W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2025 – 07:53 AM EST

PDB ID	:	3NJ0
Title	:	X-ray crystal structure of the PYL2-pyrabactin A complex
Authors	:	Peterson, F.C.; Burgie, E.S.; Bingman, C.A.; Volkman, B.F.; Phillips Jr., G.N.; Cutler, S.R.; Jensen, D.R.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2010-06-16
Resolution	:	1.89 Å(reported)

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

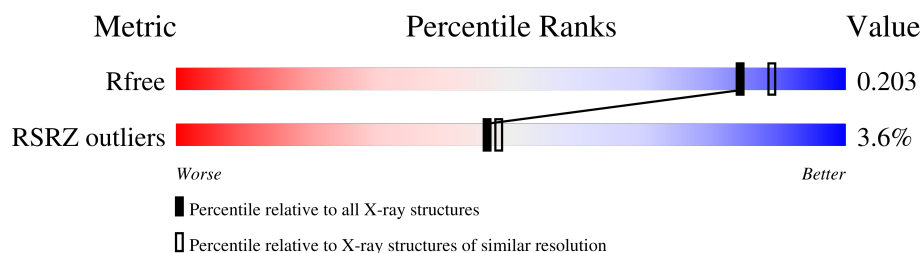|		
MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	Percentile Ranks	Value
Rfree		0.203
RSRZ outliers		3.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4879 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 Abscisic acid receptor PYL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total 1429	C 899	N 245	O 280	S 5	0	6	0
1	B	179	Total 1433	C 902	N 248	O 279	S 4	0	3	0
1	C	177	Total 1420	C 893	N 246	O 277	S 4	0	3	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O80992
A	-1	SER	-	expression tag	UNP O80992
A	0	HIS	-	expression tag	UNP O80992
B	-2	GLY	-	expression tag	UNP O80992
B	-1	SER	-	expression tag	UNP O80992
B	0	HIS	-	expression tag	UNP O80992
C	-2	GLY	-	expression tag	UNP O80992
C	-1	SER	-	expression tag	UNP O80992
C	0	HIS	-	expression tag	UNP O80992

- Molecule 2 is 4-bromo-N-(pyridin-2-ylmethyl)naphthalene-1-sulfonamide (three-letter code: PYV) (formula: $C_{16}H_{13}BrN_2O_2S$).

PYV
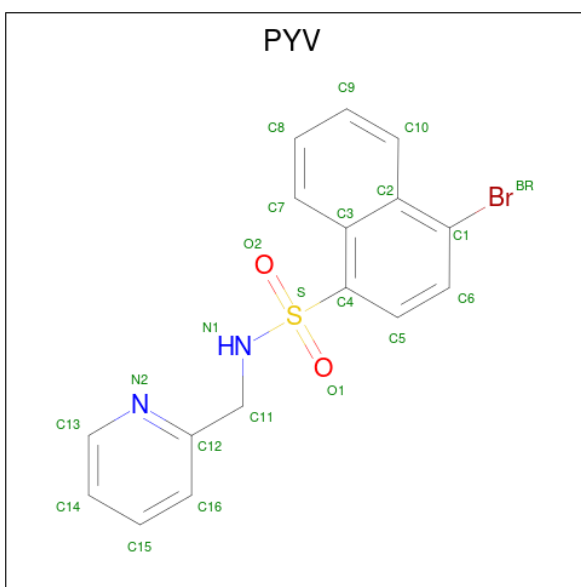
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	1
			86	2	64	8	8	4		
2	B	1	Total	Br	C	N	O	S	0	1
			86	2	64	8	8	4		
2	C	1	Total	Br	C	N	O	S	0	1
			86	2	64	8	8	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
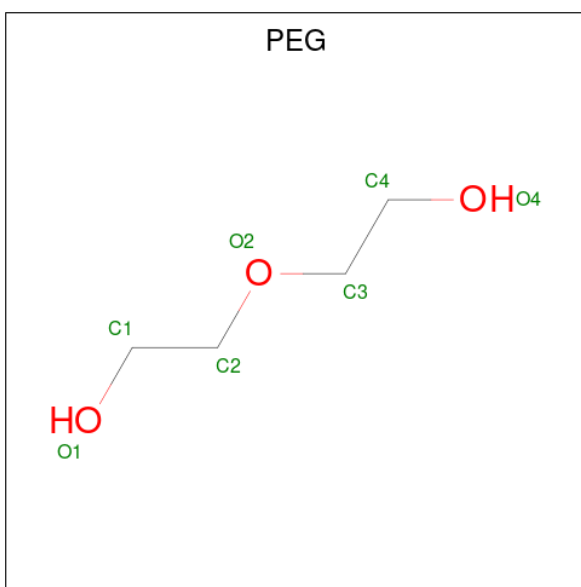
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total C O 7 4 3			0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total C O 6 3 3			0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total O 107 107		0	1
5	B	114	Total O 116 116		0	2
5	C	94	Total O 96 96		0	2

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	62.54Å 105.15Å 187.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 1.89 29.66 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.66-1.89) 97.0 (29.66-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.178 , 0.205 0.178 , 0.203	Depositor DCC
R_{free} test set	1969 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.0	EDS
L-test for twinning[2]	$<\|L\|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.036 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4879	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\|L\|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

15 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	PYV	C	300[D]	-	23,23,24	3.71	2 (8%)	31,32,34	1.97	5 (16%)
2	PYV	A	300[D]	-	23,23,24	3.72	2 (8%)	31,32,34	1.97	5 (16%)
2	PYV	C	300[C]	-	24,24,24	3.66	4 (16%)	33,34,34	2.00	6 (18%)
2	PYV	A	300[B]	-	23,23,24	4.27	5 (21%)	31,32,34	2.38	11 (35%)
2	PYV	B	300[D]	-	23,23,24	3.72	2 (8%)	31,32,34	1.96	5 (16%)
2	PYV	B	300[C]	-	24,24,24	3.63	3 (12%)	33,34,34	1.98	6 (18%)
2	PYV	C	300[A]	-	24,24,24	4.29	8 (33%)	33,34,34	1.83	10 (30%)
3	PEG	C	191	-	6,6,6	0.45	0	5,5,5	0.37	0
4	GOL	C	192	-	5,5,5	0.48	0	5,5,5	0.47	0
2	PYV	B	300[A]	-	24,24,24	4.53	8 (33%)	33,34,34	2.30	11 (33%)
2	PYV	C	300[B]	-	23,23,24	3.71	2 (8%)	31,32,34	1.97	5 (16%)
2	PYV	B	300[B]	-	23,23,24	3.70	2 (8%)	31,32,34	1.97	5 (16%)
2	PYV	A	300[A]	-	24,24,24	4.19	5 (20%)	33,34,34	2.38	13 (39%)
3	PEG	A	191	-	6,6,6	0.43	0	5,5,5	0.30	0
2	PYV	A	300[C]	-	24,24,24	3.65	3 (12%)	33,34,34	1.99	6 (18%)

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	PYV	C	300[D]	-	-	6/12/12/12	0/3/3/3
2	PYV	A	300[D]	-	-	8/12/12/12	0/3/3/3
2	PYV	C	300[C]	-	-	6/12/12/12	0/3/3/3
2	PYV	A	300[B]	-	-	3/12/12/12	0/3/3/3
2	PYV	B	300[D]	-	-	3/12/12/12	0/3/3/3
2	PYV	B	300[C]	-	-	3/12/12/12	0/3/3/3
2	PYV	C	300[A]	-	-	7/12/12/12	0/3/3/3
3	PEG	C	191	-	-	3/4/4/4	-
4	GOL	C	192	-	-	4/4/4/4	-
2	PYV	B	300[A]	-	-	2/12/12/12	0/3/3/3
2	PYV	C	300[B]	-	-	5/12/12/12	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYV	B	300[B]	-	-	2/12/12/12	0/3/3/3
2	PYV	A	300[A]	-	-	3/12/12/12	0/3/3/3
3	PEG	A	191	-	-	1/4/4/4	-
2	PYV	A	300[C]	-	-	8/12/12/12	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300[A]	PYV	C4-S	-20.50	1.56	1.77
2	A	300[A]	PYV	C4-S	-18.95	1.58	1.77
2	A	300[B]	PYV	C4-S	-18.95	1.58	1.77
2	C	300[A]	PYV	C4-S	-18.95	1.58	1.77
2	A	300[C]	PYV	C4-S	-17.13	1.59	1.77

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300[C]	PYV	O2-S-O1	-8.31	109.43	119.52
2	A	300[D]	PYV	O2-S-O1	-8.31	109.43	119.52
2	C	300[B]	PYV	O2-S-O1	-8.31	109.43	119.52
2	B	300[B]	PYV	O2-S-O1	-8.30	109.44	119.52
2	B	300[D]	PYV	O2-S-O1	-8.28	109.46	119.52

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300[C]	PYV	C3-C4-S-N1
2	A	300[C]	PYV	C5-C4-S-N1
2	A	300[C]	PYV	C3-C4-S-O1
2	A	300[C]	PYV	C5-C4-S-O1
2	A	300[D]	PYV	C3-C4-S-N1

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.
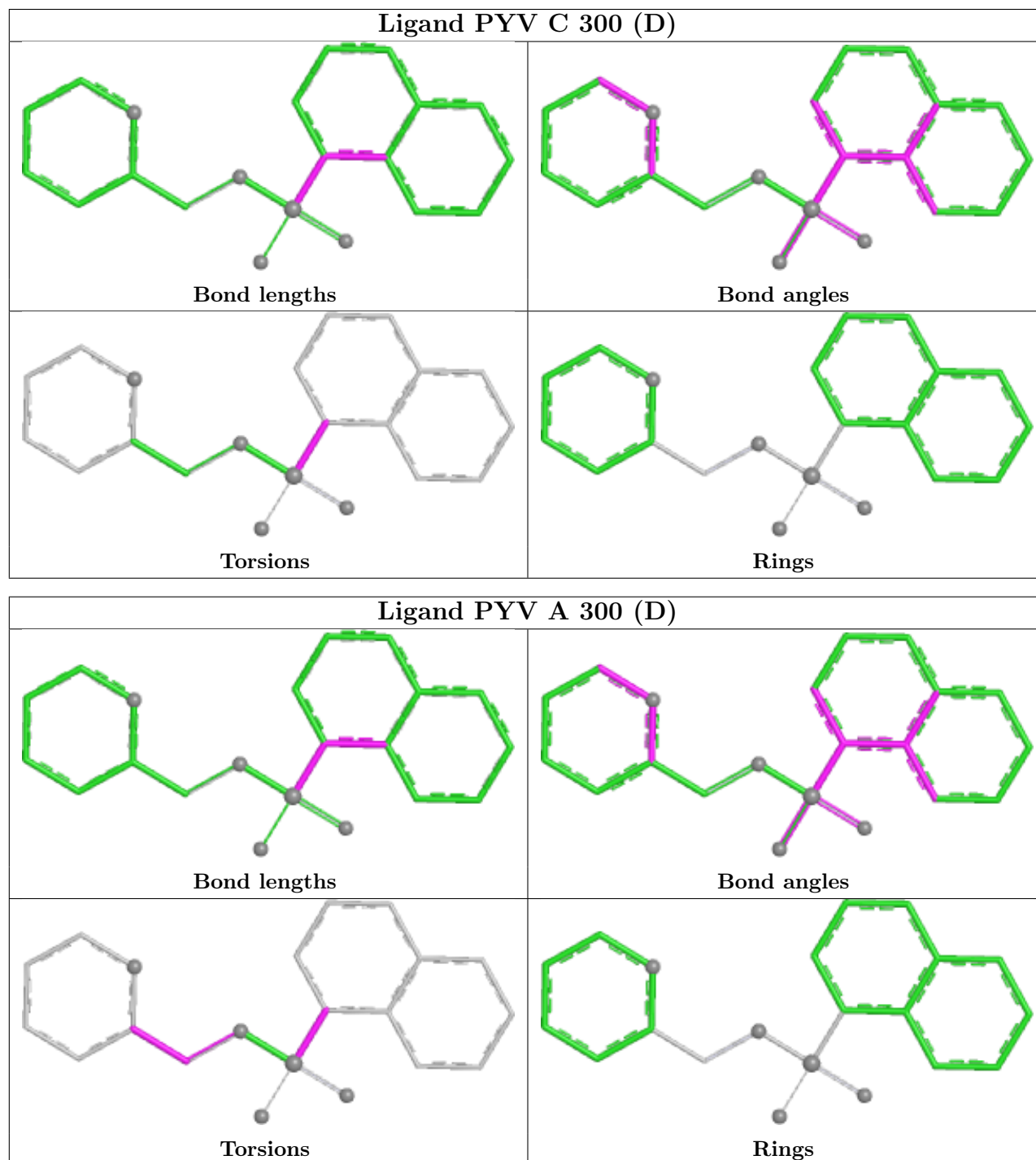
Ligand PYV C 300 (D)
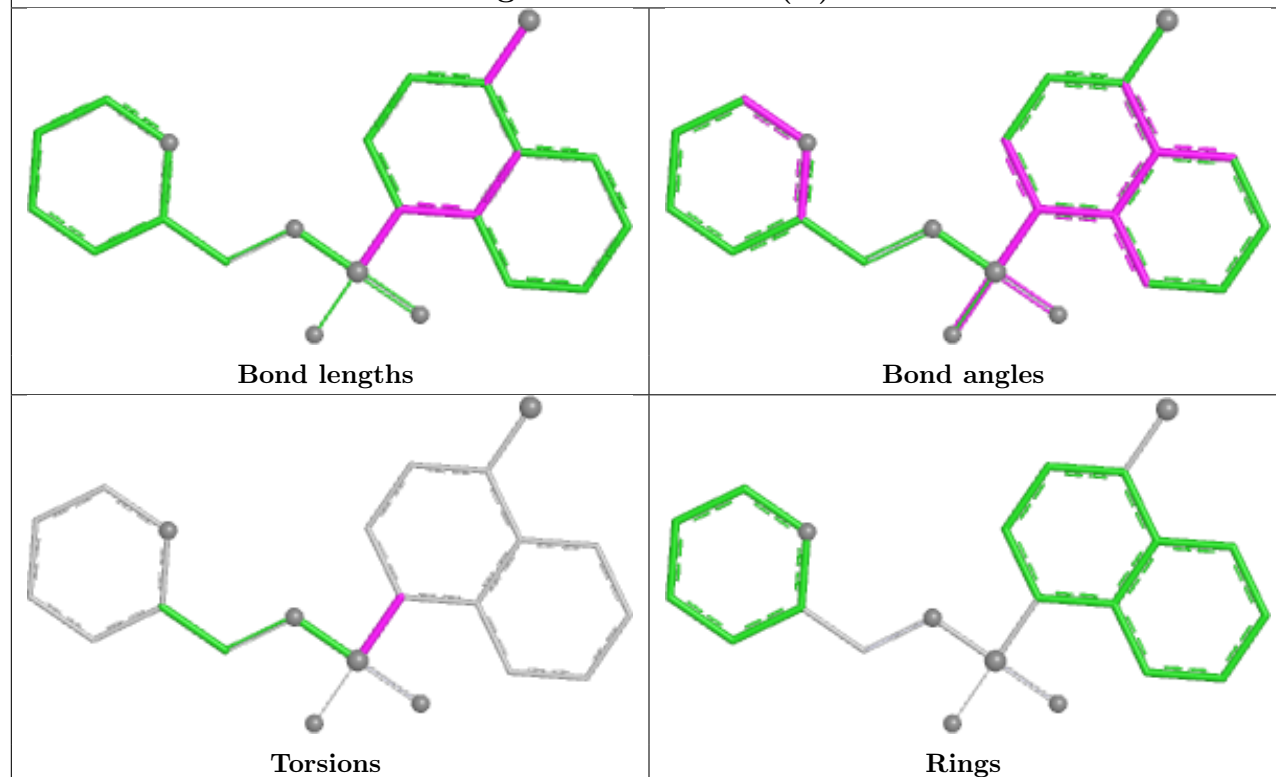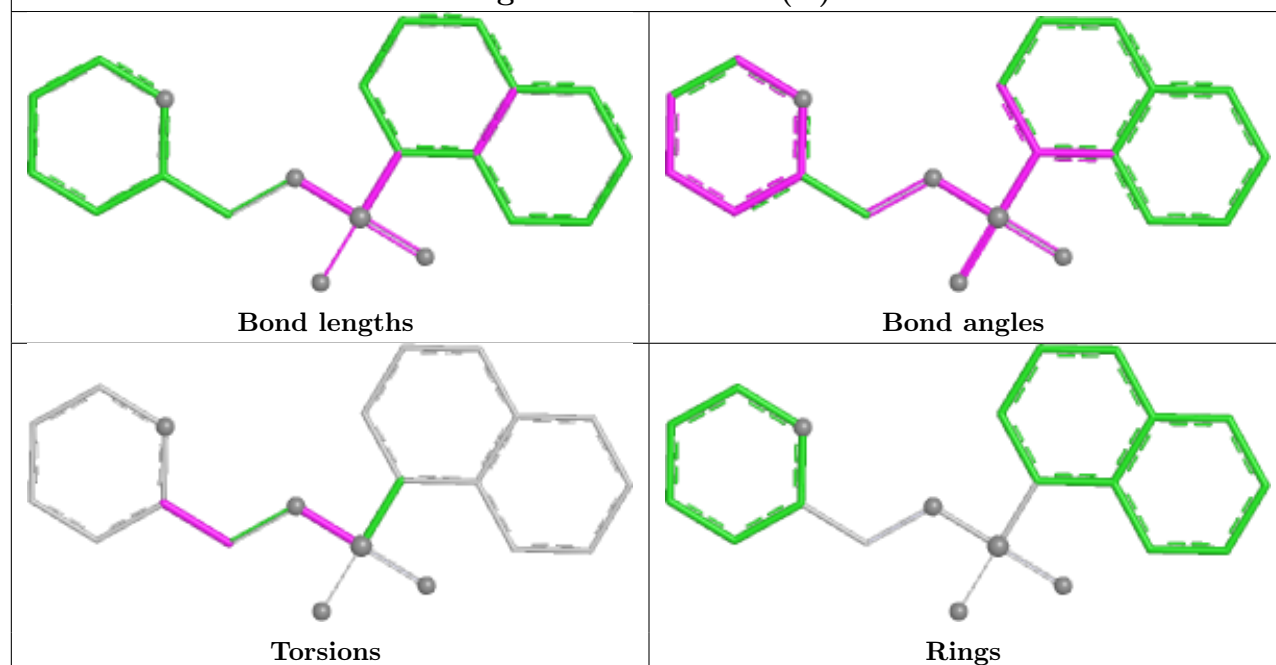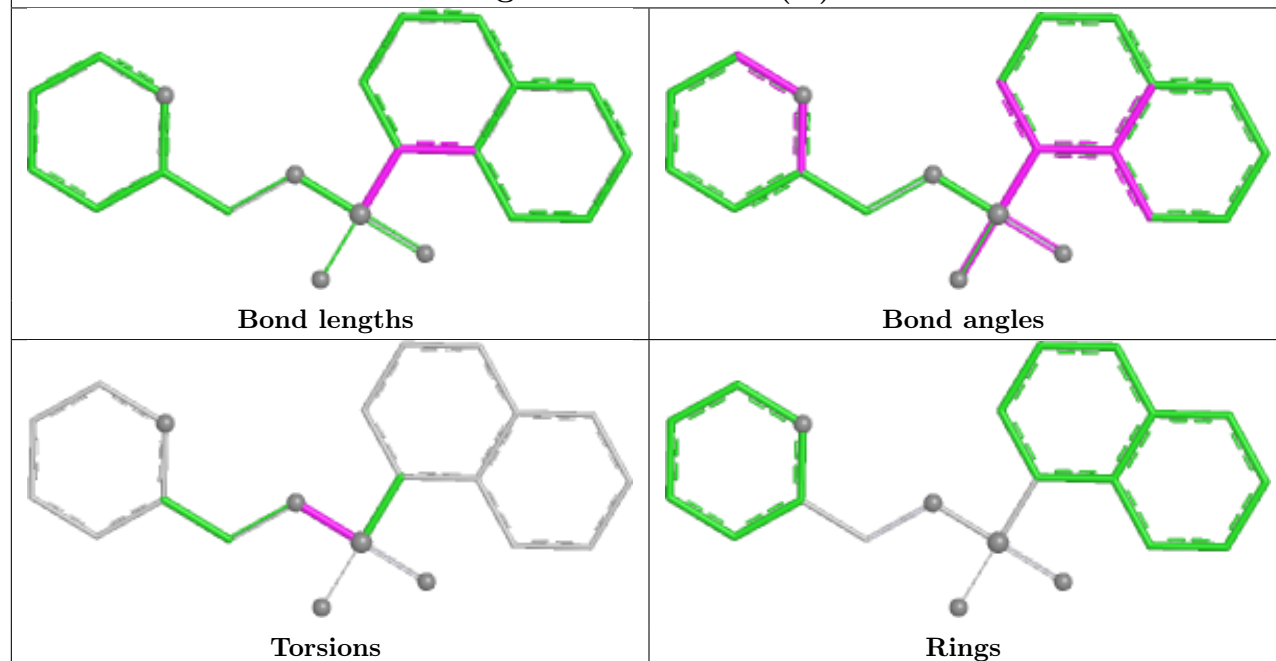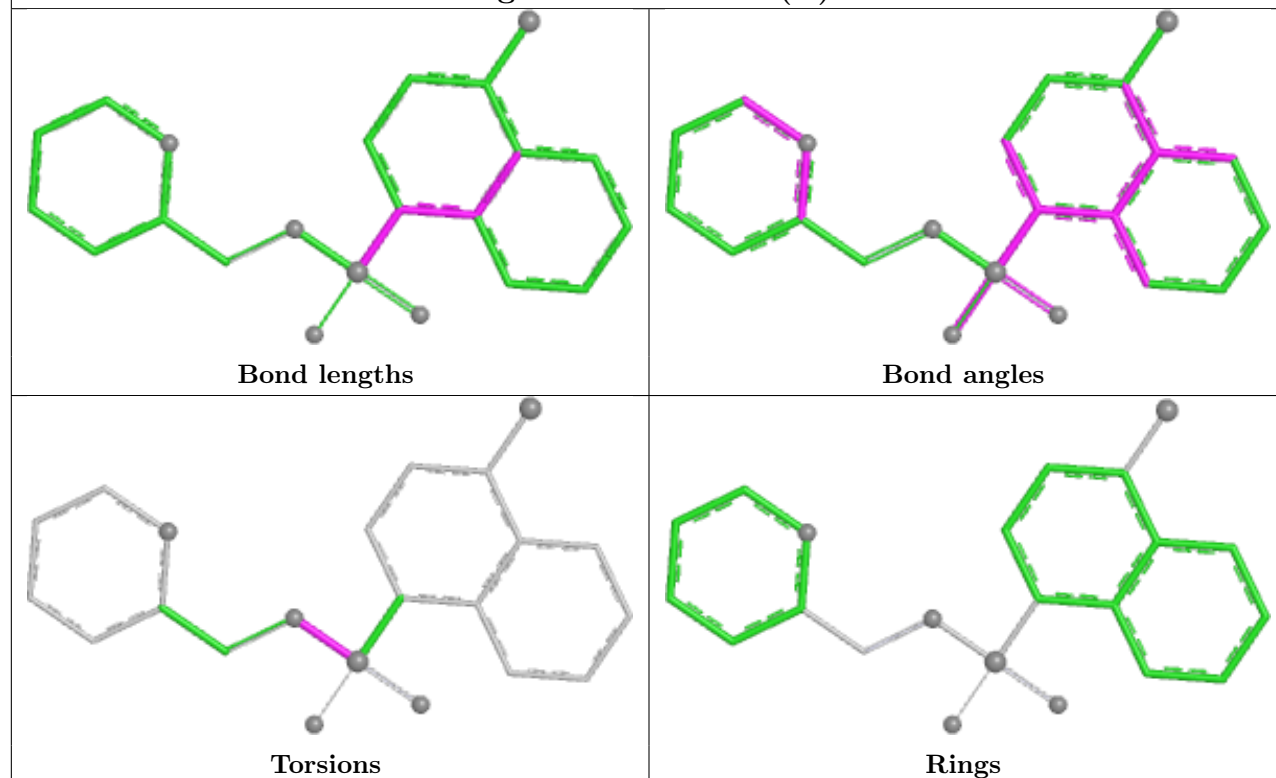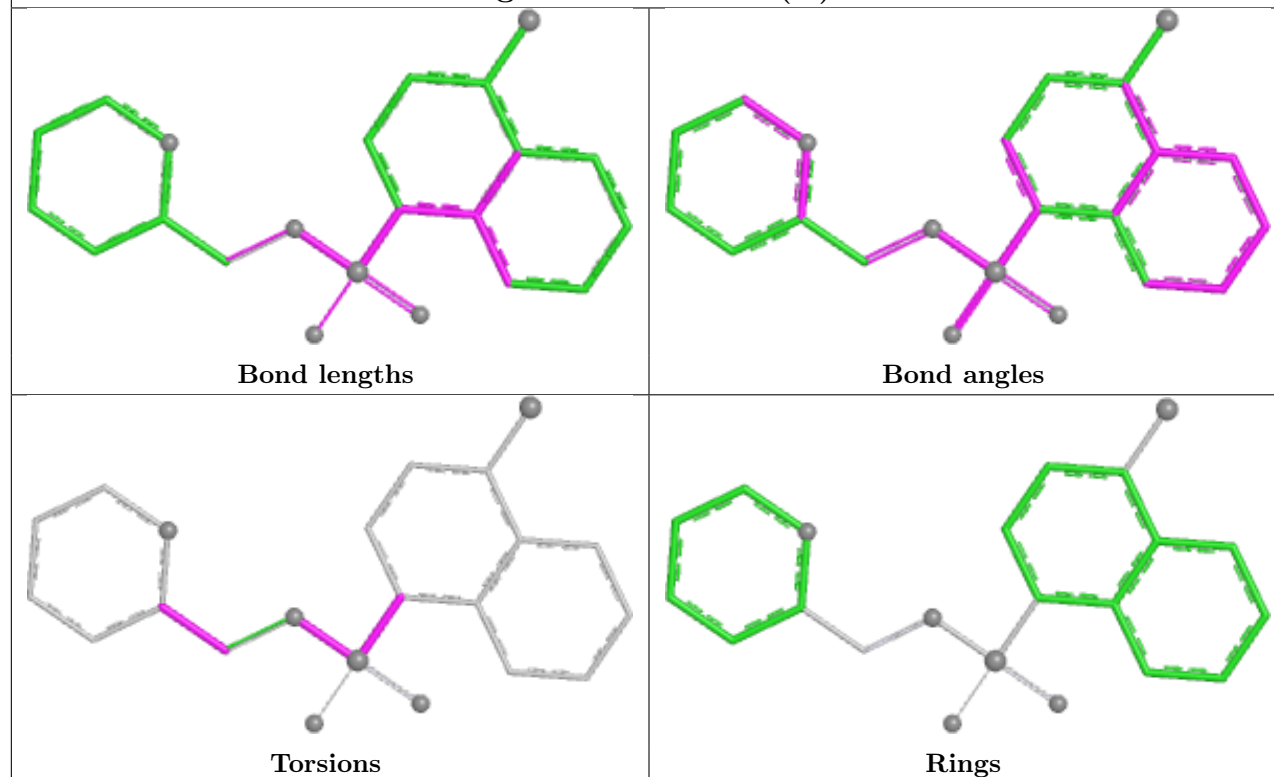
Bond lengths

Bond angles

Torsions

Rings

Ligand PYV A 300 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV C 300 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV A 300 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV B 300 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV B 300 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV C 300 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV B 300 (A)

Bond lengths

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Torsions

Rings

Ligand PYV C 300 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV B 300 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV A 300 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand PYV A 300 (C)

Bond lengths

Bond angles

Torsions

Rings
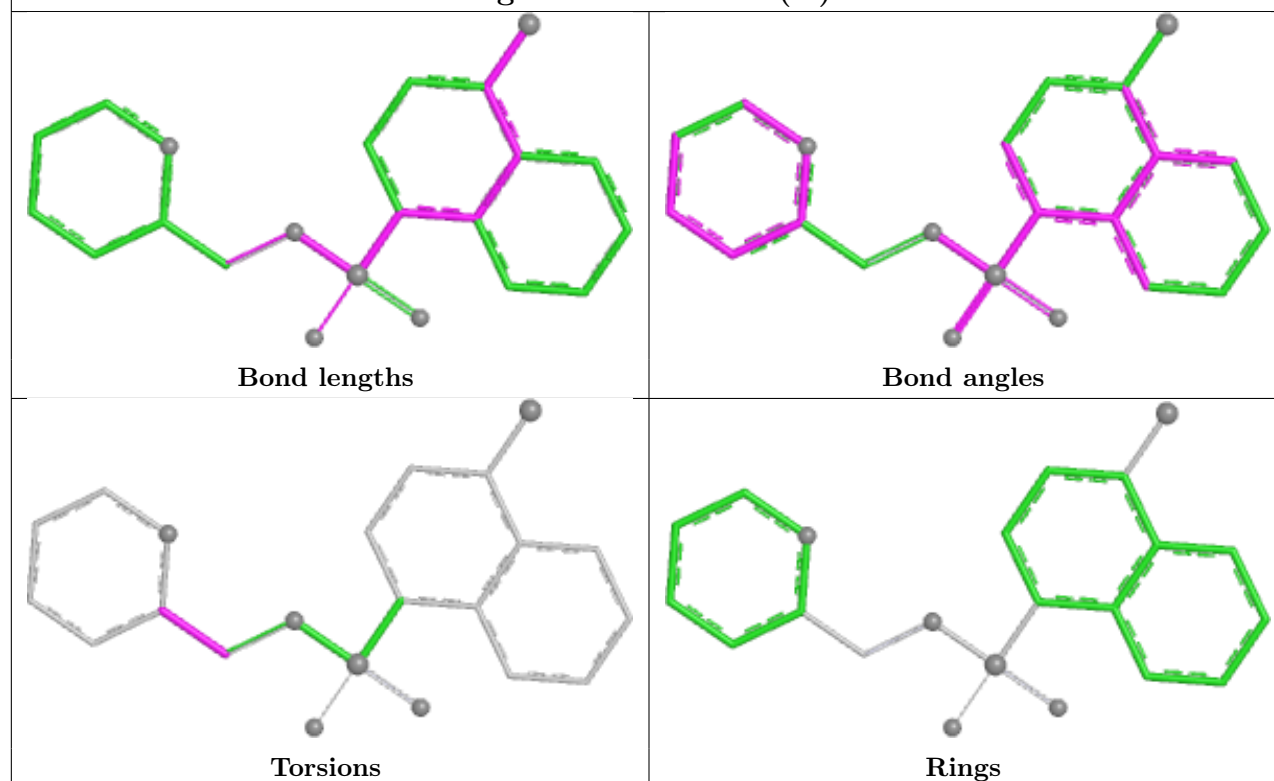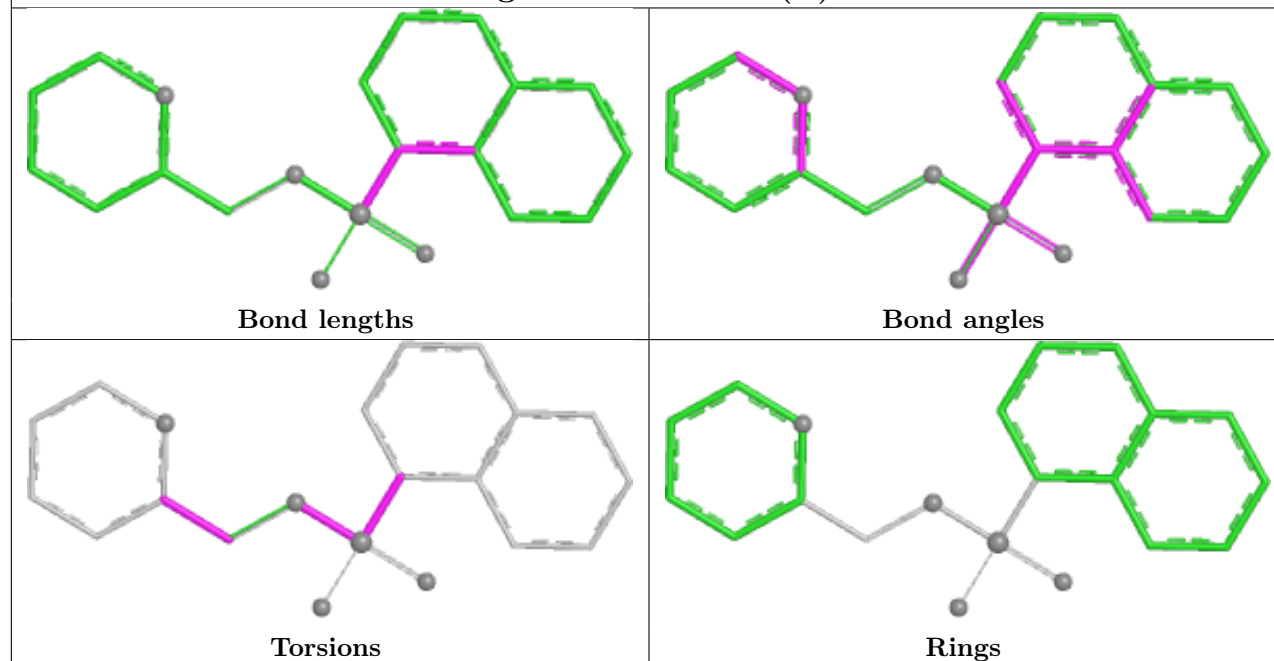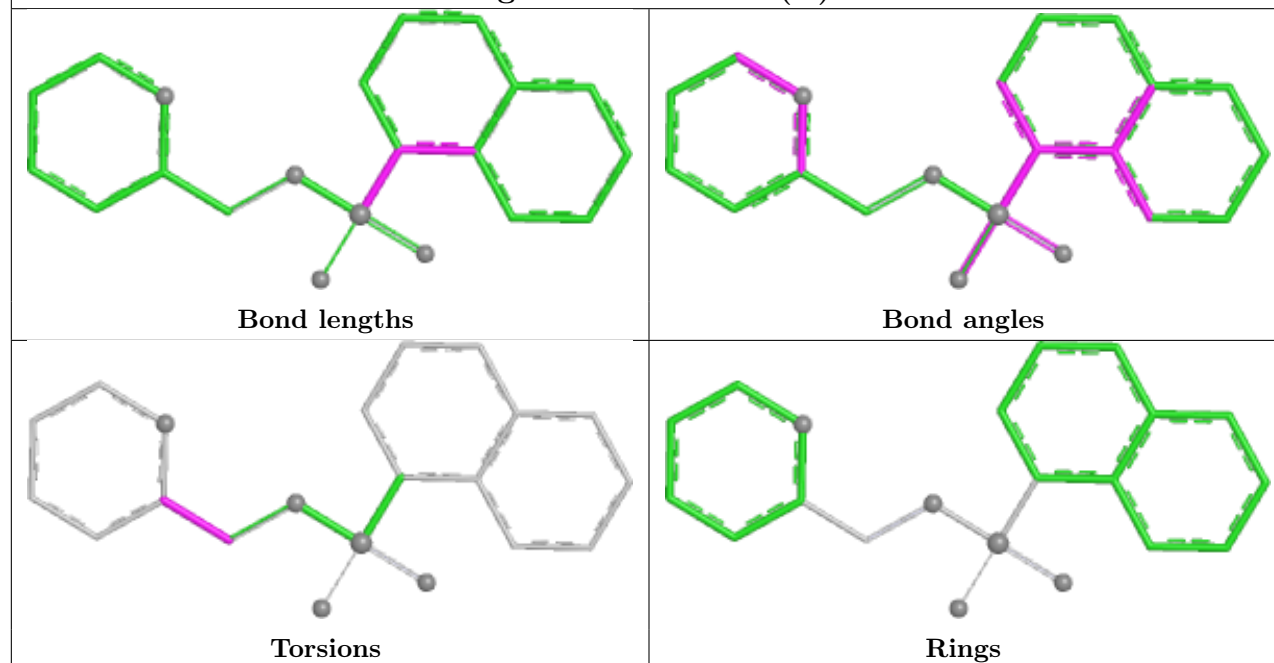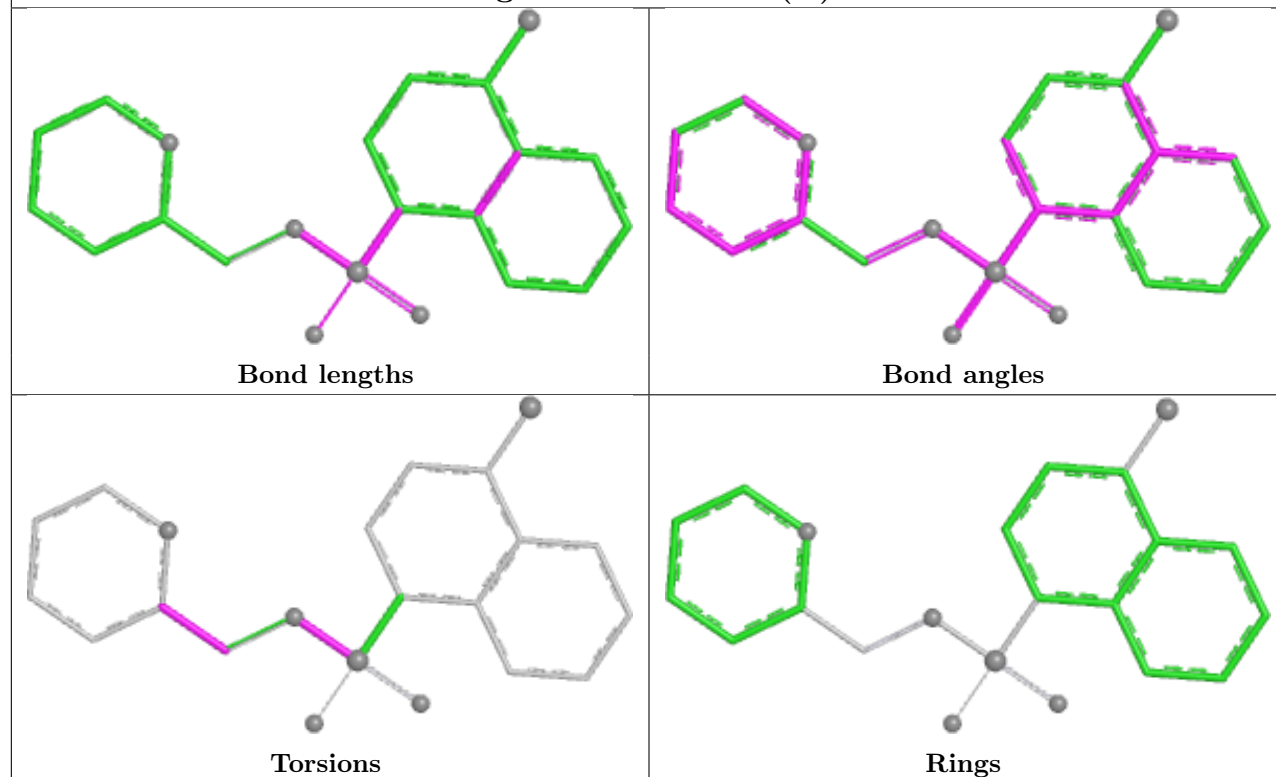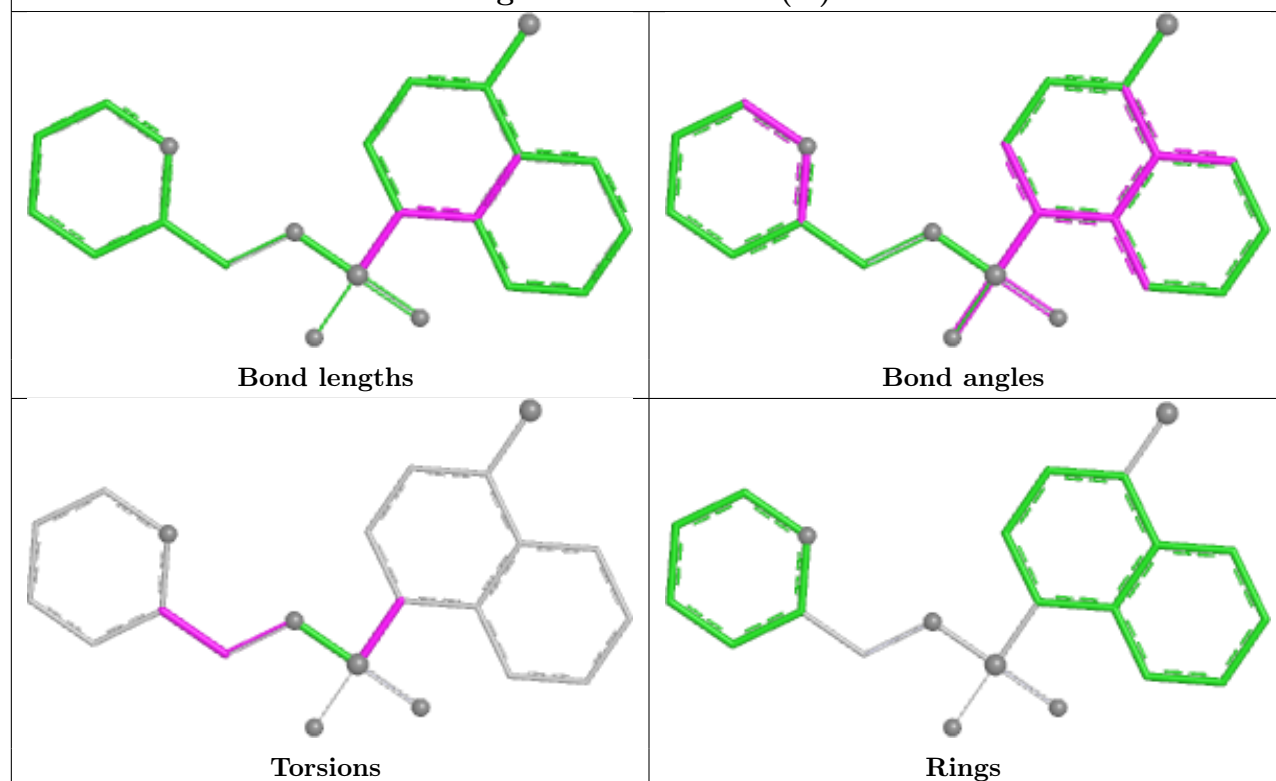
4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	177/193 (91%)	-0.17	4 (2%)	61	63	14, 28, 65, 104	6 (3%)
1	B	179/193 (92%)	-0.12	7 (3%)	44	45	16, 31, 68, 127	3 (1%)
1	C	177/193 (91%)	0.05	8 (4%)	39	40	18, 37, 80, 125	3 (1%)
All	All	533/579 (92%)	-0.08	19 (3%)	46	48	14, 32, 74, 127	12 (2%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	SER	4.0
1	B	28	PHE	3.9
1	C	28	PHE	3.6
1	B	7	VAL	3.5
1	A	119	HIS	3.4

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

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

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	C	191	7/7	0.80	0.13	49,52,55,57	7
2	PYV	B	300[B]	21/22	0.84	0.16	54,59,63,64	21
2	PYV	B	300[C]	22/22	0.84	0.16	48,58,63,63	22
2	PYV	B	300[D]	21/22	0.84	0.16	56,58,62,63	21
2	PYV	B	300[A]	22/22	0.84	0.16	43,58,63,63	22
3	PEG	A	191	7/7	0.86	0.15	48,52,58,63	0
4	GOL	C	192	6/6	0.86	0.40	71,74,76,78	6
2	PYV	C	300[D]	21/22	0.88	0.16	66,68,71,72	21
2	PYV	C	300[A]	22/22	0.88	0.16	40,68,71,72	22
2	PYV	C	300[B]	21/22	0.88	0.16	65,68,71,72	21
2	PYV	C	300[C]	22/22	0.88	0.16	47,68,71,72	22
2	PYV	A	300[D]	21/22	0.91	0.15	48,50,51,52	21
2	PYV	A	300[A]	22/22	0.91	0.15	33,50,51,52	22
2	PYV	A	300[B]	21/22	0.91	0.15	47,50,51,52	21
2	PYV	A	300[C]	22/22	0.91	0.15	48,50,51,52	22

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 PYV B 300 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
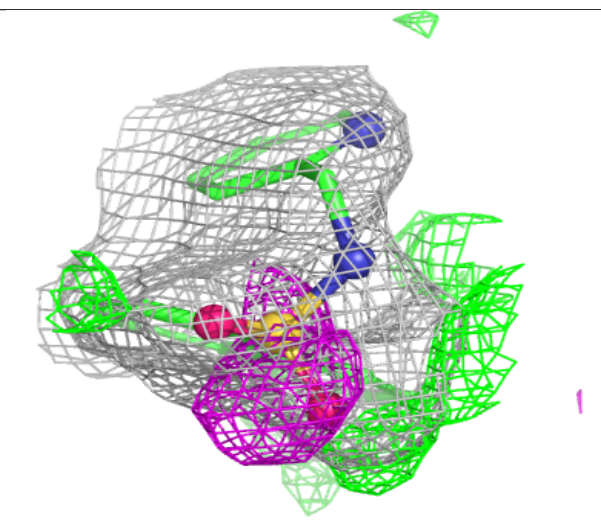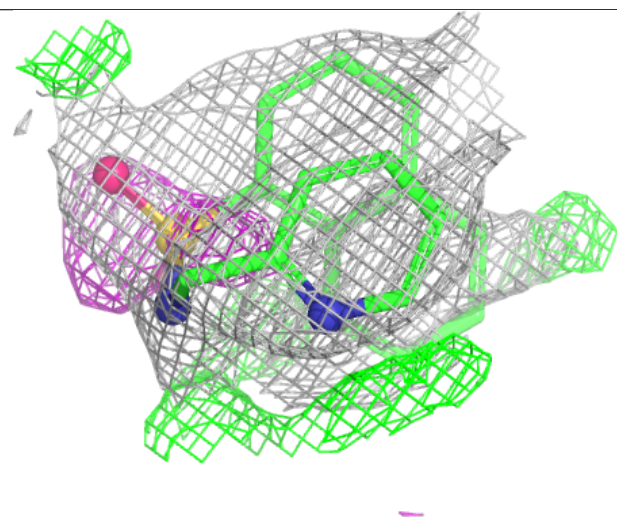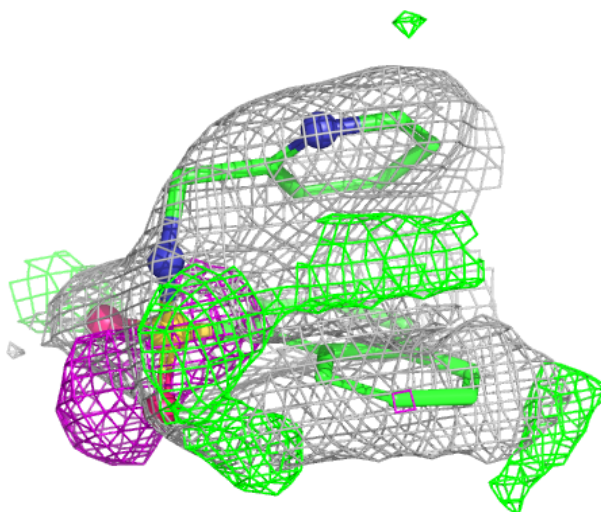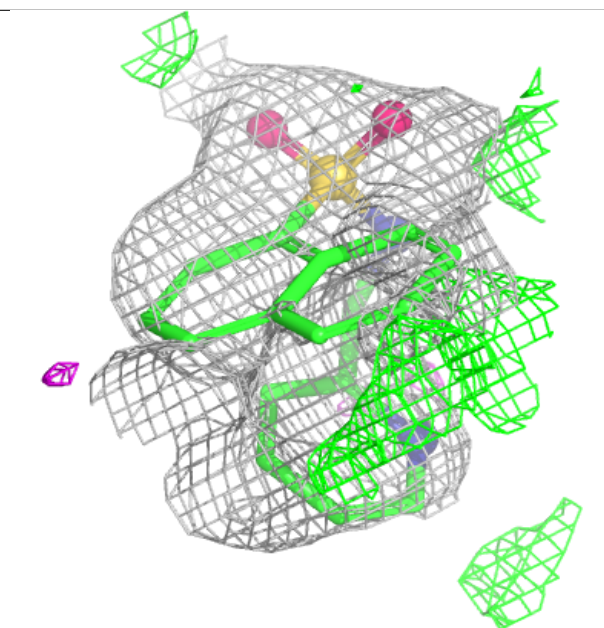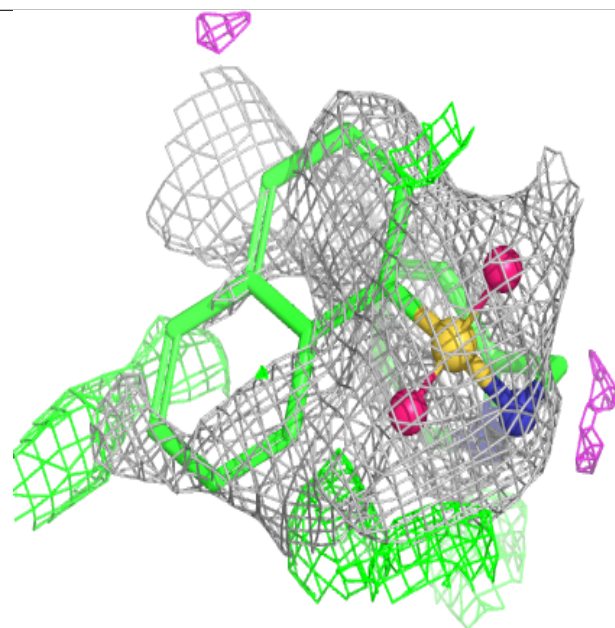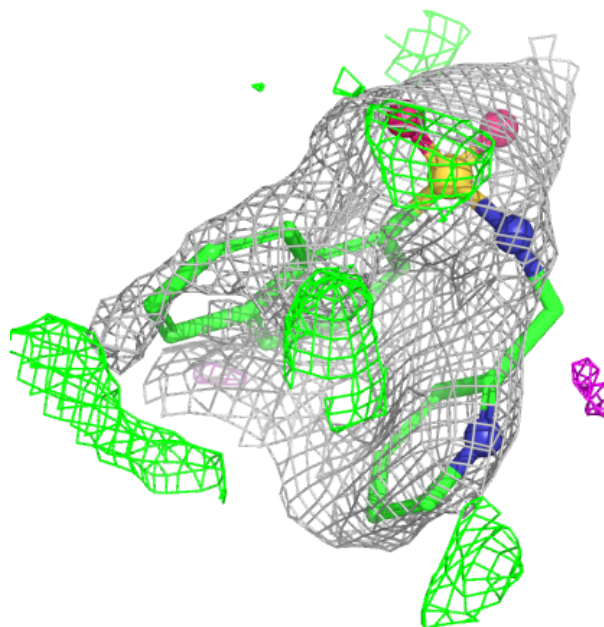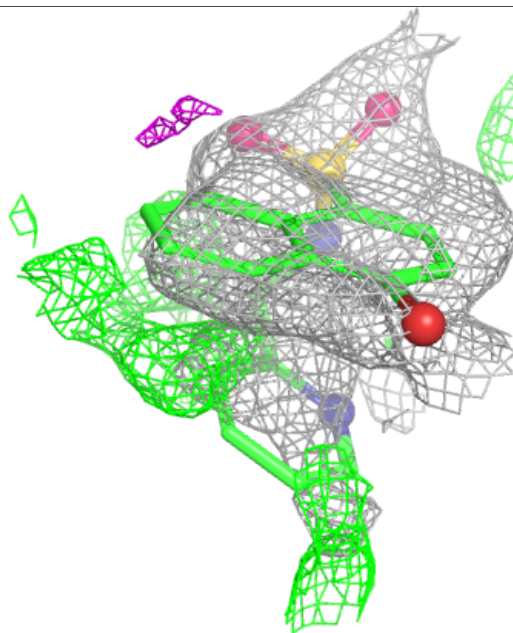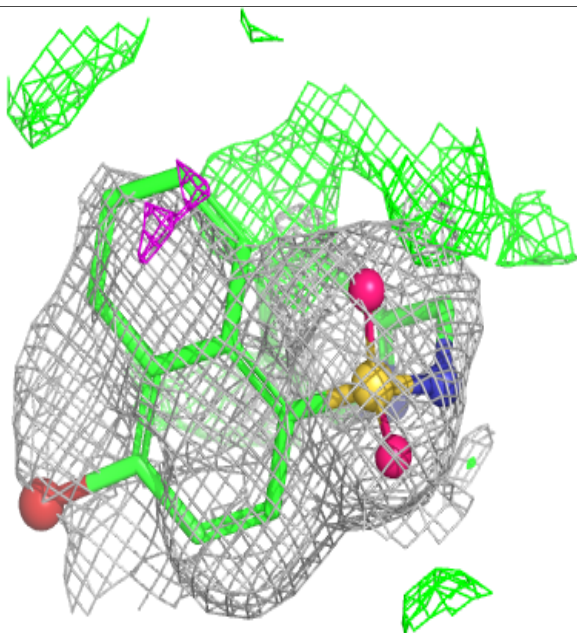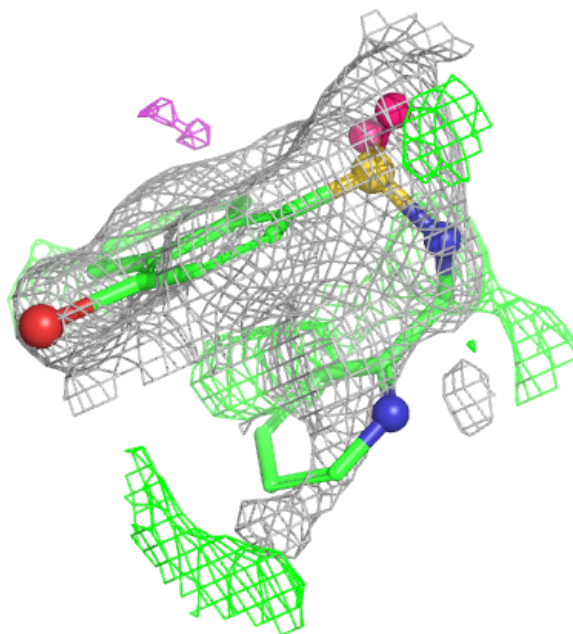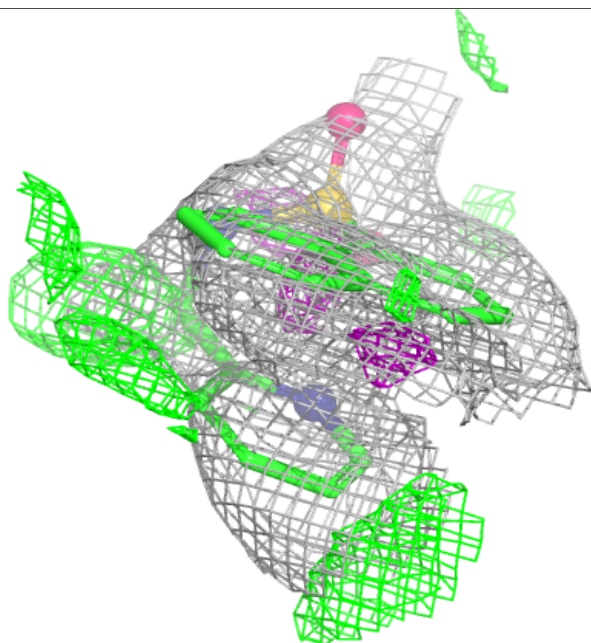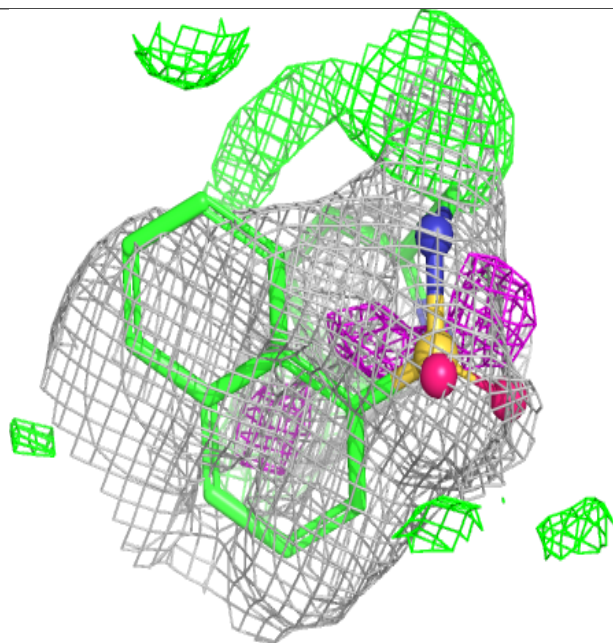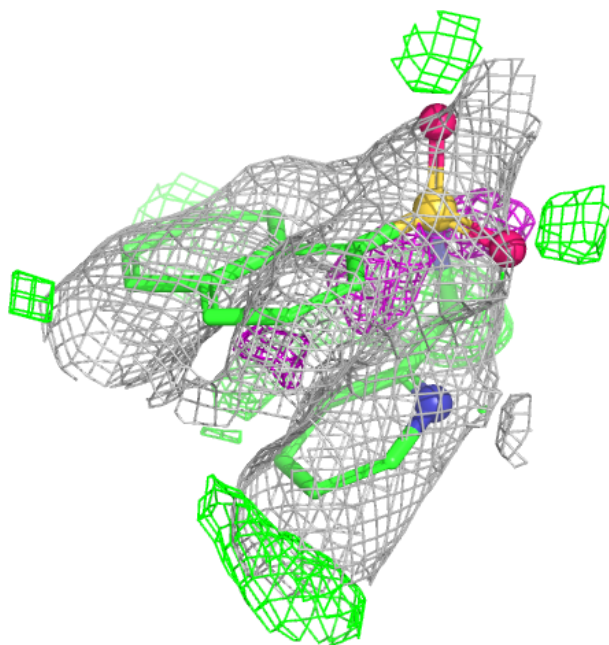
Electron density around PYV B 300 (C):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
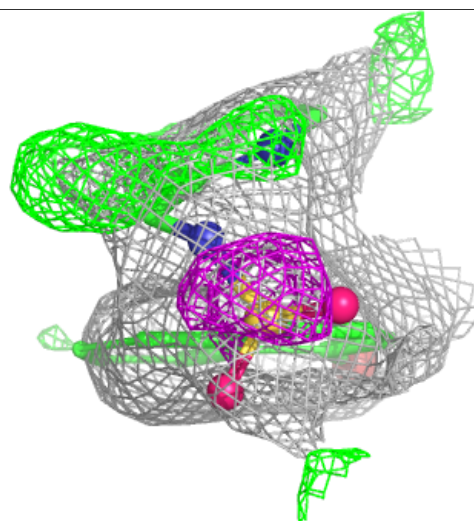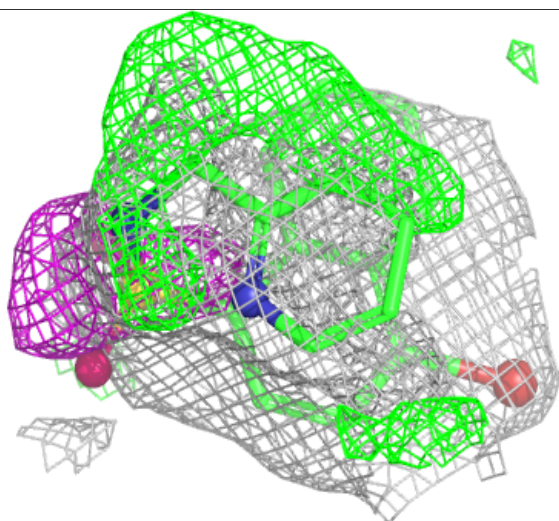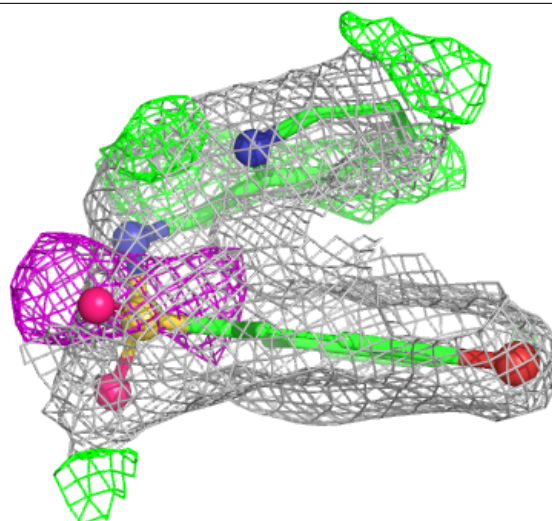
Electron density around PYV B 300 (D):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
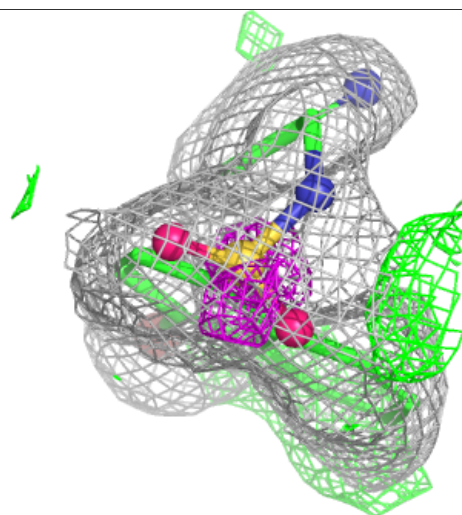and green (positive)
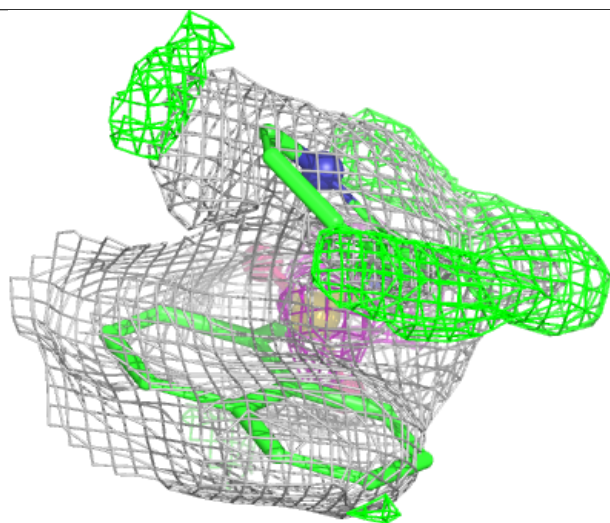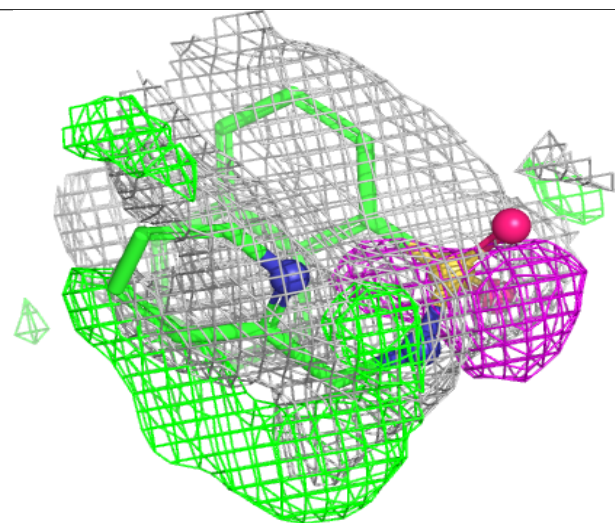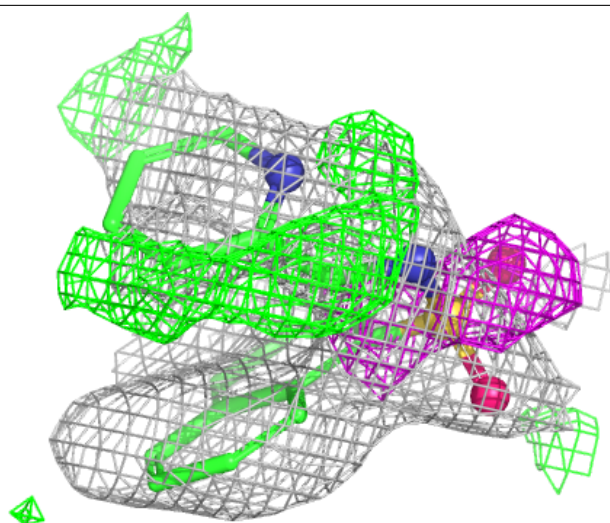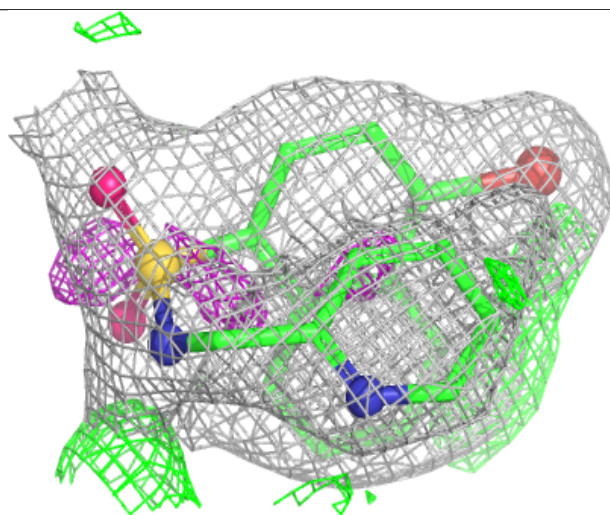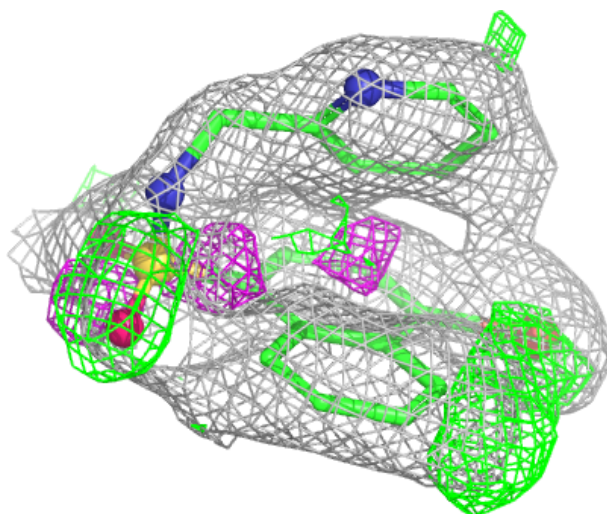
Electron density around PYV B 300 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
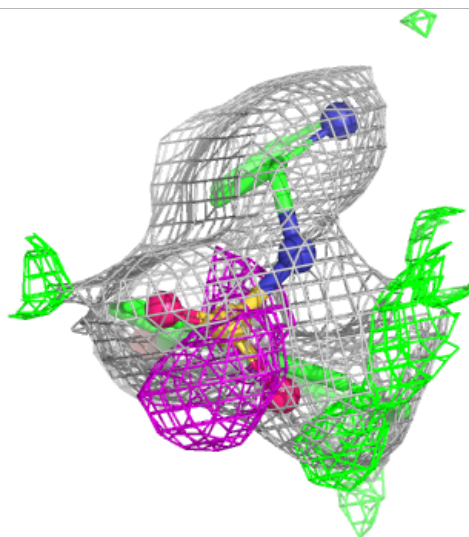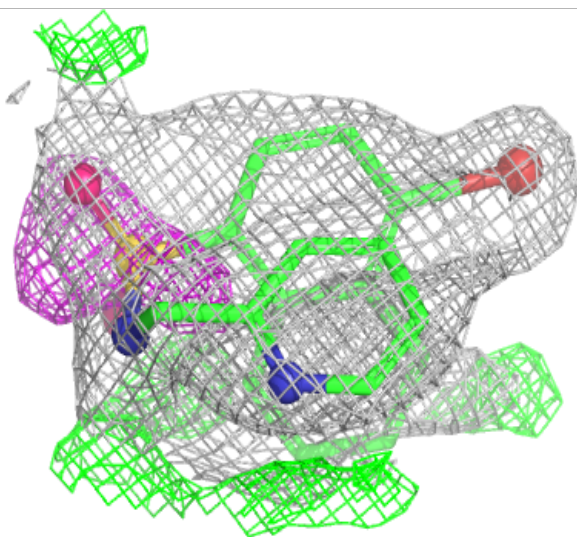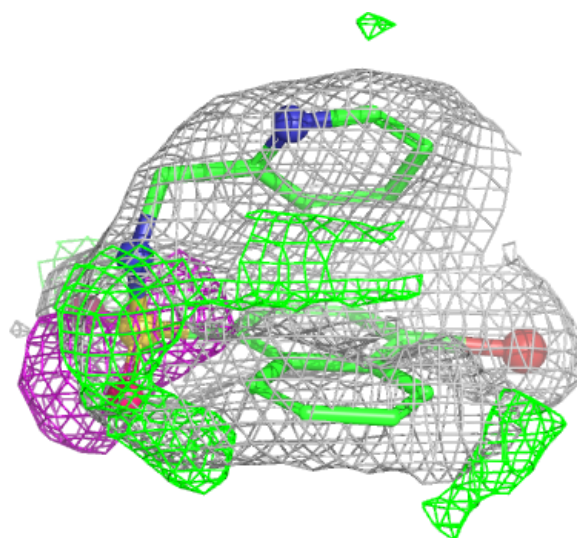
Electron density around PYV C 300 (D):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
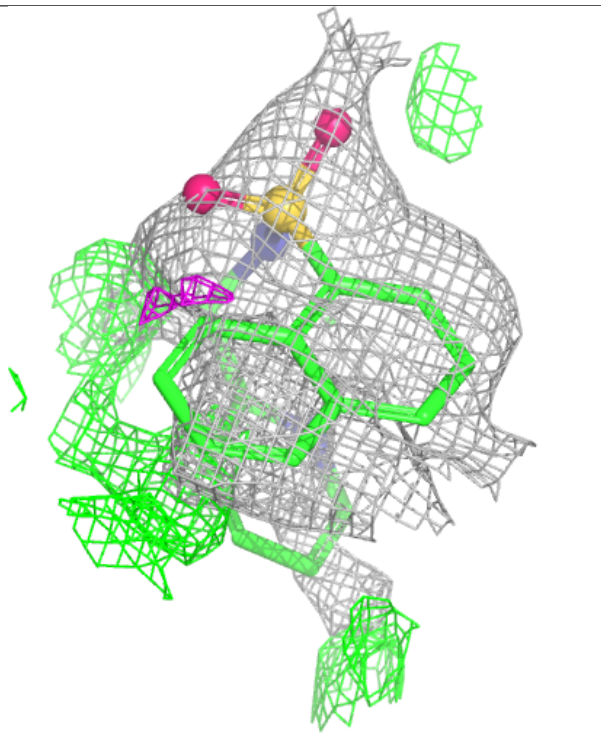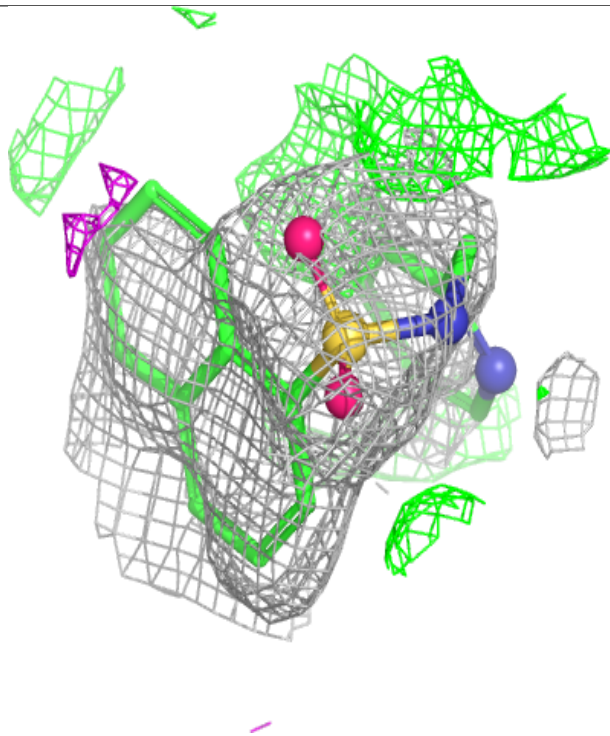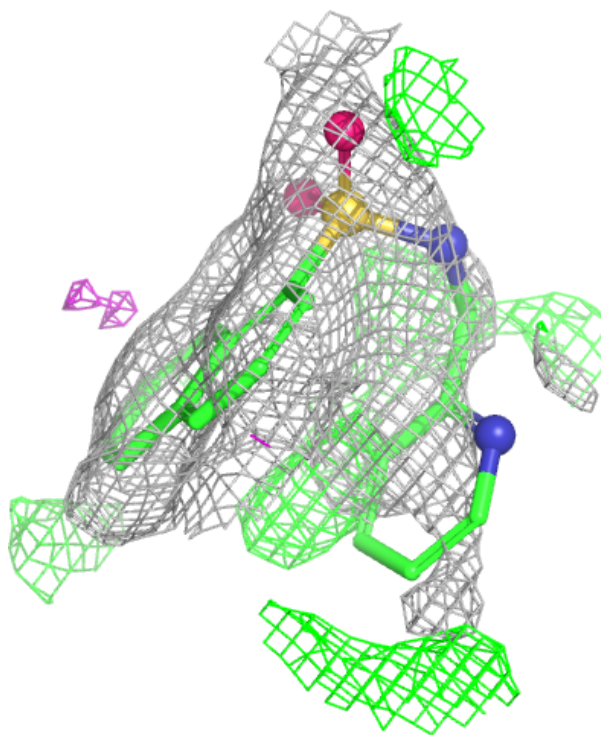
Electron density around PYV C 300 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
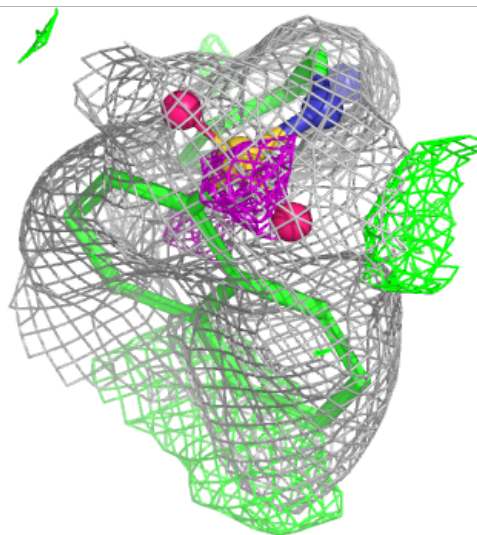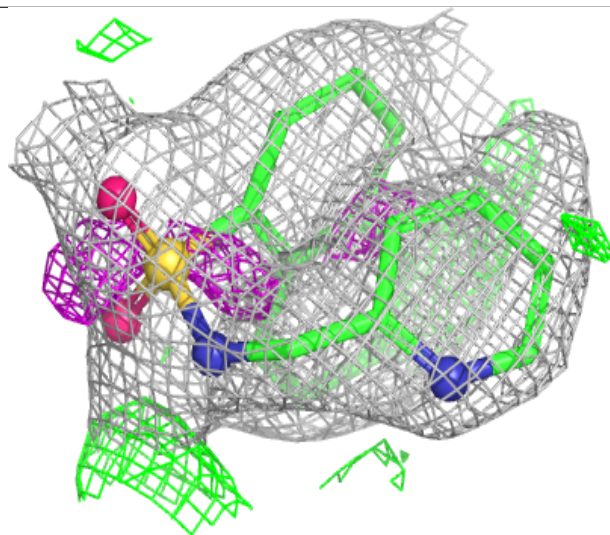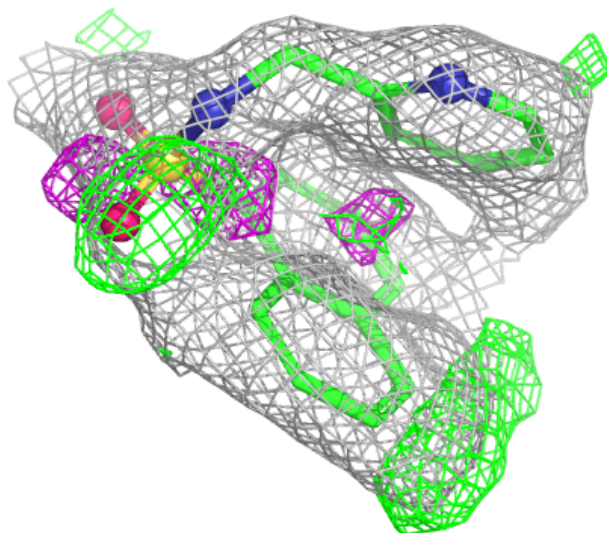and green (positive)
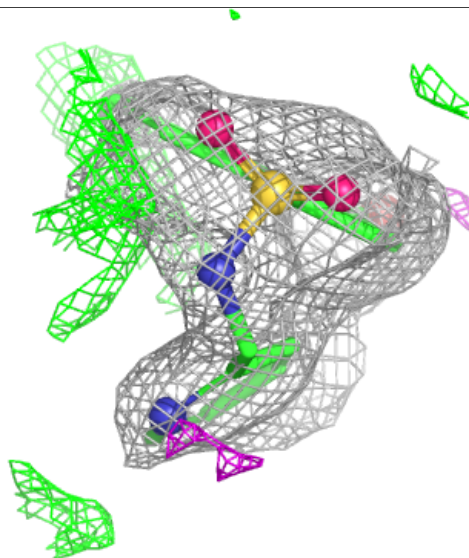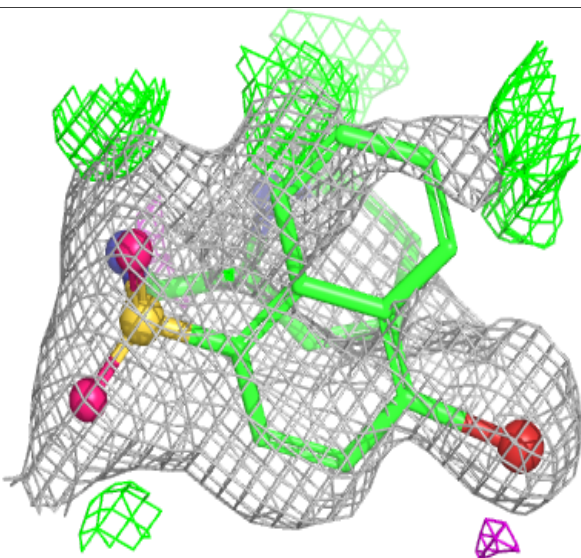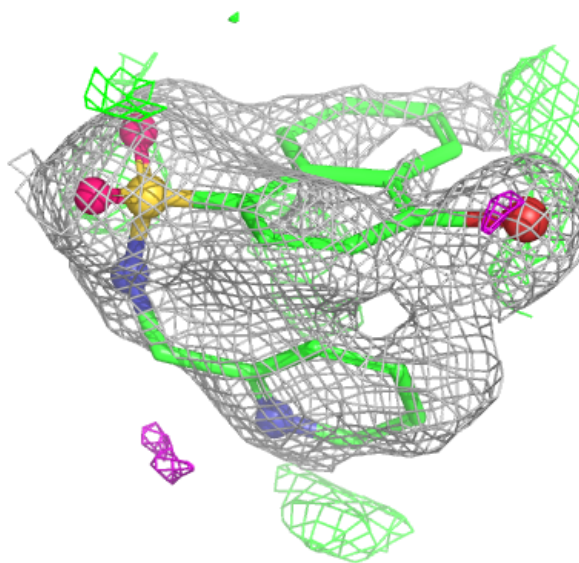
Electron density around PYV C 300 (B):

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

Electron density around PYV C 300 (C):

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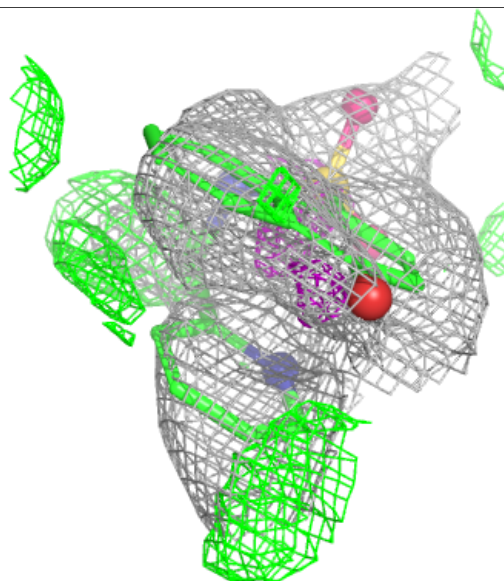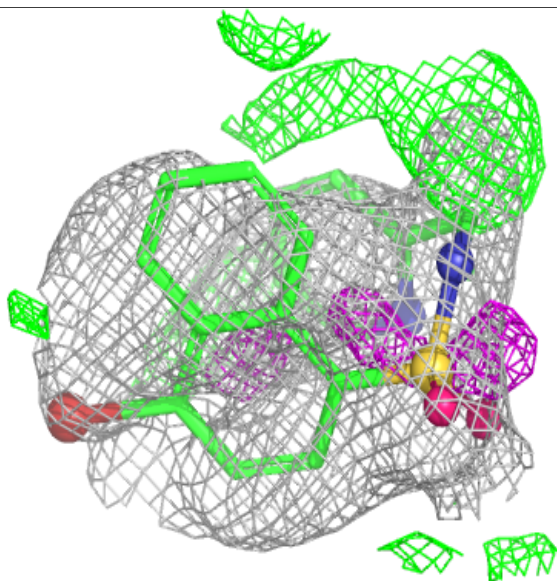and green (positive)

Electron density around PYV A 300 (D):

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

Electron density around PYV A 300 (A):

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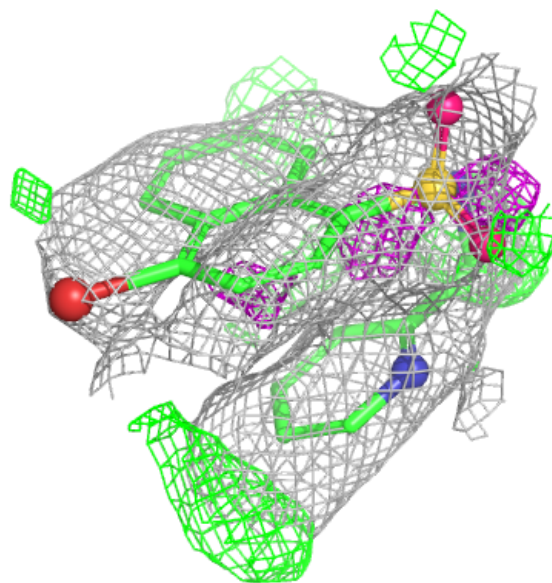and green (positive)

Electron density around PYV A 300 (B):

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

Electron density around PYV A 300 (C):

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

5.5 Other polymers ⓘ

There are no such residues in this entry.