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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

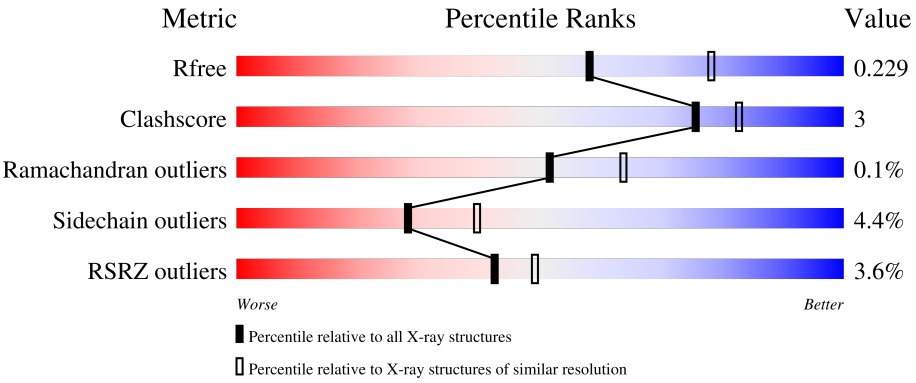
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 <=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	3% 86% 8% • 5%
1	B	317	3% 86% 9% • •
1	C	317	3% 87% 6% 6%
1	D	317	3% 85% 6% • 7%
1	E	317	3% 86% 8% 5%

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Mol	Chain	Length	Quality of chain
1	F	317	4% 86% 7% 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	PO4	D	403	-	X	-	-

2 Entry composition (i)

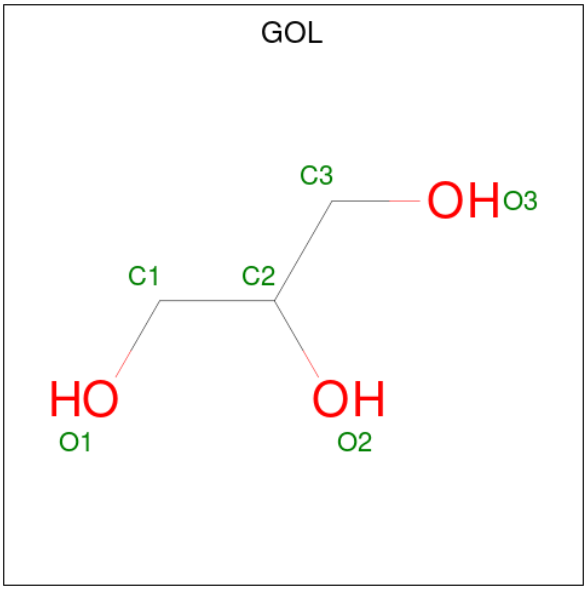
There are 6 unique types of molecules in this entry. The entry contains 14415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

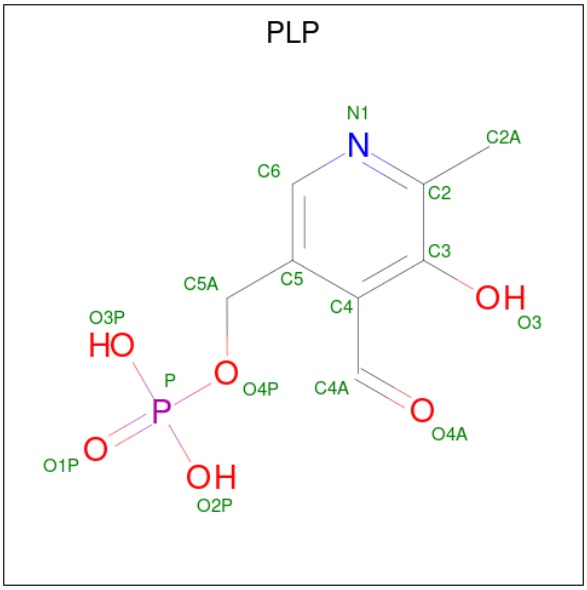
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	3	0
			2285	1437	419	419	10			
1	B	306	Total	C	N	O	S	0	4	0
			2328	1465	423	430	10			
1	C	297	Total	C	N	O	S	0	4	0
			2269	1420	424	415	10			
1	D	294	Total	C	N	O	S	0	2	0
			2231	1397	412	412	10			
1	E	300	Total	C	N	O	S	0	3	0
	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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



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

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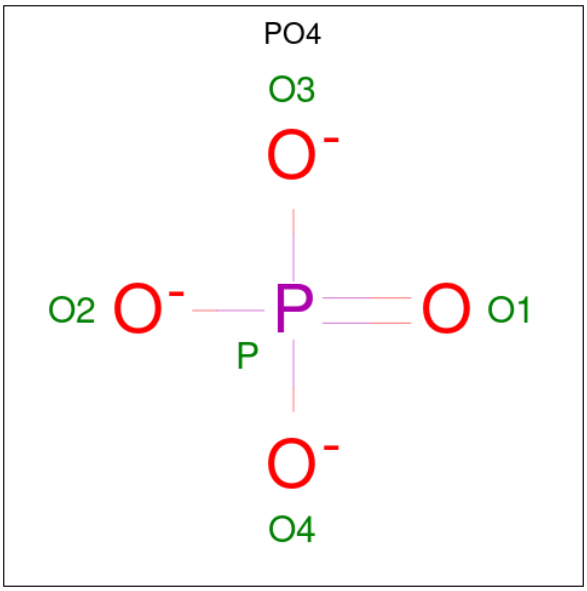
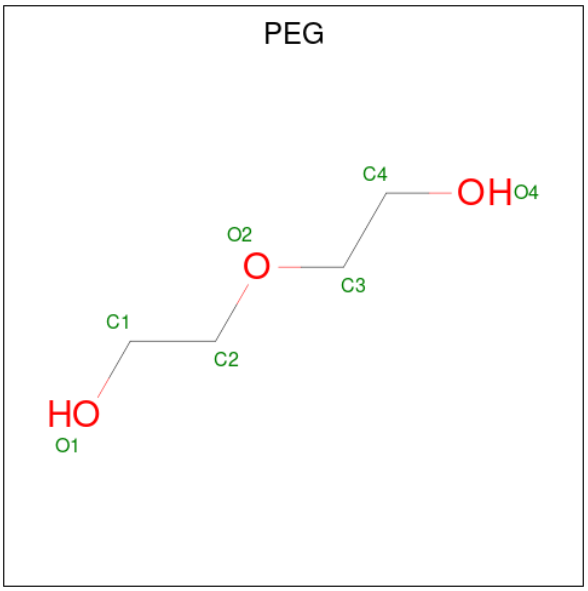
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O P 6 1 4 1	0	0
3	D	1	Total C O P 6 1 4 1	0	0
3	E	1	Total C O P 6 1 4 1	0	0
3	F	1	Total C O P 6 1 4 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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.

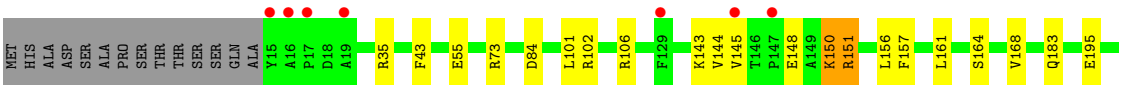
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	B	117	Total O 117 117	0	0
6	C	111	Total O 111 111	0	0
6	D	78	Total O 79 79	0	1
6	E	103	Total O 103 103	0	0
6	F	72	Total O 72 72	0	0

3 Residue-property plots (i)

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

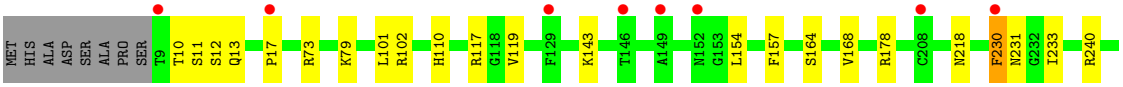
• Molecule 1: Aminotransferase, class 4

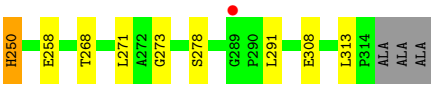
Chain A:



• Molecule 1: Aminotransferase, class 4

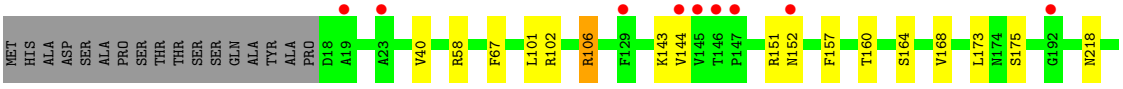
Chain B:

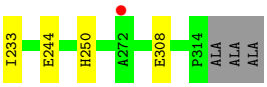




• Molecule 1: Aminotransferase, class 4

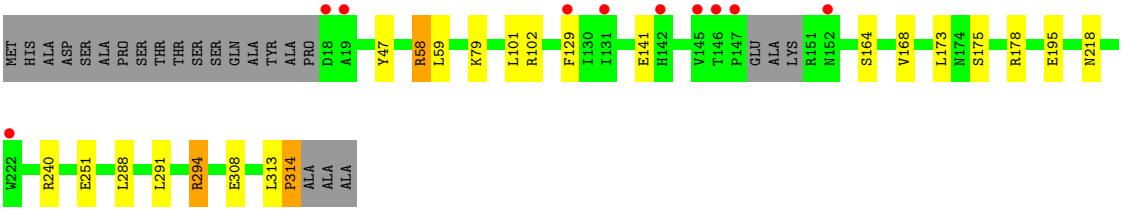
Chain C:



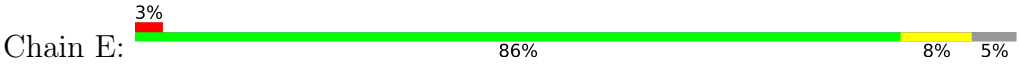


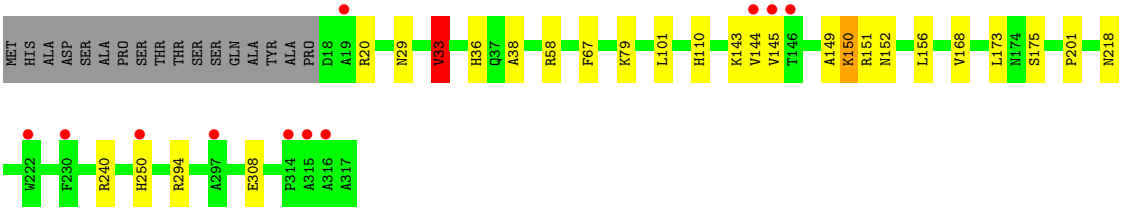
• Molecule 1: Aminotransferase, class 4

Chain D:

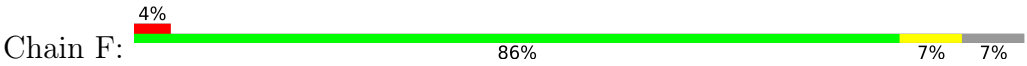


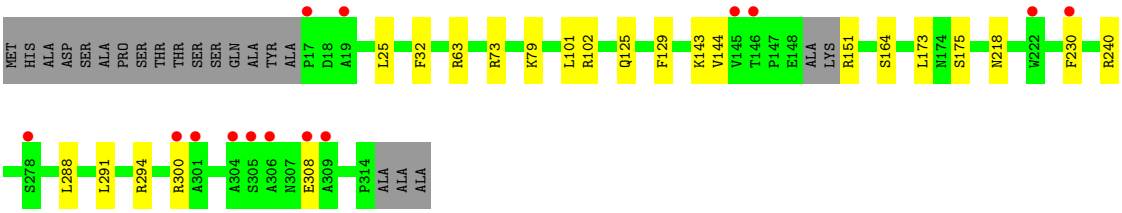
• Molecule 1: Aminotransferase, class 4





• Molecule 1: Aminotransferase, class 4





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.18 (at 2.29Å)	Xtriage
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	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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%)

All (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
1	D	195	GLU	CD-OE1	6.41	1.32	1.25
1	C	244	GLU	CD-OE2	5.63	1.31	1.25
1	A	195	GLU	CD-OE2	5.47	1.31	1.25
1	A	84	ASP	CG-OD1	5.41	1.37	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	C	250[A]	HIS	CB-CA-C	10.81	132.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	250[B]	HIS	CB-CA-C	10.81	132.02	110.40
1	D	129	PHE	CB-CA-C	9.78	129.97	110.40
1	E	250[A]	HIS	CB-CA-C	8.35	127.09	110.40
1	E	250[B]	HIS	CB-CA-C	8.35	127.09	110.40
1	A	250[A]	HIS	CA-C-O	7.10	135.01	120.10
1	A	250[B]	HIS	CA-C-O	7.10	135.01	120.10
1	A	35	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	E	33	VAL	CA-CB-CG1	6.83	121.15	110.90
1	E	294	ARG	CG-CD-NE	-6.60	97.95	111.80
1	A	250[A]	HIS	O-C-N	-6.54	112.23	122.70
1	A	250[B]	HIS	O-C-N	-6.54	112.23	122.70
1	B	250[A]	HIS	CB-CA-C	6.18	122.77	110.40
1	B	250[B]	HIS	CB-CA-C	6.18	122.77	110.40
1	F	240[A]	ARG	CB-CG-CD	6.18	127.66	111.60
1	F	240[B]	ARG	CB-CG-CD	6.18	127.66	111.60
1	C	106[A]	ARG	CG-CD-NE	5.99	124.38	111.80
1	C	106[B]	ARG	CG-CD-NE	5.99	124.38	111.80
1	C	106[A]	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	106[B]	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	102[A]	ARG	CB-CG-CD	5.60	126.17	111.60
1	B	102[B]	ARG	CB-CG-CD	5.60	126.17	111.60
1	C	58[A]	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	58[B]	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	106[A]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	106[B]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	F	240[A]	ARG	CD-NE-CZ	5.31	131.04	123.60
1	F	240[B]	ARG	CD-NE-CZ	5.31	131.04	123.60
1	A	150	LYS	CB-CA-C	-5.26	99.88	110.40
1	B	230[A]	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	B	230[B]	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	E	20	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	58[A]	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	58[B]	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	58[A]	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	58[B]	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	308	GLU	CB-CA-C	5.06	120.52	110.40
1	D	314	PRO	N-CA-C	5.04	125.20	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

All (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
1:E:29:ASN:HD22	5:E:402:PEG:H32	1.24	1.00
1:F:73[B]:ARG:CZ	1:F:230[B]:PHE:CZ	2.44	0.99
1:A:73[A]:ARG:CZ	1:A:230[A]:PHE:CZ	2.46	0.98
1:C:102[B]:ARG:HG2	1:C:102[B]:ARG:NH2	1.71	0.97
1:A:73[A]:ARG:CZ	1:A:230[A]:PHE:HZ	1.77	0.97
1:F:73[B]:ARG:NH2	1:F:230[B]:PHE:HZ	1.65	0.93
1:B:73:ARG:CZ	1:B:230[A]:PHE:CZ	2.52	0.93
1:B:117:ARG:HH11	5:B:402:PEG:H22	1.35	0.92
1:B:73:ARG:NH2	1:B:230[A]:PHE:HZ	1.67	0.91
1:A:73[A]:ARG:NH2	1:A:230[A]:PHE:CZ	2.40	0.88
1:C:102[B]:ARG:HH21	1:C:102[B]:ARG:CG	1.89	0.85
1:B:278:SER:HB2	5:B:403:PEG:H21	1.70	0.73
1:B:230[A]:PHE:CE2	3:B:404:PLP:C4	2.75	0.70
1:A:73[A]:ARG:NE	1:A:230[A]:PHE:CE1	2.62	0.68
1:B:230[A]:PHE:CD2	3:B:404:PLP:C4	2.78	0.66
1:B:117:ARG:NH1	5:B:402:PEG:H22	2.10	0.63
1:E:149:ALA:C	1:E:151:ARG:H	2.02	0.62
1:B:73:ARG:NH2	1:B:230[A]:PHE:CZ	2.59	0.62
1:A:55:GLU:OE1	1:A:73[B]:ARG:HD3	1.99	0.61
1:F:73[B]:ARG:NH2	1:F:230[B]:PHE:CZ	2.56	0.59
3:B:404:PLP:O4A	3:B:404:PLP:O3	2.18	0.59
1:B:13:GLN:HA	1:B:271:LEU:HD22	1.84	0.59
1:A:73[A]:ARG:NE	1:A:230[A]:PHE:CZ	2.71	0.57
1:E:33:VAL:CG1	1:E:38:ALA:HA	2.34	0.57
1:B:12:SER:HB3	1:B:154:LEU:HD11	1.88	0.56
1:B:250[B]:HIS:HD2	6:B:562:HOH:O	1.89	0.55
1:F:151:ARG:HH12	1:F:300:ARG:HH12	1.55	0.55
1:B:230[A]:PHE:CD2	3:B:404:PLP:C3	2.92	0.52
1:B:17:PRO:HA	6:B:607:HOH:O	2.11	0.51
1:B:230[A]:PHE:CE2	3:B:404:PLP:C4A	2.94	0.51
1:E:36:HIS:CD2	6:E:579:HOH:O	2.64	0.50
1:E:149:ALA:C	1:E:151:ARG:N	2.64	0.50
1:C:164:SER:HB3	1:D:168:VAL:CG1	2.42	0.49
1:C:40:VAL:HG11	1:D:47:TYR:CD1	2.48	0.49
1:A:148:GLU:HA	1:A:151:ARG:NH2	2.28	0.48
1:A:168:VAL:HG11	1:B:164:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:NE	1:B:230[A]:PHE:CZ	2.82	0.48
1:F:25:LEU:HD13	1:F:102:ARG:CZ	2.44	0.48
1:F:63:ARG:HB2	6:F:516:HOH:O	2.13	0.47
1:B:73:ARG:NE	1:B:230[A]:PHE:CE1	2.83	0.47
1:E:173:LEU:HG	1:E:175:SER:HB3	1.97	0.47
1:A:73[A]:ARG:NE	1:A:230[A]:PHE:HE1	2.08	0.47
1:D:102:ARG:HG3	1:D:102:ARG:NH1	2.28	0.47
1:A:161:LEU:CD1	1:A:183:GLN:HB3	2.45	0.46
1:D:102:ARG:HG3	1:D:102:ARG:HH11	1.81	0.46
1:C:164:SER:HB3	1:D:168:VAL:HG11	1.98	0.46
1:B:73:ARG:NH1	1:B:233:ILE:HD13	2.31	0.46
1:E:110:HIS:HE1	1:E:143:LYS:CB	2.29	0.46
1:F:25:LEU:HD13	1:F:102:ARG:NH1	2.31	0.45
1:E:201:PRO:HG3	6:E:587:HOH:O	2.17	0.45
5:B:403:PEG:H32	5:B:403:PEG:H12	1.82	0.45
1:E:33:VAL:HG11	1:E:38:ALA:HA	1.98	0.45
1:C:168:VAL:CG1	1:D:164:SER:HB3	2.47	0.44
1:A:73[A]:ARG:NH1	1:A:233:ILE:CD1	2.81	0.44
1:D:294[A]:ARG:HH11	1:D:294[A]:ARG:HD3	1.64	0.44
1:F:32:PHE:CE2	5:F:402:PEG:H21	2.53	0.44
1:D:173:LEU:HG	1:D:175:SER:HB3	2.00	0.43
1:A:145:VAL:HG12	1:A:150:LYS:HG3	2.01	0.42
1:A:168:VAL:CG1	1:B:164:SER:HB3	2.48	0.42
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.84	0.42
1:B:110:HIS:HB3	1:B:143:LYS:HD2	2.02	0.42
1:C:173:LEU:HG	1:C:175:SER:HB3	2.02	0.42
1:F:73[B]:ARG:NH1	1:F:230[B]:PHE:CZ	2.86	0.42
1:C:102[A]:ARG:HG3	1:C:102[A]:ARG:HH11	1.85	0.42
1:A:73[A]:ARG:NH1	1:A:233:ILE:HD13	2.35	0.41
1:D:178:ARG:NE	4:D:403:PO4:O4	2.52	0.41
1:E:168:VAL:CG1	1:F:164:SER:HB3	2.50	0.41
1:A:164:SER:HB3	1:B:168:VAL:CG1	2.50	0.41
1:B:268:THR:HA	1:B:273:GLY:O	2.21	0.41
1:A:43:PHE:CG	2:A:401:GOL:H32	2.55	0.41
1:D:294[B]:ARG:HH11	1:D:294[B]:ARG:HD2	1.63	0.41
1:E:150:LYS:C	1:E:152:ASN:N	2.74	0.41
1:C:102[A]:ARG:HG3	1:C:102[A]:ARG:NH1	2.35	0.41
1:A:294:ARG:HD2	6:A:539:HOH:O	2.20	0.41
1:F:173:LEU:HG	1:F:175:SER:HB3	2.02	0.41
2:A:405:GOL:H12	1:B:119:VAL:HG11	2.04	0.40
1:B:178:ARG:NE	4:B:405:PO4:O2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58[B]:ARG:NH1	6:D:505:HOH:O	2.49	0.40
1:D:59:LEU:HD11	1:D:313:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	106	ARG
1	A	143	LYS
1	A	144	VAL
1	A	151	ARG
1	A	156	LEU
1	A	157	PHE
1	A	240	ARG
1	A	288	LEU
1	A	308	GLU
1	B	10	THR
1	B	11	SER
1	B	79	LYS
1	B	101	LEU
1	B	157[A]	PHE
1	B	157[B]	PHE
1	B	218	ASN
1	B	231	ASN
1	B	240	ARG
1	B	291	LEU
1	B	308	GLU
1	B	313	LEU
1	C	67	PHE
1	C	101	LEU
1	C	106[A]	ARG
1	C	106[B]	ARG
1	C	143	LYS
1	C	144	VAL
1	C	151	ARG
1	C	152	ASN

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Mol	Chain	Res	Type
1	C	157	PHE
1	C	160	THR
1	C	218	ASN
1	C	233	ILE
1	C	308	GLU
1	D	79	LYS
1	D	101	LEU
1	D	218	ASN
1	D	240	ARG
1	D	251	GLU
1	D	288	LEU
1	D	291	LEU
1	D	308	GLU
1	D	314	PRO
1	E	33	VAL
1	E	58	ARG
1	E	67	PHE
1	E	79	LYS
1	E	101	LEU
1	E	150	LYS
1	E	156	LEU
1	E	218	ASN
1	E	240	ARG
1	F	79	LYS
1	F	101	LEU
1	F	125	GLN
1	F	143	LYS
1	F	144	VAL
1	F	218	ASN
1	F	288	LEU
1	F	291	LEU
1	F	294	ARG
1	F	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	HIS
1	C	218	ASN
1	C	231	ASN
1	E	29	ASN
1	E	110	HIS

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Mol	Chain	Res	Type
1	E	142	HIS
1	E	190	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
3	A	403	PLP	P-O4P	3.72	1.66	1.59
5	E	403	PEG	O4-C4	3.13	1.58	1.42
4	F	404	PO4	P-O4	-3.02	1.45	1.54
4	C	403	PO4	P-O1	2.73	1.57	1.50
3	C	402	PLP	P-O4P	2.69	1.64	1.59
5	B	402	PEG	O1-C1	2.62	1.55	1.42
5	B	402	PEG	C2-C1	2.47	1.62	1.49
3	F	403	PLP	P-O4P	2.41	1.63	1.59
3	A	403	PLP	P-O1P	-2.30	1.43	1.50
3	B	404	PLP	P-O3P	-2.30	1.46	1.54
5	E	403	PEG	C2-C1	2.26	1.61	1.49
4	D	403	PO4	P-O3	-2.18	1.48	1.54
4	A	404	PO4	P-O2	-2.17	1.48	1.54
5	E	403	PEG	O1-C1	2.14	1.53	1.42
5	B	403	PEG	C2-C1	2.12	1.60	1.49
5	E	403	PEG	C3-C4	2.12	1.60	1.49
3	B	404	PLP	O3-C3	-2.07	1.32	1.37
3	C	402	PLP	P-O2P	-2.04	1.47	1.54
4	B	405	PO4	P-O4	-2.01	1.48	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	PLP	O2P-P-O4P	2.51	117.24	105.99
4	D	403	PO4	O4-P-O2	2.44	115.80	107.97
5	B	402	PEG	C3-O2-C2	2.42	123.77	113.29
4	E	406	PO4	O3-P-O2	2.33	115.46	107.97
3	B	404	PLP	O3-C3-C2	2.15	122.17	117.49
3	C	402	PLP	O3P-P-O4P	2.13	115.55	105.99
4	C	403	PO4	O4-P-O1	-2.05	103.38	110.89
3	B	404	PLP	O4P-C5A-C5	-2.04	105.47	109.35
3	D	402	PLP	O2P-P-O4P	2.01	114.98	105.99

There are no chirality outliers.

All (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
2	E	407	GOL	O1-C1-C2-C3
2	E	407	GOL	C1-C2-C3-O3
2	F	401	GOL	C1-C2-C3-O3
2	F	401	GOL	O2-C2-C3-O3
3	A	403	PLP	C5A-O4P-P-O1P
3	B	404	PLP	C5A-O4P-P-O1P
3	F	403	PLP	C5A-O4P-P-O1P
5	B	403	PEG	C1-C2-O2-C3
5	B	401	PEG	C1-C2-O2-C3
5	B	402	PEG	O1-C1-C2-O2
5	B	401	PEG	O1-C1-C2-O2
5	B	403	PEG	O1-C1-C2-O2
2	A	402	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	E	404	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O2-C2-C3-O3
2	C	401	GOL	O1-C1-C2-O2
2	E	404	GOL	O1-C1-C2-O2
2	E	404	GOL	O2-C2-C3-O3
2	E	407	GOL	O1-C1-C2-O2
2	E	407	GOL	O2-C2-C3-O3
2	A	405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	403	PEG	O2-C3-C4-O4
5	F	402	PEG	C4-C3-O2-C2
5	B	401	PEG	C4-C3-O2-C2
2	D	401	GOL	O1-C1-C2-O2
5	B	402	PEG	C4-C3-O2-C2
3	E	405	PLP	C5A-O4P-P-O1P
2	E	401	GOL	C1-C2-C3-O3
5	E	402	PEG	C1-C2-O2-C3
5	F	402	PEG	C1-C2-O2-C3
3	B	404	PLP	C3-C4-C4A-O4A
5	B	401	PEG	O2-C3-C4-O4
3	B	404	PLP	C5-C4-C4A-O4A
2	E	401	GOL	O2-C2-C3-O3

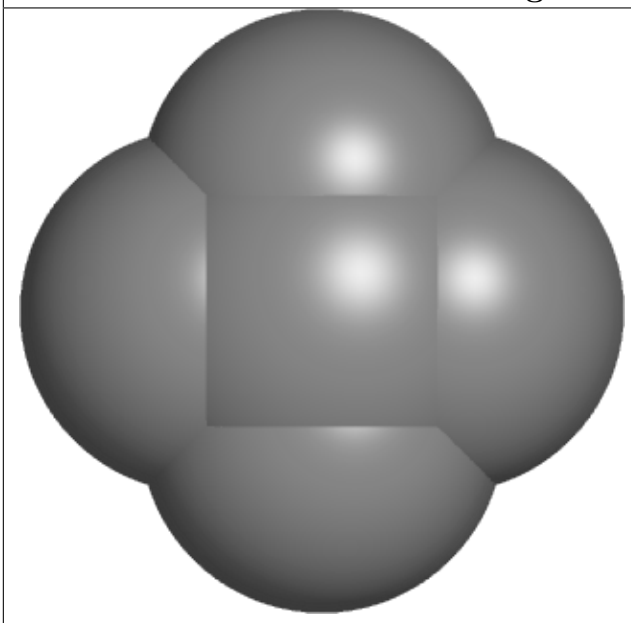
There are no ring outliers.

9 monomers are involved in 15 short contacts:

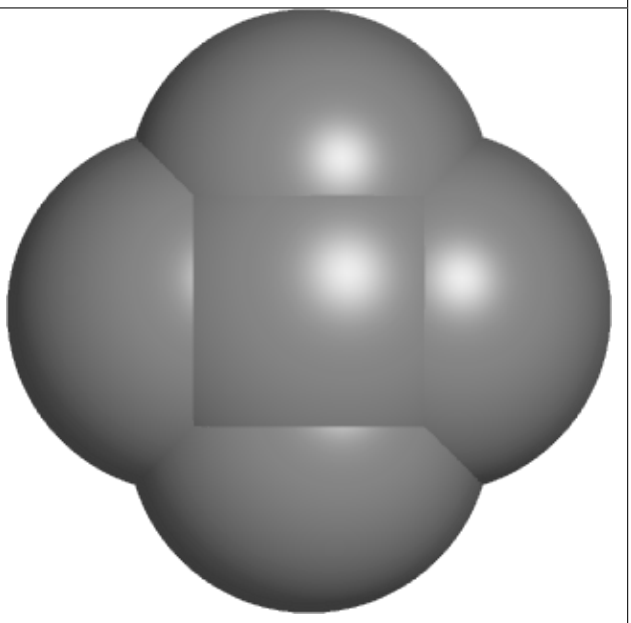
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	PO4	1	0
3	B	404	PLP	5	0
5	F	402	PEG	1	0
5	B	403	PEG	2	0
5	B	402	PEG	2	0
4	B	405	PO4	1	0
2	A	405	GOL	1	0
2	A	401	GOL	1	0
5	E	402	PEG	1	0

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 then 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.

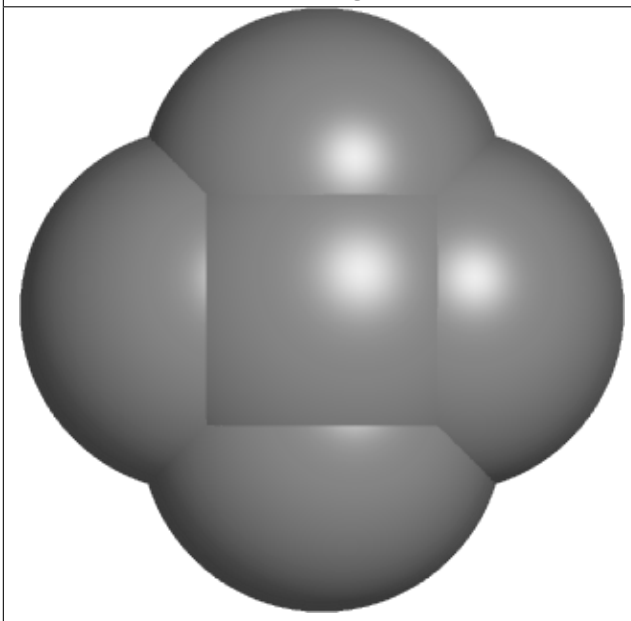
Ligand PO4 D 403



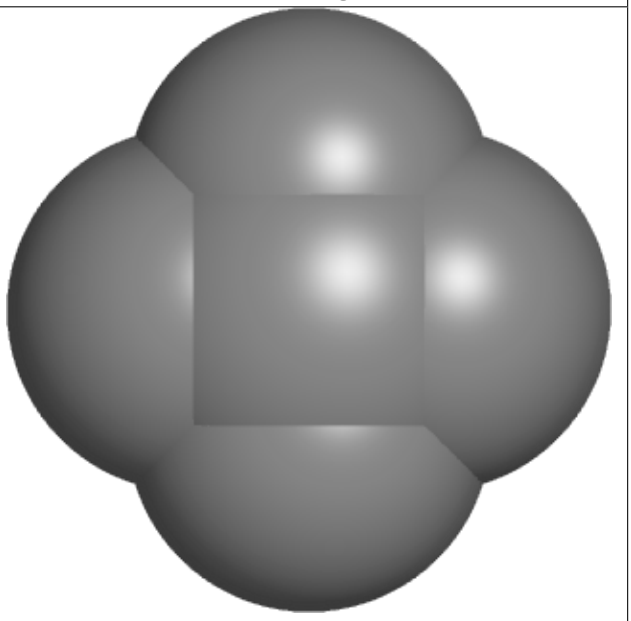
Bond lengths



Bond angles

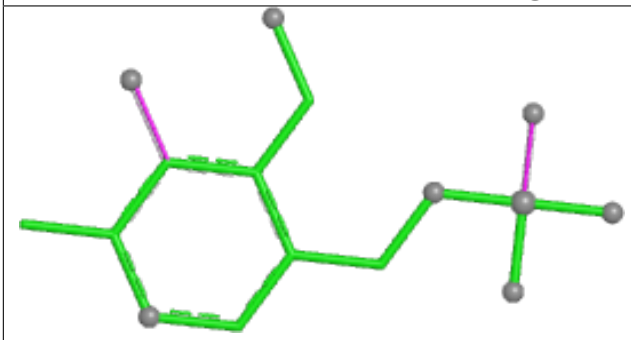


Torsions

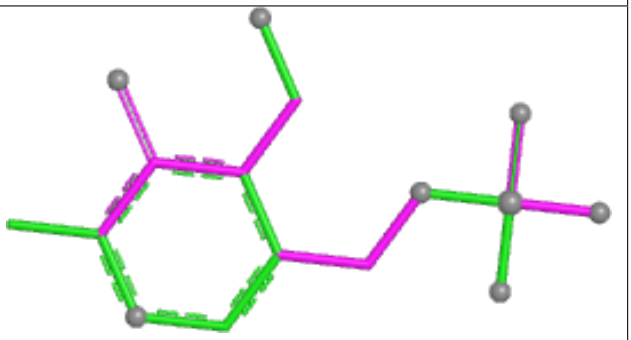


Rings

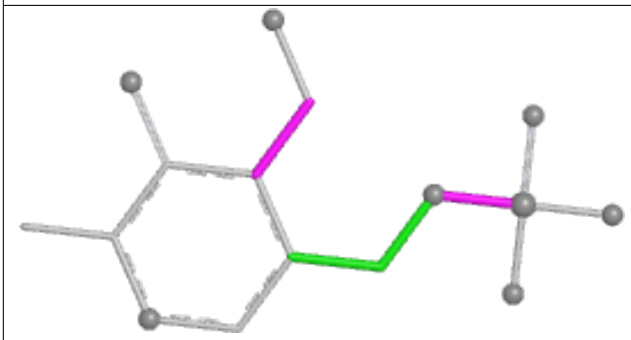
Ligand PLP B 404



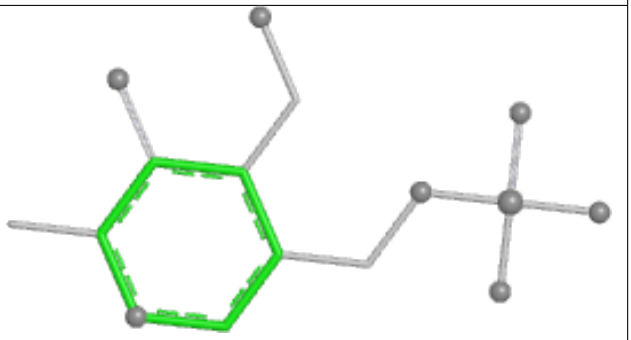
Bond lengths



Bond angles

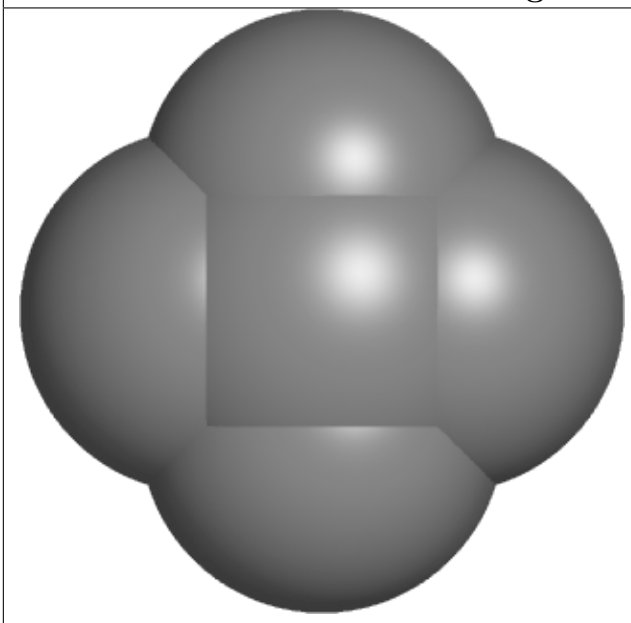


Torsions

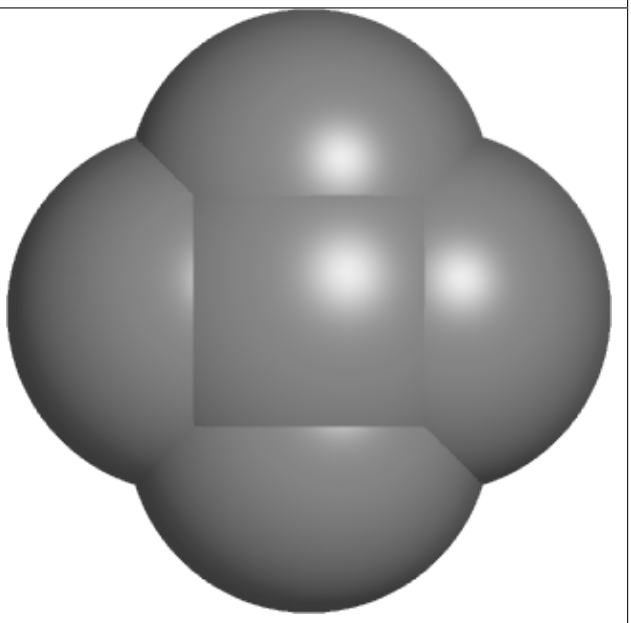


Rings

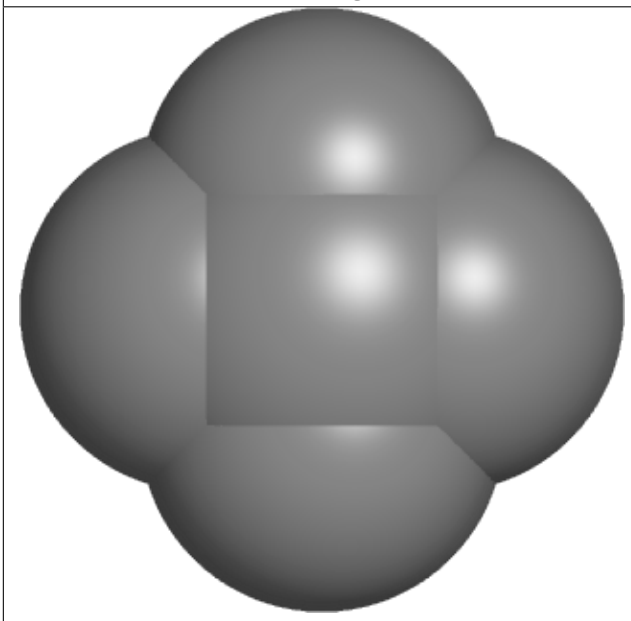
Ligand PO4 A 404



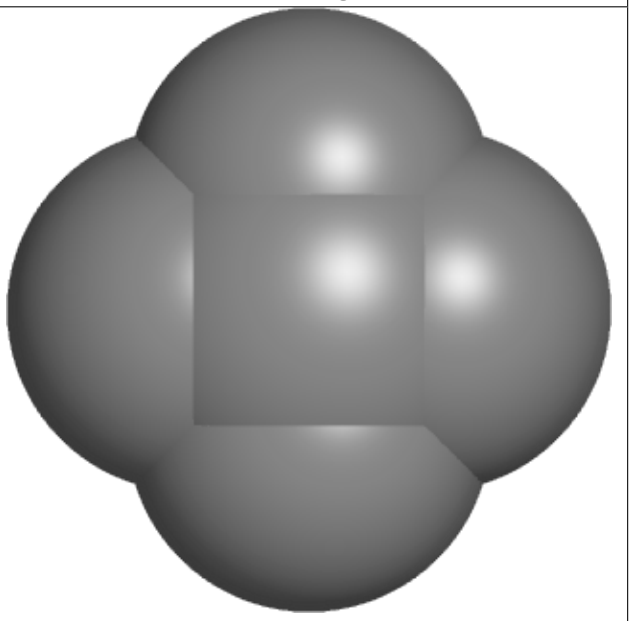
Bond lengths



Bond angles

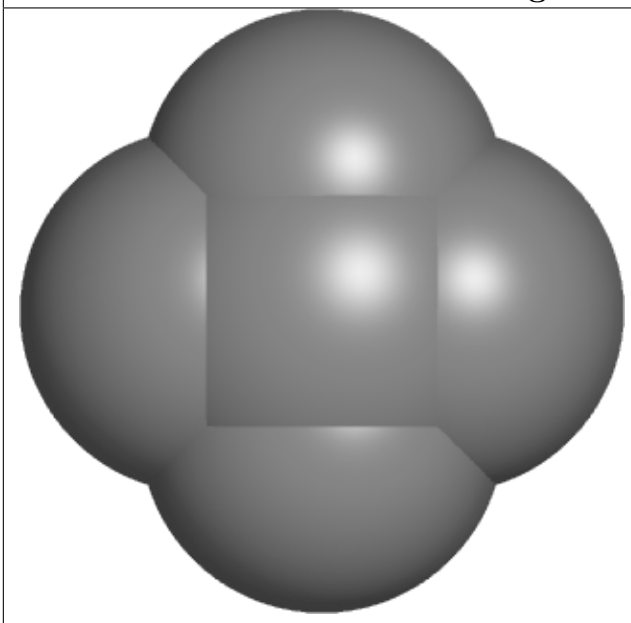


Torsions

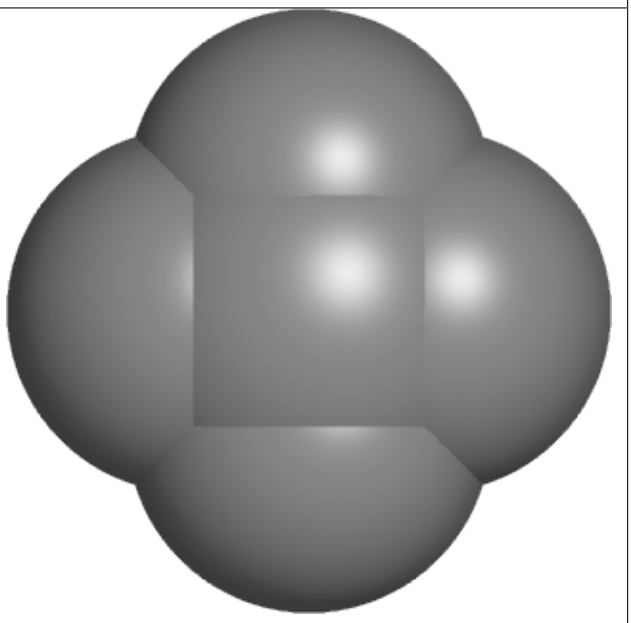


Rings

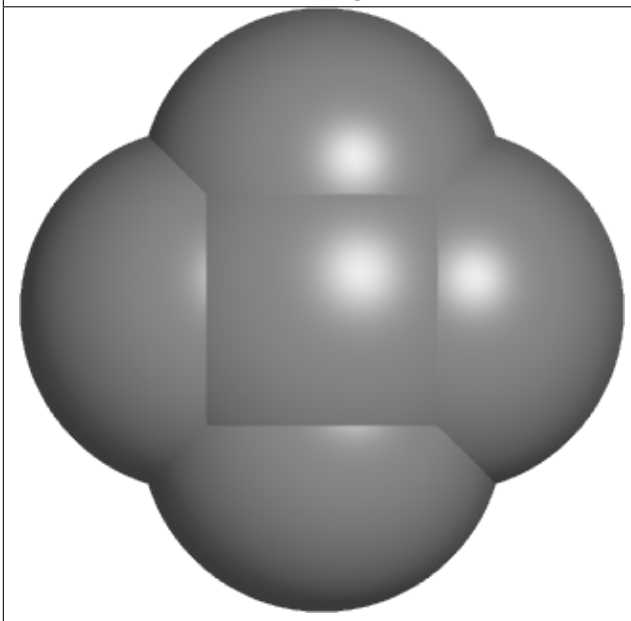
Ligand PO4 F 404



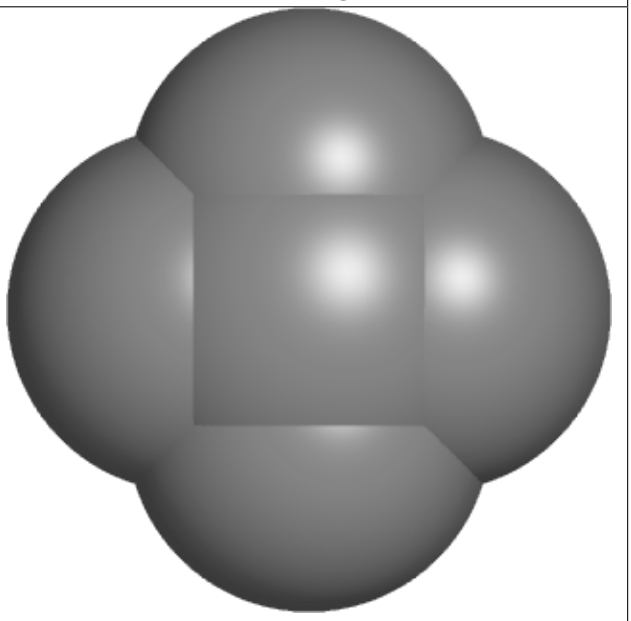
Bond lengths



Bond angles

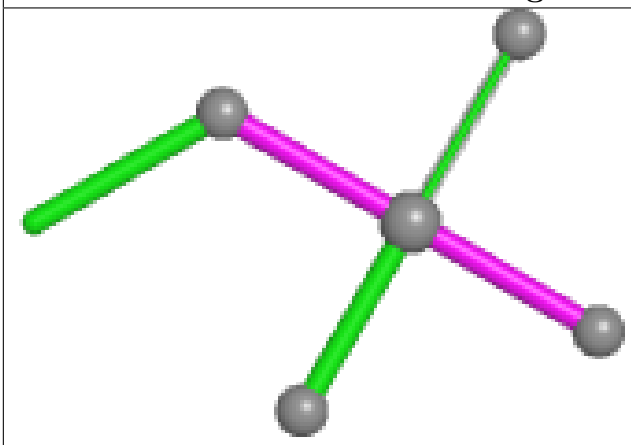


Torsions

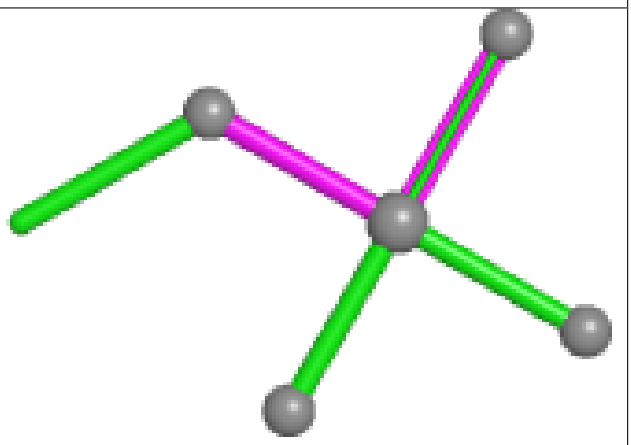


Rings

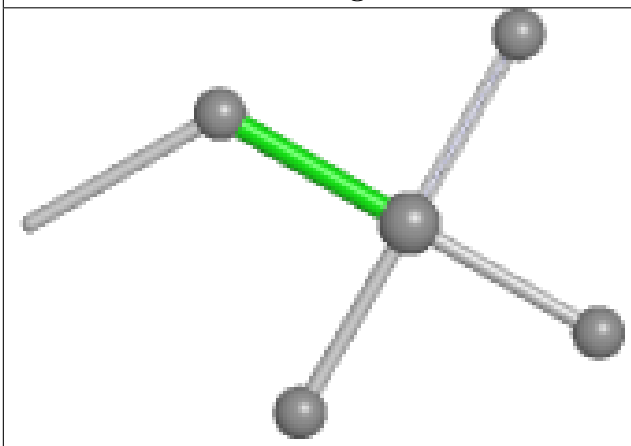
Ligand PLP C 402



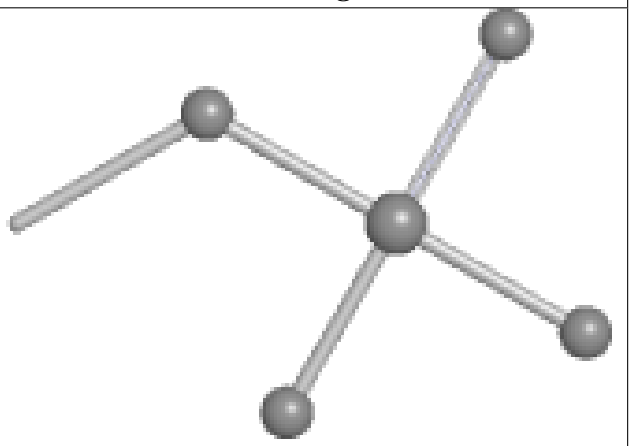
Bond lengths



Bond angles

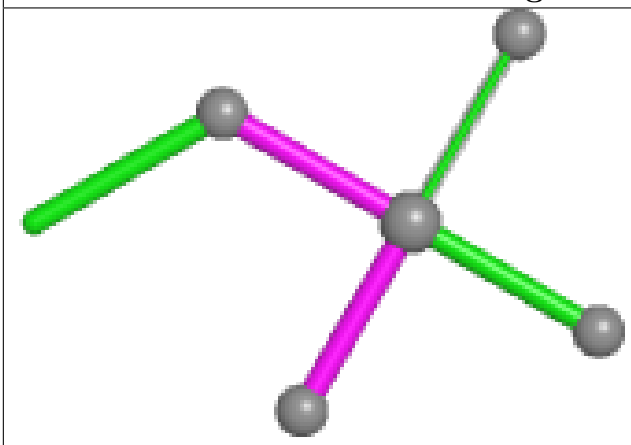


Torsions



Rings

Ligand PLP A 403



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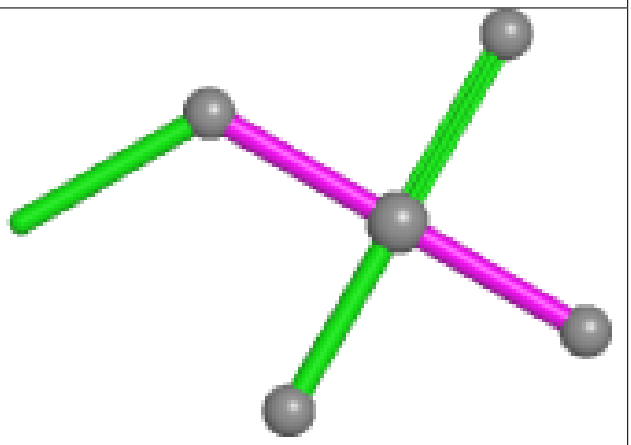
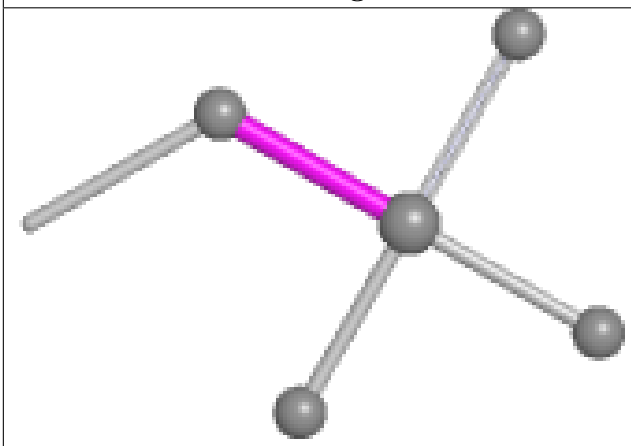
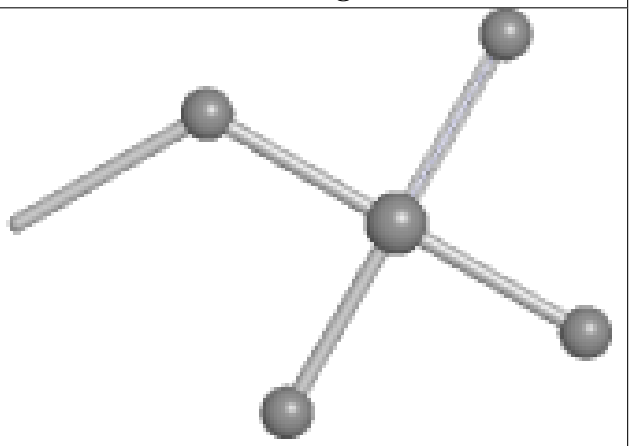


Bond angles

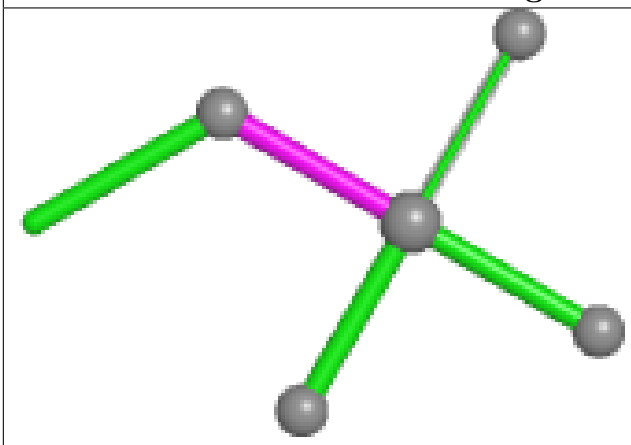


Torsions

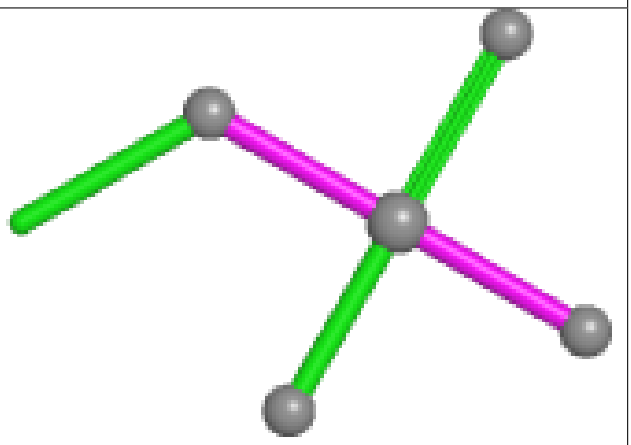


Rings

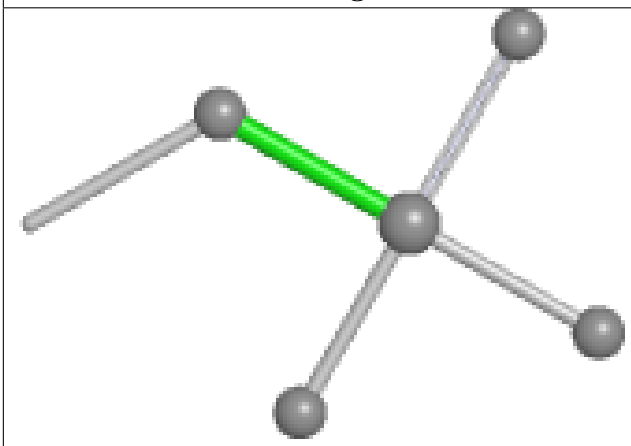
Ligand PLP D 402



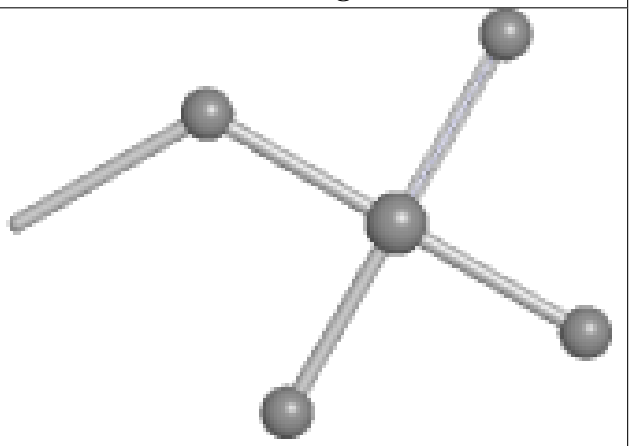
Bond lengths



Bond angles

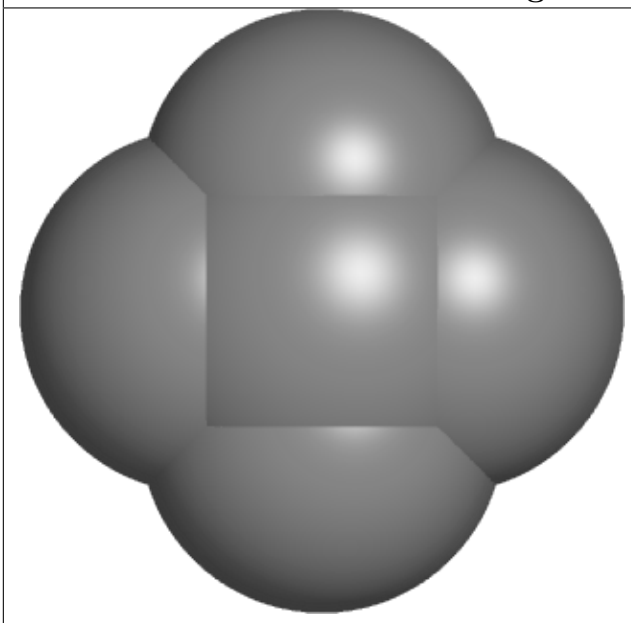


Torsions

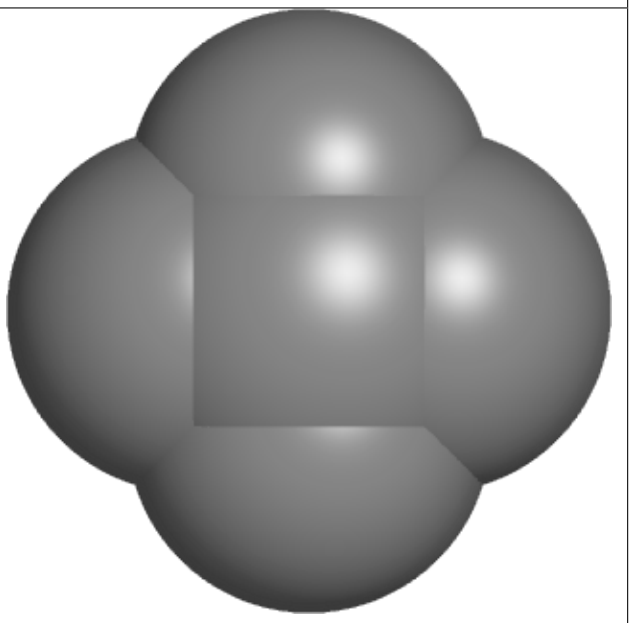


Rings

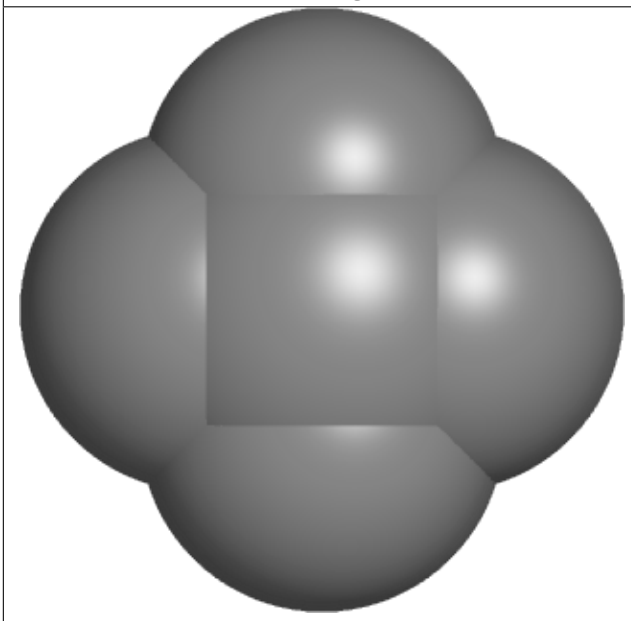
Ligand PO4 C 403



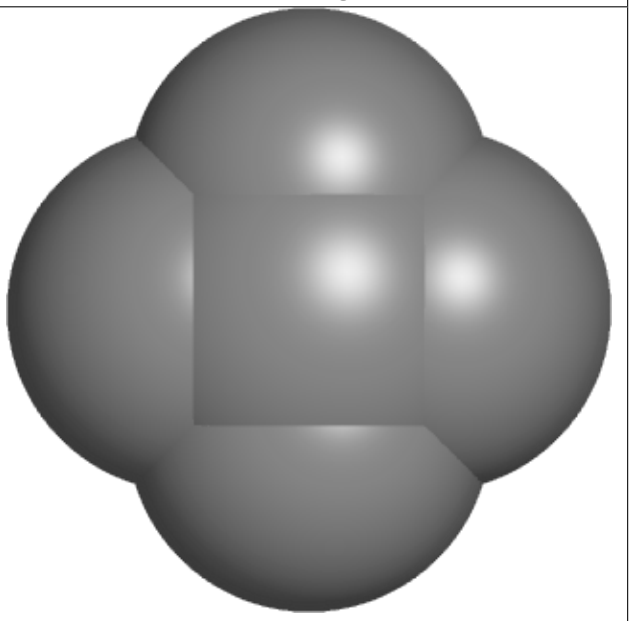
Bond lengths



Bond angles

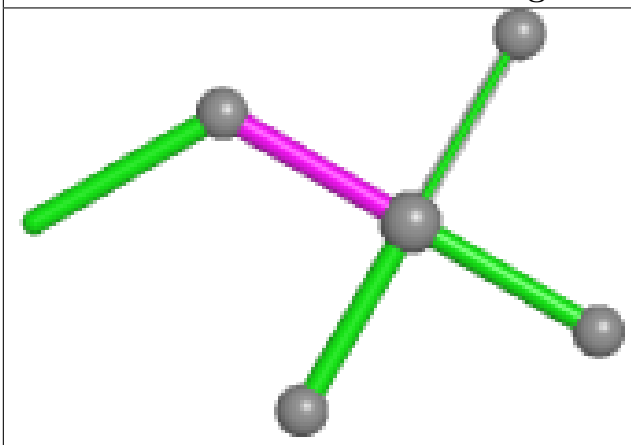


Torsions

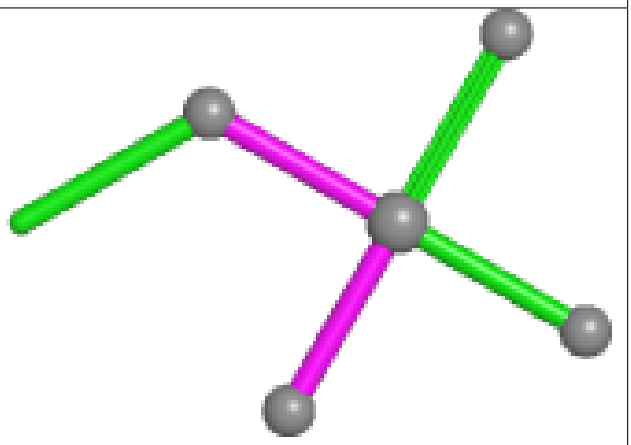


Rings

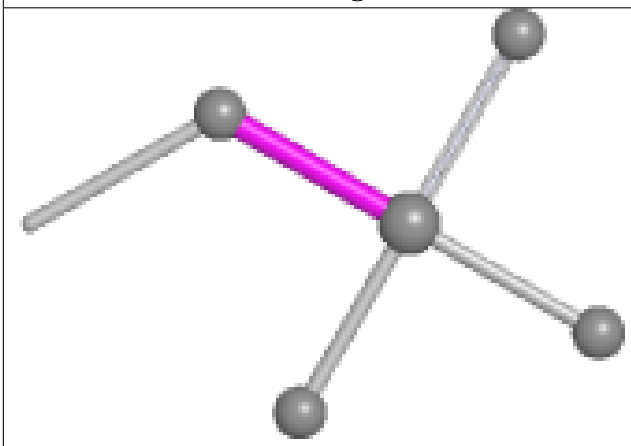
Ligand PLP F 403



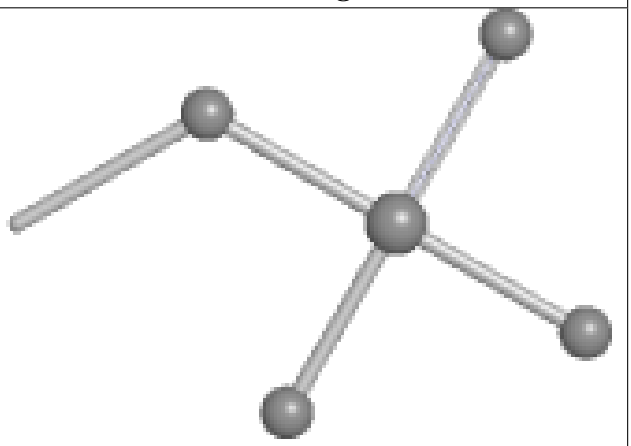
Bond lengths



Bond angles

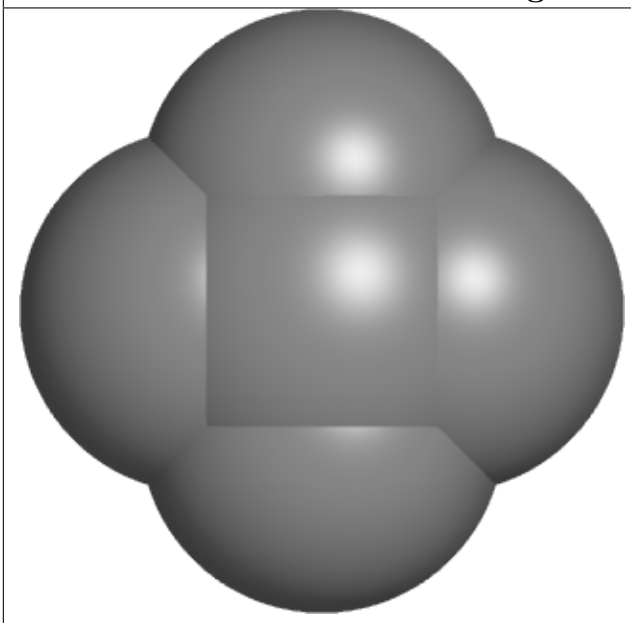


Torsions

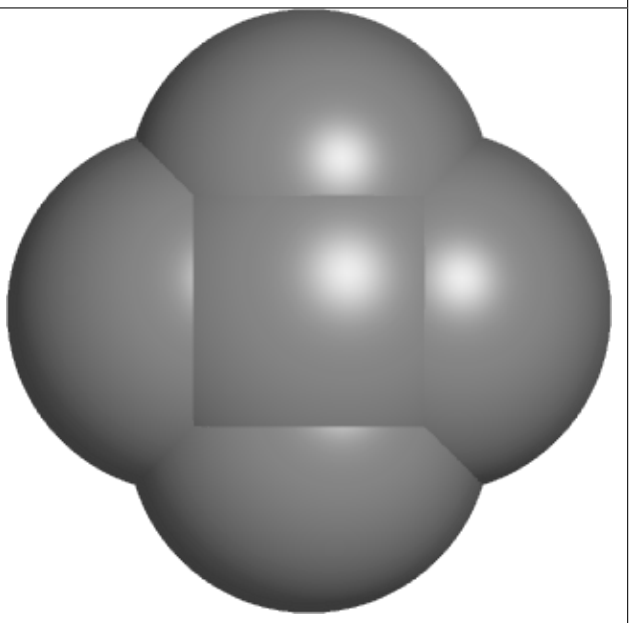


Rings

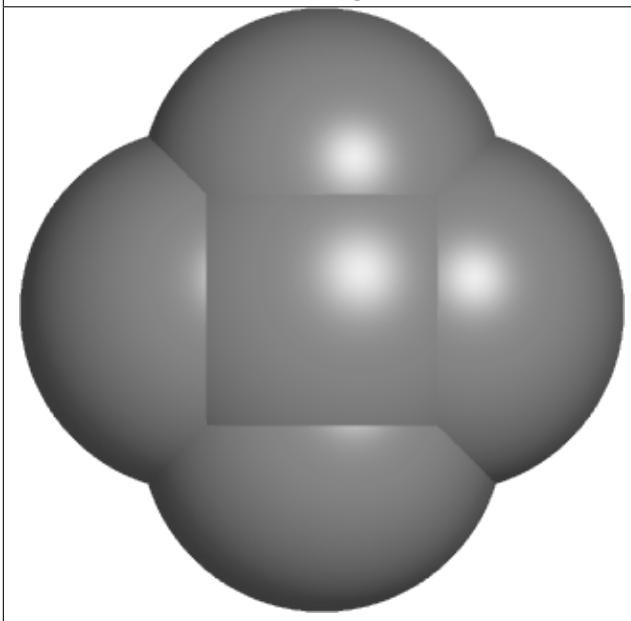
Ligand PO4 B 405



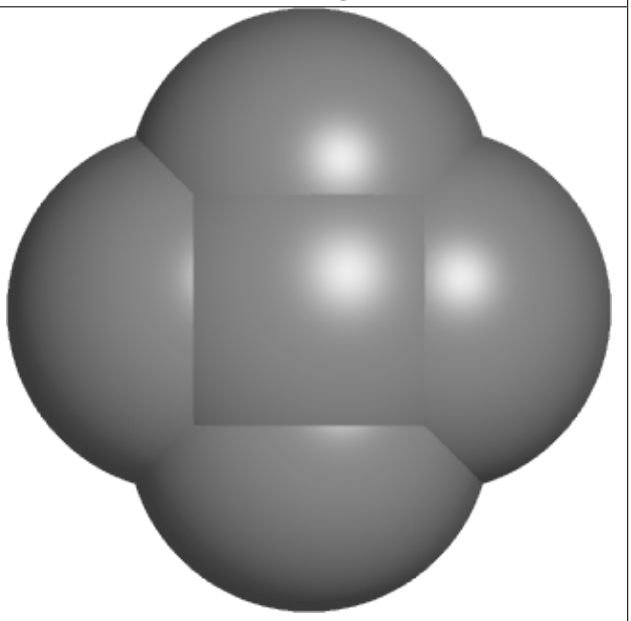
Bond lengths



Bond angles

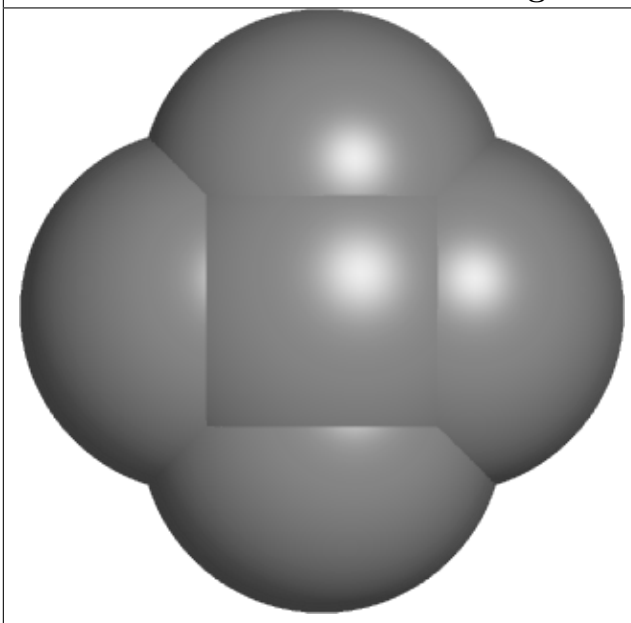


Torsions

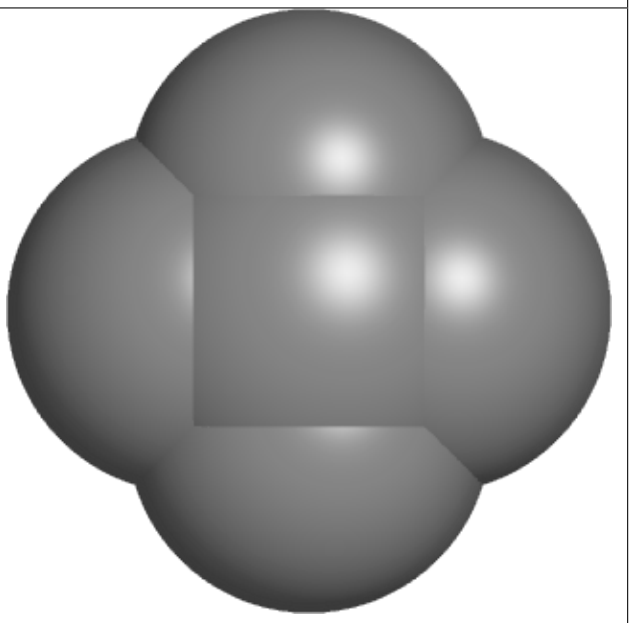


Rings

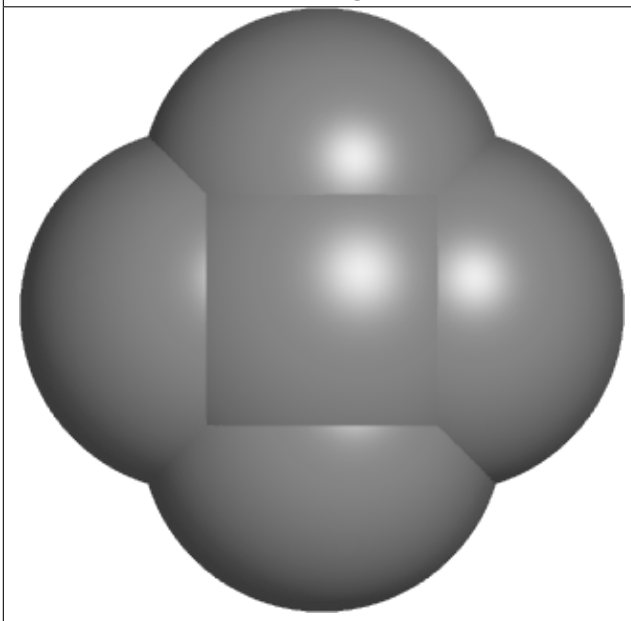
Ligand PO4 E 406



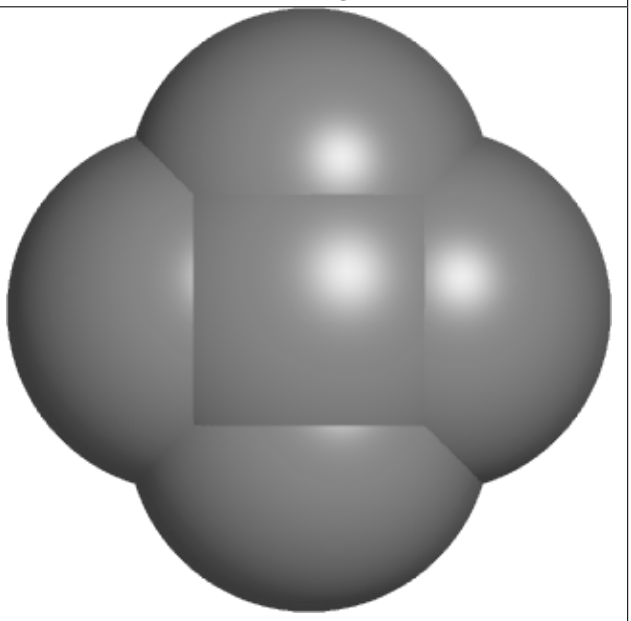
Bond lengths



Bond angles

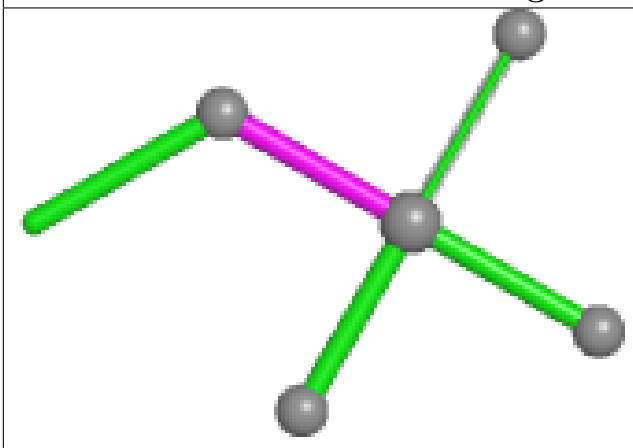


Torsions

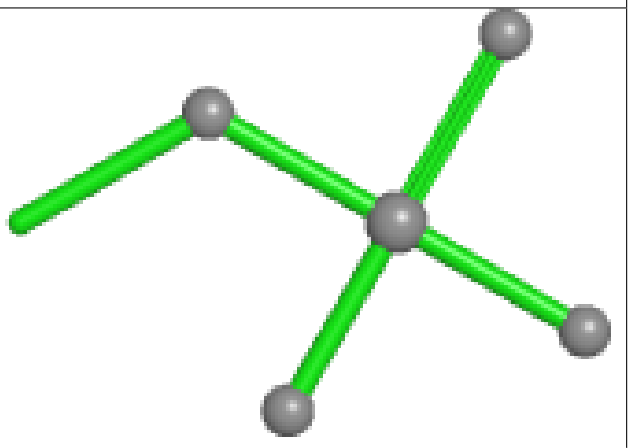


Rings

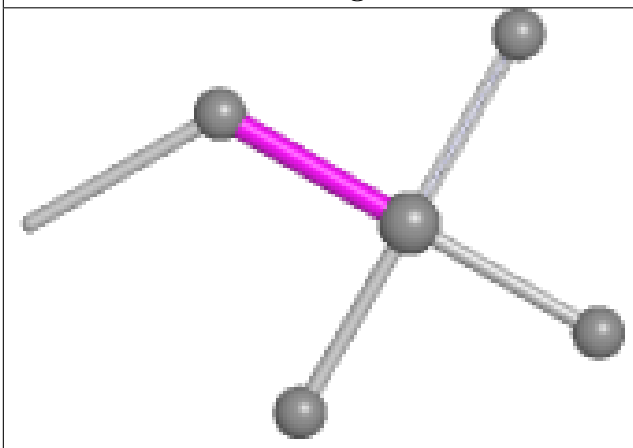
Ligand PLP E 405



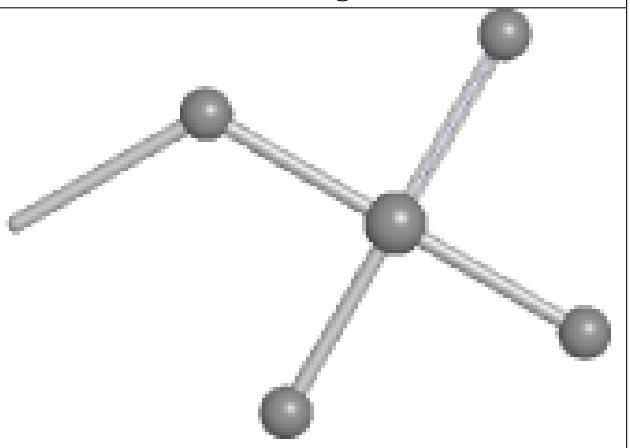
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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

All (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
1	A	129	PHE	3.9
1	C	152	ASN	3.9
1	C	129	PHE	3.7
1	F	309	ALA	3.6
1	E	144	VAL	3.4
1	A	15	TYR	3.3
1	D	145	VAL	3.3
1	C	145	VAL	3.3
1	A	147	PRO	3.1
1	A	230[A]	PHE	3.1
1	A	16	ALA	3.1
1	B	17	PRO	3.0
1	A	145	VAL	3.0
1	C	23	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	316	ALA	2.9
1	E	19	ALA	2.9
1	A	19	ALA	2.9
1	D	222	TRP	2.8
1	C	19	ALA	2.8
1	B	146	THR	2.8
1	B	152	ASN	2.8
1	F	305	SER	2.7
1	D	131	ILE	2.7
1	F	304	ALA	2.7
1	B	129	PHE	2.7
1	C	147	PRO	2.6
1	D	147	PRO	2.6
1	B	9	THR	2.6
1	C	146	THR	2.6
1	F	308	GLU	2.6
1	D	18	ASP	2.6
1	C	144	VAL	2.5
1	E	315	ALA	2.4
1	F	301	ALA	2.4
1	F	230[A]	PHE	2.4
1	F	17	PRO	2.4
1	E	222	TRP	2.4
1	F	146	THR	2.3
1	D	142	HIS	2.3
1	E	297	ALA	2.3
1	F	306	ALA	2.3
1	A	309	ALA	2.3
1	F	278	SER	2.3
1	A	222	TRP	2.2
1	E	230	PHE	2.2
1	E	146	THR	2.2
1	E	145	VAL	2.2
1	F	222	TRP	2.2
1	C	272	ALA	2.2
1	C	192	GLY	2.2
1	F	300	ARG	2.1
1	D	152	ASN	2.1
1	F	145	VAL	2.1
1	B	208	CYS	2.1
1	E	250[A]	HIS	2.1
1	F	19	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	289	GLY	2.1
1	B	230[A]	PHE	2.1
1	A	17	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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

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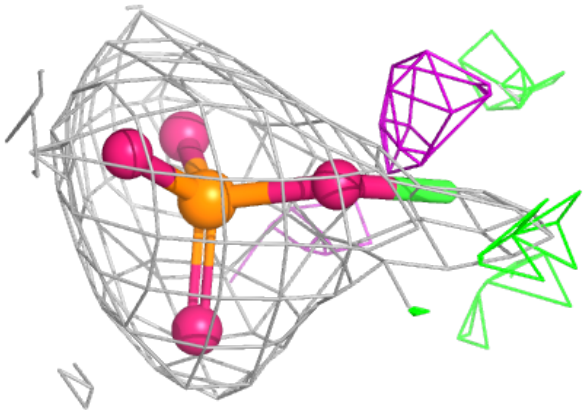
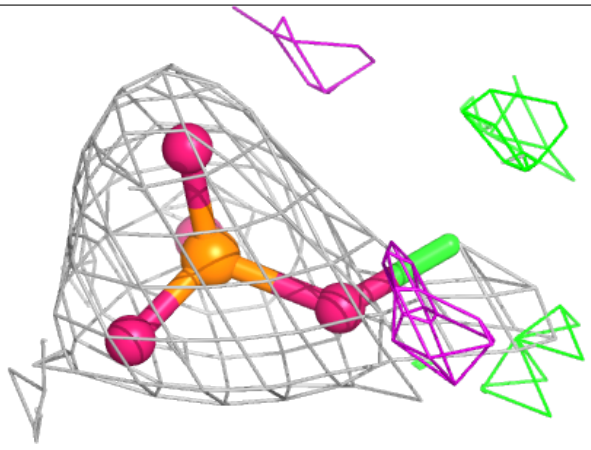
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PLP	A	403	6/16	0.98	0.20	29,34,38,39	1
4	PO4	D	403	5/5	0.98	0.18	40,41,43,46	0
3	PLP	C	402	6/16	0.98	0.24	33,39,42,57	0
4	PO4	F	404	5/5	0.98	0.19	42,46,51,55	0
3	PLP	F	403	6/16	0.98	0.17	38,40,40,41	1
4	PO4	A	404	5/5	0.99	0.20	35,36,40,42	0
4	PO4	B	405	5/5	0.99	0.16	33,33,38,39	0

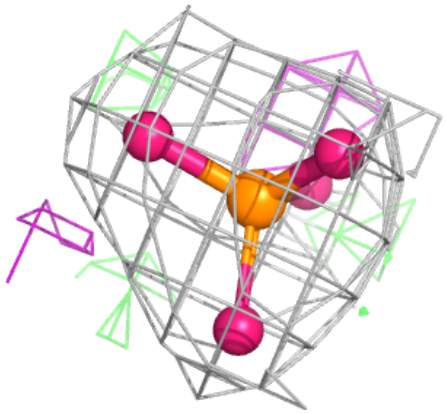
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

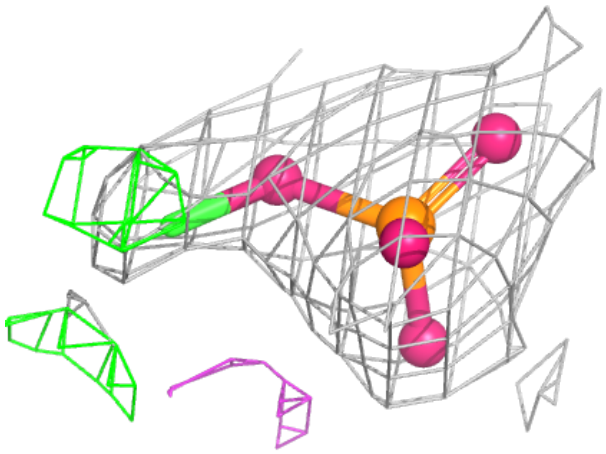


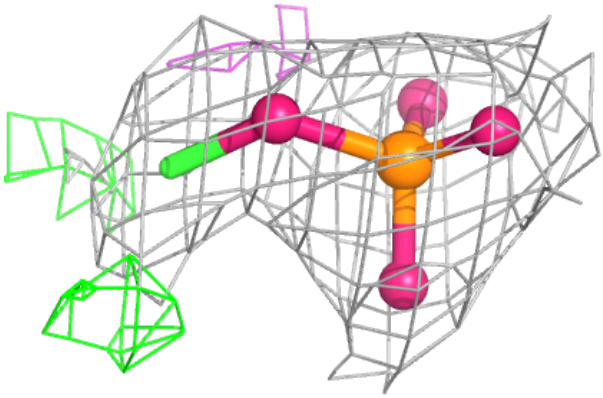


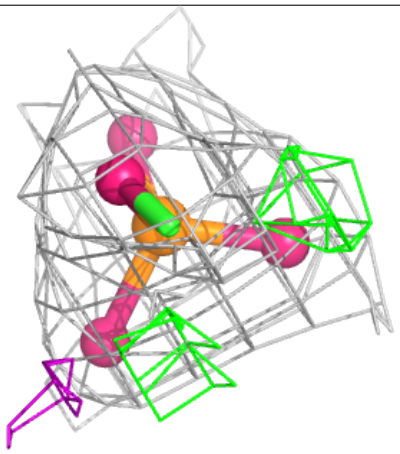


Electron density around PLP E 405:

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

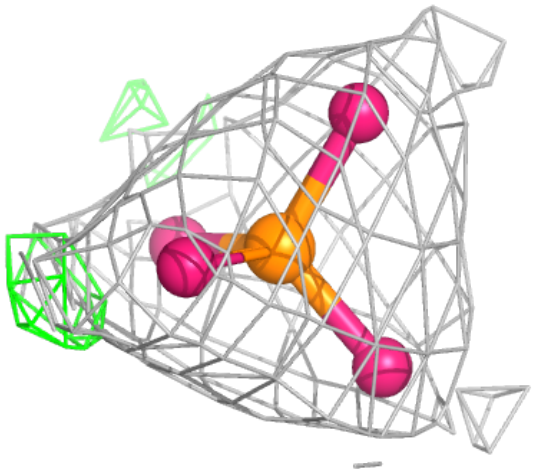


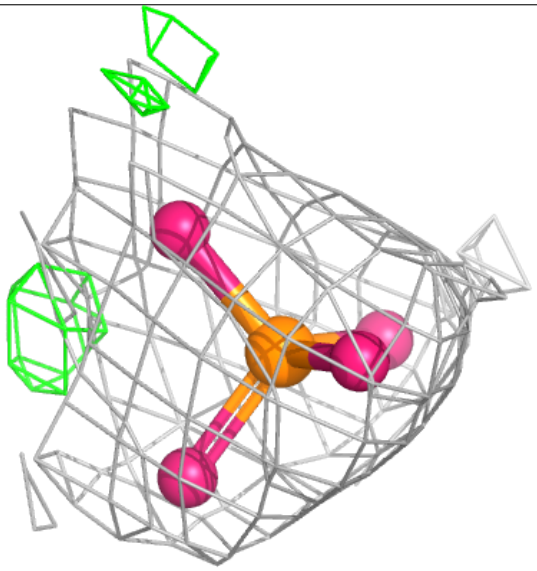


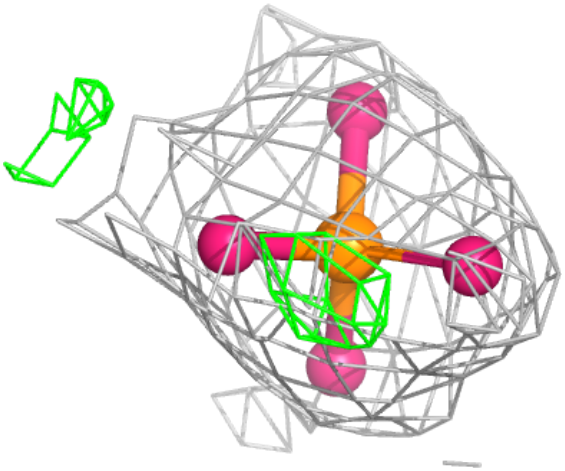


Electron density around PO4 C 403:

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

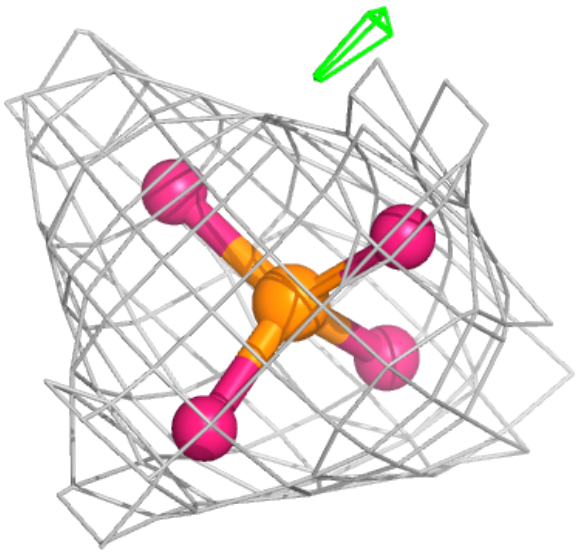


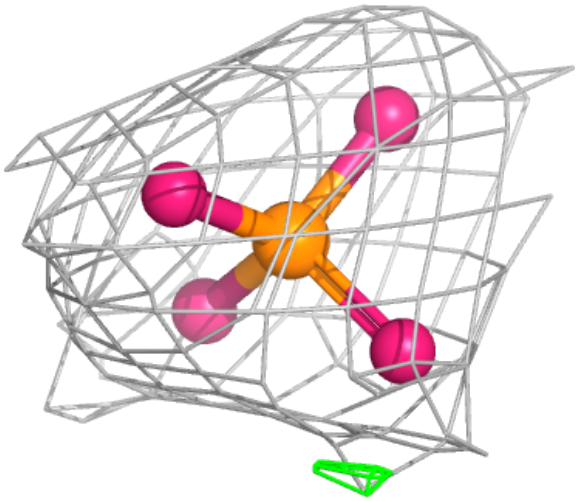


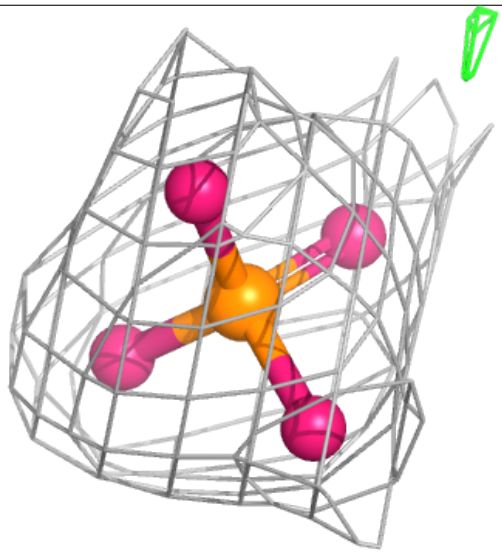


Electron density around PO4 E 406:

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

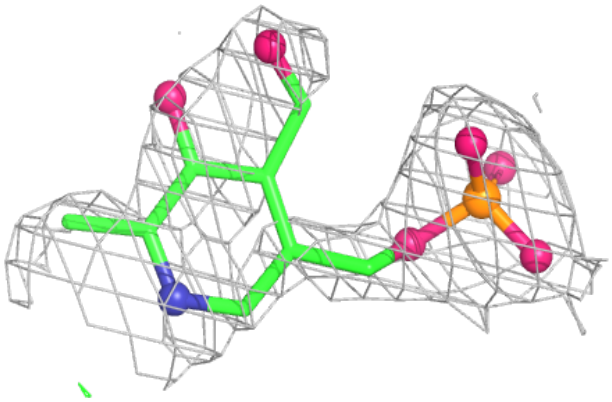


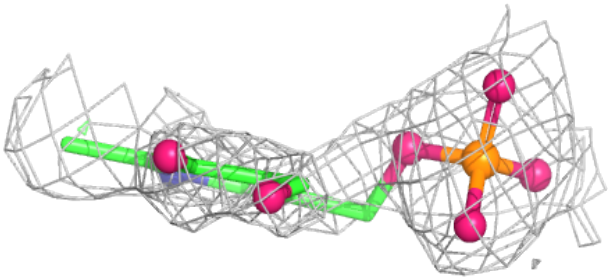


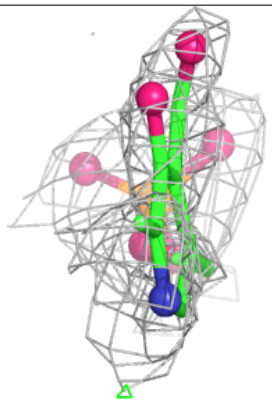


Electron density around PLP B 404:

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

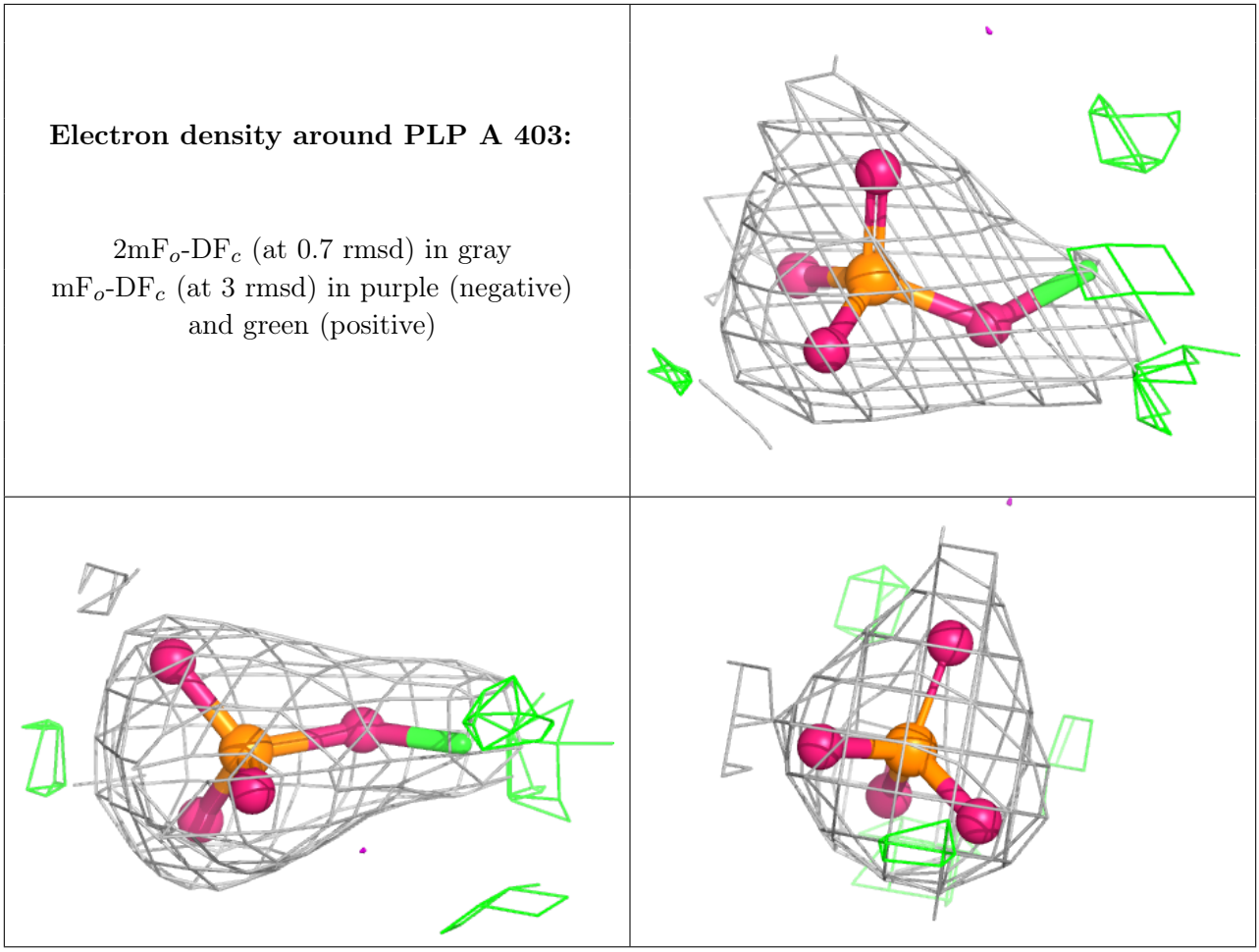






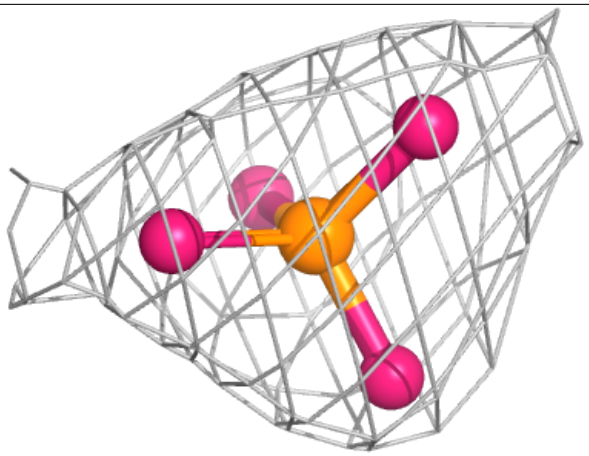
Electron density around PLP A 403:

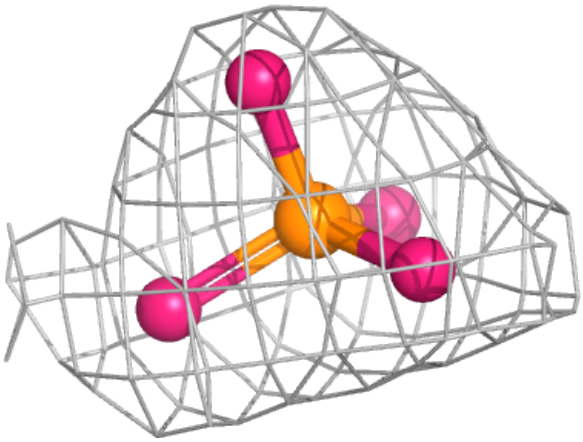
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

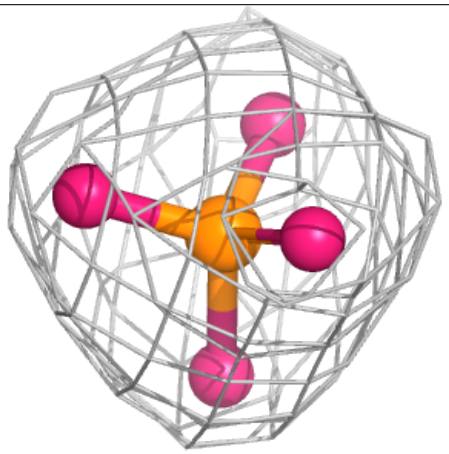


Electron density around PO4 D 403:

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

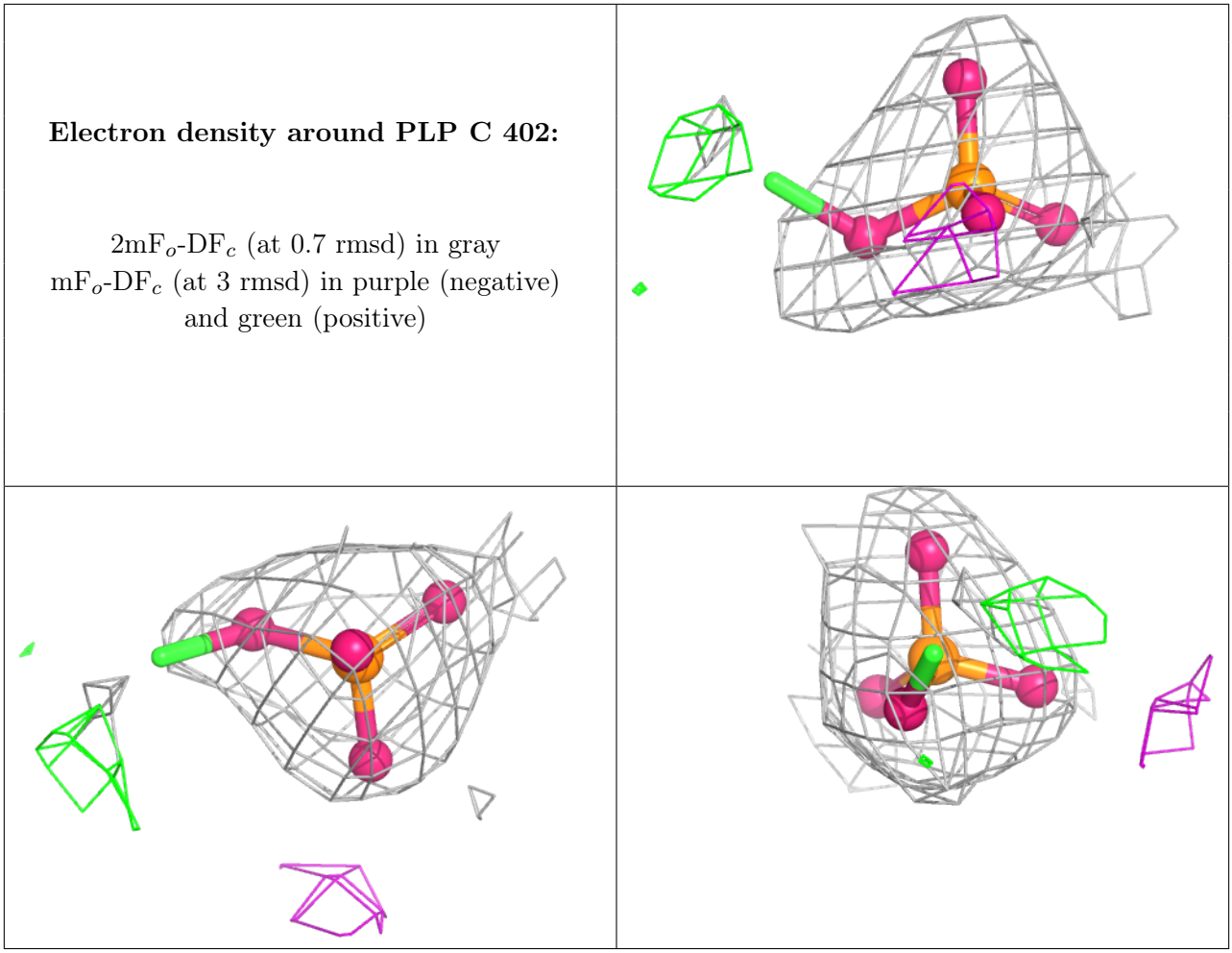






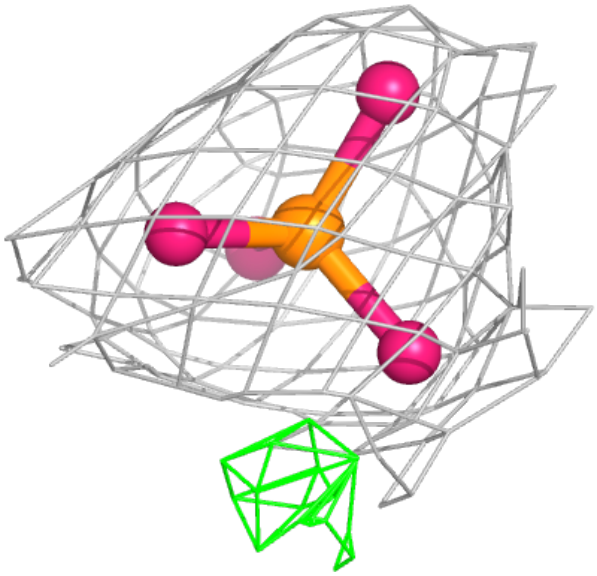
Electron density around PLP C 402:

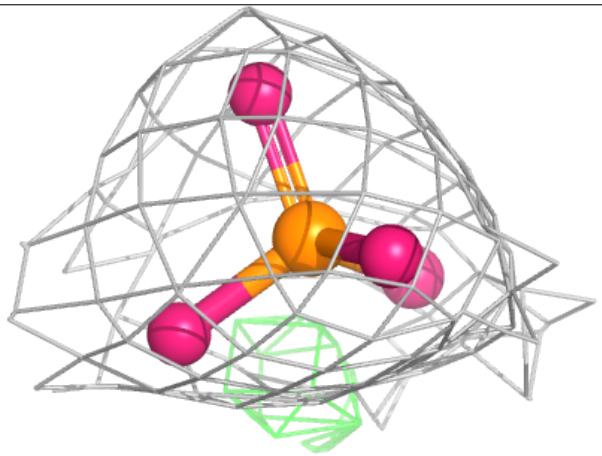
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

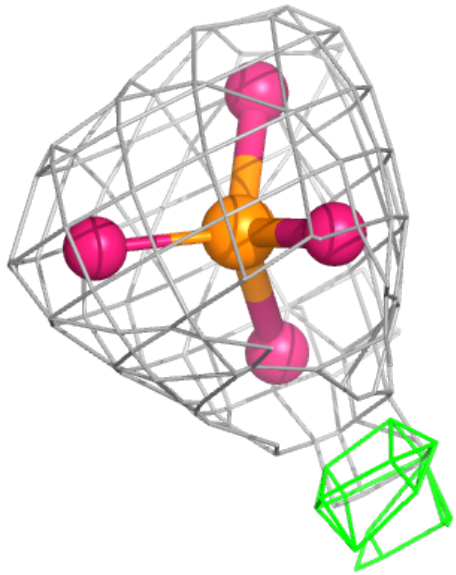


Electron density around PO4 F 404:

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

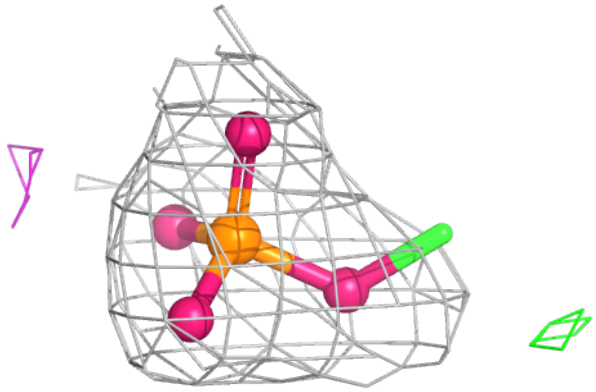


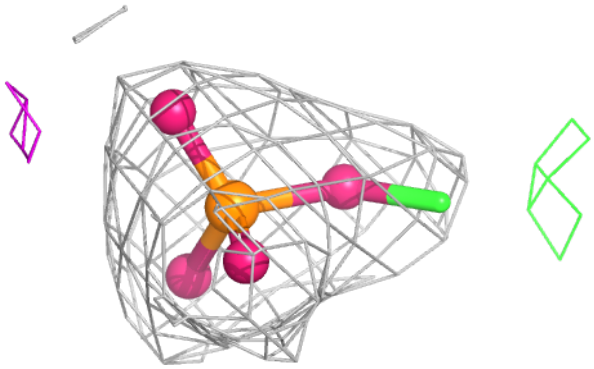


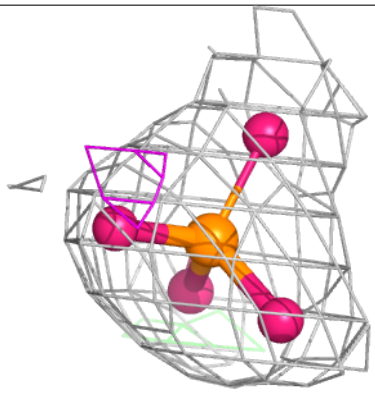


Electron density around PLP F 403:

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

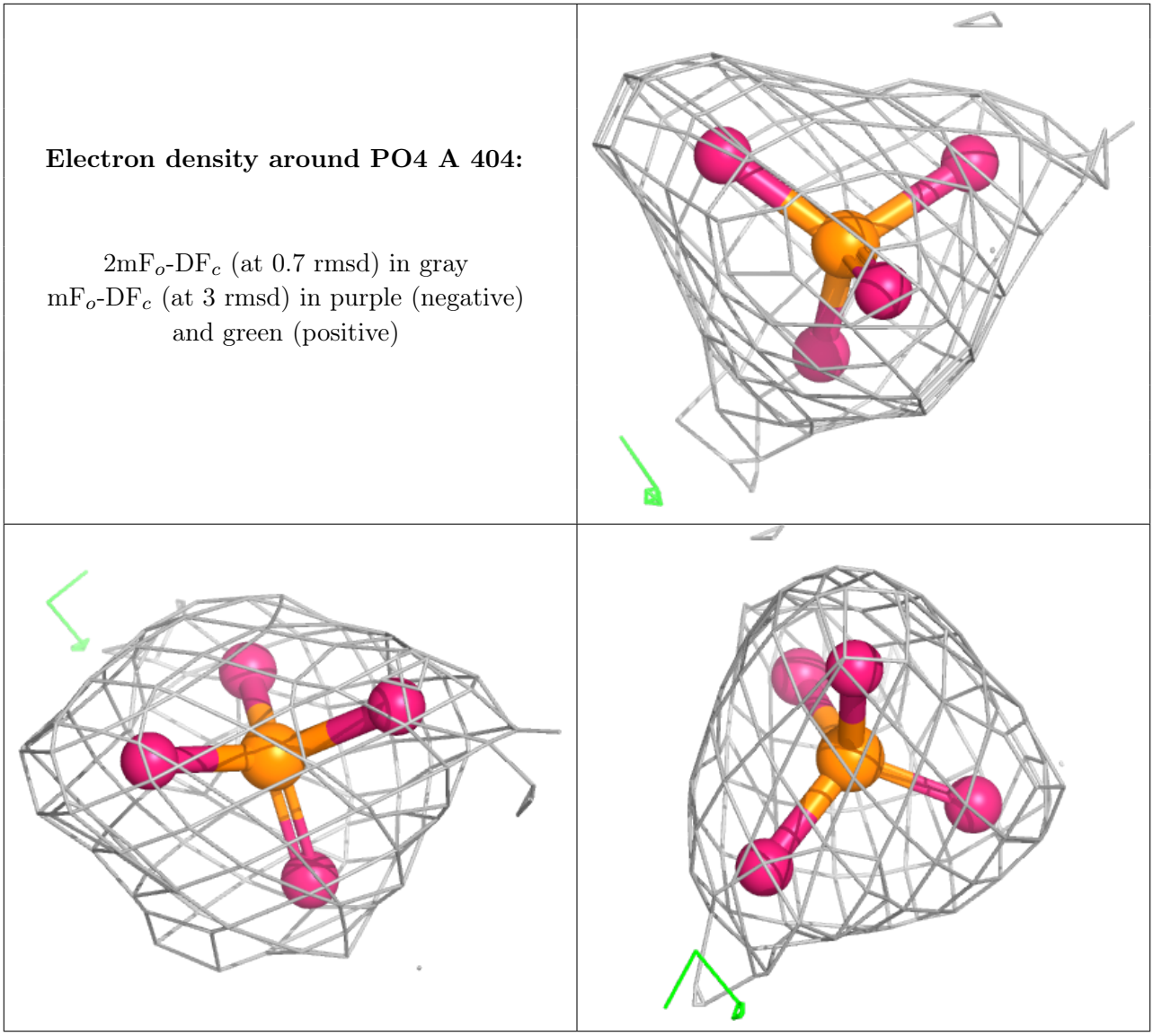






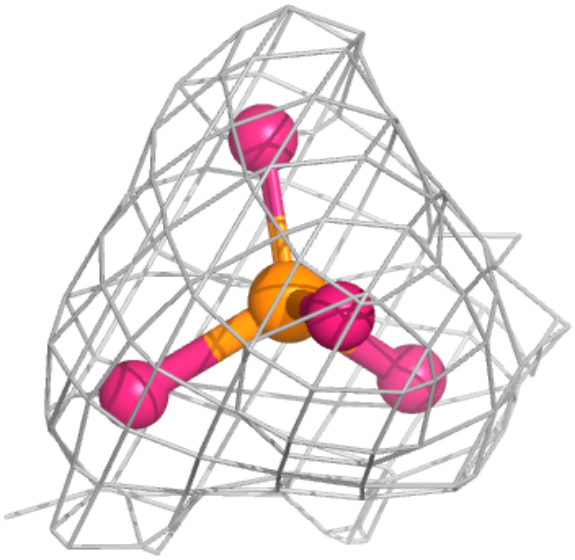
Electron density around PO4 A 404:

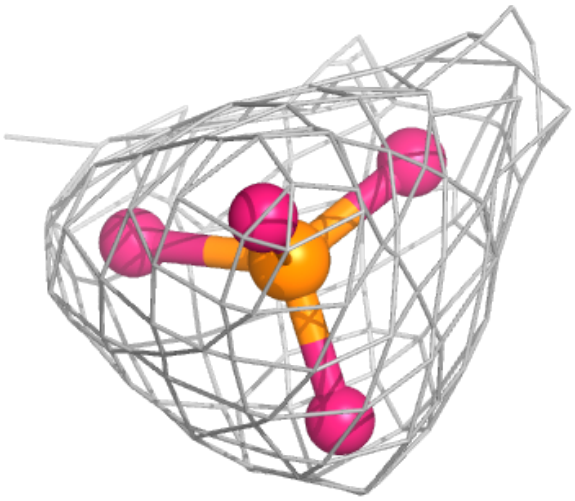
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

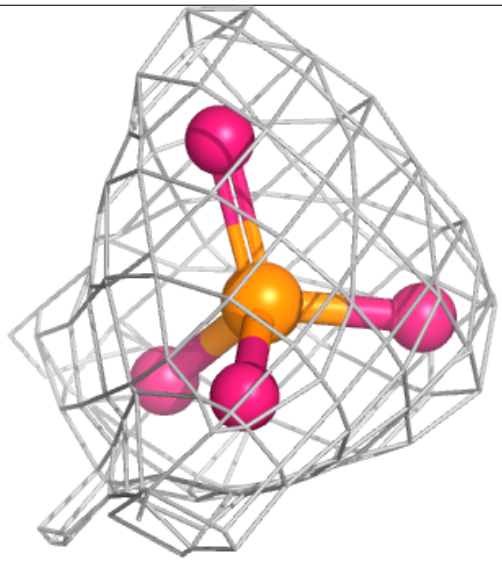


Electron density around PO4 B 405:

$2mF_o$-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.