



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:28 pm BST

PDB ID : 1EQ2
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.

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)
Xtriage (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

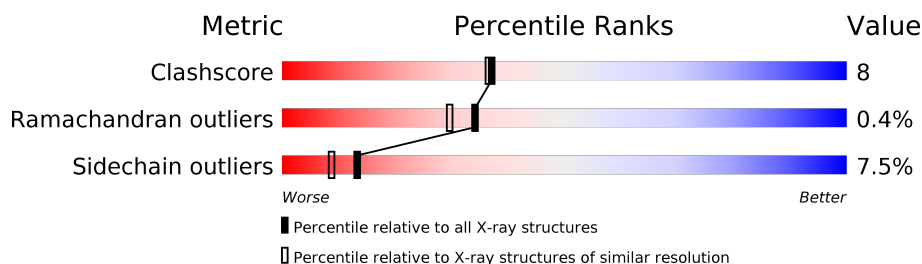
1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	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	 79% 17% . .
1	J	310	 77% 17% . .

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

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

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

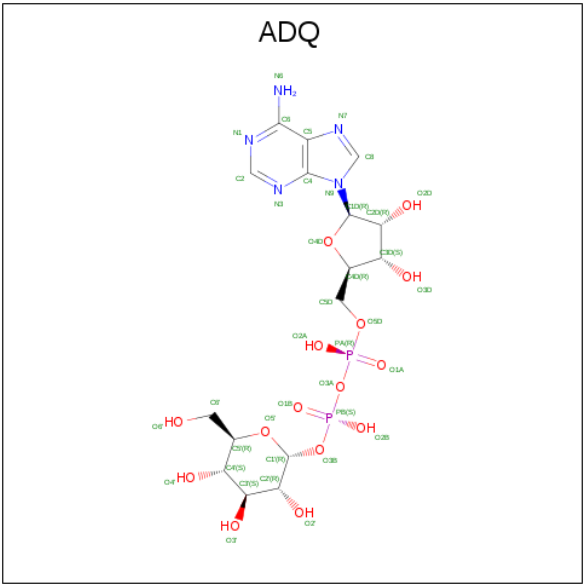
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Chain	Residue	Modelled	Actual	Comment	Reference
J	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910

-
- The chemical structure of Naproxen (NAP) is shown, highlighting its enantiomers and stereochemistry. The structure features a naphthalene ring system with a carboxylic acid group at position 1 and a chiral center at position 6. The chiral center is labeled with (S) and (R) configurations, indicating the enantiomers. The structure also shows the presence of a carboxylic acid group and a carboxylate salt form (NAP⁻).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: C₁₆H₂₅N₅O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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.

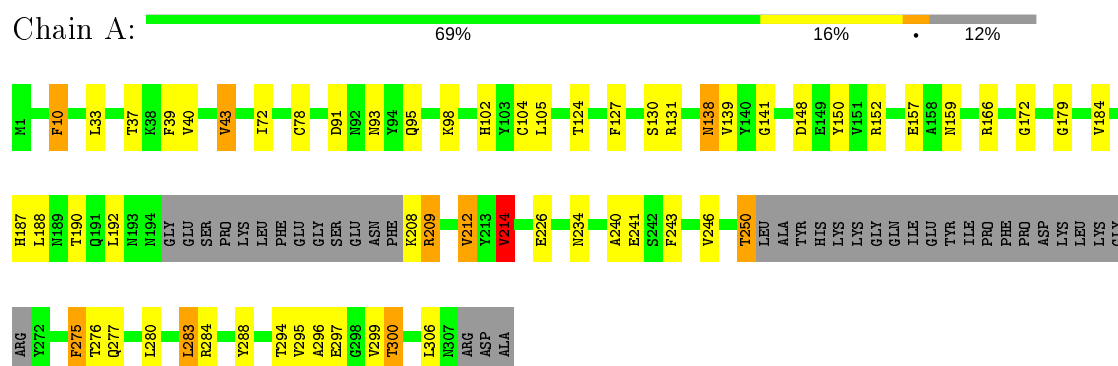
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	119	Total 119	O 119	0	0
4	C	82	Total 82	O 82	0	0
4	D	118	Total 118	O 118	0	0
4	E	105	Total 105	O 105	0	0
4	F	106	Total 106	O 106	0	0
4	G	118	Total 118	O 118	0	0
4	H	114	Total 114	O 114	0	0
4	I	123	Total 123	O 123	0	0
4	J	101	Total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

3 Residue-property plots

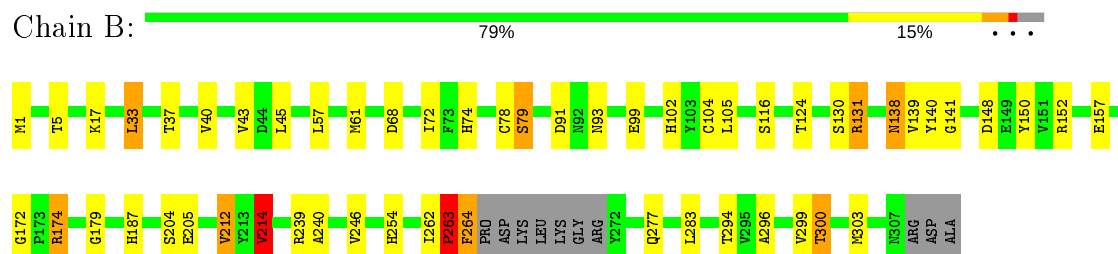
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

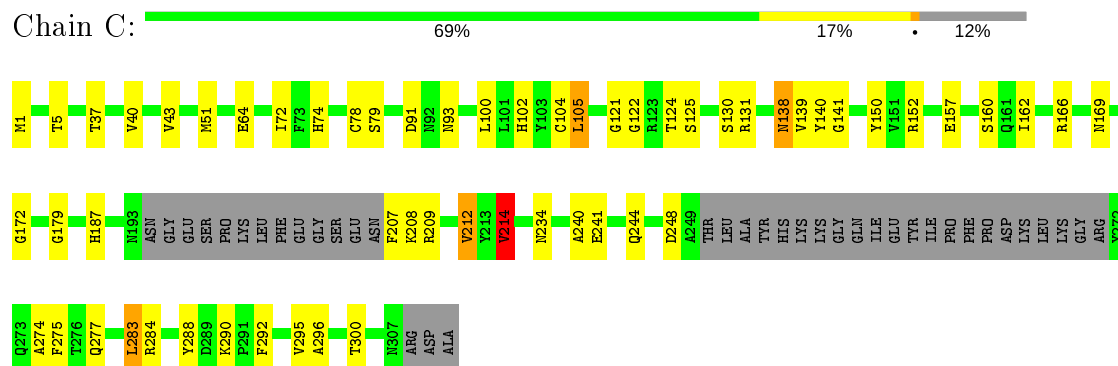
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE




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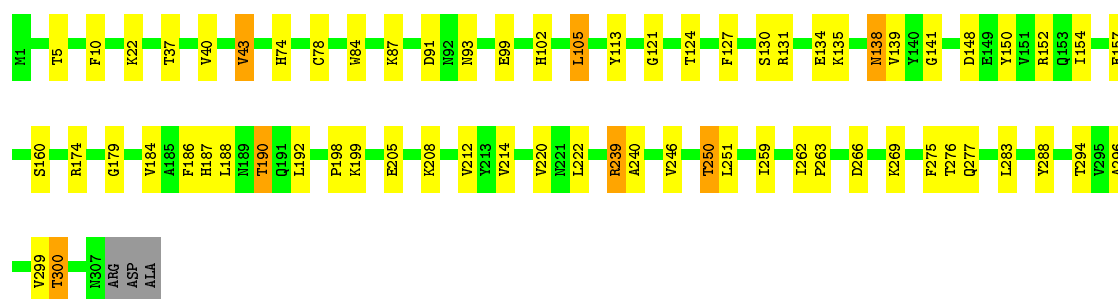


• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE




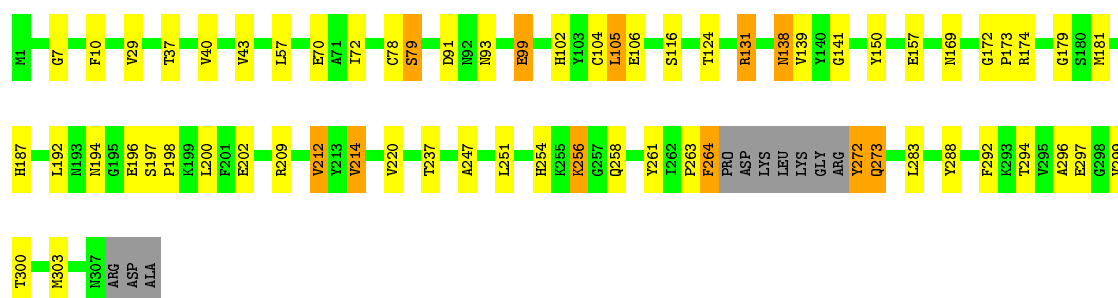
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain D:  77% 19% ..



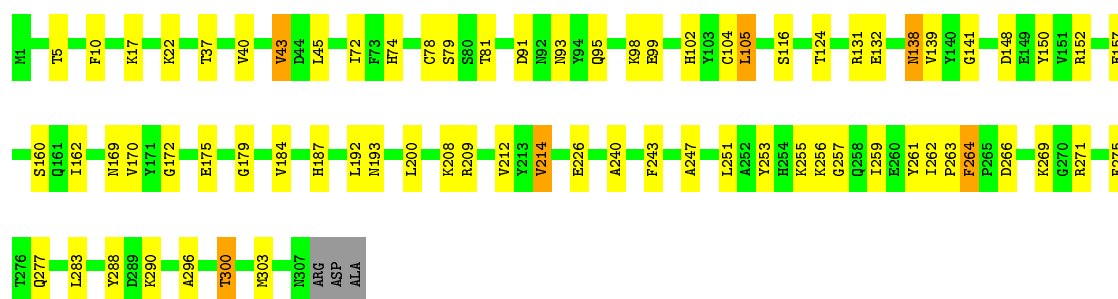
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain E:  76% 17% . .




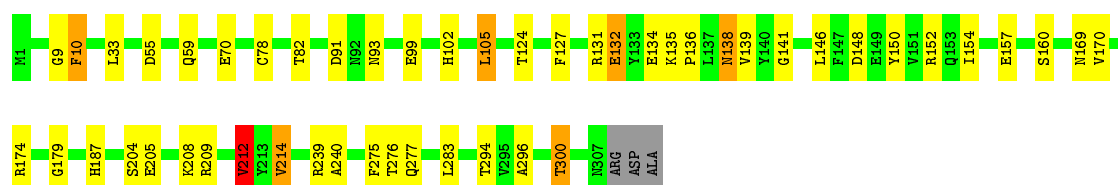
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain F:  75% 22% ..




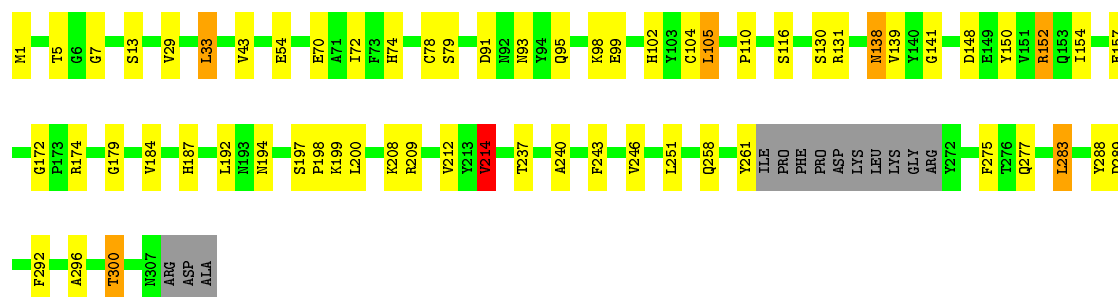
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain G:  83% 14% ..




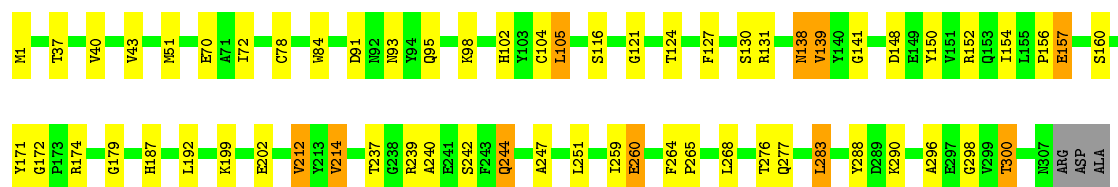
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain H:  75% 18%




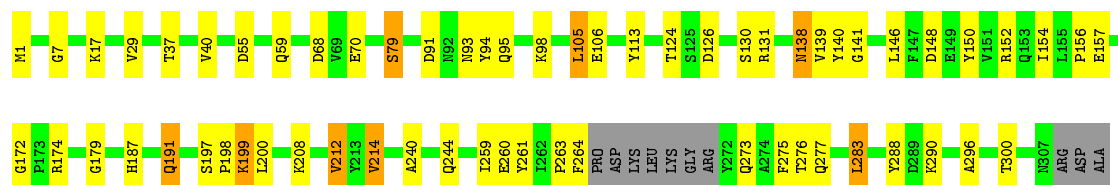
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain I:  79% 17%



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

Chain J:  77% 17%



4 Data and refinement statistics

Xtriage (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	99.46 Å 109.76 Å 181.54 Å 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.	Xtriage
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	0.59	0/2188	0.70	2/2958 (0.1%)
1	B	0.59	0/2434	0.73	4/3290 (0.1%)
1	C	0.63	0/2200	0.74	2/2973 (0.1%)
1	D	0.58	0/2492	0.74	0/3368
1	E	0.60	0/2434	0.74	2/3290 (0.1%)
1	F	0.59	0/2492	0.72	0/3368
1	G	0.59	0/2492	0.73	1/3368 (0.0%)
1	H	0.61	0/2406	0.73	2/3251 (0.1%)
1	I	0.60	0/2492	0.73	1/3368 (0.0%)
1	J	0.59	0/2434	0.73	2/3290 (0.1%)
All	All	0.60	0/24064	0.73	16/32524 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	N-CA-C	-5.76	95.45	111.00
1	J	212	VAL	CB-CA-C	-5.64	100.68	111.40
1	C	214	VAL	CB-CA-C	-5.64	100.68	111.40
1	A	212	VAL	CB-CA-C	-5.63	100.70	111.40
1	I	212	VAL	CB-CA-C	-5.62	100.73	111.40

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	2150	0	2045	36	0
1	B	2386	0	2272	29	0
1	C	2160	0	2056	30	0
1	D	2442	0	2337	39	0
1	E	2386	0	2272	35	0
1	F	2442	0	2337	42	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	2271	34	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	0	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
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	22912	368	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 368 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:H8	3:A:2500:ADQ:H5'1	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:H8	3:C:2502:ADQ:H5'1	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%)	14	8
1	B	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	41	37
1	C	265/310 (86%)	251 (95%)	13 (5%)	1 (0%)	34	30
1	D	304/310 (98%)	292 (96%)	11 (4%)	1 (0%)	41	37
1	E	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	41	37
1	F	304/310 (98%)	290 (95%)	13 (4%)	1 (0%)	41	37
1	G	304/310 (98%)	291 (96%)	11 (4%)	2 (1%)	22	16
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%)	15	9
All	All	2924/3100 (94%)	2798 (96%)	113 (4%)	13 (0%)	34	30

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 ⓘ

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%)	13	8
1	B	248/256 (97%)	226 (91%)	22 (9%)	9	6
1	C	224/256 (88%)	208 (93%)	16 (7%)	14	10
1	D	254/256 (99%)	235 (92%)	19 (8%)	13	9
1	E	248/256 (97%)	230 (93%)	18 (7%)	14	9
1	F	254/256 (99%)	235 (92%)	19 (8%)	13	9
1	G	254/256 (99%)	238 (94%)	16 (6%)	18	13
1	H	245/256 (96%)	227 (93%)	18 (7%)	14	9
1	I	254/256 (99%)	234 (92%)	20 (8%)	12	8
1	J	248/256 (97%)	229 (92%)	19 (8%)	13	8
All	All	2451/2560 (96%)	2267 (92%)	184 (8%)	13	9

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	139	VAL
1	F	157	GLU
1	J	124	THR
1	E	181	MET
1	F	79	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	95	GLN
1	G	138	ASN
1	J	169	ASN
1	F	102	HIS
1	F	254	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	78	1	3,6,7	0.76	0	0,6,8	0.00	-
1	CSO	B	78	1	3,6,7	0.56	0	0,6,8	0.00	-
1	CSO	I	78	1	3,6,7	0.71	0	0,6,8	0.00	-
1	CSO	E	78	1	3,6,7	0.83	0	0,6,8	0.00	-
1	CSO	A	78	1	3,6,7	0.60	0	0,6,8	0.00	-
1	CSO	G	78	1	3,6,7	0.77	0	0,6,8	0.00	-
1	CSO	C	78	1	3,6,7	0.77	0	0,6,8	0.00	-
1	CSO	J	78	1	3,6,7	0.69	0	0,6,8	0.00	-
1	CSO	H	78	1	3,6,7	0.68	0	0,6,8	0.00	-
1	CSO	F	78	1	3,6,7	0.62	0	0,6,8	0.00	-

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	D	78	1	-	1/1/5/7	-
1	CSO	B	78	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	I	78	1	-	1/1/5/7	-
1	CSO	E	78	1	-	0/1/5/7	-
1	CSO	A	78	1	-	0/1/5/7	-
1	CSO	G	78	1	-	1/1/5/7	-
1	CSO	C	78	1	-	0/1/5/7	-
1	CSO	J	78	1	-	1/1/5/7	-
1	CSO	H	78	1	-	1/1/5/7	-
1	CSO	F	78	1	-	1/1/5/7	-

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	I	78	CSO	N-CA-CB-SG
1	G	78	CSO	N-CA-CB-SG
1	J	78	CSO	N-CA-CB-SG
1	H	78	CSO	N-CA-CB-SG

There are no ring outliers.

9 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	F	2405	-	45,52,52	2.28	11 (24%)	56,80,80	2.02	12 (21%)
2	NAP	I	2408	-	45,52,52	2.24	10 (22%)	56,80,80	1.96	11 (19%)
3	ADQ	C	2502	-	24,29,41	1.04	2 (8%)	29,45,63	1.44	2 (6%)
3	ADQ	H	2507	-	24,29,41	1.30	3 (12%)	29,45,63	1.45	3 (10%)
2	NAP	J	2409	-	45,52,52	2.38	11 (24%)	56,80,80	1.99	9 (16%)
3	ADQ	I	2508	-	24,29,41	0.98	2 (8%)	29,45,63	1.49	4 (13%)
3	ADQ	J	2509	-	24,29,41	1.17	3 (12%)	29,45,63	1.52	4 (13%)
3	ADQ	B	2501	-	35,41,41	1.38	4 (11%)	45,63,63	1.71	9 (20%)
3	ADQ	D	2503	-	35,41,41	1.50	4 (11%)	45,63,63	1.99	9 (20%)
2	NAP	G	2406	-	45,52,52	2.25	12 (26%)	56,80,80	1.93	13 (23%)
3	ADQ	F	2505	-	35,41,41	1.48	6 (17%)	45,63,63	1.72	8 (17%)
2	NAP	E	2404	-	45,52,52	2.27	11 (24%)	56,80,80	1.99	14 (25%)
3	ADQ	G	2506	-	24,29,41	1.32	2 (8%)	29,45,63	1.41	3 (10%)
3	ADQ	E	2504	-	24,29,41	1.12	3 (12%)	29,45,63	1.52	5 (17%)
3	ADQ	A	2500	-	24,29,41	1.24	4 (16%)	29,45,63	1.48	4 (13%)
2	NAP	B	2401	-	45,52,52	2.29	10 (22%)	56,80,80	2.01	10 (17%)
2	NAP	D	2403	-	45,52,52	2.27	12 (26%)	56,80,80	1.88	10 (17%)
2	NAP	A	2400	-	45,52,52	2.37	12 (26%)	56,80,80	1.96	11 (19%)
2	NAP	H	2407	-	45,52,52	2.27	10 (22%)	56,80,80	1.99	10 (17%)
2	NAP	C	2402	-	45,52,52	2.19	9 (20%)	56,80,80	1.99	10 (17%)

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	ADQ	G	2506	-	-	1/12/32/59	0/3/3/4
2	NAP	F	2405	-	-	1/31/67/67	0/5/5/5
2	NAP	I	2408	-	-	6/31/67/67	0/5/5/5
3	ADQ	C	2502	-	-	5/12/32/59	0/3/3/4
3	ADQ	H	2507	-	-	5/12/32/59	0/3/3/4
2	NAP	J	2409	-	-	4/31/67/67	0/5/5/5
3	ADQ	I	2508	-	-	4/12/32/59	0/3/3/4
3	ADQ	J	2509	-	-	4/12/32/59	0/3/3/4
3	ADQ	B	2501	-	-	6/19/59/59	0/4/4/4
3	ADQ	D	2503	-	-	8/19/59/59	0/4/4/4
3	ADQ	F	2505	-	-	6/19/59/59	0/4/4/4
2	NAP	E	2404	-	-	7/31/67/67	0/5/5/5
2	NAP	C	2402	-	-	4/31/67/67	0/5/5/5
3	ADQ	E	2504	-	-	2/12/32/59	0/3/3/4
3	ADQ	A	2500	-	-	3/12/32/59	0/3/3/4
2	NAP	B	2401	-	-	3/31/67/67	0/5/5/5
2	NAP	D	2403	-	-	2/31/67/67	0/5/5/5
2	NAP	A	2400	-	-	3/31/67/67	0/5/5/5
2	NAP	H	2407	-	-	5/31/67/67	0/5/5/5
2	NAP	G	2406	-	1/1/12/12	10/31/67/67	0/5/5/5

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2401	NAP	P2B-O2B	8.77	1.75	1.59
2	J	2409	NAP	P2B-O2B	8.71	1.75	1.59
2	H	2407	NAP	P2B-O2B	8.52	1.75	1.59
2	E	2404	NAP	P2B-O2B	8.20	1.74	1.59
2	I	2408	NAP	P2B-O2B	8.03	1.74	1.59

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	C5N-C4N-C3N	-7.57	111.39	120.34
2	J	2409	NAP	C5N-C4N-C3N	-7.47	111.50	120.34
2	E	2404	NAP	C5N-C4N-C3N	-7.43	111.55	120.34
2	B	2401	NAP	C5N-C4N-C3N	-7.42	111.56	120.34
3	D	2503	ADQ	O3B-C1'-C2'	7.42	121.97	108.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	2406	NAP	C4B

5 of 89 torsion outliers are listed below:

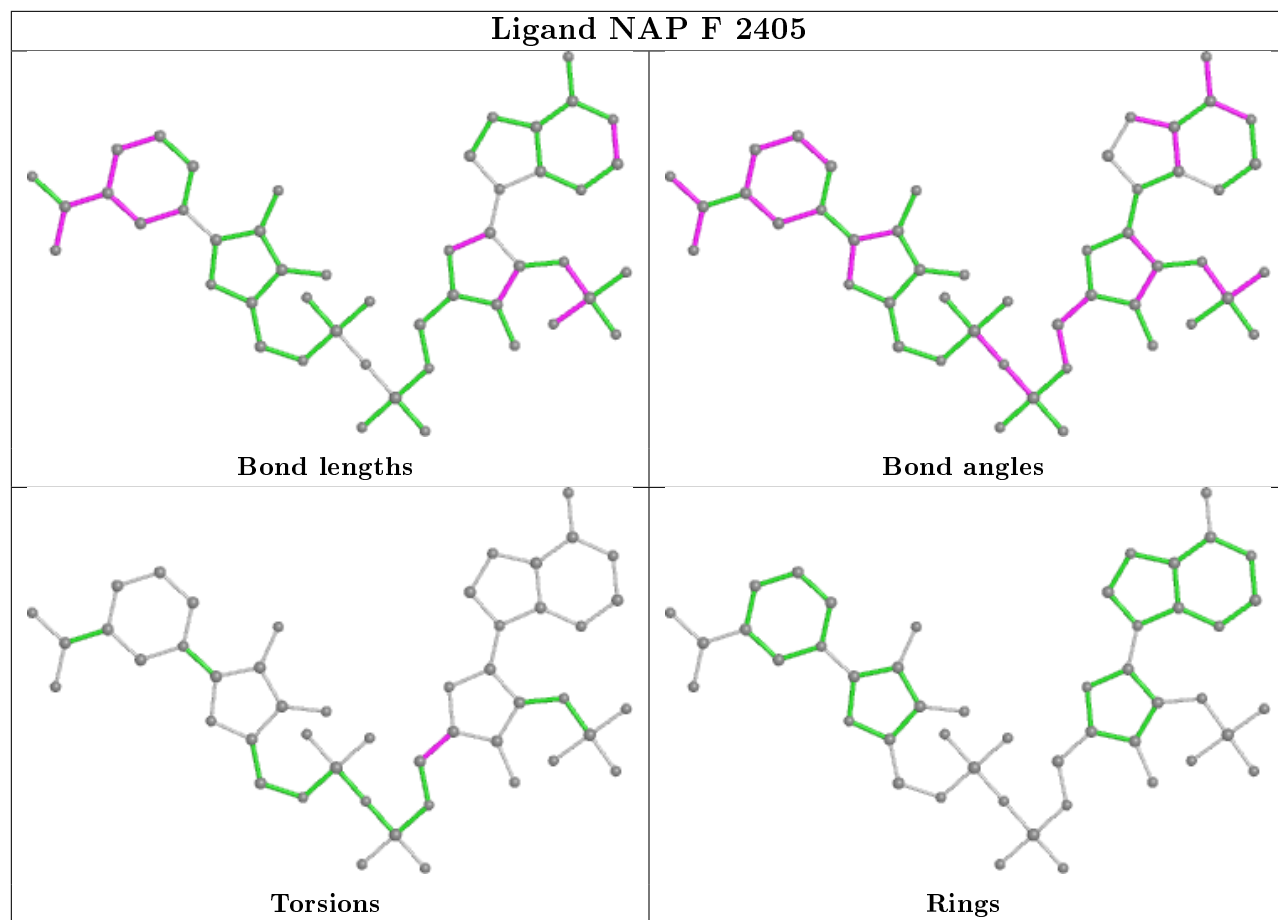
Mol	Chain	Res	Type	Atoms
3	J	2509	ADQ	C5D-O5D-PA-O2A
3	J	2509	ADQ	C5D-O5D-PA-O3A
3	C	2502	ADQ	C5D-O5D-PA-O1A
3	C	2502	ADQ	C5D-O5D-PA-O2A
3	C	2502	ADQ	C5D-O5D-PA-O3A

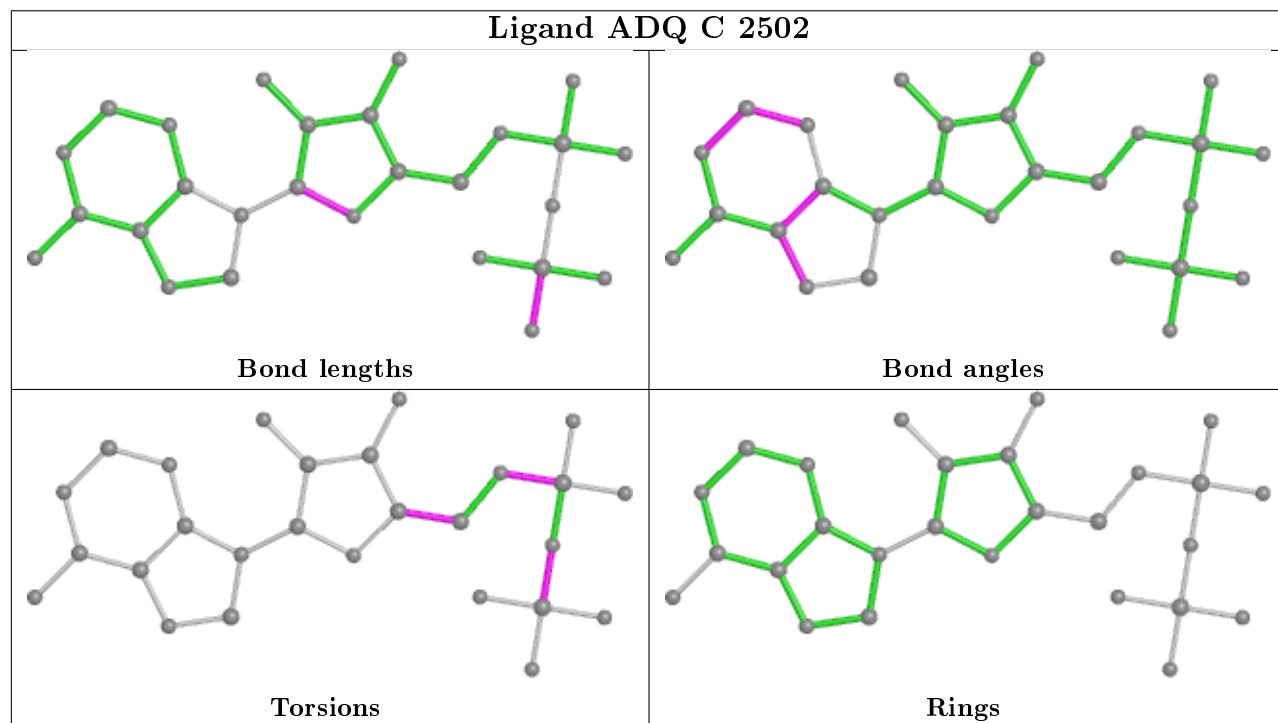
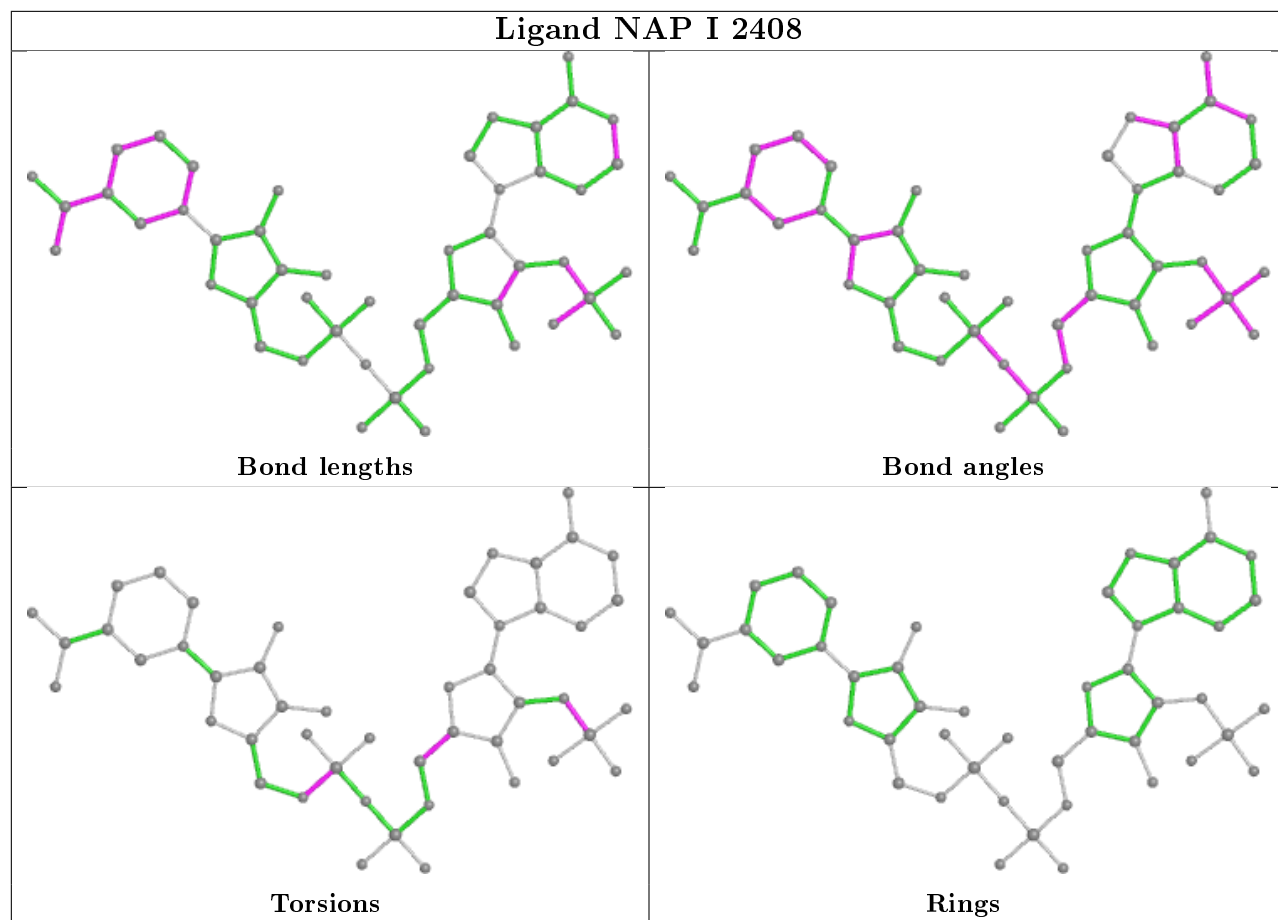
There are no ring outliers.

14 monomers are involved in 24 short contacts:

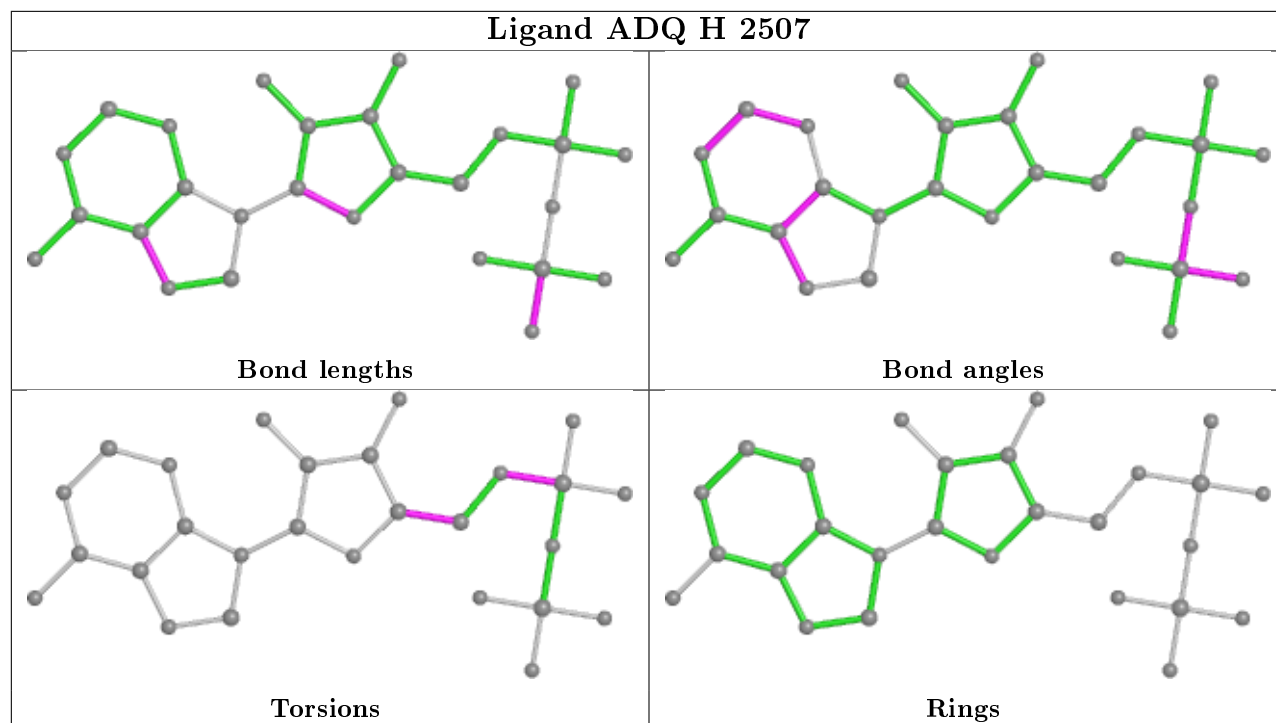
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2405	NAP	1	0
2	I	2408	NAP	1	0
3	C	2502	ADQ	2	0
3	H	2507	ADQ	1	0
3	I	2508	ADQ	3	0
3	B	2501	ADQ	2	0
2	G	2406	NAP	1	0
3	F	2505	ADQ	3	0
2	E	2404	NAP	1	0
3	E	2504	ADQ	3	0
3	A	2500	ADQ	3	0
2	B	2401	NAP	1	0
2	A	2400	NAP	1	0
2	H	2407	NAP	1	0

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.

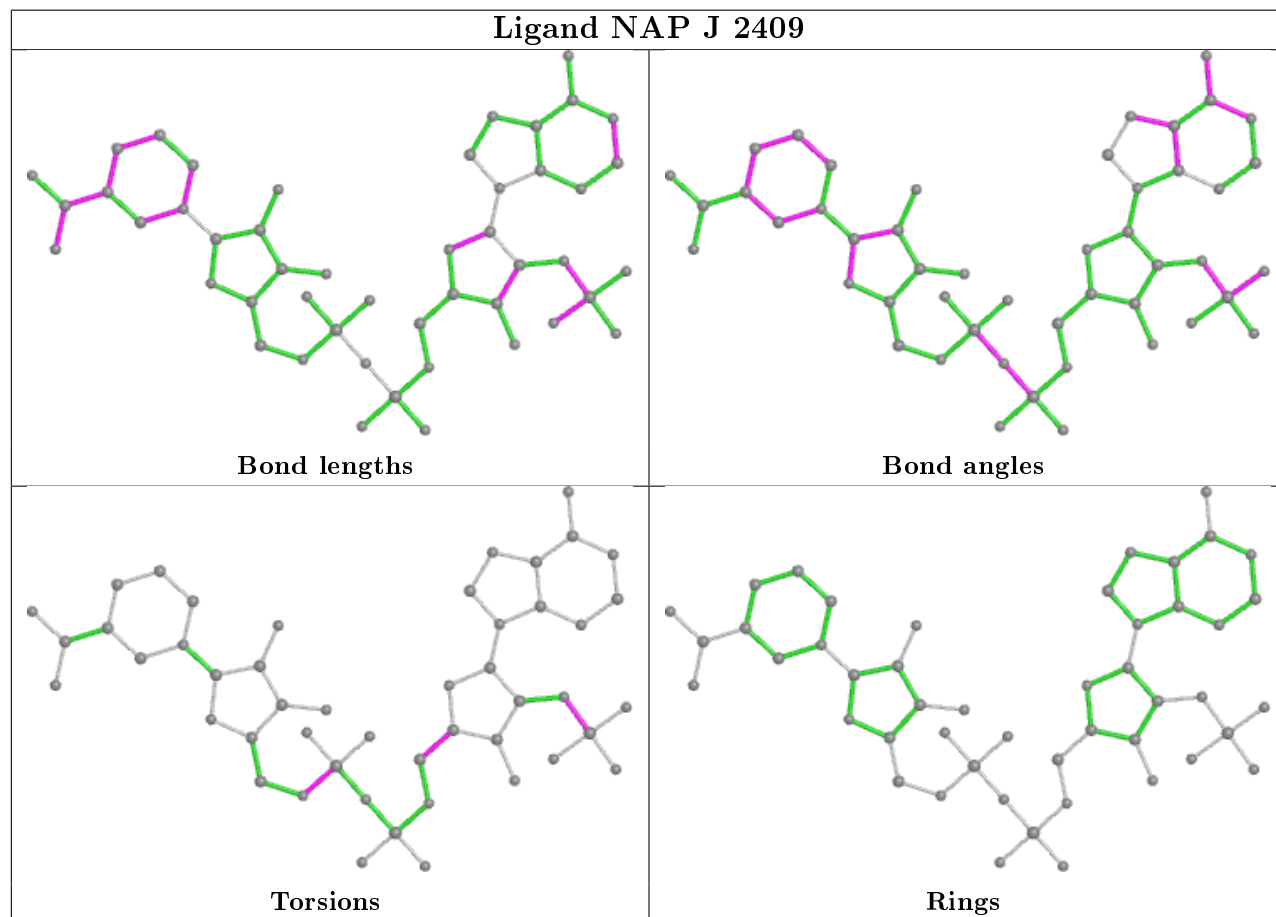


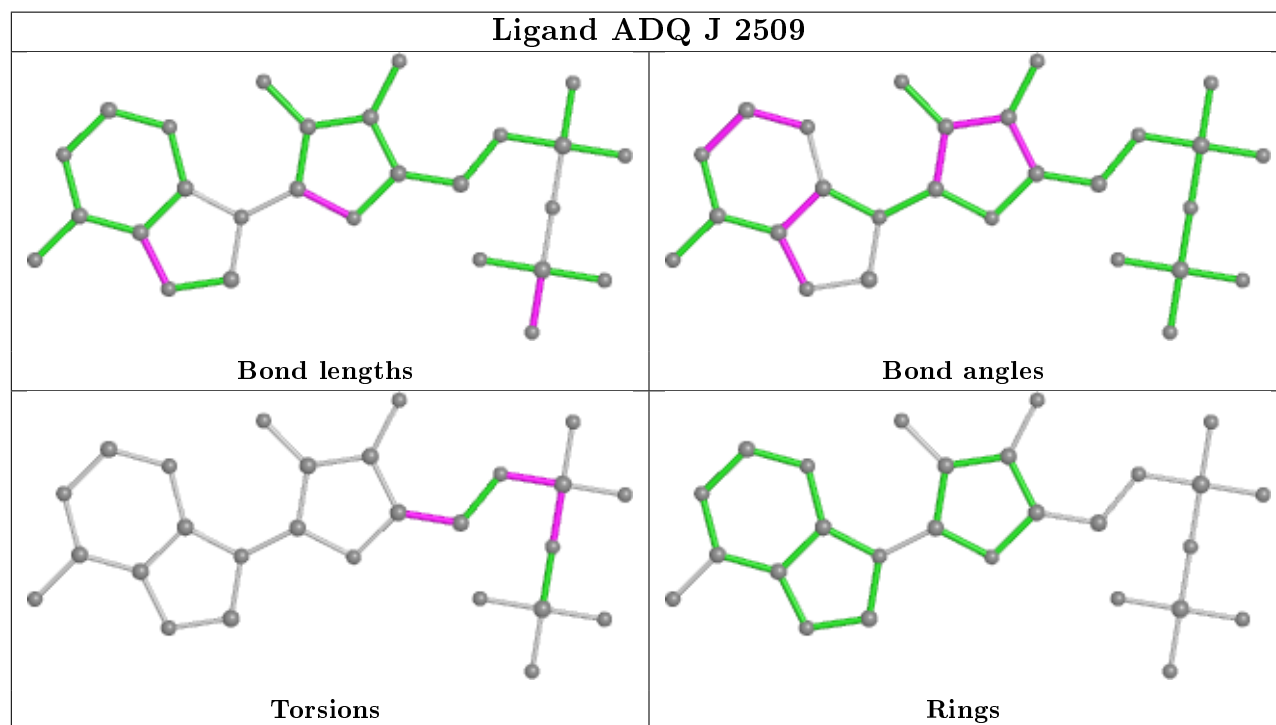
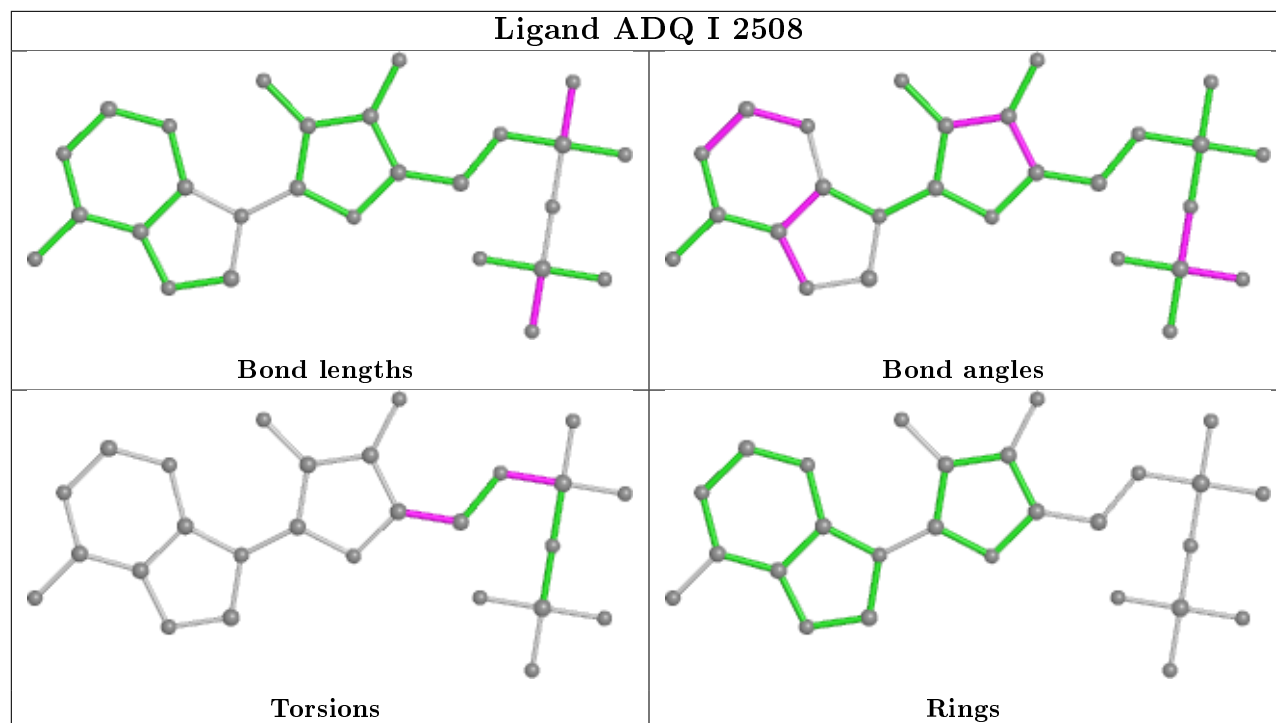


Ligand ADQ H 2507

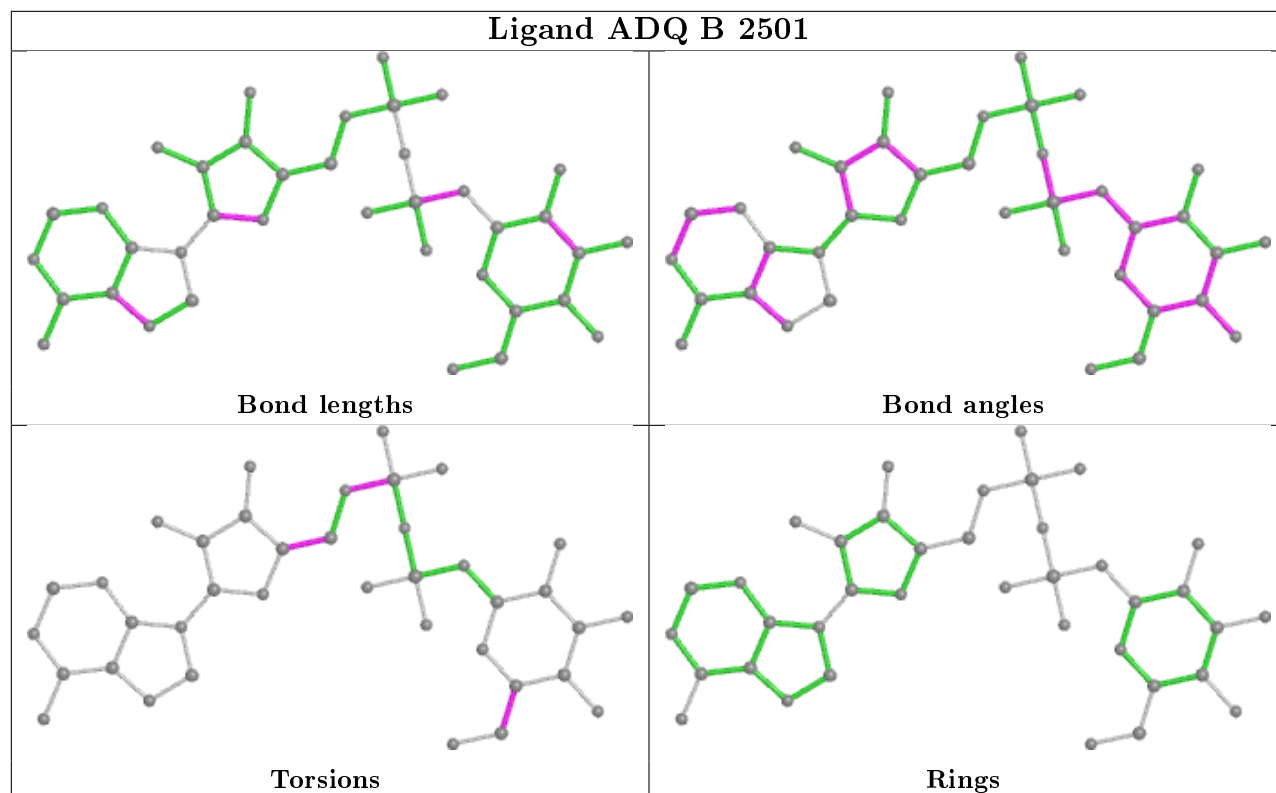


Ligand NAP J 2409

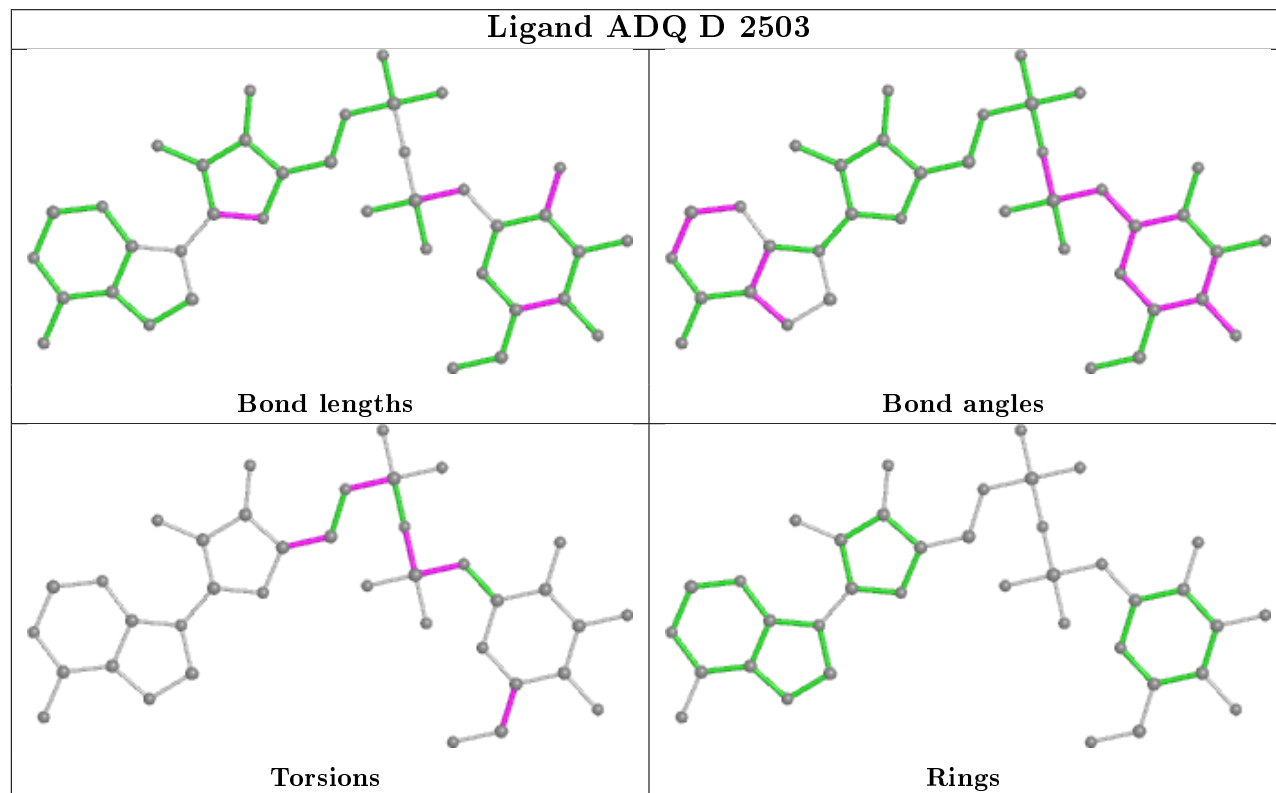




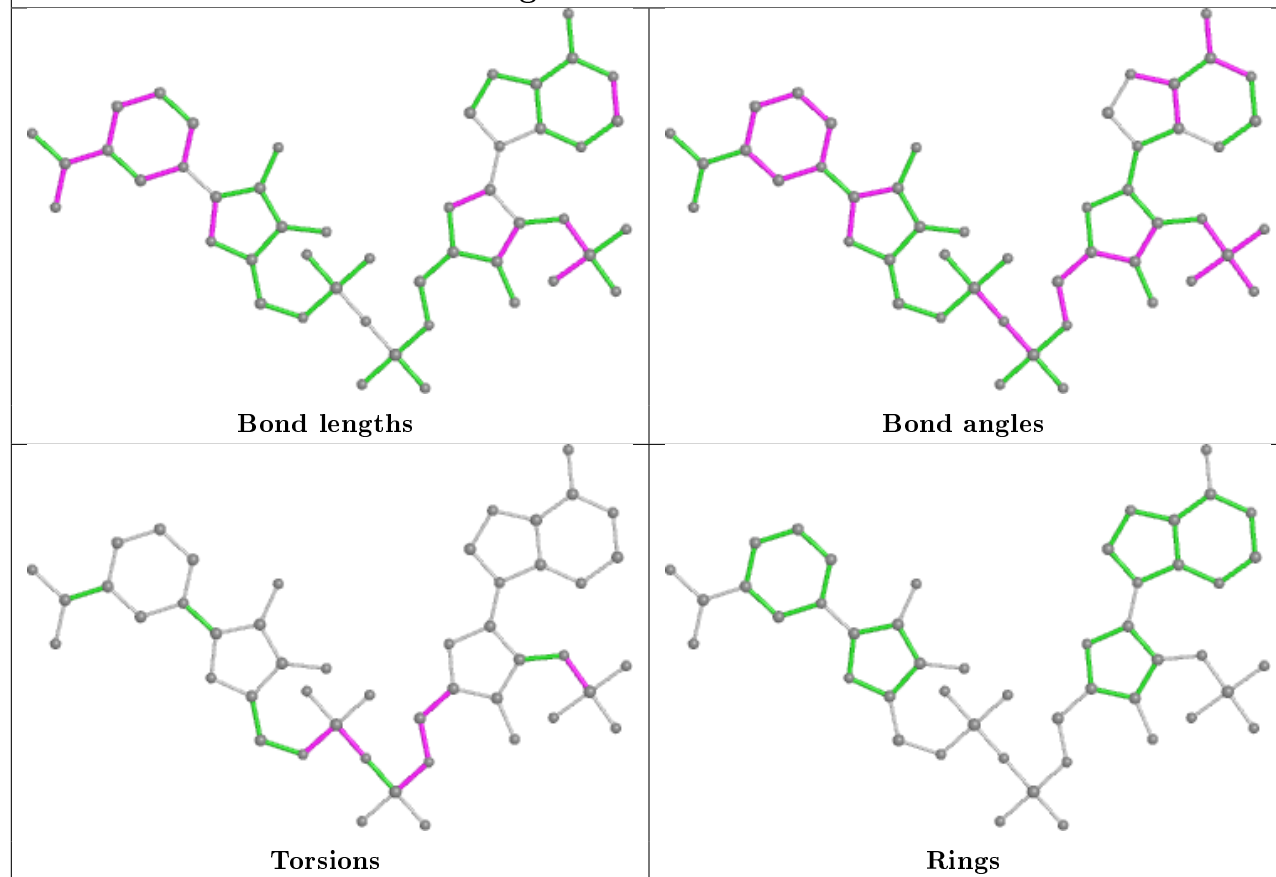
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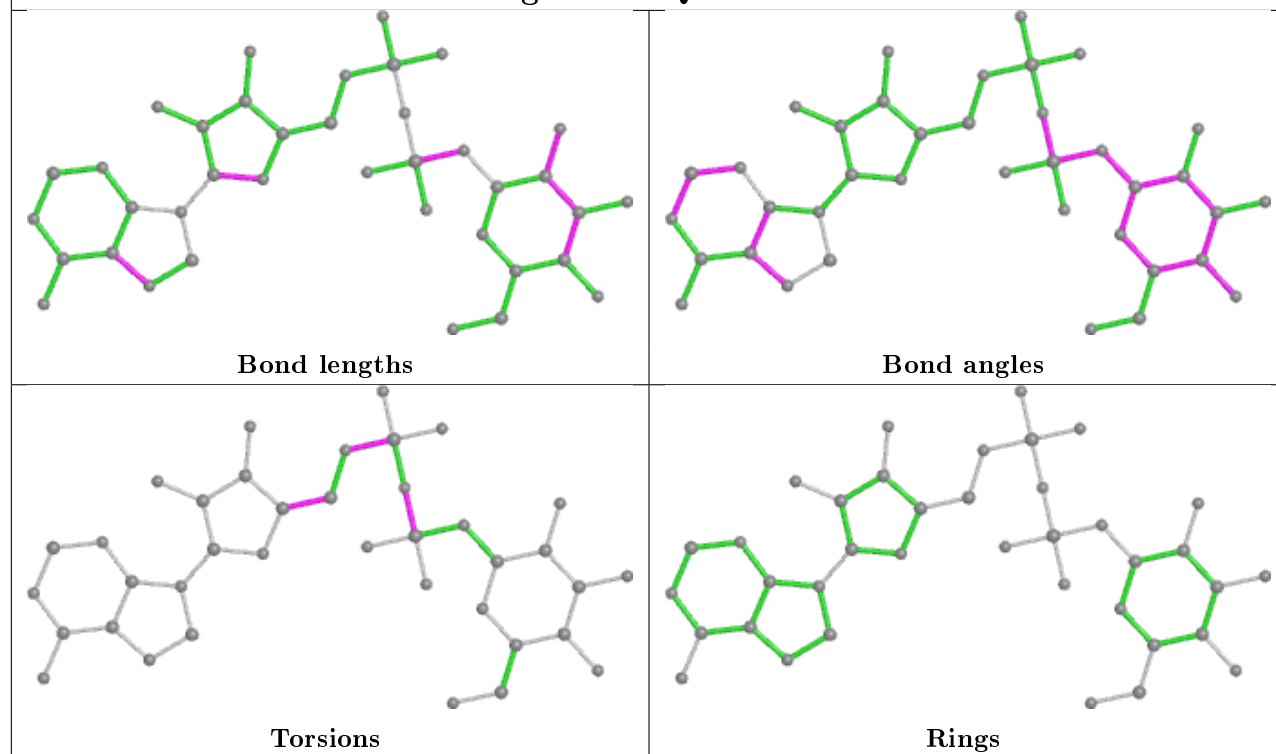
Ligand ADQ D 2503



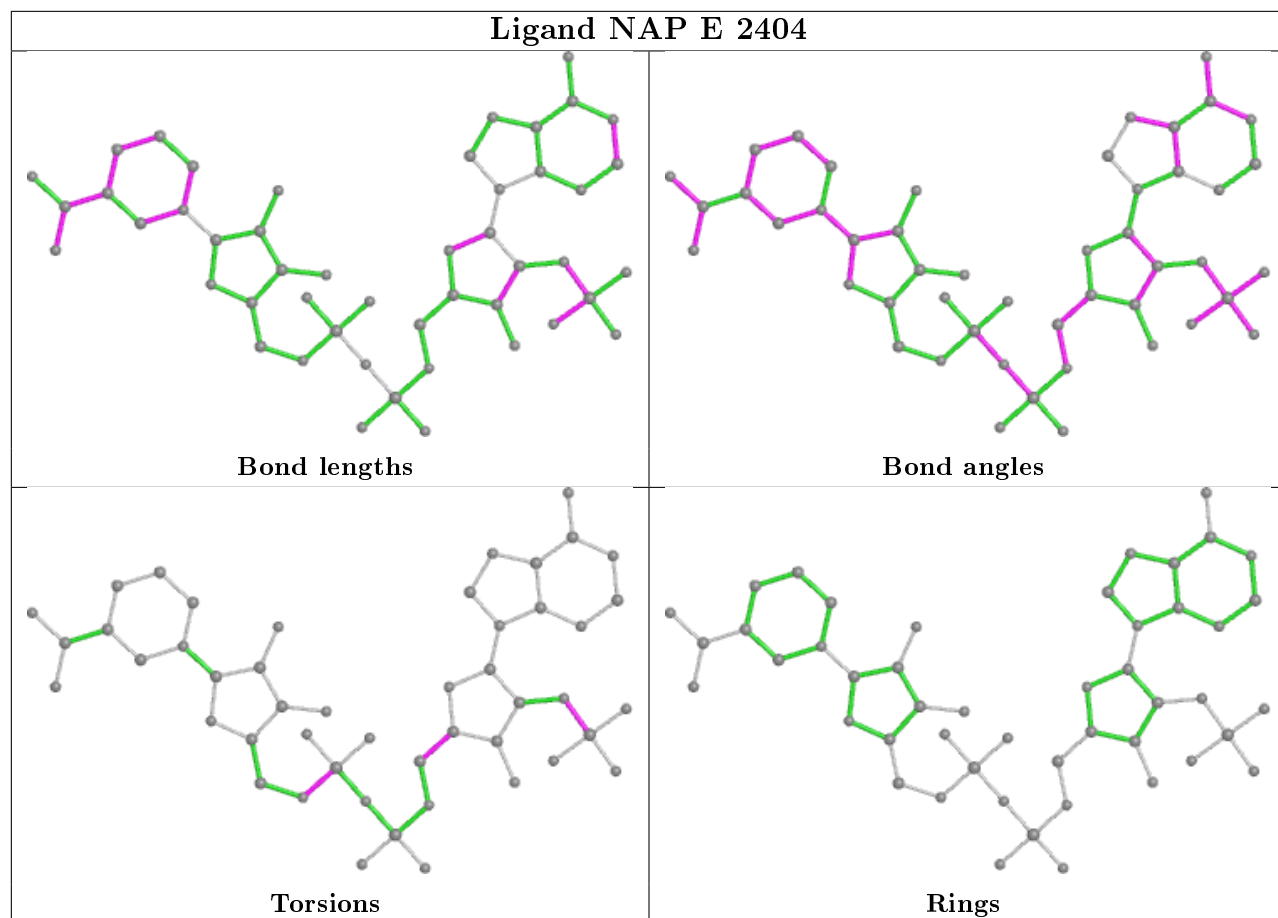
Ligand NAP G 2406



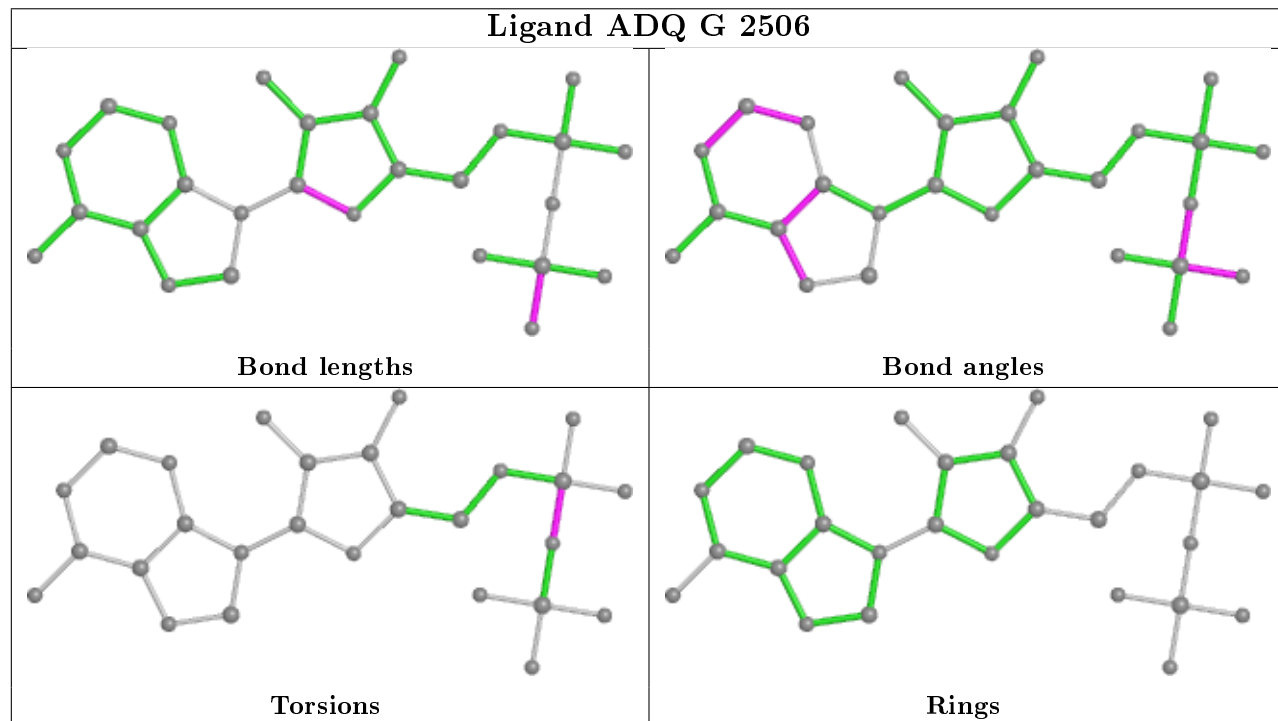
Ligand ADQ F 2505



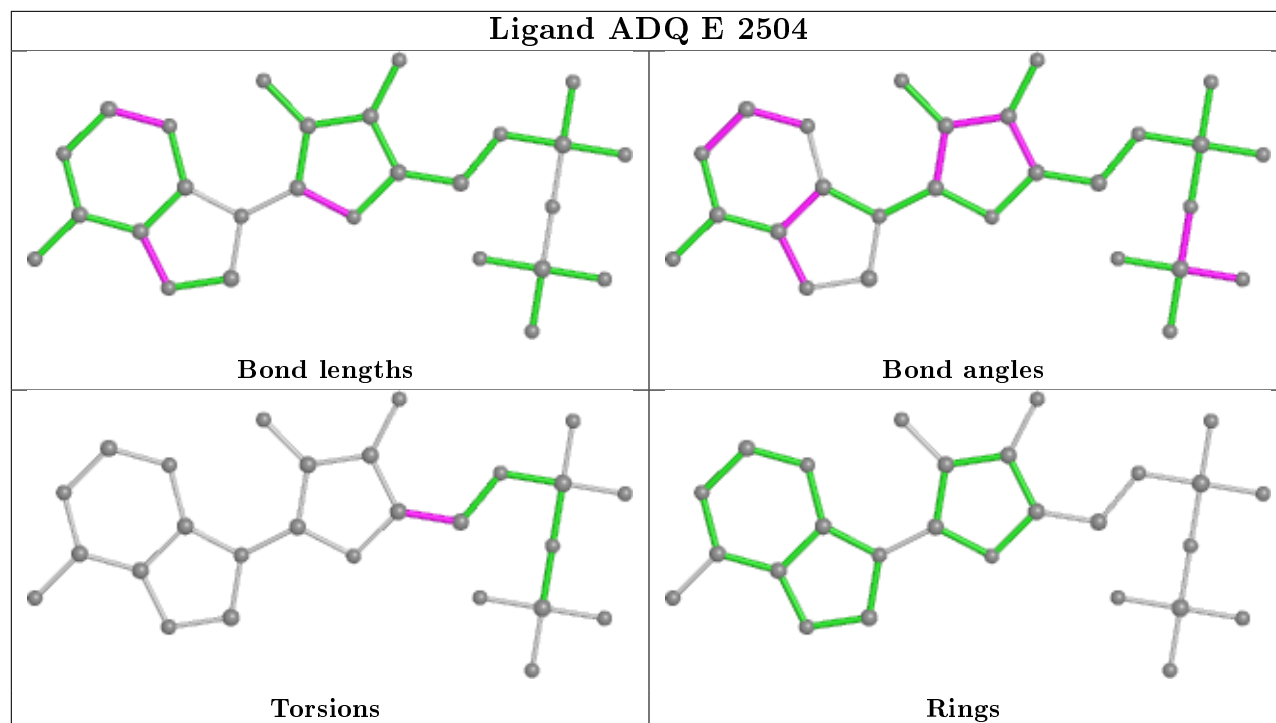
Ligand NAP E 2404



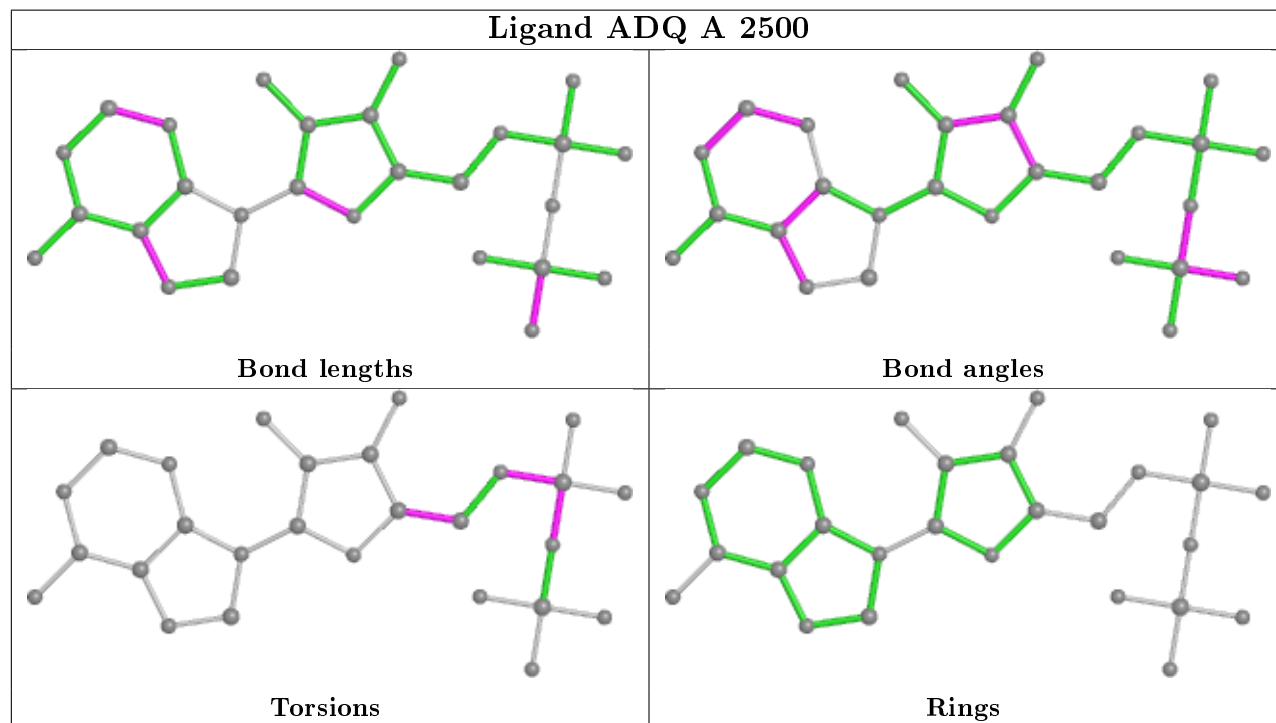
Ligand ADQ G 2506

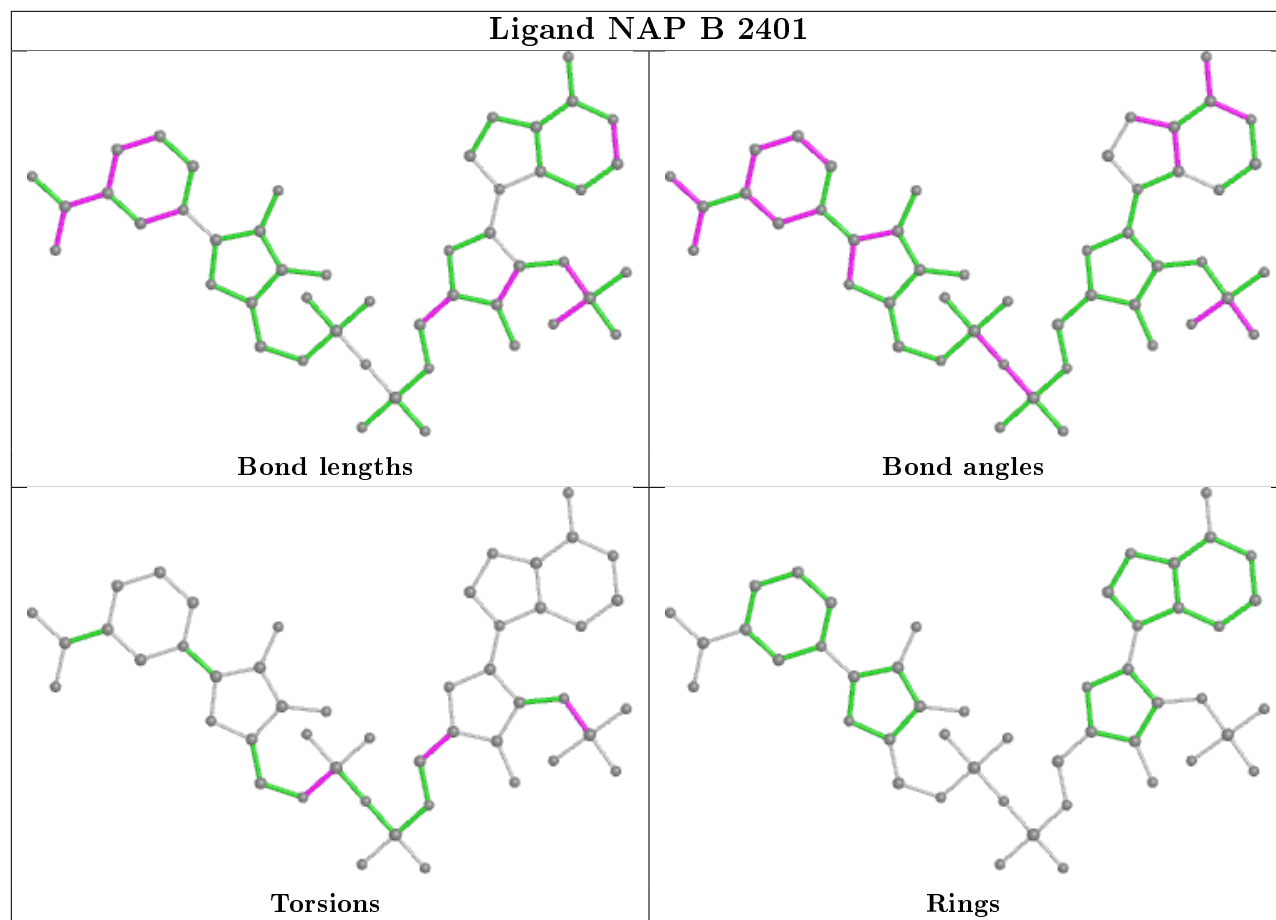


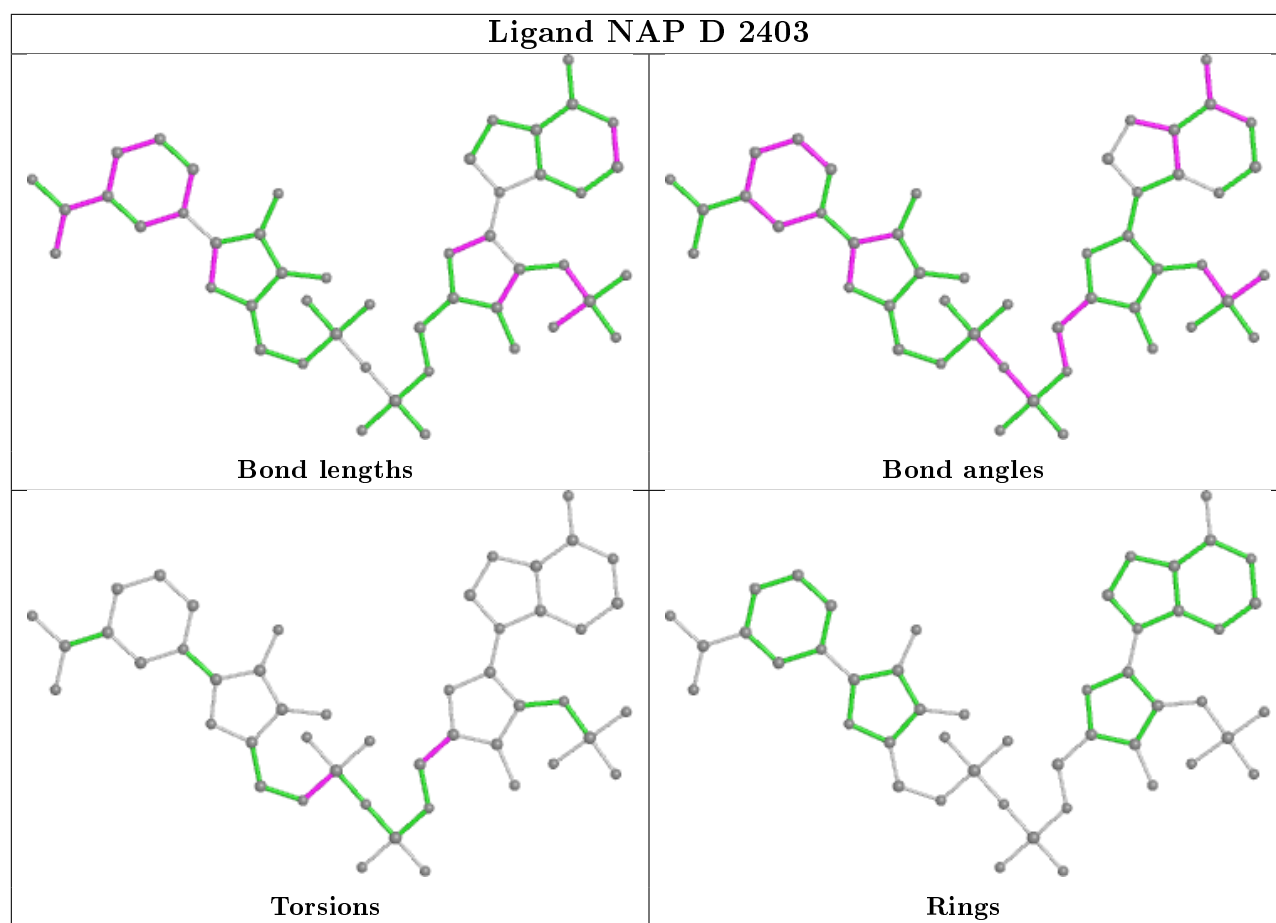
Ligand ADQ E 2504

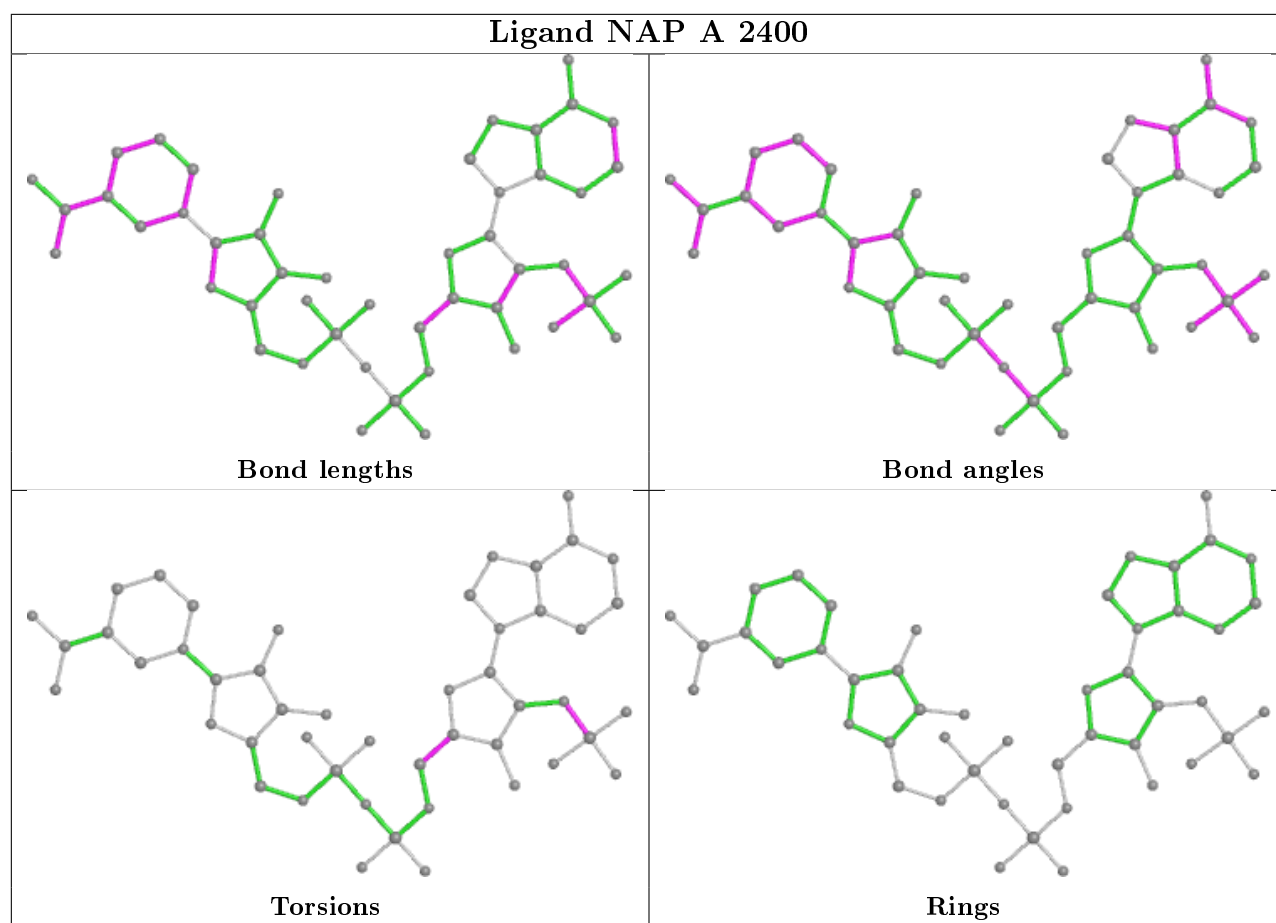


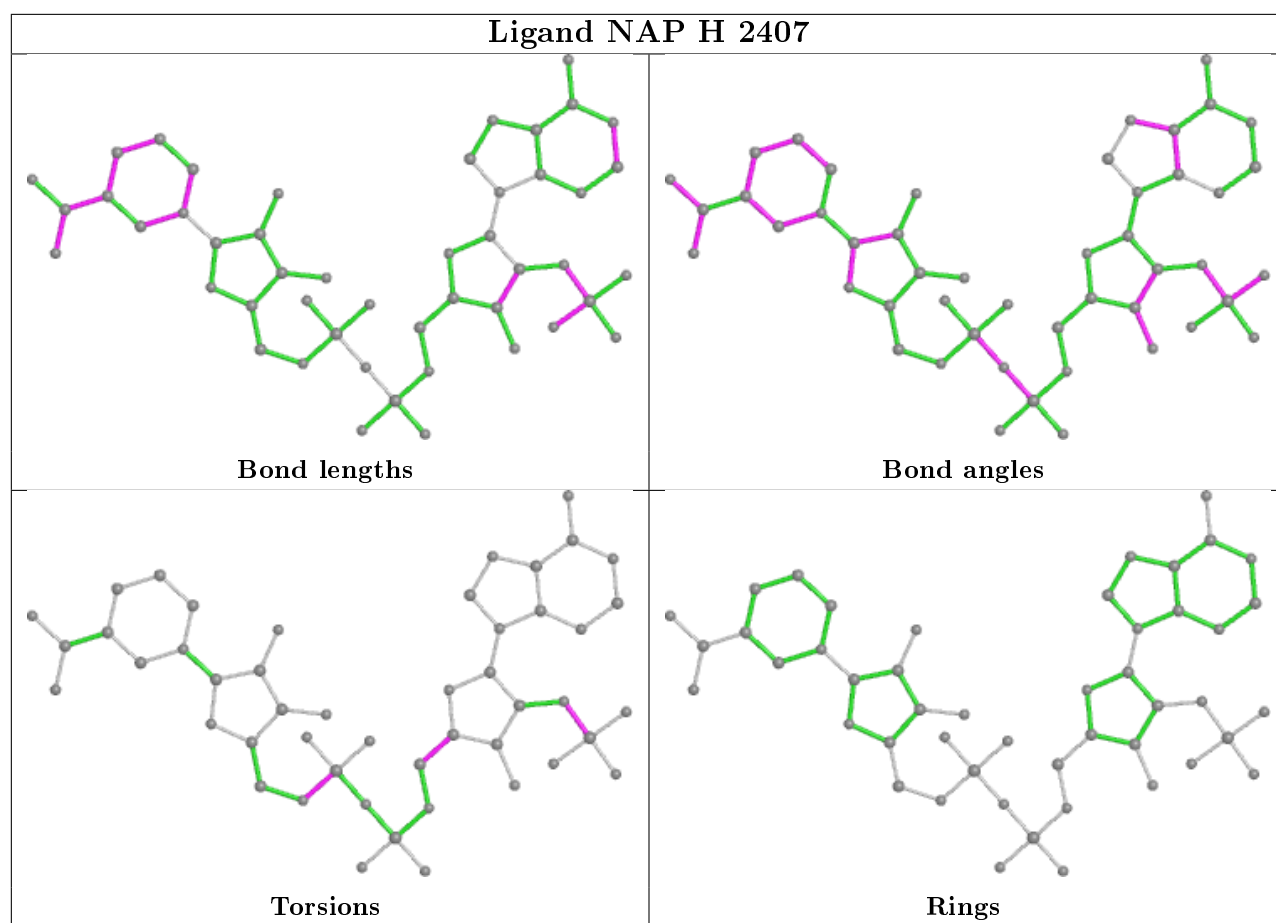
Ligand ADQ A 2500

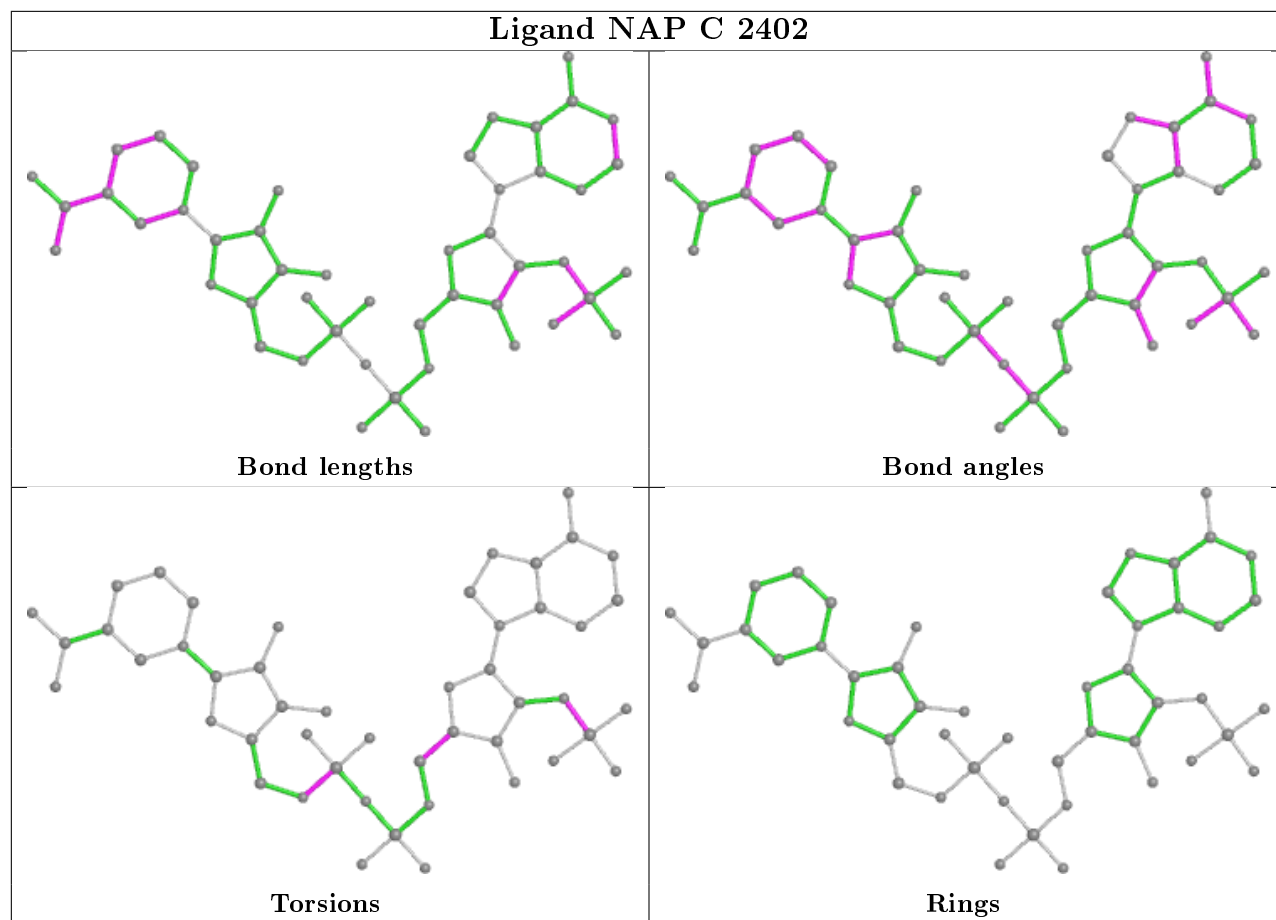












5.7 Other polymers [i](#)

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.