



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:29 pm BST

PDB ID : 1G3I
Title : CRYSTAL STRUCTURE OF THE HSLUV PROTEASE-CHAPERONE COMPLEX
Authors : Sousa, M.C.; Trame, C.B.; Tsuruta, H.; Wilbanks, S.M.; Reddy, V.S.; McKay, D.B.
Deposited on : 2000-10-24
Resolution : 3.41 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

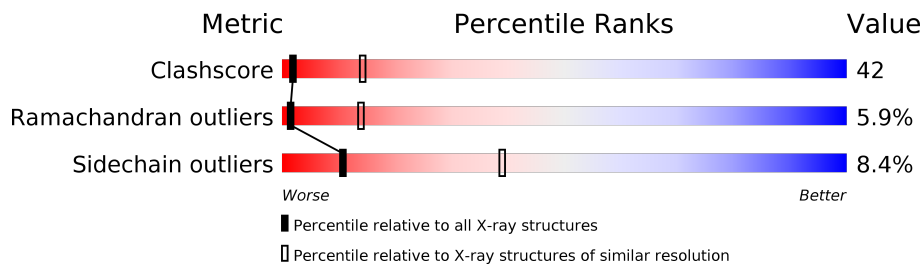
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)

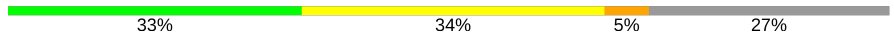
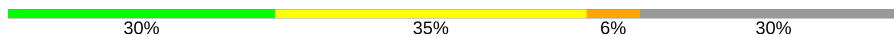
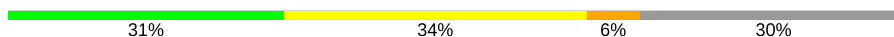
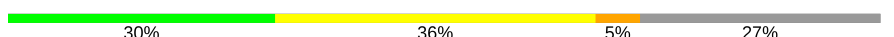

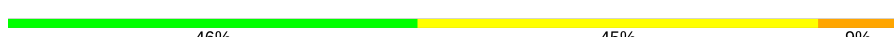
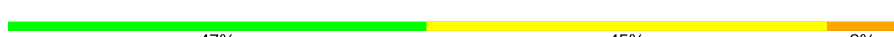



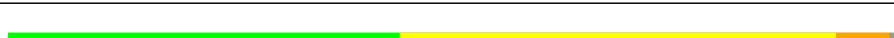

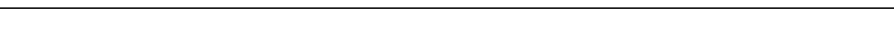
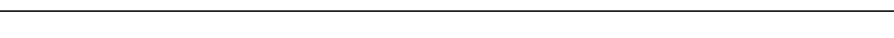
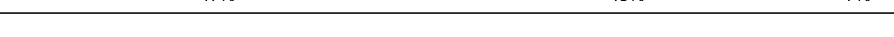
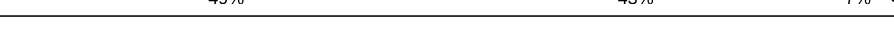
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	
1	S	444	
1	T	444	

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Mol	Chain	Length	Quality of chain
1	U	444	
1	V	444	
1	W	444	
1	X	444	
2	G	174	
2	H	174	
2	I	174	
2	J	174	
2	K	174	
2	L	174	
2	M	174	
2	N	174	
2	O	174	
2	P	174	
2	Q	174	
2	R	174	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	E	454	-	-	X	-
3	ATP	S	456	-	-	X	-
3	ATP	U	458	-	-	X	-
3	ATP	X	461	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 HSLU PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	Total 2539	C 1588	N 454	O 487	S 10	0	0	0
1	B	326	Total 2539	C 1588	N 454	O 487	S 10	0	0	0
1	C	319	Total 2484	C 1554	N 446	O 474	S 10	0	0	0
1	D	318	Total 2476	C 1548	N 445	O 473	S 10	0	0	0
1	E	317	Total 2462	C 1540	N 443	O 469	S 10	0	0	0
1	F	320	Total 2495	C 1560	N 450	O 475	S 10	0	0	0
1	S	317	Total 2468	C 1543	N 444	O 471	S 10	0	0	0
1	T	331	Total 2570	C 1602	N 461	O 497	S 10	0	0	0
1	U	322	Total 2503	C 1562	N 449	O 482	S 10	0	0	0
1	V	313	Total 2432	C 1519	N 436	O 467	S 10	0	0	0
1	W	312	Total 2428	C 1516	N 437	O 465	S 10	0	0	0
1	X	322	Total 2500	C 1562	N 446	O 482	S 10	0	0	0

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

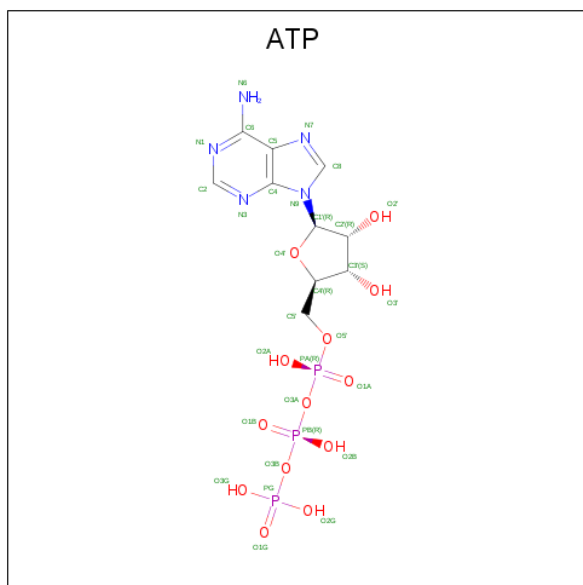
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	173	Total 1280	C 803	N 227	O 246	S 4	0	0	0
2	H	173	Total 1280	C 802	N 227	O 247	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	173	Total 1292	C 810	N 229	O 249	S 4	0	0	0
2	J	173	Total 1280	C 802	N 227	O 247	S 4	0	0	0
2	K	173	Total 1280	C 802	N 227	O 247	S 4	0	0	0
2	L	173	Total 1294	C 810	N 231	O 249	S 4	0	0	0
2	M	173	Total 1261	C 791	N 226	O 241	S 3	0	0	0
2	N	173	Total 1261	C 791	N 226	O 241	S 3	0	0	0
2	O	173	Total 1257	C 789	N 225	O 240	S 3	0	0	0
2	P	173	Total 1257	C 789	N 225	O 240	S 3	0	0	0
2	Q	173	Total 1261	C 791	N 226	O 241	S 3	0	0	0
2	R	173	Total 1257	C 789	N 225	O 240	S 3	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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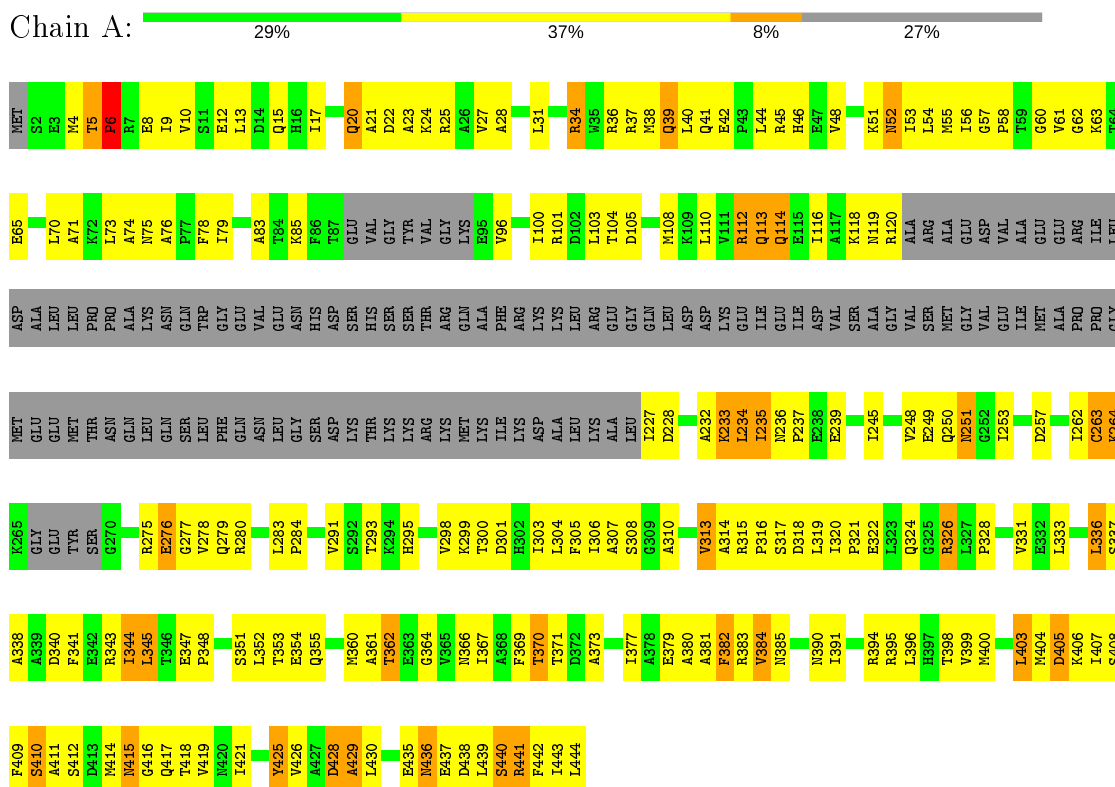
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	S	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	T	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	U	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	V	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	W	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	X	1	Total 31	C 10	N 5	O 13	P 3	0	0

3 Residue-property plots

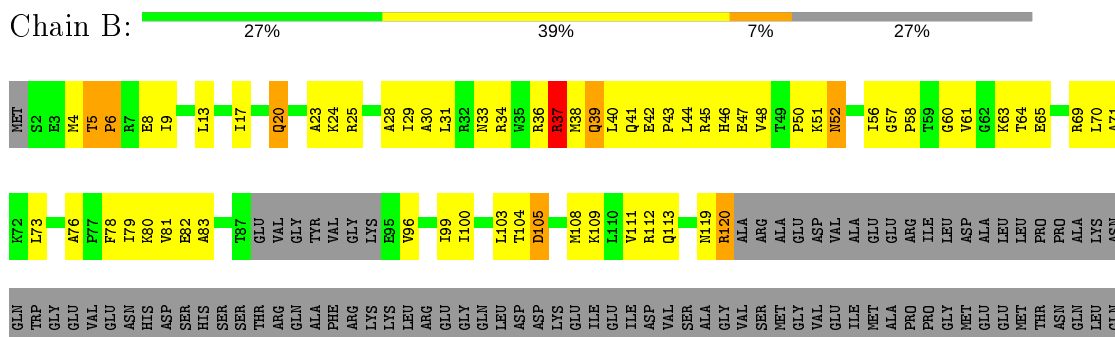
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

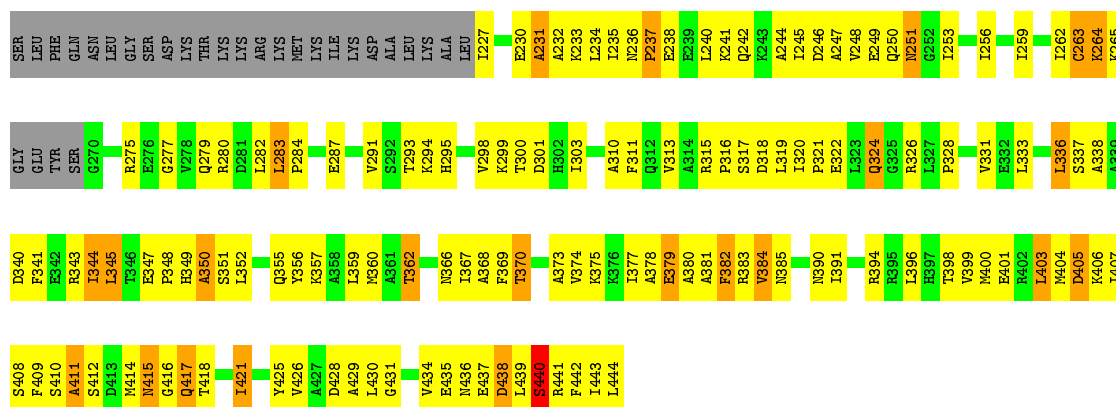
Note EDS was not executed.

- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

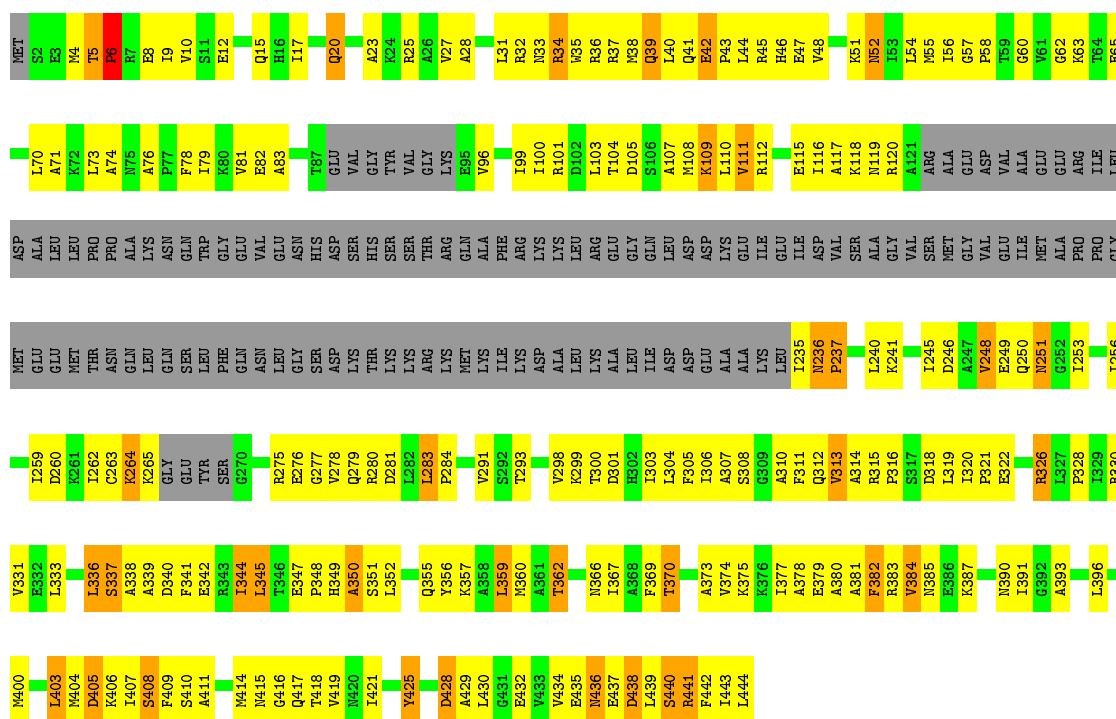
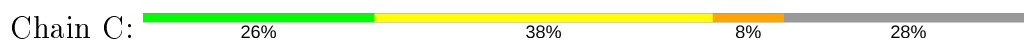


- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

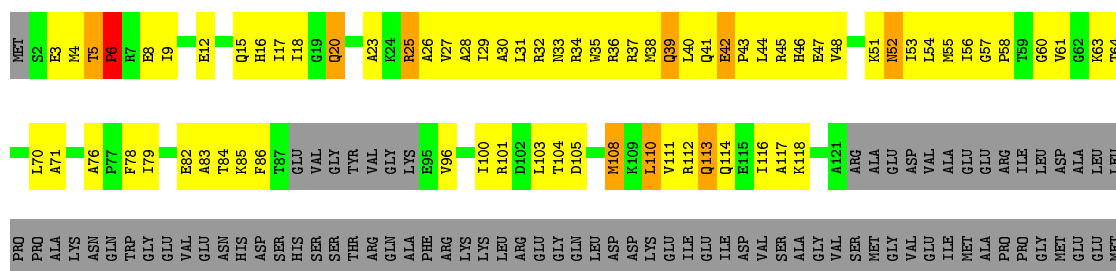
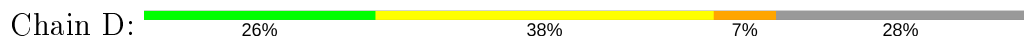


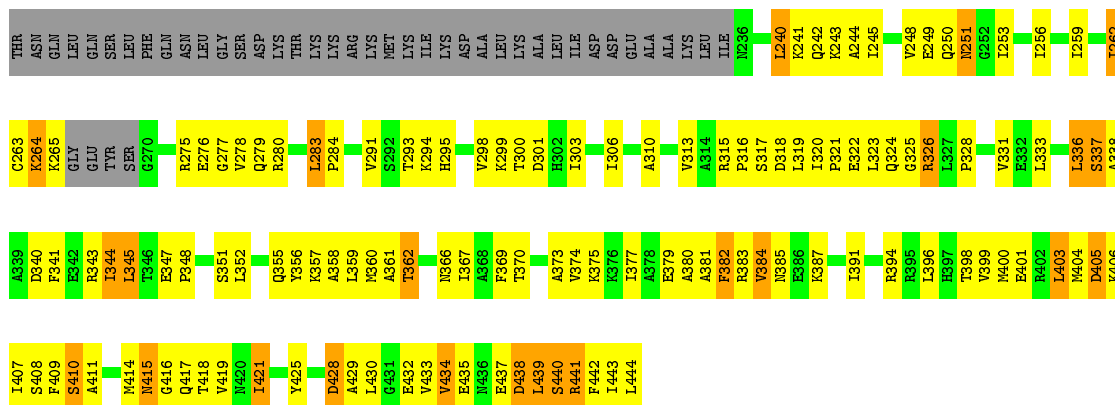


● Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

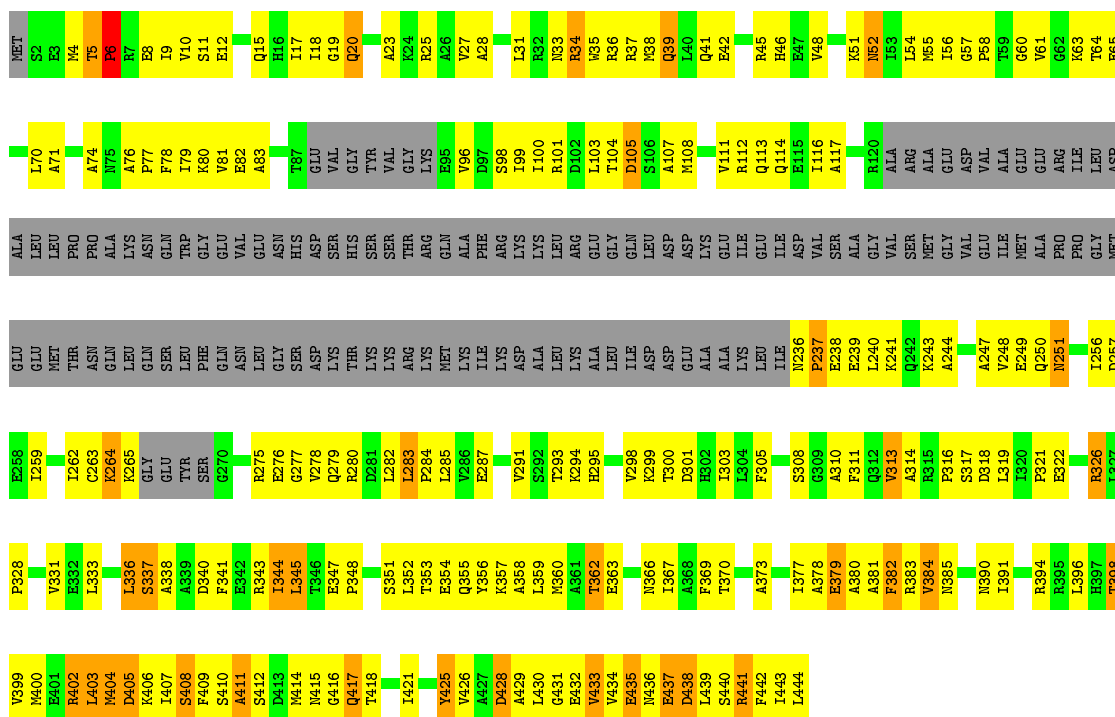
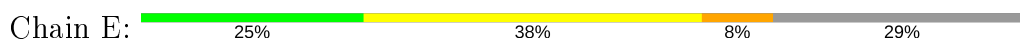


● Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

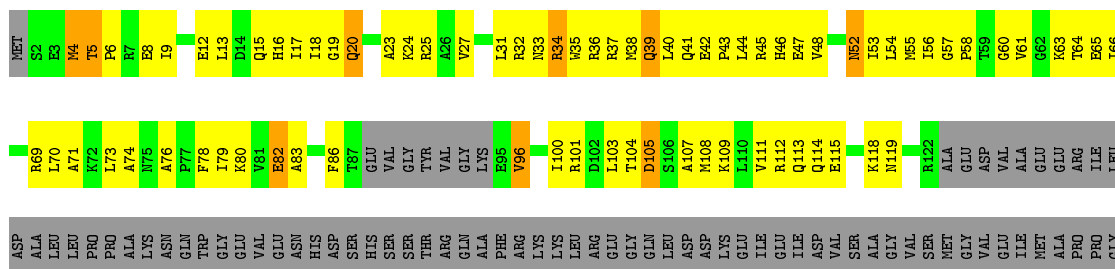
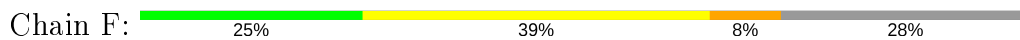


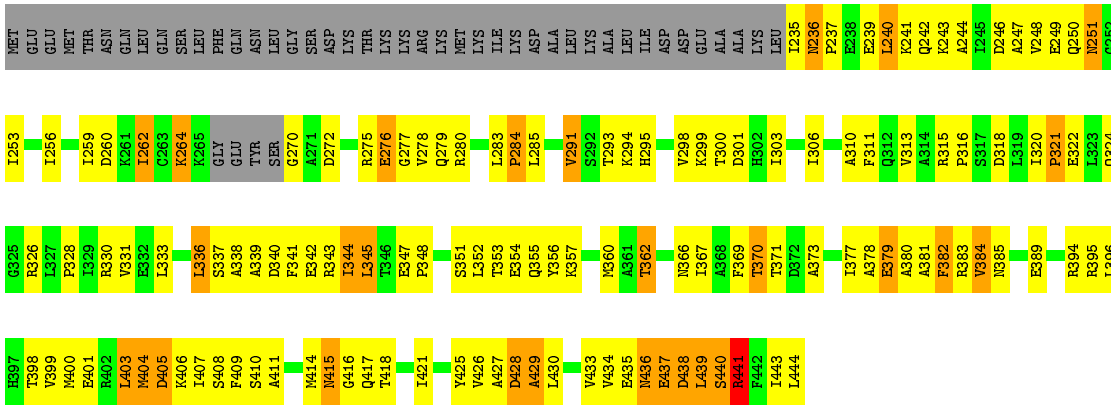


- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

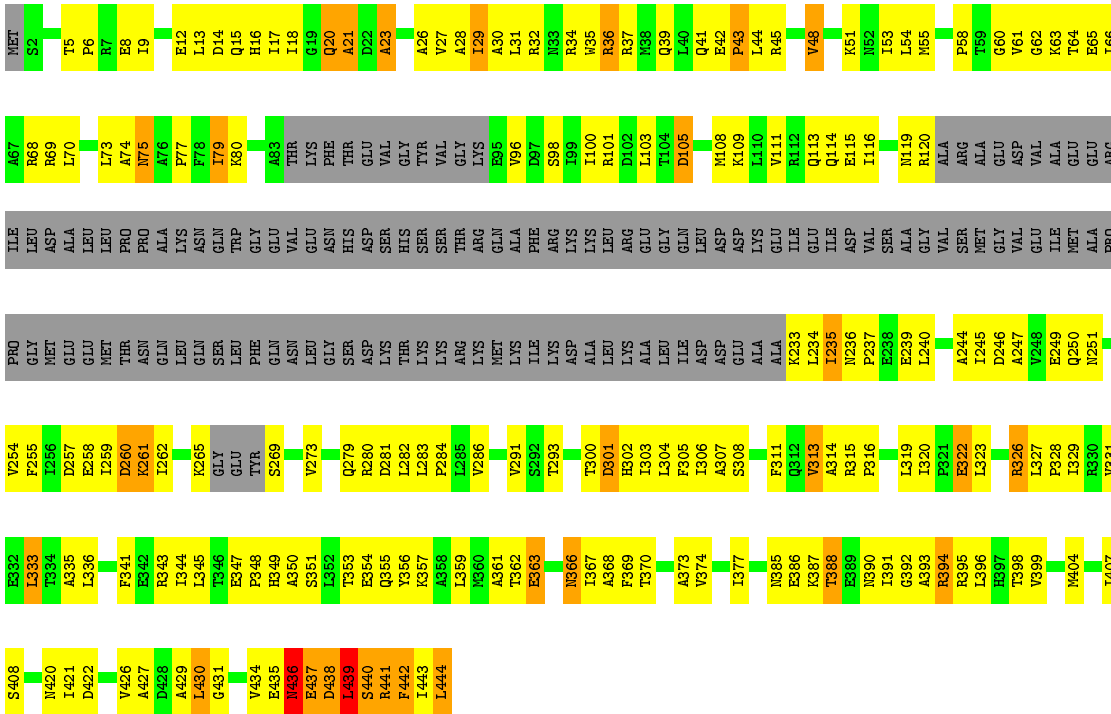


- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

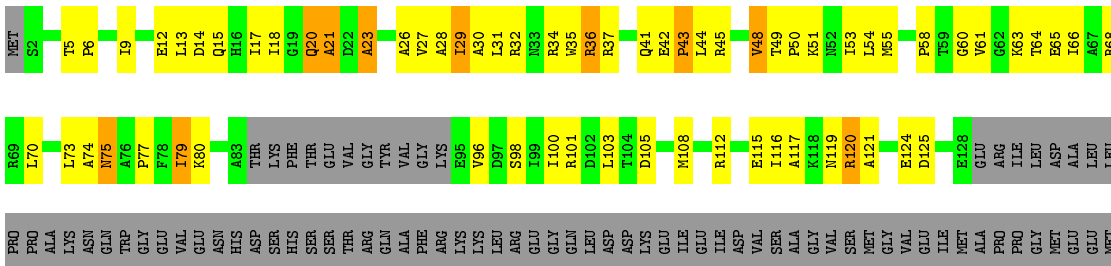


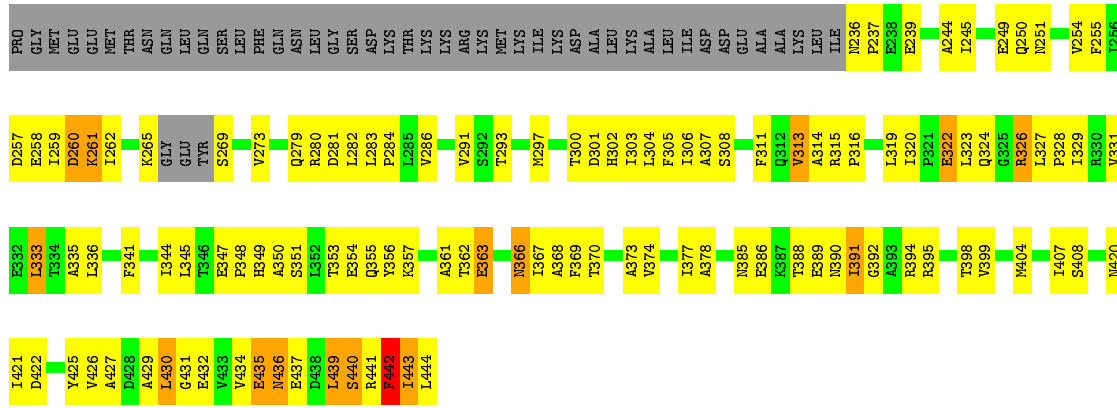


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

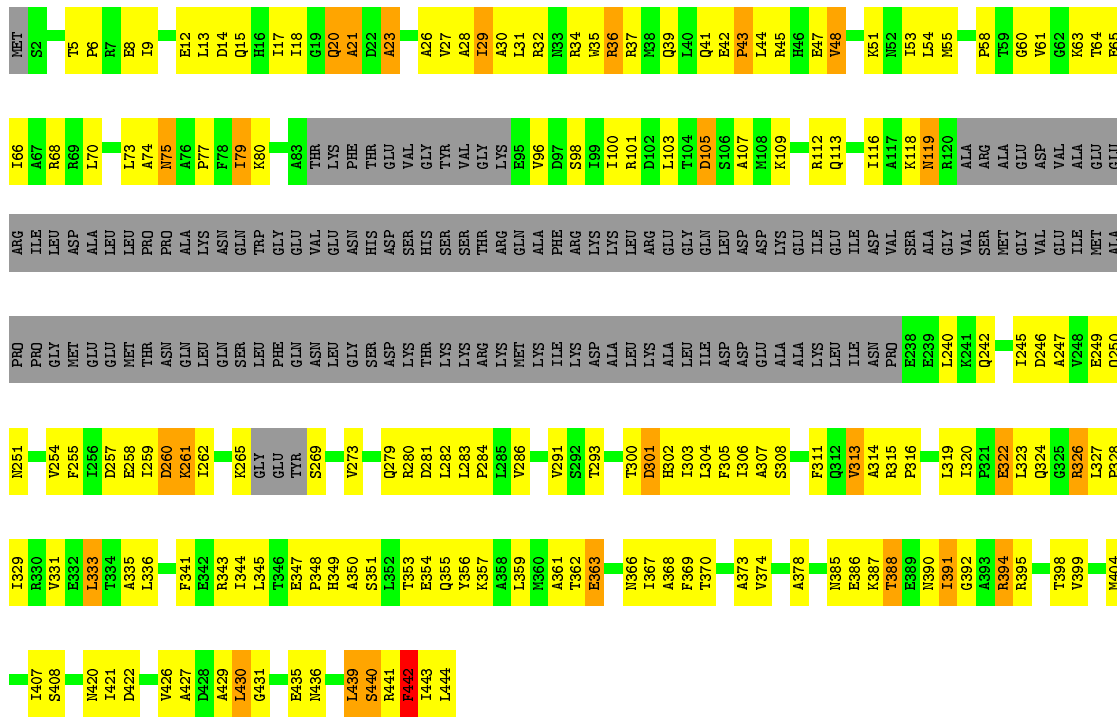
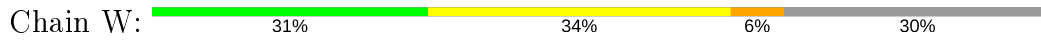


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

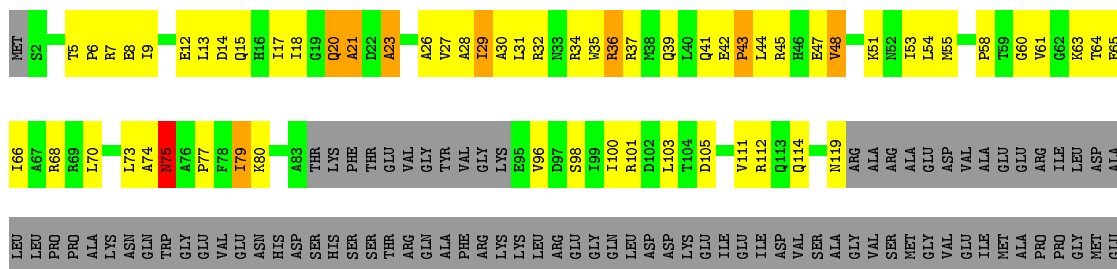
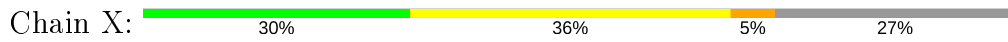


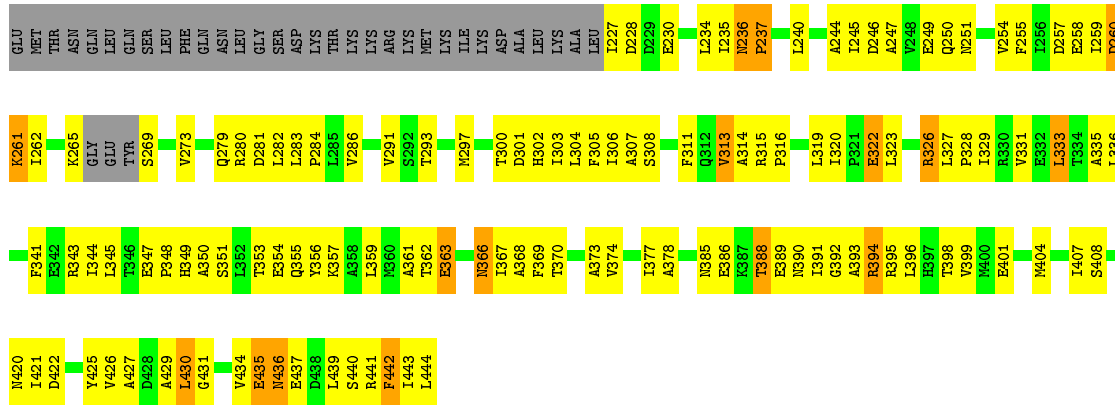


● Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

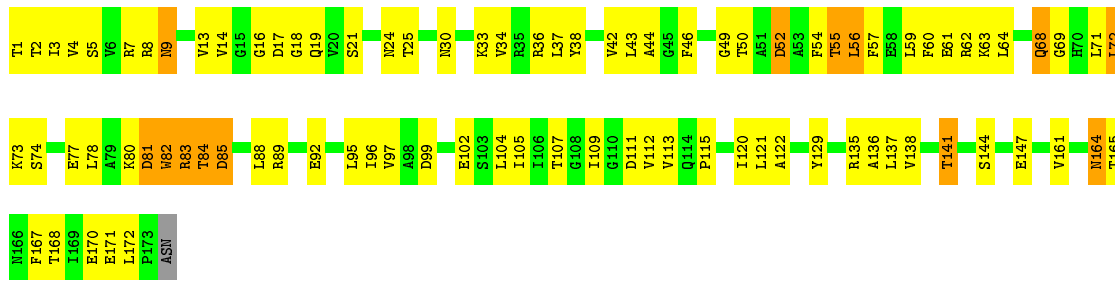


● Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

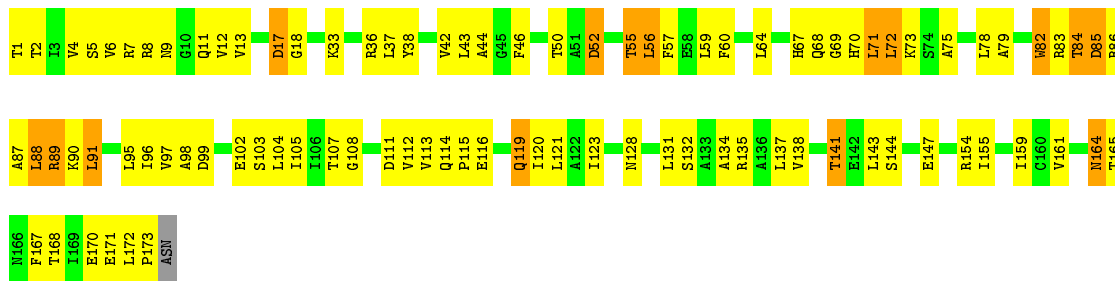




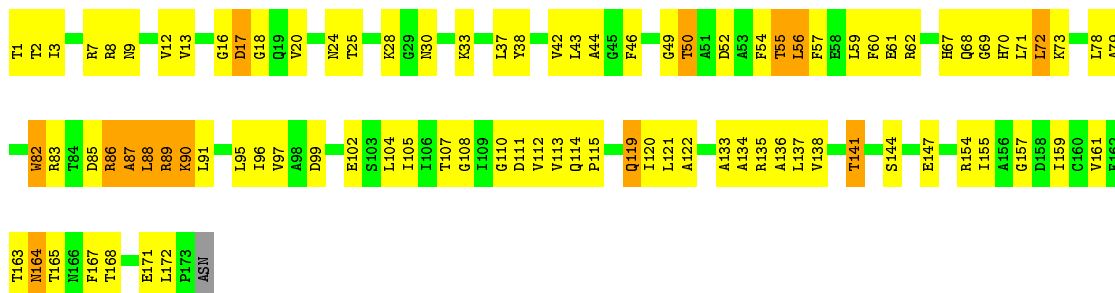
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



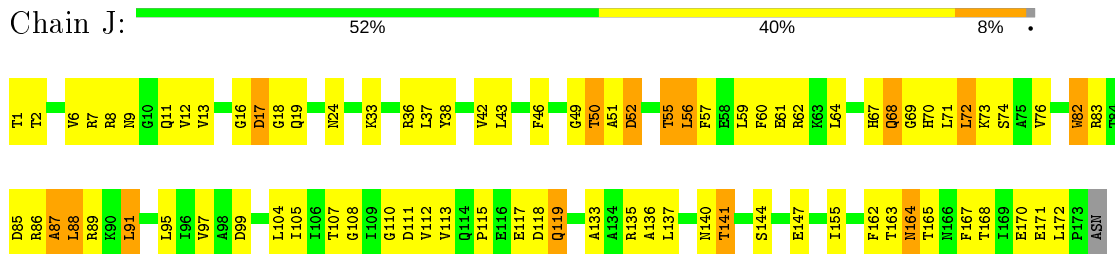
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



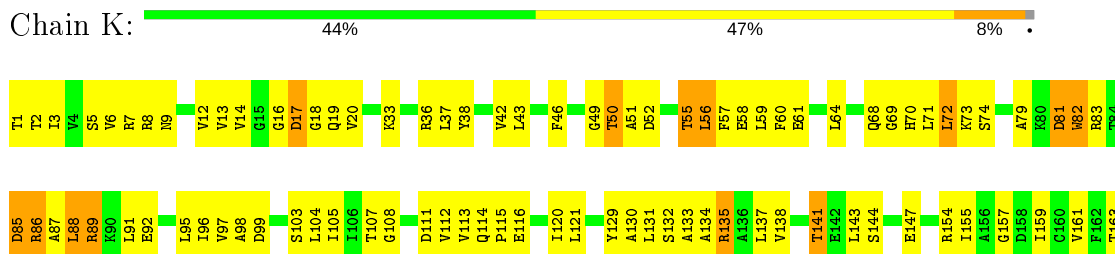
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



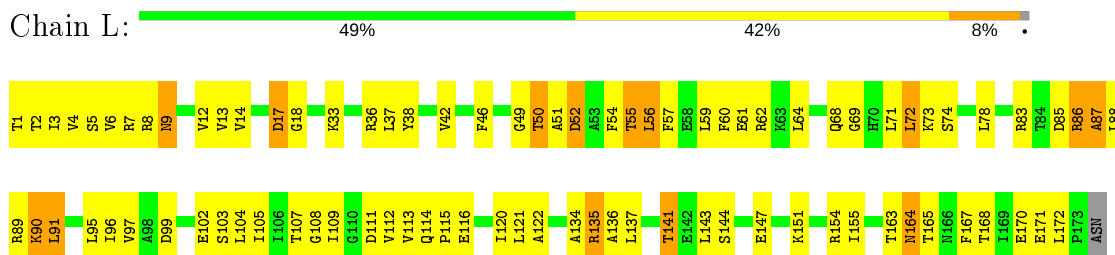
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



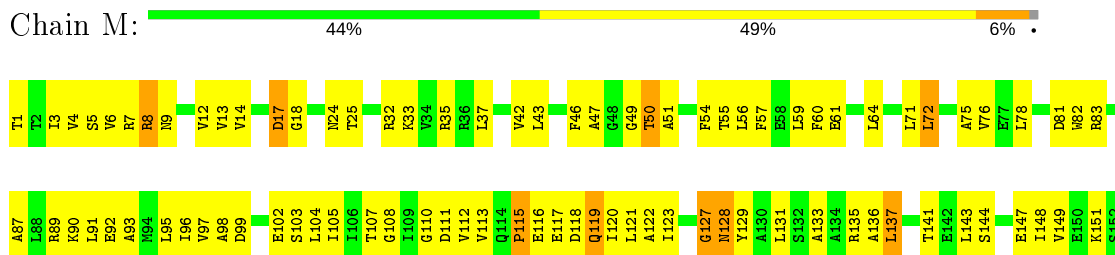
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

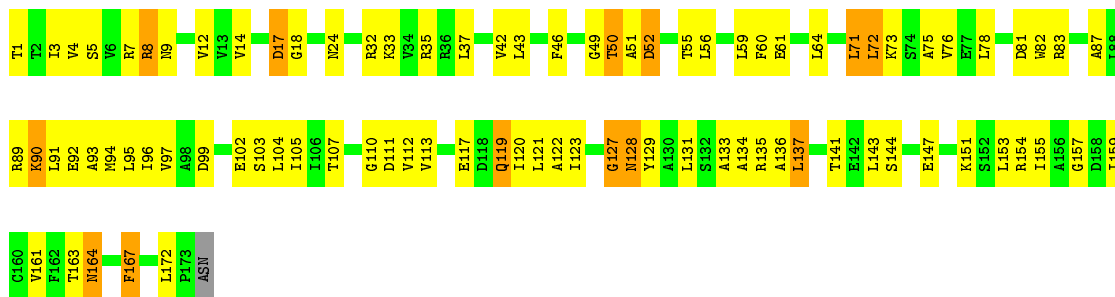


• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



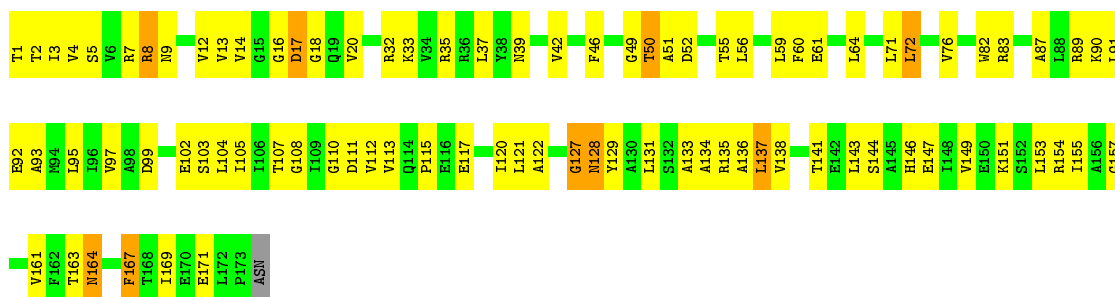
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV





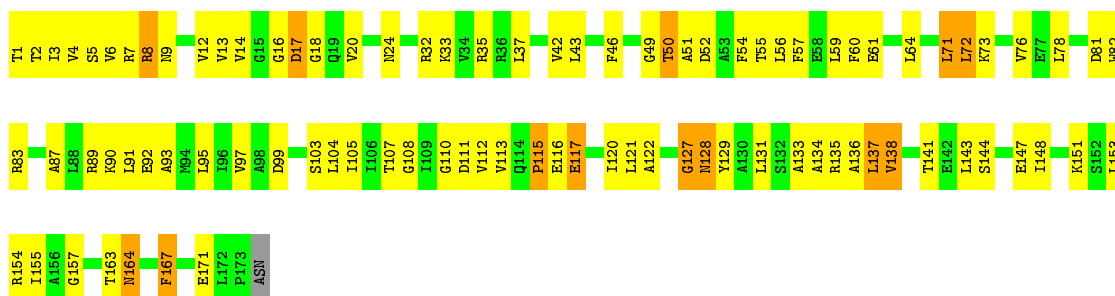
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain O: 49% 45% 5%



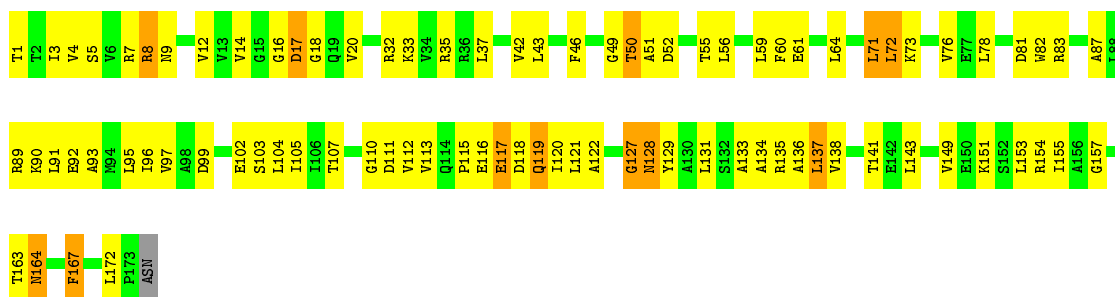
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P: 47% 45% 7%



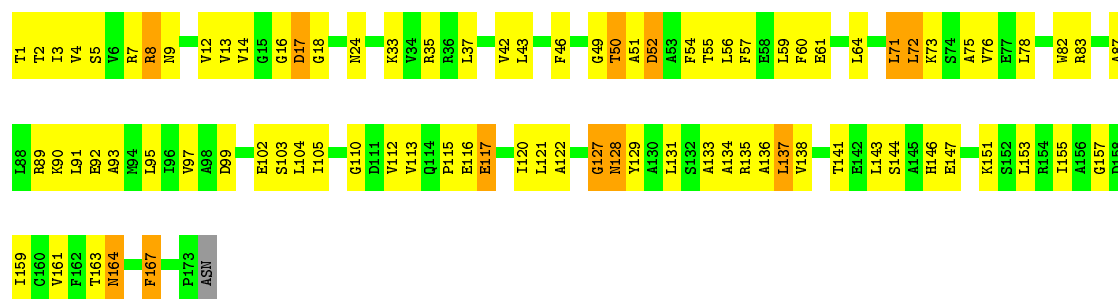
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain Q: 49% 43% 7%



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain R:  49% 43% 7%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	209.22Å 220.58Å 241.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.08 – 3.41	Depositor
% Data completeness (in resolution range)	(Not available) (30.08-3.41)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	45528	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

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: ATP

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	0.65	1/2566 (0.0%)	0.81	0/3458
1	B	0.62	0/2566	0.81	2/3458 (0.1%)
1	C	0.55	0/2511	0.78	1/3384 (0.0%)
1	D	0.64	1/2503 (0.0%)	0.82	1/3373 (0.0%)
1	E	0.67	0/2489	0.83	2/3354 (0.1%)
1	F	0.64	0/2522	0.79	0/3398
1	S	0.31	0/2494	0.55	0/3360
1	T	0.31	0/2596	0.56	0/3499
1	U	0.30	0/2529	0.55	0/3408
1	V	0.30	0/2458	0.55	0/3313
1	W	0.30	0/2453	0.55	0/3304
1	X	0.31	0/2526	0.55	0/3405
2	G	0.55	0/1294	0.76	0/1753
2	H	0.55	0/1294	0.78	0/1754
2	I	0.50	0/1306	0.73	0/1767
2	J	0.50	0/1294	0.75	0/1754
2	K	0.52	0/1294	0.74	0/1754
2	L	0.55	0/1308	0.77	0/1770
2	M	0.41	0/1275	0.66	0/1732
2	N	0.39	0/1275	0.65	0/1732
2	O	0.35	0/1271	0.62	0/1727
2	P	0.37	0/1271	0.63	0/1727
2	Q	0.45	0/1275	0.65	0/1732
2	R	0.40	0/1271	0.63	0/1727
All	All	0.49	2/45641 (0.0%)	0.70	6/61643 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	CYS	CB-SG	-8.39	1.68	1.82
1	D	263	CYS	CB-SG	-5.66	1.72	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	LEU	CA-CB-CG	-7.04	99.10	115.30
1	C	283	LEU	CA-CB-CG	-6.71	99.88	115.30
1	E	431	GLY	N-CA-C	6.00	128.10	113.10
1	B	283	LEU	CA-CB-CG	-5.45	102.76	115.30
1	D	283	LEU	CA-CB-CG	-5.20	103.34	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2539	0	2606	238	0
1	B	2539	0	2606	245	0
1	C	2484	0	2552	237	0
1	D	2476	0	2541	237	0
1	E	2462	0	2521	241	0
1	F	2495	0	2565	257	0
1	S	2468	0	2540	242	0
1	T	2570	0	2628	223	0
1	U	2503	0	2564	225	0
1	V	2432	0	2492	216	0
1	W	2428	0	2492	218	0
1	X	2500	0	2562	237	1
2	G	1280	0	1275	107	0
2	H	1280	0	1270	115	0
2	I	1292	0	1296	110	0
2	J	1280	0	1270	101	0
2	K	1280	0	1270	111	0
2	L	1294	0	1296	101	0
2	M	1261	0	1240	106	0
2	N	1261	0	1240	104	0
2	O	1257	0	1234	98	0
2	P	1257	0	1234	98	0
2	Q	1261	0	1240	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1257	0	1234	93	0
3	A	31	0	12	2	0
3	B	31	0	12	5	0
3	C	31	0	12	5	0
3	D	31	0	12	4	0
3	E	31	0	12	9	0
3	F	31	0	12	8	0
3	S	31	0	12	14	0
3	T	31	0	12	3	0
3	U	31	0	12	12	0
3	V	31	0	12	3	0
3	W	31	0	12	8	0
3	X	31	0	12	9	0
All	All	45528	0	45912	3804	1

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 42.

The worst 5 of 3804 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:F:264:LYS:NZ	1:F:279:GLN:HE22	1.38	1.21
2:Q:7:ARG:HD2	2:Q:119:GLN:OE1	1.44	1.17
1:E:264:LYS:NZ	1:E:279:GLN:HE22	1.42	1.15
2:N:7:ARG:HD2	2:N:119:GLN:HE21	1.09	1.15
1:A:264:LYS:NZ	1:A:279:GLN:HE22	1.45	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ARG:NH2	1:X:7:ARG:NH2[2_765]	2.08	0.12

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 X-ray entries followed by that with respect to entries

of similar resolution.

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	318/444 (72%)	244 (77%)	57 (18%)	17 (5%)	2	16
1	B	318/444 (72%)	241 (76%)	58 (18%)	19 (6%)	1	13
1	C	311/444 (70%)	234 (75%)	60 (19%)	17 (6%)	2	15
1	D	310/444 (70%)	235 (76%)	56 (18%)	19 (6%)	1	13
1	E	309/444 (70%)	238 (77%)	51 (16%)	20 (6%)	1	12
1	F	312/444 (70%)	240 (77%)	54 (17%)	18 (6%)	1	14
1	S	309/444 (70%)	227 (74%)	57 (18%)	25 (8%)	1	8
1	T	323/444 (73%)	236 (73%)	63 (20%)	24 (7%)	1	10
1	U	314/444 (71%)	237 (76%)	54 (17%)	23 (7%)	1	10
1	V	305/444 (69%)	228 (75%)	54 (18%)	23 (8%)	1	9
1	W	304/444 (68%)	223 (73%)	57 (19%)	24 (8%)	1	9
1	X	314/444 (71%)	235 (75%)	56 (18%)	23 (7%)	1	10
2	G	171/174 (98%)	141 (82%)	28 (16%)	2 (1%)	13	46
2	H	171/174 (98%)	139 (81%)	26 (15%)	6 (4%)	3	25
2	I	171/174 (98%)	136 (80%)	30 (18%)	5 (3%)	4	29
2	J	171/174 (98%)	136 (80%)	28 (16%)	7 (4%)	3	22
2	K	171/174 (98%)	138 (81%)	26 (15%)	7 (4%)	3	22
2	L	171/174 (98%)	137 (80%)	27 (16%)	7 (4%)	3	22
2	M	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	2	16
2	N	171/174 (98%)	129 (75%)	34 (20%)	8 (5%)	2	19
2	O	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	2	16
2	P	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	2	16
2	Q	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	2	16
2	R	171/174 (98%)	128 (75%)	33 (19%)	10 (6%)	1	14
All	All	5799/7416 (78%)	4418 (76%)	1041 (18%)	340 (6%)	1	14

5 of 340 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	235	ILE

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	436	ASN
1	A	438	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	274/373 (74%)	244 (89%)	30 (11%)	6	28
1	B	274/373 (74%)	248 (90%)	26 (10%)	8	33
1	C	268/373 (72%)	231 (86%)	37 (14%)	3	18
1	D	267/373 (72%)	237 (89%)	30 (11%)	6	26
1	E	264/373 (71%)	232 (88%)	32 (12%)	5	23
1	F	269/373 (72%)	242 (90%)	27 (10%)	7	31
1	S	267/373 (72%)	246 (92%)	21 (8%)	12	41
1	T	276/373 (74%)	258 (94%)	18 (6%)	17	49
1	U	270/373 (72%)	250 (93%)	20 (7%)	13	44
1	V	263/373 (70%)	246 (94%)	17 (6%)	17	49
1	W	262/373 (70%)	246 (94%)	16 (6%)	18	51
1	X	270/373 (72%)	252 (93%)	18 (7%)	16	49
2	G	130/140 (93%)	115 (88%)	15 (12%)	5	25
2	H	130/140 (93%)	115 (88%)	15 (12%)	5	25
2	I	133/140 (95%)	119 (90%)	14 (10%)	7	29
2	J	130/140 (93%)	118 (91%)	12 (9%)	9	35
2	K	130/140 (93%)	118 (91%)	12 (9%)	9	35
2	L	133/140 (95%)	123 (92%)	10 (8%)	13	44
2	M	125/140 (89%)	121 (97%)	4 (3%)	39	69
2	N	125/140 (89%)	119 (95%)	6 (5%)	25	59
2	O	124/140 (89%)	120 (97%)	4 (3%)	39	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	124/140 (89%)	119 (96%)	5 (4%)	31	63
2	Q	125/140 (89%)	121 (97%)	4 (3%)	39	69
2	R	124/140 (89%)	119 (96%)	5 (4%)	31	63
All	All	4757/6156 (77%)	4359 (92%)	398 (8%)	11	39

5 of 398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	437	GLU
2	I	135	ARG
1	W	246	ASP
2	G	68	GLN
2	H	82	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	24	ASN
2	M	164	ASN
1	W	385	ASN
2	H	164	ASN
2	J	164	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 carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	C	452	-	26,33,33	0.72	1 (3%)	31,52,52	1.26	4 (12%)
3	ATP	D	453	-	26,33,33	0.68	0	31,52,52	1.13	1 (3%)
3	ATP	U	458	-	26,33,33	0.59	0	31,52,52	0.97	2 (6%)
3	ATP	B	451	-	26,33,33	0.75	1 (3%)	31,52,52	1.12	3 (9%)
3	ATP	X	461	-	26,33,33	0.62	0	31,52,52	1.00	2 (6%)
3	ATP	W	460	-	26,33,33	0.63	0	31,52,52	1.01	2 (6%)
3	ATP	E	454	-	26,33,33	0.81	1 (3%)	31,52,52	1.16	3 (9%)
3	ATP	S	456	-	26,33,33	0.61	0	31,52,52	1.00	2 (6%)
3	ATP	F	455	-	26,33,33	0.80	1 (3%)	31,52,52	1.17	2 (6%)
3	ATP	A	450	-	26,33,33	0.82	1 (3%)	31,52,52	1.18	3 (9%)
3	ATP	T	457	-	26,33,33	0.66	0	31,52,52	0.98	2 (6%)
3	ATP	V	459	-	26,33,33	0.60	0	31,52,52	0.98	2 (6%)

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	ATP	C	452	-	-	5/18/38/38	0/3/3/3
3	ATP	D	453	-	-	4/18/38/38	0/3/3/3
3	ATP	U	458	-	-	4/18/38/38	0/3/3/3
3	ATP	B	451	-	-	1/18/38/38	0/3/3/3
3	ATP	X	461	-	-	6/18/38/38	0/3/3/3
3	ATP	W	460	-	-	5/18/38/38	0/3/3/3
3	ATP	E	454	-	-	5/18/38/38	0/3/3/3
3	ATP	S	456	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	F	455	-	-	5/18/38/38	0/3/3/3
3	ATP	A	450	-	-	3/18/38/38	0/3/3/3
3	ATP	T	457	-	-	3/18/38/38	0/3/3/3
3	ATP	V	459	-	-	3/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	455	ATP	C8-N7	-2.18	1.30	1.34
3	E	454	ATP	C8-N7	-2.11	1.30	1.34
3	A	450	ATP	C8-N7	-2.07	1.31	1.34
3	C	452	ATP	C8-N7	-2.06	1.31	1.34
3	B	451	ATP	C8-N7	-2.04	1.31	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	452	ATP	PA-O3A-PB	-3.53	120.71	132.83
3	W	460	ATP	C5-C6-N6	2.38	123.98	120.35
3	S	456	ATP	C5-C6-N6	2.37	123.96	120.35
3	D	453	ATP	PB-O3B-PG	2.34	140.86	132.83
3	F	455	ATP	O3G-PG-O2G	2.34	116.56	107.64

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	453	ATP	C5'-O5'-PA-O1A
3	D	453	ATP	C5'-O5'-PA-O2A
3	U	458	ATP	C5'-O5'-PA-O1A
3	W	460	ATP	C5'-O5'-PA-O1A
3	F	455	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

12 monomers are involved in 82 short contacts:

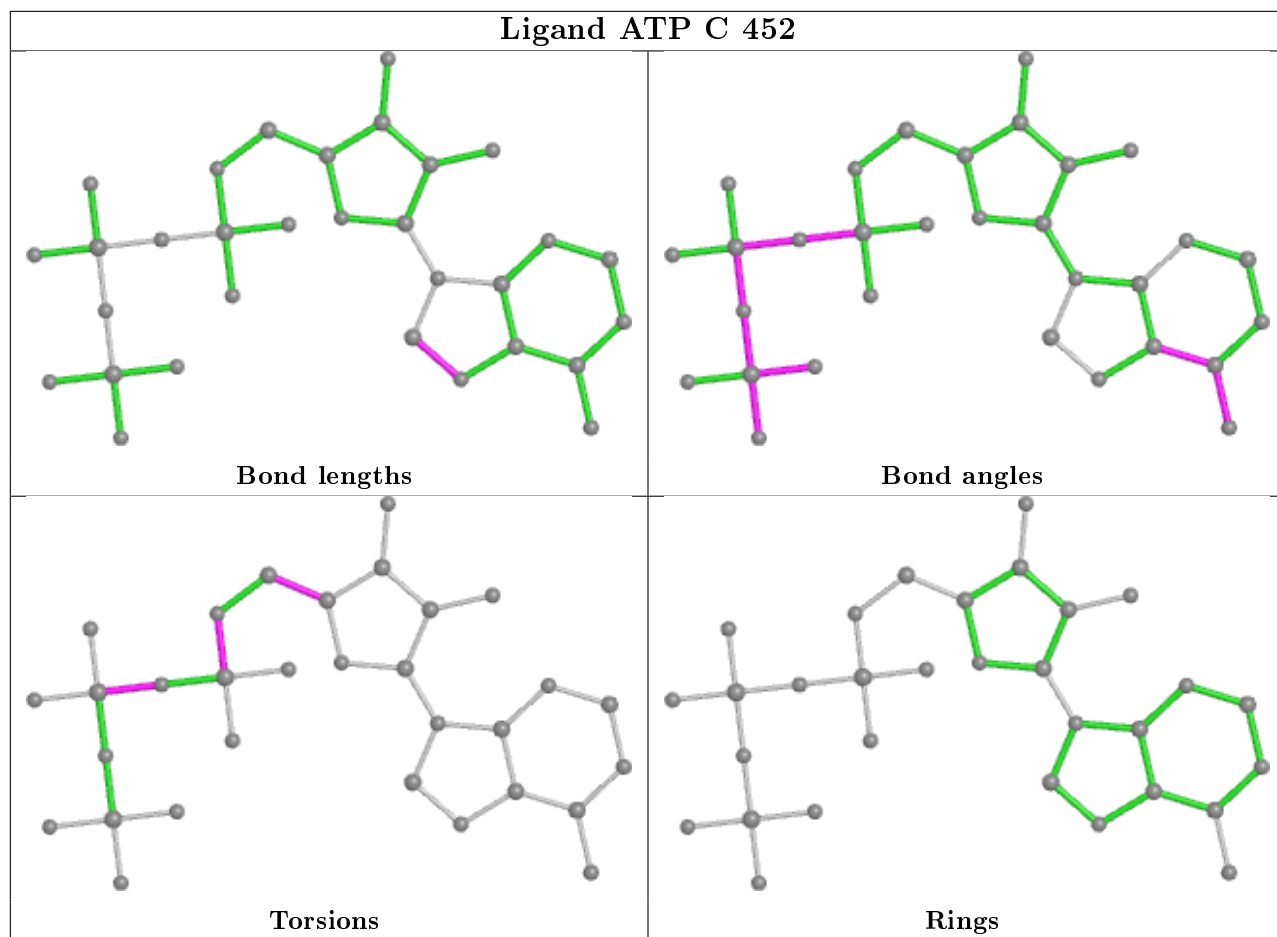
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	452	ATP	5	0
3	D	453	ATP	4	0
3	U	458	ATP	12	0

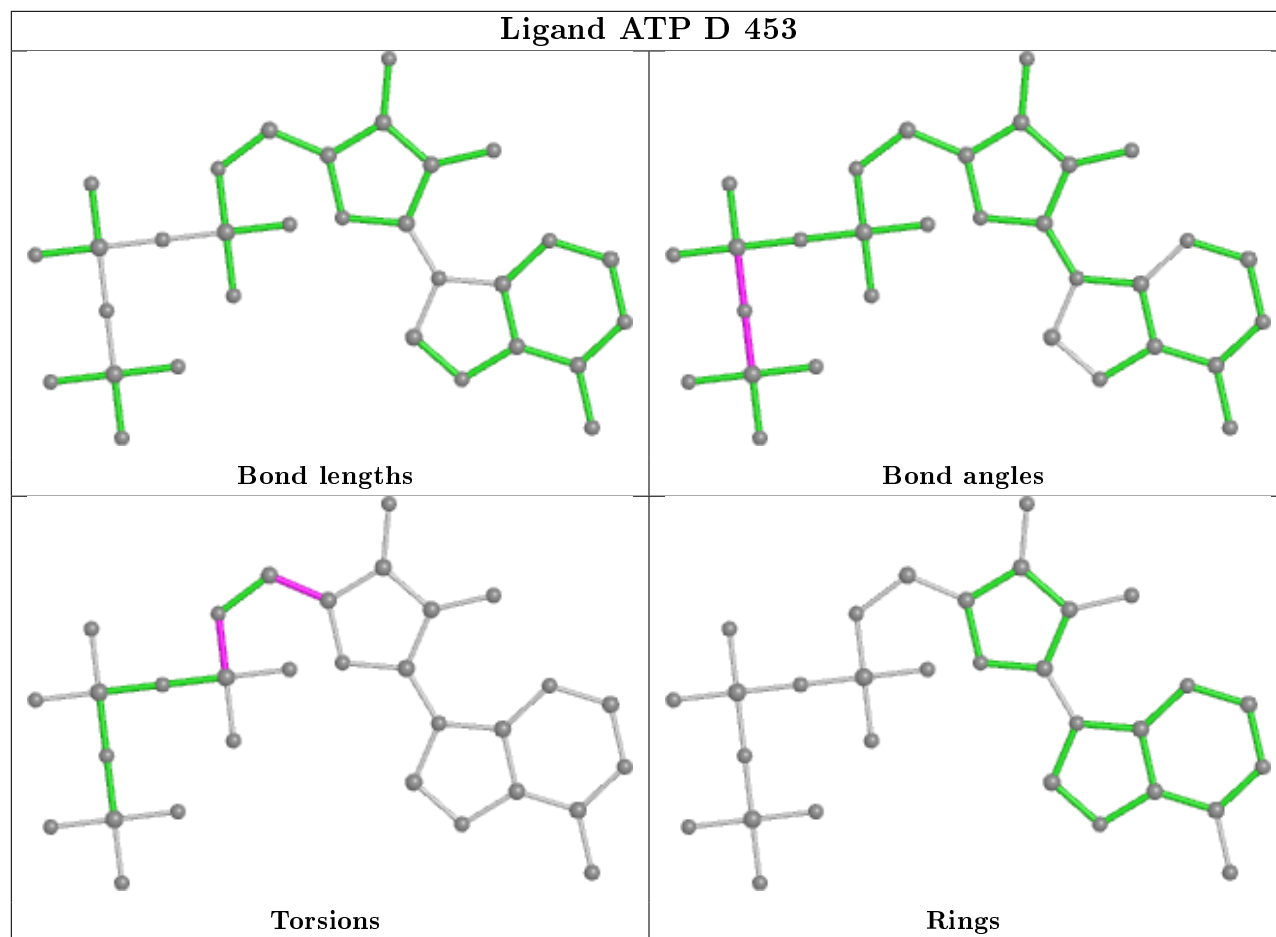
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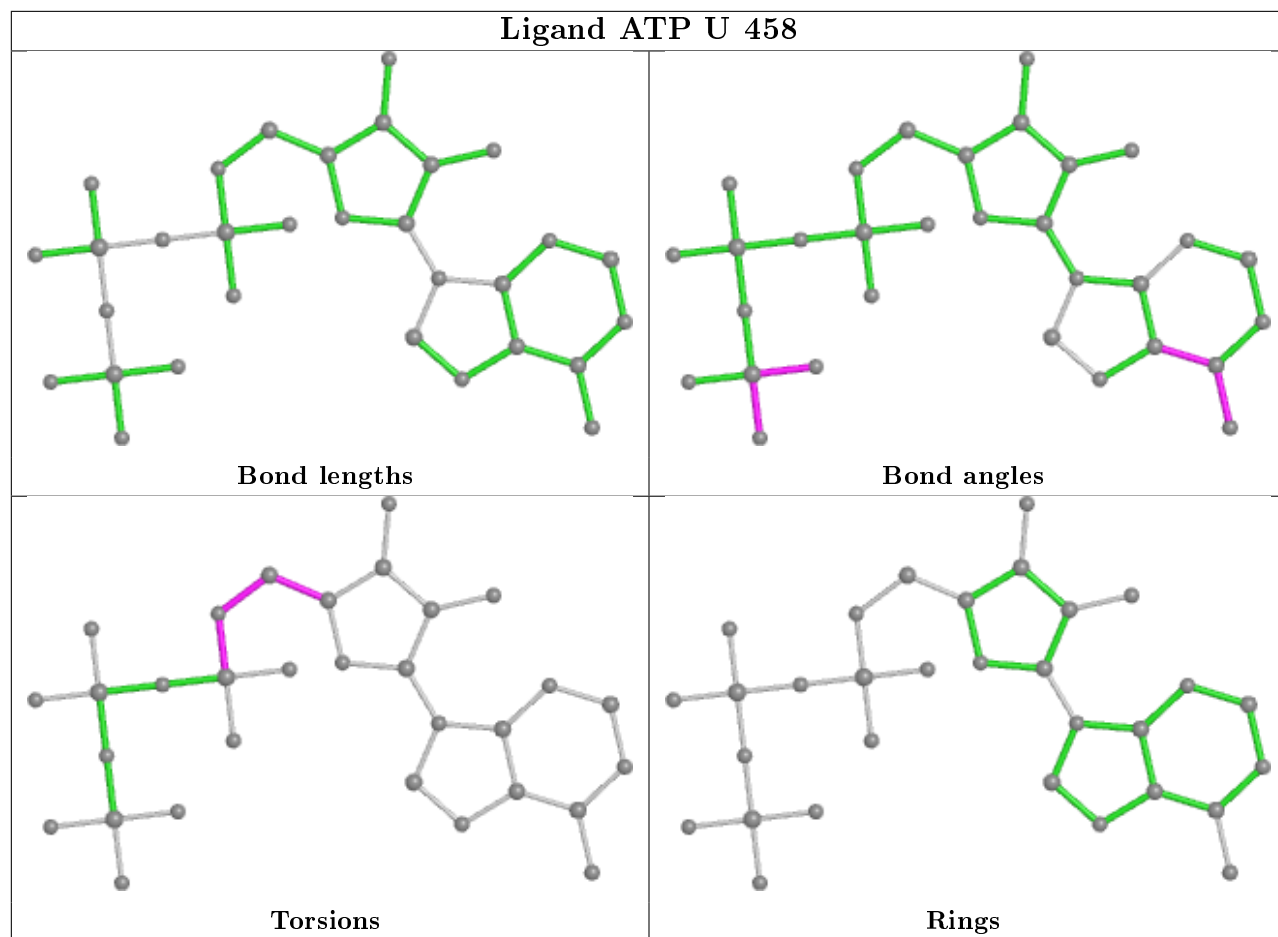
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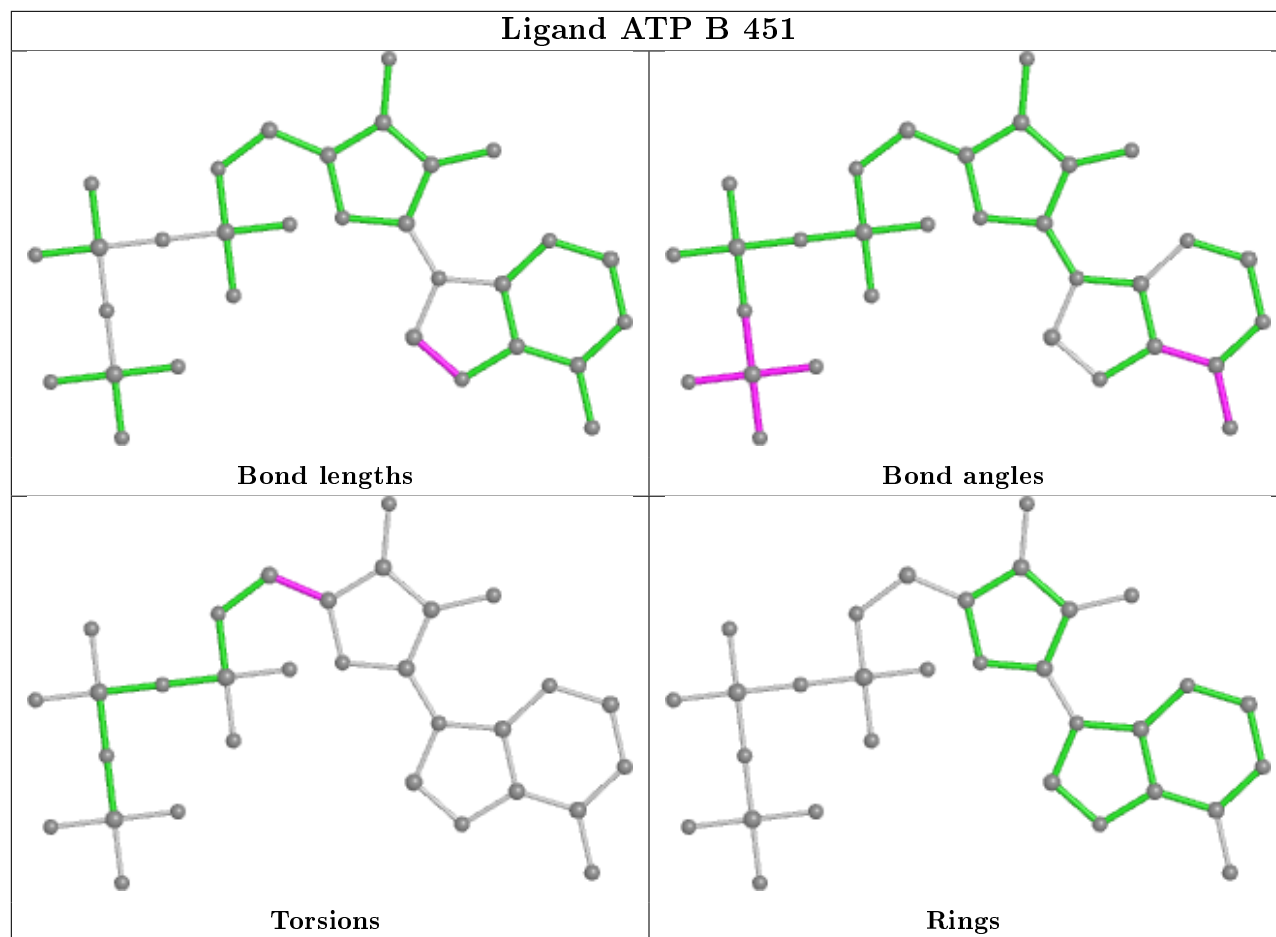
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	451	ATP	5	0
3	X	461	ATP	9	0
3	W	460	ATP	8	0
3	E	454	ATP	9	0
3	S	456	ATP	14	0
3	F	455	ATP	8	0
3	A	450	ATP	2	0
3	T	457	ATP	3	0
3	V	459	ATP	3	0

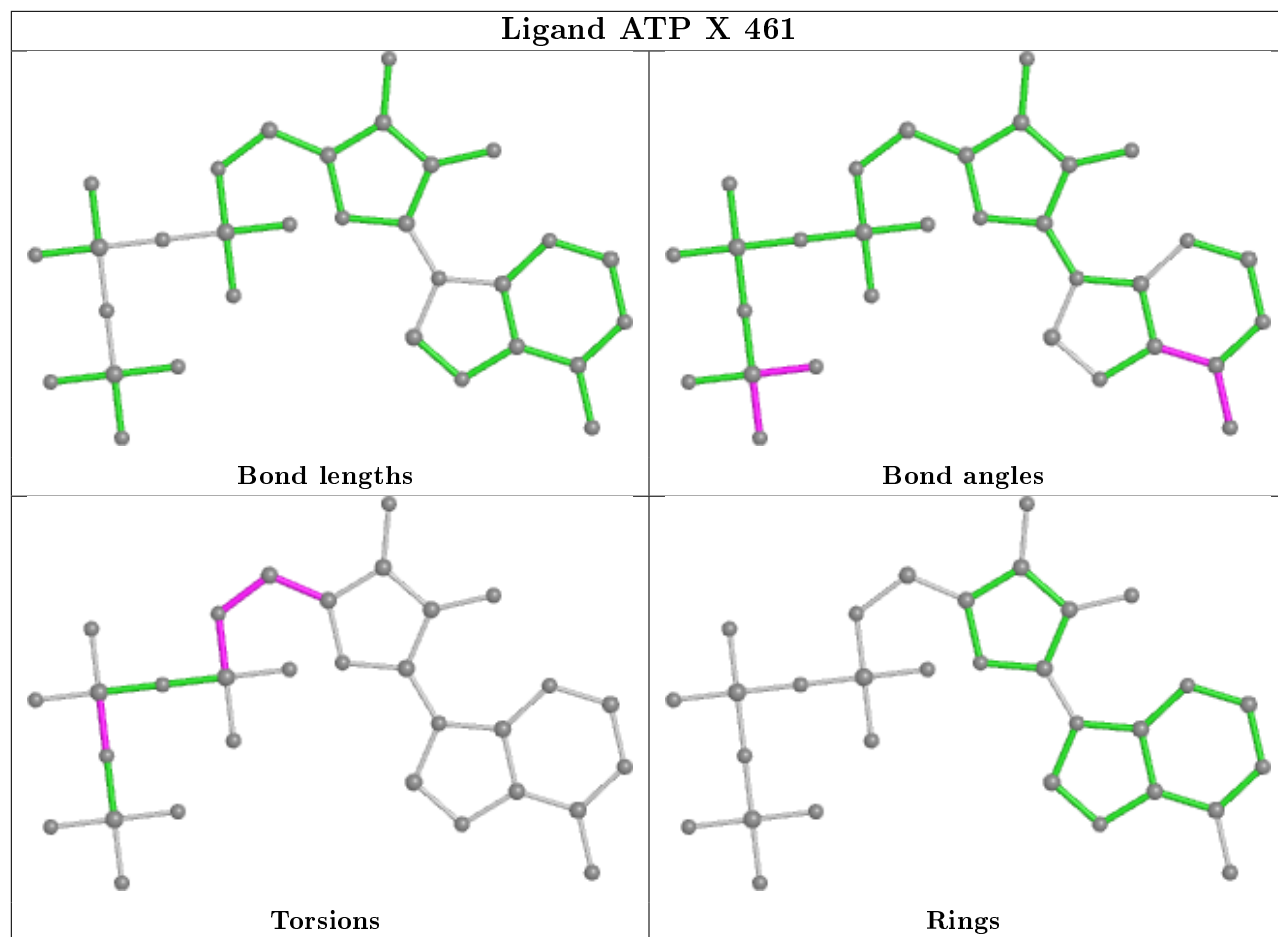
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

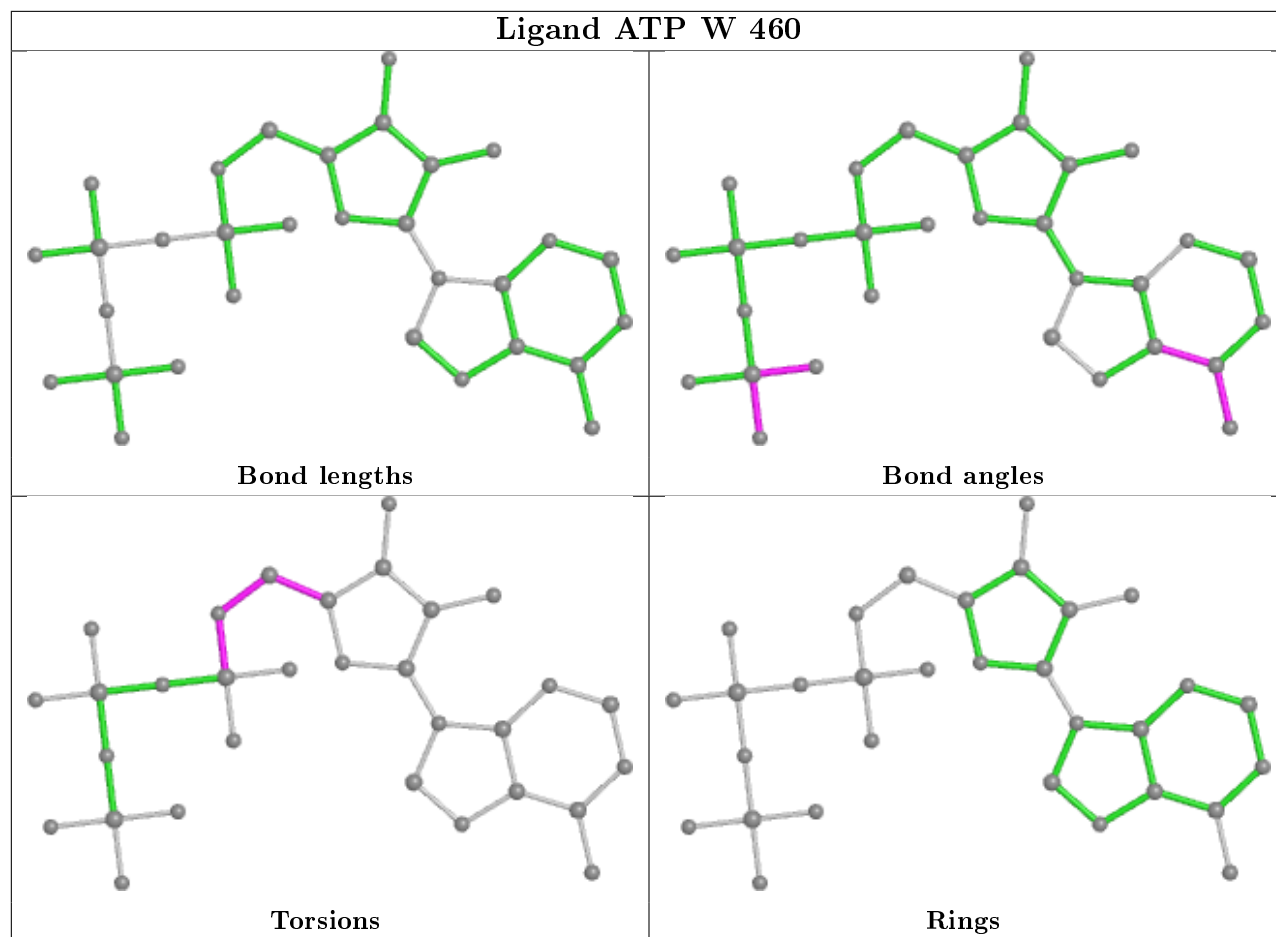


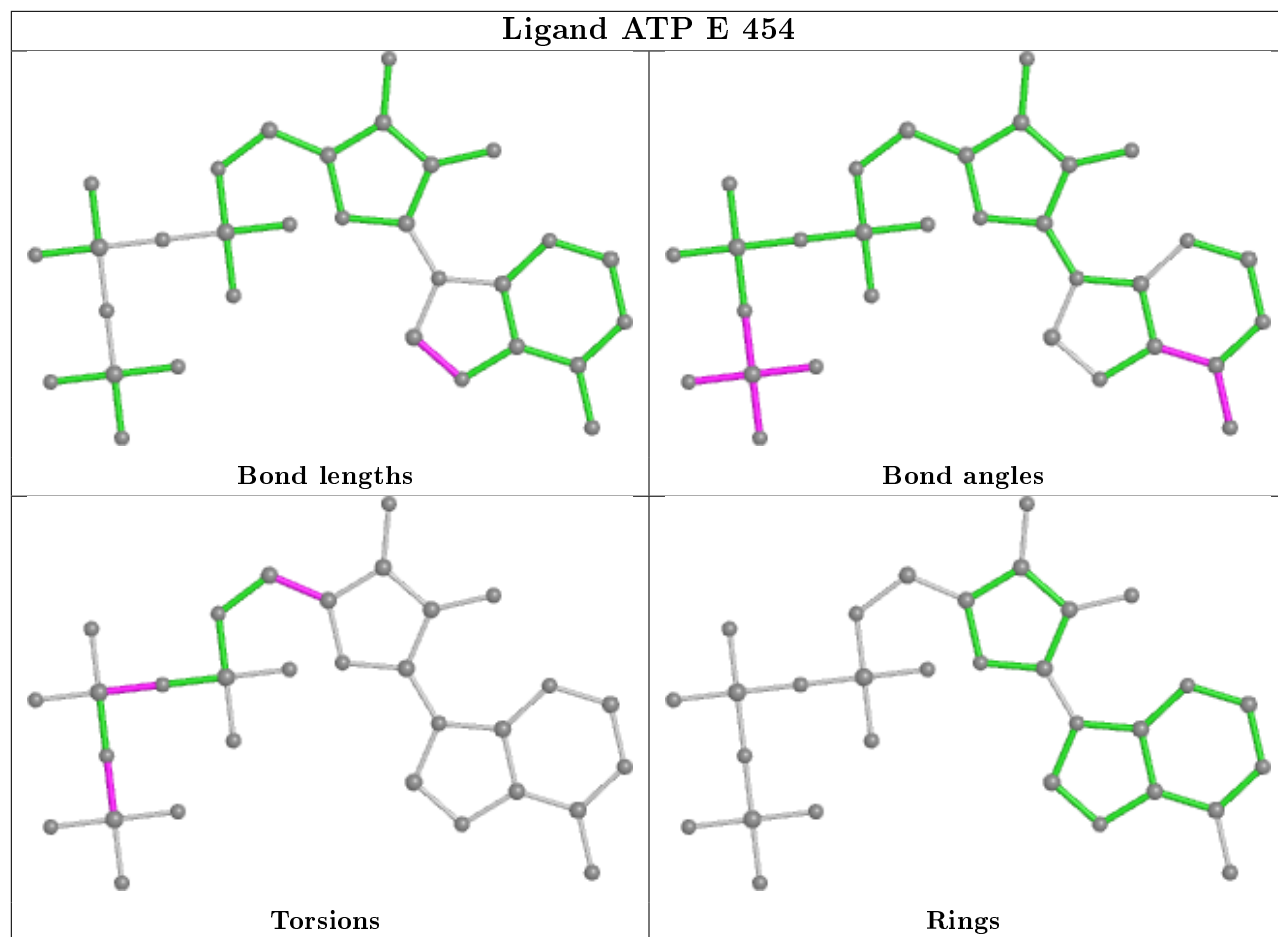


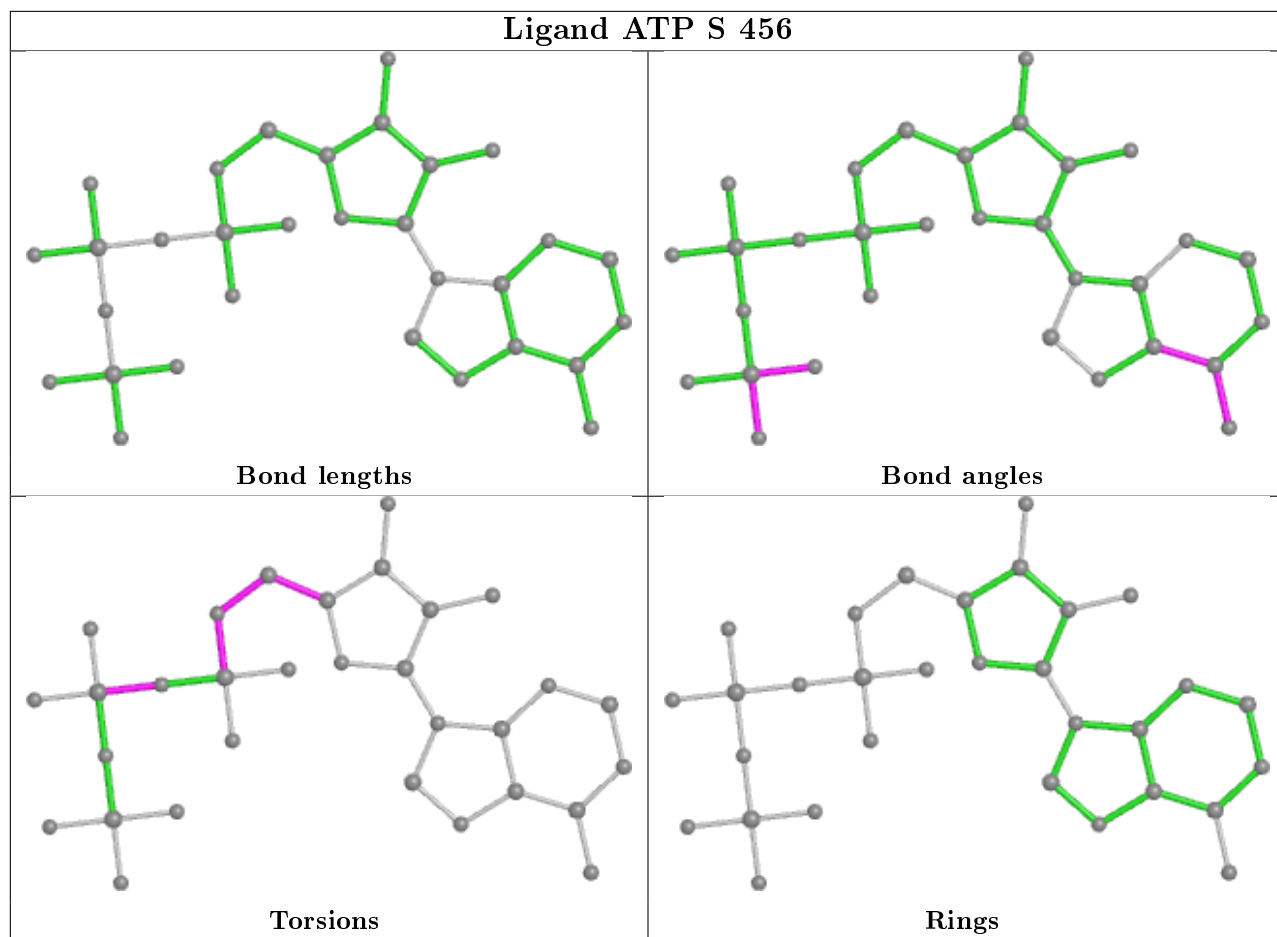


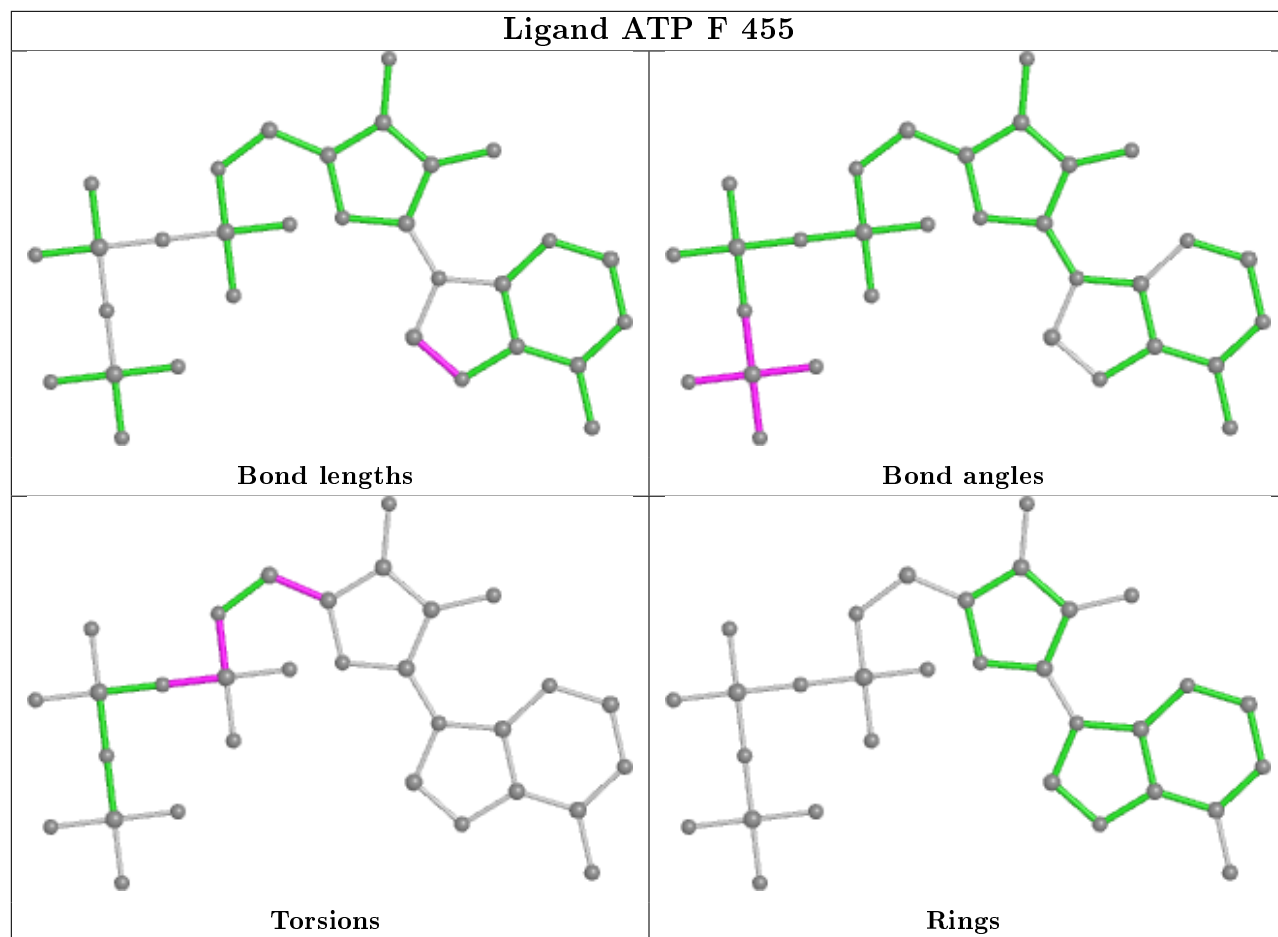


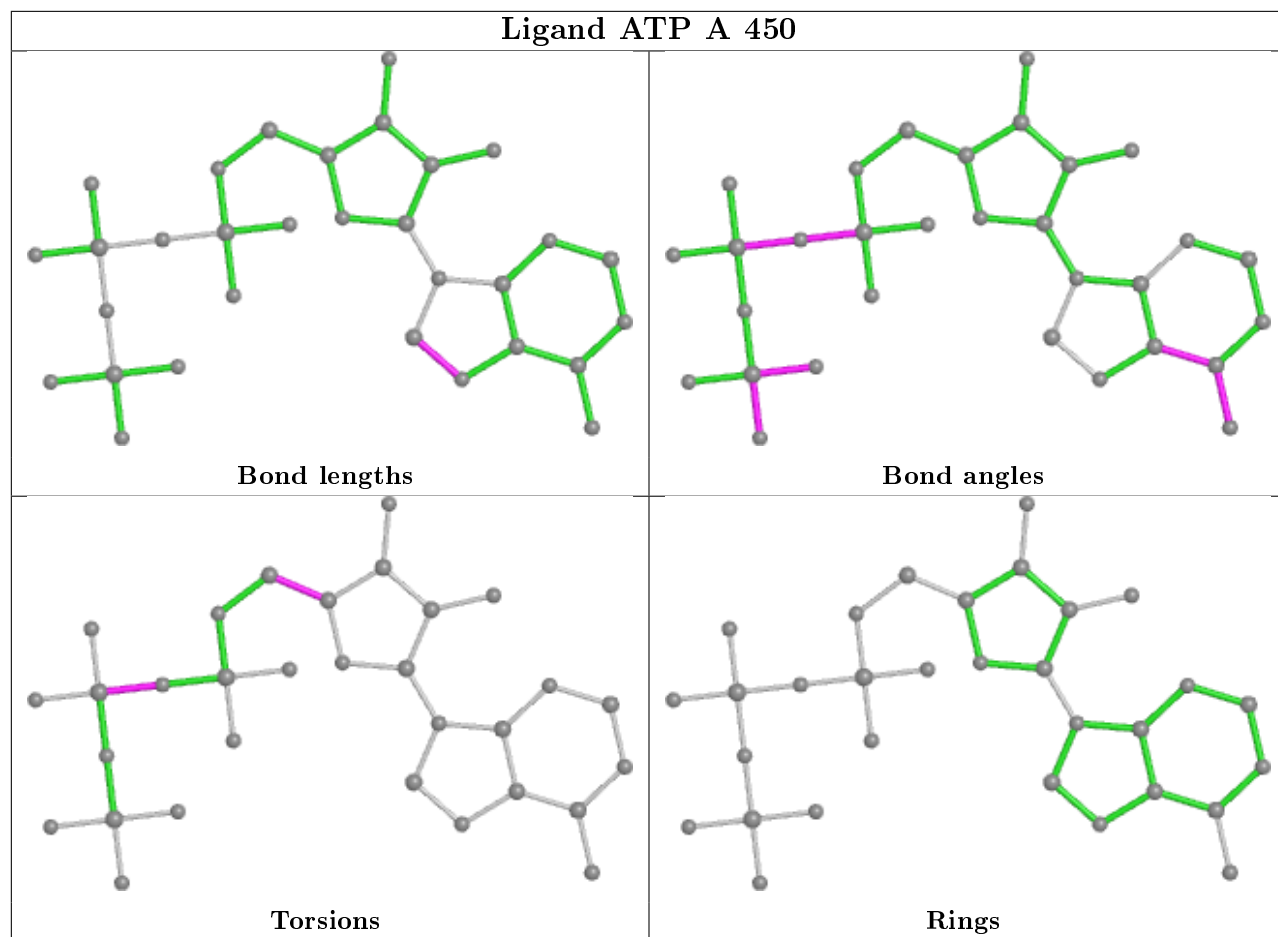


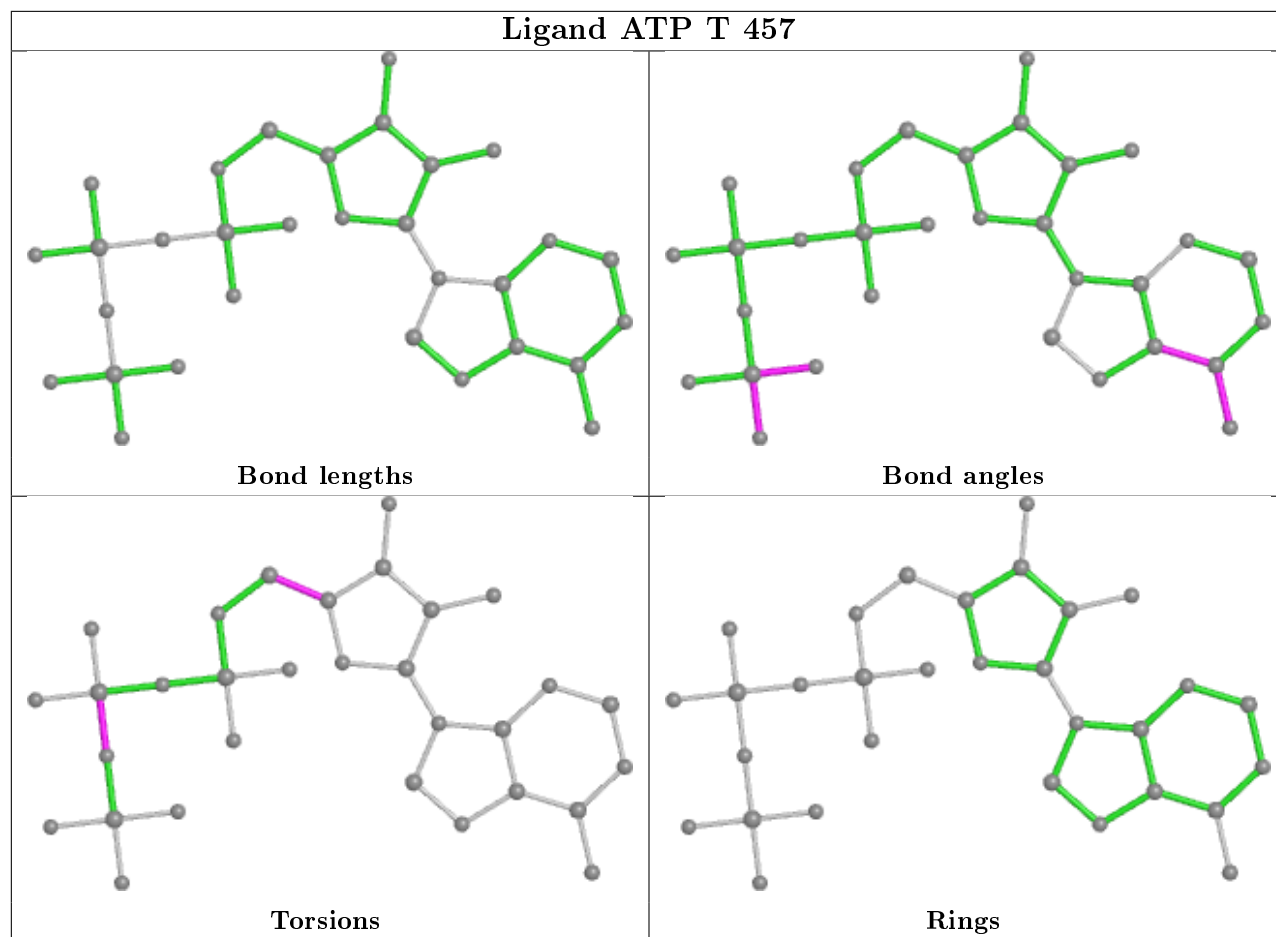


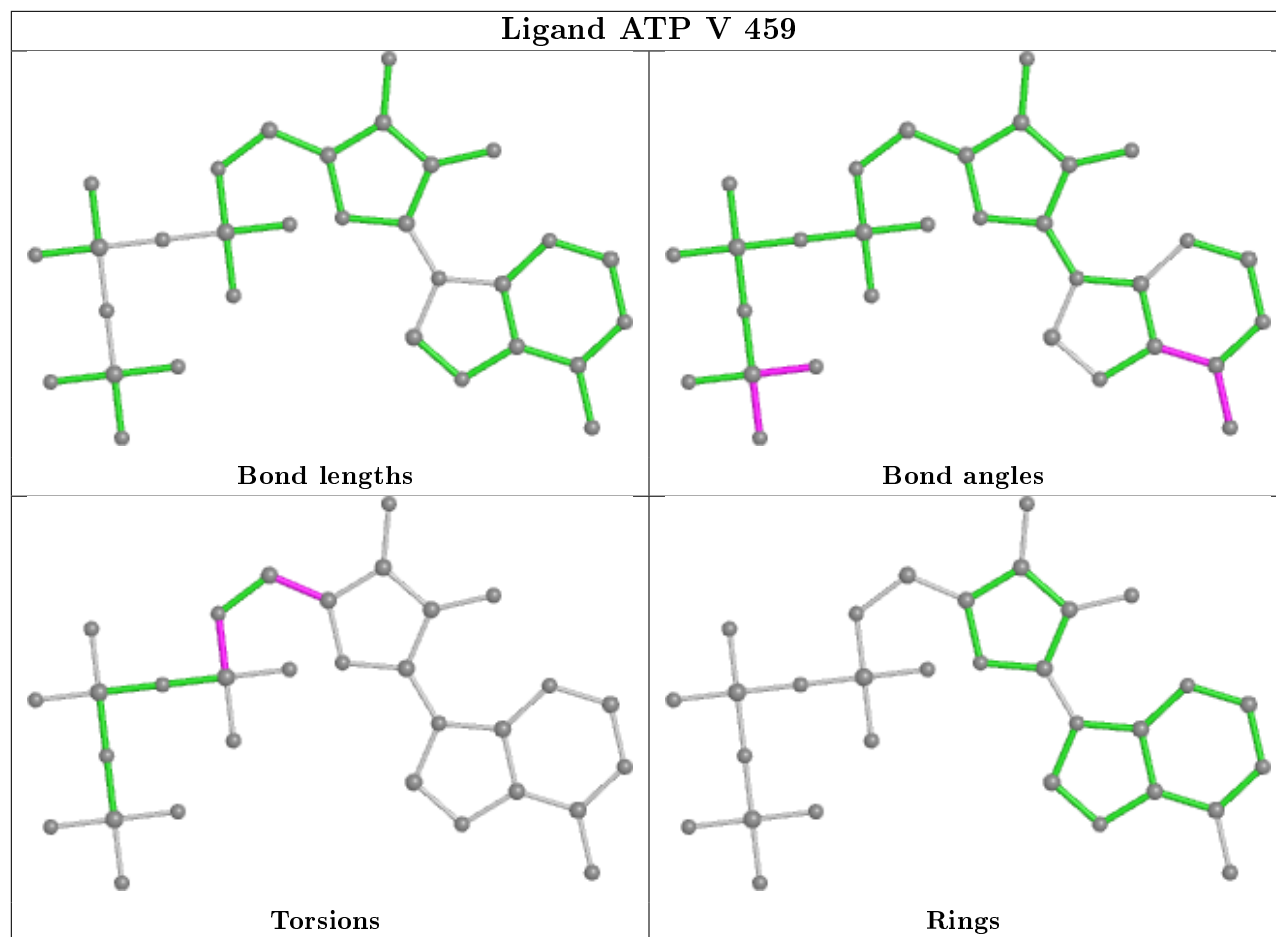












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.