



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 02:13 PM JST

PDB ID : 7CAV
Title : Versatile cis-prenyltransferase MM_0014 from Methanosarcina mazei (crystal type: co-FG+DMAPP)
Authors : Unno, H.; Hemmi, H.
Deposited on : 2020-06-10
Resolution : 1.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

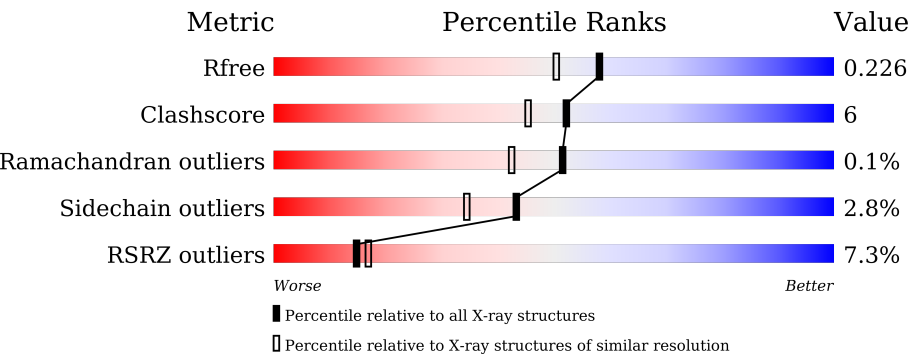
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	224	<div><div>6%</div><div>87%8%6%</div></div>
1	B	224	<div><div>6%</div><div>83%16%.</div></div>
1	C	224	<div><div>8%</div><div>77%17%. .</div></div>
1	D	224	<div><div>10%</div><div>87%7%6%</div></div>
1	E	224	<div><div>7%</div><div>78%12%. 9%</div></div>
1	F	224	<div><div>7%</div><div>81%15%. .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	224	<div> <div></div> <div>4%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	H	224	<div> <div></div> <div>7%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>

2 Entry composition

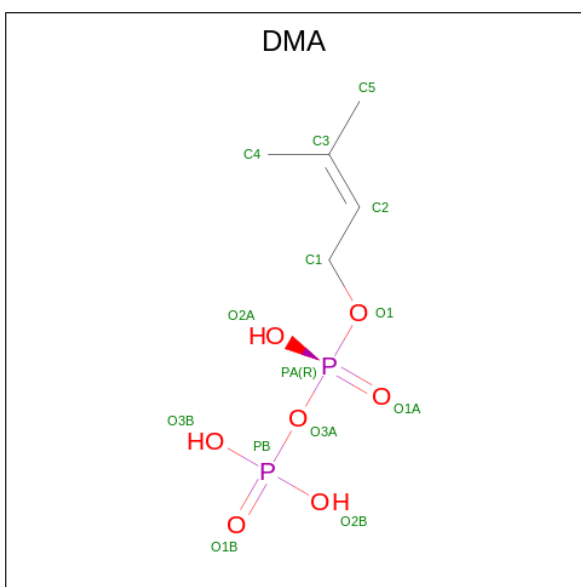
There are 7 unique types of molecules in this entry. The entry contains 14653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cis-prenyltransferase MM_0014.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1727	1117	293	310	7			
1	B	222	Total	C	N	O	S	0	0	0
			1801	1161	306	327	7			
1	C	217	Total	C	N	O	S	0	0	0
			1761	1135	300	320	6			
1	D	211	Total	C	N	O	S	0	0	0
			1718	1112	292	308	6			
1	E	204	Total	C	N	O	S	0	0	0
			1670	1084	285	295	6			
1	F	216	Total	C	N	O	S	0	0	0
			1753	1131	299	317	6			
1	G	219	Total	C	N	O	S	0	0	0
			1780	1149	302	322	7			
1	H	206	Total	C	N	O	S	0	0	0
			1686	1092	287	301	6			

- Molecule 2 is DIMETHYLALLYL DIPHOSPHATE (three-letter code: DMA) (formula: $C_5H_{12}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	7	2		
2	A	1	Total	C	O	P	0	0
			14	5	7	2		
2	C	1	Total	C	O	P	0	0
			14	5	7	2		
2	C	1	Total	C	O	P	0	0
			14	5	7	2		
2	D	1	Total	C	O	P	0	0
			14	5	7	2		
2	D	1	Total	C	O	P	0	0
			14	5	7	2		
2	E	1	Total	C	O	P	0	0
			14	5	7	2		
2	E	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

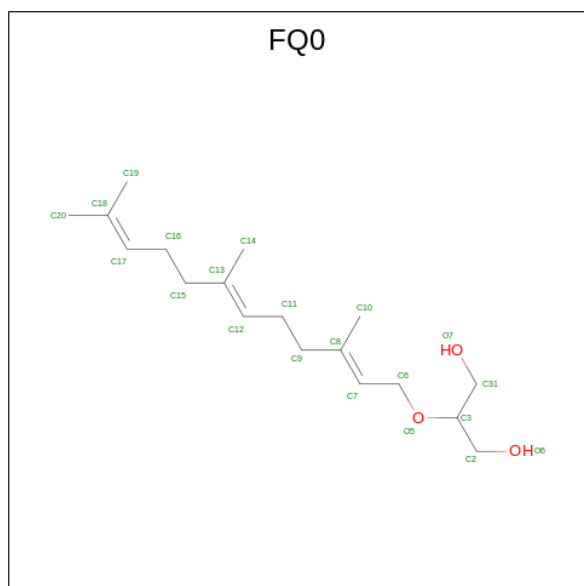
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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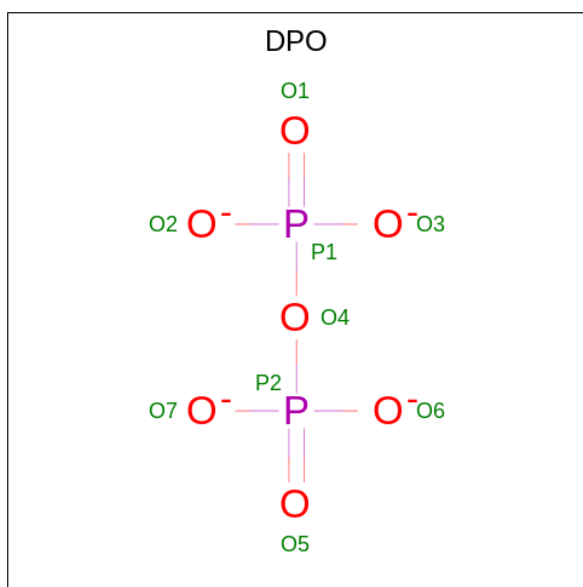
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propane-1,3-diol (three-letter code: FQ0) (formula: C₁₈H₃₂O₃) (labeled as "Ligand of Interest" by depositor).



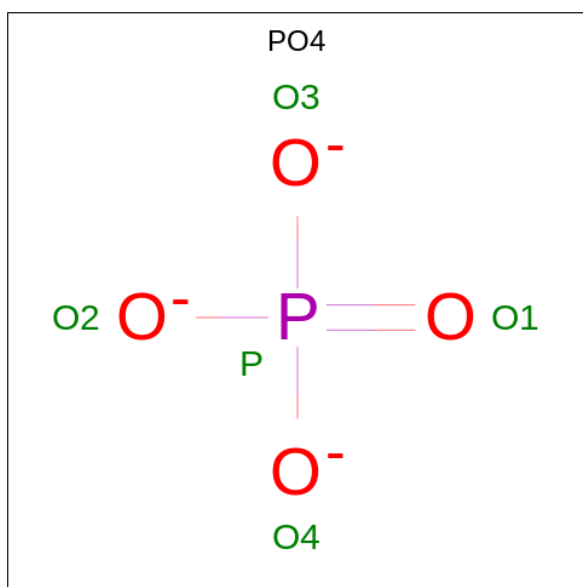
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			21	18	3		
4	F	1	Total	C	O	0	0
			21	18	3		
4	G	1	Total	C	O	0	0
			21	18	3		
4	H	1	Total	C	O	0	0
			21	18	3		

- Molecule 5 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	B	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	G	1	Total	O	P	0	0
			9	7	2		
5	G	1	Total	O	P	0	0
			9	7	2		
5	H	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	P	0	0
			5	4	1		

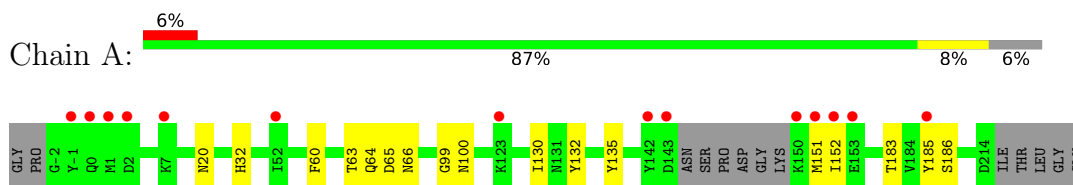
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	69	Total	O	0	0
			69	69		
7	C	55	Total	O	0	0
			55	55		
7	D	48	Total	O	0	0
			48	48		
7	E	42	Total	O	0	0
			42	42		
7	F	49	Total	O	0	0
			49	49		
7	G	78	Total	O	0	0
			78	78		
7	H	60	Total	O	0	0
			60	60		

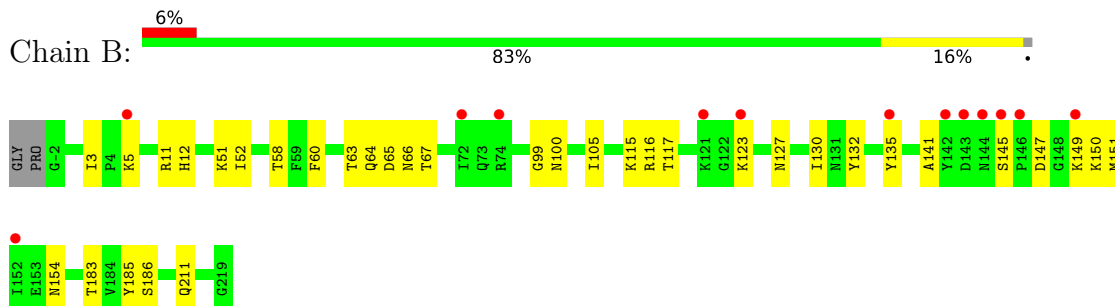
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

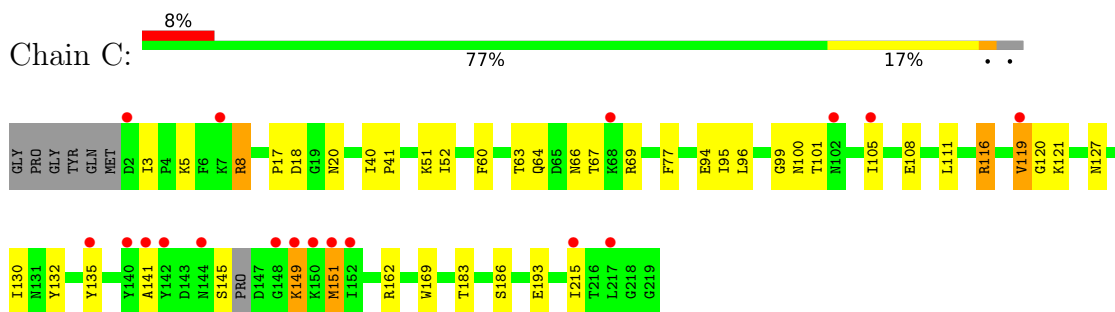
- Molecule 1: cis-prenyltransferase MM_0014



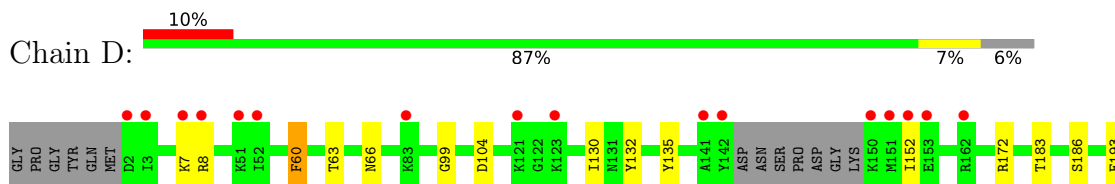
- Molecule 1: cis-prenyltransferase MM_0014

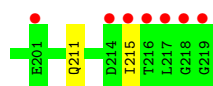


- Molecule 1: cis-prenyltransferase MM_0014

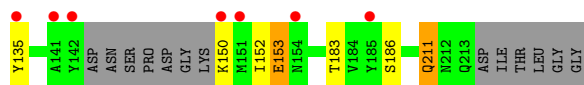
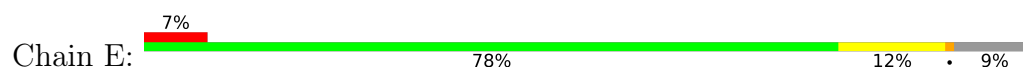


- Molecule 1: cis-prenyltransferase MM_0014

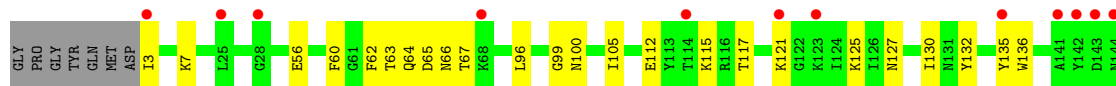
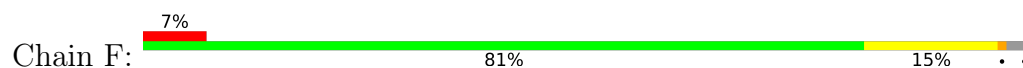




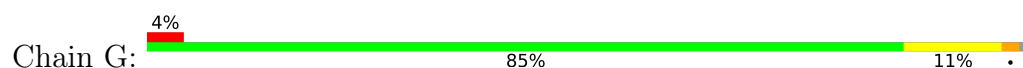
- Molecule 1: cis-prenyltransferase MM_0014



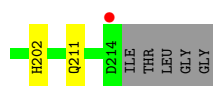
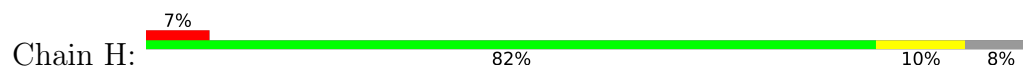
- Molecule 1: cis-prenyltransferase MM_0014



- Molecule 1: cis-prenyltransferase MM_0014



- Molecule 1: cis-prenyltransferase MM_0014



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.85Å 98.91Å 193.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 1.91 47.92 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.92-1.91) 99.8 (47.92-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	74.30 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.220 0.204 , 0.226	Depositor DCC
R_{free} test set	7541 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14653	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3700e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMA, FQ0, PO4, DPO

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	0.64	0/1769	0.76	0/2390
1	B	0.66	0/1845	0.75	0/2493
1	C	0.64	0/1802	0.73	0/2433
1	D	0.63	0/1759	0.74	0/2376
1	E	0.63	0/1711	0.70	0/2312
1	F	0.64	0/1794	0.73	0/2422
1	G	0.64	0/1822	0.74	0/2459
1	H	0.64	0/1727	0.70	0/2334
All	All	0.64	0/14229	0.73	0/19219

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1727	0	1727	14	0
1	B	1801	0	1801	21	0
1	C	1761	0	1761	36	0
1	D	1718	0	1726	12	0
1	E	1670	0	1683	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1753	0	1757	24	0
1	G	1780	0	1782	18	0
1	H	1686	0	1691	14	0
2	A	28	0	18	5	0
2	C	28	0	18	4	0
2	D	28	0	18	1	0
2	E	28	0	18	6	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
4	B	21	0	0	0	0
4	F	21	0	0	0	0
4	G	21	0	0	0	0
4	H	21	0	0	2	0
5	B	18	0	0	0	0
5	F	18	0	0	0	0
5	G	18	0	0	0	0
5	H	9	0	0	1	0
6	G	5	0	0	0	0
7	A	84	0	0	1	0
7	B	69	0	0	1	0
7	C	55	0	0	2	0
7	D	48	0	0	1	0
7	E	42	0	0	2	0
7	F	49	0	0	0	0
7	G	78	0	0	2	0
7	H	60	0	0	0	0
All	All	14653	0	14000	155	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.

All (155) 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:B:116:ARG:HH22	1:B:127:ASN:HD21	1.20	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:ARG:HG2	1:F:172:ARG:HH21	1.39	0.87
1:E:3:ILE:HG23	1:E:4:PRO:HD3	1.69	0.75
1:C:108:GLU:HA	1:C:111:LEU:HD23	1.71	0.70
1:E:116:ARG:HH21	1:E:127:ASN:HD21	1.40	0.69
1:G:122:GLY:O	1:G:123:LYS:HG3	1.93	0.68
1:E:115:LYS:O	1:E:117:THR:HG23	1.94	0.68
1:A:20:ASN:OD1	2:A:302:DMA:H12	1.93	0.68
1:C:94:GLU:OE1	1:C:116:ARG:CG	2.42	0.67
1:F:172:ARG:HH21	1:F:172:ARG:CG	2.08	0.67
1:C:66:ASN:HD21	2:C:301:DMA:H42	1.61	0.66
1:C:94:GLU:HG3	1:C:121:LYS:HA	1.76	0.66
1:G:7:LYS:H	1:G:211:GLN:HE22	1.44	0.65
1:C:94:GLU:OE1	1:C:116:ARG:HG2	1.97	0.64
1:E:99:GLY:HA3	1:E:130:ILE:O	1.97	0.64
1:G:63:THR:H	1:G:66:ASN:HD22	1.45	0.63
1:E:3:ILE:CG2	1:E:4:PRO:HD3	2.30	0.62
1:D:63:THR:H	1:D:66:ASN:HD22	1.48	0.61
1:G:205:LYS:HA	1:G:205:LYS:HE2	1.82	0.60
1:A:63:THR:H	1:A:66:ASN:HD22	1.47	0.60
1:C:69:ARG:NH1	2:C:302:DMA:O1A	2.34	0.60
1:C:94:GLU:CG	1:C:121:LYS:HA	2.31	0.59
1:B:115:LYS:O	1:B:117:THR:HG23	2.01	0.59
1:F:63:THR:HA	1:F:132:TYR:O	2.03	0.58
1:H:99:GLY:HA3	1:H:130:ILE:O	2.02	0.58
1:A:20:ASN:OD1	2:A:302:DMA:C1	2.51	0.58
1:E:135:TYR:OH	1:F:149:LYS:HA	2.03	0.58
1:H:96:LEU:HB3	1:H:127:ASN:HD22	1.68	0.58
1:F:64:GLN:HE22	1:F:100:ASN:HD22	1.51	0.58
1:C:67:THR:HG21	1:C:105:ILE:HG21	1.85	0.58
1:B:63:THR:HA	1:B:132:TYR:O	2.04	0.57
1:B:145:SER:OG	1:B:154:ASN:HB2	2.05	0.57
1:H:193:GLU:HG3	1:H:202:HIS:CE1	2.40	0.56
1:H:63:THR:HA	1:H:132:TYR:O	2.05	0.56
1:B:116:ARG:NH2	1:B:127:ASN:HD21	1.97	0.56
1:A:63:THR:H	1:A:66:ASN:ND2	2.03	0.56
1:E:7:LYS:H	1:E:211:GLN:HE22	1.53	0.55
1:G:63:THR:H	1:G:66:ASN:ND2	2.04	0.55
1:D:99:GLY:HA3	1:D:130:ILE:O	2.06	0.55
1:B:141:ALA:HB1	1:B:151:MET:HG2	1.89	0.55
1:A:185:TYR:OH	1:B:65:ASP:OD2	2.22	0.54
1:F:64:GLN:NE2	1:F:100:ASN:HD22	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLU:HA	1:C:111:LEU:CD2	2.37	0.53
1:E:63:THR:HA	1:E:132:TYR:O	2.08	0.53
2:E:302:DMA:H51	7:E:431:HOH:O	2.08	0.53
1:F:99:GLY:HA3	1:F:130:ILE:O	2.09	0.53
1:G:135:TYR:CE2	1:H:152:ILE:HG21	2.44	0.53
1:D:63:THR:H	1:D:66:ASN:ND2	2.06	0.53
1:E:63:THR:H	1:E:66:ASN:ND2	2.07	0.53
1:E:96:LEU:HB3	1:E:127:ASN:HD22	1.73	0.53
1:E:150:LYS:HG3	1:E:153:GLU:HB2	1.91	0.53
1:C:17:PRO:HD2	2:C:301:DMA:H52	1.91	0.52
1:C:64:GLN:HE22	1:C:100:ASN:HD22	1.58	0.52
1:C:3:ILE:HG21	1:C:52:ILE:CG2	2.40	0.52
1:D:60:PHE:CD2	2:D:302:DMA:H53	2.44	0.52
1:G:63:THR:HA	1:G:132:TYR:O	2.10	0.52
1:F:7:LYS:HA	1:F:7:LYS:HE2	1.92	0.52
1:G:67:THR:HG21	1:G:105:ILE:HG21	1.92	0.52
1:H:64:GLN:HE22	1:H:136:TRP:HB2	1.75	0.52
1:C:215:ILE:O	1:F:112:GLU:HA	2.10	0.51
1:F:152:ILE:HD13	1:F:152:ILE:O	2.09	0.51
1:B:116:ARG:HH22	1:B:127:ASN:ND2	1.97	0.51
1:H:116:ARG:HH21	1:H:127:ASN:HD21	1.56	0.51
1:F:183:THR:HA	1:F:186:SER:OG	2.11	0.51
1:G:150:LYS:NZ	7:G:402:HOH:O	2.38	0.51
1:C:64:GLN:NE2	1:C:100:ASN:HD22	2.08	0.51
1:G:99:GLY:HA3	1:G:130:ILE:O	2.10	0.51
1:C:94:GLU:HG2	1:C:120:GLY:O	2.11	0.50
1:D:7:LYS:H	1:D:211:GLN:HE22	1.60	0.50
1:F:67:THR:HG21	1:F:105:ILE:HG21	1.94	0.50
1:B:3:ILE:HD12	1:B:51:LYS:HG2	1.94	0.50
2:E:302:DMA:C5	7:E:431:HOH:O	2.60	0.49
1:E:116:ARG:HH21	1:E:127:ASN:ND2	2.09	0.49
2:A:301:DMA:H43	2:A:302:DMA:C2	2.42	0.49
1:B:12:HIS:HE1	1:B:58:THR:OG1	1.95	0.49
1:D:63:THR:HA	1:D:132:TYR:O	2.12	0.49
1:A:183:THR:HA	1:A:186:SER:OG	2.13	0.49
1:B:63:THR:H	1:B:66:ASN:ND2	2.11	0.48
1:C:3:ILE:HD12	1:C:51:LYS:HD2	1.95	0.48
1:E:17:PRO:HD2	2:E:301:DMA:H52	1.95	0.48
1:B:11:ARG:NH1	1:C:101:THR:O	2.46	0.48
1:C:96:LEU:HB3	1:C:127:ASN:HD22	1.79	0.48
1:E:12:HIS:HE1	1:E:58:THR:OG1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:HA3	1:A:130:ILE:O	2.13	0.48
1:B:67:THR:HG21	1:B:105:ILE:HG21	1.95	0.48
1:E:183:THR:HA	1:E:186:SER:OG	2.14	0.48
4:H:302:FQ0:C31	5:H:303:DPO:O7	2.62	0.48
1:E:63:THR:H	1:E:66:ASN:HD22	1.61	0.47
1:G:214:ASP:HB3	1:G:217:LEU:HD22	1.96	0.47
1:C:63:THR:HA	1:C:132:TYR:O	2.13	0.47
1:G:149:LYS:HA	1:H:135:TYR:OH	2.15	0.47
1:C:99:GLY:HA3	1:C:130:ILE:O	2.14	0.47
1:F:7:LYS:H	1:F:211:GLN:HE22	1.62	0.47
1:H:67:THR:HG21	1:H:105:ILE:HG21	1.95	0.46
7:B:416:HOH:O	1:C:119:VAL:HG13	2.13	0.46
1:A:32:HIS:HD2	7:A:480:HOH:O	1.98	0.46
1:H:89:ALA:O	1:H:119:VAL:HG11	2.14	0.46
1:C:8:ARG:HH12	1:C:215:ILE:HG12	1.80	0.46
1:F:151:MET:HG3	1:F:152:ILE:N	2.31	0.46
1:A:64:GLN:NE2	1:A:100:ASN:HD22	2.14	0.46
1:H:66:ASN:ND2	4:H:302:FQ0:O6	2.48	0.46
1:B:183:THR:HA	1:B:186:SER:OG	2.16	0.46
1:B:99:GLY:HA3	1:B:130:ILE:O	2.16	0.46
1:C:67:THR:CG2	1:C:105:ILE:HG21	2.46	0.45
1:C:183:THR:HA	1:C:186:SER:OG	2.17	0.45
1:G:183:THR:HA	1:G:186:SER:OG	2.16	0.45
1:F:62:PHE:HA	1:F:66:ASN:HD22	1.81	0.45
1:C:149:LYS:HA	1:D:135:TYR:OH	2.15	0.45
1:A:66:ASN:HD21	2:A:301:DMA:H52	1.82	0.45
1:B:3:ILE:HG21	1:B:52:ILE:CG2	2.47	0.45
1:A:63:THR:HA	1:A:132:TYR:O	2.16	0.45
1:C:63:THR:H	1:C:66:ASN:HD22	1.63	0.45
1:D:183:THR:HA	1:D:186:SER:OG	2.17	0.45
1:C:63:THR:H	1:C:66:ASN:ND2	2.15	0.45
1:E:152:ILE:HG21	1:F:135:TYR:CE2	2.53	0.44
1:D:7:LYS:H	1:D:211:GLN:NE2	2.15	0.44
1:A:152:ILE:HG21	1:B:135:TYR:CE2	2.53	0.44
1:E:74:ARG:HD2	1:E:105:ILE:HD12	2.00	0.44
1:E:18:ASP:HA	2:E:302:DMA:H11	2.00	0.44
1:F:7:LYS:HA	1:F:7:LYS:CE	2.48	0.44
1:F:96:LEU:O	1:F:127:ASN:HA	2.18	0.44
1:F:115:LYS:O	1:F:117:THR:HG23	2.18	0.44
1:C:95:ILE:O	1:C:116:ARG:NH1	2.51	0.43
1:H:63:THR:H	1:H:66:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:193:GLU:CG	1:H:202:HIS:CE1	3.02	0.43
1:G:64:GLN:NE2	1:G:100:ASN:HD22	2.16	0.43
1:B:64:GLN:HE22	1:B:100:ASN:HD22	1.67	0.43
1:C:135:TYR:CE2	1:D:152:ILE:HG21	2.53	0.43
1:E:20:ASN:HD22	2:E:302:DMA:H12	1.84	0.43
1:D:8:ARG:NH2	1:D:215:ILE:HD12	2.34	0.43
1:D:172:ARG:NH1	7:D:402:HOH:O	2.41	0.43
1:G:67:THR:O	1:G:74:ARG:HD2	2.18	0.43
1:F:172:ARG:CG	1:F:172:ARG:NH2	2.73	0.43
1:G:11:ARG:NH1	7:G:409:HOH:O	2.52	0.43
1:A:135:TYR:OH	1:B:149:LYS:HA	2.19	0.42
1:E:20:ASN:ND2	2:E:302:DMA:H12	2.34	0.42
1:A:65:ASP:OD2	1:B:185:TYR:OH	2.32	0.42
1:B:63:THR:H	1:B:66:ASN:HD22	1.67	0.42
2:A:301:DMA:H43	2:A:302:DMA:C3	2.50	0.42
1:C:94:GLU:HG3	7:C:408:HOH:O	2.19	0.42
1:C:141:ALA:HB1	1:C:151:MET:HG2	2.02	0.42
1:F:121:LYS:HA	1:F:121:LYS:HE2	2.01	0.42
1:E:3:ILE:HG23	1:E:4:PRO:CD	2.46	0.42
1:C:40:ILE:N	1:C:41:PRO:CD	2.84	0.41
1:F:195:TRP:HB3	1:F:196:PRO:HD3	2.02	0.41
1:C:18:ASP:HB3	1:C:169:TRP:O	2.21	0.41
1:F:56:GLU:HA	1:F:125:LYS:O	2.21	0.41
1:F:136:TRP:CH2	1:F:156:ALA:HB1	2.56	0.41
1:C:162:ARG:NH2	7:C:401:HOH:O	2.44	0.41
1:G:40:ILE:N	1:G:41:PRO:CD	2.84	0.40
1:C:20:ASN:HD22	2:C:302:DMA:H2	1.85	0.40
1:H:141:ALA:HB1	1:H:151:MET:HG3	2.04	0.40
1:C:141:ALA:O	1:C:145:SER:HB2	2.21	0.40
1:E:67:THR:HG21	1:E:105:ILE:HG21	2.03	0.40
1:G:122:GLY:C	1:G:123:LYS:HG3	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/224 (92%)	203 (98%)	4 (2%)	0	100	100
1	B	220/224 (98%)	213 (97%)	6 (3%)	1 (0%)	29	18
1	C	213/224 (95%)	211 (99%)	2 (1%)	0	100	100
1	D	207/224 (92%)	204 (99%)	3 (1%)	0	100	100
1	E	200/224 (89%)	198 (99%)	2 (1%)	0	100	100
1	F	212/224 (95%)	208 (98%)	4 (2%)	0	100	100
1	G	215/224 (96%)	208 (97%)	7 (3%)	0	100	100
1	H	202/224 (90%)	200 (99%)	2 (1%)	0	100	100
All	All	1676/1792 (94%)	1645 (98%)	30 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	LYS

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	184/193 (95%)	182 (99%)	2 (1%)	73	72
1	B	192/193 (100%)	187 (97%)	5 (3%)	46	37
1	C	188/193 (97%)	179 (95%)	9 (5%)	25	15
1	D	183/193 (95%)	180 (98%)	3 (2%)	62	58
1	E	178/193 (92%)	173 (97%)	5 (3%)	43	34
1	F	187/193 (97%)	181 (97%)	6 (3%)	39	29
1	G	189/193 (98%)	182 (96%)	7 (4%)	34	23
1	H	180/193 (93%)	176 (98%)	4 (2%)	52	45
All	All	1481/1544 (96%)	1440 (97%)	41 (3%)	43	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	A	151	MET
1	B	5	LYS
1	B	60	PHE
1	B	147	ASP
1	B	150	LYS
1	B	211	GLN
1	C	5	LYS
1	C	8	ARG
1	C	60	PHE
1	C	77	PHE
1	C	116	ARG
1	C	119	VAL
1	C	149	LYS
1	C	151	MET
1	C	193	GLU
1	D	60	PHE
1	D	104	ASP
1	D	193	GLU
1	E	3	ILE
1	E	60	PHE
1	E	83	LYS
1	E	153	GLU
1	E	211	GLN
1	F	3	ILE
1	F	60	PHE
1	F	65	ASP
1	F	151	MET
1	F	152	ILE
1	F	193	GLU
1	G	5	LYS
1	G	60	PHE
1	G	74	ARG
1	G	123	LYS
1	G	151	MET
1	G	205	LYS
1	G	217	LEU
1	H	60	PHE
1	H	150	LYS
1	H	151	MET
1	H	211	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	66	ASN
1	A	131	ASN
1	A	211	GLN
1	A	213	GLN
1	B	12	HIS
1	B	64	GLN
1	B	66	ASN
1	B	127	ASN
1	B	131	ASN
1	B	211	GLN
1	B	213	GLN
1	C	12	HIS
1	C	64	GLN
1	C	66	ASN
1	C	127	ASN
1	C	131	ASN
1	C	211	GLN
1	D	64	GLN
1	D	66	ASN
1	D	131	ASN
1	D	211	GLN
1	E	12	HIS
1	E	20	ASN
1	E	66	ASN
1	E	127	ASN
1	E	131	ASN
1	E	211	GLN
1	E	213	GLN
1	F	20	ASN
1	F	64	GLN
1	F	66	ASN
1	F	131	ASN
1	F	211	GLN
1	F	213	GLN
1	G	20	ASN
1	G	64	GLN
1	G	66	ASN
1	G	131	ASN
1	G	211	GLN
1	G	213	GLN

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Mol	Chain	Res	Type
1	H	12	HIS
1	H	64	GLN
1	H	66	ASN
1	H	127	ASN
1	H	131	ASN
1	H	211	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z > 2$
5	DPO	B	303	3	6,8,8	0.89	0	13,13,13	0.84	0
5	DPO	F	304	3	6,8,8	0.73	0	13,13,13	0.79	0
4	FQ0	G	302	-	20,20,20	0.66	0	23,23,23	0.94	0
6	PO4	G	305	3	4,4,4	0.59	0	6,6,6	0.45	0
4	FQ0	H	302	-	20,20,20	0.54	0	23,23,23	1.13	1 (4%)
2	DMA	A	302	3	11,13,13	0.79	1 (9%)	15,19,19	0.76	0
5	DPO	G	303	3	6,8,8	0.71	0	13,13,13	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMA	E	301	3	11,13,13	0.63	0	15,19,19	0.71	0
4	FQ0	F	302	-	20,20,20	0.64	0	23,23,23	1.14	1 (4%)
2	DMA	D	302	3	11,13,13	0.64	0	15,19,19	0.64	0
2	DMA	C	302	3	11,13,13	0.53	0	15,19,19	0.74	0
4	FQ0	B	302	-	20,20,20	0.62	0	23,23,23	1.01	0
5	DPO	H	303	3	6,8,8	0.74	0	13,13,13	0.72	0
2	DMA	D	301	3	11,13,13	0.72	0	15,19,19	0.75	1 (6%)
2	DMA	C	301	3	11,13,13	0.56	0	15,19,19	0.67	0
5	DPO	B	304	3	6,8,8	0.68	0	13,13,13	0.87	0
2	DMA	E	302	3	11,13,13	0.63	0	15,19,19	0.68	0
5	DPO	G	304	3	6,8,8	0.77	0	13,13,13	0.74	0
2	DMA	A	301	3	11,13,13	0.74	0	15,19,19	0.82	0
5	DPO	F	303	3	6,8,8	0.82	0	13,13,13	0.70	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
5	DPO	B	303	3	-	1/6/6/6	-
5	DPO	F	304	3	-	0/6/6/6	-
4	FQ0	G	302	-	-	1/22/22/22	-
4	FQ0	H	302	-	-	3/22/22/22	-
2	DMA	A	302	3	-	5/13/13/13	-
5	DPO	G	303	3	-	3/6/6/6	-
2	DMA	E	301	3	-	5/13/13/13	-
4	FQ0	F	302	-	-	4/22/22/22	-
2	DMA	D	302	3	-	3/13/13/13	-
2	DMA	C	302	3	-	3/13/13/13	-
4	FQ0	B	302	-	-	0/22/22/22	-
5	DPO	H	303	3	-	1/6/6/6	-
2	DMA	D	301	3	-	4/13/13/13	-
2	DMA	C	301	3	-	3/13/13/13	-
5	DPO	B	304	3	-	3/6/6/6	-
2	DMA	E	302	3	-	5/13/13/13	-
5	DPO	G	304	3	-	0/6/6/6	-
2	DMA	A	301	3	-	3/13/13/13	-
5	DPO	F	303	3	-	1/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	DMA	PB-O3B	-2.24	1.46	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	302	FQ0	O5-C3-C31	2.50	115.29	108.64
4	H	302	FQ0	C9-C8-C7	-2.21	116.64	121.12
2	D	301	DMA	O3B-PB-O2B	2.03	115.38	107.64

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DMA	C1-O1-PA-O1A
2	A	302	DMA	C2-C1-O1-PA
2	A	302	DMA	C1-C2-C3-C4
2	A	302	DMA	C1-C2-C3-C5
2	C	301	DMA	C1-O1-PA-O2A
2	C	302	DMA	C1-O1-PA-O1A
2	D	302	DMA	C1-O1-PA-O2A
2	E	301	DMA	C1-O1-PA-O1A
2	E	302	DMA	C2-C1-O1-PA
2	E	302	DMA	C1-O1-PA-O1A
4	F	302	FQ0	C2-C3-C31-O7
4	F	302	FQ0	O5-C3-C31-O7
4	H	302	FQ0	C2-C3-C31-O7
4	H	302	FQ0	O5-C3-C31-O7
5	B	303	DPO	P1-O4-P2-O7
5	B	304	DPO	P1-O4-P2-O6
5	G	303	DPO	P2-O4-P1-O2
5	G	303	DPO	P2-O4-P1-O3
4	G	302	FQ0	C12-C11-C9-C8
5	G	303	DPO	P1-O4-P2-O5
2	A	301	DMA	C1-O1-PA-O3A
2	C	301	DMA	C1-O1-PA-O3A
2	D	302	DMA	C1-O1-PA-O3A
2	E	301	DMA	C1-O1-PA-O3A
2	A	302	DMA	PB-O3A-PA-O2A
2	C	302	DMA	PB-O3A-PA-O2A
2	D	301	DMA	PB-O3A-PA-O1A
2	E	301	DMA	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	E	302	DMA	PB-O3A-PA-O2A
2	A	301	DMA	C1-O1-PA-O2A
2	C	301	DMA	C1-O1-PA-O1A
2	D	302	DMA	C1-O1-PA-O1A
2	E	301	DMA	C1-O1-PA-O2A
2	A	302	DMA	PB-O3A-PA-O1A
4	H	302	FQ0	C10-C8-C9-C11
5	B	304	DPO	P1-O4-P2-O5
4	F	302	FQ0	C31-C3-O5-C6
5	B	304	DPO	P1-O4-P2-O7
5	F	303	DPO	P1-O4-P2-O7
5	H	303	DPO	P1-O4-P2-O6
2	C	302	DMA	C2-C1-O1-PA
2	D	301	DMA	C2-C1-O1-PA
2	D	301	DMA	C1-O1-PA-O3A
2	E	302	DMA	C1-O1-PA-O3A
4	F	302	FQ0	C10-C8-C9-C11
2	D	301	DMA	PB-O3A-PA-O2A
2	E	301	DMA	PB-O3A-PA-O1A
2	E	302	DMA	PB-O3A-PA-O1A

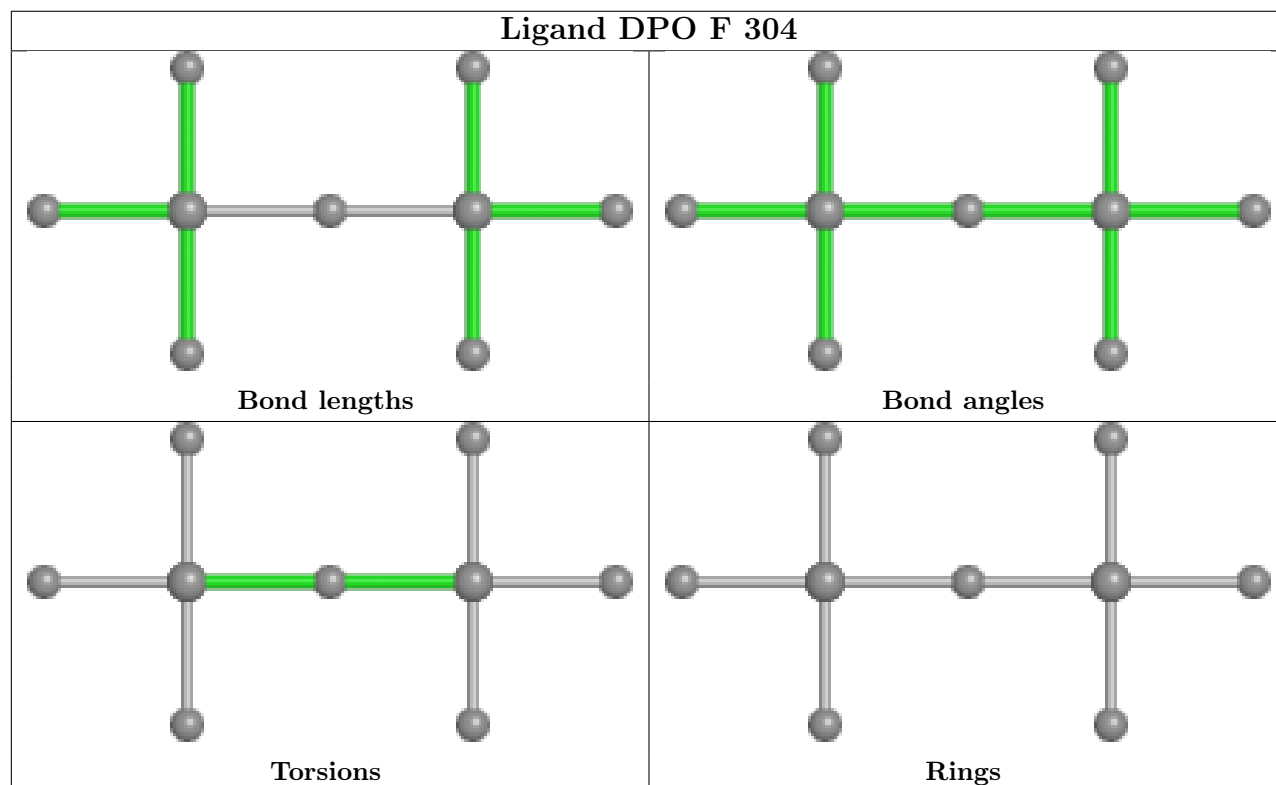
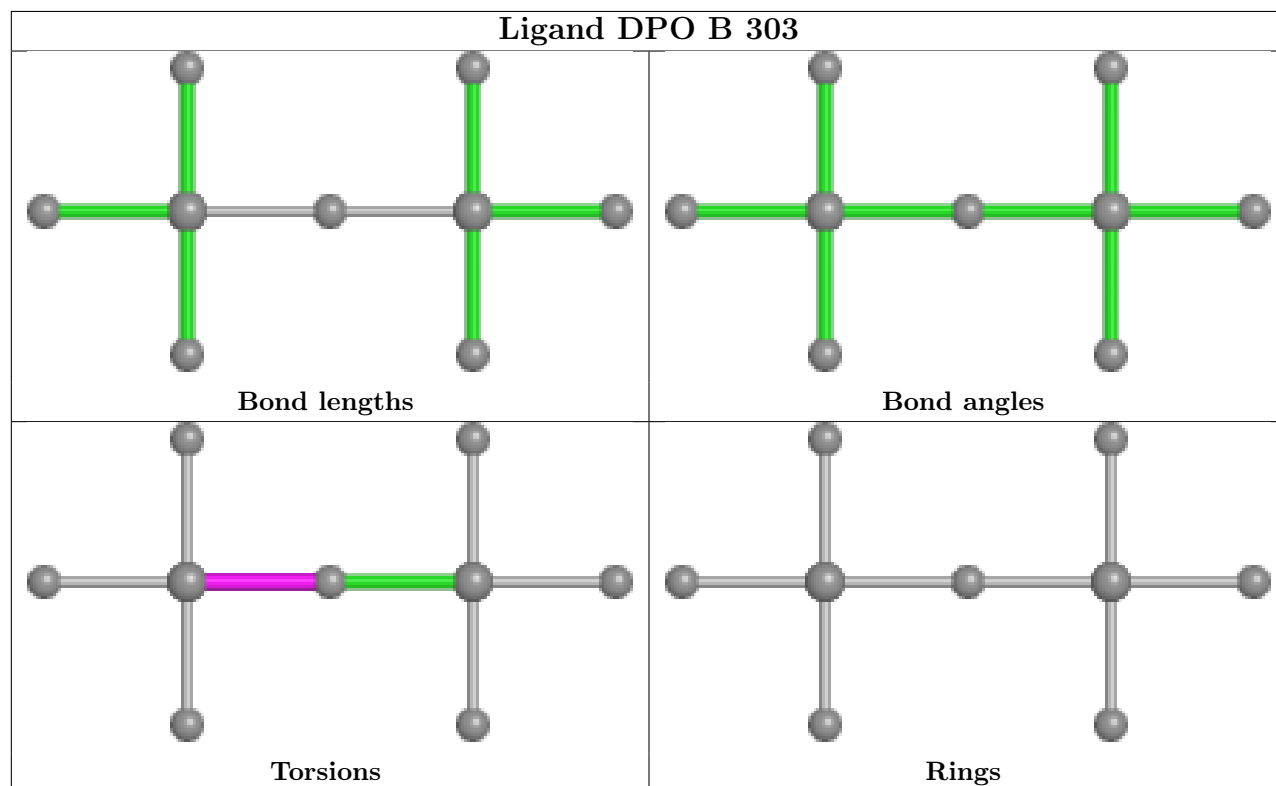
There are no ring outliers.

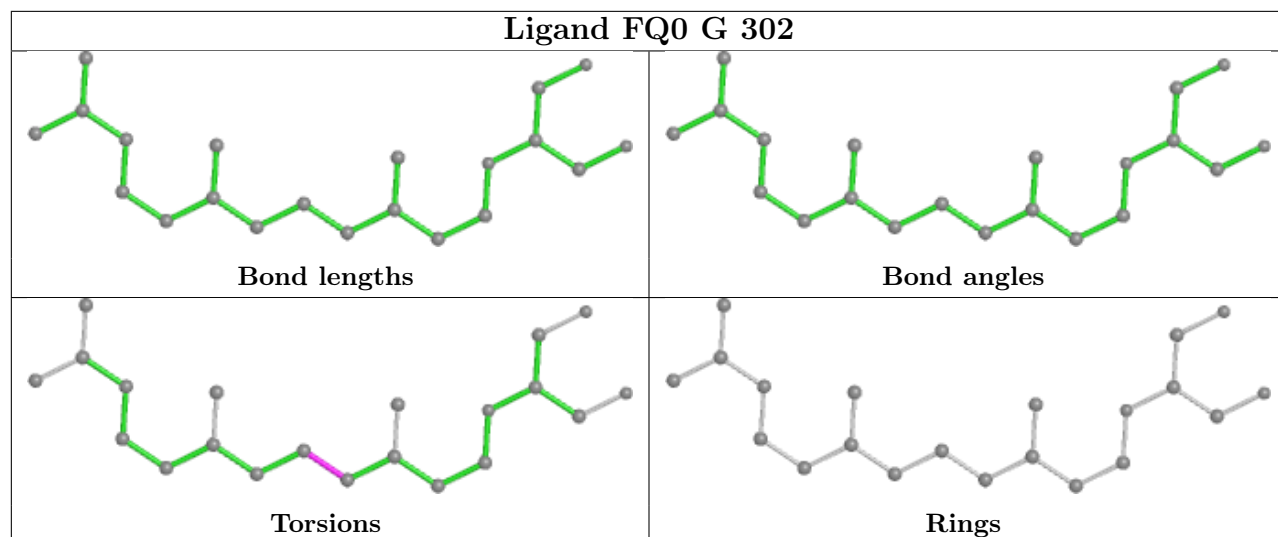
9 monomers are involved in 18 short contacts:

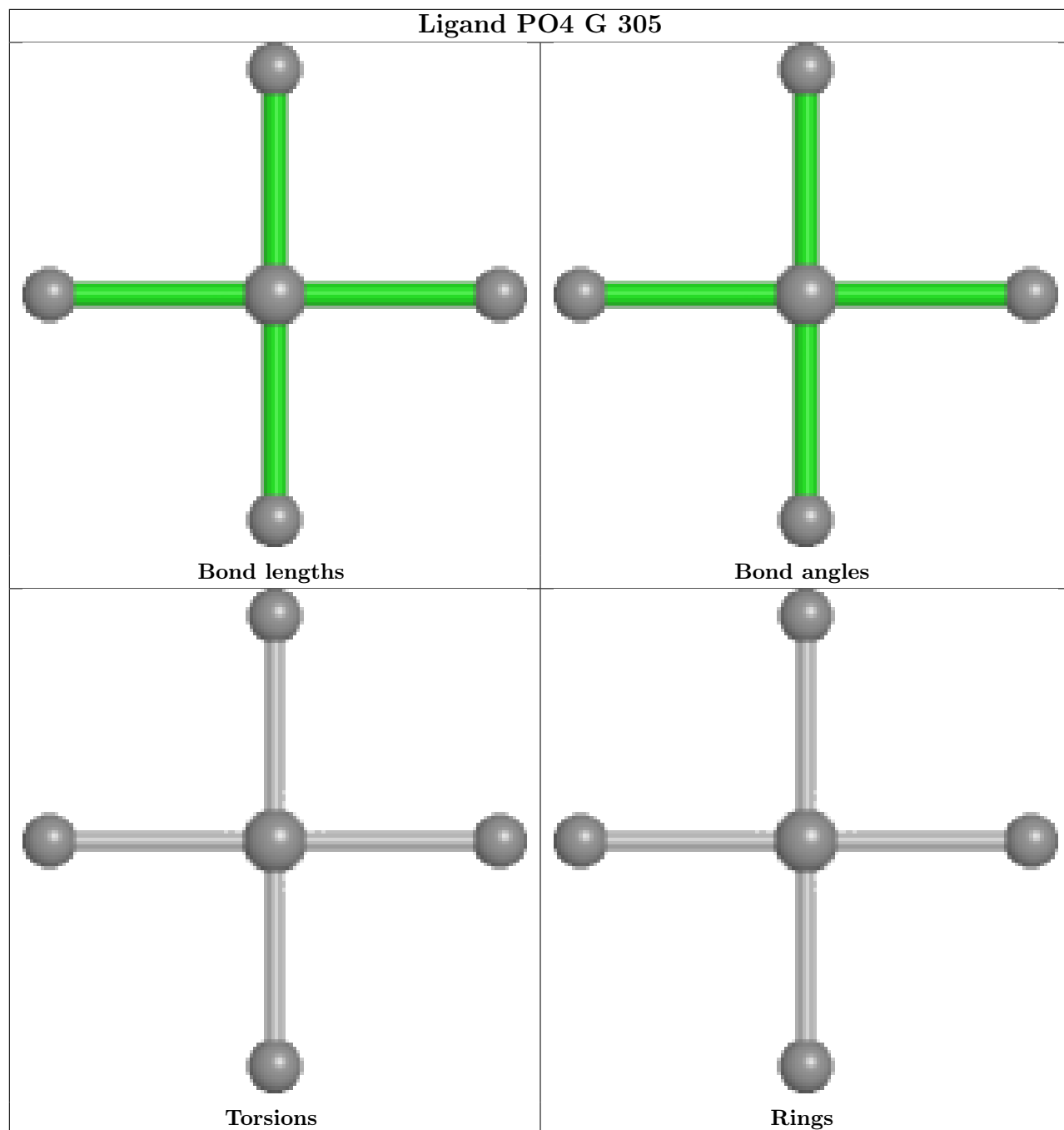
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	FQ0	2	0
2	A	302	DMA	4	0
2	E	301	DMA	1	0
2	D	302	DMA	1	0
2	C	302	DMA	2	0
5	H	303	DPO	1	0
2	C	301	DMA	2	0
2	E	302	DMA	5	0
2	A	301	DMA	3	0

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

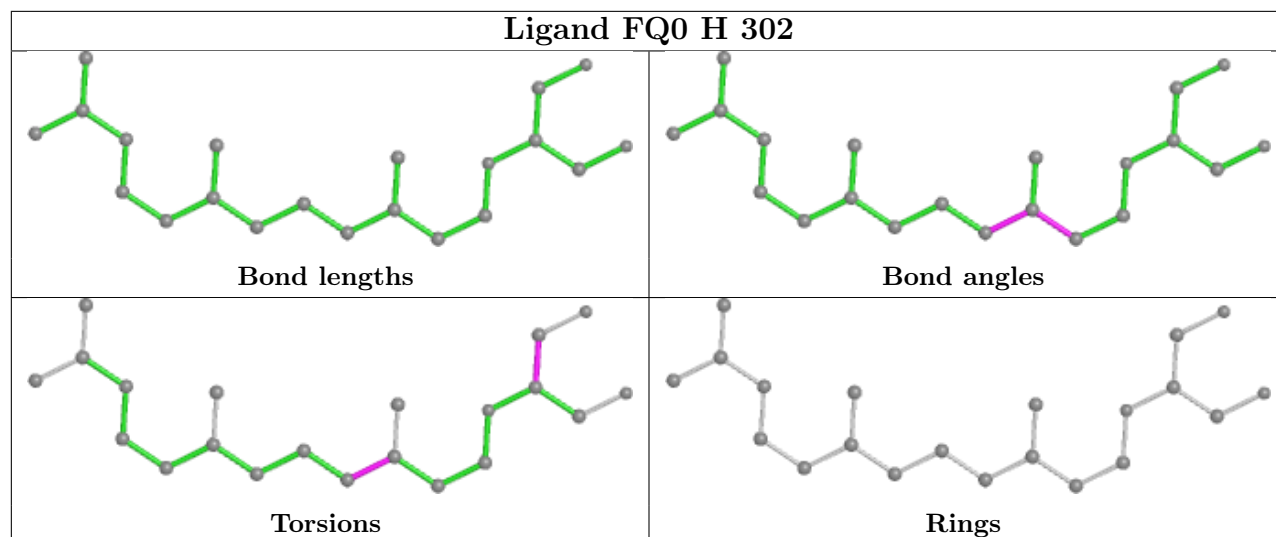
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



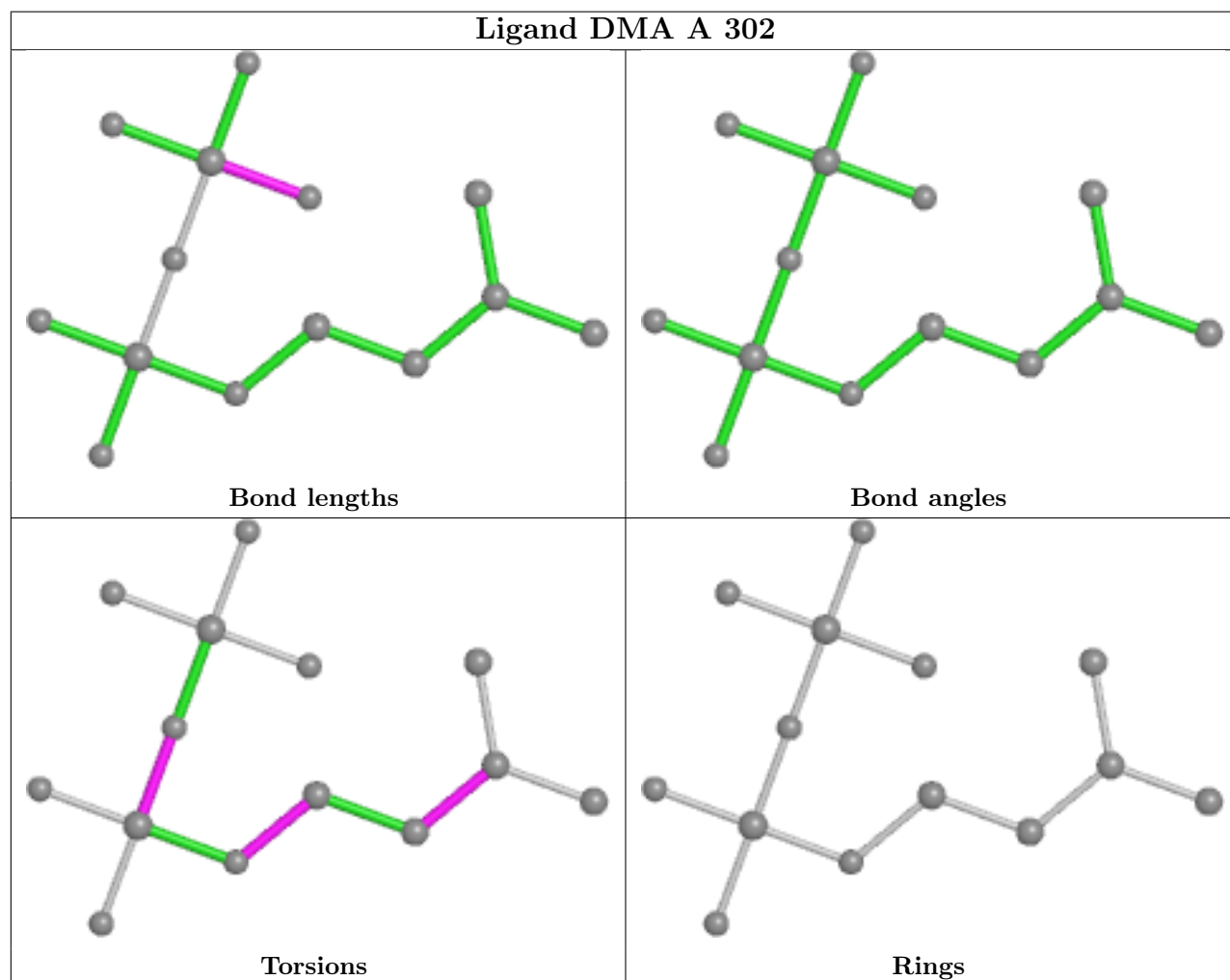


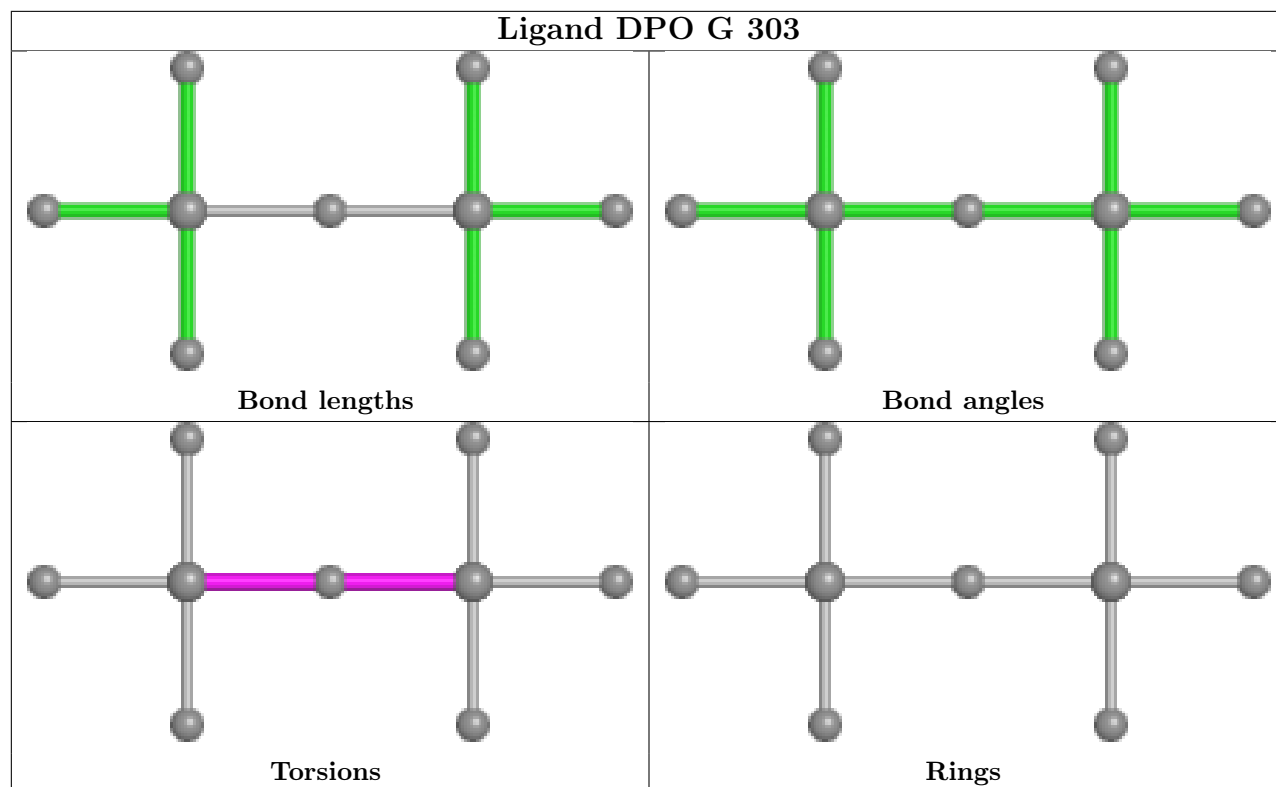


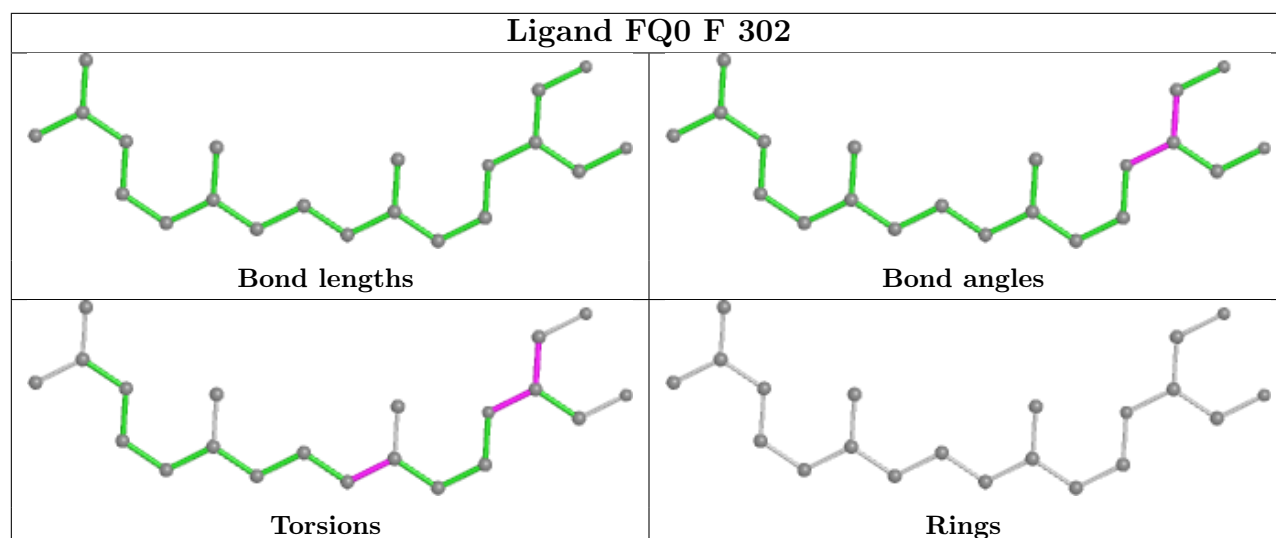
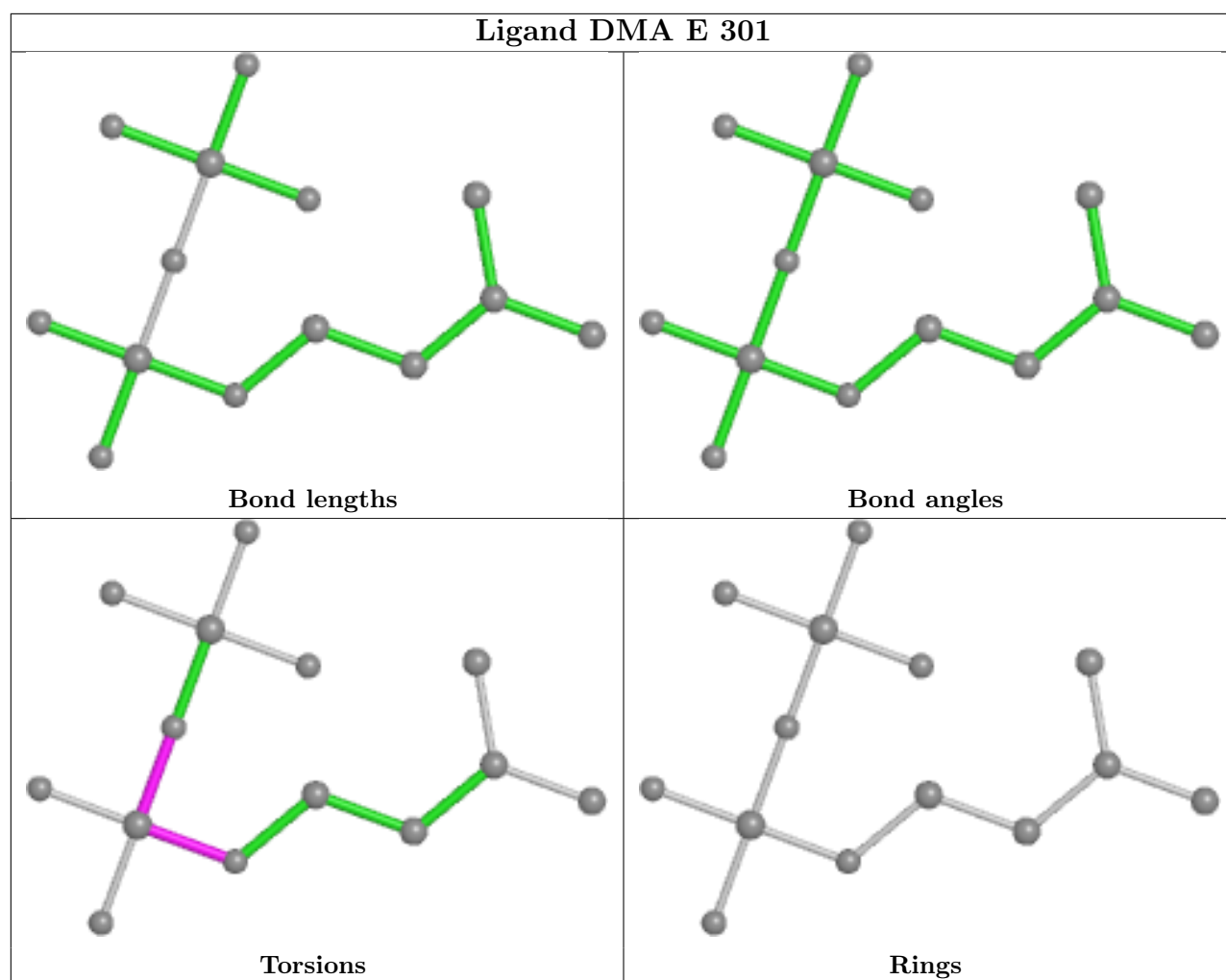
Ligand FQ0 H 302

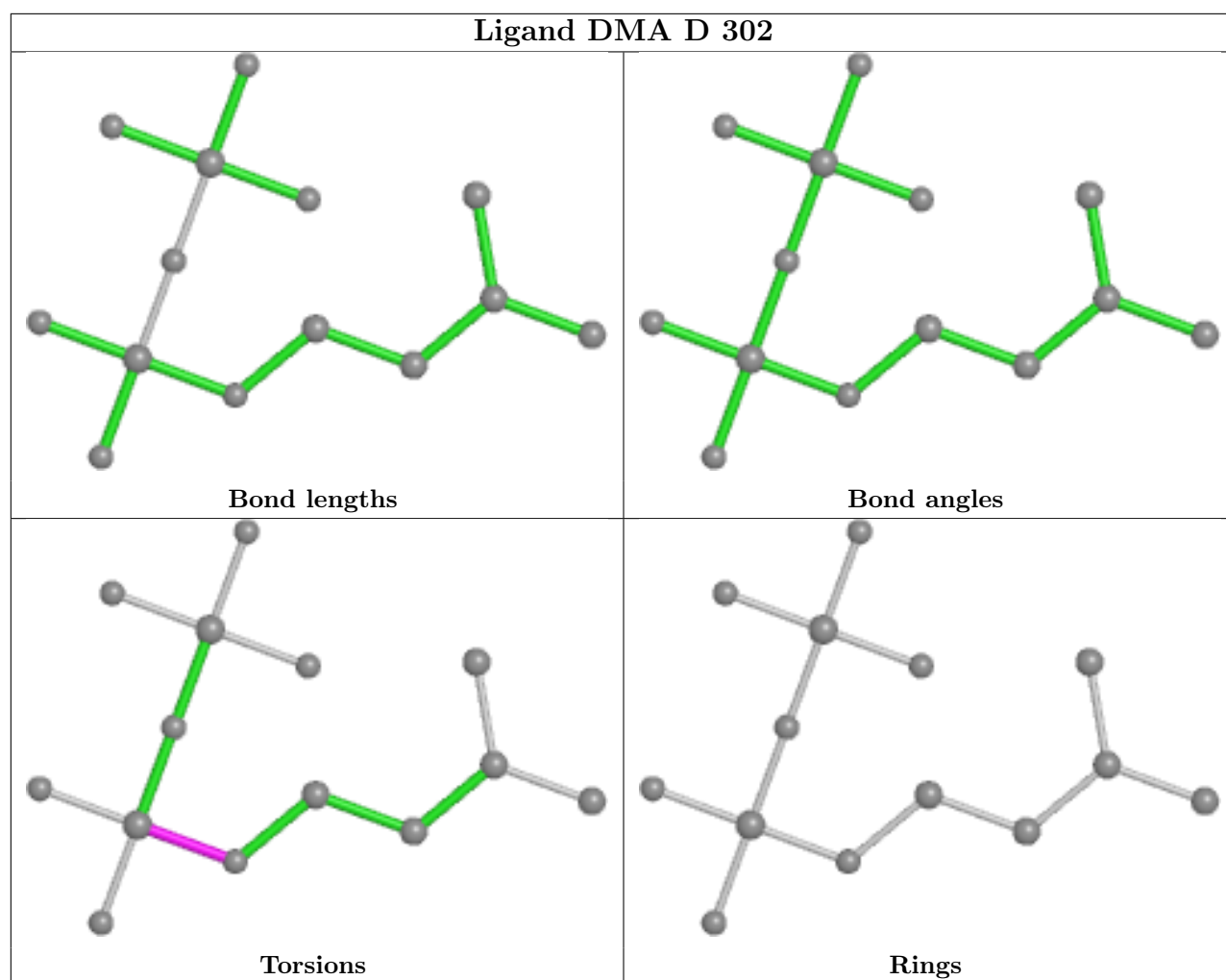


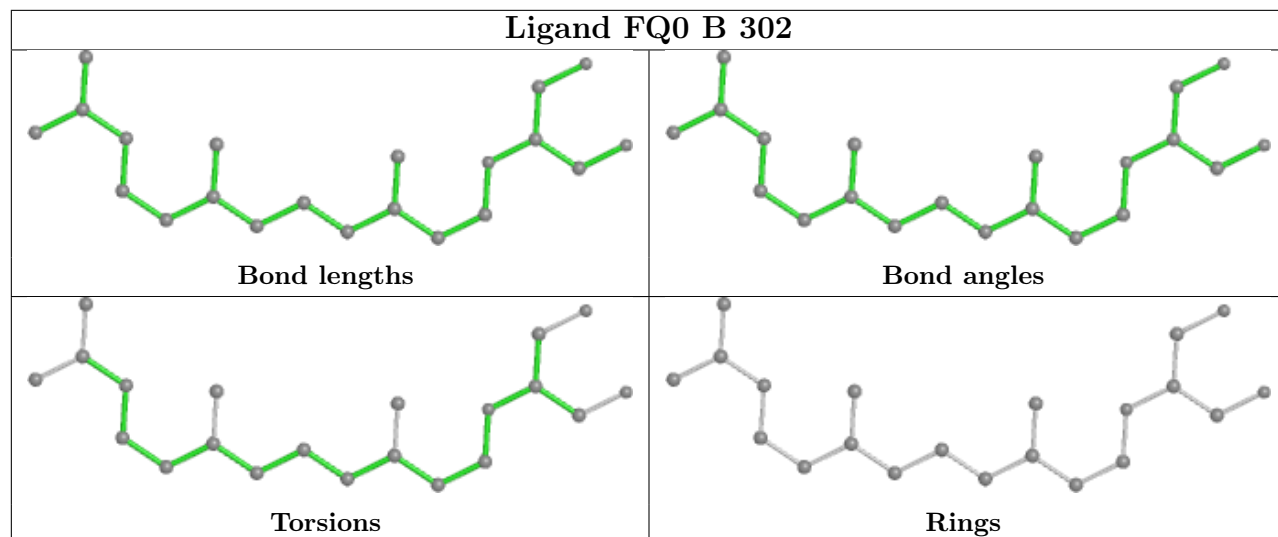
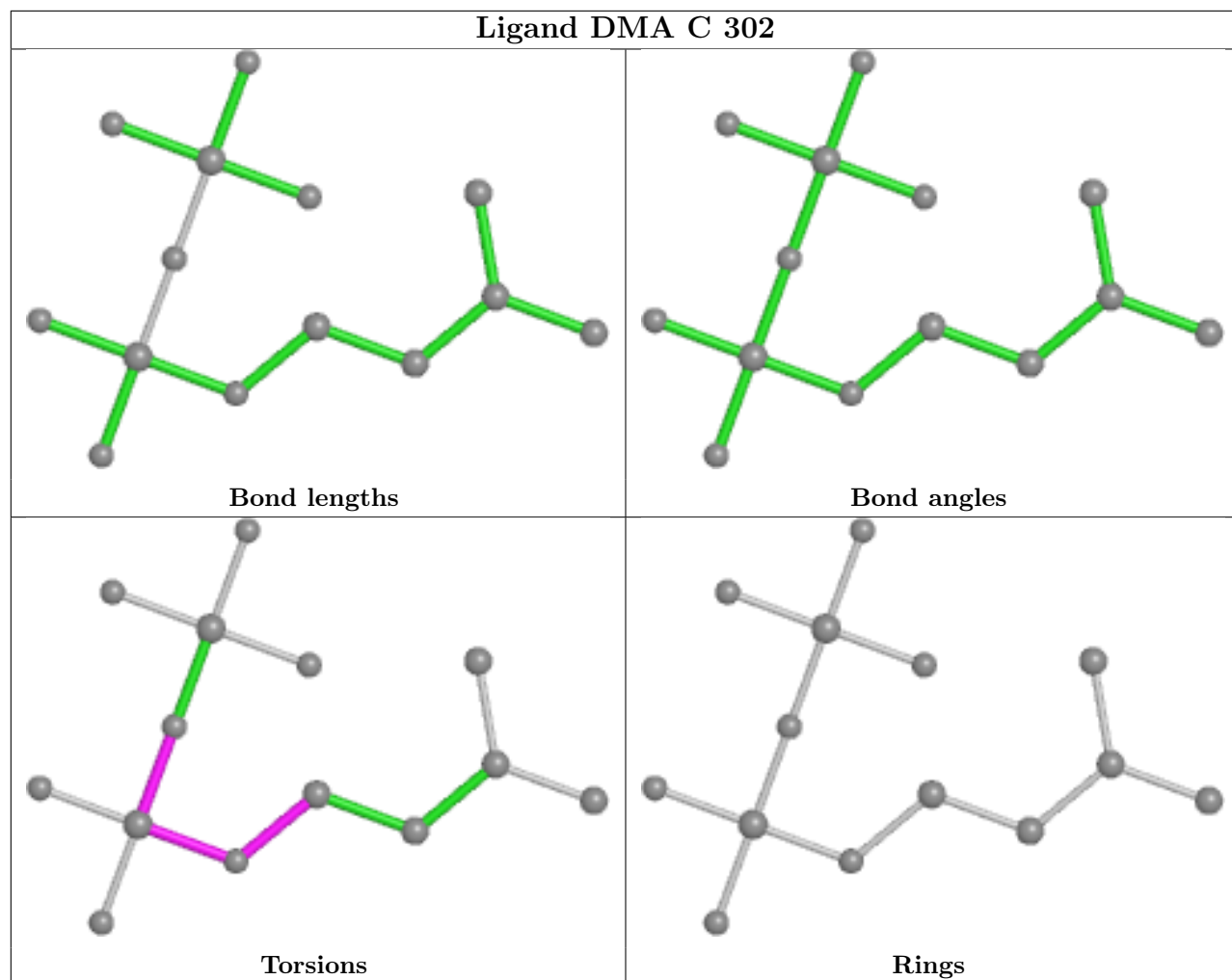
Ligand DMA A 302

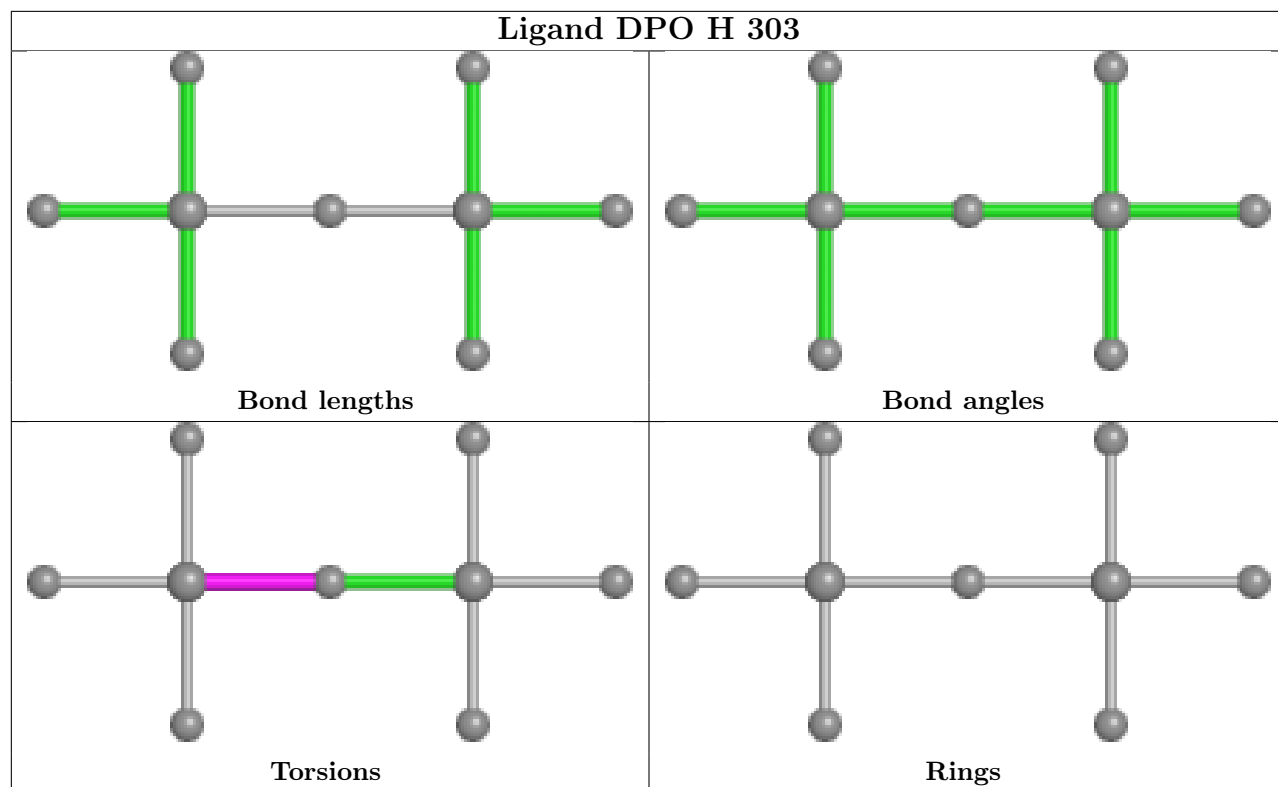


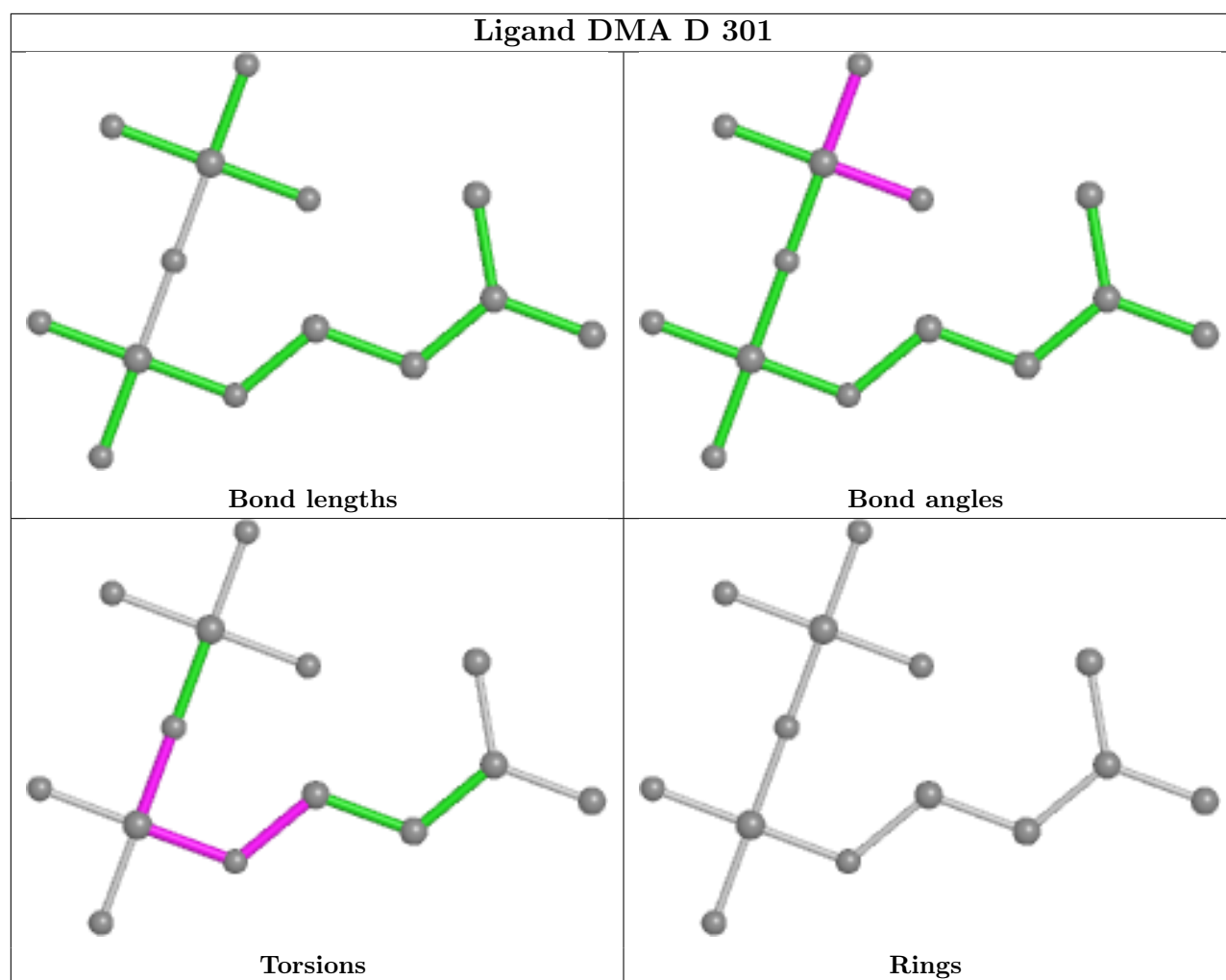


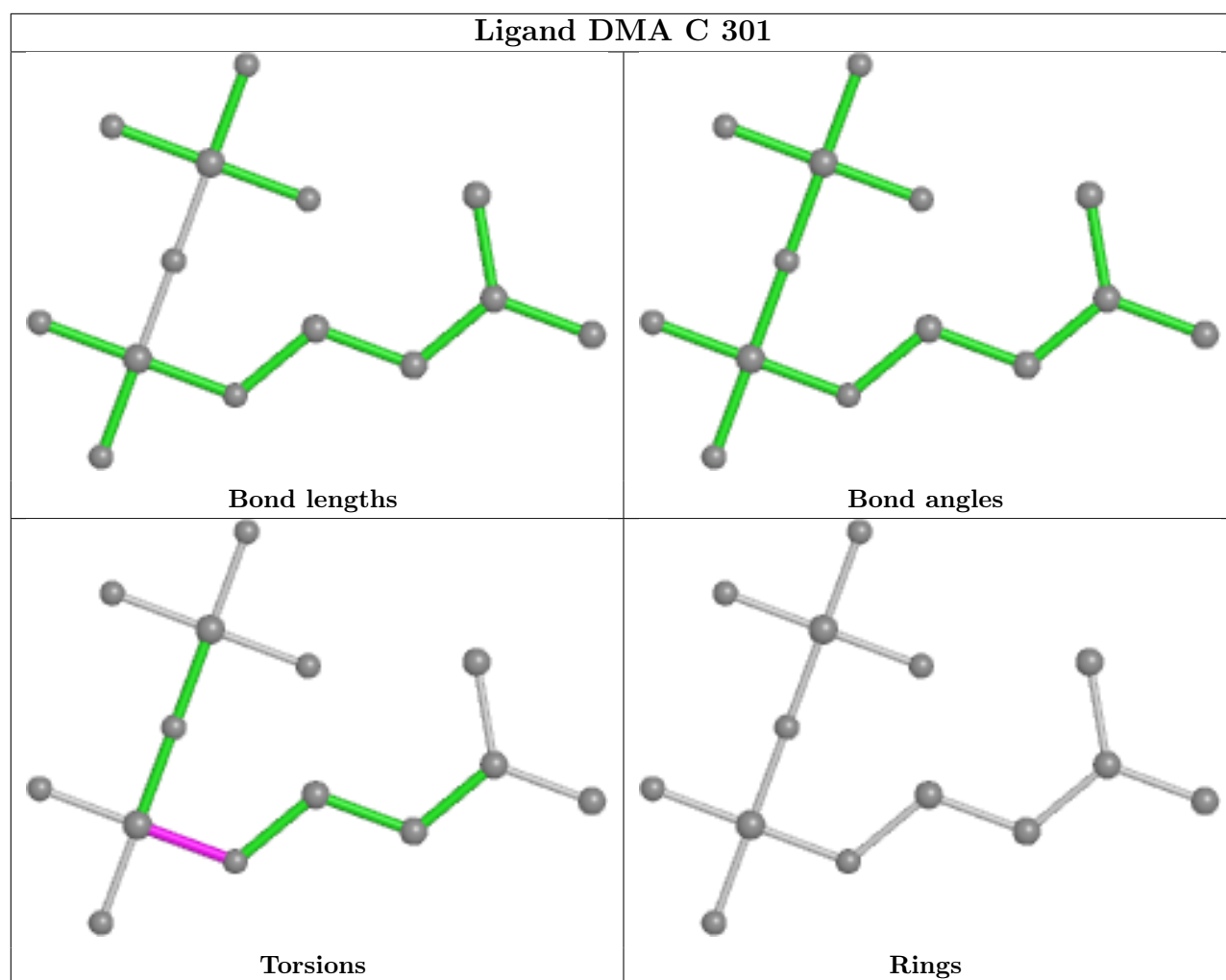


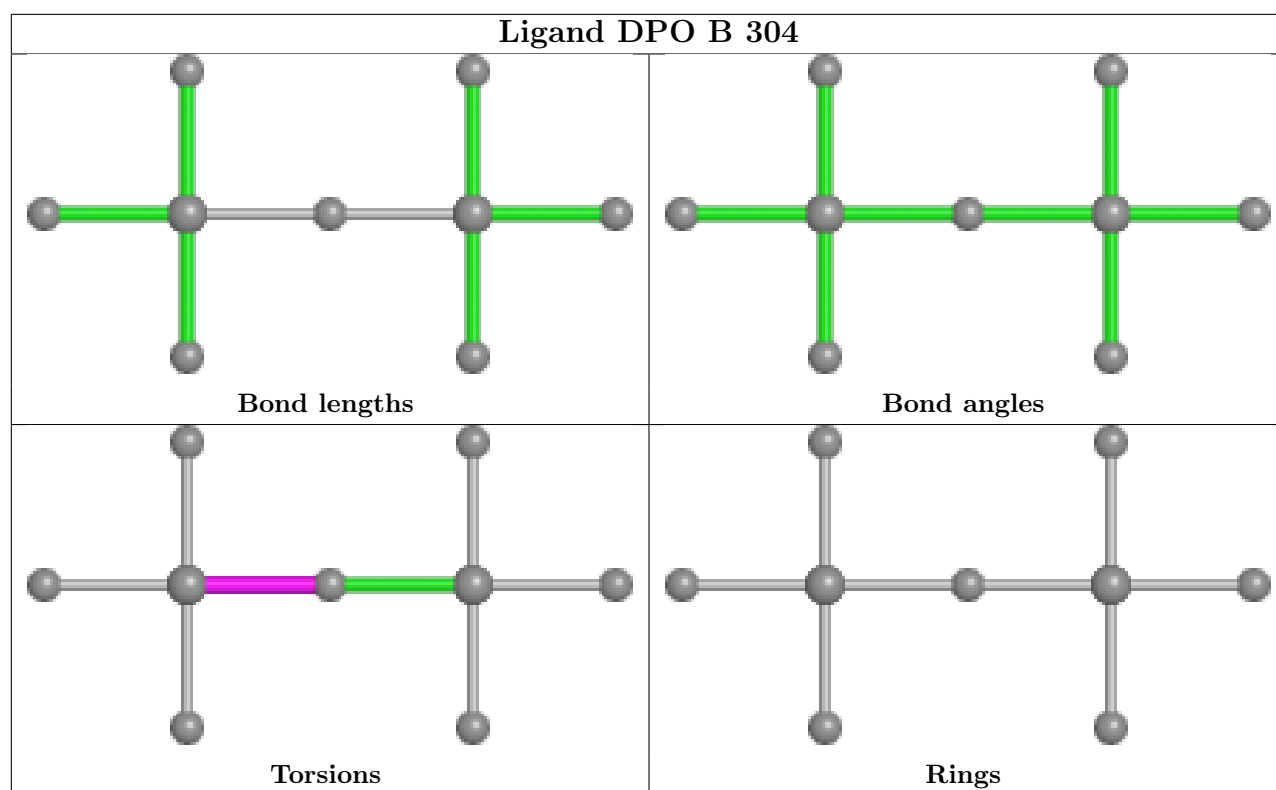


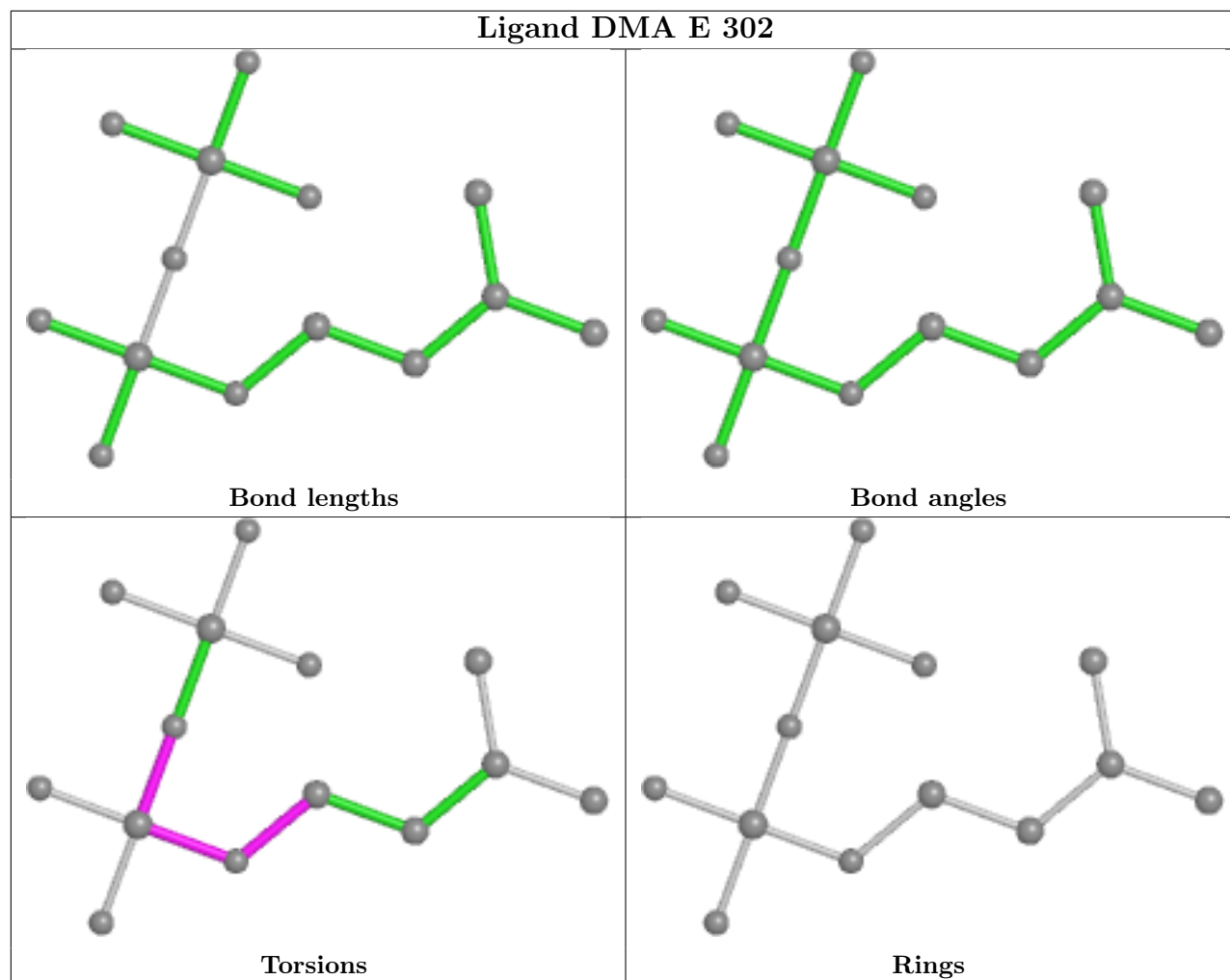


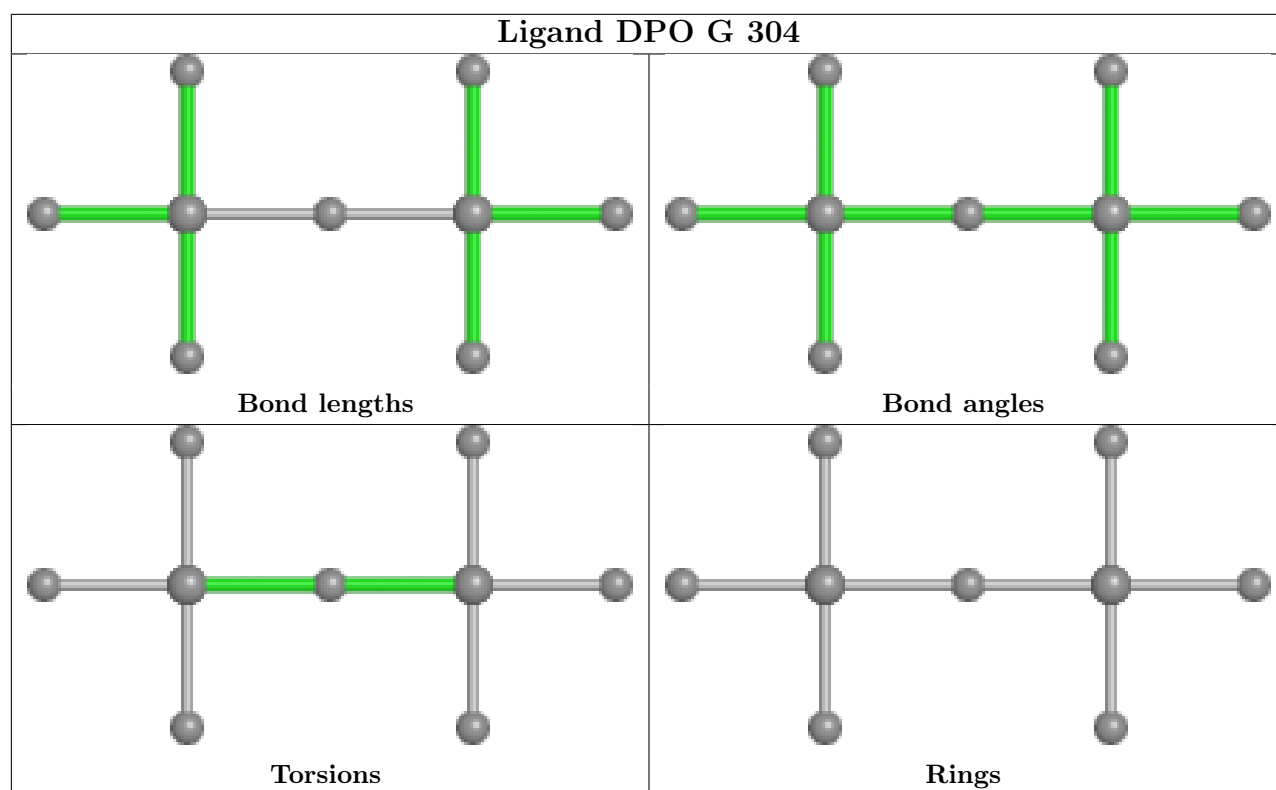


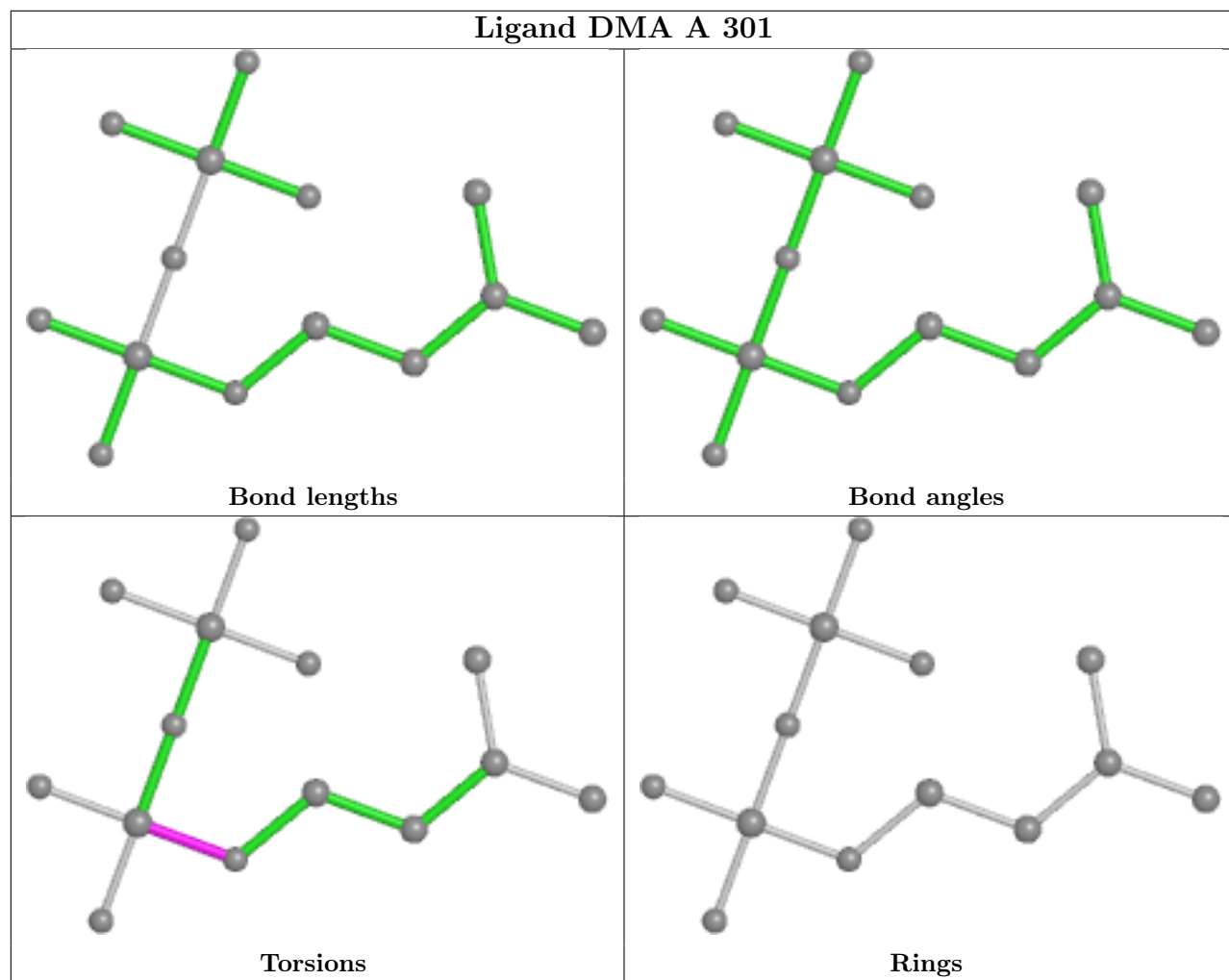


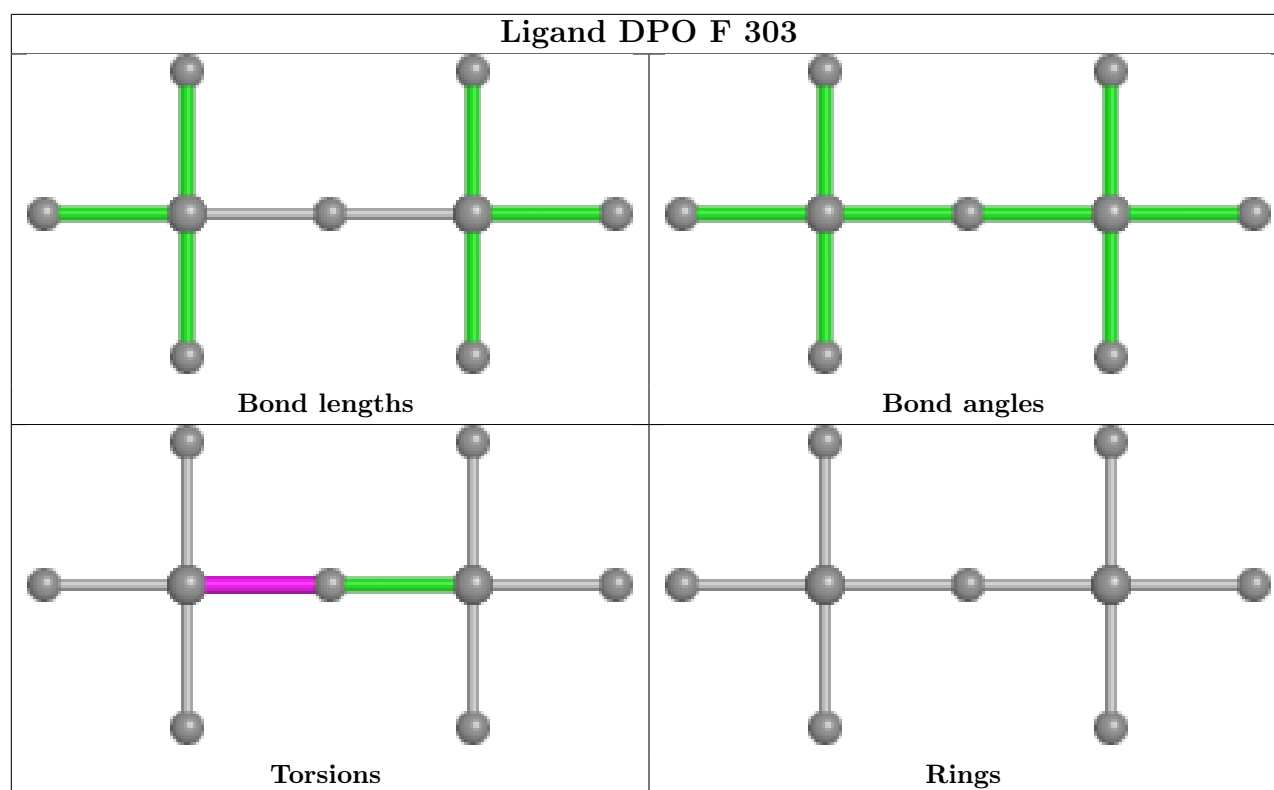












5.7 Other polymers [i](#)

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	211/224 (94%)	0.41	14 (6%) 18 20	27, 38, 67, 89	0
1	B	222/224 (99%)	0.41	13 (5%) 22 25	27, 37, 63, 88	0
1	C	217/224 (96%)	0.66	18 (8%) 11 13	29, 43, 73, 94	0
1	D	211/224 (94%)	0.64	23 (10%) 5 6	30, 44, 69, 86	0
1	E	204/224 (91%)	0.51	15 (7%) 14 16	31, 45, 73, 85	0
1	F	216/224 (96%)	0.68	16 (7%) 14 16	30, 45, 73, 104	0
1	G	219/224 (97%)	0.51	10 (4%) 32 35	30, 41, 68, 94	0
1	H	206/224 (91%)	0.42	15 (7%) 15 17	30, 42, 70, 88	0
All	All	1706/1792 (95%)	0.53	124 (7%) 15 17	27, 42, 71, 104	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	142	TYR	9.0
1	B	142	TYR	6.2
1	A	-1	TYR	6.0
1	D	150	LYS	5.9
1	H	151	MET	5.7
1	H	141	ALA	5.7
1	G	152	ILE	5.6
1	D	218	GLY	5.3
1	D	141	ALA	5.3
1	F	3	ILE	4.8
1	C	142	TYR	4.6
1	E	150	LYS	4.5
1	C	141	ALA	4.4
1	A	1	MET	4.4
1	H	2	ASP	4.3
1	F	142	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	2	ASP	4.2
1	E	71	GLN	4.1
1	F	147	ASP	4.1
1	C	151	MET	3.9
1	D	216	THR	3.9
1	D	219	GLY	3.9
1	C	152	ILE	3.9
1	F	148	GLY	3.8
1	D	215	ILE	3.8
1	C	149	LYS	3.7
1	F	141	ALA	3.6
1	B	145	SER	3.6
1	H	142	TYR	3.6
1	A	152	ILE	3.5
1	D	217	LEU	3.5
1	F	25	LEU	3.4
1	G	135	TYR	3.3
1	H	152	ILE	3.3
1	G	-1	TYR	3.3
1	E	32	HIS	3.2
1	D	162	ARG	3.2
1	D	201	GLU	3.2
1	E	141	ALA	3.2
1	D	151	MET	3.2
1	H	150	LYS	3.2
1	E	151	MET	3.1
1	D	153	GLU	3.1
1	E	185	TYR	3.1
1	D	123	LYS	3.0
1	D	52	ILE	3.0
1	E	108	GLU	3.0
1	B	144	ASN	3.0
1	B	143	ASP	3.0
1	G	149	LYS	3.0
1	E	142	TYR	2.9
1	C	215	ILE	2.9
1	C	68	LYS	2.9
1	B	72	ILE	2.9
1	A	0	GLN	2.9
1	E	3	ILE	2.9
1	E	68	LYS	2.8
1	F	123	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	151	MET	2.8
1	E	25	LEU	2.8
1	F	121	LYS	2.8
1	A	2	ASP	2.8
1	C	140	TYR	2.8
1	F	144	ASN	2.8
1	B	5	LYS	2.7
1	G	-2	GLY	2.7
1	D	83	LYS	2.7
1	H	135	TYR	2.7
1	C	7	LYS	2.7
1	D	8	ARG	2.7
1	A	150	LYS	2.7
1	C	135	TYR	2.7
1	E	135	TYR	2.7
1	D	152	ILE	2.6
1	G	5	LYS	2.6
1	H	105	ILE	2.6
1	F	135	TYR	2.6
1	B	152	ILE	2.6
1	E	72	ILE	2.6
1	C	102	ASN	2.6
1	H	102	ASN	2.6
1	A	143	ASP	2.5
1	D	7	LYS	2.5
1	B	135	TYR	2.5
1	F	151	MET	2.5
1	G	141	ALA	2.5
1	F	68	LYS	2.4
1	A	151	MET	2.4
1	A	185	TYR	2.4
1	D	121	LYS	2.4
1	A	153	GLU	2.4
1	F	28	GLY	2.4
1	C	150	LYS	2.4
1	H	155	ILE	2.4
1	C	144	ASN	2.3
1	E	154	ASN	2.3
1	C	148	GLY	2.3
1	A	7	LYS	2.3
1	H	153	GLU	2.3
1	A	142	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	190	VAL	2.2
1	C	119	VAL	2.2
1	H	214	ASP	2.2
1	D	3	ILE	2.2
1	E	28	GLY	2.2
1	C	2	ASP	2.2
1	D	142	TYR	2.2
1	B	74	ARG	2.2
1	F	143	ASP	2.2
1	C	105	ILE	2.2
1	F	114	THR	2.2
1	B	149	LYS	2.2
1	C	217	LEU	2.1
1	B	121	LYS	2.1
1	D	51	LYS	2.1
1	H	65	ASP	2.1
1	F	152	ILE	2.1
1	G	147	ASP	2.1
1	D	214	ASP	2.1
1	B	123	LYS	2.1
1	A	123	LYS	2.0
1	B	146	PRO	2.0
1	H	28	GLY	2.0
1	A	52	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

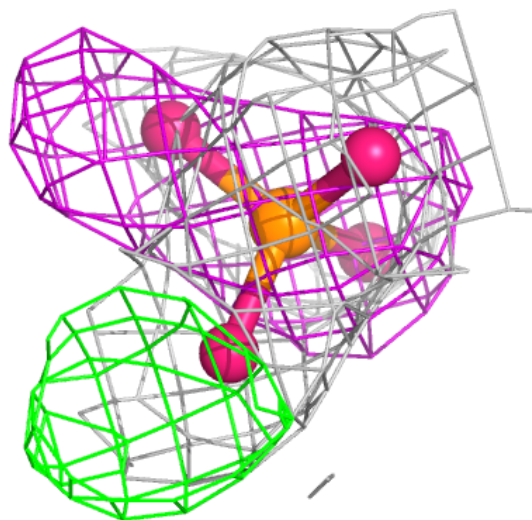
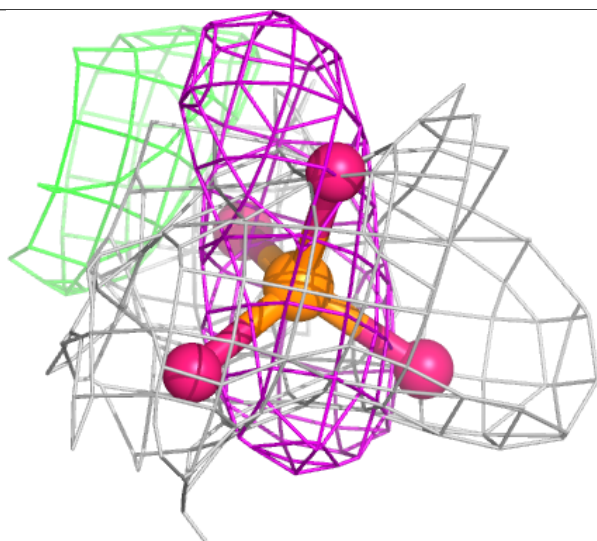
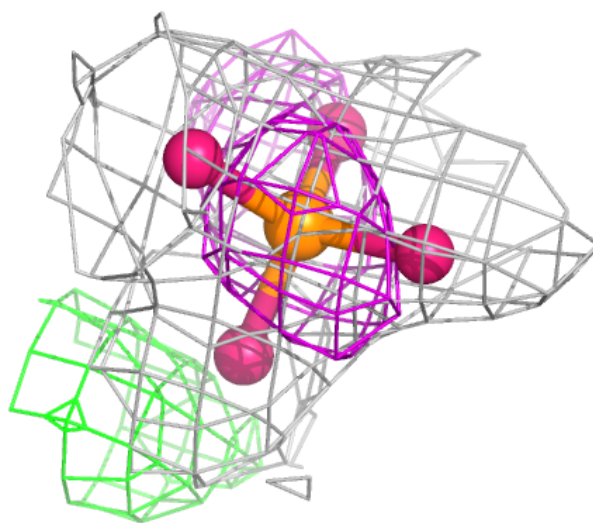
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	G	305	5/5	0.66	0.25	53,56,64,66	0
4	FQ0	G	302	21/21	0.81	0.23	36,55,75,76	0
4	FQ0	B	302	21/21	0.82	0.20	40,47,66,67	0
3	MG	G	301	1/1	0.83	0.06	45,45,45,45	0
3	MG	F	301	1/1	0.84	0.07	51,51,51,51	0
5	DPO	G	304	9/9	0.86	0.14	55,64,78,80	0
3	MG	E	303	1/1	0.86	0.06	47,47,47,47	0
5	DPO	B	304	9/9	0.89	0.12	51,57,64,67	0
4	FQ0	F	302	21/21	0.89	0.18	37,43,61,63	0
3	MG	H	301	1/1	0.89	0.12	60,60,60,60	0
4	FQ0	H	302	21/21	0.90	0.18	39,46,69,74	0
3	MG	B	301	1/1	0.91	0.06	43,43,43,43	0
5	DPO	F	304	9/9	0.91	0.17	55,60,78,80	0
2	DMA	C	301	14/14	0.95	0.14	49,52,57,58	0
3	MG	A	303	1/1	0.96	0.05	32,32,32,32	0
2	DMA	E	302	14/14	0.96	0.11	43,49,57,60	0
5	DPO	H	303	9/9	0.96	0.10	46,48,52,52	0
3	MG	C	303	1/1	0.96	0.05	45,45,45,45	0
5	DPO	B	303	9/9	0.97	0.09	38,43,47,48	0
2	DMA	C	302	14/14	0.97	0.12	43,52,59,60	0
5	DPO	F	303	9/9	0.97	0.10	44,49,54,56	0
2	DMA	D	301	14/14	0.97	0.12	33,38,44,44	0
5	DPO	G	303	9/9	0.97	0.09	44,50,51,54	0
2	DMA	E	301	14/14	0.97	0.10	41,47,52,54	0
2	DMA	A	302	14/14	0.97	0.14	28,35,51,52	0
2	DMA	A	301	14/14	0.97	0.10	31,36,37,38	0
2	DMA	D	302	14/14	0.98	0.10	34,41,45,48	0
3	MG	D	303	1/1	0.99	0.07	34,34,34,34	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.

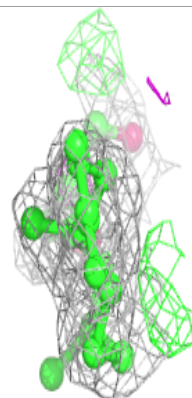
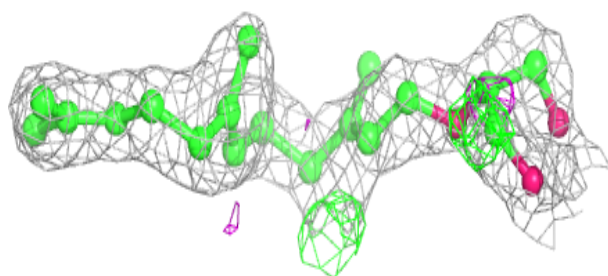
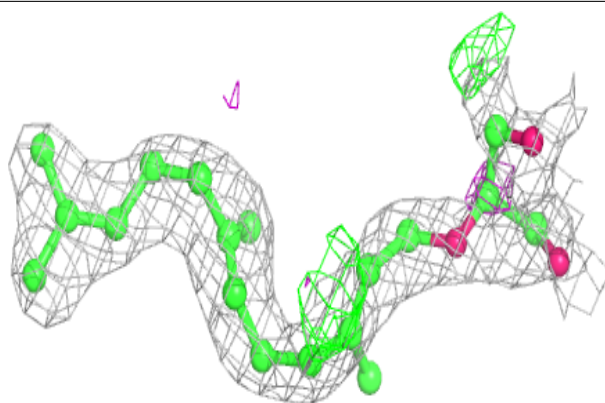
Electron density around PO4 G 305:

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

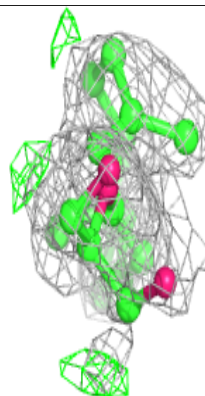
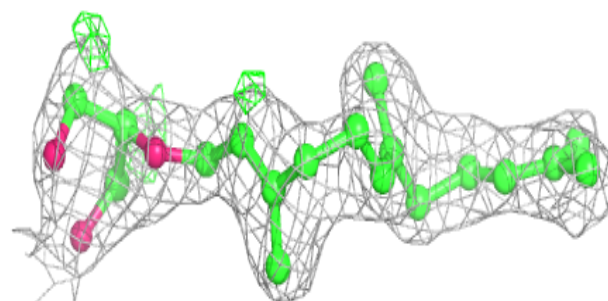
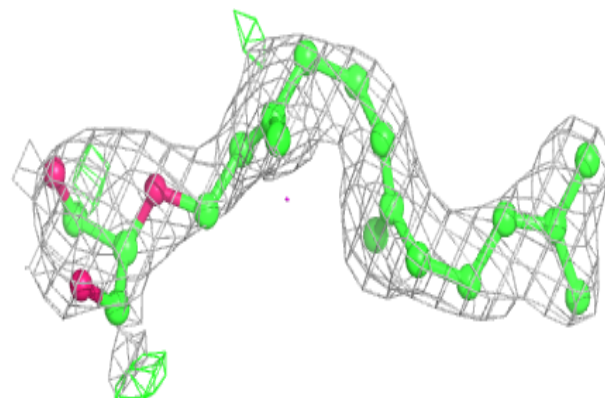


Electron density around FQ0 G 302:

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

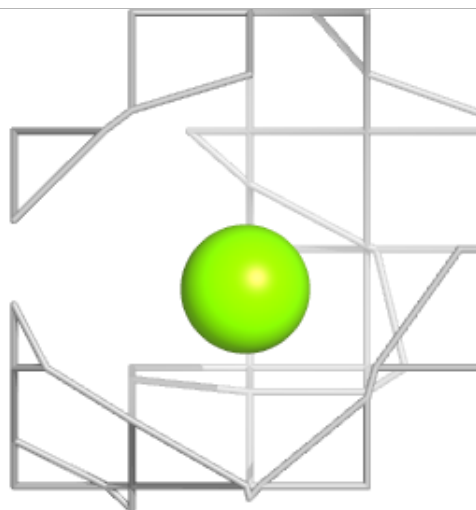
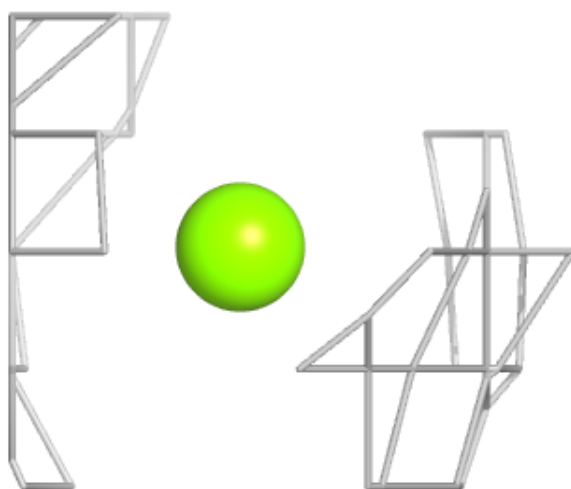
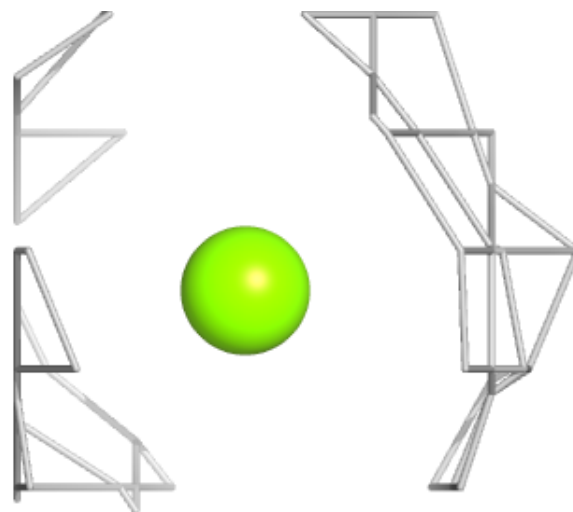
**Electron density around FQ0 B 302:**

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



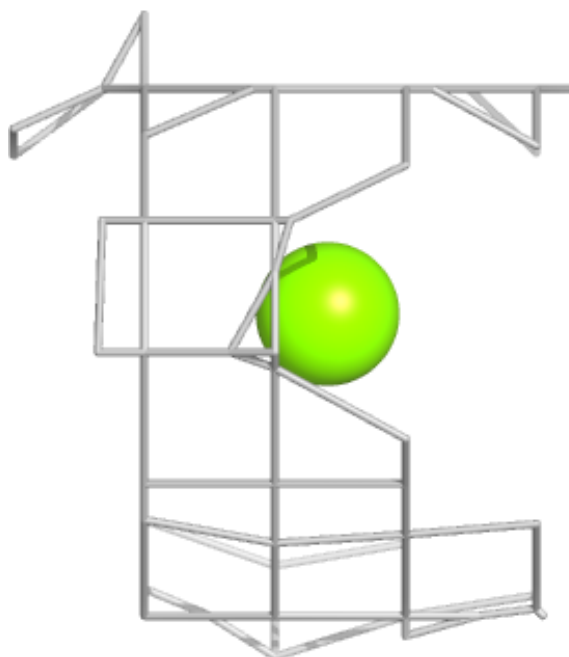
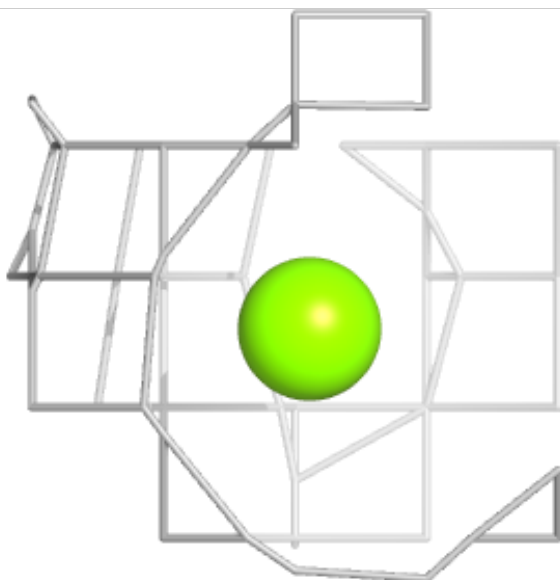
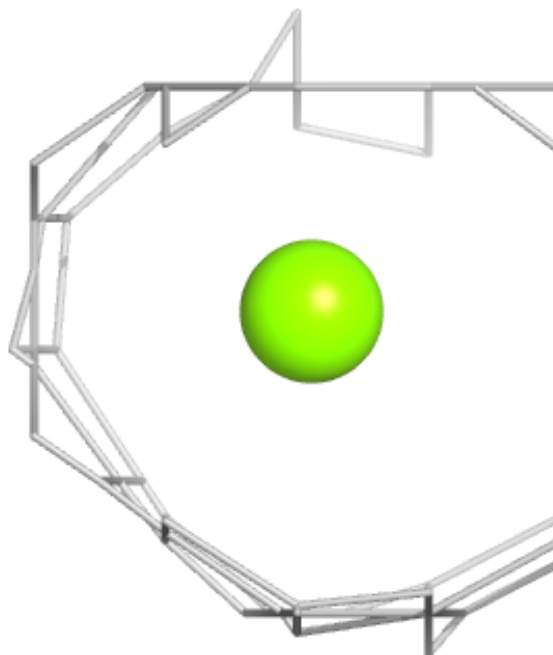
Electron density around MG G 301:

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



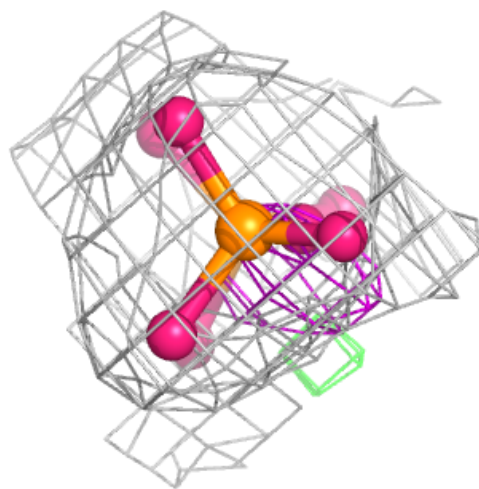
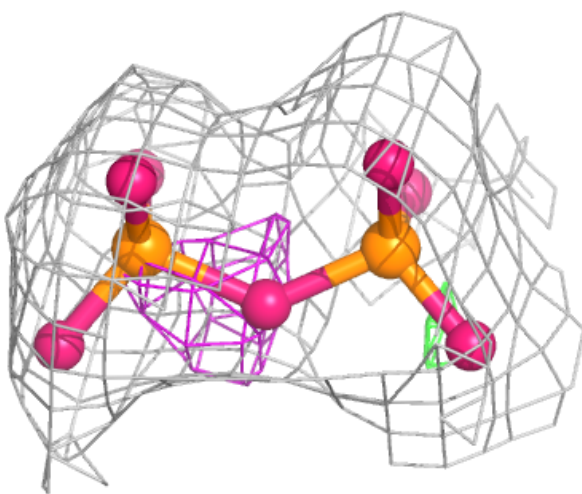
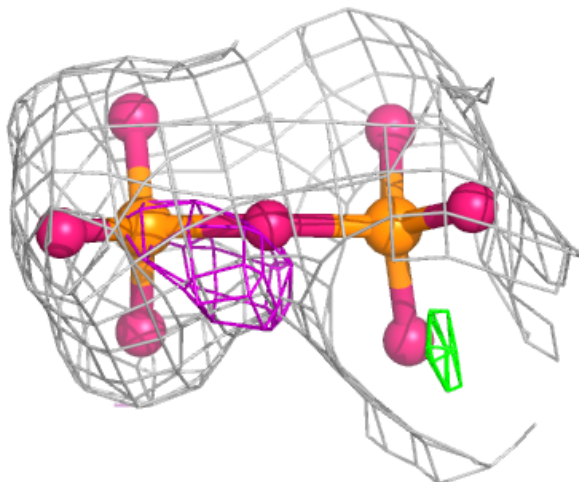
Electron density around MG F 301:

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



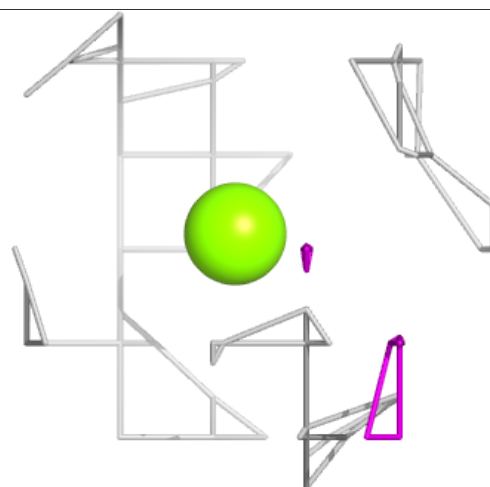
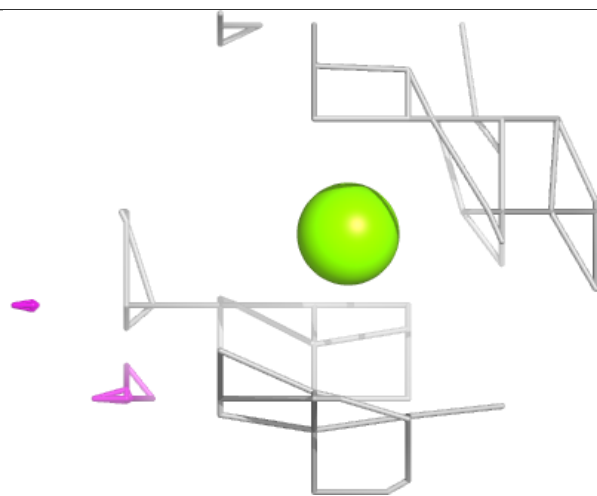
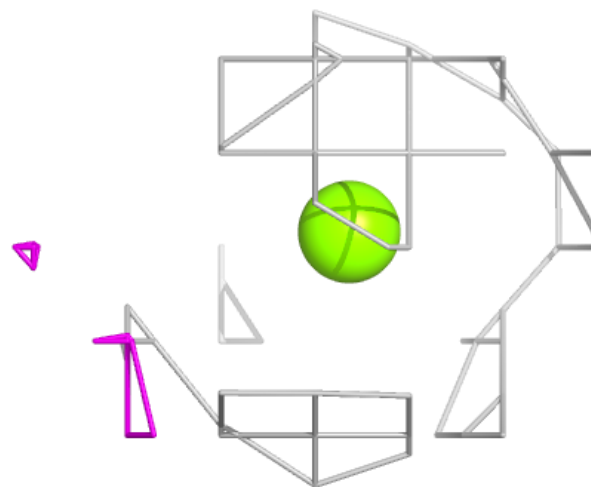
Electron density around DPO G 304:

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



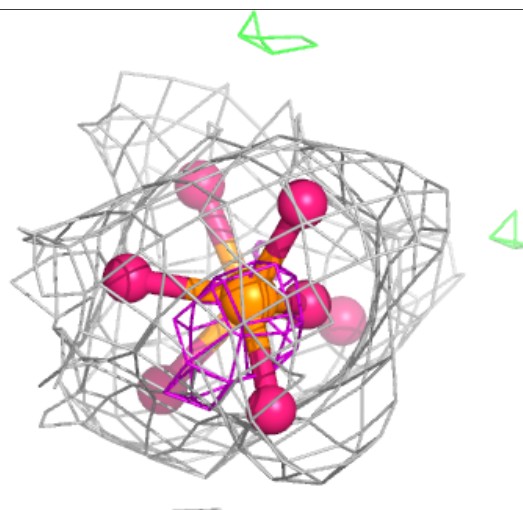
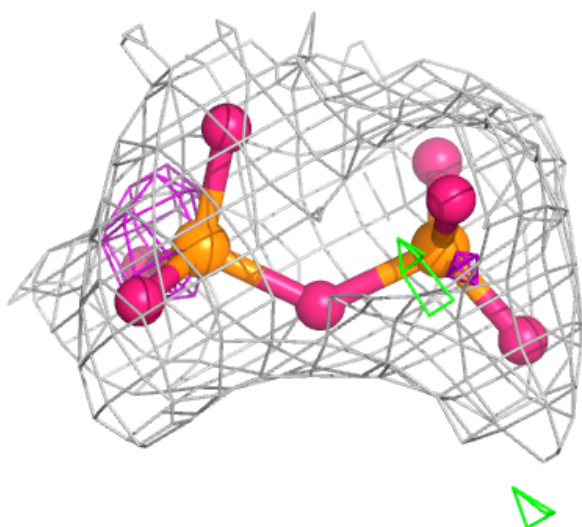
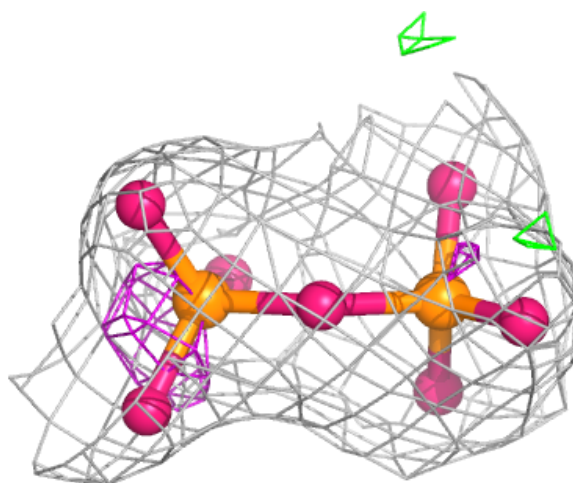
Electron density around MG E 303:

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



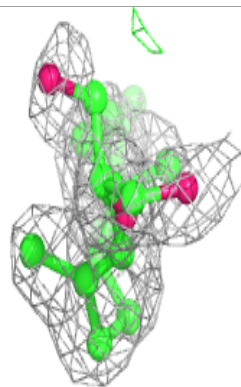
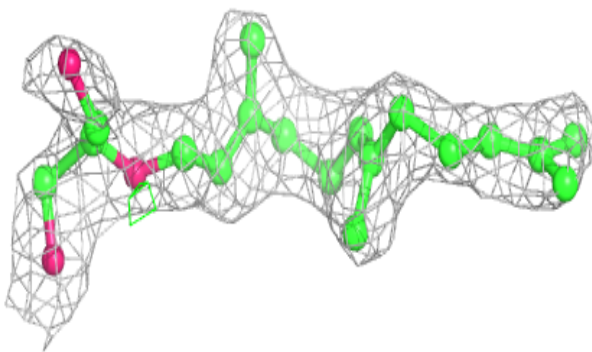
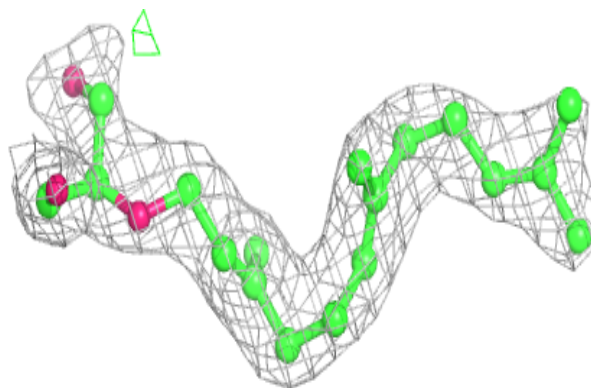
Electron density around DPO B 304:

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



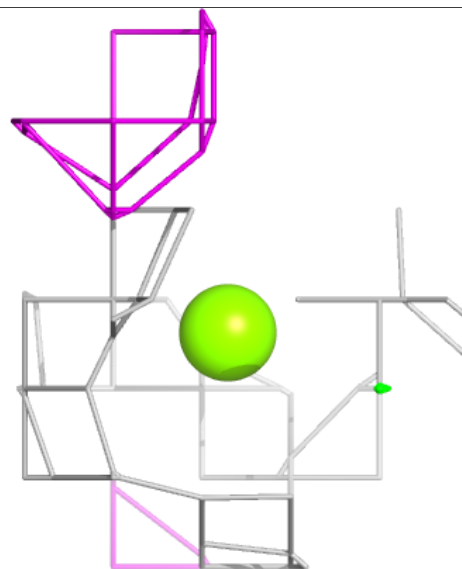
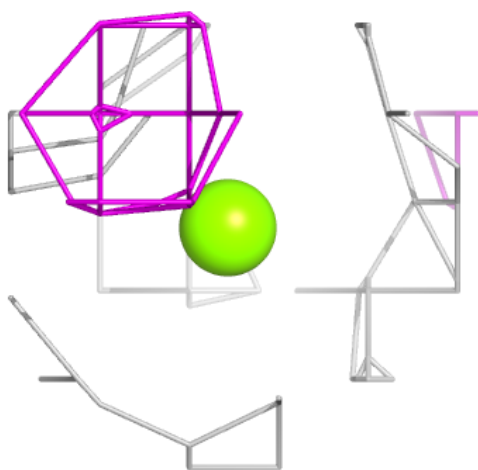
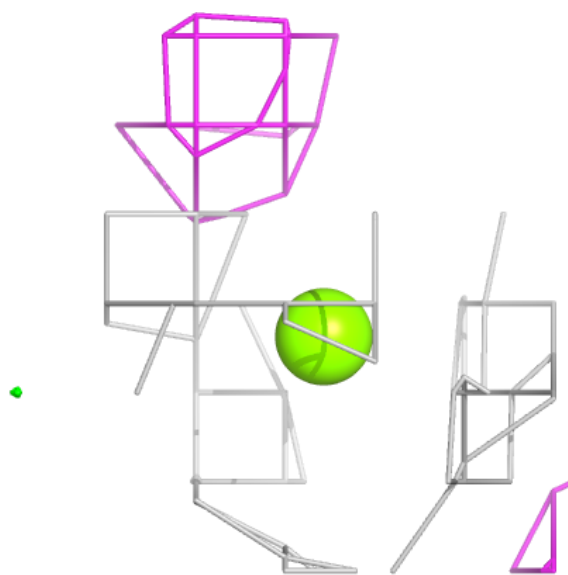
Electron density around FQ0 F 302:

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



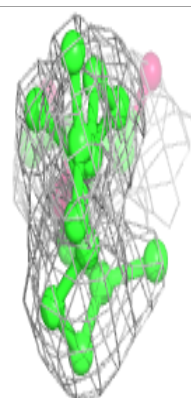
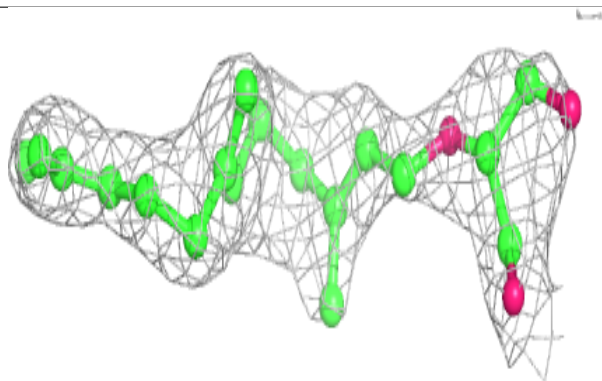
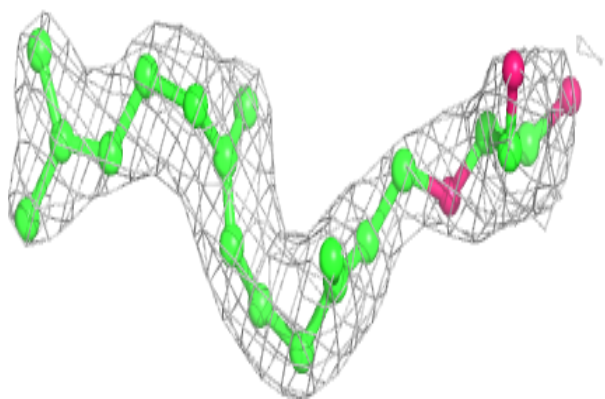
Electron density around MG H 301:

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



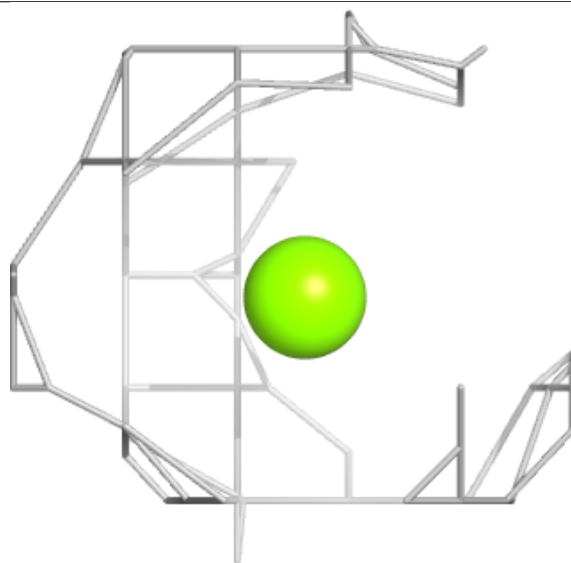
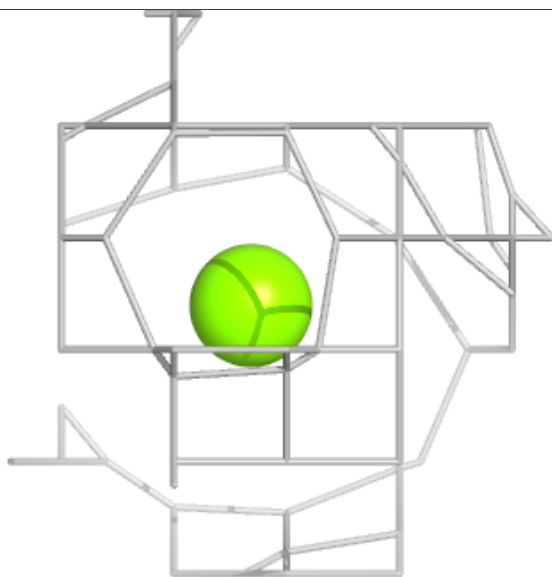
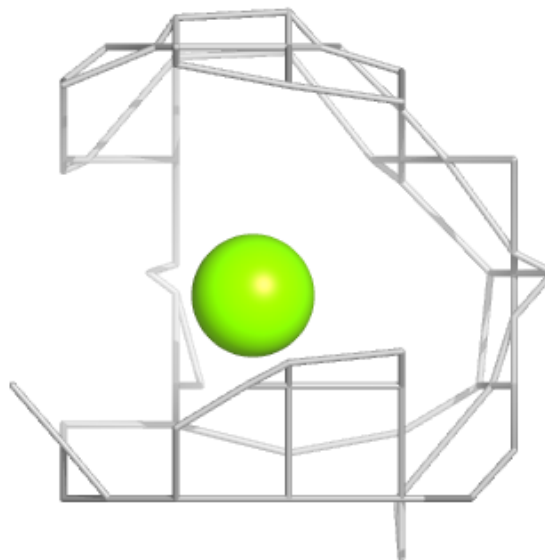
Electron density around FQ0 H 302:

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



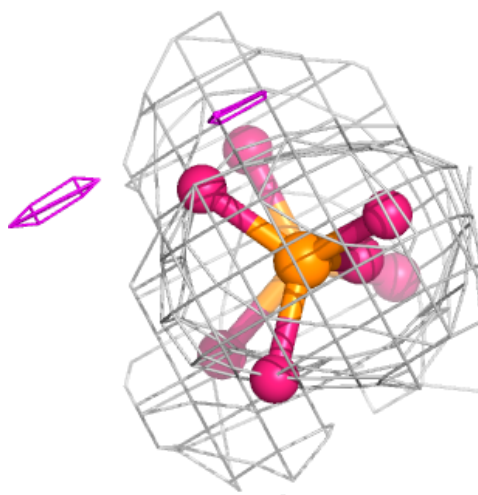
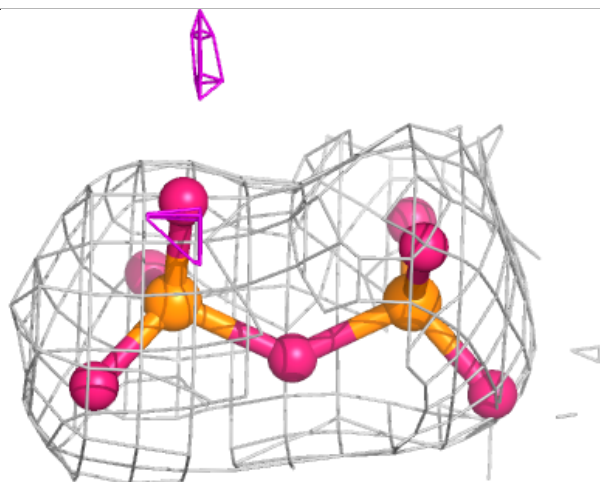
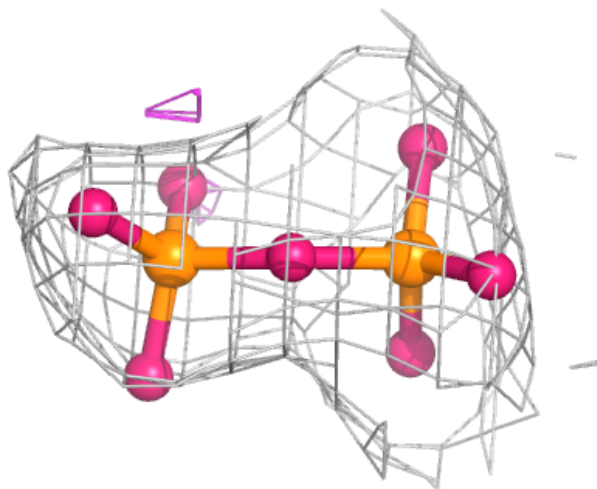
Electron density around MG B 301:

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



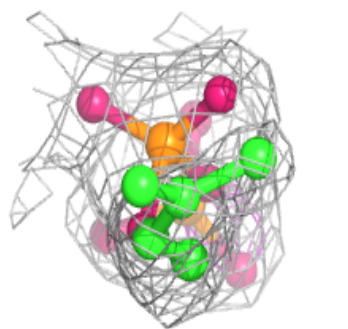
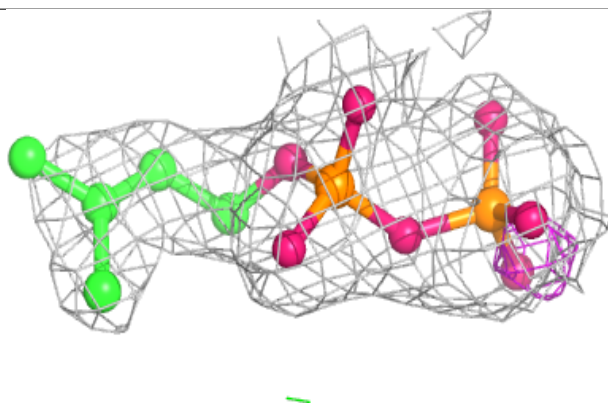
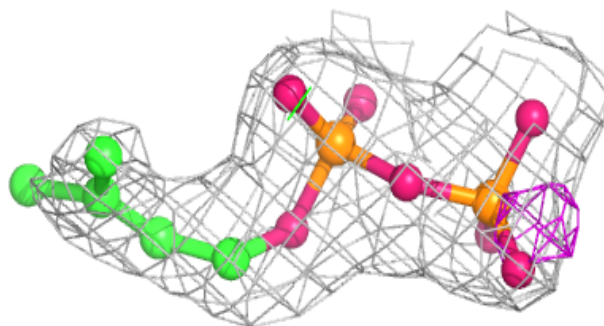
Electron density around DPO F 304:

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



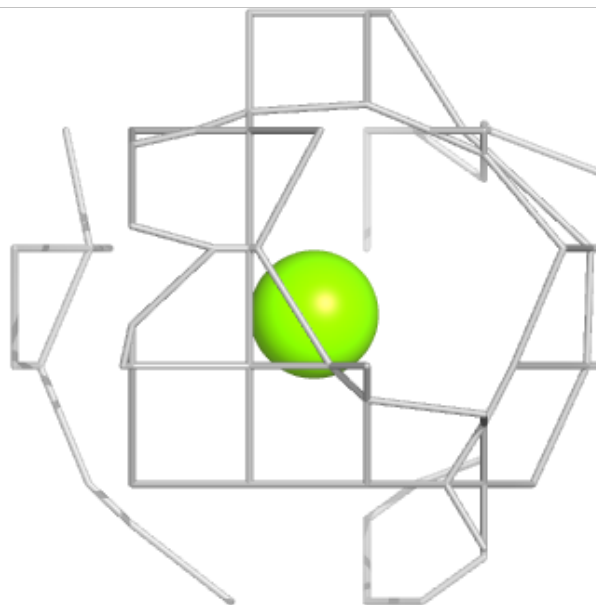
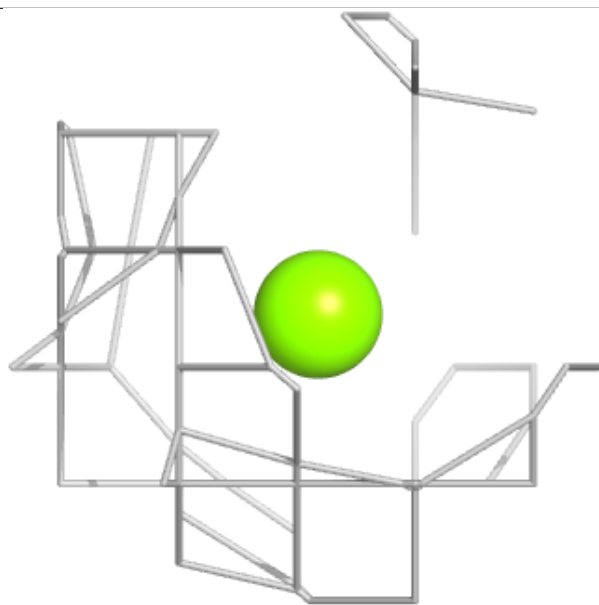
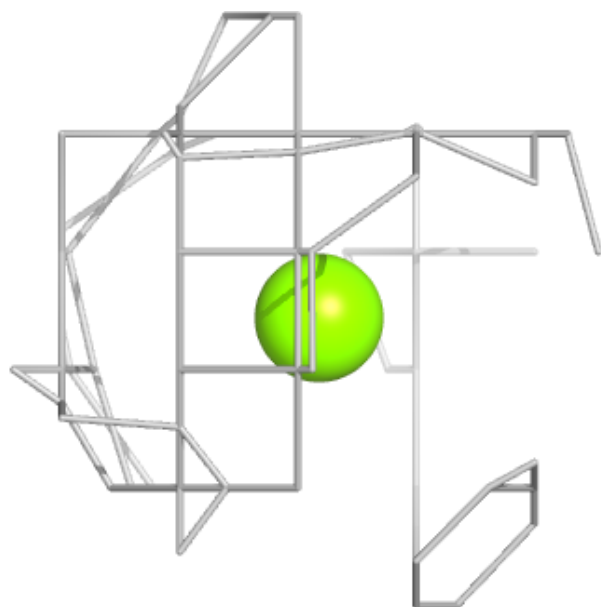
Electron density around DMA C 301:

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



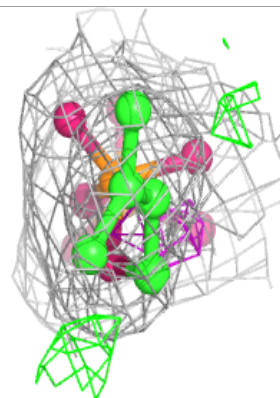
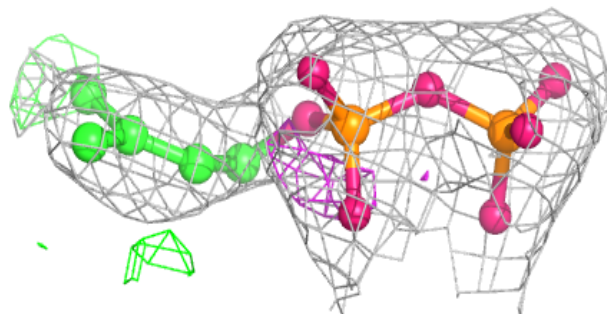
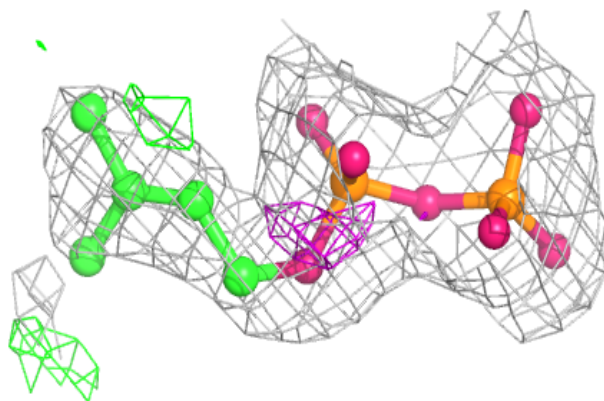
Electron density around MG A 303:

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

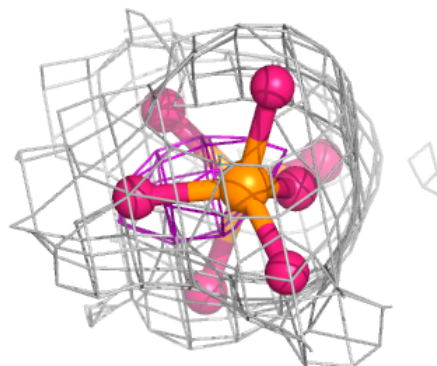
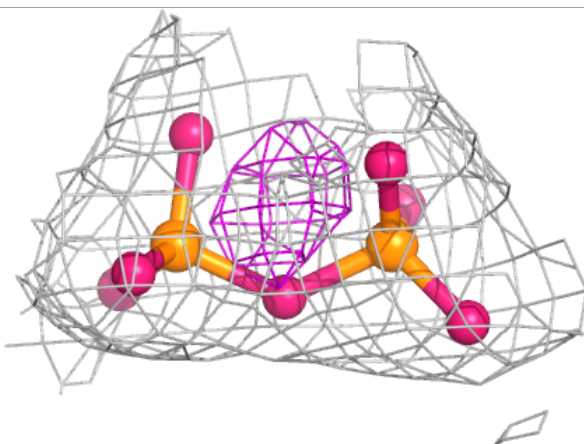
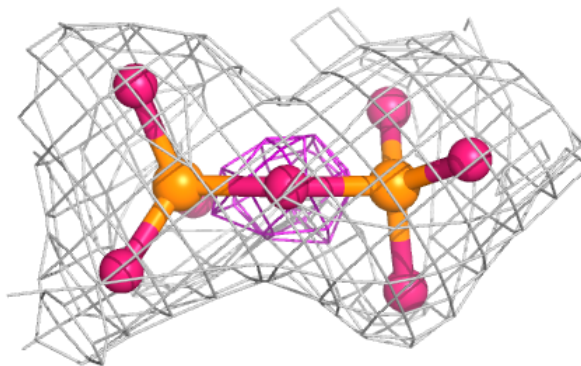


Electron density around DMA E 302:

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

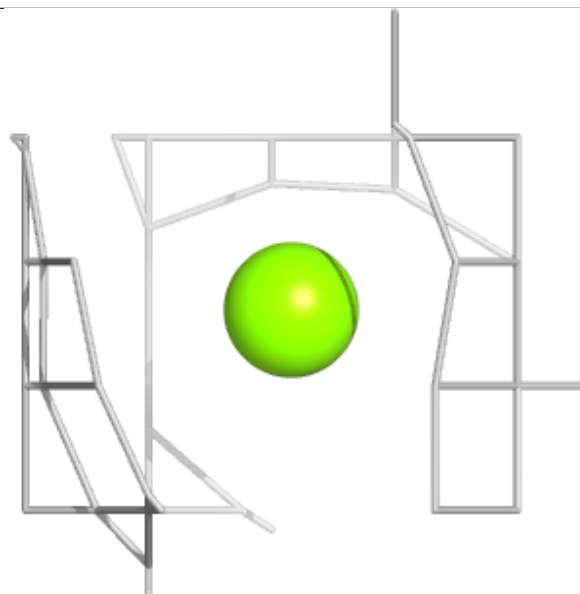
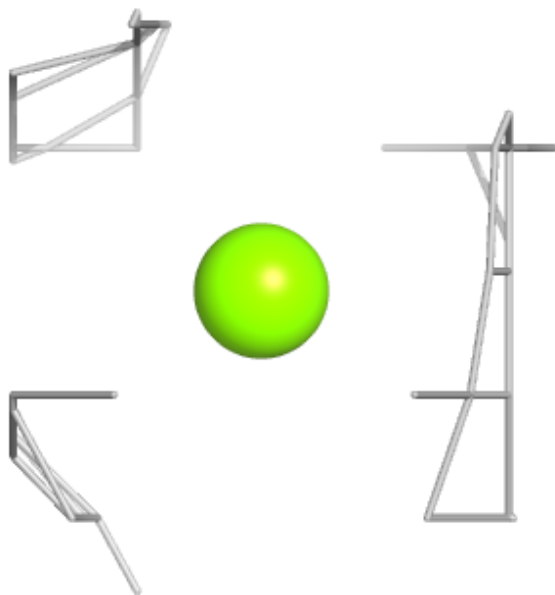
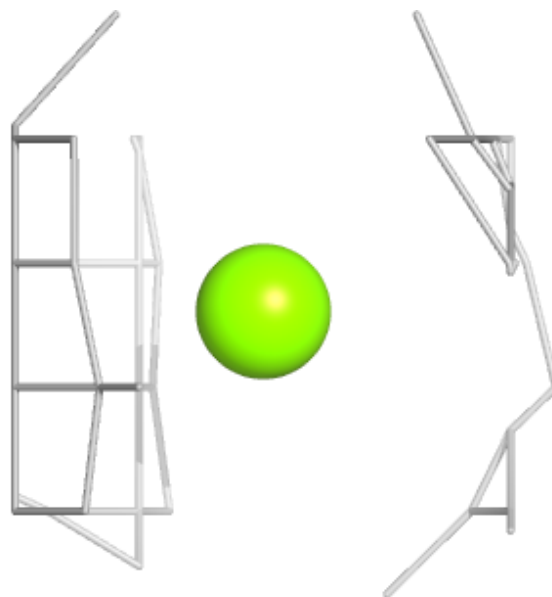
**Electron density around DPO H 303:**

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



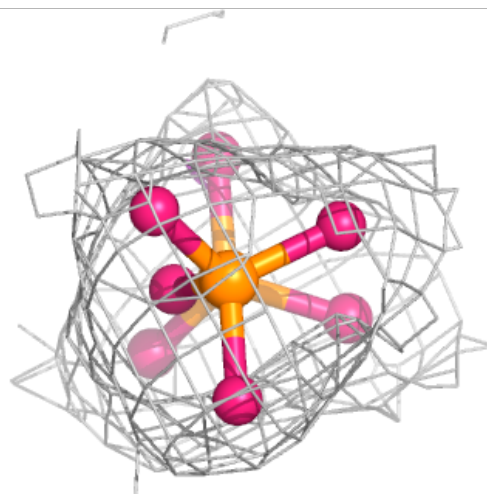
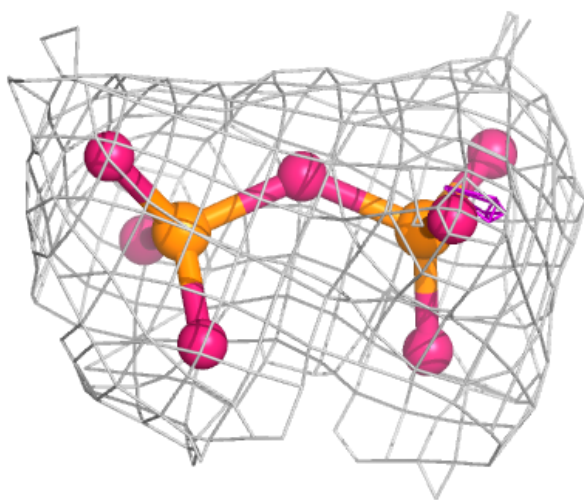
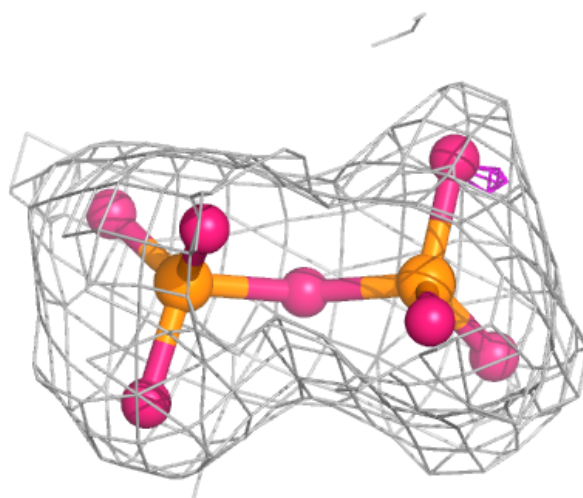
Electron density around MG C 303:

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



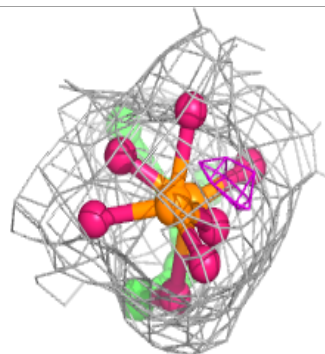
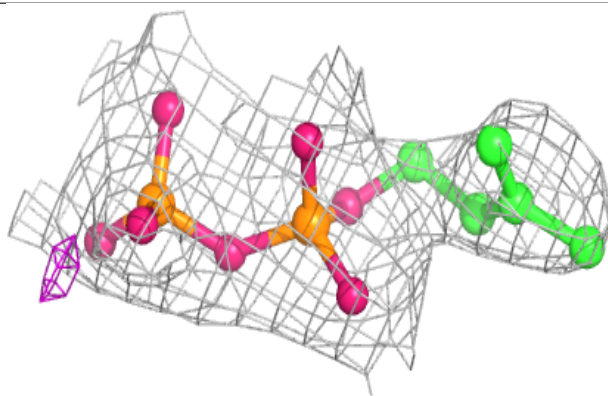
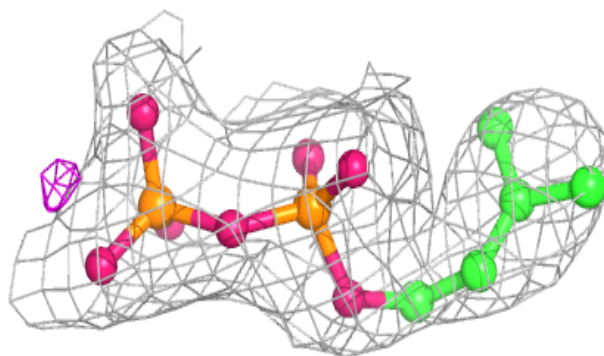
Electron density around DPO B 303:

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



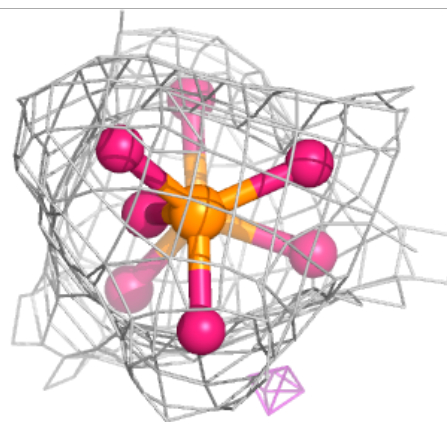
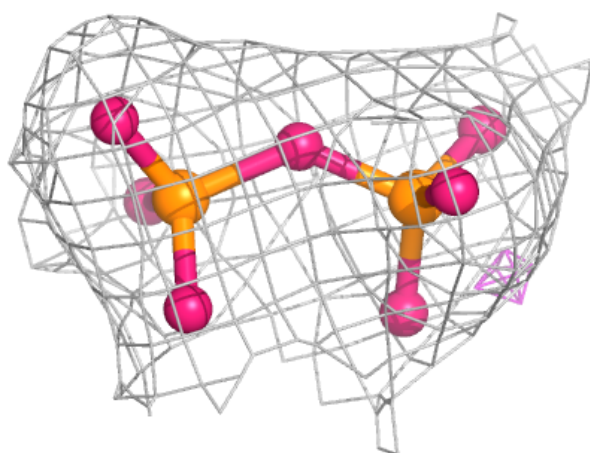
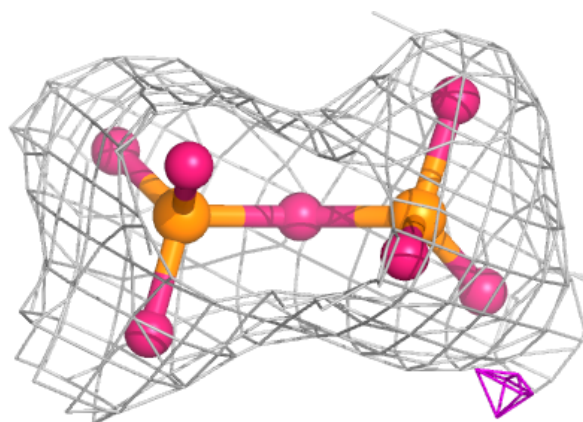
Electron density around DMA C 302:

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



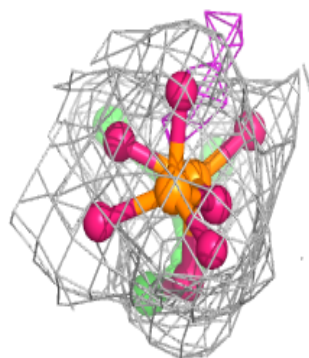
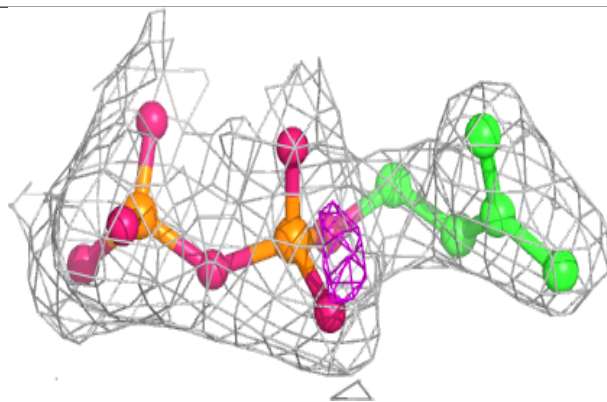
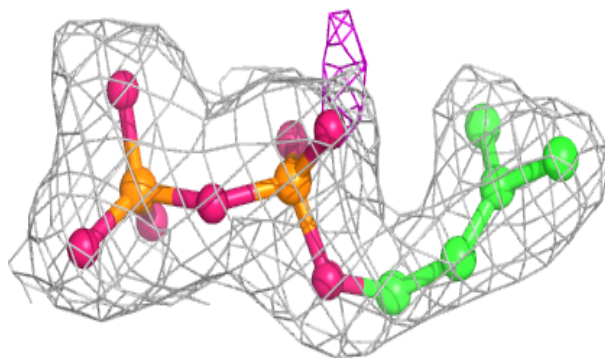
Electron density around DPO F 303:

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



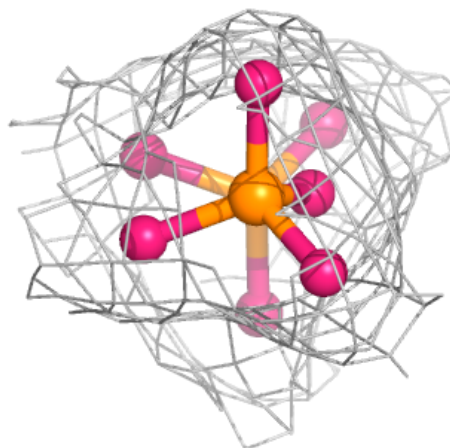
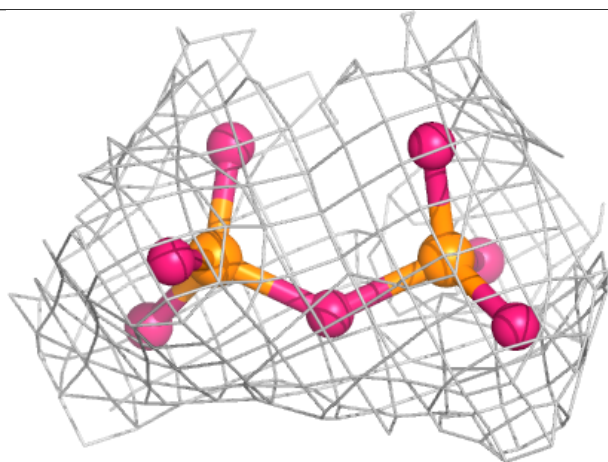
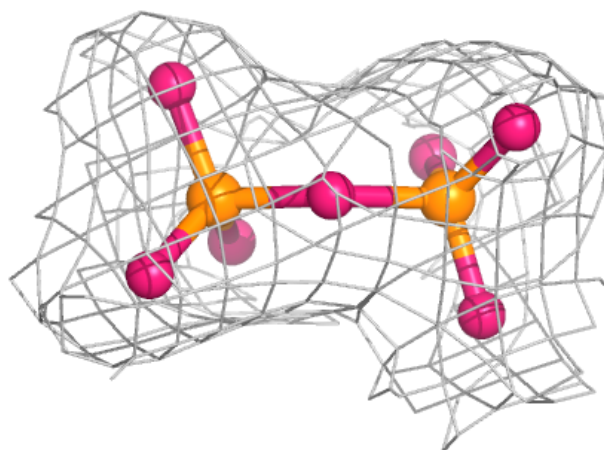
Electron density around DMA D 301:

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



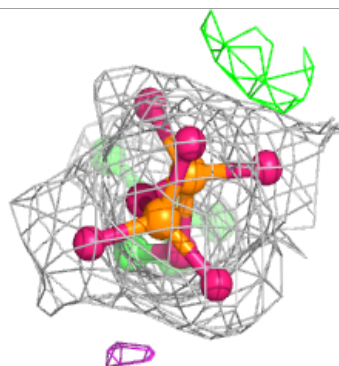
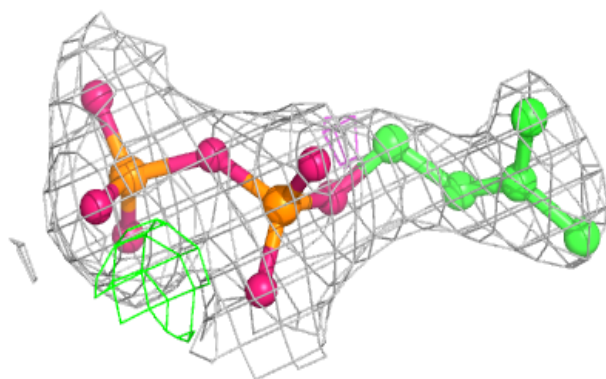
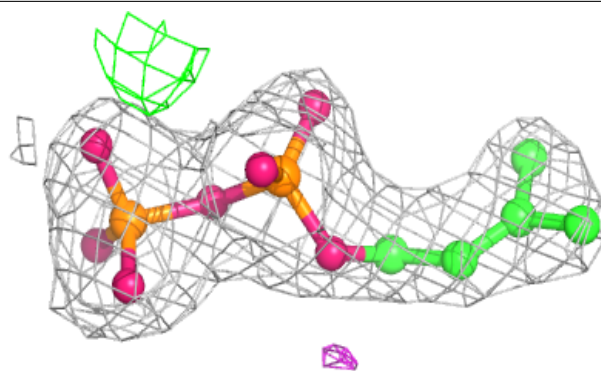
Electron density around DPO G 303:

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

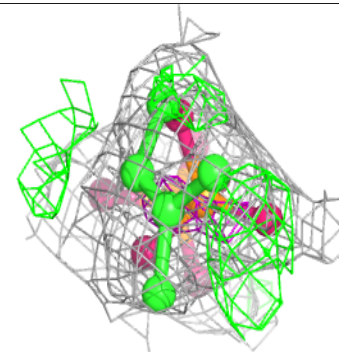
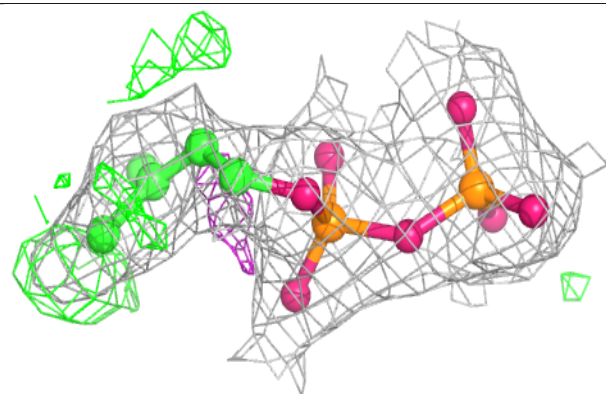
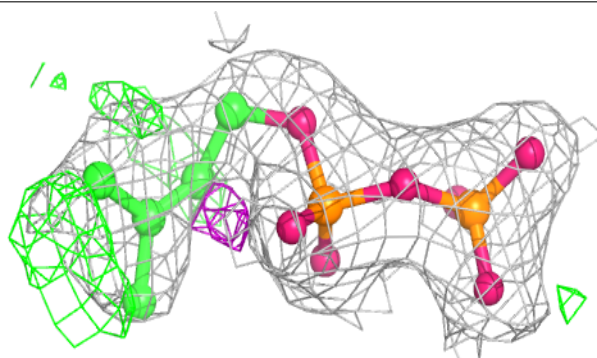


Electron density around DMA E 301:

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

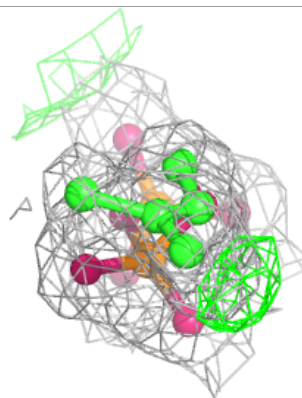
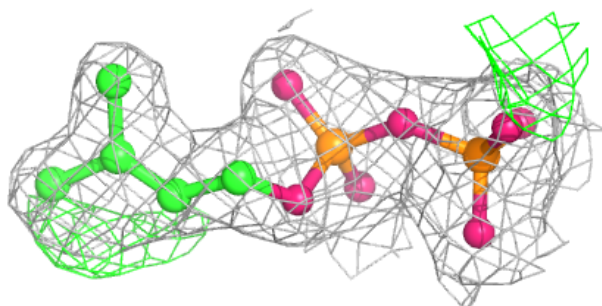
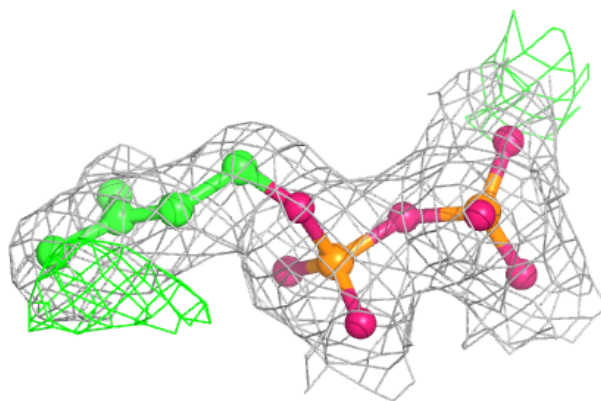
**Electron density around DMA A 302:**

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

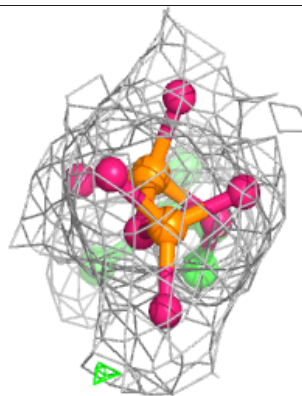
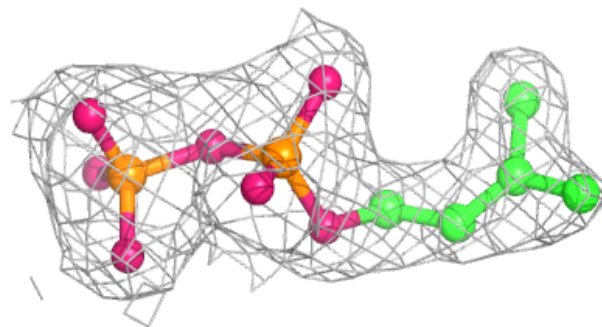
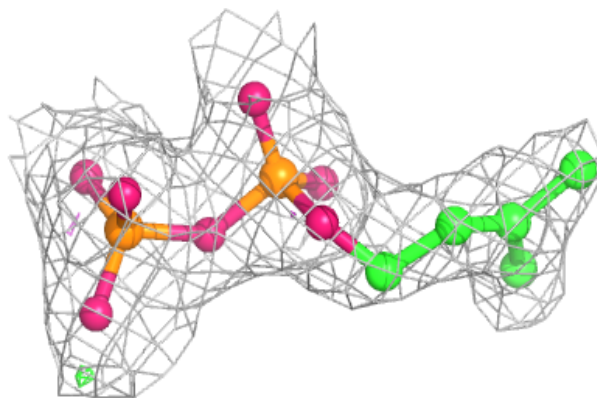


Electron density around DMA A 301:

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

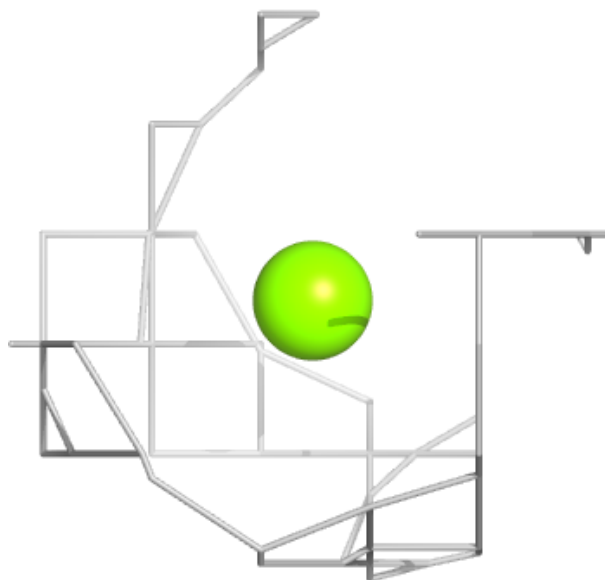
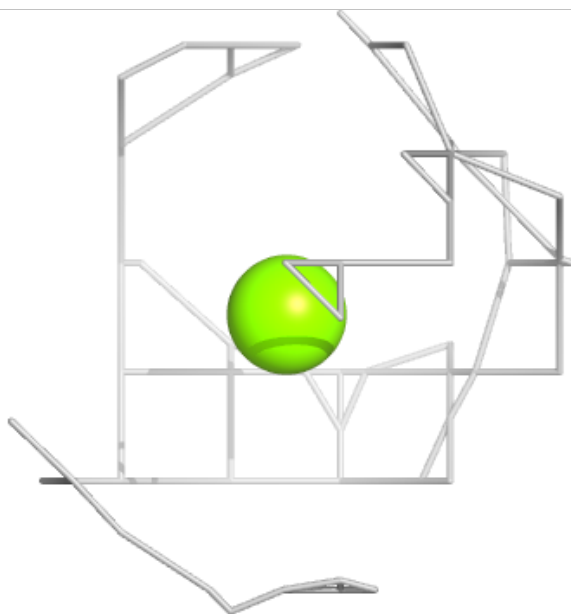
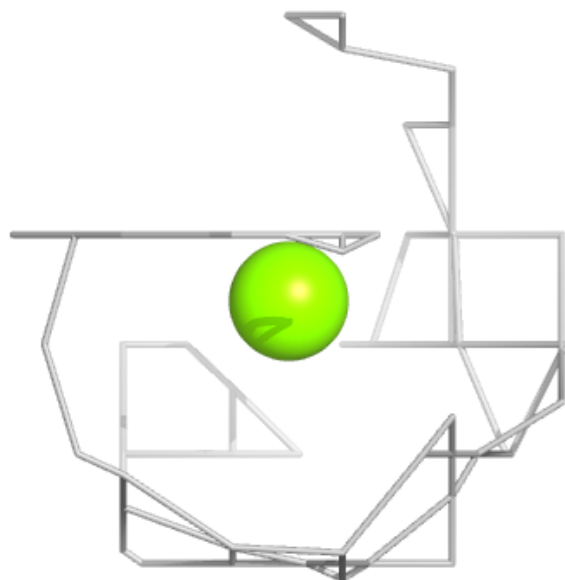
**Electron density around DMA D 302:**

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.