wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 06:41 AM JST

PDB ID	:	6LT4
EMDB ID	:	EMD-0967
Title	:	AAA+ ATPase, ClpL from Streptococcus pneumoniae: ATPrS-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:

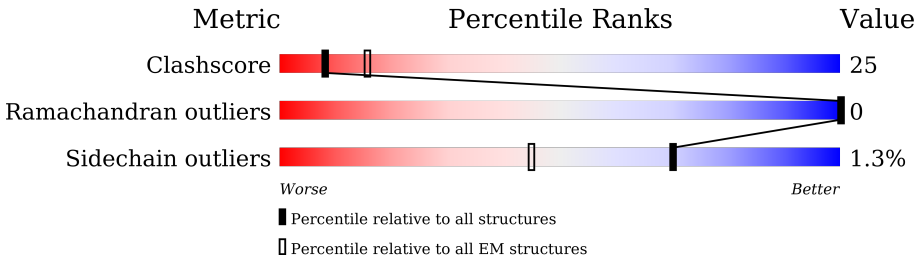
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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)
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 >=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 <=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	39% 51% 37% • 11%
1	B	701	41% 50% 38% • 11%
1	C	701	39% 52% 36% • 11%
1	D	701	41% 51% 37% • 11%
1	E	701	39% 51% 37% • 11%
1	F	701	39% 53% 35% • 11%
1	G	701	39% 52% 36% • 11%
1	H	701	42% 52% 36% • 11%

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Mol	Chain	Length	Quality of chain
1	I	701	44% 51% 37% • 11%
1	J	701	43% 52% 36% • 11%
1	K	701	40% 51% 37% • 11%
1	L	701	40% 52% 36% • 11%
1	M	701	42% 52% 36% • 11%
1	N	701	42% 51% 37% • 11%

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

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 (three-letter code: 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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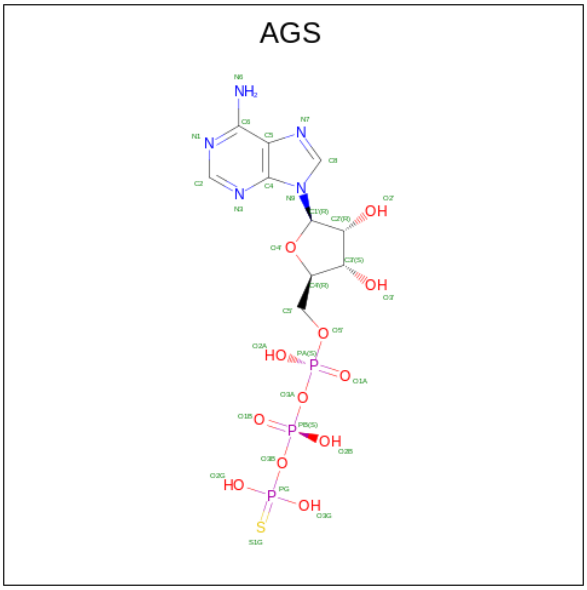
Mol	Chain	Residues	Atoms	AltConf
2	G	2	Total Mg 2 2	0
2	H	2	Total Mg 2 2	0
2	I	2	Total Mg 2 2	0
2	J	2	Total Mg 2 2	0
2	K	2	Total Mg 2 2	0
2	L	2	Total Mg 2 2	0
2	M	2	Total Mg 2 2	0
2	N	2	Total Mg 2 2	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

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

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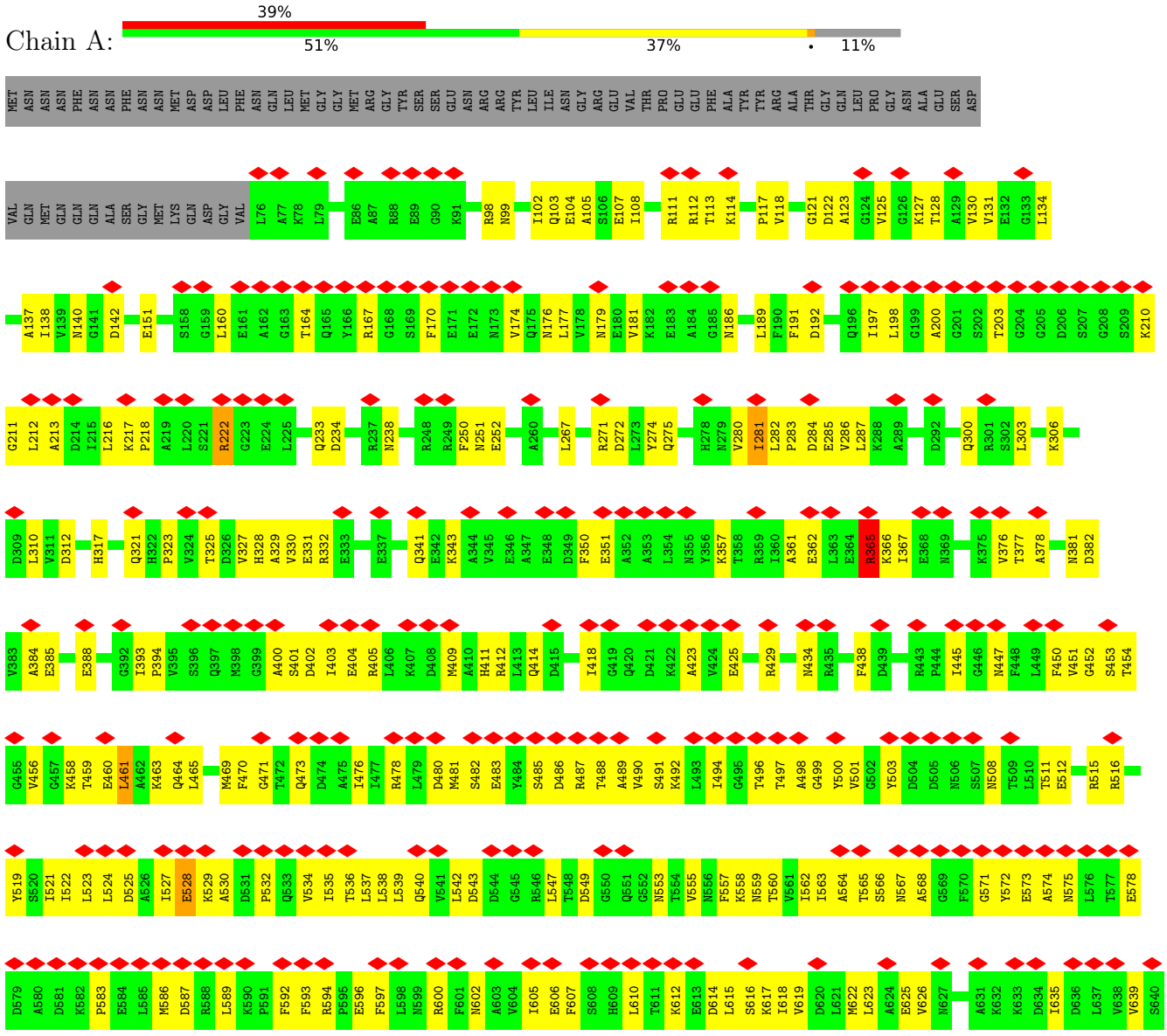
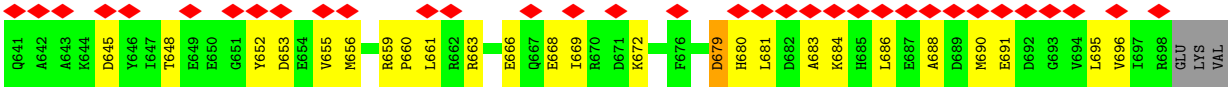
Mol	Chain	Residues	Atoms						AltConf
3	M	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	M	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	N	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	N	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

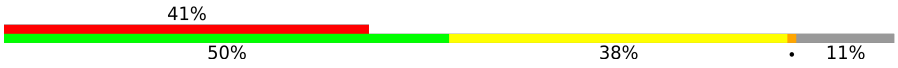
- Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

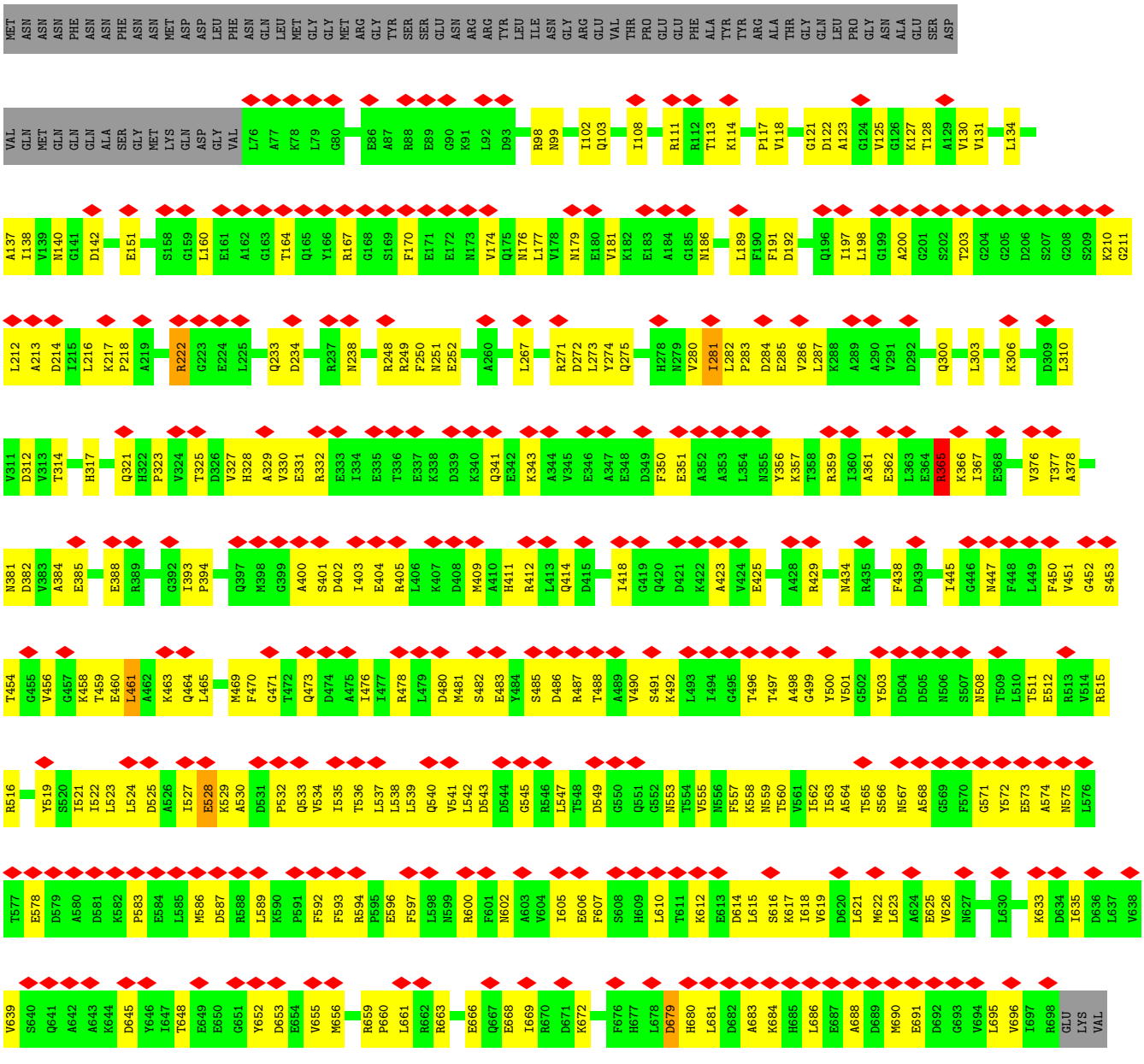




• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

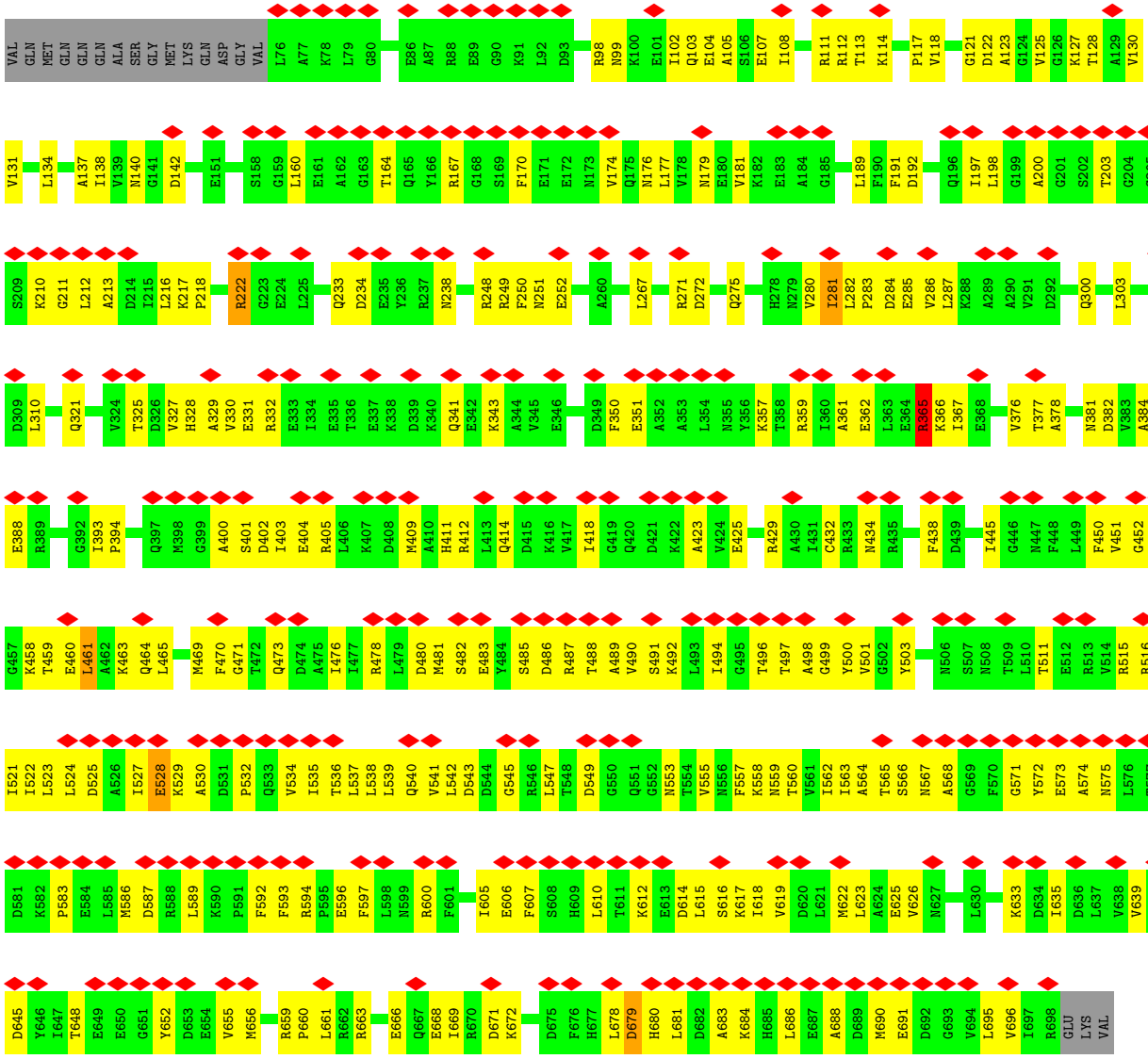
Chain B:





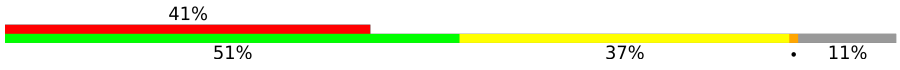
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

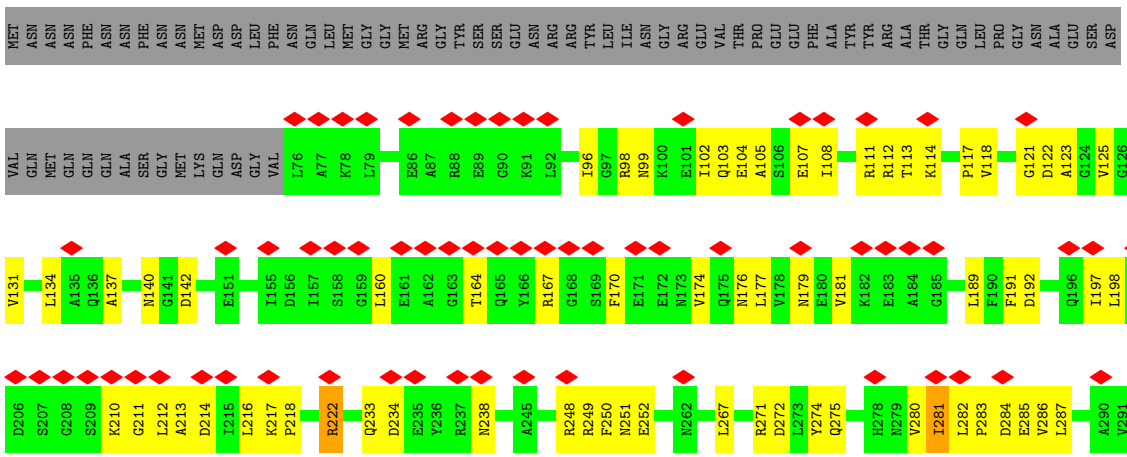
Chain C:

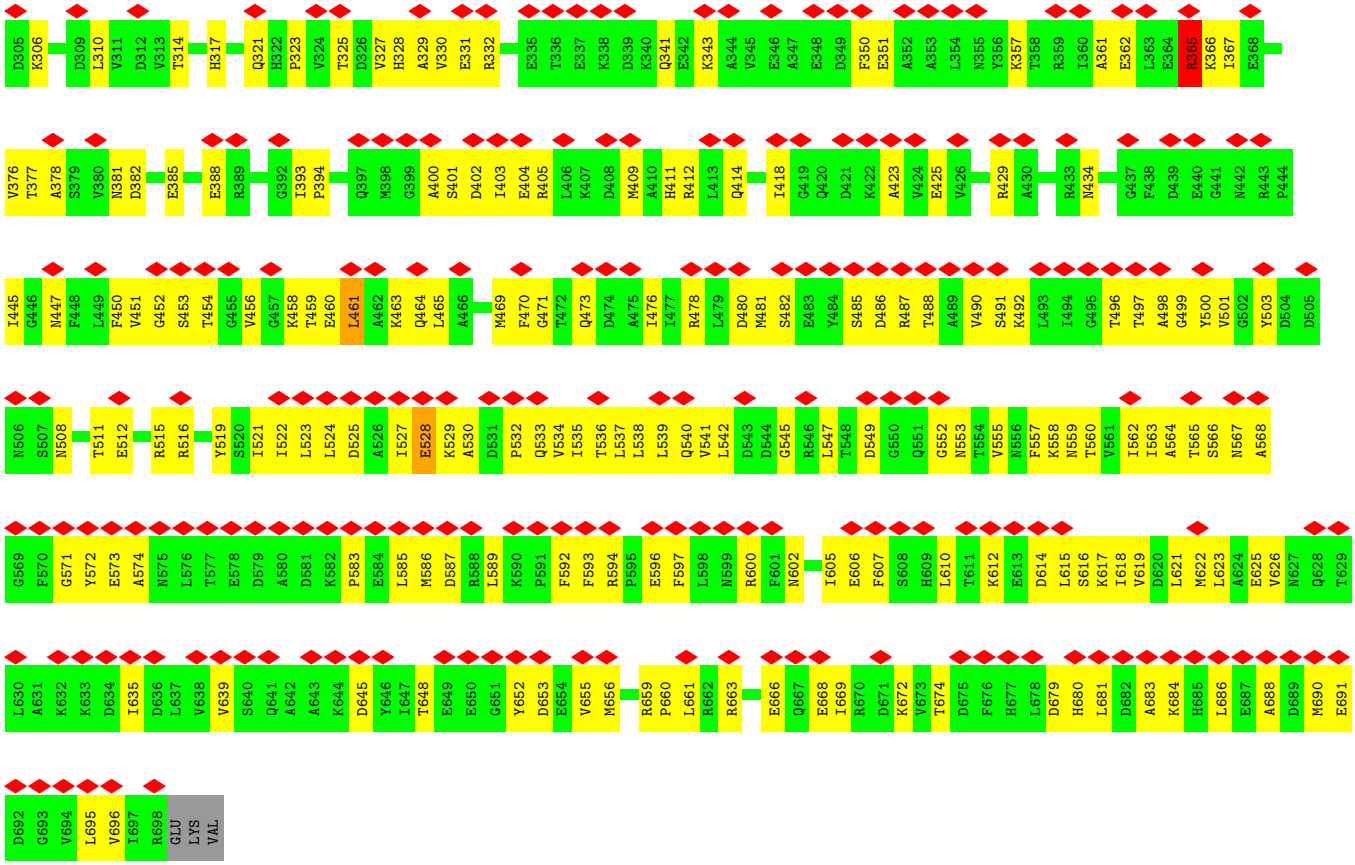


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

Chain D:

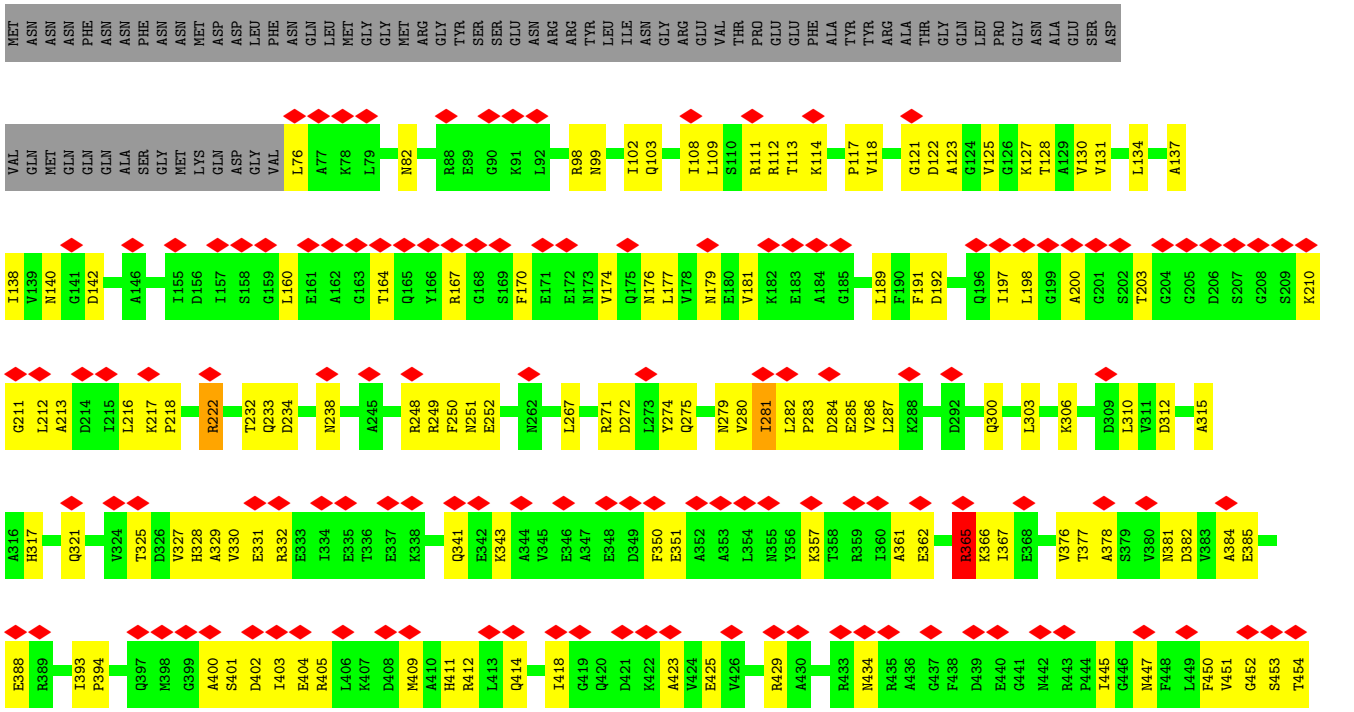


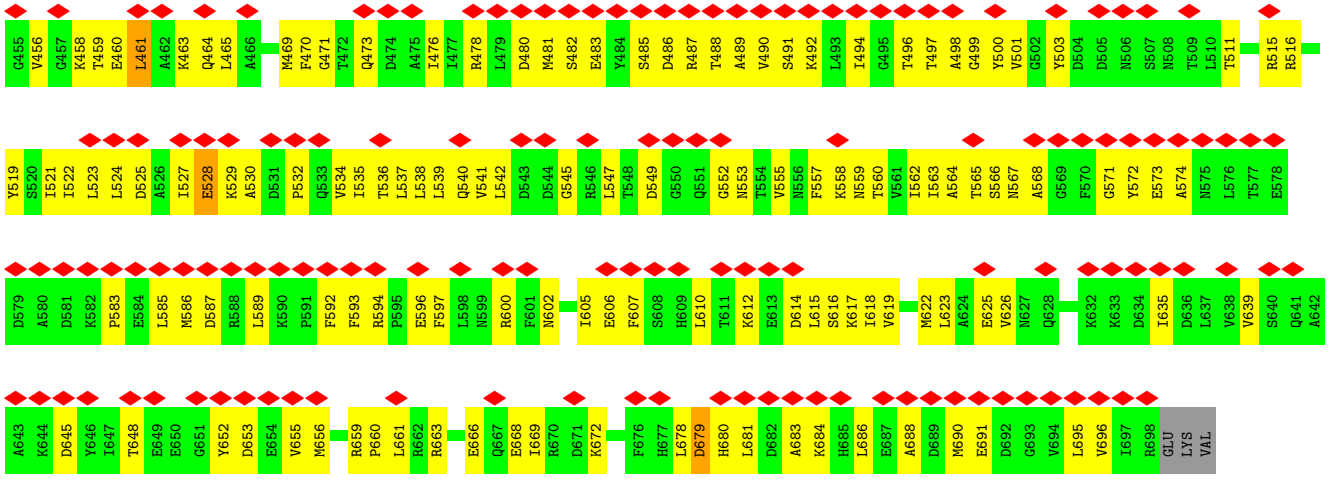




• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

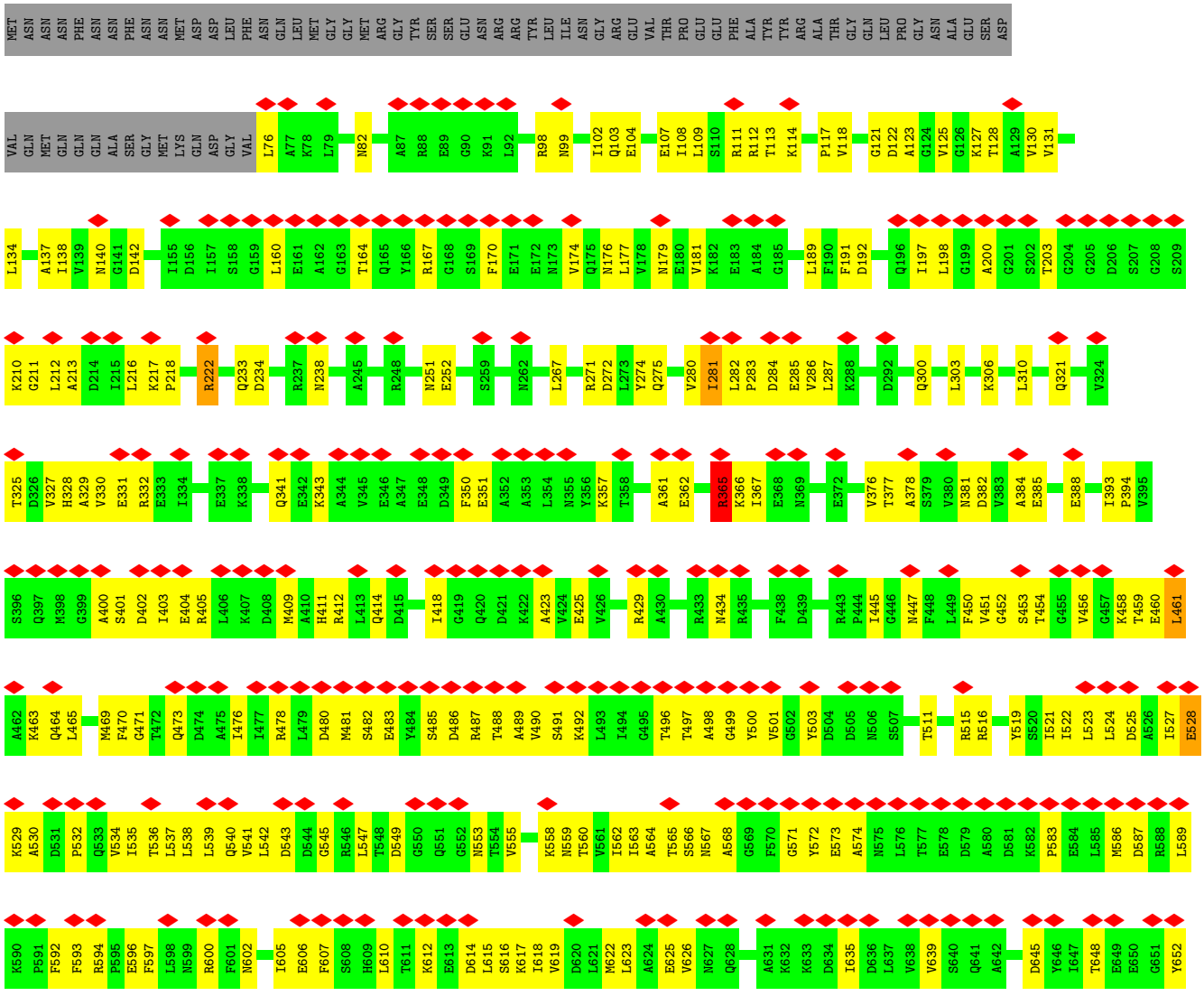
Chain E:

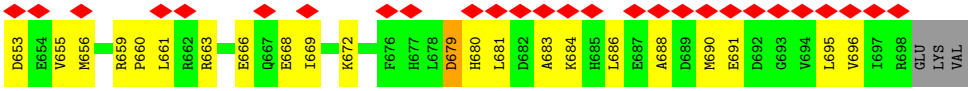




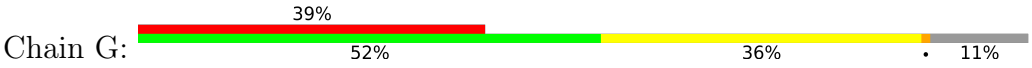
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

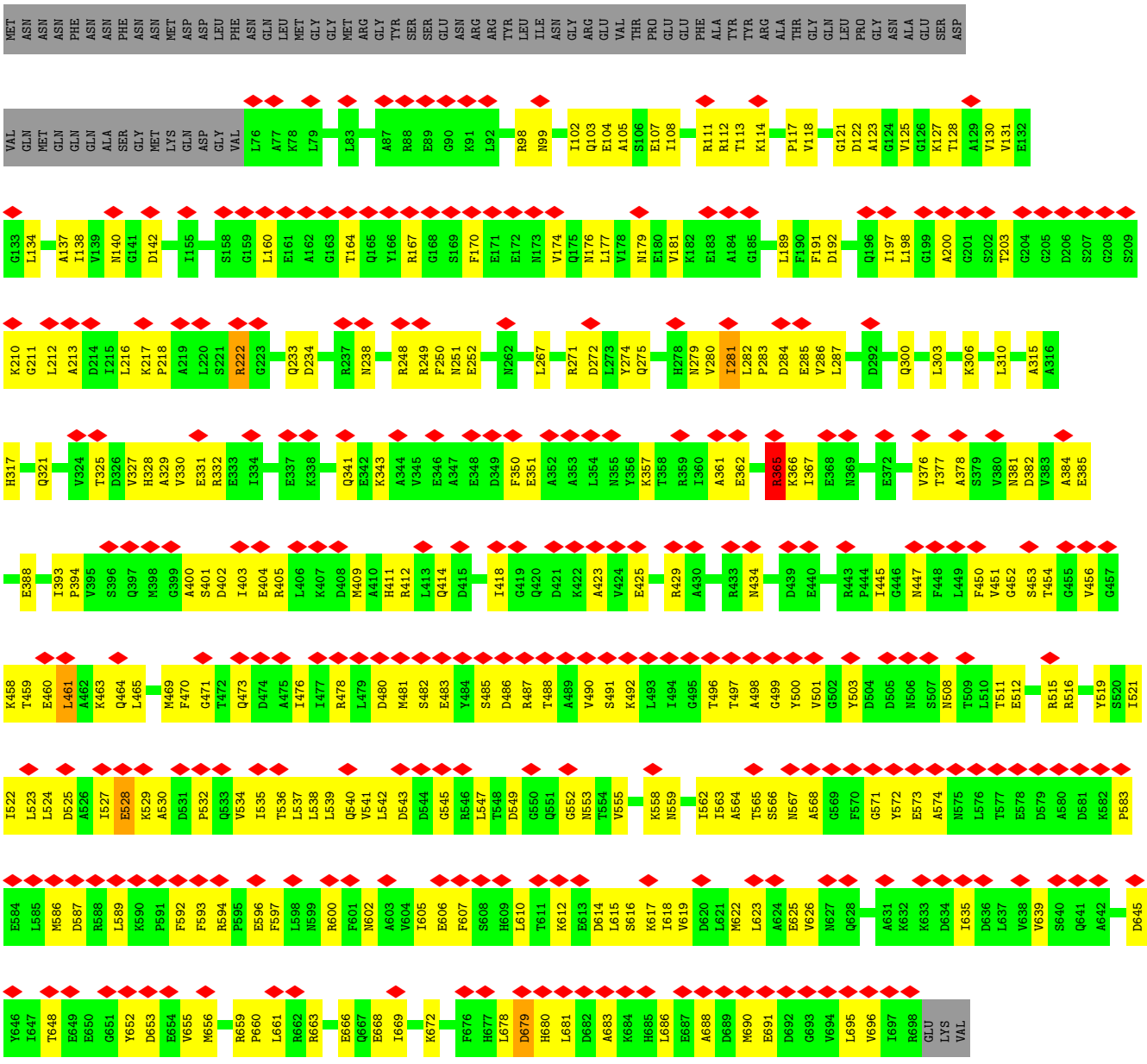
Chain F:



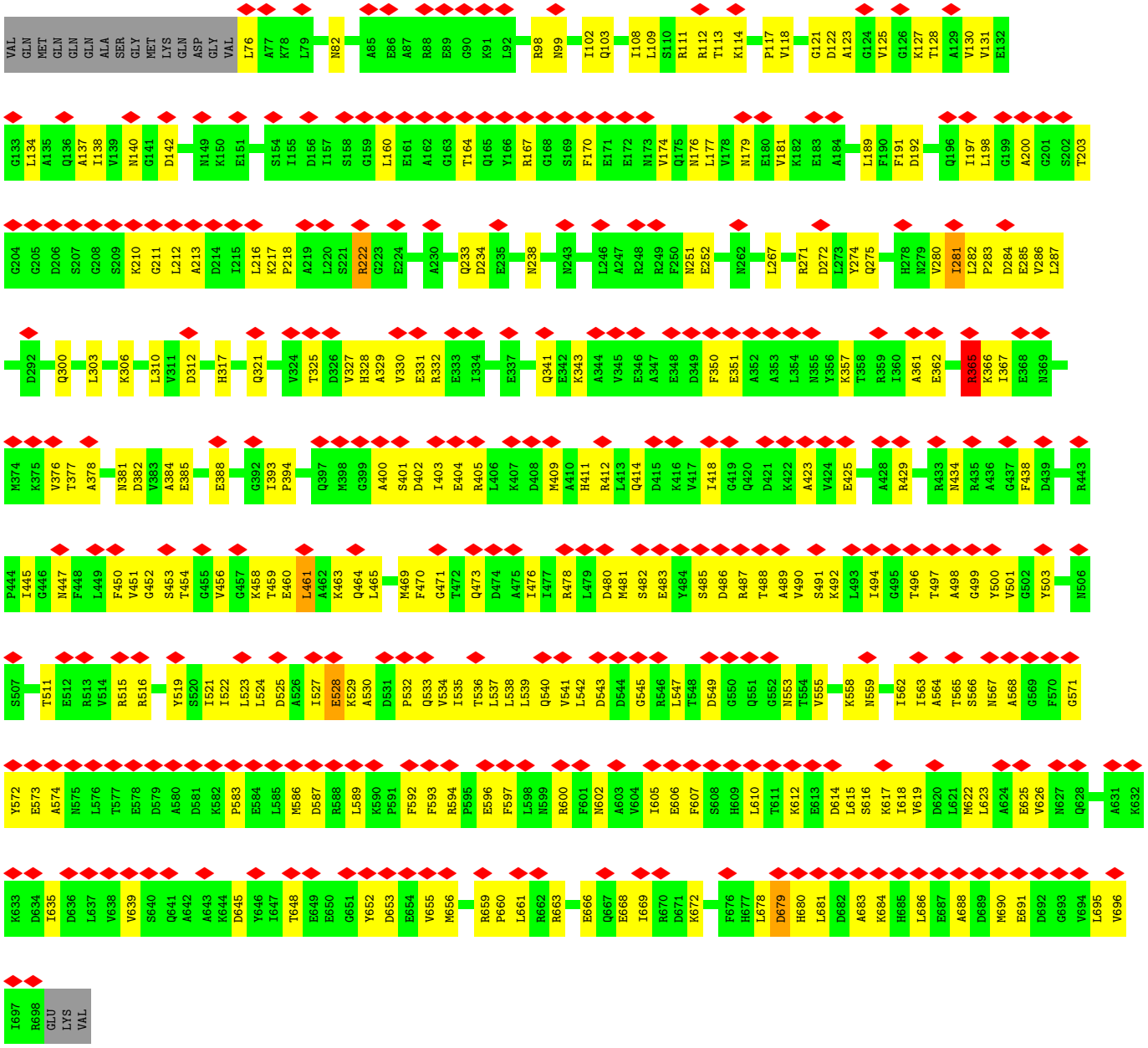


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

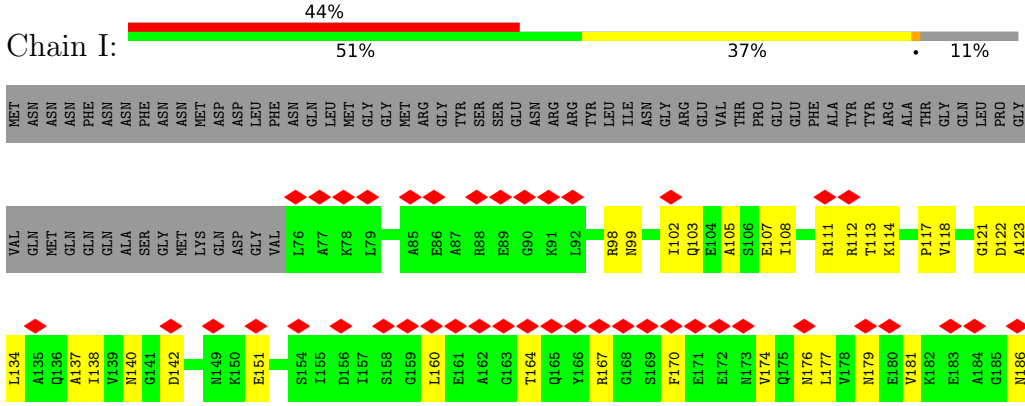


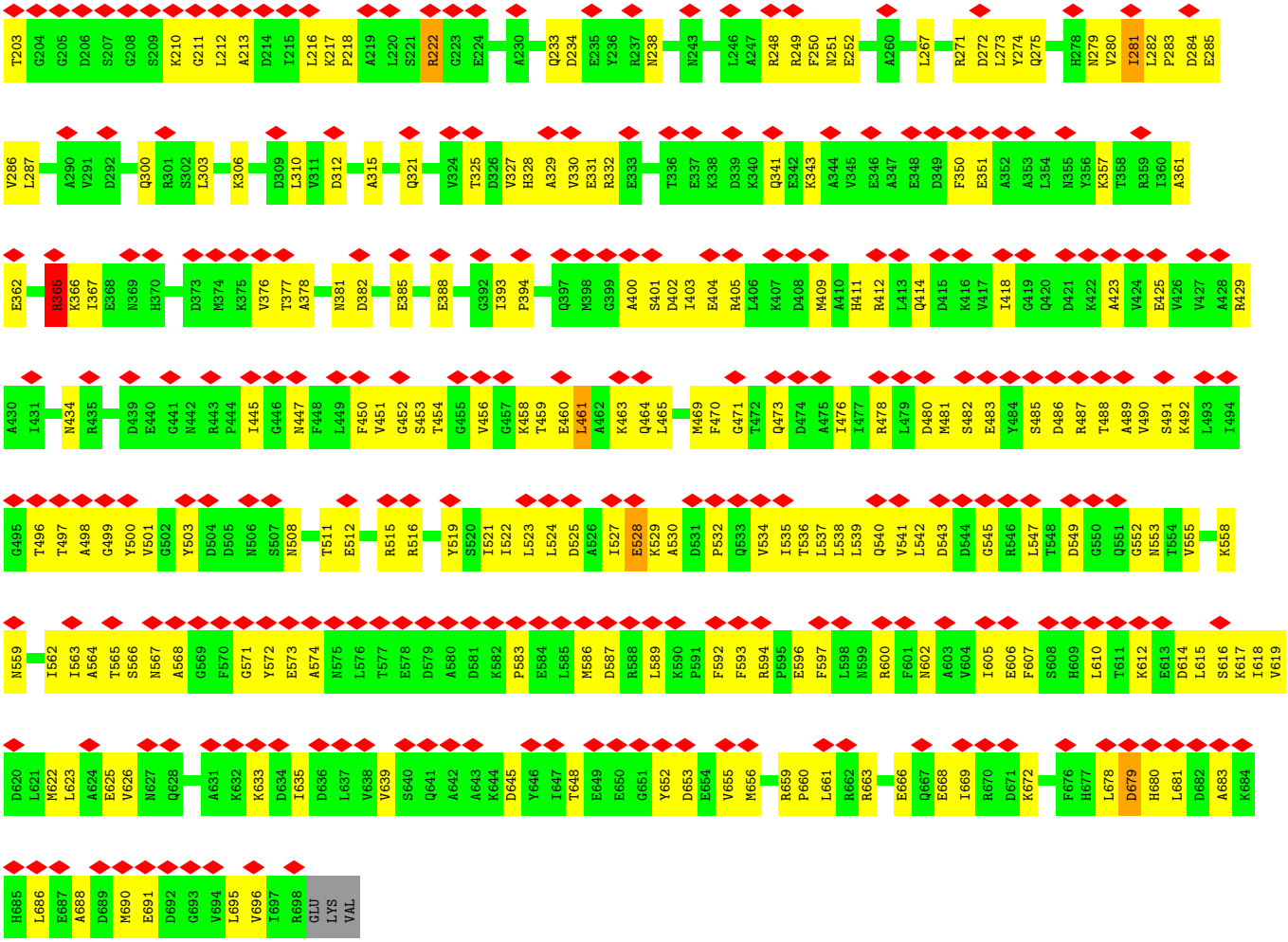


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

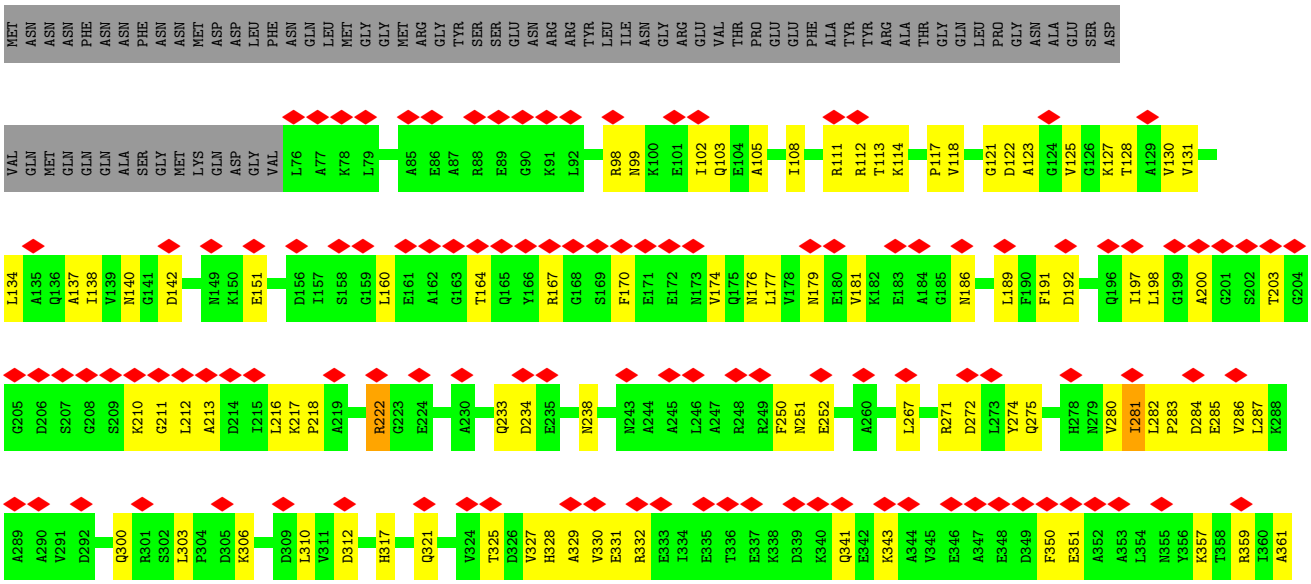


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

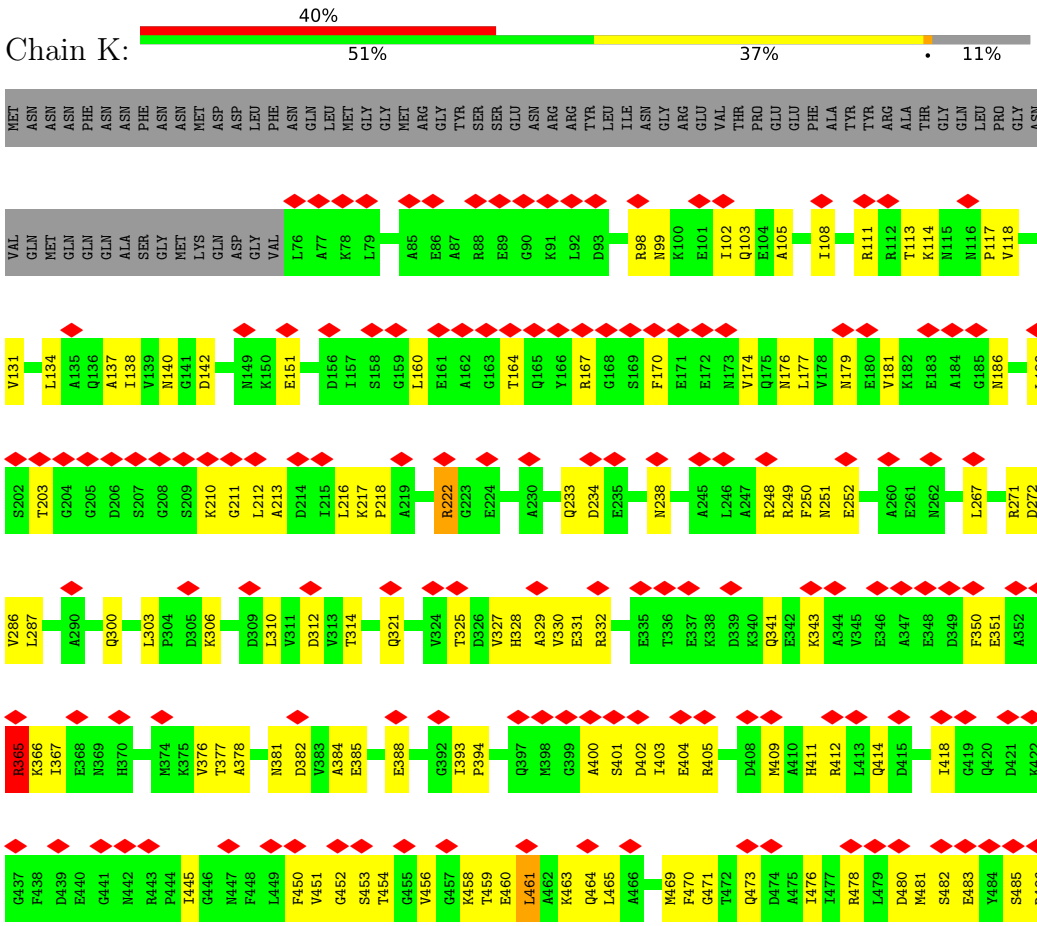


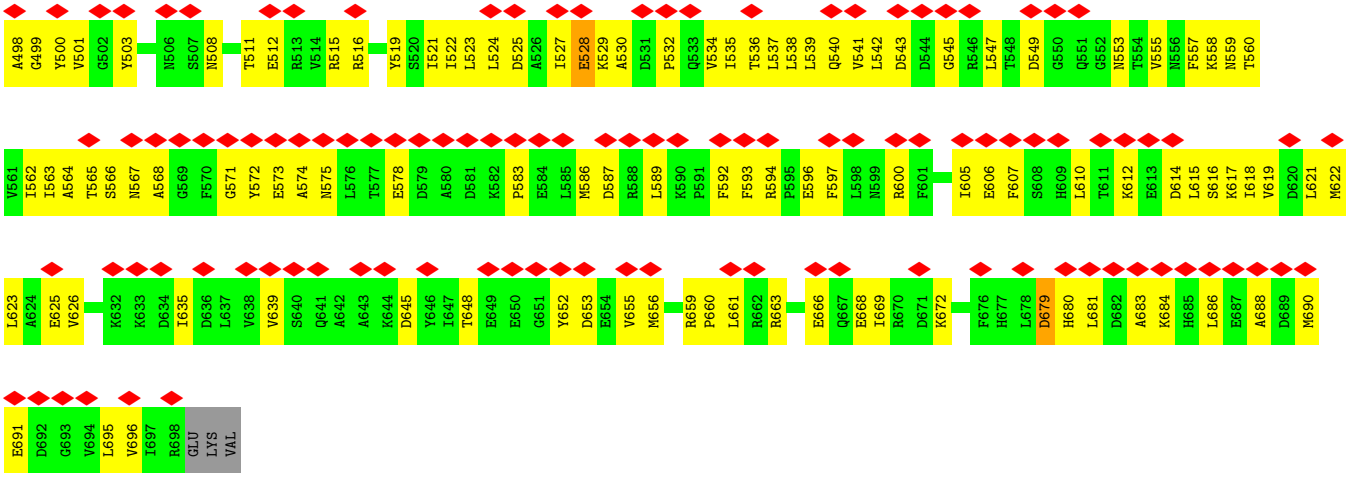


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

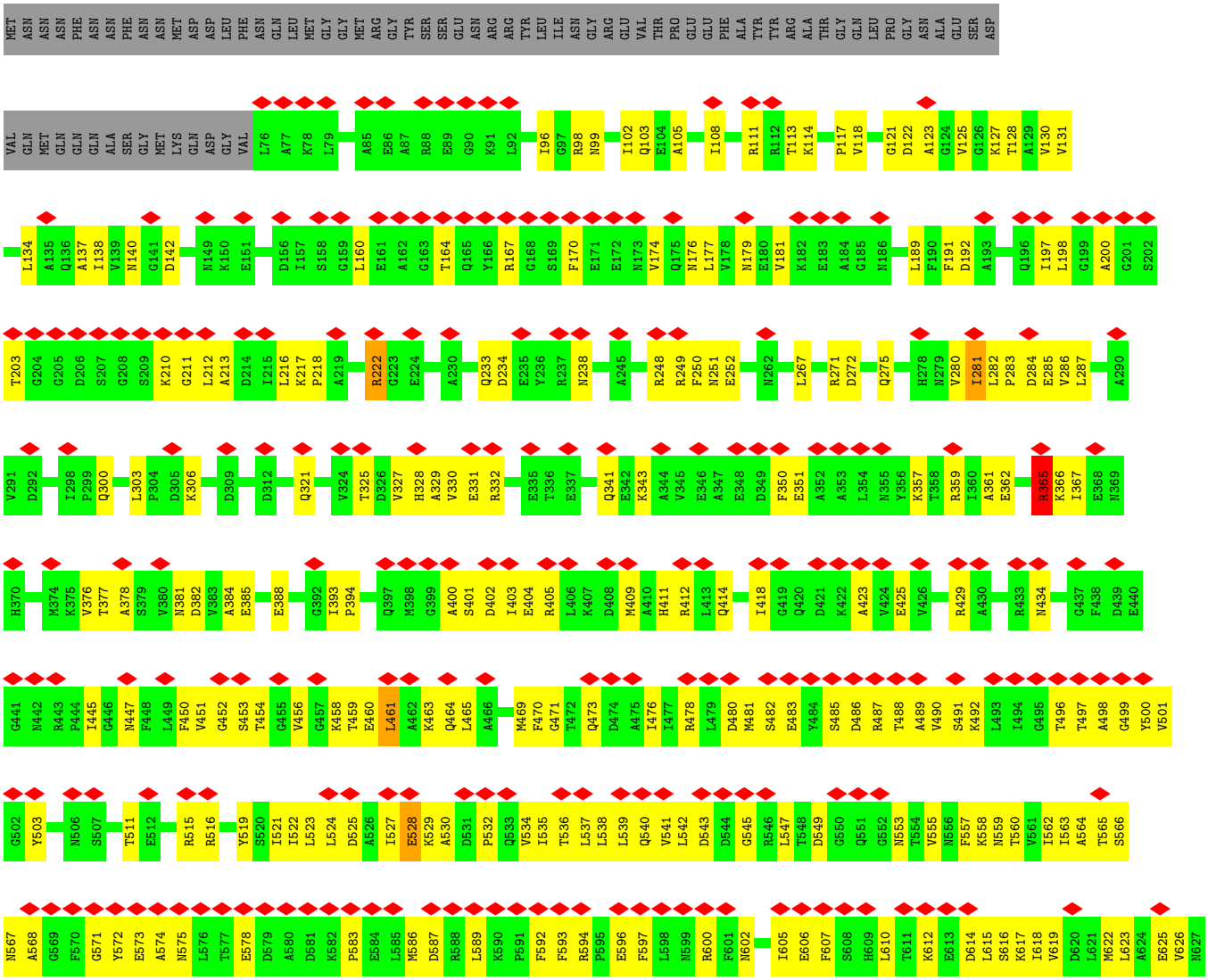


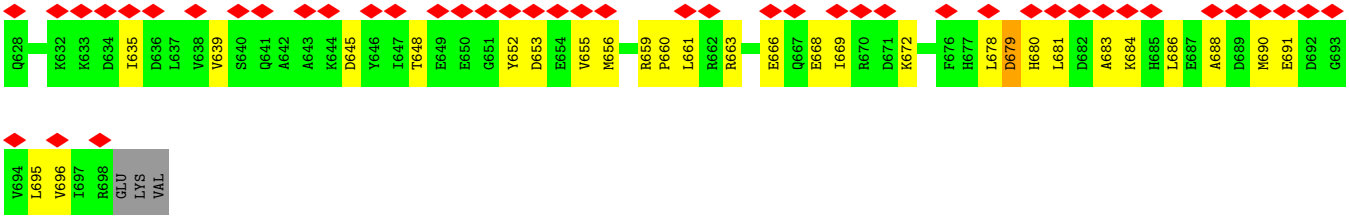
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit





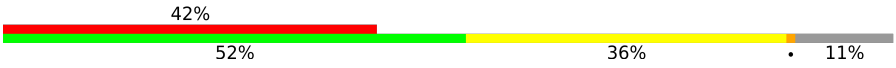
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

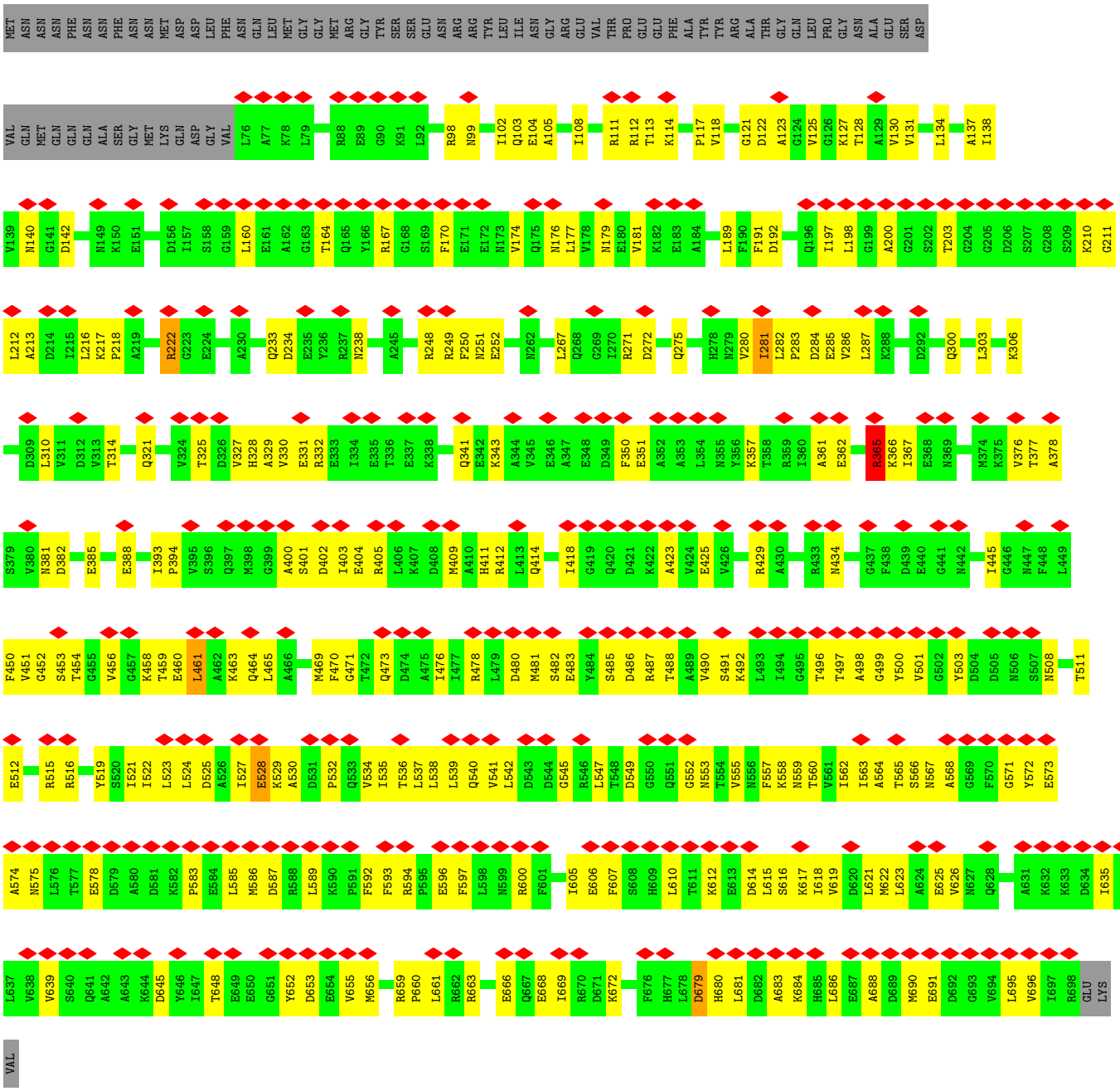




• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

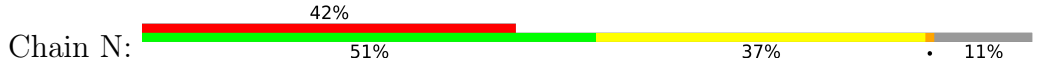
Chain M:

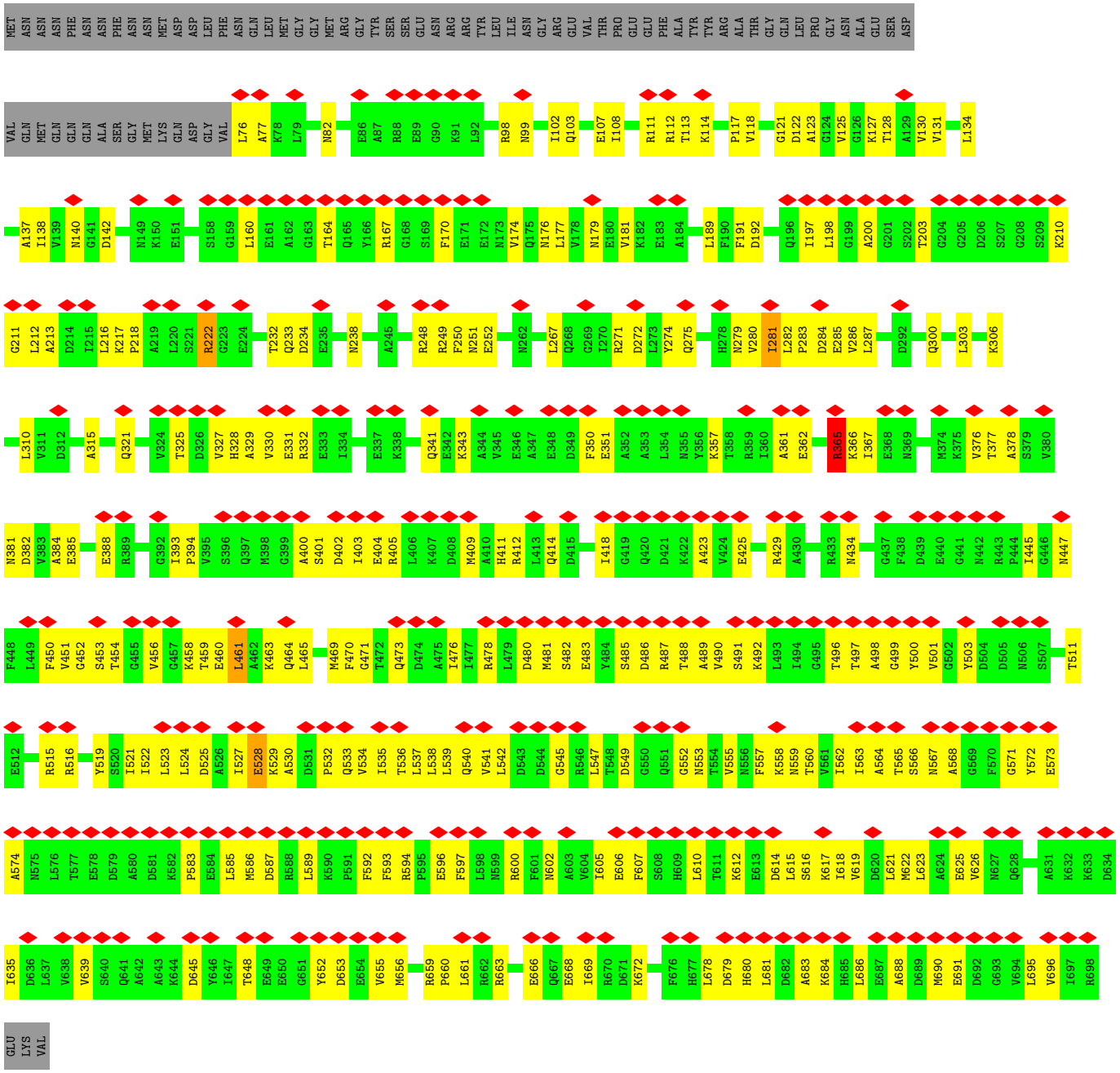




• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

Chain N:


42%
51%
37%
11%


MET ASN ASN ASN PHE ASN ASN PHE ASN ASN MET ASP ASP LEU PHE ASN GLN LEU MET GLY GLY MET ARG GLY TYR SER SER GLU ASN ARG ARG TYR LEU ILE ASN GLY ARG GLU VAL THR PRO GLU GLU PHE ALA TYR TYR ARG ALA THR GLY GLN LEU PRO GLY ASN ALA GLU SER ASP
VAL GLN MET GLN GLN GLN ALA SER GLY 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 N140 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 N179 E180 V181 K182 E183 A184 L189 F190 F191 D192 Q196 I197 L198 G199 A200 G201 S202 T203 G204 G205 D206 S207 G208 S209 K210
G211 L212 A213 D214 I215 L216 K217 P218 A219 L220 S221 R222 G223 E224 T232 Q233 D234 E235 N238 A245 R248 R249 F250 N251 E252 N262 L267 Q268 G269 I270 R271 D272 L273 Y274 Q275 H278 N279 V280 I281 L282 P283 D284 E285 V286 L287 D292 Q300 L303 K306
L310 V311 D312 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 Y356 K357 T358 R359 I360 A361 E362 R365 K366 I367 E368 N369 M374 K375 V376 T377 A378 S379 V380
N381 D382 V383 A384 E385 E388 R389 G392 I393 P394 V395 S396 Q397 M398 G399 A400 S401 D402 I403 E404 R405 L406 K407 D408 M409 A410 H411 R412 L413 Q414 D415 I418 G419 Q420 D421 K422 A423 V424 E425 R429 A430 R433 N434 G437 F438 D439 E440 G441 N442 R443 P444 I445 G446 N447
F448 L449 F450 V451 G452 S453 T454 G455 V456 G457 K458 T459 E460 L461 A462 K463 Q464 L465 M469 F470 G471 T472 Q473 D474 A475 I476 I477 R478 L479 D480 M481 S482 E483 Y484 S485 D486 R487 T488 A489 V490 S491 K492 L493 I494 G495 T496 T497 A498 G499 Y500 V501 G502 Y503 D504 D505 N506 S507 T511
E512 R515 R516 Y519 S520 I521 I522 L523 L524 D525 A526 I527 E528 K529 A530 D531 P532 Q533 V534 I535 T536 L537 L538 L539 Q540 V541 L542 D543 D544 G545 R546 L547 T548 D549 G550 Q551 G552 N553 T554 V555 N556 F557 K558 N559 T560 V561 I562 I563 A564 T565 S566 N567 A568 G569 F570 G571 Y572 E573
A574 N575 L576 T577 E578 D579 A580 D581 K582 P583 E584 L585 M586 D587 R588 L589 K590 P591 F592 F593 R594 P595 E596 F597 L598 N599 R600 F601 N602 A603 V604 I605 E606 F607 S608 H609 L610 T611 K612 E613 D614 L615 S616 K617 I618 V619 D620 L621 M622 L623 A624 E625 V626 N627 Q628 A631 K632 K633 D634
I635 D636 L637 V638 V639 S640 Q641 A642 A643 K644 D645 Y646 I647 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 I697 R698
GLU LYS VAL

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.34	0/4883	0.54	1/6603 (0.0%)
1	B	0.34	0/4883	0.54	1/6603 (0.0%)
1	C	0.34	0/4883	0.54	1/6603 (0.0%)
1	D	0.34	0/4883	0.54	1/6603 (0.0%)
1	E	0.34	0/4883	0.54	1/6603 (0.0%)
1	F	0.34	0/4883	0.54	1/6603 (0.0%)
1	G	0.34	0/4883	0.54	1/6603 (0.0%)
1	H	0.34	0/4883	0.54	1/6603 (0.0%)
1	I	0.34	0/4883	0.54	1/6603 (0.0%)
1	J	0.34	0/4883	0.54	1/6603 (0.0%)
1	K	0.34	0/4883	0.54	1/6603 (0.0%)
1	L	0.34	0/4883	0.54	1/6603 (0.0%)
1	M	0.34	0/4883	0.54	1/6603 (0.0%)
1	N	0.34	0/4883	0.54	1/6603 (0.0%)
All	All	0.34	0/68362	0.54	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(^{o})	Ideal(^{o})
1	G	365	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	L	365	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	E	365	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	K	365	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	365	ARG	NE-CZ-NH1	6.40	123.50	120.30

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	249	0
1	B	4824	0	4841	259	0
1	C	4824	0	4841	251	0
1	D	4824	0	4841	263	0
1	E	4824	0	4841	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4824	0	4841	242	0
1	G	4824	0	4841	251	0
1	H	4824	0	4841	254	0
1	I	4824	0	4841	256	0
1	J	4824	0	4841	245	0
1	K	4824	0	4841	247	0
1	L	4824	0	4841	240	0
1	M	4824	0	4841	245	0
1	N	4824	0	4841	254	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	3368	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 25.

The worst 5 of 3368 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%)	513 (99%)	7 (1%)	69	82
1	B	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	C	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	D	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	E	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	F	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	G	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	H	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	I	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	J	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	K	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	L	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	M	520/586 (89%)	513 (99%)	7 (1%)	69	82
1	N	520/586 (89%)	513 (99%)	7 (1%)	69	82
All	All	7280/8204 (89%)	7182 (99%)	98 (1%)	70	82

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	233	GLN
1	K	233	GLN
1	I	377	THR
1	J	365	ARG
1	K	473	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	176	ASN

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Mol	Chain	Res	Type
1	L	179	ASN
1	J	179	ASN
1	K	179	ASN
1	M	176	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	G	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	J	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	M	803	2	26,33,33	0.71	0	26,52,52	1.11	2 (7%)
3	AGS	D	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	H	803	2	26,33,33	0.70	0	26,52,52	1.11	2 (7%)
3	AGS	B	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	A	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	H	802	2	26,33,33	0.72	1 (3%)	26,52,52	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AGS	E	803	2	26,33,33	0.70	0	26,52,52	1.11	2 (7%)
3	AGS	D	802	2	26,33,33	0.73	1 (3%)	26,52,52	1.11	2 (7%)
3	AGS	J	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	L	802	2	26,33,33	0.73	1 (3%)	26,52,52	1.10	2 (7%)
3	AGS	L	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	F	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	B	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	A	803	2	26,33,33	0.70	0	26,52,52	1.11	2 (7%)
3	AGS	E	802	2	26,33,33	0.73	1 (3%)	26,52,52	1.11	2 (7%)
3	AGS	K	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	F	802	2	26,33,33	0.72	0	26,52,52	1.11	2 (7%)
3	AGS	N	803	2	26,33,33	0.70	0	26,52,52	1.11	2 (7%)
3	AGS	C	802	2	26,33,33	0.72	0	26,52,52	1.10	2 (7%)
3	AGS	G	803	2	26,33,33	0.71	0	26,52,52	1.11	2 (7%)
3	AGS	K	803	2	26,33,33	0.70	0	26,52,52	1.10	2 (7%)
3	AGS	N	802	2	26,33,33	0.73	0	26,52,52	1.11	2 (7%)
3	AGS	M	802	2	26,33,33	0.73	0	26,52,52	1.11	2 (7%)
3	AGS	I	803	2	26,33,33	0.70	0	26,52,52	1.11	2 (7%)
3	AGS	I	802	2	26,33,33	0.72	1 (3%)	26,52,52	1.11	2 (7%)
3	AGS	C	803	2	26,33,33	0.69	0	26,52,52	1.11	2 (7%)

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	G	802	2	-	6/17/38/38	0/3/3/3
3	AGS	J	802	2	-	6/17/38/38	0/3/3/3
3	AGS	M	803	2	-	7/17/38/38	0/3/3/3
3	AGS	D	803	2	-	7/17/38/38	0/3/3/3
3	AGS	H	803	2	-	7/17/38/38	0/3/3/3
3	AGS	B	802	2	-	6/17/38/38	0/3/3/3
3	AGS	A	802	2	-	6/17/38/38	0/3/3/3
3	AGS	H	802	2	-	6/17/38/38	0/3/3/3
3	AGS	E	803	2	-	7/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	802	2	-	6/17/38/38	0/3/3/3
3	AGS	J	803	2	-	7/17/38/38	0/3/3/3
3	AGS	L	802	2	-	6/17/38/38	0/3/3/3
3	AGS	L	803	2	-	7/17/38/38	0/3/3/3
3	AGS	F	803	2	-	7/17/38/38	0/3/3/3
3	AGS	B	803	2	-	7/17/38/38	0/3/3/3
3	AGS	A	803	2	-	7/17/38/38	0/3/3/3
3	AGS	E	802	2	-	6/17/38/38	0/3/3/3
3	AGS	K	802	2	-	6/17/38/38	0/3/3/3
3	AGS	F	802	2	-	6/17/38/38	0/3/3/3
3	AGS	N	803	2	-	7/17/38/38	0/3/3/3
3	AGS	C	802	2	-	6/17/38/38	0/3/3/3
3	AGS	G	803	2	-	7/17/38/38	0/3/3/3
3	AGS	K	803	2	-	7/17/38/38	0/3/3/3
3	AGS	N	802	2	-	6/17/38/38	0/3/3/3
3	AGS	M	802	2	-	6/17/38/38	0/3/3/3
3	AGS	I	803	2	-	7/17/38/38	0/3/3/3
3	AGS	I	802	2	-	6/17/38/38	0/3/3/3
3	AGS	C	803	2	-	7/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	AGS	PG-S1G	2.02	1.95	1.90
3	E	802	AGS	PG-S1G	2.02	1.95	1.90
3	H	802	AGS	PG-S1G	2.01	1.95	1.90
3	L	802	AGS	PG-S1G	2.01	1.95	1.90
3	I	802	AGS	PG-S1G	2.00	1.95	1.90

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	802	AGS	PA-O3A-PB	-4.28	118.13	132.83
3	I	802	AGS	PA-O3A-PB	-4.28	118.14	132.83
3	C	802	AGS	PA-O3A-PB	-4.28	118.15	132.83
3	K	802	AGS	PA-O3A-PB	-4.28	118.15	132.83
3	M	802	AGS	PA-O3A-PB	-4.28	118.15	132.83

There are no chirality outliers.

5 of 182 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-O3A
3	A	802	AGS	O4'-C4'-C5'-O5'
3	A	803	AGS	PB-O3B-PG-O2G
3	A	803	AGS	PB-O3B-PG-O3G

There are no ring outliers.

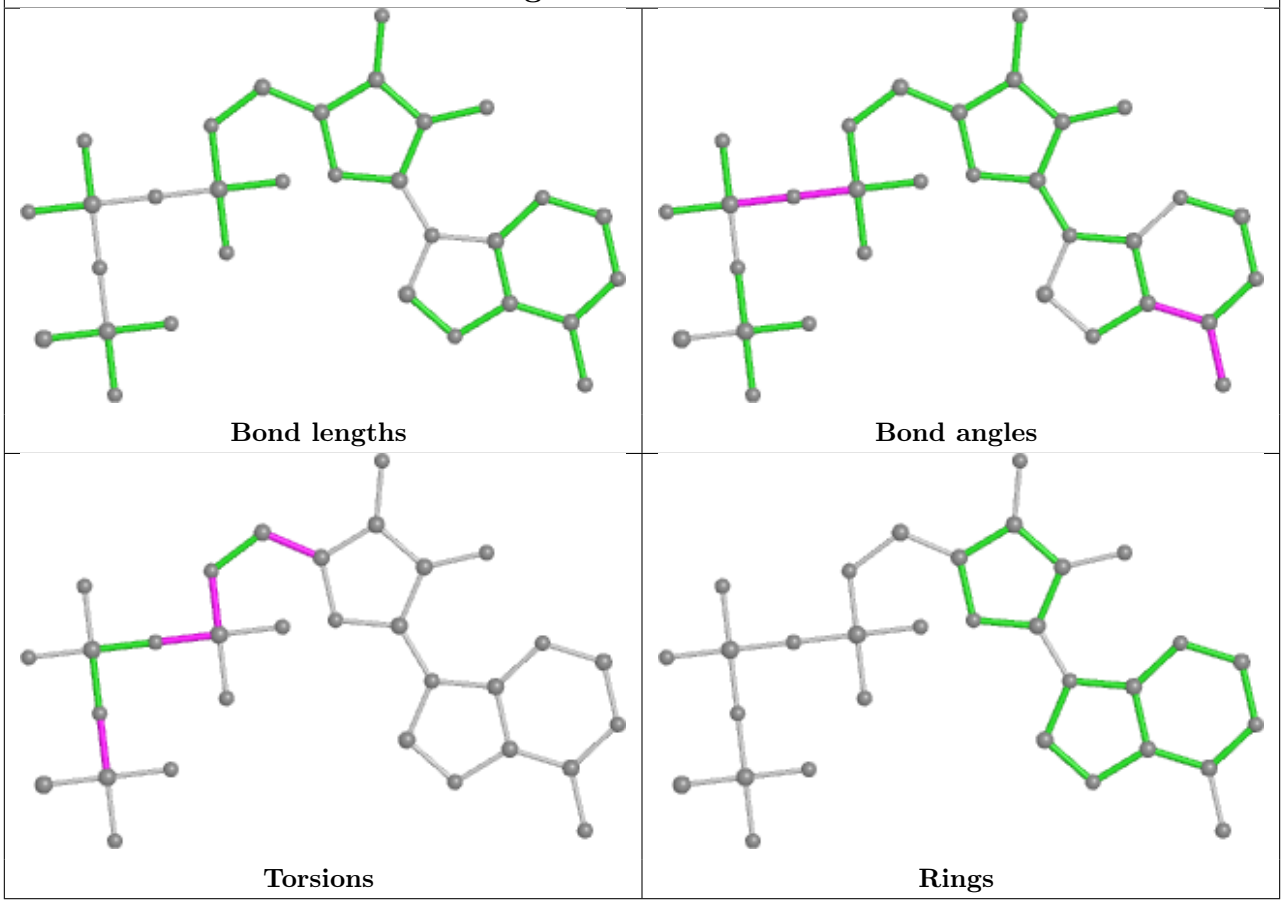
28 monomers are involved in 88 short contacts:

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

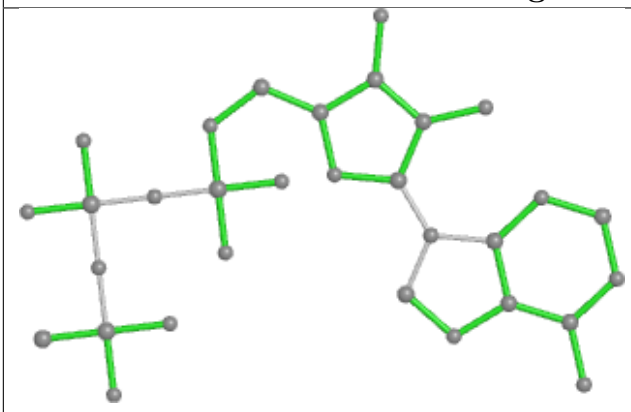
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

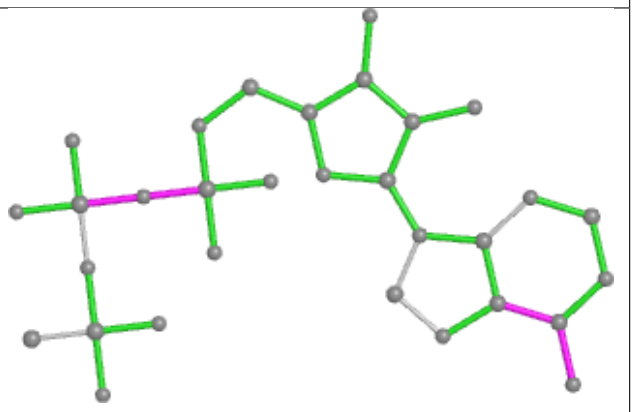
Ligand AGS G 802



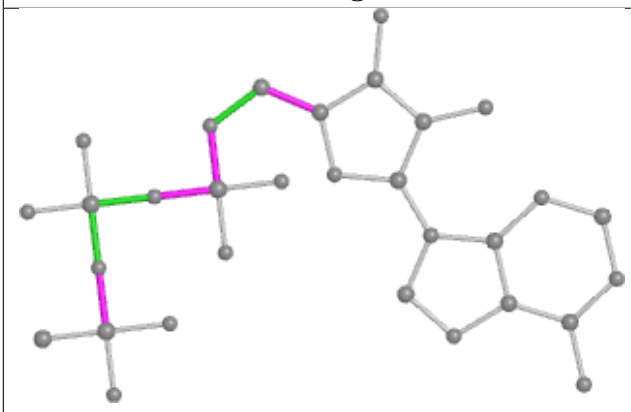
Ligand AGS J 802



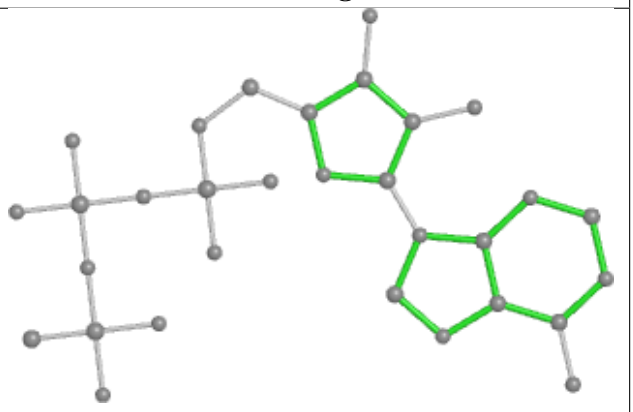
Bond lengths



Bond angles

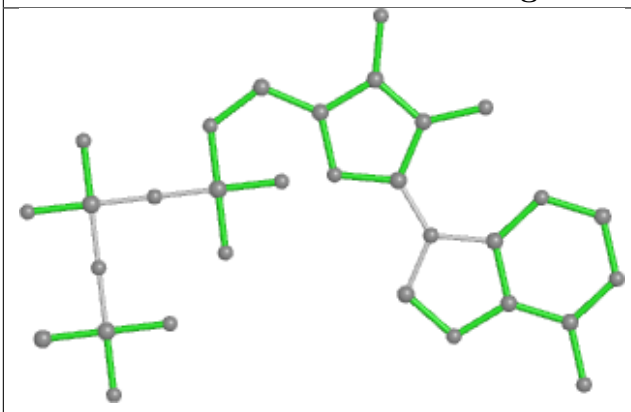


Torsions



Rings

Ligand AGS M 803



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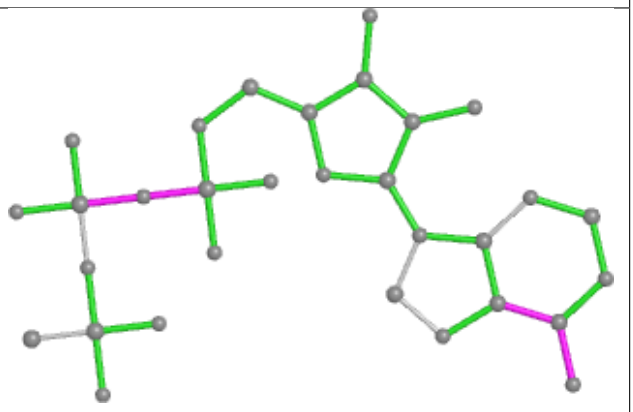
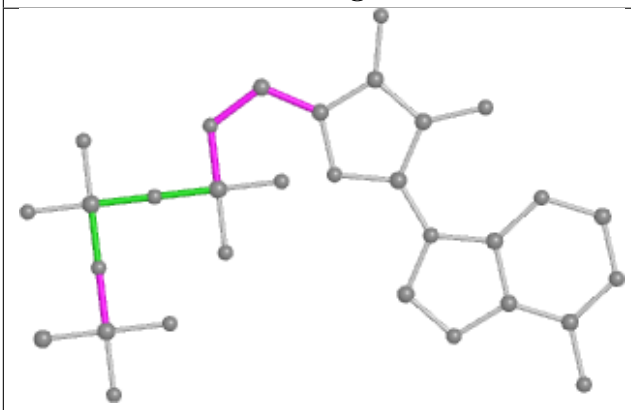


Bond angles



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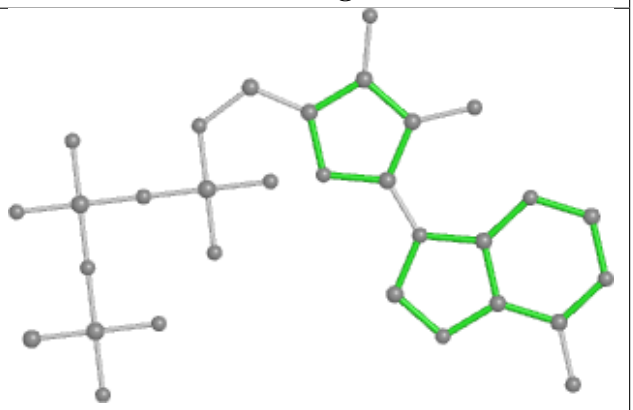
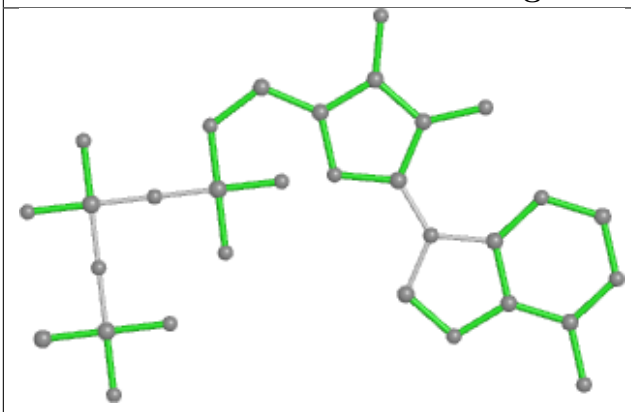


Rings

Ligand AGS D 803



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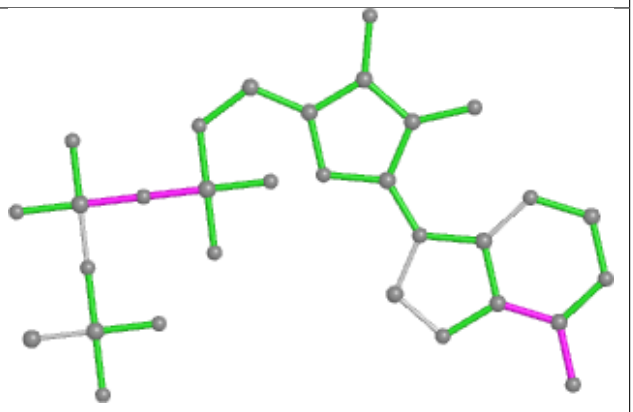
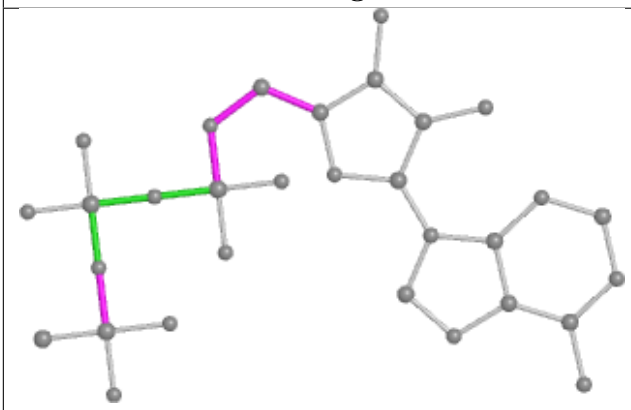


Bond angles



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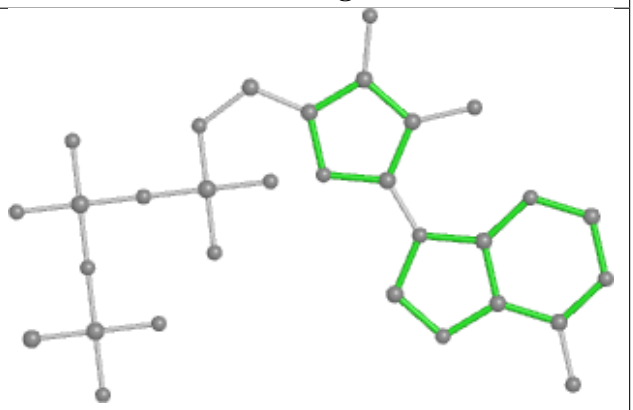
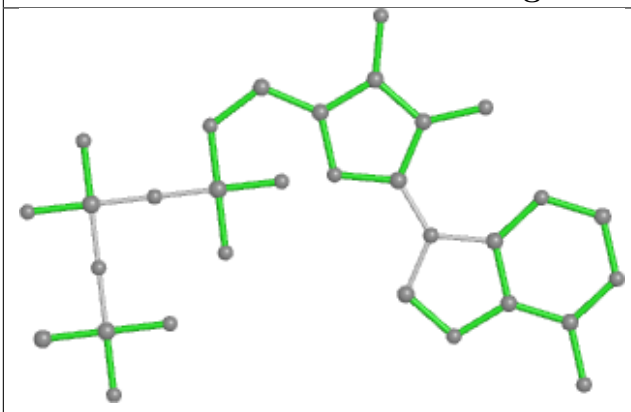


Rings

Ligand AGS H 803



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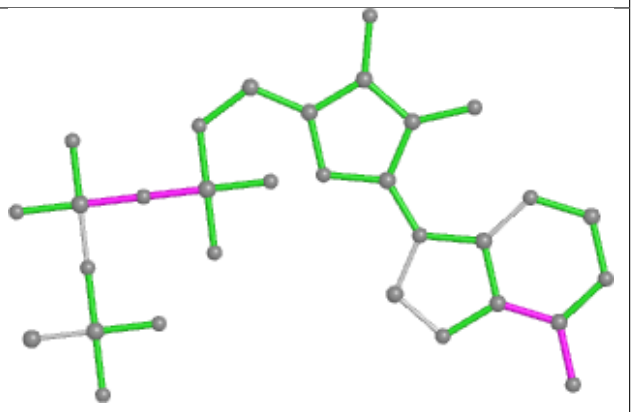
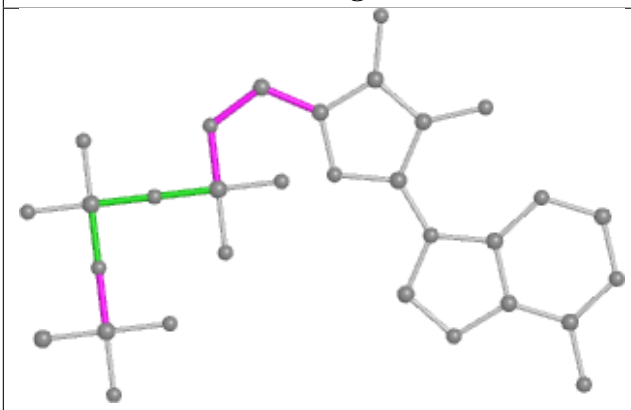
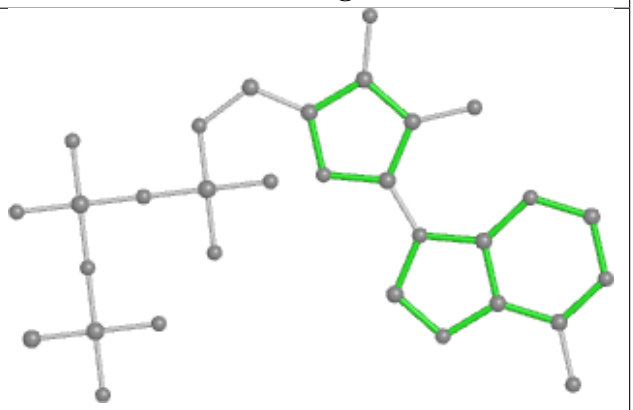


Bond angles

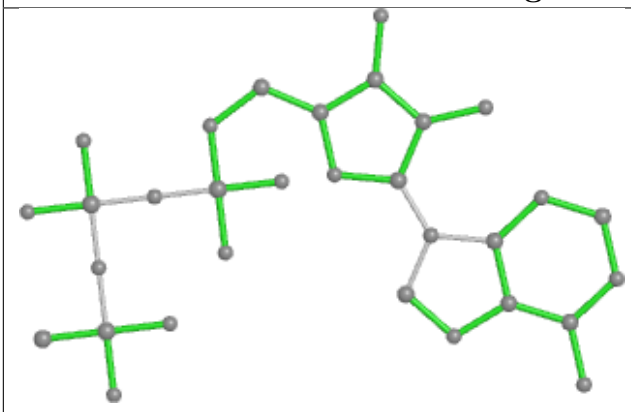


Torsions



Rings

Ligand AGS B 802



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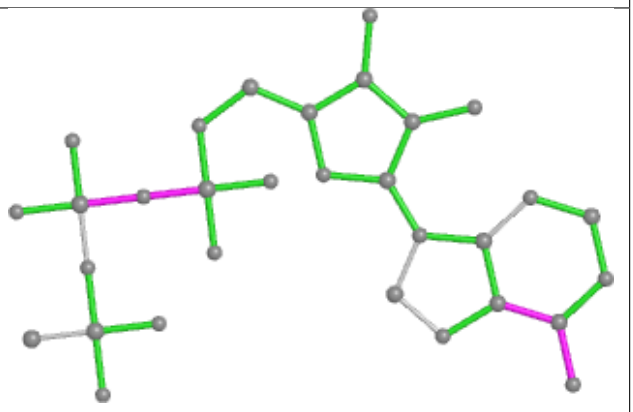
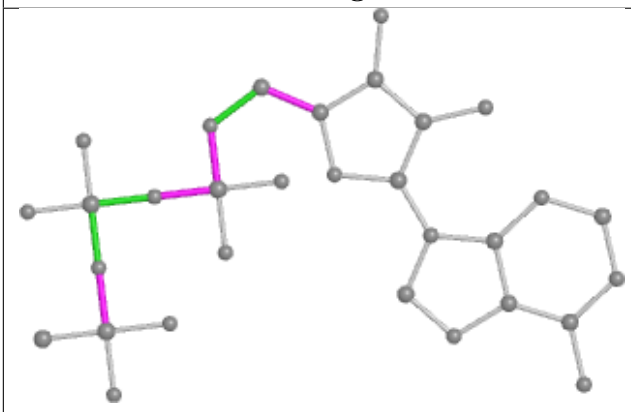


Bond angles



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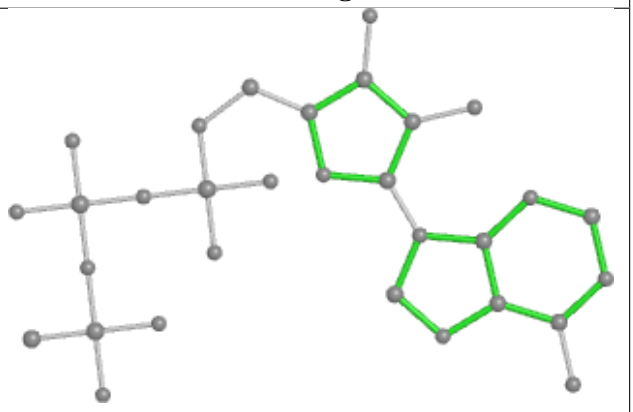
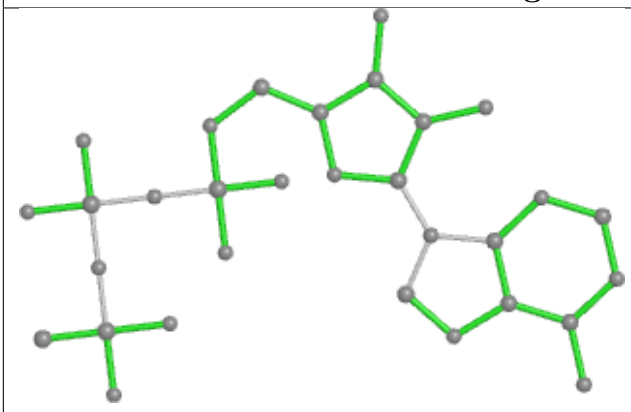


Rings

Ligand AGS A 802



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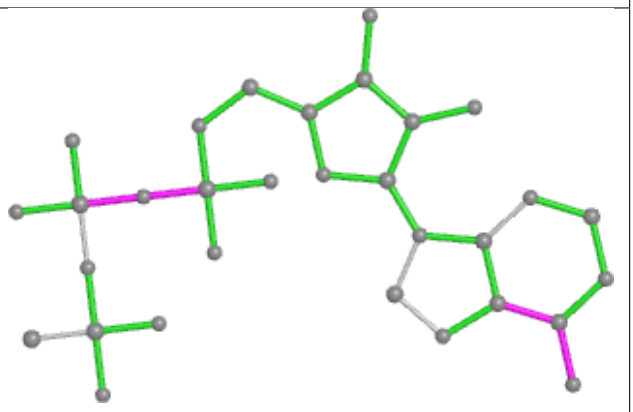

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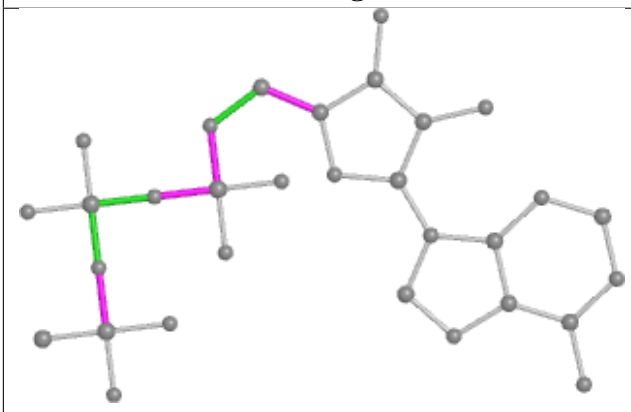

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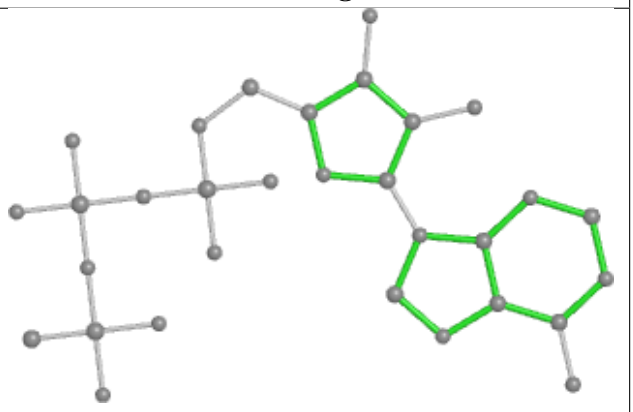
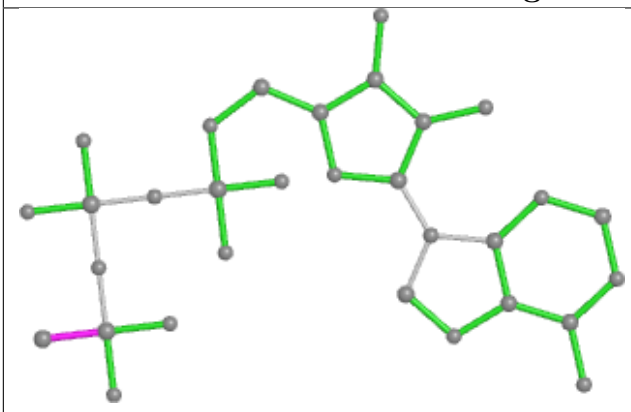


Rings

Ligand AGS H 802



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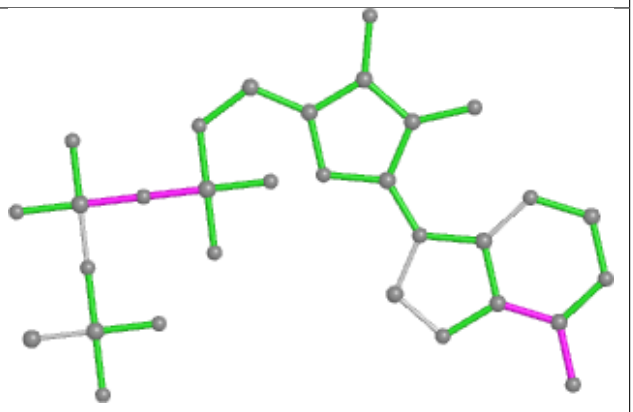

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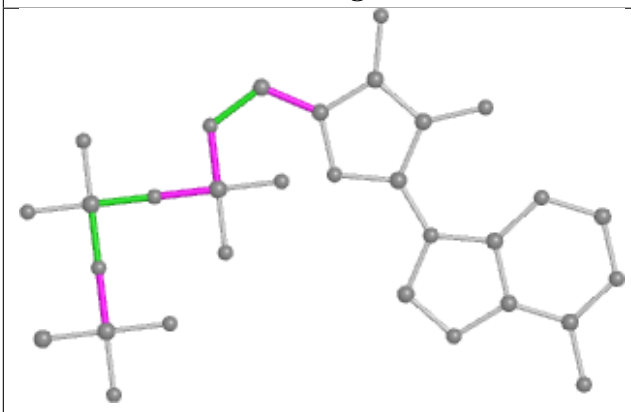

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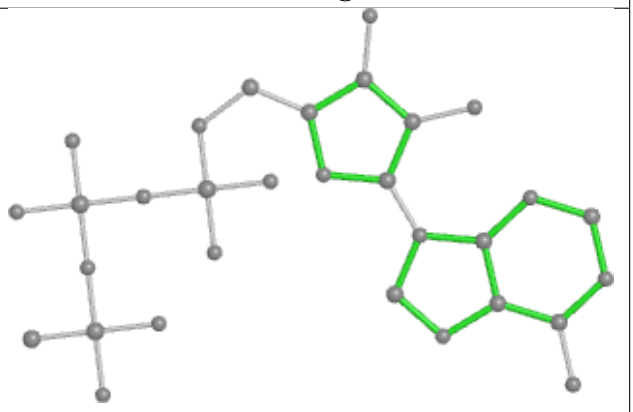
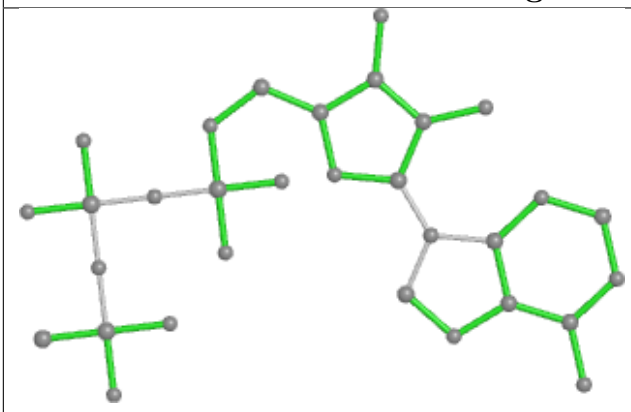


Rings

Ligand AGS E 803



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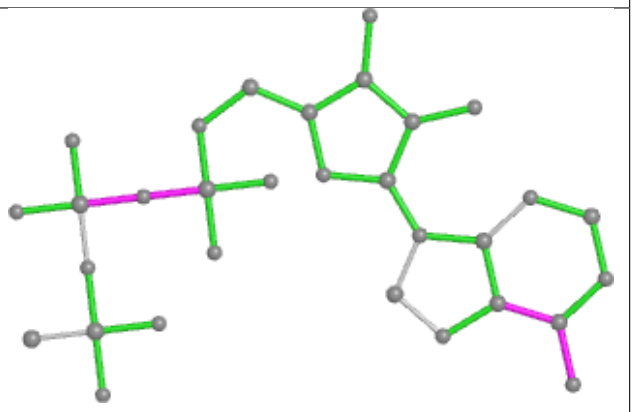
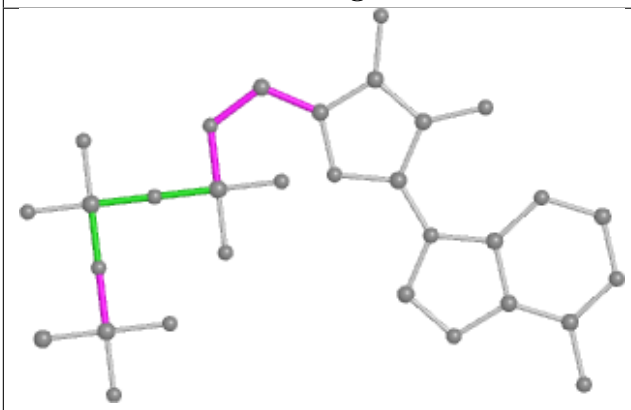


Bond angles



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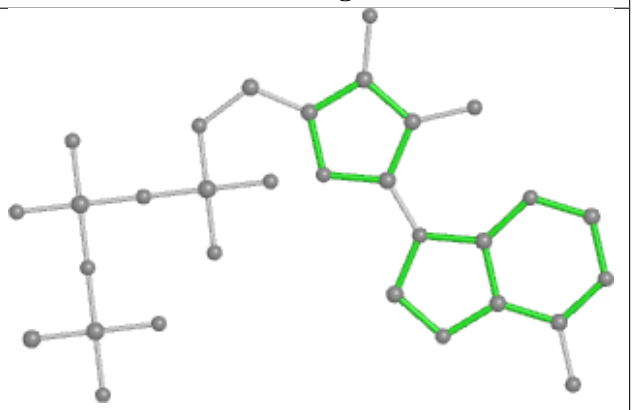
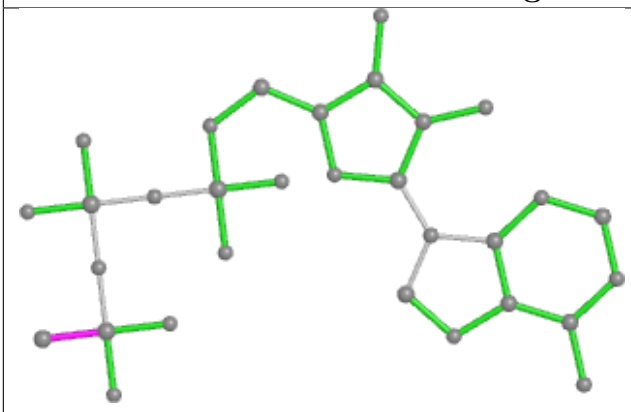


Rings

Ligand AGS D 802



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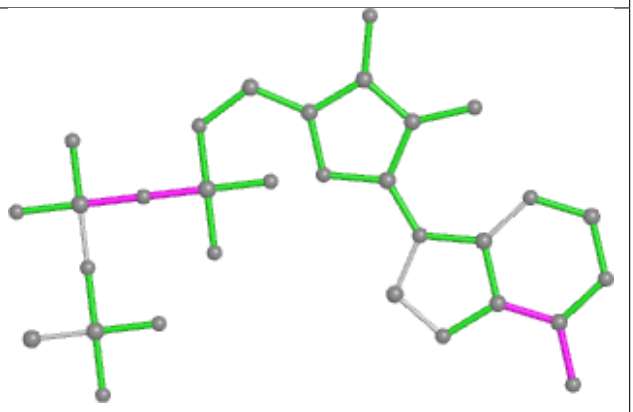
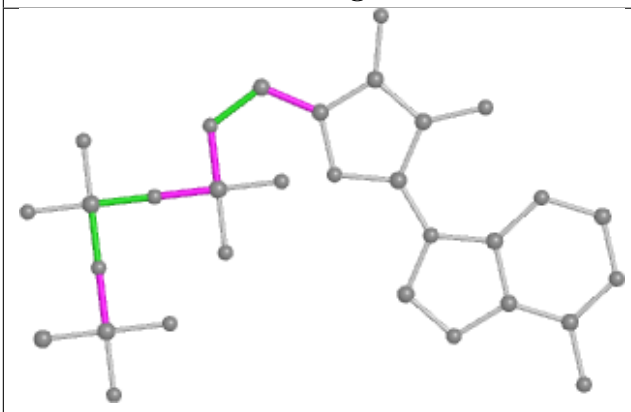


Bond angles



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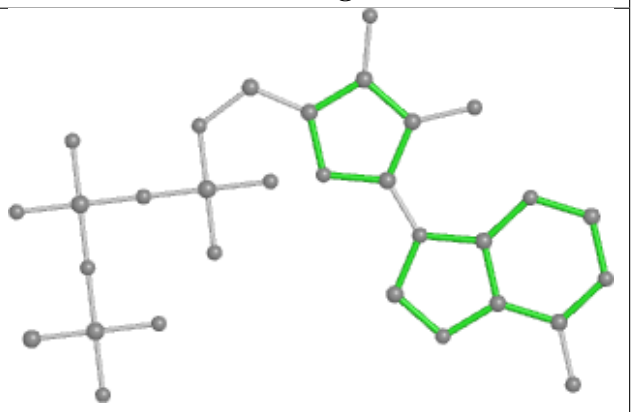
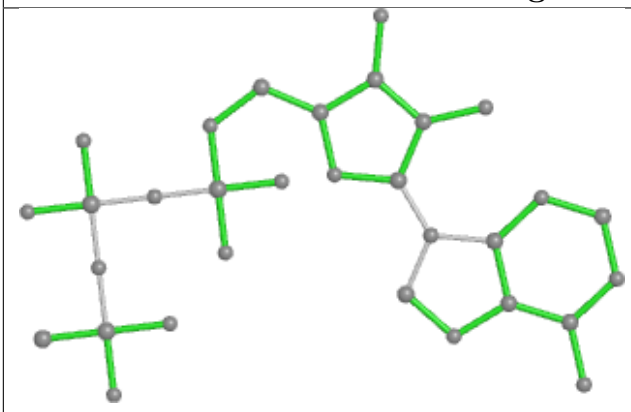


Rings

Ligand AGS J 803



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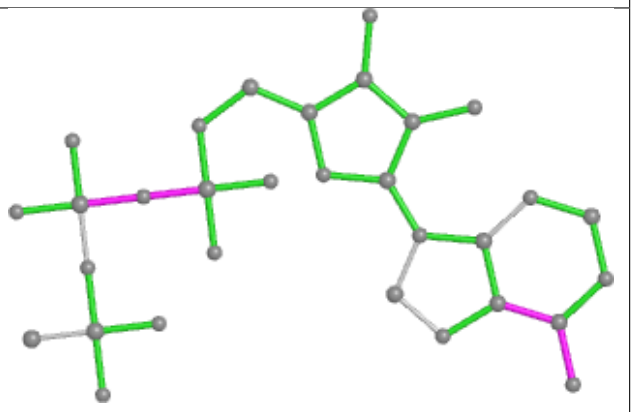
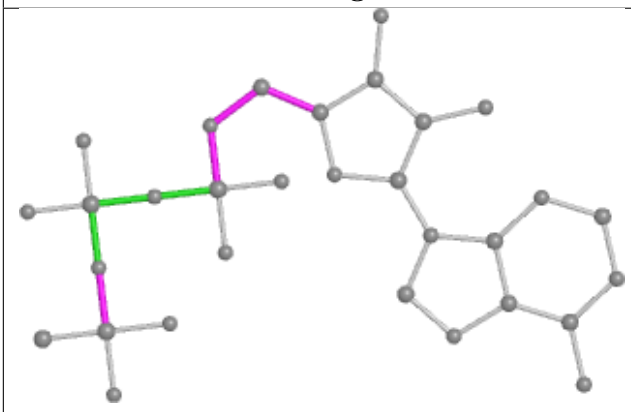


Bond angles



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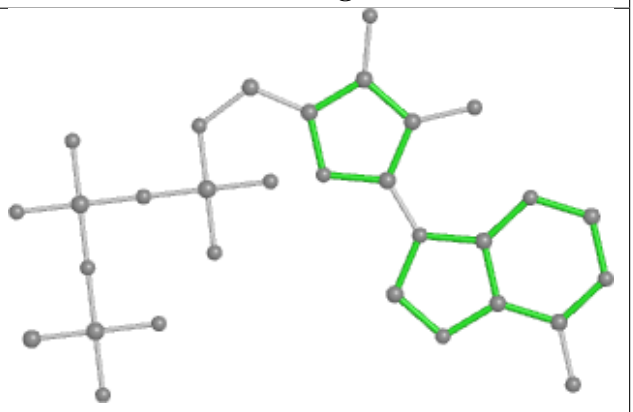
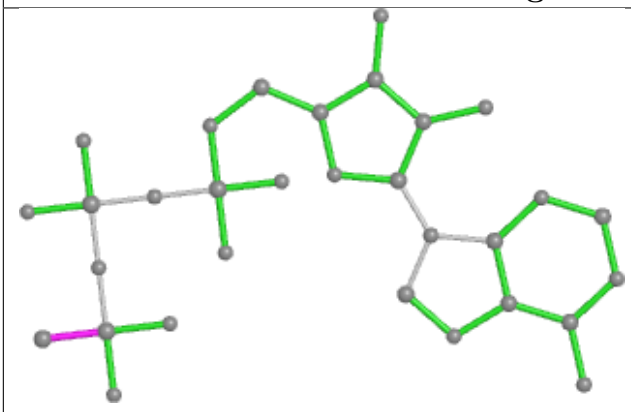


Rings

Ligand AGS L 802



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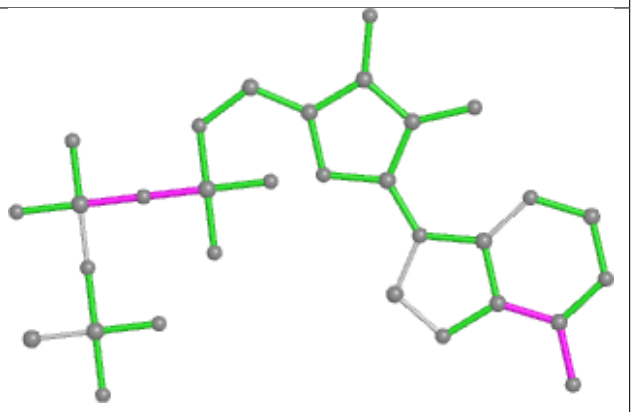
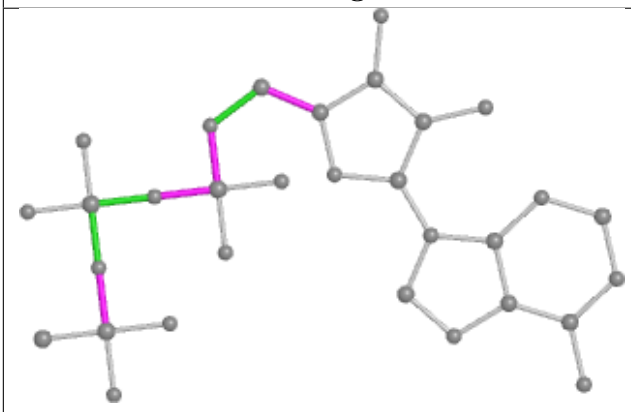


Bond angles



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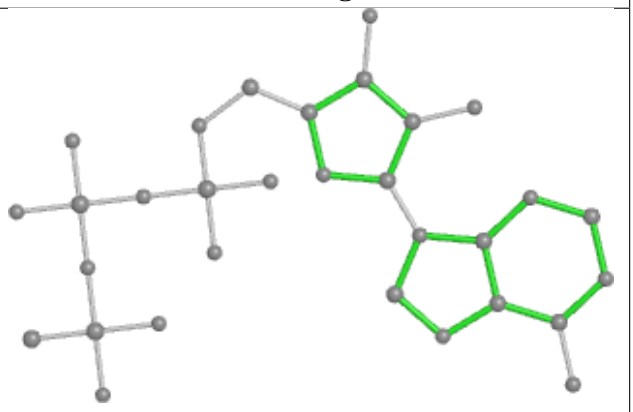
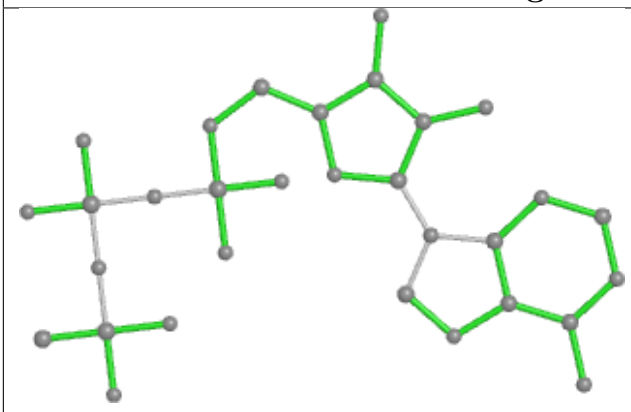


Rings

Ligand AGS L 803



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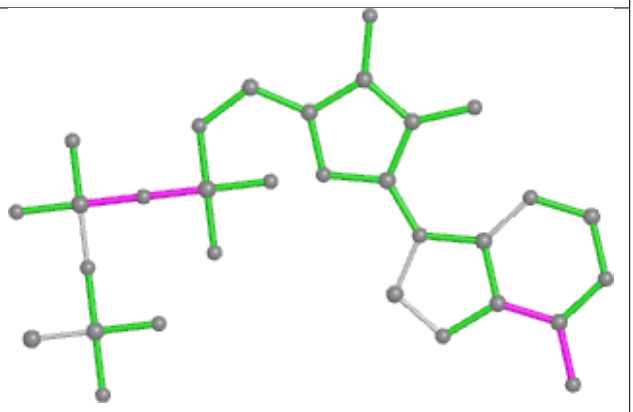
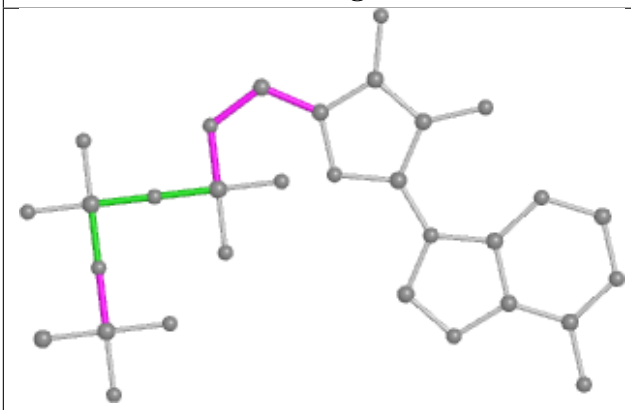
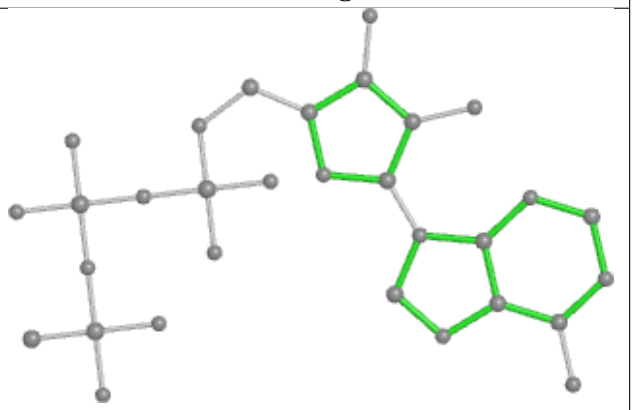


Bond angles

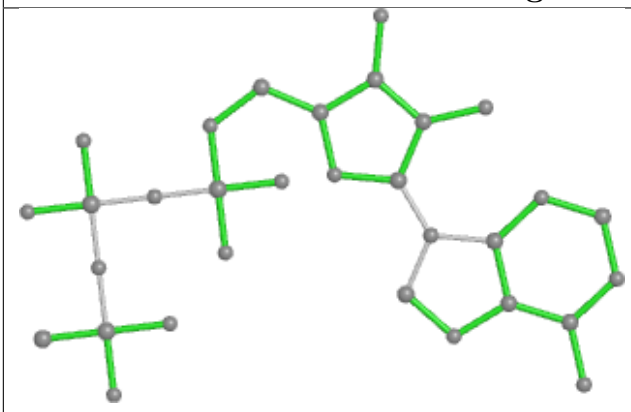


Torsions



Rings

Ligand AGS F 803



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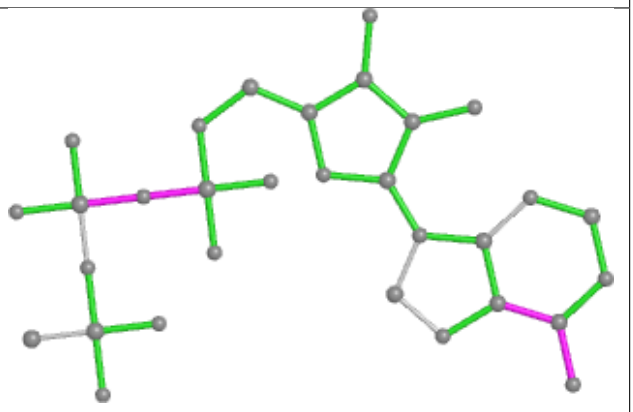
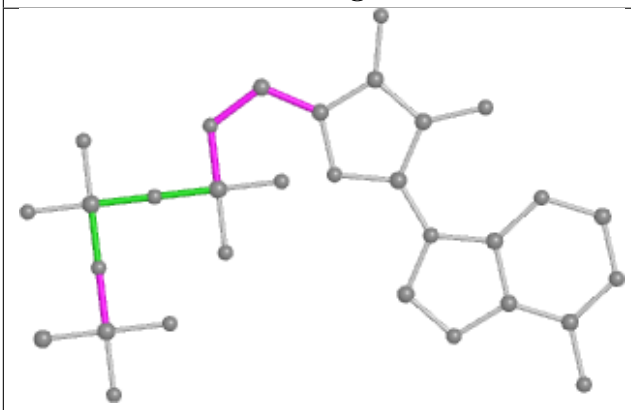
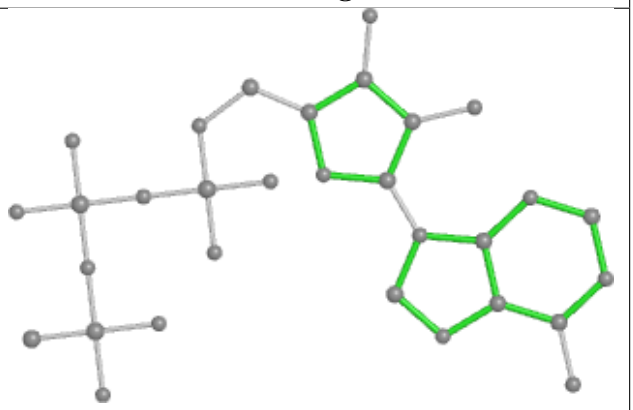


Bond angles

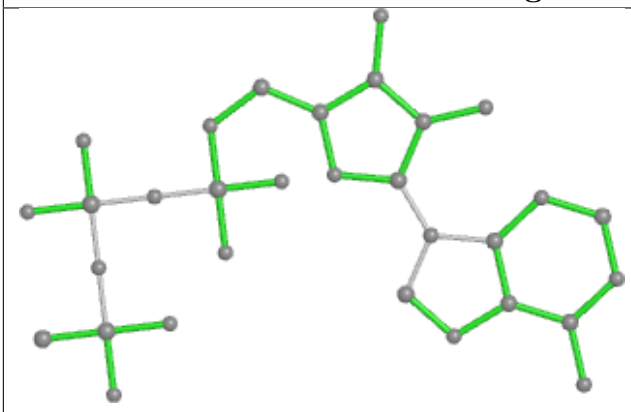


Torsions

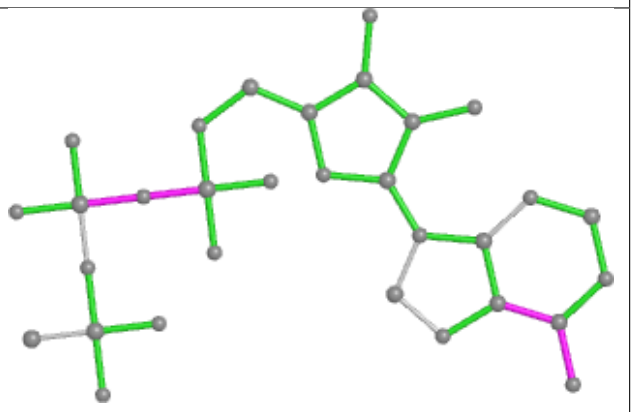


Rings

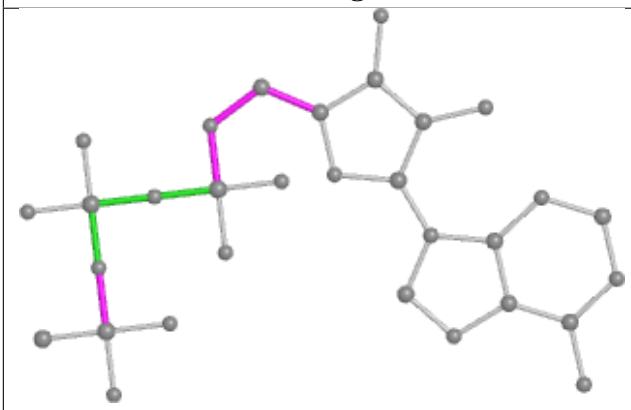
Ligand AGS B 803



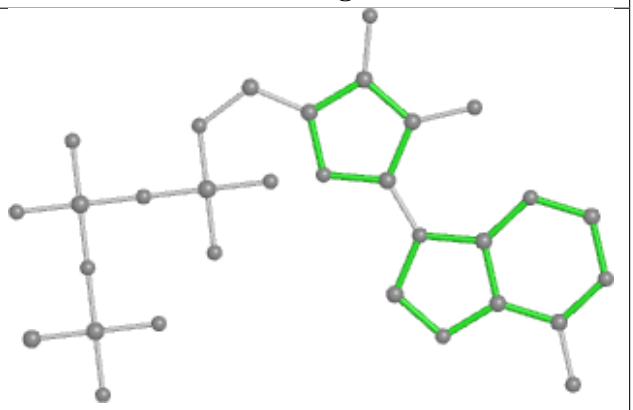
Bond lengths



Bond angles

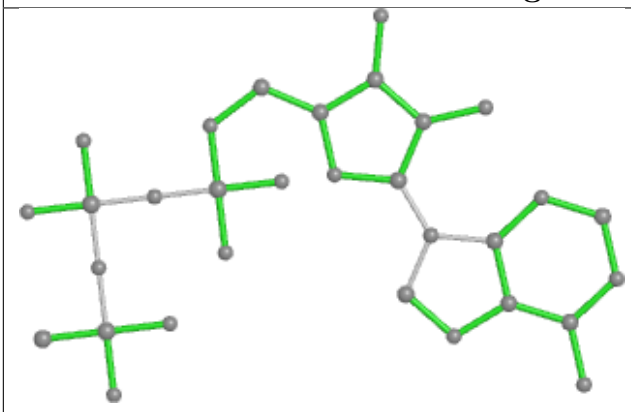


Torsions



Rings

Ligand AGS A 803



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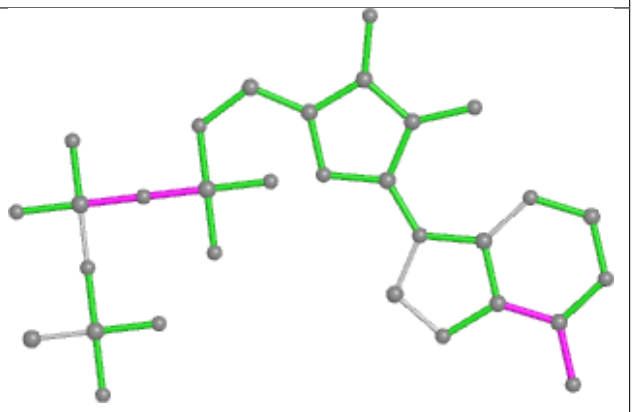

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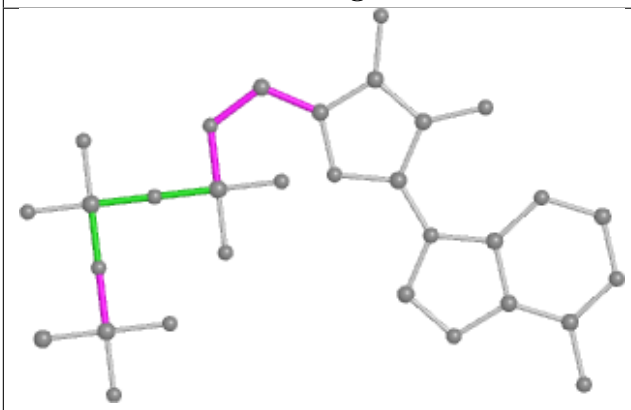

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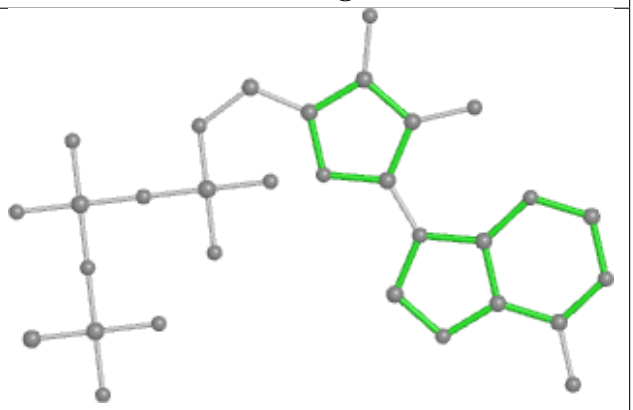
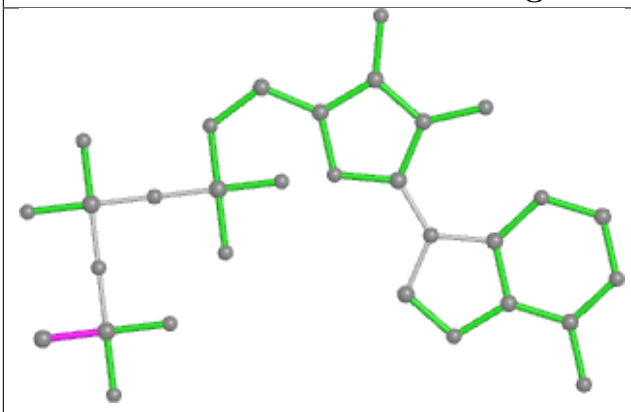


Rings

Ligand AGS E 802



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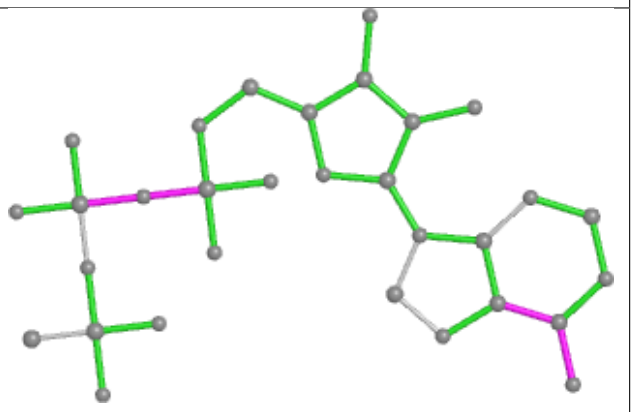

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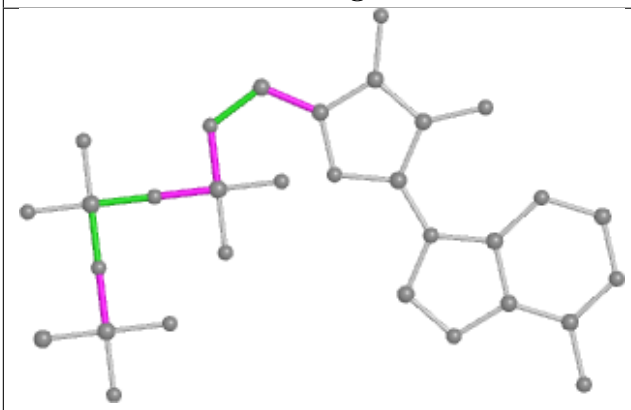

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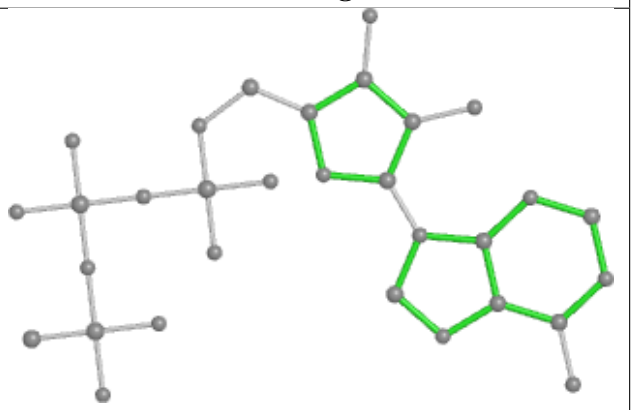
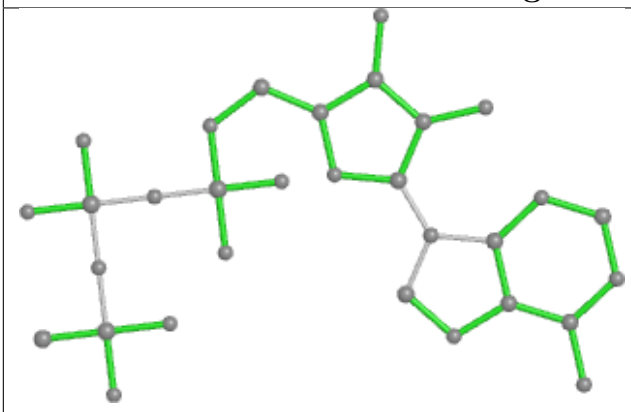


Rings

Ligand AGS K 802



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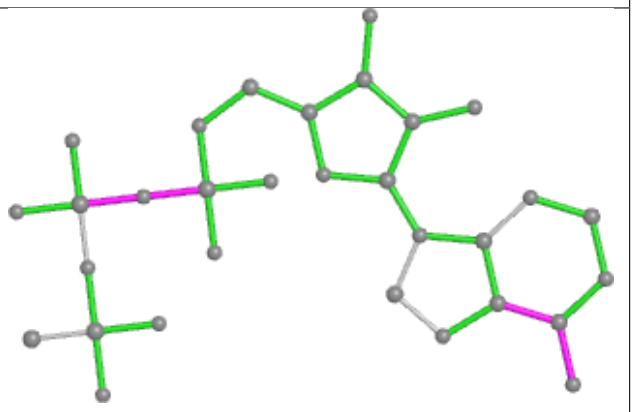
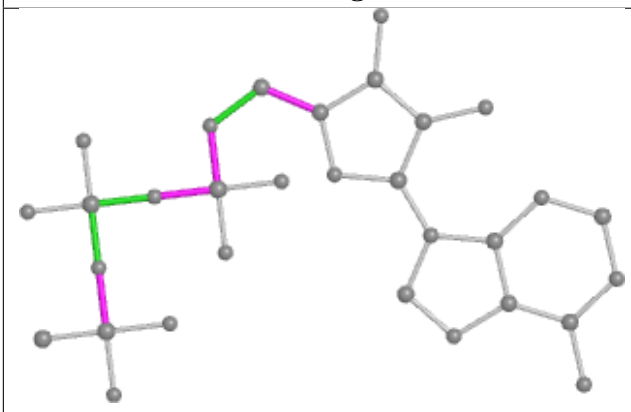


Bond angles



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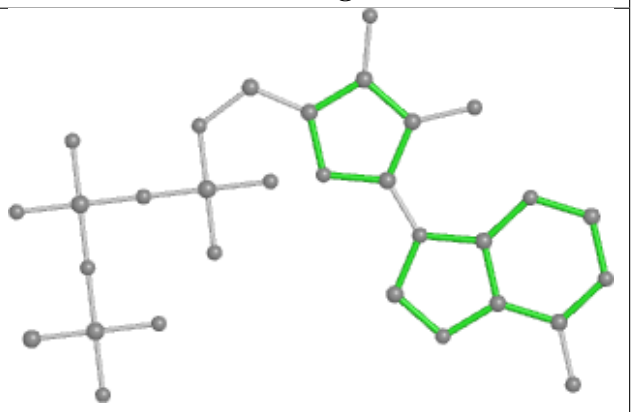
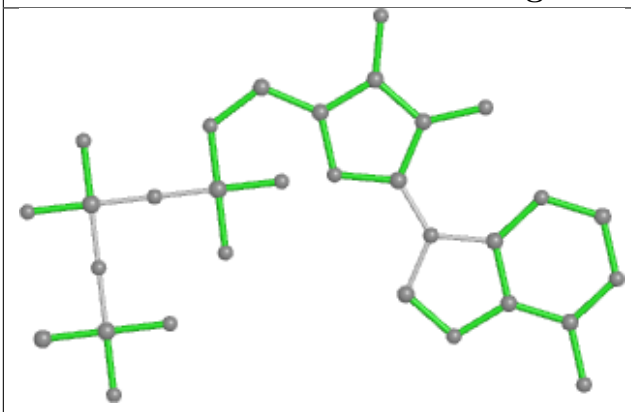
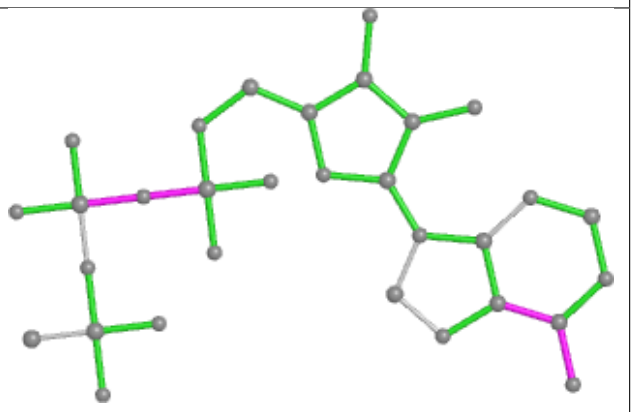


Rings

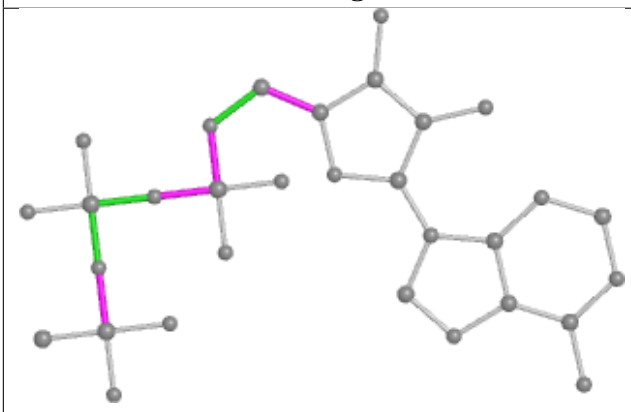
Ligand AGS F 802



Bond lengths



Bond angles



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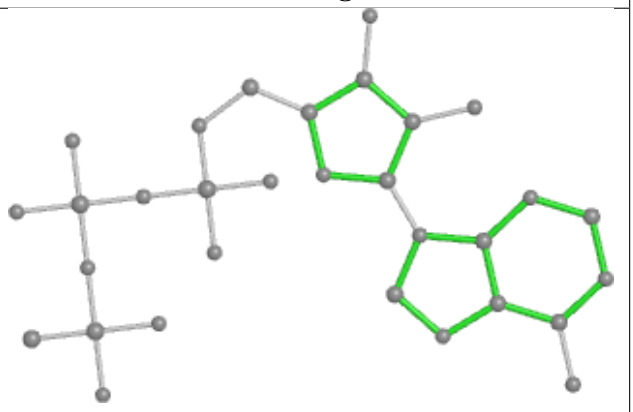
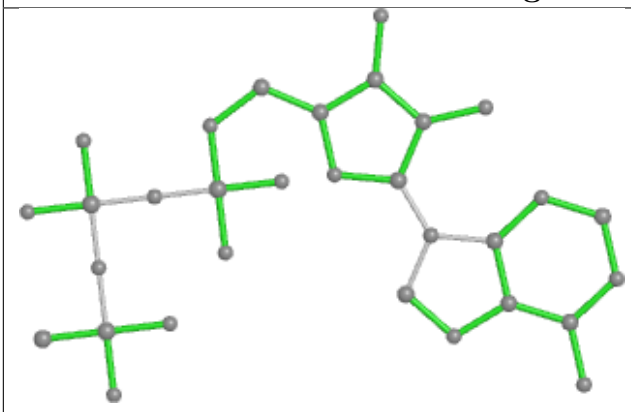


Rings

Ligand AGS N 803



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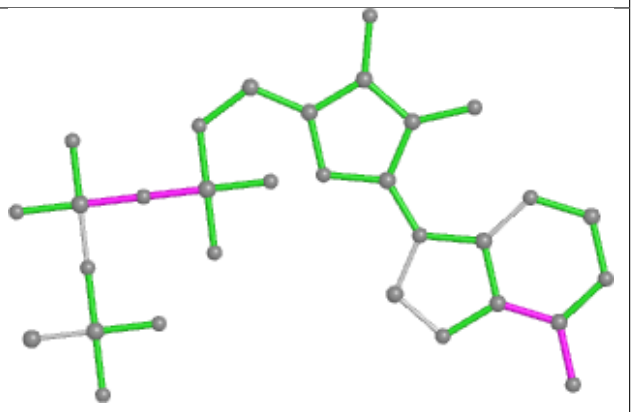
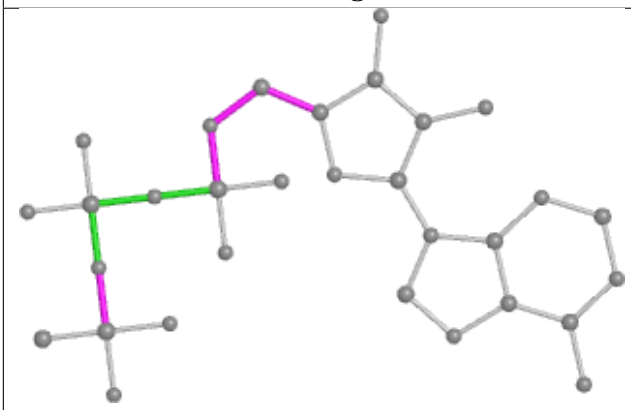


Bond angles



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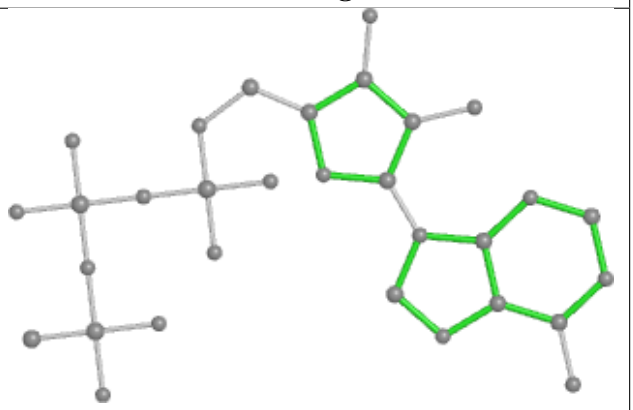
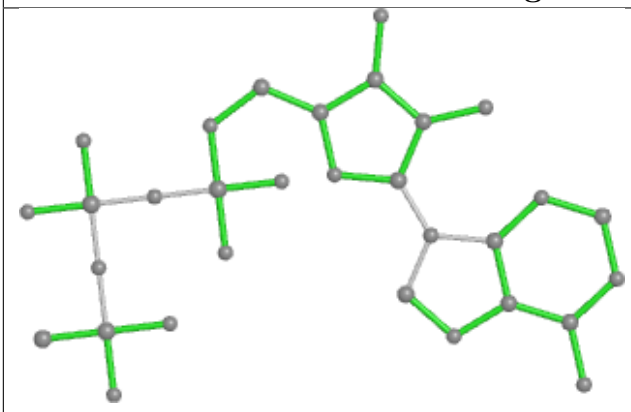


Rings

Ligand AGS C 802



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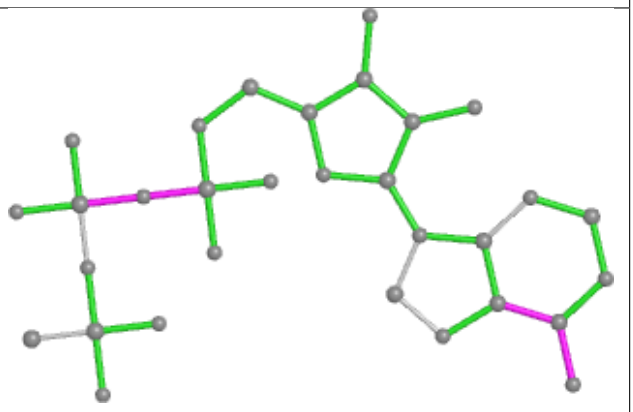

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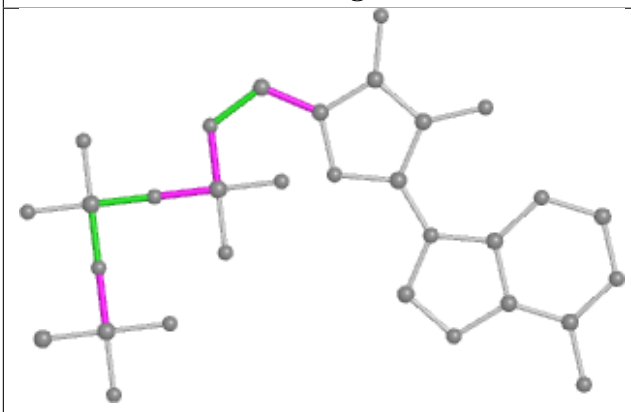

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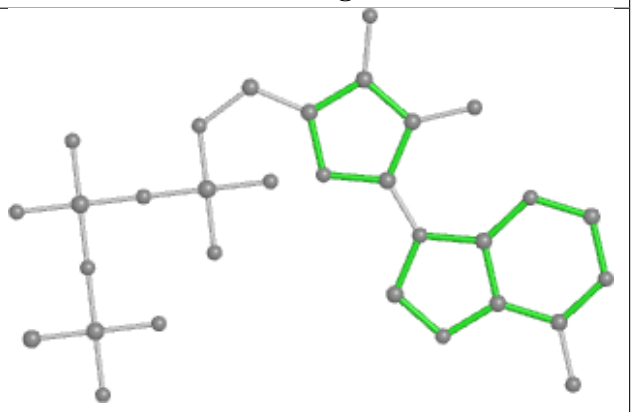
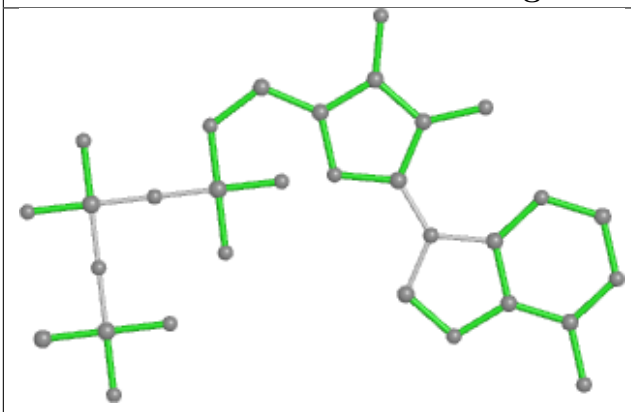


Rings

Ligand AGS G 803



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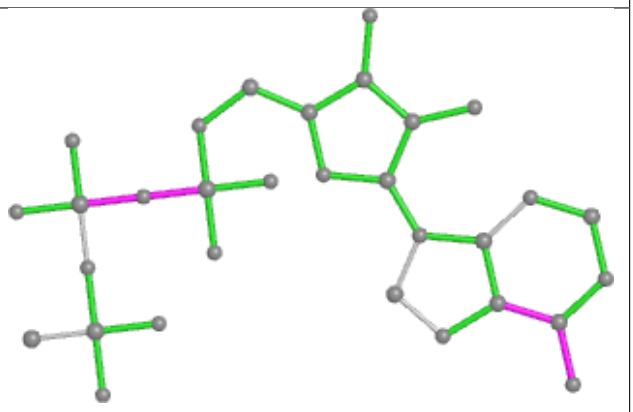
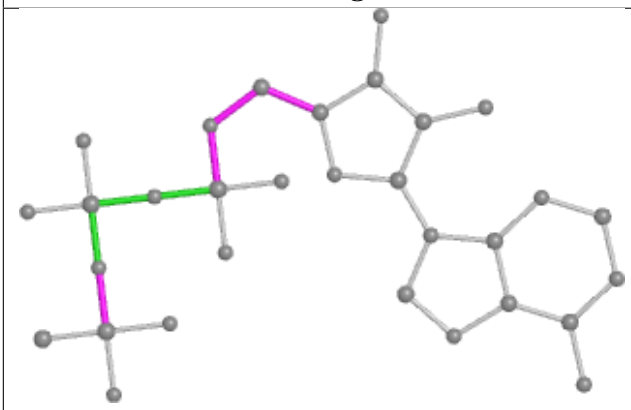


Bond angles



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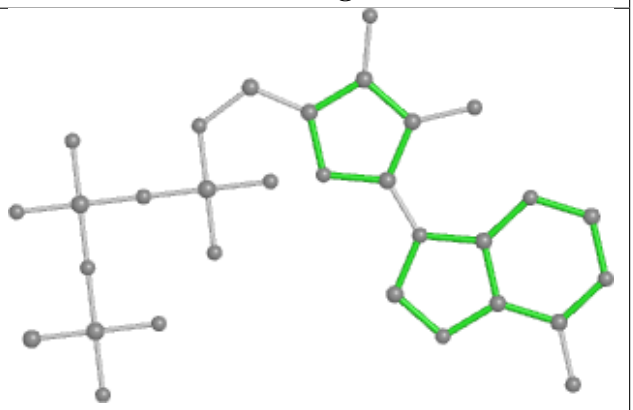
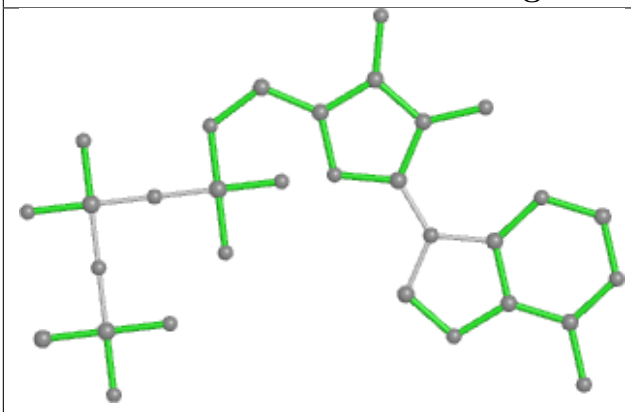


Rings

Ligand AGS K 803



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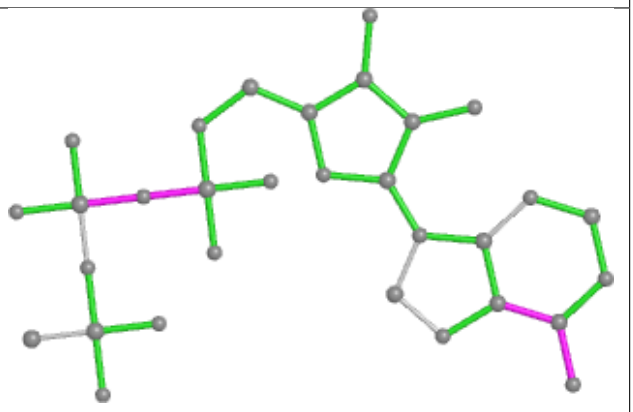
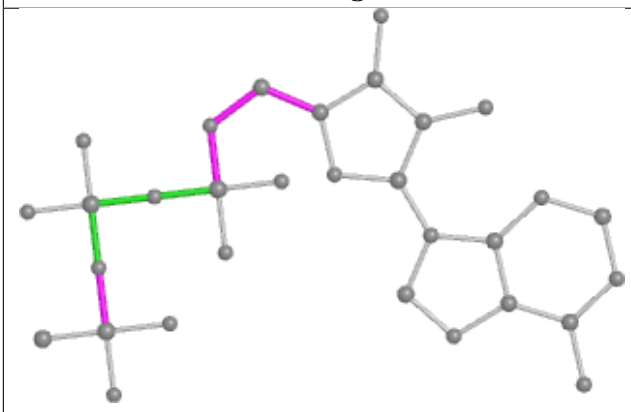


Bond angles



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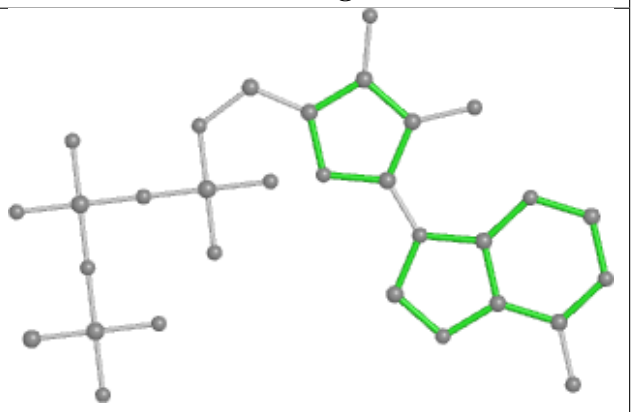
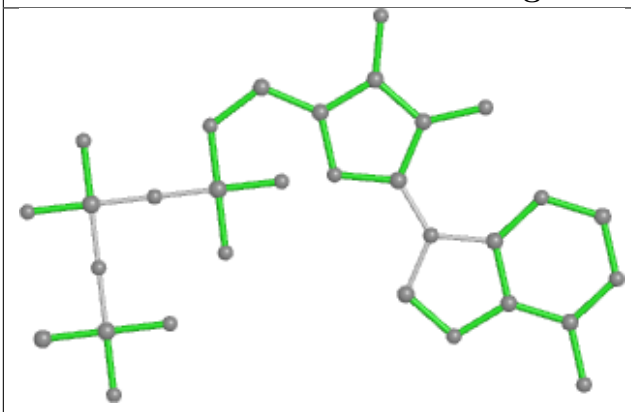
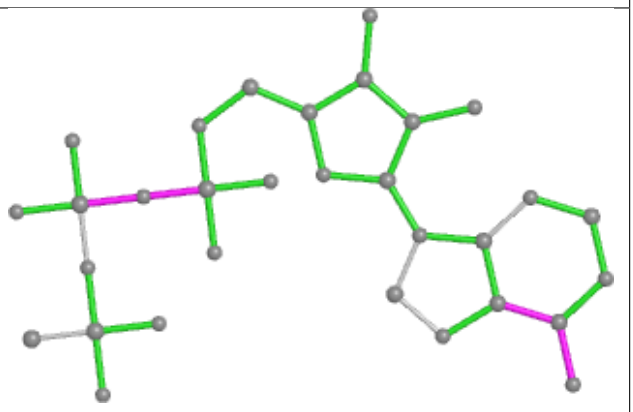


Rings

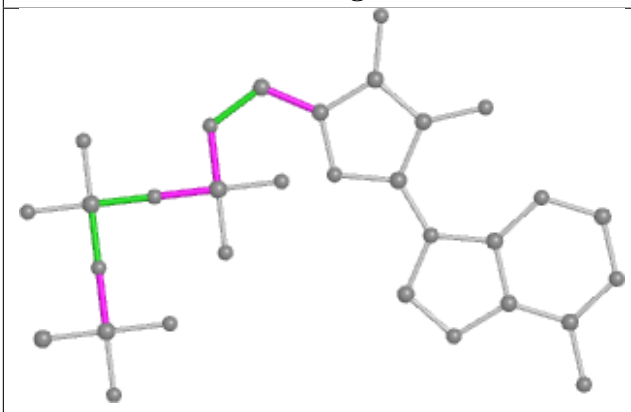
Ligand AGS N 802



Bond lengths



Bond angles



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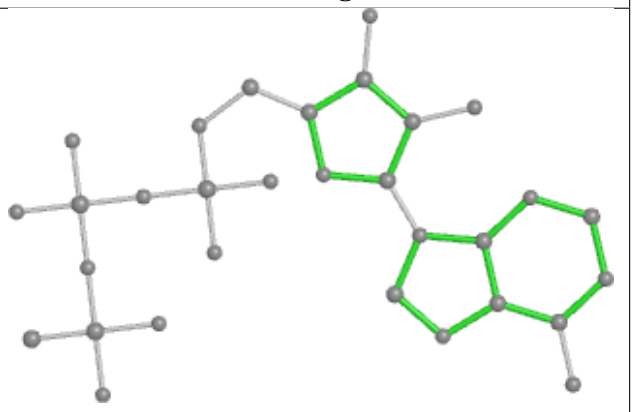
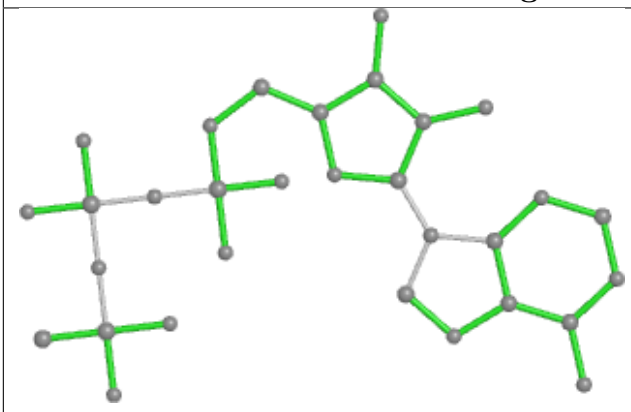
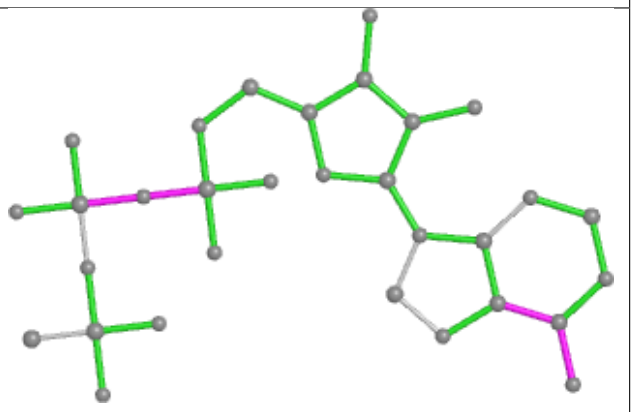


Rings

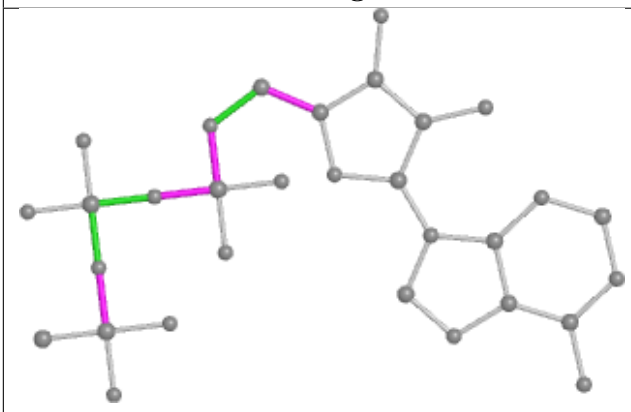
Ligand AGS M 802



Bond lengths



Bond angles



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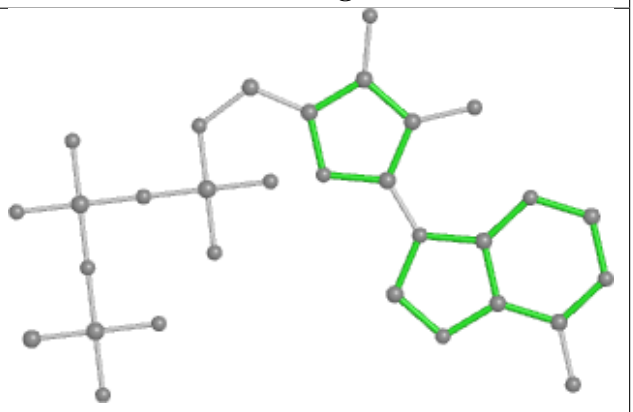
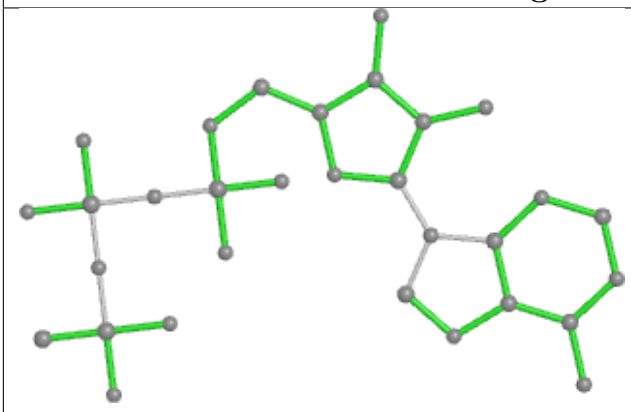


Rings

Ligand AGS I 803



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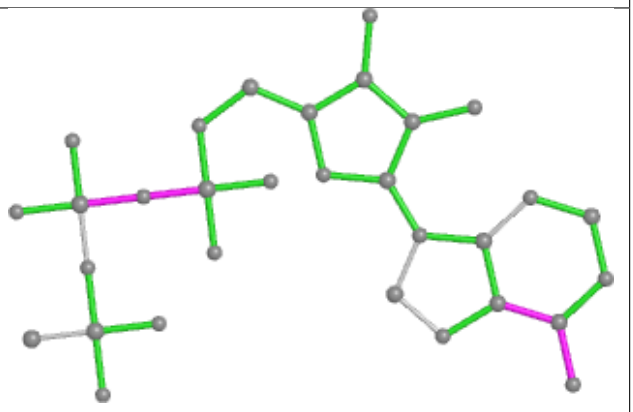
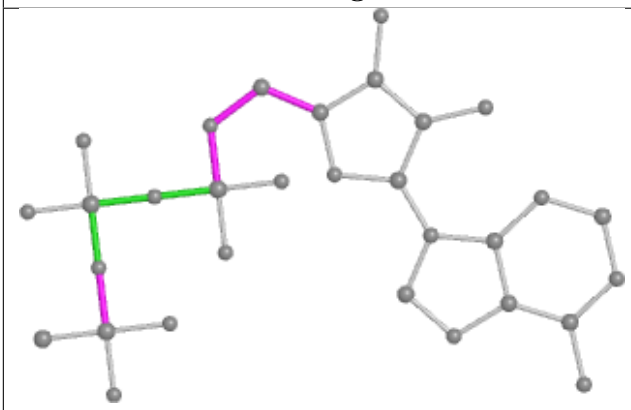


Bond angles



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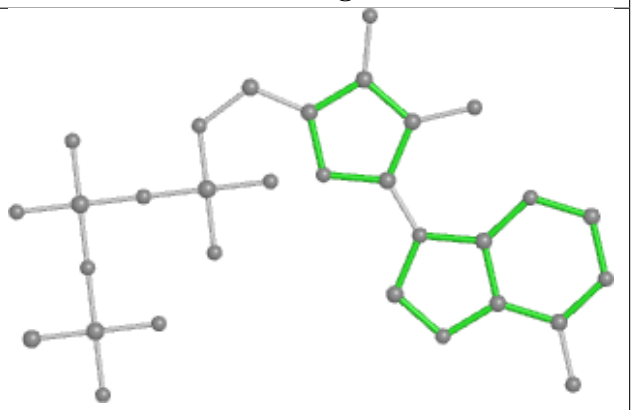
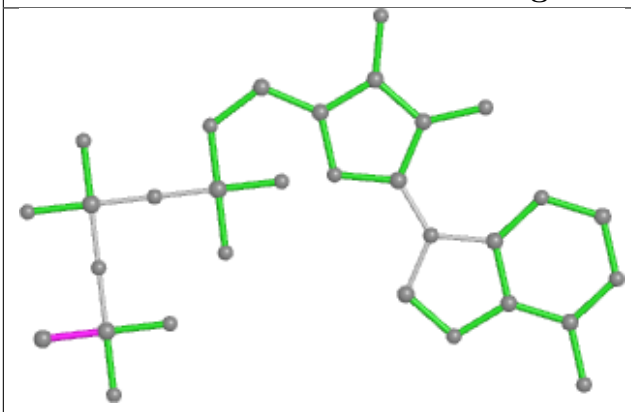
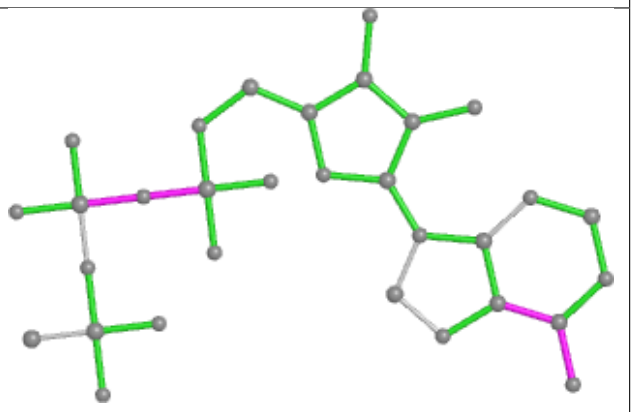


Rings

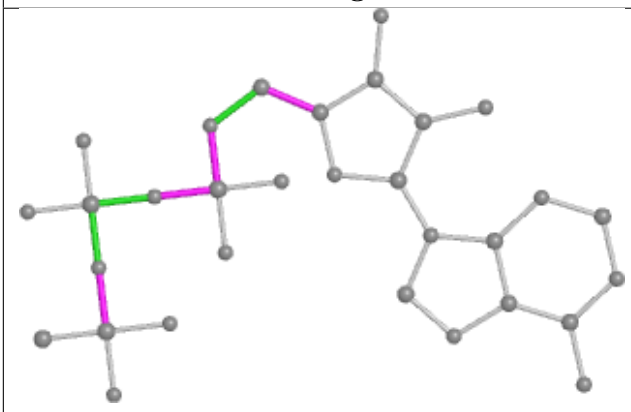
Ligand AGS I 802



Bond lengths



Bond angles



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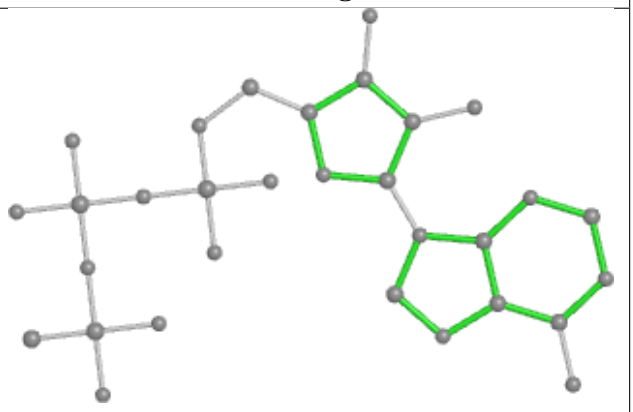
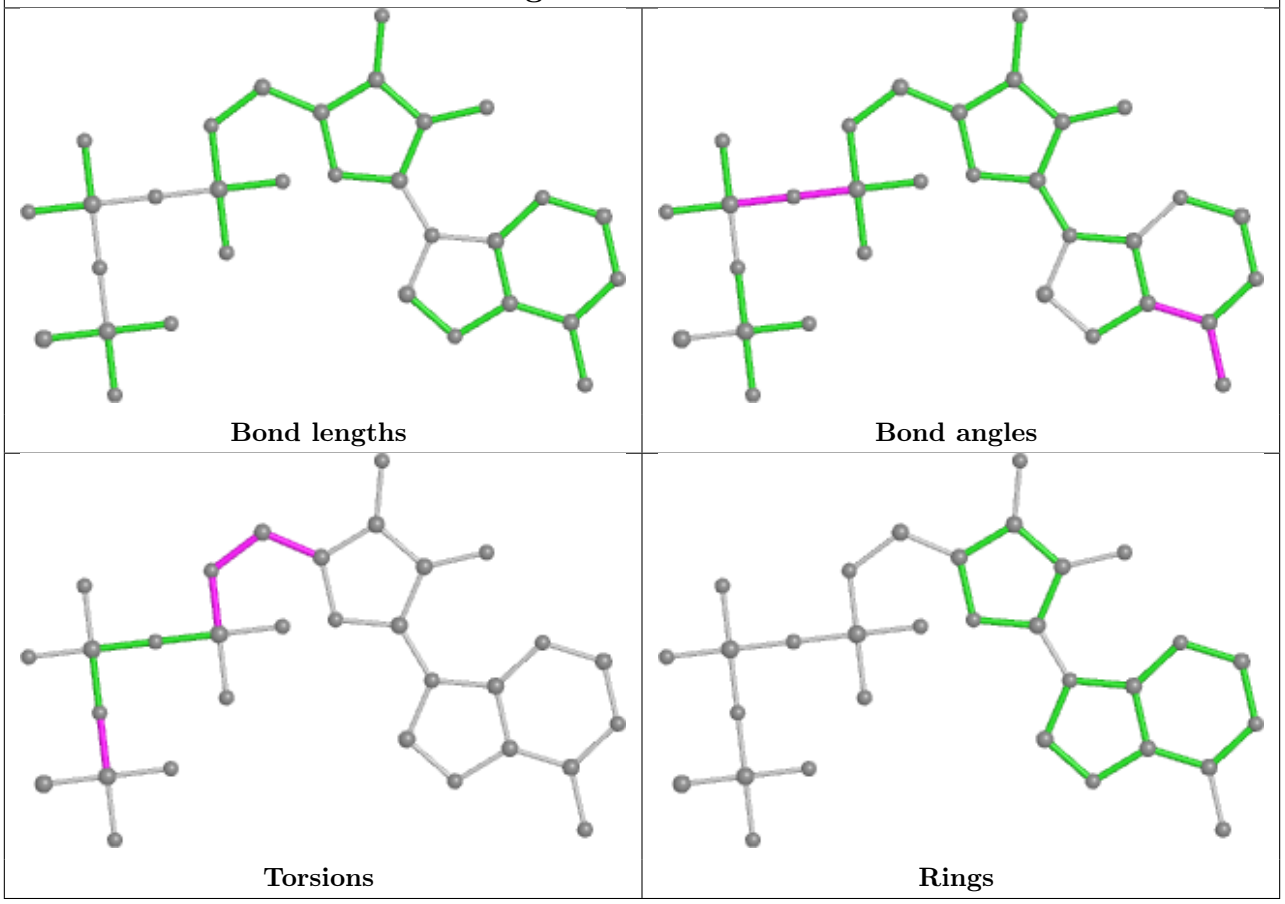


Rings

Ligand AGS C 803



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.

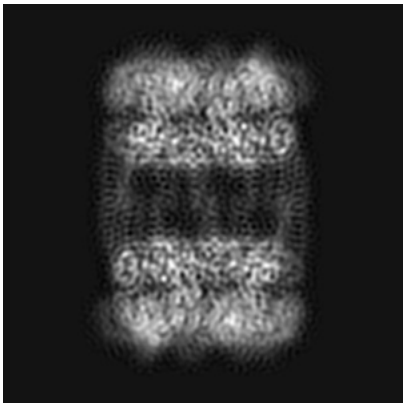
6 Map visualisation

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.

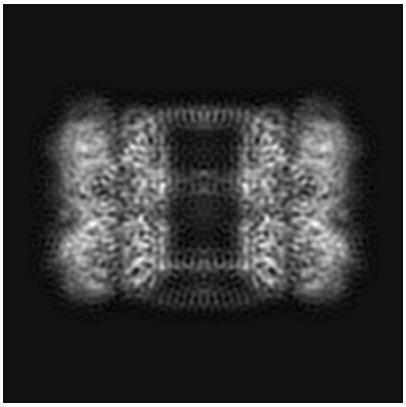
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

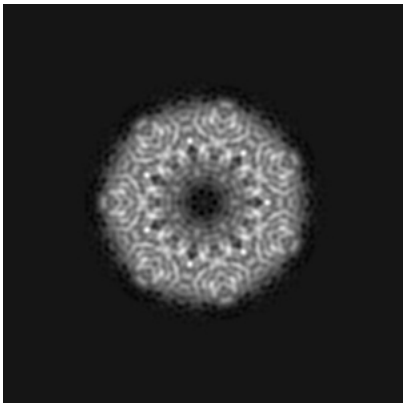
6.1.1 Primary map



X



Y

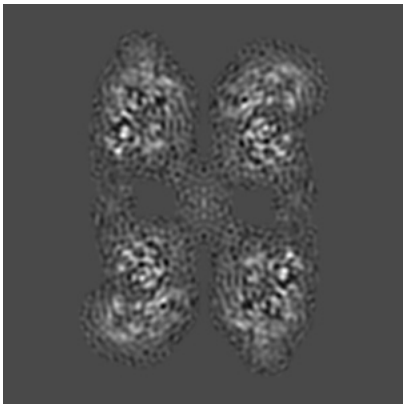


Z

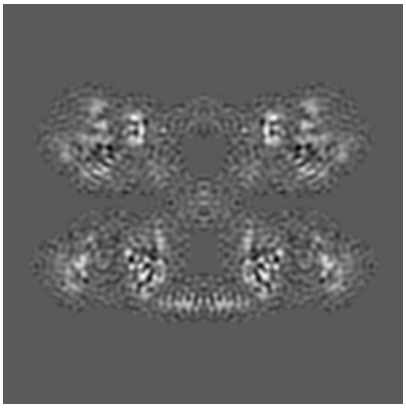
The images above show the map projected in three orthogonal directions.

6.2 Central slices

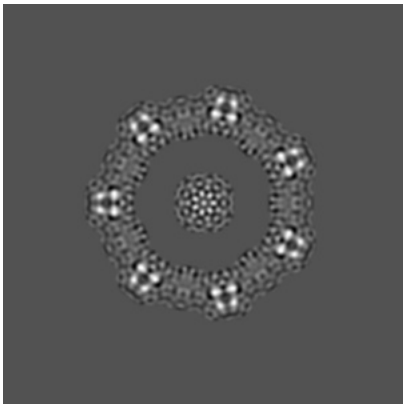
6.2.1 Primary map



X Index: 100



Y Index: 100



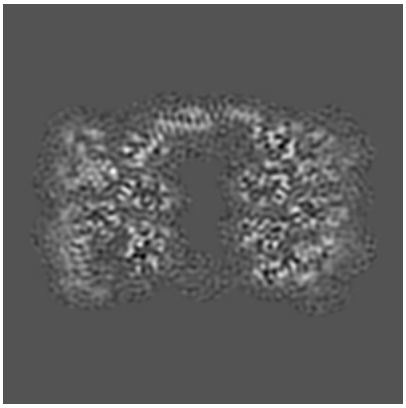
Z Index: 100

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



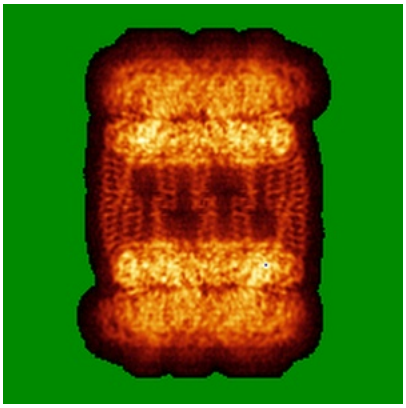
Y Index: 76

Z Index: 69

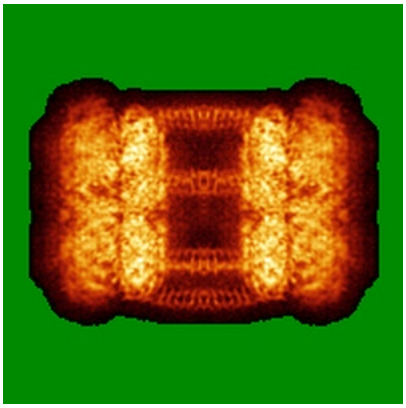
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

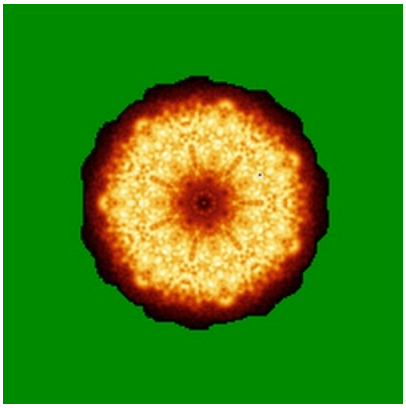
6.4.1 Primary map



X



Y

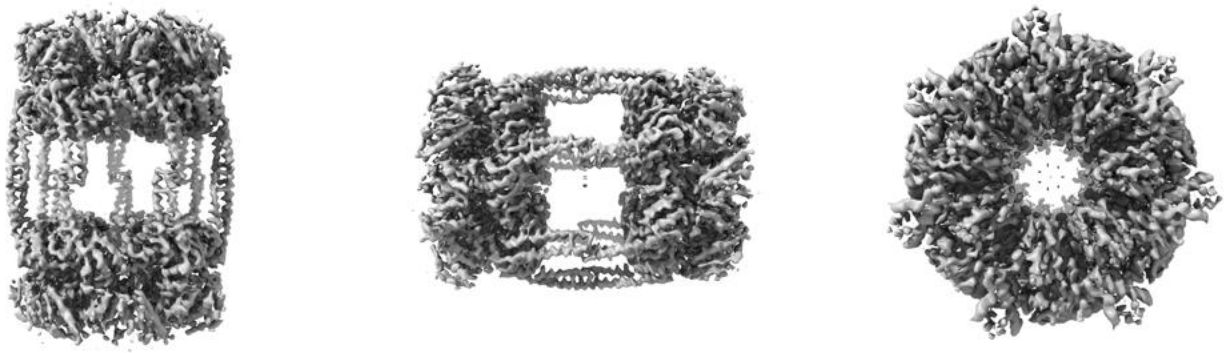


Z

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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

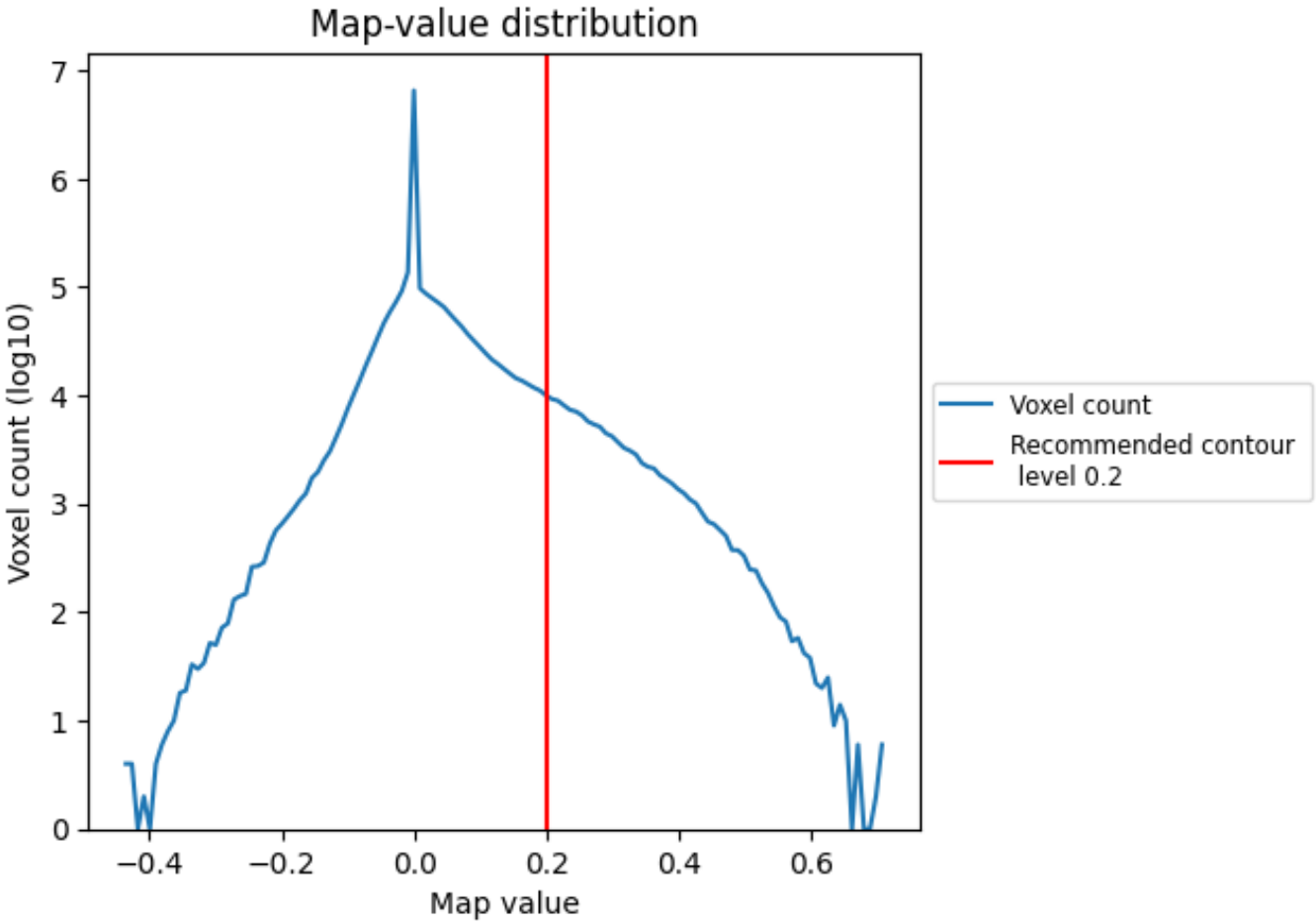
6.6 Mask visualisation (i)

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

7 Map analysis

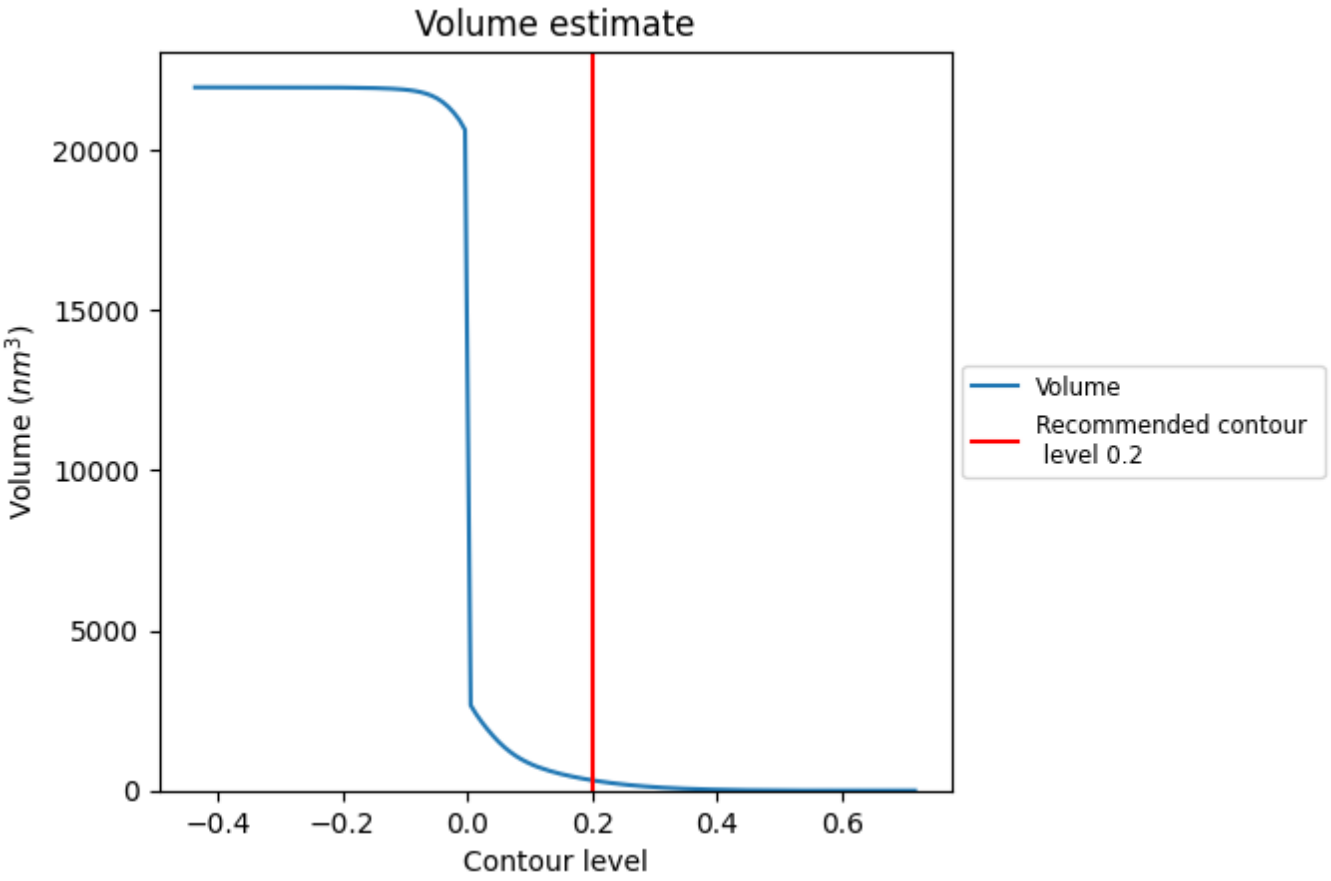
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

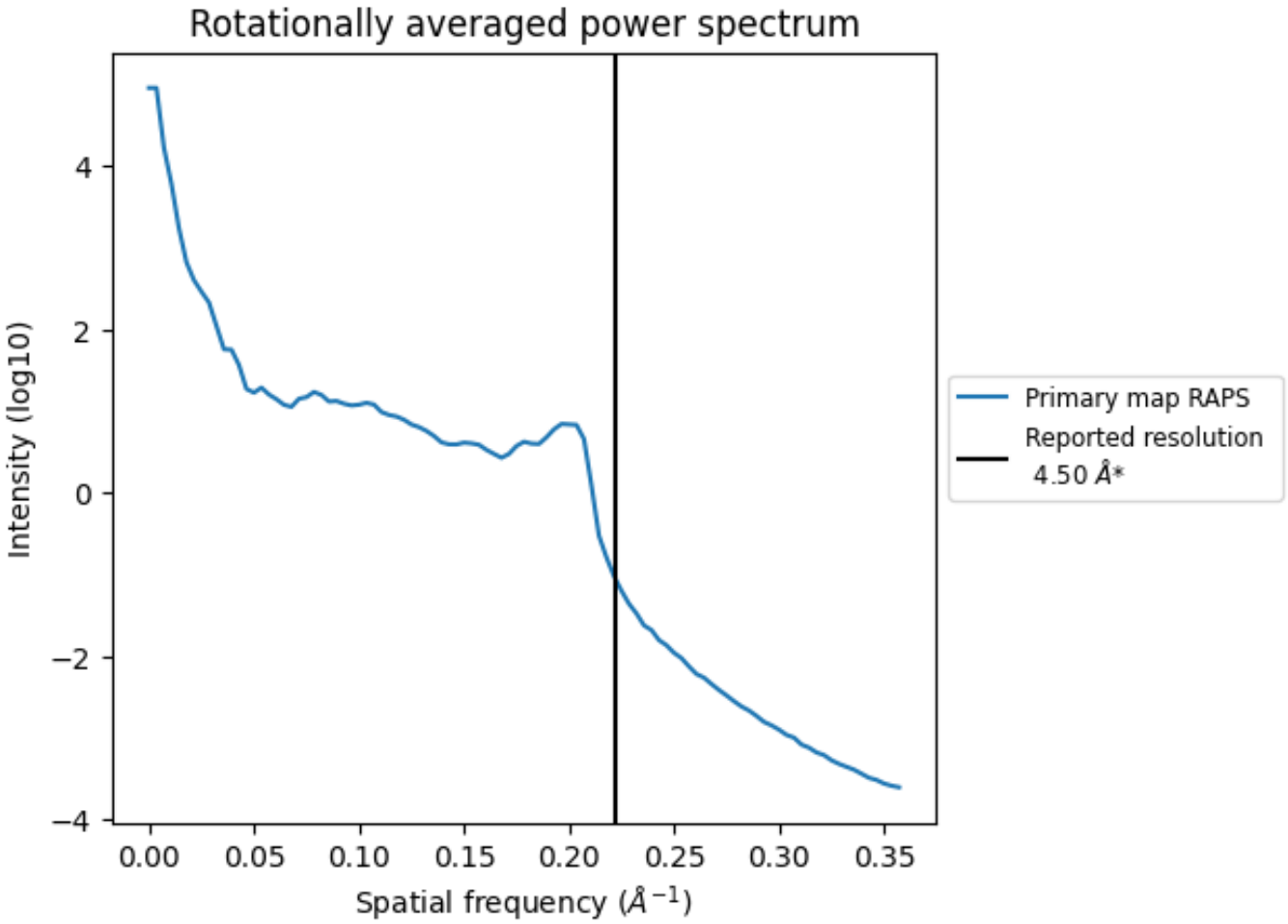
7.2 Volume estimate (i)



The volume at the recommended contour level is 322 nm^3; 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}

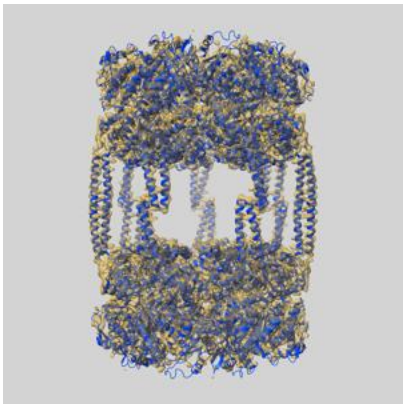
8 Fourier-Shell correlation (i)

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

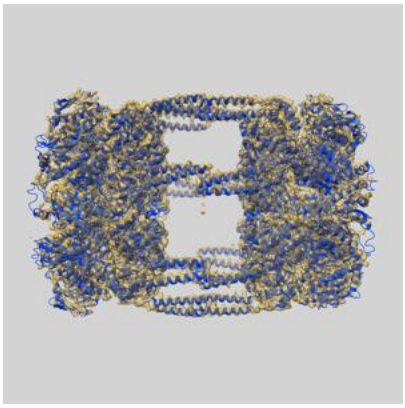
9 Map-model fit

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.

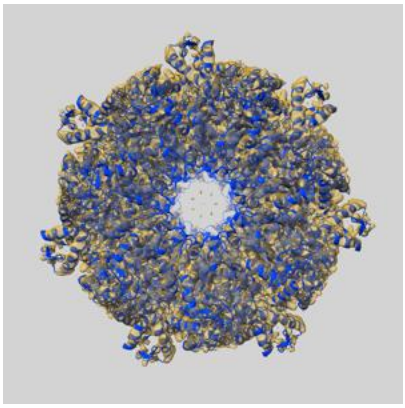
9.1 Map-model overlay



X



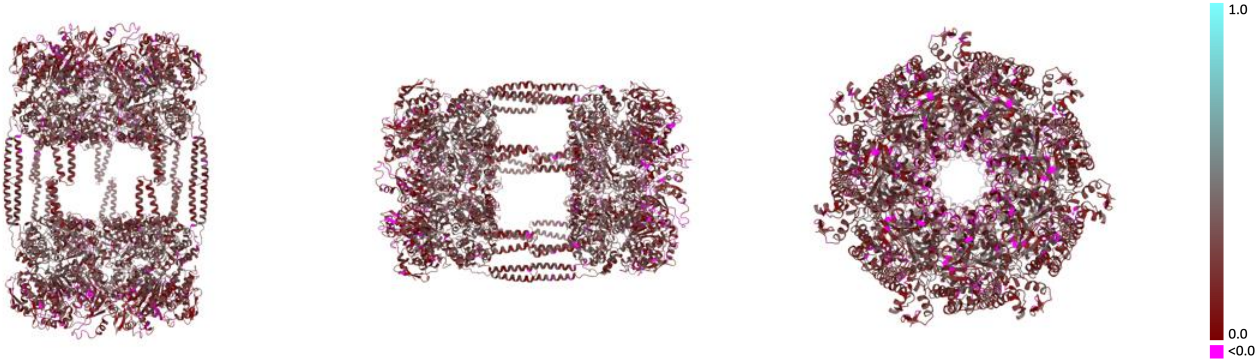
Y



Z

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.

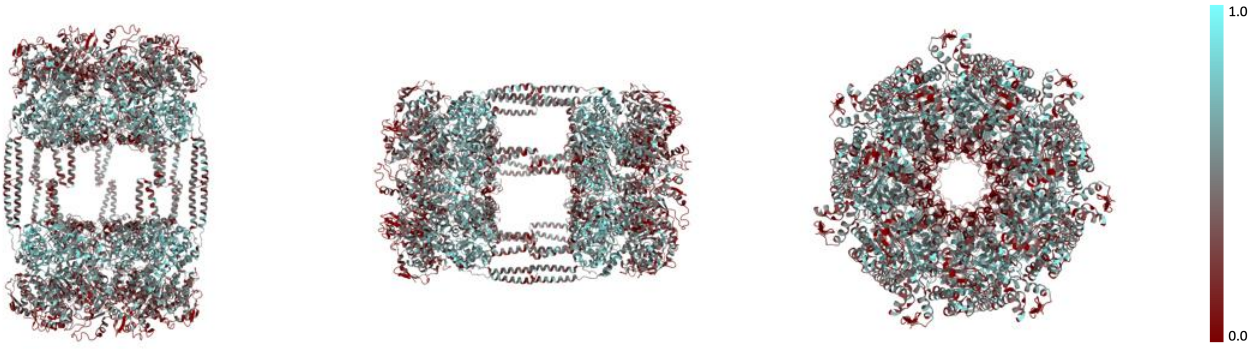
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

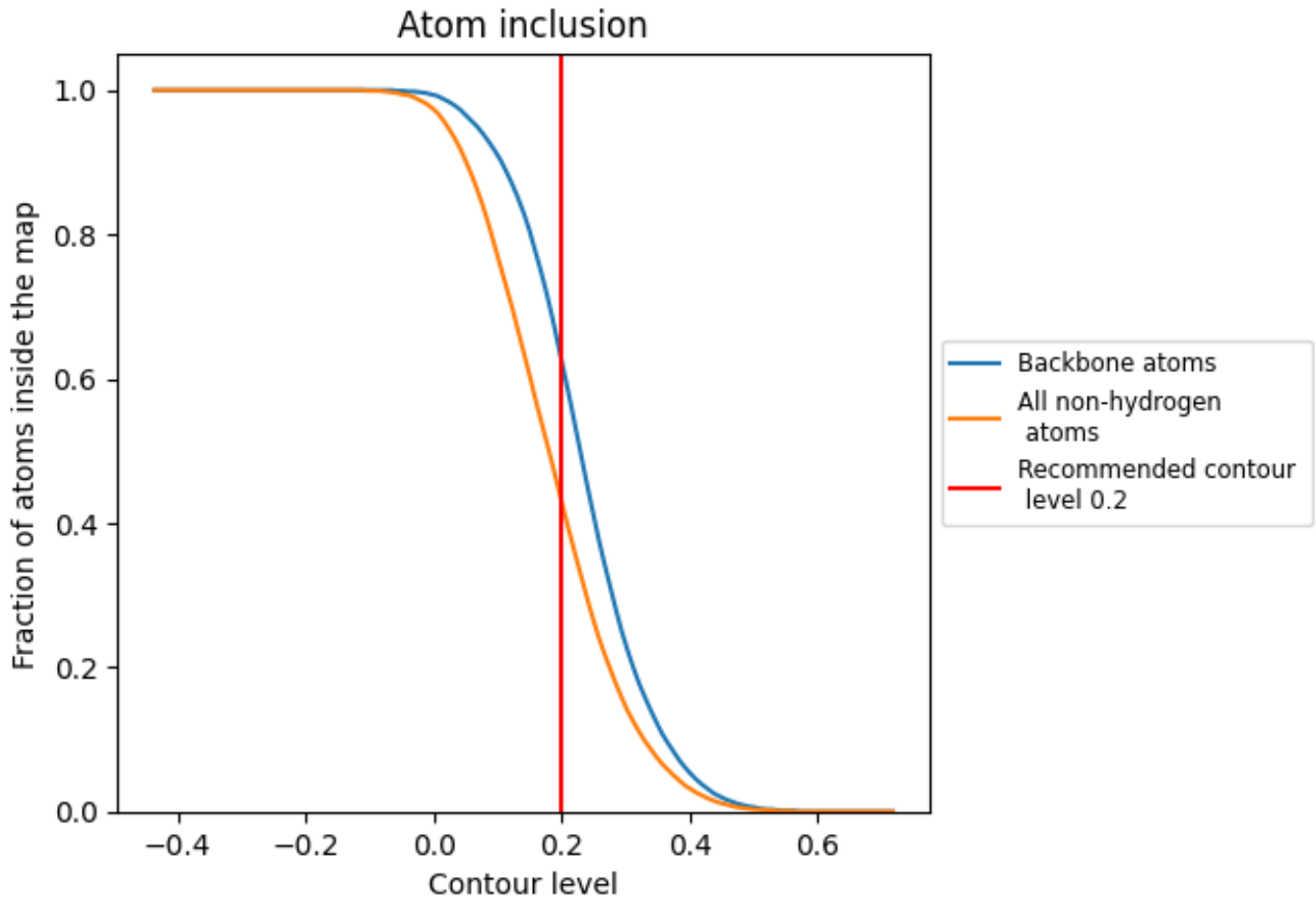
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

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