



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 03:59 PM EDT

PDB ID : 1XU7
Title : Crystal Structure of the Interface Open Conformation of Tetrameric 11b-HSD1
Authors : Hosfield, D.J.; Wu, Y.; Skene, R.J.; Hilger, M.; Jennings, A.; Snell, G.P.;
Aertgeerts, K.
Deposited on : 2004-10-25
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

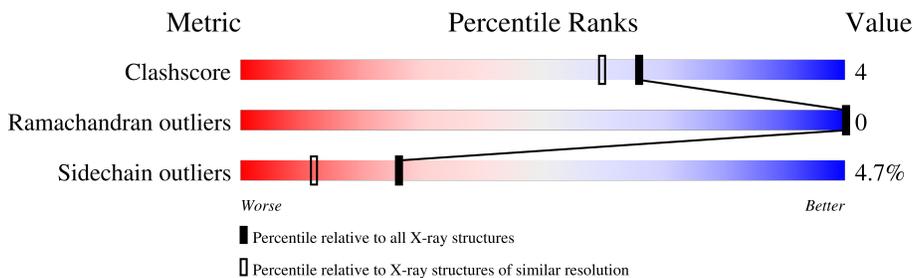
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 ≥ 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	286	
1	B	286	
1	C	286	
1	D	286	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8921 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 Corticosteroid 11-beta-dehydrogenase, isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2014	1284	341	374	15	0	10	0
1	B	262	2008	1281	340	372	15	0	10	0
1	C	262	2008	1281	340	372	15	0	9	0
1	D	261	2001	1277	339	370	15	0	10	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP P28845
A	8	LYS	-	cloning artifact	UNP P28845
A	9	HIS	-	cloning artifact	UNP P28845
A	10	GLN	-	cloning artifact	UNP P28845
A	11	HIS	-	cloning artifact	UNP P28845
A	12	GLN	-	cloning artifact	UNP P28845
A	13	HIS	-	cloning artifact	UNP P28845
A	14	GLN	-	cloning artifact	UNP P28845
A	15	HIS	-	cloning artifact	UNP P28845
A	16	GLN	-	cloning artifact	UNP P28845
A	17	HIS	-	cloning artifact	UNP P28845
A	18	GLN	-	cloning artifact	UNP P28845
A	19	HIS	-	cloning artifact	UNP P28845
A	20	GLN	-	cloning artifact	UNP P28845
A	21	GLN	-	cloning artifact	UNP P28845
A	22	PRO	-	cloning artifact	UNP P28845
A	23	LEU	-	cloning artifact	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	initiating methionine	UNP P28845
B	8	LYS	-	cloning artifact	UNP P28845
B	9	HIS	-	cloning artifact	UNP P28845

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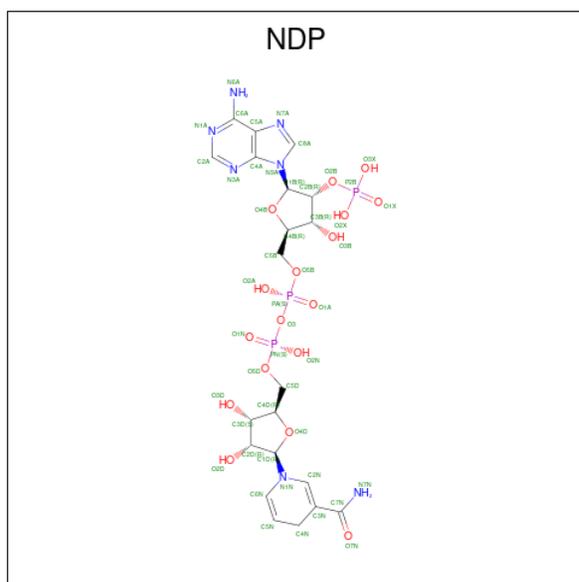
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning artifact	UNP P28845
B	17	HIS	-	cloning artifact	UNP P28845
B	18	GLN	-	cloning artifact	UNP P28845
B	19	HIS	-	cloning artifact	UNP P28845
B	20	GLN	-	cloning artifact	UNP P28845
B	21	GLN	-	cloning artifact	UNP P28845
B	22	PRO	-	cloning artifact	UNP P28845
B	23	LEU	-	cloning artifact	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	initiating methionine	UNP P28845
C	8	LYS	-	cloning artifact	UNP P28845
C	9	HIS	-	cloning artifact	UNP P28845
C	10	GLN	-	cloning artifact	UNP P28845
C	11	HIS	-	cloning artifact	UNP P28845
C	12	GLN	-	cloning artifact	UNP P28845
C	13	HIS	-	cloning artifact	UNP P28845
C	14	GLN	-	cloning artifact	UNP P28845
C	15	HIS	-	cloning artifact	UNP P28845
C	16	GLN	-	cloning artifact	UNP P28845
C	17	HIS	-	cloning artifact	UNP P28845
C	18	GLN	-	cloning artifact	UNP P28845
C	19	HIS	-	cloning artifact	UNP P28845
C	20	GLN	-	cloning artifact	UNP P28845
C	21	GLN	-	cloning artifact	UNP P28845
C	22	PRO	-	cloning artifact	UNP P28845
C	23	LEU	-	cloning artifact	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	initiating methionine	UNP P28845
D	8	LYS	-	cloning artifact	UNP P28845
D	9	HIS	-	cloning artifact	UNP P28845
D	10	GLN	-	cloning artifact	UNP P28845
D	11	HIS	-	cloning artifact	UNP P28845
D	12	GLN	-	cloning artifact	UNP P28845
D	13	HIS	-	cloning artifact	UNP P28845
D	14	GLN	-	cloning artifact	UNP P28845
D	15	HIS	-	cloning artifact	UNP P28845

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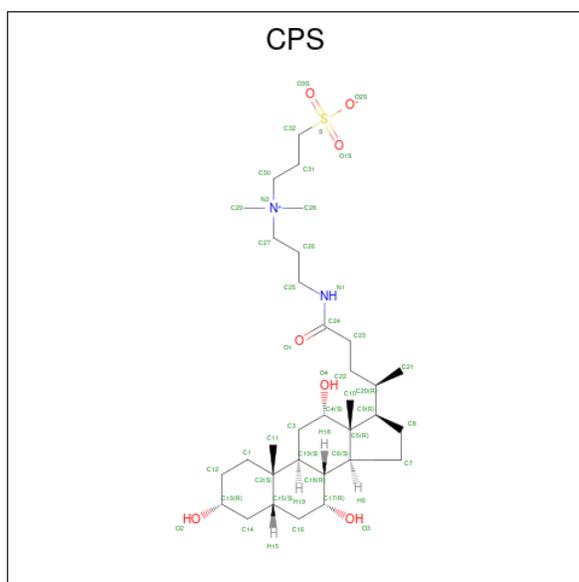
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning artifact	UNP P28845
D	23	LEU	-	cloning artifact	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	42	32	2	7	1	0	0
3	A	1	22	19	3			0	0
3	B	1	42	32	2	7	1	0	0
3	C	1	42	32	2	7	1	0	0
3	C	1	22	19	3			0	0
3	D	1	42	32	2	7	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	113	Total	O	0	0
			113	113		
4	C	140	Total	O	0	0
			140	140		
4	D	104	Total	O	0	0
			104	104		

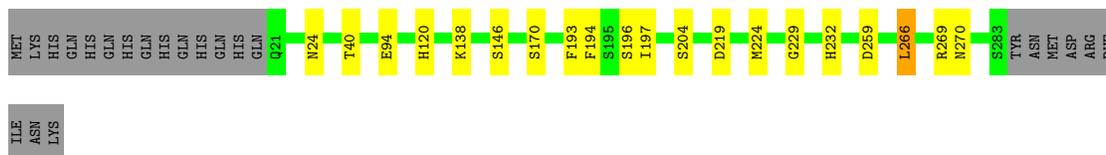
3 Residue-property plots [i](#)

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: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain A: 



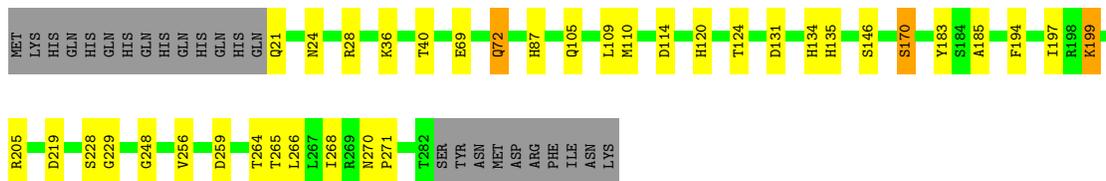
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain B: 



- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain C: 



- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain D: 



Y258	D259	L262	W263	T264	I288	R269	N270	K274	I275	L276	S281	THR	SER	TYR	ASN	MET	ASP	ARG	PHE	ILE	ASN	LYS
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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	56.43Å 159.62Å 73.54Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.1 (20.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.197 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CPS, NDP

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	0.31	0/2048	0.56	2/2766 (0.1%)
1	B	0.31	0/2042	0.58	3/2758 (0.1%)
1	C	0.31	0/2042	0.59	4/2758 (0.1%)
1	D	0.29	0/2035	0.57	3/2748 (0.1%)
All	All	0.31	0/8167	0.57	12/11030 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	219	ASP	CB-CG-OD2	6.16	123.85	118.30
1	D	219	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	219	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	259	ASP	CB-CG-OD2	5.28	123.05	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2014	0	2041	11	0
1	B	2008	0	2036	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2008	0	2038	18	0
1	D	2001	0	2029	12	0
2	A	48	0	26	0	0
2	B	48	0	26	1	0
2	C	48	0	24	4	0
2	D	48	0	24	5	0
3	A	64	0	88	2	0
3	B	42	0	58	3	0
3	C	64	0	88	5	0
3	D	42	0	58	3	0
4	A	129	0	0	2	0
4	B	113	0	0	3	0
4	C	140	0	0	4	0
4	D	104	0	0	1	0
All	All	8921	0	8536	68	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 4.

The worst 5 of 68 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)
2:D:528:NDP:N3A	2:D:528:NDP:C4A	1.73	1.50
2:D:528:NDP:O5B	2:D:528:NDP:C5B	1.64	1.46
2:C:526:NDP:O3B	2:C:526:NDP:C3B	1.64	1.43
1:A:196[A]:SER:HB2	4:B:973:HOH:O	1.80	0.81
1:C:69:GLU:O	1:C:72:GLN:HG3	1.82	0.79

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	261/286 (91%)	252 (97%)	9 (3%)	0	100	100
1	B	260/286 (91%)	249 (96%)	11 (4%)	0	100	100
1	C	260/286 (91%)	250 (96%)	10 (4%)	0	100	100
1	D	259/286 (91%)	249 (96%)	10 (4%)	0	100	100
All	All	1040/1144 (91%)	1000 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	220/243 (90%)	215 (98%)	5 (2%)	50	37
1	B	219/243 (90%)	210 (96%)	9 (4%)	30	16
1	C	219/243 (90%)	208 (95%)	11 (5%)	24	10
1	D	218/243 (90%)	202 (93%)	16 (7%)	14	4
All	All	876/972 (90%)	835 (95%)	41 (5%)	26	12

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	109	LEU
1	D	234	GLN
1	D	124[A]	THR
1	D	199	LYS
1	D	268	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	HIS
1	C	134	HIS
1	C	120	HIS

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Mol	Chain	Res	Type
1	C	270	ASN
1	B	77	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	NDP	D	528	-	45,52,52	5.80	29 (64%)	53,80,80	1.91	12 (22%)
3	CPS	A	523	-	45,45,45	1.93	10 (22%)	69,70,70	1.05	5 (7%)
2	NDP	B	524	-	45,52,52	4.04	22 (48%)	53,80,80	1.98	13 (24%)
2	NDP	C	526	-	45,52,52	4.80	24 (53%)	53,80,80	1.86	12 (22%)
3	CPS	C	2	-	25,25,45	0.55	0	37,41,70	1.08	2 (5%)
3	CPS	C	527	-	45,45,45	2.00	11 (24%)	69,70,70	1.10	6 (8%)
3	CPS	D	529	-	45,45,45	1.87	11 (24%)	69,70,70	1.07	5 (7%)
2	NDP	A	522	-	45,52,52	3.71	18 (40%)	53,80,80	1.91	11 (20%)
3	CPS	A	1	-	25,25,45	0.56	0	37,41,70	1.47	9 (24%)
3	CPS	B	525	-	45,45,45	1.86	11 (24%)	69,70,70	1.22	7 (10%)

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	NDP	D	528	-	-	7/30/77/77	0/5/5/5
3	CPS	A	523	-	-	4/25/90/90	0/4/4/4
2	NDP	B	524	-	-	6/30/77/77	0/5/5/5
2	NDP	C	526	-	-	4/30/77/77	0/5/5/5
3	CPS	C	2	-	-	-	0/4/4/4
3	CPS	C	527	-	-	2/25/90/90	0/4/4/4
3	CPS	D	529	-	-	4/25/90/90	0/4/4/4
2	NDP	A	522	-	-	6/30/77/77	0/5/5/5
3	CPS	A	1	-	-	-	0/4/4/4
3	CPS	B	525	-	-	5/25/90/90	0/4/4/4

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	NDP	C4A-N3A	27.69	1.73	1.35
2	C	526	NDP	C4A-N3A	19.80	1.63	1.35
2	B	524	NDP	C4A-N3A	14.28	1.55	1.35
2	D	528	NDP	C3B-C2B	-12.41	1.25	1.52
2	C	526	NDP	C2A-N1A	12.00	1.56	1.33

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	524	NDP	N3A-C2A-N1A	-6.26	118.89	128.68
2	A	522	NDP	N3A-C2A-N1A	-5.89	119.47	128.68
2	C	526	NDP	N3A-C2A-N1A	-5.89	119.48	128.68
2	B	524	NDP	O4D-C1D-N1N	5.78	119.36	108.06
2	D	528	NDP	N3A-C2A-N1A	-5.39	120.25	128.68

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	524	NDP	C2B-O2B-P2B-O2X
2	D	528	NDP	C2B-O2B-P2B-O2X
2	D	528	NDP	O4D-C1D-N1N-C6N

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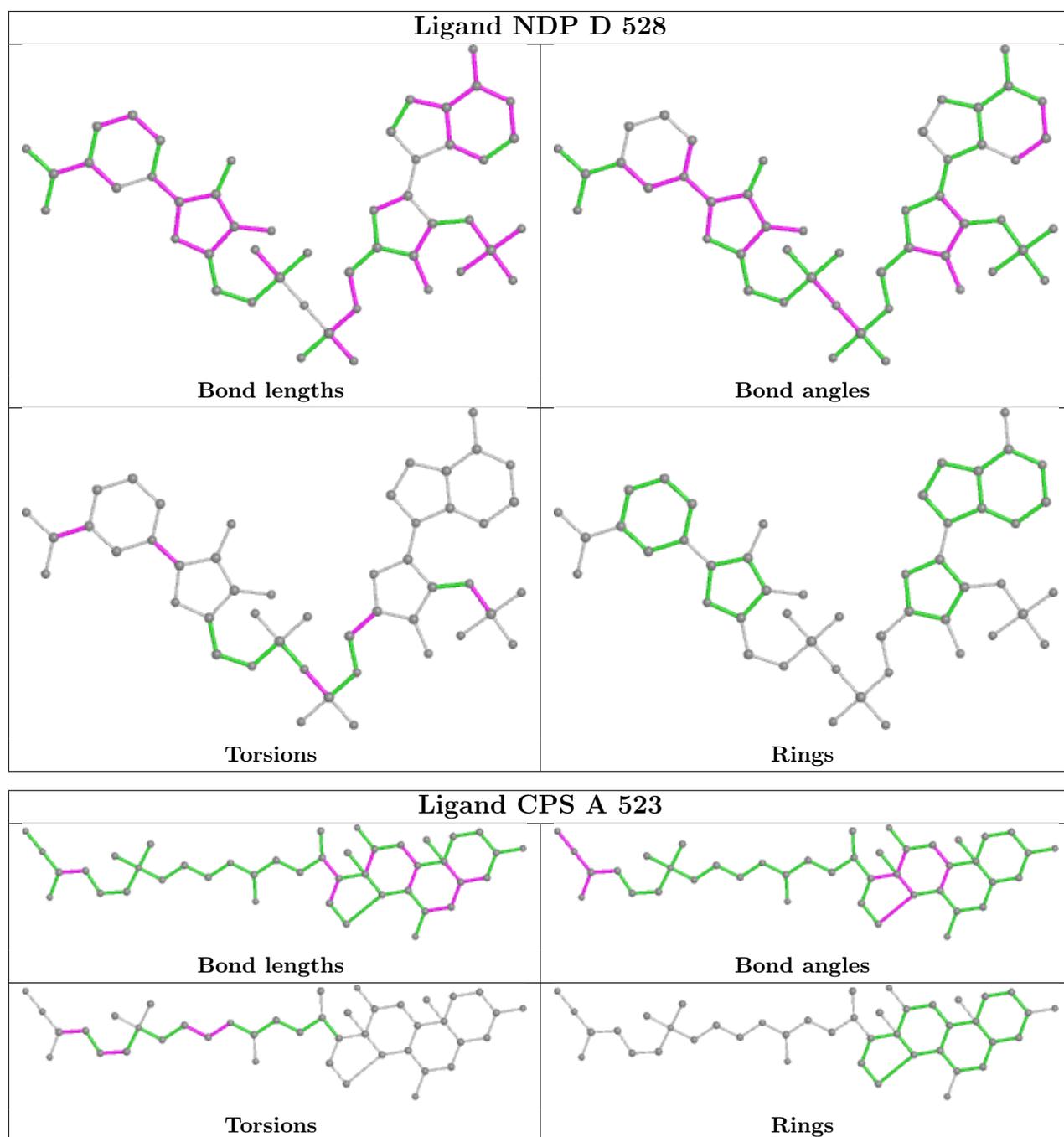
Mol	Chain	Res	Type	Atoms
3	A	523	CPS	N2-C30-C31-C32
3	D	529	CPS	C26-C27-N2-C29

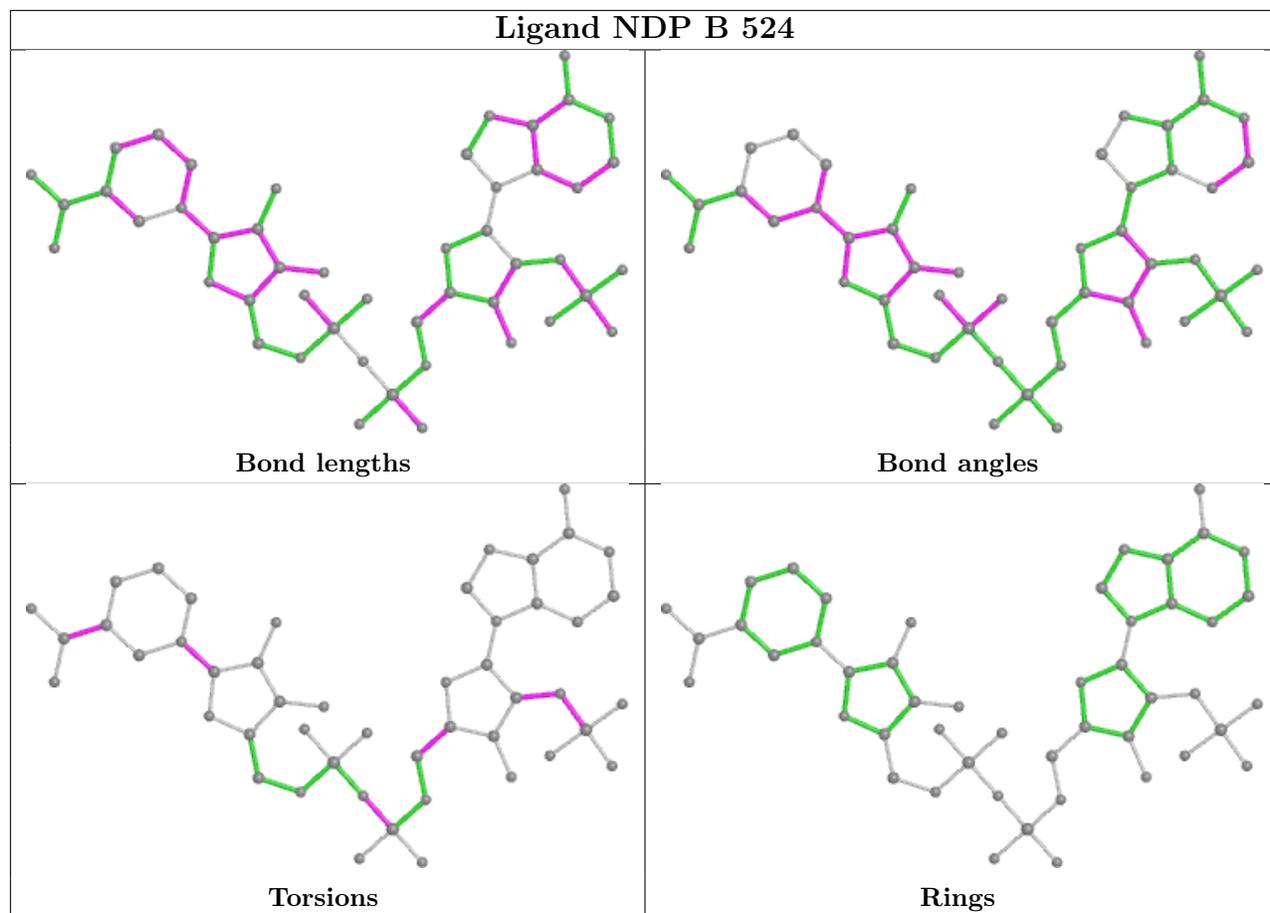
There are no ring outliers.

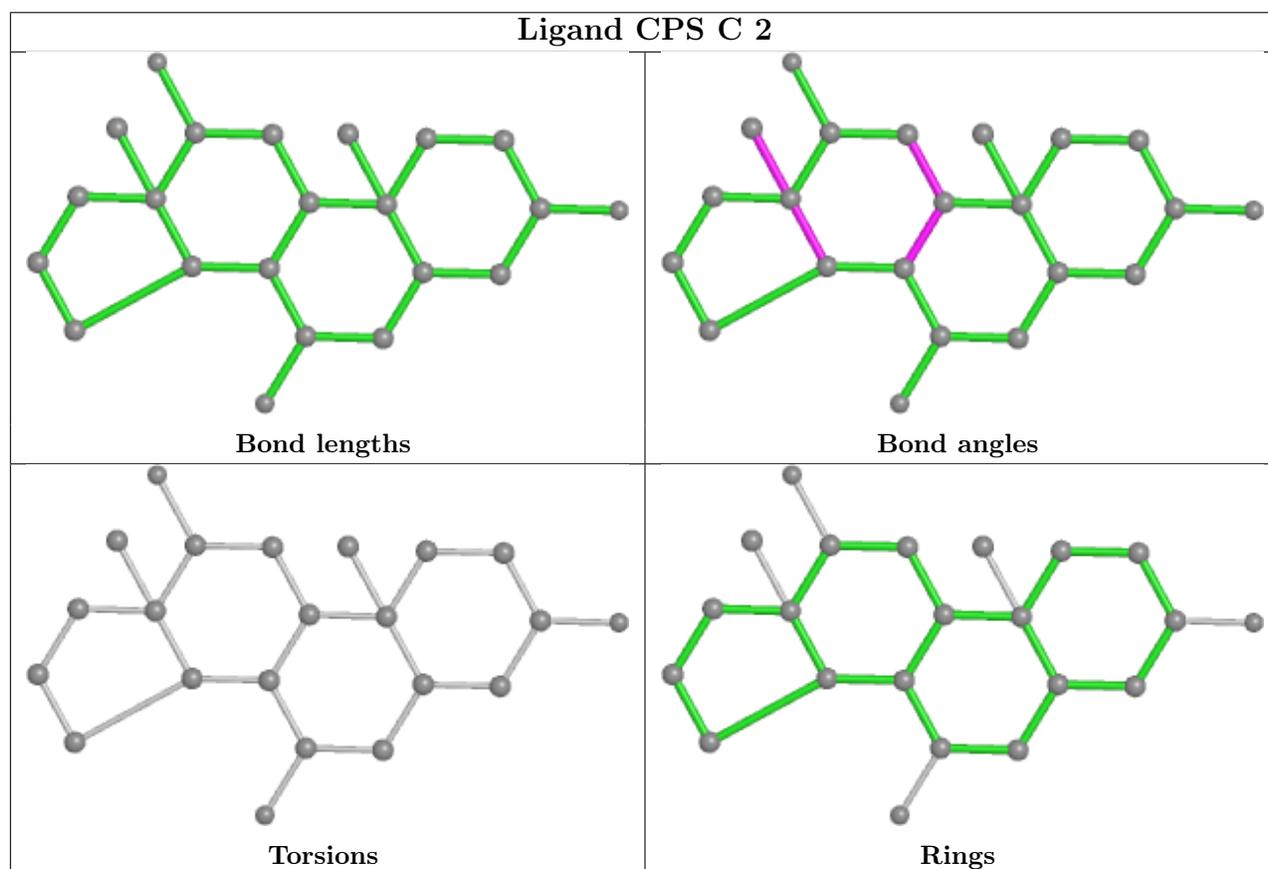
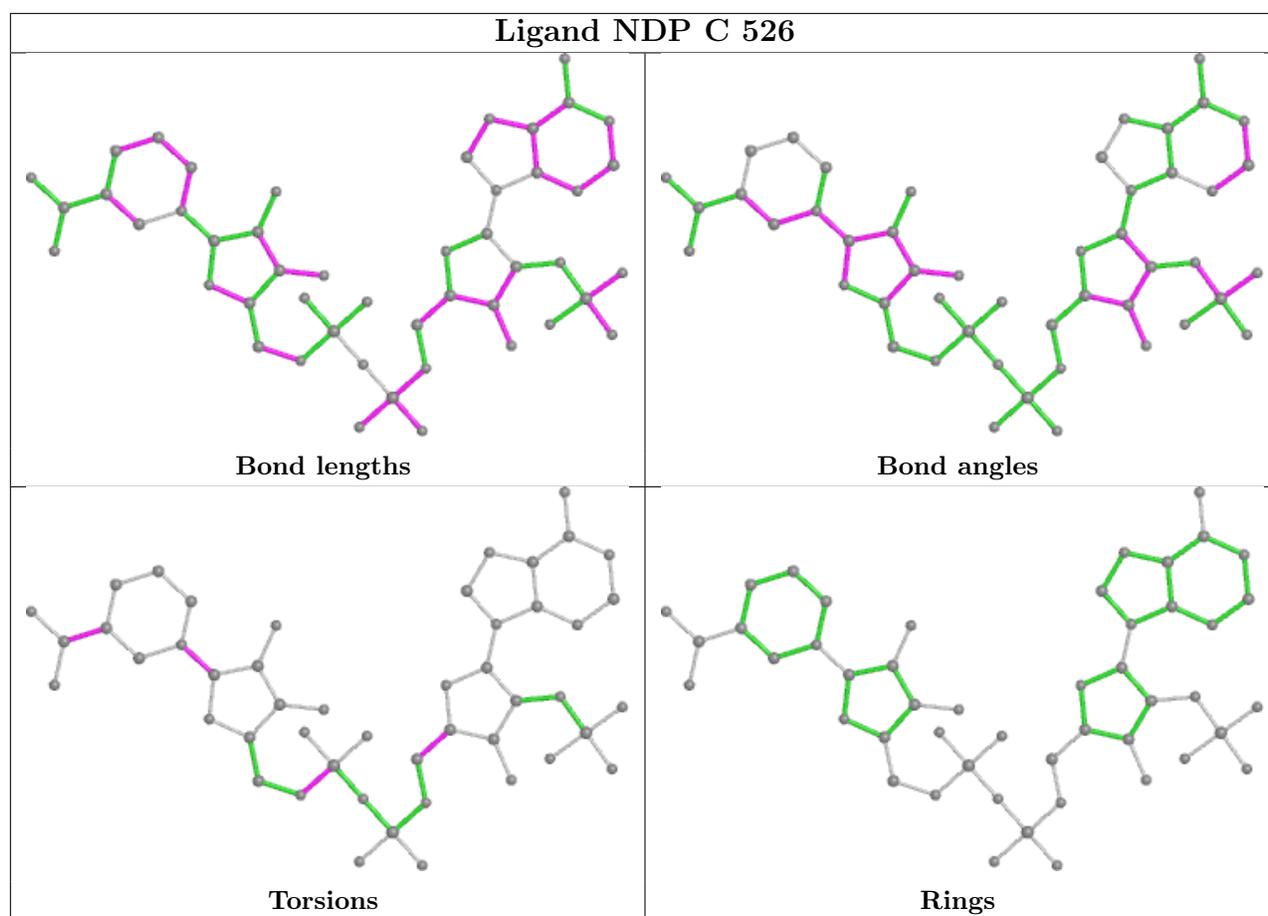
8 monomers are involved in 23 short contacts:

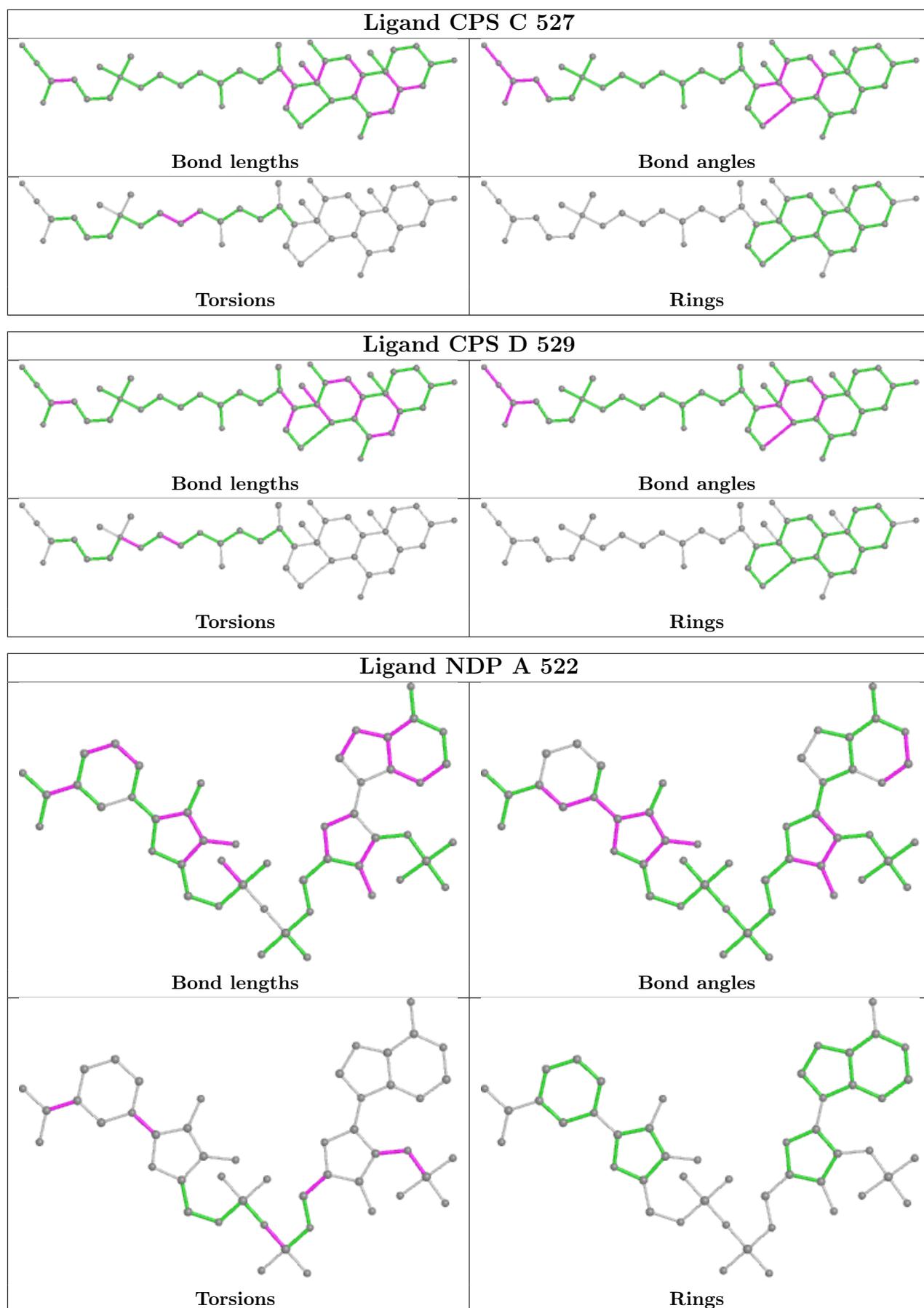
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	528	NDP	5	0
3	A	523	CPS	2	0
2	B	524	NDP	1	0
2	C	526	NDP	4	0
3	C	2	CPS	2	0
3	C	527	CPS	3	0
3	D	529	CPS	3	0
3	B	525	CPS	3	0

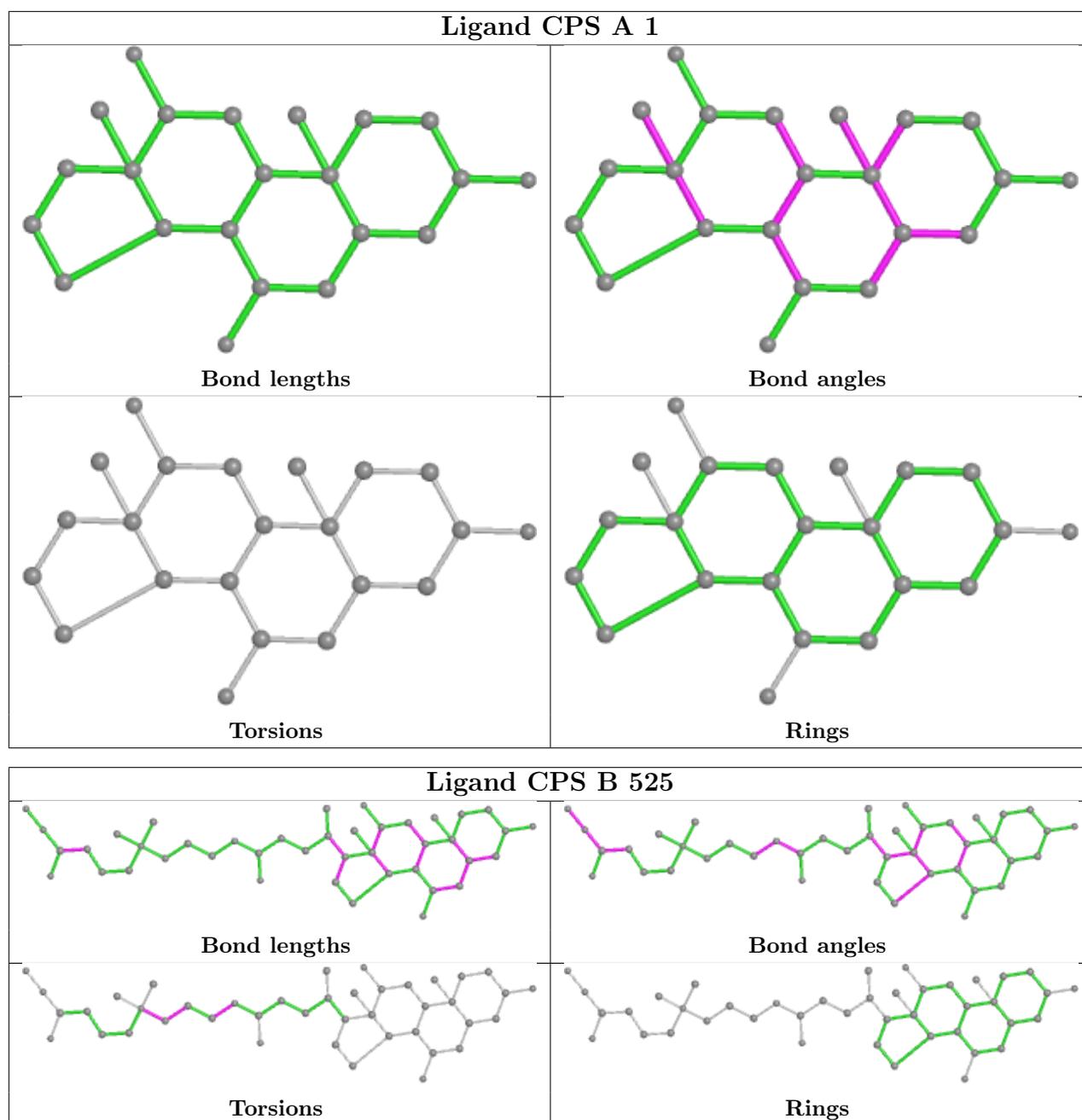
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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