



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 8HMU / pdb_00008hmu
Title : Crystal Structure of PKM2 mutant R516C
Authors : Upadhyay, S.; Kumar, A.; Patel, A.K.
Deposited on : 2022-12-05
Resolution : 2.50 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

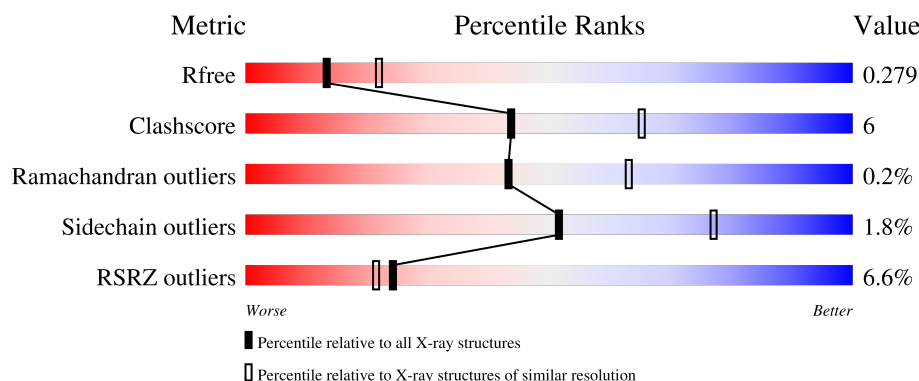
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	551	
1	B	551	
1	C	551	
1	D	551	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	B	606	-	X	-	-
3	OXL	D	602	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15451 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3839	2408	679	727	25			
1	B	464	Total	C	N	O	S	0	0	0
			3418	2145	607	642	24			
1	C	517	Total	C	N	O	S	0	0	0
			3872	2440	679	727	26			
1	D	515	Total	C	N	O	S	0	0	0
			3895	2450	684	735	26			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
A	516	CYS	ARG	engineered mutation	UNP P14618

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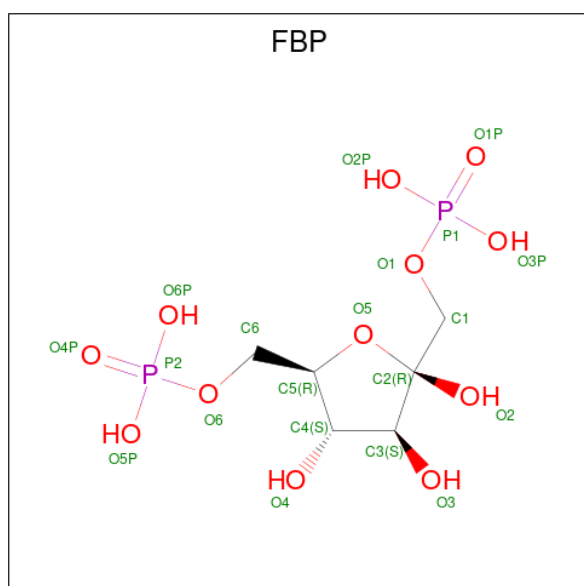
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
B	516	CYS	ARG	engineered mutation	UNP P14618
C	-19	MET	-	initiating methionine	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
C	516	CYS	ARG	engineered mutation	UNP P14618

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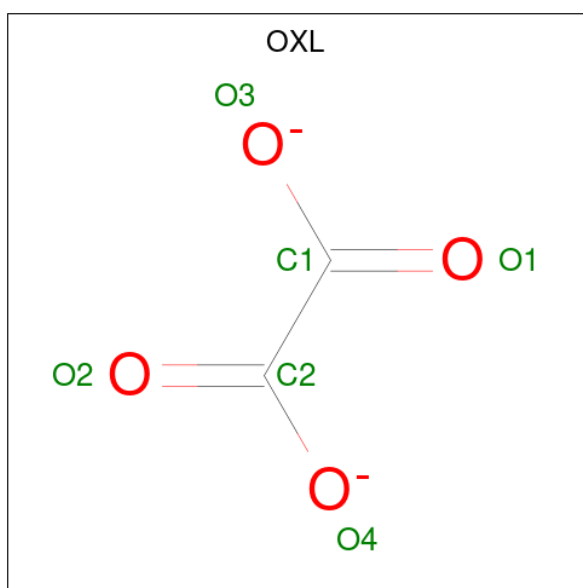
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	516	CYS	ARG	engineered mutation	UNP P14618

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			6	1	4	1		
2	B	1	Total	C	O	P	0	0
			6	1	4	1		
2	C	1	Total	C	O	P	0	0
			12	2	8	2		
2	C	1	Total	C	O	P	0	0
			6	1	4	1		
2	D	1	Total	C	O	P	0	0
			12	2	8	2		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

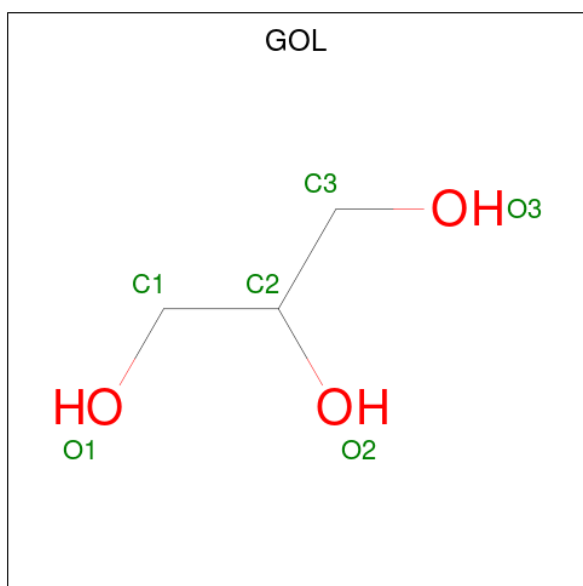
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

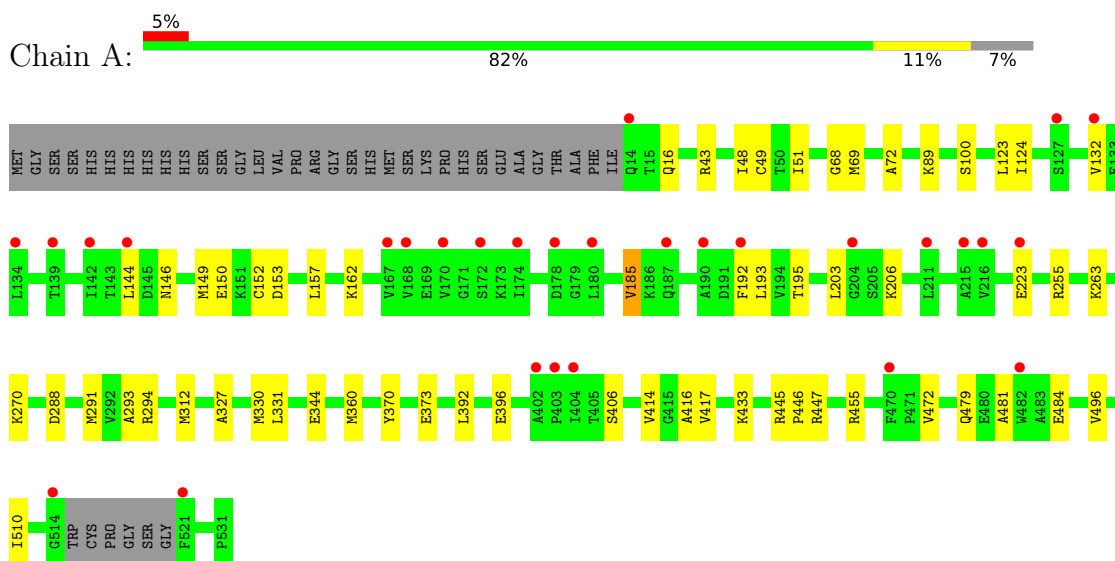
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	60	Total	O	0	0
			60	60		
8	B	48	Total	O	0	0
			48	48		
8	C	69	Total	O	0	0
			69	69		
8	D	81	Total	O	0	0
			81	81		

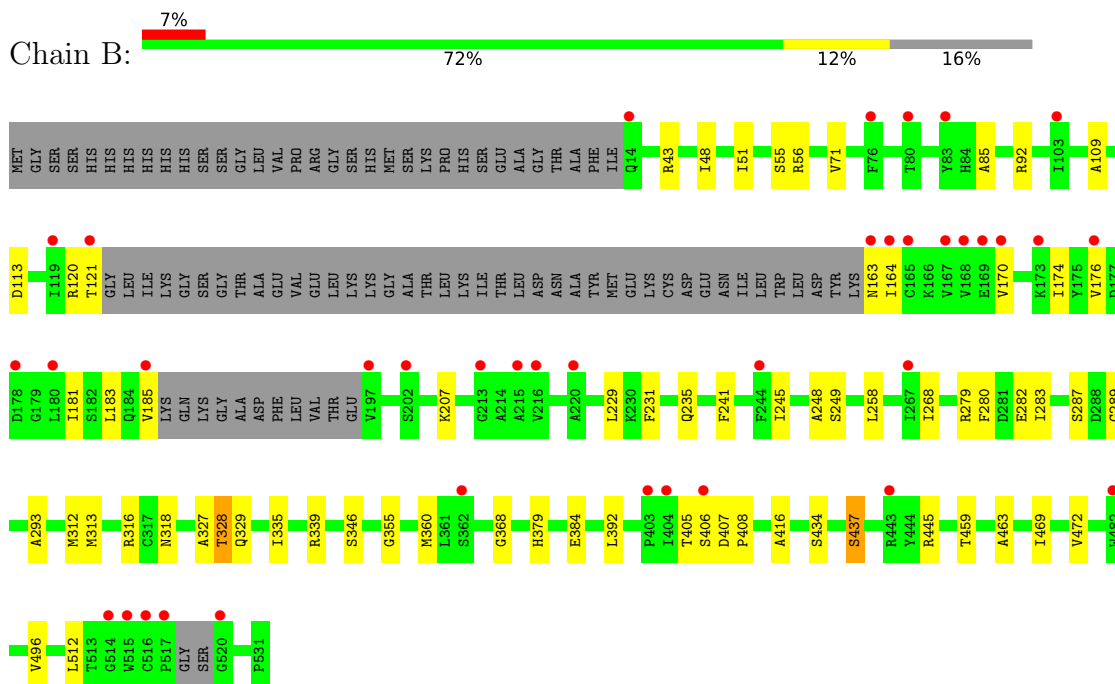
3 Residue-property plots [i](#)

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.

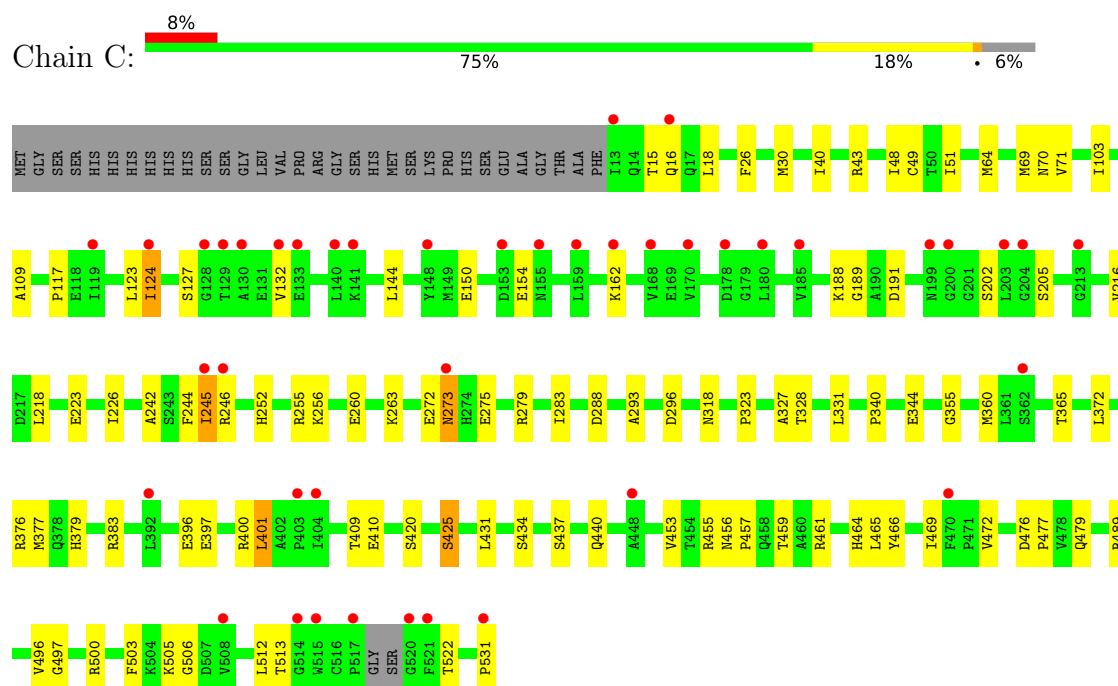
• Molecule 1: Pyruvate kinase PKM



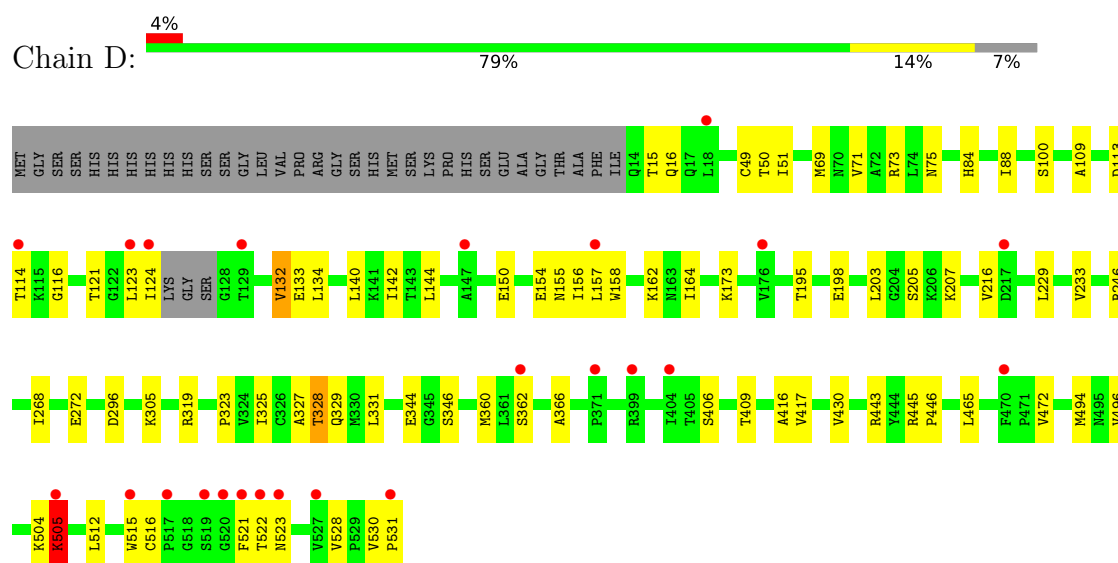
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.40Å 138.51Å 155.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.50 49.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.92-2.50) 98.2 (49.92-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.279 0.237 , 0.279	Depositor DCC
R_{free} test set	3999 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15451	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, EDO, PO4, MG, GOL, OXL

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	0.09	0/3898	0.25	0/5281
1	B	0.10	0/3471	0.27	0/4712
1	C	0.14	0/3935	0.33	0/5335
1	D	0.18	0/3958	0.36	3/5360 (0.1%)
All	All	0.13	0/15262	0.31	3/20688 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	505	LYS	N-CA-CB	8.20	121.98	110.17
1	D	504	LYS	CA-C-N	-5.03	113.04	120.94
1	D	504	LYS	C-N-CA	-5.03	113.04	120.94

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	3839	0	3828	35	0
1	B	3418	0	3371	38	0
1	C	3872	0	3864	66	0
1	D	3895	0	3908	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	18	0	0	0	0
2	D	12	0	0	0	0
3	A	6	0	0	1	0
3	B	12	0	0	1	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
4	A	4	0	6	0	0
4	B	12	0	18	1	0
4	C	8	0	12	1	0
4	D	4	0	6	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	D	20	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	B	6	0	8	0	0
7	D	6	0	8	0	0
8	A	60	0	0	1	0
8	B	48	0	0	2	0
8	C	69	0	0	0	0
8	D	81	0	0	1	0
All	All	15451	0	15029	185	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 (185) 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:C:49:CYS:HB2	1:C:69:MET:HE2	1.67	0.75
1:B:405:THR:HG22	1:B:407:ASP:H	1.50	0.73
1:D:505:LYS:HB2	1:D:530:VAL:O	1.87	0.73
1:A:51:ILE:HD11	1:A:69:MET:HE1	1.74	0.70
1:C:246:ARG:NH1	1:C:273:ASN:OD1	2.23	0.70
1:A:49:CYS:HB2	1:A:69:MET:HE3	1.73	0.69
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HG22	1:B:283:ILE:HD13	1.72	0.69
1:A:48:ILE:HB	1:A:360:MET:HG3	1.75	0.68
1:C:48:ILE:HB	1:C:360:MET:HG3	1.75	0.68
1:C:272:GLU:HG2	1:C:293:ALA:HB3	1.75	0.67
1:C:242:ALA:HB3	1:C:245:ILE:HD11	1.79	0.65
1:A:223:GLU:H	1:A:223:GLU:CD	2.05	0.63
1:C:51:ILE:HD11	1:C:69:MET:HE1	1.81	0.62
1:D:494:MET:SD	1:D:531:PRO:HD2	2.40	0.61
1:D:84:HIS:O	1:D:88:ILE:HG13	2.00	0.61
1:C:103:ILE:O	1:C:500:ARG:NH2	2.30	0.61
1:C:505:LYS:HG3	1:C:531:PRO:HG3	1.84	0.59
1:C:372:LEU:O	1:C:376:ARG:HG3	2.02	0.59
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.85	0.59
1:B:248:ALA:HB2	1:B:282:GLU:HB3	1.86	0.58
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.85	0.58
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.85	0.58
1:C:396:GLU:O	1:C:400:ARG:HG3	2.04	0.57
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.87	0.57
1:B:120:ARG:HH22	4:B:607:EDO:H21	1.70	0.57
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.86	0.56
1:A:124:ILE:HA	1:A:152:CYS:HB2	1.87	0.56
1:B:164:ILE:HD12	1:B:164:ILE:H	1.70	0.56
1:B:384:GLU:OE2	1:D:305:LYS:NZ	2.37	0.56
1:C:331:LEU:HD23	1:C:344:GLU:HB3	1.88	0.56
1:C:252:HIS:O	1:C:256:LYS:HE2	2.07	0.55
1:C:246:ARG:HB2	1:C:275:GLU:HG2	1.88	0.55
1:C:64:MET:HE1	1:C:365:THR:HB	1.89	0.55
1:C:437:SER:HA	1:C:440:GLN:NE2	2.21	0.55
1:B:279:ARG:O	1:B:283:ILE:HG13	2.07	0.55
1:C:506:GLY:H	1:C:531:PRO:HD3	1.71	0.55
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.89	0.55
1:D:121:THR:HG22	1:D:157:LEU:HD21	1.87	0.54
1:A:417:VAL:HG13	1:A:446:PRO:HB3	1.90	0.54
1:C:223:GLU:HA	1:C:226:ILE:HD12	1.89	0.54
1:D:521:PHE:HE1	1:D:523:ASN:HD22	1.55	0.53
1:A:392:LEU:O	1:A:396:GLU:HG3	2.08	0.53
1:B:85:ALA:HB2	1:B:231:PHE:HZ	1.73	0.53
1:C:144:LEU:HD22	1:C:162:LYS:HA	1.90	0.53
1:A:481:ALA:HB3	1:A:484:GLU:HB2	1.91	0.53
1:D:155:ASN:HB3	1:D:156:ILE:HD12	1.90	0.53
1:D:272:GLU:HB3	1:D:296:ASP:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:THR:HG22	1:D:366:ALA:HB2	1.90	0.52
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.92	0.52
1:A:144:LEU:HD11	1:A:162:LYS:HG2	1.91	0.52
1:D:73:ARG:HH21	1:D:113:ASP:CG	2.18	0.52
1:C:242:ALA:CB	1:C:245:ILE:HD11	2.39	0.52
1:C:260:GLU:CD	1:C:263:LYS:HD3	2.35	0.52
1:D:15:THR:O	1:D:16:GLN:HG2	2.09	0.52
1:C:124:ILE:HD11	1:C:132:VAL:HB	1.92	0.52
1:D:430:VAL:HG22	1:D:512:LEU:HD12	1.92	0.51
1:D:144:LEU:HD22	1:D:162:LYS:HA	1.92	0.51
1:C:477:PRO:O	1:C:479:GLN:NE2	2.43	0.51
1:C:255:ARG:NH2	1:C:288:ASP:OD2	2.44	0.51
1:C:16:GLN:HG2	1:C:40:ILE:HG23	1.92	0.51
1:C:43:ARG:HD3	1:C:379:HIS:HA	1.93	0.51
1:C:70:ASN:HB3	1:C:464:HIS:CG	2.45	0.51
1:C:272:GLU:HB3	1:C:296:ASP:HB2	1.92	0.51
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.94	0.50
1:D:51:ILE:HD11	1:D:69:MET:HE1	1.92	0.50
1:C:188:LYS:HG2	1:C:189:GLY:H	1.76	0.49
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.94	0.49
1:D:134:LEU:HD11	1:D:203:LEU:HD22	1.93	0.49
1:D:173:LYS:NZ	1:D:198:GLU:OE1	2.35	0.49
1:C:49:CYS:SG	1:C:69:MET:HG3	2.53	0.49
1:D:123:LEU:HD13	1:D:150:GLU:HG2	1.94	0.49
1:C:457:PRO:O	1:C:461:ARG:HG3	2.13	0.49
1:C:26:PHE:CE2	1:C:30:MET:HE2	2.47	0.49
1:C:43:ARG:HB2	1:C:383:ARG:HG3	1.95	0.49
1:C:144:LEU:HD12	1:C:191:ASP:HA	1.95	0.48
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.95	0.48
1:C:397:GLU:O	1:C:401:LEU:HD22	2.14	0.47
1:C:453:VAL:HG11	1:C:489:ARG:HB3	1.96	0.47
1:C:117:PRO:HD2	1:C:244:PHE:HB2	1.97	0.47
1:D:121:THR:OG1	1:D:207:LYS:N	2.42	0.47
1:D:140:LEU:HD21	1:D:157:LEU:HD12	1.97	0.47
1:A:146:ASN:HB3	1:A:149:MET:HE3	1.95	0.47
1:A:433:LYS:HZ1	1:A:455:ARG:H	1.61	0.47
1:B:92:ARG:NH2	1:B:235:GLN:O	2.47	0.47
1:B:327:ALA:HB1	1:B:360:MET:HE2	1.97	0.47
1:B:416:ALA:HB2	1:B:512:LEU:HD11	1.96	0.47
1:D:505:LYS:HE2	1:D:531:PRO:C	2.39	0.47
1:A:270:LYS:HG2	1:A:291:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.97	0.47
1:A:89:LYS:HE3	1:A:89:LYS:HB3	1.74	0.46
1:B:43:ARG:HD3	1:B:379:HIS:HA	1.95	0.46
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.97	0.46
1:A:263:LYS:NZ	8:A:701:HOH:O	2.29	0.46
1:B:121:THR:HG22	1:B:207:LYS:H	1.81	0.46
1:D:50:THR:OG1	1:D:73:ARG:HD3	2.16	0.46
1:D:515:TRP:CD1	1:D:516:CYS:HG	2.34	0.46
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.98	0.46
1:D:268:ILE:HG21	1:D:325:ILE:HD12	1.98	0.46
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.97	0.45
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.98	0.45
1:D:319:ARG:O	1:D:443:ARG:NH2	2.49	0.45
1:A:293:ALA:HB1	3:A:602:OXL:C2	2.47	0.45
1:B:463:ALA:HB1	1:B:469:ILE:HG21	1.96	0.45
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.98	0.45
1:C:15:THR:O	1:C:18:LEU:HG	2.16	0.45
1:C:409:THR:HG23	1:C:522:THR:O	2.16	0.45
1:B:170:VAL:HA	1:B:185:VAL:HG12	1.98	0.45
1:B:293:ALA:HB1	3:B:602:OXL:C2	2.47	0.45
1:B:445:ARG:NH1	8:B:705:HOH:O	2.47	0.45
1:C:123:LEU:HB2	1:C:150:GLU:HA	1.98	0.45
1:A:416:ALA:HB1	1:A:510:ILE:HG21	1.98	0.45
1:D:142:ILE:HD12	1:D:195:THR:HG21	1.98	0.45
1:B:355:GLY:O	1:B:445:ARG:NH2	2.50	0.45
1:C:216:VAL:HG21	4:C:605:EDO:H22	1.99	0.45
1:C:409:THR:CG2	1:C:440:GLN:HE22	2.30	0.45
1:D:114:THR:HG22	1:D:116:GLY:N	2.32	0.45
1:B:174:ILE:HB	1:B:183:LEU:HB2	1.98	0.45
1:D:445:ARG:NH1	8:D:703:HOH:O	2.49	0.45
1:B:280:PHE:CE1	1:B:313:MET:HG2	2.52	0.45
1:A:255:ARG:NH2	1:A:288:ASP:OD2	2.50	0.44
1:C:154:GLU:H	1:C:154:GLU:CD	2.25	0.44
1:A:69:MET:HE2	1:A:72:ALA:HA	1.98	0.44
1:A:185:VAL:HA	1:A:195:THR:HG22	1.98	0.44
1:A:192:PHE:O	1:A:193:LEU:HD12	2.17	0.44
1:A:294:ARG:NH2	1:A:330:MET:HG2	2.32	0.44
1:D:50:THR:HB	1:D:362:SER:HA	1.97	0.44
1:B:335:ILE:HG23	1:B:368:GLY:HA2	2.00	0.44
1:B:339:ARG:HD2	1:B:339:ARG:HA	1.78	0.44
1:C:124:ILE:HG22	1:C:205:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD21	1:D:164:ILE:HG22	1.99	0.44
1:A:291:MET:HE2	1:A:360:MET:SD	2.58	0.44
1:B:406:SER:O	1:B:408:PRO:HD3	2.18	0.44
1:C:409:THR:HG22	1:C:440:GLN:HE22	1.83	0.44
1:C:260:GLU:O	1:C:263:LYS:HG3	2.17	0.44
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.99	0.44
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.99	0.44
1:D:216:VAL:HB	1:D:246:ARG:HH22	1.81	0.44
1:C:293:ALA:HB1	3:C:602:OXL:C2	2.48	0.43
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.99	0.43
1:B:472:VAL:HG11	1:B:496:VAL:HG11	2.00	0.43
1:D:132:VAL:HG22	1:D:154:GLU:HG3	2.00	0.43
1:D:123:LEU:HA	1:D:205:SER:HB3	2.00	0.43
1:D:229:LEU:O	1:D:233:VAL:HG23	2.19	0.43
1:D:409:THR:HG23	1:D:522:THR:HB	2.01	0.43
1:B:312:MET:HE3	1:B:312:MET:HB3	1.88	0.43
1:C:246:ARG:O	1:C:279:ARG:HD3	2.19	0.43
1:D:157:LEU:HD23	1:D:158:TRP:N	2.33	0.43
1:A:43:ARG:NH2	1:A:68:GLY:O	2.48	0.43
1:B:113:ASP:HA	1:B:241:PHE:HB2	2.01	0.43
1:B:280:PHE:HE2	1:B:316:ARG:HB2	1.82	0.43
1:C:434:SER:HA	1:C:459:THR:HG21	2.00	0.43
1:C:246:ARG:HB2	1:C:275:GLU:CG	2.48	0.43
1:C:431:LEU:HD22	1:C:513:THR:HG22	2.01	0.43
1:A:16:GLN:O	1:A:447:ARG:NH1	2.52	0.43
1:C:323:PRO:HB3	1:C:465:LEU:O	2.18	0.43
1:C:505:LYS:HA	1:C:531:PRO:HD3	2.00	0.43
1:D:331:LEU:HD23	1:D:344:GLU:HB3	2.01	0.43
1:D:75:ASN:HA	1:D:113:ASP:HB3	2.00	0.42
1:C:420:SER:HA	1:C:425:SER:HB2	2.01	0.42
1:A:206:LYS:HE2	1:A:206:LYS:HB2	1.80	0.42
1:B:51:ILE:HG22	1:B:56:ARG:HG3	2.02	0.42
1:B:437:SER:OG	2:B:601:FBP:O4P	2.36	0.42
1:D:323:PRO:HB3	1:D:465:LEU:O	2.20	0.42
1:C:455:ARG:NH1	1:C:476:ASP:O	2.52	0.42
1:A:132:VAL:HG11	1:A:153:ASP:HA	2.00	0.42
1:A:445:ARG:HA	1:A:445:ARG:HD3	1.82	0.42
1:B:229:LEU:HD22	1:B:258:LEU:HD21	2.01	0.42
1:B:268:ILE:HD12	1:B:289:GLY:HA3	2.01	0.42
1:B:48:ILE:HB	1:B:360:MET:HG3	2.02	0.42
1:B:283:ILE:O	1:B:287:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.90	0.41
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.55	0.41
1:C:512:LEU:HB3	1:C:522:THR:HG21	2.01	0.41
1:A:479:GLN:HE21	1:A:479:GLN:HB3	1.68	0.41
1:B:318:ASN:ND2	8:B:704:HOH:O	2.51	0.41
1:C:246:ARG:C	1:C:283:ILE:HD11	2.46	0.41
1:D:49:CYS:SG	1:D:69:MET:HG3	2.61	0.41
1:D:173:LYS:HD2	1:D:173:LYS:HA	1.90	0.41
1:C:456:ASN:CG	1:C:459:THR:HG23	2.46	0.41
1:A:312:MET:HE3	1:A:312:MET:HB3	1.96	0.41
1:B:434:SER:HA	1:B:459:THR:HG21	2.03	0.41
1:D:515:TRP:HD1	1:D:516:CYS:HG	1.69	0.40
1:C:318:ASN:HD21	1:C:355:GLY:HA3	1.87	0.40
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/551 (92%)	491 (97%)	17 (3%)	0	100	100
1	B	456/551 (83%)	445 (98%)	10 (2%)	1 (0%)	43	63
1	C	513/551 (93%)	497 (97%)	15 (3%)	1 (0%)	43	63
1	D	511/551 (93%)	500 (98%)	10 (2%)	1 (0%)	43	63
All	All	1988/2204 (90%)	1933 (97%)	52 (3%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	328	THR

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Mol	Chain	Res	Type
1	B	328	THR
1	D	328	THR

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	401/453 (88%)	397 (99%)	4 (1%)	68	86
1	B	351/453 (78%)	343 (98%)	8 (2%)	44	72
1	C	403/453 (89%)	395 (98%)	8 (2%)	48	75
1	D	411/453 (91%)	403 (98%)	8 (2%)	50	76
All	All	1566/1812 (86%)	1538 (98%)	28 (2%)	51	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	185	VAL
1	A	406	SER
1	A	414	VAL
1	B	55	SER
1	B	163	ASN
1	B	176	VAL
1	B	181	ILE
1	B	249	SER
1	B	346	SER
1	B	392	LEU
1	B	437	SER
1	C	124	ILE
1	C	127	SER
1	C	202	SER
1	C	245	ILE
1	C	273	ASN
1	C	401	LEU
1	C	410	GLU

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Mol	Chain	Res	Type
1	C	425	SER
1	D	100	SER
1	D	124	ILE
1	D	132	VAL
1	D	133	GLU
1	D	346	SER
1	D	406	SER
1	D	505	LYS
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	146	ASN
1	A	184	GLN
1	A	210	ASN
1	A	458	GLN
1	A	479	GLN
1	B	391	HIS
1	B	491	ASN
1	C	16	GLN
1	C	252	HIS
1	C	318	ASN
1	C	439	HIS
1	C	440	GLN
1	D	16	GLN
1	D	184	GLN
1	D	199	ASN
1	D	227	GLN
1	D	391	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 7 are monoatomic - leaving 29 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
3	OXL	C	602	6	5,5,5	0.16	0	6,6,6	0.54	0
5	PO4	D	603	-	4,4,4	0.94	0	6,6,6	0.46	0
2	FBP	B	601	-	5,5,20	1.75	1 (20%)	7,7,32	0.59	0
7	GOL	B	605	-	5,5,5	0.91	0	5,5,5	1.09	0
5	PO4	C	607	-	4,4,4	0.95	0	6,6,6	0.42	0
5	PO4	D	607	-	4,4,4	0.93	0	6,6,6	0.44	0
3	OXL	B	602	6	5,5,5	2.04	2 (40%)	6,6,6	2.08	2 (33%)
5	PO4	B	608	-	4,4,4	0.96	0	6,6,6	0.46	0
4	EDO	C	604	-	3,3,3	0.42	0	2,2,2	0.38	0
2	FBP	C	601	-	10,10,20	1.86	2 (20%)	14,14,32	0.60	0
5	PO4	A	605	-	4,4,4	0.96	0	6,6,6	0.45	0
3	OXL	A	602	6	5,5,5	2.86	4 (80%)	6,6,6	2.89	4 (66%)
4	EDO	A	603	-	3,3,3	0.42	0	2,2,2	0.39	0
2	FBP	C	603	-	5,5,20	1.76	1 (20%)	7,7,32	0.62	0
2	FBP	A	601	-	5,5,20	1.72	1 (20%)	7,7,32	0.61	0
3	OXL	D	602	6	5,5,5	2.90	4 (80%)	6,6,6	2.89	4 (66%)
5	PO4	D	604	-	4,4,4	0.94	0	6,6,6	0.47	0
5	PO4	C	606	-	4,4,4	0.95	0	6,6,6	0.46	0
3	OXL	B	606	-	5,5,5	2.85	4 (80%)	6,6,6	2.89	4 (66%)
4	EDO	D	605	-	3,3,3	0.42	0	2,2,2	0.40	0
5	PO4	A	606	-	4,4,4	0.94	0	6,6,6	0.47	0
2	FBP	D	601	-	10,10,20	1.87	2 (20%)	14,14,32	0.60	0
4	EDO	B	607	-	3,3,3	0.41	0	2,2,2	0.40	0
4	EDO	B	603	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	B	604	-	3,3,3	0.43	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	D	608	-	4,4,4	0.95	0	6,6,6	0.45	0
5	PO4	A	604	-	4,4,4	0.96	0	6,6,6	0.47	0
4	EDO	C	605	-	3,3,3	0.43	0	2,2,2	0.39	0
7	GOL	D	606	-	5,5,5	0.93	0	5,5,5	1.11	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
3	OXL	C	602	6	-	4/4/4/4	-
2	FBP	B	601	-	-	1/1/3/32	-
7	GOL	B	605	-	-	2/4/4/4	-
3	OXL	B	602	6	-	4/4/4/4	-
4	EDO	C	604	-	-	0/1/1/1	-
2	FBP	C	601	-	-	1/2/6/32	-
3	OXL	A	602	6	-	4/4/4/4	-
4	EDO	A	603	-	-	0/1/1/1	-
2	FBP	C	603	-	-	0/1/3/32	-
2	FBP	A	601	-	-	0/1/3/32	-
3	OXL	D	602	6	-	2/4/4/4	-
3	OXL	B	606	-	-	4/4/4/4	-
4	EDO	D	605	-	-	0/1/1/1	-
2	FBP	D	601	-	-	2/2/6/32	-
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	C	605	-	-	0/1/1/1	-
7	GOL	D	606	-	-	1/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FBP	P1-O1	4.27	1.66	1.59
2	C	601	FBP	P1-O1	4.22	1.66	1.59
2	C	603	FBP	P2-O6	3.79	1.66	1.59
2	A	601	FBP	P2-O6	3.67	1.65	1.59
2	B	601	FBP	P2-O6	3.65	1.65	1.59
3	A	602	OXL	O2-C2	3.63	1.31	1.22
3	D	602	OXL	O1-C1	3.63	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FBP	P2-O6	3.61	1.65	1.59
3	B	602	OXL	O1-C1	3.55	1.31	1.22
2	D	601	FBP	P2-O6	3.55	1.65	1.59
3	D	602	OXL	O2-C2	3.54	1.31	1.22
3	A	602	OXL	O1-C1	3.52	1.31	1.22
3	B	606	OXL	O1-C1	3.51	1.31	1.22
3	B	606	OXL	O2-C2	3.48	1.31	1.22
3	B	606	OXL	O4-C2	-2.87	1.22	1.30
3	D	602	OXL	O4-C2	-2.85	1.22	1.30
3	B	606	OXL	O3-C1	-2.84	1.22	1.30
3	D	602	OXL	O3-C1	-2.84	1.22	1.30
3	B	602	OXL	O3-C1	-2.83	1.22	1.30
3	A	602	OXL	O3-C1	-2.83	1.22	1.30
3	A	602	OXL	O4-C2	-2.69	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	OXL	O3-C1-C2	3.96	120.52	112.83
3	B	602	OXL	O3-C1-C2	3.96	120.51	112.83
3	D	602	OXL	O4-C2-C1	3.96	120.51	112.83
3	B	606	OXL	O3-C1-C2	3.96	120.51	112.83
3	B	606	OXL	O4-C2-C1	3.96	120.50	112.83
3	A	602	OXL	O4-C2-C1	3.95	120.50	112.83
3	D	602	OXL	O3-C1-C2	3.93	120.45	112.83
3	D	602	OXL	O2-C2-C1	-3.04	114.30	120.63
3	B	606	OXL	O2-C2-C1	-3.03	114.31	120.63
3	B	606	OXL	O1-C1-C2	-3.03	114.31	120.63
3	D	602	OXL	O1-C1-C2	-3.03	114.32	120.63
3	A	602	OXL	O2-C2-C1	-3.02	114.33	120.63
3	B	602	OXL	O1-C1-C2	-3.02	114.33	120.63
3	A	602	OXL	O1-C1-C2	-3.01	114.36	120.63

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C6-O6-P2-O4P
2	C	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C6-O6-P2-O4P
3	A	602	OXL	O3-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
3	B	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	B	606	OXL	O3-C1-C2-O4
3	B	606	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O3-C1-C2-O2
7	B	605	GOL	C1-C2-C3-O3
7	B	605	GOL	O2-C2-C3-O3
3	B	606	OXL	O1-C1-C2-O4
3	B	606	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
4	B	607	EDO	O1-C1-C2-O2
7	D	606	GOL	O2-C2-C3-O3
3	D	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O2

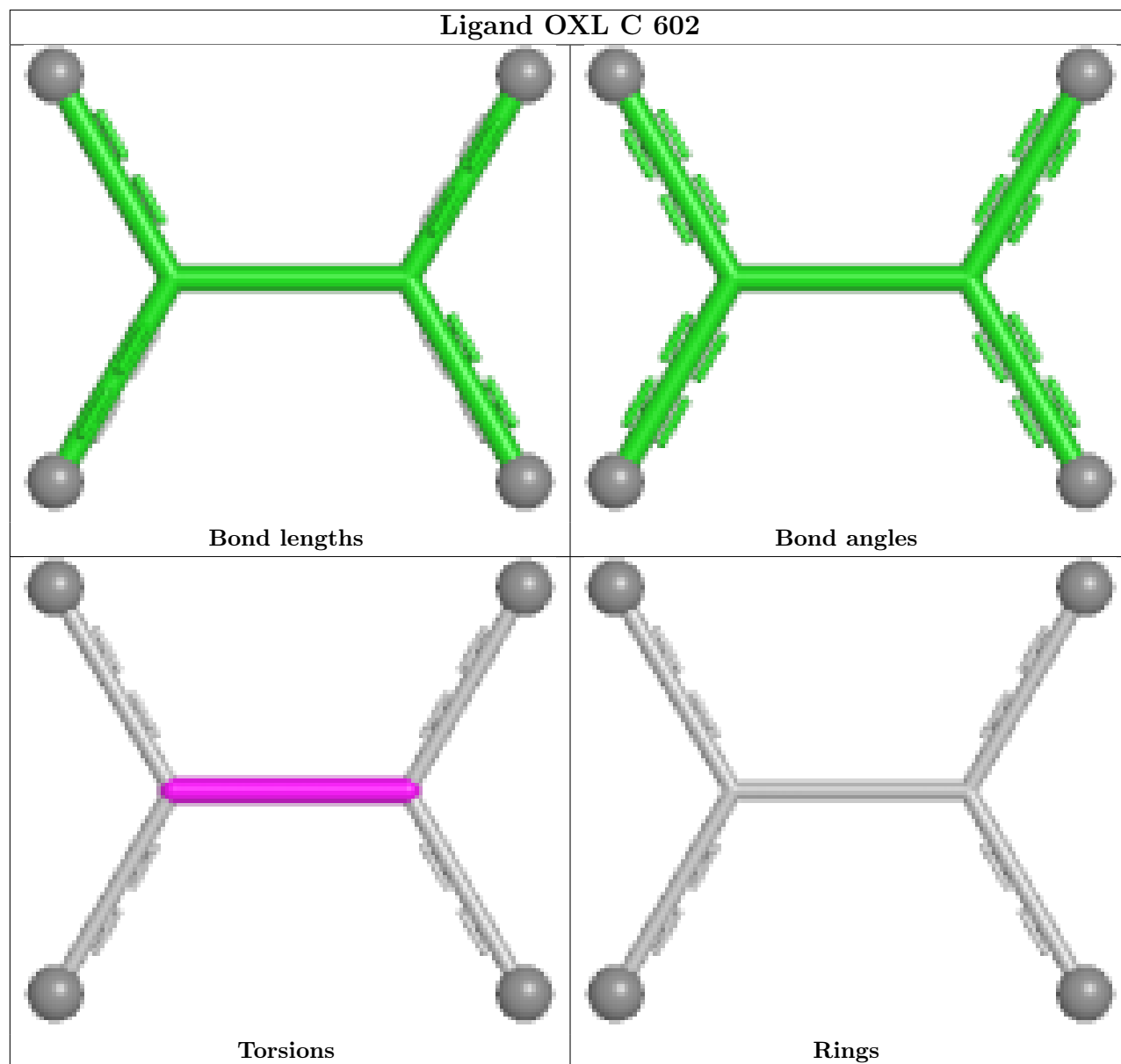
There are no ring outliers.

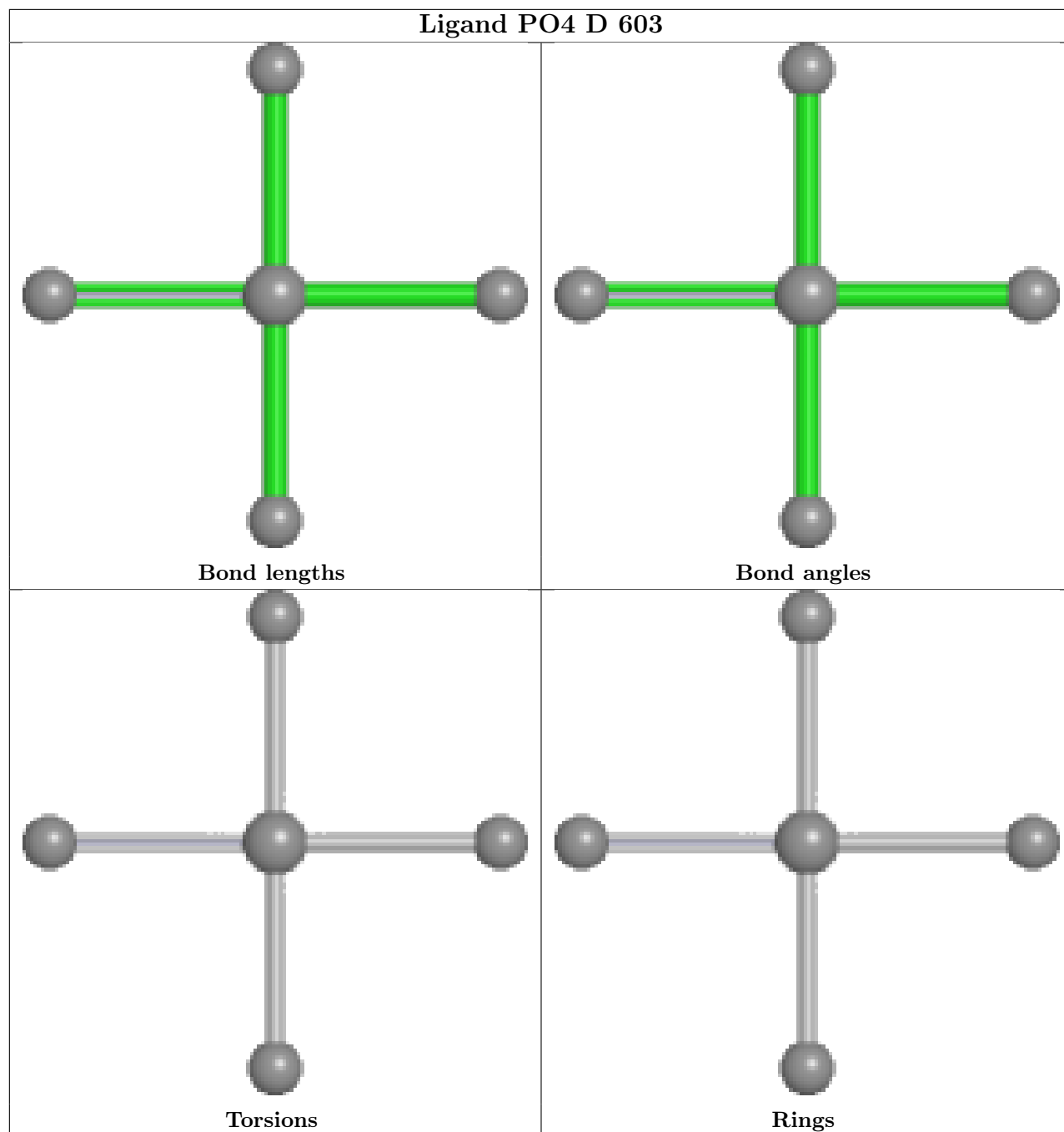
6 monomers are involved in 6 short contacts:

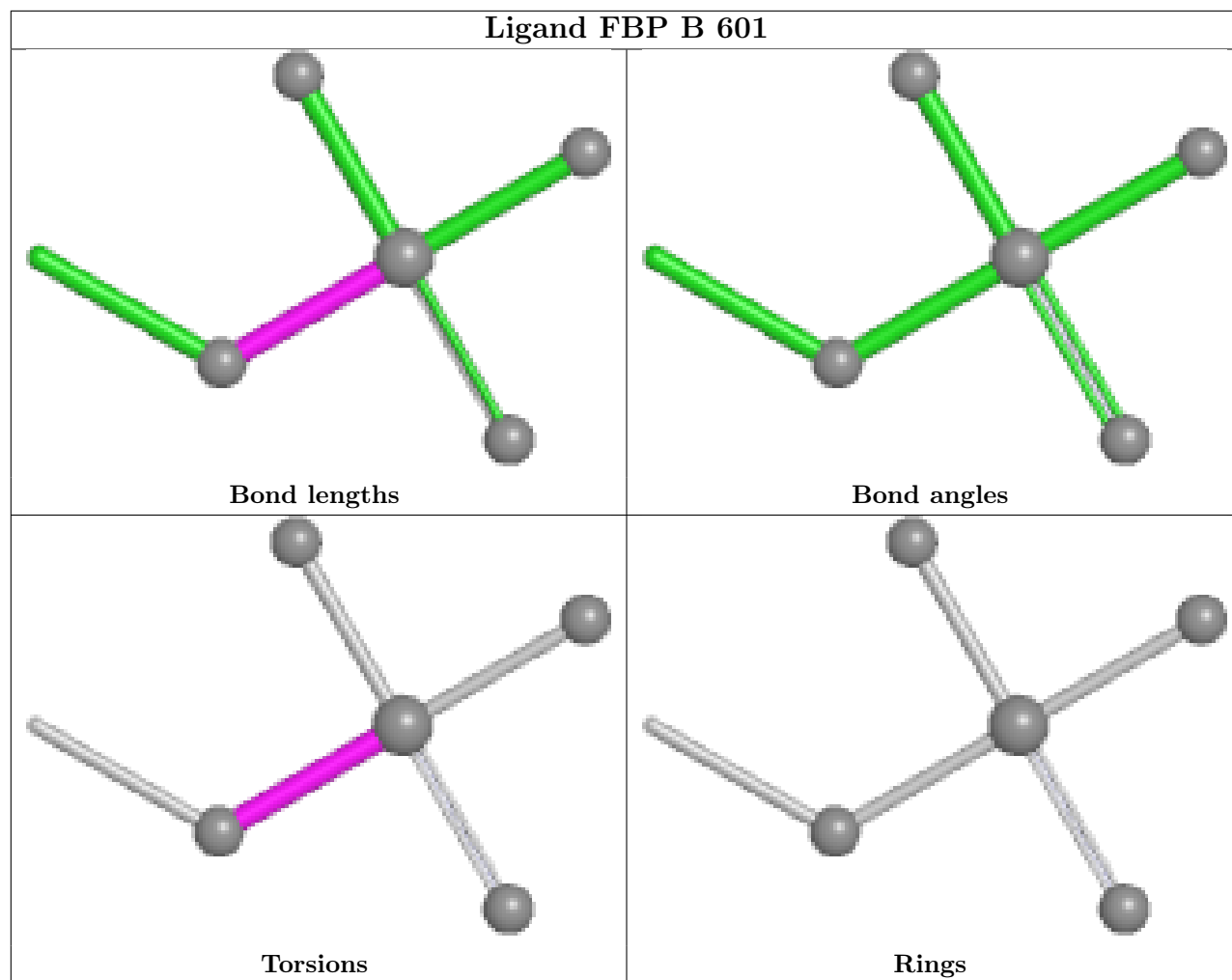
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	OXL	1	0
2	B	601	FBP	1	0
3	B	602	OXL	1	0
3	A	602	OXL	1	0
4	B	607	EDO	1	0
4	C	605	EDO	1	0

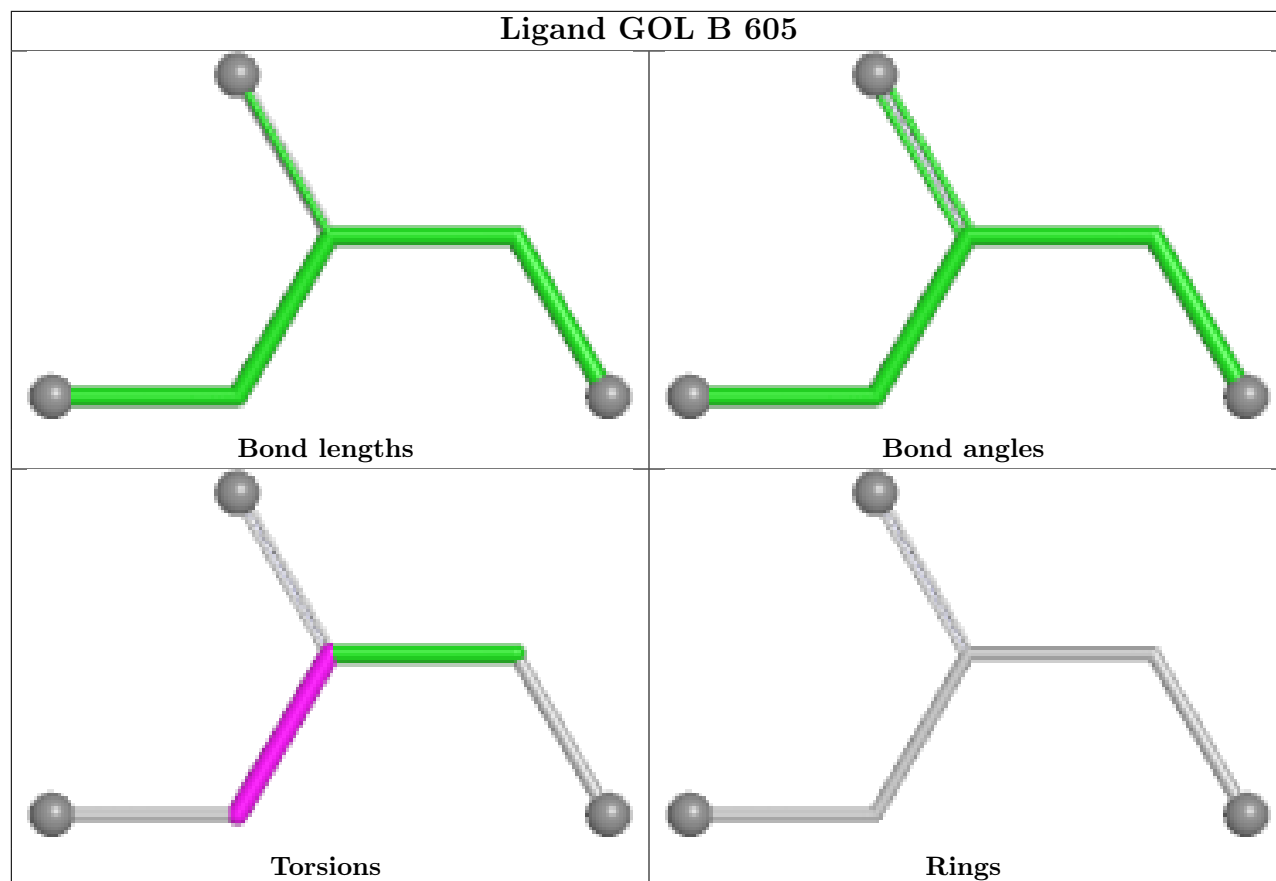
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

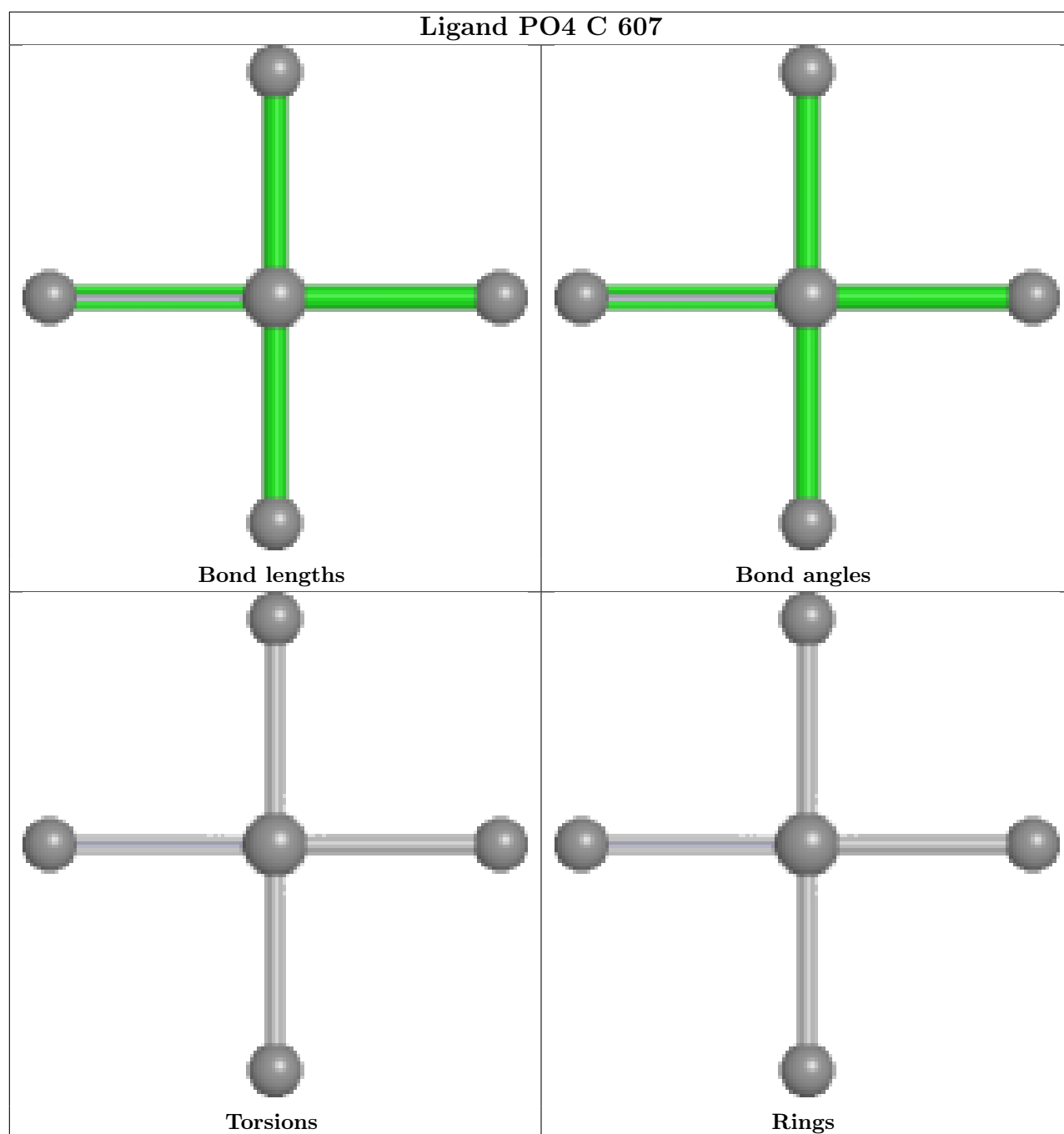
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

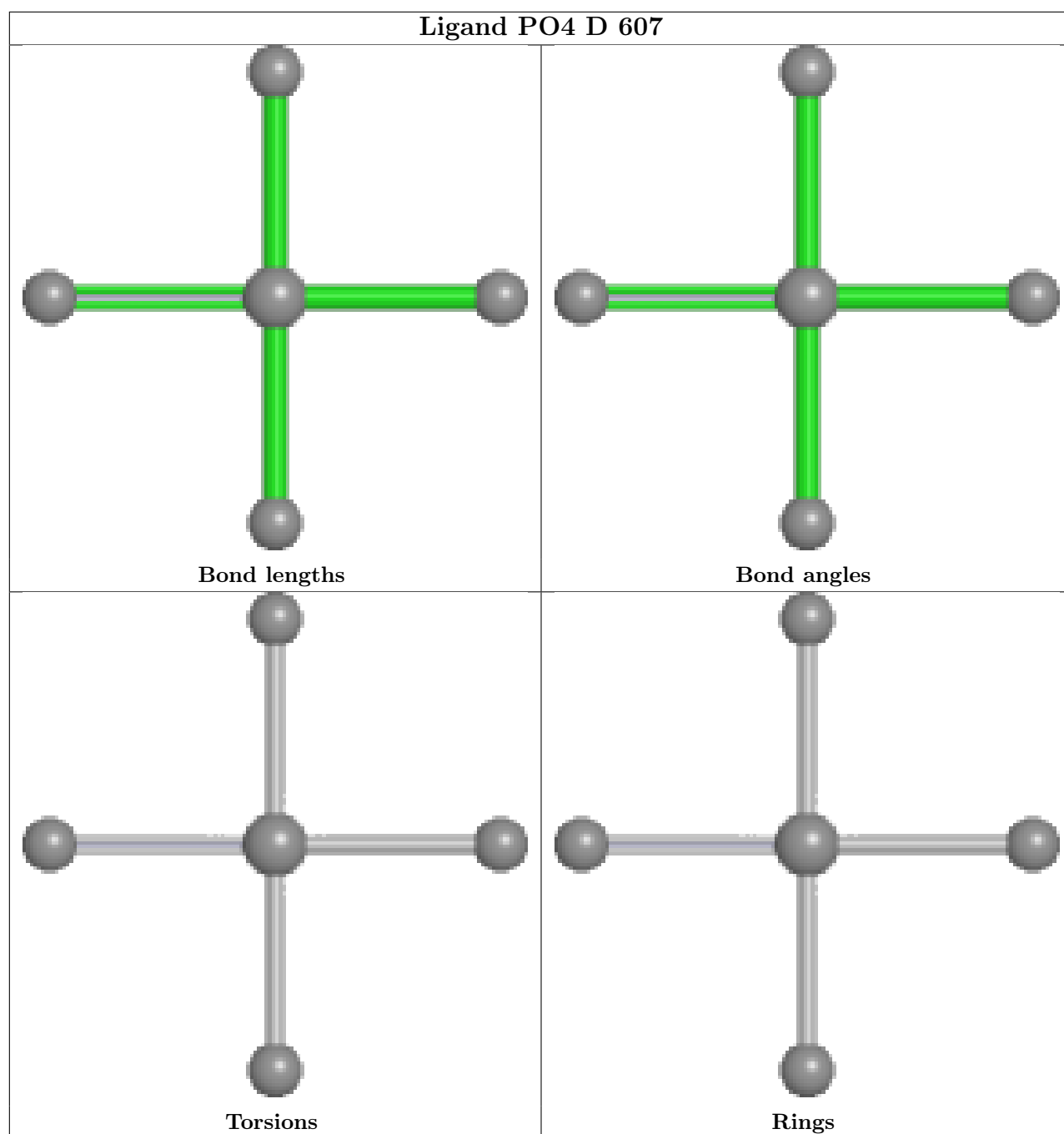


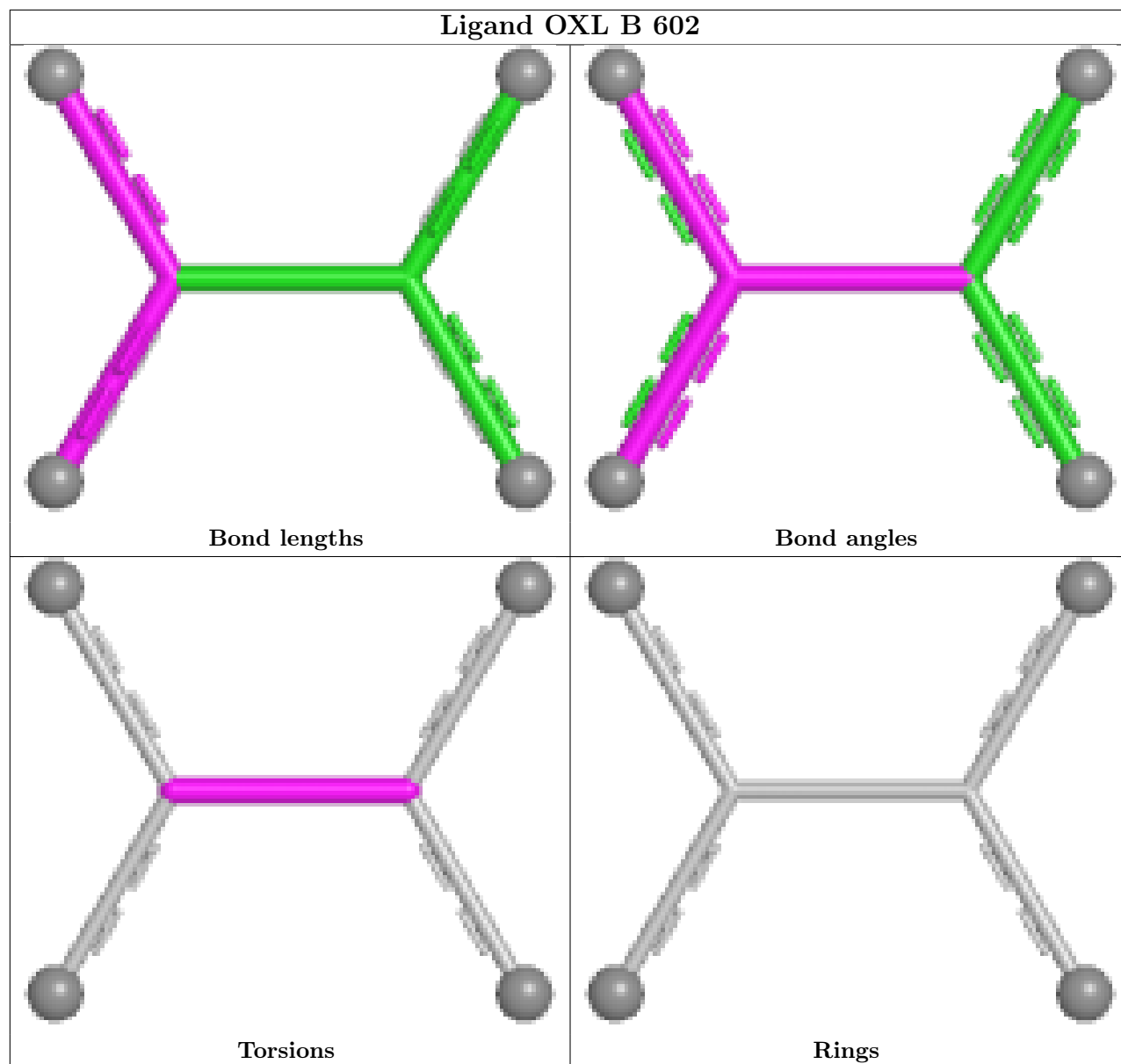


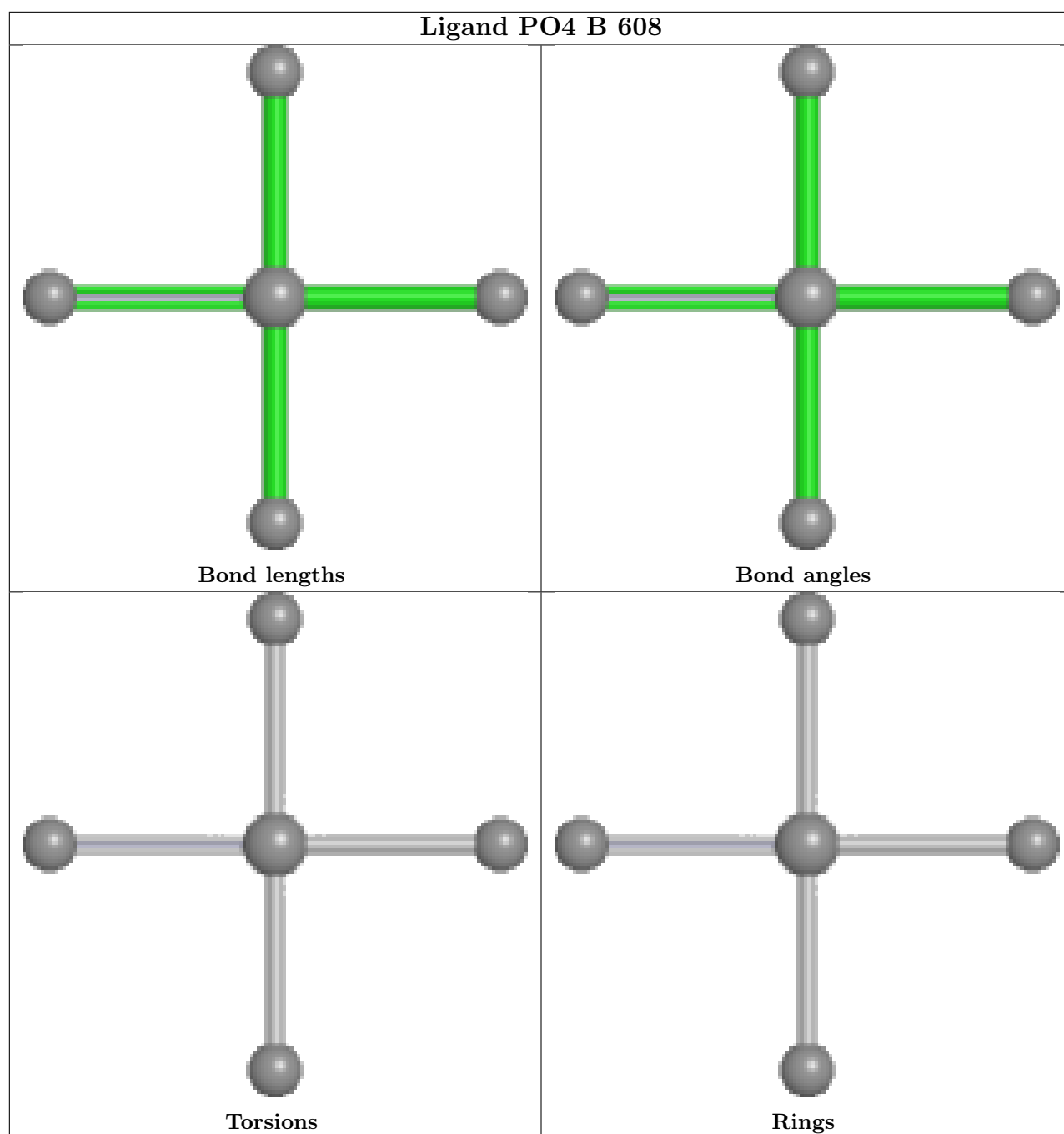


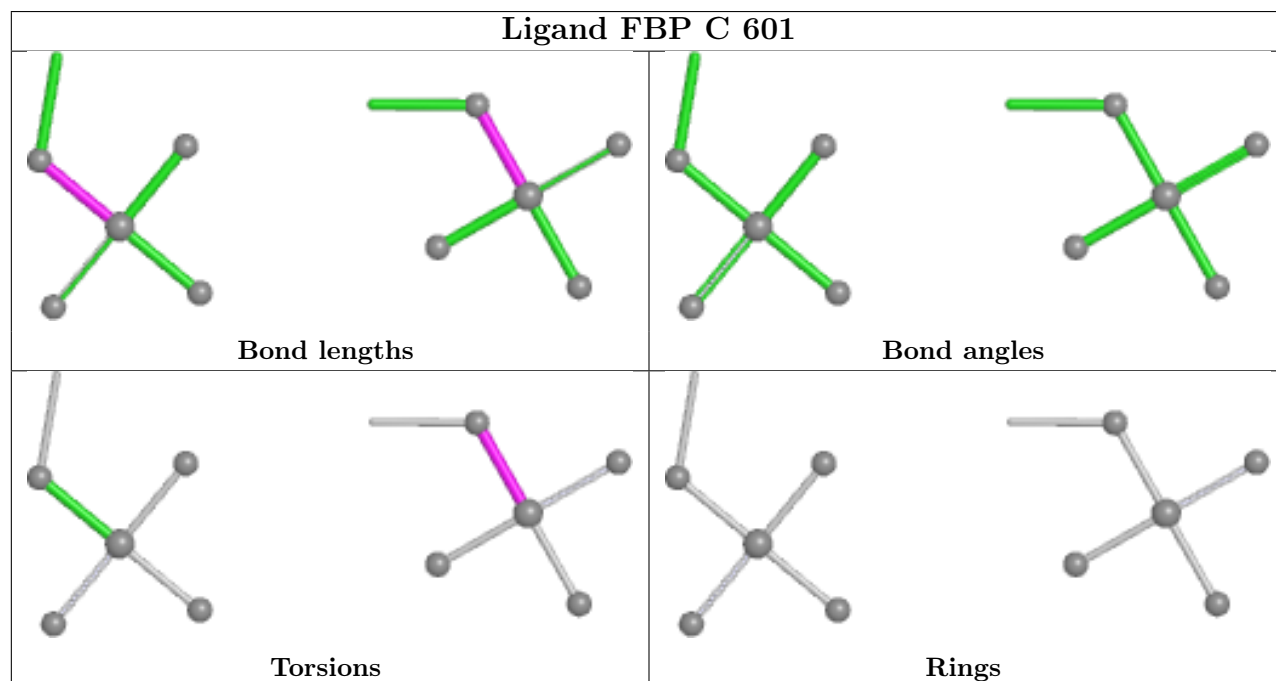
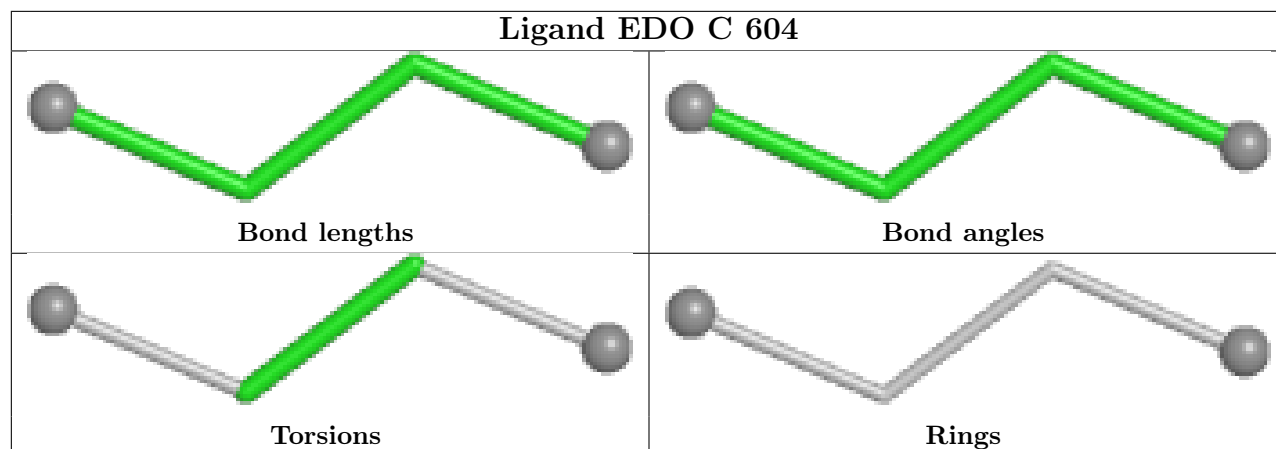


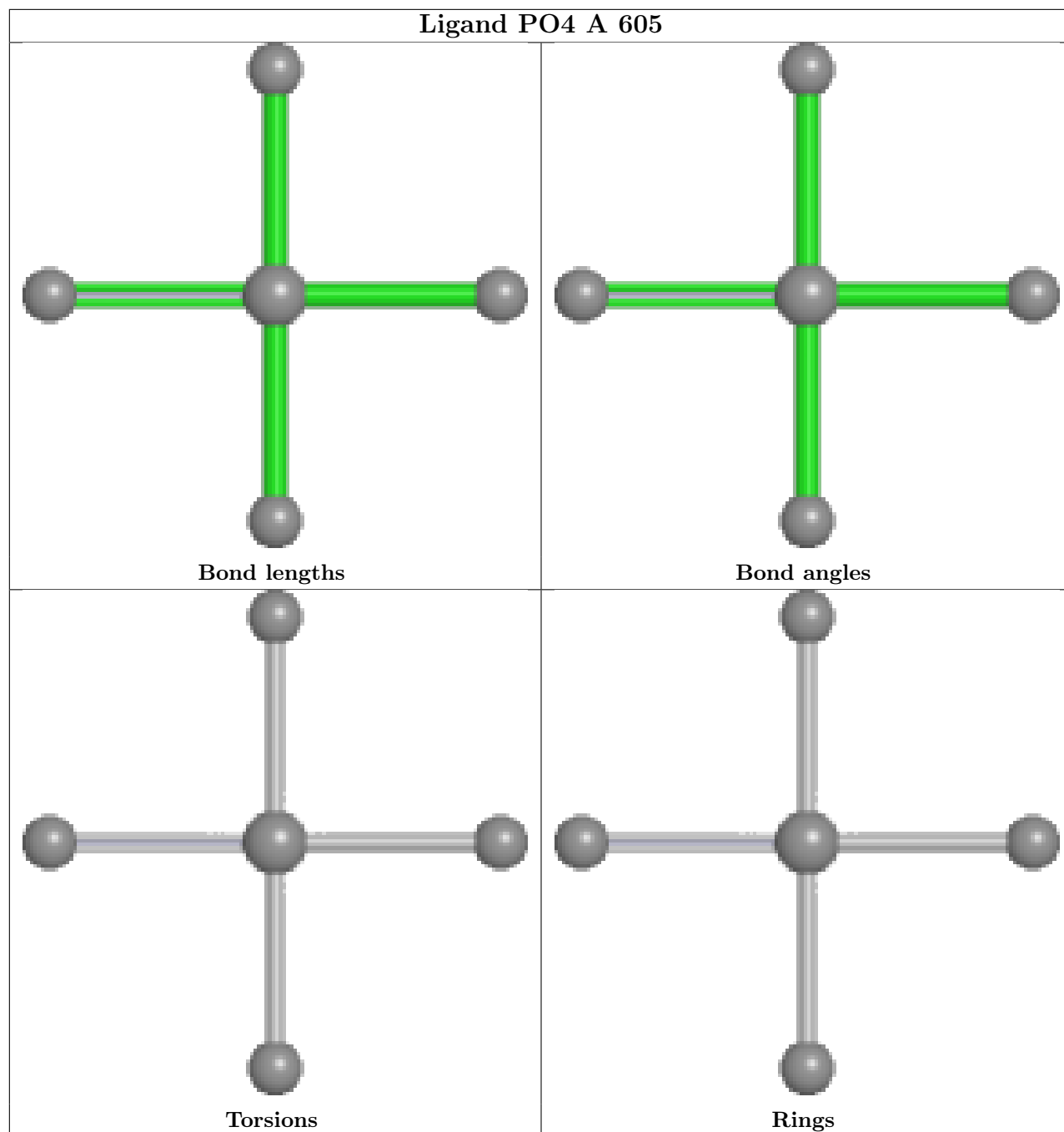


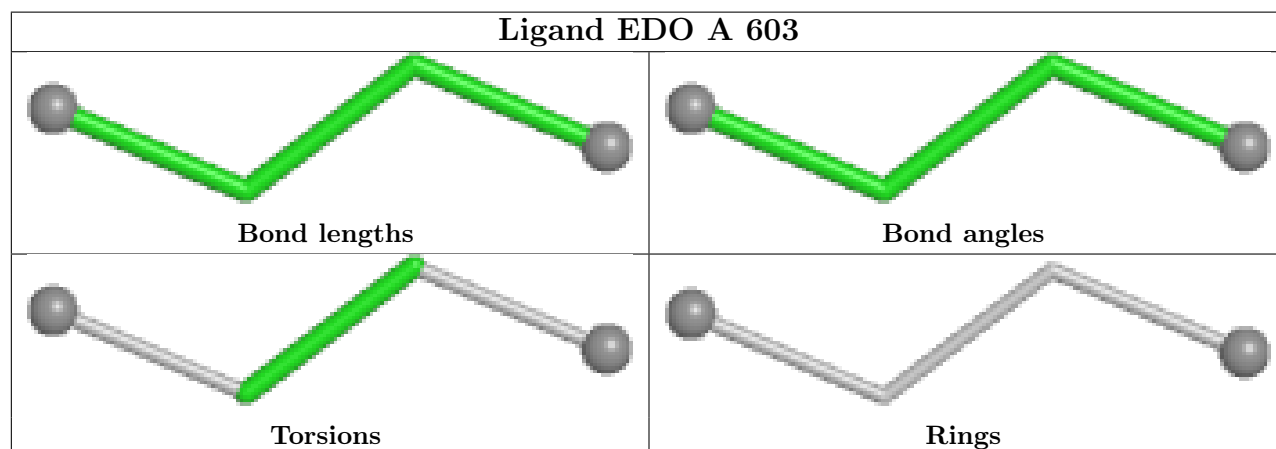
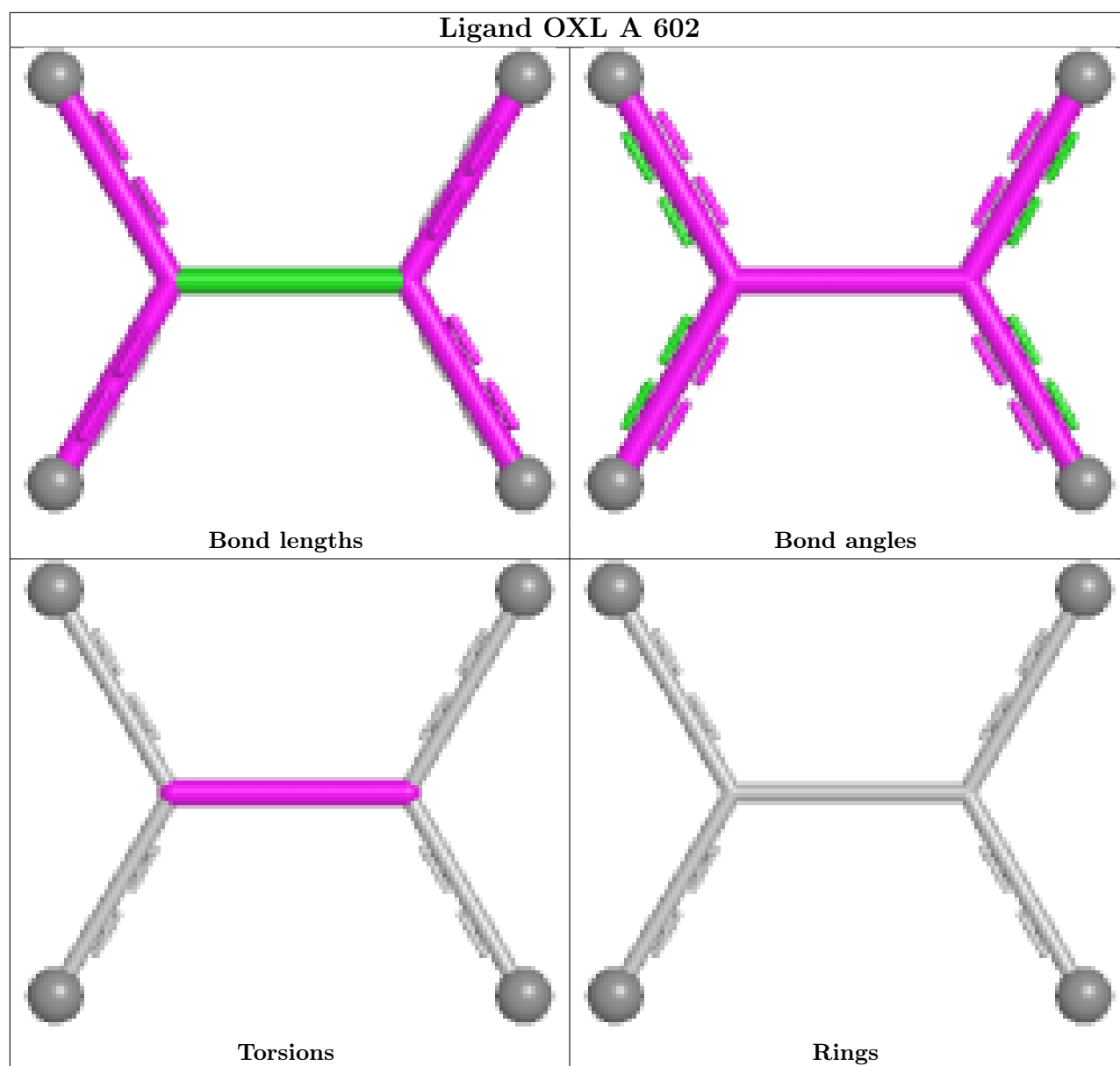


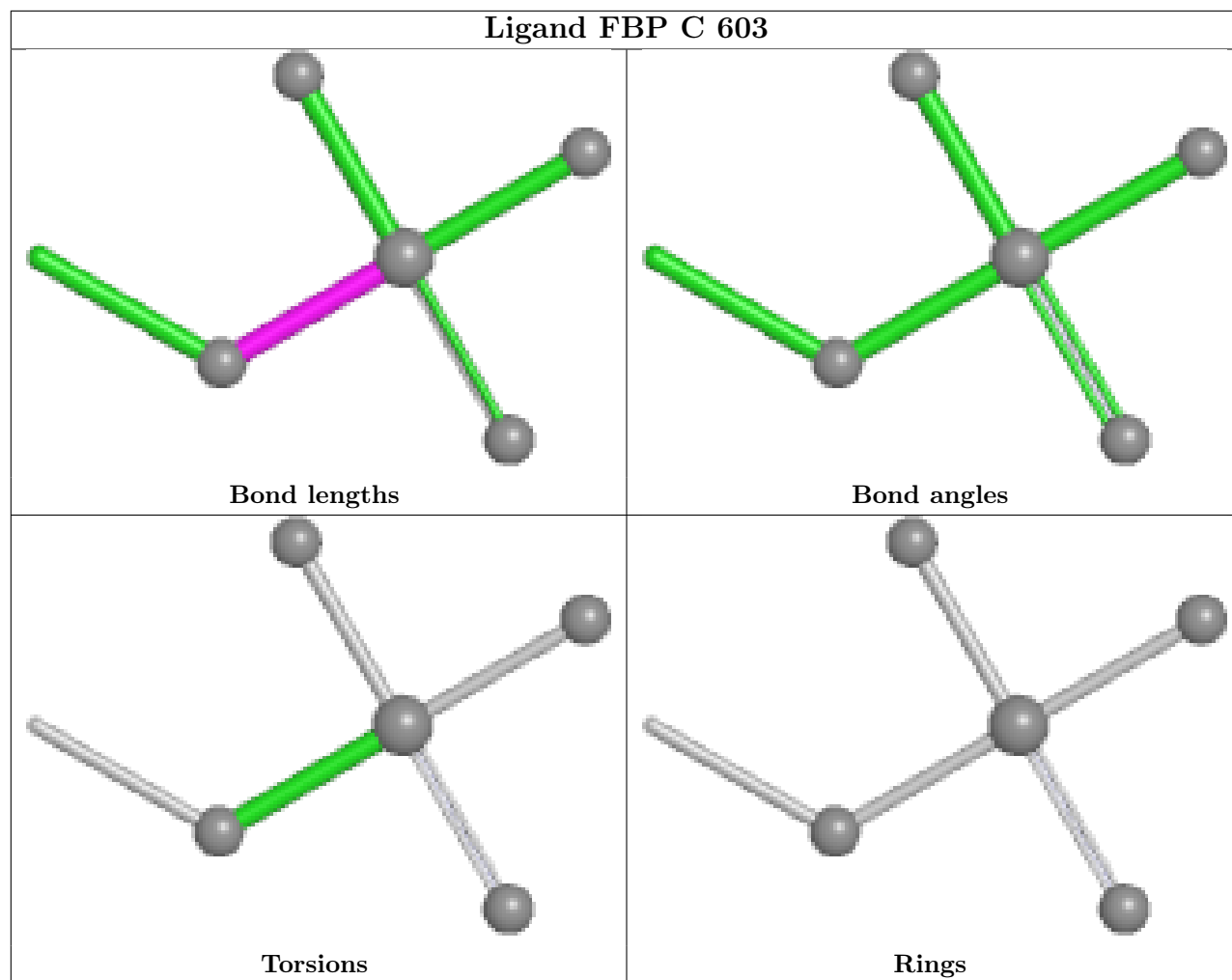


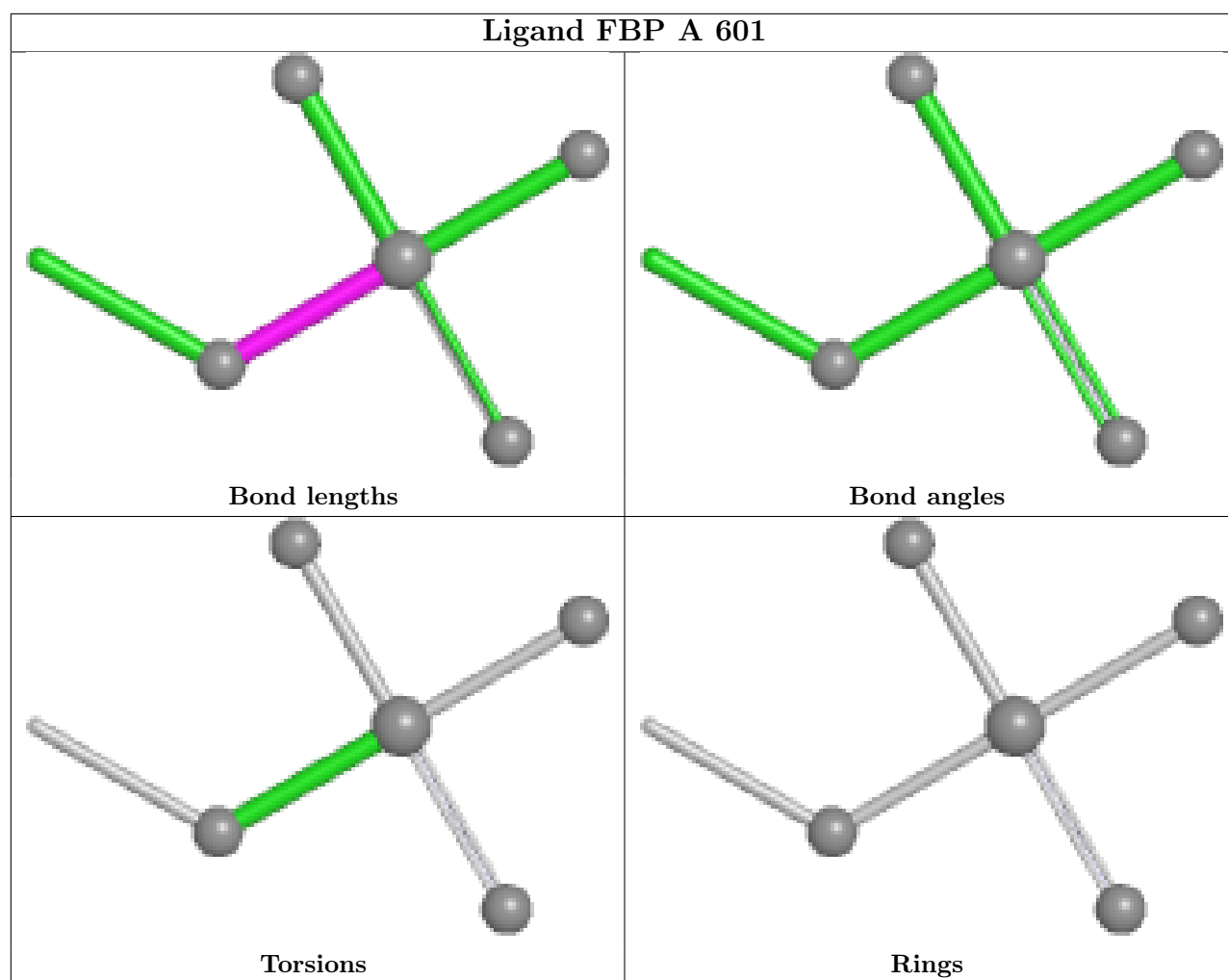


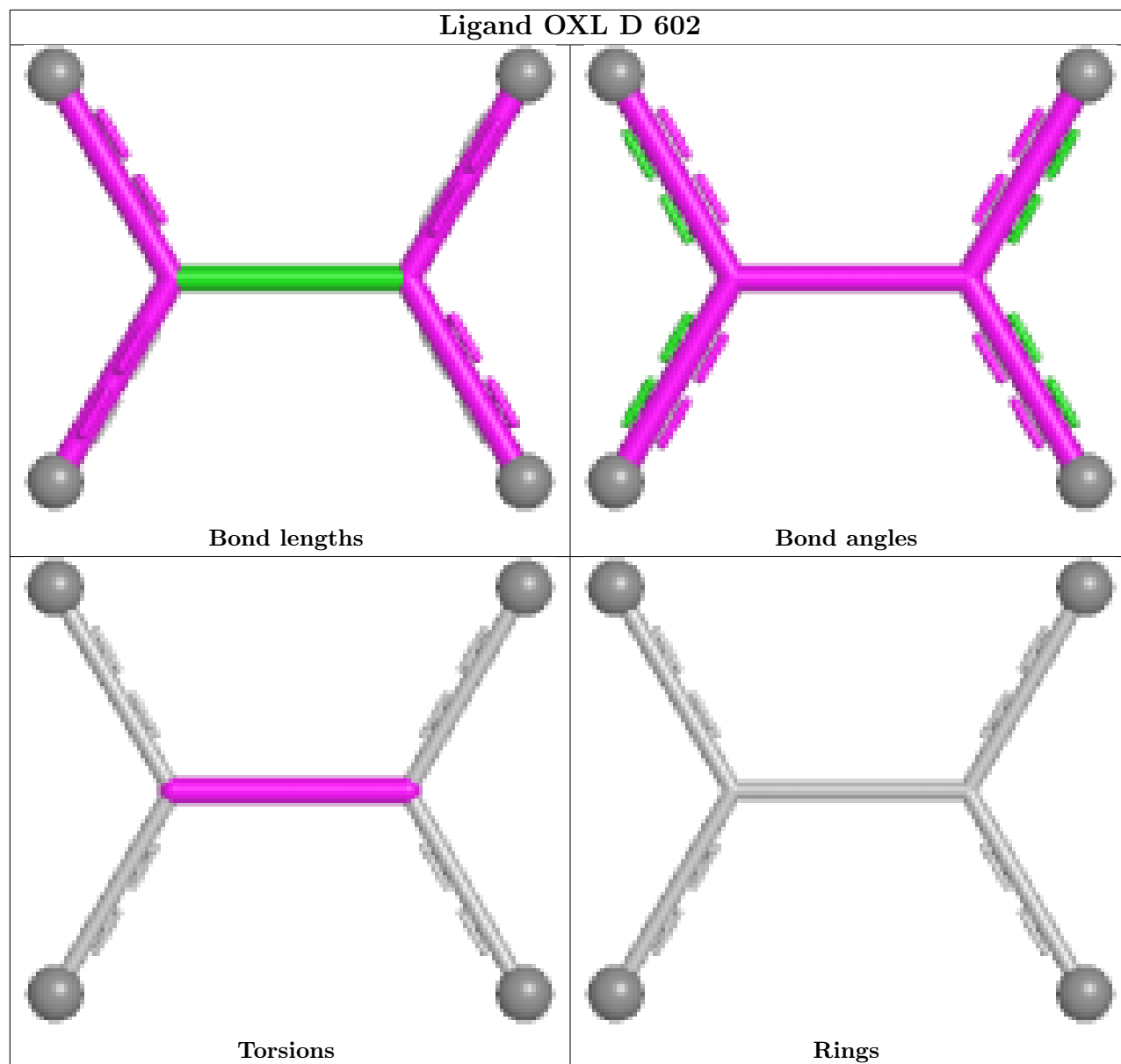


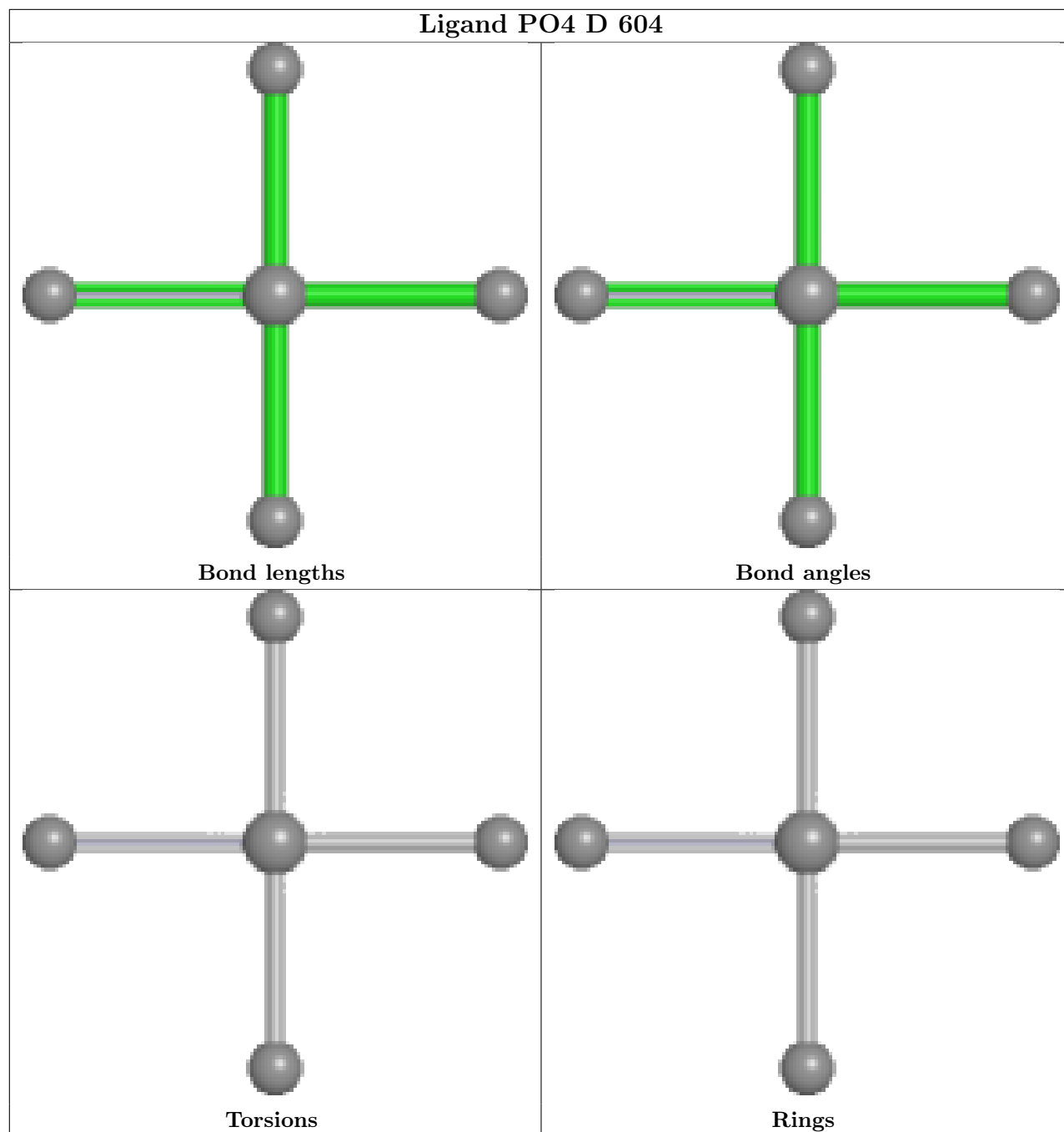


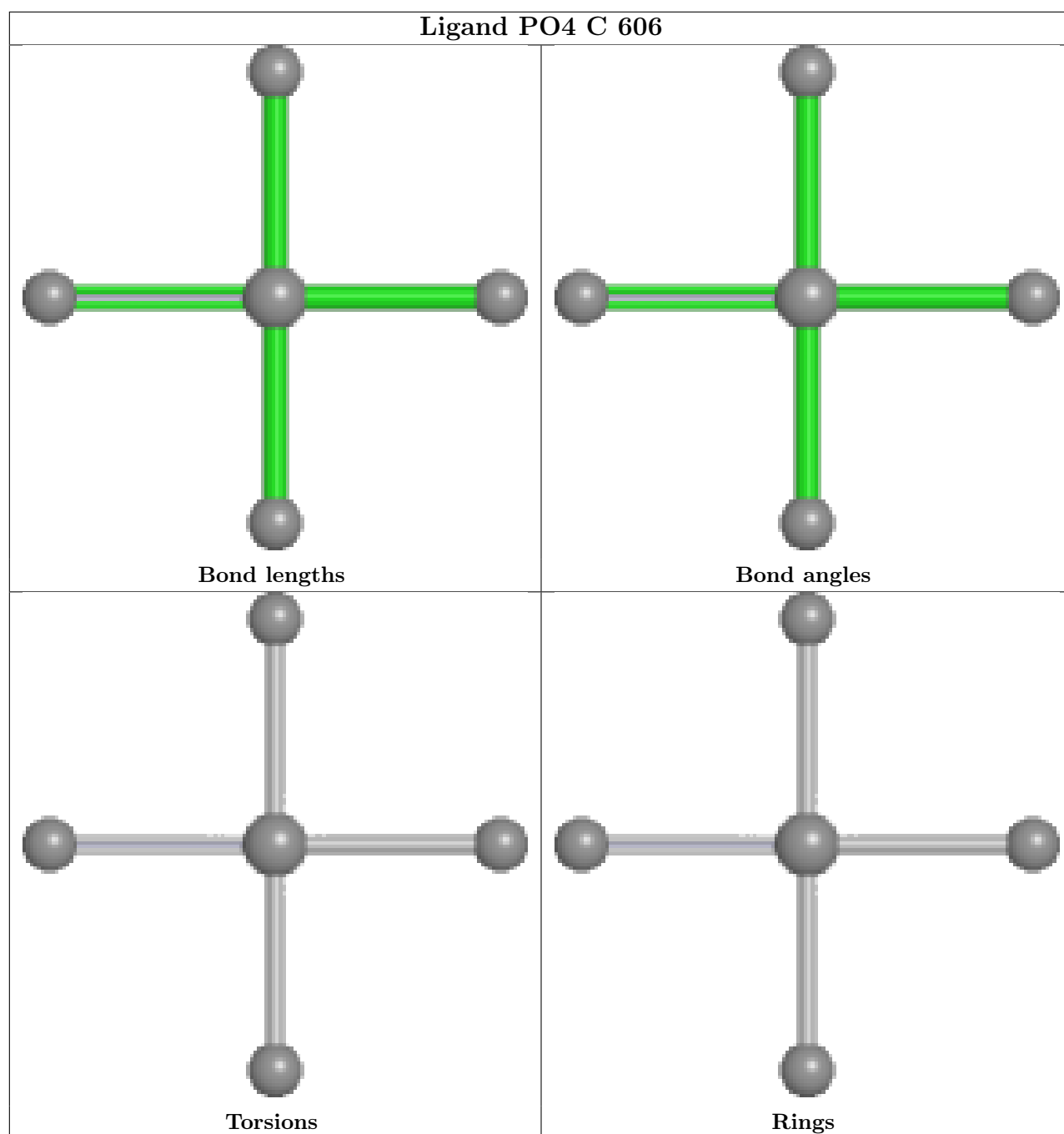


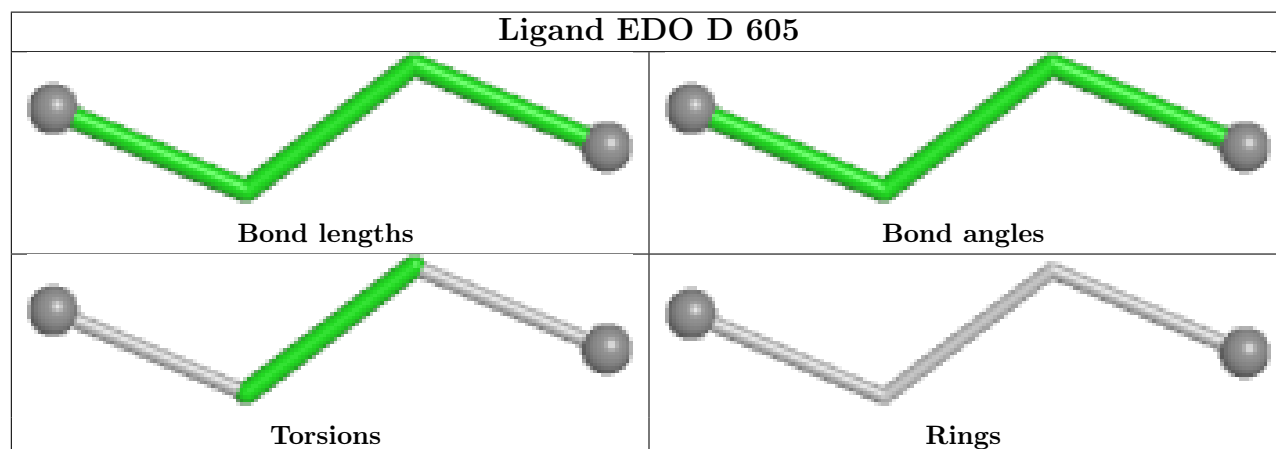
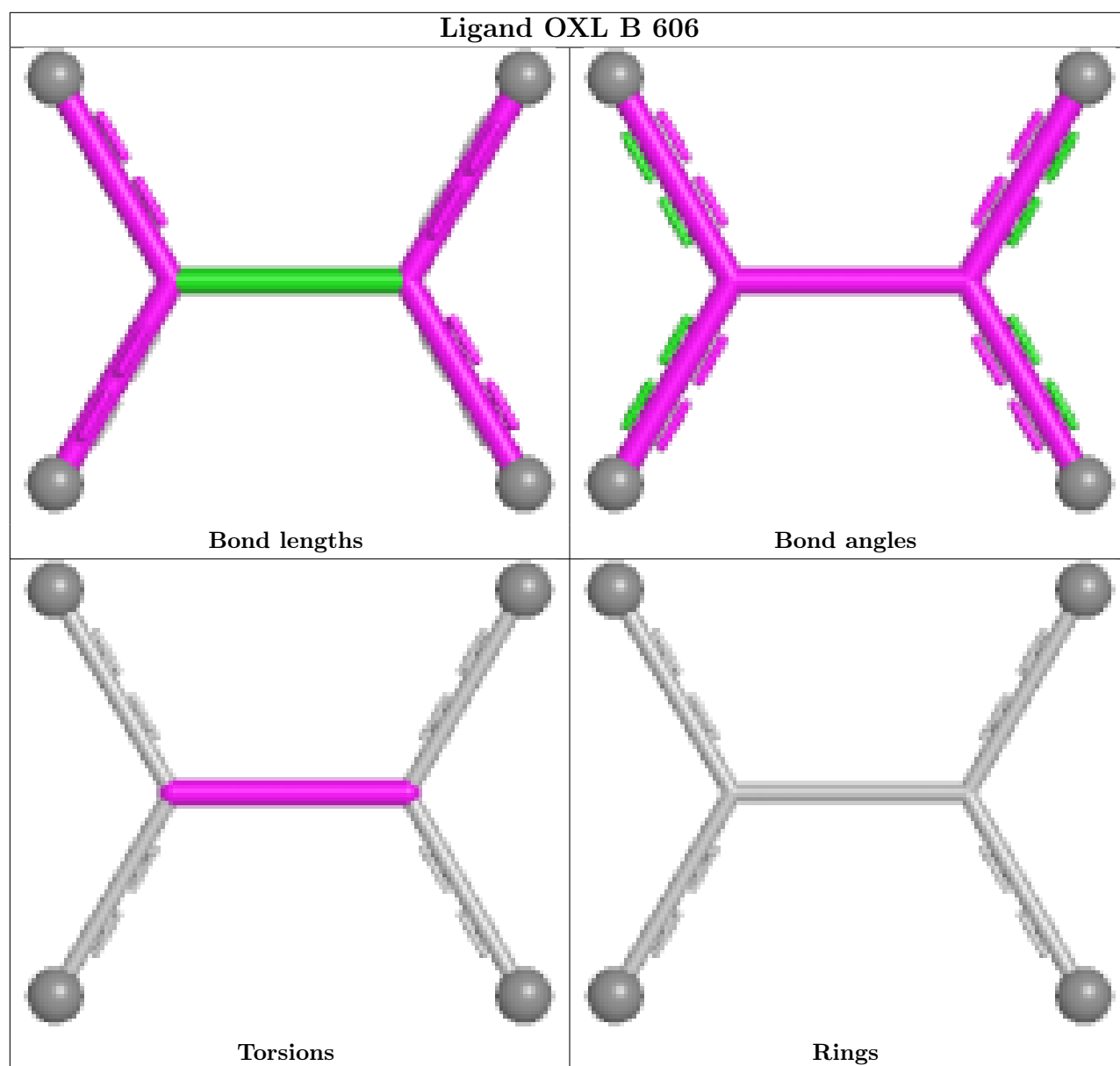


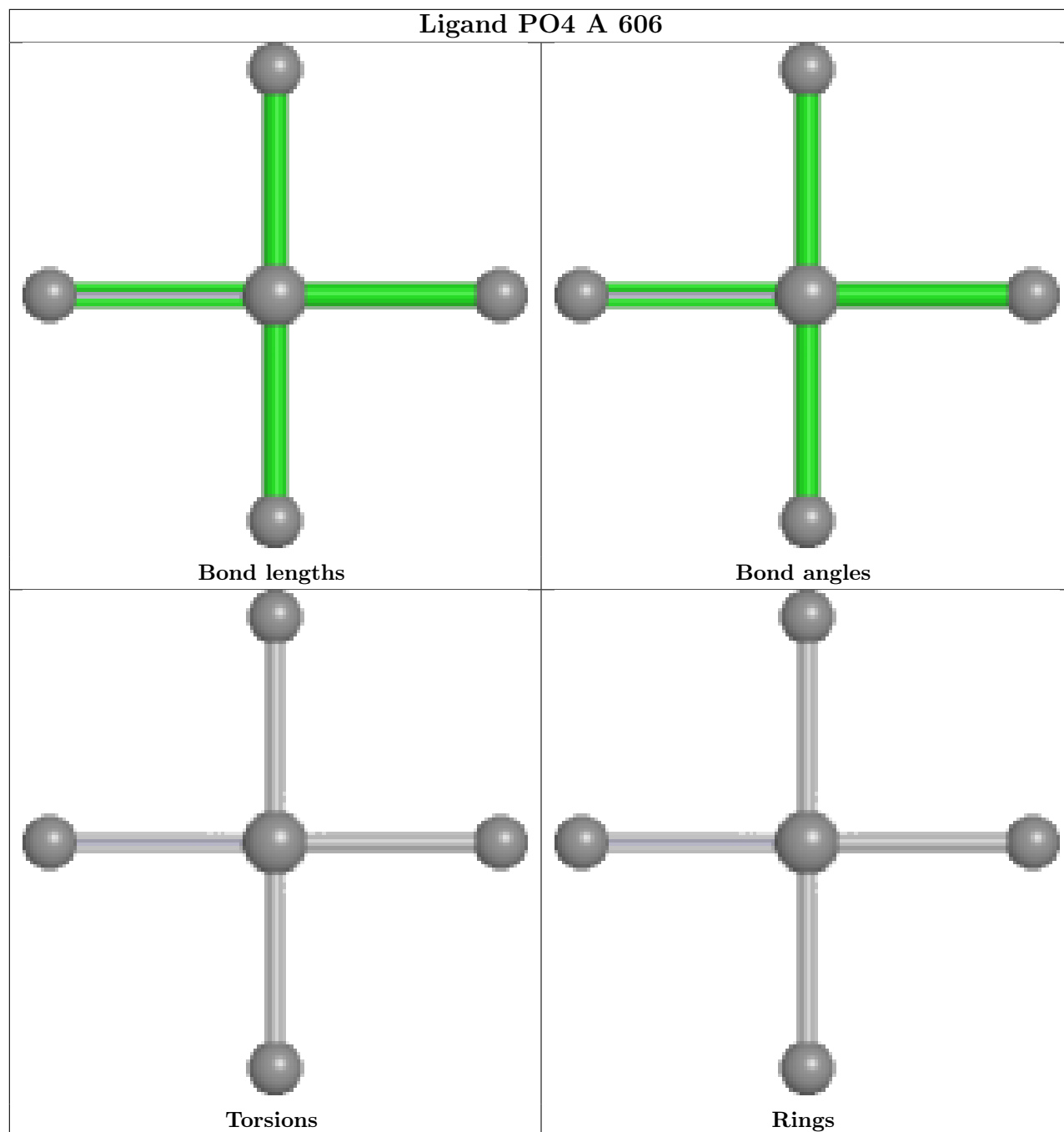


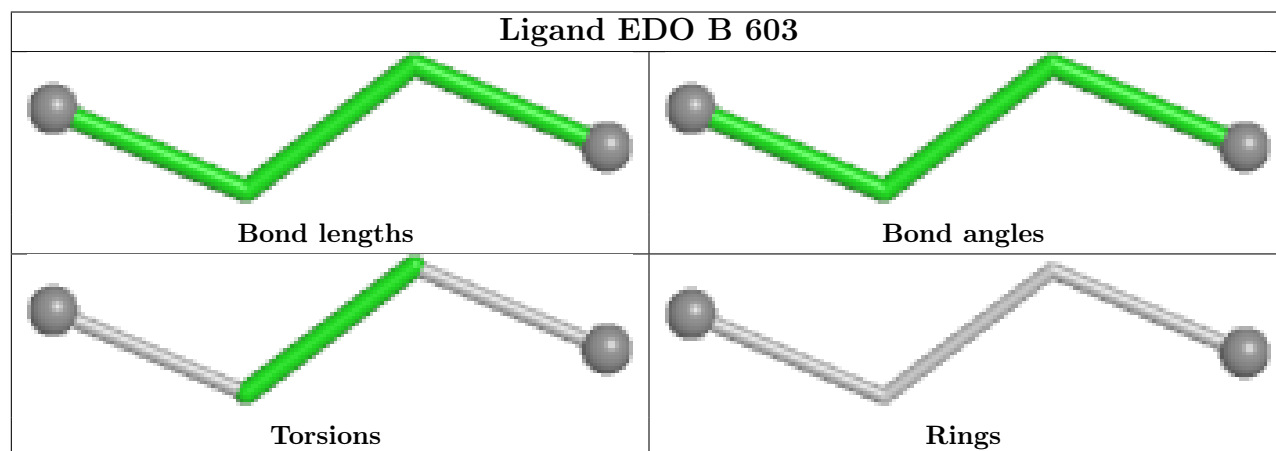
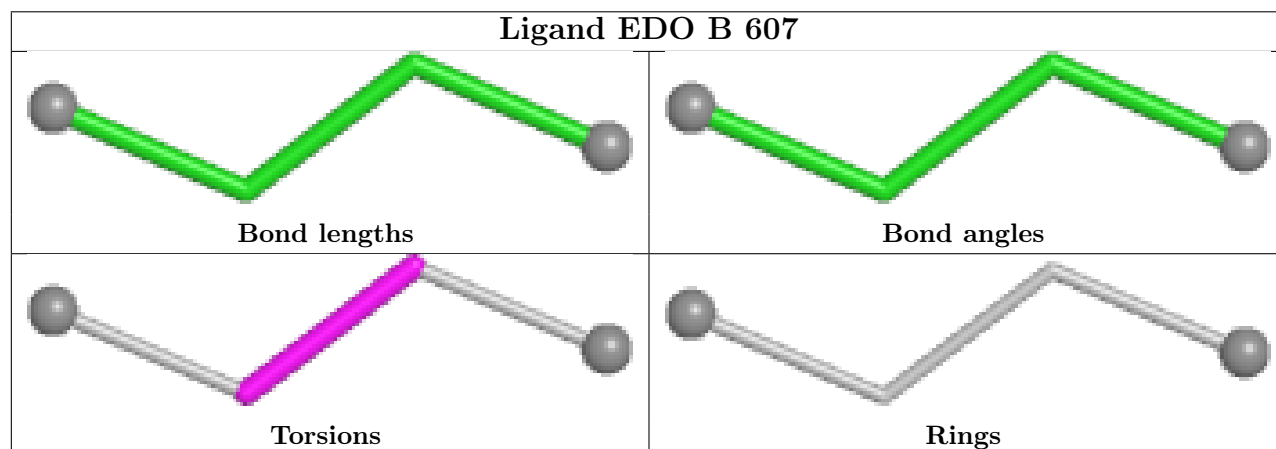
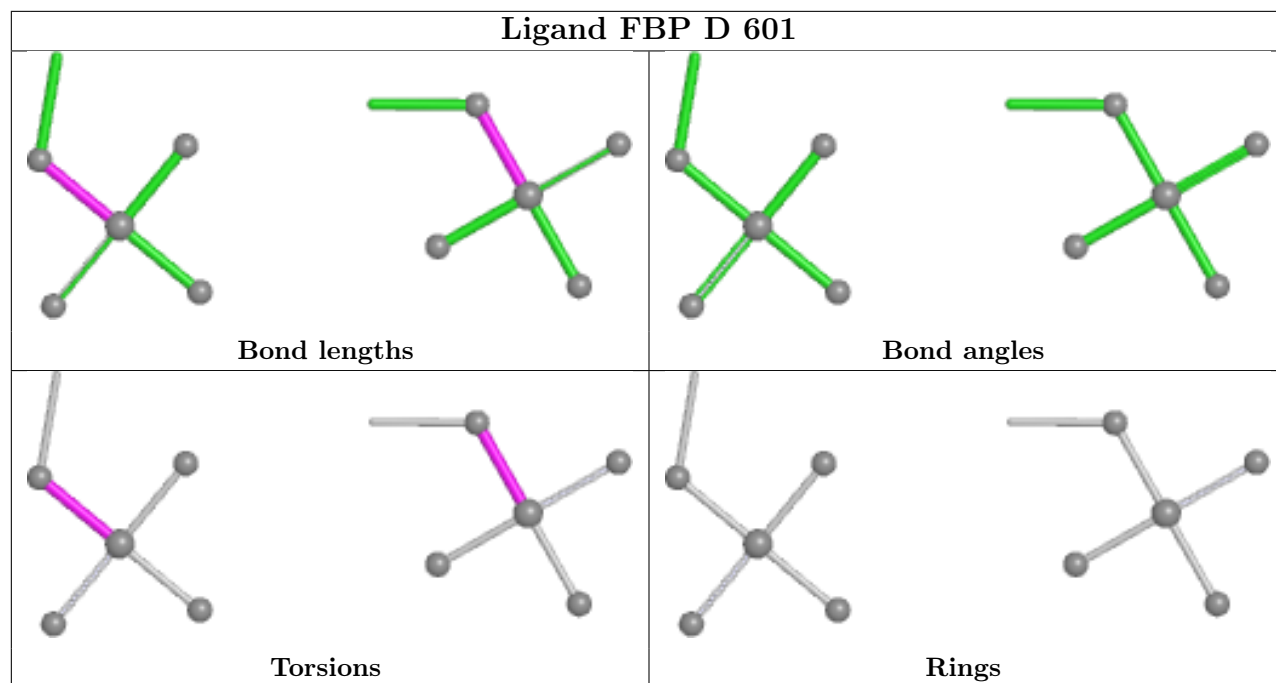


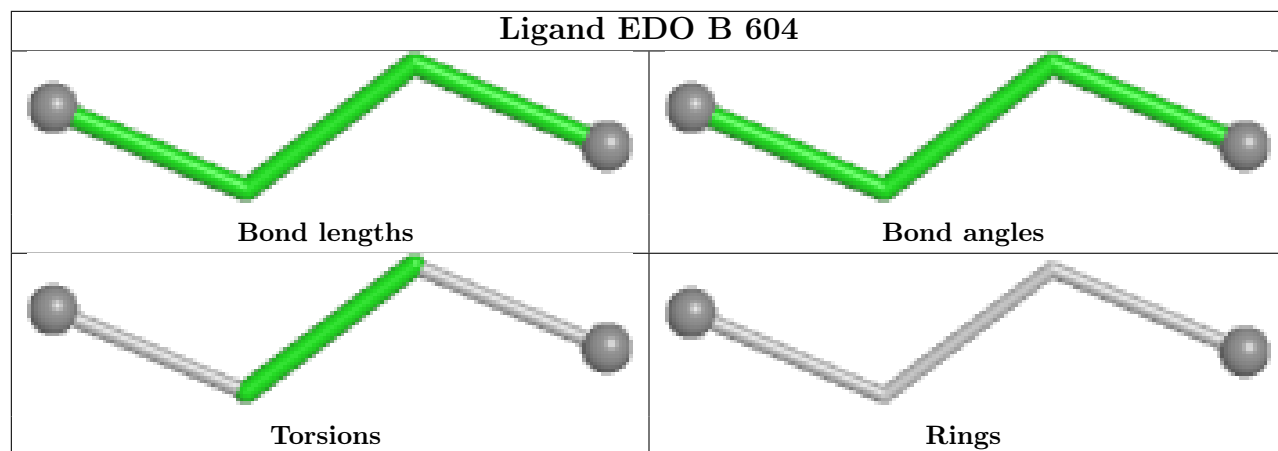


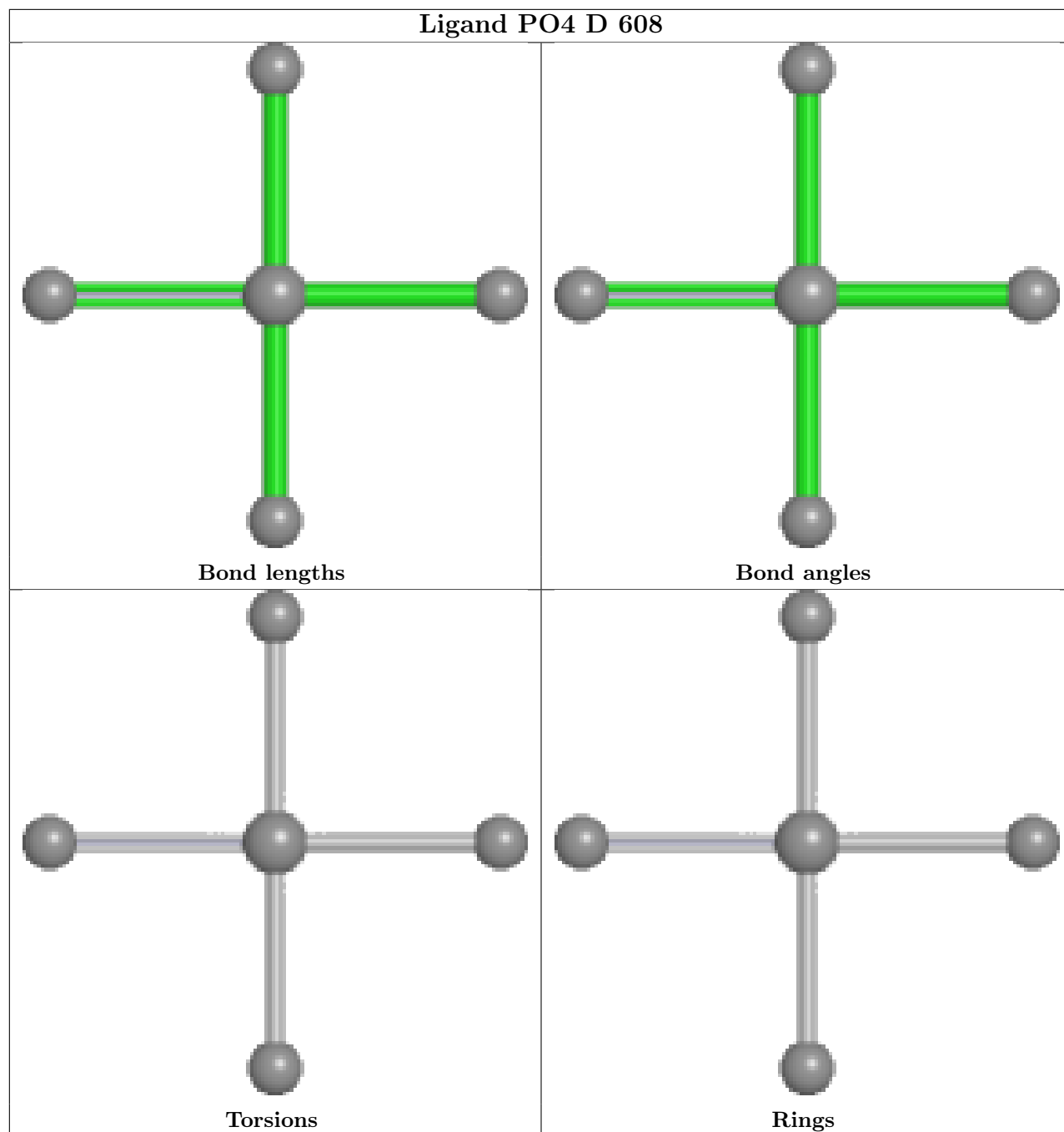


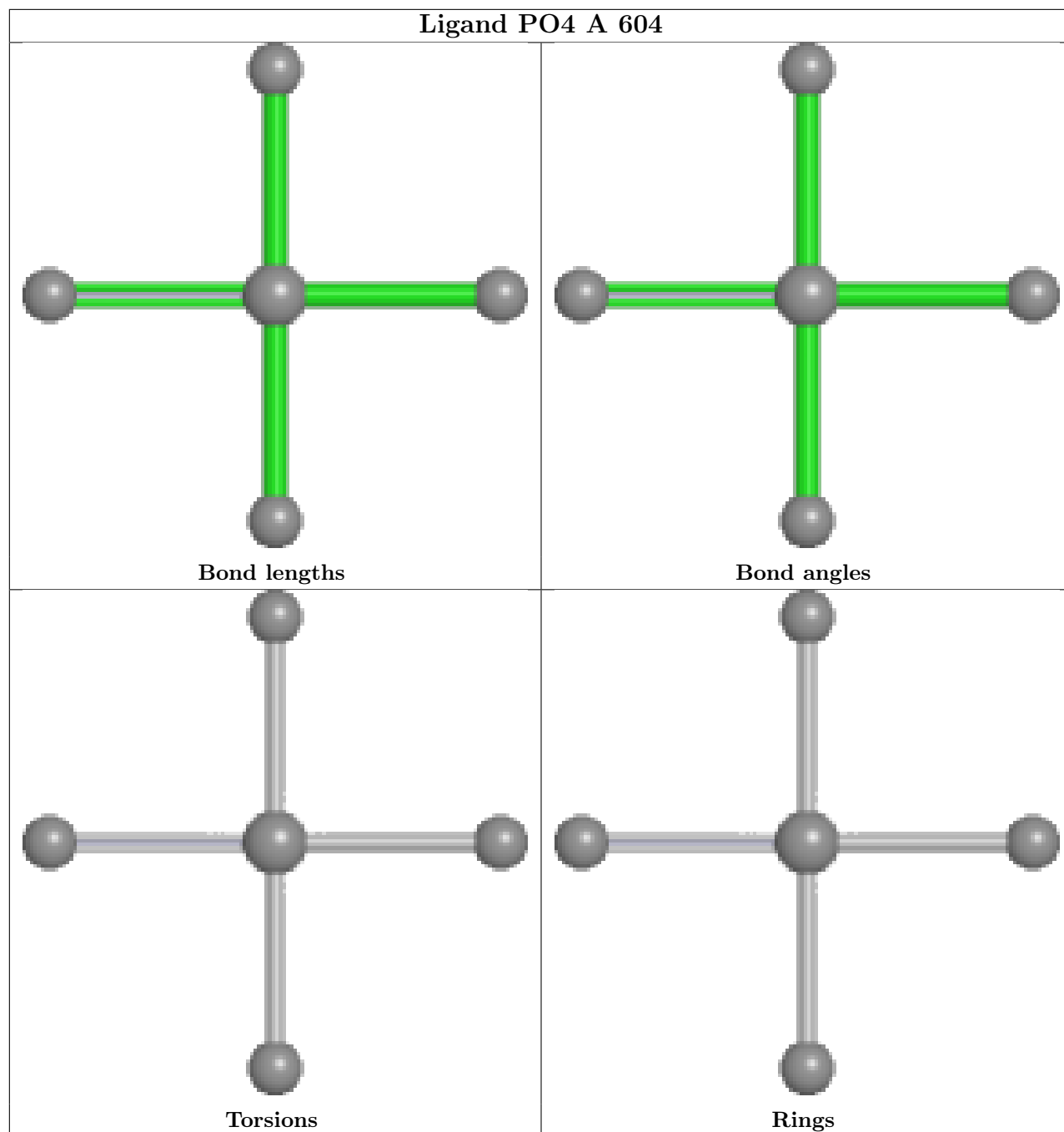


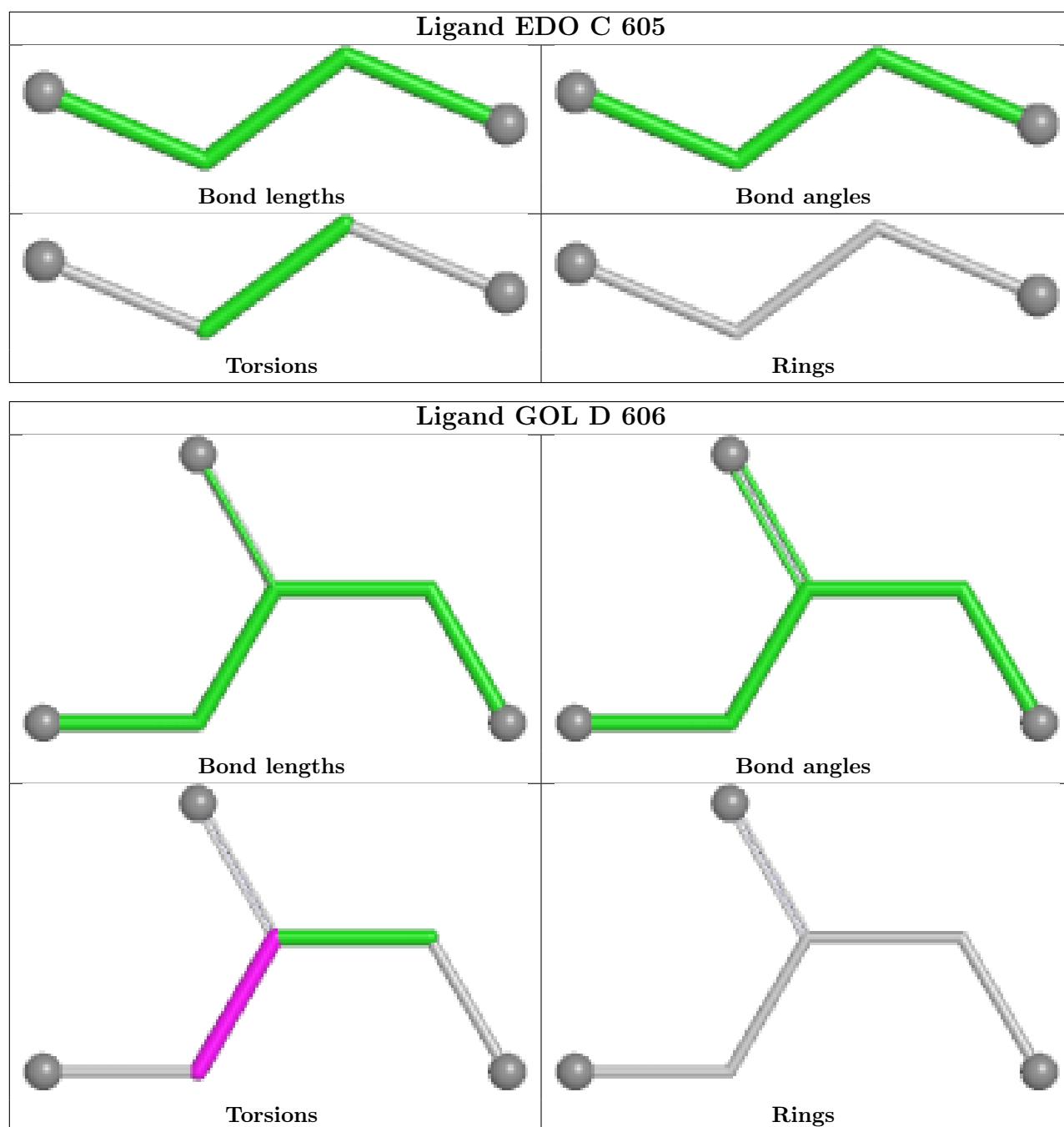












5.7 Other polymers [i](#)

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	512/551 (92%)	0.74	29 (5%)	29	26	37, 51, 103, 130	0
1	B	464/551 (84%)	0.75	38 (8%)	17	15	35, 56, 95, 115	0
1	C	517/551 (93%)	0.78	42 (8%)	18	15	38, 51, 91, 141	0
1	D	515/551 (93%)	0.61	24 (4%)	36	32	33, 48, 76, 111	0
All	All	2008/2204 (91%)	0.72	133 (6%)	24	21	33, 51, 95, 141	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	521	PHE	6.0
1	C	199	ASN	5.7
1	B	520	GLY	4.2
1	A	142	ILE	4.2
1	A	521	PHE	4.1
1	C	531	PRO	3.9
1	A	192	PHE	3.9
1	B	164	ILE	3.8
1	A	404	ILE	3.8
1	D	176	VAL	3.7
1	B	14	GLN	3.7
1	C	129	THR	3.6
1	C	520	GLY	3.6
1	C	245	ILE	3.5
1	B	185	VAL	3.4
1	D	505	LYS	3.4
1	A	168	VAL	3.4
1	A	204	GLY	3.4
1	D	362	SER	3.3
1	B	517	PRO	3.2
1	B	180	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	514	GLY	3.1
1	C	153	ASP	3.1
1	C	514	GLY	3.1
1	C	362	SER	3.0
1	C	246	ARG	3.0
1	B	515	TRP	3.0
1	C	130	ALA	3.0
1	A	187	GLN	3.0
1	B	404	ILE	3.0
1	C	515	TRP	3.0
1	D	531	PRO	2.9
1	D	470	PHE	2.9
1	D	520	GLY	2.9
1	A	139	THR	2.9
1	B	406	SER	2.9
1	C	517	PRO	2.8
1	A	190	ALA	2.8
1	C	133	GLU	2.8
1	A	470	PHE	2.8
1	B	482	TRP	2.8
1	A	514	GLY	2.8
1	A	127	SER	2.7
1	C	204	GLY	2.7
1	C	521	PHE	2.7
1	C	404	ILE	2.7
1	A	482	TRP	2.7
1	B	76	PHE	2.7
1	B	362	SER	2.7
1	C	200	GLY	2.7
1	B	197	VAL	2.7
1	B	215	ALA	2.7
1	B	167	VAL	2.6
1	B	170	VAL	2.6
1	C	16	GLN	2.6
1	B	83	TYR	2.6
1	C	168	VAL	2.6
1	B	443	ARG	2.5
1	B	403	PRO	2.5
1	B	168	VAL	2.5
1	D	18	LEU	2.5
1	A	132	VAL	2.5
1	C	155	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	399	ARG	2.5
1	C	203	LEU	2.5
1	C	273	ASN	2.5
1	A	174	ILE	2.4
1	C	178	ASP	2.4
1	D	517	PRO	2.4
1	B	121	THR	2.4
1	C	124	ILE	2.4
1	A	144	LEU	2.4
1	C	185	VAL	2.4
1	C	508	VAL	2.4
1	B	119	ILE	2.4
1	D	404	ILE	2.4
1	D	123	LEU	2.4
1	B	516	CYS	2.4
1	C	13	ILE	2.3
1	C	180	LEU	2.3
1	D	157	LEU	2.3
1	A	216	VAL	2.3
1	B	216	VAL	2.3
1	C	170	VAL	2.3
1	A	178	ASP	2.3
1	C	470	PHE	2.3
1	D	114	THR	2.3
1	C	448	ALA	2.2
1	D	147	ALA	2.2
1	D	523	ASN	2.2
1	B	80	THR	2.2
1	C	403	PRO	2.2
1	D	527	VAL	2.2
1	A	134	LEU	2.2
1	A	172	SER	2.2
1	A	403	PRO	2.2
1	A	14	GLN	2.2
1	A	211	LEU	2.2
1	A	170	VAL	2.2
1	C	132	VAL	2.2
1	A	215	ALA	2.2
1	A	402	ALA	2.2
1	D	124	ILE	2.2
1	B	178	ASP	2.2
1	A	167	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	2.1
1	B	213	GLY	2.1
1	C	128	GLY	2.1
1	D	515	TRP	2.1
1	A	223	GLU	2.1
1	C	148	TYR	2.1
1	B	165	CYS	2.1
1	D	217	ASP	2.1
1	D	519	SER	2.1
1	B	173	LYS	2.1
1	D	371	PRO	2.1
1	B	244	PHE	2.1
1	B	220	ALA	2.1
1	C	141	LYS	2.1
1	C	162	LYS	2.1
1	C	140	LEU	2.1
1	C	159	LEU	2.1
1	D	129	THR	2.1
1	C	119	ILE	2.1
1	B	202	SER	2.1
1	A	180	LEU	2.0
1	B	169	GLU	2.0
1	C	213	GLY	2.0
1	B	103	ILE	2.0
1	B	267	ILE	2.0
1	C	392	LEU	2.0
1	B	163	ASN	2.0
1	D	522	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

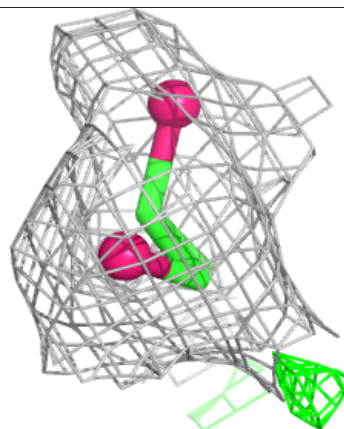
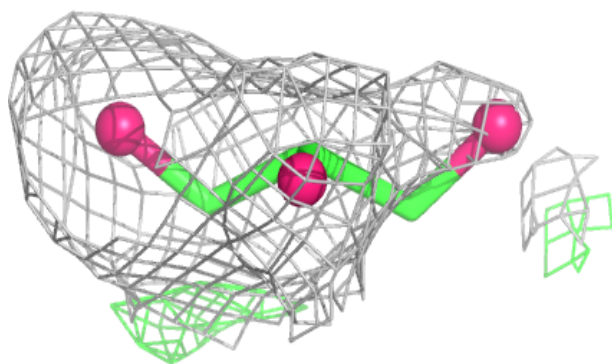
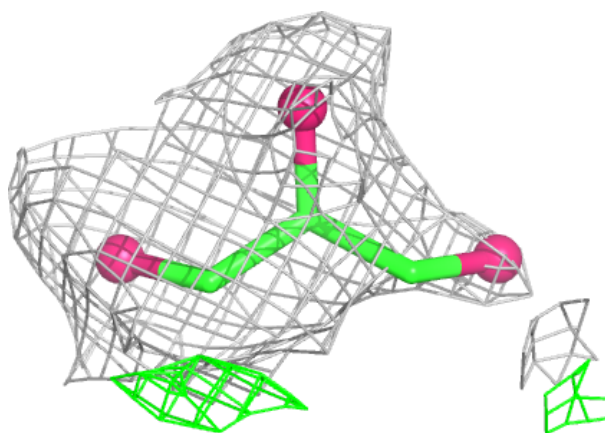
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	605	6/6	0.49	0.15	72,77,78,79	0
4	EDO	B	603	4/4	0.52	0.27	48,51,51,54	0
4	EDO	D	605	4/4	0.58	0.20	63,64,65,68	0
4	EDO	B	604	4/4	0.60	0.28	75,76,79,80	0
5	PO4	A	606	5/5	0.69	0.15	74,75,88,96	0
4	EDO	C	605	4/4	0.69	0.26	63,65,66,66	0
2	FBP	C	603	6/20	0.72	0.20	56,66,68,70	0
4	EDO	A	603	4/4	0.73	0.14	54,55,55,56	0
7	GOL	D	606	6/6	0.74	0.18	45,48,49,50	0
4	EDO	B	607	4/4	0.76	0.20	61,63,64,65	0
5	PO4	C	607	5/5	0.78	0.12	62,68,82,83	0
4	EDO	C	604	4/4	0.78	0.18	49,51,51,52	0
2	FBP	C	601	12/20	0.78	0.15	52,62,85,89	0
3	OXL	B	606	6/6	0.79	0.11	69,69,71,72	0
5	PO4	A	604	5/5	0.82	0.12	56,59,64,66	0
5	PO4	D	608	5/5	0.82	0.16	72,72,82,82	0
3	OXL	D	602	6/6	0.83	0.12	36,38,39,40	0
3	OXL	B	602	6/6	0.83	0.12	53,57,59,62	0
5	PO4	D	604	5/5	0.84	0.13	63,64,73,82	0
5	PO4	B	608	5/5	0.85	0.17	63,67,72,75	0
5	PO4	A	605	5/5	0.86	0.14	64,67,71,76	0
3	OXL	A	602	6/6	0.87	0.12	44,47,49,49	0
2	FBP	D	601	12/20	0.88	0.15	41,52,73,74	12
5	PO4	D	603	5/5	0.88	0.14	54,56,57,62	0
2	FBP	A	601	6/20	0.89	0.13	48,55,57,66	0
5	PO4	C	606	5/5	0.90	0.10	69,71,77,78	0
6	MG	D	609	1/1	0.91	0.13	40,40,40,40	0
2	FBP	B	601	6/20	0.91	0.13	54,56,63,65	0
6	MG	B	609	1/1	0.91	0.10	63,63,63,63	0
3	OXL	C	602	6/6	0.92	0.11	44,46,46,48	0
6	MG	C	608	1/1	0.93	0.11	46,46,46,46	0
6	MG	A	608	1/1	0.94	0.14	41,41,41,41	0
5	PO4	D	607	5/5	0.94	0.07	41,45,45,49	0
6	MG	C	609	1/1	0.96	0.10	42,42,42,42	0
6	MG	A	607	1/1	0.97	0.09	40,40,40,40	0
6	MG	D	610	1/1	0.98	0.04	37,37,37,37	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.

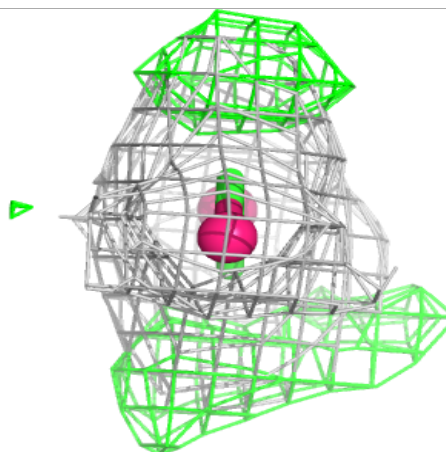
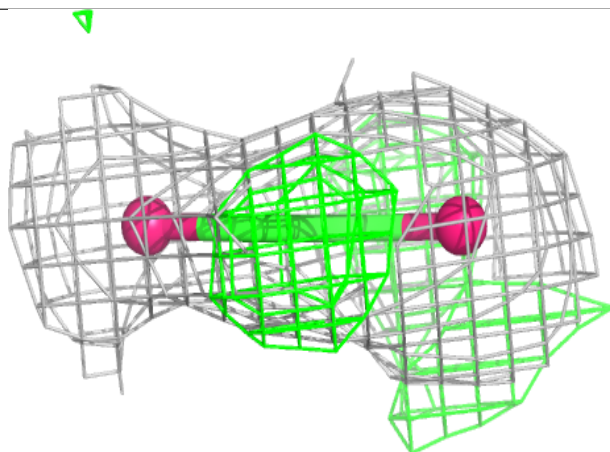
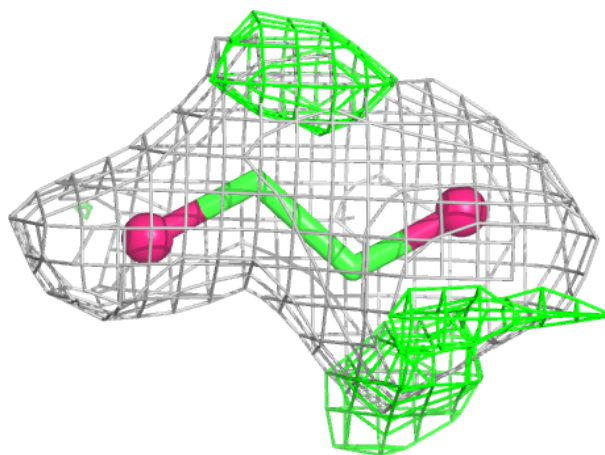
Electron density around GOL B 605:

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



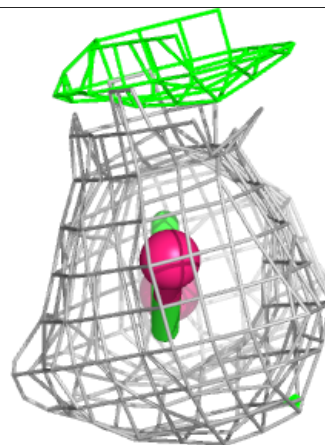
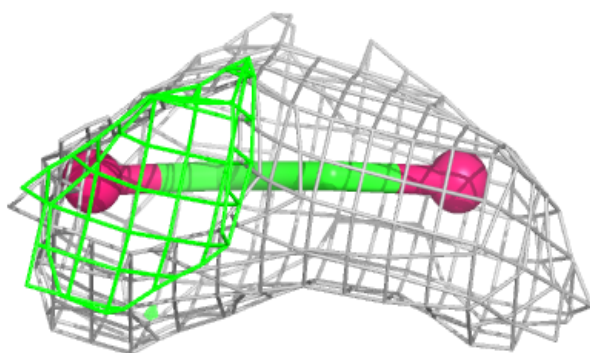
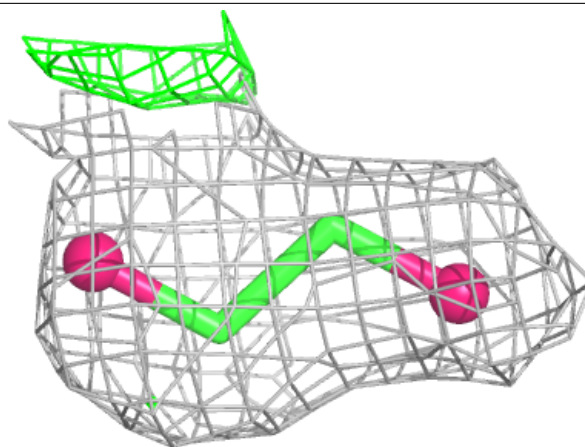
Electron density around EDO B 603:

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and green (positive)



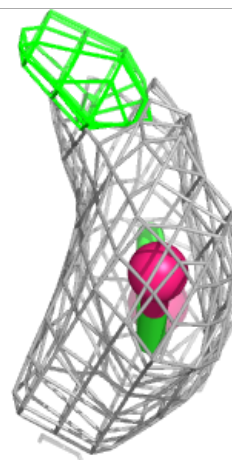
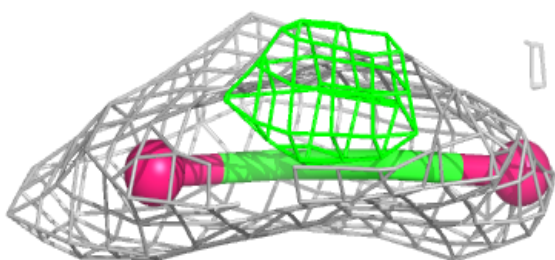
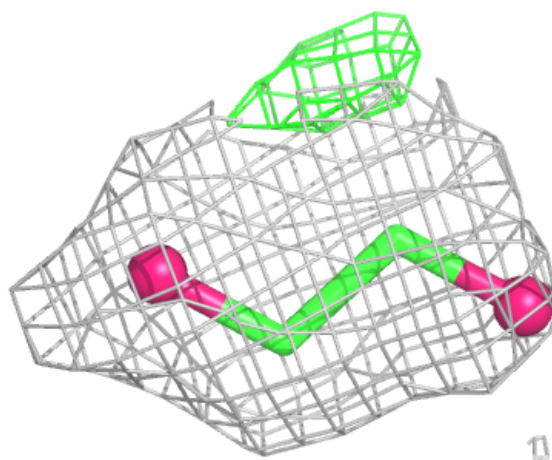
Electron density around EDO D 605:

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and green (positive)



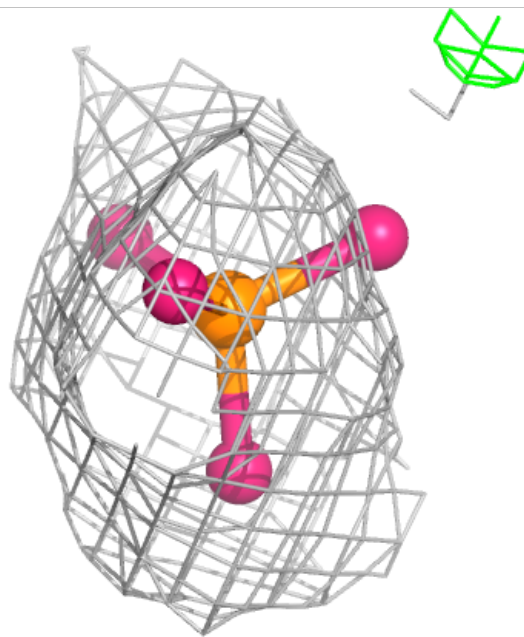
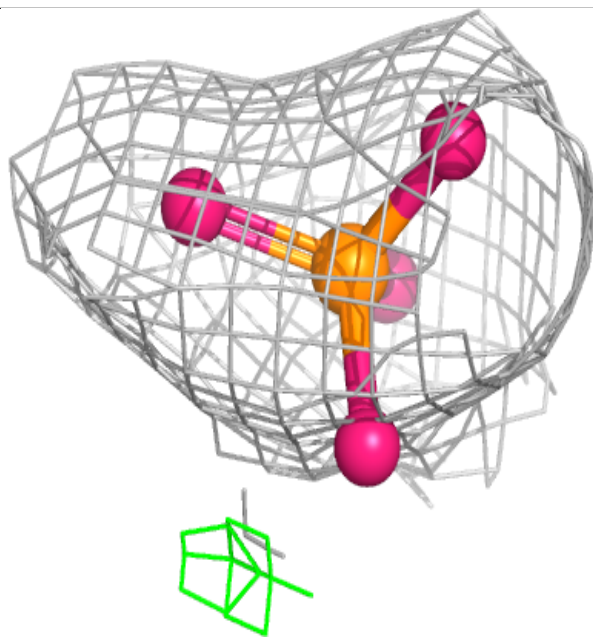
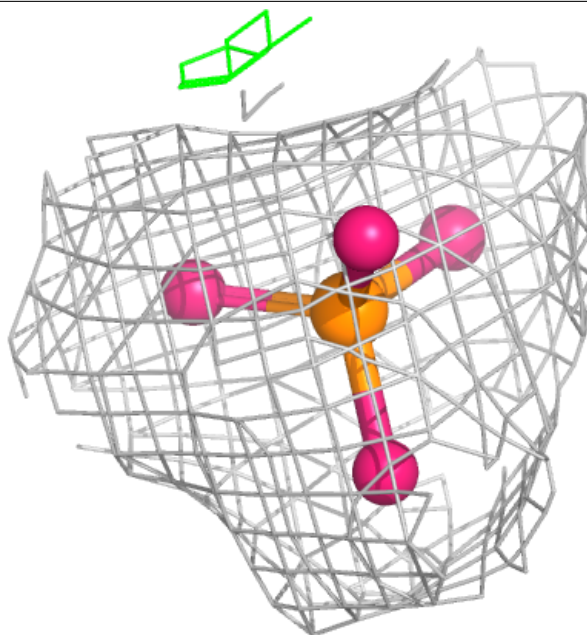
Electron density around EDO B 604:

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and green (positive)



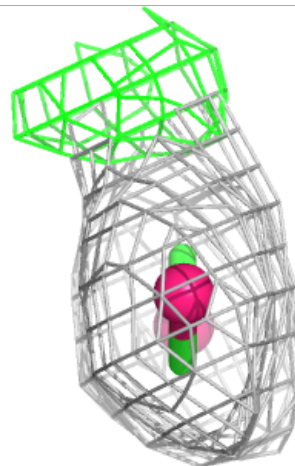
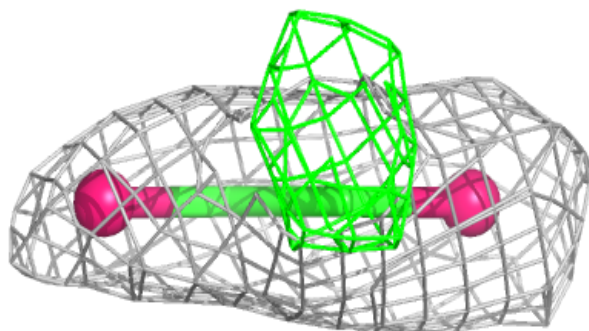
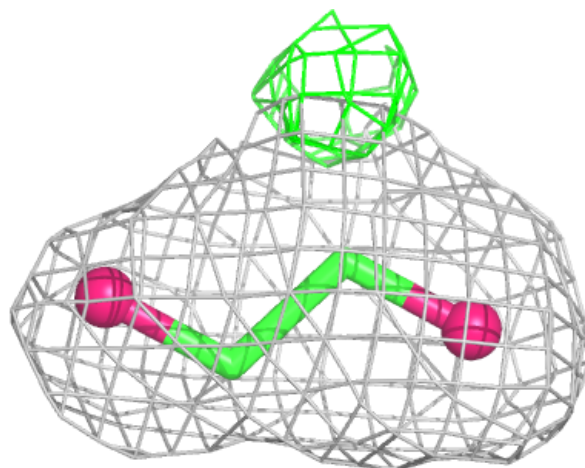
Electron density around PO4 A 606:

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and green (positive)



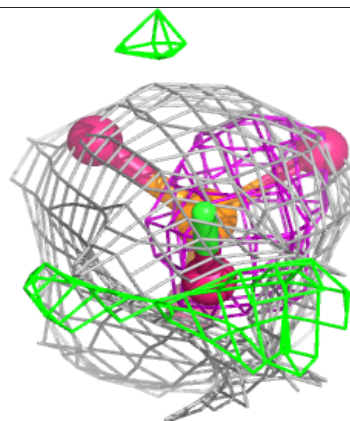
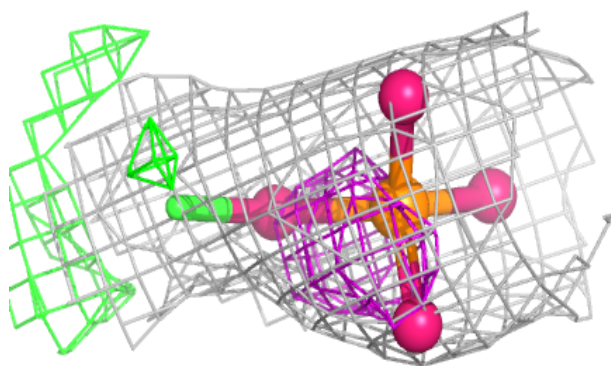
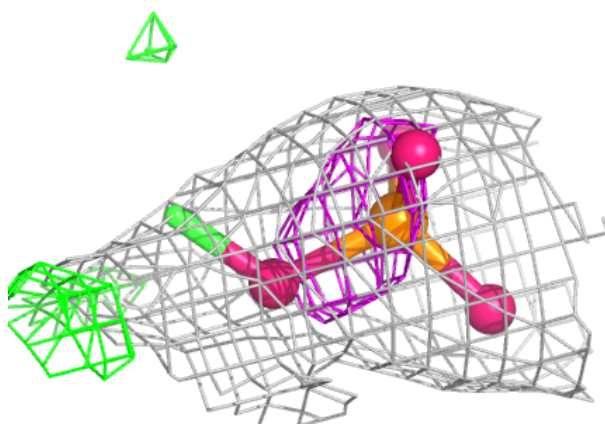
Electron density around EDO C 605:

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and green (positive)

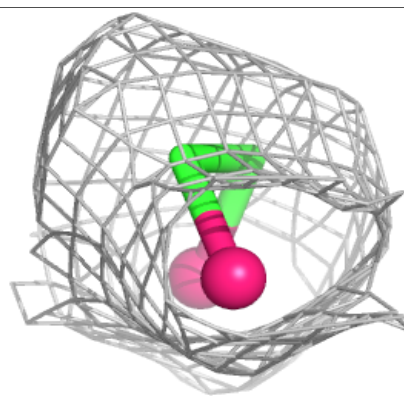
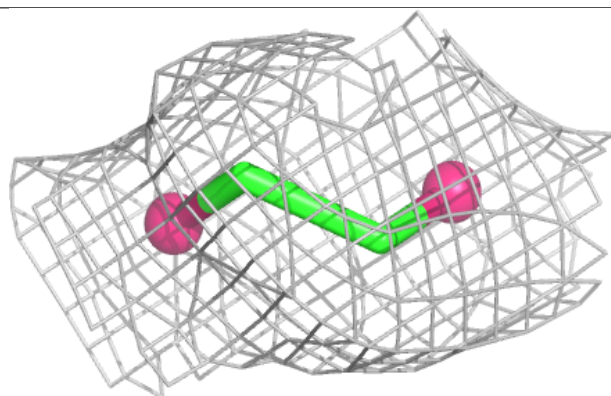
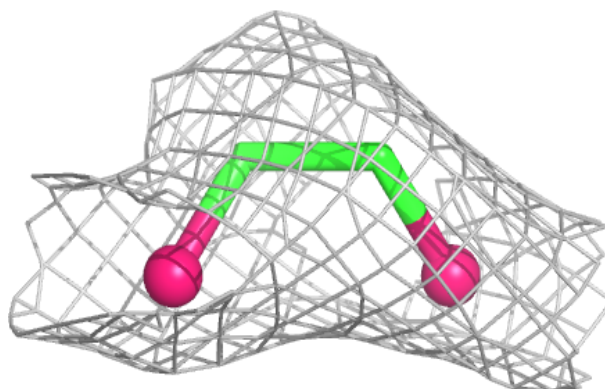


Electron density around FBP C 603:

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

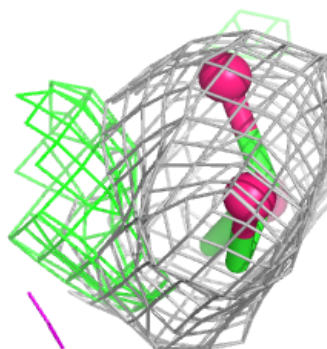
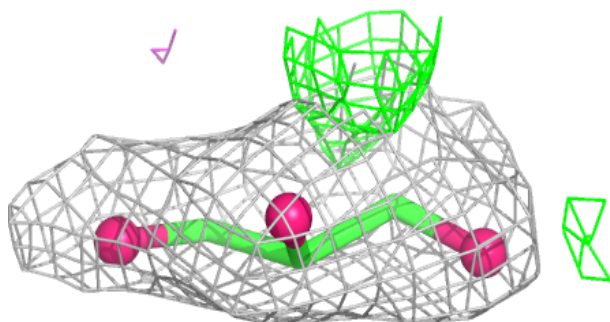
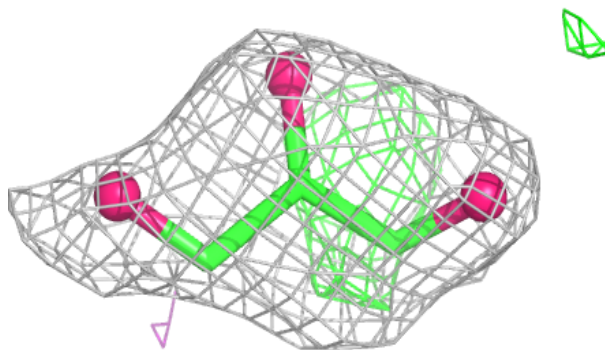
**Electron density around EDO A 603:**

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and green (positive)

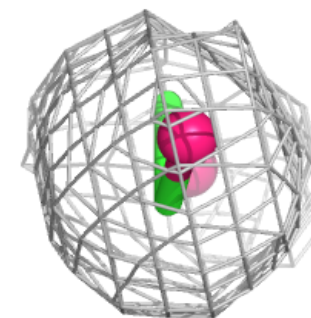
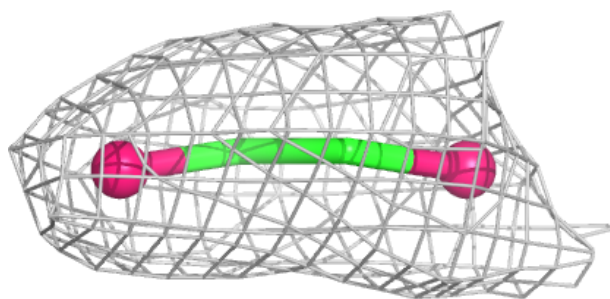
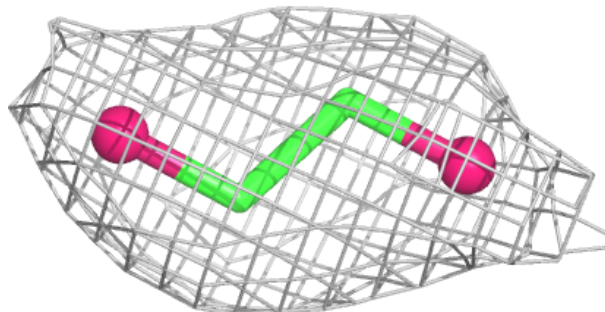


Electron density around GOL D 606:

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and green (positive)

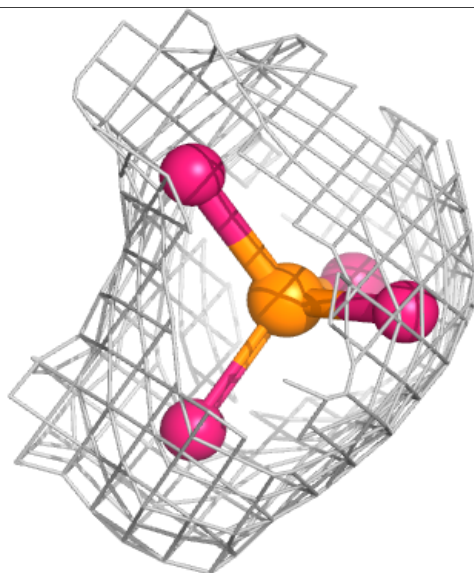
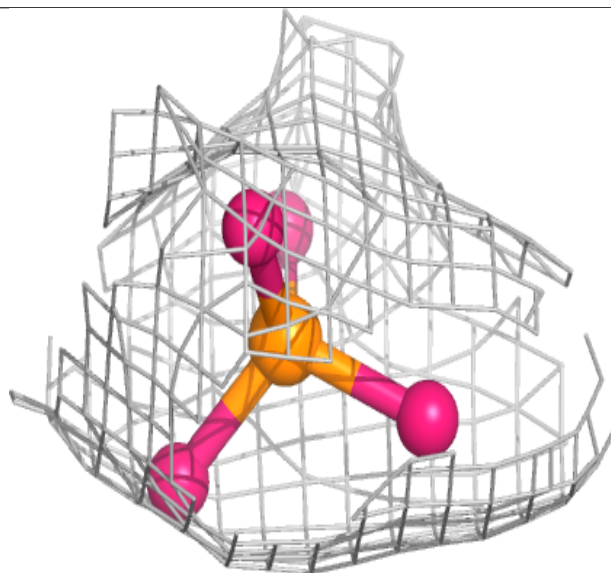
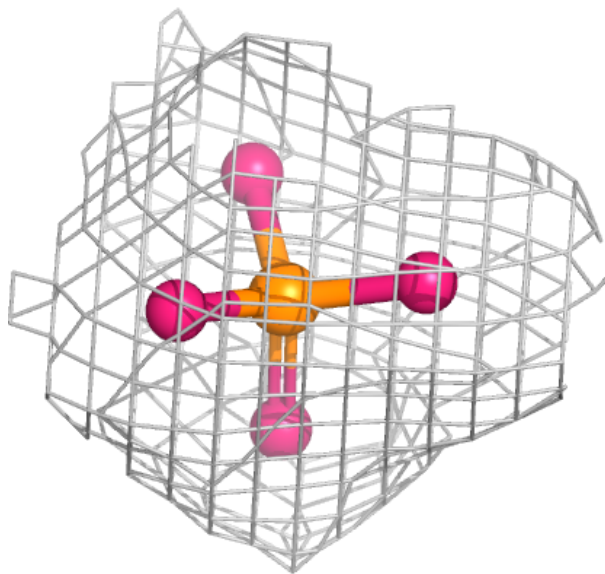
**Electron density around EDO B 607:**

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and green (positive)



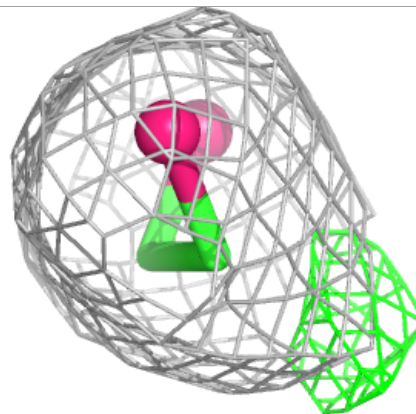
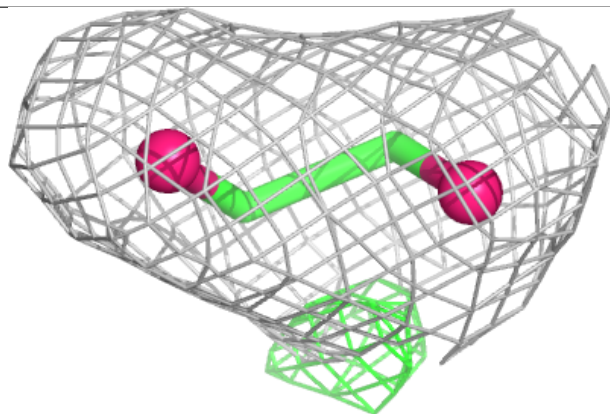
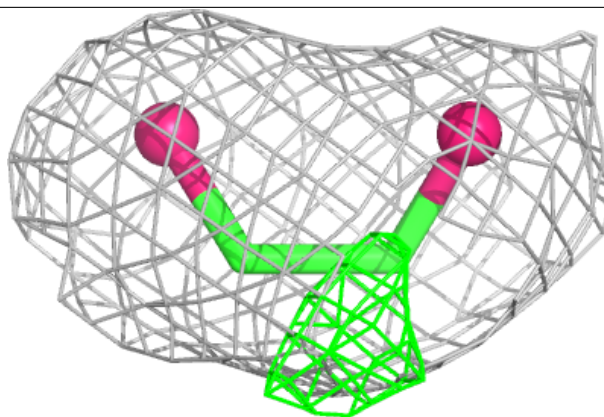
Electron density around PO4 C 607:

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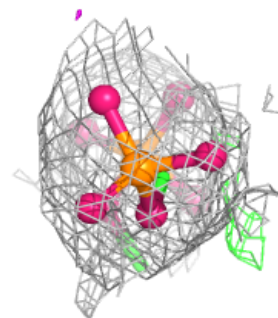
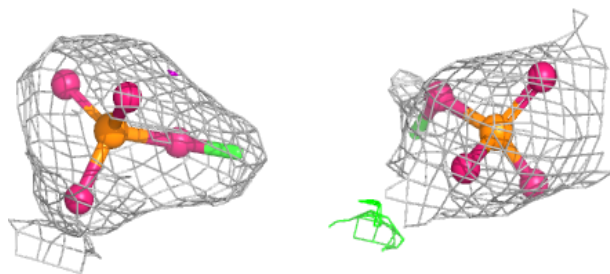
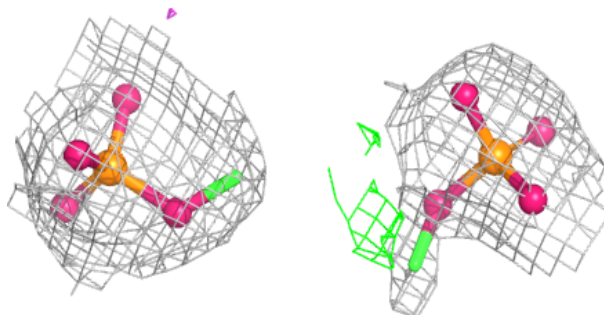


Electron density around EDO C 604:

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and green (positive)

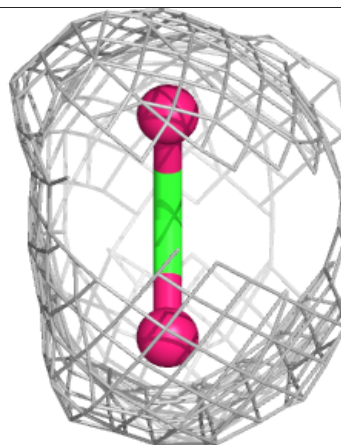
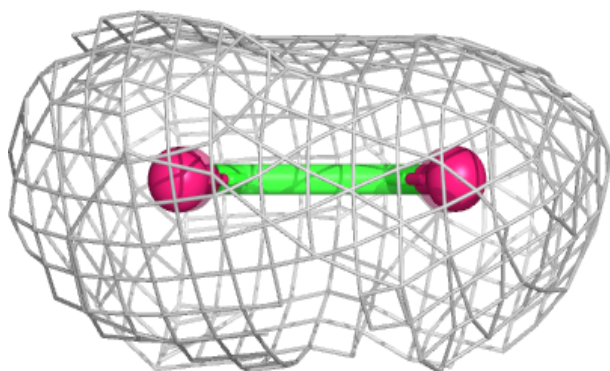
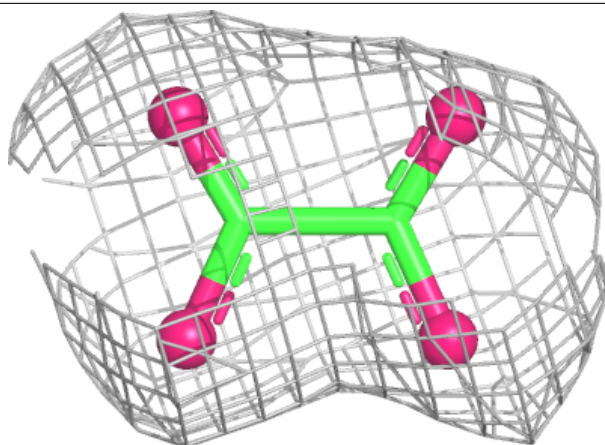
**Electron density around FBP C 601:**

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and green (positive)



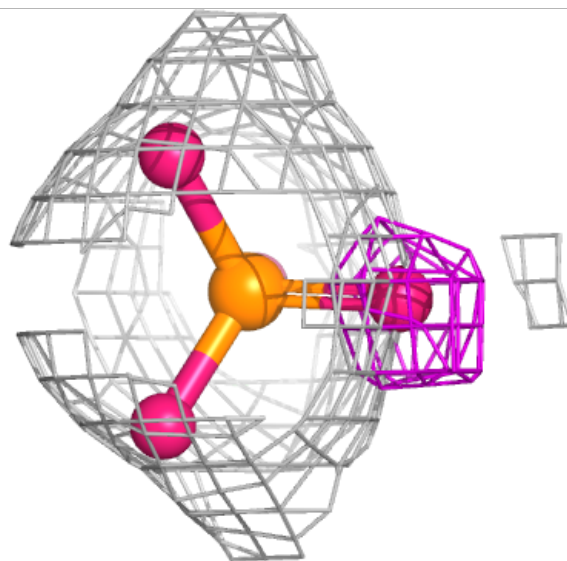
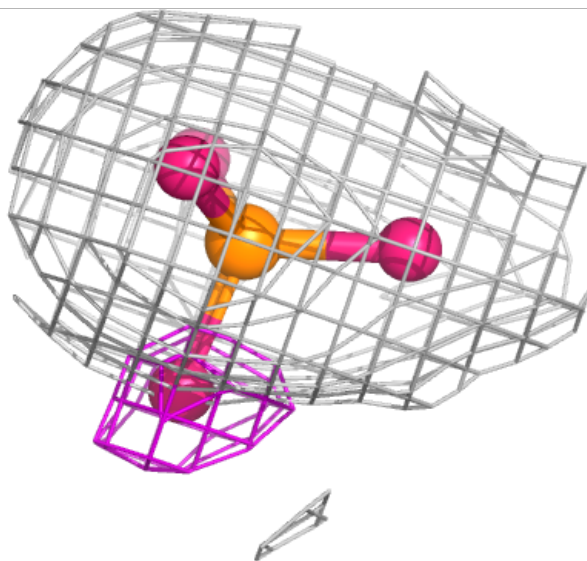
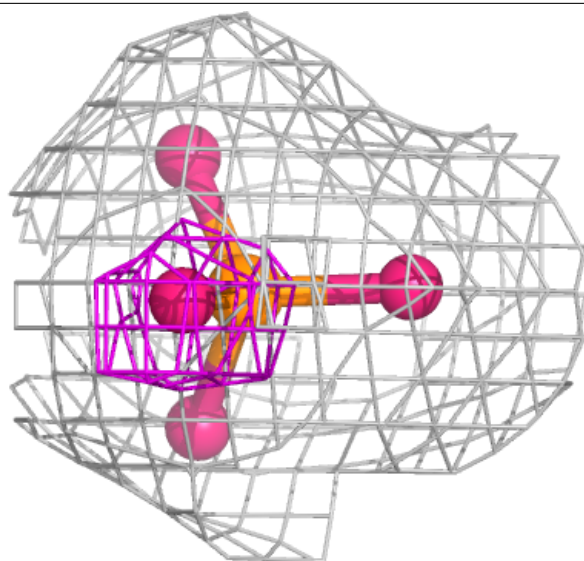
Electron density around OXL B 606:

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



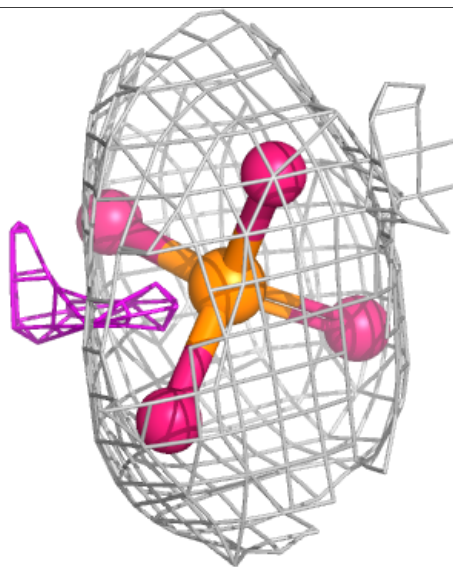
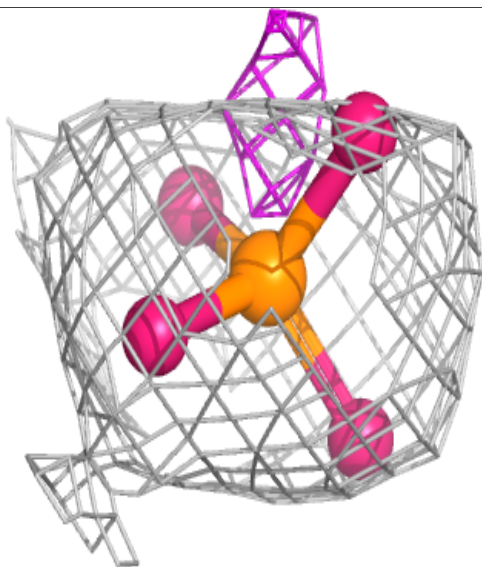
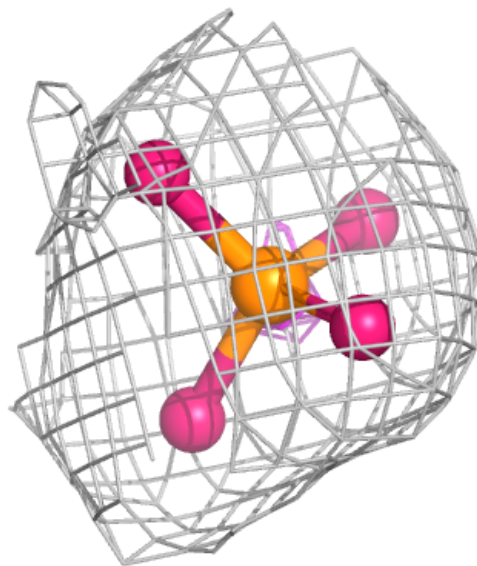
Electron density around PO4 A 604:

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



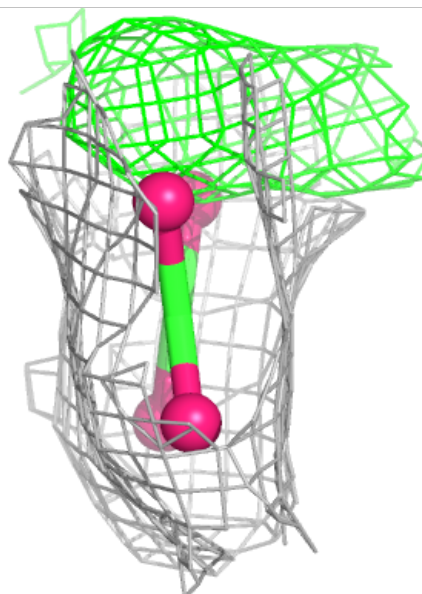
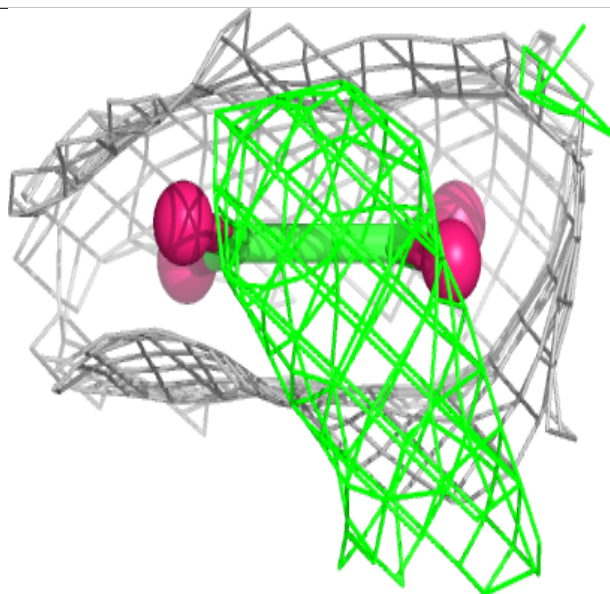
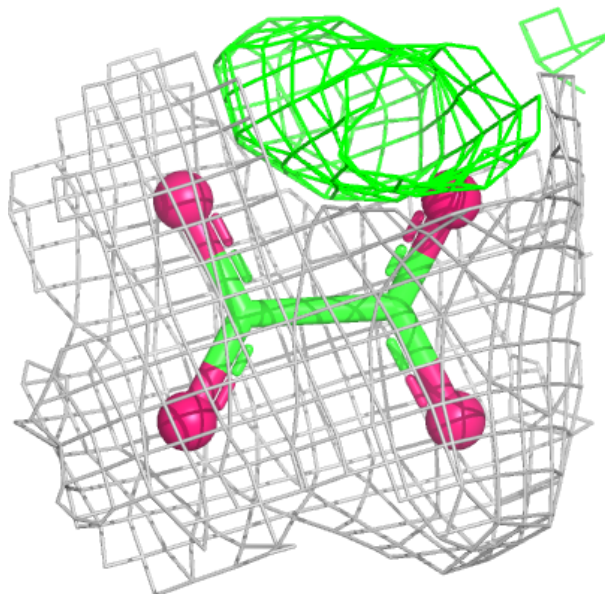
Electron density around PO4 D 608:

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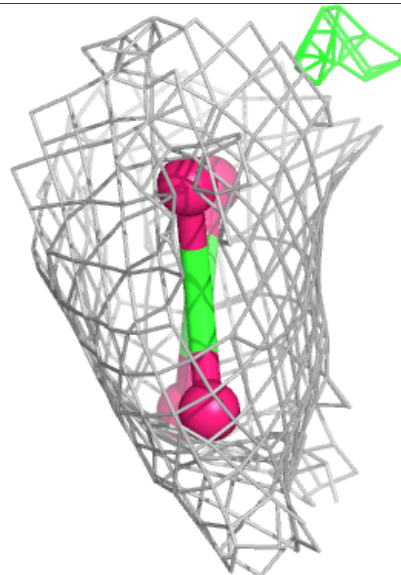
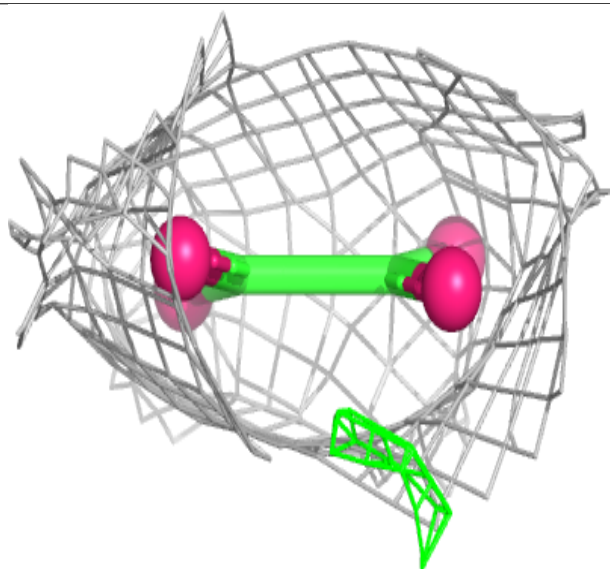
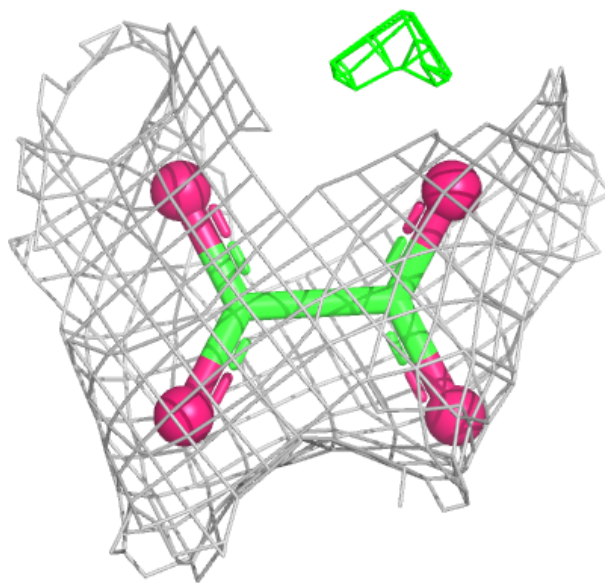
Electron density around OXL D 602:

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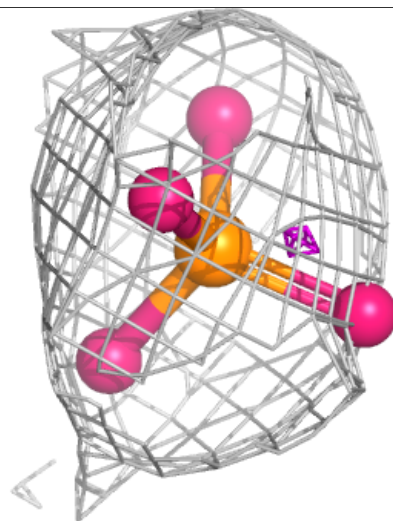
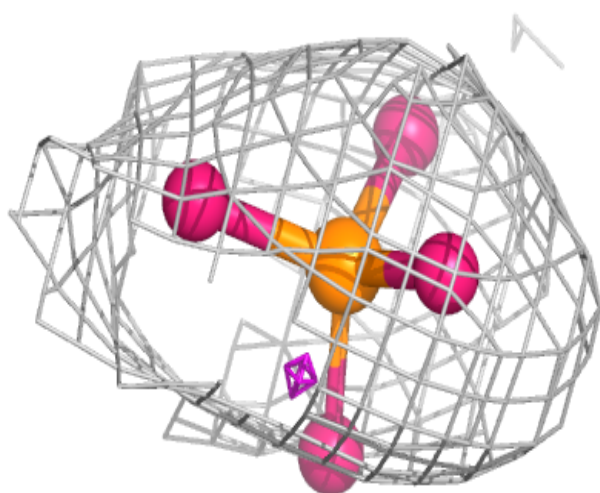
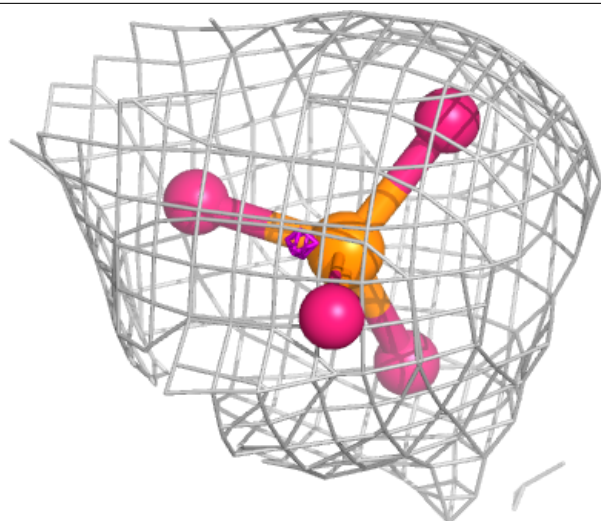
Electron density around OXL B 602:

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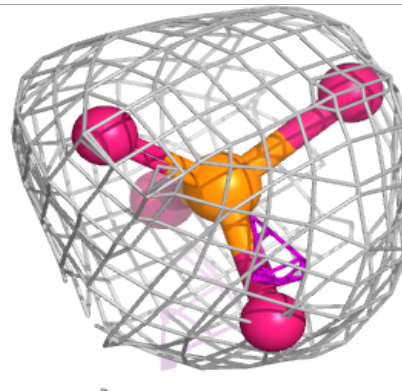
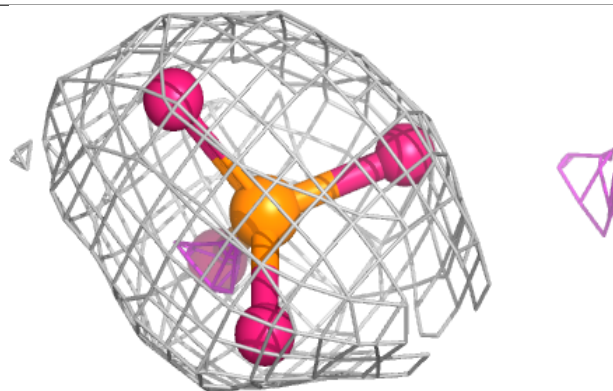
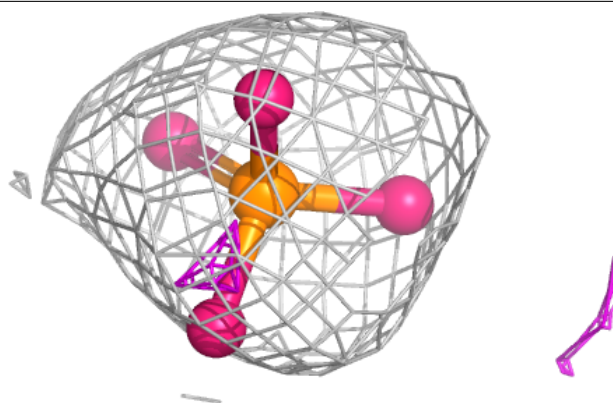
Electron density around PO4 D 604:

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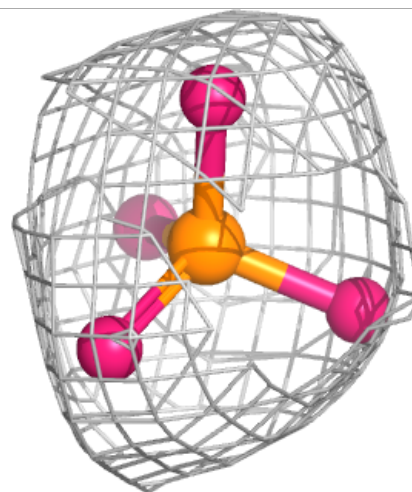
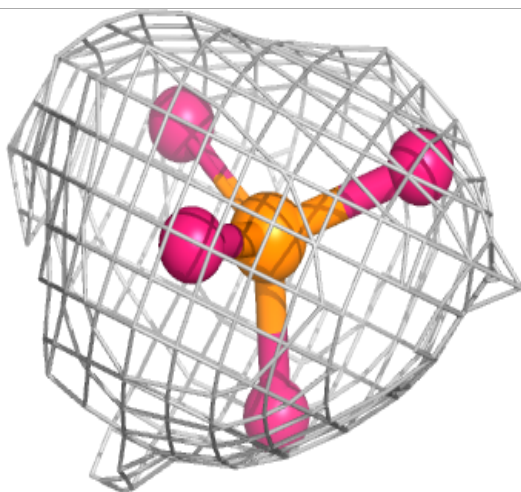
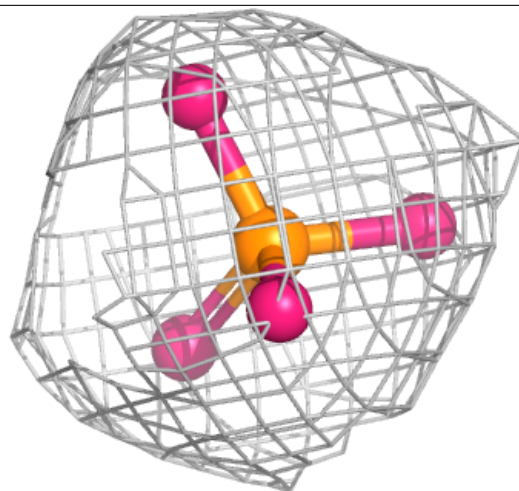
Electron density around PO4 B 608:

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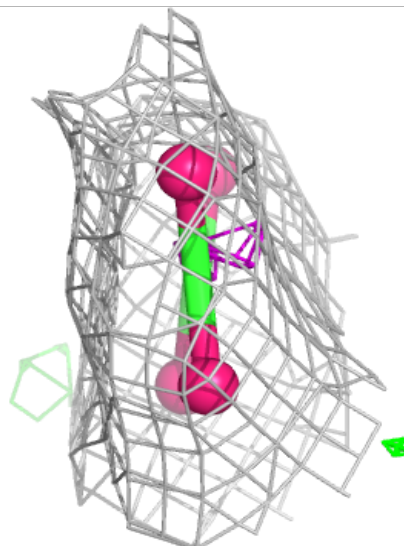
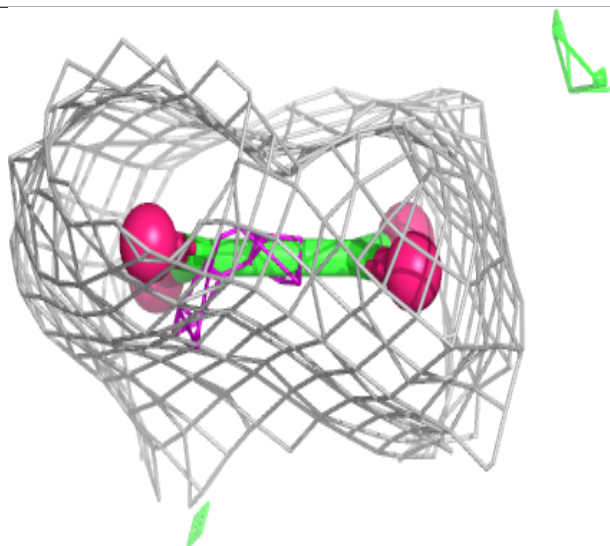
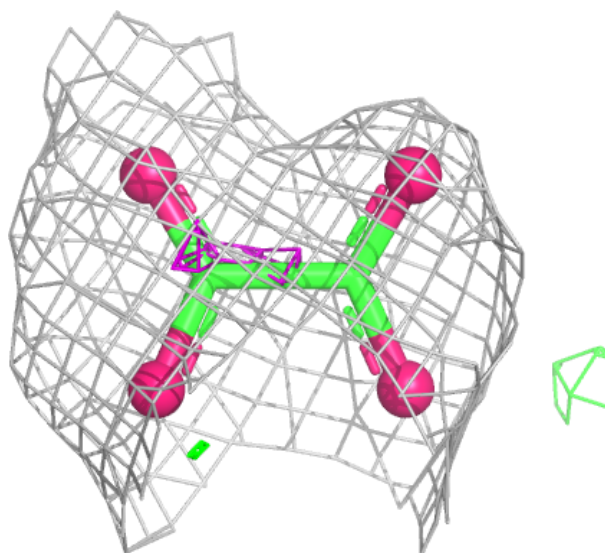
Electron density around PO4 A 605:

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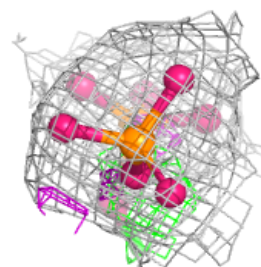
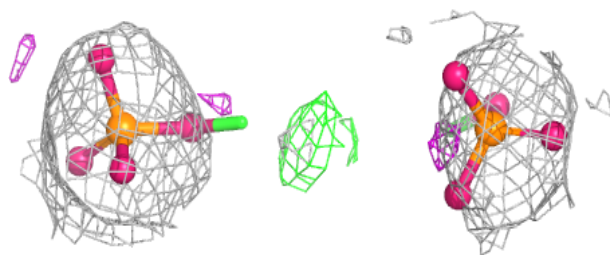
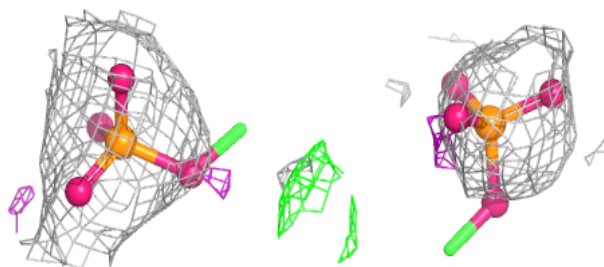
Electron density around OXL A 602:

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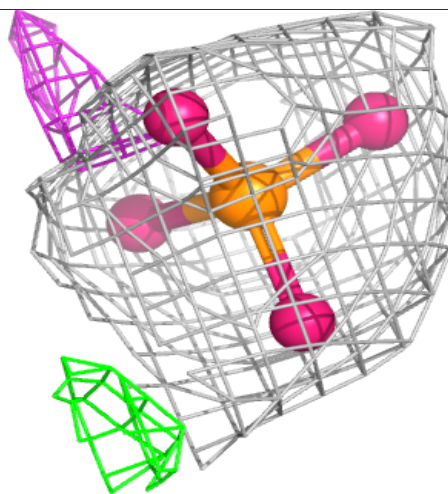
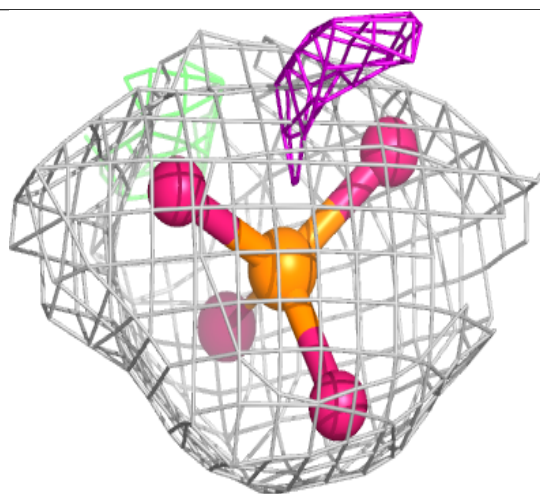
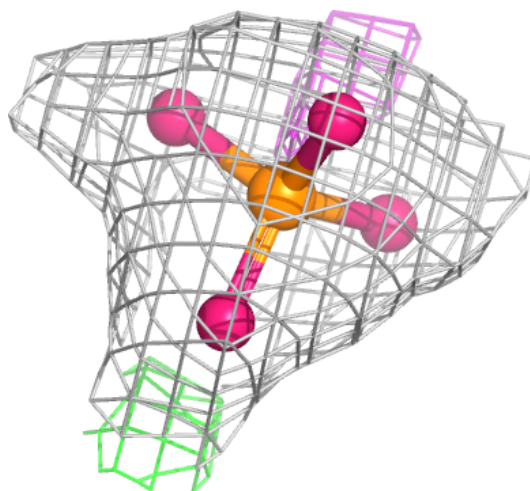
Electron density around FBP D 601:

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



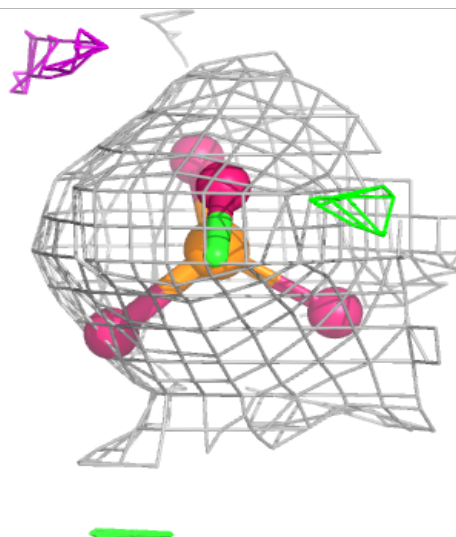
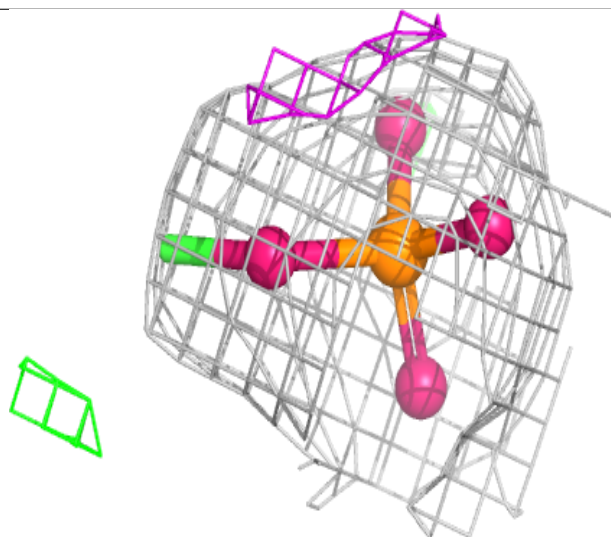
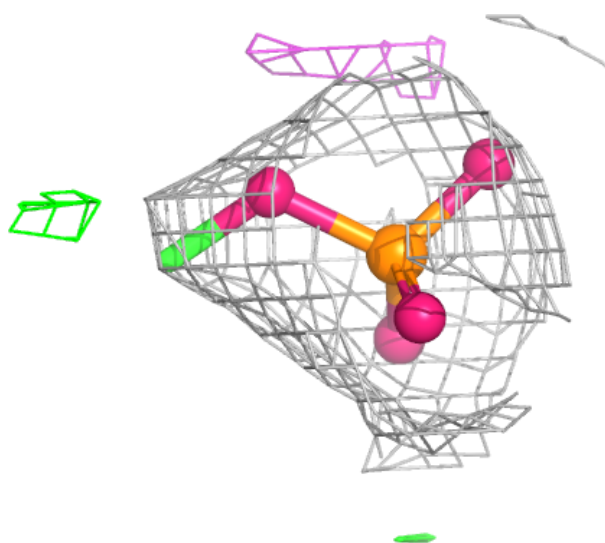
Electron density around PO4 D 603:

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and green (positive)



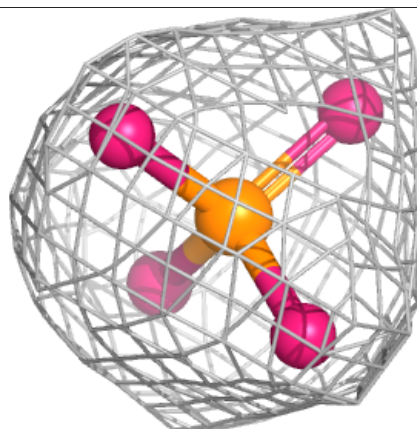
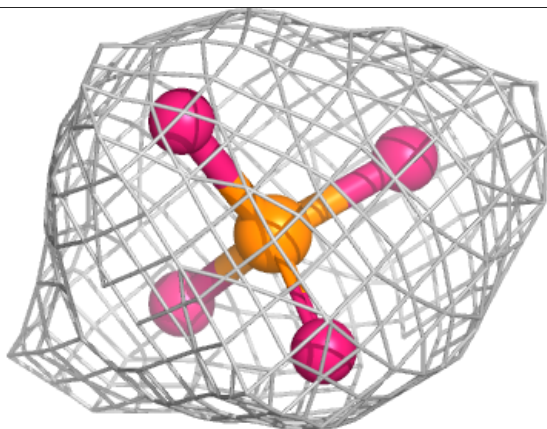
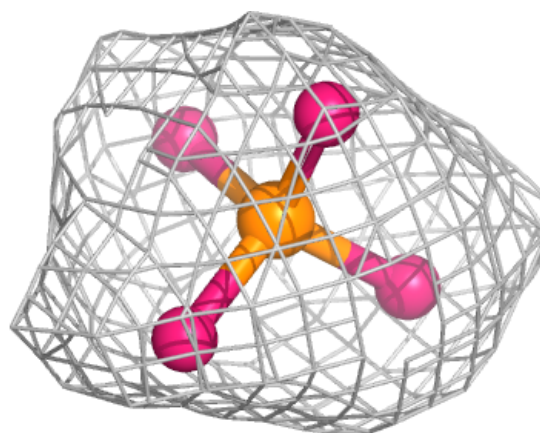
Electron density around FBP A 601:

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



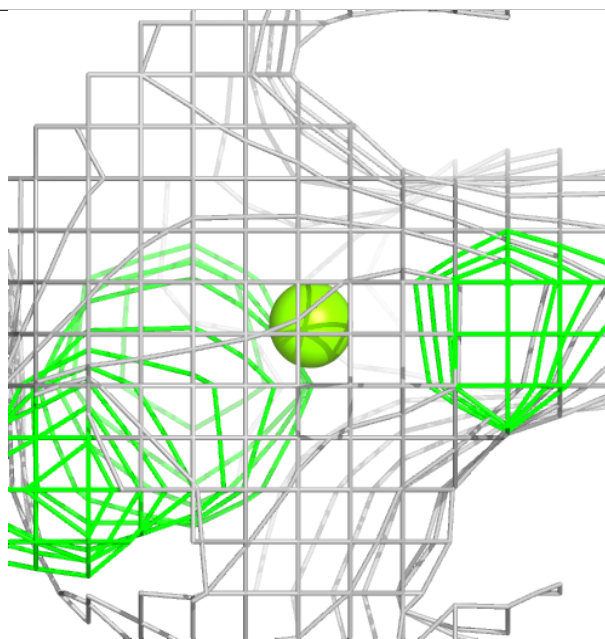
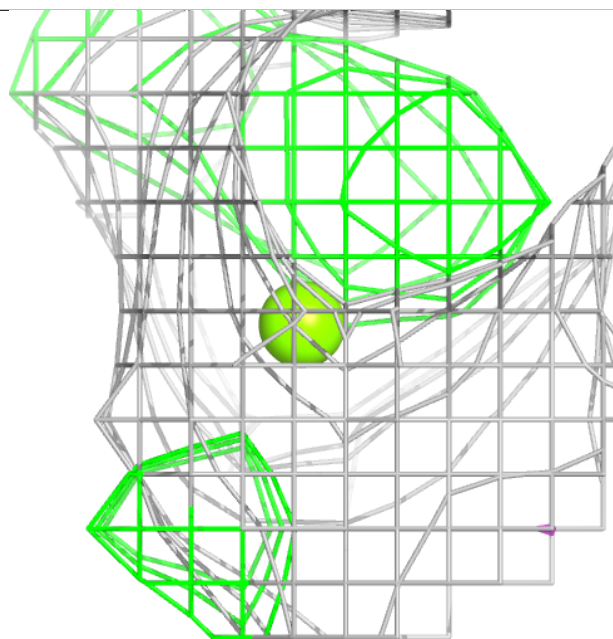
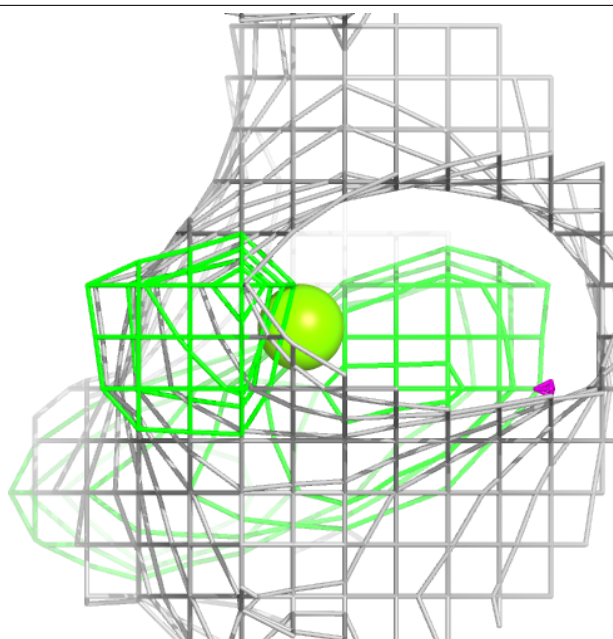
Electron density around PO4 C 606:

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



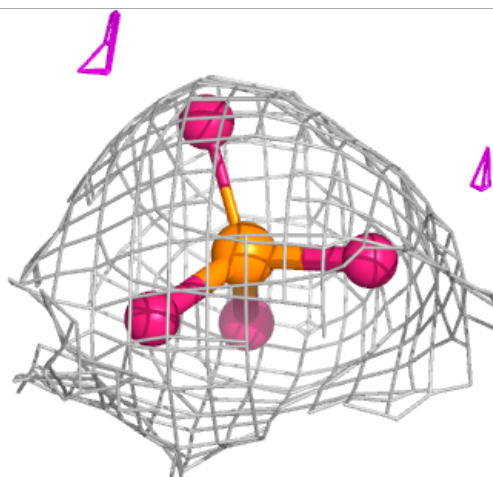
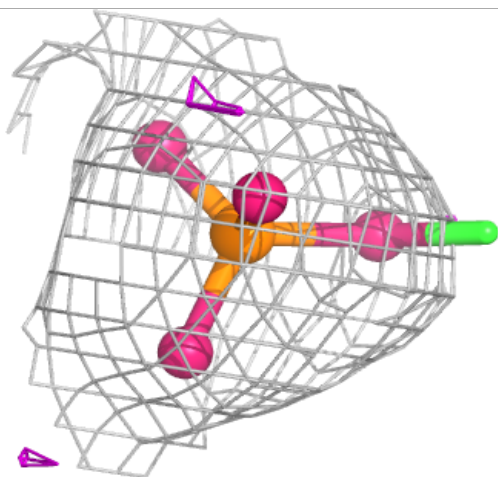
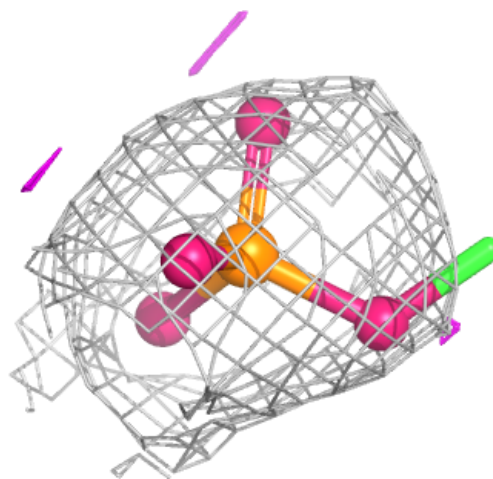
Electron density around MG D 609:

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



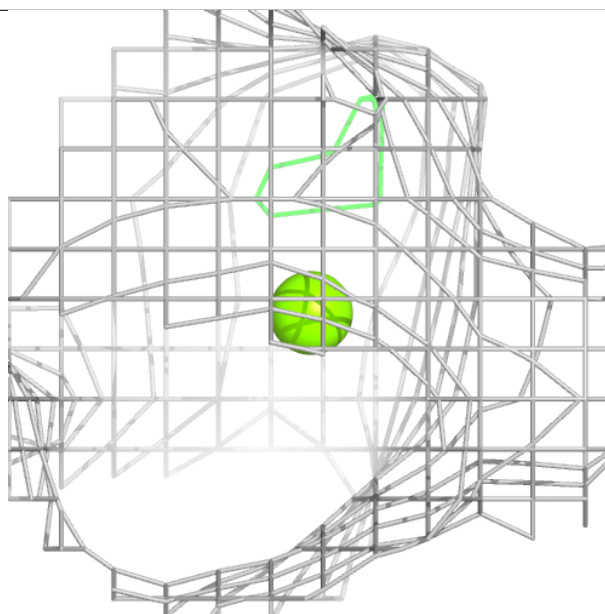
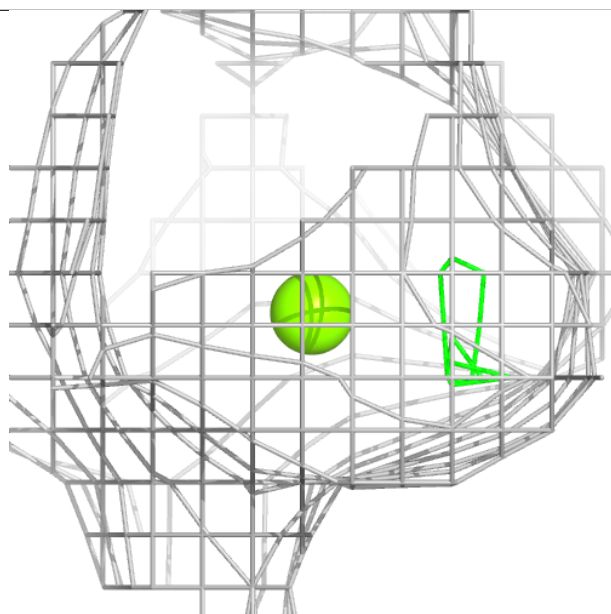
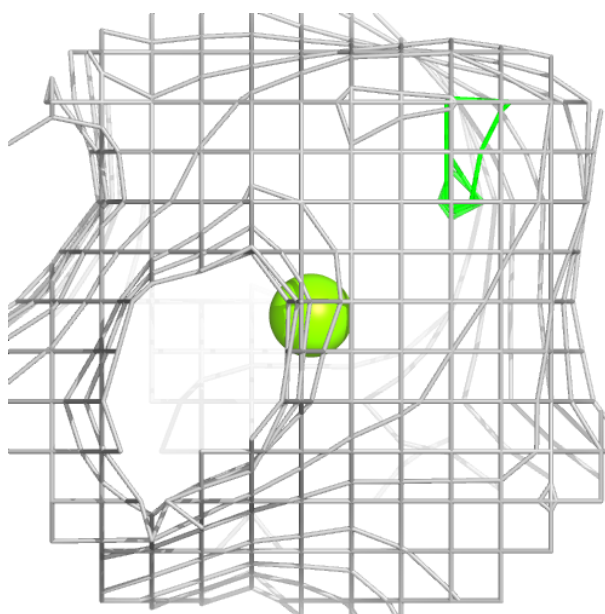
Electron density around FBP B 601:

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



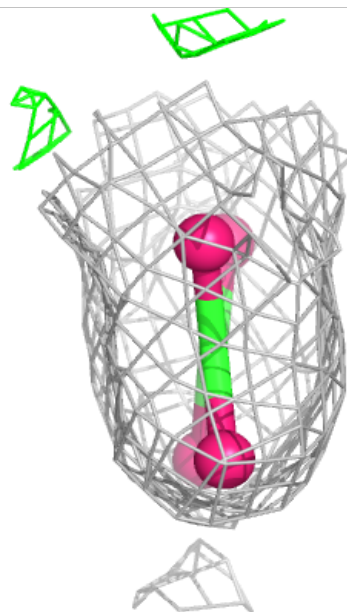
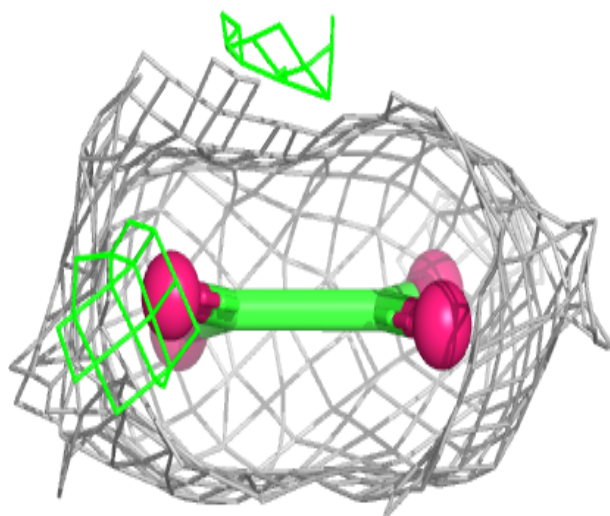
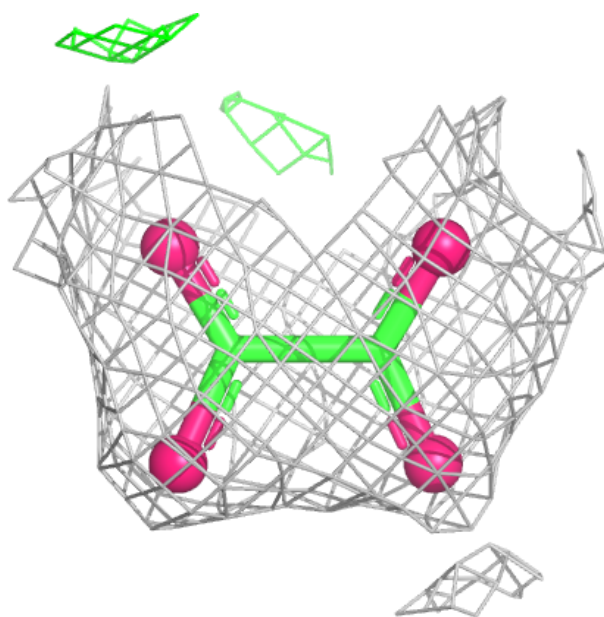
Electron density around MG B 609:

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



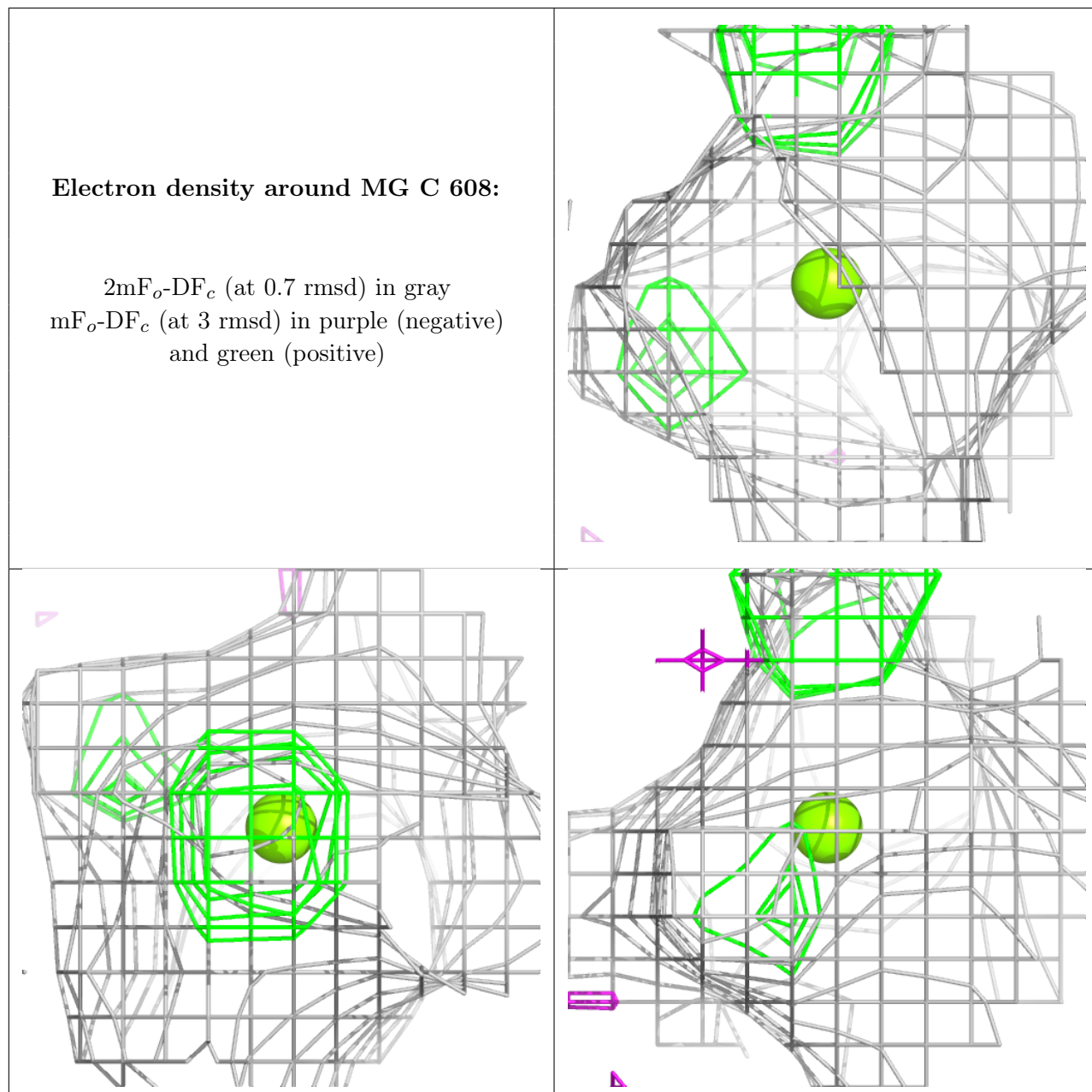
Electron density around OXL C 602:

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



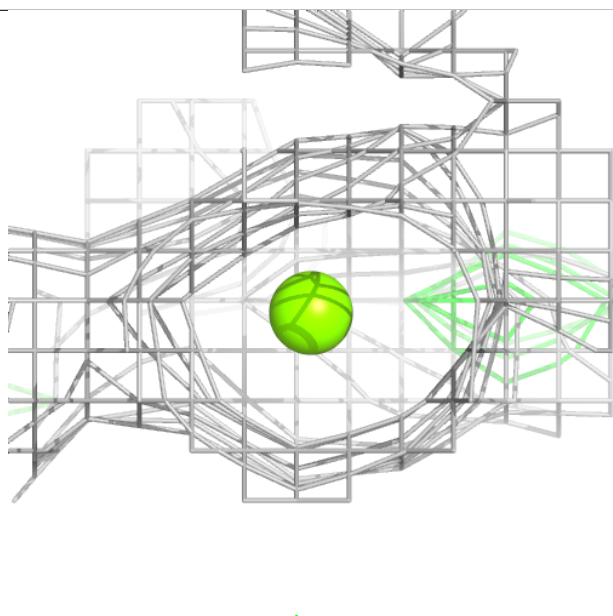
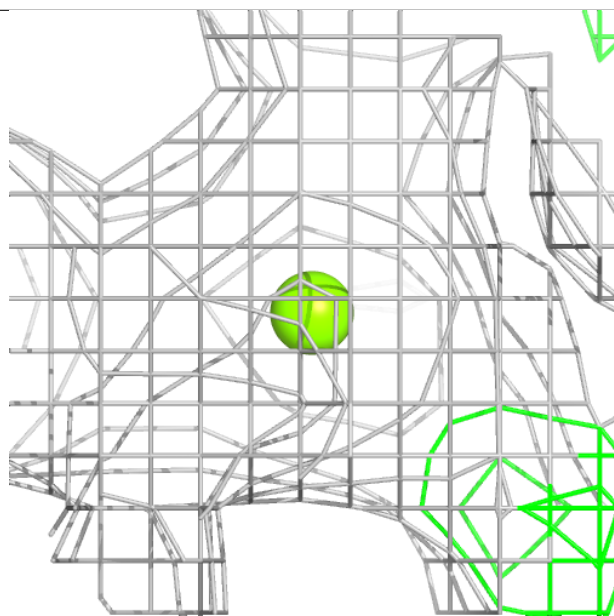
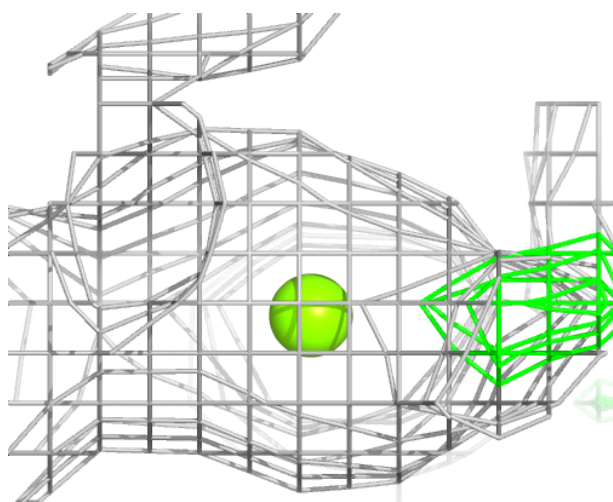
Electron density around MG C 608:

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



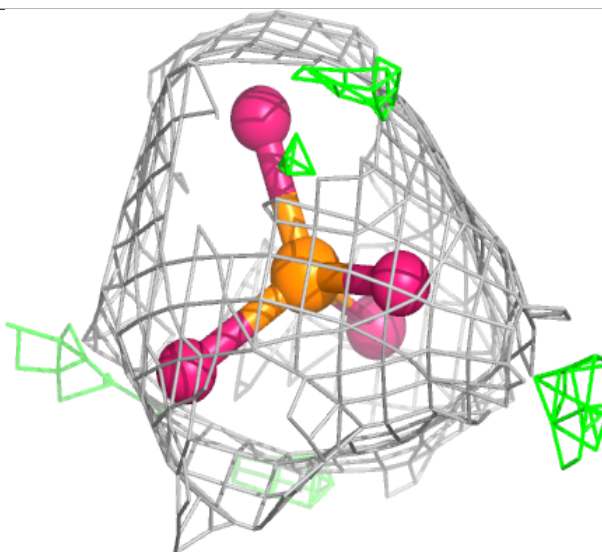
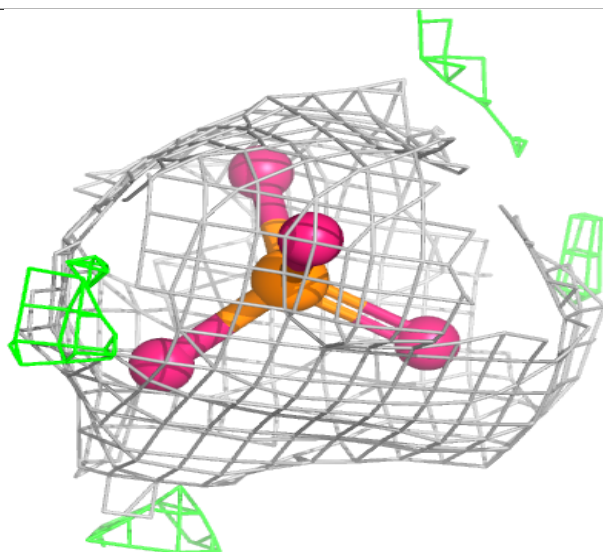
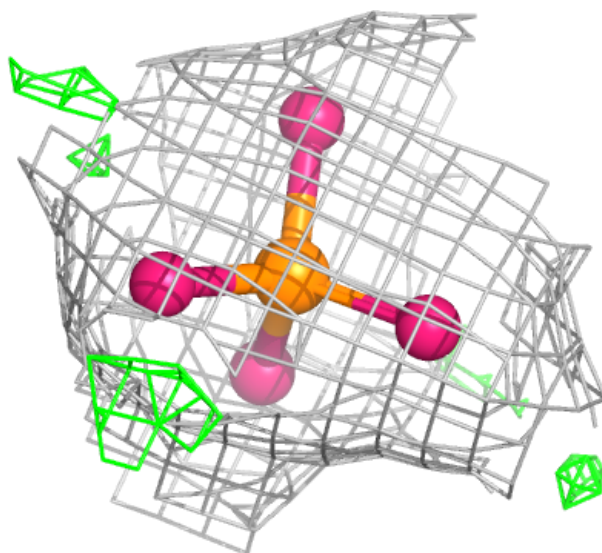
Electron density around MG A 608:

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



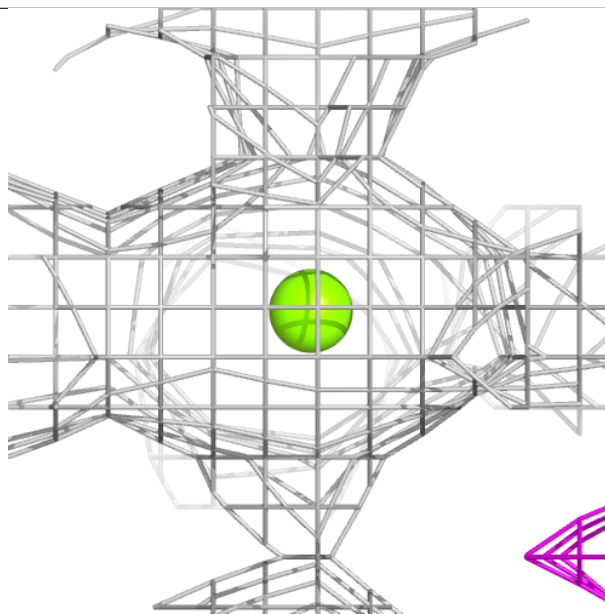
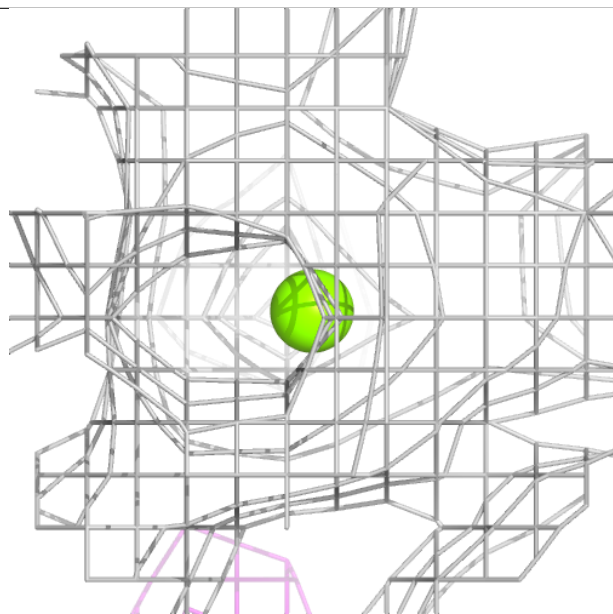
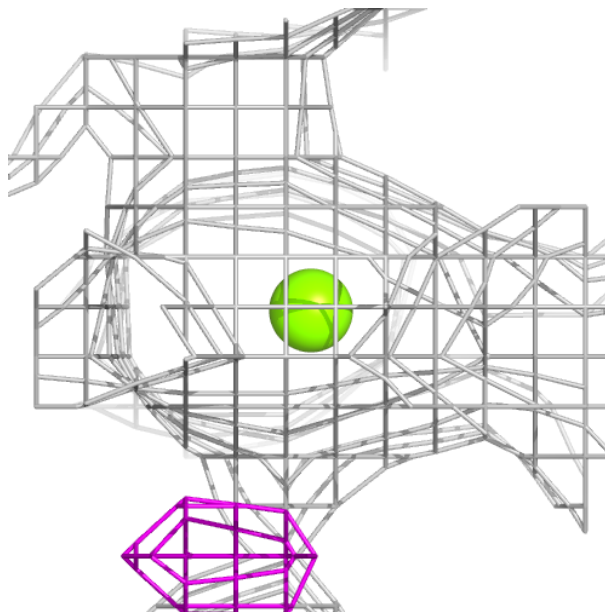
Electron density around PO4 D 607:

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



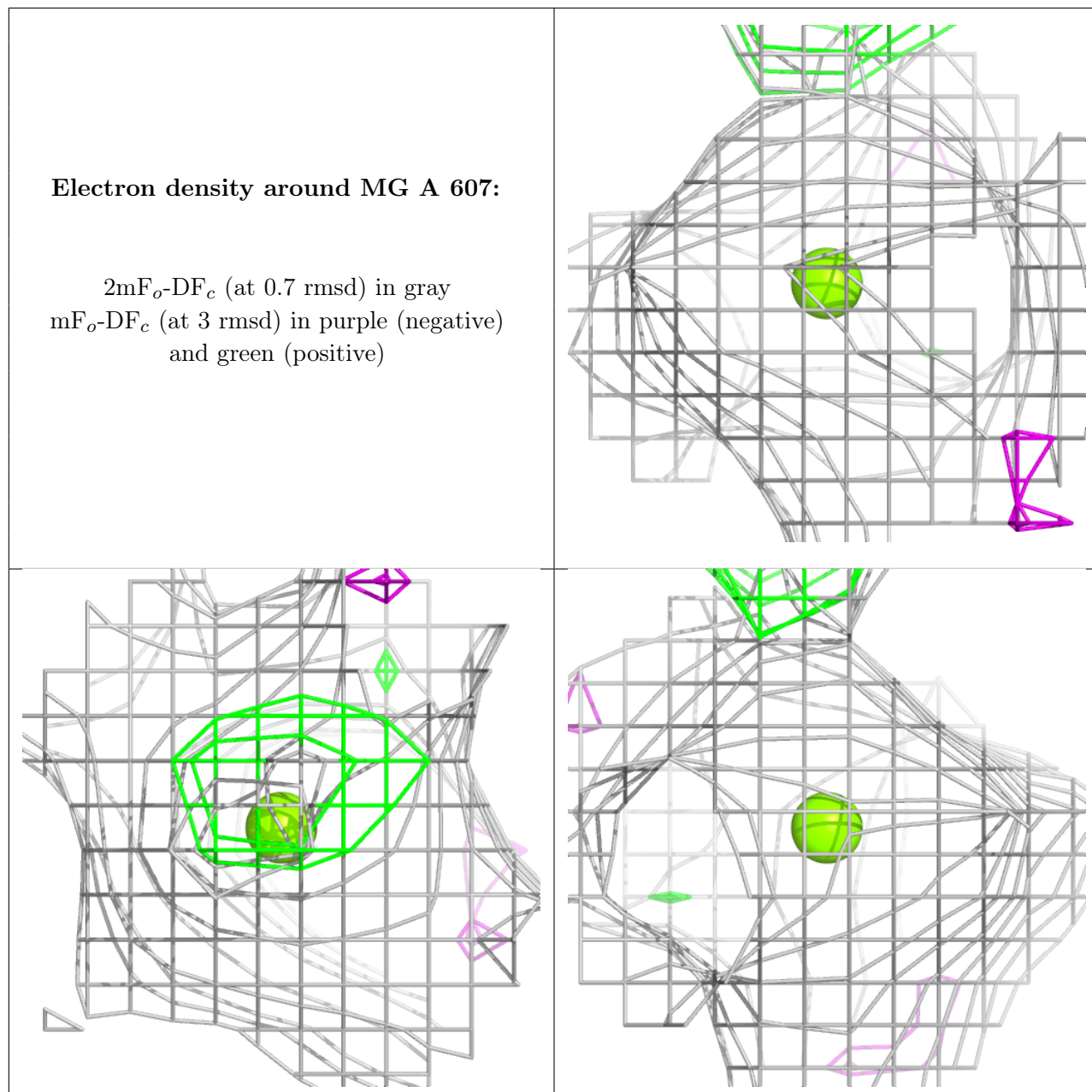
Electron density around MG C 609:

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



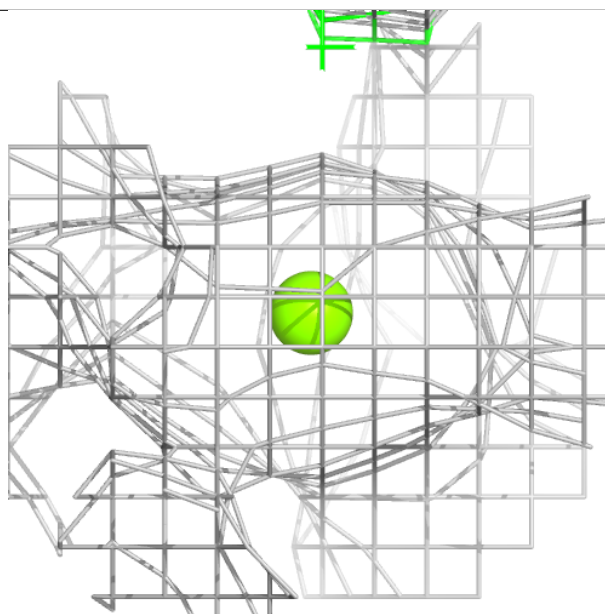
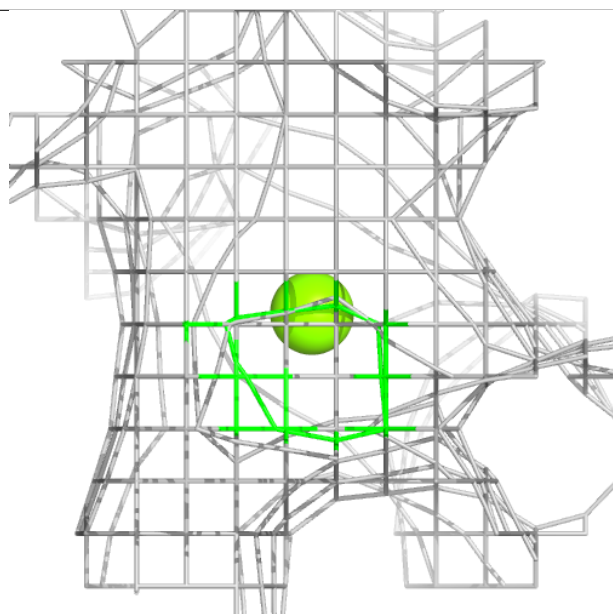
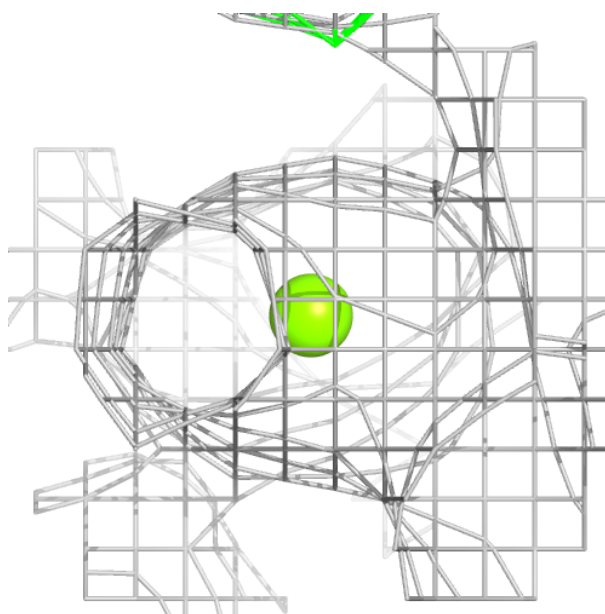
Electron density around MG A 607:

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



Electron density around MG D 610:

$2mF_o-DF_c$ (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.