



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 PM UTC

PDB ID : 7CAV / pdb_00007cav
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

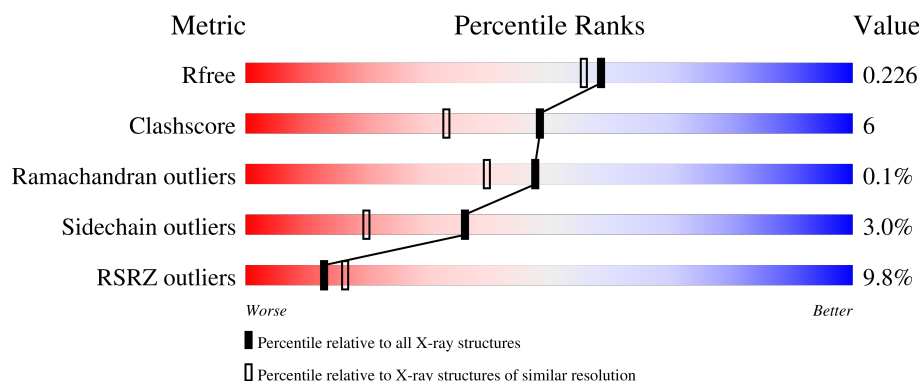
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	4% 85% 9% 6%
1	B	224	8% 84% 15% .
1	C	224	11% 76% 19% . .
1	D	224	13% 86% 7% . 6%
1	E	224	10% 77% 12% . 9%

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Mol	Chain	Length	Quality of chain
1	F	224	15% 81% 14%
1	G	224	8% 85% 11%
1	H	224	6% 81% 10% 8%

2 Entry composition

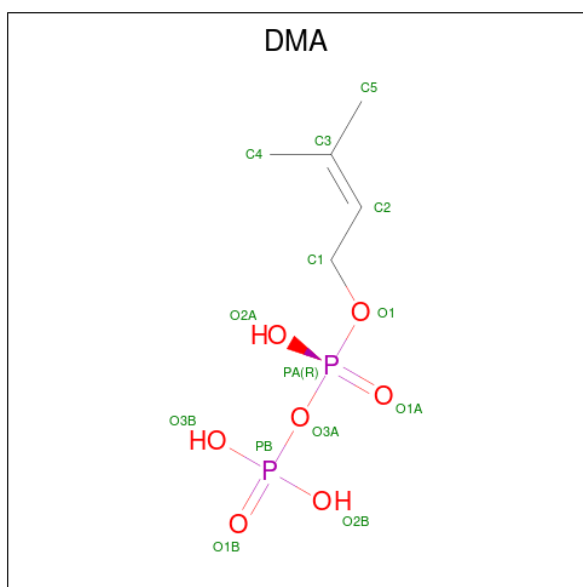
There are 7 unique types of molecules in this entry. The entry contains 14653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DMA) (formula: C₅H₁₂O₇P₂) (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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

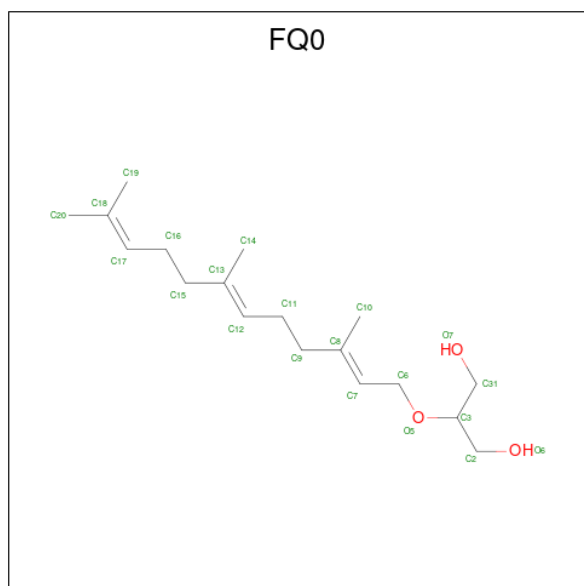
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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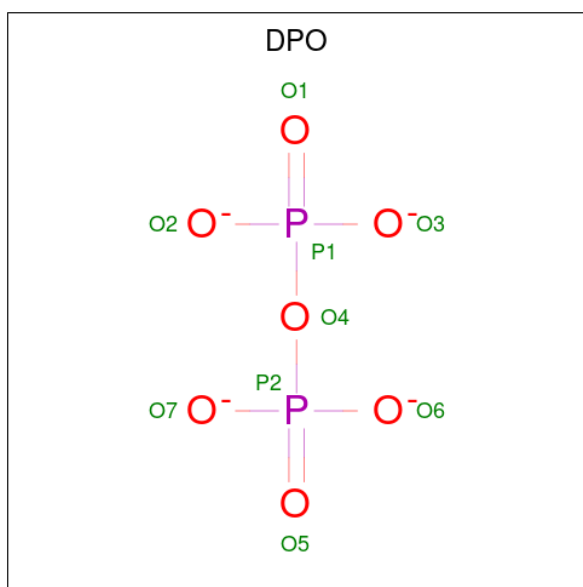
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propane-1,3-diol (CCD ID: FQ0) (formula: $C_{18}H_{32}O_3$) (labeled as "Ligand of Interest" by depositor).



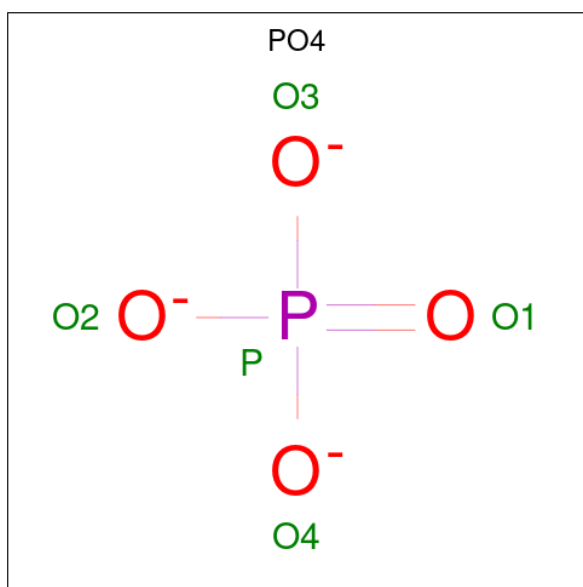
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			21	18	3		
4	F	1	Total	C	O	0	0
			21	18	3		
4	G	1	Total	C	O	0	0
			21	18	3		
4	H	1	Total	C	O	0	0
			21	18	3		

- Molecule 5 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2) (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 (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

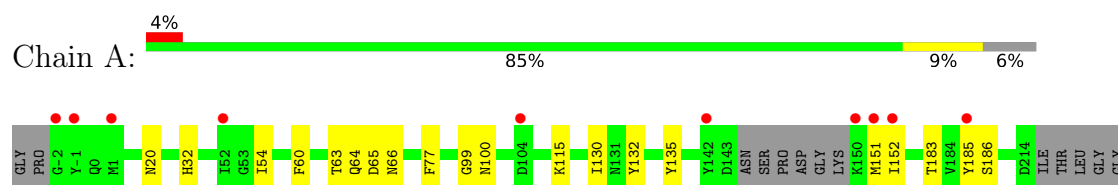
- Molecule 7 is water.

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		

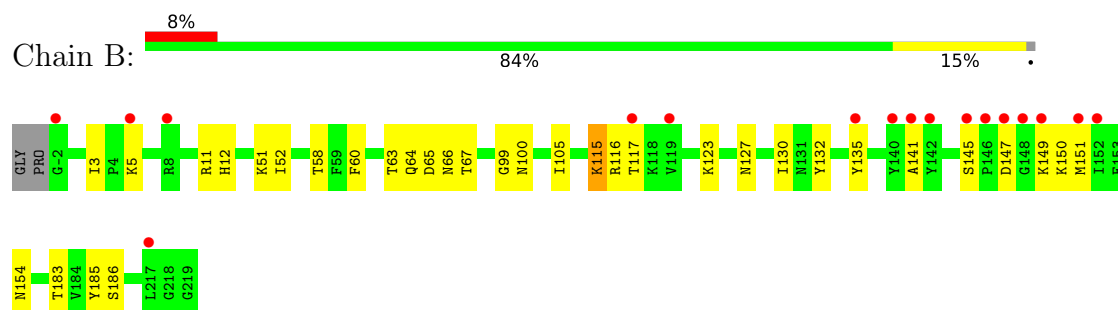
3 Residue-property plots [i](#)

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.

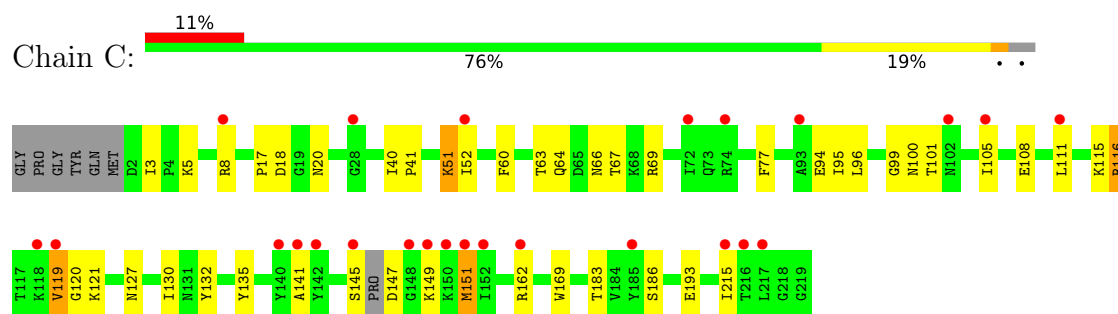
• Molecule 1: cis-prenyltransferase MM_0014



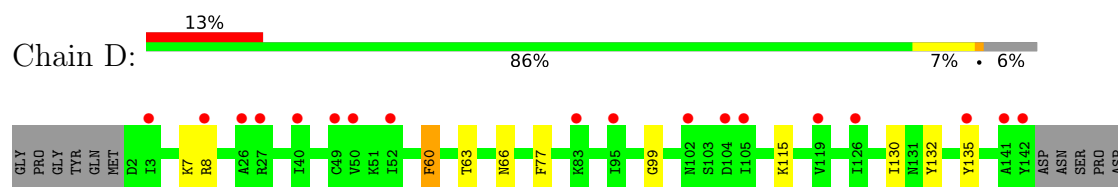
• Molecule 1: cis-prenyltransferase MM_0014

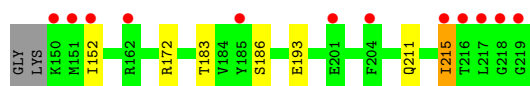


• Molecule 1: cis-prenyltransferase MM_0014

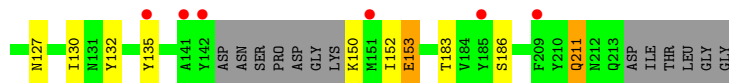
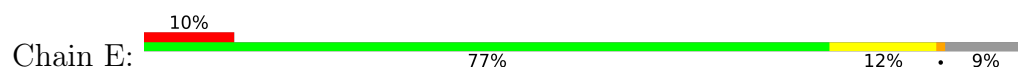


• Molecule 1: cis-prenyltransferase MM_0014

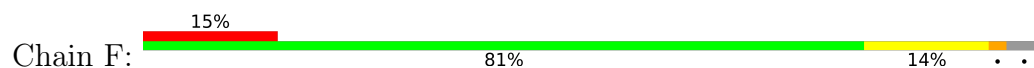




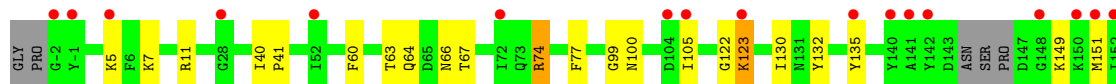
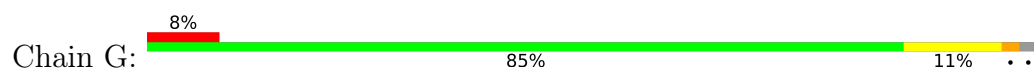
- Molecule 1: cis-prenyltransferase MM_0014



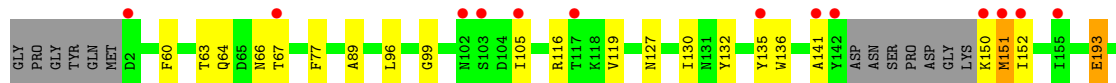
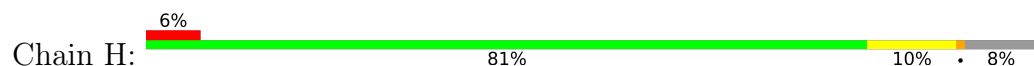
- Molecule 1: cis-prenyltransferase MM_0014



- 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) 99.9 (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 (5.10%)	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)	0.35 , 31.3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FQ0, DMA, MG, 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	0.95	0/1769	1.29	3/2390 (0.1%)
1	B	0.97	0/1845	1.26	0/2493
1	C	0.97	0/1802	1.32	3/2433 (0.1%)
1	D	0.95	0/1759	1.29	1/2376 (0.0%)
1	E	0.96	0/1711	1.29	1/2312 (0.0%)
1	F	0.97	0/1794	1.32	0/2422
1	G	0.97	0/1822	1.30	1/2459 (0.0%)
1	H	0.97	0/1727	1.27	1/2334 (0.0%)
All	All	0.96	0/14229	1.29	10/19219 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	PHE	CA-CB-CG	5.89	119.69	113.80
1	E	77	PHE	CA-CB-CG	5.79	119.59	113.80
1	D	77	PHE	CA-CB-CG	5.52	119.32	113.80
1	C	77	PHE	CA-CB-CG	5.49	119.29	113.80
1	H	77	PHE	CA-CB-CG	5.46	119.26	113.80
1	G	77	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	147	ASP	CA-C-N	5.15	125.55	119.94
1	C	147	ASP	C-N-CA	5.15	125.55	119.94
1	A	54	ILE	CA-C-N	5.13	125.65	120.00
1	A	54	ILE	C-N-CA	5.13	125.65	120.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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	1	0
7	H	60	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:122:GLY:C	1:G:123:LYS:HG3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:123:LYS:C	1:G:123:LYS:HD2	2.44	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

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%)	24	14
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%)	48	40

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%)	181 (98%)	3 (2%)	55	44
1	B	192/193 (100%)	187 (97%)	5 (3%)	40	24
1	C	188/193 (97%)	180 (96%)	8 (4%)	26	11
1	D	183/193 (95%)	179 (98%)	4 (2%)	45	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	178/193 (92%)	173 (97%)	5 (3%)	38	22
1	F	187/193 (97%)	179 (96%)	8 (4%)	26	11
1	G	189/193 (98%)	182 (96%)	7 (4%)	30	15
1	H	180/193 (93%)	175 (97%)	5 (3%)	38	22
All	All	1481/1544 (96%)	1436 (97%)	45 (3%)	36	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	A	115	LYS
1	A	151	MET
1	B	5	LYS
1	B	60	PHE
1	B	115	LYS
1	B	147	ASP
1	B	150	LYS
1	C	5	LYS
1	C	51	LYS
1	C	60	PHE
1	C	115	LYS
1	C	116	ARG
1	C	119	VAL
1	C	151	MET
1	C	193	GLU
1	D	60	PHE
1	D	115	LYS
1	D	193	GLU
1	D	215	ILE
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	115	LYS
1	F	151	MET
1	F	152	ILE
1	F	172	ARG

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Mol	Chain	Res	Type
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	193	GLU
1	H	211	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) 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	B	12	HIS
1	B	64	GLN
1	B	66	ASN
1	B	127	ASN
1	B	131	ASN
1	B	211	GLN
1	C	12	HIS
1	C	20	ASN
1	C	64	GLN
1	C	66	ASN
1	C	71	GLN
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	64	GLN

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Mol	Chain	Res	Type
1	E	66	ASN
1	E	127	ASN
1	E	131	ASN
1	E	154	ASN
1	E	211	GLN
1	F	20	ASN
1	F	66	ASN
1	F	100	ASN
1	F	211	GLN
1	F	213	GLN
1	G	20	ASN
1	G	64	GLN
1	G	66	ASN
1	G	71	GLN
1	G	131	ASN
1	G	211	GLN
1	G	213	GLN
1	H	12	HIS
1	H	64	GLN
1	H	66	ASN
1	H	71	GLN
1	H	127	ASN
1	H	131	ASN
1	H	154	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 oligosaccharides 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
2	DMA	C	302	3	12,13,13	0.59	0	15,19,19	0.64	0
4	FQ0	H	302	-	20,20,20	0.54	0	22,23,23	1.14	2 (9%)
4	FQ0	G	302	-	20,20,20	0.66	0	22,23,23	0.94	0
2	DMA	E	302	3	12,13,13	0.61	0	15,19,19	0.77	0
5	DPO	F	303	3	6,8,8	0.84	0	12,13,13	0.71	0
5	DPO	F	304	3	6,8,8	0.75	0	12,13,13	0.77	0
5	DPO	B	303	3	6,8,8	0.92	0	12,13,13	0.86	0
6	PO4	G	305	3	4,4,4	0.63	0	6,6,6	0.48	0
5	DPO	G	303	3	6,8,8	0.73	0	12,13,13	0.73	0
2	DMA	A	302	3	12,13,13	1.19	2 (16%)	15,19,19	0.76	0
4	FQ0	F	302	-	20,20,20	0.64	0	22,23,23	1.18	2 (9%)
2	DMA	A	301	3	12,13,13	0.92	0	15,19,19	0.82	0
5	DPO	B	304	3	6,8,8	0.70	0	12,13,13	0.82	0
2	DMA	D	302	3	12,13,13	0.66	0	15,19,19	0.66	0
4	FQ0	B	302	-	20,20,20	0.62	0	22,23,23	1.01	0
5	DPO	G	304	3	6,8,8	0.79	0	12,13,13	0.76	0
2	DMA	C	301	3	12,13,13	0.56	0	15,19,19	0.67	0
2	DMA	E	301	3	12,13,13	0.72	0	15,19,19	0.80	0
5	DPO	H	303	3	6,8,8	0.76	0	12,13,13	0.68	0
2	DMA	D	301	3	12,13,13	0.72	0	15,19,19	0.74	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMA	C	302	3	-	4/13/13/13	-
4	FQ0	H	302	-	-	3/22/22/22	-
4	FQ0	G	302	-	-	1/22/22/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMA	E	302	3	-	4/13/13/13	-
5	DPO	F	303	3	-	1/6/6/6	-
5	DPO	F	304	3	-	0/6/6/6	-
5	DPO	B	303	3	-	1/6/6/6	-
5	DPO	G	303	3	-	3/6/6/6	-
2	DMA	A	302	3	-	5/13/13/13	-
4	FQ0	F	302	-	-	5/22/22/22	-
2	DMA	A	301	3	-	3/13/13/13	-
5	DPO	B	304	3	-	3/6/6/6	-
2	DMA	D	302	3	-	3/13/13/13	-
4	FQ0	B	302	-	-	0/22/22/22	-
5	DPO	G	304	3	-	0/6/6/6	-
2	DMA	C	301	3	-	3/13/13/13	-
2	DMA	E	301	3	-	5/13/13/13	-
5	DPO	H	303	3	-	1/6/6/6	-
2	DMA	D	301	3	-	3/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	DMA	PA-O3A	3.09	1.62	1.59
2	A	302	DMA	PB-O3B	-2.31	1.46	1.54

All (5) 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	C2-C3-C31	-2.09	109.18	112.79
2	D	301	DMA	O3B-PB-O2B	2.02	115.38	107.80
4	H	302	FQ0	C9-C8-C7	-2.02	116.64	121.17
4	F	302	FQ0	C6-C7-C8	-2.01	122.90	126.20

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	301	DMA	C1-O1-PA-O3A
2	A	302	DMA	C2-C1-O1-PA

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

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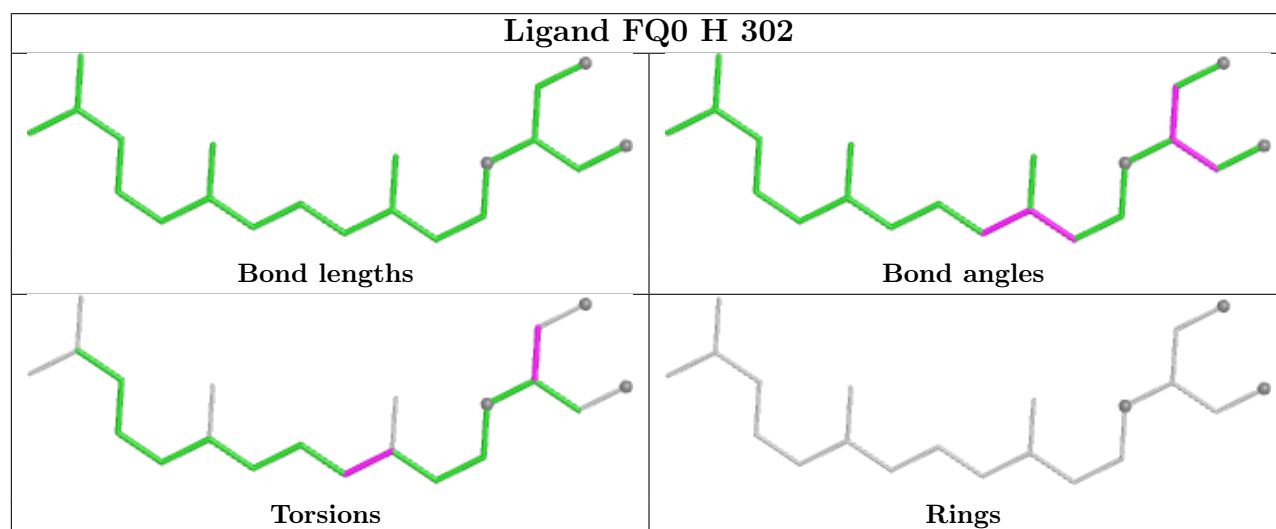
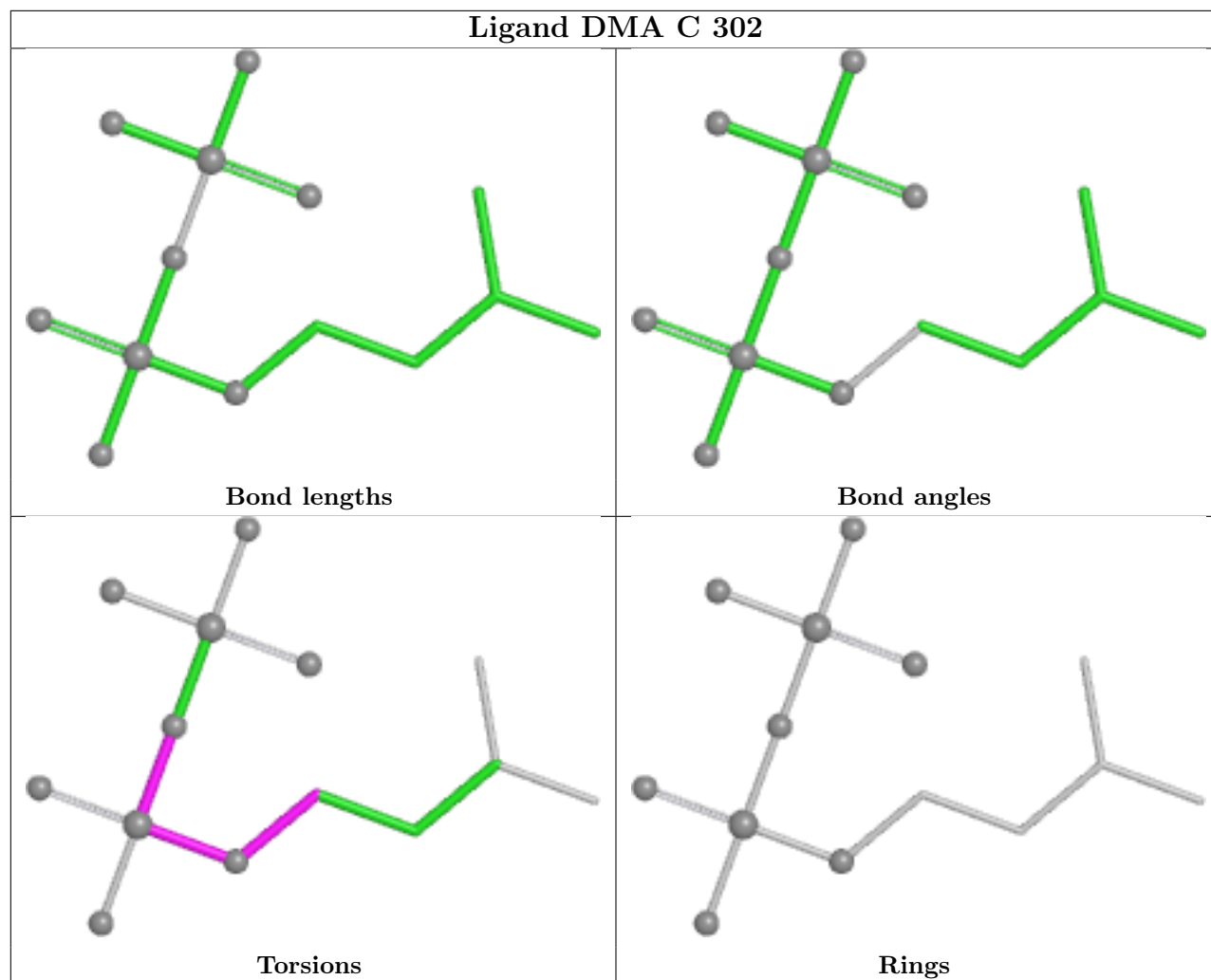
Mol	Chain	Res	Type	Atoms
2	E	302	DMA	PB-O3A-PA-O1A
4	F	302	FQ0	O6-C2-C3-C31
2	C	302	DMA	PB-O3A-PA-O1A

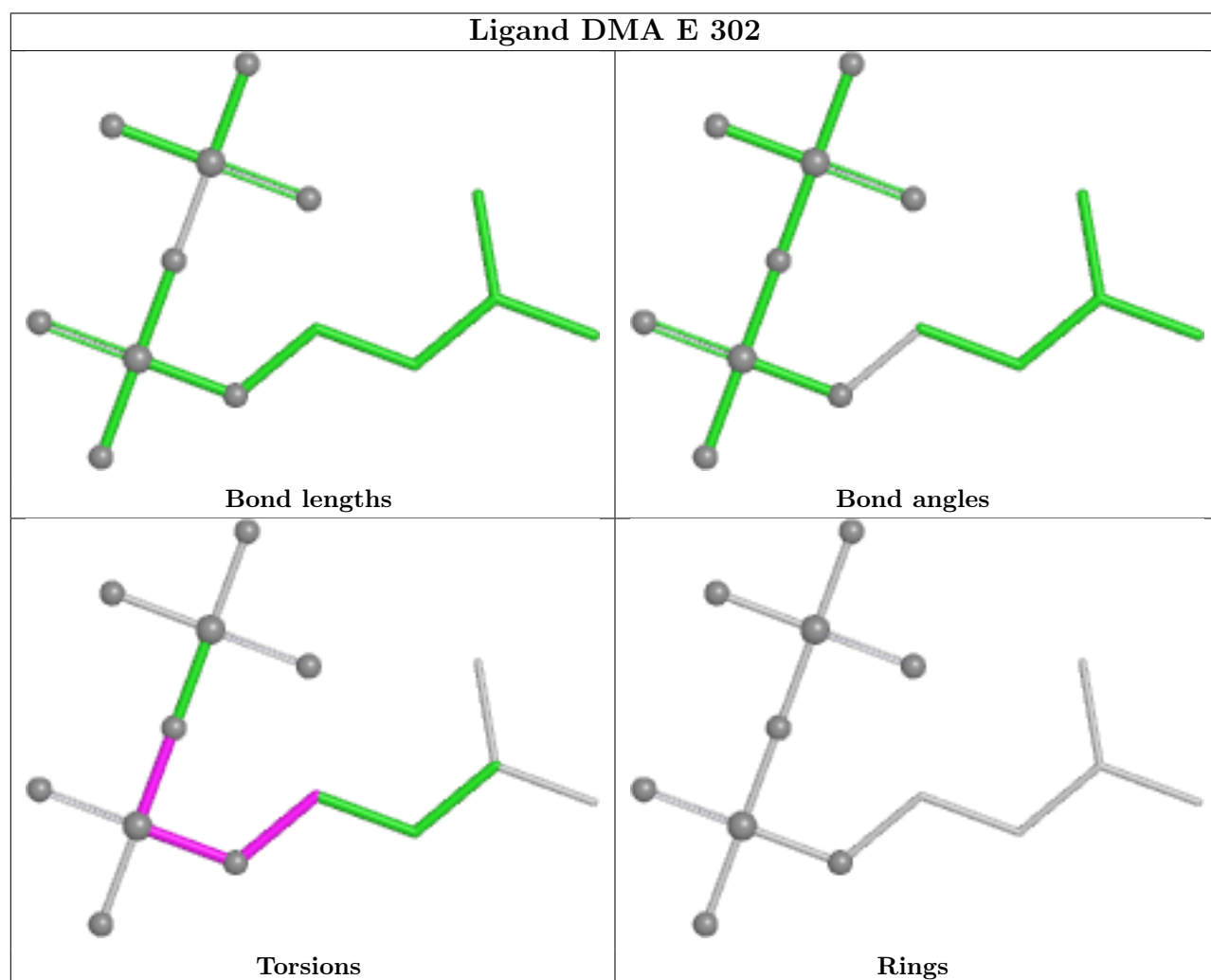
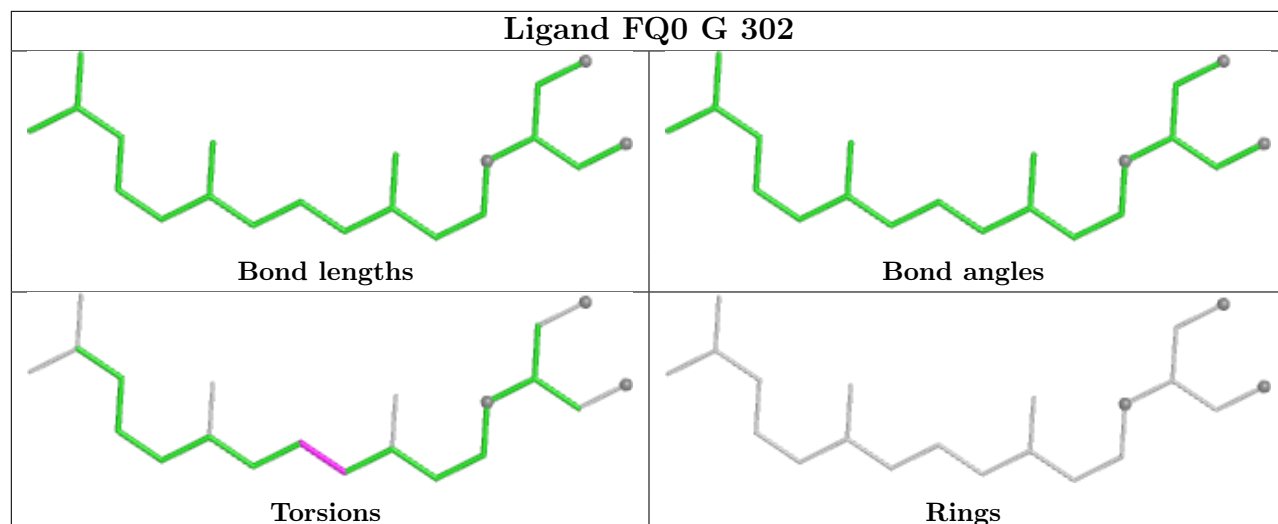
There are no ring outliers.

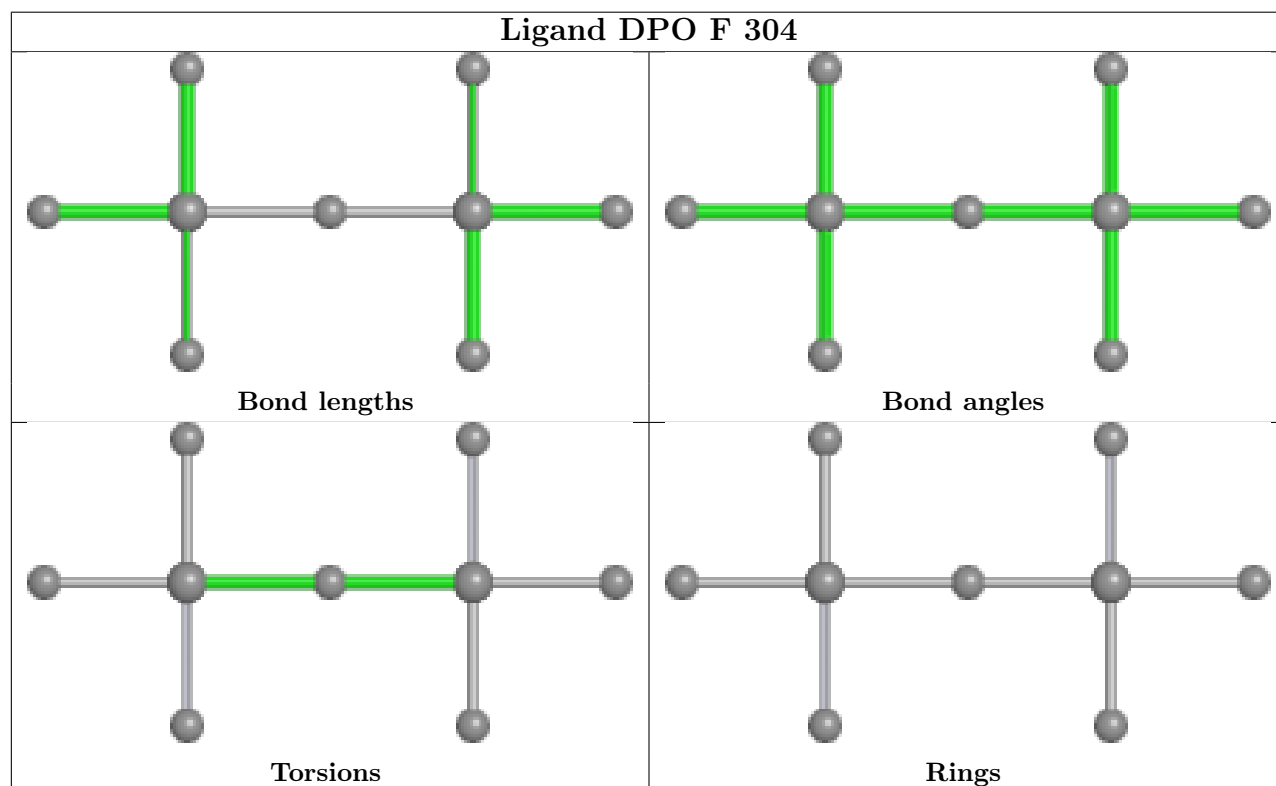
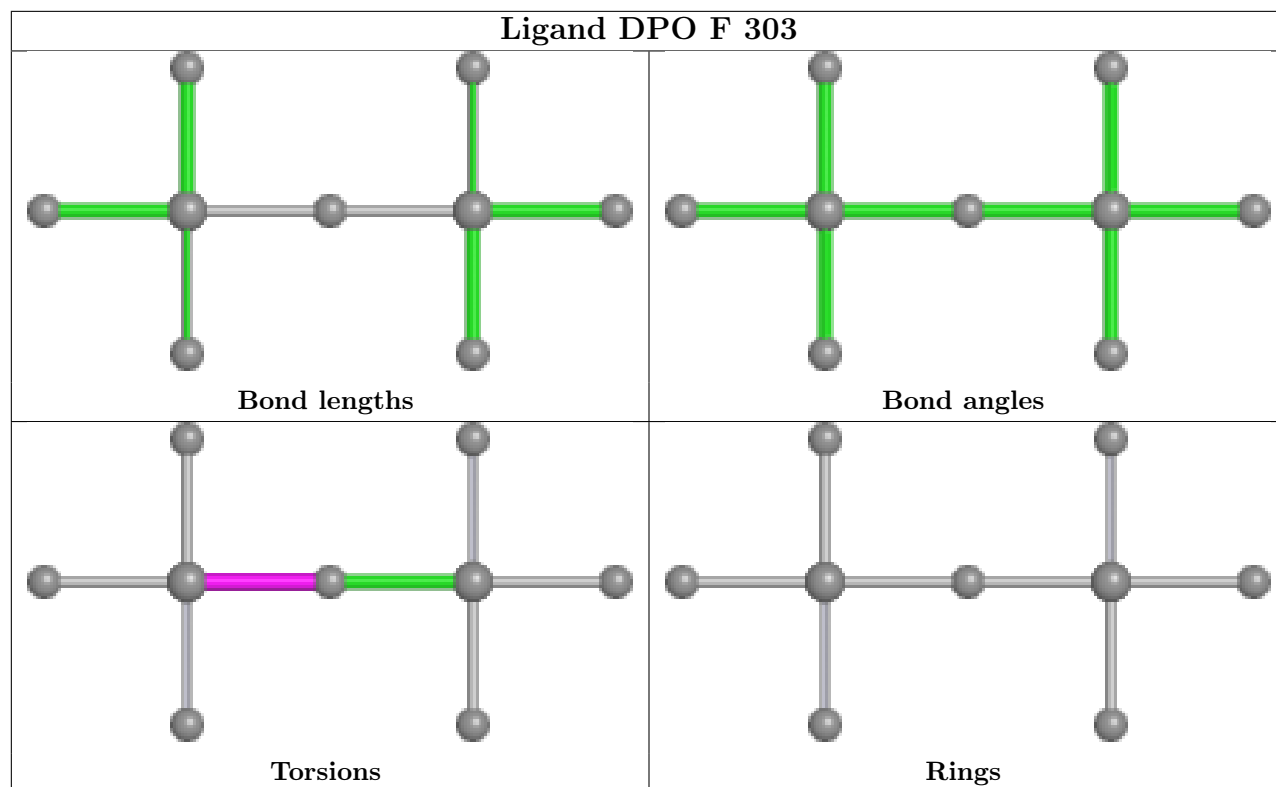
9 monomers are involved in 18 short contacts:

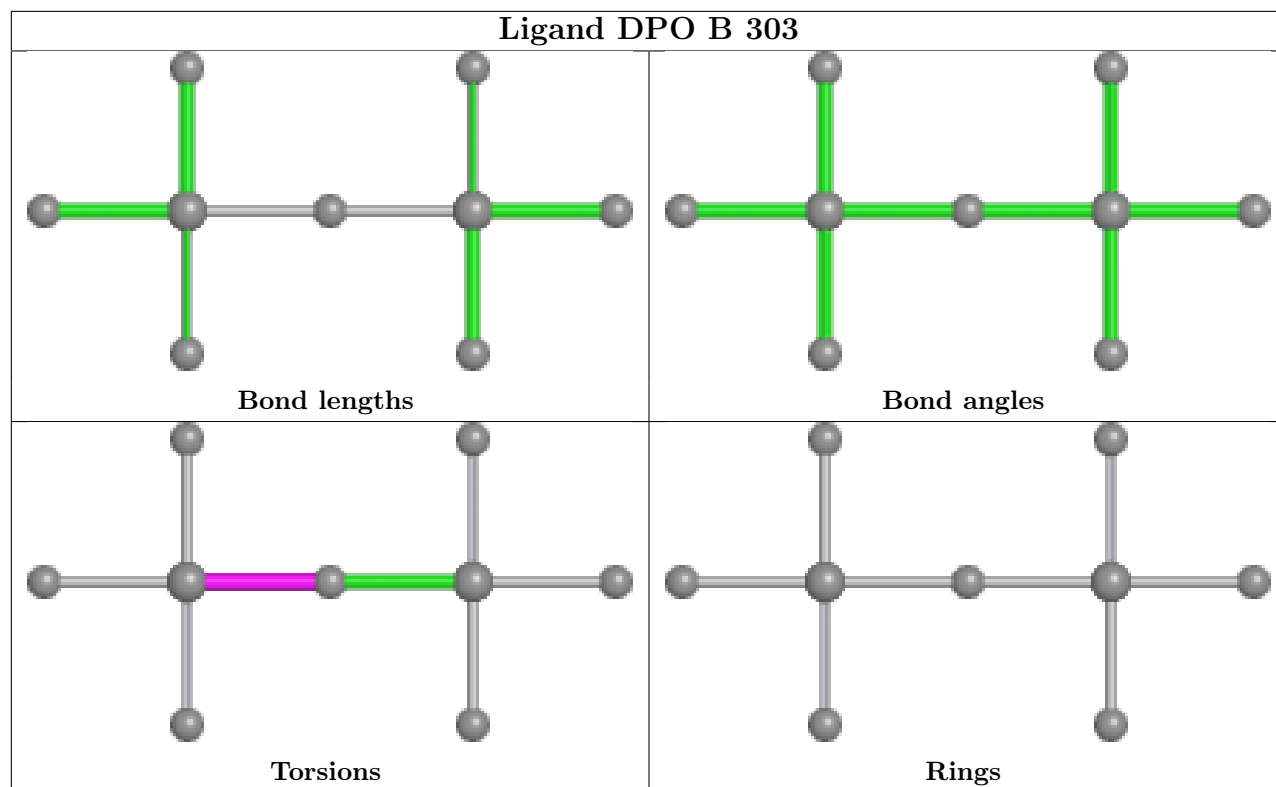
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	DMA	2	0
4	H	302	FQ0	2	0
2	E	302	DMA	5	0
2	A	302	DMA	4	0
2	A	301	DMA	3	0
2	D	302	DMA	1	0
2	C	301	DMA	2	0
2	E	301	DMA	1	0
5	H	303	DPO	1	0

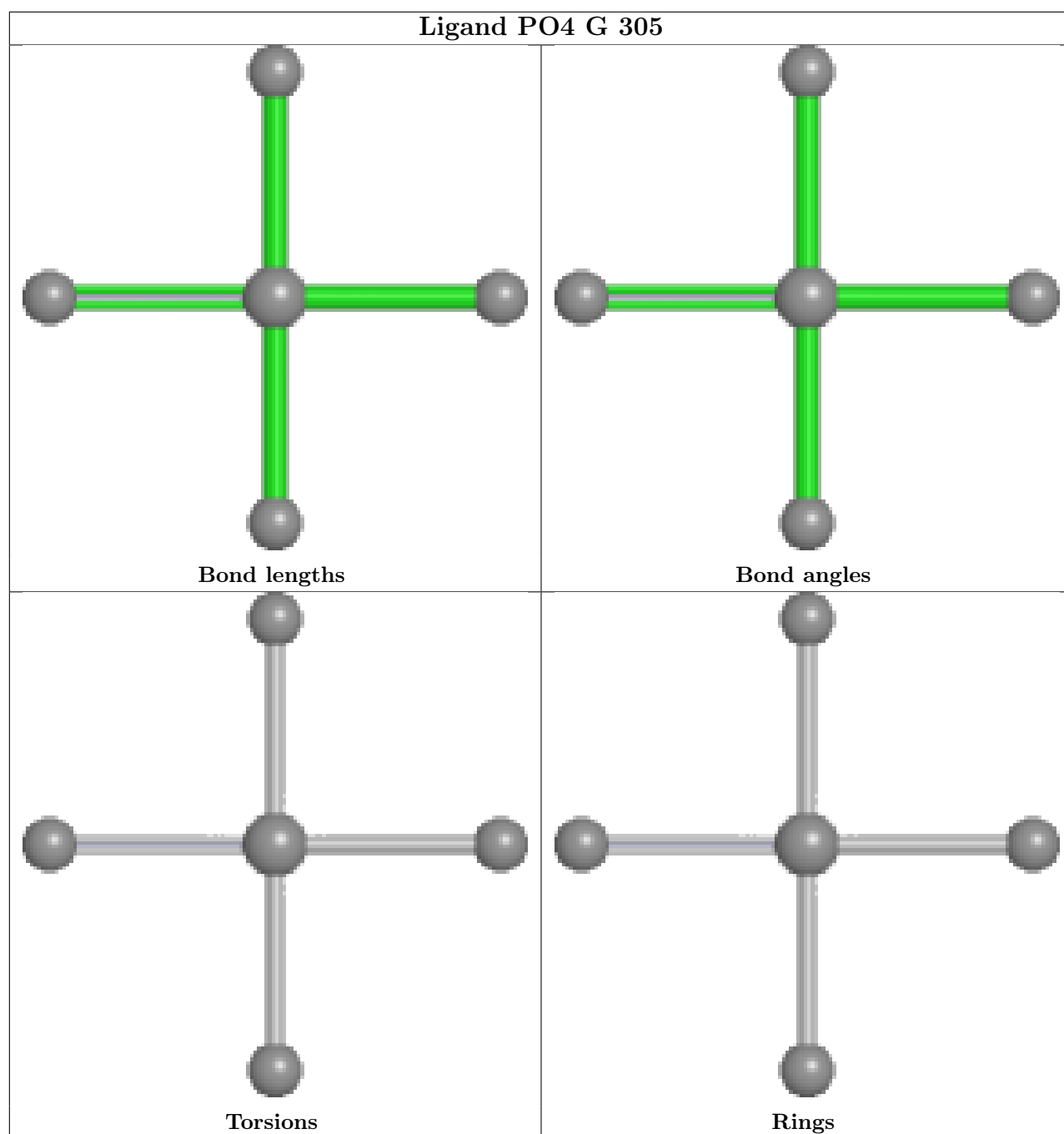
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

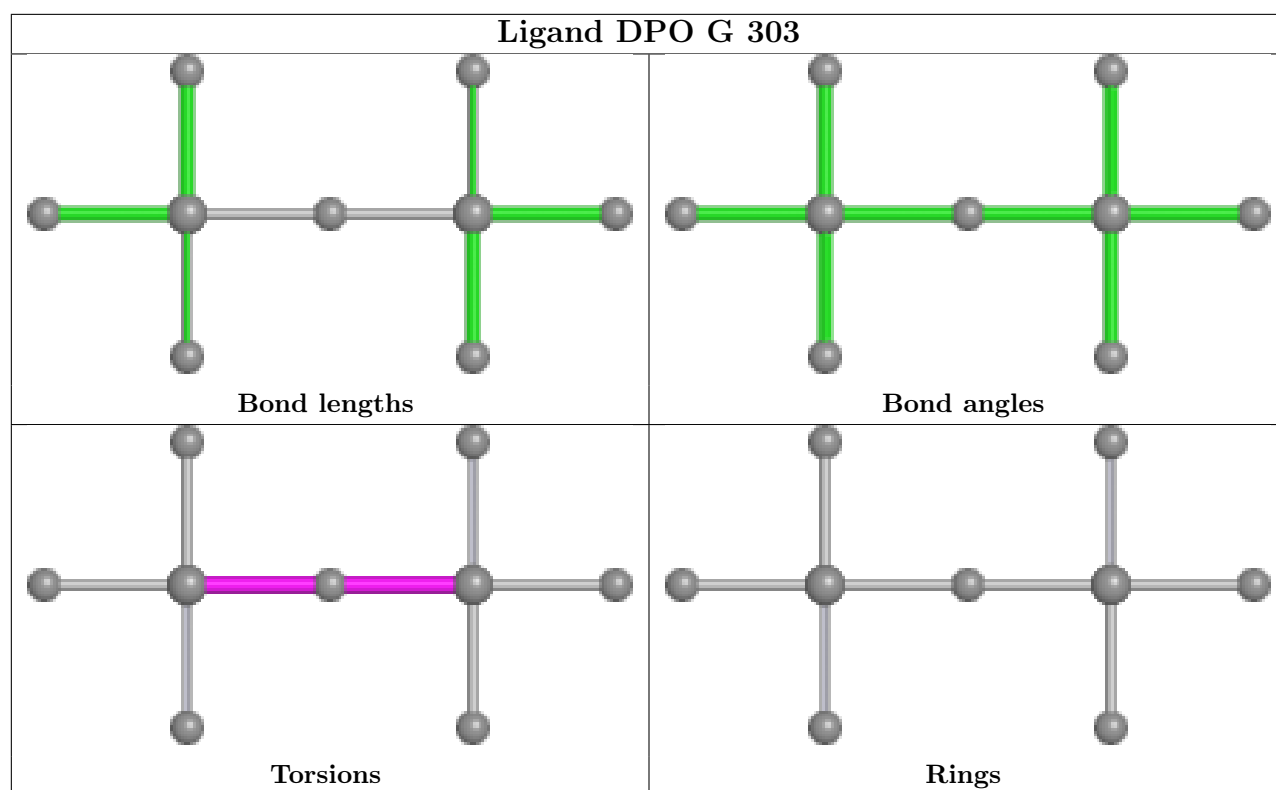


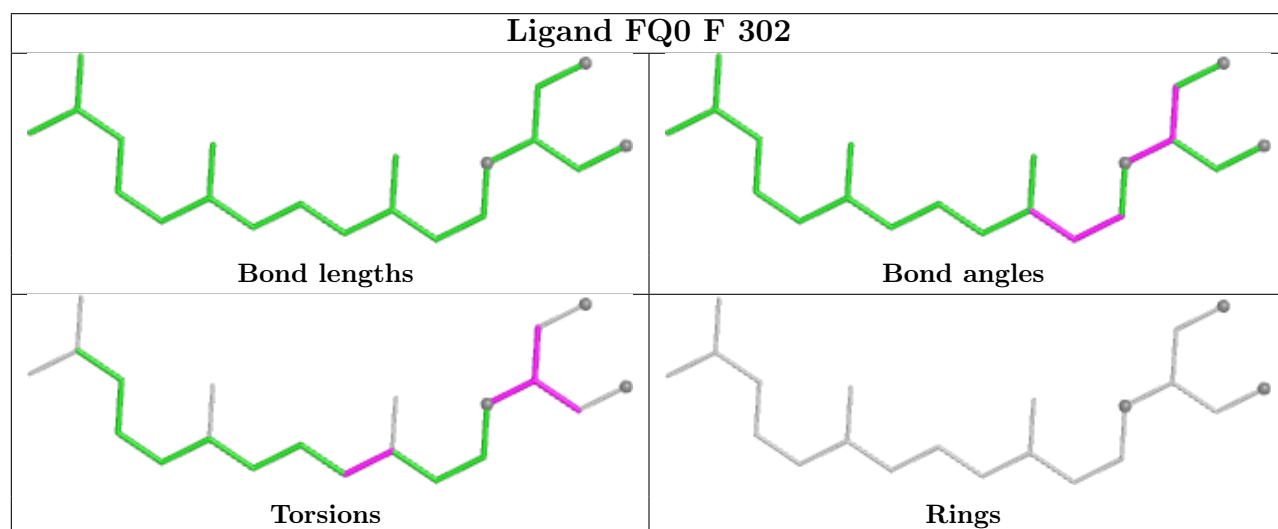
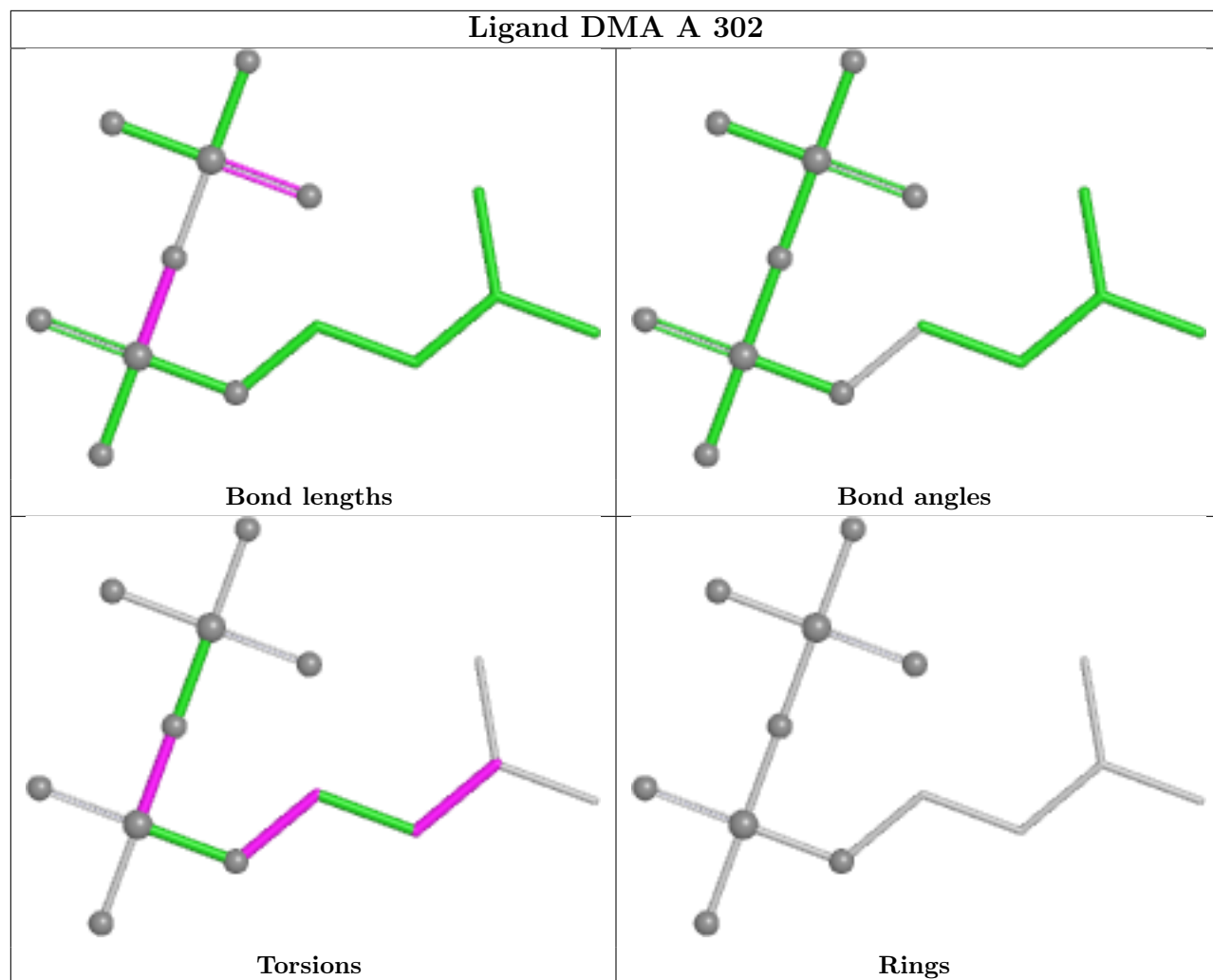


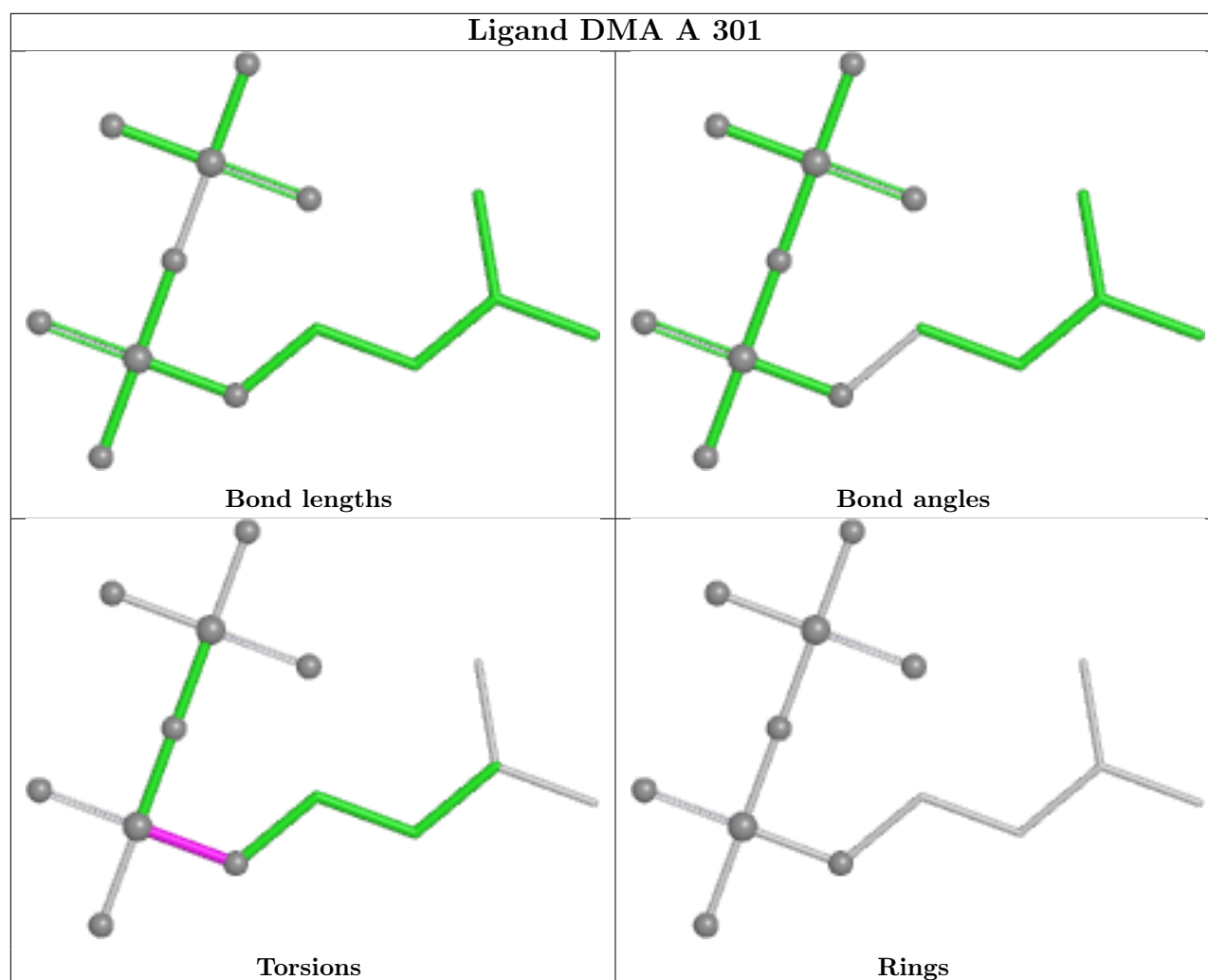


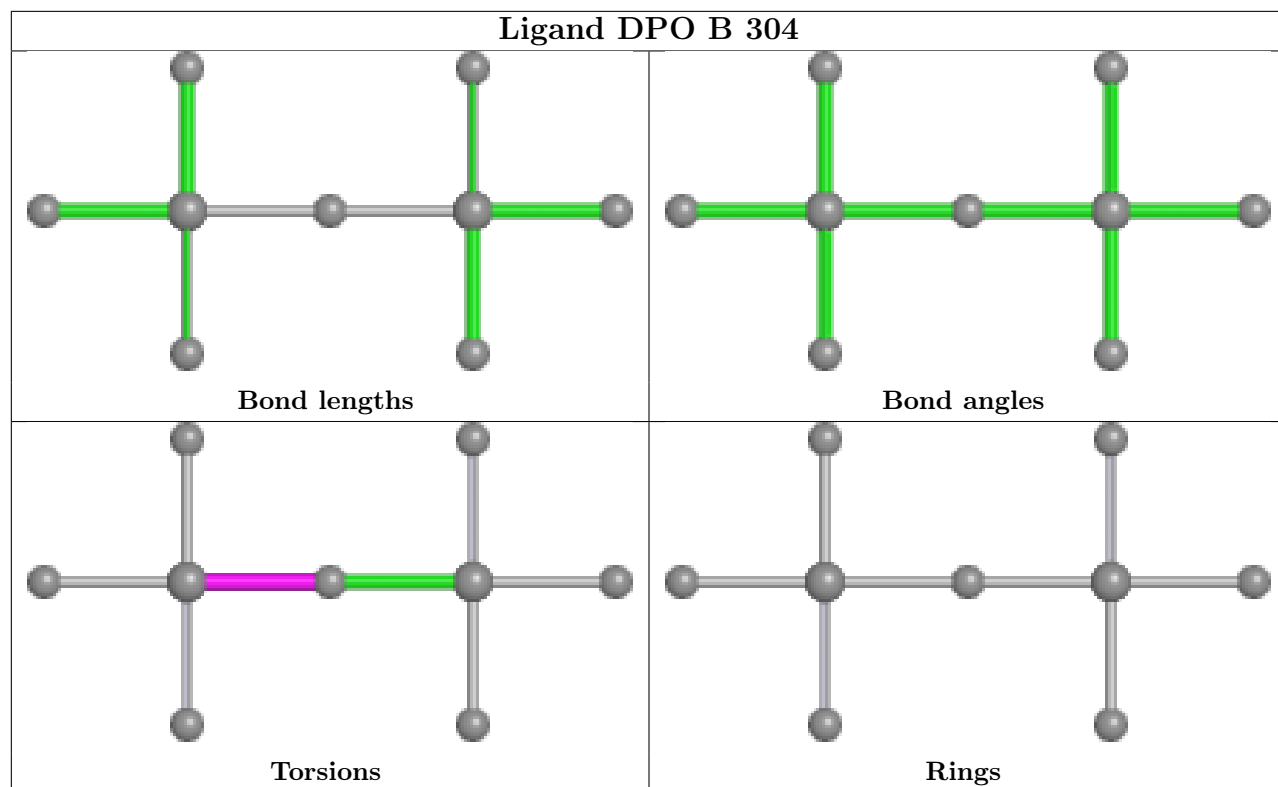




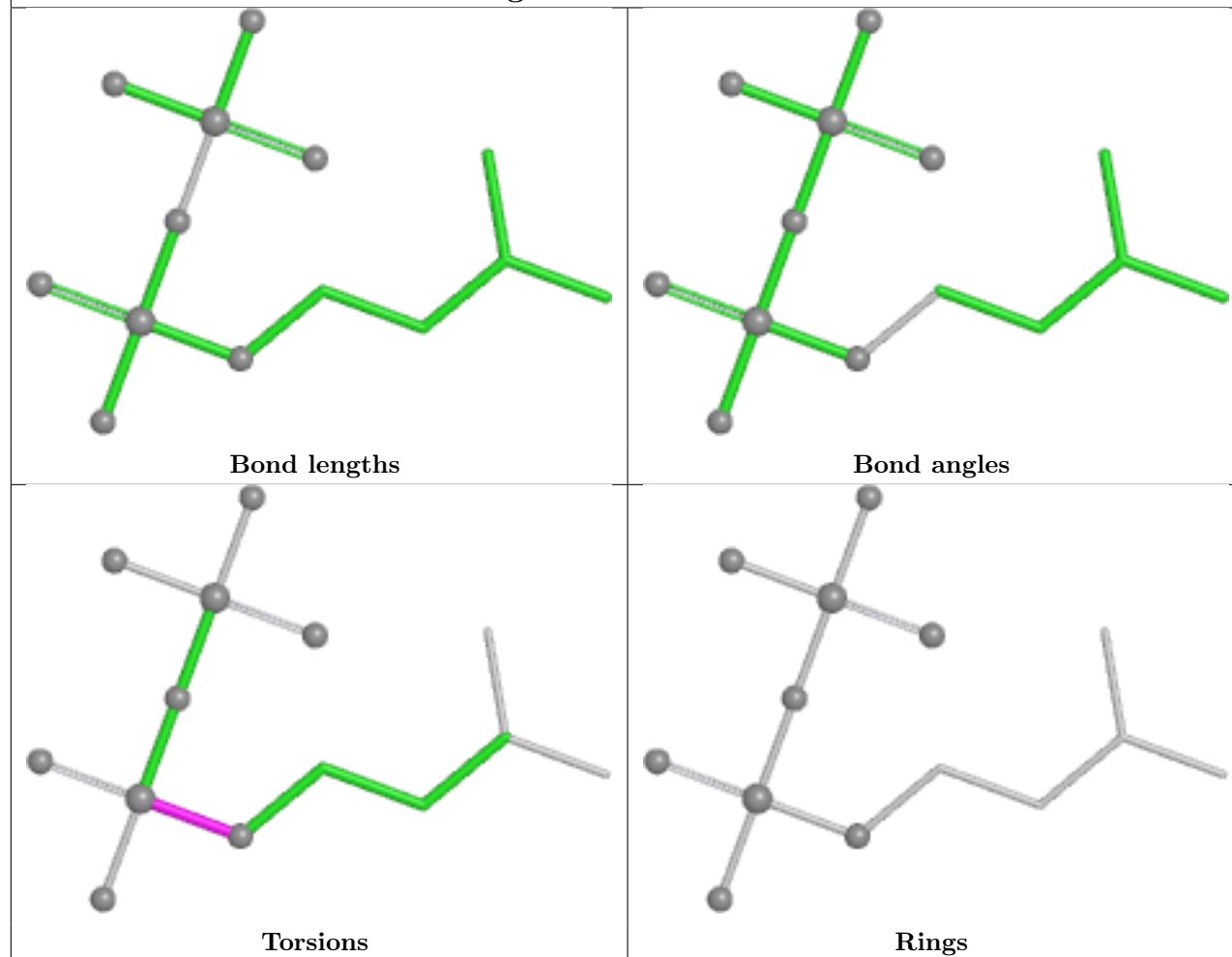




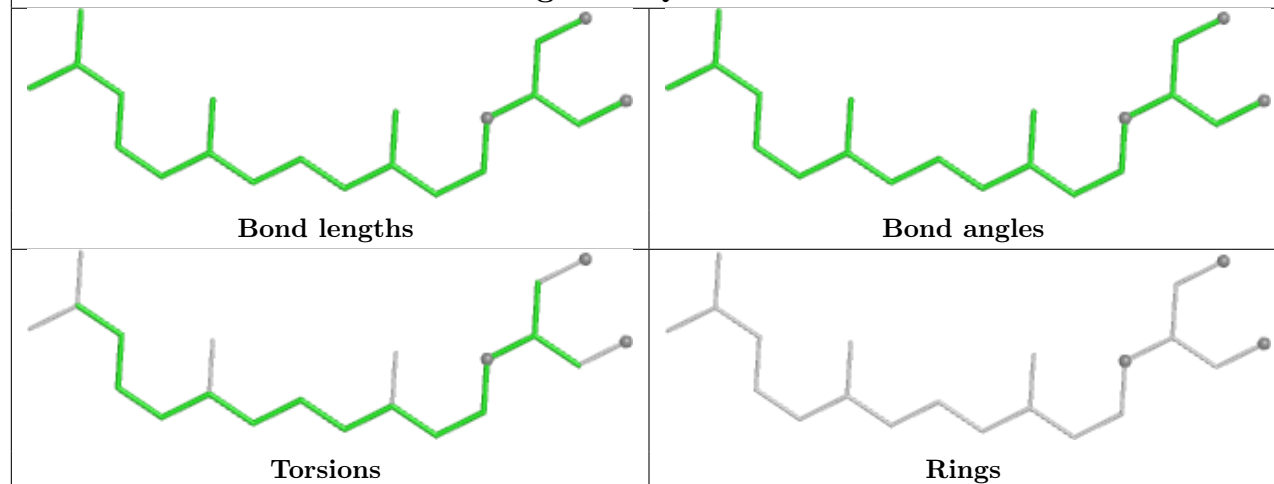


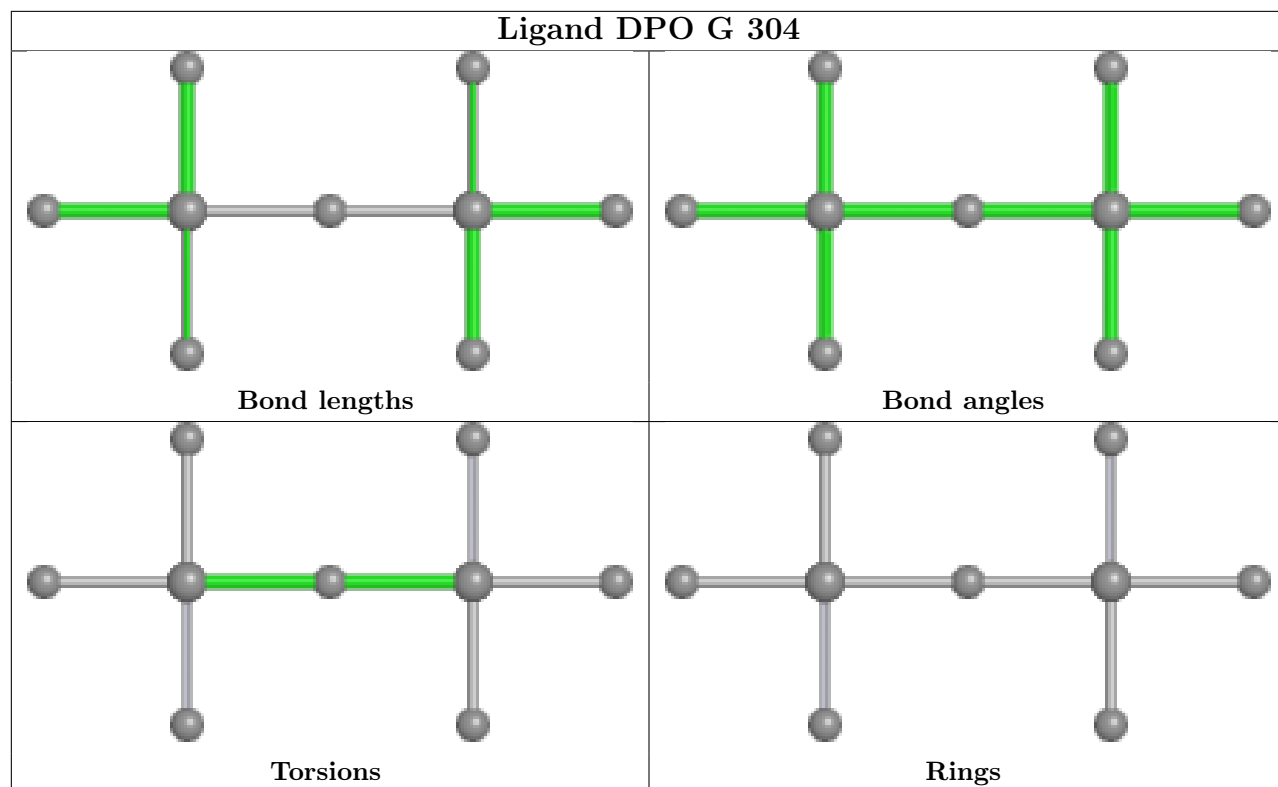


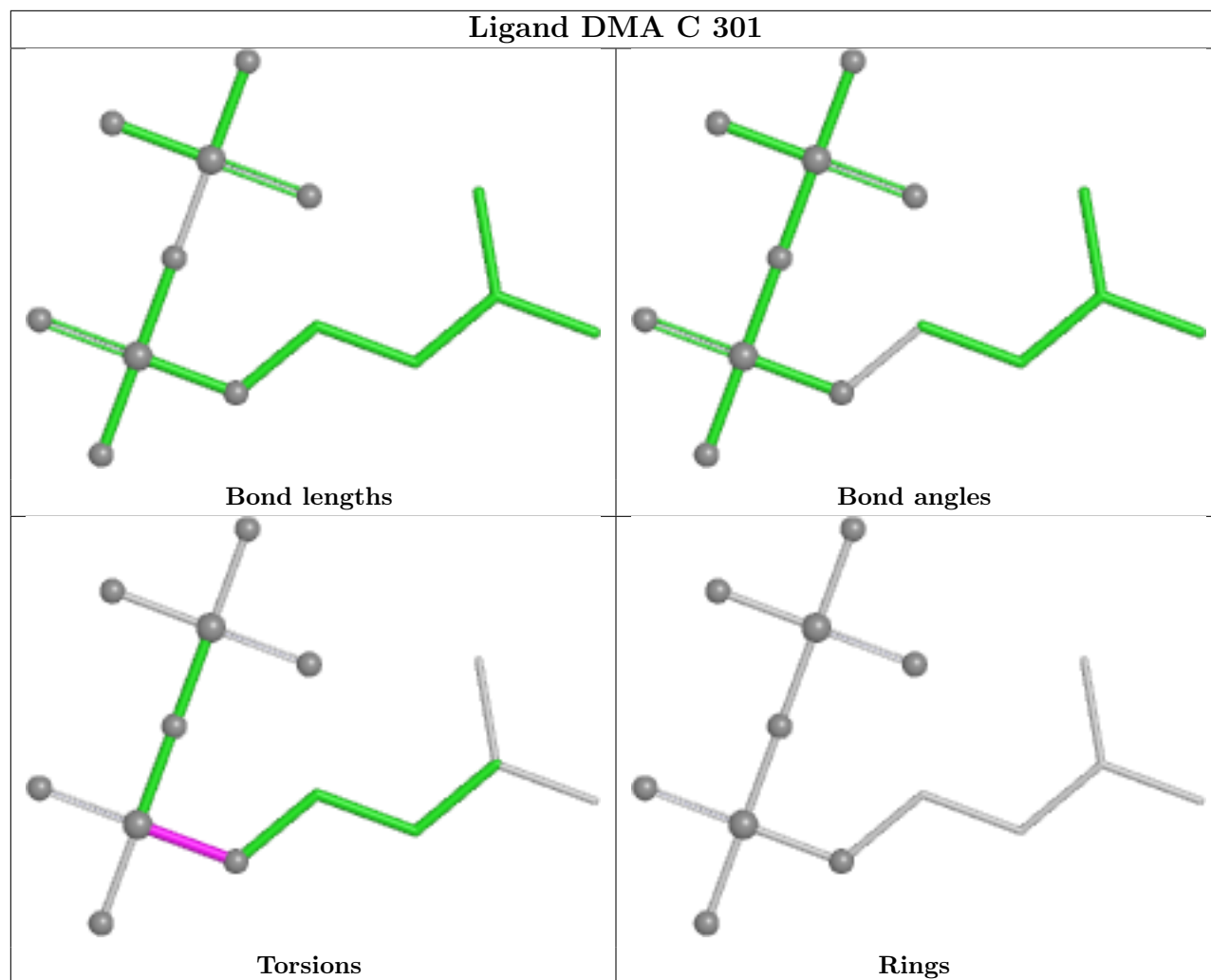
Ligand DMA D 302

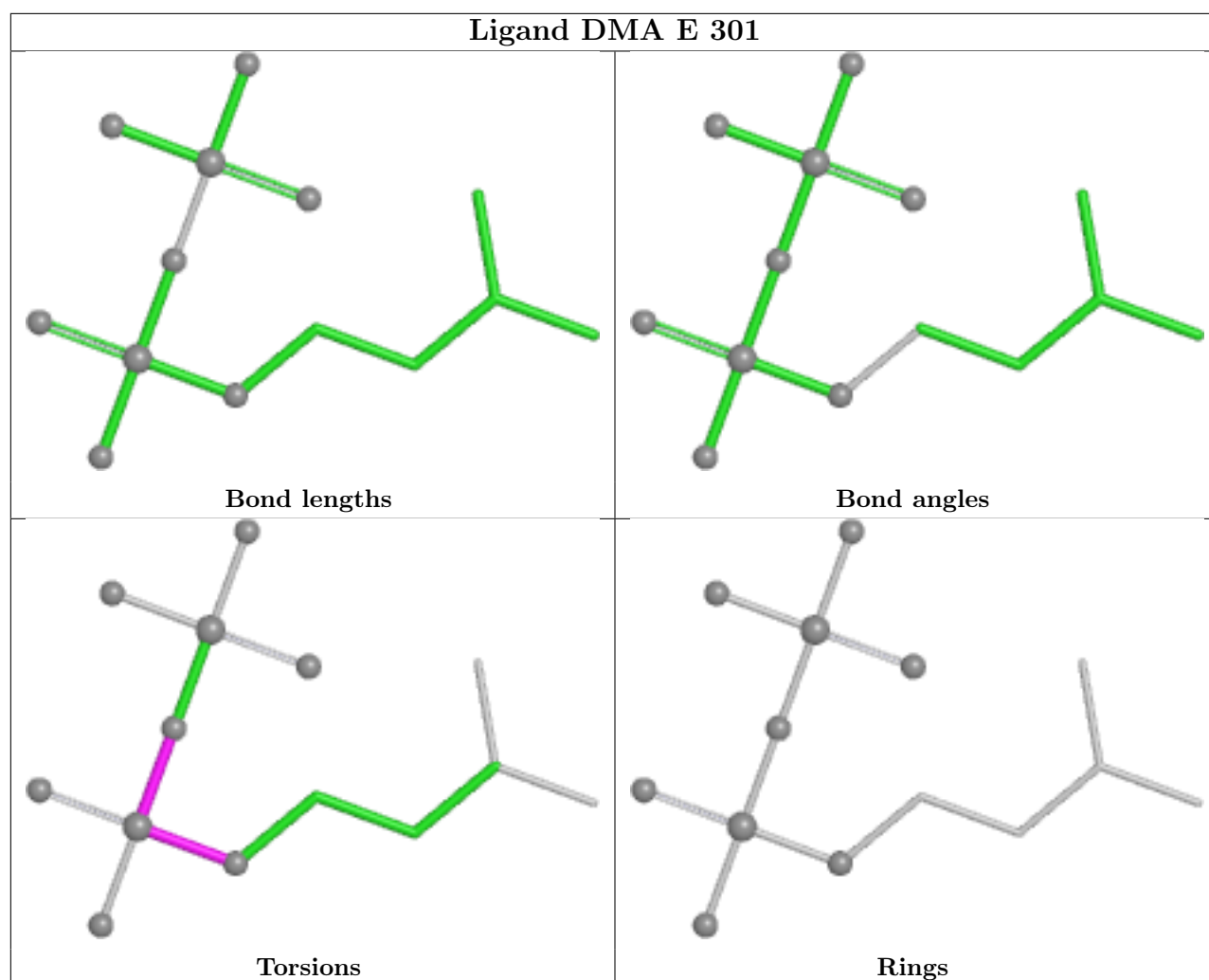


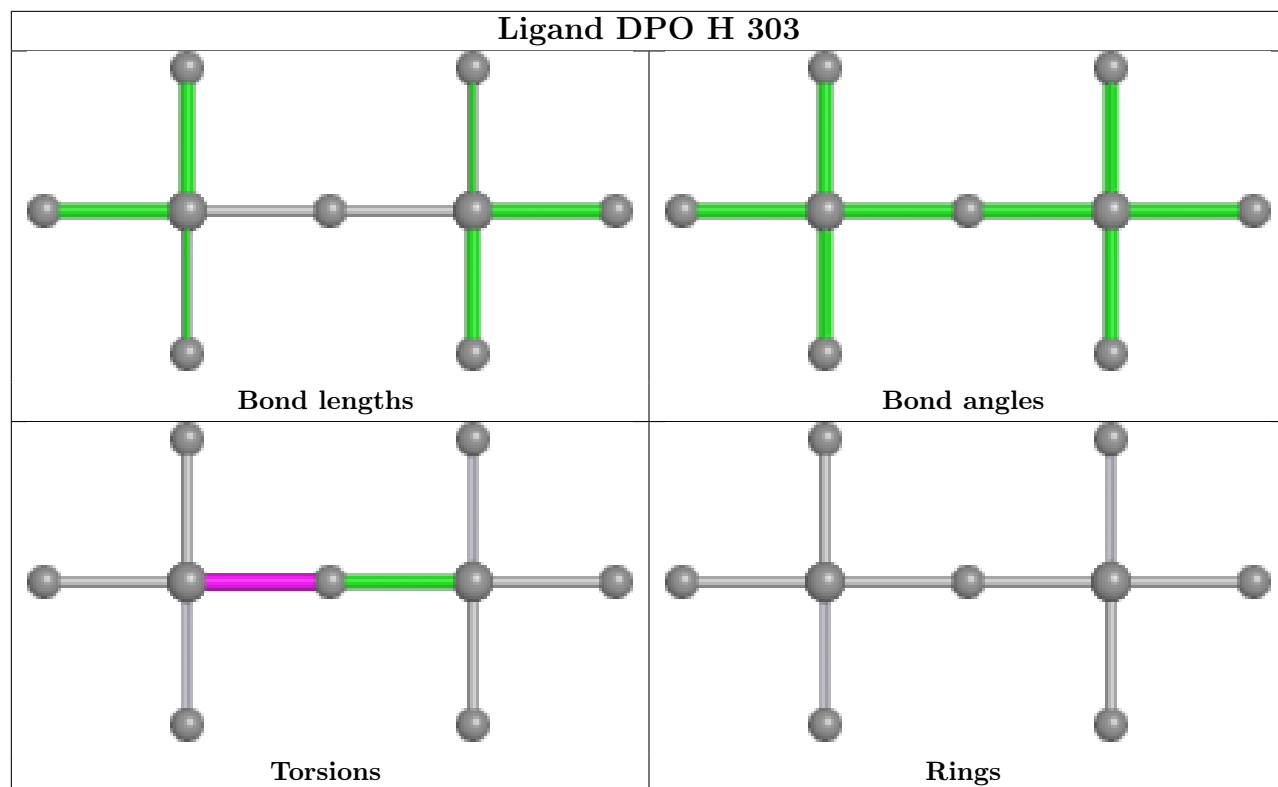
Ligand FQ0 B 302

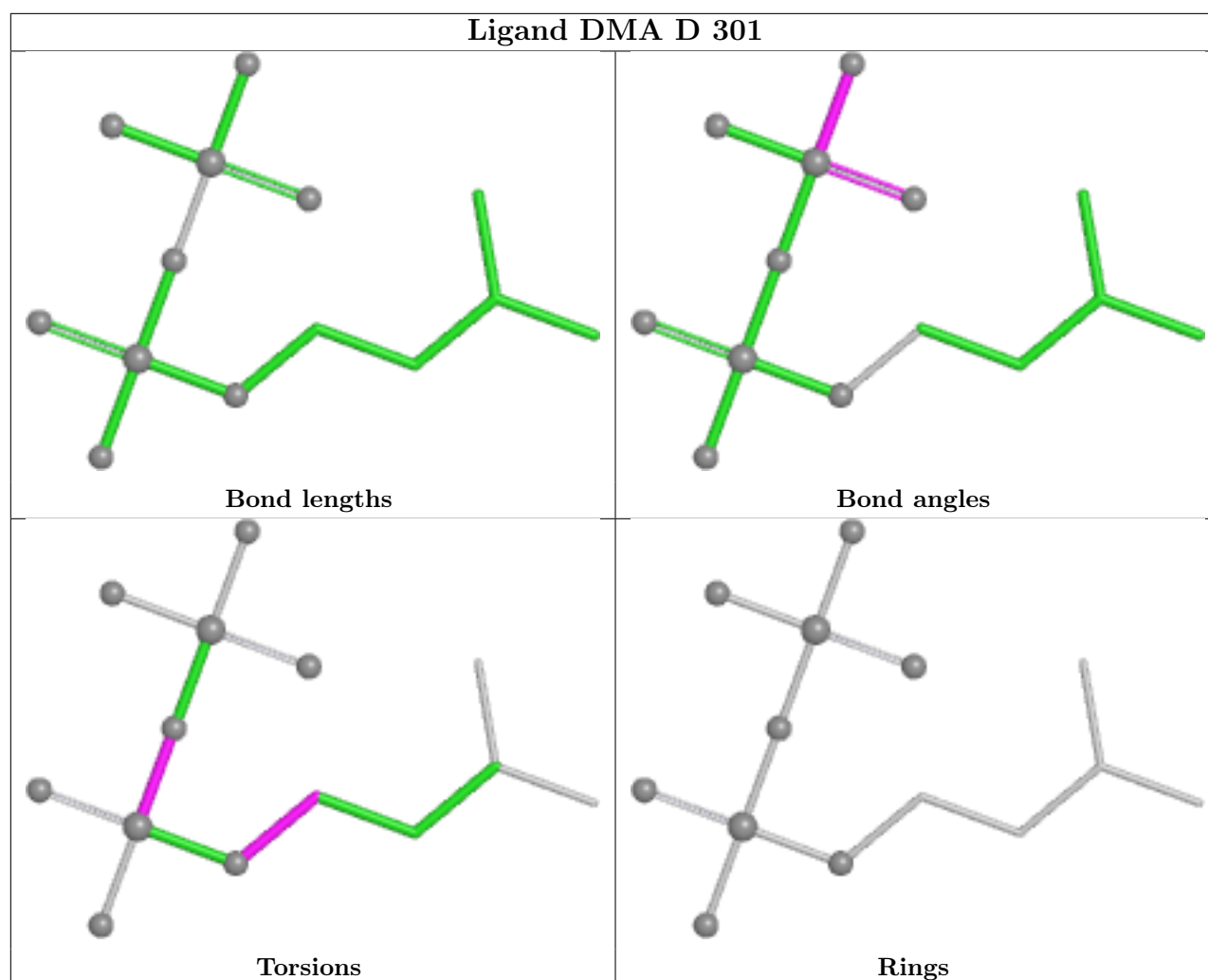












5.7 Other polymers [i](#)

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%)	0.53	10 (4%) 36 41	27, 38, 67, 89	0
1	B	222/224 (99%)	0.52	17 (7%) 19 23	27, 37, 63, 88	0
1	C	217/224 (96%)	0.89	25 (11%) 9 12	29, 43, 73, 94	0
1	D	211/224 (94%)	0.90	30 (14%) 6 8	30, 44, 69, 86	0
1	E	204/224 (91%)	0.94	22 (10%) 11 14	31, 45, 73, 85	0
1	F	216/224 (96%)	1.07	34 (15%) 5 6	30, 45, 73, 104	0
1	G	219/224 (97%)	0.68	17 (7%) 19 22	30, 41, 68, 94	0
1	H	206/224 (91%)	0.68	13 (6%) 26 30	30, 42, 70, 88	0
All	All	1706/1792 (95%)	0.78	168 (9%) 13 16	27, 42, 71, 104	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	ILE	6.4
1	G	152	ILE	6.0
1	C	152	ILE	5.8
1	F	3	ILE	5.8
1	F	152	ILE	5.0
1	B	142	TYR	5.0
1	F	145	SER	4.9
1	D	218	GLY	4.7
1	A	-1	TYR	4.7
1	B	152	ILE	4.6
1	G	142	TYR	4.3
1	H	141	ALA	4.1
1	H	142	TYR	4.0
1	G	-2	GLY	3.9
1	E	142	TYR	3.8
1	E	68	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.8
1	H	151	MET	3.6
1	D	142	TYR	3.5
1	A	52	ILE	3.5
1	C	151	MET	3.4
1	D	141	ALA	3.4
1	H	102	ASN	3.4
1	C	150	LYS	3.4
1	F	119	VAL	3.4
1	C	217	LEU	3.4
1	H	117	THR	3.4
1	A	142	TYR	3.3
1	A	152	ILE	3.3
1	B	146	PRO	3.3
1	D	52	ILE	3.3
1	C	119	VAL	3.3
1	A	151	MET	3.2
1	F	105	ILE	3.2
1	D	219	GLY	3.2
1	F	150	LYS	3.1
1	D	217	LEU	3.1
1	H	103	SER	3.1
1	D	215	ILE	3.1
1	B	-2	GLY	3.1
1	E	25	LEU	3.1
1	C	142	TYR	3.0
1	E	135	TYR	3.0
1	F	114	THR	3.0
1	D	104	ASP	3.0
1	C	145	SER	2.9
1	D	185	TYR	2.9
1	E	29	LEU	2.9
1	G	-1	TYR	2.9
1	D	216	THR	2.9
1	E	28	GLY	2.9
1	B	145	SER	2.9
1	G	148	GLY	2.9
1	F	117	THR	2.8
1	A	185	TYR	2.8
1	F	142	TYR	2.8
1	D	162	ARG	2.8
1	F	68	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	97	VAL	2.8
1	G	150	LYS	2.8
1	D	201	GLU	2.8
1	E	185	TYR	2.7
1	G	135	TYR	2.7
1	F	118	LYS	2.7
1	F	72	ILE	2.7
1	G	105	ILE	2.7
1	E	24	ALA	2.7
1	E	26	ALA	2.7
1	C	111	LEU	2.7
1	F	8	ARG	2.7
1	E	31	LYS	2.7
1	H	105	ILE	2.7
1	E	141	ALA	2.6
1	C	140	TYR	2.6
1	H	135	TYR	2.6
1	F	217	LEU	2.6
1	H	152	ILE	2.6
1	D	8	ARG	2.6
1	C	185	TYR	2.6
1	E	70	PRO	2.6
1	F	25	LEU	2.6
1	F	111	LEU	2.6
1	C	215	ILE	2.6
1	C	8	ARG	2.6
1	B	148	GLY	2.6
1	D	135	TYR	2.6
1	F	9	LEU	2.6
1	F	95	ILE	2.6
1	G	5	LYS	2.6
1	E	32	HIS	2.5
1	F	151	MET	2.5
1	C	105	ILE	2.5
1	F	215	ILE	2.5
1	G	72	ILE	2.5
1	B	151	MET	2.5
1	E	71	GLN	2.5
1	G	151	MET	2.5
1	F	122	GLY	2.5
1	D	102	ASN	2.4
1	H	155	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	140	TYR	2.4
1	H	2	ASP	2.4
1	E	117	THR	2.4
1	C	149	LYS	2.4
1	F	106	PHE	2.4
1	F	147	ASP	2.4
1	B	8	ARG	2.4
1	E	72	ILE	2.4
1	D	26	ALA	2.4
1	C	28	GLY	2.4
1	F	28	GLY	2.4
1	G	123	LYS	2.4
1	C	72	ILE	2.3
1	D	152	ILE	2.3
1	C	148	GLY	2.3
1	F	148	GLY	2.3
1	D	83	LYS	2.3
1	F	7	LYS	2.3
1	D	27	ARG	2.3
1	F	141	ALA	2.3
1	D	3	ILE	2.3
1	E	151	MET	2.3
1	D	119	VAL	2.3
1	C	141	ALA	2.3
1	D	95	ILE	2.3
1	C	216	THR	2.3
1	H	150	LYS	2.2
1	C	52	ILE	2.2
1	A	150	LYS	2.2
1	A	-2	GLY	2.2
1	F	120	GLY	2.2
1	B	141	ALA	2.2
1	D	204	PHE	2.2
1	F	140	TYR	2.2
1	D	151	MET	2.2
1	A	104	ASP	2.2
1	B	147	ASP	2.2
1	D	49	CYS	2.2
1	C	93	ALA	2.2
1	C	118	LYS	2.2
1	E	77	PHE	2.1
1	B	140	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	119	VAL	2.1
1	B	217	LEU	2.1
1	C	162	ARG	2.1
1	F	204	PHE	2.1
1	B	135	TYR	2.1
1	D	40	ILE	2.1
1	D	126	ILE	2.1
1	F	113	TYR	2.1
1	B	5	LYS	2.1
1	B	149	LYS	2.1
1	D	105	ILE	2.1
1	G	104	ASP	2.1
1	E	27	ARG	2.1
1	D	150	LYS	2.1
1	F	209	PHE	2.0
1	G	52	ILE	2.0
1	H	67	THR	2.0
1	G	28	GLY	2.0
1	C	102	ASN	2.0
1	D	50	VAL	2.0
1	F	107	PRO	2.0
1	G	141	ALA	2.0
1	E	88	ILE	2.0
1	E	209	PHE	2.0
1	B	117	THR	2.0
1	C	74	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

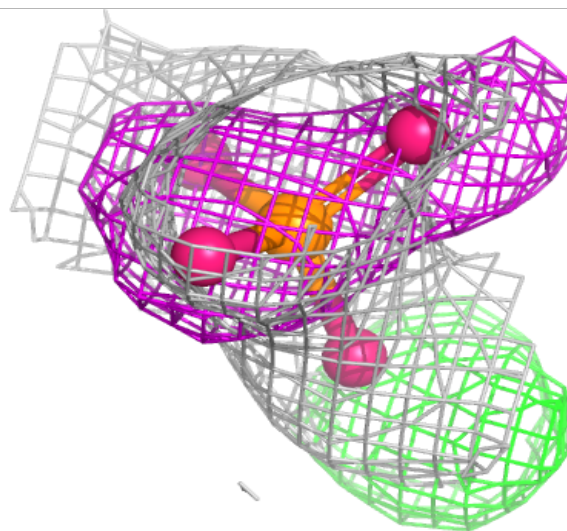
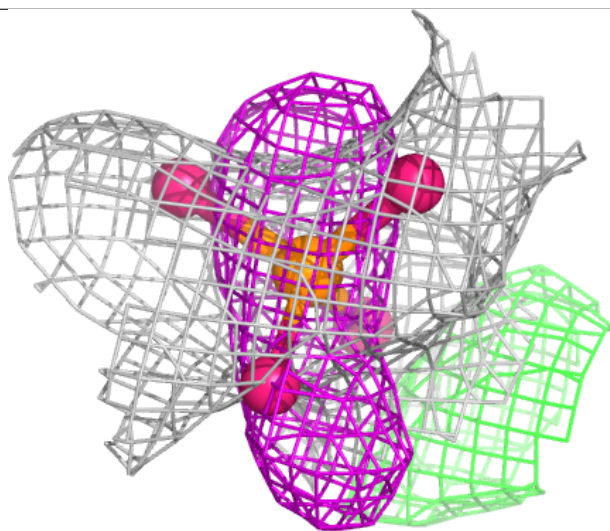
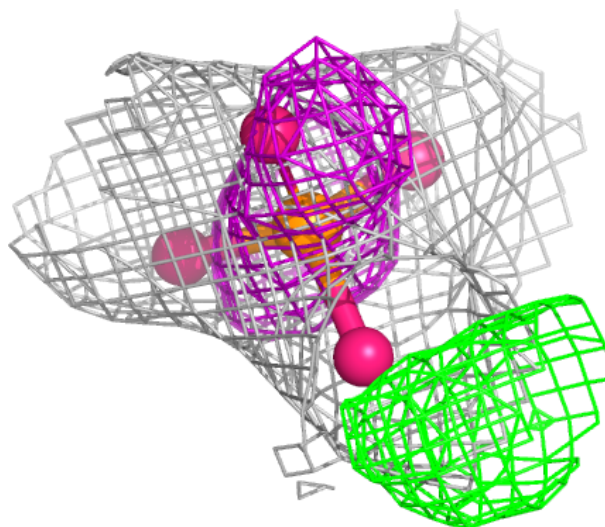
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	G	305	5/5	0.57	0.17	53,56,64,66	0
4	FQ0	G	302	21/21	0.81	0.19	36,55,75,76	0
4	FQ0	B	302	21/21	0.83	0.17	40,47,66,67	0
5	DPO	G	304	9/9	0.84	0.10	55,64,78,80	0
5	DPO	B	304	9/9	0.84	0.10	51,57,64,67	0
5	DPO	F	304	9/9	0.86	0.10	55,60,78,80	0
4	FQ0	F	302	21/21	0.88	0.13	37,43,61,63	0
4	FQ0	H	302	21/21	0.89	0.13	39,46,69,74	0
2	DMA	C	301	14/14	0.92	0.11	49,52,57,58	0
5	DPO	H	303	9/9	0.93	0.08	46,48,52,52	0
2	DMA	E	302	14/14	0.93	0.11	43,49,57,60	0
2	DMA	C	302	14/14	0.94	0.10	43,52,59,60	0
3	MG	F	301	1/1	0.95	0.06	51,51,51,51	0
3	MG	G	301	1/1	0.95	0.09	45,45,45,45	0
5	DPO	F	303	9/9	0.95	0.07	44,49,54,56	0
3	MG	H	301	1/1	0.95	0.13	60,60,60,60	0
5	DPO	G	303	9/9	0.95	0.07	44,50,51,54	0
2	DMA	A	302	14/14	0.95	0.10	28,35,51,52	0
2	DMA	E	301	14/14	0.95	0.10	41,47,52,54	0
2	DMA	A	301	14/14	0.95	0.08	31,36,37,38	0
2	DMA	D	302	14/14	0.96	0.08	34,41,45,48	0
3	MG	B	301	1/1	0.96	0.07	43,43,43,43	0
5	DPO	B	303	9/9	0.96	0.06	38,43,47,48	0
3	MG	E	303	1/1	0.96	0.06	47,47,47,47	0
2	DMA	D	301	14/14	0.96	0.09	33,38,44,44	0
3	MG	A	303	1/1	0.98	0.08	32,32,32,32	0
3	MG	C	303	1/1	0.98	0.07	45,45,45,45	0
3	MG	D	303	1/1	0.99	0.04	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.

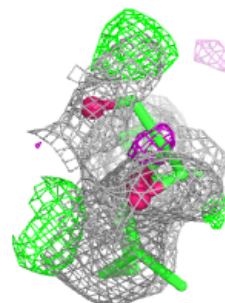
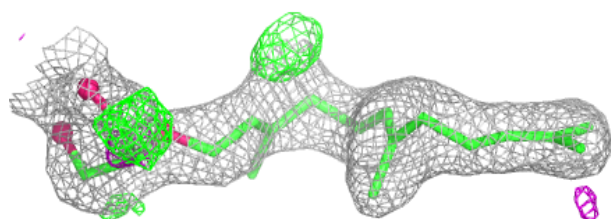
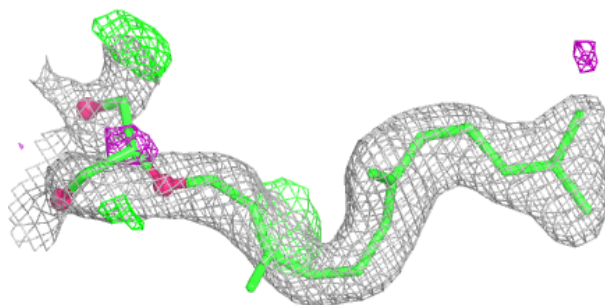
Electron density around PO4 G 305:

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

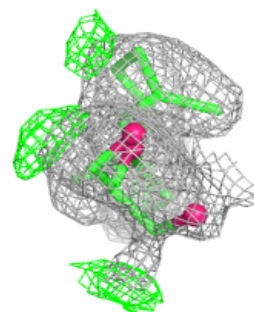
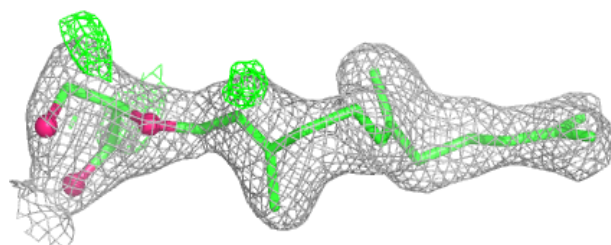
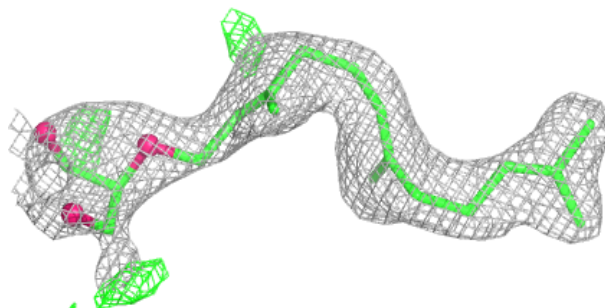


Electron density around FQ0 G 302:

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

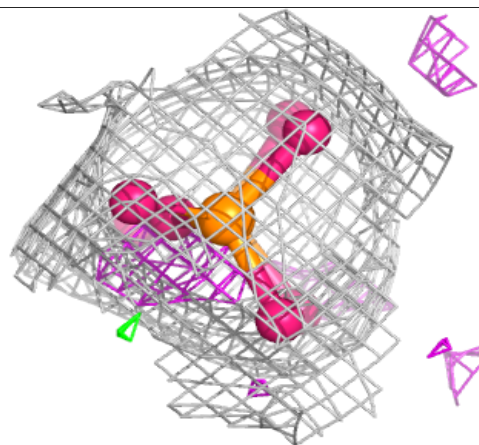
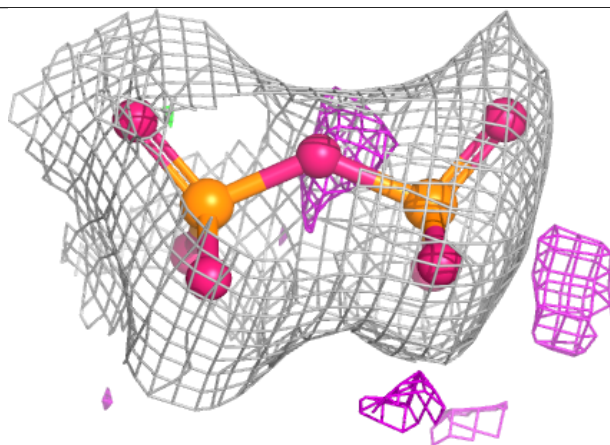
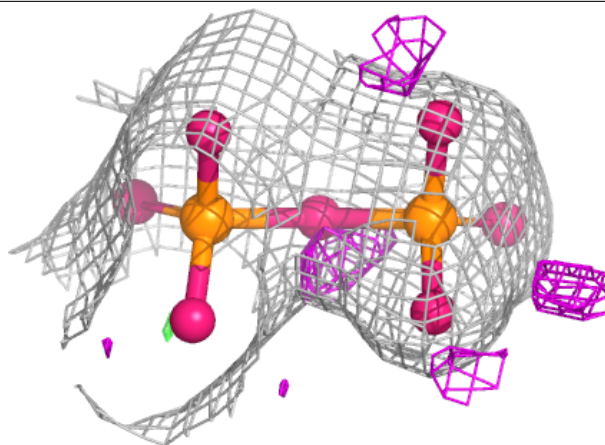
**Electron density around FQ0 B 302:**

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



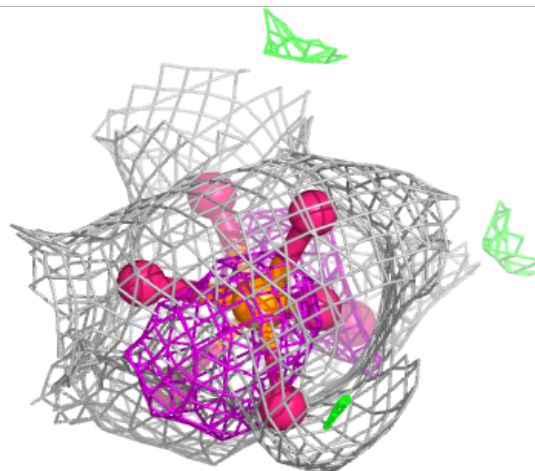
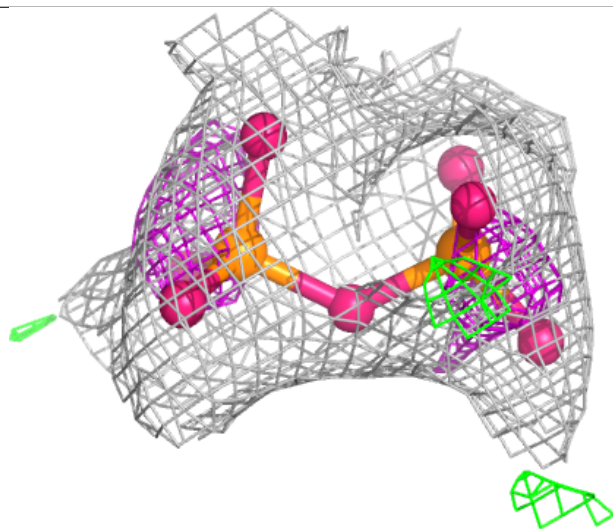
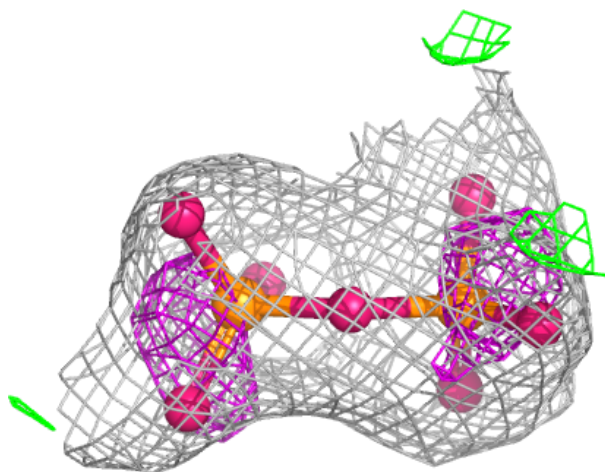
Electron density around DPO G 304:

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



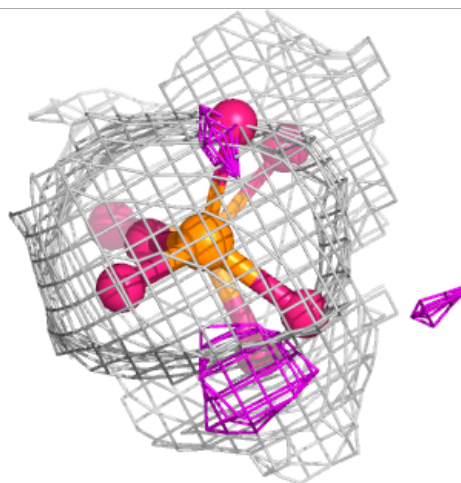
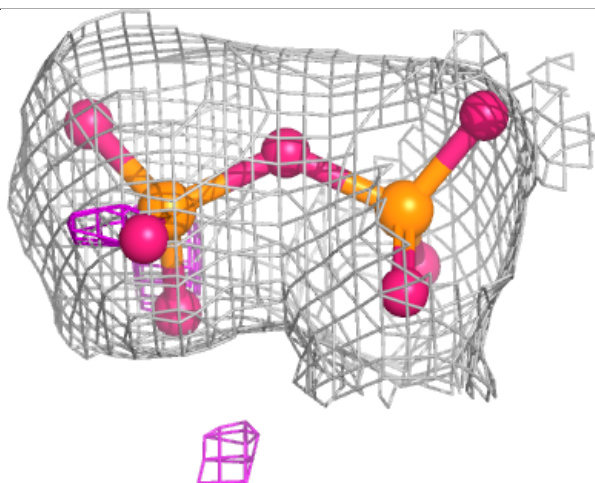
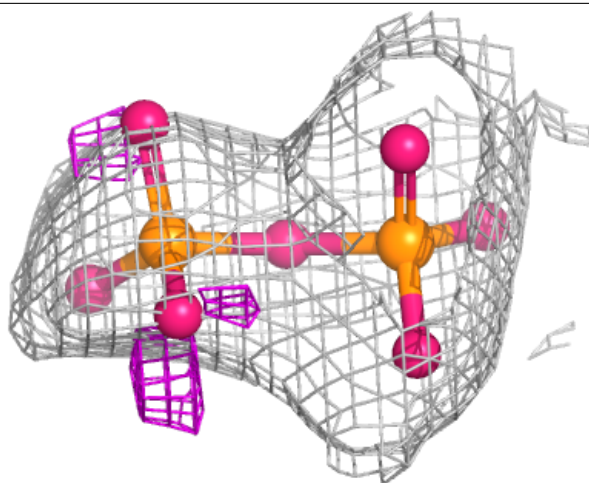
Electron density around DPO B 304:

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



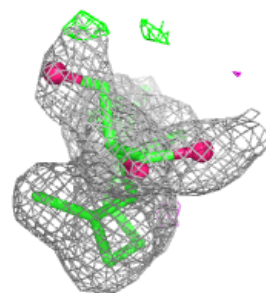
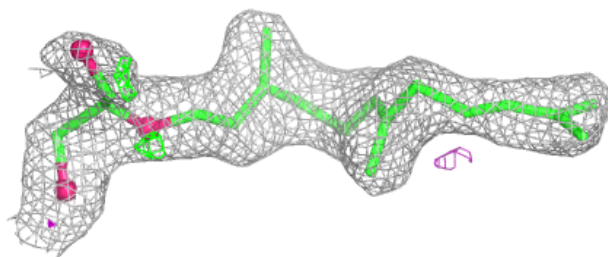
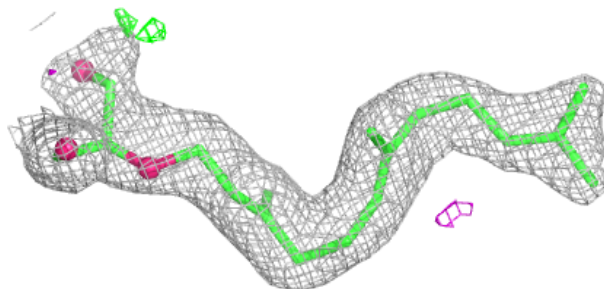
Electron density around DPO F 304:

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

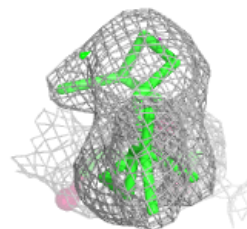
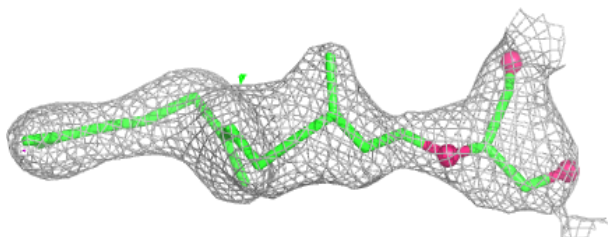
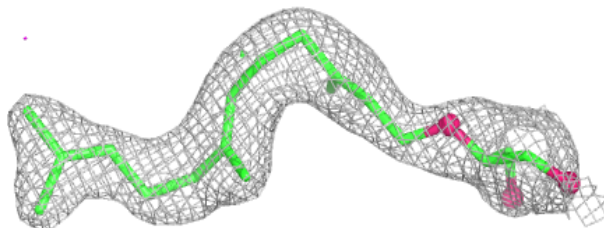


Electron density around FQ0 F 302:

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

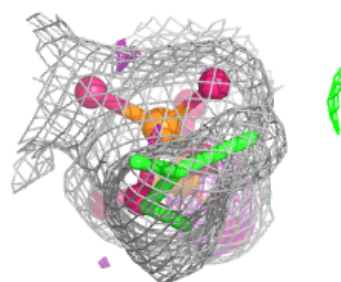
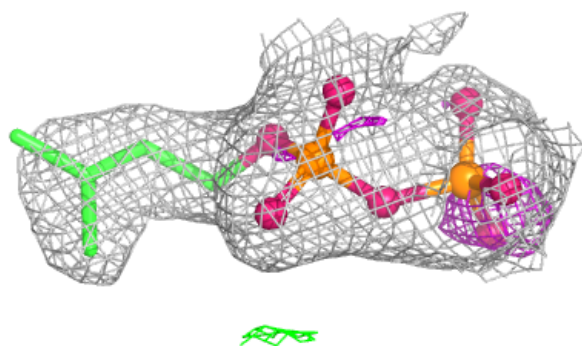
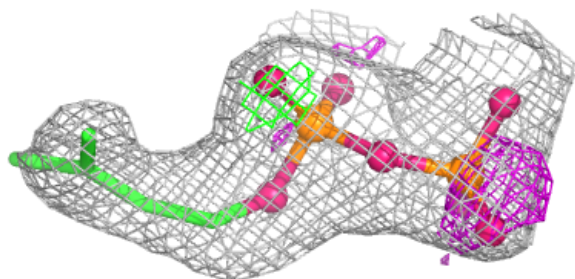
**Electron density around FQ0 H 302:**

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

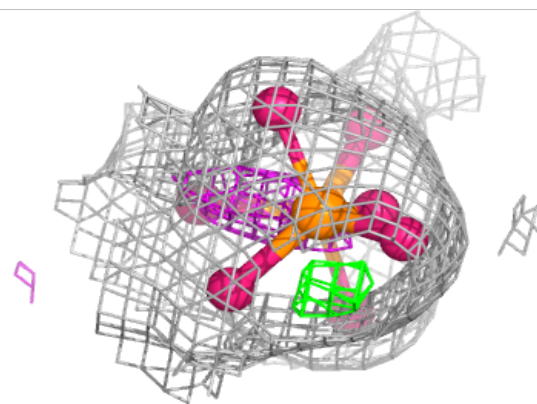
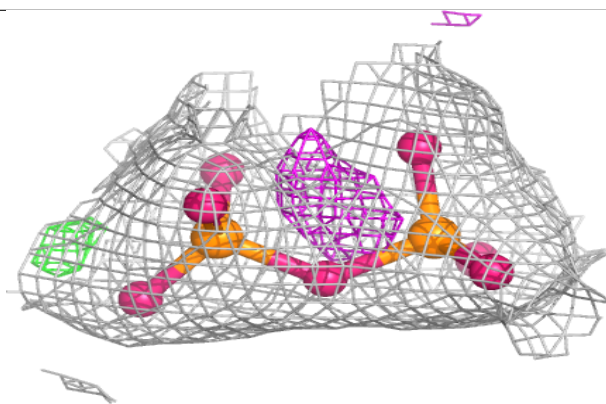
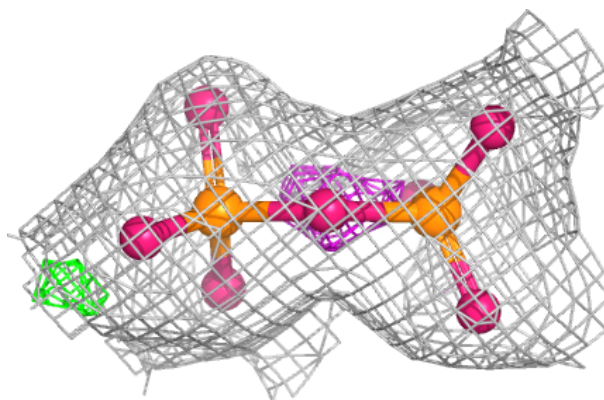


Electron density around DMA C 301:

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

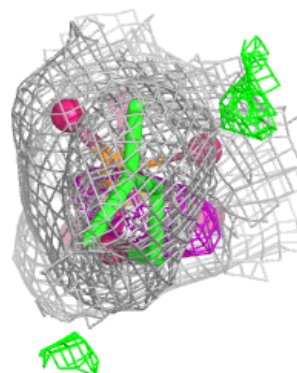
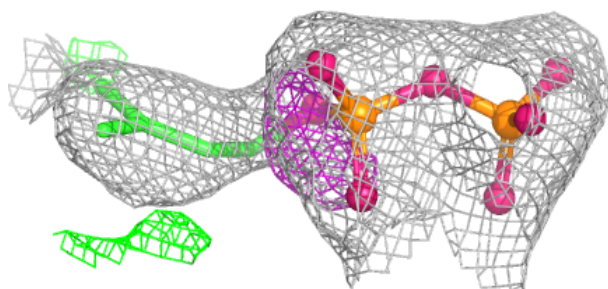
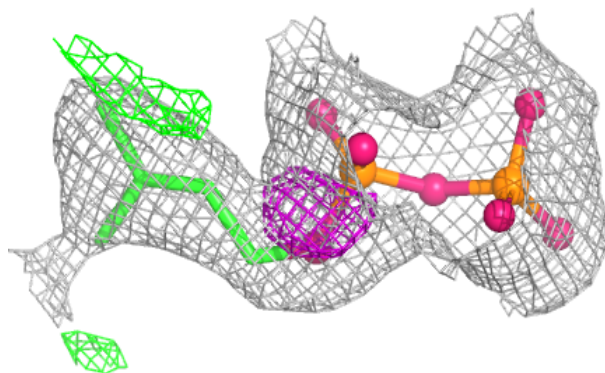
**Electron density around DPO H 303:**

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

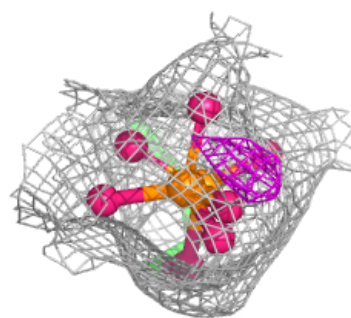
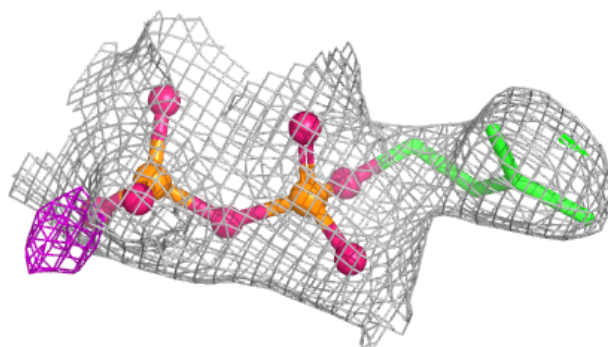
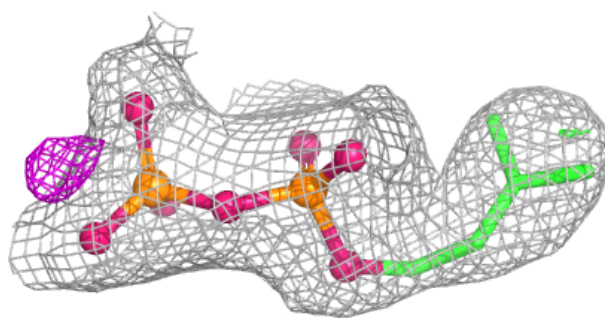


Electron density around DMA E 302:

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

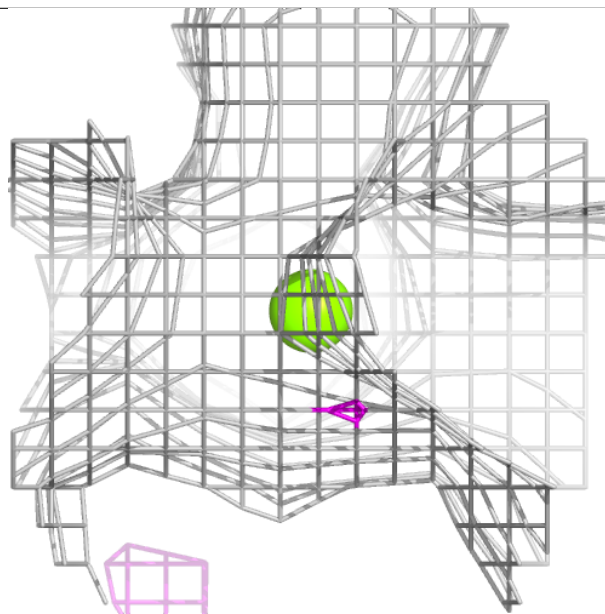
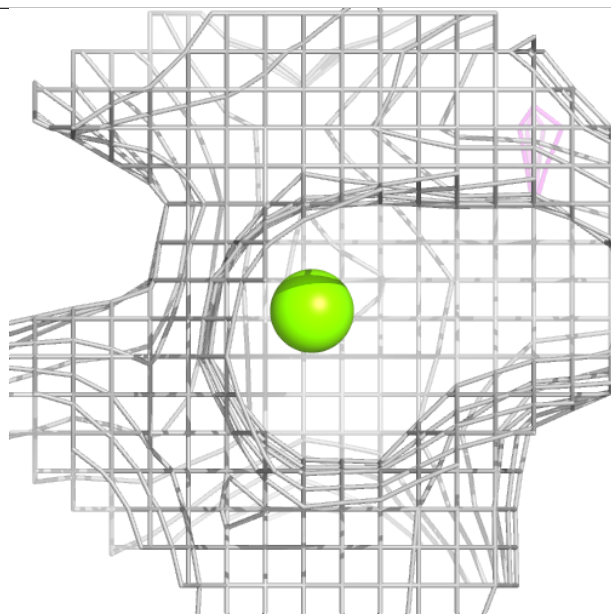
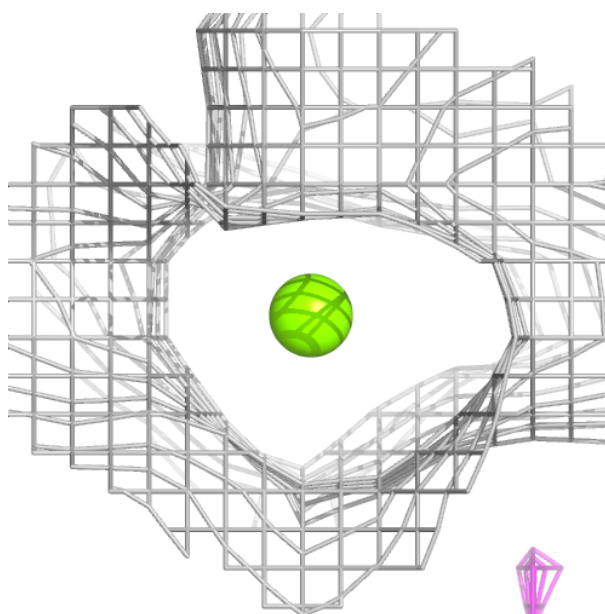
**Electron density around DMA C 302:**

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



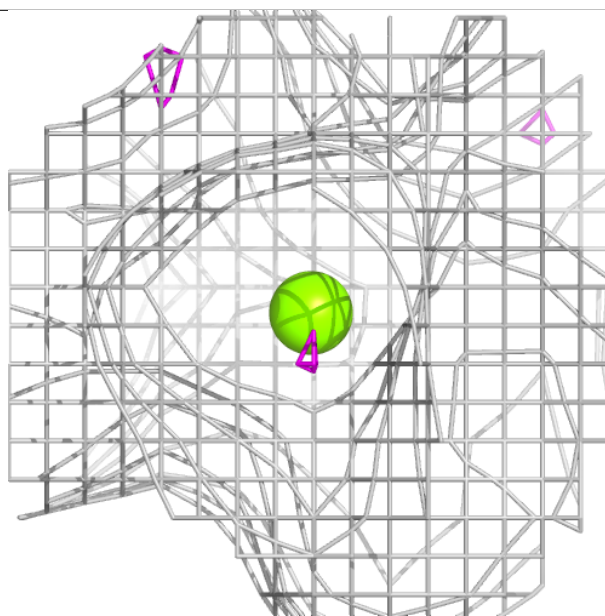
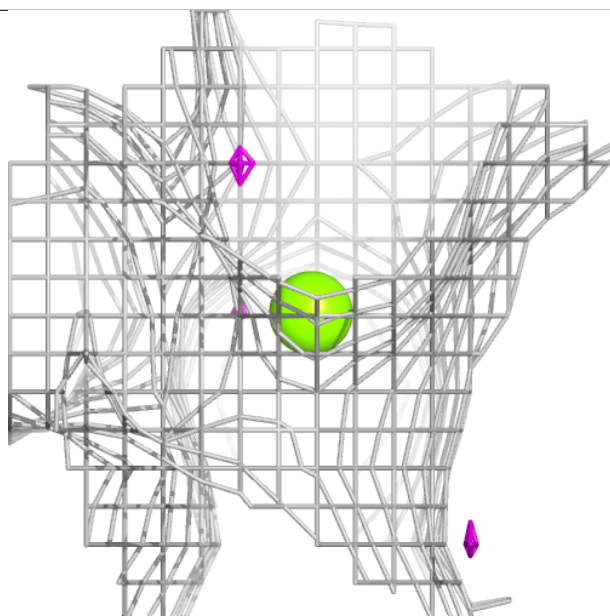
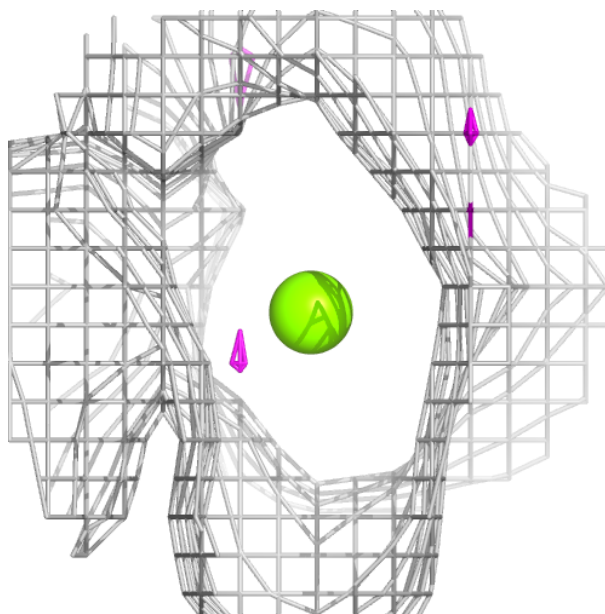
Electron density around MG F 301:

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



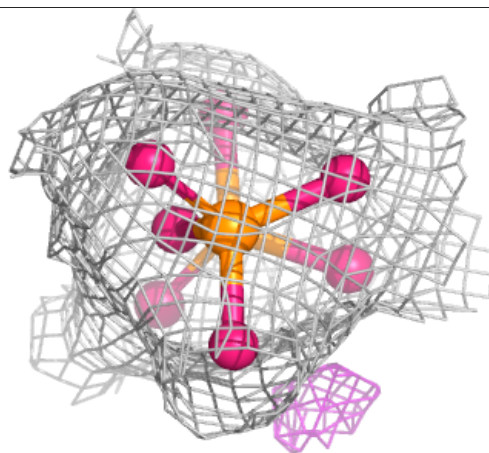
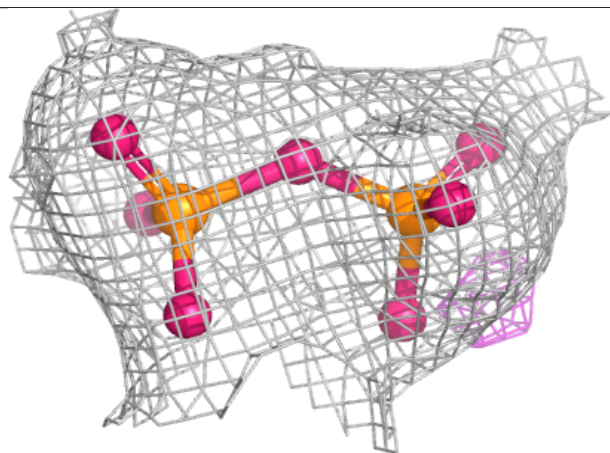
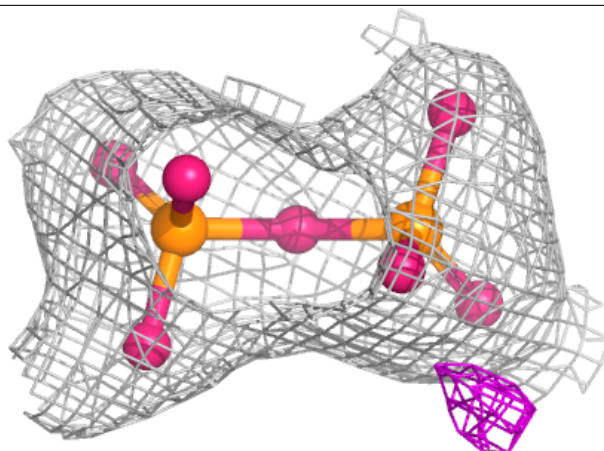
Electron density around MG G 301:

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



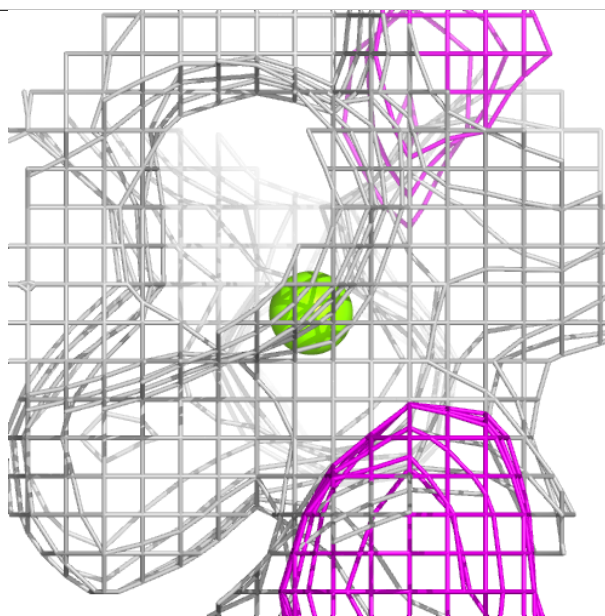
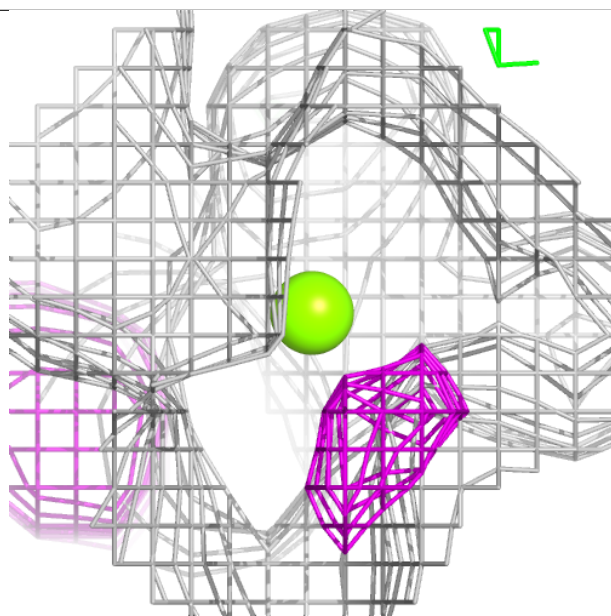
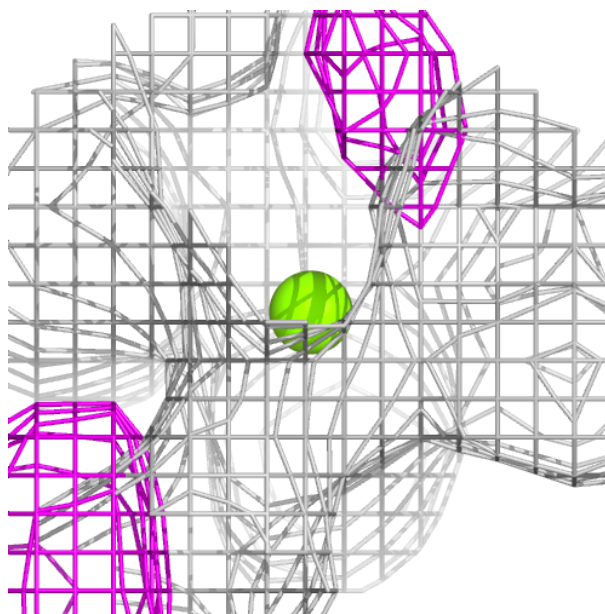
Electron density around DPO F 303:

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



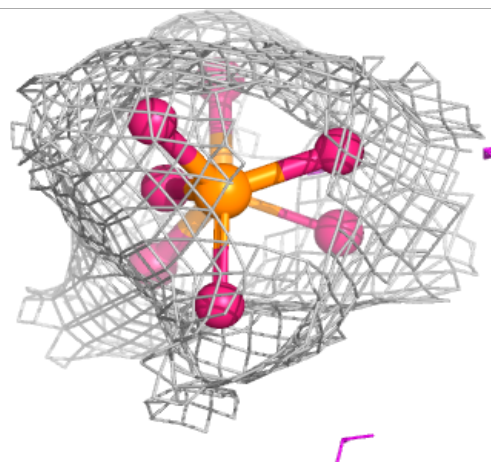
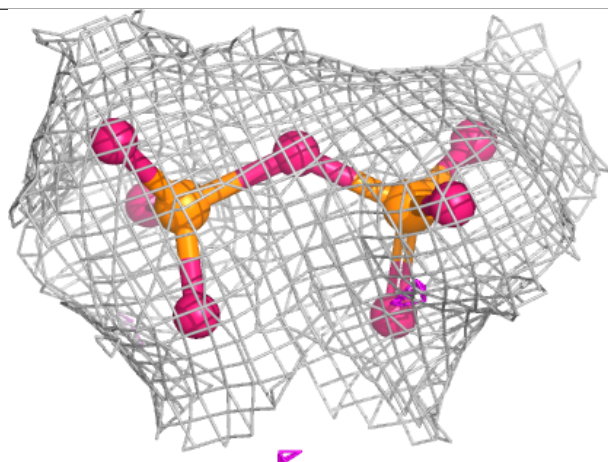
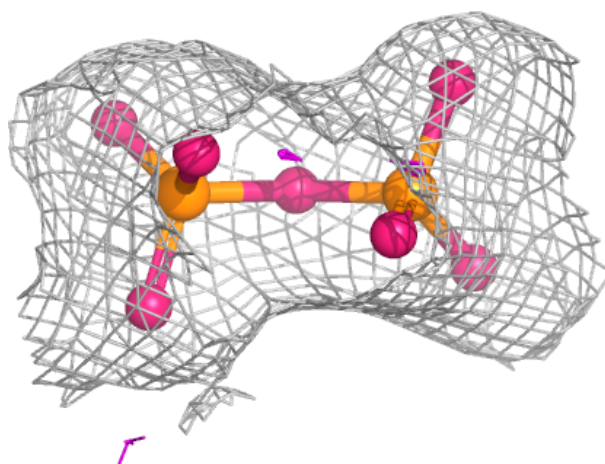
Electron density around MG H 301:

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



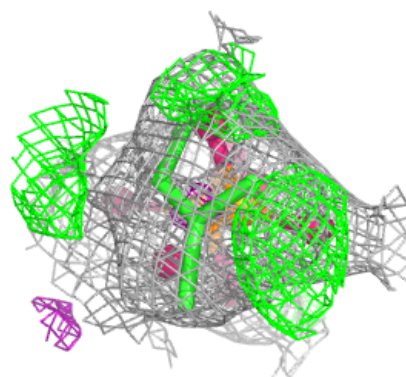
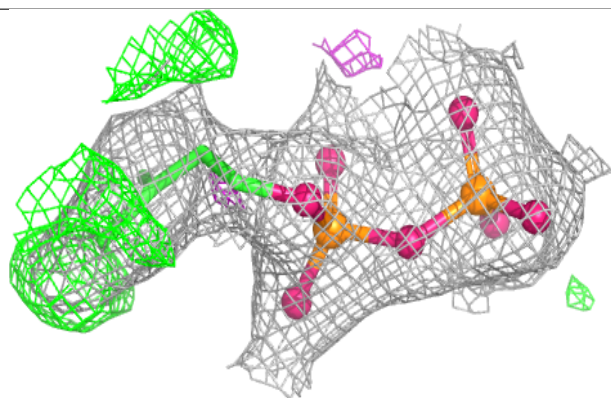
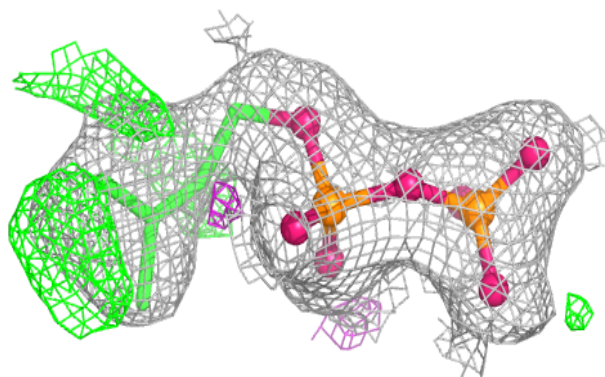
Electron density around DPO G 303:

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

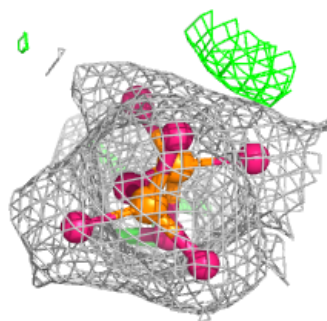
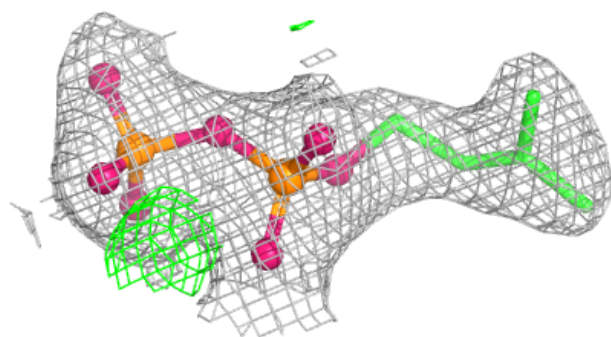
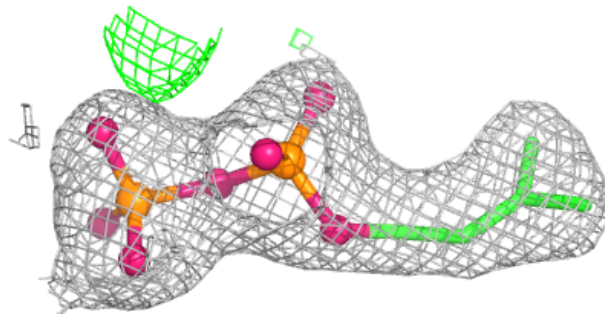


Electron density around DMA A 302:

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

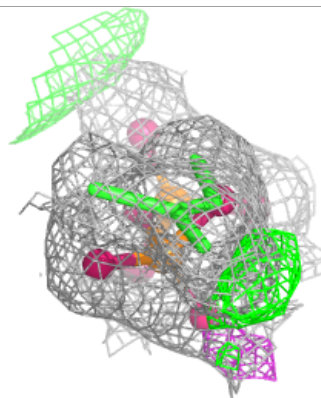
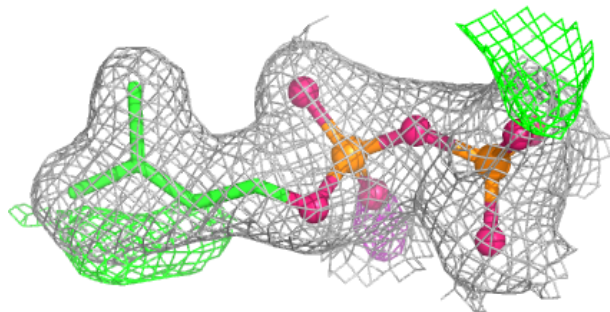
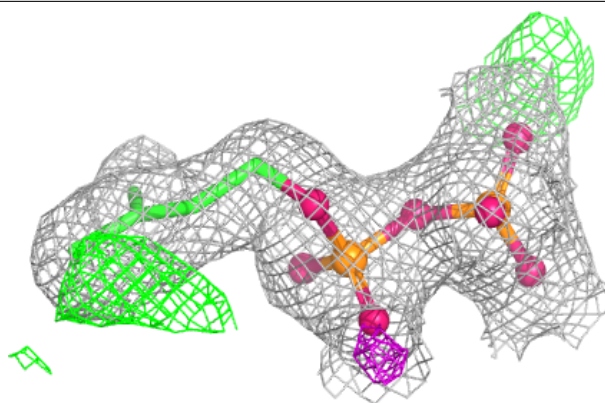
**Electron density around DMA E 301:**

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

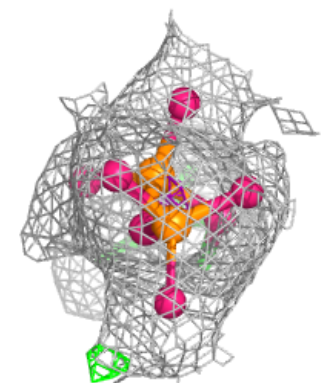
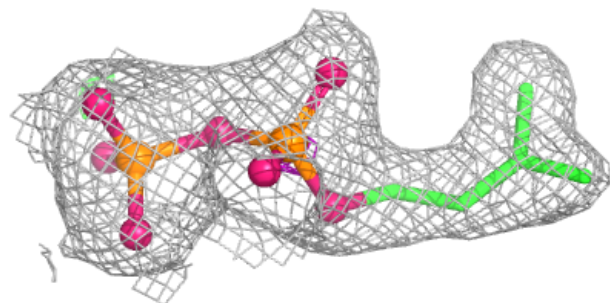
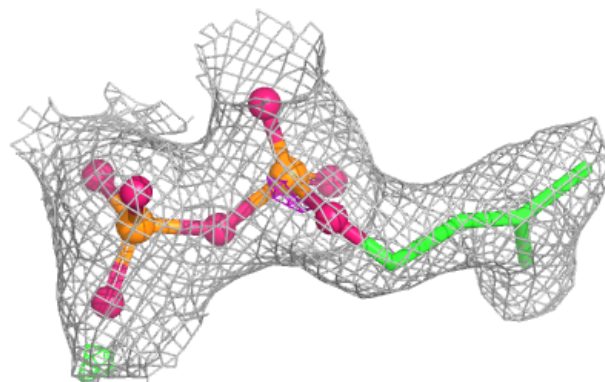


Electron density around DMA A 301:

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

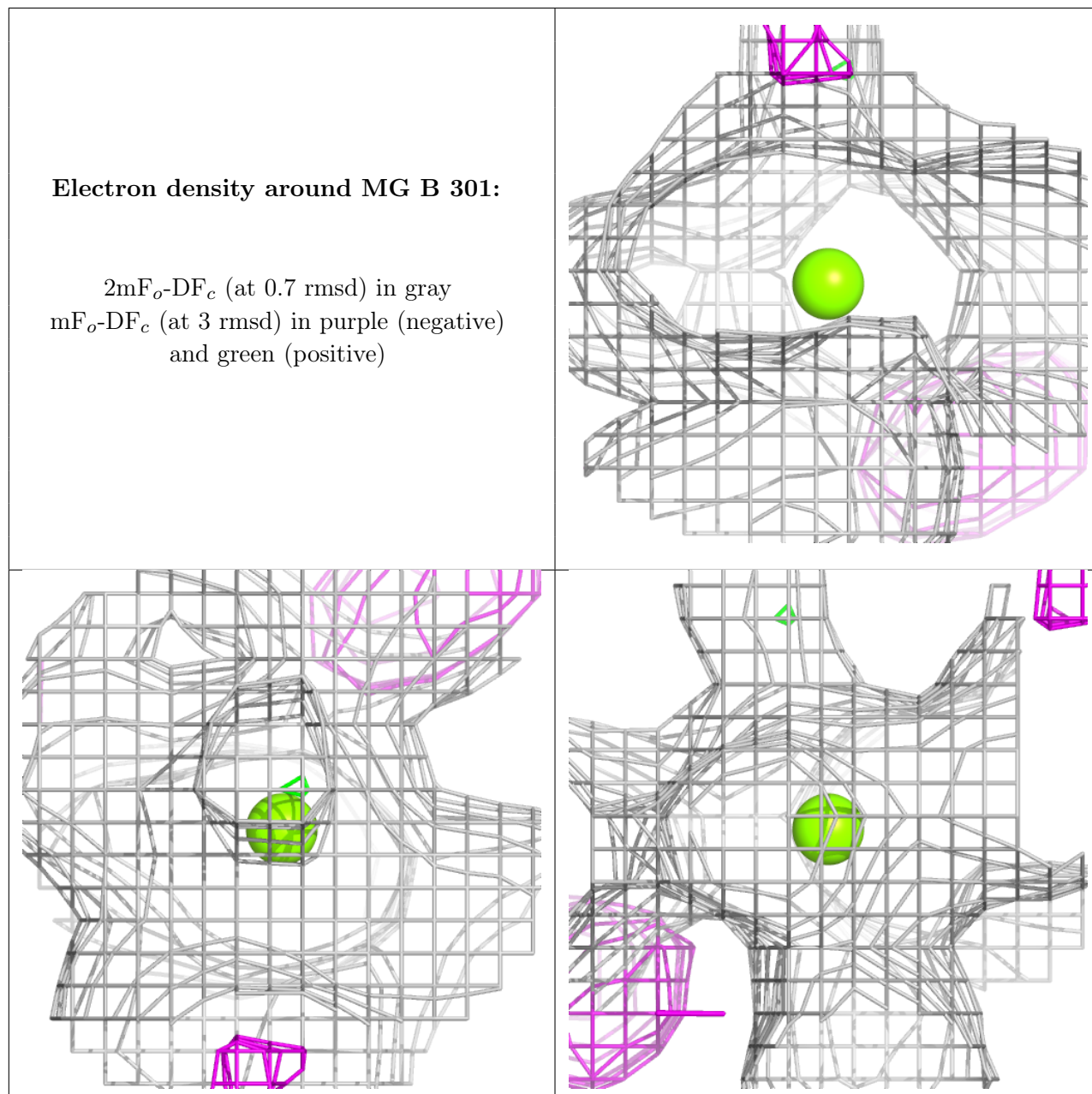
**Electron density around DMA D 302:**

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



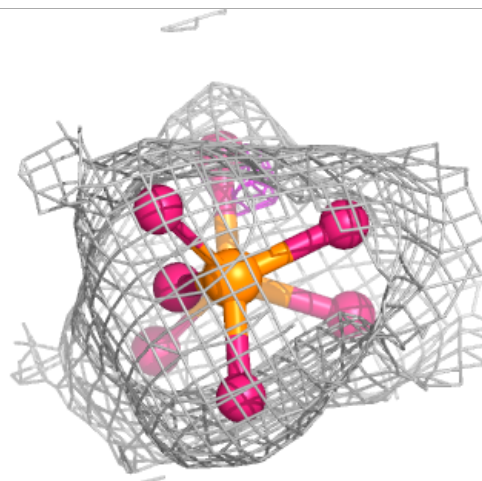
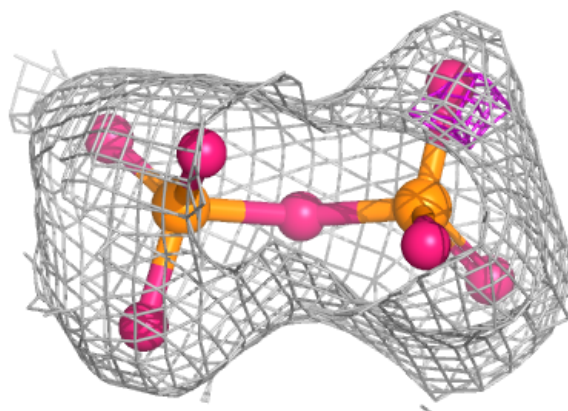
Electron density around MG B 301:

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



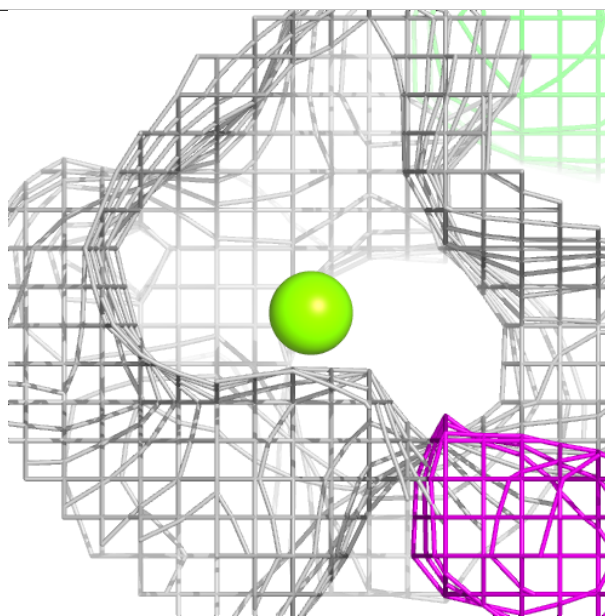
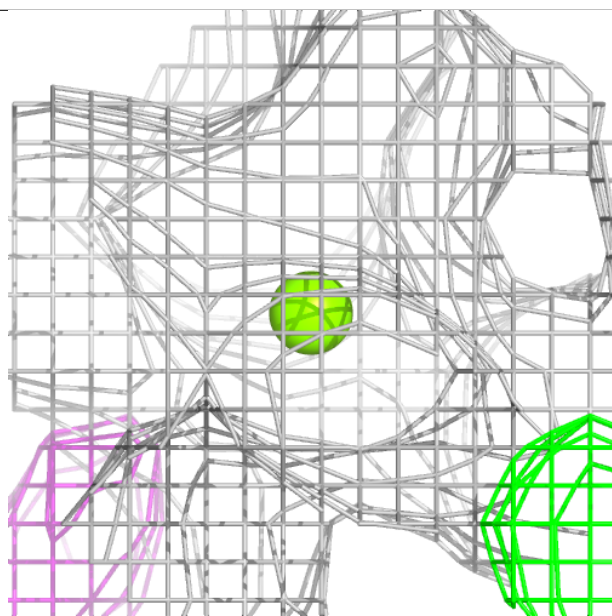
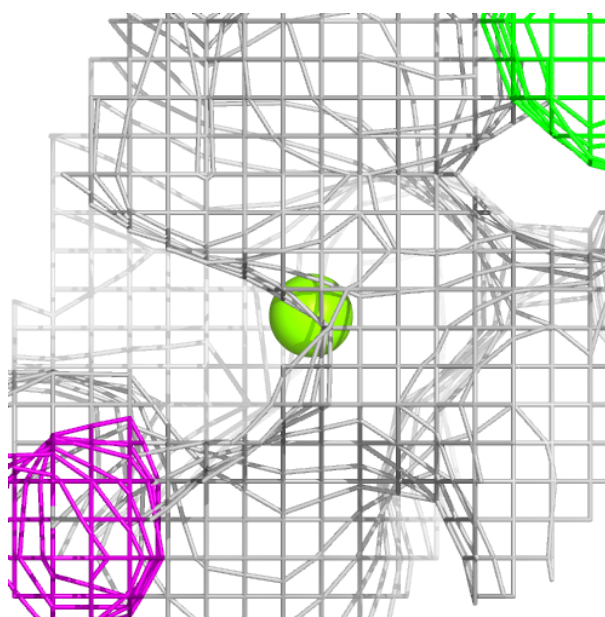
Electron density around DPO B 303:

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



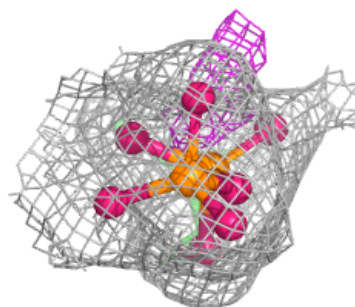
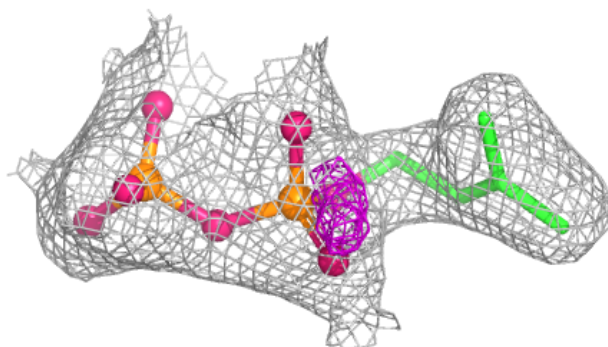
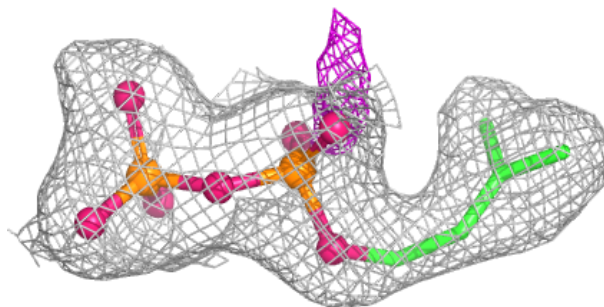
Electron density around MG E 303:

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



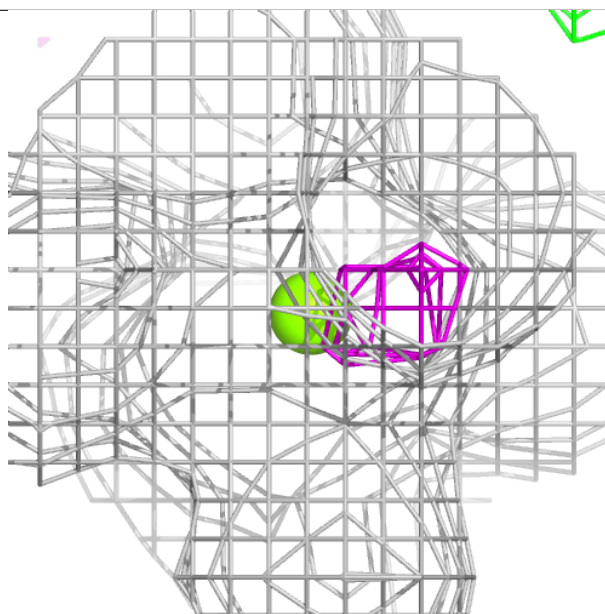
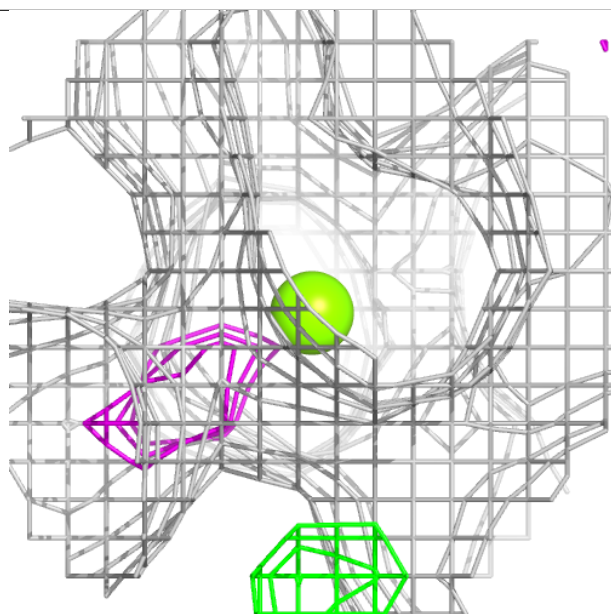
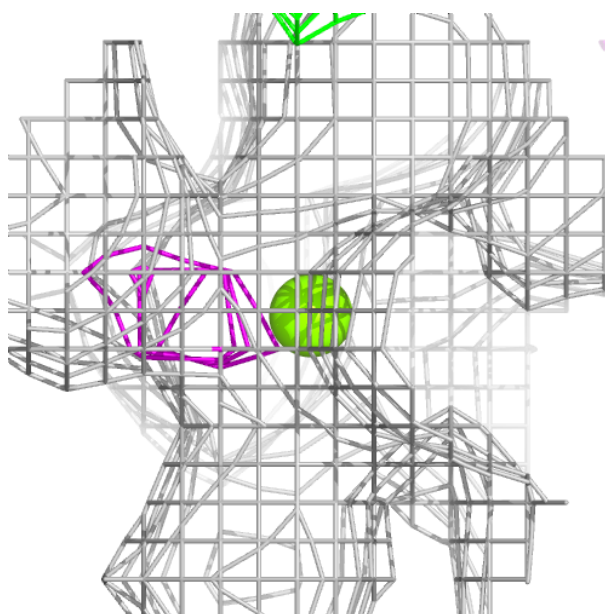
Electron density around DMA D 301:

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



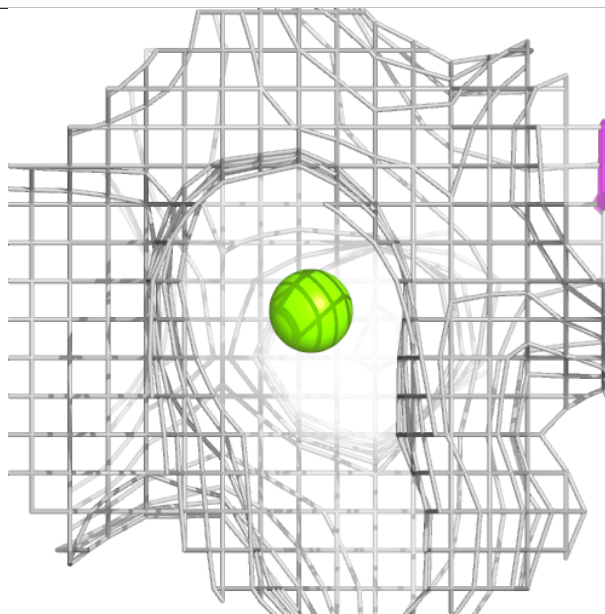
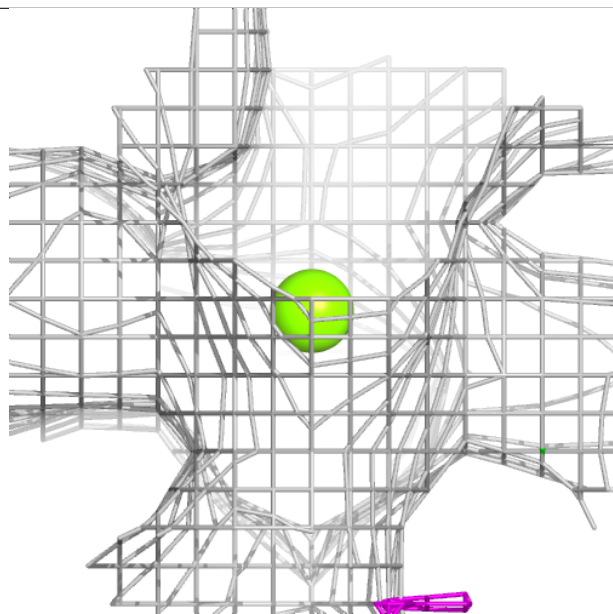
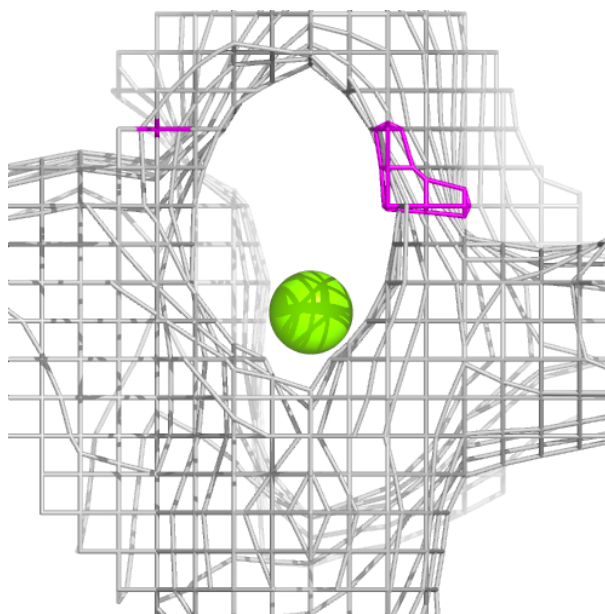
Electron density around MG A 303:

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



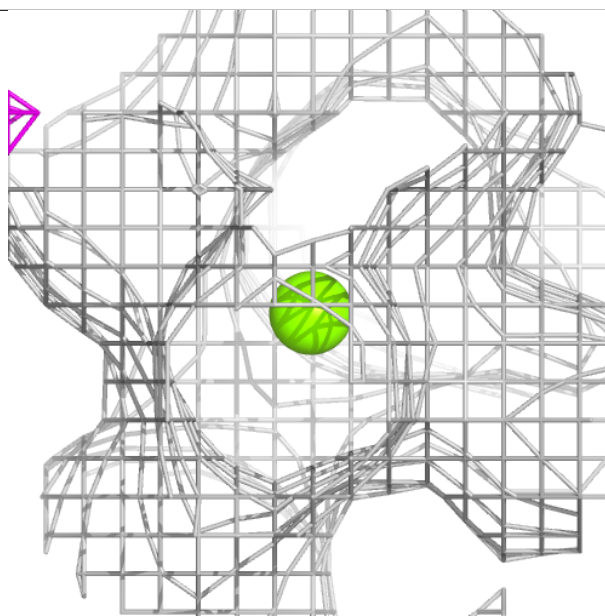
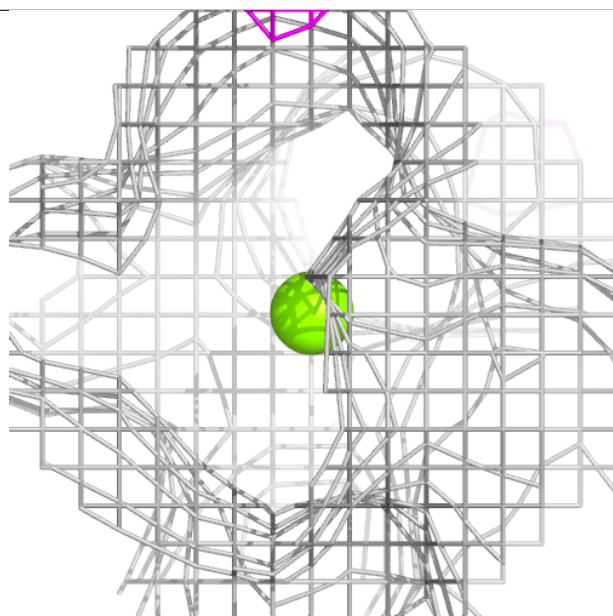
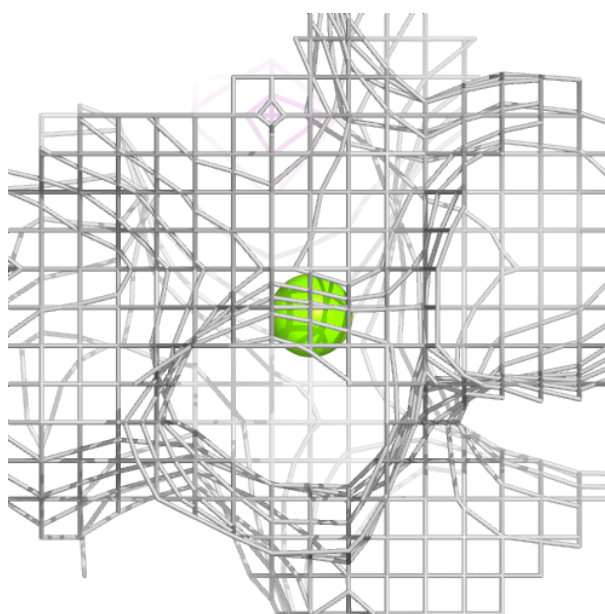
Electron density around MG C 303:

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



Electron density around 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.