



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2021 – 06:10 PM JST

PDB ID : 7CS8
Title : IiPLR1 with NADP⁺ and (-)secoisolariciresinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.60 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) : 1.13
EDS : 2.19
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.19

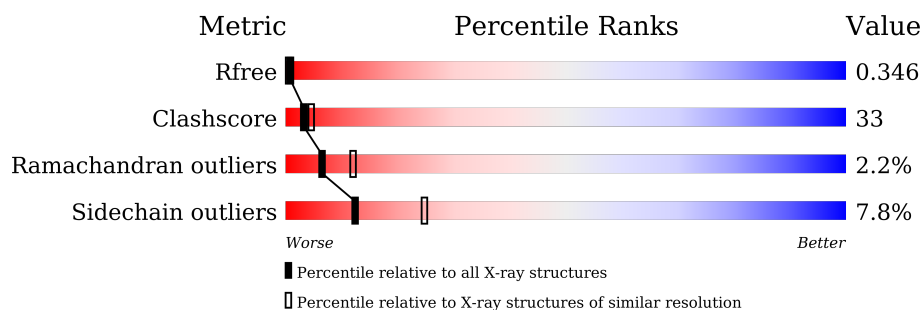
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	
1	F	317	

2 Entry composition [i](#)

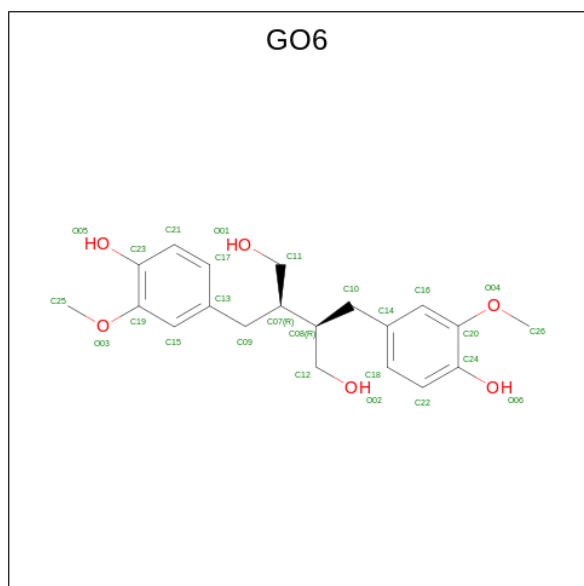
There are 4 unique types of molecules in this entry. The entry contains 14526 atoms, of which 312 are hydrogens and 0 are deuteriums.

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 Pinorensinol-lariciresinol reductase.

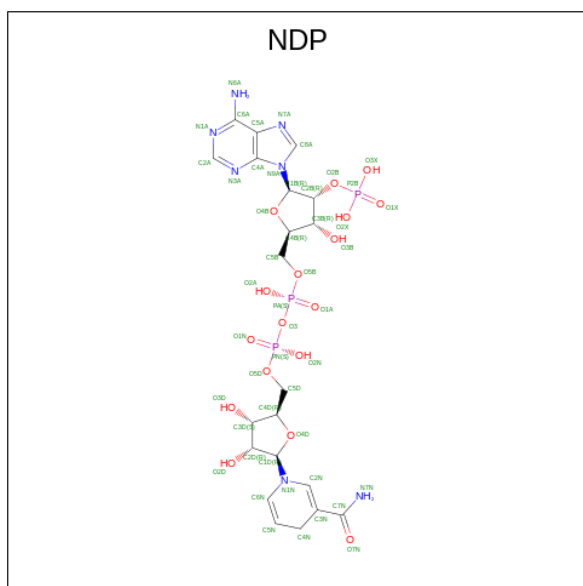
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2281	1449	386	436	10			
1	B	290	Total	C	N	O	S	0	0	0
			2281	1449	386	436	10			
1	C	288	Total	C	N	O	S	0	0	0
			2270	1442	384	434	10			
1	D	286	Total	C	N	O	S	0	0	0
			2256	1434	380	432	10			
1	E	288	Total	C	N	O	S	0	0	0
			2264	1438	382	434	10			
1	F	294	Total	C	N	O	S	0	0	0
			2320	1475	395	440	10			

- Molecule 2 is (2R,3R)-2,3-bis[(3-methoxy-4-oxidanyl-phenyl)methyl]butane-1,4-diol (three-letter code: GO6) (formula: C₂₀H₂₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 52	C 20	H 26	O 6	0	0
2	B	1	Total 52	C 20	H 26	O 6	0	0
2	C	1	Total 52	C 20	H 26	O 6	0	0
2	D	1	Total 52	C 20	H 26	O 6	0	0
2	E	1	Total 52	C 20	H 26	O 6	0	0
2	F	1	Total 52	C 20	H 26	O 6	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	B	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	C	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	D	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	E	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	F	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

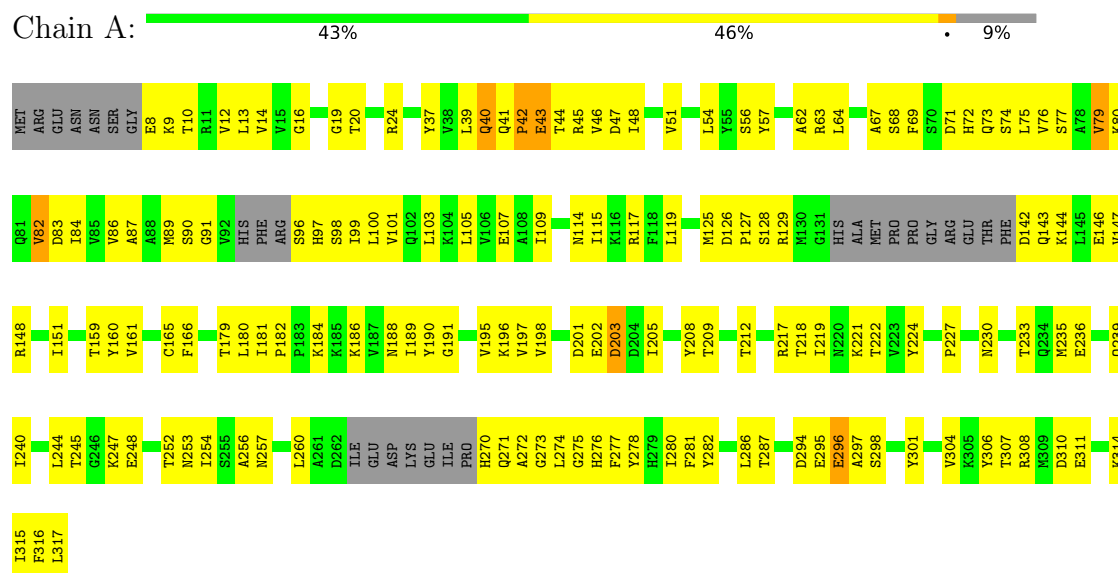
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	24	Total	O	0	0
			24	24		
4	C	12	Total	O	0	0
			12	12		
4	D	13	Total	O	0	0
			13	13		
4	E	13	Total	O	0	0
			13	13		
4	F	29	Total	O	0	0
			29	29		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pinoresinol-lariciresinol reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	244.36Å 244.36Å 76.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.73 – 2.60 46.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.73-2.60) 95.6 (46.46-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.276 , 0.346 0.278 , 0.346	Depositor DCC
R_{free} test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 12.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.408 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14526	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3549e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, GO6

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	0.45	0/2319	0.61	1/3132 (0.0%)
1	B	0.51	1/2320 (0.0%)	0.61	0/3133
1	C	0.44	0/2308	0.56	0/3117
1	D	0.44	0/2293	0.59	0/3097
1	E	0.46	0/2301	0.62	0/3107
1	F	0.48	1/2362 (0.0%)	0.64	0/3191
All	All	0.46	2/13903 (0.0%)	0.61	1/18777 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	40	GLN	C-N	-5.20	1.22	1.34
1	B	40	GLN	C-N	-5.06	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLN	C-N-CA	-5.31	108.44	121.70

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	2281	0	2282	128	0
1	B	2281	0	2280	164	0
1	C	2270	0	2270	179	0
1	D	2256	0	2260	178	0
1	E	2264	0	2266	149	0
1	F	2320	0	2320	142	0
2	A	26	26	0	0	0
2	B	26	26	0	0	0
2	C	26	26	0	2	0
2	D	26	26	0	2	0
2	E	26	26	0	1	0
2	F	26	26	0	1	0
3	A	48	26	24	11	0
3	B	48	26	23	5	0
3	C	48	26	24	9	0
3	D	48	26	23	12	0
3	E	48	26	24	5	0
3	F	48	26	24	8	0
4	A	7	0	0	7	0
4	B	24	0	0	10	0
4	C	12	0	0	9	0
4	D	13	0	0	6	0
4	E	13	0	0	6	0
4	F	29	0	0	12	0
All	All	14214	312	13820	927	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 33.

The worst 5 of 927 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:402:NDP:O4D	3:A:402:NDP:C1D	1.64	1.16
1:A:39:LEU:HD11	1:A:67:ALA:HB3	1.30	1.14
1:B:40:GLN:HG2	1:B:66:GLU:HG2	1.31	1.11
3:A:402:NDP:O4B	3:A:402:NDP:C1B	1.63	1.11
1:D:157:PRO:HB3	1:D:219:ILE:HD11	1.38	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/317 (89%)	246 (87%)	30 (11%)	6 (2%)	7	13
1	B	282/317 (89%)	251 (89%)	26 (9%)	5 (2%)	8	16
1	C	280/317 (88%)	239 (85%)	33 (12%)	8 (3%)	4	7
1	D	278/317 (88%)	237 (85%)	36 (13%)	5 (2%)	8	16
1	E	280/317 (88%)	248 (89%)	26 (9%)	6 (2%)	7	13
1	F	288/317 (91%)	254 (88%)	27 (9%)	7 (2%)	6	10
All	All	1690/1902 (89%)	1475 (87%)	178 (10%)	37 (2%)	6	12

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	A	43	GLU
1	B	122	GLU
1	B	242	GLU
1	D	242	GLU

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	247/271 (91%)	231 (94%)	16 (6%)	17	34
1	B	247/271 (91%)	220 (89%)	27 (11%)	6	11
1	C	246/271 (91%)	226 (92%)	20 (8%)	11	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	245/271 (90%)	235 (96%)	10 (4%)	30	56
1	E	245/271 (90%)	220 (90%)	25 (10%)	7	14
1	F	251/271 (93%)	233 (93%)	18 (7%)	14	29
All	All	1481/1626 (91%)	1365 (92%)	116 (8%)	12	25

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	233	THR
1	F	219	ILE
1	D	299	LYS
1	F	212	THR
1	F	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	C	34	HIS
1	D	34	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](#)

12 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	NDP	B	402	-	45,52,52	4.15	19 (42%)	53,80,80	2.00	6 (11%)
3	NDP	C	402	-	45,52,52	4.14	20 (44%)	53,80,80	2.37	5 (9%)
3	NDP	D	402	-	45,52,52	4.05	19 (42%)	53,80,80	2.19	8 (15%)
3	NDP	A	402	-	45,52,52	4.25	21 (46%)	53,80,80	2.24	5 (9%)
2	GO6	A	401	-	27,27,27	0.99	2 (7%)	30,36,36	1.23	4 (13%)
2	GO6	B	401	-	27,27,27	0.98	2 (7%)	30,36,36	1.14	4 (13%)
2	GO6	D	401	-	27,27,27	1.03	3 (11%)	30,36,36	1.29	3 (10%)
2	GO6	F	401	-	27,27,27	0.96	2 (7%)	30,36,36	1.42	4 (13%)
3	NDP	F	402	-	45,52,52	4.08	21 (46%)	53,80,80	2.20	5 (9%)
2	GO6	E	401	-	27,27,27	1.07	2 (7%)	30,36,36	1.07	2 (6%)
3	NDP	E	402	-	45,52,52	4.07	20 (44%)	53,80,80	2.25	9 (16%)
2	GO6	C	401	-	27,27,27	1.02	3 (11%)	30,36,36	1.12	4 (13%)

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	NDP	B	402	-	-	12/30/77/77	0/5/5/5
3	NDP	C	402	-	-	8/30/77/77	0/5/5/5
3	NDP	D	402	-	-	11/30/77/77	0/5/5/5
3	NDP	A	402	-	-	12/30/77/77	0/5/5/5
2	GO6	A	401	-	-	8/20/20/20	0/2/2/2
2	GO6	B	401	-	-	7/20/20/20	0/2/2/2
2	GO6	D	401	-	-	6/20/20/20	0/2/2/2
2	GO6	F	401	-	-	7/20/20/20	0/2/2/2
3	NDP	F	402	-	-	8/30/77/77	0/5/5/5
2	GO6	E	401	-	-	8/20/20/20	0/2/2/2
3	NDP	E	402	-	-	12/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GO6	C	401	-	-	15/20/20/20	0/2/2/2

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	O4B-C1B	16.08	1.63	1.41
3	B	402	NDP	O4B-C1B	15.59	1.62	1.41
3	C	402	NDP	O4B-C1B	15.46	1.62	1.41
3	E	402	NDP	O4B-C1B	14.97	1.62	1.41
3	F	402	NDP	O4B-C1B	14.42	1.61	1.41

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NDP	C5A-C6A-N6A	9.96	135.49	120.35
3	A	402	NDP	C5A-C6A-N6A	9.44	134.69	120.35
3	F	402	NDP	C5A-C6A-N6A	9.28	134.46	120.35
3	D	402	NDP	C5A-C6A-N6A	9.04	134.09	120.35
3	E	402	NDP	C5A-C6A-N6A	9.01	134.04	120.35

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GO6	C07-C08-C10-C14
2	C	401	GO6	C09-C07-C08-C10
2	C	401	GO6	C09-C07-C08-C12
2	C	401	GO6	C11-C07-C08-C10
2	C	401	GO6	C11-C07-C08-C12

There are no ring outliers.

10 monomers are involved in 55 short contacts:

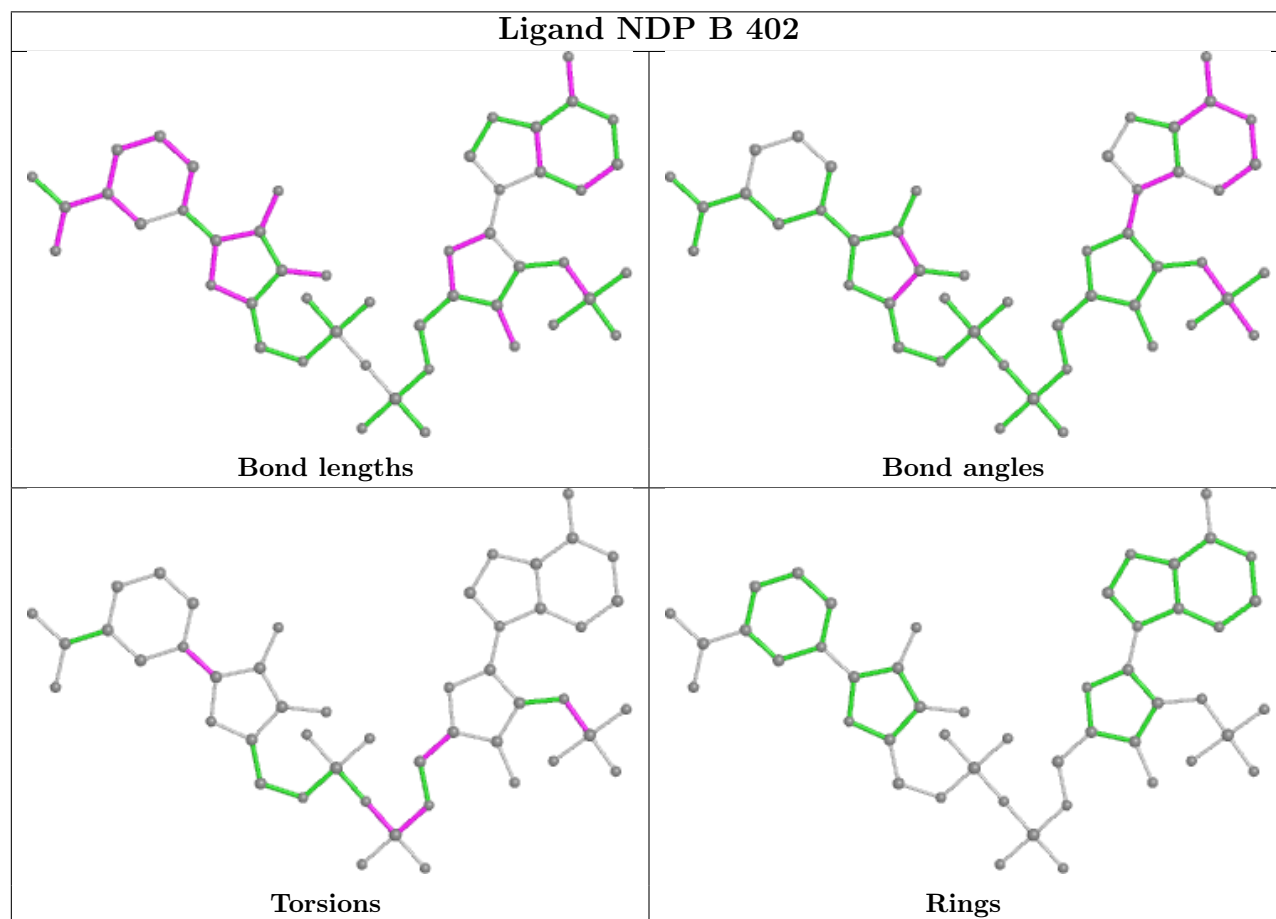
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NDP	5	0
3	C	402	NDP	9	0
3	D	402	NDP	12	0
3	A	402	NDP	11	0
2	D	401	GO6	2	0
2	F	401	GO6	1	0
3	F	402	NDP	8	0

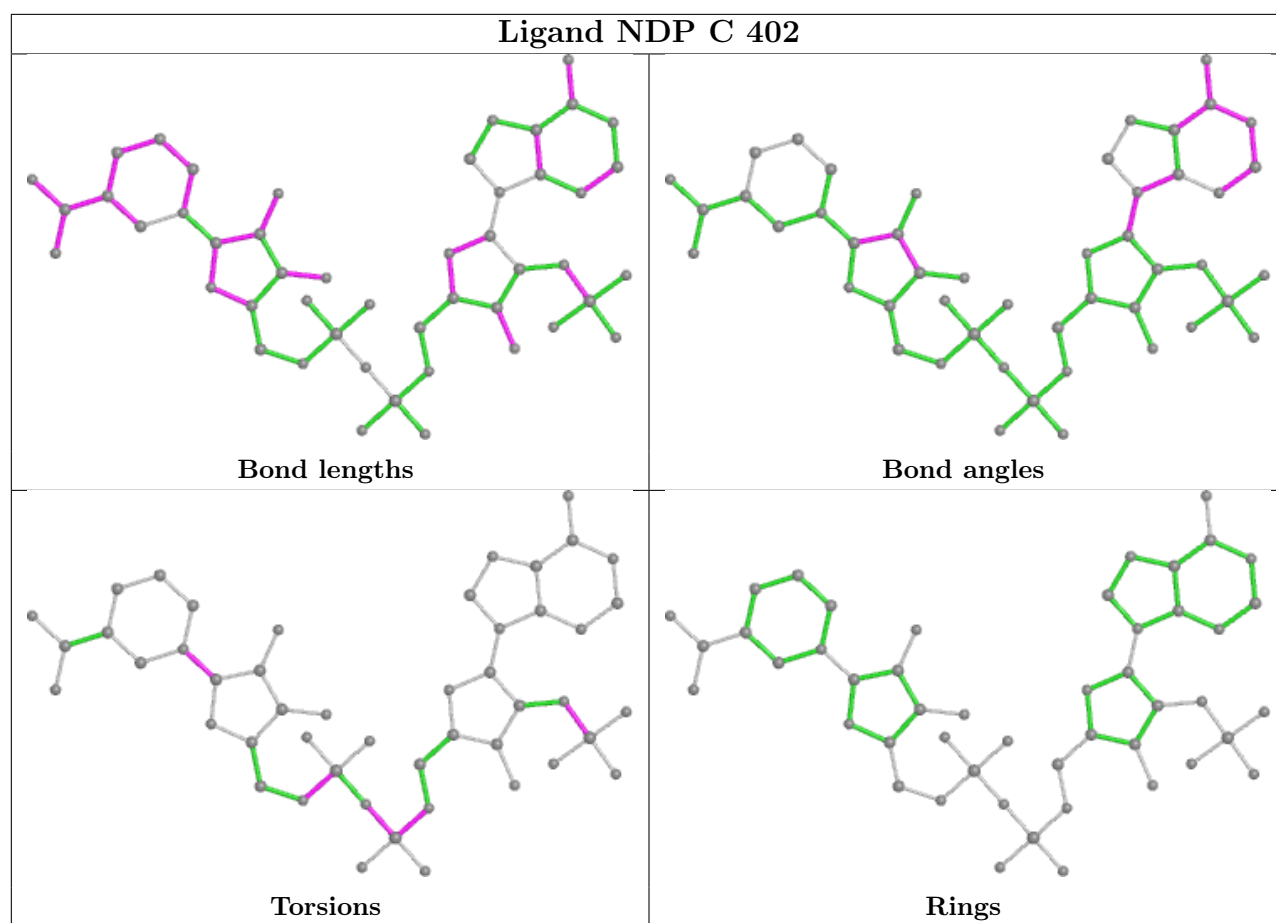
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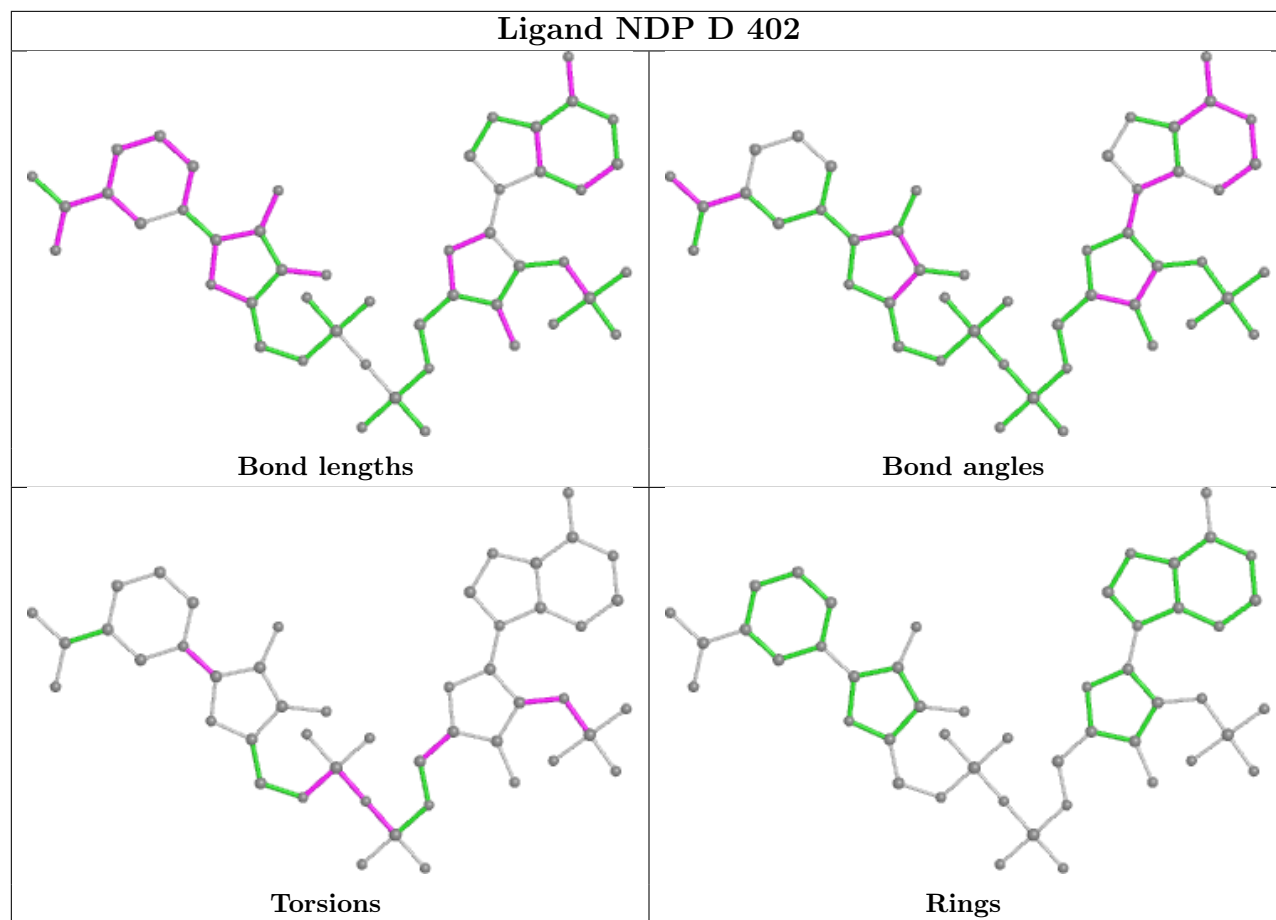
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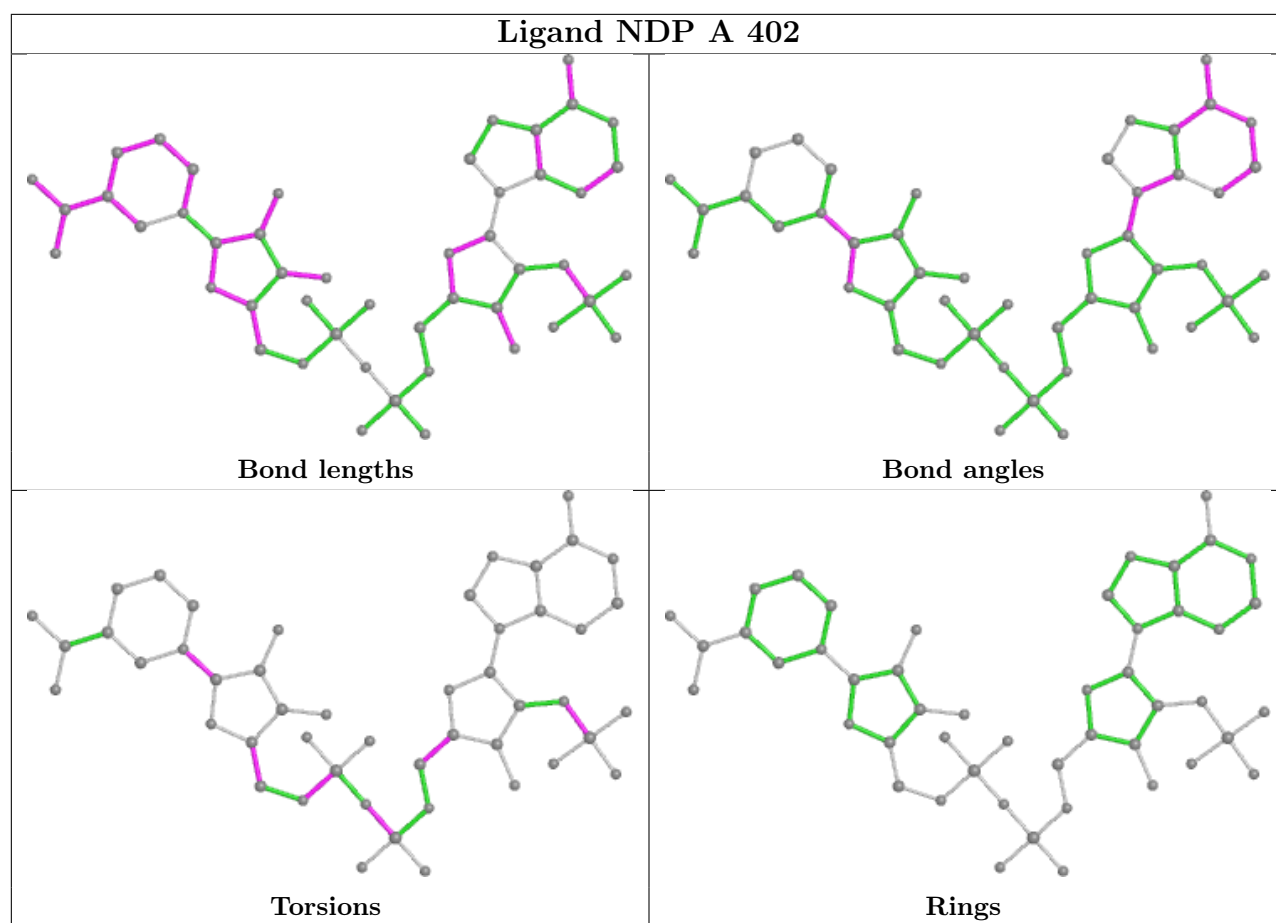
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	GO6	1	0
3	E	402	NDP	5	0
2	C	401	GO6	2	0

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.

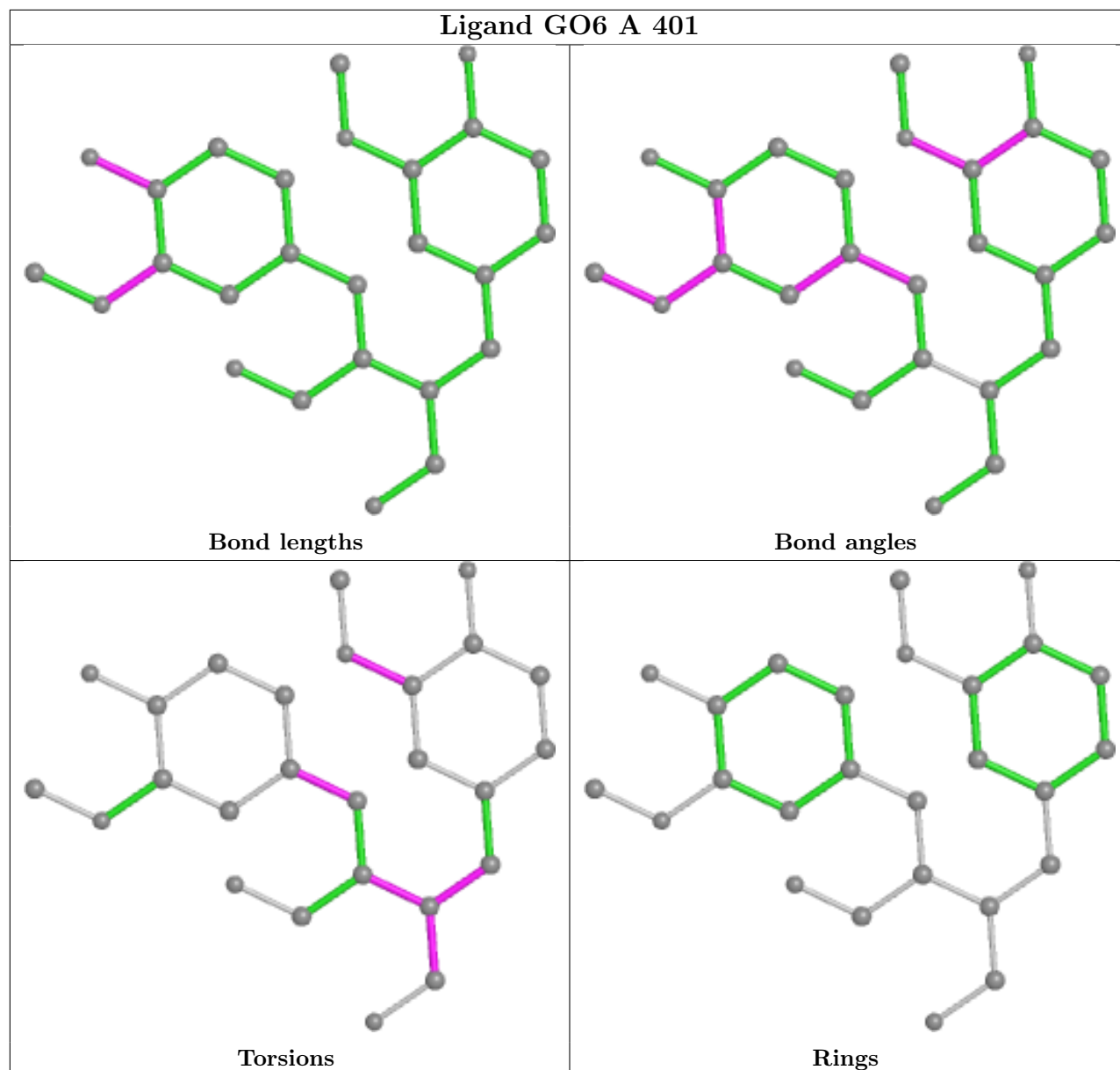




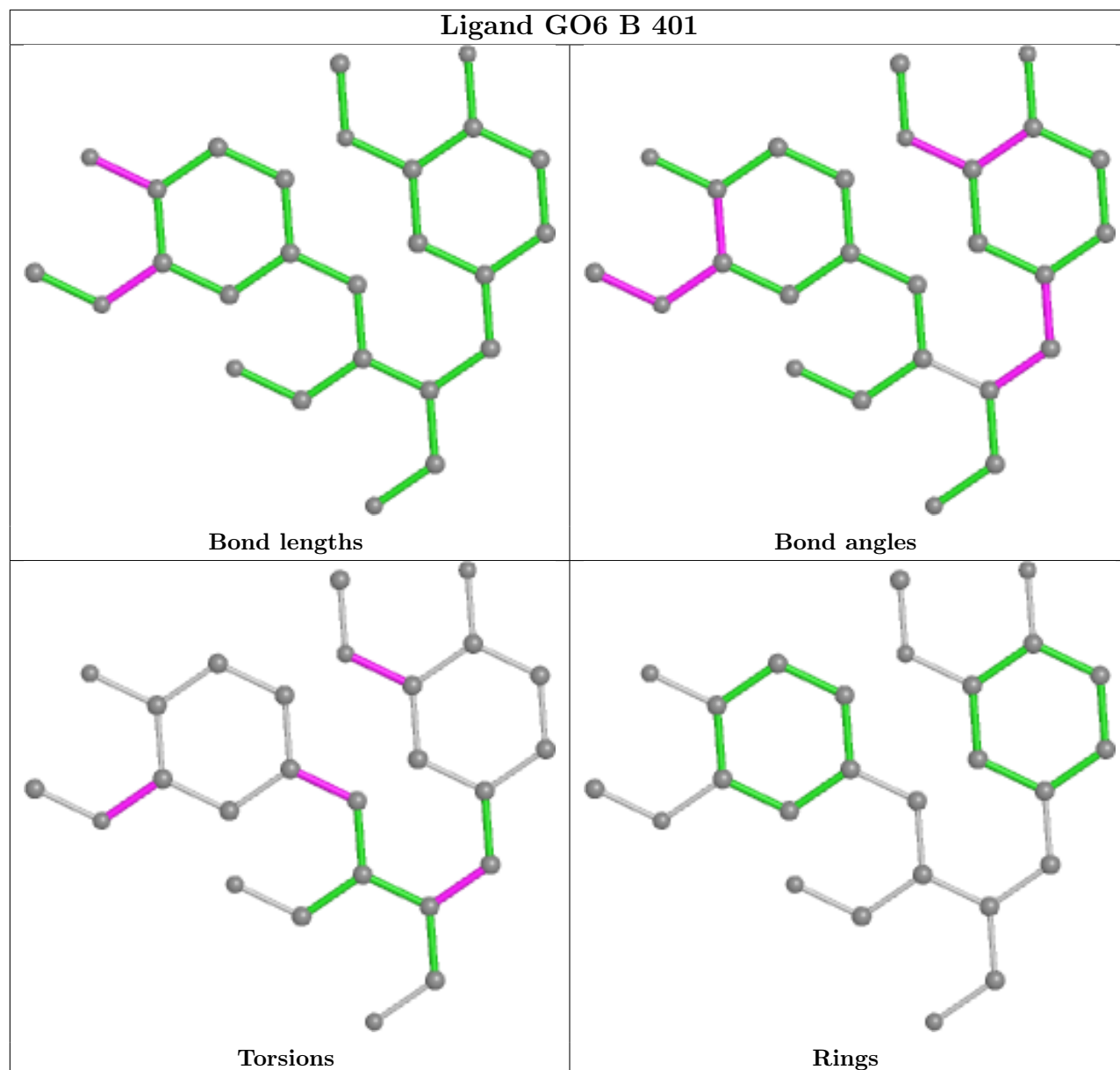


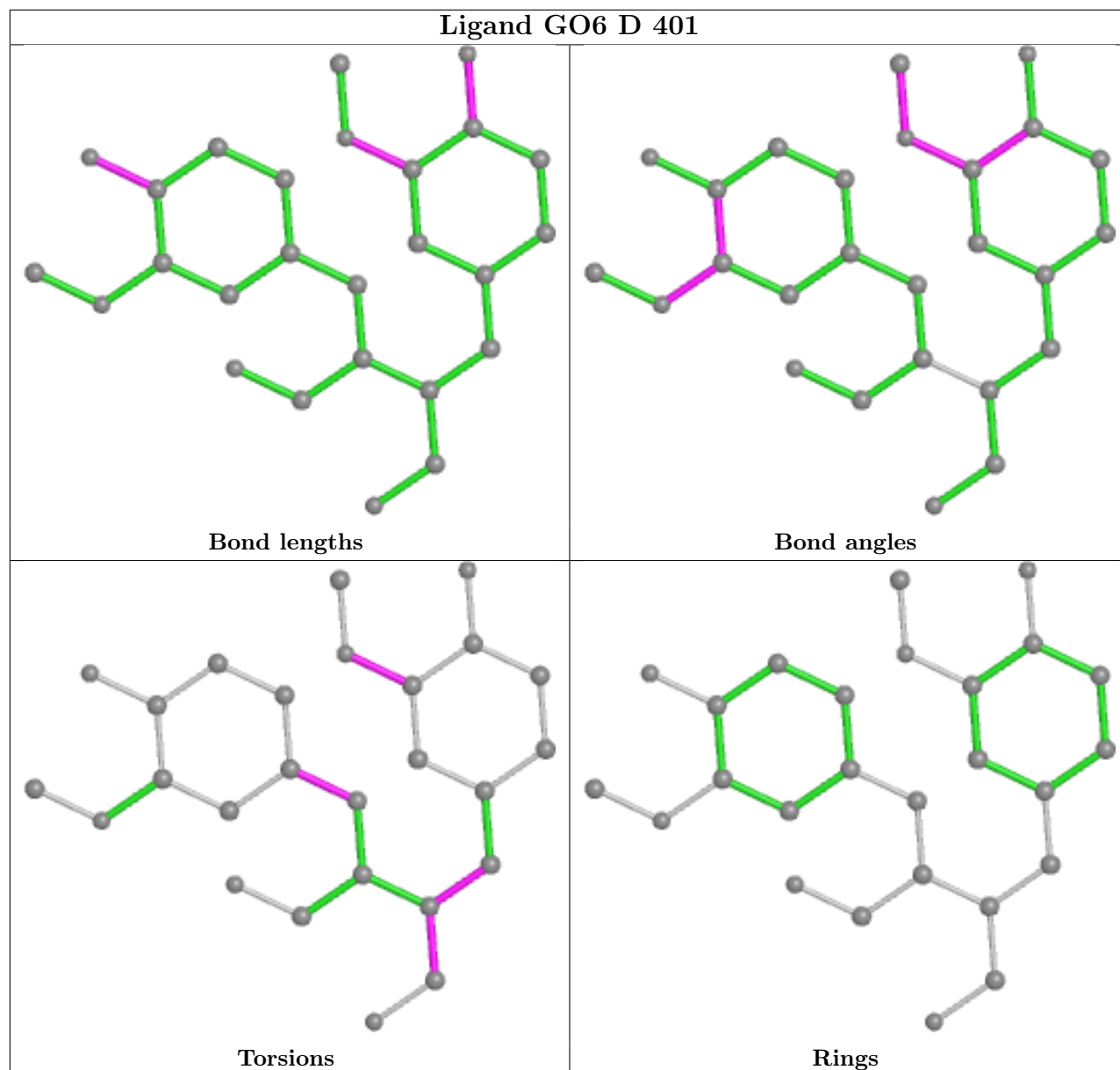


Ligand GO6 A 401

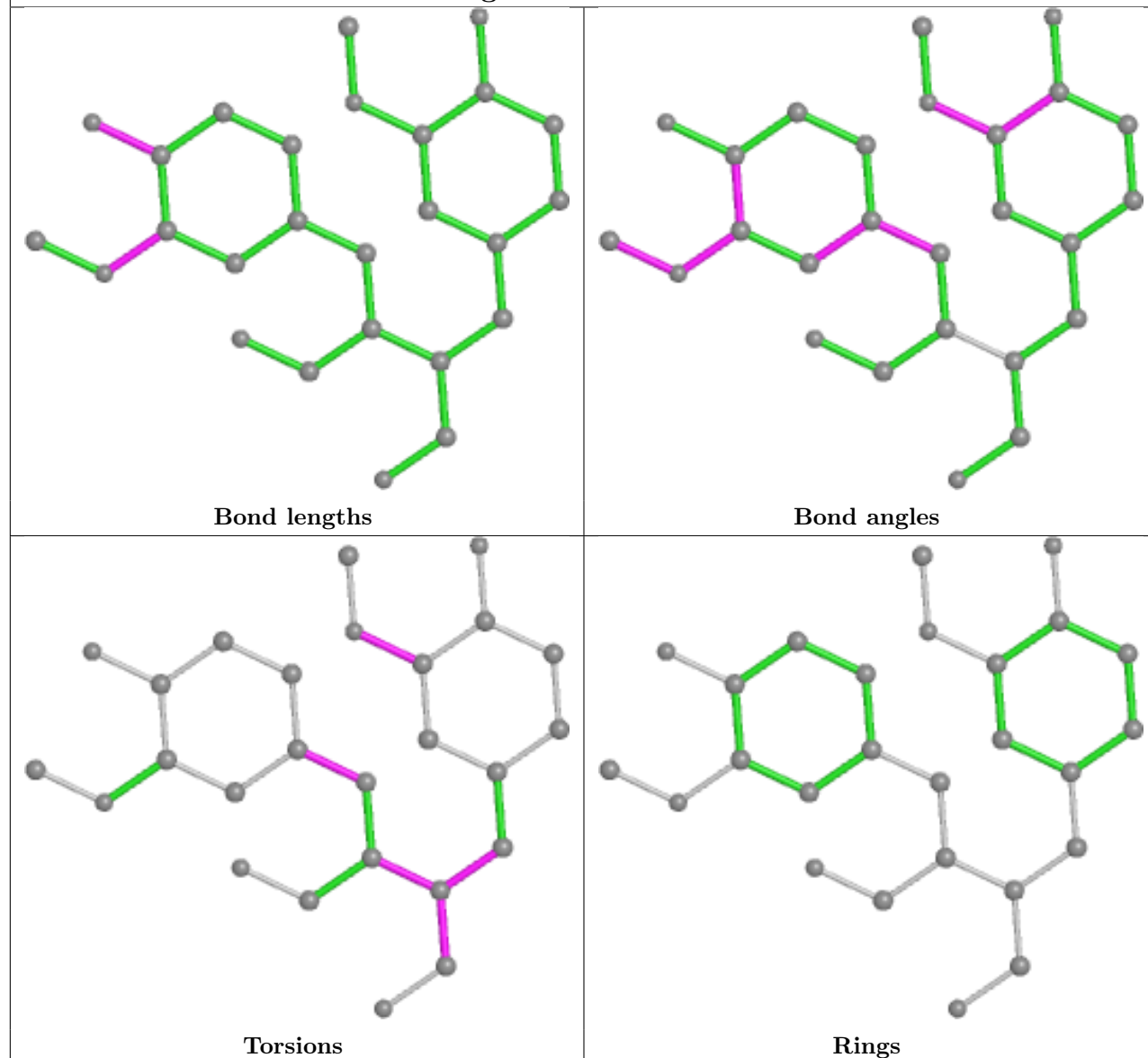


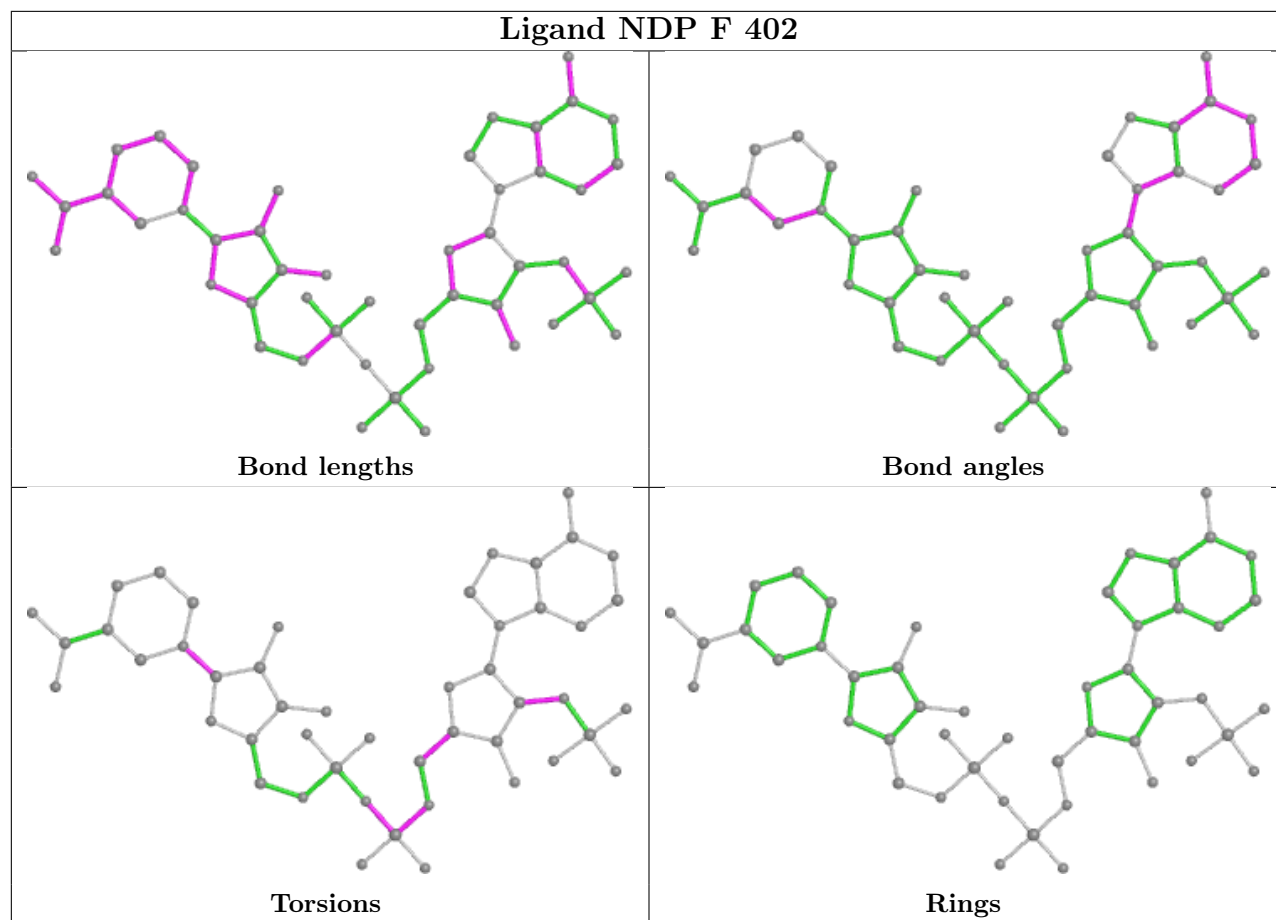
Ligand GO6 B 401



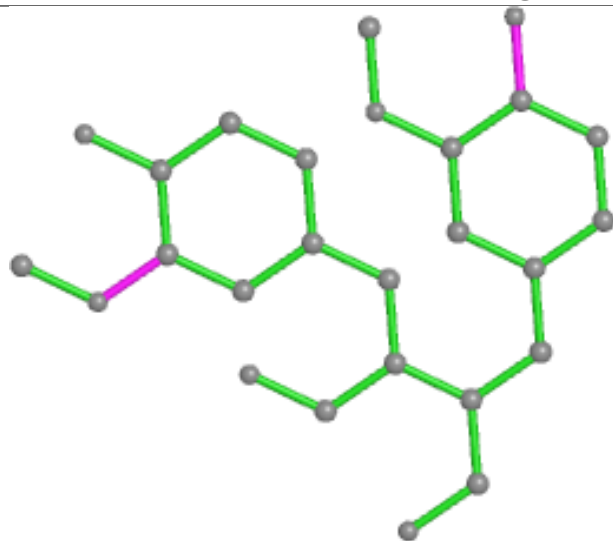


Ligand GO6 F 401

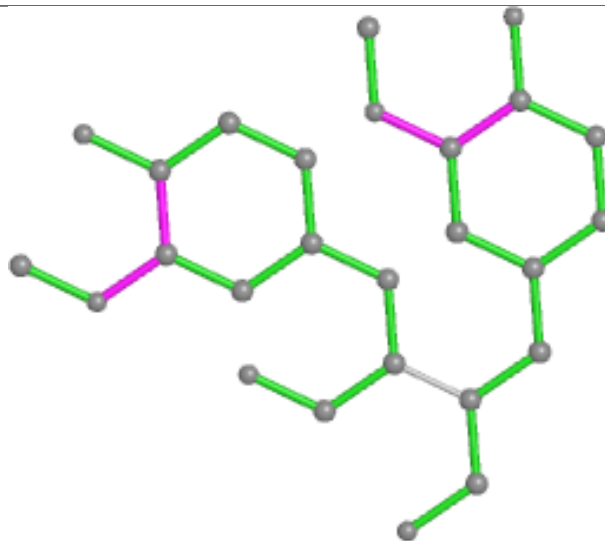




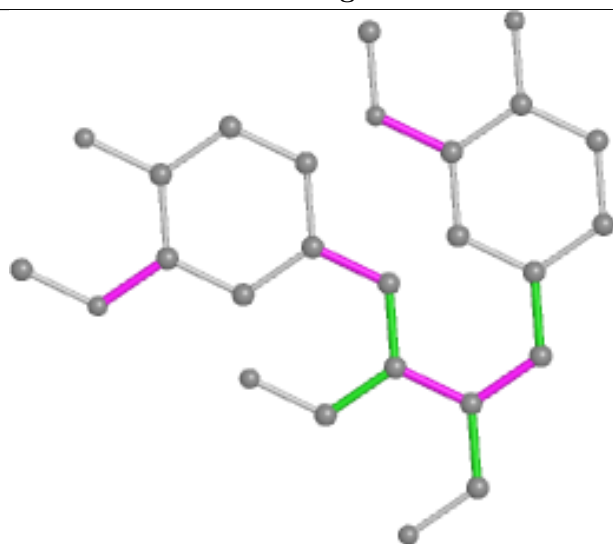
Ligand GO6 E 401



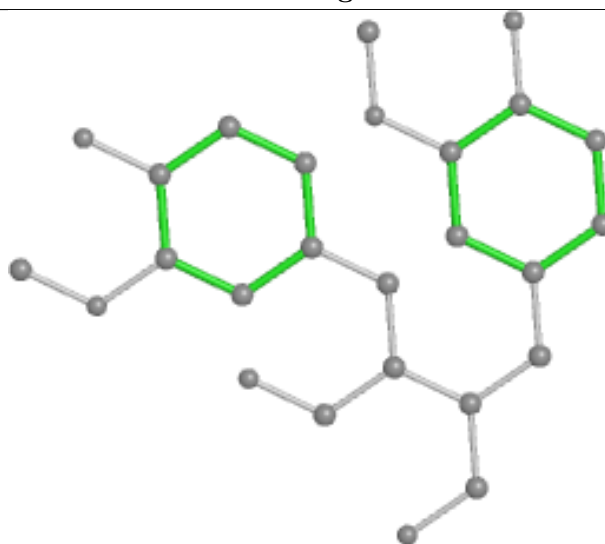
Bond lengths



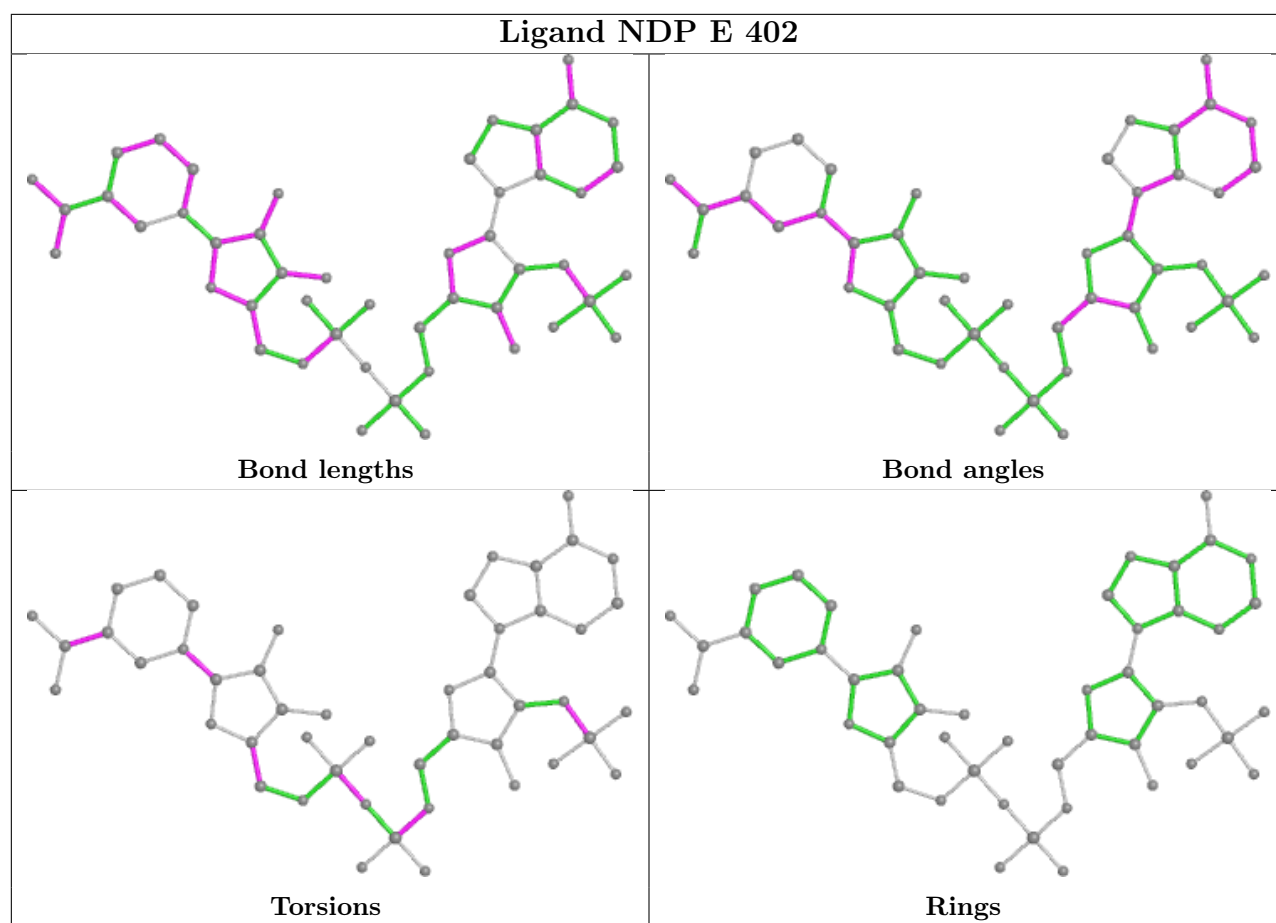
Bond angles

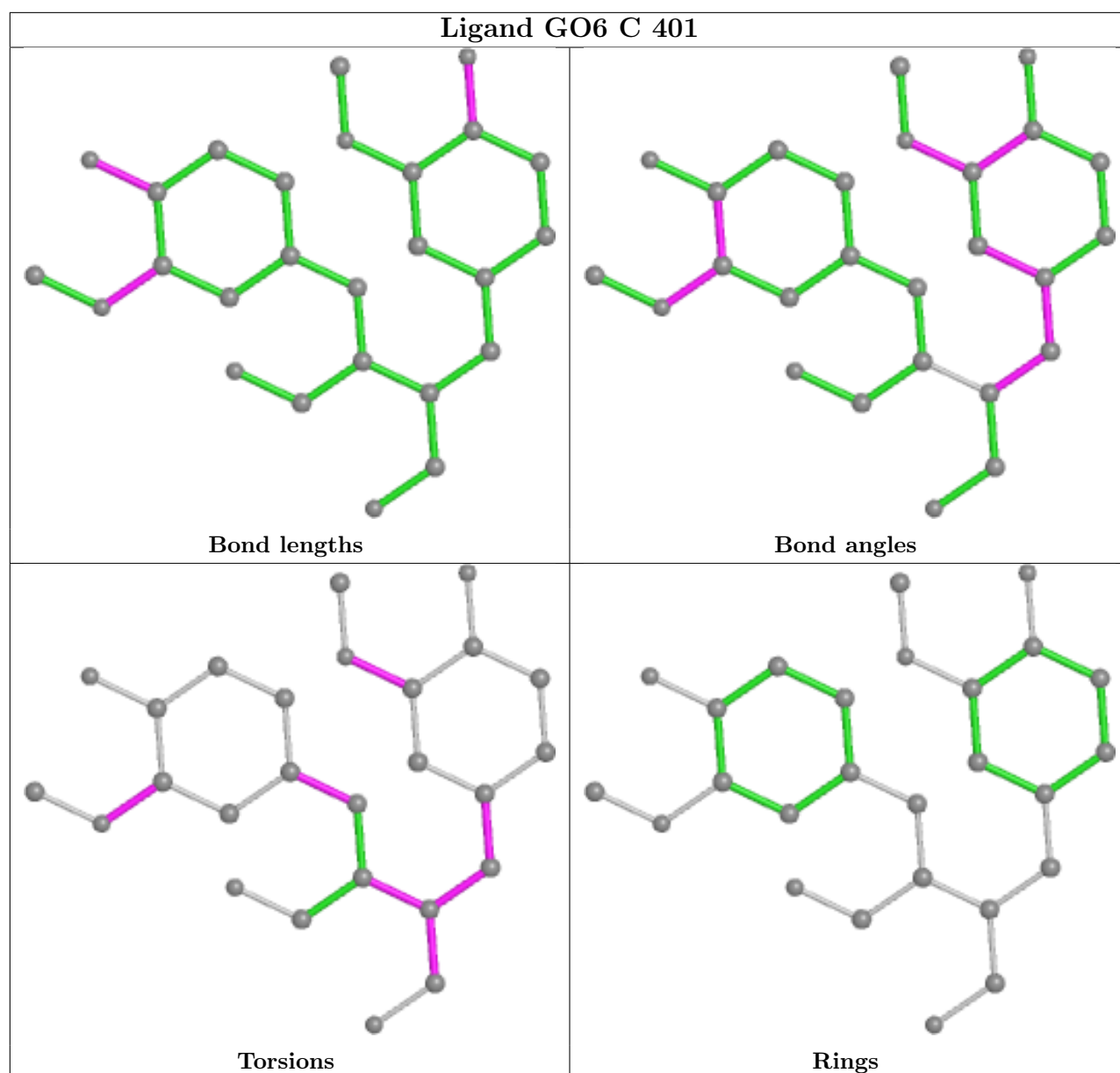


Torsions



Rings





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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

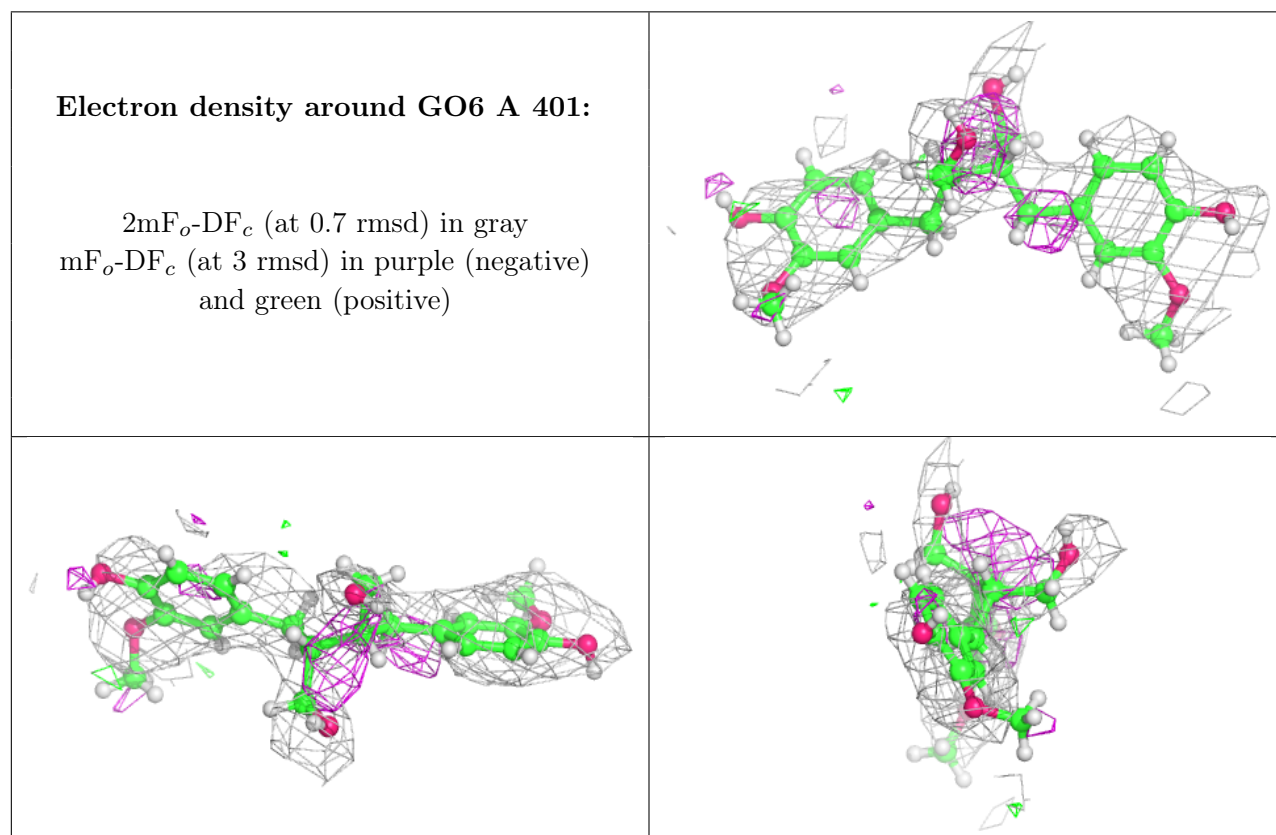
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

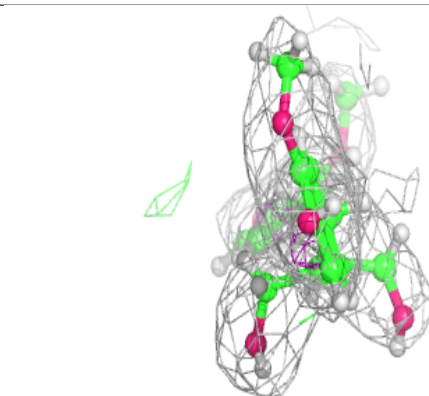
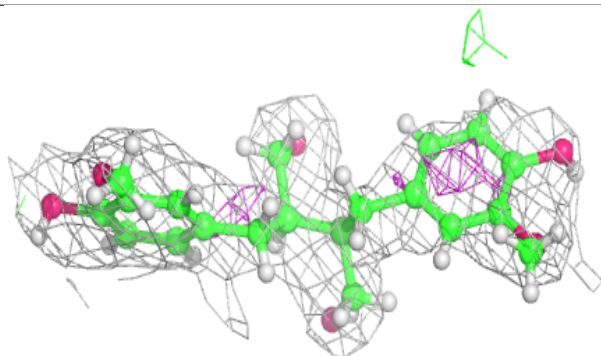
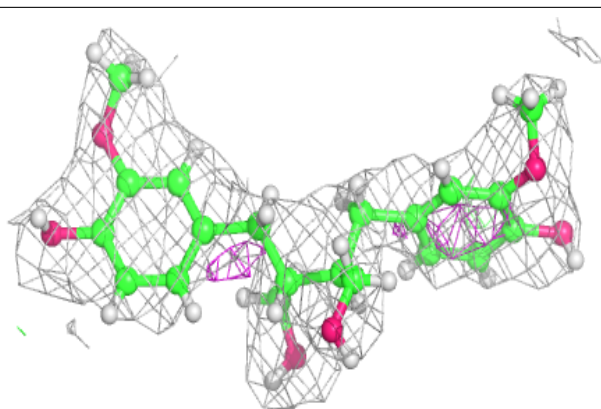
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

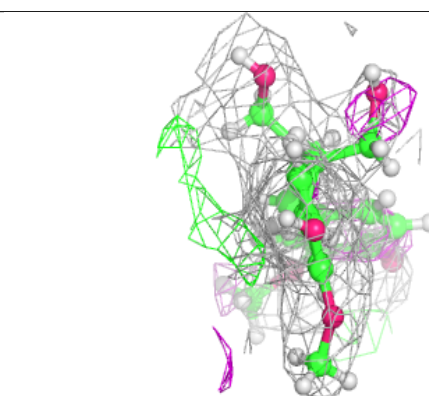
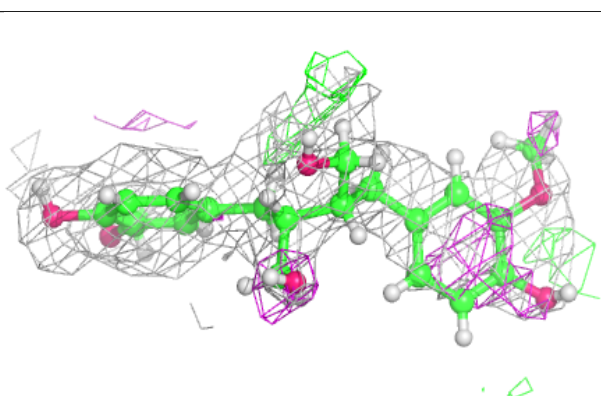
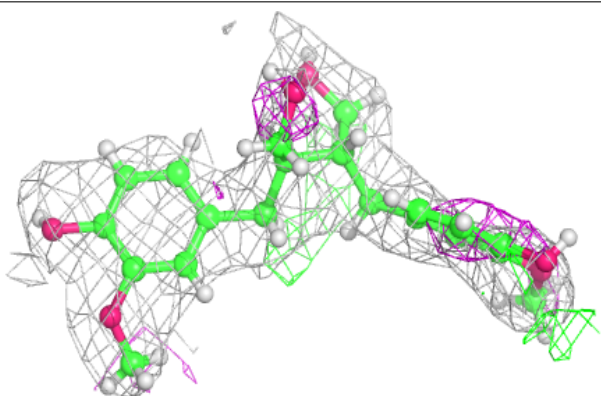


Electron density around GO6 B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

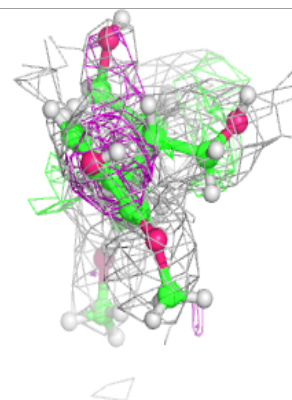
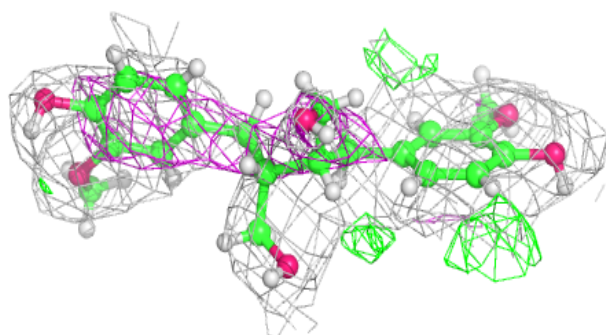
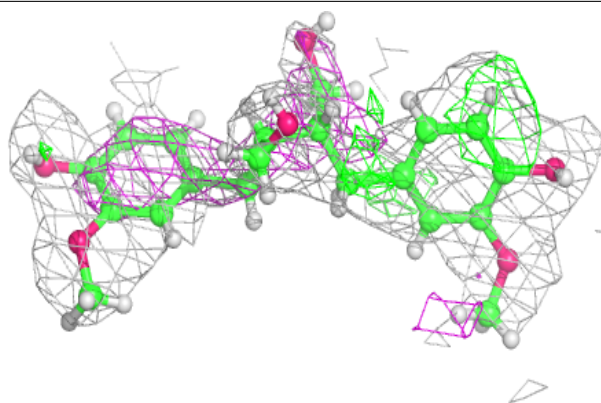
**Electron density around GO6 C 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

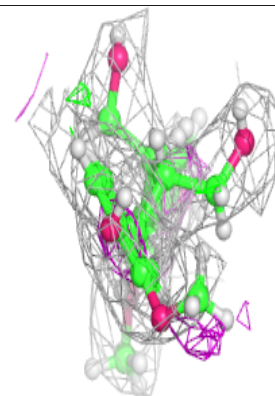
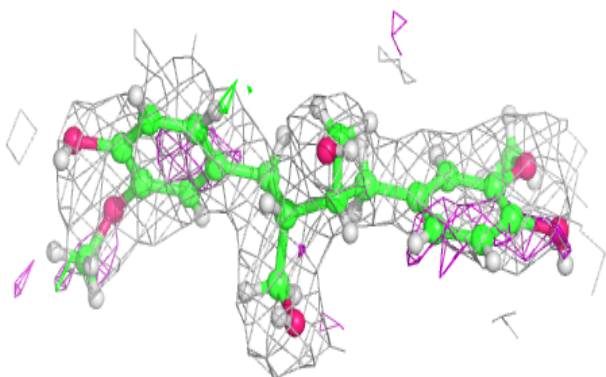
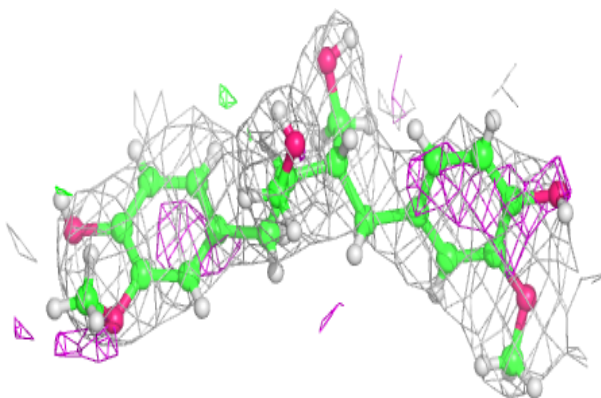


Electron density around GO6 D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

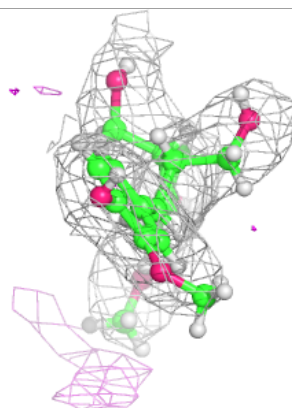
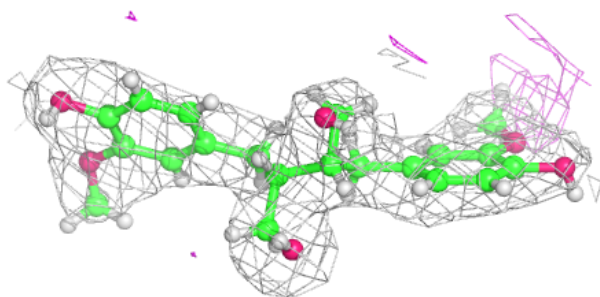
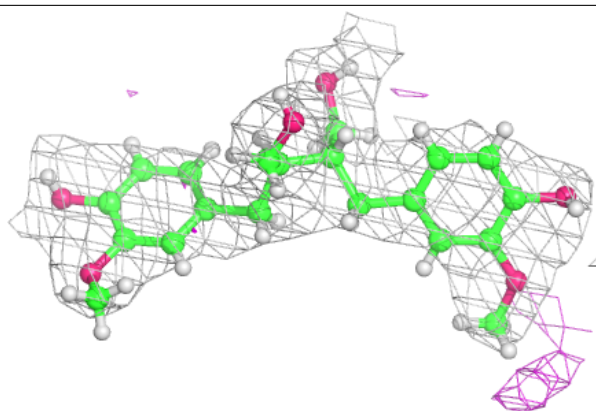
**Electron density around GO6 E 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

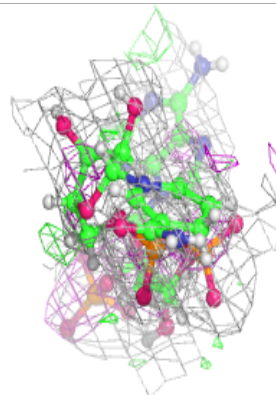
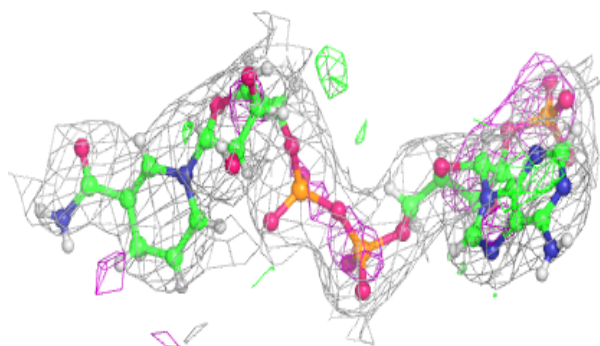
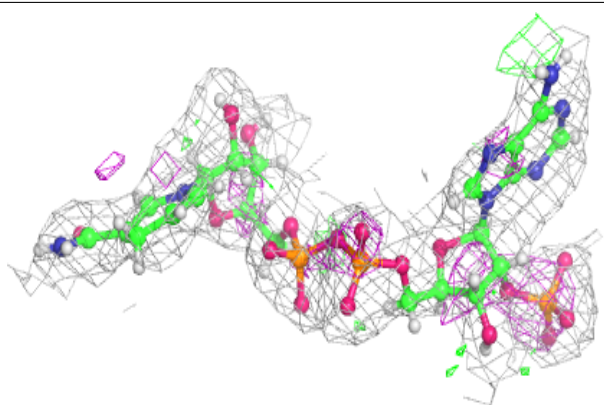


Electron density around GO6 F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

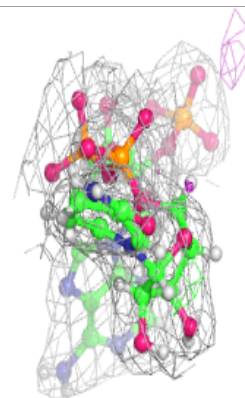
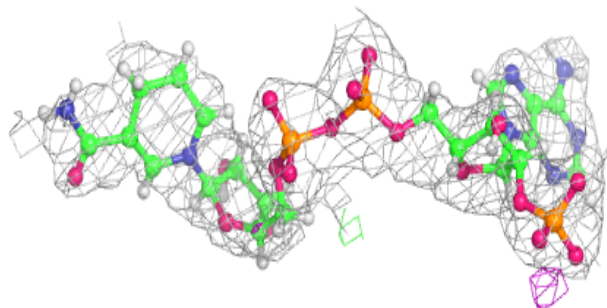
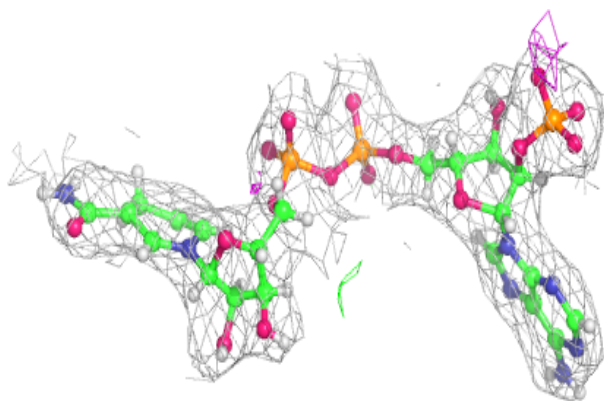
**Electron density around NDP A 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

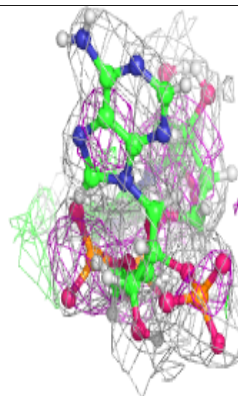
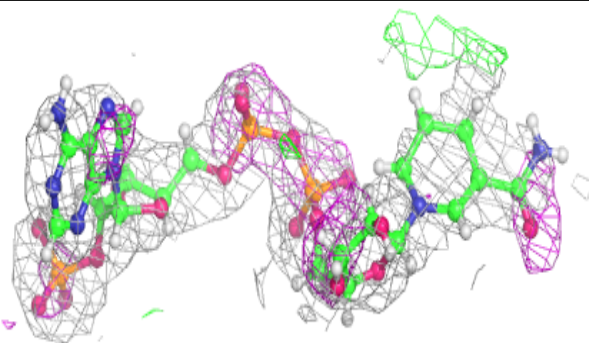
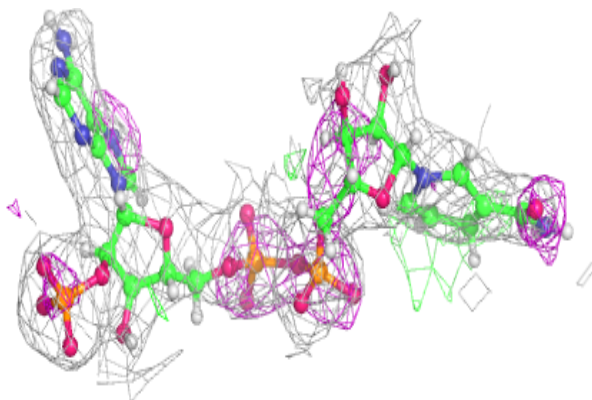


Electron density around NDP B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

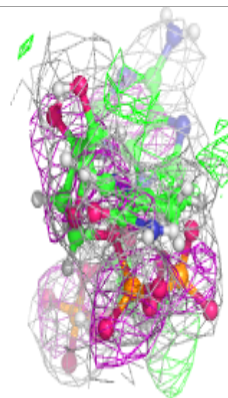
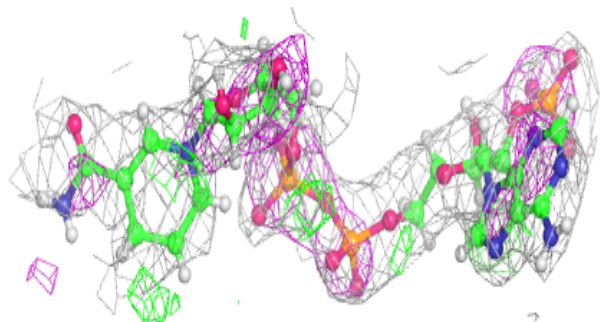
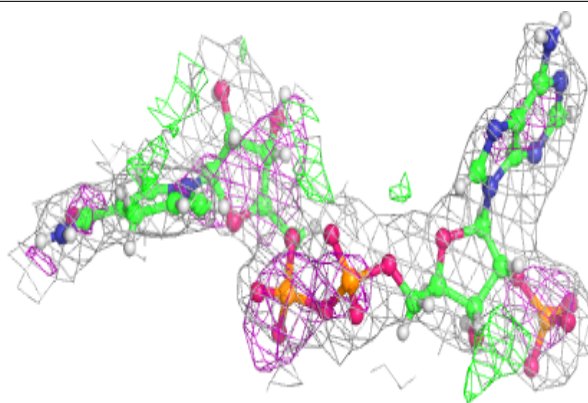
**Electron density around NDP C 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

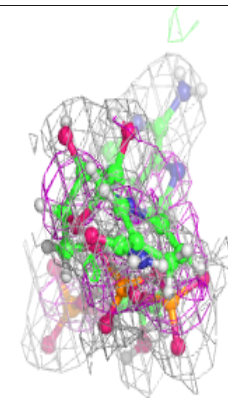
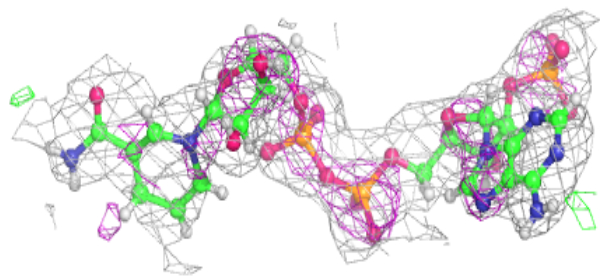
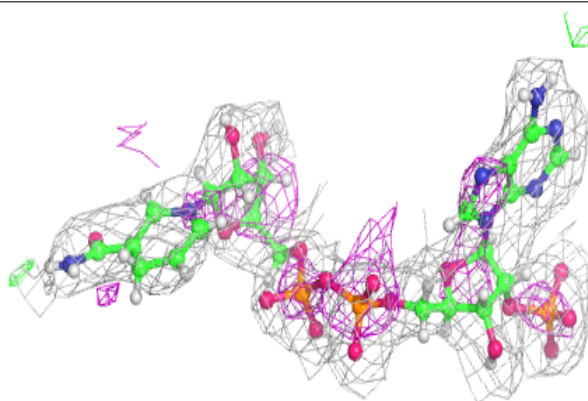


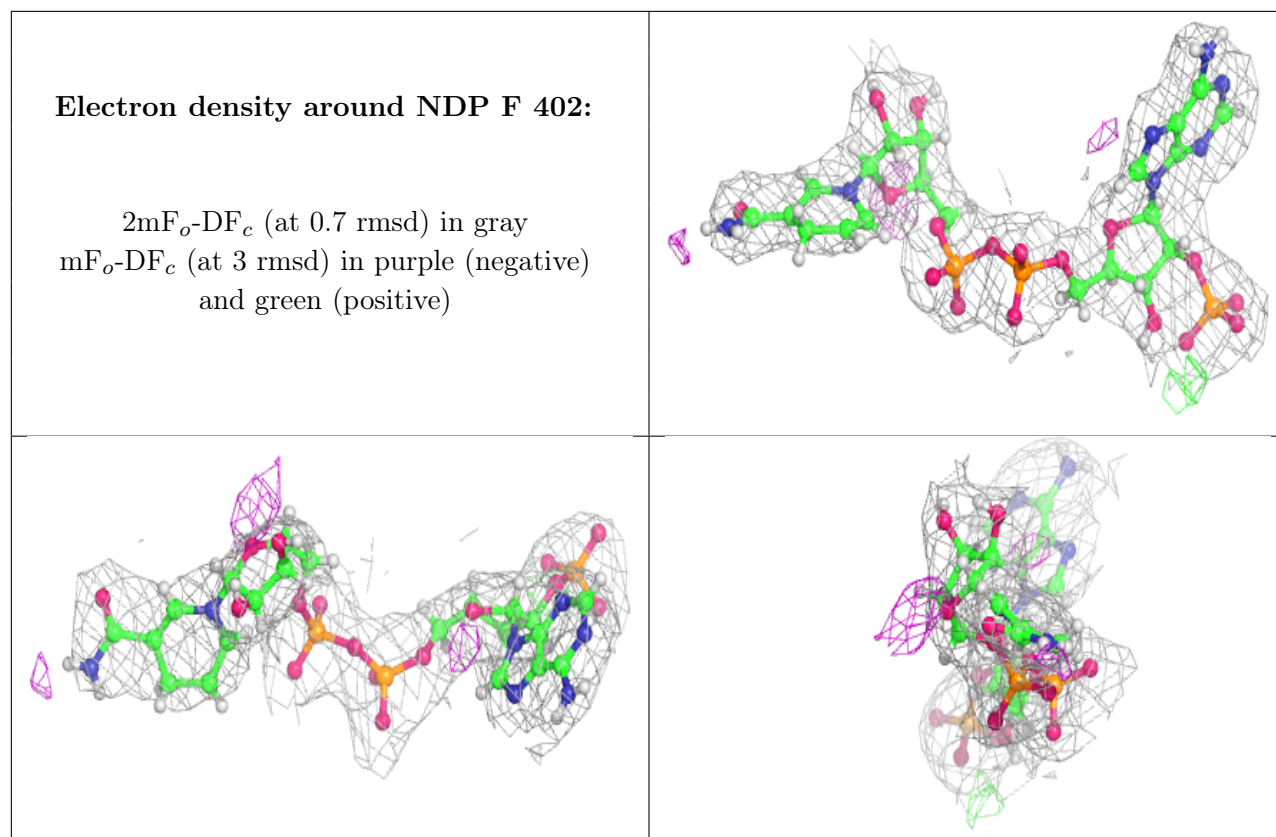
Electron density around NDP D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP E 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.