Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 04:09 PM JST

PDB ID	:	8YES
Title	:	Crystal structure of adenosylcobinamide kinase / adenosylcobinamide phosphate guanylyltransferase complexed with adenosylcobinamide-phosphate
Authors	:	Nam, Y.; Do, H.
Deposited on	:	2024-02-23
Resolution	:	2.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

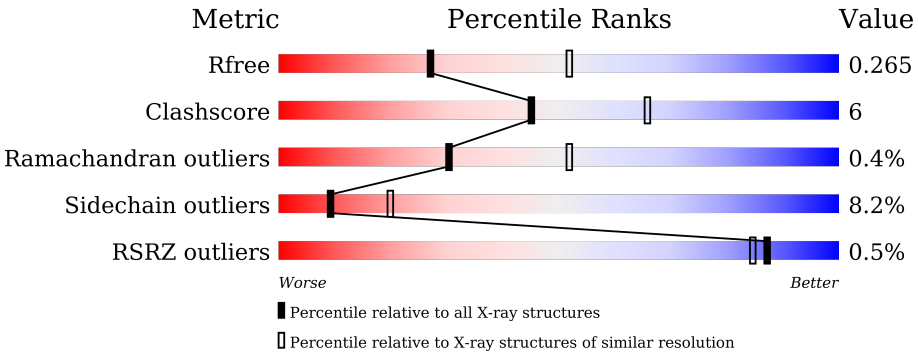
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.60 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.



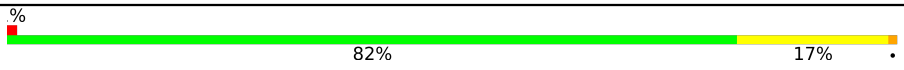
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	178	87% 11% •
1	D	178	% 86% 13% •
1	E	178	% 85% 13% ••
1	F	178	85% 12% •
2	B	179	83% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	179	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8753 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 Bifunctional adenosylcobalamin biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1349	842	251	251	5			
1	D	178	Total	C	N	O	S	0	0	0
			1349	842	251	251	5			
1	E	178	Total	C	N	O	S	0	0	0
			1349	842	251	251	5			
1	F	178	Total	C	N	O	S	0	0	0
			1349	842	251	251	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	SER	CYS	conflict	UNP A0A1I3YTB1
D	91	SER	CYS	conflict	UNP A0A1I3YTB1
E	91	SER	CYS	conflict	UNP A0A1I3YTB1
F	91	SER	CYS	conflict	UNP A0A1I3YTB1

- Molecule 2 is a protein called Bifunctional adenosylcobalamin biosynthesis protein.

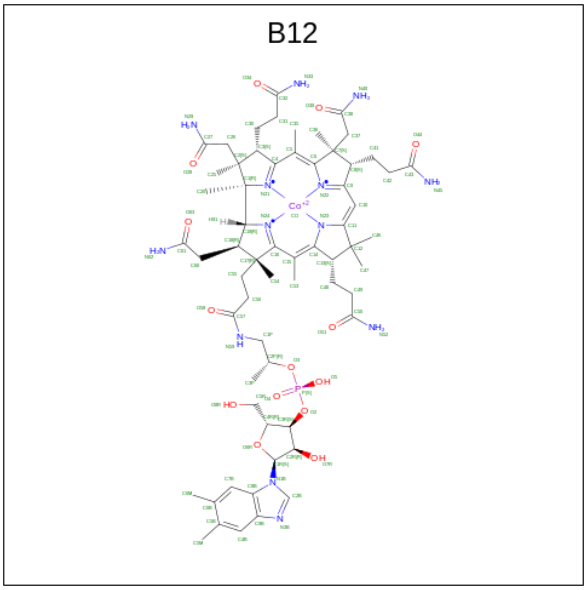
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1360	851	252	252	5			
2	C	179	Total	C	N	O	S	0	0	0
			1360	851	252	252	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	91	SER	CYS	conflict	UNP A0A1I3YTB1
C	91	SER	CYS	conflict	UNP A0A1I3YTB1

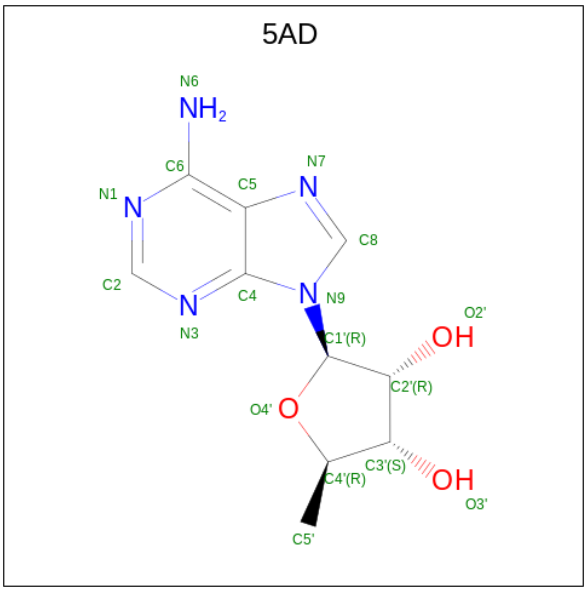
- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled

as "Ligand of Interest" by depositor).



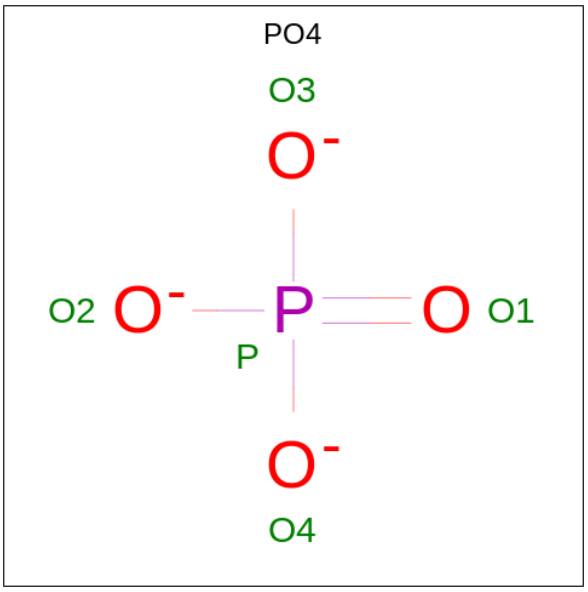
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		
3	B	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		
3	B	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		
3	D	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		
3	E	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		
3	F	1	Total	C	Co	N	O	P	0	0
			72	48	1	11	11	1		

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	10	5	3		
4	B	1	Total	C	N	O	0	0
			18	10	5	3		
4	C	1	Total	C	N	O	0	0
			18	10	5	3		
4	D	1	Total	C	N	O	0	0
			18	10	5	3		
4	E	1	Total	C	N	O	0	0
			18	10	5	3		
4	F	1	Total	C	N	O	0	0
			18	10	5	3		

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



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

- Molecule 6 is water.

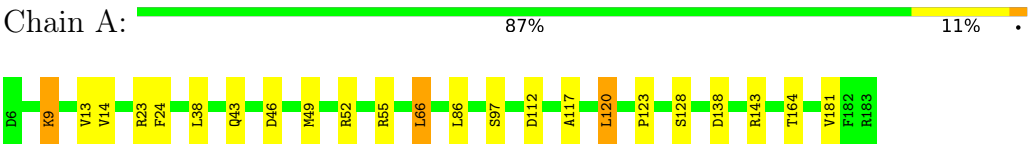
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	6	Total O 6 6	0	0
6	C	5	Total O 5 5	0	0
6	D	5	Total O 5 5	0	0
6	E	1	Total O 1 1	0	0
6	F	3	Total O 3 3	0	0

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.

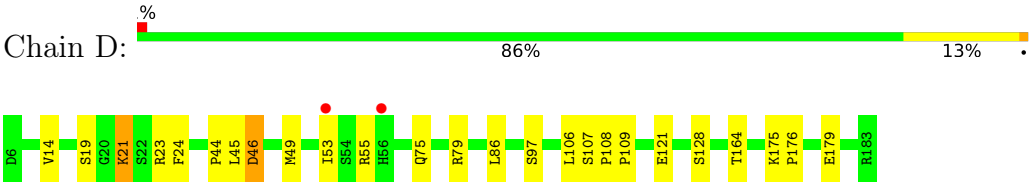
• Molecule 1: Bifunctional adenosylcobalamin biosynthesis protein

Chain A:



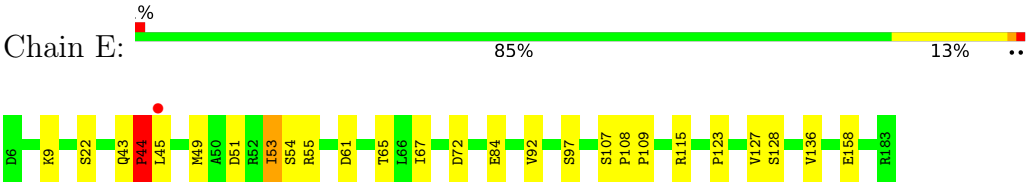
• Molecule 1: Bifunctional adenosylcobalamin biosynthesis protein

Chain D:



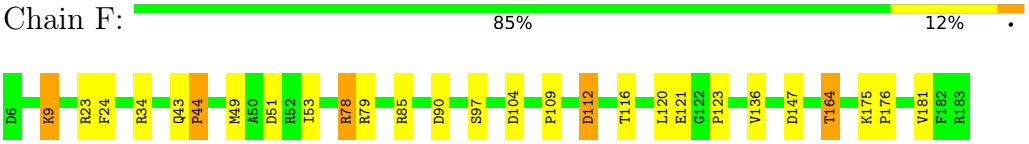
• Molecule 1: Bifunctional adenosylcobalamin biosynthesis protein

Chain E:



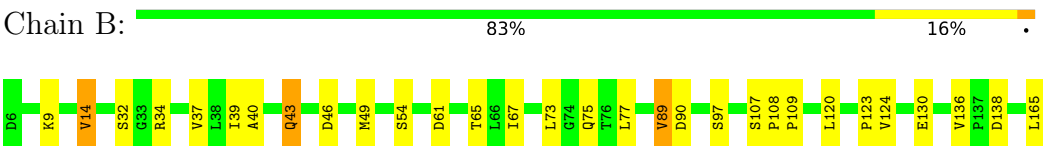
• Molecule 1: Bifunctional adenosylcobalamin biosynthesis protein

Chain F:



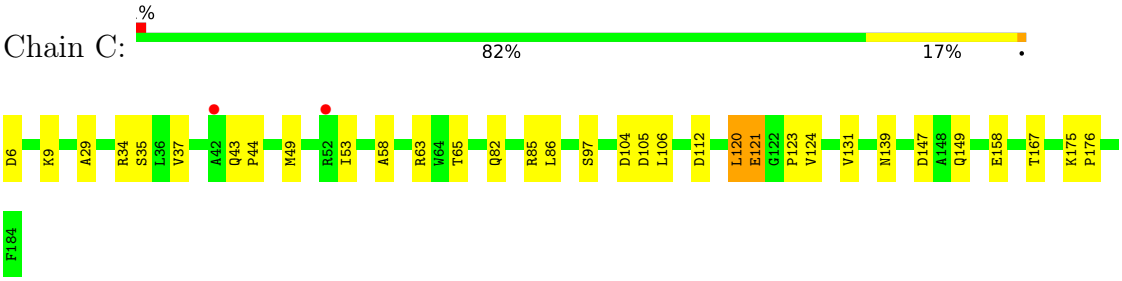
• Molecule 2: Bifunctional adenosylcobalamin biosynthesis protein

Chain B:



• Molecule 2: Bifunctional adenosylcobalamin biosynthesis protein

Chain C:


%
82%
17%
D6
K9
A29
R34
S35
L36
V37
A42
Q43
P44
M49
R52
I53
A58
R63
W64
T65
Q82
R85
L86
S97
D104
D105
L106
D112
L120
E121
G122
P123
V124
V131
N139
D147
A148
Q149
E158
T167
K175
P176
F184

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.21Å 102.92Å 129.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.60 47.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.96-2.60) 99.8 (47.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.263 0.197 , 0.265	Depositor DCC
R_{free} test set	2123 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5AD, PO4, B12

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	0.73	0/1369	0.88	0/1857
1	D	0.70	0/1369	0.85	0/1857
1	E	0.72	0/1369	0.86	0/1857
1	F	0.71	0/1369	0.86	0/1857
2	B	0.73	1/1381 (0.1%)	0.86	0/1873
2	C	0.72	0/1381	0.88	0/1873
All	All	0.72	1/8238 (0.0%)	0.87	0/11174

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	GLU	CD-OE2	5.35	1.31	1.25

There are no bond angle outliers.

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	1349	0	1378	12	0
1	D	1349	0	1378	11	0
1	E	1349	0	1378	6	0
1	F	1349	0	1378	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1360	0	1387	16	0
2	C	1360	0	1387	15	0
3	A	72	0	69	4	0
3	B	144	0	138	19	0
3	D	72	0	69	7	0
3	E	72	0	69	6	0
3	F	72	0	69	7	0
4	A	18	0	12	0	0
4	B	18	0	12	1	0
4	C	18	0	12	1	0
4	D	18	0	12	0	0
4	E	18	0	12	0	0
4	F	18	0	12	0	1
5	A	10	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
6	E	1	0	0	0	0
6	F	3	0	0	0	0
All	All	8753	0	8772	102	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (102) 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)
3:B:203:B12:H362	3:B:203:B12:H351	1.60	0.84
3:D:201:B12:H362	3:D:201:B12:H351	1.59	0.83
3:B:203:B12:H552	3:B:203:B12:H531	1.60	0.83
3:E:201:B12:H552	3:E:201:B12:H531	1.63	0.79
3:E:201:B12:H362	3:E:201:B12:H351	1.63	0.79
3:D:201:B12:H531	3:D:201:B12:H552	1.66	0.77
3:B:203:B12:H552	3:B:203:B12:C53	2.14	0.77
3:F:201:B12:H552	3:F:201:B12:H531	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:201:B12:H362	3:F:201:B12:H351	1.67	0.74
2:B:43:GLN:O	4:B:202:5AD:N6	2.25	0.69
3:B:201:B12:H552	3:B:201:B12:H531	1.76	0.67
3:B:201:B12:H362	3:B:201:B12:H351	1.76	0.67
3:F:201:B12:H552	3:F:201:B12:C53	2.26	0.66
3:B:203:B12:H451	2:C:139:ASN:HD21	1.45	0.64
3:B:201:B12:H601	3:B:201:B12:H562	1.80	0.64
1:A:117:ALA:HA	1:A:120:LEU:HD11	1.82	0.62
2:B:32:SER:O	2:B:34:ARG:NH1	2.32	0.62
1:F:85:ARG:O	1:F:123:PRO:HD2	2.00	0.61
3:F:201:B12:H562	3:F:201:B12:H601	1.82	0.61
3:B:203:B12:H531	3:B:203:B12:C55	2.31	0.61
1:F:44:PRO:HG2	1:F:53:ILE:HG21	1.83	0.59
1:D:175:LYS:HG3	1:D:176:PRO:HA	1.85	0.58
1:F:97:SER:OG	3:F:201:B12:H532	2.03	0.58
1:A:117:ALA:HA	1:A:120:LEU:CD1	2.34	0.57
1:D:19:SER:OG	1:D:21:LYS:HG2	2.04	0.57
3:D:201:B12:H552	3:D:201:B12:C53	2.34	0.56
1:F:24:PHE:CE2	1:F:164:THR:HG21	2.40	0.56
1:F:78:ARG:HG3	1:F:116:THR:HG23	1.87	0.56
3:E:201:B12:H552	3:E:201:B12:C53	2.33	0.55
1:D:46:ASP:OD1	1:D:49:MET:HB2	2.07	0.55
2:B:9:LYS:O	2:B:123:PRO:HA	2.07	0.54
1:A:9:LYS:O	1:A:123:PRO:HA	2.07	0.54
2:B:136:VAL:HG11	3:B:203:B12:H561	1.89	0.54
3:A:201:B12:H621	3:A:201:B12:H541	1.74	0.53
3:E:201:B12:H362	3:E:201:B12:C35	2.36	0.52
1:F:109:PRO:HA	1:F:112:ASP:HB3	1.92	0.52
2:B:107:SER:HB2	2:B:108:PRO:HD3	1.91	0.51
1:D:97:SER:OG	3:D:201:B12:H532	2.11	0.51
1:A:24:PHE:CE2	1:A:164:THR:HG21	2.45	0.51
2:B:73:LEU:O	2:B:77:LEU:HG	2.11	0.50
1:D:24:PHE:CE2	1:D:164:THR:HG21	2.47	0.50
1:E:97:SER:OG	3:E:201:B12:H532	2.11	0.50
3:B:203:B12:H261	4:C:201:5AD:O4'	2.11	0.50
2:C:9:LYS:O	2:C:123:PRO:HA	2.11	0.49
1:E:107:SER:HB2	1:E:108:PRO:HD3	1.94	0.49
2:B:97:SER:OG	3:B:201:B12:H532	2.12	0.49
1:F:9:LYS:O	1:F:123:PRO:HA	2.12	0.49
1:A:24:PHE:HE2	1:A:164:THR:HG21	1.77	0.49
2:B:108:PRO:HB2	2:B:109:PRO:HD3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:B12:H532	2:C:97:SER:OG	2.12	0.48
2:C:29:ALA:HA	2:C:86:LEU:CD2	2.44	0.48
3:B:201:B12:O28	3:B:201:B12:H3	2.14	0.47
1:F:116:THR:O	1:F:120:LEU:HG	2.14	0.47
2:B:14:VAL:HG23	2:B:165:LEU:HD12	1.96	0.47
2:B:40:ALA:HA	2:B:90:ASP:HB2	1.96	0.47
3:B:203:B12:H302	3:B:203:B12:H353	1.97	0.47
2:C:35:SER:O	2:C:85:ARG:HA	2.15	0.47
2:B:165:LEU:HD11	2:C:167:THR:HG21	1.96	0.46
1:E:92:VAL:HG23	1:E:127:VAL:O	2.15	0.46
2:C:6:ASP:O	2:C:6:ASP:OD1	2.33	0.46
2:C:37:VAL:HA	2:C:65:THR:O	2.15	0.46
3:D:201:B12:H351	3:D:201:B12:C36	2.36	0.45
3:B:201:B12:H562	3:B:201:B12:C60	2.44	0.45
2:B:108:PRO:HB2	2:B:109:PRO:CD	2.46	0.45
3:D:201:B12:O28	3:D:201:B12:H3	2.16	0.45
2:C:82:GLN:HA	2:C:121:GLU:HG2	1.99	0.45
3:A:201:B12:H552	3:A:201:B12:H531	1.99	0.45
1:E:44:PRO:CG	1:E:53:ILE:HG21	2.47	0.45
3:F:201:B12:H491	3:F:201:B12:H533	1.99	0.45
2:C:131:VAL:HG22	2:C:149:GLN:HG2	1.99	0.44
1:A:13:VAL:HG22	1:A:164:THR:CG2	2.48	0.44
1:A:97:SER:OG	3:A:201:B12:H532	2.18	0.44
2:C:175:LYS:HA	2:C:176:PRO:C	2.37	0.44
3:A:201:B12:H253	3:A:201:B12:H301	1.68	0.43
2:C:58:ALA:HB1	6:C:301:HOH:O	2.18	0.43
2:B:39:ILE:HB	2:B:89:VAL:HA	2.00	0.43
1:A:138:ASP:OD1	1:A:138:ASP:C	2.57	0.43
2:B:46:ASP:OD1	2:B:49:MET:HB2	2.18	0.43
1:D:121:GLU:H	1:D:121:GLU:CD	2.21	0.43
3:B:203:B12:H353	3:B:203:B12:C30	2.49	0.43
3:B:201:B12:H363	3:B:201:B12:H412	1.78	0.43
1:A:38:LEU:HD23	1:A:66:LEU:HD12	1.99	0.43
1:A:46:ASP:OD1	1:A:49:MET:HB2	2.19	0.43
1:E:9:LYS:O	1:E:123:PRO:HA	2.18	0.42
2:C:120:LEU:HD12	2:C:124:VAL:CG1	2.49	0.42
3:F:201:B12:H253	3:F:201:B12:H301	1.78	0.42
1:D:14:VAL:HA	1:D:128:SER:O	2.20	0.42
1:E:108:PRO:HB2	1:E:109:PRO:HD3	2.02	0.42
3:E:201:B12:O28	3:E:201:B12:H3	2.19	0.42
1:F:175:LYS:HA	1:F:176:PRO:C	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG11	2:B:67:ILE:HD12	2.02	0.41
1:D:107:SER:HB2	1:D:108:PRO:HD3	2.02	0.41
3:B:201:B12:H301	3:B:201:B12:H253	1.82	0.41
1:D:44:PRO:HG3	1:D:53:ILE:HB	2.02	0.41
2:C:44:PRO:HG3	2:C:53:ILE:HG13	2.03	0.41
1:A:143:ARG:HH12	3:B:201:B12:H331	1.68	0.41
3:D:201:B12:H362	3:D:201:B12:C35	2.42	0.41
1:D:106:LEU:O	1:D:109:PRO:HD2	2.21	0.40
2:B:120:LEU:CD1	2:B:124:VAL:HG11	2.52	0.40
1:A:14:VAL:HA	1:A:128:SER:O	2.21	0.40
2:C:105:ASP:OD1	2:C:106:LEU:N	2.55	0.40
1:D:175:LYS:HA	1:D:176:PRO:C	2.41	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:202:5AD:O2'	4:F:202:5AD:O2'[2_555]	2.11	0.09
1:F:43:GLN:OE1	1:F:43:GLN:OE1[2_555]	2.17	0.03

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	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
1	D	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
1	E	176/178 (99%)	157 (89%)	18 (10%)	1 (1%)	22	43
1	F	176/178 (99%)	162 (92%)	12 (7%)	2 (1%)	12	26
2	B	177/179 (99%)	166 (94%)	10 (6%)	1 (1%)	22	43
2	C	177/179 (99%)	169 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1058/1070 (99%)	990 (94%)	64 (6%)	4 (0%)	30 52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	ASP
1	E	44	PRO
1	F	90	ASP
1	F	44	PRO

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	140/140 (100%)	130 (93%)	10 (7%)	12 26
1	D	140/140 (100%)	131 (94%)	9 (6%)	14 32
1	E	140/140 (100%)	122 (87%)	18 (13%)	3 6
1	F	140/140 (100%)	126 (90%)	14 (10%)	6 13
2	B	141/141 (100%)	133 (94%)	8 (6%)	17 37
2	C	141/141 (100%)	131 (93%)	10 (7%)	12 26
All	All	842/842 (100%)	773 (92%)	69 (8%)	9 20

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	23	ARG
1	A	43	GLN
1	A	52	ARG
1	A	55	ARG
1	A	66	LEU
1	A	86	LEU
1	A	112	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	LEU
1	A	181	VAL
2	B	14	VAL
2	B	43	GLN
2	B	54	SER
2	B	65	THR
2	B	75	GLN
2	B	89	VAL
2	B	138	ASP
2	B	183	ARG
2	C	34	ARG
2	C	43	GLN
2	C	49	MET
2	C	63	ARG
2	C	104	ASP
2	C	112	ASP
2	C	120	LEU
2	C	121	GLU
2	C	147	ASP
2	C	158	GLU
1	D	21	LYS
1	D	23	ARG
1	D	45	LEU
1	D	46	ASP
1	D	55	ARG
1	D	75	GLN
1	D	79	ARG
1	D	86	LEU
1	D	179	GLU
1	E	22	SER
1	E	43	GLN
1	E	44	PRO
1	E	45	LEU
1	E	49	MET
1	E	51	ASP
1	E	53	ILE
1	E	54	SER
1	E	55	ARG
1	E	61	ASP
1	E	65	THR
1	E	67	ILE
1	E	72	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	84	GLU
1	E	115	ARG
1	E	128	SER
1	E	136	VAL
1	E	158	GLU
1	F	9	LYS
1	F	23	ARG
1	F	34	ARG
1	F	49	MET
1	F	51	ASP
1	F	78	ARG
1	F	79	ARG
1	F	104	ASP
1	F	112	ASP
1	F	121	GLU
1	F	136	VAL
1	F	147	ASP
1	F	164	THR
1	F	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
2	B	129	ASN
2	B	173	GLN
2	C	82	GLN
2	C	139	ASN
2	C	173	GLN
1	D	43	GLN
1	D	129	ASN
1	D	173	GLN
1	E	129	ASN
1	E	149	GLN
1	E	173	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

26 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	$\#\|Z\| > 2$
5	PO4	E	204	-	4,4,4	0.48	0	6,6,6	0.76	0
3	B12	E	201	-	71,79,101	1.27	6 (8%)	114,132,166	1.96	18 (15%)
4	5AD	D	202	-	17,20,20	0.62	0	15,30,30	0.94	0
3	B12	F	201	-	71,79,101	1.36	8 (11%)	114,132,166	2.08	23 (20%)
5	PO4	D	203	-	4,4,4	0.53	0	6,6,6	0.56	0
5	PO4	C	202	-	4,4,4	1.27	1 (25%)	6,6,6	0.51	0
5	PO4	E	203	-	4,4,4	1.19	0	6,6,6	0.40	0
4	5AD	E	202	-	17,20,20	0.66	0	15,30,30	1.01	1 (6%)
3	B12	B	203	-	71,79,101	1.44	7 (9%)	114,132,166	2.32	28 (24%)
3	B12	D	201	-	71,79,101	1.29	5 (7%)	114,132,166	2.09	20 (17%)
5	PO4	B	206	-	4,4,4	0.54	0	6,6,6	0.43	0
5	PO4	B	204	-	4,4,4	0.60	0	6,6,6	0.58	0
5	PO4	A	204	-	4,4,4	0.83	0	6,6,6	0.64	0
5	PO4	D	204	-	4,4,4	1.05	0	6,6,6	0.52	0
5	PO4	C	203	-	4,4,4	0.25	0	6,6,6	0.63	0
5	PO4	F	203	-	4,4,4	0.92	0	6,6,6	0.76	0
3	B12	B	201	-	71,79,101	1.46	8 (11%)	114,132,166	2.17	27 (23%)
5	PO4	C	204	-	4,4,4	0.52	0	6,6,6	0.47	0
4	5AD	A	202	-	17,20,20	0.60	0	15,30,30	1.20	3 (20%)
4	5AD	F	202	-	17,20,20	0.73	0	15,30,30	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	B12	A	201	-	71,79,101	1.48	10 (14%)	114,132,166	1.98	22 (19%)
5	PO4	A	203	-	4,4,4	0.84	0	6,6,6	0.77	0
5	PO4	D	205	-	4,4,4	0.59	0	6,6,6	0.46	0
4	5AD	C	201	-	17,20,20	0.62	0	15,30,30	1.03	2 (13%)
4	5AD	B	202	-	17,20,20	0.67	0	15,30,30	1.08	1 (6%)
5	PO4	B	205	-	4,4,4	1.29	1 (25%)	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5AD	A	202	-	-	0/0/20/20	0/3/3/3
4	5AD	F	202	-	-	0/0/20/20	0/3/3/3
4	5AD	E	202	-	-	0/0/20/20	0/3/3/3
3	B12	B	203	-	-	18/45/196/223	-
3	B12	A	201	-	-	18/45/196/223	-
4	5AD	C	201	-	-	0/0/20/20	0/3/3/3
3	B12	E	201	-	-	7/45/196/223	-
4	5AD	B	202	-	-	0/0/20/20	0/3/3/3
3	B12	B	201	-	-	9/45/196/223	-
4	5AD	D	202	-	-	0/0/20/20	0/3/3/3
3	B12	D	201	-	-	14/45/196/223	-
3	B12	F	201	-	-	11/45/196/223	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	B12	C14-N23	-5.48	1.28	1.35
3	B	203	B12	C19-N24	-5.19	1.39	1.48
3	B	203	B12	C14-N23	-5.09	1.28	1.35
3	F	201	B12	C14-N23	-4.98	1.28	1.35
3	E	201	B12	C14-N23	-4.72	1.29	1.35
3	A	201	B12	C16-C15	-4.63	1.31	1.44
3	F	201	B12	C19-N24	-4.44	1.40	1.48
3	B	201	B12	C9-N22	4.41	1.42	1.30
3	D	201	B12	C14-N23	-4.33	1.29	1.35
3	F	201	B12	C16-C15	-4.33	1.32	1.44
3	B	203	B12	C16-C15	-4.26	1.32	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	B12	C19-N24	-3.93	1.41	1.48
3	A	201	B12	C19-N24	-3.91	1.41	1.48
3	A	201	B12	C14-N23	-3.90	1.30	1.35
3	D	201	B12	C9-N22	3.70	1.40	1.30
3	E	201	B12	C19-N24	-3.67	1.42	1.48
3	E	201	B12	C16-C15	-3.62	1.34	1.44
3	E	201	B12	C9-N22	3.52	1.39	1.30
3	B	203	B12	C9-N22	3.52	1.39	1.30
3	D	201	B12	C16-C15	-3.50	1.34	1.44
3	F	201	B12	C9-N22	3.27	1.39	1.30
3	B	201	B12	C19-N24	-3.22	1.42	1.48
3	B	201	B12	C60-C61	-3.15	1.43	1.51
3	B	201	B12	C16-C15	-3.12	1.36	1.44
3	D	201	B12	C60-C61	-2.87	1.44	1.51
3	A	201	B12	C9-N22	2.82	1.37	1.30
3	B	203	B12	C60-C61	-2.69	1.44	1.51
3	A	201	B12	C1-C19	-2.65	1.49	1.55
3	A	201	B12	C56-C57	-2.42	1.46	1.51
3	A	201	B12	C54-C17	-2.34	1.50	1.54
3	B	201	B12	C56-C57	-2.27	1.47	1.51
3	B	203	B12	C14-C15	2.26	1.48	1.38
3	A	201	B12	C10-C11	-2.25	1.31	1.38
3	B	201	B12	P-O2	2.25	1.63	1.54
3	F	201	B12	C1-C2	-2.19	1.53	1.58
3	E	201	B12	C60-C61	-2.18	1.45	1.51
5	B	205	PO4	P-O3	-2.16	1.48	1.54
3	B	203	B12	C46-C12	-2.14	1.49	1.54
3	F	201	B12	C10-C9	2.12	1.45	1.39
3	A	201	B12	O58-C57	-2.12	1.19	1.23
3	F	201	B12	P-O2	2.12	1.63	1.54
3	B	201	B12	C60-C18	2.09	1.58	1.54
3	E	201	B12	P-O2	2.07	1.62	1.54
3	F	201	B12	C60-C61	-2.07	1.46	1.51
5	C	202	PO4	P-O3	-2.05	1.48	1.54
3	A	201	B12	C57-N59	-2.02	1.28	1.33

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	B12	C1-C19-N24	9.85	117.32	106.24
3	E	201	B12	C1-C19-N24	9.68	117.13	106.24
3	F	201	B12	C1-C19-N24	9.15	116.54	106.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	B12	C20-C1-C19	-9.12	100.57	109.36
3	D	201	B12	C1-C19-N24	8.76	116.10	106.24
3	B	201	B12	C20-C1-C19	-8.61	101.06	109.36
3	B	203	B12	C1-C19-N24	8.08	115.33	106.24
3	F	201	B12	C20-C1-C19	-7.88	101.77	109.36
3	F	201	B12	C2-C1-C19	7.65	130.68	118.60
3	A	201	B12	C1-C19-N24	7.50	114.68	106.24
3	D	201	B12	C20-C1-C19	-7.45	102.18	109.36
3	A	201	B12	C18-C19-N24	6.82	112.69	102.31
3	B	203	B12	C2-C1-C19	6.79	129.32	118.60
3	D	201	B12	C60-C18-C19	6.71	132.14	114.62
3	D	201	B12	C2-C1-C19	6.62	129.05	118.60
3	A	201	B12	C2P-C1P-N59	-6.52	103.32	112.93
3	E	201	B12	C20-C1-C19	-6.49	103.10	109.36
3	E	201	B12	C18-C19-N24	6.38	112.02	102.31
3	D	201	B12	C1-C19-C18	6.07	131.84	121.88
3	A	201	B12	C60-C18-C19	5.83	129.84	114.62
3	B	201	B12	C2-C1-C19	5.82	127.78	118.60
3	E	201	B12	C2-C1-C19	5.81	127.77	118.60
3	B	203	B12	C1-C19-C18	5.71	131.25	121.88
3	F	201	B12	C1-C19-C18	5.68	131.21	121.88
3	B	203	B12	C18-C17-C16	-5.66	93.79	100.67
3	A	201	B12	C20-C1-C19	-5.65	103.91	109.36
3	B	201	B12	C18-C19-N24	5.64	110.89	102.31
3	F	201	B12	C18-C17-C16	-5.64	93.82	100.67
3	B	203	B12	C18-C19-N24	5.63	110.88	102.31
3	B	201	B12	C60-C18-C19	5.59	129.20	114.62
3	B	203	B12	C56-C57-N59	5.44	125.57	116.42
3	A	201	B12	C1-C19-C18	4.95	130.01	121.88
3	E	201	B12	C60-C18-C19	4.91	127.43	114.62
3	D	201	B12	C18-C19-N24	4.90	109.77	102.31
3	B	203	B12	C56-C55-C17	4.90	124.95	115.52
3	B	203	B12	C60-C18-C19	4.81	127.17	114.62
3	D	201	B12	C18-C17-C16	-4.72	94.93	100.67
3	F	201	B12	C60-C18-C19	4.61	126.64	114.62
3	B	201	B12	C1-C19-C18	4.60	129.43	121.88
3	F	201	B12	C18-C19-N24	4.54	109.22	102.31
3	B	201	B12	C18-C17-C16	-4.24	95.51	100.67
3	F	201	B12	C13-C14-N23	4.20	114.82	109.10
3	E	201	B12	C18-C17-C16	-4.10	95.68	100.67
3	B	203	B12	C3P-C2P-C1P	3.89	118.94	111.39
3	D	201	B12	C9-C10-C11	-3.88	120.36	125.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	B12	C13-C14-N23	3.84	114.32	109.10
3	E	201	B12	C7-C6-N22	3.77	114.82	107.94
3	E	201	B12	C48-C13-C14	3.75	117.83	108.49
3	B	203	B12	O58-C57-N59	-3.75	115.94	123.01
3	E	201	B12	C1-C19-C18	3.74	128.03	121.88
3	F	201	B12	C3P-C2P-C1P	3.56	118.31	111.39
3	D	201	B12	C36-C7-C37	3.52	116.61	110.80
3	A	201	B12	C2-C1-C19	3.52	124.16	118.60
3	B	201	B12	C48-C13-C14	3.45	117.08	108.49
3	A	201	B12	C13-C14-N23	3.37	113.69	109.10
3	E	201	B12	C13-C14-N23	3.33	113.64	109.10
3	B	203	B12	C26-C2-C1	3.31	115.17	110.01
3	B	201	B12	C25-C2-C1	3.28	118.73	113.78
3	B	201	B12	C5-C6-N22	-3.27	118.89	123.88
3	D	201	B12	C20-C1-N21	-3.26	104.91	110.27
3	B	201	B12	C7-C6-N22	3.26	113.90	107.94
3	B	203	B12	C48-C13-C14	3.25	116.59	108.49
3	B	201	B12	C3P-C2P-C1P	3.25	117.70	111.39
3	B	203	B12	C13-C14-N23	3.22	113.49	109.10
3	A	201	B12	C18-C60-C61	3.22	122.02	113.97
3	A	201	B12	C48-C13-C14	3.22	116.52	108.49
3	D	201	B12	O5-P-O4	3.20	123.21	110.68
3	B	203	B12	C7-C8-C9	-3.17	96.85	100.90
3	D	201	B12	C48-C13-C14	3.16	116.37	108.49
3	A	201	B12	C9-C10-C11	-3.13	121.44	125.97
3	F	201	B12	C9-C10-C11	-3.08	121.52	125.97
3	B	201	B12	C12-C11-C10	-3.05	119.40	123.37
3	A	201	B12	C36-C7-C37	3.01	115.76	110.80
3	B	203	B12	C1P-N59-C57	2.95	129.12	122.69
3	B	203	B12	C2P-C1P-N59	-2.92	108.63	112.93
3	E	201	B12	C7-C6-C5	-2.83	123.62	128.07
3	D	201	B12	O34-C32-N33	-2.79	114.90	122.50
3	F	201	B12	C12-C11-C10	-2.71	119.85	123.37
3	B	203	B12	C9-C10-C11	-2.68	122.09	125.97
3	E	201	B12	O5-P-O4	2.66	121.11	110.68
3	B	201	B12	C9-C10-C11	-2.63	122.16	125.97
3	D	201	B12	C13-C14-N23	2.63	112.68	109.10
3	B	203	B12	C18-C60-C61	2.60	120.45	113.97
3	B	201	B12	O58-C57-C56	-2.56	117.33	122.02
3	A	201	B12	P-O3-C2P	-2.55	115.49	123.21
3	B	201	B12	C2P-C1P-N59	-2.53	109.20	112.93
3	B	203	B12	O5-P-O4	2.53	120.57	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	201	B12	C13-C14-C15	-2.53	120.46	124.32
3	B	203	B12	C55-C17-C18	2.52	116.03	111.15
3	A	201	B12	C12-C11-C10	-2.52	120.09	123.37
3	B	203	B12	C7-C6-N22	2.51	112.52	107.94
3	D	201	B12	C7-C6-N22	2.51	112.52	107.94
3	B	201	B12	C13-C12-C11	-2.51	98.13	100.97
3	F	201	B12	C26-C2-C1	2.50	113.90	110.01
3	F	201	B12	O5-P-O4	2.47	120.37	110.68
3	A	201	B12	C48-C13-C12	-2.47	109.72	116.63
3	E	201	B12	C20-C1-N21	-2.46	106.23	110.27
3	F	201	B12	C7-C6-N22	2.45	112.41	107.94
3	F	201	B12	C54-C17-C18	2.43	116.56	112.98
3	B	201	B12	O63-C61-C60	-2.40	115.81	120.87
3	B	201	B12	C13-C14-C15	-2.39	120.66	124.32
3	E	201	B12	C15-C14-N23	-2.39	123.34	126.26
3	F	201	B12	O63-C61-C60	-2.37	115.88	120.87
3	E	201	B12	C9-C10-C11	-2.37	122.55	125.97
3	D	201	B12	O63-C61-N62	2.36	128.95	122.50
3	A	201	B12	C55-C17-C16	2.35	121.30	116.65
3	E	201	B12	C47-C12-C46	-2.34	105.40	109.35
3	B	203	B12	O28-C27-N29	-2.33	116.13	122.50
3	A	201	B12	C7-C8-C9	-2.32	97.93	100.90
3	D	201	B12	C18-C60-C61	2.32	119.76	113.97
3	B	201	B12	C48-C13-C12	-2.31	110.14	116.63
4	A	202	5AD	C5-C6-N6	2.31	123.87	120.35
3	F	201	B12	C37-C7-C8	2.31	114.58	108.39
4	C	201	5AD	C5-C6-N6	2.30	123.85	120.35
4	C	201	5AD	C1'-N9-C4	-2.29	122.62	126.64
3	F	201	B12	C36-C7-C8	-2.28	107.86	112.08
4	B	202	5AD	C5-C6-N6	2.27	123.81	120.35
3	F	201	B12	C48-C13-C14	2.27	114.15	108.49
3	B	201	B12	O63-C61-N62	2.27	128.69	122.50
3	F	201	B12	O58-C57-C56	-2.26	117.89	122.02
4	A	202	5AD	C5'-C4'-C3'	2.22	118.03	115.70
4	E	202	5AD	C5-C6-N6	2.22	123.72	120.35
3	B	201	B12	C31-C30-C3	-2.21	108.35	114.73
3	B	203	B12	C35-C5-C6	2.19	125.92	122.43
3	D	201	B12	C7-C8-C9	-2.18	98.12	100.90
3	B	203	B12	O39-C38-N40	2.17	128.43	122.50
3	B	203	B12	O58-C57-C56	-2.15	118.08	122.02
3	A	201	B12	C30-C3-C2	-2.15	114.54	119.09
3	B	201	B12	C55-C17-C16	2.14	120.88	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	202	5AD	C1'-N9-C4	-2.13	122.89	126.64
3	B	201	B12	C56-C55-C17	-2.12	111.43	115.52
3	A	201	B12	C36-C7-C8	-2.12	108.16	112.08
3	B	201	B12	O2-P-O5	2.12	115.73	107.64
3	D	201	B12	C42-C41-C8	-2.11	108.63	114.73
3	B	203	B12	O3-C2P-C3P	-2.10	100.61	108.72
3	A	201	B12	O5-P-O4	2.09	118.86	110.68
3	E	201	B12	C31-C30-C3	-2.09	108.70	114.73
3	D	201	B12	C36-C7-C8	-2.07	108.25	112.08
3	B	203	B12	C12-C11-C10	-2.07	120.68	123.37
3	E	201	B12	C1P-N59-C57	-2.07	118.18	122.69
3	A	201	B12	C30-C3-C4	2.06	114.42	109.63
3	F	201	B12	C20-C1-C2	-2.05	109.86	113.28
3	B	201	B12	C10-C11-N23	2.05	127.93	124.43
3	F	201	B12	O63-C61-N62	2.04	128.08	122.50
3	A	201	B12	C5-C6-N22	-2.01	120.81	123.88

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	B12	C38-C37-C7-C6
3	A	201	B12	C38-C37-C7-C36
3	A	201	B12	C38-C37-C7-C8
3	A	201	B12	C56-C57-N59-C1P
3	A	201	B12	O58-C57-N59-C1P
3	A	201	B12	C19-C18-C60-C61
3	A	201	B12	N59-C1P-C2P-C3P
3	A	201	B12	N59-C1P-C2P-O3
3	A	201	B12	C2P-O3-P-O4
3	A	201	B12	C2P-O3-P-O5
3	B	201	B12	C42-C41-C8-C9
3	B	201	B12	C19-C18-C60-C61
3	B	201	B12	N59-C1P-C2P-C3P
3	B	203	B12	C38-C37-C7-C36
3	B	203	B12	C16-C17-C55-C56
3	B	203	B12	C54-C17-C55-C56
3	B	203	B12	C18-C17-C55-C56
3	B	203	B12	C56-C57-N59-C1P
3	B	203	B12	O58-C57-N59-C1P
3	B	203	B12	N59-C1P-C2P-C3P
3	B	203	B12	N59-C1P-C2P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	201	B12	C38-C37-C7-C6
3	D	201	B12	C38-C37-C7-C36
3	D	201	B12	C38-C37-C7-C8
3	D	201	B12	C18-C17-C55-C56
3	D	201	B12	C19-C18-C60-C61
3	D	201	B12	C1P-C2P-O3-P
3	D	201	B12	C3P-C2P-O3-P
3	E	201	B12	C19-C18-C60-C61
3	E	201	B12	N59-C1P-C2P-C3P
3	E	201	B12	C1P-C2P-O3-P
3	F	201	B12	C16-C17-C55-C56
3	F	201	B12	C18-C17-C55-C56
3	F	201	B12	C19-C18-C60-C61
3	F	201	B12	C1P-C2P-O3-P
3	F	201	B12	C3P-C2P-O3-P
3	A	201	B12	C2-C3-C30-C31
3	A	201	B12	C4-C3-C30-C31
3	B	201	B12	C18-C17-C55-C56
3	E	201	B12	C18-C17-C55-C56
3	F	201	B12	C2-C3-C30-C31
3	B	201	B12	C16-C17-C55-C56
3	D	201	B12	C16-C17-C55-C56
3	E	201	B12	C16-C17-C55-C56
3	B	203	B12	C19-C18-C60-C61
3	B	203	B12	C38-C37-C7-C8
3	B	203	B12	C42-C41-C8-C7
3	F	201	B12	C4-C3-C30-C31
3	B	203	B12	C48-C49-C50-N52
3	B	203	B12	C38-C37-C7-C6
3	F	201	B12	C3-C30-C31-C32
3	A	201	B12	C30-C31-C32-N33
3	B	201	B12	C30-C31-C32-O34
3	A	201	B12	C30-C31-C32-O34
3	B	201	B12	C30-C31-C32-N33
3	D	201	B12	C30-C31-C32-O34
3	B	203	B12	C1P-C2P-O3-P
3	B	203	B12	C3P-C2P-O3-P
3	E	201	B12	C3P-C2P-O3-P
3	D	201	B12	N59-C1P-C2P-C3P
3	F	201	B12	N59-C1P-C2P-C3P
3	E	201	B12	N59-C1P-C2P-O3
3	F	201	B12	C14-C13-C48-C49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	201	B12	C18-C60-C61-O63
3	A	201	B12	C14-C13-C48-C49
3	B	203	B12	C42-C41-C8-C9
3	A	201	B12	C18-C60-C61-N62
3	B	203	B12	C48-C49-C50-O51
3	F	201	B12	C54-C17-C55-C56
3	D	201	B12	C30-C31-C32-N33
3	B	201	B12	N59-C1P-C2P-O3
3	D	201	B12	C2P-O3-P-O4
3	D	201	B12	C2P-O3-P-O5
3	B	203	B12	C2P-C1P-N59-C57
3	A	201	B12	C3-C2-C26-C27
3	D	201	B12	C17-C18-C60-C61
3	B	201	B12	C2-C3-C30-C31

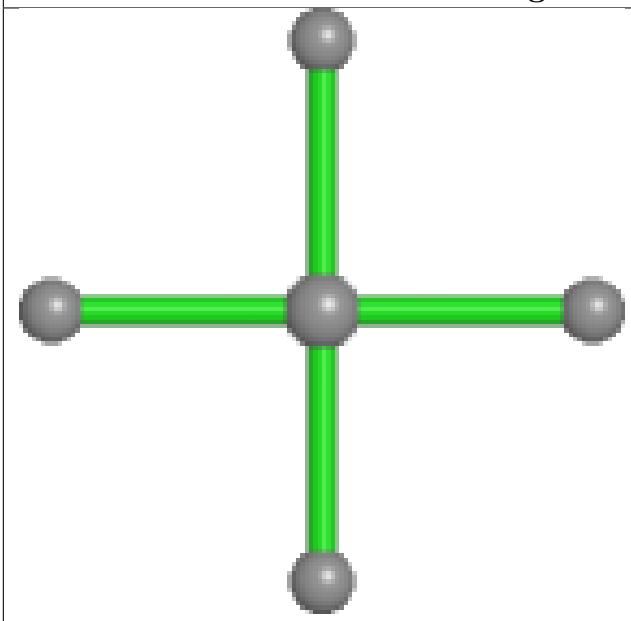
There are no ring outliers.

9 monomers are involved in 45 short contacts:

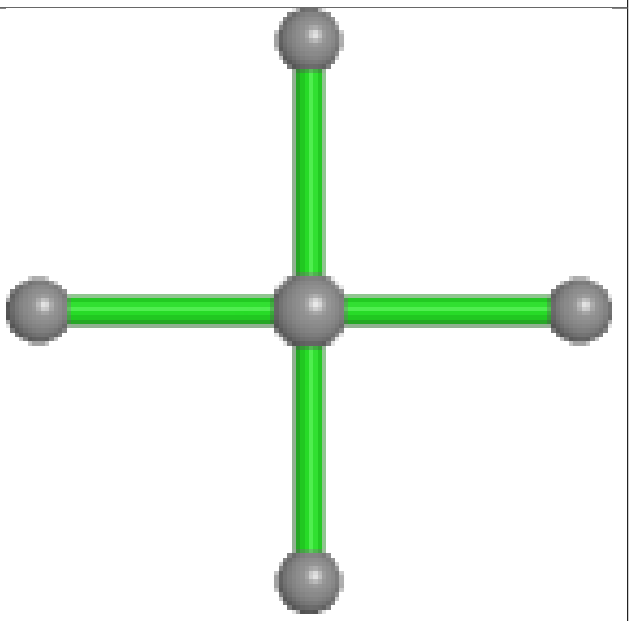
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201	B12	6	0
3	F	201	B12	7	0
3	B	203	B12	10	0
3	D	201	B12	7	0
3	B	201	B12	9	0
4	F	202	5AD	0	1
3	A	201	B12	4	0
4	C	201	5AD	1	0
4	B	202	5AD	1	0

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.

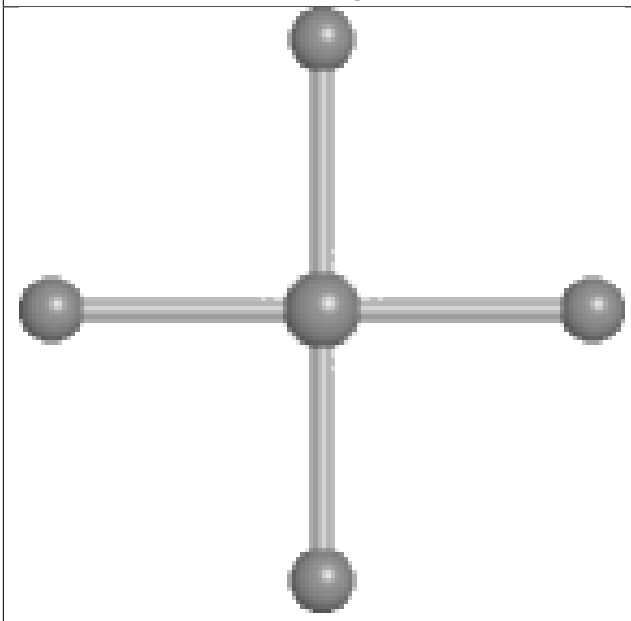
Ligand PO4 E 204



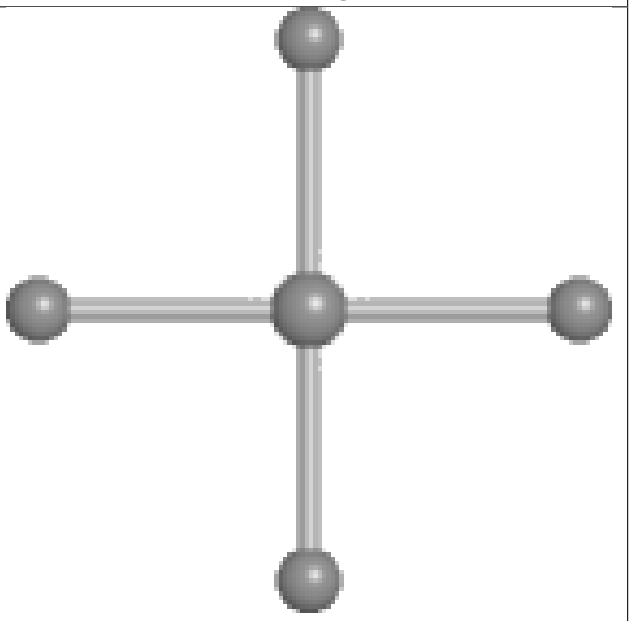
Bond lengths



Bond angles

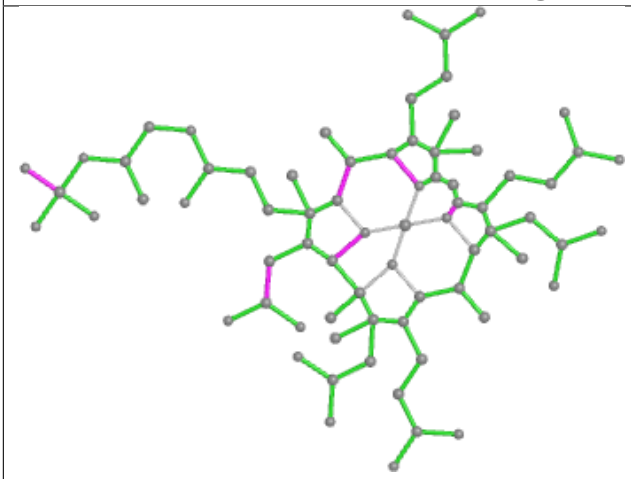


Torsions

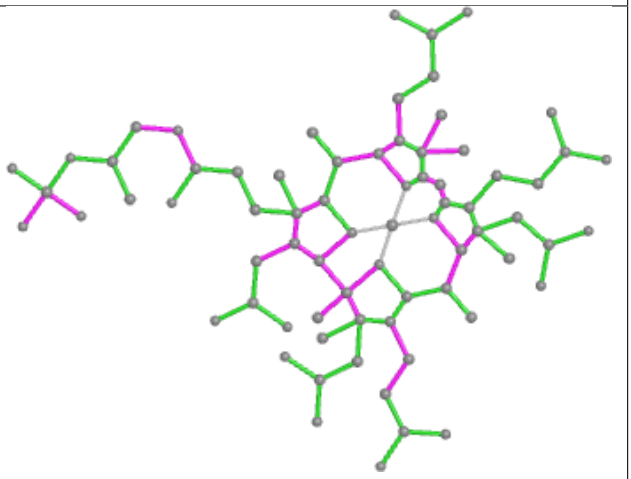


Rings

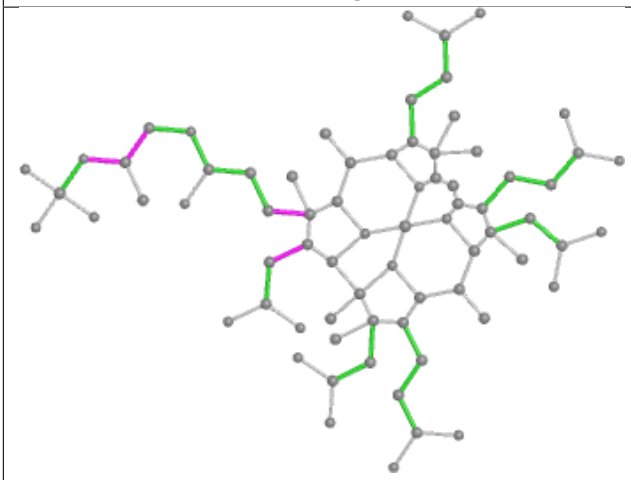
Ligand B12 E 201



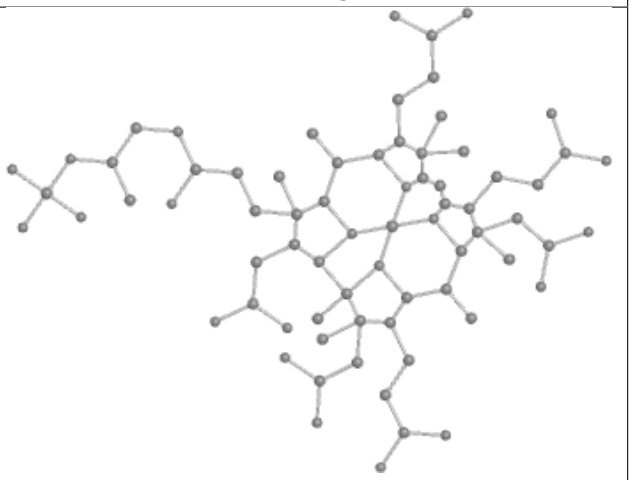
Bond lengths



Bond angles

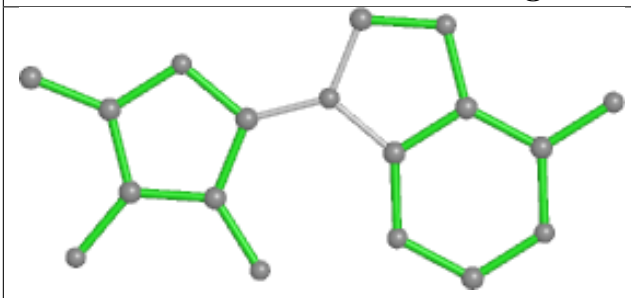


Torsions

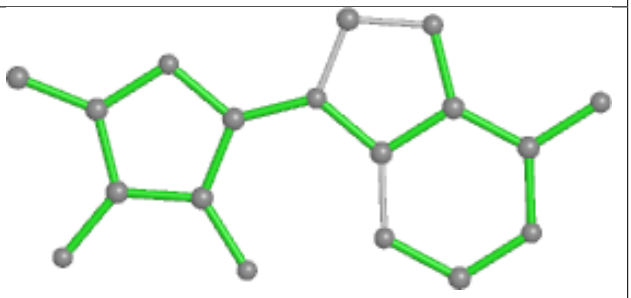


Rings

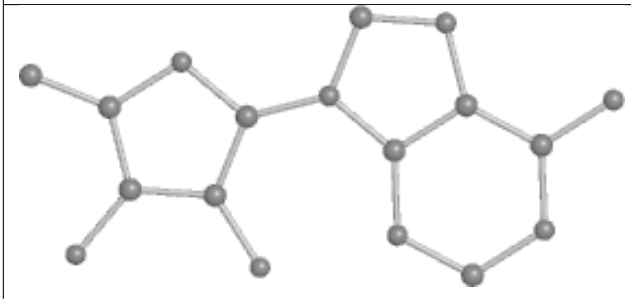
Ligand 5AD D 202



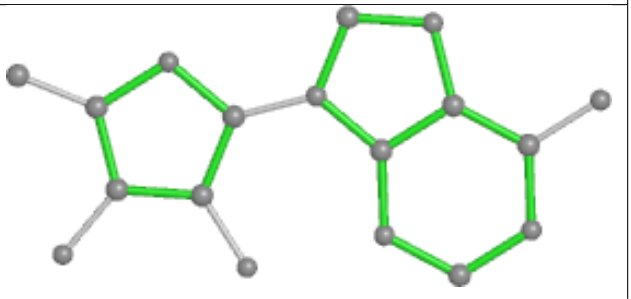
Bond lengths



Bond angles

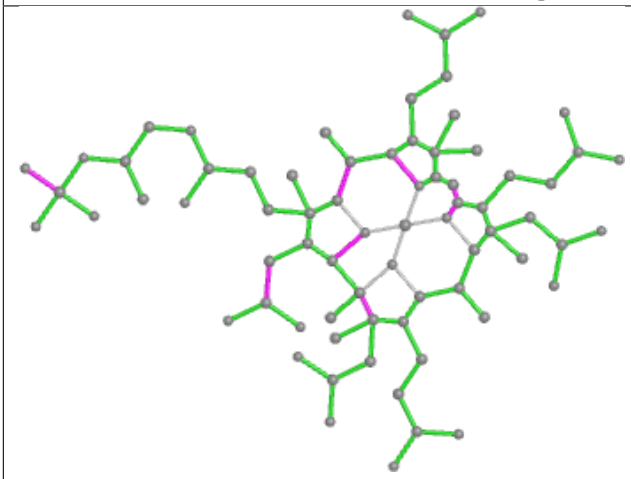


Torsions

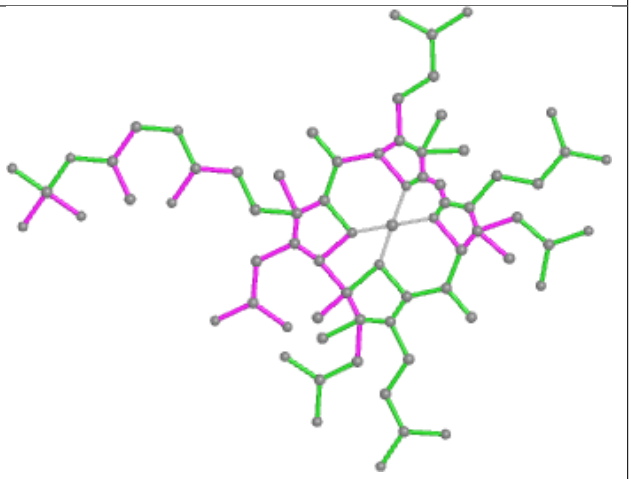


Rings

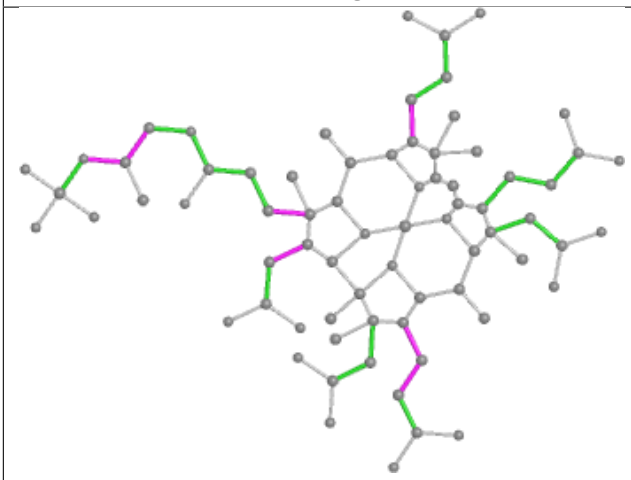
Ligand B12 F 201



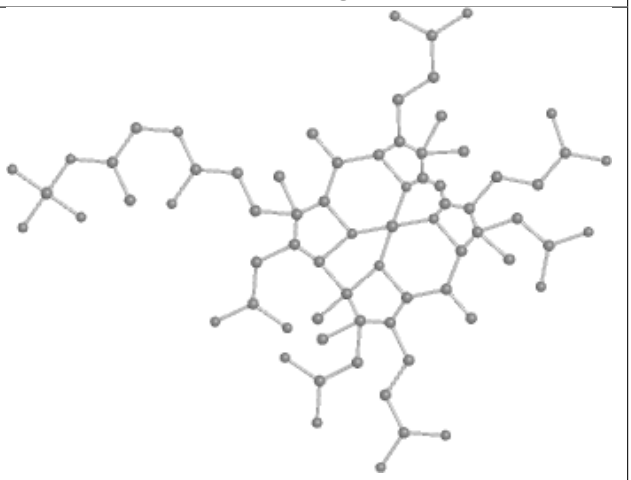
Bond lengths



Bond angles

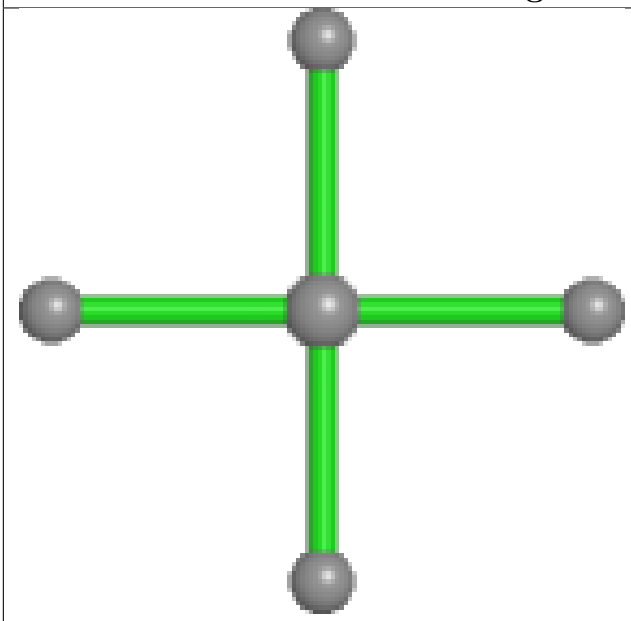


Torsions

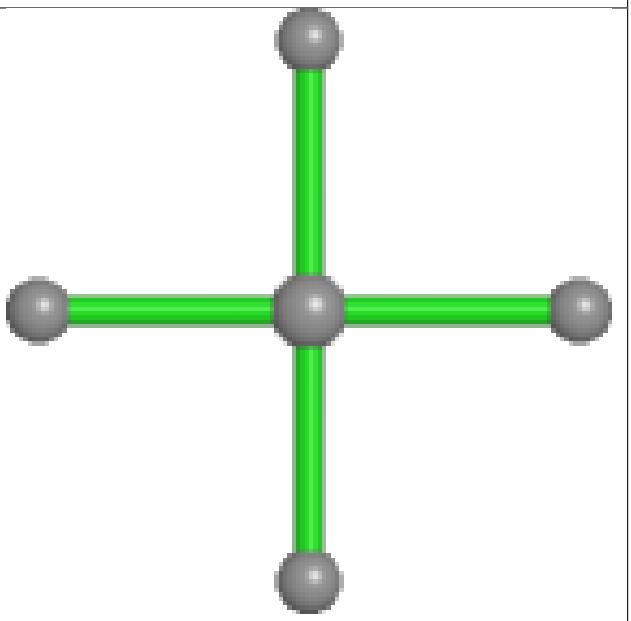


Rings

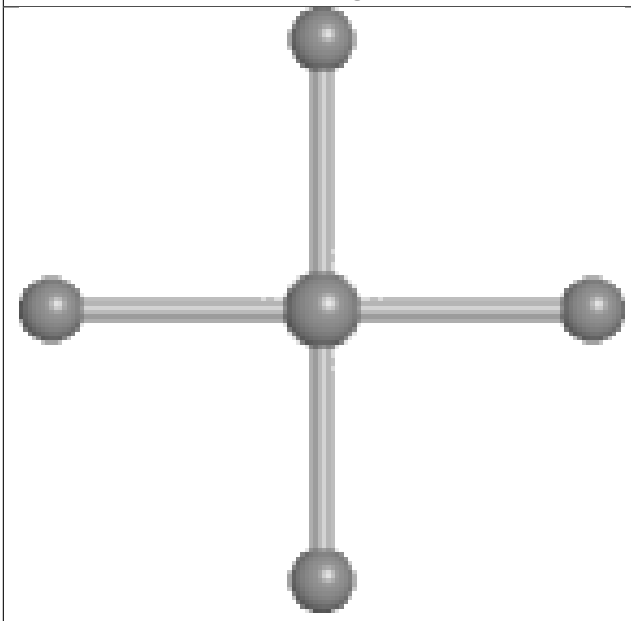
Ligand PO4 D 203



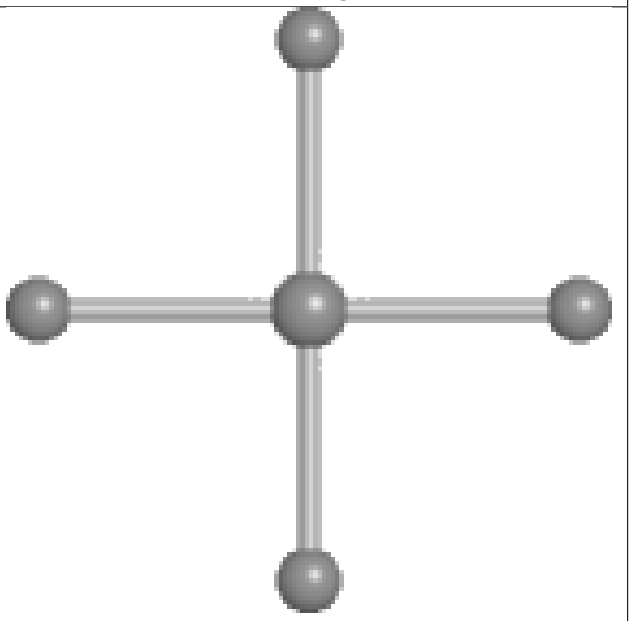
Bond lengths



Bond angles

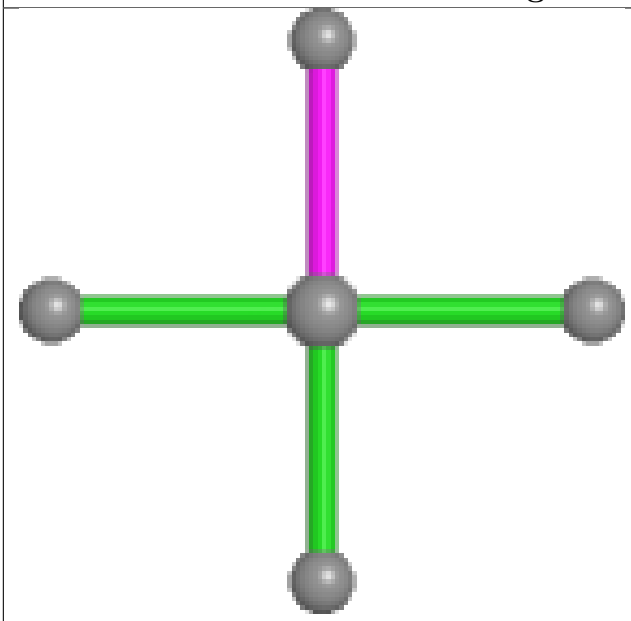


Torsions

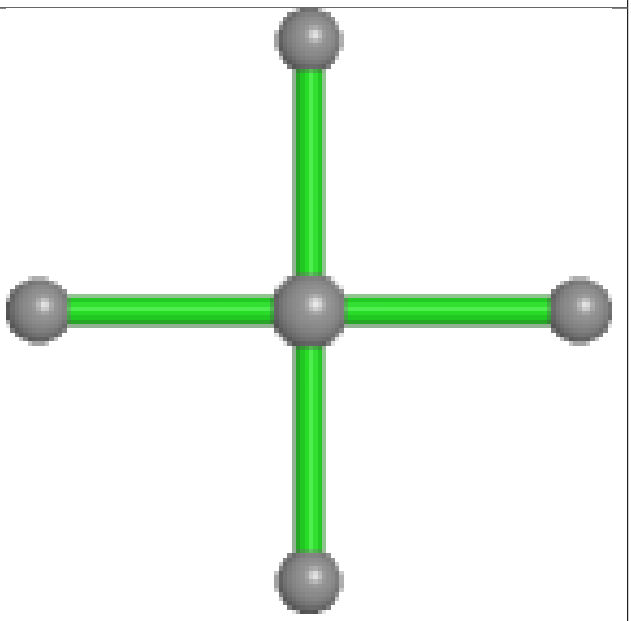


Rings

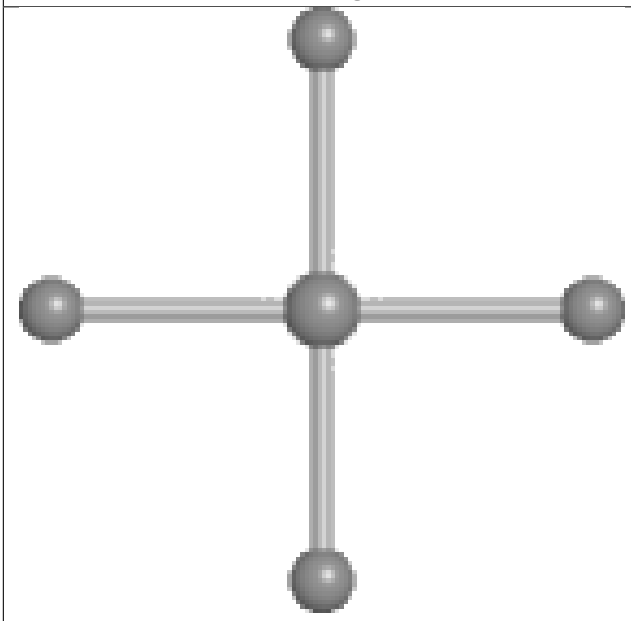
Ligand PO4 C 202



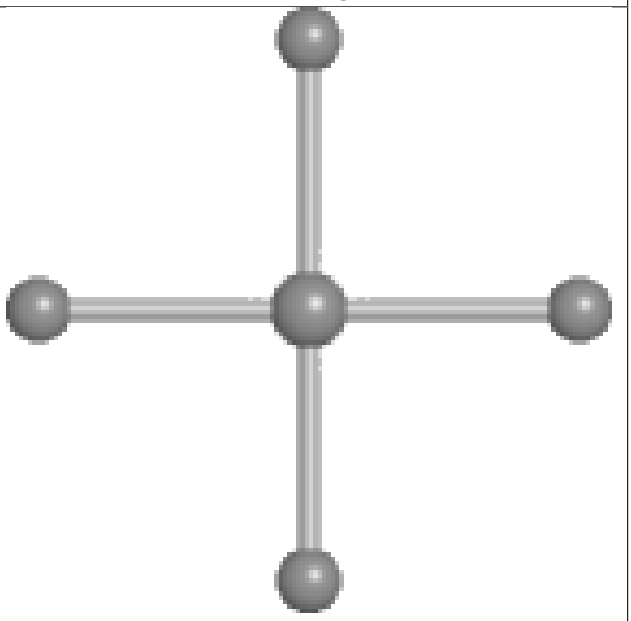
Bond lengths



Bond angles

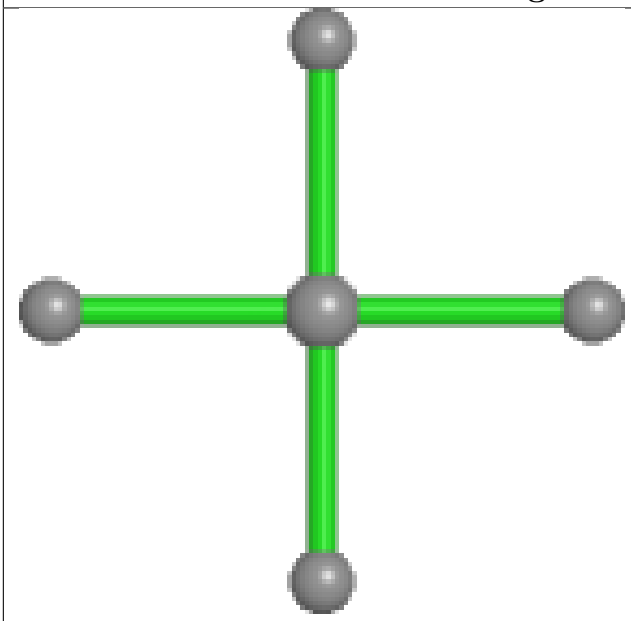


Torsions

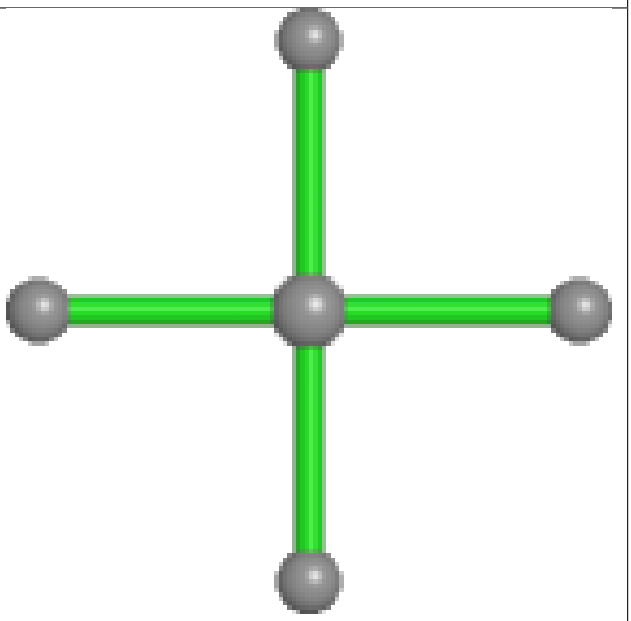


Rings

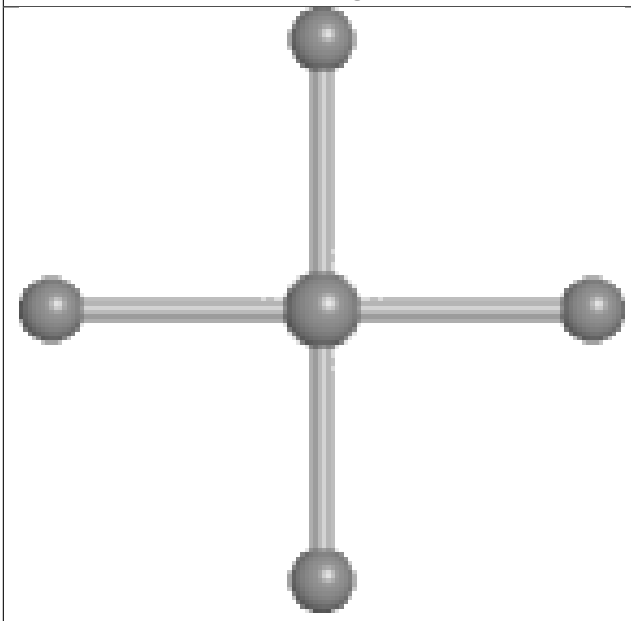
Ligand PO4 E 203



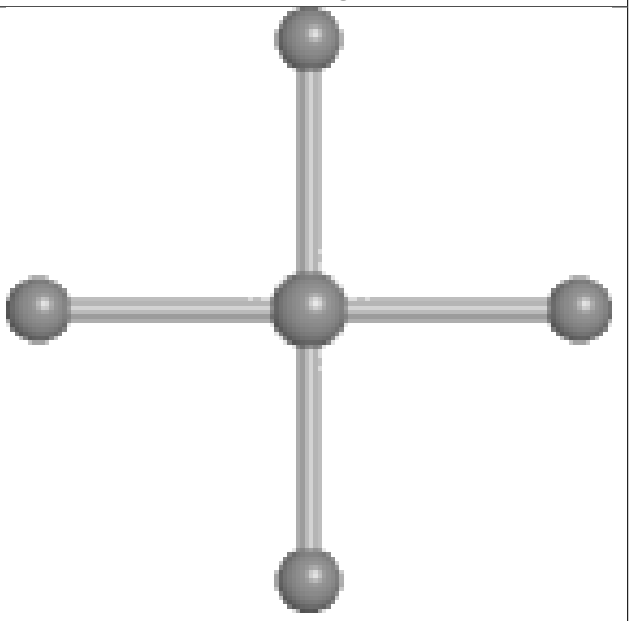
Bond lengths



Bond angles

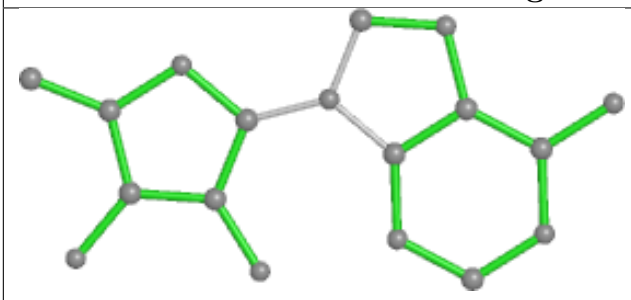


Torsions

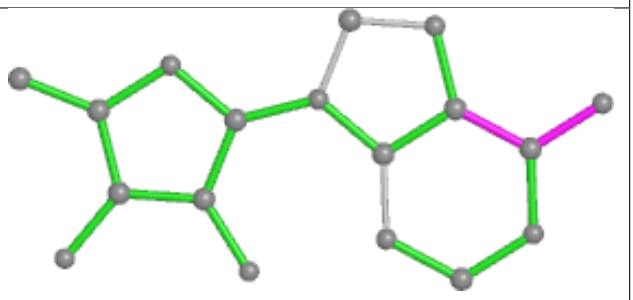


Rings

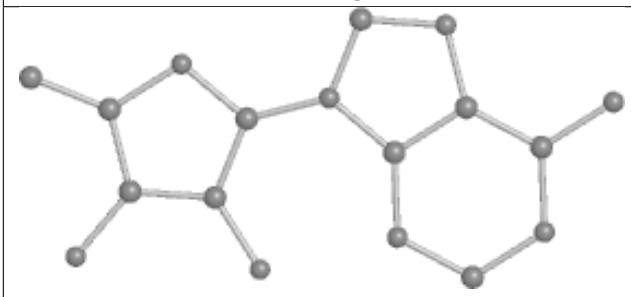
Ligand 5AD E 202



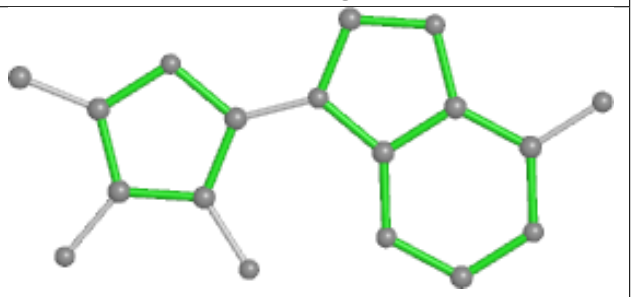
Bond lengths



Bond angles

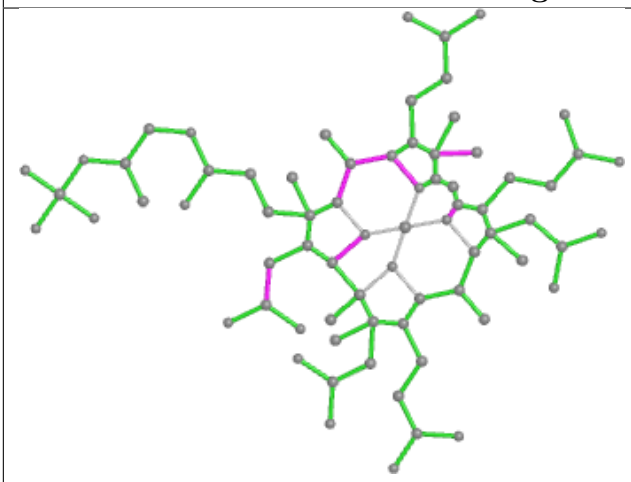


Torsions

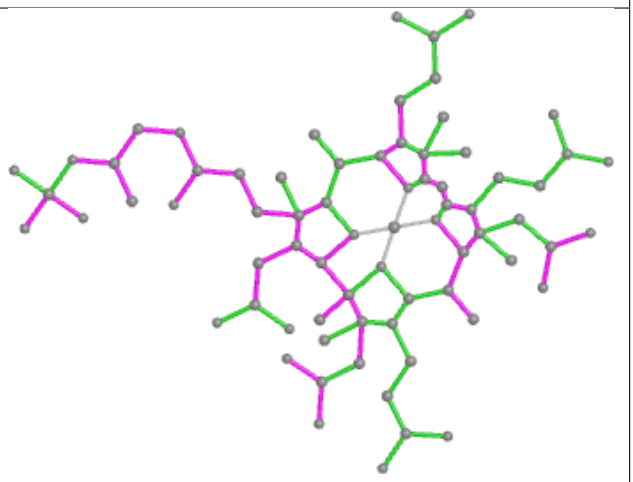


Rings

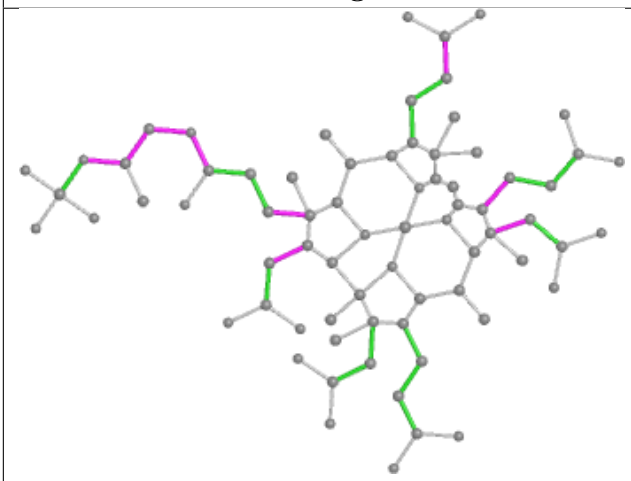
Ligand B12 B 203



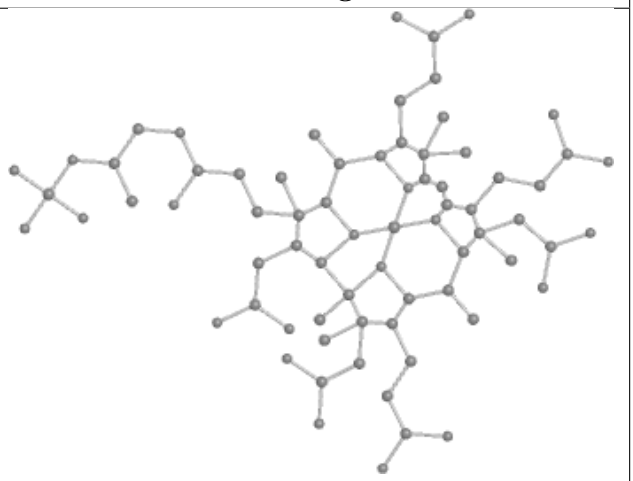
Bond lengths



Bond angles

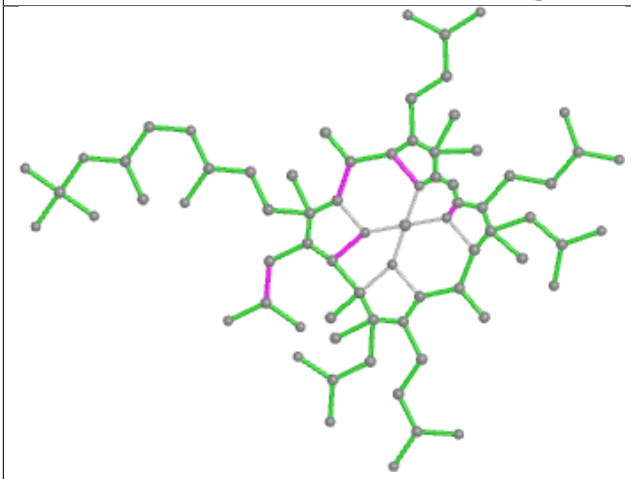


Torsions

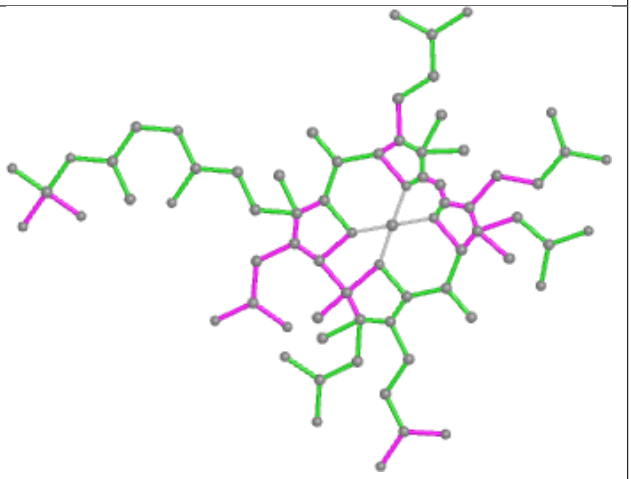


Rings

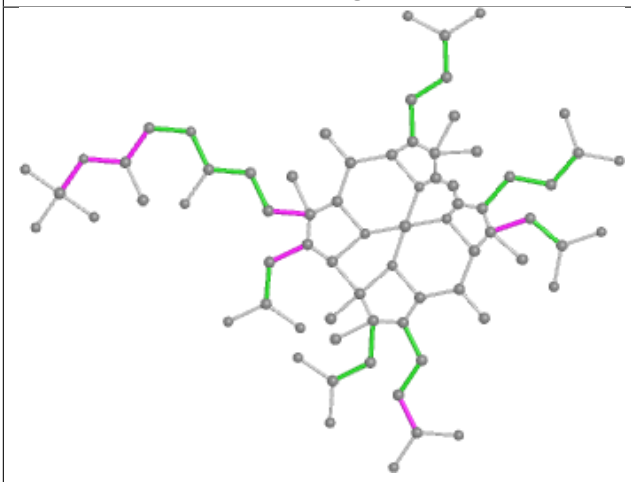
Ligand B12 D 201



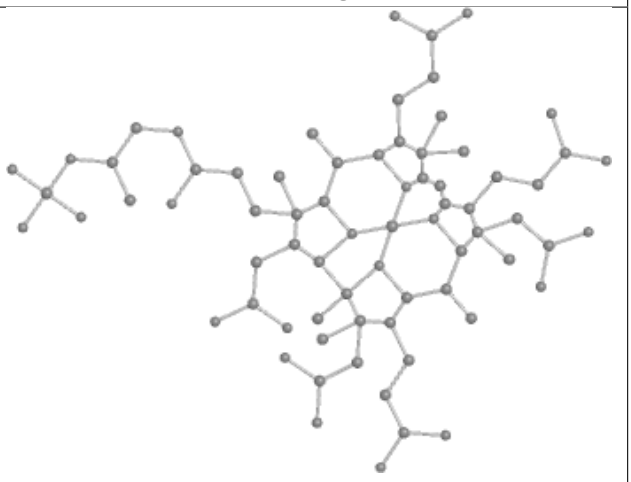
Bond lengths



Bond angles

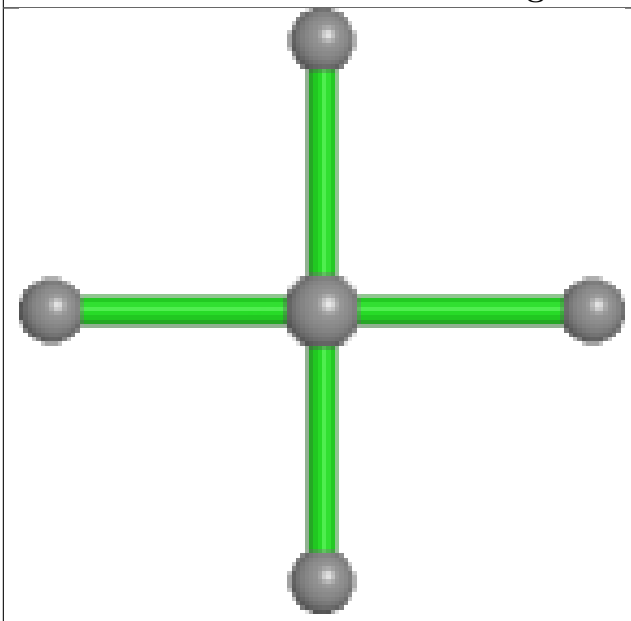


Torsions

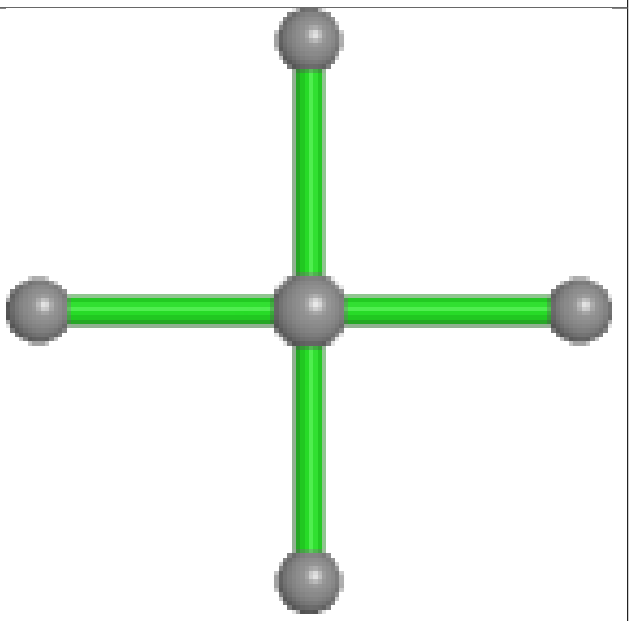


Rings

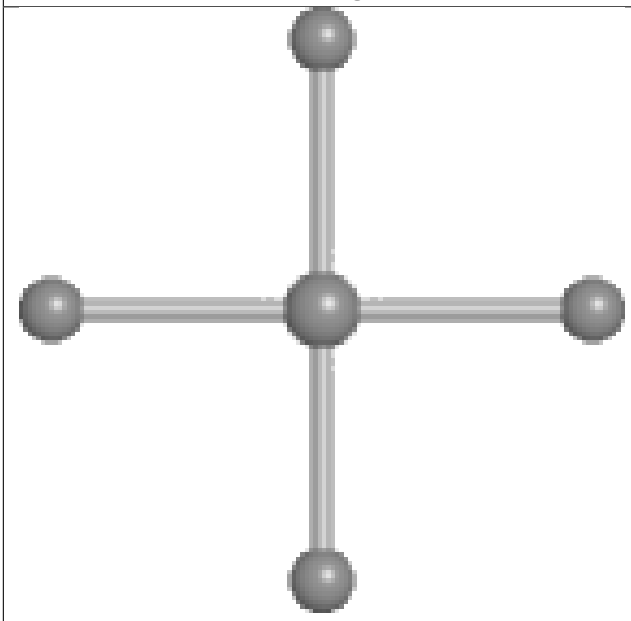
Ligand PO4 B 206



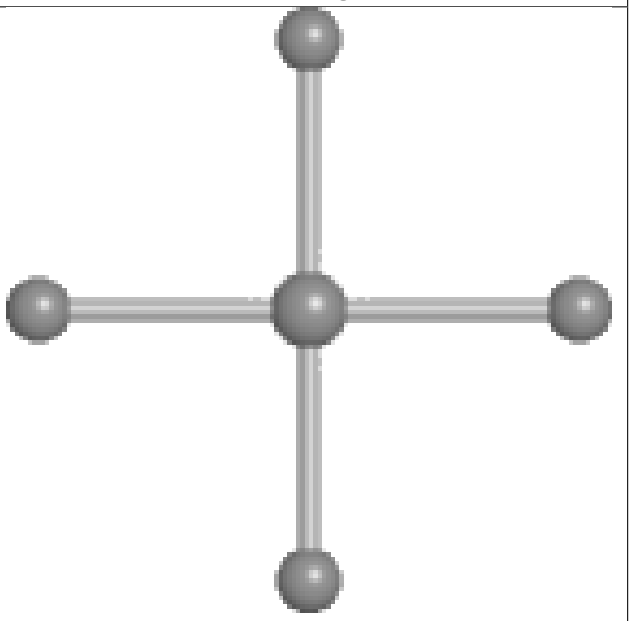
Bond lengths



Bond angles

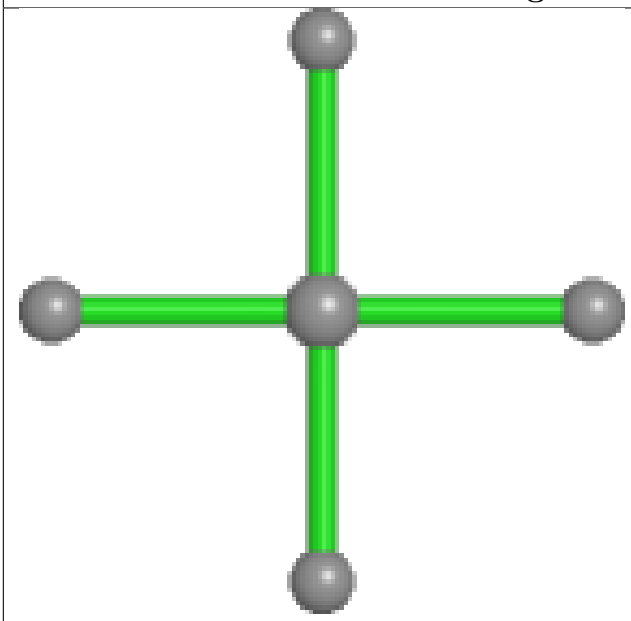


Torsions

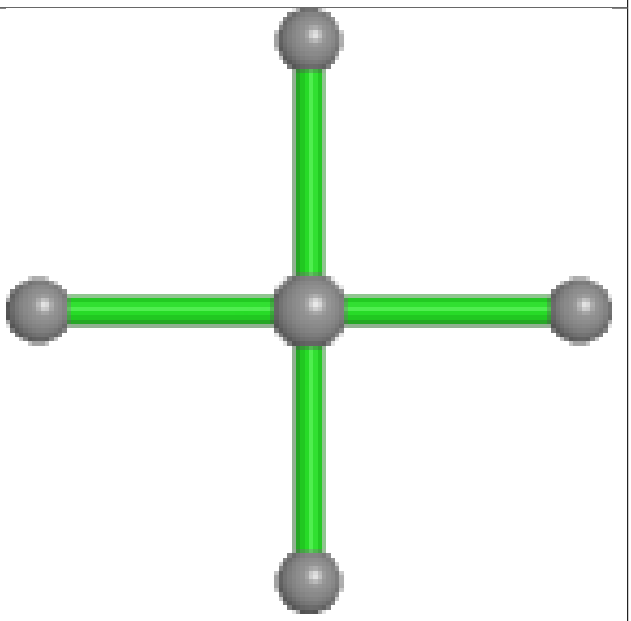


Rings

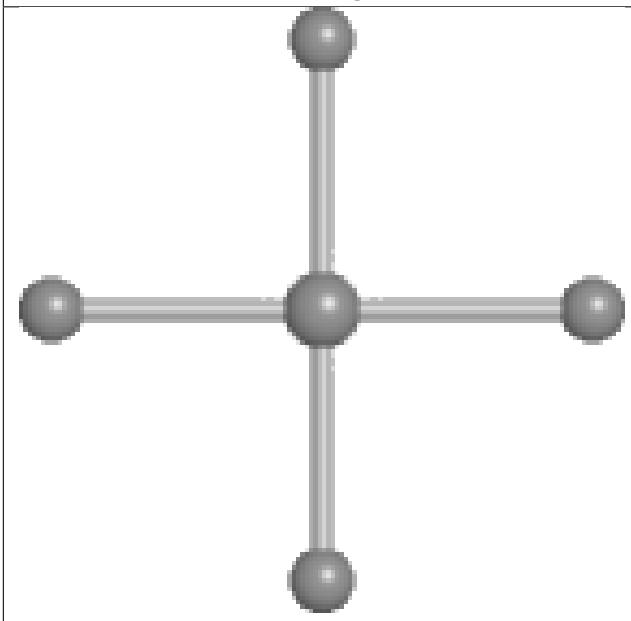
Ligand PO4 B 204



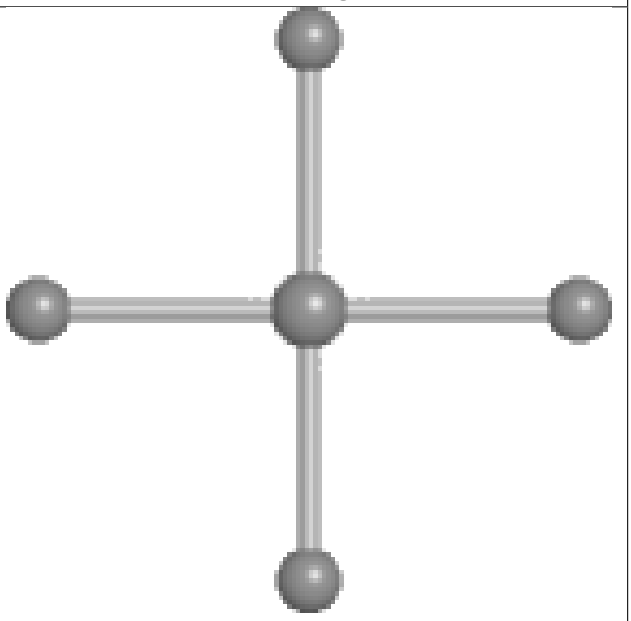
Bond lengths



Bond angles

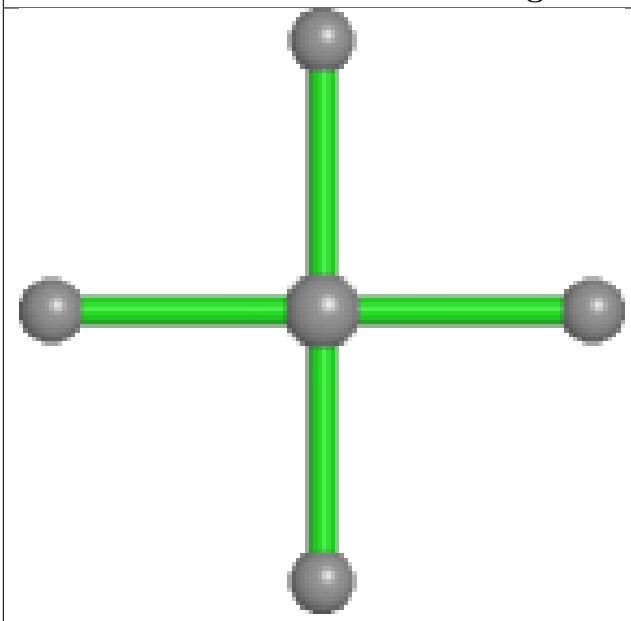


Torsions

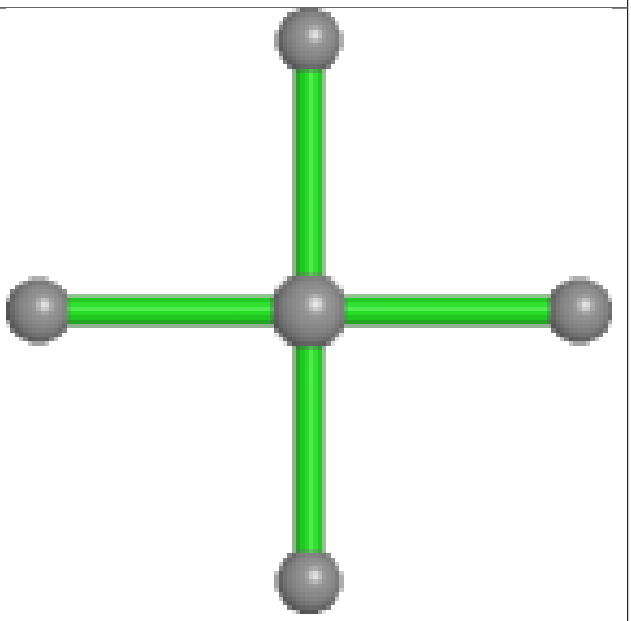


Rings

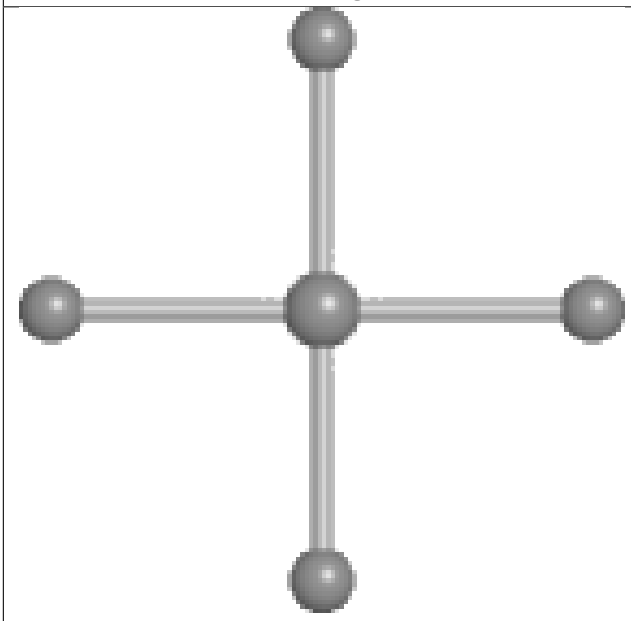
Ligand PO4 A 204



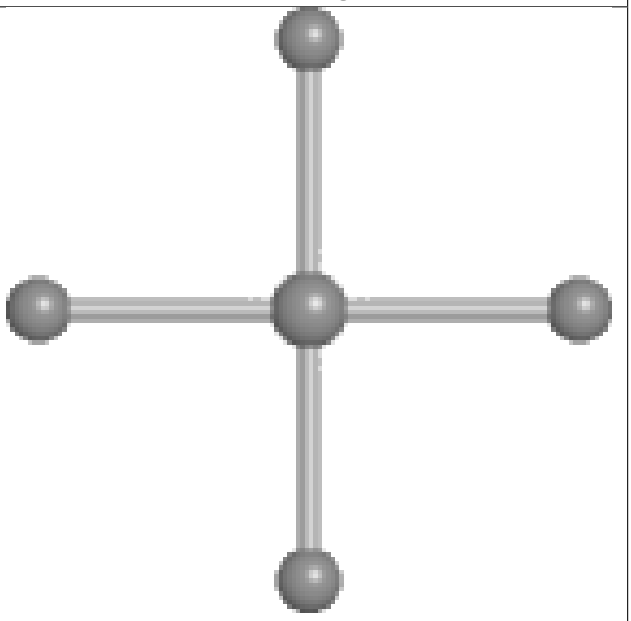
Bond lengths



Bond angles

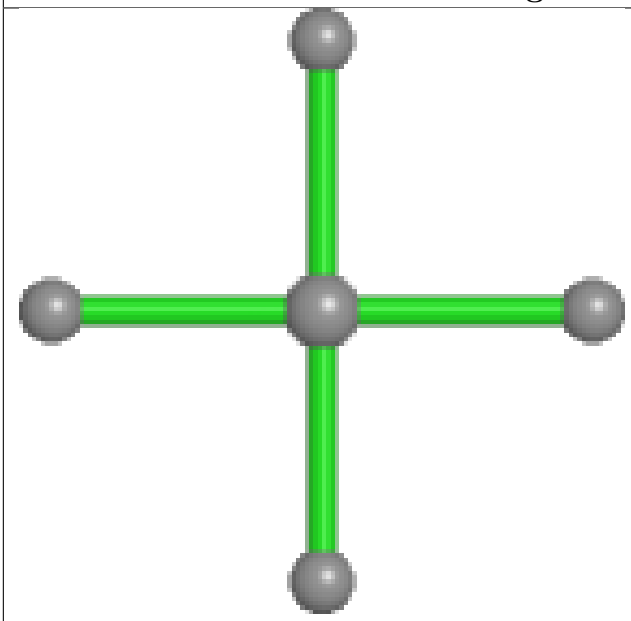


Torsions

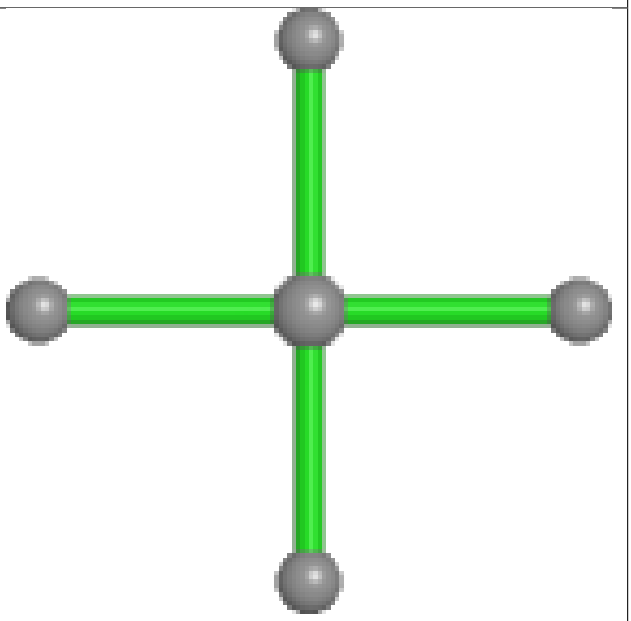


Rings

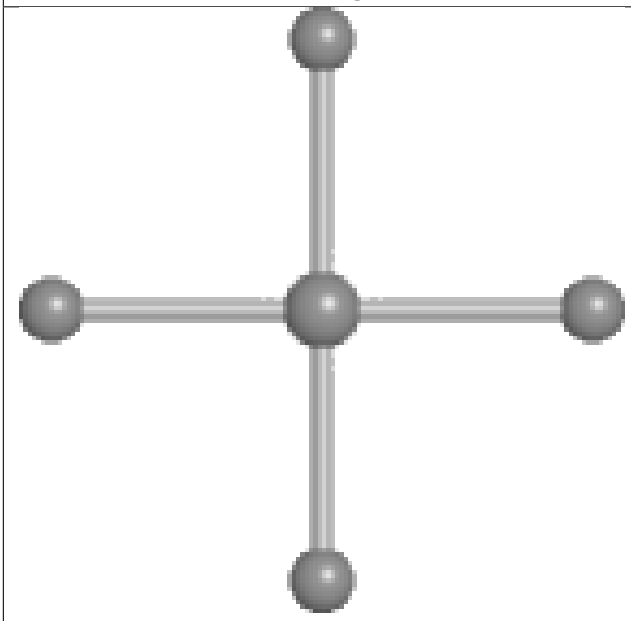
Ligand PO4 D 204



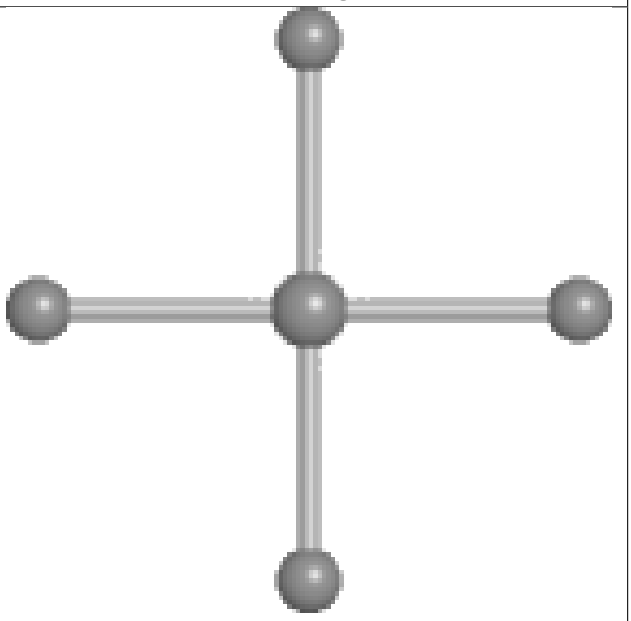
Bond lengths



Bond angles

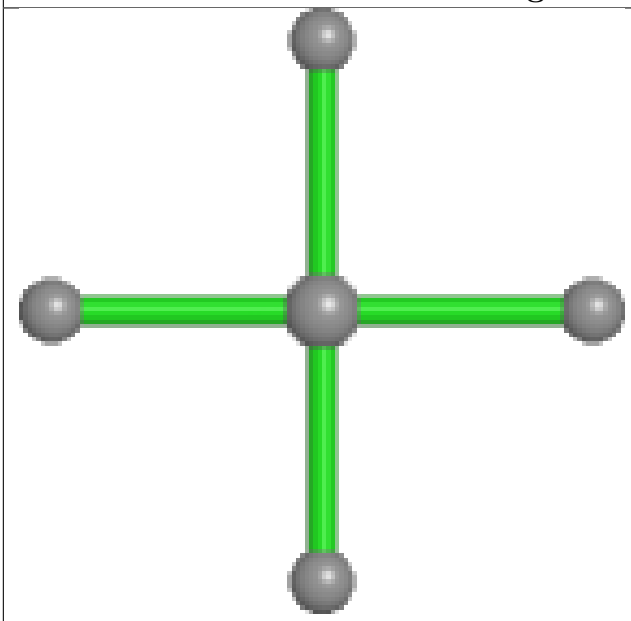


Torsions

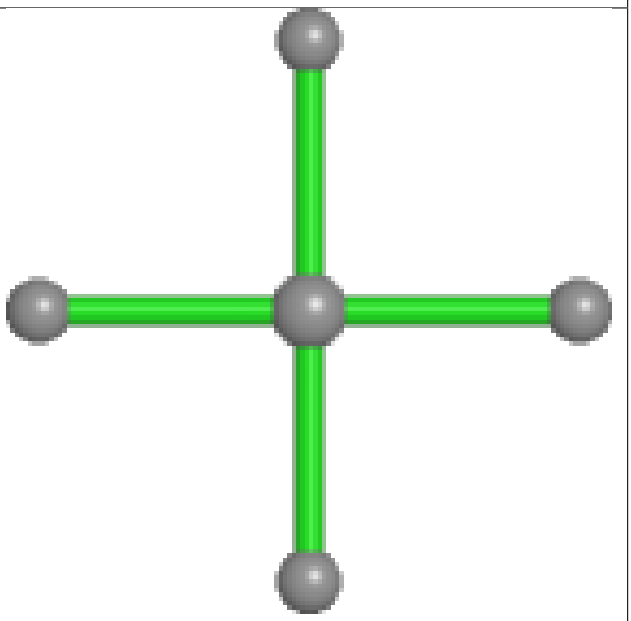


Rings

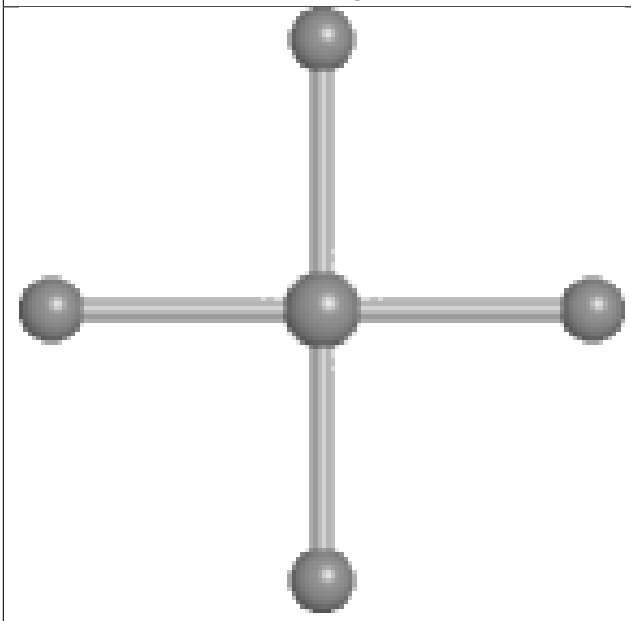
Ligand PO4 C 203



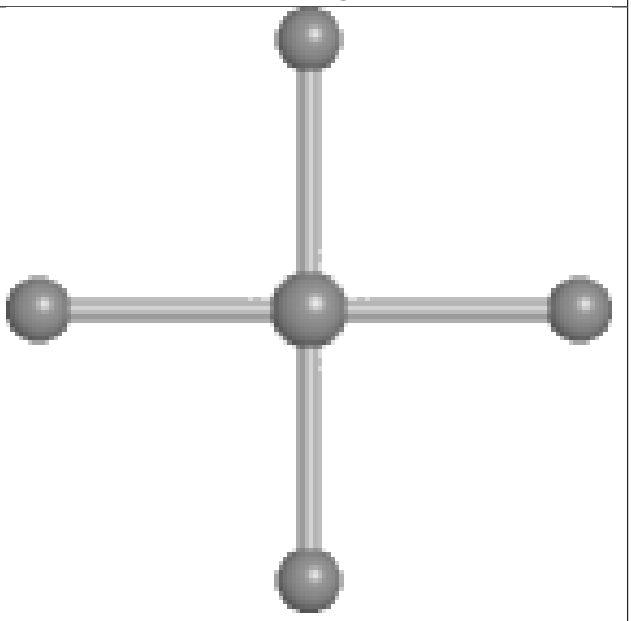
Bond lengths



Bond angles

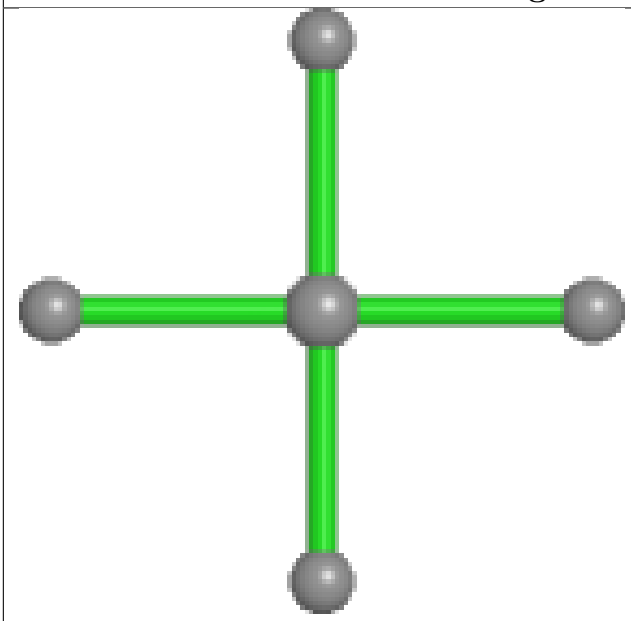


Torsions

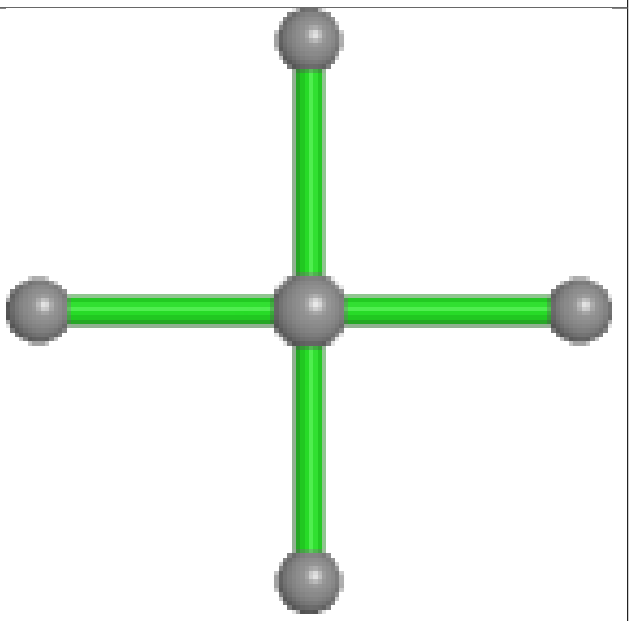


Rings

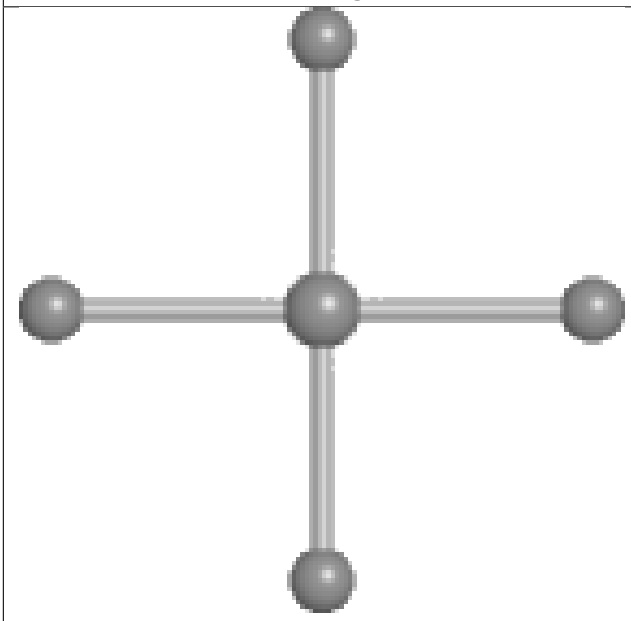
Ligand PO4 F 203



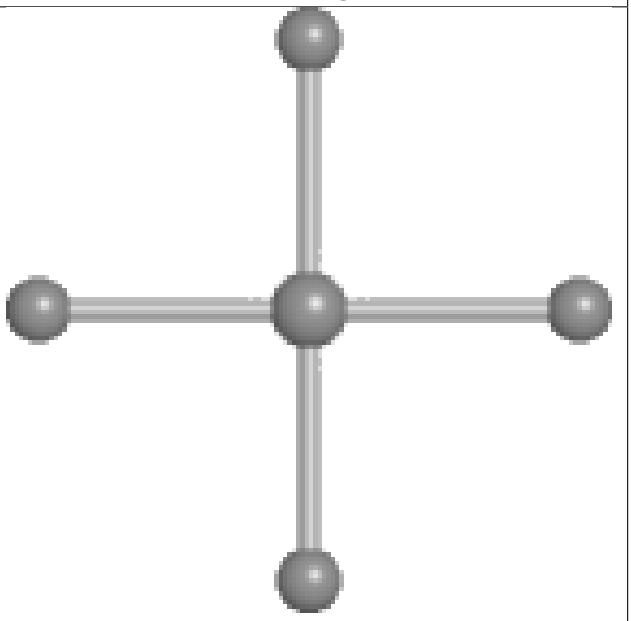
Bond lengths



Bond angles

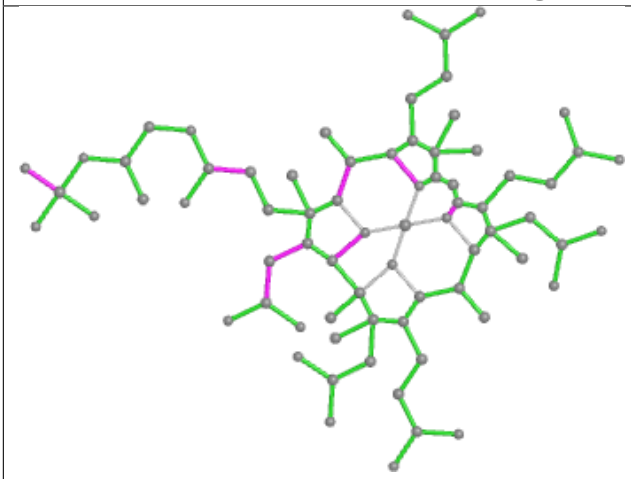


Torsions

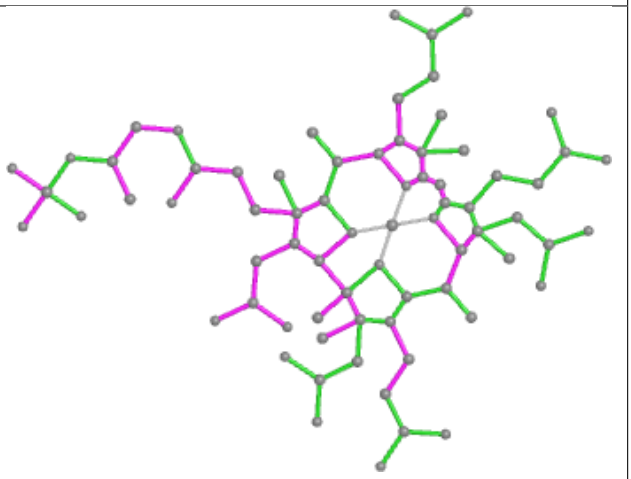


Rings

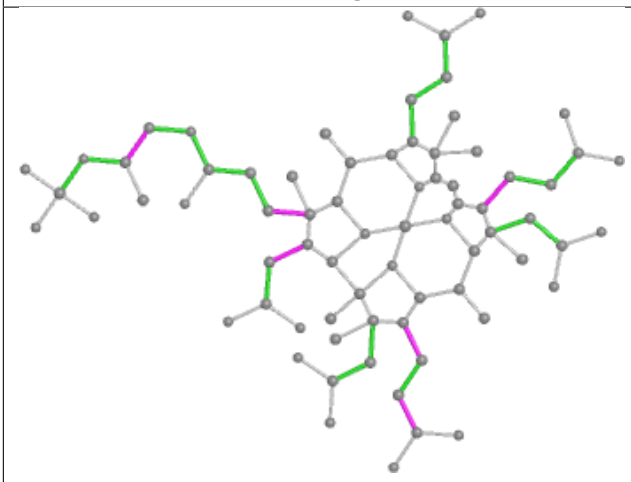
Ligand B12 B 201



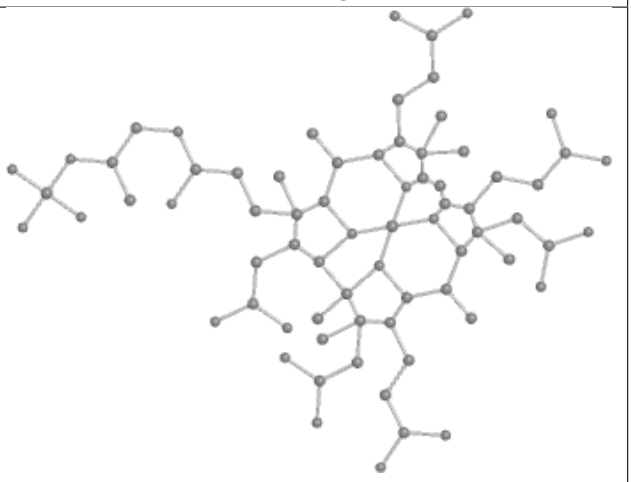
Bond lengths



Bond angles

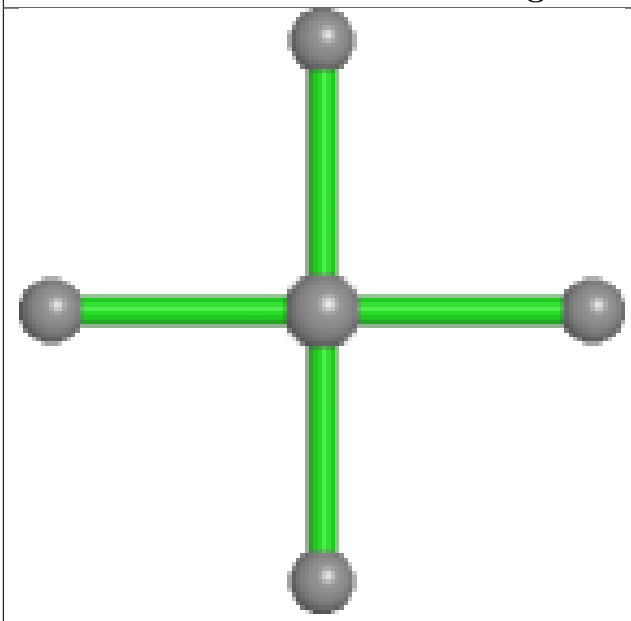


Torsions

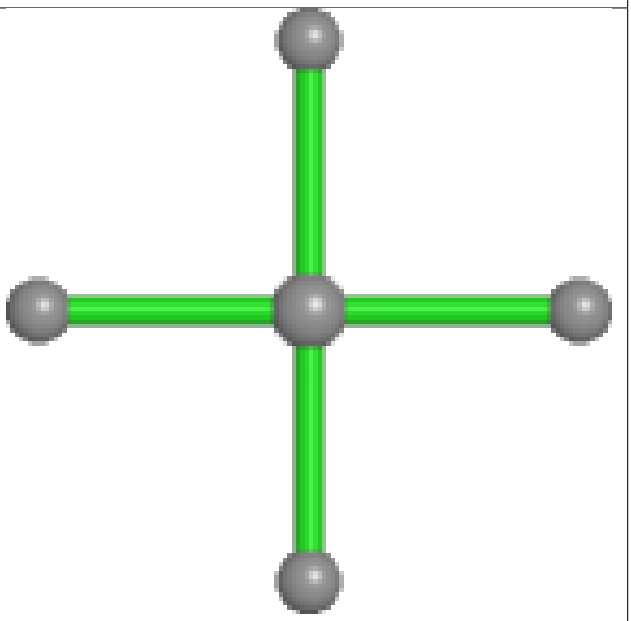


Rings

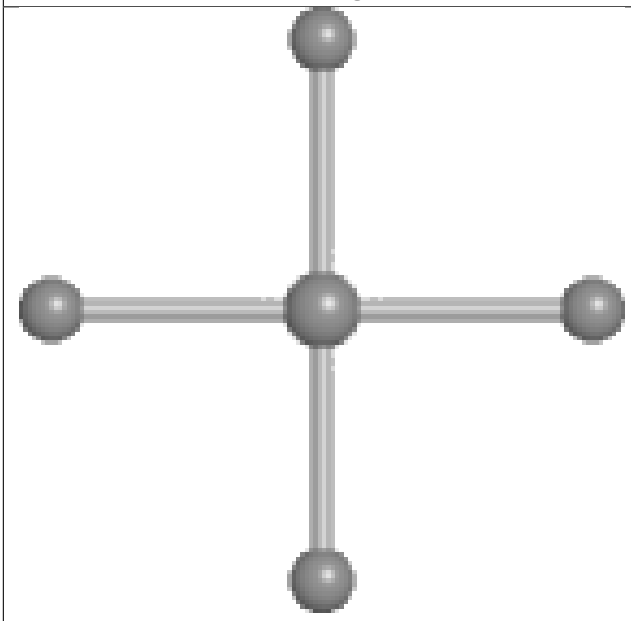
Ligand PO4 C 204



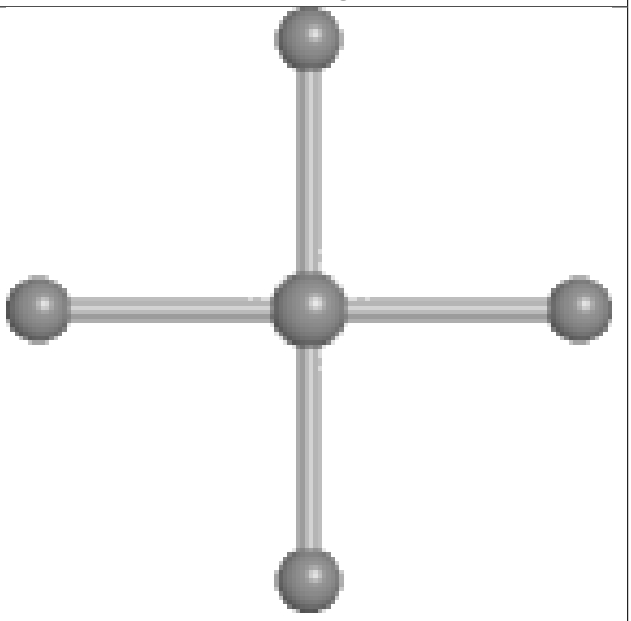
Bond lengths



Bond angles

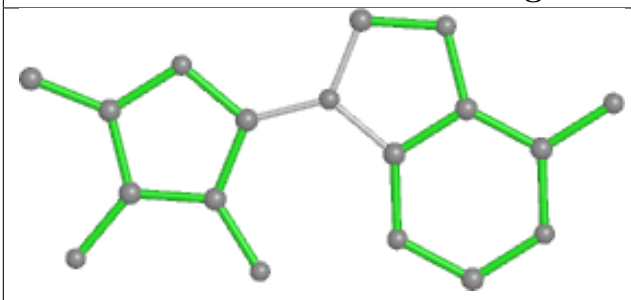


Torsions

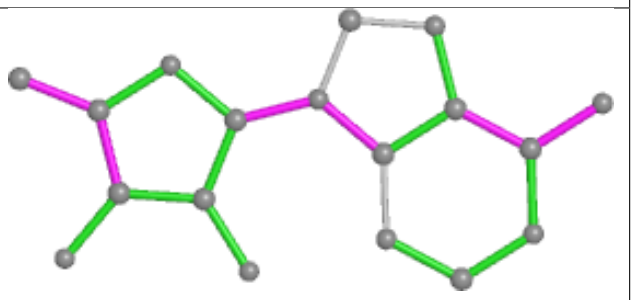


Rings

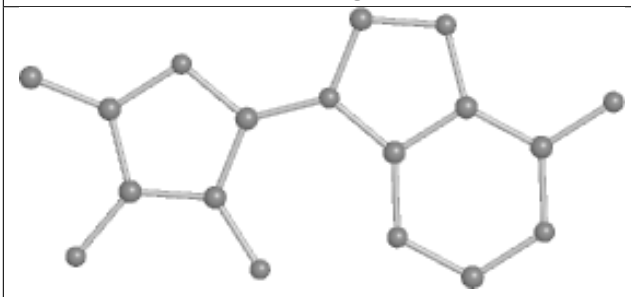
Ligand 5AD A 202



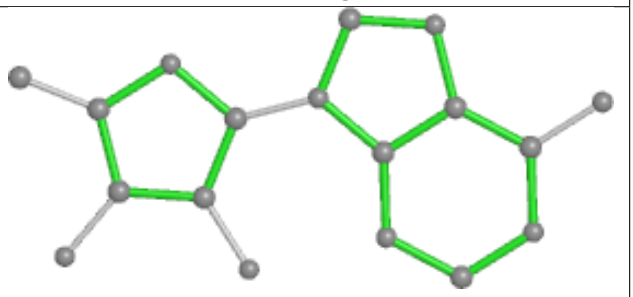
Bond lengths



Bond angles

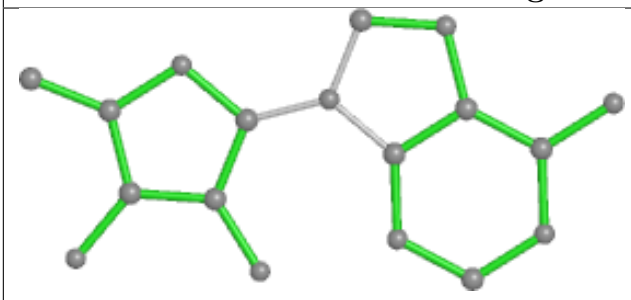


Torsions

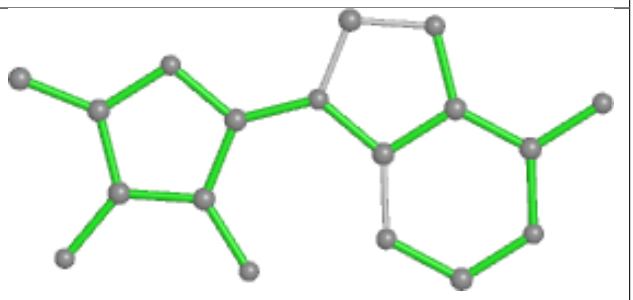


Rings

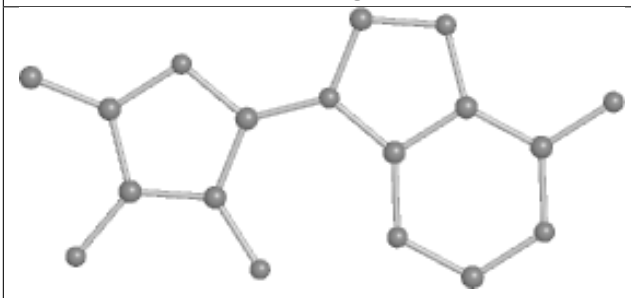
Ligand 5AD F 202



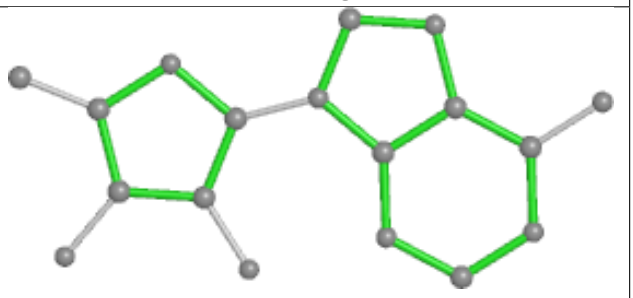
Bond lengths



Bond angles

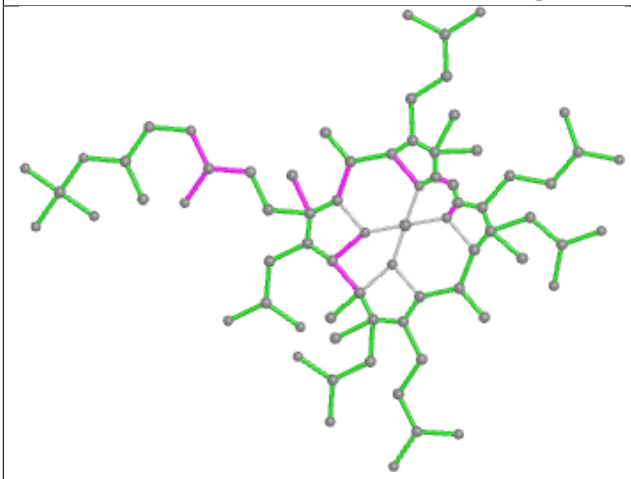


Torsions

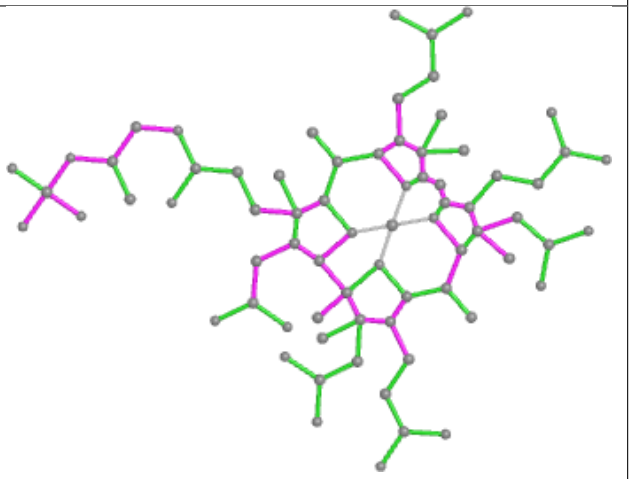


Rings

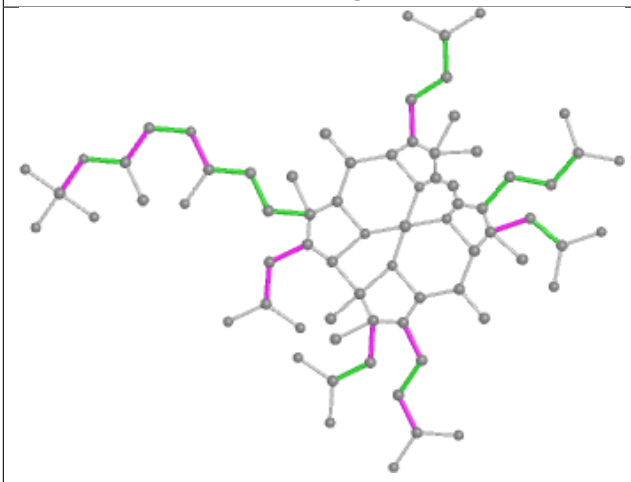
Ligand B12 A 201



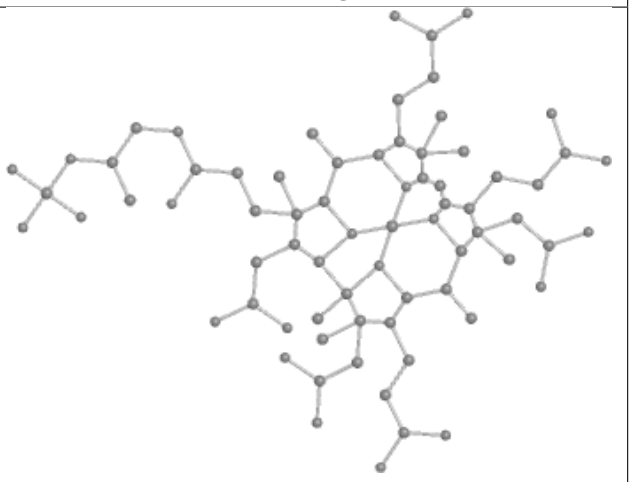
Bond lengths



Bond angles

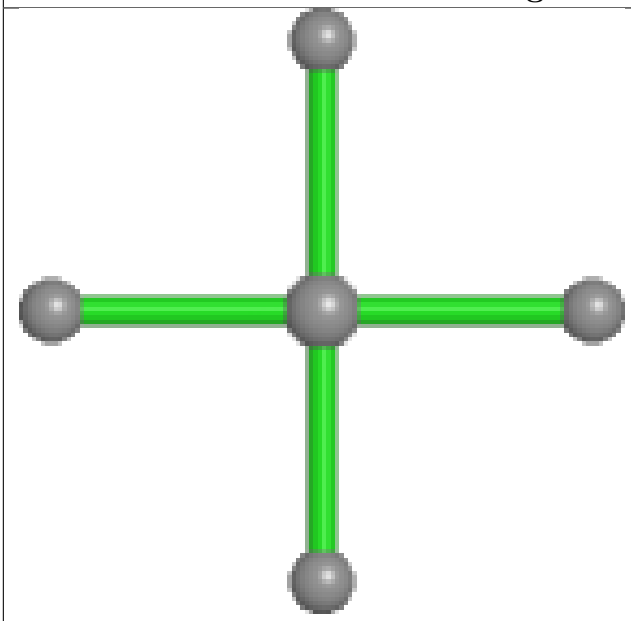


Torsions

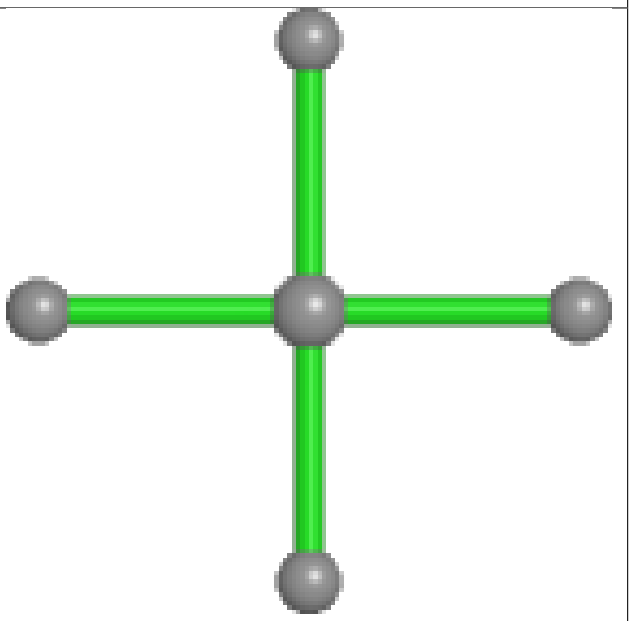


Rings

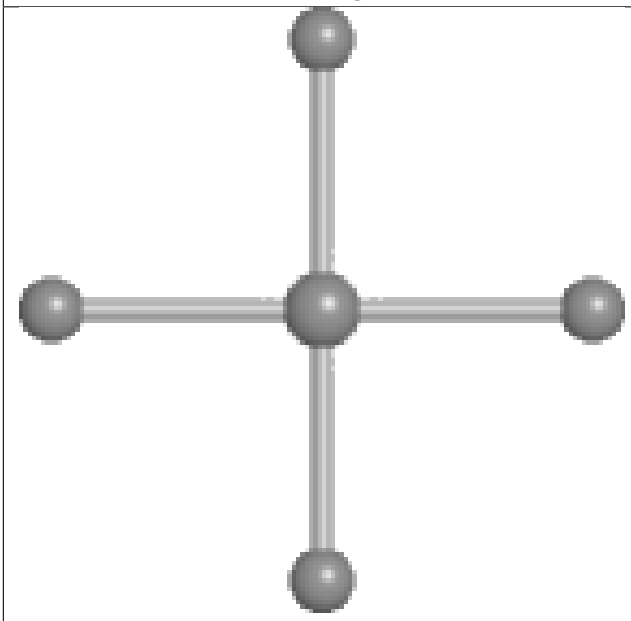
Ligand PO4 A 203



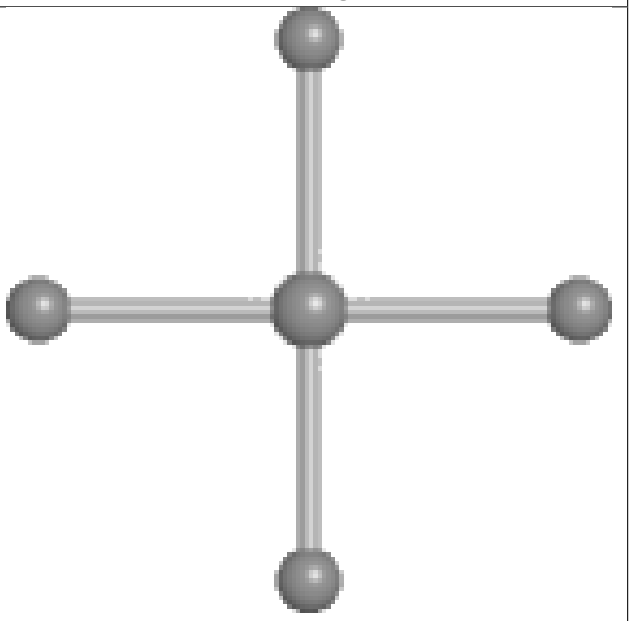
Bond lengths



Bond angles

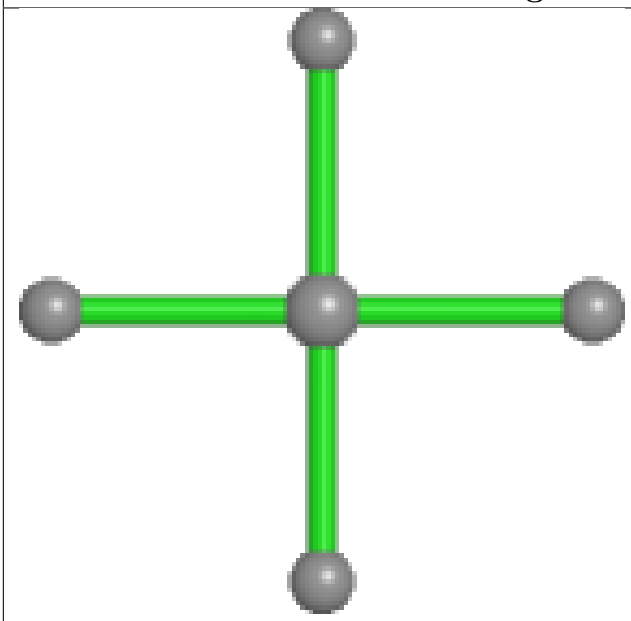


Torsions

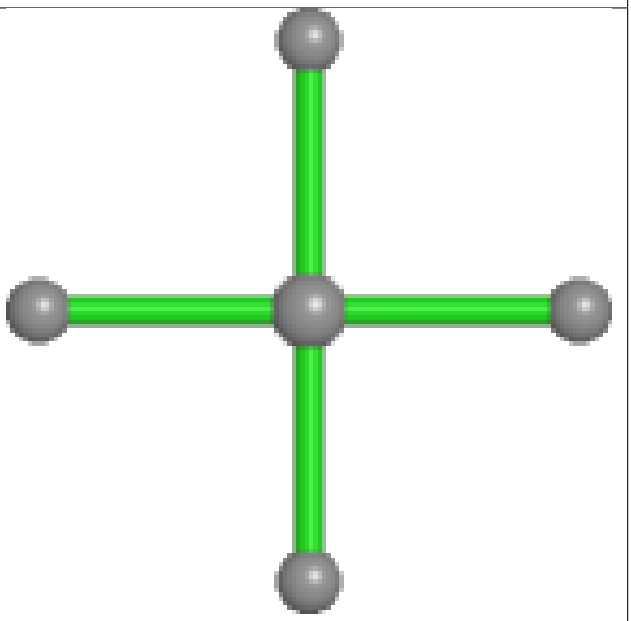


Rings

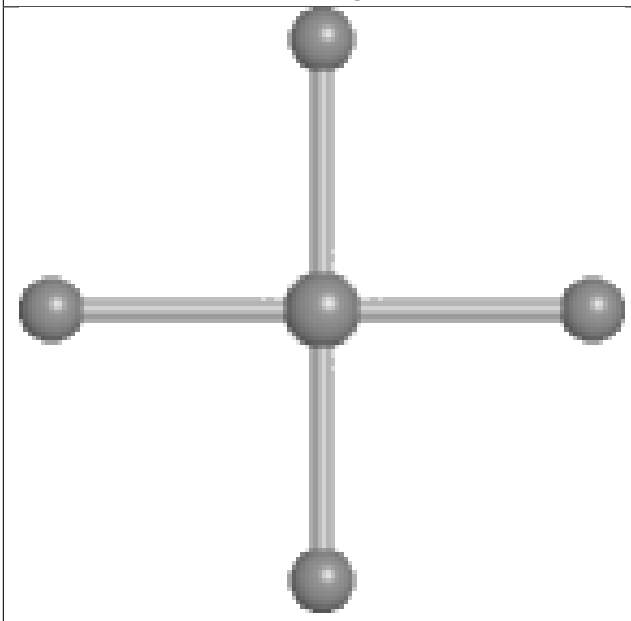
Ligand PO4 D 205



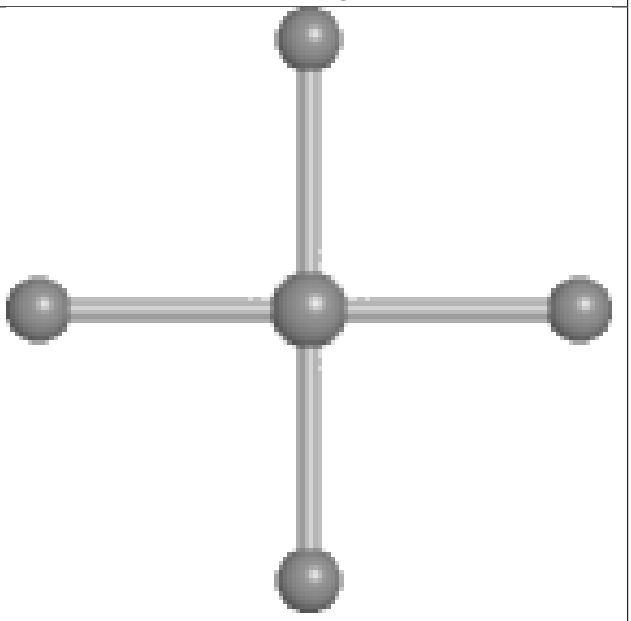
Bond lengths



Bond angles

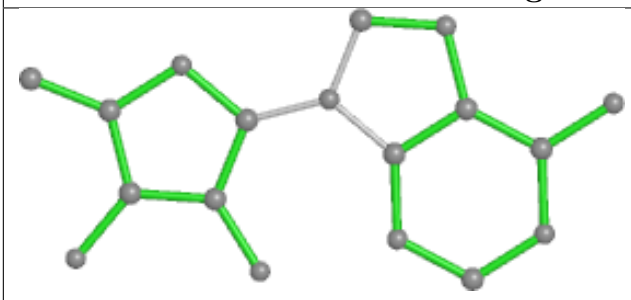


Torsions

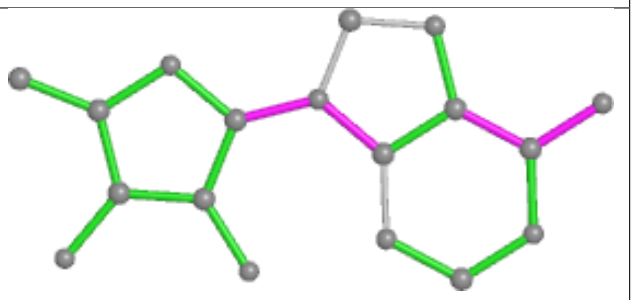


Rings

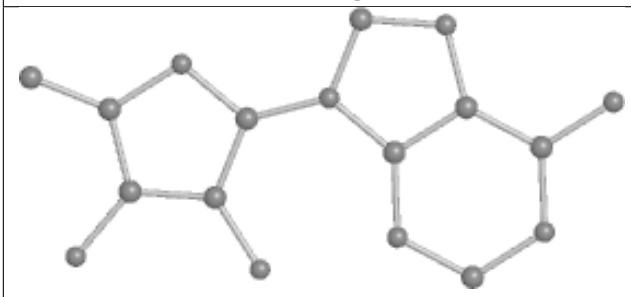
Ligand 5AD C 201



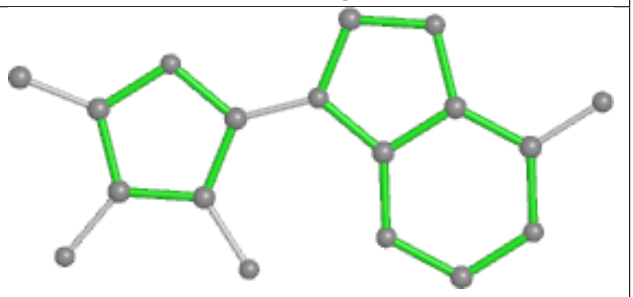
Bond lengths



Bond angles

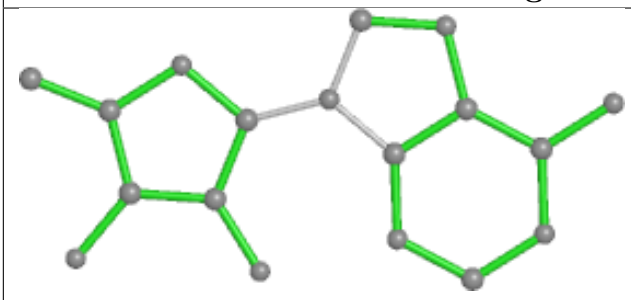


Torsions

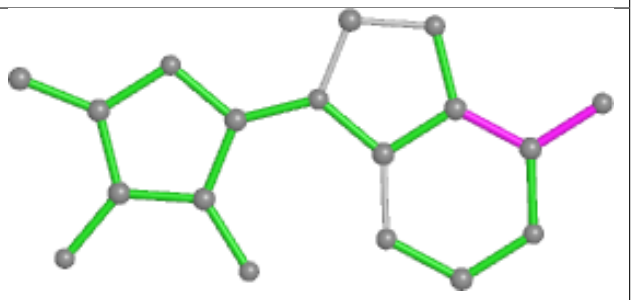


Rings

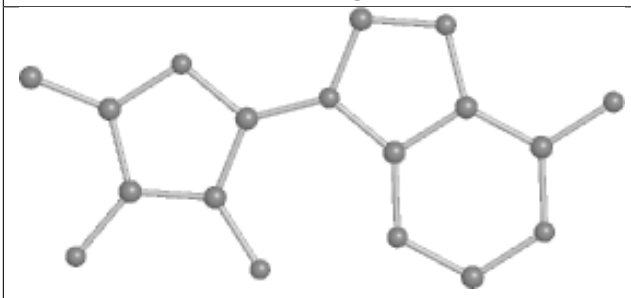
Ligand 5AD B 202



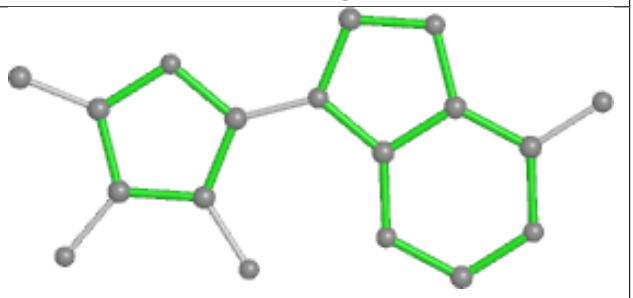
Bond lengths



Bond angles

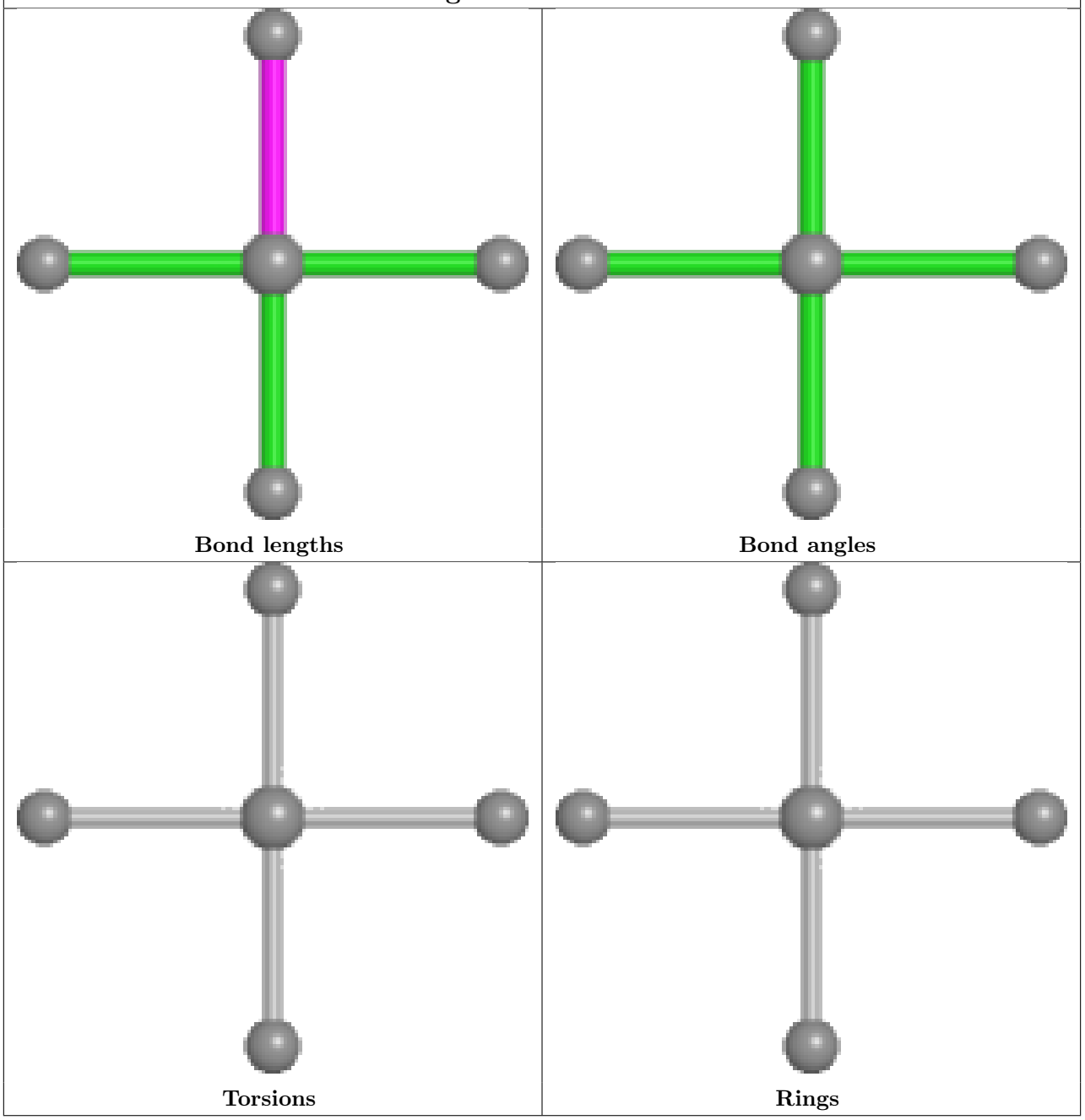


Torsions



Rings

Ligand PO4 B 205



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	178/178 (100%)	-0.41	0 100 100	37, 55, 98, 122	0
1	D	178/178 (100%)	-0.23	2 (1%) 77 74	47, 65, 112, 142	0
1	E	178/178 (100%)	-0.16	1 (0%) 85 83	45, 76, 118, 148	0
1	F	178/178 (100%)	-0.04	0 100 100	48, 77, 114, 142	0
2	B	179/179 (100%)	-0.28	0 100 100	39, 66, 105, 115	0
2	C	179/179 (100%)	-0.41	2 (1%) 77 74	39, 57, 111, 142	0
All	All	1070/1070 (100%)	-0.26	5 (0%) 87 84	37, 66, 111, 148	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	42	ALA	3.1
1	D	53	ILE	2.4
2	C	52	ARG	2.4
1	E	45	LEU	2.4
1	D	56	HIS	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

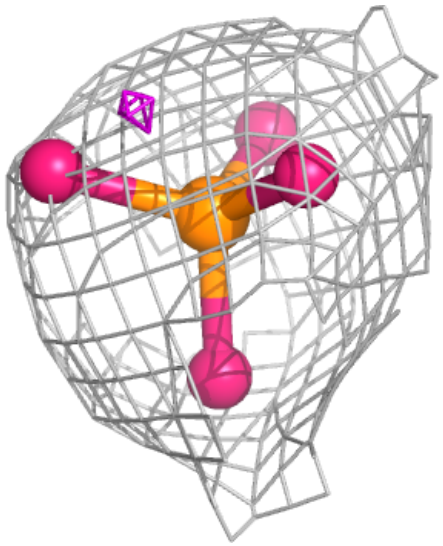
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

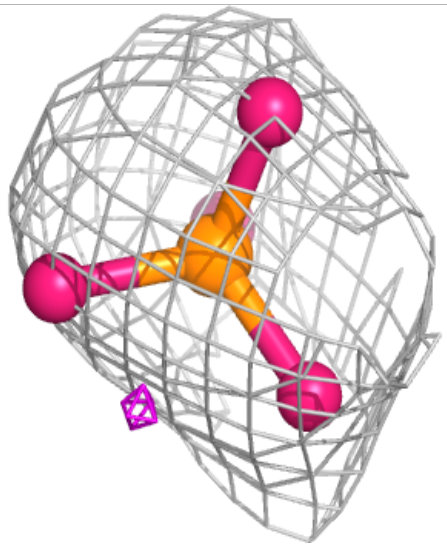
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	C	204	5/5	0.71	0.08	116,123,132,133	0
5	PO4	D	205	5/5	0.76	0.08	107,112,120,121	0
5	PO4	D	204	5/5	0.84	0.15	79,84,98,100	0
5	PO4	C	203	5/5	0.88	0.13	74,75,77,82	0
4	5AD	C	201	18/18	0.90	0.09	49,55,59,61	0
4	5AD	F	202	18/18	0.90	0.08	62,70,75,86	0
5	PO4	A	204	5/5	0.92	0.15	60,69,78,83	0
5	PO4	B	206	5/5	0.92	0.12	64,73,77,81	0
4	5AD	E	202	18/18	0.93	0.08	65,76,84,100	0
3	B12	A	201	72/91	0.94	0.11	40,54,85,112	0
4	5AD	A	202	18/18	0.94	0.07	43,51,63,68	0
4	5AD	B	202	18/18	0.94	0.07	48,54,59,61	0
3	B12	E	201	72/91	0.95	0.09	49,62,111,129	0
3	B12	B	201	72/91	0.95	0.09	40,51,77,106	0
5	PO4	E	203	5/5	0.95	0.06	64,65,75,78	0
3	B12	D	201	72/91	0.96	0.09	46,54,82,102	0
3	B12	B	203	72/91	0.96	0.08	40,52,85,106	0
3	B12	F	201	72/91	0.96	0.09	52,63,90,100	0
4	5AD	D	202	18/18	0.96	0.06	41,50,64,65	0
5	PO4	C	202	5/5	0.96	0.06	56,58,59,69	0
5	PO4	E	204	5/5	0.96	0.08	51,53,60,69	0
5	PO4	F	203	5/5	0.96	0.07	58,65,70,89	0
5	PO4	A	203	5/5	0.97	0.05	50,51,54,64	0
5	PO4	B	204	5/5	0.97	0.06	45,49,50,53	0
5	PO4	B	205	5/5	0.97	0.06	54,54,62,65	0
5	PO4	D	203	5/5	0.98	0.05	54,57,69,69	0

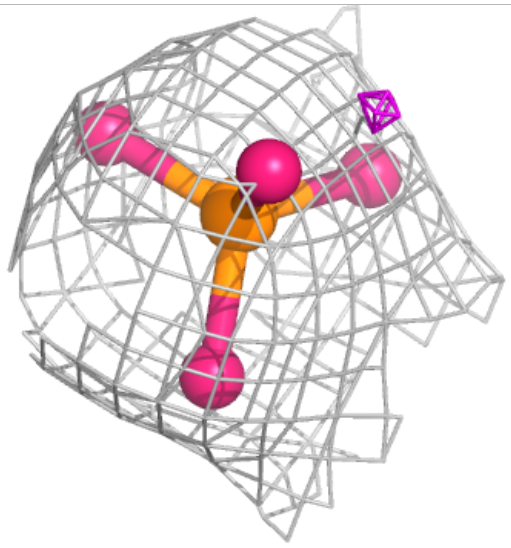
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PO4 C 204:

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

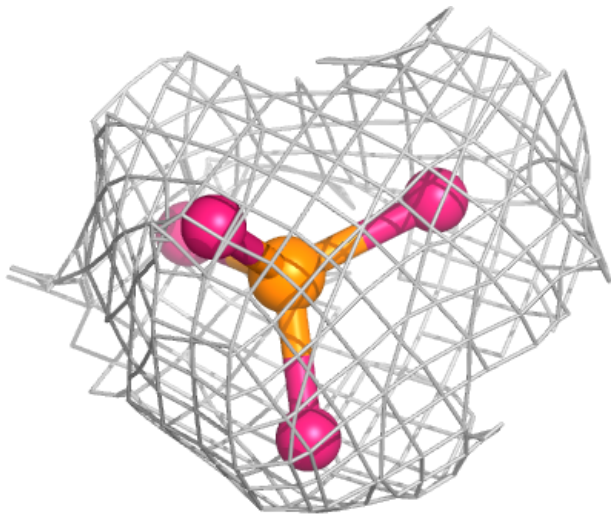


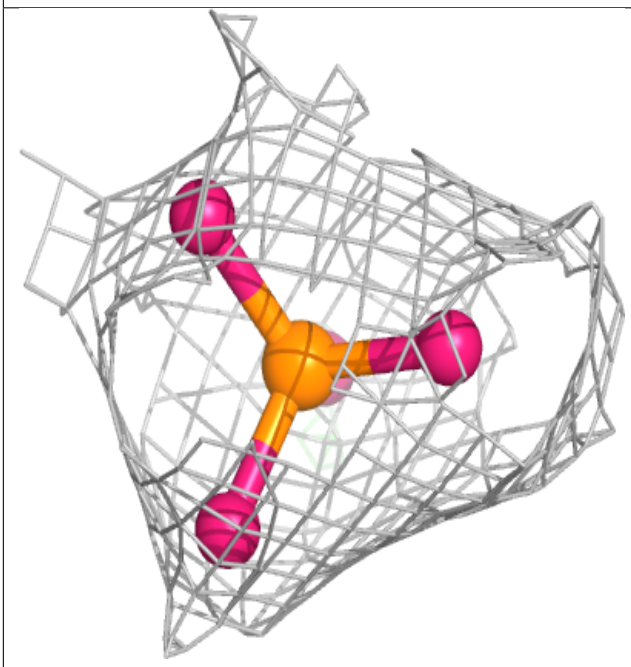


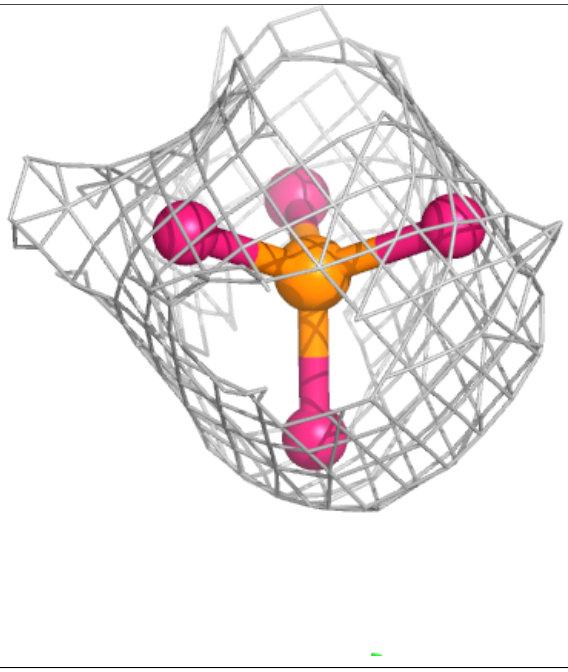


Electron density around PO4 D 205:

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

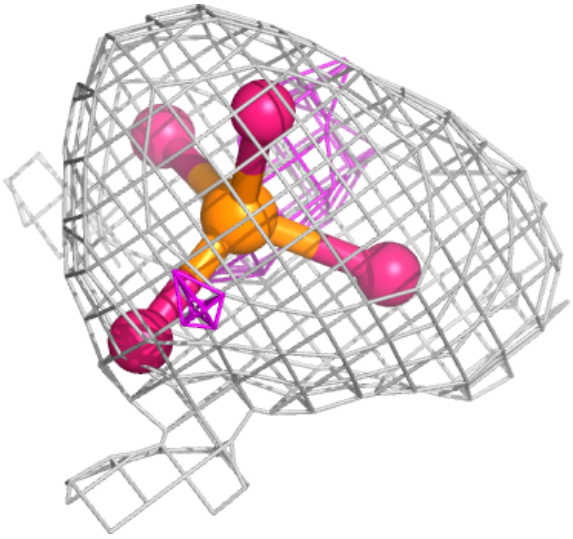


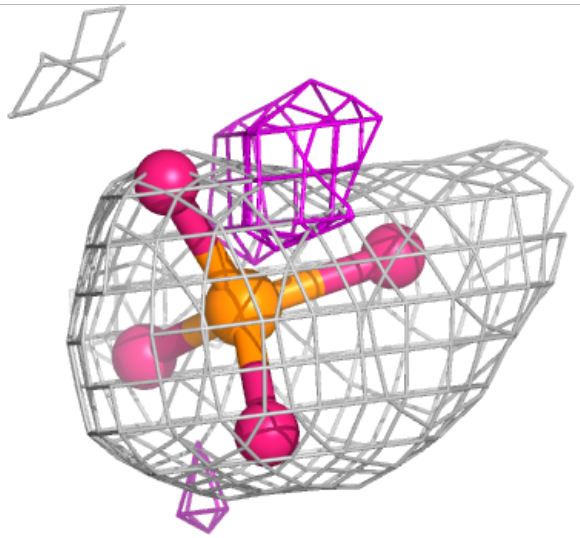


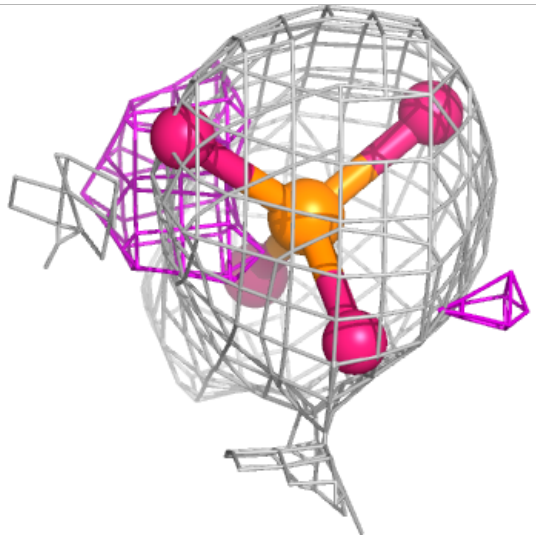


Electron density around PO4 D 204:

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

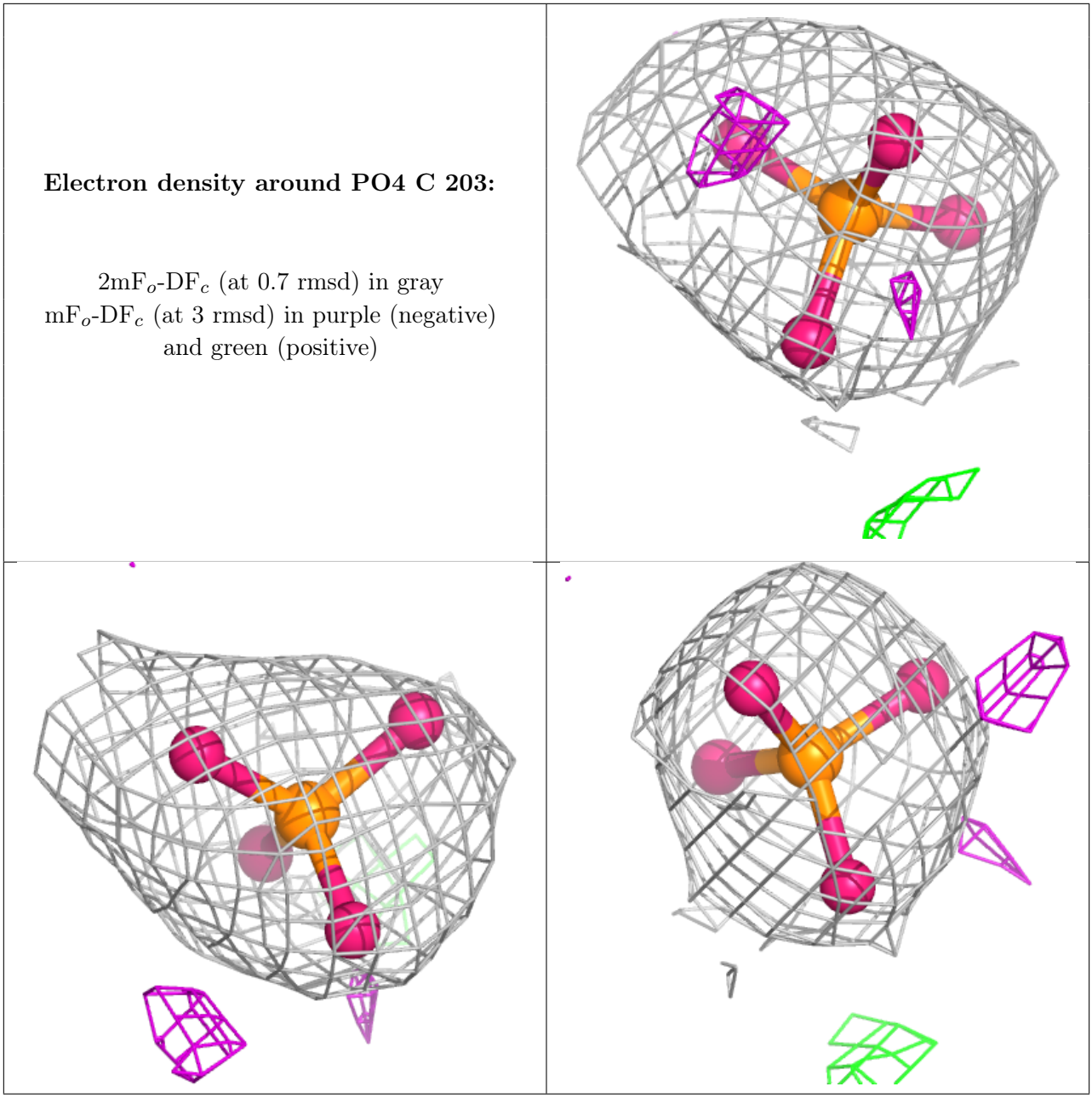






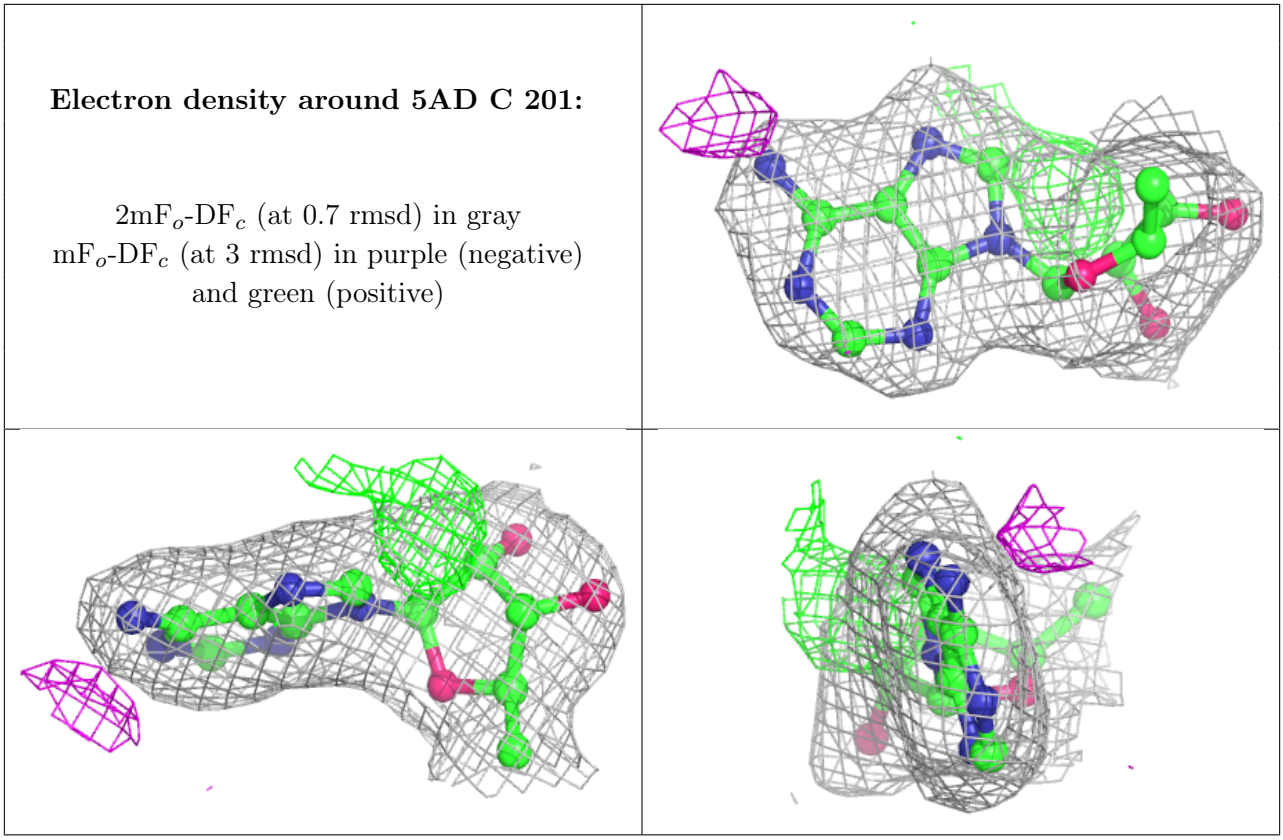
Electron density around PO4 C 203:

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



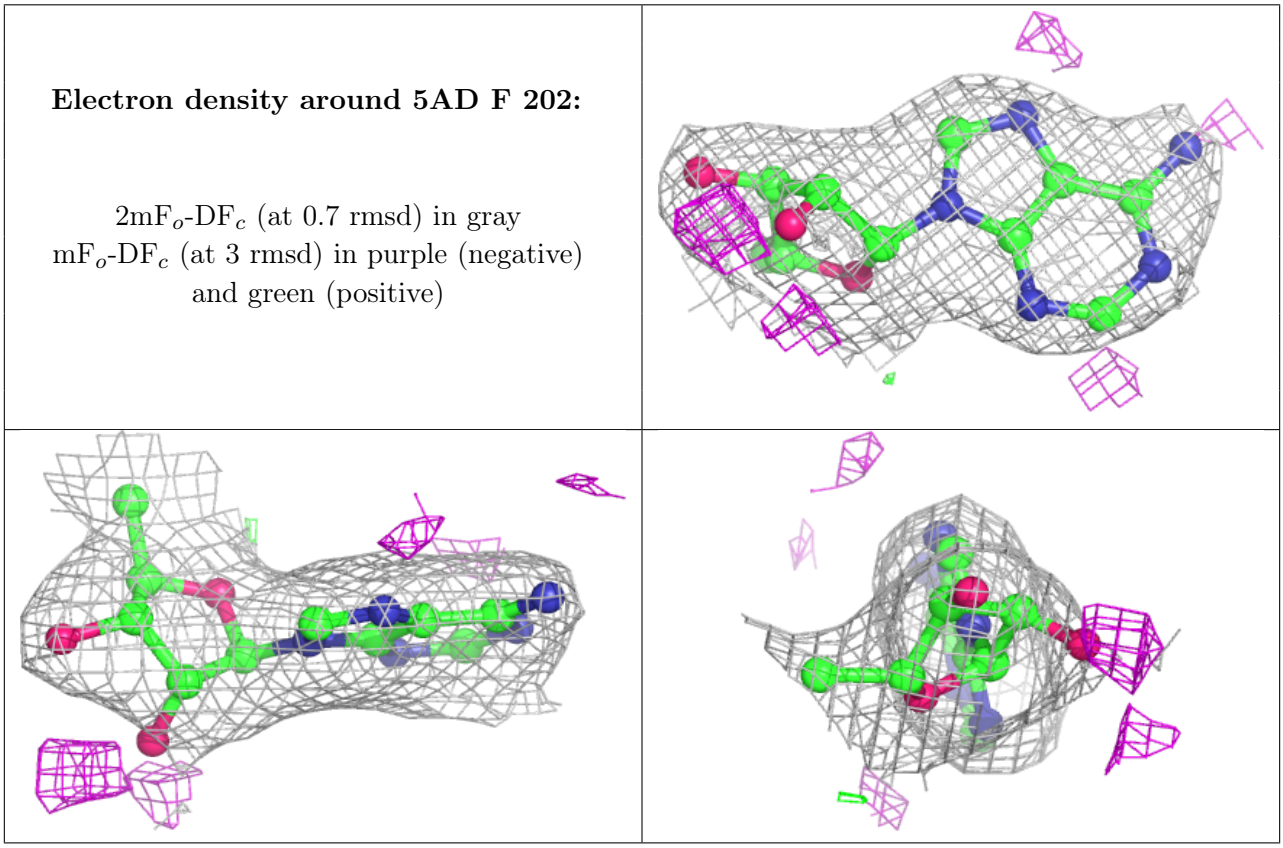
Electron density around 5AD C 201:

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



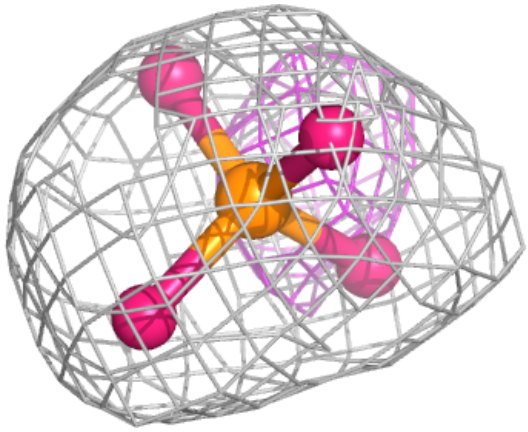
Electron density around 5AD F 202:

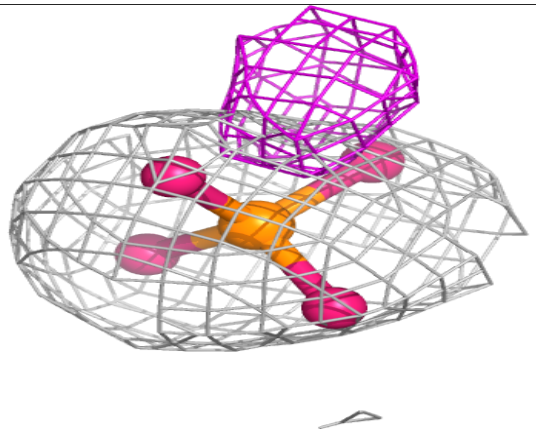
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

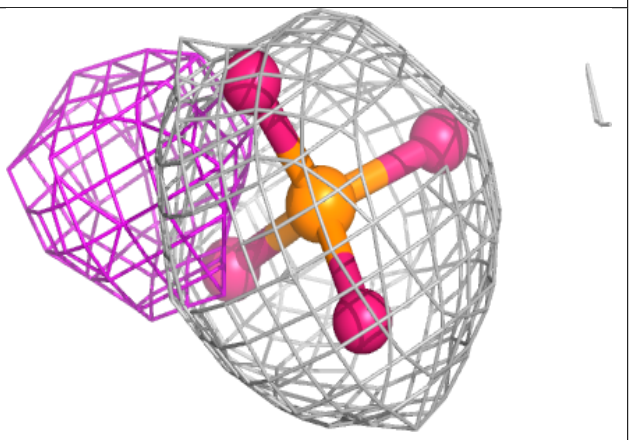


Electron density around PO4 A 204:

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

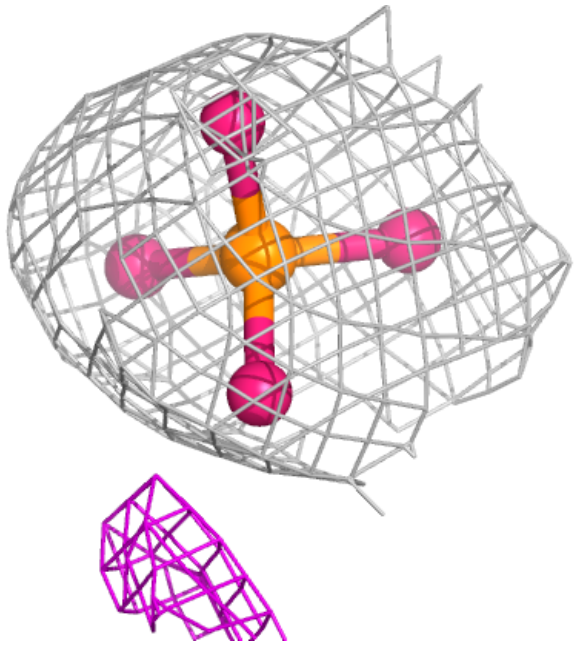


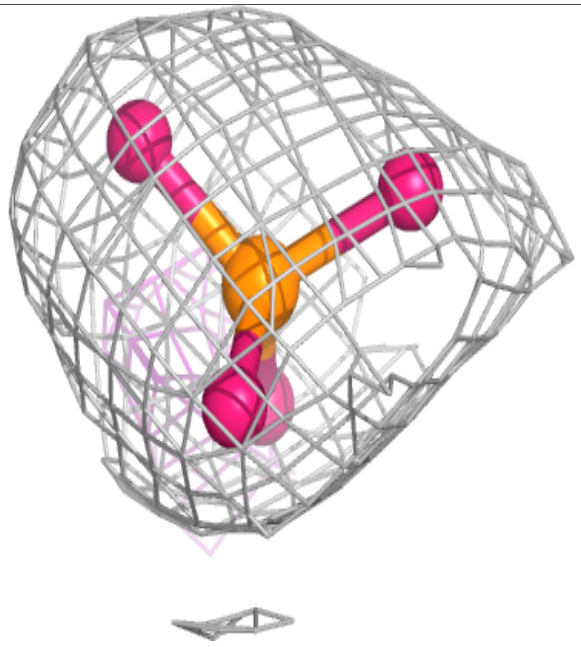


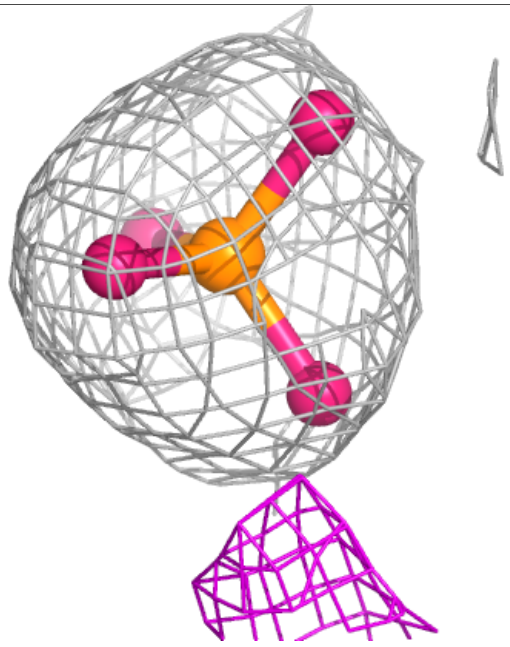


Electron density around PO4 B 206:

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

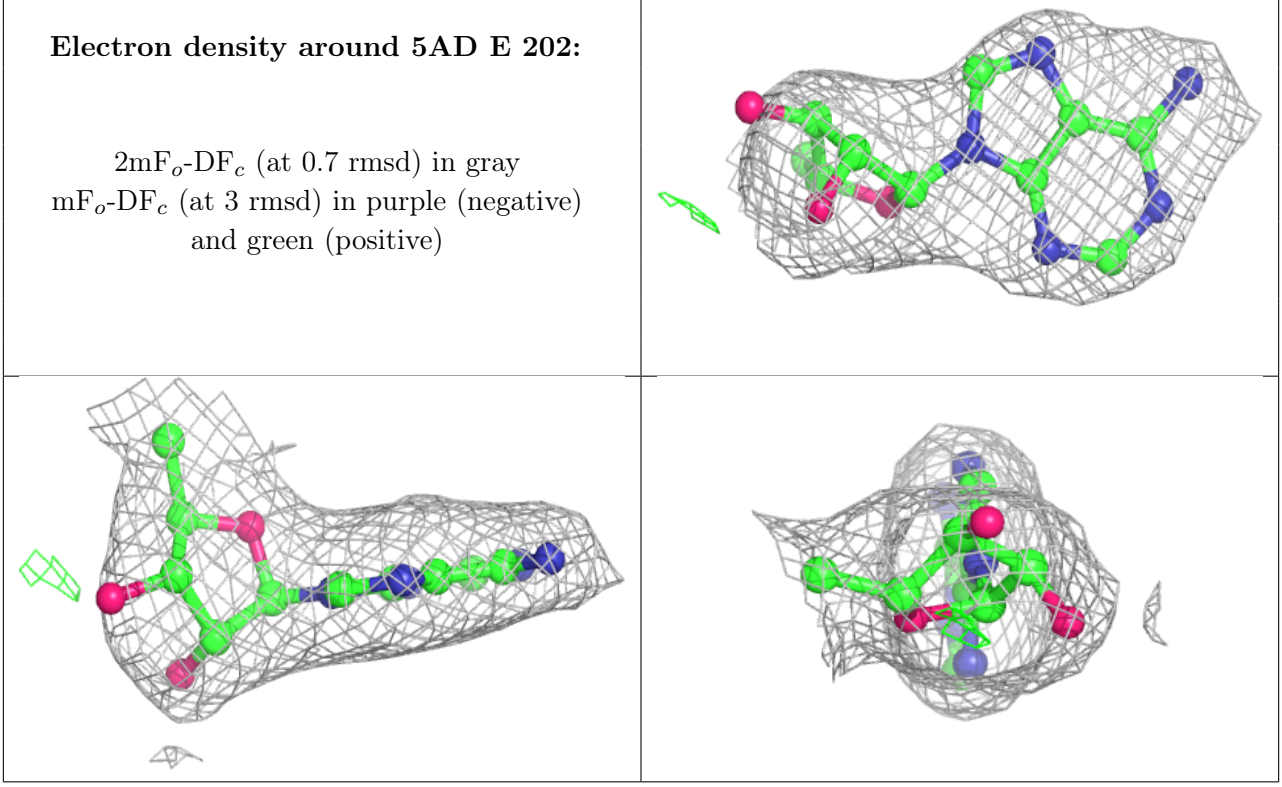






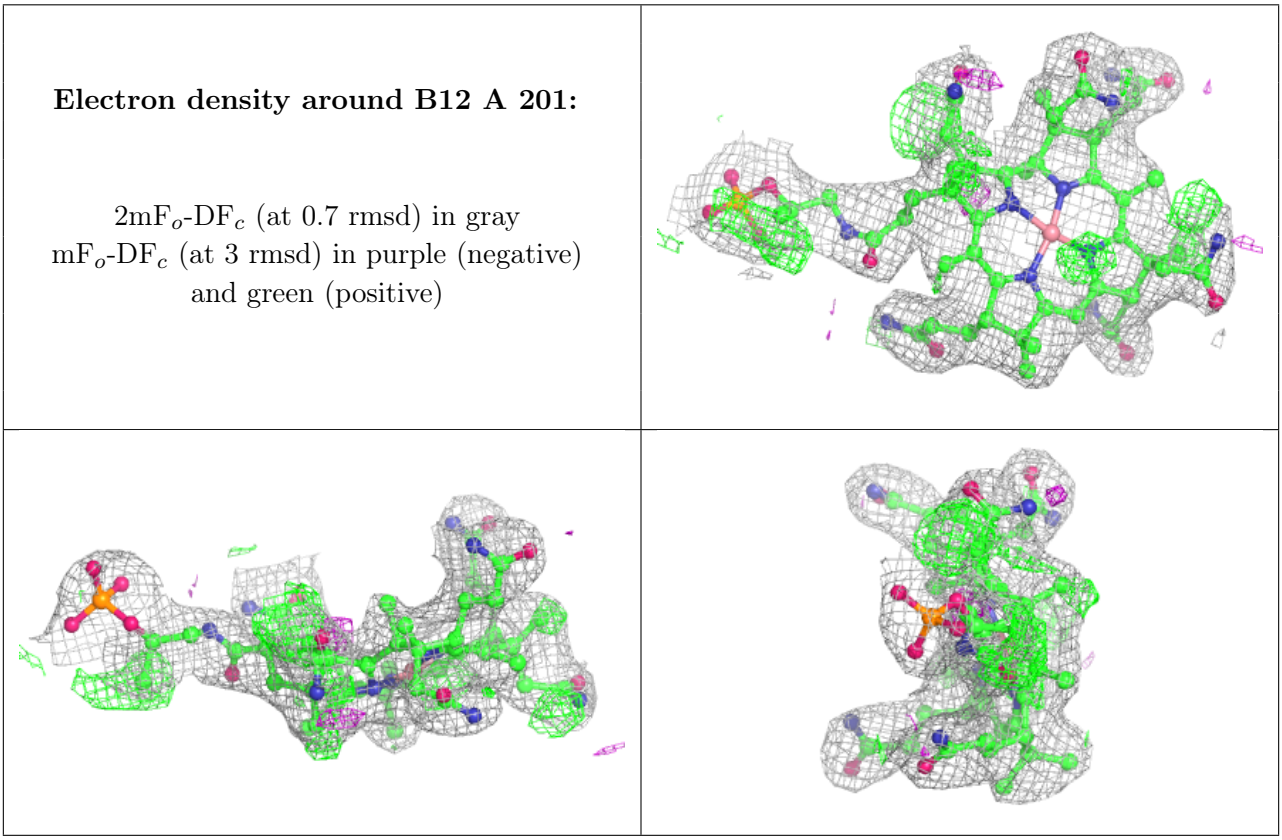
Electron density around 5AD E 202:

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



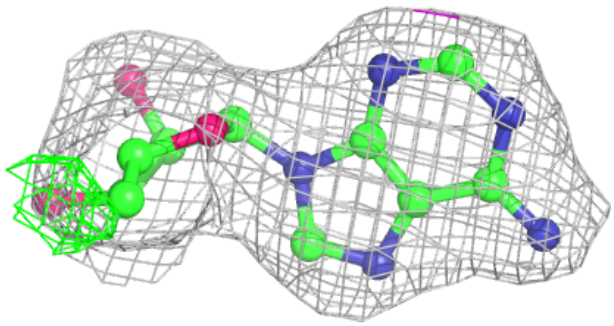
Electron density around B12 A 201:

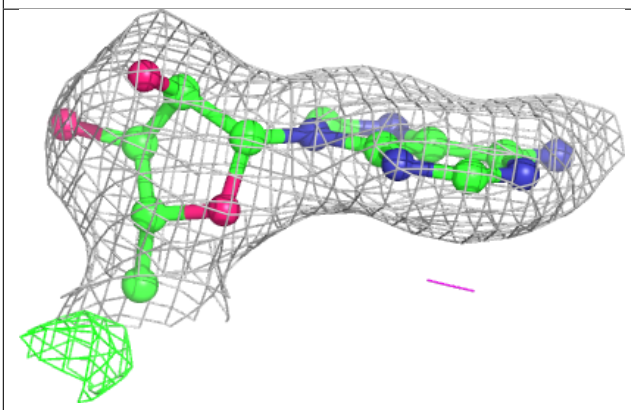
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

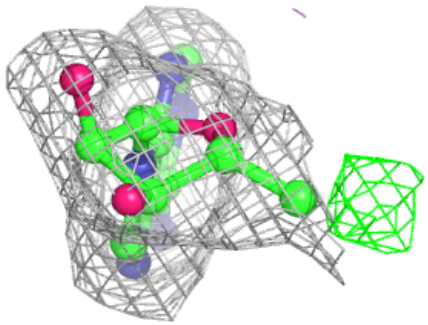


Electron density around 5AD A 202:

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

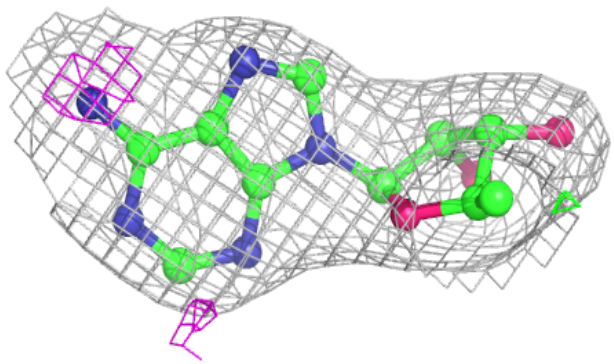


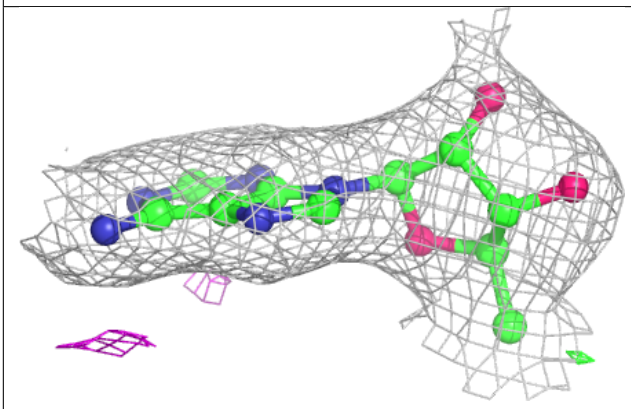


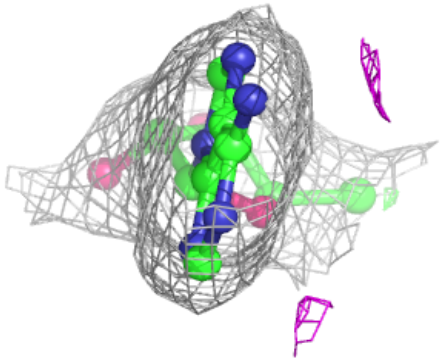


Electron density around 5AD B 202:

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

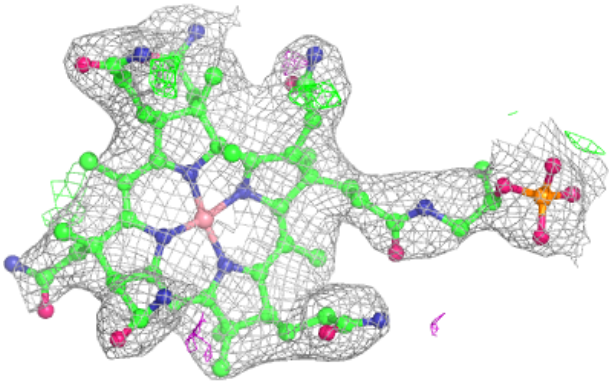


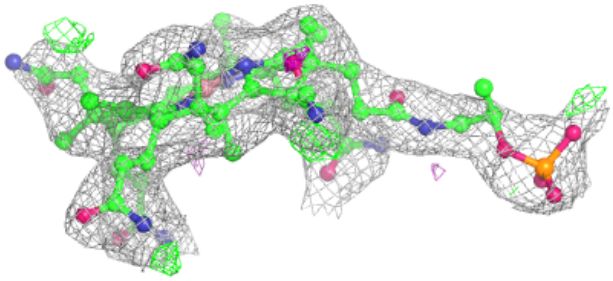


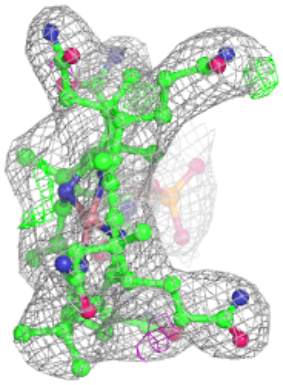


Electron density around B12 E 201:

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

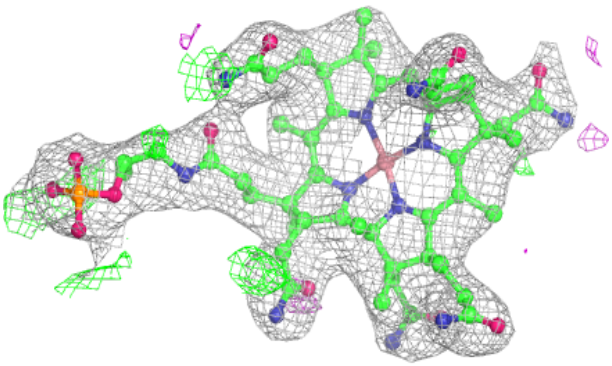


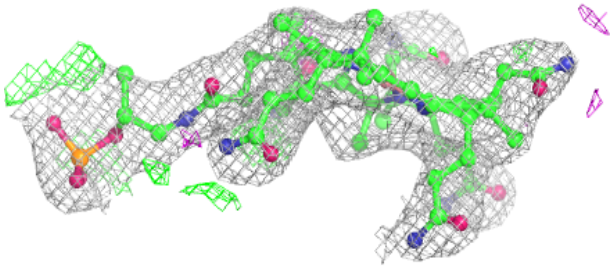


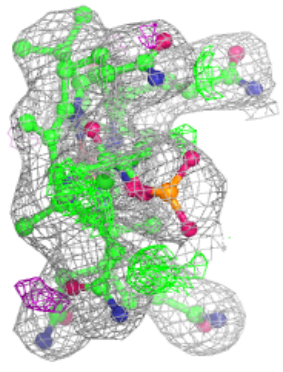


Electron density around B12 B 201:

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

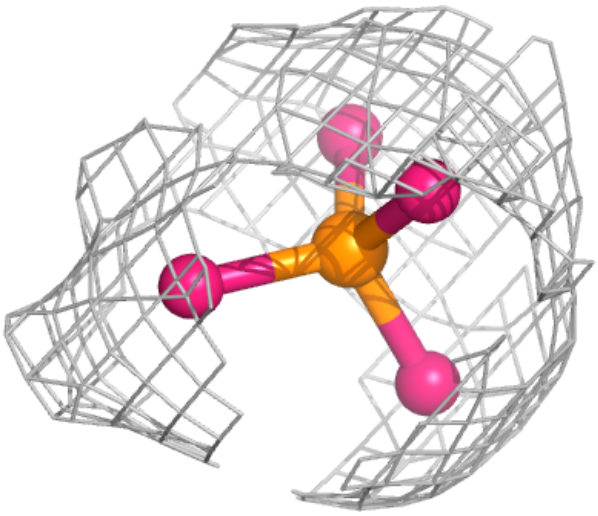


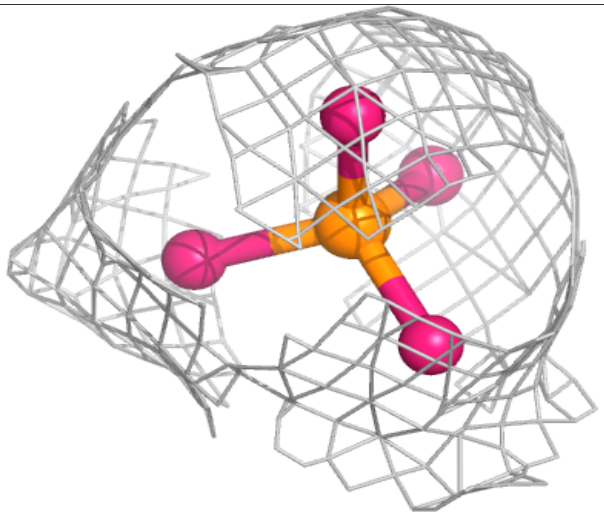


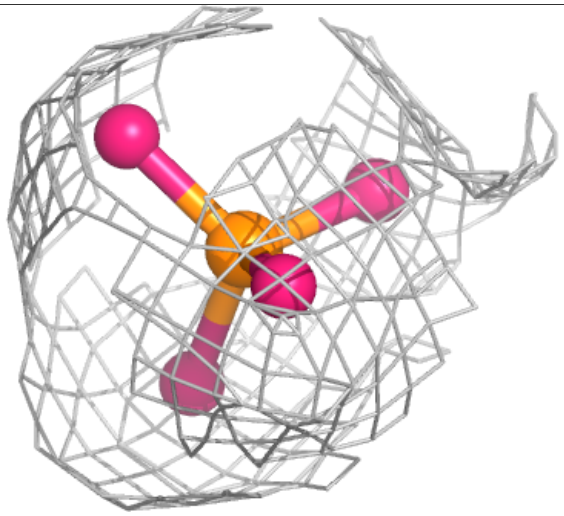


Electron density around PO4 E 203:

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

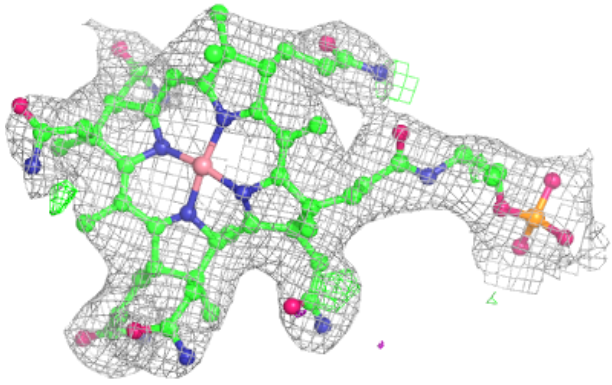


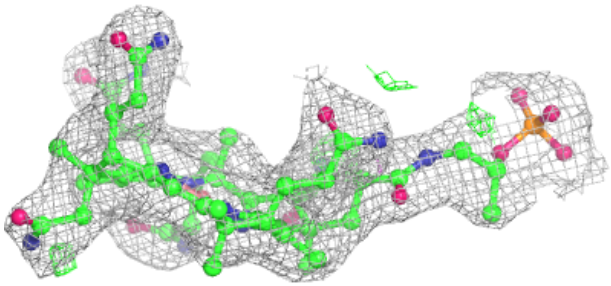


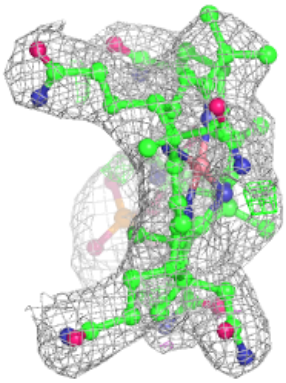


Electron density around B12 D 201:

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

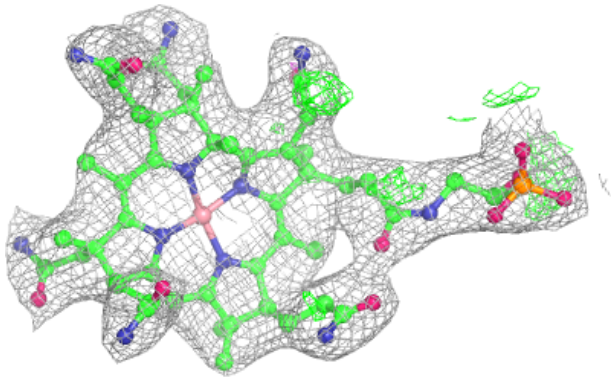


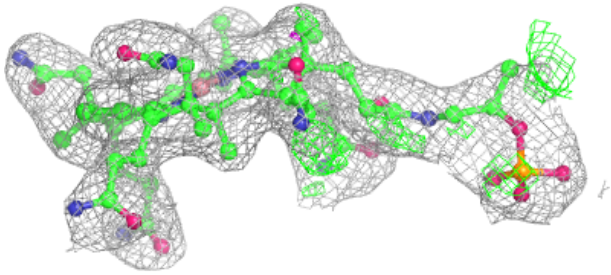


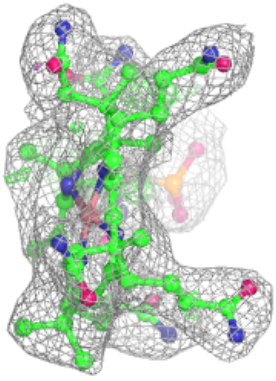


Electron density around B12 B 203:

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

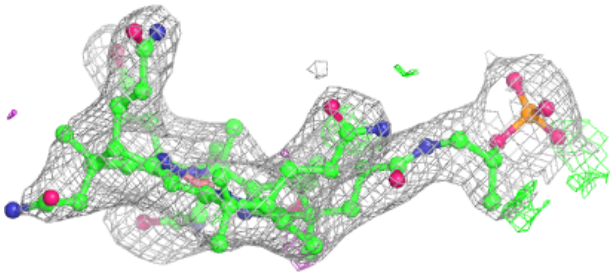


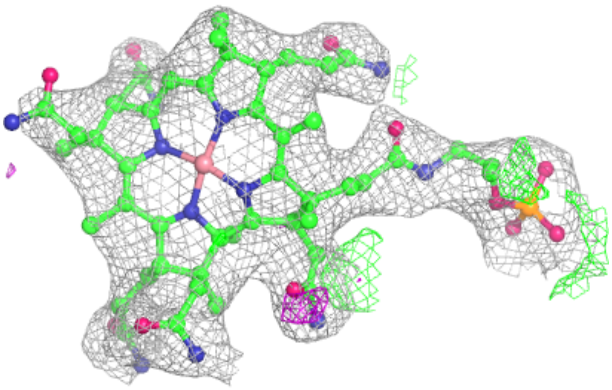


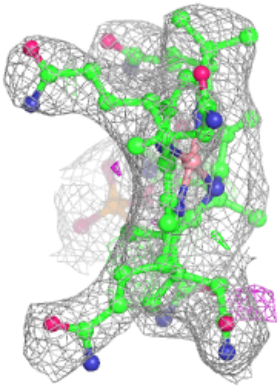


Electron density around B12 F 201:

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

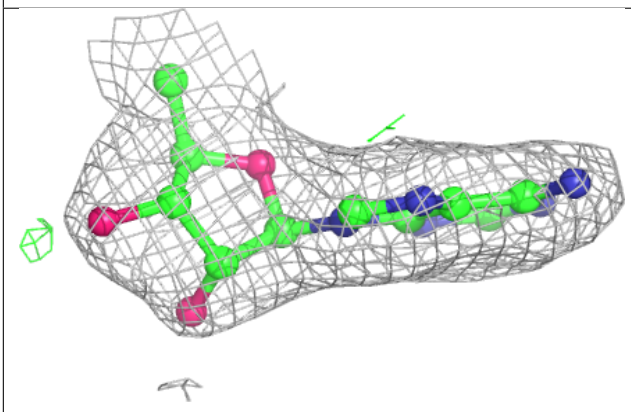


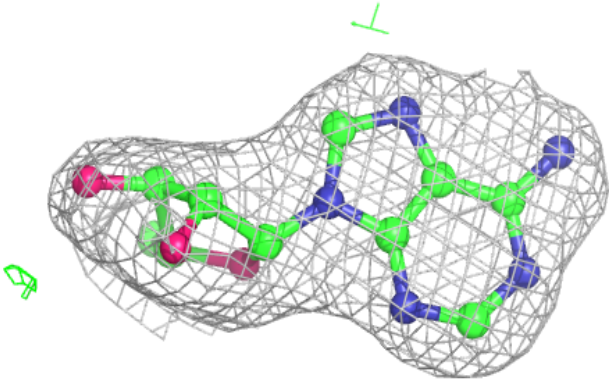


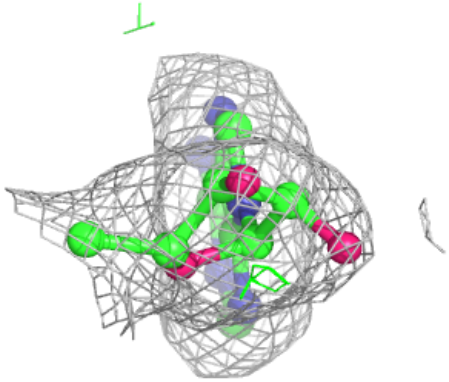


Electron density around 5AD D 202:

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

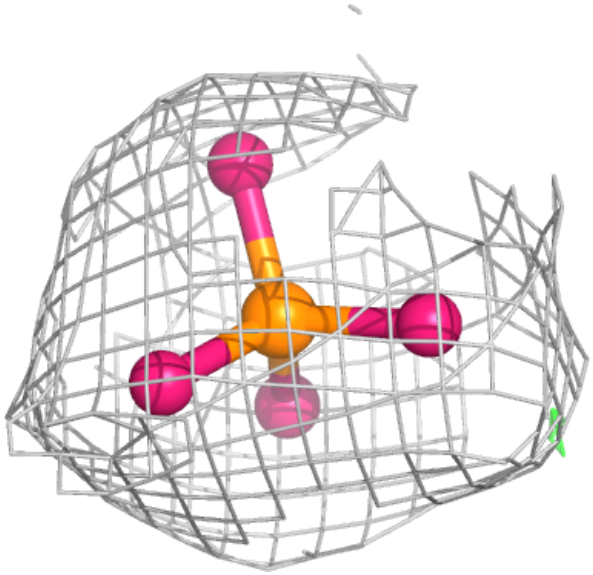


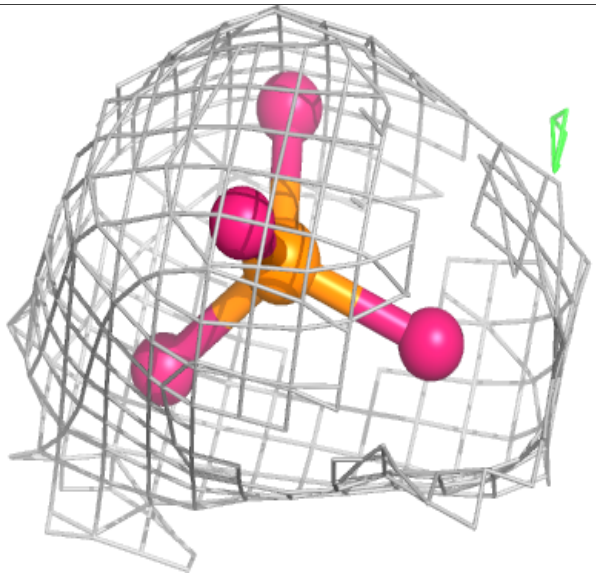


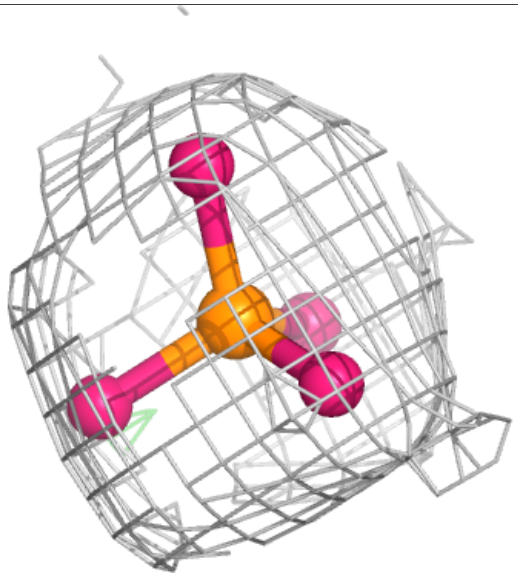


Electron density around PO4 C 202:

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

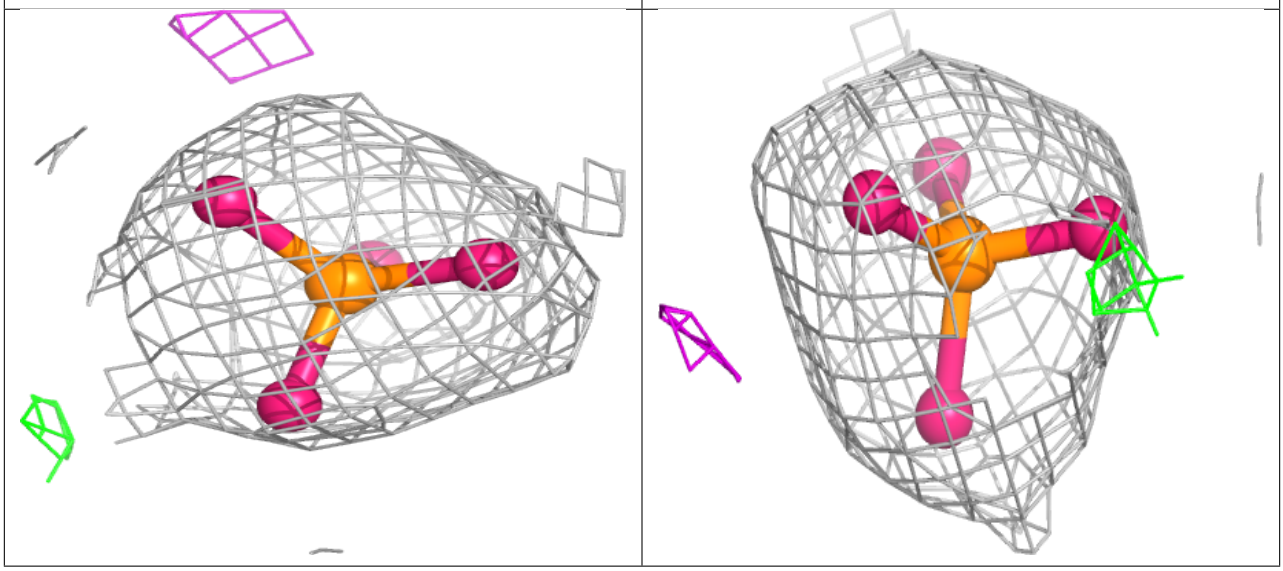






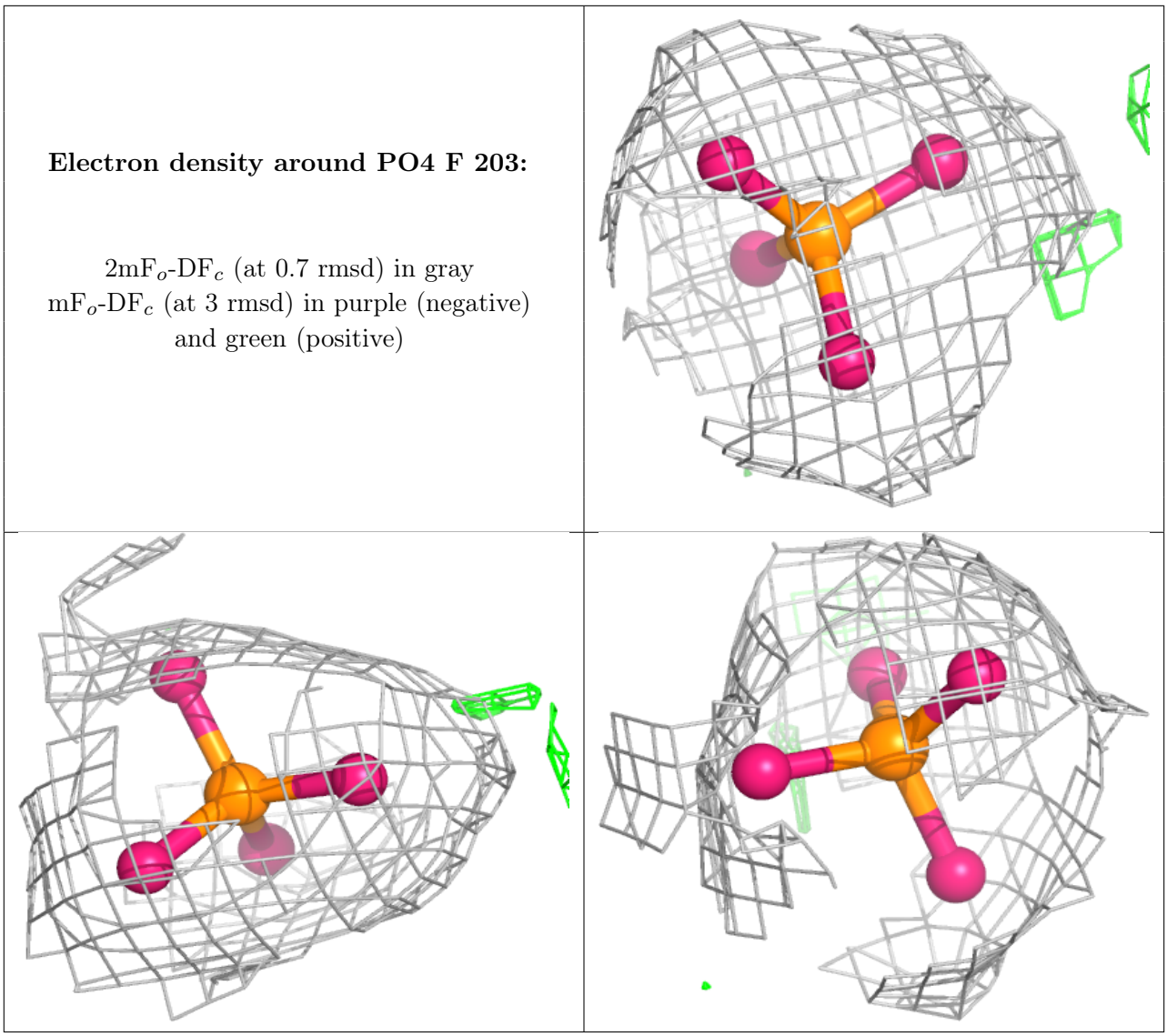
Electron density around PO4 E 204:

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



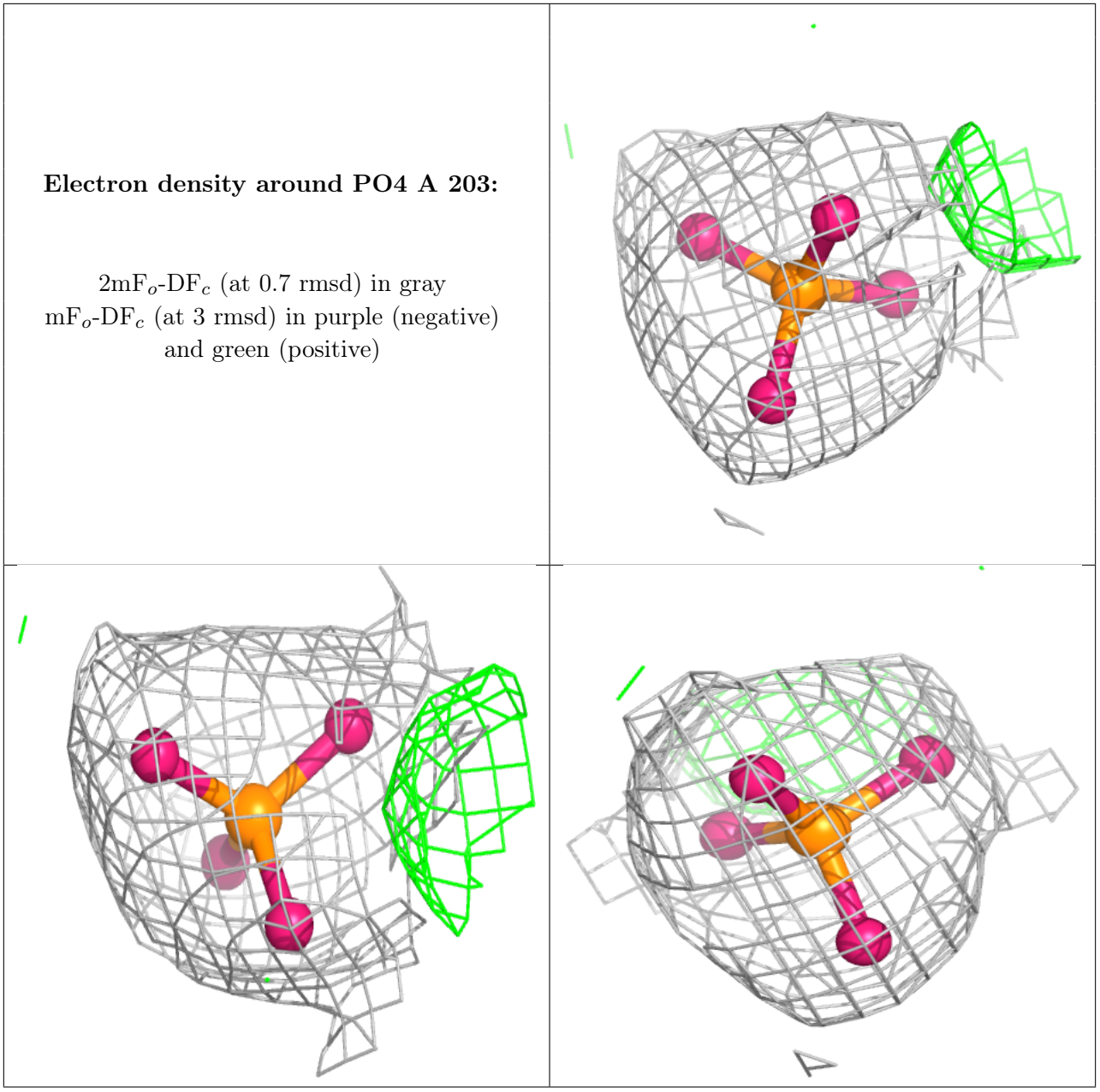
Electron density around PO4 F 203:

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



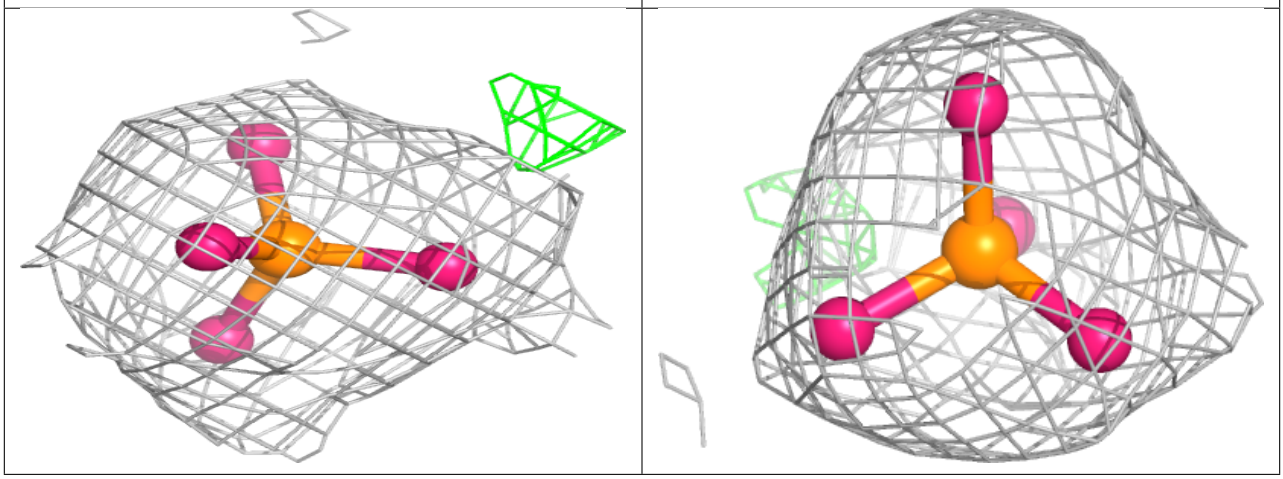
Electron density around PO4 A 203:

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



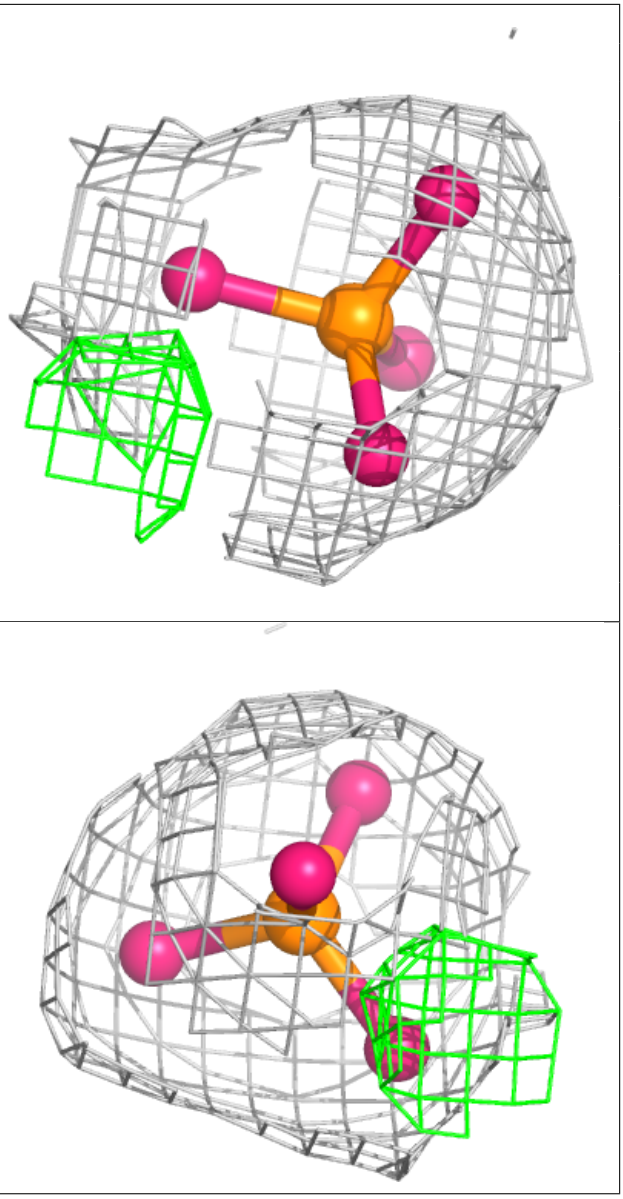
Electron density around PO4 B 204:

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



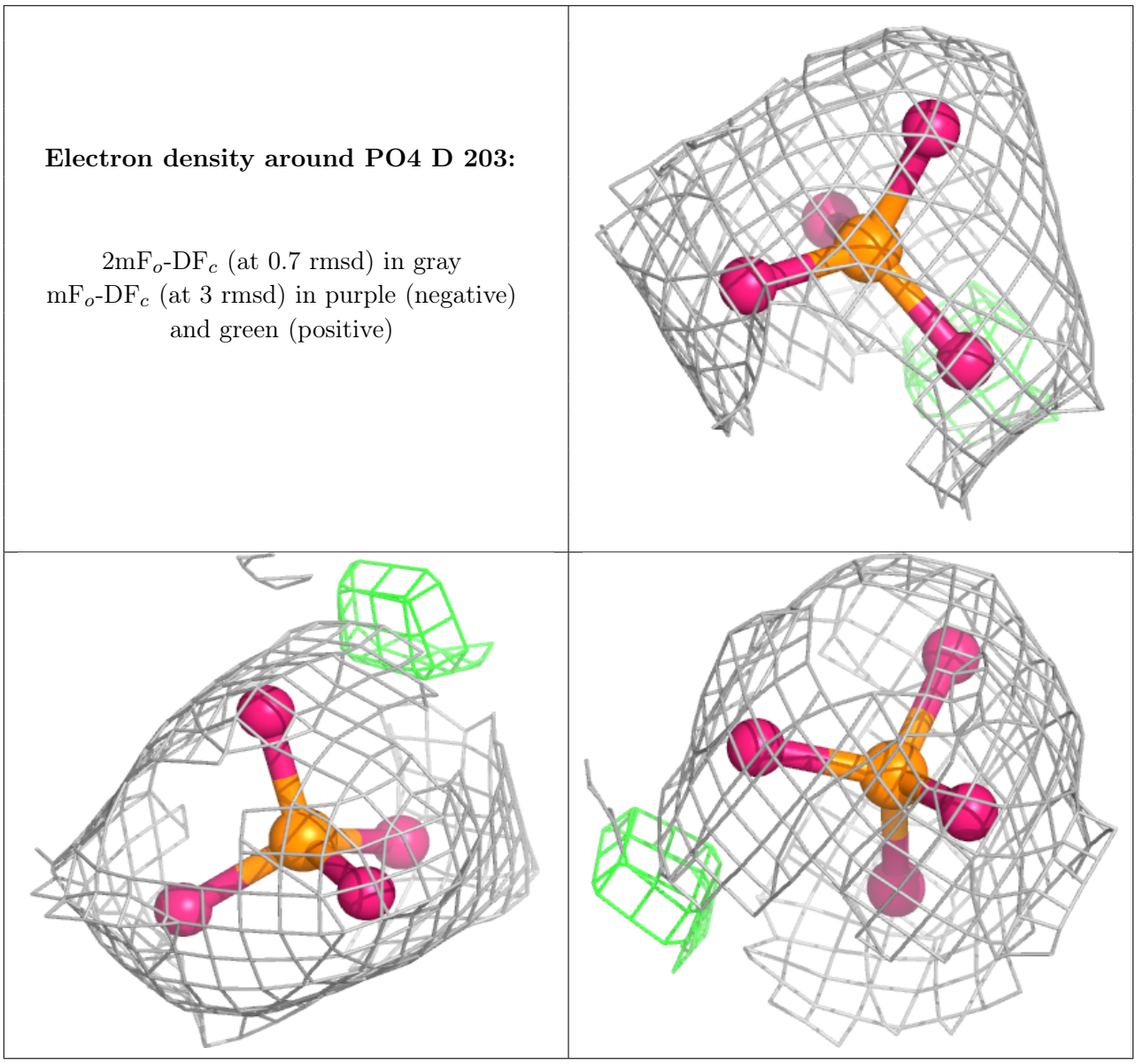
Electron density around PO4 B 205:

$2mF_o$-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 203:

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



6.5 Other polymers

There are no such residues in this entry.