



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 10:13 pm BST

PDB ID : 7Z79
Title : Crystal structure of aminotransferase-like protein from *Variovorax paradoxus*
Authors : Boyko, K.M.; Matyuta, I.O.; Nikolaeva, A.Y.; Khrenova, M.G.; Rakitina, T.V.; Popov, V.O.; Bezsudnova, E.Y.
Deposited on : 2022-03-15
Resolution : 2.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

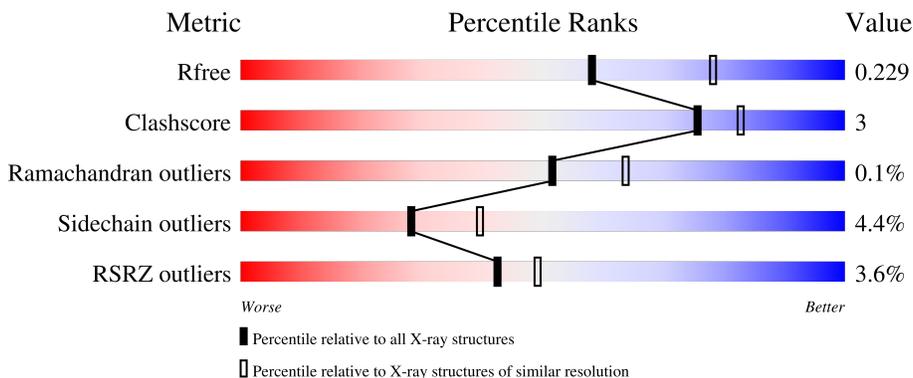
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	317	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3% 86% 8% • 5%</p>
1	B	317	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3% 86% 9% • •</p>
1	C	317	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3% 87% 6% 6%</p>
1	D	317	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3% 85% 6% • 7%</p>
1	E	317	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">3% 86% 8% 5%</p>

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Mol	Chain	Length	Quality of chain
1	F	317	<p>4% 86% 7% 7%</p>

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	PO4	D	403	-	X	-	-

2 Entry composition [i](#)

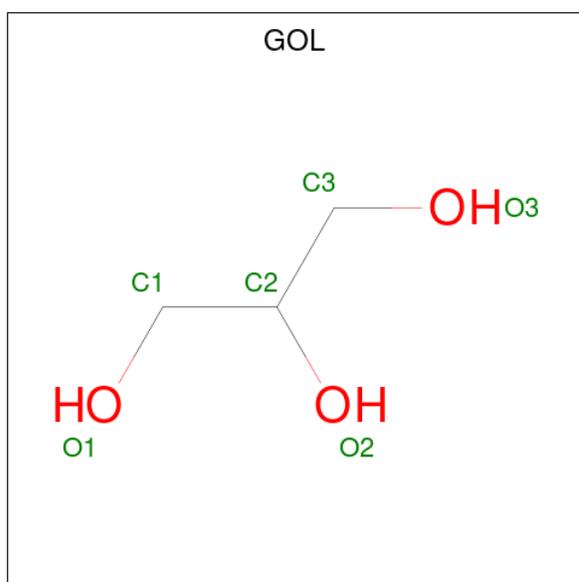
There are 6 unique types of molecules in this entry. The entry contains 14415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminotransferase, class 4.

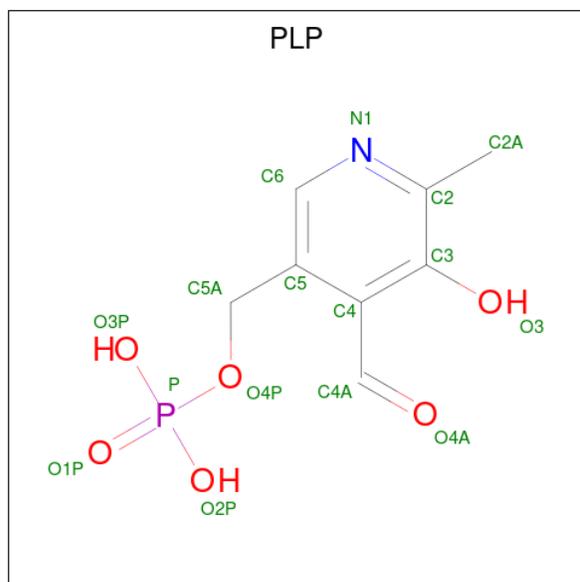
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	Total 2285	C 1437	N 419	O 419	S 10	0	3	0
1	B	306	Total 2328	C 1465	N 423	O 430	S 10	0	4	0
1	C	297	Total 2269	C 1420	N 424	O 415	S 10	0	4	0
1	D	294	Total 2231	C 1397	N 412	O 412	S 10	0	2	0
1	E	300	Total 2263	C 1421	N 412	O 420	S 10	0	3	0
1	F	296	Total 2256	C 1419	N 414	O 413	S 10	0	4	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



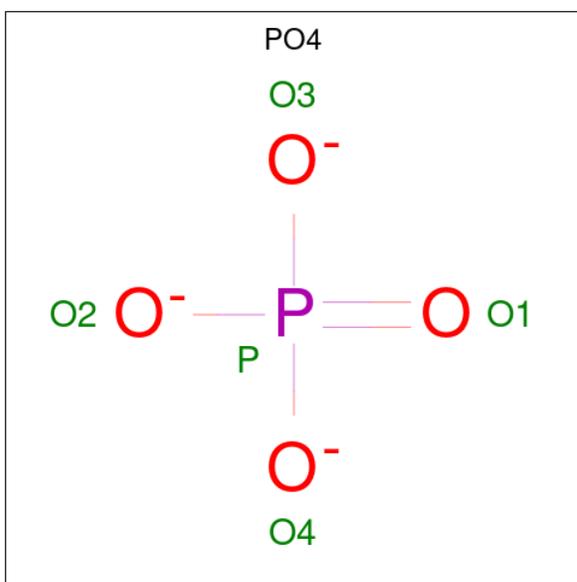
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	O	P	0	0	
			6	1	4	1			
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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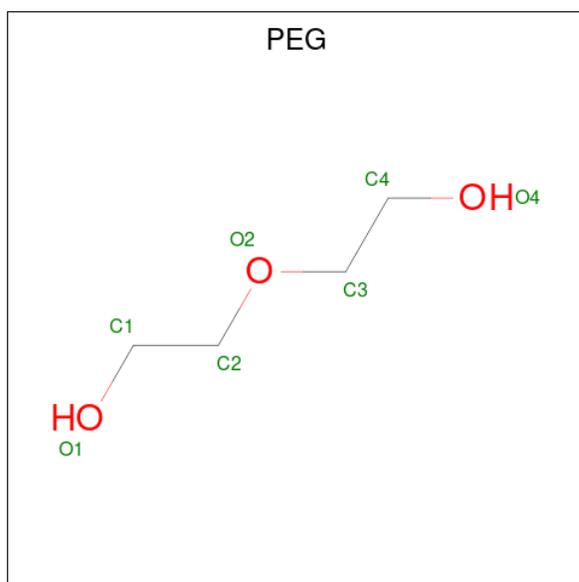
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	P	0	0
			6	1	4	1		
3	D	1	Total	C	O	P	0	0
			6	1	4	1		
3	E	1	Total	C	O	P	0	0
			6	1	4	1		
3	F	1	Total	C	O	P	0	0
			6	1	4	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

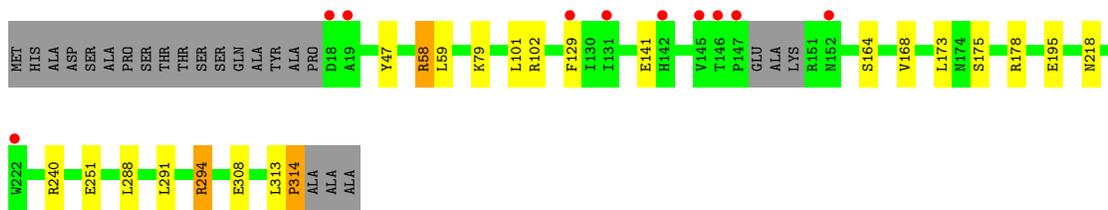
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



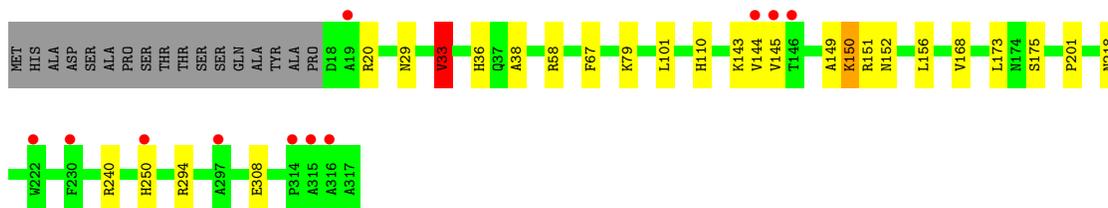
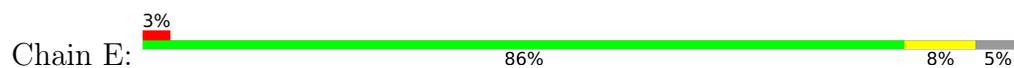
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

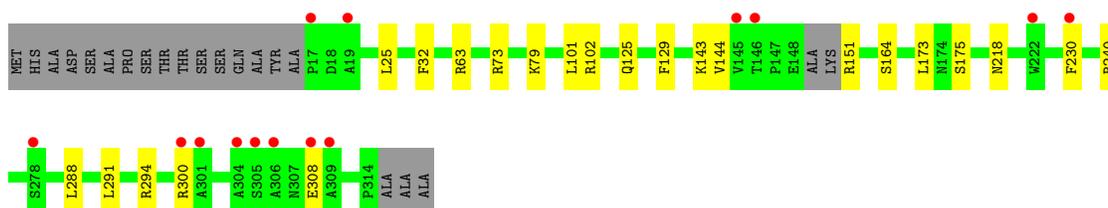
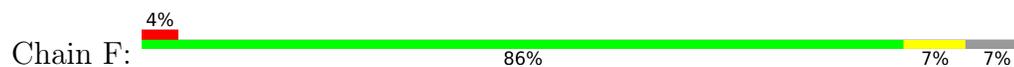
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	B	117	Total O 117 117	0	0
6	C	111	Total O 111 111	0	0
6	D	78	Total O 79 79	0	1
6	E	103	Total O 103 103	0	0
6	F	72	Total O 72 72	0	0



- Molecule 1: Aminotransferase, class 4



- Molecule 1: Aminotransferase, class 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.30Å 164.30Å 190.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	142.29 – 2.30 142.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (142.29-2.30) 99.6 (142.29-2.30)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.228 0.207 , 0.229	Depositor DCC
R_{free} test set	6635 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14415	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: PO4, PLP, GOL, PEG

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	0.84	4/2340 (0.2%)	1.12	6/3179 (0.2%)
1	B	0.80	1/2392 (0.0%)	1.09	6/3252 (0.2%)
1	C	0.76	1/2330 (0.0%)	1.14	12/3164 (0.4%)
1	D	0.83	3/2282 (0.1%)	1.21	8/3099 (0.3%)
1	E	0.77	0/2317	1.12	6/3149 (0.2%)
1	F	0.68	0/2314	1.07	5/3142 (0.2%)
All	All	0.78	9/13975 (0.1%)	1.13	43/18985 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	GLU	CD-OE2	13.27	1.40	1.25
1	A	250[A]	HIS	C-O	8.99	1.40	1.23
1	A	250[B]	HIS	C-O	8.99	1.40	1.23
1	B	258	GLU	CD-OE2	-7.63	1.17	1.25
1	D	195	GLU	CD-OE2	7.42	1.33	1.25

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294[A]	ARG	CG-CD-NE	14.88	143.05	111.80
1	D	294[B]	ARG	CG-CD-NE	14.88	143.05	111.80
1	D	294[A]	ARG	NE-CZ-NH2	11.23	125.92	120.30
1	D	294[B]	ARG	NE-CZ-NH2	11.23	125.92	120.30
1	F	129	PHE	CB-CA-C	10.96	132.33	110.40

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	2285	0	2273	19	0
1	B	2328	0	2304	25	0
1	C	2269	0	2264	11	0
1	D	2231	0	2214	12	0
1	E	2263	0	2225	11	0
1	F	2256	0	2241	12	0
2	A	18	0	24	2	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	18	0	24	0	0
2	F	6	0	8	0	0
3	A	6	0	0	0	0
3	B	16	0	5	5	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	B	21	0	30	4	0
5	E	14	0	20	1	0
5	F	7	0	10	1	0
6	A	129	0	0	1	0
6	B	117	0	0	2	0
6	C	111	0	0	1	0
6	D	79	0	0	1	0
6	E	103	0	0	2	0
6	F	72	0	0	1	0
All	All	14415	0	13658	84	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 3.

The worst 5 of 84 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:A:73[A]:ARG:NH2	1:A:230[A]:PHE:HZ	1.48	1.12
1:C:102[B]:ARG:HH21	1:C:102[B]:ARG:HG2	1.12	1.09
1:F:73[B]:ARG:CZ	1:F:230[B]:PHE:HZ	1.66	1.07
1:C:102[B]:ARG:NH1	6:C:501:HOH:O	1.72	1.06
1:B:73:ARG:CZ	1:B:230[A]:PHE:HZ	1.72	1.01

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	301/317 (95%)	293 (97%)	8 (3%)	0	100	100
1	B	308/317 (97%)	300 (97%)	8 (3%)	0	100	100
1	C	300/317 (95%)	295 (98%)	5 (2%)	0	100	100
1	D	292/317 (92%)	285 (98%)	7 (2%)	0	100	100
1	E	301/317 (95%)	290 (96%)	9 (3%)	2 (1%)	22	26
1	F	296/317 (93%)	288 (97%)	8 (3%)	0	100	100
All	All	1798/1902 (94%)	1751 (97%)	45 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	144	VAL
1	E	145	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/248 (96%)	228 (96%)	10 (4%)	30	42
1	B	244/248 (98%)	232 (95%)	12 (5%)	25	35
1	C	237/248 (96%)	224 (94%)	13 (6%)	21	30
1	D	233/248 (94%)	224 (96%)	9 (4%)	32	46
1	E	232/248 (94%)	223 (96%)	9 (4%)	32	46
1	F	235/248 (95%)	225 (96%)	10 (4%)	29	40
All	All	1419/1488 (95%)	1356 (96%)	63 (4%)	28	39

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	ARG
1	F	125	GLN
1	D	79	LYS
1	F	101	LEU
1	F	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	29	ASN
1	E	110	HIS
1	E	190	GLN
1	E	142	HIS
1	C	231	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	D	403	-	4,4,4	2.34	2 (50%)	6,6,6	1.67	2 (33%)
3	PLP	B	404	-	16,16,16	1.02	2 (12%)	20,23,23	1.81	4 (20%)
4	PO4	A	404	-	4,4,4	3.63	3 (75%)	6,6,6	1.05	0
2	GOL	E	401	-	5,5,5	0.22	0	5,5,5	0.42	0
2	GOL	E	404	-	5,5,5	0.16	0	5,5,5	0.86	0
4	PO4	F	404	-	4,4,4	1.68	1 (25%)	6,6,6	0.68	0
5	PEG	F	402	-	6,6,6	0.49	0	5,5,5	0.52	0
2	GOL	E	407	-	5,5,5	0.20	0	5,5,5	0.60	0
2	GOL	D	401	-	5,5,5	0.32	0	5,5,5	1.31	0
2	GOL	F	401	-	5,5,5	0.16	0	5,5,5	0.24	0
3	PLP	C	402	-	5,5,16	1.82	2 (40%)	7,7,23	0.93	1 (14%)
2	GOL	C	401	-	5,5,5	0.13	0	5,5,5	1.01	0
3	PLP	A	403	-	5,5,16	2.13	2 (40%)	7,7,23	1.40	1 (14%)
3	PLP	D	402	-	5,5,16	2.03	1 (20%)	7,7,23	1.10	1 (14%)
5	PEG	B	403	-	6,6,6	1.17	1 (16%)	5,5,5	1.07	0
5	PEG	B	402	-	6,6,6	1.90	2 (33%)	5,5,5	1.45	1 (20%)
4	PO4	C	403	-	4,4,4	1.60	1 (25%)	6,6,6	0.99	1 (16%)
2	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.75	0
5	PEG	B	401	-	6,6,6	1.13	0	5,5,5	1.27	0
5	PEG	E	403	-	6,6,6	2.06	4 (66%)	5,5,5	1.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	F	403	-	5,5,16	1.41	1 (20%)	7,7,23	1.28	1 (14%)
4	PO4	B	405	-	4,4,4	1.51	1 (25%)	6,6,6	0.92	0
2	GOL	A	405	-	5,5,5	0.35	0	5,5,5	1.03	0
4	PO4	E	406	-	4,4,4	1.14	0	6,6,6	1.47	1 (16%)
2	GOL	A	401	-	5,5,5	0.24	0	5,5,5	0.55	0
5	PEG	E	402	-	6,6,6	1.08	0	5,5,5	0.92	0
3	PLP	E	405	-	5,5,16	3.09	1 (20%)	7,7,23	0.67	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	PLP	B	404	-	-	3/8/8/8	0/1/1/1
2	GOL	E	401	-	-	2/4/4/4	-
2	GOL	E	404	-	-	4/4/4/4	-
5	PEG	F	402	-	-	2/4/4/4	-
2	GOL	E	407	-	-	4/4/4/4	-
2	GOL	D	401	-	-	3/4/4/4	-
2	GOL	F	401	-	-	2/4/4/4	-
3	PLP	C	402	-	-	0/1/3/8	-
2	GOL	C	401	-	-	2/4/4/4	-
3	PLP	A	403	-	-	1/1/3/8	-
3	PLP	D	402	-	-	0/1/3/8	-
5	PEG	B	403	-	-	3/4/4/4	-
5	PEG	B	402	-	-	2/4/4/4	-
2	GOL	A	402	-	-	4/4/4/4	-
5	PEG	B	401	-	-	4/4/4/4	-
5	PEG	E	403	-	-	0/4/4/4	-
3	PLP	F	403	-	-	1/1/3/8	-
2	GOL	A	405	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
5	PEG	E	402	-	-	1/4/4/4	-
3	PLP	E	405	-	-	1/1/3/8	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	405	PLP	P-O4P	6.43	1.71	1.59
4	A	404	PO4	P-O1	5.64	1.64	1.50
3	D	402	PLP	P-O4P	4.10	1.67	1.59
4	D	403	PO4	P-O1	-3.85	1.41	1.50
4	A	404	PO4	P-O4	-3.72	1.43	1.54

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	PLP	C3-C4-C4A	-5.83	111.62	119.90
4	D	403	PO4	O4-P-O1	-2.88	100.37	110.89
3	F	403	PLP	O4P-P-O1P	-2.81	98.55	109.39
3	B	404	PLP	O3P-P-O2P	2.76	118.20	107.64
3	A	403	PLP	O2P-P-O4P	2.51	117.24	105.99

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	A	405	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	E	404	GOL	O1-C1-C2-C3

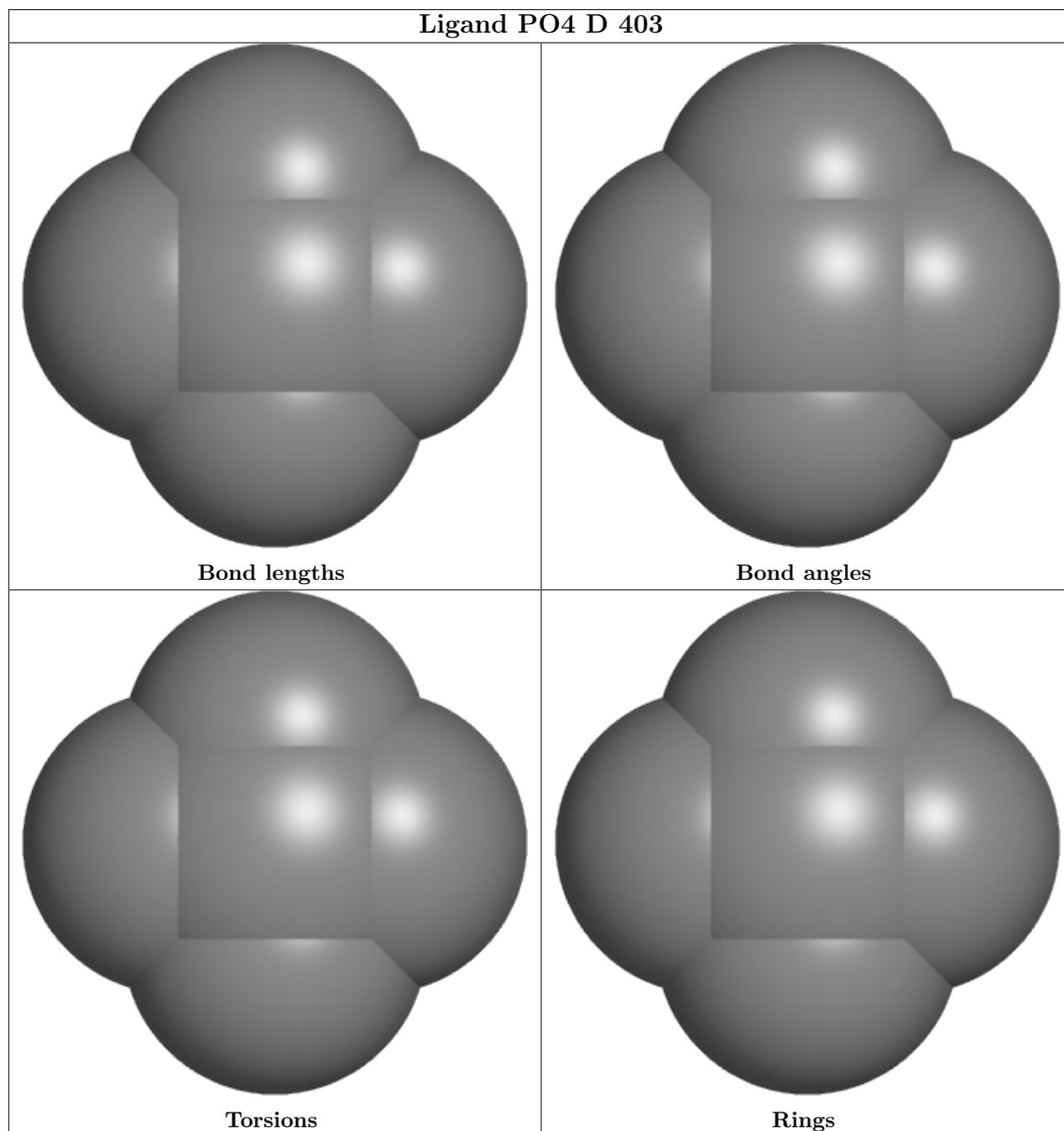
There are no ring outliers.

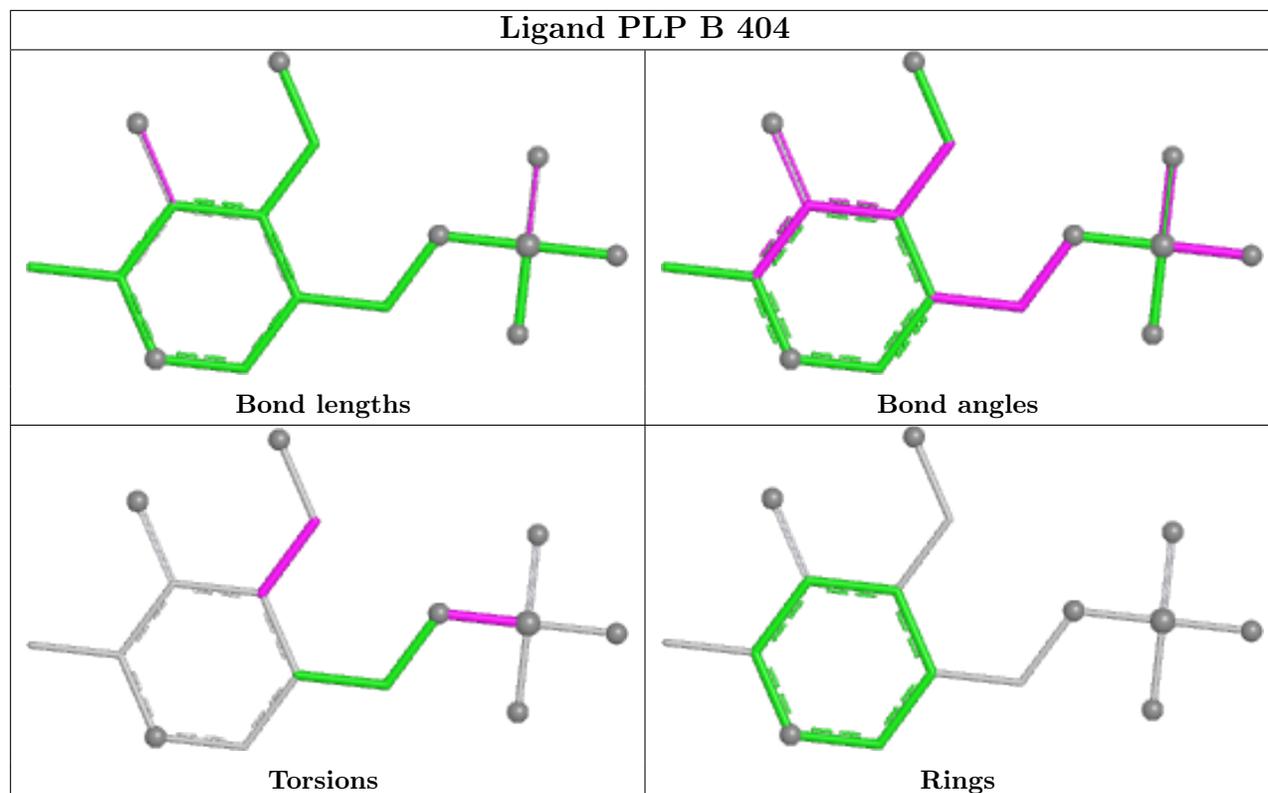
9 monomers are involved in 15 short contacts:

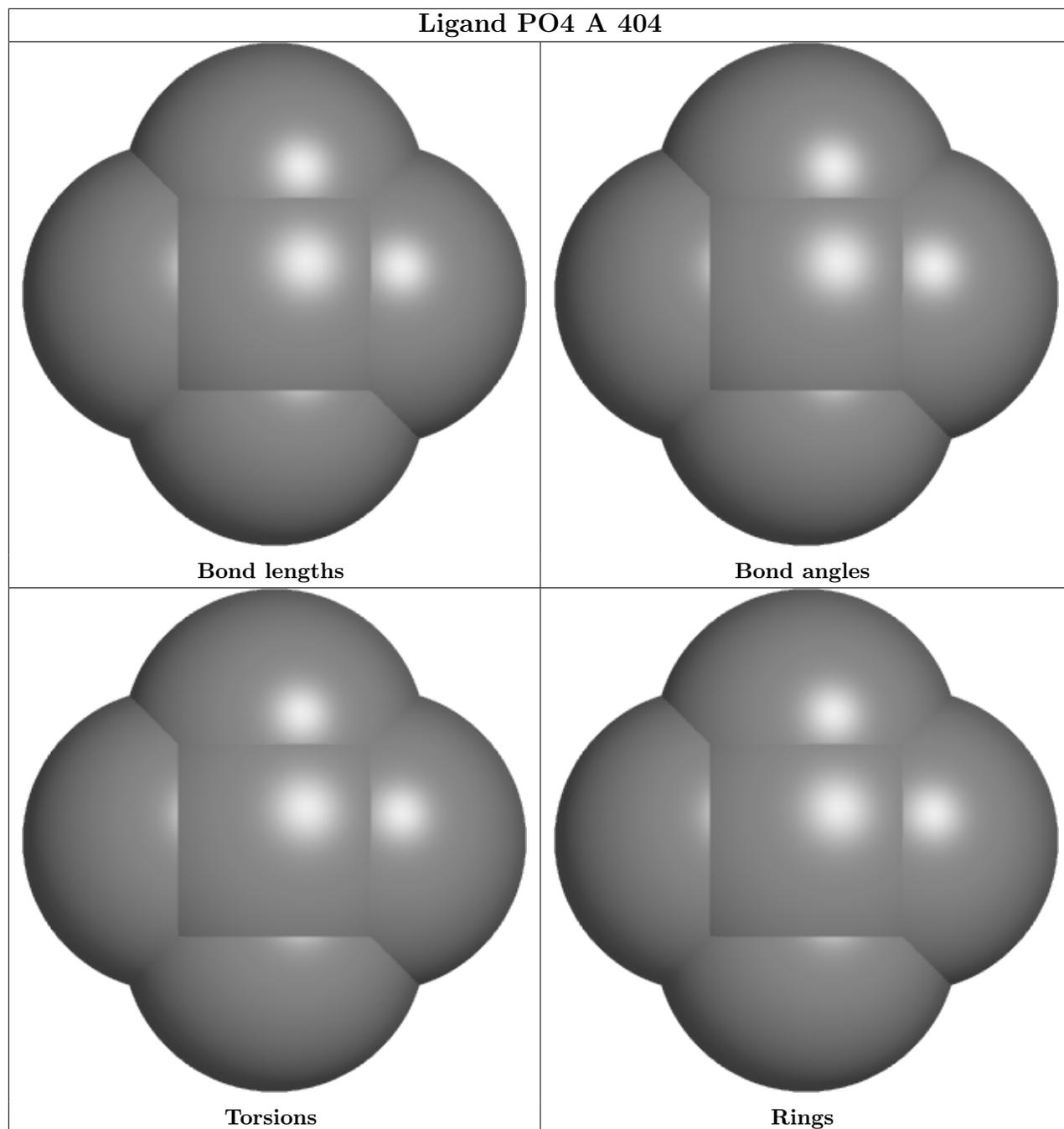
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	PO4	1	0
3	B	404	PLP	5	0
5	F	402	PEG	1	0
5	B	403	PEG	2	0
5	B	402	PEG	2	0
4	B	405	PO4	1	0
2	A	405	GOL	1	0
2	A	401	GOL	1	0
5	E	402	PEG	1	0

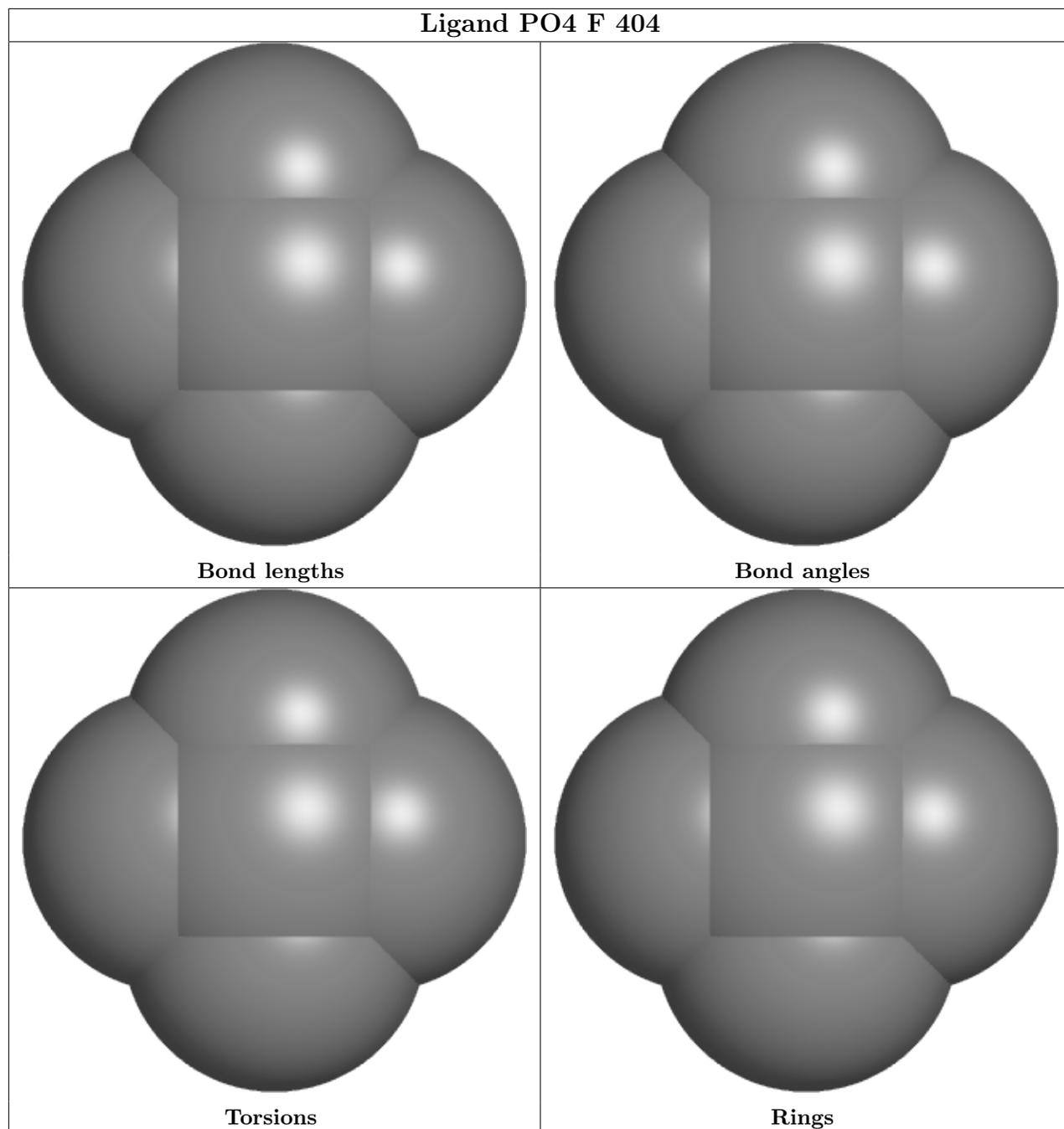
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

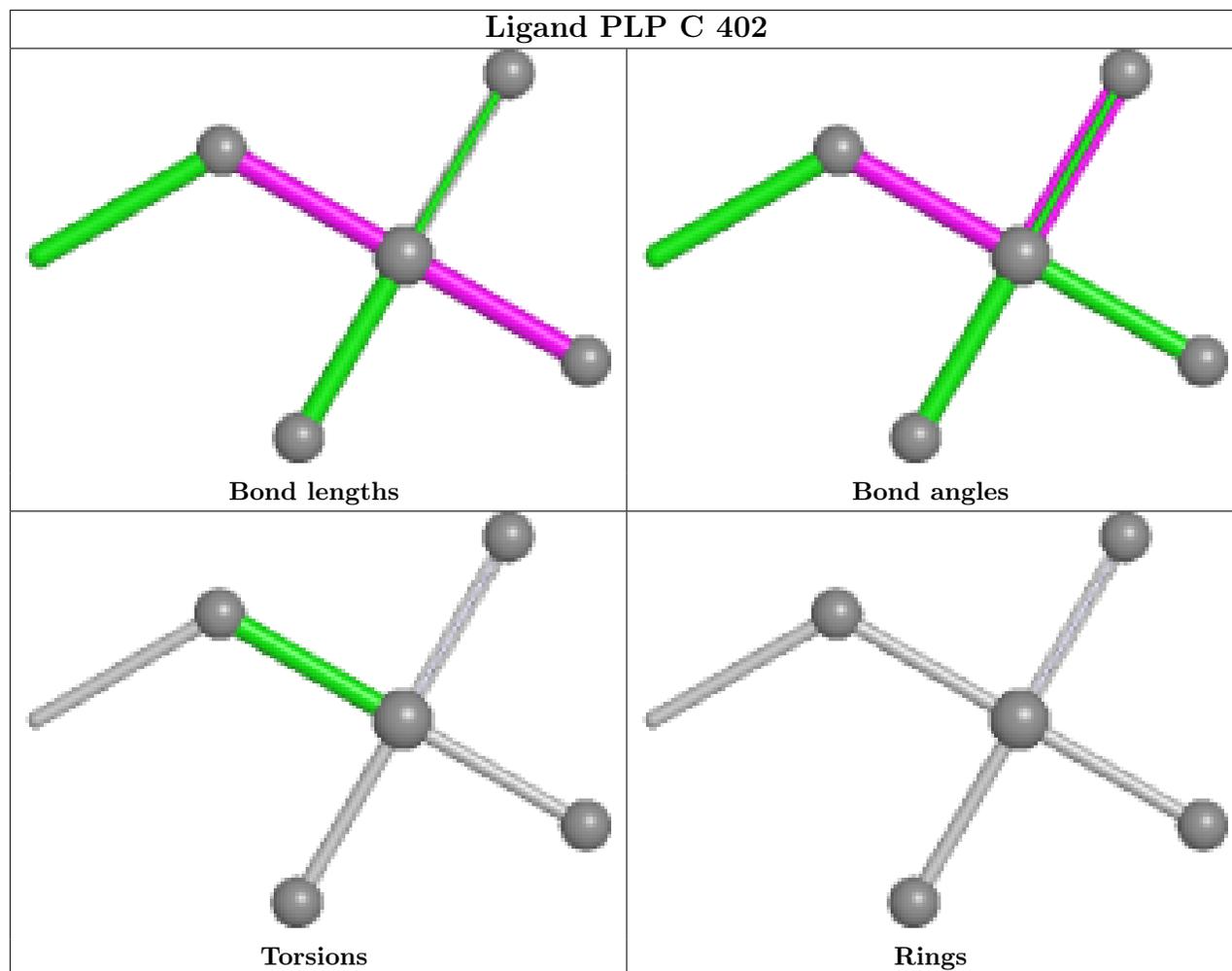
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

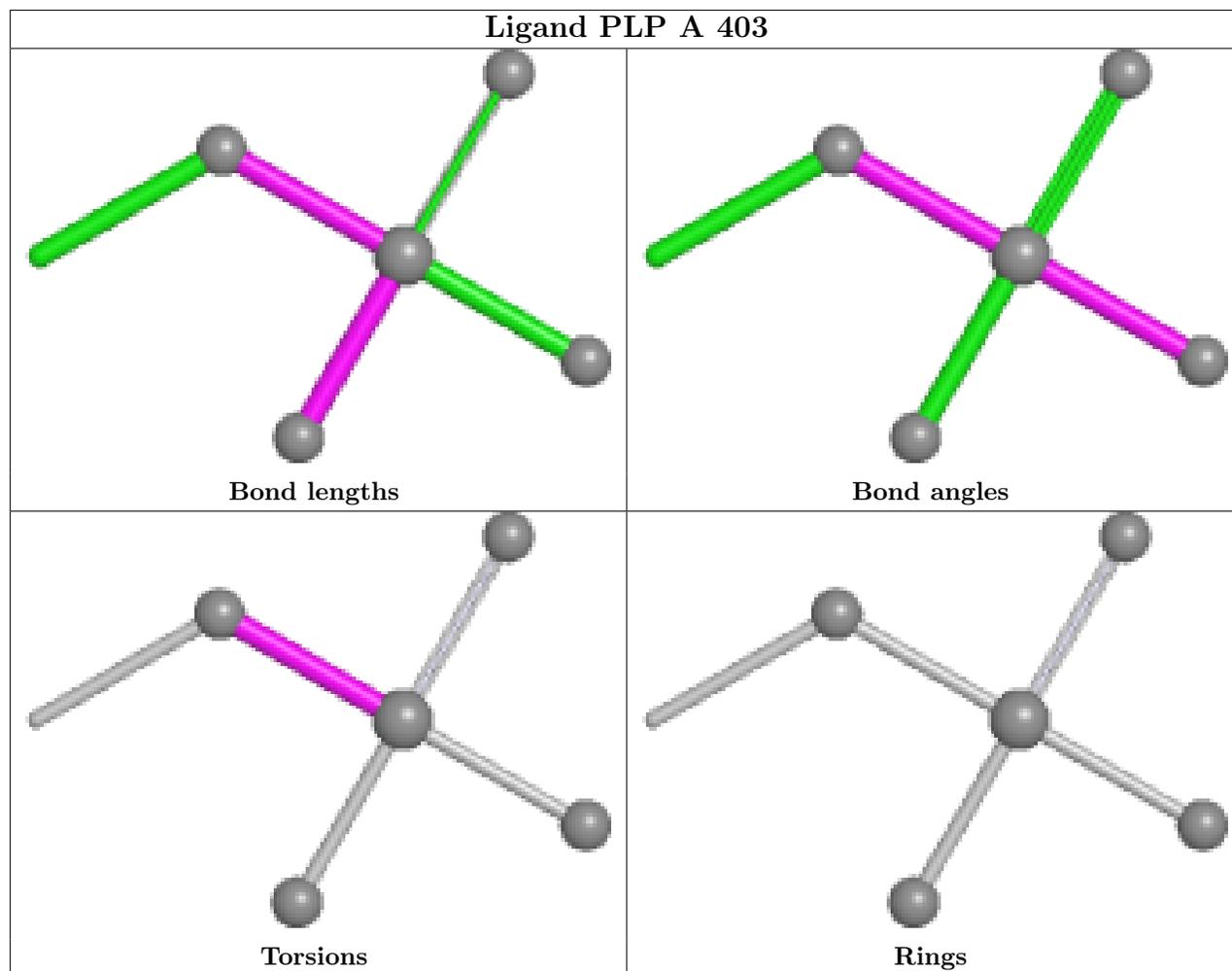


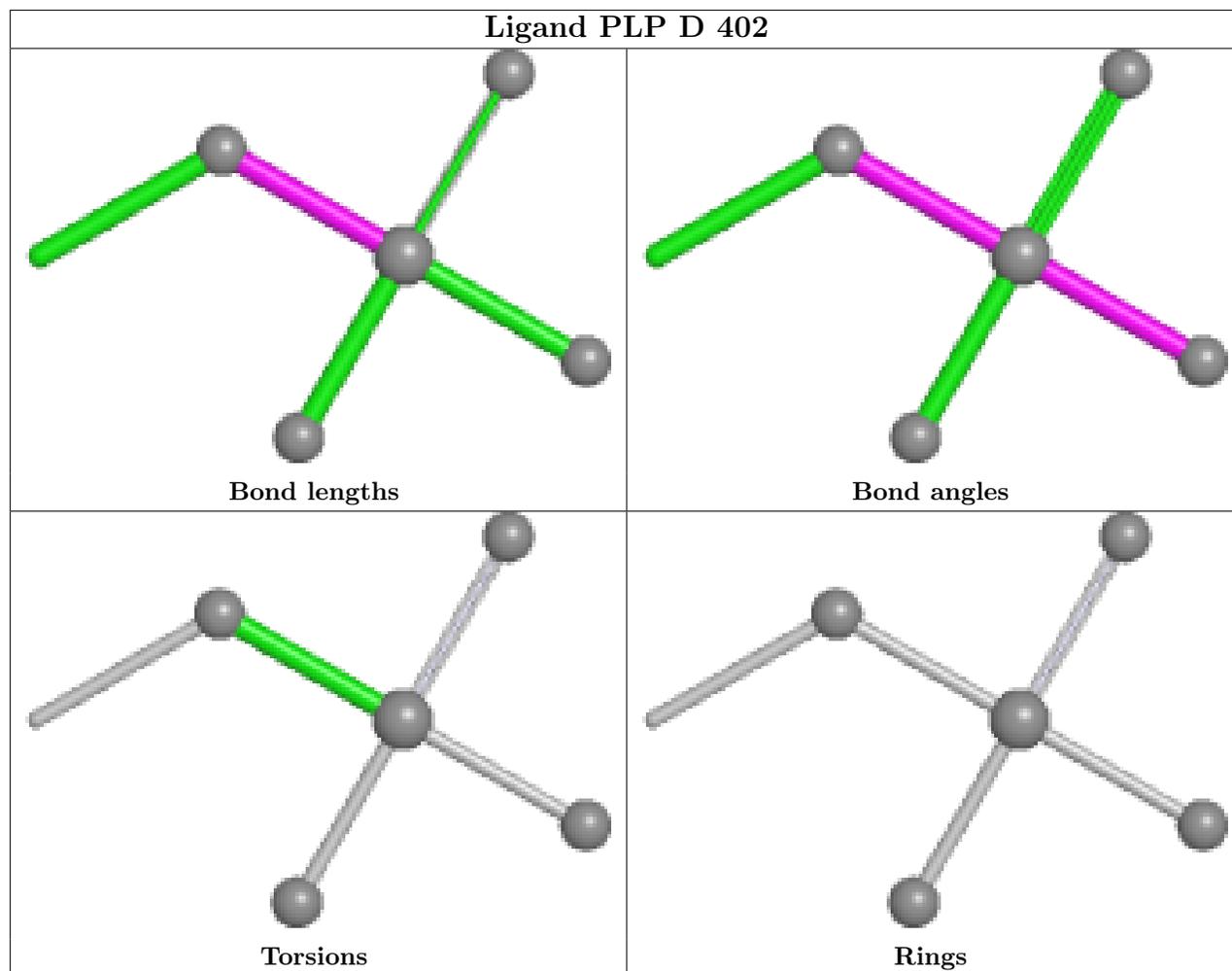


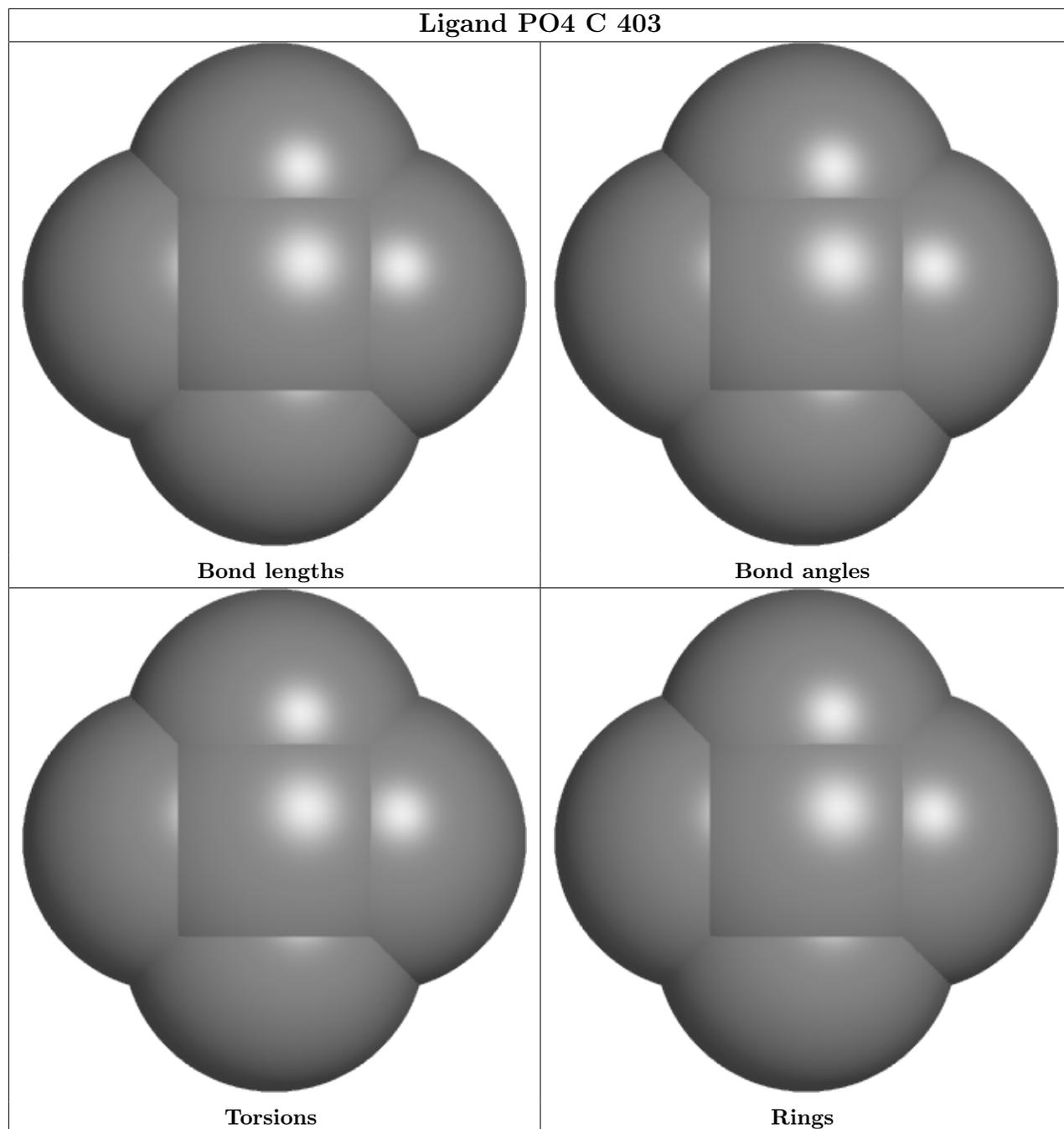


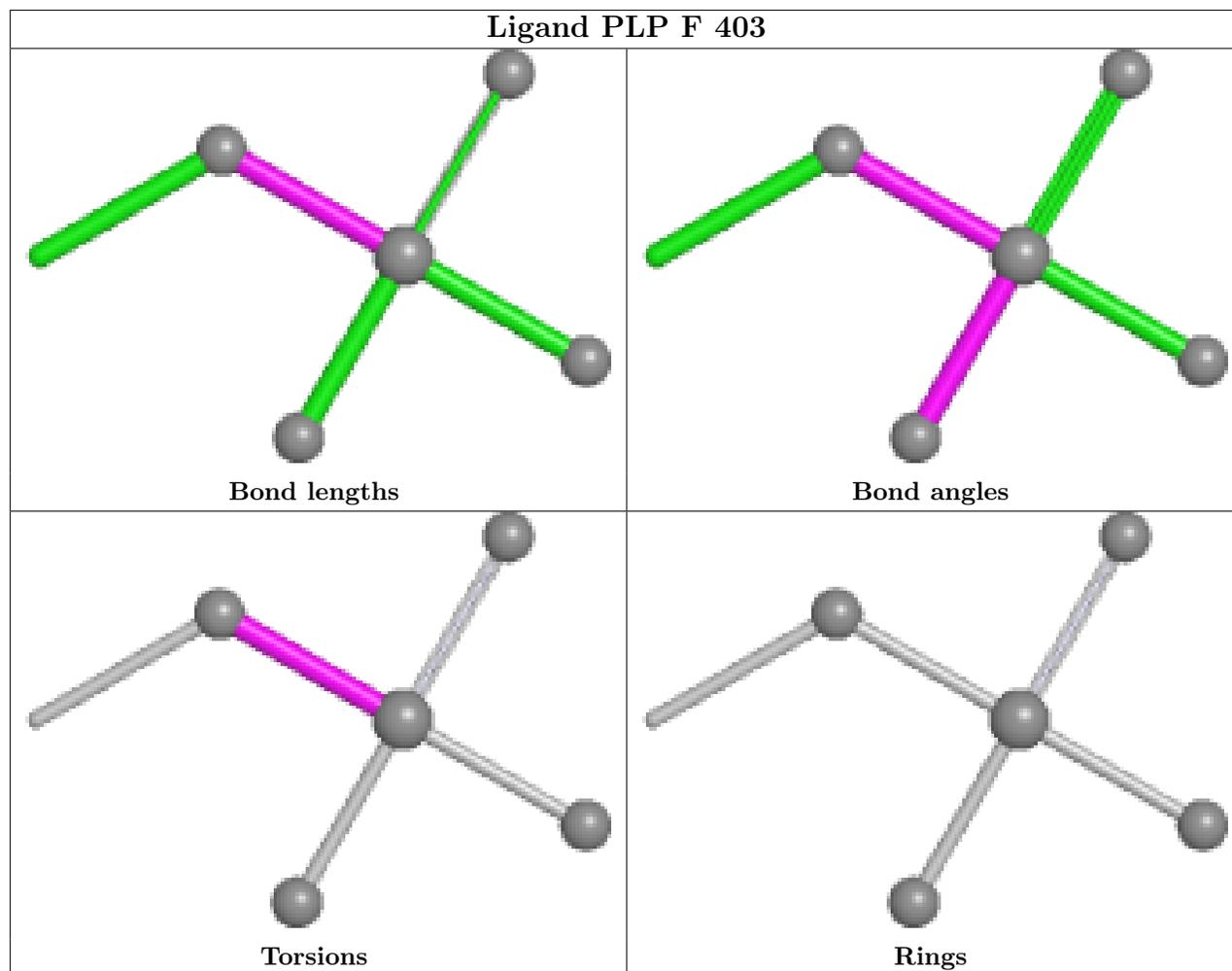


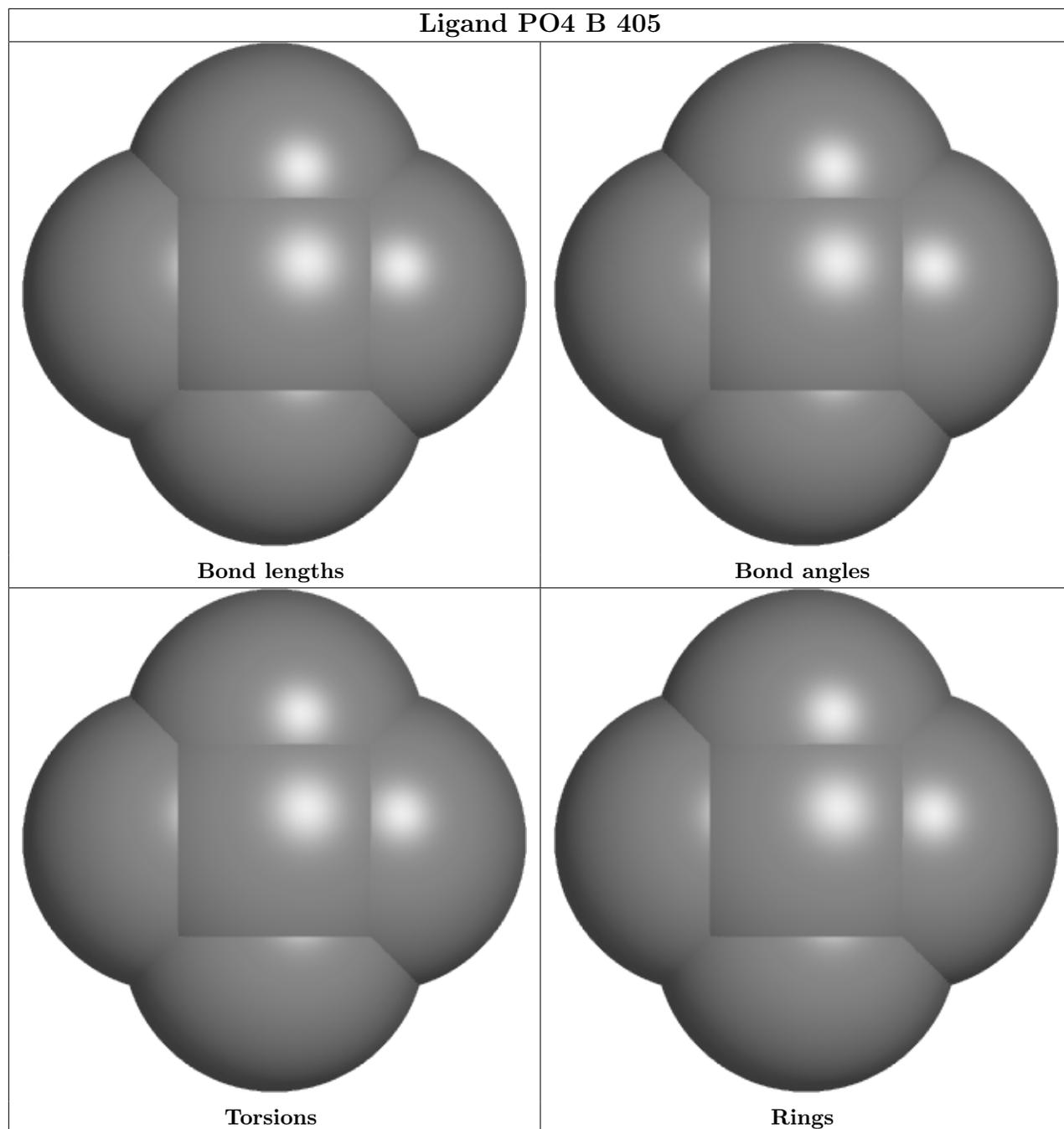




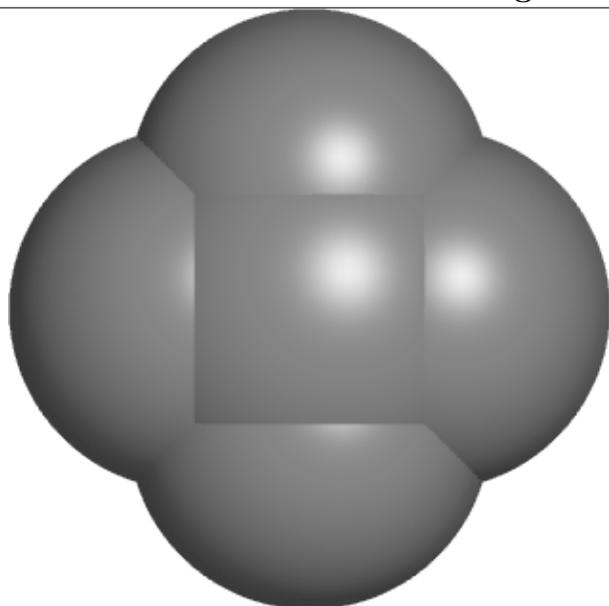




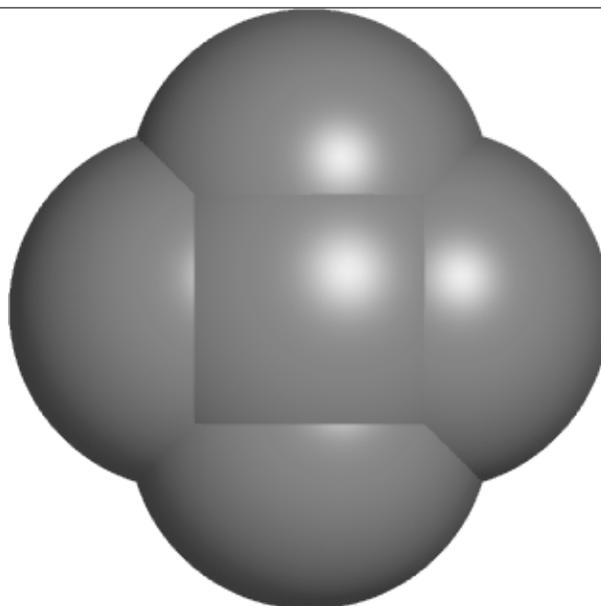




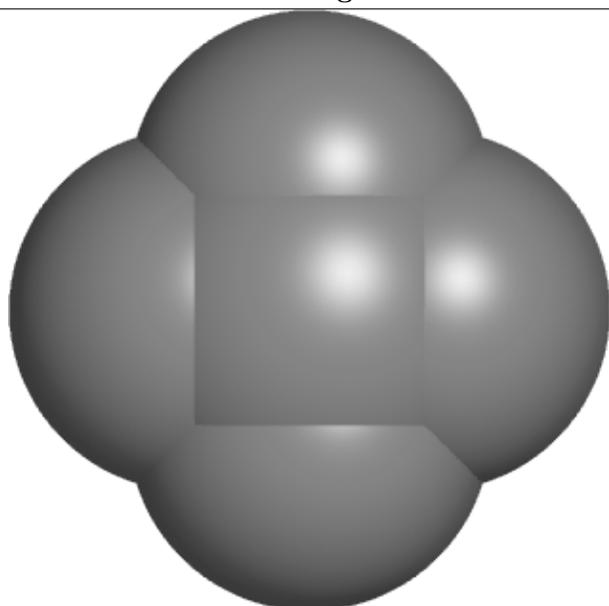
Ligand PO4 E 406



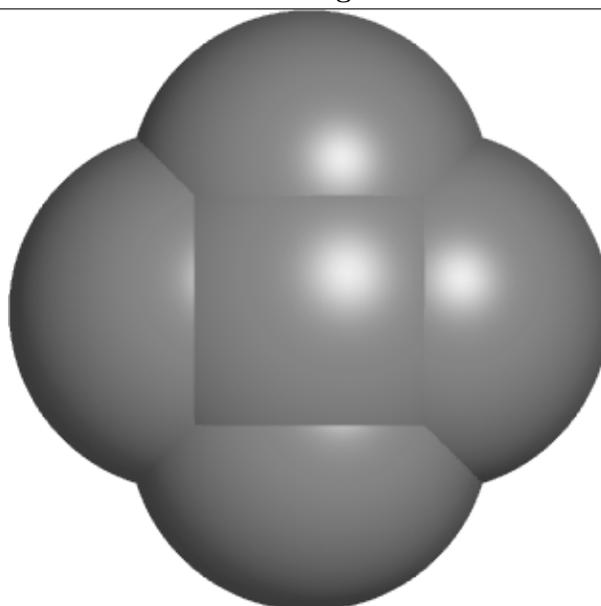
Bond lengths



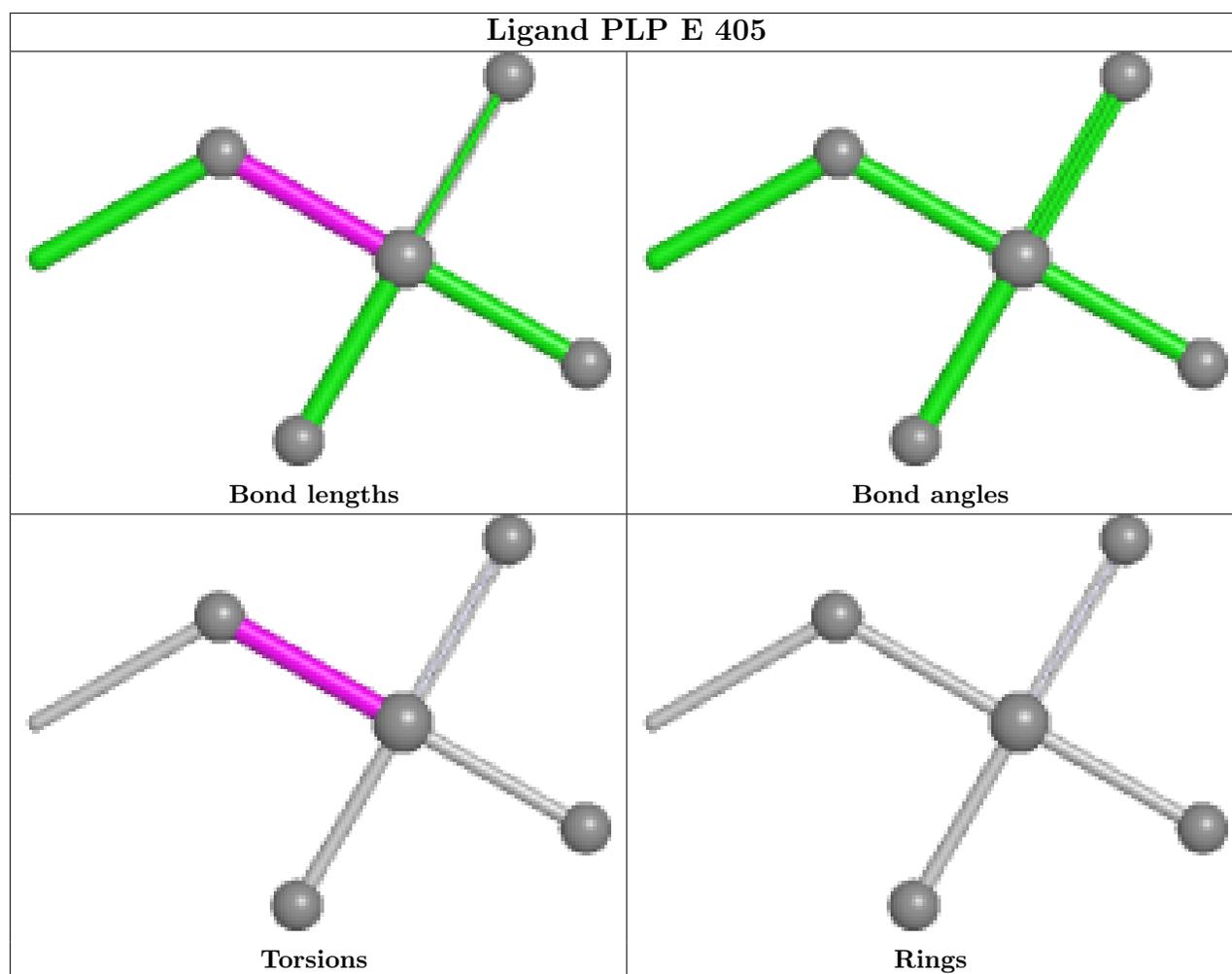
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	300/317 (94%)	0.60	10 (3%) 46 53	25, 35, 68, 124	0
1	B	306/317 (96%)	0.56	9 (2%) 51 58	26, 36, 67, 96	0
1	C	297/317 (93%)	0.57	10 (3%) 45 52	28, 39, 73, 98	0
1	D	294/317 (92%)	0.63	10 (3%) 45 52	28, 43, 76, 117	0
1	E	300/317 (94%)	0.59	11 (3%) 41 48	28, 38, 76, 103	0
1	F	296/317 (93%)	0.62	14 (4%) 31 38	31, 46, 82, 105	0
All	All	1793/1902 (94%)	0.59	64 (3%) 42 49	25, 39, 74, 124	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	THR	7.8
1	D	19	ALA	5.5
1	D	129	PHE	4.5
1	E	314	PRO	4.0
1	B	149	ALA	4.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

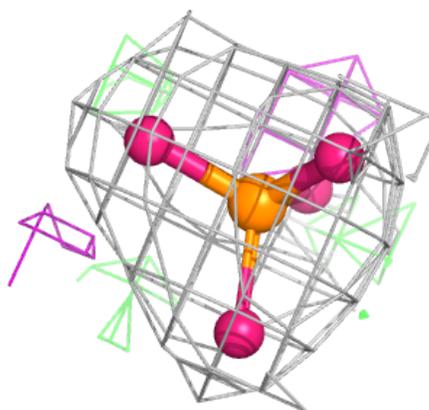
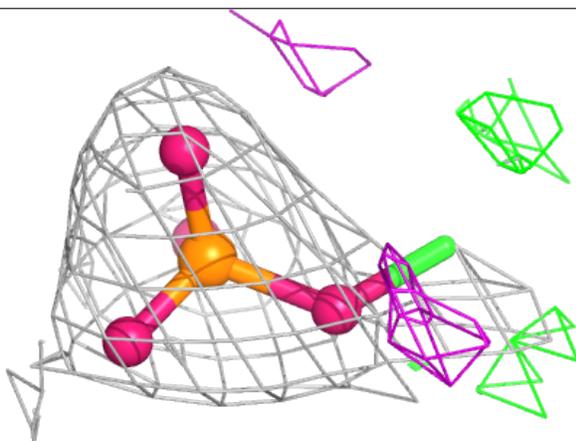
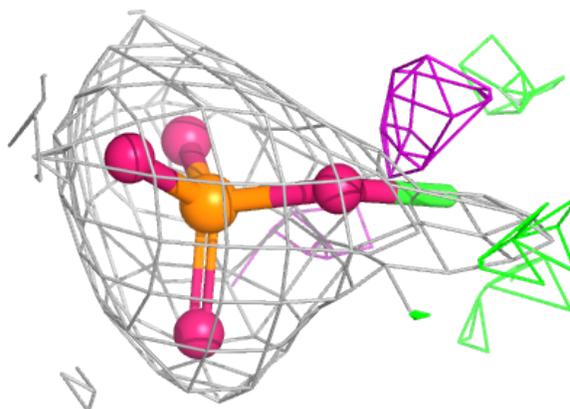
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	E	402	7/7	0.56	0.29	69,75,91,103	0
5	PEG	B	402	7/7	0.67	0.23	44,52,65,76	0
5	PEG	B	403	7/7	0.72	0.37	59,67,74,76	0
5	PEG	F	402	7/7	0.72	0.18	87,98,105,118	0
5	PEG	E	403	7/7	0.75	0.39	50,71,79,82	0
2	GOL	A	402	6/6	0.75	0.18	66,73,81,82	0
2	GOL	E	404	6/6	0.76	0.14	68,79,83,87	0
5	PEG	B	401	7/7	0.79	0.19	57,72,101,103	0
2	GOL	E	407	6/6	0.83	0.25	53,61,70,72	0
2	GOL	A	405	6/6	0.85	0.22	52,56,58,60	0
2	GOL	E	401	6/6	0.86	0.27	64,73,80,86	0
2	GOL	C	401	6/6	0.87	0.27	48,51,54,55	0
2	GOL	D	401	6/6	0.90	0.14	43,54,59,61	0
2	GOL	A	401	6/6	0.91	0.18	30,32,35,39	0
2	GOL	F	401	6/6	0.91	0.25	48,58,69,69	0
3	PLP	D	402	6/16	0.97	0.24	34,40,48,60	0
3	PLP	E	405	6/16	0.97	0.19	33,33,40,54	0
4	PO4	C	403	5/5	0.97	0.18	46,48,49,57	0
4	PO4	E	406	5/5	0.97	0.17	40,41,47,54	0
3	PLP	B	404	16/16	0.97	0.30	29,31,33,36	11
3	PLP	A	403	6/16	0.98	0.20	29,34,38,39	1
4	PO4	D	403	5/5	0.98	0.18	40,41,43,46	0
3	PLP	C	402	6/16	0.98	0.24	33,39,42,57	0
4	PO4	F	404	5/5	0.98	0.19	42,46,51,55	0
3	PLP	F	403	6/16	0.98	0.17	38,40,40,41	1
4	PO4	A	404	5/5	0.99	0.20	35,36,40,42	0
4	PO4	B	405	5/5	0.99	0.16	33,33,38,39	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.

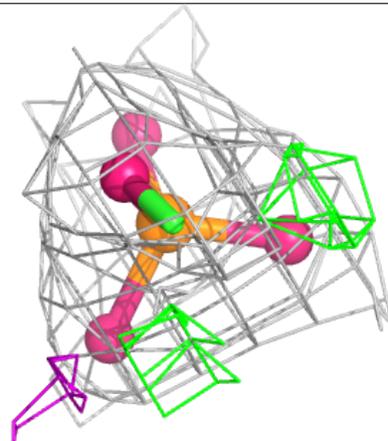
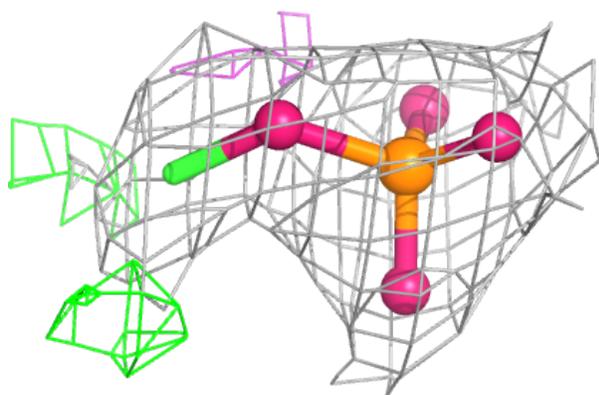
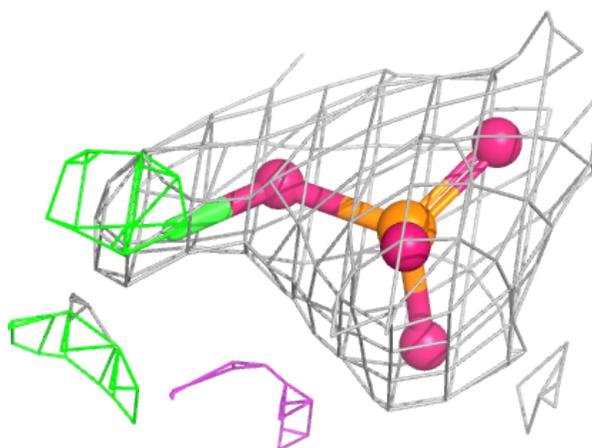
Electron density around PLP D 402:

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



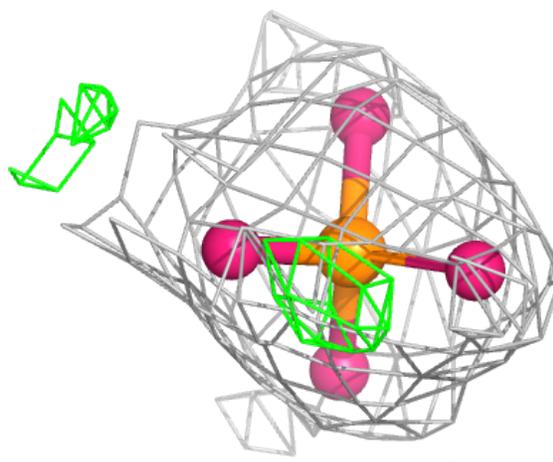
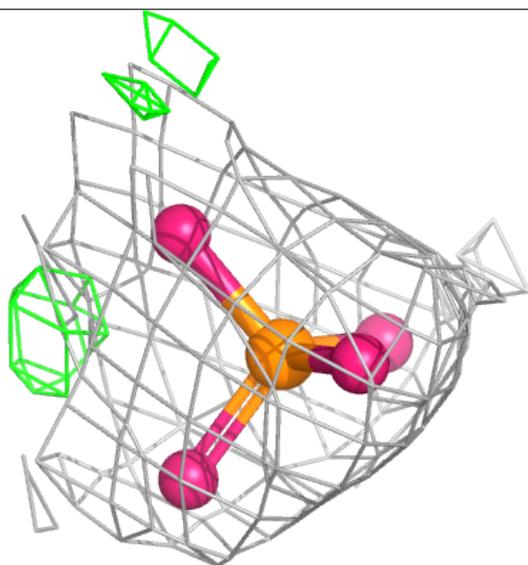
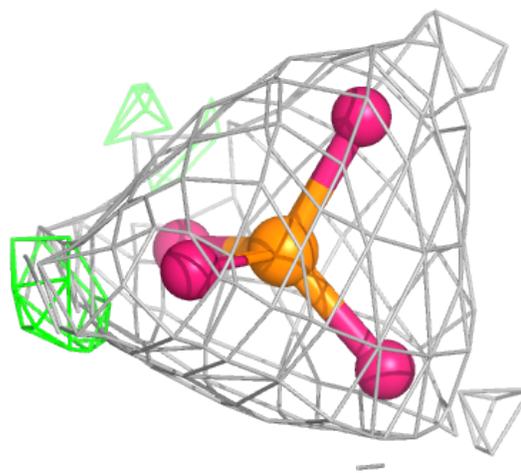
Electron density around PLP E 405:

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



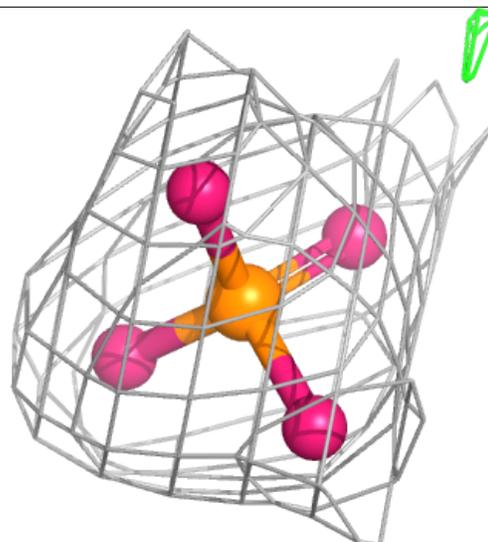
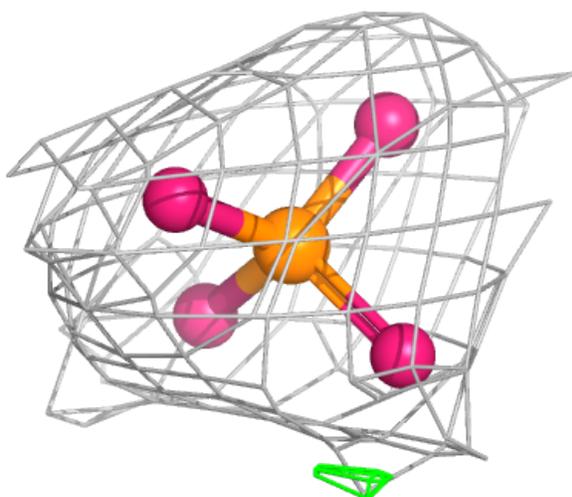
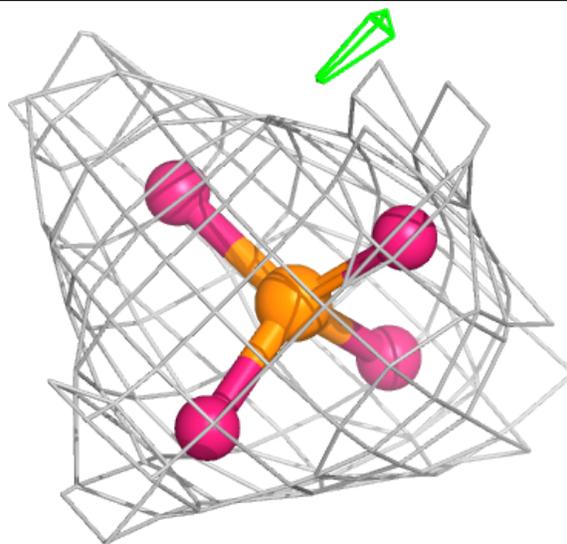
Electron density around PO4 C 403:

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



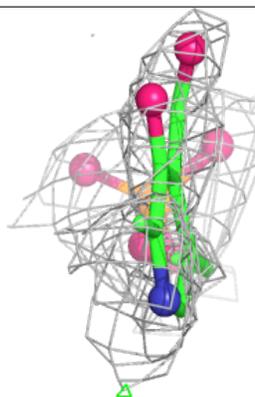
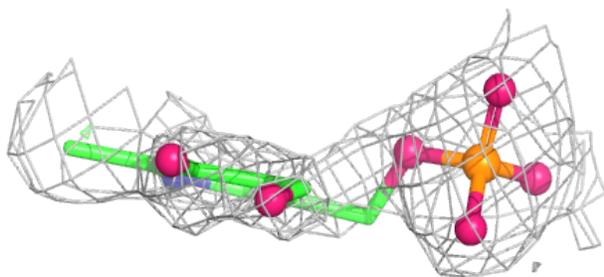
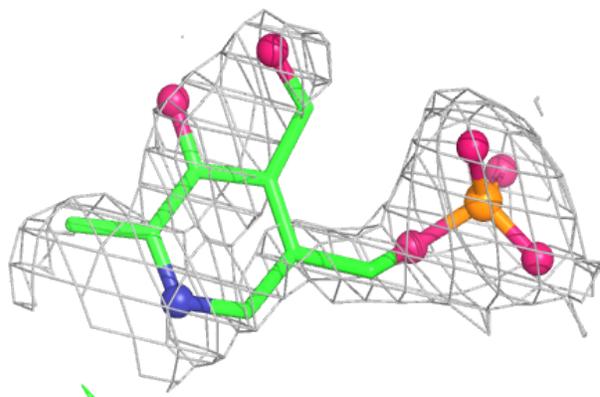
Electron density around PO4 E 406:

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and green (positive)



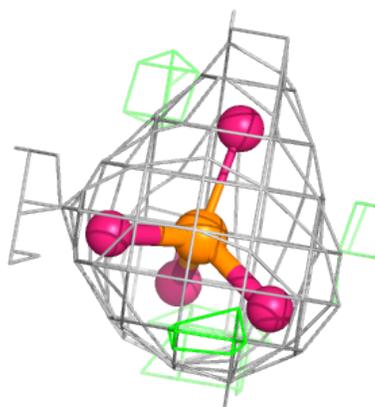
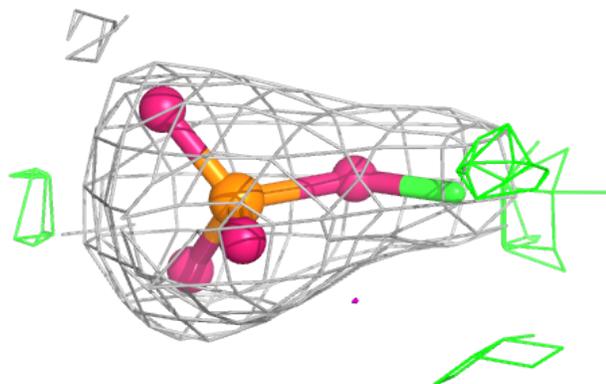
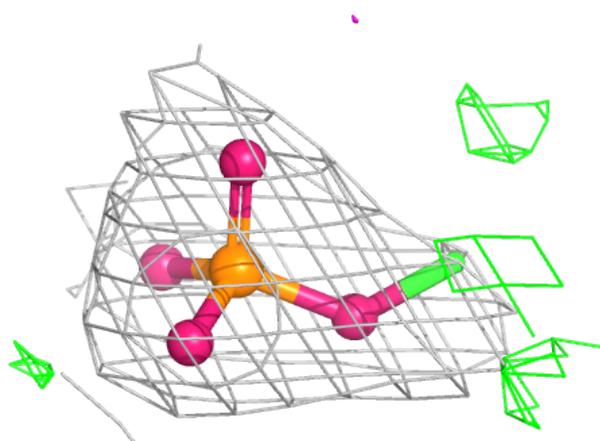
Electron density around PLP B 404:

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



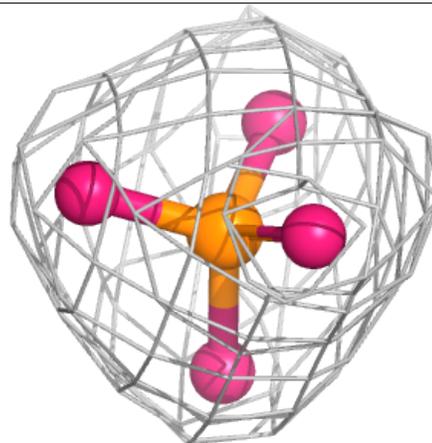
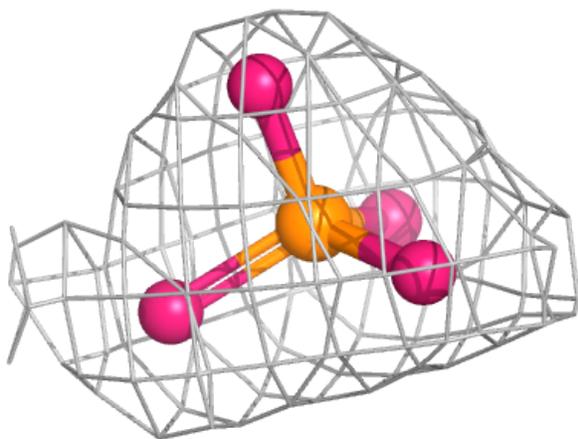
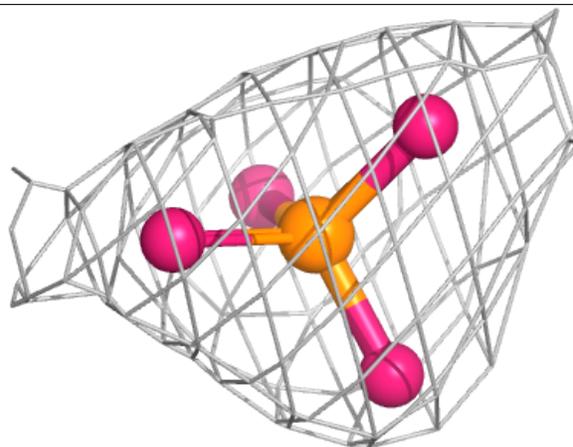
Electron density around PLP A 403:

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and green (positive)



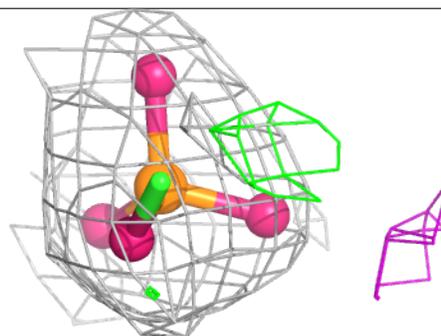
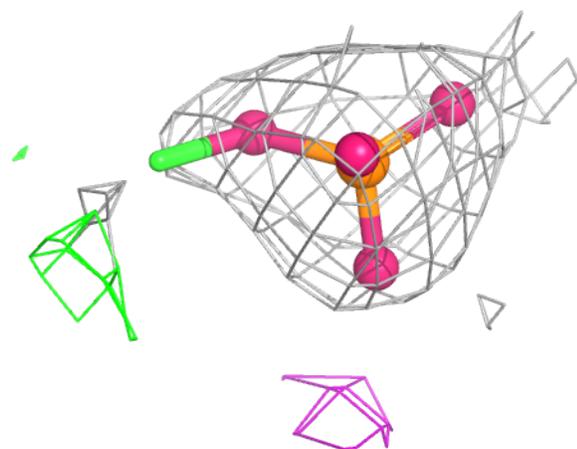
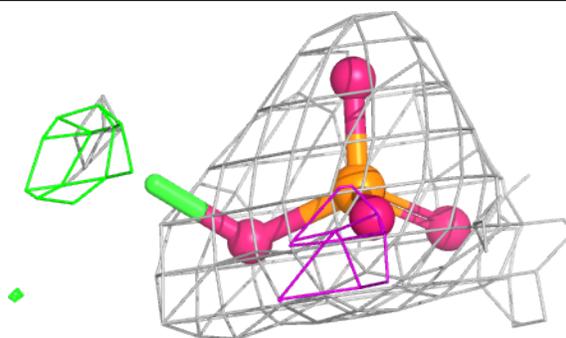
Electron density around PO4 D 403:

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and green (positive)



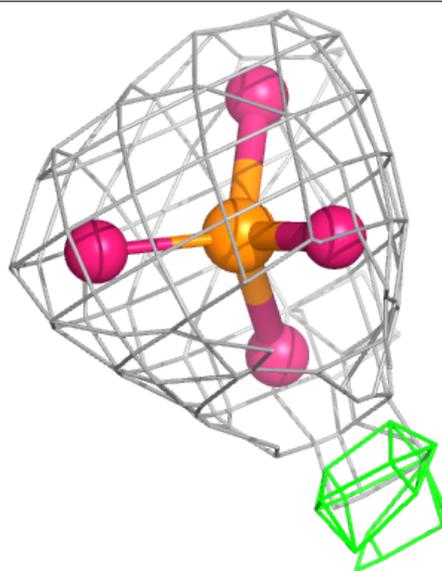
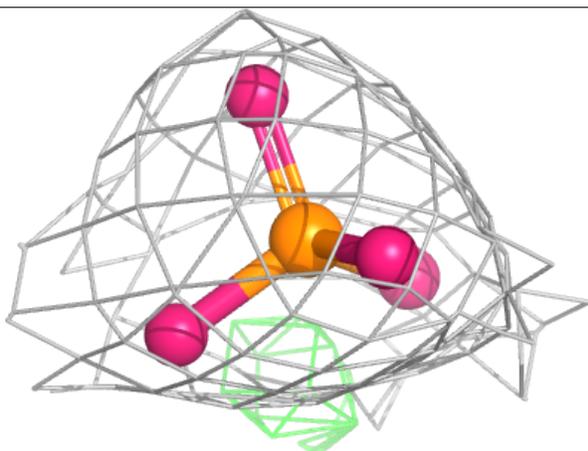
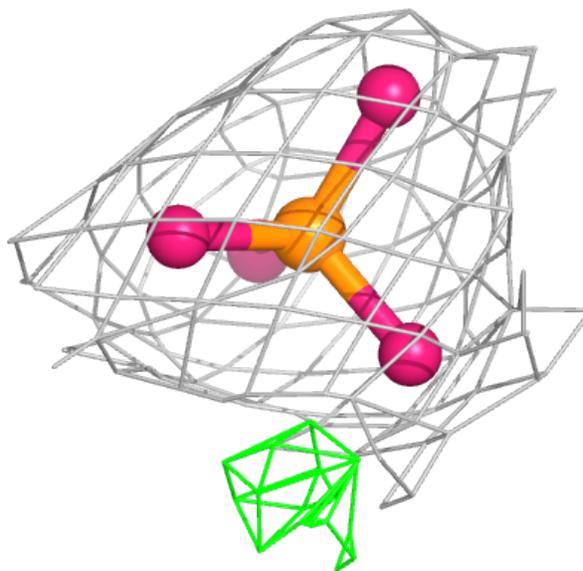
Electron density around PLP C 402:

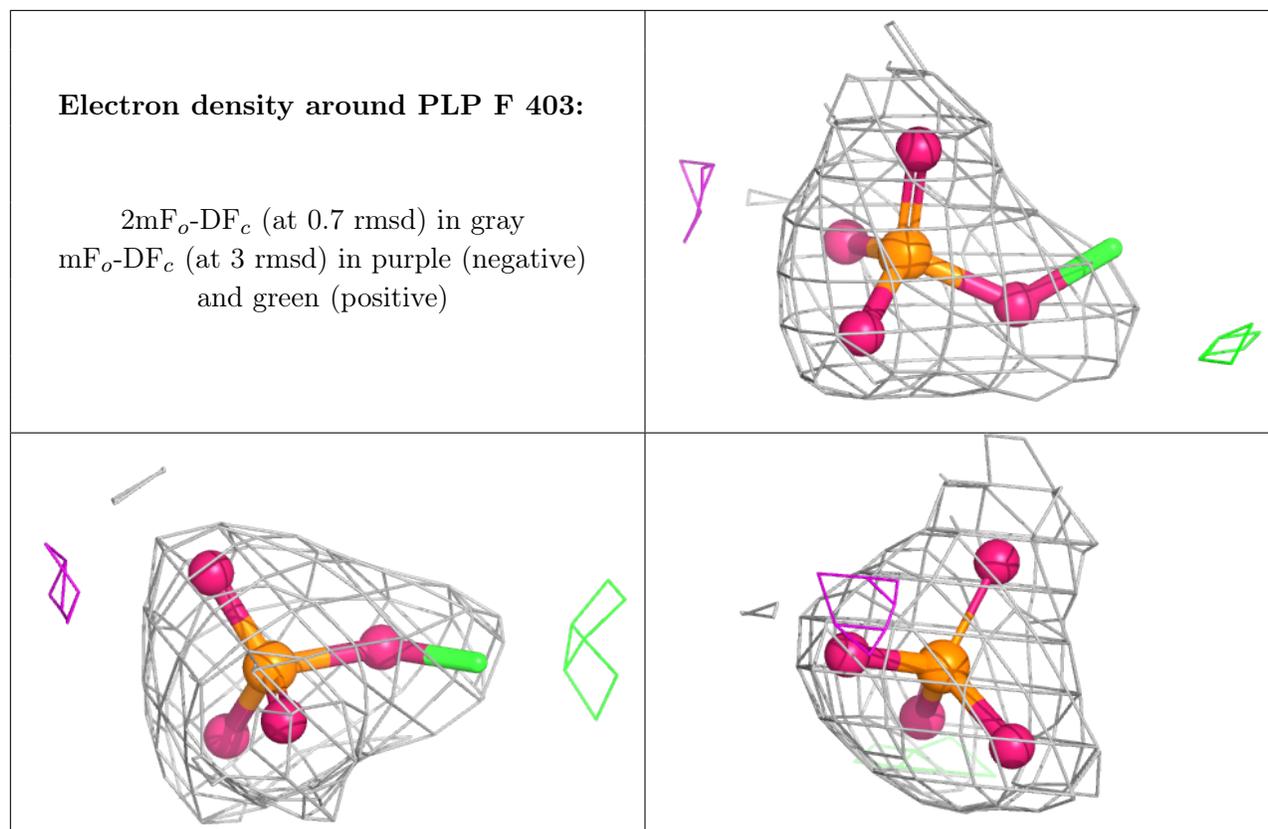
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PO4 F 404:

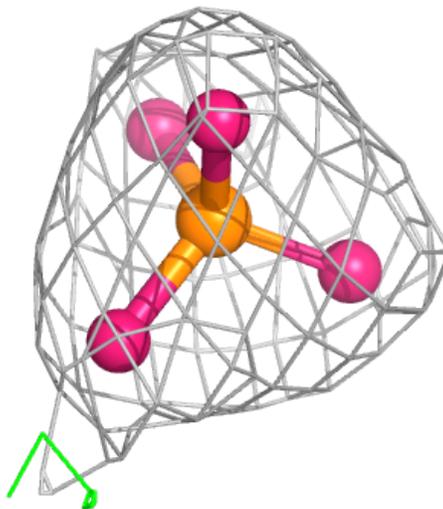
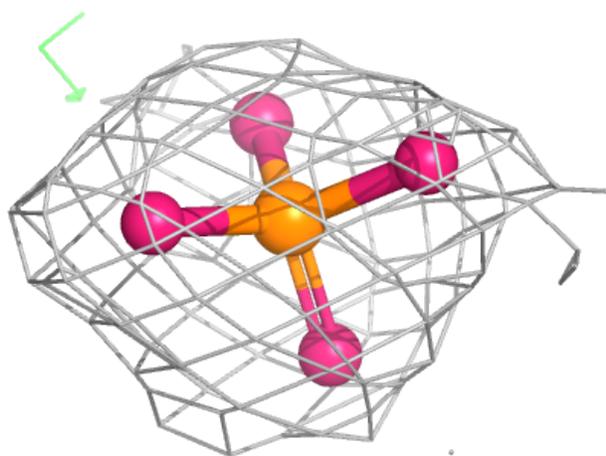
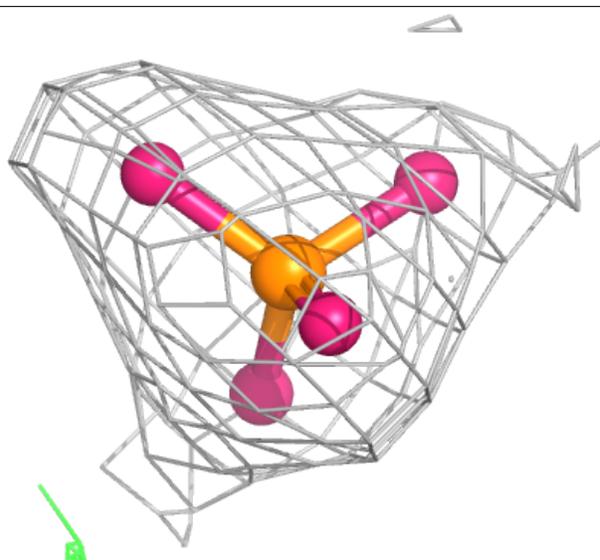
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

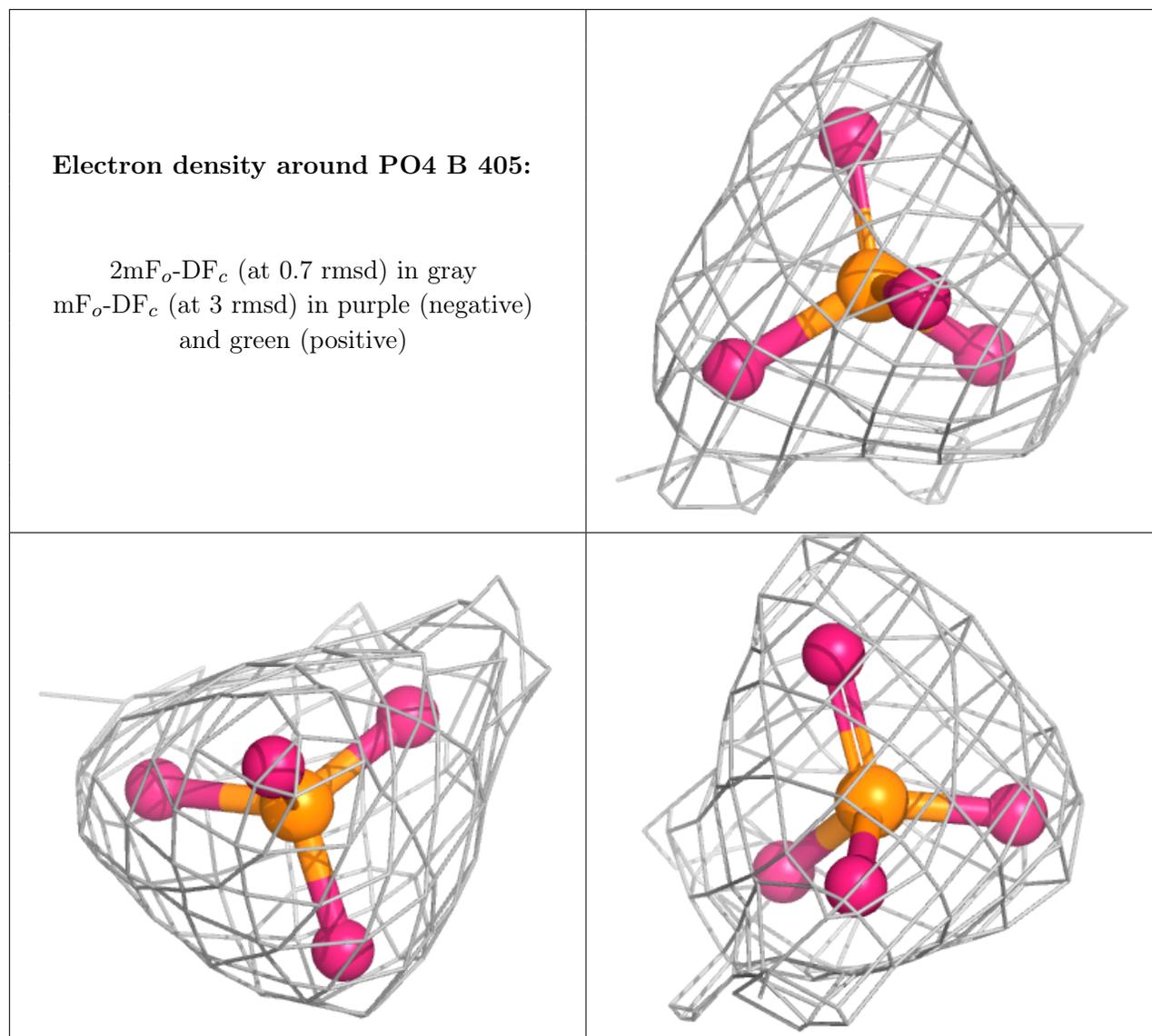




Electron density around PO4 A 404:

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.