



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:57 PM UTC

PDB ID : 8H5A / pdb_00008h5a
Title : Crystal structure of YhaJ effector binding domain (ligand-bound)
Authors : Kim, M.; Ryu, S.E.
Deposited on : 2022-10-12
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

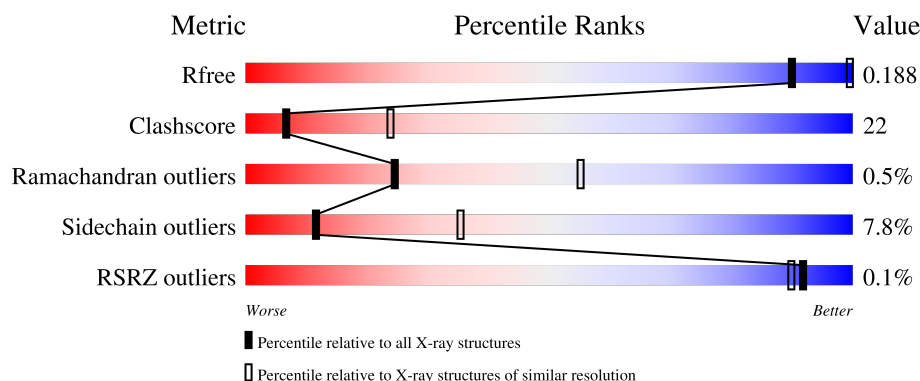
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	207	58% 32% 6% ..
1	B	207	60% 34% . ..
1	C	207	71% 23% . ..
1	D	207	58% 36%
1	E	207	63% 28% 5% ..

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Mol	Chain	Length	Quality of chain
1	F	207	
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	
1	O	207	
1	P	207	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7DV	A	301	-	-	X	-
2	7DV	B	302	-	-	X	-
2	7DV	C	301	-	-	X	-
2	7DV	E	301	-	-	X	-
2	7DV	F	301	-	-	X	-
2	7DV	H	303	-	-	X	-
2	7DV	I	301	-	-	X	-
2	7DV	J	301	-	-	X	-
2	7DV	M	301	-	-	X	-
2	7DV	N	301	-	-	X	-
2	7DV	N	302	-	-	X	-
2	7DV	P	301	-	-	X	-
2	7DV	P	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25837 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 HTH-type transcriptional regulator YhaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	B	202	Total	C	N	O	S	0	0	0
			1584	1005	276	295	8			
1	C	202	Total	C	N	O	S	0	0	0
			1580	1004	278	291	7			
1	D	203	Total	C	N	O	S	0	0	0
			1570	996	272	294	8			
1	E	202	Total	C	N	O	S	0	0	0
			1581	1003	278	293	7			
1	F	204	Total	C	N	O	S	0	0	0
			1597	1013	279	297	8			
1	G	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	H	203	Total	C	N	O	S	0	0	0
			1588	1007	277	296	8			
1	I	202	Total	C	N	O	S	0	0	0
			1581	1005	277	292	7			
1	J	200	Total	C	N	O	S	0	0	0
			1569	995	273	293	8			
1	K	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	L	201	Total	C	N	O	S	0	0	0
			1574	998	274	294	8			
1	M	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	N	203	Total	C	N	O	S	0	0	0
			1584	1005	277	294	8			
1	O	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	P	203	Total	C	N	O	S	0	0	0
			1584	1004	276	296	8			

There are 64 discrepancies between the modelled and reference sequences:

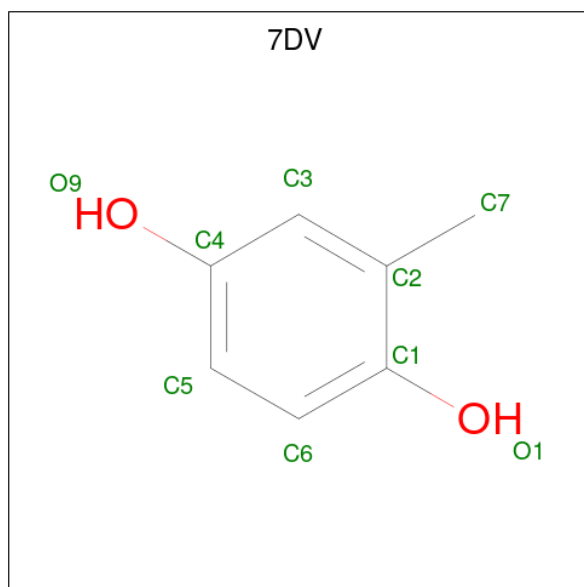
Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	-	expression tag	UNP P67661
A	93	SER	-	expression tag	UNP P67661
A	94	HIS	-	expression tag	UNP P67661
A	95	MET	-	expression tag	UNP P67661
B	92	GLY	-	expression tag	UNP P67661
B	93	SER	-	expression tag	UNP P67661
B	94	HIS	-	expression tag	UNP P67661
B	95	MET	-	expression tag	UNP P67661
C	92	GLY	-	expression tag	UNP P67661
C	93	SER	-	expression tag	UNP P67661
C	94	HIS	-	expression tag	UNP P67661
C	95	MET	-	expression tag	UNP P67661
D	92	GLY	-	expression tag	UNP P67661
D	93	SER	-	expression tag	UNP P67661
D	94	HIS	-	expression tag	UNP P67661
D	95	MET	-	expression tag	UNP P67661
E	92	GLY	-	expression tag	UNP P67661
E	93	SER	-	expression tag	UNP P67661
E	94	HIS	-	expression tag	UNP P67661
E	95	MET	-	expression tag	UNP P67661
F	92	GLY	-	expression tag	UNP P67661
F	93	SER	-	expression tag	UNP P67661
F	94	HIS	-	expression tag	UNP P67661
F	95	MET	-	expression tag	UNP P67661
G	92	GLY	-	expression tag	UNP P67661
G	93	SER	-	expression tag	UNP P67661
G	94	HIS	-	expression tag	UNP P67661
G	95	MET	-	expression tag	UNP P67661
H	92	GLY	-	expression tag	UNP P67661
H	93	SER	-	expression tag	UNP P67661
H	94	HIS	-	expression tag	UNP P67661
H	95	MET	-	expression tag	UNP P67661
I	92	GLY	-	expression tag	UNP P67661
I	93	SER	-	expression tag	UNP P67661
I	94	HIS	-	expression tag	UNP P67661
I	95	MET	-	expression tag	UNP P67661
J	92	GLY	-	expression tag	UNP P67661
J	93	SER	-	expression tag	UNP P67661
J	94	HIS	-	expression tag	UNP P67661
J	95	MET	-	expression tag	UNP P67661
K	92	GLY	-	expression tag	UNP P67661
K	93	SER	-	expression tag	UNP P67661

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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	HIS	-	expression tag	UNP P67661
K	95	MET	-	expression tag	UNP P67661
L	92	GLY	-	expression tag	UNP P67661
L	93	SER	-	expression tag	UNP P67661
L	94	HIS	-	expression tag	UNP P67661
L	95	MET	-	expression tag	UNP P67661
M	92	GLY	-	expression tag	UNP P67661
M	93	SER	-	expression tag	UNP P67661
M	94	HIS	-	expression tag	UNP P67661
M	95	MET	-	expression tag	UNP P67661
N	92	GLY	-	expression tag	UNP P67661
N	93	SER	-	expression tag	UNP P67661
N	94	HIS	-	expression tag	UNP P67661
N	95	MET	-	expression tag	UNP P67661
O	92	GLY	-	expression tag	UNP P67661
O	93	SER	-	expression tag	UNP P67661
O	94	HIS	-	expression tag	UNP P67661
O	95	MET	-	expression tag	UNP P67661
P	92	GLY	-	expression tag	UNP P67661
P	93	SER	-	expression tag	UNP P67661
P	94	HIS	-	expression tag	UNP P67661
P	95	MET	-	expression tag	UNP P67661

- Molecule 2 is 2-methylbenzene-1,4-diol (CCD ID: 7DV) (formula: C₇H₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 7 2	0	0
2	A	1	Total C O 9 7 2	0	0
2	A	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			9	7	2		
2	H	1	Total	C	O	0	0
			9	7	2		
2	H	1	Total	C	O	0	0
			9	7	2		
2	I	1	Total	C	O	0	0
			9	7	2		
2	I	1	Total	C	O	0	0
			9	7	2		
2	I	1	Total	C	O	0	0
			9	7	2		
2	J	1	Total	C	O	0	0
			9	7	2		
2	J	1	Total	C	O	0	0
			9	7	2		
2	J	1	Total	C	O	0	0
			9	7	2		
2	K	1	Total	C	O	0	0
			9	7	2		
2	K	1	Total	C	O	0	0
			9	7	2		
2	K	1	Total	C	O	0	0
			9	7	2		
2	L	1	Total	C	O	0	0
			9	7	2		
2	L	1	Total	C	O	0	0
			9	7	2		
2	L	1	Total	C	O	0	0
			9	7	2		
2	L	1	Total	C	O	0	0
			9	7	2		
2	M	1	Total	C	O	0	0
			9	7	2		
2	M	1	Total	C	O	0	0
			9	7	2		
2	M	1	Total	C	O	0	0
			9	7	2		
2	N	1	Total	C	O	0	0
			9	7	2		
2	N	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	N	1	Total	C	O	0	0
			9	7	2		
2	O	1	Total	C	O	0	0
			9	7	2		
2	O	1	Total	C	O	0	0
			9	7	2		
2	O	1	Total	C	O	0	0
			9	7	2		
2	P	1	Total	C	O	0	0
			9	7	2		
2	P	1	Total	C	O	0	0
			9	7	2		
2	P	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	I	2	Total	Na	0	0
			2	2		
3	K	1	Total	Na	0	0
			1	1		
3	L	1	Total	Na	0	0
			1	1		
3	N	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total 1	Na 1	0	0
3	P	1	Total 1	Na 1	0	0

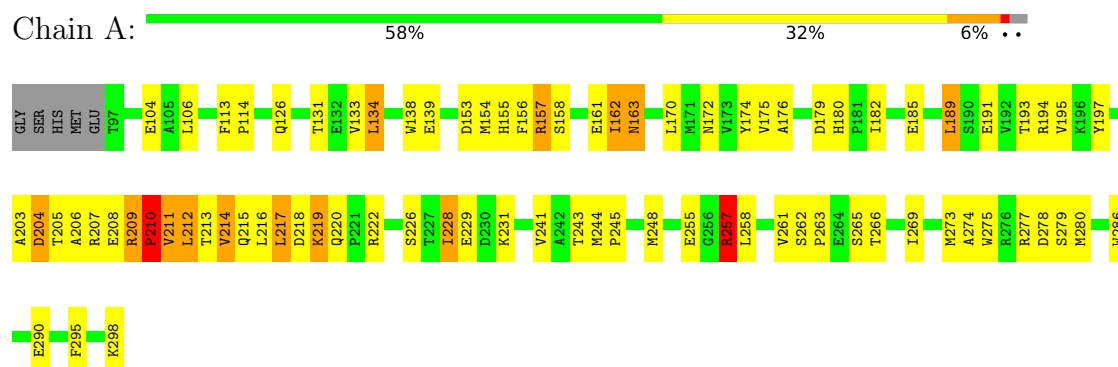
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	4	Total 4	O 4	0	0
4	C	5	Total 5	O 5	0	0
4	D	3	Total 3	O 3	0	0
4	E	3	Total 3	O 3	0	0
4	F	5	Total 5	O 5	0	0
4	G	1	Total 1	O 1	0	0
4	H	6	Total 6	O 6	0	0
4	I	6	Total 6	O 6	0	0
4	J	4	Total 4	O 4	0	0
4	K	1	Total 1	O 1	0	0
4	L	4	Total 4	O 4	0	0
4	M	9	Total 9	O 9	0	0
4	N	4	Total 4	O 4	0	0
4	O	11	Total 11	O 11	0	0
4	P	3	Total 3	O 3	0	0

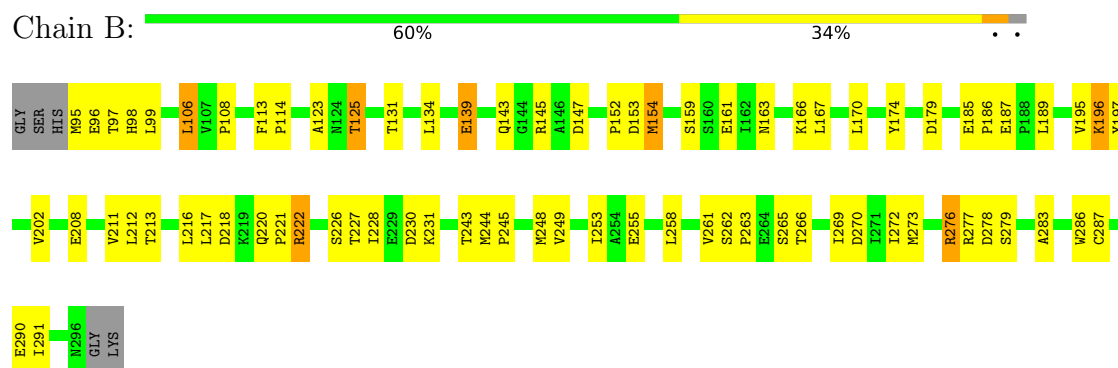
3 Residue-property plots

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

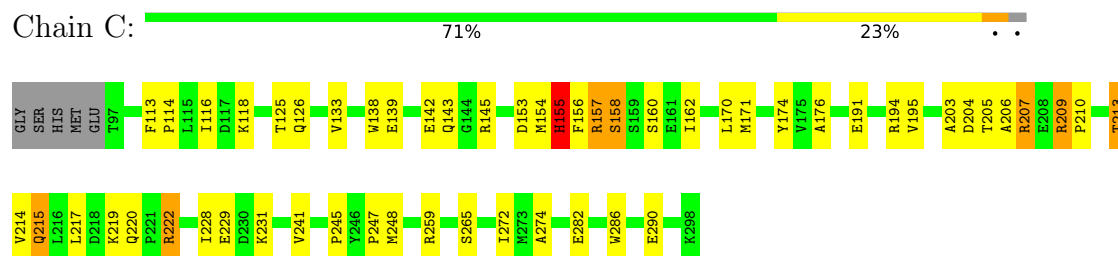
- Molecule 1: HTH-type transcriptional regulator YhaJ



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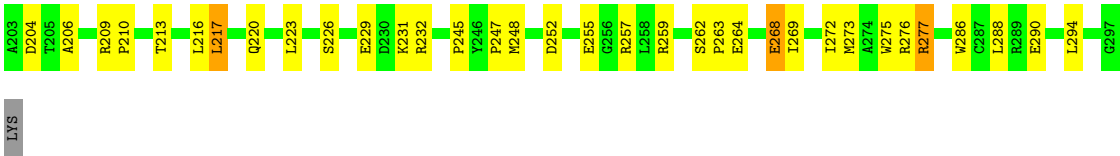


- Molecule 1: HTH-type transcriptional regulator YhaJ



- Molecule 1: HTH-type transcriptional regulator YhaJ





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	215.75Å 215.75Å 264.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.80 35.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (35.00-2.80) 99.9 (35.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.232 0.151 , 0.188	Depositor DCC
R_{free} test set	5969 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.170 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.175 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.176 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.176 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.176 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.176 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.197 for h,-h-k,-l	Xtriage

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¹Intensities estimated from amplitudes.

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

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Property	Value	Source
Reported twinning fraction	0.122 for H, K, L 0.125 for K, H, -L 0.128 for -K, $-1/3H+1/3K-2/3L$, $4/3H+2/3K-1/3L$ 0.120 for $-1/3H-2/3K-2/3L$, $-2/3H-1/3K+2/3L$, $-2/3H+2/3K-1/3L$ 0.128 for $-1/3H+1/3K-2/3L$, -K, $-4/3H-2/3K+1/3L$ 0.130 for -H, $1/3H-1/3K+2/3L$, $2/3H+4/3K+1/3L$ 0.125 for $1/3H-1/3K+2/3L$, -H, $-2/3H-4/3K-1/3L$ 0.122 for $-2/3H-1/3K+2/3L$, $-1/3H-2/3K-2/3L$, $2/3H-2/3K+1/3L$	Depositor
Outliers	0 of 112445 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25837	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 7DV

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	0.73	0/1615	1.05	3/2196 (0.1%)
1	B	0.66	0/1615	0.98	2/2198 (0.1%)
1	C	0.67	0/1611	0.98	1/2191 (0.0%)
1	D	0.68	0/1601	1.04	5/2183 (0.2%)
1	E	0.72	0/1612	1.03	3/2192 (0.1%)
1	F	0.69	0/1628	1.15	9/2214 (0.4%)
1	G	0.68	0/1611	1.01	2/2192 (0.1%)
1	H	0.69	0/1619	1.03	5/2203 (0.2%)
1	I	0.67	0/1612	1.03	3/2192 (0.1%)
1	J	0.73	1/1599 (0.1%)	1.10	5/2175 (0.2%)
1	K	0.76	2/1611 (0.1%)	1.06	5/2192 (0.2%)
1	L	0.73	0/1604	1.08	8/2182 (0.4%)
1	M	0.72	1/1611 (0.1%)	1.10	7/2192 (0.3%)
1	N	0.73	0/1615	1.02	2/2198 (0.1%)
1	O	0.71	0/1615	1.06	4/2196 (0.2%)
1	P	0.71	0/1615	1.06	4/2199 (0.2%)
All	All	0.70	4/25794 (0.0%)	1.05	68/35095 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
1	N	0	2
1	P	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	290	GLU	CD-OE2	-6.81	1.12	1.25
1	K	180	HIS	CE1-NE2	5.66	1.38	1.32
1	M	183	HIS	CE1-NE2	5.62	1.38	1.32
1	K	183	HIS	CG-ND1	5.58	1.44	1.38

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	157	ARG	CB-CG-CD	14.07	143.66	111.30
1	O	191	GLU	CB-CA-C	10.23	131.69	110.31
1	O	140	ARG	CB-CG-CD	8.99	131.98	111.30
1	N	229	GLU	CB-CG-CD	8.94	127.79	112.60
1	N	161	GLU	CB-CA-C	-8.90	96.01	110.79

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ALA	Mainchain
1	D	278	ASP	Peptide
1	E	156	PHE	Peptide
1	F	156	PHE	Peptide
1	G	214	VAL	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1584	0	1629	108	0
1	B	1584	0	1617	86	1
1	C	1580	0	1625	76	0
1	D	1570	0	1583	84	0
1	E	1581	0	1621	81	0
1	F	1597	0	1633	85	1
1	G	1580	0	1618	66	0
1	H	1588	0	1620	96	0
1	I	1581	0	1626	94	0
1	J	1569	0	1596	66	1
1	K	1580	0	1619	74	0
1	L	1574	0	1600	84	1
1	M	1580	0	1619	73	0
1	N	1584	0	1615	56	2
1	O	1584	0	1628	62	0
1	P	1584	0	1610	59	0
2	A	27	0	0	6	0
2	B	27	0	0	8	0
2	C	27	0	0	7	0
2	D	36	0	0	5	0
2	E	27	0	0	9	0
2	F	27	0	0	7	0
2	G	27	0	0	2	0
2	H	27	0	0	8	0
2	I	27	0	0	8	0
2	J	27	0	0	7	0
2	K	27	0	0	2	0
2	L	36	0	0	2	0
2	M	27	0	0	7	0
2	N	27	0	0	9	0
2	O	27	0	0	4	0
2	P	27	0	0	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	6	0	0	5	0
4	I	6	0	0	0	0
4	J	4	0	0	1	0
4	K	1	0	0	0	0
4	L	4	0	0	0	0
4	M	9	0	0	2	0
4	N	4	0	0	0	0
4	O	11	0	0	1	0
4	P	3	0	0	0	0
All	All	25837	0	25859	1110	3

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 22.

The worst 5 of 1110 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:275:TRP:CZ3	1:L:280:MET:HE2	1.57	1.40
1:L:275:TRP:CZ3	1:L:280:MET:CE	2.08	1.36
1:I:134:LEU:CD1	2:I:301:7DV:O9	1.80	1.29
1:L:275:TRP:HZ3	1:L:280:MET:CE	1.43	1.29
1:K:174:TYR:OH	1:K:241:VAL:HG12	1.19	1.26

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:285:SER:OG	1:N:282:GLU:OE1[8_544]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:OD1	1:F:163:ASN:ND2[6_555]	2.05	0.15
1:J:277:ARG:NH1	1:N:285:SER:OG[8_544]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/207 (97%)	185 (92%)	14 (7%)	1 (0%)	24	55
1	B	200/207 (97%)	193 (96%)	7 (4%)	0	100	100
1	C	200/207 (97%)	186 (93%)	11 (6%)	3 (2%)	8	28
1	D	201/207 (97%)	189 (94%)	12 (6%)	0	100	100
1	E	200/207 (97%)	186 (93%)	10 (5%)	4 (2%)	6	21
1	F	202/207 (98%)	192 (95%)	10 (5%)	0	100	100
1	G	200/207 (97%)	187 (94%)	12 (6%)	1 (0%)	24	55
1	H	201/207 (97%)	189 (94%)	12 (6%)	0	100	100
1	I	200/207 (97%)	188 (94%)	10 (5%)	2 (1%)	12	38
1	J	196/207 (95%)	187 (95%)	9 (5%)	0	100	100
1	K	200/207 (97%)	189 (94%)	9 (4%)	2 (1%)	12	38
1	L	197/207 (95%)	188 (95%)	9 (5%)	0	100	100
1	M	200/207 (97%)	191 (96%)	7 (4%)	2 (1%)	12	38
1	N	201/207 (97%)	191 (95%)	10 (5%)	0	100	100
1	O	200/207 (97%)	189 (94%)	9 (4%)	2 (1%)	12	38
1	P	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
All	All	3199/3312 (97%)	3022 (94%)	160 (5%)	17 (0%)	24	55

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	157	ARG
1	O	208	GLU
1	O	210	PRO
1	C	215	GLN
1	E	206	ALA

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	173/177 (98%)	154 (89%)	19 (11%)	6	20
1	B	173/177 (98%)	165 (95%)	8 (5%)	24	58
1	C	172/177 (97%)	161 (94%)	11 (6%)	16	44
1	D	169/177 (96%)	155 (92%)	14 (8%)	10	32
1	E	172/177 (97%)	158 (92%)	14 (8%)	11	33
1	F	174/177 (98%)	157 (90%)	17 (10%)	7	25
1	G	172/177 (97%)	165 (96%)	7 (4%)	27	62
1	H	173/177 (98%)	160 (92%)	13 (8%)	12	37
1	I	172/177 (97%)	159 (92%)	13 (8%)	12	36
1	J	172/177 (97%)	156 (91%)	16 (9%)	8	27
1	K	172/177 (97%)	165 (96%)	7 (4%)	27	62
1	L	172/177 (97%)	158 (92%)	14 (8%)	11	33
1	M	172/177 (97%)	157 (91%)	15 (9%)	9	30
1	N	172/177 (97%)	151 (88%)	21 (12%)	5	16
1	O	173/177 (98%)	160 (92%)	13 (8%)	12	37
1	P	172/177 (97%)	159 (92%)	13 (8%)	12	36
All	All	2755/2832 (97%)	2540 (92%)	215 (8%)	11	35

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	280	MET

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Mol	Chain	Res	Type
1	L	192	VAL
1	O	248	MET
1	J	154	MET
1	J	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	155	HIS
1	P	163	ASN
1	J	126	GLN
1	I	172	ASN
1	P	184	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 16 are monoatomic - leaving 50 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7DV	C	303	-	9,9,9	1.16	1 (11%)	12,12,12	2.18	4 (33%)
2	7DV	E	301	-	9,9,9	1.47	2 (22%)	12,12,12	1.94	4 (33%)
2	7DV	D	302	-	9,9,9	1.11	1 (11%)	12,12,12	1.14	0
2	7DV	I	301	-	9,9,9	1.32	2 (22%)	12,12,12	1.78	2 (16%)
2	7DV	M	302	-	9,9,9	1.87	4 (44%)	12,12,12	1.18	1 (8%)
2	7DV	F	303	-	9,9,9	0.80	0	12,12,12	0.79	0
2	7DV	P	303	-	9,9,9	1.09	0	12,12,12	1.57	3 (25%)
2	7DV	D	304	-	9,9,9	1.14	1 (11%)	12,12,12	1.46	2 (16%)
2	7DV	J	303	-	9,9,9	1.04	0	12,12,12	1.49	2 (16%)
2	7DV	I	303	-	9,9,9	0.95	0	12,12,12	1.17	1 (8%)
2	7DV	A	302	-	9,9,9	1.09	1 (11%)	12,12,12	1.04	1 (8%)
2	7DV	C	302	-	9,9,9	0.96	0	12,12,12	0.82	0
2	7DV	J	302	-	9,9,9	0.88	0	12,12,12	1.04	0
2	7DV	M	301	-	9,9,9	1.82	3 (33%)	12,12,12	2.41	4 (33%)
2	7DV	J	301	-	9,9,9	1.25	1 (11%)	12,12,12	1.30	2 (16%)
2	7DV	L	301	-	9,9,9	0.94	0	12,12,12	0.92	0
2	7DV	A	301	-	9,9,9	0.90	0	12,12,12	1.32	2 (16%)
2	7DV	G	303	-	9,9,9	0.99	0	12,12,12	1.54	2 (16%)
2	7DV	B	303	-	9,9,9	1.18	1 (11%)	12,12,12	1.22	2 (16%)
2	7DV	O	302	-	9,9,9	1.25	0	12,12,12	1.54	2 (16%)
2	7DV	B	302	-	9,9,9	0.94	0	12,12,12	0.60	0
2	7DV	E	302	-	9,9,9	1.53	1 (11%)	12,12,12	1.29	2 (16%)
2	7DV	P	302	-	9,9,9	0.89	0	12,12,12	1.96	4 (33%)
2	7DV	G	301	-	9,9,9	1.47	1 (11%)	12,12,12	2.16	3 (25%)
2	7DV	G	302	-	9,9,9	1.06	0	12,12,12	0.93	1 (8%)
2	7DV	L	304	-	9,9,9	1.16	0	12,12,12	1.40	2 (16%)
2	7DV	K	303	-	9,9,9	1.36	2 (22%)	12,12,12	0.88	0
2	7DV	H	303	-	9,9,9	1.06	0	12,12,12	0.95	0
2	7DV	K	302	-	9,9,9	1.64	3 (33%)	12,12,12	1.11	2 (16%)
2	7DV	N	303	-	9,9,9	1.06	1 (11%)	12,12,12	1.35	2 (16%)
2	7DV	L	303	-	9,9,9	1.16	1 (11%)	12,12,12	0.95	1 (8%)
2	7DV	B	301	-	9,9,9	1.42	3 (33%)	12,12,12	1.41	1 (8%)
2	7DV	M	303	-	9,9,9	1.02	0	12,12,12	1.41	2 (16%)
2	7DV	N	301	-	9,9,9	1.46	1 (11%)	12,12,12	1.19	1 (8%)
2	7DV	K	301	-	9,9,9	1.13	1 (11%)	12,12,12	0.85	0
2	7DV	H	301	-	9,9,9	1.03	1 (11%)	12,12,12	1.17	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7DV	H	302	-	9,9,9	0.99	0	12,12,12	1.11	0
2	7DV	L	302	-	9,9,9	1.16	0	12,12,12	0.96	0
2	7DV	F	301	-	9,9,9	1.69	3 (33%)	12,12,12	1.45	2 (16%)
2	7DV	F	302	-	9,9,9	1.15	1 (11%)	12,12,12	1.50	2 (16%)
2	7DV	P	301	-	9,9,9	1.04	0	12,12,12	0.92	0
2	7DV	A	303	-	9,9,9	1.02	0	12,12,12	1.26	2 (16%)
2	7DV	I	302	-	9,9,9	1.06	0	12,12,12	0.91	0
2	7DV	O	303	-	9,9,9	1.01	0	12,12,12	1.35	1 (8%)
2	7DV	E	303	-	9,9,9	1.16	2 (22%)	12,12,12	1.37	2 (16%)
2	7DV	D	303	-	9,9,9	0.85	0	12,12,12	0.70	0
2	7DV	O	301	-	9,9,9	1.66	2 (22%)	12,12,12	2.45	4 (33%)
2	7DV	N	302	-	9,9,9	1.15	1 (11%)	12,12,12	1.32	1 (8%)
2	7DV	D	301	-	9,9,9	1.19	0	12,12,12	1.55	3 (25%)
2	7DV	C	301	-	9,9,9	1.07	0	12,12,12	1.46	3 (25%)

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	7DV	C	303	-	-	-	0/1/1/1
2	7DV	E	301	-	-	-	0/1/1/1
2	7DV	D	302	-	-	-	0/1/1/1
2	7DV	I	301	-	-	-	0/1/1/1
2	7DV	M	302	-	-	-	0/1/1/1
2	7DV	F	303	-	-	-	0/1/1/1
2	7DV	P	303	-	-	-	0/1/1/1
2	7DV	D	304	-	-	-	0/1/1/1
2	7DV	J	303	-	-	-	0/1/1/1
2	7DV	I	303	-	-	-	0/1/1/1
2	7DV	A	302	-	-	-	0/1/1/1
2	7DV	C	302	-	-	-	0/1/1/1
2	7DV	J	302	-	-	-	0/1/1/1
2	7DV	M	301	-	-	-	0/1/1/1
2	7DV	J	301	-	-	-	0/1/1/1
2	7DV	L	301	-	-	-	0/1/1/1
2	7DV	A	301	-	-	-	0/1/1/1
2	7DV	G	303	-	-	-	0/1/1/1
2	7DV	B	303	-	-	-	0/1/1/1
2	7DV	O	302	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7DV	B	302	-	-	-	0/1/1/1
2	7DV	E	302	-	-	-	0/1/1/1
2	7DV	P	302	-	-	-	0/1/1/1
2	7DV	G	301	-	-	-	0/1/1/1
2	7DV	G	302	-	-	-	0/1/1/1
2	7DV	L	304	-	-	-	0/1/1/1
2	7DV	K	303	-	-	-	0/1/1/1
2	7DV	H	303	-	-	-	0/1/1/1
2	7DV	K	302	-	-	-	0/1/1/1
2	7DV	N	303	-	-	-	0/1/1/1
2	7DV	L	303	-	-	-	0/1/1/1
2	7DV	B	301	-	-	-	0/1/1/1
2	7DV	M	303	-	-	-	0/1/1/1
2	7DV	N	301	-	-	-	0/1/1/1
2	7DV	K	301	-	-	-	0/1/1/1
2	7DV	H	301	-	-	-	0/1/1/1
2	7DV	H	302	-	-	-	0/1/1/1
2	7DV	L	302	-	-	-	0/1/1/1
2	7DV	F	301	-	-	-	0/1/1/1
2	7DV	F	302	-	-	-	0/1/1/1
2	7DV	P	301	-	-	-	0/1/1/1
2	7DV	A	303	-	-	-	0/1/1/1
2	7DV	I	302	-	-	-	0/1/1/1
2	7DV	O	303	-	-	-	0/1/1/1
2	7DV	E	303	-	-	-	0/1/1/1
2	7DV	D	303	-	-	-	0/1/1/1
2	7DV	O	301	-	-	-	0/1/1/1
2	7DV	N	302	-	-	-	0/1/1/1
2	7DV	D	301	-	-	-	0/1/1/1
2	7DV	C	301	-	-	-	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	302	7DV	O1-C1	3.62	1.43	1.36
2	K	302	7DV	O1-C1	3.54	1.43	1.36
2	E	302	7DV	O1-C1	3.33	1.43	1.36
2	M	301	7DV	O1-C1	3.28	1.42	1.36
2	O	301	7DV	O1-C1	3.25	1.42	1.36

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	301	7DV	C7-C2-C1	5.85	126.70	120.69
2	M	301	7DV	C7-C2-C1	5.37	126.21	120.69
2	C	303	7DV	C7-C2-C1	4.69	125.51	120.69
2	E	301	7DV	C7-C2-C1	4.68	125.50	120.69
2	G	301	7DV	O1-C1-C2	4.30	125.88	117.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 106 short contacts:

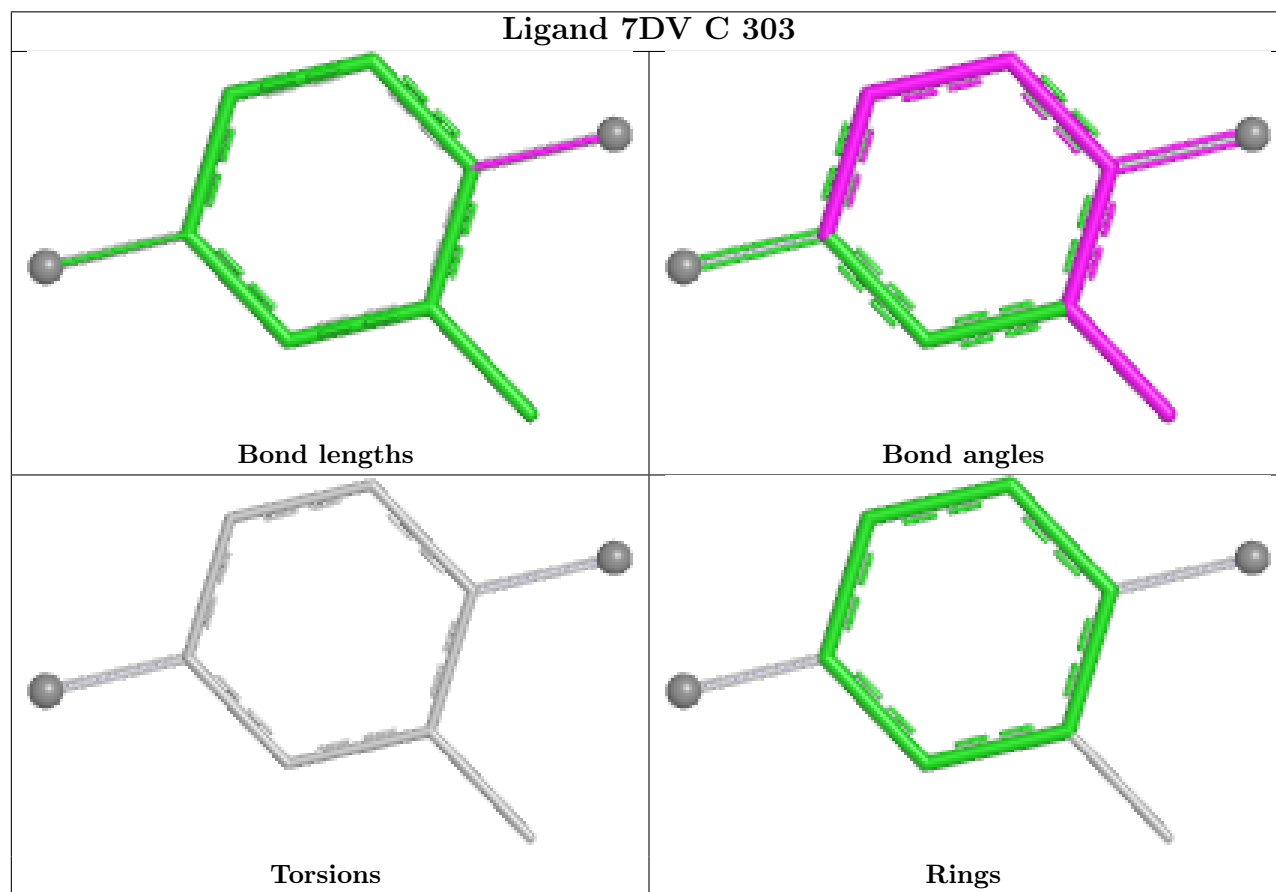
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	7DV	8	0
2	D	302	7DV	2	0
2	I	301	7DV	7	0
2	M	302	7DV	2	0
2	P	303	7DV	2	0
2	D	304	7DV	1	0
2	C	302	7DV	3	0
2	J	302	7DV	2	0
2	M	301	7DV	5	0
2	J	301	7DV	5	0
2	A	301	7DV	6	0
2	O	302	7DV	2	0
2	B	302	7DV	5	0
2	E	302	7DV	1	0
2	P	302	7DV	8	0
2	G	301	7DV	1	0
2	G	302	7DV	1	0
2	H	303	7DV	4	0
2	K	302	7DV	1	0
2	B	301	7DV	3	0
2	N	301	7DV	5	0
2	K	301	7DV	1	0
2	H	301	7DV	1	0
2	H	302	7DV	3	0
2	L	302	7DV	2	0
2	F	301	7DV	5	0
2	F	302	7DV	2	0
2	P	301	7DV	5	0
2	I	302	7DV	1	0
2	O	301	7DV	2	0

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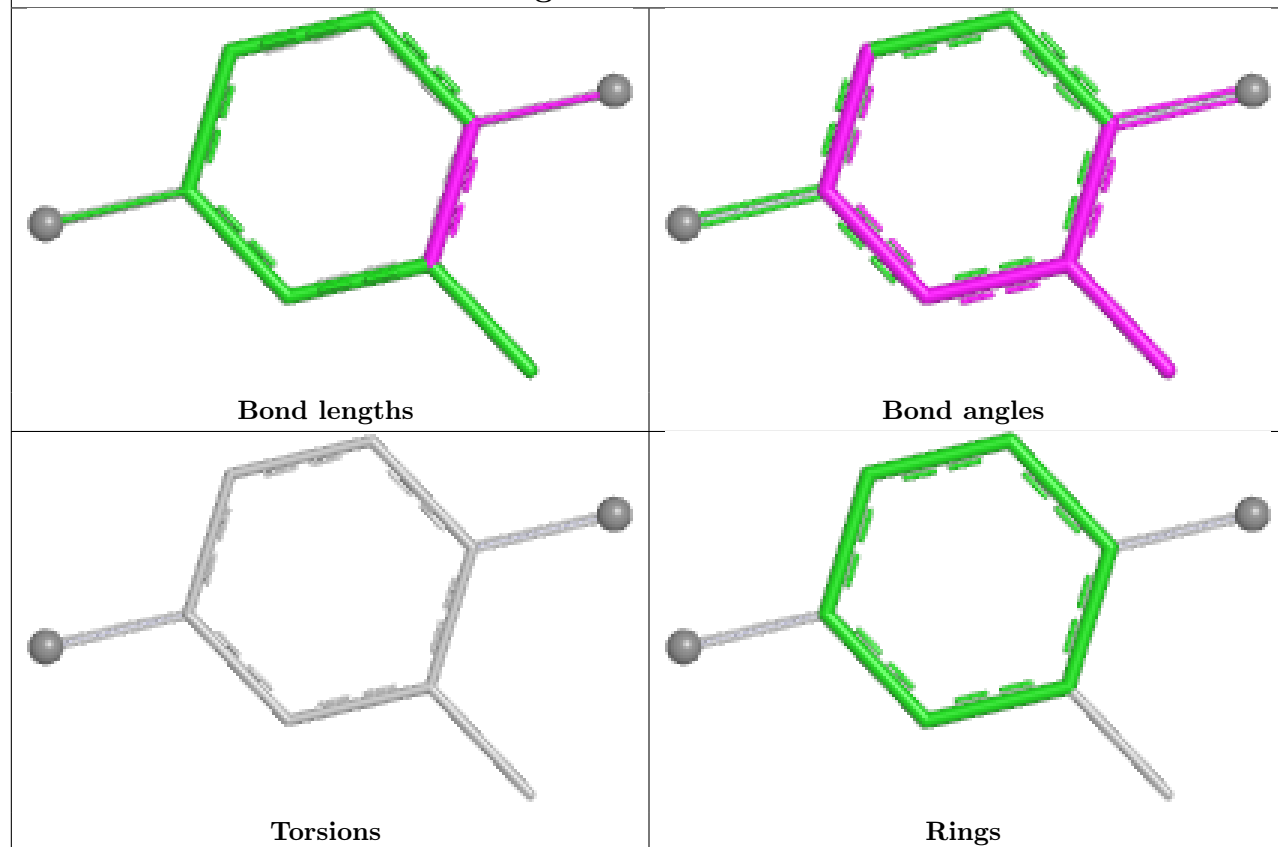
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	302	7DV	4	0
2	D	301	7DV	2	0
2	C	301	7DV	4	0

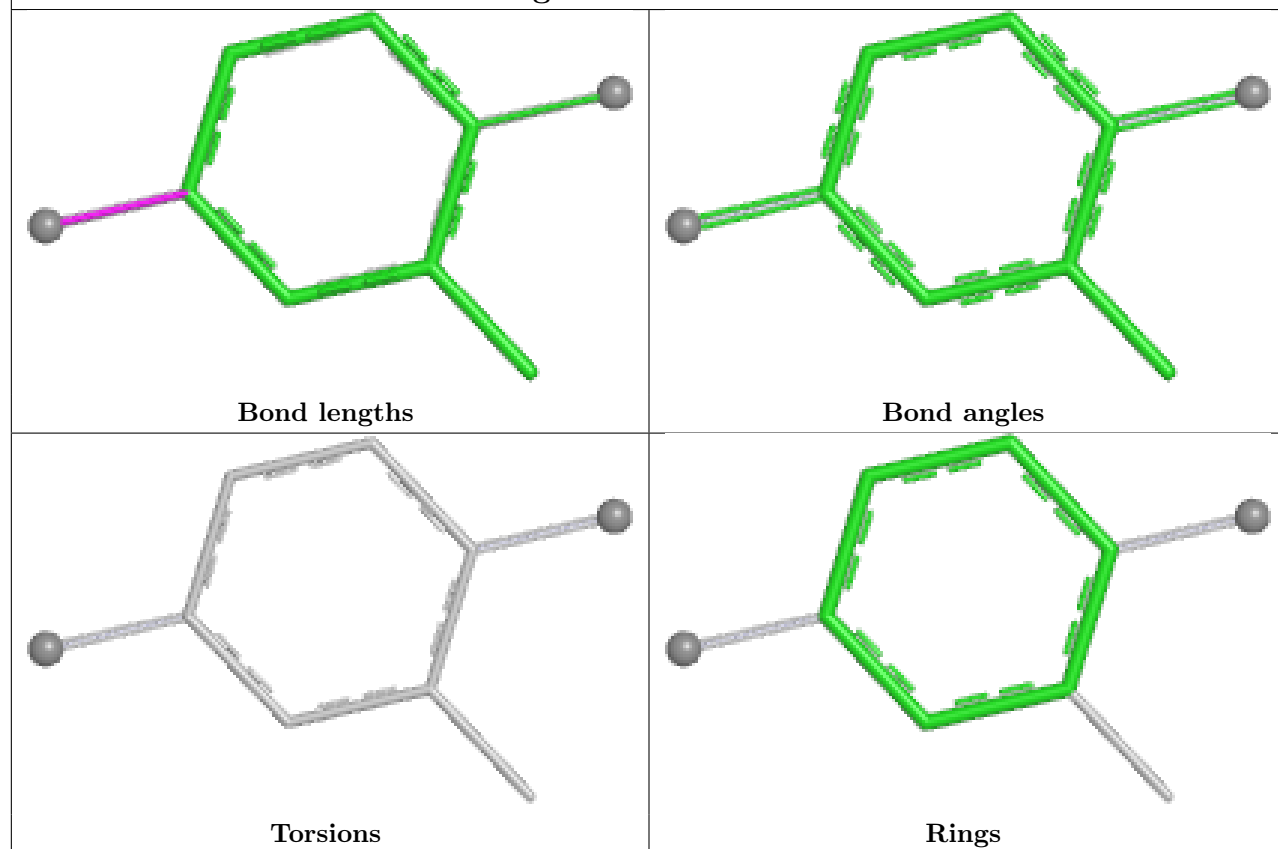
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



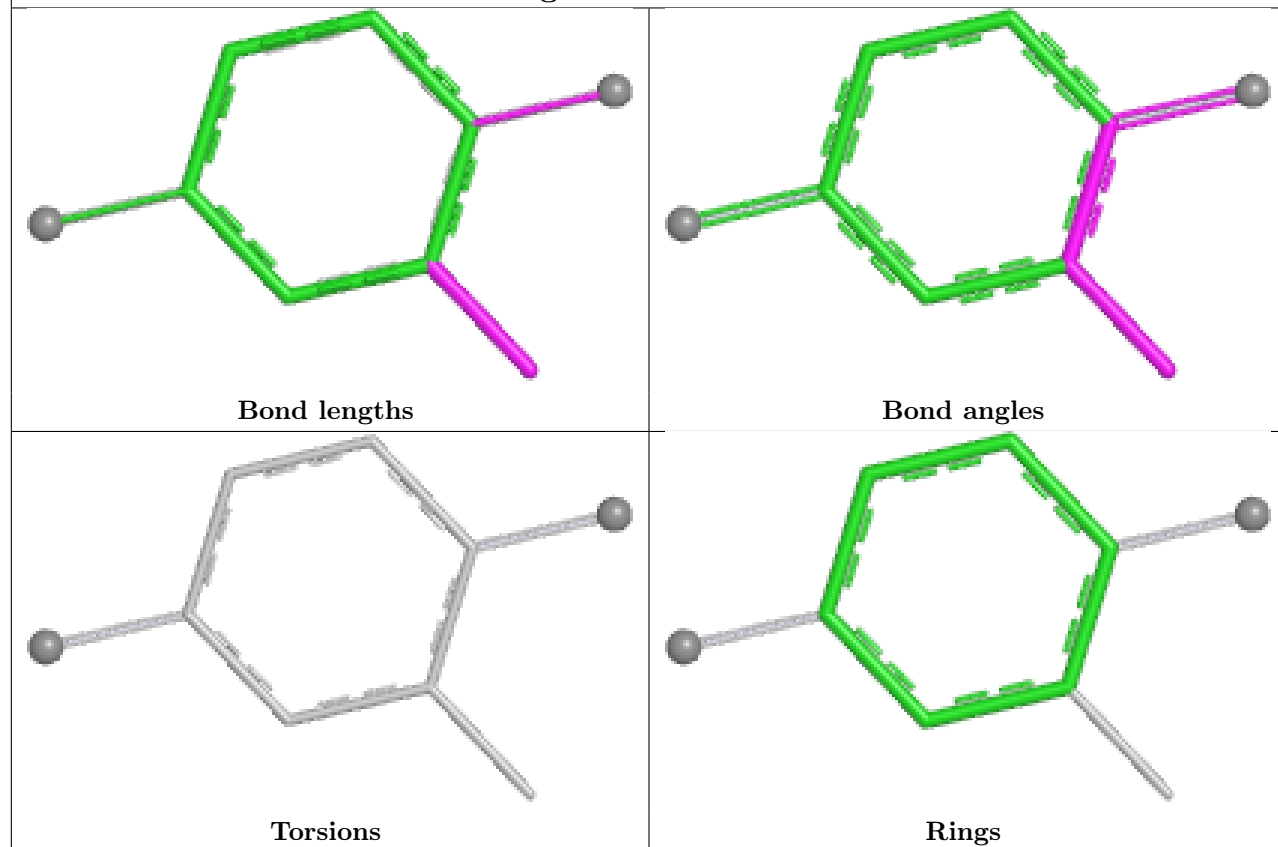
Ligand 7DV E 301



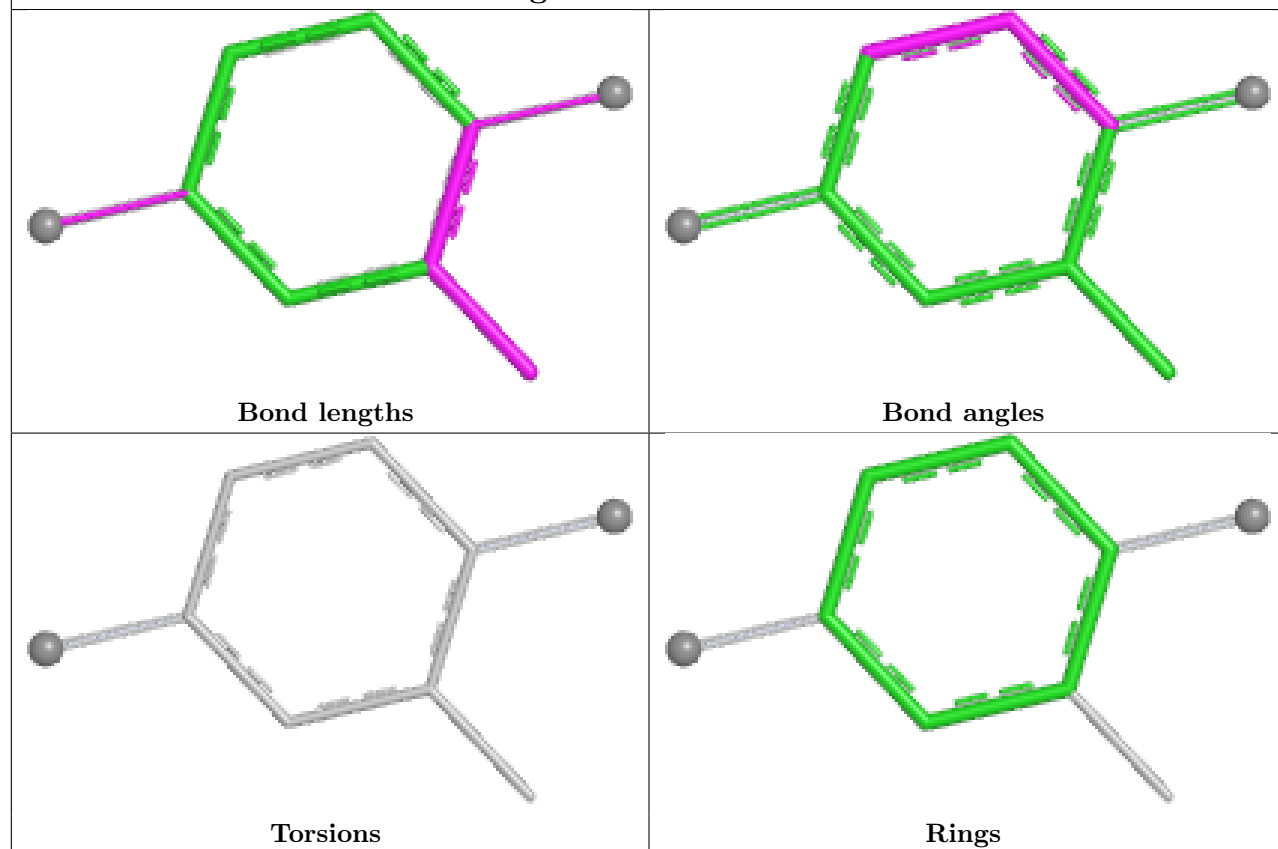
Ligand 7DV D 302



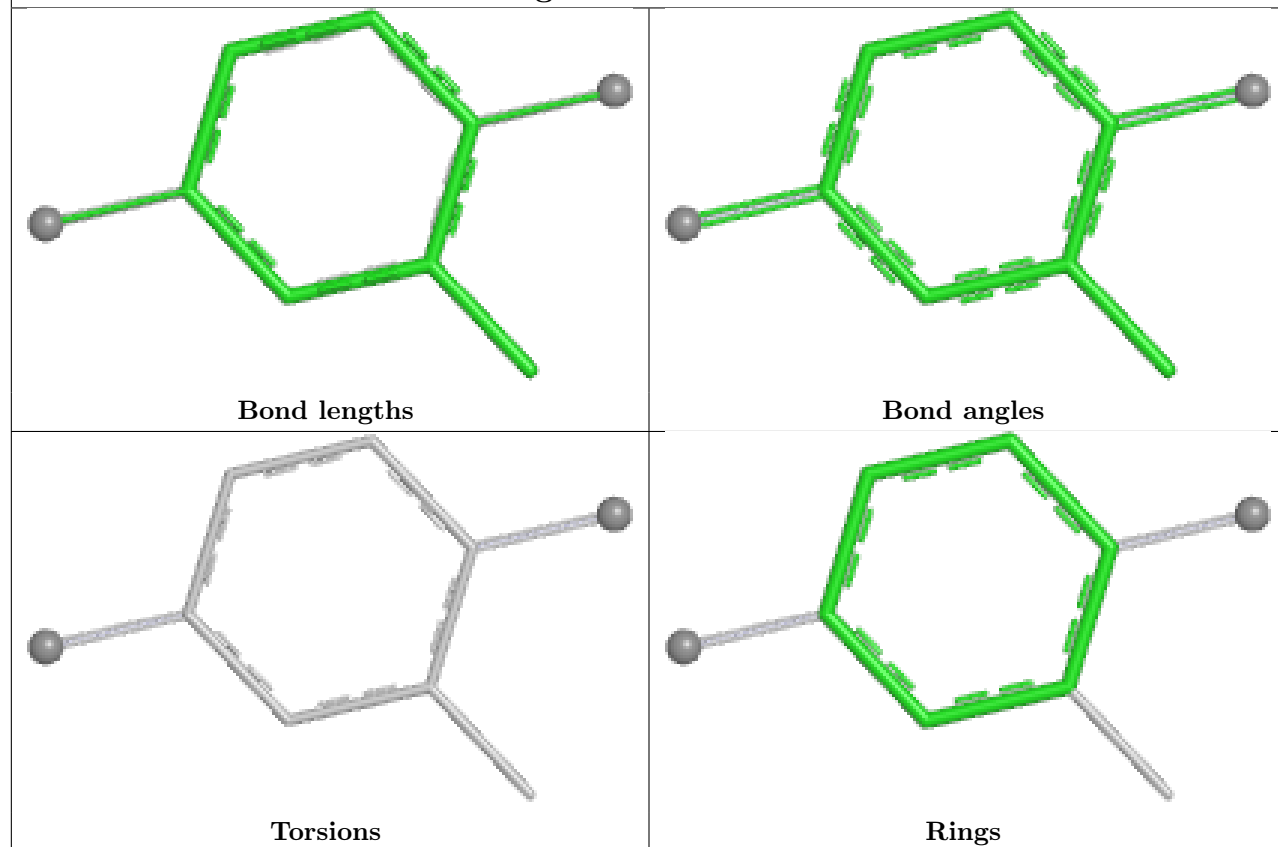
Ligand 7DV I 301



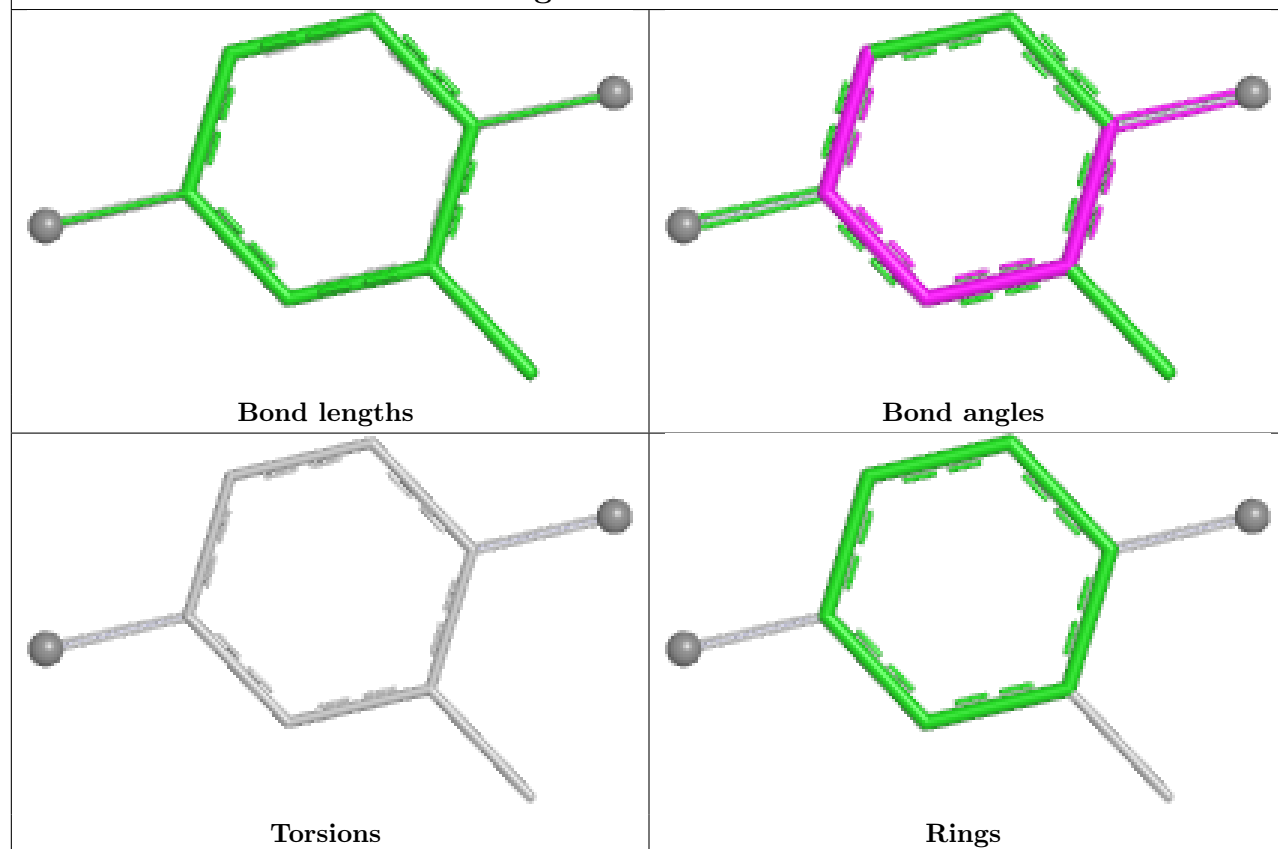
Ligand 7DV M 302



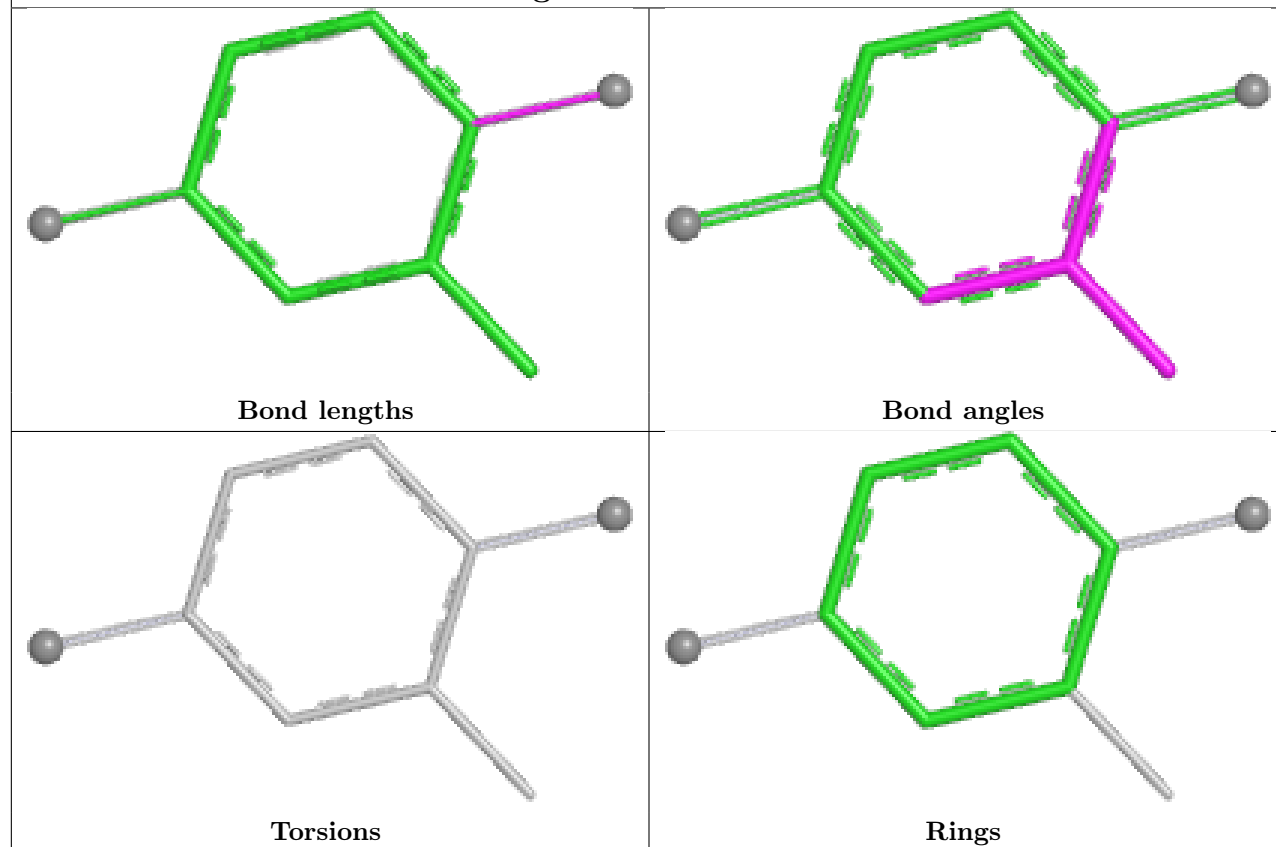
Ligand 7DV F 303



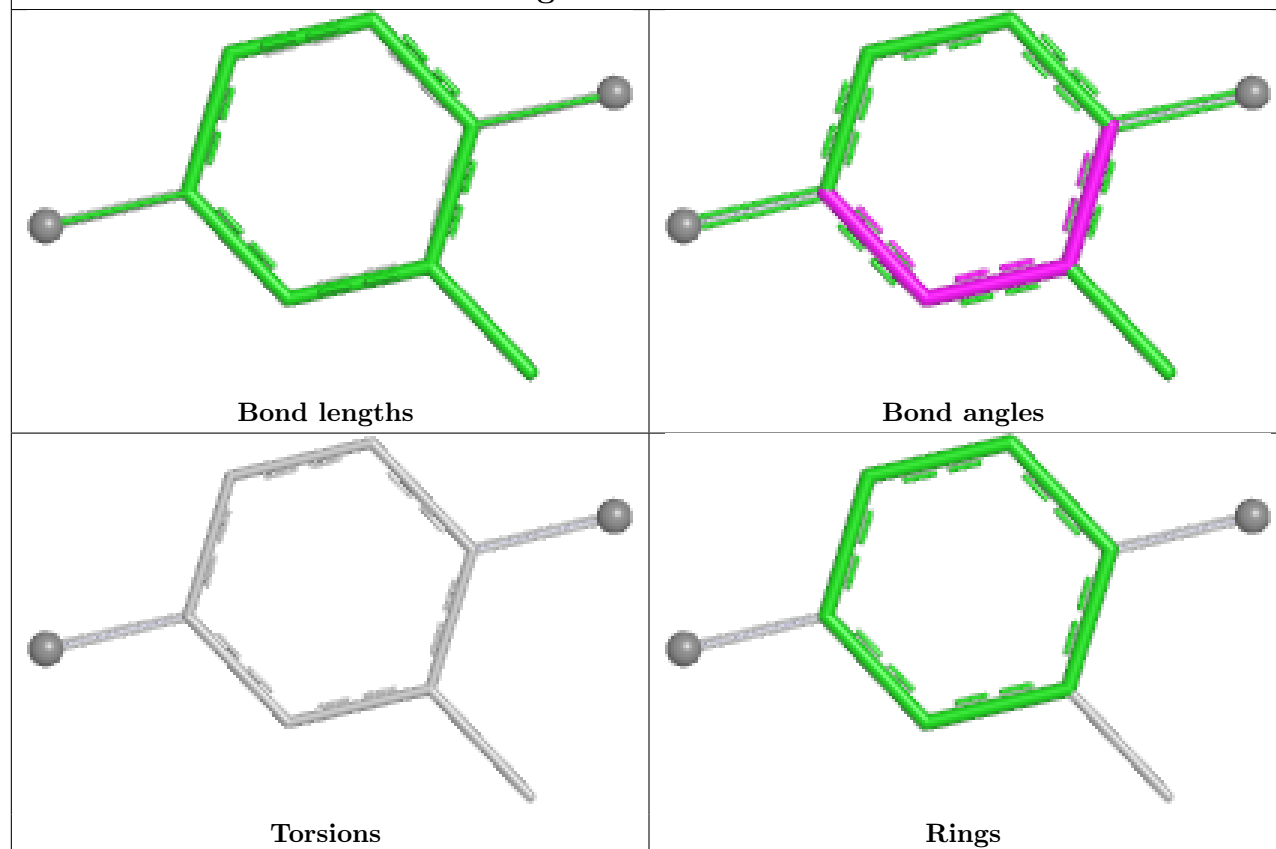
Ligand 7DV P 303



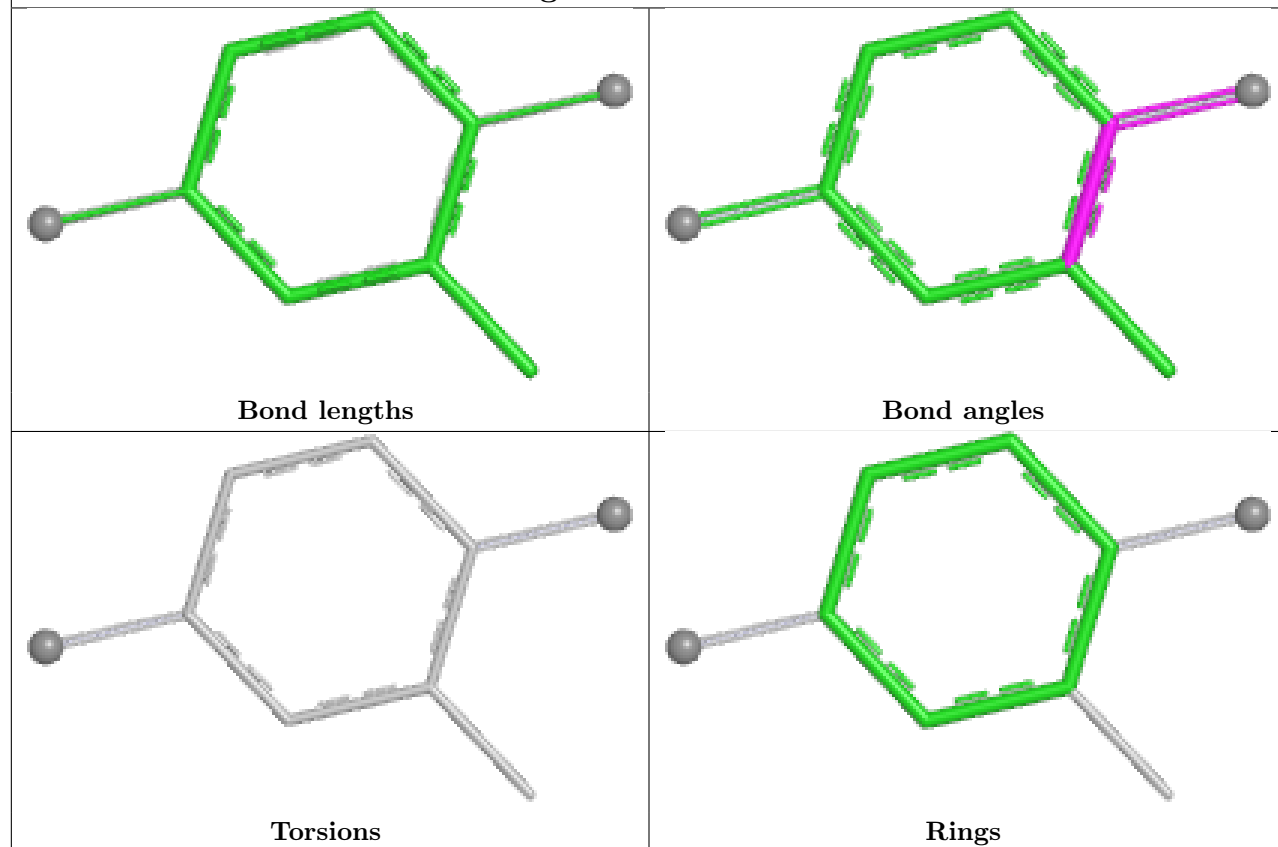
Ligand 7DV D 304



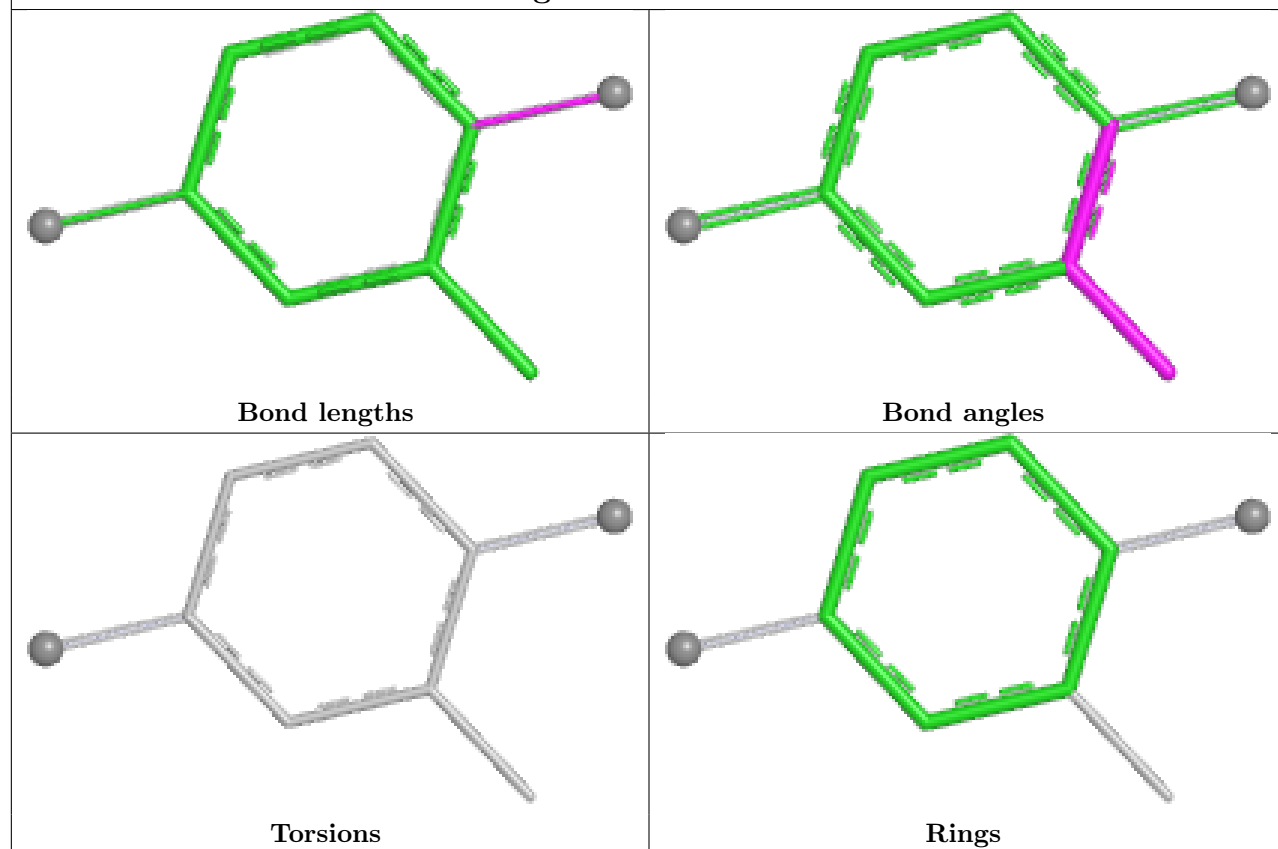
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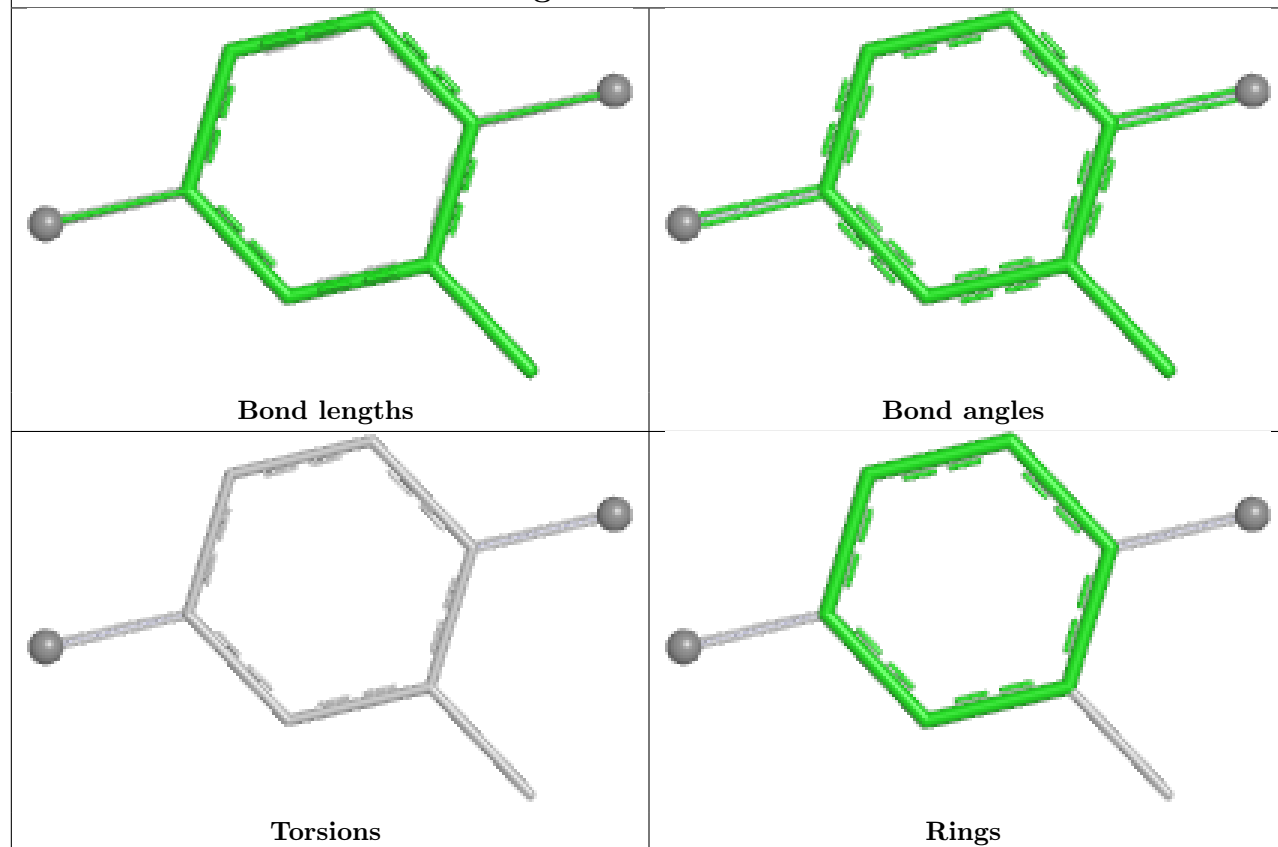
Ligand 7DV I 303



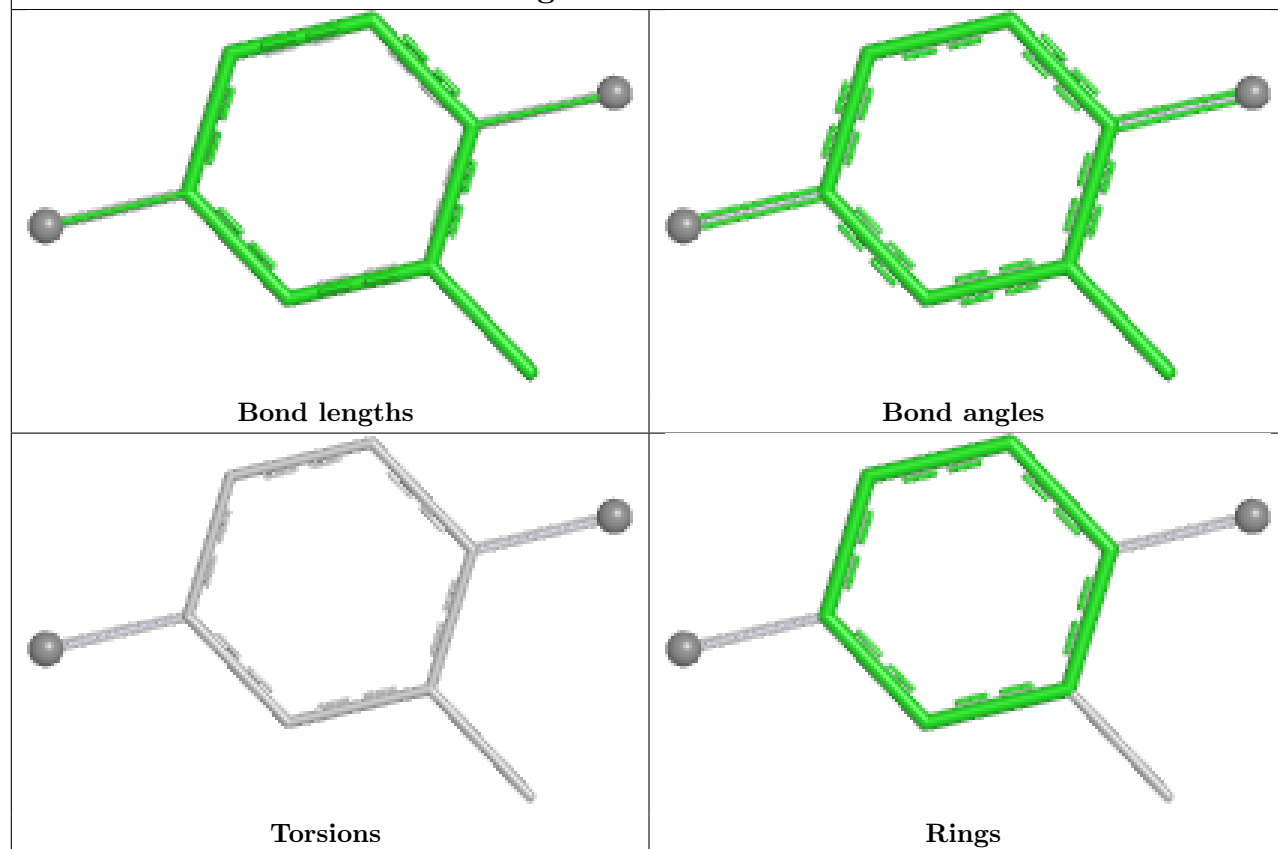
Ligand 7DV A 302



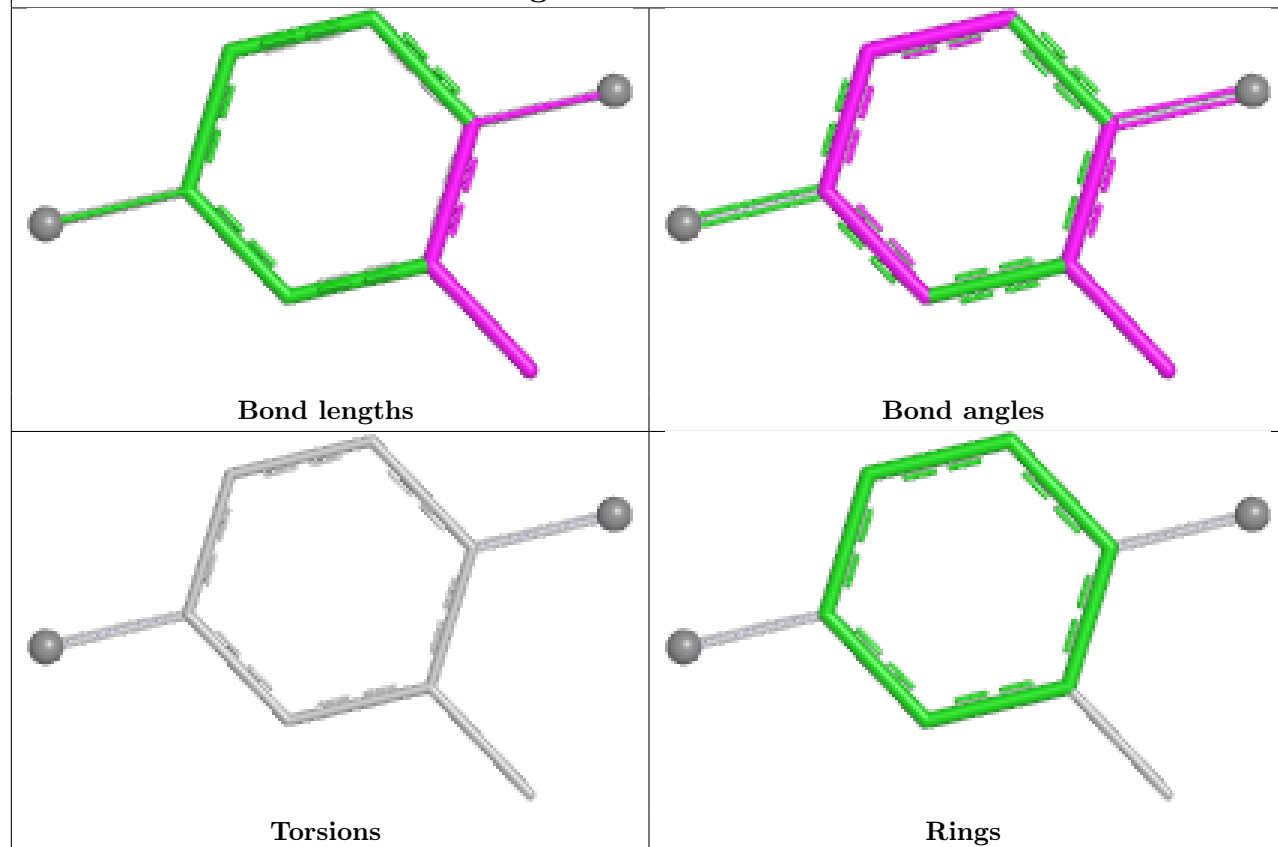
Ligand 7DV C 302



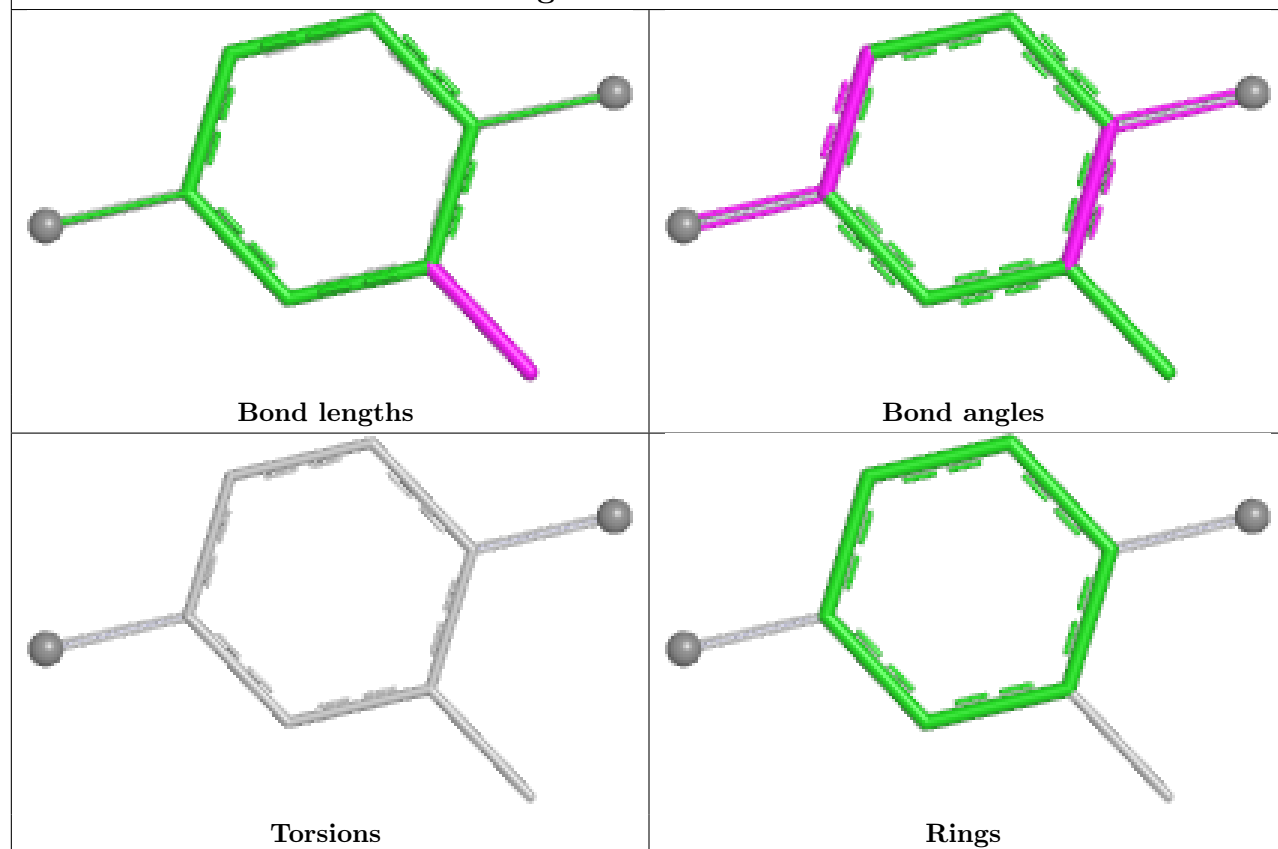
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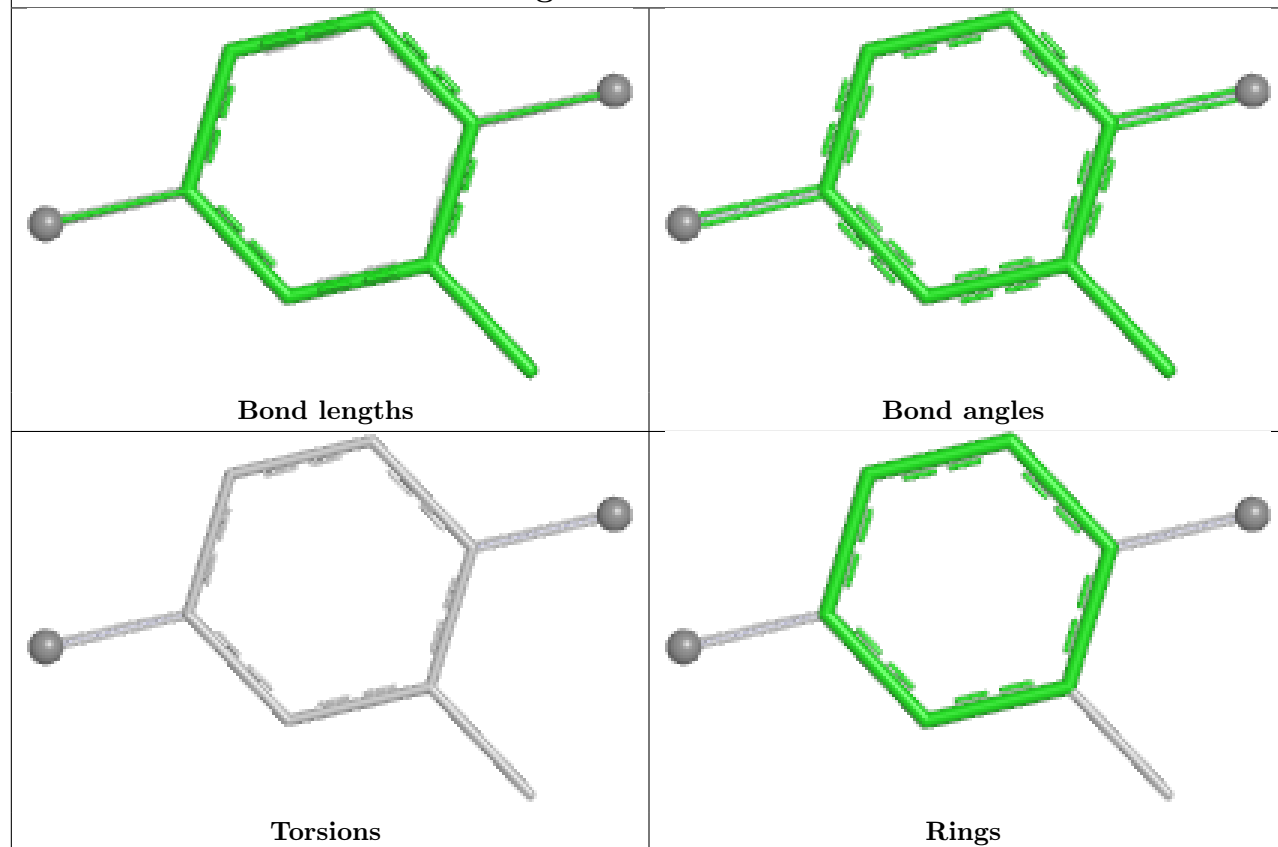
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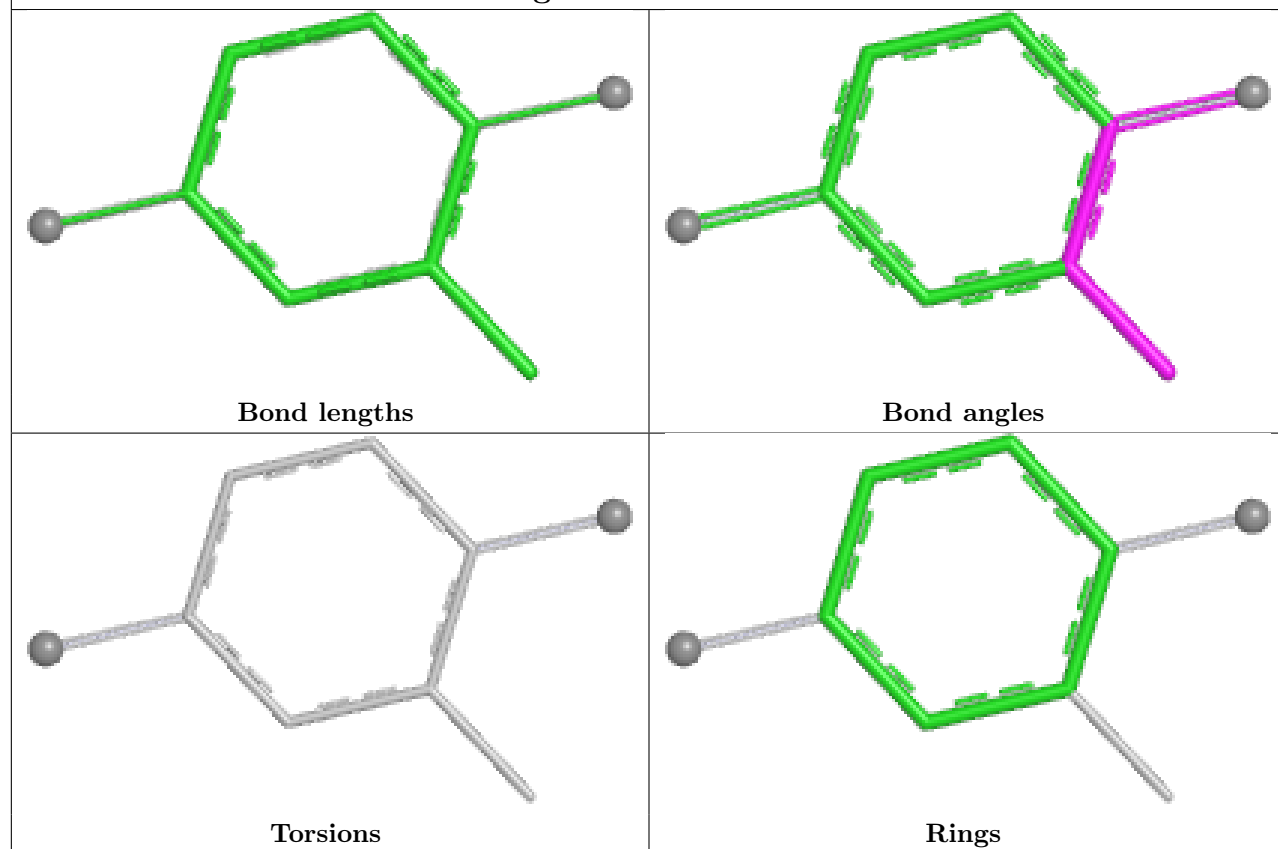
Ligand 7DV J 301



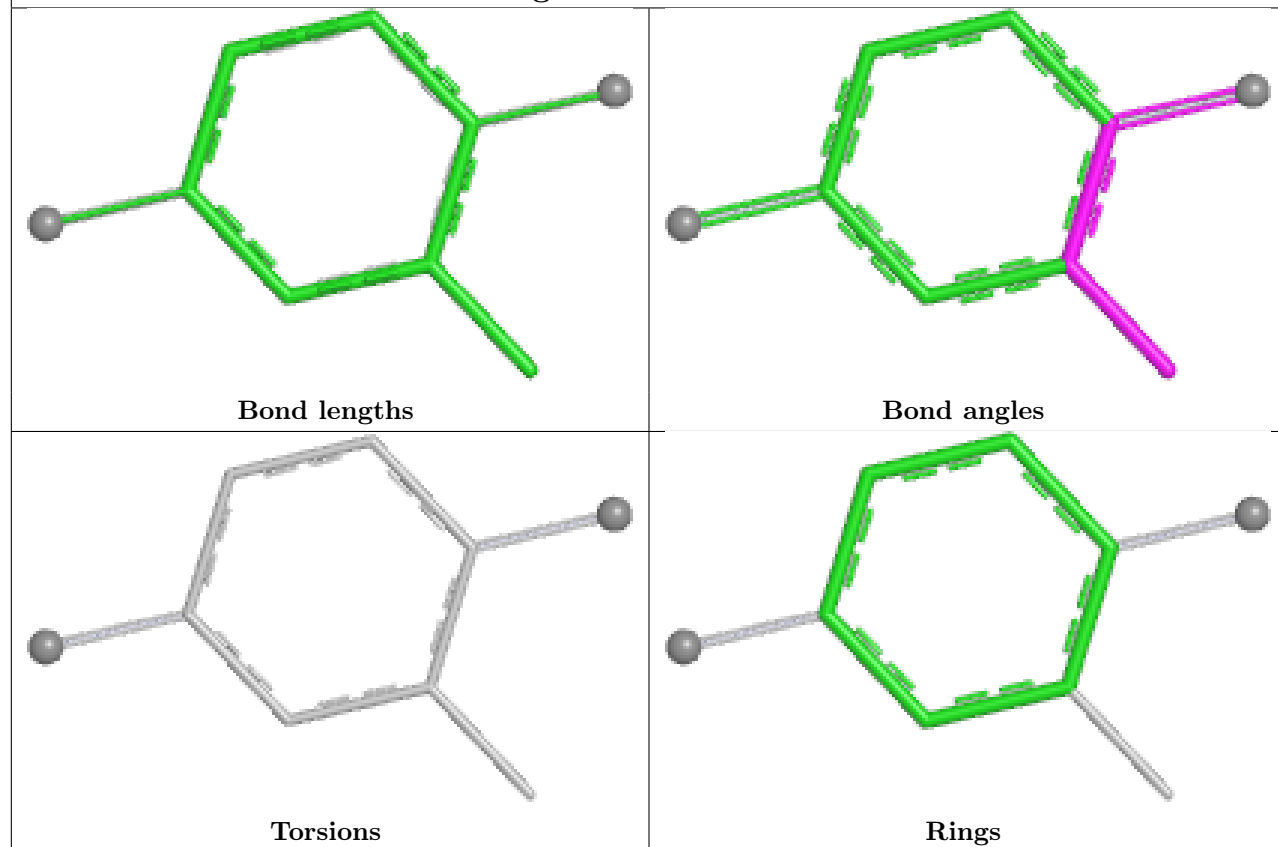
Ligand 7DV L 301



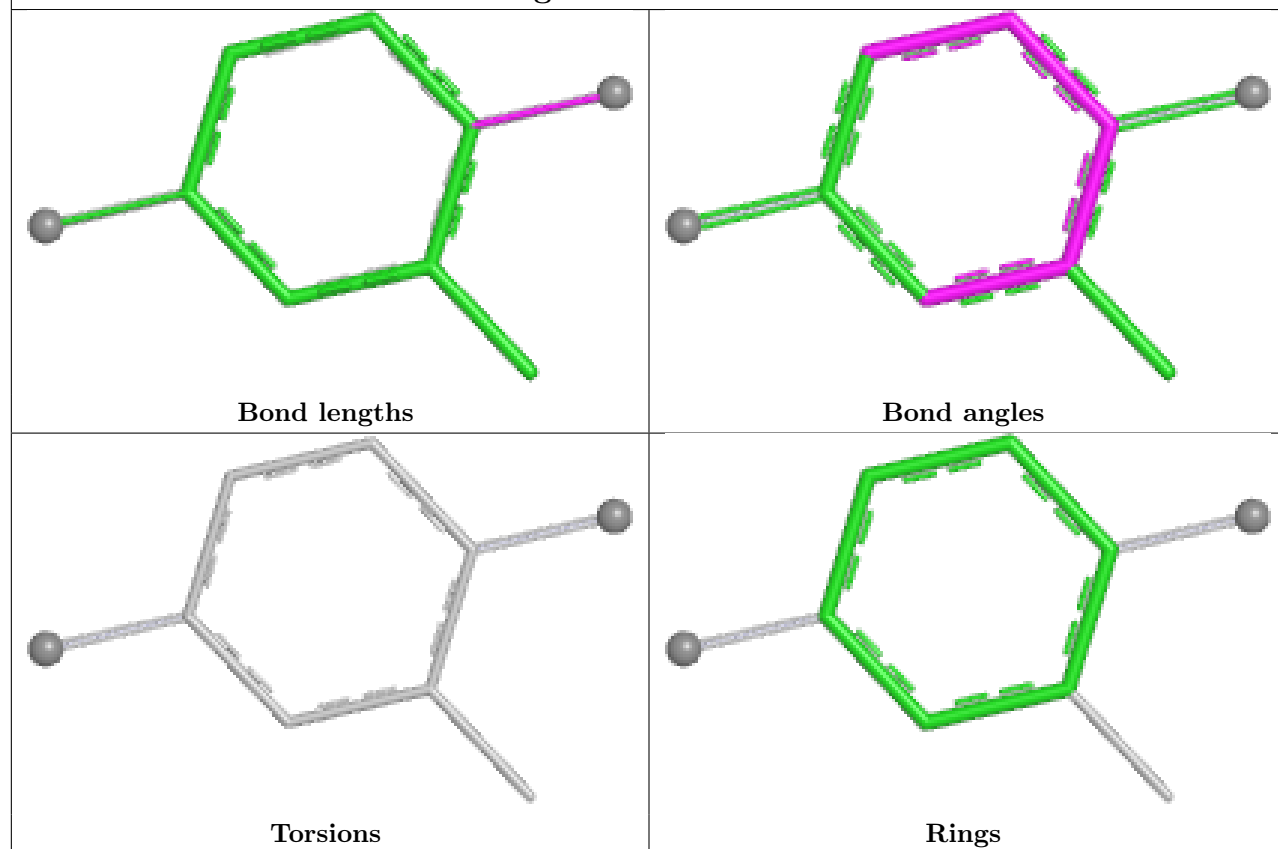
Ligand 7DV A 301



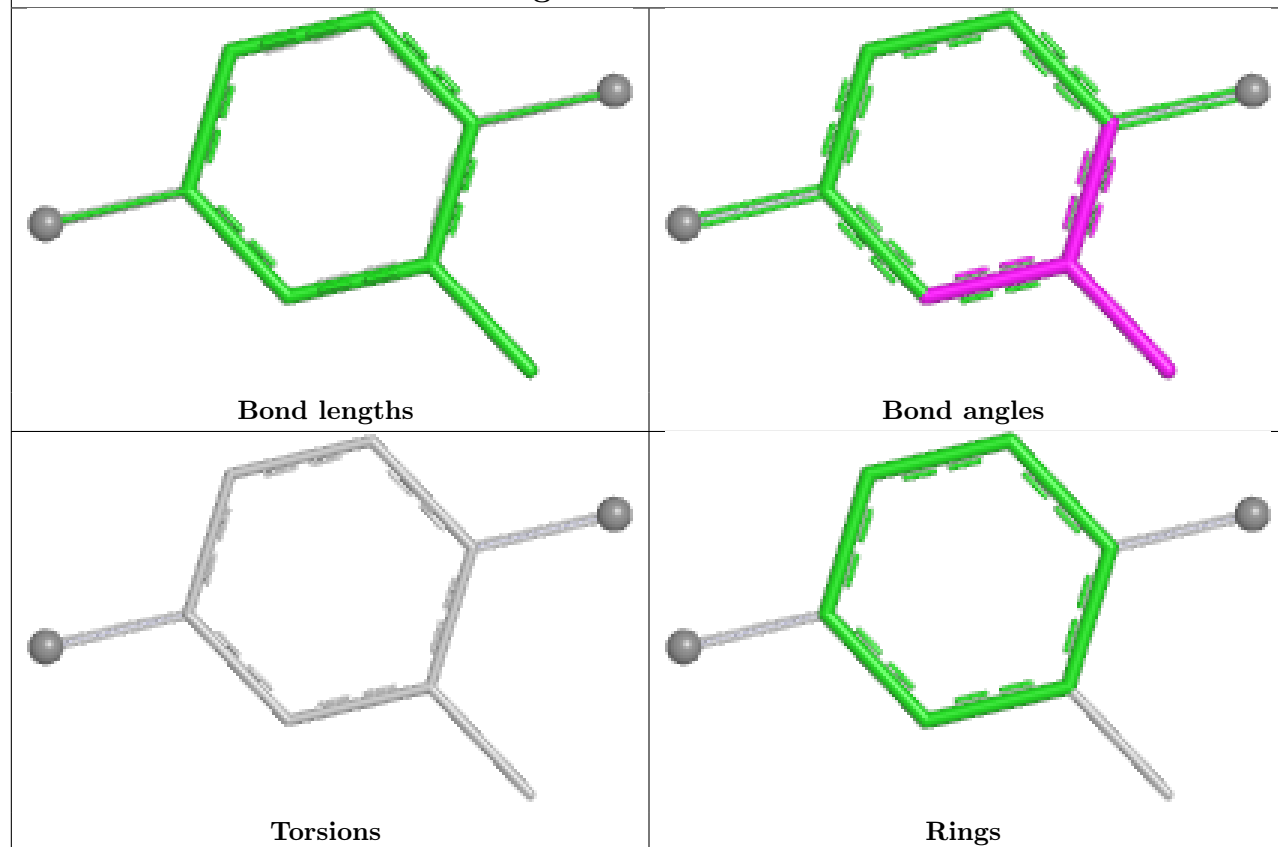
Ligand 7DV G 303



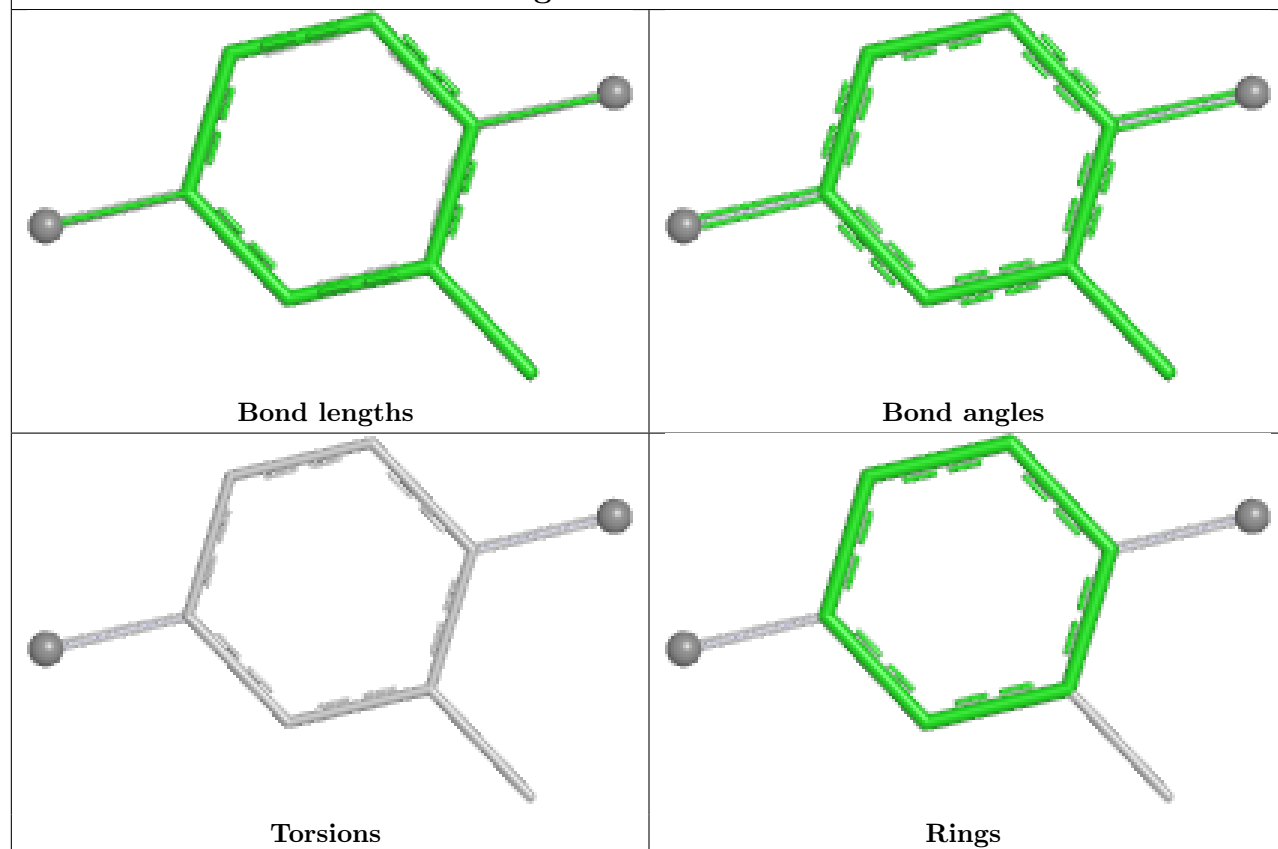
Ligand 7DV B 303



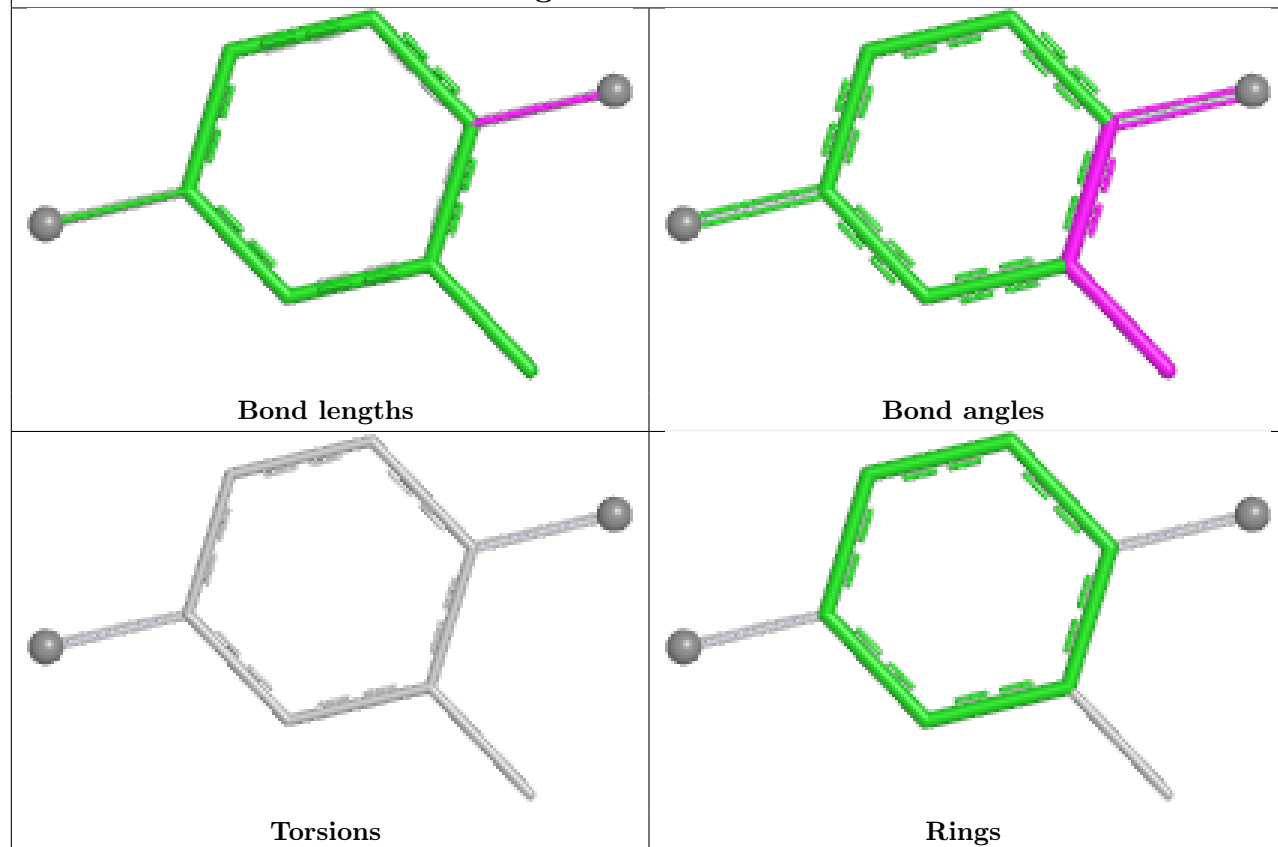
Ligand 7DV O 302



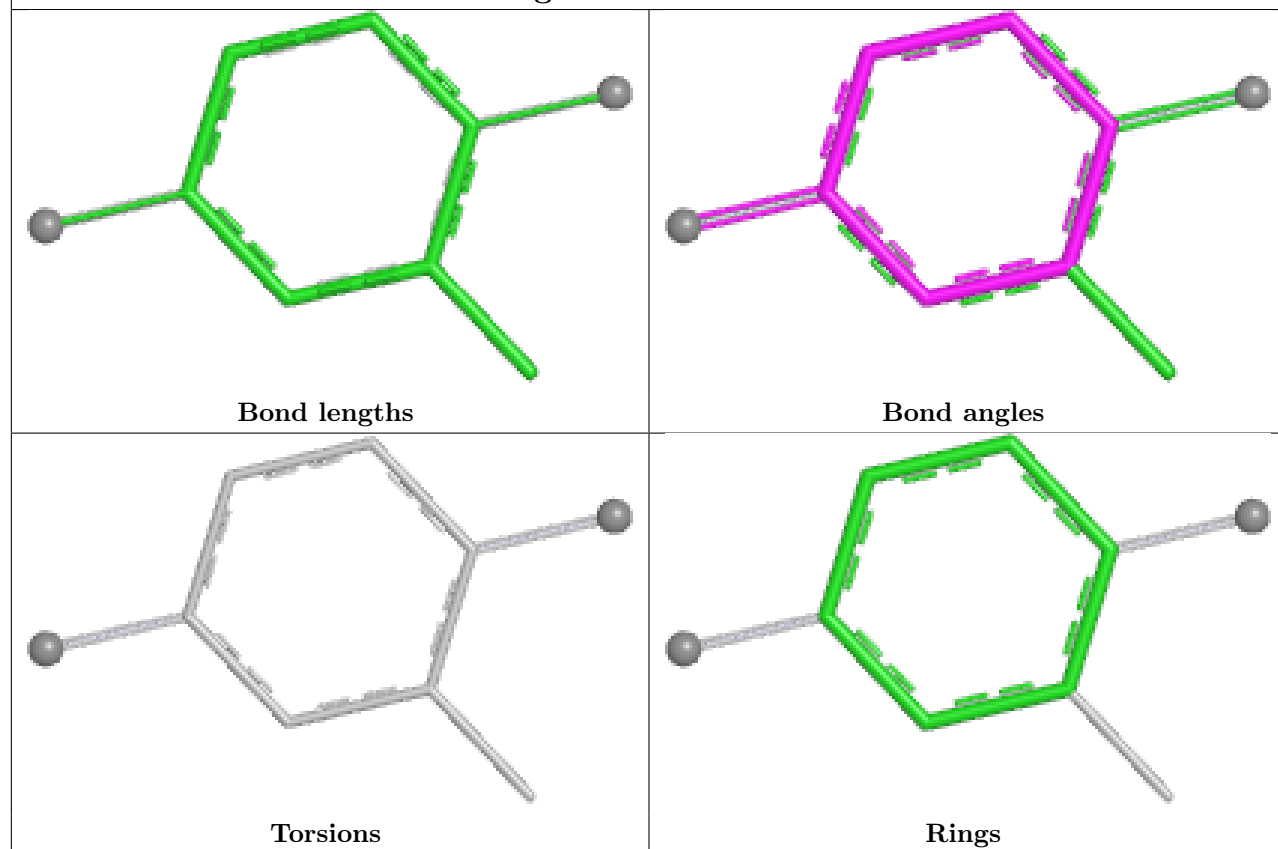
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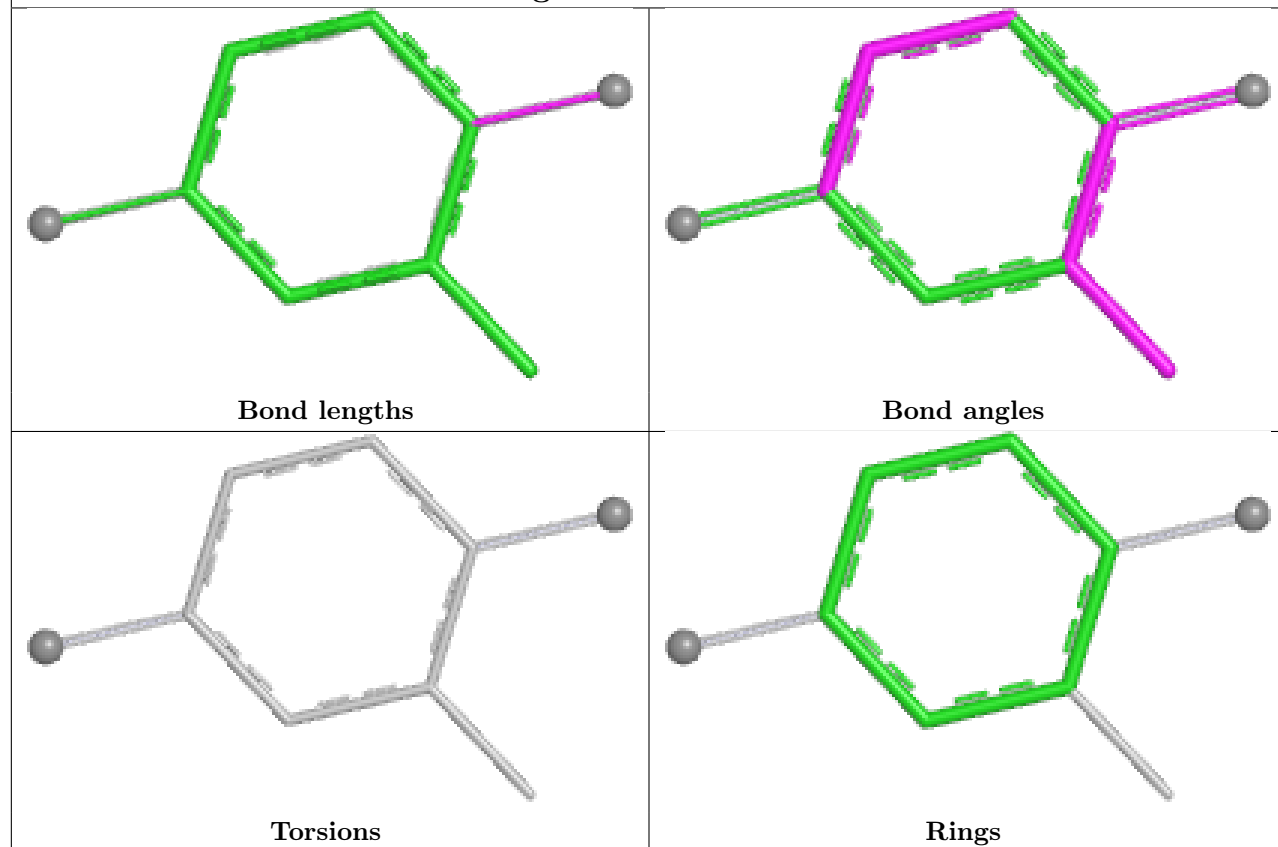
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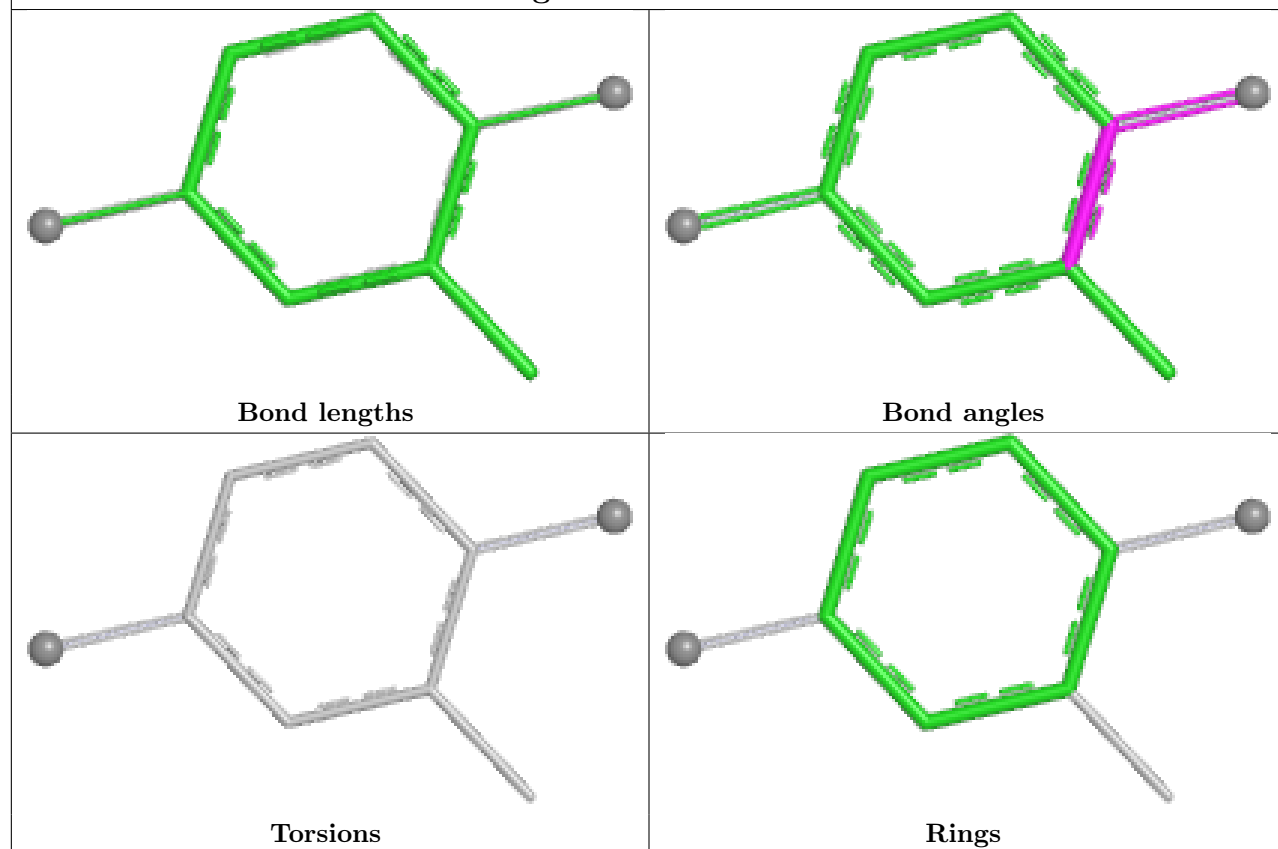
Ligand 7DV P 302



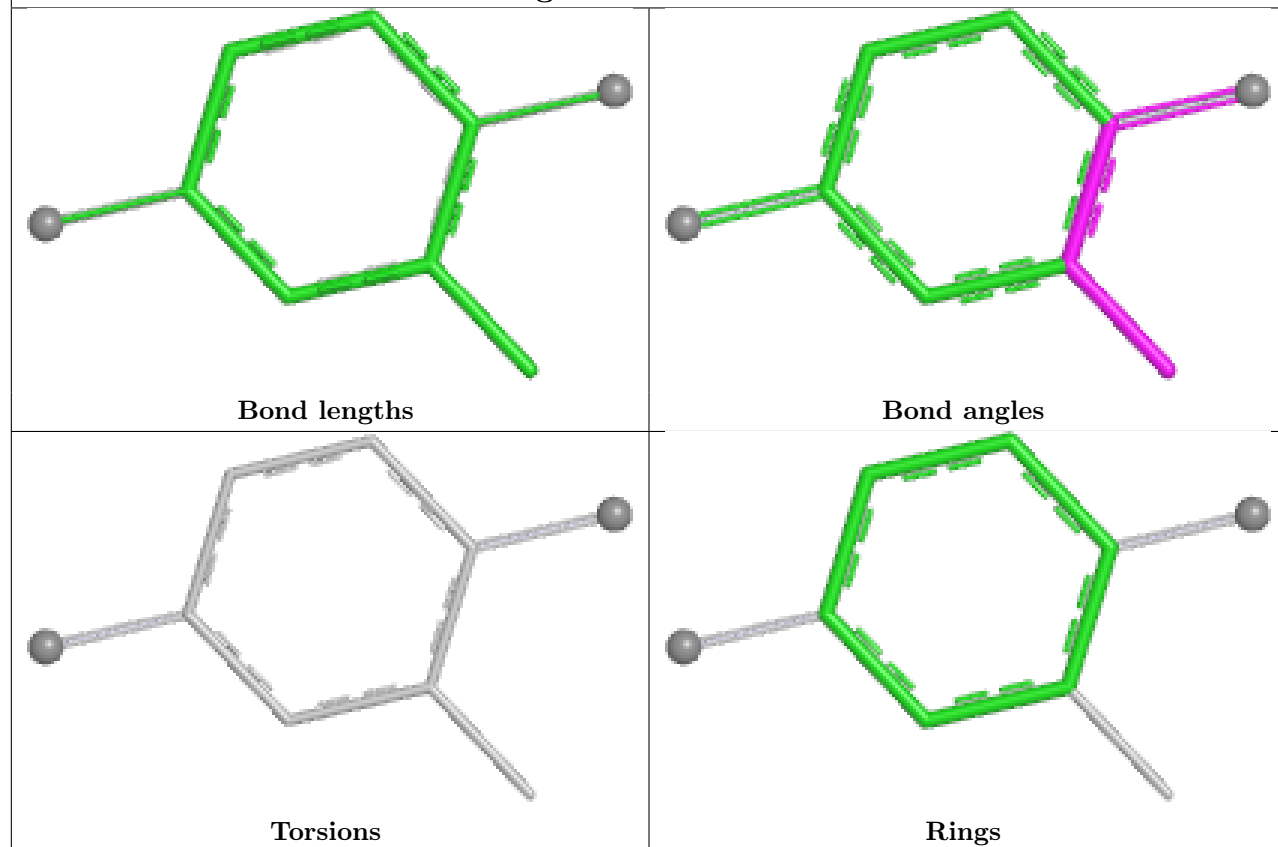
Ligand 7DV G 301



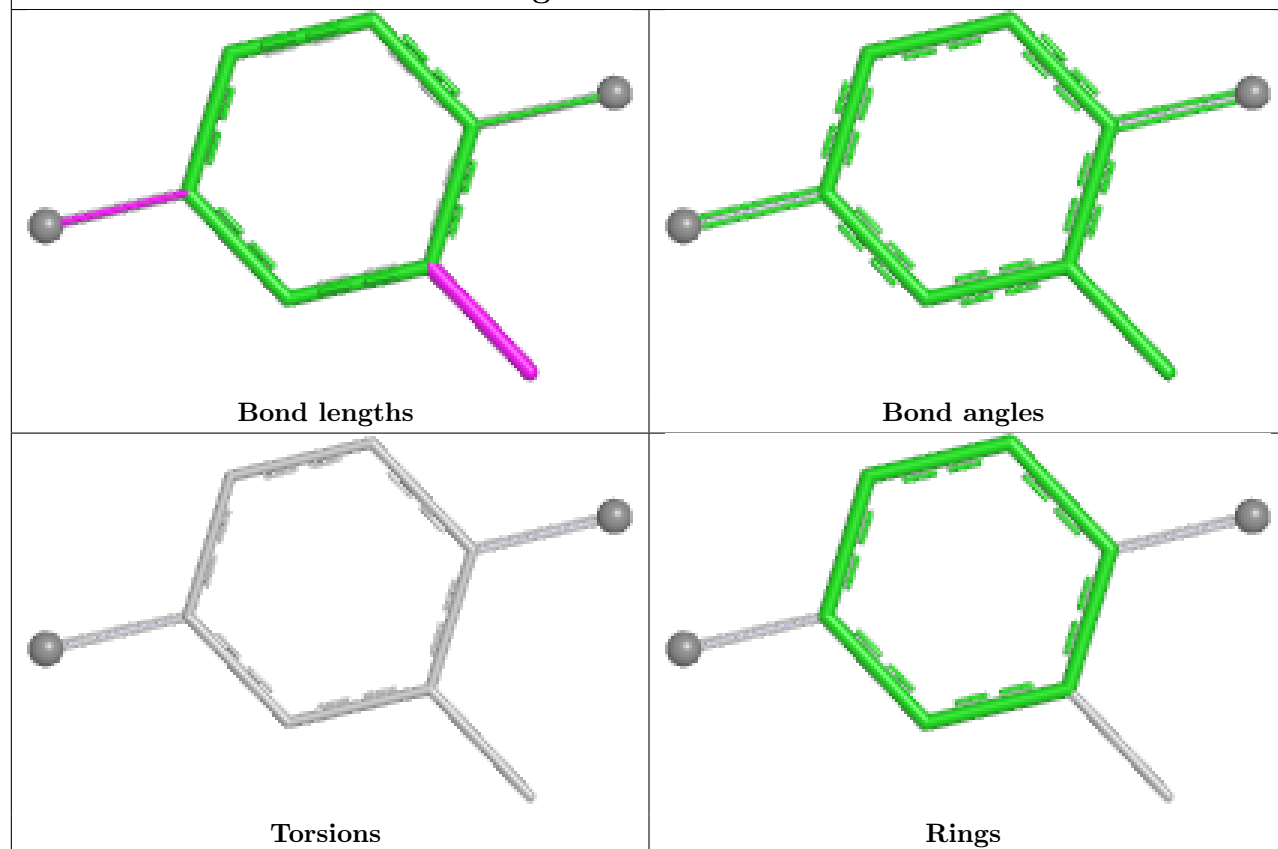
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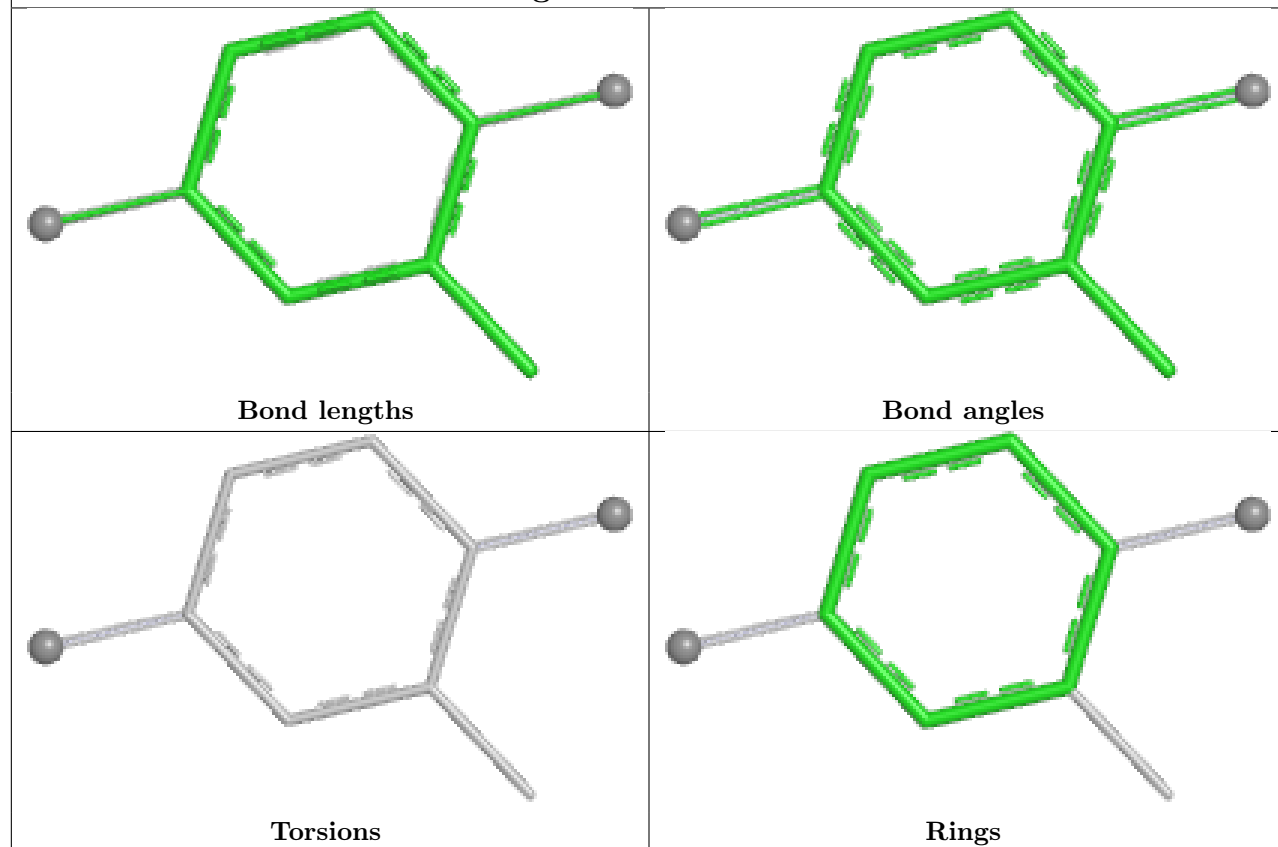
Ligand 7DV L 304



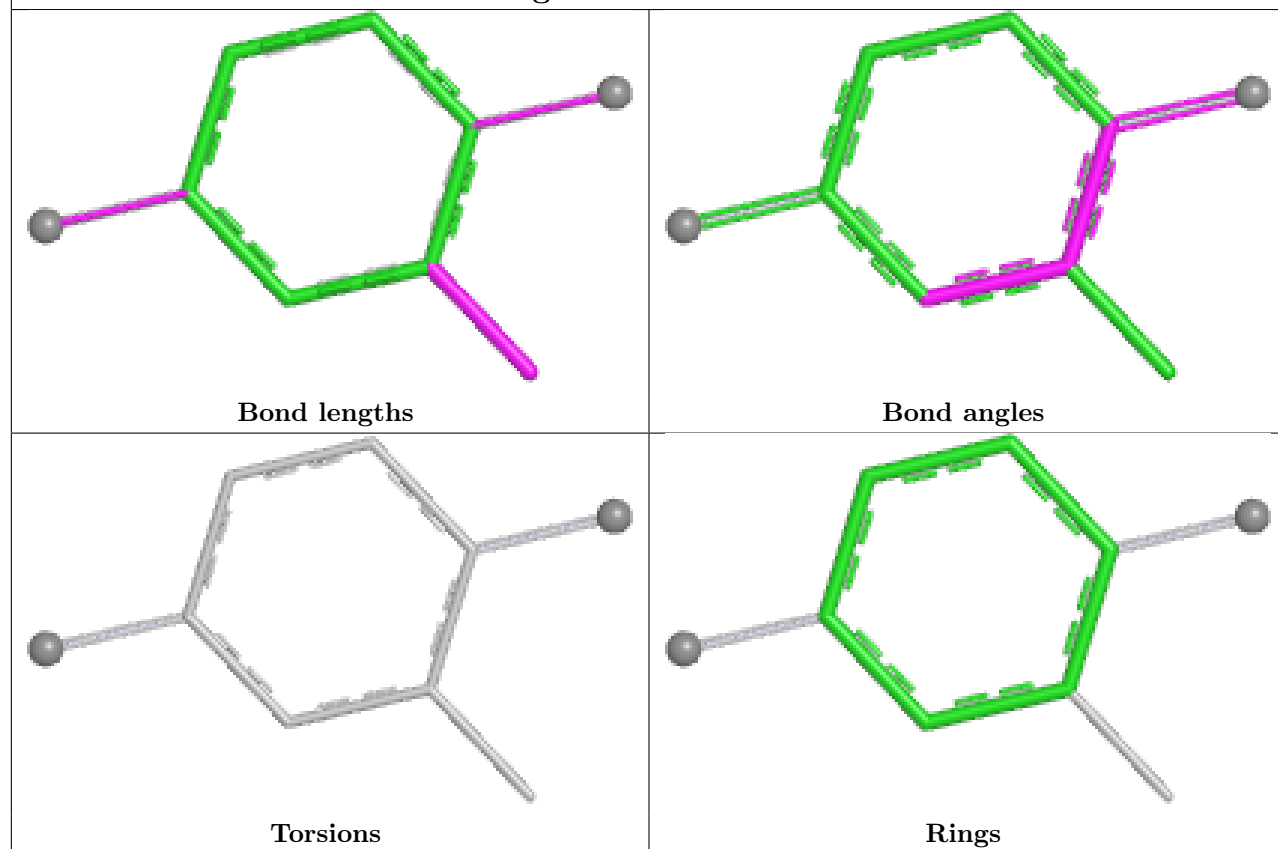
Ligand 7DV K 303



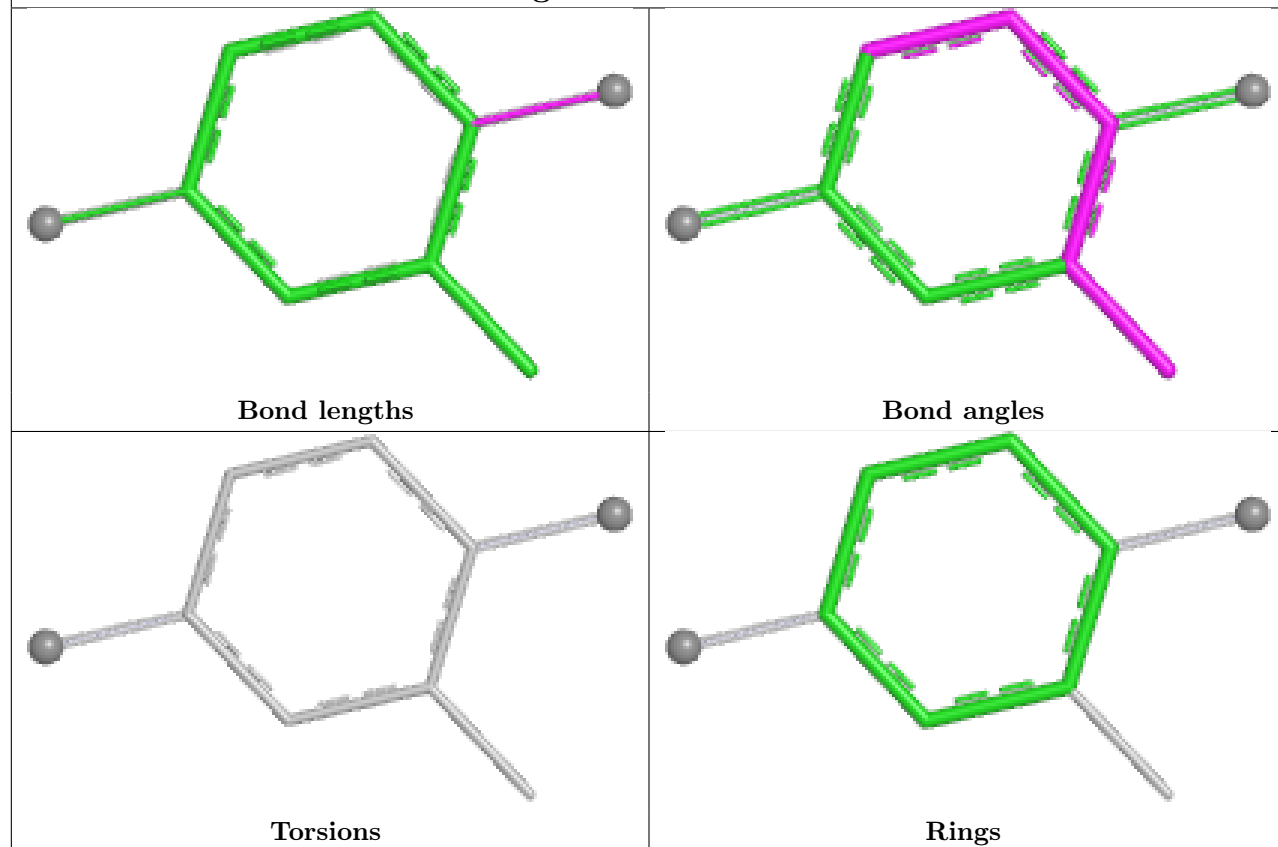
Ligand 7DV H 303



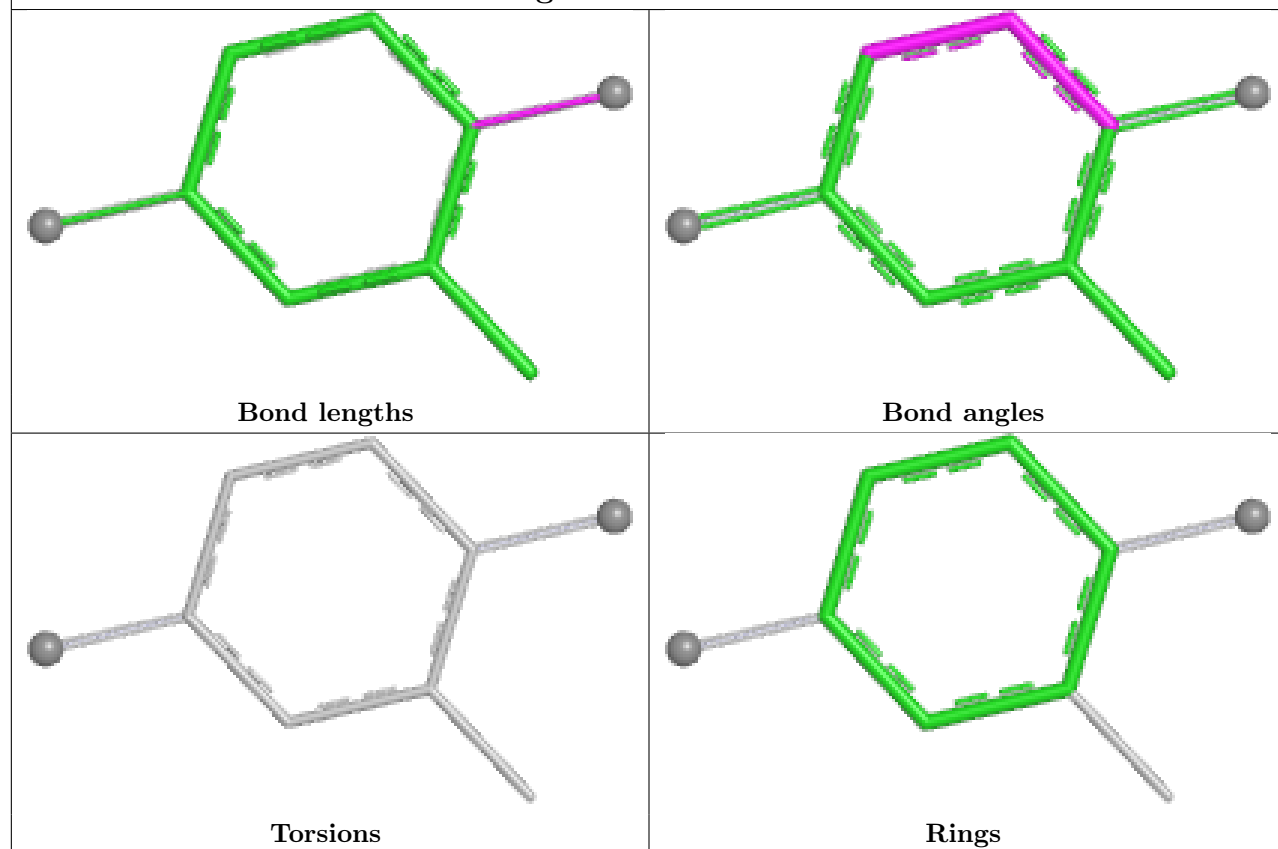
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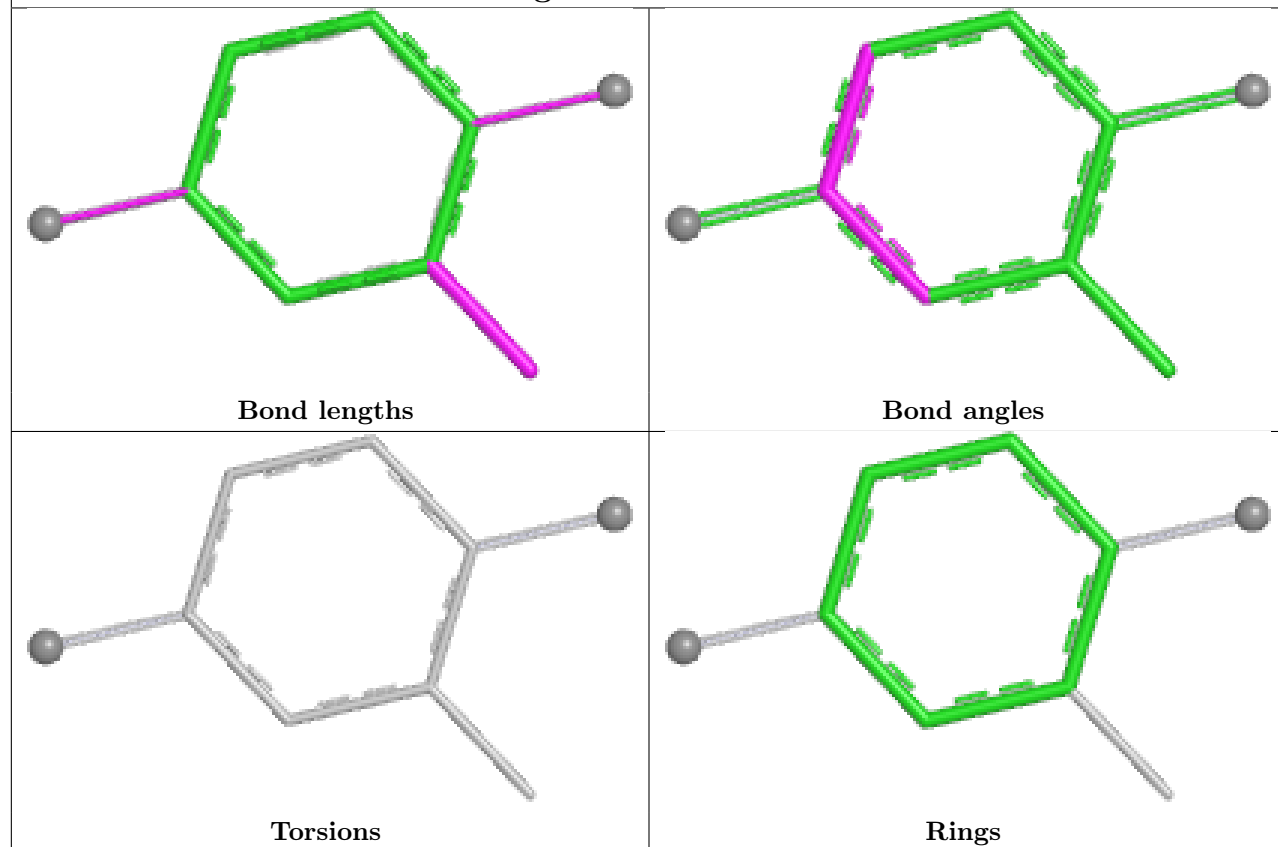
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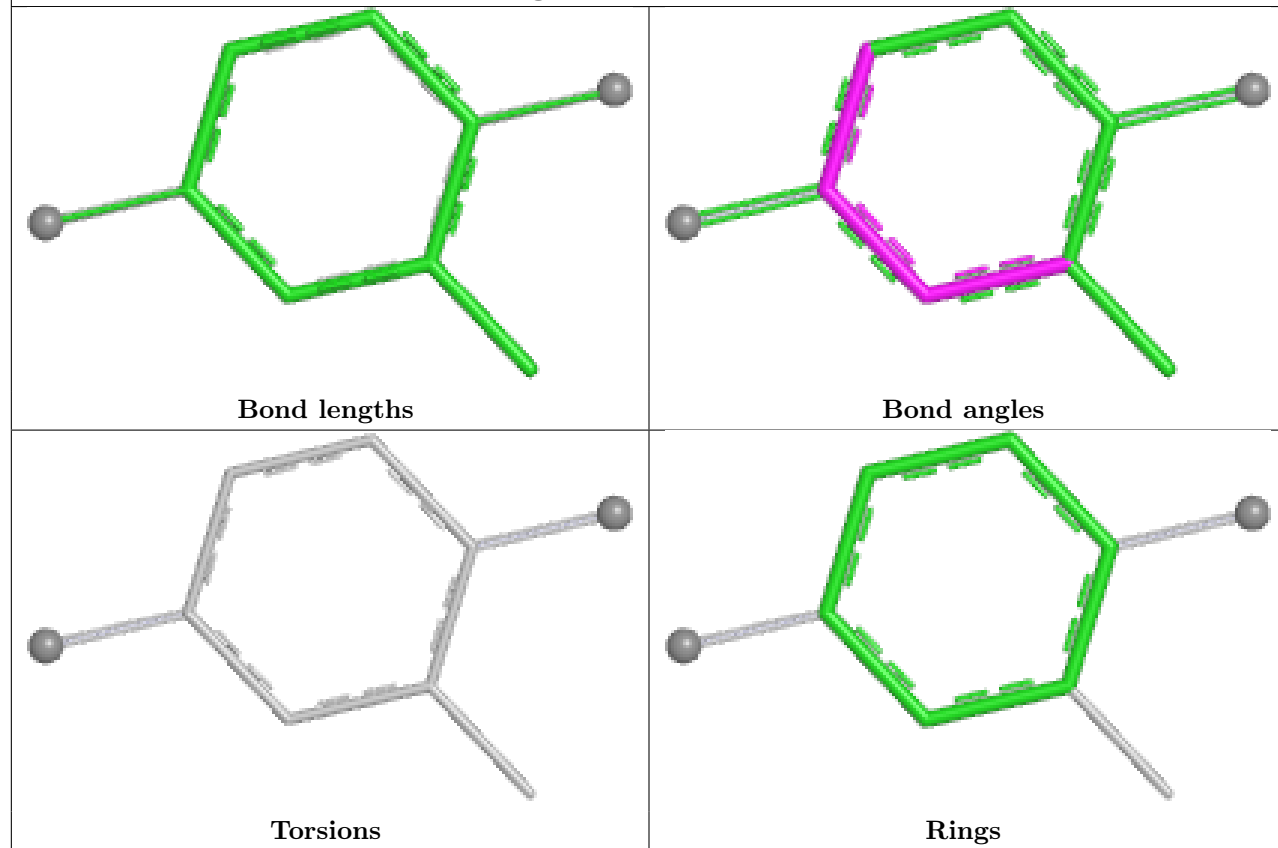
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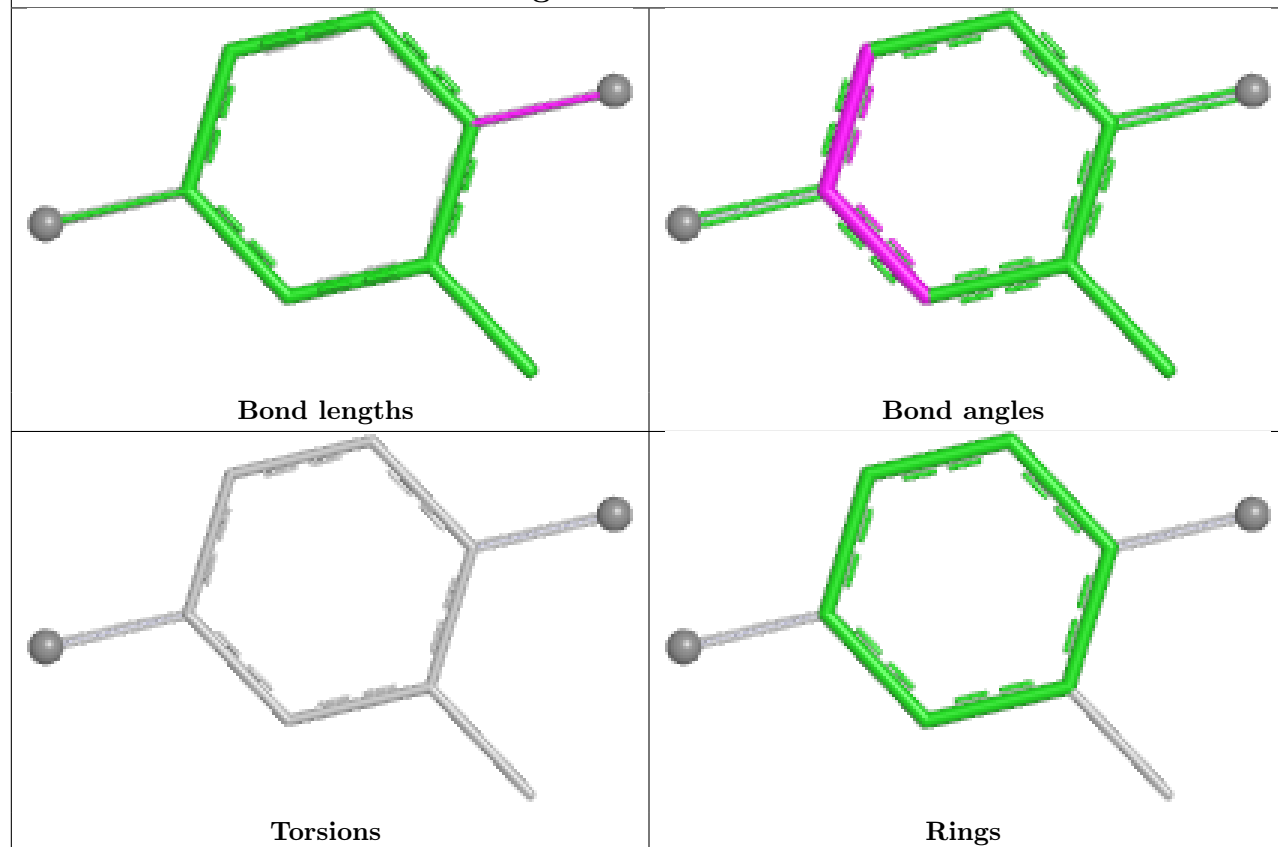
Ligand 7DV B 301



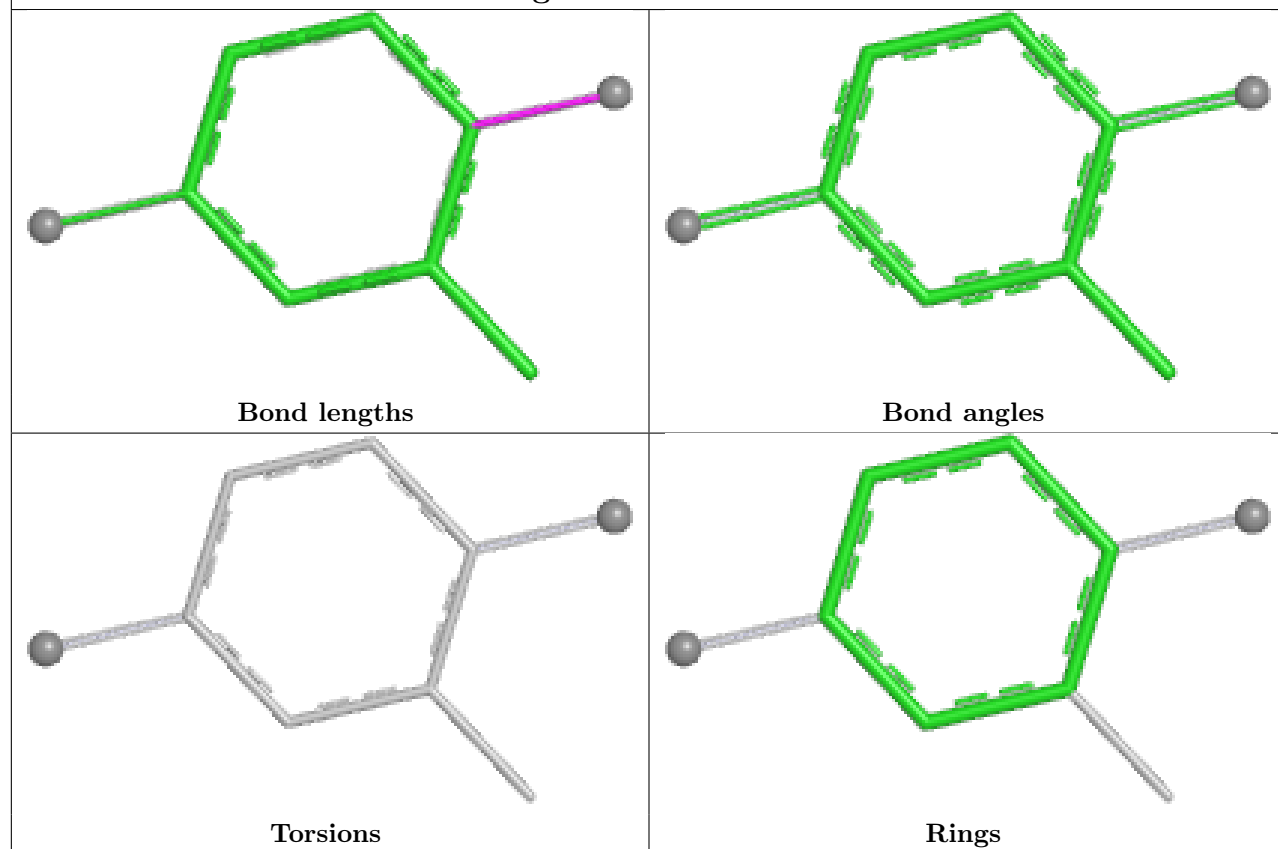
Ligand 7DV M 303



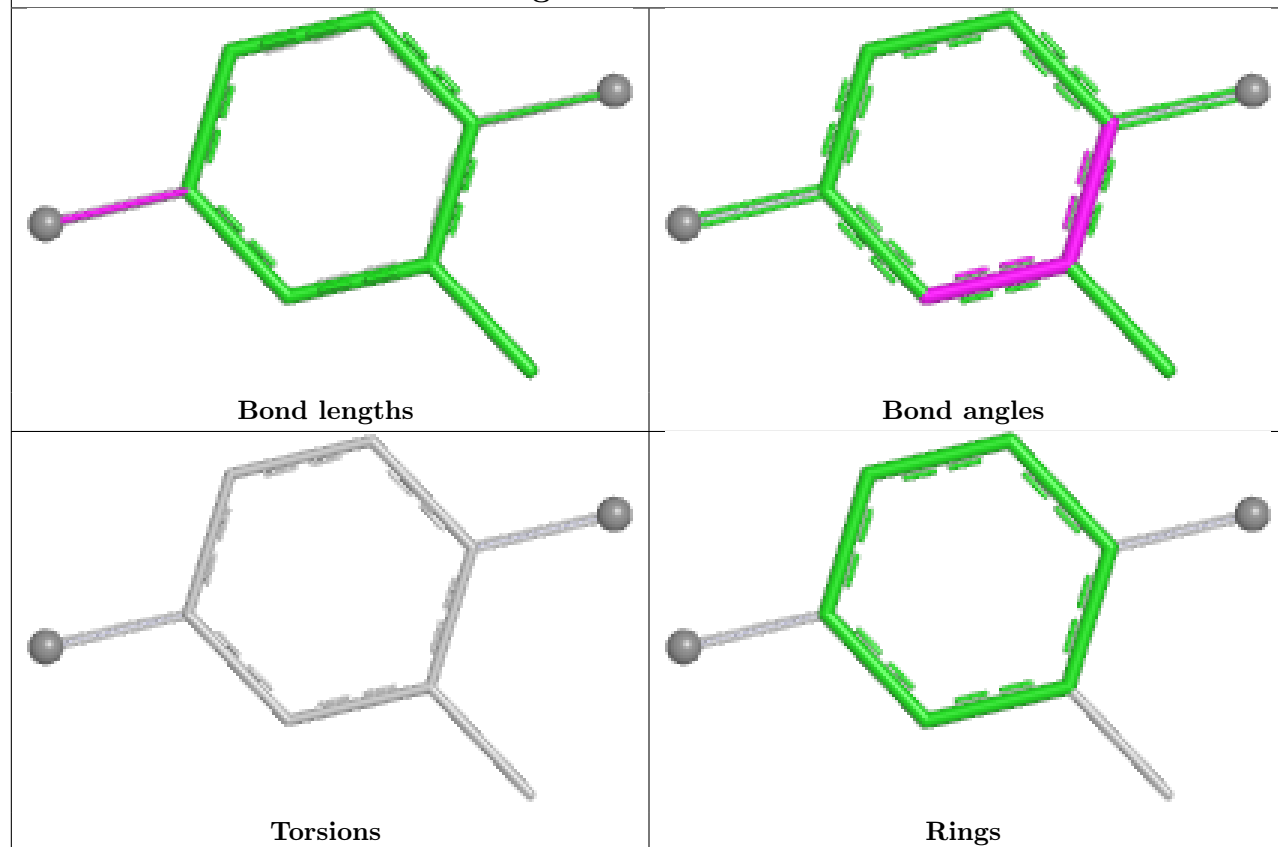
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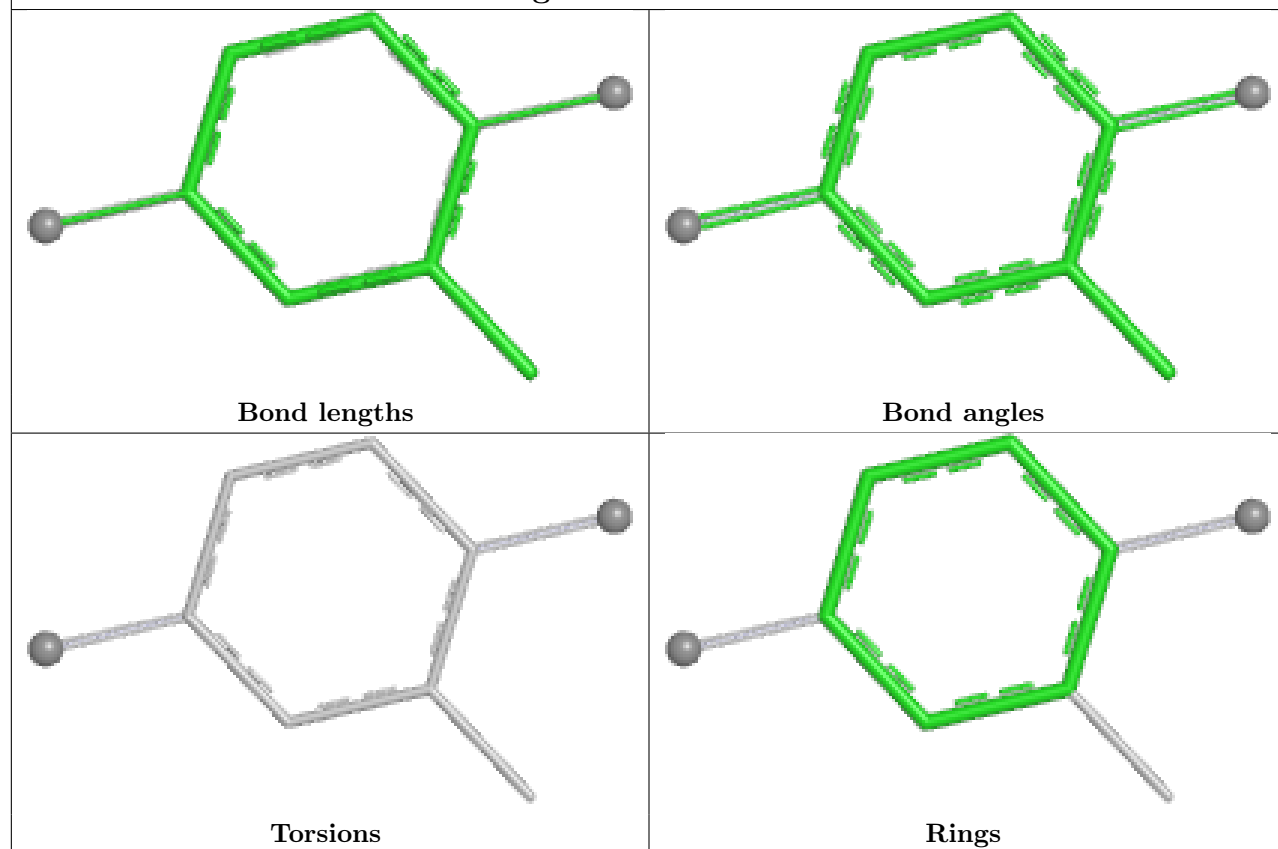
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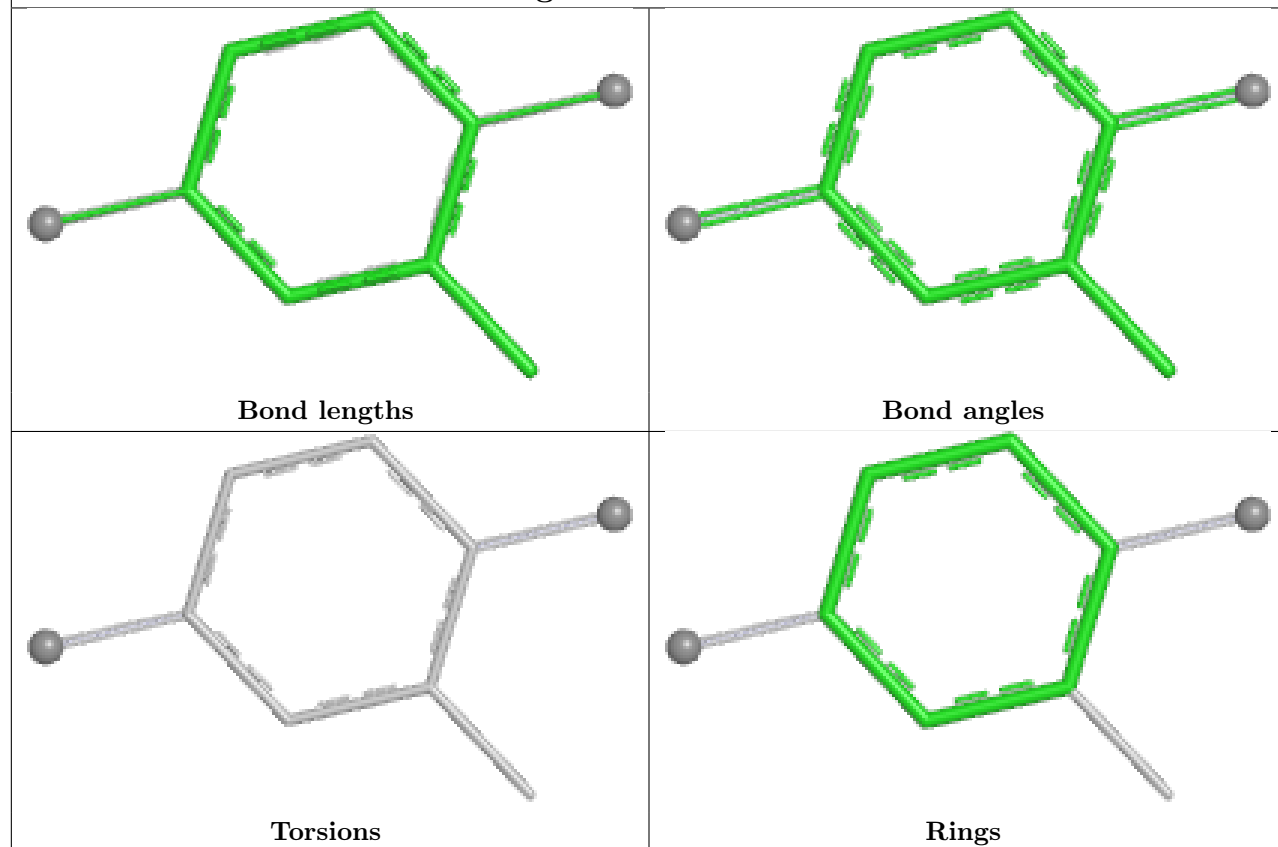
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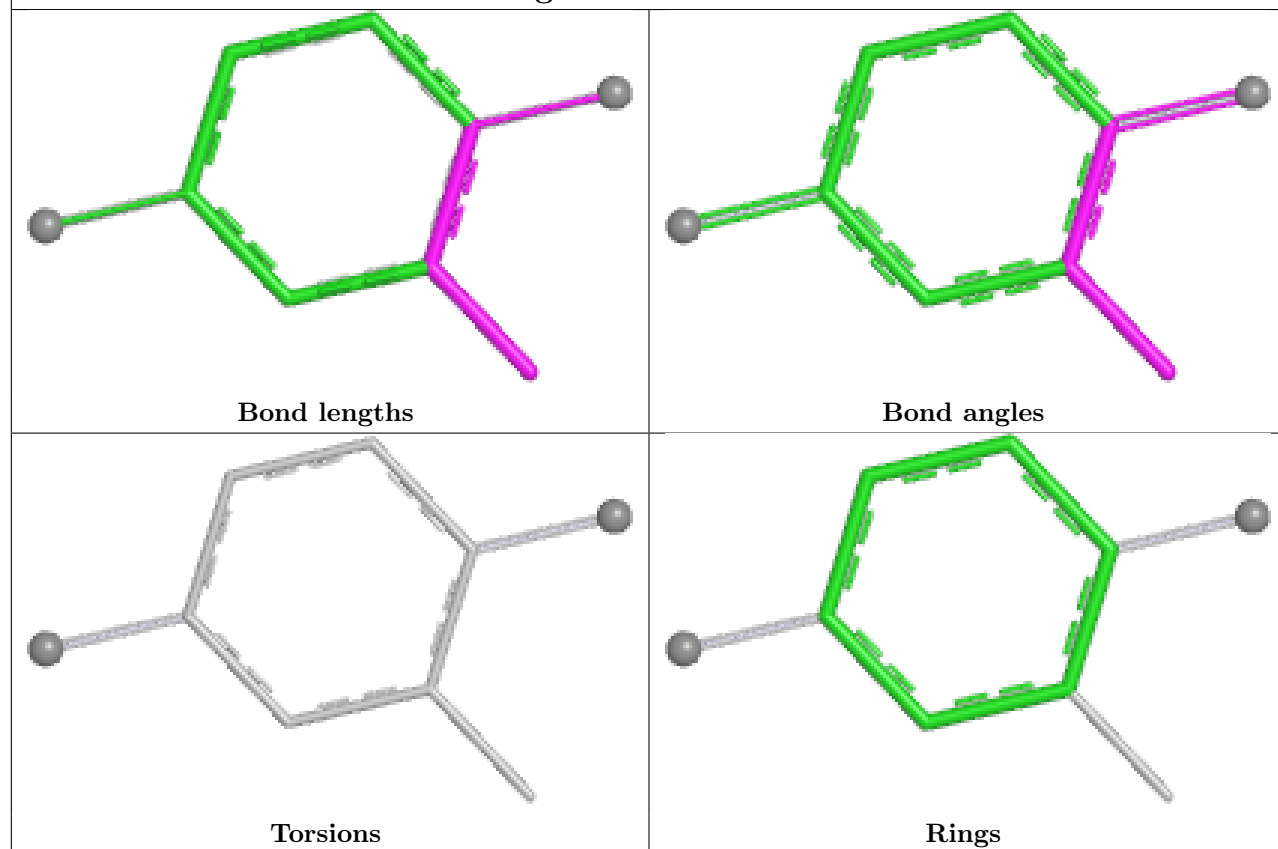
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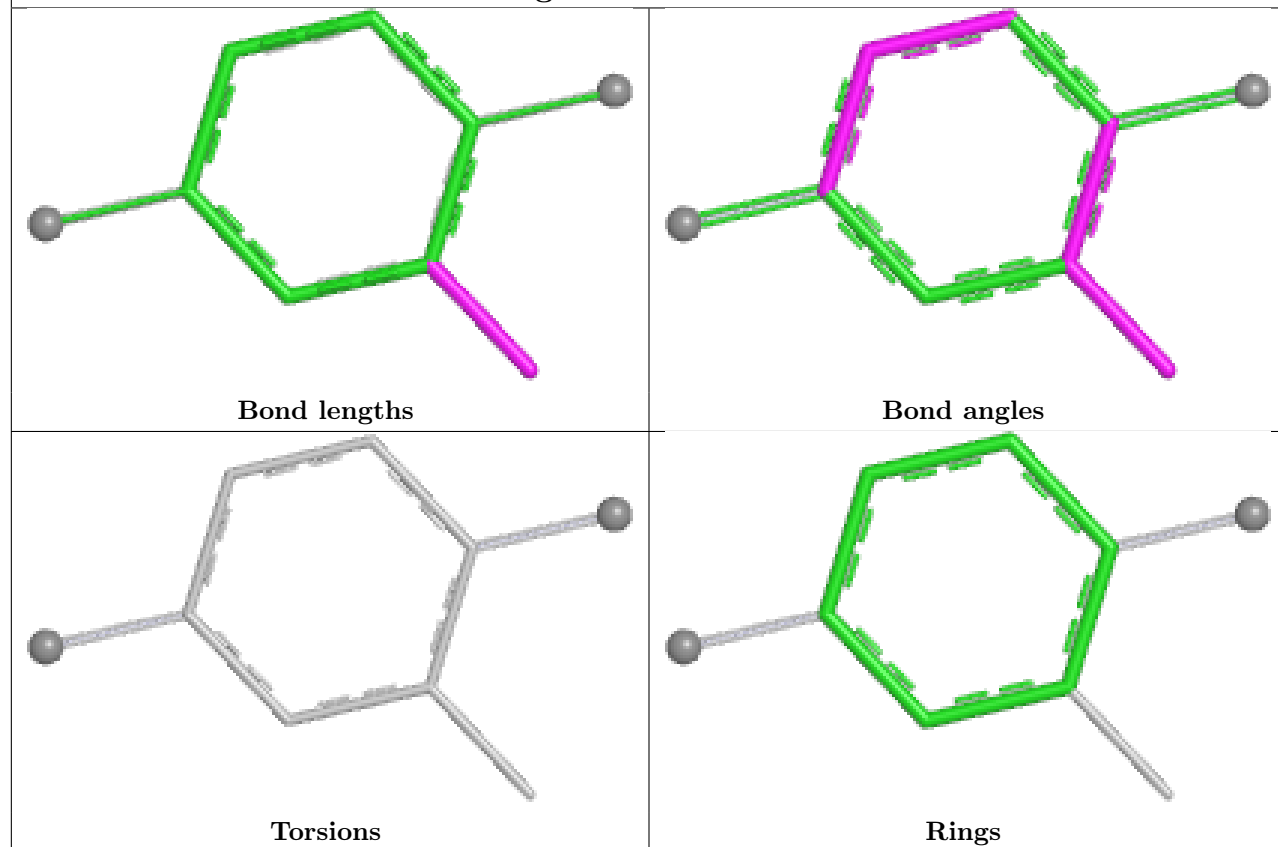
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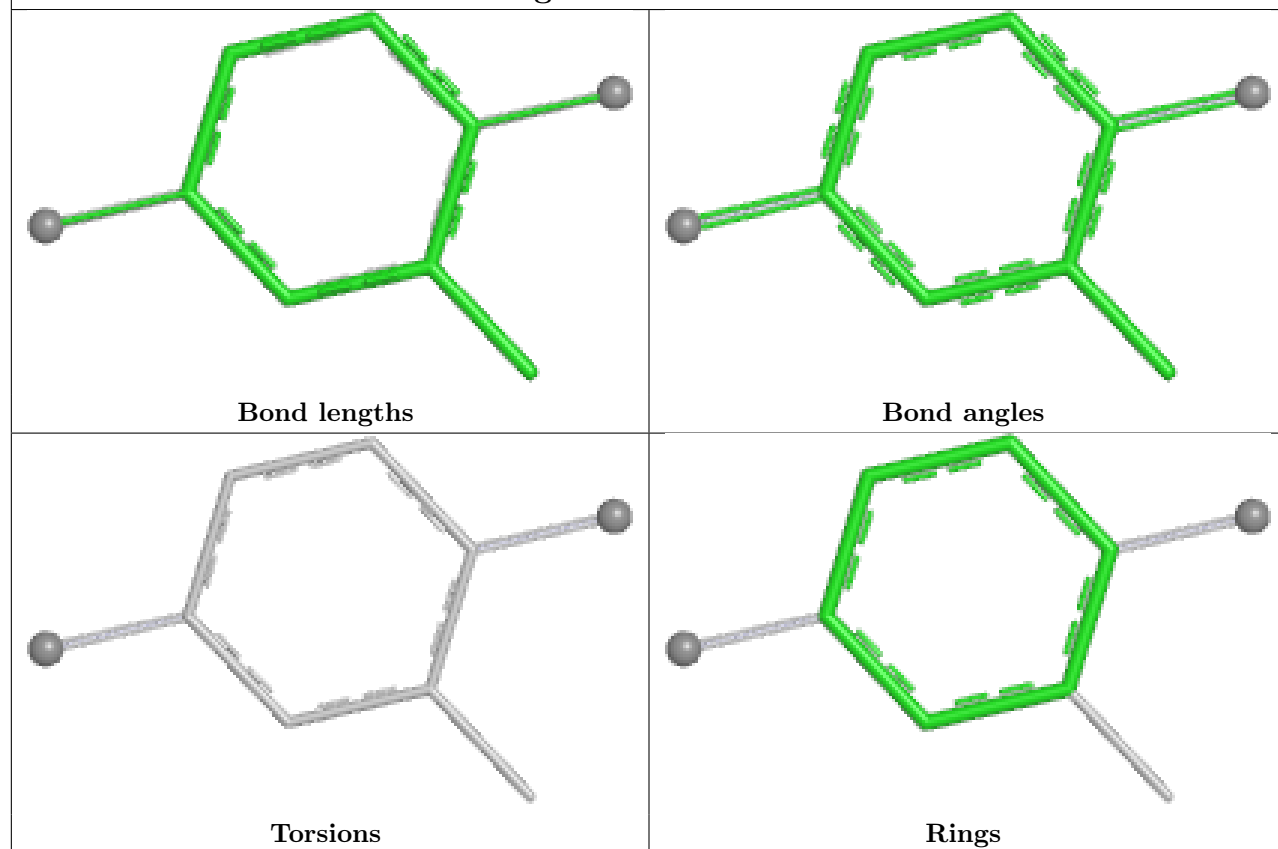
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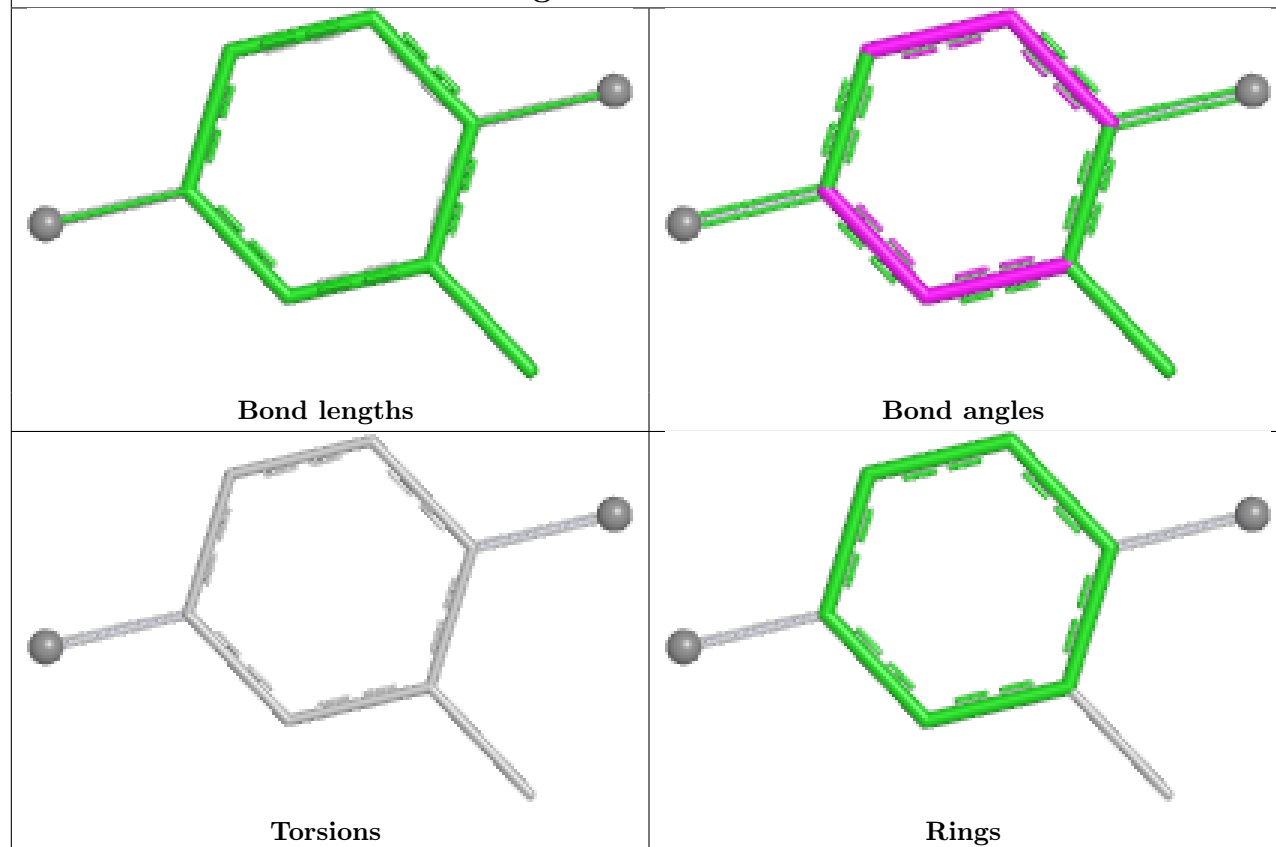
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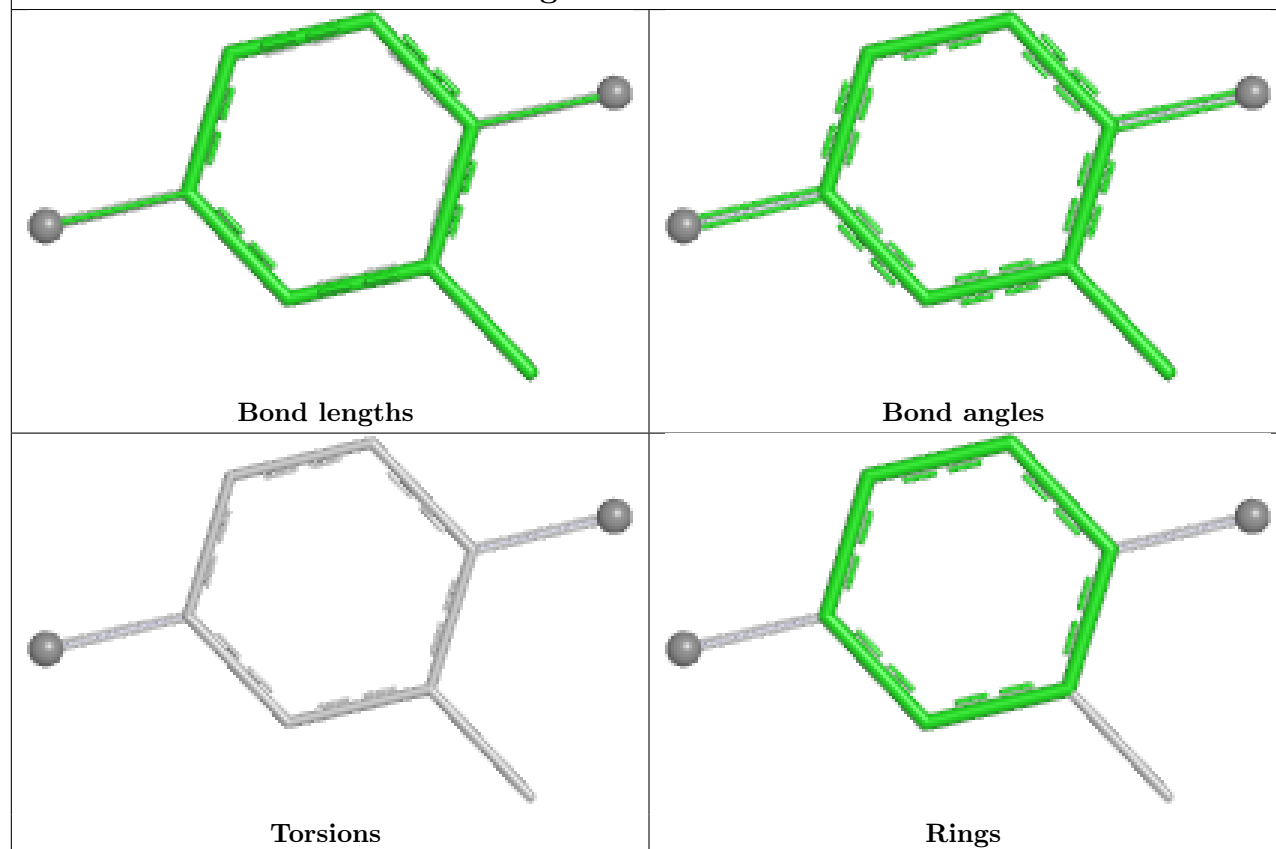
Ligand 7DV P 301



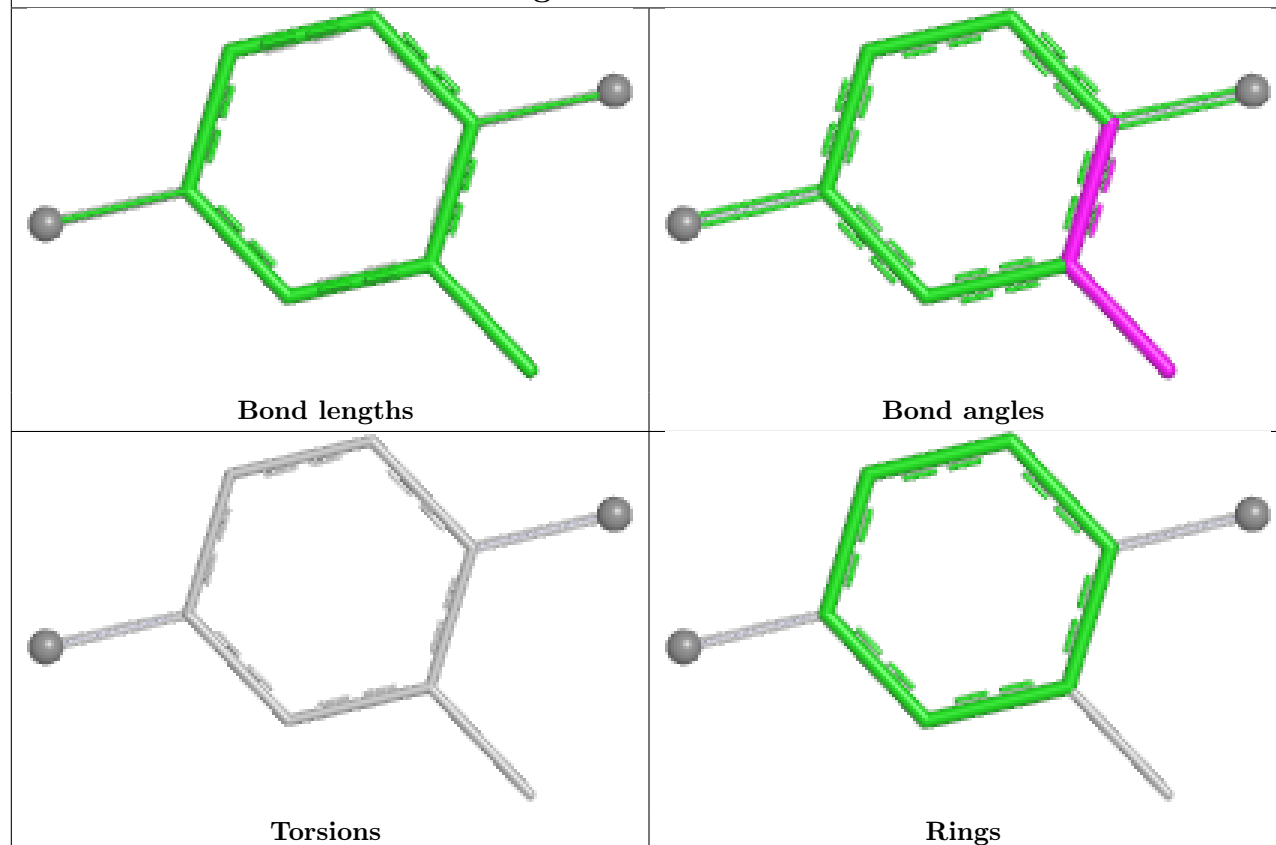
Ligand 7DV A 303



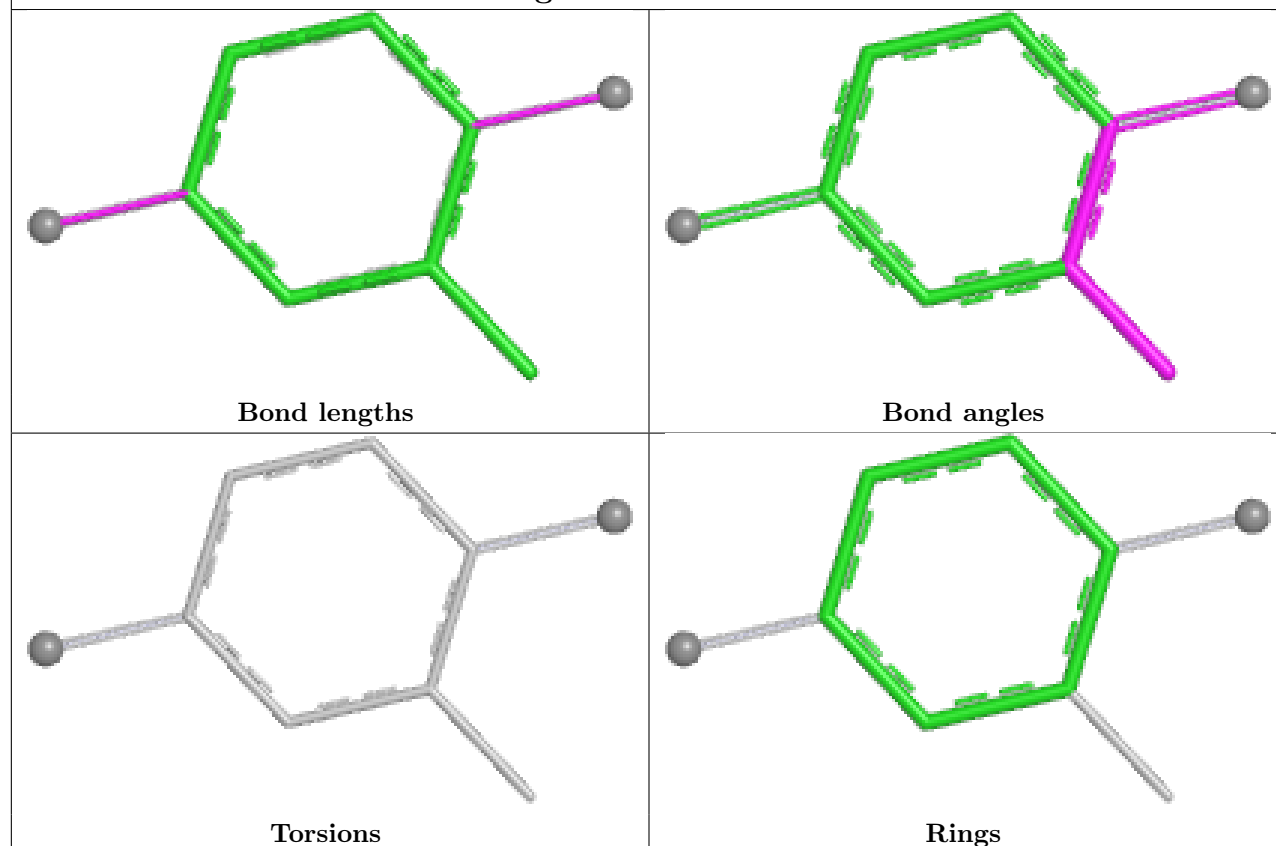
Ligand 7DV I 302



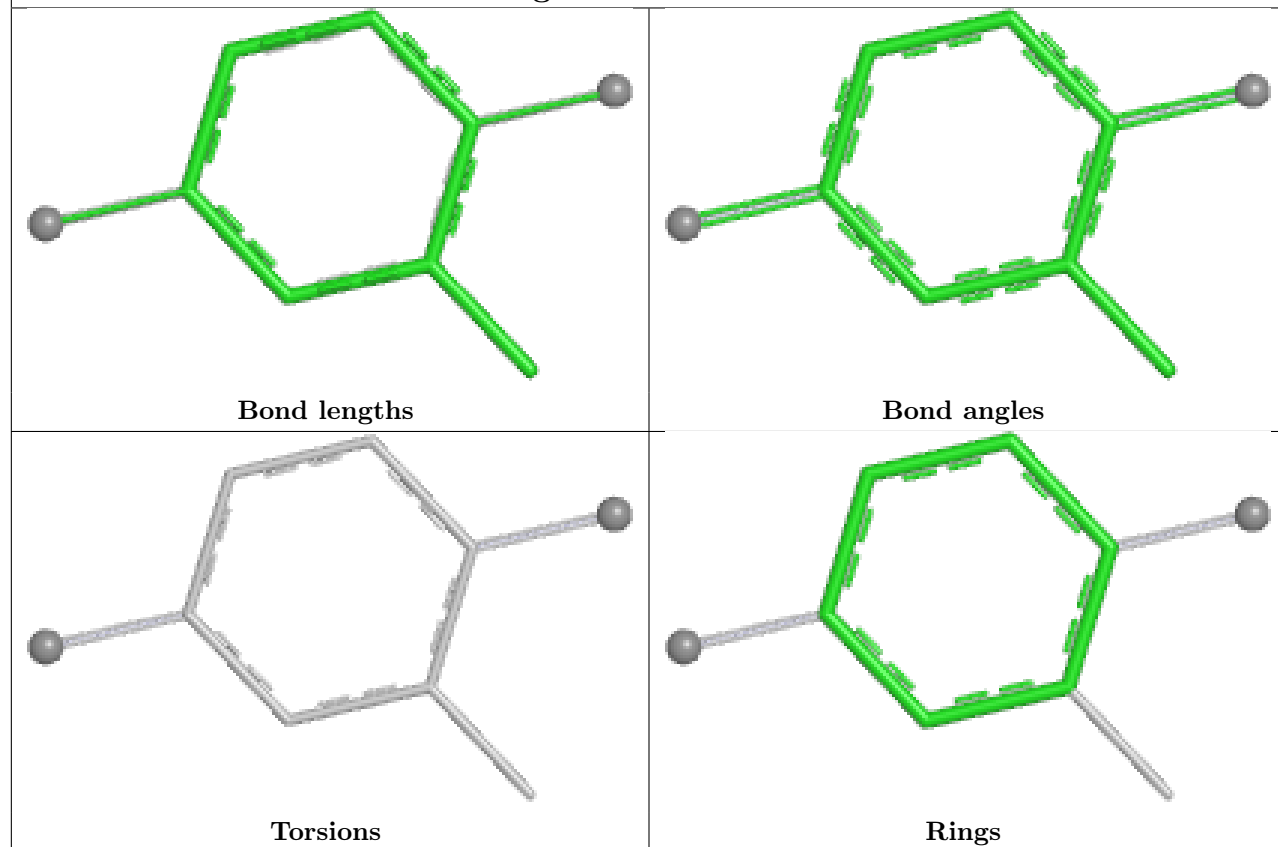
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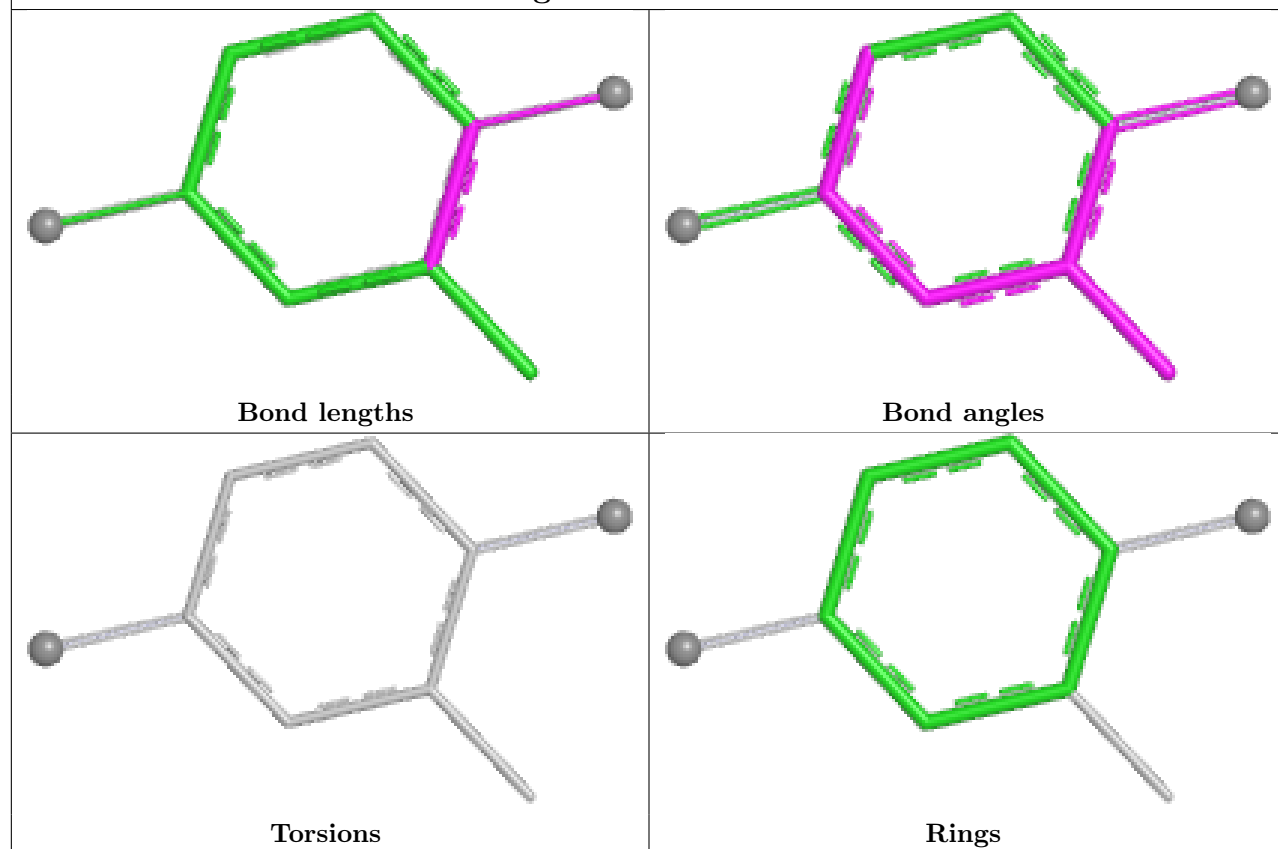
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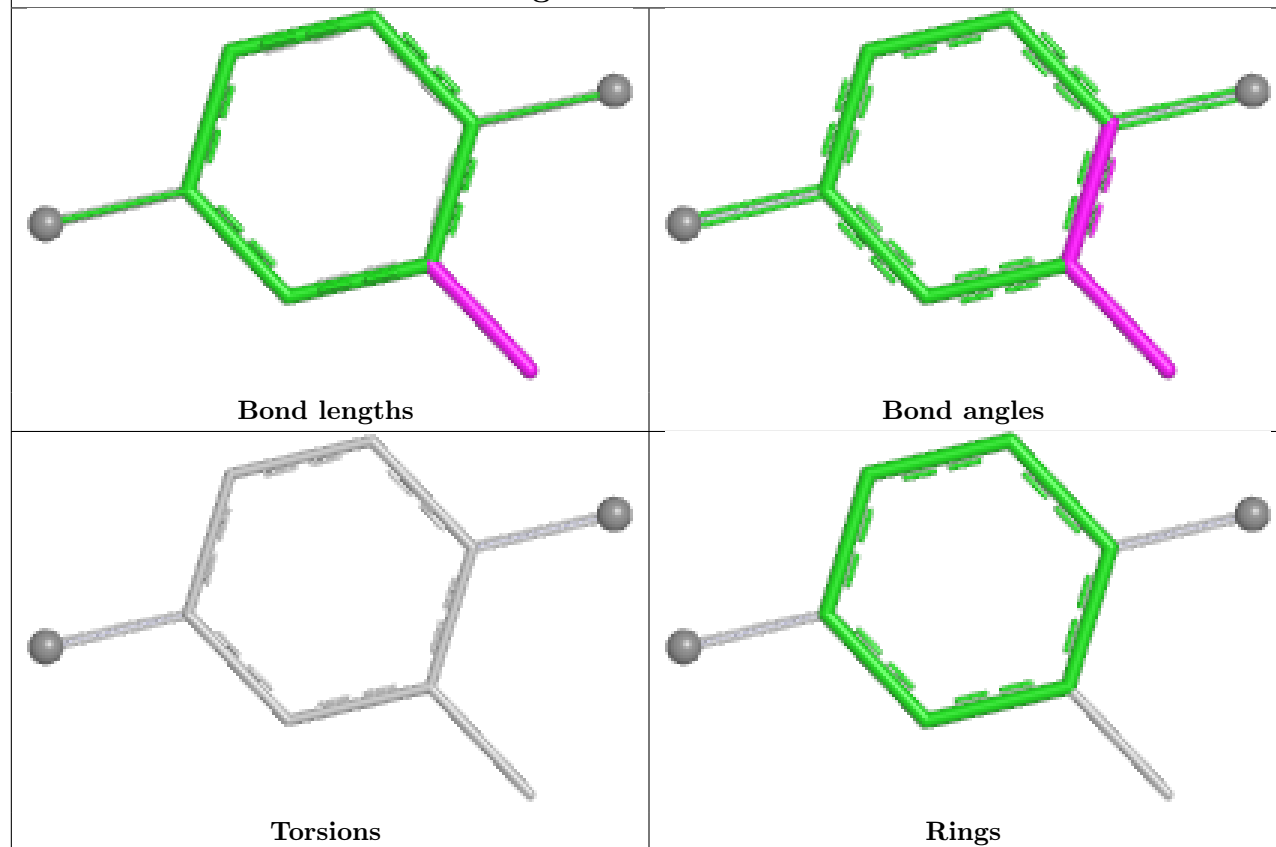
Ligand 7DV D 303



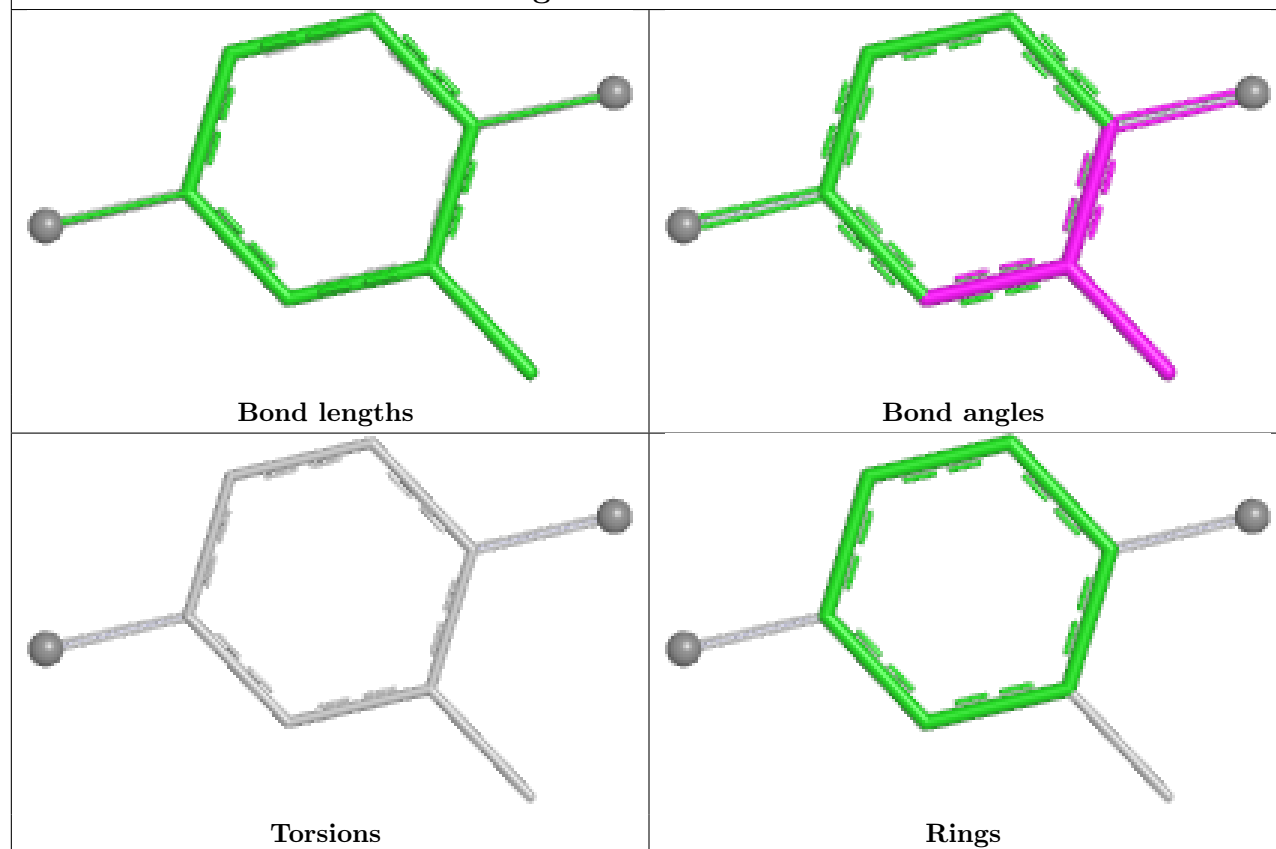
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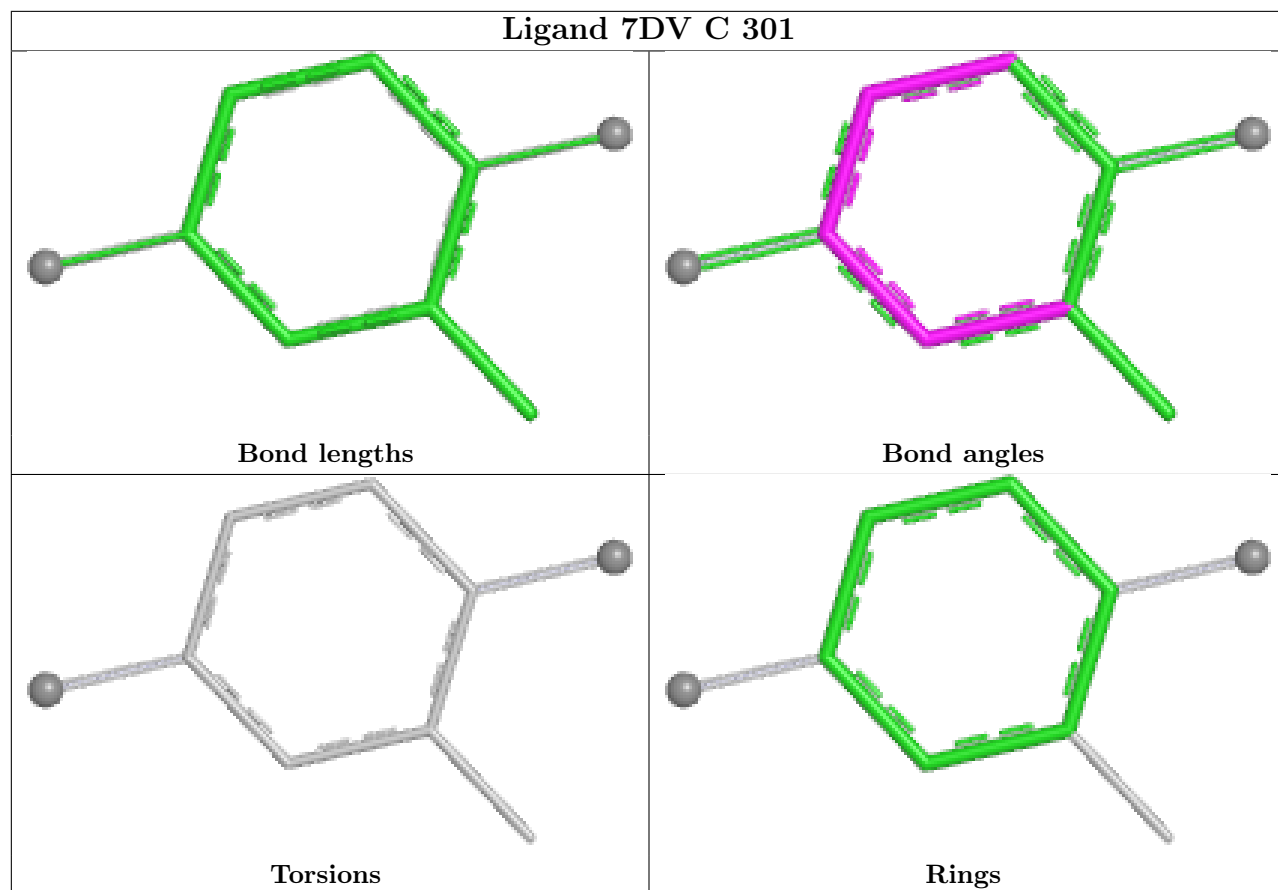


Ligand 7DV N 302



Ligand 7DV D 301





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	202/207 (97%)	-0.27	0 100 100	45, 65, 81, 97	0
1	B	202/207 (97%)	-0.26	0 100 100	49, 69, 85, 96	0
1	C	202/207 (97%)	-0.29	0 100 100	45, 65, 82, 94	0
1	D	203/207 (98%)	-0.26	0 100 100	49, 69, 83, 96	0
1	E	202/207 (97%)	-0.37	0 100 100	43, 62, 80, 95	0
1	F	204/207 (98%)	-0.34	0 100 100	42, 66, 83, 104	0
1	G	202/207 (97%)	-0.32	0 100 100	44, 62, 81, 103	0
1	H	203/207 (98%)	-0.30	0 100 100	50, 68, 84, 111	0
1	I	202/207 (97%)	-0.30	1 (0%) 87 82	44, 64, 80, 101	0
1	J	200/207 (96%)	-0.29	0 100 100	43, 69, 84, 106	0
1	K	202/207 (97%)	-0.29	1 (0%) 87 82	42, 63, 80, 95	0
1	L	201/207 (97%)	-0.30	0 100 100	49, 68, 79, 85	0
1	M	202/207 (97%)	-0.35	0 100 100	45, 62, 81, 95	0
1	N	203/207 (98%)	-0.33	1 (0%) 87 82	43, 66, 81, 110	0
1	O	202/207 (97%)	-0.34	0 100 100	44, 62, 83, 92	0
1	P	203/207 (98%)	-0.27	1 (0%) 87 82	48, 69, 82, 95	0
All	All	3235/3312 (97%)	-0.30	4 (0%) 92 90	42, 66, 83, 111	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	274	ALA	2.4
1	I	216	LEU	2.1
1	P	149	VAL	2.1
1	K	204	ASP	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	7DV	G	303	9/9	0.71	0.18	63,65,73,78	0
2	7DV	E	303	9/9	0.74	0.14	41,53,70,75	0
2	7DV	A	303	9/9	0.80	0.15	50,70,81,86	0
2	7DV	E	302	9/9	0.81	0.13	83,89,97,101	0
2	7DV	I	302	9/9	0.82	0.14	56,67,76,77	0
2	7DV	O	303	9/9	0.82	0.15	50,56,72,73	0
2	7DV	M	302	9/9	0.84	0.11	58,67,79,82	0
2	7DV	O	301	9/9	0.84	0.17	58,88,98,107	0
2	7DV	K	303	9/9	0.84	0.12	62,70,82,82	0
2	7DV	O	302	9/9	0.85	0.14	46,63,69,72	0
2	7DV	I	303	9/9	0.86	0.15	60,66,80,82	0
2	7DV	M	303	9/9	0.86	0.13	41,48,55,59	0
2	7DV	J	302	9/9	0.86	0.10	63,73,77,79	0
2	7DV	K	301	9/9	0.86	0.19	68,84,98,100	0
2	7DV	E	301	9/9	0.86	0.18	65,85,104,108	0
2	7DV	G	301	9/9	0.87	0.16	50,64,73,80	0
2	7DV	D	302	9/9	0.88	0.10	54,72,85,89	0
2	7DV	B	302	9/9	0.88	0.11	67,81,94,94	0
3	NA	F	304	1/1	0.88	0.10	59,59,59,59	0
2	7DV	C	303	9/9	0.89	0.10	57,62,65,81	0
2	7DV	A	301	9/9	0.89	0.16	64,74,83,85	0
2	7DV	F	302	9/9	0.89	0.10	58,68,74,74	0
2	7DV	A	302	9/9	0.89	0.10	38,53,64,71	0
2	7DV	G	302	9/9	0.90	0.11	57,65,71,75	0
2	7DV	L	301	9/9	0.90	0.12	49,59,64,65	0
2	7DV	N	301	9/9	0.90	0.14	71,80,89,96	0
3	NA	E	304	1/1	0.90	0.12	43,43,43,43	0

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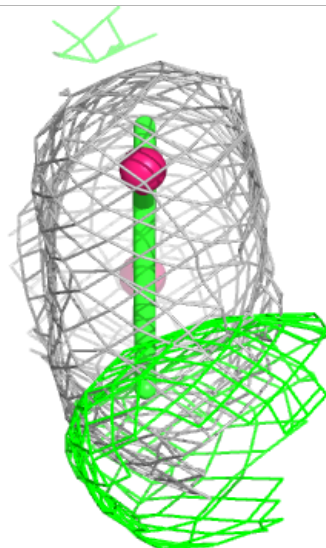
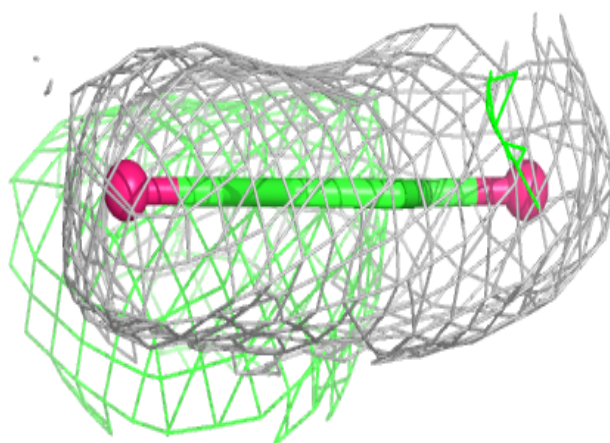
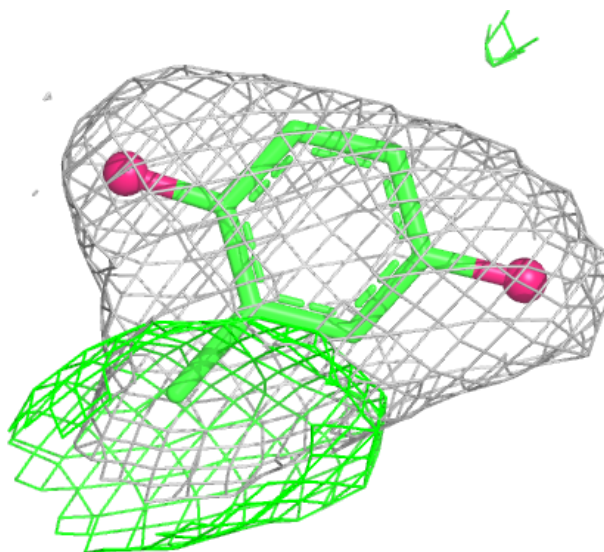
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7DV	N	303	9/9	0.90	0.11	48,69,87,91	0
2	7DV	M	301	9/9	0.91	0.15	60,72,83,83	0
2	7DV	N	302	9/9	0.91	0.11	66,82,90,94	0
2	7DV	C	302	9/9	0.91	0.09	42,54,61,88	0
2	7DV	J	301	9/9	0.91	0.13	68,72,86,87	0
2	7DV	F	303	9/9	0.92	0.09	65,73,81,84	0
2	7DV	C	301	9/9	0.92	0.14	62,67,72,87	0
2	7DV	F	301	9/9	0.92	0.10	47,56,65,70	0
2	7DV	B	303	9/9	0.92	0.10	66,71,83,88	0
2	7DV	P	302	9/9	0.92	0.08	42,51,58,64	0
3	NA	D	305	1/1	0.92	0.11	45,45,45,45	0
2	7DV	H	302	9/9	0.92	0.07	51,57,64,65	0
2	7DV	H	303	9/9	0.92	0.08	53,65,70,79	0
3	NA	I	305	1/1	0.92	0.16	55,55,55,55	0
3	NA	O	304	1/1	0.92	0.17	55,55,55,55	0
2	7DV	P	303	9/9	0.93	0.09	46,61,73,83	0
3	NA	A	304	1/1	0.93	0.19	59,59,59,59	0
2	7DV	I	301	9/9	0.93	0.11	68,73,79,81	0
2	7DV	B	301	9/9	0.93	0.11	49,62,71,76	0
2	7DV	D	301	9/9	0.93	0.10	52,60,65,65	0
3	NA	I	304	1/1	0.93	0.10	48,48,48,48	0
2	7DV	P	301	9/9	0.93	0.11	62,66,75,76	0
2	7DV	K	302	9/9	0.93	0.09	63,70,77,80	0
3	NA	G	304	1/1	0.94	0.20	55,55,55,55	0
2	7DV	J	303	9/9	0.94	0.09	65,78,79,87	0
2	7DV	L	303	9/9	0.94	0.09	55,64,76,78	0
2	7DV	D	303	9/9	0.94	0.10	61,77,80,83	0
2	7DV	L	302	9/9	0.95	0.09	62,71,78,81	0
3	NA	C	304	1/1	0.95	0.11	48,48,48,48	0
2	7DV	H	301	9/9	0.95	0.09	65,69,75,76	0
3	NA	K	304	1/1	0.96	0.18	52,52,52,52	0
3	NA	N	305	1/1	0.96	0.13	42,42,42,42	0
2	7DV	D	304	9/9	0.96	0.11	58,62,73,78	0
2	7DV	L	304	9/9	0.97	0.09	46,54,63,83	0
3	NA	P	304	1/1	0.97	0.12	48,48,48,48	0
3	NA	H	304	1/1	0.98	0.13	41,41,41,41	0
3	NA	L	305	1/1	0.98	0.12	54,54,54,54	0
3	NA	N	304	1/1	0.98	0.08	64,64,64,64	0
3	NA	B	304	1/1	0.99	0.07	44,44,44,44	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.

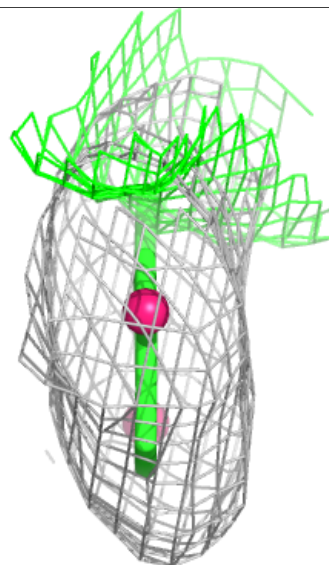
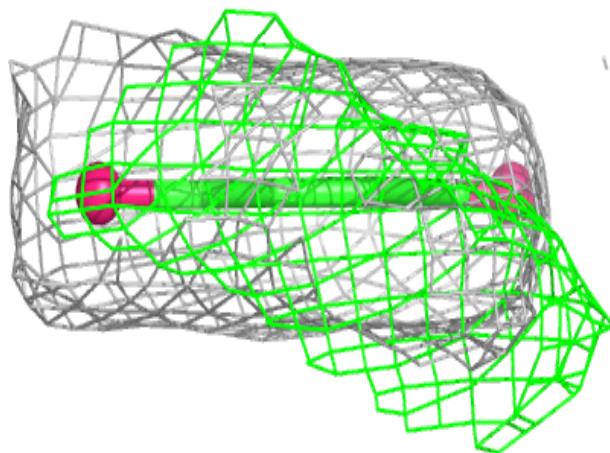
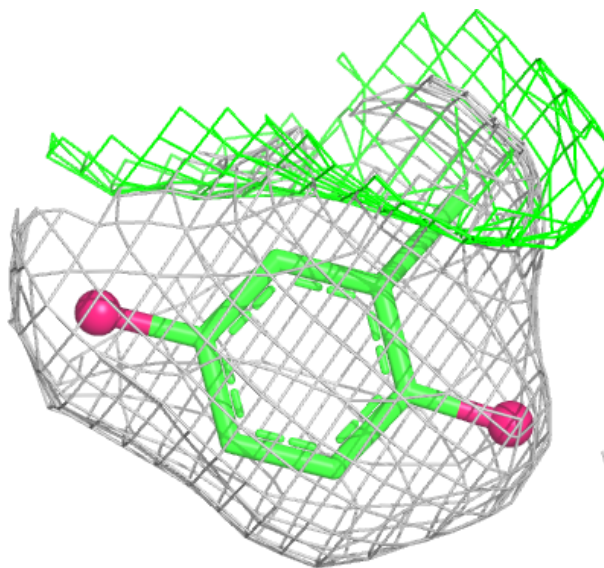
Electron density around 7DV G 303:

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



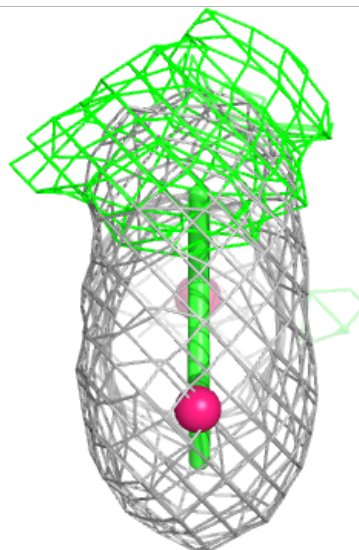
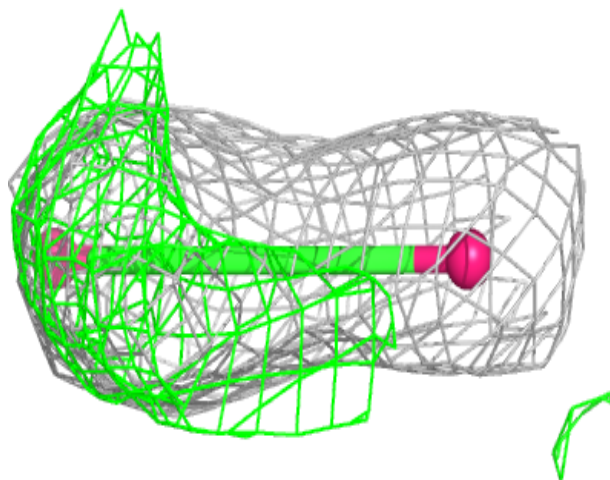
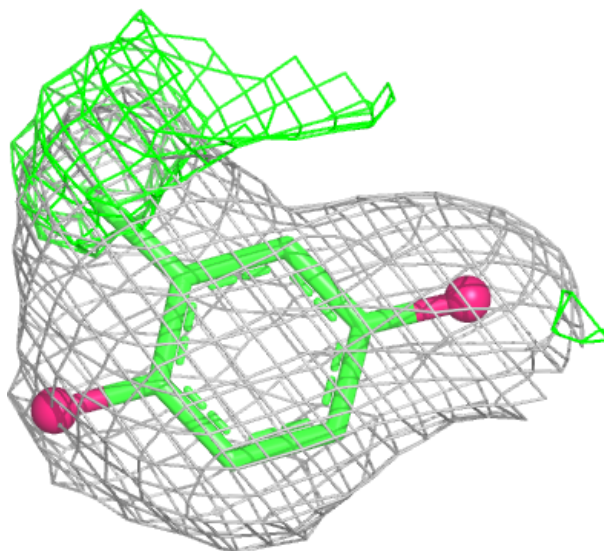
Electron density around 7DV E 303:

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



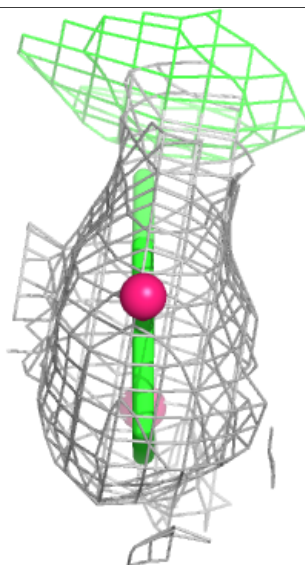
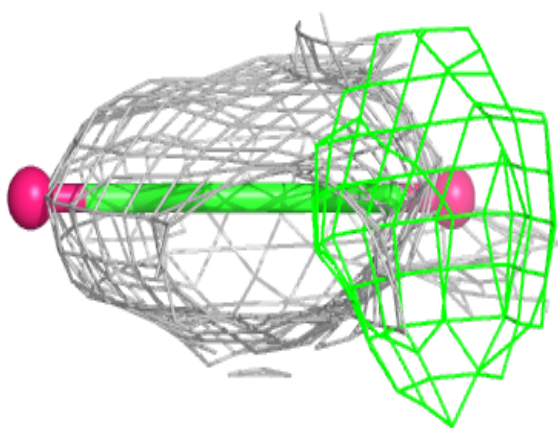
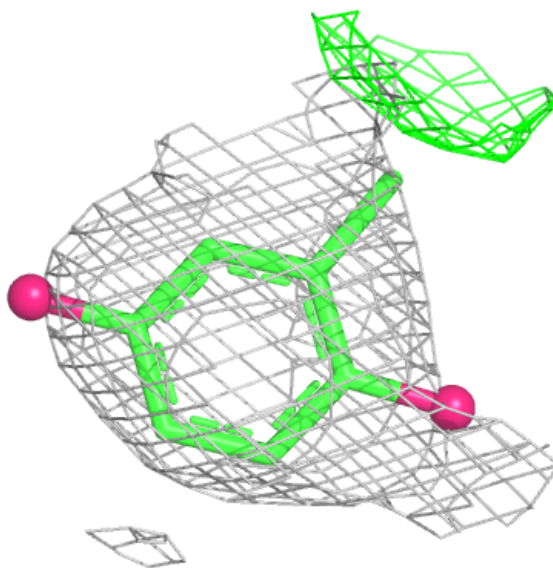
Electron density around 7DV A 303:

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



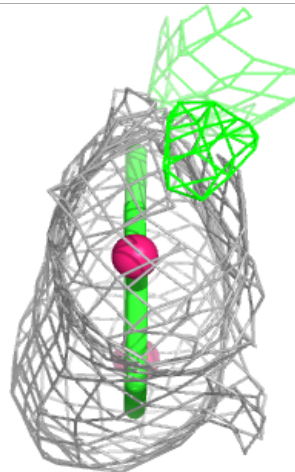
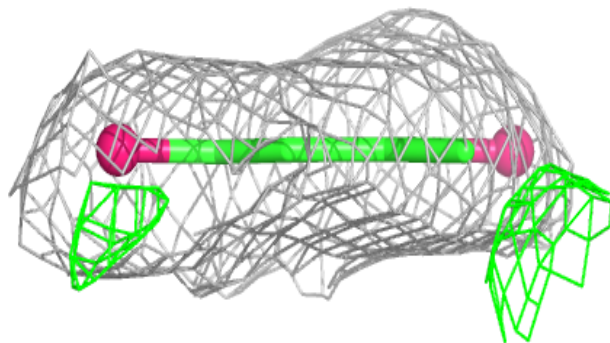
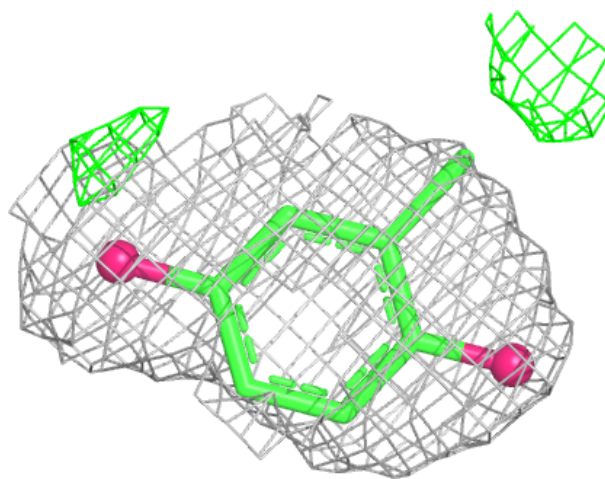
Electron density around 7DV E 302:

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



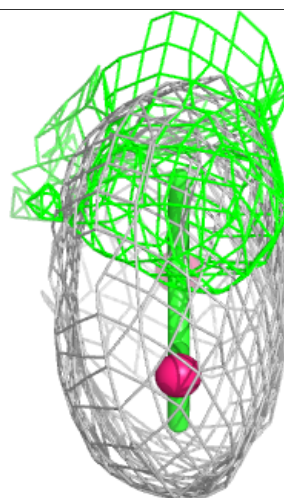
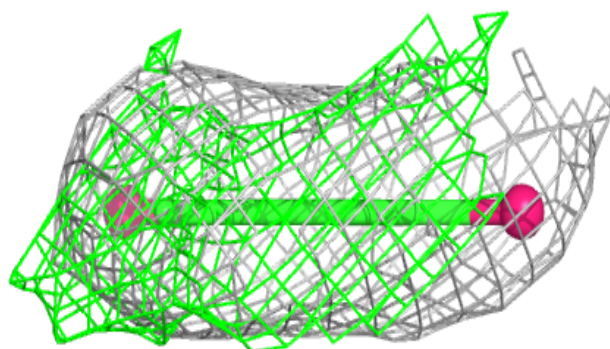
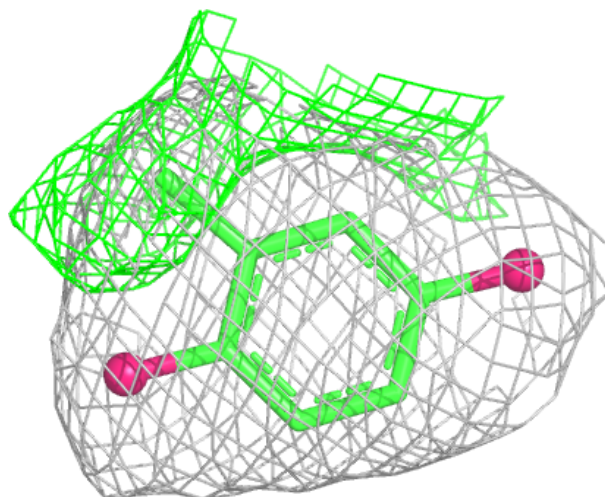
Electron density around 7DV I 302:

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



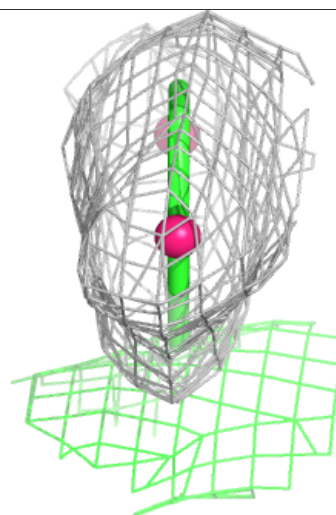
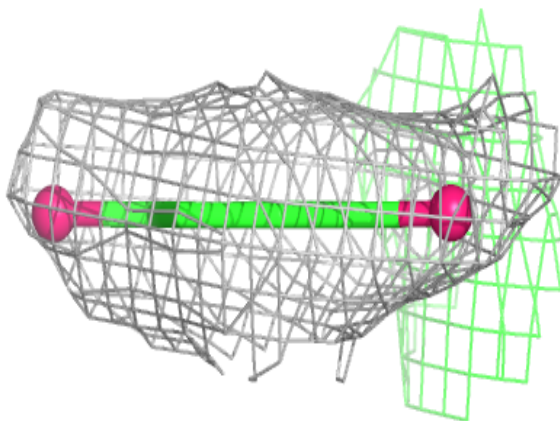
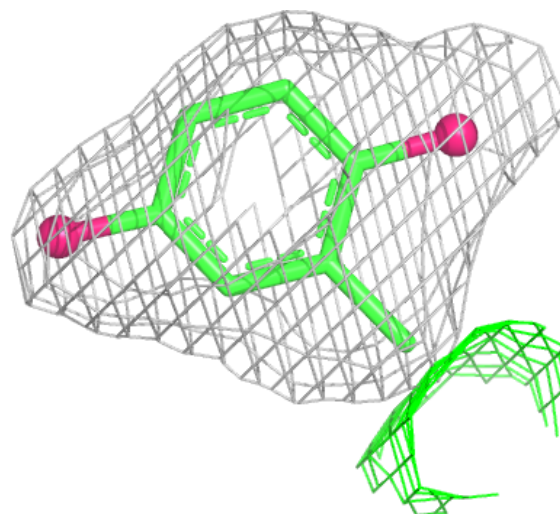
Electron density around 7DV O 303:

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



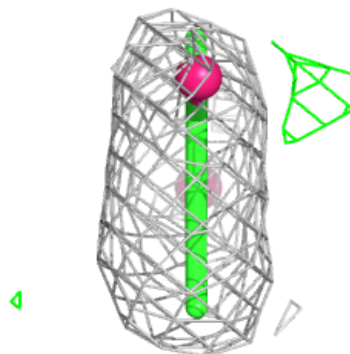
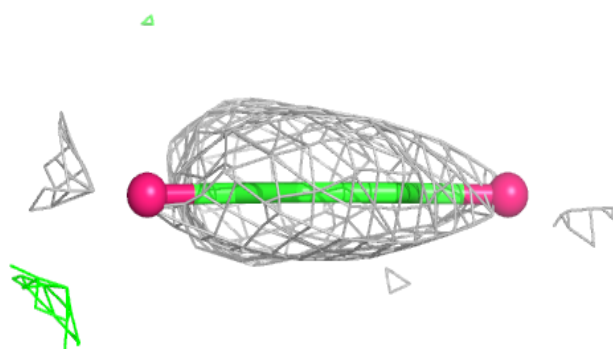
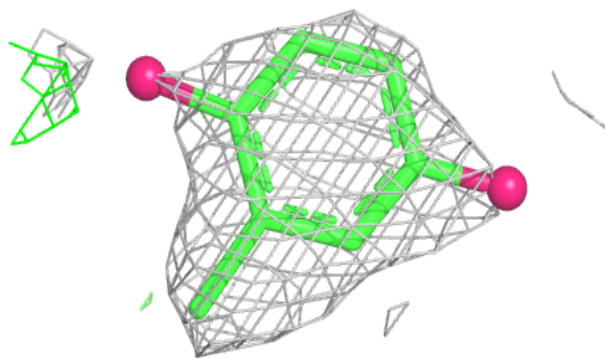
Electron density around 7DV M 302:

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



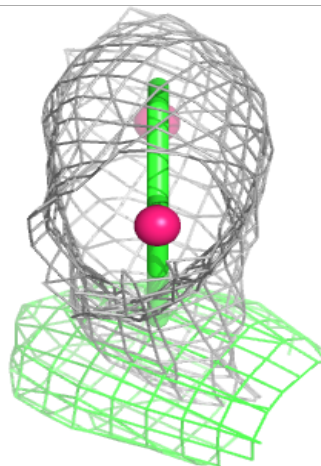
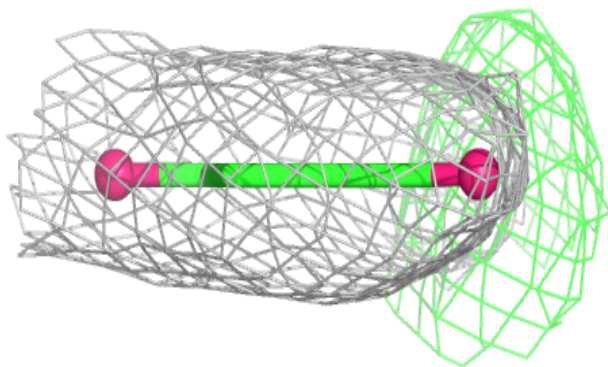
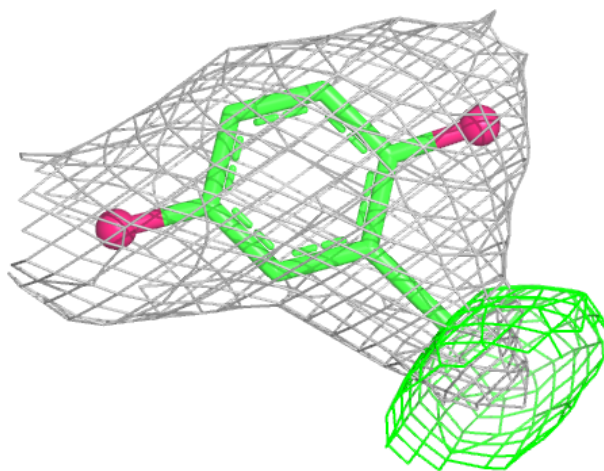
Electron density around 7DV O 301:

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



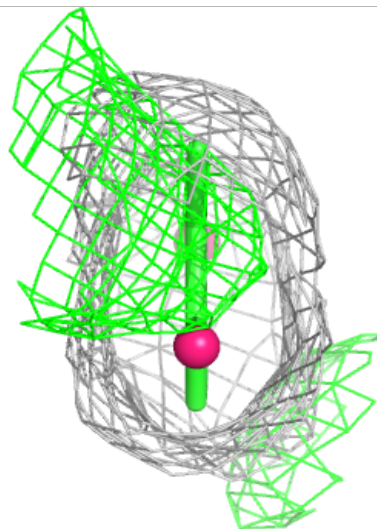
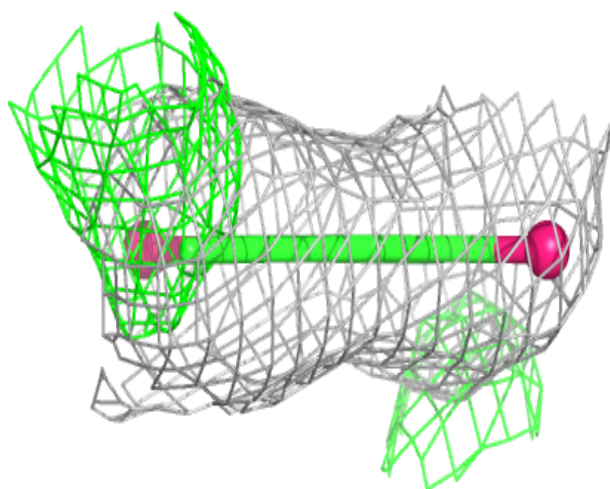
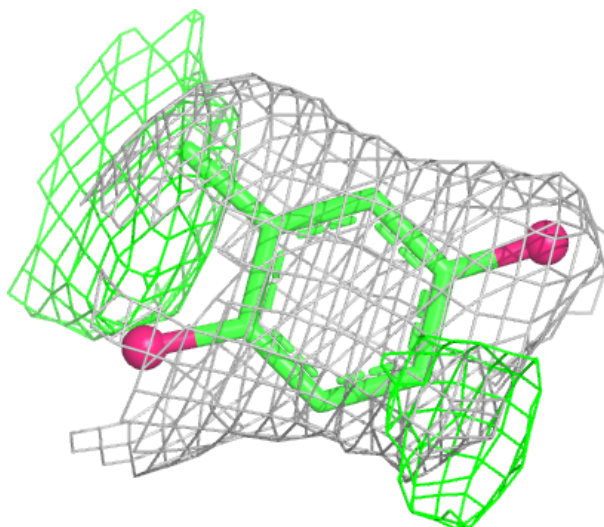
Electron density around 7DV K 303:

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



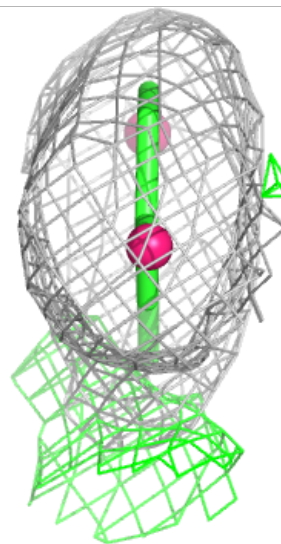
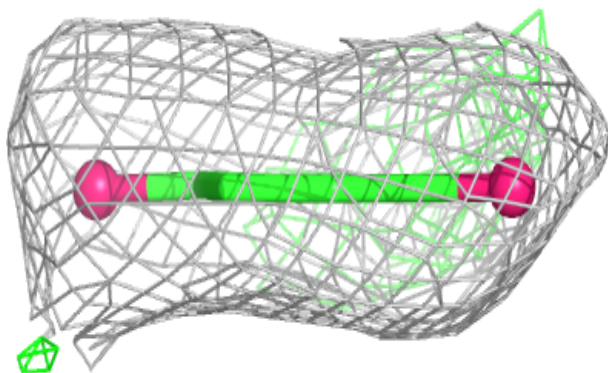
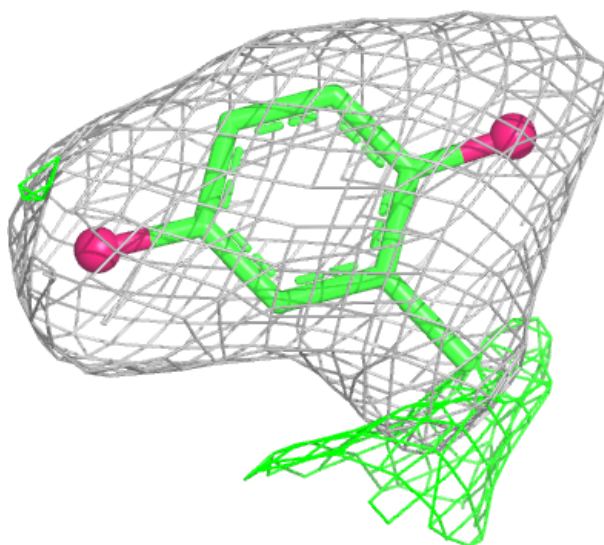
Electron density around 7DV O 302:

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



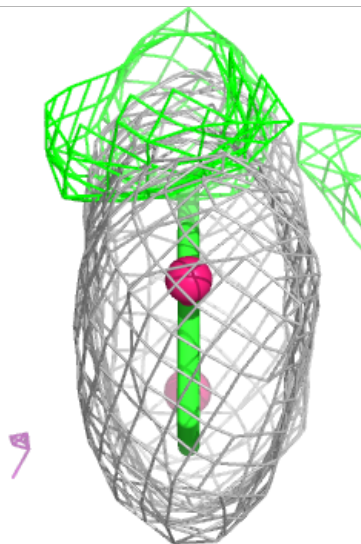
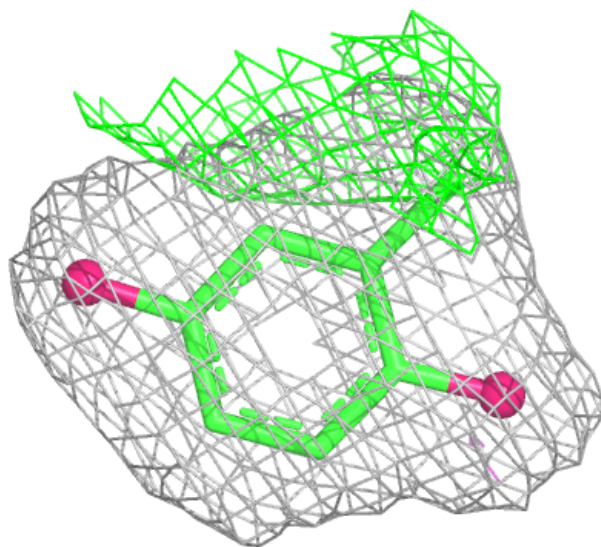
Electron density around 7DV I 303:

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



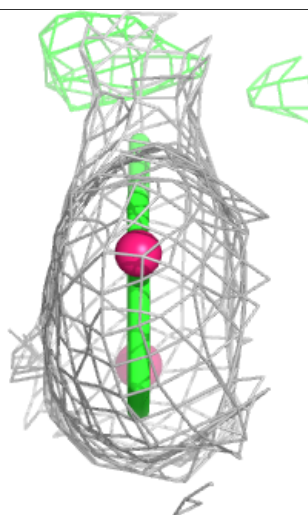
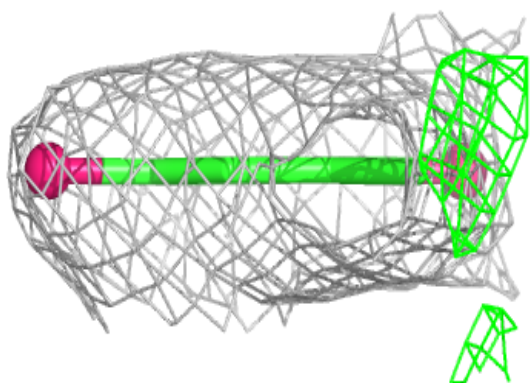
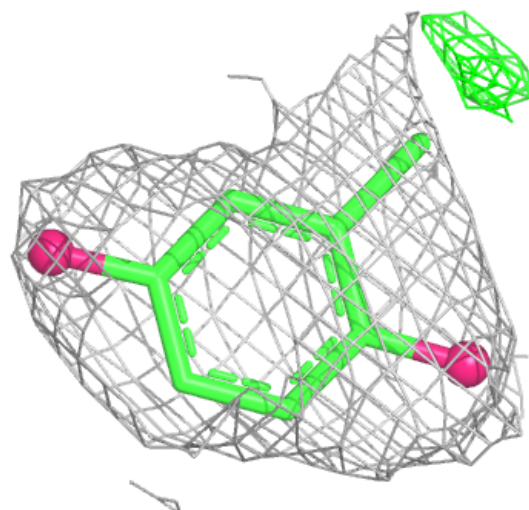
Electron density around 7DV M 303:

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



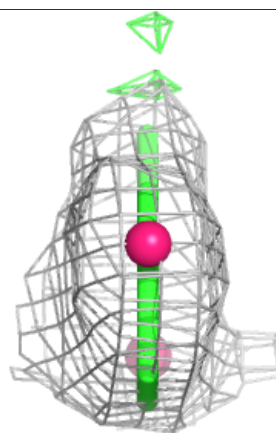
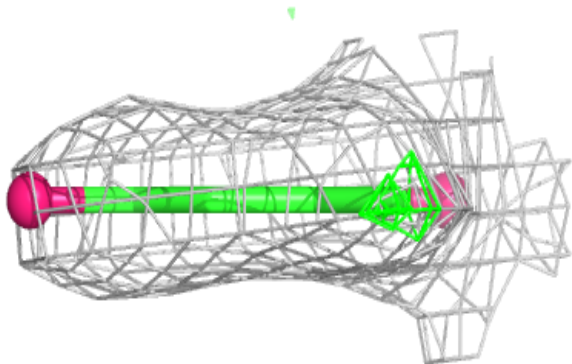
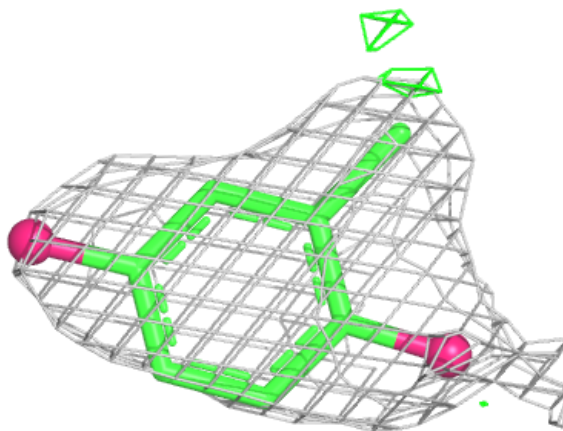
Electron density around 7DV J 302:

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



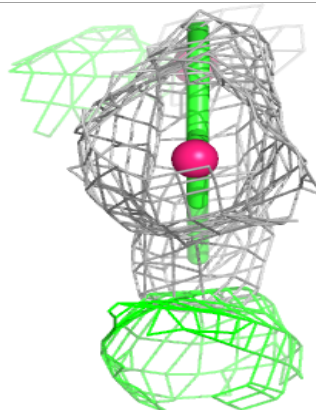
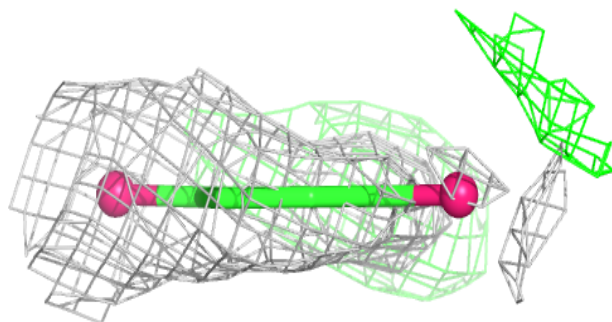
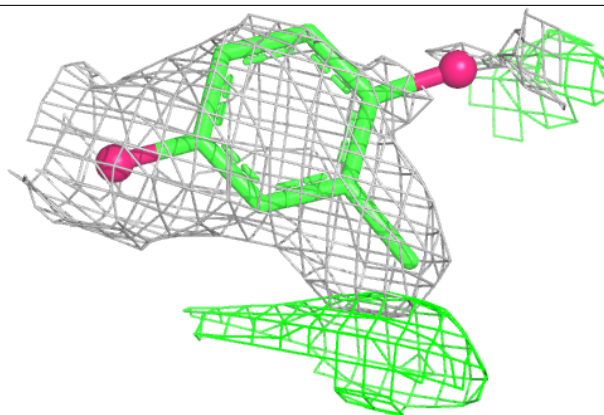
Electron density around 7DV K 301:

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

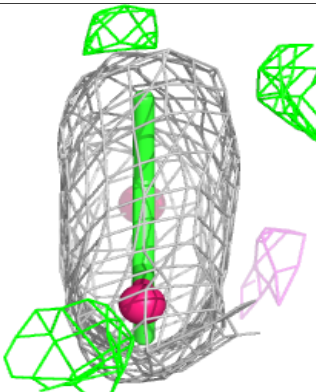
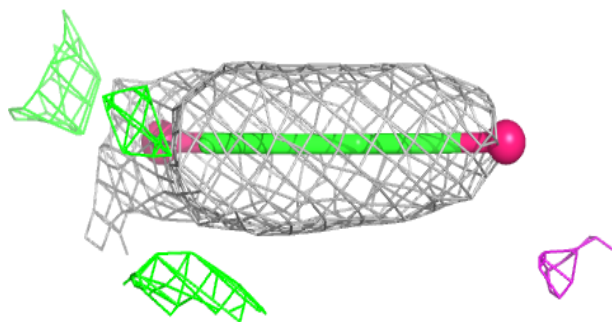
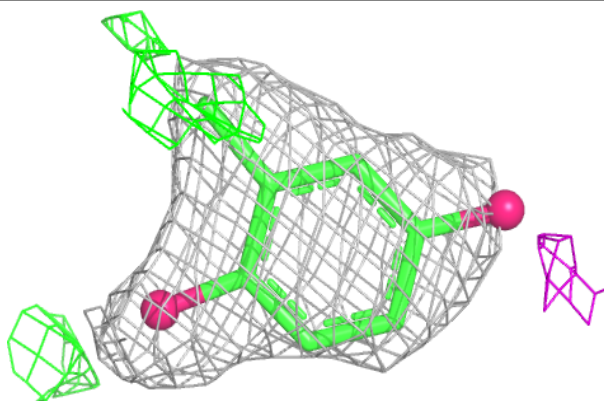


Electron density around 7DV E 301:

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

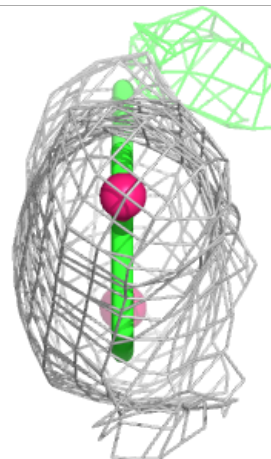
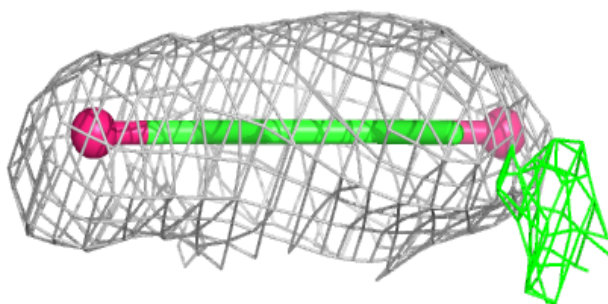
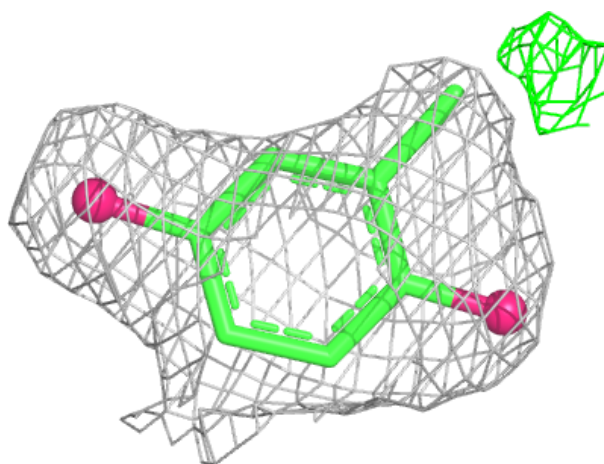
**Electron density around 7DV G 301:**

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



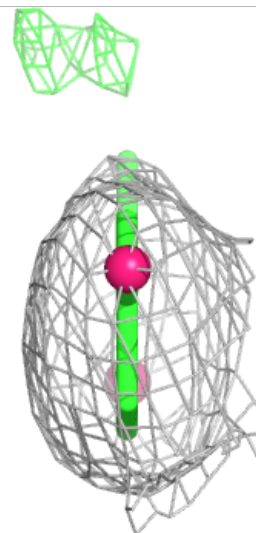
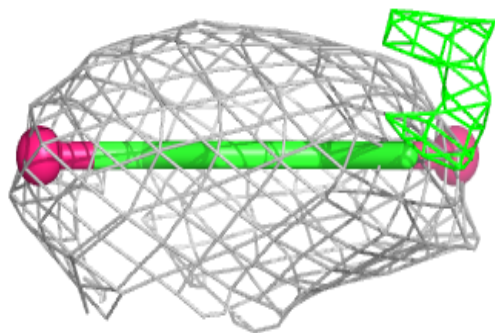
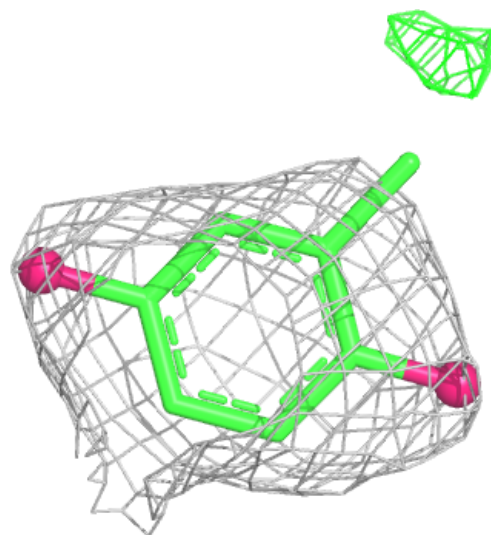
Electron density around 7DV D 302:

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



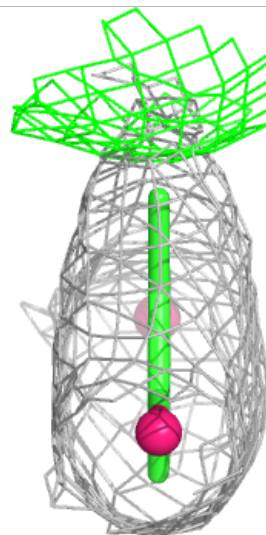
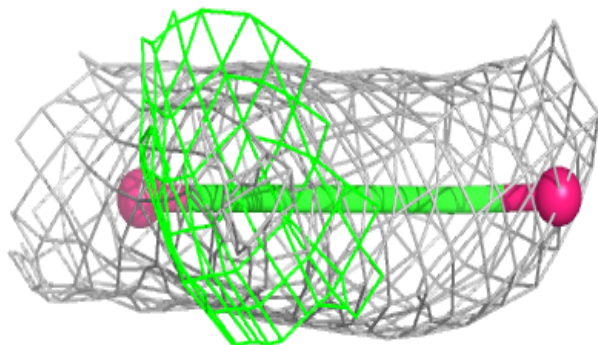
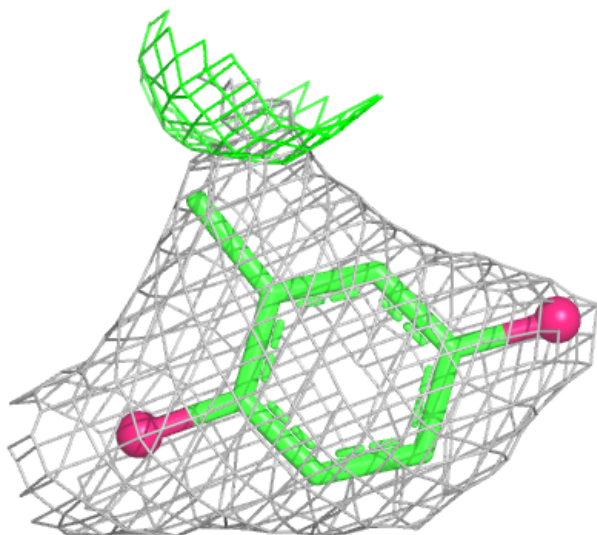
Electron density around 7DV B 302:

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



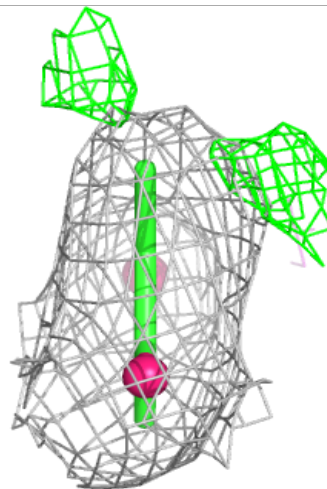
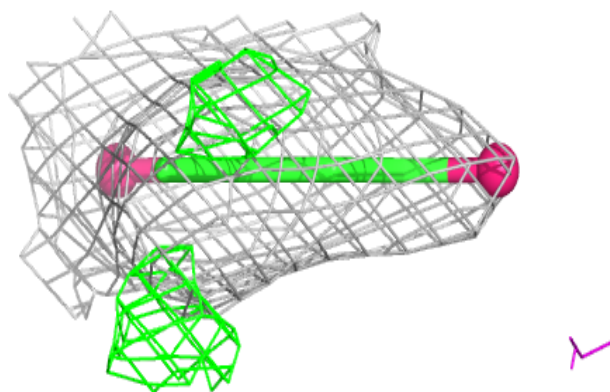
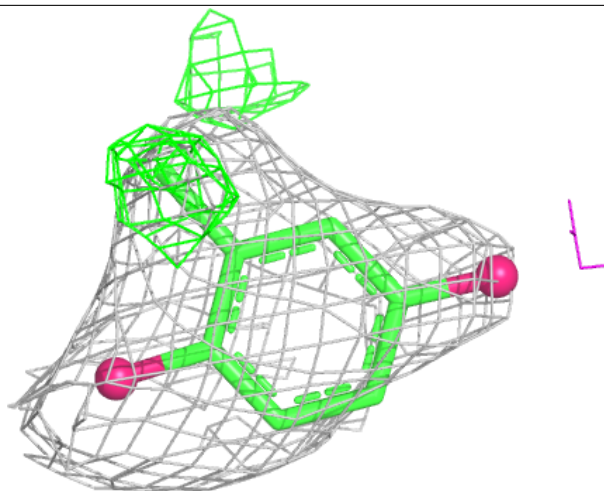
Electron density around 7DV C 303:

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



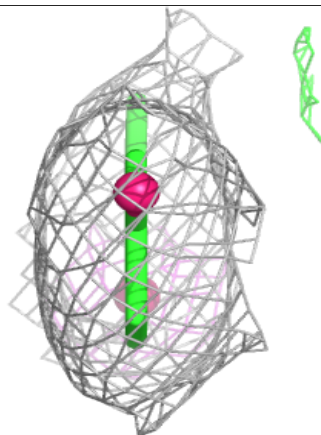
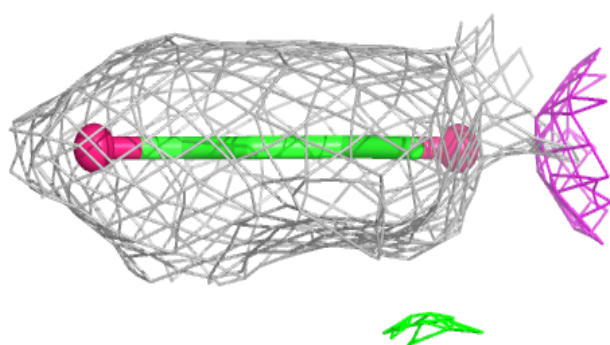
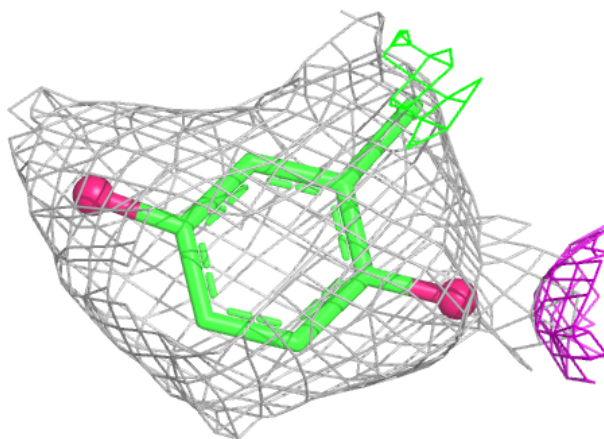
Electron density around 7DV A 301:

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and green (positive)



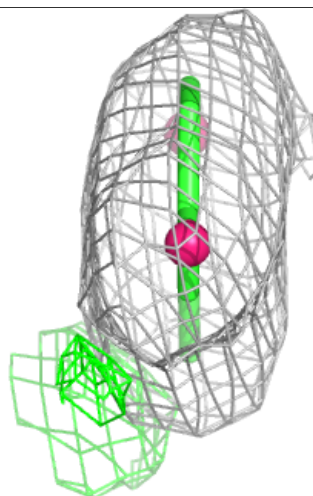
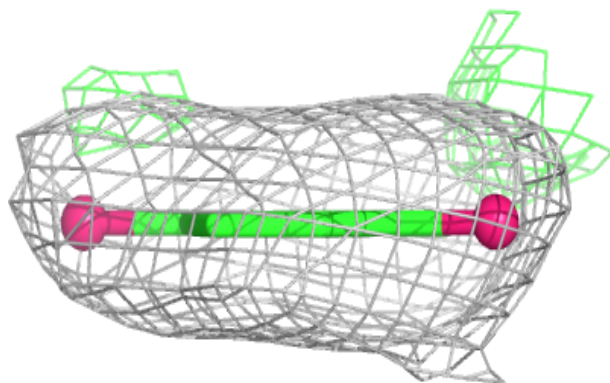
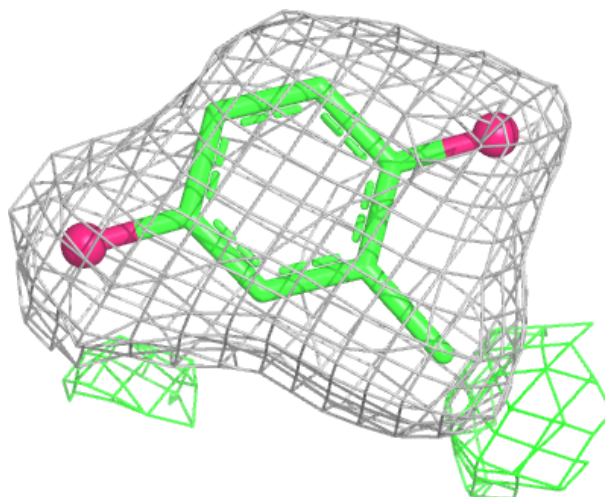
Electron density around 7DV F 302:

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



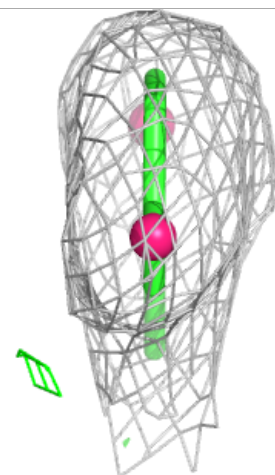
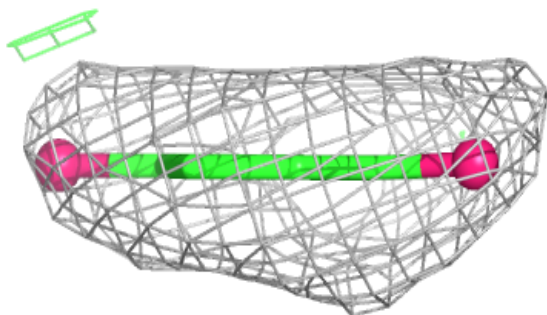
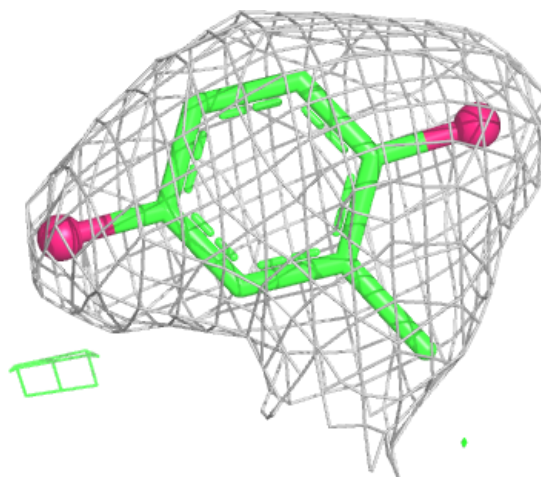
Electron density around 7DV A 302:

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



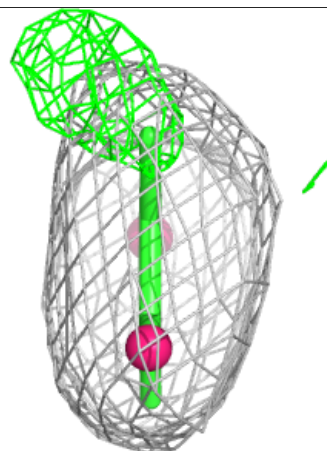
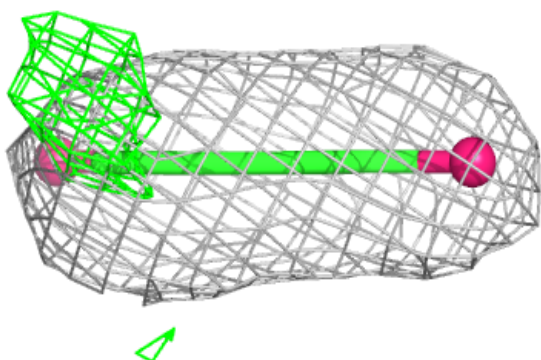
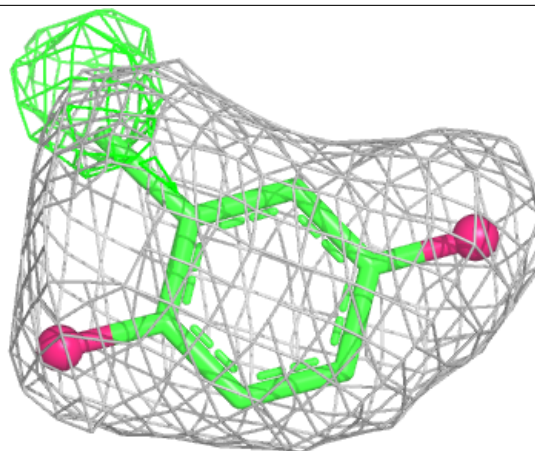
Electron density around 7DV G 302:

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



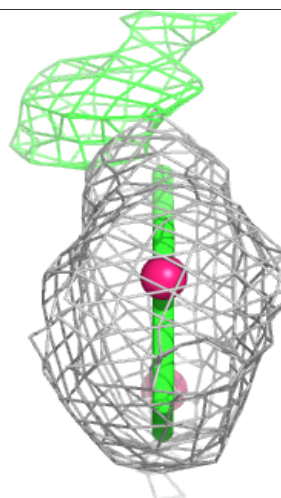
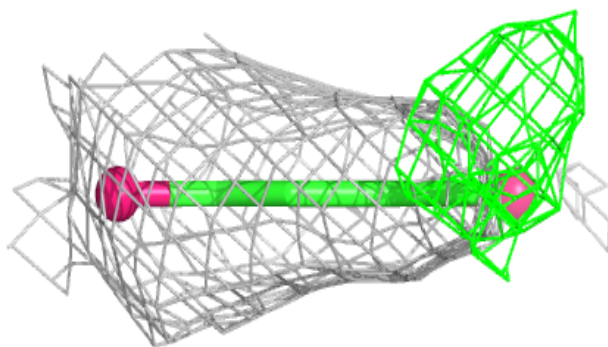
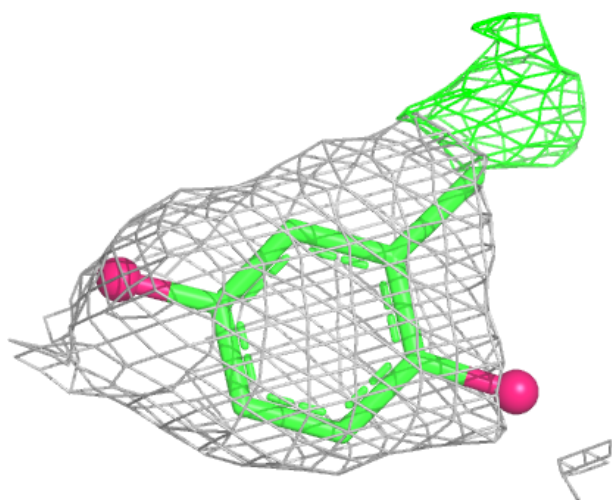
Electron density around 7DV L 301:

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



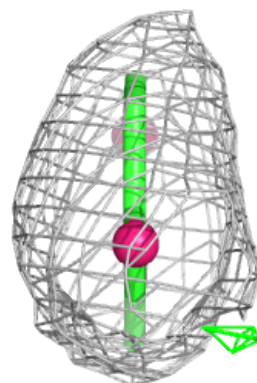
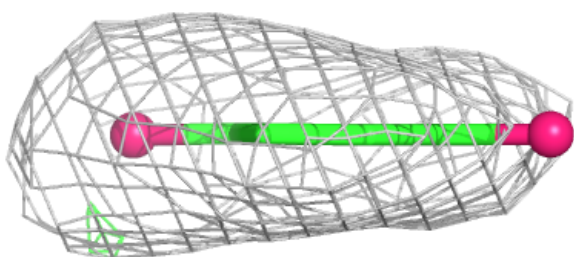
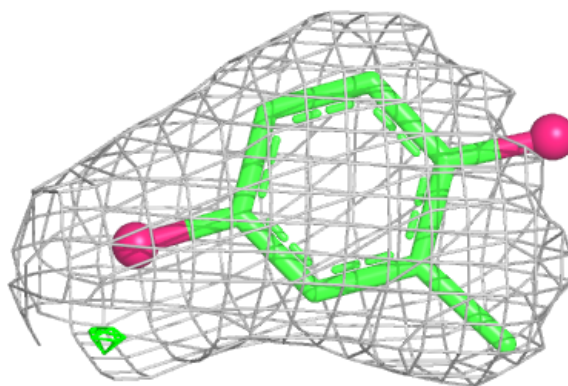
Electron density around 7DV N 301:

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

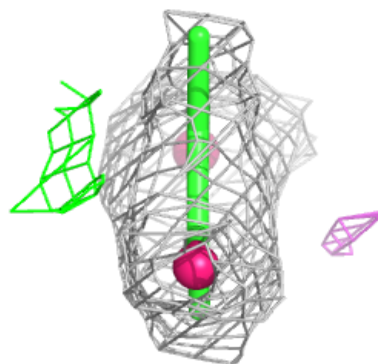
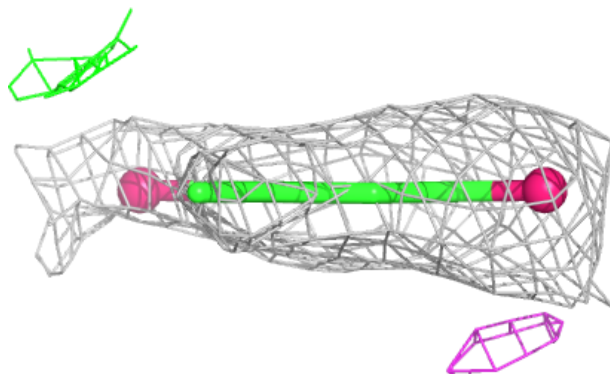
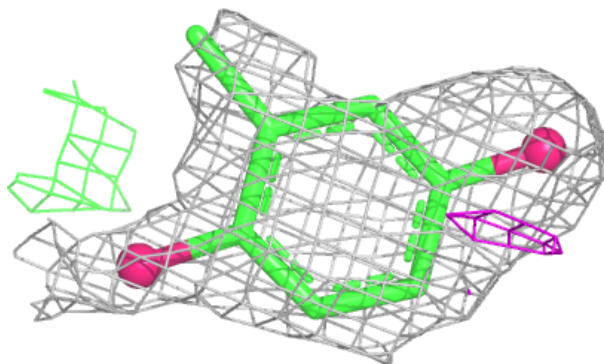


Electron density around 7DV N 303:

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

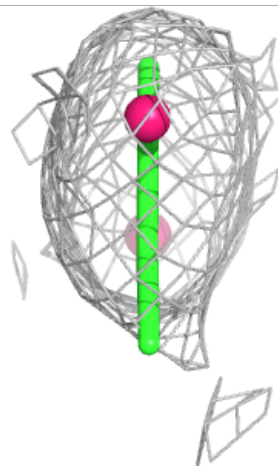
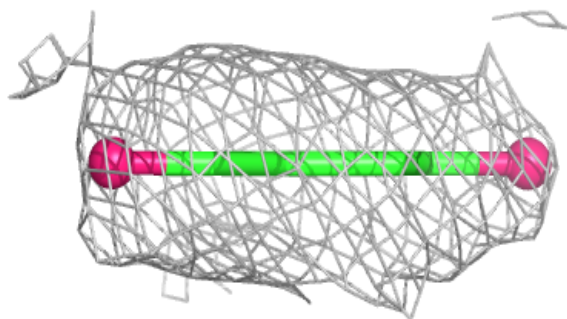
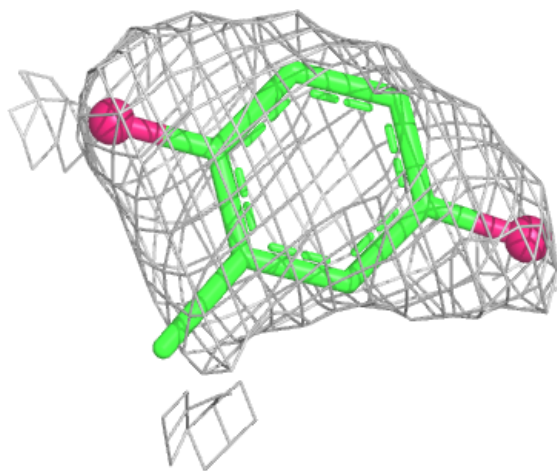
**Electron density around 7DV M 301:**

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



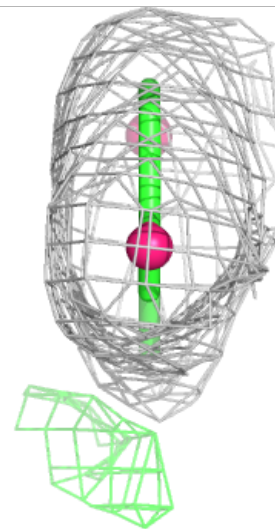
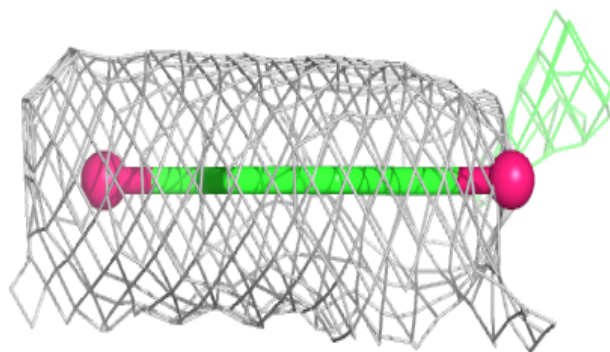
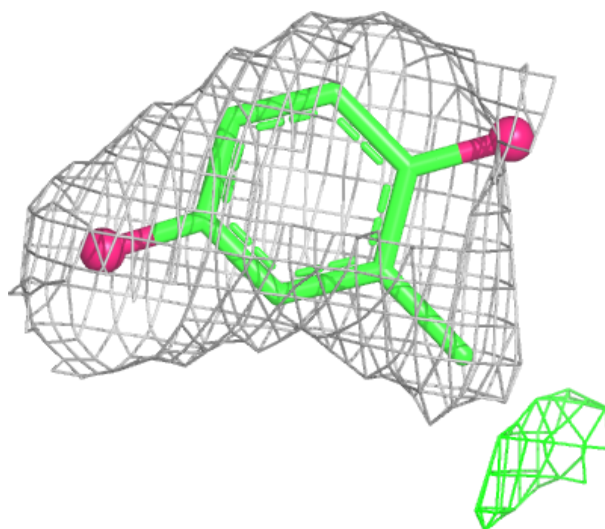
Electron density around 7DV N 302:

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



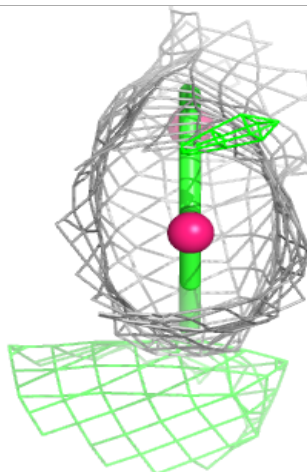
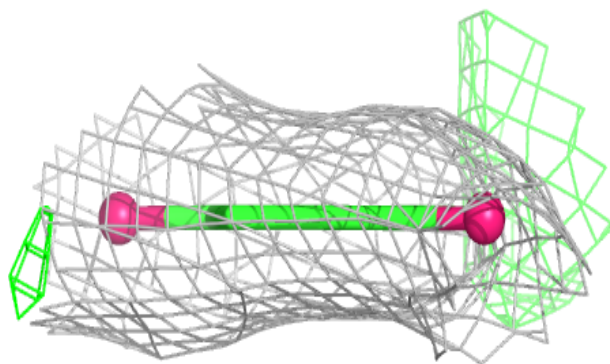
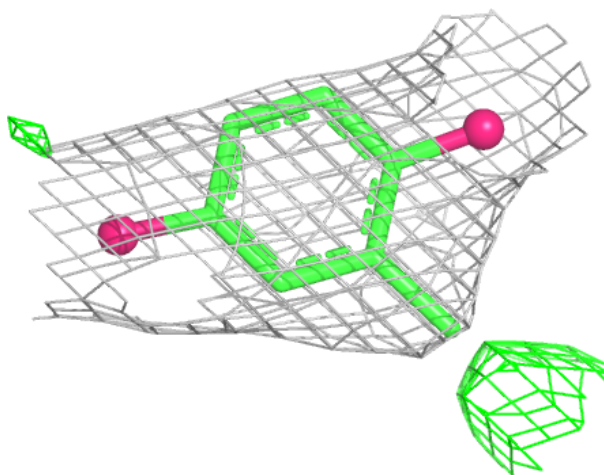
Electron density around 7DV C 302:

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



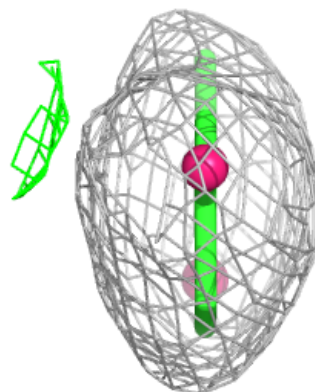
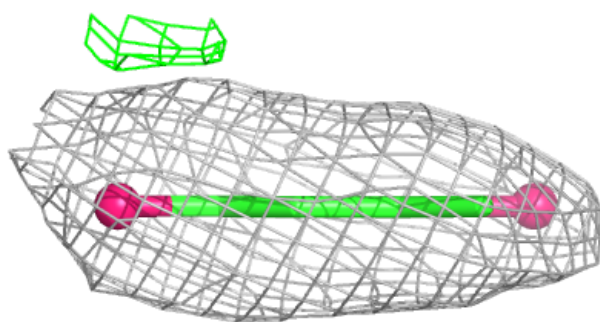
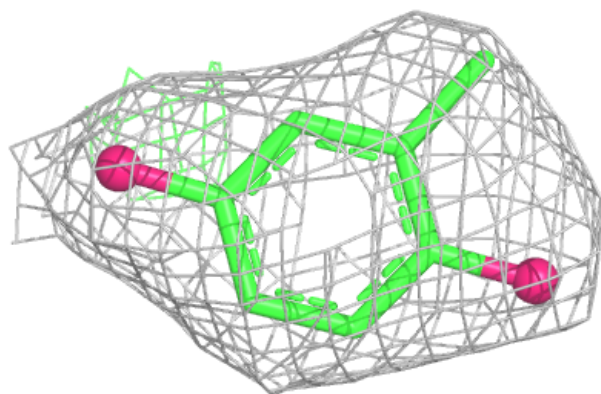
Electron density around 7DV J 301:

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

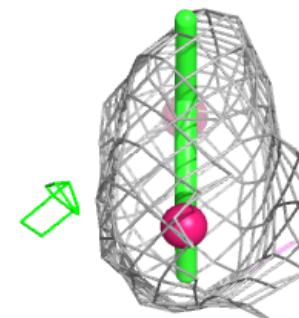
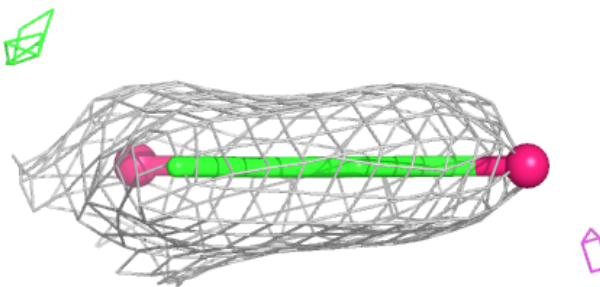
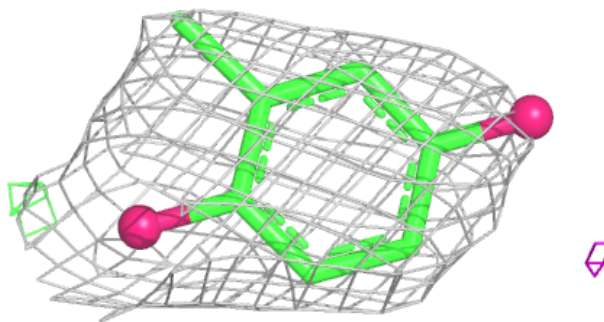


Electron density around 7DV F 303:

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

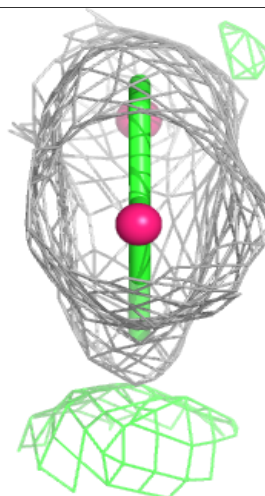
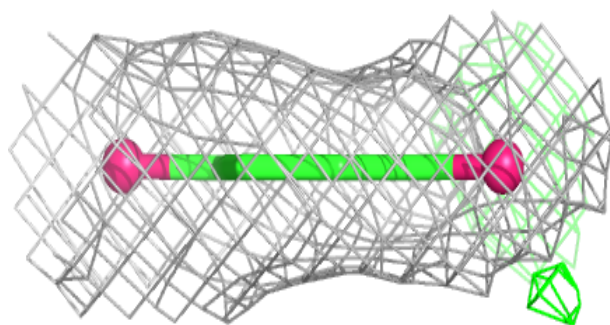
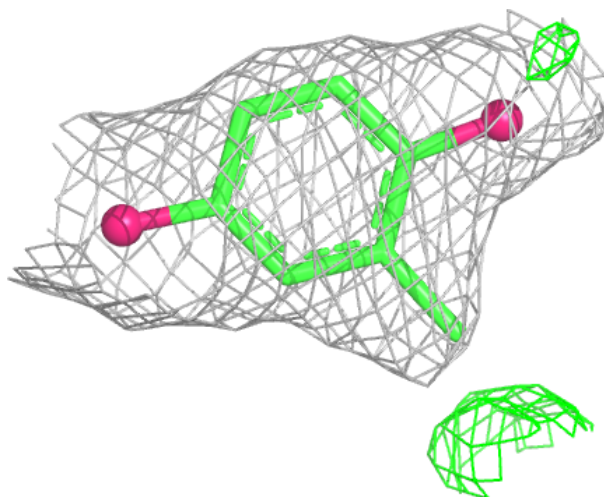
**Electron density around 7DV C 301:**

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



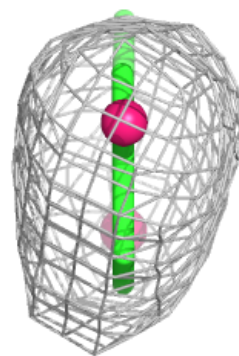
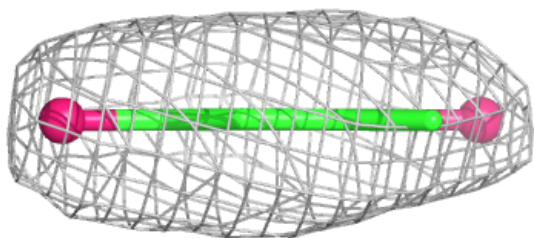
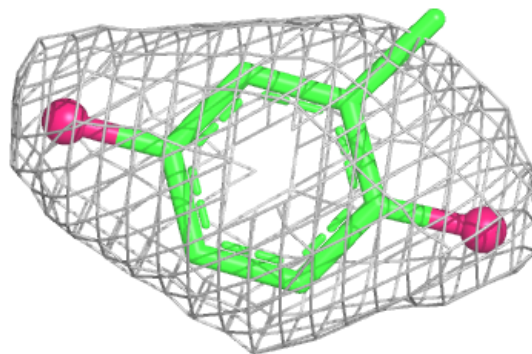
Electron density around 7DV F 301:

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



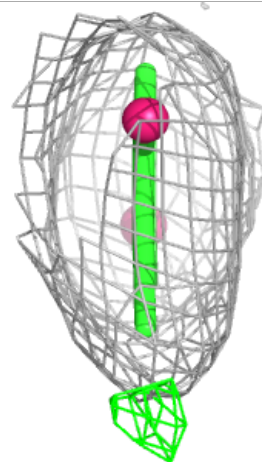
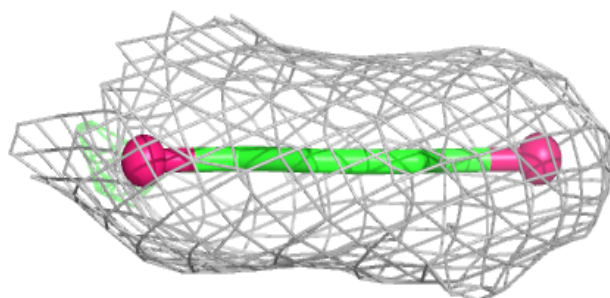
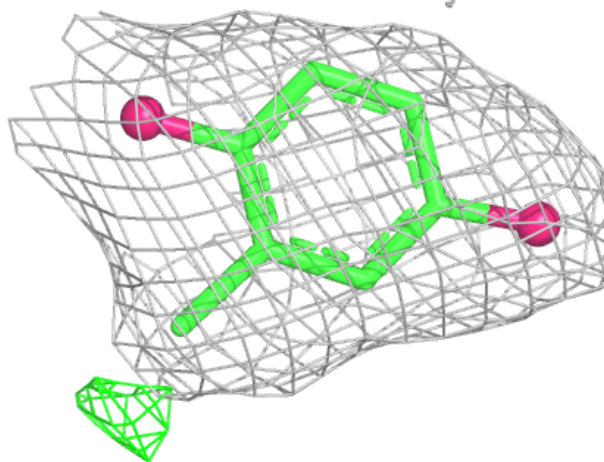
Electron density around 7DV B 303:

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



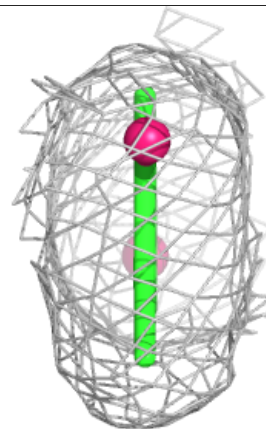
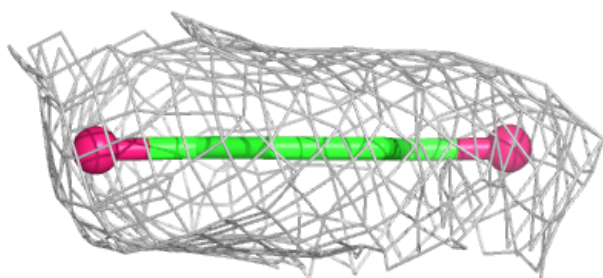
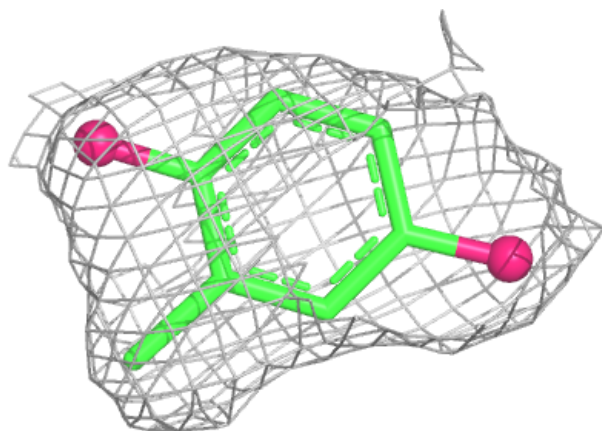
Electron density around 7DV P 302:

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

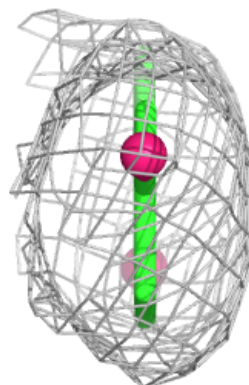
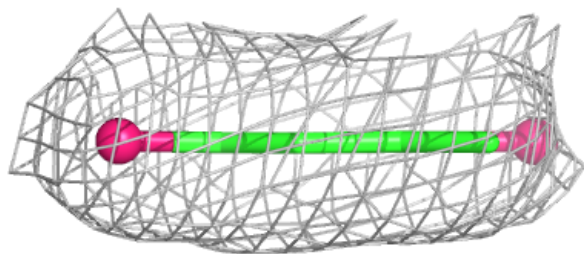
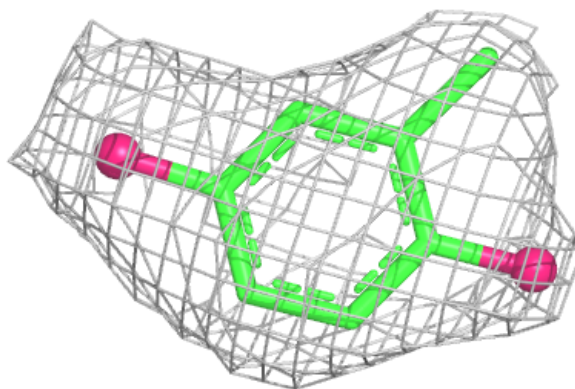


Electron density around 7DV H 302:

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

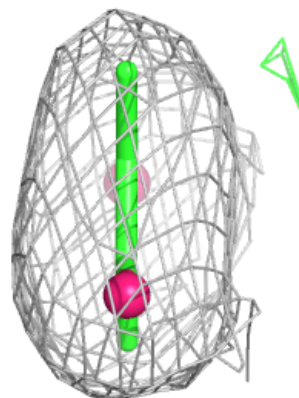
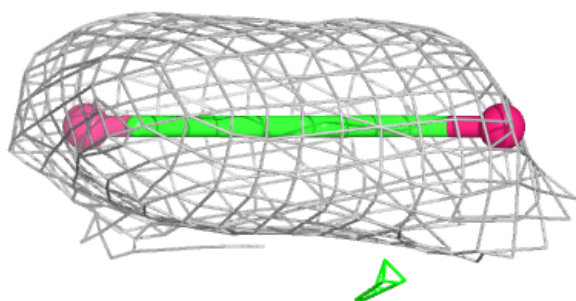
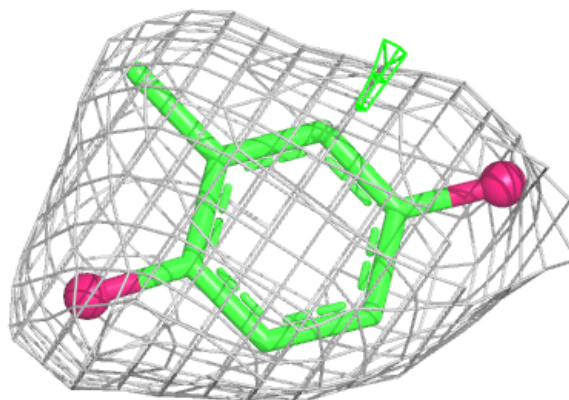
**Electron density around 7DV H 303:**

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

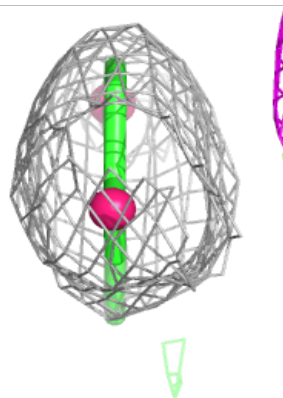
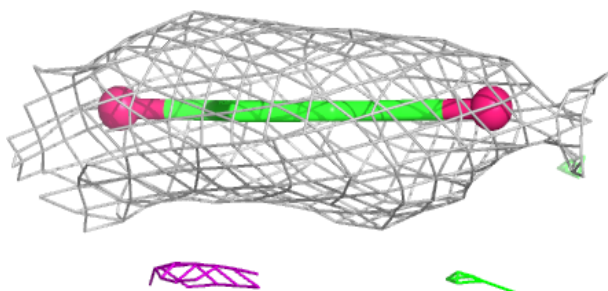
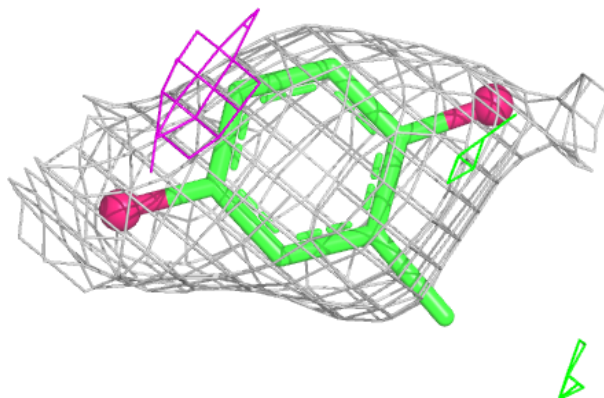


Electron density around 7DV P 303:

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

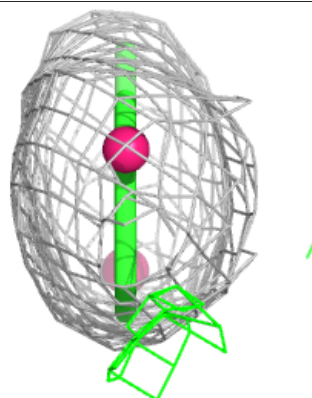
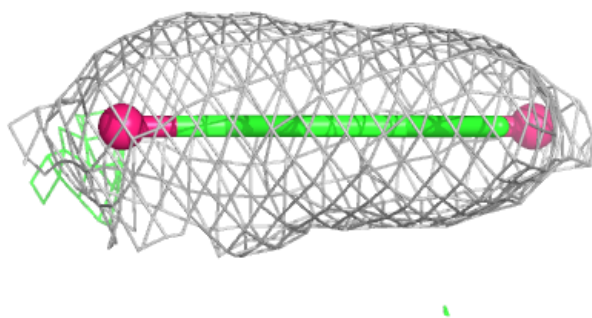
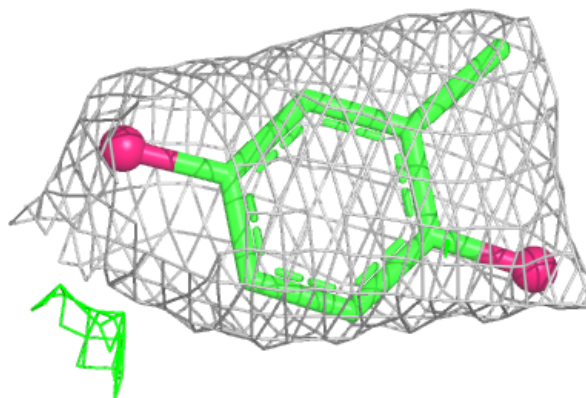
**Electron density around 7DV I 301:**

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



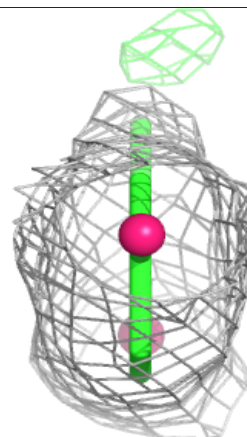
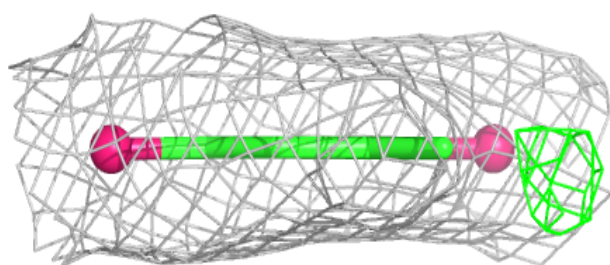
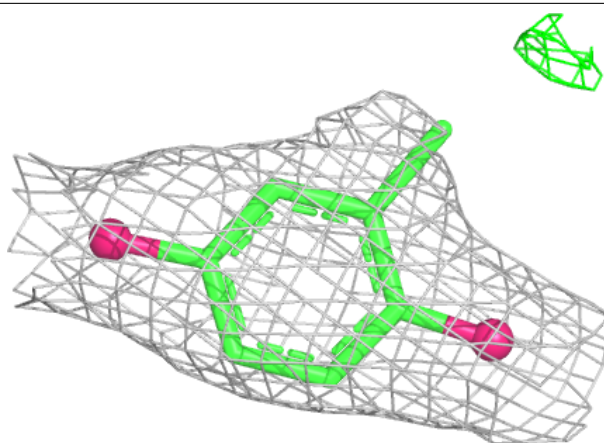
Electron density around 7DV B 301:

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

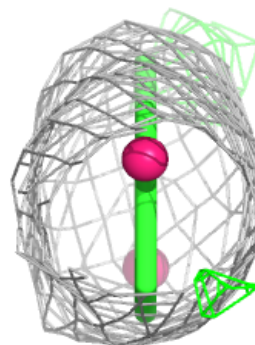
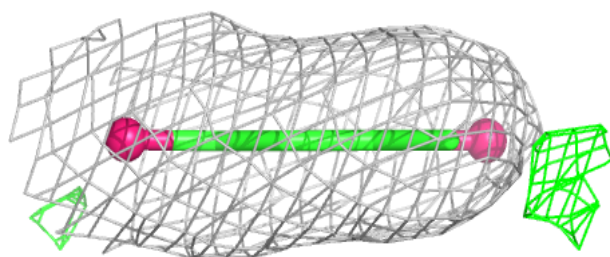
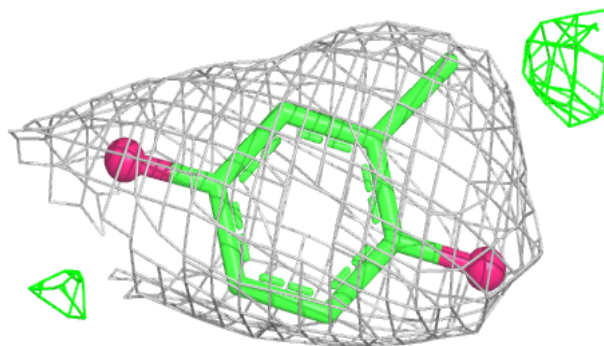


Electron density around 7DV D 301:

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

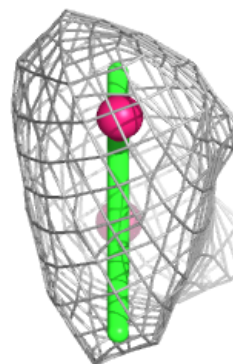
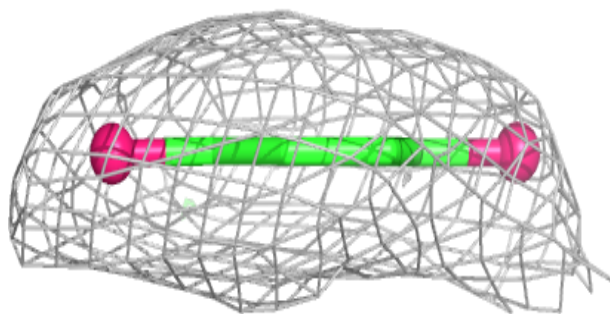
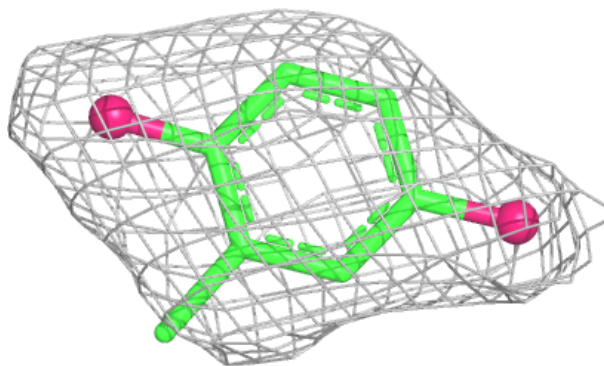
**Electron density around 7DV P 301:**

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



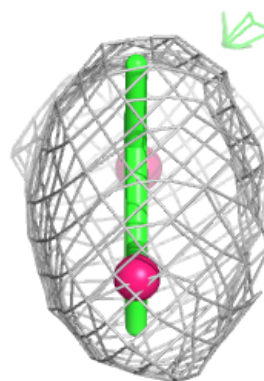
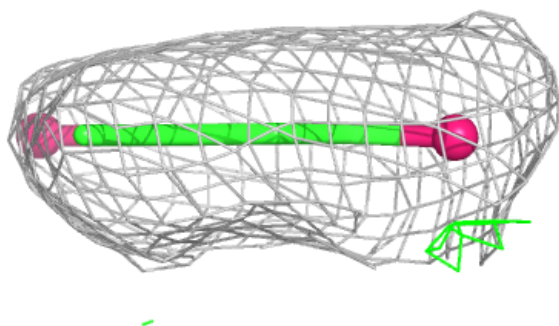
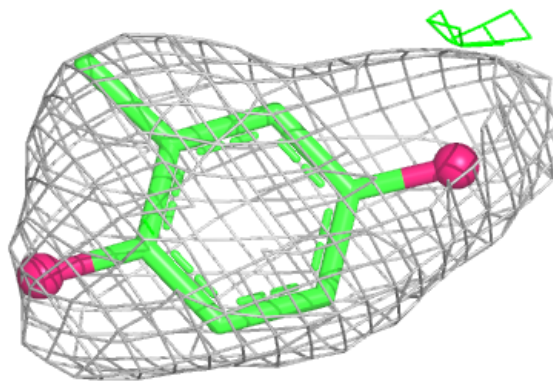
Electron density around 7DV K 302:

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

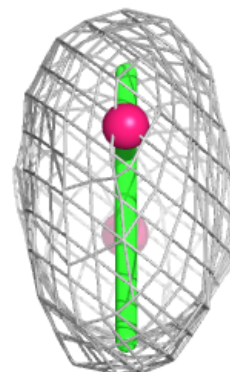
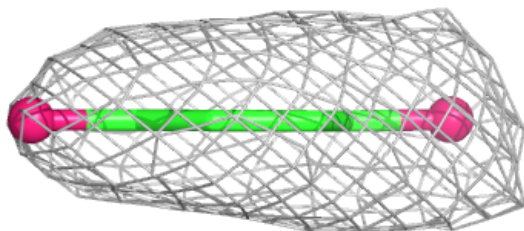
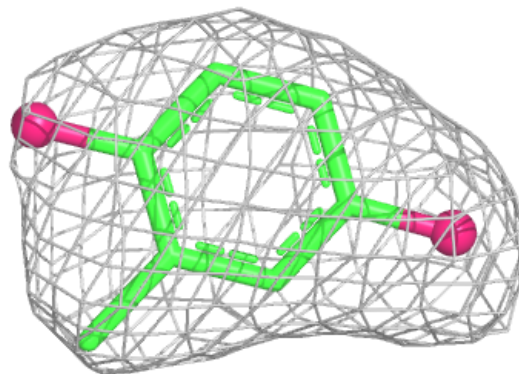


Electron density around 7DV J 303:

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

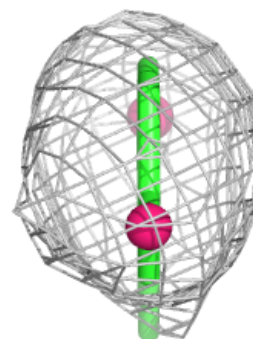
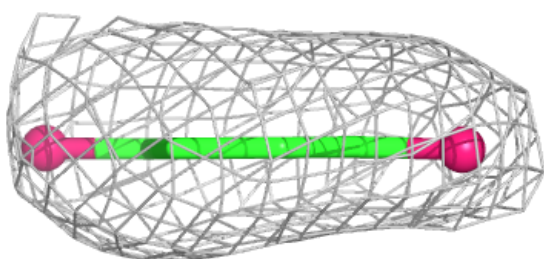
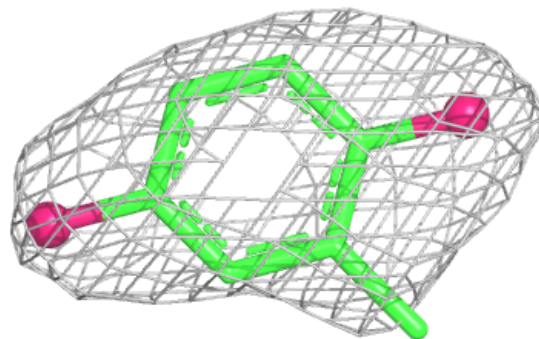
**Electron density around 7DV L 303:**

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

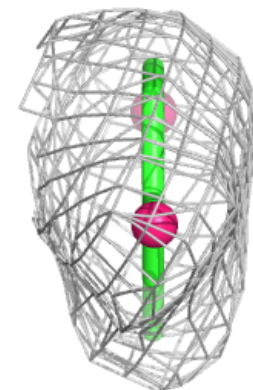
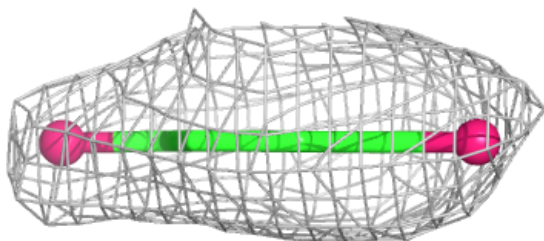
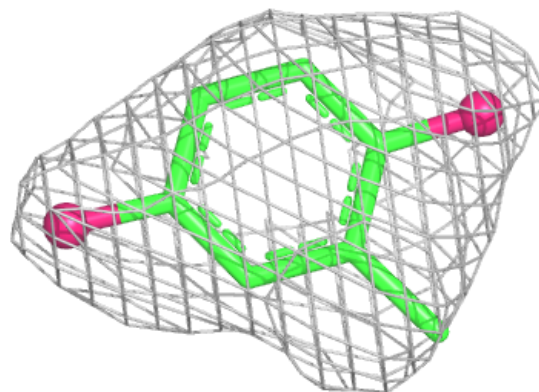


Electron density around 7DV D 303:

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

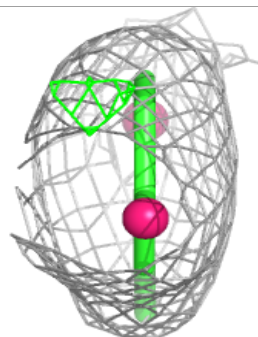
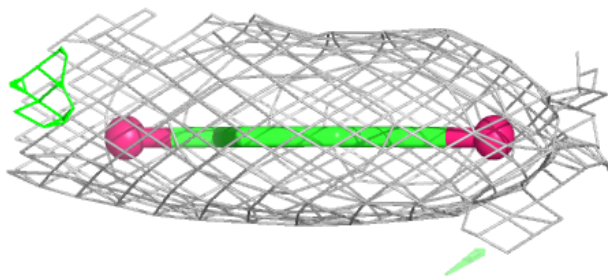
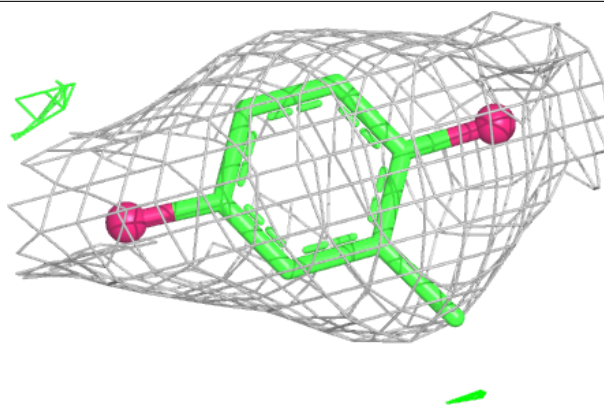
**Electron density around 7DV L 302:**

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

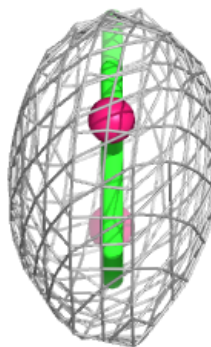
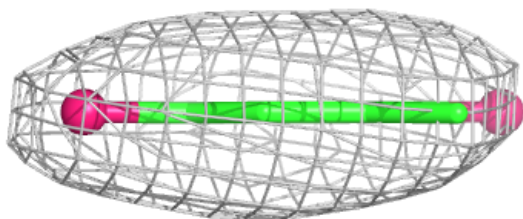
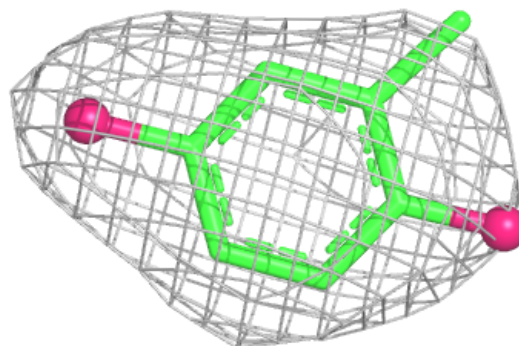


Electron density around 7DV H 301:

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

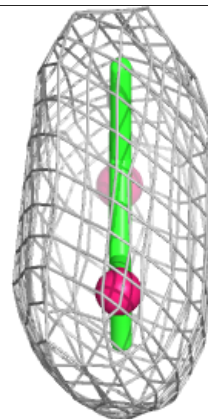
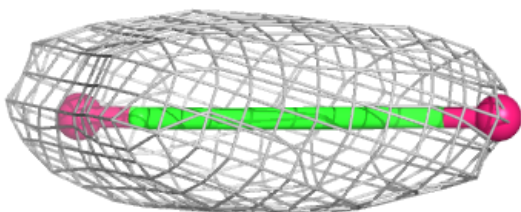
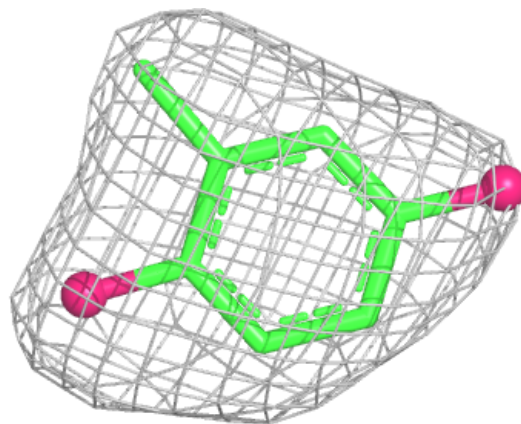
**Electron density around 7DV D 304:**

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



Electron density around 7DV L 304:

$2mF_o - DF_c$ (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.