



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:54 PM UTC

PDB ID : 5H47 / pdb_00005h47
Title : Crystal structure of AOL complexed with 2-MeSe-Fuc
Authors : Kato, R.; Nishikawa, Y.; Makyio, H.
Deposited on : 2016-10-31
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	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

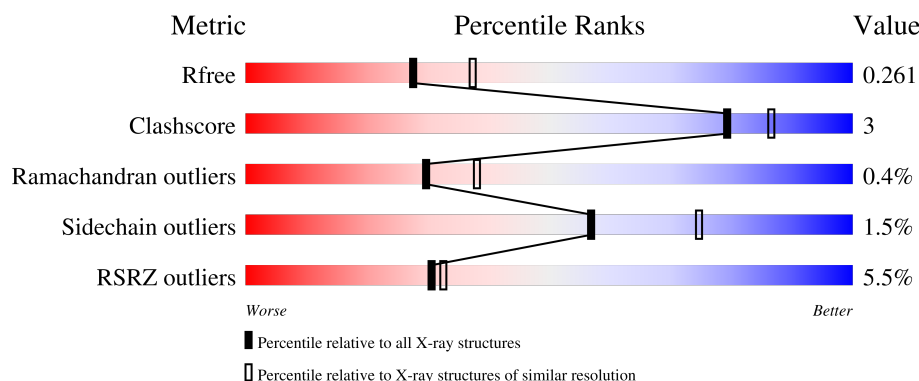
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	311	94% 6%
1	B	311	94% 6%
1	C	311	91% 8%
1	D	311	2% 94% 5%
1	E	311	92% 7%

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Mol	Chain	Length	Quality of chain
1	F	311	% 93% 7%
1	G	311	93% 7%
1	H	311	% 91% 8%
1	I	311	% 96% .
1	J	311	4% 95% 5%
1	K	311	13% 91% 9%
1	L	311	42% 82% 18%

2 Entry composition

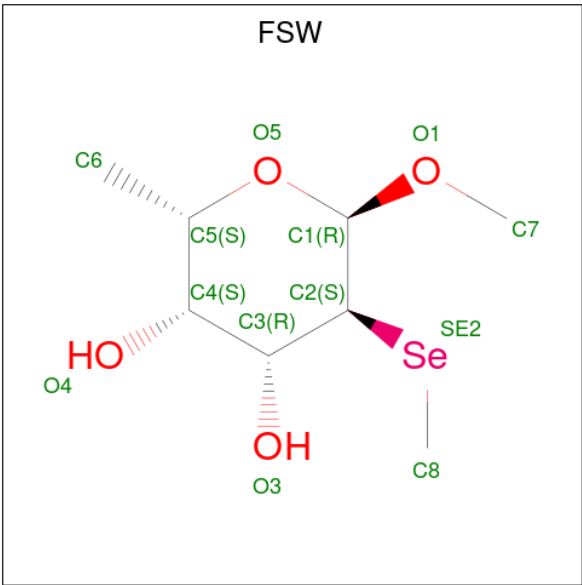
There are 3 unique types of molecules in this entry. The entry contains 31809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	B	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	C	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	D	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	E	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	F	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	G	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	H	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	I	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	J	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	K	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			
1	L	310	Total	C	N	O	S	0	0	0
			2436	1551	423	457	5			

- Molecule 2 is methyl 6-deoxy-2-Se-methyl-2-seleno-alpha-L-galactopyranoside (CCD ID: FSW) (formula: C₈H₁₆O₄Se).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	A	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	B	1	Total	C	O	Se	0	0
			13	8	4	1		
2	C	1	Total	C	O	Se	0	0
			13	8	4	1		
2	C	1	Total	C	O	Se	0	0
			13	8	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	C	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	D	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	E	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	F	1	Total 13	C 8	O 4	Se 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	G	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	H	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	I	1	Total 13	C 8	O 4	Se 1	0	0
2	J	1	Total 13	C 8	O 4	Se 1	0	0
2	J	1	Total 13	C 8	O 4	Se 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	J	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	K	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		
2	L	1	Total	C	O	Se	0	0
			13	8	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	188	Total	O	0	0
			188	188		
3	C	156	Total	O	0	0
			156	156		

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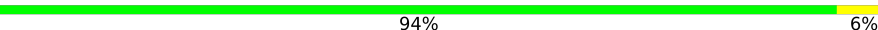
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	179	Total 179	O 179	0	0
3	E	150	Total 150	O 150	0	0
3	F	160	Total 160	O 160	0	0
3	G	121	Total 121	O 121	0	0
3	H	139	Total 139	O 139	0	0
3	I	124	Total 124	O 124	0	0
3	J	107	Total 107	O 107	0	0
3	K	61	Total 61	O 61	0	0
3	L	47	Total 47	O 47	0	0

3 Residue-property plots [i](#)

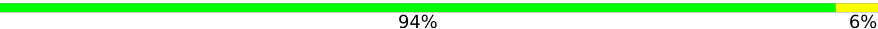
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein

Chain A: 



- Molecule 1: Uncharacterized protein

Chain B: 

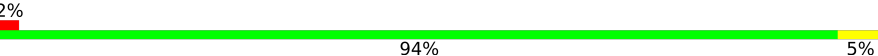


- Molecule 1: Uncharacterized protein

Chain C: 



- Molecule 1: Uncharacterized protein

Chain D: 

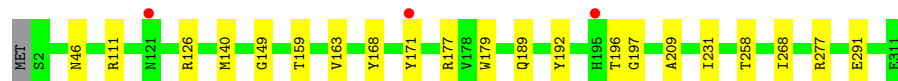
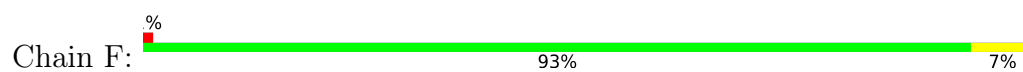


- Molecule 1: Uncharacterized protein

Chain E: 



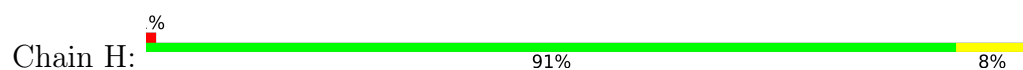
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



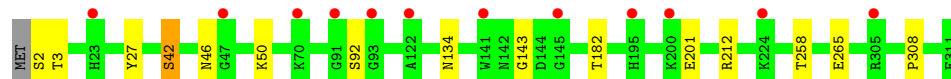
- Molecule 1: Uncharacterized protein



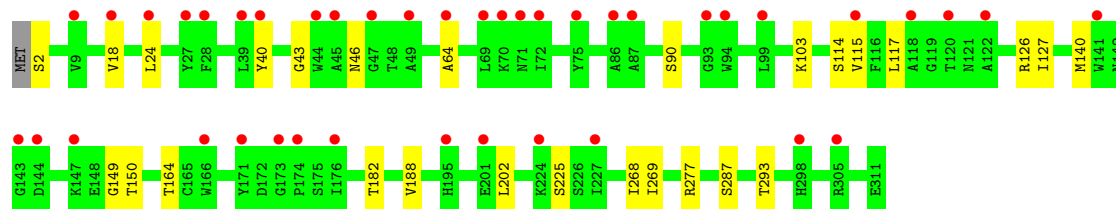
- Molecule 1: Uncharacterized protein



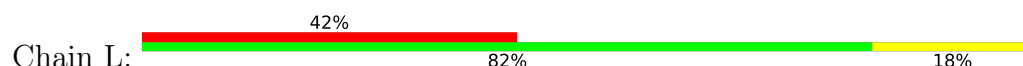
- Molecule 1: Uncharacterized protein

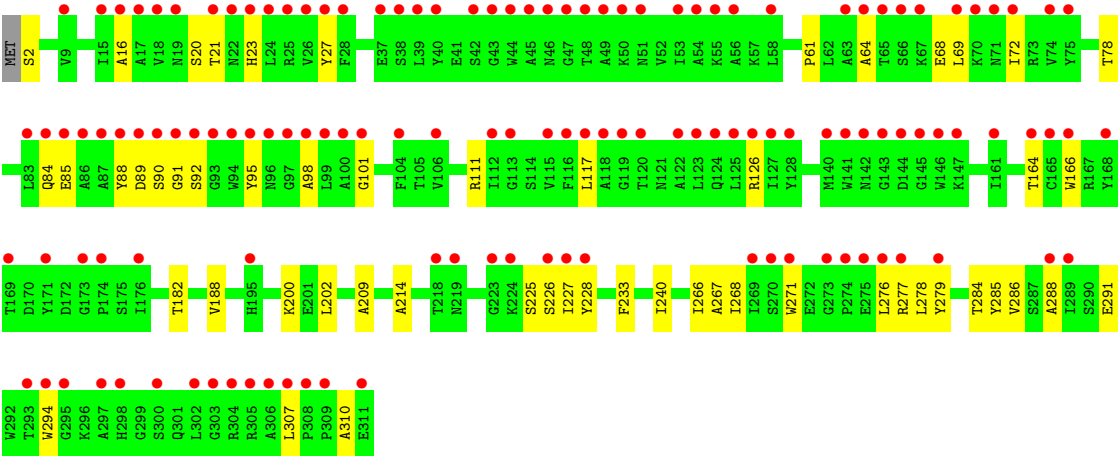


- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.97Å 214.32Å 126.53Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	39.99 – 2.30 39.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.99-2.30) 100.0 (39.99-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.216 , 0.258 0.219 , 0.261	Depositor DCC
R_{free} test set	11932 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31809	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FSW

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	0.95	0/2504	0.93	0/3413
1	B	0.94	0/2504	0.94	2/3413 (0.1%)
1	C	0.92	0/2504	0.93	2/3413 (0.1%)
1	D	0.97	1/2504 (0.0%)	0.95	0/3413
1	E	0.90	1/2504 (0.0%)	0.91	0/3413
1	F	0.89	0/2504	0.95	2/3413 (0.1%)
1	G	0.87	0/2504	0.93	0/3413
1	H	0.89	0/2504	0.94	2/3413 (0.1%)
1	I	0.88	0/2504	0.93	2/3413 (0.1%)
1	J	0.93	0/2504	0.98	2/3413 (0.1%)
1	K	0.88	0/2504	0.97	2/3413 (0.1%)
1	L	0.93	0/2504	1.02	2/3413 (0.1%)
All	All	0.91	2/30048 (0.0%)	0.95	16/40956 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	210	PRO	C-O	-5.31	1.20	1.25
1	E	3	THR	N-CA	5.19	1.50	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	209	ALA	CA-C-N	-7.00	114.55	119.66
1	L	209	ALA	C-N-CA	-7.00	114.55	119.66
1	H	70	LYS	N-CA-C	-5.87	105.79	113.12
1	C	140	MET	N-CA-C	5.71	118.09	109.23
1	C	14	GLY	N-CA-C	-5.64	104.86	112.14
1	B	140	MET	N-CA-C	5.49	117.75	109.23
1	J	265	GLU	N-CA-C	-5.49	102.33	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	209	ALA	CA-C-N	-5.38	115.79	119.66
1	F	209	ALA	C-N-CA	-5.38	115.79	119.66
1	I	209	ALA	CA-C-N	-5.38	115.79	119.66
1	I	209	ALA	C-N-CA	-5.38	115.79	119.66
1	B	297	ALA	N-CA-C	5.25	117.00	111.28
1	H	23	HIS	N-CA-C	-5.22	98.75	107.99
1	K	24	LEU	N-CA-C	5.15	117.46	108.76
1	J	143	GLY	N-CA-C	5.15	122.21	115.47
1	K	115	VAL	N-CA-C	5.14	117.14	108.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2436	0	2348	9	0
1	B	2436	0	2348	11	0
1	C	2436	0	2348	16	0
1	D	2436	0	2348	9	0
1	E	2436	0	2348	11	0
1	F	2436	0	2348	11	0
1	G	2436	0	2348	17	0
1	H	2436	0	2348	18	0
1	I	2436	0	2348	8	0
1	J	2436	0	2348	5	0
1	K	2436	0	2348	12	0
1	L	2436	0	2348	32	0
2	A	78	0	0	2	0
2	B	78	0	0	0	0
2	C	78	0	0	5	0
2	D	78	0	0	1	0
2	E	78	0	0	3	0
2	F	78	0	0	2	0
2	G	78	0	0	3	0
2	H	78	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	78	0	0	0	0
2	J	78	0	0	0	0
2	K	78	0	0	1	0
2	L	78	0	0	6	0
3	A	209	0	0	2	0
3	B	188	0	0	3	0
3	C	156	0	0	1	0
3	D	179	0	0	1	0
3	E	150	0	0	0	0
3	F	160	0	0	1	0
3	G	121	0	0	5	0
3	H	139	0	0	4	0
3	I	124	0	0	2	0
3	J	107	0	0	0	0
3	K	61	0	0	0	0
3	L	47	0	0	3	0
All	All	31809	0	28176	156	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 3.

All (156) 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:L:88:TYR:CZ	2:L:1001:FSW:O4	1.99	1.15
1:C:2:SER:N	3:C:1101:HOH:O	1.99	0.96
1:L:88:TYR:CE1	2:L:1001:FSW:O4	2.20	0.93
1:B:2:SER:N	3:B:1101:HOH:O	2.06	0.87
1:L:88:TYR:CE2	2:L:1001:FSW:O4	2.31	0.83
1:C:140:MET:CE	1:C:149:GLY:HA3	2.10	0.81
1:H:2:SER:N	3:H:1102:HOH:O	2.16	0.77
1:C:140:MET:HE3	1:C:149:GLY:HA3	1.67	0.76
1:G:140:MET:HE3	1:G:149:GLY:HA3	1.68	0.73
1:H:272:GLU:O	3:H:1101:HOH:O	2.08	0.72
1:A:2:SER:N	3:A:1102:HOH:O	2.23	0.71
1:L:268:ILE:HD13	1:L:278:LEU:HD13	1.73	0.70
1:I:190:ARG:HD3	1:I:202:LEU:HD23	1.72	0.70
1:F:291:GLU:OE1	2:F:1006:FSW:O3	2.09	0.70
1:C:140:MET:HE3	1:C:149:GLY:CA	2.21	0.69
1:L:23:HIS:HB3	1:L:69:LEU:HD11	1.76	0.66
1:E:167:ARG:NH1	1:E:171:TYR:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:MET:HE2	1:K:149:GLY:HA2	1.79	0.64
1:L:276:LEU:HD12	1:L:294:TRP:HB3	1.80	0.63
1:G:111:ARG:HG3	1:G:159:THR:O	2.02	0.60
1:I:300:SER:HB2	3:I:1203:HOH:O	2.02	0.59
1:K:140:MET:HE1	2:K:1003:FSW:SE2	2.52	0.59
1:G:140:MET:HE1	2:G:1003:FSW:C2	2.33	0.59
1:L:268:ILE:HD12	1:L:277:ARG:O	2.02	0.59
1:G:140:MET:HE1	2:G:1003:FSW:SE2	2.52	0.58
1:B:190:ARG:HD2	1:B:202:LEU:HD23	1.86	0.58
1:L:166:TRP:CD1	1:L:227:ILE:HD13	2.39	0.58
1:F:168:TYR:HB2	1:F:171:TYR:HB2	1.86	0.57
1:L:188:VAL:HG21	1:L:202:LEU:HD22	1.85	0.57
1:A:190:ARG:HD2	1:A:202:LEU:HD23	1.84	0.57
1:G:268:ILE:HD13	1:G:278:LEU:HD13	1.84	0.57
1:B:268:ILE:HD13	1:B:278:LEU:HD13	1.86	0.57
1:A:237:ASP:OD2	3:A:1101:HOH:O	2.17	0.56
1:L:95:TYR:HE2	2:L:1002:FSW:C8	2.18	0.56
1:H:20:SER:OG	1:H:68:GLU:OE1	2.24	0.55
1:H:98:ALA:HB2	2:H:1002:FSW:C8	2.38	0.54
1:L:111:ARG:HD2	3:L:1108:HOH:O	2.07	0.53
1:I:190:ARG:CD	1:I:202:LEU:HD23	2.36	0.53
1:C:291:GLU:OE1	2:C:1006:FSW:O3	2.27	0.52
1:B:130:GLN:OE1	3:B:1102:HOH:O	2.18	0.52
1:C:95:TYR:HE1	2:C:1002:FSW:C8	2.21	0.52
1:K:268:ILE:HD12	1:K:277:ARG:O	2.10	0.52
1:B:111:ARG:HG3	1:B:160:GLY:HA2	1.90	0.52
1:L:284:THR:O	1:L:288:ALA:HB3	2.10	0.52
1:C:268:ILE:HD12	1:C:277:ARG:O	2.10	0.51
1:E:35:ILE:HD12	1:E:62:LEU:HD11	1.91	0.51
1:L:78:THR:HG22	1:L:84:GLN:OE1	2.10	0.51
1:L:88:TYR:CD1	2:L:1001:FSW:O4	2.64	0.51
1:G:2:SER:N	3:G:1104:HOH:O	2.43	0.51
1:L:214:ALA:O	1:L:233:PHE:HA	2.10	0.50
2:A:1004:FSW:O1	2:A:1004:FSW:C8	2.60	0.50
1:E:140:MET:HE1	2:E:1003:FSW:C8	2.42	0.50
1:G:277:ARG:CD	1:G:293:THR:HG22	2.42	0.50
1:L:285:TYR:HA	3:L:1105:HOH:O	2.11	0.50
1:H:305:ARG:NH2	3:H:1104:HOH:O	2.36	0.50
1:A:268:ILE:HD13	1:A:278:LEU:HD13	1.93	0.49
1:C:36:ARG:HD3	1:C:48:THR:O	2.13	0.49
1:K:188:VAL:HG21	1:K:202:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:ARG:HG3	1:I:160:GLY:HA2	1.94	0.49
1:H:98:ALA:CB	2:H:1002:FSW:C8	2.90	0.49
1:H:170:ASP:HB3	1:H:224:LYS:HG3	1.94	0.49
1:I:111:ARG:NH1	3:I:1105:HOH:O	2.44	0.49
1:F:140:MET:HE2	1:F:149:GLY:HA2	1.95	0.48
1:C:138:GLU:OE1	2:C:1003:FSW:O3	2.31	0.48
1:G:189:GLN:NE2	1:G:251:TYR:OH	2.46	0.48
1:B:140:MET:HE2	1:B:149:GLY:HA2	1.96	0.48
1:C:111:ARG:HG3	1:C:159:THR:O	2.14	0.47
1:J:2:SER:OG	1:J:3:THR:N	2.46	0.47
1:L:117:LEU:HD21	1:L:126:ARG:CG	2.45	0.47
1:H:111:ARG:HD2	3:H:1146:HOH:O	2.13	0.47
1:K:277:ARG:CD	1:K:293:THR:HG22	2.44	0.47
2:G:1005:FSW:O1	3:G:1102:HOH:O	2.20	0.47
1:B:111:ARG:NH1	3:B:1106:HOH:O	2.44	0.47
1:A:111:ARG:HG3	1:A:160:GLY:HA2	1.97	0.47
1:B:30:ASP:C	1:B:30:ASP:OD1	2.58	0.46
1:E:277:ARG:CD	1:E:293:THR:HG22	2.45	0.46
1:L:21:THR:O	1:L:271:TRP:CE2	2.68	0.46
1:L:117:LEU:HD21	1:L:126:ARG:HG3	1.97	0.46
1:F:111:ARG:HG3	1:F:159:THR:O	2.15	0.46
1:H:111:ARG:HG3	1:H:160:GLY:HA2	1.97	0.46
1:L:16:ALA:HB1	1:L:64:ALA:HB3	1.98	0.46
1:L:27:TYR:OH	1:L:72:ILE:HG21	2.15	0.46
1:L:61:PRO:HB3	1:L:111:ARG:HA	1.98	0.46
1:C:3:THR:HG21	1:C:310:ALA:O	2.16	0.46
1:K:117:LEU:HD21	1:K:126:ARG:CG	2.46	0.46
1:L:240:ILE:HG12	1:L:266:ILE:HD11	1.97	0.46
1:D:131:LYS:NZ	3:D:1108:HOH:O	2.48	0.46
1:K:40:TYR:HA	1:K:43:GLY:O	2.17	0.45
1:F:111:ARG:HD2	3:F:1190:HOH:O	2.16	0.45
1:F:126:ARG:CD	1:F:140:MET:HB3	2.46	0.45
1:L:98:ALA:O	1:L:101:GLY:N	2.50	0.45
1:D:111:ARG:HG3	1:D:159:THR:O	2.17	0.45
1:E:111:ARG:HG3	1:E:159:THR:O	2.17	0.45
1:B:266:ILE:HG22	1:B:267:ALA:N	2.30	0.45
1:D:268:ILE:HD12	1:D:277:ARG:O	2.17	0.45
1:F:268:ILE:HD12	1:F:277:ARG:O	2.16	0.45
1:E:138:GLU:OE1	2:E:1003:FSW:O3	2.35	0.45
1:E:179:TRP:CZ2	1:E:231:ILE:HD11	2.51	0.44
1:I:111:ARG:HG3	1:I:159:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:HD2	1:D:202:LEU:HD23	1.99	0.44
1:G:7:GLN:NE2	1:J:134:ASN:HD21	2.16	0.44
1:G:7:GLN:HE22	1:J:134:ASN:HD21	1.64	0.44
1:G:11:PHE:HB2	1:J:212:ARG:NH1	2.33	0.44
1:F:189:GLN:OE1	2:F:1004:FSW:O4	2.36	0.44
1:I:39:LEU:C	1:I:39:LEU:HD12	2.43	0.44
1:D:61:PRO:HB3	1:D:111:ARG:HA	1.99	0.44
1:H:111:ARG:HG3	1:H:159:THR:O	2.18	0.44
1:G:88:TYR:OH	3:G:1103:HOH:O	2.20	0.43
1:K:140:MET:HE2	1:K:149:GLY:CA	2.45	0.43
1:F:163:VAL:HA	1:F:177:ARG:O	2.17	0.43
1:G:305:ARG:HD3	3:G:1217:HOH:O	2.17	0.43
1:H:278:LEU:HB2	1:H:292:TRP:HB3	2.01	0.43
1:G:277:ARG:HD3	1:G:293:THR:HG22	2.01	0.43
1:H:189:GLN:NE2	2:H:1004:FSW:O4	2.49	0.43
1:K:117:LEU:HD21	1:K:126:ARG:HG2	1.99	0.43
1:L:2:SER:N	3:L:1105:HOH:O	2.50	0.43
1:L:89:ASP:O	1:L:91:GLY:N	2.51	0.43
1:I:277:ARG:CD	1:I:293:THR:HG22	2.49	0.43
1:C:140:MET:HE1	2:C:1003:FSW:SE2	2.68	0.43
1:H:193:ASP:OD2	1:H:199:TYR:OH	2.13	0.42
1:D:40:TYR:HA	1:D:43:GLY:O	2.20	0.42
1:J:27:TYR:CD2	1:J:27:TYR:N	2.87	0.42
1:L:266:ILE:HG22	1:L:267:ALA:N	2.35	0.42
1:C:140:MET:CE	1:C:149:GLY:CA	2.86	0.42
1:C:191:ALA:HB3	1:C:199:TYR:CD2	2.55	0.42
1:L:307:LEU:O	1:L:310:ALA:HB3	2.18	0.42
1:E:175:SER:OG	1:E:193:ASP:OD1	2.35	0.42
1:L:20:SER:OG	1:L:68:GLU:OE1	2.27	0.42
1:L:85:GLU:OE2	2:L:1002:FSW:O4	2.37	0.42
1:B:205:ILE:HG22	1:B:251:TYR:CE2	2.55	0.42
1:K:269:ILE:HG13	1:K:277:ARG:HB2	2.00	0.42
1:G:111:ARG:HD2	3:G:1127:HOH:O	2.19	0.42
1:H:39:LEU:HD12	1:H:39:LEU:C	2.45	0.42
1:G:140:MET:HE3	1:G:149:GLY:CA	2.44	0.42
1:H:291:GLU:OE1	2:H:1006:FSW:O3	2.38	0.42
1:A:149:GLY:HA2	2:A:1003:FSW:C8	2.50	0.41
1:E:212:ARG:NH1	1:H:11:PHE:HB2	2.35	0.41
1:D:126:ARG:HD3	1:D:140:MET:HB3	2.02	0.41
1:G:193:ASP:HB2	1:G:196:THR:CG2	2.51	0.41
1:C:83:LEU:HB3	1:C:99:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:SER:CB	1:H:157:PRO:HG2	2.50	0.41
1:E:291:GLU:OE1	2:E:1006:FSW:O3	2.39	0.41
1:B:282:ASN:OD1	1:B:282:ASN:C	2.64	0.41
1:K:18:VAL:HG13	1:K:64:ALA:HB1	2.03	0.41
1:H:39:LEU:HD13	1:H:41:GLU:HG2	2.03	0.41
1:L:228:TYR:N	1:L:228:TYR:CD1	2.88	0.41
1:A:277:ARG:CD	1:A:293:THR:HG22	2.51	0.40
1:L:279:TYR:CE1	1:L:291:GLU:HG3	2.56	0.40
1:D:189:GLN:OE1	2:D:1004:FSW:O4	2.40	0.40
1:F:192:TYR:CE2	1:F:197:GLY:HA2	2.55	0.40
1:D:190:ARG:CD	1:D:202:LEU:HD23	2.52	0.40
1:K:114:SER:HA	1:K:127:ILE:HD13	2.02	0.40
1:A:61:PRO:HG3	1:A:110:SER:O	2.22	0.40
1:A:89:ASP:O	1:A:90:SER:C	2.63	0.40
1:C:37:GLU:OE1	2:C:1001:FSW:O4	2.40	0.40
1:F:179:TRP:CZ2	1:F:231:ILE:HD11	2.56	0.40

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	308/311 (99%)	302 (98%)	6 (2%)	0	100	100
1	B	308/311 (99%)	299 (97%)	8 (3%)	1 (0%)	36	46
1	C	308/311 (99%)	298 (97%)	9 (3%)	1 (0%)	36	46
1	D	308/311 (99%)	293 (95%)	14 (4%)	1 (0%)	36	46
1	E	308/311 (99%)	297 (96%)	9 (3%)	2 (1%)	21	27
1	F	308/311 (99%)	296 (96%)	11 (4%)	1 (0%)	36	46
1	G	308/311 (99%)	301 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	308/311 (99%)	296 (96%)	11 (4%)	1 (0%)	36	46
1	I	308/311 (99%)	296 (96%)	12 (4%)	0	100	100
1	J	308/311 (99%)	290 (94%)	14 (4%)	4 (1%)	9	10
1	K	308/311 (99%)	283 (92%)	23 (8%)	2 (1%)	21	27
1	L	308/311 (99%)	281 (91%)	25 (8%)	2 (1%)	21	27
All	All	3696/3732 (99%)	3532 (96%)	149 (4%)	15 (0%)	30	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	90	SER
1	B	46	ASN
1	J	42	SER
1	J	46	ASN
1	D	46	ASN
1	E	46	ASN
1	H	46	ASN
1	K	46	ASN
1	C	46	ASN
1	J	308	PRO
1	K	225	SER
1	L	286	VAL
1	F	46	ASN
1	J	92	SER
1	E	286	VAL

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	251/252 (100%)	246 (98%)	5 (2%)	48	67
1	B	251/252 (100%)	250 (100%)	1 (0%)	84	92
1	C	251/252 (100%)	246 (98%)	5 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	251/252 (100%)	249 (99%)	2 (1%)	73	86
1	E	251/252 (100%)	247 (98%)	4 (2%)	55	73
1	F	251/252 (100%)	249 (99%)	2 (1%)	73	86
1	G	251/252 (100%)	246 (98%)	5 (2%)	48	67
1	H	251/252 (100%)	249 (99%)	2 (1%)	73	86
1	I	251/252 (100%)	249 (99%)	2 (1%)	73	86
1	J	251/252 (100%)	246 (98%)	5 (2%)	48	67
1	K	251/252 (100%)	244 (97%)	7 (3%)	38	56
1	L	251/252 (100%)	245 (98%)	6 (2%)	43	62
All	All	3012/3024 (100%)	2966 (98%)	46 (2%)	57	75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	90	SER
1	A	92	SER
1	A	199	TYR
1	A	266	ILE
1	B	258	THR
1	C	24	LEU
1	C	39	LEU
1	C	62	LEU
1	C	182	THR
1	C	266	ILE
1	D	39	LEU
1	D	90	SER
1	E	62	LEU
1	E	127	ILE
1	E	182	THR
1	E	201	GLU
1	F	196	THR
1	F	258	THR
1	G	70	LYS
1	G	90	SER
1	G	120	THR
1	G	123	LEU
1	G	199	TYR
1	H	24	LEU

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Mol	Chain	Res	Type
1	H	266	ILE
1	I	42	SER
1	I	105	THR
1	J	42	SER
1	J	50	LYS
1	J	182	THR
1	J	201	GLU
1	J	258	THR
1	K	2	SER
1	K	90	SER
1	K	103	LYS
1	K	150	THR
1	K	164	THR
1	K	182	THR
1	K	287	SER
1	L	92	SER
1	L	164	THR
1	L	182	THR
1	L	200	LYS
1	L	225	SER
1	L	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	247	HIS
1	B	7	GLN
1	B	32	HIS
1	B	134	ASN
1	B	249	GLN
1	C	7	GLN
1	C	219	ASN
1	C	249	GLN
1	C	298	HIS
1	D	121	ASN
1	D	137	GLN
1	D	151	ASN
1	E	7	GLN
1	E	134	ASN
1	E	238	ASN
1	E	247	HIS

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Mol	Chain	Res	Type
1	F	7	GLN
1	F	71	ASN
1	F	84	GLN
1	F	124	GLN
1	F	134	ASN
1	F	195	HIS
1	F	242	GLN
1	F	247	HIS
1	F	298	HIS
1	G	189	GLN
1	G	238	ASN
1	G	301	GLN
1	H	7	GLN
1	H	124	GLN
1	H	134	ASN
1	H	137	GLN
1	H	142	ASN
1	H	151	ASN
1	H	189	GLN
1	H	238	ASN
1	I	7	GLN
1	I	71	ASN
1	I	134	ASN
1	I	247	HIS
1	I	298	HIS
1	J	71	ASN
1	J	134	ASN
1	J	238	ASN
1	J	249	GLN
1	J	301	GLN
1	K	7	GLN
1	K	71	ASN
1	K	134	ASN
1	K	242	GLN
1	K	249	GLN
1	K	301	GLN
1	L	23	HIS
1	L	32	HIS
1	L	71	ASN
1	L	134	ASN
1	L	242	GLN
1	L	247	HIS

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 ⓘ

72 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FSW	A	1004	-	10,13,13	1.07	2 (20%)	14,18,18	2.26	2 (14%)
2	FSW	E	1005	-	10,13,13	1.03	1 (10%)	14,18,18	1.86	4 (28%)
2	FSW	I	1003	-	10,13,13	0.83	0	14,18,18	2.41	3 (21%)
2	FSW	I	1004	-	10,13,13	0.99	1 (10%)	14,18,18	2.58	4 (28%)
2	FSW	B	1006	-	10,13,13	1.29	1 (10%)	14,18,18	2.89	4 (28%)
2	FSW	L	1006	-	10,13,13	1.17	1 (10%)	14,18,18	2.02	6 (42%)
2	FSW	D	1004	-	10,13,13	1.03	1 (10%)	14,18,18	2.47	4 (28%)
2	FSW	E	1004	-	10,13,13	0.75	0	14,18,18	2.61	5 (35%)
2	FSW	A	1006	-	10,13,13	1.09	2 (20%)	14,18,18	2.46	3 (21%)
2	FSW	G	1005	-	10,13,13	1.29	2 (20%)	14,18,18	3.28	6 (42%)
2	FSW	J	1003	-	10,13,13	0.98	1 (10%)	14,18,18	2.52	4 (28%)
2	FSW	J	1002	-	10,13,13	0.93	1 (10%)	14,18,18	1.33	2 (14%)
2	FSW	I	1006	-	10,13,13	0.95	1 (10%)	14,18,18	2.42	4 (28%)
2	FSW	F	1001	-	10,13,13	0.65	0	14,18,18	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FSW	H	1001	-	10,13,13	1.12	1 (10%)	14,18,18	3.01	3 (21%)
2	FSW	H	1005	-	10,13,13	1.40	1 (10%)	14,18,18	2.87	4 (28%)
2	FSW	A	1005	-	10,13,13	1.16	1 (10%)	14,18,18	2.72	6 (42%)
2	FSW	J	1005	-	10,13,13	0.63	0	14,18,18	0.70	0
2	FSW	B	1003	-	10,13,13	1.10	2 (20%)	14,18,18	2.24	4 (28%)
2	FSW	K	1002	-	10,13,13	0.68	0	14,18,18	1.57	4 (28%)
2	FSW	I	1001	-	10,13,13	1.11	1 (10%)	14,18,18	2.66	5 (35%)
2	FSW	E	1006	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	C	1005	-	10,13,13	1.60	1 (10%)	14,18,18	3.62	6 (42%)
2	FSW	F	1002	-	10,13,13	0.91	1 (10%)	14,18,18	2.47	4 (28%)
2	FSW	D	1003	-	10,13,13	0.95	1 (10%)	14,18,18	2.19	6 (42%)
2	FSW	F	1004	-	10,13,13	0.93	1 (10%)	14,18,18	2.38	4 (28%)
2	FSW	H	1003	-	10,13,13	1.20	2 (20%)	14,18,18	2.39	4 (28%)
2	FSW	A	1001	-	10,13,13	0.89	1 (10%)	14,18,18	2.83	5 (35%)
2	FSW	E	1001	-	10,13,13	0.66	0	14,18,18	0.71	0
2	FSW	B	1002	-	10,13,13	0.53	0	14,18,18	2.26	3 (21%)
2	FSW	A	1003	-	10,13,13	0.94	1 (10%)	14,18,18	2.50	3 (21%)
2	FSW	G	1002	-	10,13,13	0.72	0	14,18,18	1.07	0
2	FSW	G	1006	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	D	1001	-	10,13,13	1.75	2 (20%)	14,18,18	3.10	8 (57%)
2	FSW	E	1003	-	10,13,13	0.82	0	14,18,18	2.18	5 (35%)
2	FSW	I	1002	-	10,13,13	1.21	1 (10%)	14,18,18	3.12	6 (42%)
2	FSW	J	1001	-	10,13,13	1.50	1 (10%)	14,18,18	2.92	6 (42%)
2	FSW	K	1006	-	10,13,13	1.10	1 (10%)	14,18,18	1.37	1 (7%)
2	FSW	L	1002	-	10,13,13	0.69	0	14,18,18	1.59	5 (35%)
2	FSW	B	1001	-	10,13,13	1.31	1 (10%)	14,18,18	2.97	5 (35%)
2	FSW	D	1006	-	10,13,13	0.95	1 (10%)	14,18,18	2.64	7 (50%)
2	FSW	B	1004	-	10,13,13	1.09	1 (10%)	14,18,18	0.99	1 (7%)
2	FSW	F	1006	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	F	1005	-	10,13,13	1.31	1 (10%)	14,18,18	1.28	1 (7%)
2	FSW	H	1004	-	10,13,13	1.13	1 (10%)	14,18,18	1.37	3 (21%)
2	FSW	J	1006	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	E	1002	-	10,13,13	1.33	2 (20%)	14,18,18	2.48	4 (28%)
2	FSW	K	1001	-	10,13,13	0.65	0	14,18,18	0.70	0
2	FSW	K	1003	-	10,13,13	1.28	1 (10%)	14,18,18	2.53	7 (50%)
2	FSW	K	1004	-	10,13,13	1.03	1 (10%)	14,18,18	2.25	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FSW	J	1004	-	10,13,13	1.04	1 (10%)	14,18,18	2.47	5 (35%)
2	FSW	L	1005	-	10,13,13	0.66	0	14,18,18	0.72	0
2	FSW	C	1002	-	10,13,13	0.86	1 (10%)	14,18,18	0.70	0
2	FSW	C	1003	-	10,13,13	0.90	0	14,18,18	2.29	4 (28%)
2	FSW	D	1002	-	10,13,13	1.69	1 (10%)	14,18,18	2.19	4 (28%)
2	FSW	I	1005	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	H	1006	-	10,13,13	0.64	0	14,18,18	0.71	0
2	FSW	H	1002	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	L	1001	-	10,13,13	0.64	0	14,18,18	0.66	0
2	FSW	G	1003	-	10,13,13	1.00	1 (10%)	14,18,18	1.25	2 (14%)
2	FSW	G	1001	-	10,13,13	0.64	0	14,18,18	0.71	0
2	FSW	L	1003	-	10,13,13	1.34	1 (10%)	14,18,18	1.67	3 (21%)
2	FSW	B	1005	-	10,13,13	1.18	2 (20%)	14,18,18	2.53	6 (42%)
2	FSW	C	1001	-	10,13,13	1.19	1 (10%)	14,18,18	2.92	6 (42%)
2	FSW	D	1005	-	10,13,13	1.22	1 (10%)	14,18,18	2.54	6 (42%)
2	FSW	L	1004	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	C	1004	-	10,13,13	0.88	1 (10%)	14,18,18	0.51	0
2	FSW	C	1006	-	10,13,13	0.65	0	14,18,18	0.71	0
2	FSW	F	1003	-	10,13,13	0.62	0	14,18,18	2.46	3 (21%)
2	FSW	K	1005	-	10,13,13	0.99	1 (10%)	14,18,18	1.61	4 (28%)
2	FSW	G	1004	-	10,13,13	1.03	1 (10%)	14,18,18	2.62	4 (28%)
2	FSW	A	1002	-	10,13,13	0.84	0	14,18,18	2.78	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSW	A	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1003	-	-	1/2/24/24	0/1/1/1
2	FSW	I	1004	-	-	1/2/24/24	0/1/1/1
2	FSW	B	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1006	-	-	1/2/24/24	0/1/1/1
2	FSW	D	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1005	-	-	2/2/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSW	J	1003	-	-	2/2/24/24	0/1/1/1
2	FSW	J	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1006	-	-	2/2/24/24	0/1/1/1
2	FSW	F	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1005	-	-	2/2/24/24	0/1/1/1
2	FSW	J	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1002	-	-	2/2/24/24	0/1/1/1
2	FSW	I	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1002	-	-	1/2/24/24	0/1/1/1
2	FSW	D	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	E	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1001	-	-	2/2/24/24	0/1/1/1
2	FSW	E	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1002	-	-	1/2/24/24	0/1/1/1
2	FSW	J	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1006	-	-	2/2/24/24	0/1/1/1
2	FSW	L	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1006	-	-	1/2/24/24	0/1/1/1
2	FSW	B	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1004	-	-	1/2/24/24	0/1/1/1
2	FSW	J	1006	-	-	2/2/24/24	0/1/1/1
2	FSW	E	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	K	1001	-	-	2/2/24/24	0/1/1/1
2	FSW	K	1003	-	-	2/2/24/24	0/1/1/1
2	FSW	K	1004	-	-	2/2/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSW	J	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1005	-	-	2/2/24/24	0/1/1/1
2	FSW	C	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1003	-	-	1/2/24/24	0/1/1/1
2	FSW	D	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	I	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	H	1002	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1001	-	-	1/2/24/24	0/1/1/1
2	FSW	G	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1003	-	-	0/2/24/24	0/1/1/1
2	FSW	B	1005	-	-	1/2/24/24	0/1/1/1
2	FSW	C	1001	-	-	0/2/24/24	0/1/1/1
2	FSW	D	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	L	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	C	1006	-	-	0/2/24/24	0/1/1/1
2	FSW	F	1003	-	-	2/2/24/24	0/1/1/1
2	FSW	K	1005	-	-	0/2/24/24	0/1/1/1
2	FSW	G	1004	-	-	0/2/24/24	0/1/1/1
2	FSW	A	1002	-	-	0/2/24/24	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	FSW	O1-C1	4.95	1.48	1.40
2	D	1002	FSW	O1-C1	4.93	1.48	1.40
2	C	1005	FSW	O1-C1	4.08	1.47	1.40
2	J	1001	FSW	O1-C1	3.62	1.46	1.40
2	H	1005	FSW	O1-C1	3.62	1.46	1.40
2	F	1005	FSW	O1-C1	3.53	1.46	1.40
2	B	1001	FSW	O1-C1	3.47	1.46	1.40
2	I	1002	FSW	O1-C1	3.45	1.46	1.40
2	L	1003	FSW	O1-C1	3.25	1.45	1.40
2	B	1006	FSW	O1-C1	3.21	1.45	1.40
2	K	1003	FSW	O1-C1	3.20	1.45	1.40
2	E	1002	FSW	O1-C1	3.20	1.45	1.40
2	L	1006	FSW	O1-C1	3.15	1.45	1.40
2	G	1005	FSW	O1-C1	3.13	1.45	1.40
2	A	1005	FSW	O1-C1	3.13	1.45	1.40
2	K	1006	FSW	O1-C1	3.09	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1004	FSW	O1-C1	3.01	1.45	1.40
2	I	1001	FSW	O1-C1	2.98	1.45	1.40
2	D	1005	FSW	O1-C1	2.91	1.45	1.40
2	C	1001	FSW	O1-C1	2.76	1.44	1.40
2	G	1003	FSW	O1-C1	2.73	1.44	1.40
2	G	1004	FSW	O1-C1	2.71	1.44	1.40
2	E	1005	FSW	O1-C1	2.65	1.44	1.40
2	H	1003	FSW	O1-C1	2.63	1.44	1.40
2	H	1001	FSW	O1-C1	2.59	1.44	1.40
2	B	1005	FSW	O1-C1	2.53	1.44	1.40
2	I	1006	FSW	O1-C1	2.52	1.44	1.40
2	D	1006	FSW	O1-C1	2.52	1.44	1.40
2	J	1002	FSW	O1-C1	2.43	1.44	1.40
2	K	1004	FSW	O1-C1	2.42	1.44	1.40
2	B	1003	FSW	O1-C1	2.39	1.44	1.40
2	A	1006	FSW	O1-C1	2.37	1.44	1.40
2	C	1002	FSW	O1-C1	2.34	1.44	1.40
2	A	1003	FSW	O1-C1	2.33	1.44	1.40
2	D	1004	FSW	O1-C1	2.28	1.44	1.40
2	J	1004	FSW	O1-C1	2.27	1.44	1.40
2	G	1005	FSW	O5-C1	2.27	1.47	1.41
2	H	1004	FSW	O1-C1	2.26	1.44	1.40
2	K	1005	FSW	O1-C1	2.26	1.44	1.40
2	F	1002	FSW	O1-C1	2.25	1.44	1.40
2	B	1005	FSW	O5-C1	2.24	1.47	1.41
2	A	1004	FSW	O5-C1	2.24	1.47	1.41
2	I	1004	FSW	O1-C1	2.21	1.43	1.40
2	A	1004	FSW	O1-C1	2.20	1.43	1.40
2	E	1002	FSW	O5-C1	2.19	1.47	1.41
2	D	1003	FSW	O1-C1	2.13	1.43	1.40
2	A	1006	FSW	O5-C1	2.13	1.47	1.41
2	J	1003	FSW	O1-C1	2.11	1.43	1.40
2	C	1004	FSW	O1-C1	2.10	1.43	1.40
2	F	1004	FSW	O1-C1	2.07	1.43	1.40
2	H	1003	FSW	O5-C1	2.07	1.47	1.41
2	B	1003	FSW	O5-C1	2.06	1.47	1.41
2	A	1001	FSW	O1-C1	2.05	1.43	1.40
2	D	1001	FSW	O5-C1	2.04	1.47	1.41

All (226) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1005	FSW	O4-C4-C3	-8.89	89.41	110.38
2	B	1001	FSW	O4-C4-C5	8.58	128.66	109.74
2	G	1005	FSW	O4-C4-C5	8.52	128.54	109.74
2	B	1006	FSW	O4-C4-C5	8.14	127.70	109.74
2	C	1005	FSW	C3-C4-C5	8.13	122.18	109.81
2	G	1004	FSW	O4-C4-C5	7.77	126.88	109.74
2	A	1006	FSW	O4-C4-C5	7.74	126.82	109.74
2	I	1004	FSW	O4-C4-C5	7.55	126.39	109.74
2	I	1003	FSW	O4-C4-C5	7.22	125.67	109.74
2	C	1001	FSW	O4-C4-C5	7.19	125.61	109.74
2	A	1001	FSW	O4-C4-C5	7.13	125.48	109.74
2	E	1004	FSW	O4-C4-C5	7.09	125.38	109.74
2	D	1004	FSW	O4-C4-C5	7.04	125.27	109.74
2	A	1003	FSW	O4-C4-C3	7.04	126.97	110.38
2	C	1005	FSW	O4-C4-C3	-6.95	93.99	110.38
2	I	1006	FSW	O4-C4-C5	6.82	124.78	109.74
2	D	1001	FSW	O4-C4-C5	6.79	124.72	109.74
2	I	1002	FSW	O4-C4-C5	6.73	124.59	109.74
2	H	1001	FSW	O4-C4-C3	6.59	125.92	110.38
2	C	1003	FSW	O4-C4-C5	6.56	124.21	109.74
2	F	1003	FSW	O4-C4-C5	6.54	124.16	109.74
2	B	1005	FSW	O4-C4-C5	6.53	124.14	109.74
2	I	1002	FSW	O1-C1-C2	6.43	119.21	107.94
2	D	1002	FSW	O1-C1-C2	6.32	119.01	107.94
2	J	1001	FSW	O4-C4-C3	6.30	125.24	110.38
2	J	1004	FSW	O4-C4-C5	6.30	123.64	109.74
2	H	1003	FSW	O4-C4-C5	6.26	123.54	109.74
2	A	1004	FSW	O4-C4-C5	6.22	123.46	109.74
2	D	1006	FSW	O4-C4-C5	6.06	123.11	109.74
2	A	1005	FSW	O4-C4-C3	5.98	124.47	110.38
2	H	1001	FSW	O1-C1-C2	5.92	118.31	107.94
2	F	1004	FSW	O4-C4-C5	5.91	122.77	109.74
2	B	1003	FSW	O4-C4-C5	5.83	122.59	109.74
2	E	1003	FSW	O4-C4-C5	5.83	122.59	109.74
2	A	1002	FSW	C2-C3-C4	-5.79	102.03	111.09
2	J	1003	FSW	O4-C4-C3	5.76	123.96	110.38
2	A	1002	FSW	O4-C4-C5	5.76	122.45	109.74
2	I	1001	FSW	O4-C4-C5	5.69	122.30	109.74
2	E	1002	FSW	O4-C4-C5	5.69	122.29	109.74
2	I	1001	FSW	O4-C4-C3	5.66	123.72	110.38
2	K	1003	FSW	O4-C4-C5	5.62	122.14	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1005	FSW	O4-C4-C5	-5.55	97.49	109.74
2	H	1001	FSW	O4-C4-C5	5.43	121.73	109.74
2	J	1003	FSW	O4-C4-C5	5.38	121.60	109.74
2	B	1002	FSW	O4-C4-C5	5.29	121.41	109.74
2	K	1004	FSW	O4-C4-C5	5.29	121.40	109.74
2	F	1002	FSW	O4-C4-C3	5.16	122.53	110.38
2	D	1005	FSW	C2-C3-C4	-5.15	103.02	111.09
2	K	1004	FSW	O4-C4-C3	5.11	122.42	110.38
2	J	1001	FSW	O4-C4-C5	4.97	120.71	109.74
2	D	1001	FSW	O4-C4-C3	4.95	122.04	110.38
2	C	1001	FSW	O4-C4-C3	4.87	121.86	110.38
2	A	1005	FSW	C2-C3-C4	-4.77	103.62	111.09
2	E	1002	FSW	C2-C3-C4	-4.69	103.75	111.09
2	F	1004	FSW	O4-C4-C3	4.66	121.35	110.38
2	J	1004	FSW	O4-C4-C3	4.65	121.34	110.38
2	G	1005	FSW	C1-O5-C5	4.64	121.54	113.63
2	D	1005	FSW	O4-C4-C3	4.63	121.30	110.38
2	F	1002	FSW	O4-C4-C5	4.60	119.88	109.74
2	F	1002	FSW	C2-C3-C4	-4.55	103.97	111.09
2	I	1002	FSW	O4-C4-C3	4.46	120.89	110.38
2	J	1001	FSW	O1-C1-C2	4.46	115.76	107.94
2	A	1003	FSW	C2-C3-C4	-4.41	104.19	111.09
2	F	1003	FSW	C2-C3-C4	-4.37	104.25	111.09
2	A	1004	FSW	C2-C3-C4	-4.37	104.25	111.09
2	D	1006	FSW	O4-C4-C3	4.28	120.46	110.38
2	B	1001	FSW	O4-C4-C3	4.27	120.45	110.38
2	E	1004	FSW	O4-C4-C3	4.21	120.30	110.38
2	G	1004	FSW	C2-C3-C4	-4.07	104.72	111.09
2	K	1003	FSW	O4-C4-C3	4.03	119.87	110.38
2	B	1002	FSW	O4-C4-C3	3.99	119.77	110.38
2	D	1003	FSW	O4-C4-C5	3.97	118.50	109.74
2	B	1006	FSW	O1-C1-C2	3.89	114.77	107.94
2	D	1001	FSW	O5-C5-C6	3.88	115.36	106.74
2	E	1005	FSW	O4-C4-C3	-3.87	101.26	110.38
2	D	1003	FSW	O4-C4-C3	3.85	119.46	110.38
2	I	1001	FSW	O1-C1-C2	3.81	114.61	107.94
2	G	1005	FSW	C7-O1-C1	3.79	119.02	113.26
2	B	1005	FSW	O4-C4-C3	3.79	119.31	110.38
2	G	1005	FSW	C2-C3-C4	-3.72	105.27	111.09
2	B	1002	FSW	C2-C3-C4	-3.72	105.27	111.09
2	B	1006	FSW	C2-C3-C4	-3.72	105.27	111.09
2	B	1003	FSW	O4-C4-C3	3.69	119.08	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1006	FSW	O1-C1-C2	3.66	114.36	107.94
2	A	1005	FSW	O1-C1-C2	3.65	114.34	107.94
2	F	1005	FSW	O1-C1-C2	3.64	114.32	107.94
2	C	1005	FSW	O1-C1-C2	3.63	114.30	107.94
2	J	1001	FSW	O3-C3-C2	3.61	119.26	109.24
2	K	1005	FSW	O1-C1-C2	3.61	114.27	107.94
2	A	1001	FSW	O4-C4-C3	3.58	118.82	110.38
2	I	1004	FSW	C2-C3-C4	-3.57	105.50	111.09
2	E	1002	FSW	O4-C4-C3	3.55	118.75	110.38
2	A	1001	FSW	C7-O1-C1	3.53	118.63	113.26
2	D	1001	FSW	C7-O1-C1	3.53	118.63	113.26
2	L	1006	FSW	C1-O5-C5	3.53	119.65	113.63
2	D	1001	FSW	O1-C1-C2	3.52	114.12	107.94
2	C	1001	FSW	O1-C1-C2	3.50	114.08	107.94
2	L	1006	FSW	O1-C1-C2	3.50	114.07	107.94
2	K	1003	FSW	C3-C4-C5	3.49	115.11	109.81
2	D	1005	FSW	O4-C4-C5	3.48	117.42	109.74
2	D	1006	FSW	O1-C1-C2	3.43	113.95	107.94
2	H	1003	FSW	O4-C4-C3	3.41	118.41	110.38
2	A	1002	FSW	O4-C4-C3	3.39	118.37	110.38
2	A	1001	FSW	O1-C1-C2	3.39	113.88	107.94
2	K	1006	FSW	O1-C1-C2	3.38	113.87	107.94
2	H	1005	FSW	C7-O1-C1	3.37	118.38	113.26
2	I	1003	FSW	C2-C3-C4	-3.34	105.85	111.09
2	B	1001	FSW	O1-C1-C2	3.33	113.78	107.94
2	D	1001	FSW	O3-C3-C2	3.32	118.44	109.24
2	A	1006	FSW	C2-C3-C4	-3.28	105.95	111.09
2	H	1003	FSW	O5-C5-C6	3.26	113.98	106.74
2	E	1003	FSW	O4-C4-C3	3.24	118.02	110.38
2	C	1003	FSW	O4-C4-C3	3.24	118.01	110.38
2	L	1006	FSW	C7-O1-C1	3.21	118.14	113.26
2	D	1004	FSW	O4-C4-C3	3.19	117.91	110.38
2	C	1005	FSW	C1-O5-C5	3.19	119.07	113.63
2	B	1006	FSW	O4-C4-C3	3.19	117.89	110.38
2	J	1004	FSW	C2-C3-C4	-3.16	106.14	111.09
2	G	1003	FSW	C2-C3-C4	-3.13	106.18	111.09
2	K	1002	FSW	O5-C1-C2	3.13	116.78	110.02
2	A	1001	FSW	C2-C3-C4	-3.12	106.20	111.09
2	C	1001	FSW	C1-O5-C5	3.08	118.88	113.63
2	C	1003	FSW	C2-C3-C4	-3.06	106.30	111.09
2	D	1003	FSW	C3-C4-C5	3.04	114.44	109.81
2	D	1004	FSW	C2-C3-C4	-3.03	106.35	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1001	FSW	C2-C3-C4	-3.01	106.38	111.09
2	I	1002	FSW	C2-C3-C4	-2.98	106.43	111.09
2	G	1005	FSW	O5-C1-C2	2.96	116.41	110.02
2	D	1003	FSW	C2-C3-C4	-2.94	106.49	111.09
2	L	1003	FSW	C7-O1-C1	2.91	117.69	113.26
2	B	1005	FSW	C2-C3-C4	-2.90	106.54	111.09
2	F	1003	FSW	O4-C4-C3	2.90	117.21	110.38
2	L	1006	FSW	O4-C4-C5	2.90	116.13	109.74
2	E	1002	FSW	O3-C3-C2	2.89	117.24	109.24
2	A	1005	FSW	O3-C3-C4	2.87	117.14	110.38
2	D	1002	FSW	O3-C3-C2	2.84	117.11	109.24
2	A	1005	FSW	O4-C4-C5	2.83	115.99	109.74
2	E	1005	FSW	O4-C4-C5	2.82	115.96	109.74
2	E	1004	FSW	C2-C3-C4	-2.82	106.68	111.09
2	C	1005	FSW	C7-O1-C1	2.79	117.50	113.26
2	I	1001	FSW	C2-C3-C4	-2.78	106.73	111.09
2	J	1003	FSW	C1-O5-C5	2.78	118.37	113.63
2	K	1003	FSW	C7-O1-C1	2.77	117.47	113.26
2	D	1005	FSW	O5-C5-C4	-2.74	104.62	109.55
2	K	1002	FSW	C3-C4-C5	-2.66	105.78	109.81
2	L	1002	FSW	O1-C1-C2	2.64	112.57	107.94
2	D	1006	FSW	O3-C3-C2	2.63	116.52	109.24
2	I	1006	FSW	O4-C4-C3	2.62	116.55	110.38
2	H	1004	FSW	C2-C3-C4	-2.62	106.99	111.09
2	L	1002	FSW	O5-C5-C4	-2.59	104.89	109.55
2	L	1003	FSW	C1-O5-C5	2.57	118.02	113.63
2	D	1002	FSW	C2-C3-C4	-2.57	107.07	111.09
2	D	1003	FSW	O5-C5-C6	2.56	112.43	106.74
2	G	1005	FSW	O5-C5-C6	2.56	112.42	106.74
2	C	1001	FSW	O5-C5-C6	2.53	112.35	106.74
2	I	1002	FSW	C7-O1-C1	2.52	117.09	113.26
2	K	1003	FSW	O5-C5-C6	2.51	112.31	106.74
2	E	1003	FSW	C2-C3-C4	-2.51	107.16	111.09
2	B	1001	FSW	C7-O1-C1	2.51	117.07	113.26
2	L	1006	FSW	O5-C5-C4	2.50	114.05	109.55
2	D	1002	FSW	C7-O1-C1	2.49	117.05	113.26
2	B	1003	FSW	O5-C5-C4	-2.49	105.07	109.55
2	I	1003	FSW	O4-C4-C3	2.48	116.23	110.38
2	B	1005	FSW	C1-O5-C5	2.48	117.86	113.63
2	J	1004	FSW	O5-C5-C6	2.44	112.16	106.74
2	F	1002	FSW	O3-C3-C2	2.44	116.00	109.24
2	I	1004	FSW	O3-C3-C2	2.44	116.00	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1004	FSW	C3-C4-C5	2.42	113.50	109.81
2	J	1001	FSW	C7-O1-C1	2.42	116.94	113.26
2	K	1005	FSW	C2-C3-C4	-2.41	107.31	111.09
2	K	1003	FSW	O5-C5-C4	-2.39	105.25	109.55
2	H	1004	FSW	O4-C4-C5	2.39	115.00	109.74
2	G	1004	FSW	O3-C3-C2	2.37	115.81	109.24
2	I	1002	FSW	O3-C3-C2	2.36	115.80	109.24
2	F	1004	FSW	O5-C5-C4	-2.35	105.33	109.55
2	H	1005	FSW	O4-C4-C5	2.35	114.92	109.74
2	J	1002	FSW	C2-C3-C4	-2.34	107.42	111.09
2	F	1004	FSW	O5-C5-C6	2.34	111.93	106.74
2	D	1006	FSW	C3-C4-C5	2.34	113.37	109.81
2	A	1003	FSW	O4-C4-C5	2.33	114.89	109.74
2	B	1004	FSW	O5-C1-O1	2.33	116.35	110.94
2	L	1002	FSW	O5-C5-C6	2.31	111.87	106.74
2	H	1003	FSW	C1-O5-C5	2.31	117.57	113.63
2	H	1005	FSW	C3-C4-C5	2.30	113.30	109.81
2	I	1006	FSW	C2-C3-C4	-2.27	107.54	111.09
2	A	1006	FSW	O4-C4-C3	2.26	115.70	110.38
2	I	1004	FSW	O4-C4-C3	2.25	115.68	110.38
2	D	1006	FSW	C2-C3-C4	-2.25	107.57	111.09
2	K	1005	FSW	O4-C4-C3	2.24	115.65	110.38
2	D	1003	FSW	O5-C5-C4	-2.24	105.53	109.55
2	E	1005	FSW	C7-O1-C1	2.22	116.63	113.26
2	I	1001	FSW	O3-C3-C2	2.22	115.38	109.24
2	G	1003	FSW	O1-C1-C2	2.21	111.81	107.94
2	A	1002	FSW	O3-C3-C2	2.20	115.34	109.24
2	K	1003	FSW	O3-C3-C2	2.20	115.34	109.24
2	K	1002	FSW	O5-C5-C4	-2.20	105.60	109.55
2	L	1006	FSW	C2-C3-C4	2.20	114.52	111.09
2	K	1002	FSW	O5-C1-O1	-2.20	105.83	110.94
2	B	1003	FSW	O5-C5-C6	2.17	111.56	106.74
2	B	1005	FSW	O3-C3-C2	2.15	115.19	109.24
2	H	1004	FSW	C7-O1-C1	2.14	116.51	113.26
2	B	1001	FSW	C6-C5-C4	2.14	117.00	113.08
2	E	1005	FSW	O3-C3-C2	2.13	115.15	109.24
2	E	1004	FSW	O3-C3-C2	2.13	115.14	109.24
2	D	1004	FSW	C7-O1-C1	2.13	116.49	113.26
2	A	1005	FSW	C3-C4-C5	2.12	113.04	109.81
2	D	1001	FSW	C2-C3-C4	-2.12	107.77	111.09
2	C	1001	FSW	O3-C3-C2	2.11	115.10	109.24
2	D	1005	FSW	C7-O1-C1	2.11	116.47	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1005	FSW	O3-C3-C4	2.10	115.33	110.38
2	J	1002	FSW	O3-C3-C2	2.09	115.04	109.24
2	E	1003	FSW	C7-O1-C1	-2.08	110.10	113.26
2	B	1005	FSW	O5-C5-C6	2.08	111.35	106.74
2	J	1003	FSW	C2-C3-C4	-2.07	107.85	111.09
2	L	1003	FSW	O5-C5-C4	-2.07	105.83	109.55
2	K	1005	FSW	O3-C3-C4	2.05	115.22	110.38
2	G	1004	FSW	O4-C4-C3	2.05	115.21	110.38
2	C	1003	FSW	O1-C1-C2	2.05	111.53	107.94
2	L	1002	FSW	O5-C1-O1	-2.04	106.18	110.94
2	J	1004	FSW	O5-C5-C4	-2.04	105.88	109.55
2	L	1002	FSW	C1-O5-C5	-2.03	110.17	113.63
2	D	1001	FSW	O5-C5-C4	-2.03	105.90	109.55
2	A	1002	FSW	O5-C1-C2	2.03	114.40	110.02
2	E	1003	FSW	O5-C5-C6	2.01	111.21	106.74
2	E	1004	FSW	O5-C5-C6	2.01	111.20	106.74
2	D	1006	FSW	C7-O1-C1	2.00	116.30	113.26

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	FSW	C2-C1-O1-C7
2	B	1005	FSW	O5-C1-O1-C7
2	F	1003	FSW	C2-C1-O1-C7
2	G	1005	FSW	C2-C1-O1-C7
2	K	1001	FSW	C2-C1-O1-C7
2	K	1002	FSW	C2-C1-O1-C7
2	K	1004	FSW	C2-C1-O1-C7
2	L	1005	FSW	O5-C1-O1-C7
2	L	1005	FSW	C2-C1-O1-C7
2	L	1006	FSW	O5-C1-O1-C7
2	A	1005	FSW	O5-C1-O1-C7
2	C	1003	FSW	O5-C1-O1-C7
2	G	1005	FSW	O5-C1-O1-C7
2	I	1004	FSW	O5-C1-O1-C7
2	K	1004	FSW	O5-C1-O1-C7
2	F	1003	FSW	O5-C1-O1-C7
2	K	1001	FSW	O5-C1-O1-C7
2	K	1002	FSW	O5-C1-O1-C7
2	H	1004	FSW	O5-C1-O1-C7
2	K	1006	FSW	O5-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
2	I	1003	FSW	O5-C1-O1-C7
2	K	1003	FSW	O5-C1-O1-C7
2	J	1006	FSW	O5-C1-O1-C7
2	F	1002	FSW	O5-C1-O1-C7
2	I	1006	FSW	O5-C1-O1-C7
2	D	1001	FSW	O5-C1-O1-C7
2	J	1003	FSW	O5-C1-O1-C7
2	D	1001	FSW	C2-C1-O1-C7
2	I	1006	FSW	C2-C1-O1-C7
2	J	1003	FSW	C2-C1-O1-C7
2	K	1003	FSW	C2-C1-O1-C7
2	K	1006	FSW	C2-C1-O1-C7
2	J	1006	FSW	C2-C1-O1-C7
2	D	1006	FSW	C2-C1-O1-C7
2	I	1002	FSW	C2-C1-O1-C7
2	L	1001	FSW	O5-C1-O1-C7

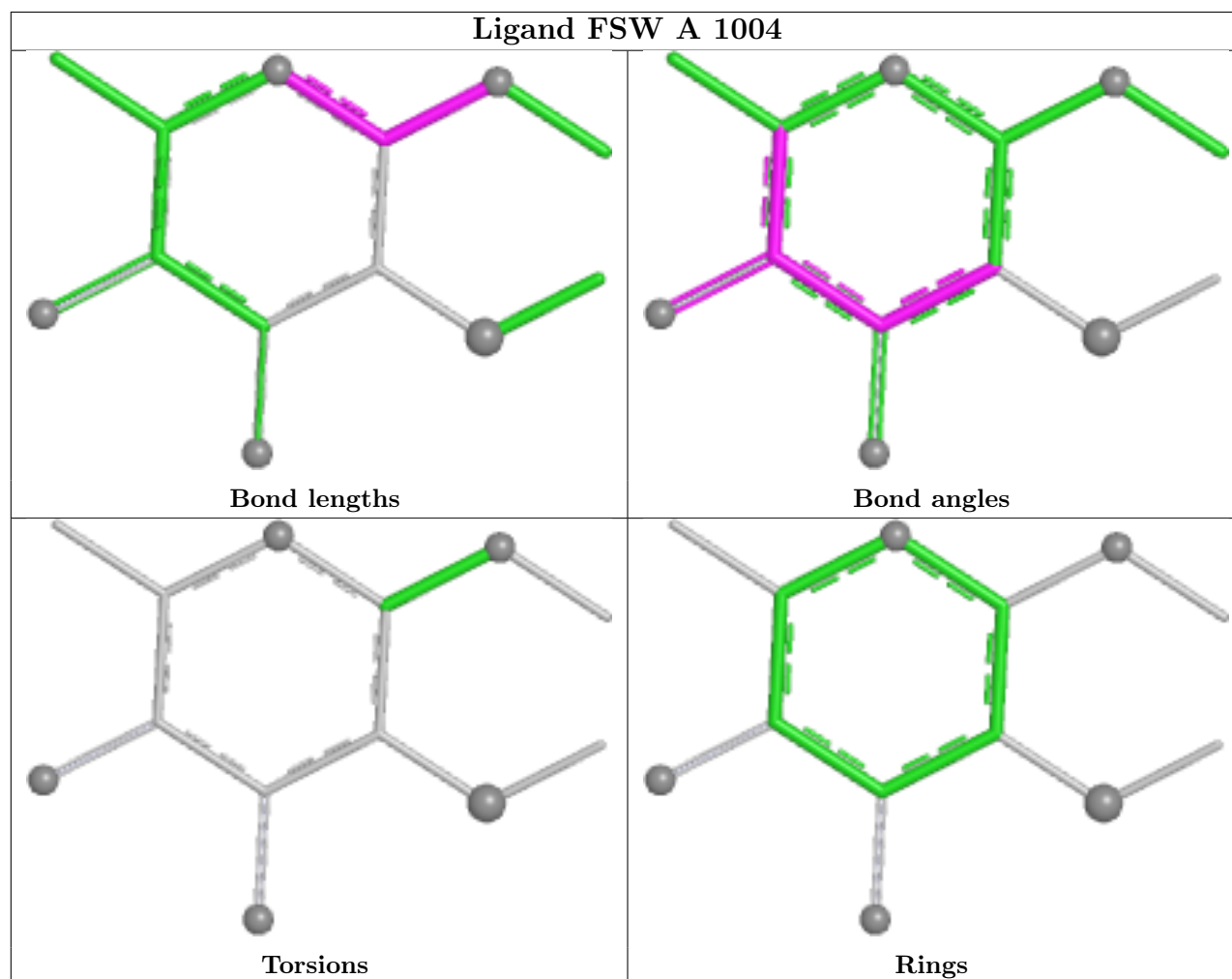
There are no ring outliers.

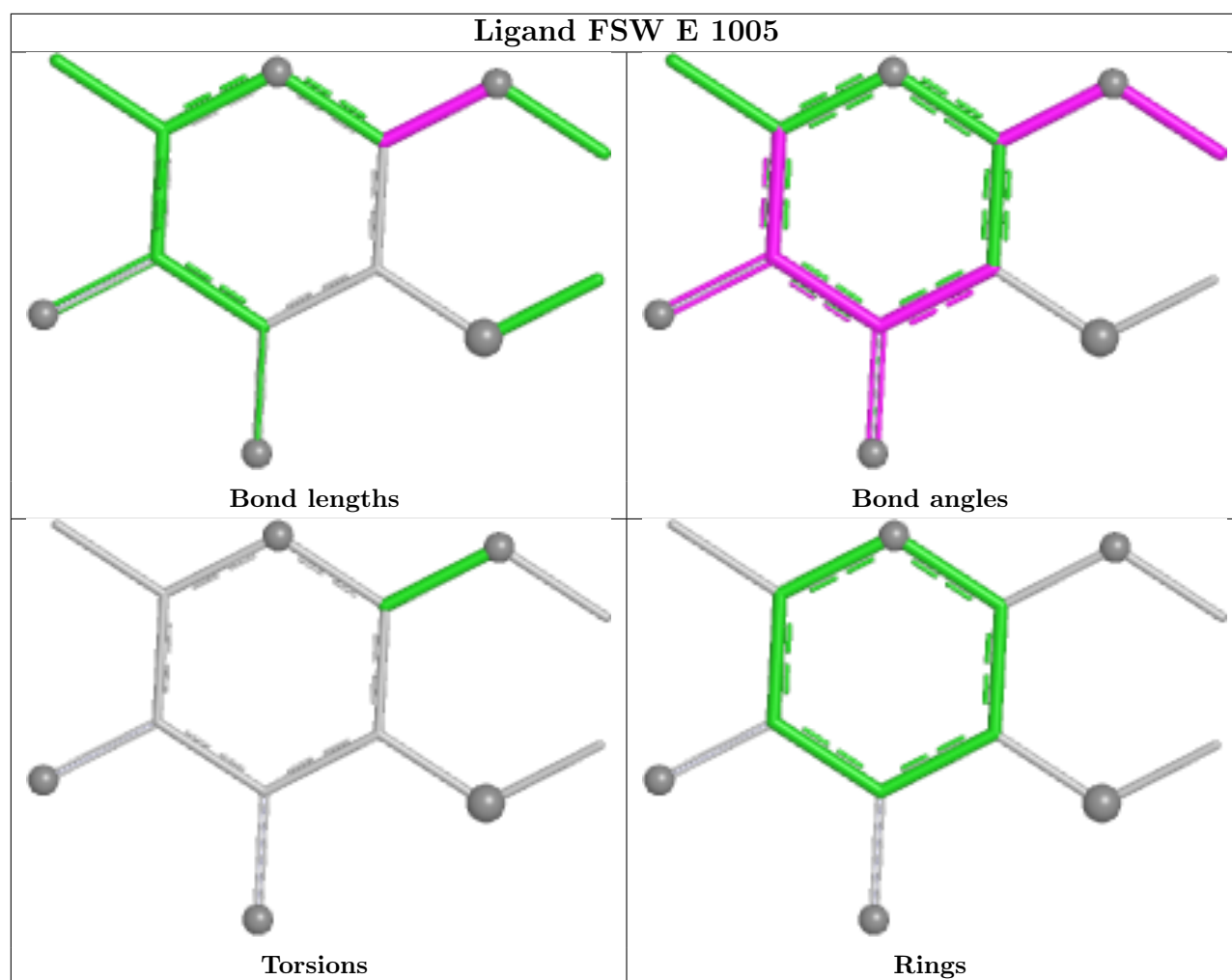
19 monomers are involved in 27 short contacts:

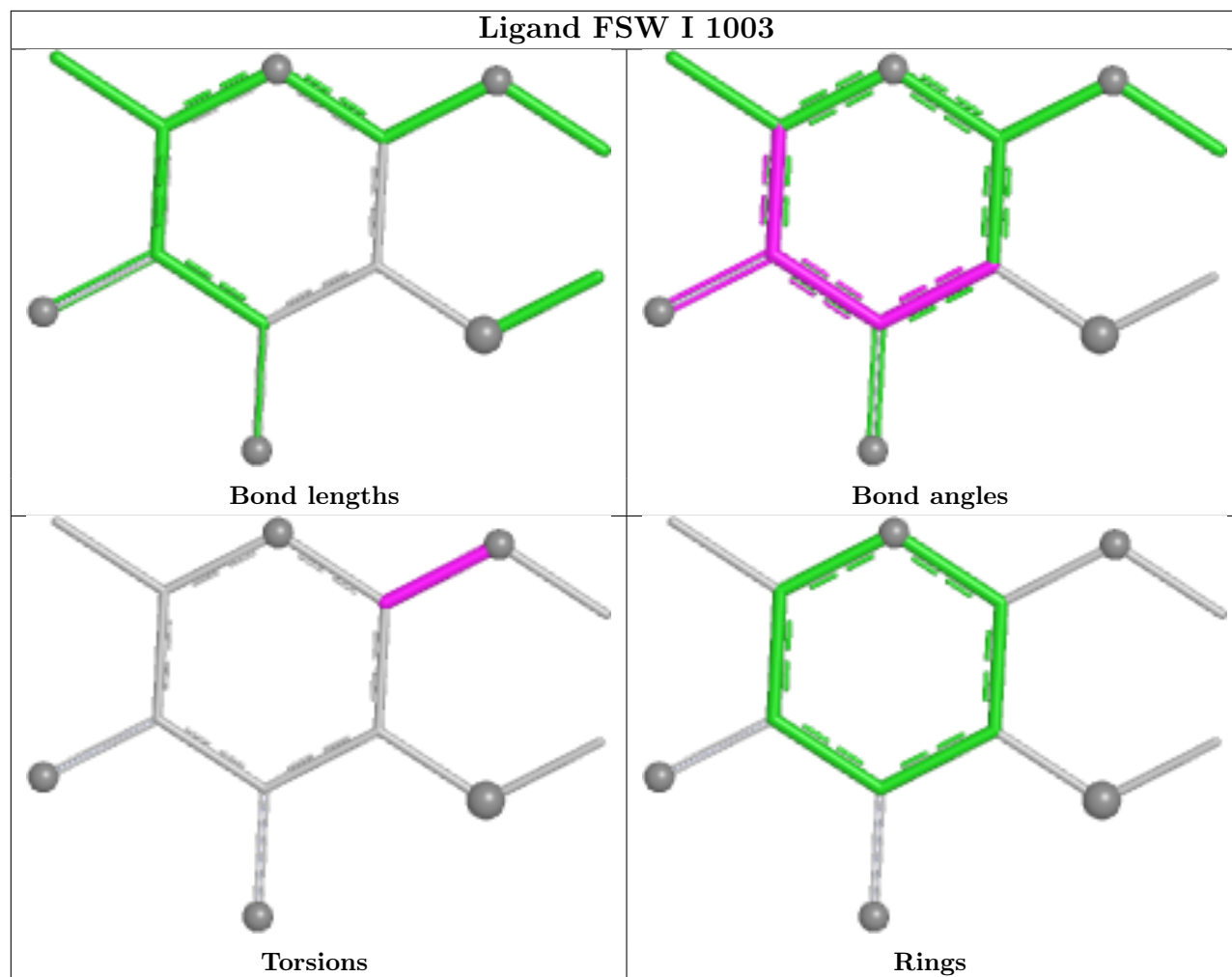
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	FSW	1	0
2	D	1004	FSW	1	0
2	G	1005	FSW	1	0
2	E	1006	FSW	1	0
2	F	1004	FSW	1	0
2	A	1003	FSW	1	0
2	E	1003	FSW	2	0
2	L	1002	FSW	2	0
2	F	1006	FSW	1	0
2	H	1004	FSW	1	0
2	K	1003	FSW	1	0
2	C	1002	FSW	1	0
2	C	1003	FSW	2	0
2	H	1006	FSW	1	0
2	H	1002	FSW	2	0
2	L	1001	FSW	4	0
2	G	1003	FSW	2	0
2	C	1001	FSW	1	0
2	C	1006	FSW	1	0

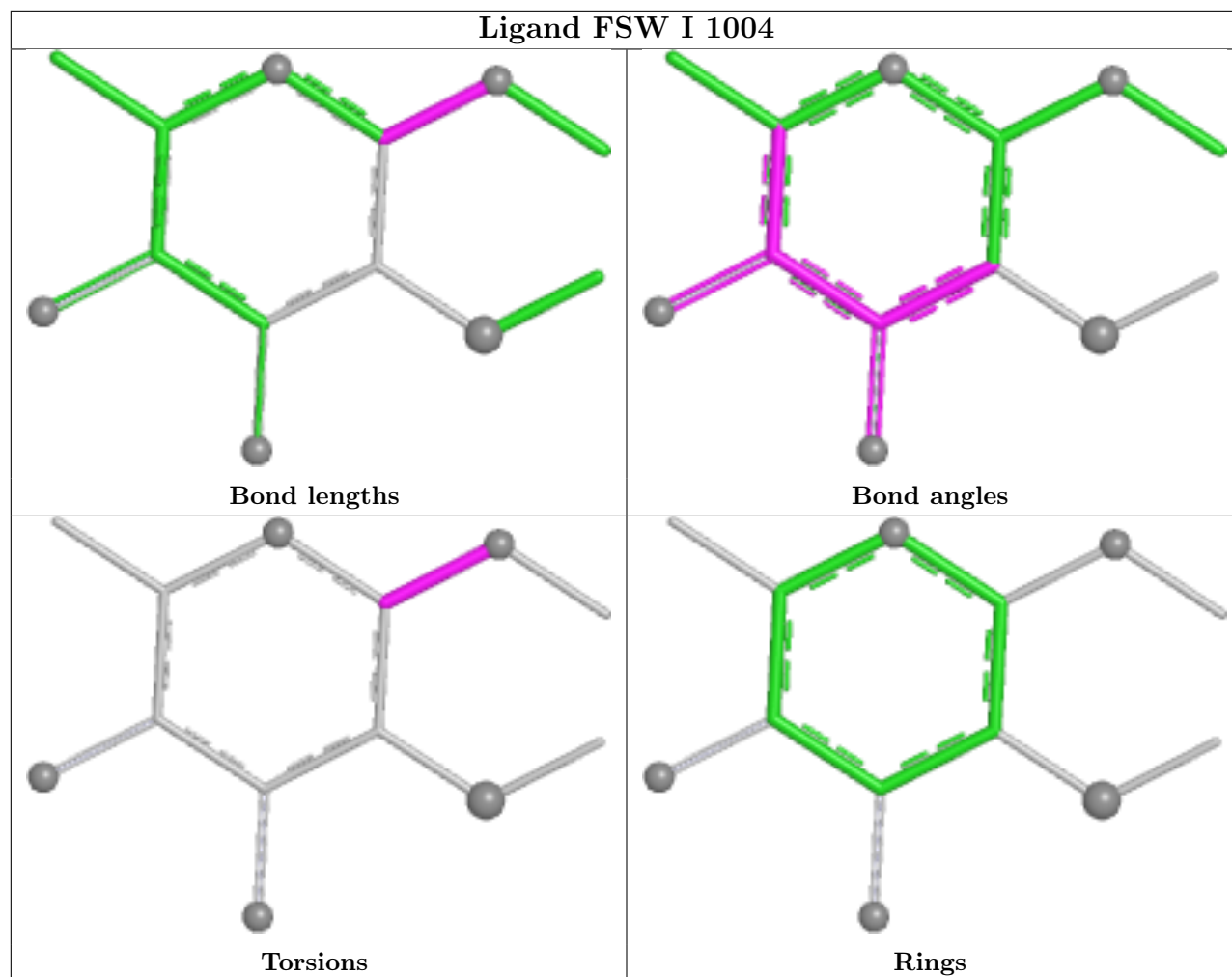
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

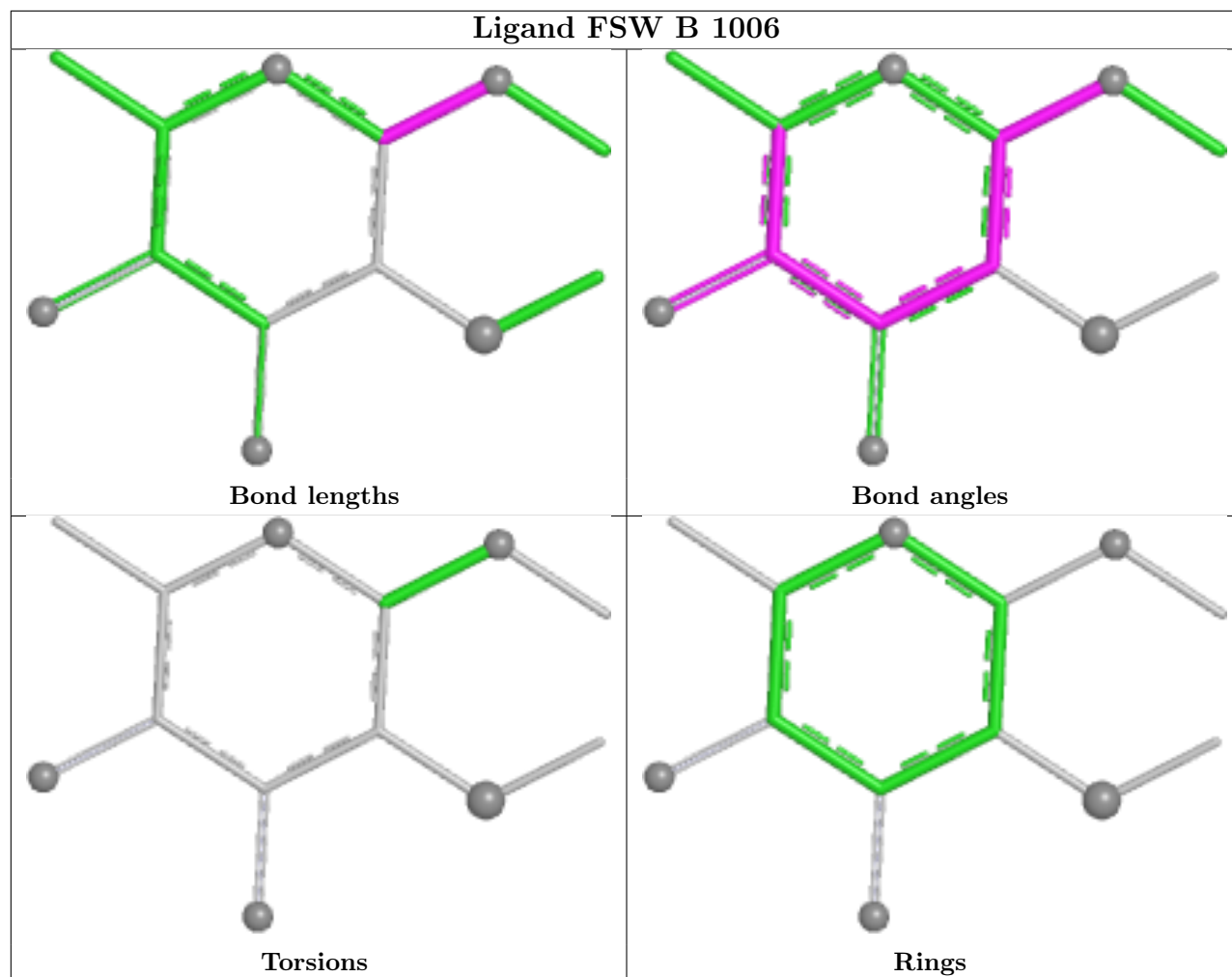
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

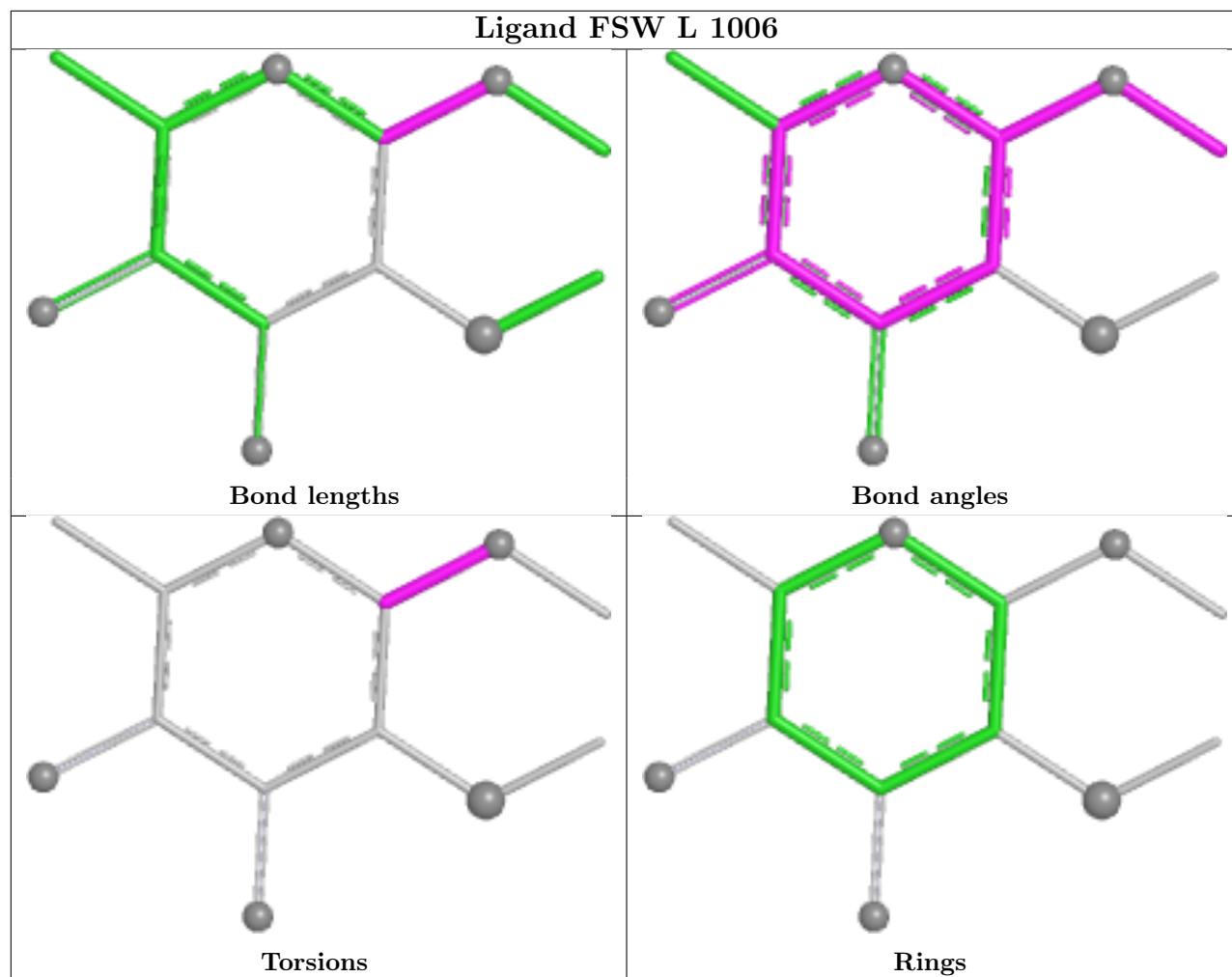


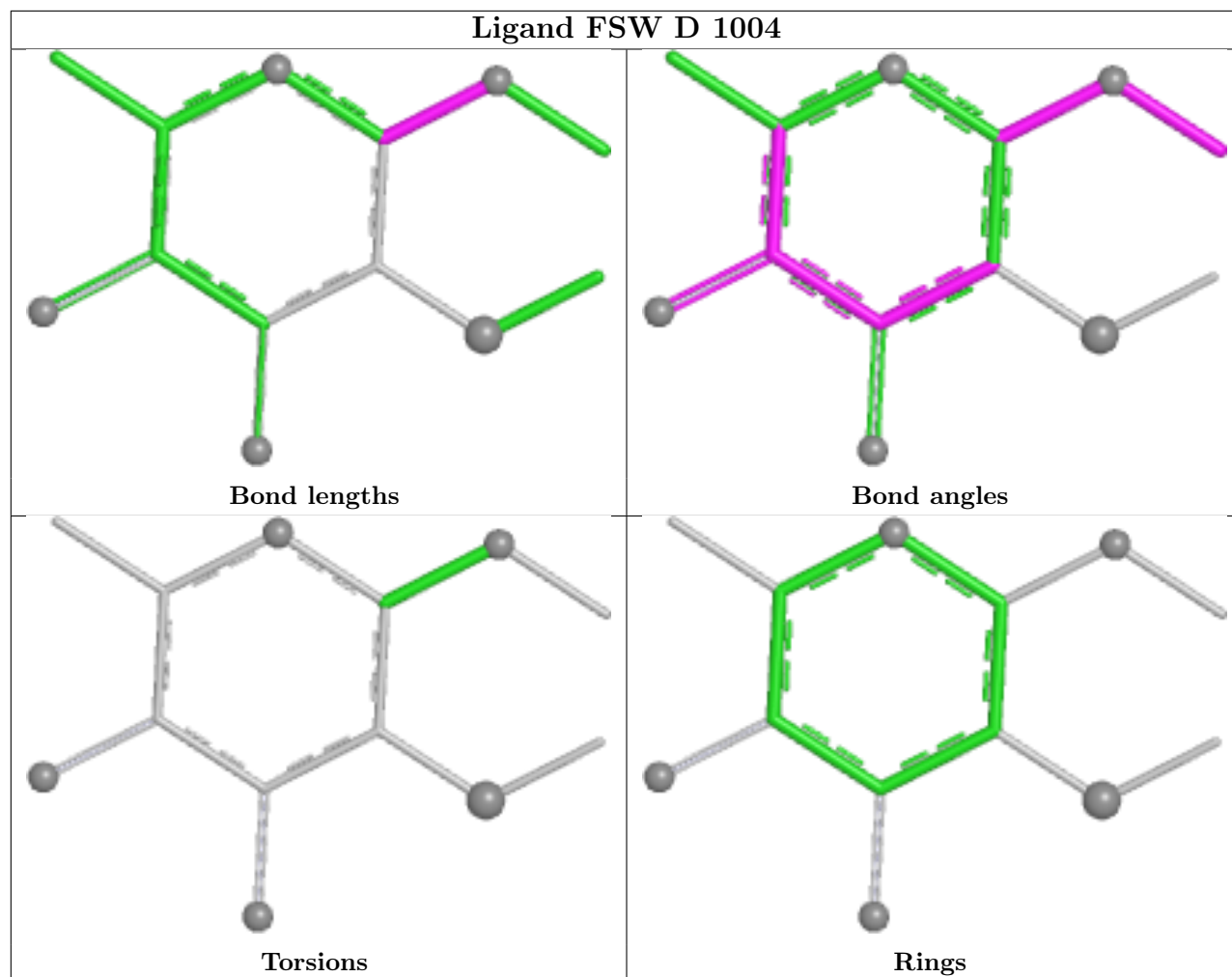


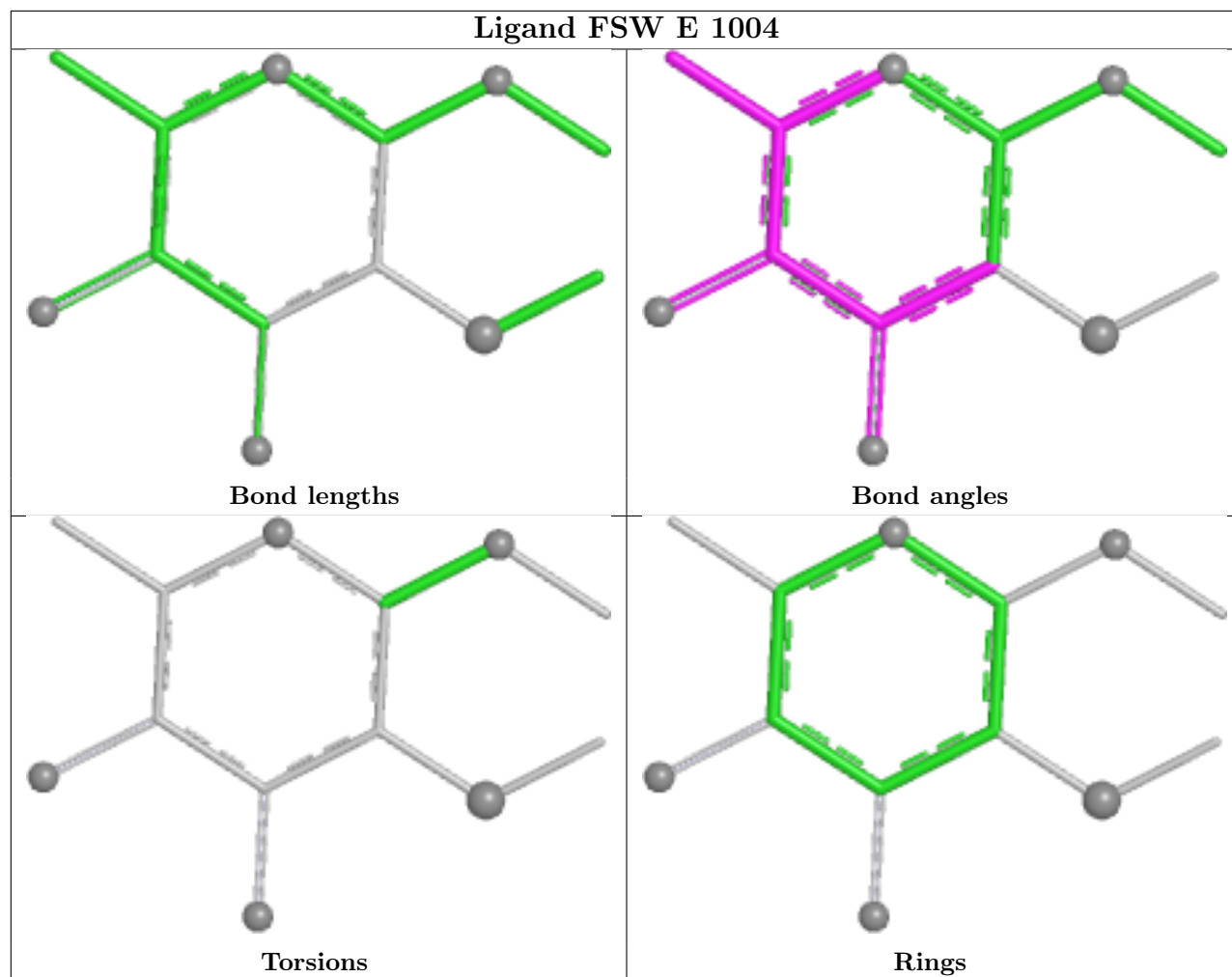


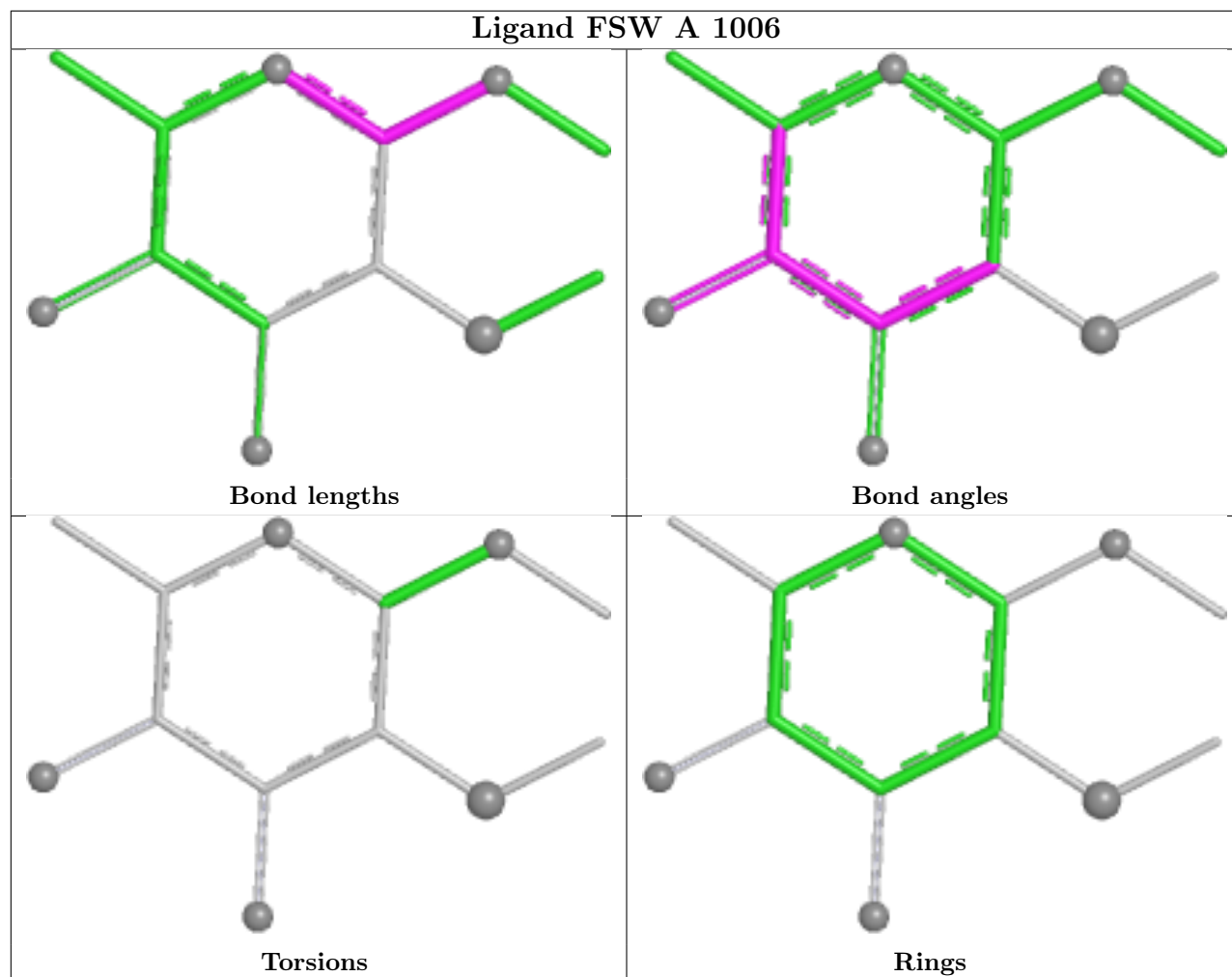


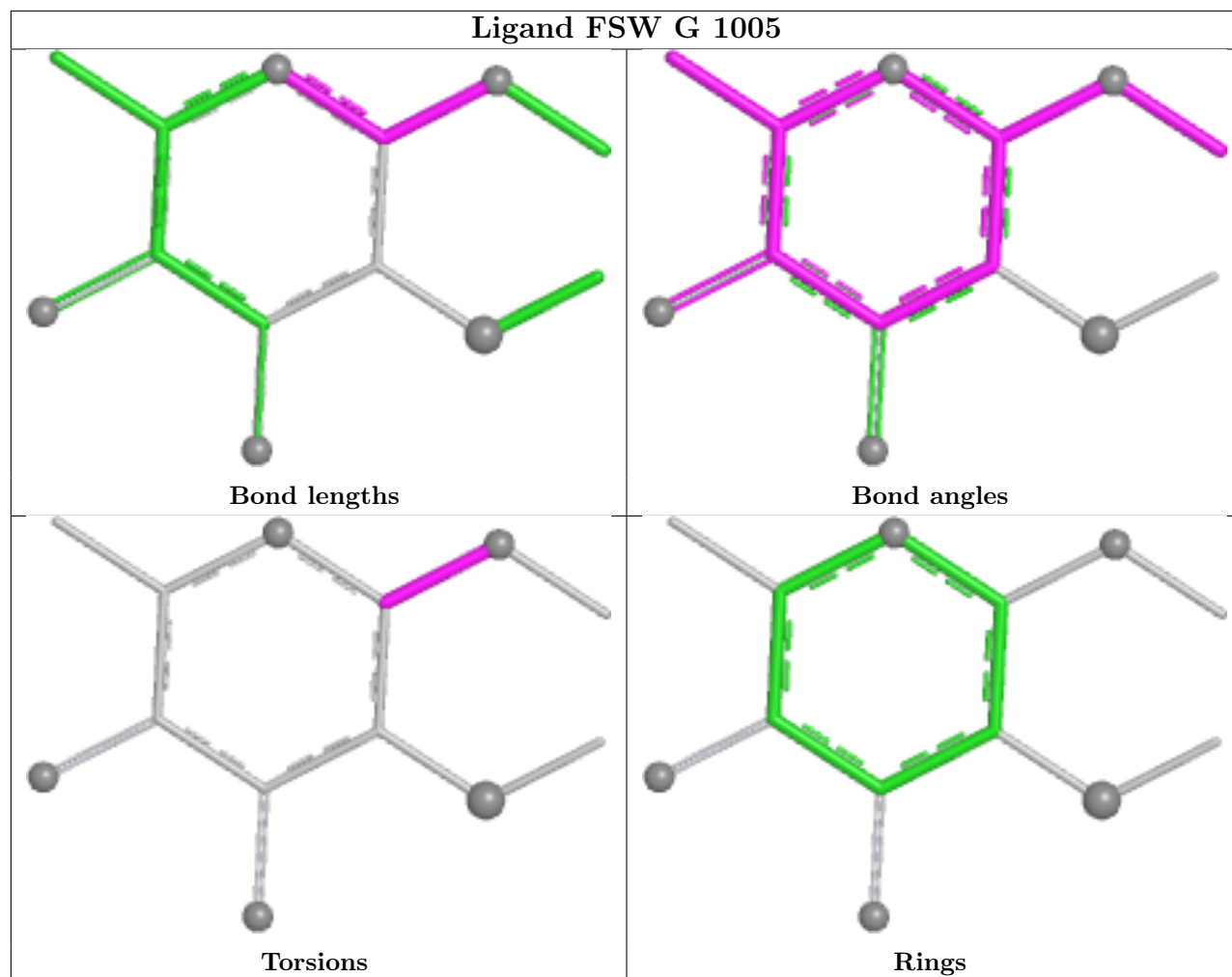


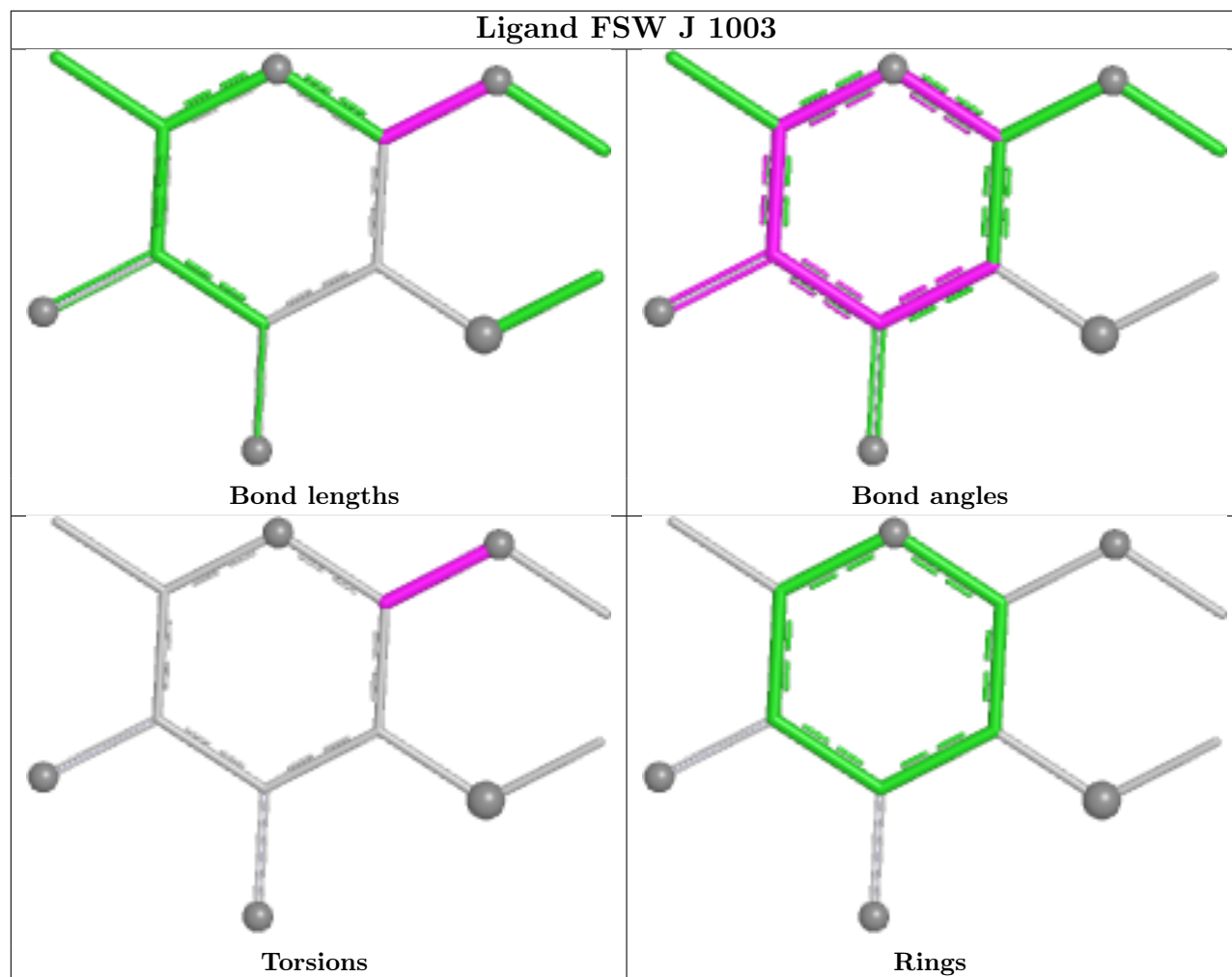


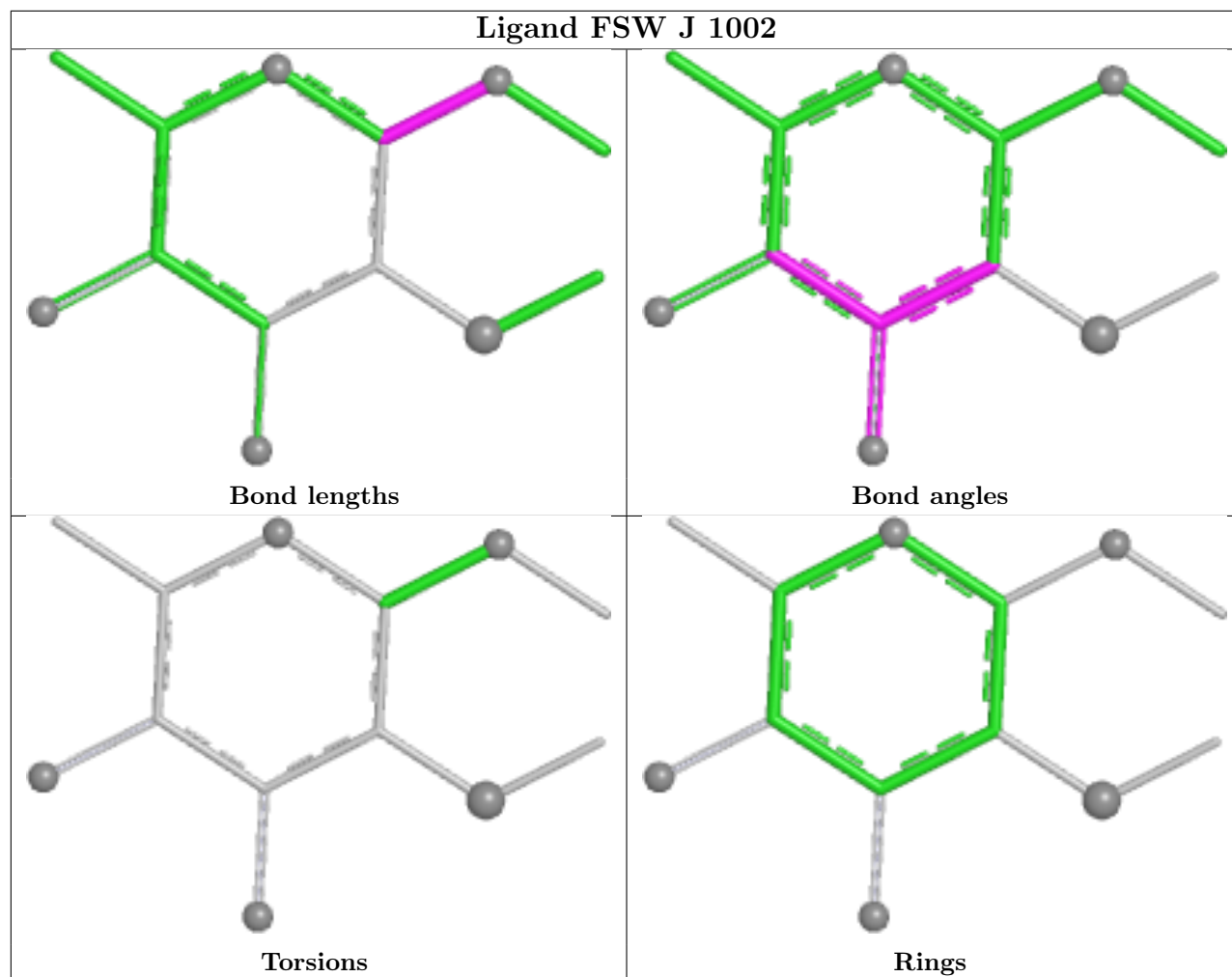


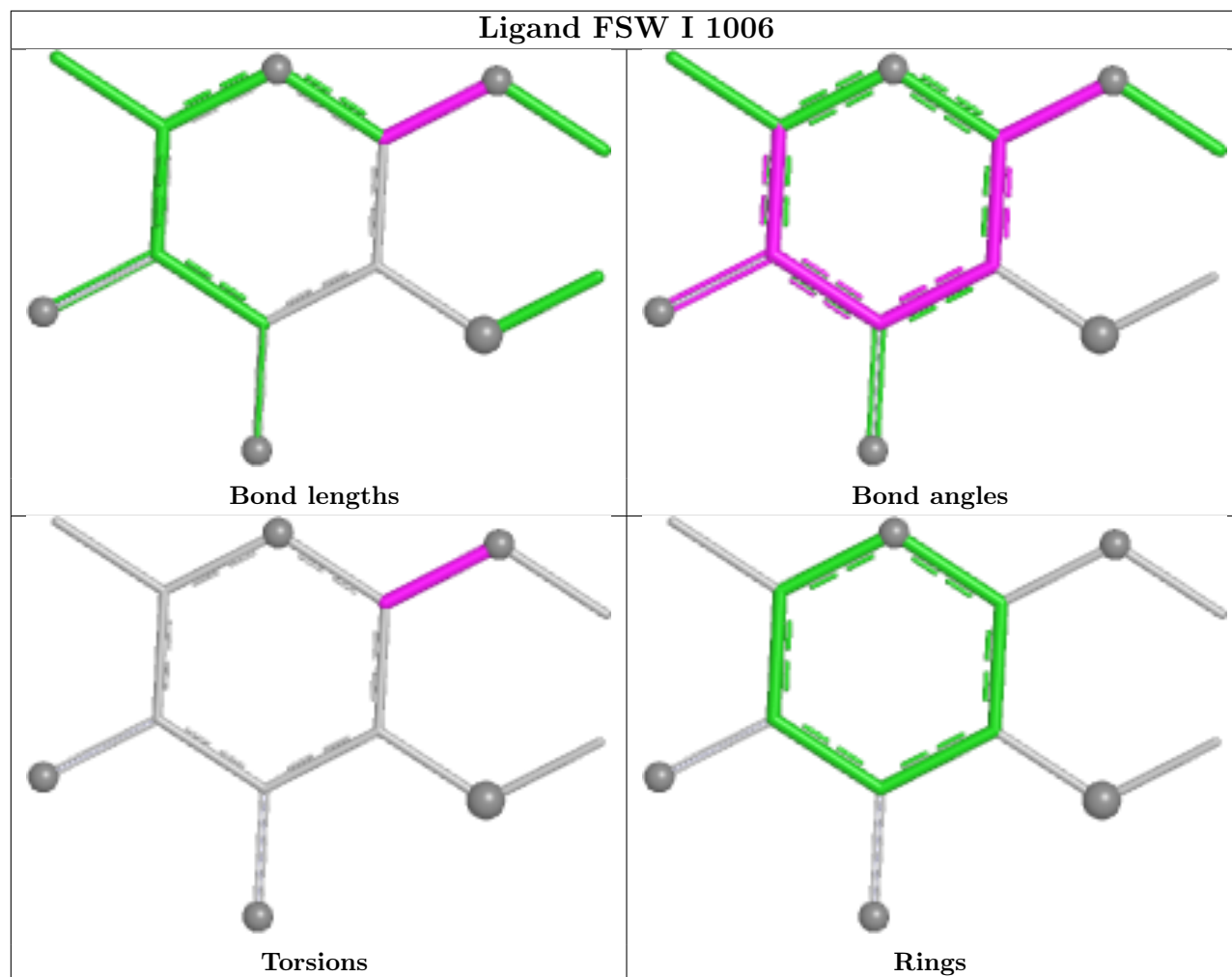


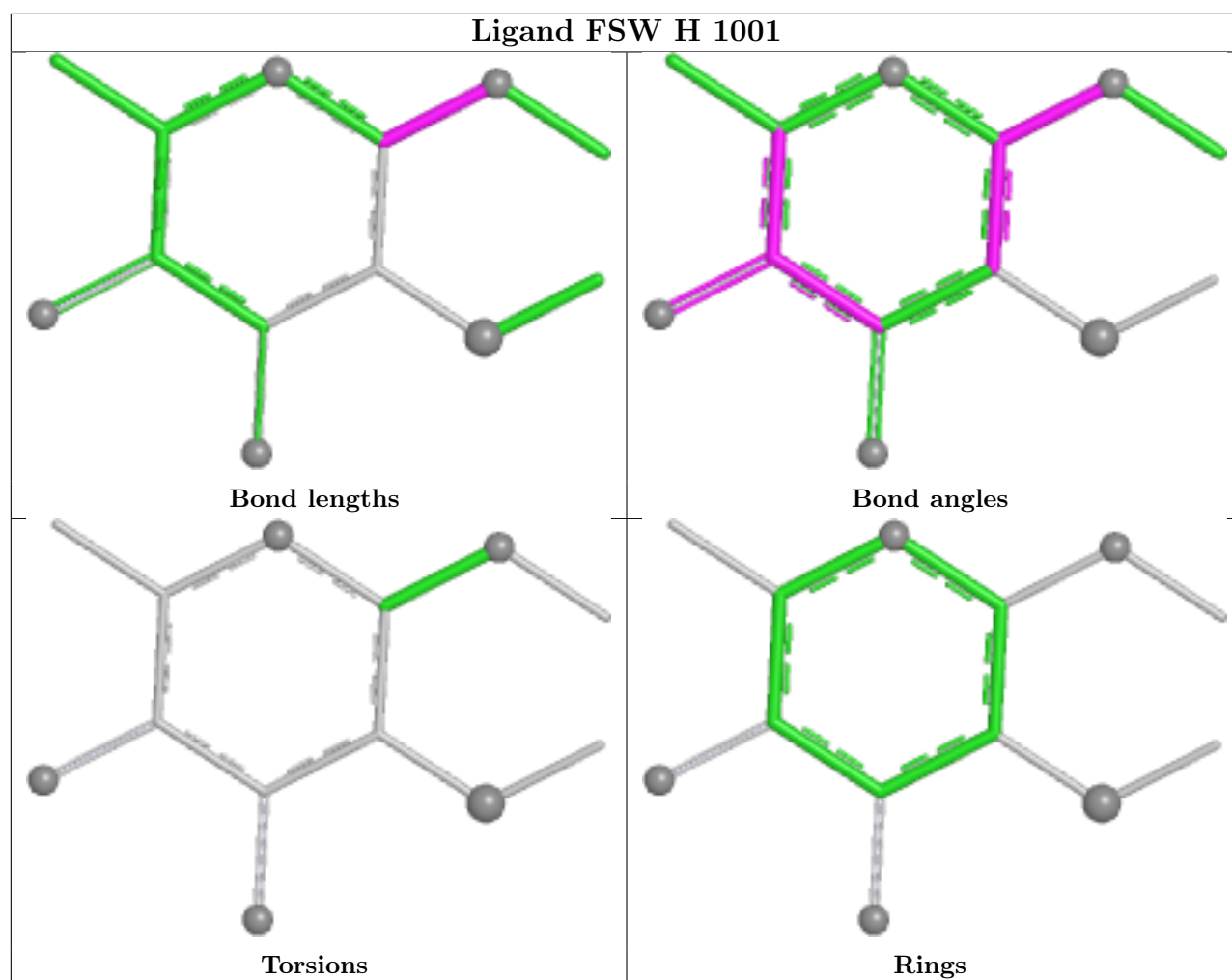


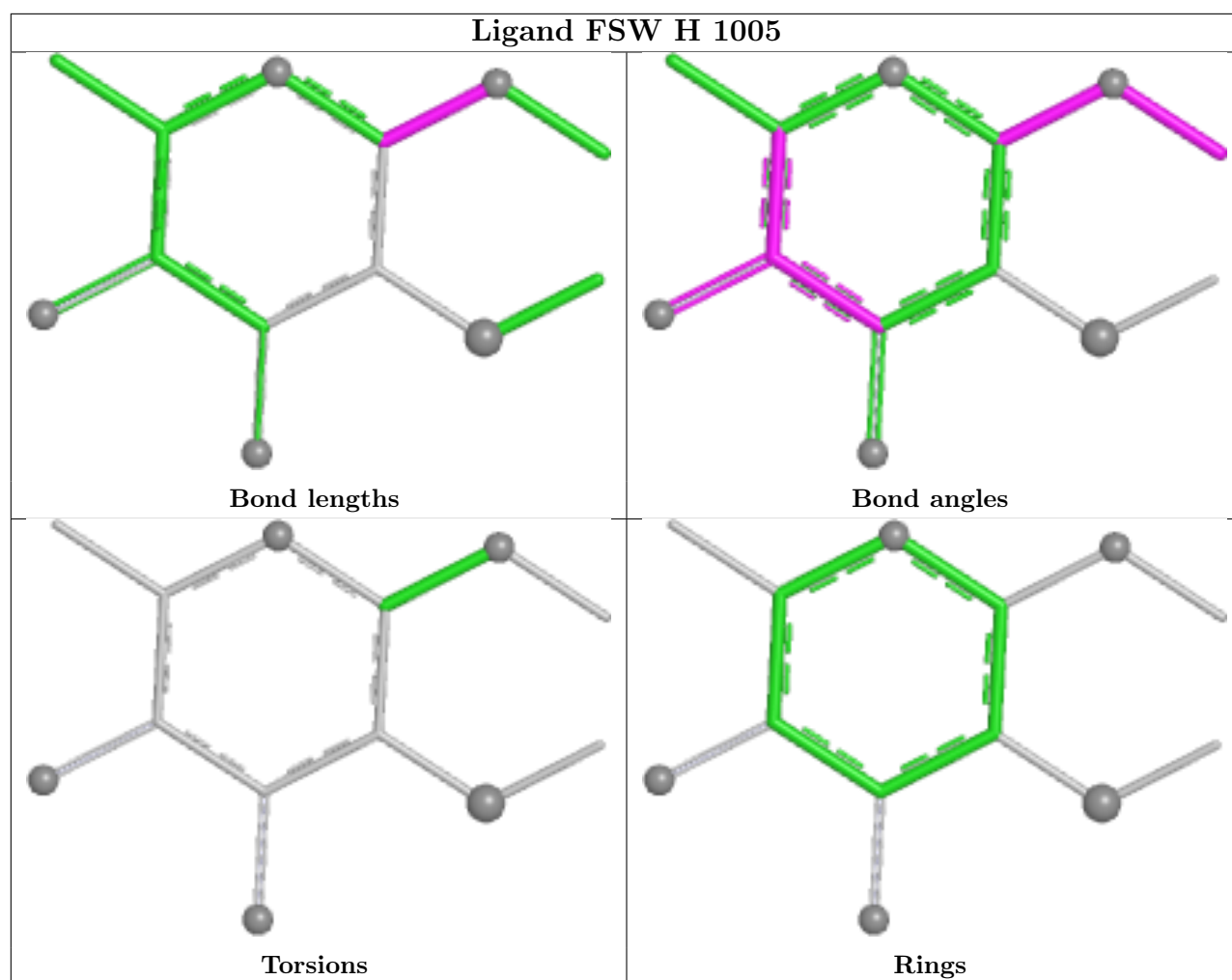


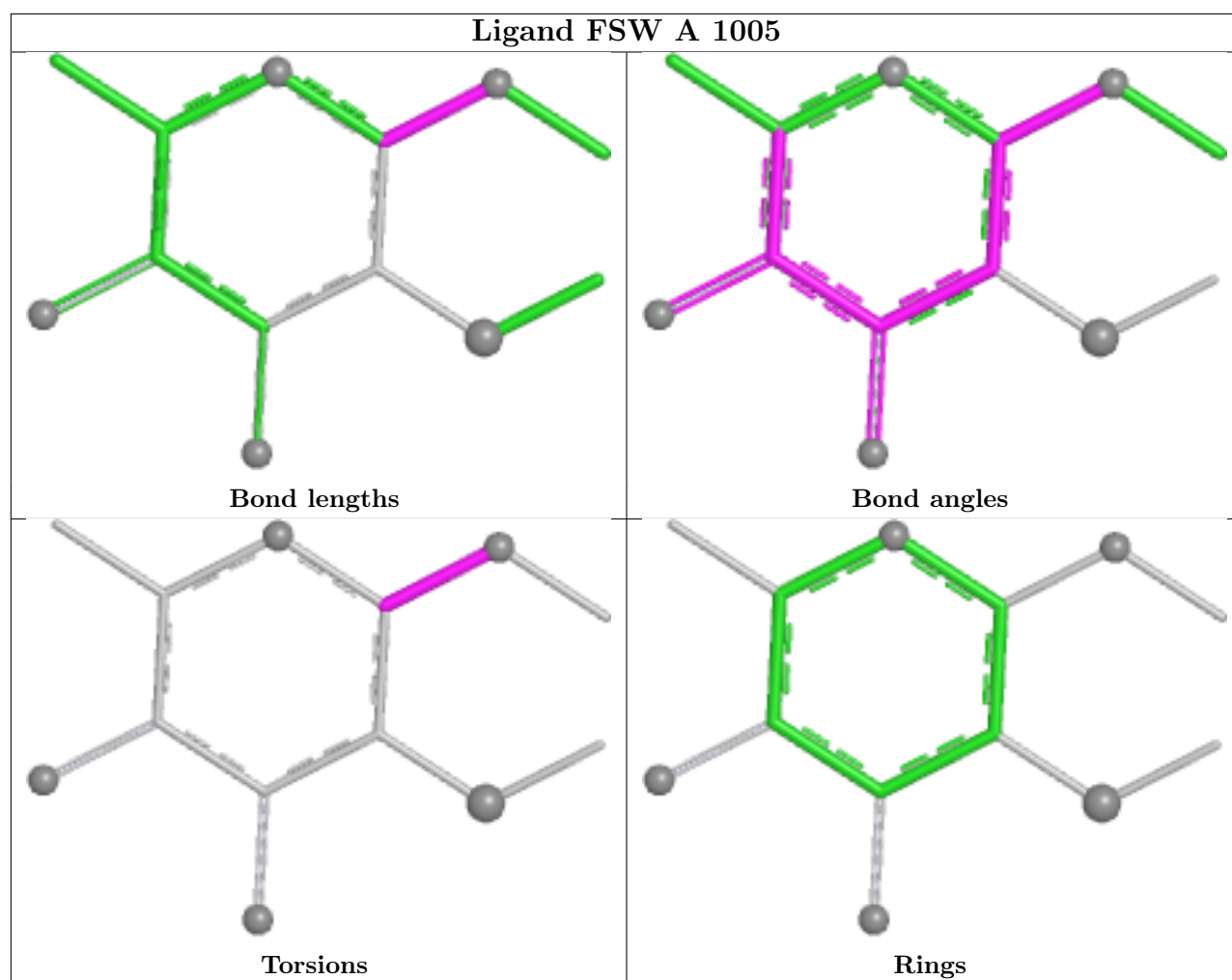


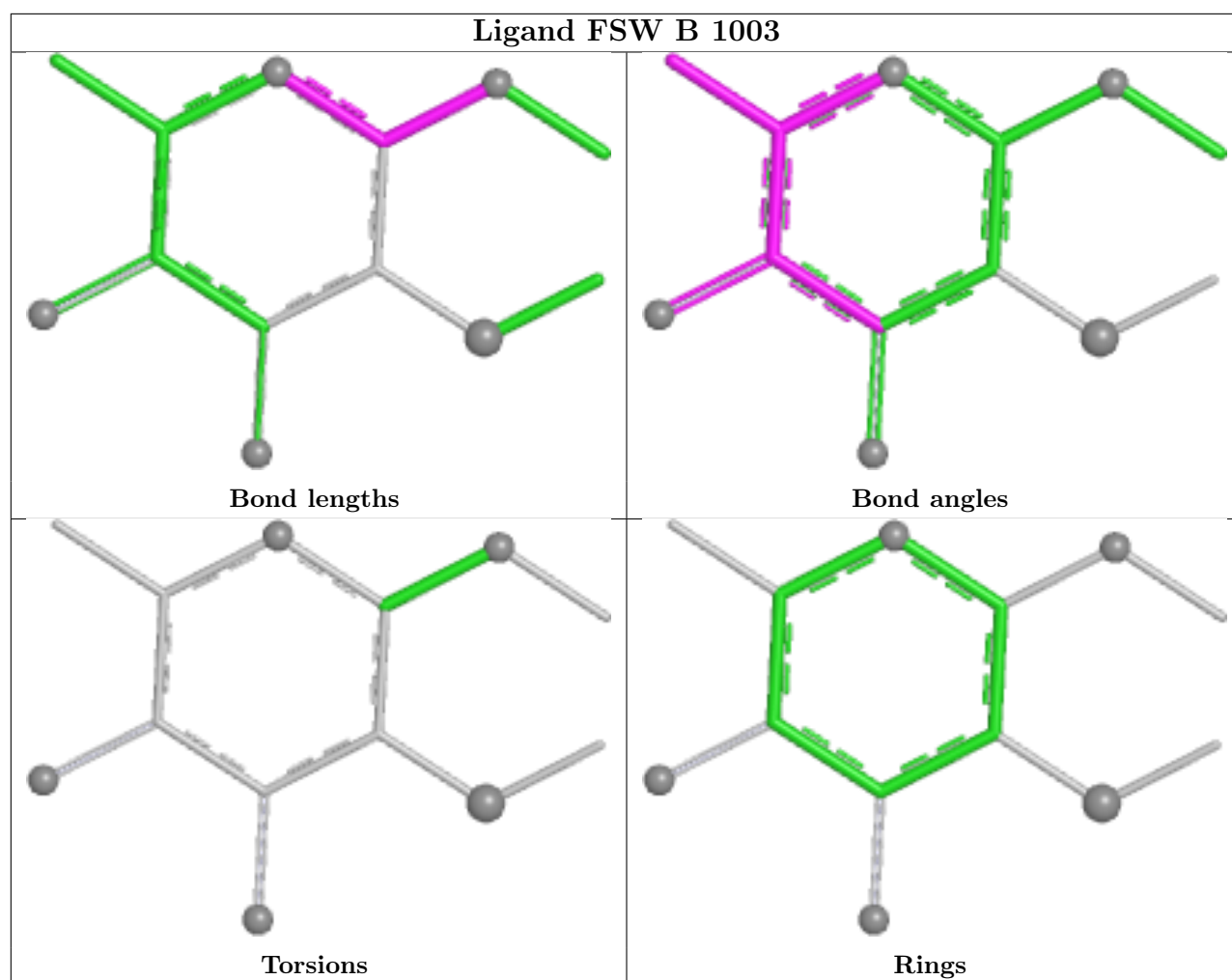


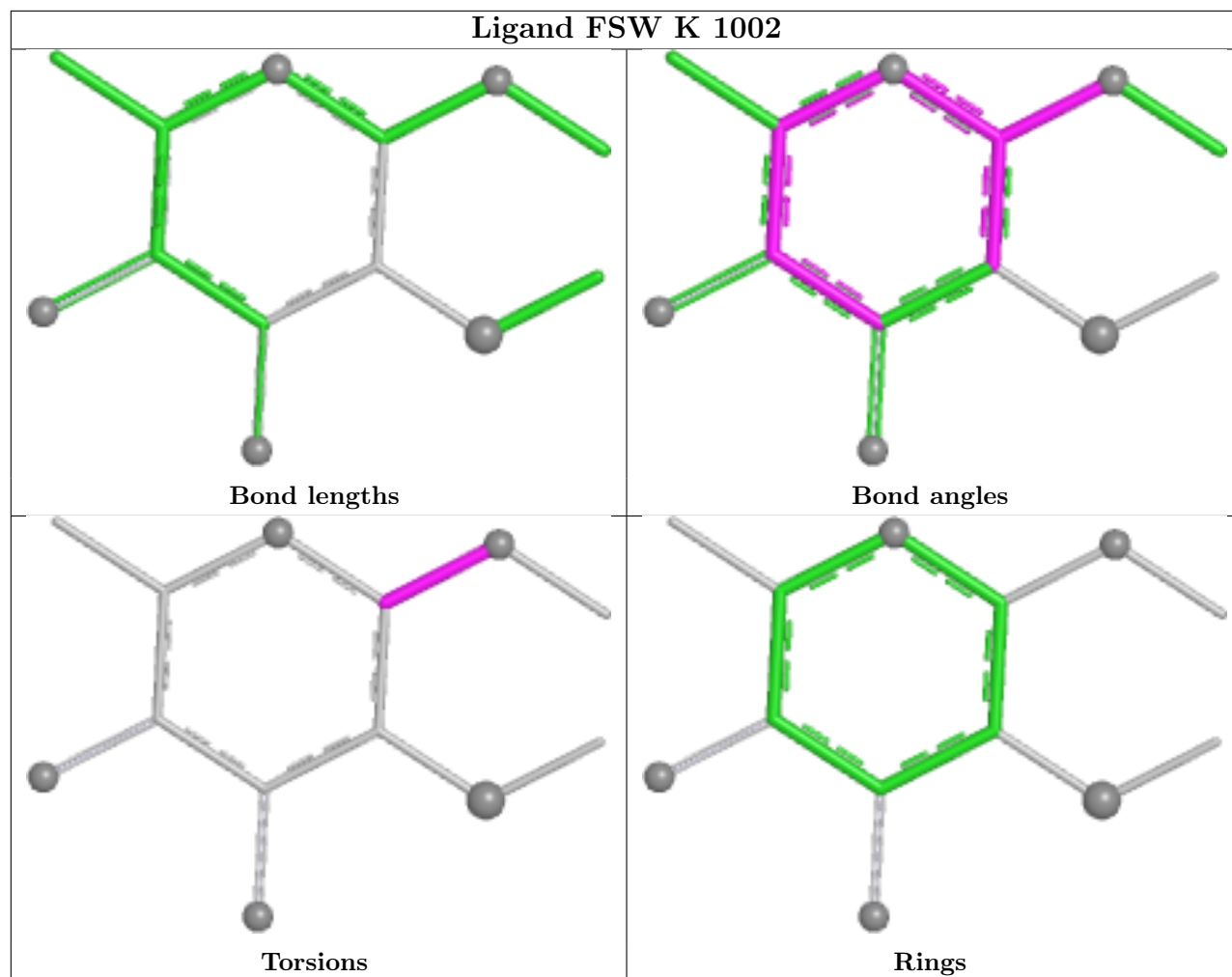


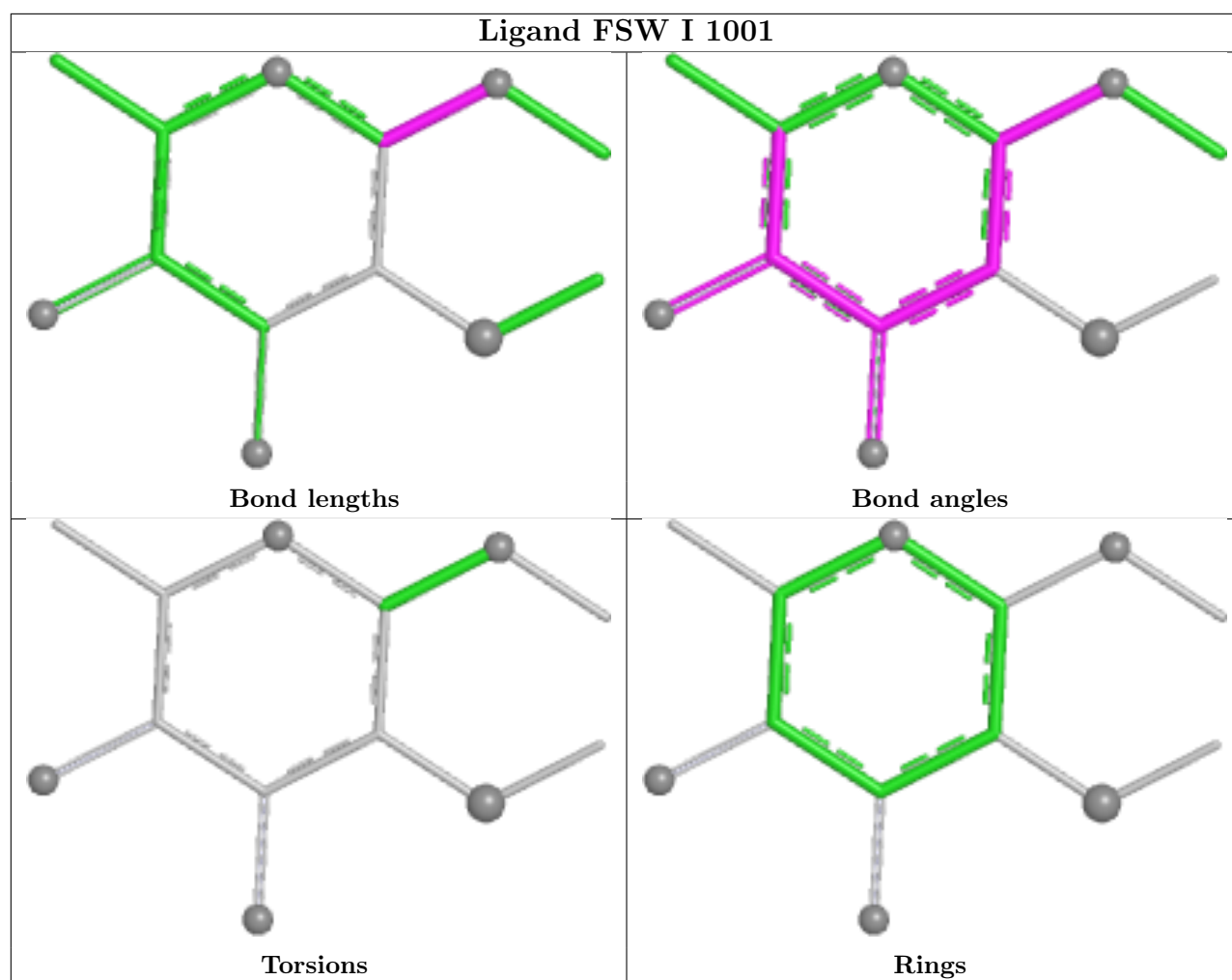


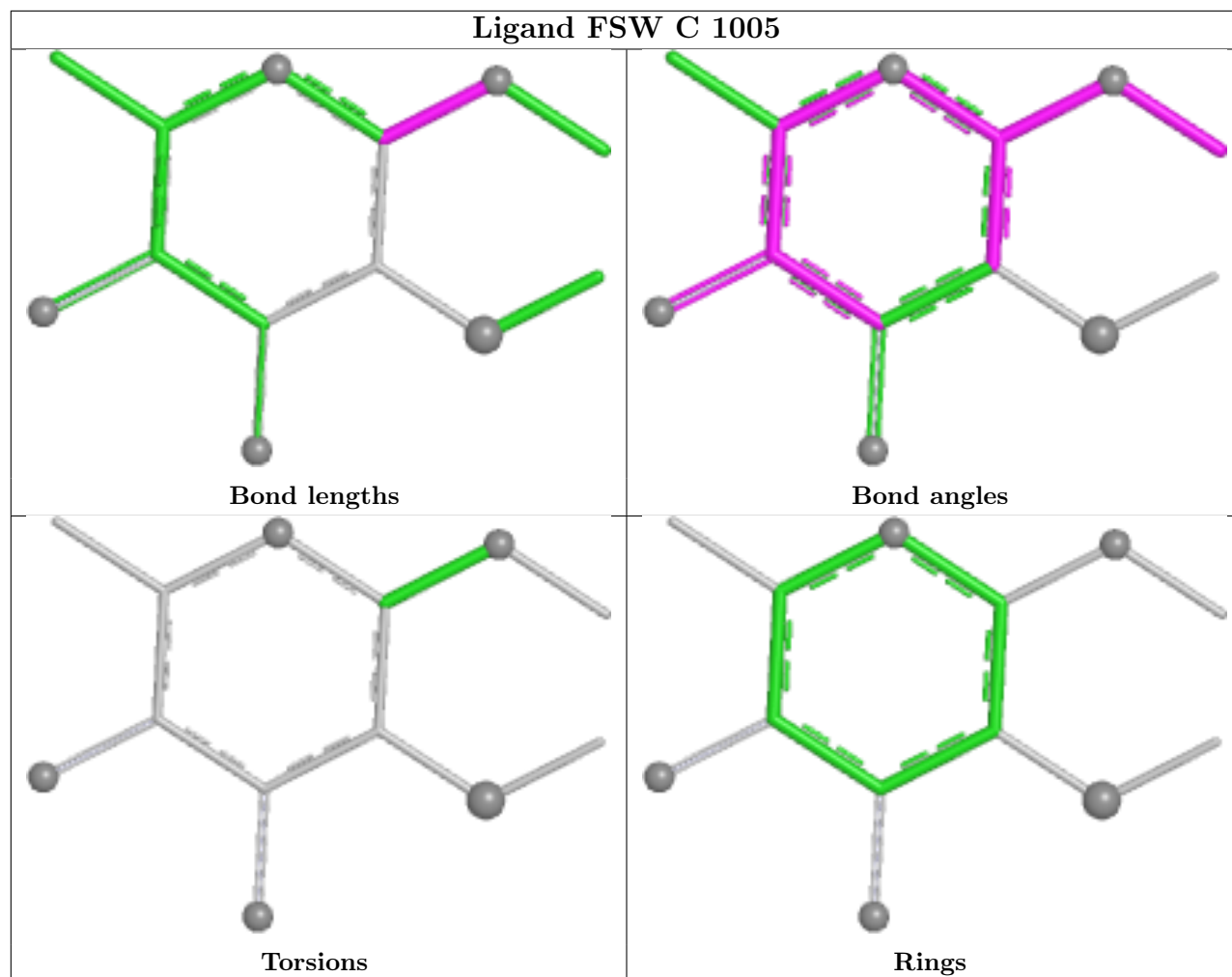


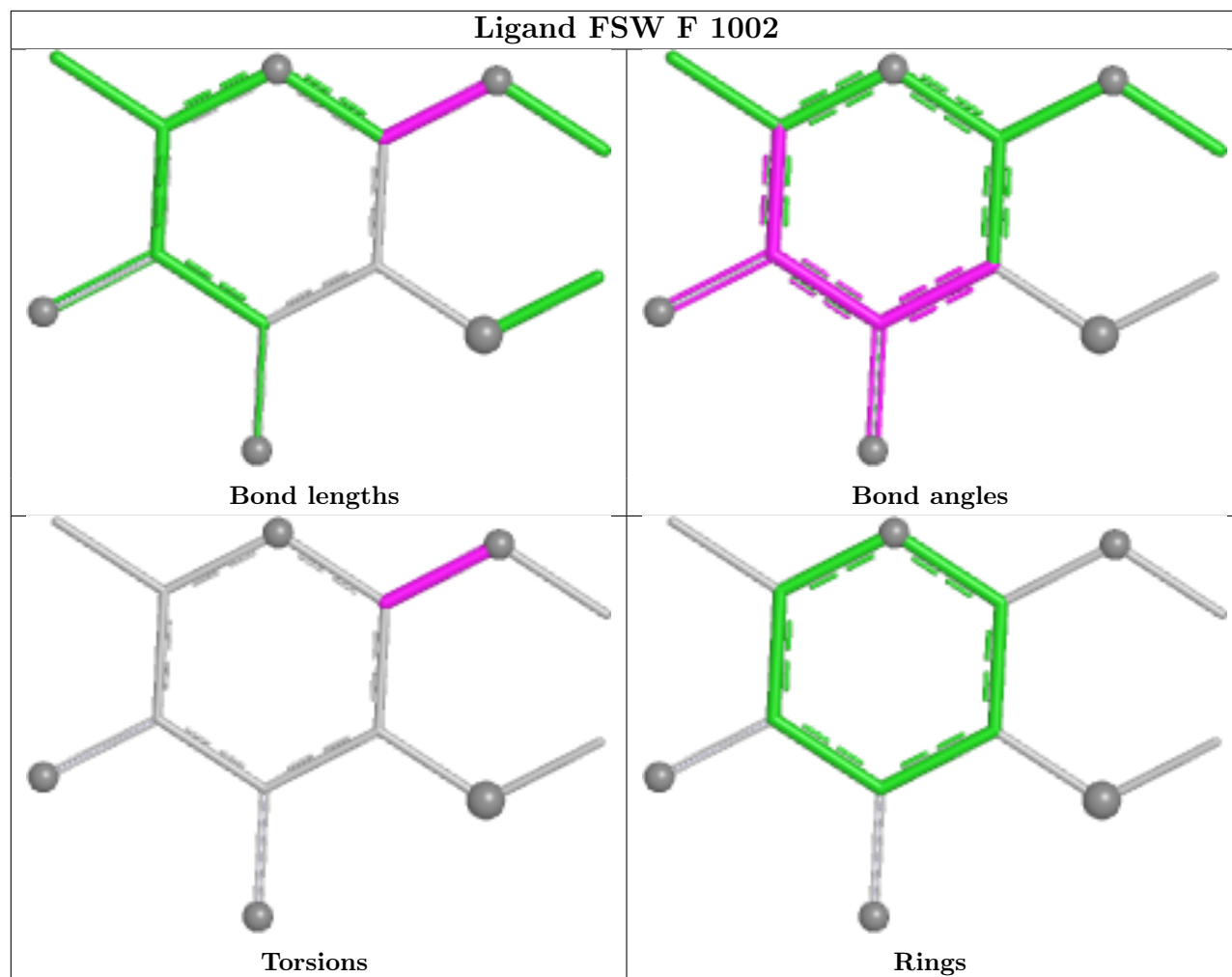


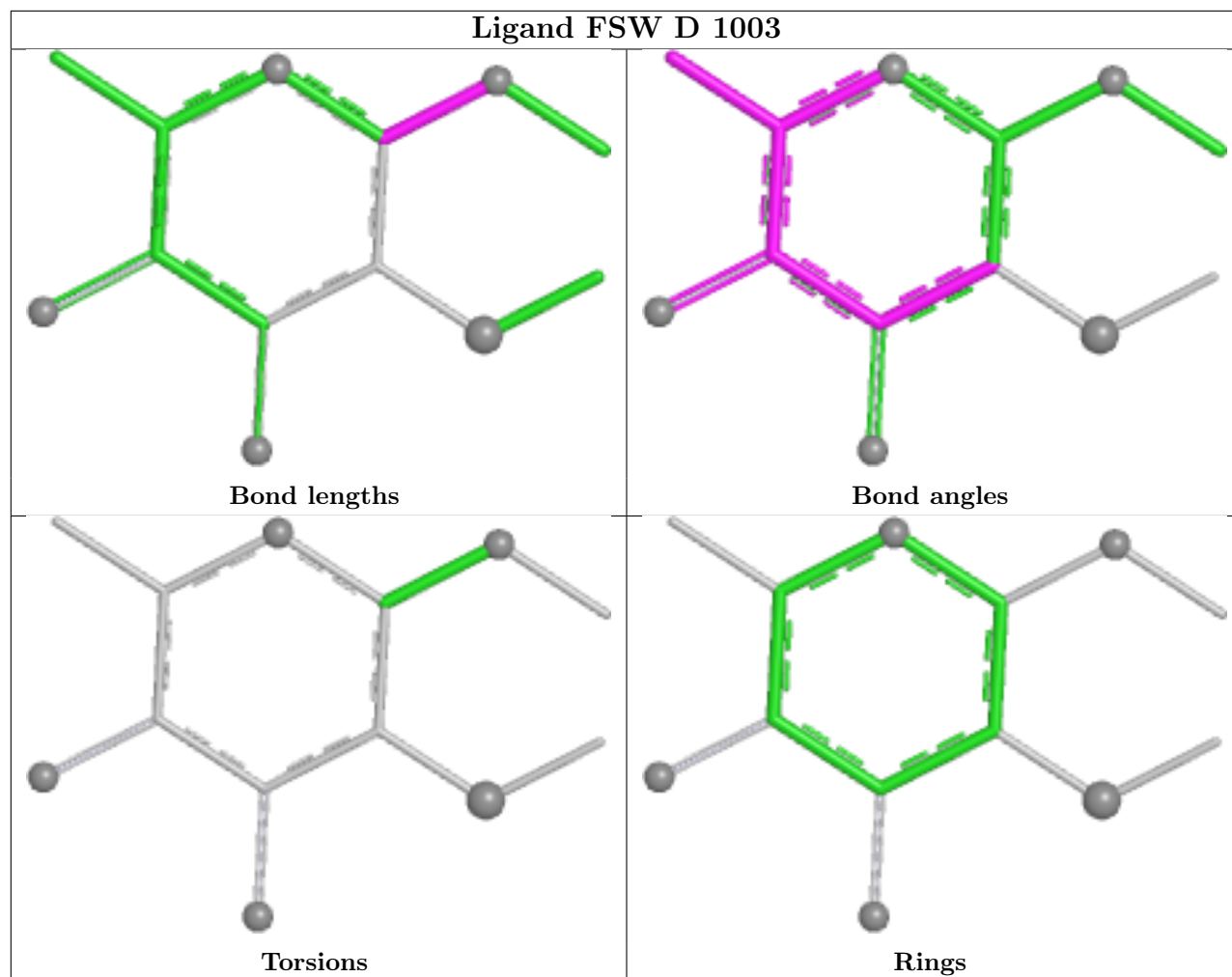


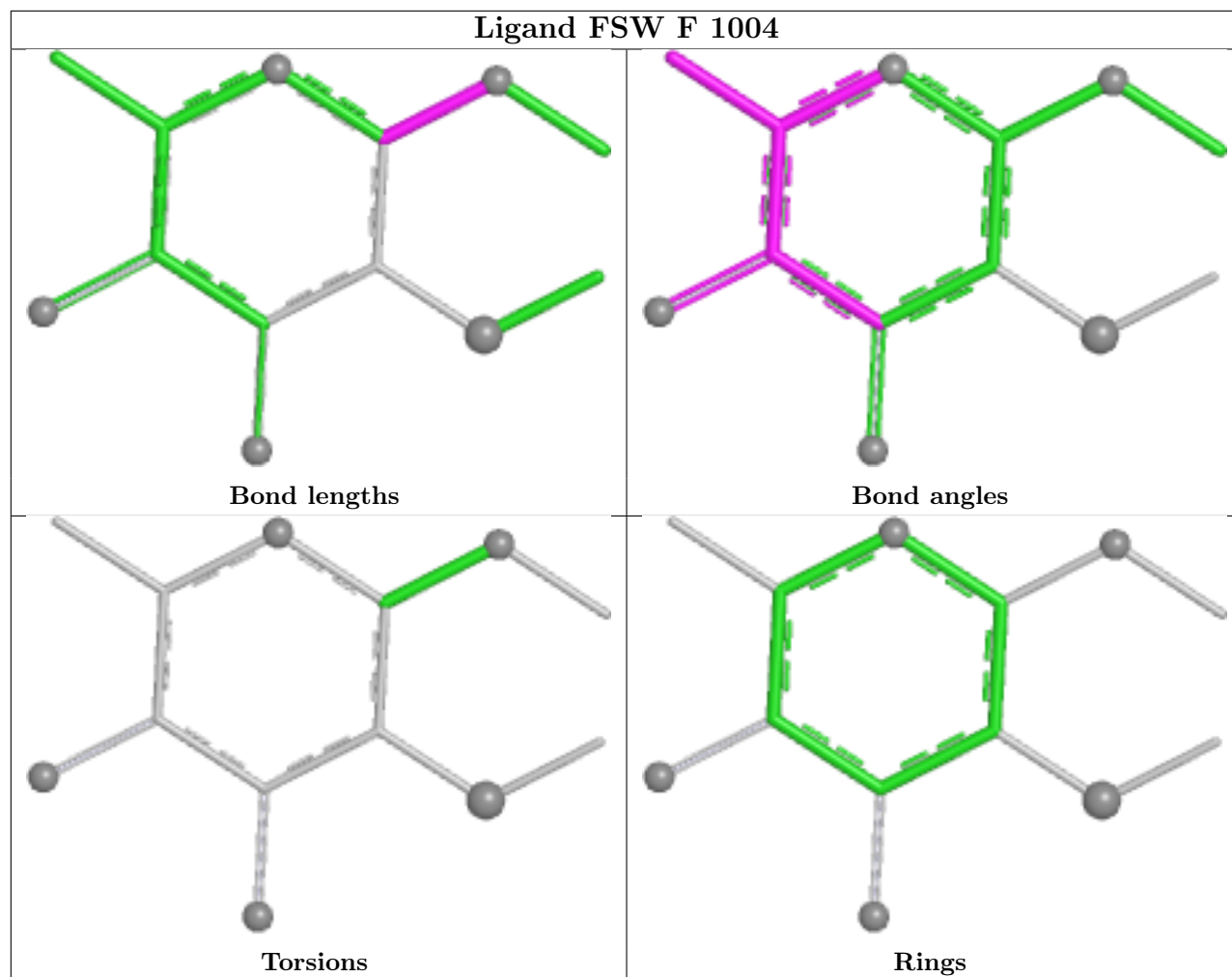


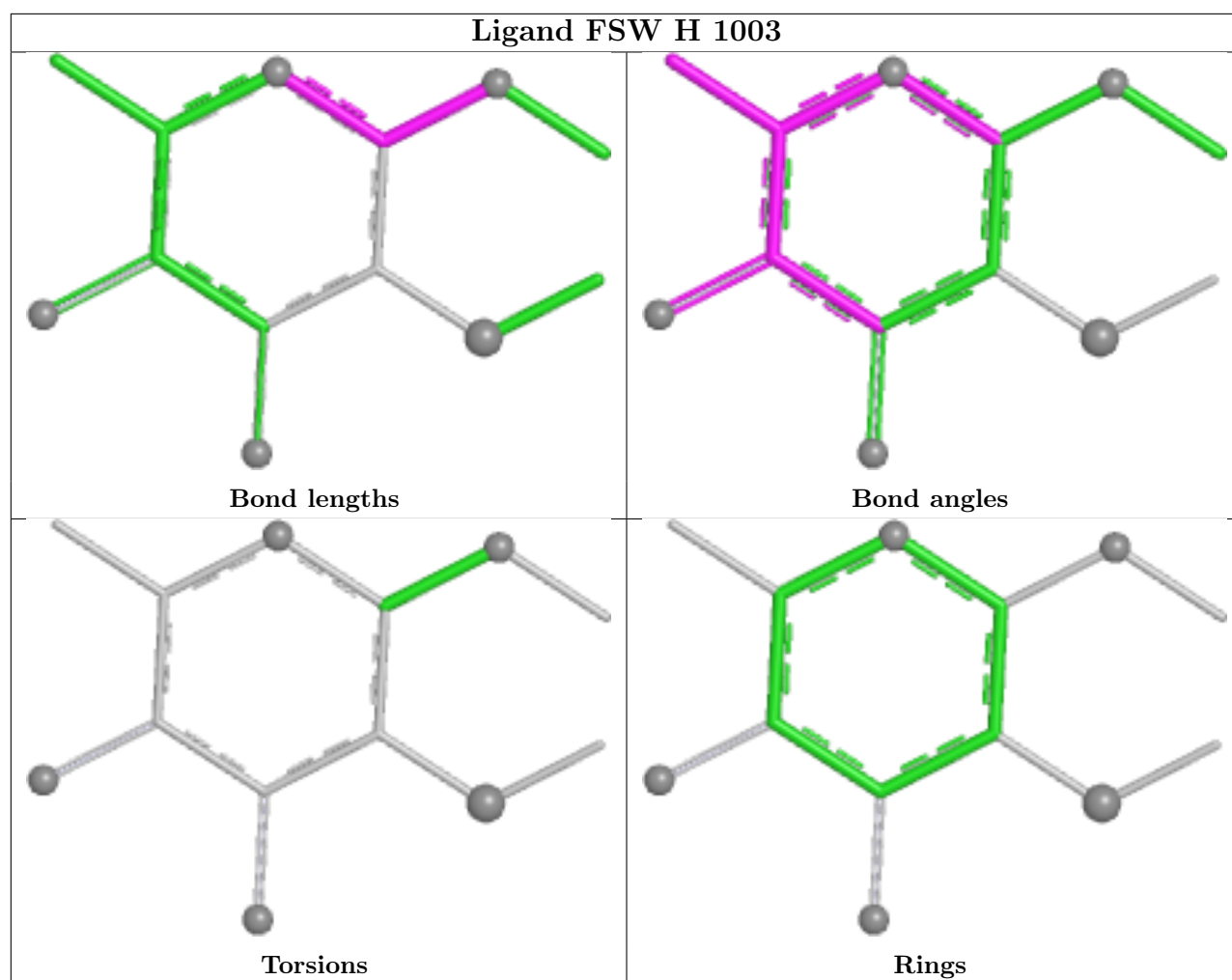


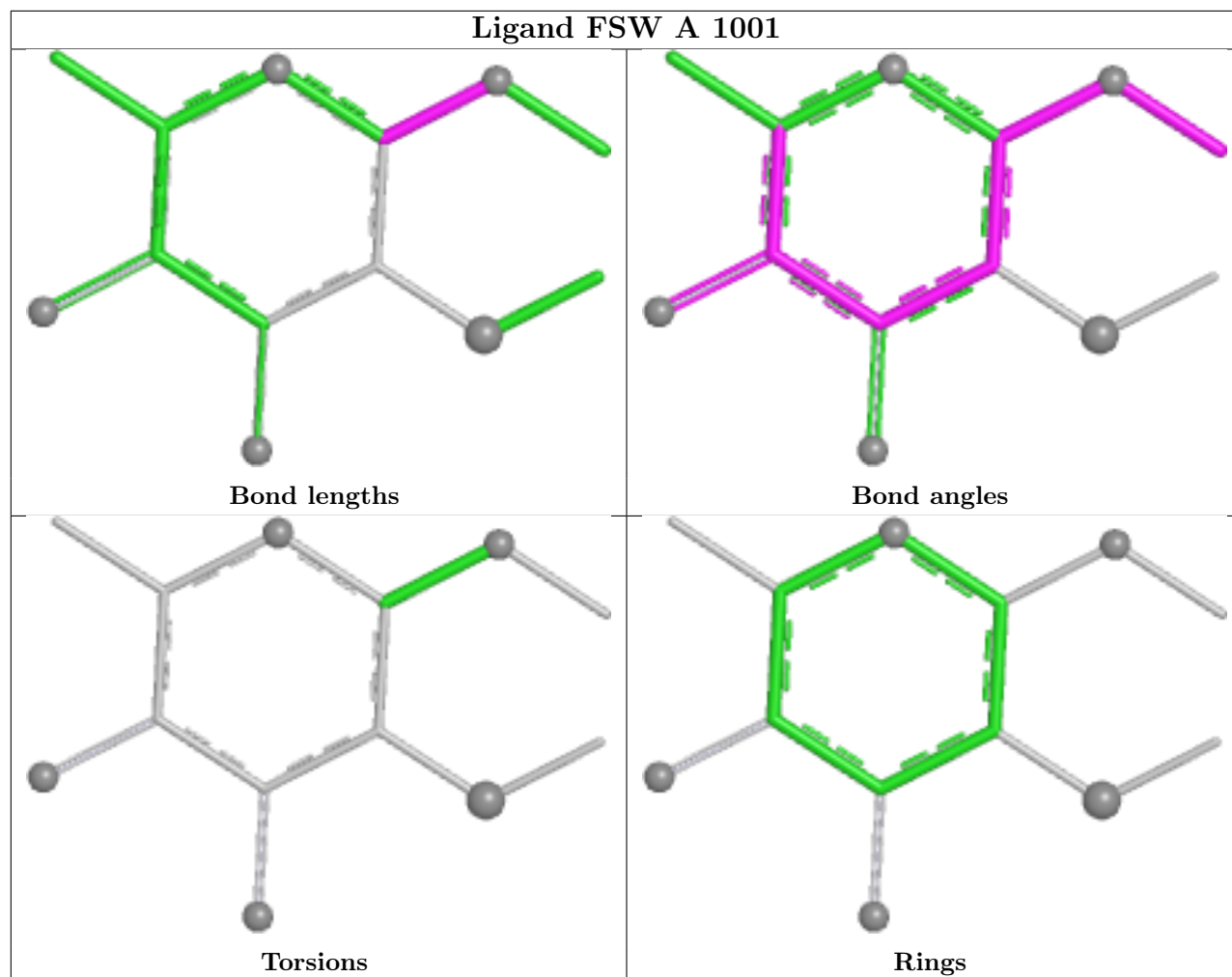


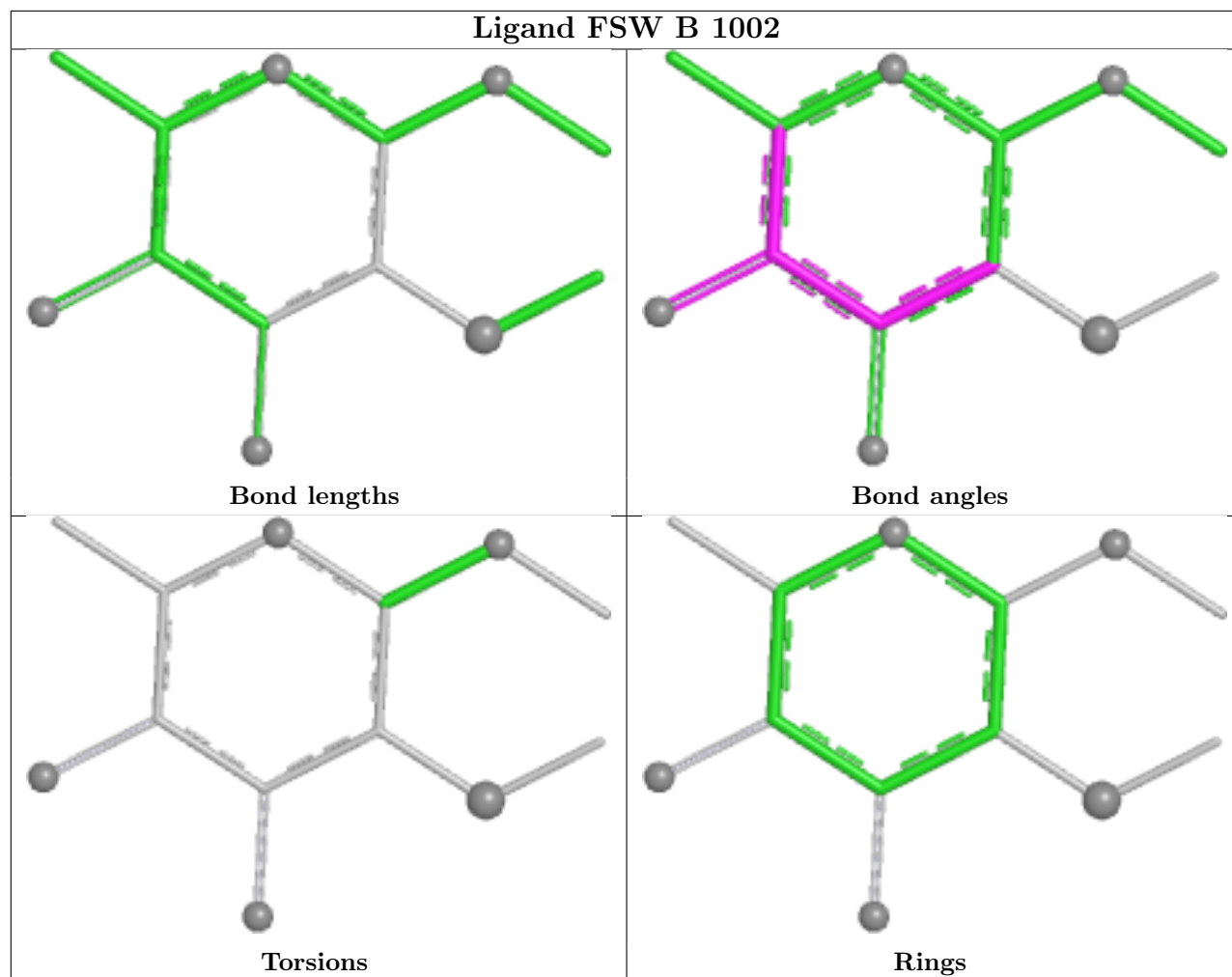


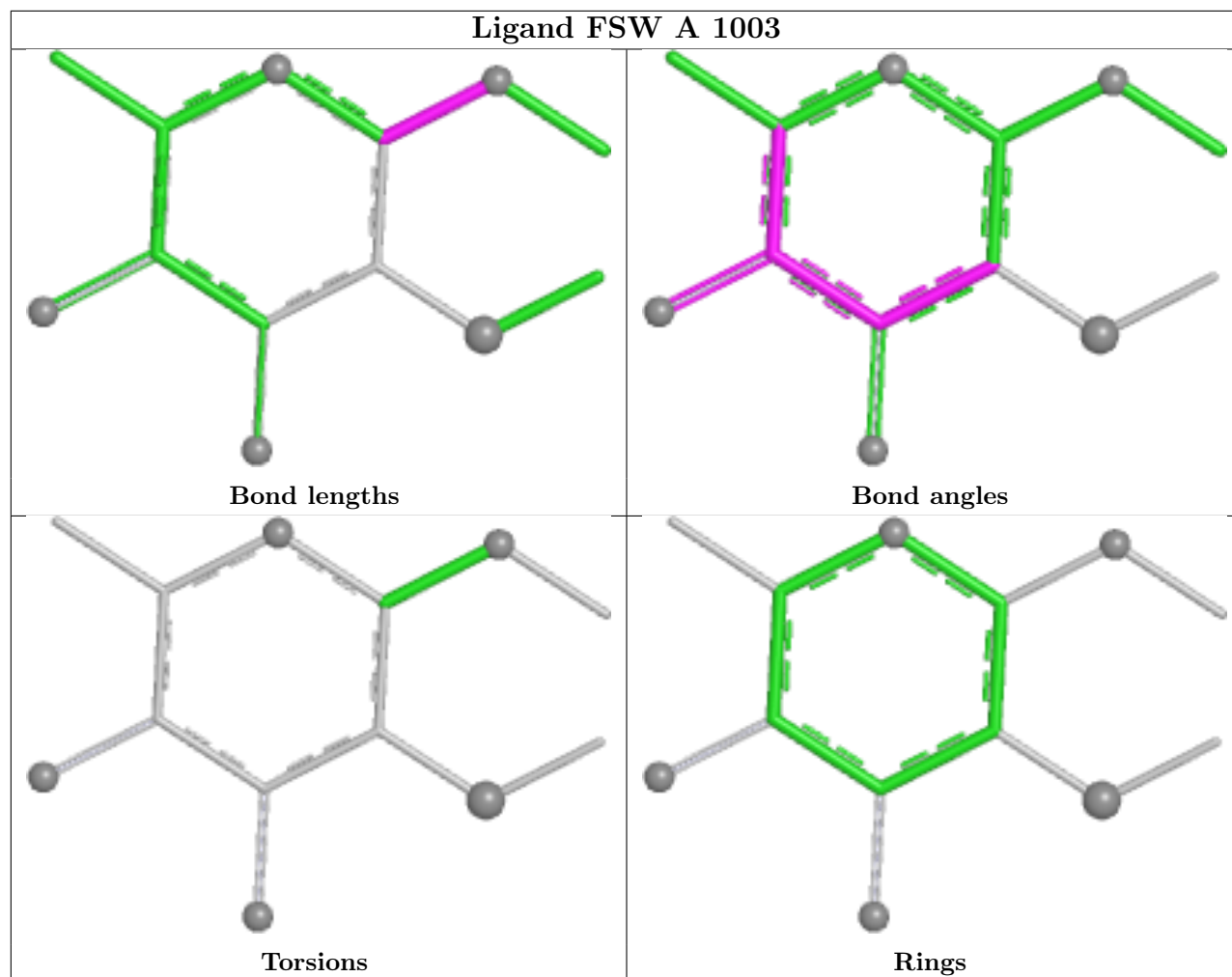


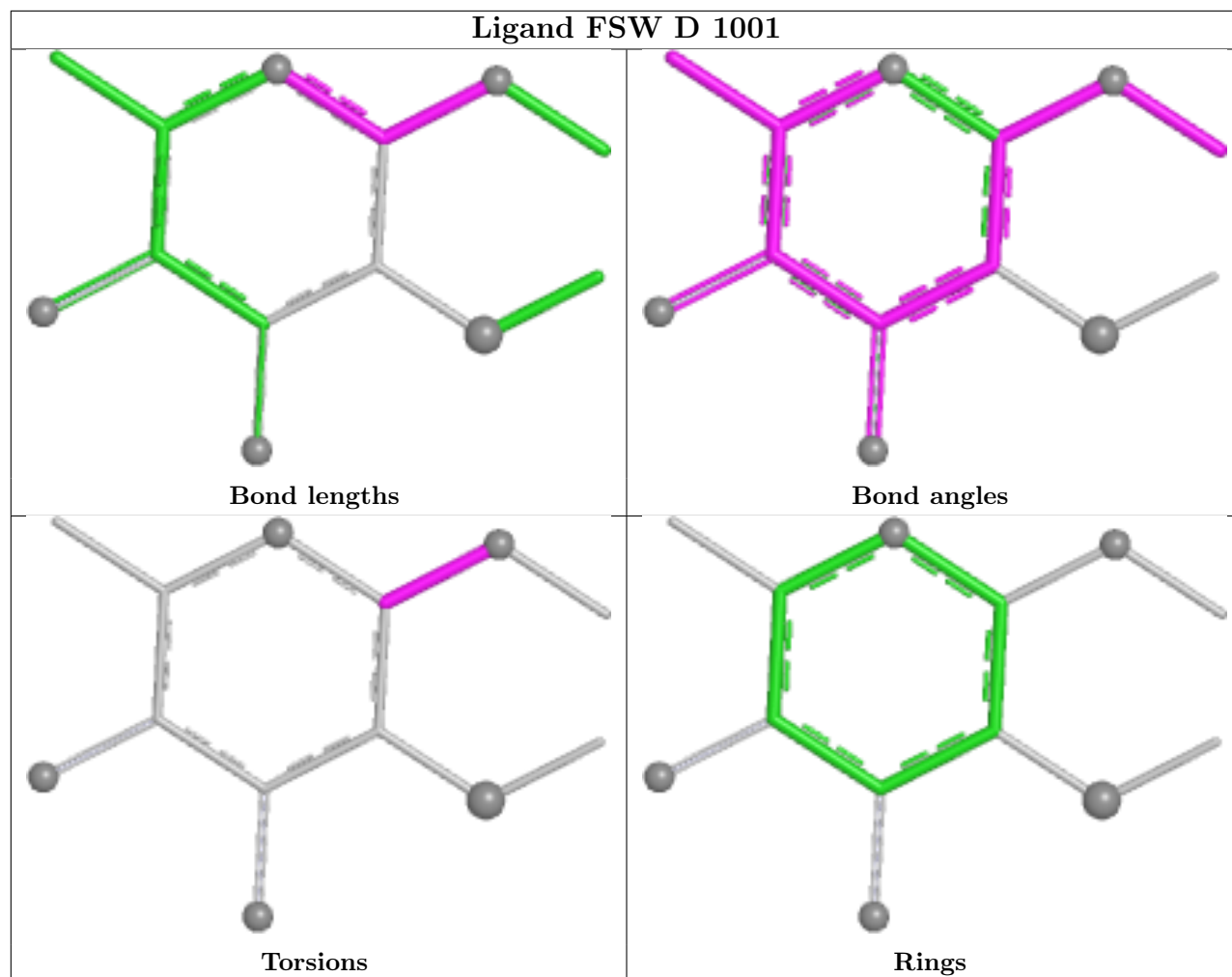


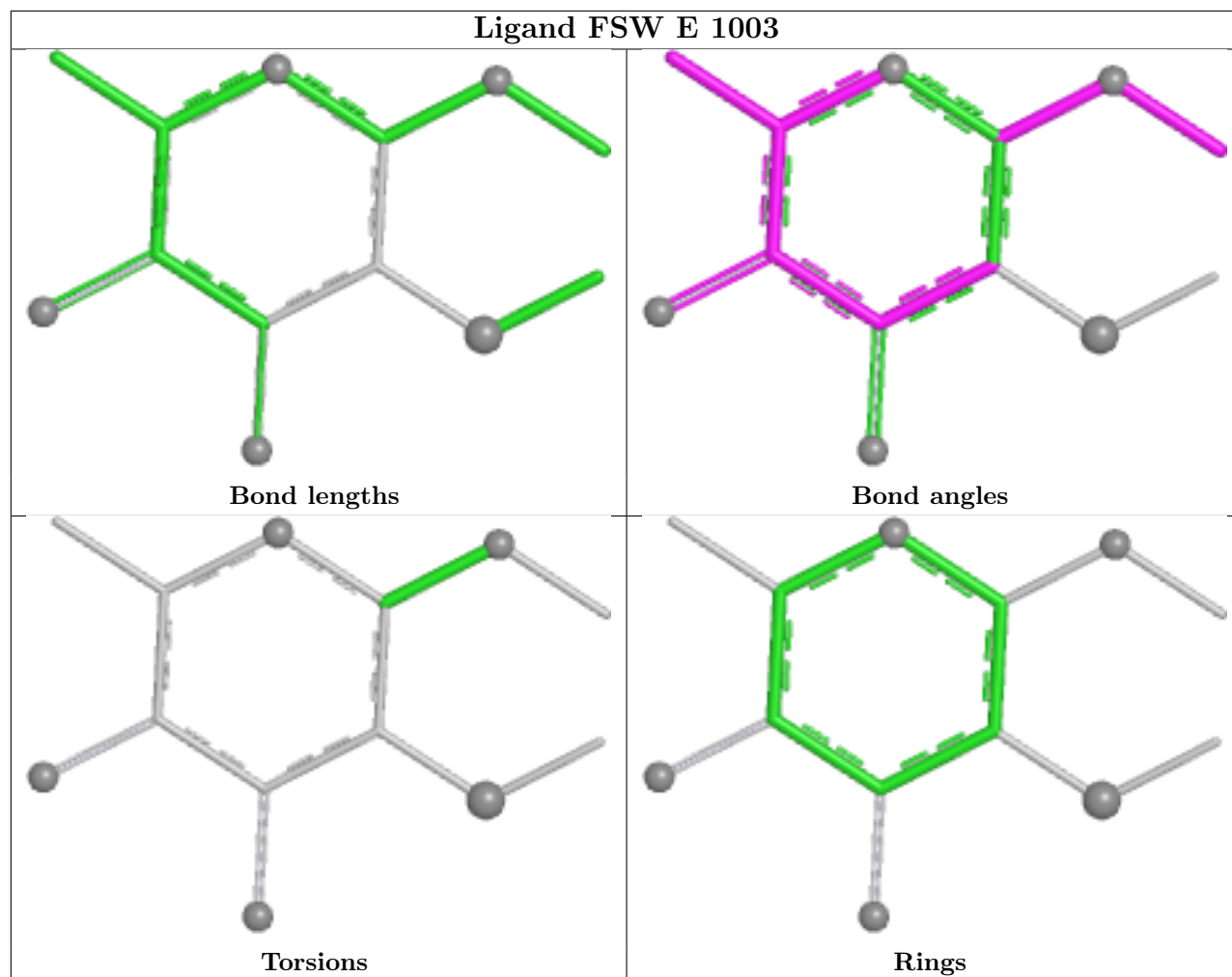


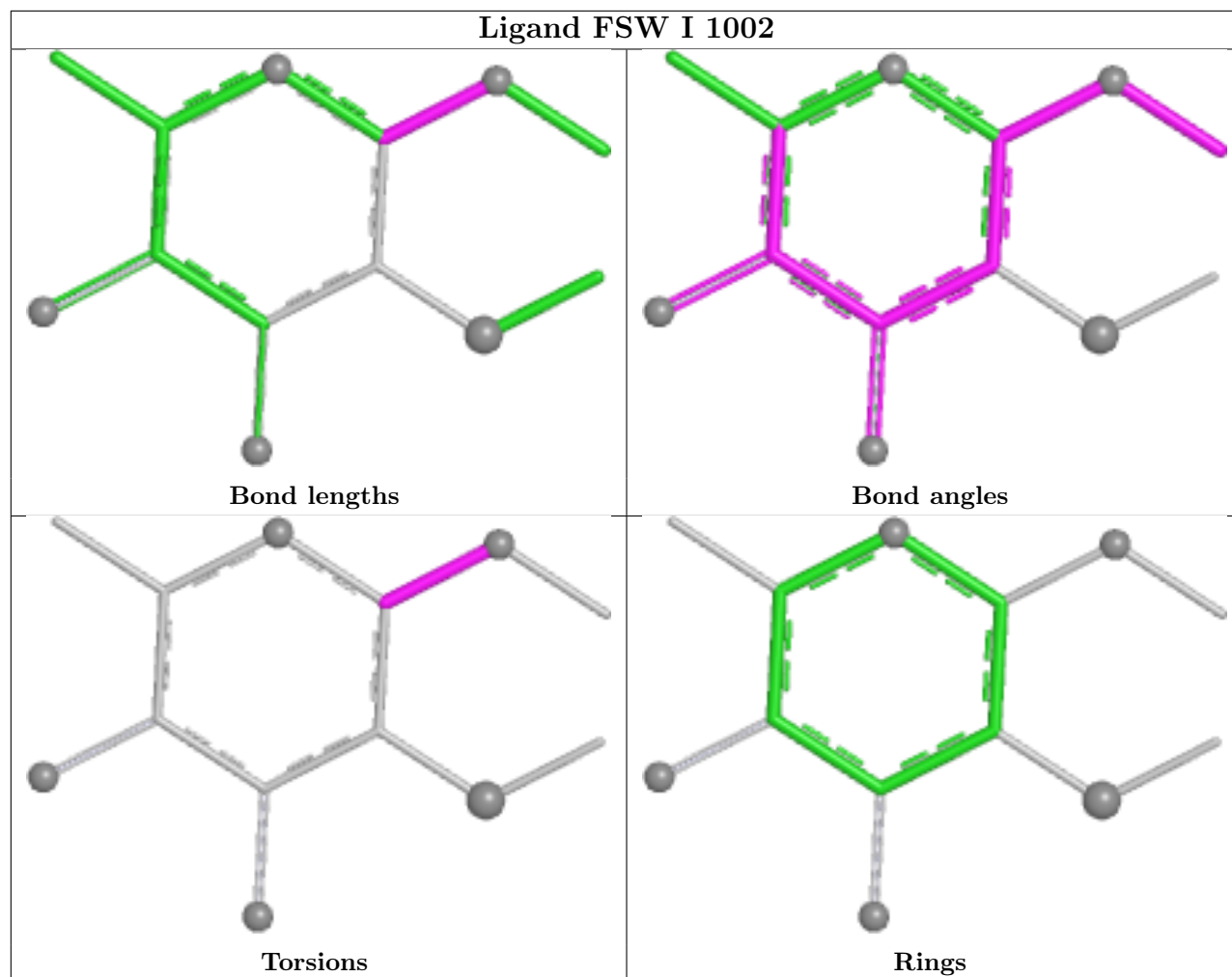


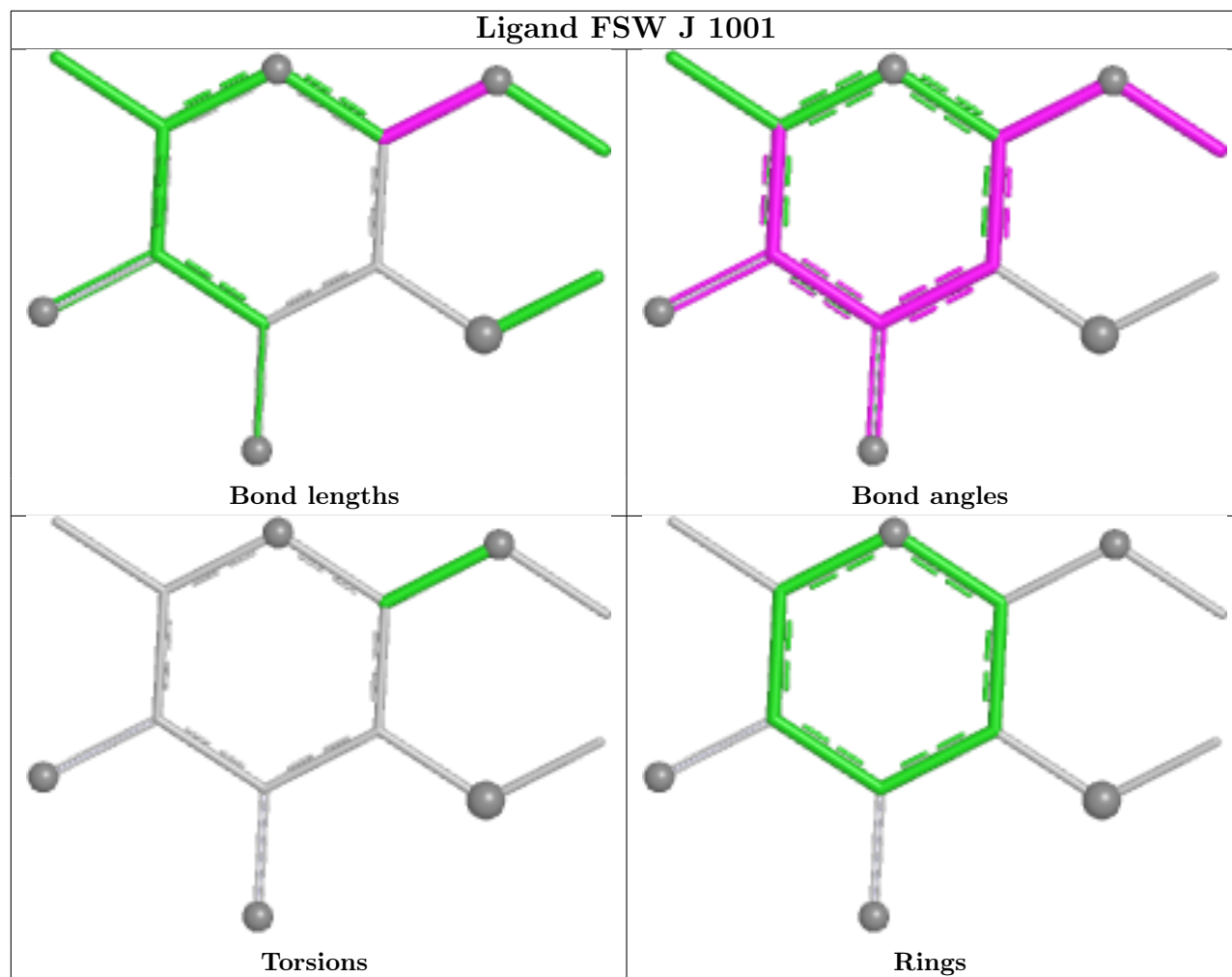


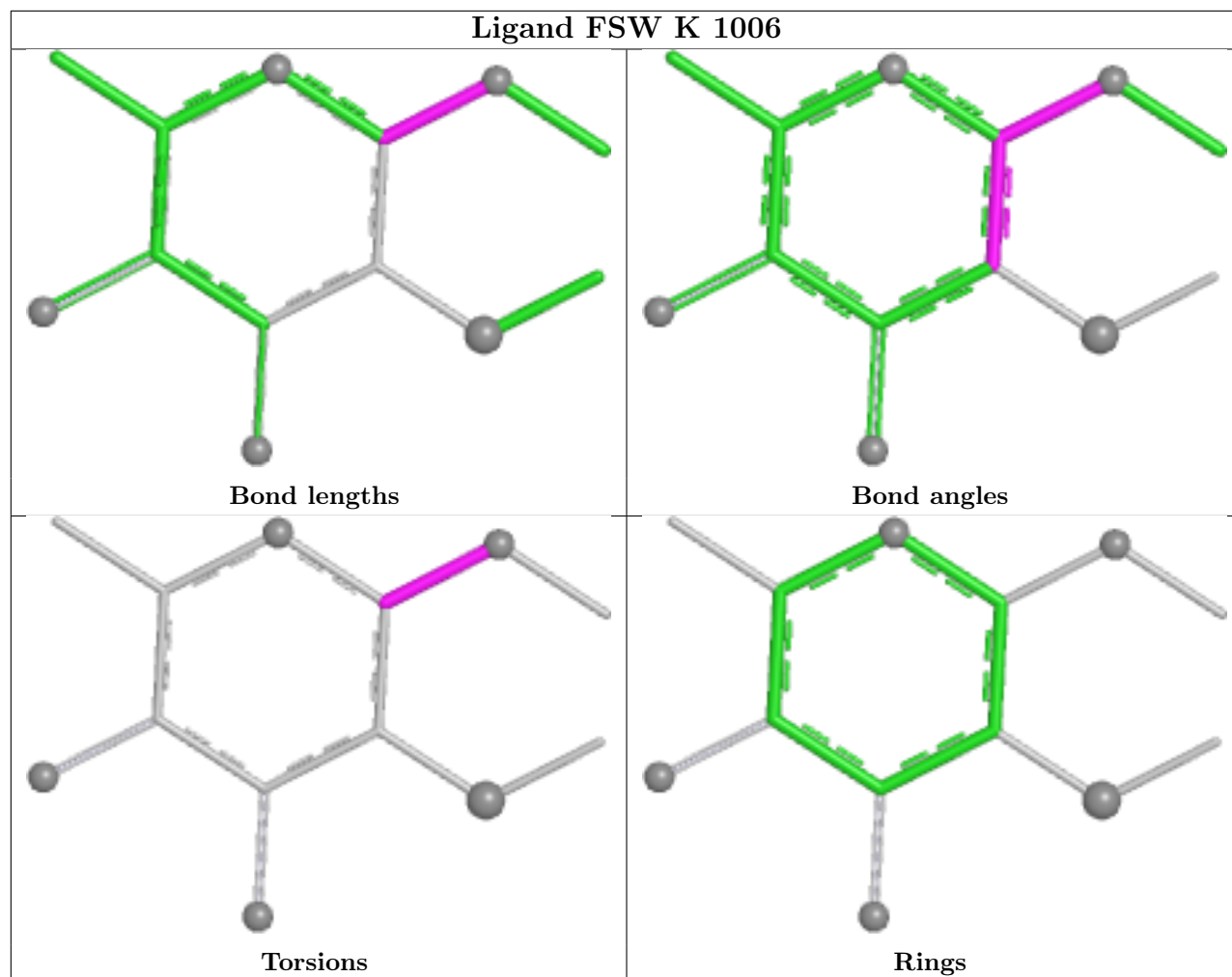


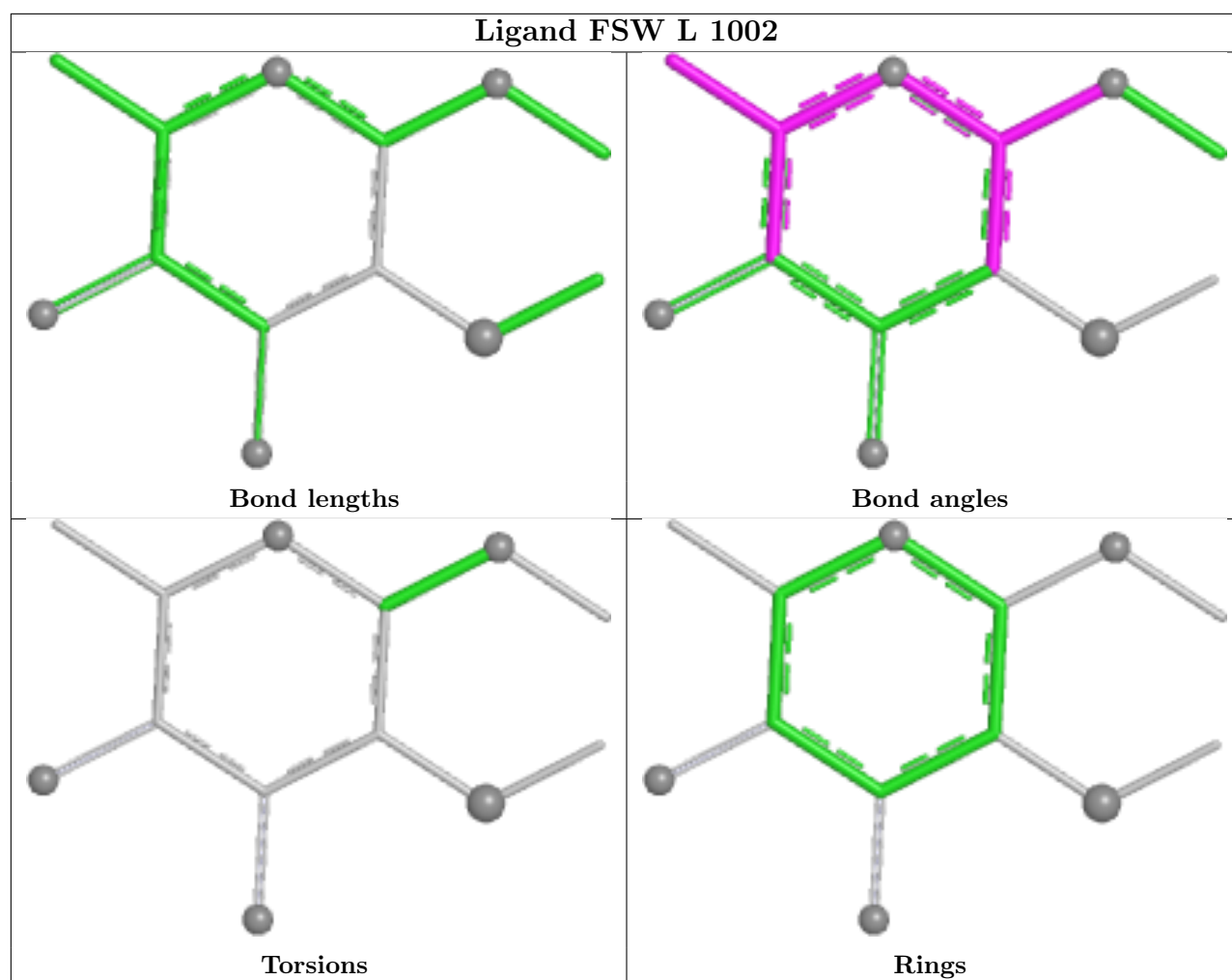


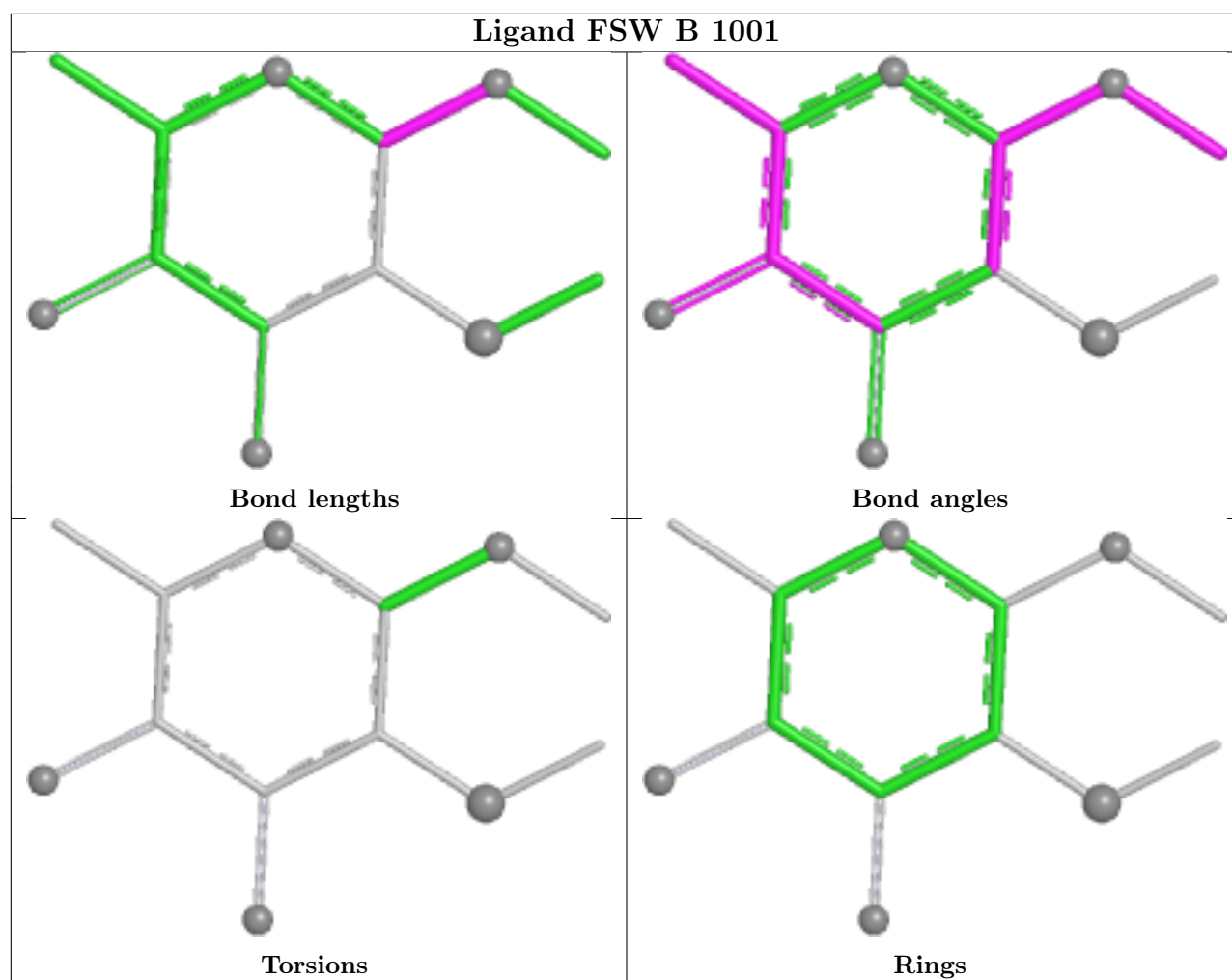


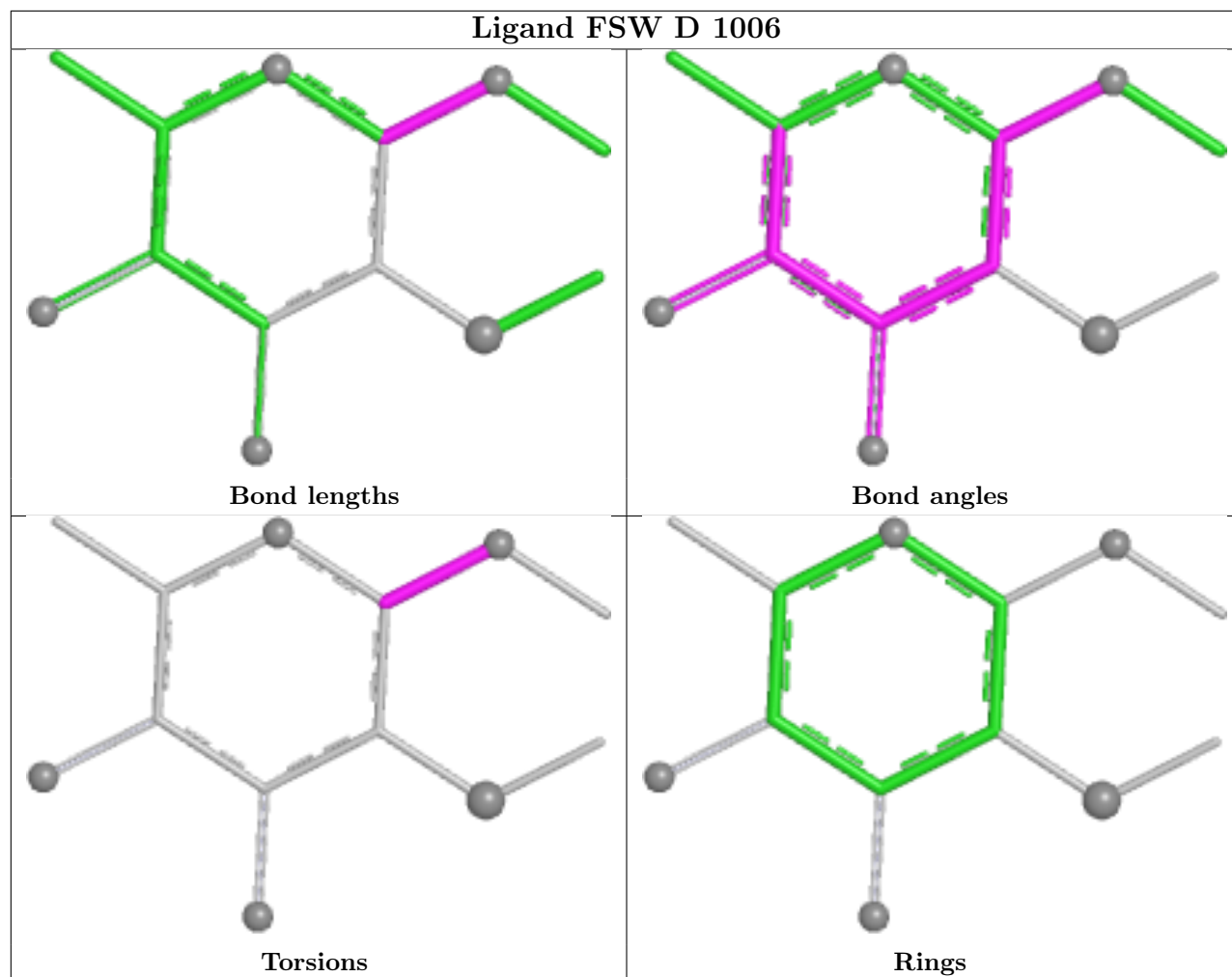


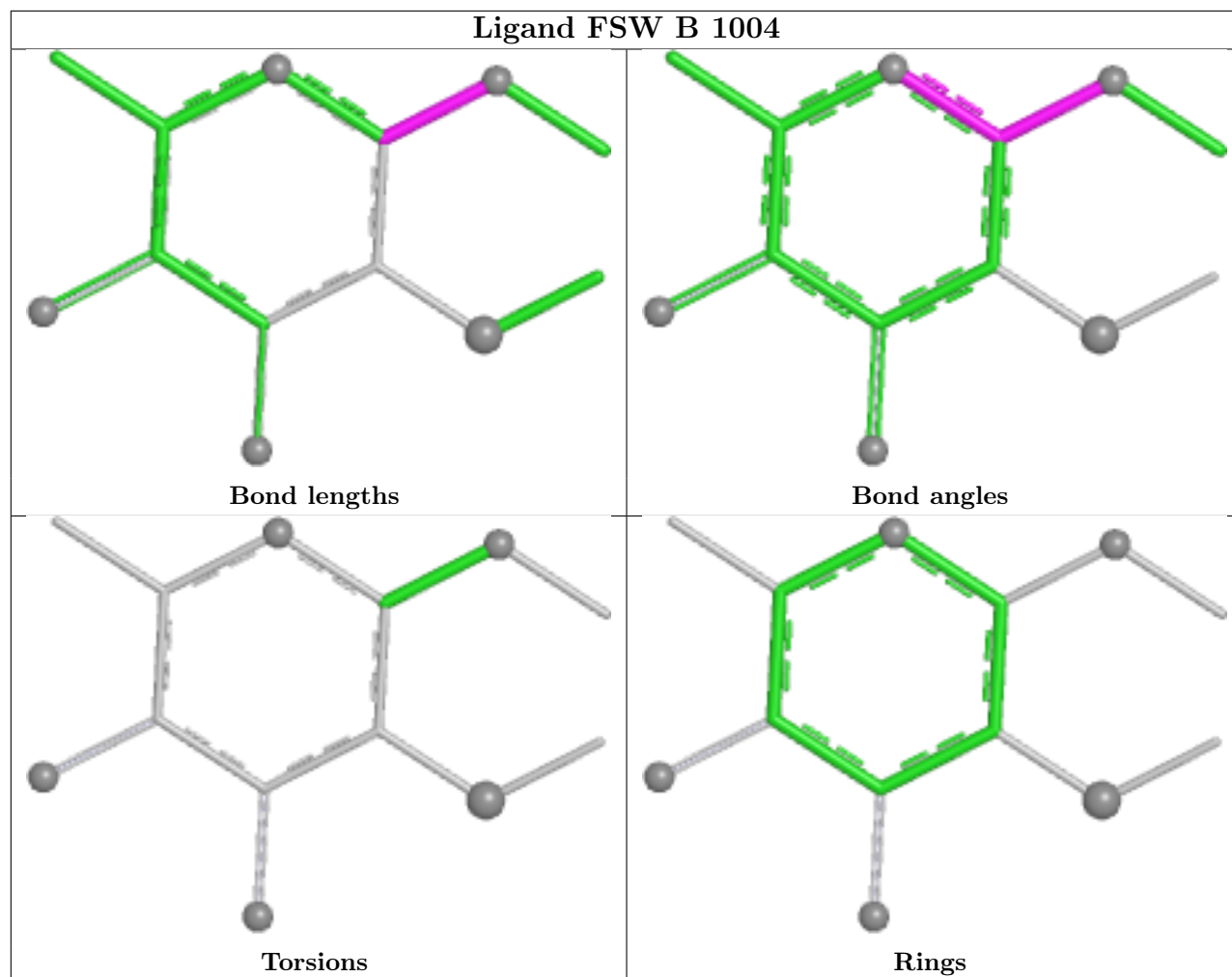


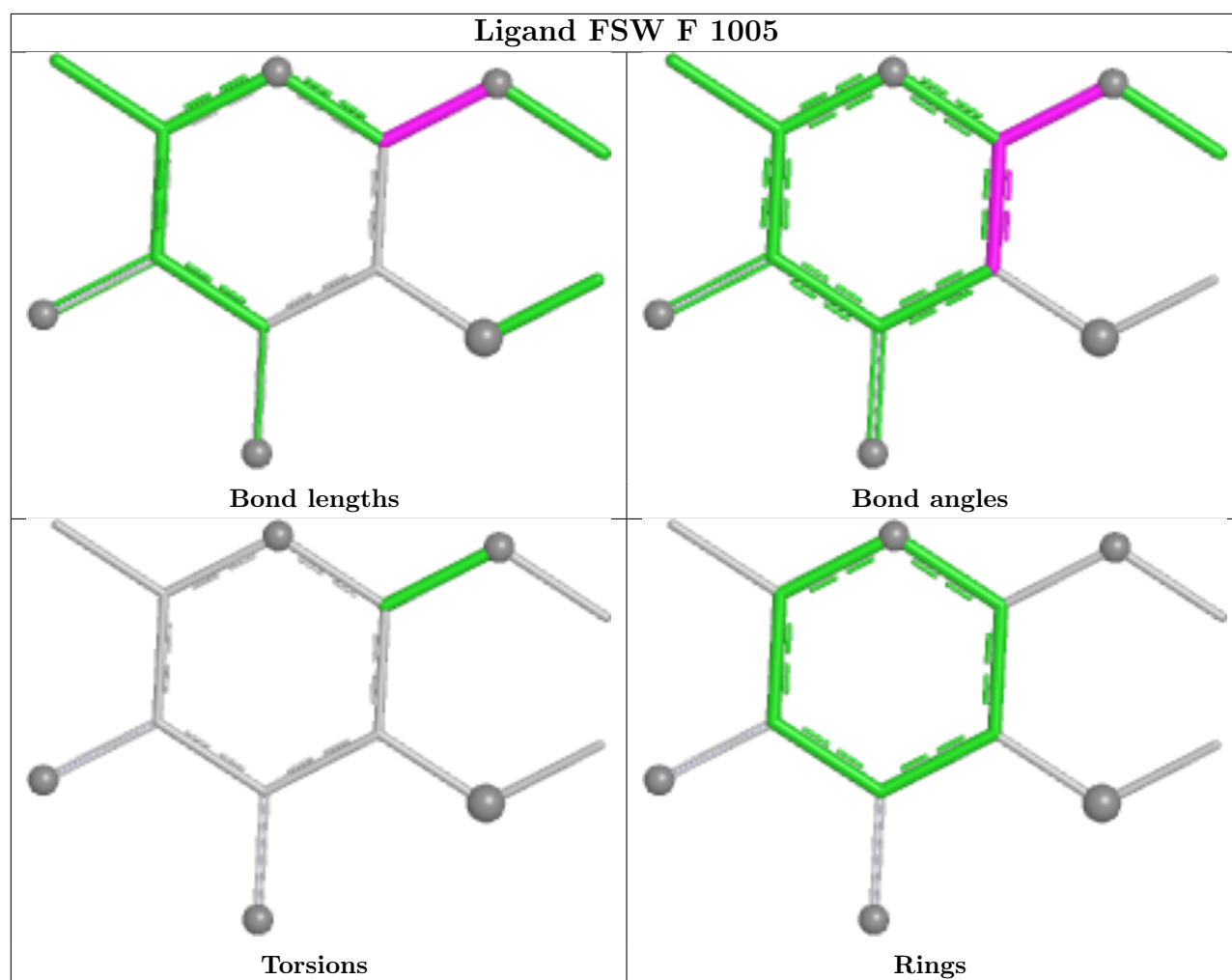


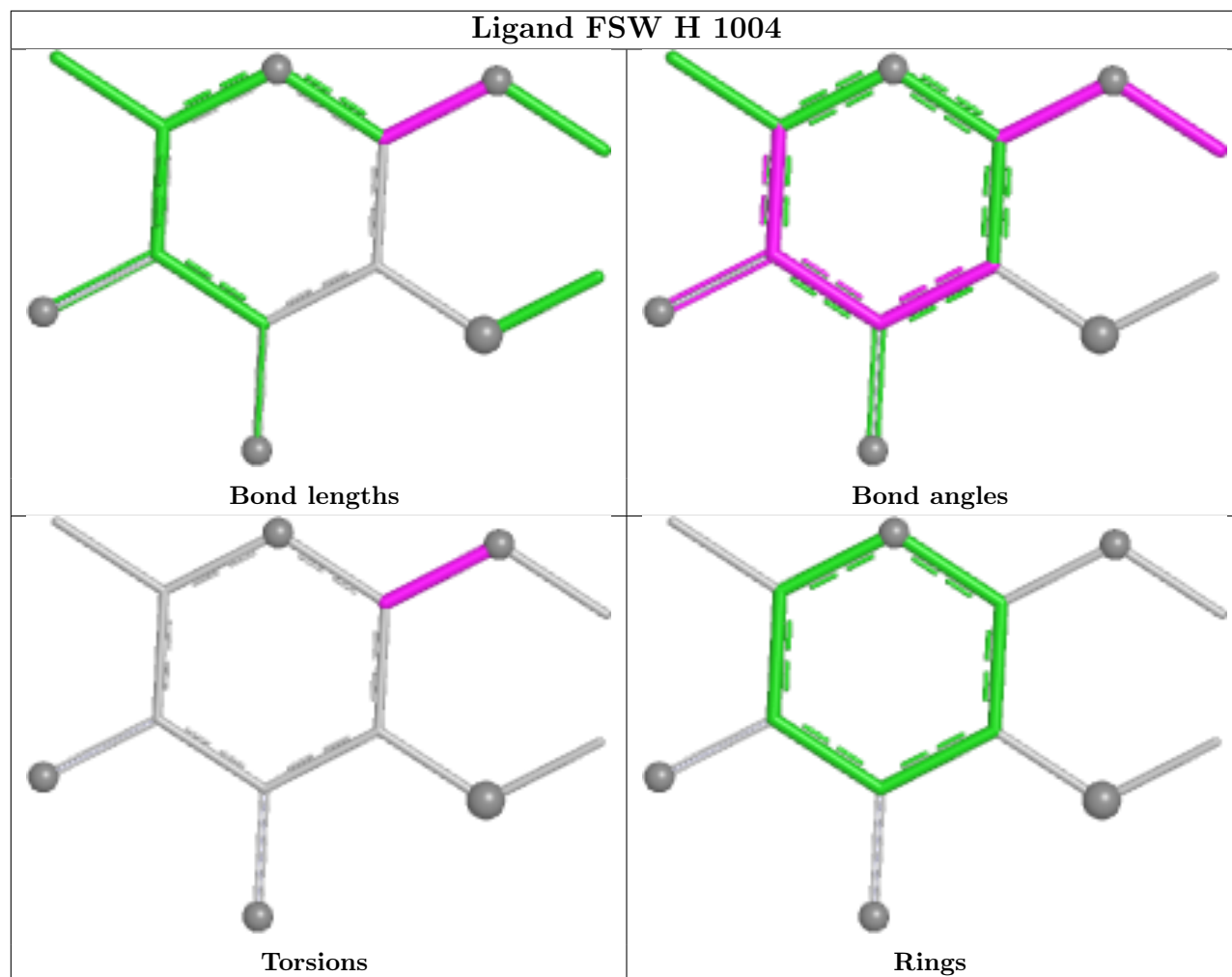


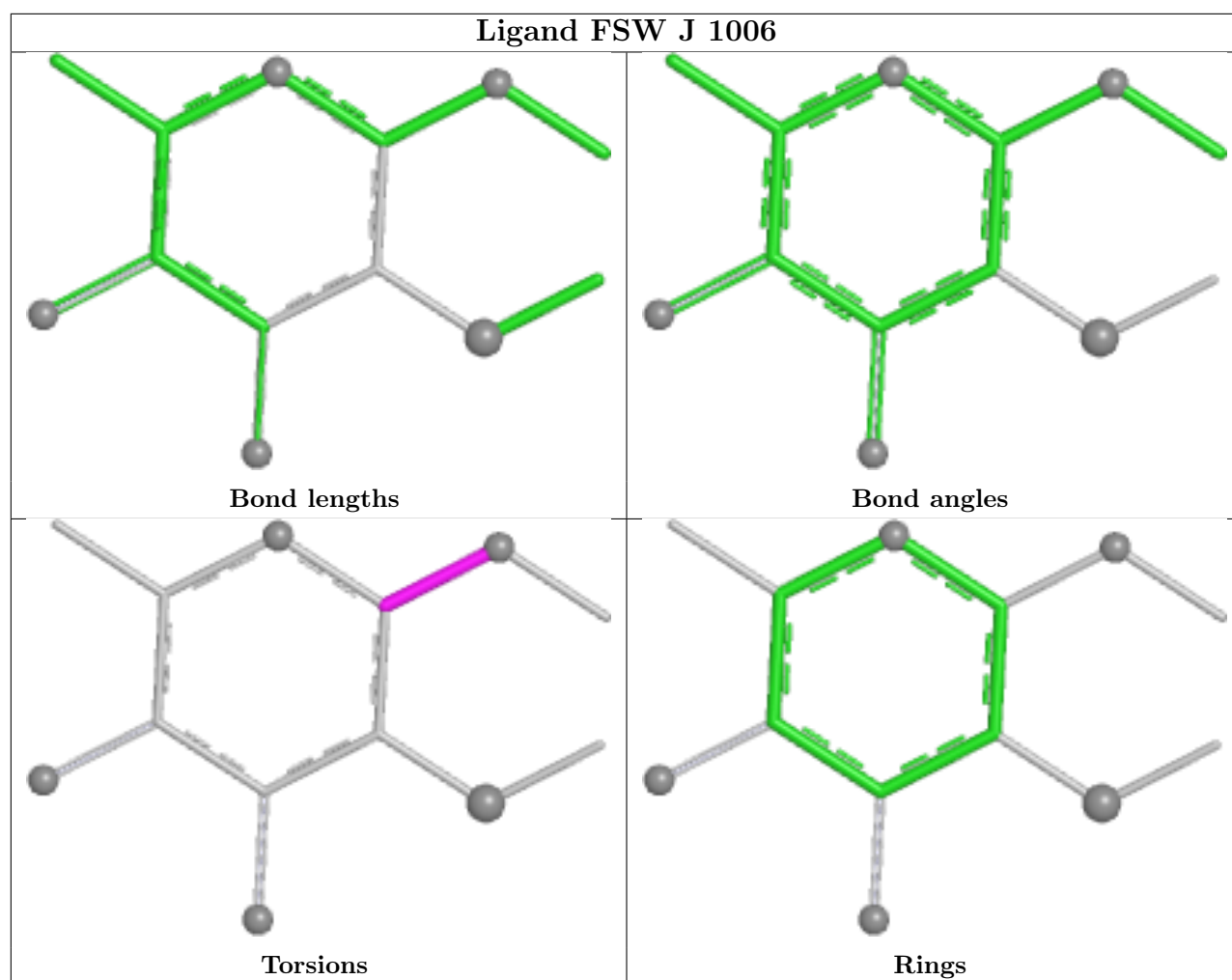


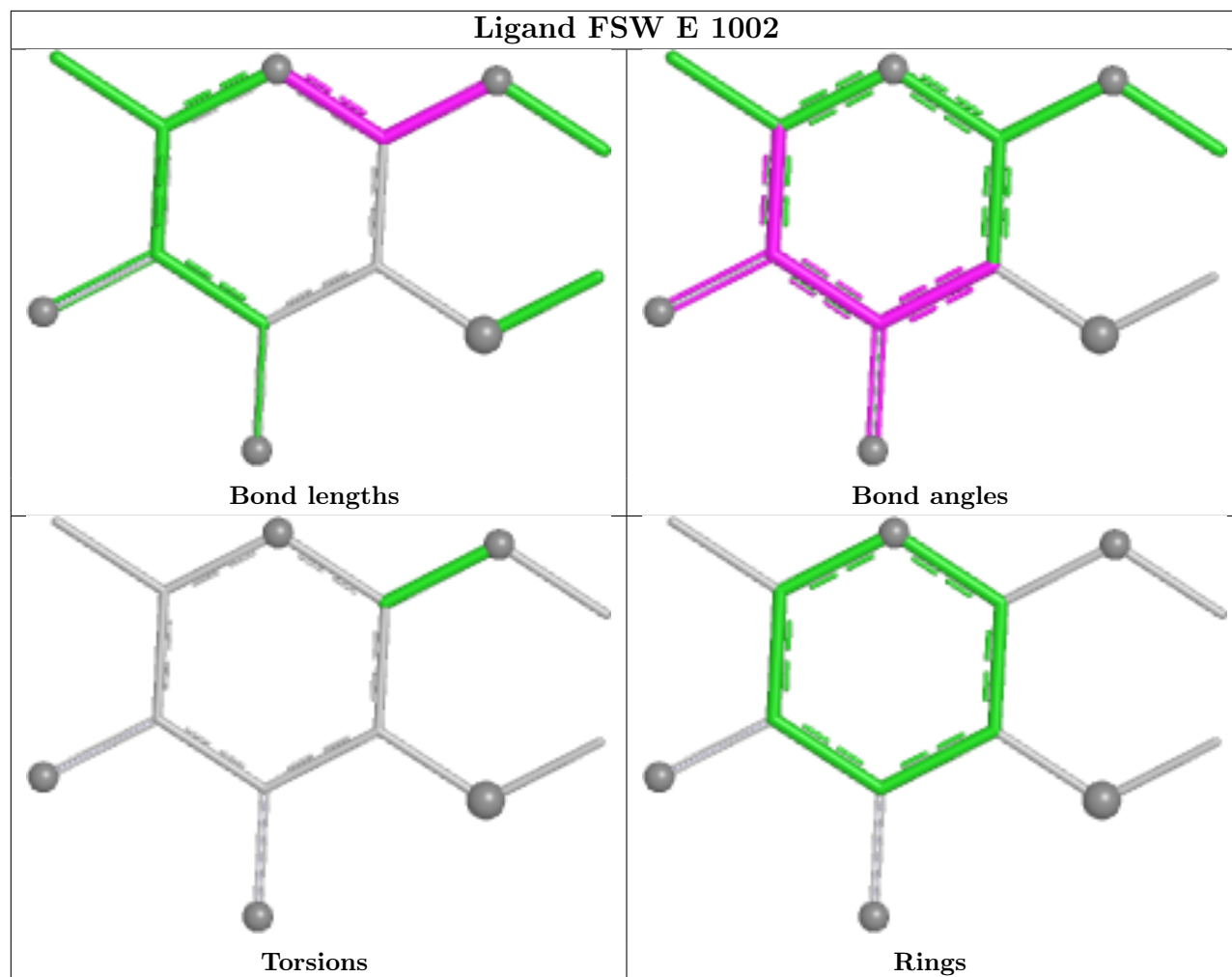


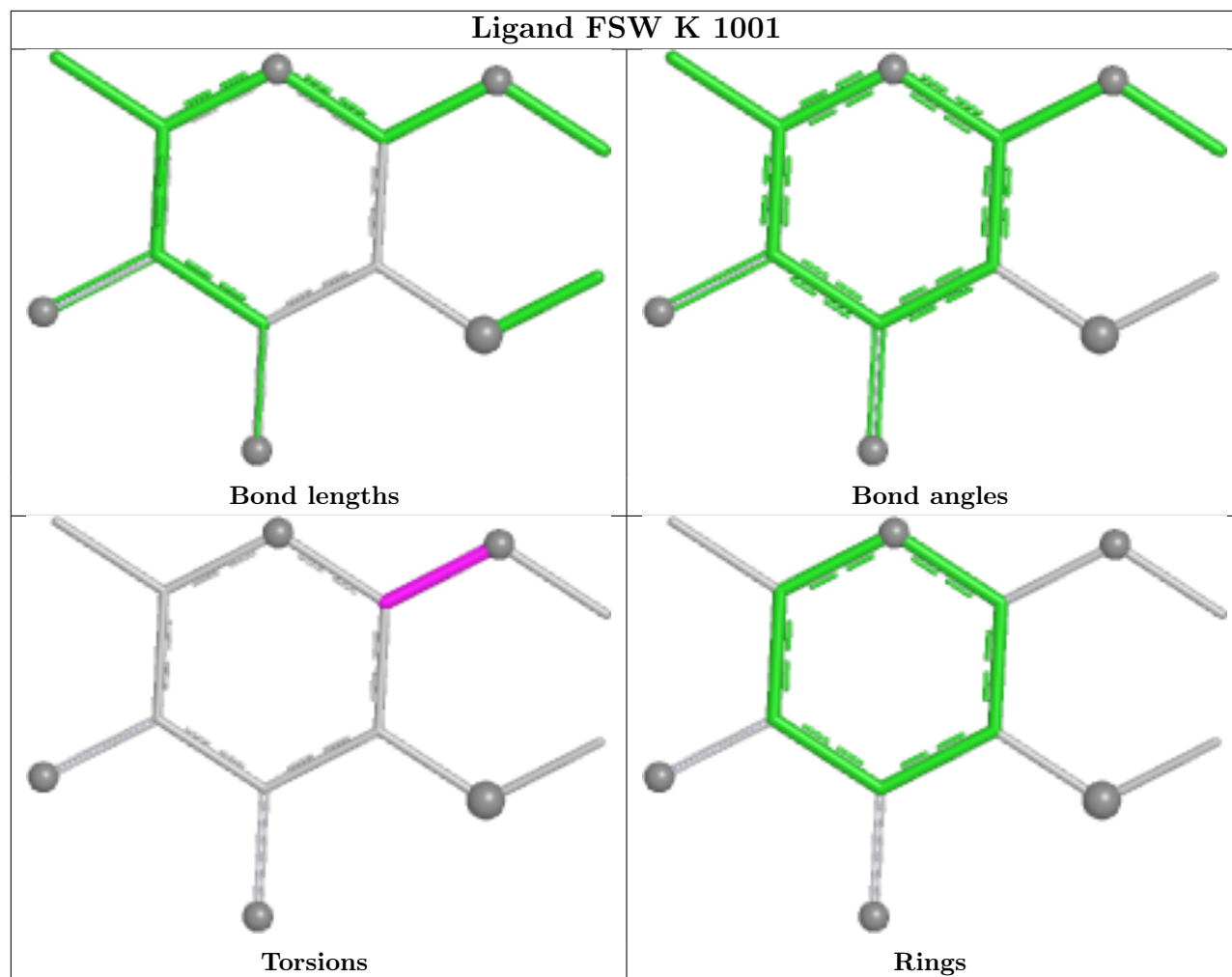


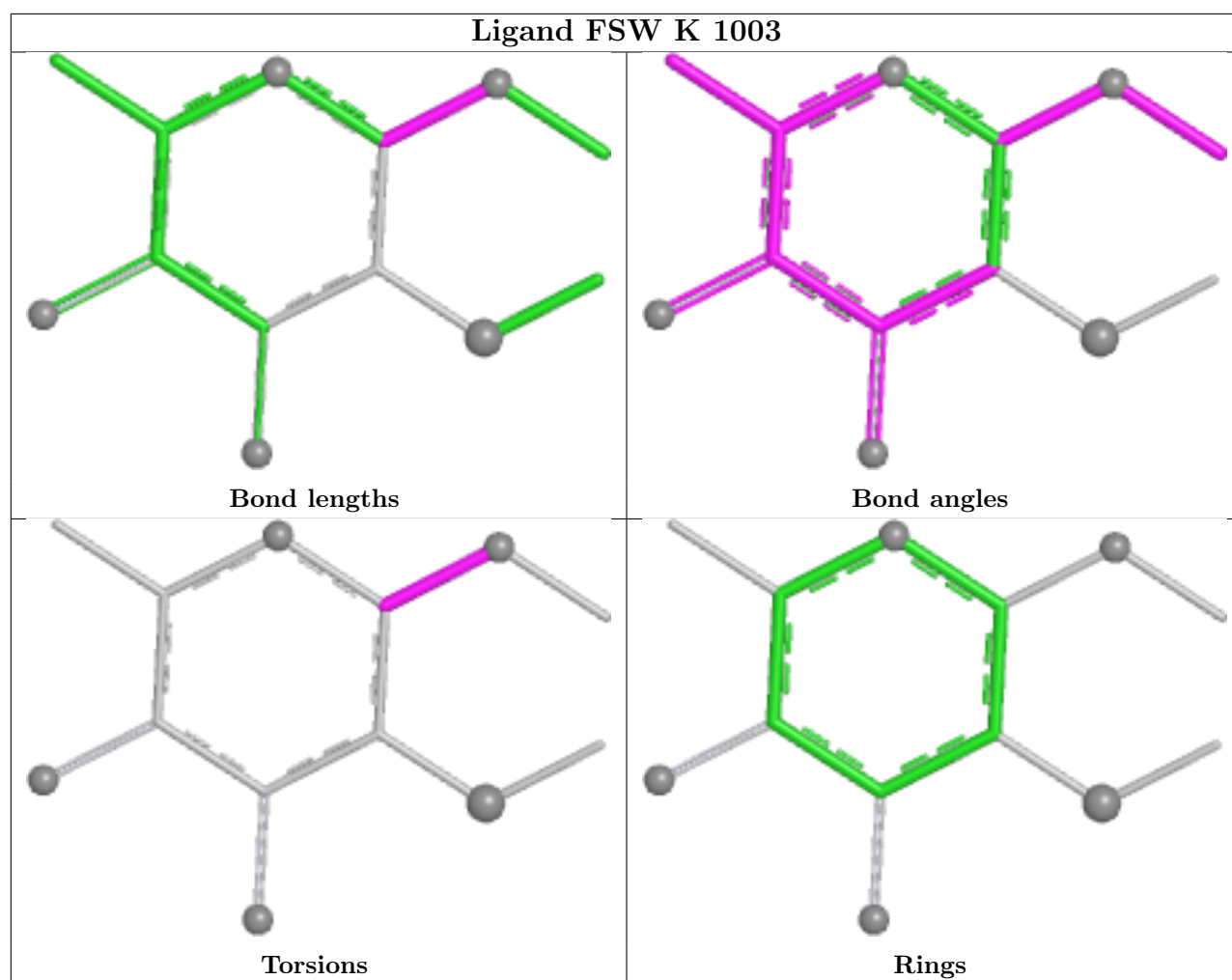


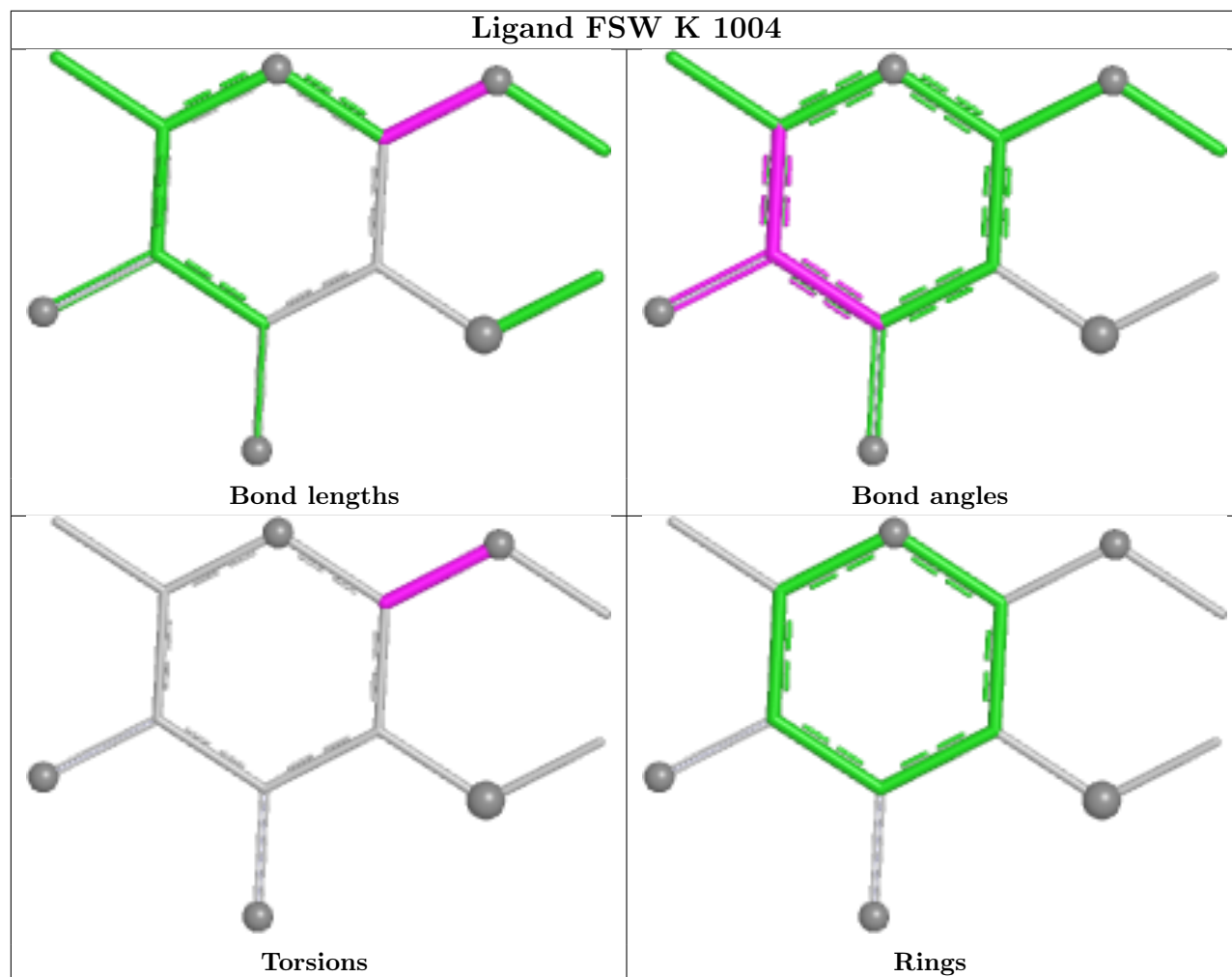


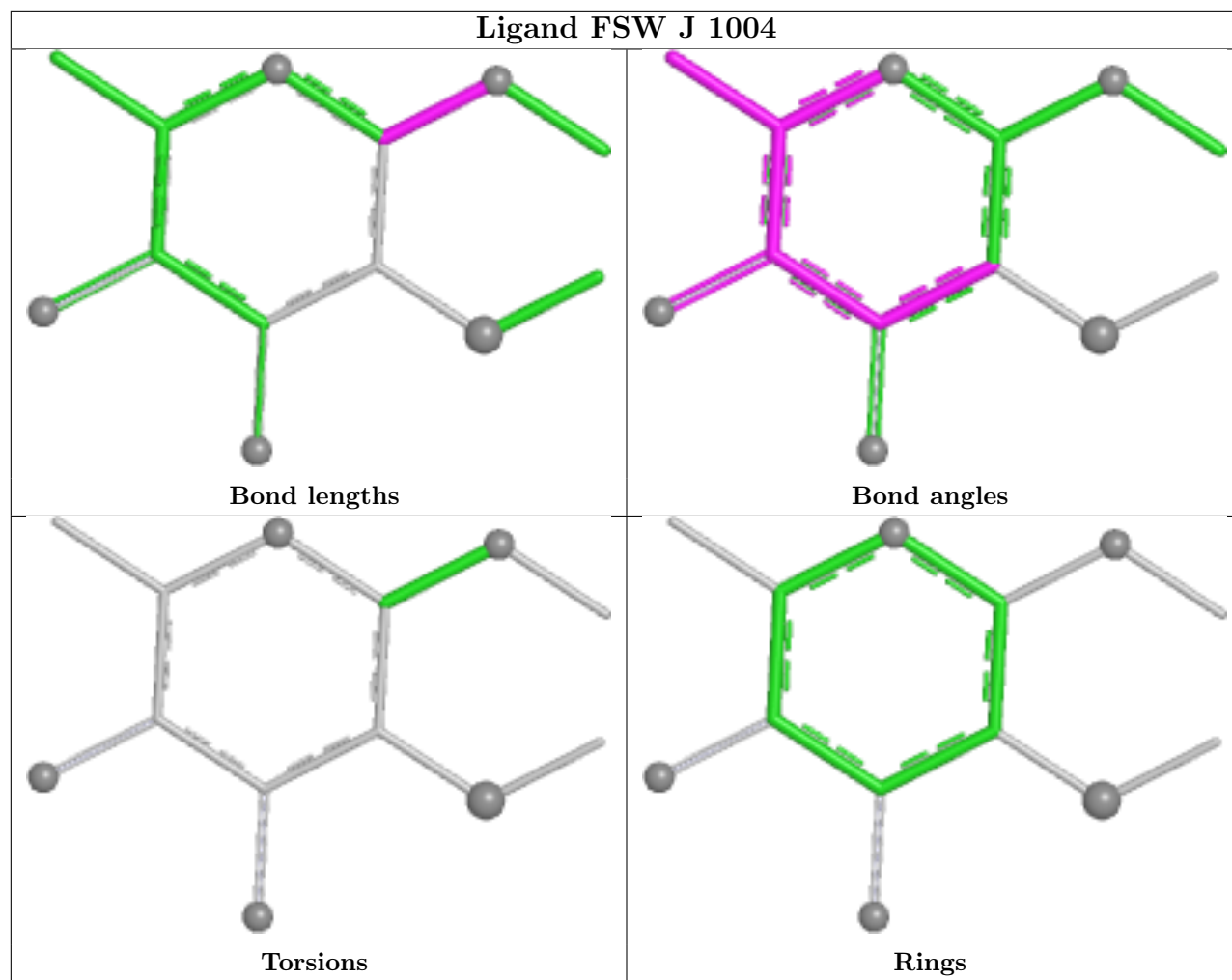


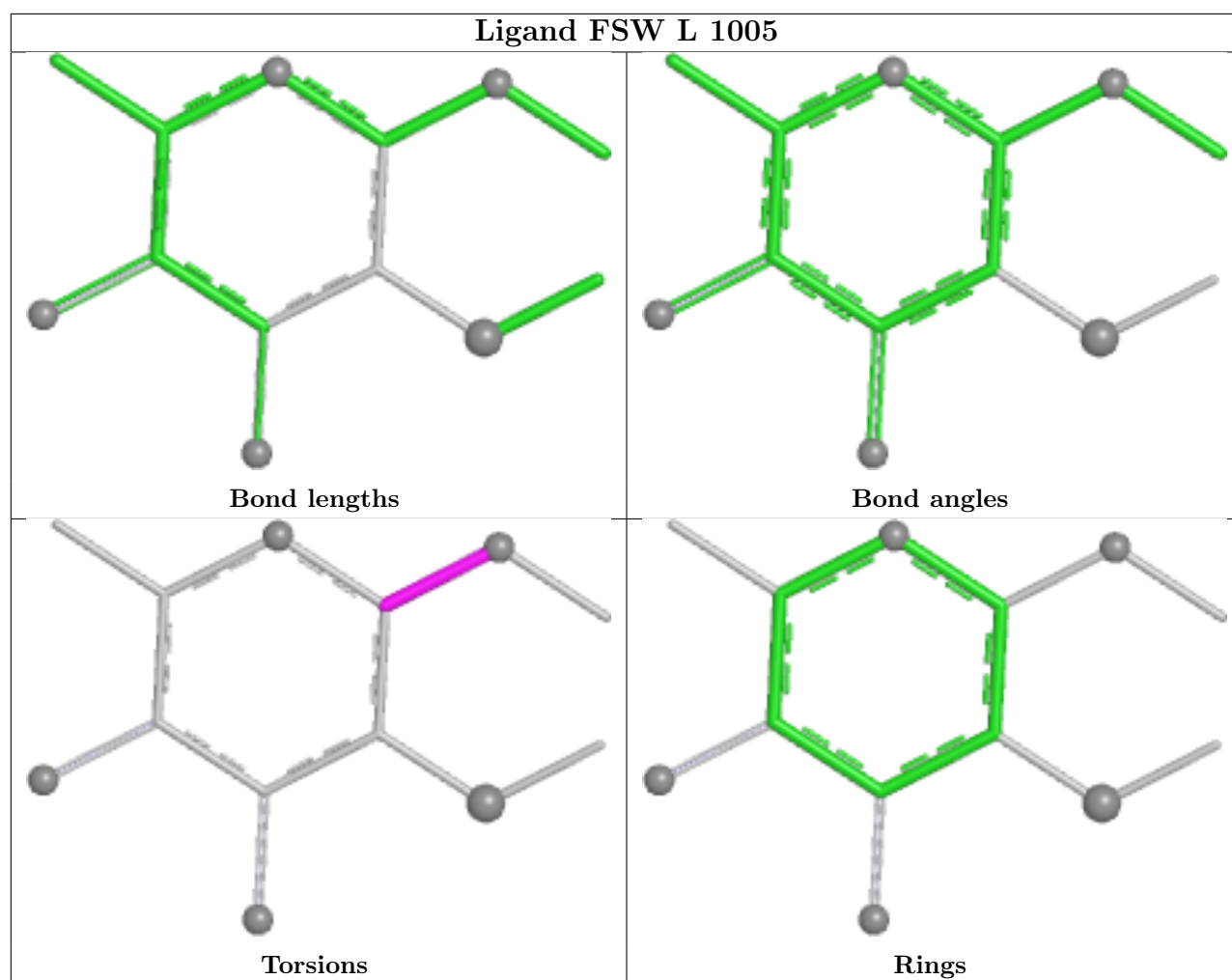


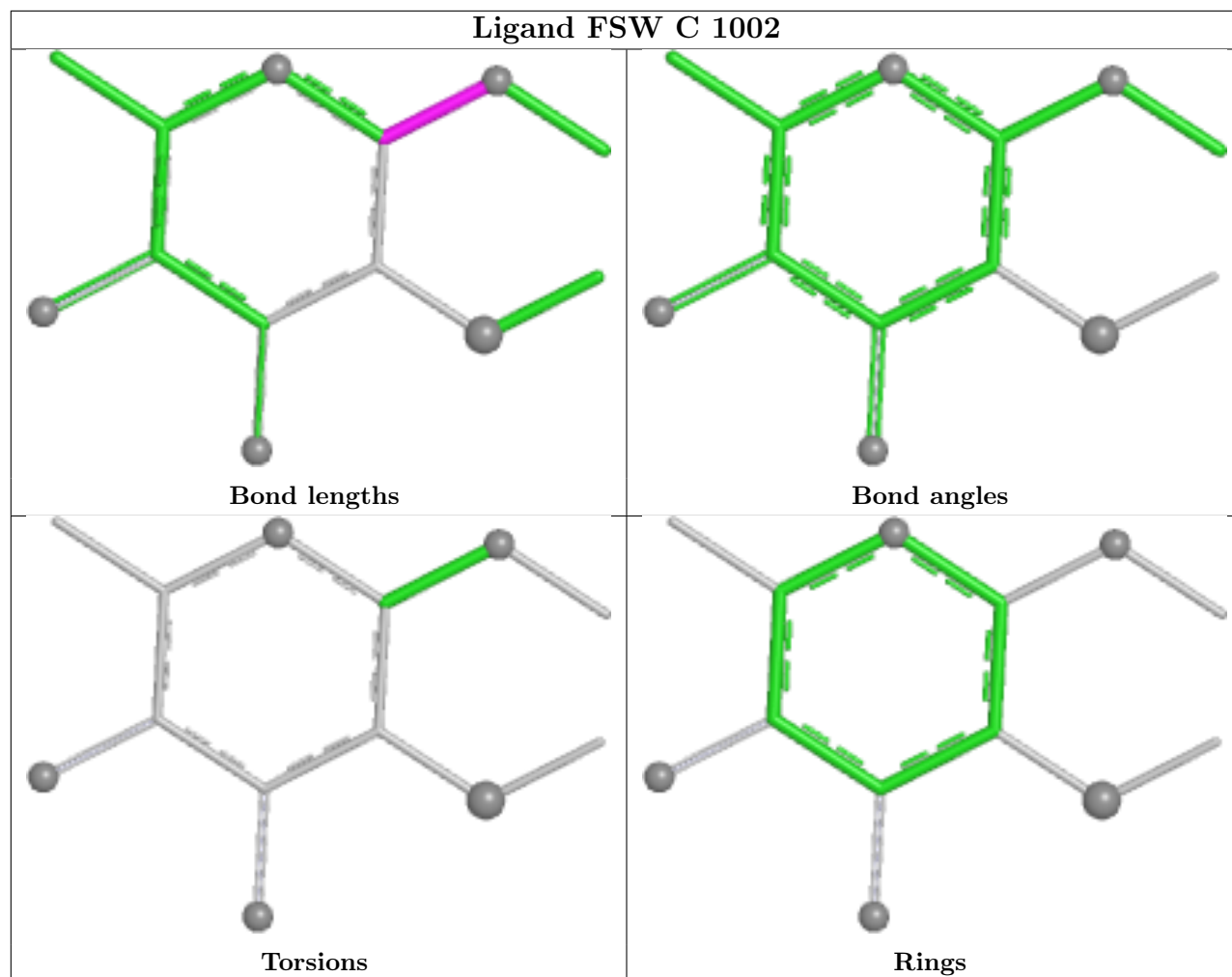


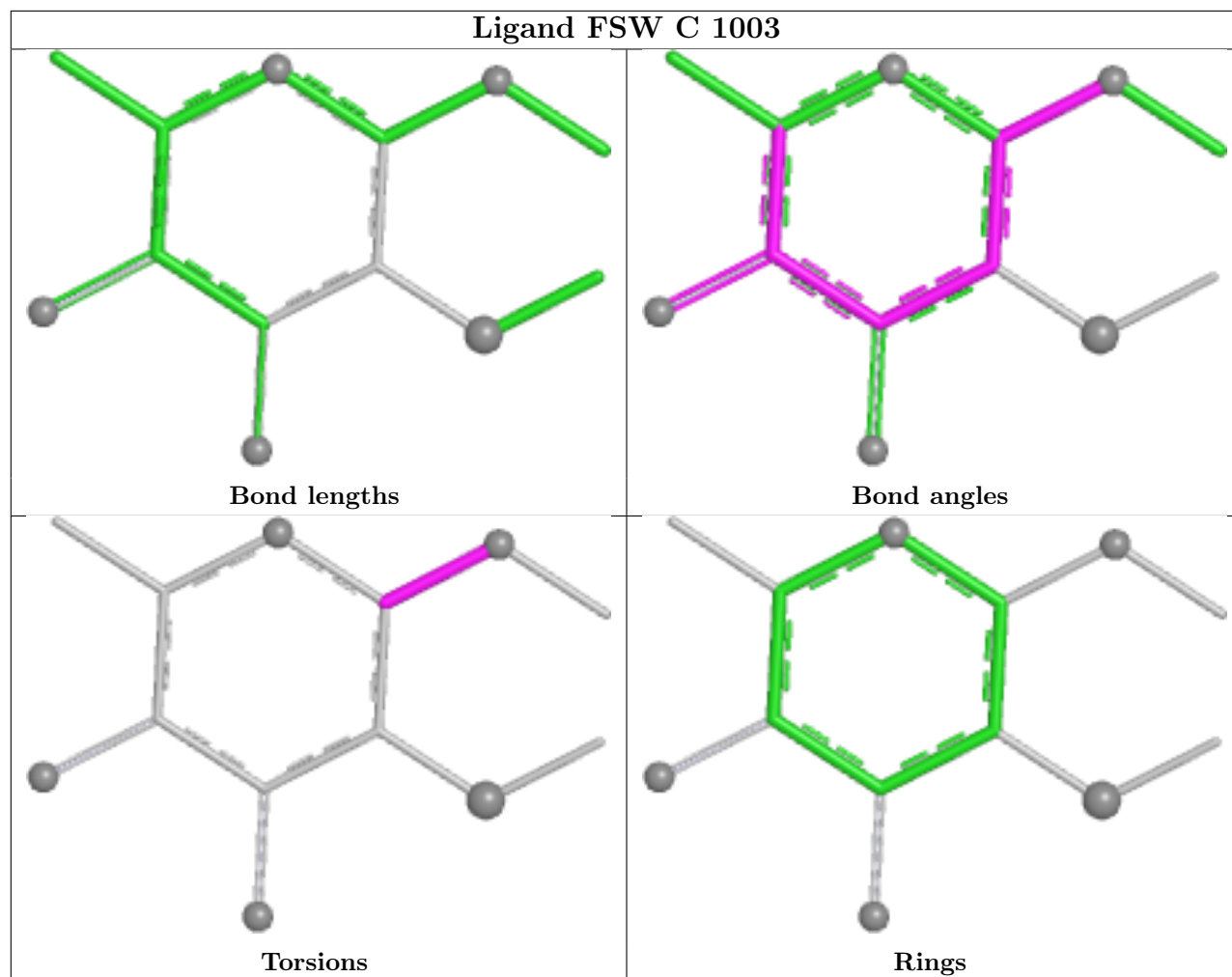


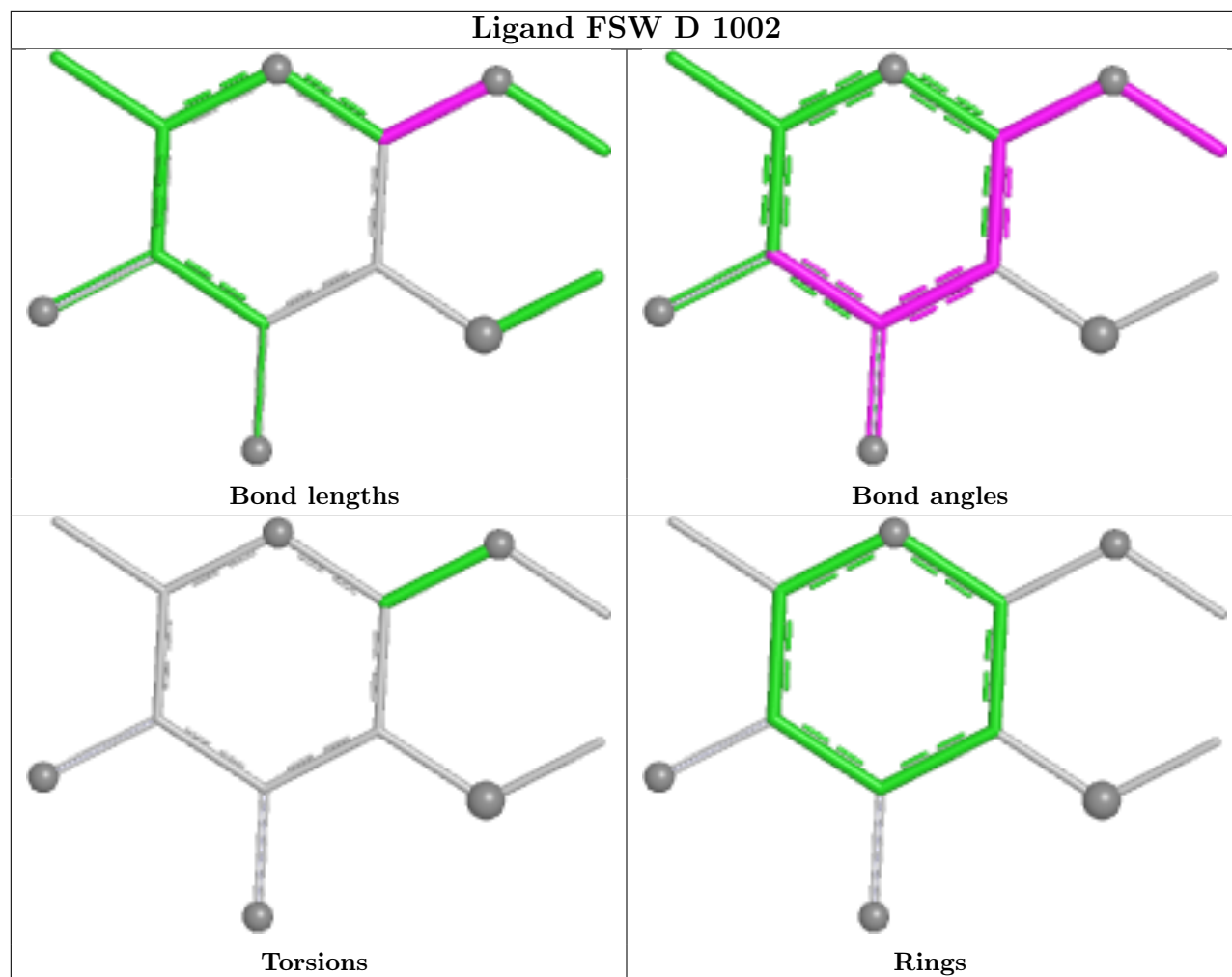


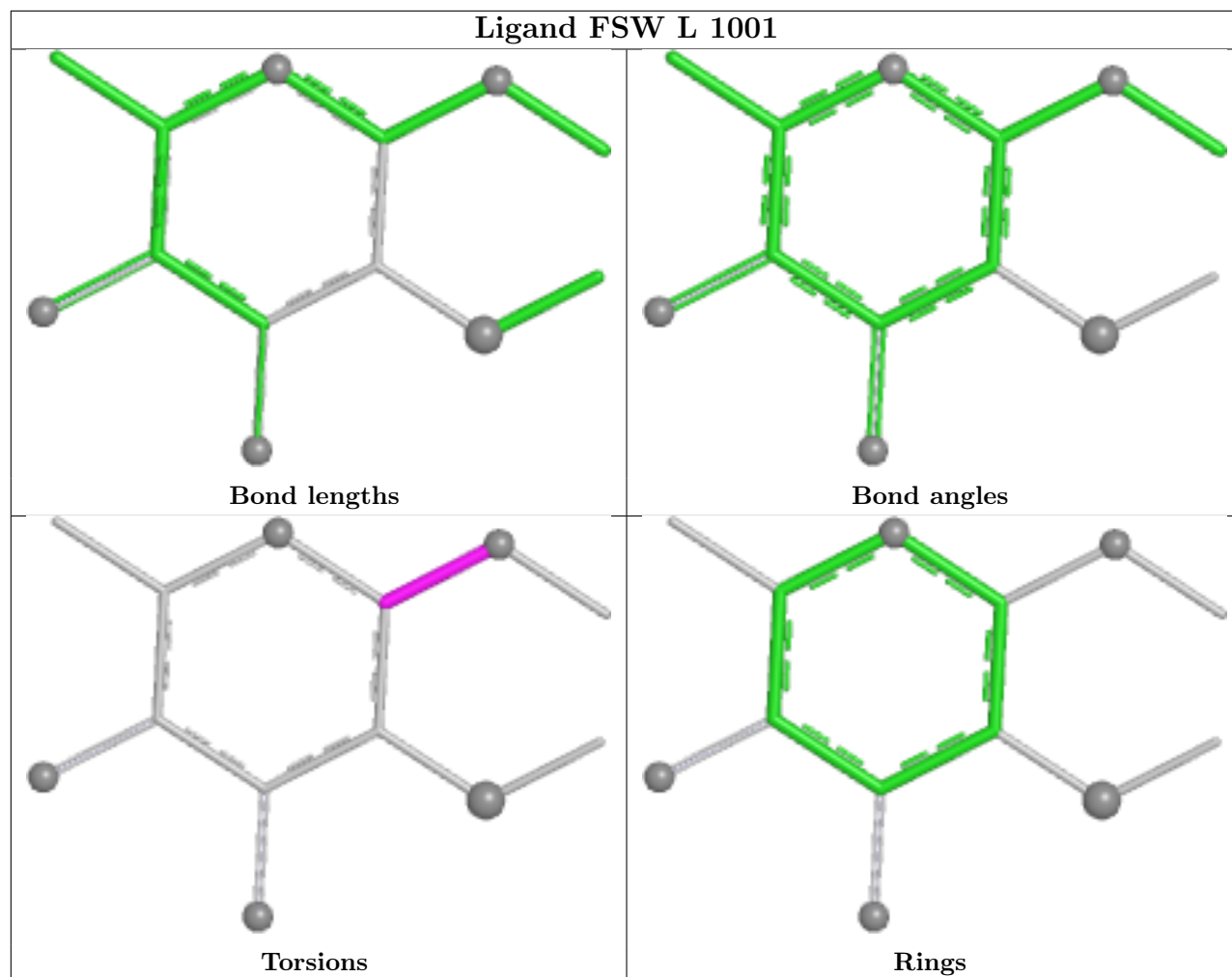


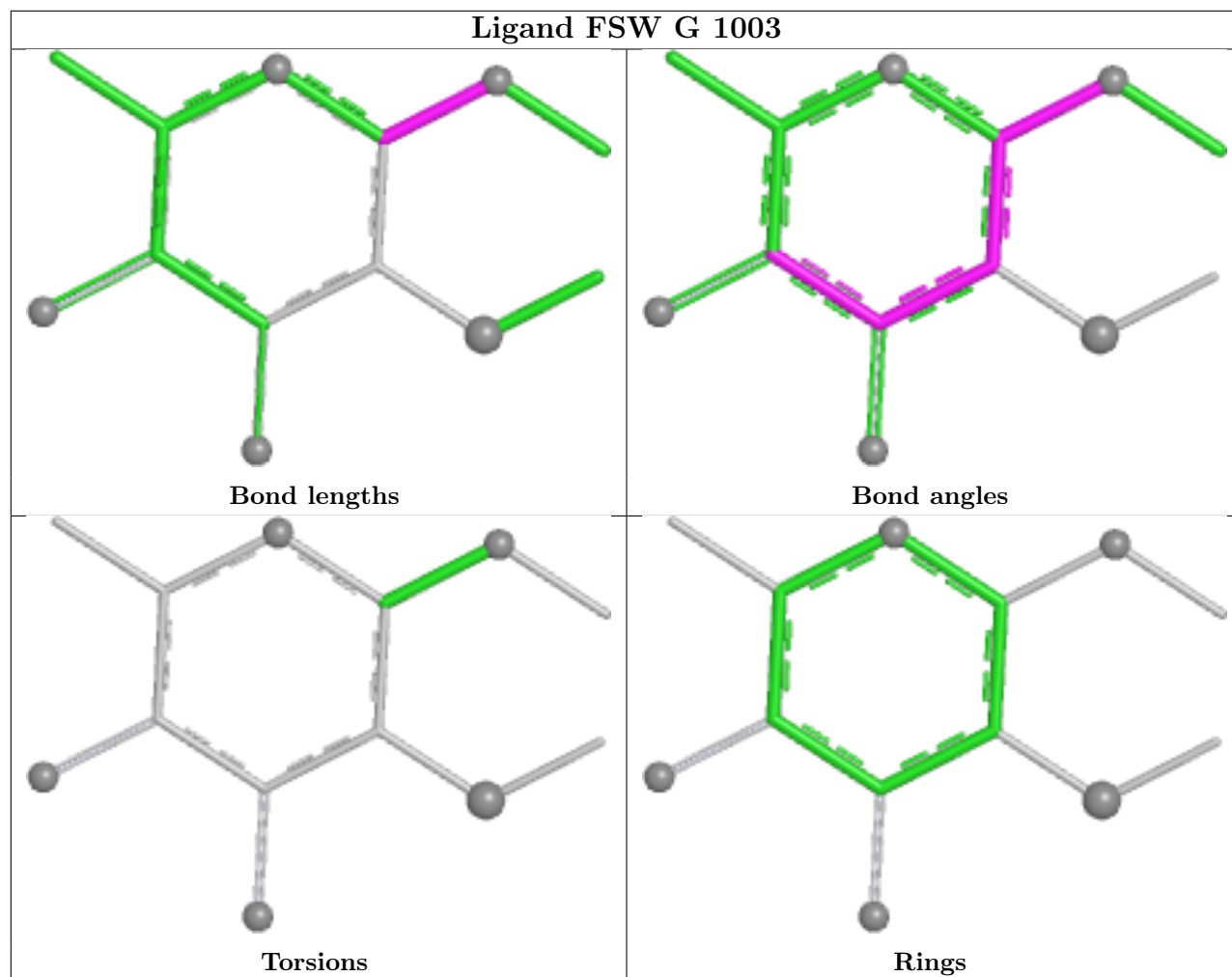


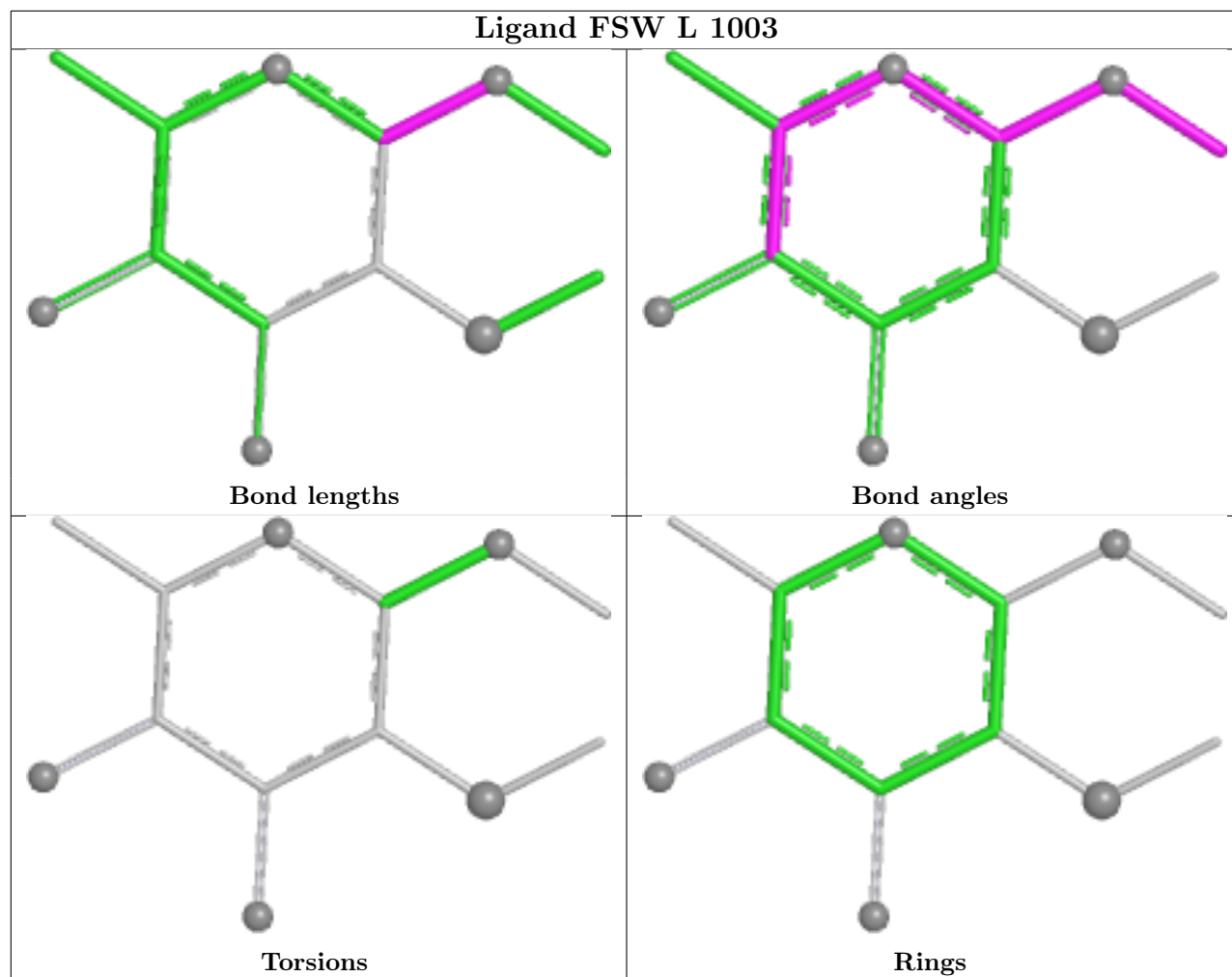


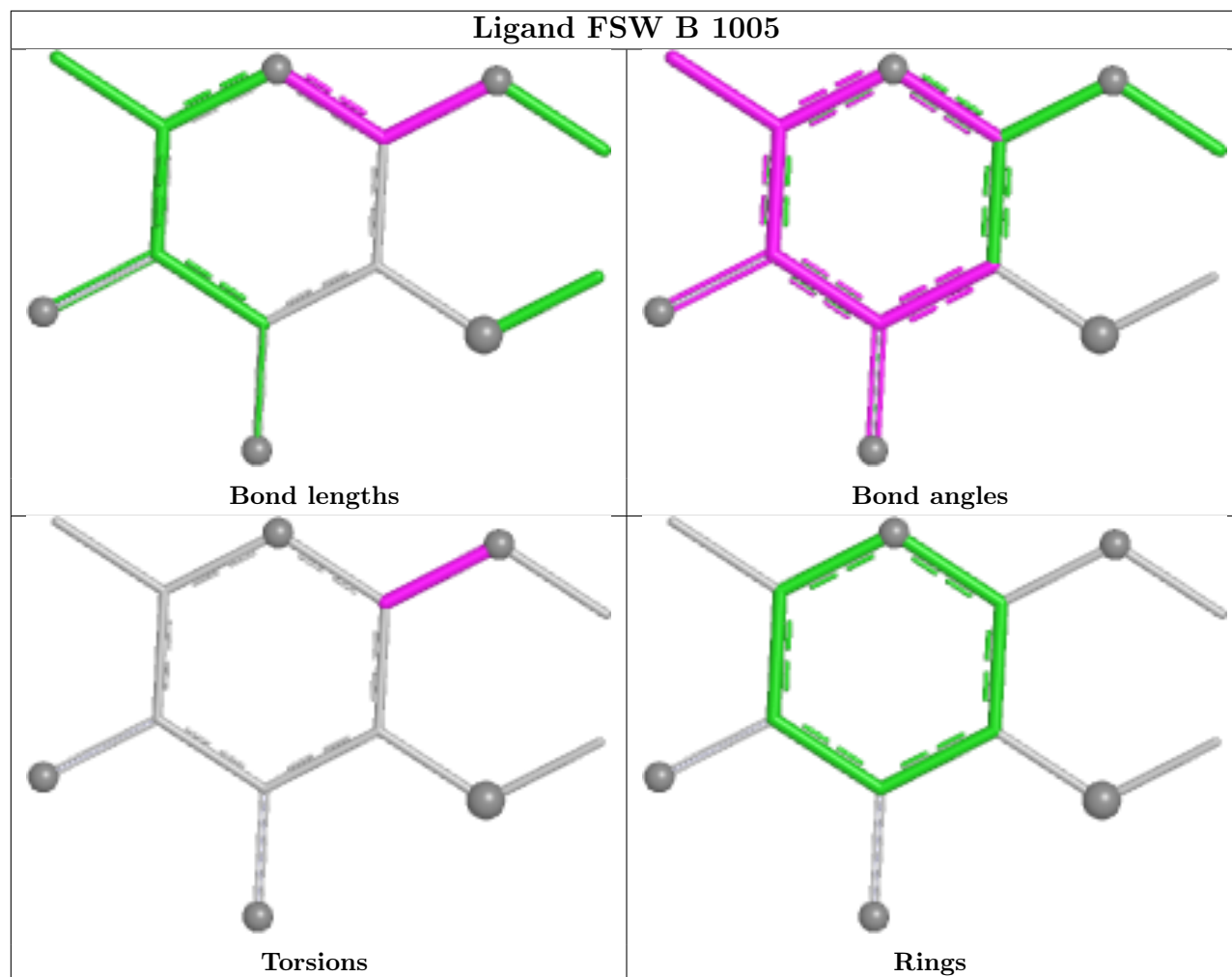


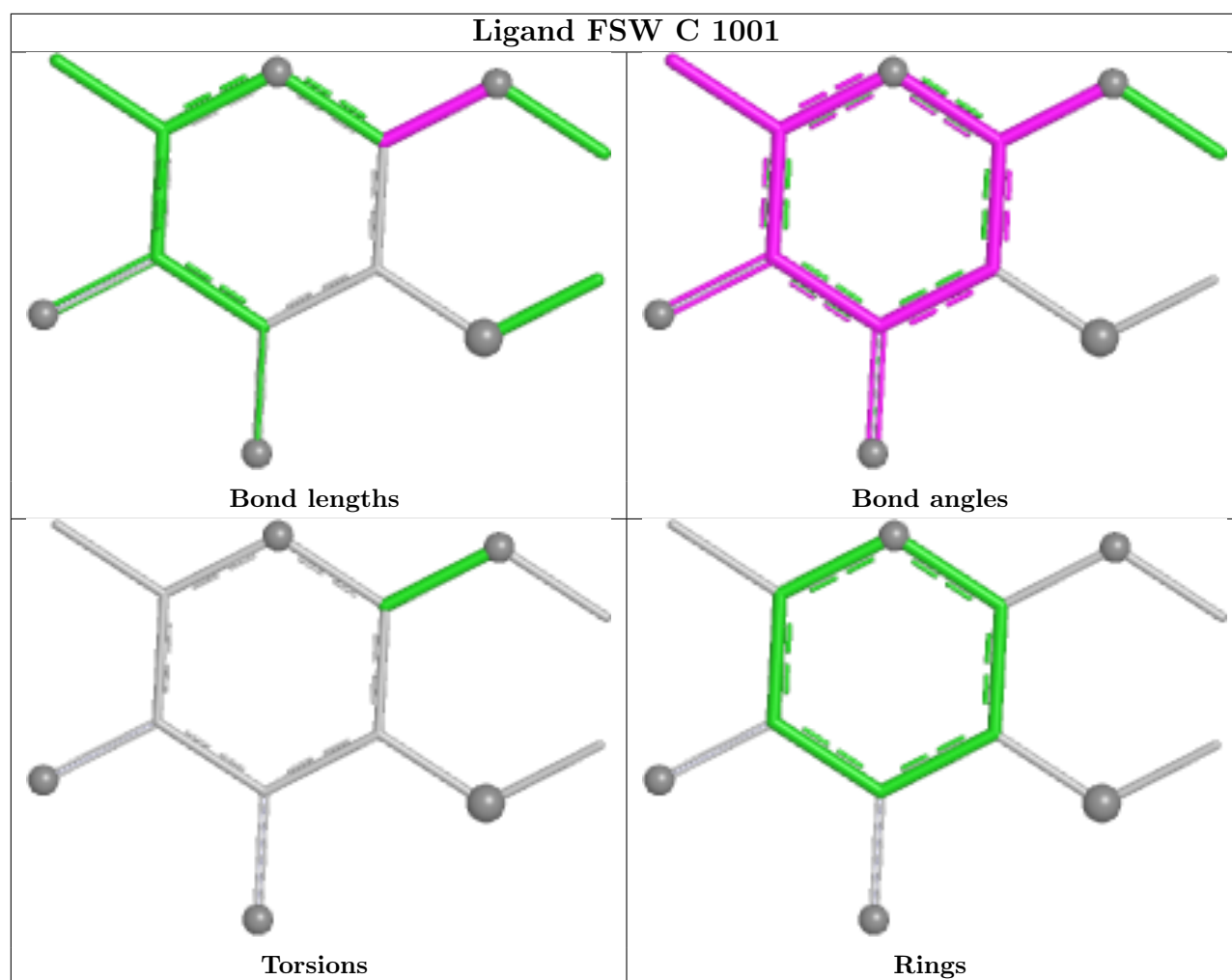


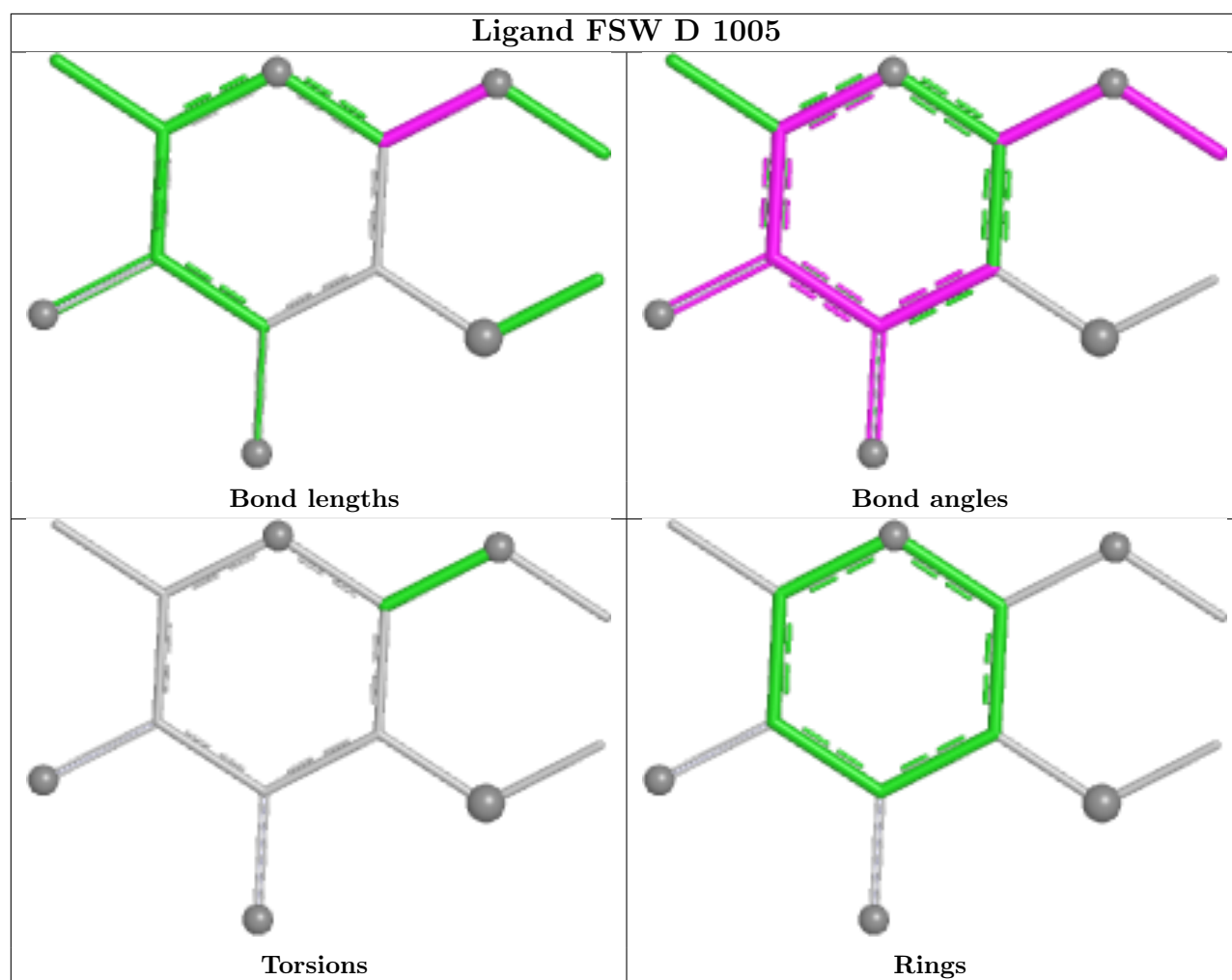


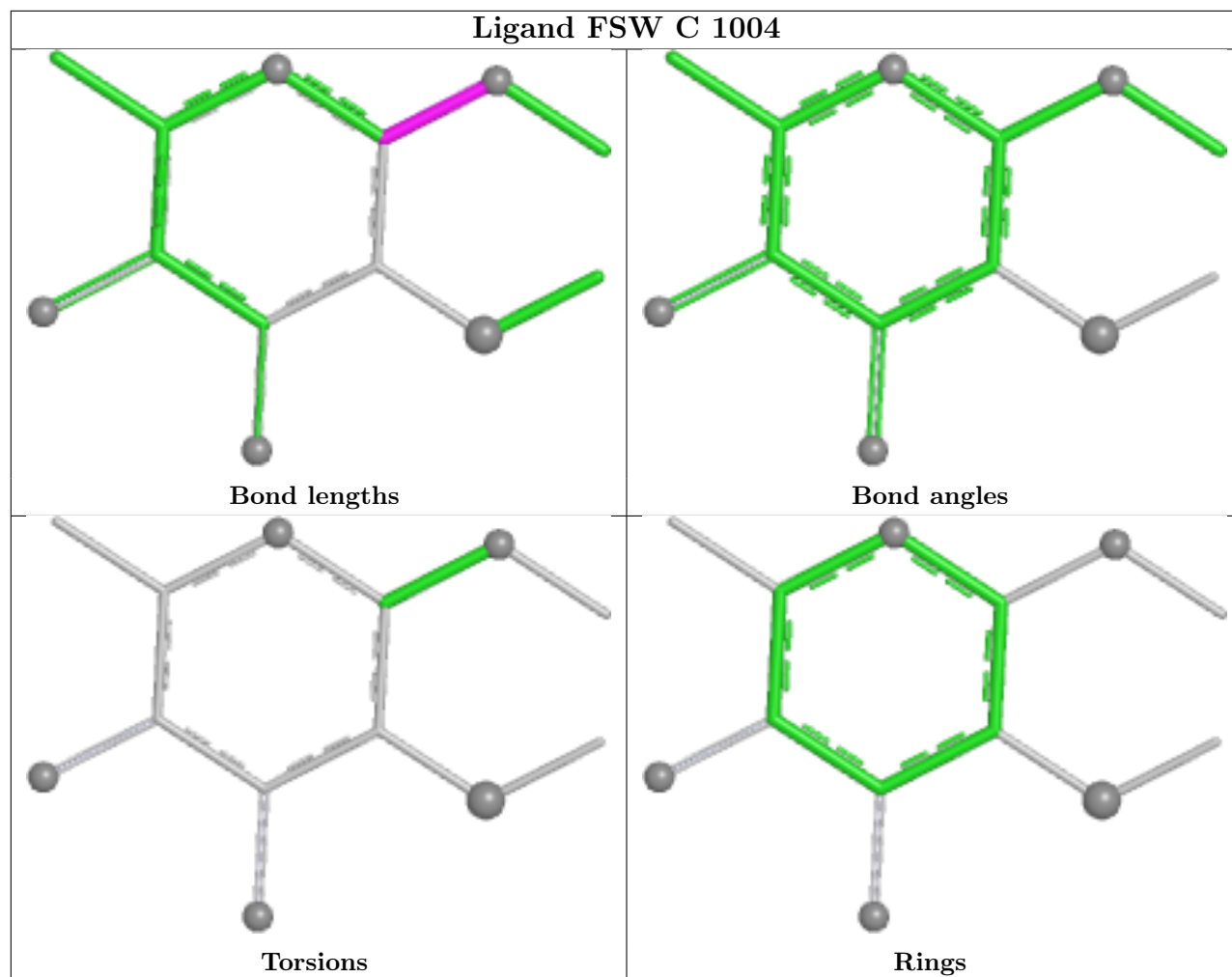


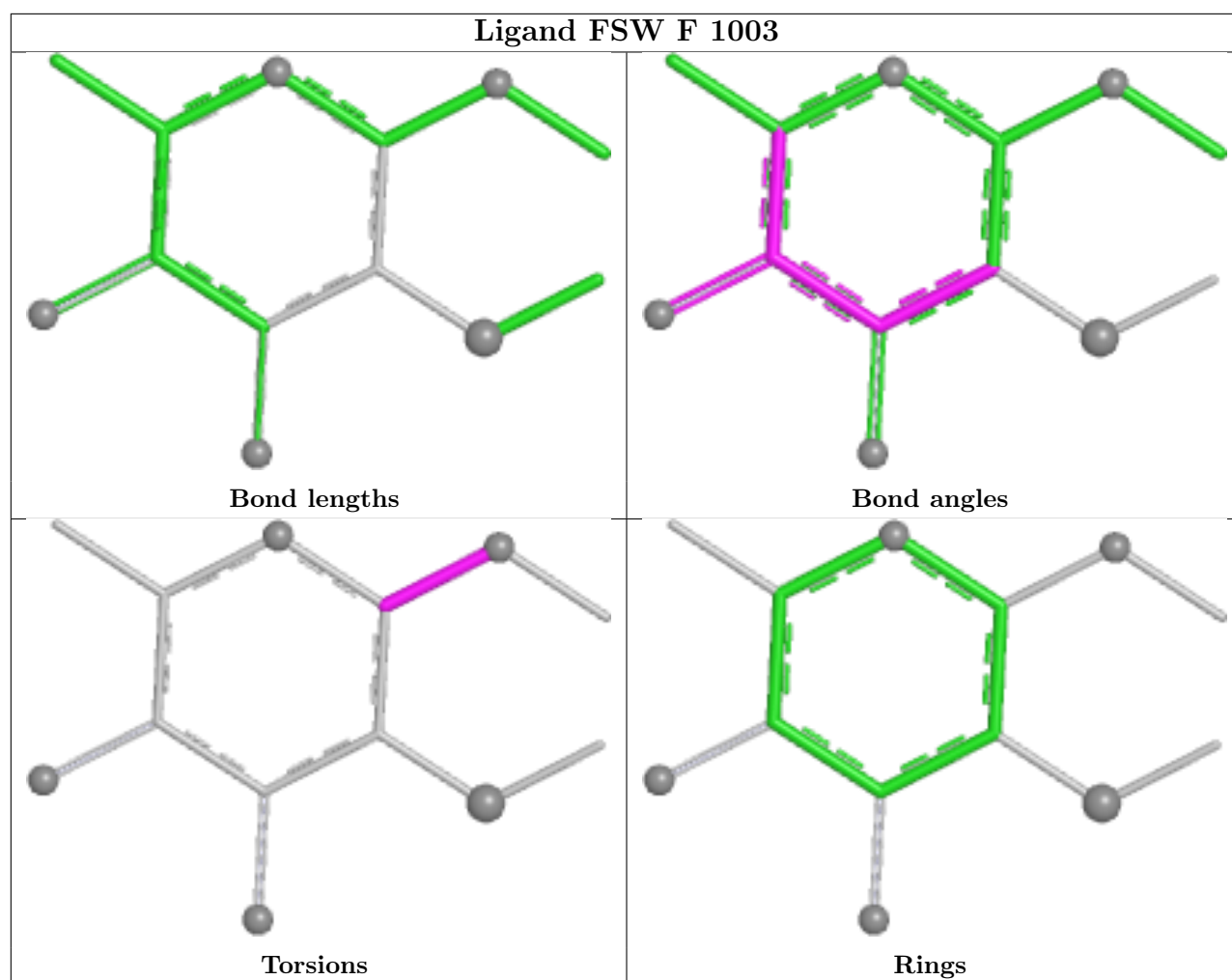


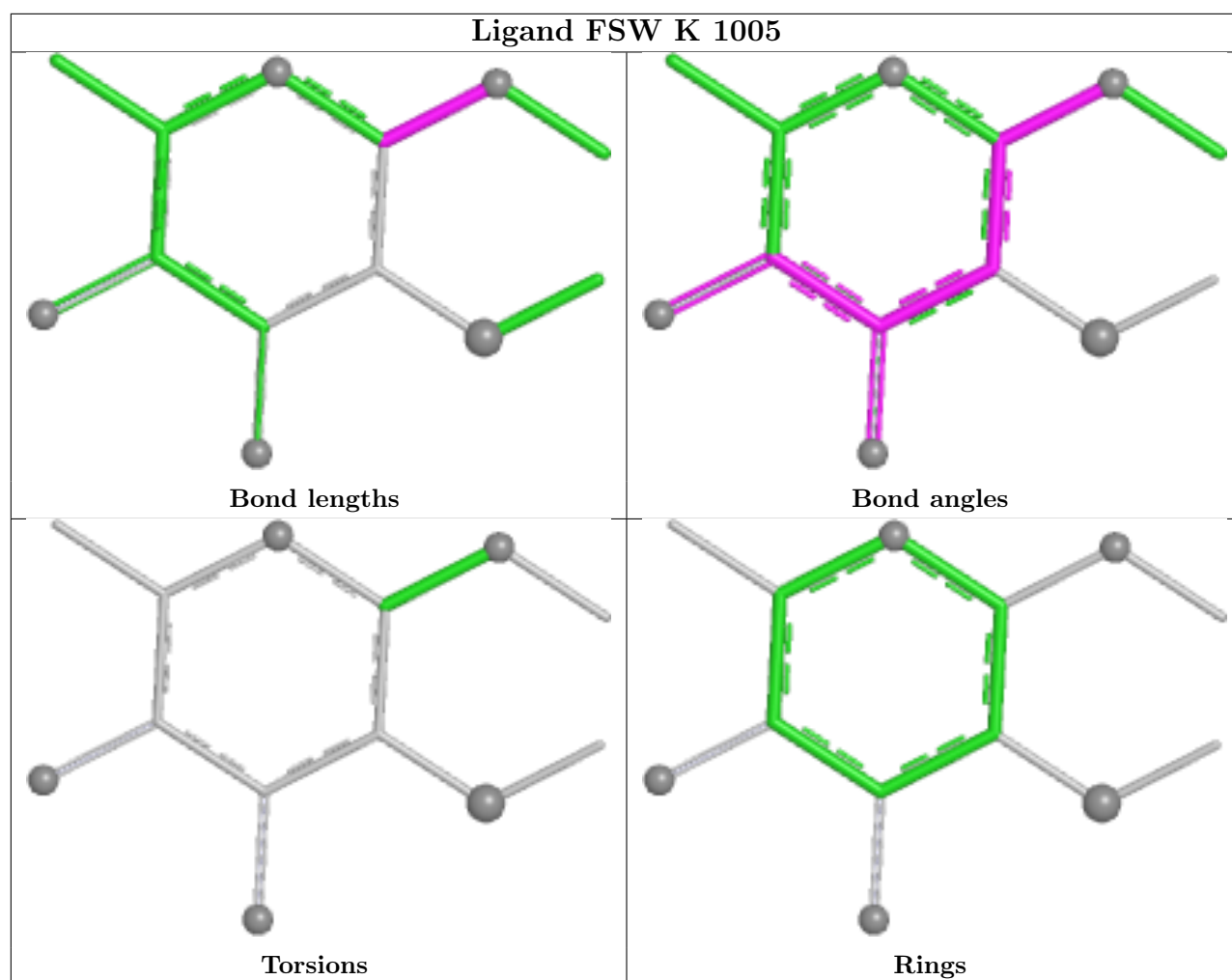


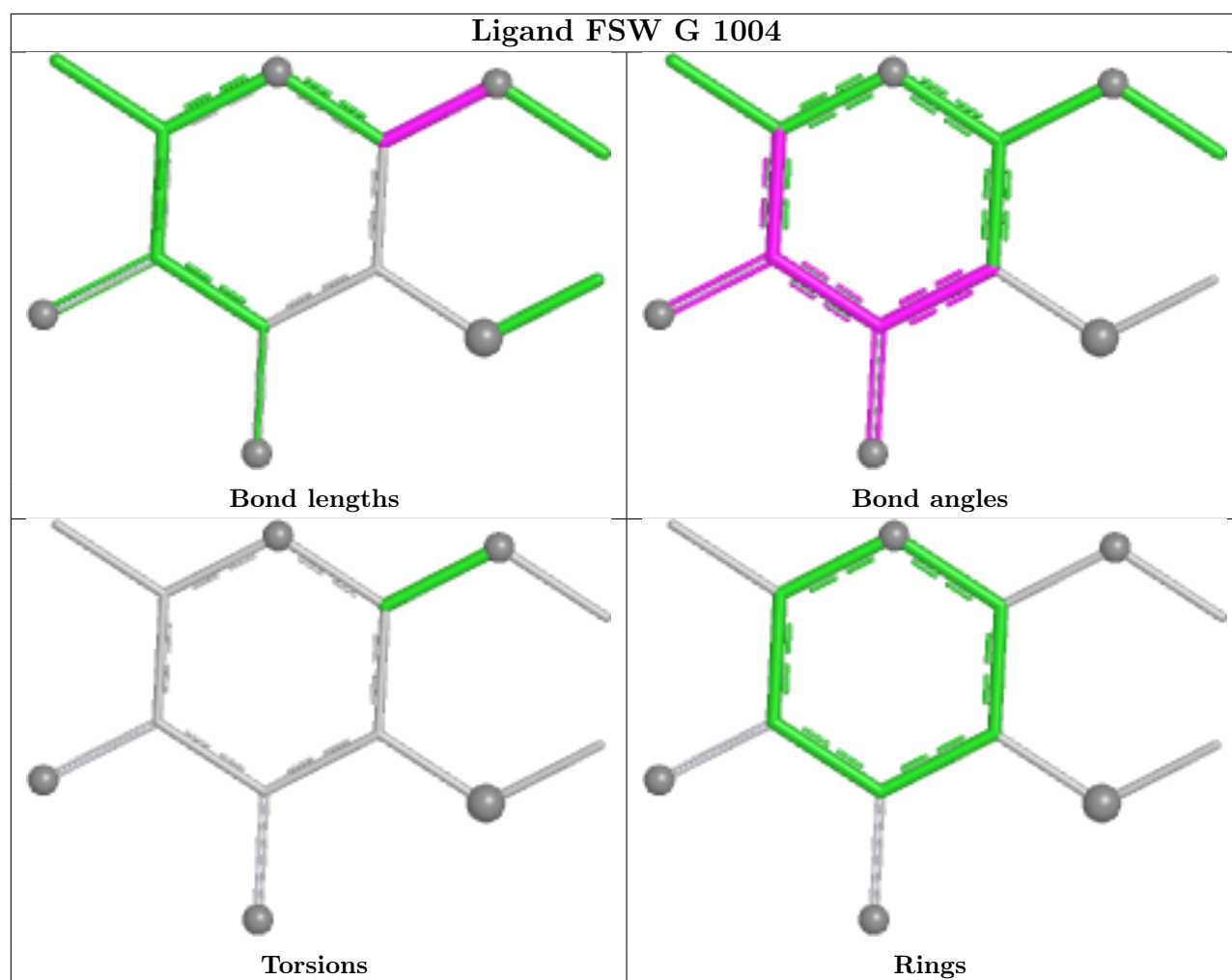


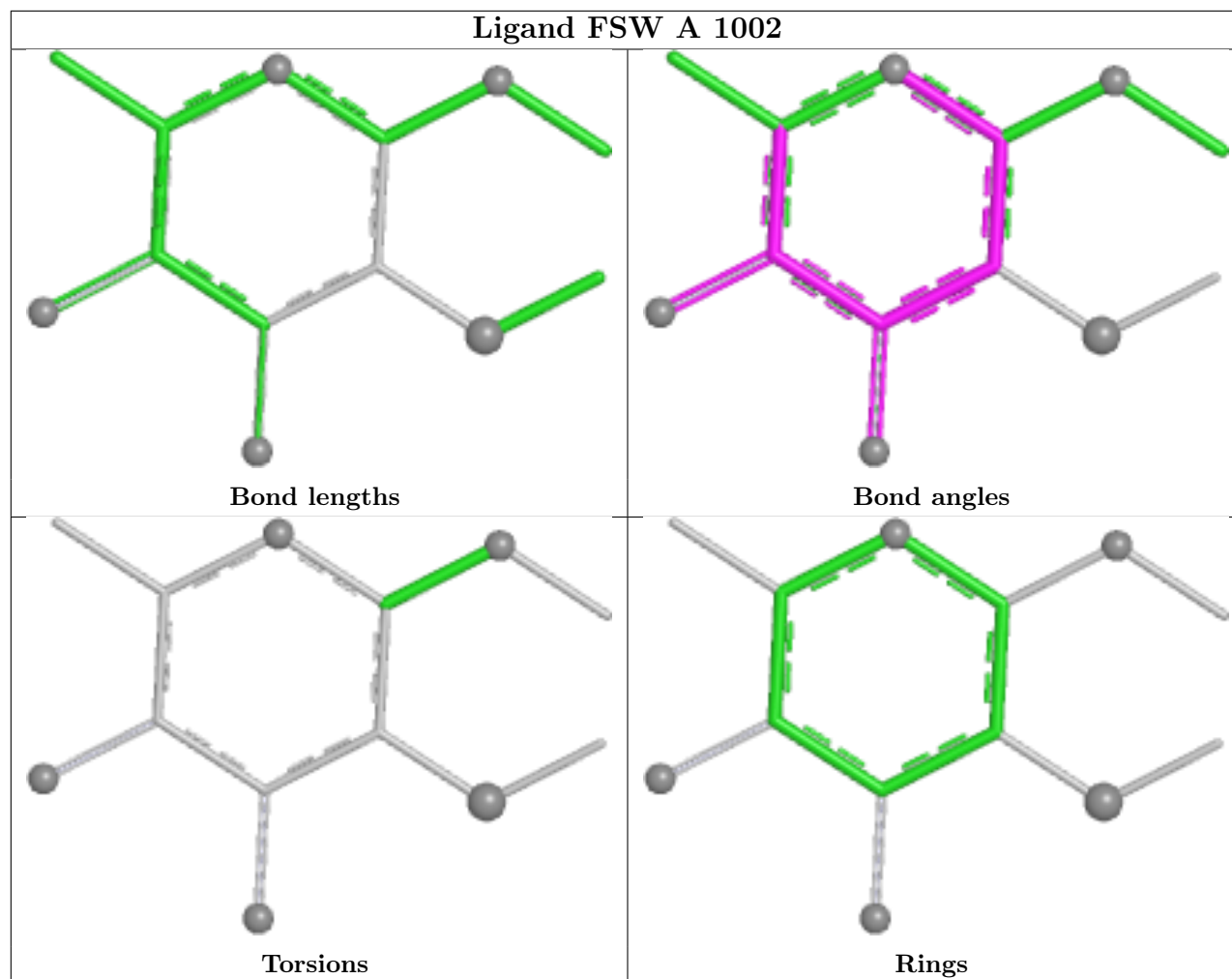












5.7 Other polymers [i](#)

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 ⓘ

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	310/311 (99%)	-0.46	1 (0%) 90 90	20, 29, 46, 79	0
1	B	310/311 (99%)	-0.34	1 (0%) 90 90	21, 31, 49, 82	0
1	C	310/311 (99%)	-0.14	1 (0%) 90 90	24, 37, 55, 80	0
1	D	310/311 (99%)	0.03	6 (1%) 66 68	23, 36, 60, 82	0
1	E	310/311 (99%)	-0.11	1 (0%) 90 90	24, 37, 59, 79	0
1	F	310/311 (99%)	0.12	3 (0%) 79 80	24, 41, 64, 84	0
1	G	310/311 (99%)	-0.05	1 (0%) 90 90	27, 40, 58, 82	0
1	H	310/311 (99%)	0.05	4 (1%) 75 76	26, 41, 63, 84	0
1	I	310/311 (99%)	0.07	3 (0%) 79 80	25, 41, 63, 112	0
1	J	310/311 (99%)	0.52	12 (3%) 43 45	29, 46, 66, 90	0
1	K	310/311 (99%)	0.91	41 (13%) 7 8	31, 55, 81, 94	0
1	L	310/311 (99%)	1.85	132 (42%) 0 0	30, 65, 101, 123	0
All	All	3720/3732 (99%)	0.20	206 (5%) 30 32	20, 40, 74, 123	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	39	LEU	6.6
1	L	27	TYR	5.8
1	L	122	ALA	5.7
1	L	195	HIS	5.4
1	L	141	TRP	5.3
1	L	174	PRO	5.3
1	L	93	GLY	5.2
1	L	87	ALA	5.2
1	L	17	ALA	4.9
1	L	86	ALA	4.8
1	L	44	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
1	L	124	GLN	4.7
1	L	123	LEU	4.7
1	L	49	ALA	4.5
1	L	88	TYR	4.5
1	L	64	ALA	4.5
1	L	118	ALA	4.4
1	L	23	HIS	4.4
1	I	195	HIS	4.3
1	L	28	PHE	4.2
1	L	269	ILE	4.0
1	L	18	VAL	4.0
1	J	195	HIS	3.9
1	L	48	THR	3.9
1	L	70	LYS	3.9
1	L	71	ASN	3.9
1	B	195	HIS	3.8
1	L	24	LEU	3.8
1	L	43	GLY	3.8
1	L	218	THR	3.7
1	L	56	ALA	3.7
1	L	173	GLY	3.7
1	L	117	LEU	3.6
1	L	125	LEU	3.6
1	L	277	ARG	3.6
1	L	298	HIS	3.6
1	L	116	PHE	3.6
1	K	70	LYS	3.6
1	K	122	ALA	3.5
1	L	304	ARG	3.5
1	L	26	VAL	3.4
1	L	25	ARG	3.4
1	L	297	ALA	3.4
1	L	119	GLY	3.4
1	L	166	TRP	3.4
1	L	307	LEU	3.4
1	K	49	ALA	3.4
1	F	195	HIS	3.4
1	L	91	GLY	3.4
1	L	308	PRO	3.4
1	L	147	LYS	3.4
1	L	145	GLY	3.3
1	L	99	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	168	TYR	3.3
1	L	279	TYR	3.3
1	L	16	ALA	3.3
1	L	89	ASP	3.3
1	L	142	ASN	3.3
1	L	69	LEU	3.3
1	L	67	LYS	3.3
1	L	65	THR	3.3
1	L	271	TRP	3.3
1	G	195	HIS	3.2
1	L	106	VAL	3.2
1	C	195	HIS	3.2
1	L	169	THR	3.1
1	L	15	ILE	3.1
1	L	37	GLU	3.1
1	L	94	TRP	3.1
1	L	96	ASN	3.1
1	L	113	GLY	3.0
1	L	146	TRP	3.0
1	L	140	MET	3.0
1	K	141	TRP	3.0
1	L	274	PRO	3.0
1	L	92	SER	2.9
1	L	104	PHE	2.9
1	L	53	ILE	2.9
1	L	224	LYS	2.9
1	L	100	ALA	2.9
1	L	115	VAL	2.9
1	K	72	ILE	2.9
1	L	46	ASN	2.9
1	L	40	TYR	2.8
1	L	171	TYR	2.8
1	L	83	LEU	2.8
1	L	294	TRP	2.8
1	L	72	ILE	2.8
1	K	195	HIS	2.8
1	K	118	ALA	2.8
1	L	50	LYS	2.8
1	D	119	GLY	2.8
1	L	128	TYR	2.8
1	K	24	LEU	2.8
1	L	126	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	127	ILE	2.8
1	K	39	LEU	2.8
1	L	176	ILE	2.7
1	L	90	SER	2.7
1	L	303	GLY	2.7
1	K	144	ASP	2.7
1	L	289	ILE	2.7
1	L	309	PRO	2.7
1	L	85	GLU	2.7
1	D	173	GLY	2.7
1	K	93	GLY	2.6
1	H	195	HIS	2.6
1	L	54	ALA	2.6
1	L	9	VAL	2.6
1	L	66	SER	2.6
1	L	302	LEU	2.6
1	J	224	LYS	2.6
1	J	145	GLY	2.6
1	A	195	HIS	2.6
1	D	195	HIS	2.6
1	K	87	ALA	2.5
1	L	288	ALA	2.5
1	K	176	ILE	2.5
1	K	69	LEU	2.5
1	L	276	LEU	2.5
1	L	98	ALA	2.5
1	K	224	LYS	2.5
1	L	101	GLY	2.5
1	K	201	GLU	2.5
1	L	51	ASN	2.5
1	L	305	ARG	2.5
1	K	174	PRO	2.5
1	L	228	TYR	2.4
1	E	50	LYS	2.4
1	H	200	LYS	2.4
1	L	219	ASN	2.4
1	L	47	GLY	2.4
1	L	120	THR	2.4
1	L	164	THR	2.4
1	K	305	ARG	2.4
1	L	227	ILE	2.4
1	L	22	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	75	TYR	2.3
1	L	95	TYR	2.3
1	L	293	THR	2.3
1	L	38	SER	2.3
1	L	226	SER	2.3
1	L	84	GLN	2.3
1	D	91	GLY	2.3
1	L	143	GLY	2.3
1	L	63	ALA	2.3
1	K	18	VAL	2.3
1	K	147	LYS	2.3
1	F	171	TYR	2.3
1	J	305	ARG	2.3
1	J	23	HIS	2.3
1	L	311	GLU	2.3
1	L	161	ILE	2.3
1	K	143	GLY	2.3
1	K	27	TYR	2.3
1	L	75	TYR	2.3
1	J	91	GLY	2.2
1	I	201	GLU	2.2
1	K	45	ALA	2.2
1	K	120	THR	2.2
1	K	94	TRP	2.2
1	J	200	LYS	2.2
1	L	19	ASN	2.2
1	L	21	THR	2.2
1	L	270	SER	2.2
1	D	143	GLY	2.2
1	J	93	GLY	2.2
1	L	273	GLY	2.2
1	L	295	GLY	2.2
1	K	64	ALA	2.2
1	L	300	SER	2.2
1	K	171	TYR	2.2
1	K	99	LEU	2.2
1	K	9	VAL	2.2
1	L	97	GLY	2.2
1	K	227	ILE	2.1
1	L	55	LYS	2.1
1	K	298	HIS	2.1
1	L	165	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	42	SER	2.1
1	L	58	LEU	2.1
1	L	112	ILE	2.1
1	K	115	VAL	2.1
1	L	74	VAL	2.1
1	J	141	TRP	2.1
1	K	28	PHE	2.1
1	K	44	TRP	2.1
1	K	47	GLY	2.1
1	K	173	GLY	2.1
1	J	122	ALA	2.1
1	L	306	ALA	2.1
1	L	275	GLU	2.1
1	I	173	GLY	2.1
1	J	47	GLY	2.1
1	L	223	GLY	2.1
1	K	166	TRP	2.1
1	J	70	LYS	2.0
1	H	175	SER	2.0
1	K	86	ALA	2.0
1	L	144	ASP	2.0
1	K	40	TYR	2.0
1	H	201	GLU	2.0
1	L	45	ALA	2.0
1	F	121	ASN	2.0
1	K	71	ASN	2.0
1	D	200	LYS	2.0

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
2	FSW	L	1001	13/13	0.60	0.26	88,110,127,130	0
2	FSW	K	1002	13/13	0.77	0.25	78,91,109,185	0
2	FSW	L	1002	13/13	0.79	0.28	105,123,133,136	0
2	FSW	L	1005	13/13	0.80	0.20	66,74,85,88	0
2	FSW	D	1002	13/13	0.82	0.19	52,67,88,93	0
2	FSW	J	1001	13/13	0.82	0.18	55,67,80,83	0
2	FSW	K	1001	13/13	0.83	0.19	78,89,94,94	0
2	FSW	L	1006	13/13	0.83	0.19	77,89,100,100	0
2	FSW	F	1006	13/13	0.86	0.18	55,65,76,77	0
2	FSW	G	1006	13/13	0.87	0.15	40,51,66,69	0
2	FSW	J	1006	13/13	0.87	0.16	48,56,82,84	0
2	FSW	E	1001	13/13	0.88	0.17	51,60,65,65	0
2	FSW	J	1005	13/13	0.89	0.15	57,63,72,72	0
2	FSW	L	1003	13/13	0.89	0.12	43,46,55,68	0
2	FSW	D	1001	13/13	0.90	0.15	50,57,69,79	0
2	FSW	E	1006	13/13	0.90	0.14	52,62,69,76	0
2	FSW	I	1002	13/13	0.92	0.14	41,60,73,75	0
2	FSW	F	1001	13/13	0.92	0.13	56,60,75,75	0
2	FSW	H	1006	13/13	0.92	0.14	44,54,70,77	0
2	FSW	K	1003	13/13	0.92	0.14	52,57,70,80	0
2	FSW	K	1006	13/13	0.92	0.14	64,76,88,92	0
2	FSW	J	1002	13/13	0.93	0.13	47,54,60,62	0
2	FSW	K	1005	13/13	0.93	0.12	58,67,78,84	0
2	FSW	D	1006	13/13	0.94	0.12	47,54,65,70	0
2	FSW	I	1005	13/13	0.94	0.12	40,47,60,68	0
2	FSW	G	1001	13/13	0.94	0.11	50,54,73,74	0
2	FSW	C	1006	13/13	0.94	0.13	34,39,50,57	0
2	FSW	H	1001	13/13	0.94	0.11	50,57,67,69	0
2	FSW	H	1002	13/13	0.94	0.12	43,48,52,57	0
2	FSW	H	1003	13/13	0.94	0.11	36,44,57,70	0
2	FSW	F	1005	13/13	0.94	0.13	56,64,72,73	0
2	FSW	B	1006	13/13	0.95	0.11	30,41,56,60	0
2	FSW	H	1004	13/13	0.95	0.10	34,36,40,42	0
2	FSW	H	1005	13/13	0.95	0.12	51,61,70,71	0
2	FSW	L	1004	13/13	0.95	0.12	47,54,56,57	0
2	FSW	C	1001	13/13	0.95	0.10	36,40,53,57	0
2	FSW	G	1005	13/13	0.95	0.12	51,57,73,80	0
2	FSW	F	1004	13/13	0.96	0.11	37,40,44,45	0
2	FSW	E	1005	13/13	0.96	0.10	47,52,60,61	0
2	FSW	I	1006	13/13	0.96	0.10	35,39,56,58	0
2	FSW	B	1005	13/13	0.96	0.10	41,46,56,59	0

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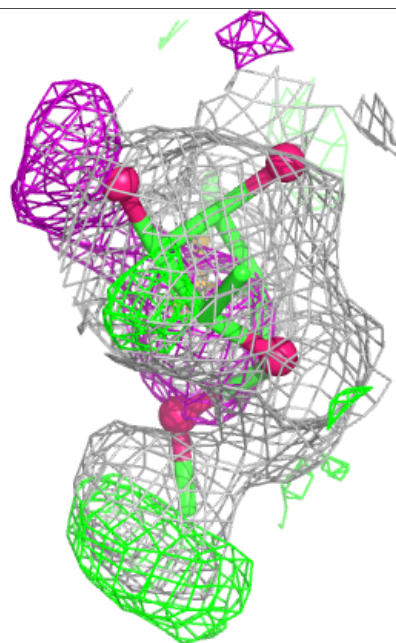
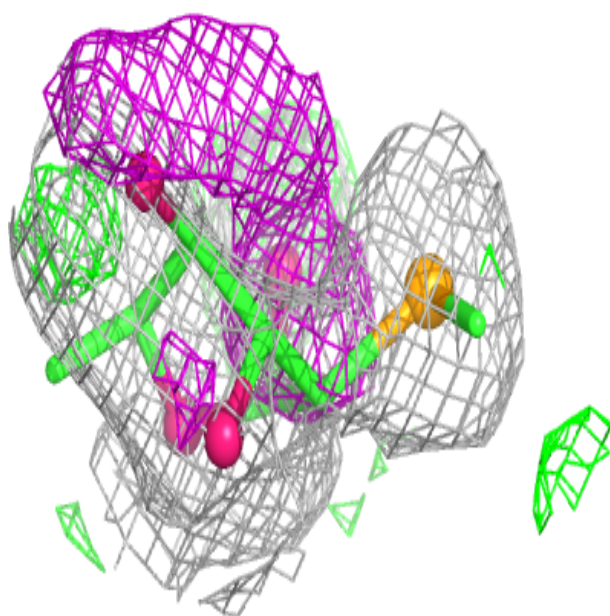
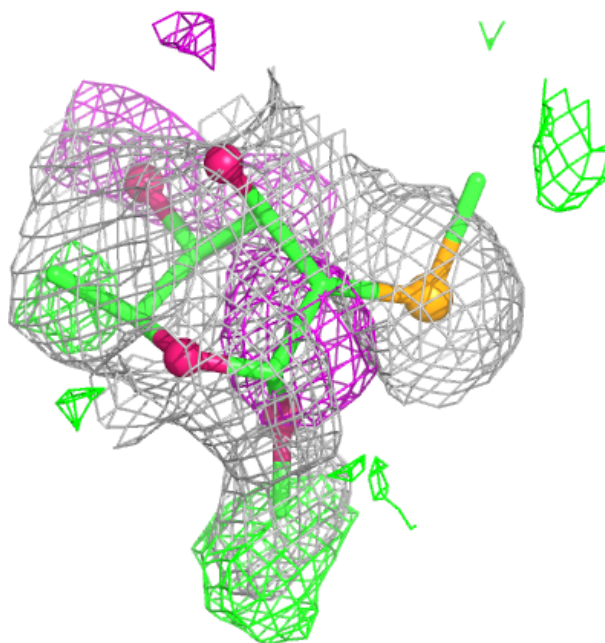
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FSW	A	1001	13/13	0.96	0.08	30,38,52,55	0
2	FSW	I	1001	13/13	0.96	0.10	40,47,61,61	0
2	FSW	E	1002	13/13	0.97	0.09	30,37,40,44	0
2	FSW	E	1003	13/13	0.97	0.09	34,39,46,61	0
2	FSW	G	1003	13/13	0.97	0.08	37,40,52,53	0
2	FSW	C	1005	13/13	0.97	0.09	33,40,49,51	0
2	FSW	K	1004	13/13	0.97	0.09	42,48,53,54	0
2	FSW	I	1003	13/13	0.97	0.09	40,52,59,60	0
2	FSW	I	1004	13/13	0.97	0.08	34,41,45,48	0
2	FSW	D	1003	13/13	0.97	0.08	34,38,44,48	0
2	FSW	D	1005	13/13	0.97	0.09	42,49,54,55	0
2	FSW	F	1003	13/13	0.97	0.09	36,39,49,50	0
2	FSW	A	1006	13/13	0.97	0.09	28,35,50,54	0
2	FSW	J	1003	13/13	0.97	0.09	40,43,53,53	0
2	FSW	A	1004	13/13	0.97	0.08	25,28,37,49	0
2	FSW	C	1003	13/13	0.98	0.07	34,38,51,57	0
2	FSW	F	1002	13/13	0.98	0.08	34,39,44,47	0
2	FSW	C	1004	13/13	0.98	0.07	28,33,36,37	0
2	FSW	B	1003	13/13	0.98	0.08	29,33,42,53	0
2	FSW	A	1005	13/13	0.98	0.08	33,43,52,55	0
2	FSW	A	1003	13/13	0.98	0.07	32,34,39,42	0
2	FSW	B	1001	13/13	0.98	0.08	35,39,49,53	0
2	FSW	J	1004	13/13	0.98	0.08	35,41,43,47	0
2	FSW	G	1002	13/13	0.98	0.07	37,38,40,40	0
2	FSW	C	1002	13/13	0.98	0.07	32,38,48,50	0
2	FSW	G	1004	13/13	0.98	0.07	35,40,42,43	0
2	FSW	E	1004	13/13	0.99	0.05	30,32,35,36	0
2	FSW	B	1002	13/13	0.99	0.06	25,27,30,30	0
2	FSW	A	1002	13/13	0.99	0.06	25,27,32,37	0
2	FSW	D	1004	13/13	0.99	0.06	30,32,36,37	0
2	FSW	B	1004	13/13	0.99	0.05	24,27,28,31	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.

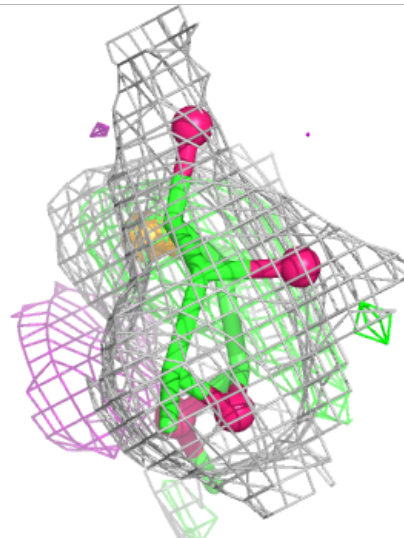
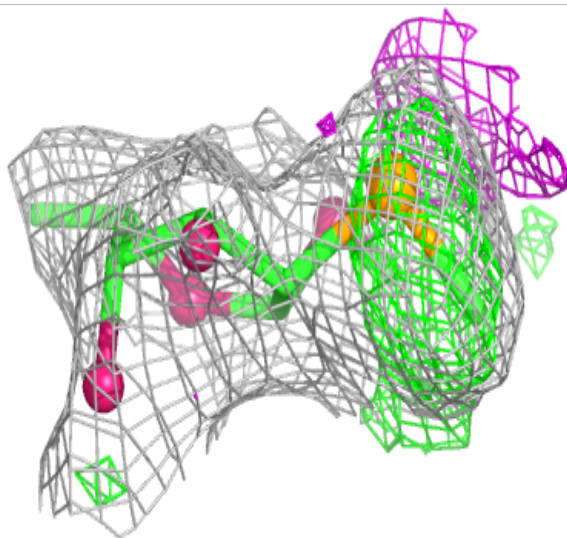
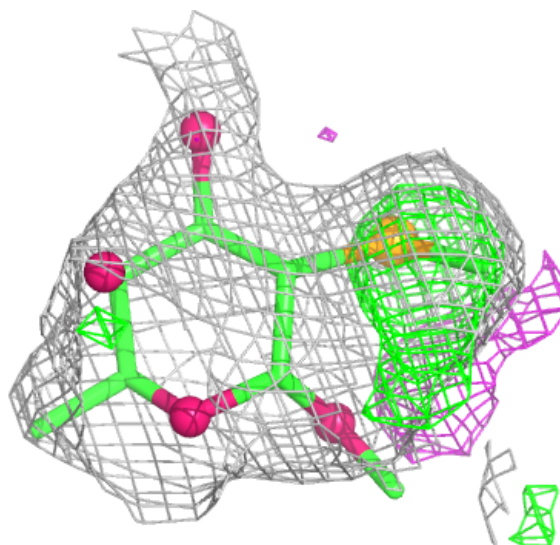
Electron density around FSW L 1001:

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



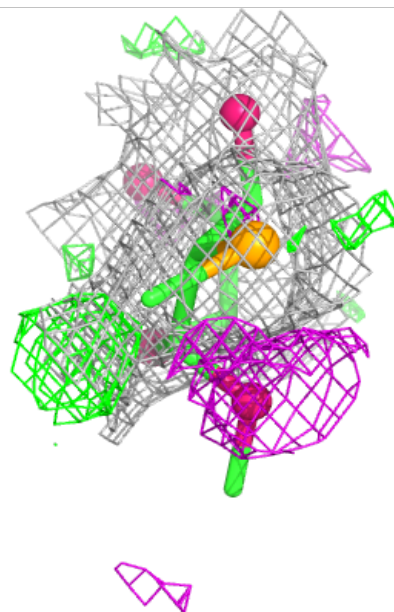
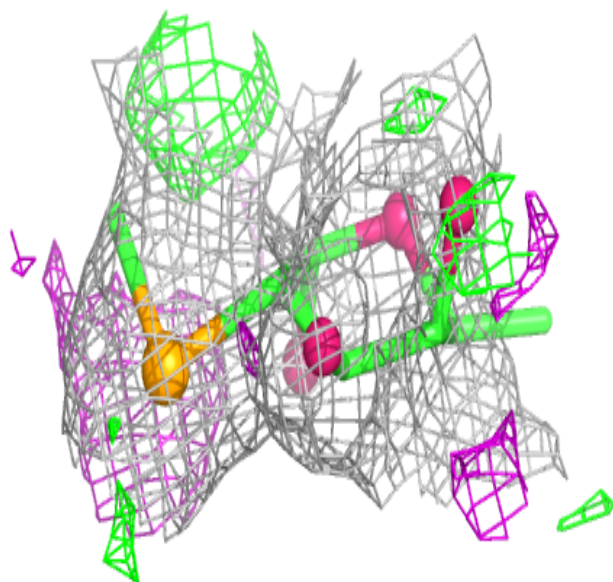
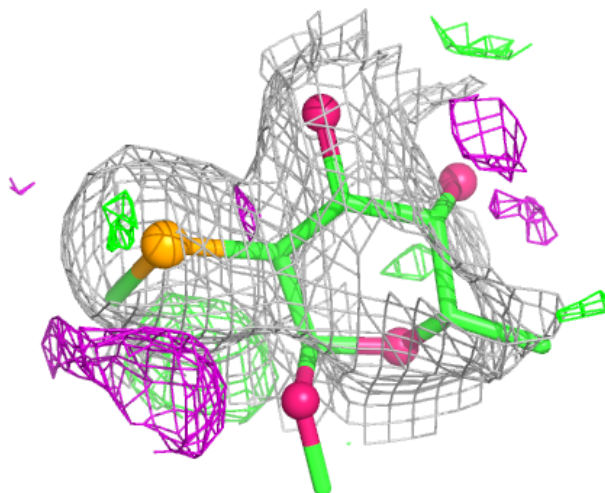
Electron density around FSW K 1002:

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



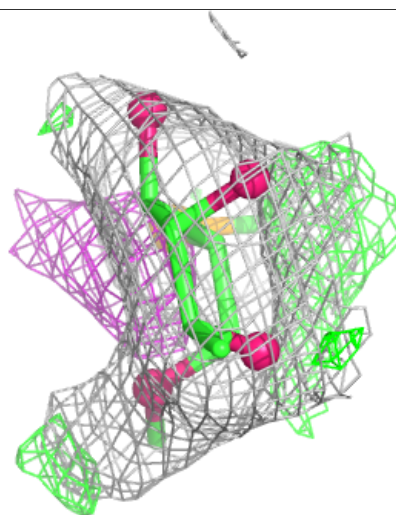
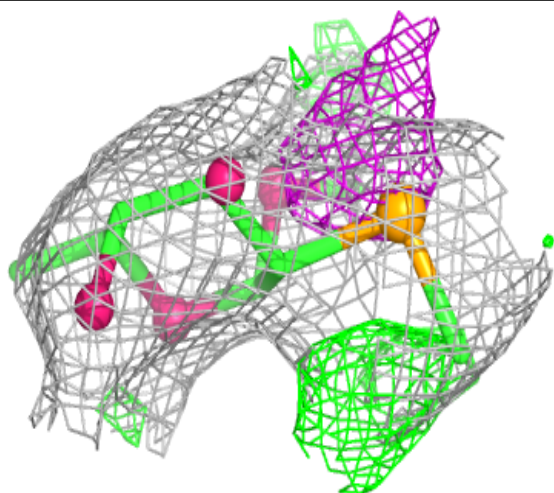
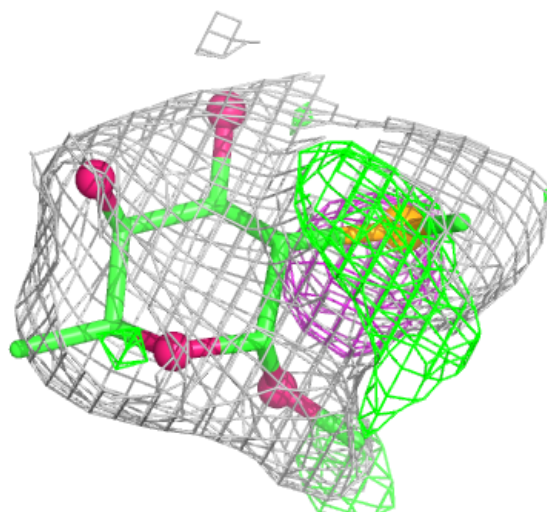
Electron density around FSW L 1002:

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



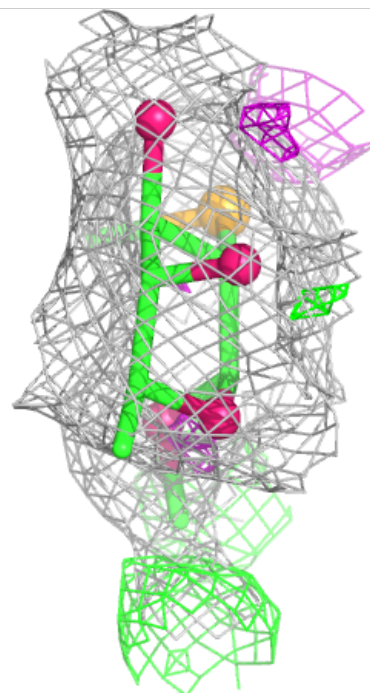
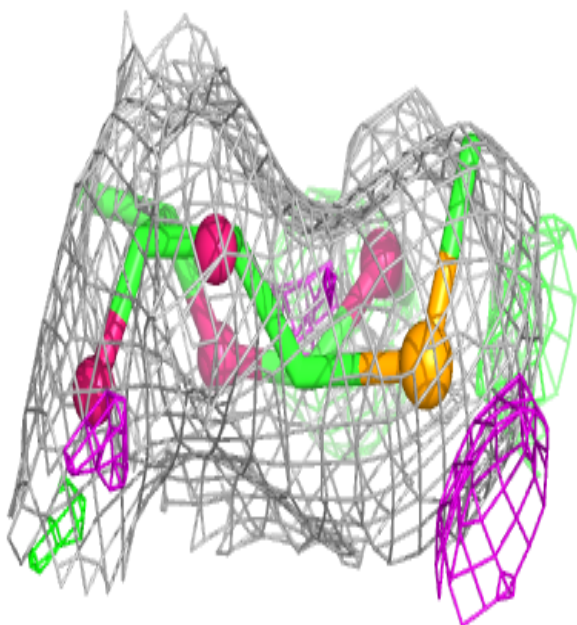
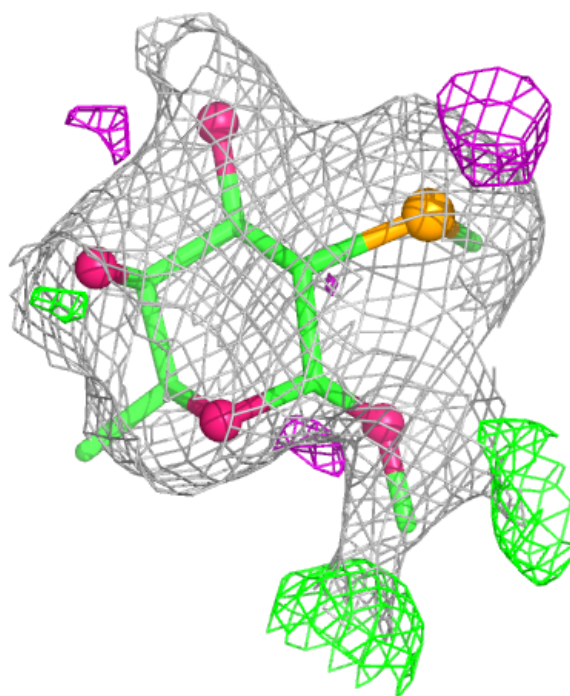
Electron density around FSW L 1005:

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



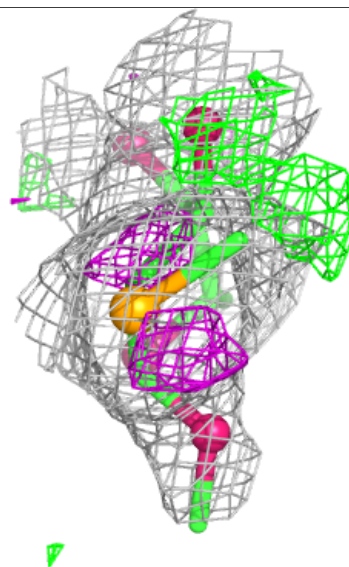
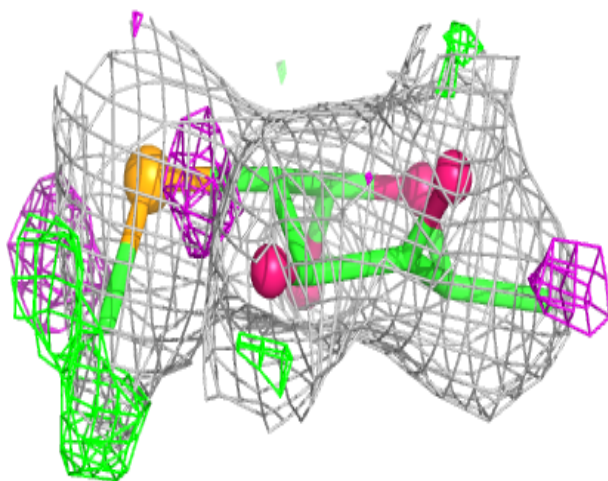
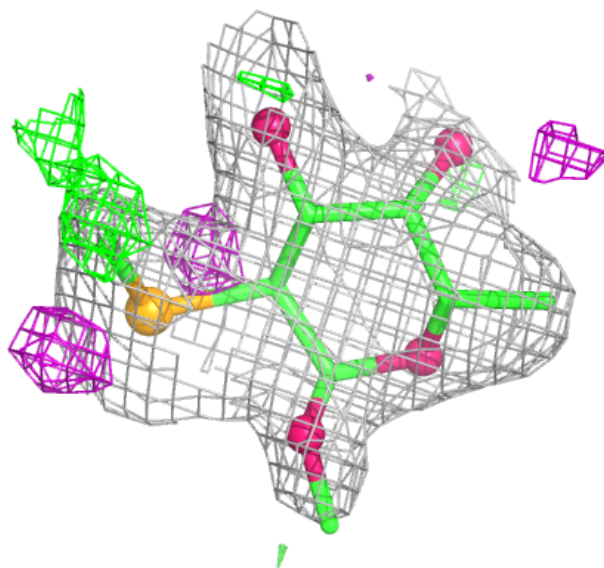
Electron density around FSW D 1002:

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



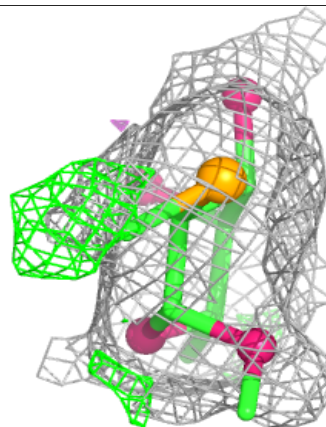
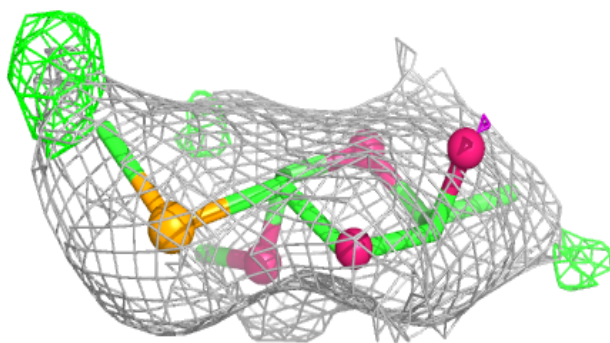
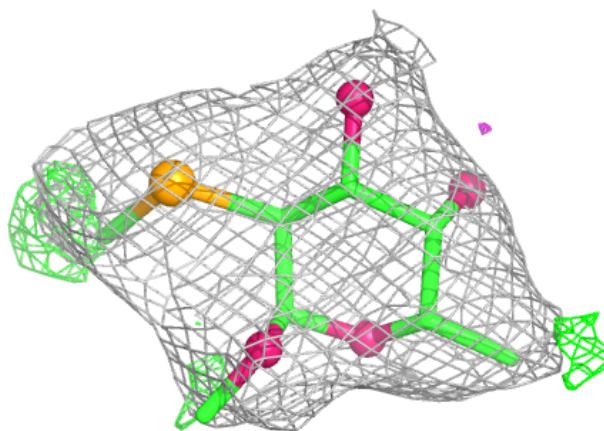
Electron density around FSW J 1001:

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

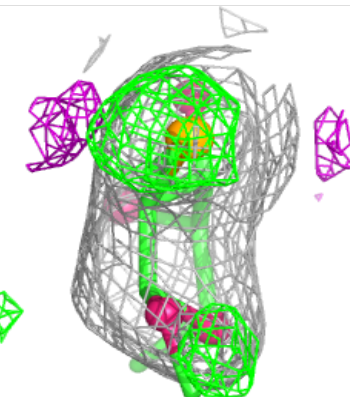
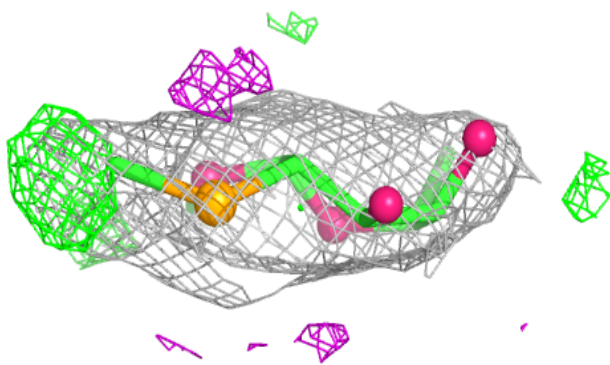
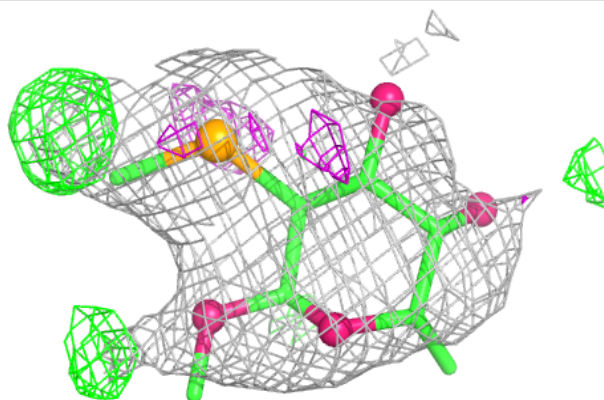


Electron density around FSW K 1001:

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and green (positive)

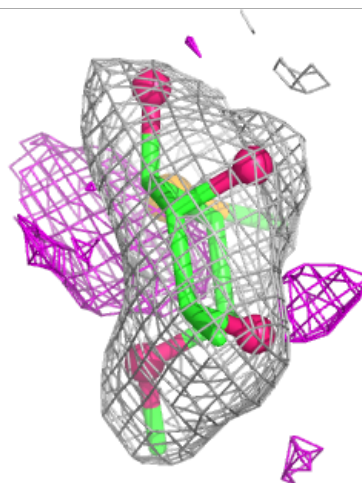
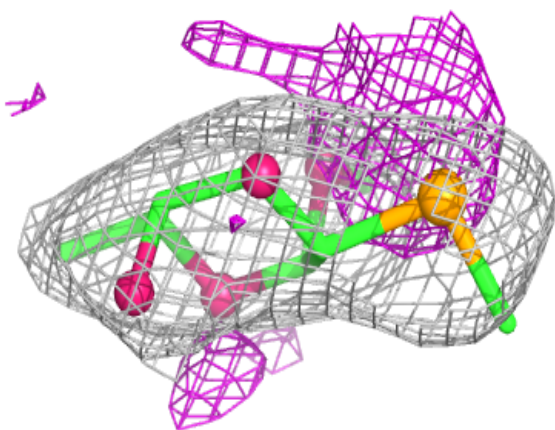
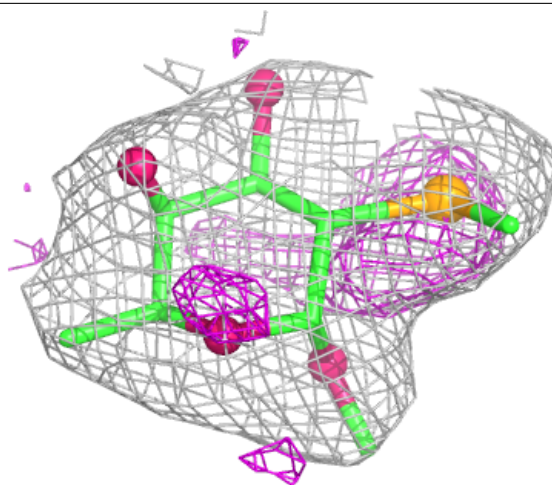
**Electron density around FSW L 1006:**

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and green (positive)



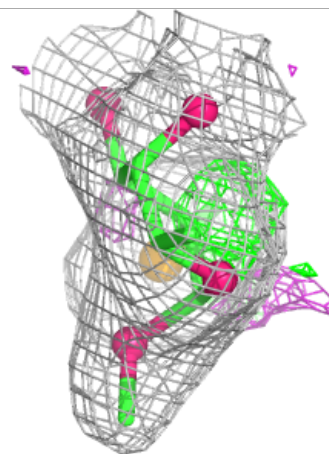
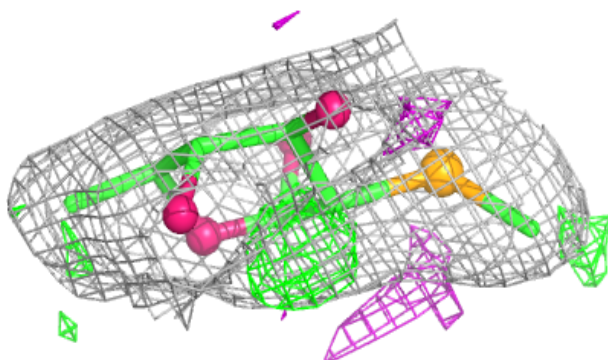
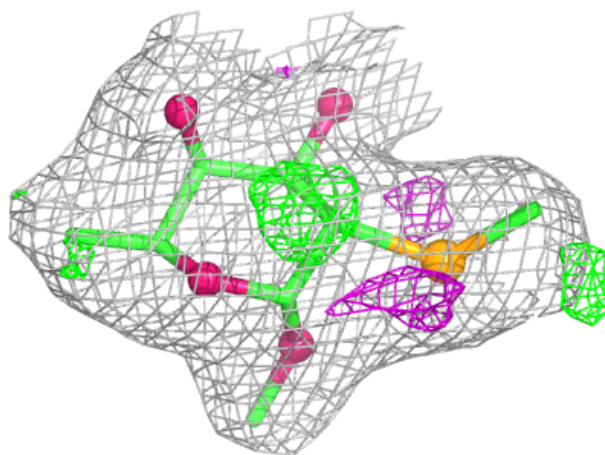
Electron density around FSW J 1006:

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and green (positive)



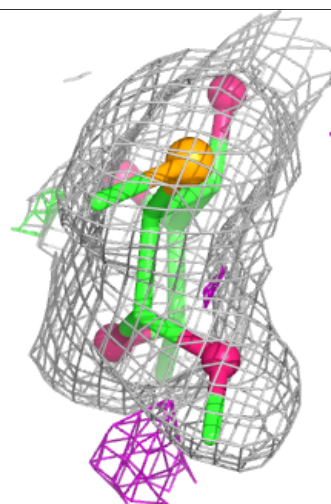
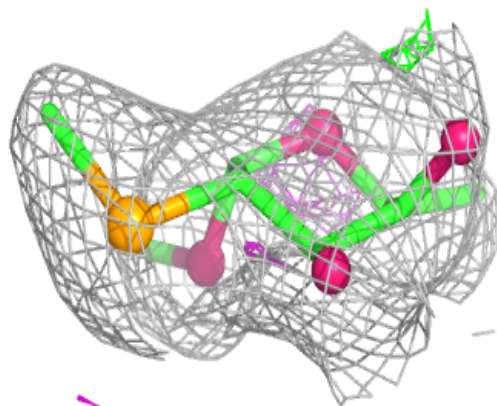
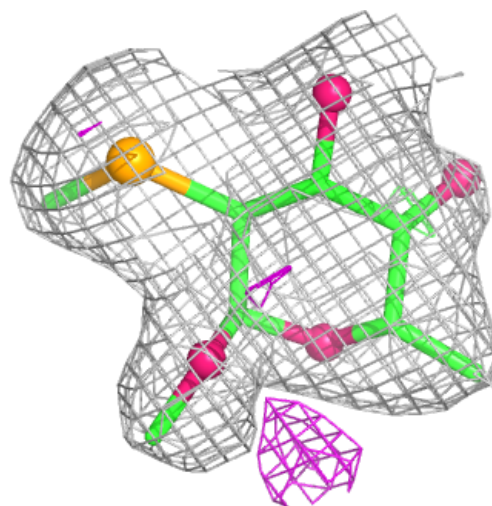
Electron density around FSW L 1003:

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



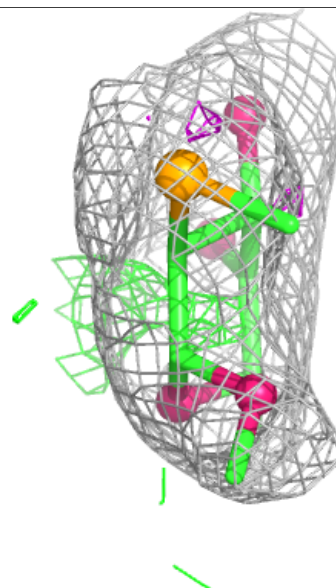
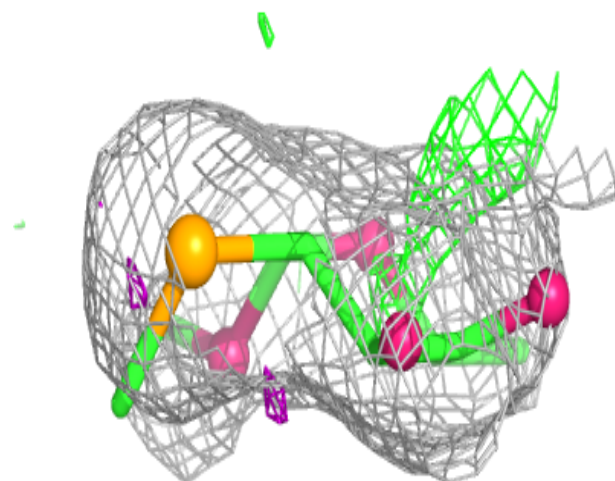
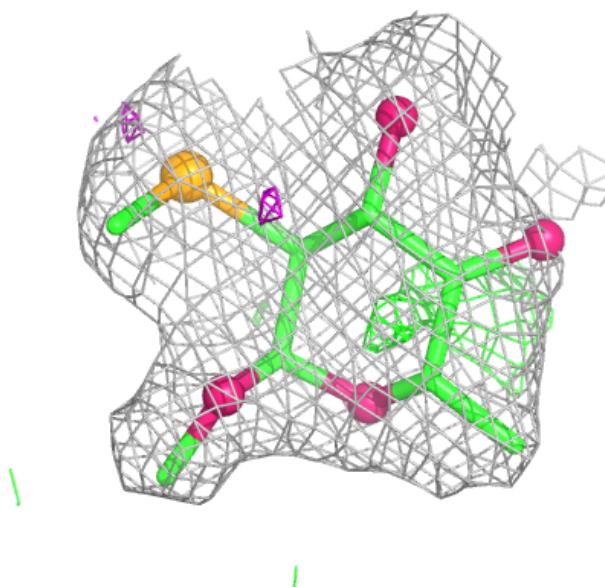
Electron density around FSW D 1001:

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



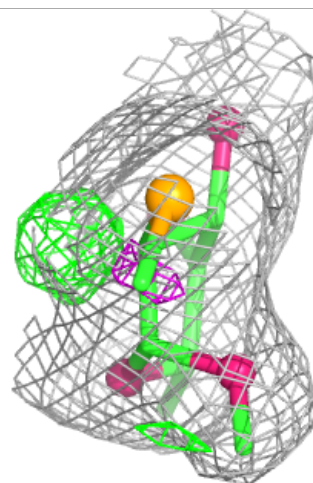
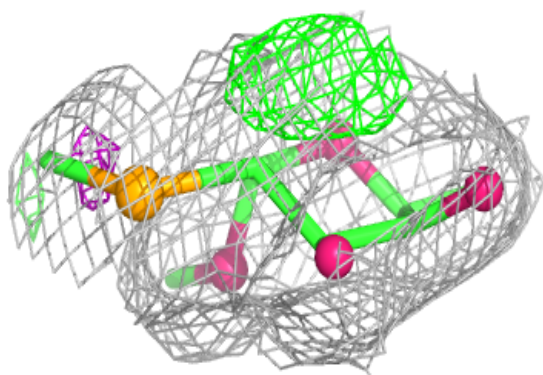
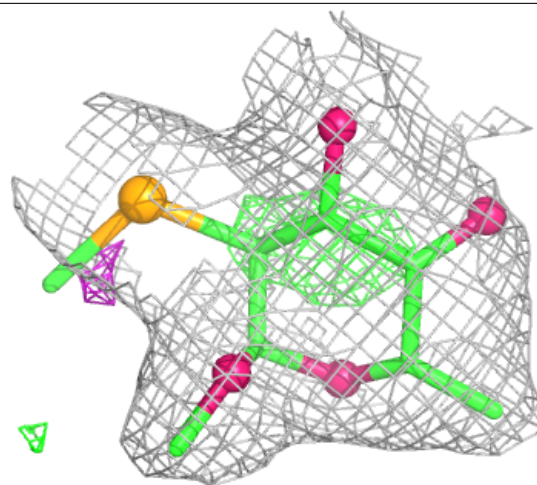
Electron density around FSW I 1002:

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and green (positive)



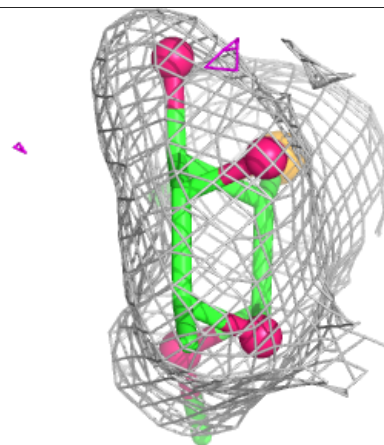
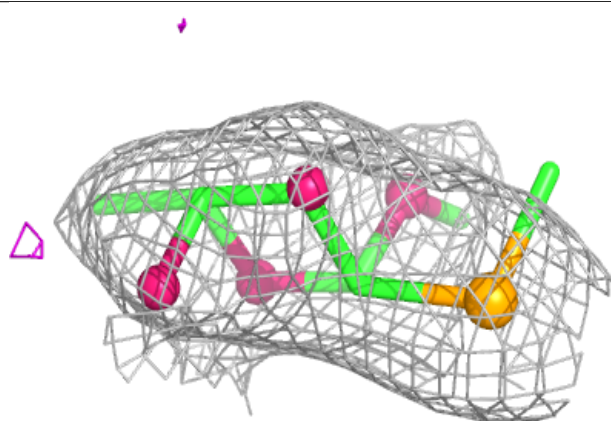
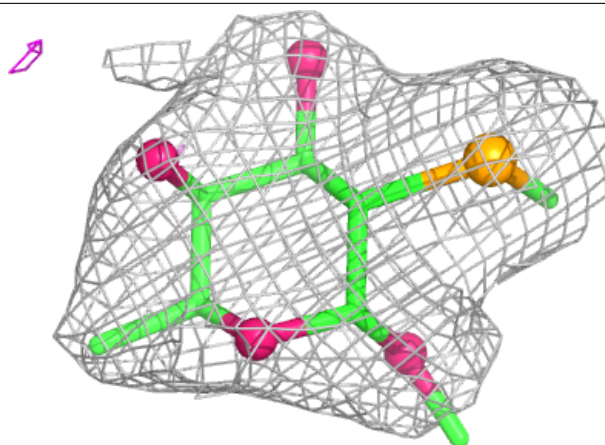
Electron density around FSW K 1003:

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and green (positive)



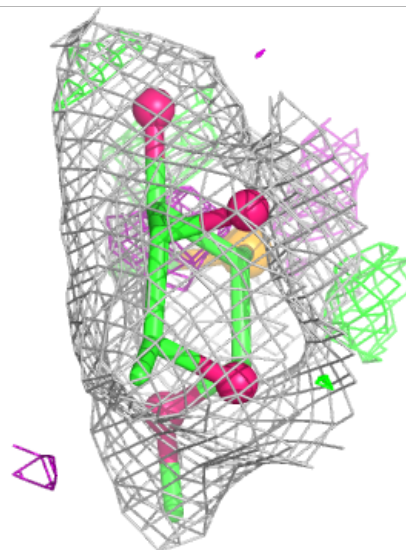
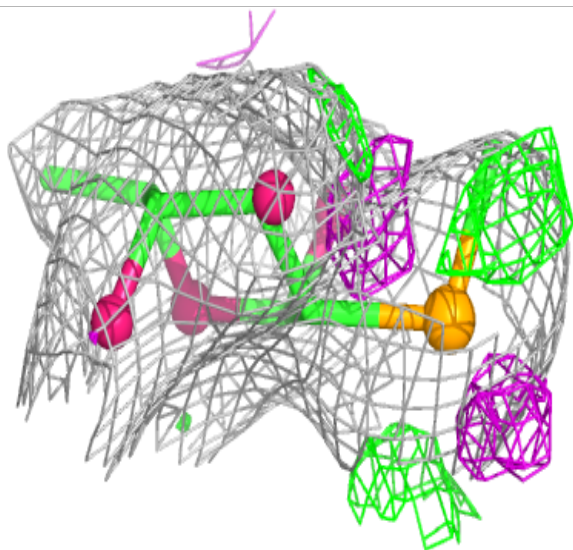
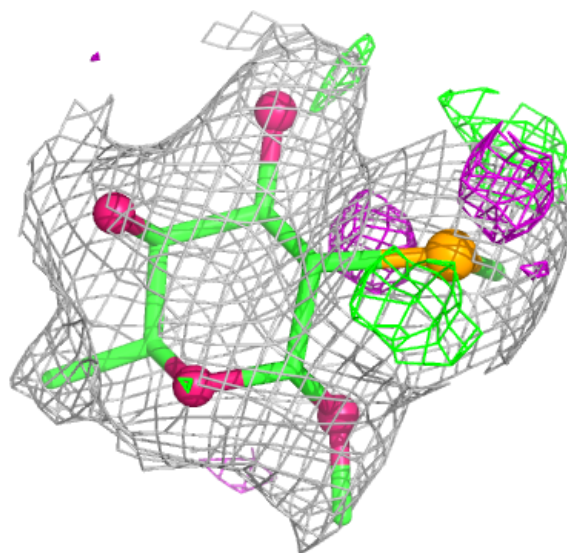
Electron density around FSW K 1006:

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and green (positive)



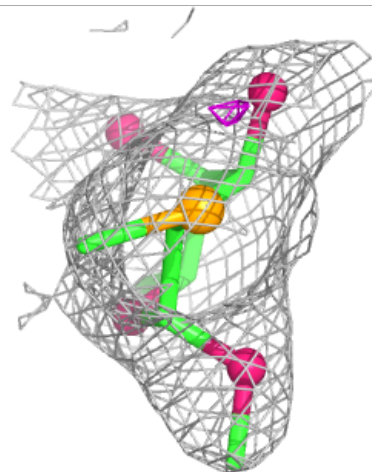
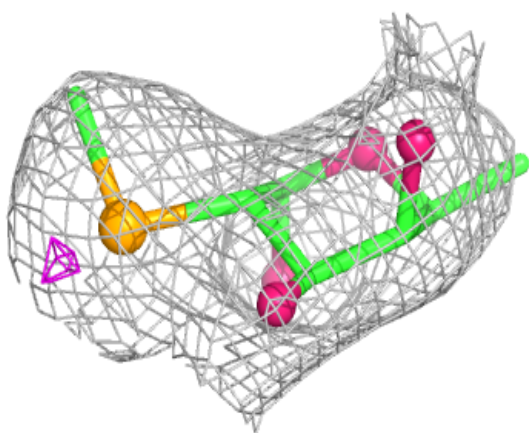
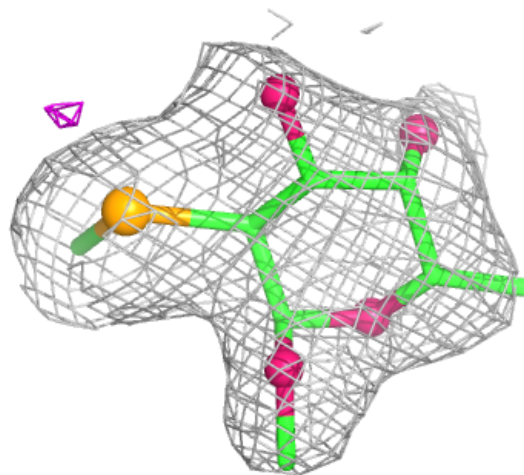
Electron density around FSW J 1002:

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



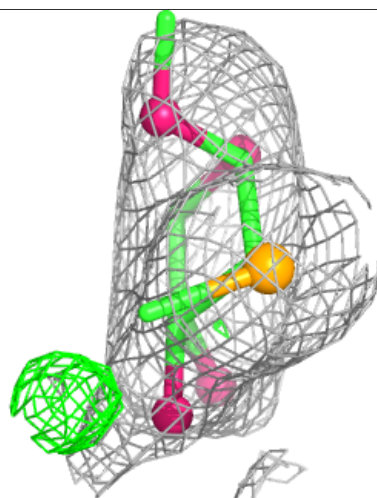
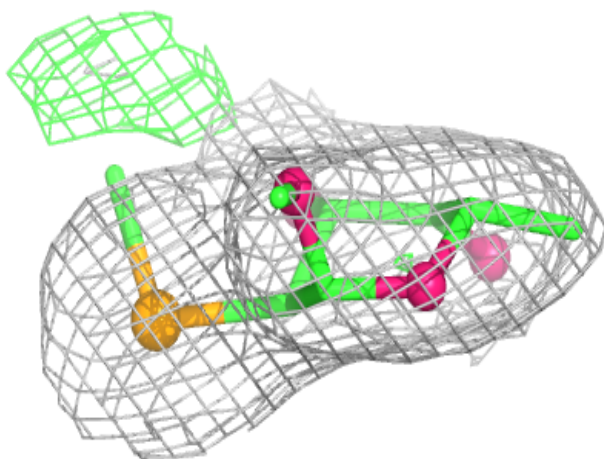
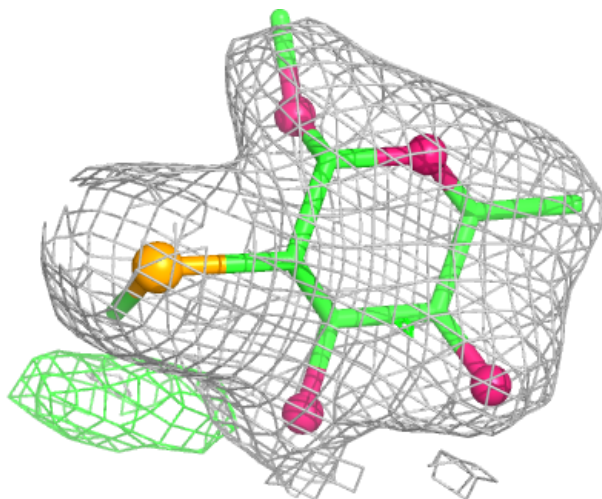
Electron density around FSW K 1005:

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



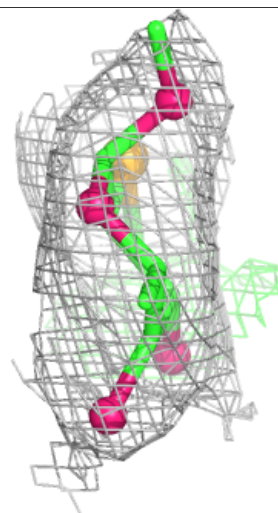
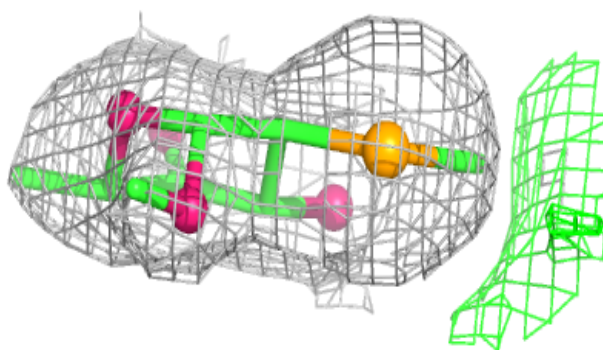
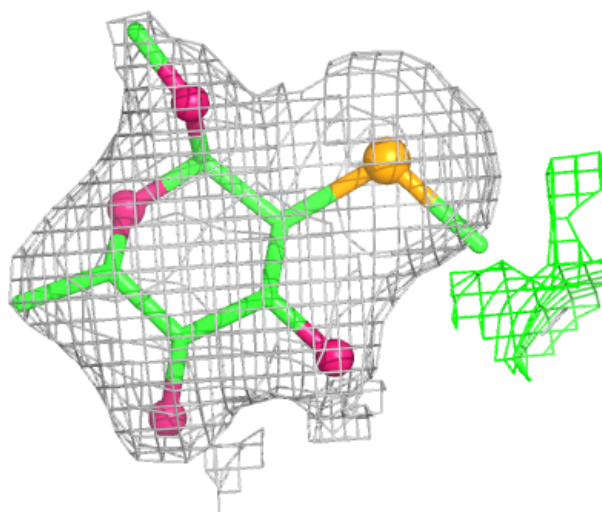
Electron density around FSW D 1006:

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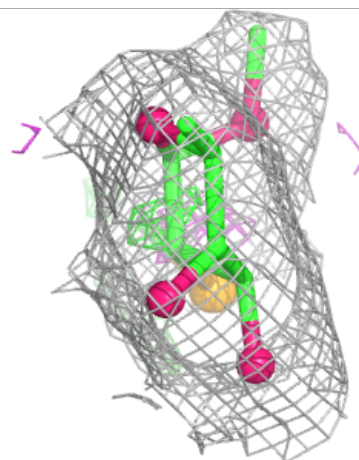
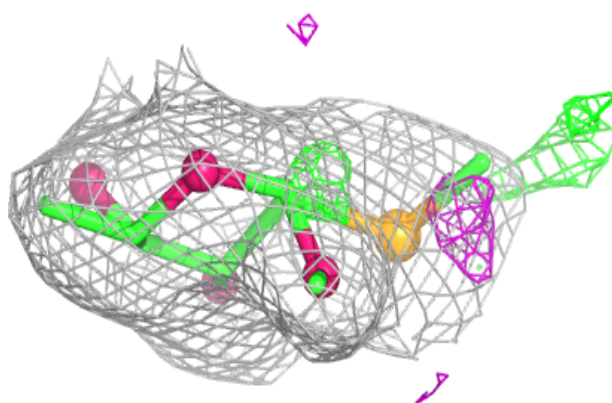
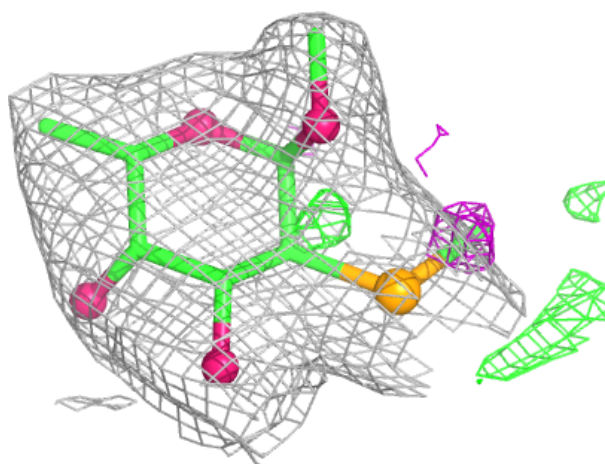
Electron density around FSW H 1001:

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and green (positive)



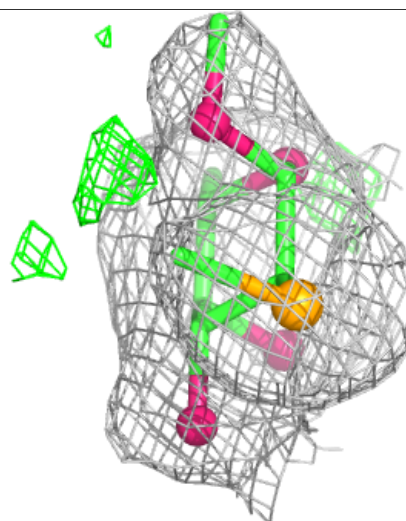
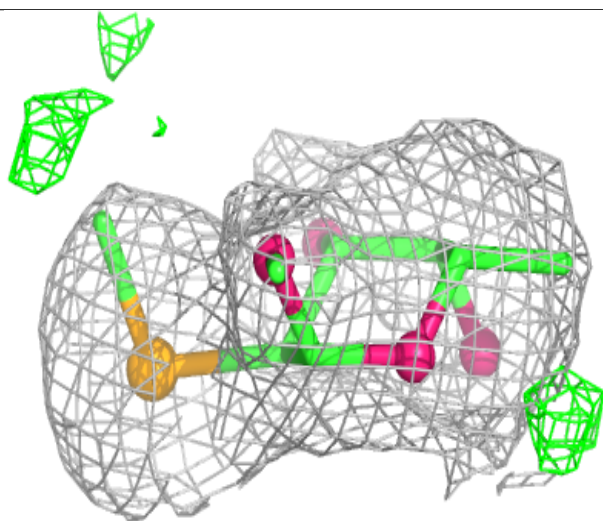
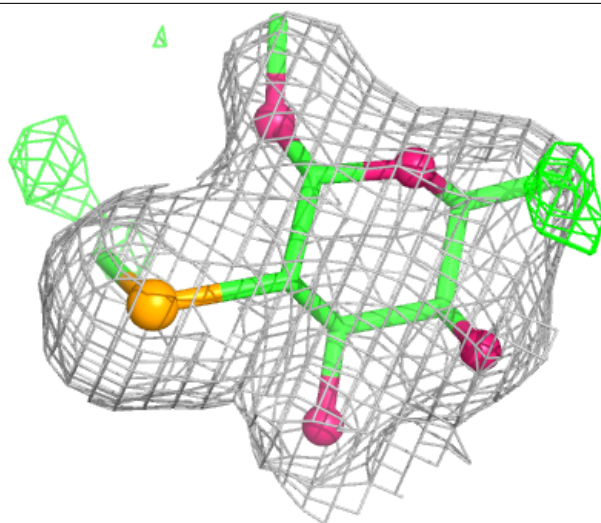
Electron density around FSW H 1003:

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



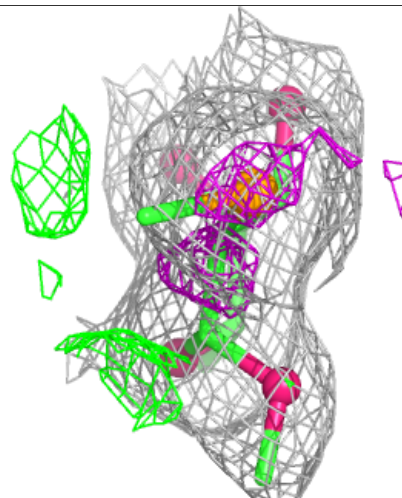
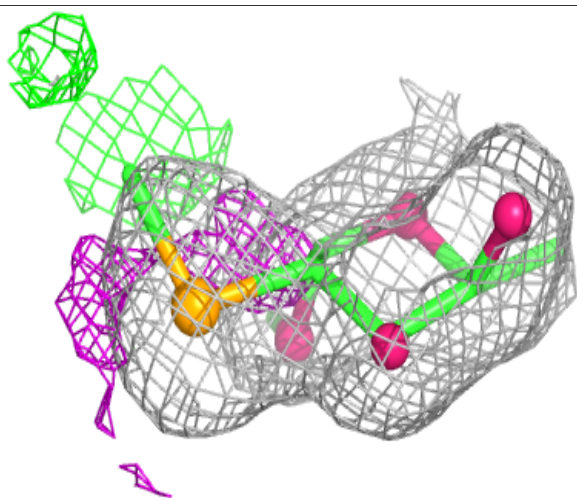
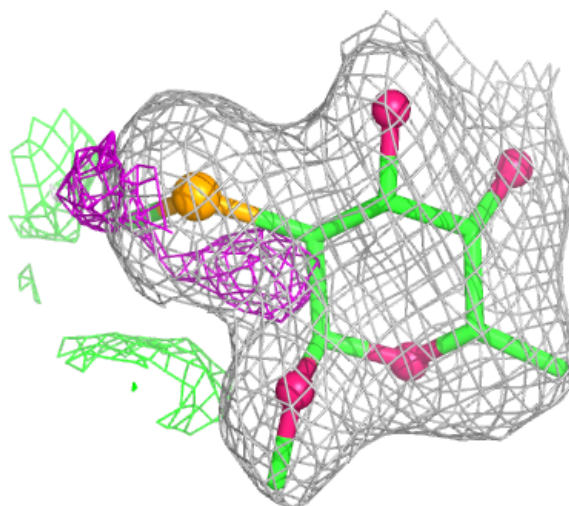
Electron density around FSW F 1005:

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



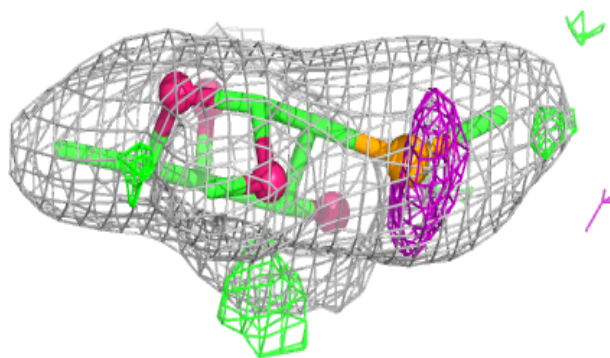
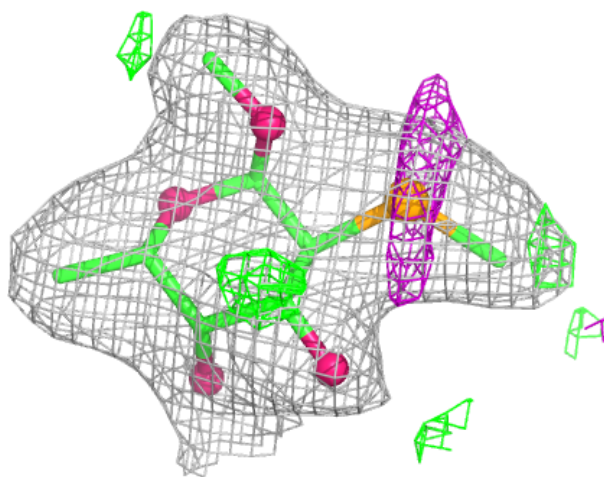
Electron density around FSW B 1006:

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



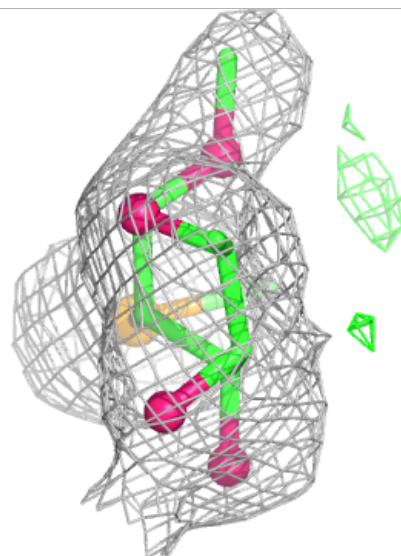
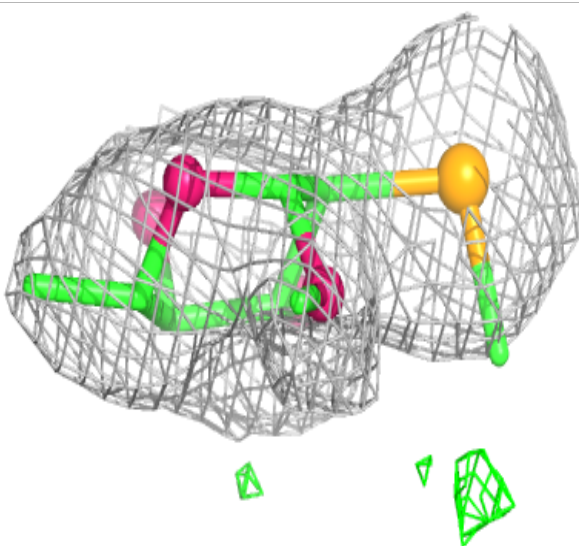
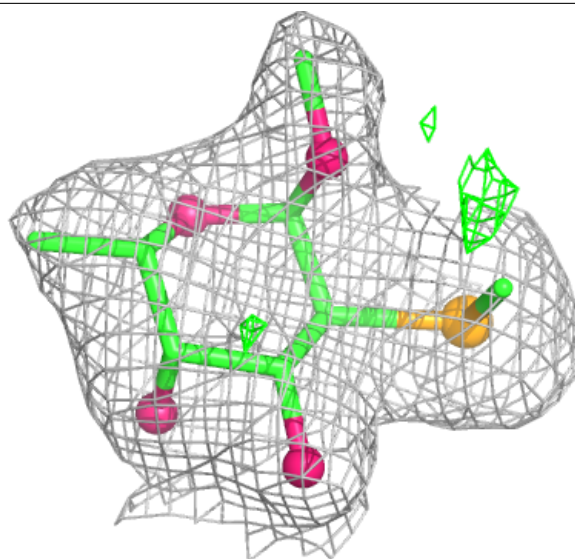
Electron density around FSW H 1004:

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



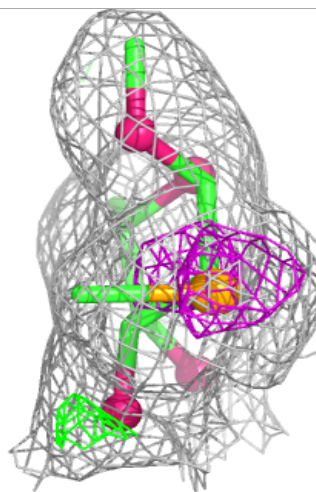
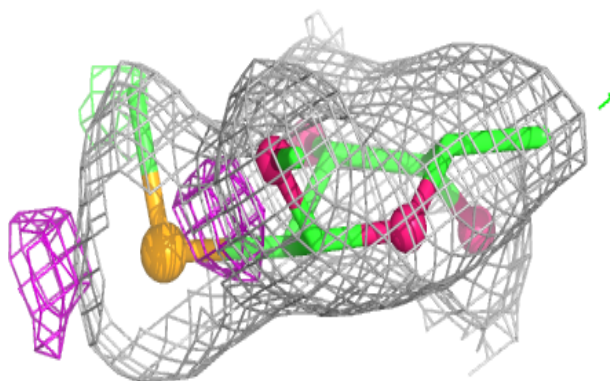
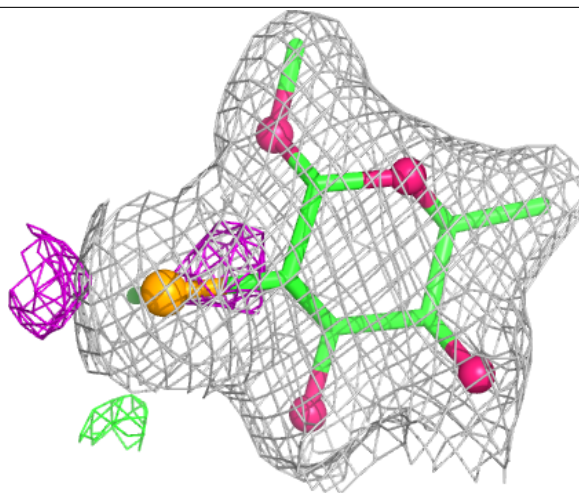
Electron density around FSW H 1005:

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



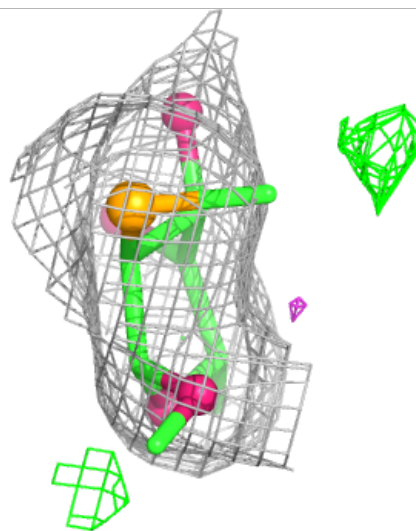
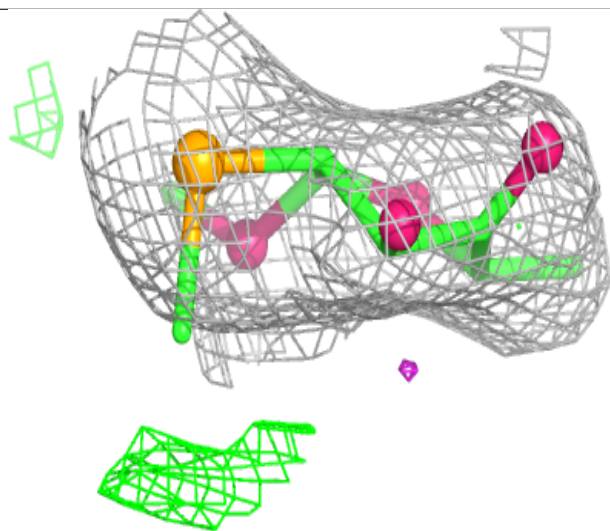
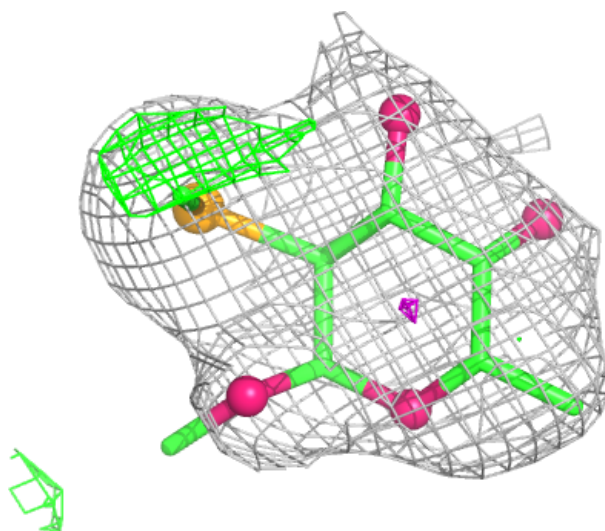
Electron density around FSW C 1001:

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



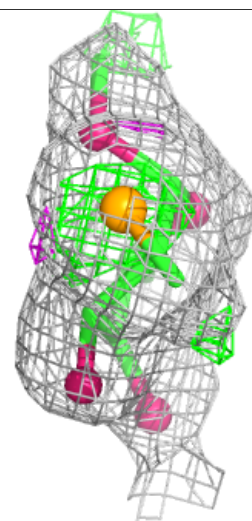
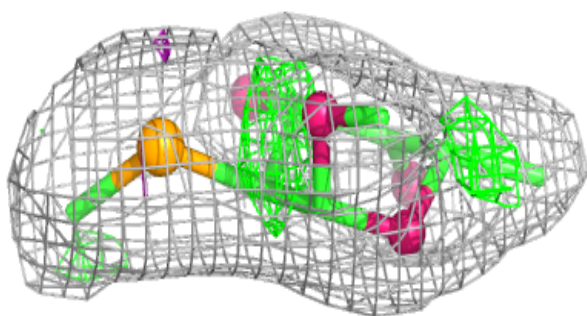
Electron density around FSW G 1005:

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



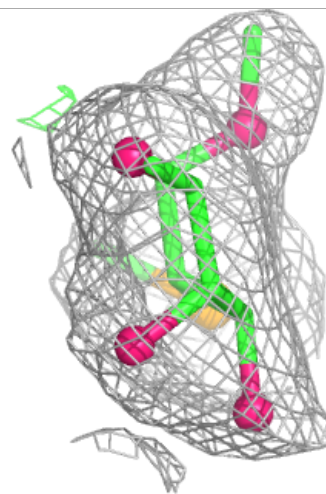
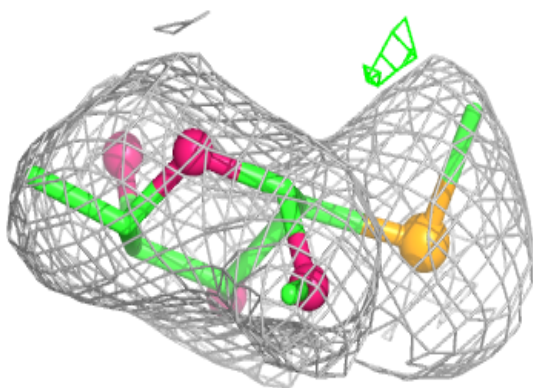
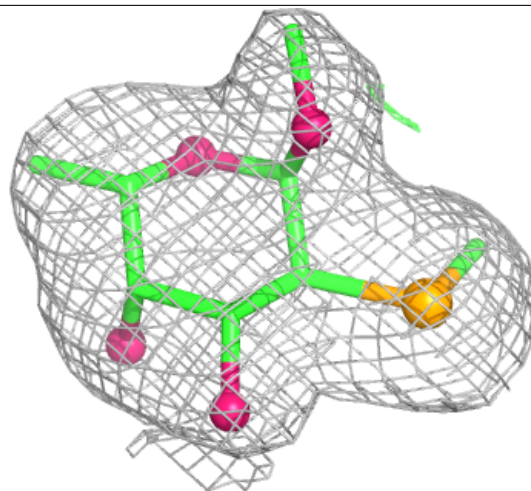
Electron density around FSW F 1004:

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



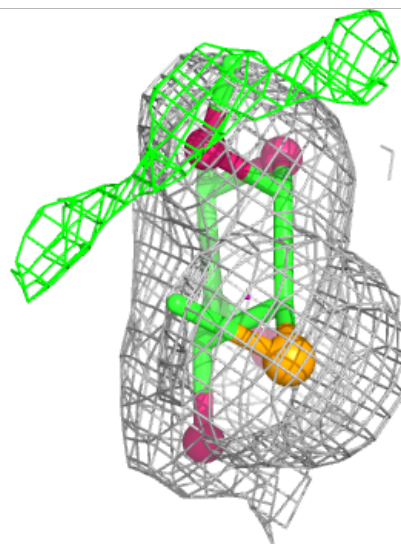
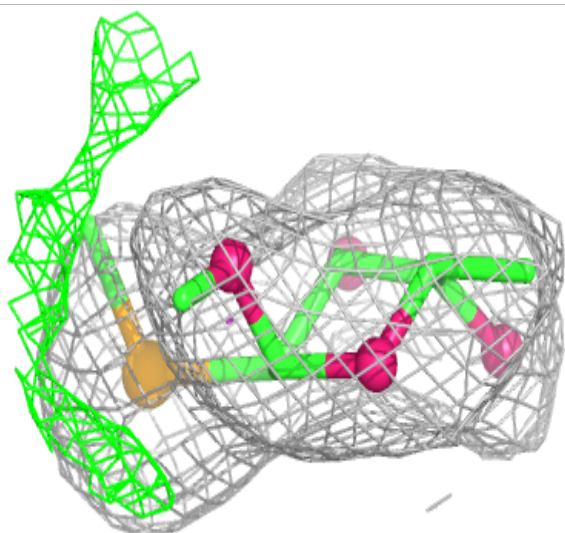
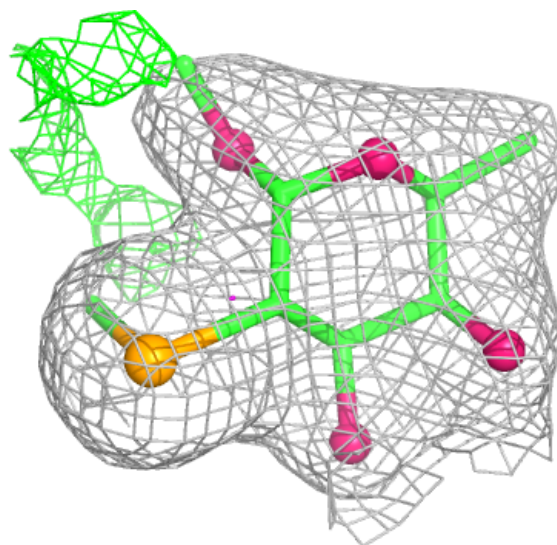
Electron density around FSW E 1005:

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



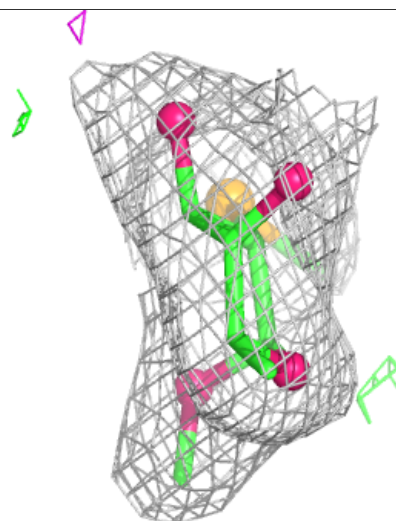
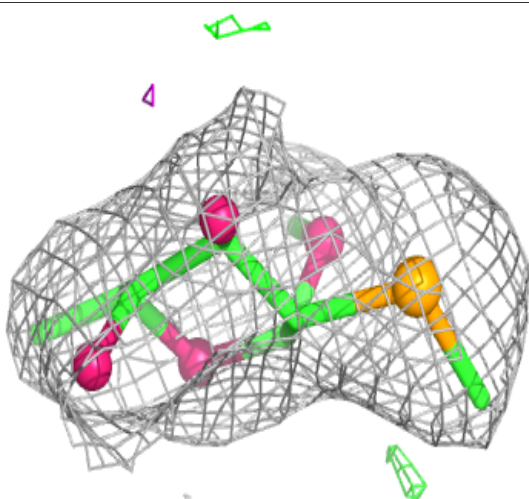
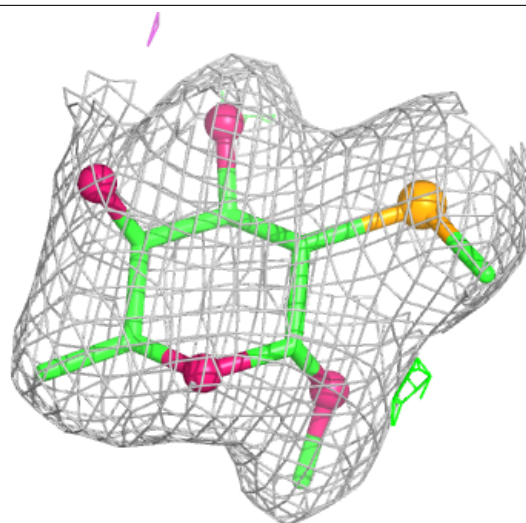
Electron density around FSW I 1006:

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



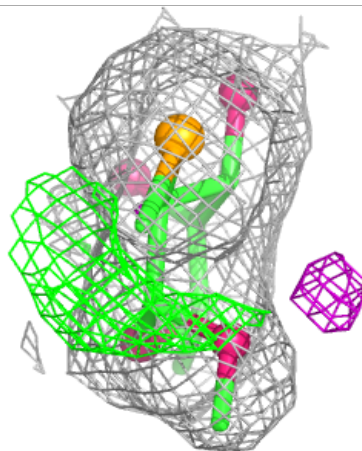
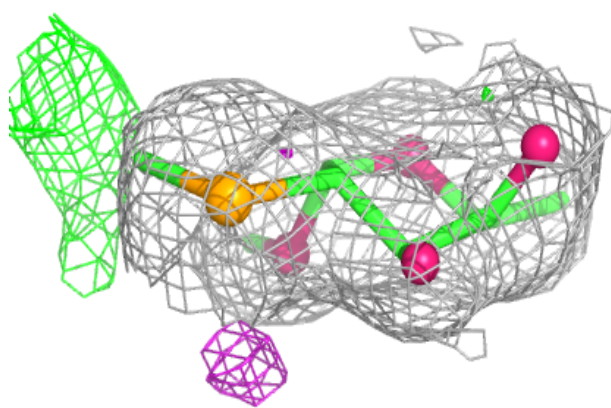
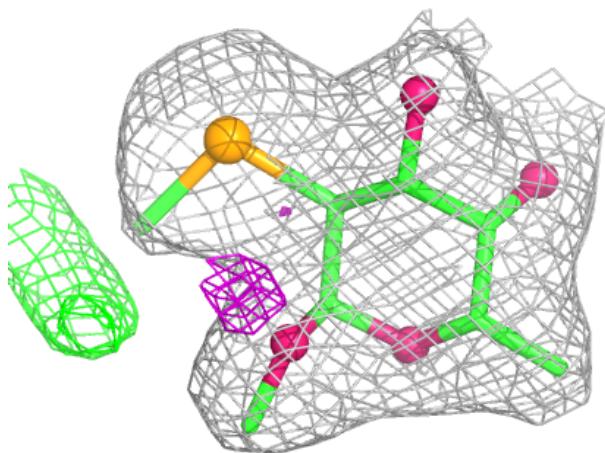
Electron density around FSW B 1005:

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



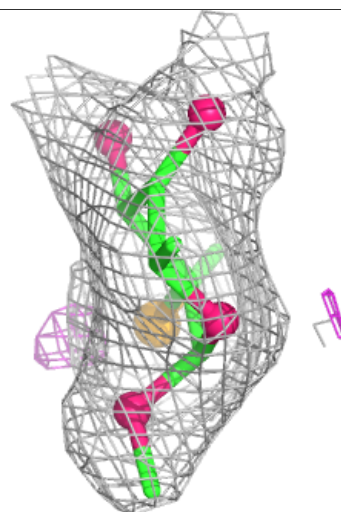
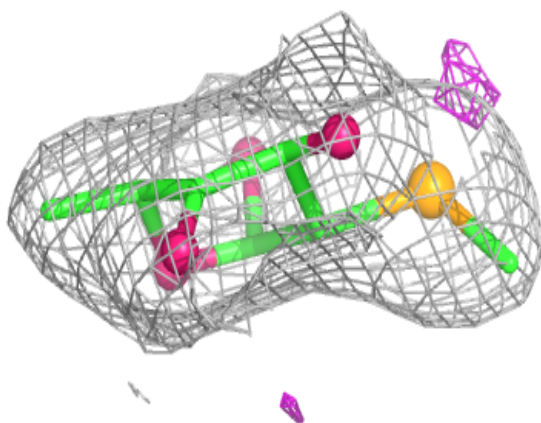
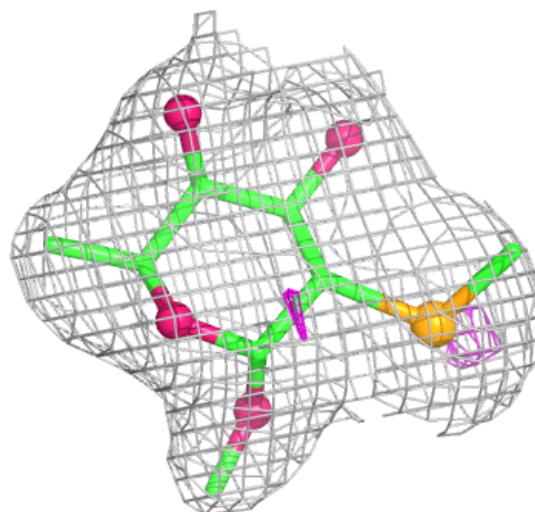
Electron density around FSW A 1001:

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



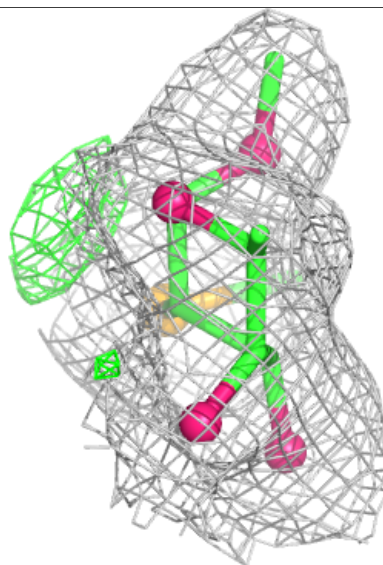
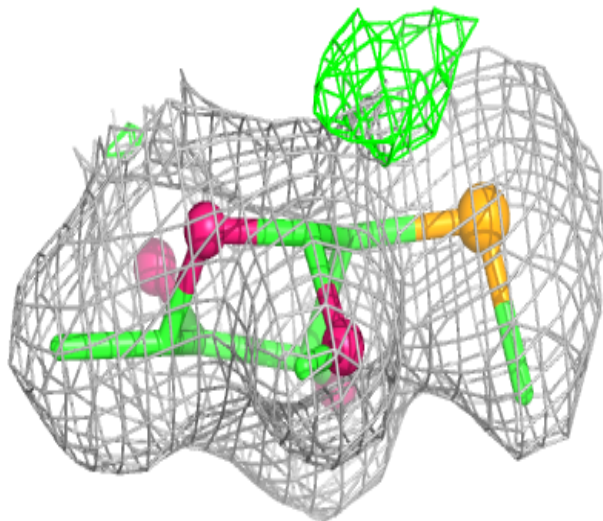
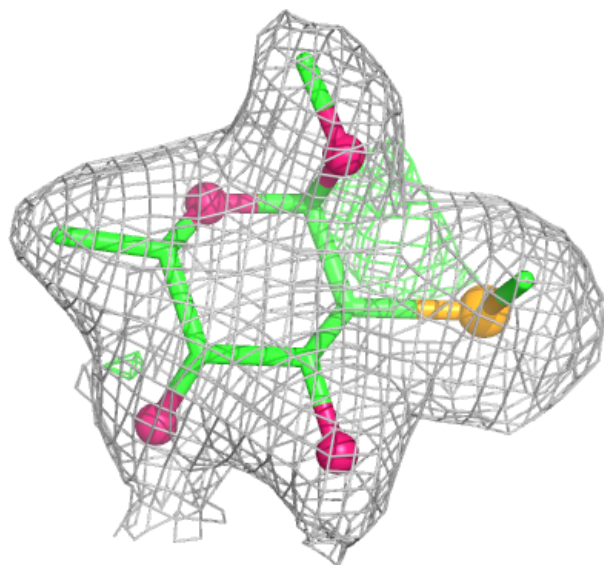
Electron density around FSW I 1001:

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



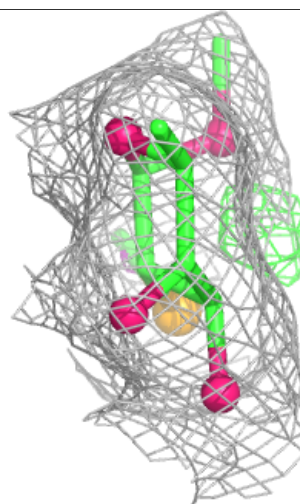
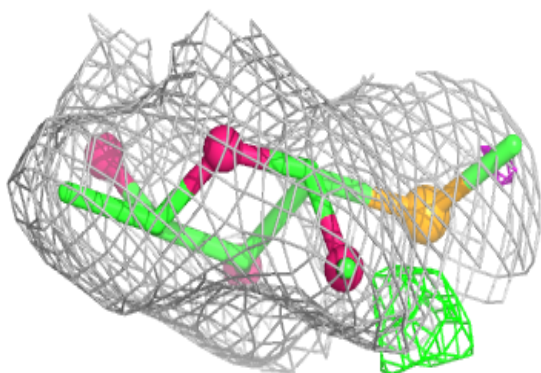
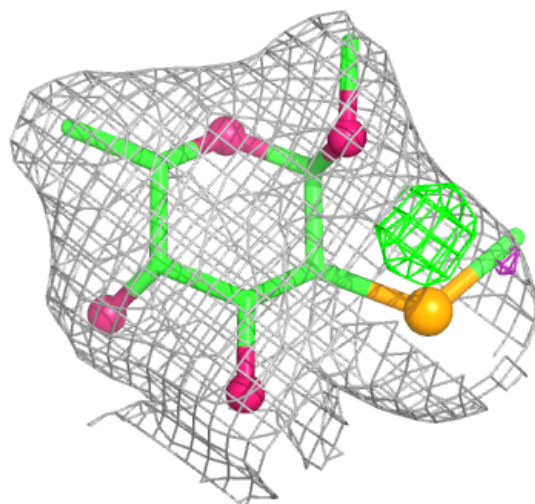
Electron density around FSW E 1002:

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



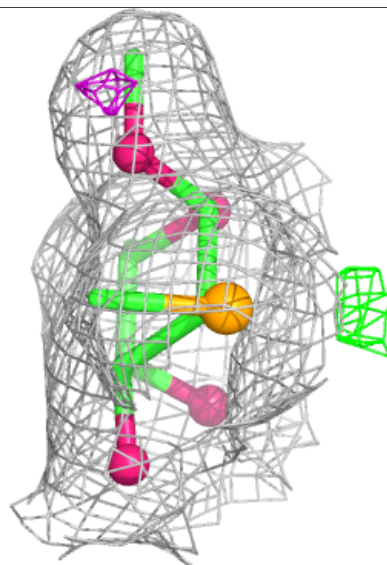
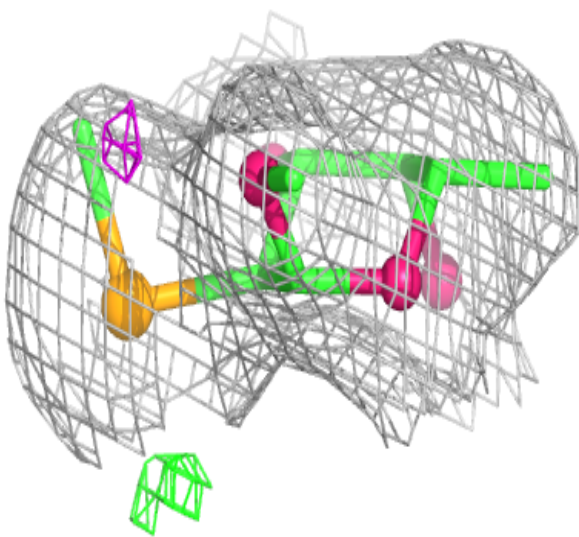
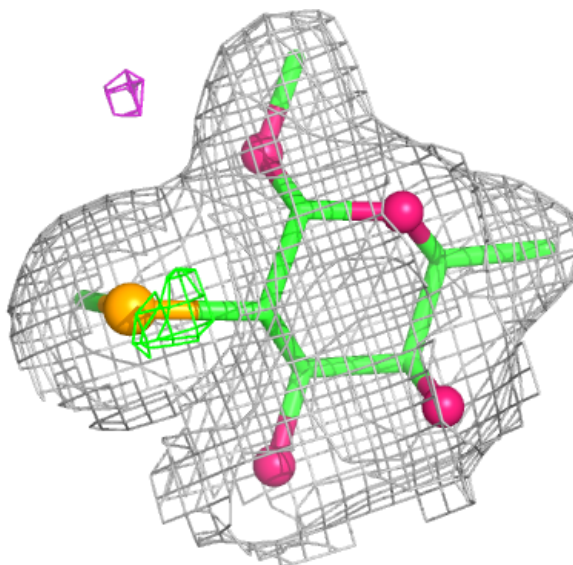
Electron density around FSW E 1003:

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



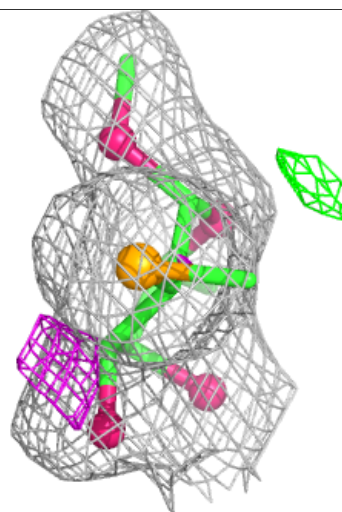
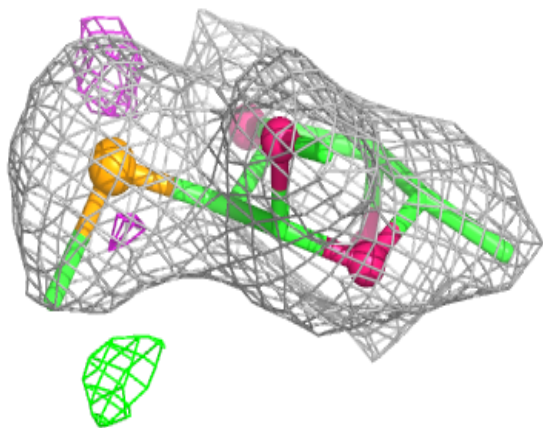
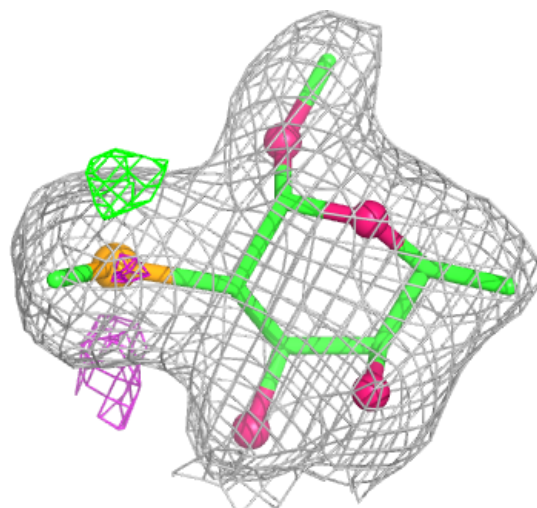
Electron density around FSW G 1003:

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



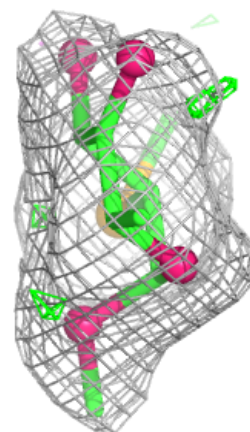
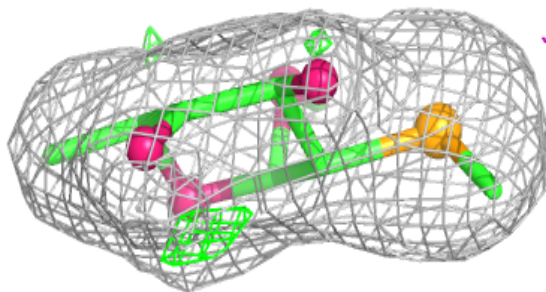
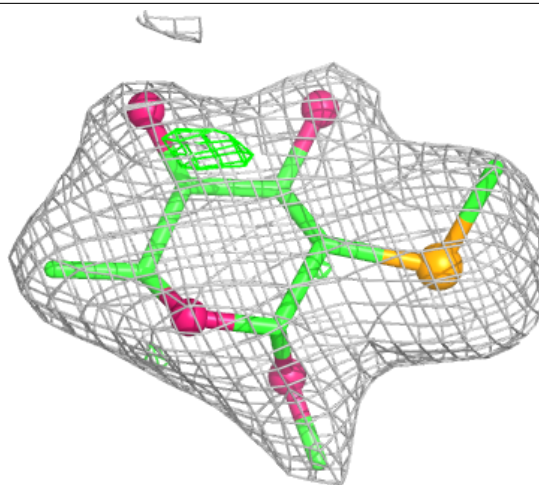
Electron density around FSW C 1005:

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



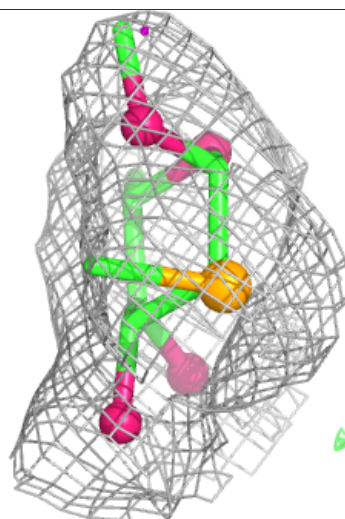
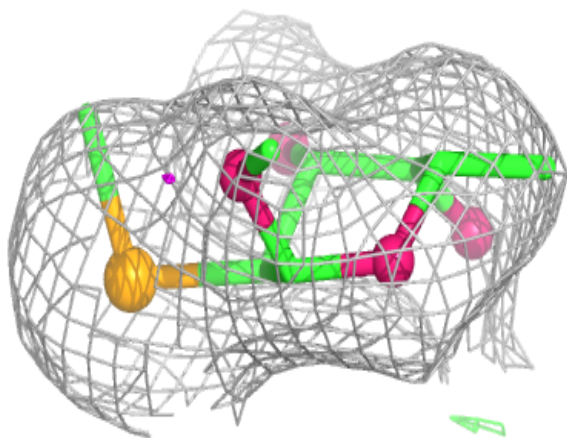
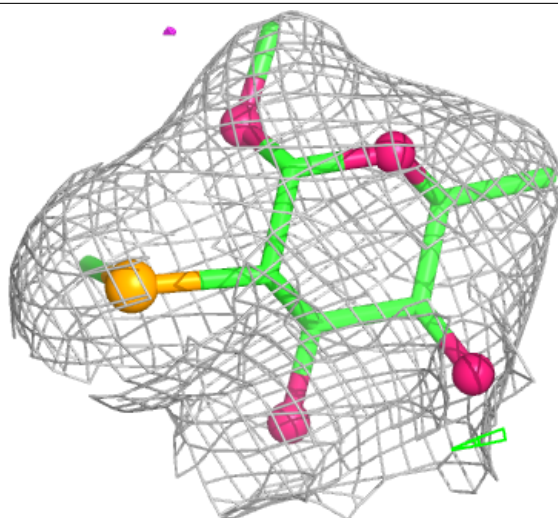
Electron density around FSW K 1004:

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



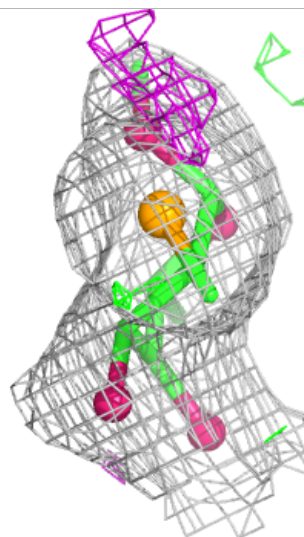
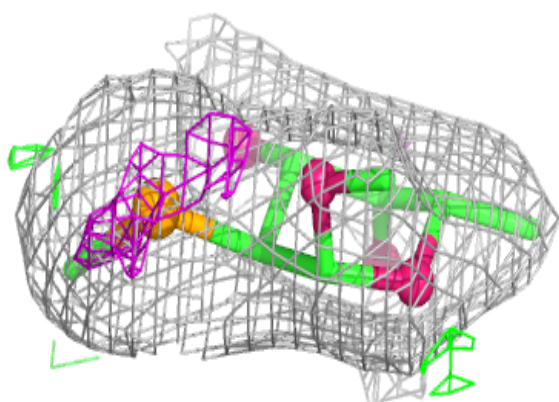
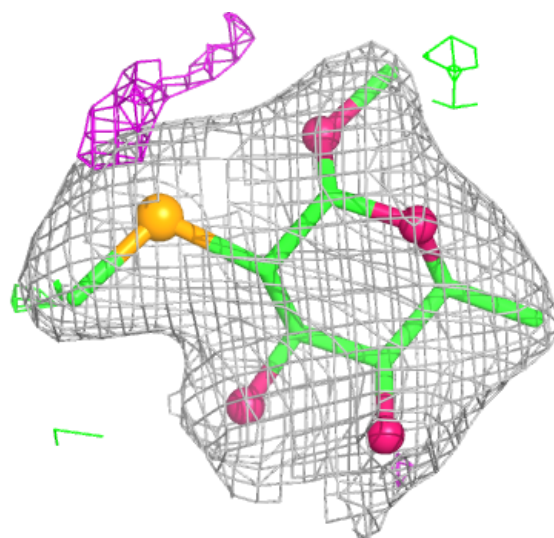
Electron density around FSW I 1003:

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



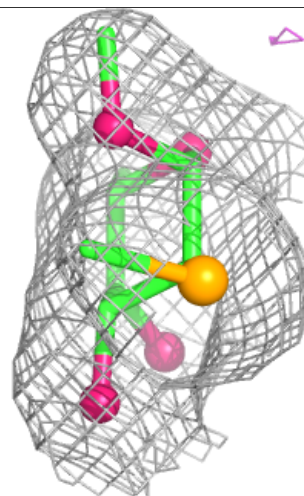
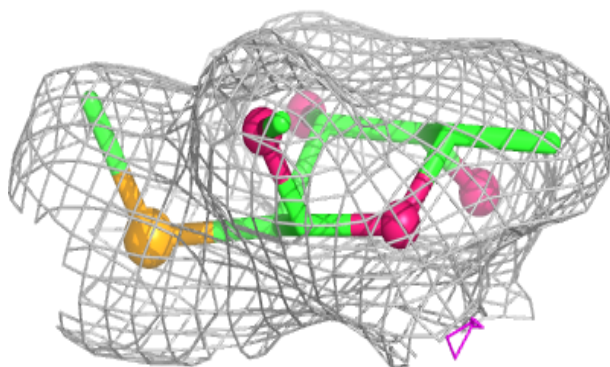
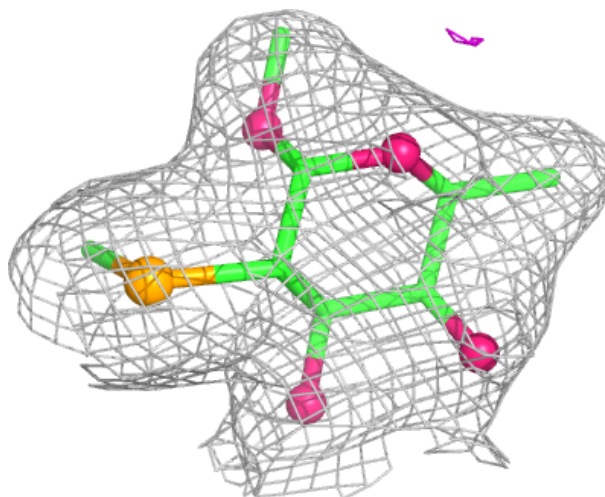
Electron density around FSW I 1004:

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



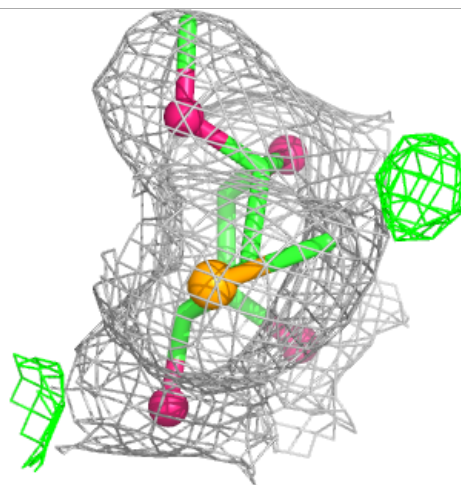
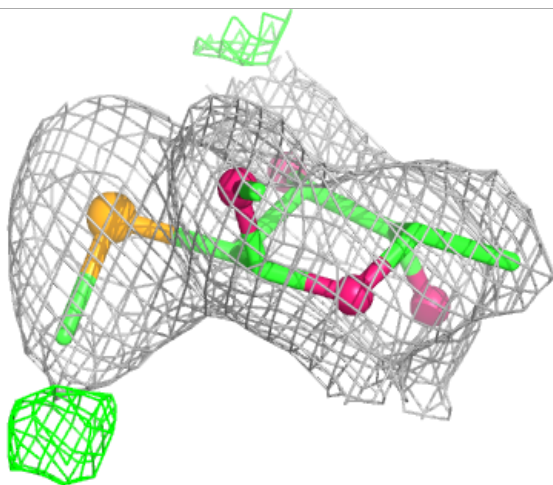
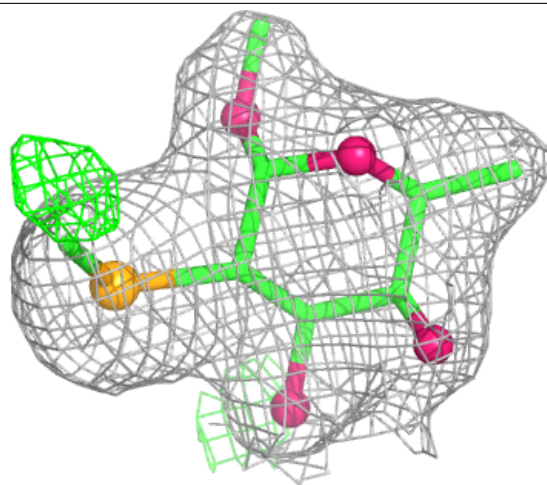
Electron density around FSW D 1003:

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



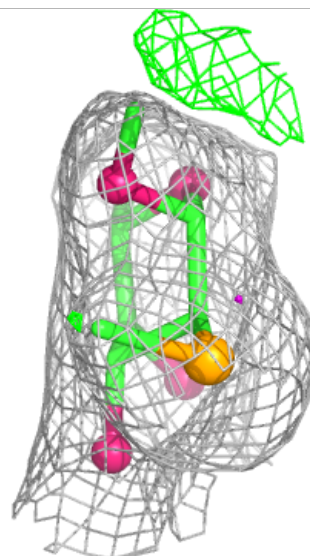
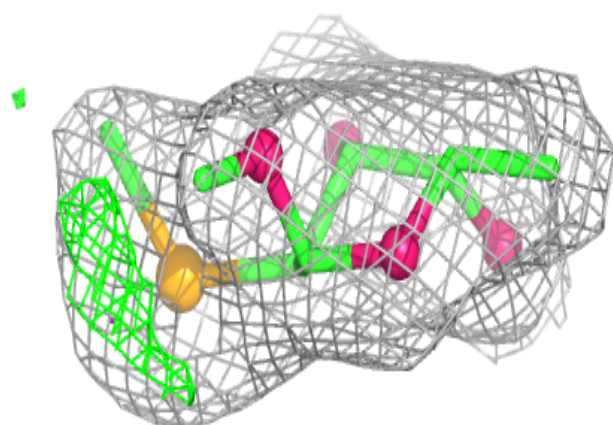
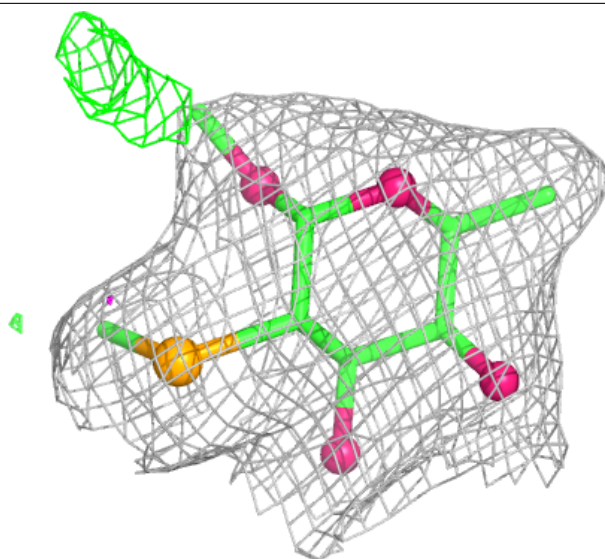
Electron density around FSW D 1005:

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



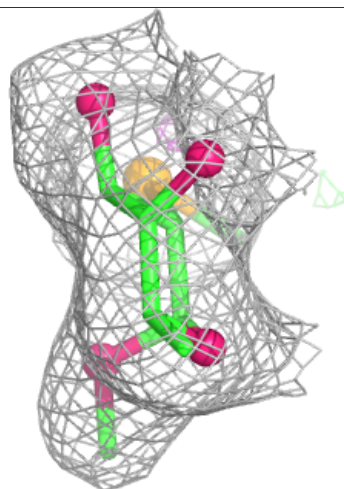
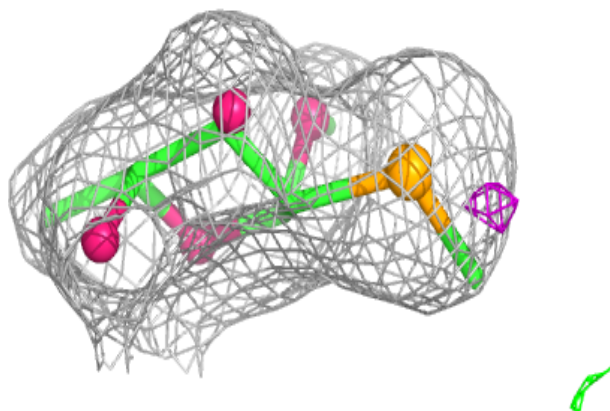
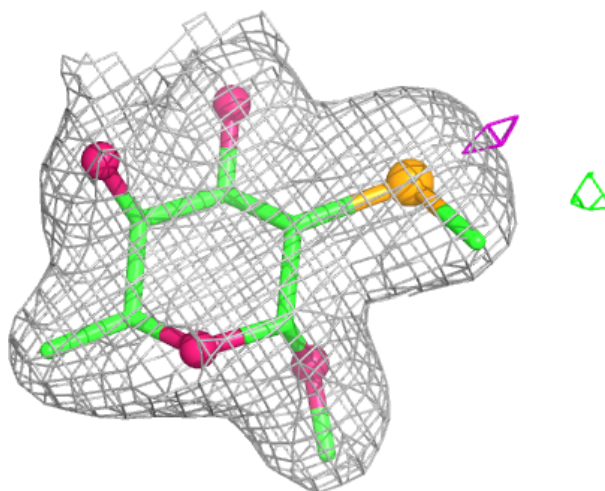
Electron density around FSW F 1003:

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



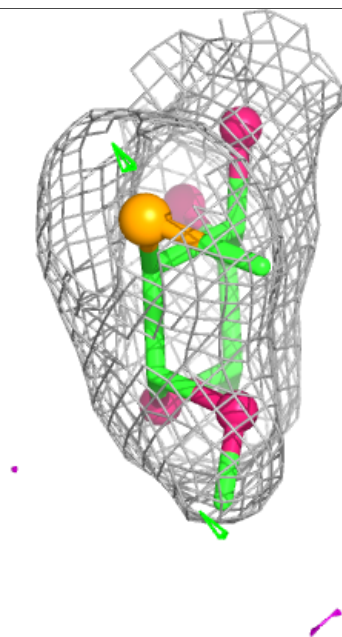
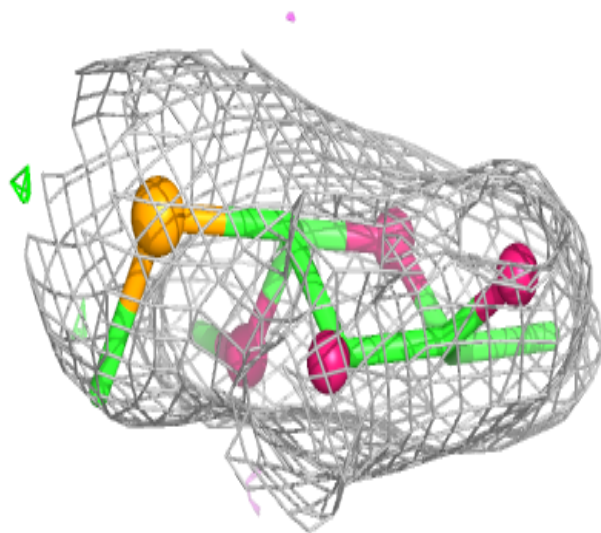
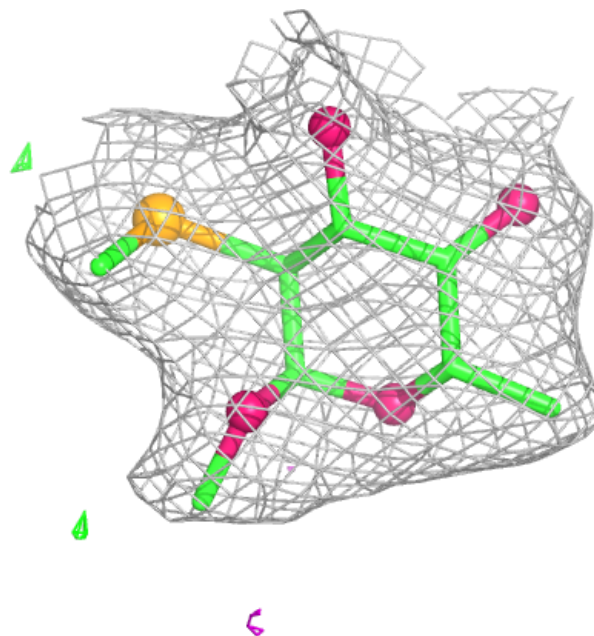
Electron density around FSW A 1006:

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



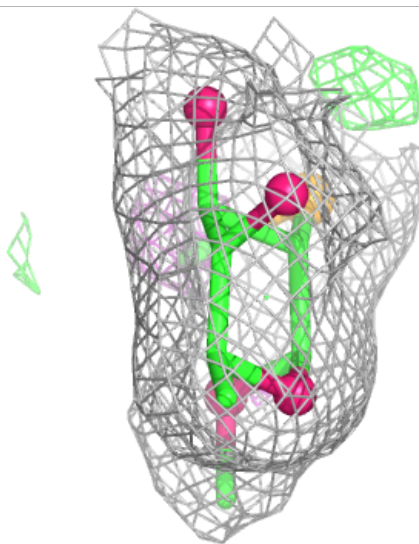
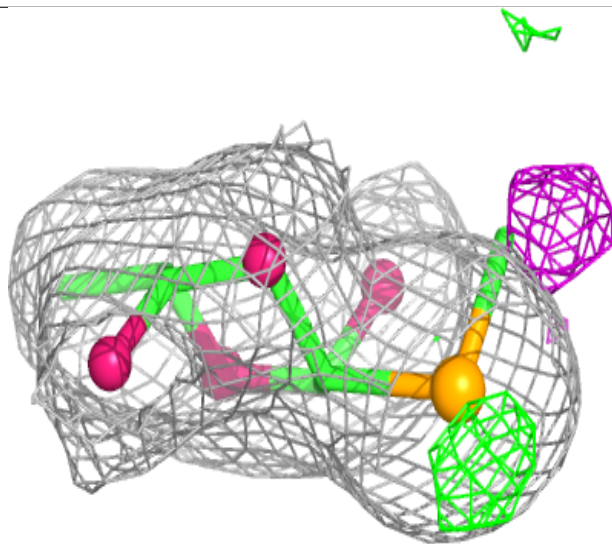
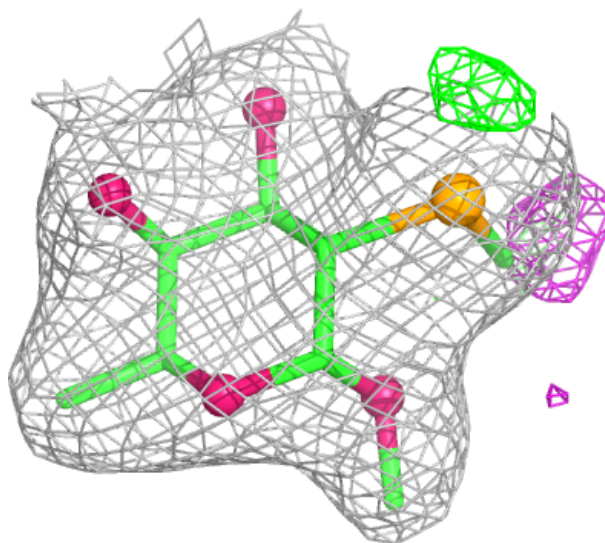
Electron density around FSW J 1003:

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



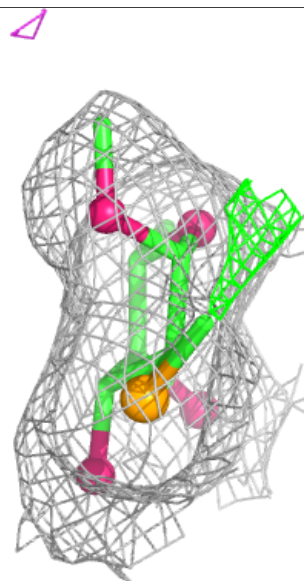
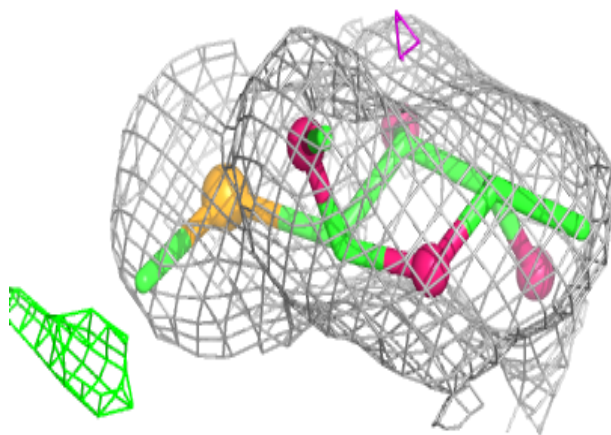
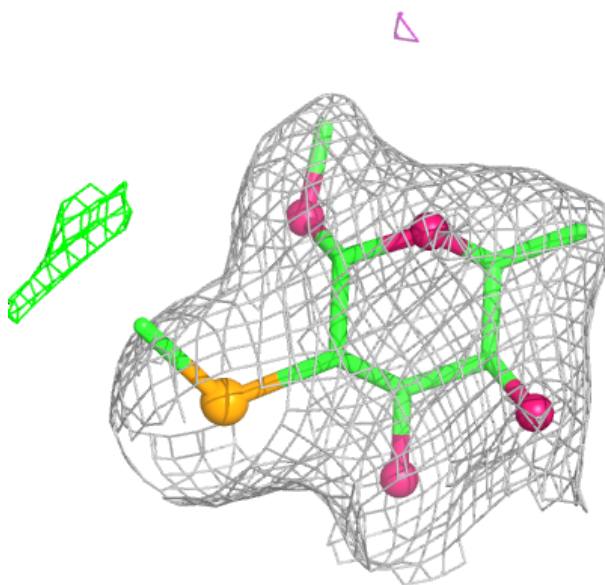
Electron density around FSW A 1004:

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



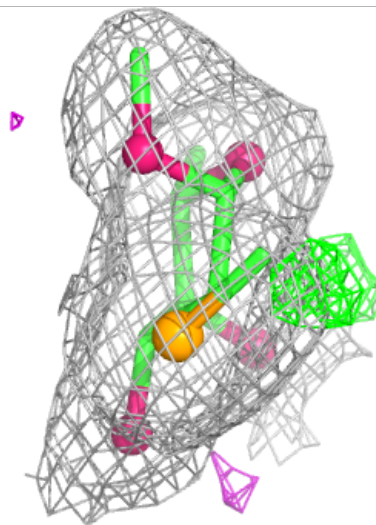
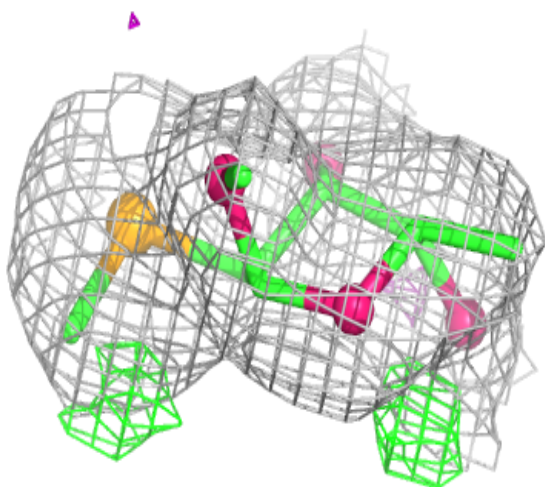
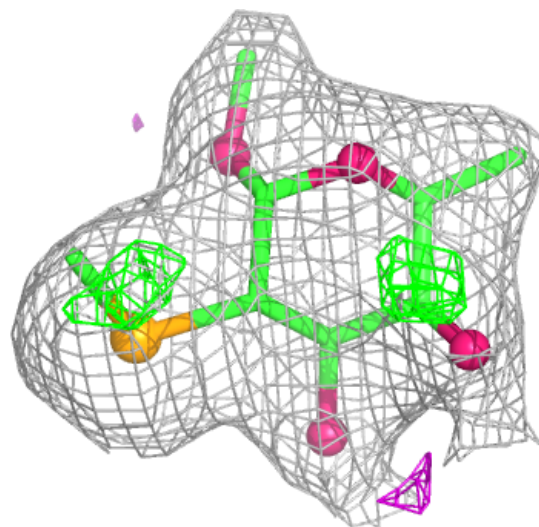
Electron density around FSW C 1003:

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



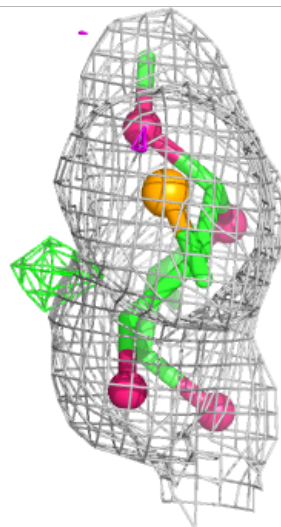
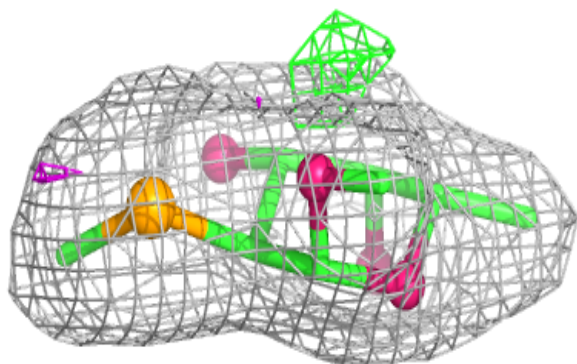
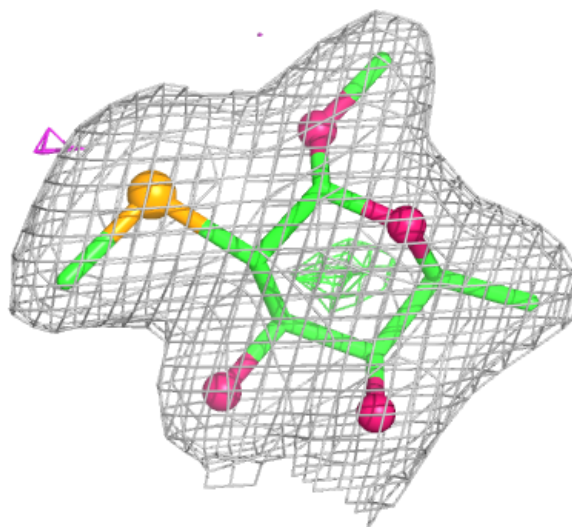
Electron density around FSW F 1002:

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



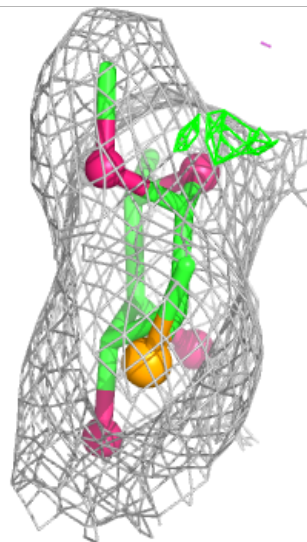
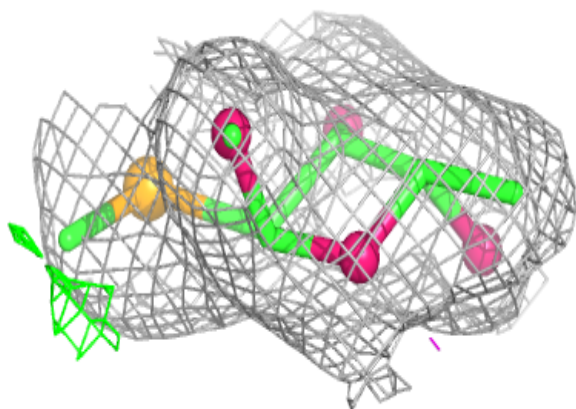
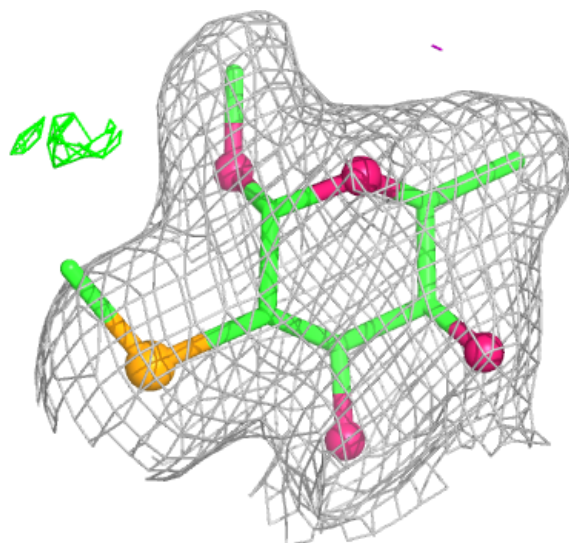
Electron density around FSW C 1004:

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



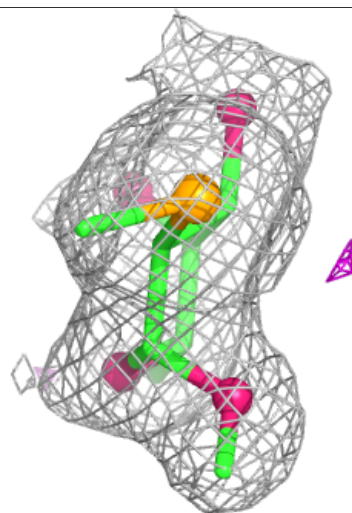
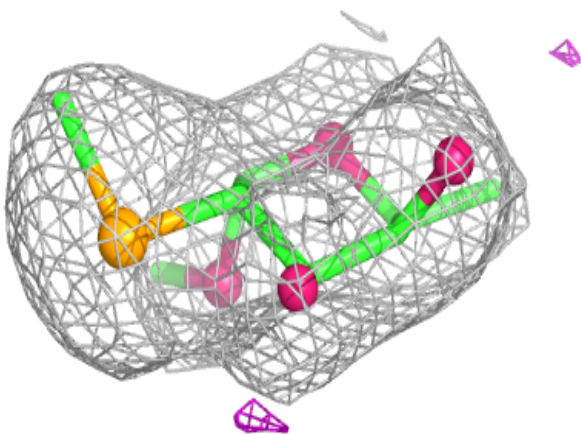
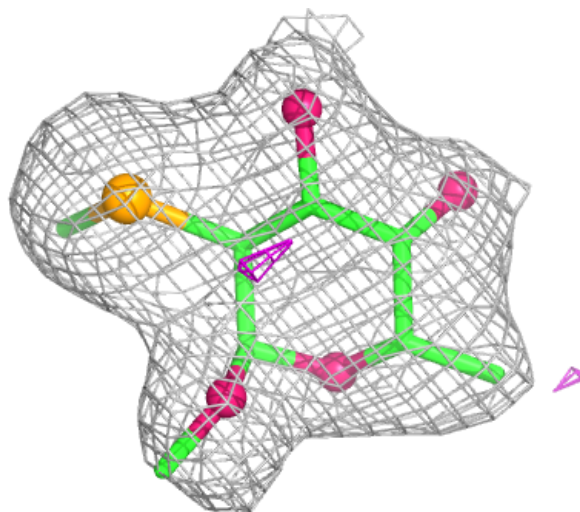
Electron density around FSW B 1003:

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



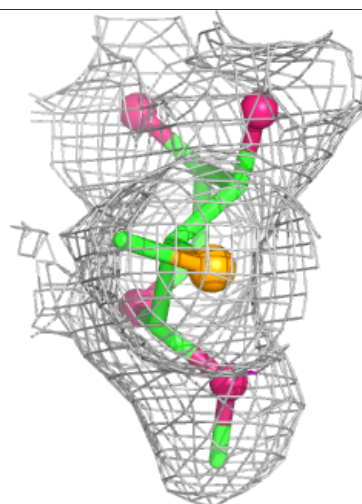
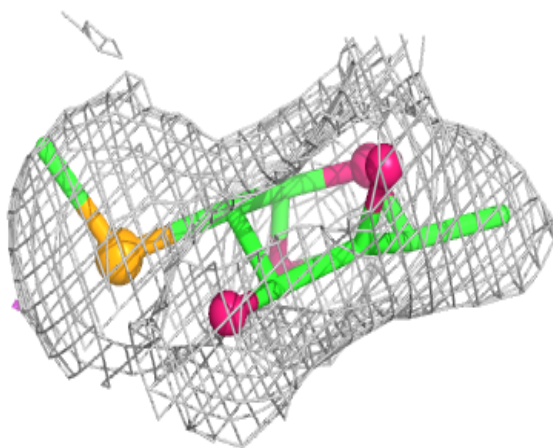
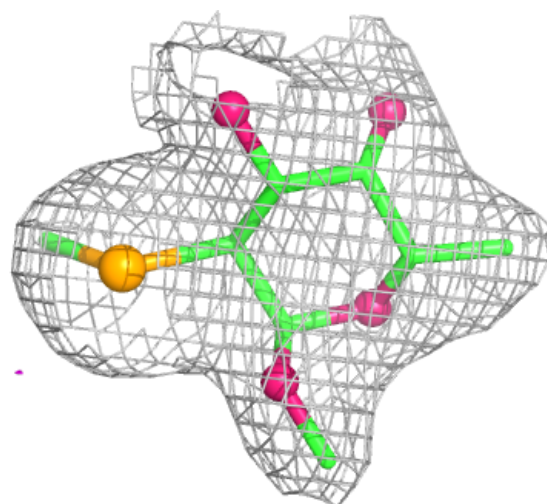
Electron density around FSW A 1005:

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



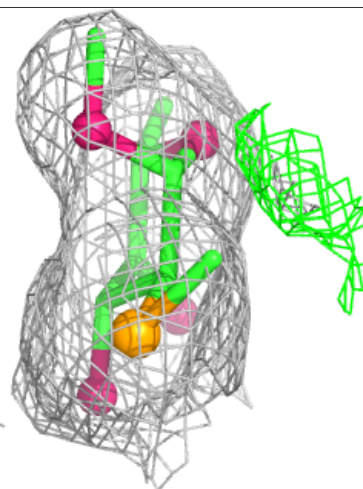
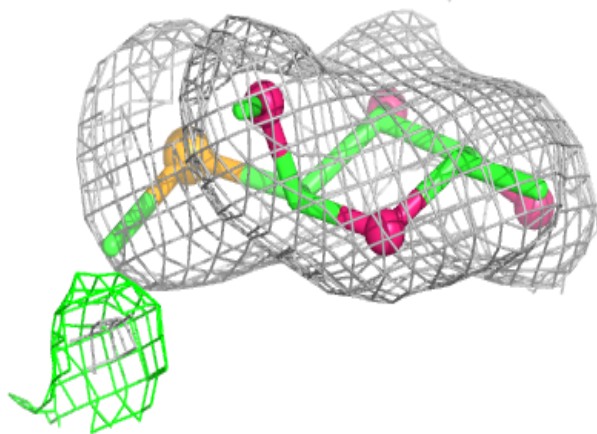
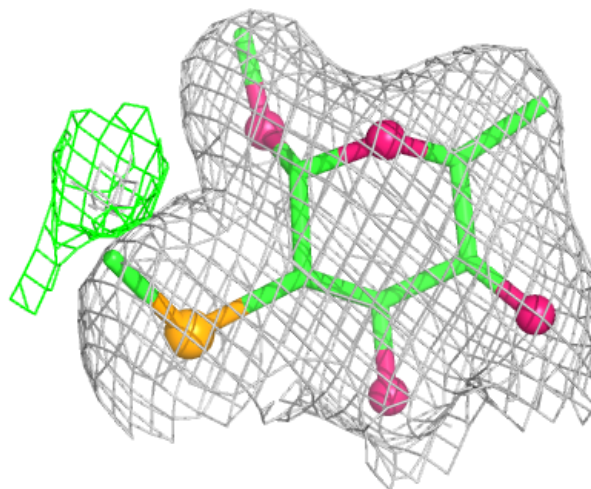
Electron density around FSW A 1003:

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



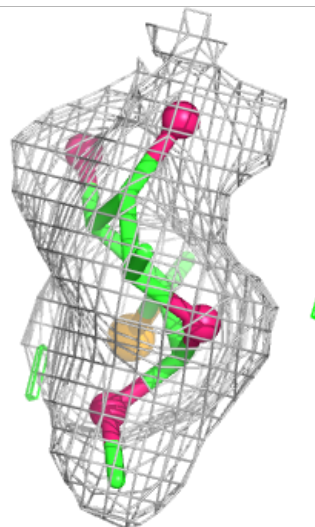
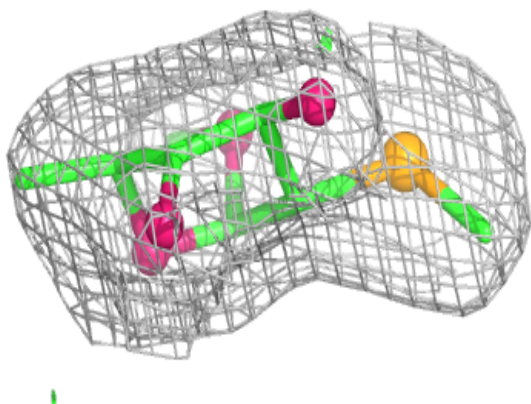
Electron density around FSW B 1001:

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



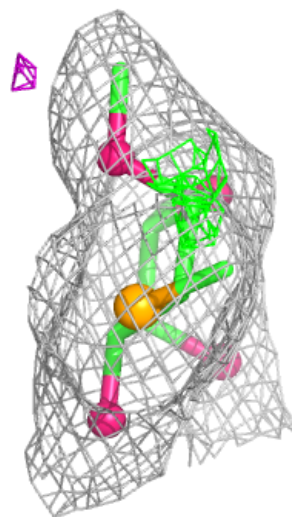
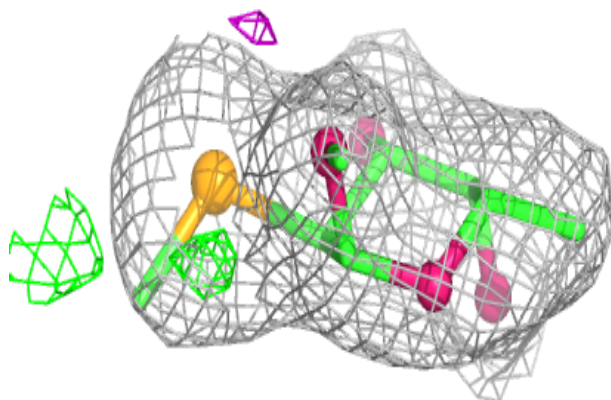
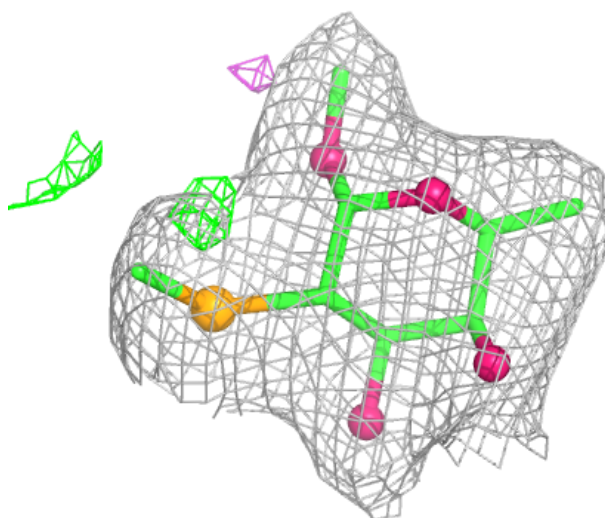
Electron density around FSW J 1004:

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



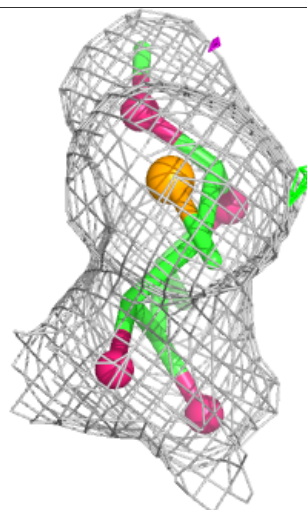
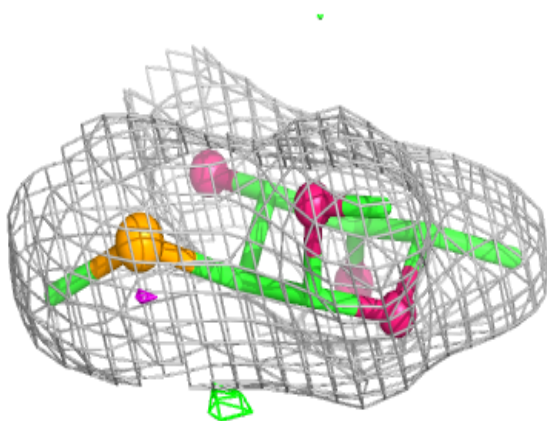
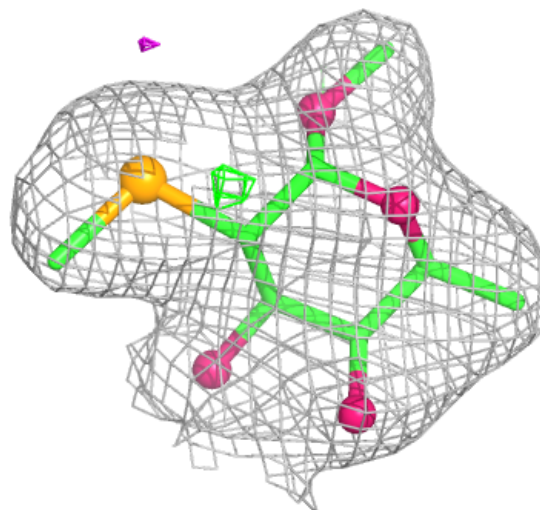
Electron density around FSW C 1002:

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



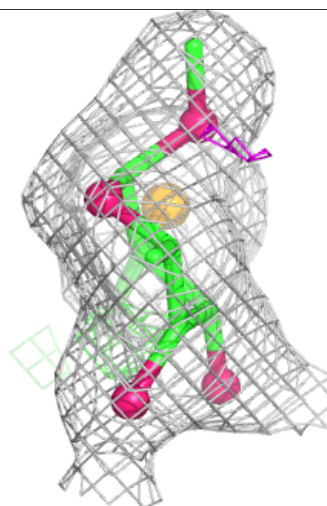
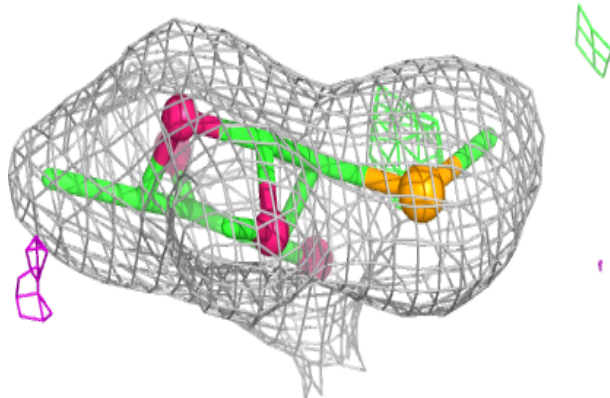
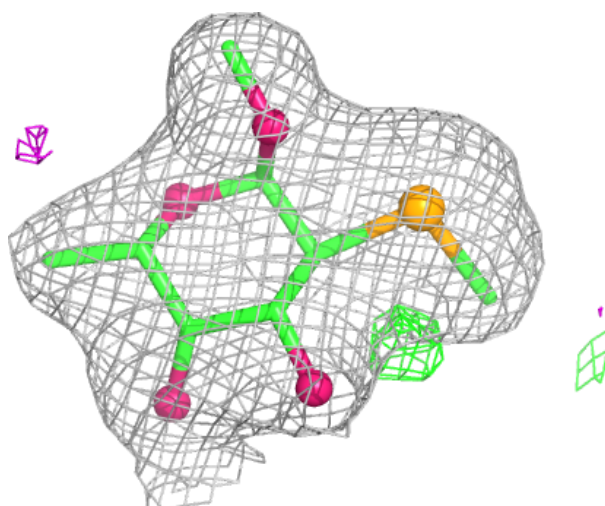
Electron density around FSW G 1004:

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



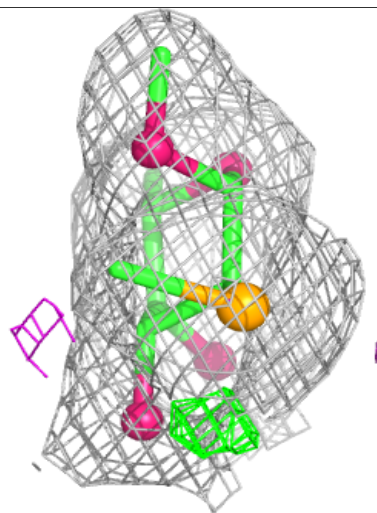
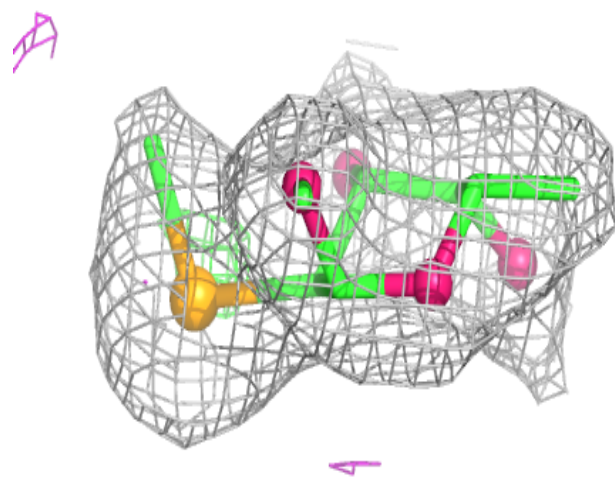
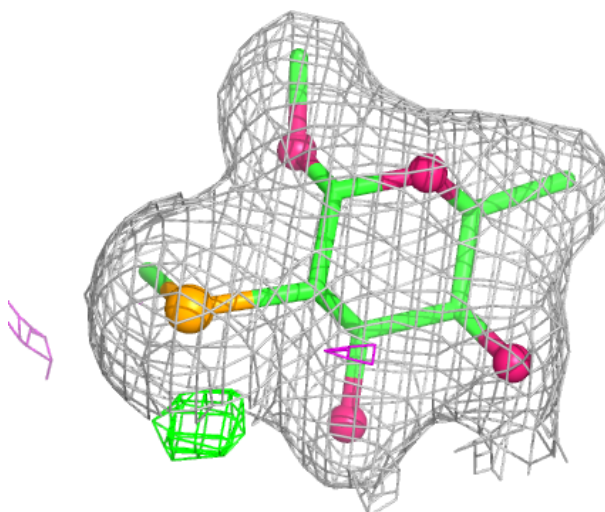
Electron density around FSW E 1004:

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



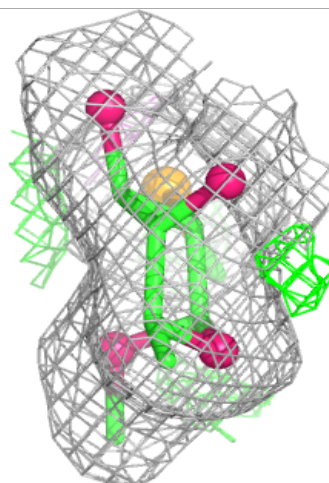
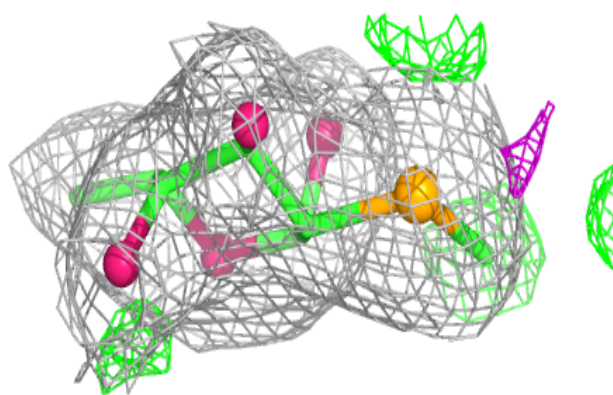
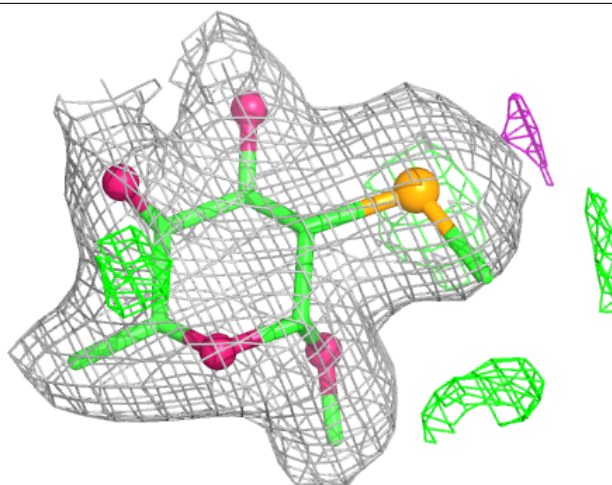
Electron density around FSW B 1002:

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



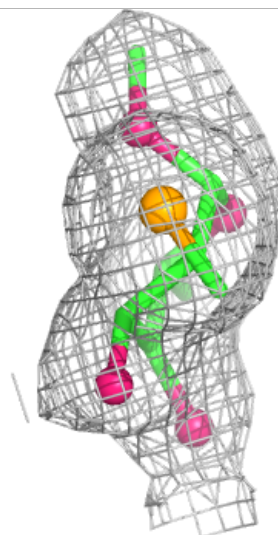
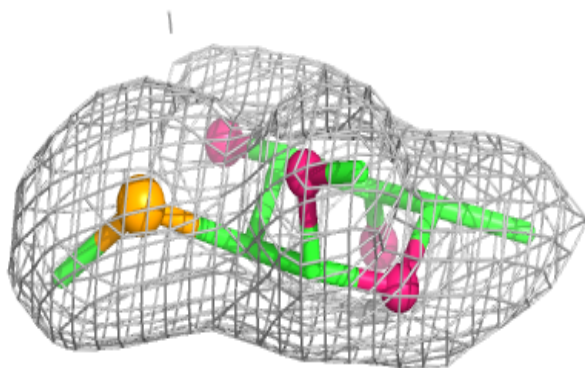
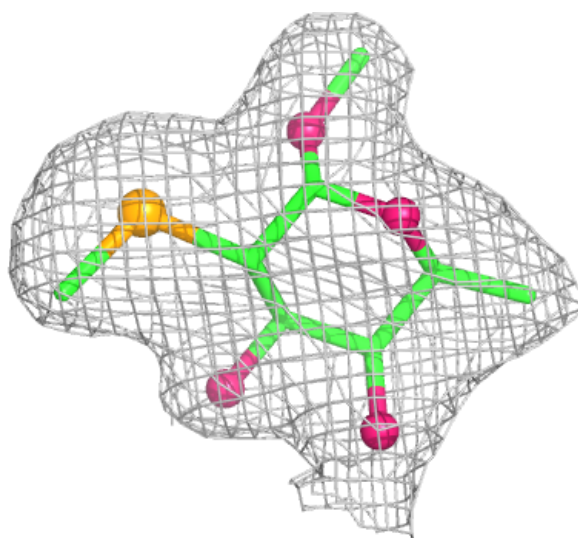
Electron density around FSW A 1002:

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



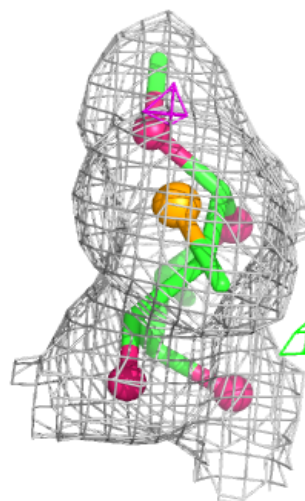
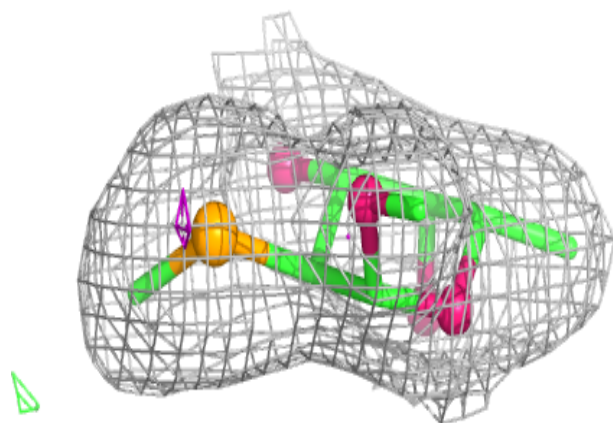
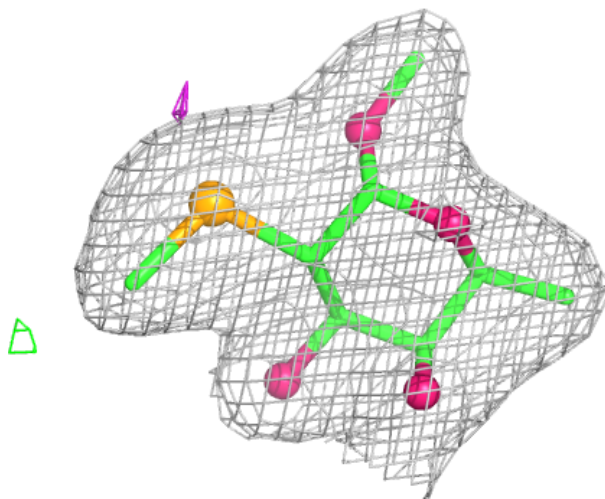
Electron density around FSW D 1004:

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



Electron density around FSW B 1004:

$2mF_o-DF_c$ (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.