



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:49 PM UTC

PDB ID : 7QYY / pdb_00007qyy
Title : Vanadium-dependent bromoperoxidase from *Corallina pilulifera* in complex with chloride
Authors : Isupov, M.N.; Mitchell, D.; Littelchild, J.A.; Garcia-Rodriguez, E.
Deposited on : 2022-01-29
Resolution : 2.00 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

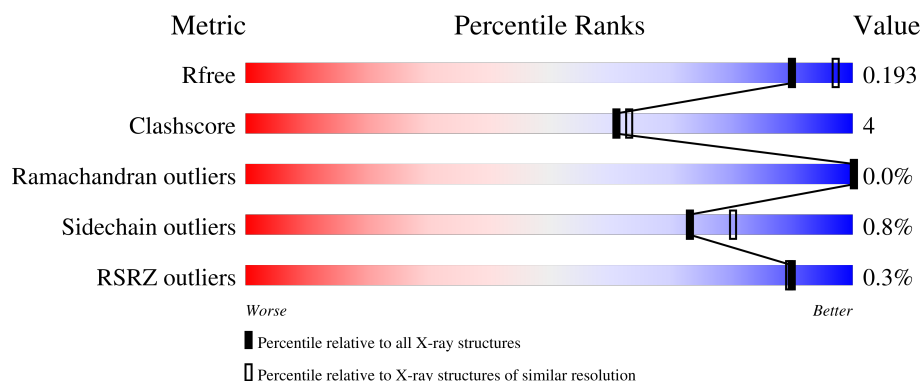
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	AAA	598	92% 8%
1	BBB	598	92% 8%
1	CCC	598	92% 8%
1	DDD	598	93% 7%

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
4	GOL	AAA	613	-	-	X	-
4	GOL	AAA	615	-	-	X	-
4	GOL	AAA	619	-	-	X	-
4	GOL	BBB	602	-	-	X	-
4	GOL	BBB	614	-	-	X	-
4	GOL	BBB	619	-	-	X	-
4	GOL	BBB	621	-	-	X	-
4	GOL	BBB	622	-	-	X	-
4	GOL	CCC	606	-	-	X	-
4	GOL	CCC	613	-	-	X	-
4	GOL	CCC	615	-	-	X	-
4	GOL	CCC	616	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22702 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 Vanadium-dependent bromoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	597	Total	C	N	O	S	0	27	0
			4745	3036	777	925	7			
1	BBB	597	Total	C	N	O	S	0	27	0
			4746	3032	778	929	7			
1	CCC	597	Total	C	N	O	S	0	31	0
			4768	3049	777	935	7			
1	DDD	597	Total	C	N	O	S	0	32	0
			4769	3053	778	931	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	423	ALA	PRO	conflict	UNP O81959
BBB	423	ALA	PRO	conflict	UNP O81959
CCC	423	ALA	PRO	conflict	UNP O81959
DDD	423	ALA	PRO	conflict	UNP O81959

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	P	0	0
			5	4	1		
2	AAA	1	Total	O	P	0	0
			5	4	1		
2	AAA	1	Total	O	P	0	0
			5	4	1		
2	BBB	1	Total	O	P	0	0
			5	4	1		
2	BBB	1	Total	O	P	0	0
			5	4	1		
2	CCC	1	Total	O	P	0	0
			5	4	1		
2	CCC	1	Total	O	P	0	0
			5	4	1		
2	DDD	1	Total	O	P	0	0
			5	4	1		
2	DDD	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Ca	0	0
			1	1		
3	BBB	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CCC	1	Total	Ca	0	0
			1	1		
3	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	2	Total	Na	0	0
			2	2		
5	BBB	1	Total	Na	0	0
			1	1		
5	CCC	1	Total	Na	0	0
			1	1		
5	DDD	1	Total	Na	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	4	Total 4	Cl 4	0	0
6	BBB	5	Total 5	Cl 5	0	0
6	CCC	3	Total 3	Cl 3	0	0
6	DDD	4	Total 4	Cl 4	0	0

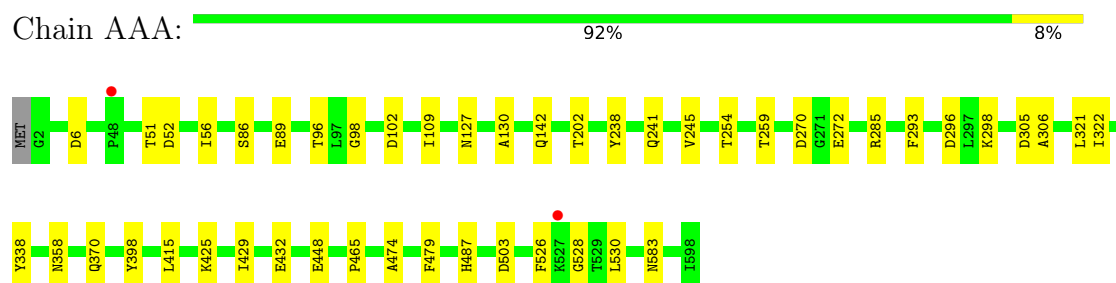
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	815	Total 815	O 815	0	0
7	BBB	792	Total 792	O 792	0	0
7	CCC	822	Total 822	O 822	0	0
7	DDD	785	Total 785	O 785	0	0

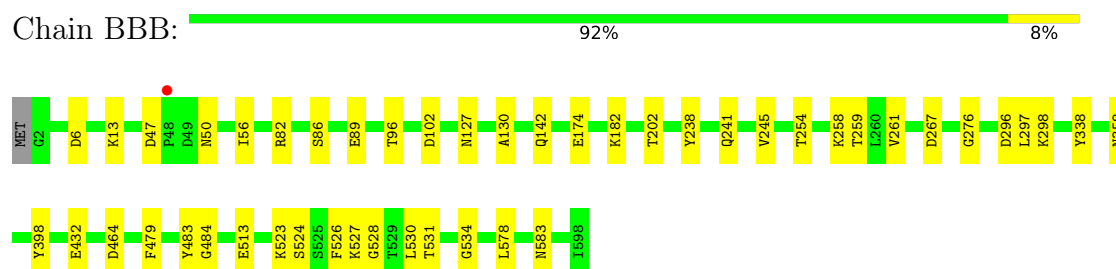
3 Residue-property plots

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.

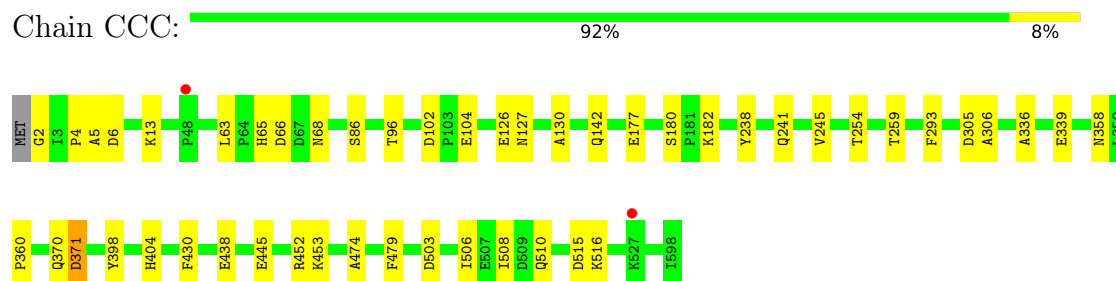
- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase

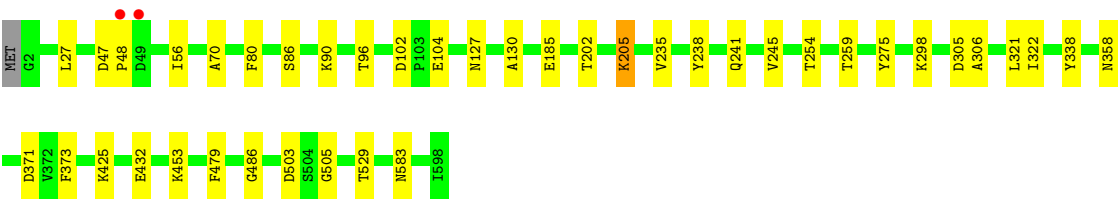


- Molecule 1: Vanadium-dependent bromoperoxidase



- Molecule 1: Vanadium-dependent bromoperoxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	182.12Å 182.12Å 177.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.96-2.00) 94.3 (19.96-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.146 , 0.193 0.146 , 0.193	Depositor DCC
R_{free} test set	10625 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22702	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, PO4, CL, NA

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	AAA	0.78	1/4923 (0.0%)	1.09	8/6686 (0.1%)
1	BBB	0.76	0/4920	1.07	5/6685 (0.1%)
1	CCC	0.79	2/4956 (0.0%)	1.09	10/6731 (0.1%)
1	DDD	0.76	0/4958	1.07	9/6737 (0.1%)
All	All	0.78	3/19757 (0.0%)	1.08	32/26839 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	404	HIS	CE1-NE2	7.43	1.40	1.32
1	AAA	487	HIS	CE1-NE2	5.50	1.38	1.32
1	CCC	2	GLY	N-CA	5.24	1.53	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	254	THR	CA-CB-OG1	-7.57	98.24	109.60
1	AAA	254	THR	CA-CB-OG1	-7.44	98.44	109.60
1	BBB	254	THR	CA-CB-OG1	-7.23	98.75	109.60
1	DDD	254	THR	CA-CB-OG1	-7.20	98.80	109.60
1	DDD	259	THR	CA-CB-OG1	-6.65	99.62	109.60
1	BBB	358	ASN	CA-CB-CG	-6.29	106.31	112.60
1	AAA	96	THR	CA-CB-OG1	-6.12	100.43	109.60
1	AAA	259	THR	CA-CB-OG1	-6.03	100.55	109.60
1	CCC	259	THR	CA-CB-OG1	-5.80	100.89	109.60
1	CCC	503	ASP	CA-C-N	-5.77	112.64	122.56
1	CCC	503	ASP	C-N-CA	-5.77	112.64	122.56
1	CCC	371	ASP	CA-CB-CG	5.77	118.37	112.60
1	BBB	96	THR	CA-CB-OG1	-5.69	101.06	109.60
1	CCC	358	ASN	CA-CB-CG	-5.64	106.96	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	503	ASP	CA-C-N	-5.50	113.10	122.56
1	AAA	503	ASP	C-N-CA	-5.50	113.10	122.56
1	DDD	96	THR	CA-CB-OG1	-5.50	101.36	109.60
1	DDD	529	THR	CA-CB-OG1	-5.44	101.43	109.60
1	AAA	270	ASP	CA-CB-CG	-5.43	107.17	112.60
1	CCC	336	ALA	CA-C-N	-5.43	112.06	120.31
1	CCC	336	ALA	C-N-CA	-5.43	112.06	120.31
1	DDD	202	THR	CA-CB-OG1	-5.42	101.47	109.60
1	DDD	358	ASN	CA-CB-CG	-5.25	107.35	112.60
1	AAA	202	THR	CA-CB-OG1	-5.24	101.74	109.60
1	BBB	259	THR	CA-CB-OG1	-5.23	101.75	109.60
1	DDD	80	PHE	CA-CB-CG	5.19	118.99	113.80
1	BBB	202	THR	CA-CB-OG1	-5.13	101.91	109.60
1	CCC	96	THR	CA-CB-OG1	-5.13	101.91	109.60
1	DDD	503	ASP	CA-C-N	-5.11	113.77	122.56
1	DDD	503	ASP	C-N-CA	-5.11	113.77	122.56
1	CCC	452	ARG	CG-CD-NE	-5.11	100.77	112.00
1	AAA	358	ASN	CA-CB-CG	-5.05	107.55	112.60

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	AAA	4745	0	4719	37	0
1	BBB	4746	0	4694	52	0
1	CCC	4768	0	4728	34	0
1	DDD	4769	0	4741	28	0
2	AAA	15	0	0	0	0
2	BBB	10	0	0	0	0
2	CCC	10	0	0	0	0
2	DDD	10	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DDD	1	0	0	0	0
4	AAA	108	0	143	28	0
4	BBB	114	0	151	32	0
4	CCC	102	0	136	24	0
4	DDD	66	0	88	4	0
5	AAA	2	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	4	0	0	0	0
6	BBB	5	0	0	0	0
6	CCC	3	0	0	0	0
6	DDD	4	0	0	1	0
7	AAA	815	0	0	12	1
7	BBB	792	0	0	8	0
7	CCC	822	0	0	12	1
7	DDD	785	0	0	6	1
All	All	22702	0	19400	165	2

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 4.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AAA:621:GOL:H32	7:AAA:926:HOH:O	1.48	1.10
1:BBB:527[B]:LYS:HD2	1:BBB:527[B]:LYS:C	1.78	1.09
1:CCC:66:ASP:OD2	4:CCC:606:GOL:H12	1.58	1.03
1:BBB:527[B]:LYS:HD2	1:BBB:527[B]:LYS:O	1.58	1.01
1:BBB:527[B]:LYS:C	1:BBB:527[B]:LYS:CD	2.35	0.98
1:AAA:298[A]:LYS:HE2	4:AAA:613:GOL:H31	1.48	0.94
4:BBB:621:GOL:H31	7:BBB:771:HOH:O	1.68	0.92
1:BBB:258[A]:LYS:NZ	4:BBB:621:GOL:H32	1.91	0.85
4:CCC:613:GOL:H11	1:DDD:583:ASN:HD22	1.41	0.85
4:CCC:613:GOL:H2	7:CCC:740:HOH:O	1.78	0.81
1:BBB:258[A]:LYS:HZ3	4:BBB:621:GOL:H32	1.44	0.81
4:BBB:620:GOL:H12	7:BBB:1218:HOH:O	1.80	0.80
4:AAA:619:GOL:H31	7:BBB:1152:HOH:O	1.83	0.79
1:BBB:174:GLU:HG3	4:BBB:611:GOL:H11	1.65	0.79
1:BBB:531:THR:H	4:BBB:614:GOL:H11	1.46	0.79
1:BBB:261:VAL:HG21	4:BBB:622:GOL:H32	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:296[B]:ASP:OD1	4:AAA:613:GOL:H11	1.83	0.78
4:CCC:619:GOL:H11	7:CCC:1348:HOH:O	1.83	0.77
1:CCC:180[B]:SER:HB2	4:CCC:616:GOL:H11	1.67	0.77
1:CCC:445[A]:GLU:HG2	7:CCC:721:HOH:O	1.86	0.75
1:BBB:298:LYS:HG3	4:BBB:619:GOL:H12	1.69	0.75
1:BBB:298:LYS:HE3	4:BBB:619:GOL:H31	1.69	0.74
1:CCC:177[B]:GLU:OE2	1:CCC:516:LYS:HD3	1.87	0.74
1:CCC:180[A]:SER:HB3	4:CCC:616:GOL:H11	1.70	0.72
1:CCC:438[A]:GLU:OE1	7:CCC:704:HOH:O	2.07	0.72
1:CCC:68:ASN:HB2	4:CCC:606:GOL:H11	1.73	0.70
1:AAA:6:ASP:HB3	7:AAA:1224:HOH:O	1.91	0.69
1:BBB:182:LYS:HZ1	4:BBB:611:GOL:H12	1.58	0.69
1:BBB:534:GLY:HA3	4:BBB:614:GOL:H12	1.74	0.68
1:CCC:68:ASN:HD22	4:CCC:606:GOL:H11	1.57	0.68
1:AAA:298[B]:LYS:HG3	4:AAA:613:GOL:H12	1.74	0.68
1:AAA:583:ASN:ND2	4:AAA:619:GOL:O2	2.26	0.68
4:AAA:615:GOL:H2	7:AAA:808:HOH:O	1.94	0.67
1:BBB:531:THR:H	4:BBB:614:GOL:C1	2.07	0.66
1:BBB:82:ARG:HE	4:BBB:618:GOL:C1	2.09	0.65
1:AAA:296[A]:ASP:OD1	4:AAA:613:GOL:H11	1.97	0.65
1:BBB:523:LYS:HE3	7:BBB:718:HOH:O	1.96	0.65
1:BBB:526:PHE:HB2	4:BBB:616:GOL:H2	1.79	0.64
1:AAA:285:ARG:HH12	4:BBB:602:GOL:H11	1.63	0.64
1:AAA:583:ASN:CB	4:AAA:619:GOL:O2	2.46	0.64
1:CCC:6:ASP:HB3	7:CCC:1271:HOH:O	1.99	0.62
1:CCC:371:ASP:OD1	4:CCC:615:GOL:H32	1.99	0.62
1:BBB:6:ASP:HB3	7:BBB:1250:HOH:O	1.99	0.62
1:BBB:258[B]:LYS:HE3	4:BBB:621:GOL:H32	1.80	0.62
1:BBB:527[B]:LYS:CD	1:BBB:528[B]:GLY:N	2.64	0.61
1:AAA:272[B]:GLU:OE2	4:AAA:606:GOL:C1	2.50	0.60
1:BBB:530:LEU:HA	4:BBB:614:GOL:H11	1.82	0.60
1:BBB:531:THR:N	4:BBB:614:GOL:H11	2.16	0.60
1:BBB:267:ASP:OD2	4:BBB:602:GOL:H11	2.02	0.59
4:BBB:617:GOL:H12	7:BBB:802:HOH:O	2.01	0.59
1:DDD:298[B]:LYS:HD2	4:DDD:609:GOL:H11	1.83	0.59
1:CCC:180[A]:SER:OG	4:CCC:616:GOL:H2	2.03	0.58
1:AAA:429[A]:ILE:HD12	7:AAA:736:HOH:O	2.02	0.58
1:AAA:425:LYS:HE2	7:AAA:1295:HOH:O	2.04	0.57
1:AAA:272[B]:GLU:OE2	4:AAA:606:GOL:H11	2.05	0.57
4:AAA:618:GOL:H2	7:AAA:743:HOH:O	2.05	0.57
1:DDD:298[A]:LYS:HD3	7:DDD:825:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:298[A]:LYS:HG3	4:AAA:613:GOL:H12	1.86	0.57
4:AAA:615:GOL:H12	1:BBB:583:ASN:CB	2.36	0.56
1:CCC:68:ASN:HD22	4:CCC:606:GOL:C1	2.18	0.56
1:CCC:13:LYS:HE2	1:DDD:27:LEU:HD21	1.86	0.56
1:CCC:453[B]:LYS:NZ	7:CCC:709:HOH:O	2.32	0.56
4:CCC:613:GOL:H11	1:DDD:583:ASN:ND2	2.17	0.55
1:AAA:102:ASP:HB2	1:AAA:109[A]:ILE:HD11	1.88	0.55
4:CCC:607:GOL:O1	4:CCC:611:GOL:H32	2.07	0.54
1:BBB:258[A]:LYS:HZ2	4:BBB:621:GOL:H32	1.72	0.54
1:CCC:180[B]:SER:HB2	4:CCC:616:GOL:C1	2.37	0.54
1:BBB:13:LYS:NZ	7:BBB:716:HOH:O	2.40	0.54
4:CCC:613:GOL:H11	1:DDD:583:ASN:HB3	1.90	0.54
1:BBB:527[B]:LYS:HD2	1:BBB:528[B]:GLY:N	2.20	0.54
1:AAA:272[B]:GLU:OE2	4:AAA:606:GOL:O1	2.25	0.54
4:AAA:615:GOL:H12	1:BBB:583:ASN:HB2	1.90	0.54
1:BBB:182:LYS:NZ	4:BBB:611:GOL:H12	2.23	0.54
1:AAA:285:ARG:HH12	4:BBB:602:GOL:C1	2.22	0.53
4:AAA:615:GOL:C1	7:AAA:808:HOH:O	2.57	0.53
1:AAA:298[A]:LYS:CG	4:AAA:613:GOL:H12	2.39	0.52
4:CCC:613:GOL:C1	1:DDD:583:ASN:HD22	2.18	0.52
1:BBB:527[B]:LYS:HD3	1:BBB:528[B]:GLY:N	2.26	0.51
1:AAA:429[A]:ILE:HD11	7:AAA:1334:HOH:O	2.11	0.50
4:AAA:615:GOL:H32	7:AAA:718:HOH:O	2.11	0.50
1:DDD:205[A]:LYS:HB3	7:DDD:1164:HOH:O	2.12	0.49
1:DDD:104[B]:GLU:HG3	7:DDD:731:HOH:O	2.12	0.48
1:AAA:89:GLU:OE2	4:AAA:615:GOL:H11	2.13	0.48
1:CCC:453[B]:LYS:CE	7:CCC:709:HOH:O	2.62	0.48
1:BBB:297:LEU:HB3	4:BBB:619:GOL:H2	1.95	0.48
1:AAA:52:ASP:OD1	4:AAA:620:GOL:H31	2.13	0.48
1:DDD:185:GLU:OE2	7:DDD:702:HOH:O	2.20	0.48
1:CCC:180[B]:SER:OG	1:CCC:182:LYS:HG2	2.14	0.47
1:CCC:339:GLU:HG3	1:DDD:275:TYR:CZ	2.49	0.47
1:BBB:47:ASP:OD1	1:BBB:47:ASP:C	2.57	0.47
1:AAA:298[A]:LYS:CD	4:AAA:613:GOL:H12	2.44	0.47
1:BBB:578:LEU:HD23	1:CCC:4:PRO:HB3	1.97	0.47
1:DDD:70:ALA:HB3	4:DDD:607:GOL:H32	1.96	0.47
1:BBB:267:ASP:OD2	4:BBB:602:GOL:C1	2.63	0.47
1:AAA:305:ASP:O	1:AAA:306:ALA:HB3	2.15	0.46
4:CCC:615:GOL:C3	7:CCC:1132:HOH:O	2.63	0.46
1:BBB:261:VAL:HG21	4:BBB:622:GOL:C3	2.42	0.46
1:CCC:127:ASN:HB3	1:CCC:130:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:527[B]:LYS:O	1:BBB:527[B]:LYS:CD	2.44	0.46
1:DDD:235[B]:VAL:HG21	4:DDD:613:GOL:H32	1.98	0.46
1:AAA:241:GLN:O	1:AAA:245[A]:VAL:HG22	2.16	0.46
1:BBB:127:ASN:HB3	1:BBB:130:ALA:HB2	1.99	0.45
4:CCC:615:GOL:H32	7:CCC:1132:HOH:O	2.16	0.45
1:BBB:261:VAL:HG11	4:BBB:622:GOL:H11	1.98	0.45
4:CCC:616:GOL:H11	7:CCC:763:HOH:O	2.15	0.45
1:BBB:47:ASP:O	1:BBB:50:ASN:HB3	2.16	0.45
1:BBB:296[B]:ASP:OD2	4:BBB:609:GOL:O2	2.20	0.45
1:BBB:464:ASP:OD2	4:BBB:619:GOL:O2	2.28	0.45
4:CCC:613:GOL:H11	1:DDD:583:ASN:CB	2.47	0.45
1:DDD:505:GLY:HA2	4:DDD:606:GOL:H12	1.99	0.45
1:AAA:526:PHE:CZ	1:AAA:528[A]:GLY:HA3	2.52	0.45
1:BBB:56[A]:ILE:HD11	1:BBB:432:GLU:CD	2.42	0.45
1:BBB:241:GLN:O	1:BBB:245[A]:VAL:HG22	2.17	0.45
1:DDD:241:GLN:O	1:DDD:245[A]:VAL:HG22	2.16	0.45
1:DDD:425:LYS:CE	7:DDD:888:HOH:O	2.64	0.45
4:AAA:615:GOL:C2	7:AAA:808:HOH:O	2.57	0.44
1:CCC:126:GLU:HG2	1:DDD:371:ASP:HB3	1.99	0.44
1:CCC:515[B]:ASP:OD1	1:CCC:516:LYS:N	2.50	0.44
1:AAA:127:ASN:HB3	1:AAA:130:ALA:HB2	1.99	0.44
1:CCC:371:ASP:OD2	4:CCC:615:GOL:H11	2.16	0.44
1:DDD:127:ASN:HB3	1:DDD:130:ALA:HB2	1.99	0.44
4:AAA:619:GOL:H11	1:BBB:89:GLU:HB2	2.00	0.44
4:AAA:615:GOL:H12	1:BBB:583:ASN:HB3	1.99	0.43
4:CCC:608:GOL:O3	7:CCC:705:HOH:O	2.21	0.43
1:AAA:530:LEU:HA	4:AAA:612:GOL:H31	2.01	0.43
1:AAA:298[B]:LYS:HE3	4:AAA:613:GOL:H31	2.00	0.43
1:DDD:56[A]:ILE:HD11	1:DDD:432:GLU:CD	2.43	0.43
1:DDD:453[B]:LYS:HG3	7:DDD:784:HOH:O	2.19	0.43
1:AAA:56[B]:ILE:HG13	1:AAA:415:LEU:HD21	2.00	0.42
1:BBB:513:GLU:HG3	1:BBB:524:SER:HB2	2.01	0.42
1:CCC:241:GLN:O	1:CCC:245[A]:VAL:HG22	2.19	0.42
4:AAA:621:GOL:H2	7:AAA:1214:HOH:O	2.19	0.42
1:DDD:486:GLY:HA3	6:DDD:616:CL:CL	2.57	0.42
1:AAA:142:GLN:HG2	1:AAA:398:TYR:CD1	2.54	0.42
1:BBB:483:TYR:HA	1:BBB:484:GLY:HA2	1.92	0.42
1:CCC:102[B]:ASP:OD1	1:CCC:104:GLU:N	2.49	0.42
1:CCC:305:ASP:O	1:CCC:306:ALA:HB3	2.20	0.41
1:DDD:238:TYR:CD1	1:DDD:238:TYR:C	2.98	0.41
1:AAA:293:PHE:CG	1:AAA:474:ALA:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:321:LEU:O	1:AAA:322:ILE:C	2.63	0.41
4:BBB:615:GOL:H11	7:BBB:716:HOH:O	2.21	0.41
1:BBB:261:VAL:HG11	4:BBB:622:GOL:H32	2.01	0.41
1:AAA:56[A]:ILE:HD11	1:AAA:432:GLU:CD	2.45	0.41
1:AAA:448:GLU:OE2	1:AAA:465:PRO:HB3	2.21	0.41
1:CCC:5:ALA:CB	4:CCC:614:GOL:H32	2.51	0.41
1:CCC:63:LEU:O	1:CCC:65:HIS:CE1	2.74	0.41
1:CCC:142:GLN:HG2	1:CCC:398:TYR:CD1	2.56	0.41
1:DDD:305:ASP:O	1:DDD:306:ALA:HB3	2.21	0.41
1:AAA:98:GLY:HA2	1:AAA:305:ASP:O	2.21	0.41
1:AAA:238:TYR:CD1	1:AAA:238:TYR:C	2.99	0.41
1:BBB:276:GLY:H	4:BBB:601:GOL:C3	2.33	0.40
1:CCC:238:TYR:CD1	1:CCC:238:TYR:C	2.99	0.40
1:BBB:142:GLN:HG2	1:BBB:398:TYR:CD1	2.56	0.40
1:CCC:293:PHE:CG	1:CCC:474:ALA:HA	2.56	0.40
1:CCC:430:PHE:CE1	4:CCC:606:GOL:H32	2.56	0.40
1:DDD:47:ASP:HA	1:DDD:48:PRO:HD3	1.87	0.40
1:DDD:321:LEU:O	1:DDD:322:ILE:C	2.64	0.40
1:AAA:51:THR:HB	1:CCC:506:ILE:CD1	2.52	0.40
1:CCC:510[B]:GLN:HG3	7:CCC:1272:HOH:O	2.20	0.40
7:AAA:1388:HOH:O	1:DDD:90:LYS:HB2	2.22	0.40
1:BBB:238:TYR:CD1	1:BBB:238:TYR:C	3.00	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AAA:807:HOH:O	7:DDD:1043:HOH:O[3_565]	2.16	0.04
7:CCC:919:HOH:O	7:CCC:919:HOH:O[2_665]	2.19	0.01

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	AAA	623/598 (104%)	611 (98%)	12 (2%)	0	100	100
1	BBB	622/598 (104%)	613 (99%)	9 (1%)	0	100	100
1	CCC	626/598 (105%)	615 (98%)	11 (2%)	0	100	100
1	DDD	627/598 (105%)	614 (98%)	12 (2%)	1 (0%)	43	42
All	All	2498/2392 (104%)	2453 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	373	PHE

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	AAA	517/491 (105%)	511 (99%)	6 (1%)	63	70
1	BBB	516/491 (105%)	512 (99%)	4 (1%)	73	80
1	CCC	520/491 (106%)	513 (99%)	7 (1%)	61	68
1	DDD	521/491 (106%)	515 (99%)	6 (1%)	63	70
All	All	2074/1964 (106%)	2051 (99%)	23 (1%)	73	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	86[A]	SER
1	AAA	86[B]	SER
1	AAA	86[C]	SER
1	AAA	338	TYR
1	AAA	370	GLN
1	AAA	479	PHE
1	BBB	86[A]	SER
1	BBB	86[B]	SER
1	BBB	338	TYR
1	BBB	479	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CCC	86[A]	SER
1	CCC	86[B]	SER
1	CCC	360	PRO
1	CCC	370	GLN
1	CCC	479	PHE
1	CCC	508[A]	ILE
1	CCC	508[B]	ILE
1	DDD	86[A]	SER
1	DDD	86[B]	SER
1	DDD	205[A]	LYS
1	DDD	205[B]	LYS
1	DDD	338	TYR
1	DDD	479	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 99 ligands modelled in this entry, 25 are monoatomic - leaving 74 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	PO4	CCC	601	-	4,4,4	0.96	0	6,6,6	0.67	0
4	GOL	BBB	612	-	5,5,5	0.24	0	5,5,5	0.65	0
4	GOL	BBB	616	-	5,5,5	0.08	0	5,5,5	0.49	0
4	GOL	CCC	604	-	5,5,5	0.29	0	5,5,5	0.24	0
4	GOL	CCC	611	-	5,5,5	0.20	0	5,5,5	0.67	0
4	GOL	DDD	607	-	5,5,5	0.26	0	5,5,5	0.44	0
4	GOL	CCC	613	-	5,5,5	0.66	0	5,5,5	1.46	1 (20%)
4	GOL	AAA	615	-	5,5,5	0.58	0	5,5,5	1.00	0
2	PO4	BBB	603	-	4,4,4	1.09	0	6,6,6	1.18	0
4	GOL	BBB	622	-	5,5,5	0.18	0	5,5,5	0.58	0
4	GOL	CCC	615	-	5,5,5	0.36	0	5,5,5	0.97	0
4	GOL	DDD	611	-	5,5,5	0.29	0	5,5,5	0.60	0
4	GOL	BBB	617	-	5,5,5	0.12	0	5,5,5	0.54	0
2	PO4	AAA	622	-	4,4,4	2.27	1 (25%)	6,6,6	0.80	0
4	GOL	AAA	609	-	5,5,5	0.21	0	5,5,5	0.47	0
4	GOL	CCC	607	-	5,5,5	0.15	0	5,5,5	0.43	0
4	GOL	BBB	618	-	5,5,5	0.23	0	5,5,5	0.72	0
4	GOL	CCC	608	-	5,5,5	0.26	0	5,5,5	0.41	0
4	GOL	DDD	606	5	5,5,5	0.45	0	5,5,5	0.52	0
4	GOL	AAA	620	-	5,5,5	0.24	0	5,5,5	0.59	0
4	GOL	DDD	614	-	5,5,5	0.31	0	5,5,5	0.58	0
2	PO4	DDD	602	-	4,4,4	2.24	2 (50%)	6,6,6	0.93	0
4	GOL	DDD	610	-	5,5,5	0.17	0	5,5,5	0.34	0
4	GOL	CCC	614	-	5,5,5	0.22	0	5,5,5	0.88	0
4	GOL	BBB	620	-	5,5,5	0.10	0	5,5,5	0.29	0
4	GOL	CCC	606	-	5,5,5	0.24	0	5,5,5	0.19	0
4	GOL	AAA	612	-	5,5,5	0.14	0	5,5,5	0.22	0
4	GOL	DDD	608	-	5,5,5	0.17	0	5,5,5	0.34	0
4	GOL	BBB	613	-	5,5,5	0.25	0	5,5,5	0.49	0
4	GOL	BBB	615	-	5,5,5	0.16	0	5,5,5	0.90	0
4	GOL	AAA	610	-	5,5,5	0.17	0	5,5,5	0.38	0
4	GOL	DDD	613	-	5,5,5	0.22	0	5,5,5	0.54	0
4	GOL	CCC	616	-	5,5,5	0.12	0	5,5,5	0.53	0
4	GOL	DDD	601	-	5,5,5	0.18	0	5,5,5	0.34	0
4	GOL	AAA	605	5	5,5,5	0.41	0	5,5,5	0.79	0
4	GOL	BBB	610	-	5,5,5	0.27	0	5,5,5	0.49	0
2	PO4	CCC	603	-	4,4,4	0.89	0	6,6,6	0.48	0
4	GOL	DDD	612	-	5,5,5	0.36	0	5,5,5	0.86	0
4	GOL	AAA	613	-	5,5,5	0.15	0	5,5,5	0.21	0
4	GOL	AAA	619	-	5,5,5	0.16	0	5,5,5	0.66	0
4	GOL	BBB	606	-	5,5,5	0.12	0	5,5,5	0.27	0
4	GOL	CCC	612	-	5,5,5	0.34	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	BBB	608	-	5,5,5	0.16	0	5,5,5	0.53	0
4	GOL	BBB	601	-	5,5,5	0.17	0	5,5,5	0.69	0
4	GOL	AAA	618	5	5,5,5	0.22	0	5,5,5	0.47	0
4	GOL	AAA	611	-	5,5,5	0.26	0	5,5,5	0.64	0
4	GOL	BBB	619	-	5,5,5	0.16	0	5,5,5	0.52	0
2	PO4	AAA	603	-	4,4,4	2.15	2 (50%)	6,6,6	0.70	0
4	GOL	BBB	602	-	5,5,5	0.30	0	5,5,5	0.74	0
2	PO4	AAA	601	-	4,4,4	0.65	0	6,6,6	1.11	1 (16%)
4	GOL	CCC	617	-	5,5,5	0.27	0	5,5,5	0.70	0
4	GOL	AAA	607	-	5,5,5	0.22	0	5,5,5	0.59	0
2	PO4	BBB	605	-	4,4,4	1.97	1 (25%)	6,6,6	1.06	1 (16%)
4	GOL	AAA	604	-	5,5,5	0.43	0	5,5,5	0.56	0
4	GOL	BBB	607	5	5,5,5	0.42	0	5,5,5	0.53	0
4	GOL	CCC	609	-	5,5,5	0.29	0	5,5,5	0.63	0
4	GOL	CCC	618	-	5,5,5	0.17	0	5,5,5	0.34	0
2	PO4	DDD	604	-	4,4,4	1.60	1 (25%)	6,6,6	0.89	0
4	GOL	AAA	614	-	5,5,5	0.31	0	5,5,5	0.48	0
4	GOL	AAA	606	-	5,5,5	0.39	0	5,5,5	1.40	1 (20%)
4	GOL	AAA	617	-	5,5,5	0.22	0	5,5,5	0.60	0
4	GOL	AAA	608	-	5,5,5	0.20	0	5,5,5	0.62	0
4	GOL	BBB	611	-	5,5,5	0.25	0	5,5,5	0.78	0
4	GOL	DDD	609	-	5,5,5	0.11	0	5,5,5	0.27	0
4	GOL	BBB	614	-	5,5,5	0.19	0	5,5,5	0.71	0
4	GOL	AAA	621	-	5,5,5	0.27	0	5,5,5	0.73	0
4	GOL	BBB	621	-	5,5,5	0.29	0	5,5,5	0.76	0
4	GOL	CCC	610	-	5,5,5	0.19	0	5,5,5	0.50	0
4	GOL	CCC	619	-	5,5,5	0.12	0	5,5,5	0.22	0
4	GOL	CCC	605	5	5,5,5	0.40	0	5,5,5	0.44	0
4	GOL	DDD	605	-	5,5,5	0.24	0	5,5,5	0.49	0
4	GOL	BBB	609	-	5,5,5	0.27	0	5,5,5	0.46	0
4	GOL	CCC	620	-	5,5,5	0.21	0	5,5,5	0.55	0
4	GOL	AAA	616	-	5,5,5	0.15	0	5,5,5	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	BBB	612	-	-	0/4/4/4	-
4	GOL	BBB	616	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	CCC	604	-	-	0/4/4/4	-
4	GOL	CCC	611	-	-	2/4/4/4	-
4	GOL	DDD	607	-	-	2/4/4/4	-
4	GOL	CCC	613	-	-	2/4/4/4	-
4	GOL	AAA	615	-	-	0/4/4/4	-
4	GOL	BBB	622	-	-	4/4/4/4	-
4	GOL	CCC	615	-	-	0/4/4/4	-
4	GOL	DDD	611	-	-	0/4/4/4	-
4	GOL	BBB	617	-	-	4/4/4/4	-
4	GOL	CCC	608	-	-	1/4/4/4	-
4	GOL	AAA	609	-	-	0/4/4/4	-
4	GOL	CCC	607	-	-	0/4/4/4	-
4	GOL	BBB	618	-	-	2/4/4/4	-
4	GOL	DDD	606	5	-	0/4/4/4	-
4	GOL	DDD	614	-	-	2/4/4/4	-
4	GOL	AAA	620	-	-	2/4/4/4	-
4	GOL	DDD	610	-	-	0/4/4/4	-
4	GOL	CCC	614	-	-	2/4/4/4	-
4	GOL	BBB	620	-	-	1/4/4/4	-
4	GOL	CCC	606	-	-	2/4/4/4	-
4	GOL	AAA	612	-	-	2/4/4/4	-
4	GOL	DDD	608	-	-	4/4/4/4	-
4	GOL	BBB	613	-	-	1/4/4/4	-
4	GOL	BBB	615	-	-	2/4/4/4	-
4	GOL	AAA	610	-	-	0/4/4/4	-
4	GOL	DDD	613	-	-	1/4/4/4	-
4	GOL	CCC	616	-	-	0/4/4/4	-
4	GOL	DDD	601	-	-	2/4/4/4	-
4	GOL	AAA	605	5	-	0/4/4/4	-
4	GOL	BBB	610	-	-	0/4/4/4	-
4	GOL	DDD	612	-	-	2/4/4/4	-
4	GOL	AAA	613	-	-	2/4/4/4	-
4	GOL	AAA	619	-	-	2/4/4/4	-
4	GOL	BBB	606	-	-	0/4/4/4	-
4	GOL	CCC	612	-	-	3/4/4/4	-
4	GOL	BBB	608	-	-	2/4/4/4	-
4	GOL	BBB	601	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	AAA	618	5	-	2/4/4/4	-
4	GOL	AAA	611	-	-	2/4/4/4	-
4	GOL	BBB	619	-	-	2/4/4/4	-
4	GOL	BBB	602	-	-	4/4/4/4	-
4	GOL	CCC	617	-	-	2/4/4/4	-
4	GOL	AAA	607	-	-	2/4/4/4	-
4	GOL	AAA	604	-	-	0/4/4/4	-
4	GOL	BBB	607	5	-	0/4/4/4	-
4	GOL	CCC	609	-	-	2/4/4/4	-
4	GOL	CCC	618	-	-	2/4/4/4	-
4	GOL	AAA	614	-	-	3/4/4/4	-
4	GOL	AAA	606	-	-	4/4/4/4	-
4	GOL	AAA	617	-	-	4/4/4/4	-
4	GOL	AAA	608	-	-	0/4/4/4	-
4	GOL	BBB	611	-	-	3/4/4/4	-
4	GOL	DDD	609	-	-	3/4/4/4	-
4	GOL	BBB	614	-	-	1/4/4/4	-
4	GOL	AAA	621	-	-	2/4/4/4	-
4	GOL	BBB	621	-	-	4/4/4/4	-
4	GOL	CCC	610	-	-	2/4/4/4	-
4	GOL	CCC	619	-	-	1/4/4/4	-
4	GOL	CCC	605	5	-	0/4/4/4	-
4	GOL	DDD	605	-	-	0/4/4/4	-
4	GOL	BBB	609	-	-	2/4/4/4	-
4	GOL	CCC	620	-	-	0/4/4/4	-
4	GOL	AAA	616	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	622	PO4	P-O1	4.14	1.60	1.50
2	BBB	605	PO4	P-O3	3.50	1.64	1.54
2	DDD	602	PO4	P-O1	3.44	1.58	1.50
2	AAA	603	PO4	P-O4	-2.85	1.46	1.54
2	DDD	604	PO4	P-O4	-2.39	1.47	1.54
2	DDD	602	PO4	P-O2	-2.37	1.47	1.54
2	AAA	603	PO4	P-O3	-2.31	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	CCC	613	GOL	O1-C1-C2	2.53	121.78	110.38
4	AAA	606	GOL	O2-C2-C3	-2.34	99.50	109.18
2	BBB	605	PO4	O4-P-O1	-2.22	103.09	110.95
2	AAA	601	PO4	O3-P-O2	2.15	114.61	107.91

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	606	GOL	O1-C1-C2-C3
4	AAA	611	GOL	O1-C1-C2-C3
4	AAA	612	GOL	C1-C2-C3-O3
4	AAA	613	GOL	C1-C2-C3-O3
4	AAA	614	GOL	C1-C2-C3-O3
4	AAA	614	GOL	O2-C2-C3-O3
4	AAA	616	GOL	O1-C1-C2-C3
4	AAA	617	GOL	C1-C2-C3-O3
4	AAA	617	GOL	O2-C2-C3-O3
4	AAA	618	GOL	C1-C2-C3-O3
4	AAA	618	GOL	O2-C2-C3-O3
4	BBB	601	GOL	O1-C1-C2-C3
4	BBB	602	GOL	C1-C2-C3-O3
4	BBB	609	GOL	O1-C1-C2-C3
4	BBB	611	GOL	C1-C2-C3-O3
4	BBB	615	GOL	C1-C2-C3-O3
4	BBB	616	GOL	O1-C1-C2-C3
4	BBB	617	GOL	C1-C2-C3-O3
4	BBB	618	GOL	O1-C1-C2-O2
4	BBB	618	GOL	O1-C1-C2-C3
4	BBB	619	GOL	C1-C2-C3-O3
4	BBB	619	GOL	O2-C2-C3-O3
4	BBB	621	GOL	C1-C2-C3-O3
4	BBB	622	GOL	C1-C2-C3-O3
4	CCC	606	GOL	O1-C1-C2-C3
4	CCC	609	GOL	O1-C1-C2-C3
4	CCC	611	GOL	C1-C2-C3-O3
4	CCC	611	GOL	O2-C2-C3-O3
4	CCC	612	GOL	C1-C2-C3-O3
4	CCC	617	GOL	O1-C1-C2-C3
4	DDD	601	GOL	C1-C2-C3-O3
4	DDD	607	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	DDD	609	GOL	O2-C2-C3-O3
4	AAA	613	GOL	O2-C2-C3-O3
4	BBB	622	GOL	O2-C2-C3-O3
4	CCC	609	GOL	O1-C1-C2-O2
4	CCC	614	GOL	O2-C2-C3-O3
4	DDD	607	GOL	O1-C1-C2-O2
4	AAA	606	GOL	C1-C2-C3-O3
4	AAA	614	GOL	O1-C1-C2-C3
4	AAA	616	GOL	C1-C2-C3-O3
4	AAA	617	GOL	O1-C1-C2-C3
4	AAA	619	GOL	C1-C2-C3-O3
4	AAA	620	GOL	O1-C1-C2-C3
4	AAA	621	GOL	O1-C1-C2-C3
4	BBB	602	GOL	O1-C1-C2-C3
4	BBB	608	GOL	O1-C1-C2-C3
4	BBB	608	GOL	C1-C2-C3-O3
4	BBB	617	GOL	O1-C1-C2-C3
4	BBB	620	GOL	C1-C2-C3-O3
4	BBB	621	GOL	O1-C1-C2-C3
4	BBB	622	GOL	O1-C1-C2-C3
4	CCC	613	GOL	C1-C2-C3-O3
4	CCC	614	GOL	C1-C2-C3-O3
4	DDD	608	GOL	O1-C1-C2-C3
4	DDD	608	GOL	C1-C2-C3-O3
4	DDD	609	GOL	C1-C2-C3-O3
4	DDD	612	GOL	C1-C2-C3-O3
4	AAA	611	GOL	O1-C1-C2-O2
4	AAA	617	GOL	O1-C1-C2-O2
4	AAA	621	GOL	O1-C1-C2-O2
4	BBB	602	GOL	O1-C1-C2-O2
4	BBB	602	GOL	O2-C2-C3-O3
4	BBB	609	GOL	O1-C1-C2-O2
4	BBB	611	GOL	O2-C2-C3-O3
4	BBB	615	GOL	O2-C2-C3-O3
4	BBB	616	GOL	O1-C1-C2-O2
4	BBB	621	GOL	O2-C2-C3-O3
4	BBB	622	GOL	O1-C1-C2-O2
4	CCC	606	GOL	O1-C1-C2-O2
4	CCC	612	GOL	O2-C2-C3-O3
4	DDD	601	GOL	O2-C2-C3-O3
4	AAA	606	GOL	O1-C1-C2-O2
4	AAA	606	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	AAA	612	GOL	O2-C2-C3-O3
4	AAA	616	GOL	O1-C1-C2-O2
4	AAA	616	GOL	O2-C2-C3-O3
4	AAA	620	GOL	O1-C1-C2-O2
4	BBB	601	GOL	O1-C1-C2-O2
4	CCC	612	GOL	O1-C1-C2-O2
4	CCC	617	GOL	O1-C1-C2-O2
4	AAA	619	GOL	O2-C2-C3-O3
4	BBB	617	GOL	O2-C2-C3-O3
4	CCC	613	GOL	O2-C2-C3-O3
4	BBB	611	GOL	O1-C1-C2-O2
4	BBB	613	GOL	O1-C1-C2-O2
4	BBB	616	GOL	O2-C2-C3-O3
4	DDD	613	GOL	O2-C2-C3-O3
4	DDD	614	GOL	O1-C1-C2-O2
4	DDD	614	GOL	O2-C2-C3-O3
4	CCC	618	GOL	C1-C2-C3-O3
4	CCC	618	GOL	O2-C2-C3-O3
4	BBB	614	GOL	O1-C1-C2-O2
4	BBB	621	GOL	O1-C1-C2-O2
4	AAA	607	GOL	C1-C2-C3-O3
4	CCC	610	GOL	O1-C1-C2-C3
4	AAA	607	GOL	O2-C2-C3-O3
4	BBB	617	GOL	O1-C1-C2-O2
4	DDD	608	GOL	O1-C1-C2-O2
4	DDD	608	GOL	O2-C2-C3-O3
4	DDD	612	GOL	O2-C2-C3-O3
4	DDD	609	GOL	O1-C1-C2-C3
4	CCC	608	GOL	O1-C1-C2-O2
4	CCC	619	GOL	O2-C2-C3-O3
4	CCC	610	GOL	O1-C1-C2-O2

There are no ring outliers.

34 monomers are involved in 88 short contacts:

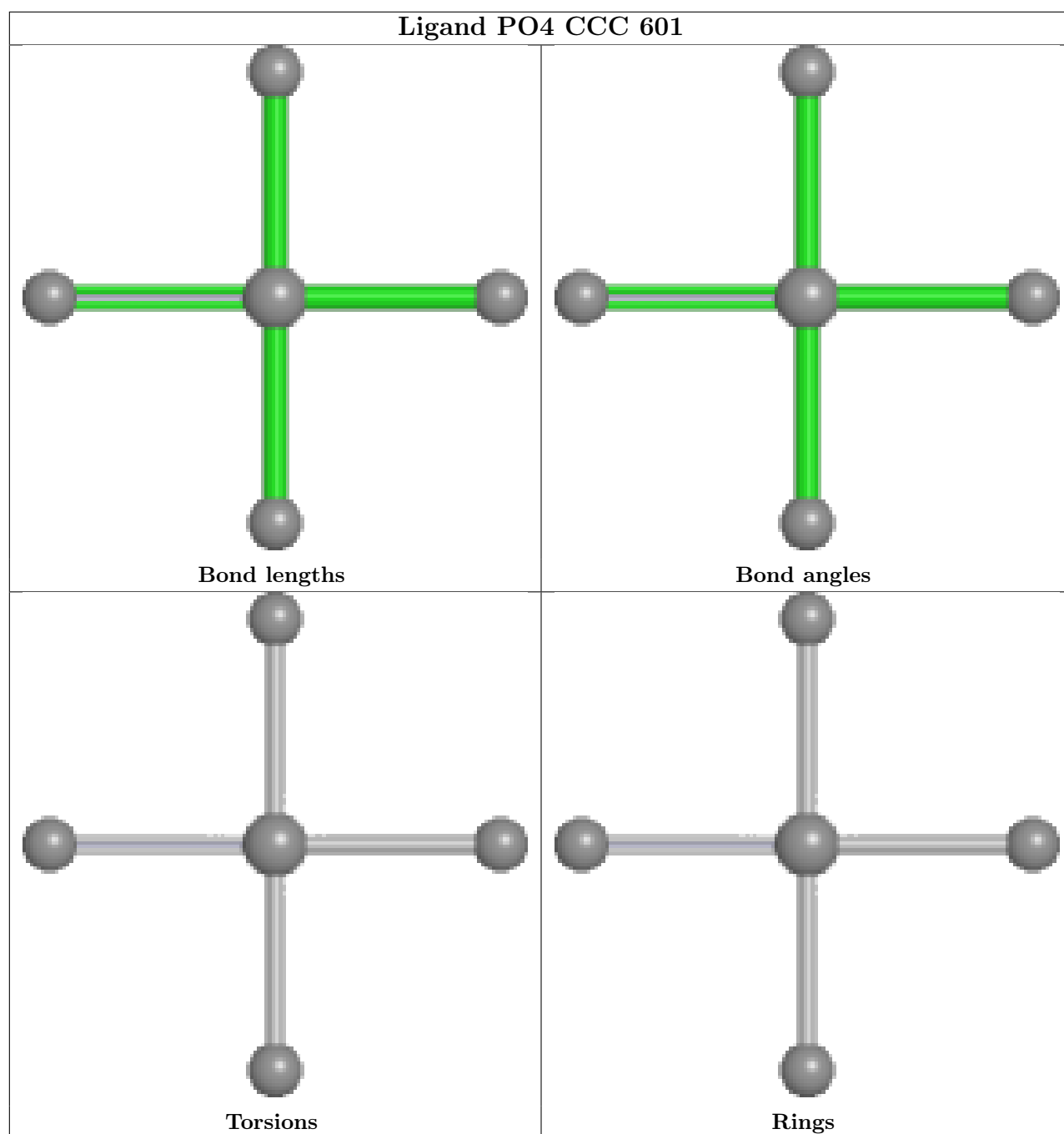
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	616	GOL	1	0
4	CCC	611	GOL	1	0
4	DDD	607	GOL	1	0
4	CCC	613	GOL	6	0
4	AAA	615	GOL	8	0
4	BBB	622	GOL	4	0

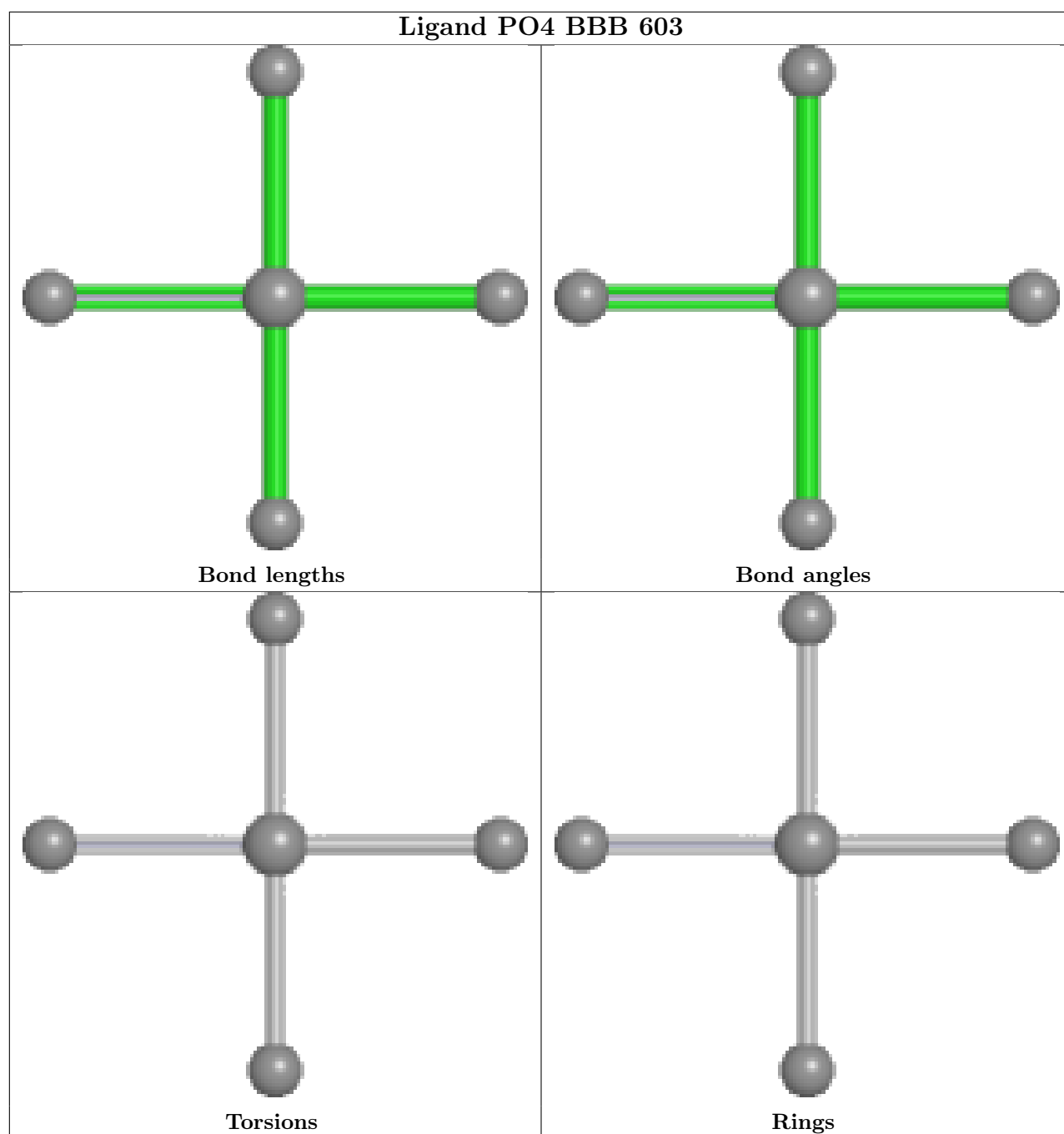
Continued on next page...

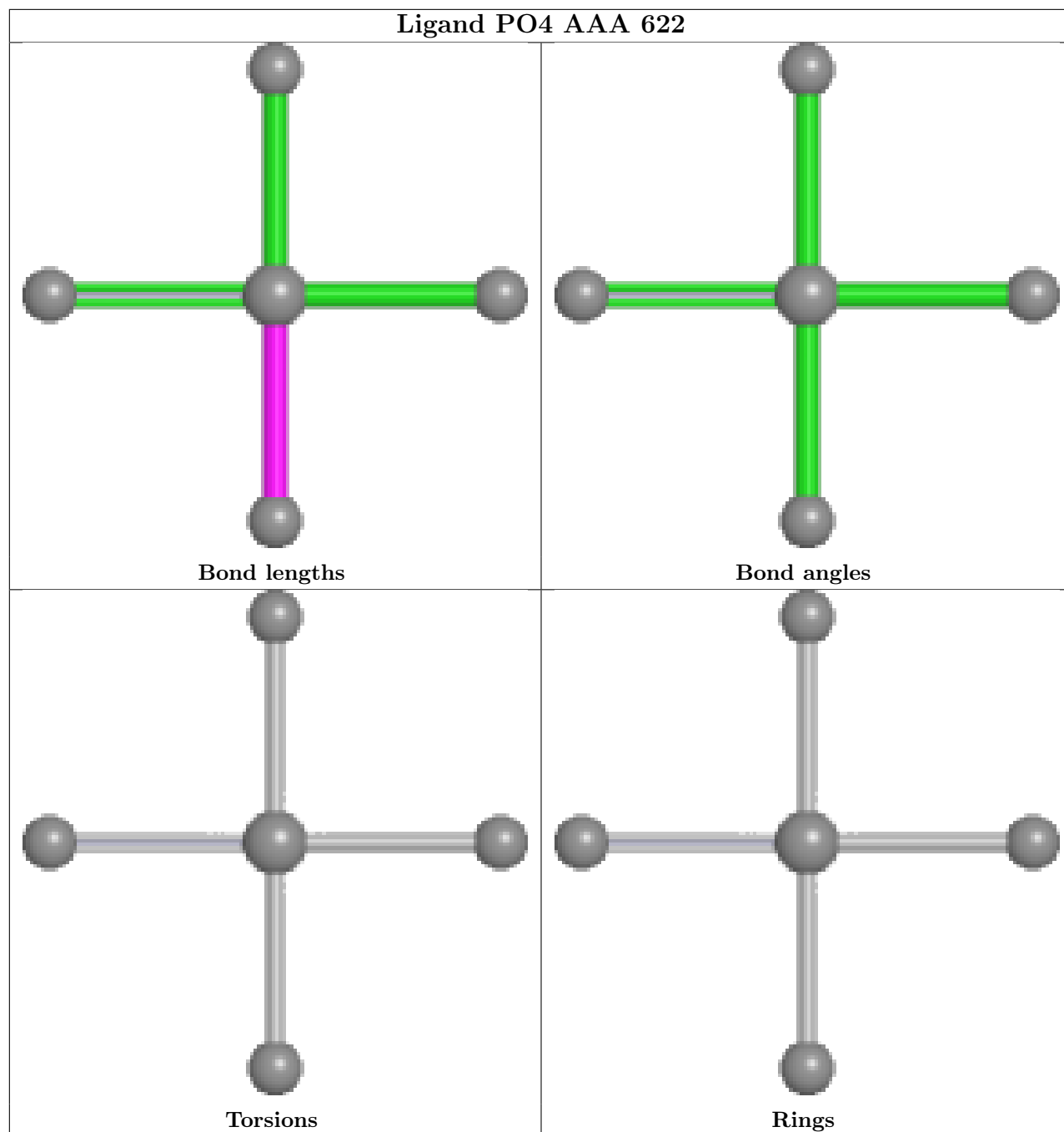
Continued from previous page...

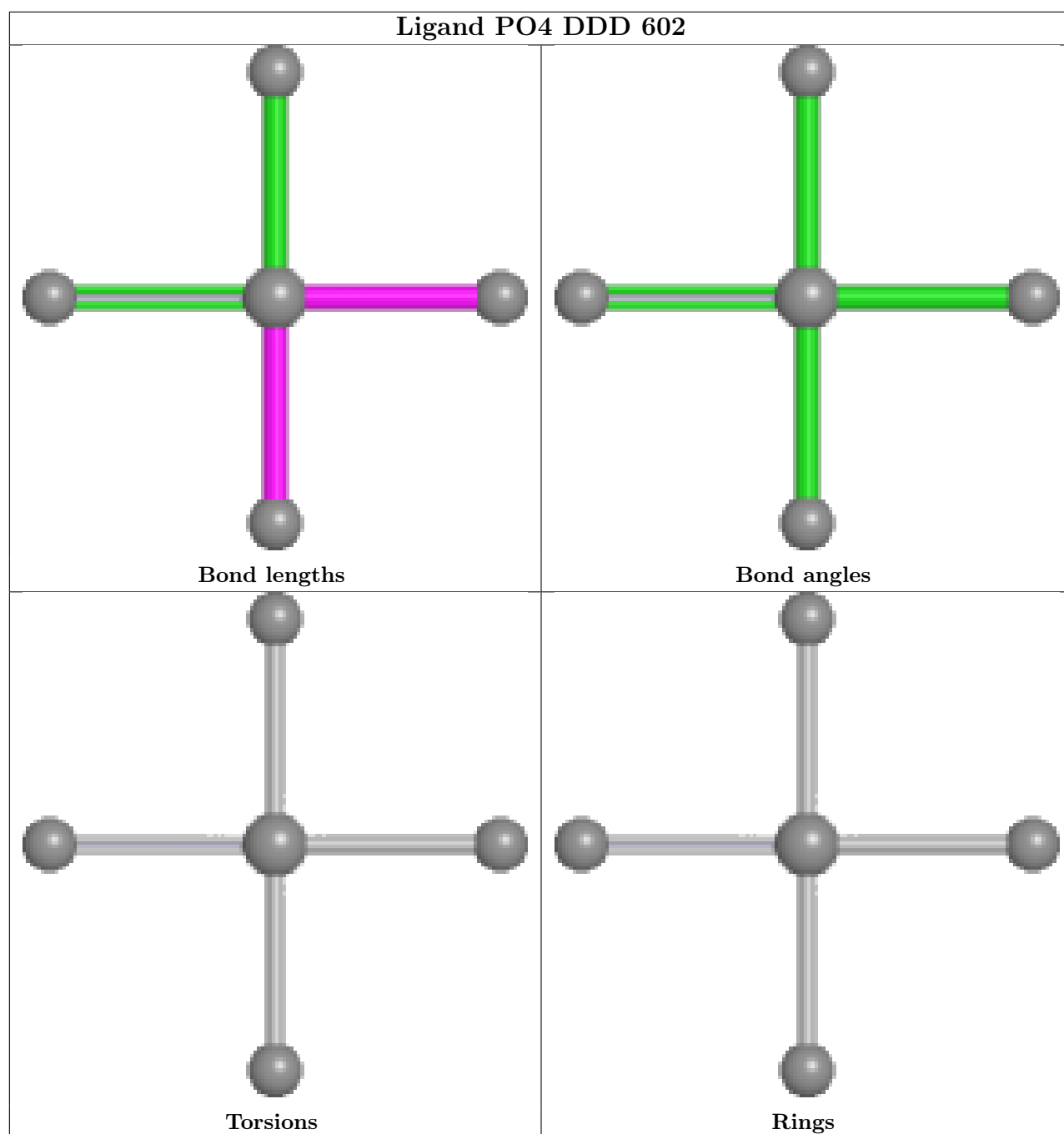
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	615	GOL	4	0
4	BBB	617	GOL	1	0
4	CCC	607	GOL	1	0
4	BBB	618	GOL	1	0
4	CCC	608	GOL	1	0
4	DDD	606	GOL	1	0
4	AAA	620	GOL	1	0
4	CCC	614	GOL	1	0
4	BBB	620	GOL	1	0
4	CCC	606	GOL	5	0
4	AAA	612	GOL	1	0
4	BBB	615	GOL	1	0
4	DDD	613	GOL	1	0
4	CCC	616	GOL	5	0
4	AAA	613	GOL	8	0
4	AAA	619	GOL	4	0
4	BBB	601	GOL	1	0
4	AAA	618	GOL	1	0
4	BBB	619	GOL	4	0
4	BBB	602	GOL	4	0
4	AAA	606	GOL	3	0
4	BBB	611	GOL	3	0
4	DDD	609	GOL	1	0
4	BBB	614	GOL	5	0
4	AAA	621	GOL	2	0
4	BBB	621	GOL	5	0
4	CCC	619	GOL	1	0
4	BBB	609	GOL	1	0

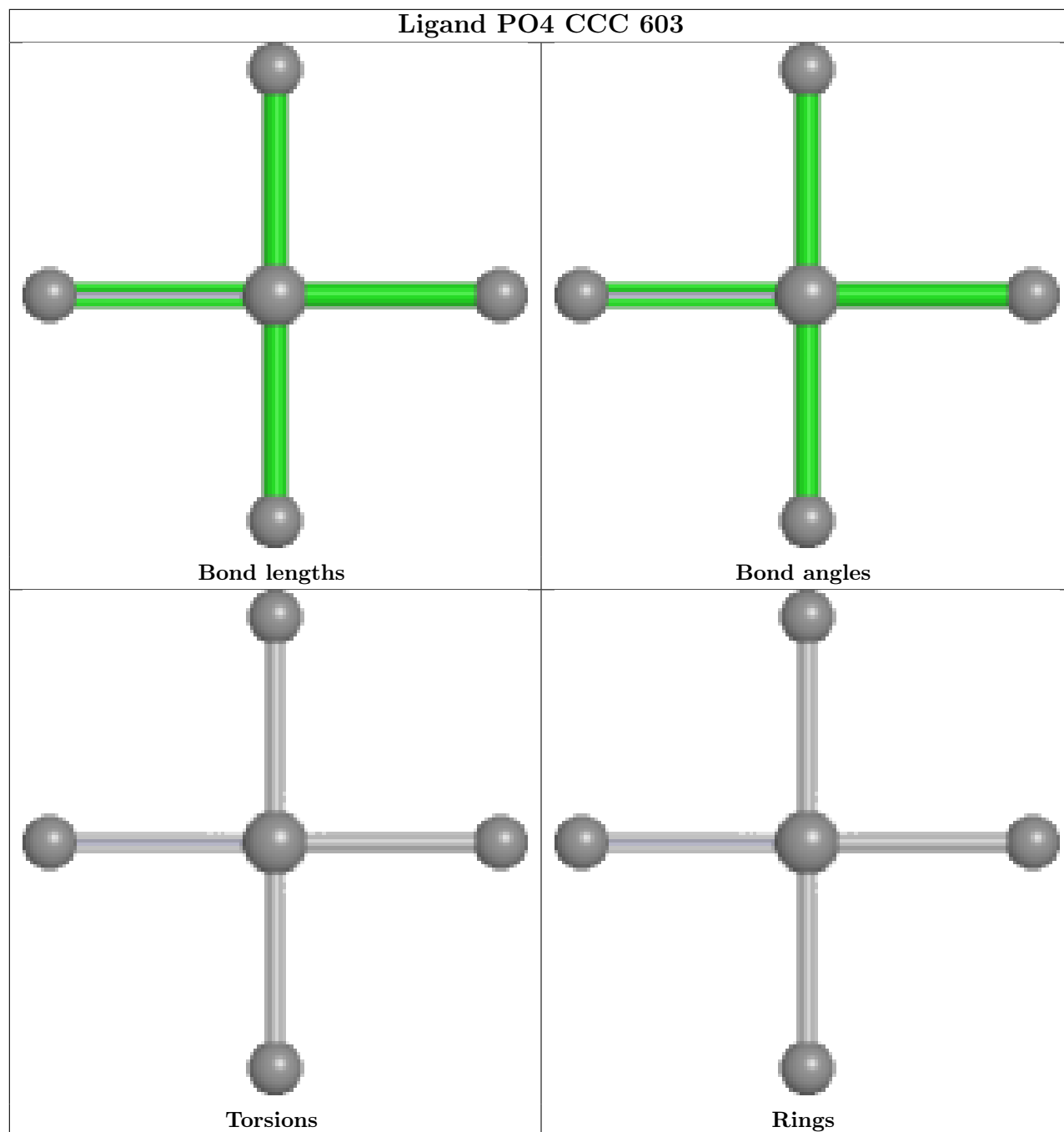
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

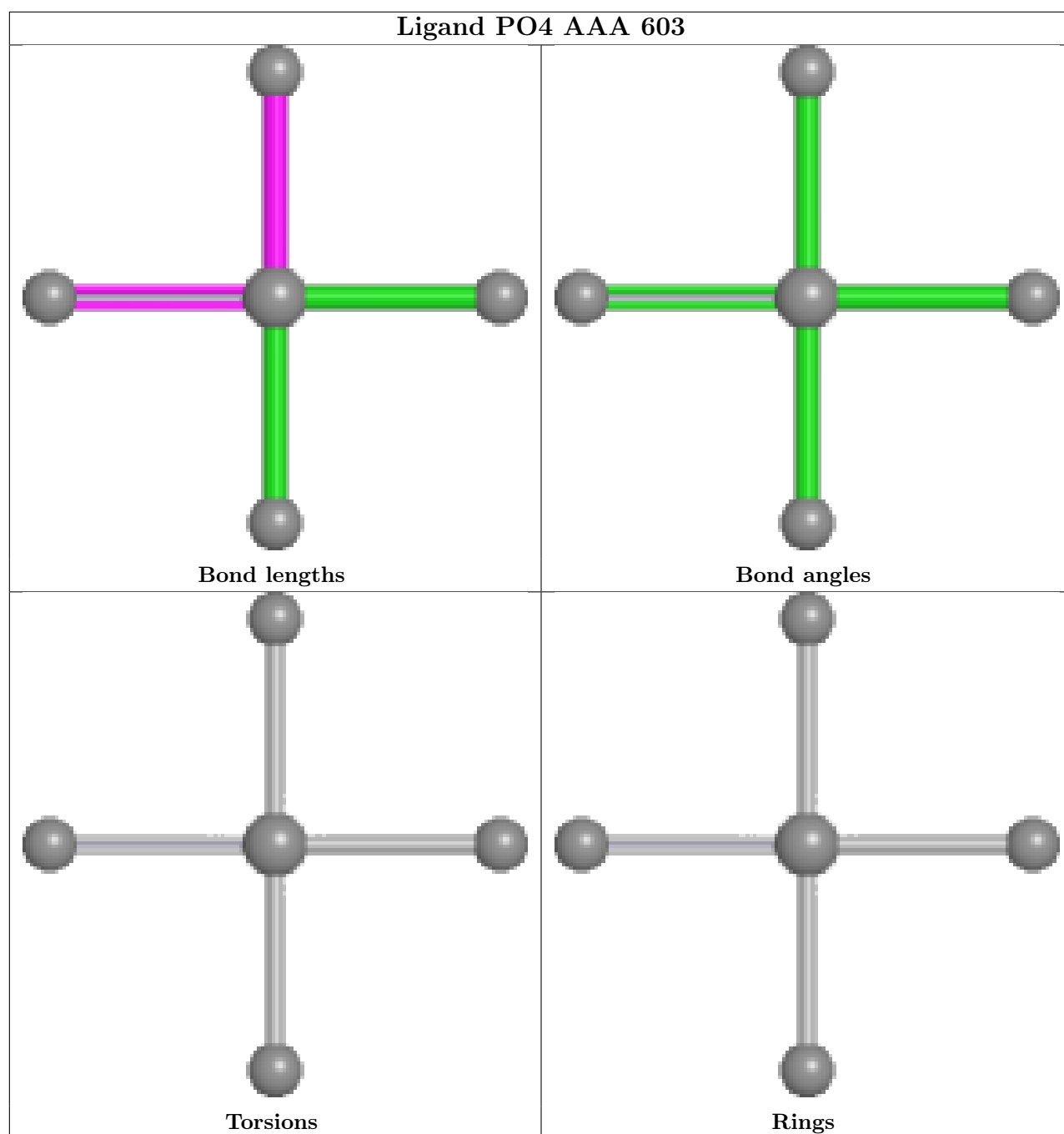


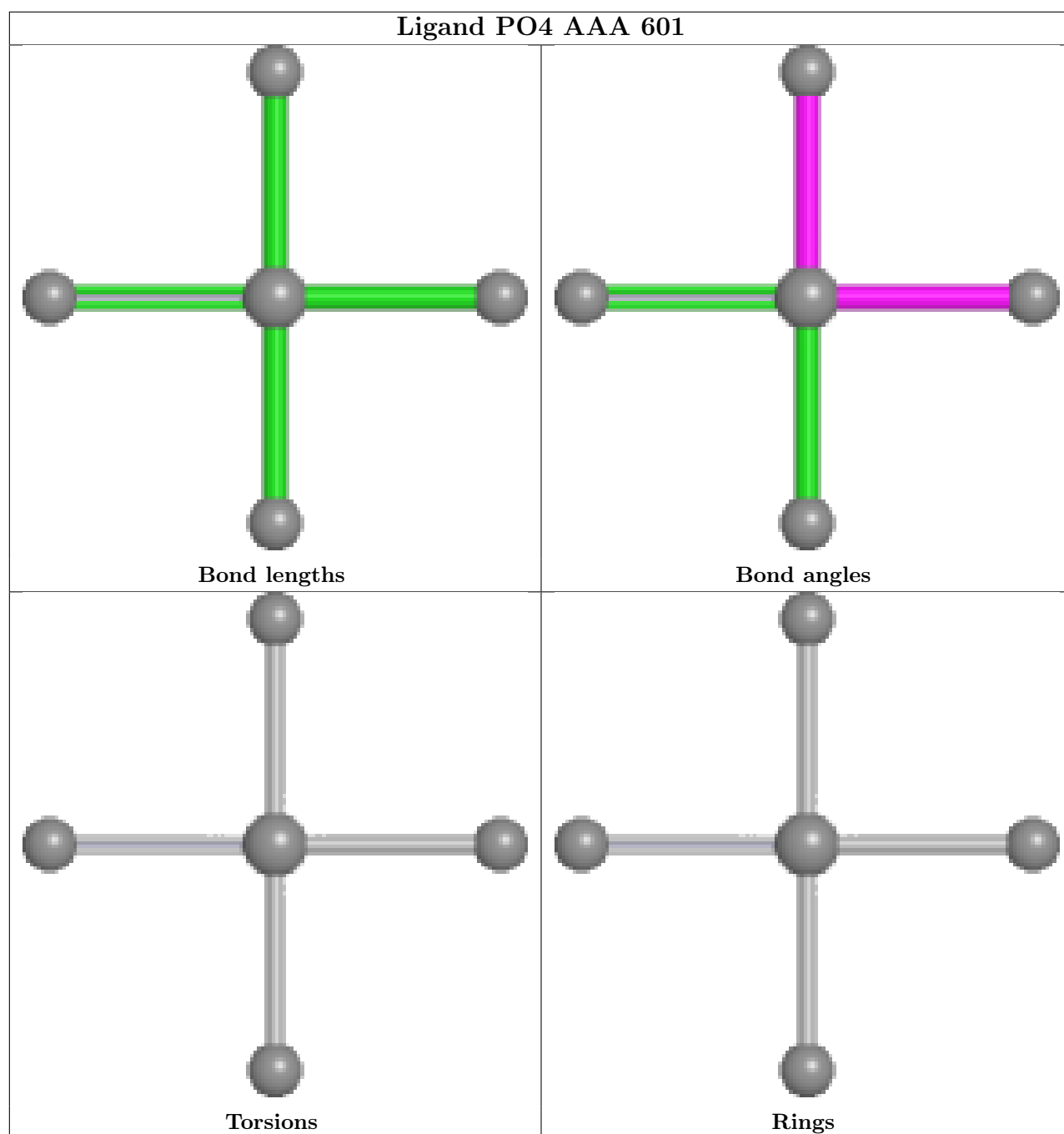


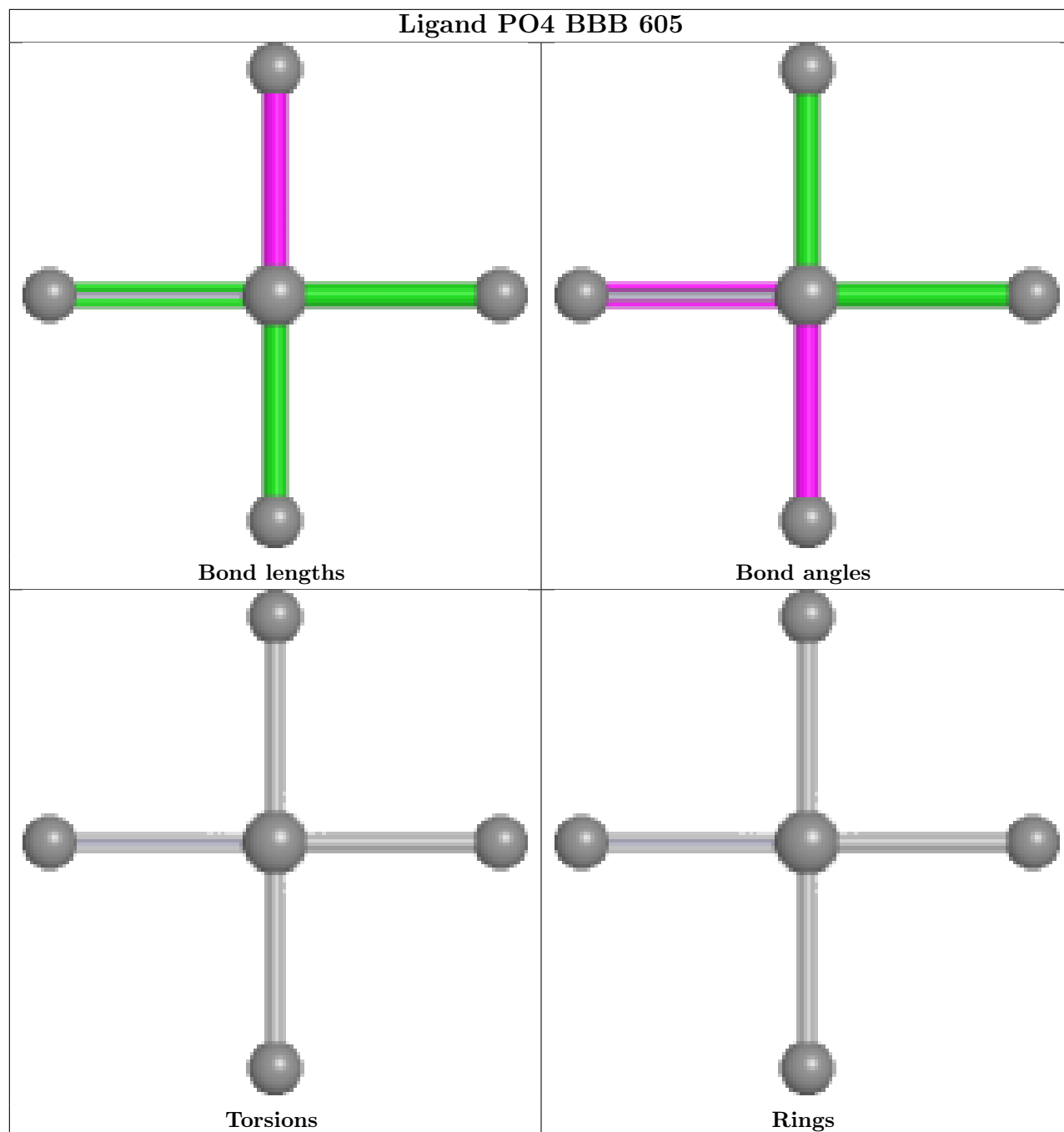


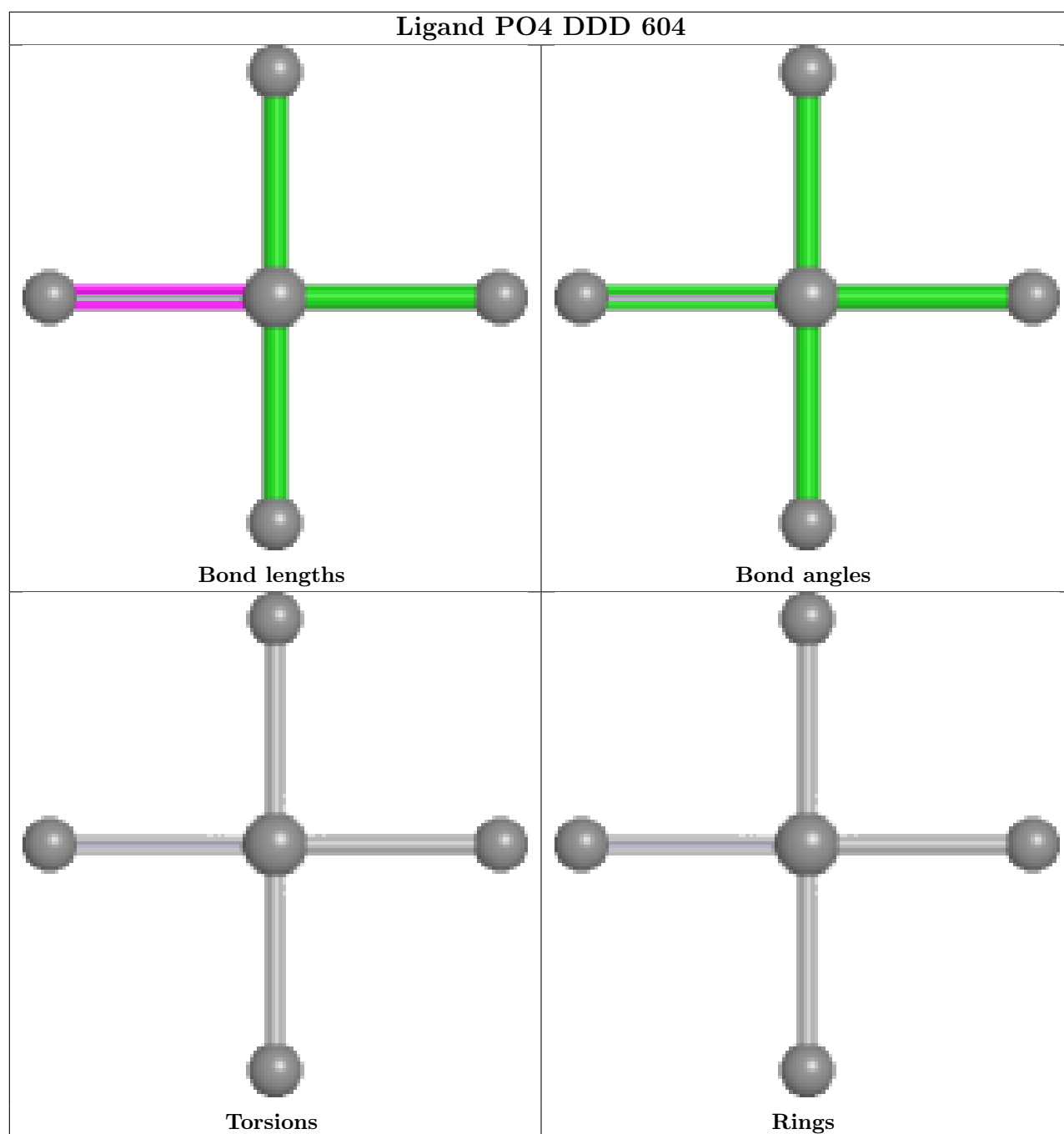












5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	597/598 (99%)	-0.73	2 (0%) 90 89	9, 19, 36, 93	27 (4%)
1	BBB	597/598 (99%)	-0.77	1 (0%) 91 90	10, 19, 34, 78	27 (4%)
1	CCC	597/598 (99%)	-0.80	2 (0%) 90 89	9, 18, 31, 104	31 (5%)
1	DDD	597/598 (99%)	-0.75	2 (0%) 90 89	9, 19, 35, 91	32 (5%)
All	All	2388/2392 (99%)	-0.76	7 (0%) 90 89	9, 19, 34, 104	117 (4%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	48	PRO	4.6
1	BBB	48	PRO	3.7
1	AAA	48	PRO	3.4
1	CCC	527[A]	LYS	3.3
1	DDD	48	PRO	3.3
1	AAA	527[A]	LYS	2.8
1	DDD	49[A]	ASP	2.4

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 ⓘ

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
4	GOL	AAA	617	6/6	0.72	0.21	23,27,35,40	6
4	GOL	BBB	620	6/6	0.72	0.17	32,38,42,56	6
4	GOL	CCC	617	6/6	0.75	0.18	13,24,29,35	6
4	GOL	AAA	614	6/6	0.80	0.18	31,54,75,76	0
4	GOL	BBB	615	6/6	0.80	0.18	37,74,90,92	0
4	GOL	CCC	618	6/6	0.80	0.15	28,48,57,77	6
4	GOL	CCC	613	6/6	0.81	0.17	28,38,54,57	0
4	GOL	BBB	602	6/6	0.83	0.23	18,25,45,50	6
4	GOL	BBB	616	6/6	0.83	0.17	26,37,58,63	6
4	GOL	CCC	612	6/6	0.84	0.14	30,51,64,71	0
4	GOL	BBB	613	6/6	0.84	0.15	25,46,57,68	0
4	GOL	BBB	601	6/6	0.84	0.13	43,46,62,80	0
4	GOL	BBB	621	6/6	0.84	0.15	26,31,46,59	6
4	GOL	CCC	616	6/6	0.85	0.20	26,43,61,66	6
2	PO4	AAA	622	5/5	0.86	0.15	40,43,60,84	0
4	GOL	AAA	616	6/6	0.86	0.17	31,41,44,49	6
4	GOL	CCC	615	6/6	0.86	0.14	22,31,37,47	6
4	GOL	BBB	618	6/6	0.87	0.17	21,34,47,47	6
5	NA	AAA	624	1/1	0.88	0.15	39,39,39,39	0
4	GOL	AAA	620	6/6	0.89	0.15	28,49,90,93	0
4	GOL	CCC	614	6/6	0.89	0.16	14,28,38,43	6
4	GOL	BBB	611	6/6	0.89	0.15	24,57,68,110	0
4	GOL	AAA	621	6/6	0.89	0.20	25,27,40,68	6
4	GOL	BBB	614	6/6	0.89	0.15	14,46,63,72	0
4	GOL	CCC	610	6/6	0.89	0.12	27,42,61,72	0
4	GOL	DDD	612	6/6	0.89	0.13	34,46,61,67	0
4	GOL	AAA	615	6/6	0.89	0.15	29,37,49,49	0
4	GOL	DDD	614	6/6	0.90	0.12	22,45,73,82	0
4	GOL	AAA	613	6/6	0.90	0.13	38,46,64,99	0
4	GOL	AAA	608	6/6	0.91	0.13	32,36,58,72	0
4	GOL	AAA	611	6/6	0.91	0.13	30,45,79,81	0
4	GOL	BBB	622	6/6	0.91	0.13	20,21,31,42	6
4	GOL	AAA	606	6/6	0.91	0.12	30,45,59,64	0
4	GOL	DDD	609	6/6	0.91	0.12	30,35,53,91	0
4	GOL	AAA	607	6/6	0.91	0.13	26,47,64,71	0
4	GOL	DDD	613	6/6	0.91	0.13	22,47,59,68	0
4	GOL	BBB	617	6/6	0.91	0.13	30,50,70,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	BBB	612	6/6	0.91	0.12	32,35,79,82	0
4	GOL	AAA	618	6/6	0.92	0.09	31,44,54,62	0
4	GOL	CCC	611	6/6	0.92	0.13	20,54,64,77	0
4	GOL	CCC	609	6/6	0.92	0.09	36,40,45,52	0
4	GOL	DDD	601	6/6	0.92	0.17	22,53,63,108	0
4	GOL	DDD	608	6/6	0.92	0.12	29,42,52,70	0
4	GOL	CCC	620	6/6	0.93	0.10	31,47,49,61	0
4	GOL	AAA	619	6/6	0.93	0.15	23,34,103,107	0
4	GOL	CCC	608	6/6	0.93	0.09	24,30,37,41	0
4	GOL	BBB	619	6/6	0.93	0.13	26,40,56,78	6
5	NA	CCC	621	1/1	0.93	0.10	36,36,36,36	0
4	GOL	DDD	611	6/6	0.94	0.07	27,33,54,56	0
4	GOL	CCC	619	6/6	0.94	0.09	34,50,58,71	0
4	GOL	CCC	607	6/6	0.94	0.12	24,45,61,82	0
4	GOL	AAA	612	6/6	0.94	0.10	22,58,63,69	0
4	GOL	BBB	609	6/6	0.94	0.13	29,35,54,100	0
4	GOL	BBB	610	6/6	0.94	0.09	28,32,42,55	0
4	GOL	AAA	610	6/6	0.95	0.07	22,35,52,56	0
4	GOL	DDD	610	6/6	0.95	0.08	25,35,43,51	0
4	GOL	DDD	607	6/6	0.95	0.08	27,38,60,65	0
4	GOL	BBB	608	6/6	0.95	0.13	25,45,65,82	0
5	NA	DDD	615	1/1	0.95	0.11	41,41,41,41	0
4	GOL	CCC	605	6/6	0.96	0.07	20,21,25,29	0
4	GOL	CCC	606	6/6	0.96	0.10	17,29,52,117	0
4	GOL	AAA	609	6/6	0.96	0.06	27,33,41,41	0
4	GOL	AAA	605	6/6	0.96	0.08	22,25,28,29	0
6	CL	BBB	627	1/1	0.96	0.12	41,41,41,41	0
6	CL	CCC	622	1/1	0.96	0.05	26,26,26,26	0
6	CL	DDD	616	1/1	0.96	0.06	31,31,31,31	0
2	PO4	DDD	604	5/5	0.97	0.08	33,37,38,65	0
4	GOL	DDD	606	6/6	0.97	0.06	18,21,25,28	0
4	GOL	AAA	604	6/6	0.97	0.06	22,24,25,27	0
6	CL	AAA	625	1/1	0.97	0.05	31,31,31,31	0
6	CL	BBB	624	1/1	0.97	0.04	30,30,30,30	0
2	PO4	BBB	605	5/5	0.97	0.07	26,30,39,39	0
2	PO4	CCC	603	5/5	0.97	0.08	36,37,46,49	0
5	NA	AAA	623	1/1	0.97	0.13	47,47,47,47	0
4	GOL	CCC	604	6/6	0.98	0.07	18,21,23,26	0
2	PO4	AAA	603	5/5	0.98	0.05	22,22,30,38	5
4	GOL	DDD	605	6/6	0.98	0.07	20,34,37,38	0
4	GOL	BBB	606	6/6	0.98	0.04	16,23,28,30	0
6	CL	BBB	628	1/1	0.98	0.05	31,31,31,31	0

Continued on next page...

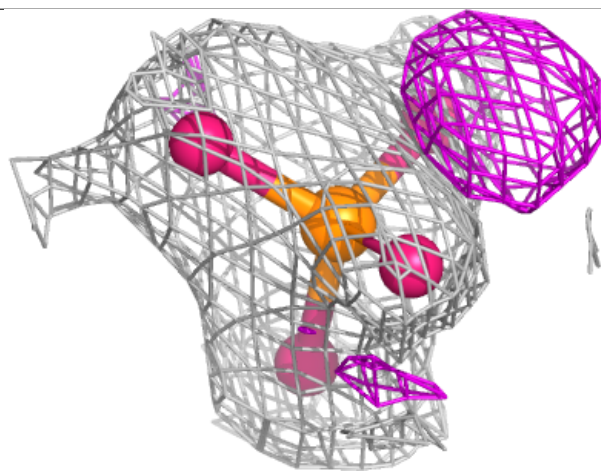
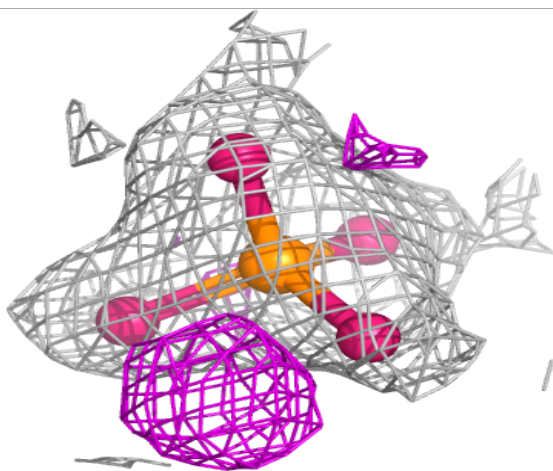
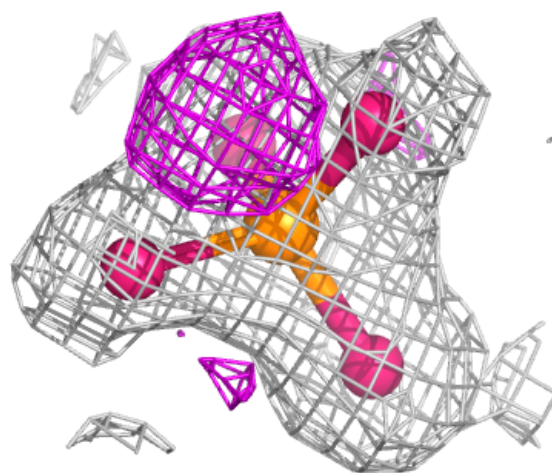
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	BBB	623	1/1	0.98	0.09	36,36,36,36	0
6	CL	CCC	624	1/1	0.98	0.06	33,33,33,33	0
4	GOL	BBB	607	6/6	0.98	0.06	19,24,25,26	0
6	CL	DDD	619	1/1	0.98	0.05	31,31,31,31	0
6	CL	AAA	628	1/1	0.99	0.06	30,30,30,30	0
3	CA	CCC	602	1/1	0.99	0.05	21,21,21,21	0
6	CL	BBB	625	1/1	0.99	0.04	22,22,22,22	0
6	CL	BBB	626	1/1	0.99	0.09	34,34,34,34	0
2	PO4	CCC	601	5/5	0.99	0.04	15,16,20,21	0
2	PO4	BBB	603	5/5	0.99	0.04	18,18,20,27	0
2	PO4	DDD	602	5/5	0.99	0.04	20,20,23,24	0
2	PO4	AAA	601	5/5	0.99	0.03	18,18,22,27	0
3	CA	BBB	604	1/1	0.99	0.04	18,18,18,18	0
6	CL	DDD	617	1/1	0.99	0.03	24,24,24,24	0
6	CL	DDD	618	1/1	0.99	0.09	30,30,30,30	0
6	CL	AAA	627	1/1	0.99	0.07	31,31,31,31	0
3	CA	DDD	603	1/1	1.00	0.04	17,17,17,17	0
3	CA	AAA	602	1/1	1.00	0.03	19,19,19,19	0
6	CL	CCC	623	1/1	1.00	0.04	26,26,26,26	0
6	CL	AAA	626	1/1	1.00	0.07	28,28,28,28	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.

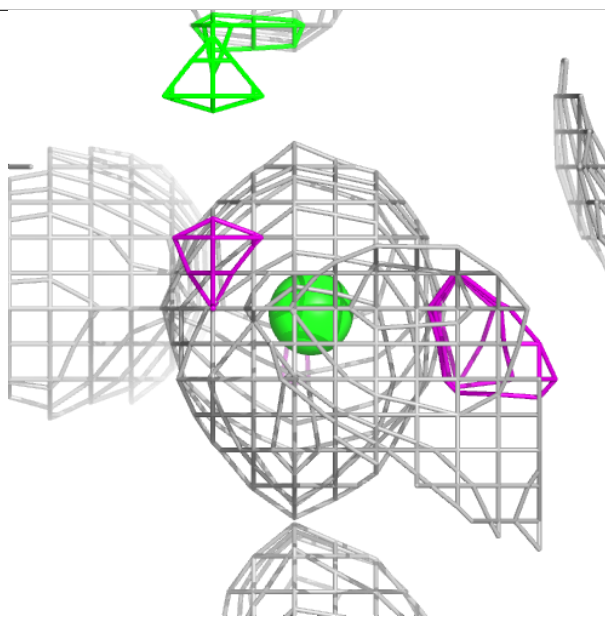
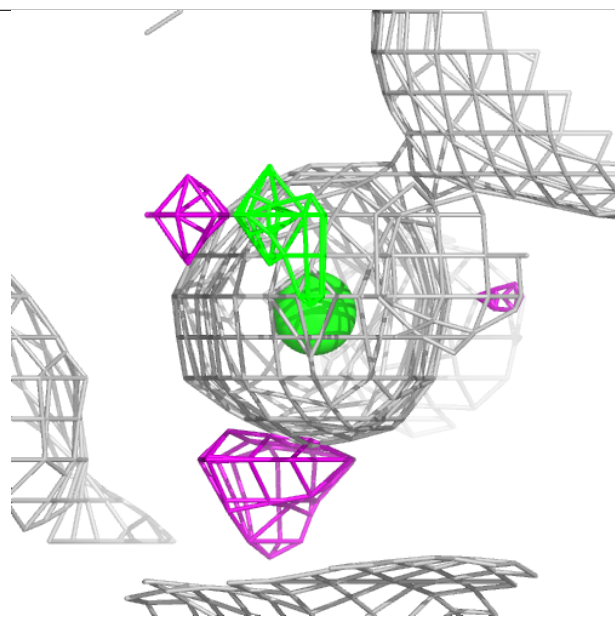
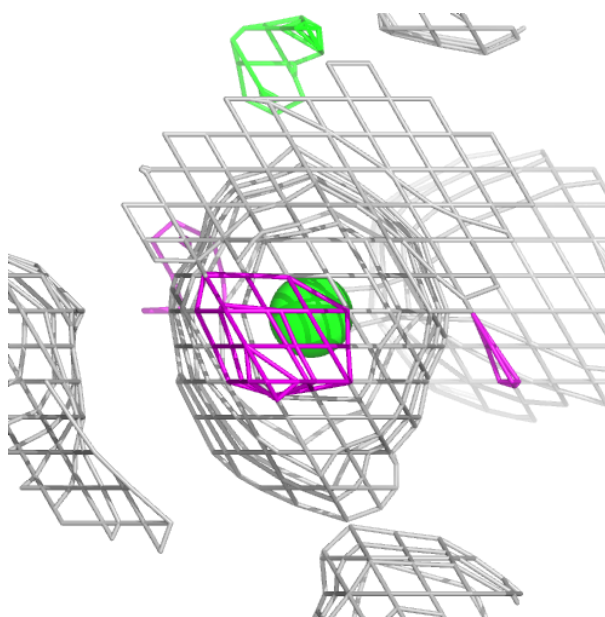
Electron density around PO4 AAA 622:

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



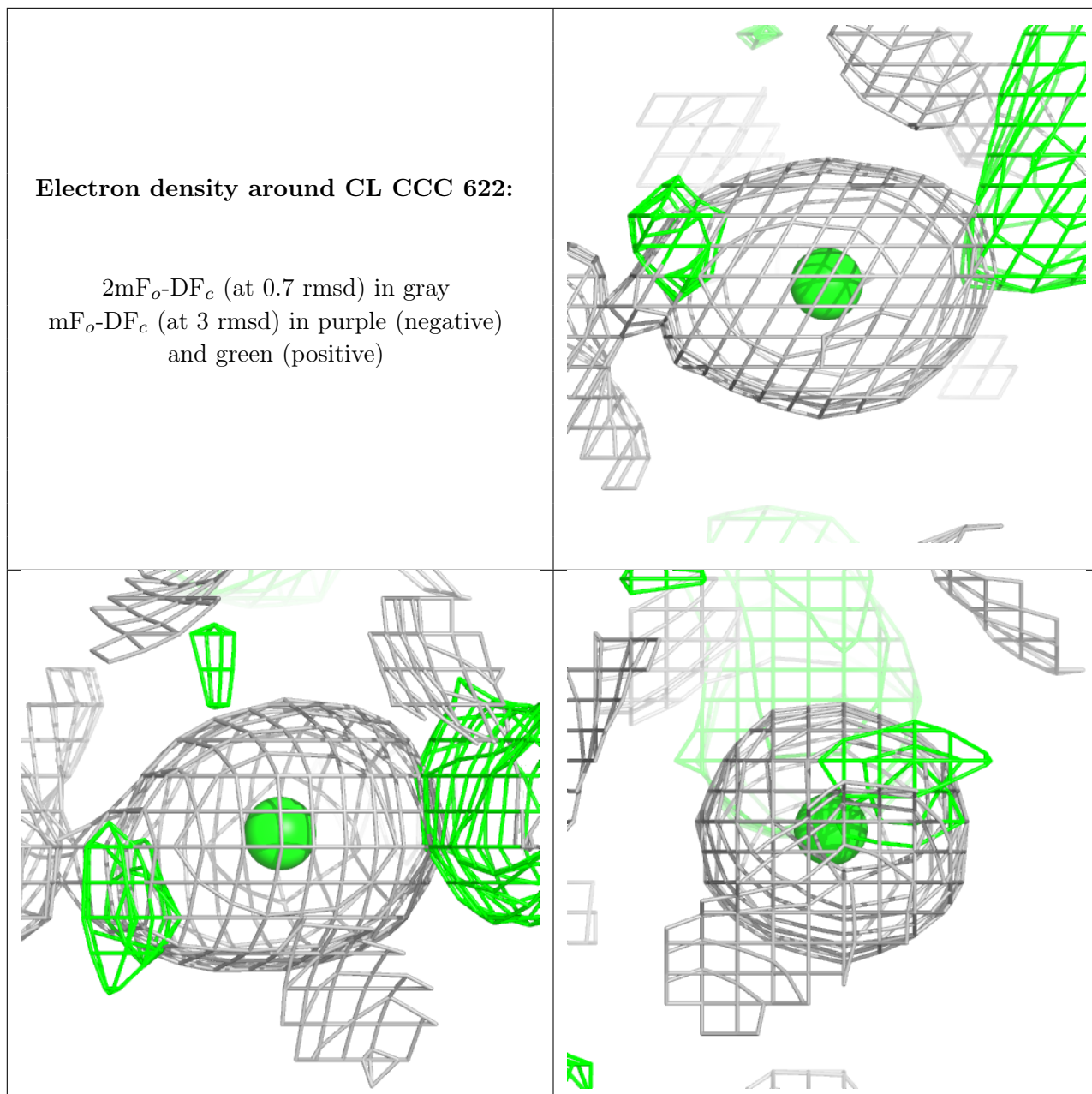
Electron density around CL BBB 627:

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



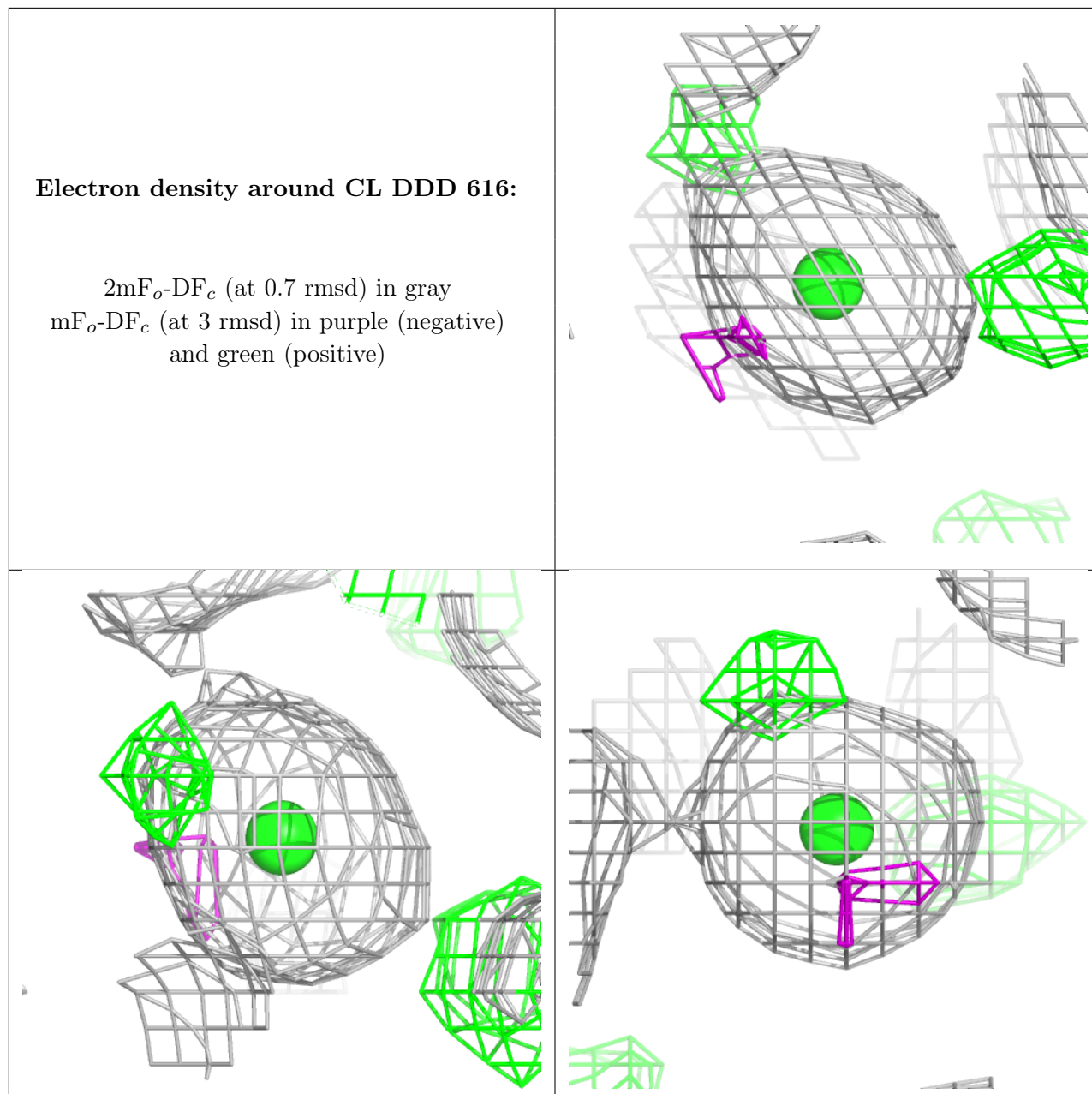
Electron density around CL CCC 622:

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



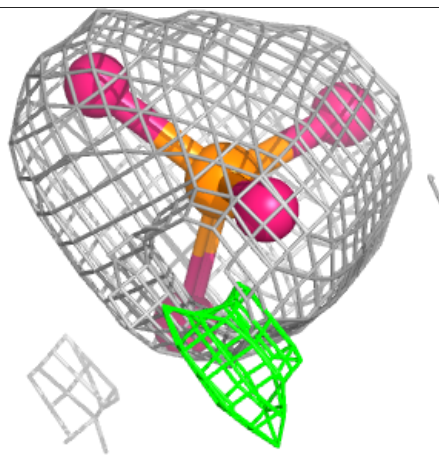
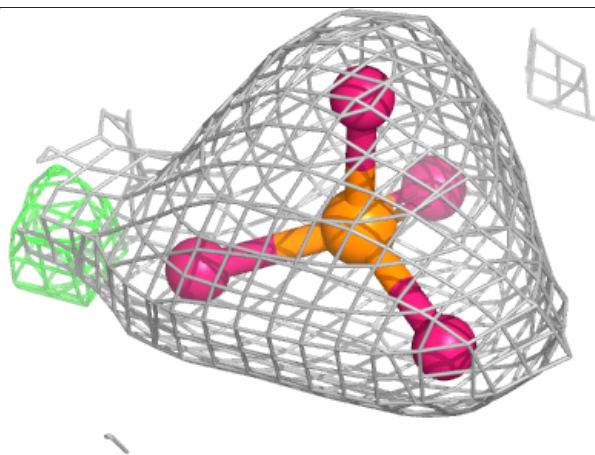
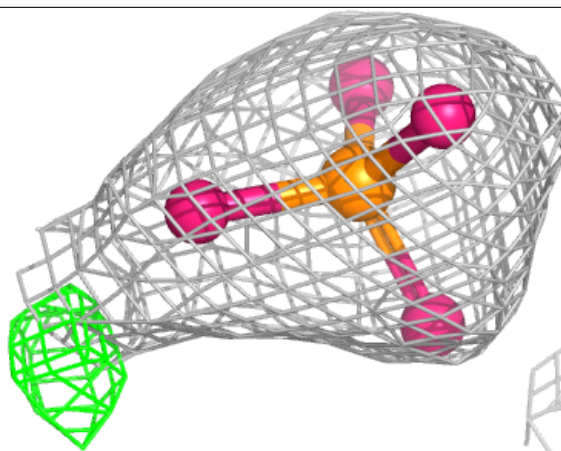
Electron density around CL DDD 616:

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



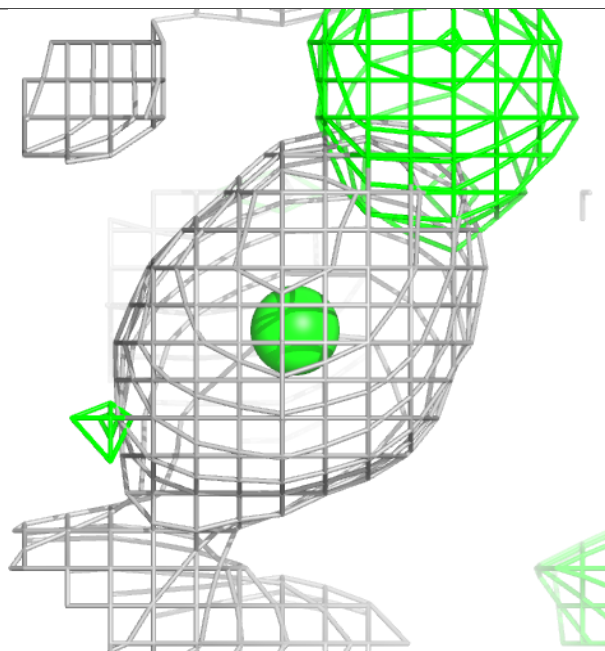
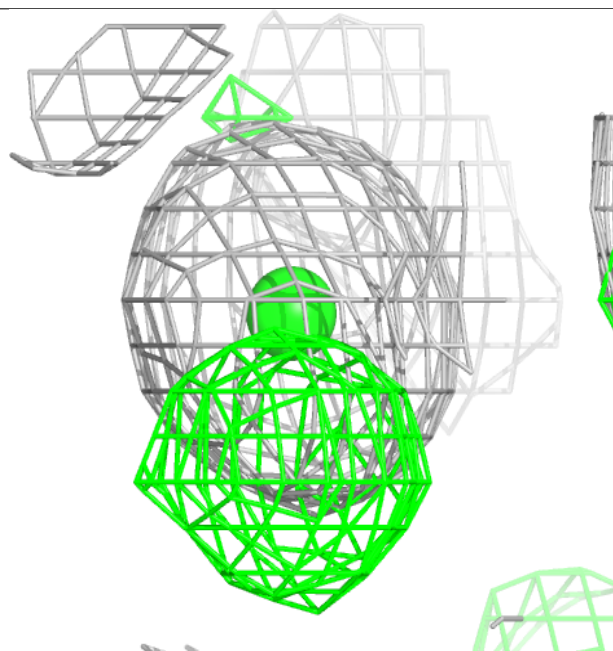
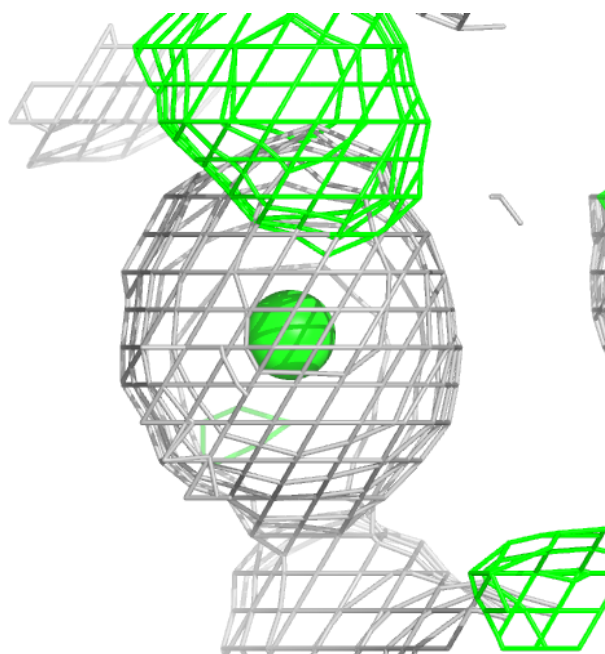
Electron density around PO4 DDD 604:

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



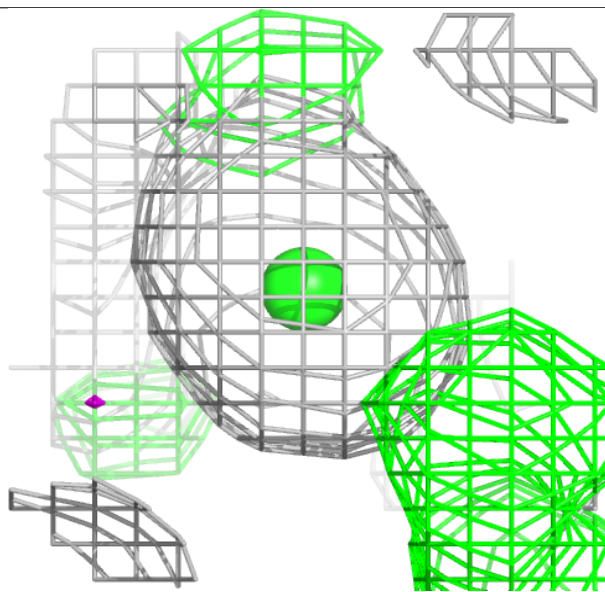
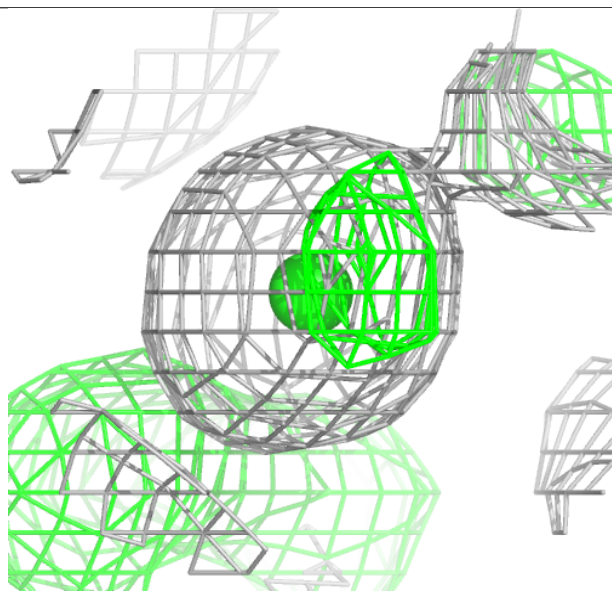
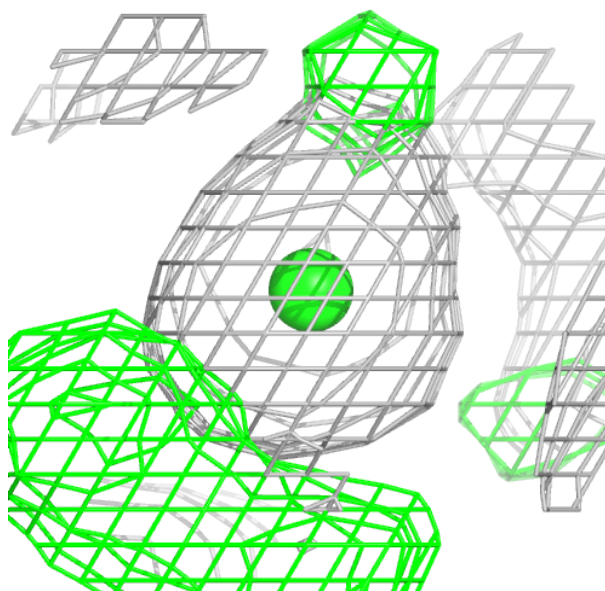
Electron density around CL AAA 625:

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



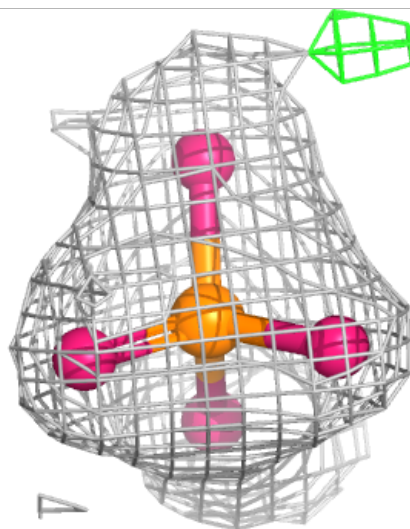
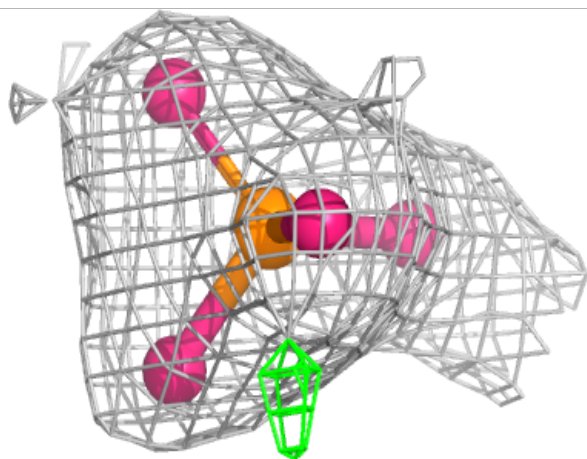
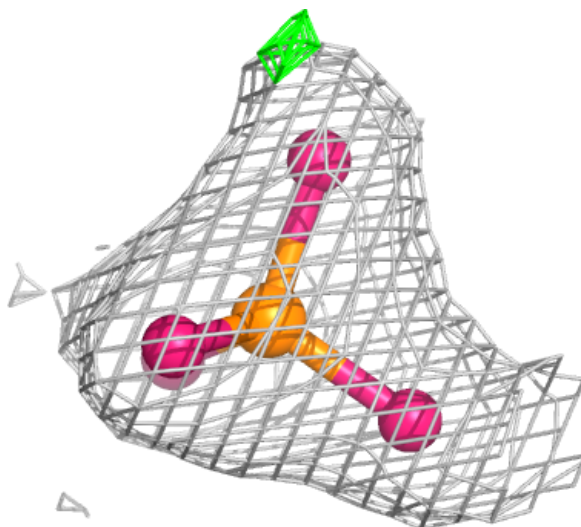
Electron density around CL BBB 624:

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



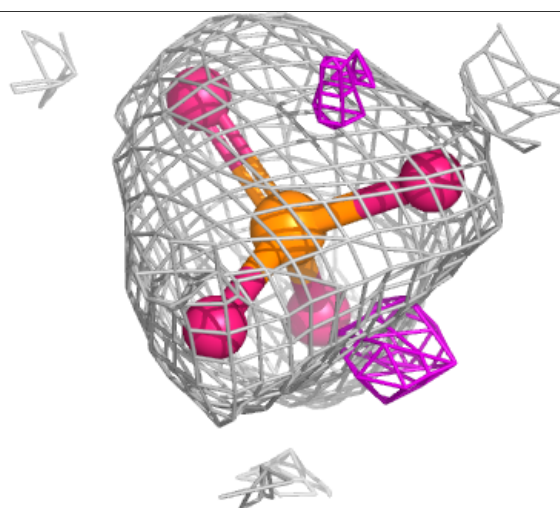
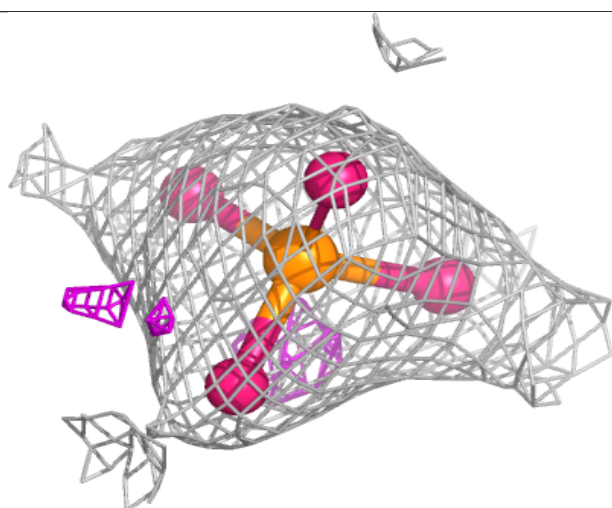
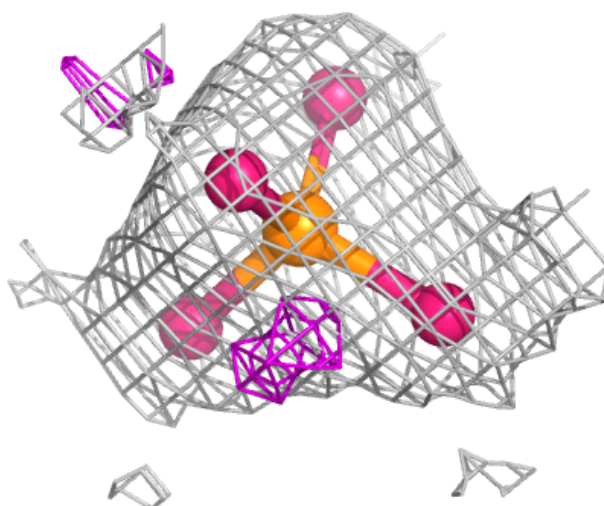
Electron density around PO4 BBB 605:

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



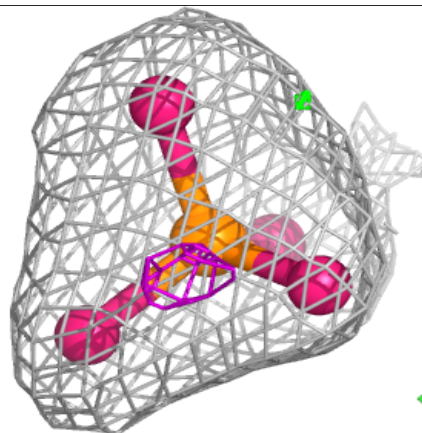
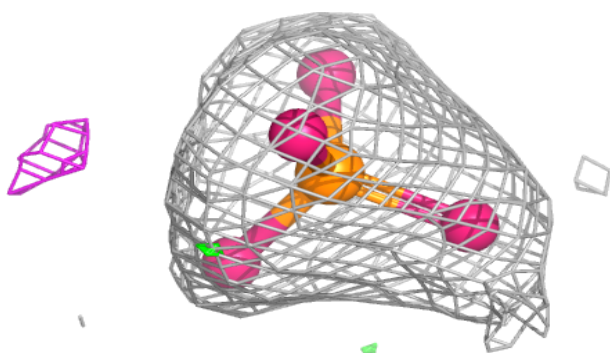
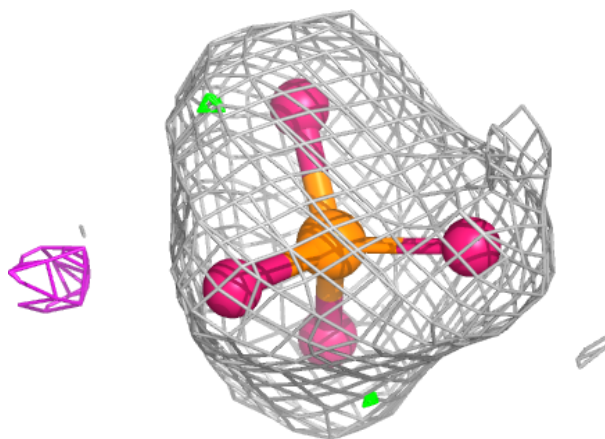
Electron density around PO4 CCC 603:

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



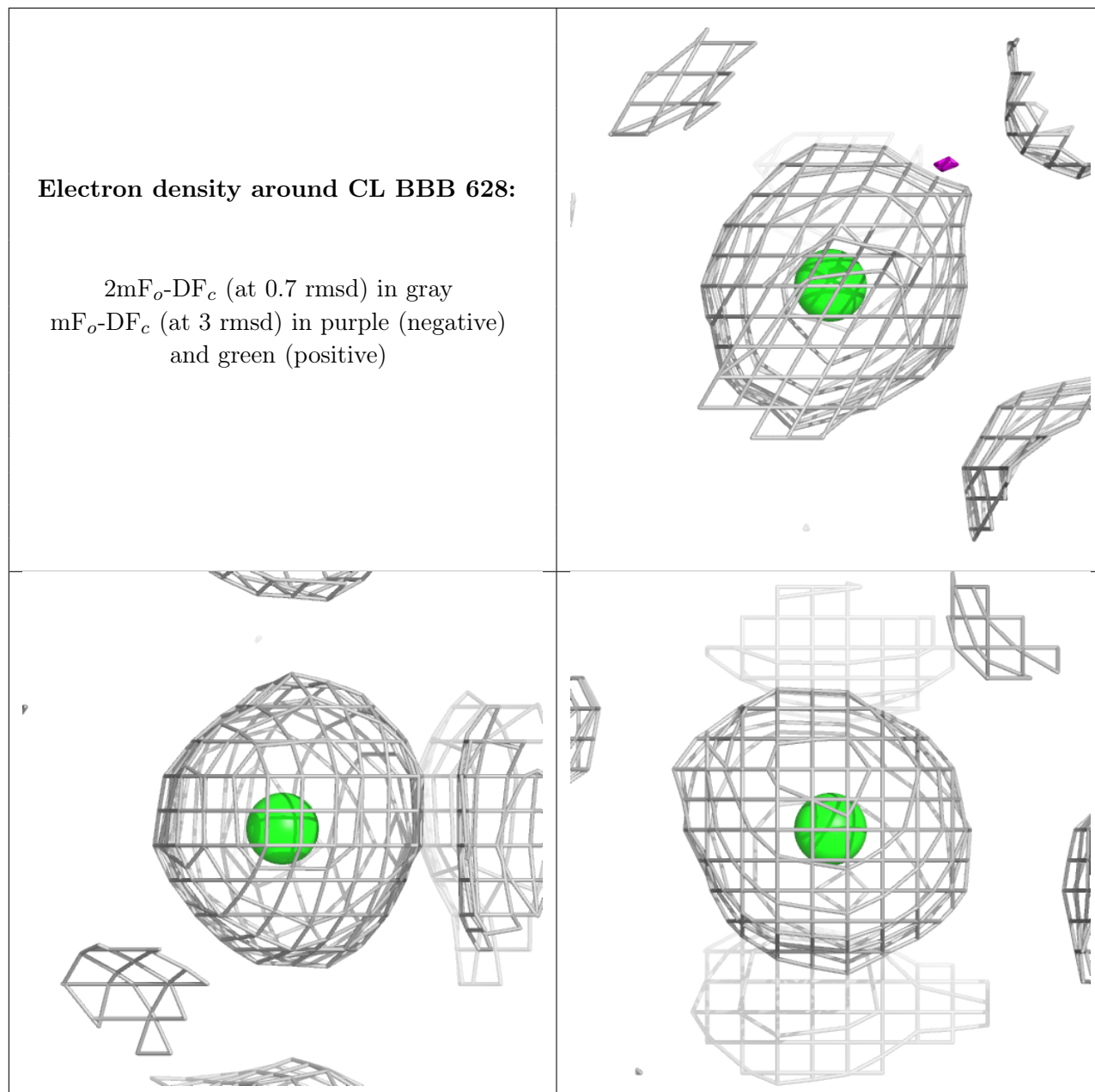
Electron density around PO4 AAA 603:

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



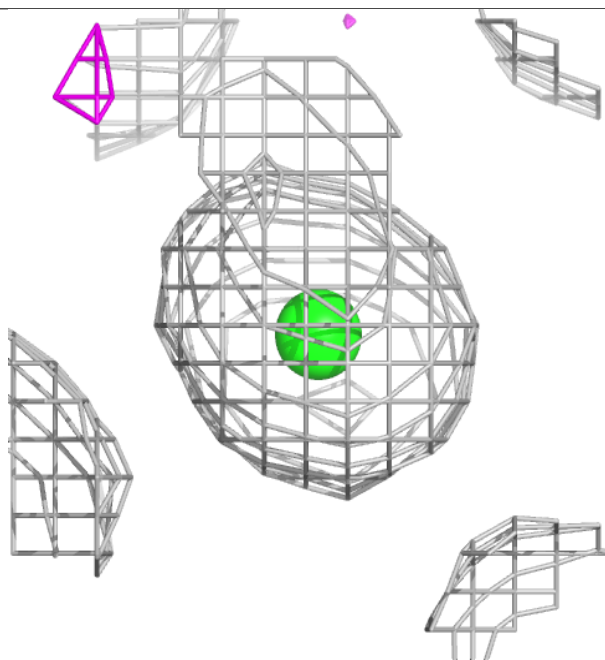
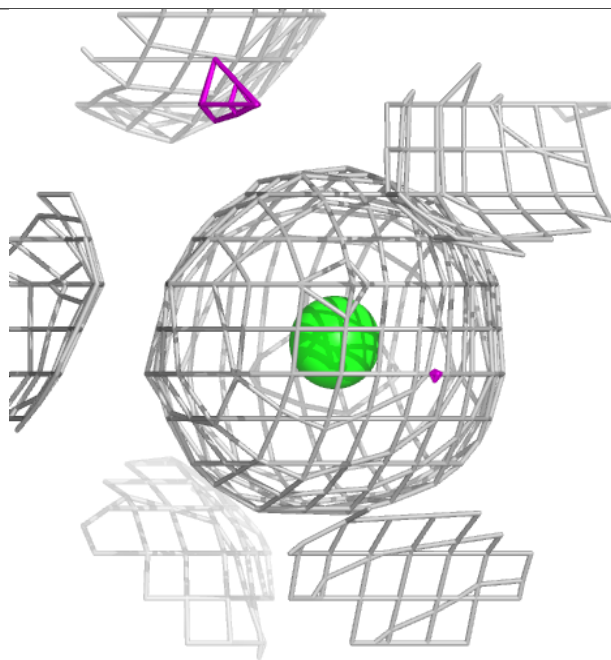
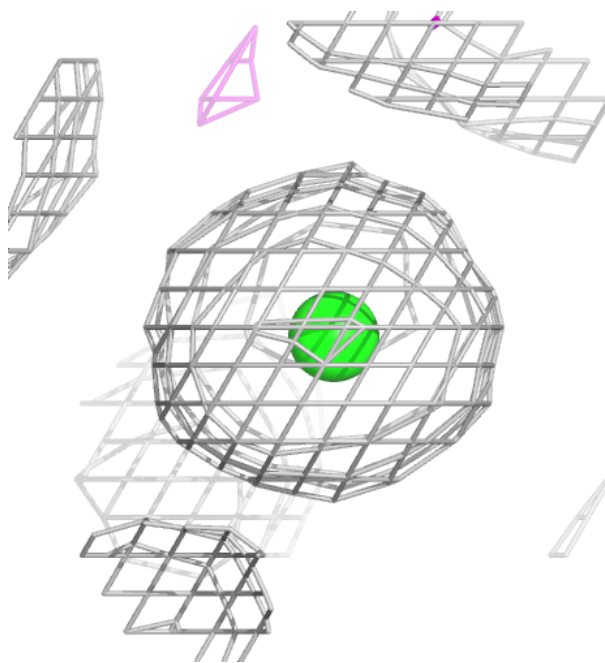
Electron density around CL BBB 628:

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



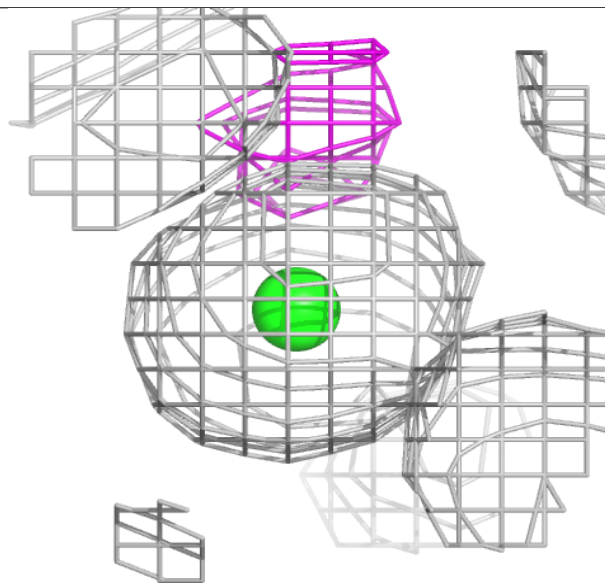
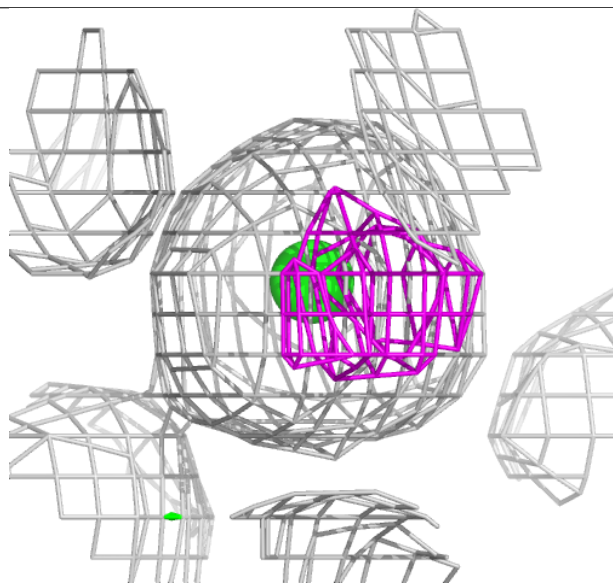
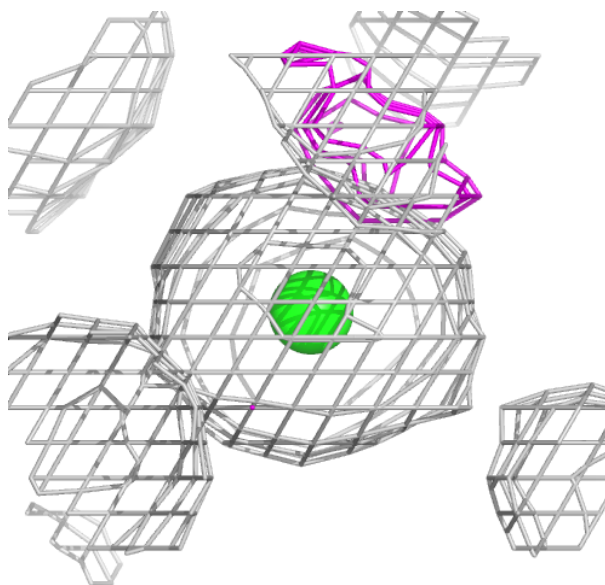
Electron density around CL CCC 624:

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



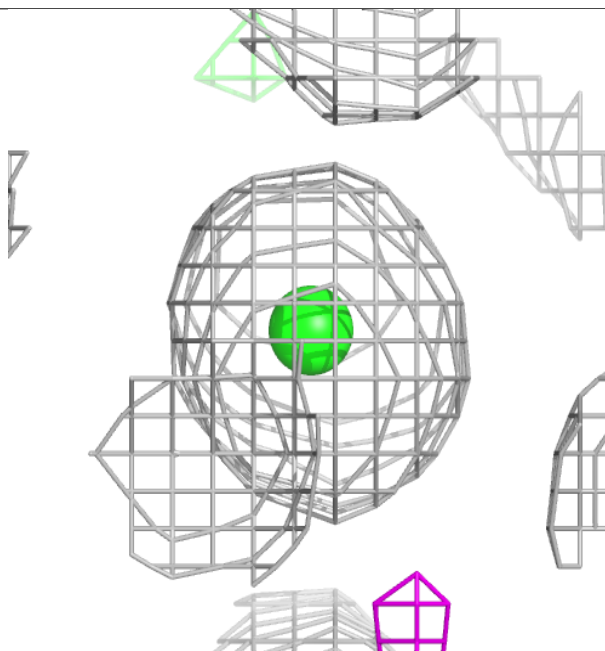
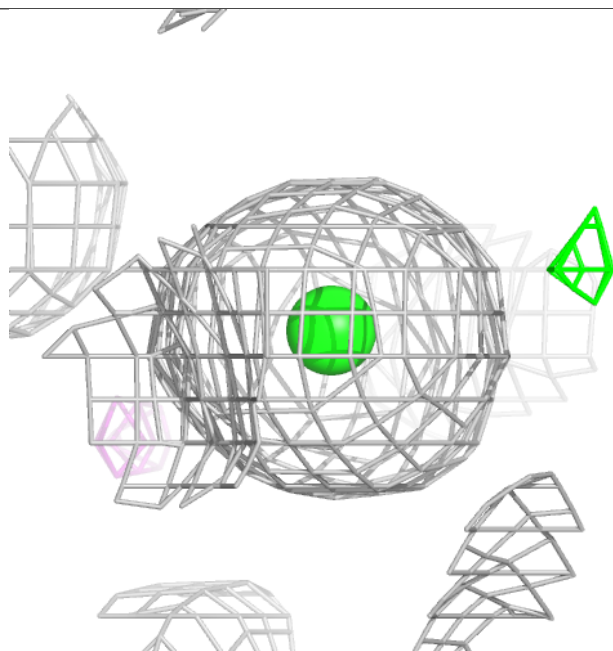
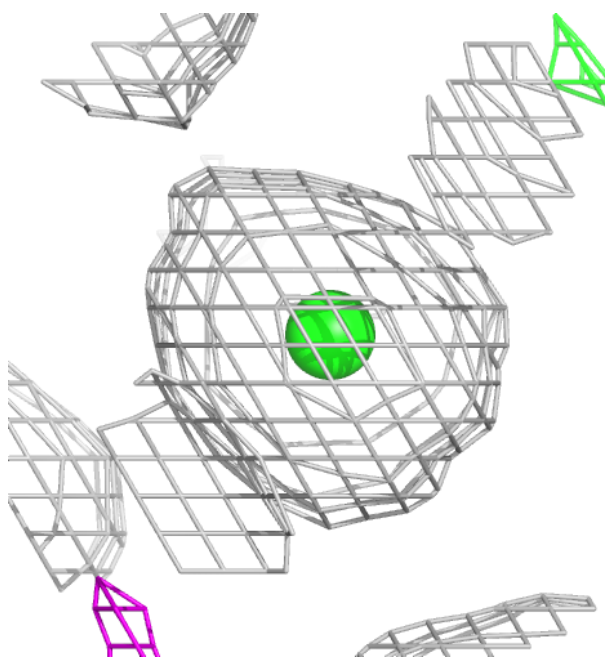
Electron density around CL DDD 619:

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



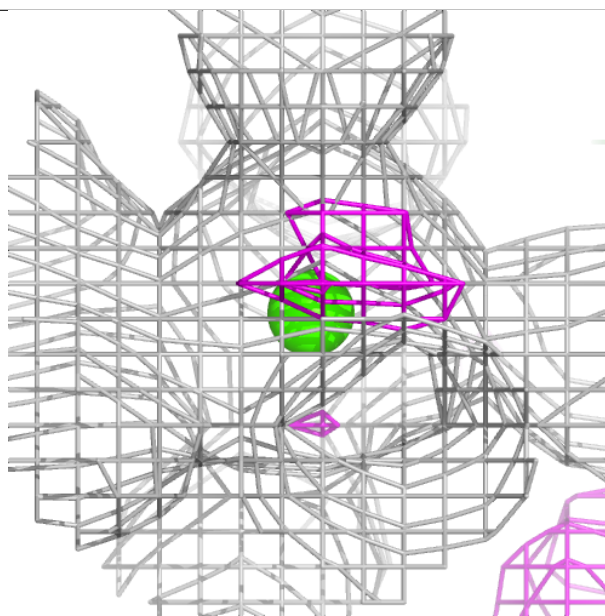
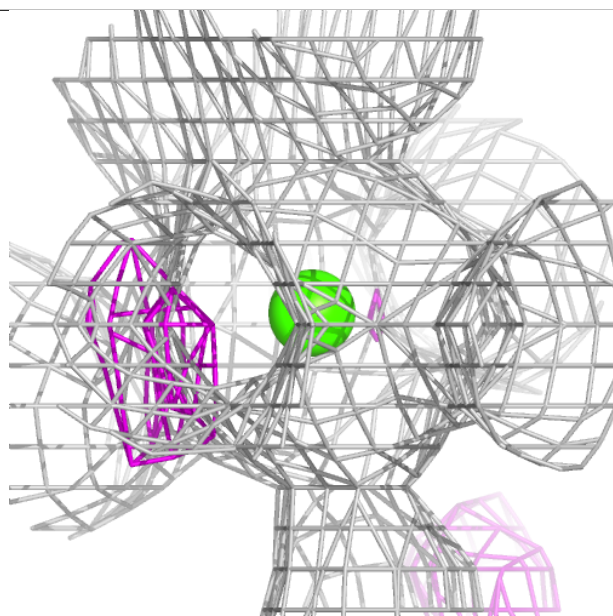
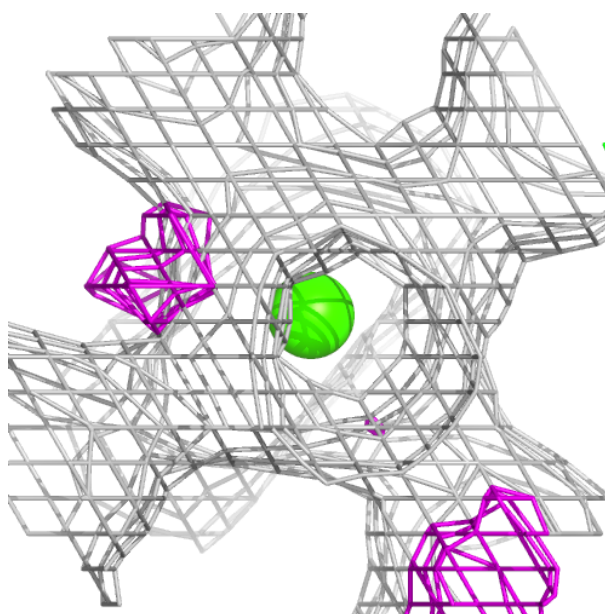
Electron density around CL AAA 628:

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



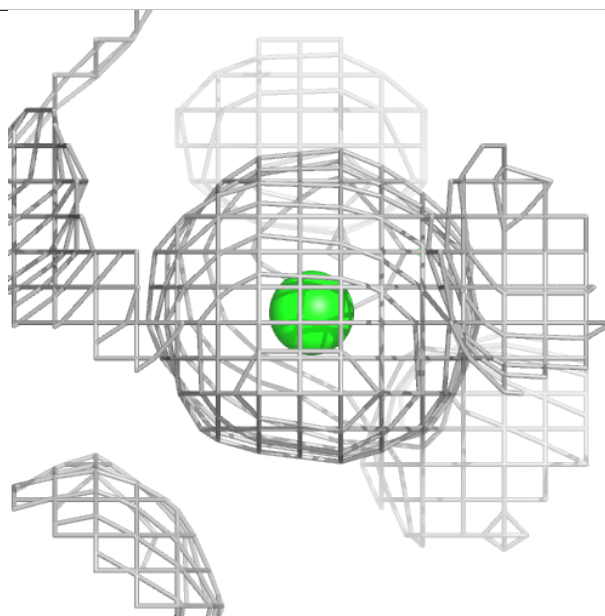
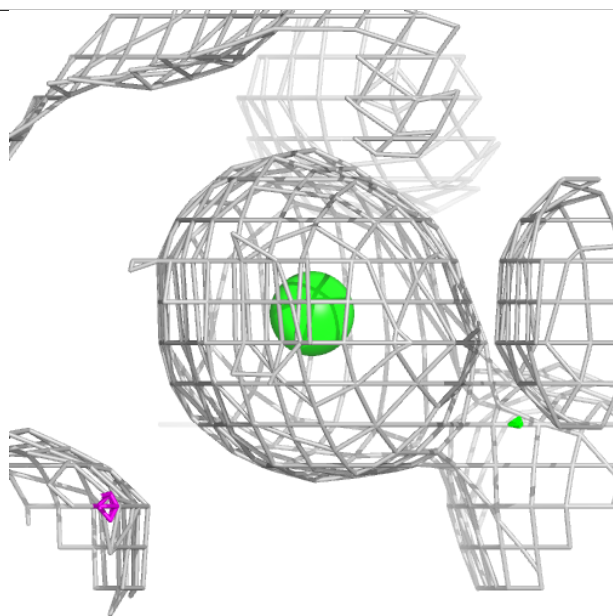
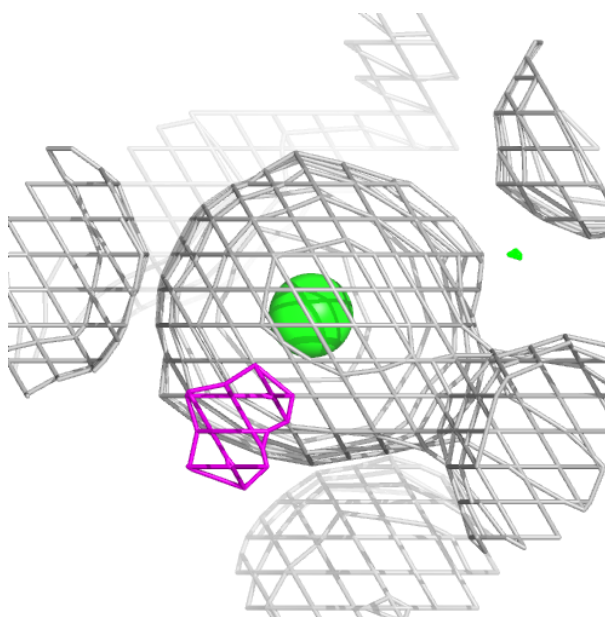
Electron density around CA CCC 602:

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



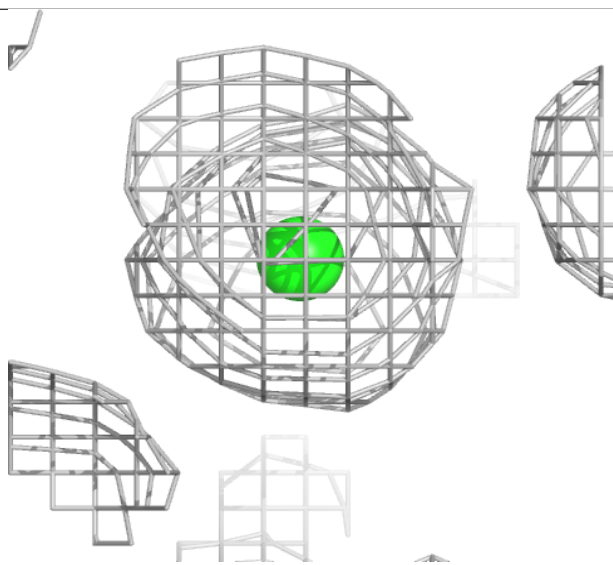
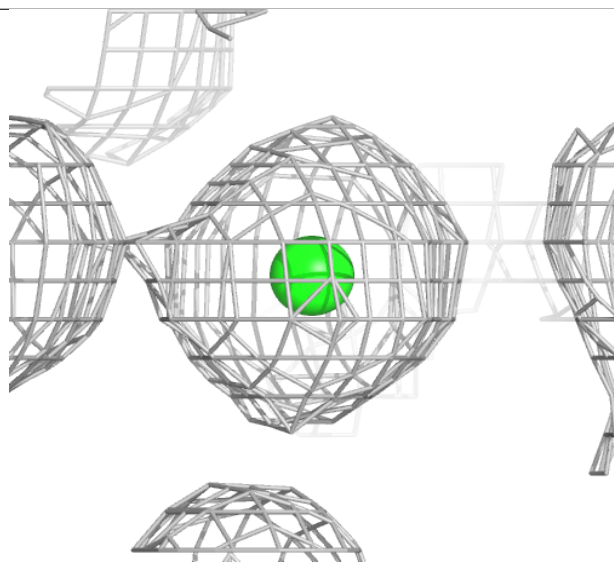
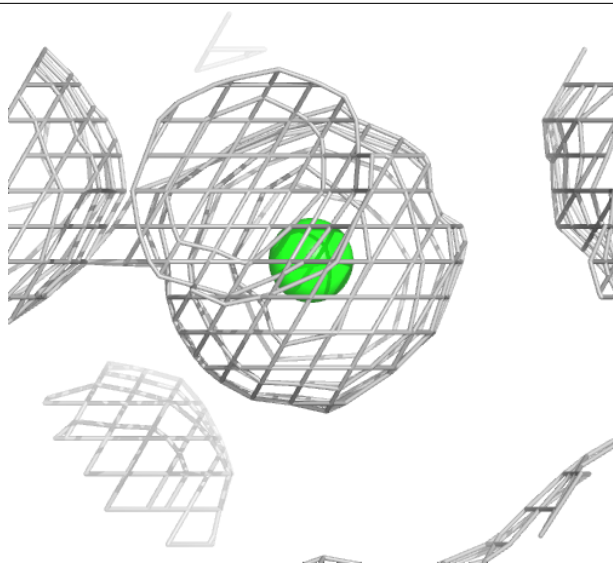
Electron density around CL BBB 625:

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



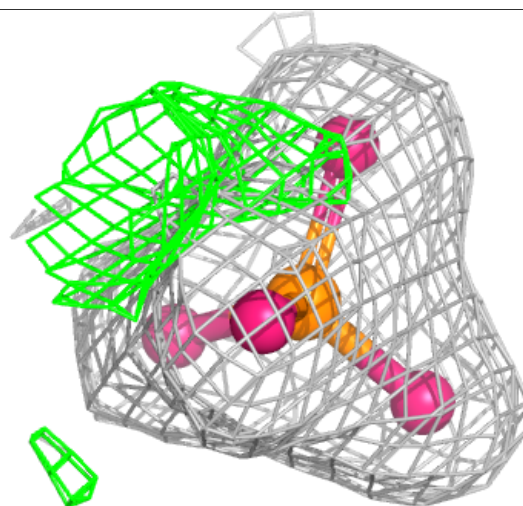
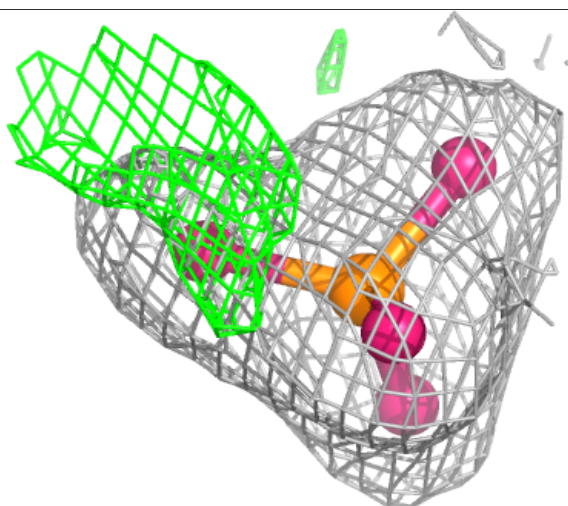
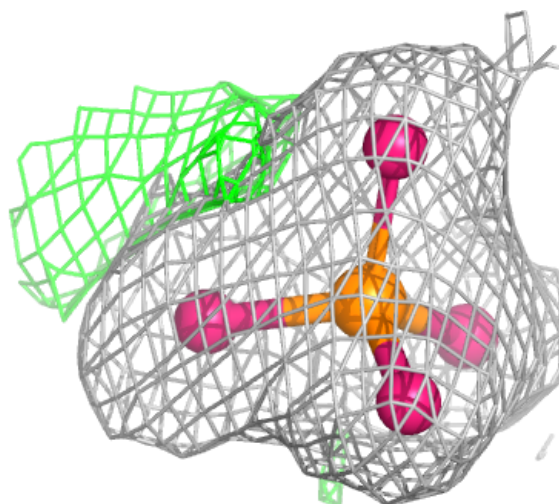
Electron density around CL BBB 626:

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



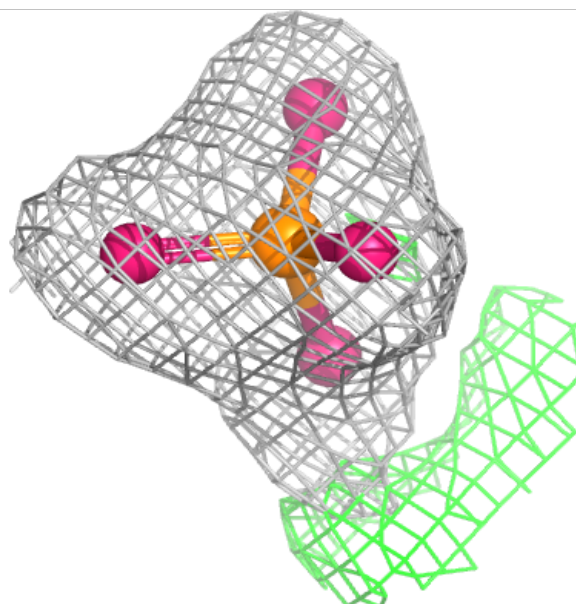
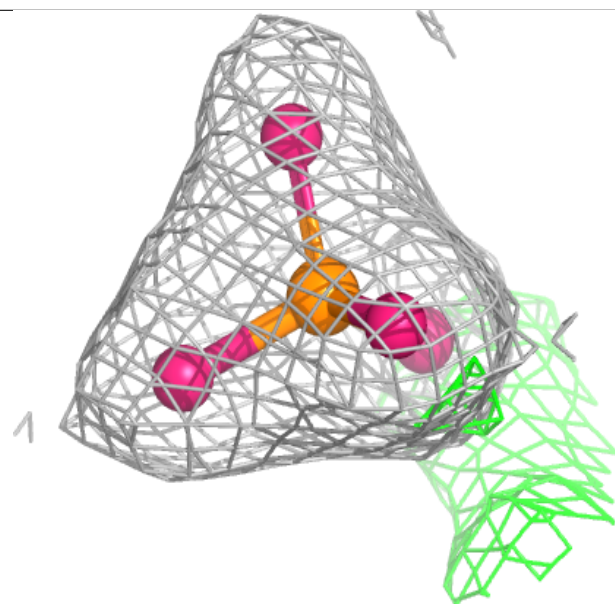
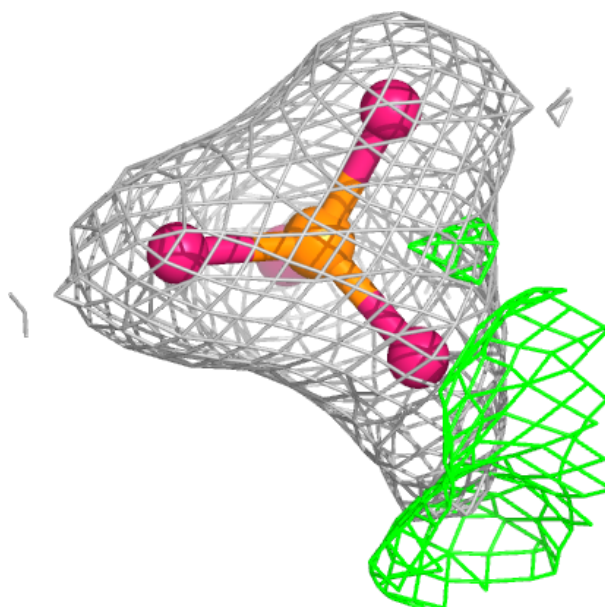
Electron density around PO4 CCC 601:

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



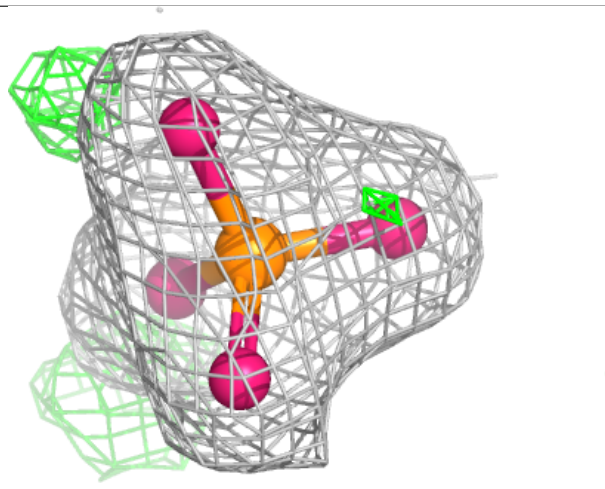
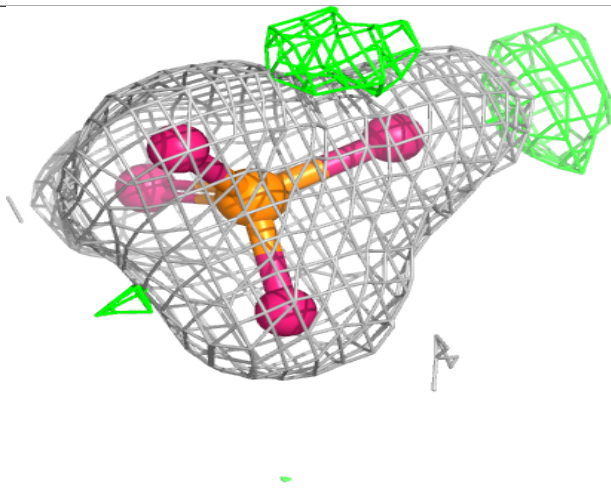
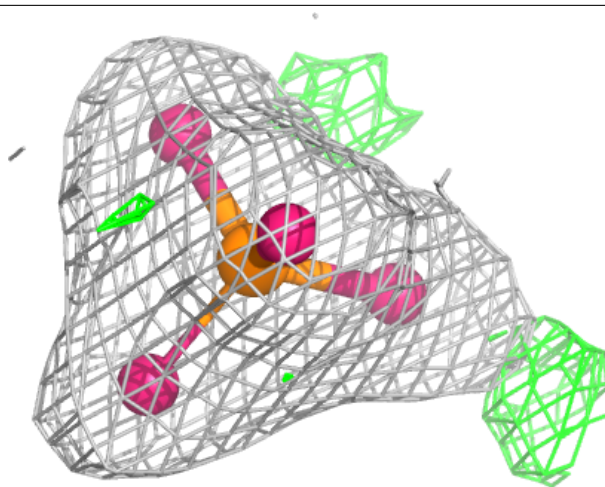
Electron density around PO4 BBB 603:

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



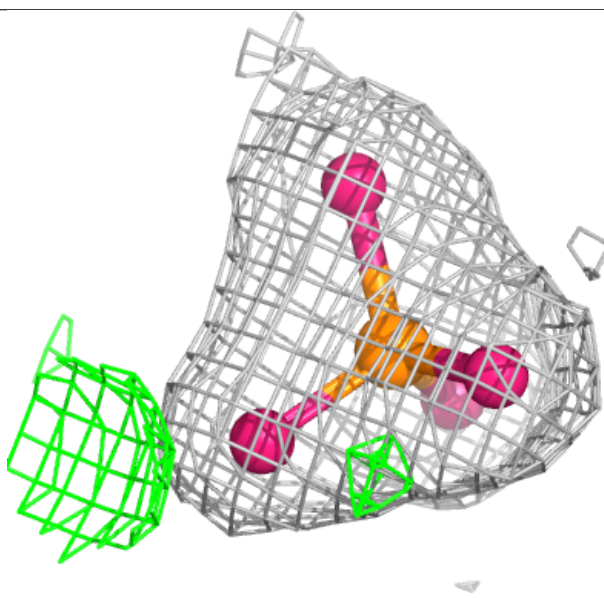
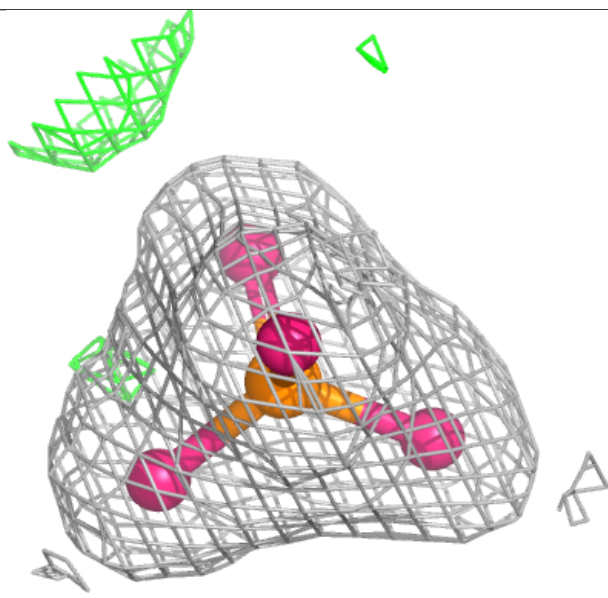
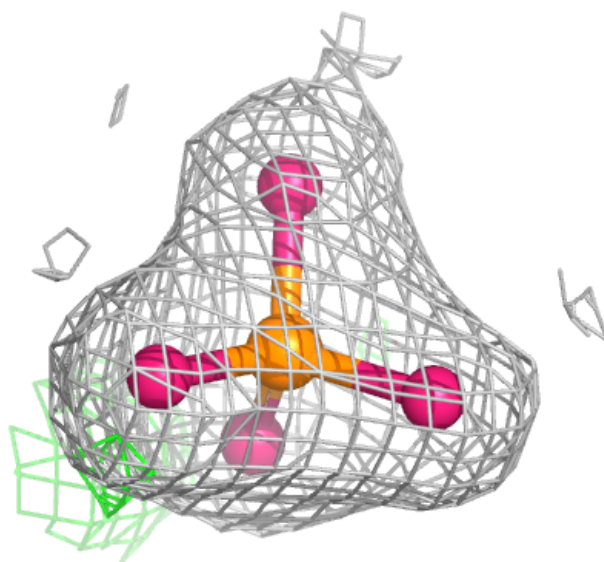
Electron density around PO4 DDD 602:

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



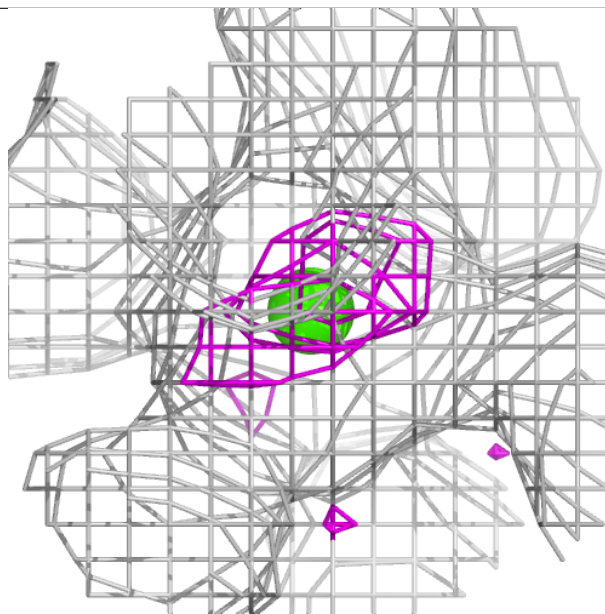
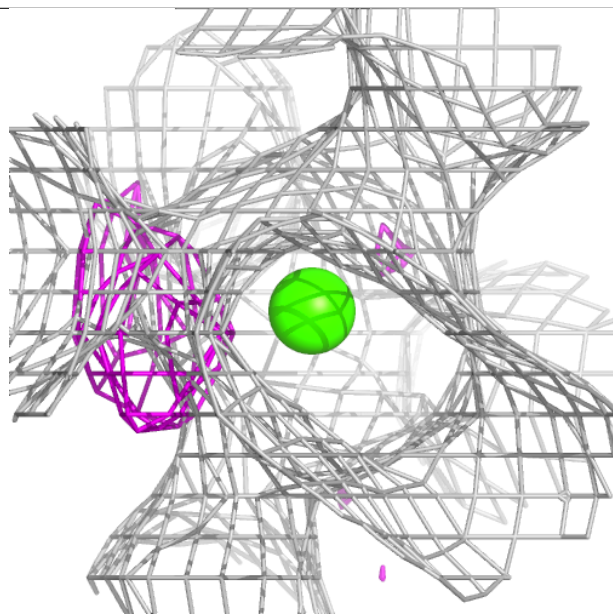
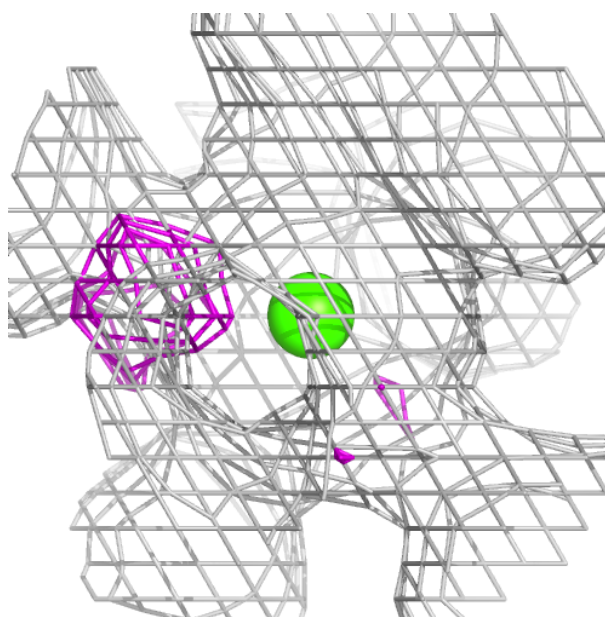
Electron density around PO4 AAA 601:

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



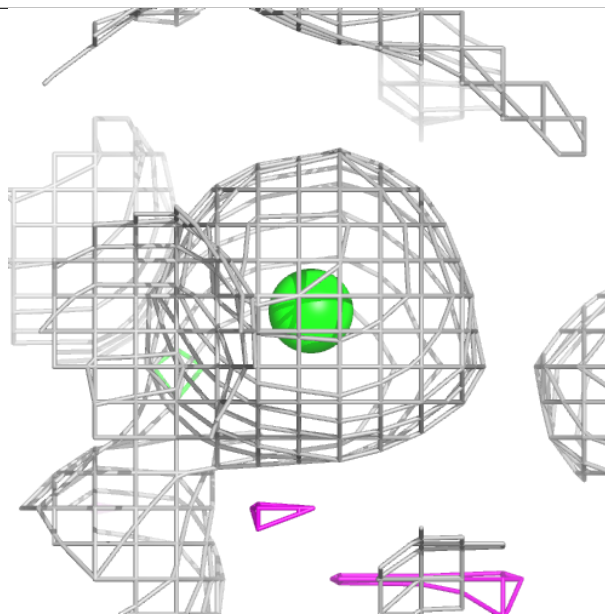
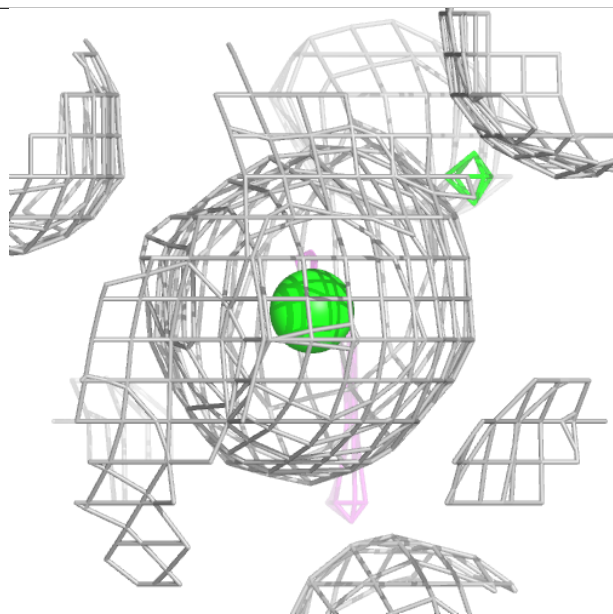
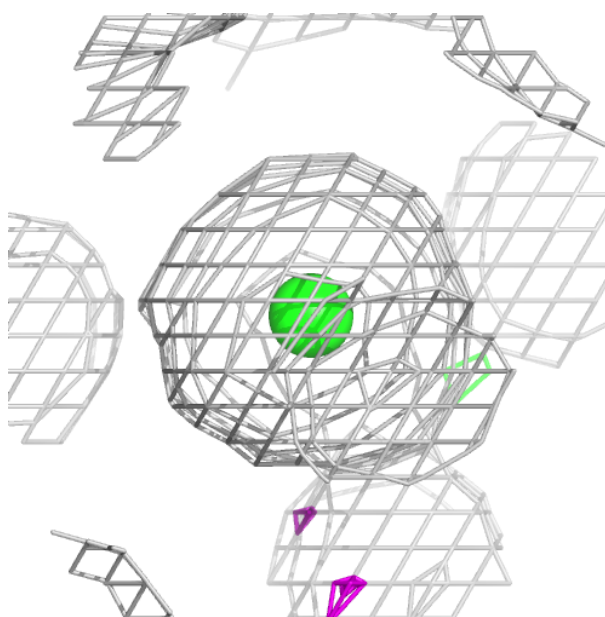
Electron density around CA BBB 604:

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



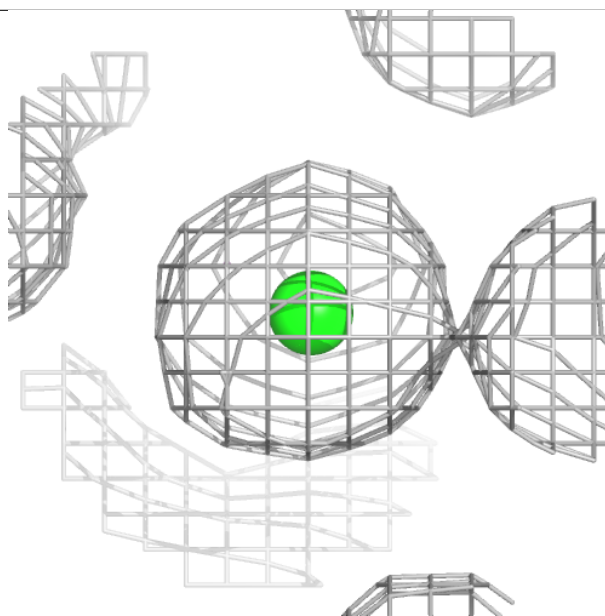
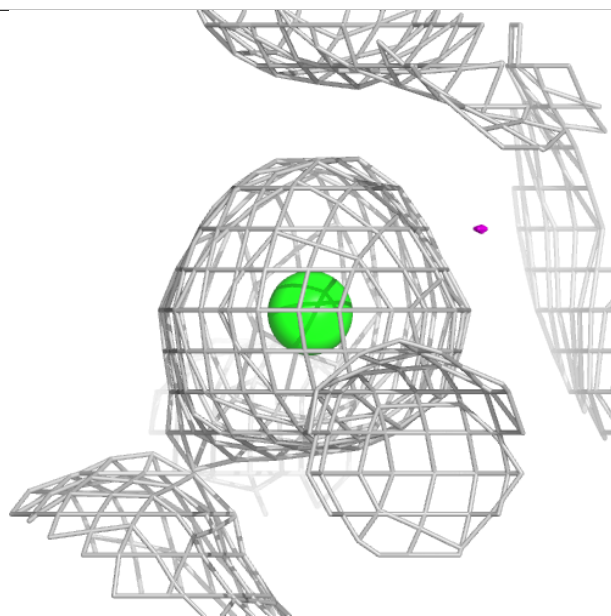
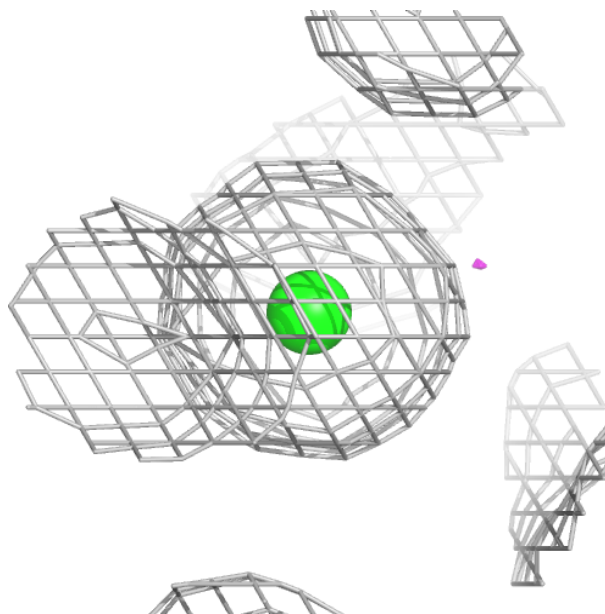
Electron density around CL DDD 617:

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



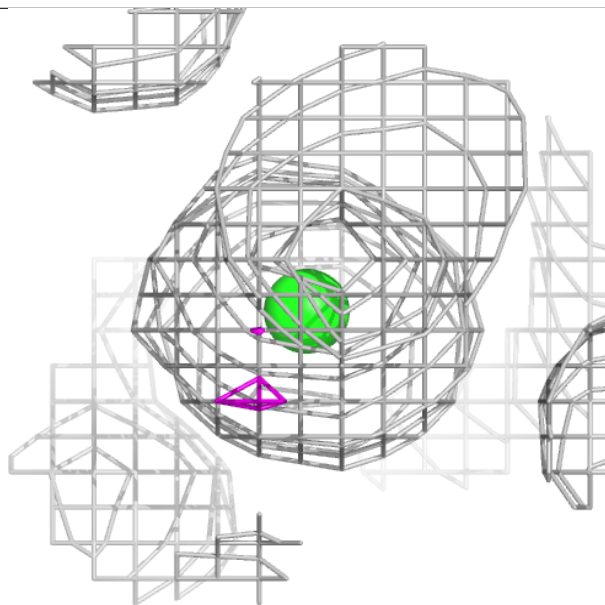
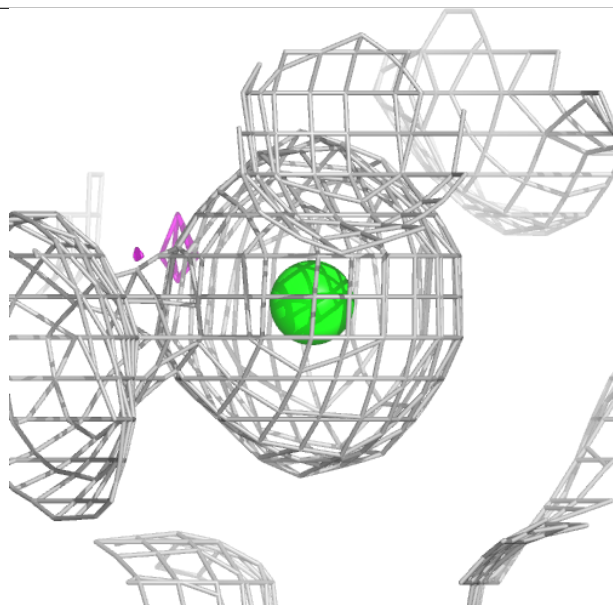
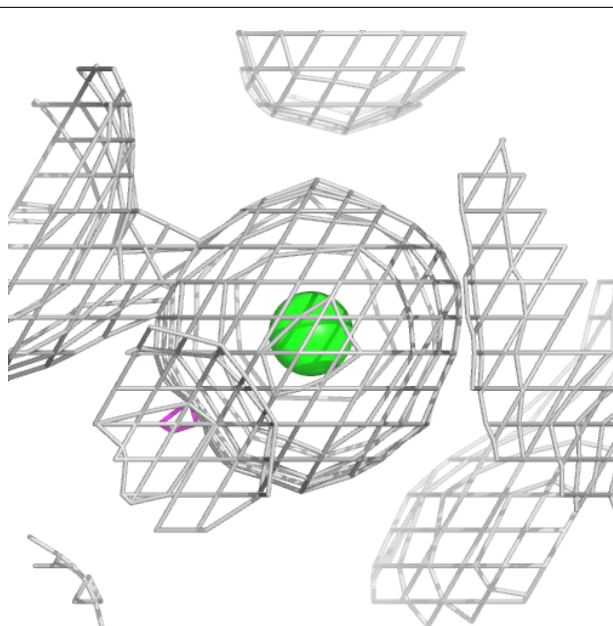
Electron density around CL DDD 618:

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



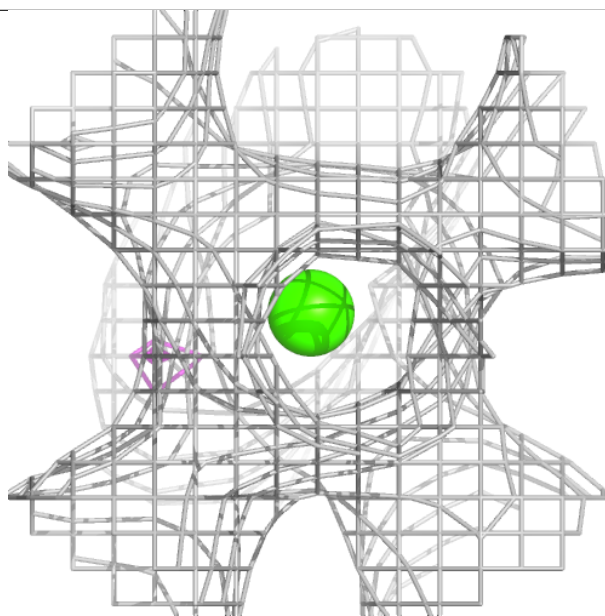
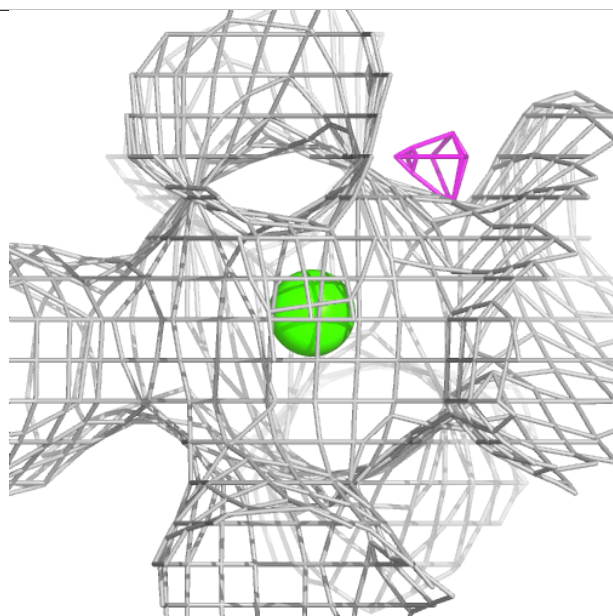
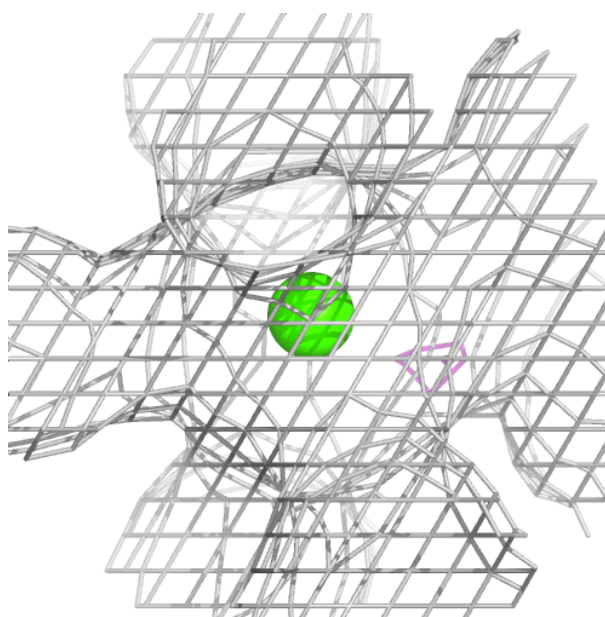
Electron density around CL AAA 627:

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



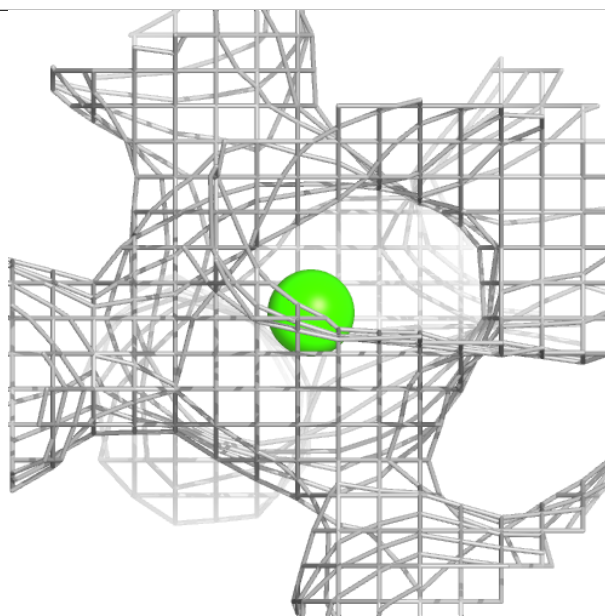
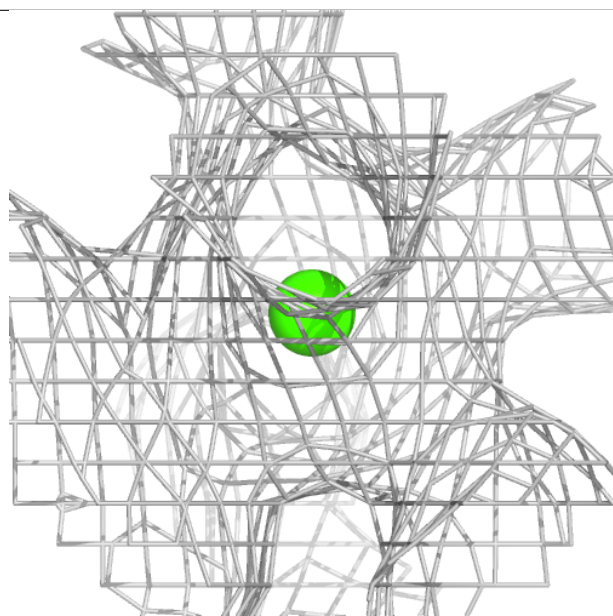
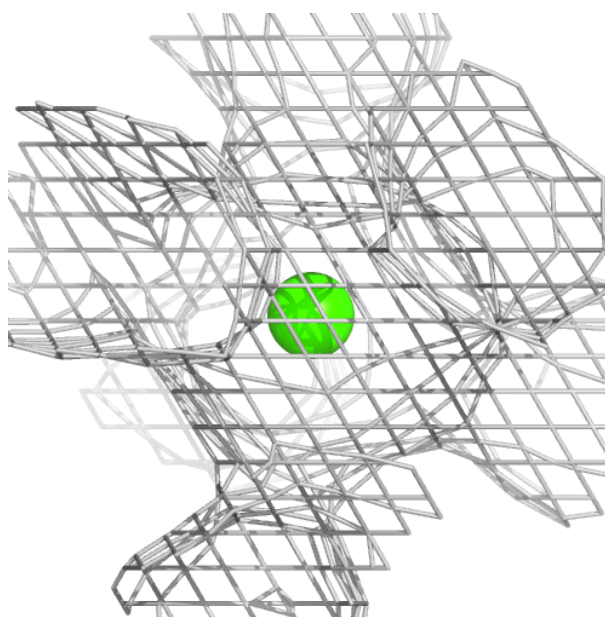
Electron density around CA DDD 603:

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



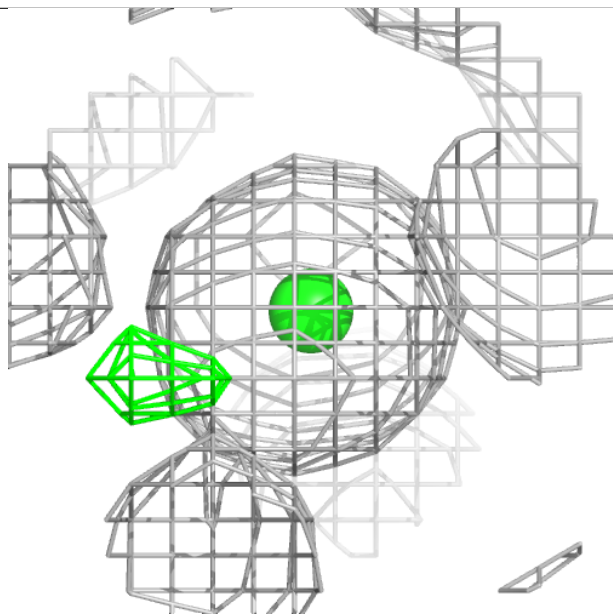
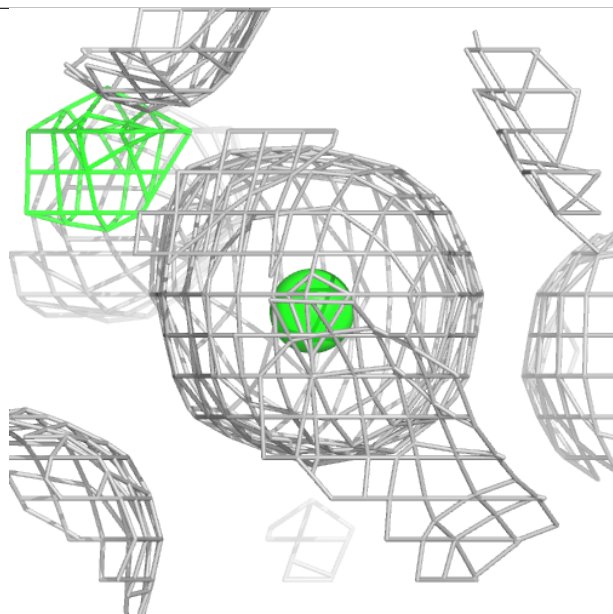
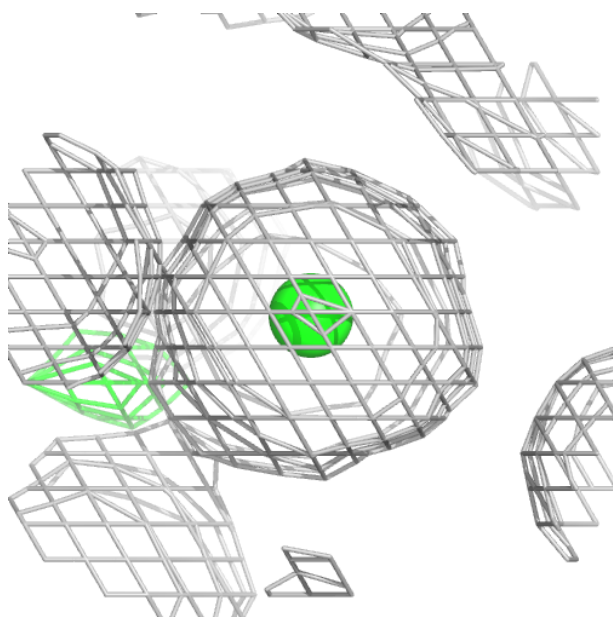
Electron density around CA AAA 602:

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



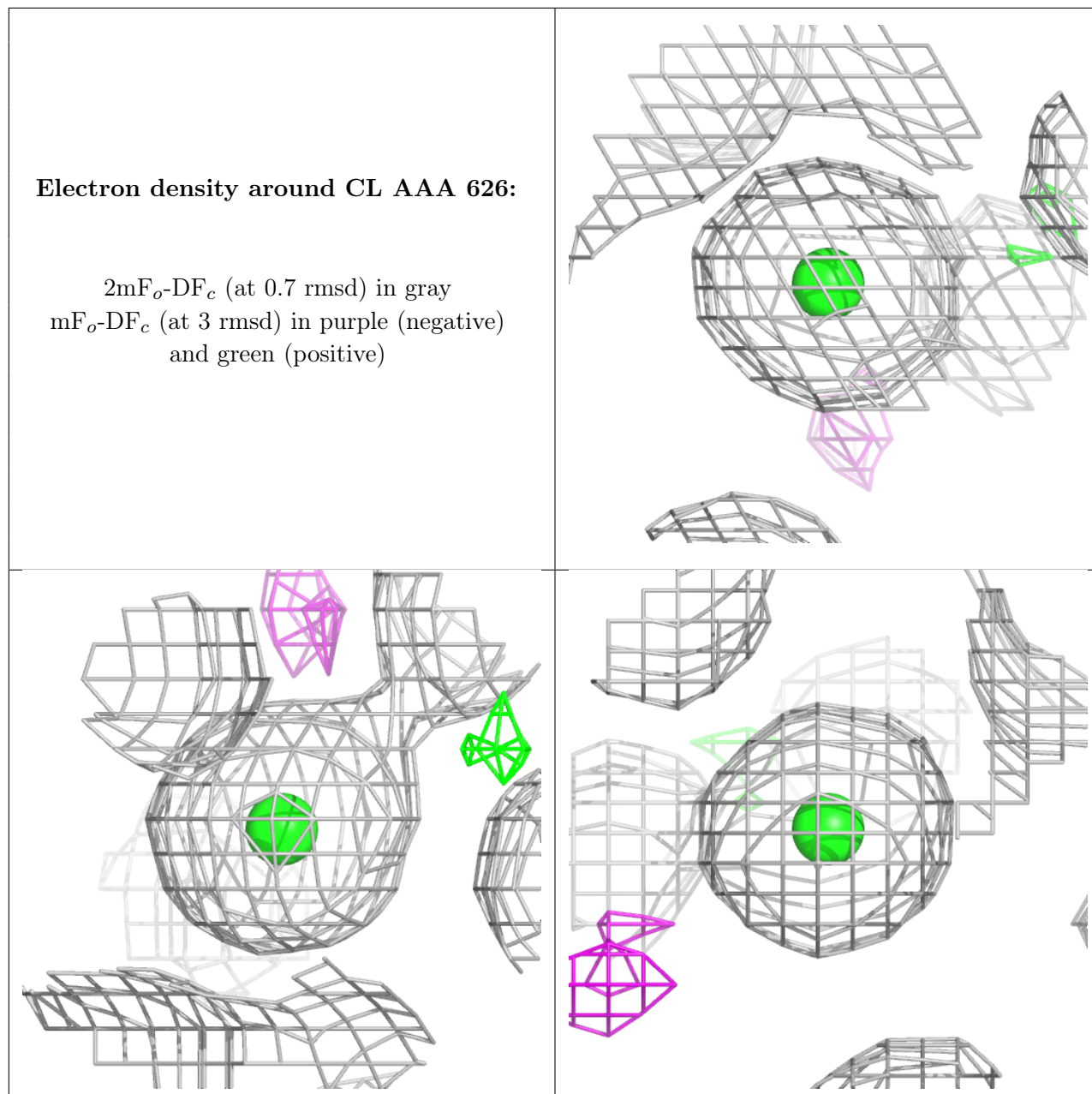
Electron density around CL CCC 623:

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



Electron density around CL AAA 626:

$2mF_o-DF_c$ (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.