



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:18 PM UTC

PDB ID : 1XU7 / pdb_00001xu7
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 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)
Xtriage (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

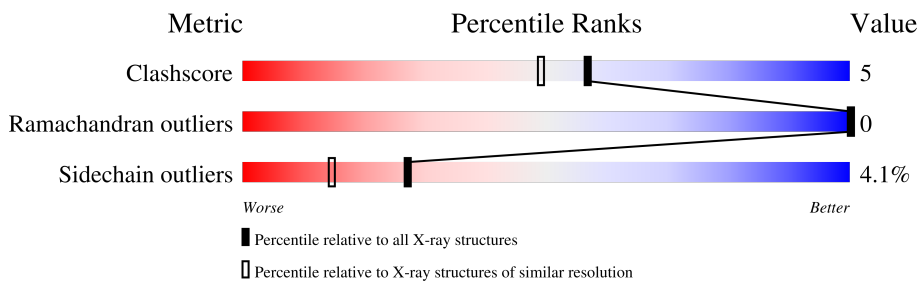
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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

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

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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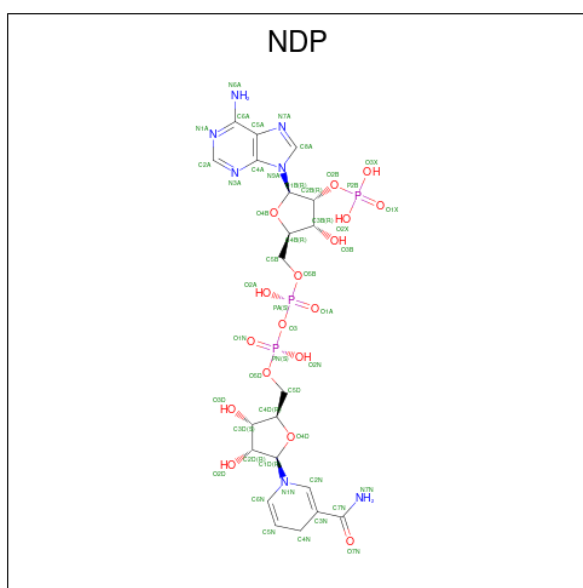
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	cloning artifact	UNP P28845
B	11	HIS	-	cloning artifact	UNP P28845
B	12	GLN	-	cloning artifact	UNP P28845
B	13	HIS	-	cloning artifact	UNP P28845
B	14	GLN	-	cloning artifact	UNP P28845
B	15	HIS	-	cloning artifact	UNP P28845
B	16	GLN	-	cloning 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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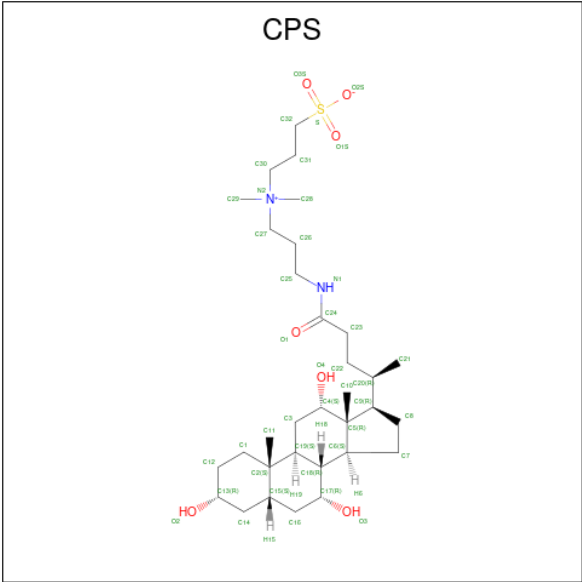
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	cloning artifact	UNP P28845
D	17	HIS	-	cloning artifact	UNP P28845
D	18	GLN	-	cloning artifact	UNP P28845
D	19	HIS	-	cloning artifact	UNP P28845
D	20	GLN	-	cloning artifact	UNP P28845
D	21	GLN	-	cloning artifact	UNP P28845
D	22	PRO	-	cloning 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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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



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

- 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		

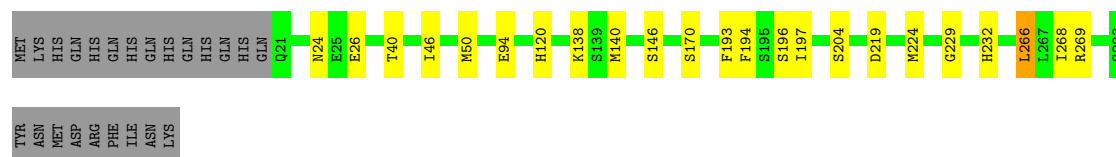
3 Residue-property plots [i](#)

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.

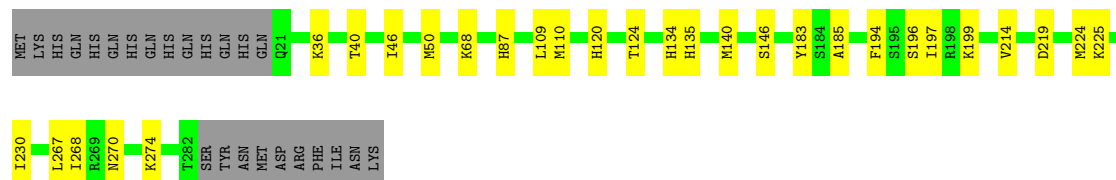
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain A: 



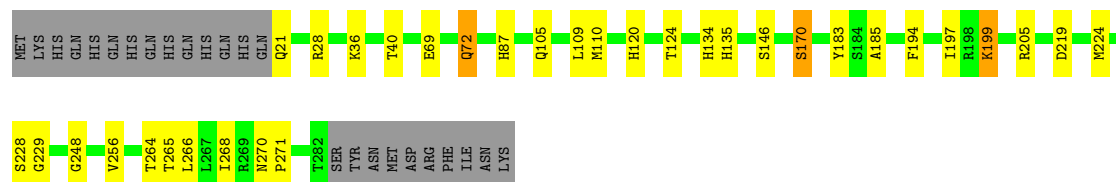
- Molecule 1: Corticosteroid 11-beta-dehydrogenase, isozyme 1

Chain B: 



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

Chain C: 



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

Chain D: 





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	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.	Xtriage
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: NDP, CPS

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	0.37	0/2048	0.75	0/2766
1	B	0.38	0/2042	0.77	0/2758
1	C	0.38	0/2042	0.76	0/2758
1	D	0.37	0/2035	0.76	0/2748
All	All	0.37	0/8167	0.76	0/11030

There are no bond length outliers.

There are no bond angle outliers.

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	15	0
1	B	2008	0	2036	15	0
1	C	2008	0	2038	20	0
1	D	2001	0	2029	14	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	79	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 5.

The worst 5 of 79 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1040/1144 (91%)	1000 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	220/243 (90%)	214 (97%)	6 (3%)	39	27
1	B	219/243 (90%)	212 (97%)	7 (3%)	34	22
1	C	219/243 (90%)	210 (96%)	9 (4%)	27	15
1	D	218/243 (90%)	204 (94%)	14 (6%)	16	6
All	All	876/972 (90%)	840 (96%)	36 (4%)	27	15

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	170	SER
1	D	281	SER
1	D	199	LYS
1	D	262	LEU
1	B	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	105	GLN
1	C	270	ASN
1	D	270	ASN
1	C	120	HIS
1	D	21	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	CPS	C	527	-	45,45,45	2.03	11 (24%)	70,70,70	1.06	4 (5%)
3	CPS	A	1	-	25,25,45	0.57	0	39,41,70	1.45	9 (23%)
3	CPS	C	2	-	25,25,45	0.57	0	39,41,70	1.09	2 (5%)
3	CPS	B	525	-	45,45,45	1.89	11 (24%)	70,70,70	1.18	6 (8%)
2	NDP	C	526	-	51,52,52	4.58	26 (50%)	71,80,80	2.29	19 (26%)
2	NDP	A	522	-	51,52,52	3.95	24 (47%)	71,80,80	2.34	18 (25%)
2	NDP	B	524	-	51,52,52	4.16	28 (54%)	71,80,80	2.40	19 (26%)
2	NDP	D	528	-	51,52,52	5.41	35 (68%)	71,80,80	2.33	18 (25%)
3	CPS	A	523	-	45,45,45	1.96	10 (22%)	70,70,70	1.01	4 (5%)
3	CPS	D	529	-	45,45,45	1.90	11 (24%)	70,70,70	1.03	4 (5%)

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	CPS	C	527	-	-	2/25/90/90	0/4/4/4
3	CPS	A	1	-	-	-	0/4/4/4
3	CPS	C	2	-	-	-	0/4/4/4
3	CPS	B	525	-	-	5/25/90/90	0/4/4/4
2	NDP	C	526	-	-	3/34/77/77	0/5/5/5
2	NDP	A	522	-	-	5/34/77/77	0/5/5/5
2	NDP	B	524	-	-	6/34/77/77	0/5/5/5
2	NDP	D	528	-	-	7/34/77/77	0/5/5/5
3	CPS	A	523	-	-	4/25/90/90	0/4/4/4
3	CPS	D	529	-	-	4/25/90/90	0/4/4/4

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	NDP	C4A-N3A	21.10	1.73	1.34
2	C	526	NDP	C4A-N3A	15.27	1.63	1.34
2	D	528	NDP	C3B-C2B	-12.67	1.25	1.53
2	C	526	NDP	C2A-N1A	12.56	1.56	1.33
2	B	524	NDP	C4A-N3A	11.20	1.55	1.34

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	528	NDP	C5A-C4A-N9A	9.23	115.87	105.81
2	B	524	NDP	C5A-C4A-N9A	9.06	115.69	105.81
2	A	522	NDP	C5A-C4A-N9A	8.75	115.35	105.81
2	C	526	NDP	C5A-C4A-N9A	8.54	115.12	105.81
2	D	528	NDP	N9A-C8A-N7A	-6.72	104.40	113.94

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

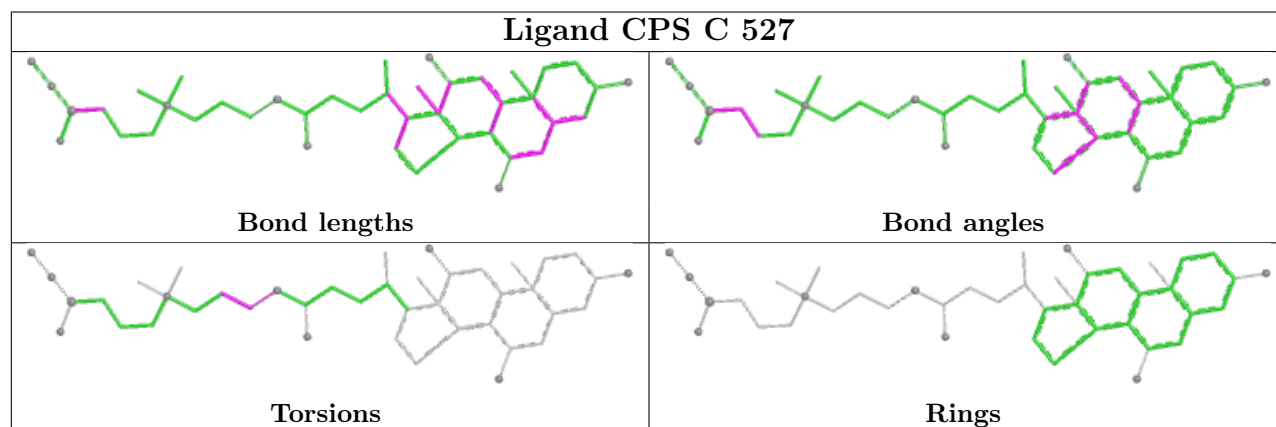
Mol	Chain	Res	Type	Atoms
2	D	528	NDP	O4D-C1D-N1N-C6N
3	A	523	CPS	N2-C30-C31-C32
3	D	529	CPS	C26-C27-N2-C30
3	B	525	CPS	C26-C25-N1-C24
3	B	525	CPS	C26-C27-N2-C28

There are no ring outliers.

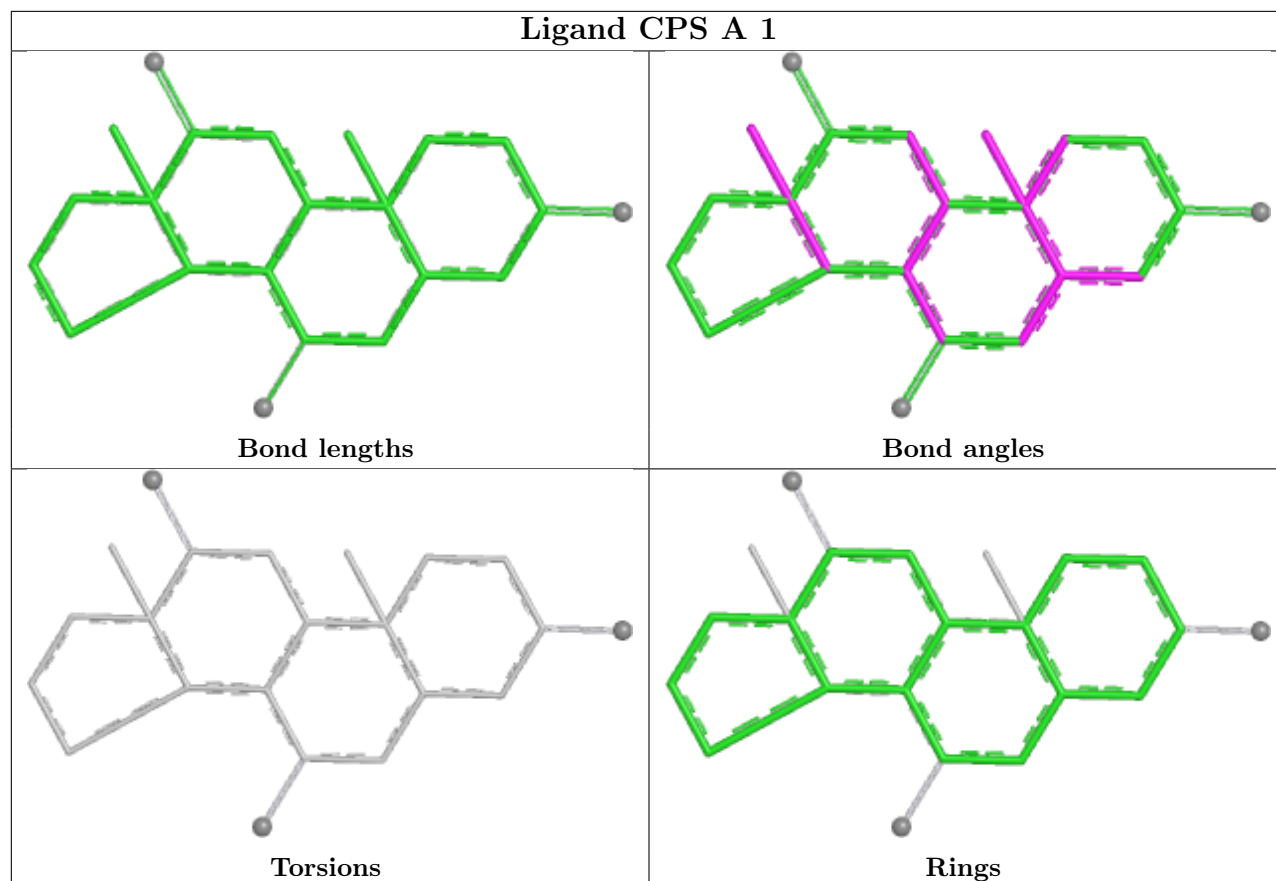
8 monomers are involved in 23 short contacts:

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

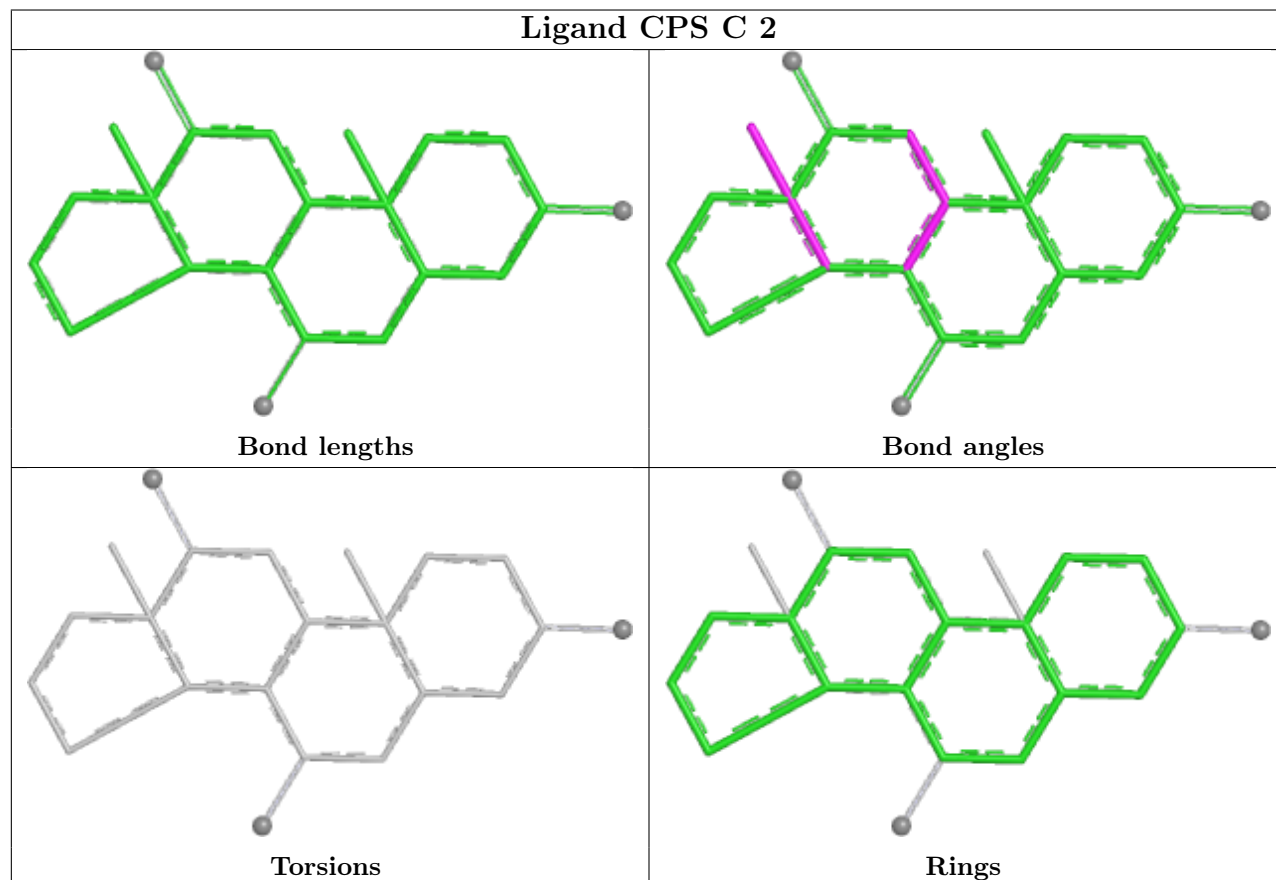
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



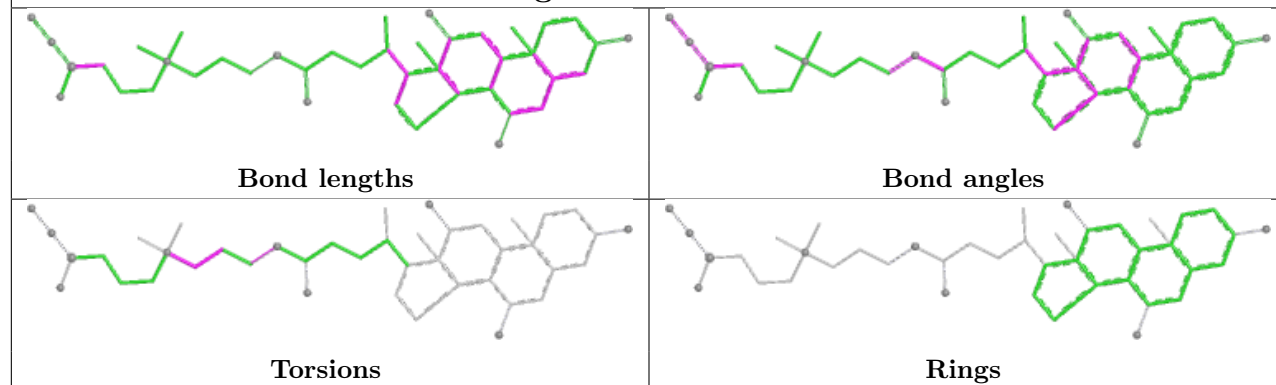
Ligand CPS A 1



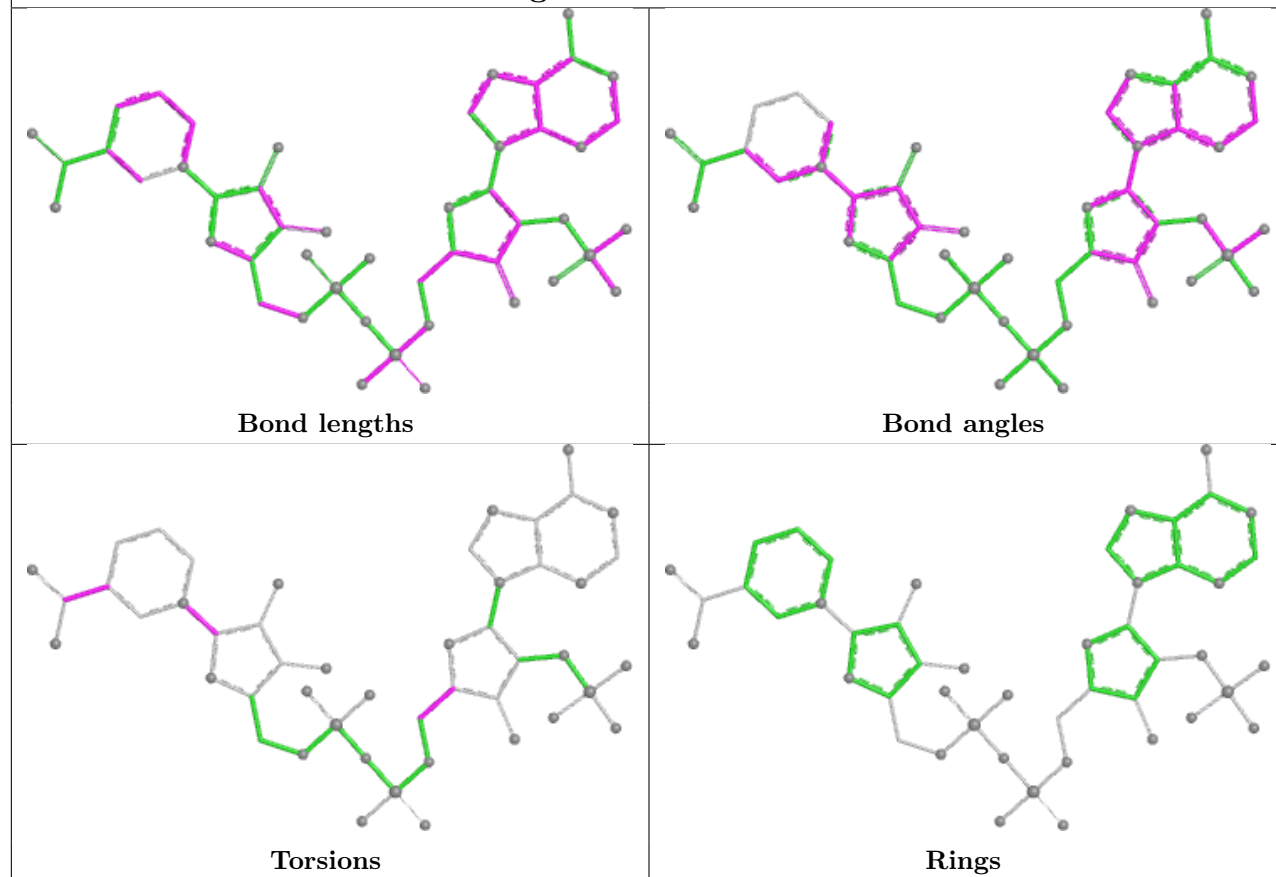
Ligand CPS C 2

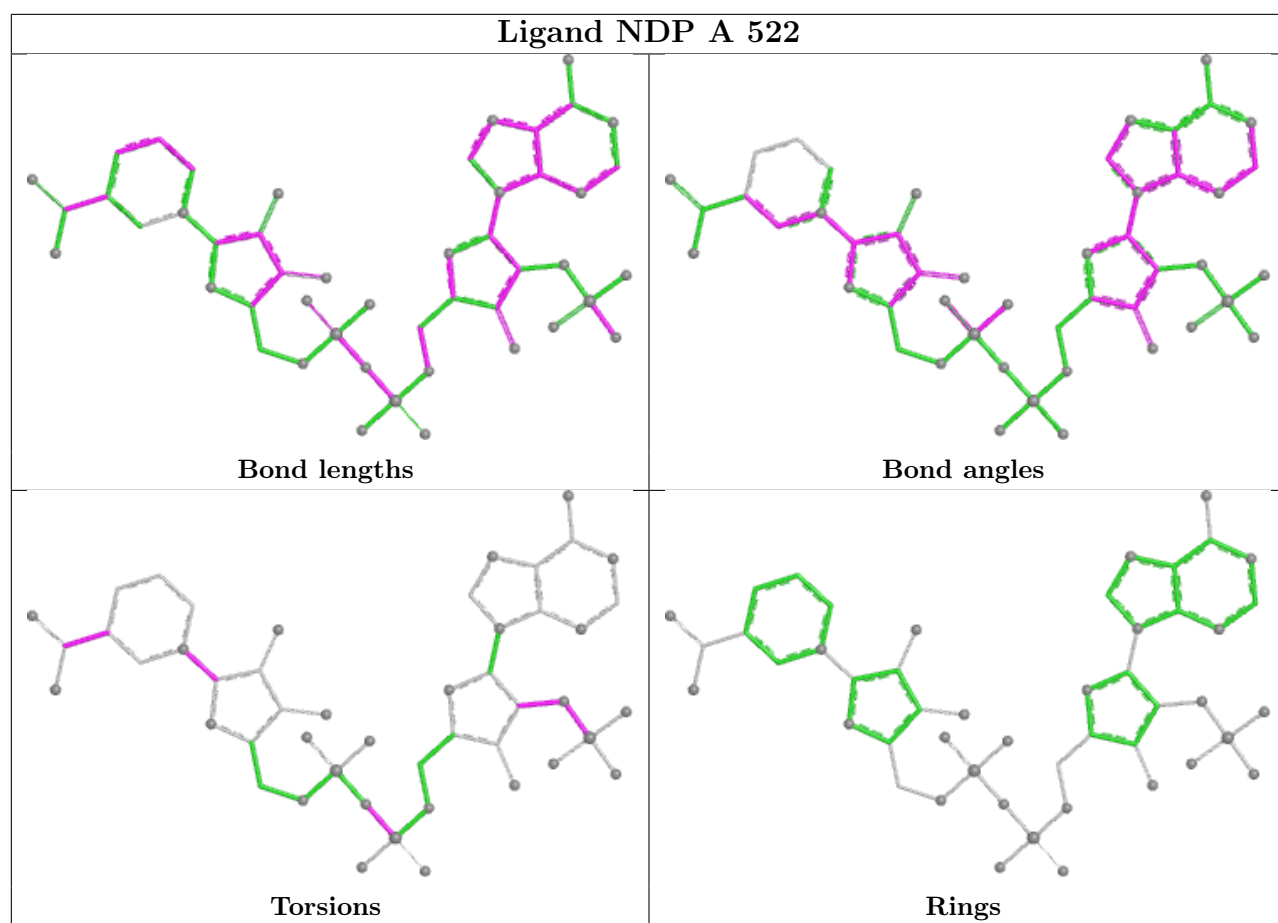


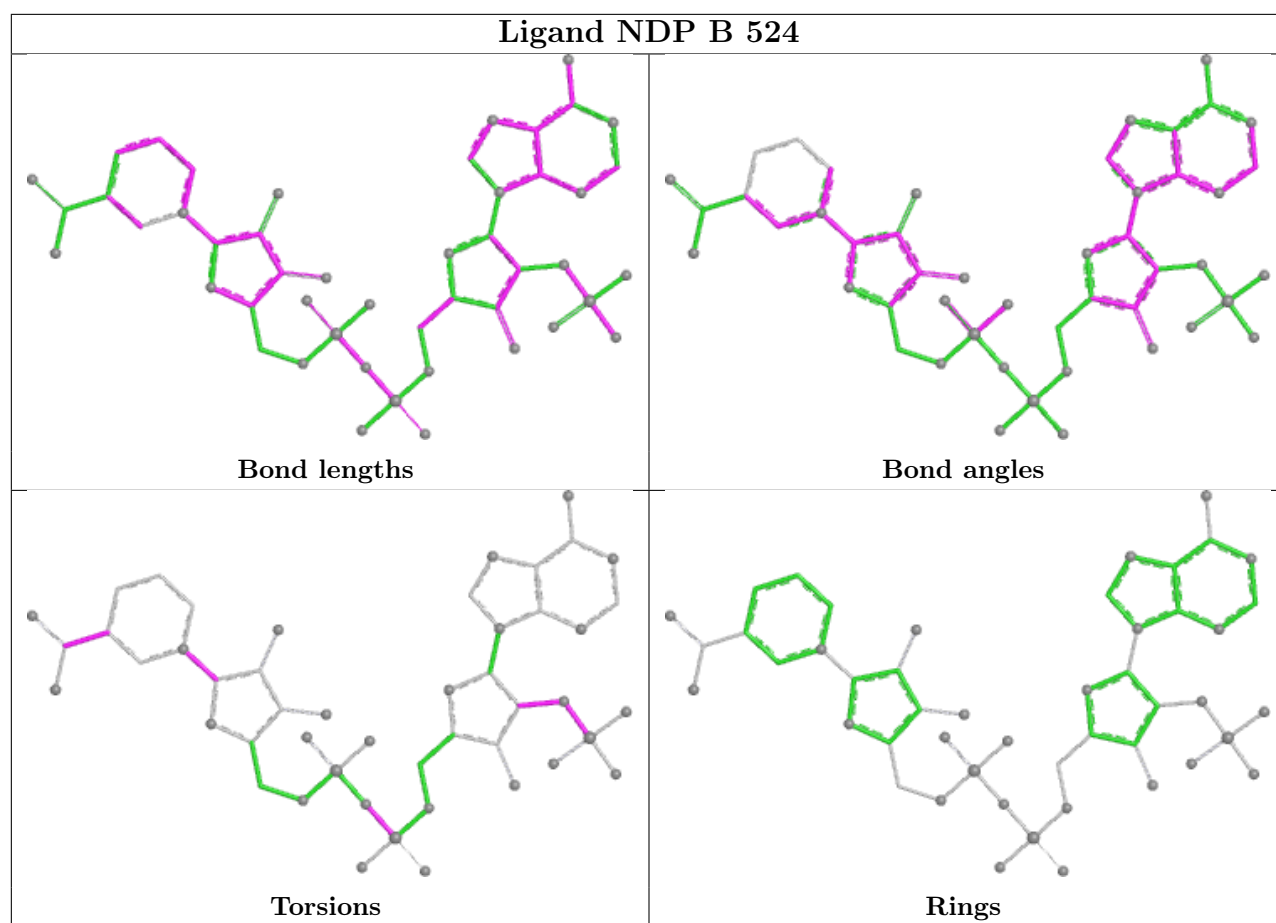
Ligand CPS B 525

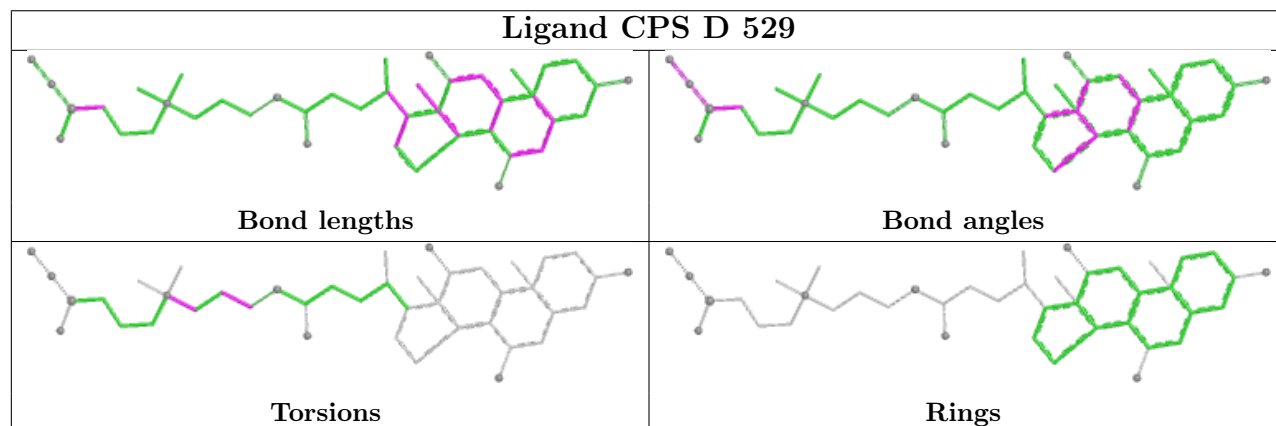
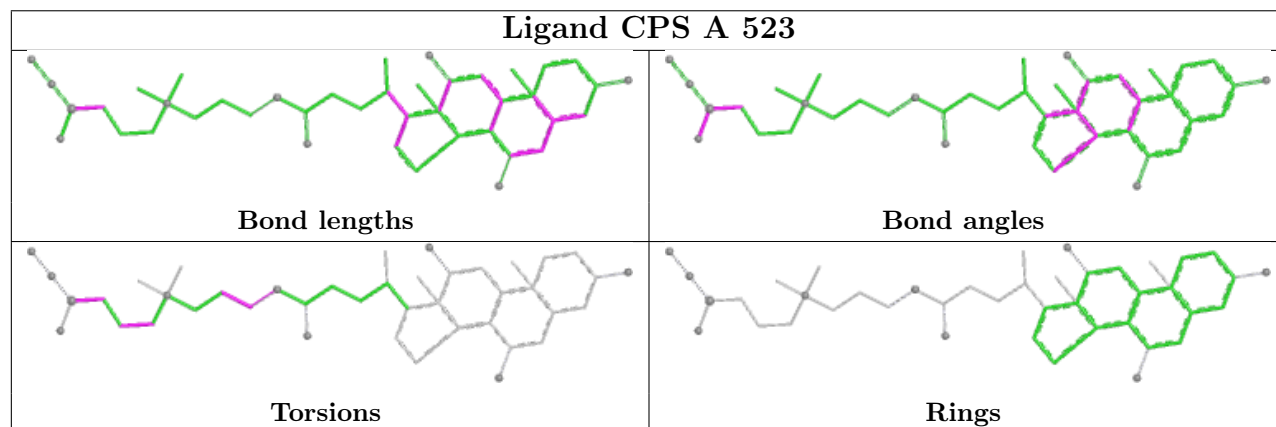
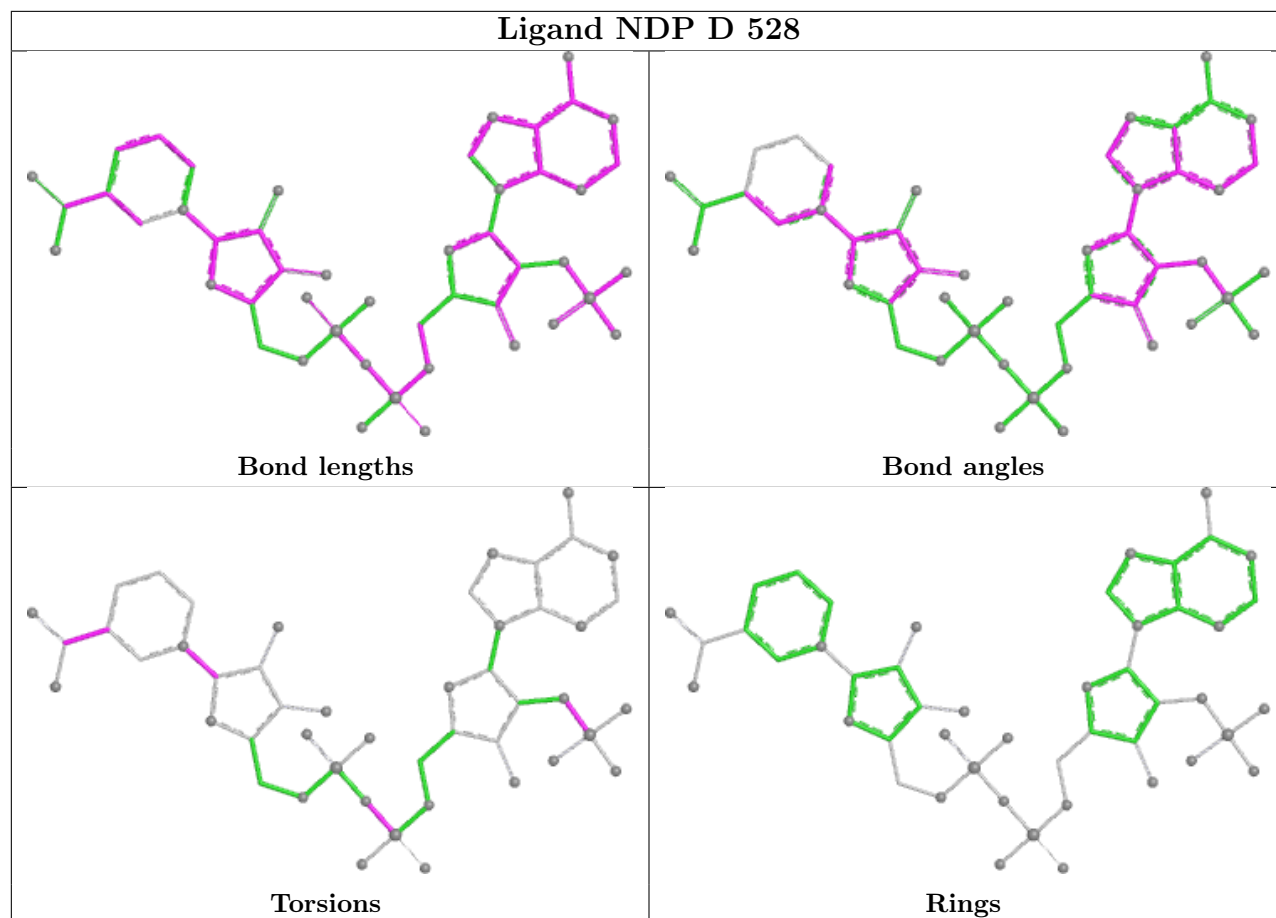


Ligand NDP C 526









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.