



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2026 – 02:08 AM UTC

PDB ID : 8UPP / pdb_00008upp
Title : Campylobacter jejuni ketol-acid reductoisomerase in complex with NADPH and Hoe704
Authors : Lin, X.; Lv, Y.; Lonhienne, T.; Guddat, L.W.
Deposited on : 2023-10-23
Resolution : 1.78 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

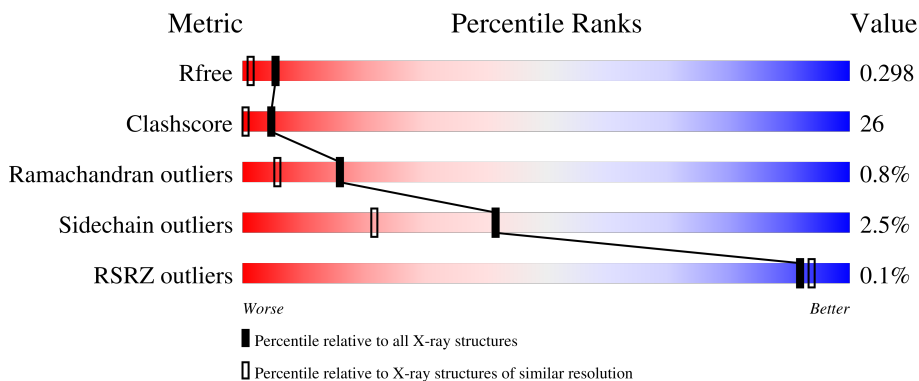
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	65% 32% ..
1	B	330	64% 33% ..
1	C	330	62% 34% ..
1	D	330	69% 28% ..
1	E	330	65% 33% ..

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Mol	Chain	Length	Quality of chain
1	F	330	 67% 31% ..
1	G	330	 63% 35% ..
1	H	330	 59% 39% ..
1	I	330	 56% 40% ...
1	J	330	 62% 35% ...
1	K	330	 66% 31% ..
1	L	330	 60% 37% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32370 atoms, of which 96 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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	327	2495	1582	424	473	16	0	1	0
1	H	327	2495	1582	424	473	16	0	1	0
1	K	327	2495	1582	424	473	16	0	1	0
1	I	327	2495	1582	424	473	16	0	1	0
1	D	327	2495	1582	424	473	16	0	1	0
1	G	327	2495	1582	424	473	16	0	1	0
1	J	327	2495	1582	424	473	16	0	1	0
1	E	327	2495	1582	424	473	16	0	1	0
1	L	327	2495	1582	424	473	16	0	1	0
1	C	327	2495	1582	424	473	16	0	1	0
1	F	327	2495	1582	424	473	16	0	1	0
1	A	327	2495	1582	424	473	16	0	1	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

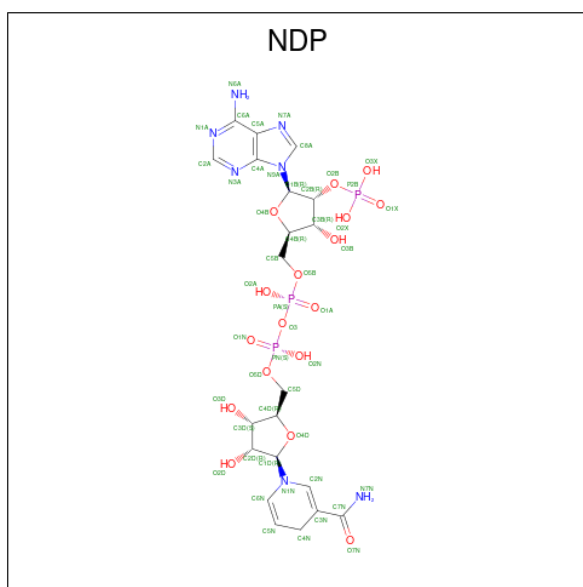
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0

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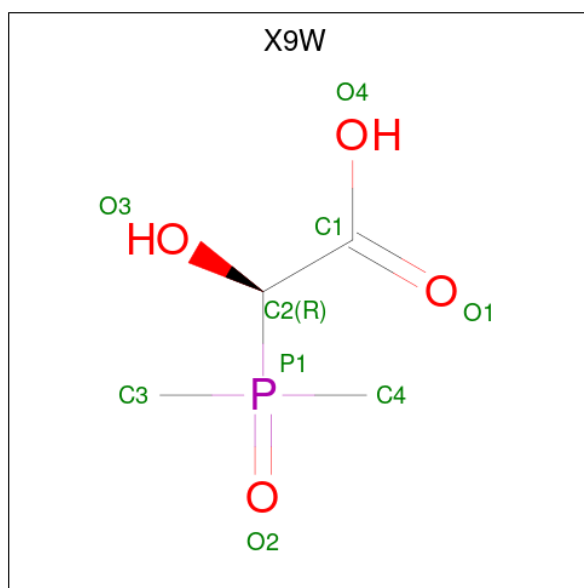
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	2	Total Mg 2 2	0	0
2	I	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	L	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (2R)-(dimethylphosphoryl)(hydroxy)acetic acid (CCD ID: X9W) (formula: C₄H₉O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	H	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	H	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	I	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	D	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	G	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	J	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	E	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	L	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	C	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	F	1	Total	C	H	O	P	0	0
			17	4	8	4	1		
4	A	1	Total	C	H	O	P	0	0
			17	4	8	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	142	Total	O	0	0
			142	142		
5	H	141	Total	O	0	0
			141	141		
5	K	114	Total	O	0	0
			114	114		
5	I	135	Total	O	0	0
			135	135		
5	D	127	Total	O	0	0
			127	127		
5	G	136	Total	O	0	0
			136	136		
5	J	145	Total	O	0	0
			145	145		
5	E	142	Total	O	0	0
			142	142		

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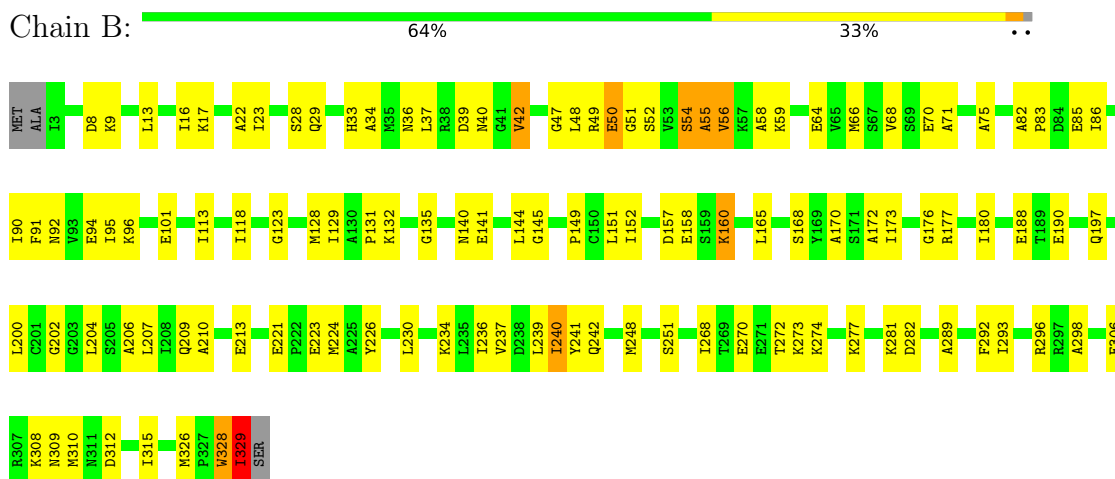
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	123	Total 123	O 123	0	0
5	C	124	Total 124	O 124	0	0
5	F	146	Total 146	O 146	0	0
5	A	151	Total 151	O 151	0	0

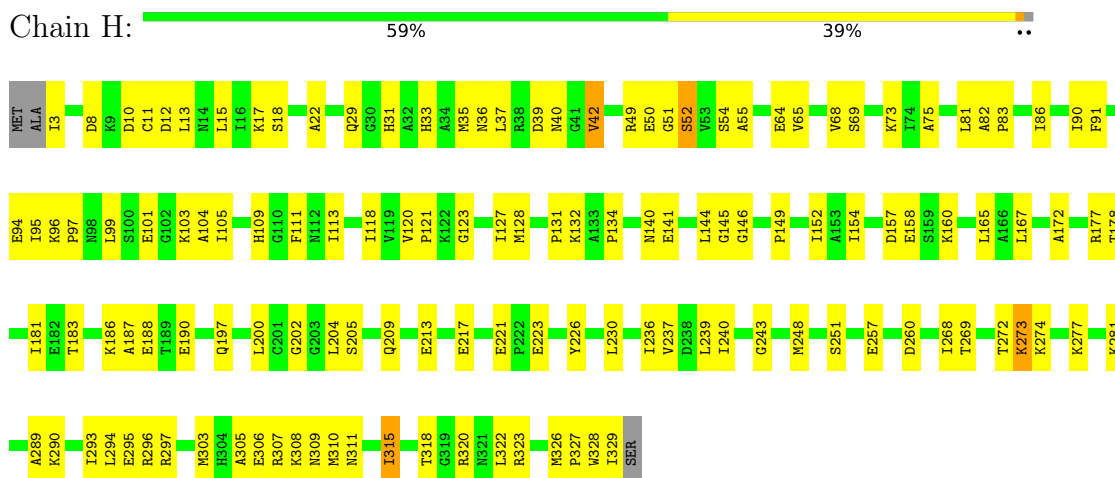
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

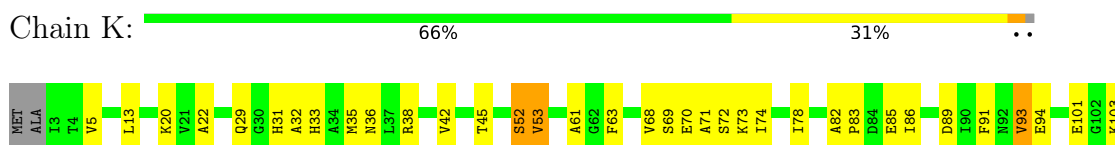
- Molecule 1: Ketol-acid reductoisomerase

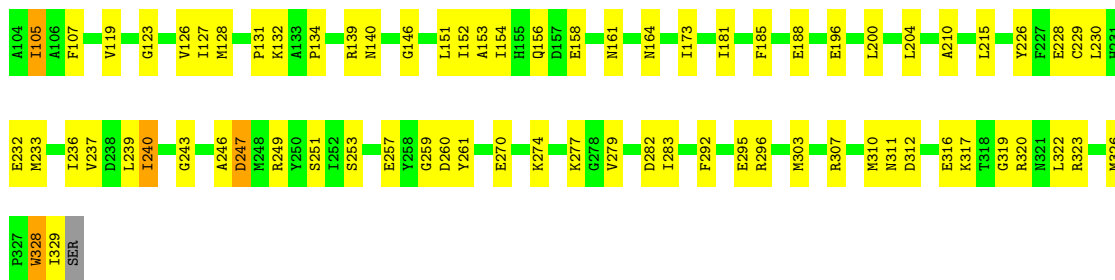


- Molecule 1: Ketol-acid reductoisomerase

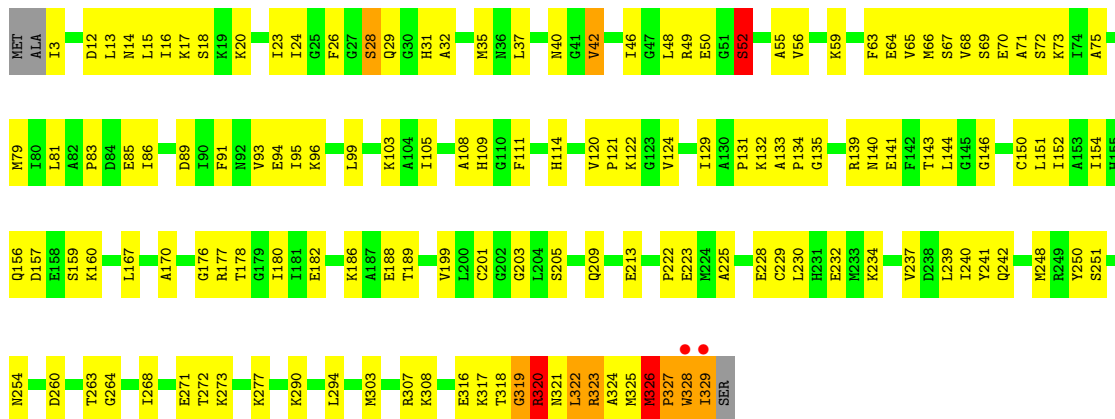


- Molecule 1: Ketol-acid reductoisomerase





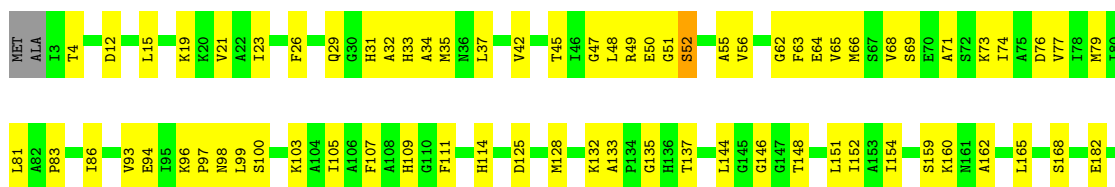
• Molecule 1: Ketol-acid reductoisomerase

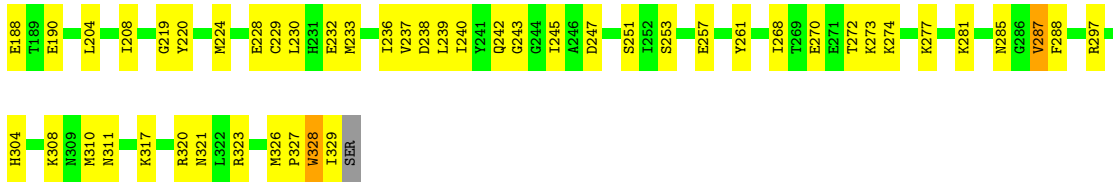


• Molecule 1: Ketol-acid reductoisomerase



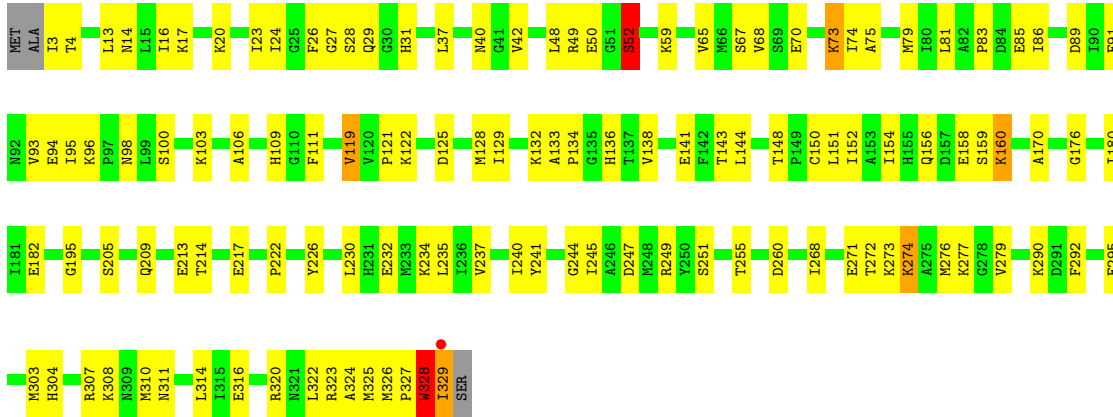
• Molecule 1: Ketol-acid reductoisomerase





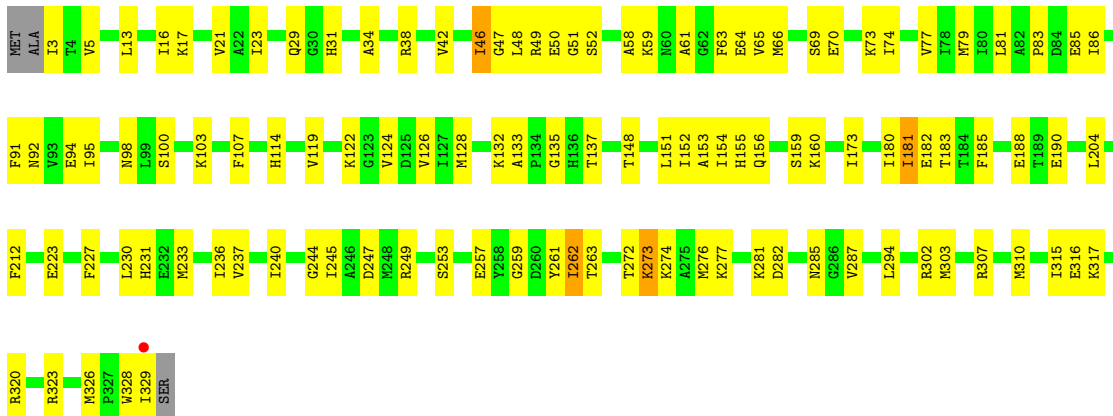
- Molecule 1: Ketol-acid reductoisomerase

Chain J: 62% 35% ...



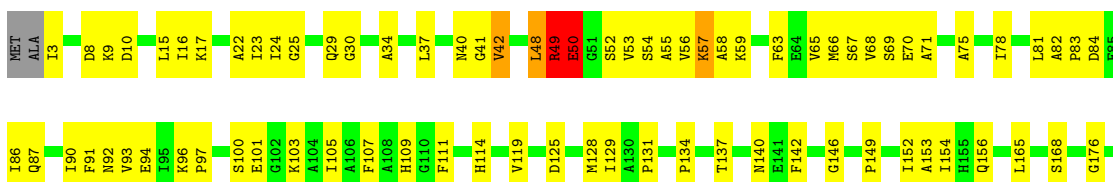
- Molecule 1: Ketol-acid reductoisomerase

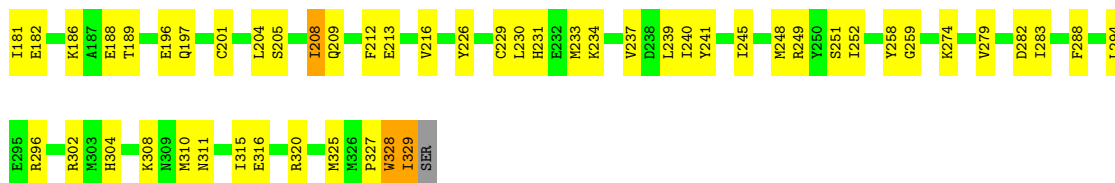
Chain E: 65% 33% ..



- Molecule 1: Ketol-acid reductoisomerase

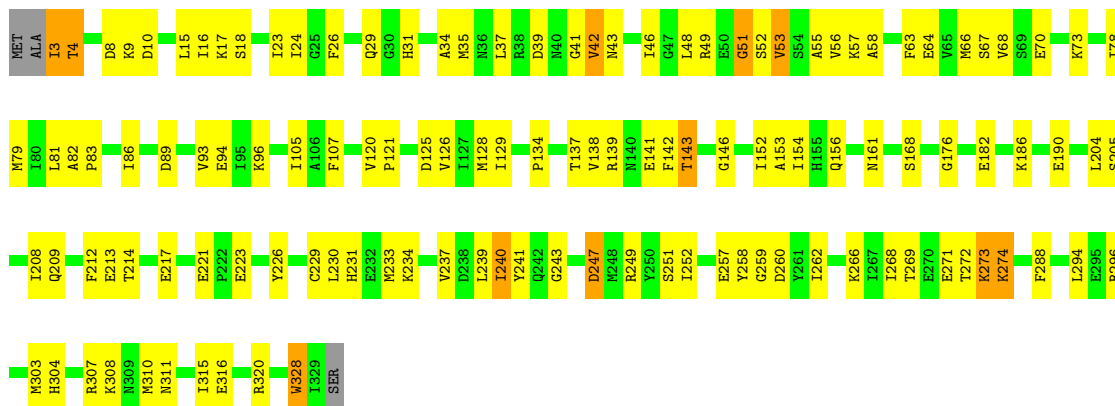
Chain L: 60% 37% ...





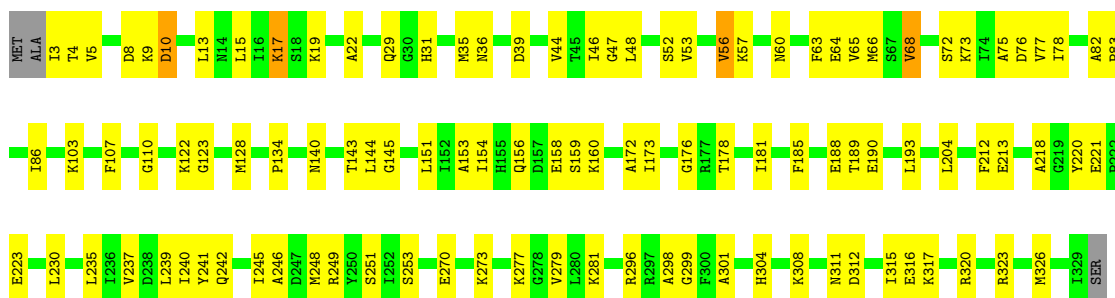
• Molecule 1: Ketol-acid reductoisomerase

Chain C: 62% 34%



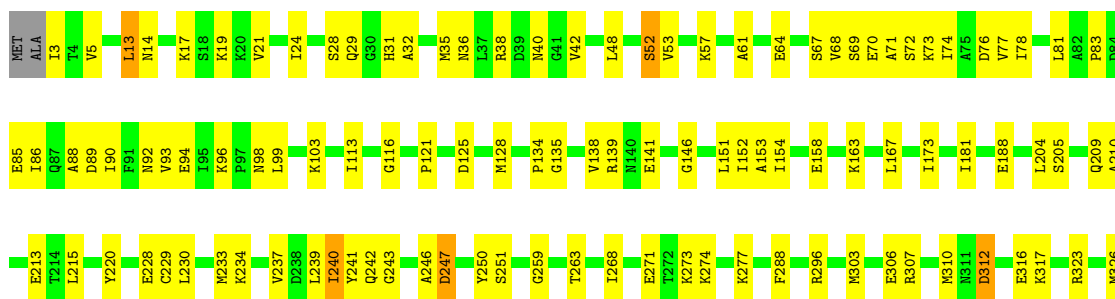
• Molecule 1: Ketol-acid reductoisomerase

Chain F: 67% 31%



• Molecule 1: Ketol-acid reductoisomerase

Chain A: 65% 32%





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.95Å 111.95Å 111.94Å 110.91° 107.73° 109.76°	Depositor
Resolution (Å)	34.35 – 1.78 34.35 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.35-1.78) 93.2 (34.35-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.264 , 0.298 0.264 , 0.298	Depositor DCC
R_{free} test set	1907 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 21.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage

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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.

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Property	Value	Source
Estimated twinning fraction	0.096 for -k,h+k+1,-h 0.096 for -l,-h,h+k+1 0.097 for -k,-l,h+k+1 0.097 for h+k+1,-h,-k 0.089 for h+k+1,-l,-h 0.089 for -l,h+k+1,-k 0.109 for -h-k-l,h,l 0.109 for k,-h-k-l,l 0.108 for l,k,-h-k-l 0.108 for -h-k-l,k,h 0.108 for h,-h-k-l,k 0.108 for h,l,-h-k-l 0.108 for l,h,k 0.108 for k,l,h 0.457 for -h-k-l,l,k 0.096 for -h,-l,-k 0.468 for l,-h-k-l,h 0.097 for -l,-k,-h 0.457 for k,h,-h-k-l 0.089 for -k,-h,-l 0.096 for h+k+1,-k,-l 0.098 for -h,h+k+1,-l 0.090 for -h,-k,h+k+1	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32370	wwPDB-VP
Average B, all atoms (\AA^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MG, NDP, X9W

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	0.39	0/2539	0.58	0/3422
1	B	0.38	0/2539	0.57	1/3422 (0.0%)
1	C	0.37	0/2539	0.54	0/3422
1	D	0.40	0/2539	0.55	0/3422
1	E	0.49	1/2539 (0.0%)	0.54	0/3422
1	F	0.43	0/2539	0.56	0/3422
1	G	0.40	0/2539	0.55	0/3422
1	H	0.36	0/2539	0.56	0/3422
1	I	0.39	1/2539 (0.0%)	0.55	0/3422
1	J	0.39	0/2539	0.57	0/3422
1	K	0.39	0/2539	0.57	0/3422
1	L	0.37	0/2539	0.56	0/3422
All	All	0.40	2/30468 (0.0%)	0.56	1/41064 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	46	ILE	C-N	14.11	1.40	1.33
1	I	46	ILE	C-N	-5.17	1.31	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	329	ILE	N-CA-C	-6.08	93.98	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	TRP	Peptide
1	I	326	MET	Peptide
1	J	50	GLU	Peptide
1	L	49	ARG	Peptide

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	2495	0	2516	131	0
1	B	2495	0	2516	144	0
1	C	2495	0	2516	124	0
1	D	2495	0	2516	148	0
1	E	2495	0	2516	133	0
1	F	2495	0	2516	126	0
1	G	2495	0	2516	141	0
1	H	2495	0	2516	142	1
1	I	2495	0	2516	195	0
1	J	2495	0	2516	160	1
1	K	2495	0	2516	116	0
1	L	2495	0	2516	139	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	48	0	26	9	0
3	B	48	0	26	7	0
3	C	48	0	26	7	0
3	D	48	0	26	10	0
3	E	48	0	26	7	0
3	F	48	0	26	4	0
3	G	48	0	26	5	0
3	H	48	0	26	12	0
3	I	48	0	26	9	0
3	J	48	0	26	7	0
3	K	48	0	26	7	0
3	L	48	0	26	7	0
4	A	9	8	0	0	0
4	B	9	8	0	0	0
4	C	9	8	0	0	0
4	D	9	8	0	1	0
4	E	9	8	0	0	0
4	F	9	8	0	1	0
4	G	9	8	0	1	0
4	H	18	16	0	1	0
4	I	9	8	0	1	0
4	J	9	8	0	1	0
4	L	9	8	0	0	0
5	A	151	0	0	22	0
5	B	142	0	0	31	0
5	C	124	0	0	18	0
5	D	127	0	0	24	0
5	E	142	0	0	20	0
5	F	146	0	0	26	1
5	G	136	0	0	16	0
5	H	141	0	0	24	0
5	I	135	0	0	30	0
5	J	145	0	0	25	1
5	K	114	0	0	23	0
5	L	123	0	0	30	0
All	All	32274	96	30504	1571	2

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 26.

The worst 5 of 1571 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)
1:H:157:ASP:O	1:H:160:LYS:NZ	1.72	1.22
1:C:73:LYS:NZ	5:C:501:HOH:O	1.80	1.15
1:J:17:LYS:NZ	1:J:40:ASN:O	1.80	1.14
1:H:178:THR:HG23	1:K:326:MET:HE3	1.27	1.14
1:G:66:MET:HE3	1:G:71:ALA:HA	1.25	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:GLU:OE1	1:J:160:LYS:NZ[1_565]	1.75	0.45
5:J:642:HOH:O	5:F:629:HOH:O[1_655]	2.16	0.04

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	326/330 (99%)	306 (94%)	18 (6%)	2 (1%)	21	9
1	B	326/330 (99%)	308 (94%)	14 (4%)	4 (1%)	10	2
1	C	326/330 (99%)	312 (96%)	11 (3%)	3 (1%)	14	4
1	D	326/330 (99%)	308 (94%)	17 (5%)	1 (0%)	36	22
1	E	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	21	9
1	F	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	21	9
1	G	326/330 (99%)	311 (95%)	13 (4%)	2 (1%)	21	9
1	H	326/330 (99%)	310 (95%)	15 (5%)	1 (0%)	36	22
1	I	326/330 (99%)	305 (94%)	16 (5%)	5 (2%)	8	1
1	J	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	21	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	326/330 (99%)	312 (96%)	12 (4%)	2 (1%)	21	9
1	L	326/330 (99%)	306 (94%)	15 (5%)	5 (2%)	8	1
All	All	3912/3960 (99%)	3717 (95%)	164 (4%)	31 (1%)	16	6

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	SER
1	B	55	ALA
1	B	56	VAL
1	K	52	SER
1	K	328	TRP

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	262/263 (100%)	256 (98%)	6 (2%)	44	25
1	B	262/263 (100%)	257 (98%)	5 (2%)	50	32
1	C	262/263 (100%)	252 (96%)	10 (4%)	29	9
1	D	262/263 (100%)	256 (98%)	6 (2%)	44	25
1	E	262/263 (100%)	254 (97%)	8 (3%)	35	14
1	F	262/263 (100%)	257 (98%)	5 (2%)	50	32
1	G	262/263 (100%)	259 (99%)	3 (1%)	65	51
1	H	262/263 (100%)	259 (99%)	3 (1%)	65	51
1	I	262/263 (100%)	253 (97%)	9 (3%)	32	12
1	J	262/263 (100%)	253 (97%)	9 (3%)	32	12
1	K	262/263 (100%)	255 (97%)	7 (3%)	39	19
1	L	262/263 (100%)	255 (97%)	7 (3%)	39	19
All	All	3144/3156 (100%)	3066 (98%)	78 (2%)	42	22

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	ILE
1	F	68	VAL
1	C	42	VAL
1	C	273	LYS
1	A	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	161	ASN
1	F	242	GLN
1	A	98	ASN
1	G	29	GLN
1	D	87	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

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
4	X9W	I	403	2	3,8,8	1.98	1 (33%)	7,12,12	2.22	4 (57%)
4	X9W	F	401	2	3,8,8	1.45	0	7,12,12	2.19	2 (28%)
4	X9W	B	404	2	3,8,8	2.18	1 (33%)	7,12,12	1.45	0
4	X9W	E	401	2	3,8,8	2.30	1 (33%)	7,12,12	1.42	2 (28%)
4	X9W	L	404	2	3,8,8	1.13	0	7,12,12	1.49	1 (14%)
3	NDP	I	404	-	51,52,52	2.59	6 (11%)	71,80,80	1.47	12 (16%)
3	NDP	B	403	-	51,52,52	2.47	10 (19%)	71,80,80	1.53	14 (19%)
3	NDP	A	404	-	51,52,52	2.42	7 (13%)	71,80,80	1.56	18 (25%)
3	NDP	G	403	-	51,52,52	2.87	10 (19%)	71,80,80	1.53	15 (21%)
3	NDP	D	403	-	51,52,52	2.44	6 (11%)	71,80,80	1.48	15 (21%)
3	NDP	E	404	-	51,52,52	2.61	8 (15%)	71,80,80	1.57	16 (22%)
4	X9W	J	403	2	3,8,8	1.80	1 (33%)	7,12,12	2.16	3 (42%)
4	X9W	C	401	2	3,8,8	1.62	0	7,12,12	1.73	2 (28%)
3	NDP	L	403	-	51,52,52	2.63	9 (17%)	71,80,80	1.41	9 (12%)
3	NDP	H	404	-	51,52,52	2.78	8 (15%)	71,80,80	1.52	11 (15%)
4	X9W	H	403	2	3,8,8	1.52	0	7,12,12	2.47	3 (42%)
3	NDP	C	404	-	51,52,52	2.73	9 (17%)	71,80,80	1.49	13 (18%)
4	X9W	G	404	2	3,8,8	2.58	1 (33%)	7,12,12	1.81	2 (28%)
4	X9W	H	405	2	3,8,8	1.77	1 (33%)	7,12,12	1.88	2 (28%)
3	NDP	K	403	-	51,52,52	2.57	9 (17%)	71,80,80	1.54	17 (23%)
4	X9W	A	401	2	3,8,8	1.50	0	7,12,12	1.42	2 (28%)
3	NDP	F	404	-	51,52,52	2.68	9 (17%)	71,80,80	1.43	11 (15%)
4	X9W	D	404	2	3,8,8	1.78	1 (33%)	7,12,12	1.61	2 (28%)
3	NDP	J	404	-	51,52,52	2.61	7 (13%)	71,80,80	1.54	17 (23%)

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
4	X9W	I	403	2	-	3/4/10/10	-
4	X9W	F	401	2	-	3/4/10/10	-
4	X9W	B	404	2	-	1/4/10/10	-
4	X9W	E	401	2	-	2/4/10/10	-
4	X9W	L	404	2	-	2/4/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	I	404	-	-	11/34/77/77	0/5/5/5
3	NDP	B	403	-	-	14/34/77/77	0/5/5/5
3	NDP	A	404	-	-	9/34/77/77	0/5/5/5
3	NDP	G	403	-	-	8/34/77/77	0/5/5/5
3	NDP	D	403	-	-	8/34/77/77	0/5/5/5
3	NDP	E	404	-	-	7/34/77/77	0/5/5/5
4	X9W	J	403	2	-	2/4/10/10	-
4	X9W	C	401	2	-	1/4/10/10	-
3	NDP	L	403	-	-	8/34/77/77	0/5/5/5
3	NDP	H	404	-	-	12/34/77/77	0/5/5/5
4	X9W	H	403	2	-	2/4/10/10	-
3	NDP	C	404	-	-	6/34/77/77	0/5/5/5
4	X9W	G	404	2	-	3/4/10/10	-
4	X9W	H	405	2	-	3/4/10/10	-
3	NDP	K	403	-	-	13/34/77/77	0/5/5/5
4	X9W	A	401	2	-	2/4/10/10	-
3	NDP	F	404	-	-	6/34/77/77	0/5/5/5
4	X9W	D	404	2	-	2/4/10/10	-
3	NDP	J	404	-	-	11/34/77/77	0/5/5/5

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	403	NDP	P2B-O2B	15.90	1.87	1.59
3	I	404	NDP	P2B-O2B	15.30	1.86	1.59
3	H	404	NDP	P2B-O2B	15.28	1.86	1.59
3	K	403	NDP	P2B-O2B	15.21	1.86	1.59
3	J	404	NDP	P2B-O2B	14.67	1.85	1.59

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	403	X9W	C4-P1-C3	4.68	112.98	106.33
3	B	403	NDP	O2B-P2B-O1X	-4.29	94.03	109.33
3	A	404	NDP	P2B-O2B-C2B	-4.21	112.18	123.43
3	H	404	NDP	O2B-P2B-O1X	-4.12	94.63	109.33
3	J	404	NDP	O2B-P2B-O1X	-3.98	95.13	109.33

There are no chirality outliers.

5 of 139 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	NDP	C5D-O5D-PN-O3
3	B	403	NDP	C5D-O5D-PN-O1N
3	B	403	NDP	O4D-C4D-C5D-O5D
3	H	404	NDP	C5B-O5B-PA-O1A
3	H	404	NDP	C5B-O5B-PA-O2A

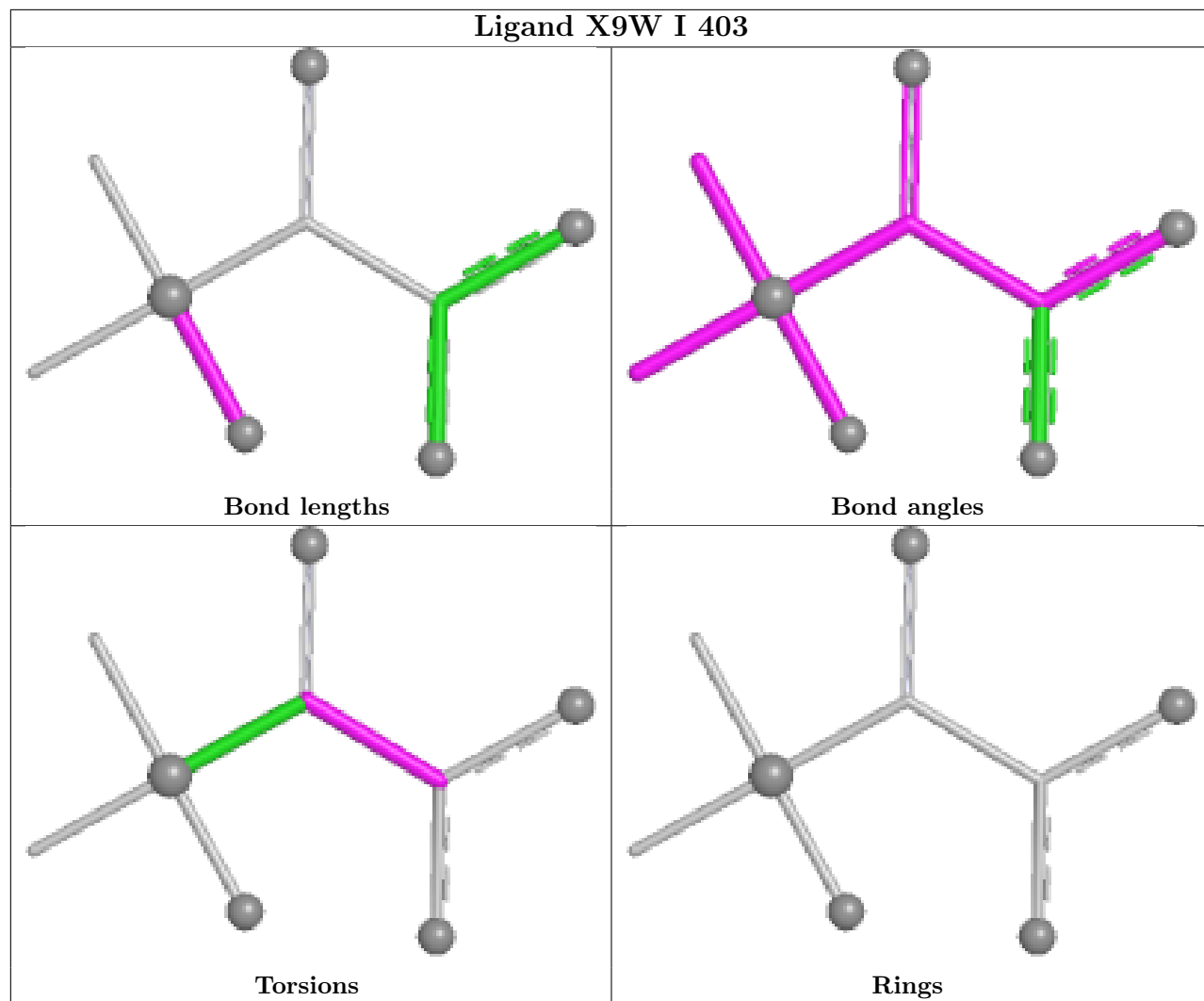
There are no ring outliers.

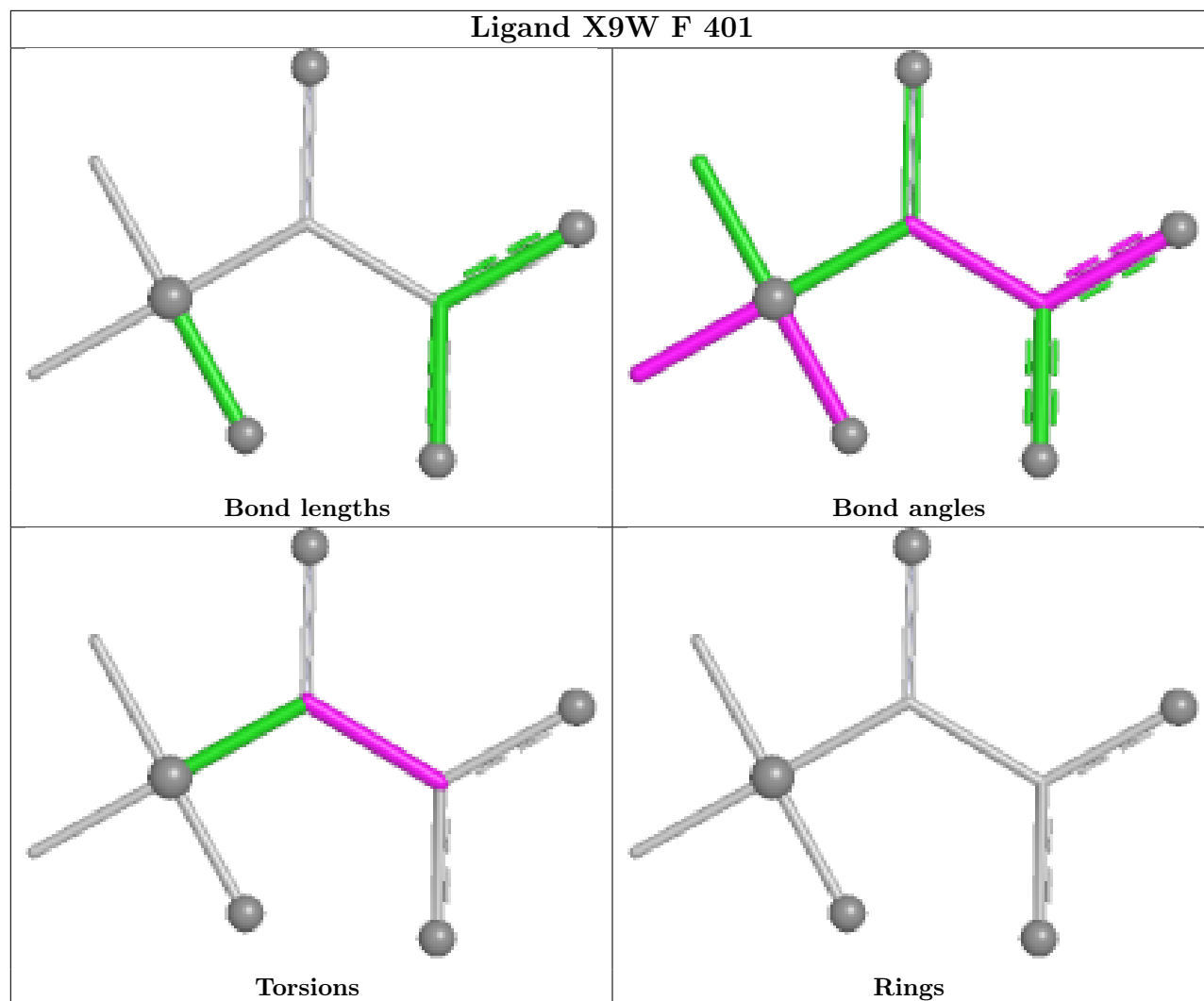
18 monomers are involved in 95 short contacts:

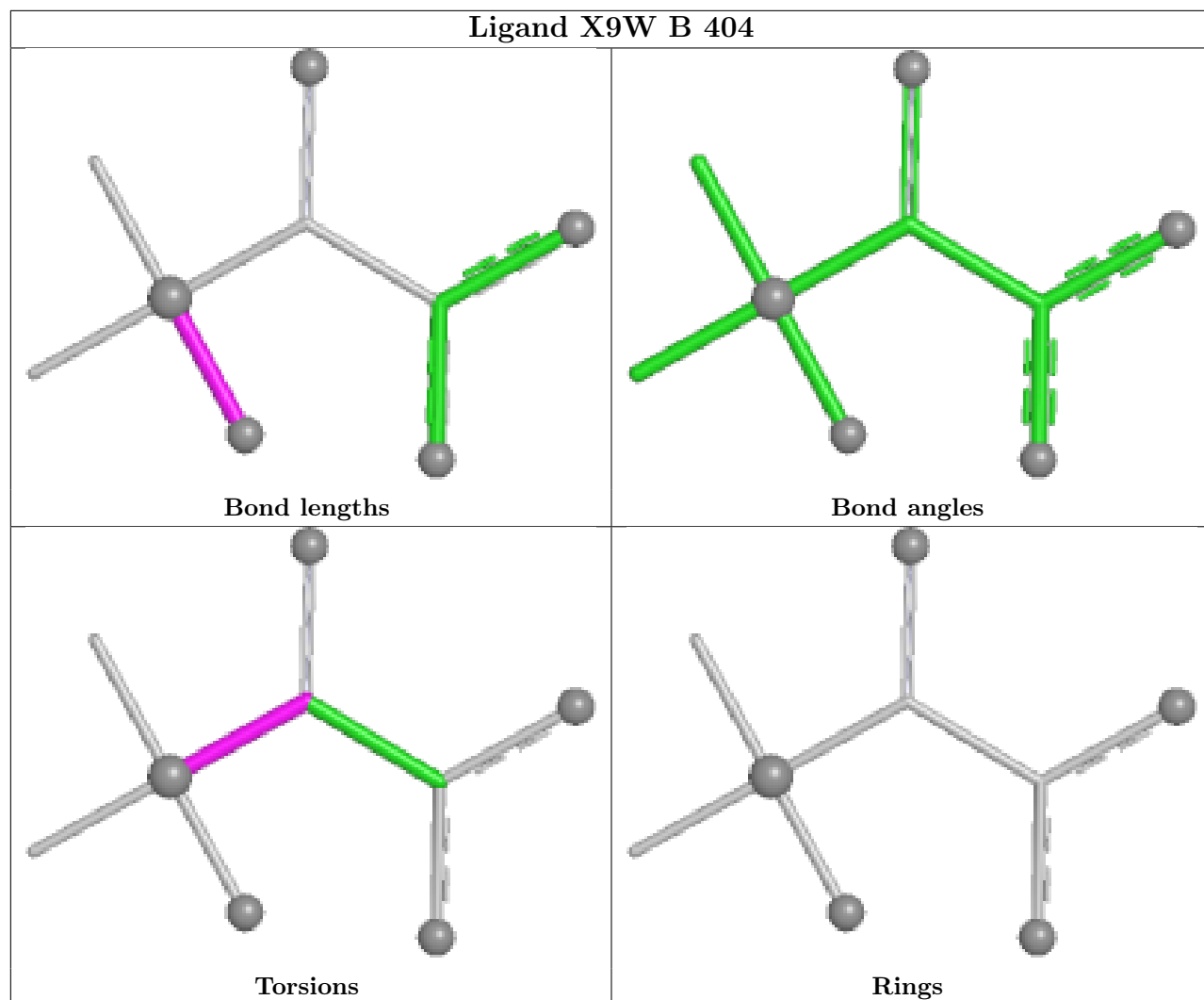
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	403	X9W	1	0
4	F	401	X9W	1	0
3	I	404	NDP	9	0
3	B	403	NDP	7	0
3	A	404	NDP	9	0
3	G	403	NDP	5	0
3	D	403	NDP	10	0
3	E	404	NDP	7	0
4	J	403	X9W	1	0
3	L	403	NDP	7	0
3	H	404	NDP	12	0
4	H	403	X9W	1	0
3	C	404	NDP	7	0
4	G	404	X9W	1	0
3	K	403	NDP	7	0
3	F	404	NDP	4	0
4	D	404	X9W	1	0
3	J	404	NDP	7	0

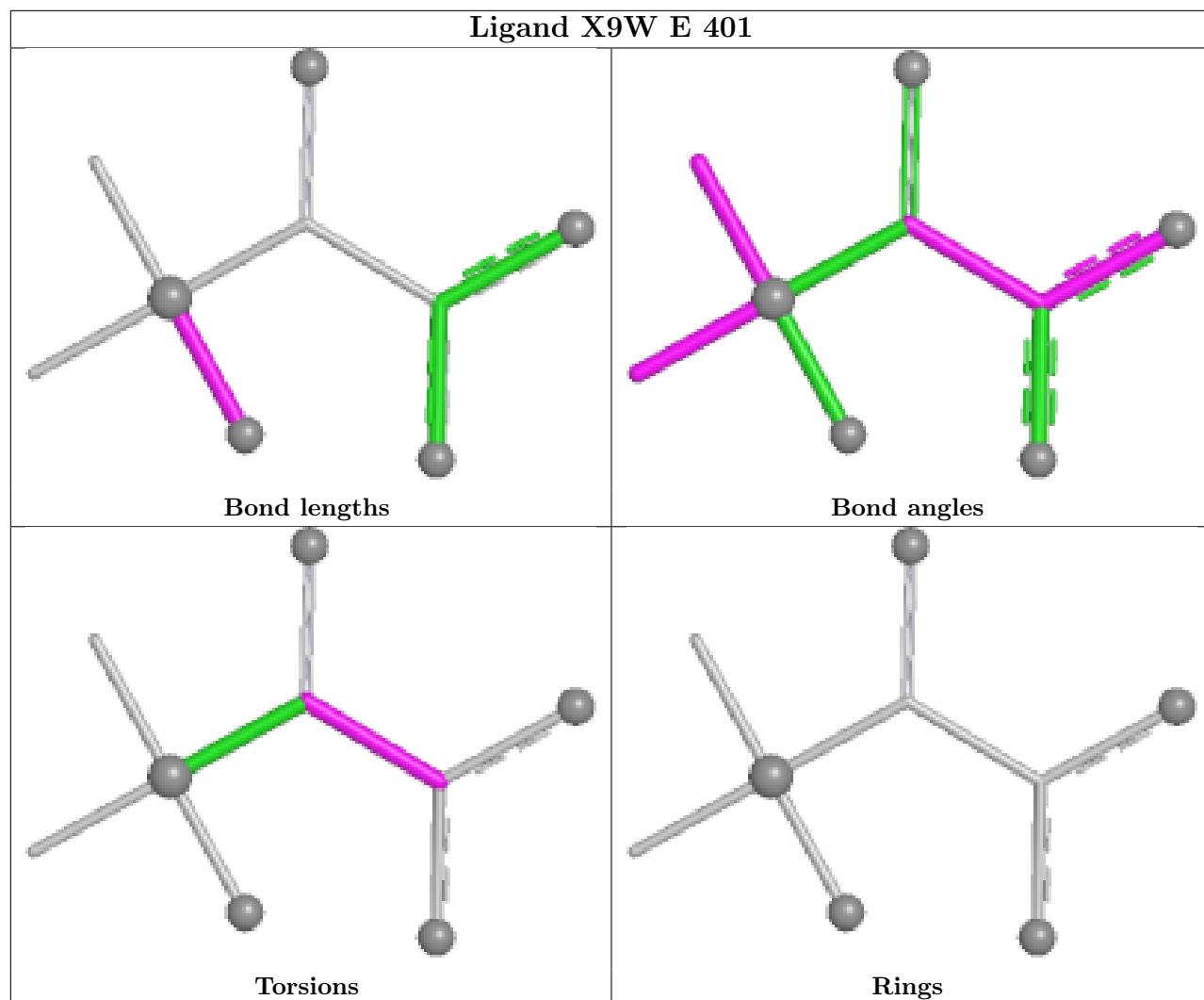
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

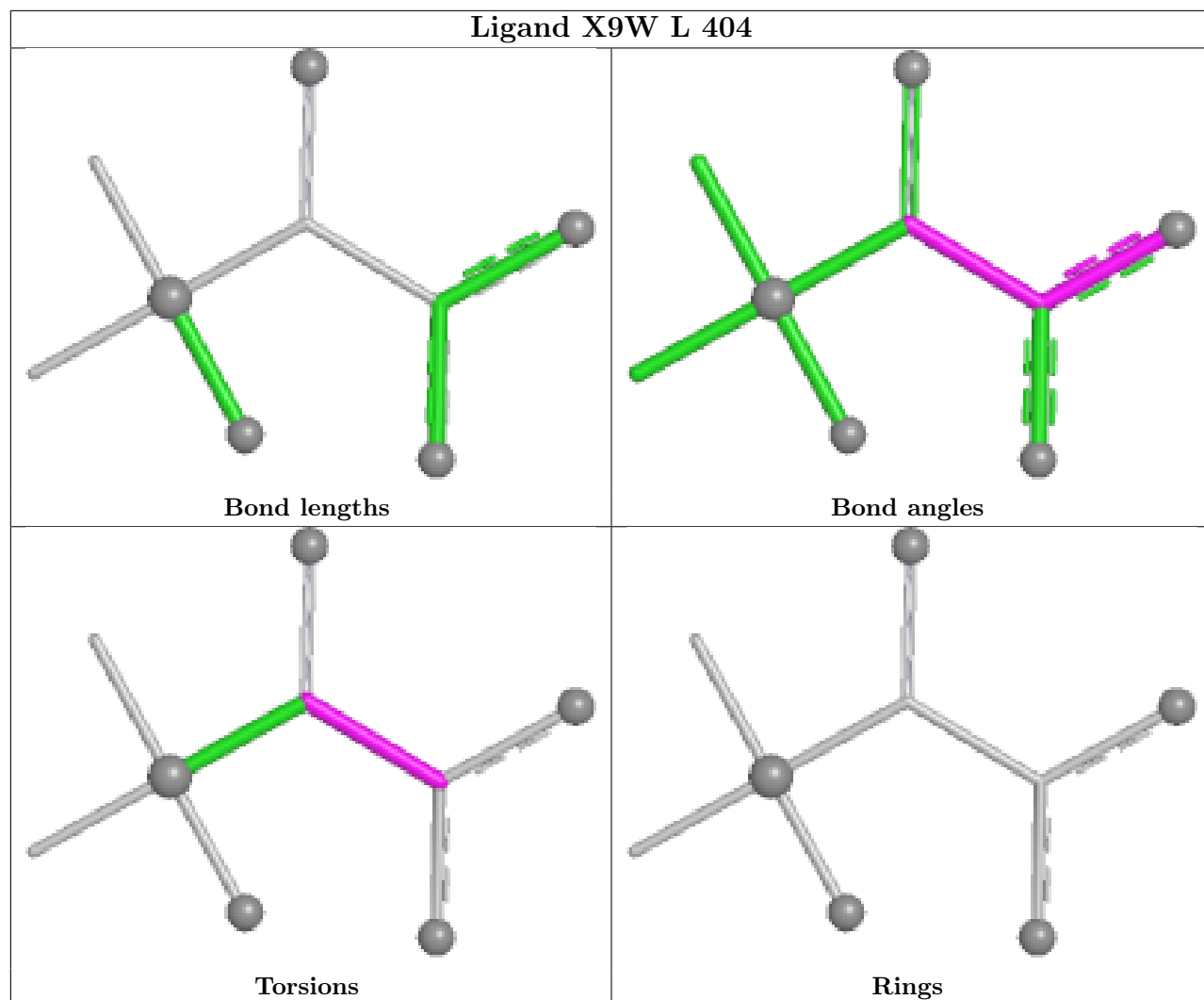
equivalents in the CSD to analyse the geometry.

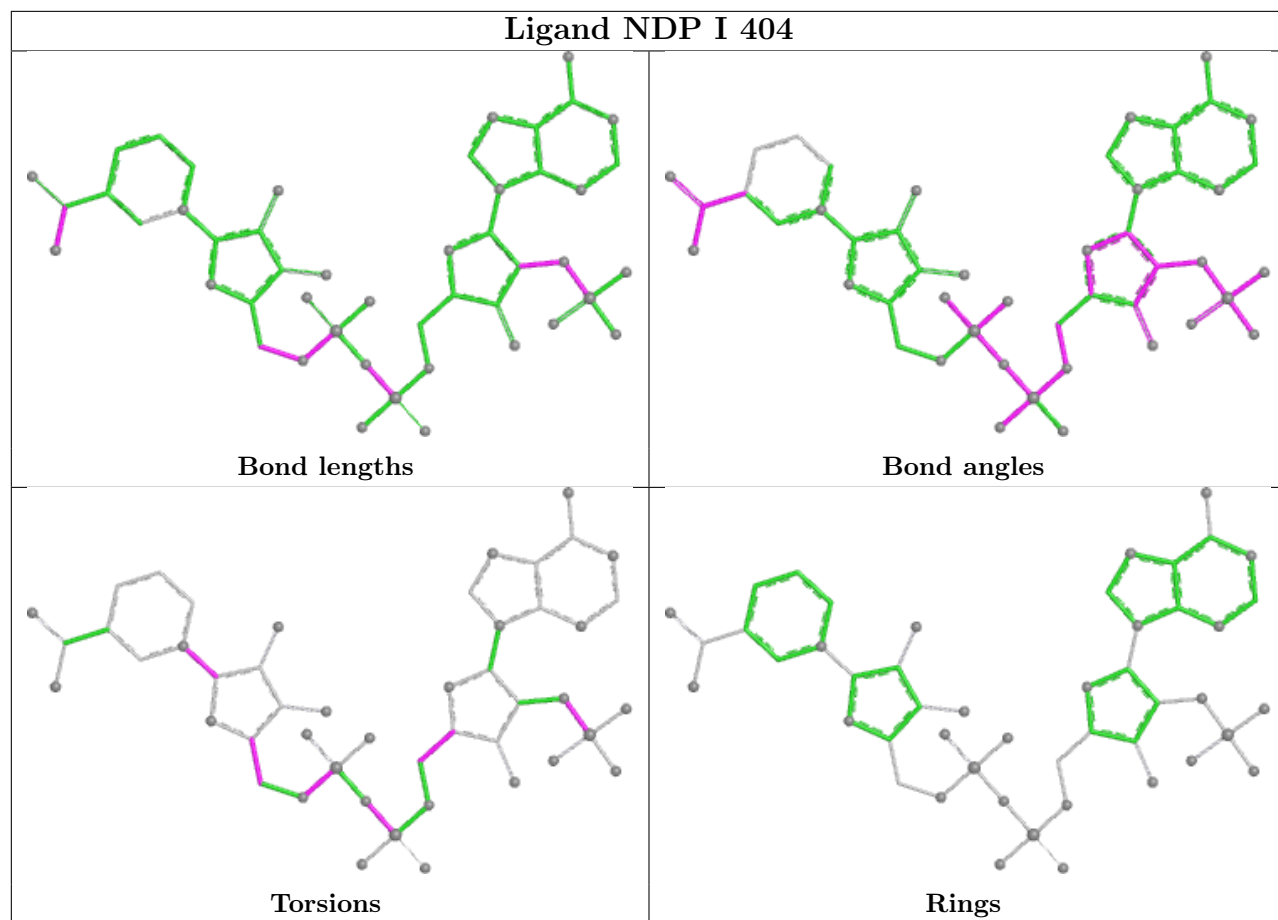


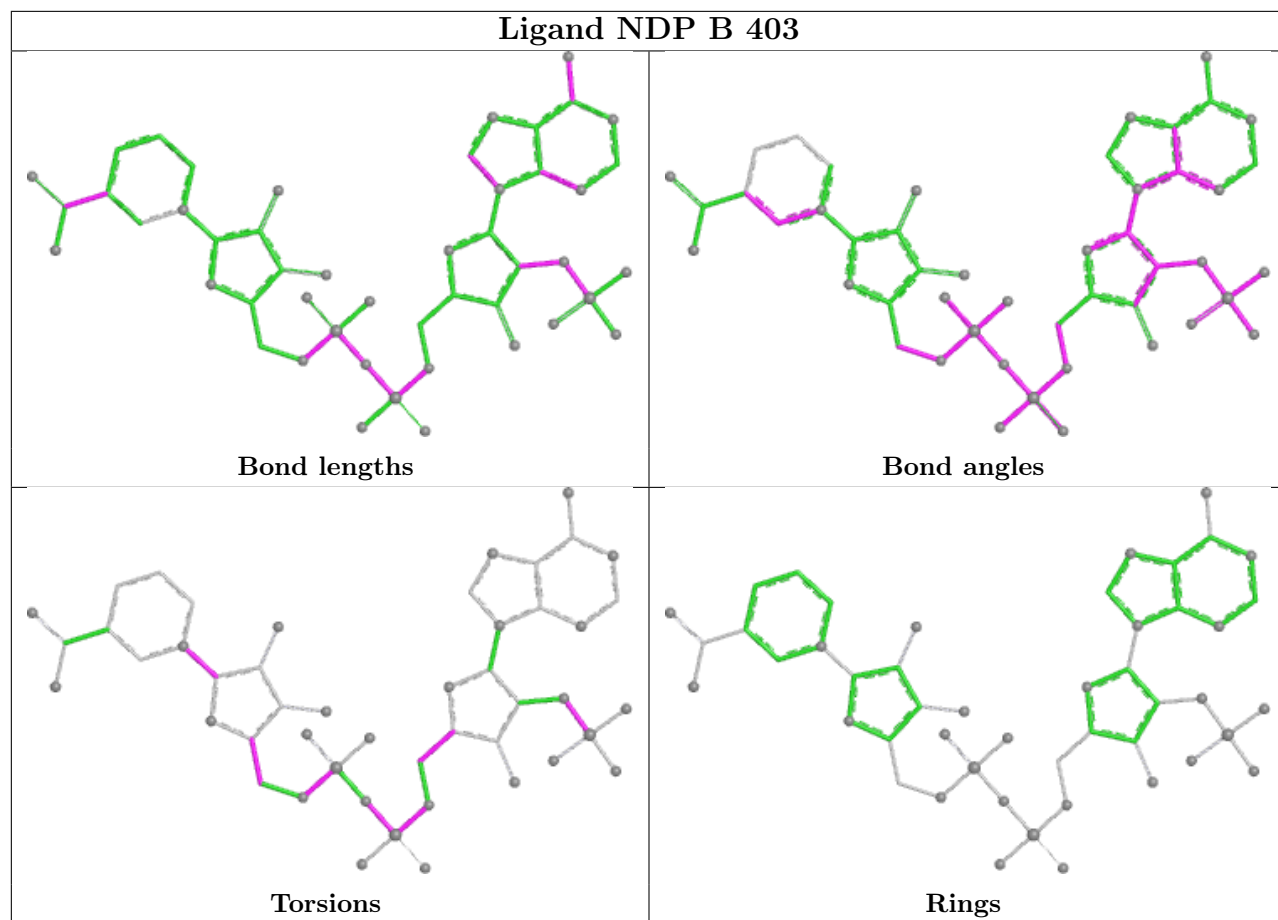


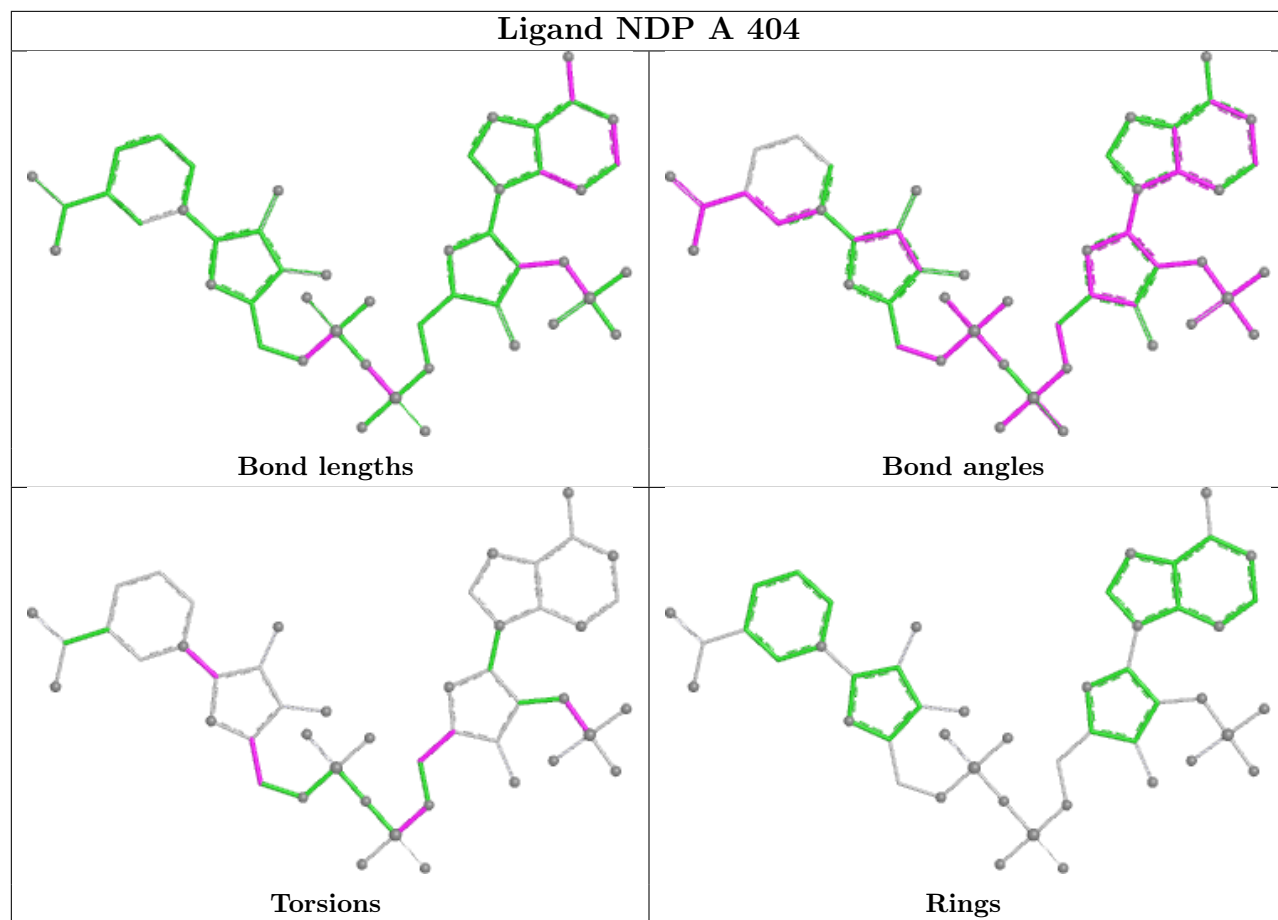


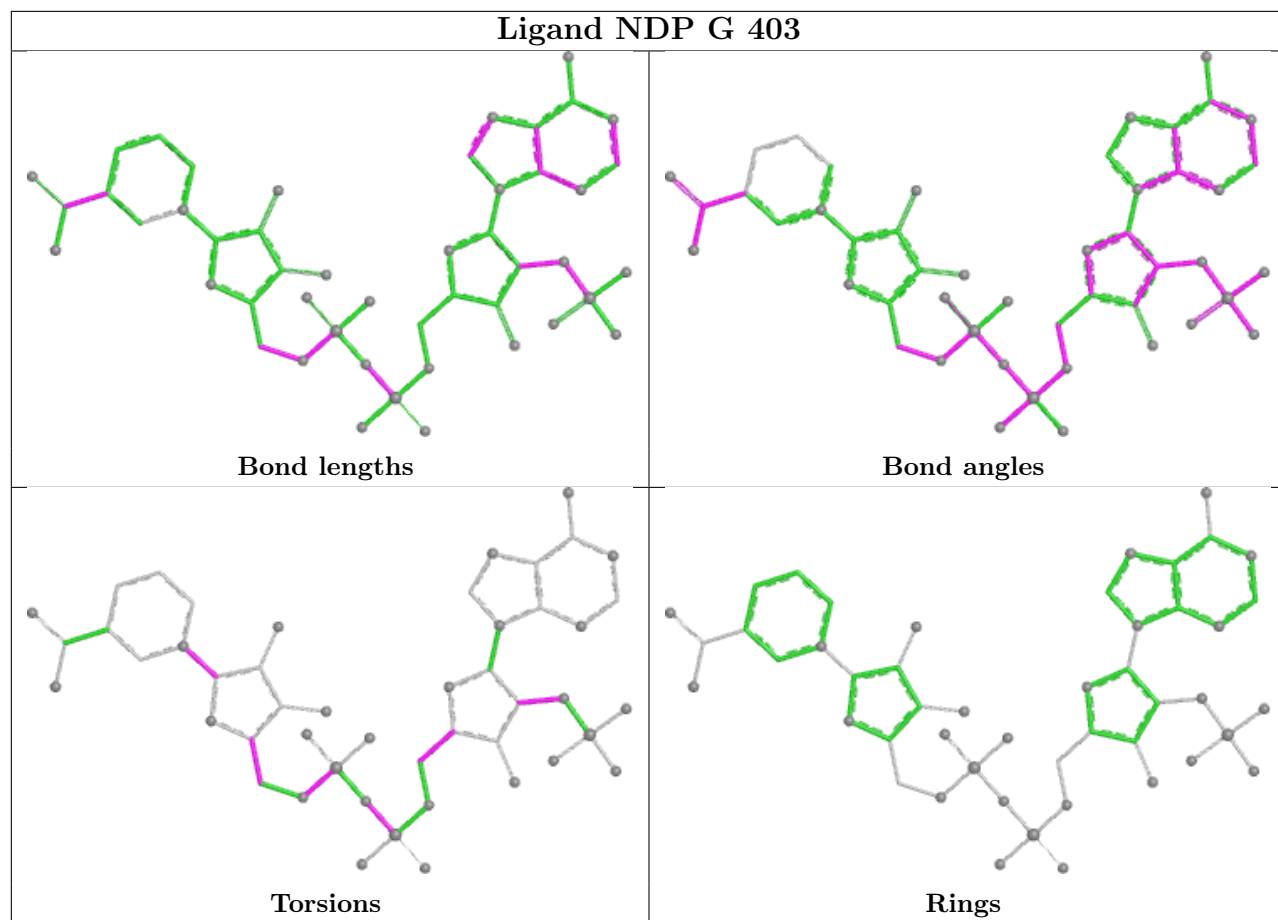


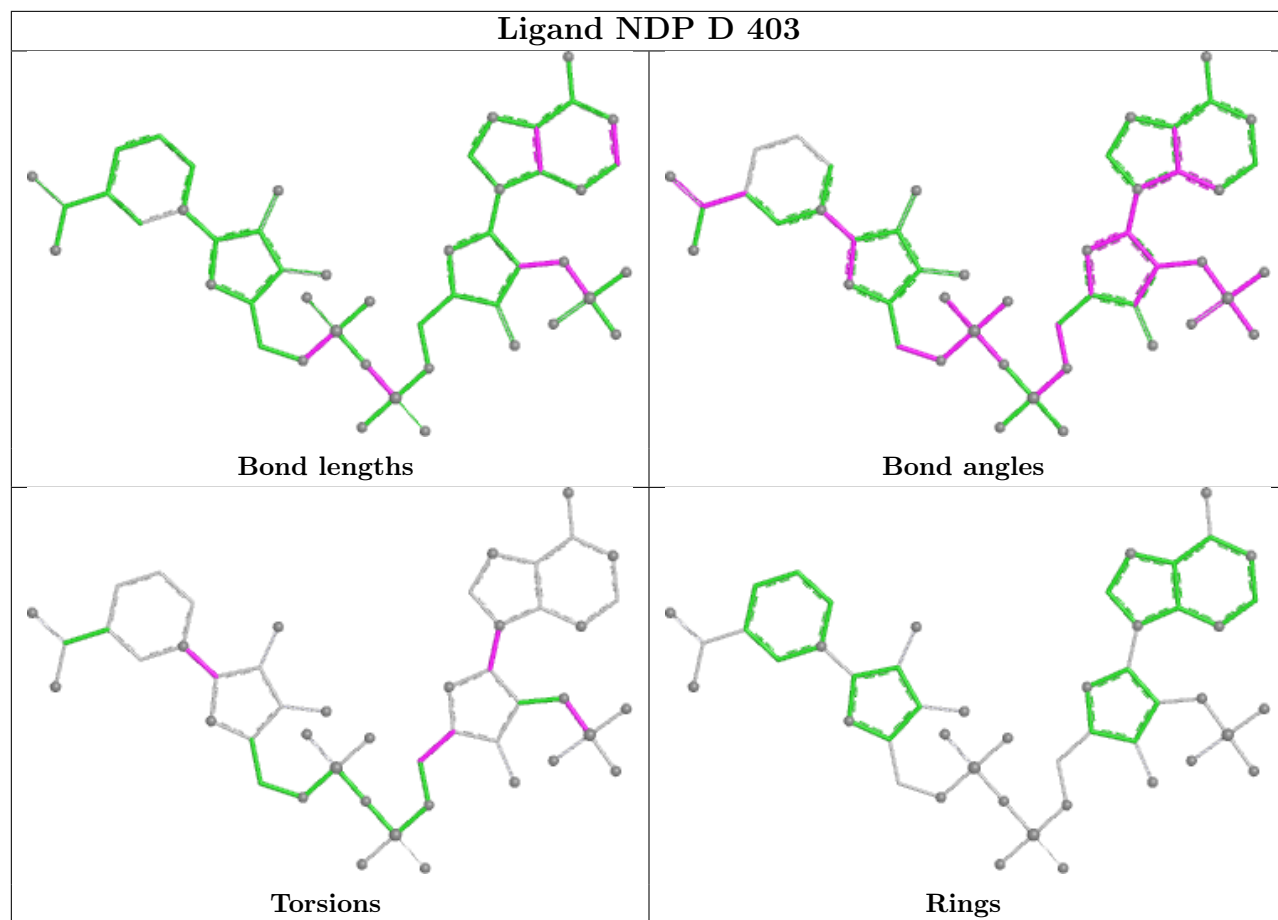


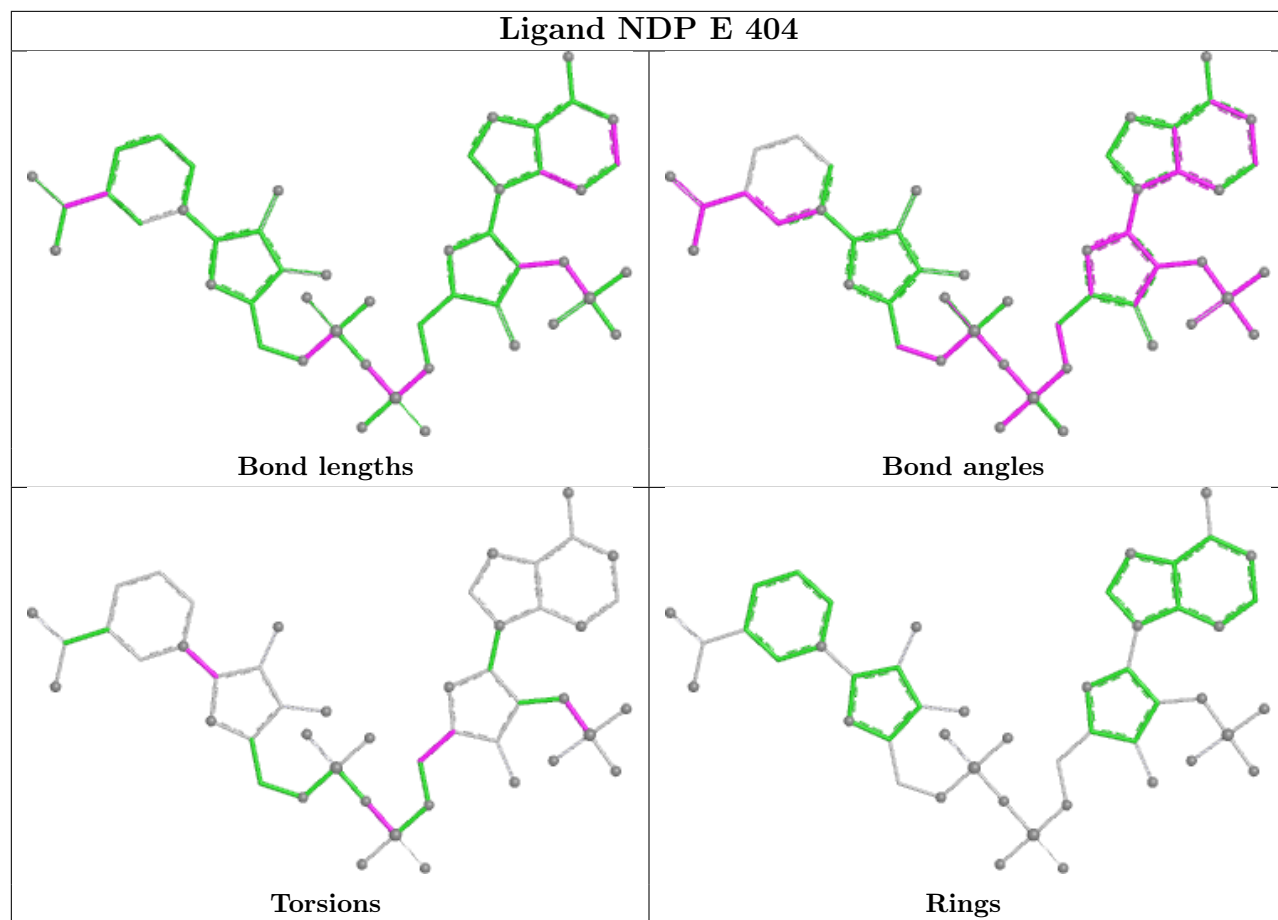


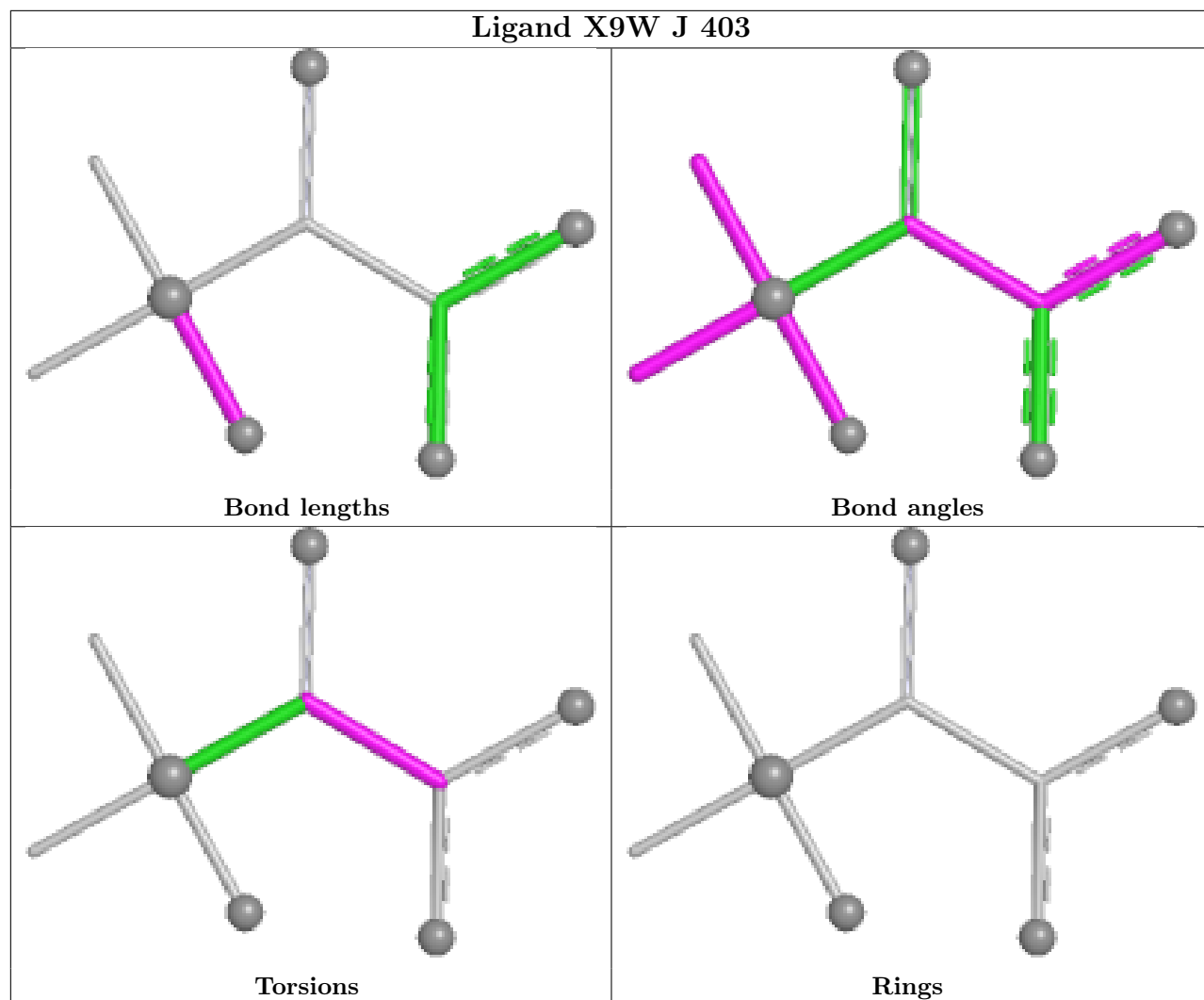


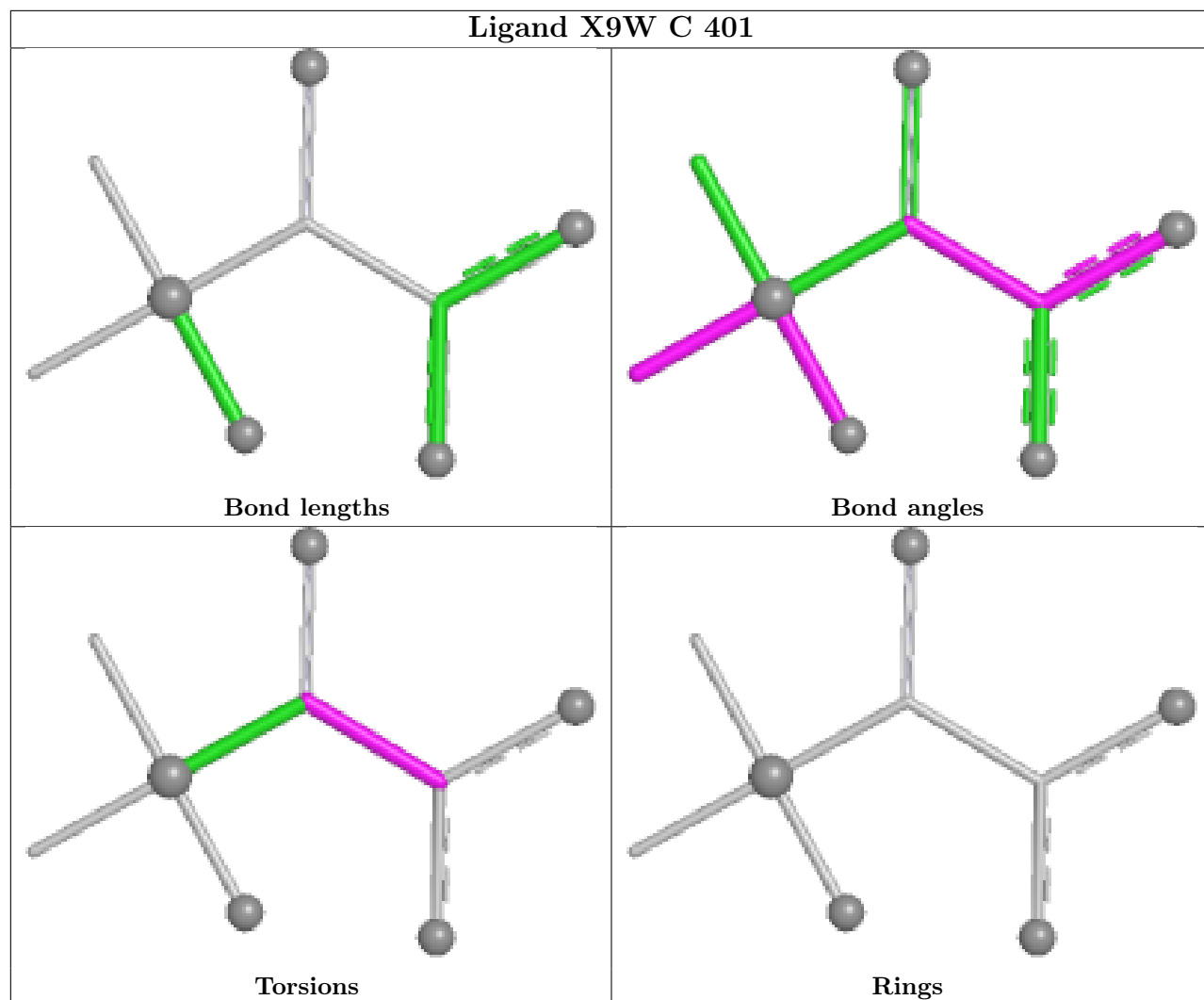


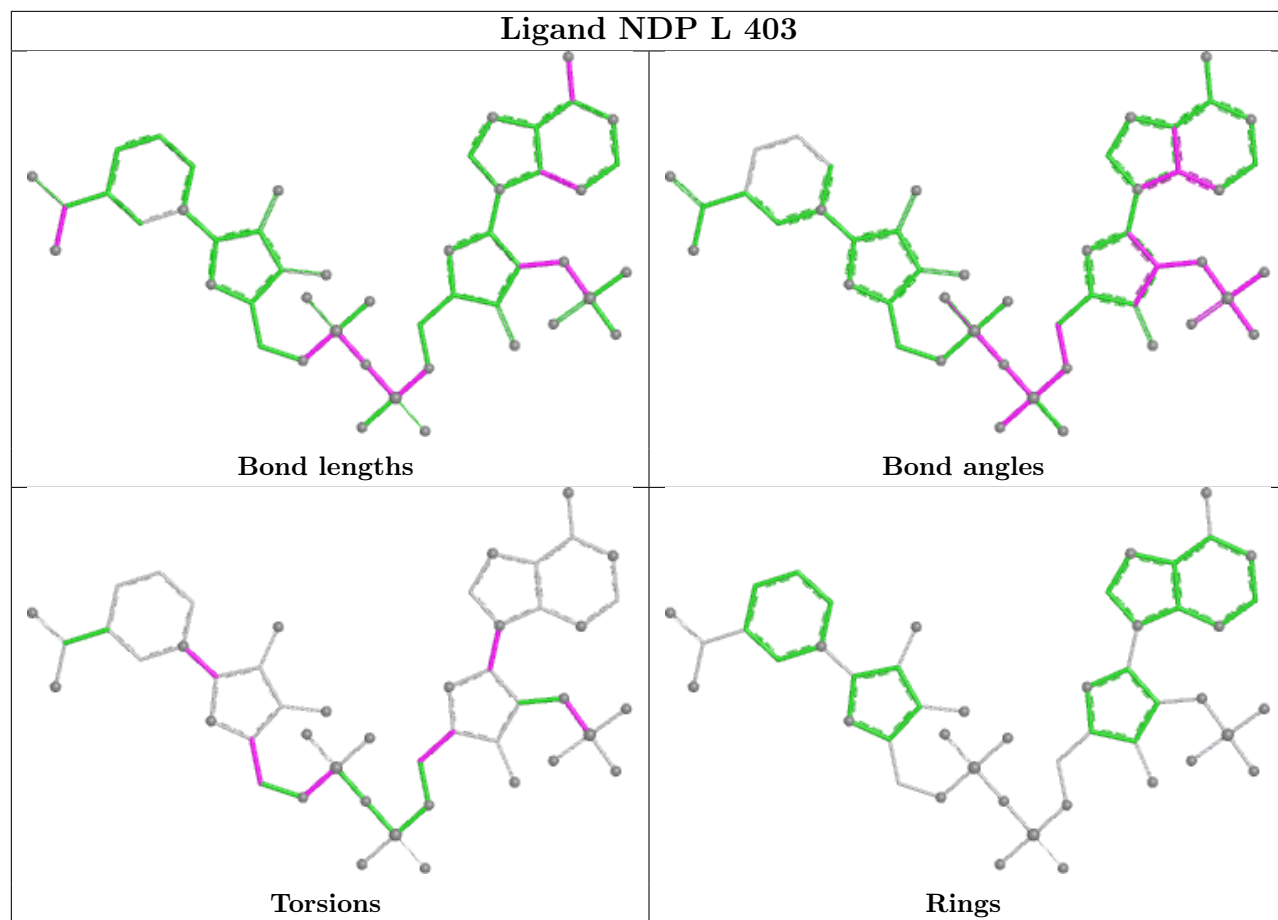


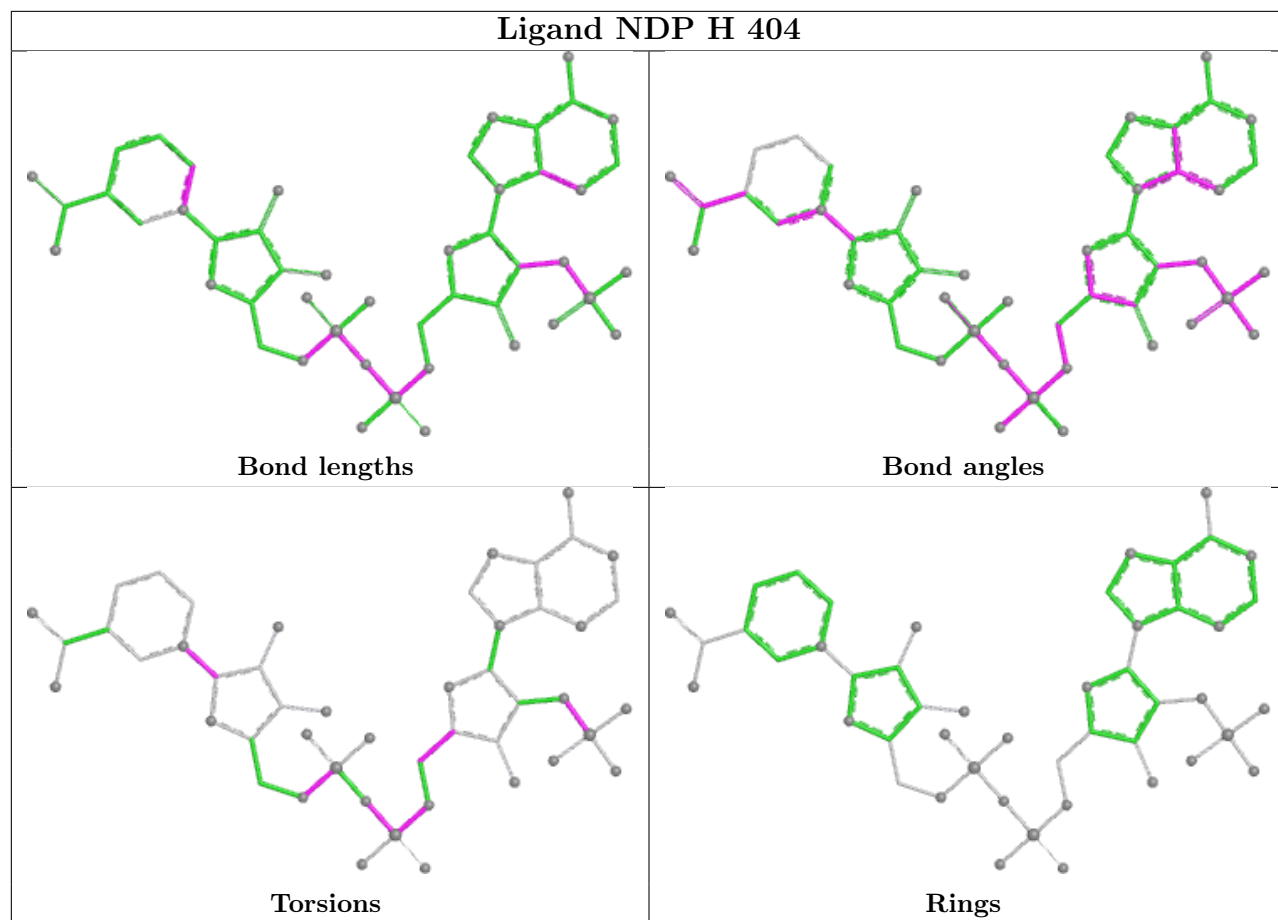


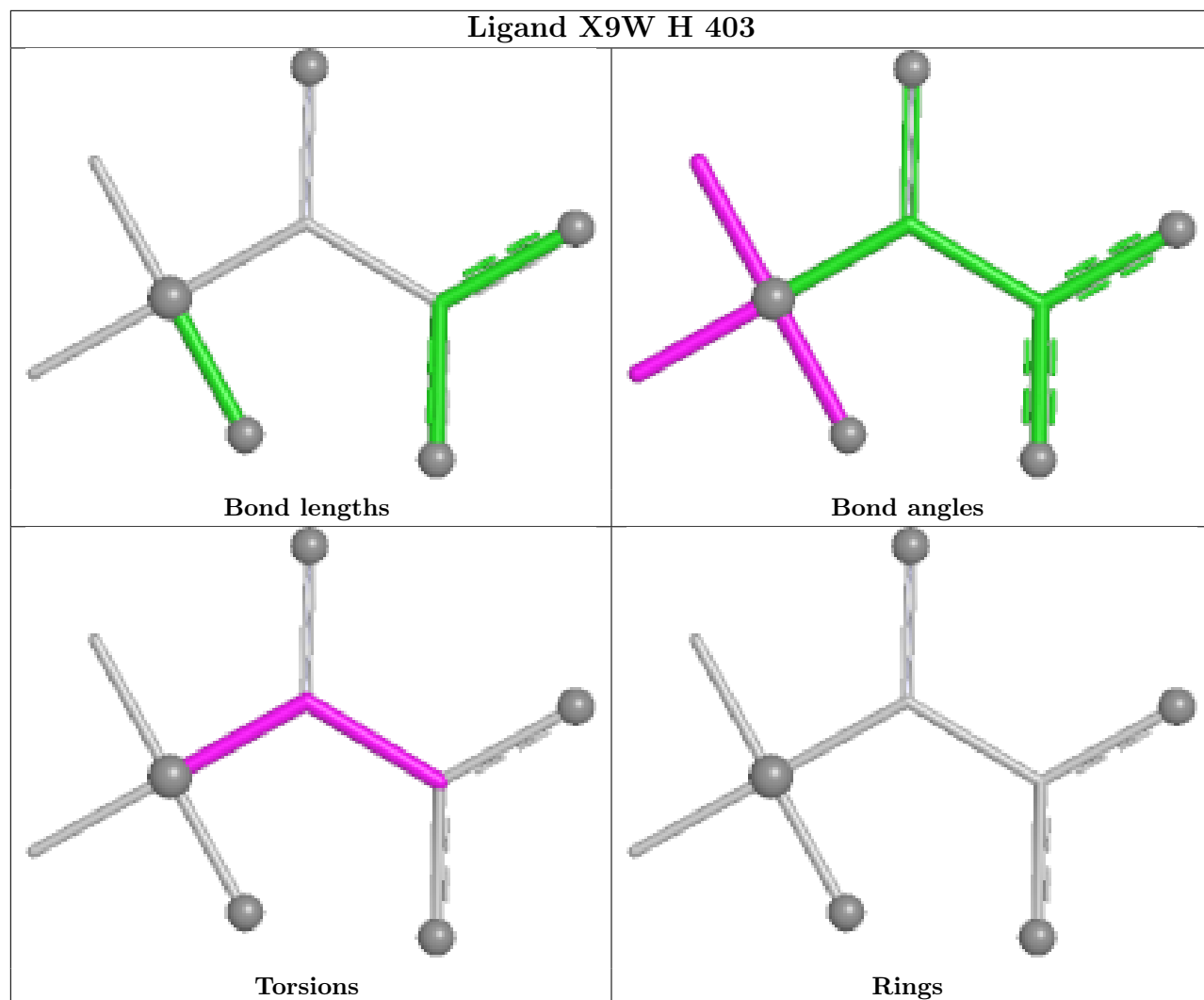


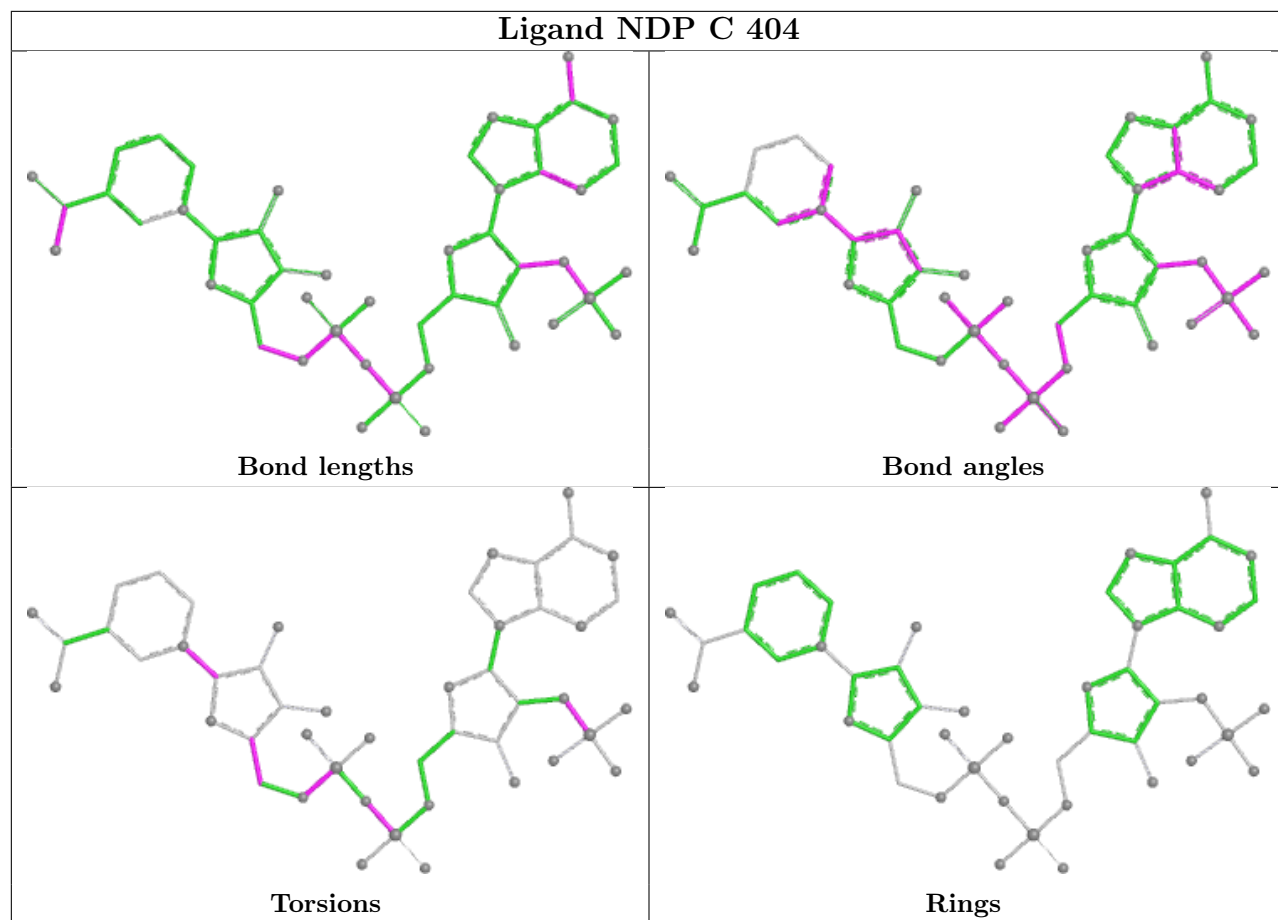


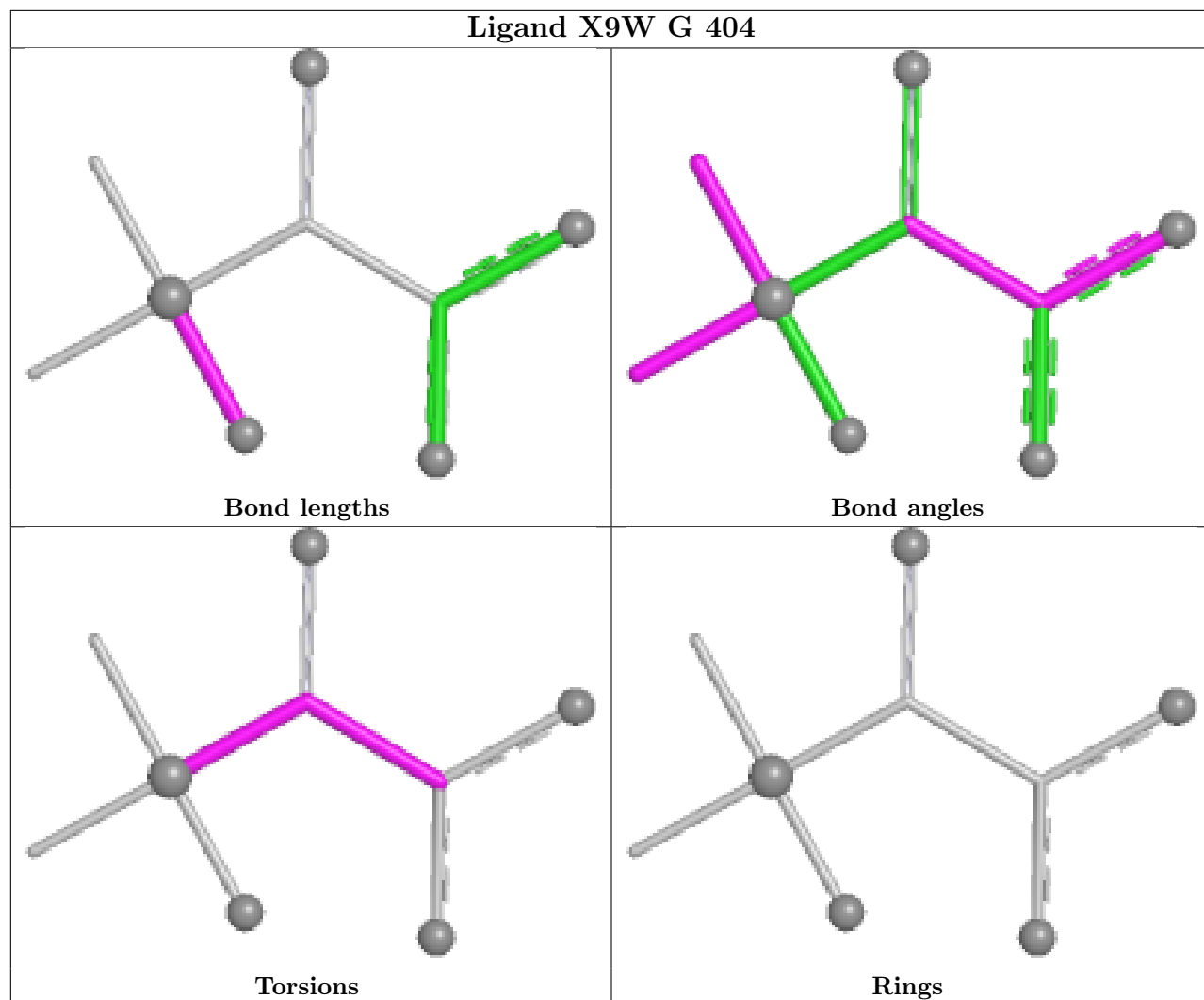


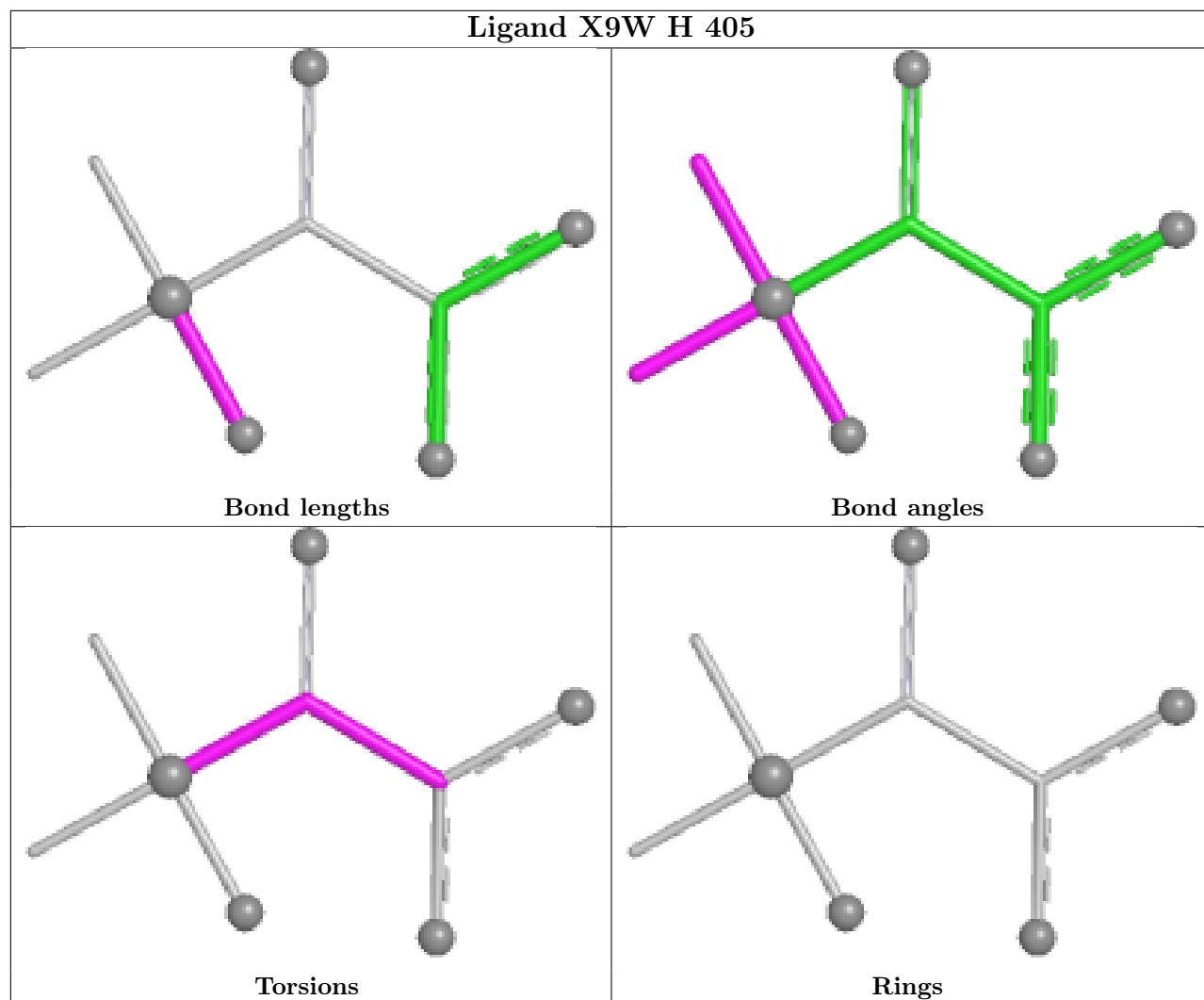


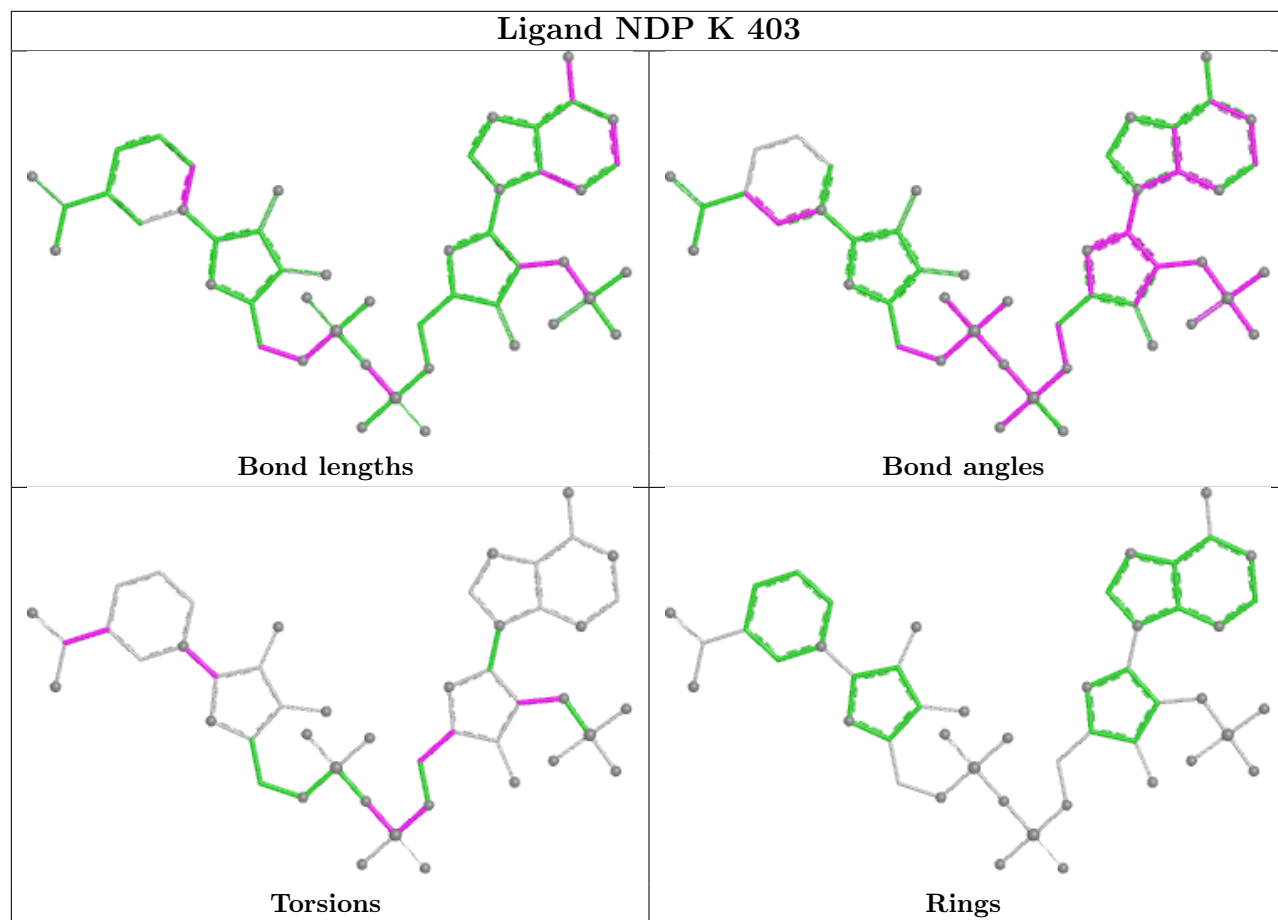


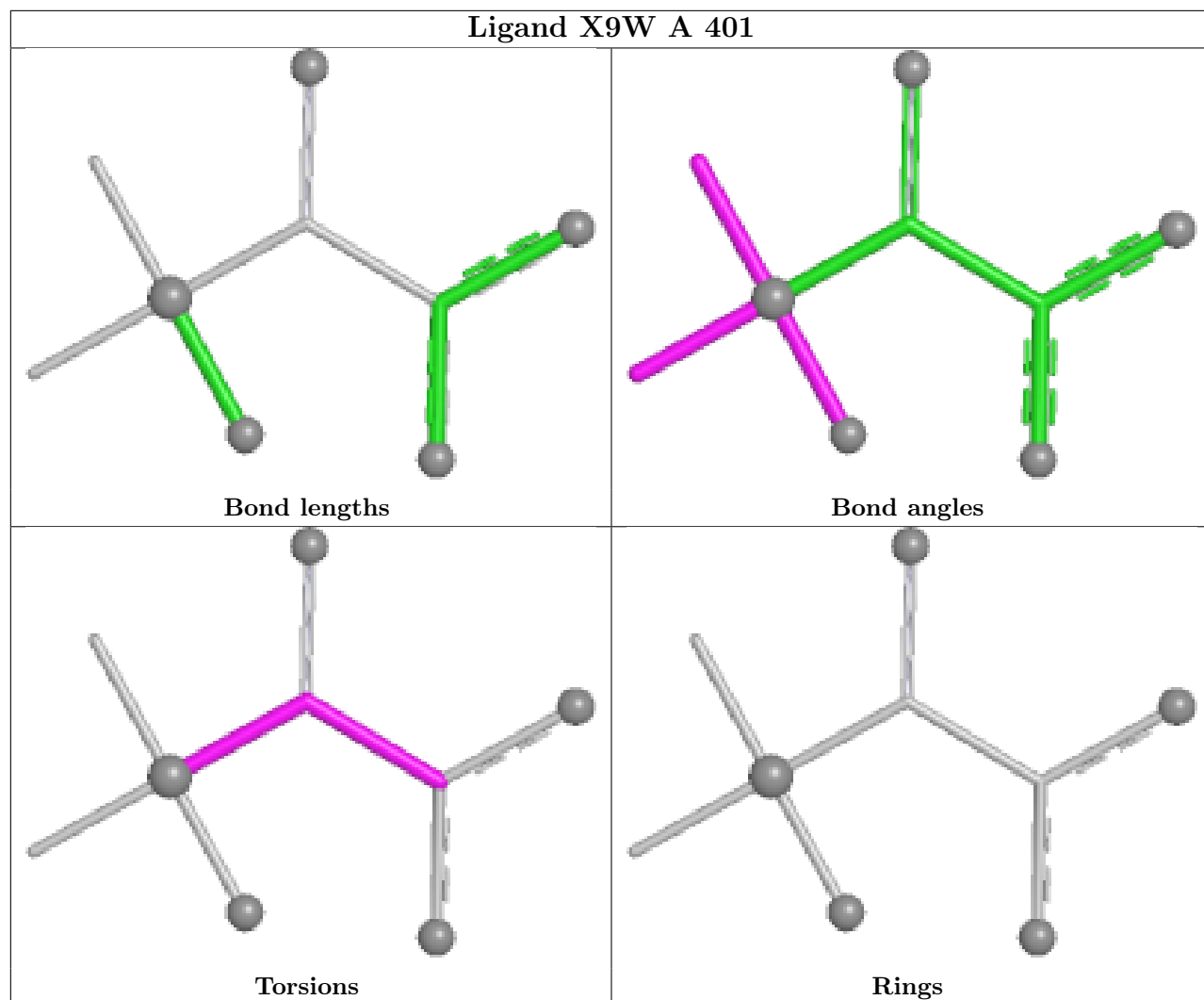


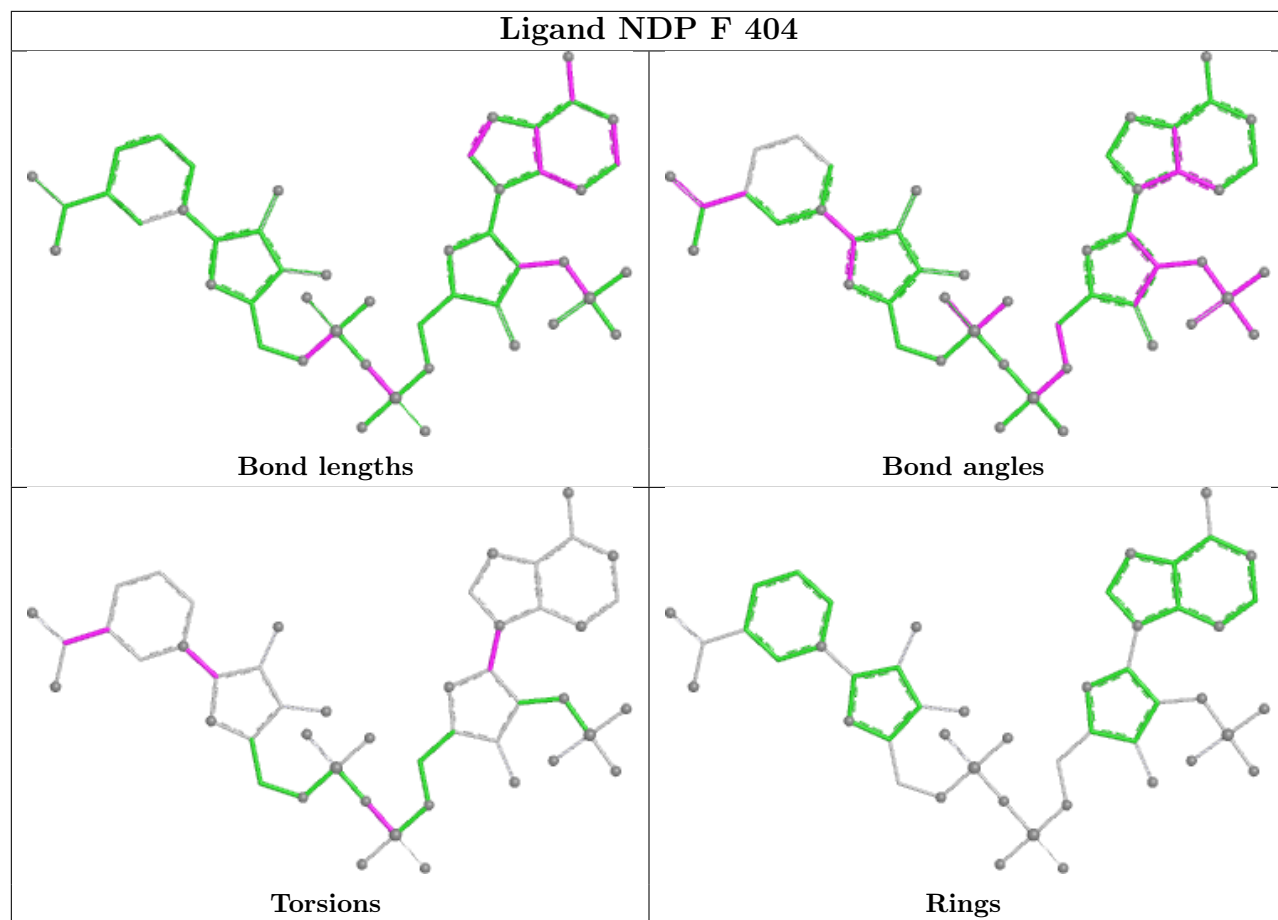


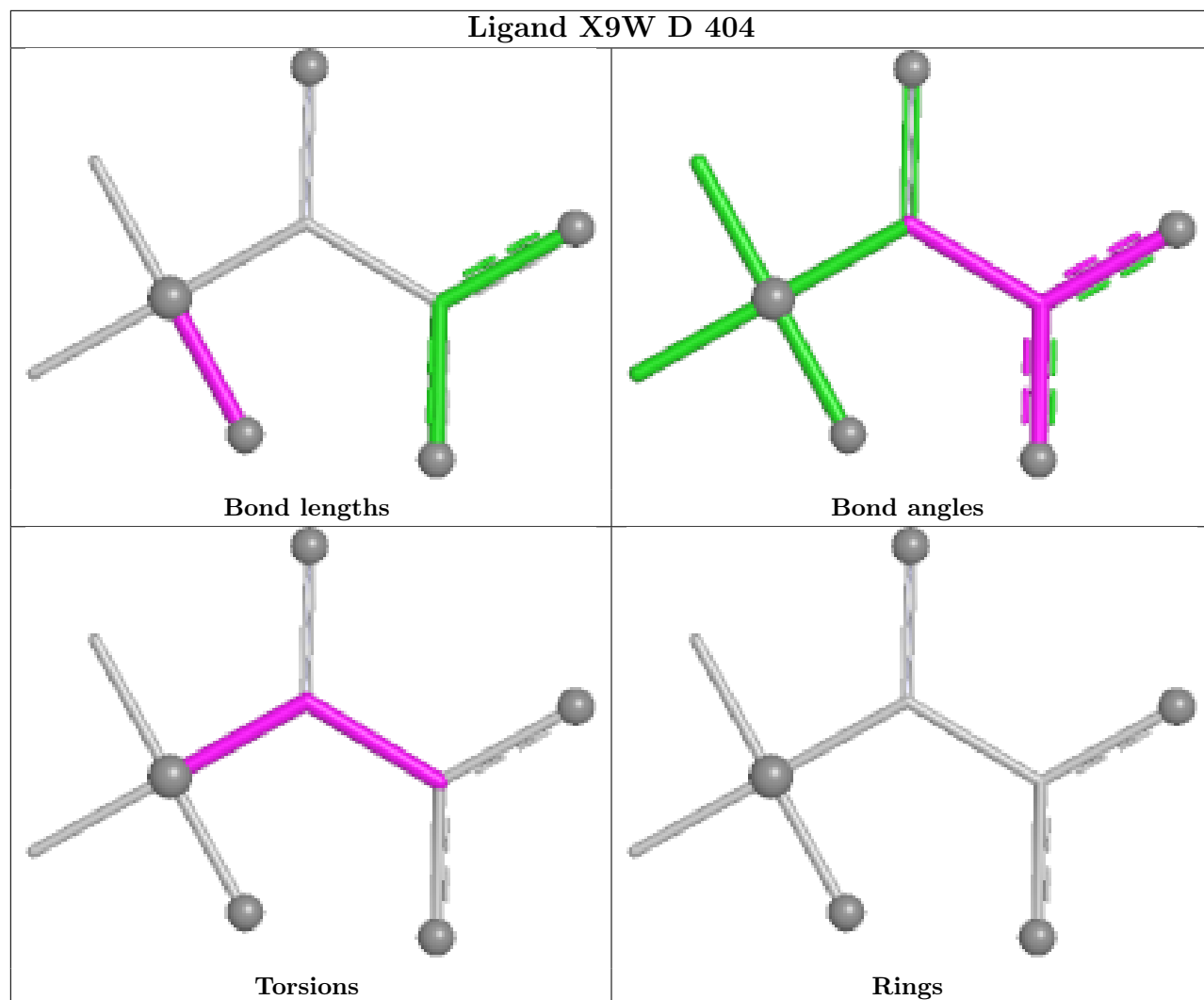


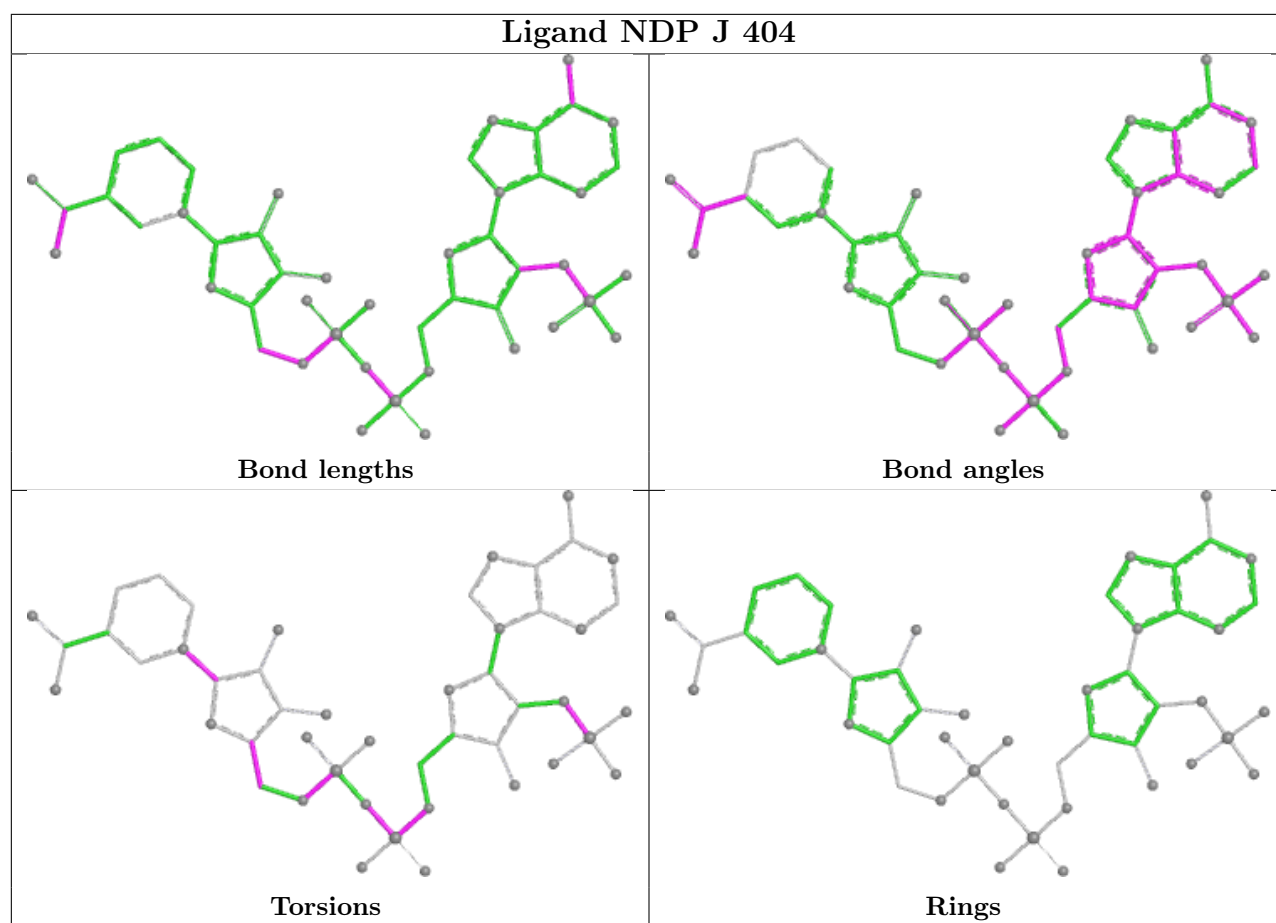












5.7 Other polymers [\(i\)](#)

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](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/330 (99%)	-1.06	1 (0%) 90 93	13, 23, 36, 65	1 (0%)
1	B	327/330 (99%)	-1.04	0 100 100	14, 25, 41, 74	1 (0%)
1	C	327/330 (99%)	-1.01	0 100 100	15, 25, 43, 73	1 (0%)
1	D	327/330 (99%)	-1.06	0 100 100	14, 22, 39, 61	1 (0%)
1	E	327/330 (99%)	-1.06	1 (0%) 90 93	14, 22, 36, 80	1 (0%)
1	F	327/330 (99%)	-1.07	0 100 100	14, 22, 40, 58	1 (0%)
1	G	327/330 (99%)	-1.08	0 100 100	13, 22, 35, 60	1 (0%)
1	H	327/330 (99%)	-1.02	0 100 100	13, 24, 40, 58	1 (0%)
1	I	327/330 (99%)	-1.01	2 (0%) 85 89	14, 24, 42, 120	1 (0%)
1	J	327/330 (99%)	-1.02	1 (0%) 90 93	14, 23, 39, 79	1 (0%)
1	K	327/330 (99%)	-1.05	0 100 100	13, 23, 36, 65	1 (0%)
1	L	327/330 (99%)	-1.02	0 100 100	15, 26, 43, 71	1 (0%)
All	All	3924/3960 (99%)	-1.04	5 (0%) 92 94	13, 24, 40, 120	12 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	329	ILE	3.9
1	I	328	TRP	3.1
1	E	329	ILE	2.9
1	A	329	ILE	2.3
1	I	329	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

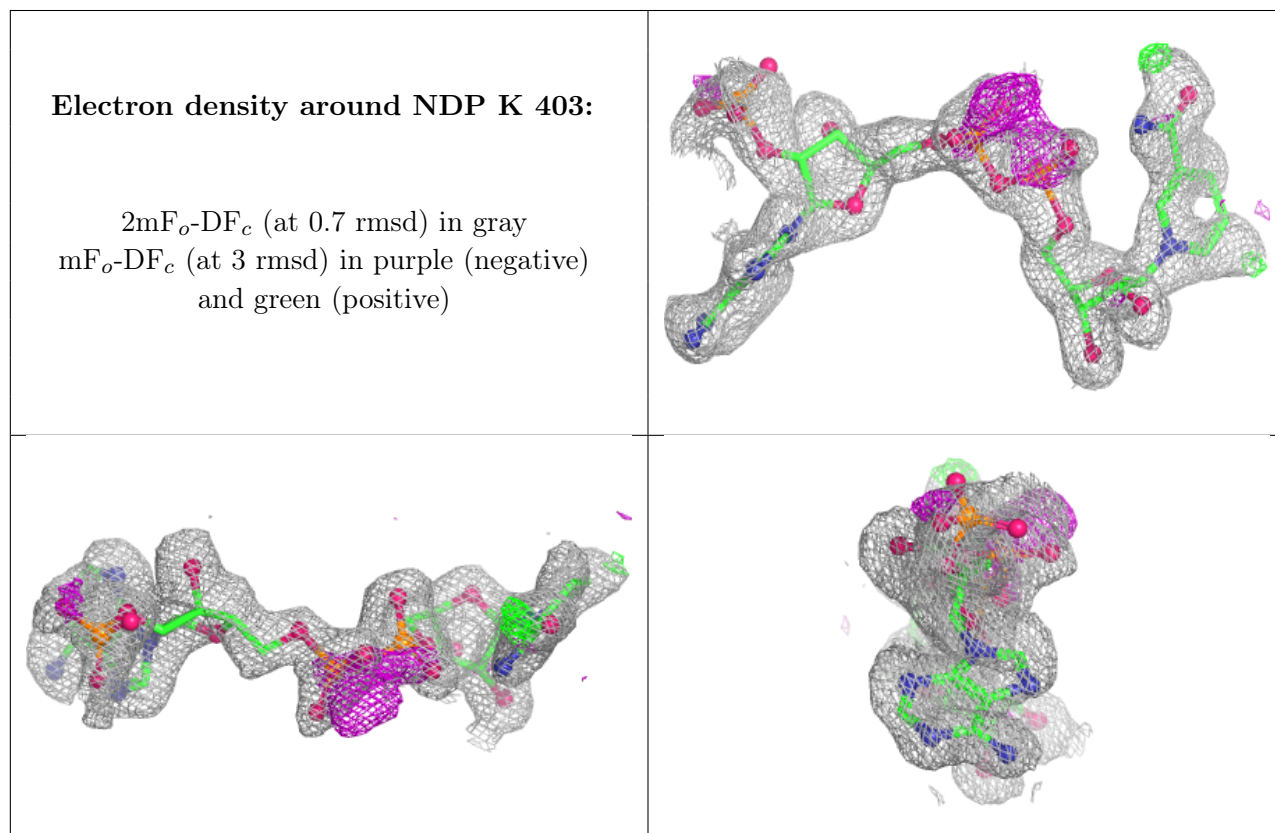
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	K	403	48/48	0.98	0.05	23,35,54,56	0
3	NDP	E	404	48/48	0.98	0.05	21,33,52,56	0
3	NDP	A	404	48/48	0.98	0.06	22,35,49,51	0
2	MG	J	401	1/1	0.99	0.05	16,16,16,16	0
2	MG	L	401	1/1	0.99	0.03	19,19,19,19	0
2	MG	F	403	1/1	0.99	0.02	19,19,19,19	0
3	NDP	B	403	48/48	0.99	0.04	22,28,40,43	0
3	NDP	H	404	48/48	0.99	0.04	22,29,43,45	0
2	MG	B	401	1/1	0.99	0.04	16,16,16,16	0
3	NDP	I	404	48/48	0.99	0.04	19,27,33,41	0
3	NDP	D	403	48/48	0.99	0.05	16,31,39,43	0
3	NDP	G	403	48/48	0.99	0.04	19,31,52,56	0
3	NDP	J	404	48/48	0.99	0.04	19,28,36,39	0
2	MG	I	401	1/1	0.99	0.03	17,17,17,17	0
3	NDP	L	403	48/48	0.99	0.04	22,32,42,43	0
3	NDP	C	404	48/48	0.99	0.05	20,32,41,45	0
3	NDP	F	404	48/48	0.99	0.04	16,29,41,46	0
2	MG	G	401	1/1	0.99	0.04	15,15,15,15	0
4	X9W	B	404	9/9	0.99	0.05	15,18,22,22	0
4	X9W	H	403	9/9	0.99	0.06	15,20,25,25	0
4	X9W	H	405	9/9	0.99	0.04	14,17,23,23	0
4	X9W	I	403	9/9	0.99	0.04	14,17,22,22	0
4	X9W	G	404	9/9	0.99	0.04	16,18,22,22	0
4	X9W	J	403	9/9	0.99	0.03	14,17,22,22	0
4	X9W	L	404	9/9	0.99	0.04	15,22,30,30	0
4	X9W	C	401	9/9	0.99	0.04	16,22,28,28	0
4	X9W	F	401	9/9	0.99	0.04	13,18,22,22	0
4	X9W	A	401	9/9	0.99	0.03	15,20,27,27	0
2	MG	H	401	1/1	1.00	0.03	18,18,18,18	0
2	MG	G	402	1/1	1.00	0.01	15,15,15,15	0
2	MG	H	402	1/1	1.00	0.05	18,18,18,18	0
2	MG	J	402	1/1	1.00	0.04	15,15,15,15	0

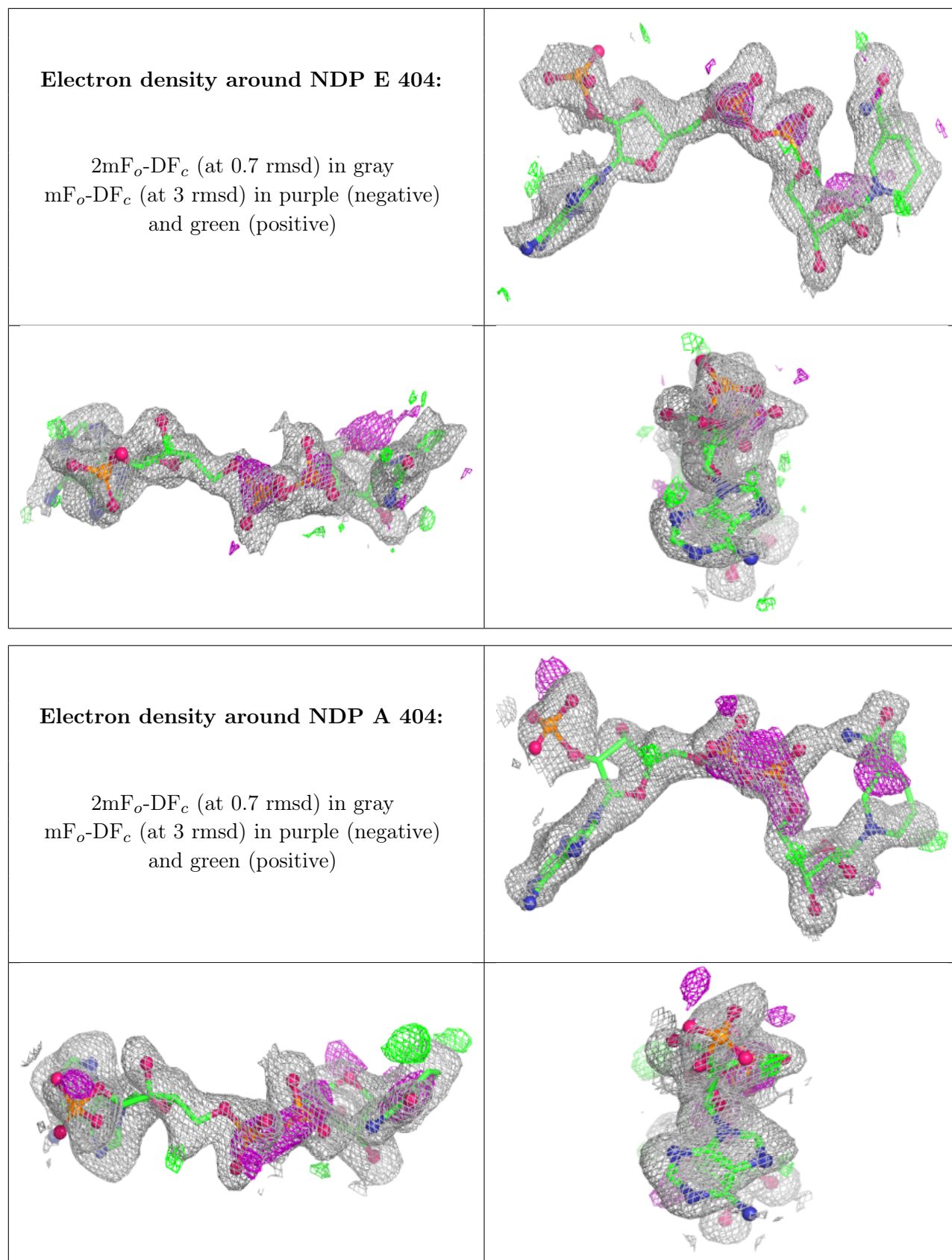
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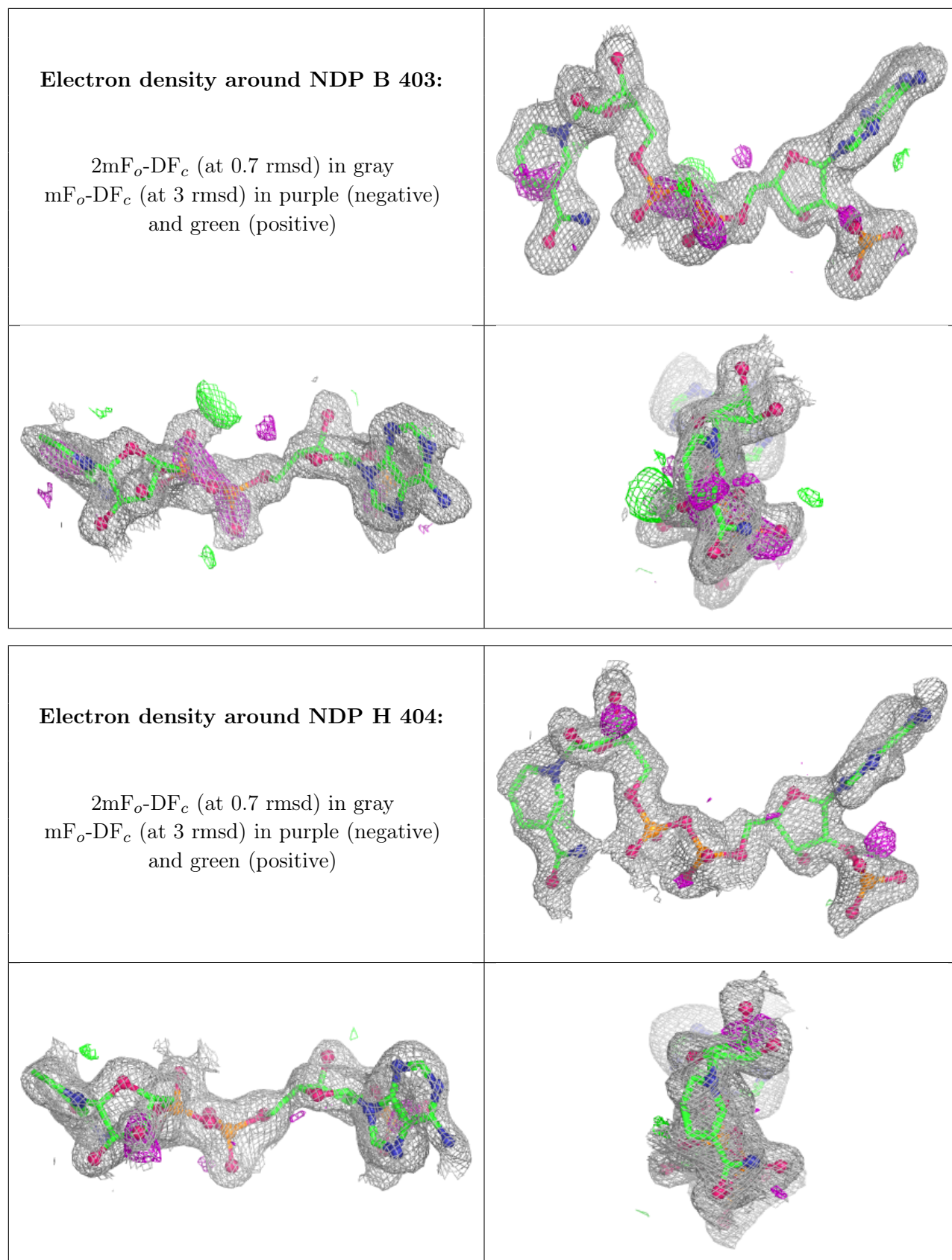
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	E	402	1/1	1.00	0.04	17,17,17,17	0
2	MG	E	403	1/1	1.00	0.01	16,16,16,16	0
2	MG	K	401	1/1	1.00	0.01	16,16,16,16	0
2	MG	L	402	1/1	1.00	0.02	18,18,18,18	0
2	MG	C	402	1/1	1.00	0.02	14,14,14,14	0
2	MG	C	403	1/1	1.00	0.06	19,19,19,19	0
2	MG	F	402	1/1	1.00	0.04	18,18,18,18	0
2	MG	K	402	1/1	1.00	0.03	17,17,17,17	0
4	X9W	D	404	9/9	1.00	0.03	14,17,21,25	0
2	MG	A	402	1/1	1.00	0.04	17,17,17,17	0
2	MG	A	403	1/1	1.00	0.05	18,18,18,18	0
4	X9W	E	401	9/9	1.00	0.03	12,17,22,22	0
2	MG	B	402	1/1	1.00	0.02	17,17,17,17	0
2	MG	I	402	1/1	1.00	0.03	15,15,15,15	0
2	MG	D	401	1/1	1.00	0.02	18,18,18,18	0
2	MG	D	402	1/1	1.00	0.02	20,20,20,20	0

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.

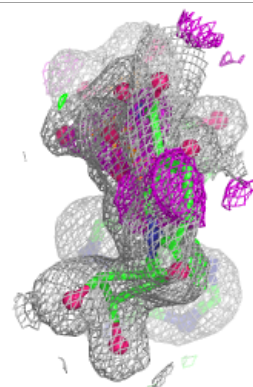
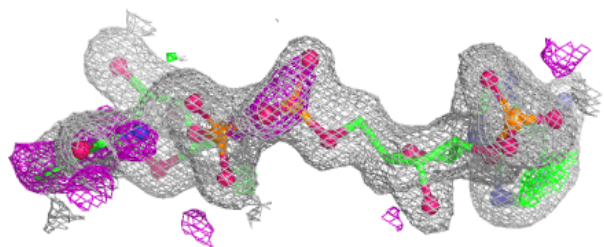
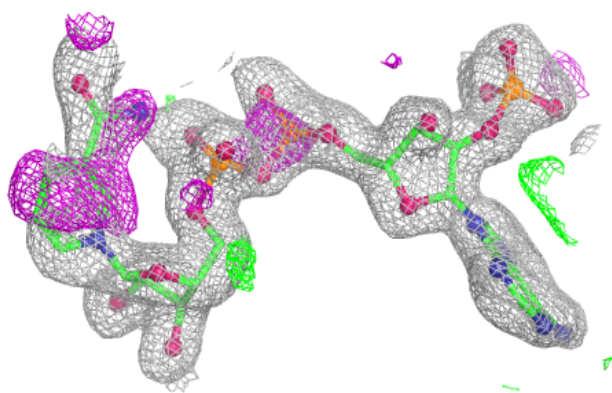




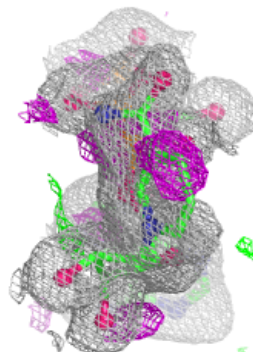
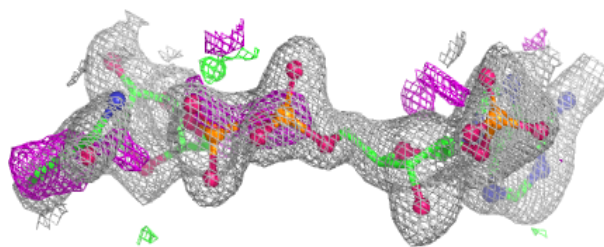
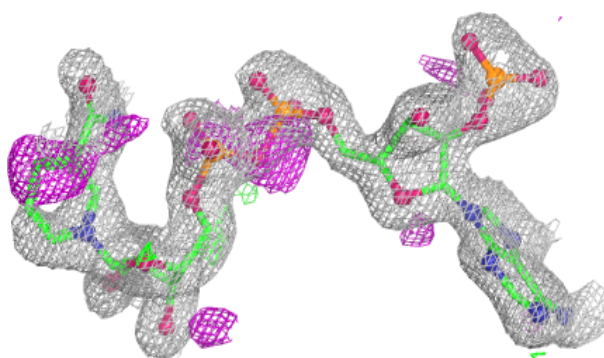


Electron density around NDP I 404:

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

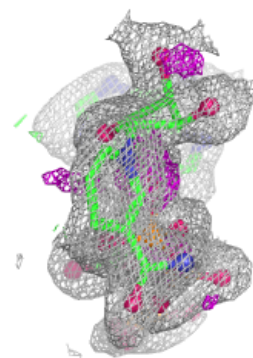
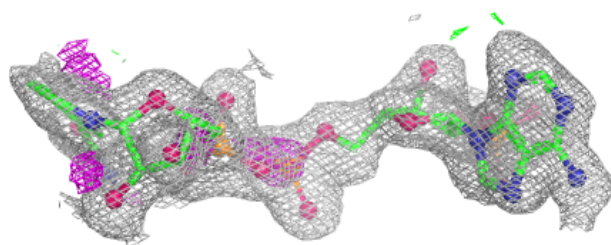
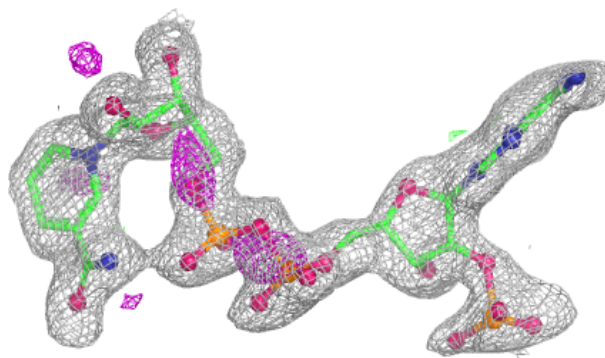
**Electron density around NDP D 403:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

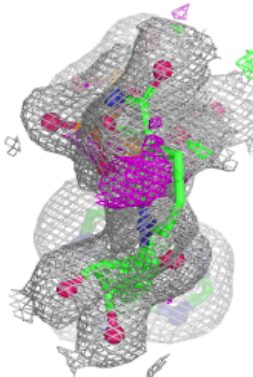
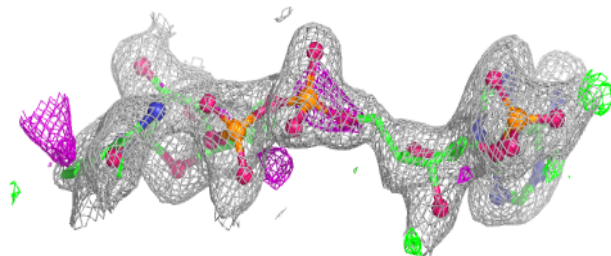
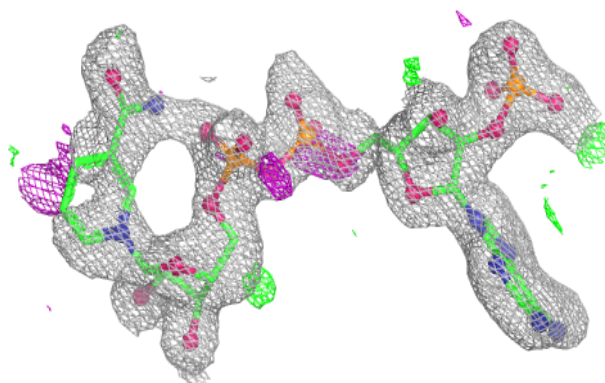


Electron density around NDP G 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

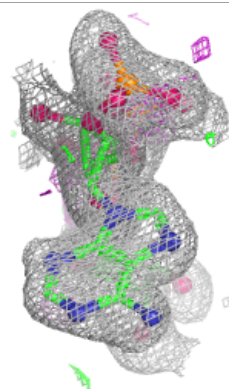
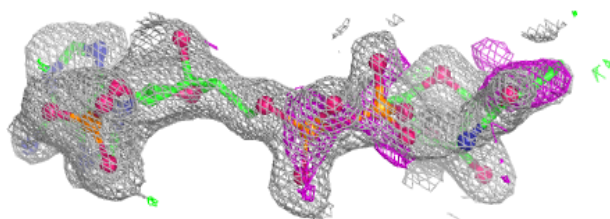
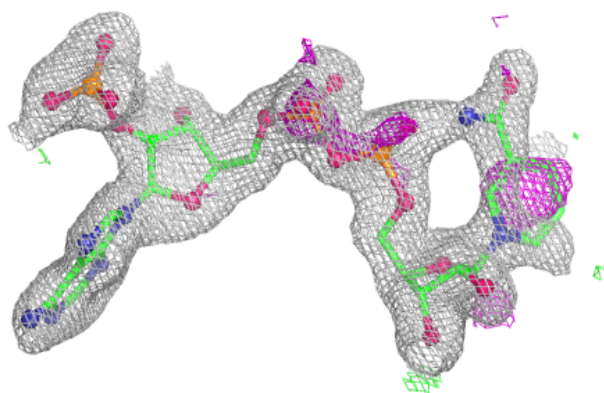
**Electron density around NDP J 404:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

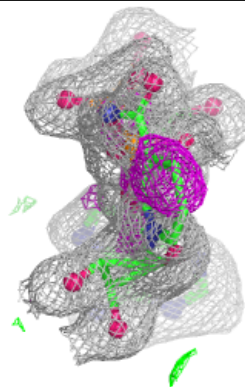
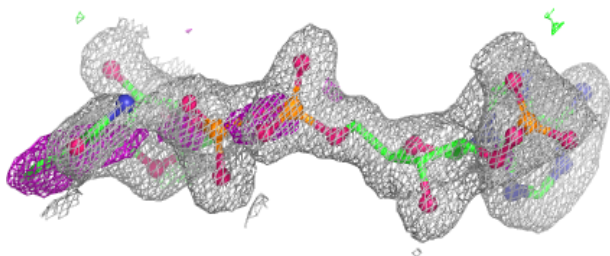
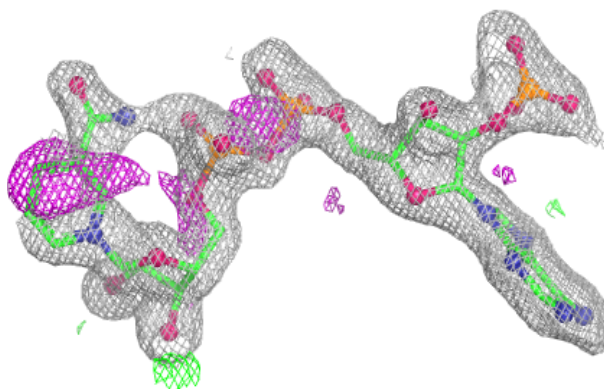


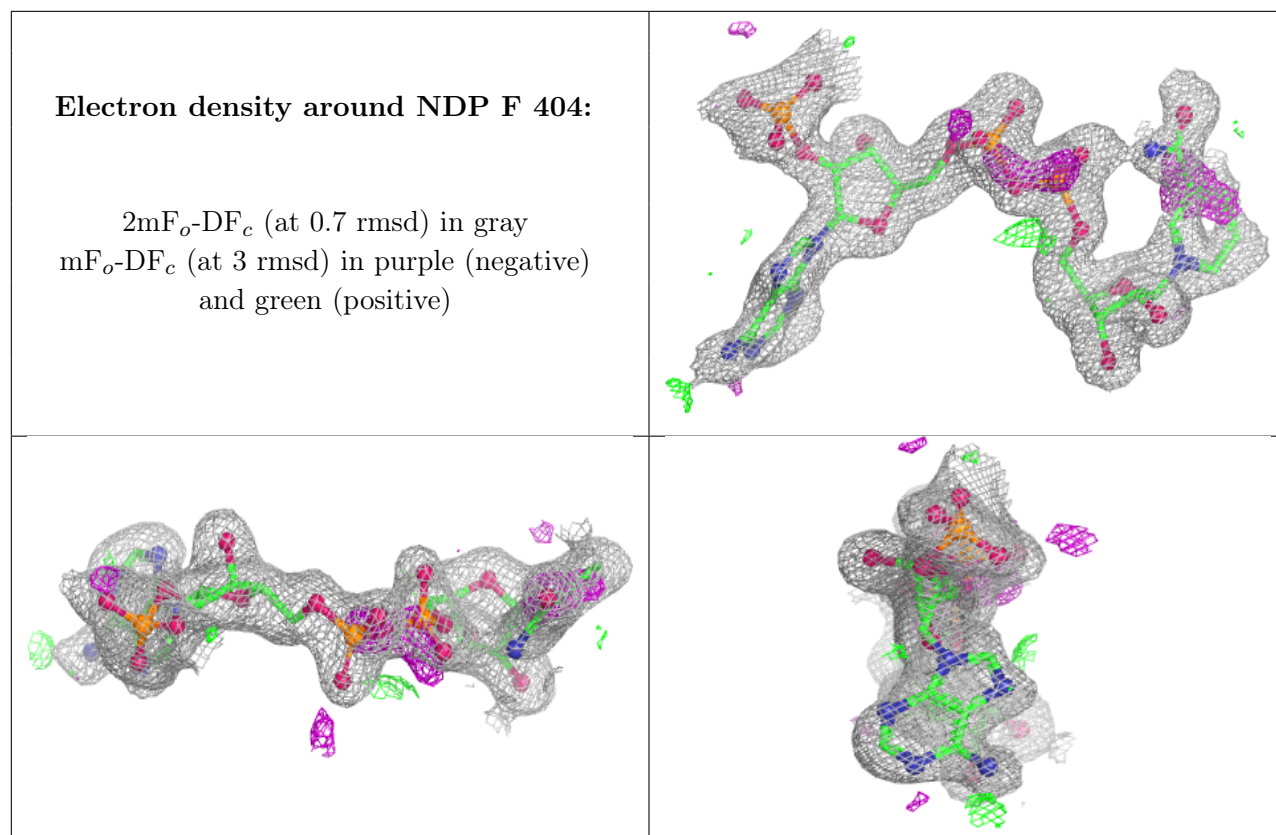
Electron density around NDP L 403:

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

**Electron density around NDP C 404:**

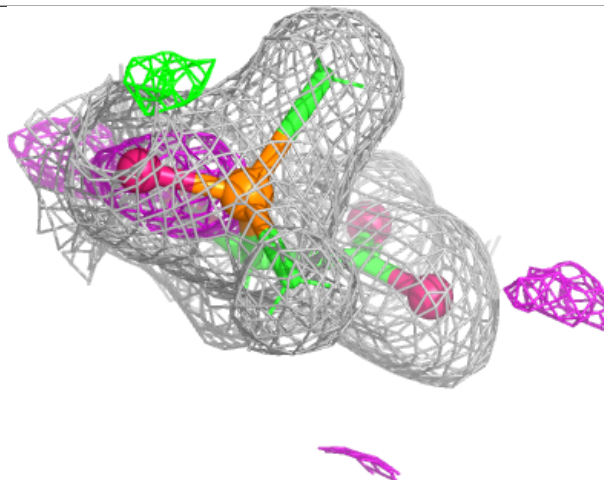
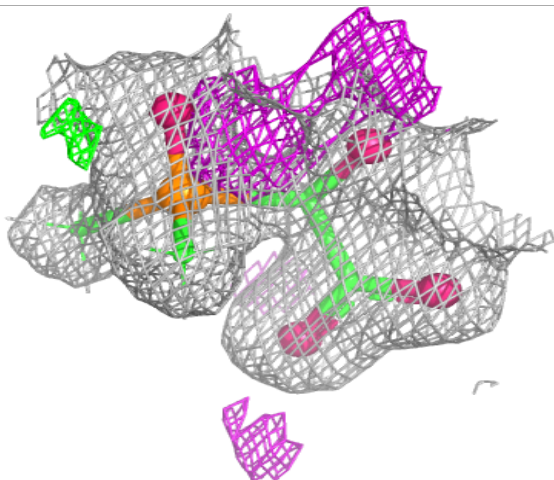
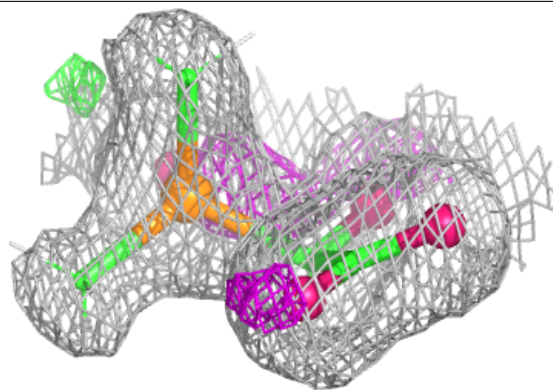
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





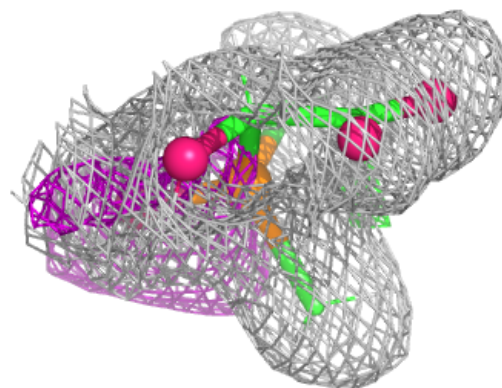
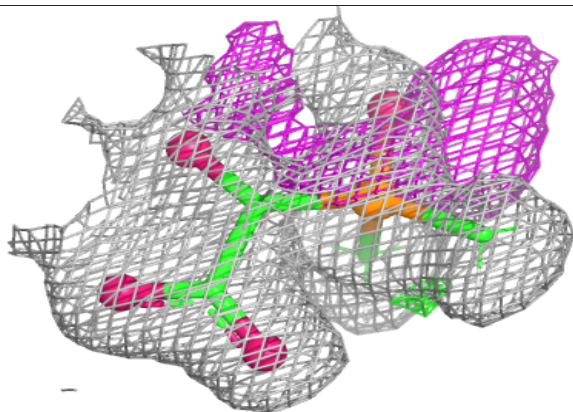
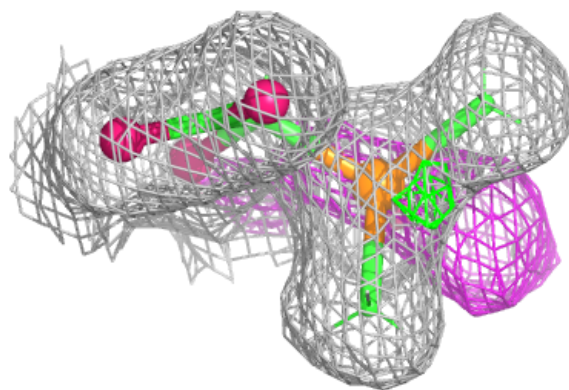
Electron density around X9W B 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

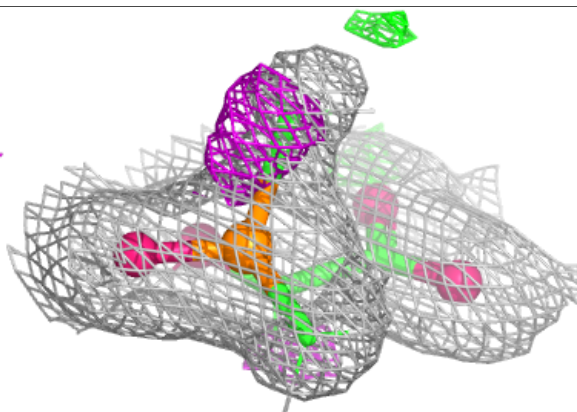
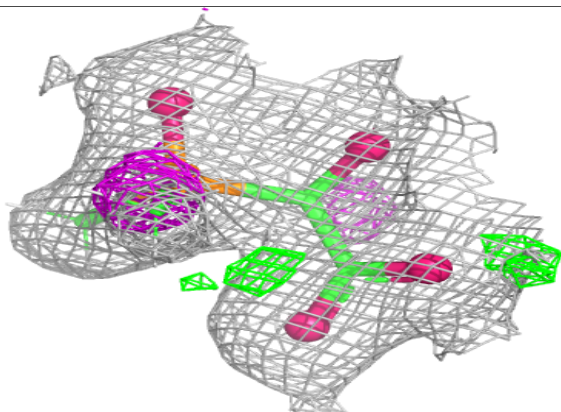
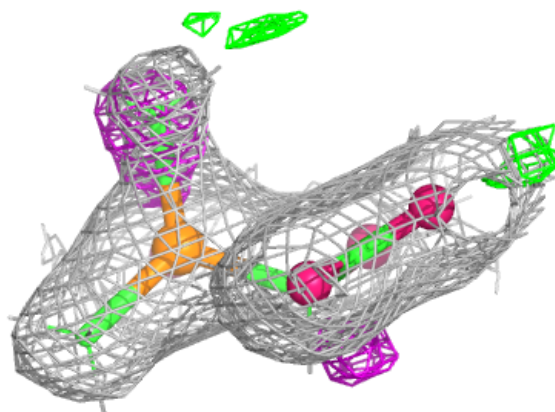


Electron density around X9W H 403:

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

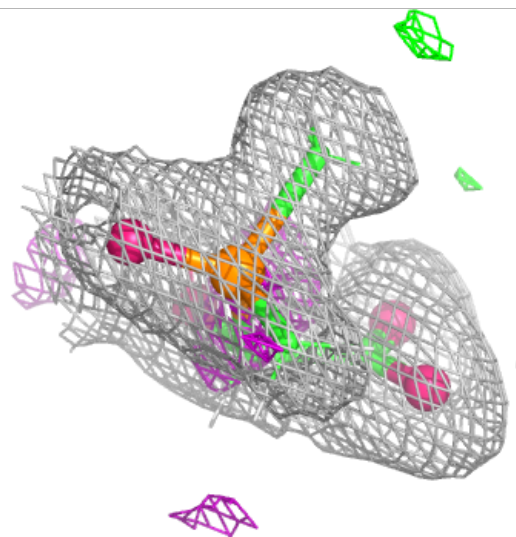
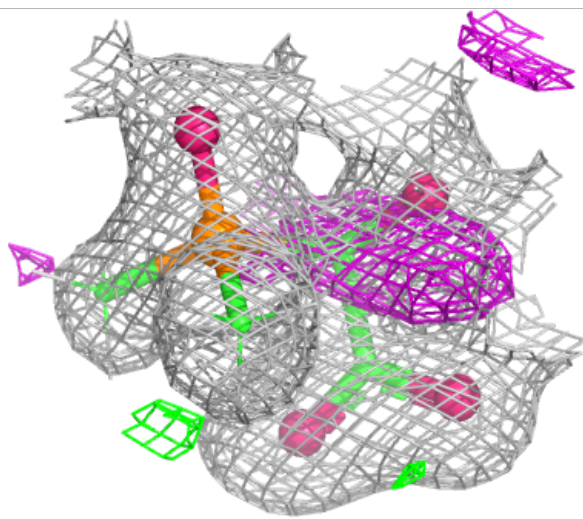
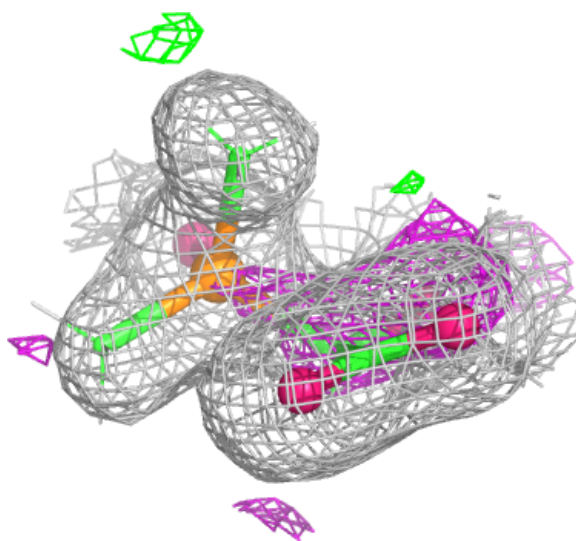
**Electron density around X9W H 405:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



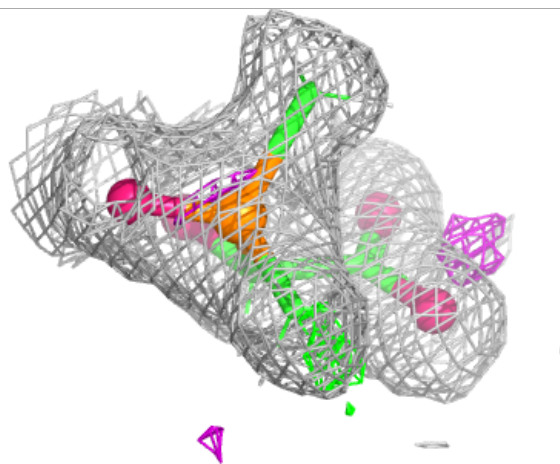
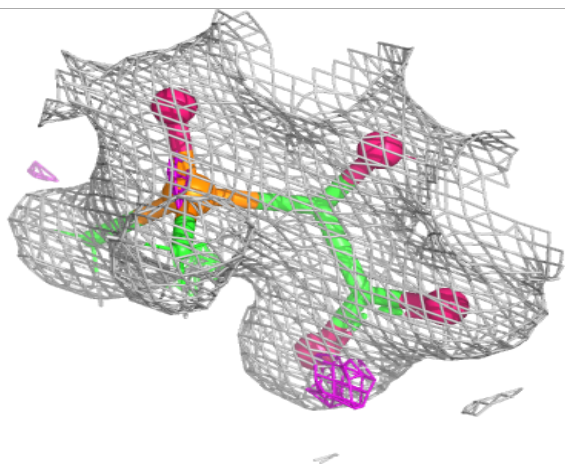
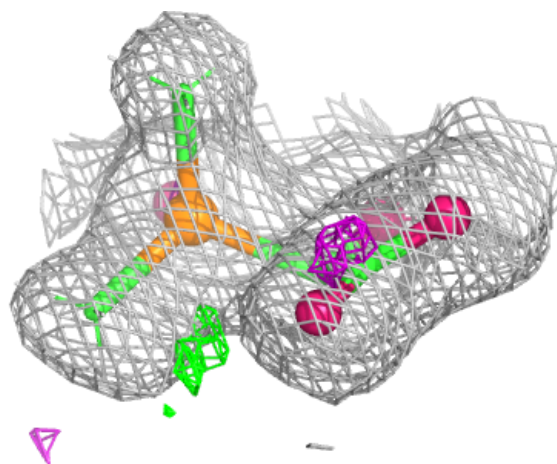
Electron density around X9W I 403:

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



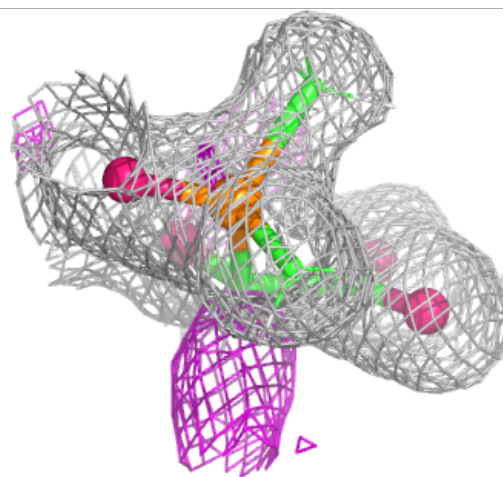
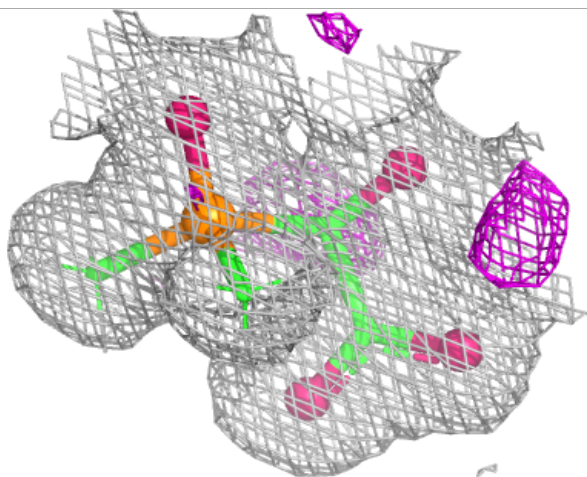
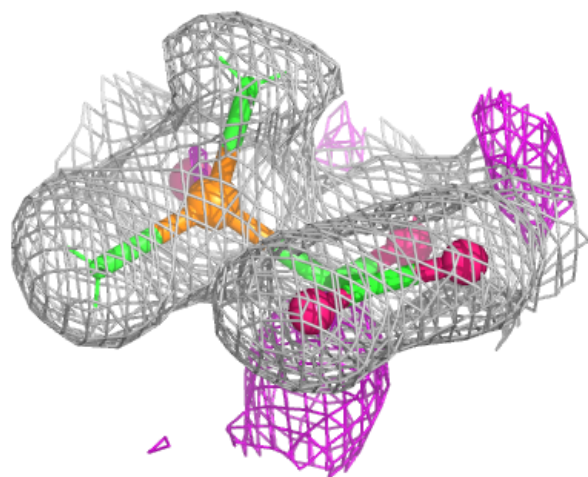
Electron density around X9W G 404:

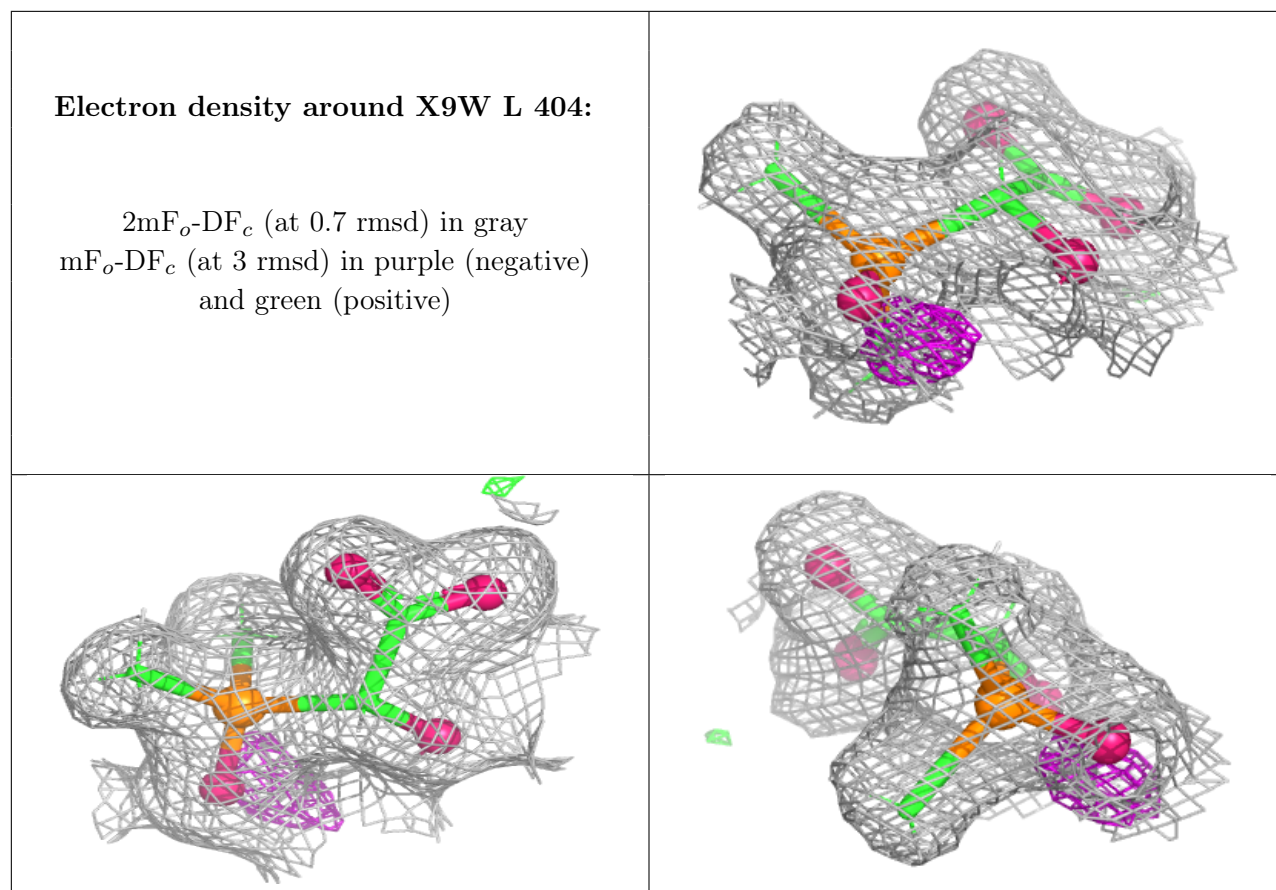
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around X9W J 403:

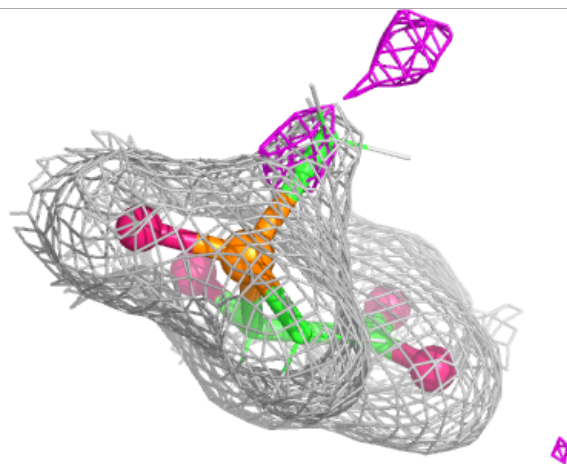
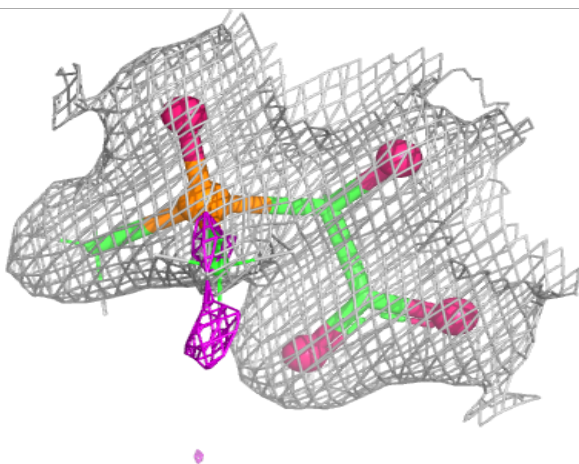
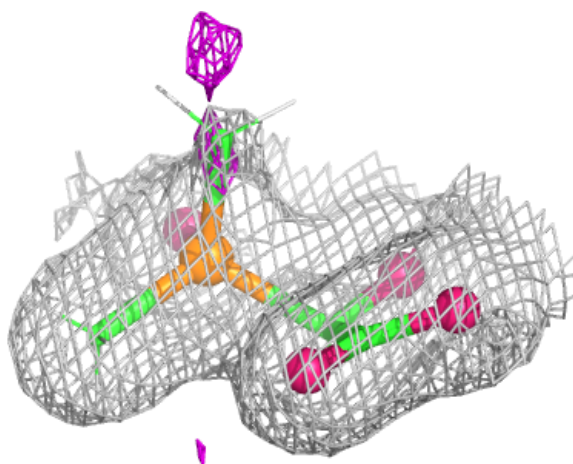
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





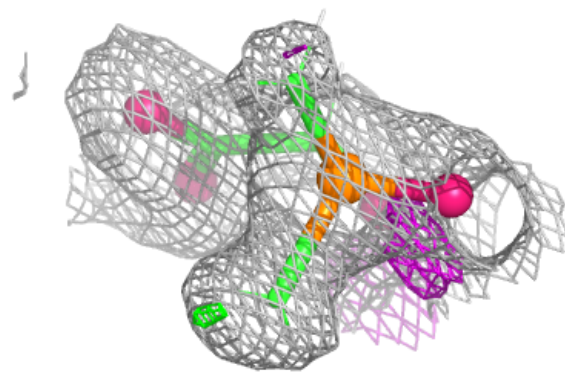
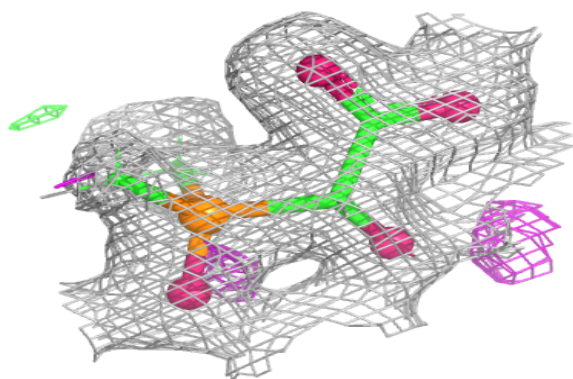
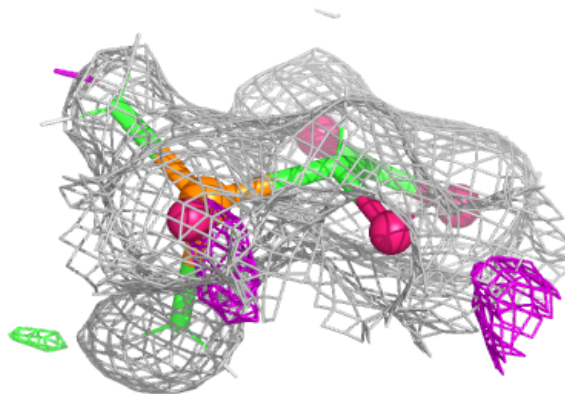
Electron density around X9W C 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

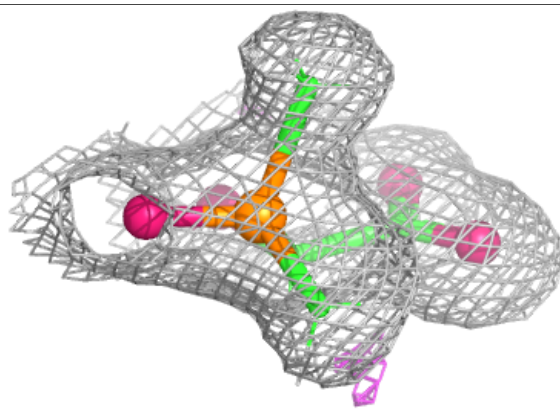
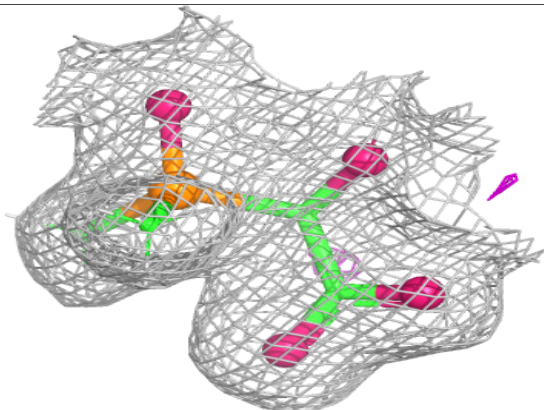
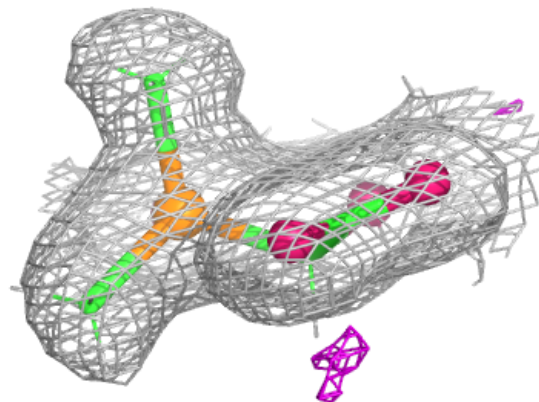


Electron density around X9W F 401:

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

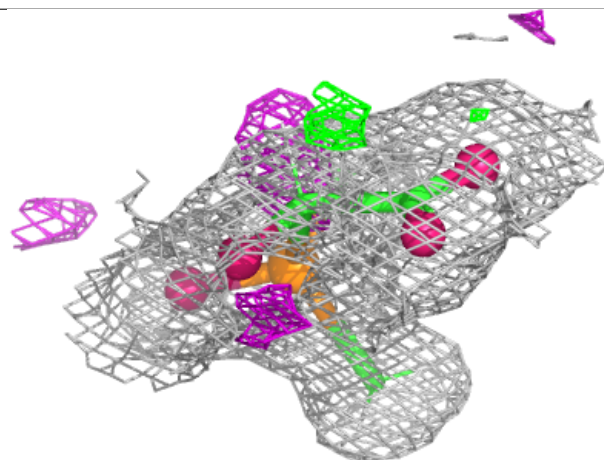
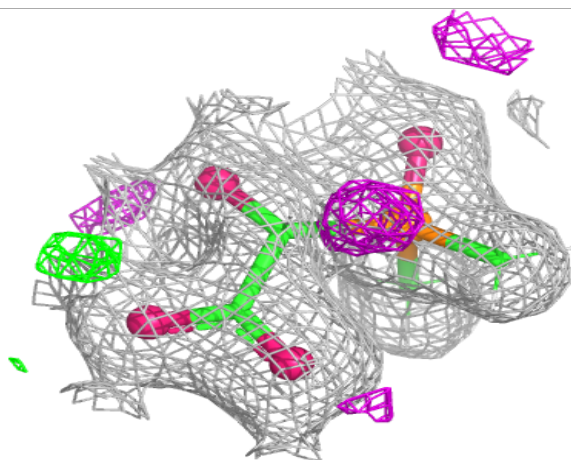
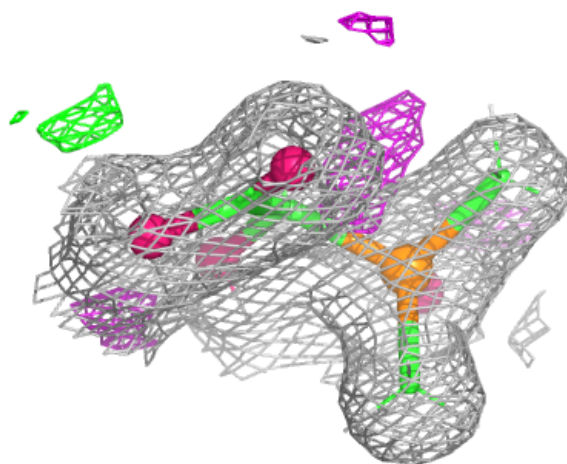
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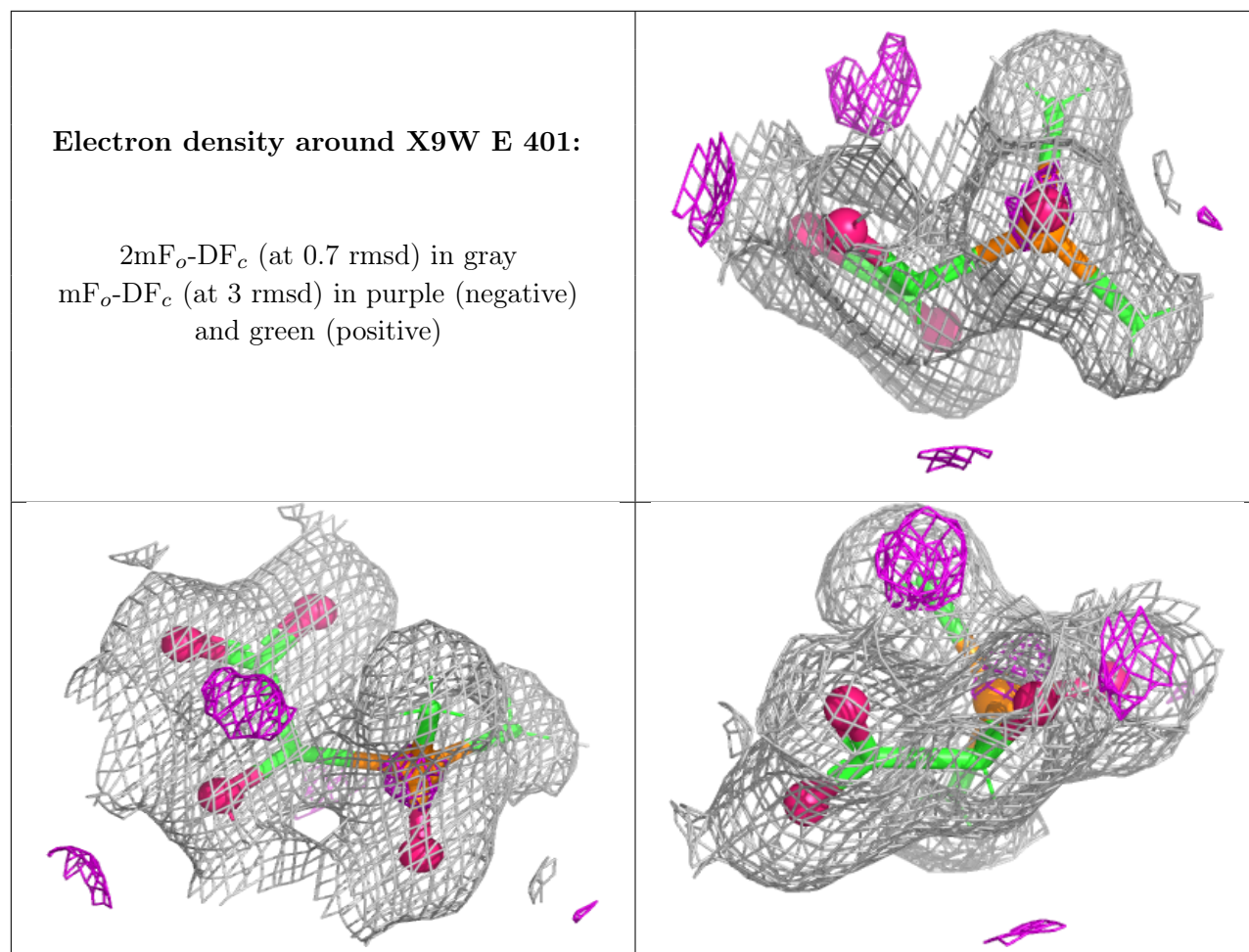
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around X9W D 404:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.