



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:11 AM UTC

PDB ID : 1G3I / pdb_00001g3i
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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

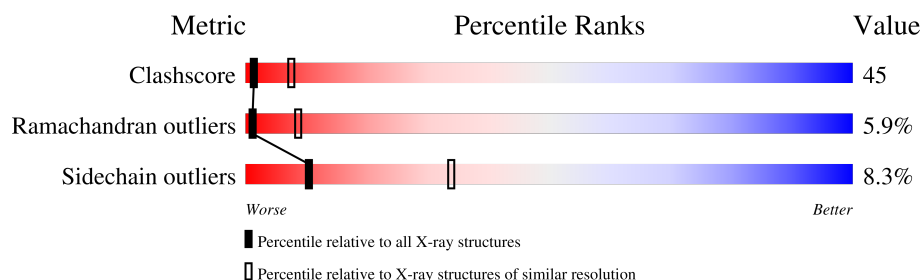
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)

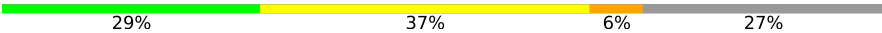
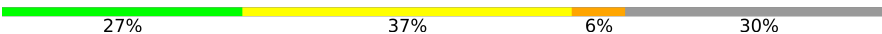
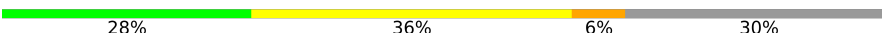
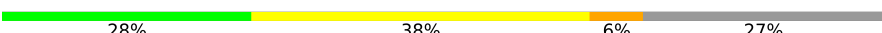
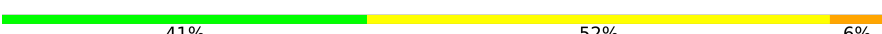
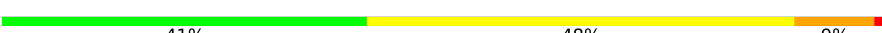
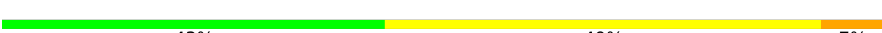
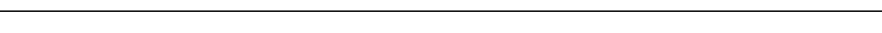
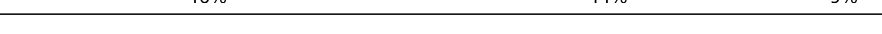
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	24% 39% 10% • 27%
1	B	444	22% 39% 10% • 27%
1	C	444	23% 37% 11% • 28%
1	D	444	22% 40% 9% • 28%
1	E	444	22% 39% 9% • 29%
1	F	444	21% 37% 13% • 28%
1	S	444	26% 38% 7% • 29%
1	T	444	28% 39% 7% • 25%

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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

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

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

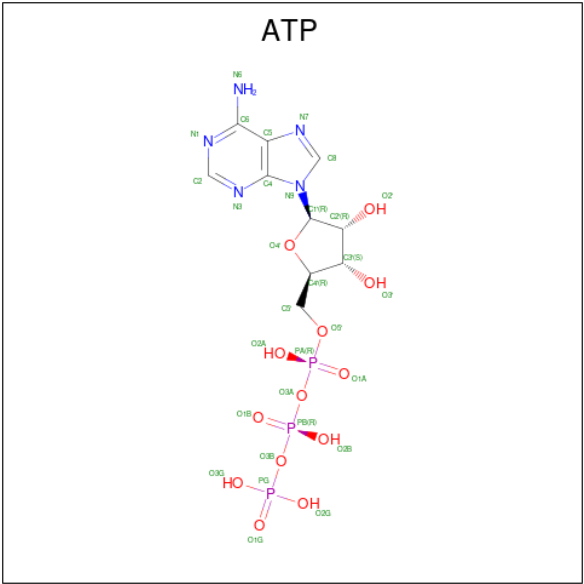
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	173	Total	C	N	O	S	0	0	0
			1280	803	227	246	4			
2	H	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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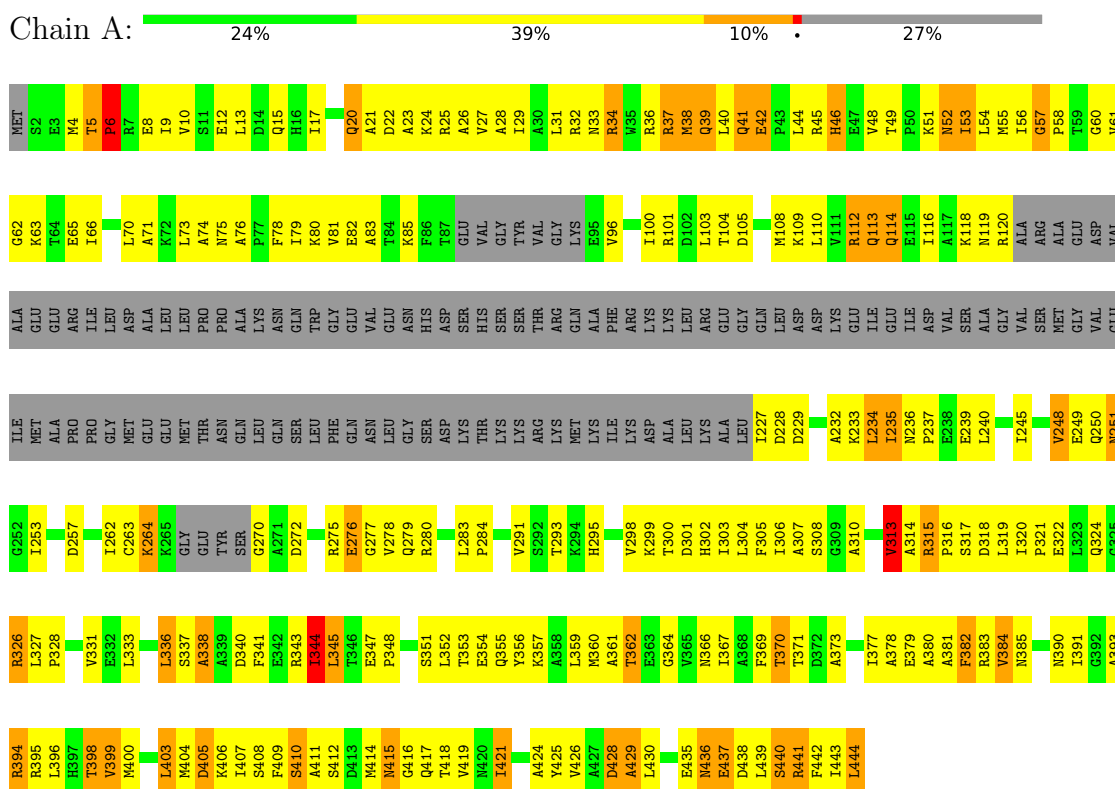
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	T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

3 Residue-property plots

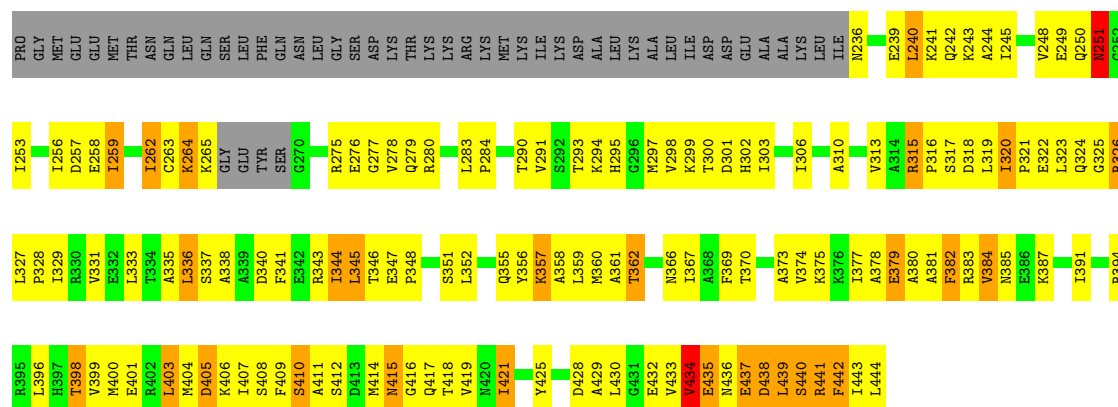
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

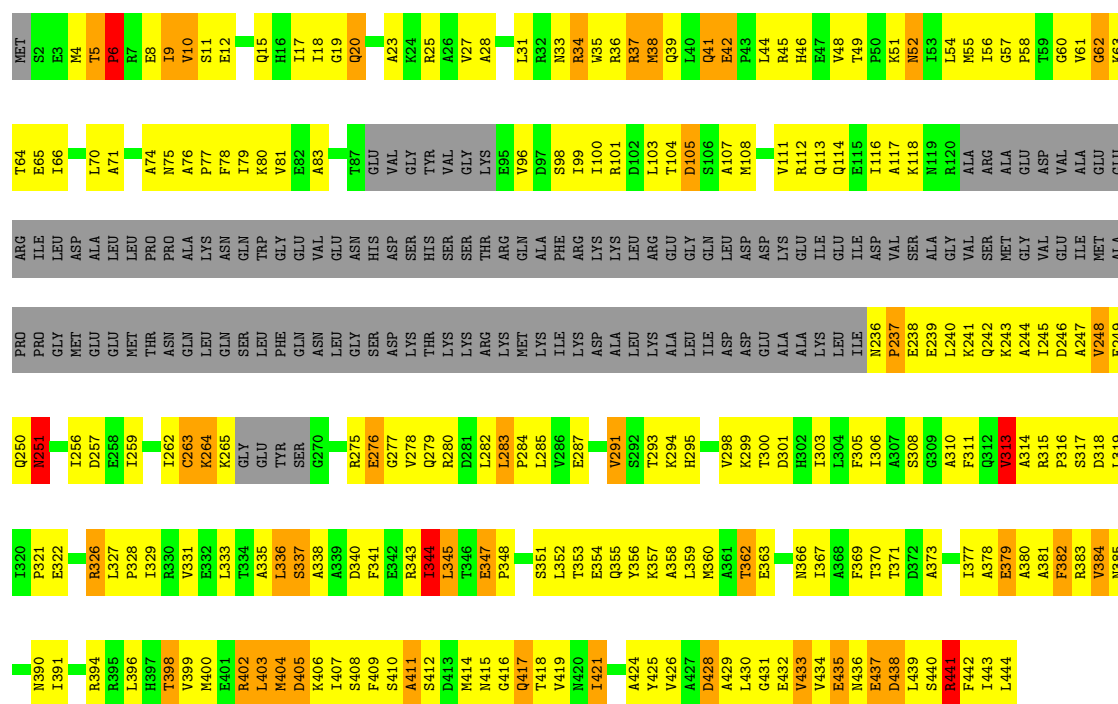
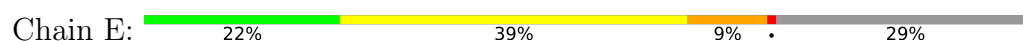
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



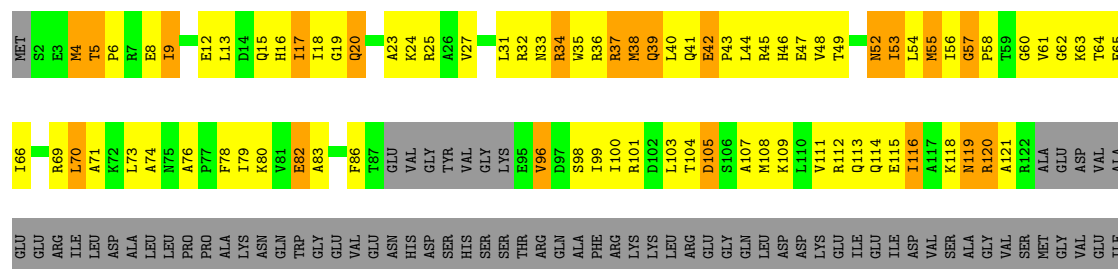
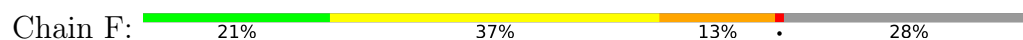


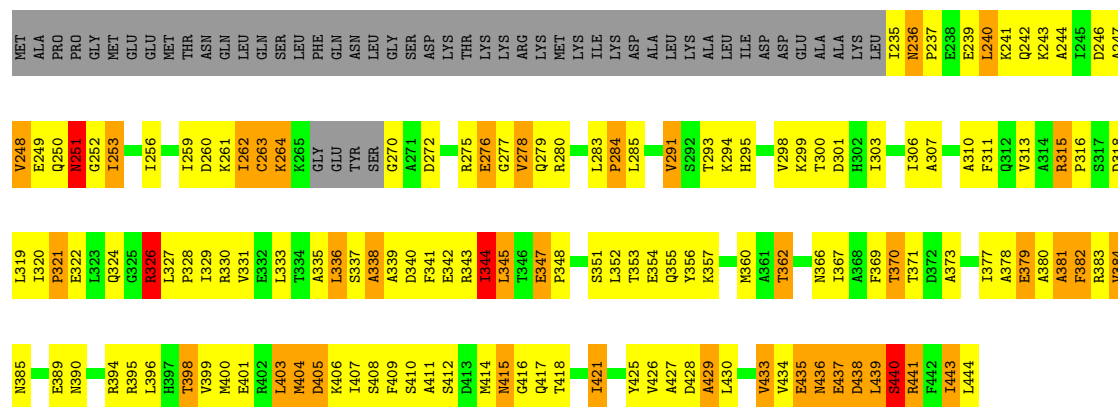


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



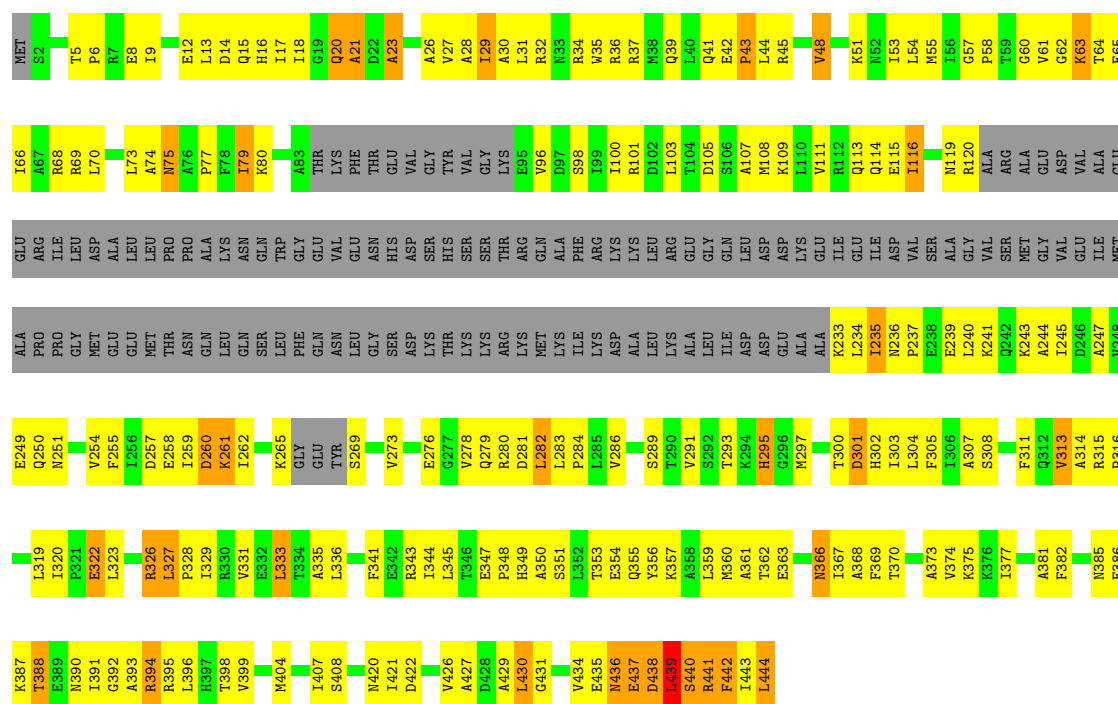
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU





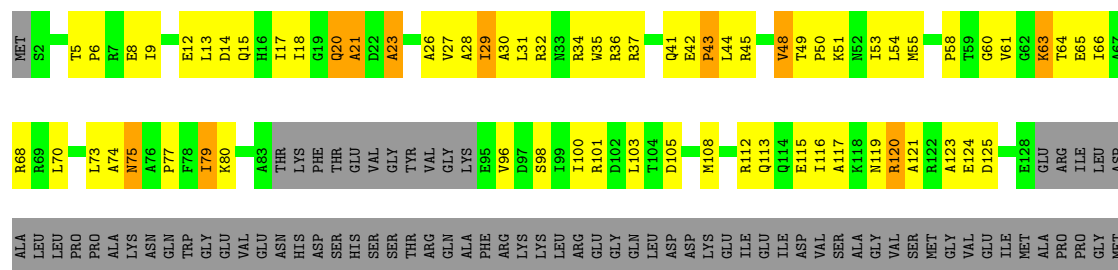
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

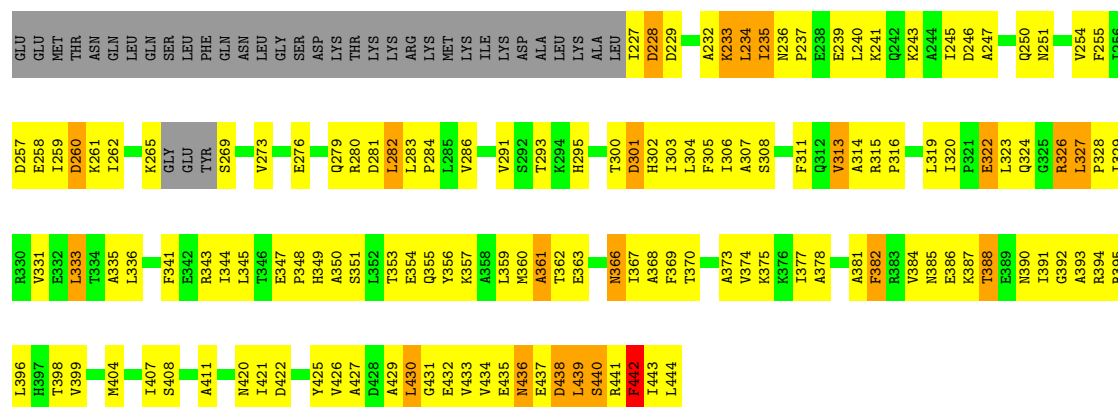
Chain S: 26% 38% 7% 29%



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

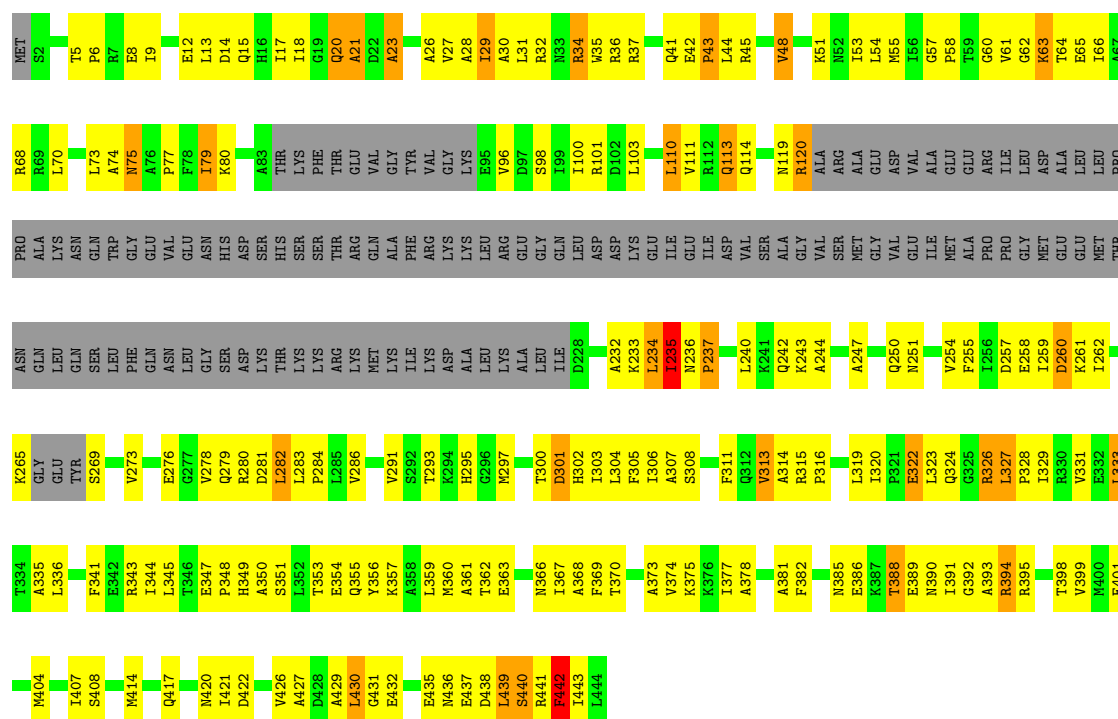
Chain T: 28% 39% 7% 25%





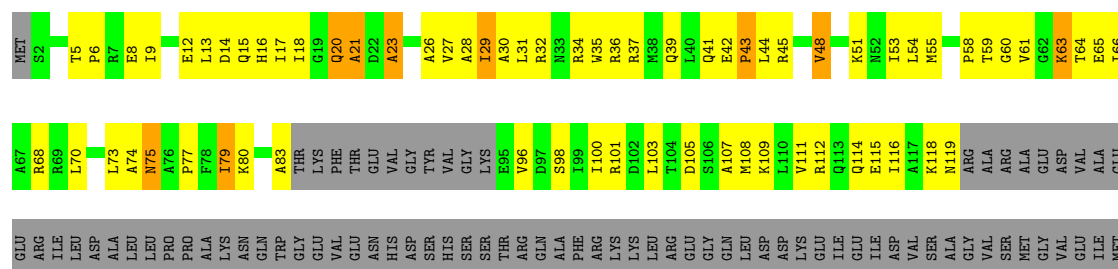
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

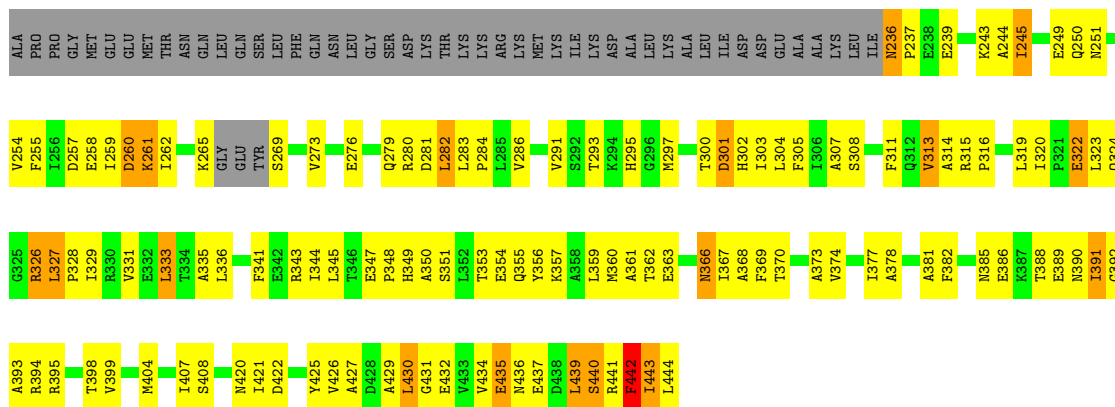
Chain U: 29% 37% 6% 27%



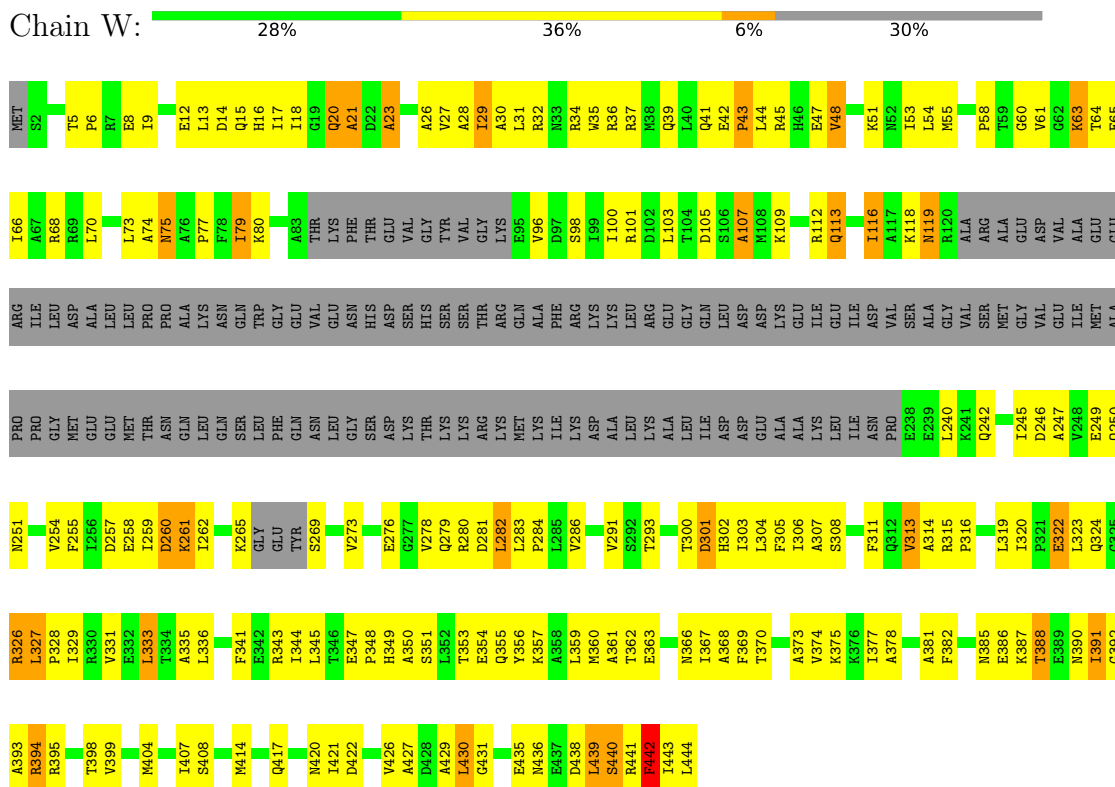
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain V: 27% 37% 6% 30%

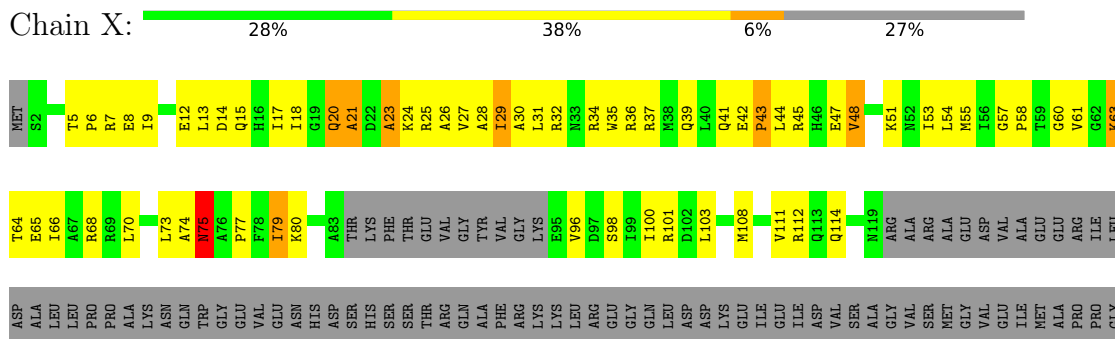


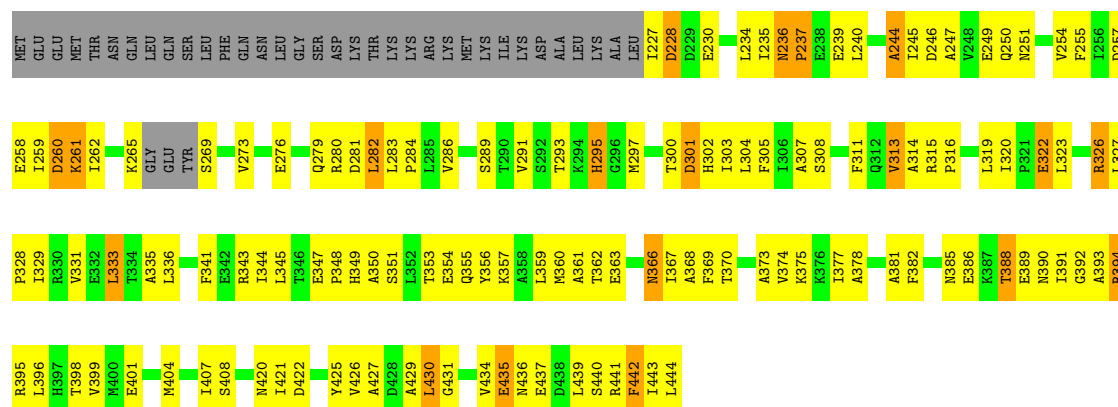


- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



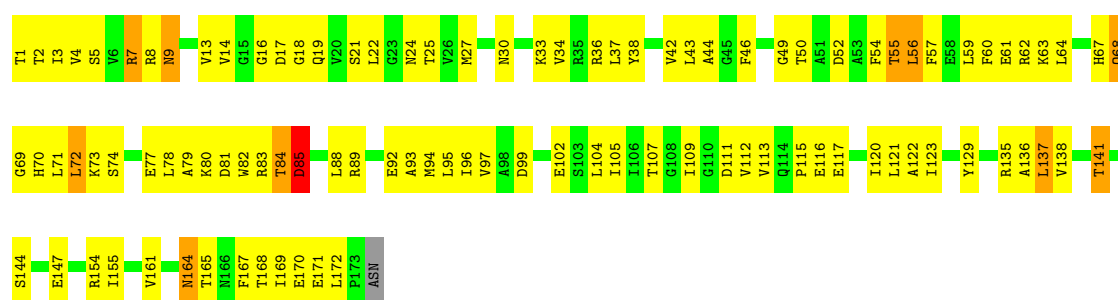
- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU





• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain G: 41% 52% 6% ..



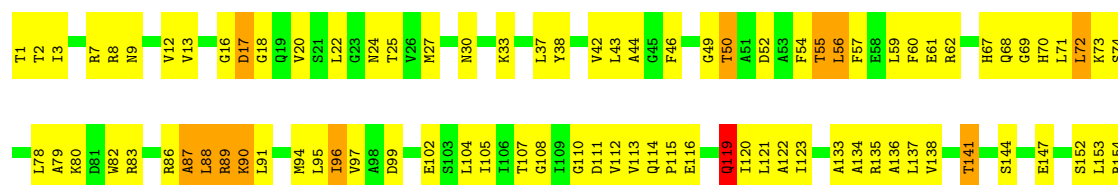
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

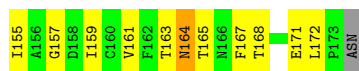
Chain H: 41% 48% 9% ..



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

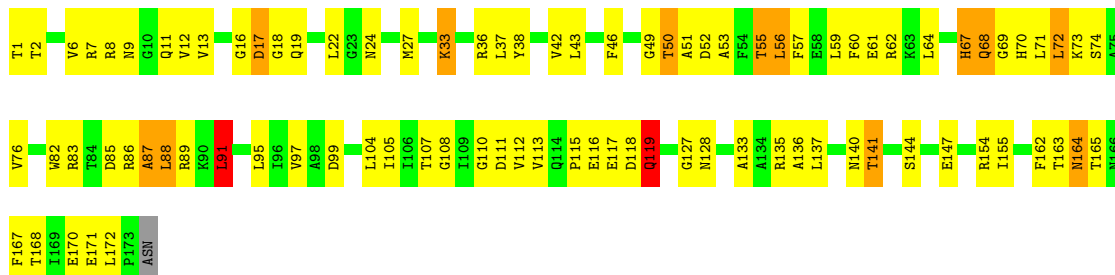
Chain I: 43% 49% 7% ..





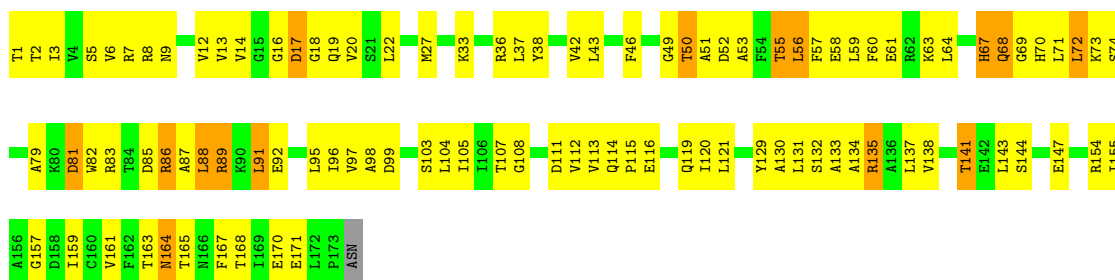
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain J: 48% 44% 7% ..



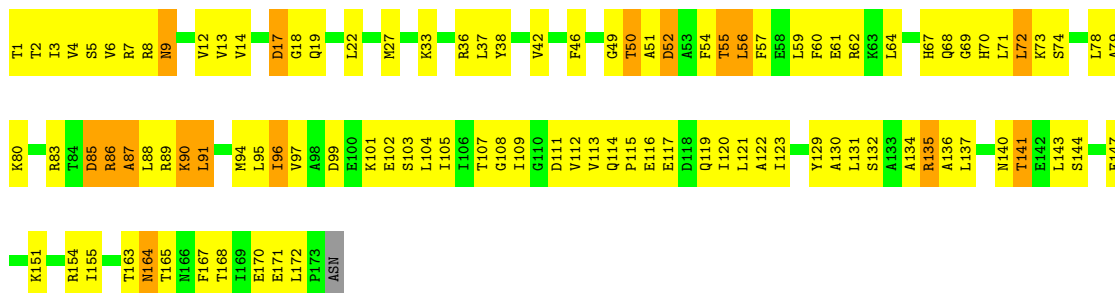
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain K: 41% 50% 9% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

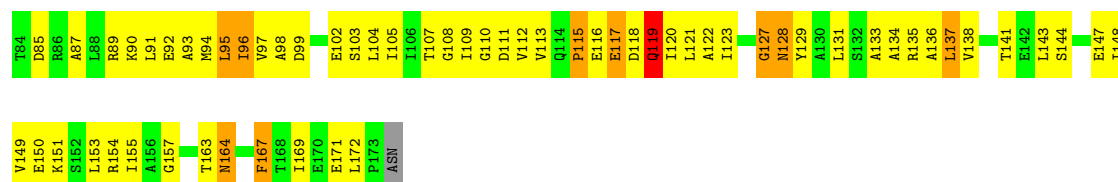
Chain L: 40% 51% 9% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

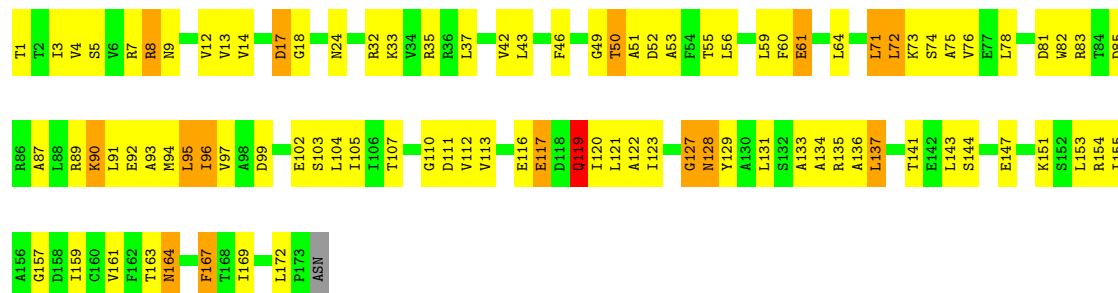
Chain M: 40% 51% 9% ..

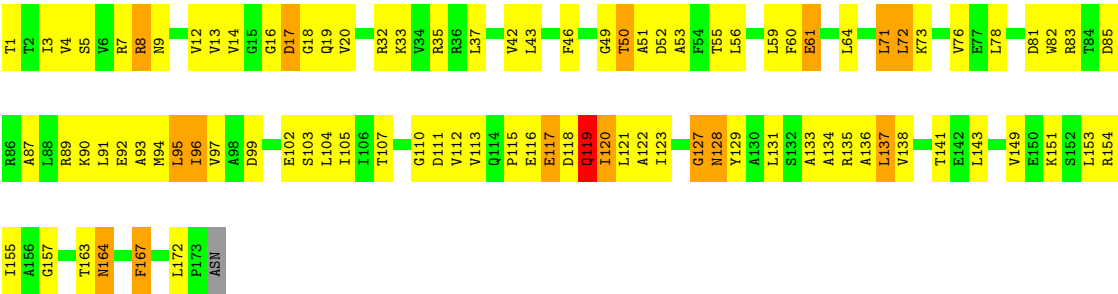




• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N: 45% 45% 9% ..





● Molecule 2: ATP-DEPENDENT PROTEASE HSLV



4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	45528	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.85	2/2566 (0.1%)	1.20	20/3458 (0.6%)
1	B	0.86	0/2566	1.21	24/3458 (0.7%)
1	C	0.77	1/2511 (0.0%)	1.19	31/3384 (0.9%)
1	D	0.85	1/2503 (0.0%)	1.24	26/3373 (0.8%)
1	E	0.89	1/2489 (0.0%)	1.27	28/3354 (0.8%)
1	F	0.86	3/2522 (0.1%)	1.23	29/3398 (0.9%)
1	S	0.38	0/2494	0.95	12/3360 (0.4%)
1	T	0.38	0/2596	0.97	13/3499 (0.4%)
1	U	0.37	0/2529	0.96	16/3408 (0.5%)
1	V	0.38	0/2458	0.96	13/3313 (0.4%)
1	W	0.36	0/2453	0.95	9/3304 (0.3%)
1	X	0.38	0/2526	0.93	10/3405 (0.3%)
2	G	0.73	0/1294	1.07	6/1753 (0.3%)
2	H	0.74	2/1294 (0.2%)	1.12	7/1754 (0.4%)
2	I	0.67	0/1306	1.04	6/1767 (0.3%)
2	J	0.67	0/1294	1.05	5/1754 (0.3%)
2	K	0.69	0/1294	1.06	3/1754 (0.2%)
2	L	0.73	0/1308	1.11	7/1770 (0.4%)
2	M	0.51	0/1275	0.99	6/1732 (0.3%)
2	N	0.48	0/1275	0.97	5/1732 (0.3%)
2	O	0.45	0/1271	0.92	3/1727 (0.2%)
2	P	0.45	0/1271	0.92	2/1727 (0.1%)
2	Q	0.61	3/1275 (0.2%)	0.99	5/1732 (0.3%)
2	R	0.50	0/1271	0.94	2/1727 (0.1%)
All	All	0.64	13/45641 (0.0%)	1.07	288/61643 (0.5%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	120	ILE	N-CA	-7.60	1.37	1.46
2	Q	119	GLN	CA-C	-7.30	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	53	ILE	CA-CB	-7.13	1.45	1.54
1	A	313	VAL	CA-CB	-6.84	1.47	1.55
2	Q	119	GLN	C-N	-6.63	1.24	1.33

The worst 5 of 288 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	N-CA-C	-10.51	97.16	110.19
1	W	116	ILE	N-CA-C	-10.49	101.99	113.43
2	M	119	GLN	OE1-CD-NE2	-10.24	112.36	122.60
2	Q	119	GLN	OE1-CD-NE2	-10.11	112.49	122.60
1	E	37	ARG	N-CA-C	-9.89	98.25	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2539	0	2606	269	0
1	B	2539	0	2606	272	0
1	C	2484	0	2552	261	0
1	D	2476	0	2541	264	0
1	E	2462	0	2521	263	0
1	F	2495	0	2565	279	0
1	S	2468	0	2540	260	0
1	T	2570	0	2628	239	0
1	U	2503	0	2564	242	0
1	V	2432	0	2492	230	0
1	W	2428	0	2492	234	0
1	X	2500	0	2562	256	1
2	G	1280	0	1275	112	0
2	H	1280	0	1270	124	0
2	I	1292	0	1296	116	0
2	J	1280	0	1270	108	0
2	K	1280	0	1270	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1294	0	1296	114	0
2	M	1261	0	1240	112	0
2	N	1261	0	1240	111	0
2	O	1257	0	1234	102	0
2	P	1257	0	1234	101	0
2	Q	1261	0	1240	101	0
2	R	1257	0	1234	99	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	4131	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 45.

The worst 5 of 4131 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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	1	10
1	B	318/444 (72%)	241 (76%)	58 (18%)	19 (6%)	1	8
1	C	311/444 (70%)	234 (75%)	60 (19%)	17 (6%)	1	10
1	D	310/444 (70%)	235 (76%)	56 (18%)	19 (6%)	1	8
1	E	309/444 (70%)	238 (77%)	51 (16%)	20 (6%)	1	7
1	F	312/444 (70%)	240 (77%)	54 (17%)	18 (6%)	1	9
1	S	309/444 (70%)	227 (74%)	57 (18%)	25 (8%)	1	4
1	T	323/444 (73%)	236 (73%)	63 (20%)	24 (7%)	1	5
1	U	314/444 (71%)	237 (76%)	54 (17%)	23 (7%)	1	5
1	V	305/444 (69%)	228 (75%)	54 (18%)	23 (8%)	1	5
1	W	304/444 (68%)	223 (73%)	57 (19%)	24 (8%)	1	5
1	X	314/444 (71%)	235 (75%)	56 (18%)	23 (7%)	1	5
2	G	171/174 (98%)	141 (82%)	28 (16%)	2 (1%)	10	35
2	H	171/174 (98%)	139 (81%)	26 (15%)	6 (4%)	3	16
2	I	171/174 (98%)	136 (80%)	30 (18%)	5 (3%)	3	19
2	J	171/174 (98%)	136 (80%)	28 (16%)	7 (4%)	2	14
2	K	171/174 (98%)	138 (81%)	26 (15%)	7 (4%)	2	14
2	L	171/174 (98%)	137 (80%)	27 (16%)	7 (4%)	2	14
2	M	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	1	10
2	N	171/174 (98%)	129 (75%)	34 (20%)	8 (5%)	2	12
2	O	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	1	10
2	P	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	1	10
2	Q	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	1	10
2	R	171/174 (98%)	128 (75%)	33 (19%)	10 (6%)	1	9
All	All	5799/7416 (78%)	4418 (76%)	1041 (18%)	340 (6%)	1	9

5 of 340 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	235	ILE
1	A	417	GLN
1	A	436	ASN
1	A	438	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	22
1	B	274/373 (74%)	242 (88%)	32 (12%)	5	20
1	C	268/373 (72%)	231 (86%)	37 (14%)	3	14
1	D	267/373 (72%)	234 (88%)	33 (12%)	4	18
1	E	264/373 (71%)	232 (88%)	32 (12%)	5	18
1	F	269/373 (72%)	235 (87%)	34 (13%)	4	17
1	S	267/373 (72%)	250 (94%)	17 (6%)	16	41
1	T	276/373 (74%)	261 (95%)	15 (5%)	20	46
1	U	270/373 (72%)	254 (94%)	16 (6%)	18	43
1	V	263/373 (70%)	251 (95%)	12 (5%)	24	49
1	W	262/373 (70%)	249 (95%)	13 (5%)	22	48
1	X	270/373 (72%)	258 (96%)	12 (4%)	25	50
2	G	130/140 (93%)	117 (90%)	13 (10%)	7	25
2	H	130/140 (93%)	116 (89%)	14 (11%)	6	22
2	I	133/140 (95%)	122 (92%)	11 (8%)	10	34
2	J	130/140 (93%)	118 (91%)	12 (9%)	8	29
2	K	130/140 (93%)	119 (92%)	11 (8%)	10	32
2	L	133/140 (95%)	123 (92%)	10 (8%)	12	37
2	M	125/140 (89%)	118 (94%)	7 (6%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	125/140 (89%)	117 (94%)	8 (6%)	16	41
2	O	124/140 (89%)	117 (94%)	7 (6%)	19	45
2	P	124/140 (89%)	117 (94%)	7 (6%)	19	45
2	Q	125/140 (89%)	118 (94%)	7 (6%)	19	45
2	R	124/140 (89%)	117 (94%)	7 (6%)	19	45
All	All	4757/6156 (77%)	4360 (92%)	397 (8%)	10	34

5 of 397 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	119	GLN
2	O	95	LEU
2	J	68	GLN
2	L	56	LEU
2	Q	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	75	ASN
1	V	417	GLN
1	T	366	ASN
1	U	385	ASN
1	W	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	32,33,33	1.02	1 (3%)	48,52,52	0.89	2 (4%)
3	ATP	W	460	-	32,33,33	0.69	1 (3%)	48,52,52	0.74	1 (2%)
3	ATP	D	453	-	32,33,33	0.91	1 (3%)	48,52,52	0.93	1 (2%)
3	ATP	A	450	-	32,33,33	0.74	1 (3%)	48,52,52	0.91	3 (6%)
3	ATP	E	454	-	32,33,33	1.05	3 (9%)	48,52,52	0.91	3 (6%)
3	ATP	U	458	-	32,33,33	0.82	3 (9%)	48,52,52	0.73	1 (2%)
3	ATP	F	455	-	32,33,33	0.87	1 (3%)	48,52,52	0.91	2 (4%)
3	ATP	S	456	-	32,33,33	0.77	1 (3%)	48,52,52	0.74	1 (2%)
3	ATP	B	451	-	32,33,33	0.83	1 (3%)	48,52,52	0.81	2 (4%)
3	ATP	X	461	-	32,33,33	0.55	0	48,52,52	0.74	1 (2%)
3	ATP	V	459	-	32,33,33	0.74	1 (3%)	48,52,52	0.72	1 (2%)
3	ATP	T	457	-	32,33,33	0.72	1 (3%)	48,52,52	0.72	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	452	-	-	4/22/38/38	0/3/3/3
3	ATP	W	460	-	-	4/22/38/38	0/3/3/3
3	ATP	D	453	-	-	3/22/38/38	0/3/3/3
3	ATP	A	450	-	-	2/22/38/38	0/3/3/3
3	ATP	E	454	-	-	4/22/38/38	0/3/3/3
3	ATP	U	458	-	-	4/22/38/38	0/3/3/3
3	ATP	F	455	-	-	4/22/38/38	0/3/3/3
3	ATP	S	456	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	451	-	-	0/22/38/38	0/3/3/3
3	ATP	X	461	-	-	6/22/38/38	0/3/3/3
3	ATP	V	459	-	-	3/22/38/38	0/3/3/3
3	ATP	T	457	-	-	4/22/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	452	ATP	PB-O3B	5.21	1.65	1.59
3	D	453	ATP	PB-O3B	4.25	1.64	1.59
3	E	454	ATP	PB-O3B	4.19	1.64	1.59
3	B	451	ATP	PB-O3B	3.71	1.63	1.59
3	F	455	ATP	PB-O3B	3.35	1.63	1.59

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	453	ATP	O2A-PA-O3A	-2.76	99.82	107.27
3	E	454	ATP	C2'-C1'-N9	-2.52	107.05	113.30
3	E	454	ATP	O3B-PG-O1G	-2.42	98.29	111.04
3	F	455	ATP	O3G-PG-O2G	2.34	116.56	107.80
3	W	460	ATP	O3G-PG-O2G	2.33	116.53	107.80

There are no chirality outliers.

5 of 44 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	D	453	ATP	C5'-O5'-PA-O3A
3	F	455	ATP	C5'-O5'-PA-O1A
3	F	455	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

12 monomers are involved in 82 short contacts:

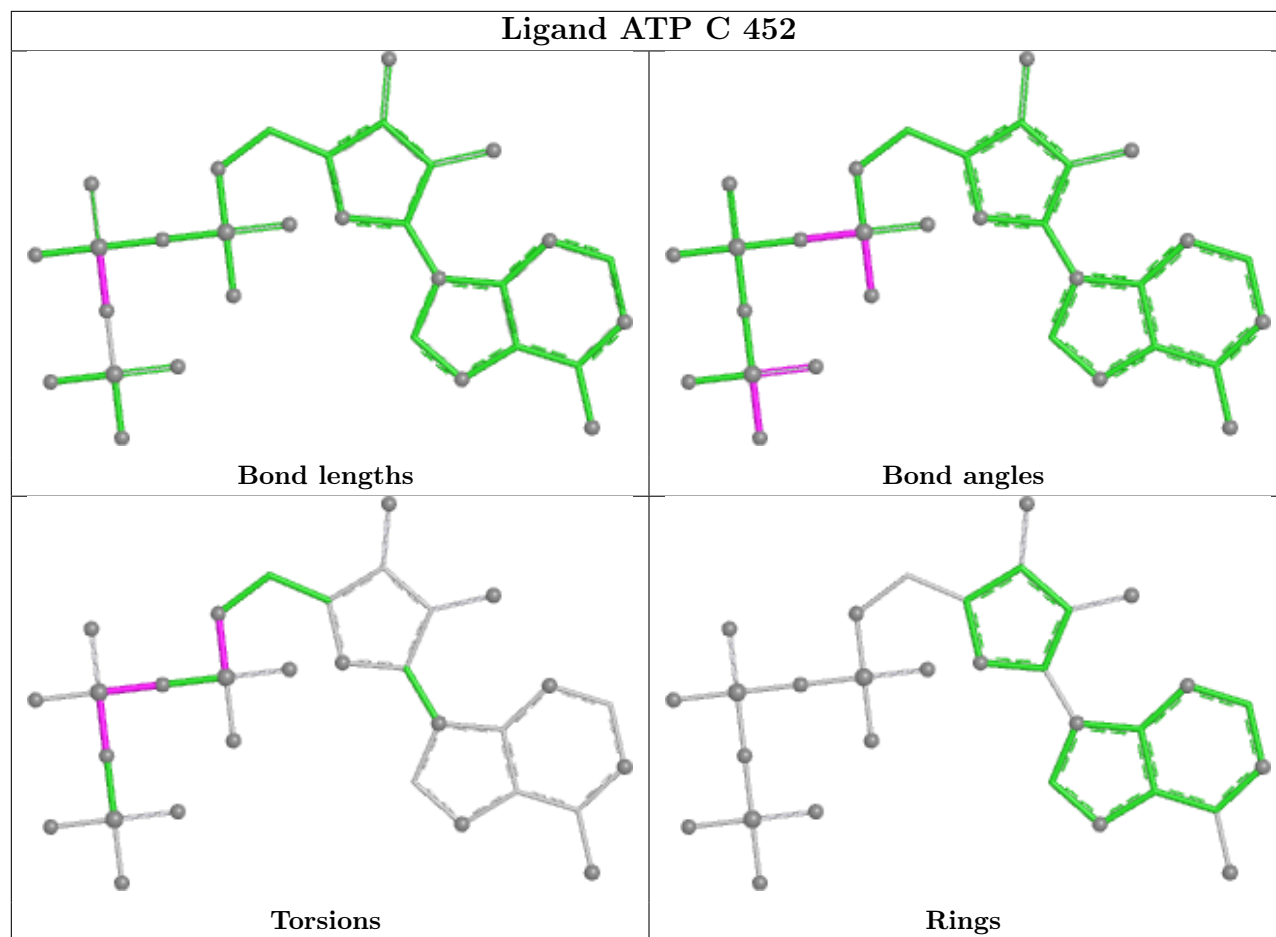
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	452	ATP	5	0
3	W	460	ATP	8	0
3	D	453	ATP	4	0

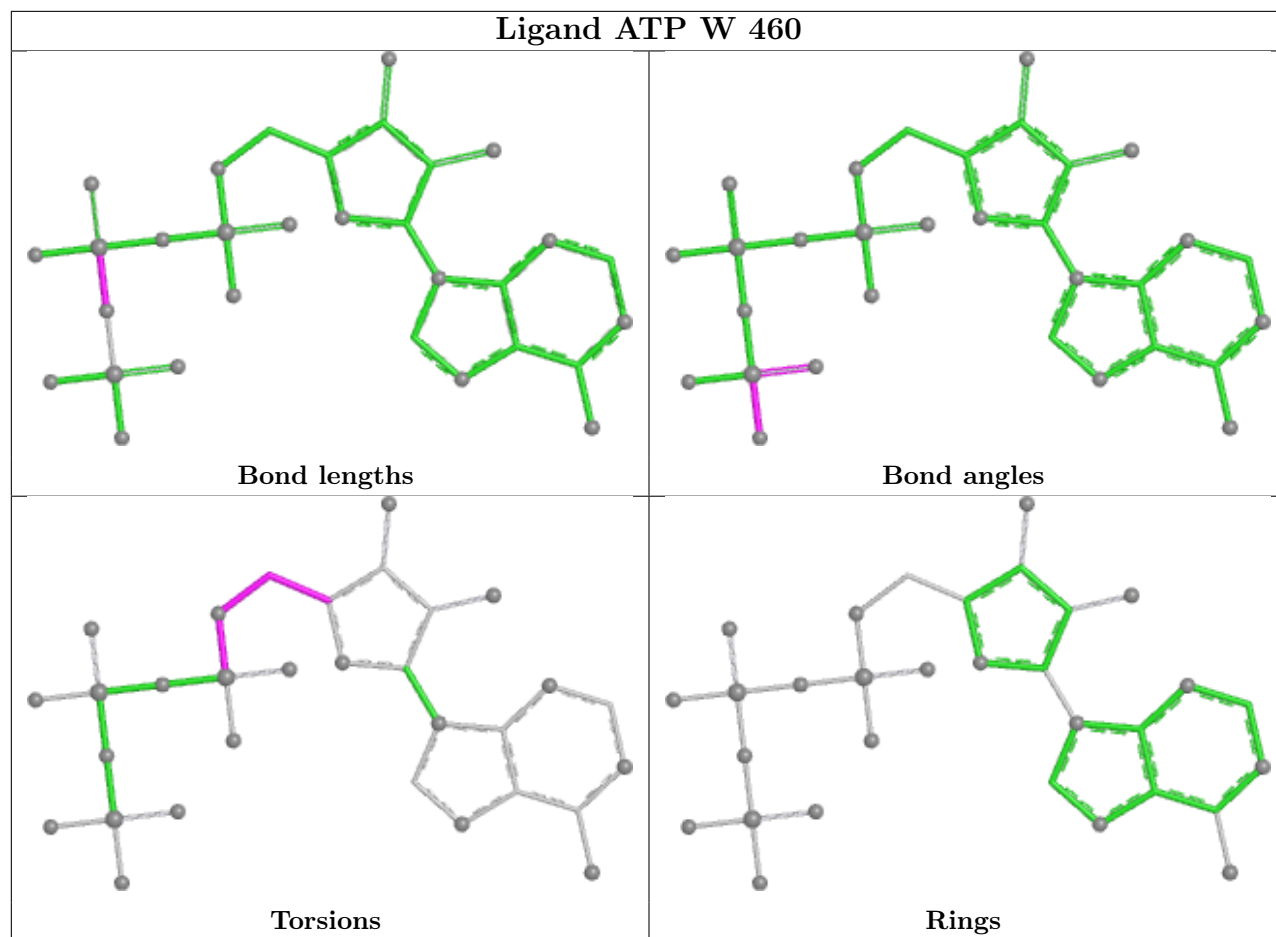
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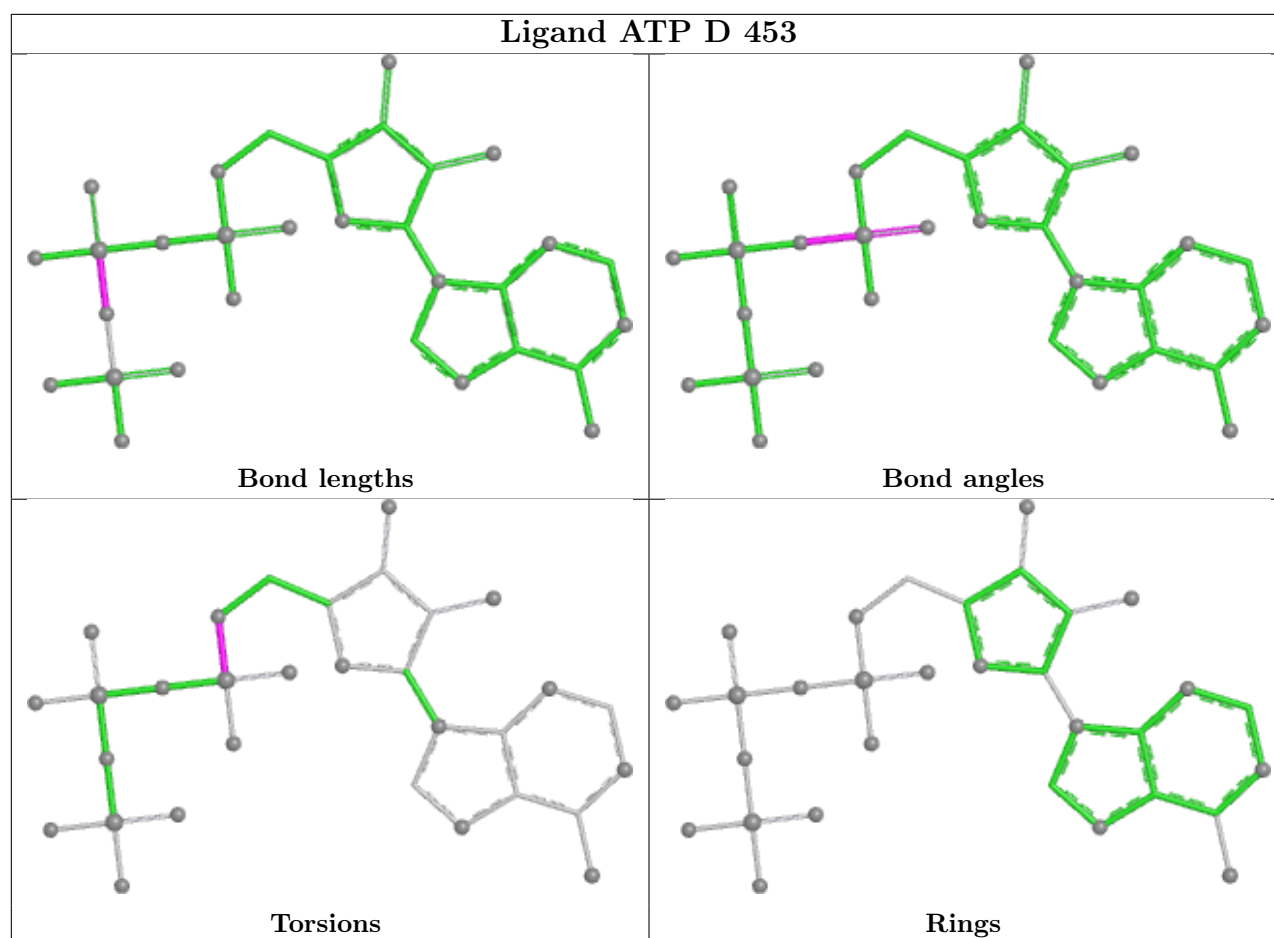
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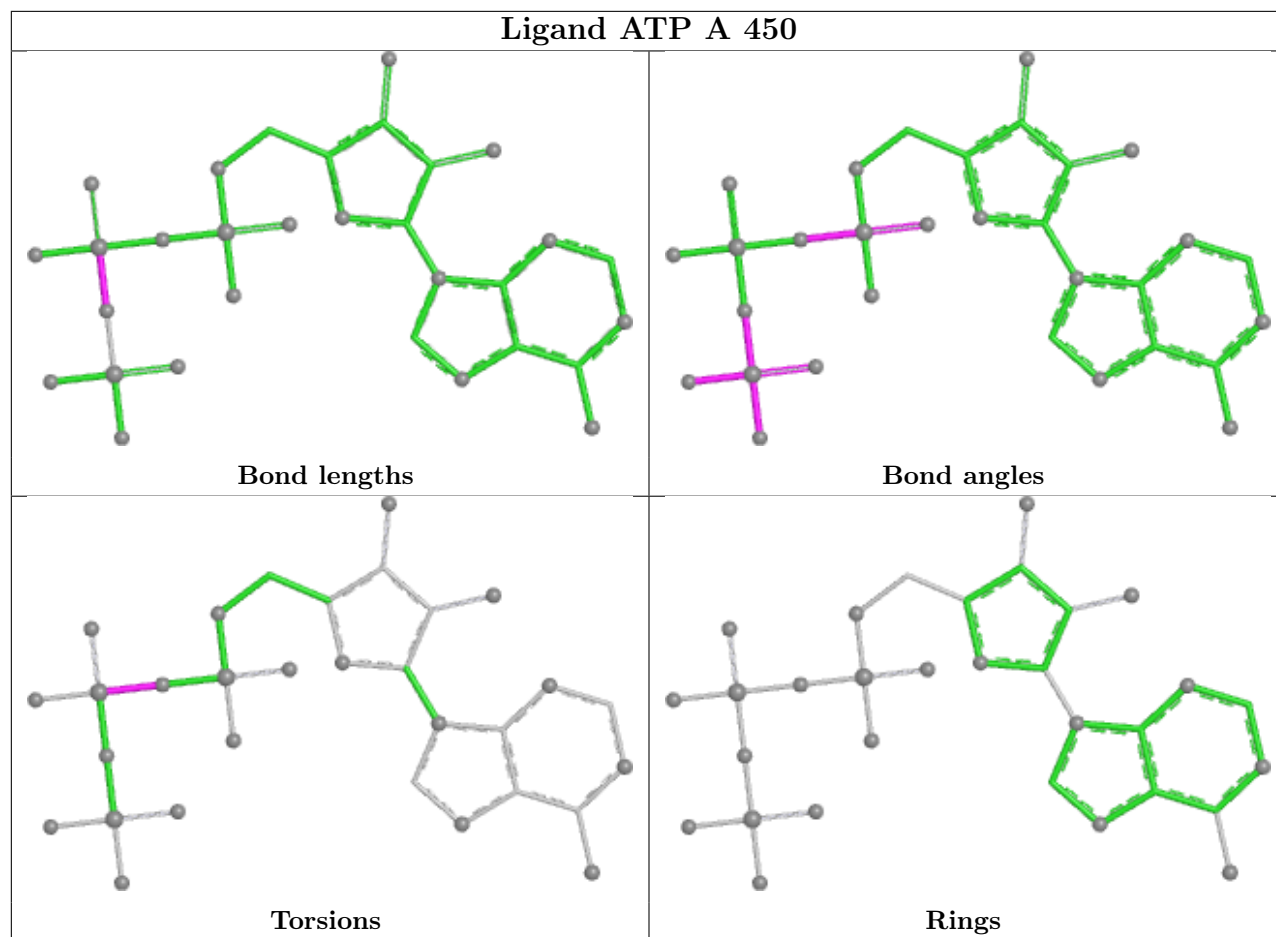
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	ATP	2	0
3	E	454	ATP	9	0
3	U	458	ATP	12	0
3	F	455	ATP	8	0
3	S	456	ATP	14	0
3	B	451	ATP	5	0
3	X	461	ATP	9	0
3	V	459	ATP	3	0
3	T	457	ATP	3	0

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.

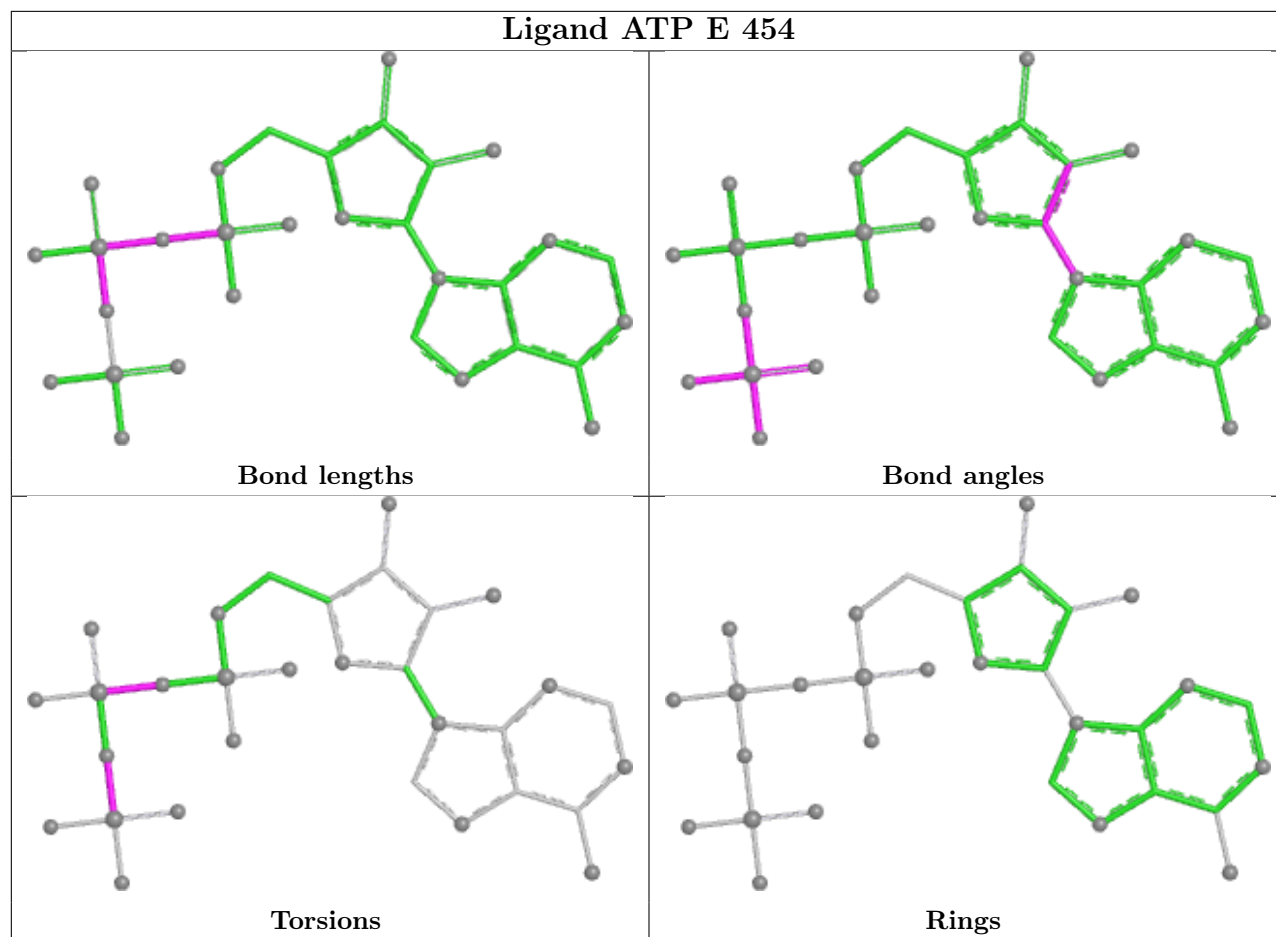


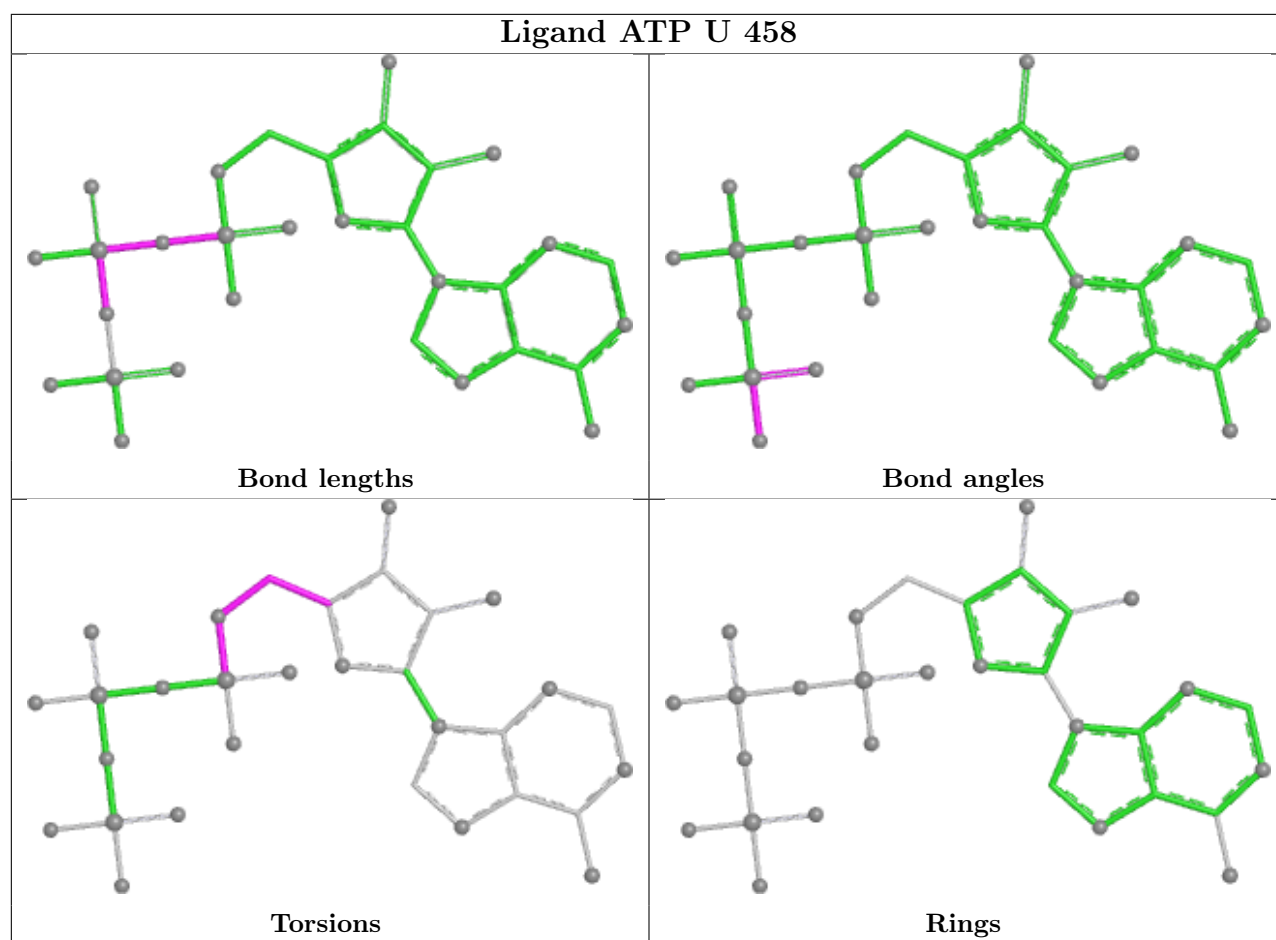


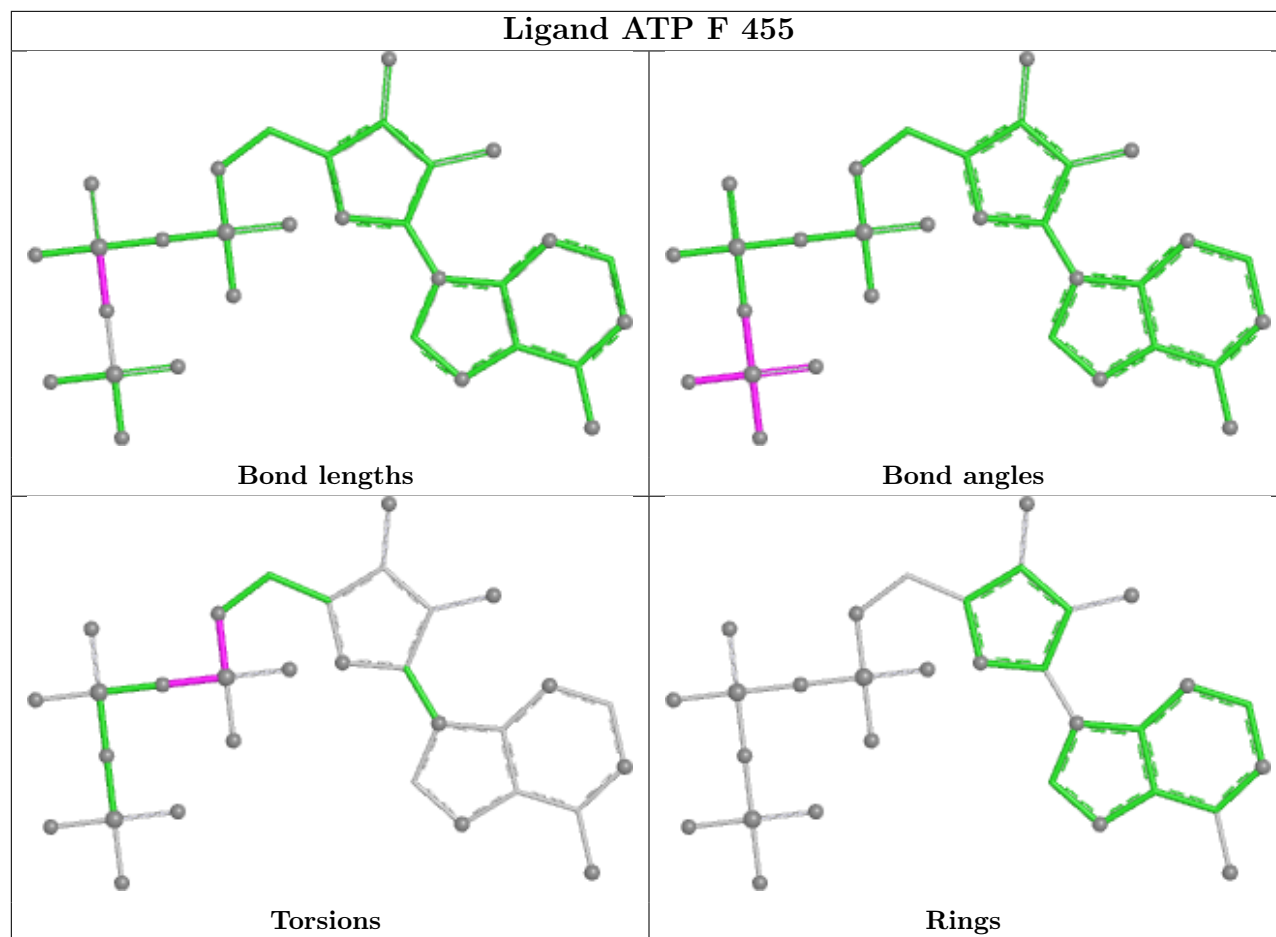


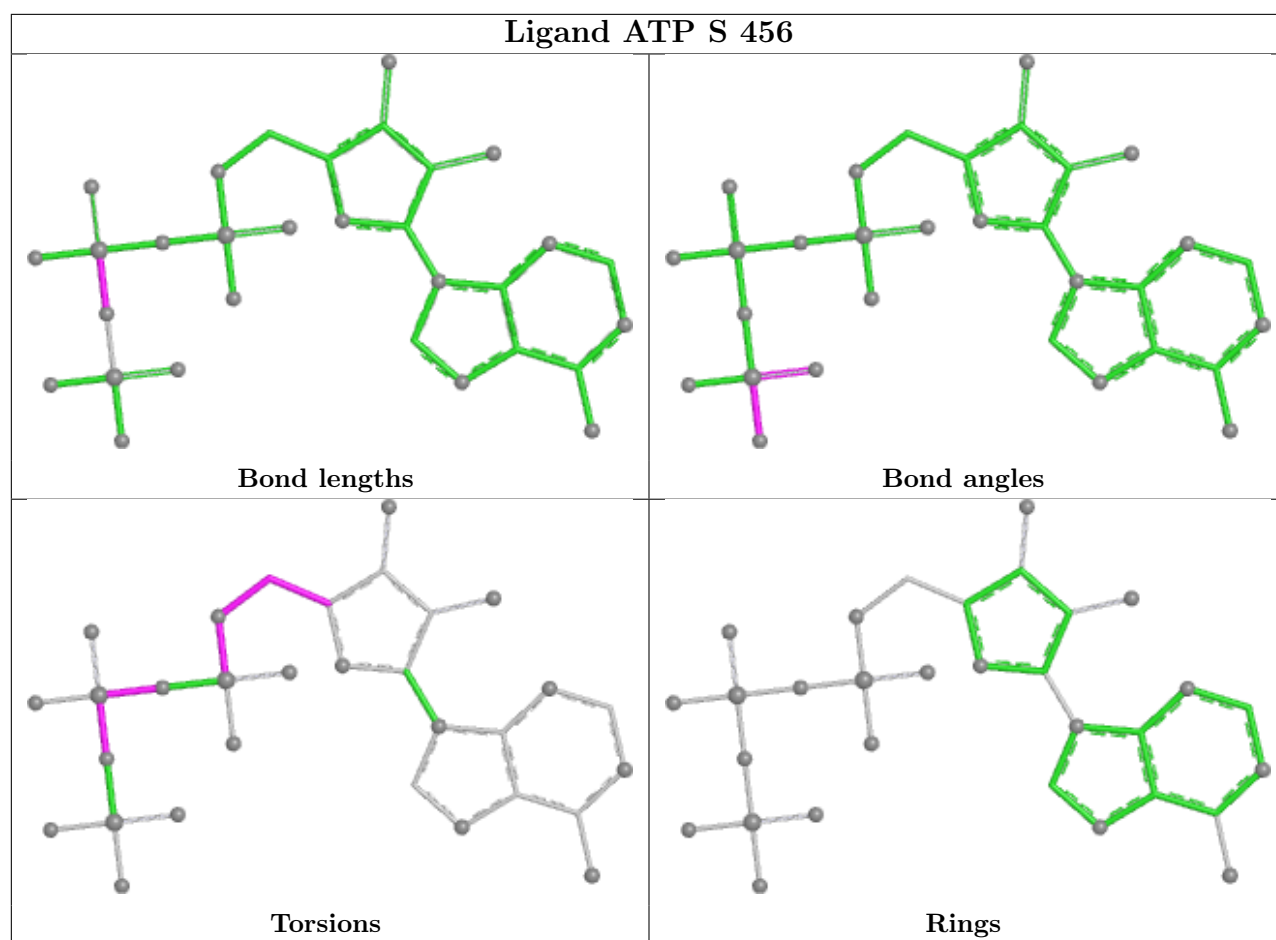


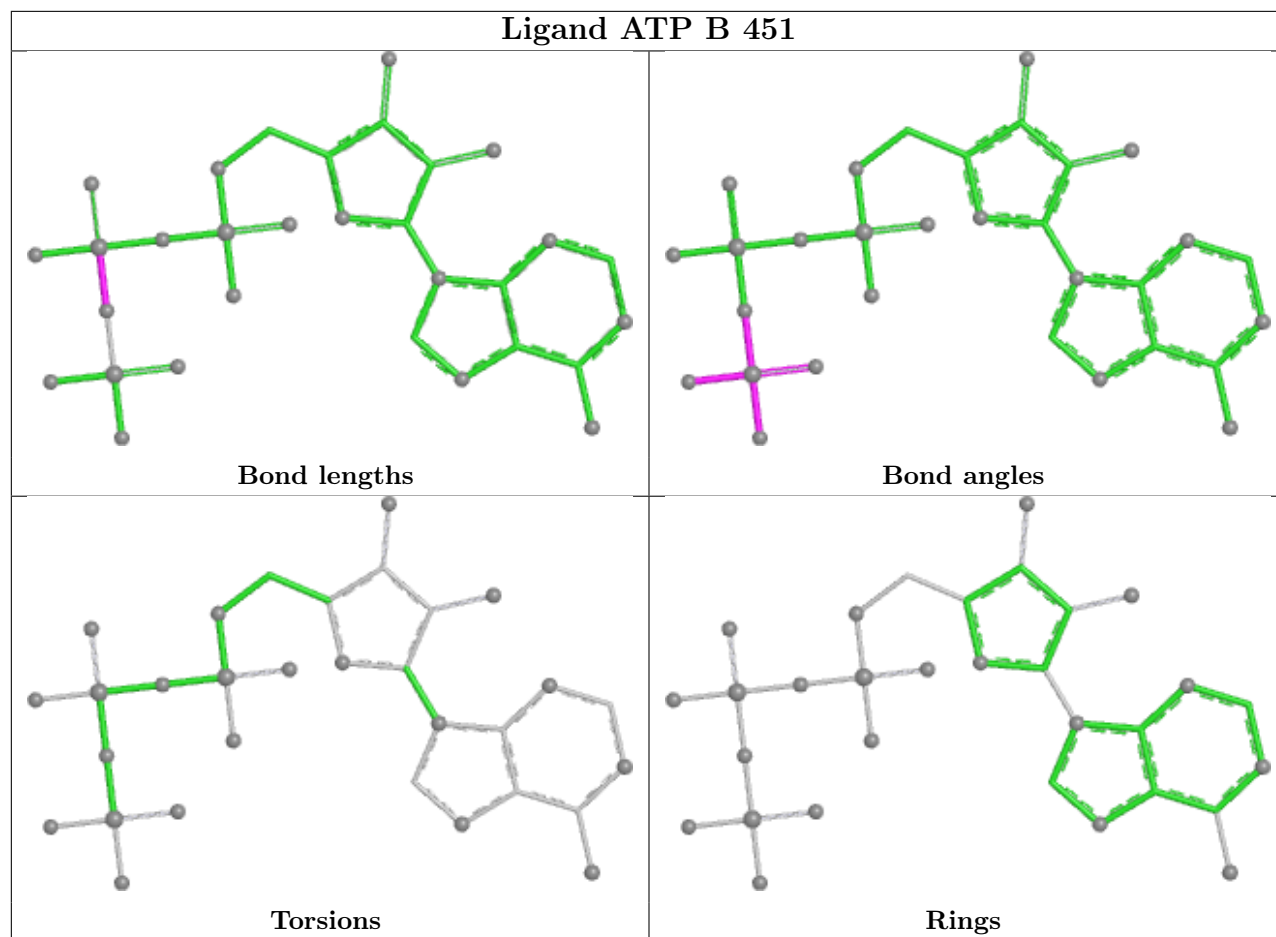
Ligand ATP E 454

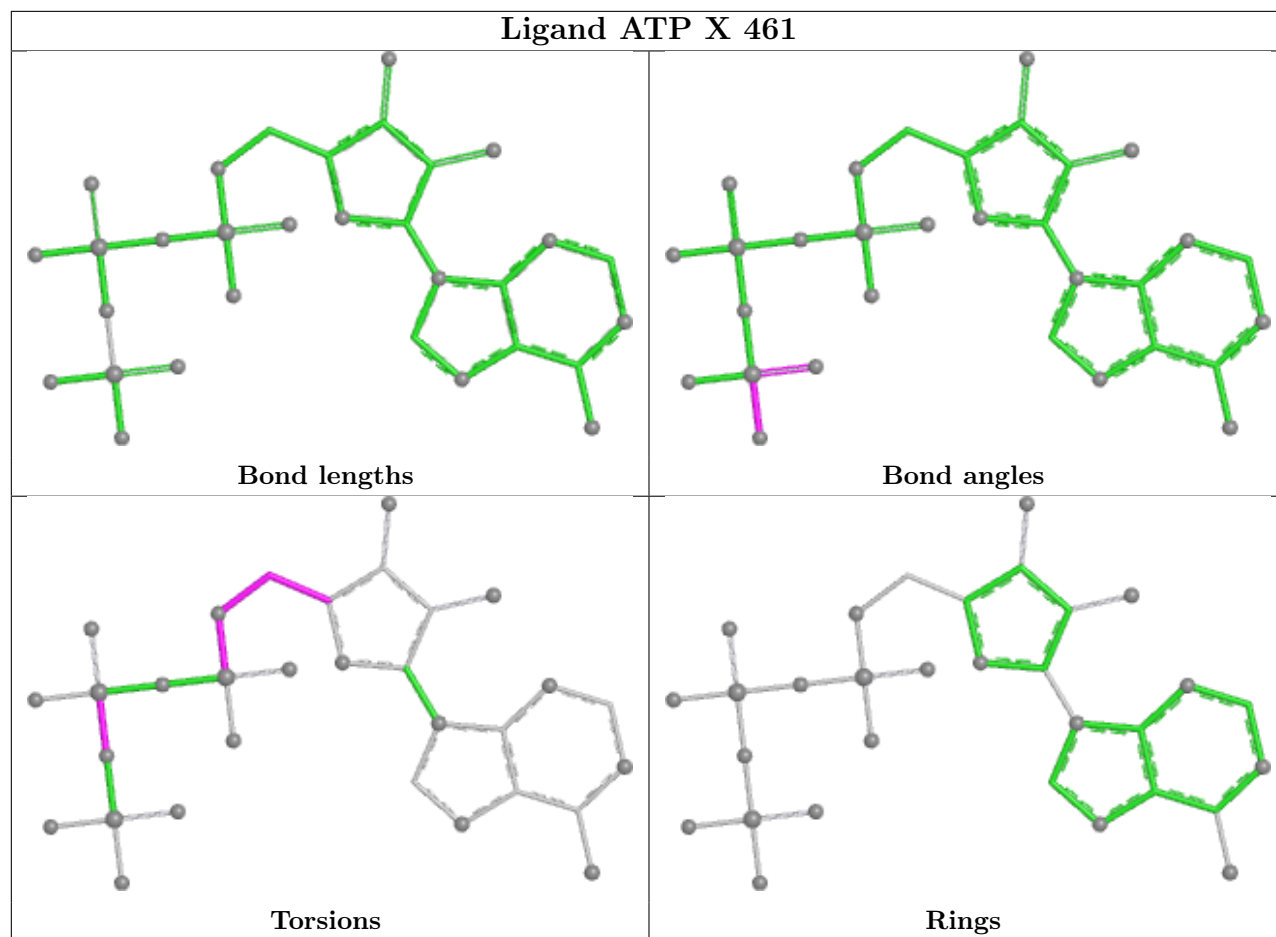




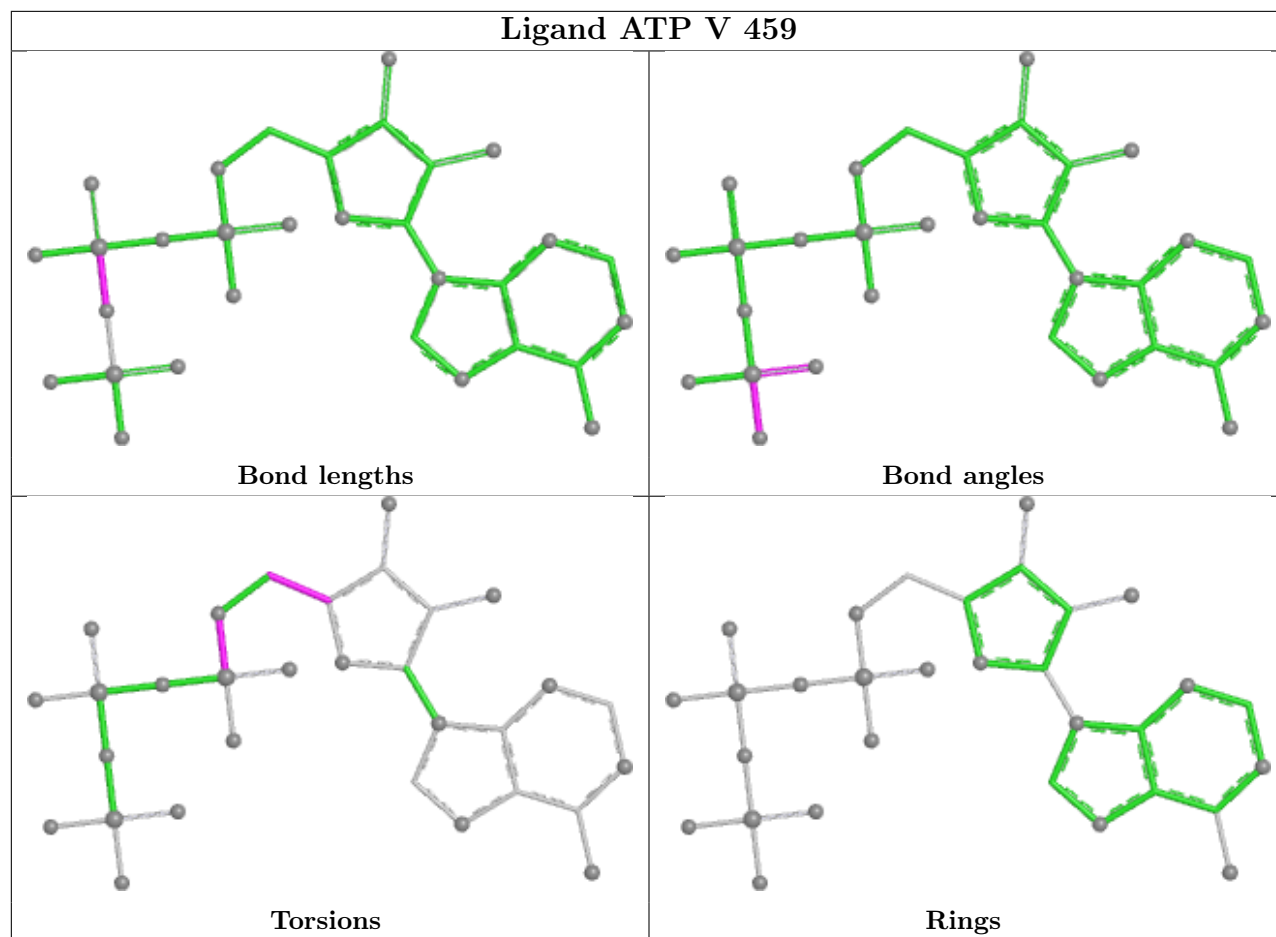


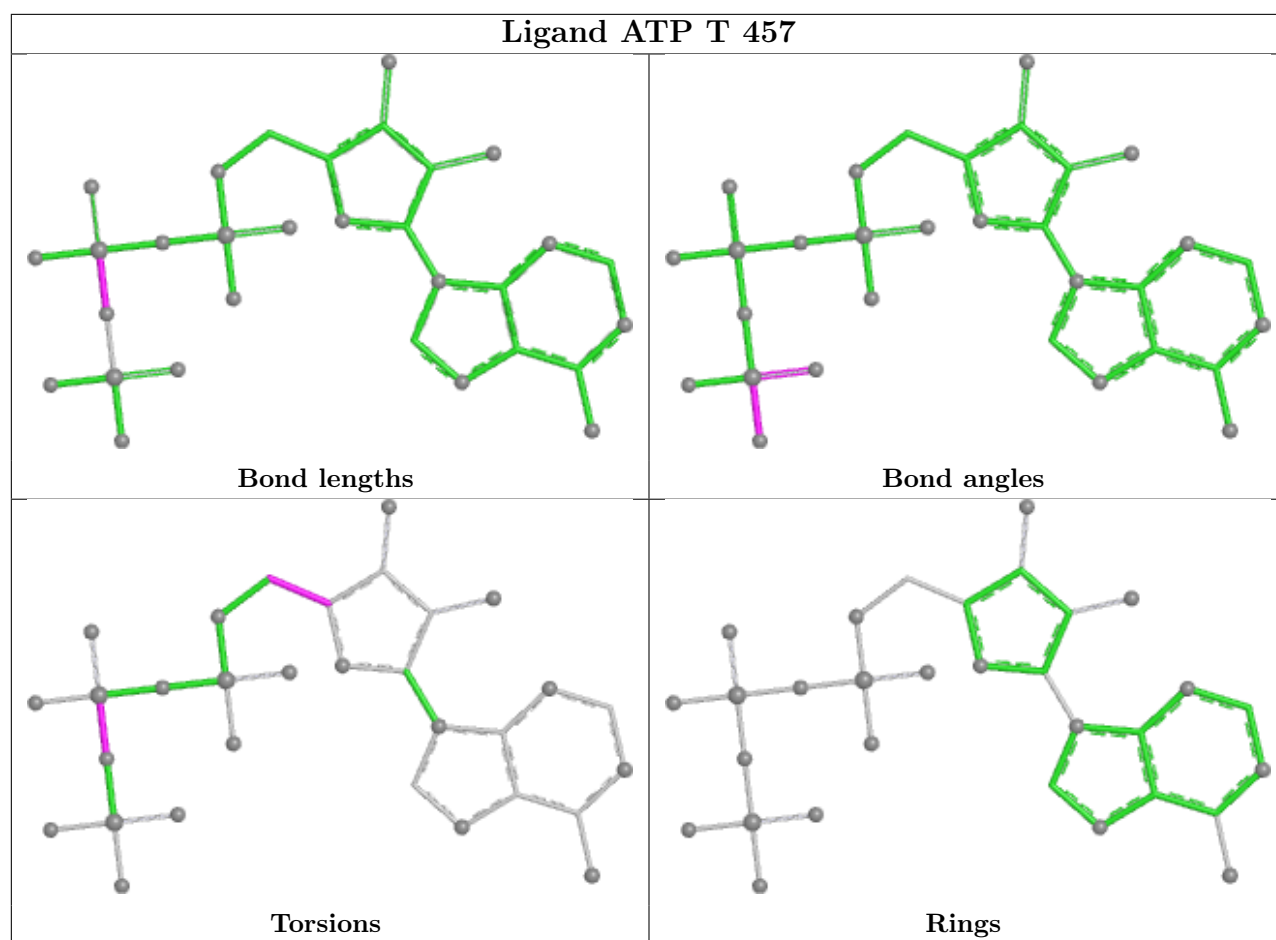






Ligand ATP V 459





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.