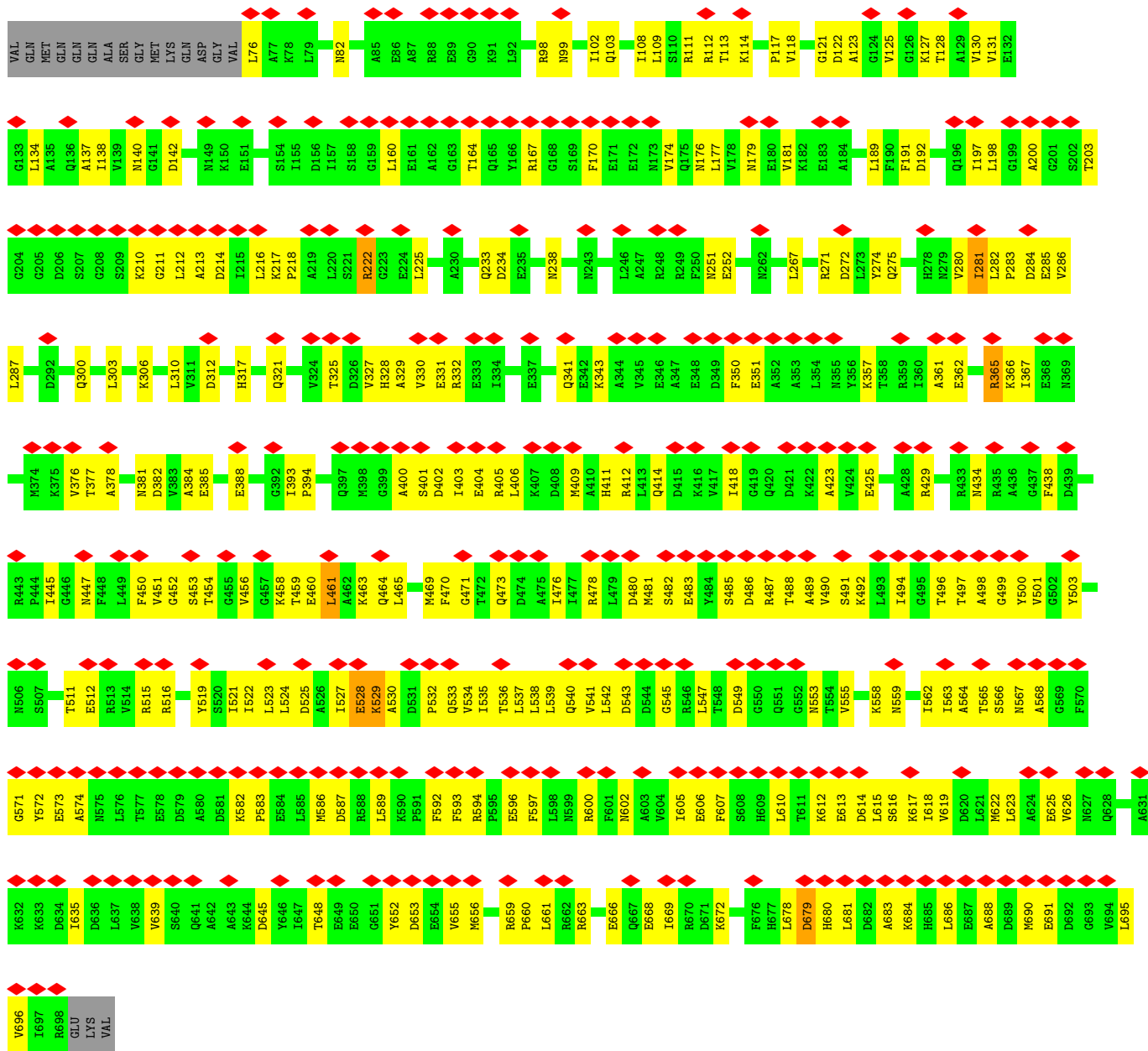
● Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



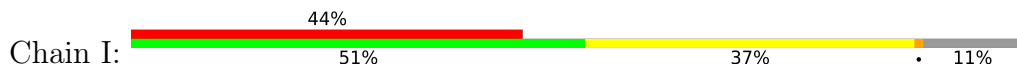


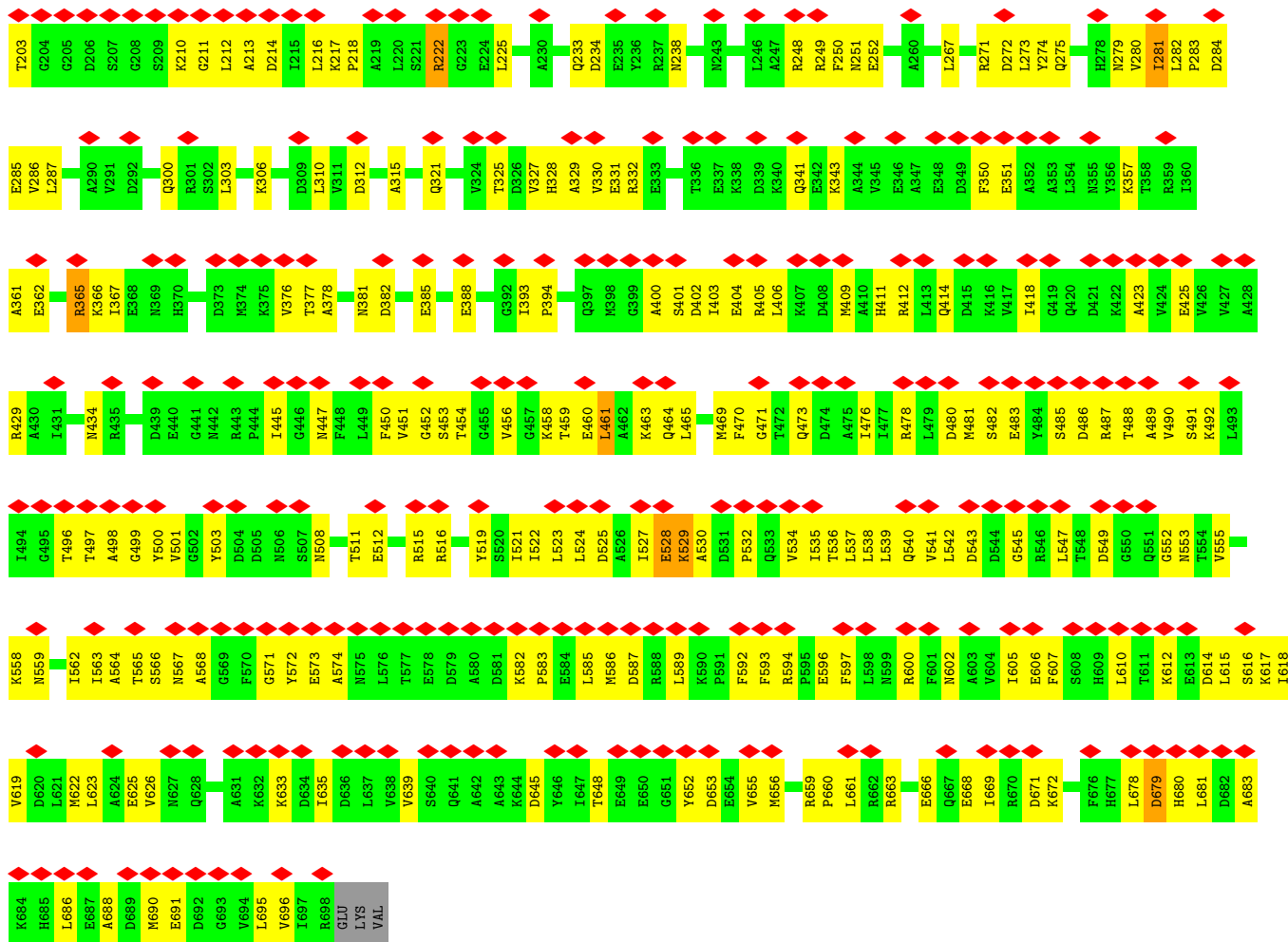
● Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



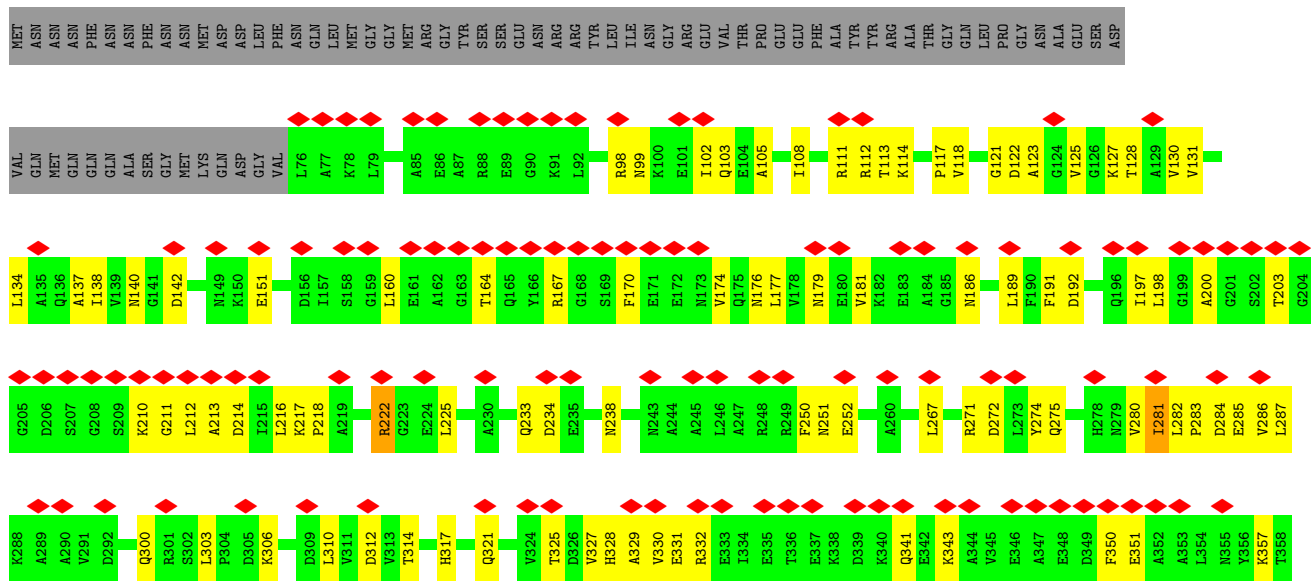
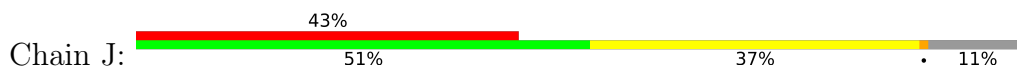


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



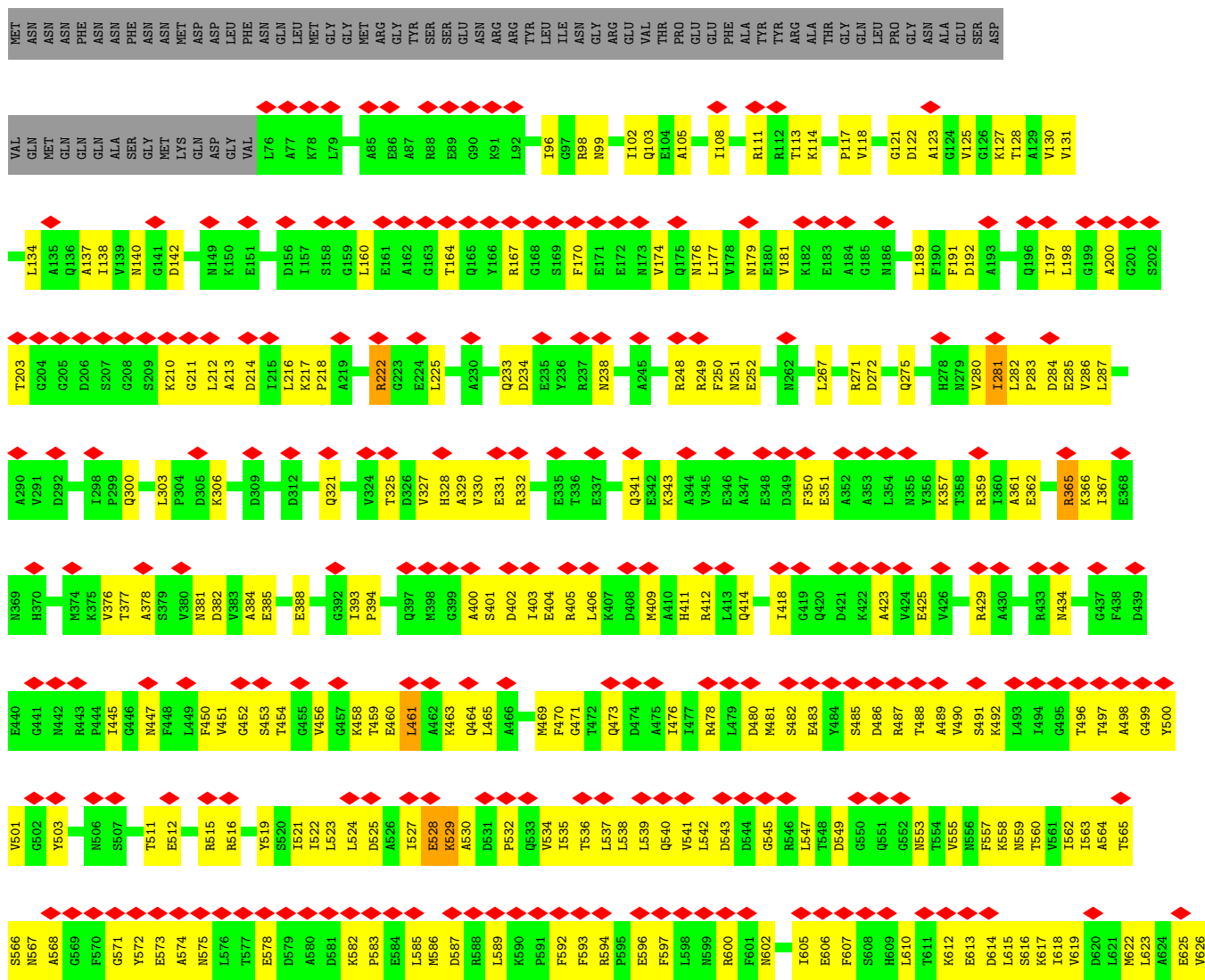
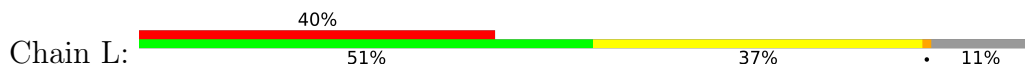


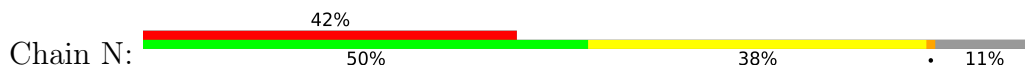
● Molecule 1: ATP-dependent Clp protease, ATP-binding subunit





● Molecule 1: ATP-dependent Clp protease, ATP-binding subunit





MET	ASN	ASN	ASN	PHE	ASN	ASN	PHE	ASN	ASN	MET	MET	ASP	ASP	LEU	PHE	ASN	GLN	GLN	MET	GLY	MET	GLY	MET	ARG	ARG	GLY	TYR	SER	SER	GLU	GLU	ARG	ASN	ASN	ARG	TYR	LEU	LEU	ILE	ASN	ASN	GLY	ARG	GLU	GLU	VAL	THR	THR	GLN	LEU	PRO	PRO	GLY	ASN	ALA	ALA	GLU	SER	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																
VAL	GLN	MET	GLN	GLN	GLN	ALA	SER	GLY	ASN	MET	LYS	GLN	ASP	GLY	VAL	L76	A77	K78	L79	N82	E86	A87	R88	E89	G90	K91	L92	R98	N99	I102	Q103	E107	I108	R111	R112	T113	K114	P117	V118	G121	D122	A123	G124	V125	G126	K127	T128	A129	V130	V131	L134	A137	I138	V139	M140	G141	D142	N149	K150	E151	S158	G159	L160	E161	A162	G163	T164	Q165	Y166	R167	G168	S169	F170	E171	E172	N173	V174	Q175	N176	L177	V178	M179	E180	V181	K182	E183	A184	L189	F190	F191	D192	Q196	I197	L198	G199	A200	G201	S202	T203	G204	G205	D206	G208	S209	R210	G211	L212	A213	D214	L215	L216	K217	P218	A219	L220	S221	R222	G223	E224	L225	T232	Q233	D234	E235	M238	A245	R248	R249	F250	N251	E252	M262	L267	Q268	G269	L270	R271	D272	L273	Y274	Q275	H278	M279	V280	L281	P283	D284	E285	V286	L287	D292	Q300	L303	K306	L310	V311	D312	V313	T314	A315	Q321	V324	T325	D326	V327	H328	A329	V330	E331	R332	E333	I334	E337	K338	Q341	E342	K343	A344	V345	E346	A347	E348	D349	F350	E351	A352	A353	L354	N355	V356	K357	T358	R359	L360	E362	R365	K366	L367	E368	K369	K374	K375	V376	T377	A378	S379	V380	N381	D382	V383	A384	Y451	E385	E388	R389	G392	L393	P394	V395	S396	Q397	M398	G399	A400	S401	D402	L403	E404	R405	L406	K407	D408	M409	A410	H411	R412	L413	Q414	D415	I418	Q419	Q420	D421	K422	A423	V424	E425	R429	A430	R433	M434	G437	F438	D439	E440	G441	N442	R443	P444	L445	G446	M447	F448	L449	F450	Y451	G452	S453	T454	G455	G456	G457	K458	T459	E460	L461	A462	K463	O464	L465	M469	F470	Q471	T472	Q473	D474	A475	L476	L477	R478	L479	D480	M481	S482	E483	Y484	S485	D486	R487	T488	A489	V490	S491	K492	L493	I494	G495	T496	T497	A498	G499	S500	V501	G502	A503	D504	D505	N506	S507	T511	E512	R515	R516	Y519	S520	I521	L522	L523	L524	D525	A526	E528	K529	A530	D531	P532	G533	V534	I535	T536	L537	L538	L539	Q540	V541	L542	D543	D544	G545	R546	L547	T548	D549	G550	Q551	G552	N553	V554	V555	N556	F557	K558	N559	T560	V561	I562	I563	A564	T565	S566	M567	A568	G569	F570	G571	Y572	E573	A574	N575	L576	T577	E578	D579	A580	D581	K582	P583	E584	L585	M586	D587	R588	L589	R590	P591	F592	F593	R594	E596	F597	L598	H599	R600	F601	M602	A603	R546	V604	I605	E606	F607	S608	H609	L610	T611	K612	E613	D614	L615	S616	K617	I618	V619	D620	L621	M622	L623	A624	E625	V626	N627	O628	A631	K632	R633	D634	I635	D636	L637	V638	V639	S640	Q641	A642	A643	R644	D645	Y646	T647	T648	E649	E650	G651	Y652	D653	E654	V655	M656	R659	P660	L661	R662	R663	E666	Q667	E668	I669	R670	D671	K672	F676	H677	L678	D679	H680	L681	D682	A683	K684	H685	L686	E687	A688	D689	M690	E691	D692	G693	V694	L695	V696

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49797	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.717	Depositor
Minimum map value	-0.436	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	280.0, 280.0, 280.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4, 1.4, 1.4	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: MG, 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	A	0.29	0/4883	0.57	1/6603 (0.0%)
1	B	0.29	0/4883	0.57	1/6603 (0.0%)
1	C	0.29	0/4883	0.57	1/6603 (0.0%)
1	D	0.29	0/4883	0.57	1/6603 (0.0%)
1	E	0.28	0/4883	0.57	1/6603 (0.0%)
1	F	0.29	0/4883	0.57	1/6603 (0.0%)
1	G	0.29	0/4883	0.57	1/6603 (0.0%)
1	H	0.29	0/4883	0.57	1/6603 (0.0%)
1	I	0.29	0/4883	0.57	1/6603 (0.0%)
1	J	0.28	0/4883	0.57	1/6603 (0.0%)
1	K	0.29	0/4883	0.57	1/6603 (0.0%)
1	L	0.29	0/4883	0.57	1/6603 (0.0%)
1	M	0.29	0/4883	0.57	1/6603 (0.0%)
1	N	0.29	0/4883	0.57	1/6603 (0.0%)
All	All	0.29	0/68362	0.57	14/92442 (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
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	2
All	All	0	40

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	LYS	N-CA-C	-8.88	103.57	114.75
1	N	529	LYS	N-CA-C	-8.87	103.57	114.75
1	E	529	LYS	N-CA-C	-8.87	103.58	114.75
1	M	529	LYS	N-CA-C	-8.87	103.58	114.75
1	D	529	LYS	N-CA-C	-8.86	103.58	114.75

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	ILE	Peptide
1	A	528	GLU	Peptide
1	A	679	ASP	Peptide
1	B	281	ILE	Peptide
1	B	528	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4824	0	4841	259	0
1	B	4824	0	4841	269	0
1	C	4824	0	4841	263	0
1	D	4824	0	4841	274	0
1	E	4824	0	4841	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4824	0	4841	251	0
1	G	4824	0	4841	263	0
1	H	4824	0	4841	264	0
1	I	4824	0	4841	267	0
1	J	4824	0	4841	253	0
1	K	4824	0	4841	258	0
1	L	4824	0	4841	253	0
1	M	4824	0	4841	258	0
1	N	4824	0	4841	266	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
3	A	62	0	24	6	0
3	B	62	0	24	7	0
3	C	62	0	24	6	0
3	D	62	0	24	7	0
3	E	62	0	24	6	0
3	F	62	0	24	6	0
3	G	62	0	24	6	0
3	H	62	0	24	6	0
3	I	62	0	24	6	0
3	J	62	0	24	6	0
3	K	62	0	24	7	0
3	L	62	0	24	7	0
3	M	62	0	24	6	0
3	N	62	0	24	6	0
All	All	68432	0	68110	3519	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 26.

The worst 5 of 3519 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:103:GLN:NE2	1:I:321:GLN:OE1	1.97	0.95
1:M:365:ARG:HH11	1:M:365:ARG:HG3	1.32	0.95
1:D:365:ARG:HH11	1:D:365:ARG:HG3	1.31	0.95
1:K:365:ARG:HG3	1:K:365:ARG:HH11	1.32	0.95
1:B:365:ARG:HH11	1:B:365:ARG:HG3	1.32	0.95

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	A	621/701 (89%)	574 (92%)	47 (8%)	0	100	100
1	B	621/701 (89%)	574 (92%)	47 (8%)	0	100	100
1	C	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	D	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	E	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	F	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	G	621/701 (89%)	574 (92%)	47 (8%)	0	100	100
1	H	621/701 (89%)	574 (92%)	47 (8%)	0	100	100
1	I	621/701 (89%)	574 (92%)	47 (8%)	0	100	100
1	J	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	K	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	L	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	M	621/701 (89%)	573 (92%)	48 (8%)	0	100	100
1	N	621/701 (89%)	572 (92%)	49 (8%)	0	100	100
All	All	8694/9814 (89%)	8026 (92%)	668 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	B	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	C	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	D	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	E	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	F	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	G	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	H	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	I	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	J	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	K	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	L	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	M	520/586 (89%)	512 (98%)	8 (2%)	57 70
1	N	520/586 (89%)	512 (98%)	8 (2%)	57 70
All	All	7280/8204 (89%)	7168 (98%)	112 (2%)	55 70

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	225	LEU
1	N	473	GLN
1	I	690	MET
1	N	461	LEU
1	M	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	176	ASN

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Mol	Chain	Res	Type
1	M	179	ASN
1	I	175	GLN
1	M	176	ASN
1	N	179	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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	AGS	H	802	2	32,33,33	0.81	4 (12%)	45,52,52	0.83	1 (2%)
3	AGS	G	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	A	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	H	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	E	802	2	32,33,33	0.81	4 (12%)	45,52,52	0.83	1 (2%)
3	AGS	J	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	M	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	M	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	L	802	2	32,33,33	0.81	4 (12%)	45,52,52	0.83	1 (2%)
3	AGS	D	803	2	32,33,33	0.49	0	45,52,52	0.79	1 (2%)
3	AGS	F	803	2	32,33,33	0.49	0	45,52,52	0.79	1 (2%)
3	AGS	N	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	I	802	2	32,33,33	0.81	4 (12%)	45,52,52	0.83	1 (2%)
3	AGS	K	802	2	32,33,33	0.80	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	L	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	N	803	2	32,33,33	0.49	0	45,52,52	0.79	1 (2%)
3	AGS	K	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	I	803	2	32,33,33	0.49	0	45,52,52	0.79	1 (2%)
3	AGS	A	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	J	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	C	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	B	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	D	802	2	32,33,33	0.81	4 (12%)	45,52,52	0.83	1 (2%)
3	AGS	F	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	E	803	2	32,33,33	0.49	0	45,52,52	0.79	1 (2%)
3	AGS	B	803	2	32,33,33	0.50	0	45,52,52	0.79	1 (2%)
3	AGS	C	802	2	32,33,33	0.81	3 (9%)	45,52,52	0.83	1 (2%)
3	AGS	G	802	2	32,33,33	0.80	3 (9%)	45,52,52	0.83	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
3	AGS	H	802	2	-	6/21/38/38	0/3/3/3
3	AGS	G	803	2	-	10/21/38/38	0/3/3/3
3	AGS	A	802	2	-	6/21/38/38	0/3/3/3
3	AGS	H	803	2	-	10/21/38/38	0/3/3/3
3	AGS	E	802	2	-	6/21/38/38	0/3/3/3
3	AGS	J	802	2	-	6/21/38/38	0/3/3/3
3	AGS	M	802	2	-	6/21/38/38	0/3/3/3
3	AGS	M	803	2	-	10/21/38/38	0/3/3/3
3	AGS	L	802	2	-	6/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	803	2	-	10/21/38/38	0/3/3/3
3	AGS	F	803	2	-	10/21/38/38	0/3/3/3
3	AGS	N	802	2	-	6/21/38/38	0/3/3/3
3	AGS	I	802	2	-	6/21/38/38	0/3/3/3
3	AGS	K	802	2	-	6/21/38/38	0/3/3/3
3	AGS	L	803	2	-	10/21/38/38	0/3/3/3
3	AGS	N	803	2	-	10/21/38/38	0/3/3/3
3	AGS	K	803	2	-	10/21/38/38	0/3/3/3
3	AGS	I	803	2	-	10/21/38/38	0/3/3/3
3	AGS	A	803	2	-	10/21/38/38	0/3/3/3
3	AGS	J	803	2	-	10/21/38/38	0/3/3/3
3	AGS	C	803	2	-	10/21/38/38	0/3/3/3
3	AGS	B	802	2	-	6/21/38/38	0/3/3/3
3	AGS	D	802	2	-	6/21/38/38	0/3/3/3
3	AGS	F	802	2	-	6/21/38/38	0/3/3/3
3	AGS	E	803	2	-	10/21/38/38	0/3/3/3
3	AGS	B	803	2	-	10/21/38/38	0/3/3/3
3	AGS	C	802	2	-	6/21/38/38	0/3/3/3
3	AGS	G	802	2	-	6/21/38/38	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	802	AGS	PB-O3B	-2.32	1.57	1.59
3	D	802	AGS	PB-O3B	-2.31	1.57	1.59
3	E	802	AGS	PB-O3B	-2.31	1.57	1.59
3	F	802	AGS	PB-O3B	-2.29	1.57	1.59
3	G	802	AGS	PB-O3B	-2.29	1.57	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	802	AGS	PB-O3B-PG	-4.92	115.16	133.17
3	N	802	AGS	PB-O3B-PG	-4.91	115.19	133.17
3	A	802	AGS	PB-O3B-PG	-4.91	115.19	133.17
3	H	802	AGS	PB-O3B-PG	-4.91	115.20	133.17
3	E	802	AGS	PB-O3B-PG	-4.91	115.20	133.17

There are no chirality outliers.

5 of 224 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	AGS	PB-O3B-PG-O2G
3	A	802	AGS	C5'-O5'-PA-O2A
3	A	802	AGS	C5'-O5'-PA-O3A
3	A	803	AGS	PB-O3B-PG-O2G
3	A	803	AGS	PB-O3B-PG-O3G

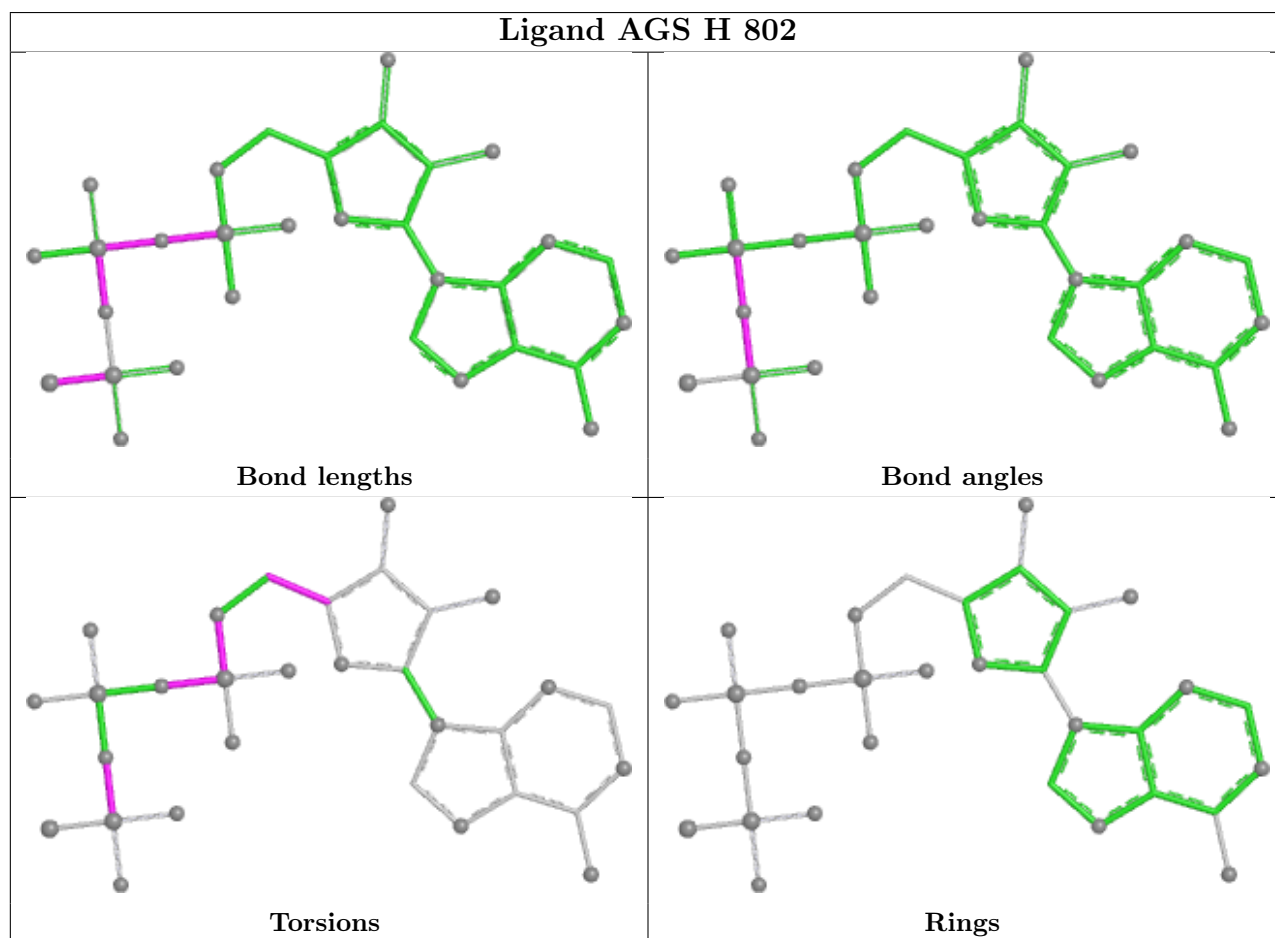
There are no ring outliers.

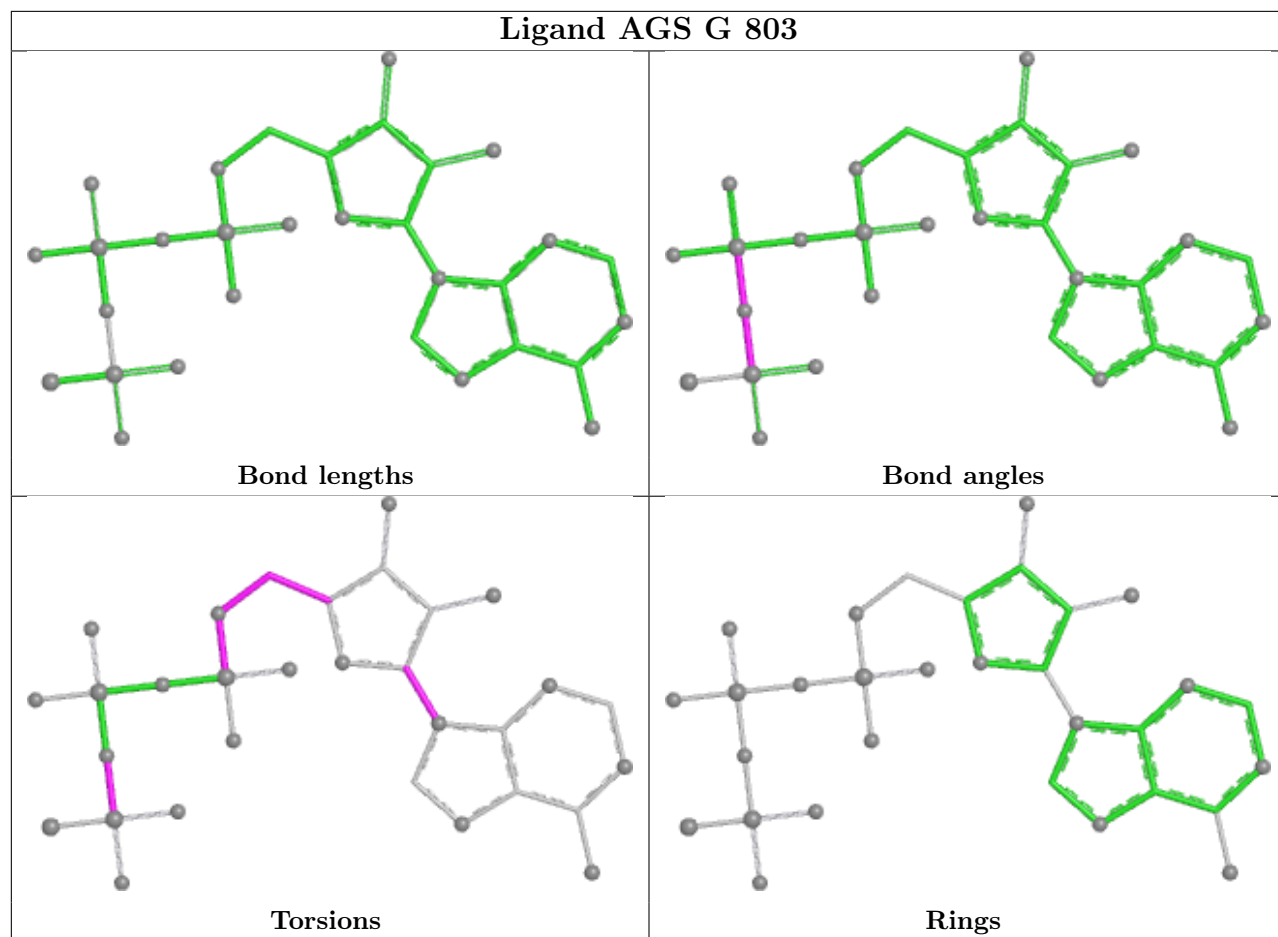
28 monomers are involved in 88 short contacts:

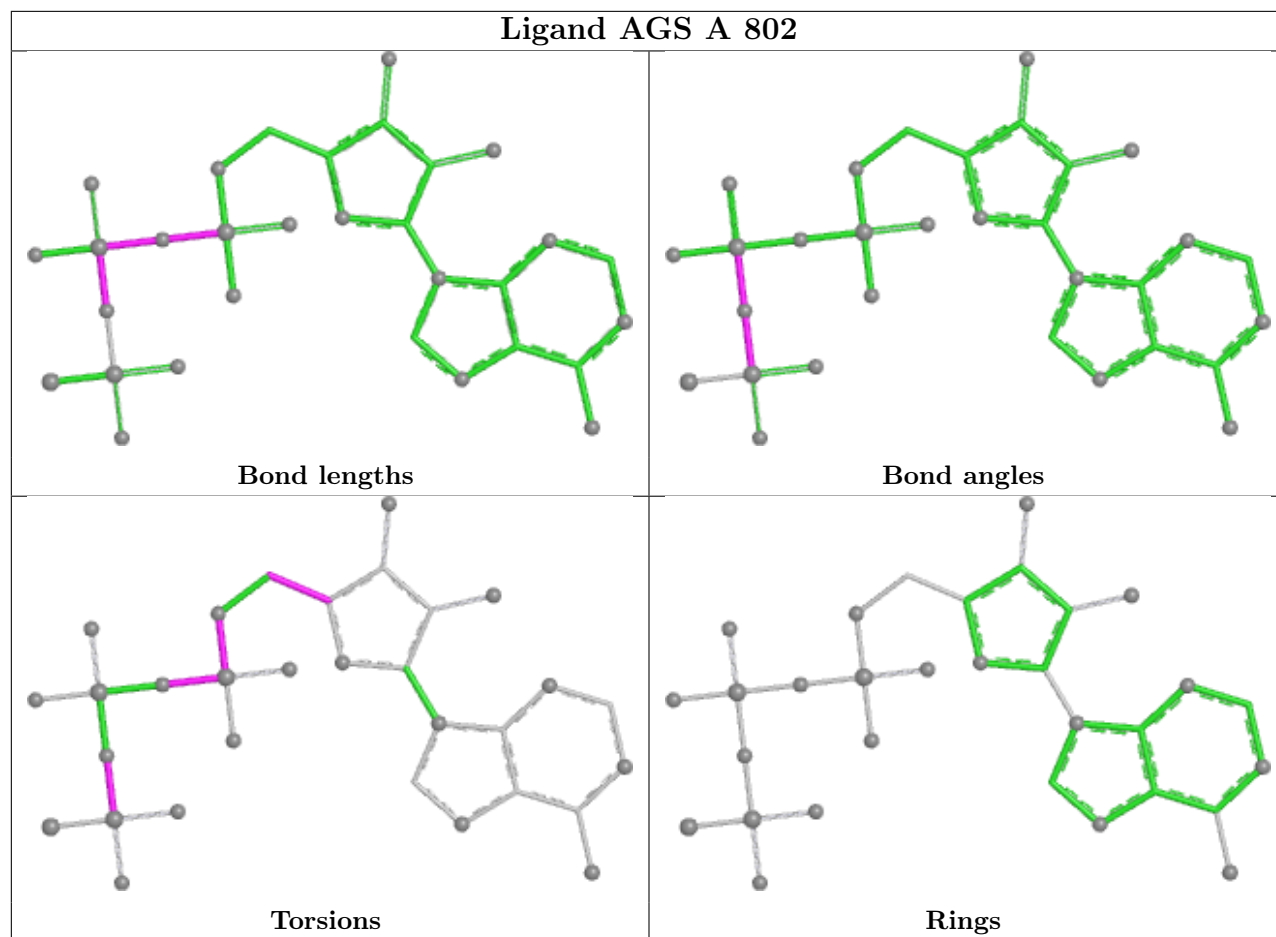
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	802	AGS	3	0
3	G	803	AGS	3	0
3	A	802	AGS	3	0
3	H	803	AGS	3	0
3	E	802	AGS	3	0
3	J	802	AGS	3	0
3	M	802	AGS	3	0
3	M	803	AGS	3	0
3	L	802	AGS	4	0
3	D	803	AGS	3	0
3	F	803	AGS	3	0
3	N	802	AGS	3	0
3	I	802	AGS	3	0
3	K	802	AGS	3	0
3	L	803	AGS	3	0
3	N	803	AGS	3	0
3	K	803	AGS	4	0
3	I	803	AGS	3	0
3	A	803	AGS	3	0
3	J	803	AGS	3	0
3	C	803	AGS	3	0
3	B	802	AGS	3	0
3	D	802	AGS	4	0
3	F	802	AGS	3	0
3	E	803	AGS	3	0
3	B	803	AGS	4	0
3	C	802	AGS	3	0
3	G	802	AGS	3	0

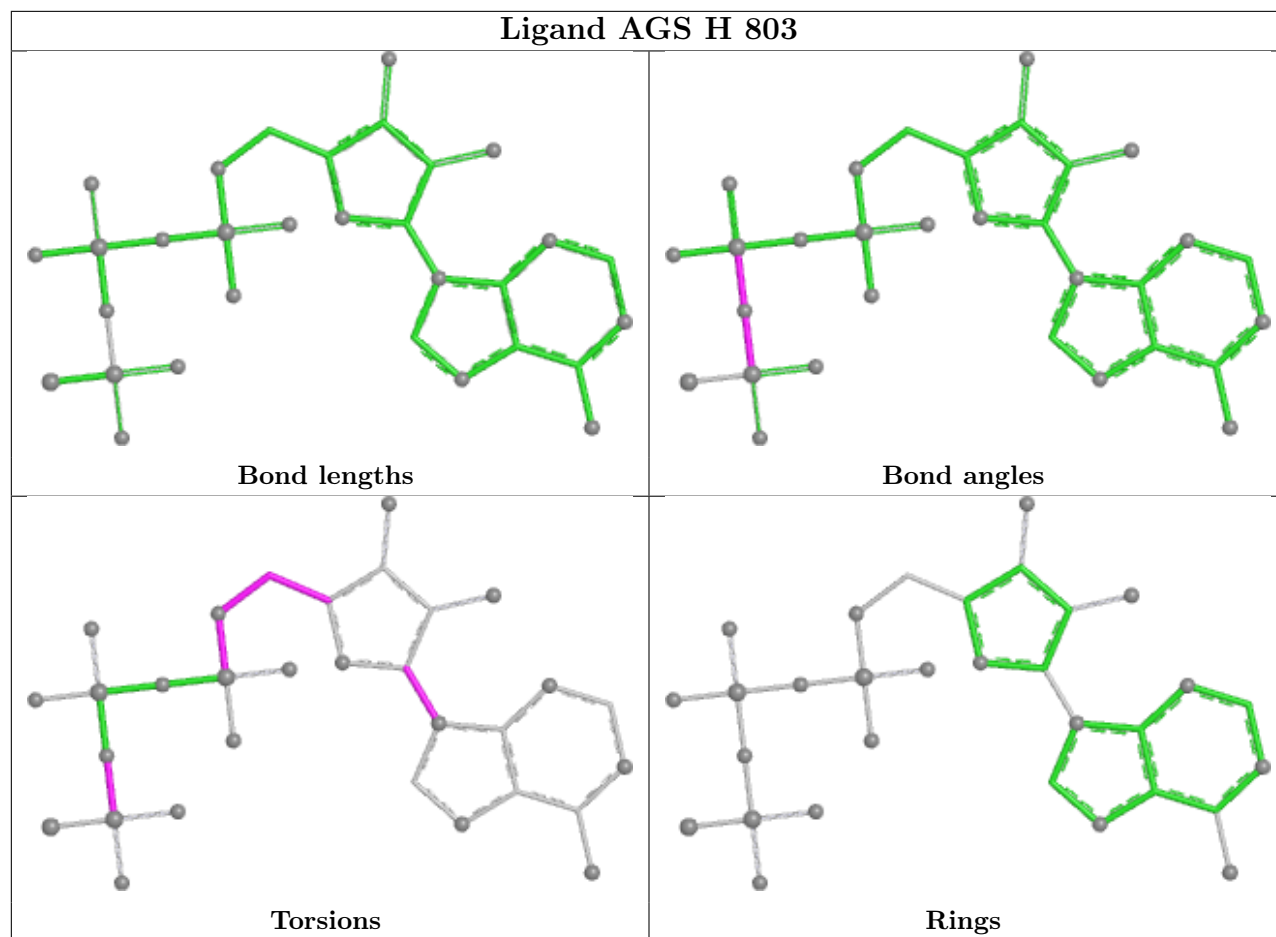
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

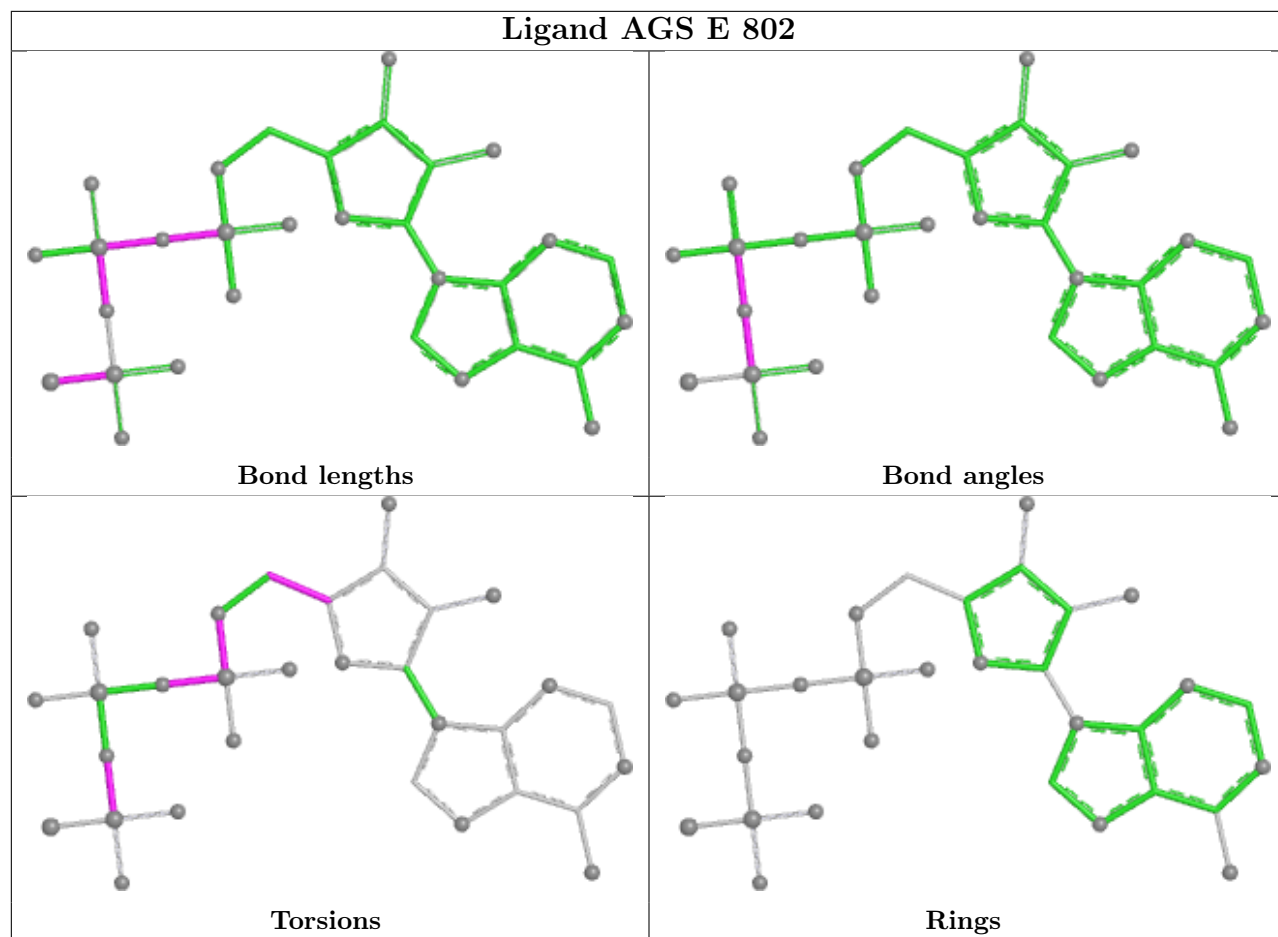
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

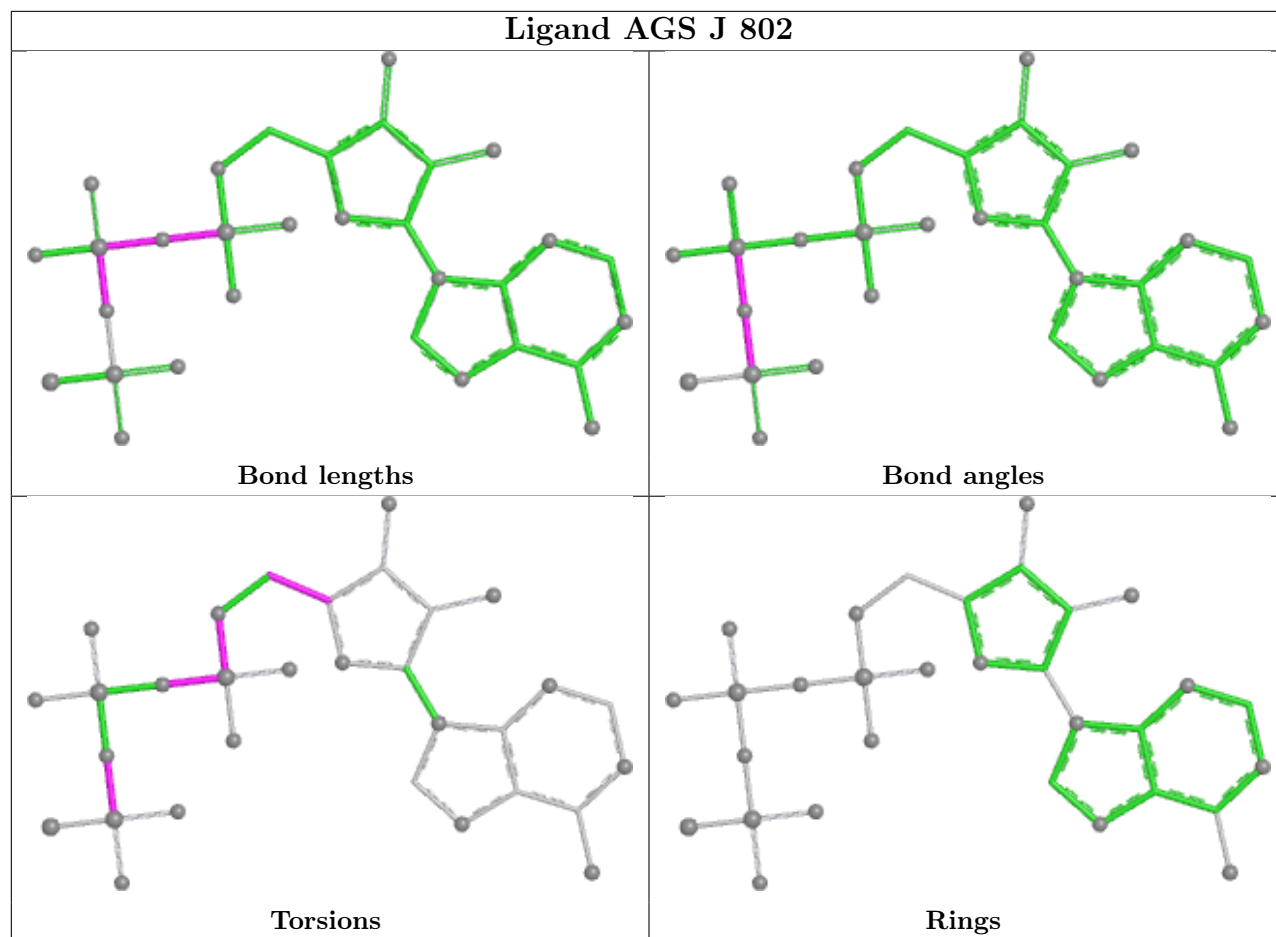


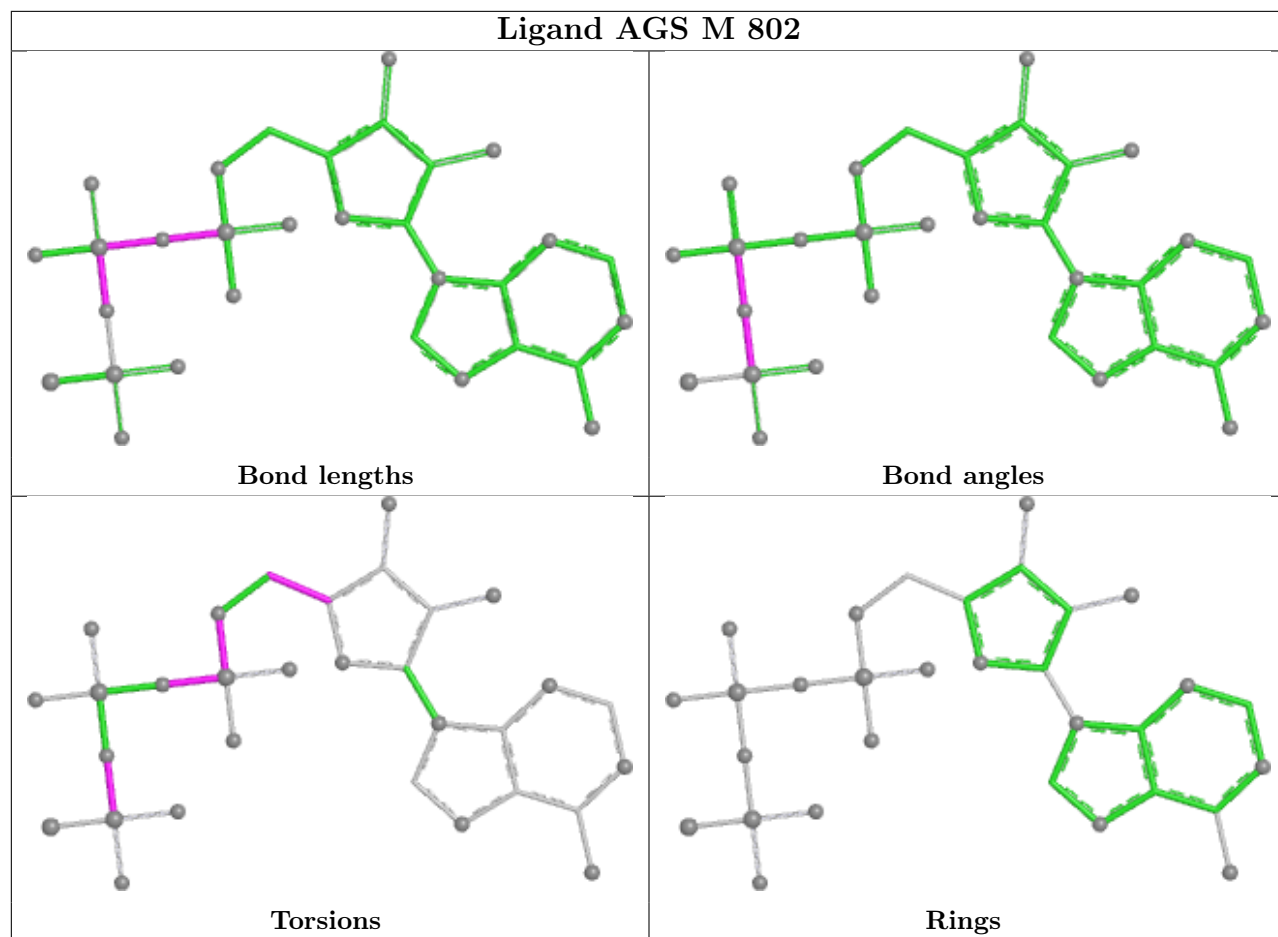


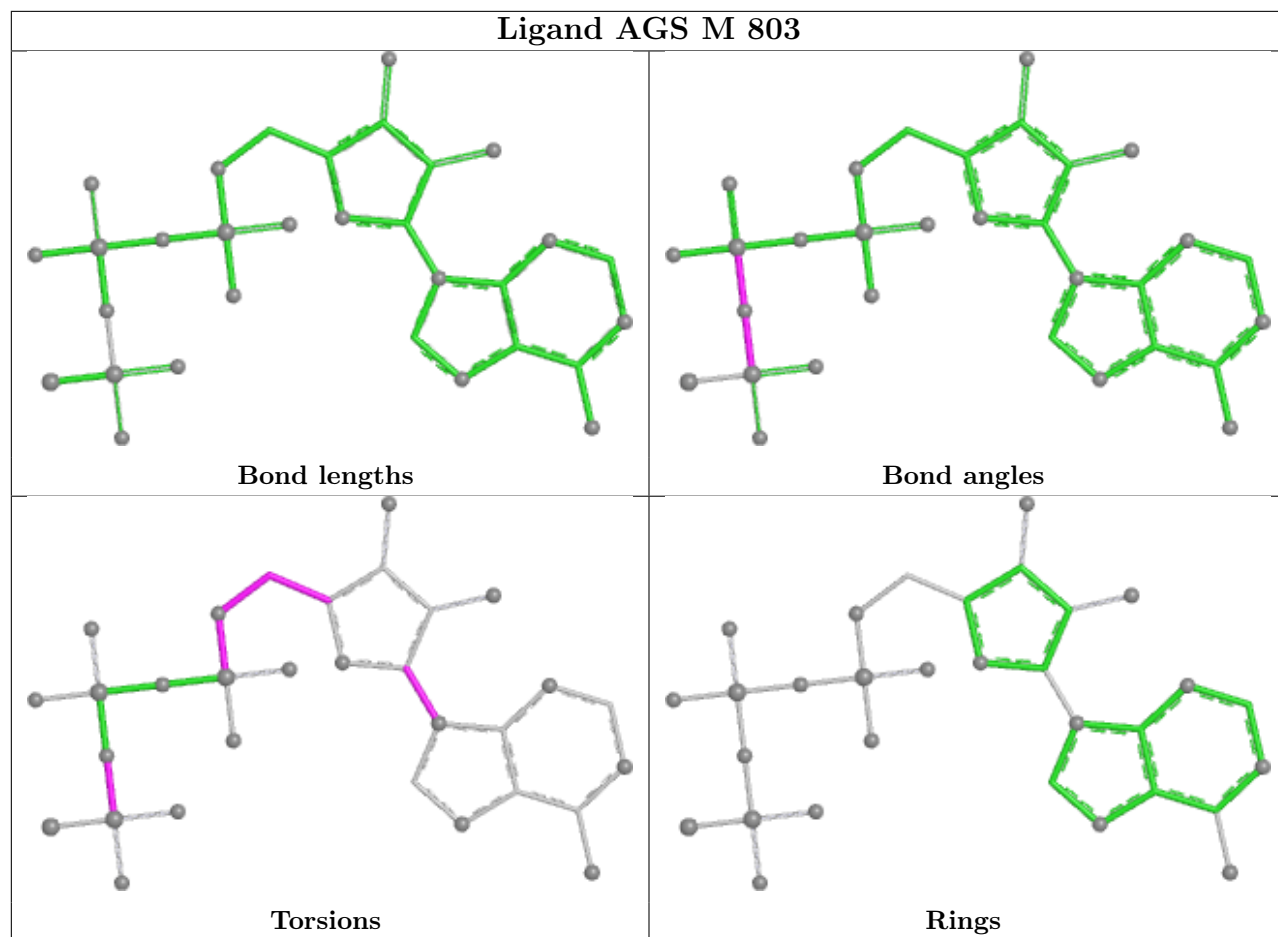


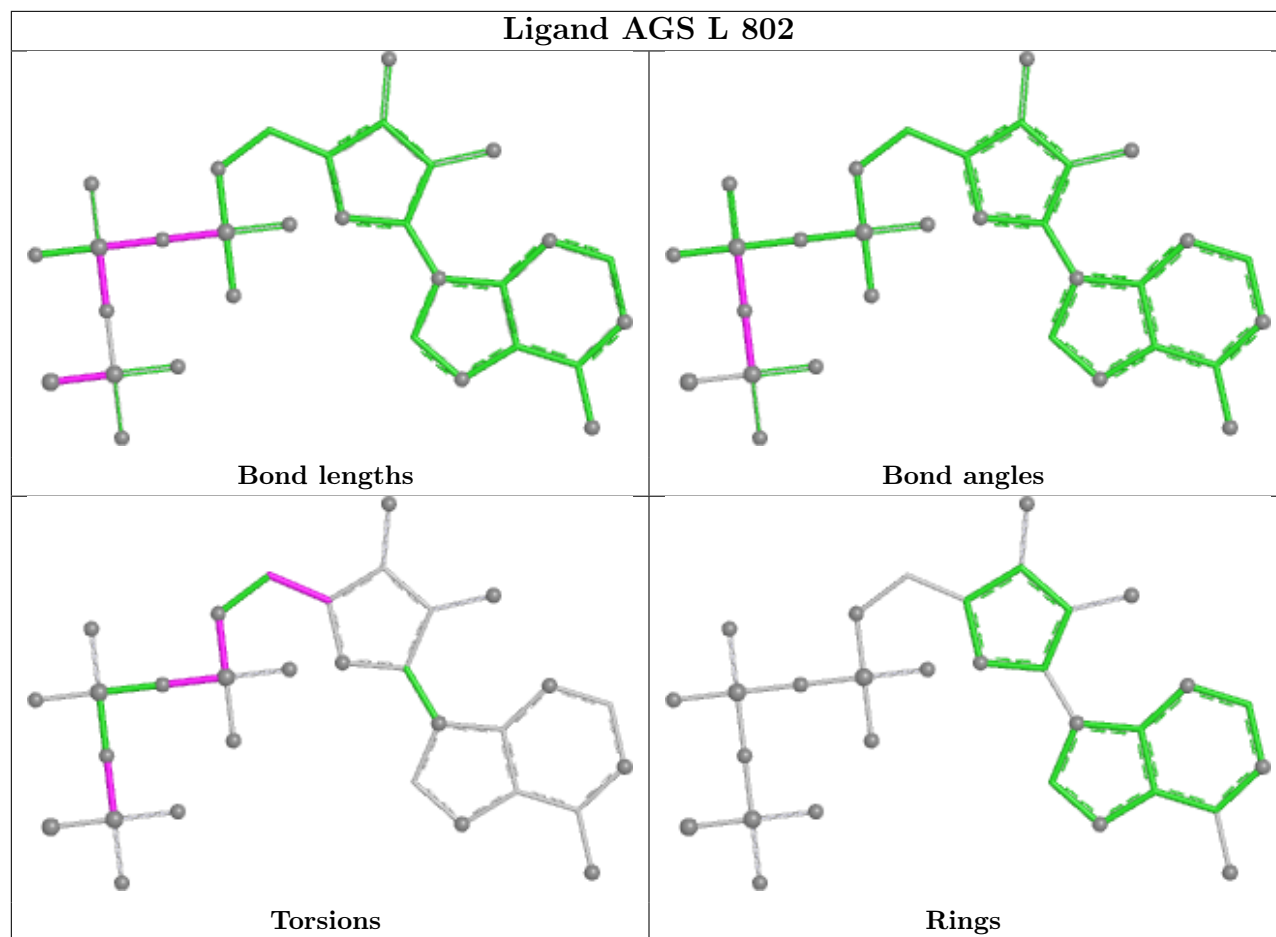


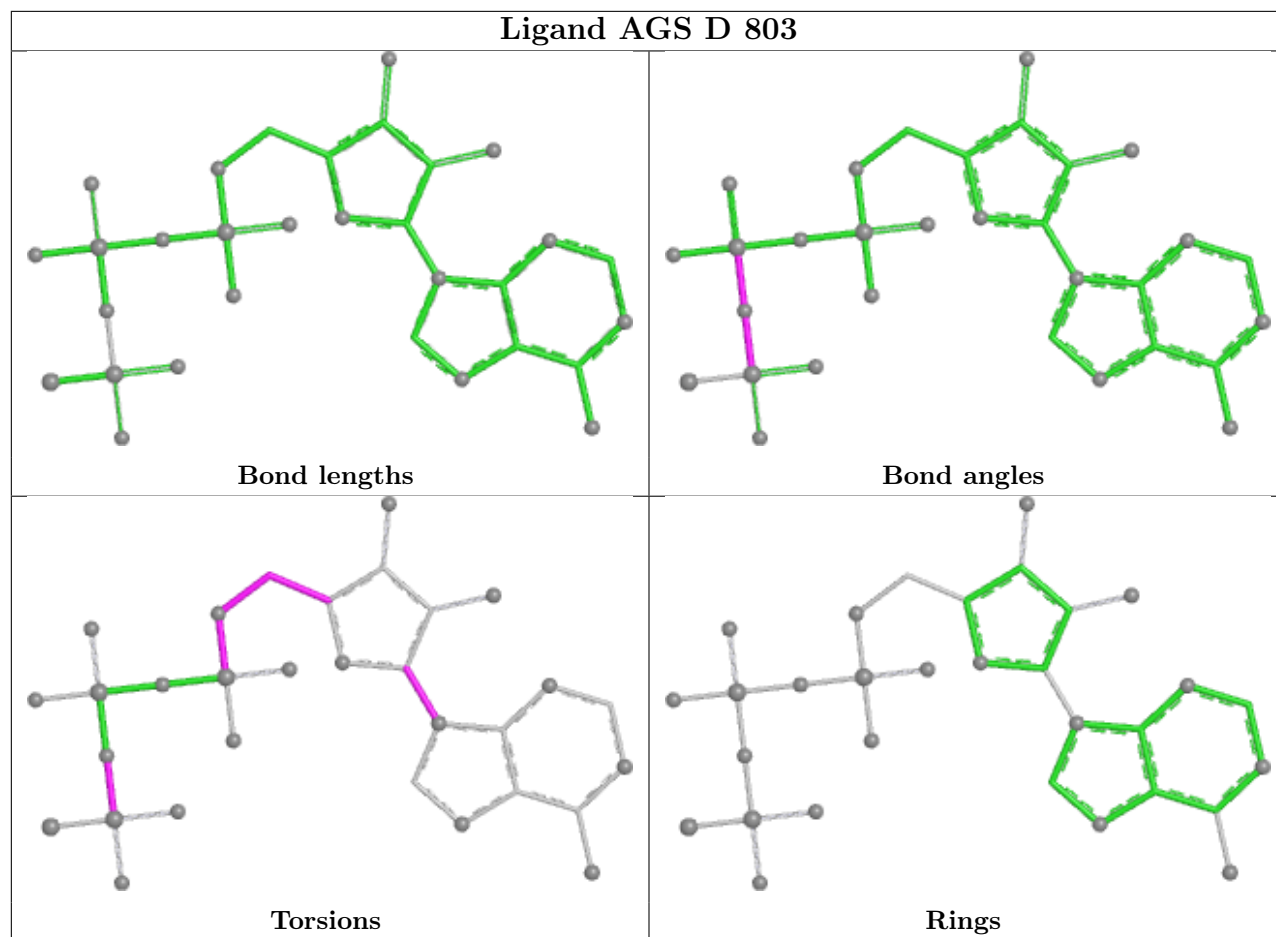


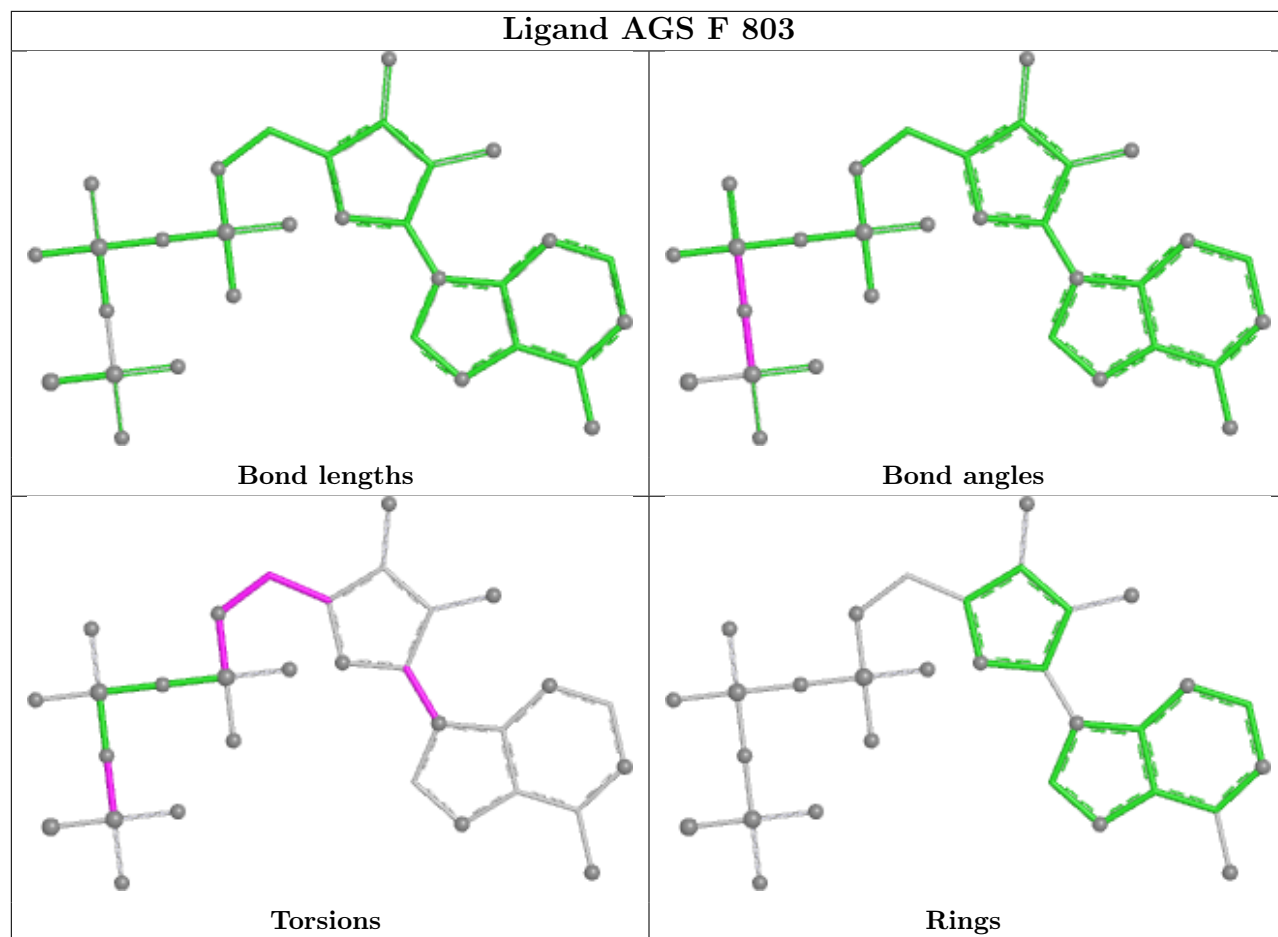


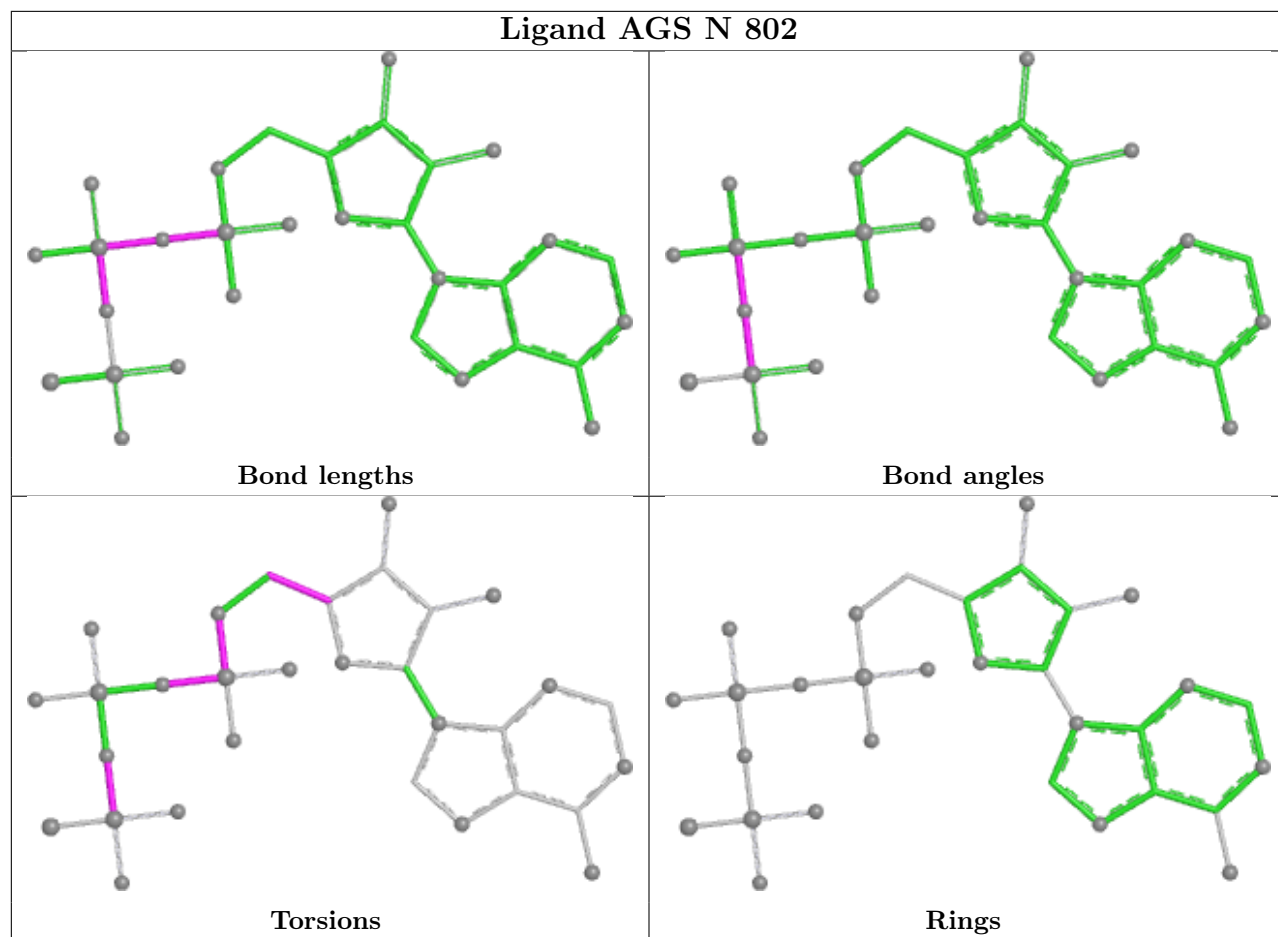


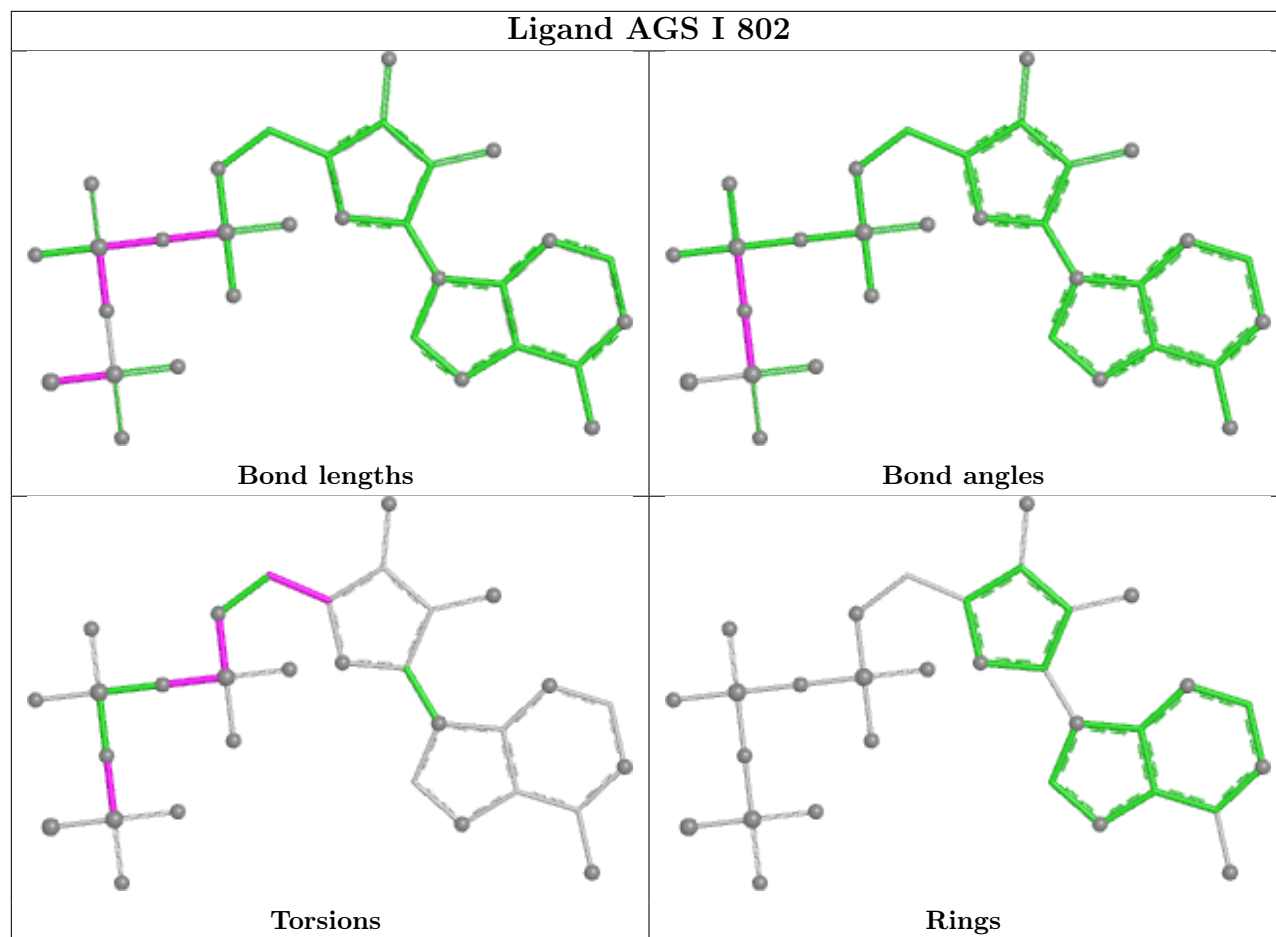


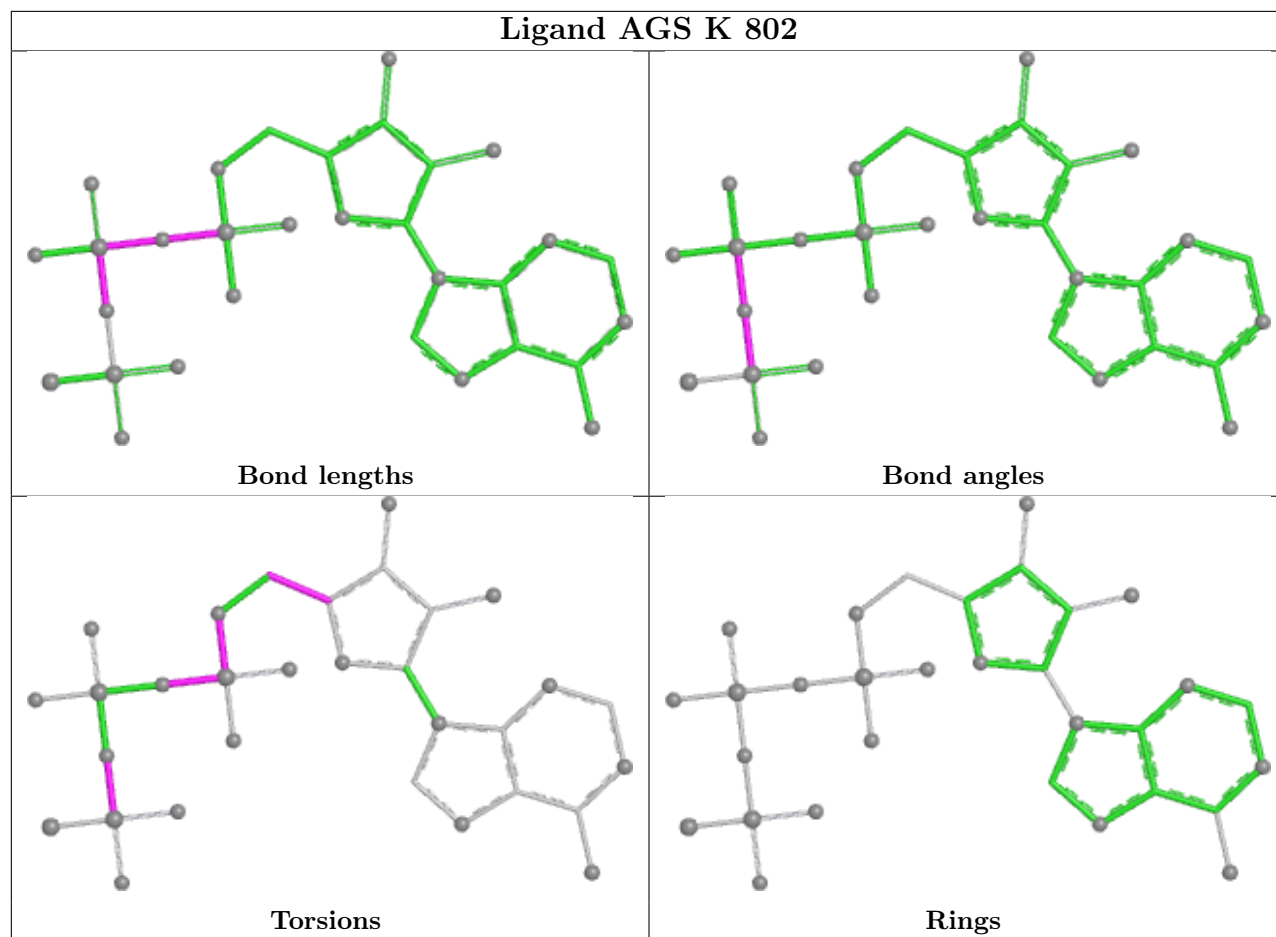


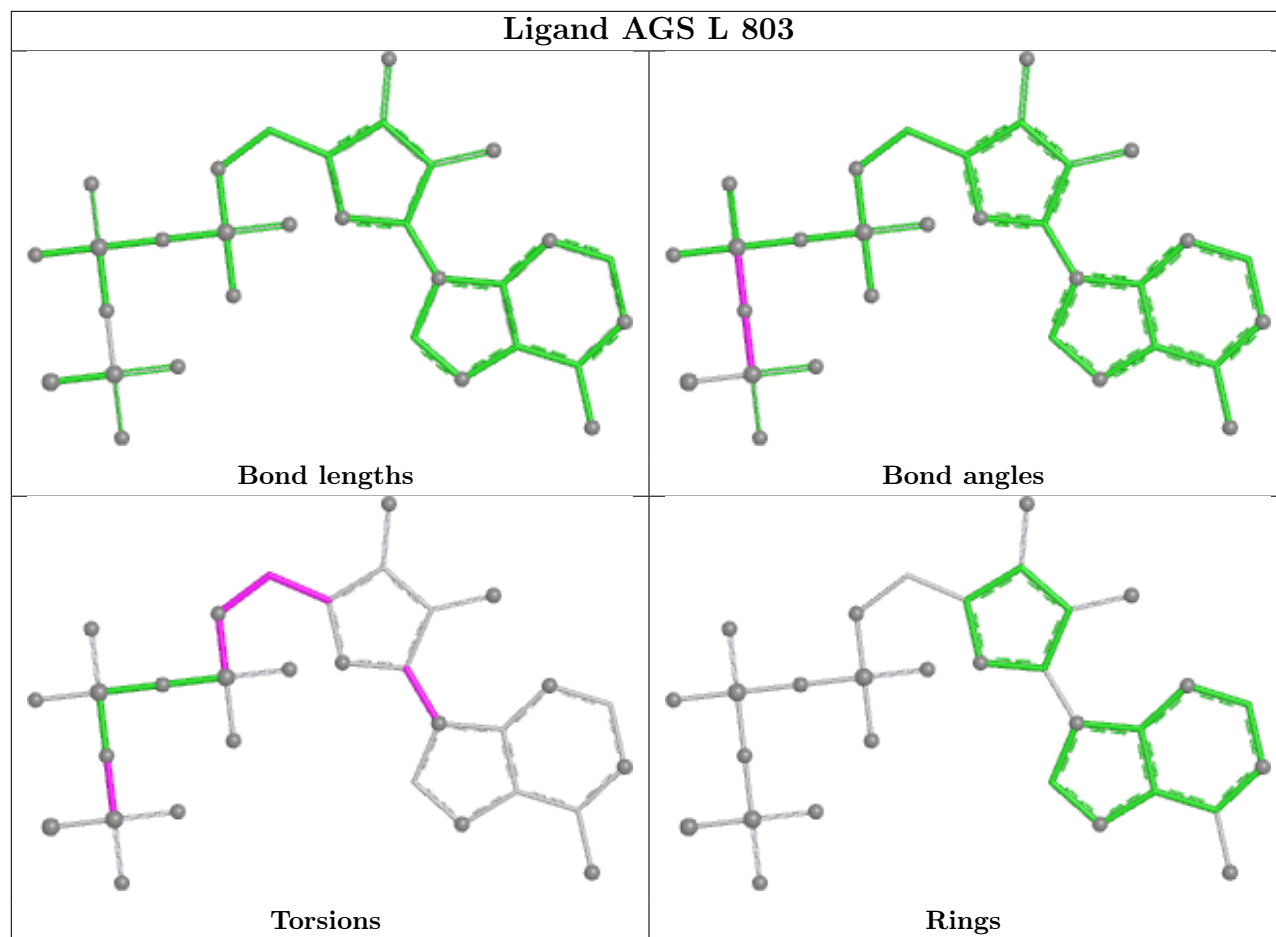


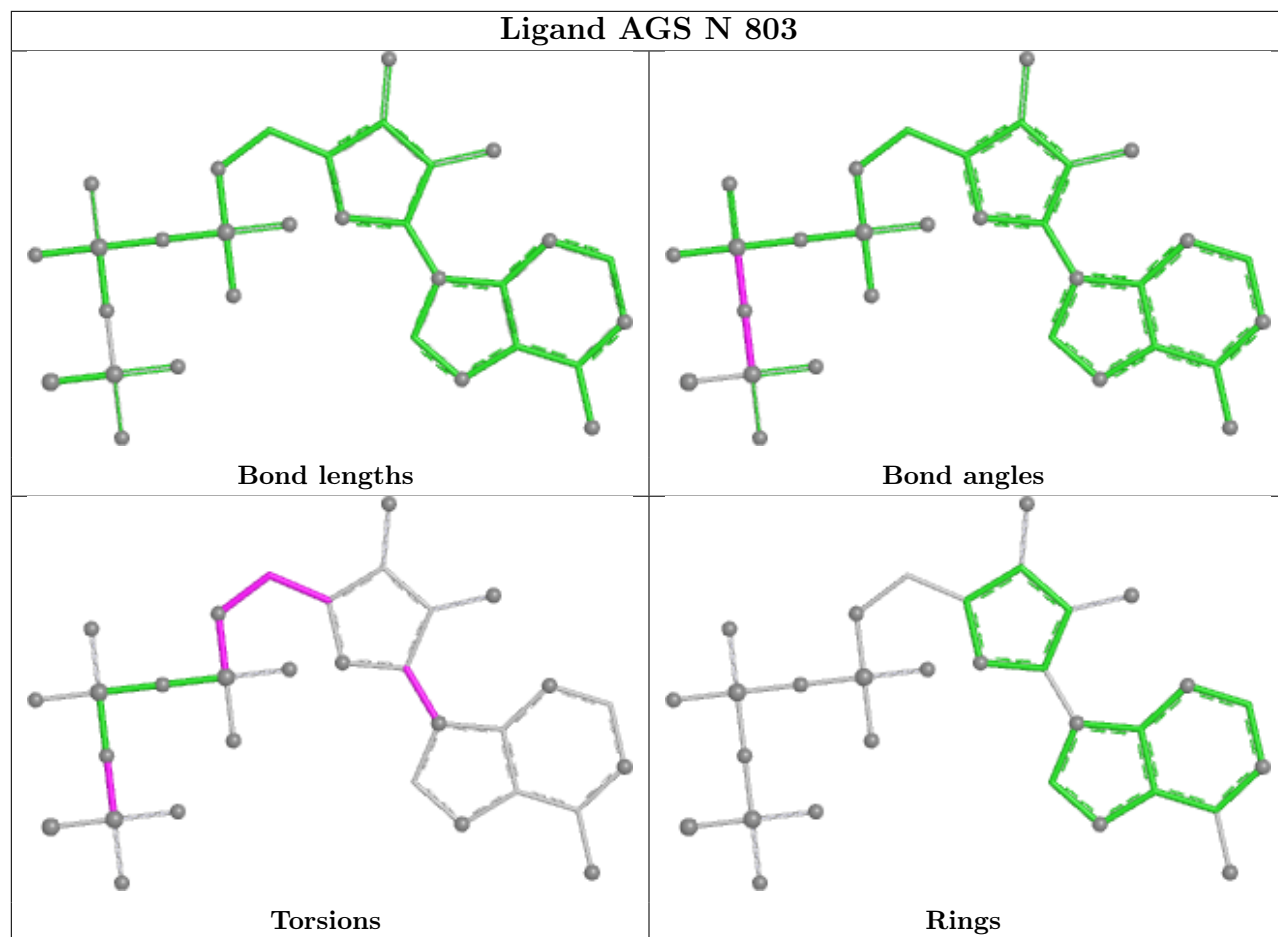


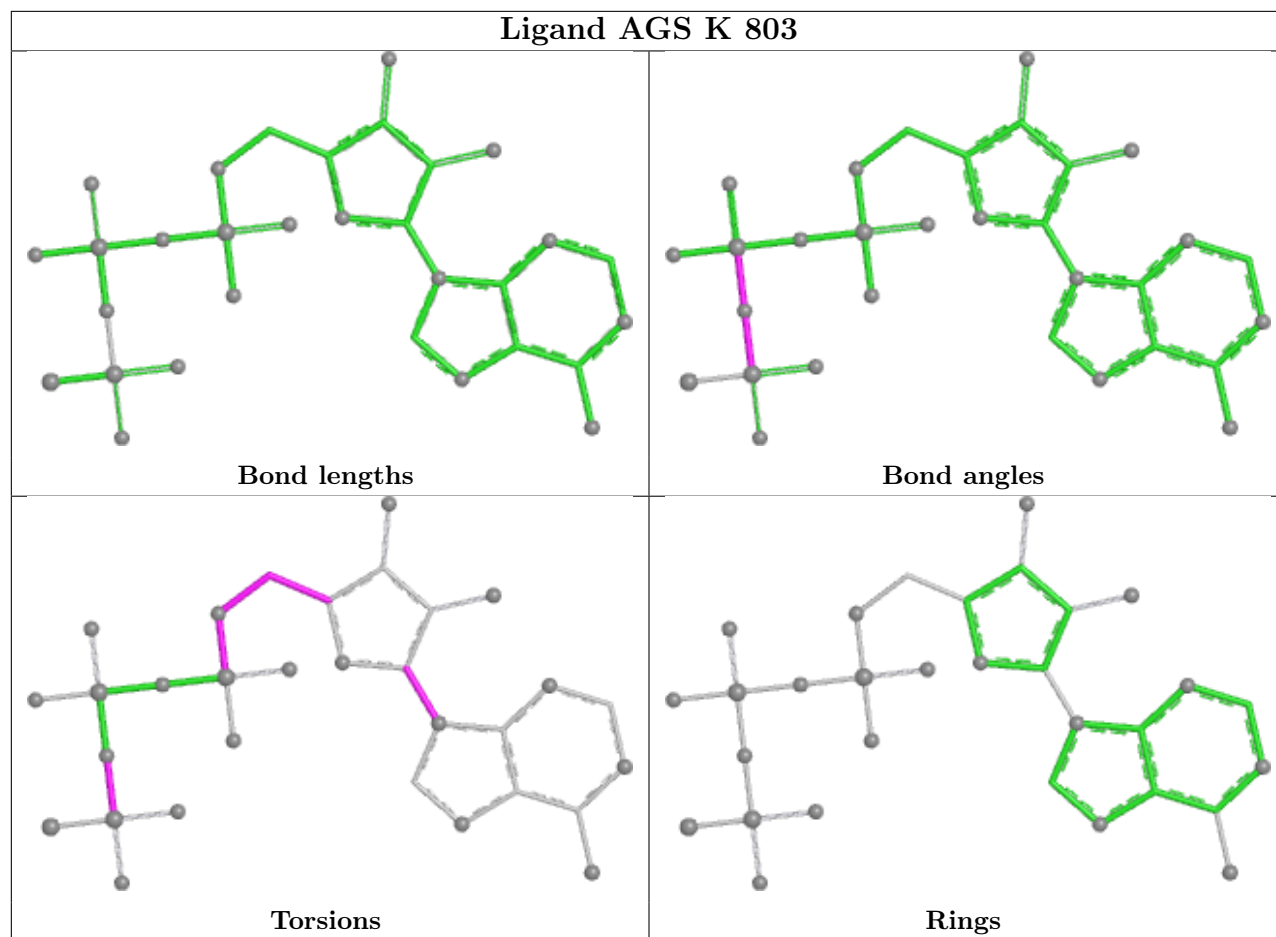


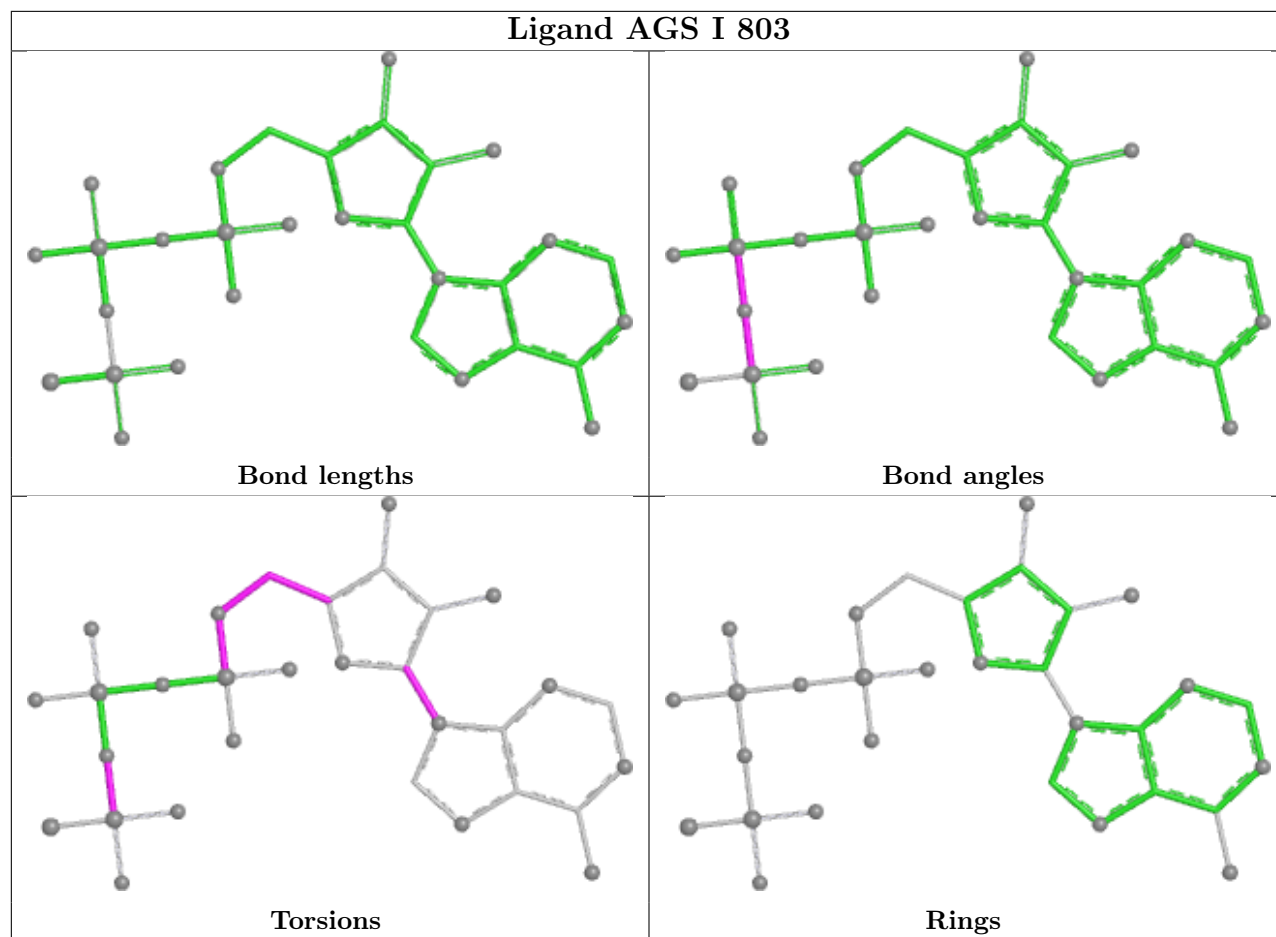


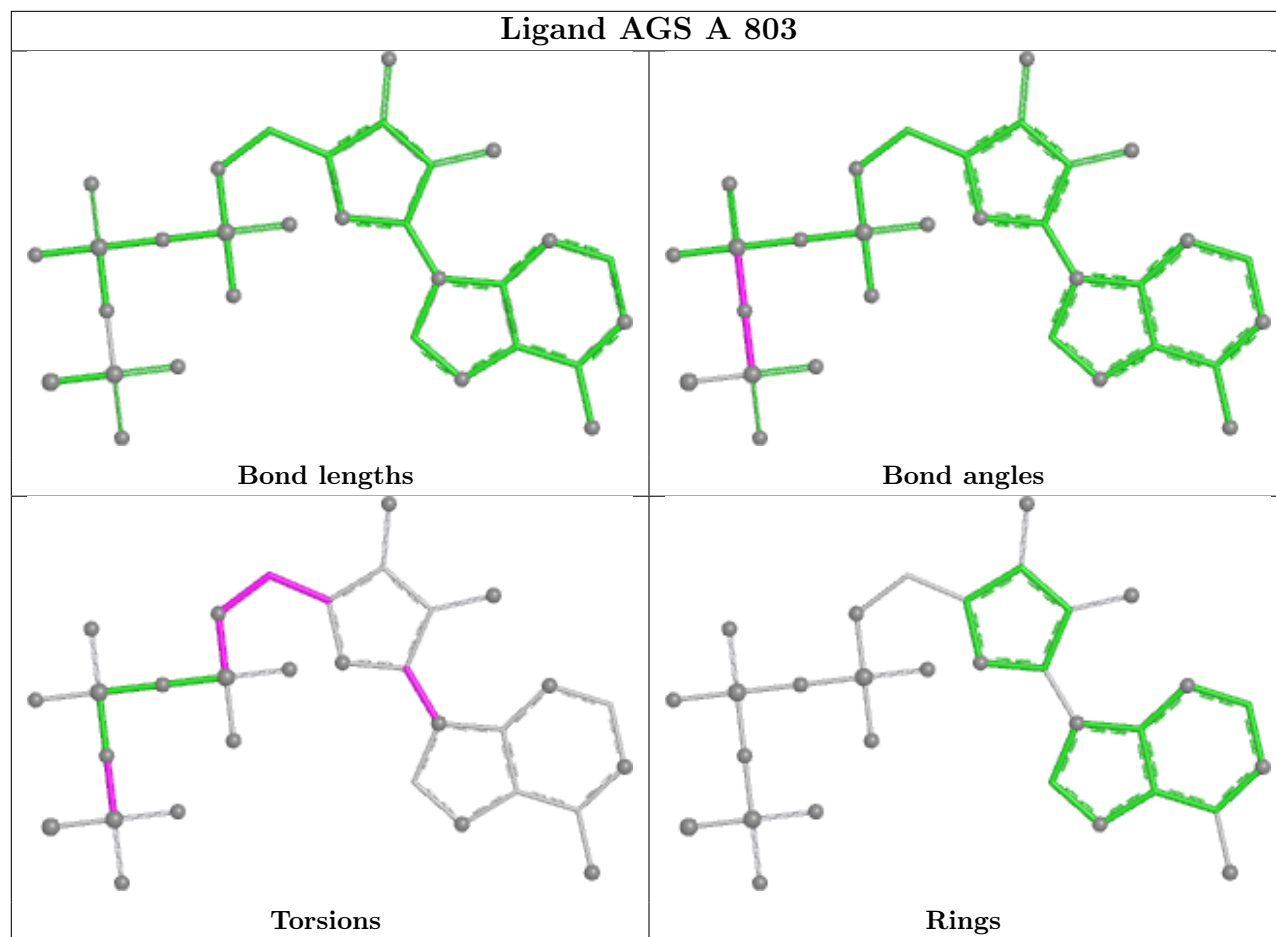


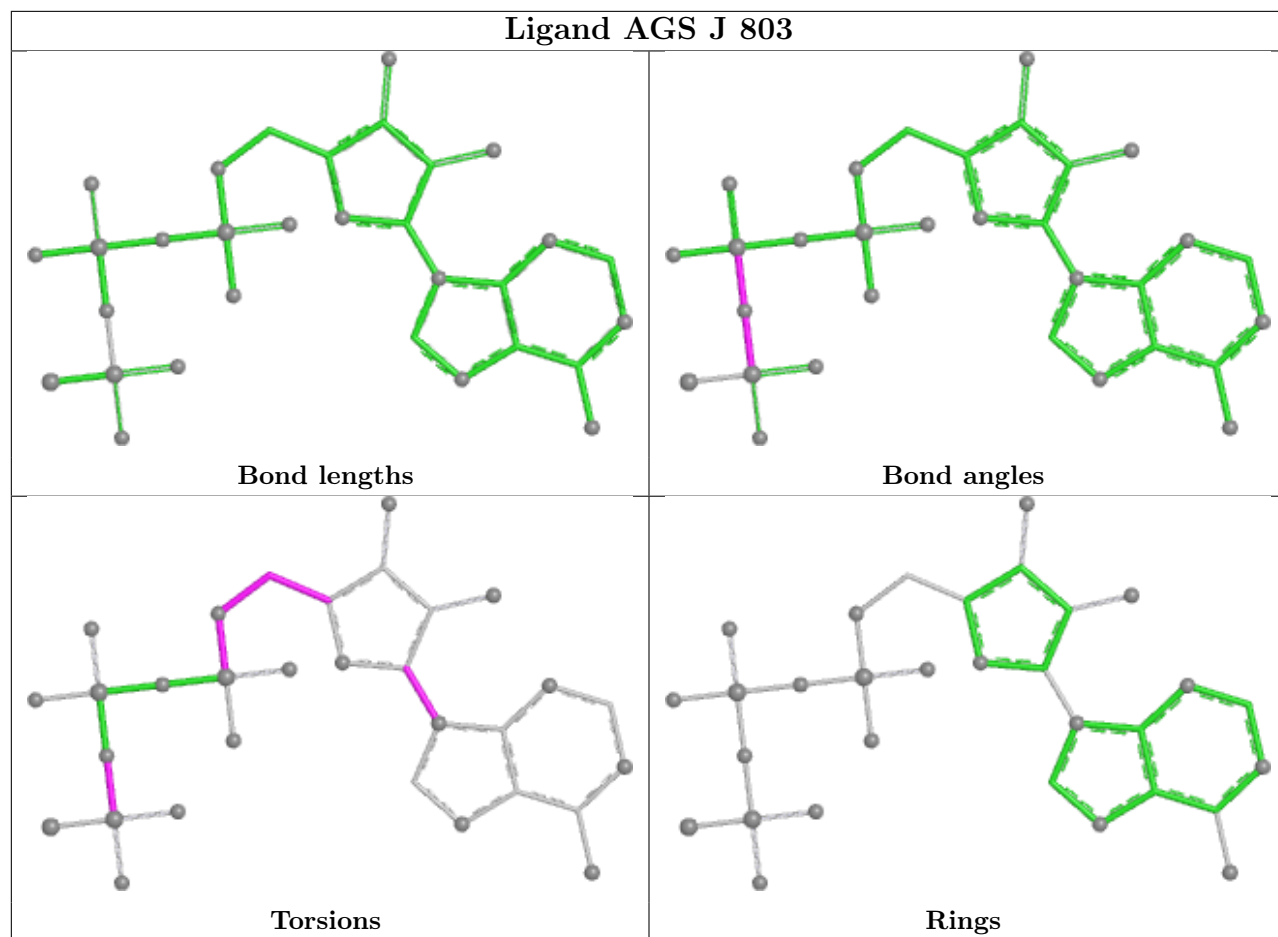


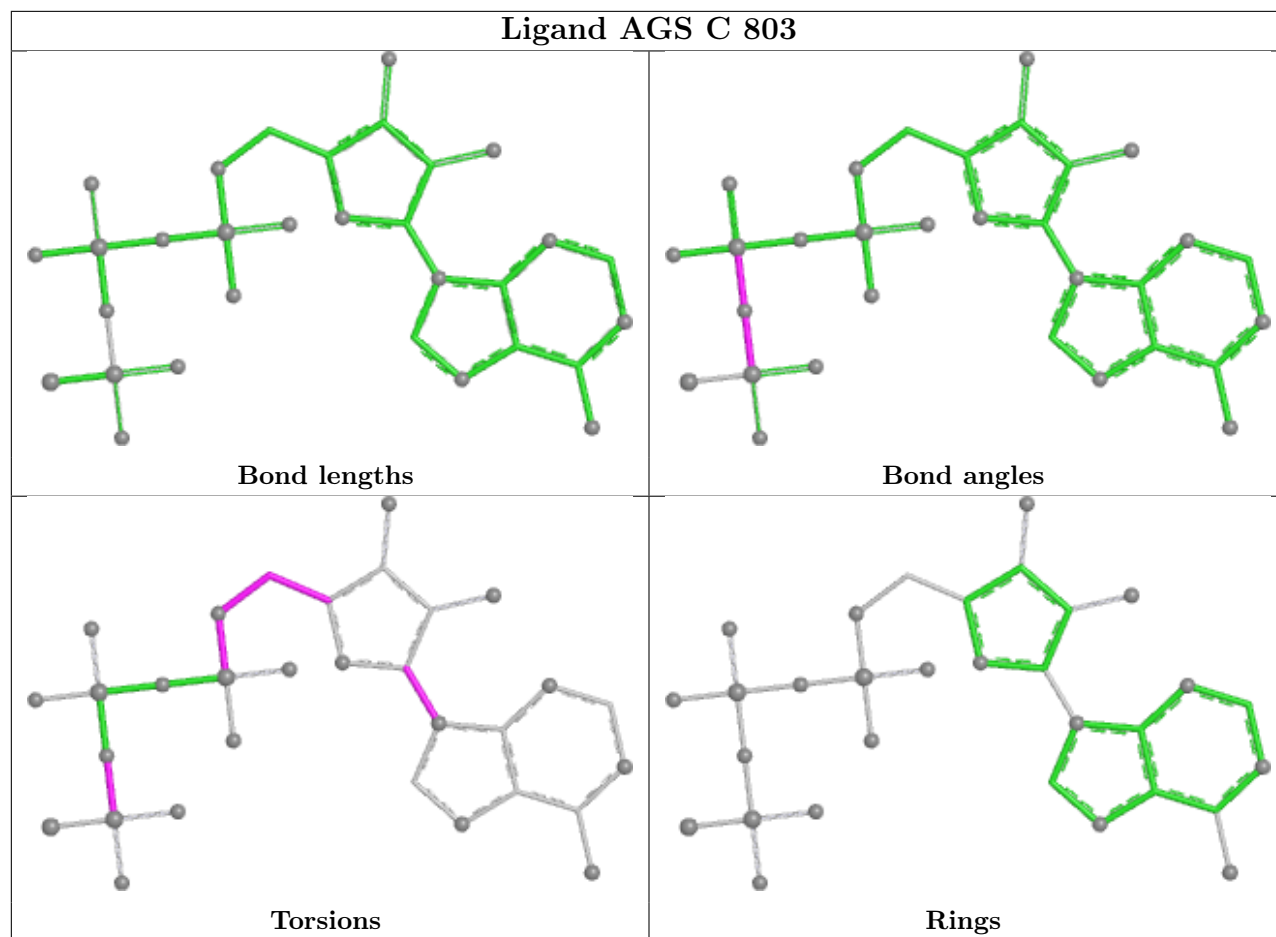


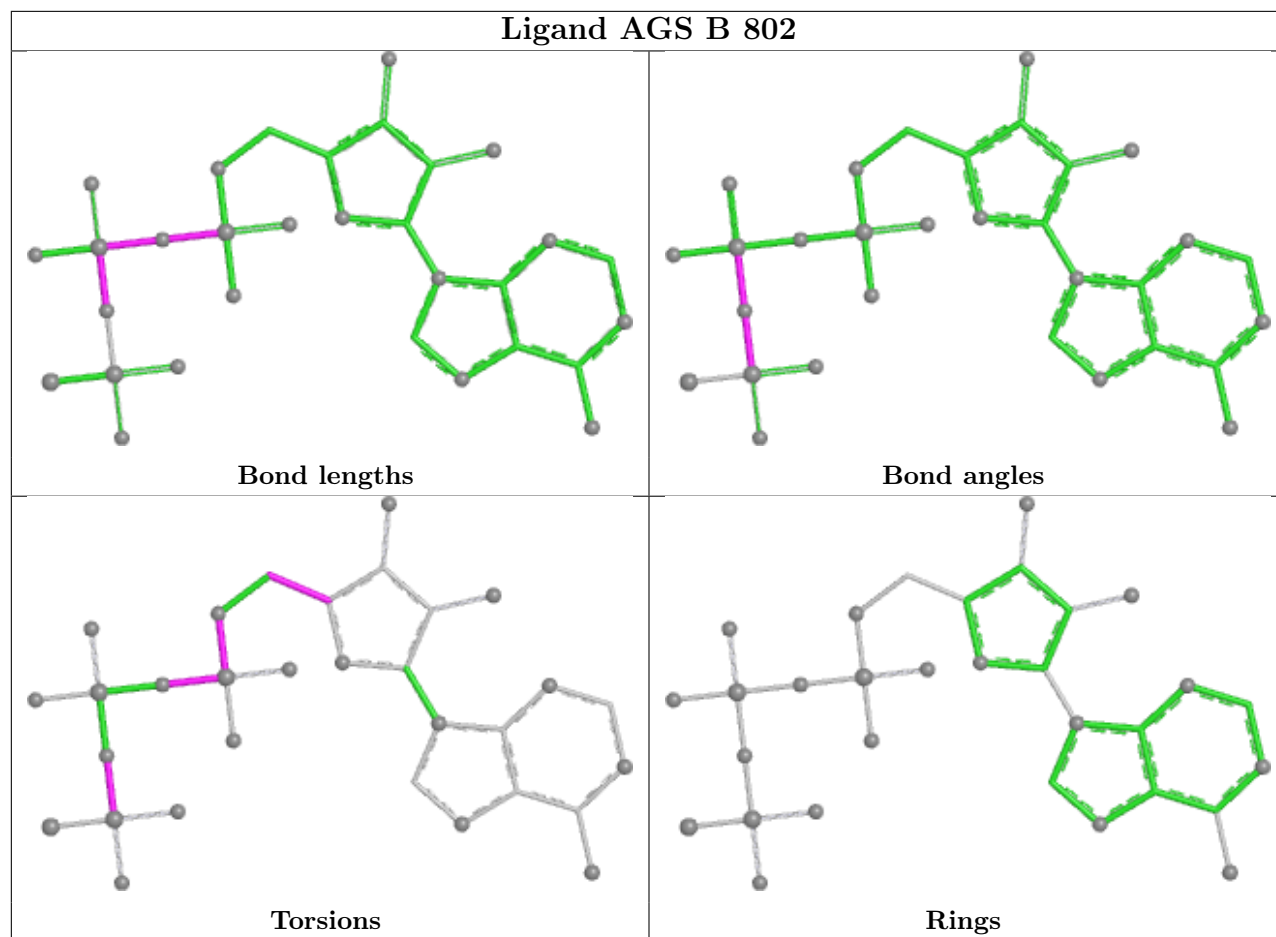


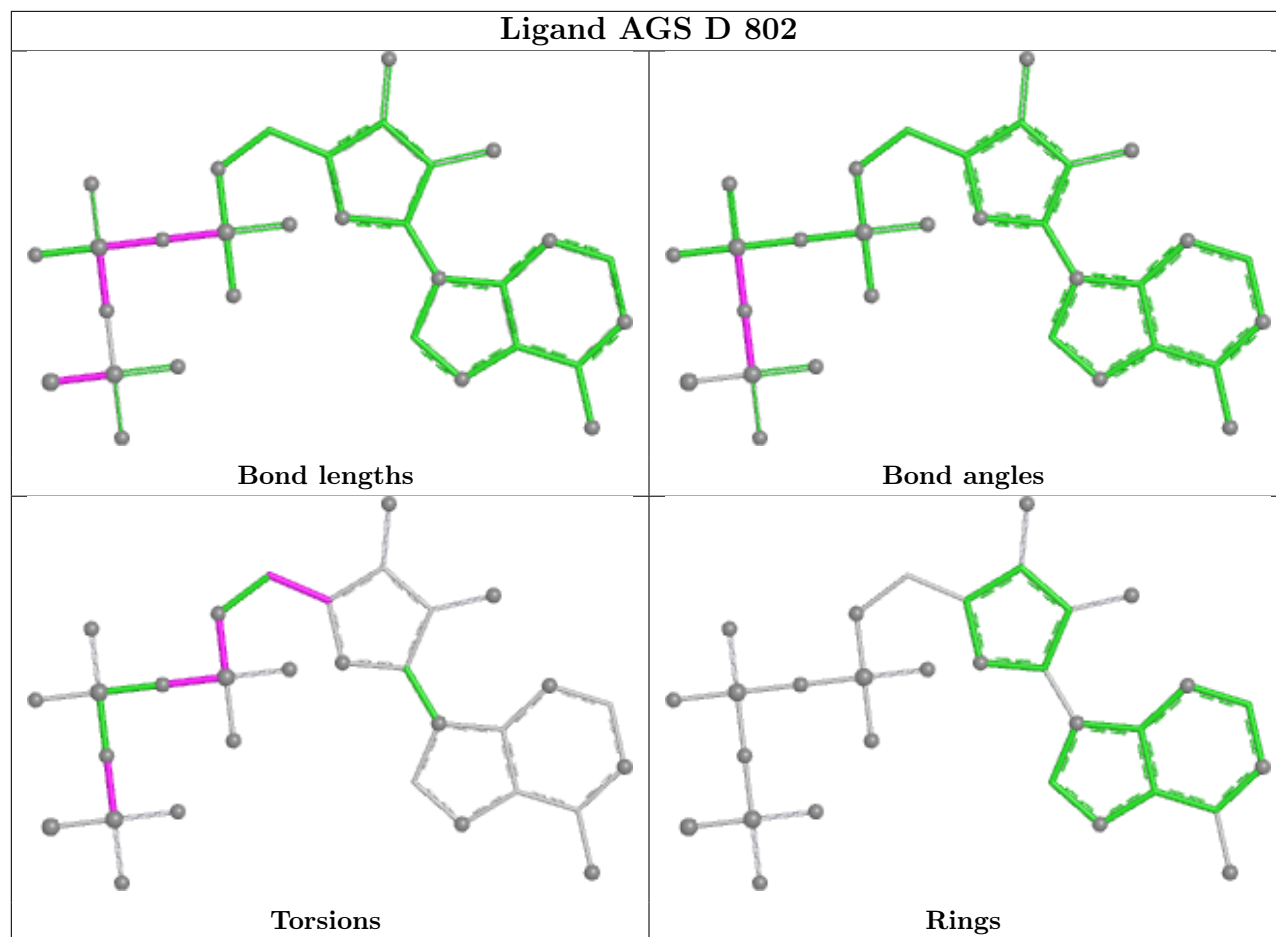


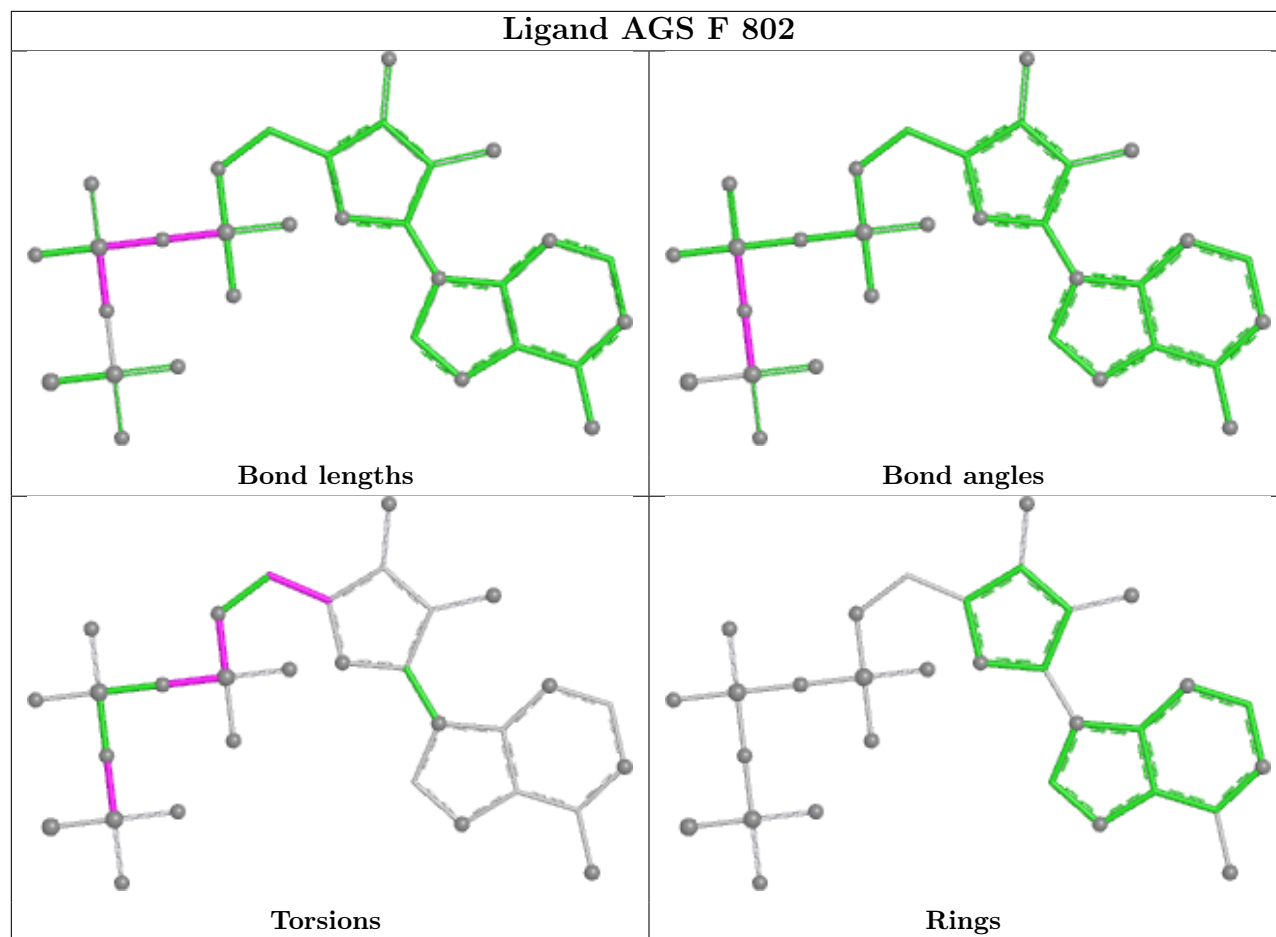


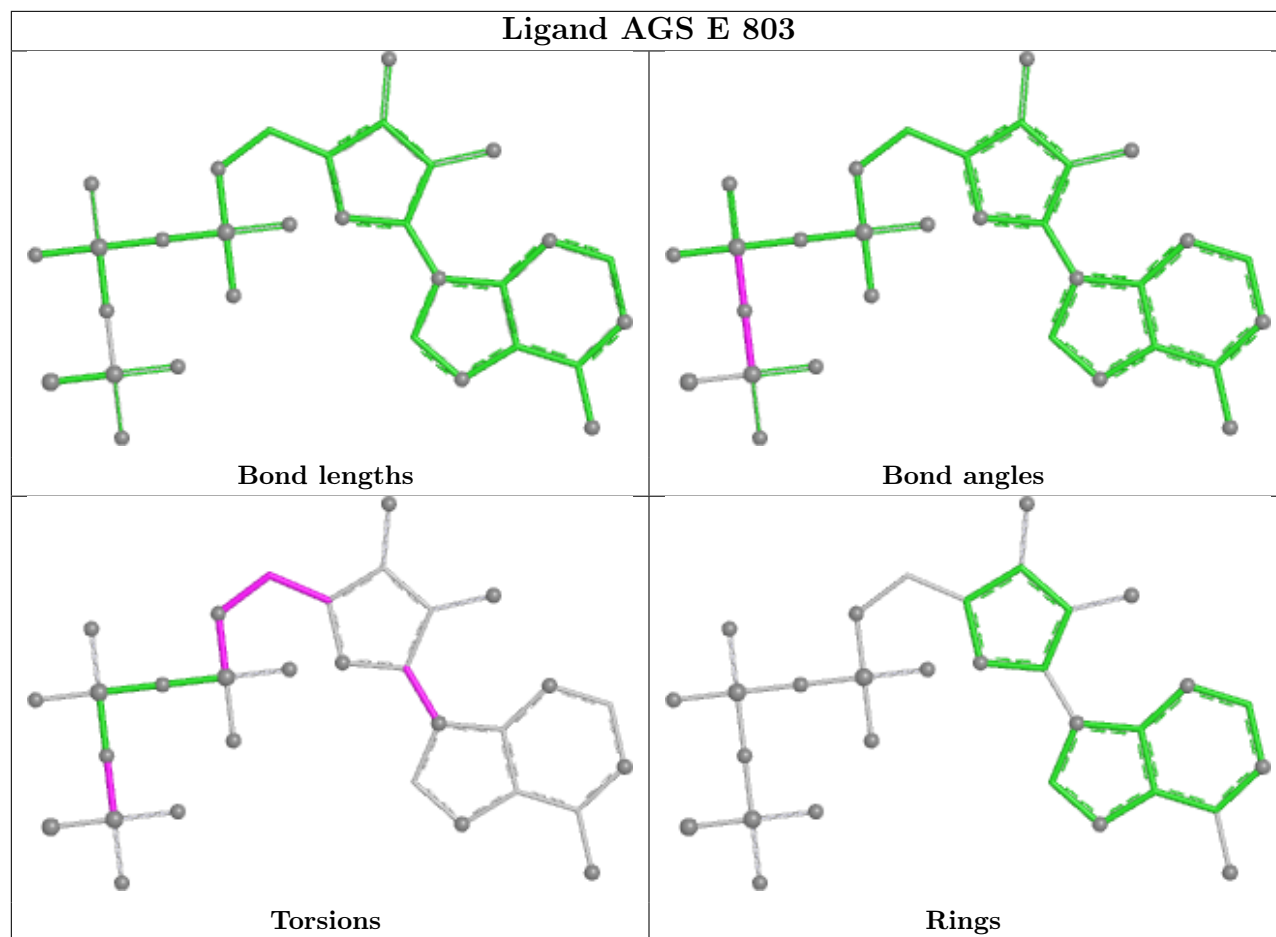


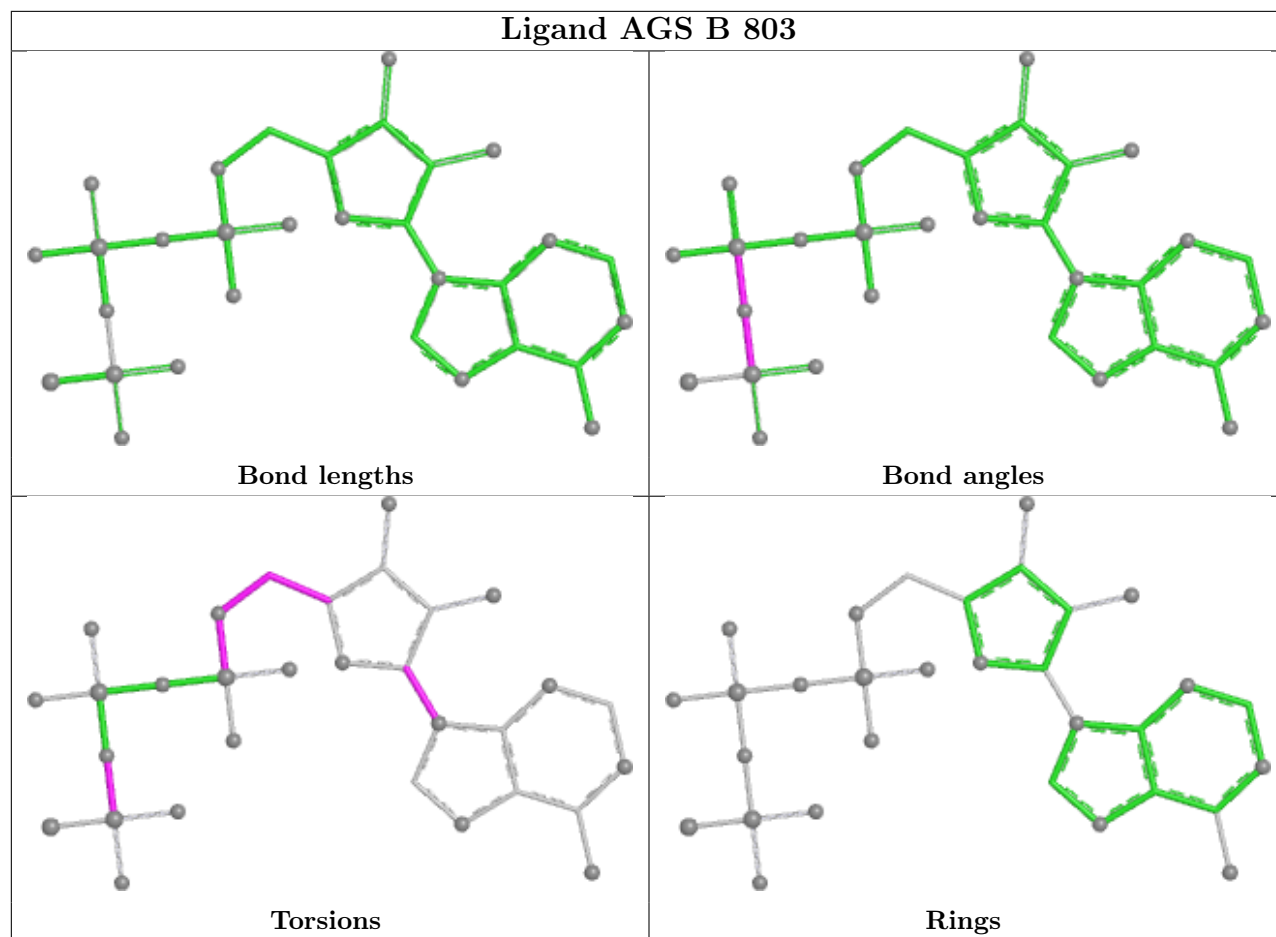


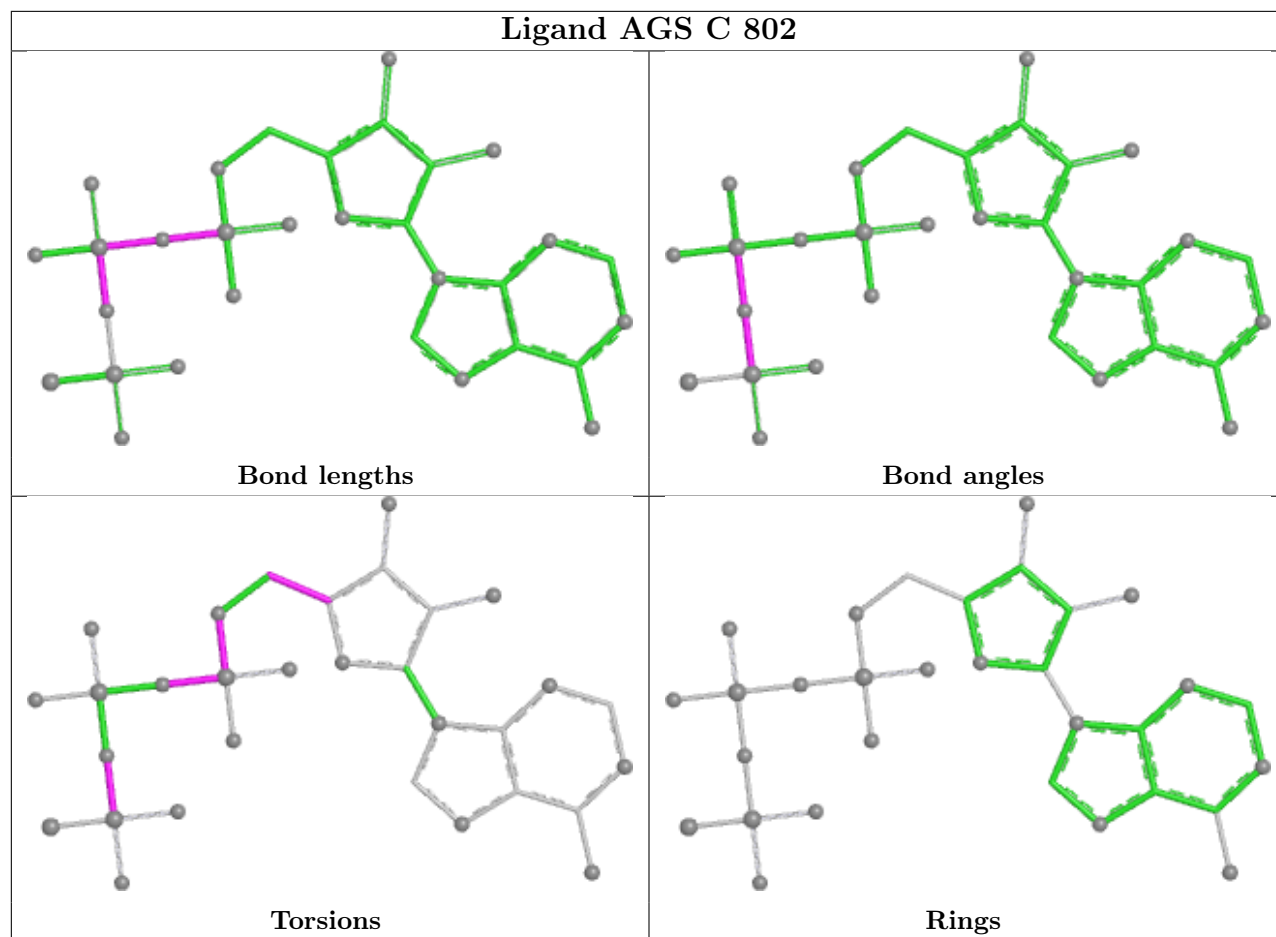


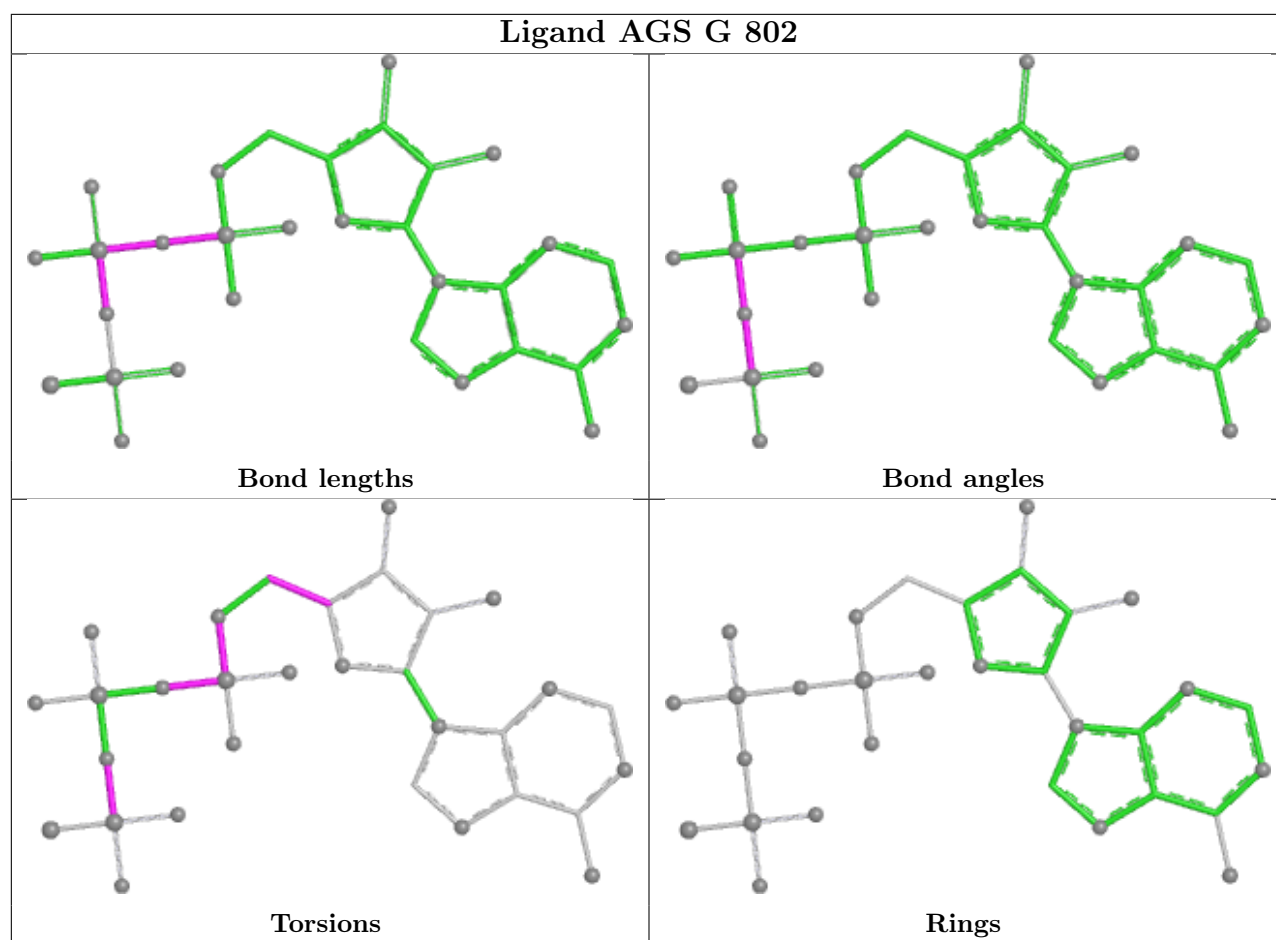












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

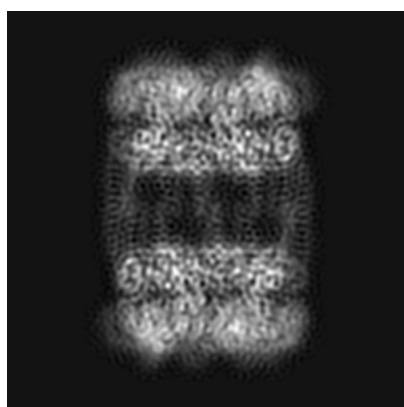
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0967. These allow visual inspection of the internal detail of the map and identification of artifacts.

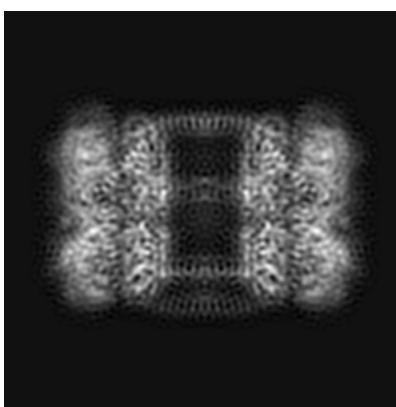
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

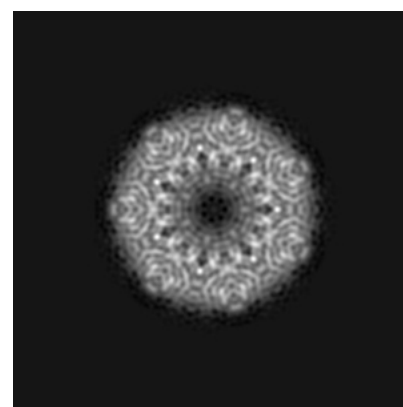
6.1.1 Primary map



X



Y

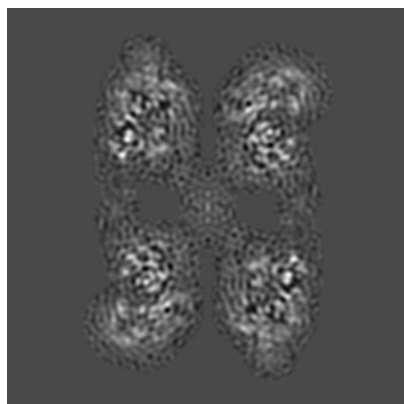


Z

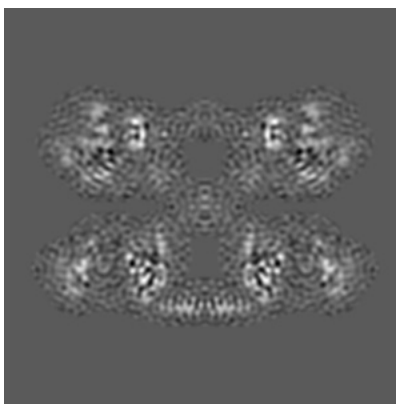
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

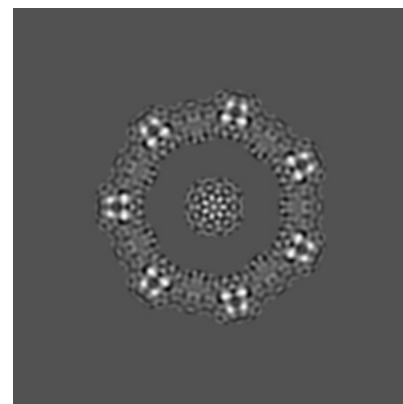
6.2.1 Primary map



X Index: 100



Y Index: 100

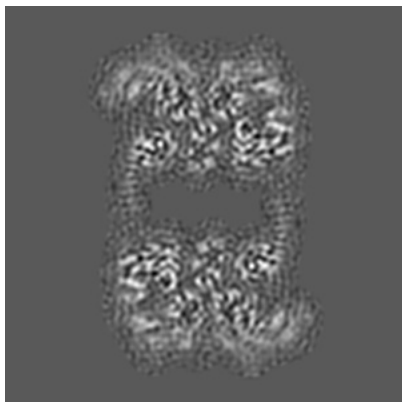


Z Index: 100

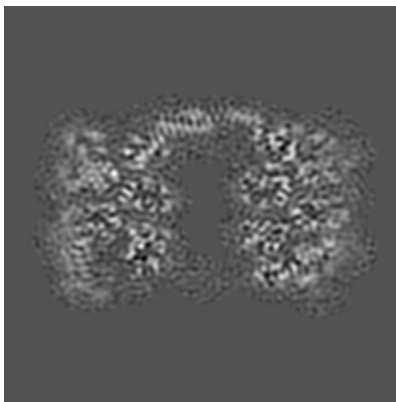
The images above show central slices of the map in three orthogonal directions.

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

6.3.1 Primary map



X Index: 78



Y Index: 76

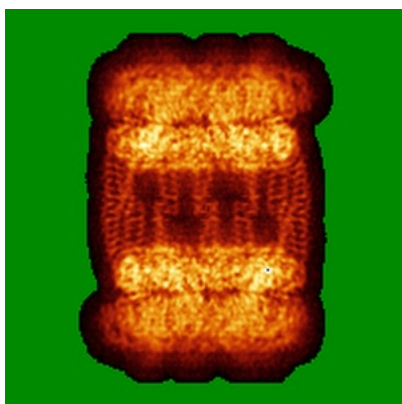


Z Index: 69

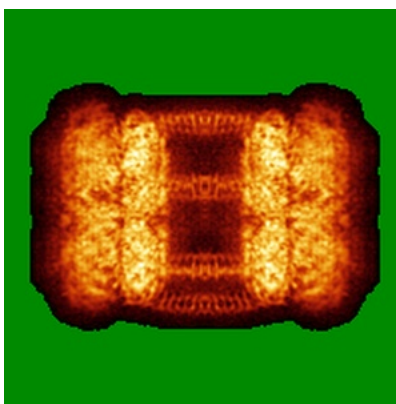
The images above show the largest variance slices of the map in three orthogonal directions.

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

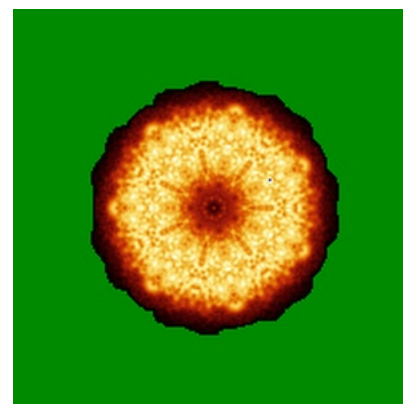
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

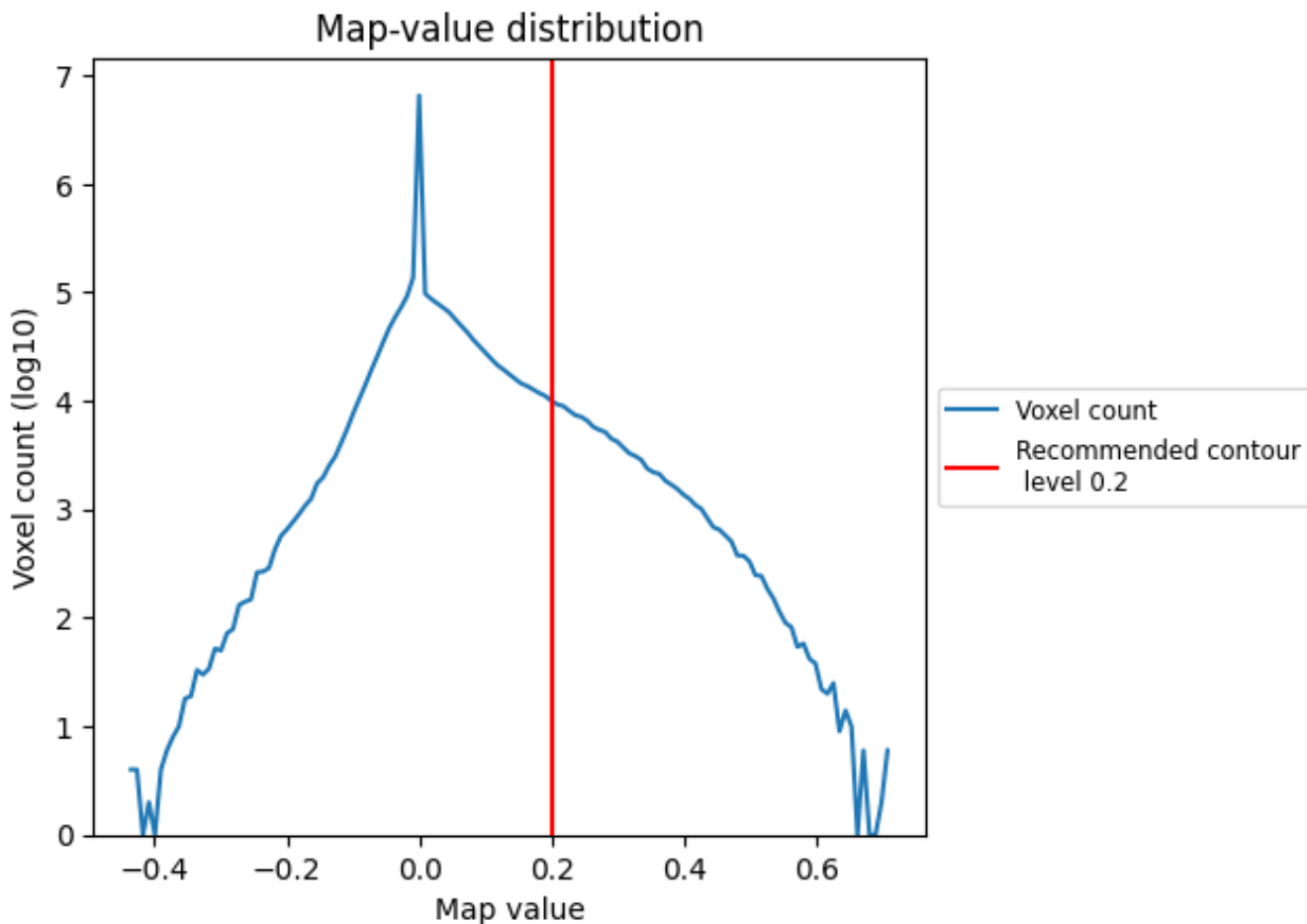
6.6 Mask visualisation

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

7 Map analysis [i](#)

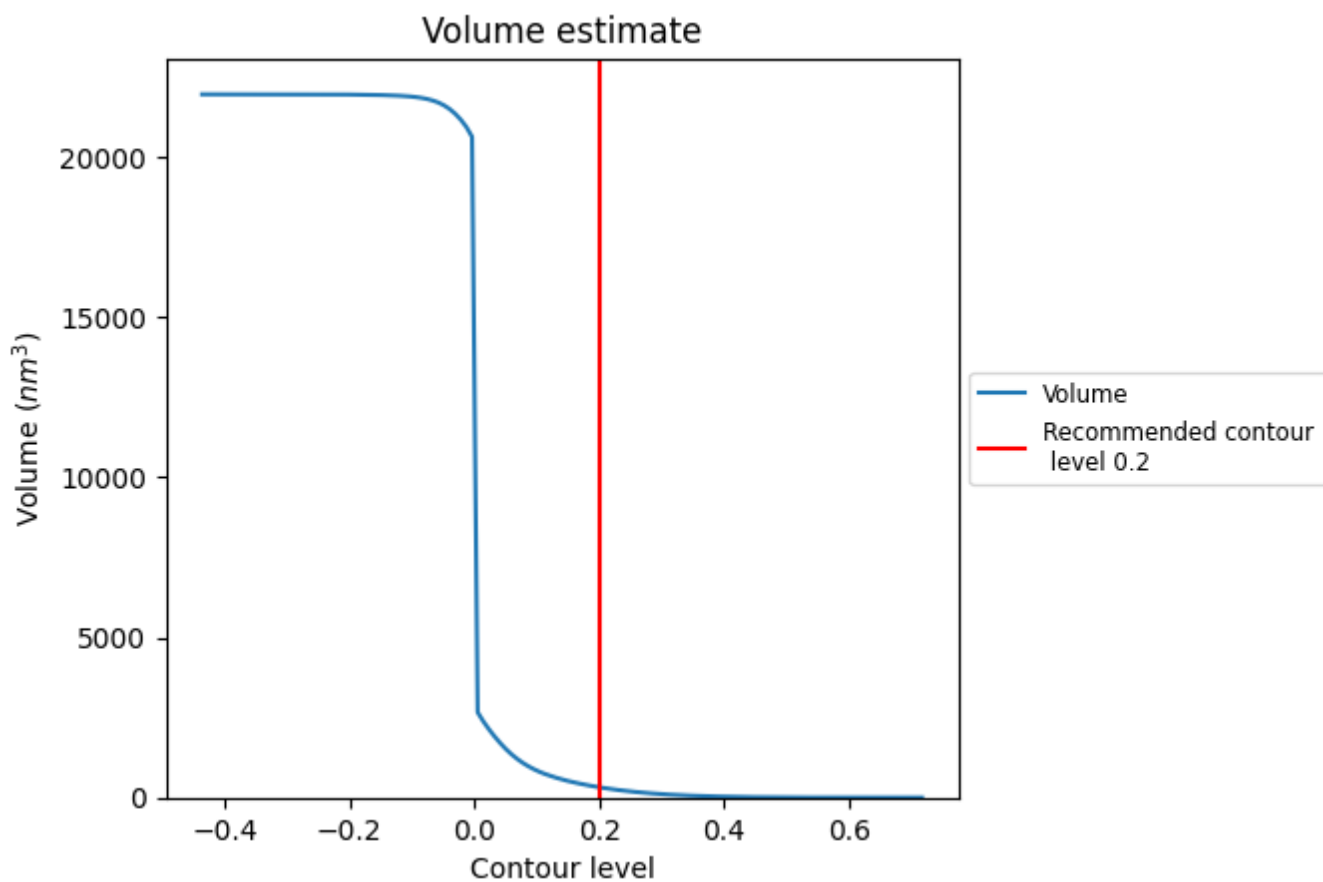
This section contains the results of statistical analysis of the map.

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.

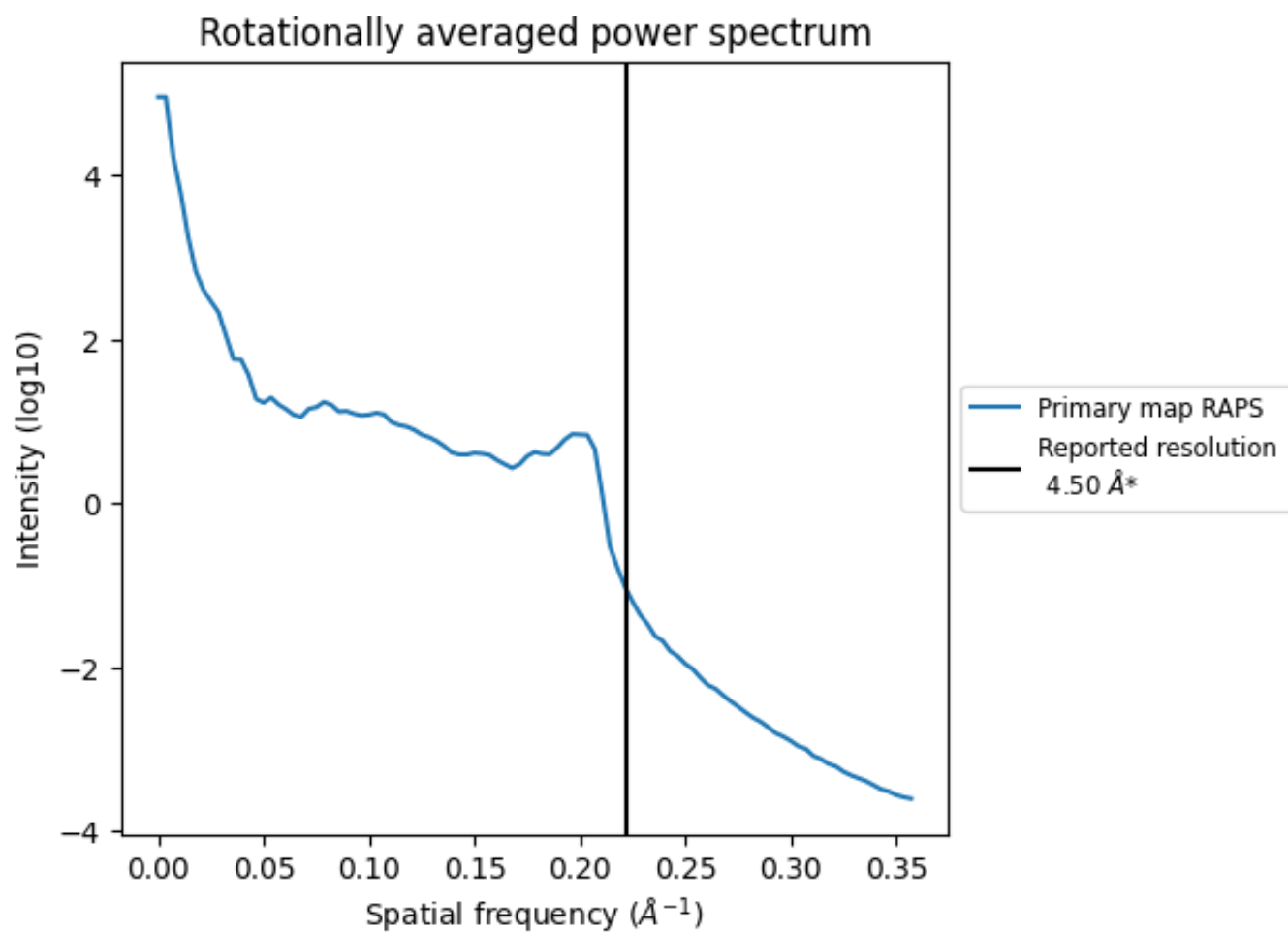
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 322 nm³; this corresponds to an approximate mass of 291 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

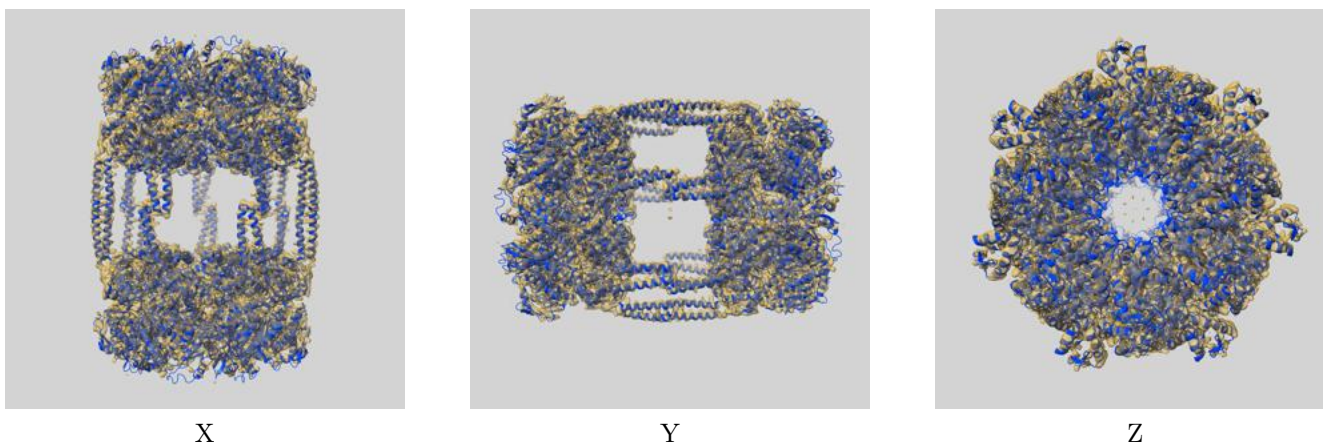
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

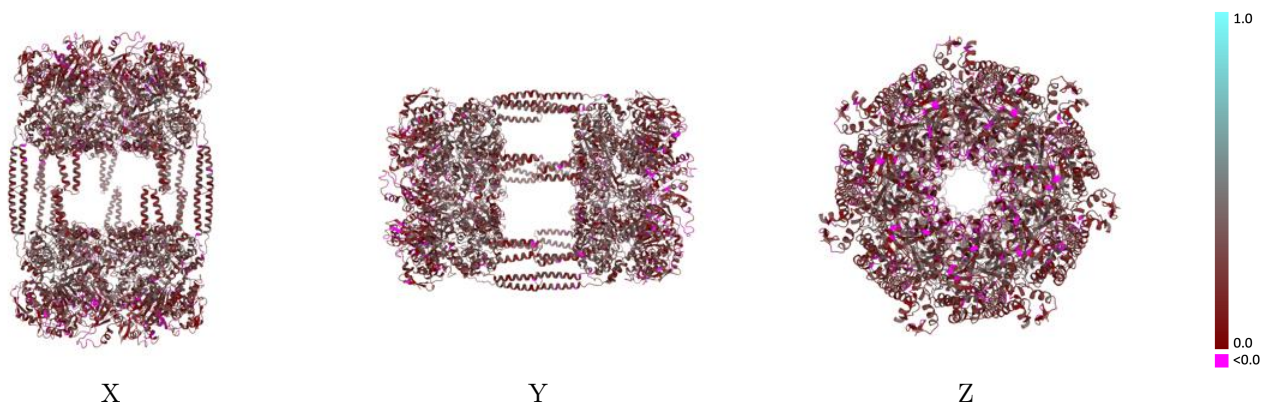
This section contains information regarding the fit between EMDB map EMD-0967 and PDB model 6LT4. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



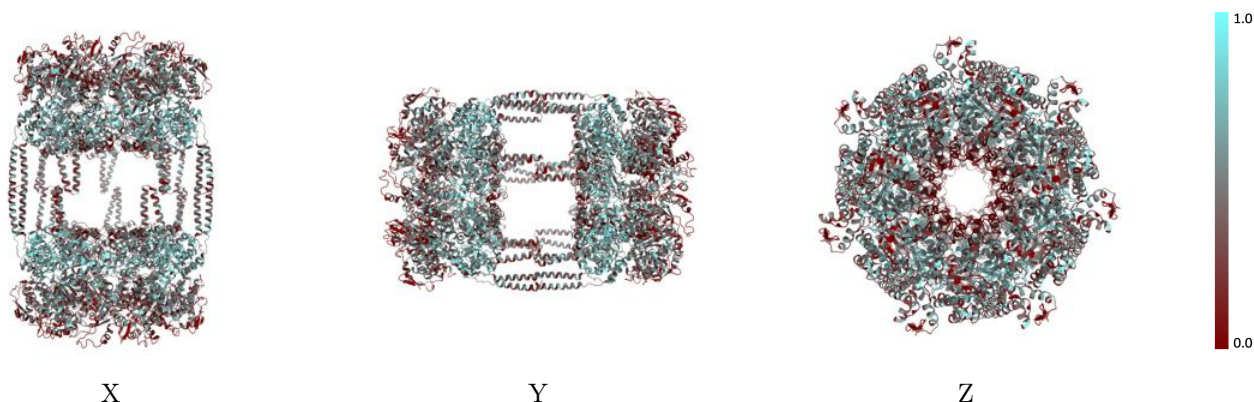
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



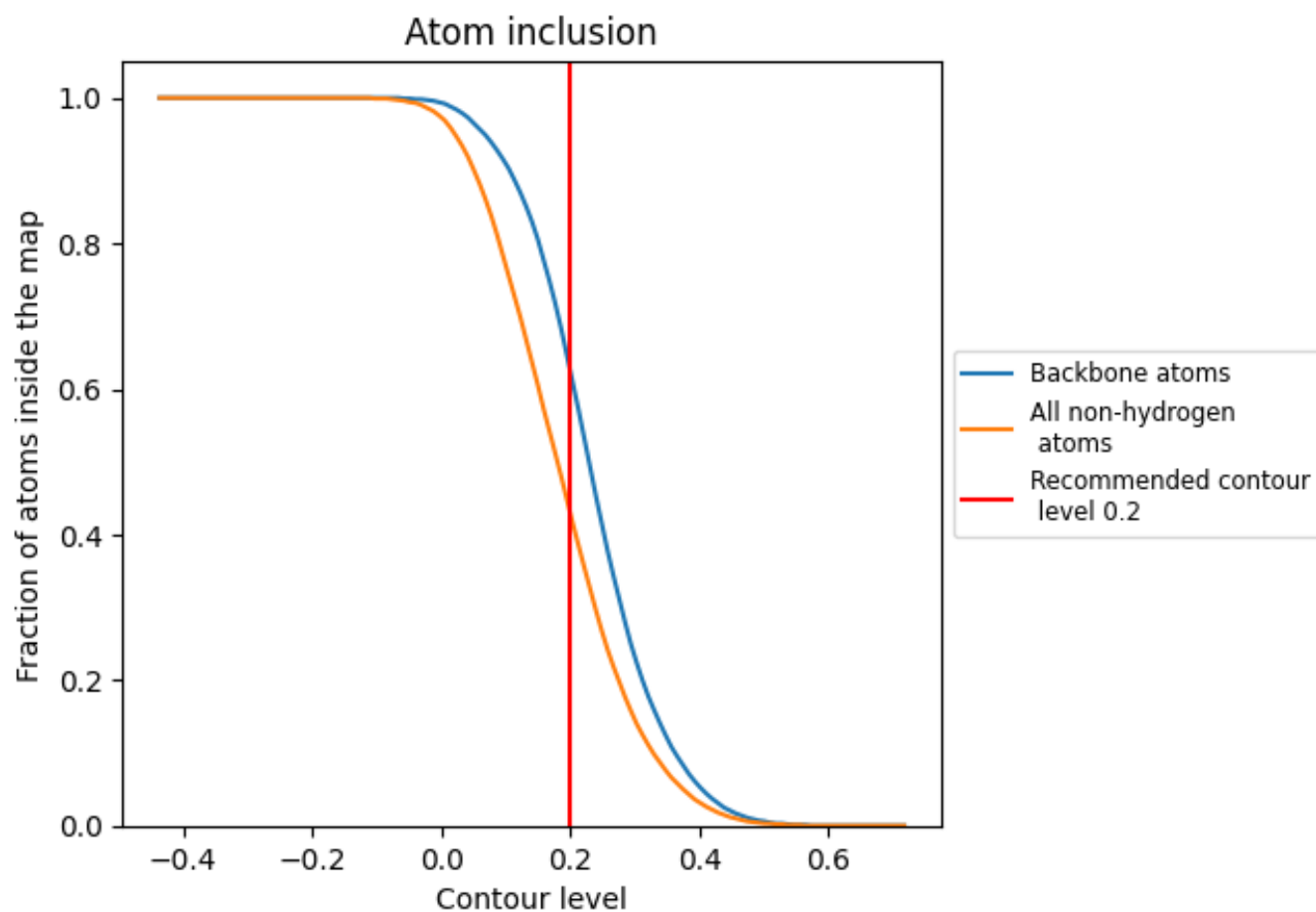
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4290	0.2270
A	0.4310	0.2300
B	0.4260	0.2310
C	0.4260	0.2310
D	0.4350	0.2300
E	0.4370	0.2310
F	0.4290	0.2230
G	0.4300	0.2260
H	0.4250	0.2260
I	0.4210	0.2160
J	0.4250	0.2240
K	0.4320	0.2320
L	0.4340	0.2330
M	0.4240	0.2240
N	0.4280	0.2240

