



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 1MX5 / pdb\_00001mx5  
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with homatropine, a cocaine analogue  
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.  
Deposited on : 2002-10-01  
Resolution : 2.80 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](mailto: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>.

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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

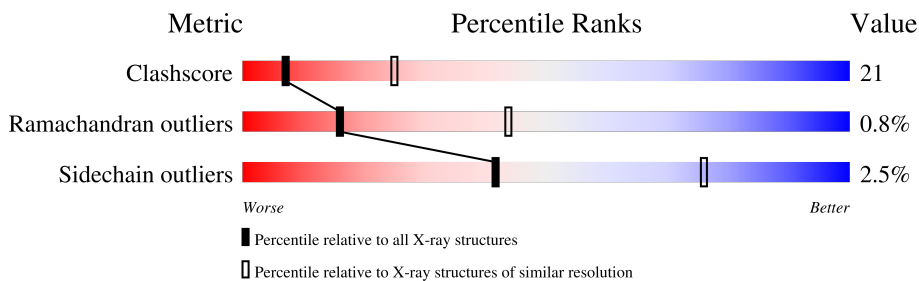
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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  $\geq 3$ , 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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	279	X	-	-	-
2	NAG	D	479	X	-	-	-
2	NAG	F	679	X	-	-	-
3	SIA	B	282	-	-	X	-
4	CL	A	11	-	-	X	-
4	CL	E	15	-	-	X	-
5	HTQ	A	111	-	-	X	-
5	HTQ	B	212	-	-	X	-
5	HTQ	E	515	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26960 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 liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4130	2662	685	763	20	0	0	0
1	B	531	4124	2659	684	761	20	0	0	0
1	C	531	4124	2659	684	761	20	0	0	0
1	D	532	4130	2662	685	763	20	0	0	0
1	E	531	4124	2659	684	761	20	0	0	0
1	F	531	4124	2659	684	761	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

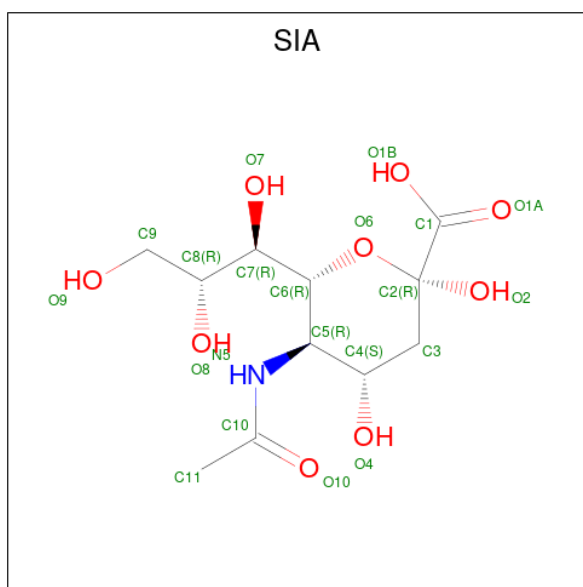
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141
F	?	-	GLN	deletion	UNP P23141

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).

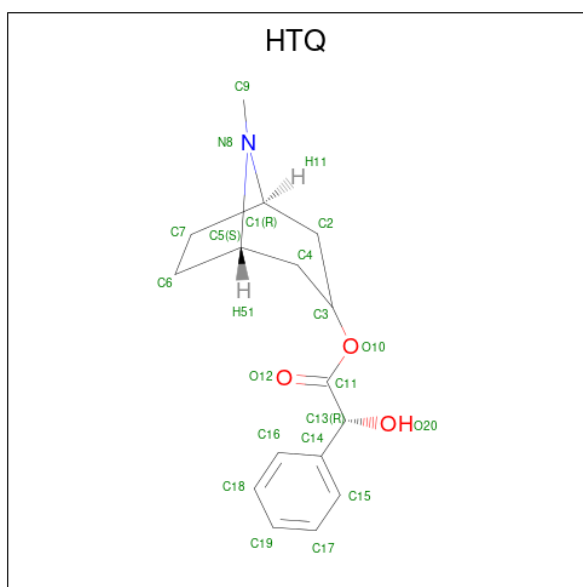


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	21	11	1	9	0	0
3	B	1	21	11	1	9	0	0
3	F	1	21	11	1	9	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	E	1	1	1	0	0

- Molecule 5 is HOMOTROPINE (CCD ID: HTQ) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			20	16	1	3		
5	A	1	Total	C	N	O	0	1
			40	32	2	6		
5	B	1	Total	C	N	O	0	0
			20	16	1	3		
5	B	1	Total	C	N	O	0	1
			40	32	2	6		
5	C	1	Total	C	N	O	0	0
			20	16	1	3		
5	C	1	Total	C	N	O	0	1
			40	32	2	6		
5	D	1	Total	C	N	O	0	0
			20	16	1	3		
5	D	1	Total	C	N	O	0	1
			40	32	2	6		
5	E	1	Total	C	N	O	0	0
			20	16	1	3		
5	E	1	Total	C	N	O	0	1
			40	32	2	6		
5	F	1	Total	C	N	O	0	0
			20	16	1	3		
5	F	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 6 is water.

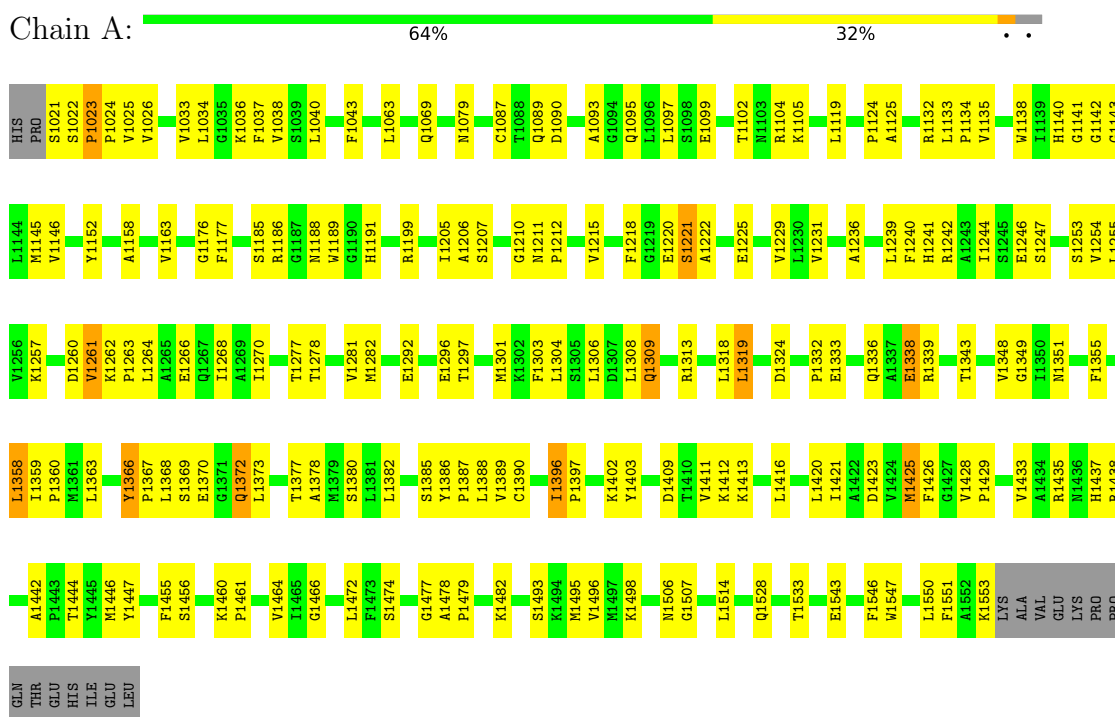
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	249	Total O 249 249	0	0
6	B	303	Total O 303 303	0	0
6	C	289	Total O 289 289	0	0
6	D	291	Total O 291 291	0	0
6	E	295	Total O 295 295	0	0
6	F	254	Total O 254 254	0	0

### 3 Residue-property plots

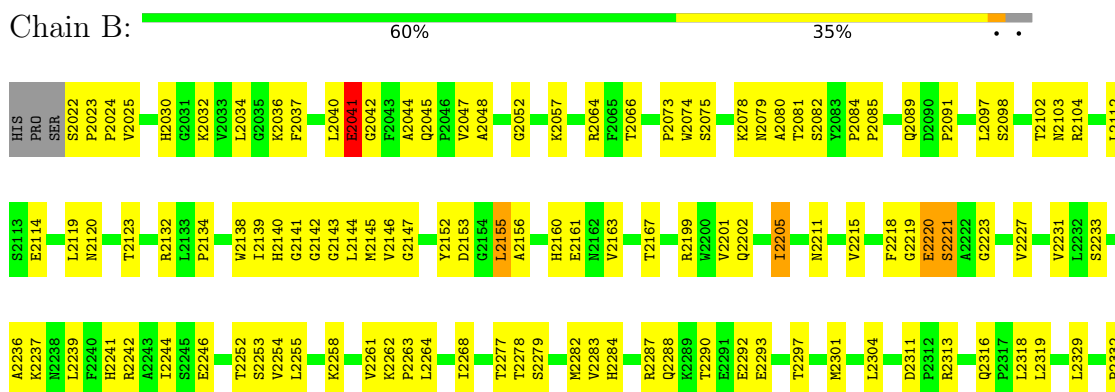
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

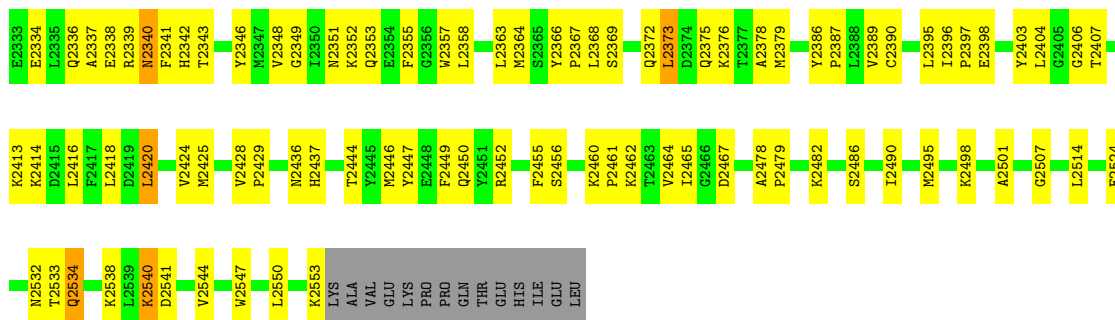
Note EDS was not executed.

- Molecule 1: liver Carboxylesterase I

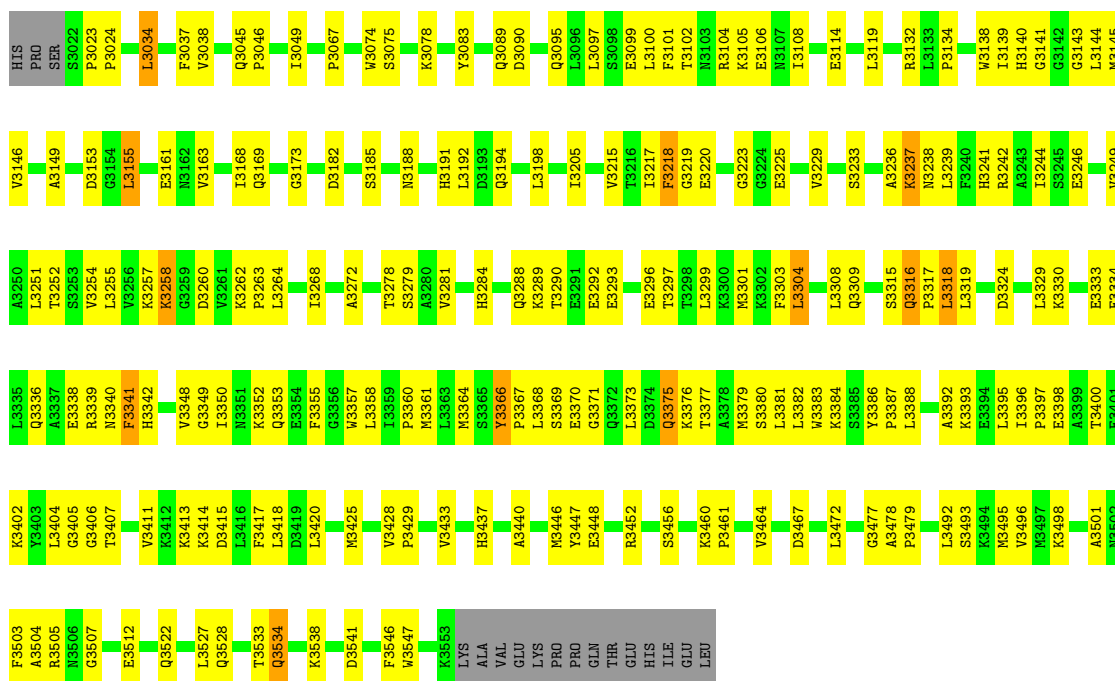


- Molecule 1: liver Carboxylesterase I

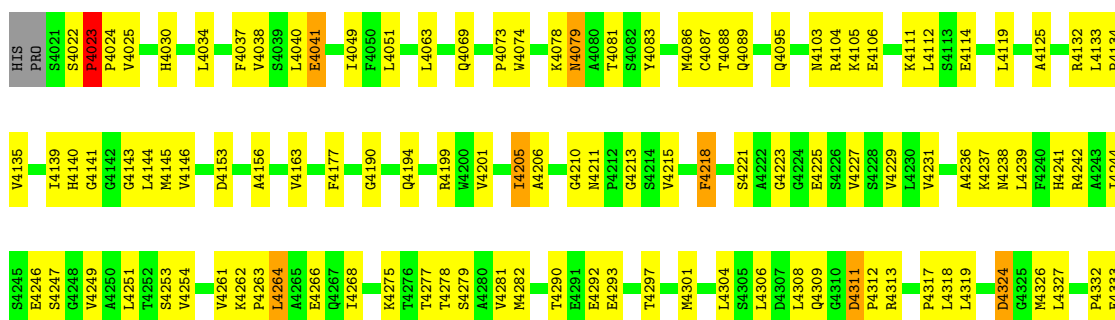


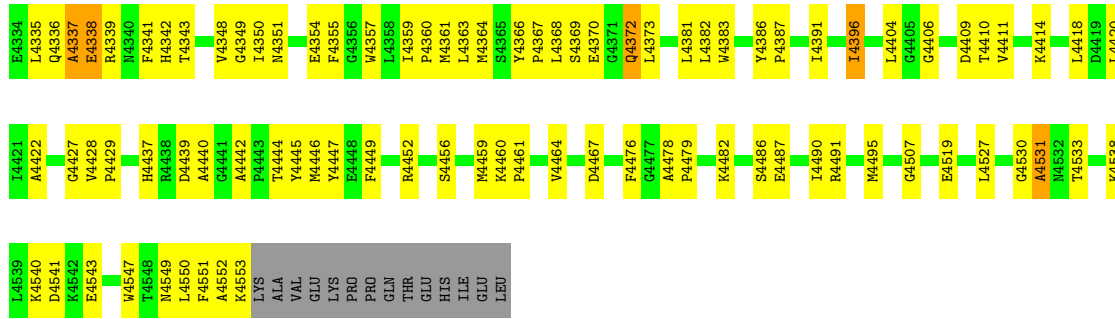


• Molecule 1: liver Carboxylesterase I

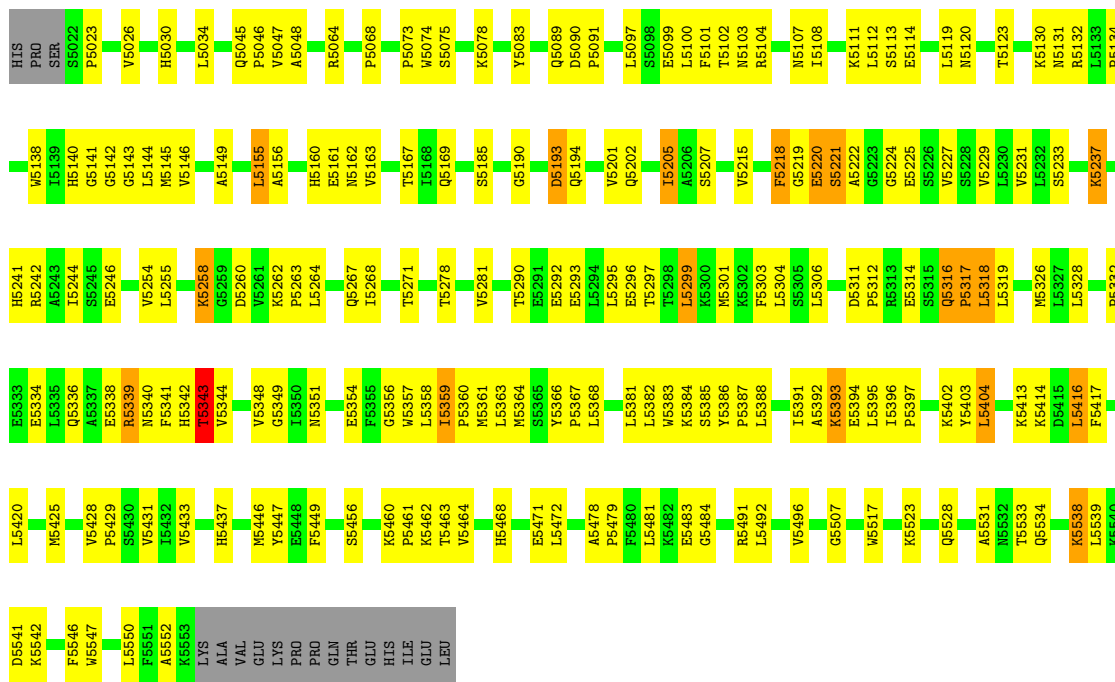


• Molecule 1: liver Carboxylesterase I





• Molecule 1: liver Carboxylesterase I



• Molecule 1: liver Carboxylesterase I



V6348	P6429	D6541
G6349	S6430	R6542
I6350	V6431	E6543
N6351	I6432	V6544
E6354	V6433	M6547
F6355	A6434	K6553
G6356	R6435	LYS
W6357	A6440	ALA
L6358	G6441	VAL
I6359	A6442	GLU
P6360	M6446	LYS
R6361	Y6447	PRO
L6363	E6448	PRO
Y6366	F6449	GLN
P6367	R6452	THR
L6368	F6455	GLU
S6369	S6456	HIS
E6370	K6460	ILE
G6371	Q6372	GLU
Q6372	L6373	LEU
D6374	P6461	
Q6375	V6464	
K6376	I6465	
S6385	G6466	
Y6386	D6467	
P6387	R6468	
L6388	L6472	
V6389	A6478	
C6390	P6479	
I6396	F6480	
P6397	L6481	
E6398	K6482	
E6401	E6488	
K6402	R6491	
Y6403	K6498	
L6404	A6501	
G6405	R6505	
D6409	M6506	
K6412	G6507	
K6413	L6514	
K6414	L6416	
D6415	F6417	
L6416	L6418	
F6417	Q6522	
L6418	Q6534	
D6419	K6538	
L6420	L6539	
D6423	K6540	
V6428		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.40Å 178.80Å 199.60Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80	Depositor
% Data completeness (in resolution range)	92.3 (19.96-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.158 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: SIA, HTQ, CL, NAG

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	0.40	0/4236	0.90	9/5754 (0.2%)
1	B	0.40	0/4230	0.90	4/5746 (0.1%)
1	C	0.40	0/4230	0.91	5/5746 (0.1%)
1	D	0.40	0/4236	0.92	11/5754 (0.2%)
1	E	0.40	0/4230	0.93	13/5746 (0.2%)
1	F	0.40	0/4230	0.91	5/5746 (0.1%)
All	All	0.40	0/25392	0.91	47/34492 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3303	PHE	N-CA-C	8.62	120.76	111.36
1	F	6075	SER	N-CA-C	8.48	121.75	111.40
1	D	4552	ALA	N-CA-C	-8.13	103.36	113.20
1	B	2114	GLU	N-CA-C	-8.02	102.94	112.89
1	B	2075	SER	N-CA-C	7.80	119.69	111.03

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	4130	0	4131	174	0
1	B	4124	0	4126	190	0
1	C	4124	0	4126	187	0
1	D	4130	0	4131	152	0
1	E	4124	0	4126	186	0
1	F	4124	0	4126	159	0
2	A	14	0	13	0	0
2	B	14	0	13	3	0
2	C	14	0	13	0	0
2	D	14	0	13	2	0
2	E	28	0	26	2	0
2	F	14	0	13	2	0
3	A	21	0	18	5	0
3	B	21	0	18	17	0
3	F	21	0	18	5	0
4	A	1	0	0	5	0
4	E	1	0	0	2	0
5	A	60	0	63	21	0
5	B	60	0	63	15	0
5	C	60	0	63	13	0
5	D	60	0	63	13	0
5	E	60	0	63	15	0
5	F	60	0	63	13	0
6	A	249	0	0	13	0
6	B	303	0	0	26	0
6	C	289	0	0	27	0
6	D	291	0	0	16	0
6	E	295	0	0	22	0
6	F	254	0	0	25	0
All	All	26960	0	25289	1056	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 21.

The worst 5 of 1056 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:E:5221:SER:HB3	4:E:15:CL:CL	1.58	1.39
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.17	1.08
1:C:3258:LYS:H	1:C:3258:LYS:HE2	1.19	1.02
1:B:2304:LEU:HD13	5:B:212:HTQ:H171	1.39	1.01
1:B:2079:ASN:HB3	3:B:282:SIA:H113	1.41	1.00

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 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	530/548 (97%)	495 (93%)	33 (6%)	2 (0%)	30	60
1	B	529/548 (96%)	496 (94%)	28 (5%)	5 (1%)	14	41
1	C	529/548 (96%)	488 (92%)	38 (7%)	3 (1%)	21	51
1	D	530/548 (97%)	503 (95%)	23 (4%)	4 (1%)	16	44
1	E	529/548 (96%)	495 (94%)	27 (5%)	7 (1%)	9	31
1	F	529/548 (96%)	493 (93%)	32 (6%)	4 (1%)	16	44
All	All	3176/3288 (97%)	2970 (94%)	181 (6%)	25 (1%)	16	44

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2253	SER
1	C	3237	LYS
1	E	5393	LYS
1	E	5462	LYS
1	F	6341	PHE

### 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	448/463 (97%)	439 (98%)	9 (2%)	48	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	447/463 (96%)	436 (98%)	11 (2%)	42	76
1	C	447/463 (96%)	433 (97%)	14 (3%)	35	70
1	D	448/463 (97%)	437 (98%)	11 (2%)	42	76
1	E	447/463 (96%)	433 (97%)	14 (3%)	35	70
1	F	447/463 (96%)	439 (98%)	8 (2%)	51	82
All	All	2684/2778 (97%)	2617 (98%)	67 (2%)	42	76

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5404	LEU
1	F	6155	LEU
1	F	6366	TYR
1	C	3258	LYS
1	C	3218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4537	GLN
1	E	5437	HIS
1	E	5045	GLN
1	E	5284	HIS
1	F	6069	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

Of 30 ligands modelled in this entry, 2 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
5	HTQ	D	414	-	22,22,22	2.15	11 (50%)	30,31,31	1.95	4 (13%)
3	SIA	F	682	-	21,21,21	1.27	2 (9%)	24,31,31	1.11	2 (8%)
5	HTQ	E	5[Y]	-	22,22,22	2.16	8 (36%)	30,31,31	1.20	3 (10%)
2	NAG	A	179	1	14,14,15	0.64	0	17,19,21	0.72	1 (5%)
5	HTQ	A	111	-	22,22,22	2.03	8 (36%)	30,31,31	1.64	5 (16%)
5	HTQ	B	212	-	22,22,22	2.01	9 (40%)	30,31,31	1.58	4 (13%)
5	HTQ	C	313	-	22,22,22	2.14	10 (45%)	30,31,31	1.35	3 (10%)
5	HTQ	E	5[Z]	-	22,22,22	2.15	9 (40%)	30,31,31	1.40	2 (6%)
2	NAG	E	580	-	14,14,15	0.56	0	17,19,21	0.66	1 (5%)
5	HTQ	D	4[Y]	-	22,22,22	2.13	8 (36%)	30,31,31	1.31	3 (10%)
2	NAG	B	279	1	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
3	SIA	A	182	-	21,21,21	1.11	2 (9%)	24,31,31	1.33	5 (20%)
5	HTQ	E	515	-	22,22,22	2.11	10 (45%)	30,31,31	1.39	2 (6%)
5	HTQ	C	3[Y]	-	22,22,22	2.15	8 (36%)	30,31,31	1.41	3 (10%)
5	HTQ	B	2[Y]	-	22,22,22	2.09	9 (40%)	30,31,31	1.10	2 (6%)
5	HTQ	F	6[Y]	-	22,22,22	2.17	8 (36%)	30,31,31	1.28	2 (6%)
5	HTQ	A	1[Y]	-	22,22,22	2.21	11 (50%)	30,31,31	1.41	3 (10%)
5	HTQ	D	4[Z]	-	22,22,22	2.06	8 (36%)	30,31,31	1.15	2 (6%)
2	NAG	E	579	1	14,14,15	0.57	0	17,19,21	0.70	1 (5%)
2	NAG	F	679	1	14,14,15	0.63	0	17,19,21	0.67	0
5	HTQ	C	3[Z]	-	22,22,22	2.20	9 (40%)	30,31,31	1.34	4 (13%)
5	HTQ	B	2[Z]	-	22,22,22	2.13	9 (40%)	30,31,31	1.28	3 (10%)
5	HTQ	F	616	-	22,22,22	2.01	10 (45%)	30,31,31	1.29	2 (6%)
5	HTQ	F	6[Z]	-	22,22,22	2.18	9 (40%)	30,31,31	1.42	3 (10%)
5	HTQ	A	1[Z]	-	22,22,22	2.23	9 (40%)	30,31,31	1.71	4 (13%)
2	NAG	C	379	1	14,14,15	0.58	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	479	1	14,14,15	0.54	0	17,19,21	0.65	0
3	SIA	B	282	-	21,21,21	1.32	2 (9%)	24,31,31	1.40	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HTQ	D	414	-	-	5/12/33/33	0/4/3/3
3	SIA	F	682	-	-	1/20/38/38	0/1/1/1
5	HTQ	E	5[Y]	-	-	4/12/33/33	0/4/3/3
2	NAG	A	179	1	-	4/6/23/26	0/1/1/1
5	HTQ	A	111	-	-	1/12/33/33	0/4/3/3
5	HTQ	B	212	-	-	1/12/33/33	0/4/3/3
5	HTQ	C	313	-	-	5/12/33/33	0/4/3/3
5	HTQ	E	5[Z]	-	-	5/12/33/33	0/4/3/3
2	NAG	E	580	-	-	4/6/23/26	0/1/1/1
5	HTQ	D	4[Y]	-	-	5/12/33/33	0/4/3/3
2	NAG	B	279	1	1/1/5/7	2/6/23/26	0/1/1/1
3	SIA	A	182	-	-	2/20/38/38	0/1/1/1
5	HTQ	E	515	-	-	5/12/33/33	0/4/3/3
5	HTQ	C	3[Y]	-	-	1/12/33/33	0/4/3/3
5	HTQ	B	2[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	F	6[Y]	-	-	5/12/33/33	0/4/3/3
5	HTQ	A	1[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	D	4[Z]	-	-	3/12/33/33	0/4/3/3
2	NAG	E	579	1	-	2/6/23/26	0/1/1/1
2	NAG	F	679	1	1/1/5/7	4/6/23/26	0/1/1/1
5	HTQ	C	3[Z]	-	-	5/12/33/33	0/4/3/3
5	HTQ	B	2[Z]	-	-	6/12/33/33	0/4/3/3
5	HTQ	F	616	-	-	4/12/33/33	0/4/3/3
5	HTQ	F	6[Z]	-	-	4/12/33/33	0/4/3/3
5	HTQ	A	1[Z]	-	-	5/12/33/33	0/4/3/3
2	NAG	C	379	1	-	4/6/23/26	0/1/1/1
2	NAG	D	479	1	1/1/5/7	2/6/23/26	0/1/1/1
3	SIA	B	282	-	-	1/20/38/38	0/1/1/1

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	682	SIA	C4-C5	3.84	1.56	1.53
5	B	2[Z]	HTQ	C4-C3	3.78	1.61	1.52
5	D	4[Y]	HTQ	C4-C3	3.75	1.61	1.52
5	E	5[Y]	HTQ	C4-C3	3.74	1.61	1.52
5	C	3[Z]	HTQ	C4-C3	3.68	1.60	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	414	HTQ	C3-O10-C11	9.43	132.54	117.72
5	A	1[Z]	HTQ	C3-O10-C11	8.08	130.41	117.72
5	A	111	HTQ	C3-O10-C11	6.62	128.12	117.72
5	E	5[Z]	HTQ	C3-O10-C11	6.42	127.81	117.72
5	B	212	HTQ	C3-O10-C11	6.25	127.54	117.72

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	279	NAG	C1
2	D	479	NAG	C1
2	F	679	NAG	C1

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
2	B	279	NAG	O7-C7-N2-C2
2	E	580	NAG	C8-C7-N2-C2
2	E	580	NAG	O7-C7-N2-C2

There are no ring outliers.

26 monomers are involved in 125 short contacts:

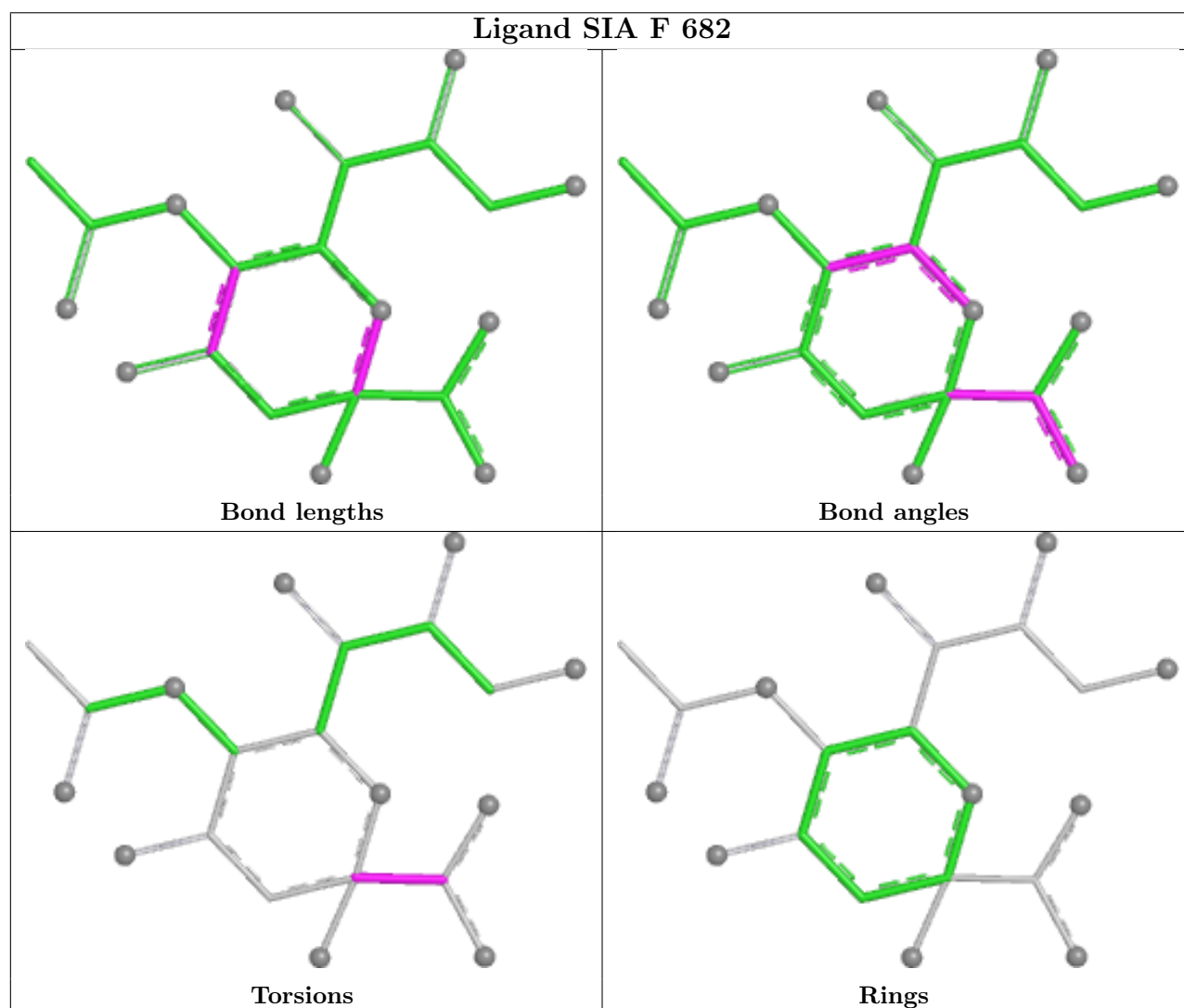
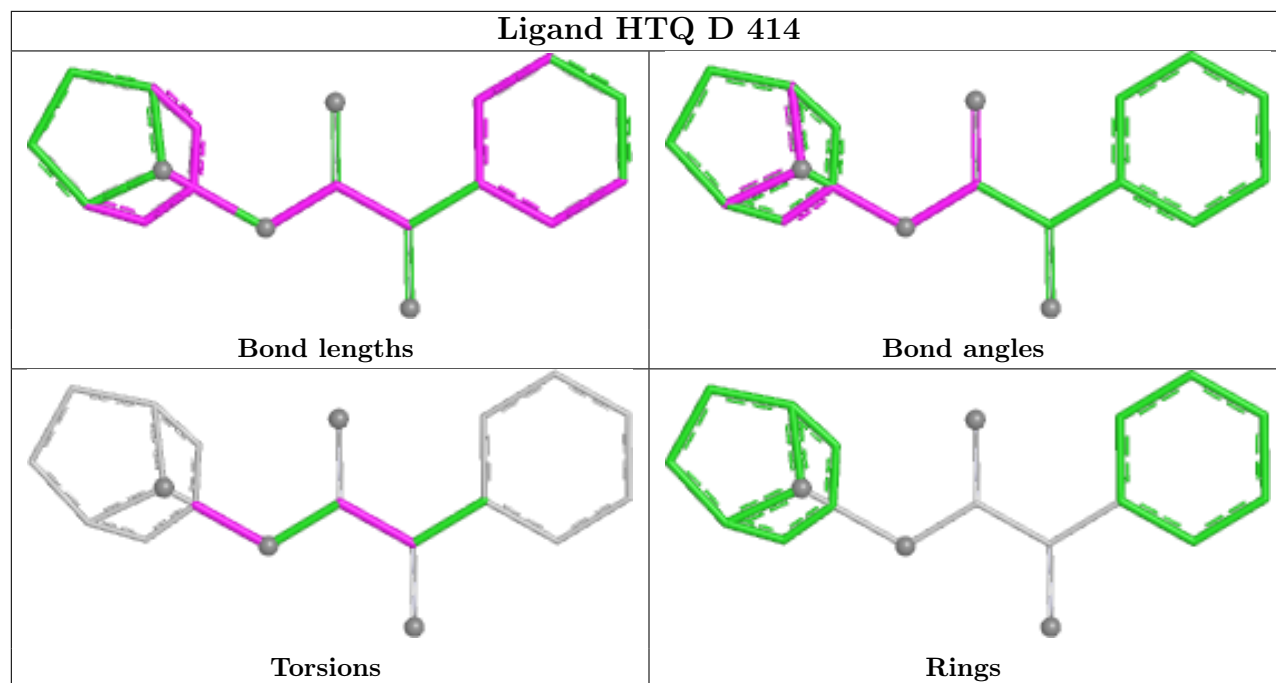
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	414	HTQ	7	0
3	F	682	SIA	5	0
5	E	5[Y]	HTQ	2	0
5	A	111	HTQ	13	0
5	B	212	HTQ	10	0
5	C	313	HTQ	4	0

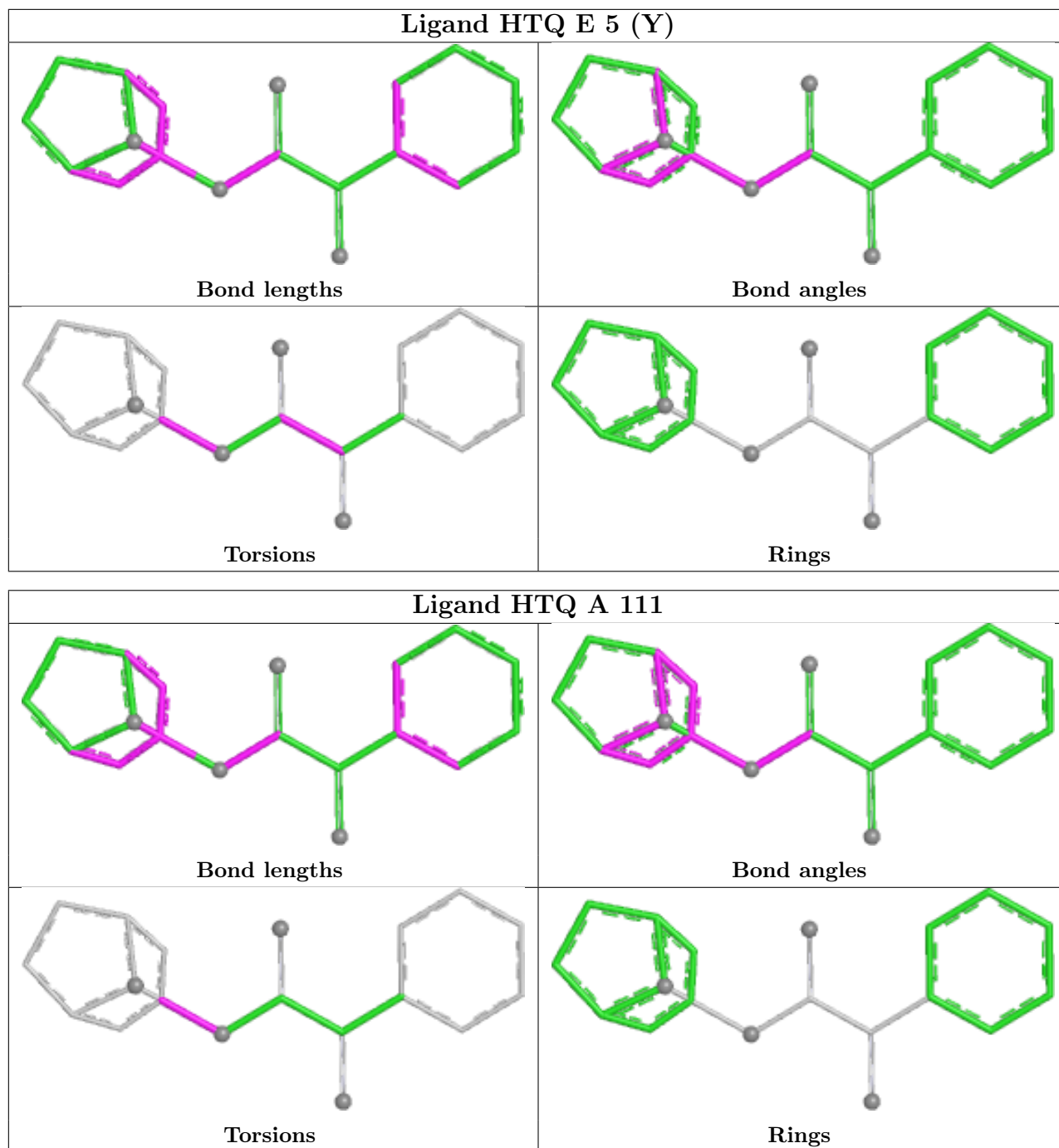
*Continued on next page...*

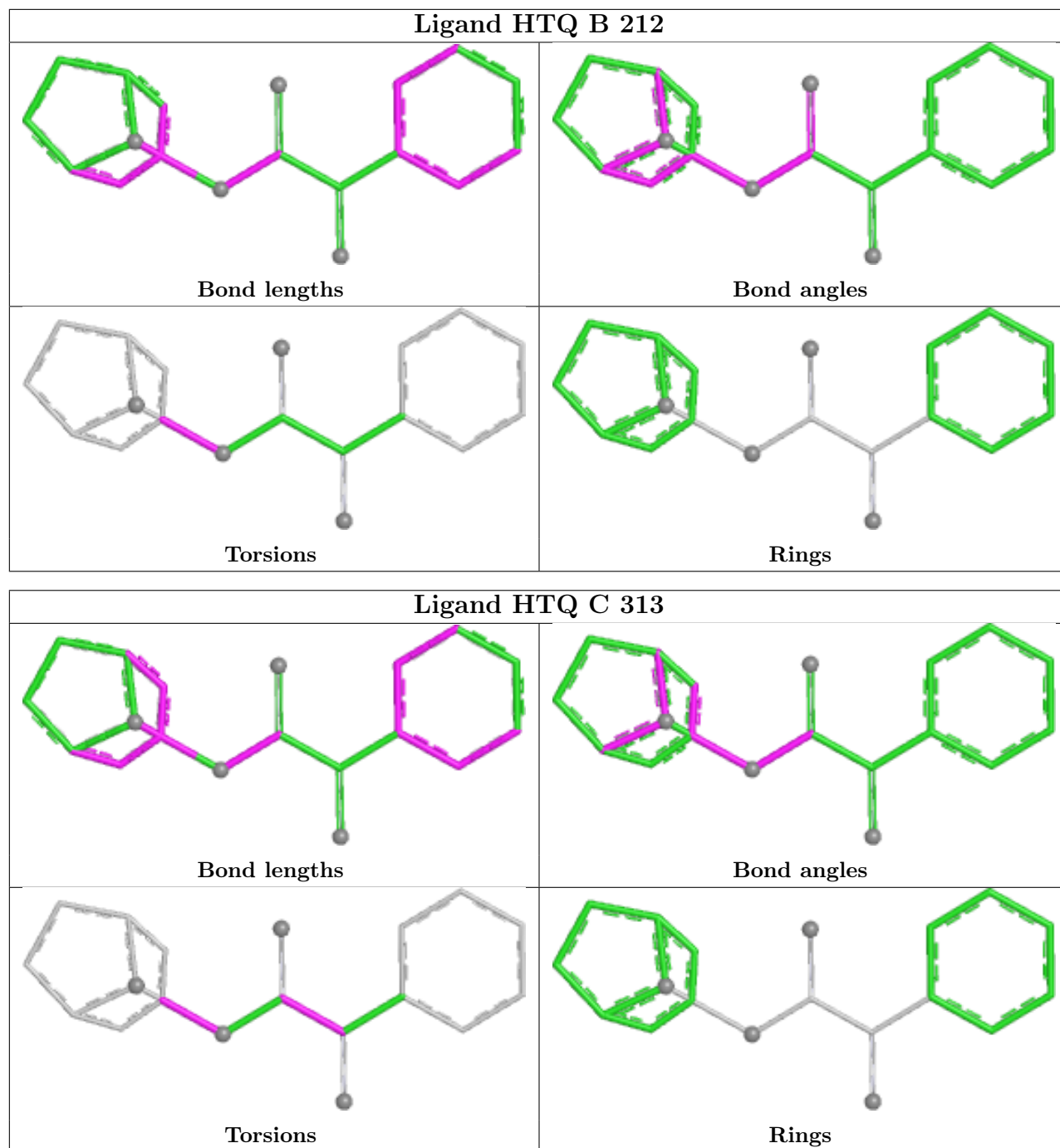
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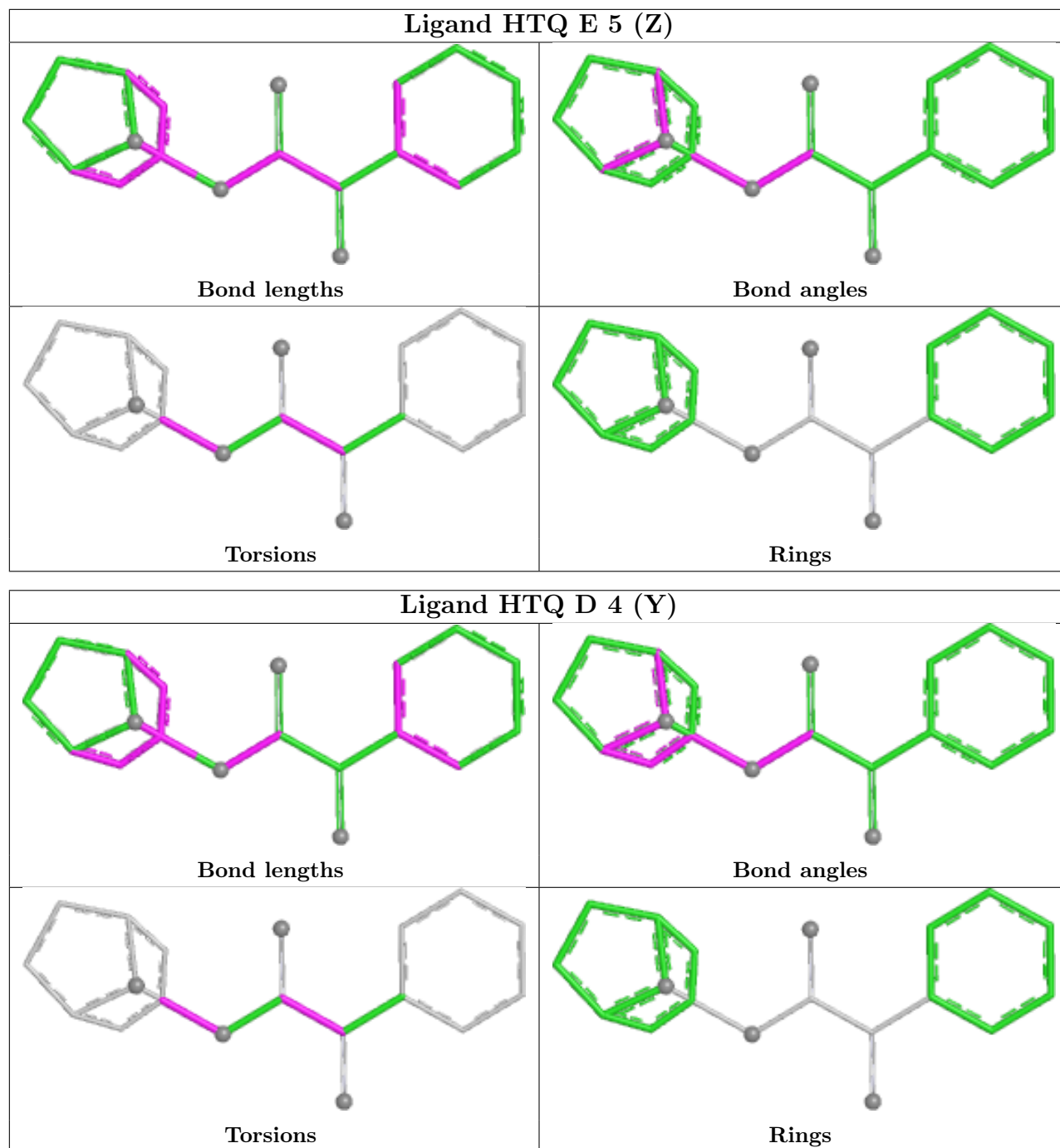
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5[Z]	HTQ	1	0
2	E	580	NAG	2	0
5	D	4[Y]	HTQ	3	0
2	B	279	NAG	3	0
3	A	182	SIA	5	0
5	E	515	HTQ	12	0
5	C	3[Y]	HTQ	4	0
5	B	2[Y]	HTQ	4	0
5	F	6[Y]	HTQ	3	0
5	A	1[Y]	HTQ	4	0
5	D	4[Z]	HTQ	3	0
2	E	579	NAG	2	0
2	F	679	NAG	2	0
5	C	3[Z]	HTQ	5	0
5	B	2[Z]	HTQ	1	0
5	F	616	HTQ	7	0
5	F	6[Z]	HTQ	3	0
5	A	1[Z]	HTQ	4	0
2	D	479	NAG	2	0
3	B	282	SIA	17	0

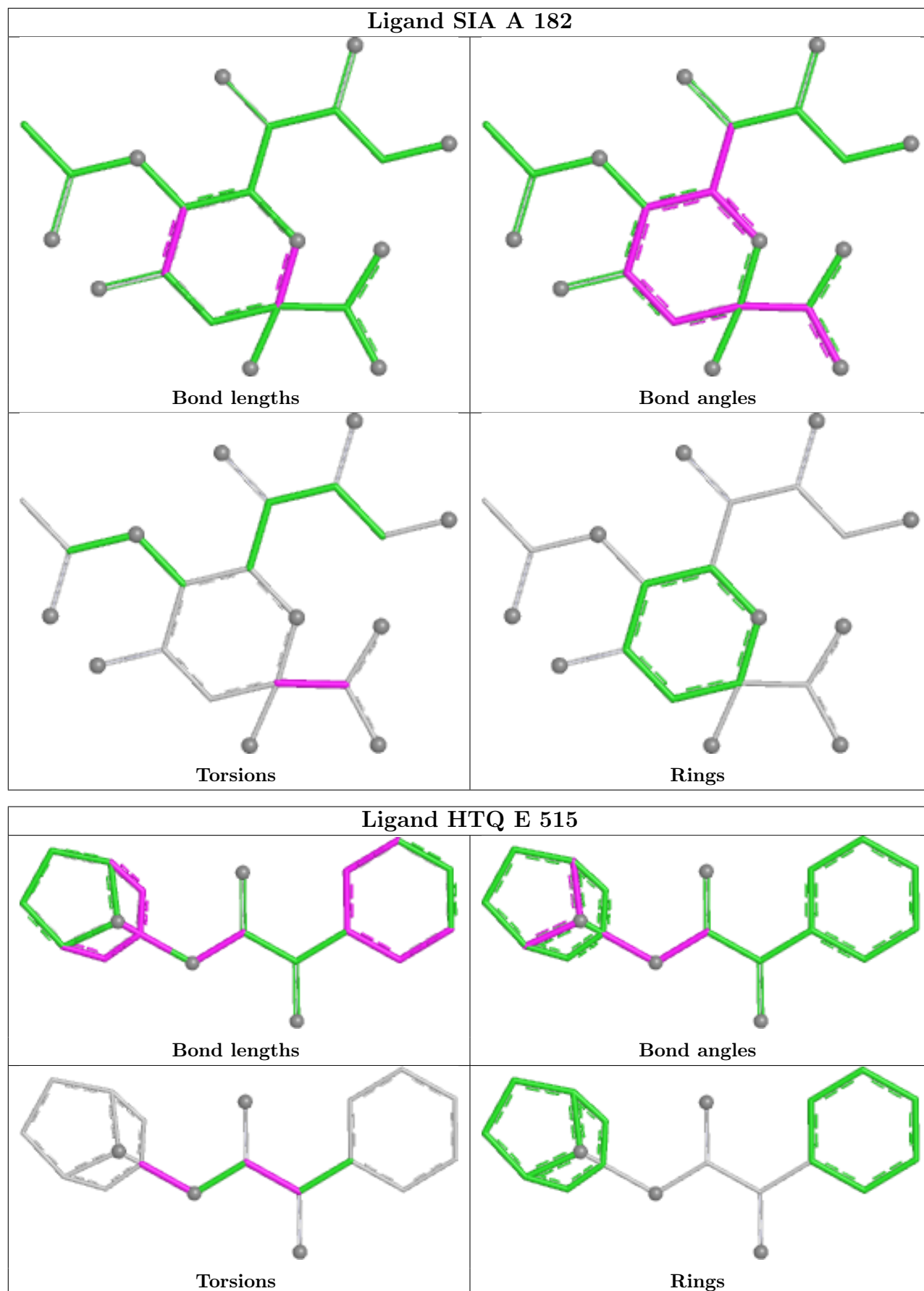
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

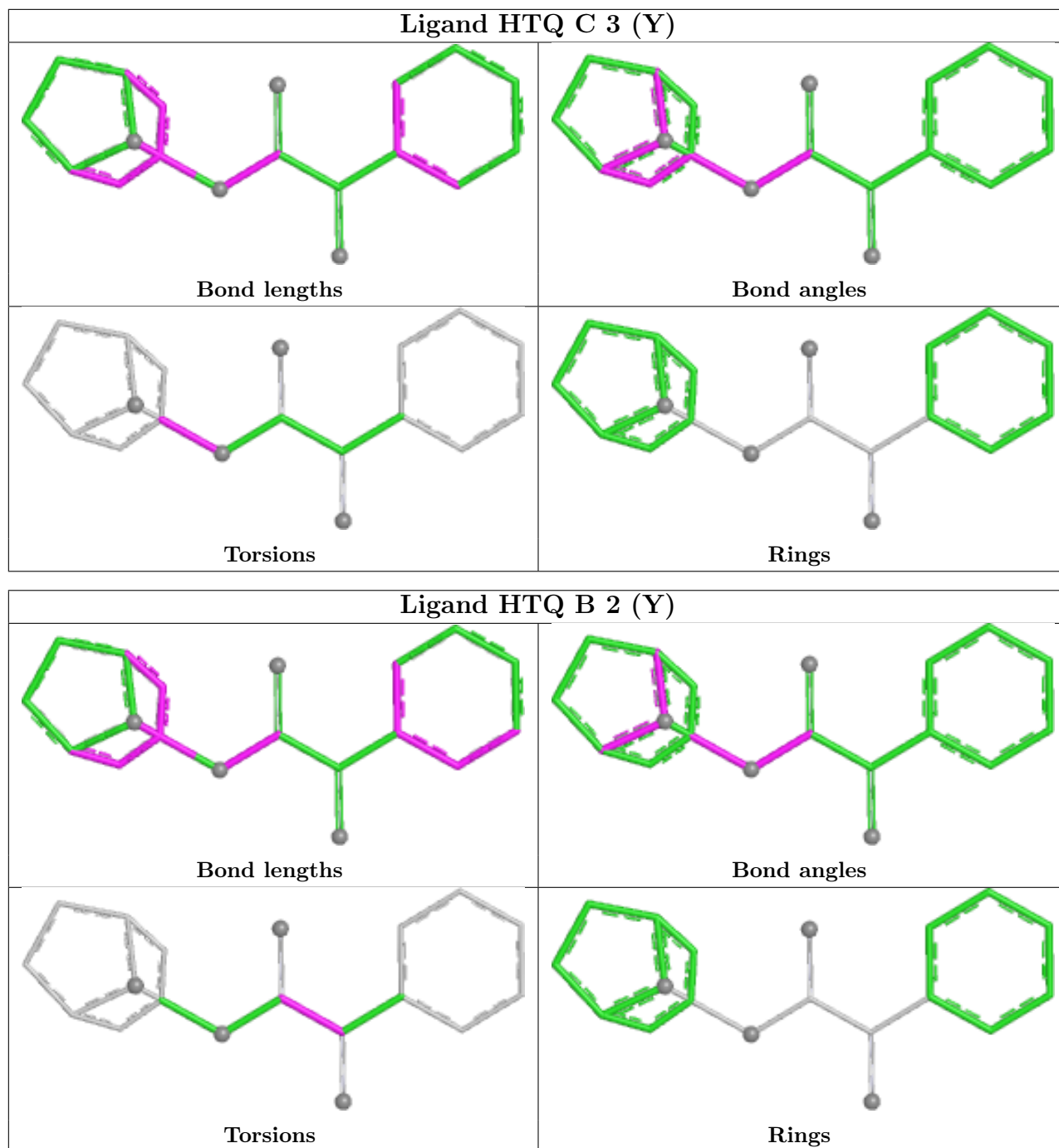


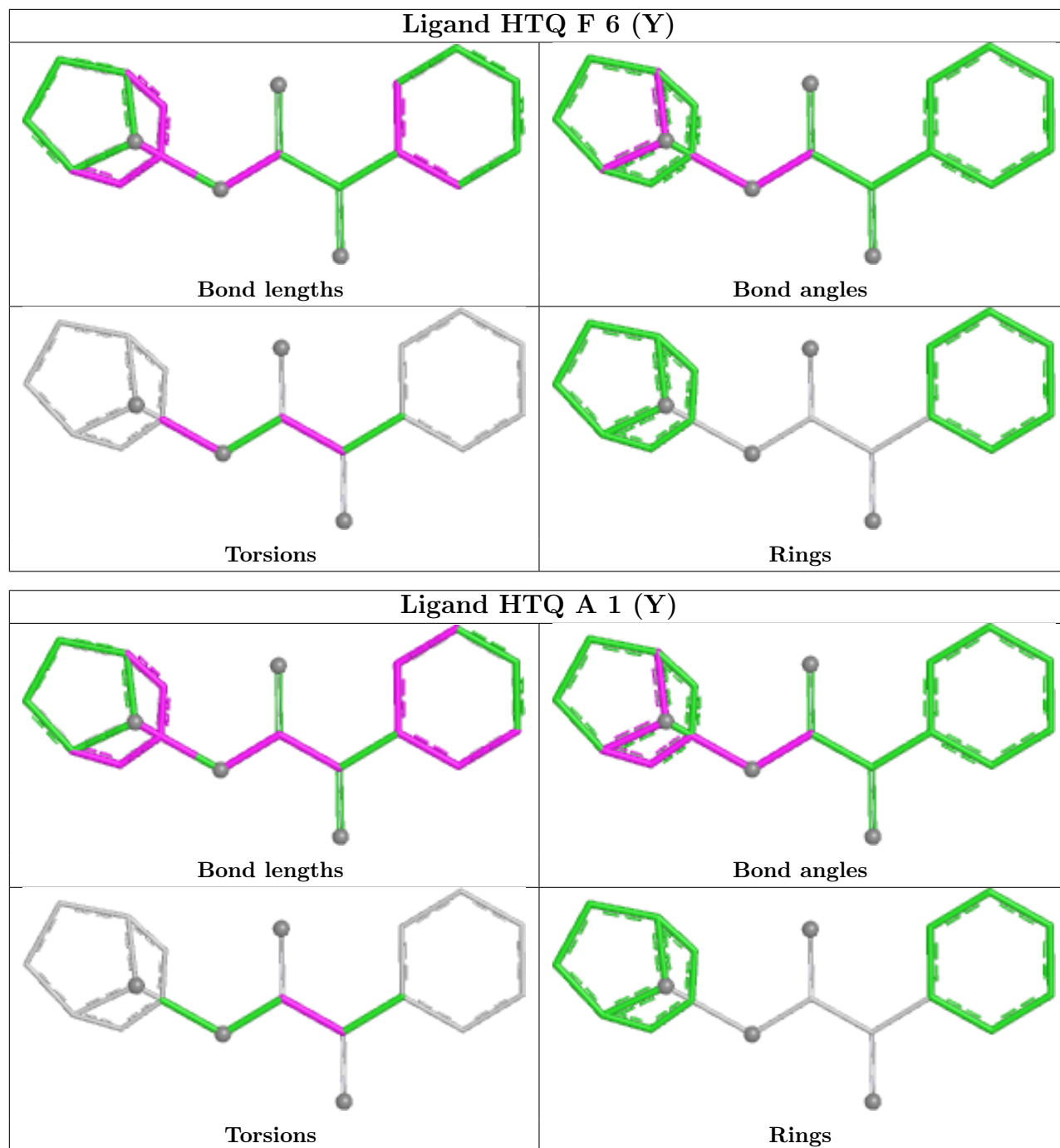


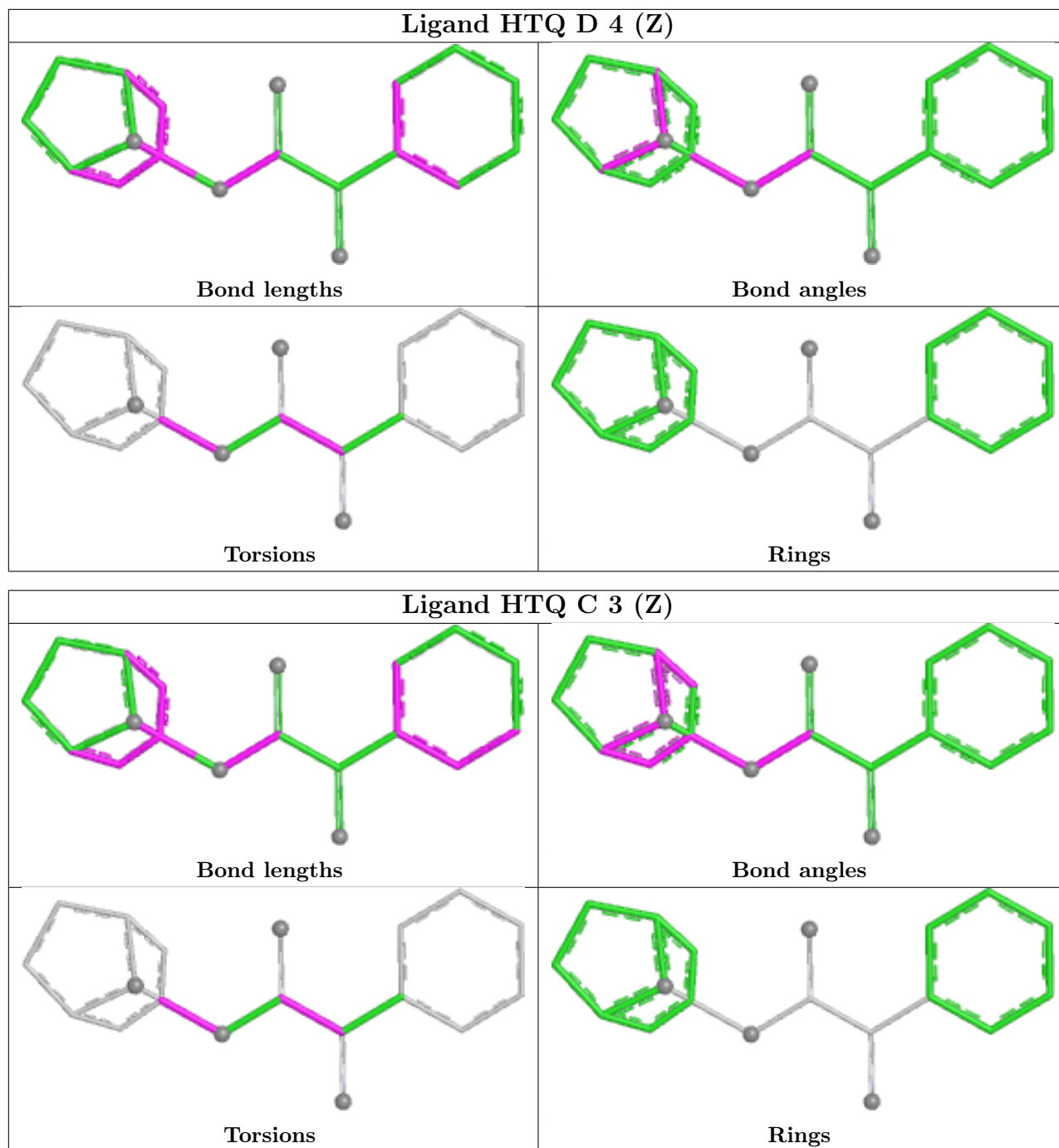


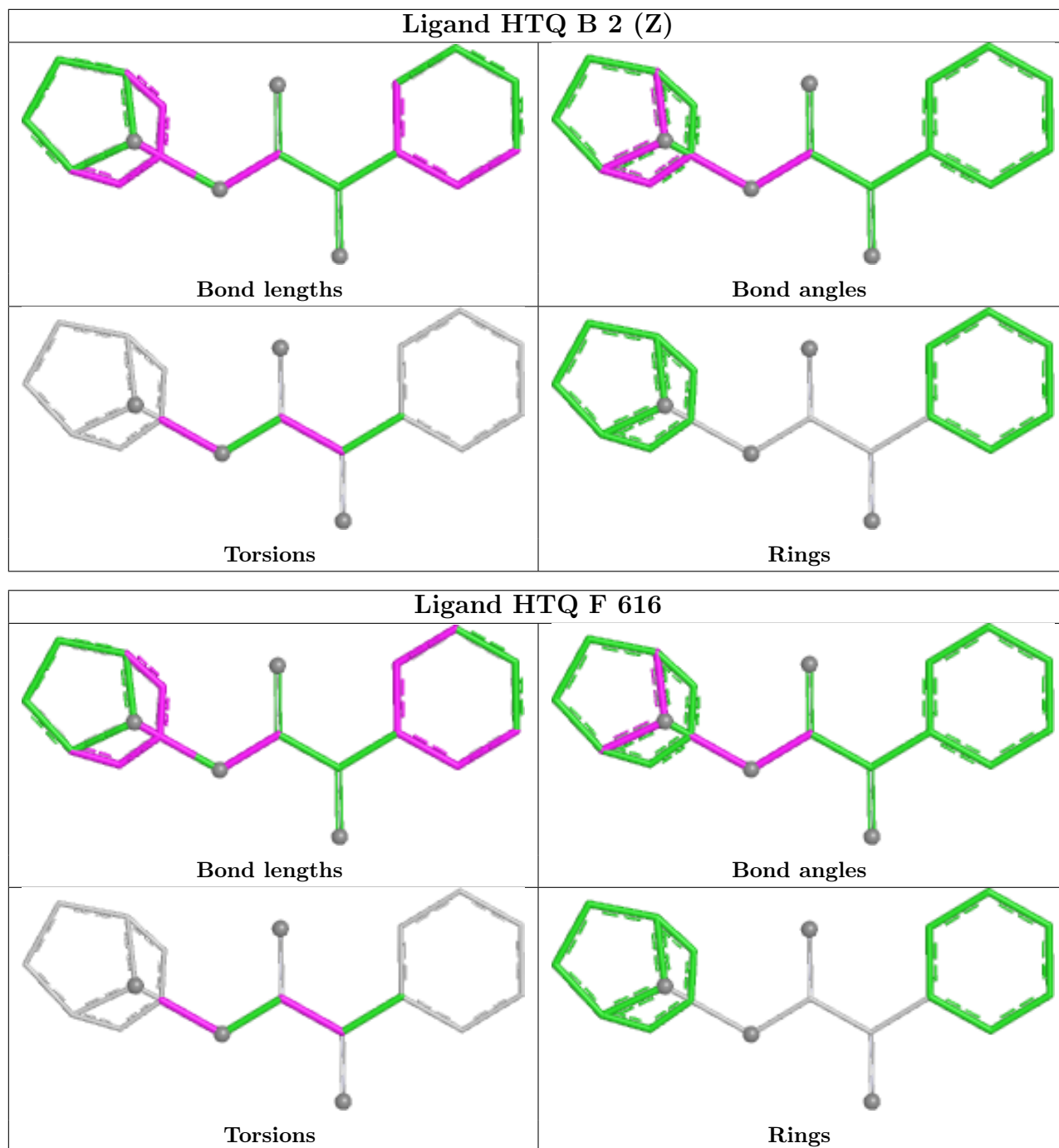


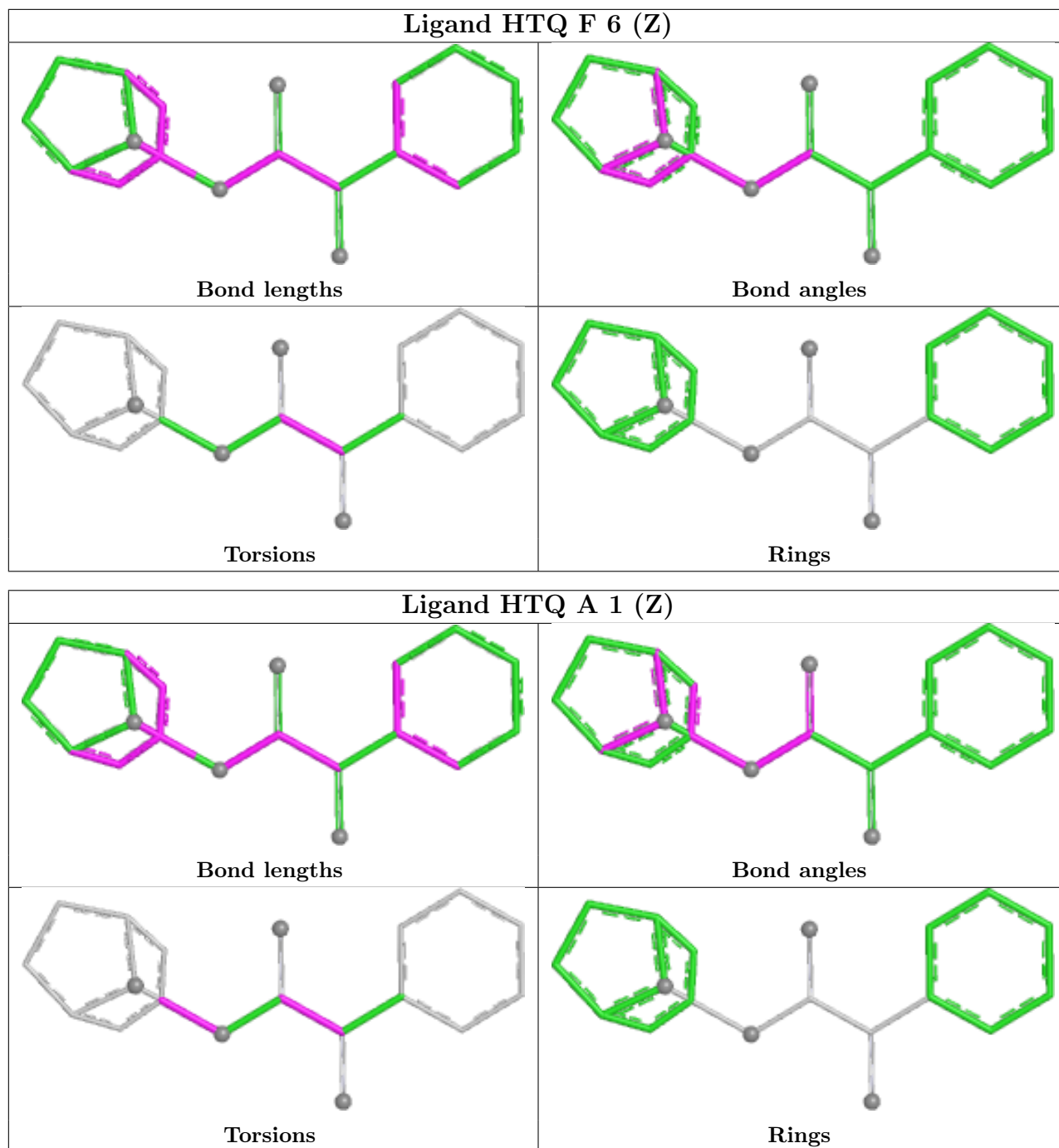


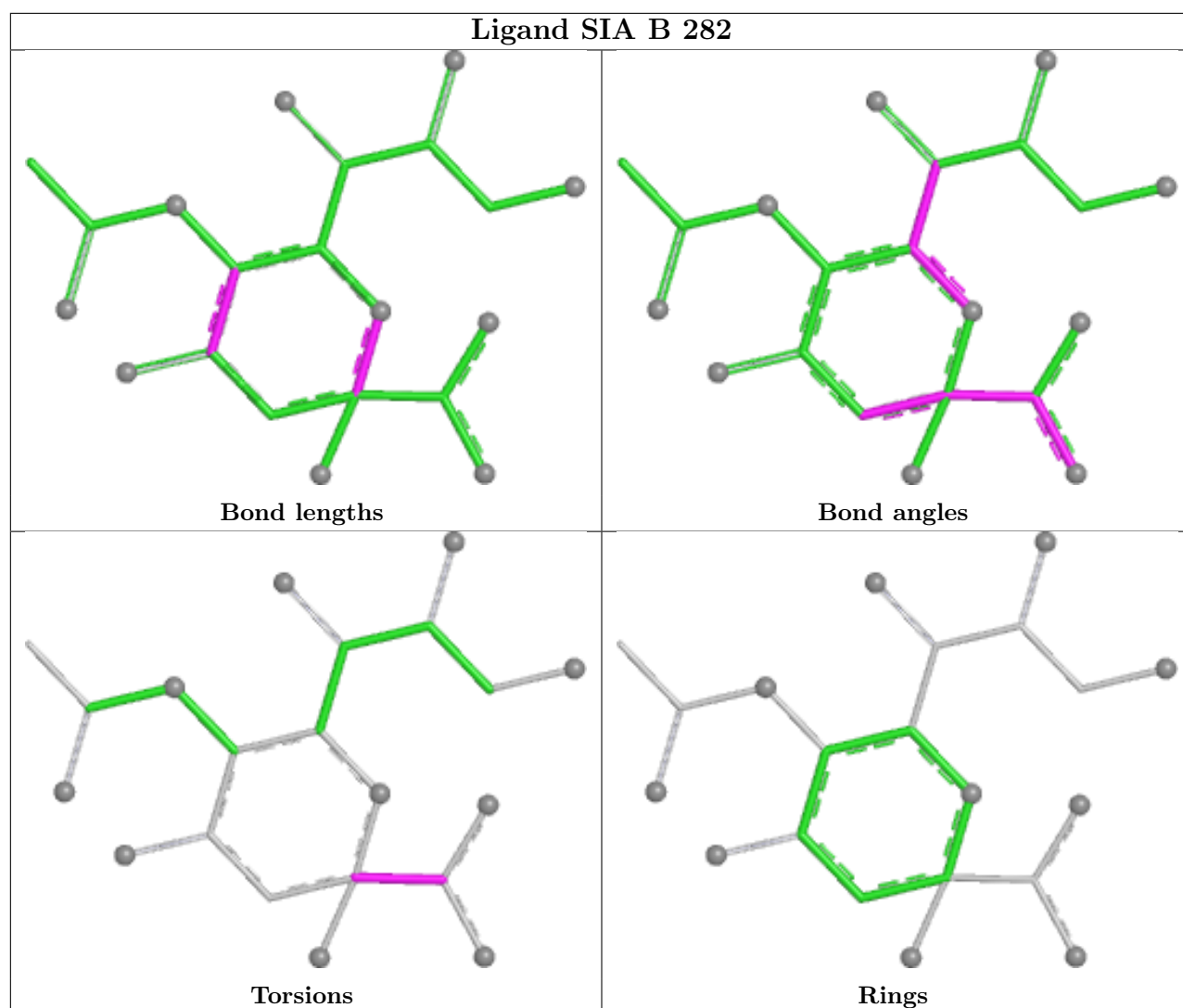












## 5.7 Other polymers [i](#)

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.