



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:15 AM UTC

PDB ID : 1EQ2 / pdb_00001eq2
Title : THE CRYSTAL STRUCTURE OF ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE
Authors : Deacon, A.M.; Ni, Y.S.; Coleman Jr., W.G.; Ealick, S.E.
Deposited on : 2000-03-31
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

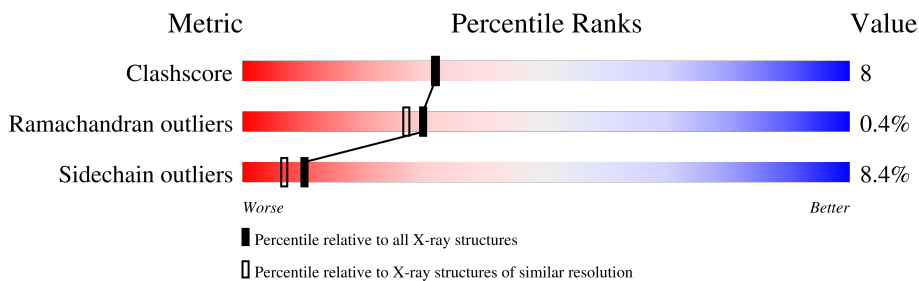
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)



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	310	
1	B	310	
1	C	310	
1	D	310	
1	E	310	
1	F	310	
1	G	310	
1	H	310	

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Mol	Chain	Length	Quality of chain
1	I	310	 76% 19% . . .
1	J	310	 75% 19% . . .

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
2	NAP	G	2406	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25435 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 ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2150	C 1375	N 349	O 417	S 9	0	0	0
1	B	300	Total 2386	C 1531	N 384	O 462	S 9	0	0	0
1	C	272	Total 2160	C 1385	N 348	O 418	S 9	0	0	0
1	D	307	Total 2442	C 1566	N 396	O 471	S 9	0	0	0
1	E	300	Total 2386	C 1531	N 384	O 462	S 9	0	0	0
1	F	307	Total 2442	C 1566	N 396	O 471	S 9	0	0	0
1	G	307	Total 2442	C 1566	N 396	O 471	S 9	0	0	0
1	H	297	Total 2360	C 1511	N 381	O 459	S 9	0	0	0
1	I	307	Total 2442	C 1566	N 396	O 471	S 9	0	0	0
1	J	300	Total 2386	C 1531	N 384	O 462	S 9	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

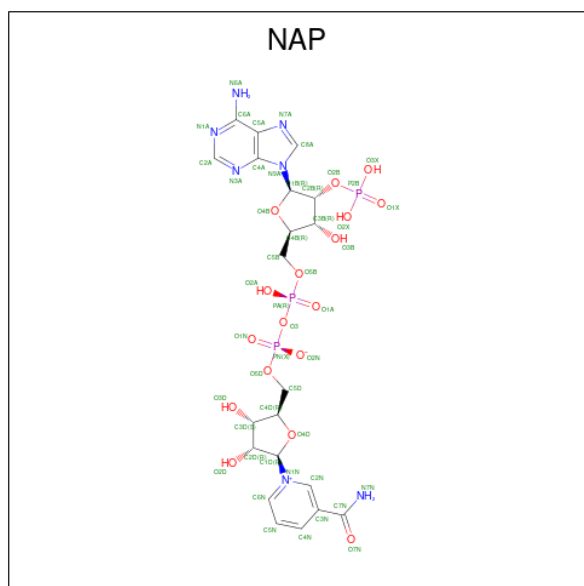
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	CSO	CYS	modified residue	UNP P67910
B	78	CSO	CYS	modified residue	UNP P67910
C	78	CSO	CYS	modified residue	UNP P67910
D	78	CSO	CYS	modified residue	UNP P67910
E	78	CSO	CYS	modified residue	UNP P67910
F	78	CSO	CYS	modified residue	UNP P67910
G	78	CSO	CYS	modified residue	UNP P67910
H	78	CSO	CYS	modified residue	UNP P67910
I	78	CSO	CYS	modified residue	UNP P67910

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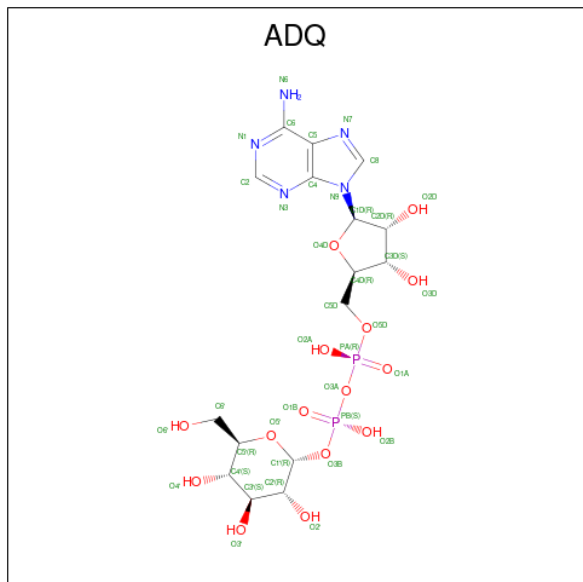
Chain	Residue	Modelled	Actual	Comment	Reference
J	78	CSO	CYS	modified residue	UNP P67910

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: ADQ) (formula: $C_{16}H_{25}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	119	Total 119	O 119	0	0
4	C	82	Total 82	O 82	0	0
4	D	118	Total 118	O 118	0	0
4	E	105	Total 105	O 105	0	0
4	F	106	Total 106	O 106	0	0
4	G	118	Total 118	O 118	0	0
4	H	114	Total 114	O 114	0	0
4	I	123	Total 123	O 123	0	0
4	J	101	Total 101	O 101	0	0

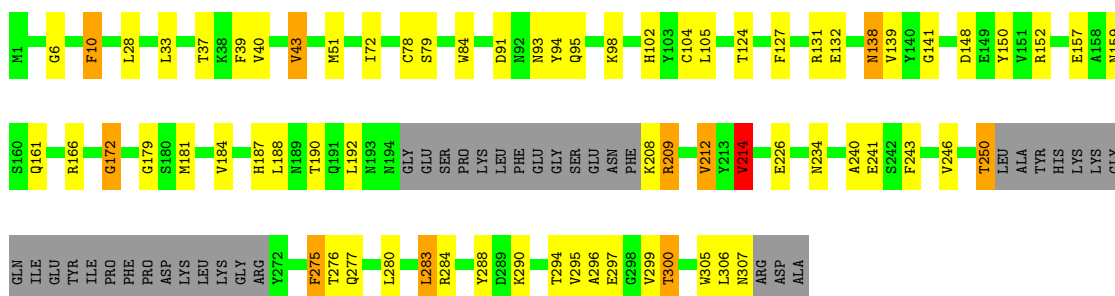
3 Residue-property plots [i](#)

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

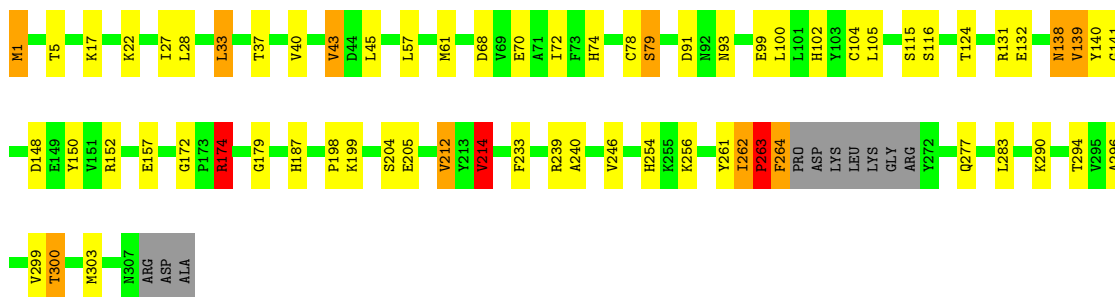
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain A: 



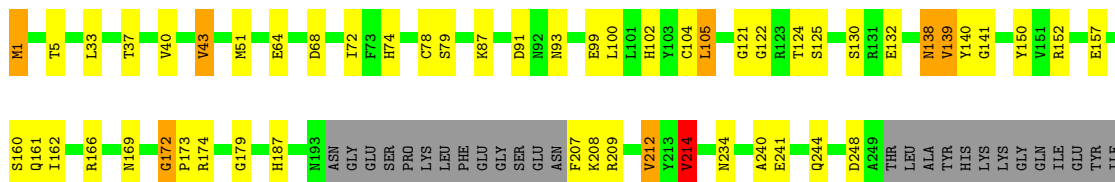
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain B: 



- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

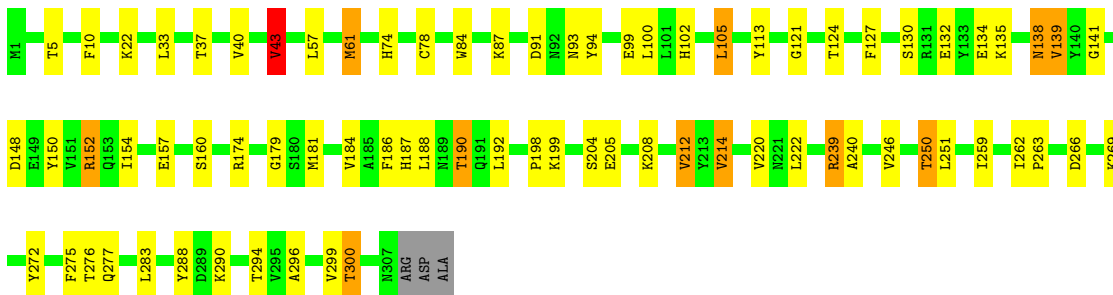
Chain C: 





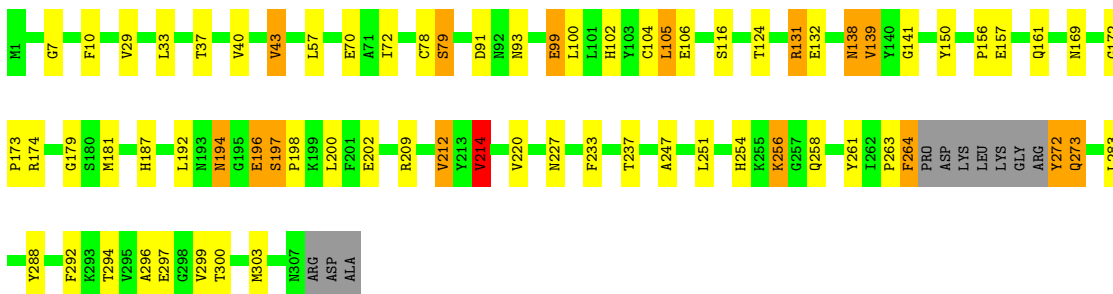
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain D: 75% 21%



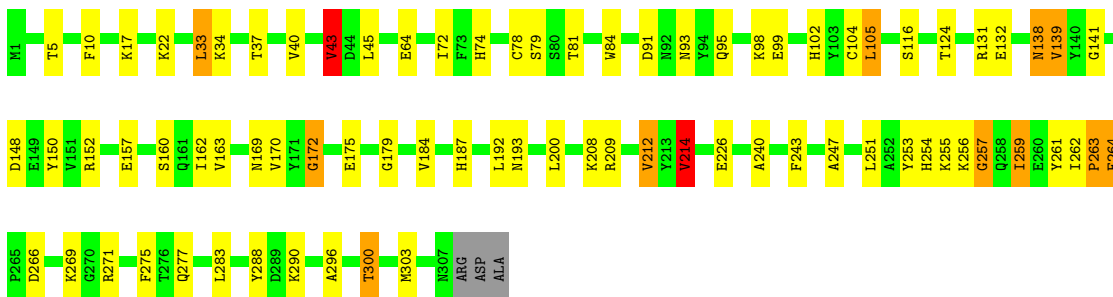
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain E: 74% 18% 5%



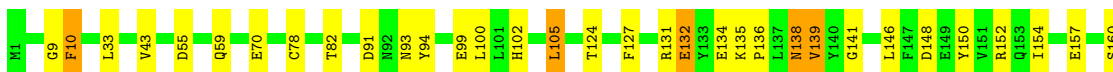
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain F: 74% 21%



- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain G: 81% 16%





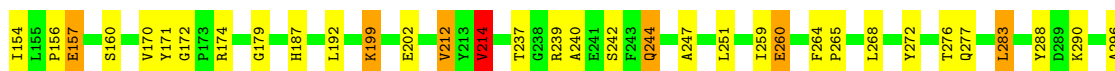
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain H: 74% 19%



- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain I: 76% 19%



- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain J: 75% 19%



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, α , β , γ	99.46Å 109.76Å 181.54Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	25435	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: CSO, NAP, ADQ

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	0.68	1/2188 (0.0%)	1.01	12/2958 (0.4%)
1	B	0.68	0/2434	1.06	18/3290 (0.5%)
1	C	0.72	0/2200	1.01	9/2973 (0.3%)
1	D	0.69	1/2492 (0.0%)	1.02	9/3368 (0.3%)
1	E	0.69	0/2434	1.04	12/3290 (0.4%)
1	F	0.69	0/2492	1.04	11/3368 (0.3%)
1	G	0.69	0/2492	1.03	11/3368 (0.3%)
1	H	0.69	1/2406 (0.0%)	1.03	13/3251 (0.4%)
1	I	0.69	0/2492	1.02	9/3368 (0.3%)
1	J	0.68	0/2434	1.02	8/3290 (0.2%)
All	All	0.69	3/24064 (0.0%)	1.03	112/32524 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	MET	SD-CE	5.39	1.93	1.79
1	D	61	MET	SD-CE	5.32	1.92	1.79
1	H	24	ILE	CA-CB	5.00	1.60	1.54

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	N-CA-C	-11.19	95.45	110.55
1	A	214	VAL	CB-CA-C	-8.48	100.93	112.04
1	F	43	VAL	N-CA-C	8.24	120.02	110.62
1	B	262	ILE	CA-C-N	7.84	129.64	119.84
1	B	262	ILE	C-N-CA	7.84	129.64	119.84

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	2150	0	2045	39	0
1	B	2386	0	2272	30	0
1	C	2160	0	2056	32	0
1	D	2442	0	2337	41	0
1	E	2386	0	2272	37	0
1	F	2442	0	2337	44	0
1	G	2442	0	2337	38	0
1	H	2360	0	2245	36	0
1	I	2442	0	2337	34	0
1	J	2386	0	2272	36	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	0	0
3	A	27	0	12	3	0
3	B	38	0	23	2	0
3	C	27	0	12	2	0
3	D	38	0	23	1	0
3	E	27	0	12	3	0
3	F	38	0	23	3	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
3	I	27	0	12	3	0
3	J	27	0	12	0	0
4	A	70	0	0	4	0
4	B	119	0	0	5	0
4	C	82	0	0	5	0
4	D	118	0	0	4	0
4	E	105	0	0	2	0
4	F	106	0	0	6	0
4	G	118	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	114	0	0	4	0
4	I	123	0	0	6	0
4	J	101	0	0	7	0
All	All	25435	0	22913	382	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 8.

The worst 5 of 382 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)
3:A:2500:ADQ:H5'1	3:A:2500:ADQ:H8	1.30	1.13
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:H8	1.39	1.04
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:H8	1.41	1.01
3:C:2502:ADQ:H5'1	3:C:2502:ADQ:H8	1.40	1.00
1:F:296:ALA:O	1:F:300:THR:HG23	1.64	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	266/310 (86%)	254 (96%)	9 (3%)	3 (1%)	11 7
1	B	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	36 35
1	C	265/310 (86%)	251 (95%)	13 (5%)	1 (0%)	30 27
1	D	304/310 (98%)	292 (96%)	11 (4%)	1 (0%)	36 35
1	E	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	36 35
1	F	304/310 (98%)	290 (95%)	13 (4%)	1 (0%)	36 35
1	G	304/310 (98%)	291 (96%)	11 (4%)	2 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	292/310 (94%)	282 (97%)	10 (3%)	0	100	100
1	I	304/310 (98%)	290 (95%)	14 (5%)	0	100	100
1	J	295/310 (95%)	280 (95%)	12 (4%)	3 (1%)	12	8
All	All	2924/3100 (94%)	2798 (96%)	113 (4%)	13 (0%)	30	27

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	B	263	PRO
1	F	264	PHE
1	J	263	PRO
1	J	259	ILE

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	222/256 (87%)	205 (92%)	17 (8%)	12	8
1	B	248/256 (97%)	224 (90%)	24 (10%)	8	5
1	C	224/256 (88%)	205 (92%)	19 (8%)	10	7
1	D	254/256 (99%)	232 (91%)	22 (9%)	9	6
1	E	248/256 (97%)	227 (92%)	21 (8%)	10	7
1	F	254/256 (99%)	232 (91%)	22 (9%)	9	6
1	G	254/256 (99%)	237 (93%)	17 (7%)	15	11
1	H	245/256 (96%)	226 (92%)	19 (8%)	11	8
1	I	254/256 (99%)	231 (91%)	23 (9%)	9	6
1	J	248/256 (97%)	227 (92%)	21 (8%)	10	7
All	All	2451/2560 (96%)	2246 (92%)	205 (8%)	10	7

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	160	SER
1	H	33	LEU
1	J	198	PRO
1	F	263	PRO
1	G	105	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	138	ASN
1	J	227	ASN
1	G	187	HIS
1	J	221	ASN
1	I	273	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](#)

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	B	78	1	3,6,7	0.57	0	1,6,8	0.21	0
1	CSO	G	78	1	3,6,7	0.80	0	1,6,8	0.07	0
1	CSO	H	78	1	3,6,7	0.70	0	1,6,8	0.41	0
1	CSO	D	78	1	3,6,7	0.79	0	1,6,8	0.60	0
1	CSO	I	78	1	3,6,7	0.73	0	1,6,8	0.45	0
1	CSO	F	78	1	3,6,7	0.62	0	1,6,8	0.71	0
1	CSO	J	78	1	3,6,7	0.71	0	1,6,8	0.43	0
1	CSO	A	78	1	3,6,7	0.62	0	1,6,8	0.11	0
1	CSO	E	78	1	3,6,7	0.86	0	1,6,8	0.03	0
1	CSO	C	78	1	3,6,7	0.80	0	1,6,8	0.35	0

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
1	CSO	B	78	1	-	0/1/5/7	-
1	CSO	G	78	1	-	1/1/5/7	-
1	CSO	H	78	1	-	1/1/5/7	-
1	CSO	D	78	1	-	1/1/5/7	-
1	CSO	I	78	1	-	1/1/5/7	-
1	CSO	F	78	1	-	1/1/5/7	-
1	CSO	J	78	1	-	1/1/5/7	-
1	CSO	A	78	1	-	0/1/5/7	-
1	CSO	E	78	1	-	0/1/5/7	-
1	CSO	C	78	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	78	CSO	N-CA-CB-SG
1	F	78	CSO	N-CA-CB-SG
1	G	78	CSO	N-CA-CB-SG
1	H	78	CSO	N-CA-CB-SG
1	I	78	CSO	N-CA-CB-SG

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	78	CSO	1	0
1	G	78	CSO	1	0
1	H	78	CSO	1	0
1	D	78	CSO	1	0
1	I	78	CSO	1	0
1	F	78	CSO	1	0
1	J	78	CSO	1	0
1	A	78	CSO	1	0
1	E	78	CSO	1	0
1	C	78	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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
2	NAP	E	2404	-	50,52,52	2.61	12 (24%)	71,80,80	1.80	11 (15%)
2	NAP	I	2408	-	50,52,52	2.75	12 (24%)	71,80,80	1.79	9 (12%)
2	NAP	D	2403	-	50,52,52	2.58	13 (26%)	71,80,80	1.74	8 (11%)
2	NAP	B	2401	-	50,52,52	2.62	12 (24%)	71,80,80	1.78	8 (11%)
3	ADQ	G	2506	-	28,29,41	1.37	5 (17%)	43,45,63	1.89	8 (18%)
3	ADQ	D	2503	-	40,41,41	1.76	8 (20%)	60,63,63	2.09	16 (26%)
3	ADQ	A	2500	-	28,29,41	1.44	3 (10%)	43,45,63	2.00	9 (20%)
2	NAP	G	2406	-	50,52,52	2.44	14 (28%)	71,80,80	1.78	11 (15%)
3	ADQ	J	2509	-	28,29,41	1.37	3 (10%)	43,45,63	2.02	8 (18%)
2	NAP	C	2402	-	50,52,52	2.37	11 (22%)	71,80,80	1.82	8 (11%)
3	ADQ	C	2502	-	28,29,41	1.26	4 (14%)	43,45,63	1.92	7 (16%)
3	ADQ	H	2507	-	28,29,41	1.37	4 (14%)	43,45,63	1.99	9 (20%)
3	ADQ	I	2508	-	28,29,41	1.23	5 (17%)	43,45,63	1.96	11 (25%)
3	ADQ	B	2501	-	40,41,41	1.42	3 (7%)	60,63,63	1.90	13 (21%)
2	NAP	H	2407	-	50,52,52	2.50	12 (24%)	71,80,80	1.76	7 (9%)
2	NAP	A	2400	-	50,52,52	2.59	13 (26%)	71,80,80	1.77	10 (14%)
2	NAP	J	2409	-	50,52,52	2.61	11 (22%)	71,80,80	1.81	6 (8%)
2	NAP	F	2405	-	50,52,52	2.42	11 (22%)	71,80,80	1.86	9 (12%)
3	ADQ	F	2505	-	40,41,41	1.51	7 (17%)	60,63,63	1.86	13 (21%)
3	ADQ	E	2504	-	28,29,41	1.42	5 (17%)	43,45,63	1.98	9 (20%)

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
2	NAP	E	2404	-	-	8/35/67/67	0/5/5/5
2	NAP	I	2408	-	-	8/35/67/67	0/5/5/5
2	NAP	D	2403	-	-	3/35/67/67	0/5/5/5
2	NAP	B	2401	-	-	2/35/67/67	0/5/5/5
3	ADQ	G	2506	-	-	1/16/32/59	0/3/3/4
3	ADQ	D	2503	-	-	8/23/59/59	0/4/4/4
3	ADQ	A	2500	-	-	2/16/32/59	0/3/3/4
2	NAP	G	2406	-	1/1/12/12	12/35/67/67	0/5/5/5
3	ADQ	J	2509	-	-	4/16/32/59	0/3/3/4
2	NAP	C	2402	-	-	3/35/67/67	0/5/5/5
3	ADQ	C	2502	-	-	5/16/32/59	0/3/3/4
3	ADQ	H	2507	-	-	5/16/32/59	0/3/3/4
3	ADQ	I	2508	-	-	4/16/32/59	0/3/3/4
3	ADQ	B	2501	-	-	5/23/59/59	0/4/4/4
2	NAP	H	2407	-	-	7/35/67/67	0/5/5/5
2	NAP	A	2400	-	-	3/35/67/67	0/5/5/5
2	NAP	J	2409	-	-	5/35/67/67	0/5/5/5
2	NAP	F	2405	-	-	3/35/67/67	0/5/5/5
3	ADQ	F	2505	-	-	5/23/59/59	0/4/4/4
3	ADQ	E	2504	-	-	2/16/32/59	0/3/3/4

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2408	NAP	PA-O3	-10.01	1.48	1.59
2	B	2401	NAP	P2B-O2B	9.33	1.75	1.59
2	J	2409	NAP	P2B-O2B	9.26	1.75	1.59
2	H	2407	NAP	P2B-O2B	9.06	1.75	1.59
2	E	2404	NAP	P2B-O2B	8.71	1.74	1.59

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	C5N-C4N-C3N	-9.13	111.39	120.36
2	J	2409	NAP	C5N-C4N-C3N	-9.02	111.50	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2404	NAP	C5N-C4N-C3N	-8.97	111.55	120.36
2	B	2401	NAP	C5N-C4N-C3N	-8.96	111.56	120.36
2	H	2407	NAP	C5N-C4N-C3N	-8.88	111.63	120.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	2406	NAP	C4B

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2400	NAP	C2B-C1B-N9A-C8A
2	B	2401	NAP	C2B-C1B-N9A-C8A
2	B	2401	NAP	C2B-C1B-N9A-C4A
2	C	2402	NAP	C2B-C1B-N9A-C8A
2	C	2402	NAP	C2B-C1B-N9A-C4A

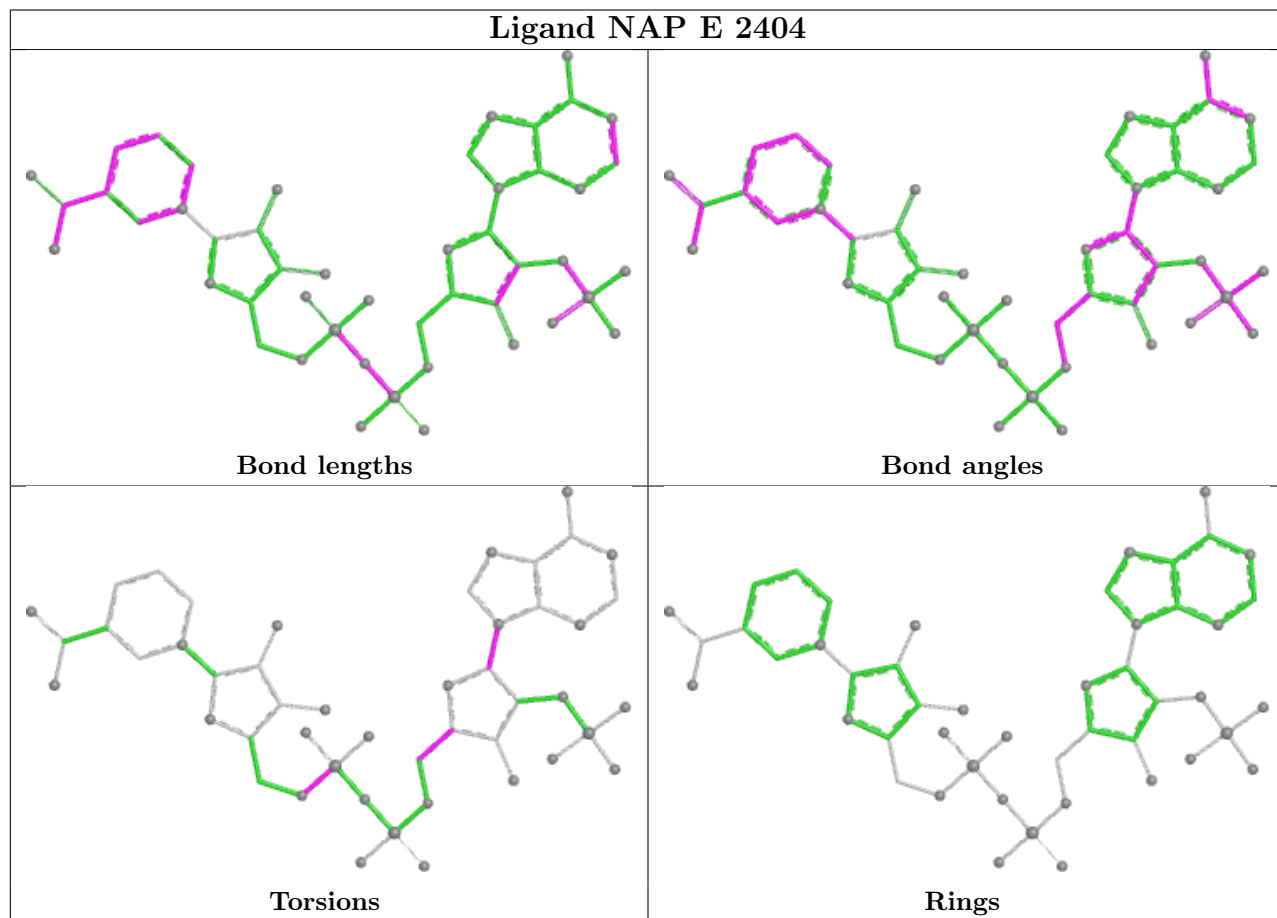
There are no ring outliers.

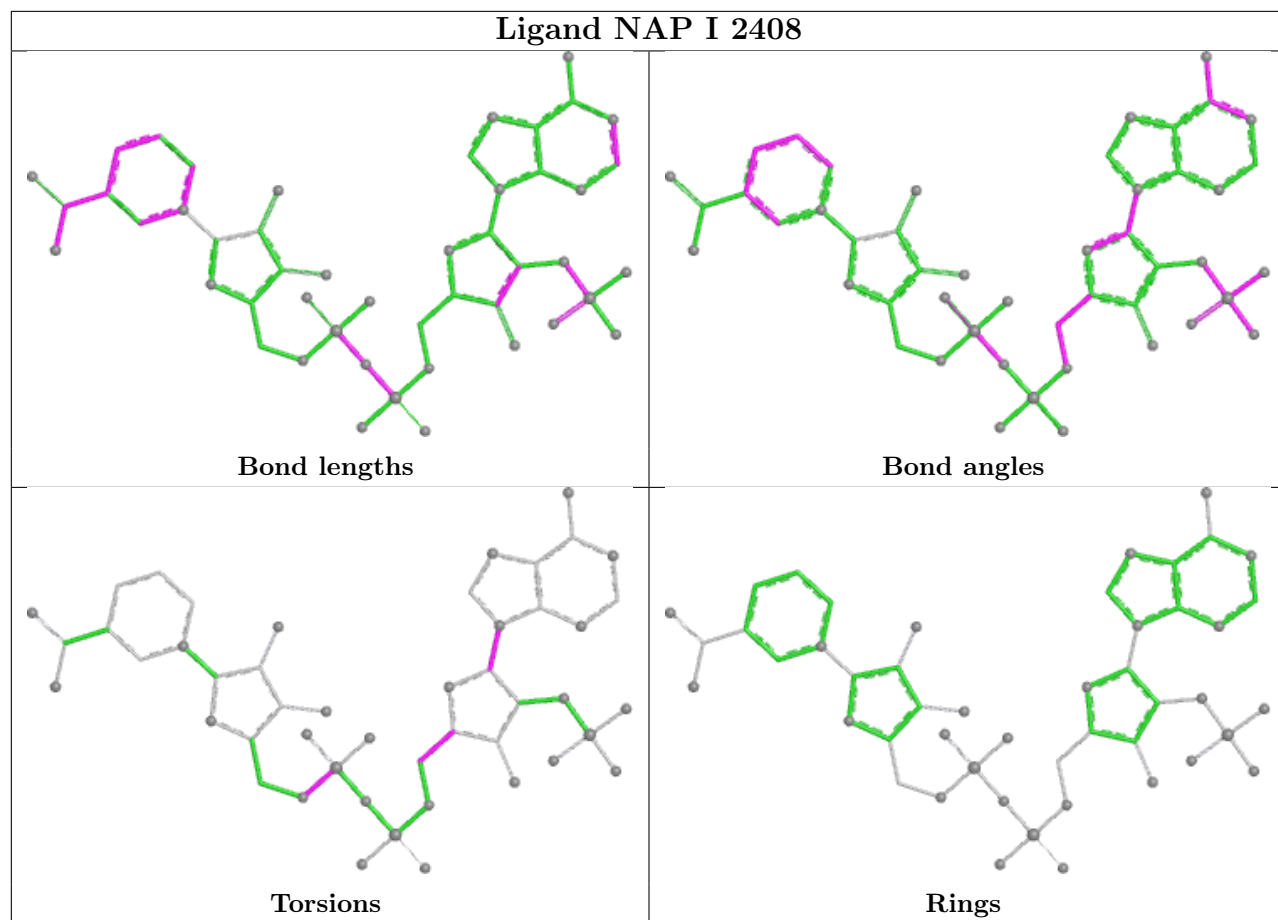
15 monomers are involved in 25 short contacts:

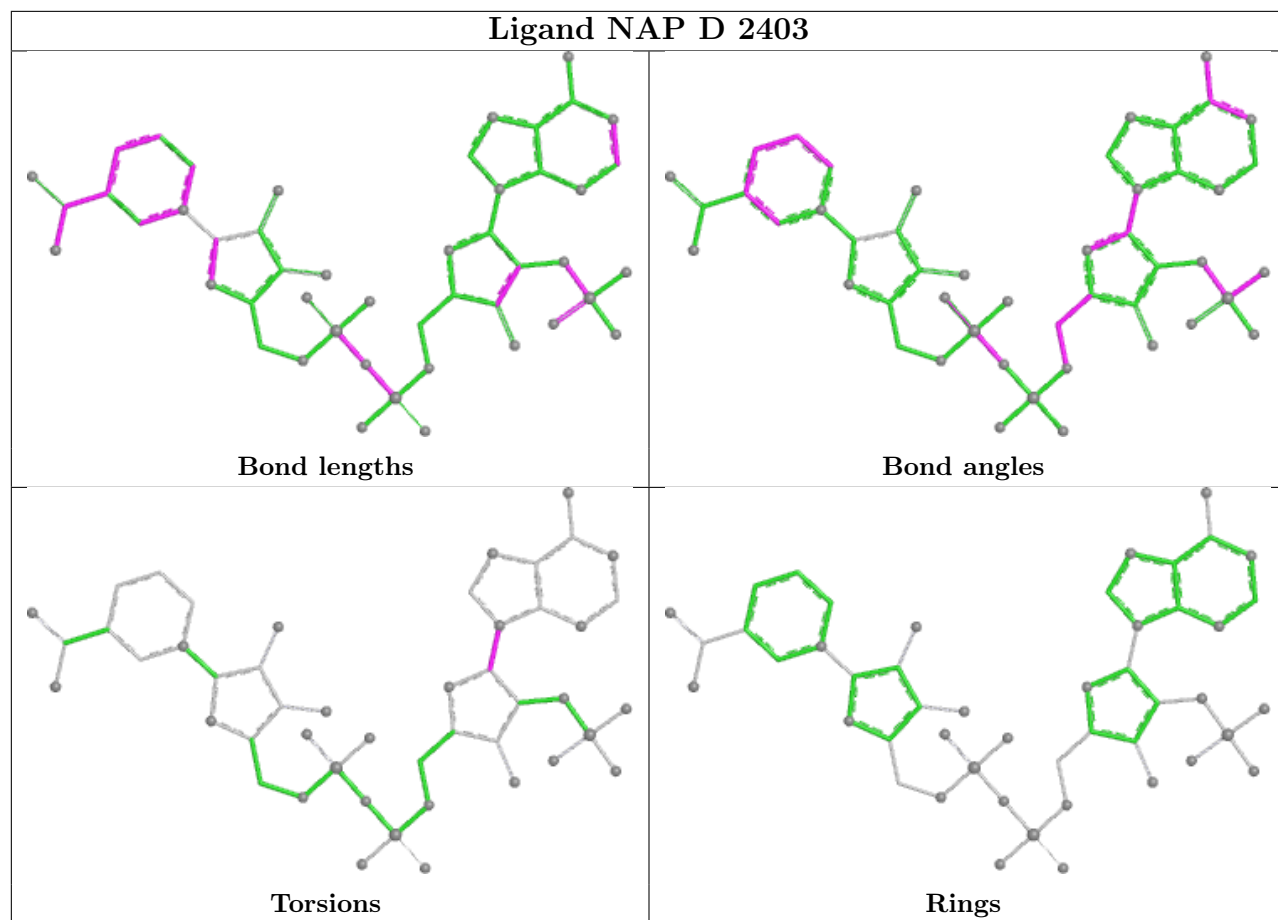
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2404	NAP	1	0
2	I	2408	NAP	1	0
2	B	2401	NAP	1	0
3	D	2503	ADQ	1	0
3	A	2500	ADQ	3	0
2	G	2406	NAP	1	0
3	C	2502	ADQ	2	0
3	H	2507	ADQ	1	0
3	I	2508	ADQ	3	0
3	B	2501	ADQ	2	0
2	H	2407	NAP	1	0
2	A	2400	NAP	1	0
2	F	2405	NAP	1	0
3	F	2505	ADQ	3	0
3	E	2504	ADQ	3	0

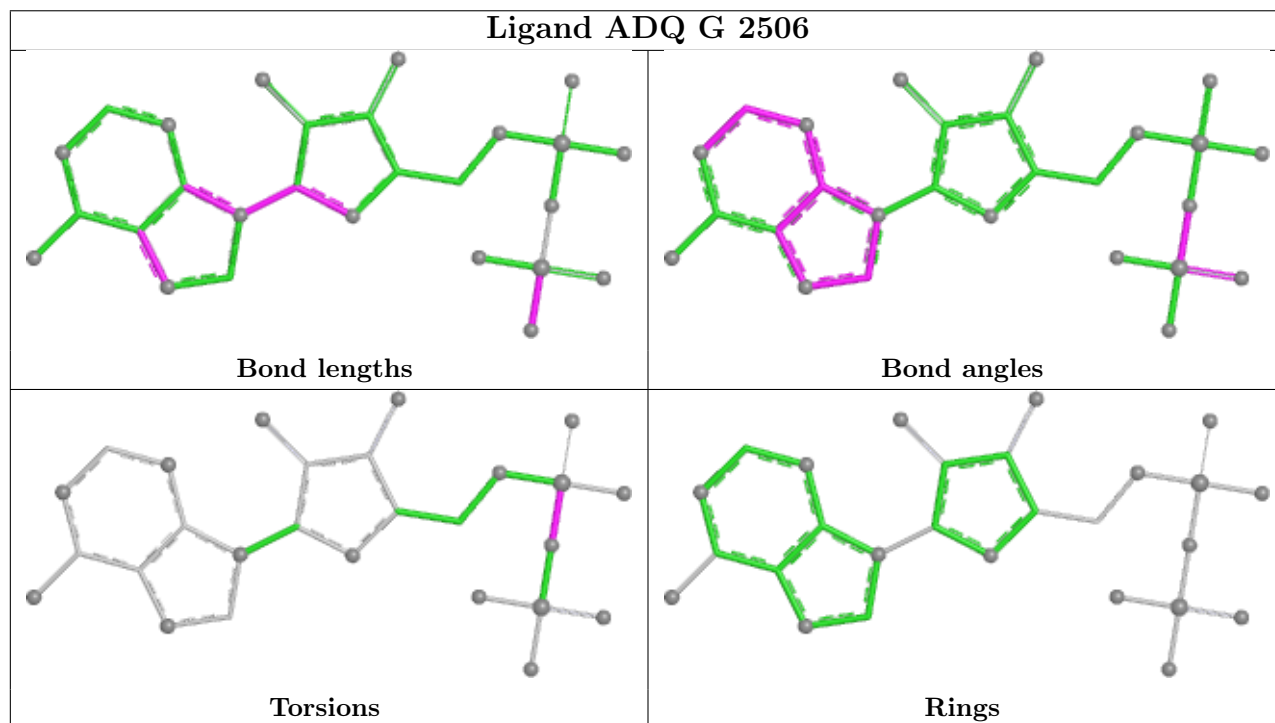
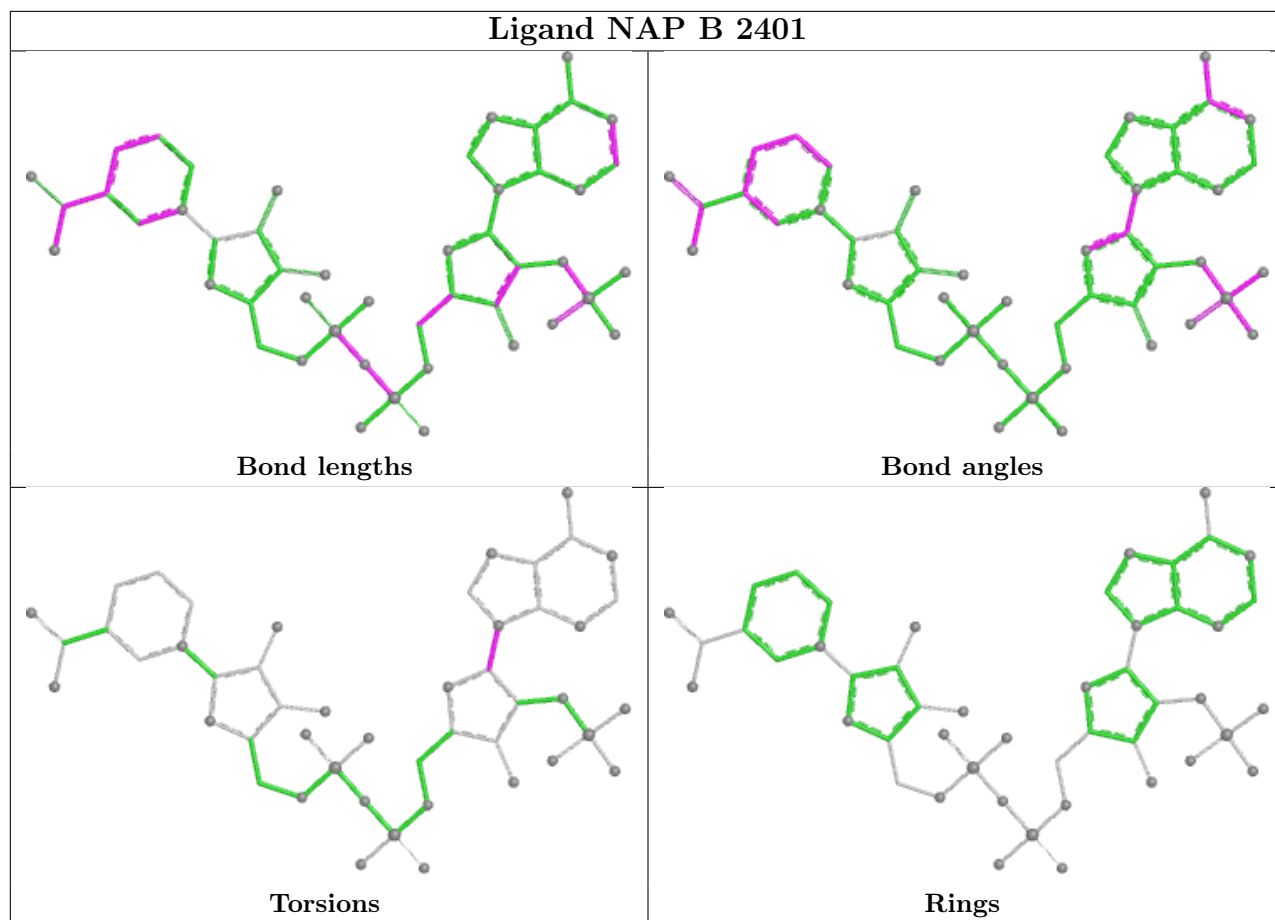
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

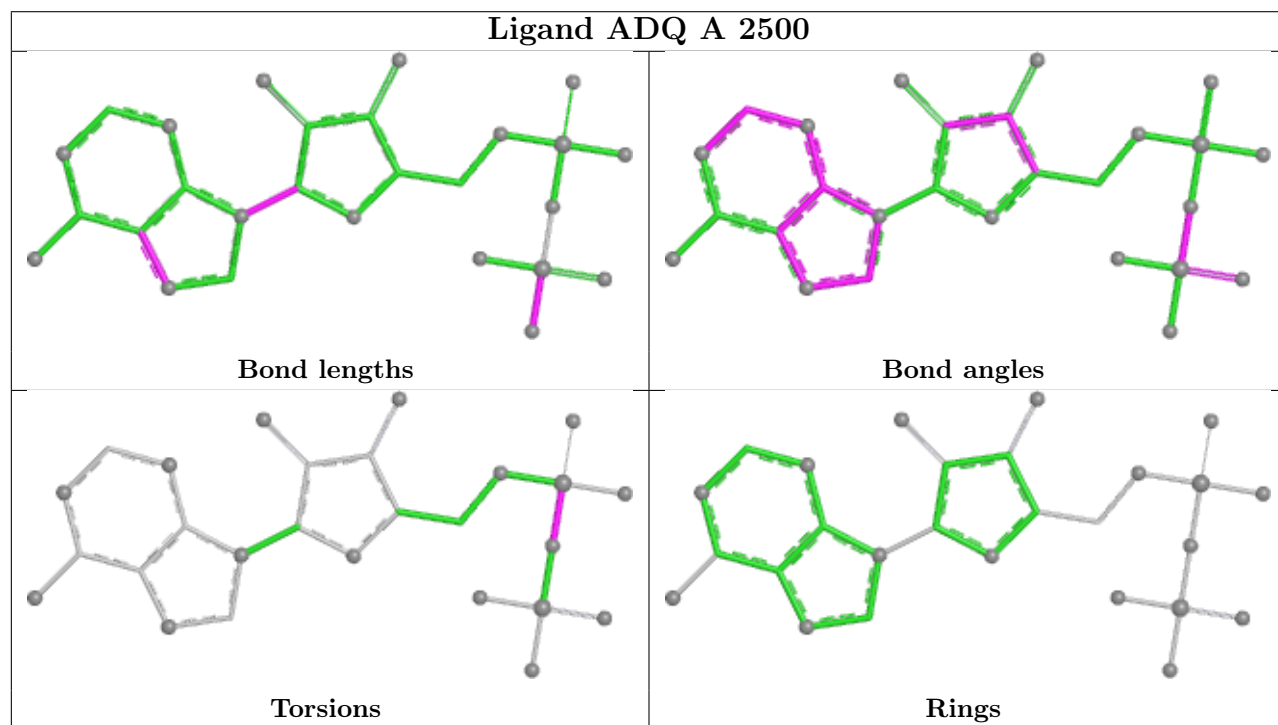
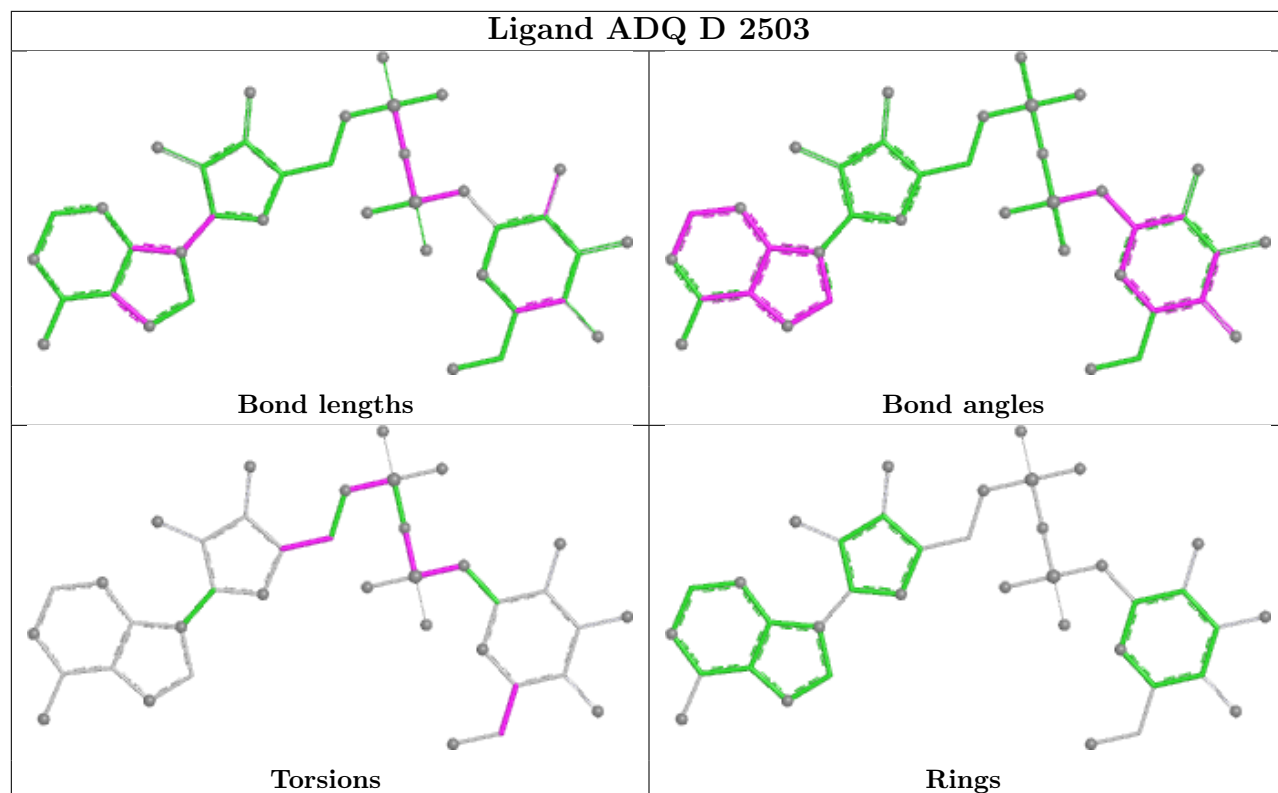
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

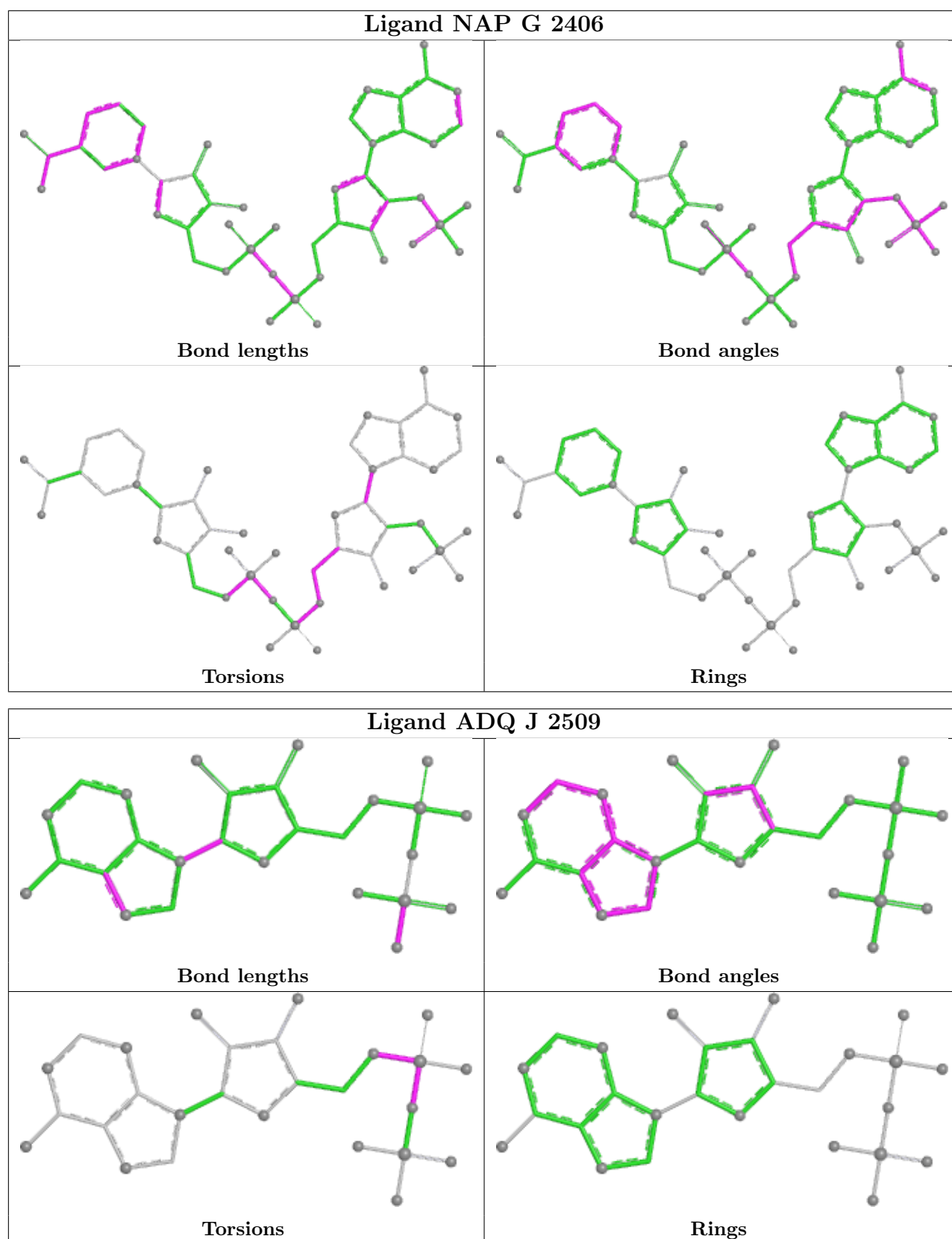


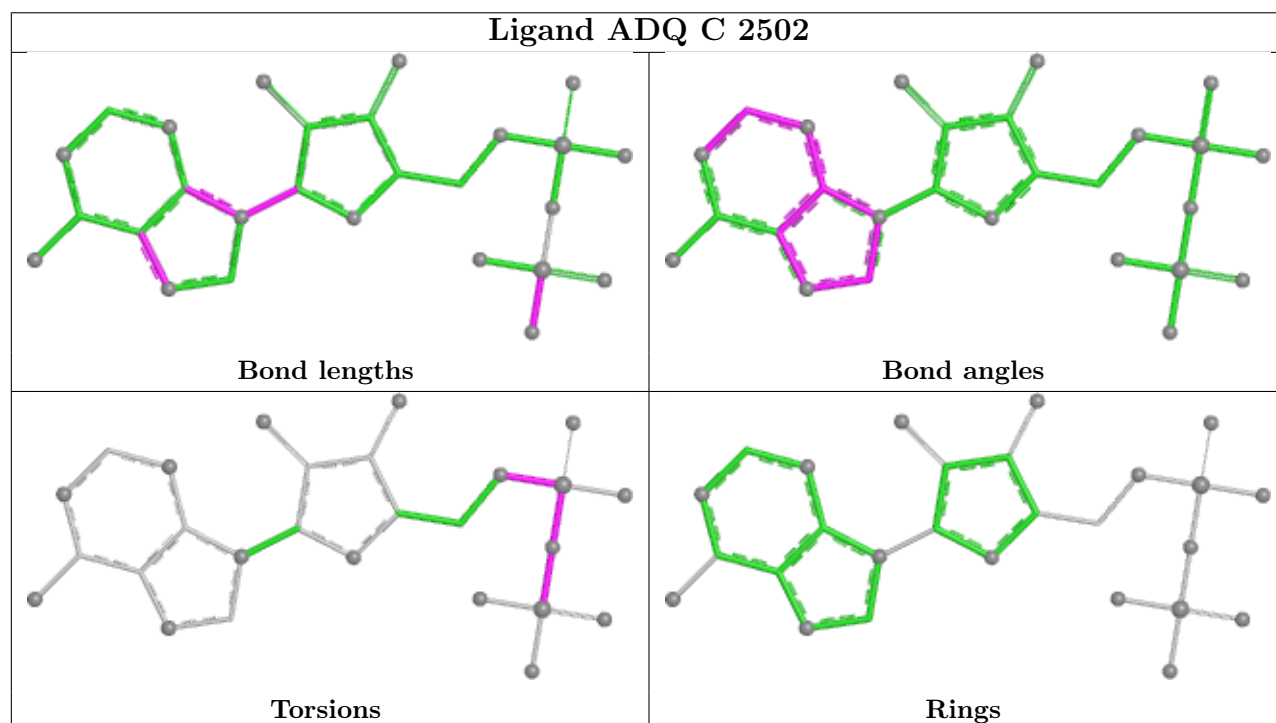
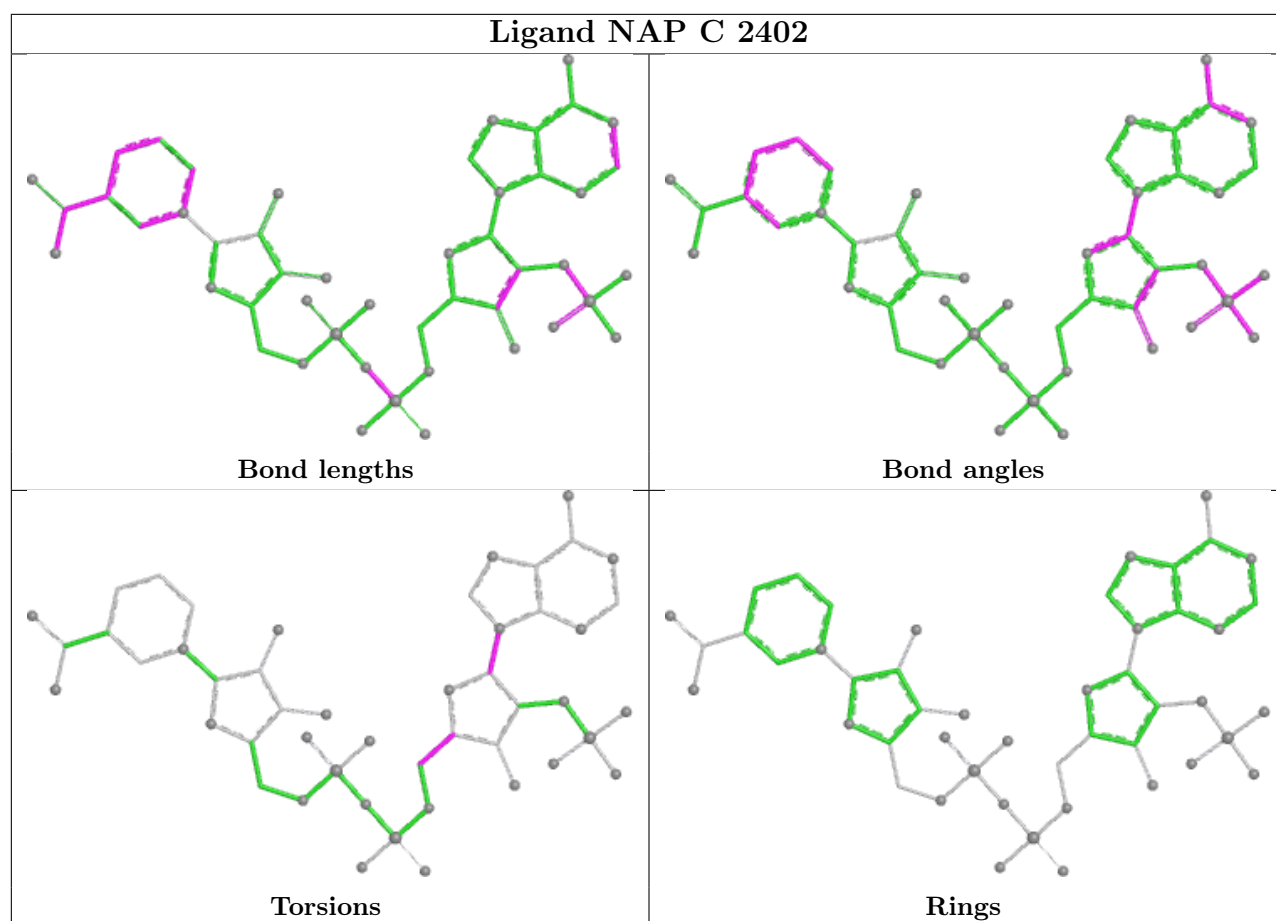


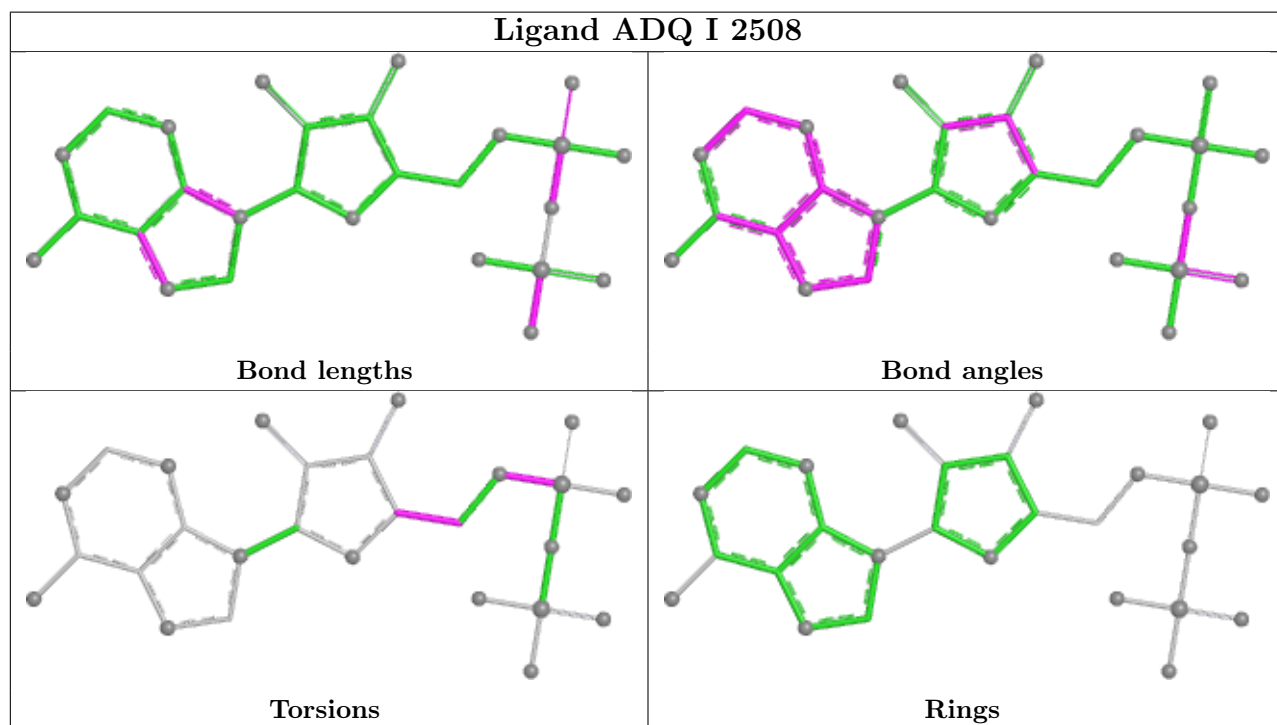
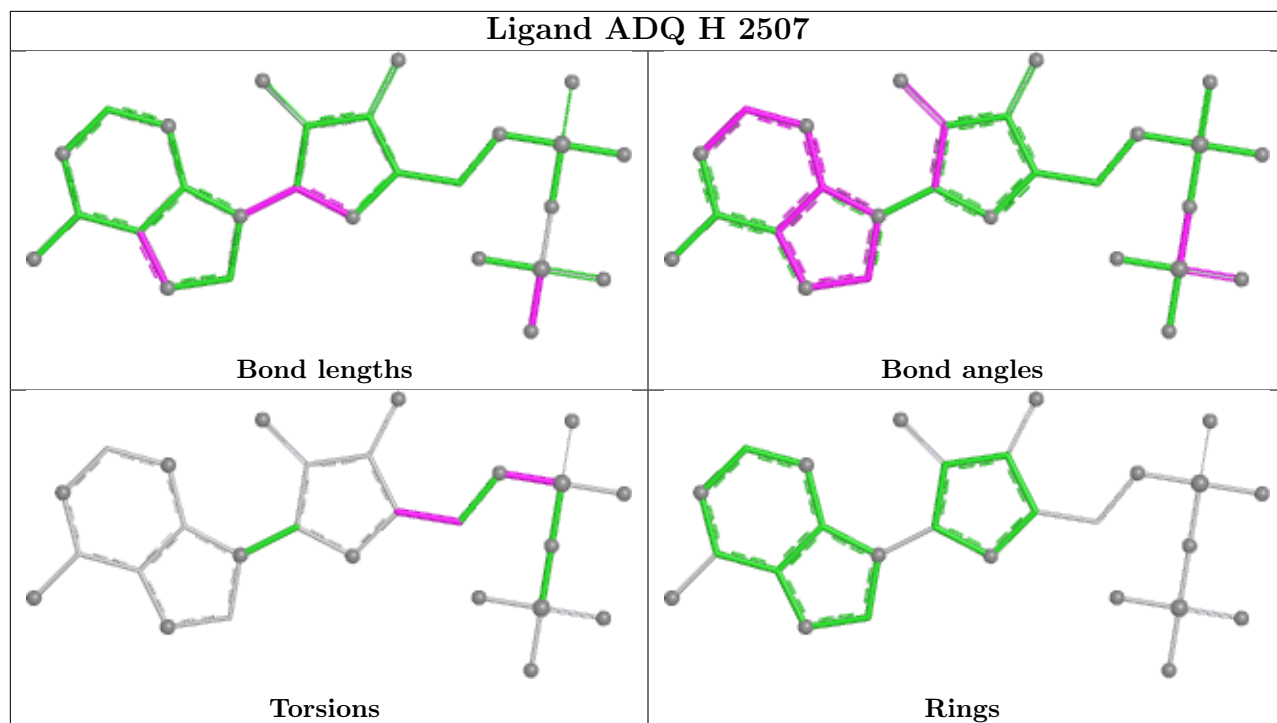


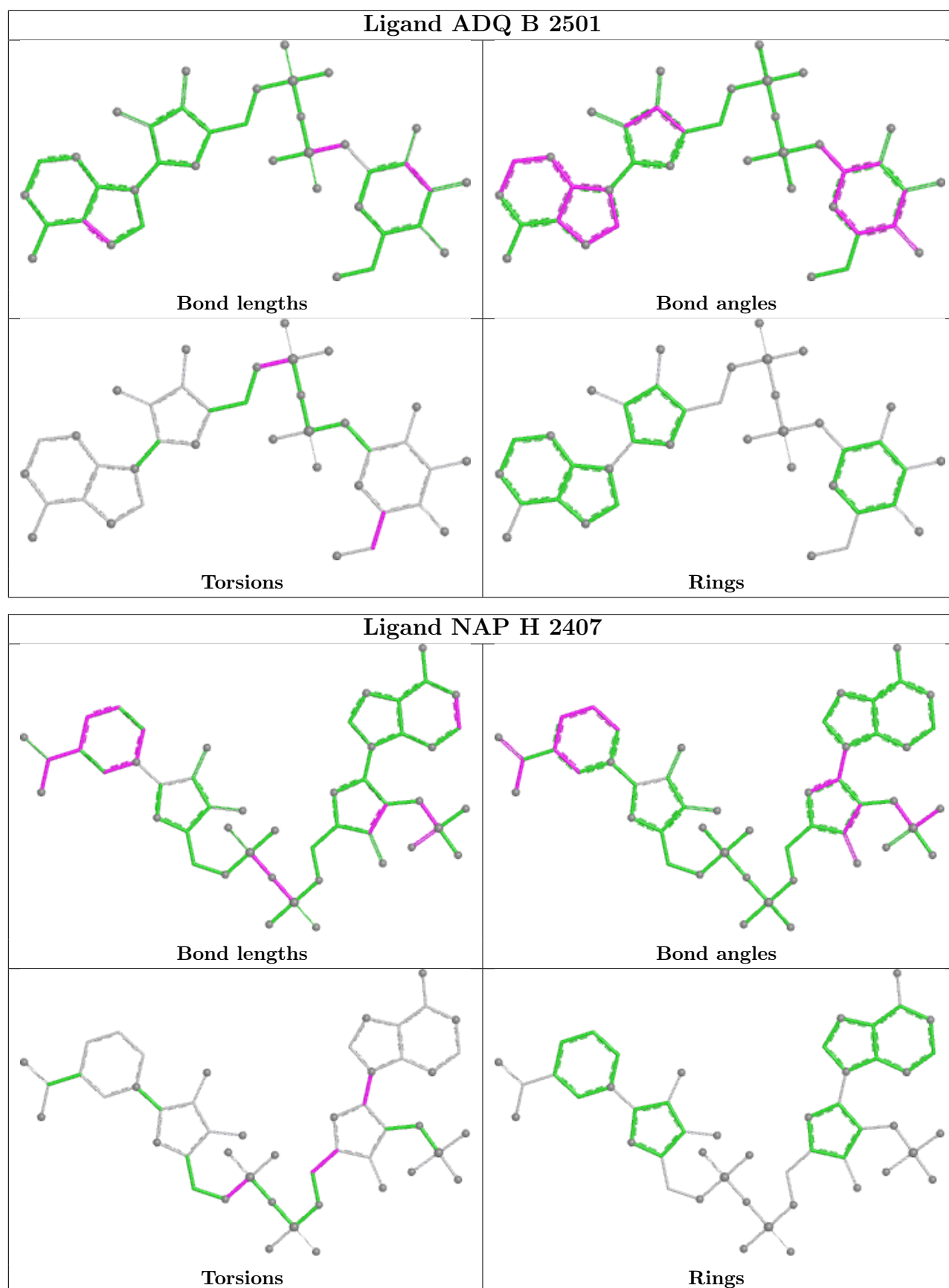


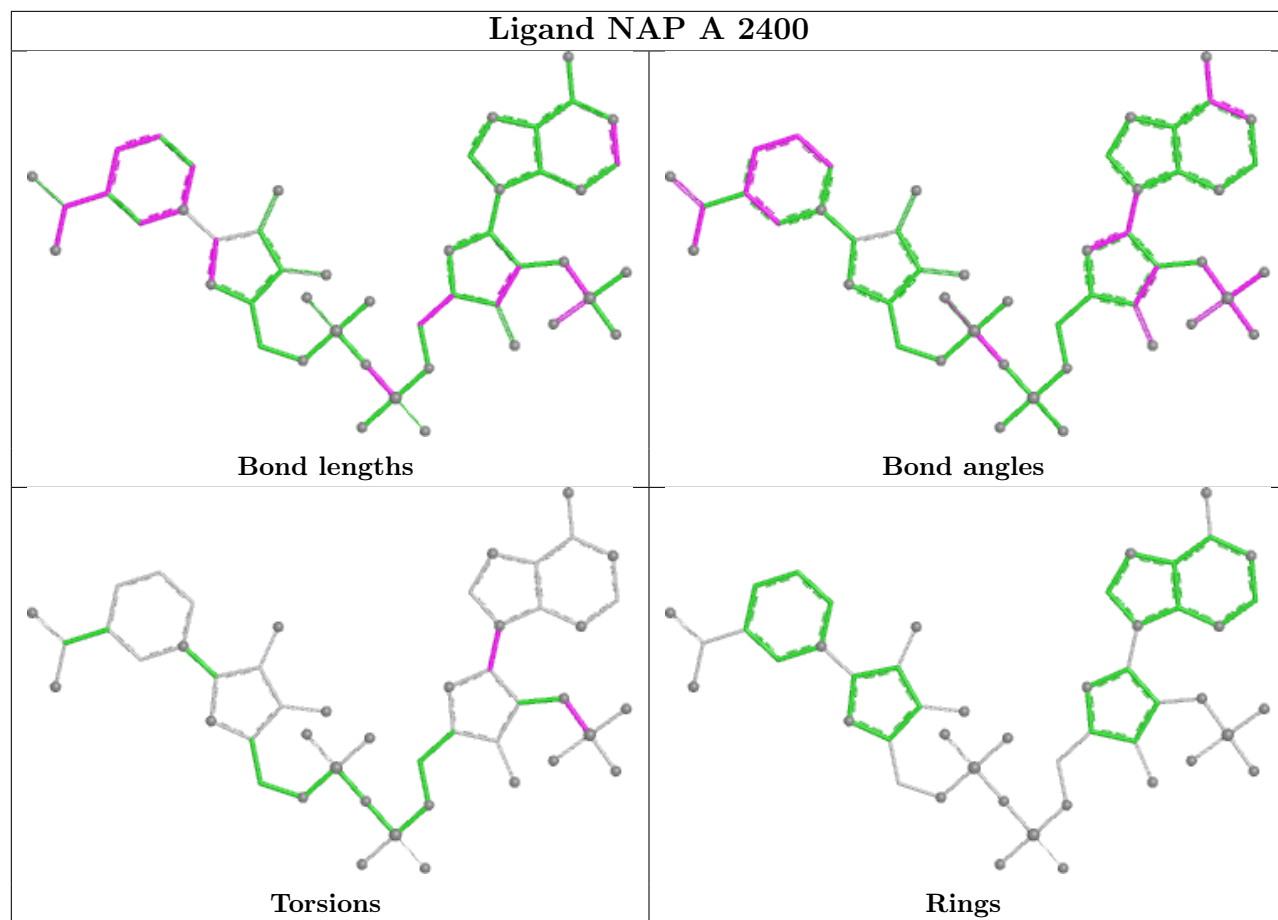


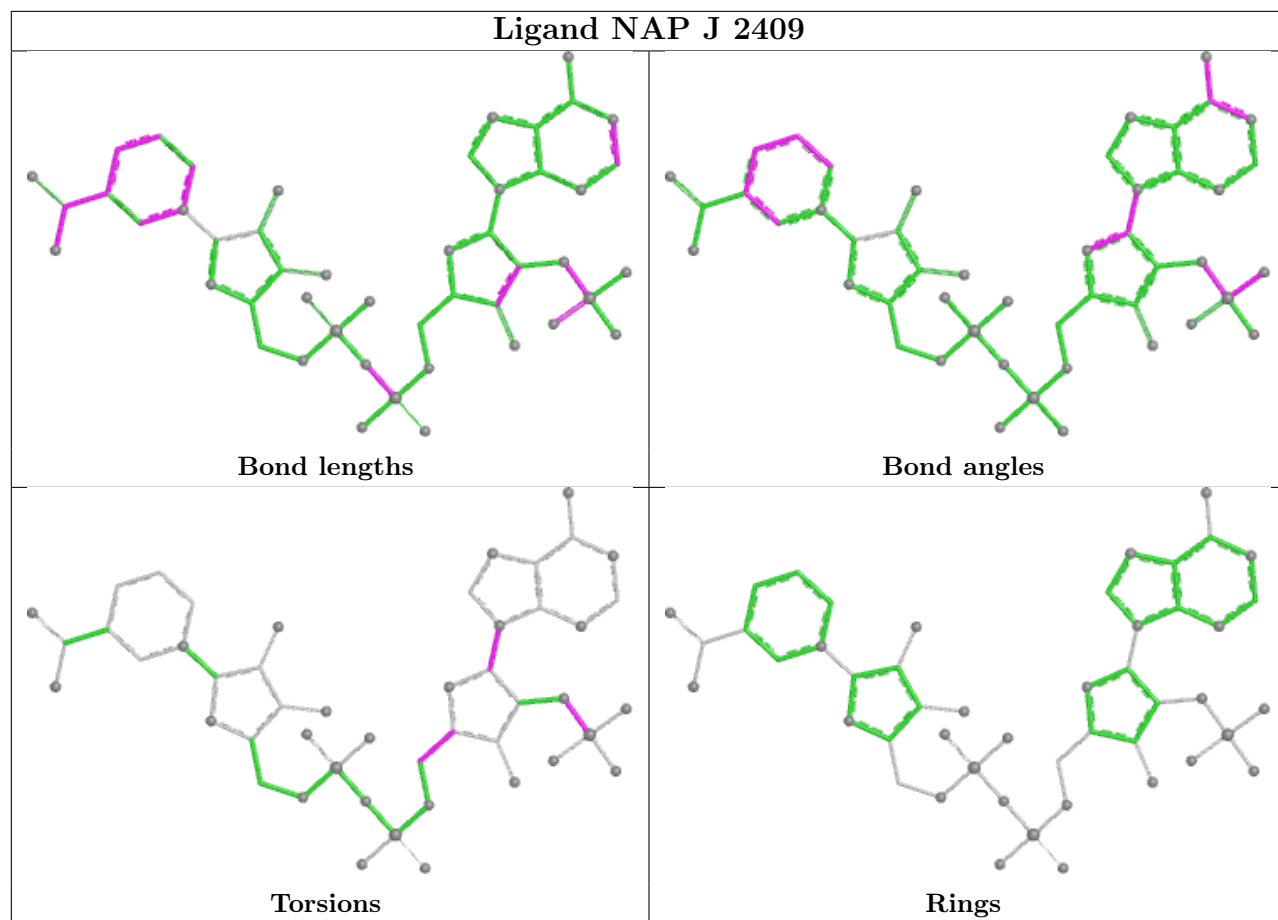


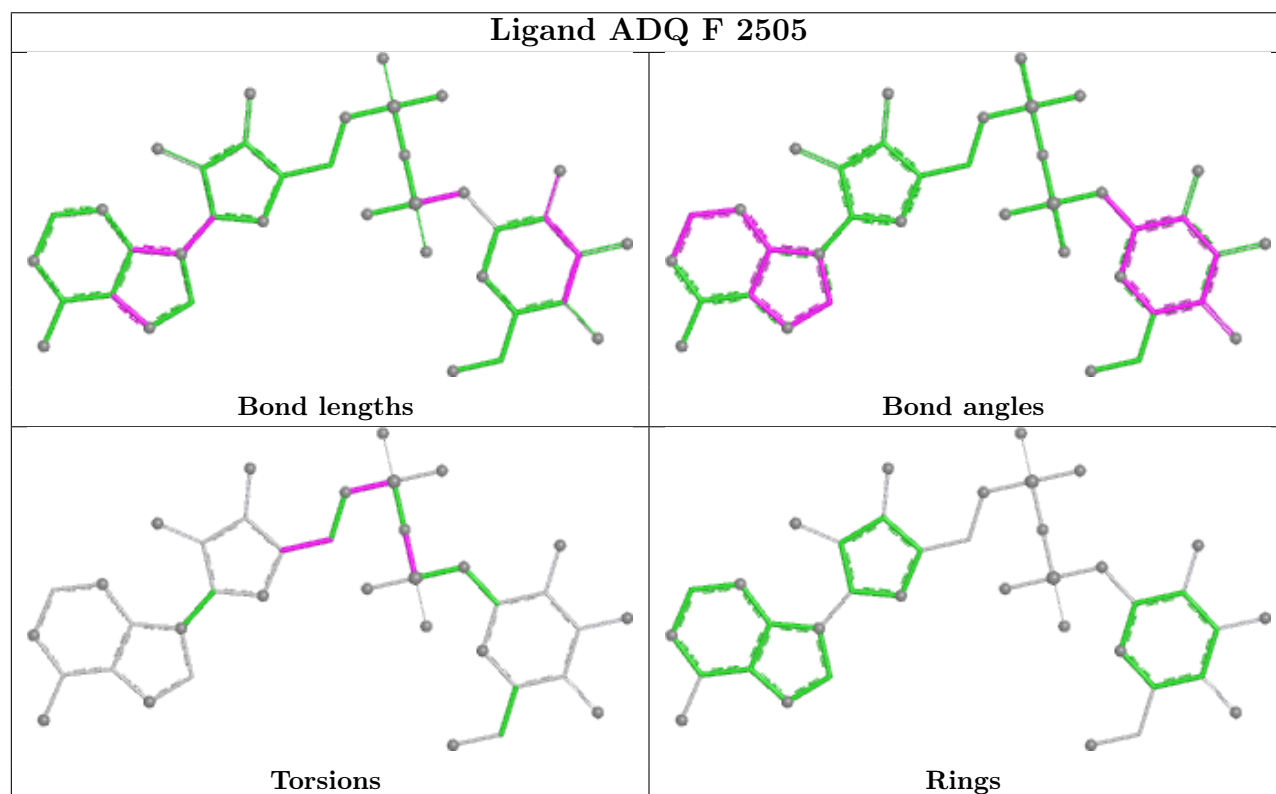
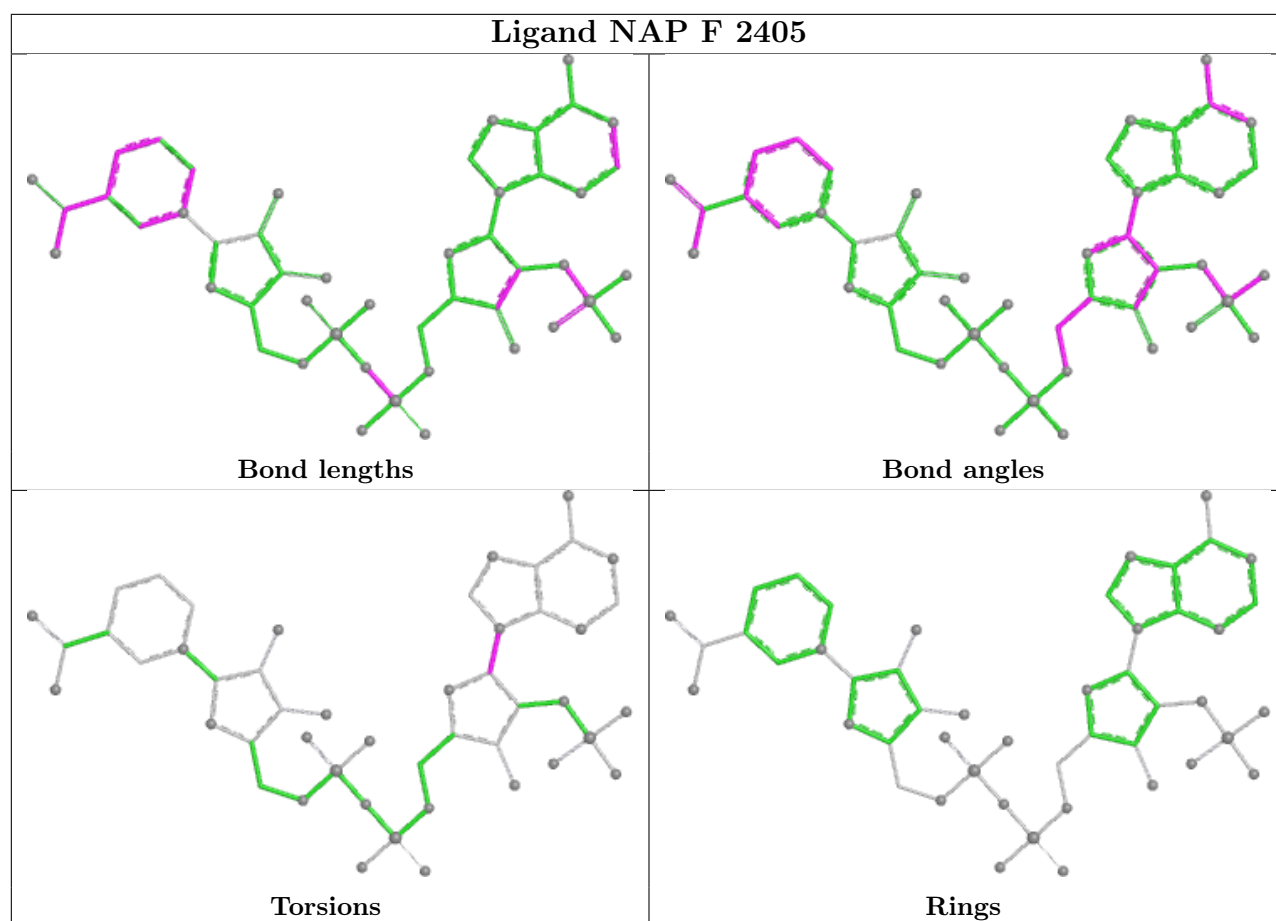


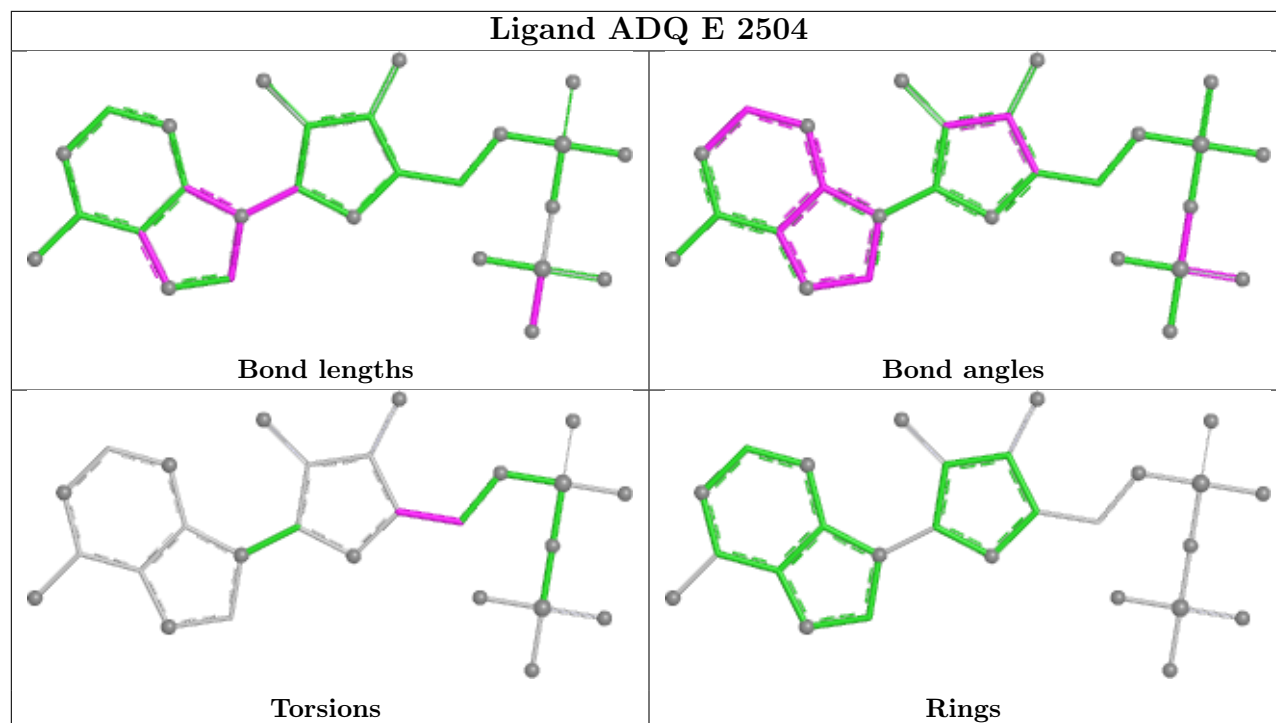












5.7 Other polymers [i](#)

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 [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.