Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:07 PM UTC

PDB ID	:	7C5Q / pdb_00007c5q
Title	:	Crystal Structure of H177A mutant Glyceraldehyde-3-phosphate dehydrogenase1 from Escherichia coli complexed with BPG at 2.13 Angstrom resolution
Authors	:	Zhang, L.; Liu, M.R.; Bao, L.Y.; Yao, Y.C.; Bostrom, I.K.; Wang, Y.D.; Chen, A.Q.; Li, J.X.; Gu, S.H.; Ji, C.N.
Deposited on	:	2020-05-20
Resolution	:	2.13 Å(reported)

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

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

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

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

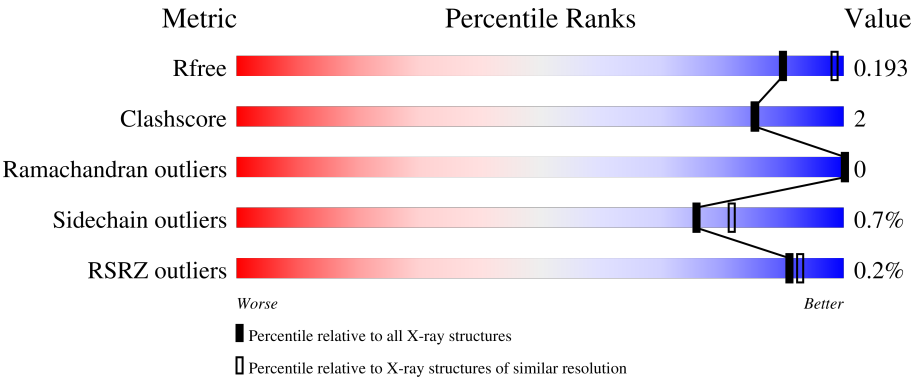
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	O	352	90% 5% 5%
1	P	352	89% 5% 5%
1	Q	352	90% · 5%
1	R	352	91% · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G3H	Q	402	-	-	X	-
3	G3H	R	402	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21814 atoms, of which 10407 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	O	334	Total	C	H	N	O	S	0	14	0
			5171	1624	2596	432	512	7			
1	P	333	Total	C	H	N	O	S	0	7	0
			5113	1606	2571	427	502	7			
1	Q	333	Total	C	H	N	O	S	0	2	0
			5069	1593	2550	423	496	7			
1	R	333	Total	C	H	N	O	S	0	0	0
			5053	1588	2543	422	493	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-18	HIS	-	expression tag	UNP A0A140NCK4
O	-17	HIS	-	expression tag	UNP A0A140NCK4
O	-16	HIS	-	expression tag	UNP A0A140NCK4
O	-15	HIS	-	expression tag	UNP A0A140NCK4
O	-14	HIS	-	expression tag	UNP A0A140NCK4
O	-13	HIS	-	expression tag	UNP A0A140NCK4
O	-12	SER	-	expression tag	UNP A0A140NCK4
O	-11	SER	-	expression tag	UNP A0A140NCK4
O	-10	GLY	-	expression tag	UNP A0A140NCK4
O	-9	LEU	-	expression tag	UNP A0A140NCK4
O	-8	VAL	-	expression tag	UNP A0A140NCK4
O	-7	PRO	-	expression tag	UNP A0A140NCK4
O	-6	ARG	-	expression tag	UNP A0A140NCK4
O	-5	GLY	-	expression tag	UNP A0A140NCK4
O	-4	SER	-	expression tag	UNP A0A140NCK4
O	-3	HIS	-	expression tag	UNP A0A140NCK4
O	-2	MET	-	expression tag	UNP A0A140NCK4
O	-1	ALA	-	expression tag	UNP A0A140NCK4
O	0	SER	-	expression tag	UNP A0A140NCK4
O	177	ALA	HIS	engineered mutation	UNP A0A140NCK4
P	-18	HIS	-	expression tag	UNP A0A140NCK4

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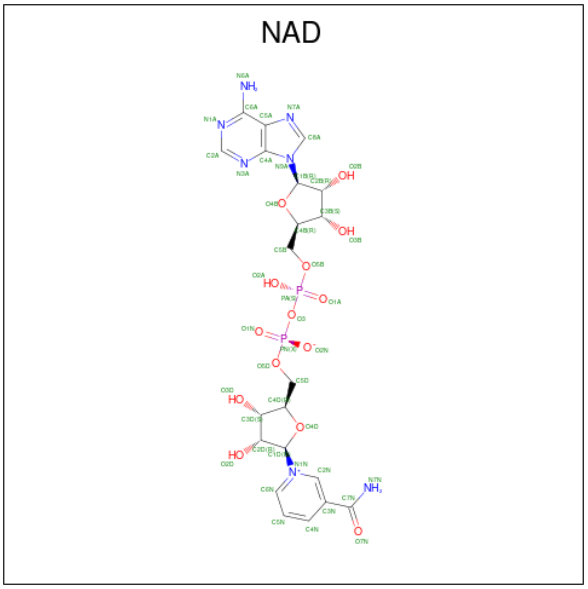
Chain	Residue	Modelled	Actual	Comment	Reference
P	-17	HIS	-	expression tag	UNP A0A140NCK4
P	-16	HIS	-	expression tag	UNP A0A140NCK4
P	-15	HIS	-	expression tag	UNP A0A140NCK4
P	-14	HIS	-	expression tag	UNP A0A140NCK4
P	-13	HIS	-	expression tag	UNP A0A140NCK4
P	-12	SER	-	expression tag	UNP A0A140NCK4
P	-11	SER	-	expression tag	UNP A0A140NCK4
P	-10	GLY	-	expression tag	UNP A0A140NCK4
P	-9	LEU	-	expression tag	UNP A0A140NCK4
P	-8	VAL	-	expression tag	UNP A0A140NCK4
P	-7	PRO	-	expression tag	UNP A0A140NCK4
P	-6	ARG	-	expression tag	UNP A0A140NCK4
P	-5	GLY	-	expression tag	UNP A0A140NCK4
P	-4	SER	-	expression tag	UNP A0A140NCK4
P	-3	HIS	-	expression tag	UNP A0A140NCK4
P	-2	MET	-	expression tag	UNP A0A140NCK4
P	-1	ALA	-	expression tag	UNP A0A140NCK4
P	0	SER	-	expression tag	UNP A0A140NCK4
P	177	ALA	HIS	engineered mutation	UNP A0A140NCK4
Q	-18	HIS	-	expression tag	UNP A0A140NCK4
Q	-17	HIS	-	expression tag	UNP A0A140NCK4
Q	-16	HIS	-	expression tag	UNP A0A140NCK4
Q	-15	HIS	-	expression tag	UNP A0A140NCK4
Q	-14	HIS	-	expression tag	UNP A0A140NCK4
Q	-13	HIS	-	expression tag	UNP A0A140NCK4
Q	-12	SER	-	expression tag	UNP A0A140NCK4
Q	-11	SER	-	expression tag	UNP A0A140NCK4
Q	-10	GLY	-	expression tag	UNP A0A140NCK4
Q	-9	LEU	-	expression tag	UNP A0A140NCK4
Q	-8	VAL	-	expression tag	UNP A0A140NCK4
Q	-7	PRO	-	expression tag	UNP A0A140NCK4
Q	-6	ARG	-	expression tag	UNP A0A140NCK4
Q	-5	GLY	-	expression tag	UNP A0A140NCK4
Q	-4	SER	-	expression tag	UNP A0A140NCK4
Q	-3	HIS	-	expression tag	UNP A0A140NCK4
Q	-2	MET	-	expression tag	UNP A0A140NCK4
Q	-1	ALA	-	expression tag	UNP A0A140NCK4
Q	0	SER	-	expression tag	UNP A0A140NCK4
Q	177	ALA	HIS	engineered mutation	UNP A0A140NCK4
R	-18	HIS	-	expression tag	UNP A0A140NCK4
R	-17	HIS	-	expression tag	UNP A0A140NCK4
R	-16	HIS	-	expression tag	UNP A0A140NCK4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	HIS	-	expression tag	UNP A0A140NCK4
R	-14	HIS	-	expression tag	UNP A0A140NCK4
R	-13	HIS	-	expression tag	UNP A0A140NCK4
R	-12	SER	-	expression tag	UNP A0A140NCK4
R	-11	SER	-	expression tag	UNP A0A140NCK4
R	-10	GLY	-	expression tag	UNP A0A140NCK4
R	-9	LEU	-	expression tag	UNP A0A140NCK4
R	-8	VAL	-	expression tag	UNP A0A140NCK4
R	-7	PRO	-	expression tag	UNP A0A140NCK4
R	-6	ARG	-	expression tag	UNP A0A140NCK4
R	-5	GLY	-	expression tag	UNP A0A140NCK4
R	-4	SER	-	expression tag	UNP A0A140NCK4
R	-3	HIS	-	expression tag	UNP A0A140NCK4
R	-2	MET	-	expression tag	UNP A0A140NCK4
R	-1	ALA	-	expression tag	UNP A0A140NCK4
R	0	SER	-	expression tag	UNP A0A140NCK4
R	177	ALA	HIS	engineered mutation	UNP A0A140NCK4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



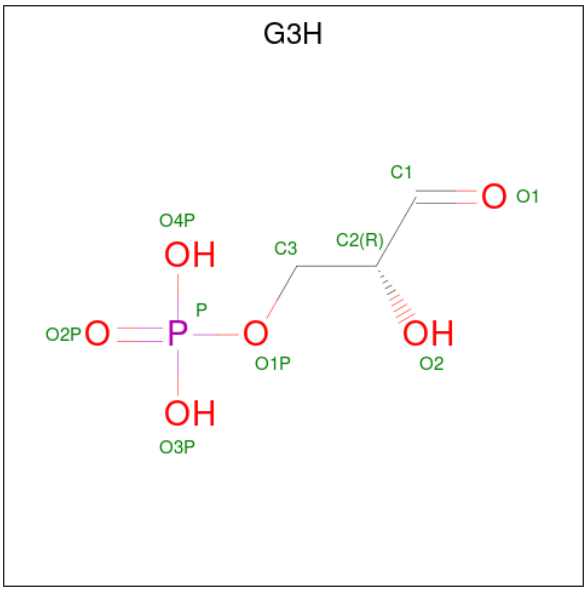
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	O	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	P	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

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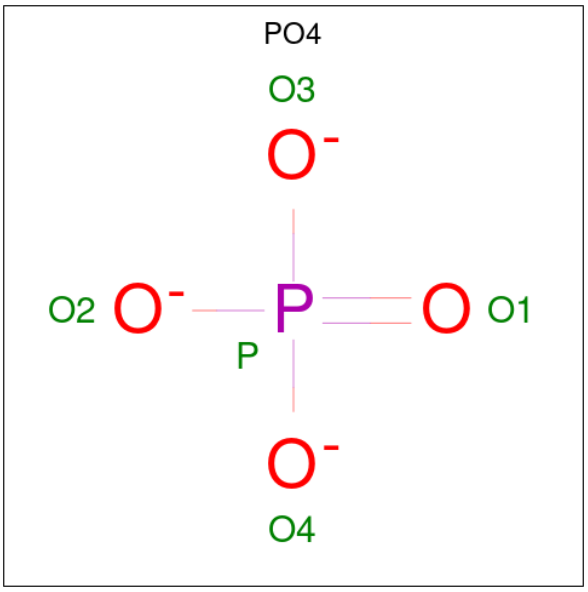
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	Q	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	R	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: $C_3H_7O_6P$) (labeled as "Ligand of Interest" by depositor).



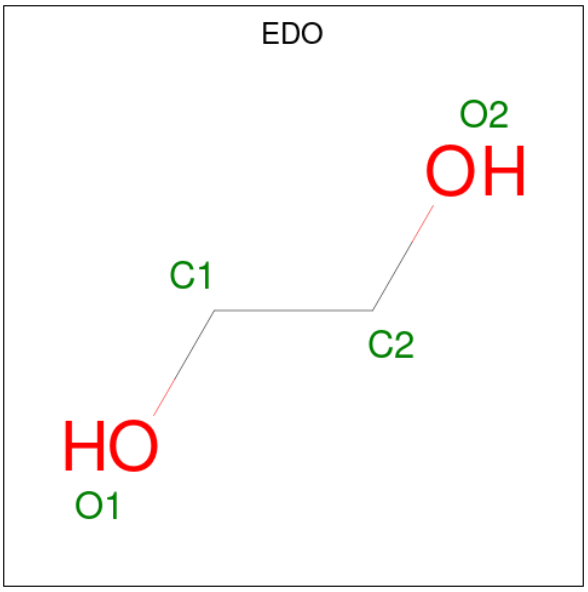
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	H	O	P	0	0
			15	3	5	6	1		
3	Q	1	Total	C	H	O	P	0	0
			15	3	5	6	1		
3	R	1	Total	C	H	O	P	0	0
			15	3	5	6	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total O P 5 4 1	0	0
4	O	1	Total O P 5 4 1	0	0
4	O	1	Total O P 5 4 1	0	0
4	P	1	Total O P 5 4 1	0	0
4	P	1	Total O P 5 4 1	0	0
4	Q	1	Total O P 5 4 1	0	0
4	Q	1	Total O P 5 4 1	0	0
4	R	1	Total O P 5 4 1	0	0
4	R	1	Total O P 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

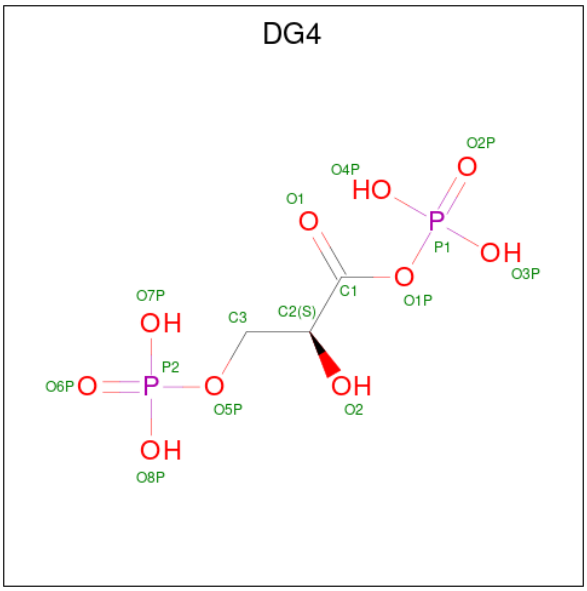


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C H O 10 2 6 2	0	0
5	Q	1	Total C H O 20 4 12 4	0	1
5	R	1	Total C H O 10 2 6 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	2	Total Cl 2 2	0	0
6	P	1	Total Cl 1 1	0	0
6	Q	1	Total Cl 1 1	0	0
6	R	1	Total Cl 1 1	0	0

- Molecule 7 is phosphono (2S)-2-oxidanyl-3-phosphonooxy-propanoate (CCD ID: DG4) (formula: $C_3H_8O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	H	O	P	0	0
			19	3	4	10	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	O	276	Total	O	0	0
			276	276		
8	P	270	Total	O	0	0
			270	270		
8	Q	253	Total	O	0	1
			254	254		
8	R	173	Total	O	0	1
			174	174		

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: Glyceraldehyde-3-phosphate dehydrogenase

Chain O:

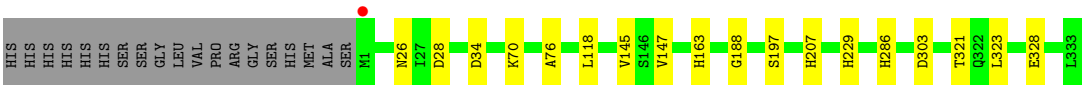




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain P:

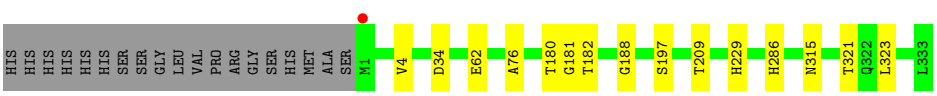




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain Q:

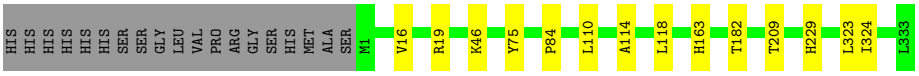




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.67Å 89.67Å 341.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.13 48.08 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.08-2.13) 99.9 (48.08-2.13)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.138 , 0.190 0.141 , 0.193	Depositor DCC
R_{free} test set	3931 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21814	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: CL, G3H, DG4, EDO, PO4, NAD

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	O	0.45	0/2665	0.64	0/3617
1	P	0.45	0/2600	0.62	0/3529
1	Q	0.45	0/2568	0.61	0/3483
1	R	0.43	0/2550	0.62	0/3460
All	All	0.45	0/10383	0.62	0/14089

There are no bond length outliers.

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	O	2575	2596	2531	9	0
1	P	2542	2571	2552	11	0
1	Q	2519	2550	2538	10	0
1	R	2510	2543	2545	10	0
2	O	44	26	25	1	0
2	P	44	26	24	0	0
2	Q	44	26	25	2	0
2	R	44	26	23	2	0
3	O	10	5	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	10	5	5	5	0
3	R	10	5	5	4	0
4	O	15	0	0	0	0
4	P	10	0	0	1	0
4	Q	10	0	0	0	0
4	R	10	0	0	1	0
5	O	4	6	6	0	0
5	Q	8	12	12	0	0
5	R	4	6	6	1	0
6	O	2	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
7	P	15	4	0	3	0
8	O	276	0	0	1	0
8	P	270	0	0	2	0
8	Q	254	0	0	0	0
8	R	174	0	0	0	0
All	All	11407	10407	10302	46	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 2.

All (46) 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:R:182:THR:HG21	3:R:402:G3H:H32	1.61	0.81
1:R:182:THR:CG2	3:R:402:G3H:H32	2.26	0.65
1:P:28:ASP:OD1	1:P:70:LYS:NZ	2.27	0.62
2:Q:401:NAD:PN	3:Q:402:G3H:H2	2.45	0.57
1:R:19:ARG:HH22	5:R:405:EDO:H12	1.70	0.57
2:R:401:NAD:O2D	3:R:402:G3H:O1P	2.20	0.54
1:Q:315:ASN:HD22	2:Q:401:NAD:H72N	1.57	0.53
7:P:402:DG4:O4P	7:P:402:DG4:O2	2.27	0.51
1:R:209:THR:HG22	1:R:229:HIS:HA	1.93	0.51
2:R:401:NAD:O2D	3:R:402:G3H:H2	2.12	0.49
1:Q:209:THR:HG22	1:Q:229:HIS:HA	1.95	0.48
1:O:118:LEU:CD1	1:O:145[B]:VAL:HG23	2.43	0.48
1:R:118:LEU:C	1:R:118:LEU:HD23	2.39	0.48
1:Q:181:GLY:HA3	3:Q:402:G3H:H11	1.96	0.47
1:Q:182:THR:HG23	3:Q:402:G3H:H31	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:402:G3H:H11	8:O:687:HOH:O	2.16	0.45
1:R:163:HIS:ND1	4:R:403:PO4:O1	2.36	0.45
1:R:323:LEU:C	1:R:323:LEU:HD23	2.42	0.45
1:Q:323:LEU:C	1:Q:323:LEU:HD23	2.42	0.45
1:Q:180:THR:HB	3:Q:402:G3H:H32	1.99	0.45
1:Q:181:GLY:CA	3:Q:402:G3H:H11	2.47	0.44
1:O:268:GLU:HG3	1:O:325:ARG:NE	2.33	0.44
1:Q:188:GLY:O	1:Q:197:SER:HB2	2.18	0.44
1:P:163:HIS:ND1	4:P:403:PO4:O2	2.38	0.44
1:P:118:LEU:HD11	1:P:147:VAL:HG13	1.99	0.43
1:O:315:ASN:O	2:O:401:NAD:H4N	2.18	0.43
1:P:286:HIS:HA	1:P:321:THR:HG21	2.01	0.43
1:O:286:HIS:HA	1:O:321:THR:HG21	2.01	0.42
1:P:328[B]:GLU:OE2	8:P:501:HOH:O	2.21	0.42
1:Q:286:HIS:HA	1:Q:321:THR:HG21	2.01	0.42
1:O:34:ASP:O	1:O:76:ALA:HA	2.20	0.42
1:P:26:ASN:HB2	8:P:731:HOH:O	2.19	0.42
1:Q:34:ASP:O	1:Q:76:ALA:HA	2.19	0.42
1:P:34:ASP:O	1:P:76:ALA:HA	2.20	0.42
1:R:75:TYR:CZ	1:R:84:PRO:HG2	2.55	0.42
1:P:188:GLY:O	1:P:197:SER:HB2	2.20	0.42
1:R:110:LEU:HA	1:R:114:ALA:O	2.19	0.42
7:P:402:DG4:O1	7:P:402:DG4:O8P	2.38	0.41
1:O:243:LEU:O	1:O:308:LYS:HA	2.21	0.41
1:P:118:LEU:CD1	1:P:145[B]:VAL:HG13	2.50	0.41
1:O:188:GLY:O	1:O:197:SER:HB2	2.21	0.41
1:O:182:THR:HG21	3:O:402:G3H:H32	2.03	0.40
1:O:323:LEU:HD23	1:O:323:LEU:C	2.45	0.40
1:P:207:HIS:HE1	7:P:402:DG4:O2	2.03	0.40
1:P:323:LEU:HD23	1:P:323:LEU:C	2.46	0.40
1:R:16:VAL:HG13	1:R:324:ILE:HD11	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	O	346/352 (98%)	331 (96%)	15 (4%)	0	100	100
1	P	338/352 (96%)	325 (96%)	13 (4%)	0	100	100
1	Q	333/352 (95%)	323 (97%)	10 (3%)	0	100	100
1	R	331/352 (94%)	316 (96%)	15 (4%)	0	100	100
All	All	1348/1408 (96%)	1295 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	O	286/288 (99%)	283 (99%)	3 (1%)	68	74
1	P	278/288 (96%)	276 (99%)	2 (1%)	76	81
1	Q	274/288 (95%)	272 (99%)	2 (1%)	76	81
1	R	272/288 (94%)	271 (100%)	1 (0%)	84	88
All	All	1110/1152 (96%)	1102 (99%)	8 (1%)	76	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	125	GLU
1	O	192	LYS
1	O	313	TYR
1	P	229	HIS
1	P	303	ASP
1	Q	4	VAL
1	Q	62	GLU
1	R	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	O	153	ASN
1	P	26	ASN
1	Q	50	ASN
1	Q	153	ASN
1	Q	257	ASN
1	Q	315	ASN
1	R	153	ASN
1	R	257	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	Q	401	-	46,48,48	3.28	15 (32%)	64,73,73	1.99	16 (25%)
4	PO4	Q	403	-	4,4,4	0.73	0	6,6,6	0.82	0
5	EDO	O	405	-	3,3,3	0.50	0	2,2,2	0.24	0
2	NAD	R	401	-	46,48,48	3.62	17 (36%)	64,73,73	1.81	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	G3H	R	402	-	8,9,9	1.77	3 (37%)	7,12,12	1.43	1 (14%)
4	PO4	P	403	-	4,4,4	0.87	0	6,6,6	0.75	0
5	EDO	Q	405[A]	-	3,3,3	0.53	0	2,2,2	0.24	0
3	G3H	O	402	-	8,9,9	1.28	1 (12%)	7,12,12	1.33	1 (14%)
5	EDO	R	405	-	3,3,3	0.45	0	2,2,2	0.83	0
4	PO4	R	404	-	4,4,4	0.87	0	6,6,6	0.62	0
4	PO4	O	403	-	4,4,4	0.97	0	6,6,6	0.59	0
7	DG4	P	402	-	12,14,14	1.67	3 (25%)	15,21,21	2.09	4 (26%)
4	PO4	O	404	-	4,4,4	0.80	0	6,6,6	0.57	0
3	G3H	Q	402	-	8,9,9	1.01	0	7,12,12	1.48	1 (14%)
5	EDO	Q	405[B]	-	3,3,3	0.44	0	2,2,2	0.46	0
4	PO4	P	404	-	4,4,4	0.86	0	6,6,6	0.53	0
4	PO4	R	403	-	4,4,4	0.64	0	6,6,6	0.80	0
4	PO4	O	408	-	4,4,4	0.81	0	6,6,6	0.56	0
4	PO4	Q	404	-	4,4,4	0.83	0	6,6,6	0.55	0
2	NAD	O	401	-	46,48,48	3.39	18 (39%)	64,73,73	1.80	13 (20%)
2	NAD	P	401	-	46,48,48	3.45	19 (41%)	64,73,73	1.80	15 (23%)

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
2	NAD	Q	401	-	-	5/30/62/62	0/5/5/5
5	EDO	Q	405[B]	-	-	0/1/1/1	-
2	NAD	O	401	-	-	5/30/62/62	0/5/5/5
5	EDO	O	405	-	-	1/1/1/1	-
3	G3H	O	402	-	-	5/7/8/8	-
2	NAD	R	401	-	-	4/30/62/62	0/5/5/5
3	G3H	R	402	-	-	3/7/8/8	-
5	EDO	R	405	-	-	0/1/1/1	-
2	NAD	P	401	-	-	4/30/62/62	0/5/5/5
5	EDO	Q	405[A]	-	-	1/1/1/1	-
7	DG4	P	402	-	-	8/13/15/15	-
3	G3H	Q	402	-	-	5/7/8/8	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	401	NAD	O4D-C1D	15.24	1.60	1.40
2	P	401	NAD	O4D-C1D	14.75	1.60	1.40
2	Q	401	NAD	O4D-C1D	14.34	1.59	1.40
2	O	401	NAD	O4D-C1D	13.70	1.58	1.40
2	O	401	NAD	O4B-C1B	8.02	1.60	1.42
2	R	401	NAD	O4B-C1B	7.97	1.60	1.42
2	P	401	NAD	O4B-C1B	7.49	1.59	1.42
2	Q	401	NAD	O4B-C1B	7.15	1.58	1.42
2	R	401	NAD	C7N-N7N	6.76	1.45	1.33
2	R	401	NAD	C2B-C1B	-6.73	1.32	1.53
2	R	401	NAD	O4B-C4B	-6.65	1.30	1.45
2	Q	401	NAD	C2B-C1B	-6.64	1.32	1.53
2	Q	401	NAD	O4B-C4B	-6.61	1.30	1.45
2	P	401	NAD	C2B-C1B	-6.58	1.32	1.53
2	O	401	NAD	C2B-C1B	-6.49	1.33	1.53
2	P	401	NAD	O4B-C4B	-6.44	1.30	1.45
2	O	401	NAD	C7N-N7N	6.01	1.44	1.33
2	O	401	NAD	O4B-C4B	-5.85	1.32	1.45
2	P	401	NAD	C7N-N7N	5.78	1.43	1.33
2	O	401	NAD	PA-O3	4.97	1.64	1.59
2	R	401	NAD	O4D-C4D	-4.86	1.34	1.45
2	O	401	NAD	O4D-C4D	-4.86	1.34	1.45
2	Q	401	NAD	O4D-C4D	-4.71	1.34	1.45
2	P	401	NAD	O4D-C4D	-4.71	1.34	1.45
2	O	401	NAD	C6A-N6A	4.41	1.45	1.34
2	P	401	NAD	C6A-N6A	4.39	1.45	1.34
2	Q	401	NAD	C6A-N6A	4.26	1.45	1.34
2	R	401	NAD	PA-O3	4.23	1.64	1.59
2	R	401	NAD	C6A-N6A	4.21	1.45	1.34
7	P	402	DG4	P1-O1P	4.15	1.67	1.59
2	Q	401	NAD	C7N-N7N	3.62	1.39	1.33
2	R	401	NAD	C5A-C4A	-3.38	1.33	1.39
2	P	401	NAD	PA-O3	3.34	1.63	1.59
2	R	401	NAD	PN-O3	3.32	1.63	1.59
2	P	401	NAD	C5A-C4A	-3.27	1.33	1.39
2	O	401	NAD	PN-O3	3.23	1.63	1.59
3	R	402	G3H	C3-C2	3.12	1.55	1.51
2	R	401	NAD	O2B-C2B	3.06	1.50	1.43
2	R	401	NAD	O3D-C3D	-3.04	1.35	1.43
2	Q	401	NAD	C5A-C4A	-3.04	1.33	1.39
2	P	401	NAD	O7N-C7N	-3.03	1.18	1.24
2	Q	401	NAD	C5A-N7A	-3.03	1.33	1.39
2	O	401	NAD	C5A-C4A	-3.00	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	401	NAD	O7N-C7N	-2.95	1.18	1.24
2	Q	401	NAD	O3D-C3D	-2.92	1.35	1.43
2	Q	401	NAD	O2B-C2B	2.91	1.50	1.43
2	O	401	NAD	O3D-C3D	-2.85	1.35	1.43
2	R	401	NAD	O2D-C2D	2.79	1.49	1.43
2	P	401	NAD	O2B-C2B	2.73	1.49	1.43
2	R	401	NAD	O7N-C7N	-2.72	1.19	1.24
2	R	401	NAD	C5B-C4B	2.69	1.59	1.51
2	O	401	NAD	C2N-N1N	2.68	1.37	1.35
2	P	401	NAD	O2D-C2D	2.67	1.49	1.43
2	R	401	NAD	O3B-C3B	-2.66	1.36	1.43
2	P	401	NAD	O3D-C3D	-2.62	1.36	1.43
2	R	401	NAD	C5A-N7A	-2.48	1.34	1.39
2	P	401	NAD	C2N-N1N	2.46	1.37	1.35
2	Q	401	NAD	O7N-C7N	-2.44	1.19	1.24
2	P	401	NAD	C5B-C4B	2.38	1.58	1.51
2	P	401	NAD	C3N-C7N	2.38	1.54	1.50
3	R	402	G3H	O2-C2	-2.35	1.39	1.43
2	P	401	NAD	O3B-C3B	-2.33	1.37	1.43
3	R	402	G3H	P-O1P	2.31	1.67	1.60
7	P	402	DG4	P2-O7P	-2.28	1.46	1.54
2	Q	401	NAD	C5B-C4B	2.28	1.58	1.51
2	Q	401	NAD	C3N-C7N	2.26	1.54	1.50
2	O	401	NAD	O2B-C2B	2.26	1.48	1.43
2	O	401	NAD	C5B-C4B	2.25	1.58	1.51
3	O	402	G3H	P-O1P	2.24	1.67	1.60
2	O	401	NAD	C3N-C7N	2.18	1.53	1.50
2	Q	401	NAD	C2N-N1N	2.17	1.37	1.35
2	O	401	NAD	C5A-N7A	-2.13	1.35	1.39
2	P	401	NAD	C5N-C4N	-2.10	1.35	1.38
2	O	401	NAD	O2D-C2D	2.04	1.48	1.43
7	P	402	DG4	P2-O5P	2.02	1.66	1.60
2	P	401	NAD	PA-O5B	2.01	1.67	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	401	NAD	O7N-C7N-C3N	7.32	128.55	119.60
2	R	401	NAD	N3A-C2A-N1A	-5.49	120.28	128.58
2	P	401	NAD	N3A-C2A-N1A	-5.35	120.49	128.58
2	O	401	NAD	N3A-C2A-N1A	-5.28	120.59	128.58
2	Q	401	NAD	N3A-C2A-N1A	-5.13	120.82	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	401	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	O	401	NAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	R	401	NAD	C5A-C4A-N3A	-4.71	120.24	126.72
2	P	401	NAD	C5A-C4A-N3A	-4.53	120.47	126.72
7	P	402	DG4	O3P-P1-O1P	4.51	118.47	105.32
2	R	401	NAD	C4D-O4D-C1D	-4.14	106.13	109.92
2	Q	401	NAD	O7N-C7N-N7N	-4.04	116.78	122.62
2	P	401	NAD	C6N-N1N-C2N	-4.01	118.47	121.88
2	P	401	NAD	O4B-C1B-N9A	-3.98	100.44	108.09
2	R	401	NAD	N9A-C8A-N7A	-3.91	108.38	113.94
2	O	401	NAD	N9A-C8A-N7A	-3.90	108.41	113.94
2	P	401	NAD	N9A-C8A-N7A	-3.87	108.44	113.94
2	O	401	NAD	N6A-C6A-N1A	-3.87	109.77	118.38
7	P	402	DG4	O5P-C3-C2	3.85	118.80	107.96
2	Q	401	NAD	N9A-C8A-N7A	-3.68	108.71	113.94
7	P	402	DG4	O7P-P2-O5P	3.53	115.87	106.67
2	O	401	NAD	C6N-N1N-C2N	-3.39	118.99	121.88
2	P	401	NAD	C2A-N3A-C4A	3.32	119.94	111.83
2	R	401	NAD	C2A-N3A-C4A	3.26	119.79	111.83
2	R	401	NAD	C6N-N1N-C2N	-3.24	119.12	121.88
2	P	401	NAD	O7N-C7N-N7N	-3.23	117.94	122.62
2	Q	401	NAD	C2A-N3A-C4A	3.19	119.63	111.83
2	O	401	NAD	C2A-N3A-C4A	3.13	119.48	111.83
2	R	401	NAD	N3A-C4A-N9A	2.99	132.25	127.17
2	P	401	NAD	N3A-C4A-N9A	2.96	132.20	127.17
2	Q	401	NAD	N6A-C6A-N1A	-2.96	111.79	118.38
7	P	402	DG4	O2-C2-C1	-2.91	101.88	109.45
2	R	401	NAD	N6A-C6A-N1A	-2.76	112.22	118.38
3	O	402	G3H	O1P-P-O2P	2.75	113.87	106.44
2	O	401	NAD	N3A-C4A-N9A	2.73	131.81	127.17
2	P	401	NAD	N6A-C6A-N1A	-2.73	112.29	118.38
3	Q	402	G3H	O4P-P-O1P	2.72	113.77	106.67
2	Q	401	NAD	C5A-N7A-C8A	2.70	107.70	103.45
2	Q	401	NAD	C4D-O4D-C1D	-2.69	107.46	109.92
2	P	401	NAD	O3-PA-O1A	-2.68	102.64	110.70
2	Q	401	NAD	N3A-C4A-N9A	2.64	131.66	127.17
2	Q	401	NAD	C6N-N1N-C2N	-2.63	119.64	121.88
2	Q	401	NAD	C3N-C7N-N7N	-2.61	114.52	117.74
2	O	401	NAD	C5A-N7A-C8A	2.61	107.55	103.45
2	R	401	NAD	C3N-C7N-N7N	2.53	120.86	117.74
2	O	401	NAD	O2N-PN-O3	2.50	114.03	107.27
2	Q	401	NAD	C5A-C4A-N9A	2.41	108.43	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	401	NAD	O7N-C7N-N7N	-2.39	119.16	122.62
2	R	401	NAD	O3-PA-O1A	-2.38	103.56	110.70
2	P	401	NAD	C2B-C1B-N9A	2.35	119.14	113.30
2	R	401	NAD	C5A-N7A-C8A	2.34	107.13	103.45
2	O	401	NAD	C5A-C6A-N6A	2.34	129.07	123.29
2	P	401	NAD	C4A-N9A-C8A	2.33	108.19	105.74
2	R	401	NAD	O2N-PN-O3	2.27	113.42	107.27
2	R	401	NAD	C2N-C3N-C4N	2.25	120.87	118.26
2	P	401	NAD	O7N-C7N-C3N	2.23	122.33	119.60
2	O	401	NAD	C4D-O4D-C1D	-2.22	107.89	109.92
2	P	401	NAD	O2A-PA-O3	2.14	113.05	107.27
2	Q	401	NAD	C6A-C5A-C4A	2.13	120.09	117.18
3	R	402	G3H	O3P-P-O2P	-2.12	102.59	110.83
2	R	401	NAD	O2A-PA-O3	2.08	112.89	107.27
2	Q	401	NAD	O4B-C1B-N9A	-2.07	104.12	108.09
2	Q	401	NAD	C4A-C5A-N7A	-2.06	108.23	110.58
2	O	401	NAD	C5A-C4A-N9A	2.04	108.03	105.81
2	R	401	NAD	C2N-N1N-C1D	2.04	123.63	119.13
2	P	401	NAD	C2N-N1N-C1D	2.02	123.59	119.13

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N
2	O	401	NAD	C2D-C1D-N1N-C2N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	P	401	NAD	O4D-C1D-N1N-C2N
2	P	401	NAD	O4D-C1D-N1N-C6N
2	P	401	NAD	C2D-C1D-N1N-C2N
2	P	401	NAD	C2D-C1D-N1N-C6N
2	Q	401	NAD	O4D-C1D-N1N-C2N
2	Q	401	NAD	O4D-C1D-N1N-C6N
2	Q	401	NAD	C2D-C1D-N1N-C2N
2	Q	401	NAD	C2D-C1D-N1N-C6N
2	R	401	NAD	O4D-C1D-N1N-C2N
2	R	401	NAD	O4D-C1D-N1N-C6N
2	R	401	NAD	C2D-C1D-N1N-C2N
2	R	401	NAD	C2D-C1D-N1N-C6N
3	O	402	G3H	C3-O1P-P-O3P
3	O	402	G3H	C3-O1P-P-O4P

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	Q	402	G3H	O1-C1-C2-C3
3	Q	402	G3H	C3-O1P-P-O3P
3	R	402	G3H	O1-C1-C2-C3
3	R	402	G3H	C1-C2-C3-O1P
3	R	402	G3H	O2-C2-C3-O1P
7	P	402	DG4	C1-C2-C3-O5P
7	P	402	DG4	O2-C2-C3-O5P
7	P	402	DG4	C2-C3-O5P-P2
7	P	402	DG4	C3-O5P-P2-O8P
7	P	402	DG4	C3-O5P-P2-O7P
5	O	405	EDO	O1-C1-C2-O2
3	O	402	G3H	C3-O1P-P-O2P
3	Q	402	G3H	C3-O1P-P-O2P
3	O	402	G3H	C2-C3-O1P-P
3	Q	402	G3H	C3-O1P-P-O4P
7	P	402	DG4	C1-O1P-P1-O2P
7	P	402	DG4	O1-C1-C2-O2
3	Q	402	G3H	C2-C3-O1P-P
2	Q	401	NAD	C2B-C1B-N9A-C8A
5	Q	405[A]	EDO	O1-C1-C2-O2
2	O	401	NAD	O4B-C4B-C5B-O5B
7	P	402	DG4	C3-O5P-P2-O6P
3	O	402	G3H	C1-C2-C3-O1P

There are no ring outliers.

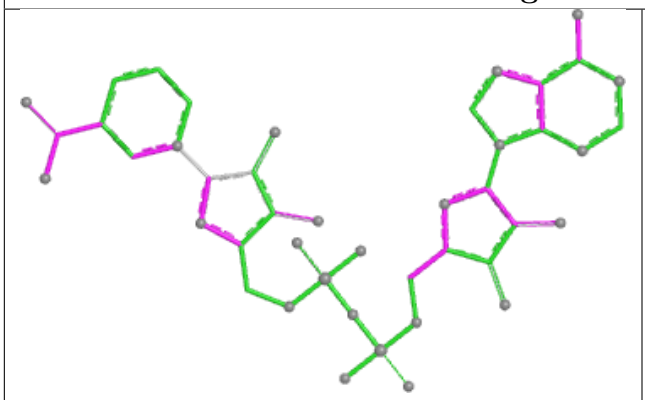
10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	NAD	2	0
2	R	401	NAD	2	0
3	R	402	G3H	4	0
4	P	403	PO4	1	0
3	O	402	G3H	2	0
5	R	405	EDO	1	0
7	P	402	DG4	3	0
3	Q	402	G3H	5	0
4	R	403	PO4	1	0
2	O	401	NAD	1	0

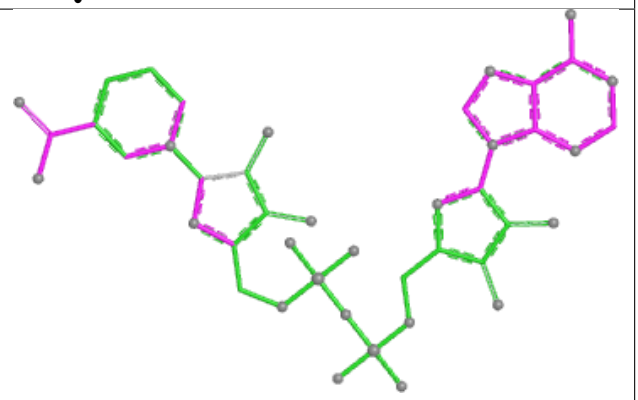
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

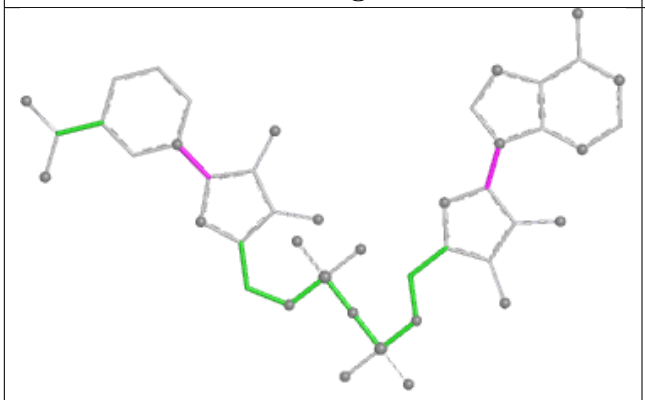
Ligand NAD Q 401



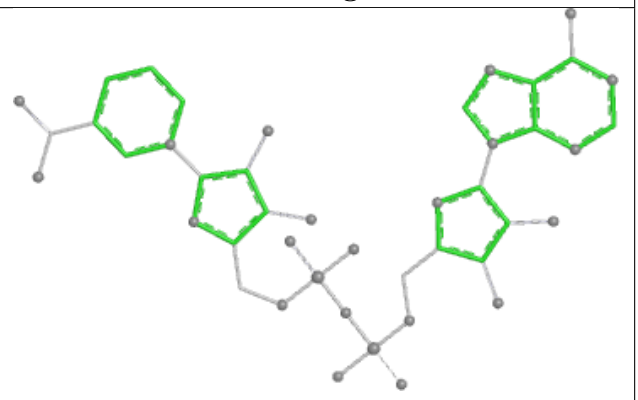
Bond lengths



Bond angles

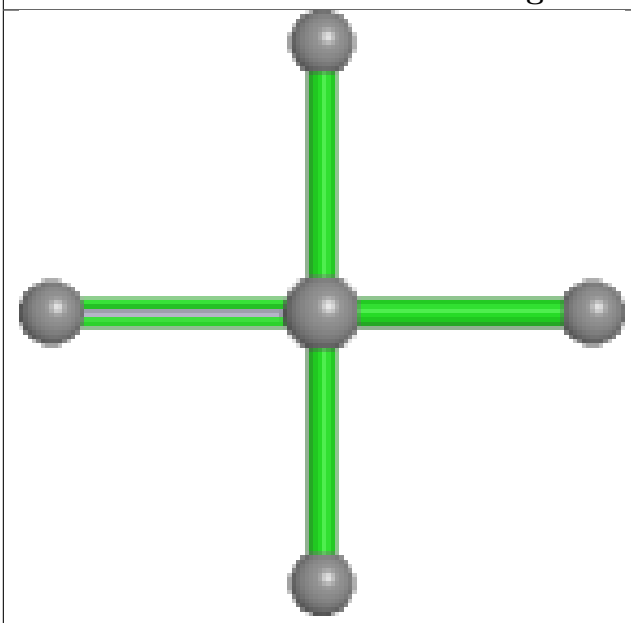


Torsions

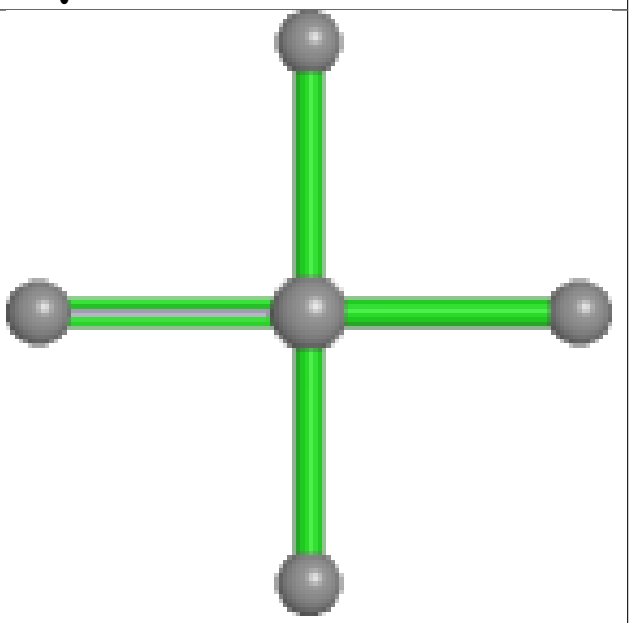


Rings

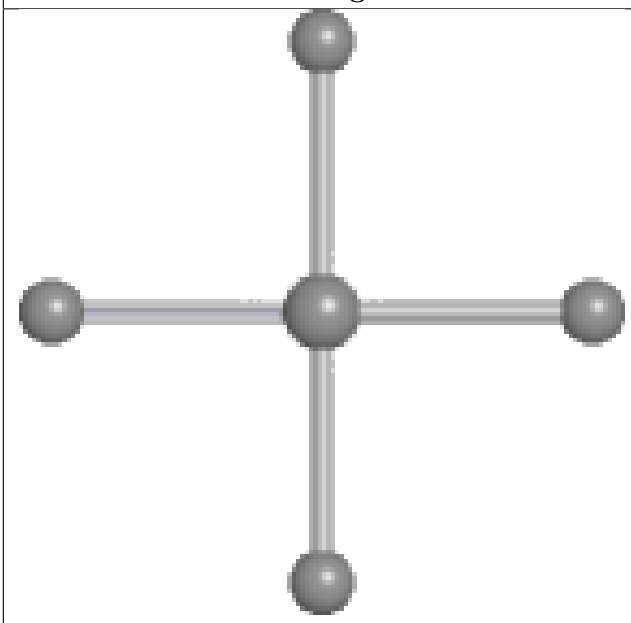
Ligand PO4 Q 403



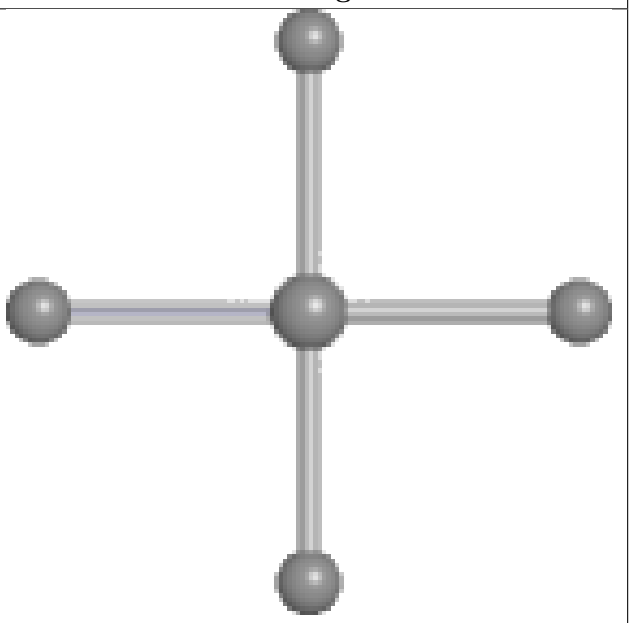
Bond lengths



Bond angles

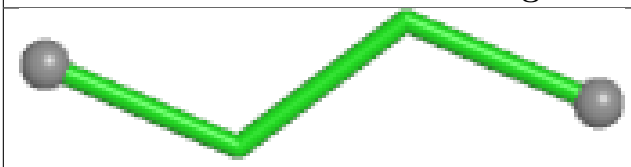


Torsions

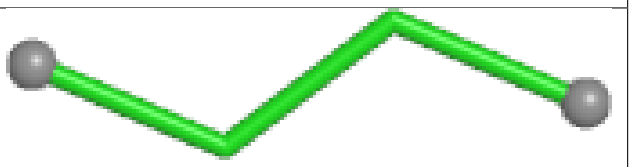


Rings

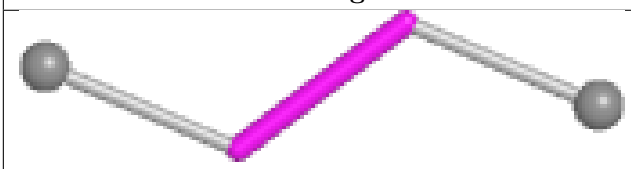
Ligand EDO O 405



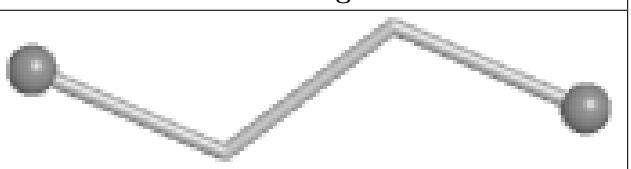
Bond lengths



Bond angles

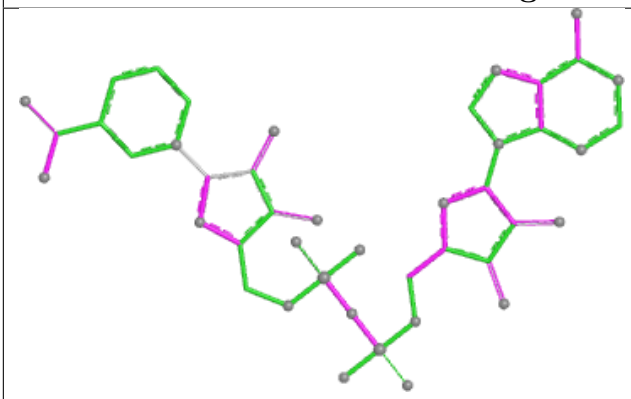


Torsions

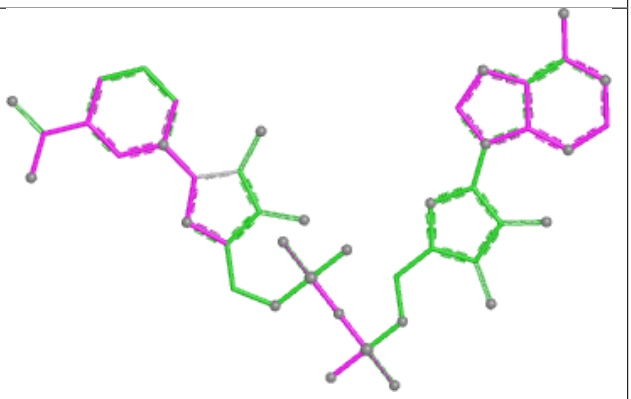


Rings

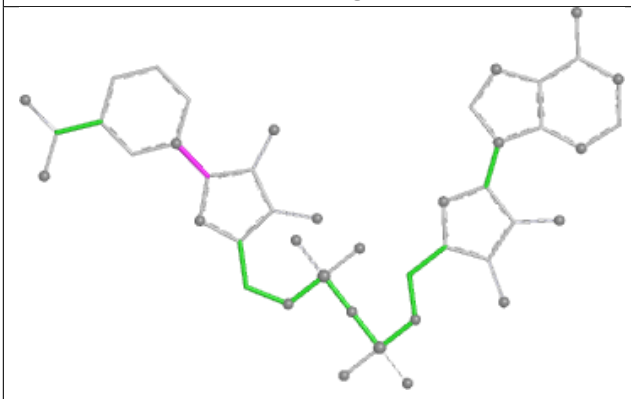
Ligand NAD R 401



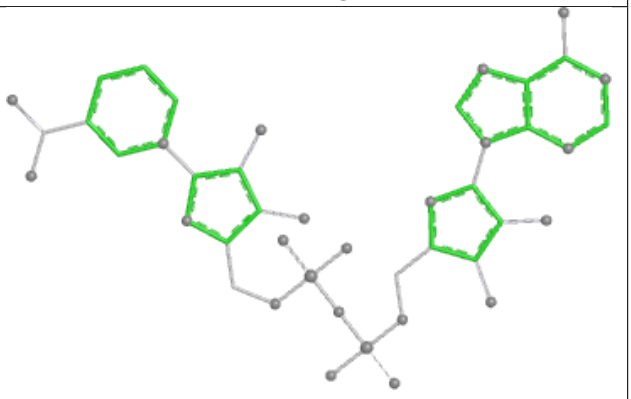
Bond lengths



Bond angles

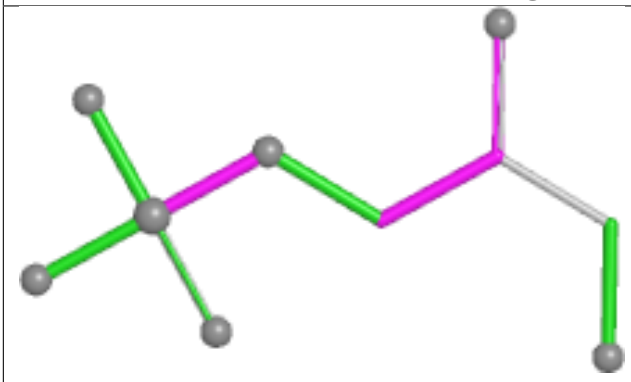


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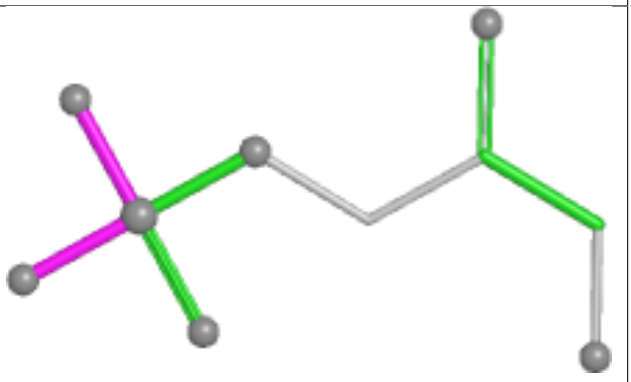


Rings

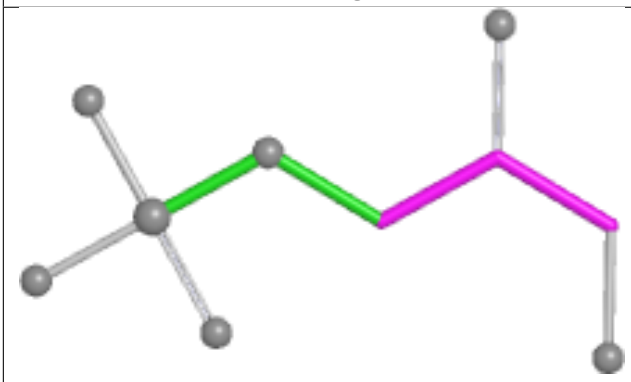
Ligand G3H R 402



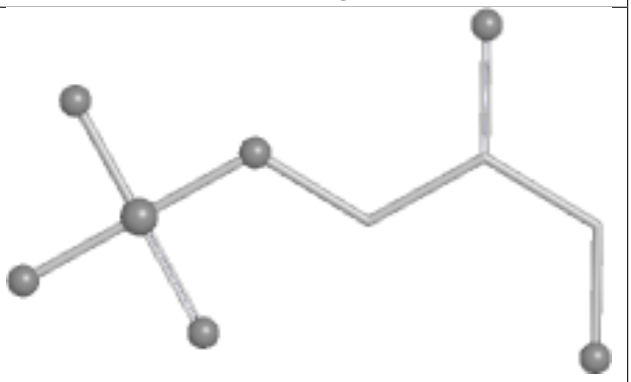
Bond lengths



Bond angles

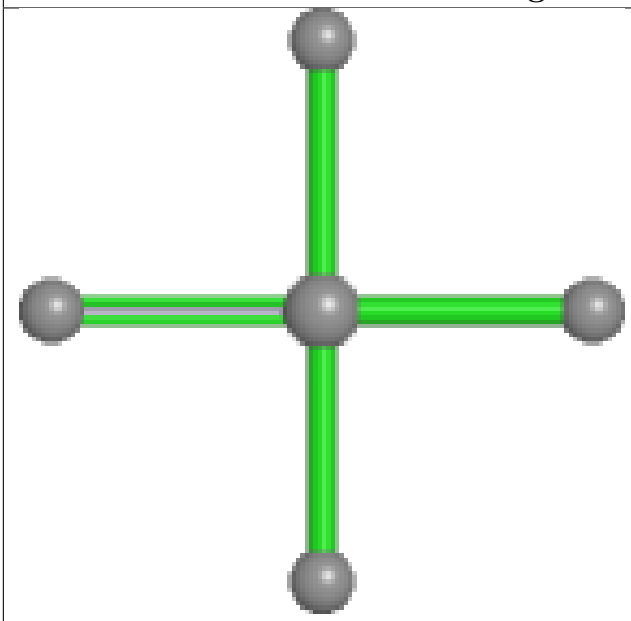


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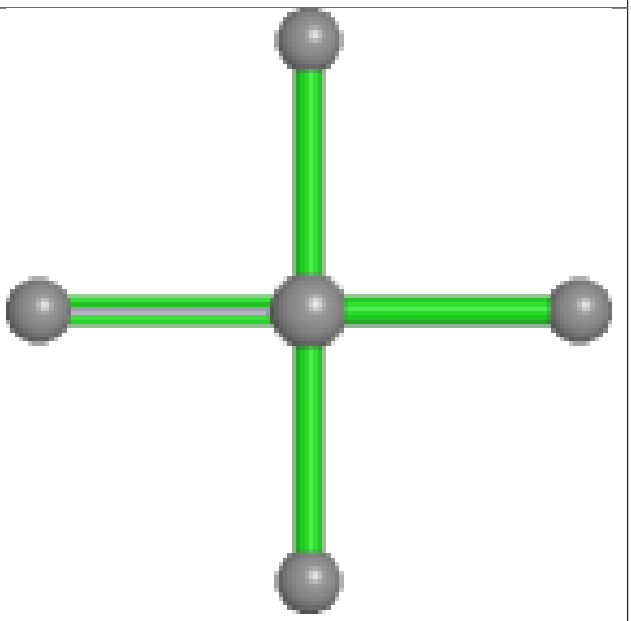


Rings

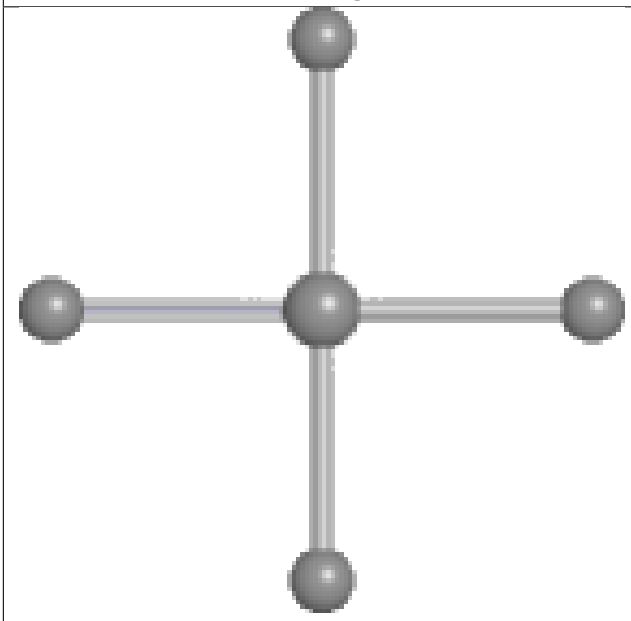
Ligand PO4 P 403



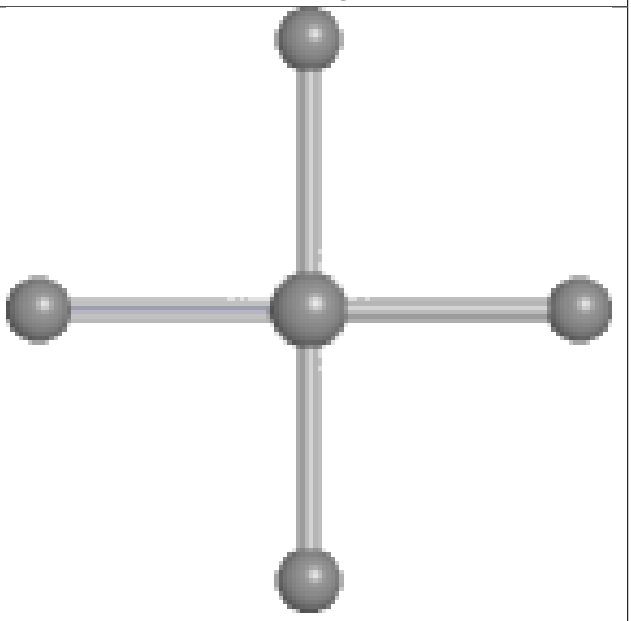
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Bond angles

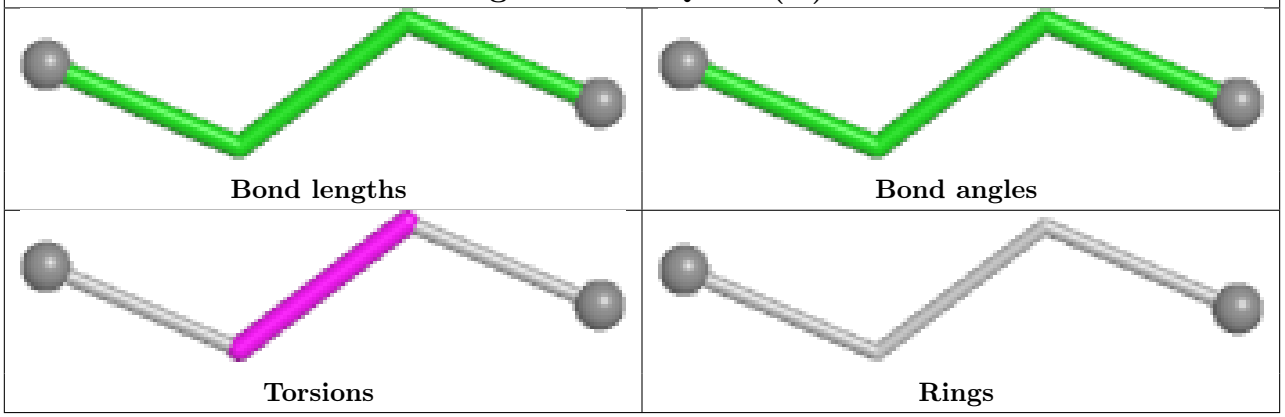


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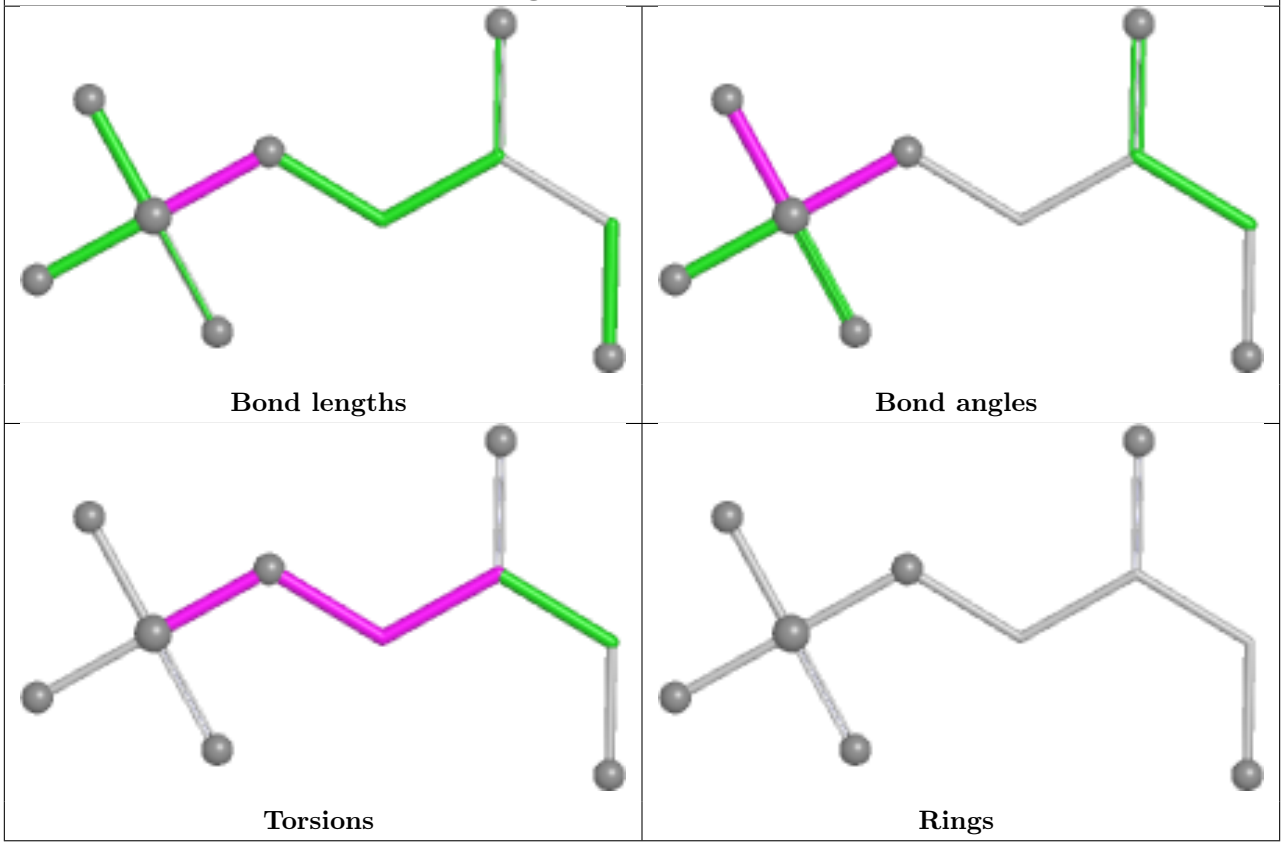


Rings

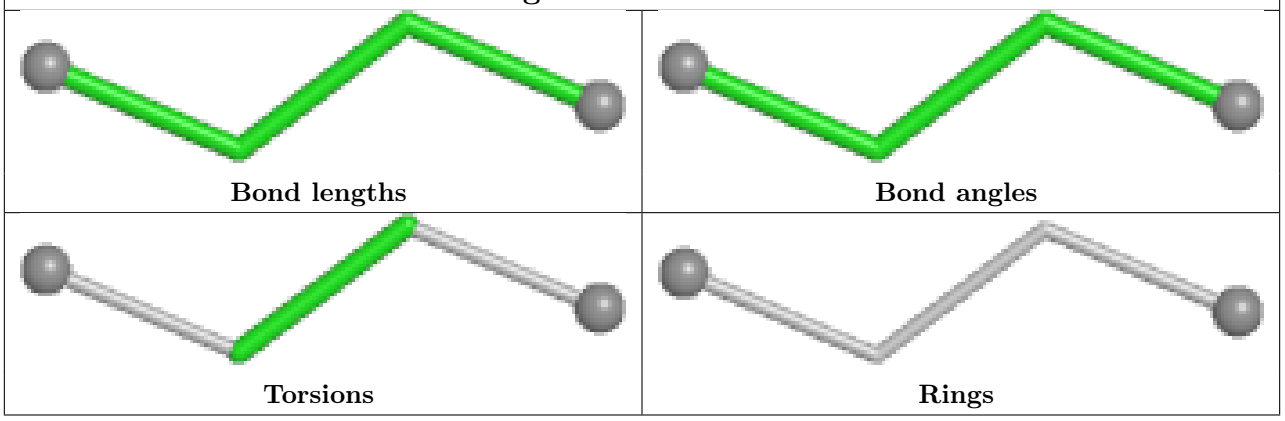
Ligand EDO Q 405 (A)



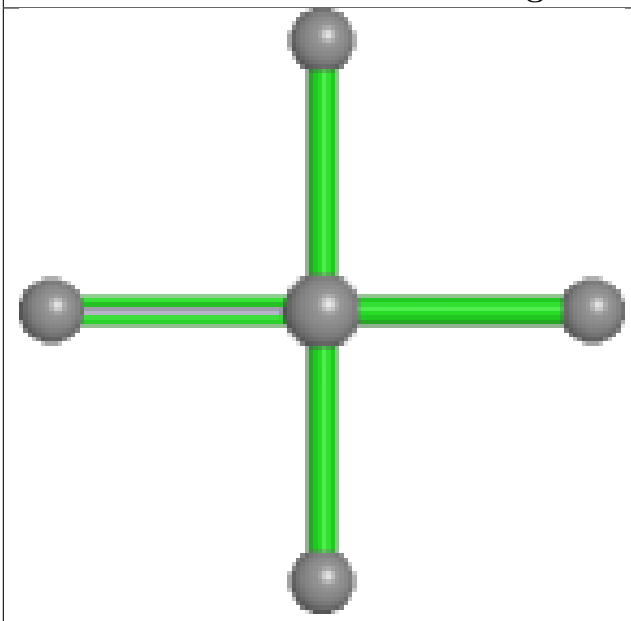
Ligand G3H O 402



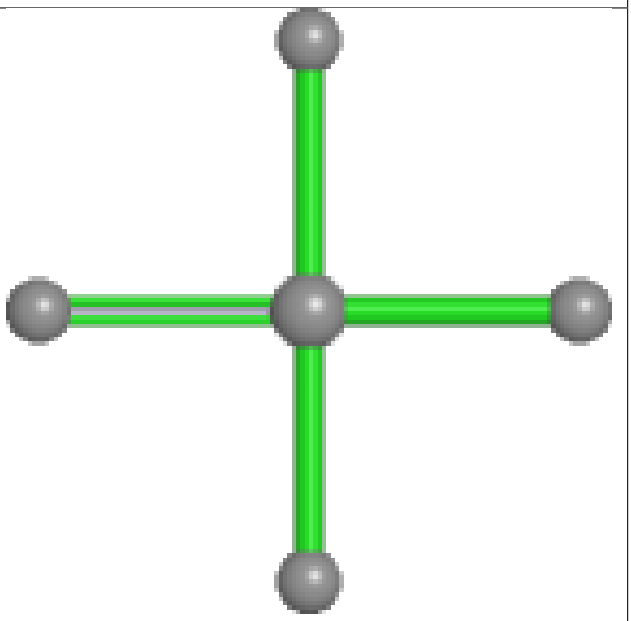
Ligand EDO R 405



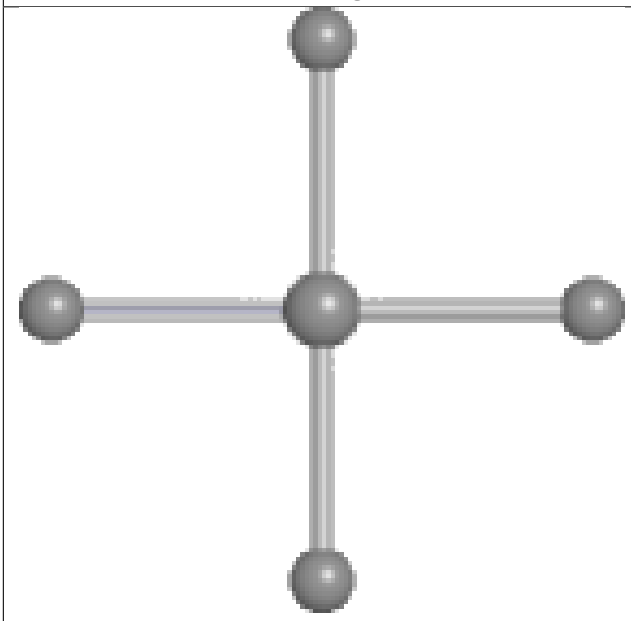
Ligand PO4 R 404



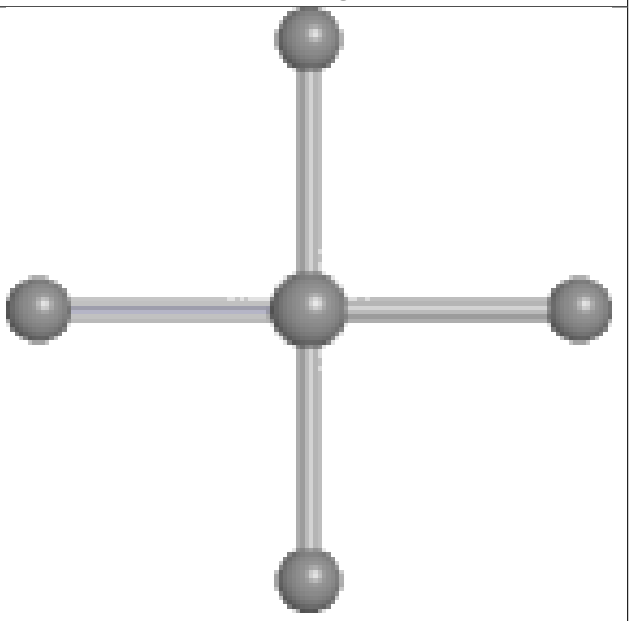
Bond lengths



Bond angles

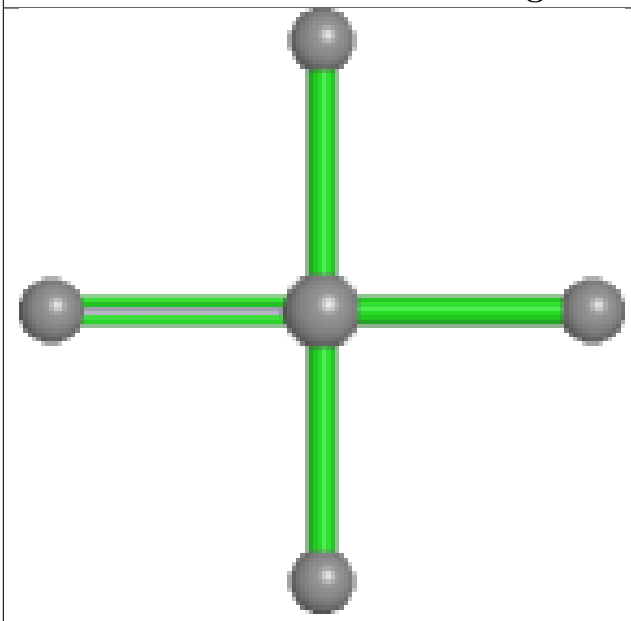


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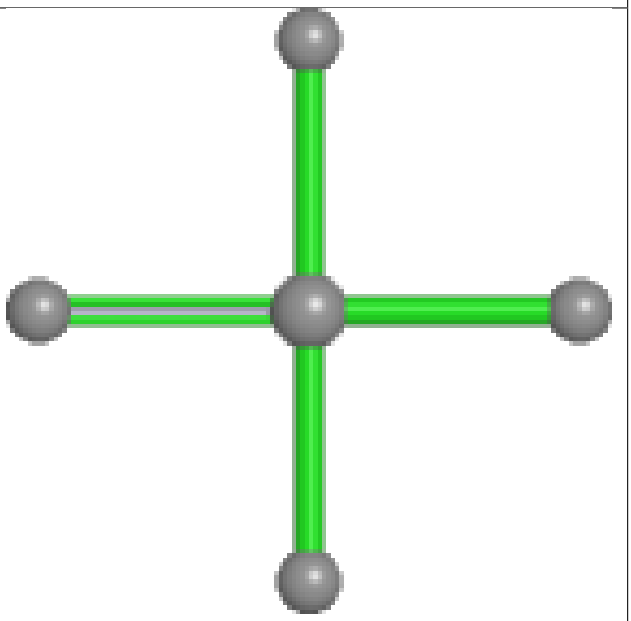


Rings

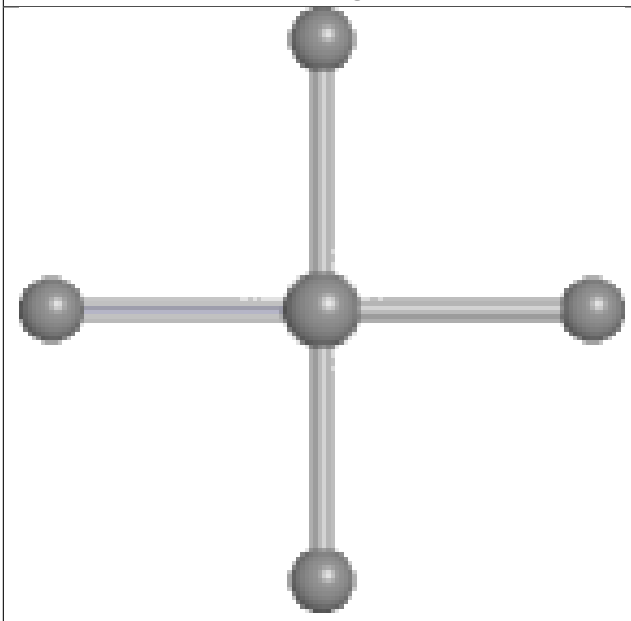
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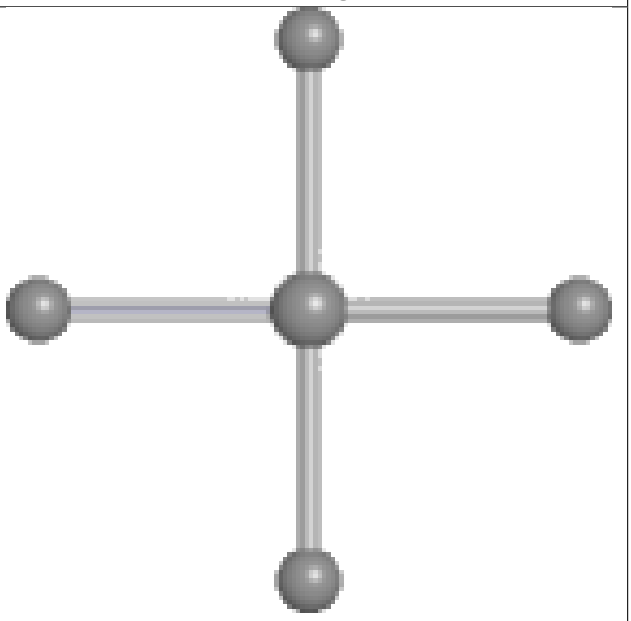
Bond lengths



Bond angles

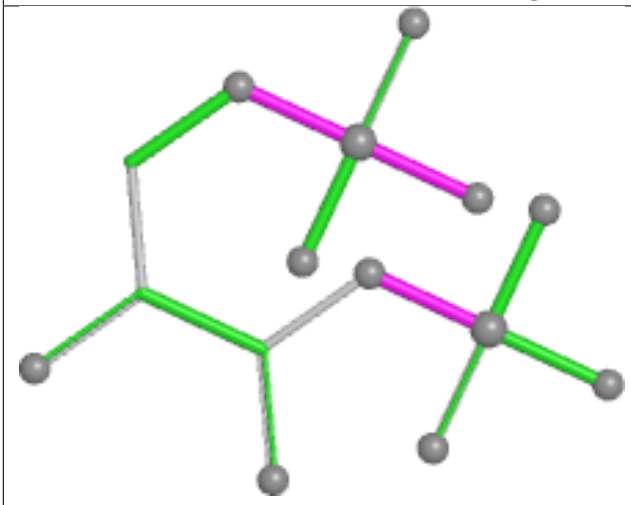


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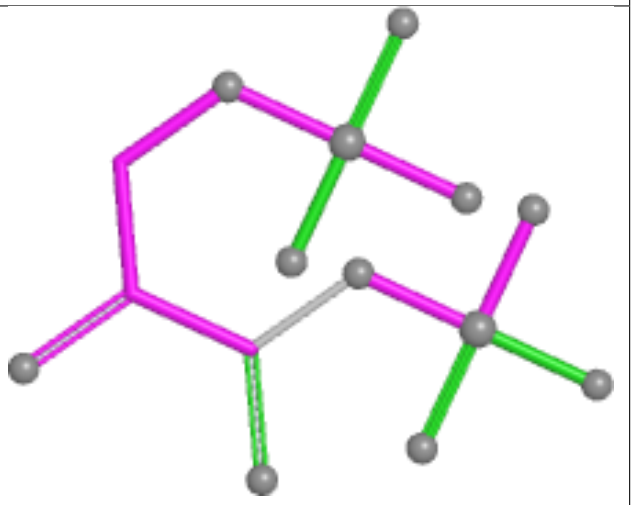


Rings

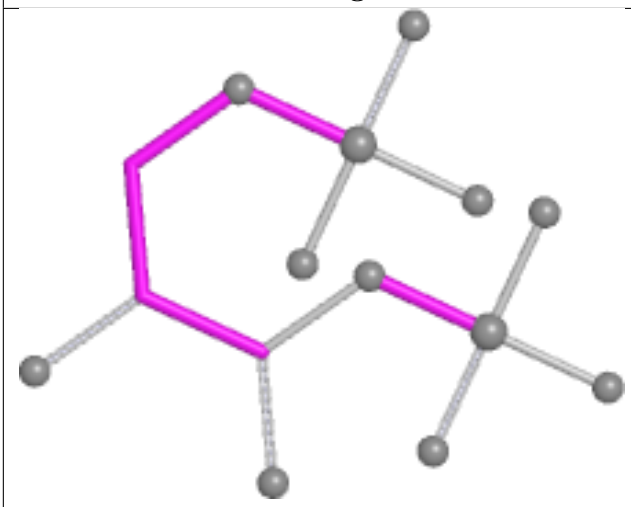
Ligand DG4 P 402



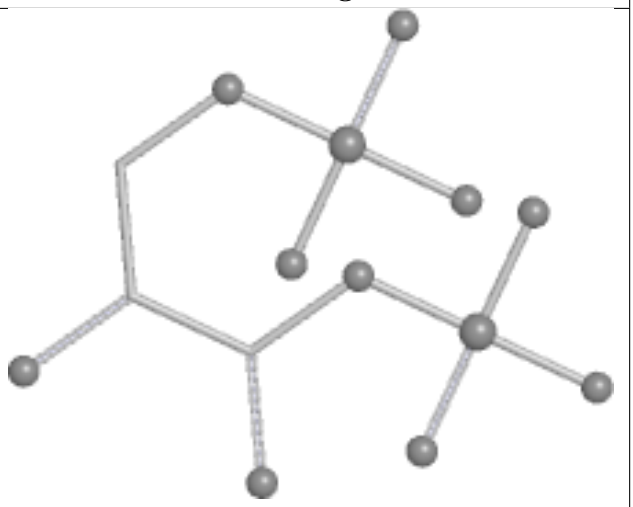
Bond lengths



Bond angles

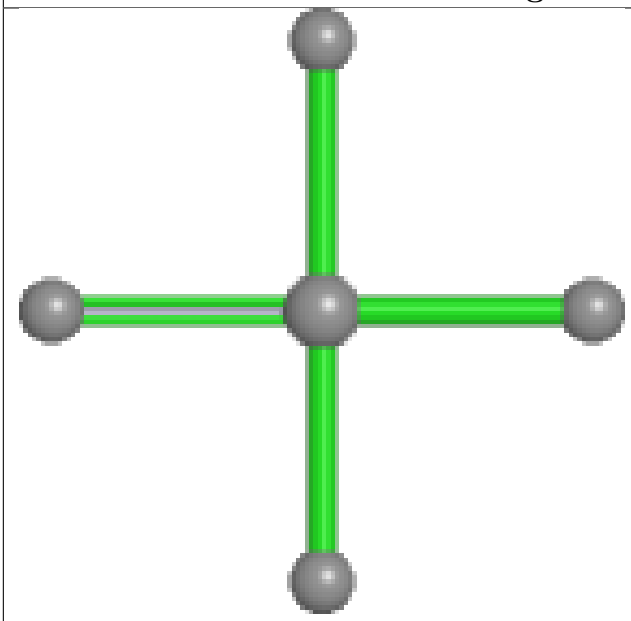


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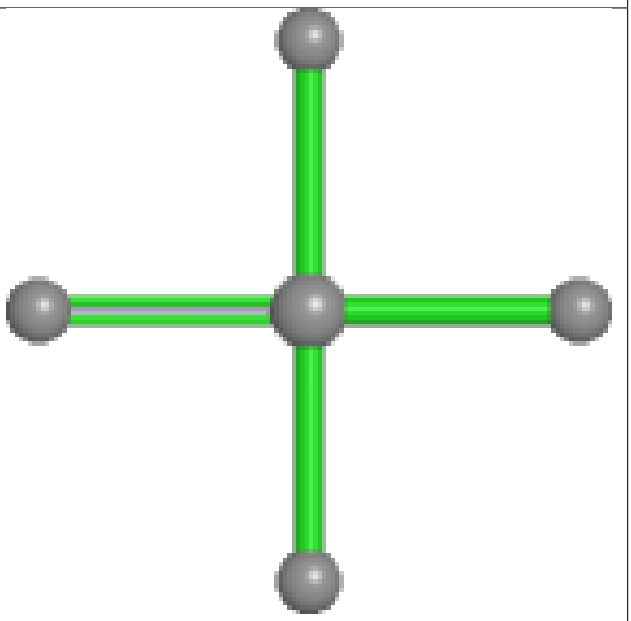


Rings

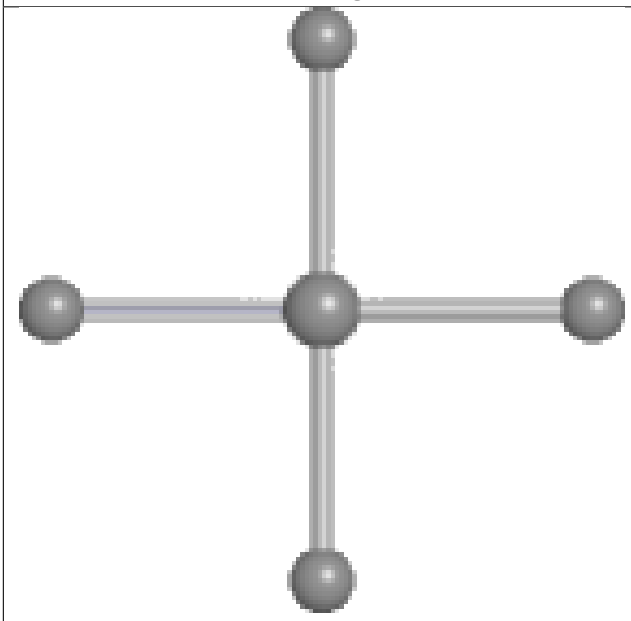
Ligand PO4 O 404



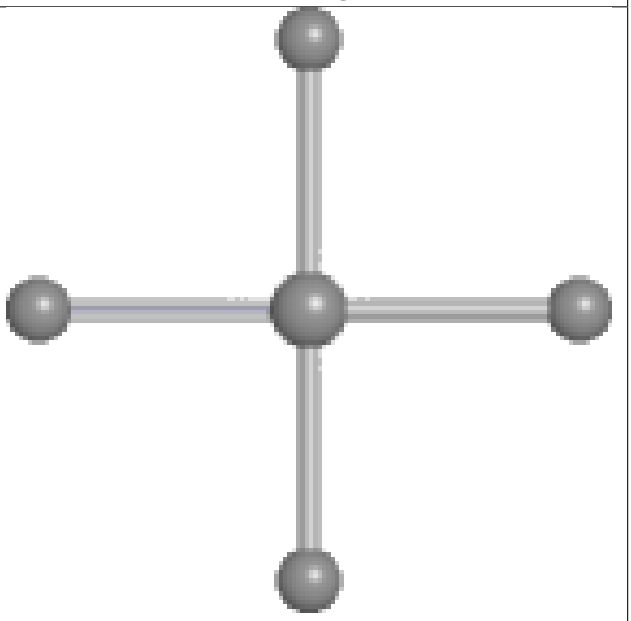
Bond lengths



Bond angles

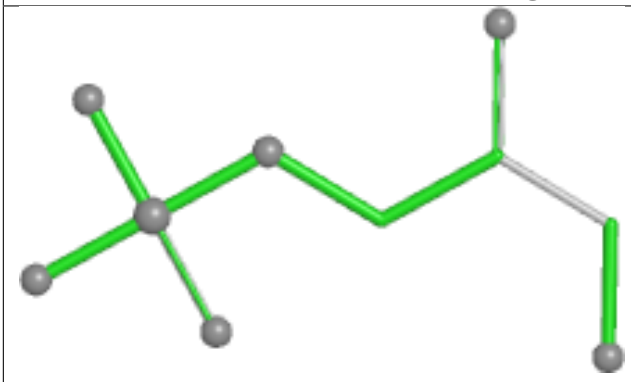


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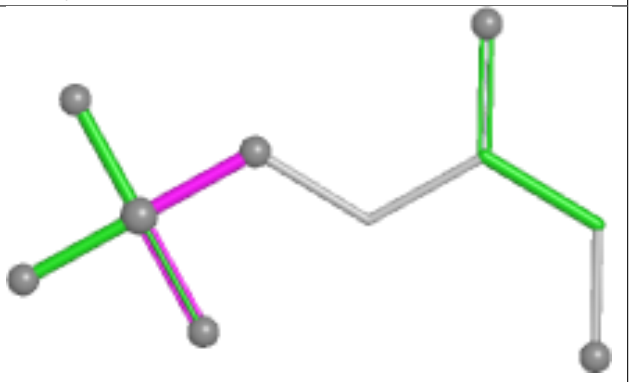


Rings

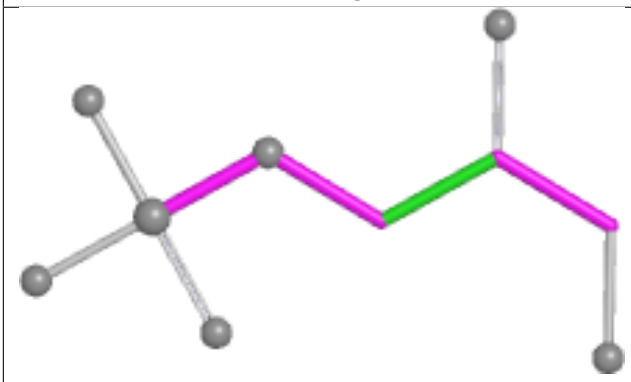
Ligand G3H Q 402



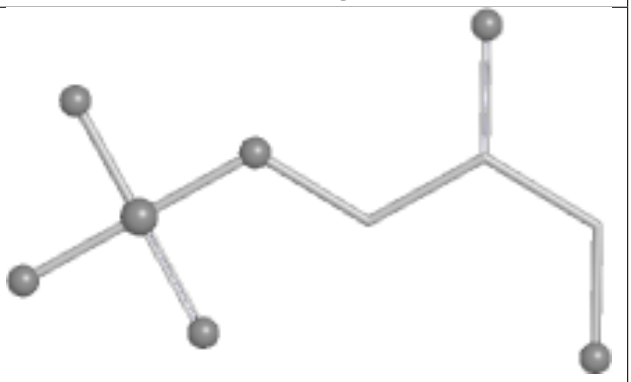
Bond lengths



Bond angles

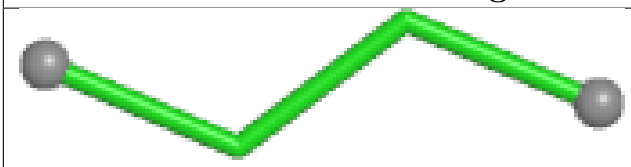


Torsions

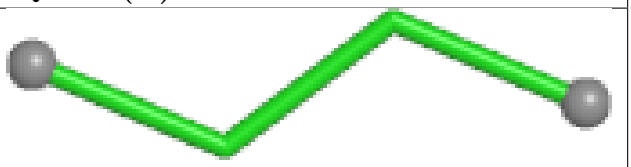


Rings

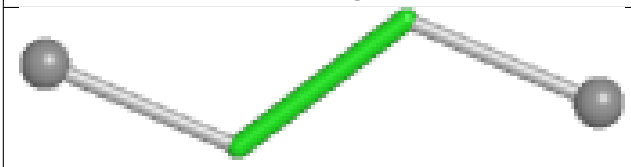
Ligand EDO Q 405 (B)



Bond lengths



Bond angles

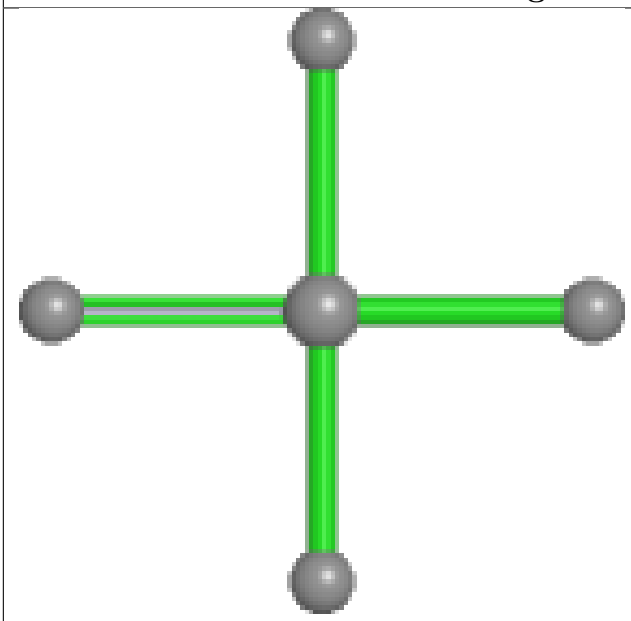


Torsions

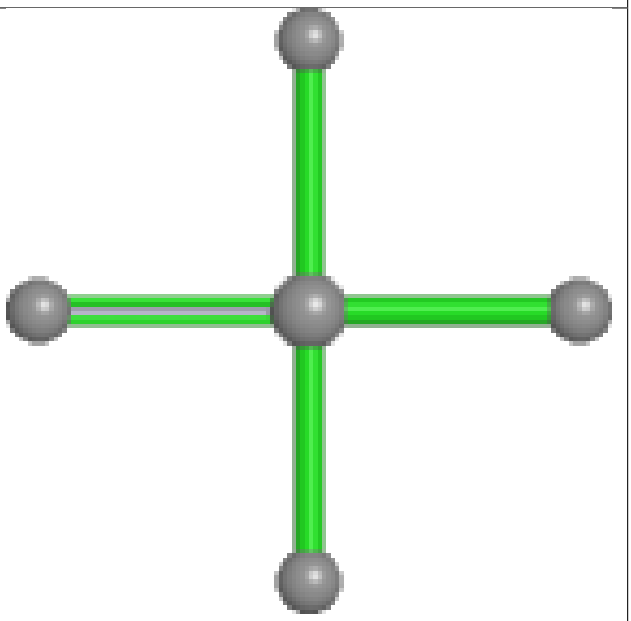


Rings

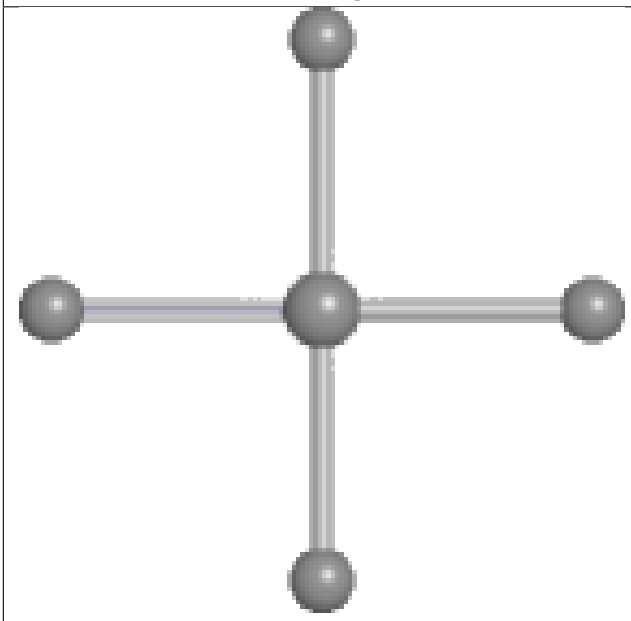
Ligand PO4 P 404



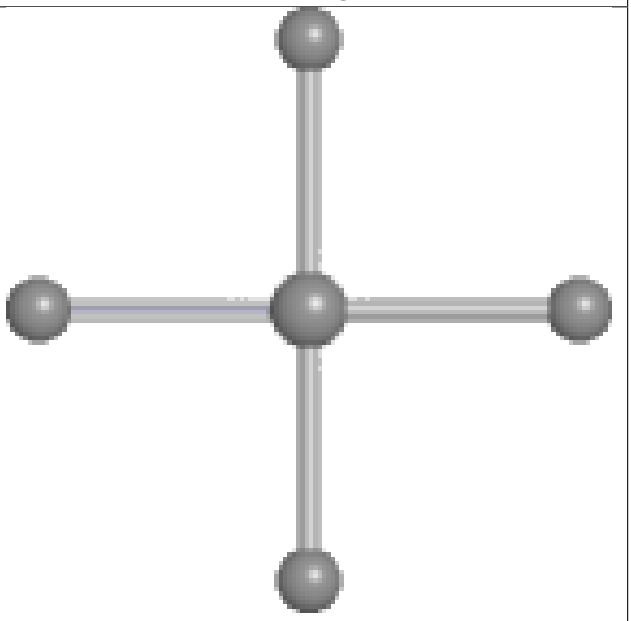
Bond lengths



Bond angles

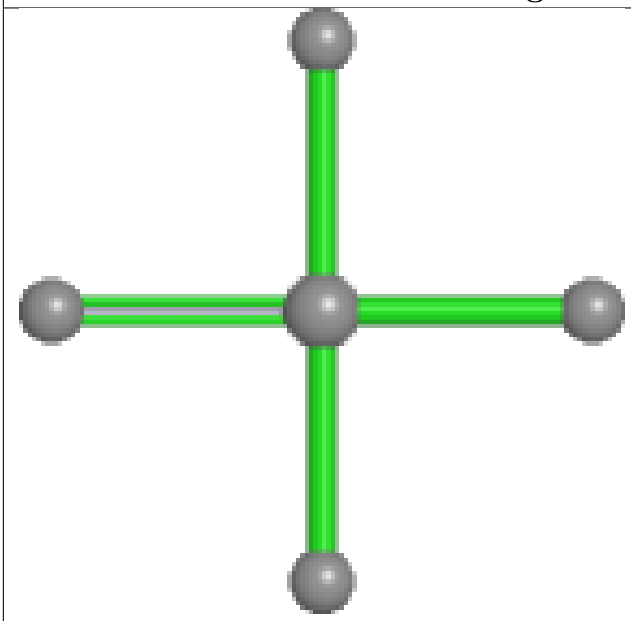


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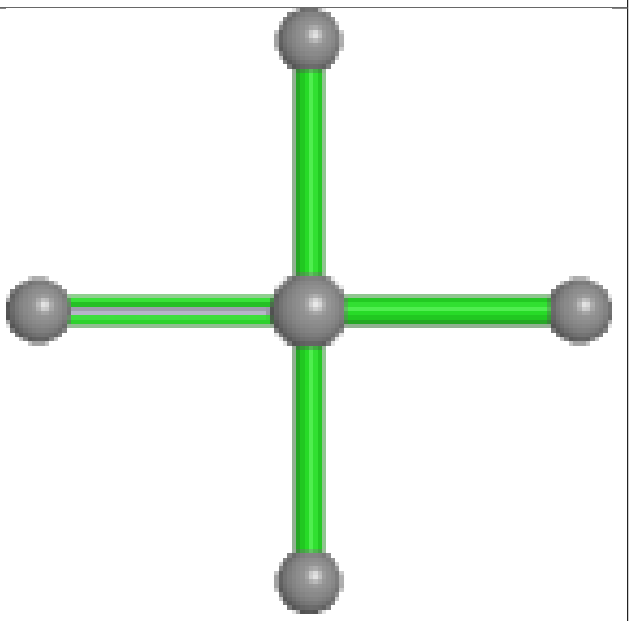


Rings

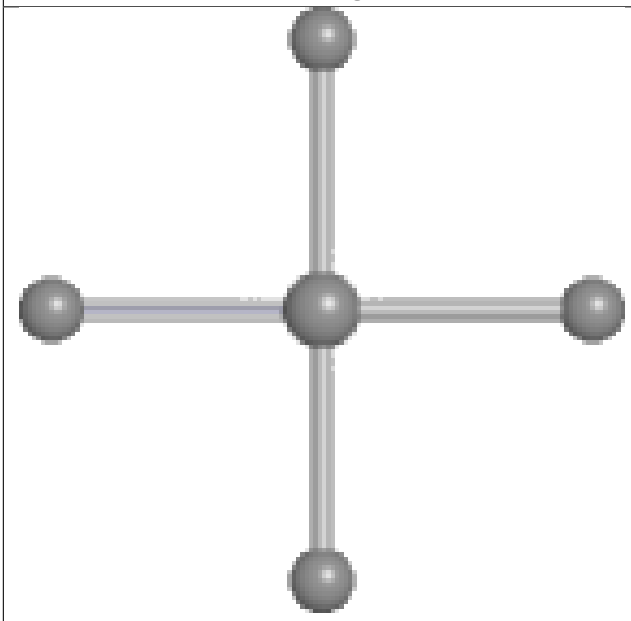
Ligand PO4 R 403



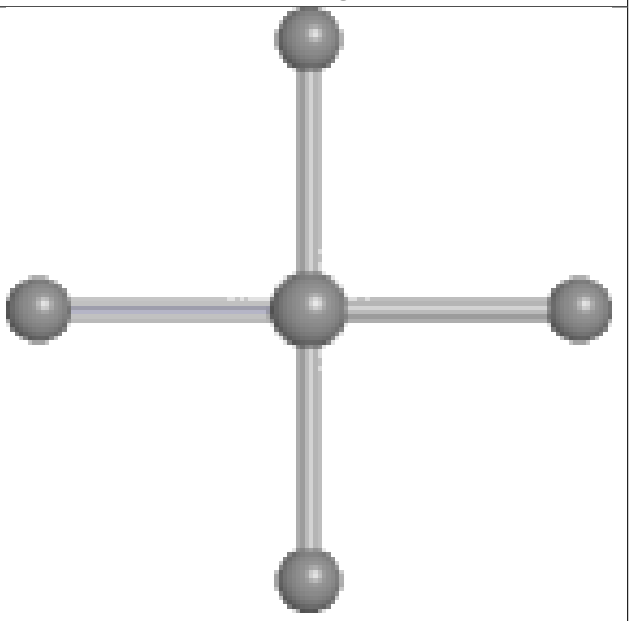
Bond lengths



Bond angles

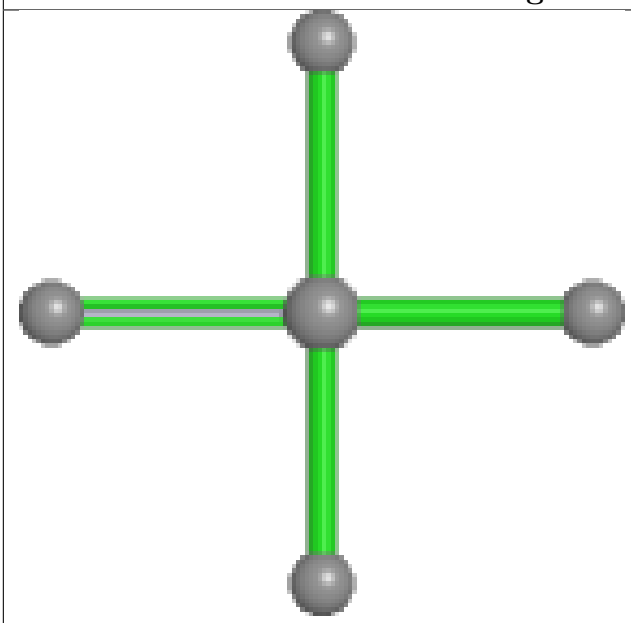


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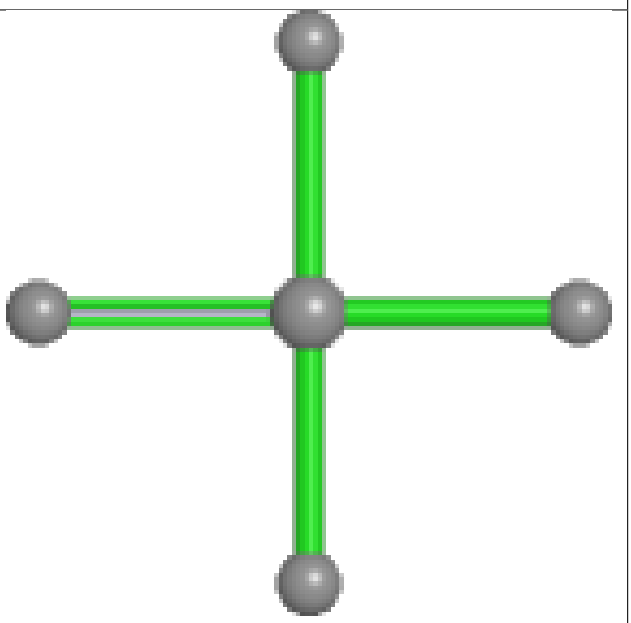


Rings

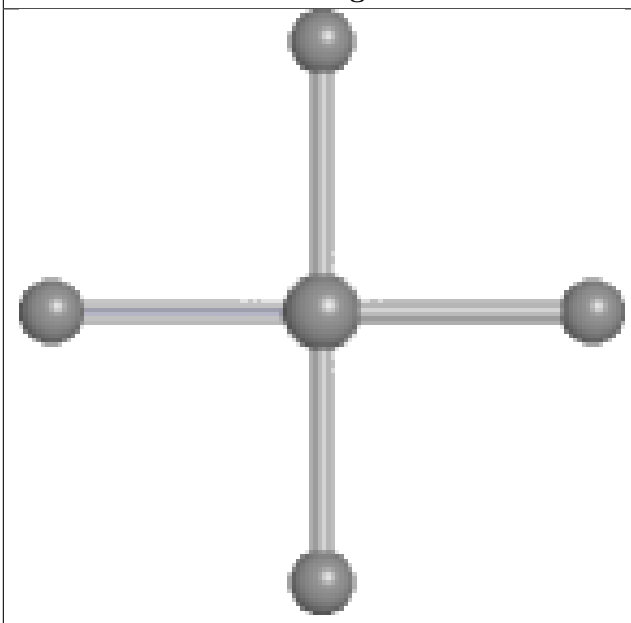
Ligand PO4 O 408



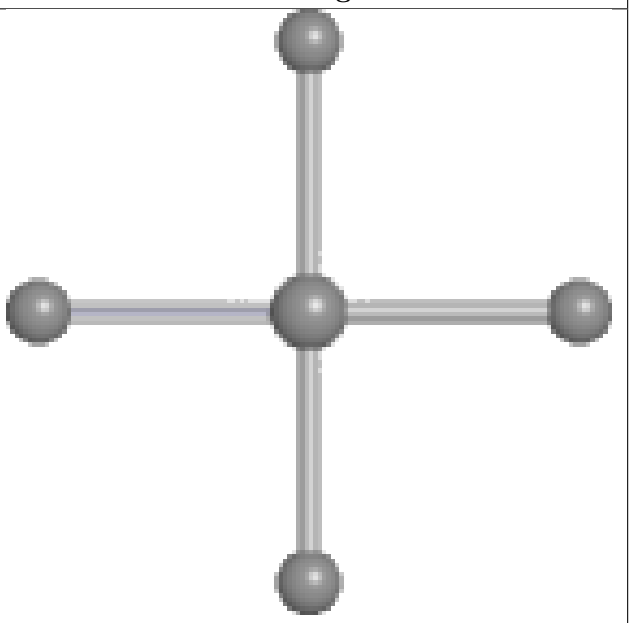
Bond lengths



Bond angles

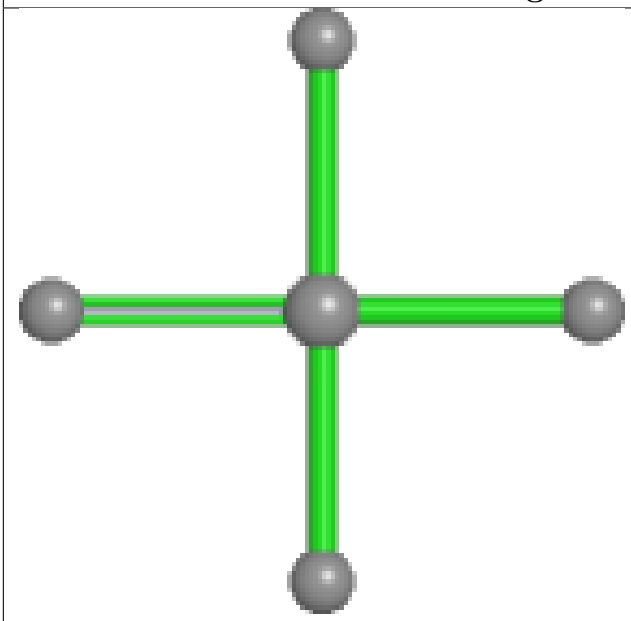


Torsions

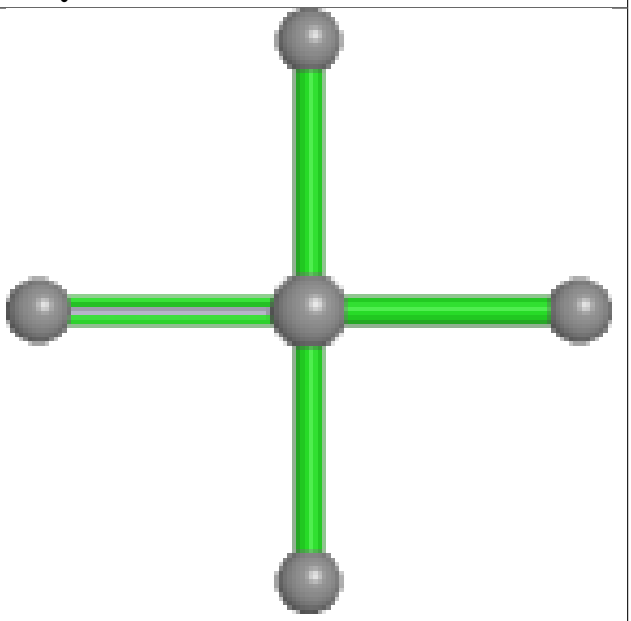


Rings

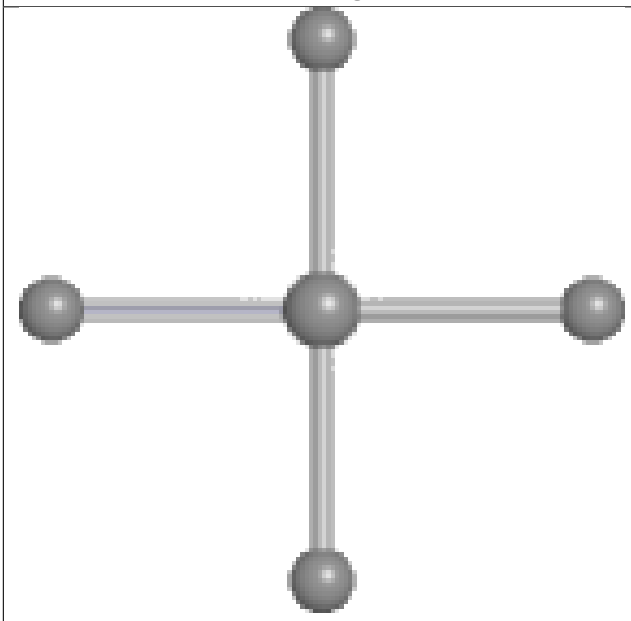
Ligand PO4 Q 404



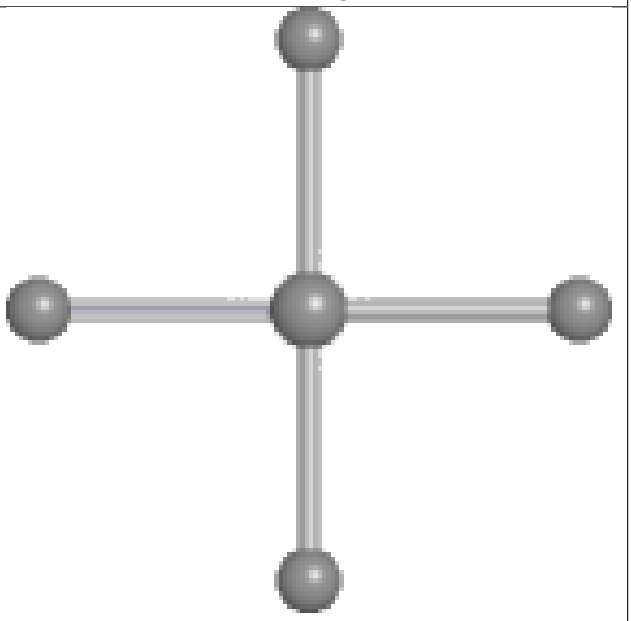
Bond lengths



Bond angles

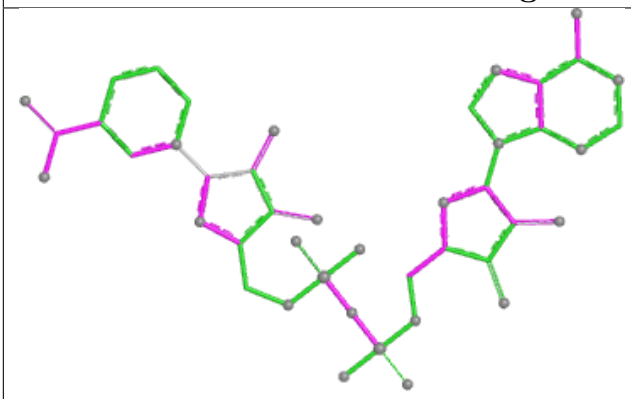


Torsions

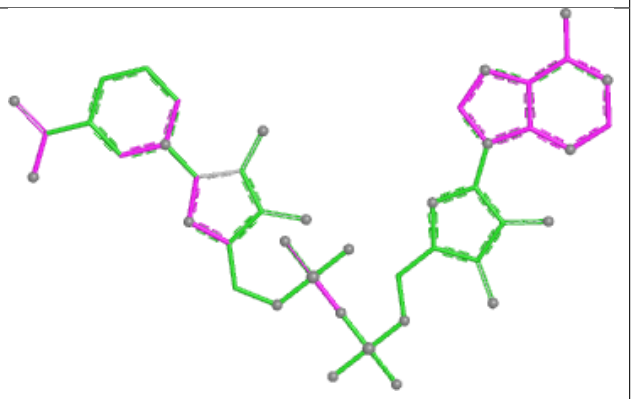


Rings

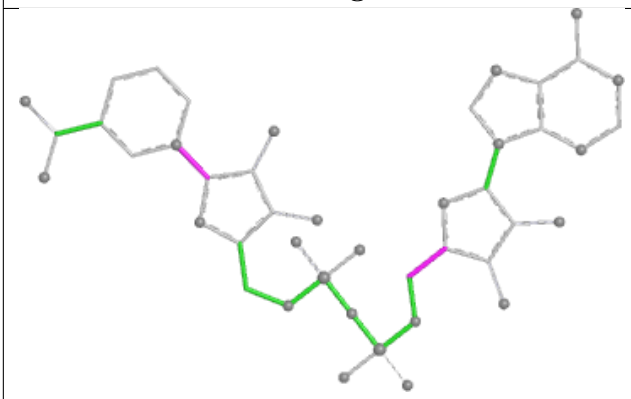
Ligand NAD O 401



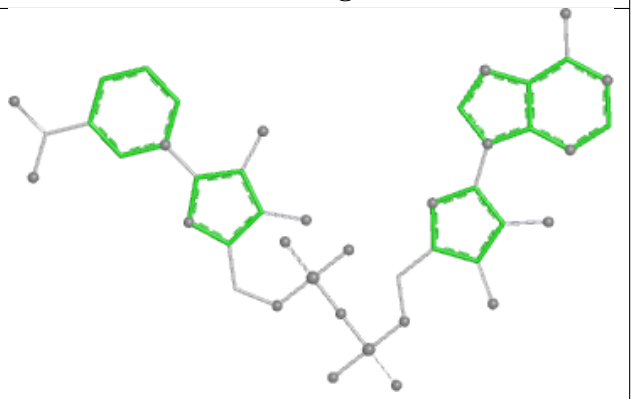
Bond lengths



Bond angles

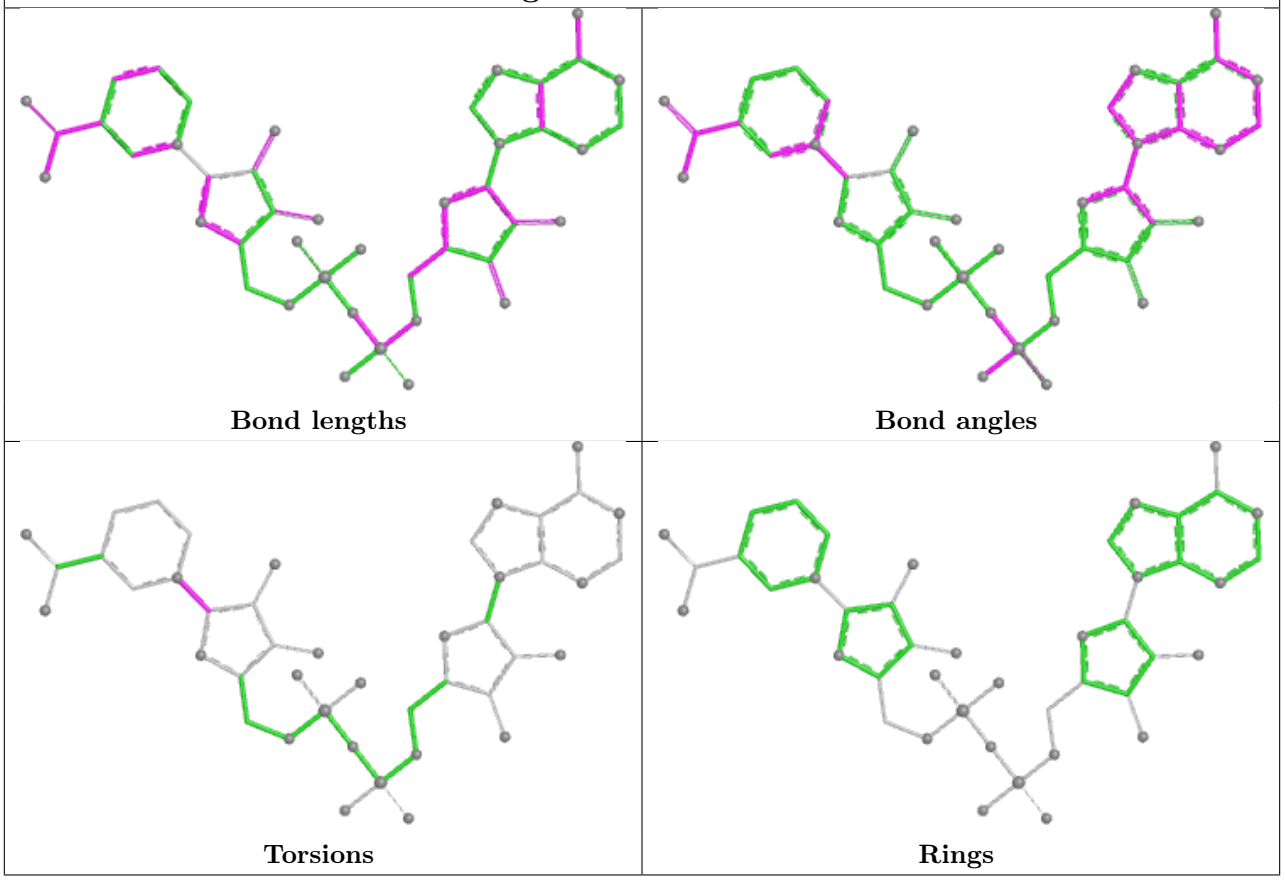


Torsions



Rings

Ligand NAD P 401



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	O	334/352 (94%)	-0.96	0 100 100	9, 21, 37, 63	7 (2%)
1	P	333/352 (94%)	-0.90	1 (0%) 90 92	11, 22, 44, 68	4 (1%)
1	Q	333/352 (94%)	-0.84	1 (0%) 90 92	13, 23, 45, 78	1 (0%)
1	R	333/352 (94%)	-0.53	0 100 100	15, 28, 55, 76	0
All	All	1333/1408 (94%)	-0.81	2 (0%) 91 93	9, 23, 47, 78	12 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	1	MET	2.8
1	P	1	MET	2.5

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 oligosaccharides in this entry.

6.4 Ligands

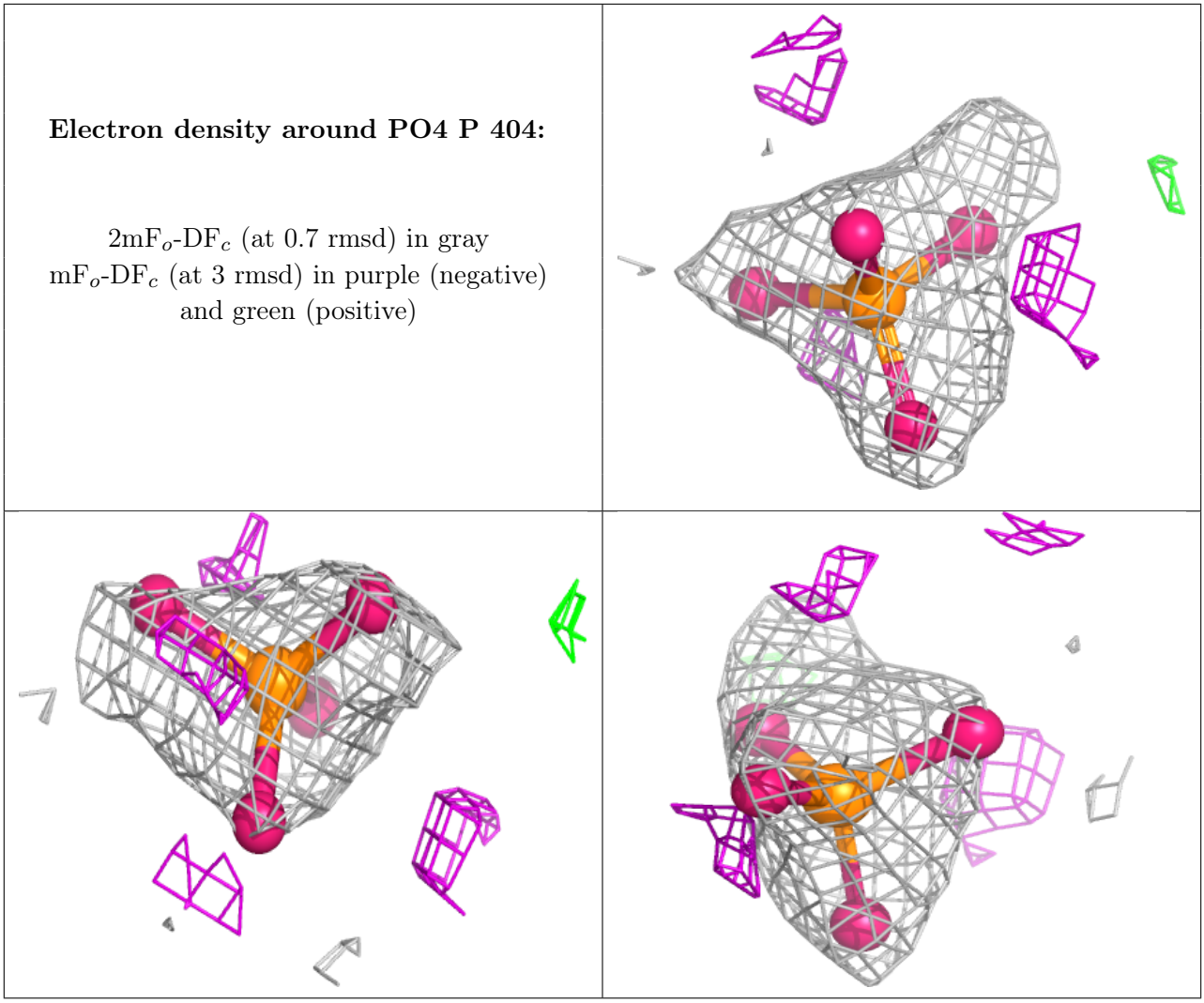
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	PO4	P	404	5/5	0.75	0.11	66,72,78,96	0
5	EDO	Q	405[A]	4/4	0.75	0.19	25,38,46,46	10
5	EDO	Q	405[B]	4/4	0.75	0.19	23,29,37,37	10
4	PO4	Q	404	5/5	0.79	0.11	61,65,92,109	0
4	PO4	O	404	5/5	0.84	0.11	54,62,85,88	0
4	PO4	R	404	5/5	0.85	0.09	55,56,88,90	0
5	EDO	O	405	4/4	0.87	0.13	34,41,46,49	0
5	EDO	R	405	4/4	0.87	0.11	30,43,53,64	0
4	PO4	O	408	5/5	0.88	0.14	41,45,51,107	0
7	DG4	P	402	15/15	0.88	0.14	11,38,53,55	19
3	G3H	Q	402	10/10	0.90	0.16	19,29,52,63	15
3	G3H	R	402	10/10	0.90	0.14	25,43,51,54	15
4	PO4	Q	403	5/5	0.92	0.12	32,51,65,66	0
4	PO4	P	403	5/5	0.92	0.11	37,48,52,58	0
4	PO4	R	403	5/5	0.92	0.15	35,52,55,62	0
3	G3H	O	402	10/10	0.93	0.11	21,35,47,52	15
4	PO4	O	403	5/5	0.97	0.08	28,34,39,51	0
2	NAD	R	401	44/44	0.98	0.05	18,23,31,38	0
6	CL	O	406	1/1	0.98	0.05	27,27,27,27	0
6	CL	R	406	1/1	0.98	0.04	29,29,29,29	0
2	NAD	Q	401	44/44	0.98	0.05	13,20,30,33	0
6	CL	Q	406	1/1	0.99	0.05	26,26,26,26	0
2	NAD	P	401	44/44	0.99	0.04	13,19,26,31	0
2	NAD	O	401	44/44	0.99	0.04	11,17,22,25	0
6	CL	P	405	1/1	1.00	0.03	22,22,22,22	0
6	CL	O	407	1/1	1.00	0.02	20,20,20,20	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.

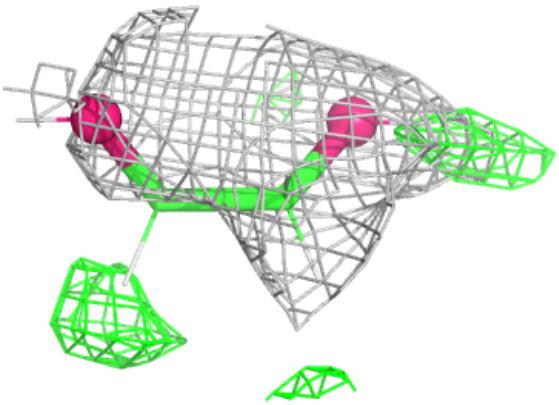
Electron density around PO4 P 404:

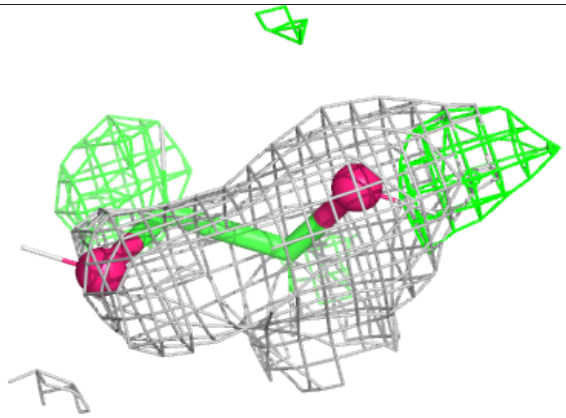
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

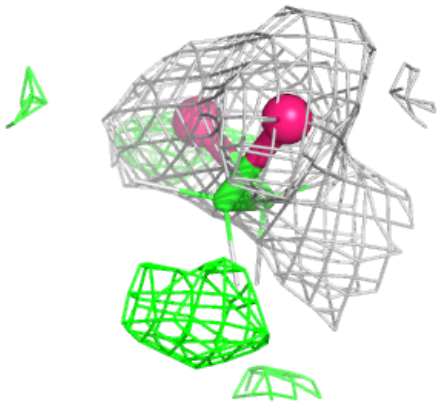


Electron density around EDO Q 405 (A):

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

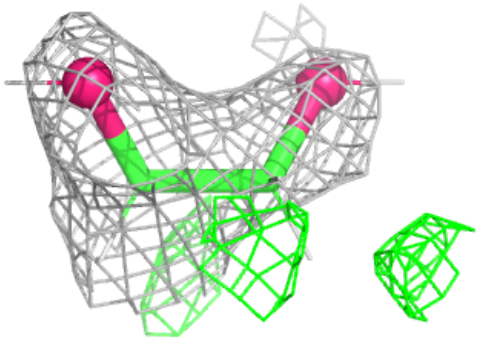


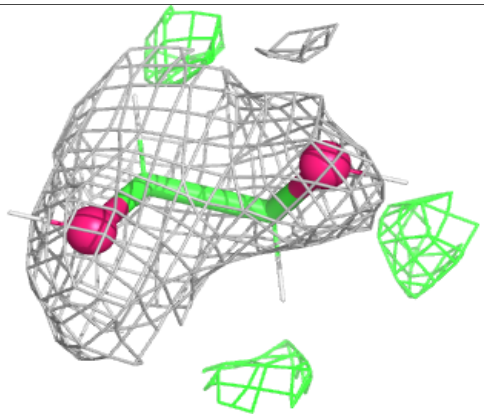


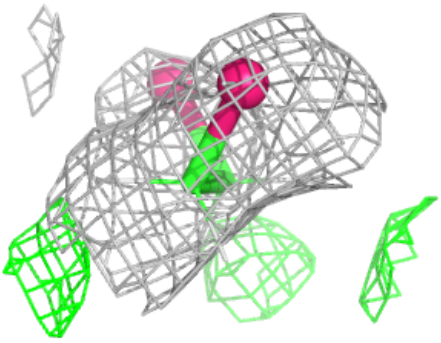


Electron density around EDO Q 405 (B):

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

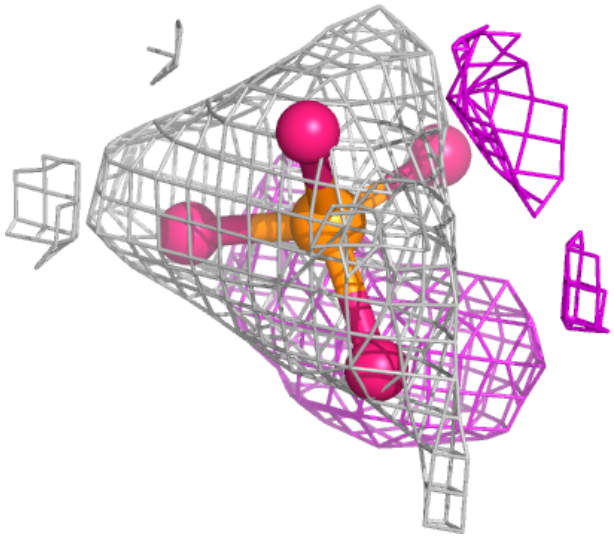


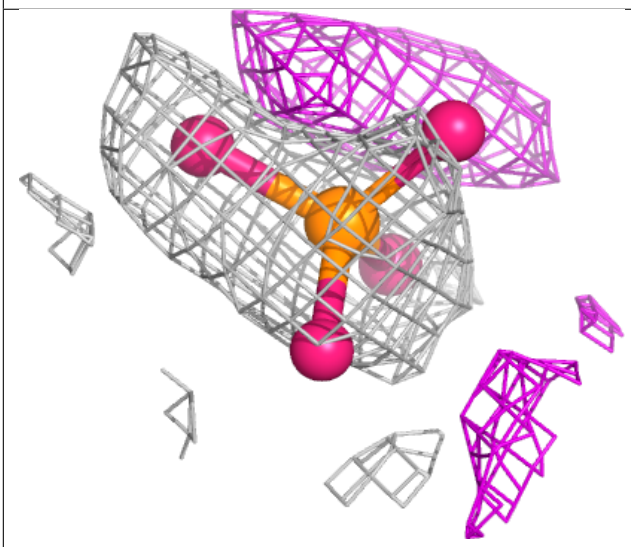


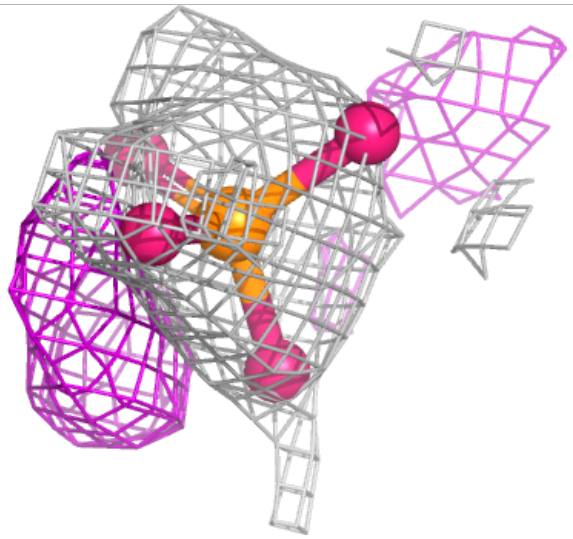


Electron density around PO4 Q 404:

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

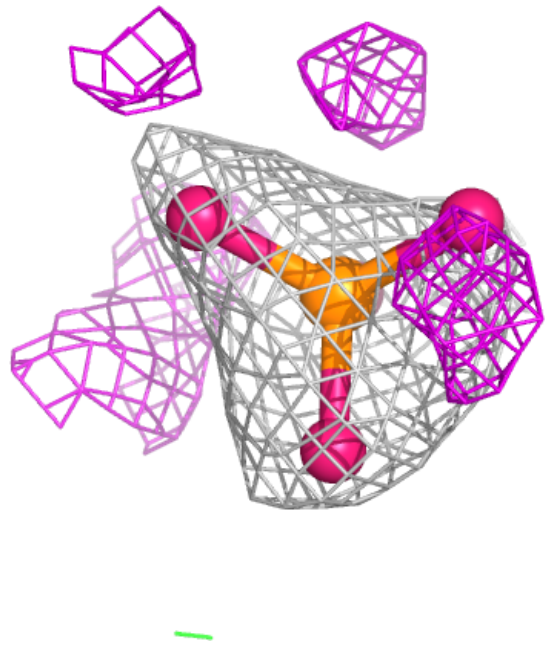


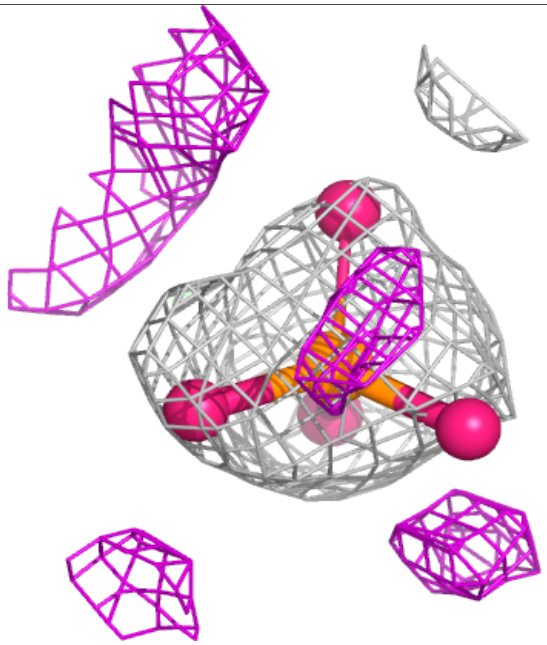


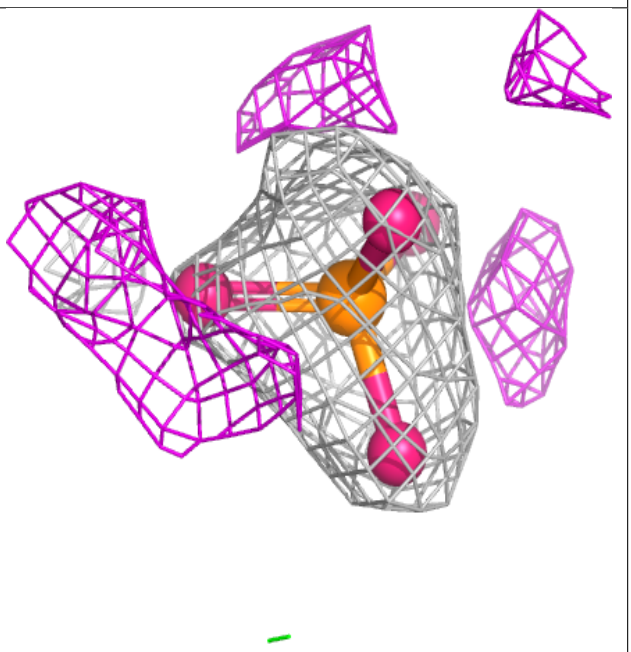


Electron density around PO4 O 404:

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

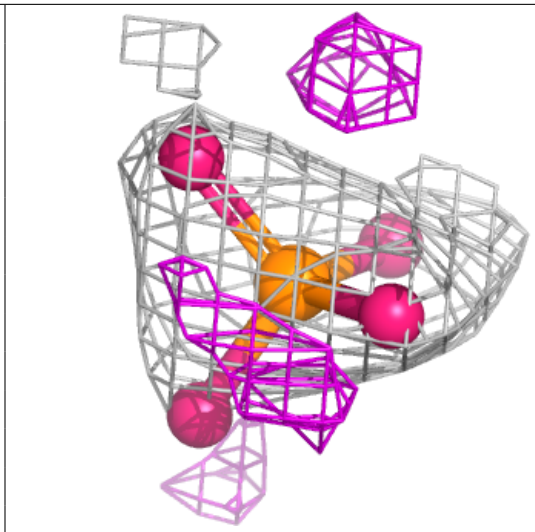


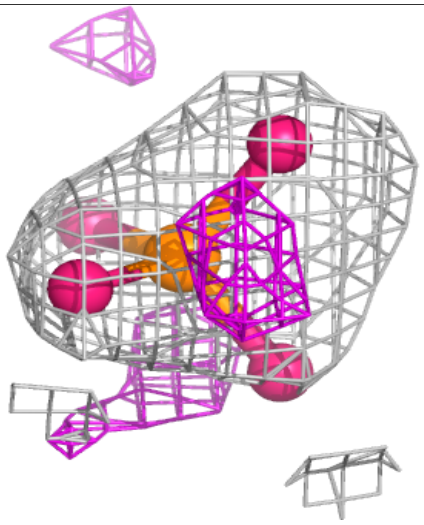


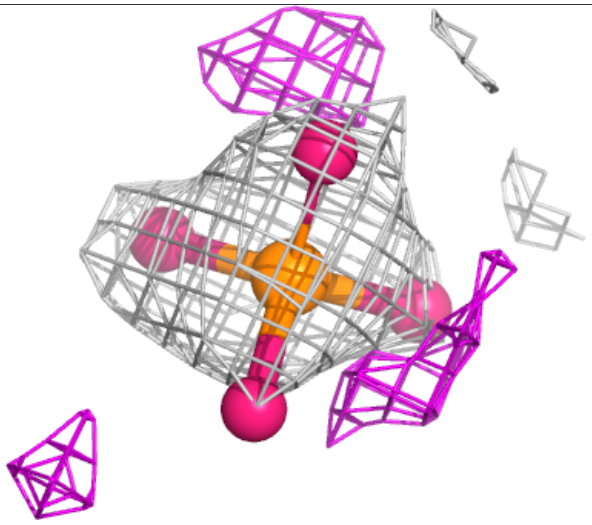


Electron density around PO4 R 404:

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

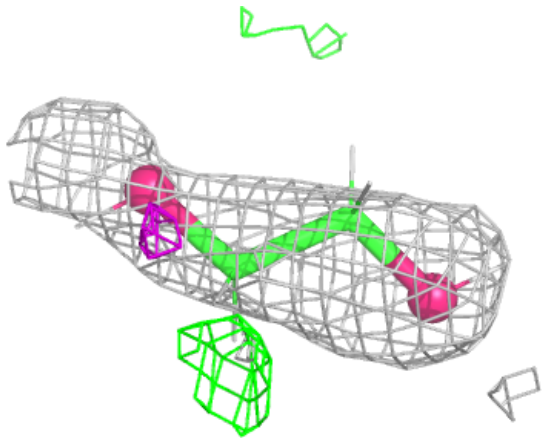


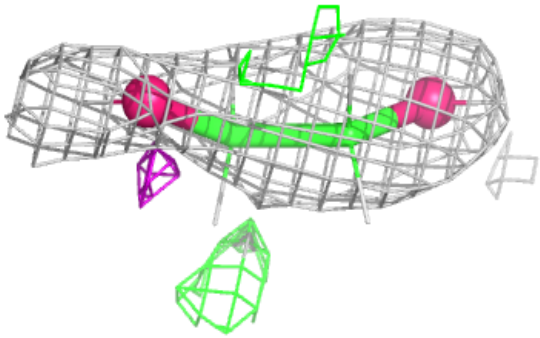


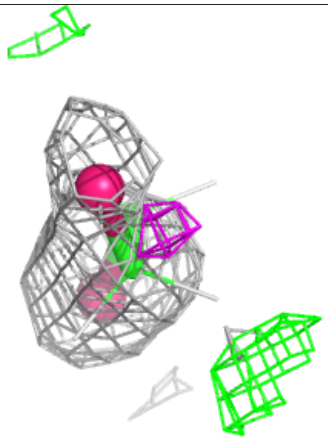


Electron density around EDO O 405:

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

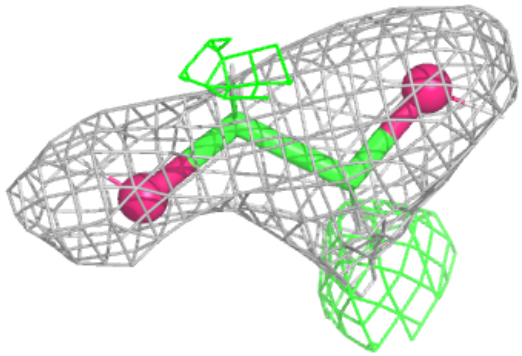


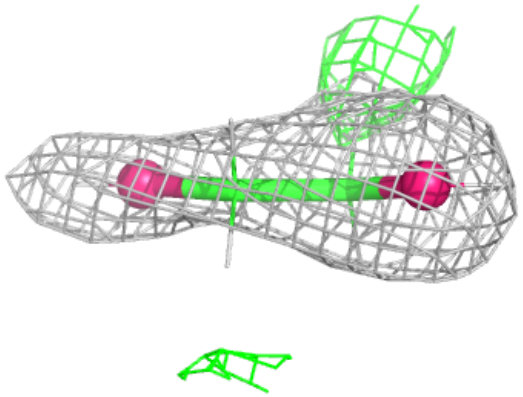


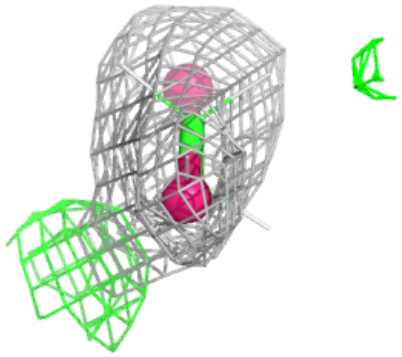


Electron density around EDO R 405:

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

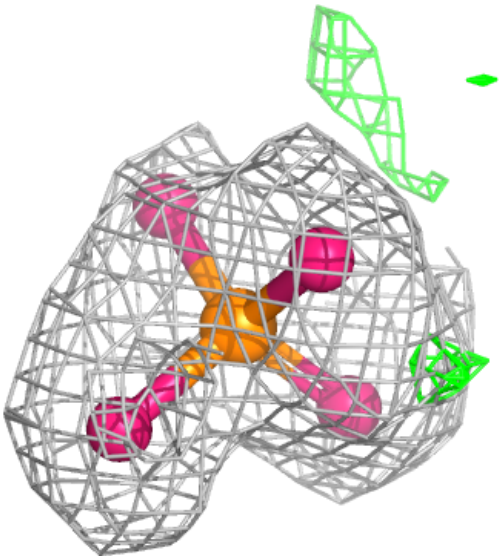


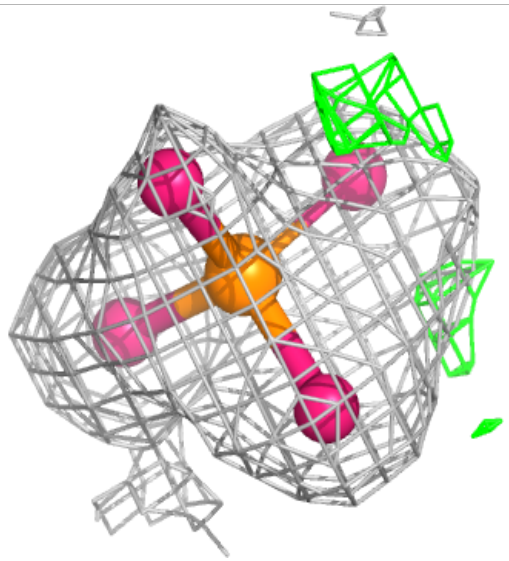


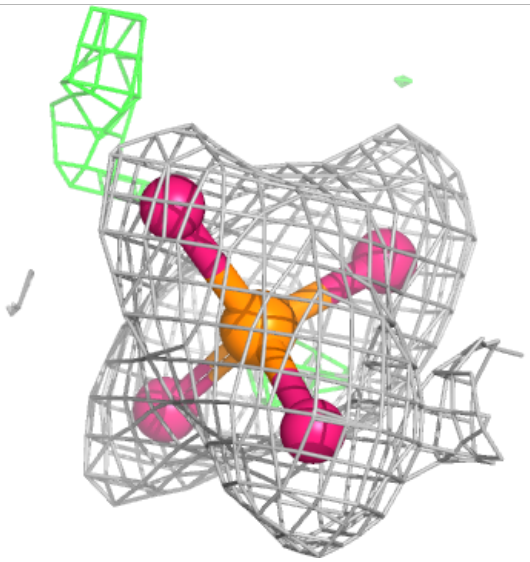


Electron density around PO4 O 408:

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

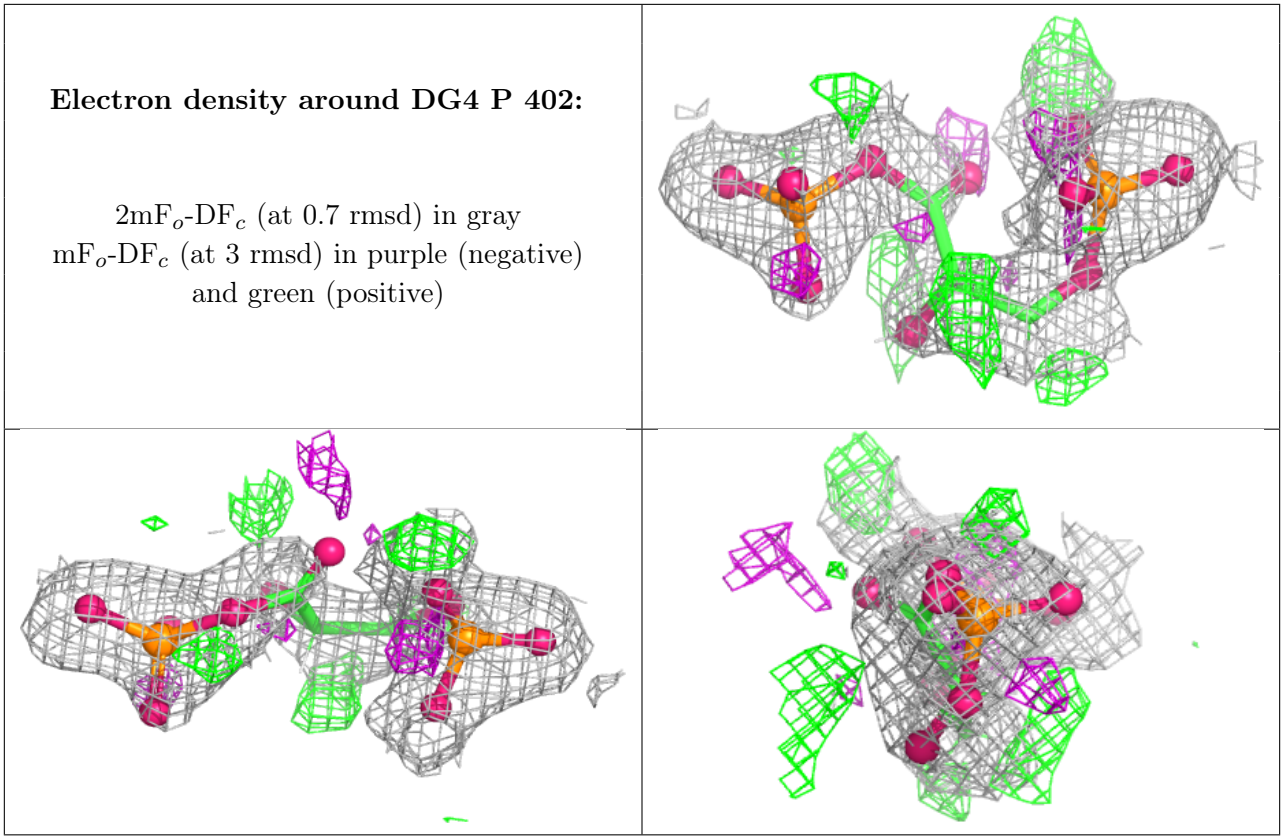






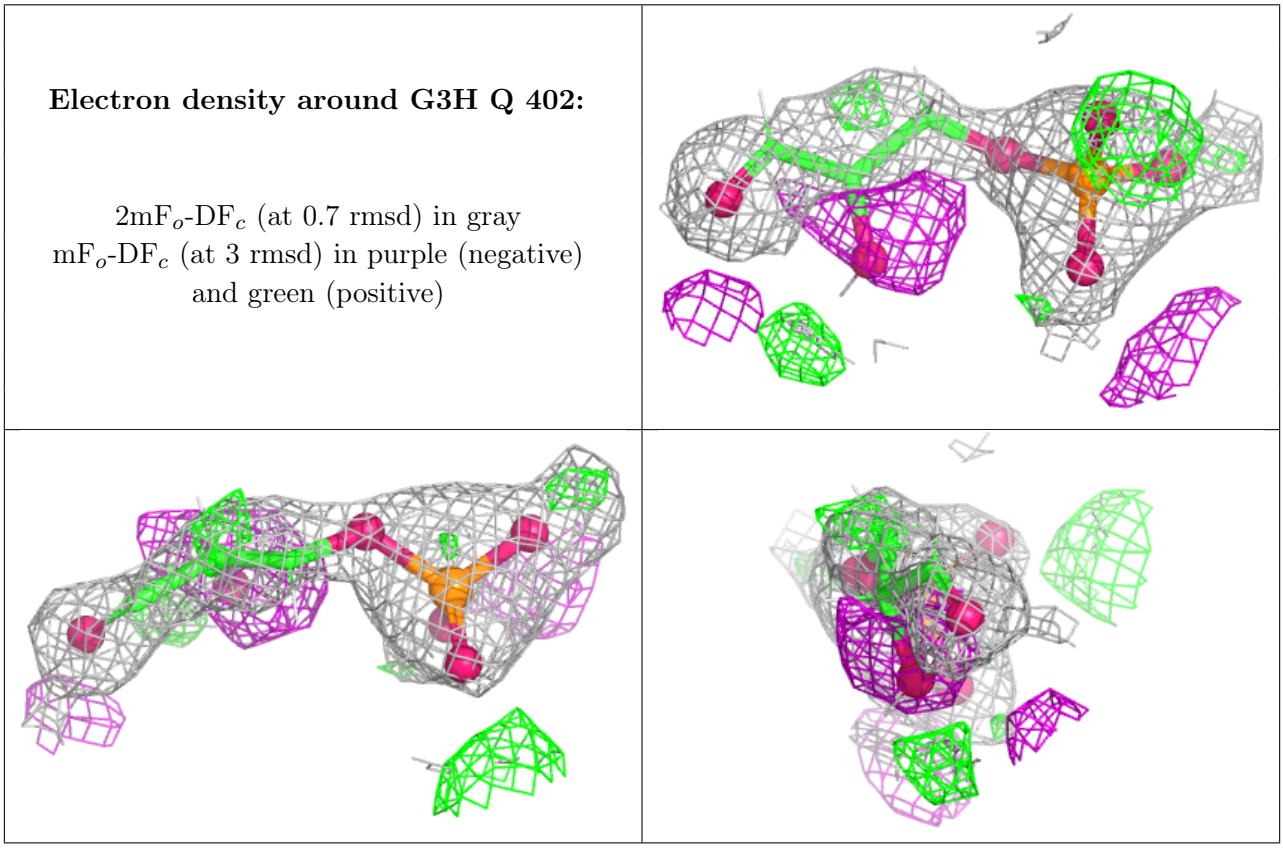
Electron density around DG4 P 402:

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



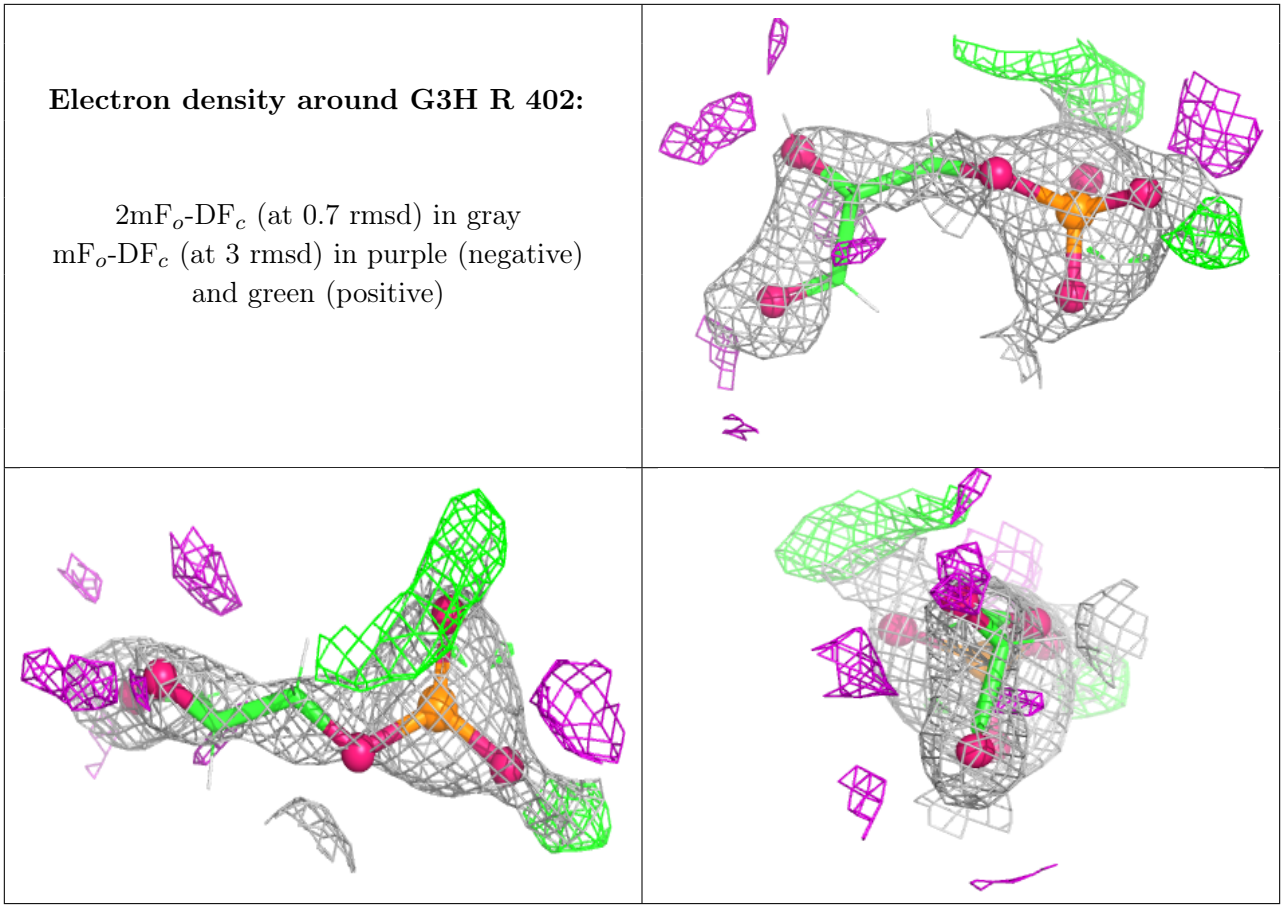
Electron density around G3H Q 402:

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



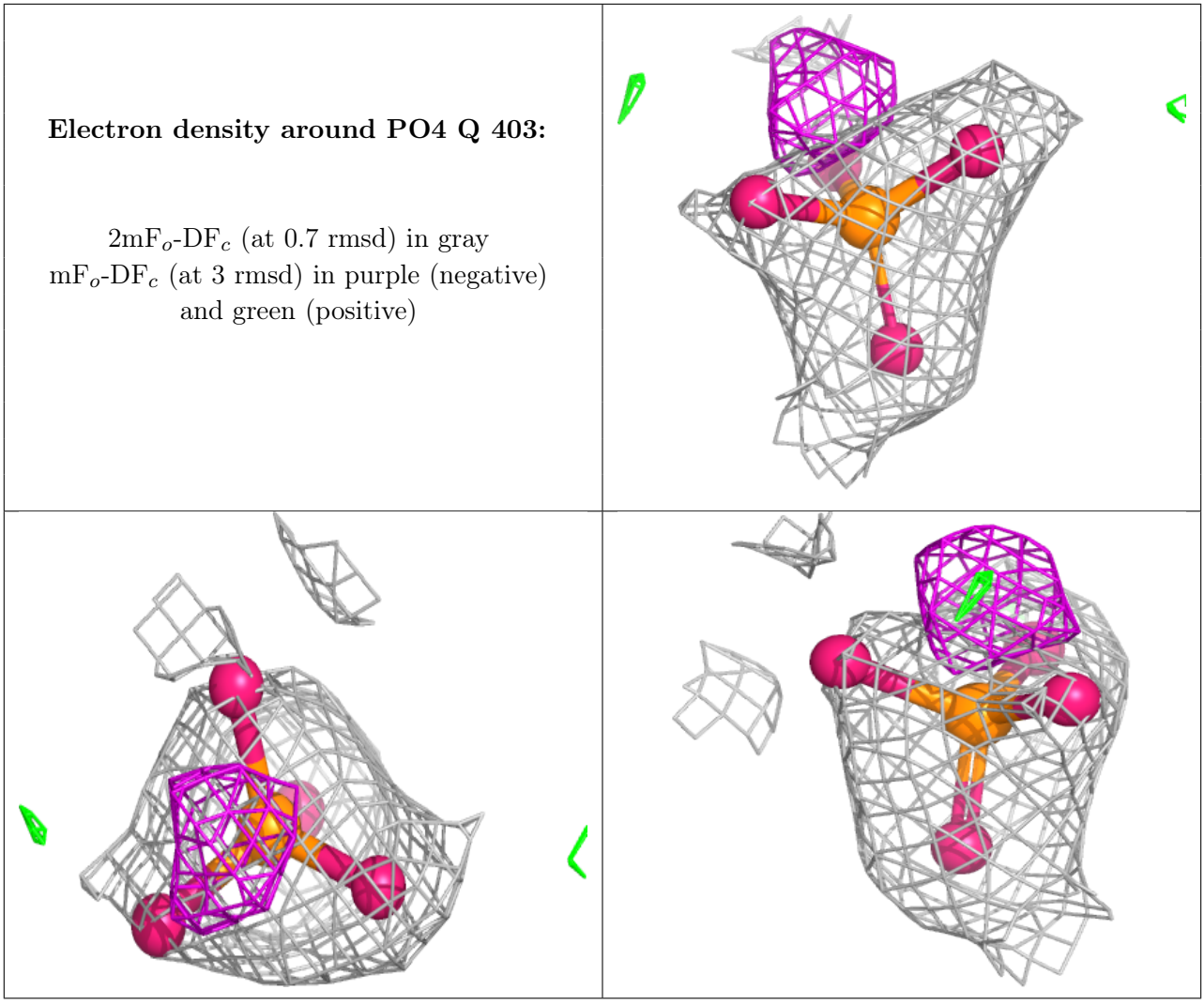
Electron density around G3H R 402:

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



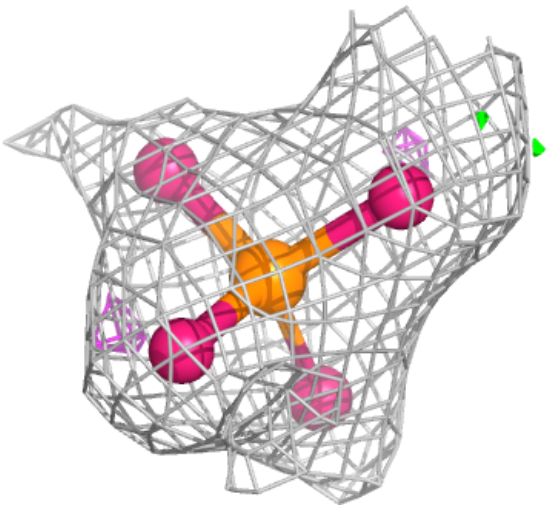
Electron density around PO4 Q 403:

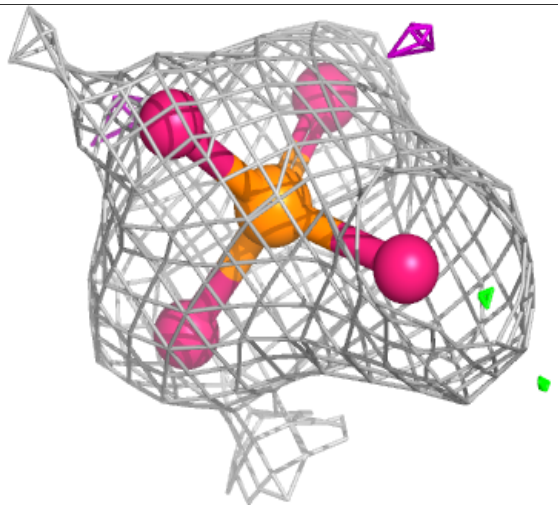
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

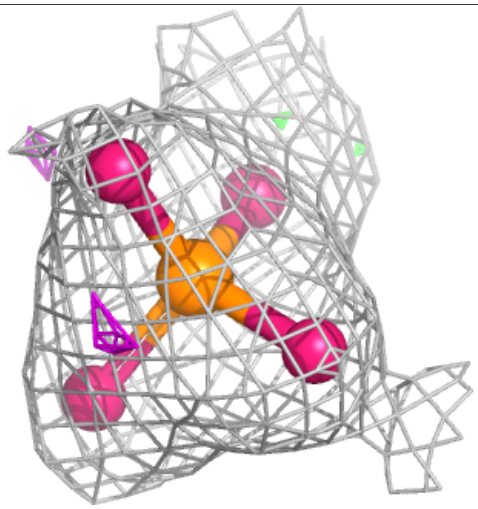


Electron density around PO4 P 403:

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

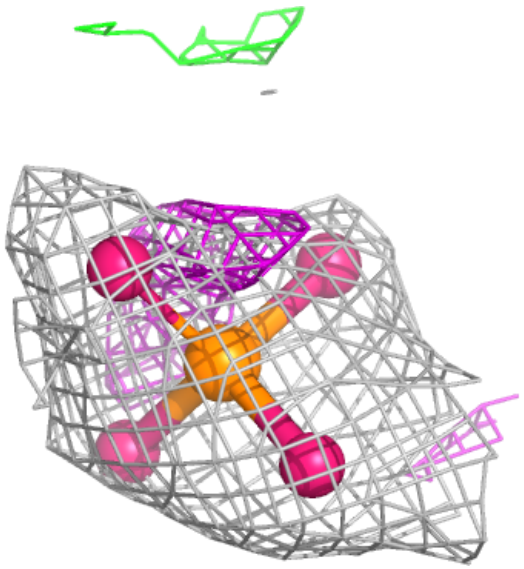


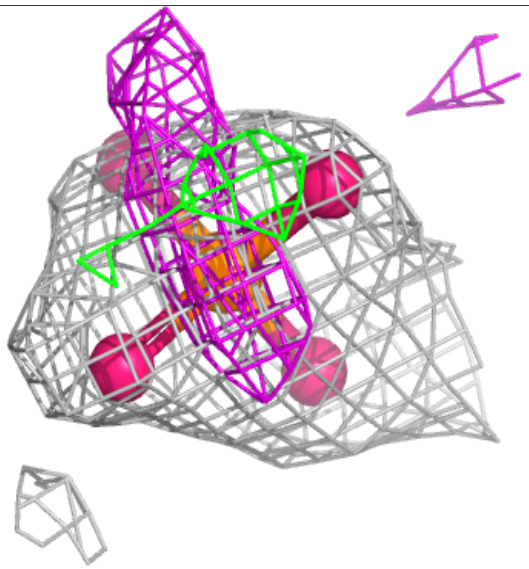


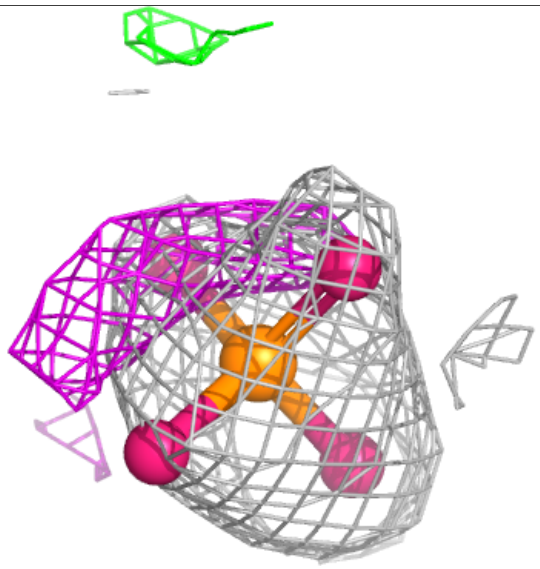


Electron density around PO4 R 403:

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

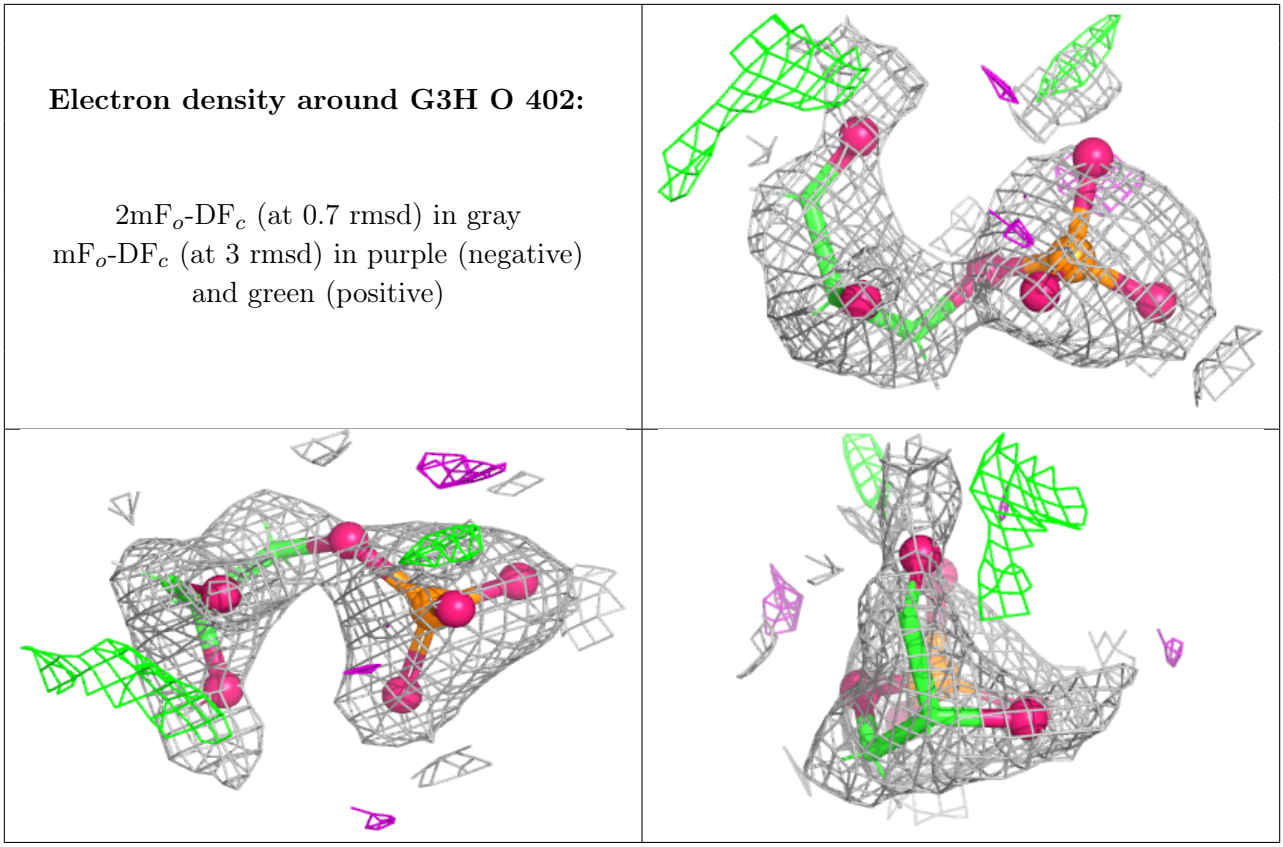






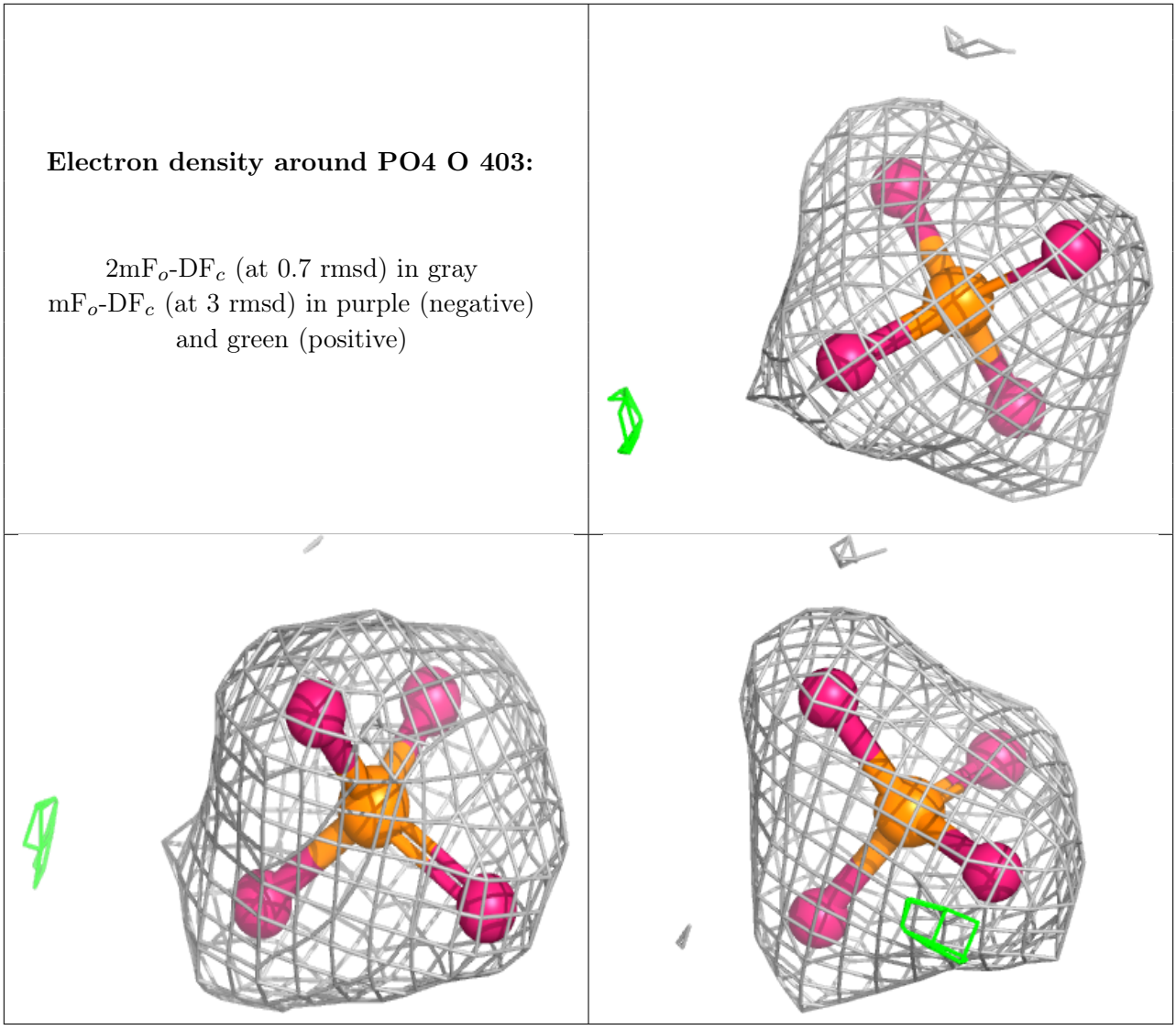
Electron density around G3H O 402:

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



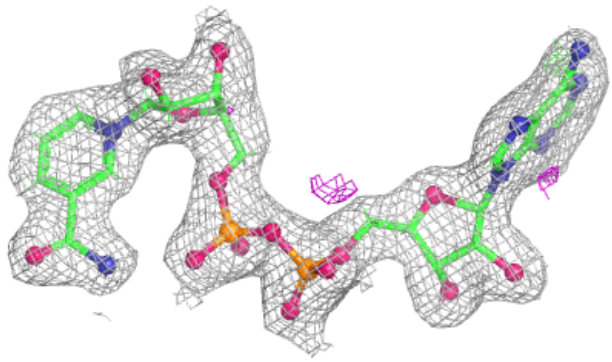
Electron density around PO4 O 403:

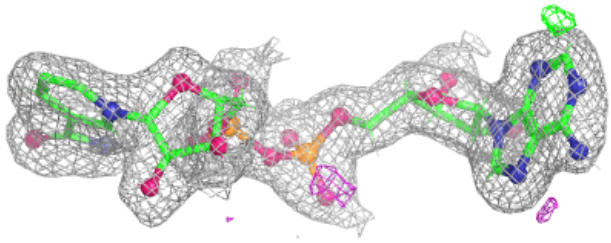
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

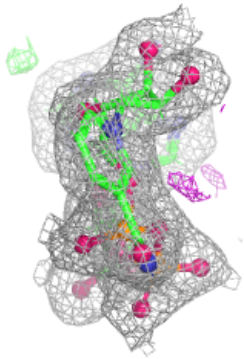


Electron density around NAD R 401:

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

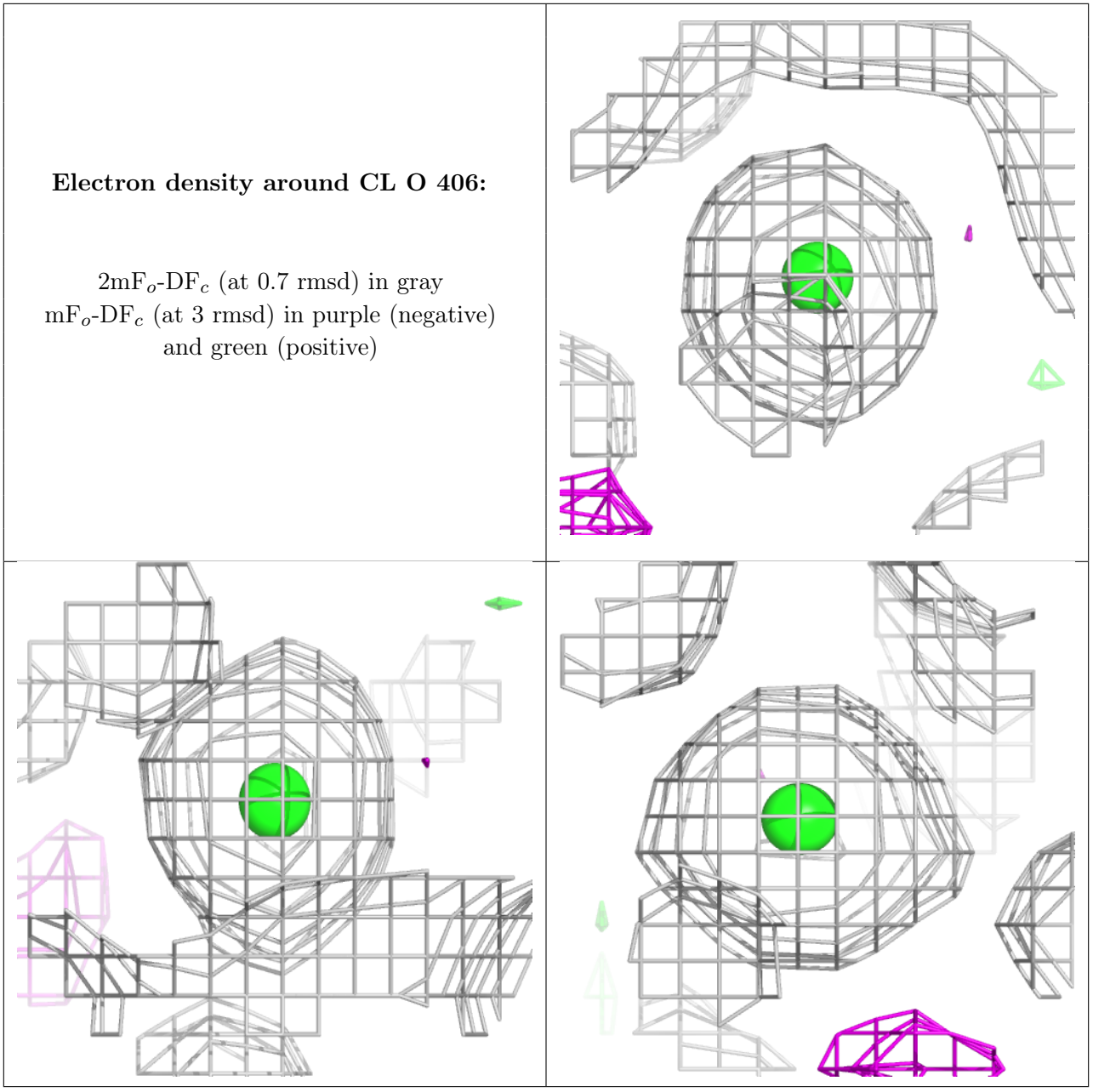






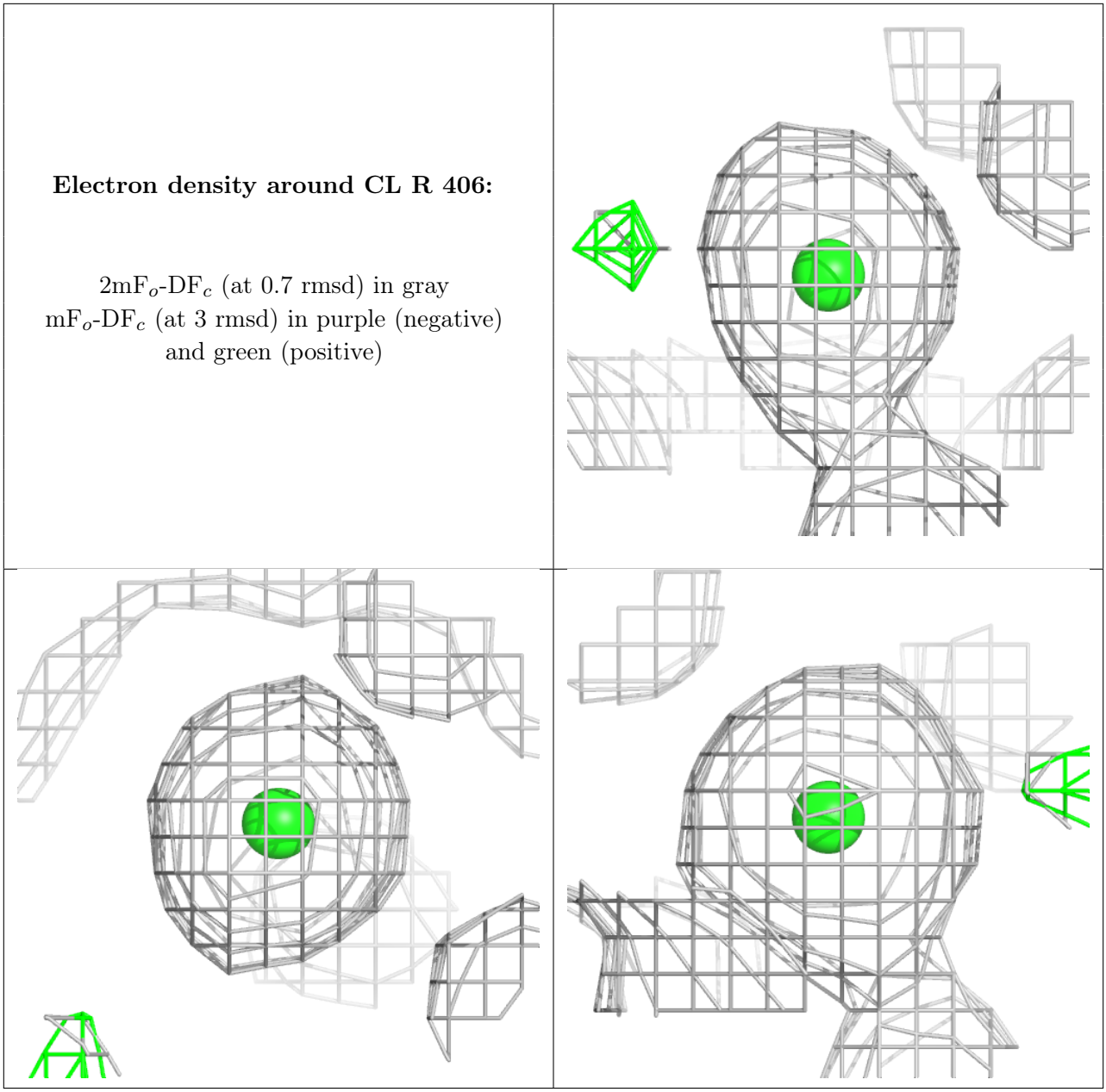
Electron density around CL O 406:

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



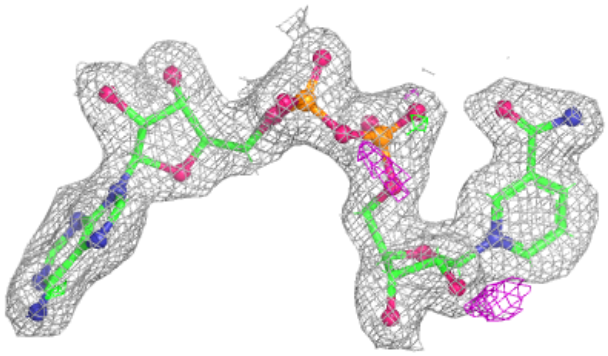
Electron density around CL R 406:

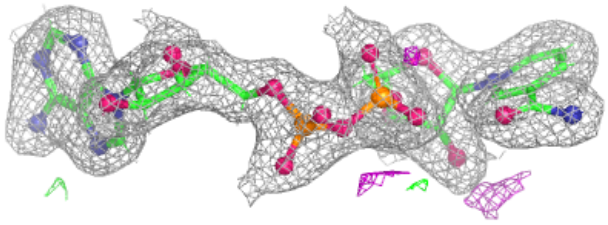
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

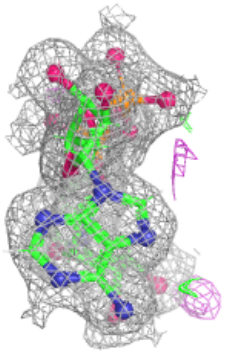


Electron density around NAD Q 401:

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

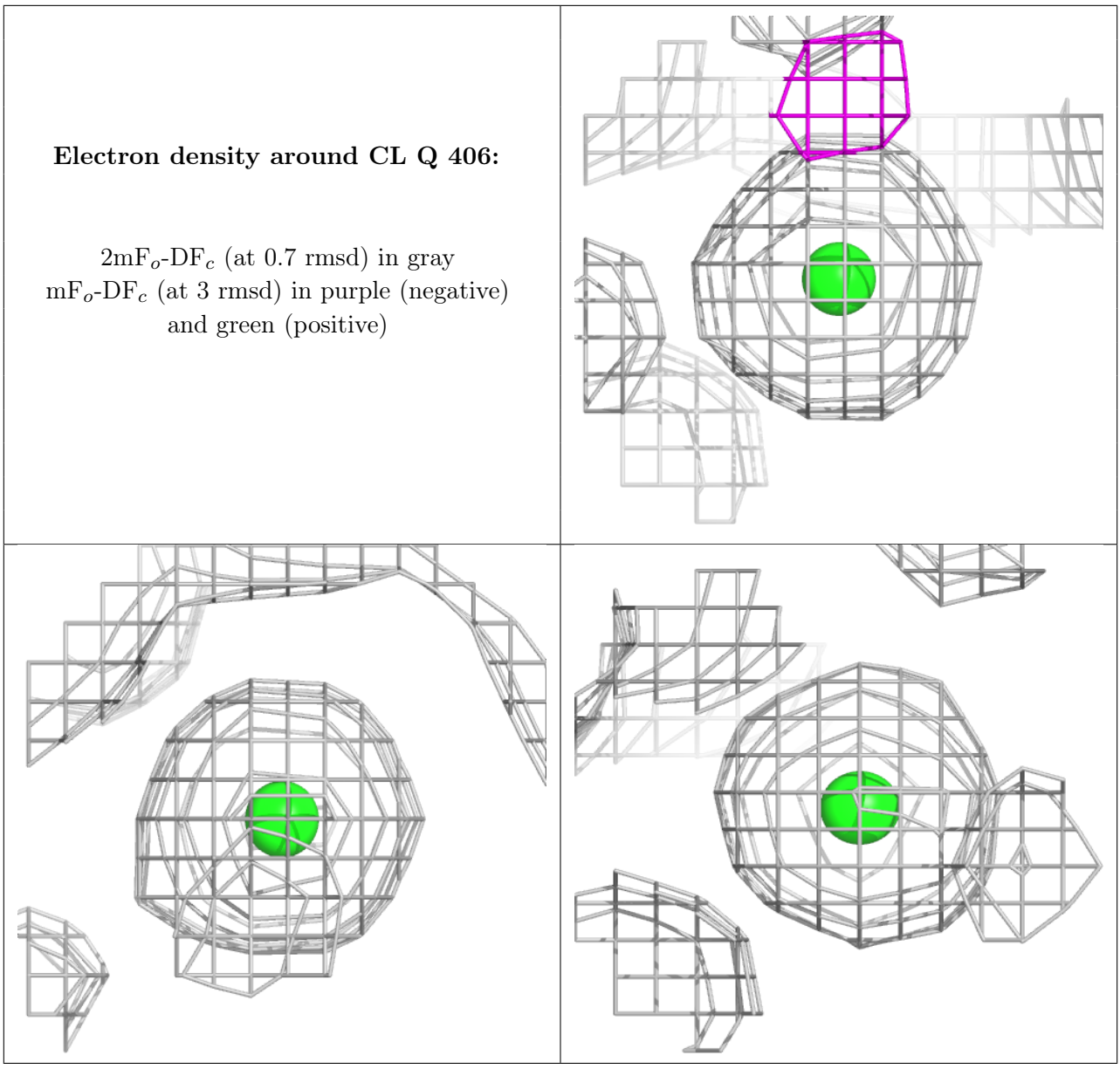






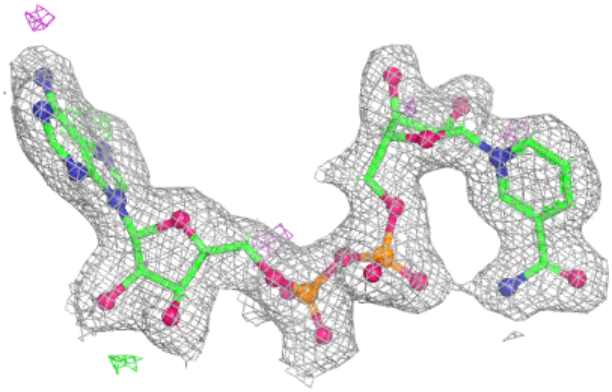
Electron density around CL Q 406:

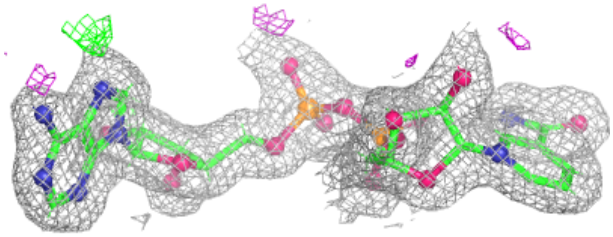
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

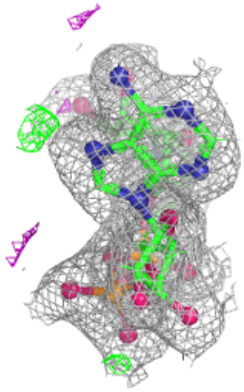


Electron density around NAD P 401:

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

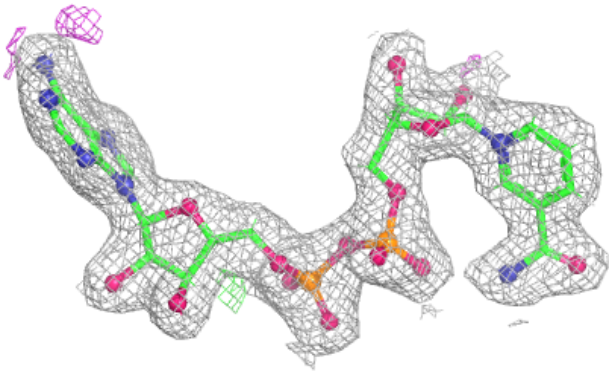


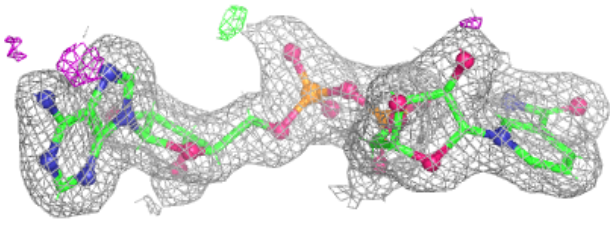


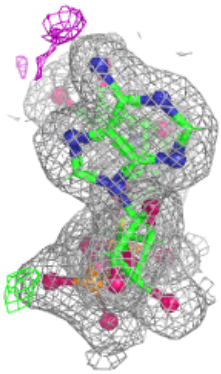


Electron density around NAD O 401:

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

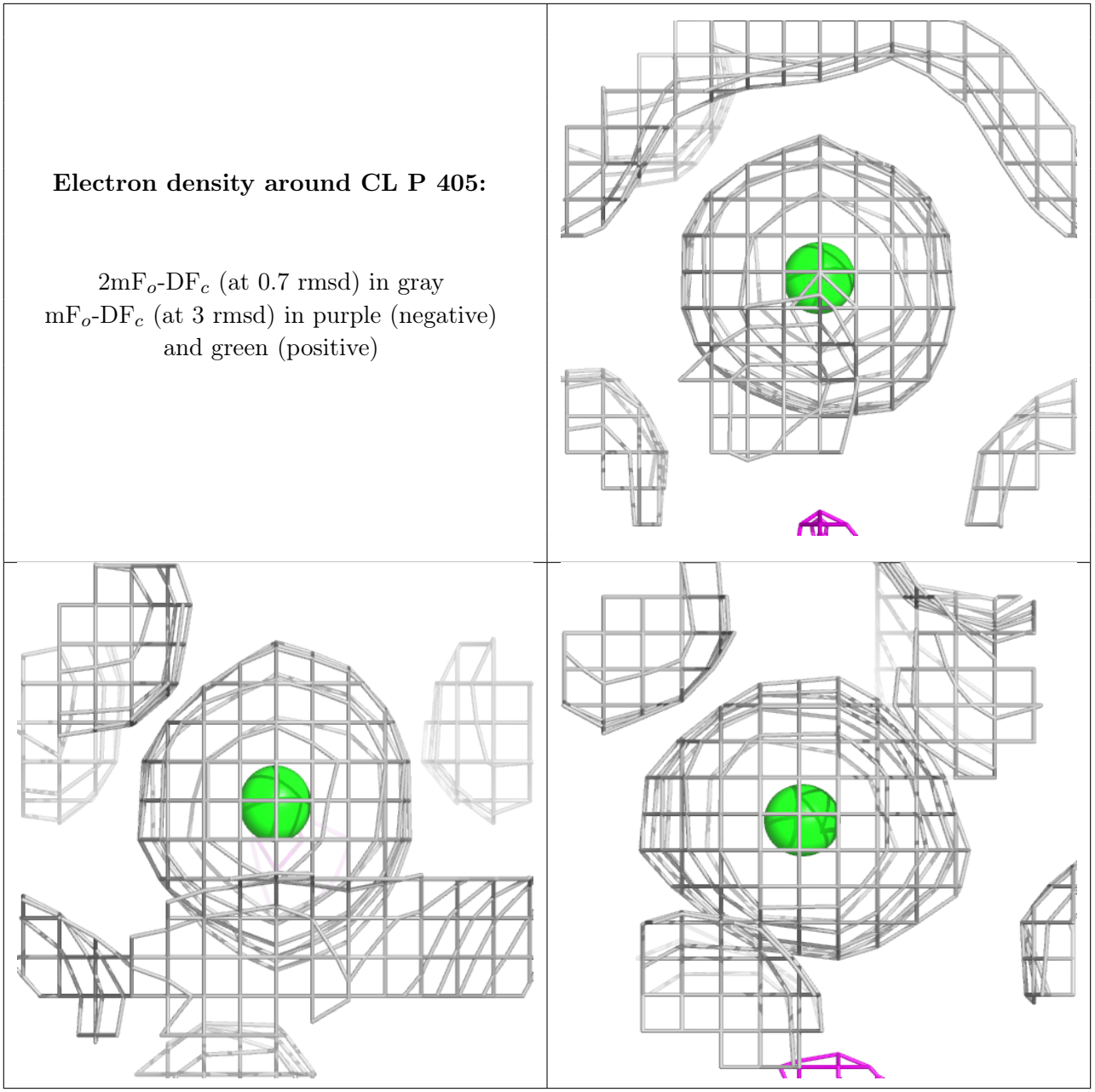






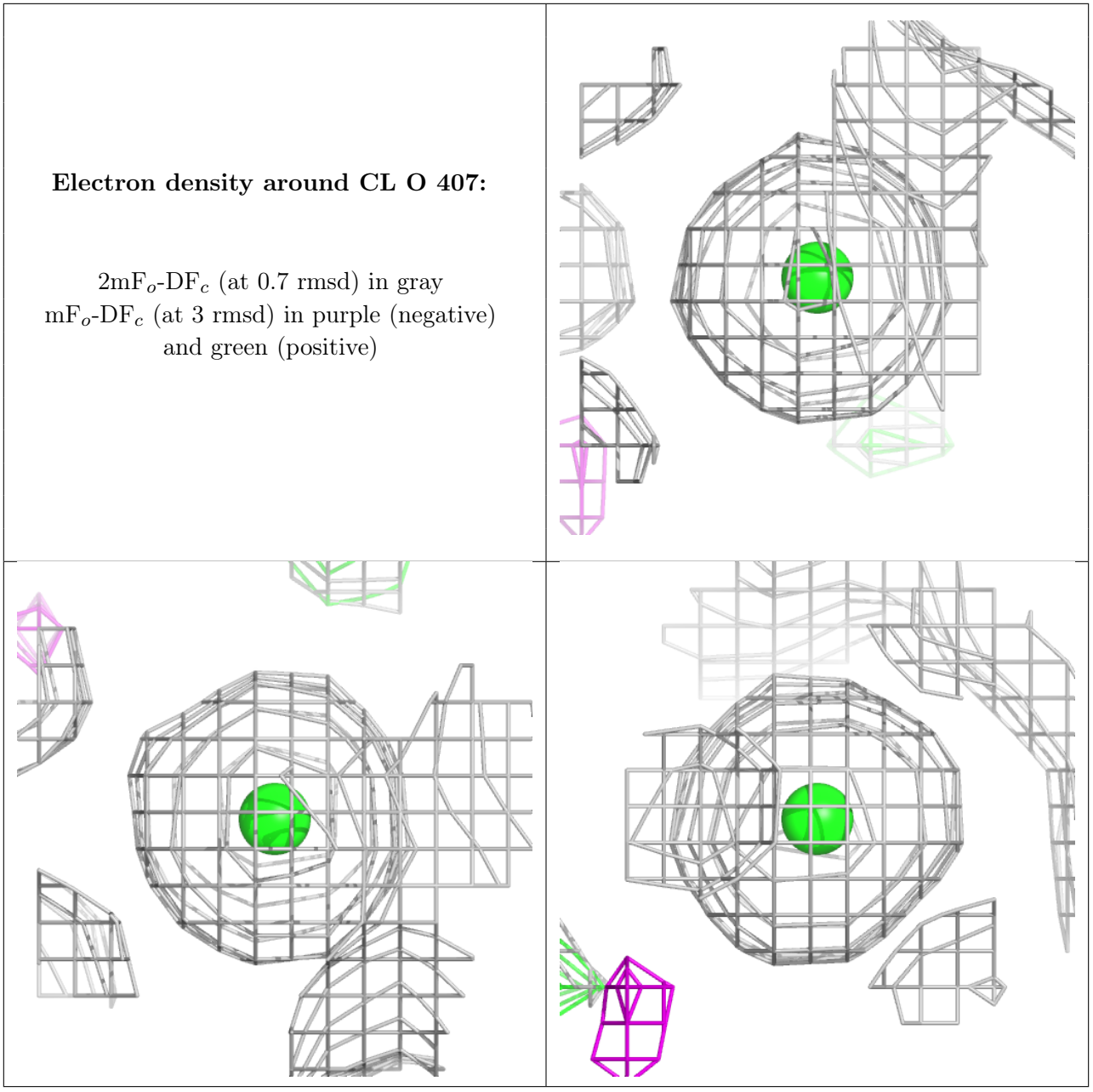
Electron density around CL P 405:

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



Electron density around CL O 407:

$2mF_o$-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.