



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 8, 2021 – 11:57 AM EST

PDB ID : 7KPE
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, E88Q mutant with pyruvate bound in the active site and R,R-bislysine at the allosteric site
Authors : Saran, S.; Sanders, D.A.R.
Deposited on : 2020-11-11
Resolution : 2.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

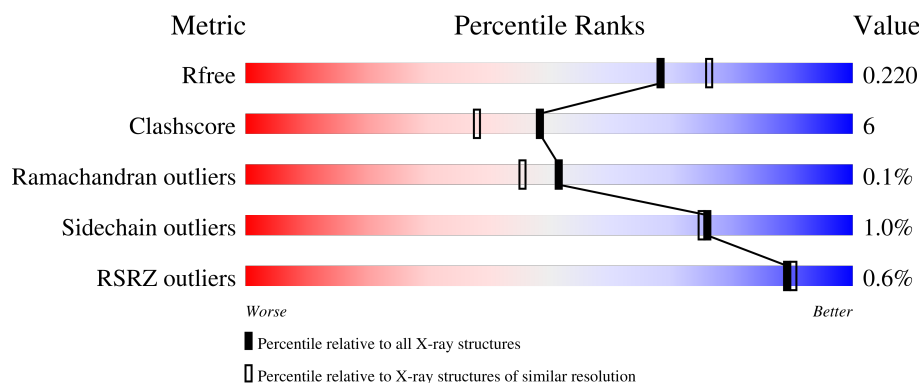
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.06 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	310	 89% 6% 5%
1	B	310	 89% 6% 5%
1	C	310	 88% 8% 5%
1	D	310	 2% 82% 10% 5%
1	E	310	 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	<div> <div></div> <div>%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

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
3	ACT	F	304	-	-	X	-
5	PGE	A	304	-	-	X	-
5	PGE	B	303	-	-	X	-
5	PGE	F	307	-	-	X	-
7	PEG	C	303	-	-	X	-
8	GOL	F	308	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14821 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2268	1443	376	436	13			
1	B	296	Total	C	N	O	S	0	0	0
			2275	1447	379	436	13			
1	C	296	Total	C	N	O	S	0	0	0
			2276	1447	379	437	13			
1	D	293	Total	C	N	O	S	0	0	0
			2244	1427	372	432	13			
1	E	295	Total	C	N	O	S	0	0	0
			2260	1436	375	436	13			
1	F	296	Total	C	N	O	S	0	0	0
			2259	1435	376	435	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	88	GLN	GLU	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	88	GLN	GLU	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	88	GLN	GLU	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	88	GLN	GLU	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	88	GLN	GLU	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	88	GLN	GLU	engineered mutation	UNP Q9PPB4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



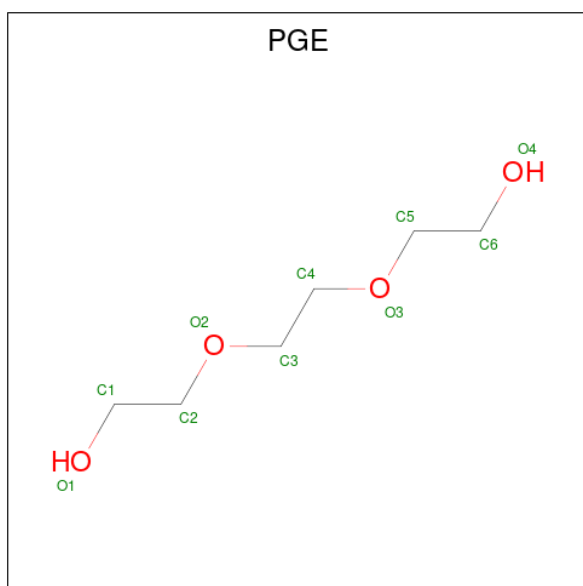
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



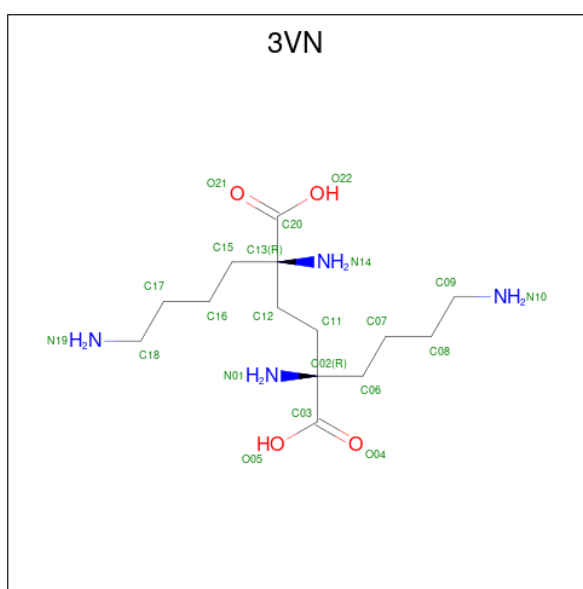
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



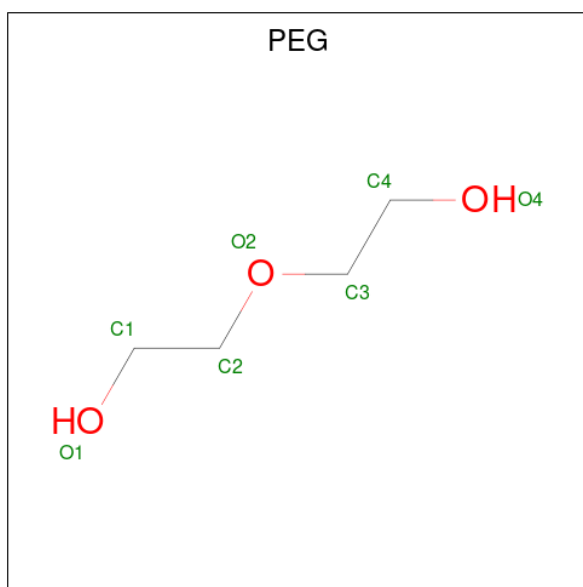
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula: C₁₄H₃₀N₄O₄) (labeled as "Ligand of Interest" by depositor).



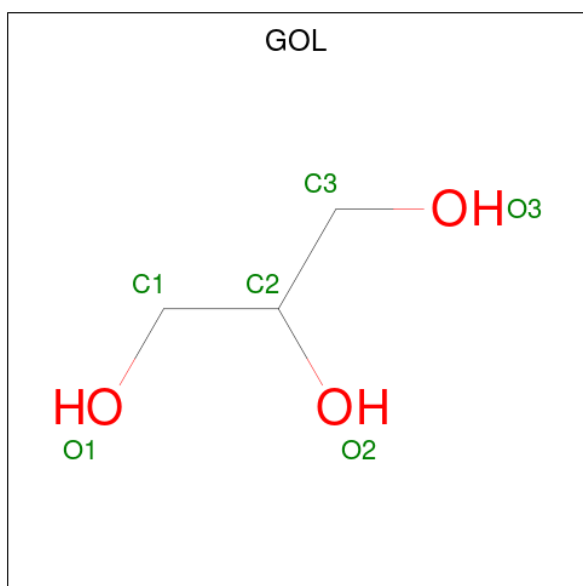
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			22	14	4	4		
6	D	1	Total	C	N	O	0	0
			22	14	4	4		
6	F	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

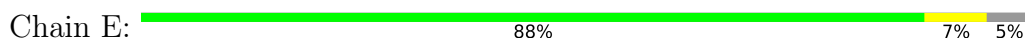
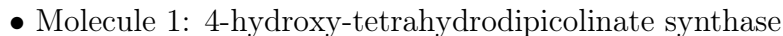


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

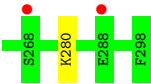
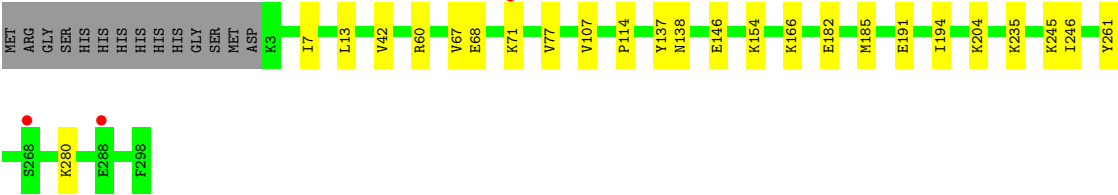
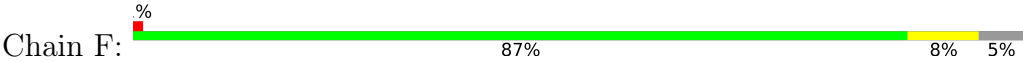
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	206	Total	O	0	0
			206	206		
9	B	188	Total	O	0	0
			188	188		
9	C	183	Total	O	0	0
			183	183		
9	D	155	Total	O	0	0
			155	155		
9	E	171	Total	O	0	0
			171	171		
9	F	156	Total	O	0	0
			156	156		

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase





- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.20Å 231.95Å 199.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.06 45.88 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.88-2.06) 94.0 (45.88-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.240 0.193 , 0.220	Depositor DCC
R_{free} test set	6103 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14821	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, KPI, GOL, PGE, 3VN, EDO, PEG, MG

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	0.37	0/2292	0.46	0/3102
1	B	0.36	0/2299	0.49	0/3109
1	C	0.40	0/2300	0.47	0/3109
1	D	0.81	0/2268	0.69	2/3070 (0.1%)
1	E	0.39	0/2284	0.51	0/3090
1	F	0.38	0/2283	0.52	0/3090
All	All	0.48	0/13726	0.53	2/18570 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ILE	N-CA-C	-6.97	92.19	111.00
1	D	66	ALA	N-CA-CB	6.73	119.53	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	KPI	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2287	29	0
1	B	2275	0	2310	19	0
1	C	2276	0	2310	28	0
1	D	2244	0	2263	44	0
1	E	2260	0	2278	15	0
1	F	2259	0	2272	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	4	0	3	0	0
3	C	4	0	3	1	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	12	0	9	15	0
4	A	4	0	6	0	0
4	F	8	0	12	1	0
5	A	10	0	14	11	0
5	B	10	0	14	9	0
5	E	10	0	14	5	0
5	F	10	0	14	8	0
6	B	22	0	28	0	0
6	D	22	0	28	3	0
6	F	22	0	28	0	0
7	C	14	0	20	13	0
7	D	7	0	10	0	0
8	F	6	0	8	2	0
9	A	206	0	0	3	0
9	B	188	0	0	1	0
9	C	183	0	0	2	0
9	D	155	0	0	2	0
9	E	171	0	0	0	0
9	F	156	0	0	2	0
All	All	14821	0	13937	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 165 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:F:60:ARG:CD	3:F:304:ACT:H1	1.45	1.44
1:F:60:ARG:HD3	3:F:304:ACT:CH3	1.54	1.33
1:F:60:ARG:HH11	3:F:304:ACT:H3	1.06	1.17
1:F:60:ARG:NH1	3:F:304:ACT:H3	1.60	1.16
1:A:154:LYS:HE3	5:A:304:PGE:H2	1.31	1.08

There are no symmetry-related clashes.

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	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	B	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	C	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	D	290/310 (94%)	283 (98%)	6 (2%)	1 (0%)	41	32
1	E	292/310 (94%)	288 (99%)	4 (1%)	0	100	100
1	F	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
All	All	1754/1860 (94%)	1726 (98%)	27 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	66	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/260 (94%)	243 (100%)	1 (0%)	91	91
1	B	247/260 (95%)	244 (99%)	3 (1%)	71	69
1	C	247/260 (95%)	247 (100%)	0	100	100
1	D	242/260 (93%)	234 (97%)	8 (3%)	38	31
1	E	244/260 (94%)	243 (100%)	1 (0%)	91	91
1	F	243/260 (94%)	242 (100%)	1 (0%)	91	91
All	All	1467/1560 (94%)	1453 (99%)	14 (1%)	76	75

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	86	THR
1	D	104	ILE
1	F	280	LYS
1	D	231	LYS
1	E	21	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	C	88	GLN
1	C	242	ASN
1	D	59	HIS
1	E	19	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	KPI	E	166	1	10,13,14	0.64	0	6,15,17	3.14	3 (50%)
1	KPI	C	166	1	10,13,14	1.39	1 (10%)	6,15,17	2.95	3 (50%)
1	KPI	B	166	1	10,13,14	1.39	1 (10%)	6,15,17	3.13	3 (50%)
1	KPI	F	166	1	10,13,14	0.61	0	6,15,17	3.15	3 (50%)
1	KPI	A	166	1	10,13,14	0.62	0	6,15,17	3.12	2 (33%)
1	KPI	D	166	1	10,13,14	0.65	0	6,15,17	3.10	3 (50%)

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
1	KPI	E	166	1	-	2/9/14/16	-
1	KPI	C	166	1	-	1/9/14/16	-
1	KPI	B	166	1	-	1/9/14/16	-
1	KPI	F	166	1	-	1/9/14/16	-
1	KPI	A	166	1	-	1/9/14/16	-
1	KPI	D	166	1	-	2/9/14/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O-C	4.11	1.36	1.19
1	C	166	KPI	O-C	4.10	1.36	1.19

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	KPI	C1-CX1-CX2	-6.27	110.98	117.92
1	F	166	KPI	C1-CX1-CX2	-6.21	111.04	117.92
1	D	166	KPI	C1-CX1-CX2	-6.20	111.05	117.92
1	B	166	KPI	C1-CX1-CX2	-6.11	111.16	117.92
1	E	166	KPI	C1-CX1-CX2	-6.05	111.22	117.92

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	CX2-CX1-NZ-CE
1	E	166	KPI	CX2-CX1-NZ-CE
1	E	166	KPI	C1-CX1-NZ-CE
1	A	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z > 2$
6	3VN	F	301	-	15,21,21	1.14	1 (6%)	12,28,28	1.68	2 (16%)
6	3VN	D	301	-	15,21,21	1.17	1 (6%)	12,28,28	1.48	2 (16%)
3	ACT	F	302	-	1,3,3	1.99	0	0,3,3	-	-
3	ACT	A	302	-	1,3,3	0.55	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	F	306	-	3,3,3	0.54	0	2,2,2	0.73	0
6	3VN	B	301	-	15,21,21	1.21	1 (6%)	12,28,28	1.43	2 (16%)
3	ACT	E	302	-	1,3,3	0.60	0	0,3,3	-	-
8	GOL	F	308	-	5,5,5	0.42	0	5,5,5	0.78	0
7	PEG	D	304	-	6,6,6	0.32	0	5,5,5	0.59	0
5	PGE	B	303	-	9,9,9	0.41	0	8,8,8	0.72	0
4	EDO	F	305	-	3,3,3	0.62	0	2,2,2	0.22	0
5	PGE	E	303	-	9,9,9	0.37	0	8,8,8	0.45	0
7	PEG	C	304	-	6,6,6	0.49	0	5,5,5	1.14	1 (20%)
3	ACT	D	305	-	1,3,3	1.07	0	0,3,3	-	-
5	PGE	A	304	-	9,9,9	0.55	0	8,8,8	1.25	1 (12%)
7	PEG	C	303	-	6,6,6	0.31	0	5,5,5	0.82	0
3	ACT	F	304	-	1,3,3	0.69	0	0,3,3	-	-
3	ACT	F	303	-	1,3,3	1.27	0	0,3,3	-	-
4	EDO	A	303	-	3,3,3	0.24	0	2,2,2	0.43	0
3	ACT	C	305	-	1,3,3	0.97	0	0,3,3	-	-
5	PGE	F	307	-	9,9,9	0.36	0	8,8,8	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	306	-	-	1/1/1/1	-
7	PEG	C	303	-	-	2/4/4/4	-
8	GOL	F	308	-	-	2/4/4/4	-
7	PEG	D	304	-	-	3/4/4/4	-
5	PGE	B	303	-	-	3/7/7/7	-
4	EDO	A	303	-	-	1/1/1/1	-
6	3VN	F	301	-	-	2/19/31/31	-
4	EDO	F	305	-	-	0/1/1/1	-
5	PGE	E	303	-	-	5/7/7/7	-
6	3VN	B	301	-	-	0/19/31/31	-
6	3VN	D	301	-	-	1/19/31/31	-
7	PEG	C	304	-	-	2/4/4/4	-
5	PGE	A	304	-	-	4/7/7/7	-
5	PGE	F	307	-	-	4/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	3VN	C06-C02	2.43	1.57	1.55
6	D	301	3VN	C06-C02	2.36	1.57	1.55
6	F	301	3VN	C06-C02	2.18	1.57	1.55

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	3VN	C16-C15-C13	-3.38	109.20	115.20
6	F	301	3VN	C07-C06-C02	-2.94	109.98	115.20
6	D	301	3VN	C07-C06-C02	-2.76	110.31	115.20
6	B	301	3VN	C07-C06-C02	-2.39	110.96	115.20
6	D	301	3VN	C16-C15-C13	-2.26	111.19	115.20

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	308	GOL	O1-C1-C2-C3
5	E	303	PGE	O2-C3-C4-O3
5	A	304	PGE	O3-C5-C6-O4
7	D	304	PEG	O1-C1-C2-O2
7	D	304	PEG	O2-C3-C4-O4

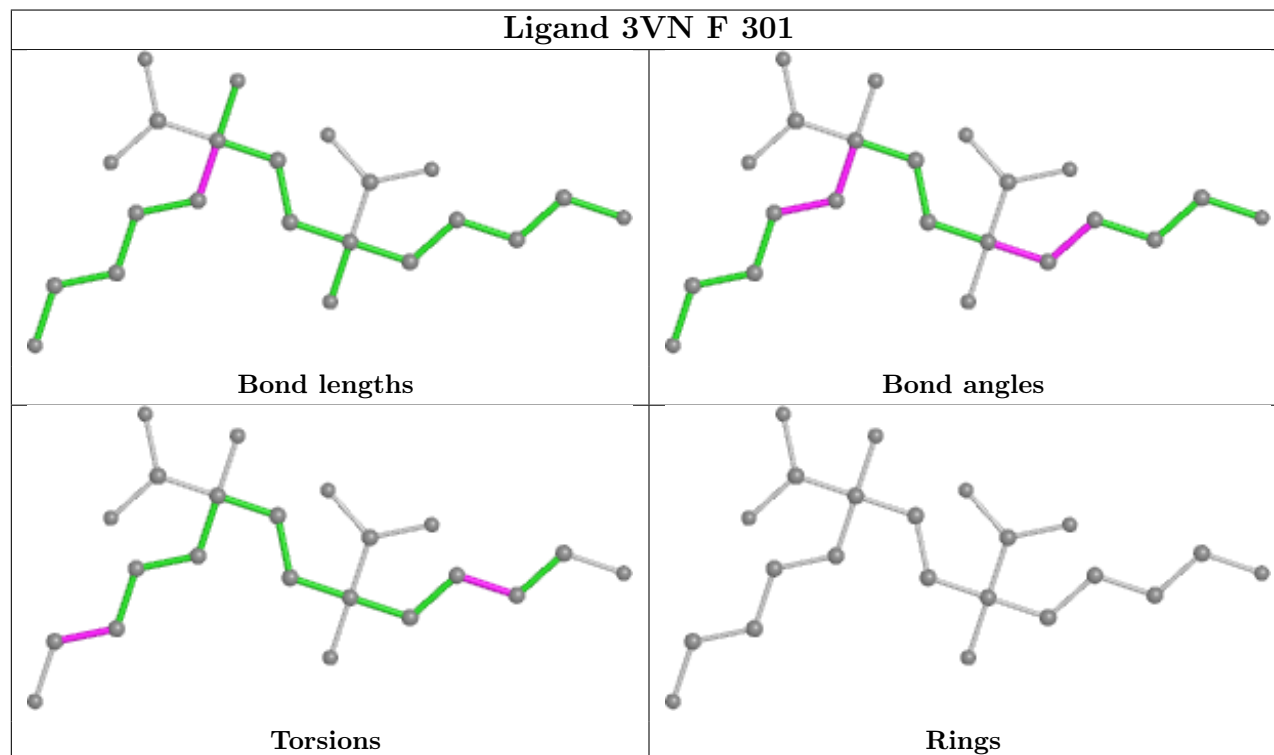
There are no ring outliers.

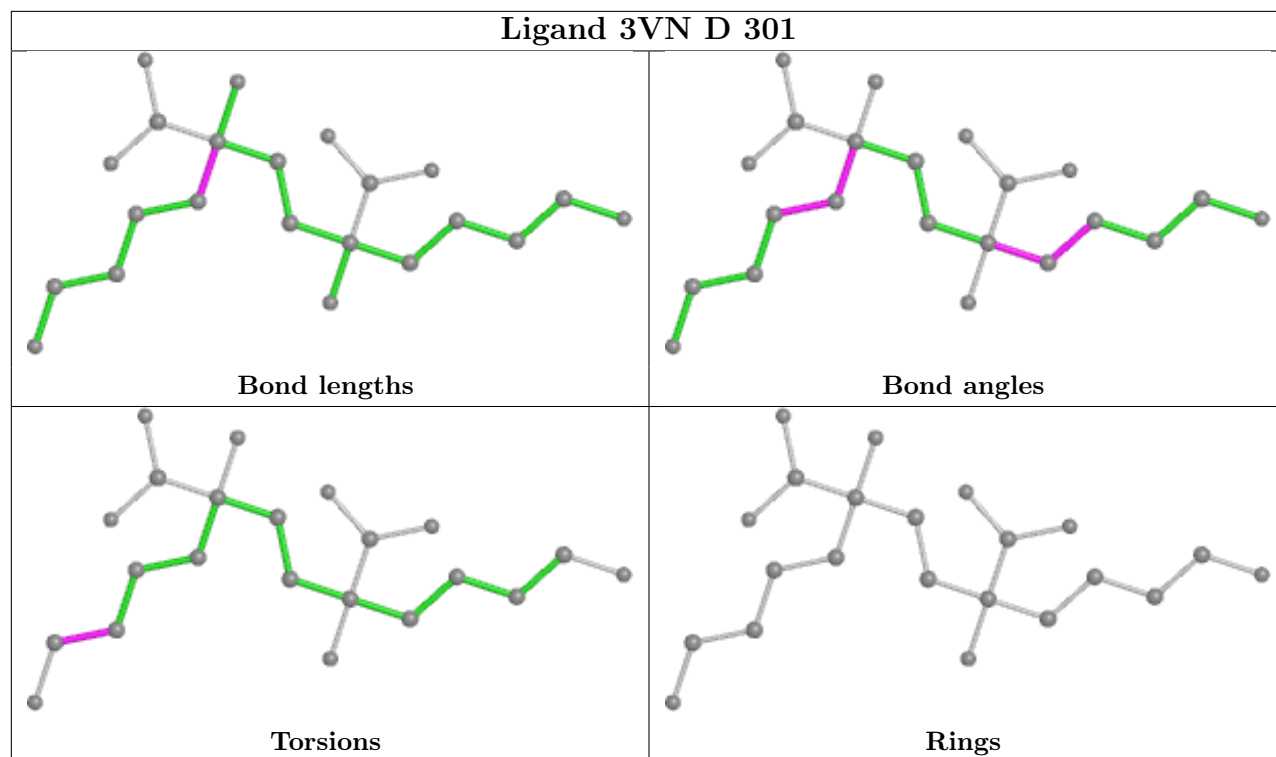
12 monomers are involved in 68 short contacts:

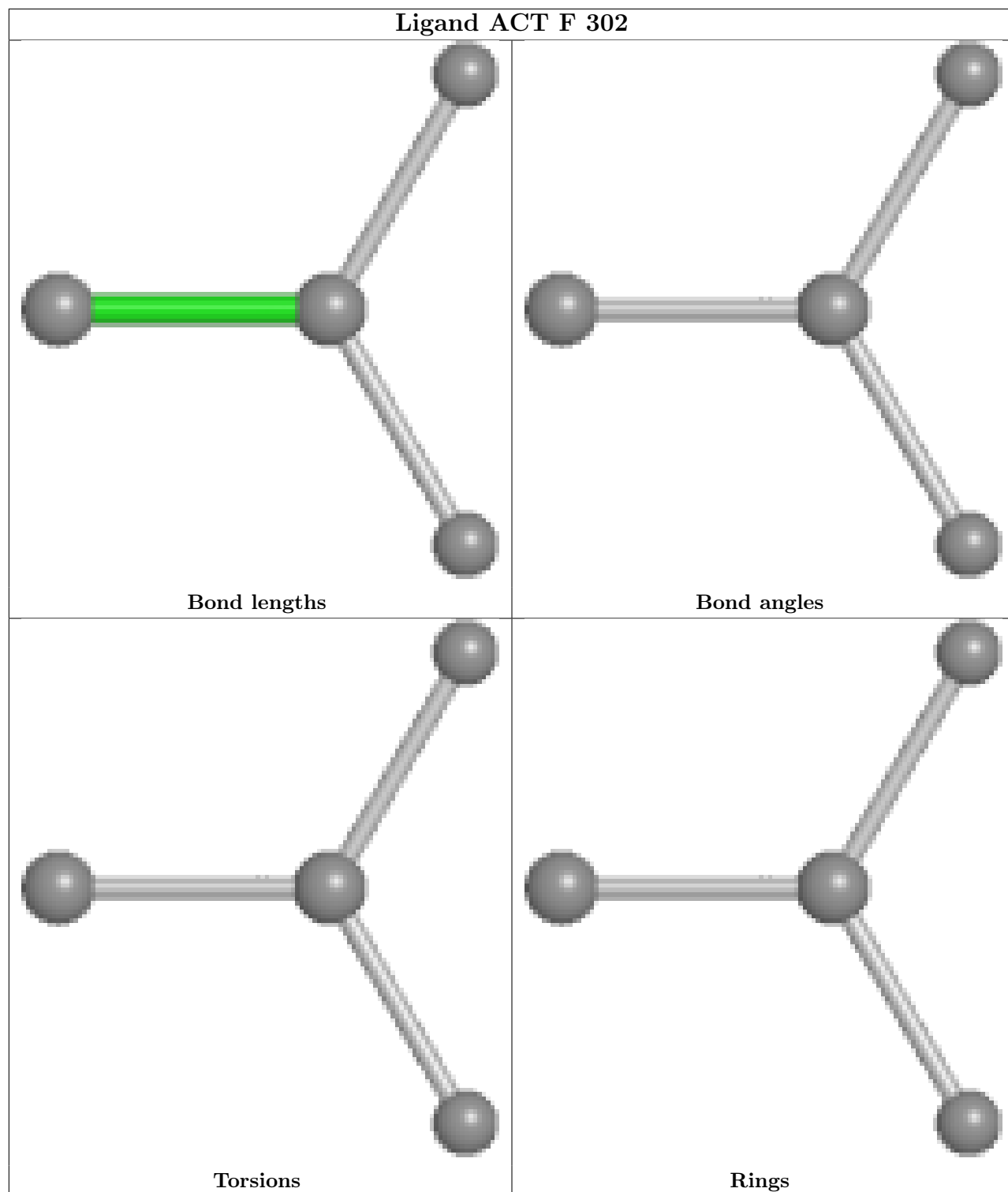
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	3VN	3	0
4	F	306	EDO	1	0
8	F	308	GOL	2	0
5	B	303	PGE	9	0
5	E	303	PGE	5	0
7	C	304	PEG	1	0
5	A	304	PGE	11	0
7	C	303	PEG	12	0
3	F	304	ACT	14	0
3	F	303	ACT	1	0
3	C	305	ACT	1	0
5	F	307	PGE	8	0

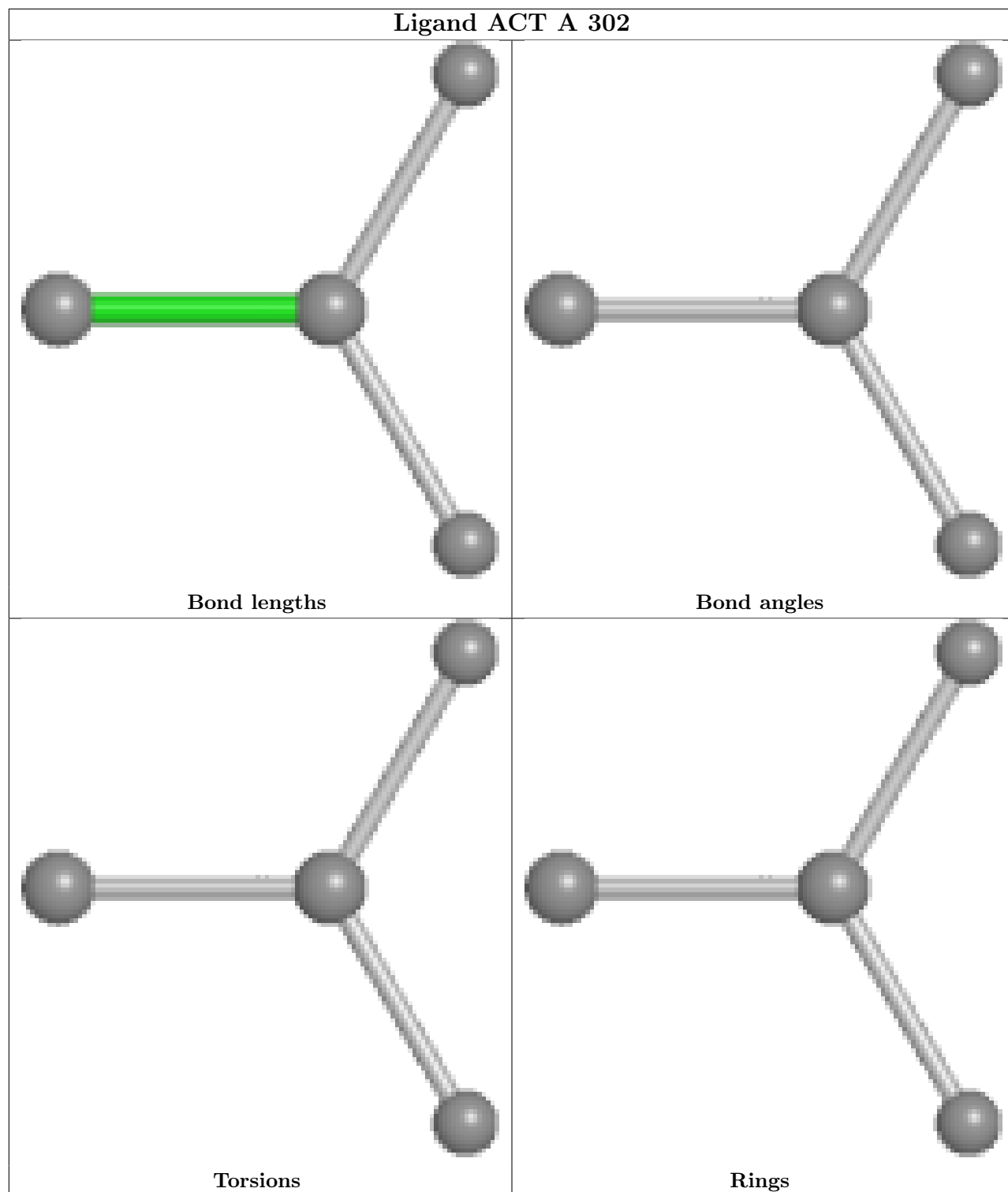
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

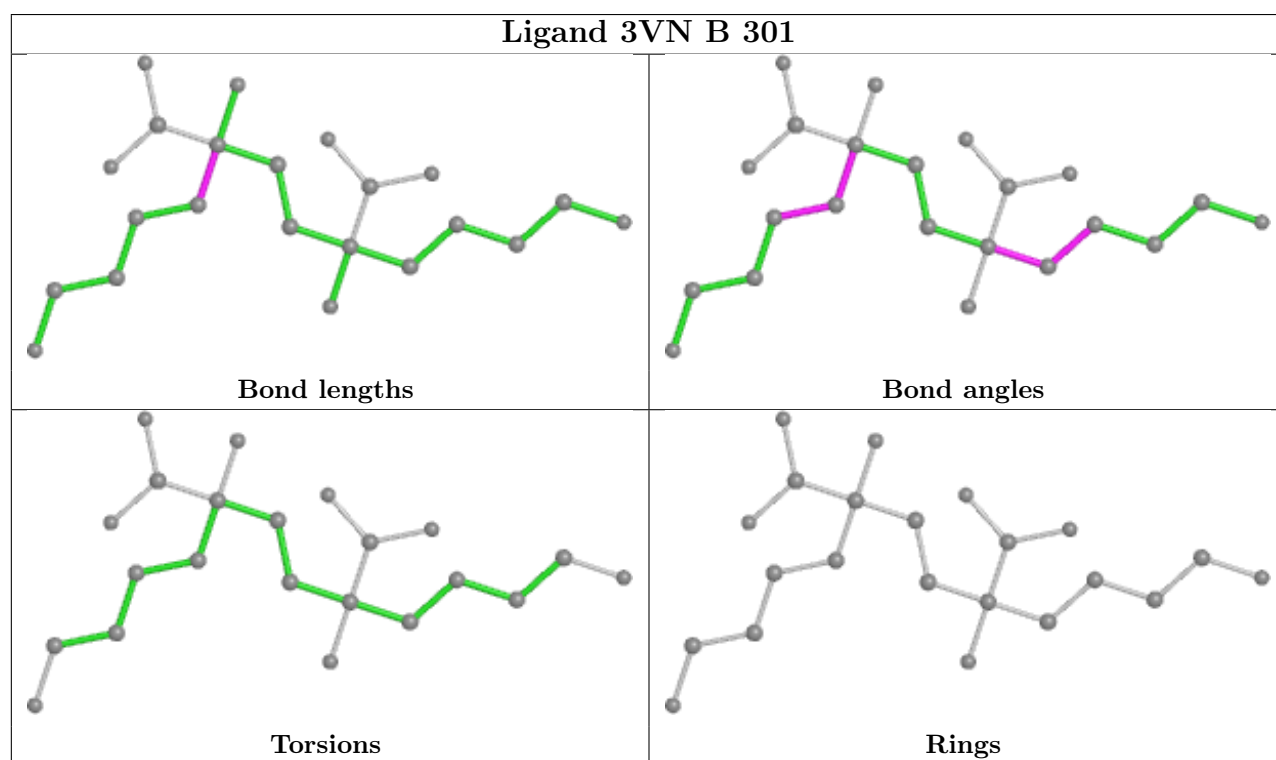
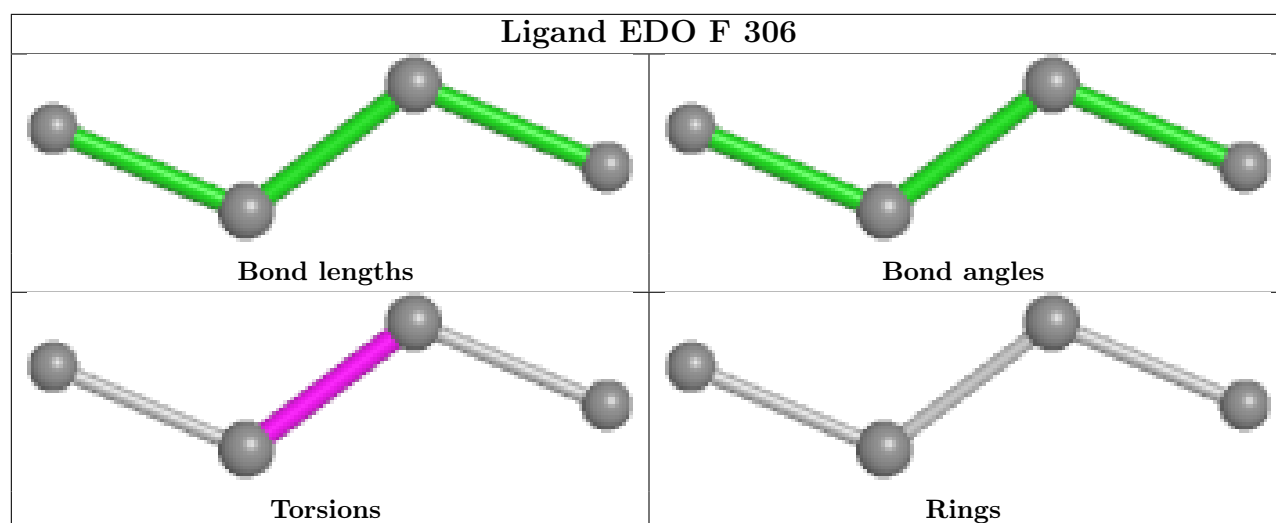
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

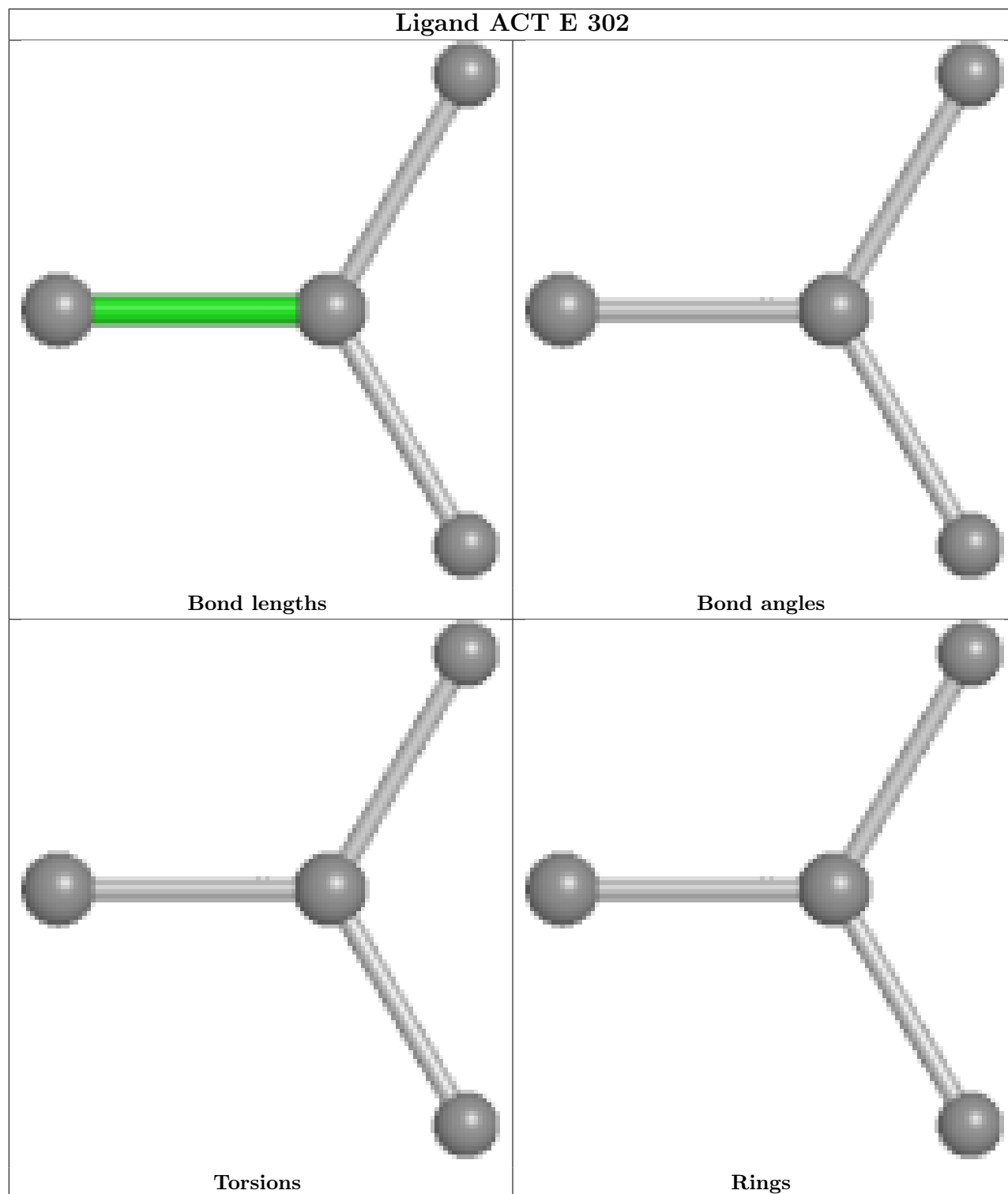


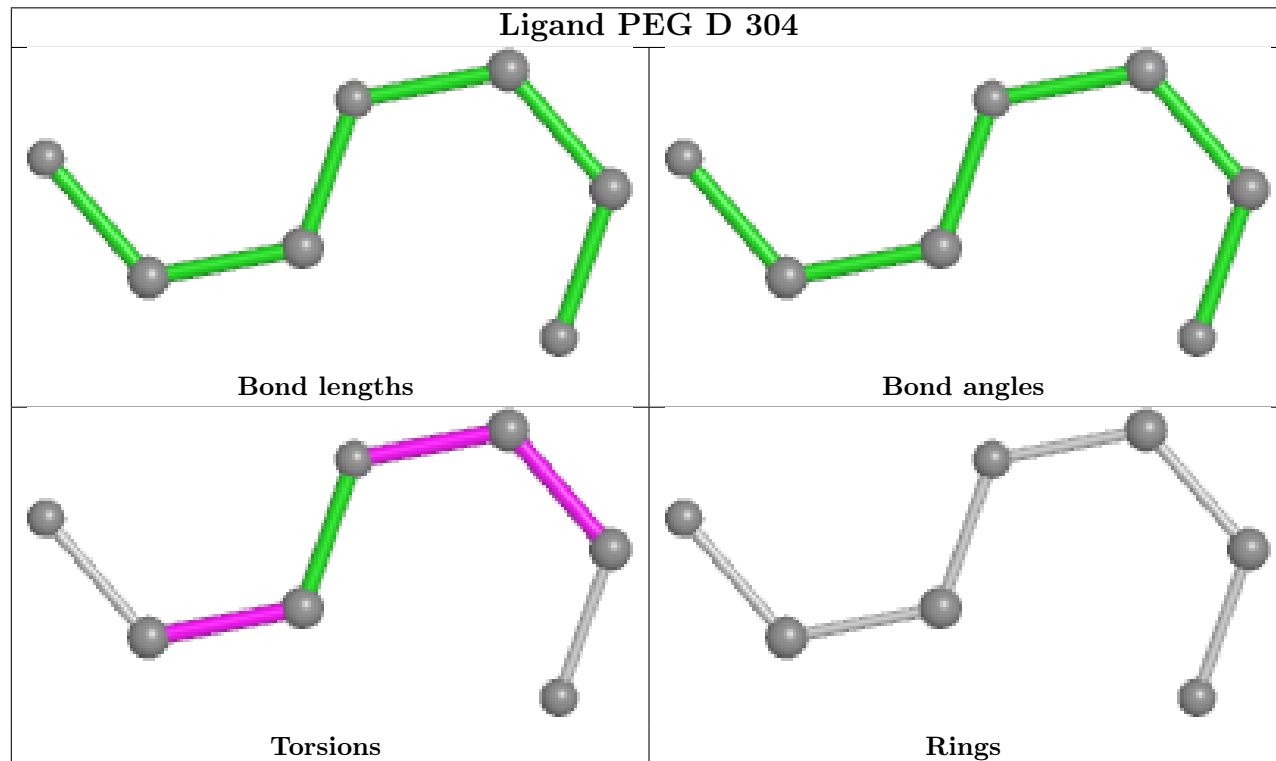
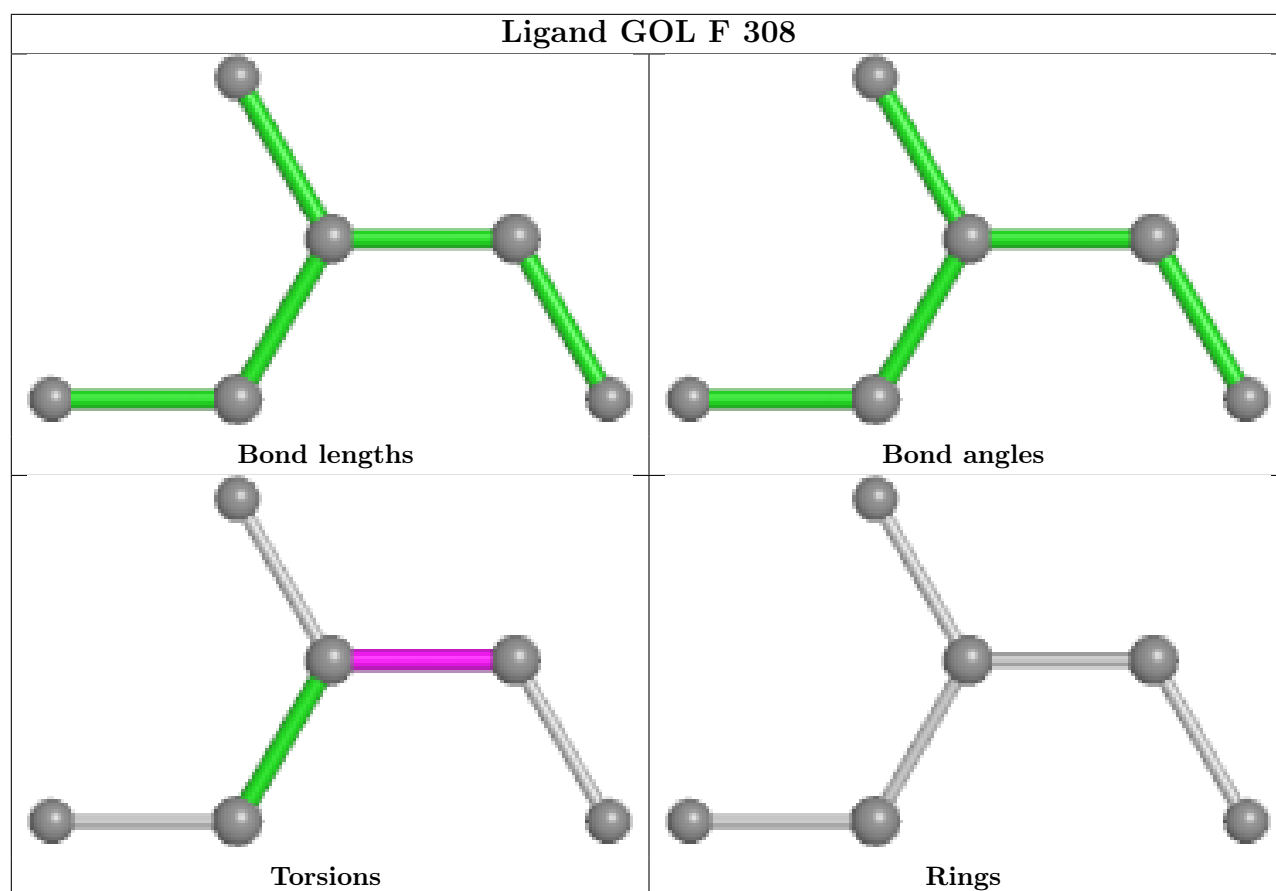


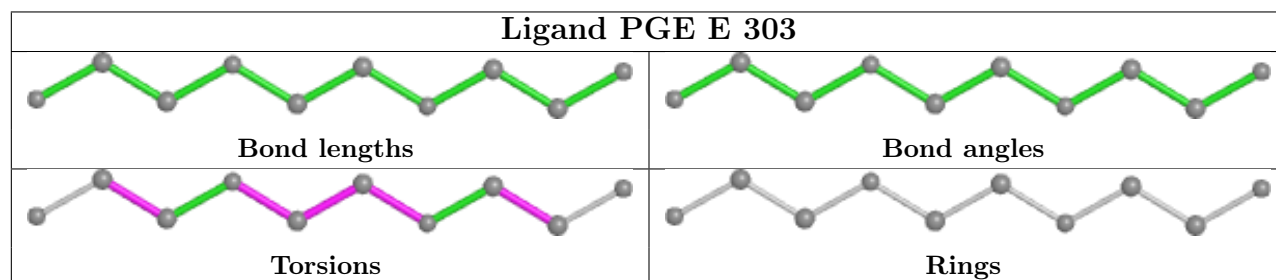
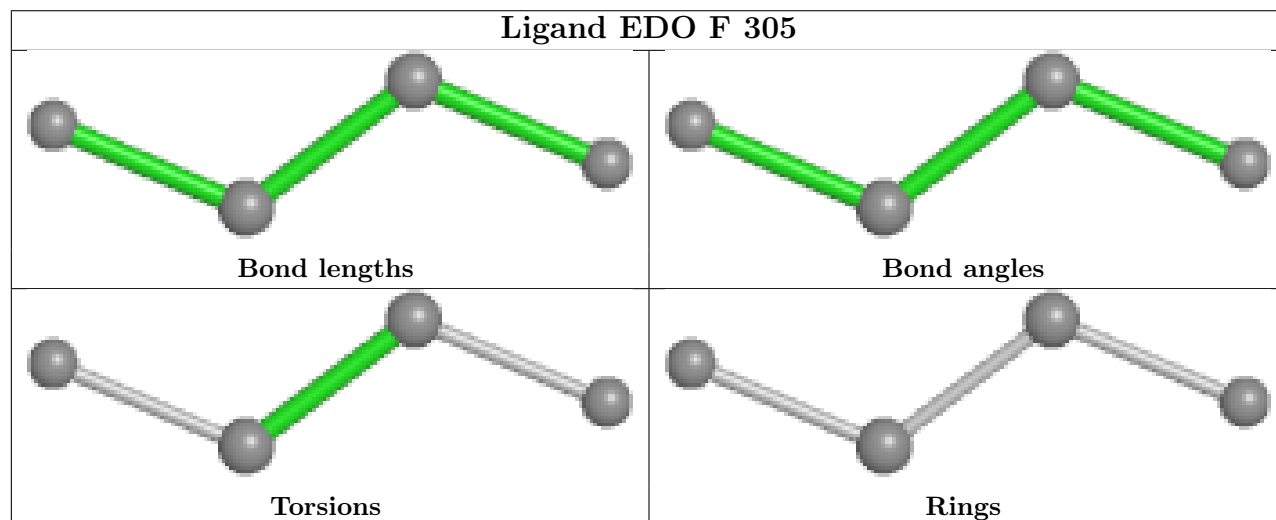
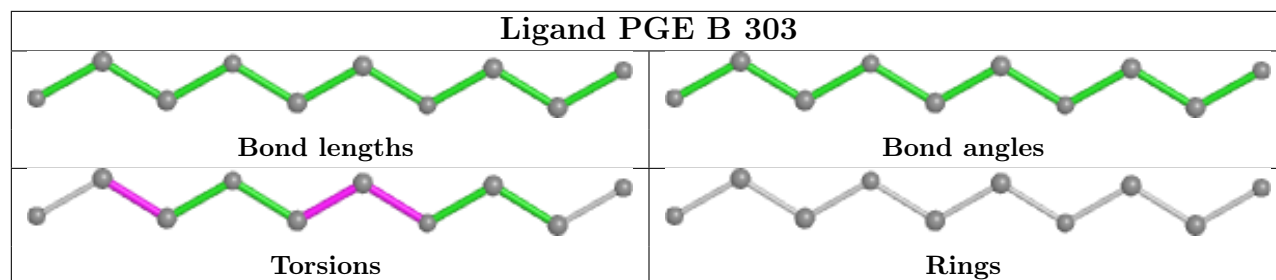


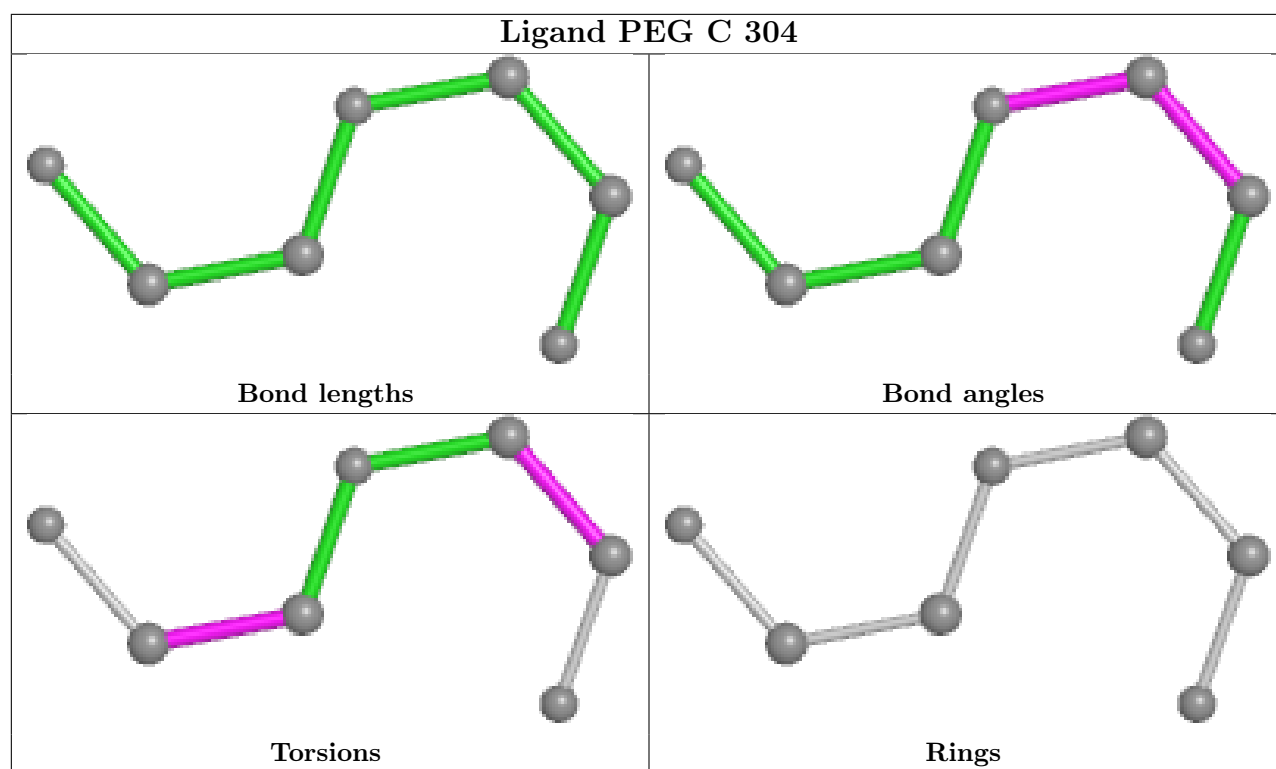


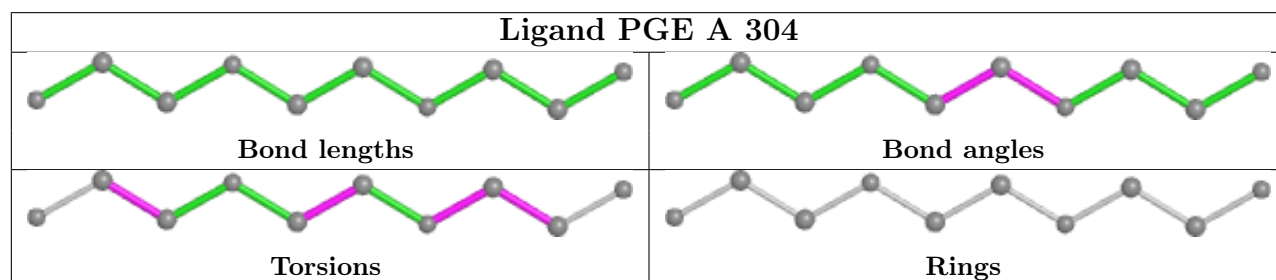
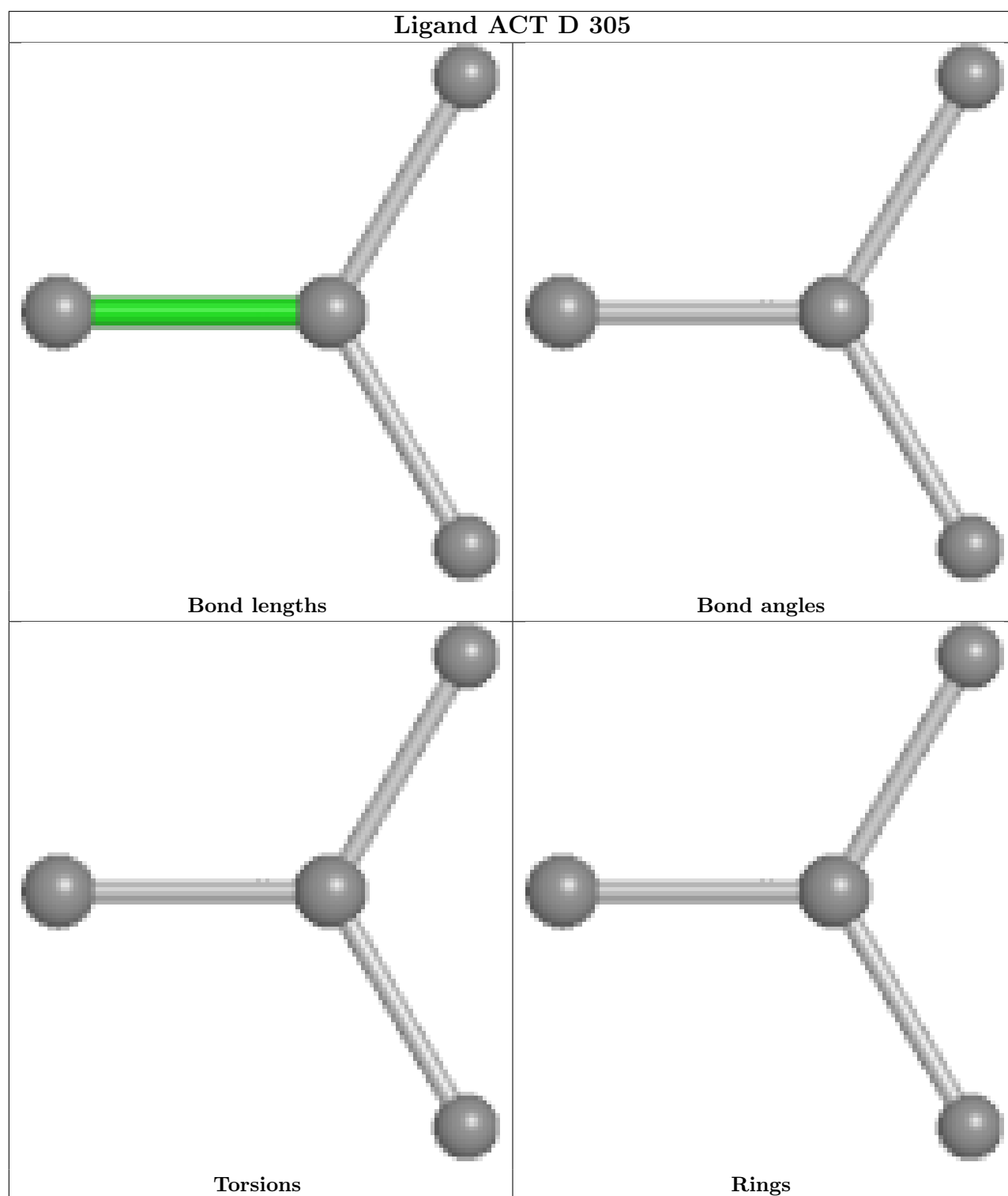


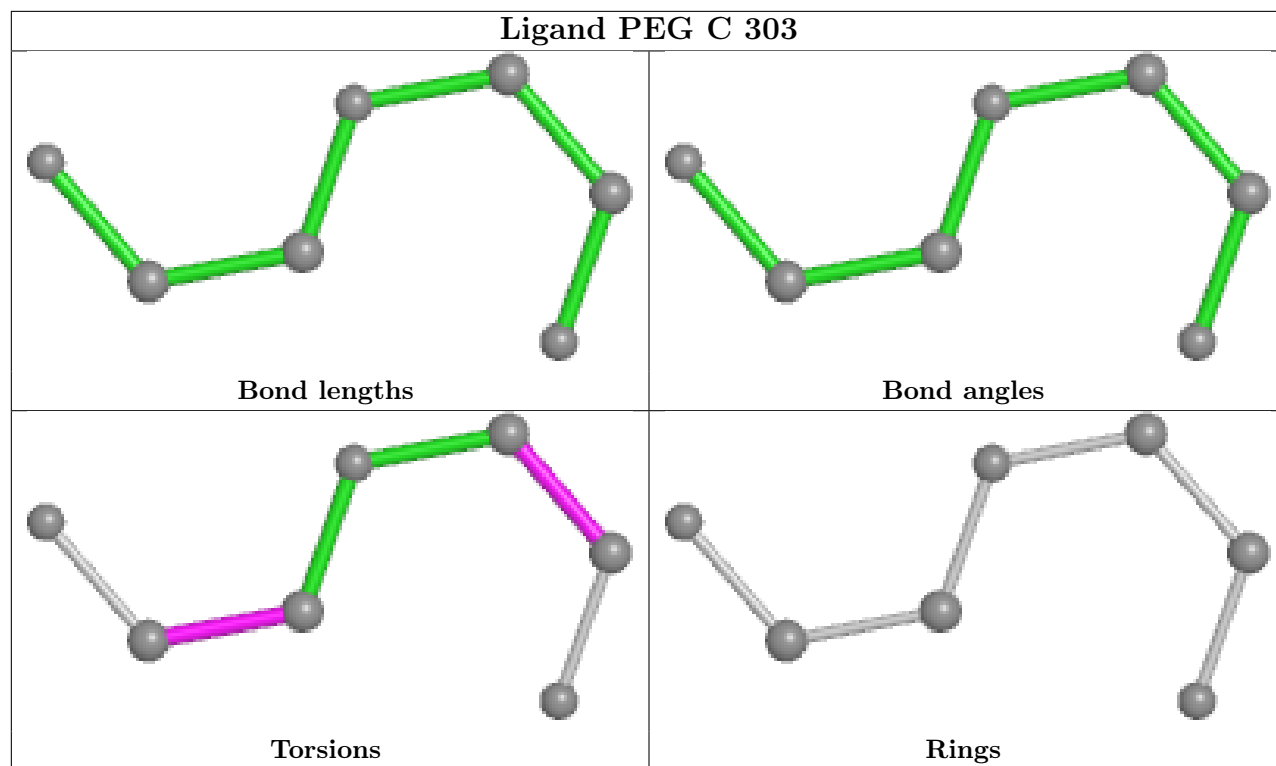


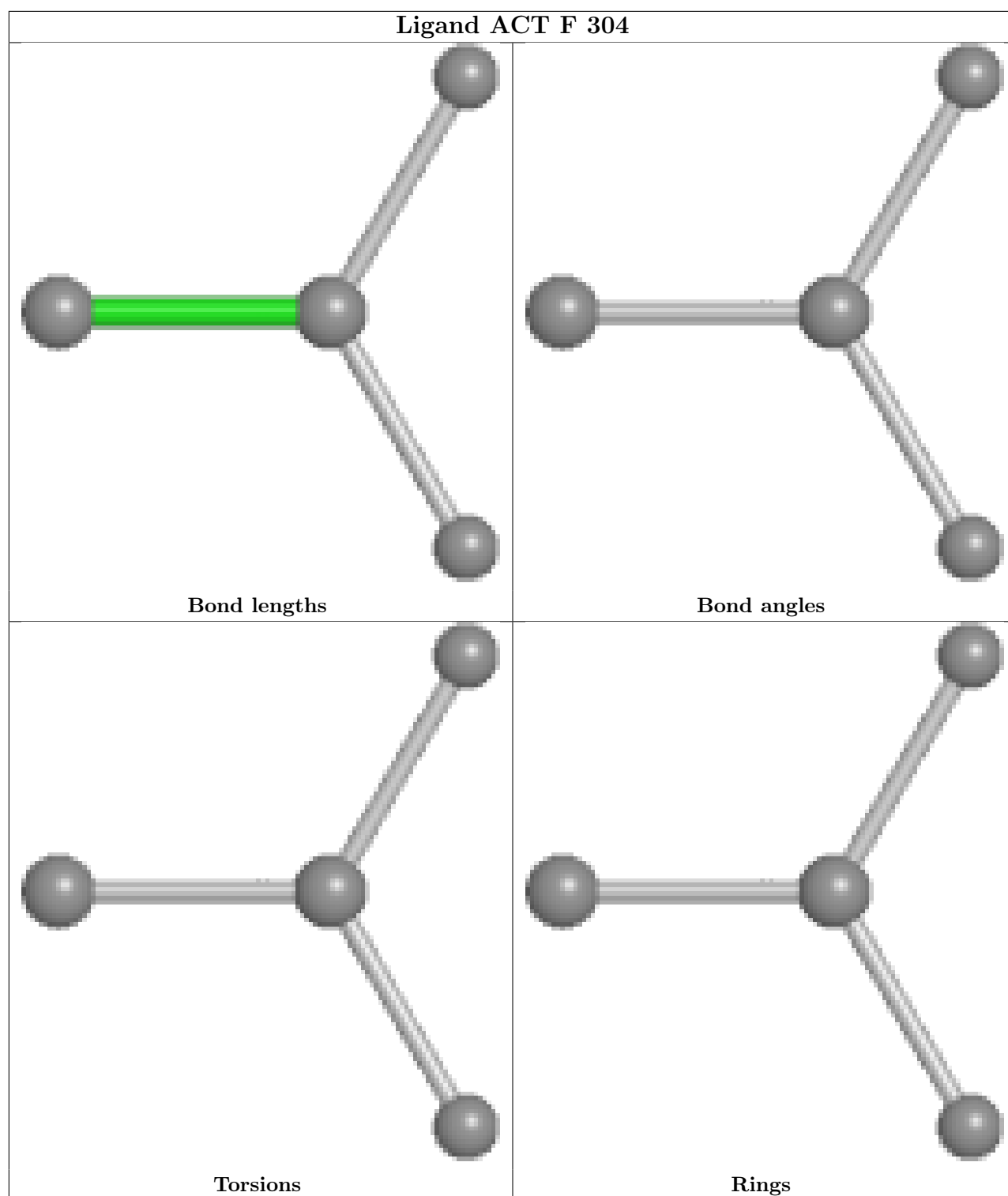


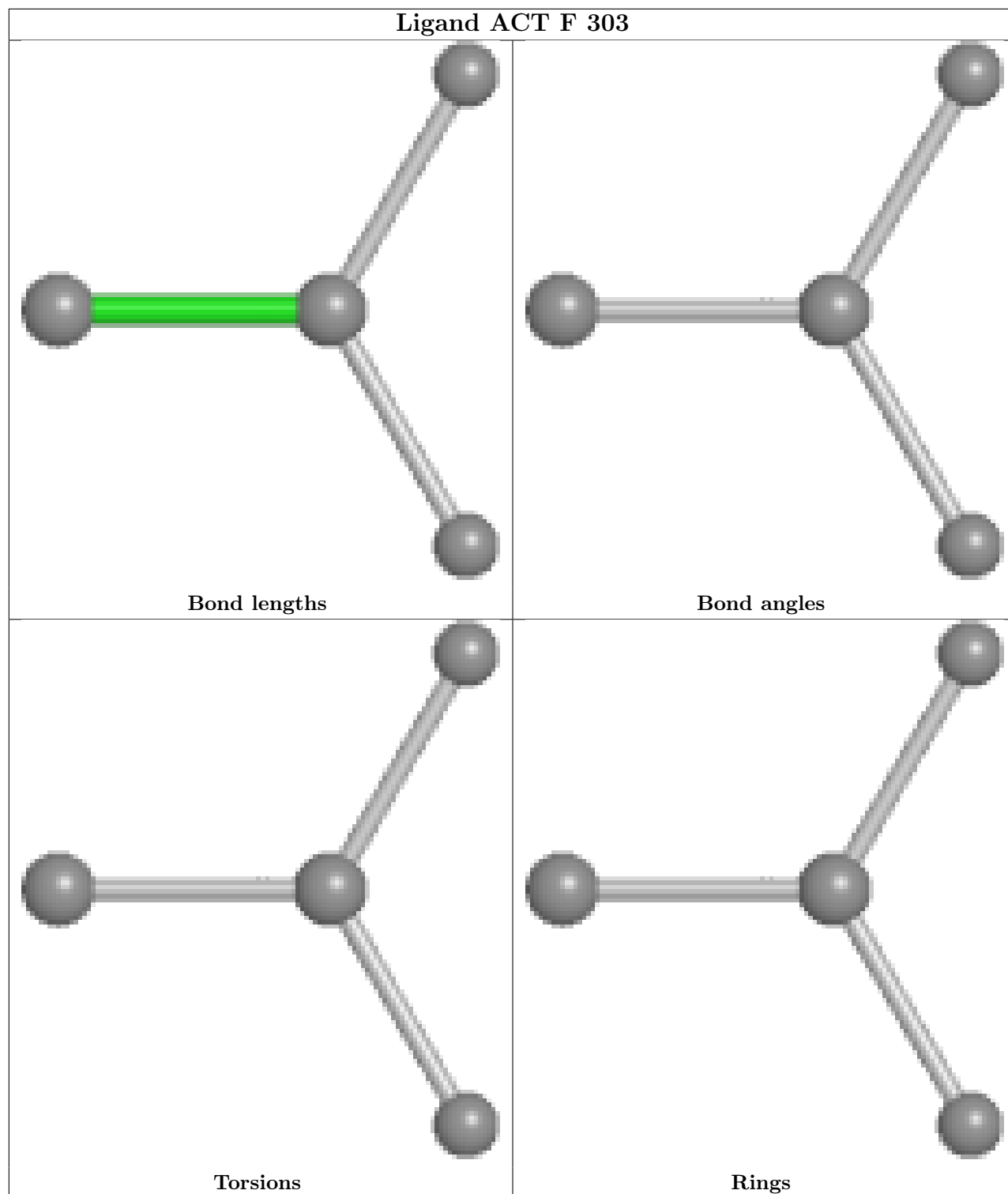


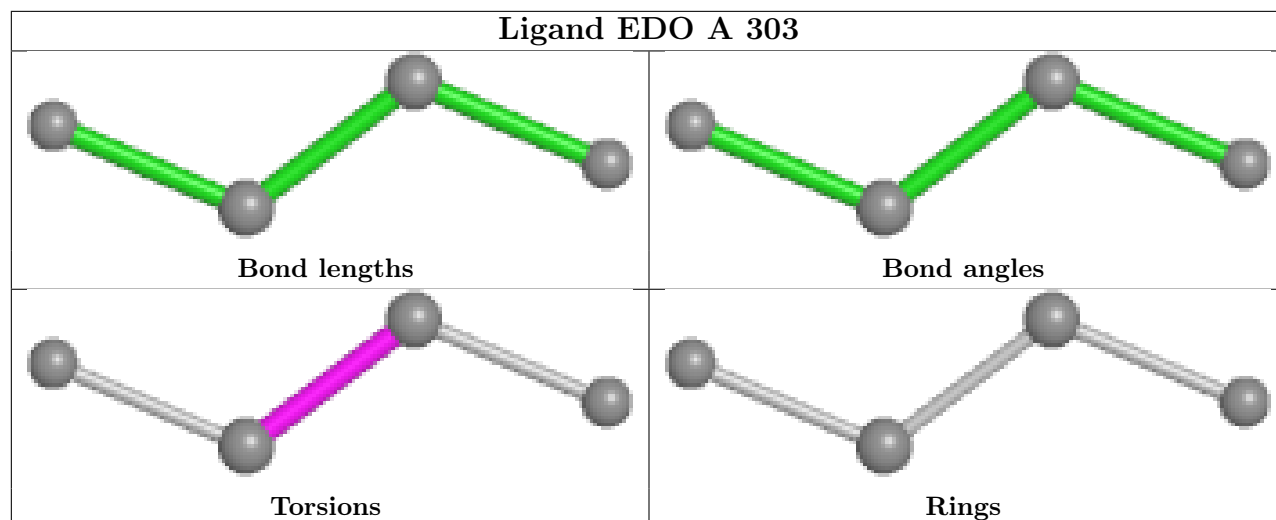


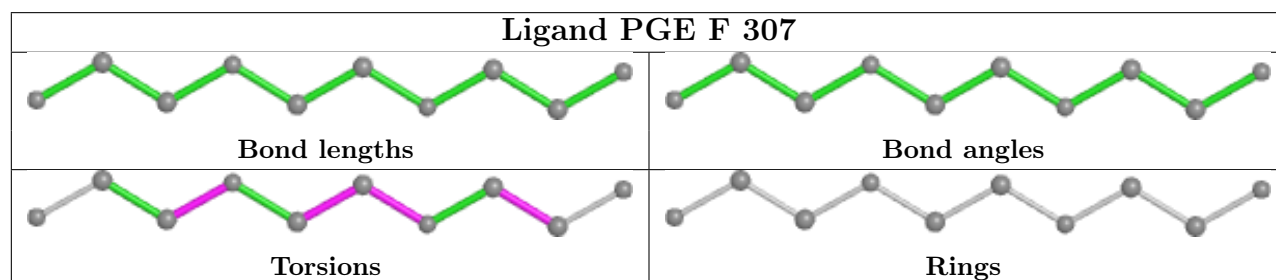
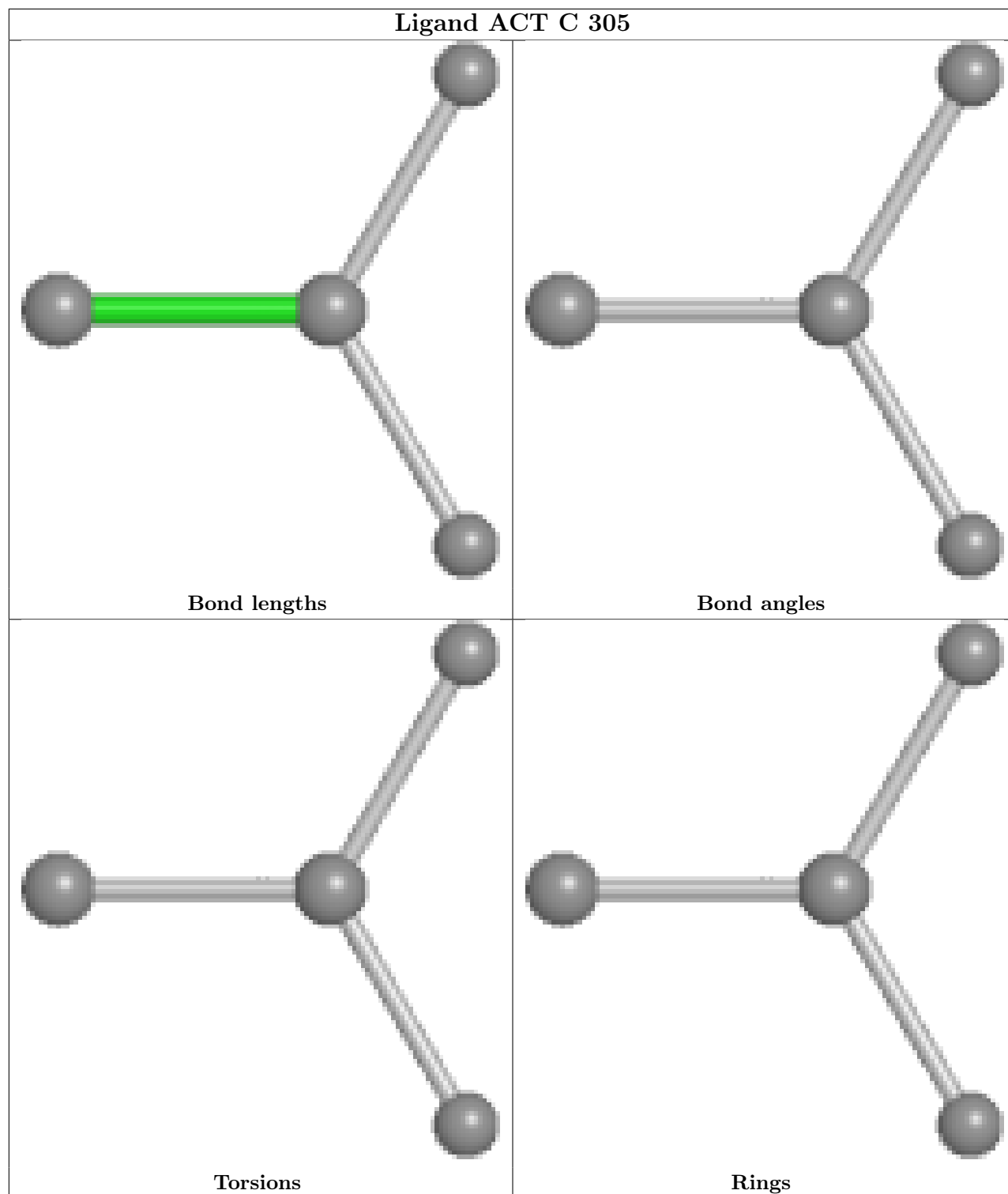












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/310 (95%)	-0.22	0 100 100	21, 27, 38, 49	0
1	B	295/310 (95%)	-0.28	1 (0%) 94 94	22, 27, 40, 46	0
1	C	295/310 (95%)	-0.21	0 100 100	21, 27, 38, 51	0
1	D	292/310 (94%)	-0.07	6 (2%) 63 65	22, 27, 38, 48	0
1	E	294/310 (94%)	-0.25	0 100 100	22, 31, 43, 51	0
1	F	295/310 (95%)	-0.09	3 (1%) 82 83	22, 31, 47, 54	0
All	All	1766/1860 (94%)	-0.19	10 (0%) 89 90	21, 28, 42, 54	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	160	GLU	3.1
1	D	131	ASP	2.8
1	D	68	GLU	2.8
1	F	288	GLU	2.7
1	F	268	SER	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KPI	E	166	14/15	0.78	0.18	24,27,36,39	0
1	KPI	C	166	14/15	0.79	0.23	21,23,35,37	0
1	KPI	D	166	14/15	0.81	0.18	21,26,37,42	0
1	KPI	B	166	14/15	0.82	0.17	20,23,32,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	KPI	A	166	14/15	0.83	0.19	22,24,38,42	0
1	KPI	F	166	14/15	0.84	0.19	22,27,41,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	MG	A	301	1/1	-0.08	0.16	30,30,30,30	0
2	MG	D	303	1/1	0.60	0.22	30,30,30,30	0
8	GOL	F	308	6/6	0.61	0.46	20,20,20,20	0
3	ACT	F	303	4/4	0.78	0.32	20,20,20,20	0
3	ACT	C	305	4/4	0.78	0.31	20,20,20,20	0
3	ACT	E	302	4/4	0.79	0.39	20,20,20,20	0
3	ACT	A	302	4/4	0.79	0.36	20,20,20,20	0
2	MG	E	301	1/1	0.79	0.30	30,30,30,30	0
5	PGE	A	304	10/10	0.80	0.32	20,20,20,20	0
2	MG	C	302	1/1	0.80	0.33	30,30,30,30	0
5	PGE	F	307	10/10	0.81	0.34	20,20,20,20	0
7	PEG	C	304	7/7	0.82	0.38	20,20,20,20	0
2	MG	B	302	1/1	0.83	0.09	30,30,30,30	0
3	ACT	F	304	4/4	0.83	0.36	20,20,20,20	0
5	PGE	B	303	10/10	0.84	0.23	20,20,20,20	0
7	PEG	D	304	7/7	0.84	0.17	20,20,20,20	0
3	ACT	F	302	4/4	0.84	0.31	20,20,20,20	0
2	MG	C	301	1/1	0.85	0.08	30,30,30,30	0
6	3VN	D	301	22/22	0.85	0.22	30,39,50,52	0
7	PEG	C	303	7/7	0.85	0.17	20,20,20,20	0
6	3VN	F	301	22/22	0.86	0.31	53,65,69,71	0
3	ACT	D	305	4/4	0.88	0.35	20,20,20,20	0
5	PGE	E	303	10/10	0.91	0.28	20,20,20,20	0
4	EDO	A	303	4/4	0.91	0.14	20,20,20,20	0
4	EDO	F	306	4/4	0.92	0.39	20,20,20,20	0
6	3VN	B	301	22/22	0.92	0.17	28,34,38,42	0

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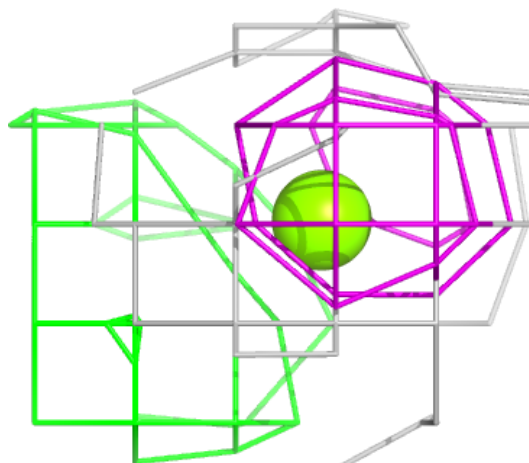
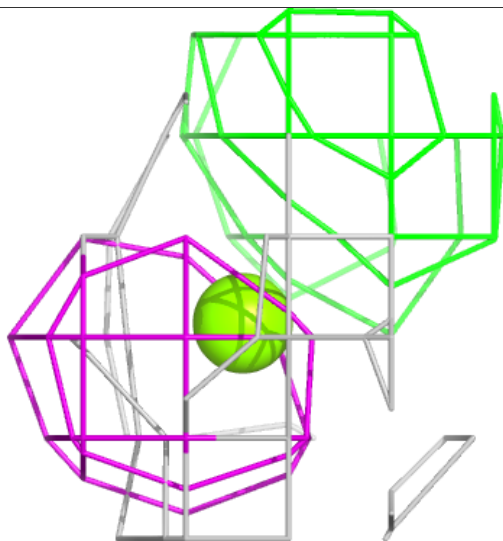
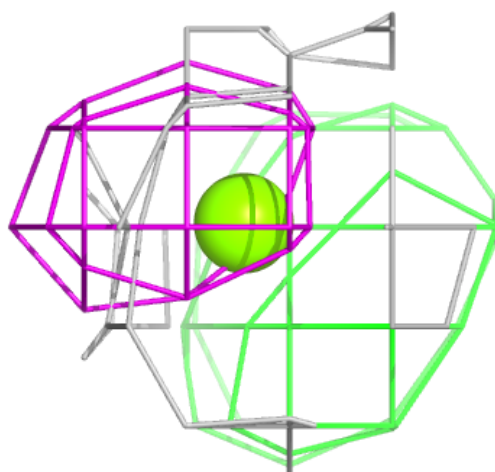
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	D	302	1/1	0.97	0.30	30,30,30,30	0
4	EDO	F	305	4/4	0.97	0.08	20,20,20,20	0

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

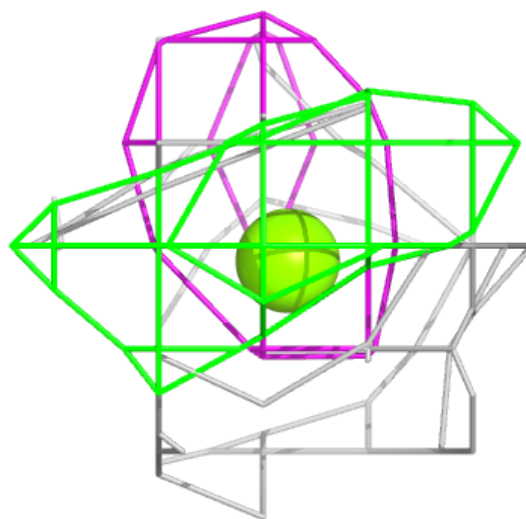
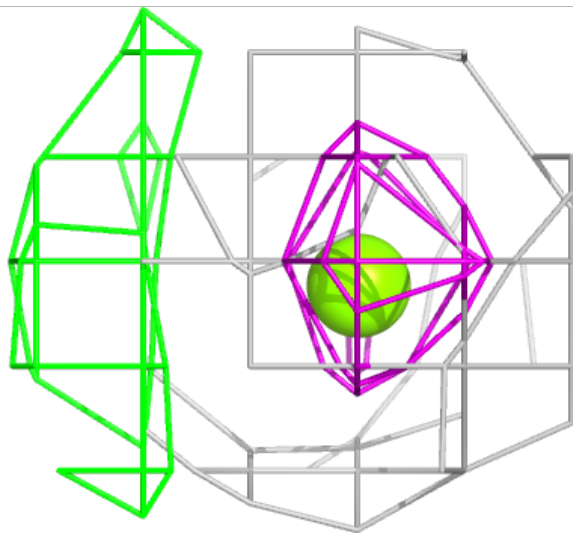
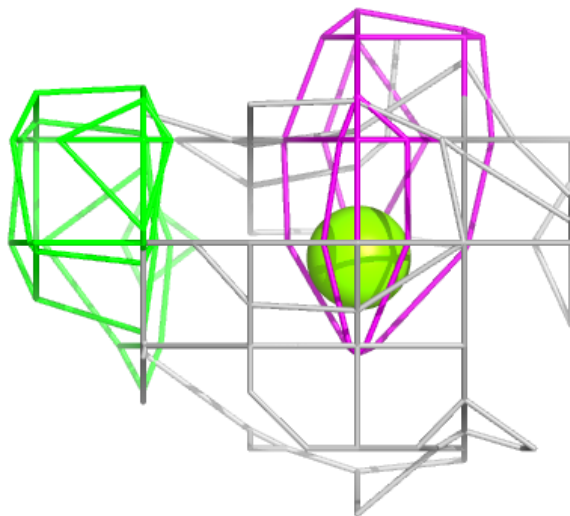
Electron density around MG A 301:

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



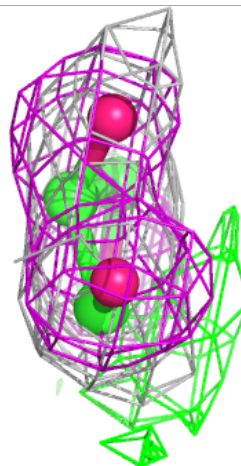
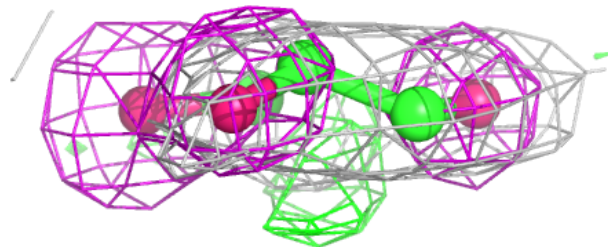
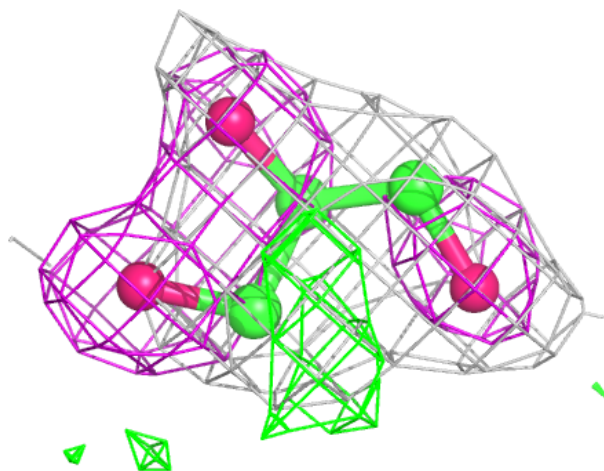
Electron density around MG D 303:

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



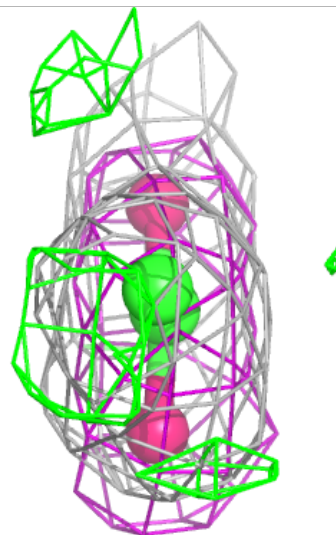
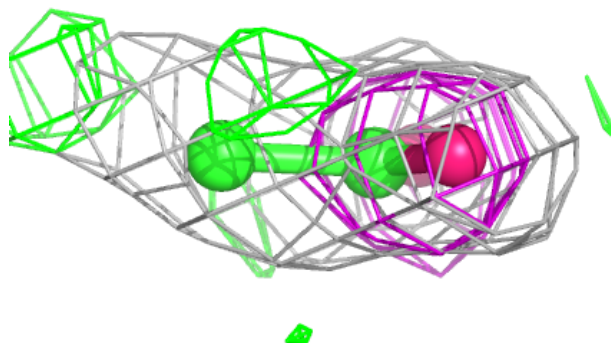
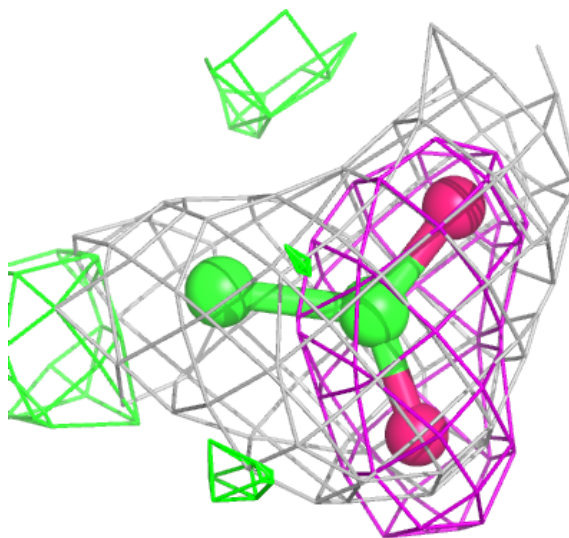
Electron density around GOL F 308:

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



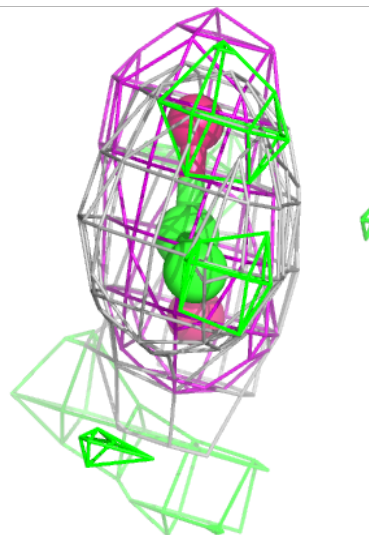
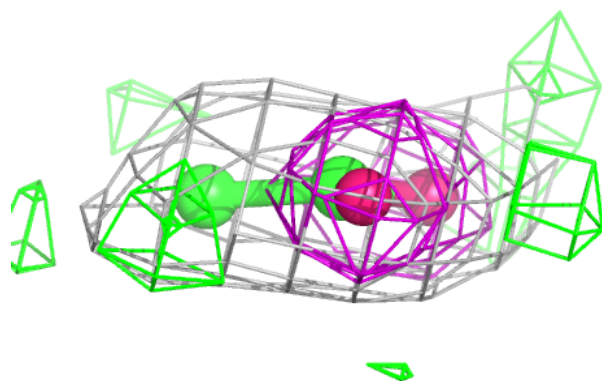
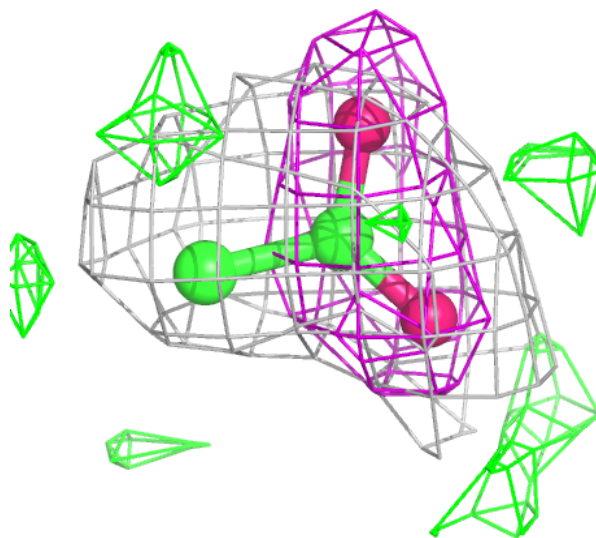
Electron density around ACT F 303:

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



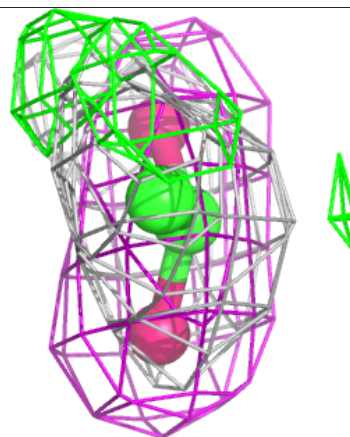
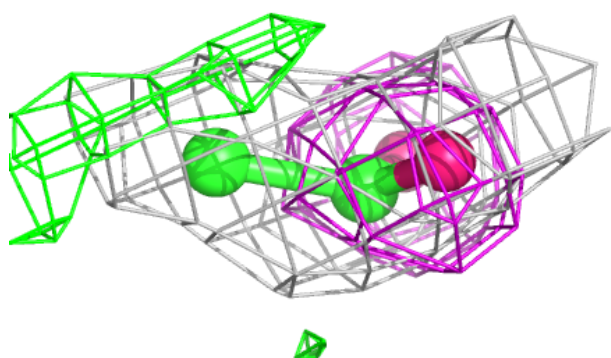
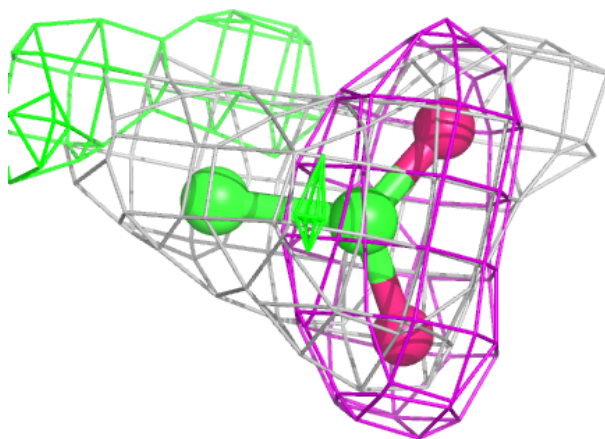
Electron density around ACT C 305:

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



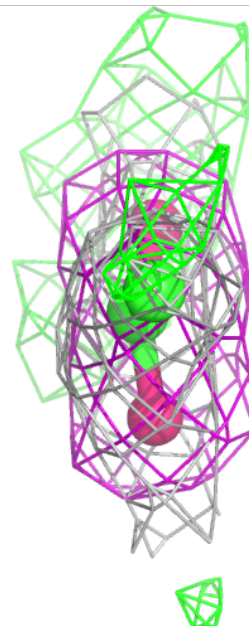
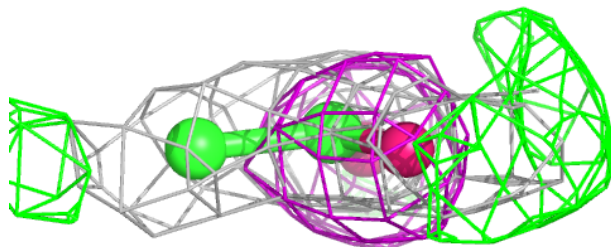
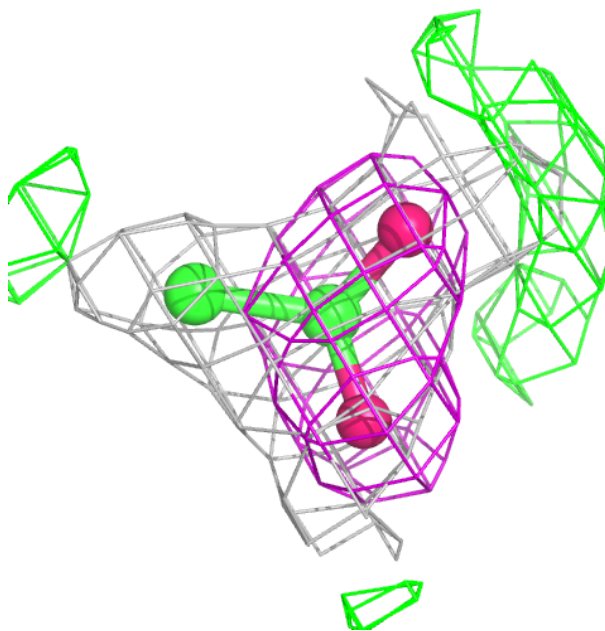
Electron density around ACT E 302:

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



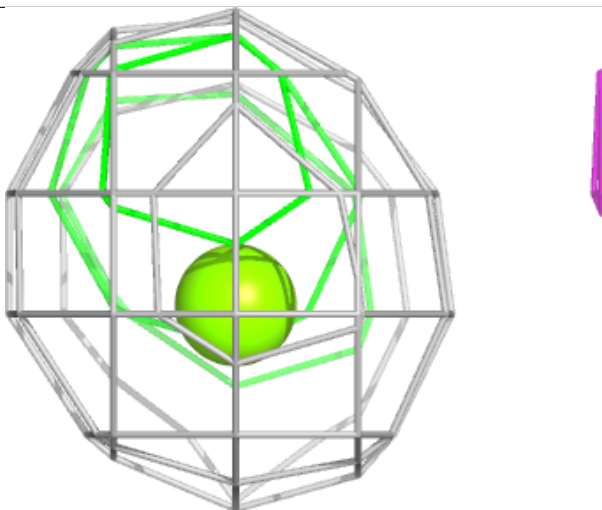
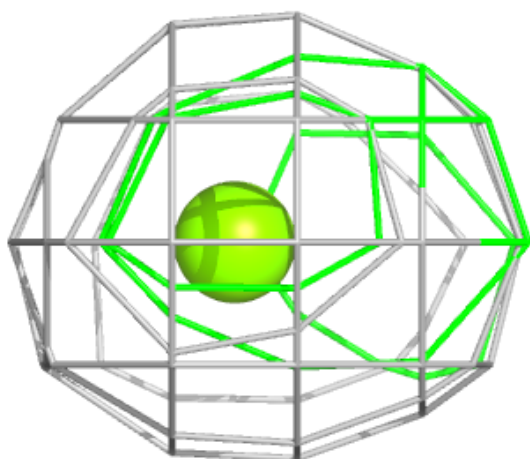
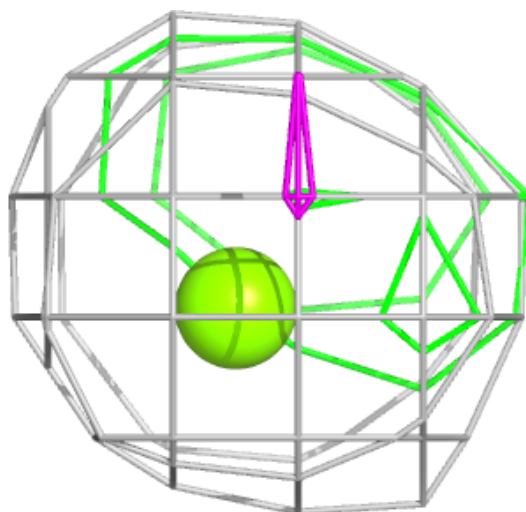
Electron density around ACT A 302:

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



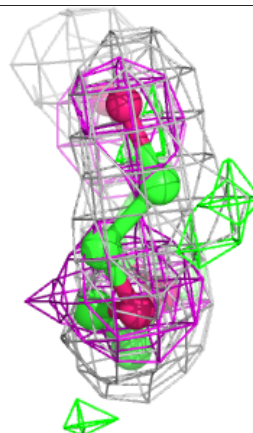
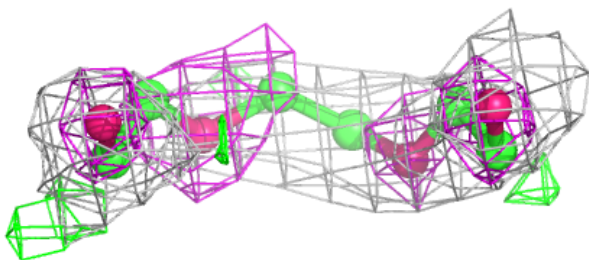
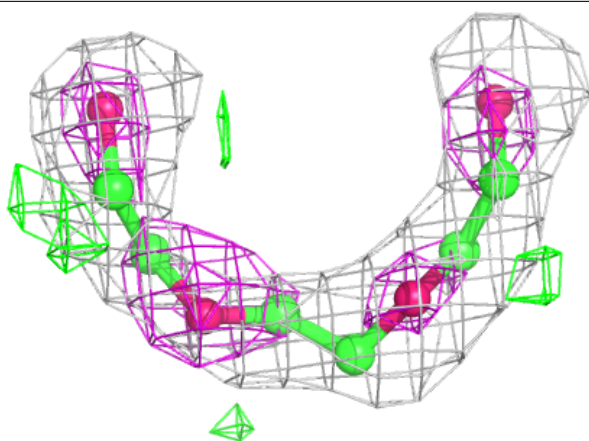
Electron density around MG E 301:

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



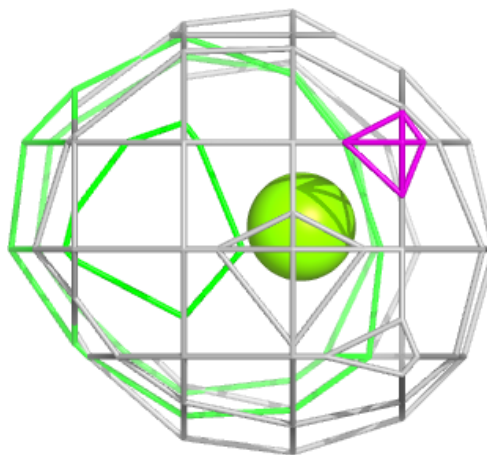
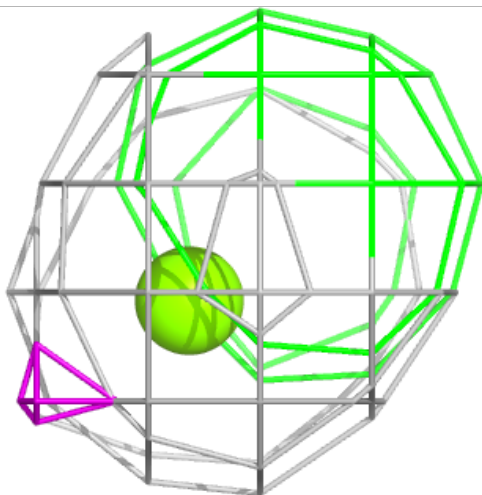
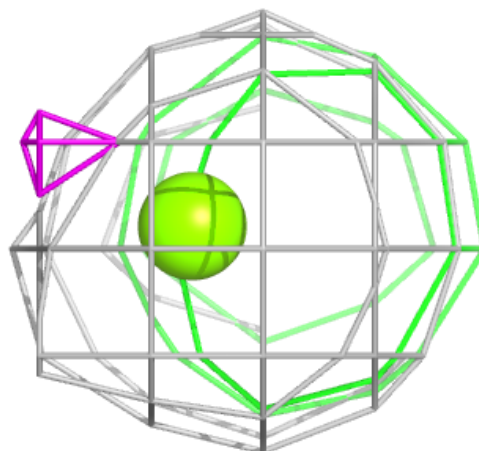
Electron density around PGE A 304:

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



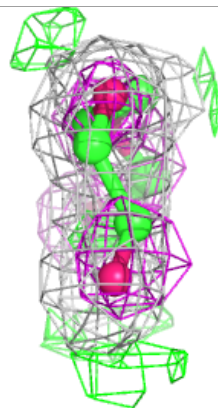
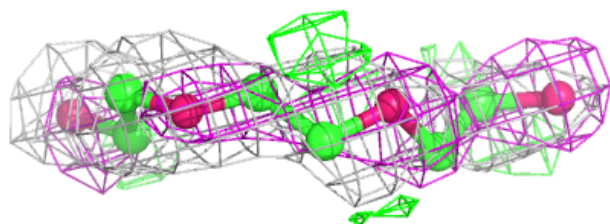
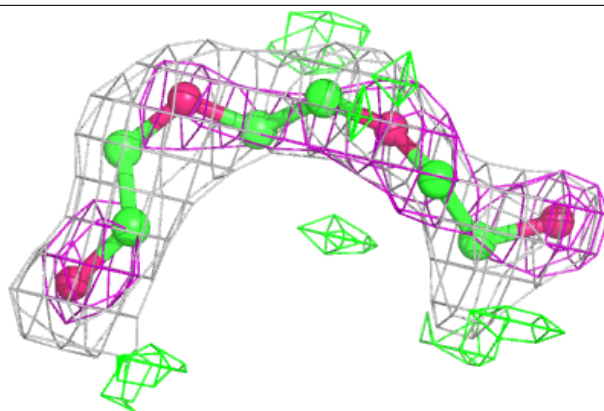
Electron density around MG C 302:

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

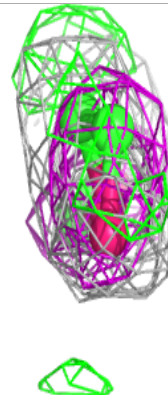
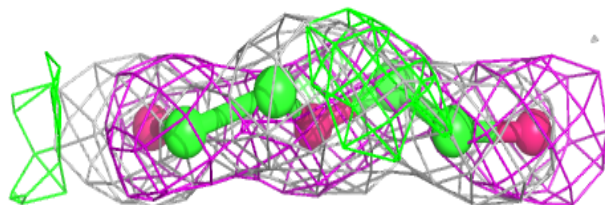
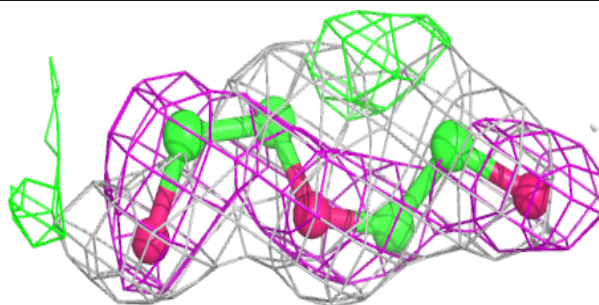


Electron density around PGE F 307:

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

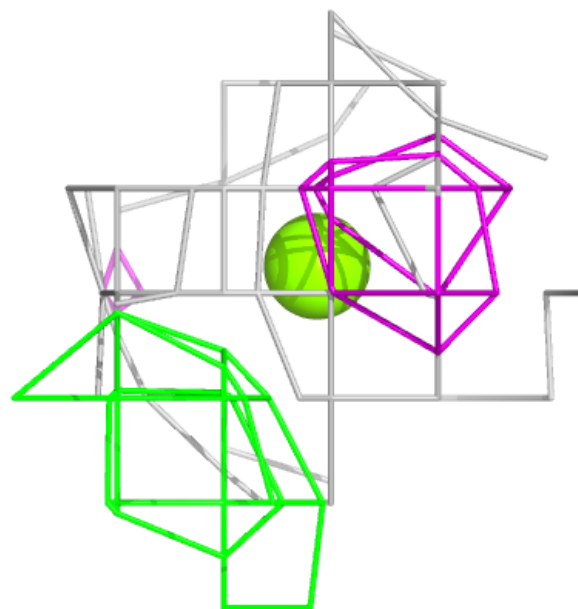
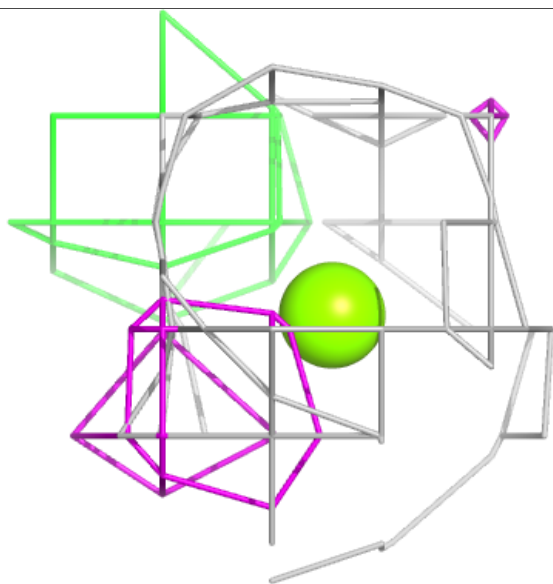
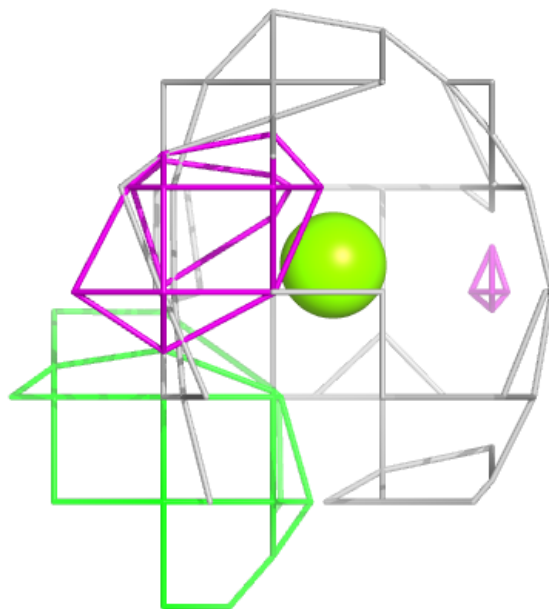
**Electron density around PEG C 304:**

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



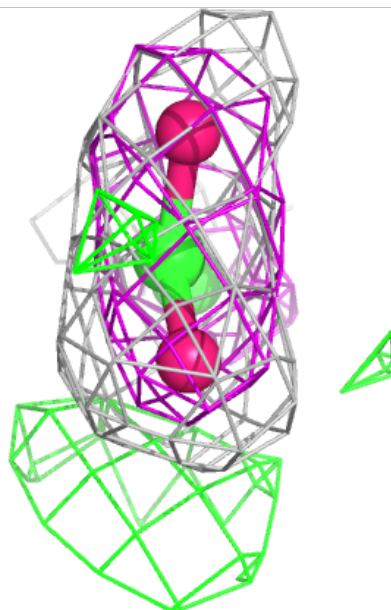
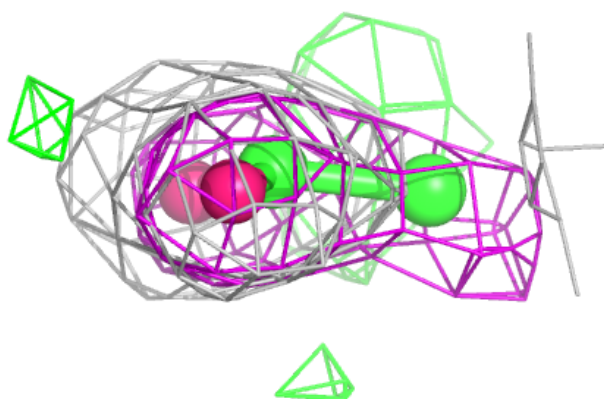
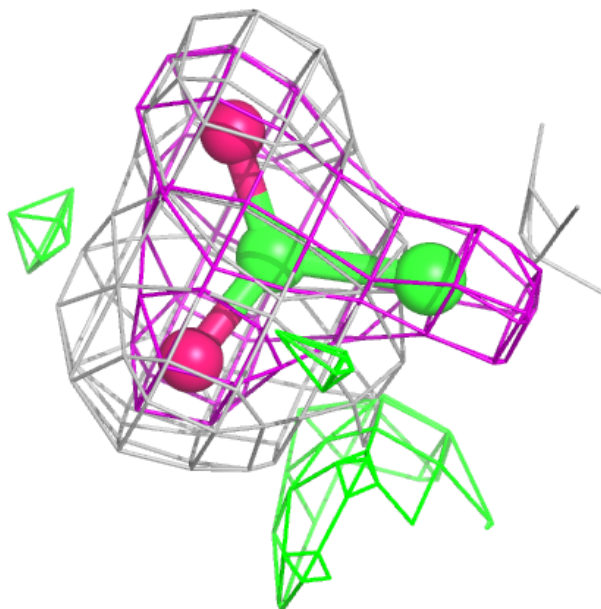
Electron density around MG B 302:

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



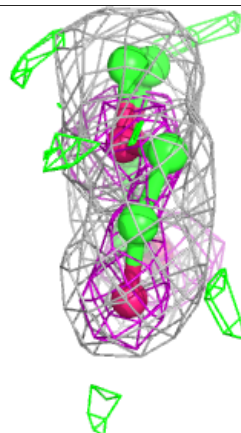
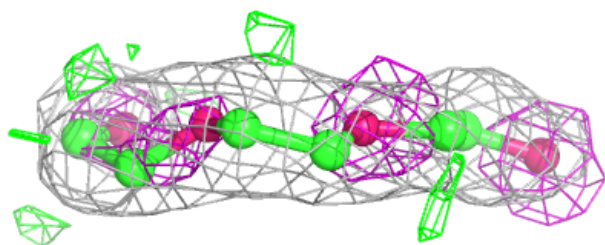
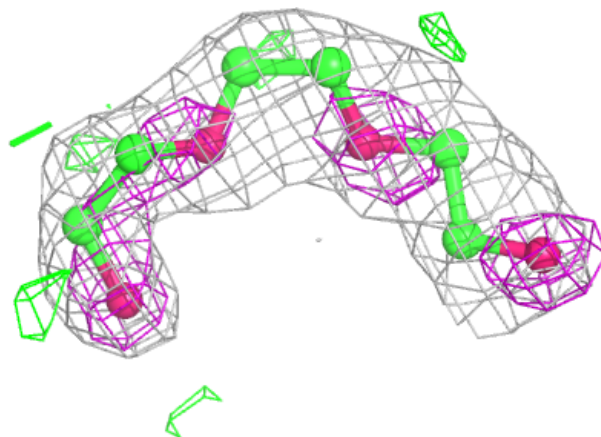
Electron density around ACT F 304:

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

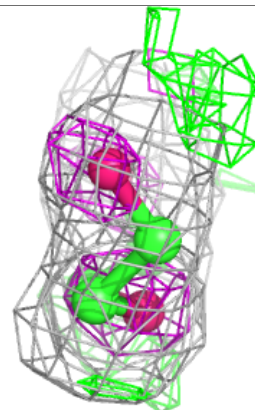
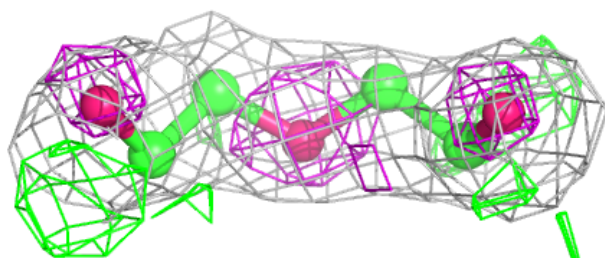
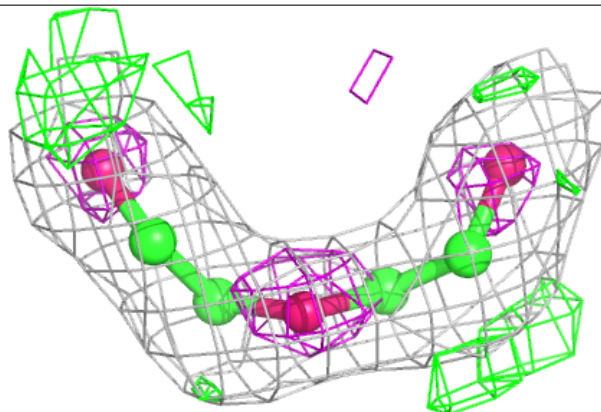


Electron density around PGE B 303:

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

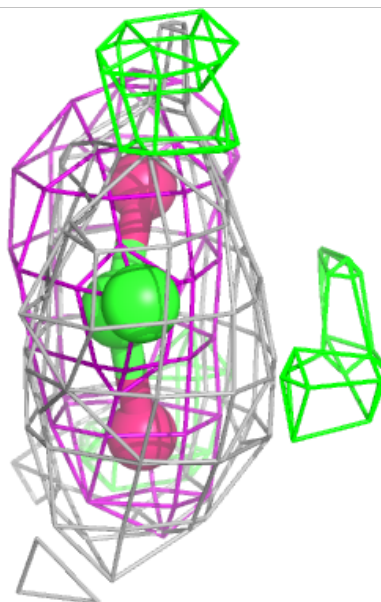
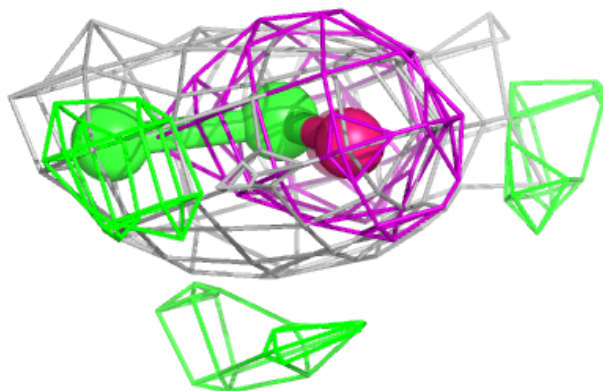
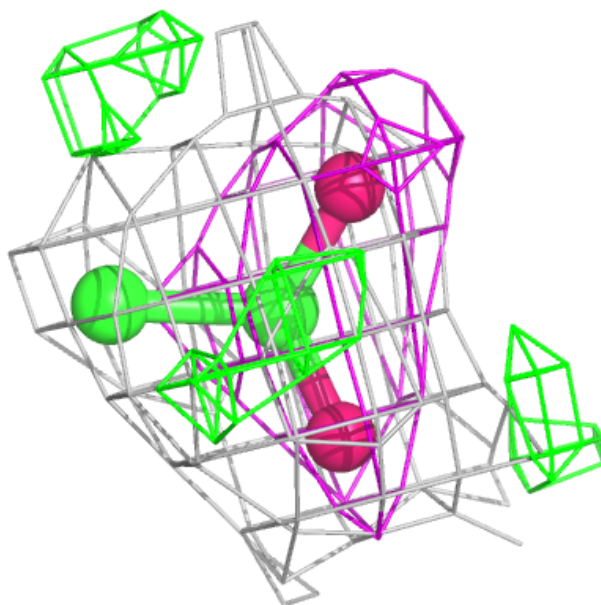
**Electron density around PEG D 304:**

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



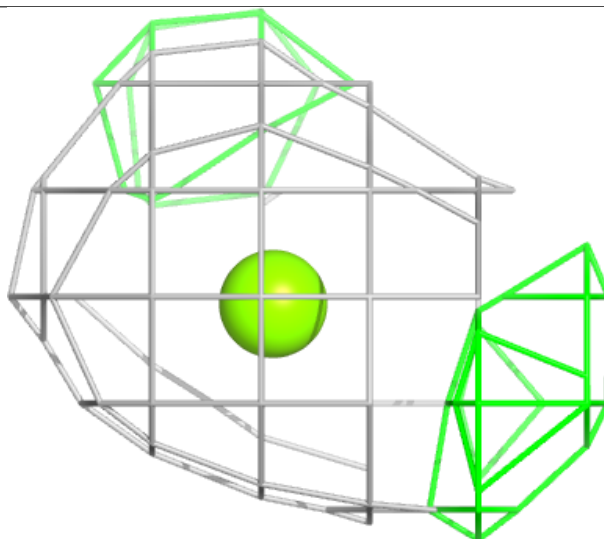
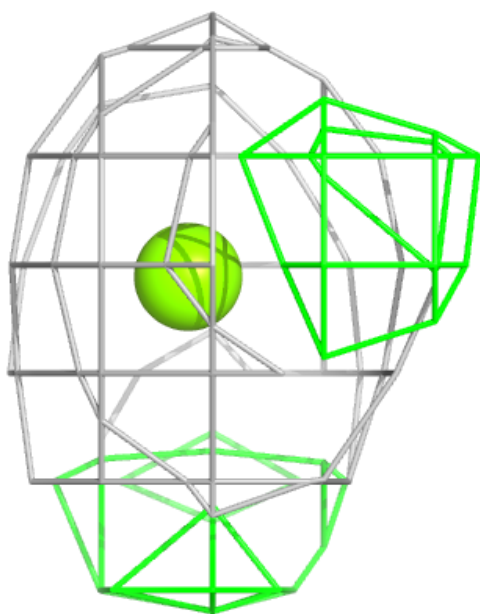
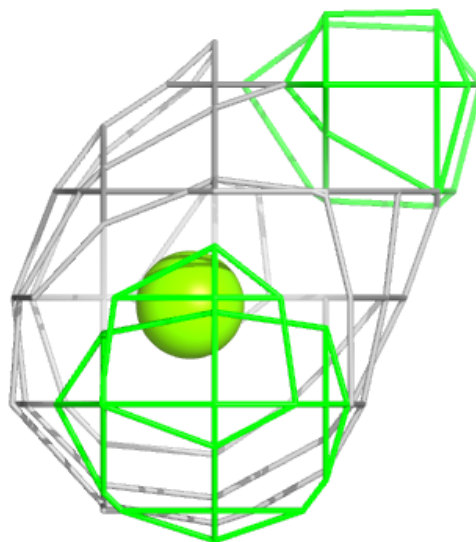
Electron density around ACT F 302:

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



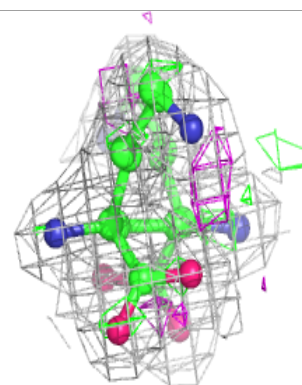
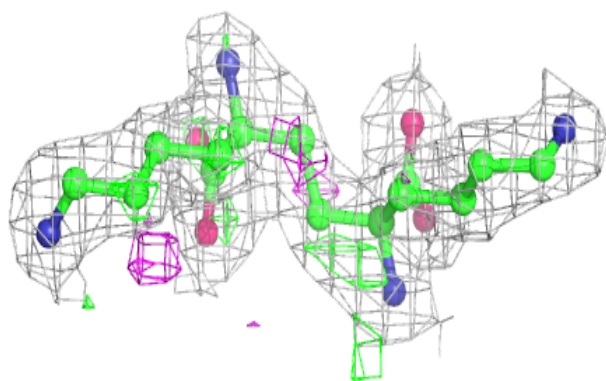
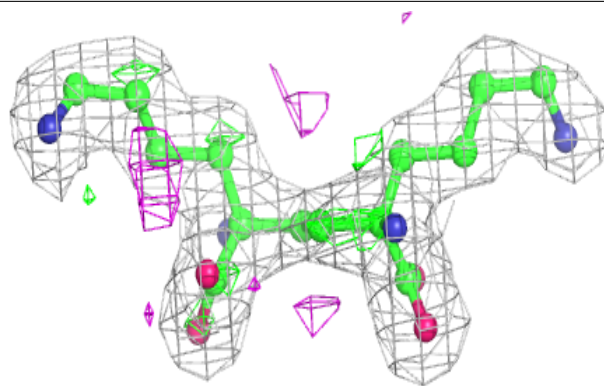
Electron density around MG C 301:

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

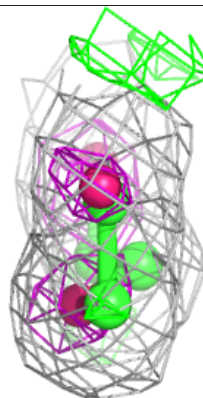
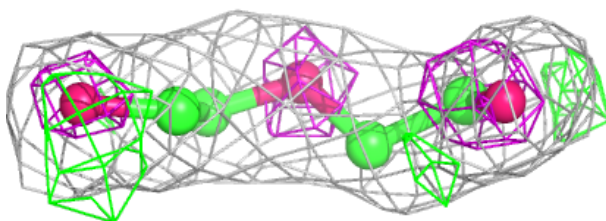
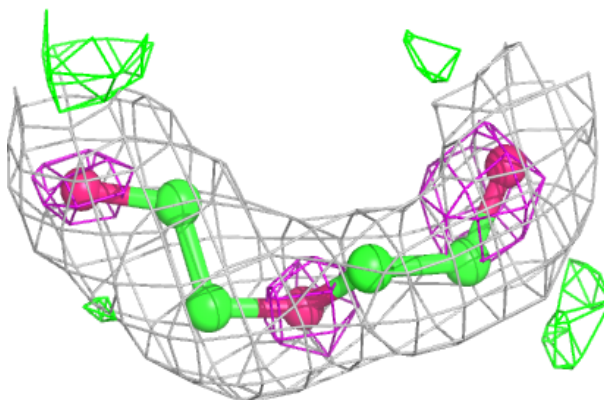


Electron density around 3VN D 301:

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

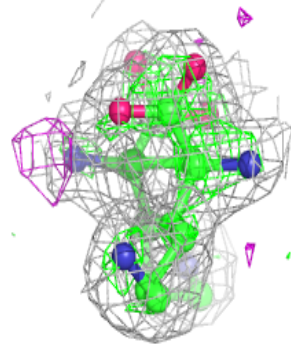
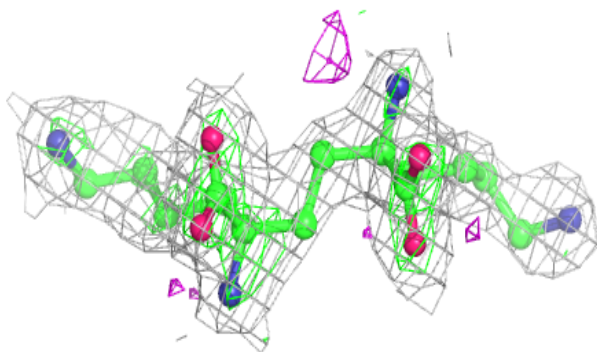
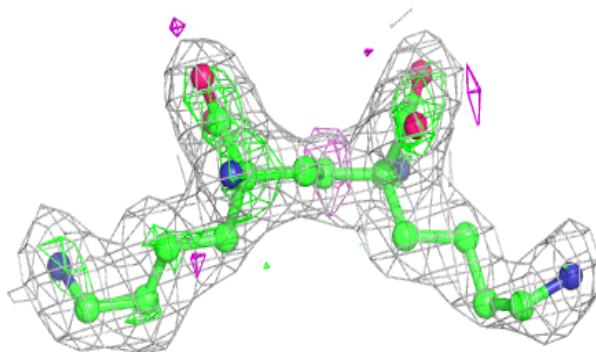
**Electron density around PEG C 303:**

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



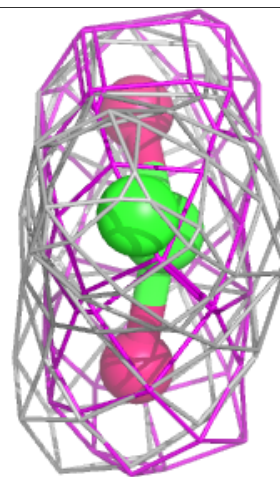
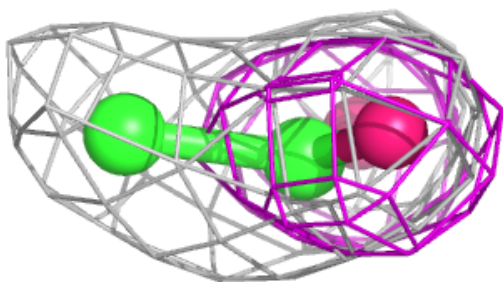
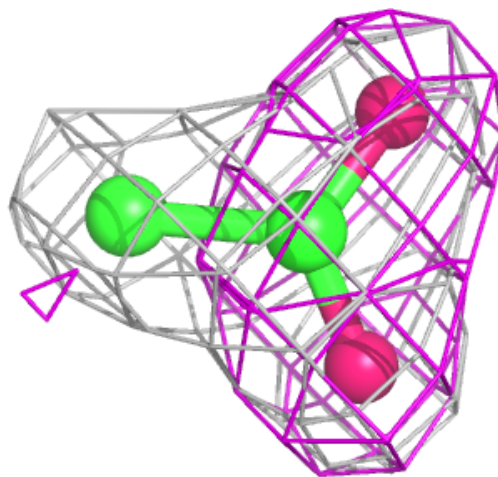
Electron density around 3VN F 301:

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



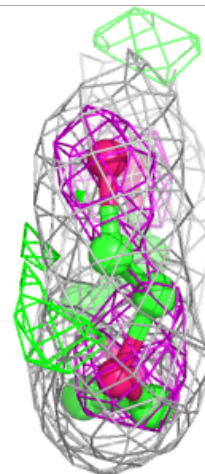
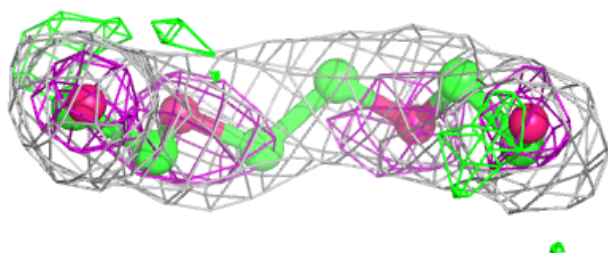
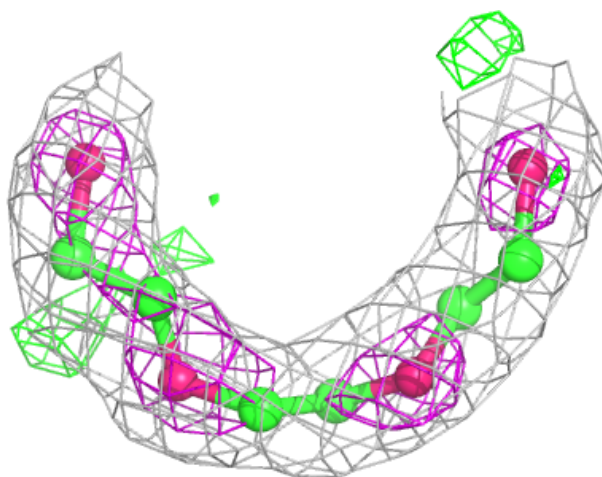
Electron density around ACT D 305:

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



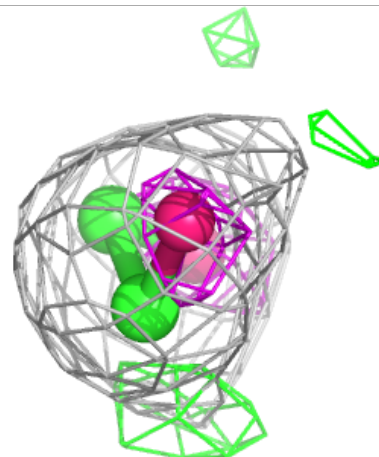
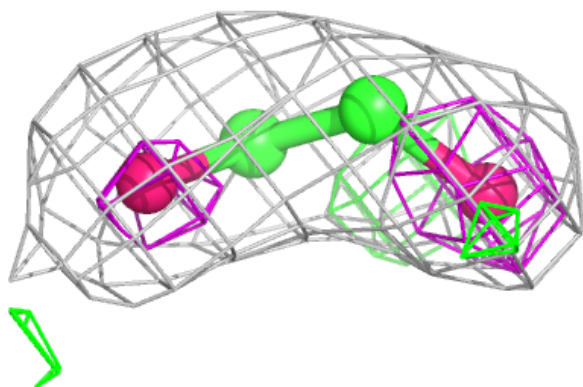
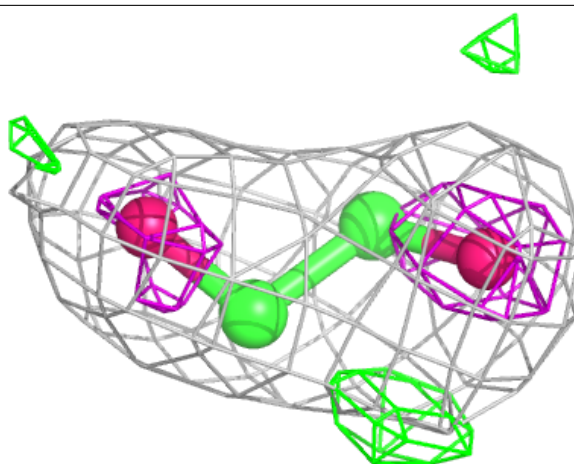
Electron density around PGE E 303:

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



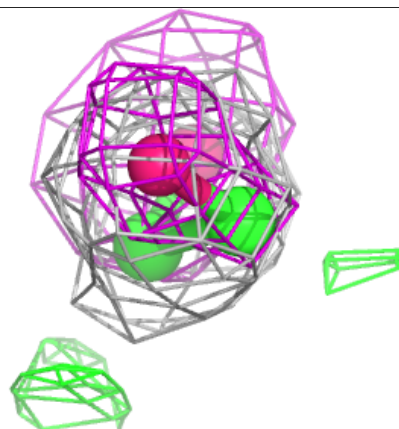
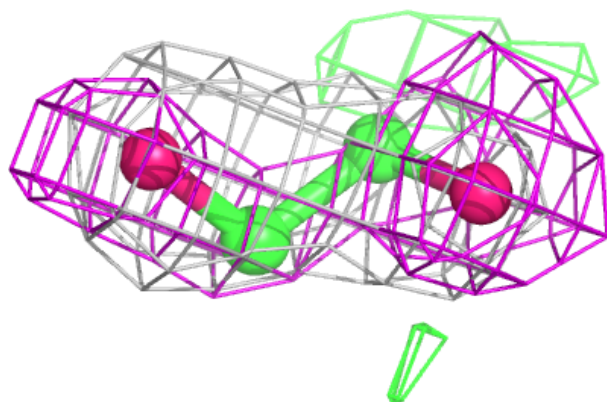
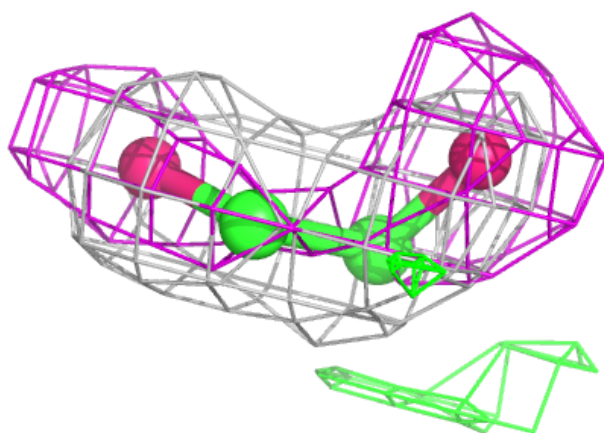
Electron density around EDO A 303:

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

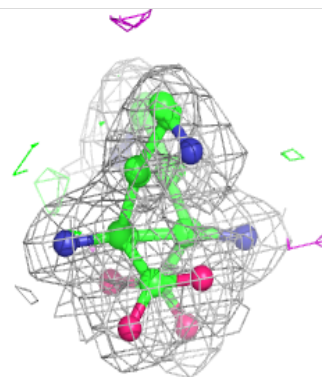
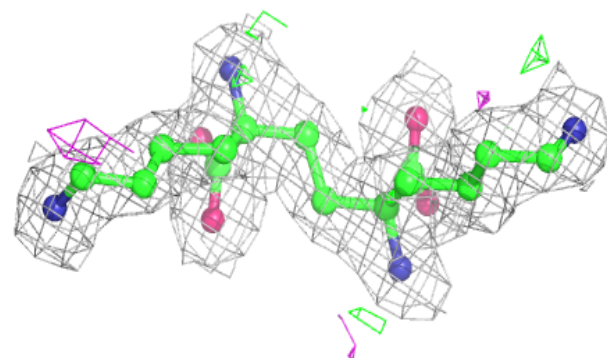
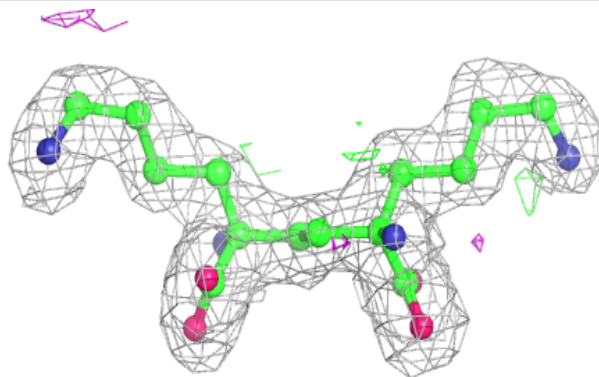


Electron density around EDO F 306:

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

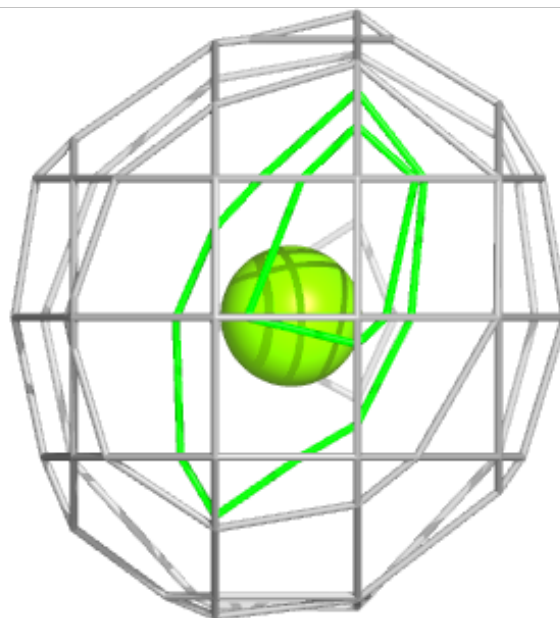
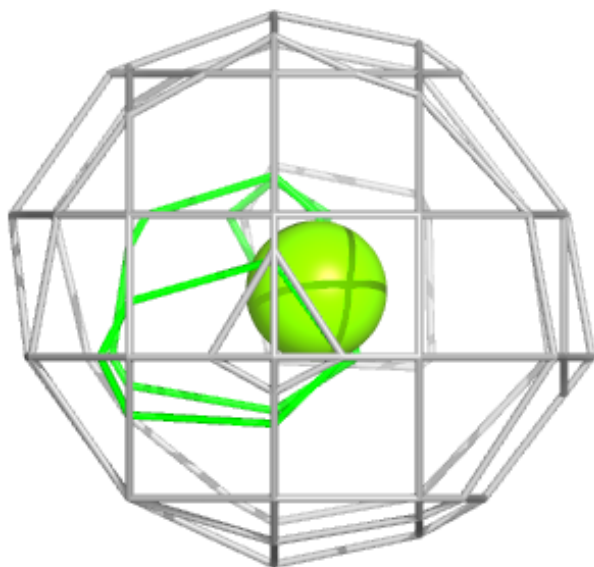
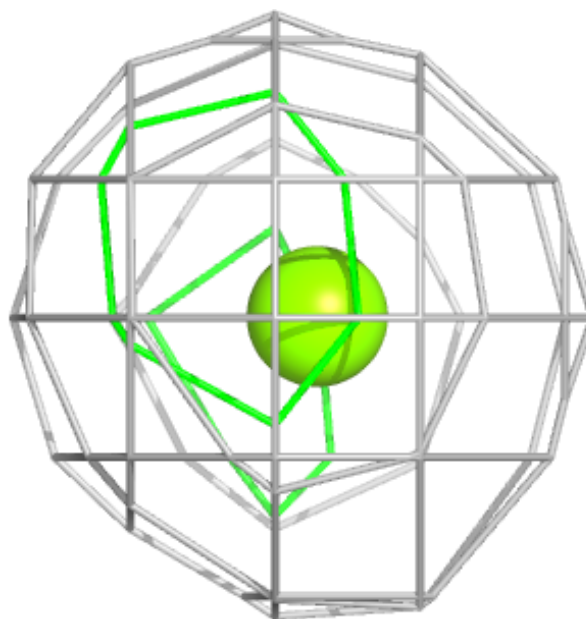
**Electron density around 3VN B 301:**

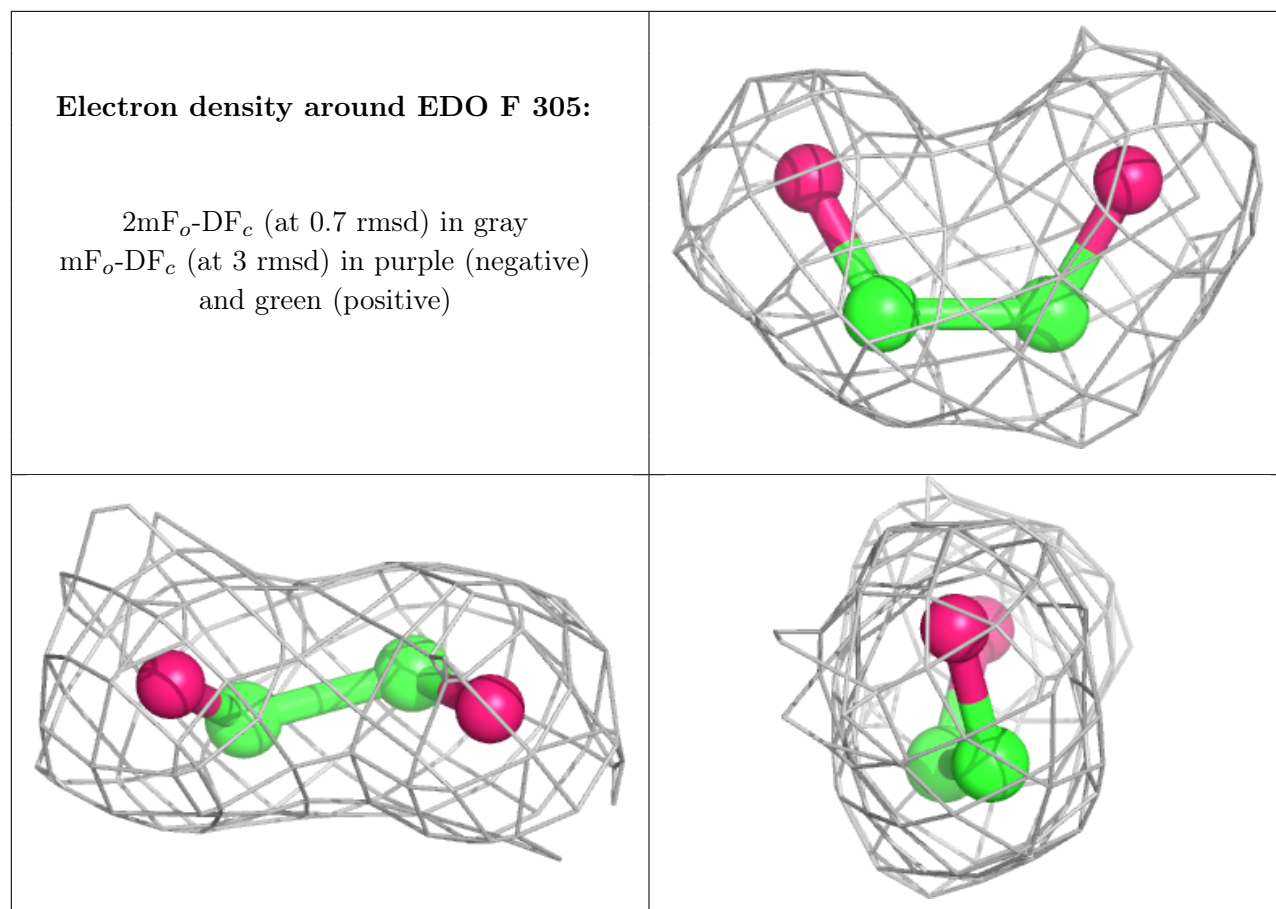
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 302:

$2mF_o-DF_c$ (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.