wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2025 – 03:17 pm GMT

PDB ID	:	8Q67
Title	:	Crystal structure of a homohexameric MCM from M. acidophilum
Authors	:	Noble, O.W.; Degut, C.; Hodgkinson, M.R.; Chong, J.P.J.; Plevin, M.J.
Deposited on	:	2023-08-11
Resolution	:	2.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

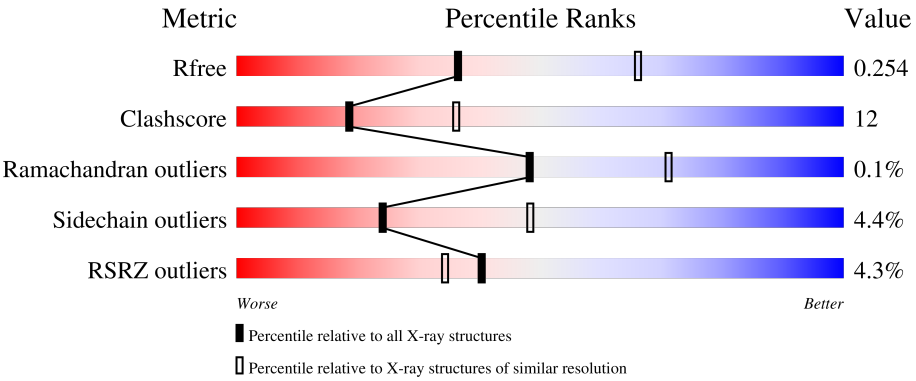
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.59 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	601	4% 79% 15%
1	B	601	5% 74% 20% 5%
1	C	601	3% 77% 18%
1	D	601	4% 80% 16%
1	E	601	4% 71% 23%

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Mol	Chain	Length	Quality of chain
1	F	601	

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	PO4	A	702	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 54511 atoms, of which 27391 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.

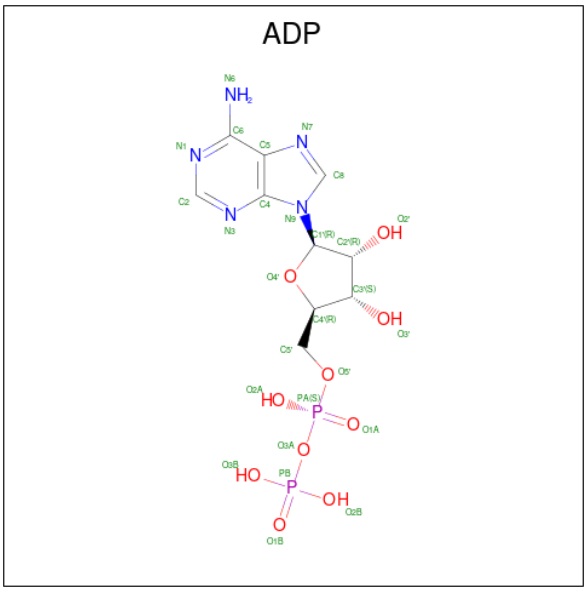
- Molecule 1 is a protein called DNA helicase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	574	Total	C	H	N	O	S	0	2	0
			9022	2846	4546	752	864	14			
1	B	572	Total	C	H	N	O	S	0	0	0
			8988	2834	4530	750	860	14			
1	C	574	Total	C	H	N	O	S	0	0	0
			9023	2849	4545	752	863	14			
1	D	577	Total	C	H	N	O	S	0	0	0
			9065	2864	4561	757	869	14			
1	E	574	Total	C	H	N	O	S	0	0	0
			9022	2847	4547	752	862	14			
1	F	582	Total	C	H	N	O	S	0	0	0
			9146	2886	4606	762	878	14			

There are 12 discrepancies between the modelled and reference sequences:

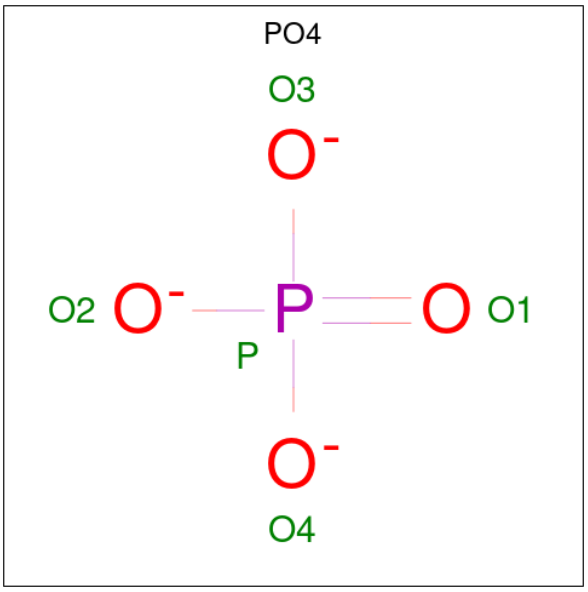
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A218NN99
A	391	GLN	GLU	engineered mutation	UNP A0A218NN99
B	0	GLY	-	expression tag	UNP A0A218NN99
B	391	GLN	GLU	engineered mutation	UNP A0A218NN99
C	0	GLY	-	expression tag	UNP A0A218NN99
C	391	GLN	GLU	engineered mutation	UNP A0A218NN99
D	0	GLY	-	expression tag	UNP A0A218NN99
D	391	GLN	GLU	engineered mutation	UNP A0A218NN99
E	0	GLY	-	expression tag	UNP A0A218NN99
E	391	GLN	GLU	engineered mutation	UNP A0A218NN99
F	0	GLY	-	expression tag	UNP A0A218NN99
F	391	GLN	GLU	engineered mutation	UNP A0A218NN99

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	1	0
			38	10	11	5	10	2		
2	B	1	Total	C	H	N	O	P	1	0
			38	10	11	5	10	2		
2	C	1	Total	C	H	N	O	P	7	0
			39	10	12	5	10	2		
2	E	1	Total	C	H	N	O	P	3	0
			38	10	11	5	10	2		
2	F	1	Total	C	H	N	O	P	5	0
			38	10	11	5	10	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

- Molecule 5 is water.

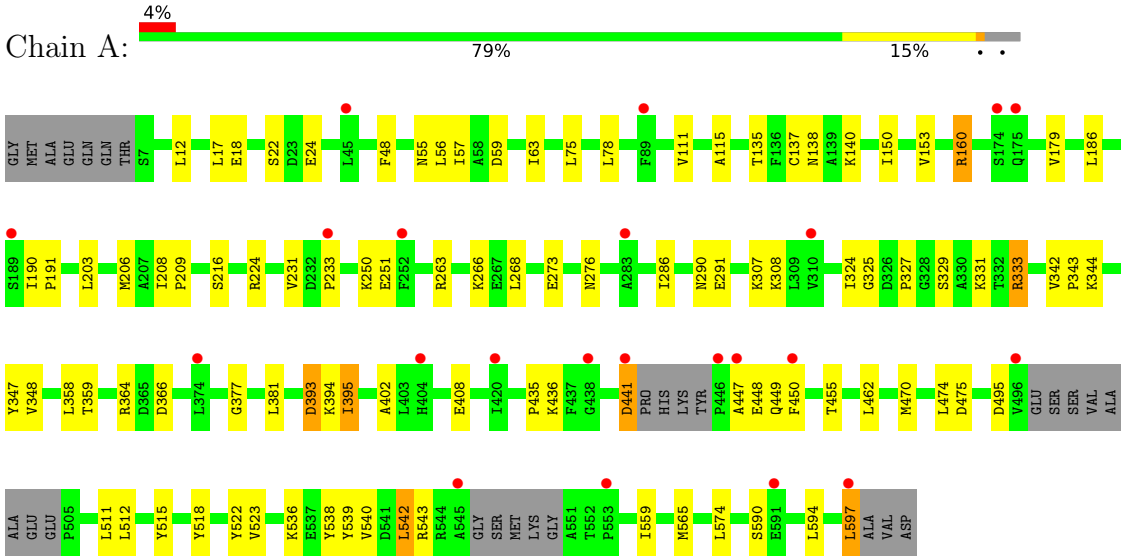
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	1	Total O 1 1	0	0
5	C	3	Total O 3 3	0	0
5	D	1	Total O 1 1	0	0
5	F	2	Total O 2 2	0	0

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.

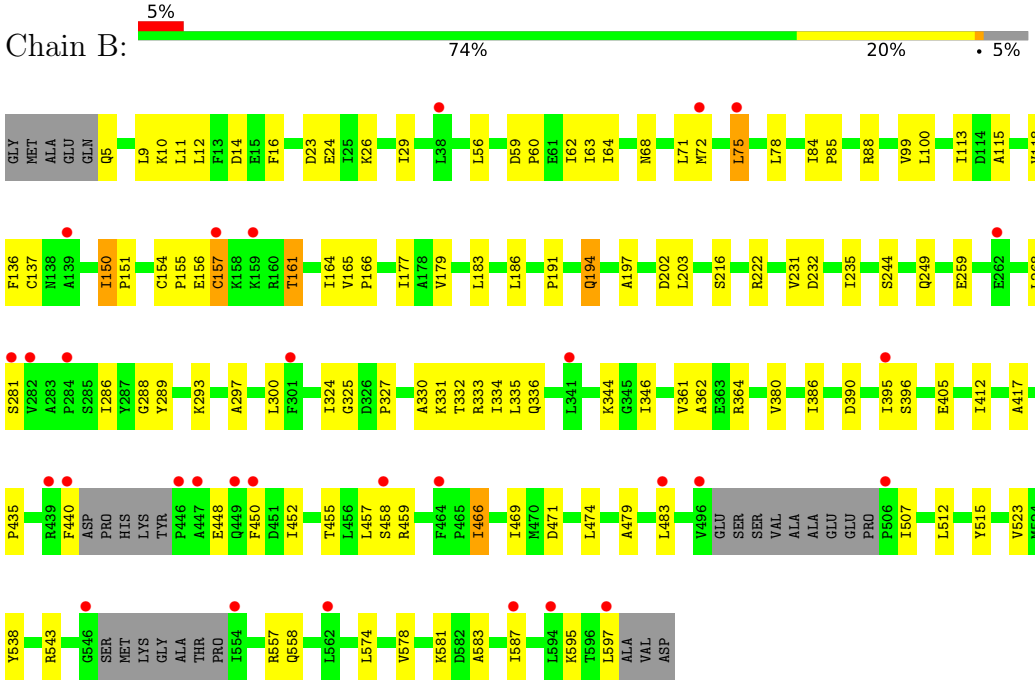
• Molecule 1: DNA helicase

Chain A:



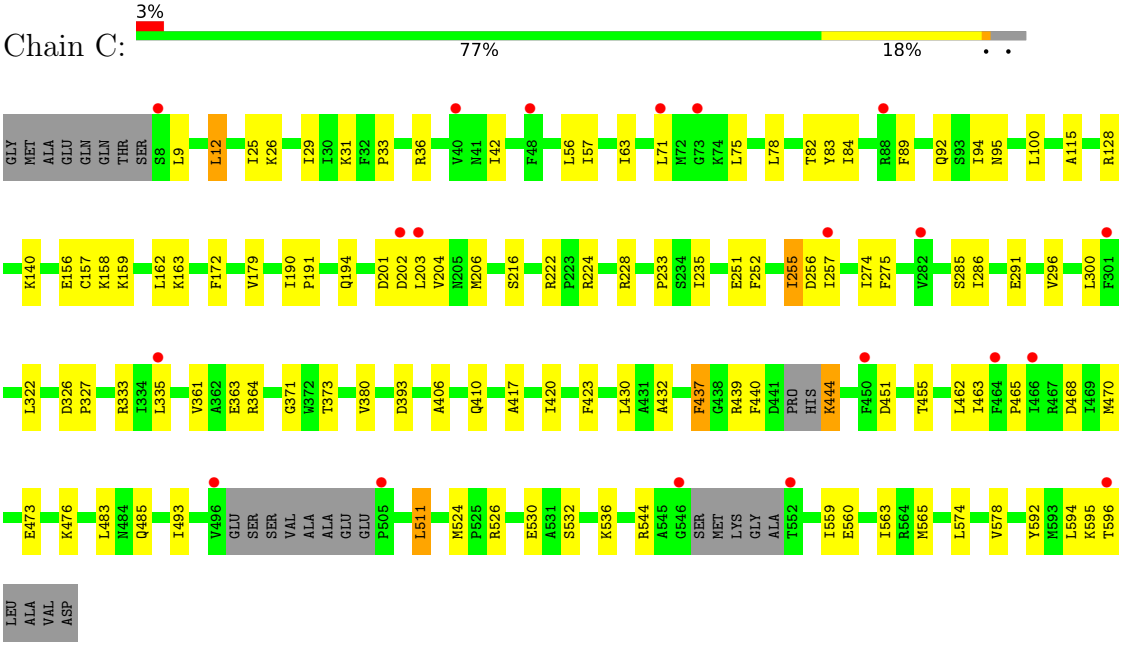
• Molecule 1: DNA helicase

Chain B:



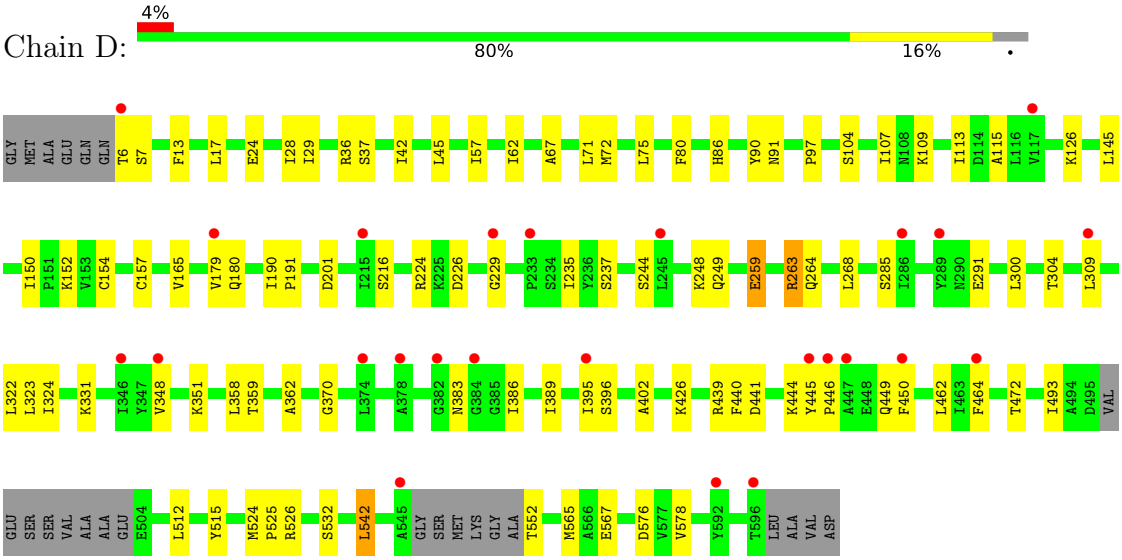
• Molecule 1: DNA helicase

Chain C:



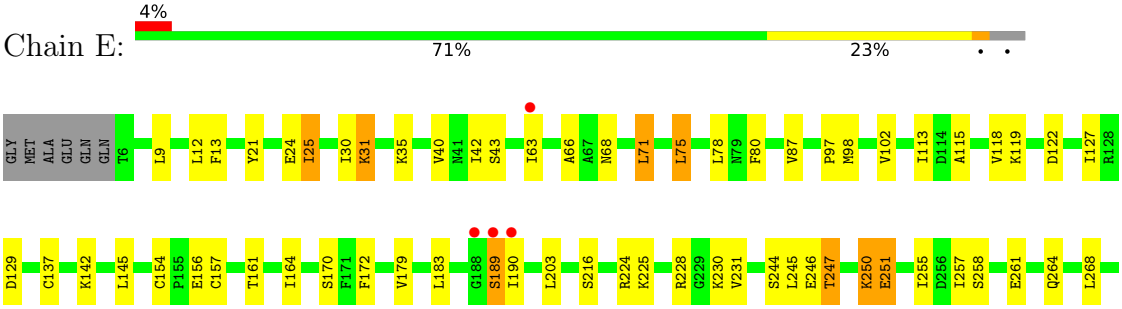
• Molecule 1: DNA helicase

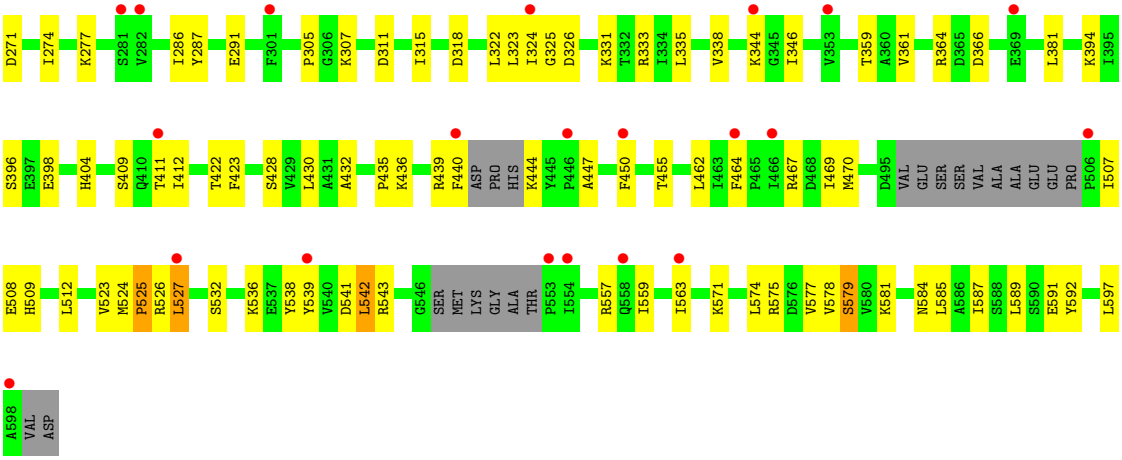
Chain D:



• Molecule 1: DNA helicase

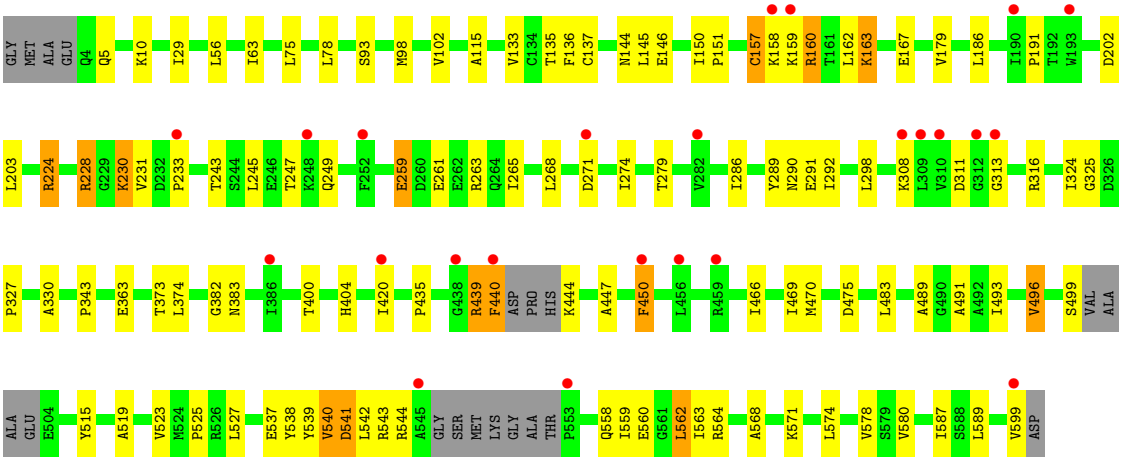
Chain E:





• Molecule 1: DNA helicase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	228.70Å 127.49Å 177.04Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	57.15 – 2.59 57.15 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (57.15-2.59) 98.0 (57.15-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.253 0.231 , 0.254	Depositor DCC
R_{free} test set	155226 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	54511	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: ZN, ADP, PO4

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	0.96	0/4559	0.74	0/6163
1	B	0.79	0/4531	0.70	0/6121
1	C	0.84	0/4554	0.71	0/6155
1	D	0.76	0/4583	0.72	0/6198
1	E	0.96	0/4550	0.80	0/6147
1	F	0.88	0/4616	0.70	0/6239
All	All	0.87	0/27393	0.73	0/37023

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	A	4476	4546	4541	98	0
1	B	4458	4530	4530	120	0
1	C	4478	4545	4545	96	0
1	D	4504	4561	4560	92	0
1	E	4475	4547	4547	154	0
1	F	4540	4606	4606	109	0
2	A	27	11	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	11	12	5	0
2	C	27	12	12	1	0
2	E	27	11	12	3	0
2	F	27	11	12	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	6	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
All	All	27120	27391	27389	643	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 12.

The worst 5 of 643 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:F:324:ILE:HD13	1:F:450:PHE:CD2	1.50	1.47
1:F:324:ILE:HD13	1:F:450:PHE:CE2	1.59	1.38
1:F:324:ILE:CD1	1:F:450:PHE:CE2	2.21	1.23
1:E:324:ILE:HG12	1:E:450:PHE:CD1	1.78	1.17
1:E:324:ILE:HG21	1:E:450:PHE:CE1	1.80	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/601 (94%)	547 (96%)	20 (4%)	1 (0%)	44	66
1	B	564/601 (94%)	543 (96%)	21 (4%)	0	100	100
1	C	566/601 (94%)	546 (96%)	19 (3%)	1 (0%)	44	66
1	D	571/601 (95%)	547 (96%)	23 (4%)	1 (0%)	44	66
1	E	566/601 (94%)	542 (96%)	23 (4%)	1 (0%)	44	66
1	F	574/601 (96%)	557 (97%)	16 (3%)	1 (0%)	44	66
All	All	3409/3606 (94%)	3282 (96%)	122 (4%)	5 (0%)	48	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	ASP
1	D	249	GLN
1	E	189	SER
1	F	343	PRO
1	A	233	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	494/513 (96%)	475 (96%)	19 (4%)	28	54
1	B	491/513 (96%)	479 (98%)	12 (2%)	44	70
1	C	493/513 (96%)	471 (96%)	22 (4%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	496/513 (97%)	487 (98%)	9 (2%)	54 77
1	E	492/513 (96%)	458 (93%)	34 (7%)	13 28
1	F	501/513 (98%)	466 (93%)	35 (7%)	12 27
All	All	2967/3078 (96%)	2836 (96%)	131 (4%)	24 48

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	440	PHE
1	F	469	ILE
1	F	599	VAL
1	C	483	LEU
1	C	444	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	ADP	E	701	-	24,29,29	1.47	5 (20%)	29,45,45	2.07	6 (20%)
2	ADP	B	701	-	24,29,29	1.13	2 (8%)	29,45,45	1.54	3 (10%)
3	PO4	C	702	-	4,4,4	1.68	1 (25%)	6,6,6	1.08	0
3	PO4	D	702	-	4,4,4	0.93	0	6,6,6	0.46	0
2	ADP	F	701	-	24,29,29	1.23	3 (12%)	29,45,45	2.01	10 (34%)
3	PO4	E	702	-	4,4,4	1.83	1 (25%)	6,6,6	0.66	0
3	PO4	A	702	-	4,4,4	3.22	4 (100%)	6,6,6	0.96	0
3	PO4	D	701	-	4,4,4	1.68	0	6,6,6	0.60	0
2	ADP	C	701	-	24,29,29	1.05	2 (8%)	29,45,45	1.39	3 (10%)
3	PO4	F	702	-	4,4,4	1.93	3 (75%)	6,6,6	0.75	0
2	ADP	A	701	-	24,29,29	1.58	6 (25%)	29,45,45	2.24	9 (31%)
3	PO4	B	702	-	4,4,4	1.81	2 (50%)	6,6,6	0.64	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
2	ADP	E	701	-	-	4/12/32/32	0/3/3/3
2	ADP	B	701	-	-	4/12/32/32	0/3/3/3
2	ADP	F	701	-	-	3/12/32/32	0/3/3/3
2	ADP	C	701	-	-	7/12/32/32	0/3/3/3
2	ADP	A	701	-	-	6/12/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ADP	C2'-C1'	-3.62	1.48	1.53
3	A	702	PO4	P-O3	-3.36	1.44	1.54
3	A	702	PO4	P-O2	-3.23	1.44	1.54
3	A	702	PO4	P-O4	-3.21	1.44	1.54
3	A	702	PO4	P-O1	-3.06	1.43	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	701	ADP	PA-O3A-PB	-7.56	106.89	132.83
2	A	701	ADP	PA-O3A-PB	-5.86	112.71	132.83
2	B	701	ADP	PA-O3A-PB	-5.64	113.47	132.83
2	F	701	ADP	PA-O3A-PB	-5.49	113.99	132.83
2	A	701	ADP	N3-C2-N1	-4.72	121.30	128.68

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C5'-O5'-PA-O2A
2	C	701	ADP	C5'-O5'-PA-O1A
2	E	701	ADP	C4'-C5'-O5'-PA

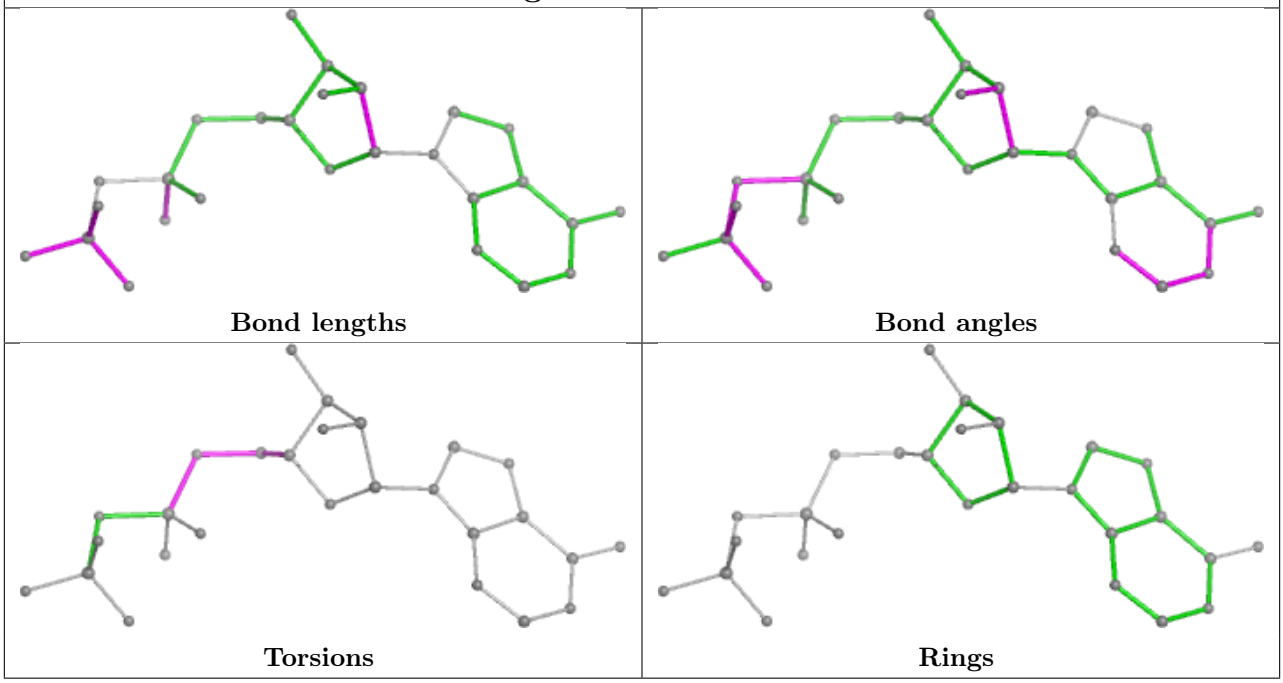
There are no ring outliers.

5 monomers are involved in 14 short contacts:

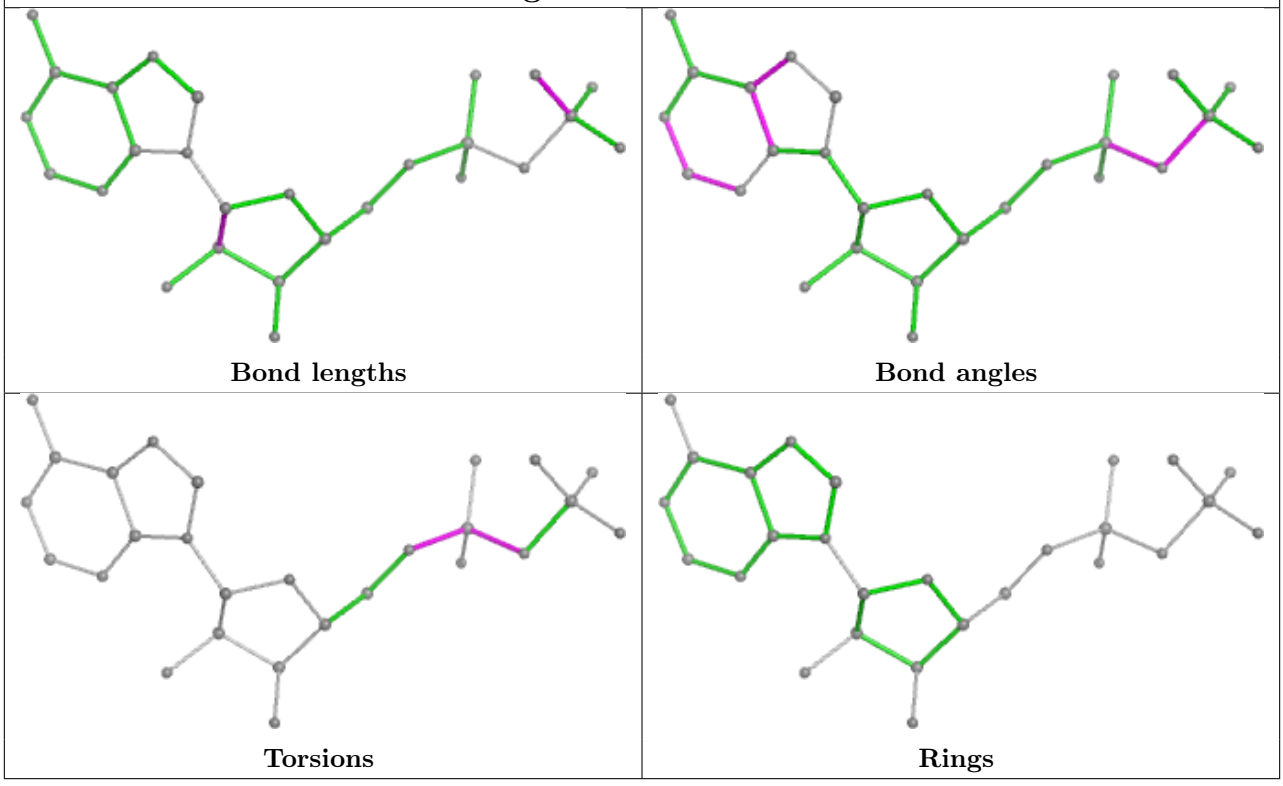
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	ADP	3	0
2	B	701	ADP	5	0
2	F	701	ADP	3	0
2	C	701	ADP	1	0
2	A	701	ADP	2	0

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.

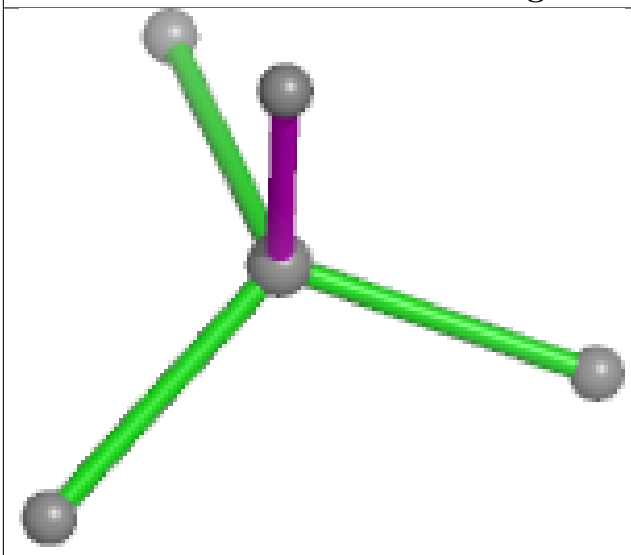
Ligand ADP E 701



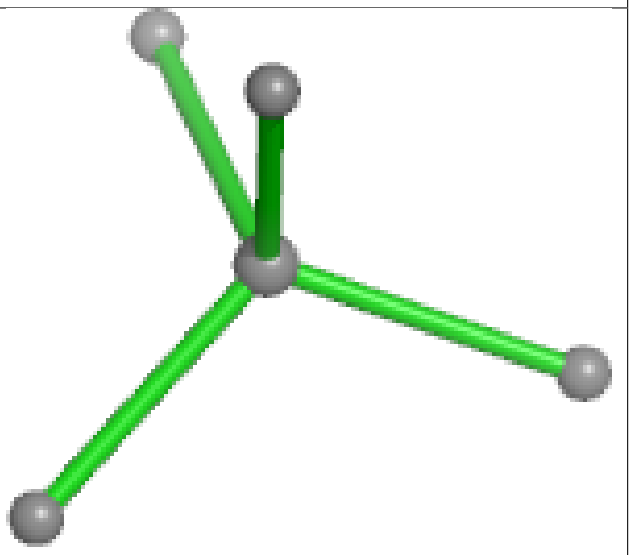
Ligand ADP B 701



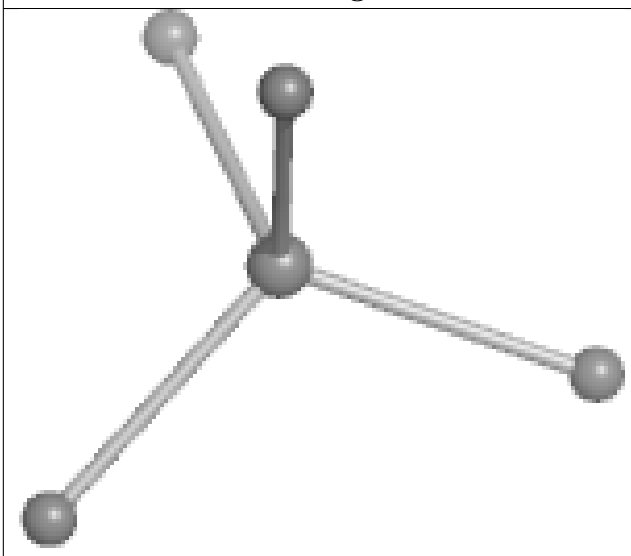
Ligand PO4 C 702



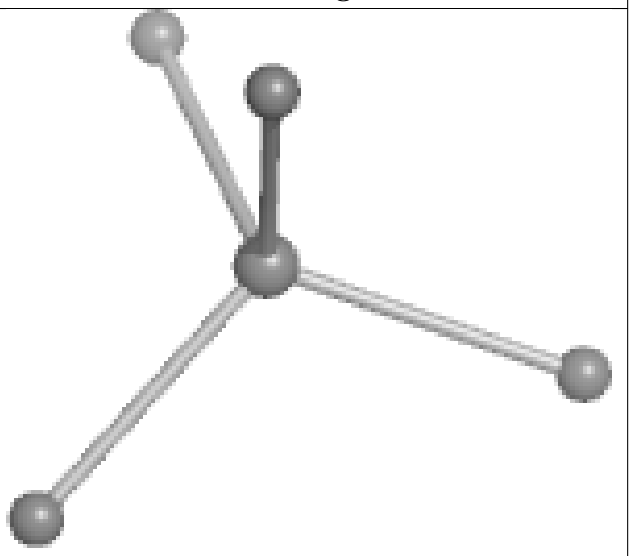
Bond lengths



Bond angles

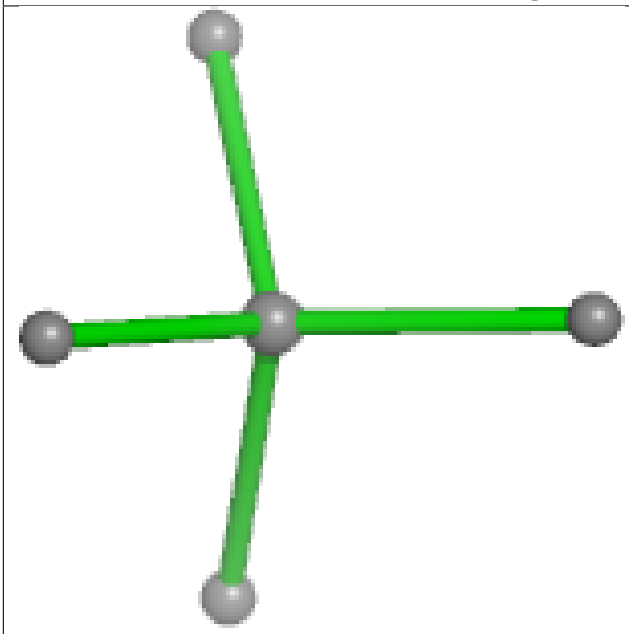


Torsions

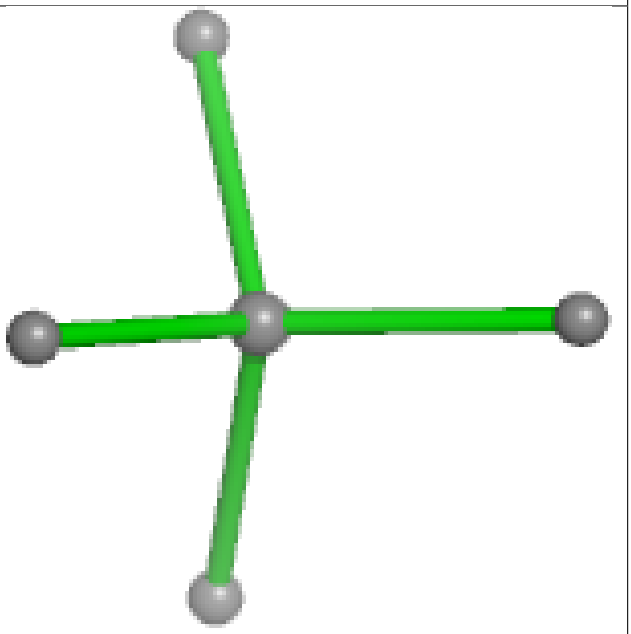


Rings

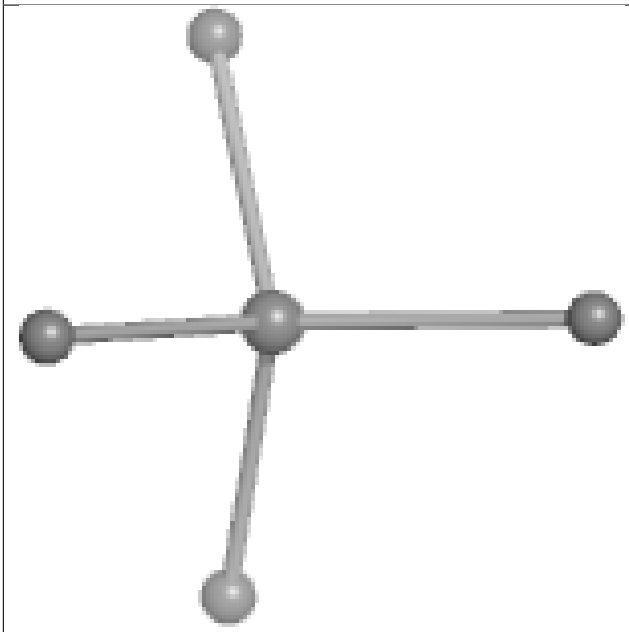
Ligand PO4 D 702



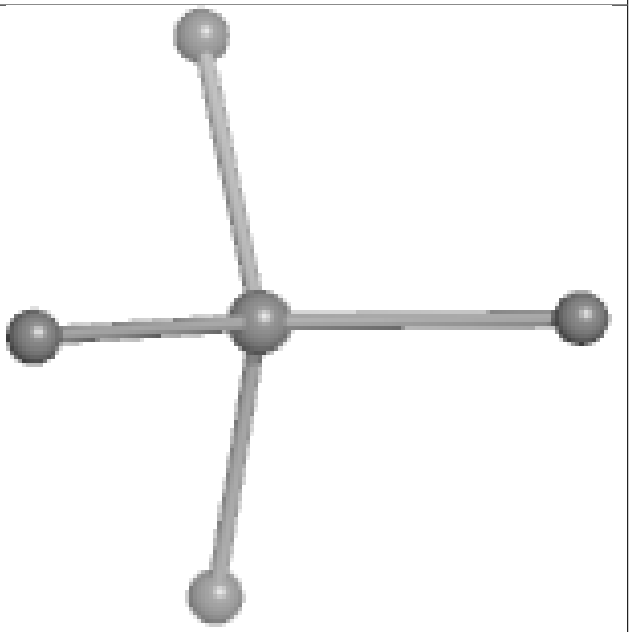
Bond lengths



Bond angles

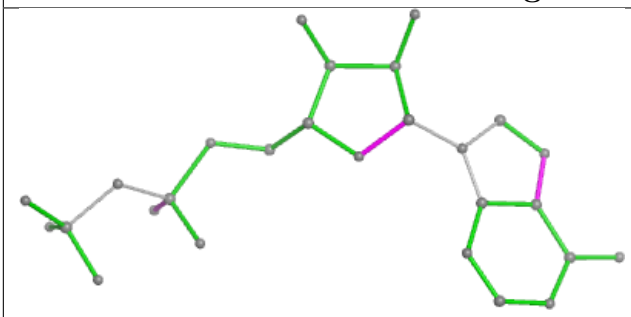


Torsions

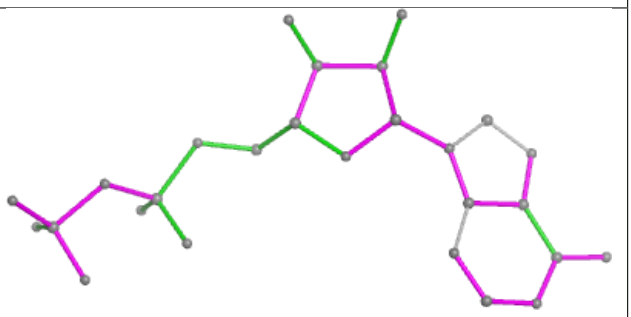


Rings

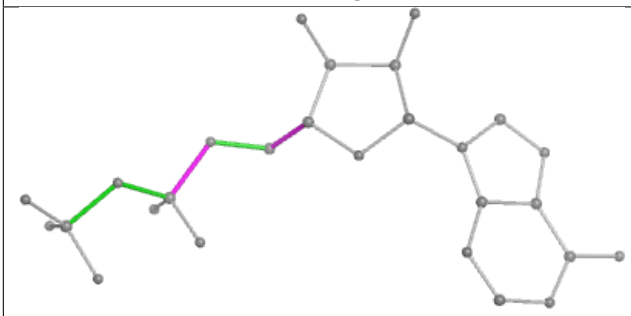
Ligand ADP F 701



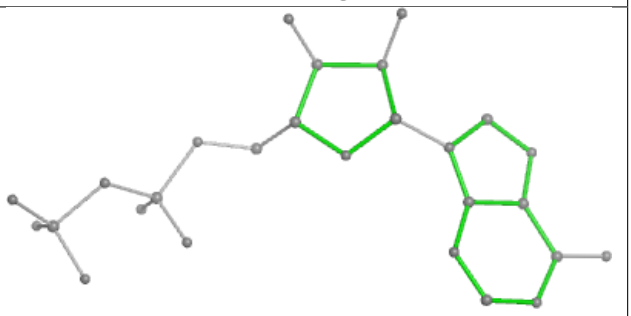
Bond lengths



Bond angles

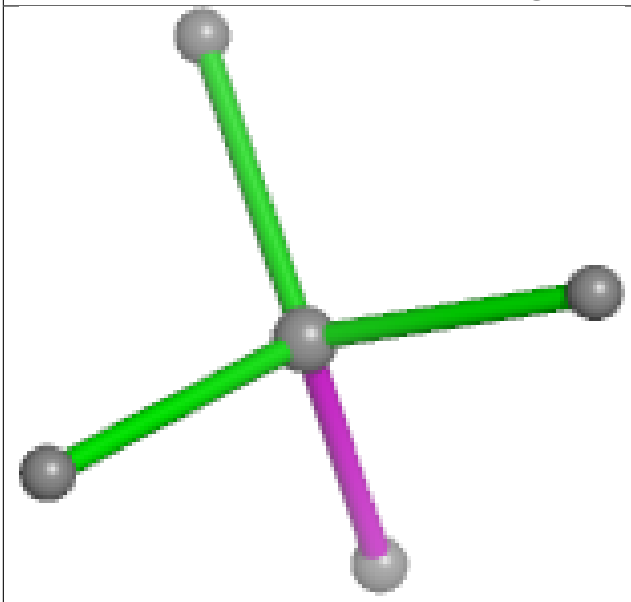


Torsions

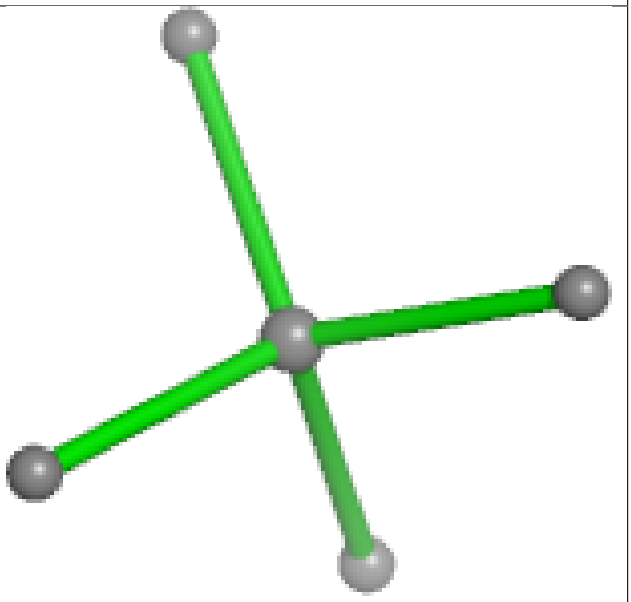


Rings

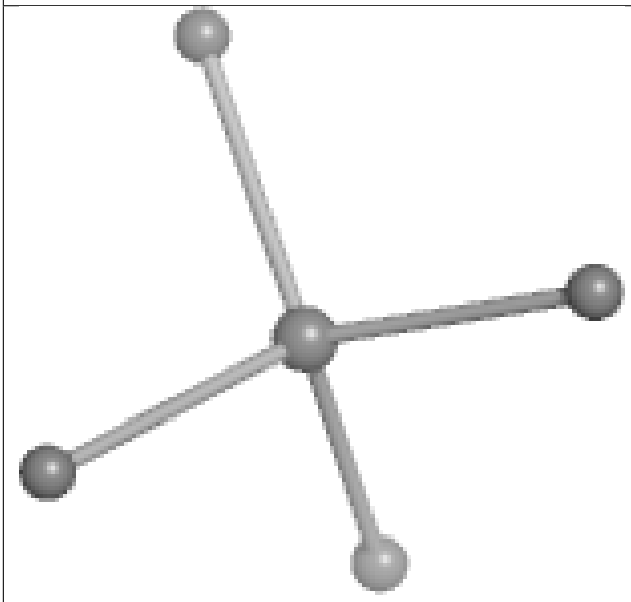
Ligand PO4 E 702



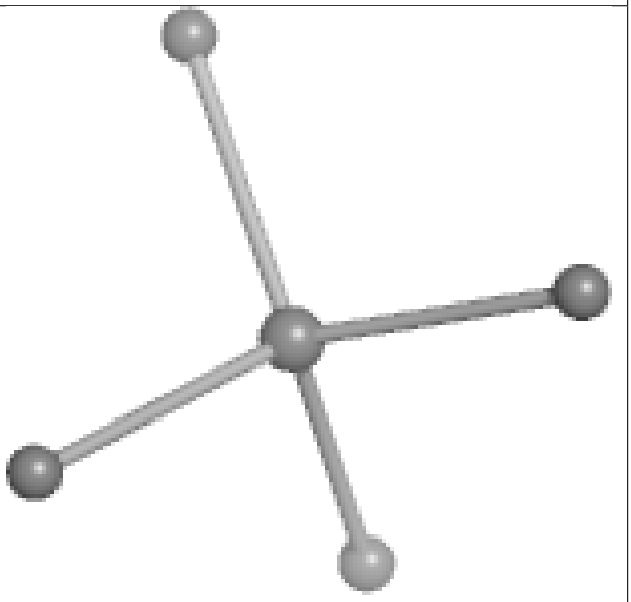
Bond lengths



Bond angles

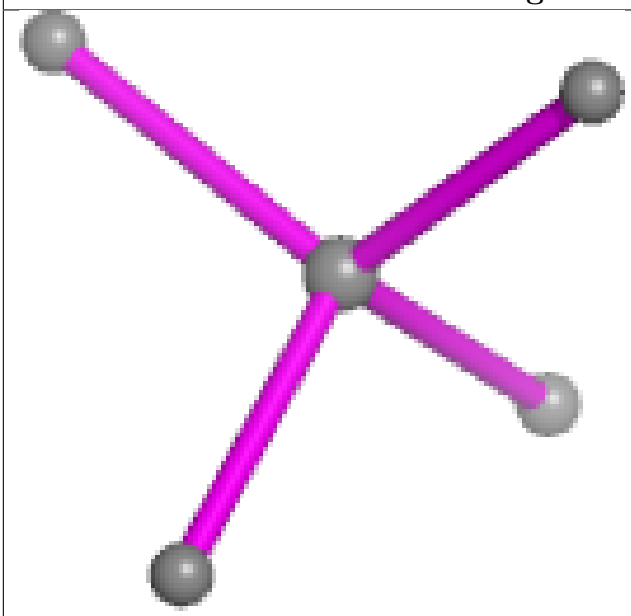


Torsions

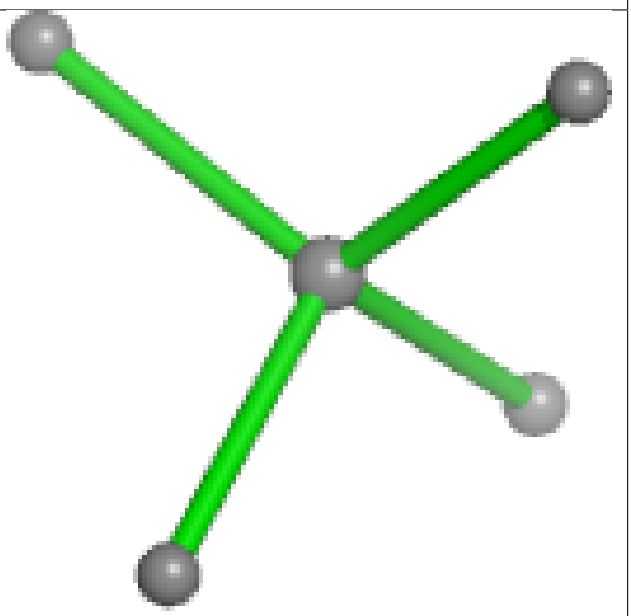


Rings

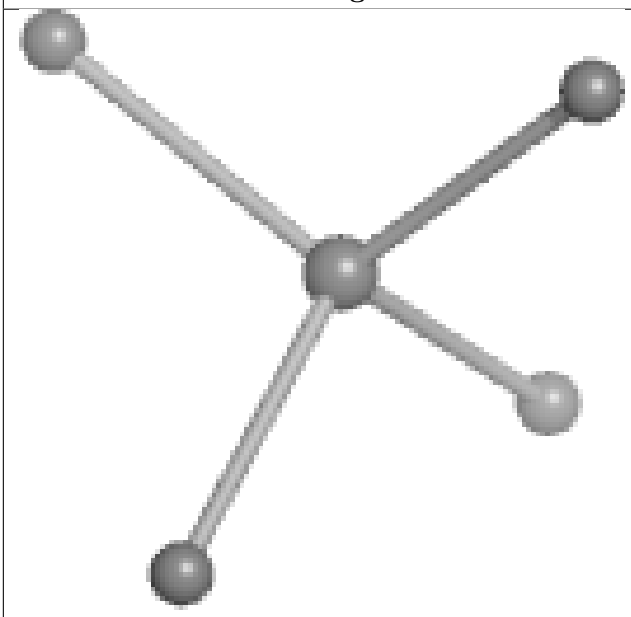
Ligand PO4 A 702



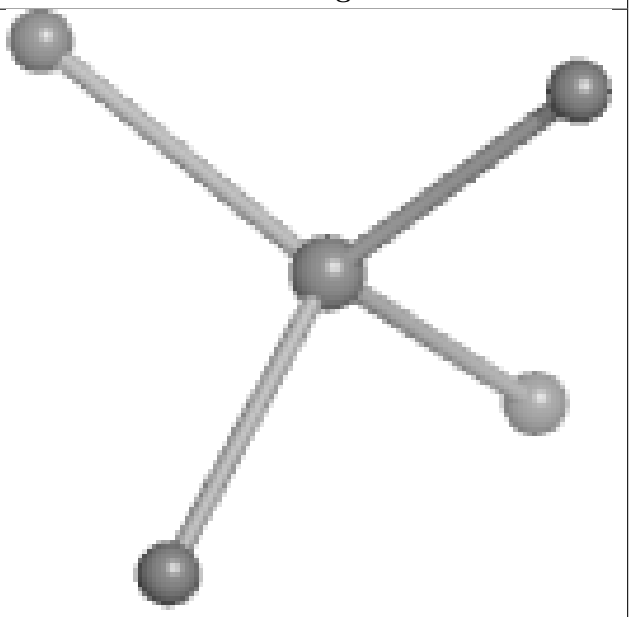
Bond lengths



Bond angles

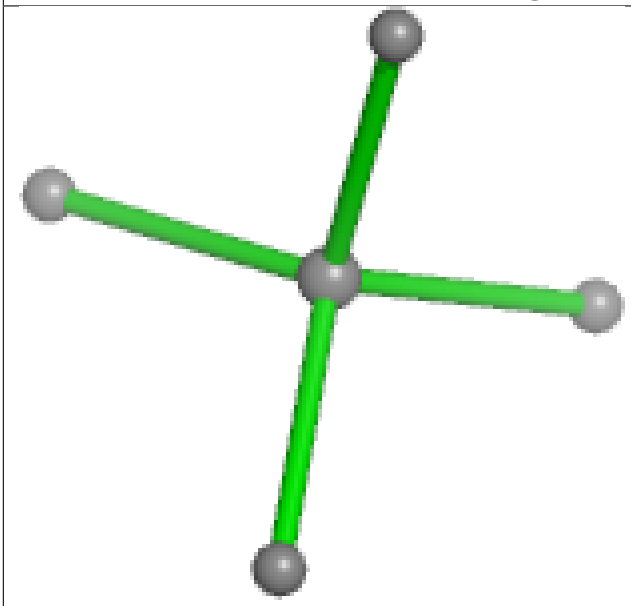


Torsions

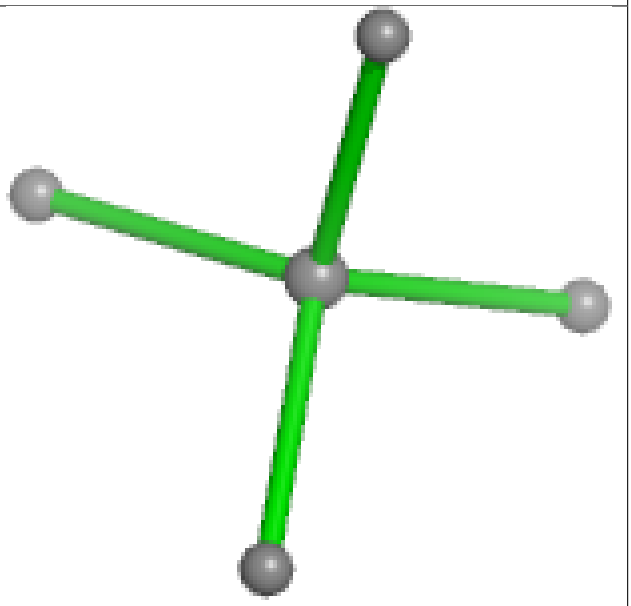


Rings

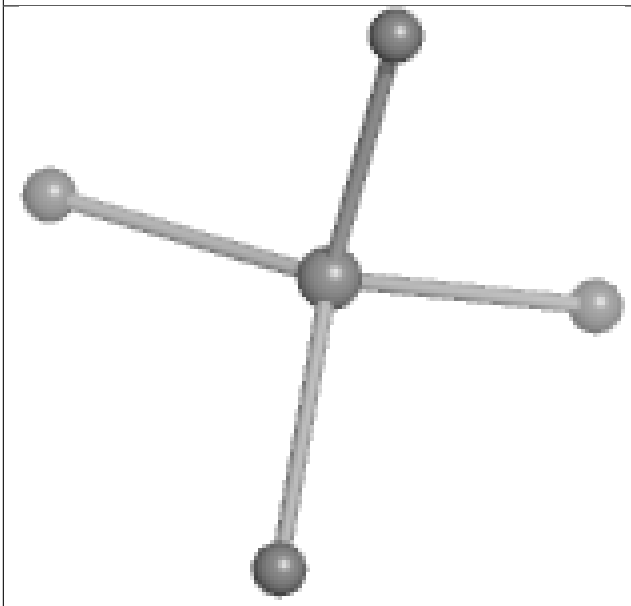
Ligand PO4 D 701



Bond lengths



Bond angles



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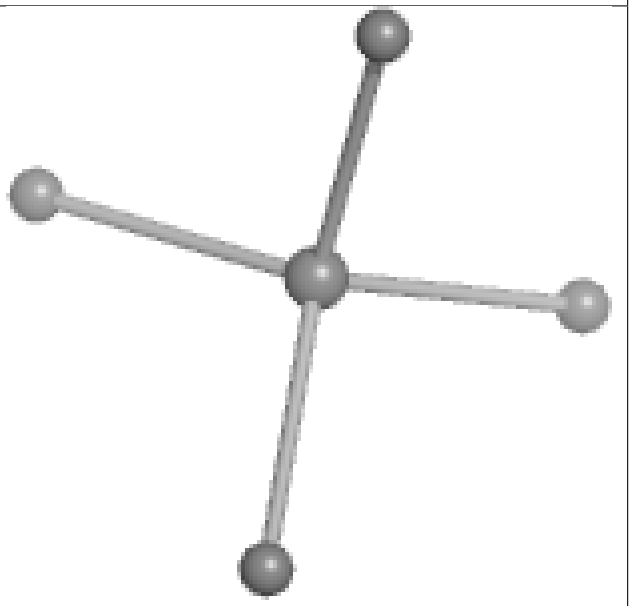
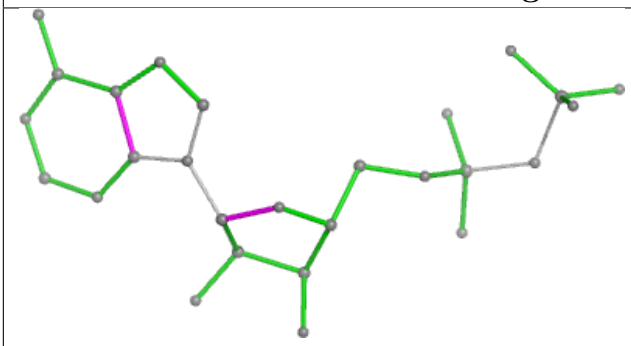
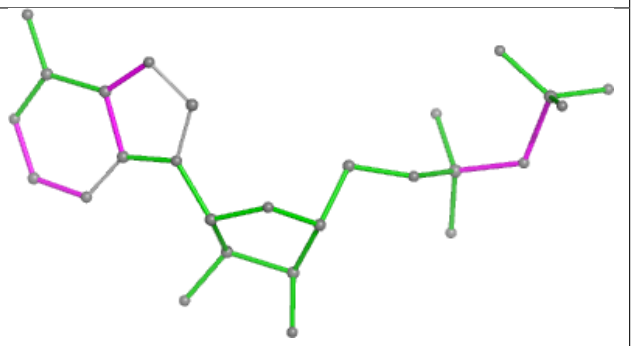


Rings

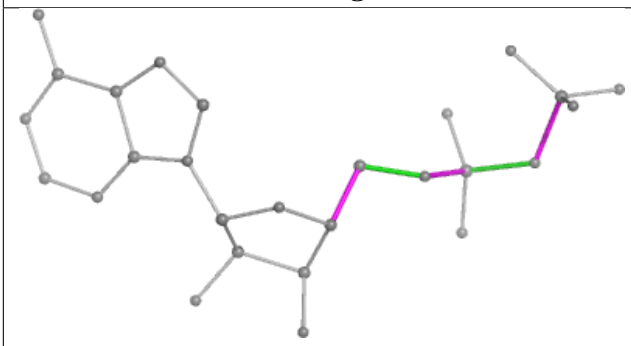
Ligand ADP C 701



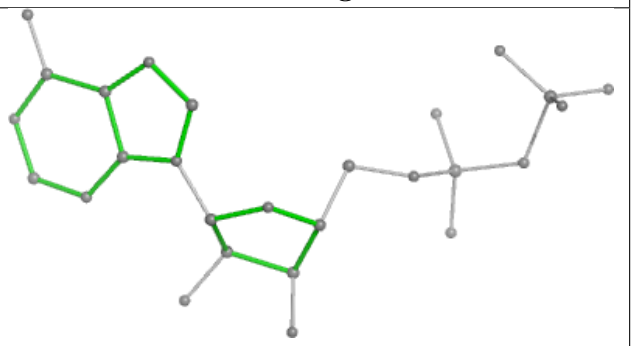
Bond lengths



Bond angles

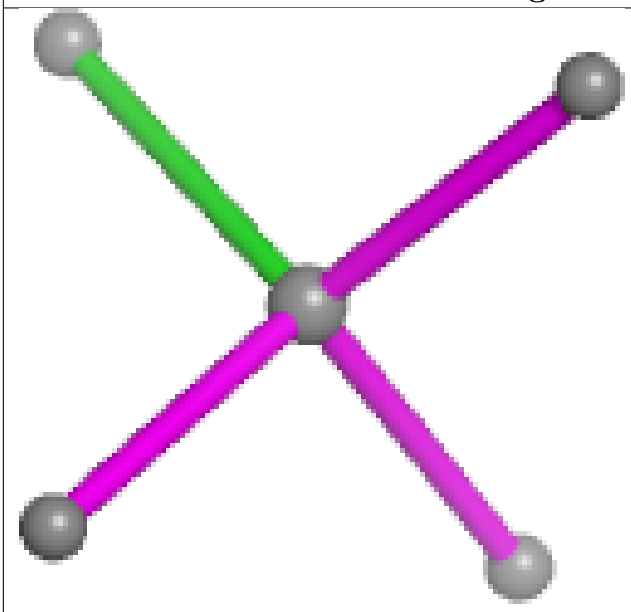


Torsions

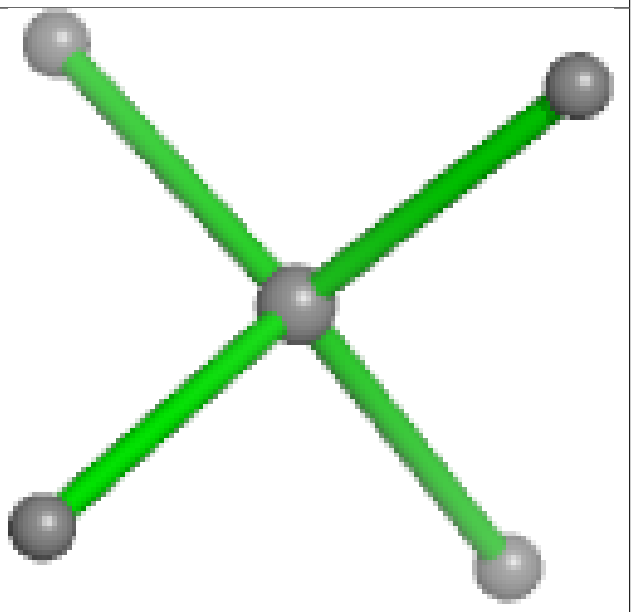


Rings

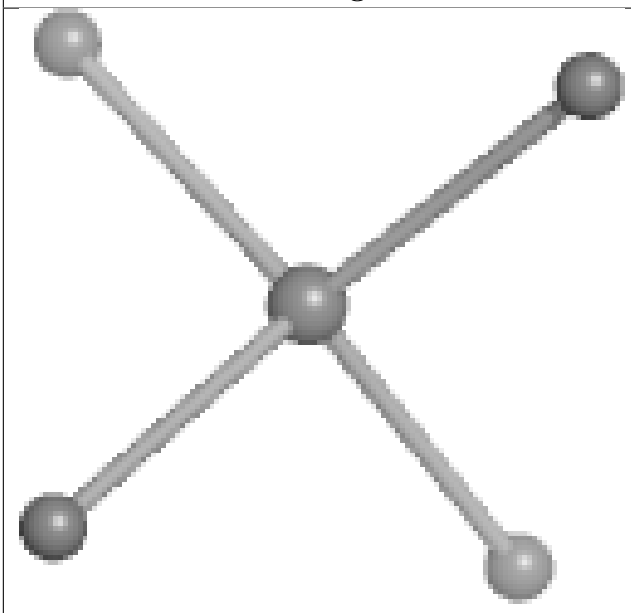
Ligand PO4 F 702



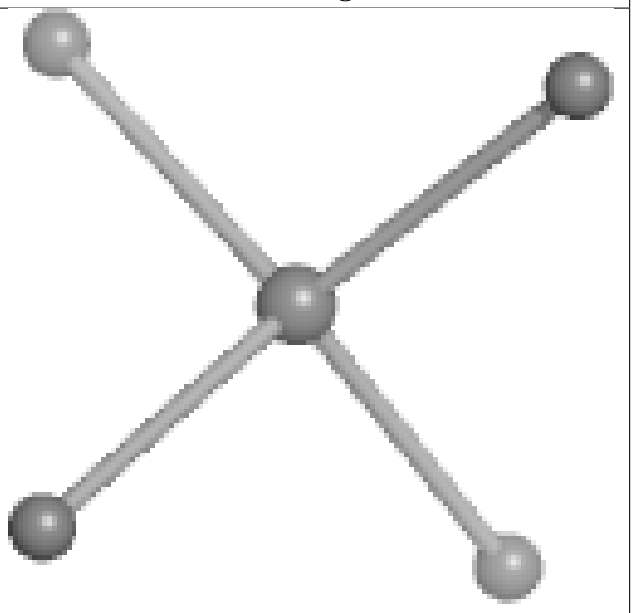
Bond lengths



Bond angles

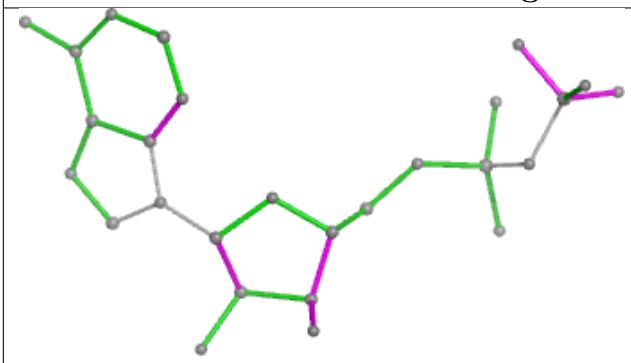


Torsions

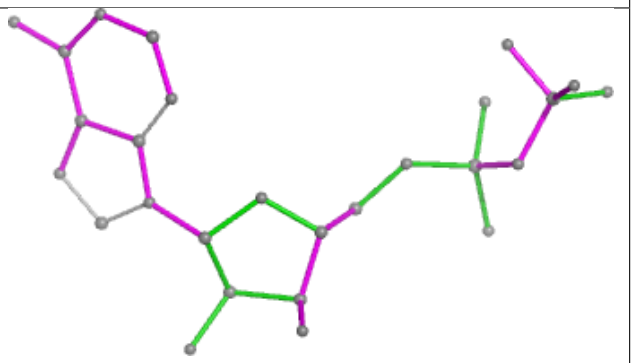


Rings

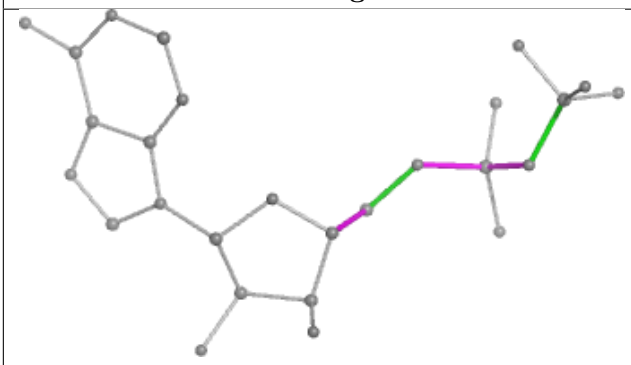
Ligand ADP A 701



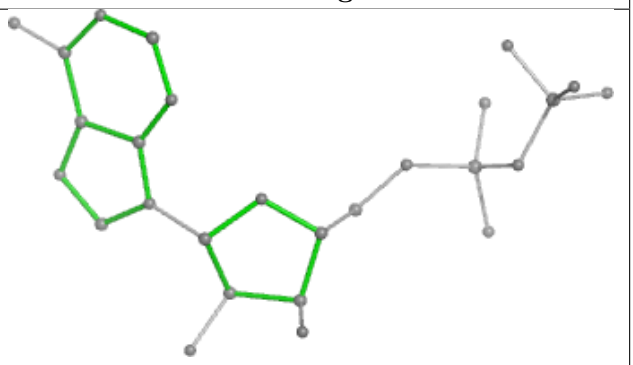
Bond lengths



Bond angles

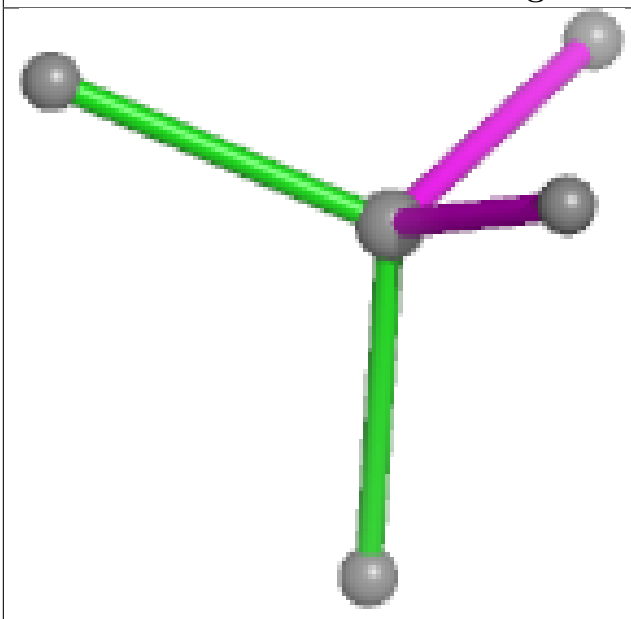


Torsions

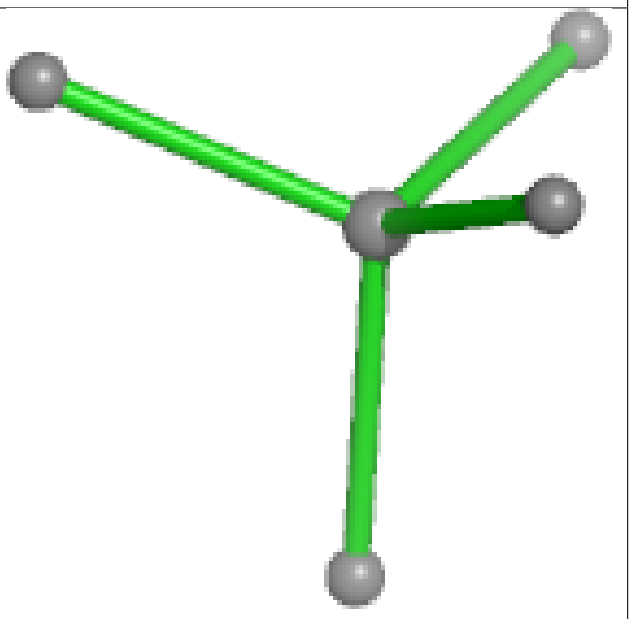


Rings

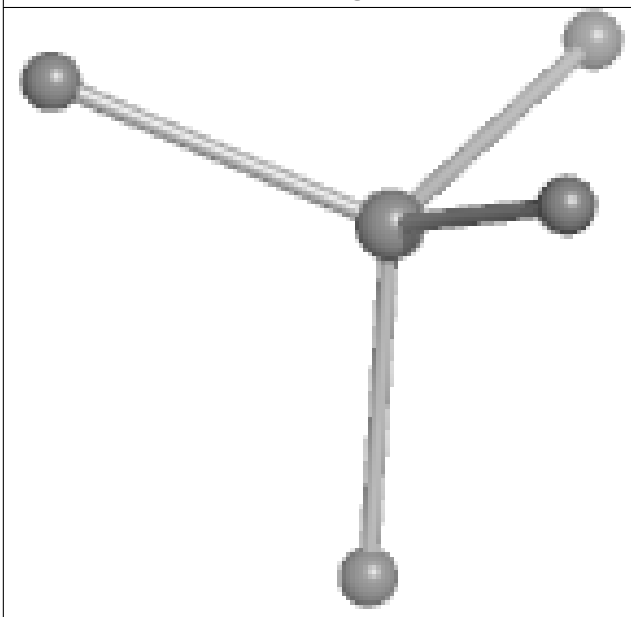
Ligand PO4 B 702



Bond lengths



Bond angles



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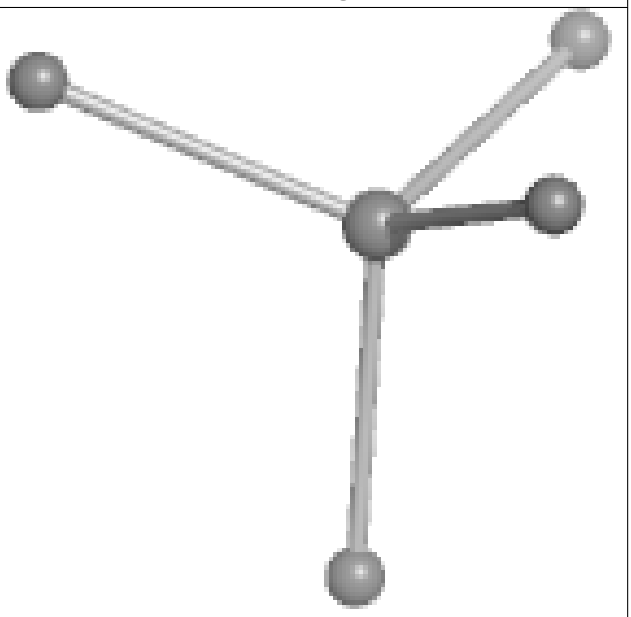


Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	574/601 (95%)	0.32	22 (3%)	44	38	49, 95, 127, 159	1 (0%)
1	B	572/601 (95%)	0.58	31 (5%)	32	27	76, 108, 143, 160	0
1	C	574/601 (95%)	0.34	20 (3%)	47	41	71, 102, 130, 167	0
1	D	577/601 (96%)	0.40	25 (4%)	40	34	76, 100, 138, 177	0
1	E	574/601 (95%)	0.48	25 (4%)	39	33	71, 115, 145, 181	0
1	F	582/601 (96%)	0.41	24 (4%)	42	36	65, 104, 139, 169	0
All	All	3453/3606 (95%)	0.42	147 (4%)	40	34	49, 103, 139, 181	1 (0%)

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	596	THR	6.5
1	B	446	PRO	6.1
1	F	545	ALA	5.6
1	B	282	VAL	5.5
1	E	282	VAL	5.0

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)

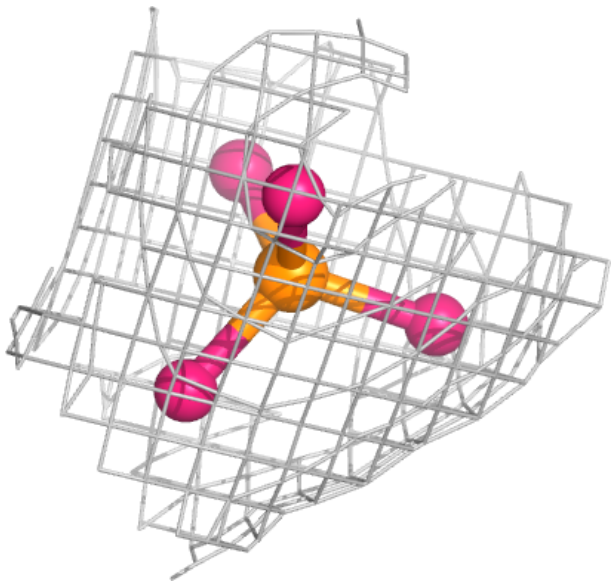
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

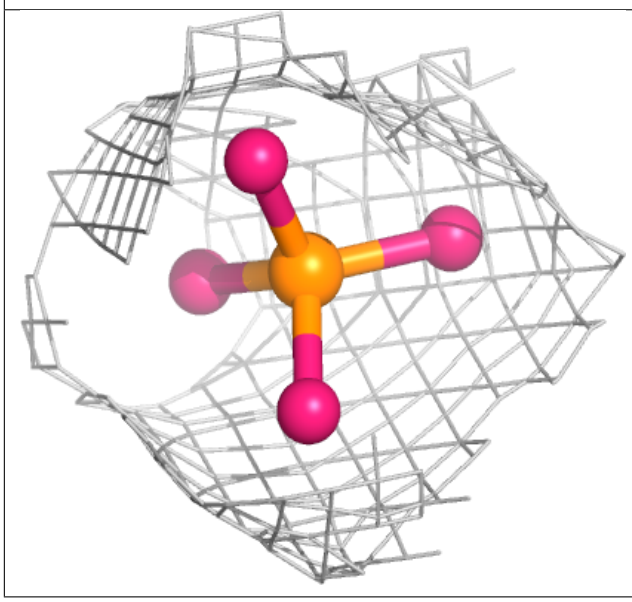
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	C	702	5/5	0.66	0.11	109,112,122,134	0
3	PO4	B	702	5/5	0.78	0.09	102,107,119,125	0
3	PO4	D	701	5/5	0.83	0.09	101,101,123,125	0
3	PO4	A	702	5/5	0.85	0.07	97,106,115,119	0
3	PO4	F	702	5/5	0.87	0.07	95,95,102,107	0
3	PO4	E	702	5/5	0.88	0.08	100,101,103,117	0
2	ADP	A	701	27/27	0.88	0.18	85,102,126,129	19
2	ADP	C	701	27/27	0.89	0.15	82,96,117,124	17
3	PO4	D	702	5/5	0.90	0.08	97,98,102,104	0
2	ADP	B	701	27/27	0.92	0.12	88,100,126,127	13
4	ZN	B	703	1/1	0.92	0.06	152,152,152,152	0
2	ADP	E	701	27/27	0.93	0.14	98,113,138,143	15
2	ADP	F	701	27/27	0.94	0.15	88,97,121,128	18
4	ZN	D	703	1/1	0.97	0.07	68,68,68,68	1
4	ZN	C	703	1/1	0.98	0.05	107,107,107,107	0
4	ZN	F	703	1/1	0.98	0.05	118,118,118,118	1
4	ZN	E	703	1/1	0.99	0.03	127,127,127,127	0
4	ZN	A	703	1/1	0.99	0.05	95,95,95,95	1

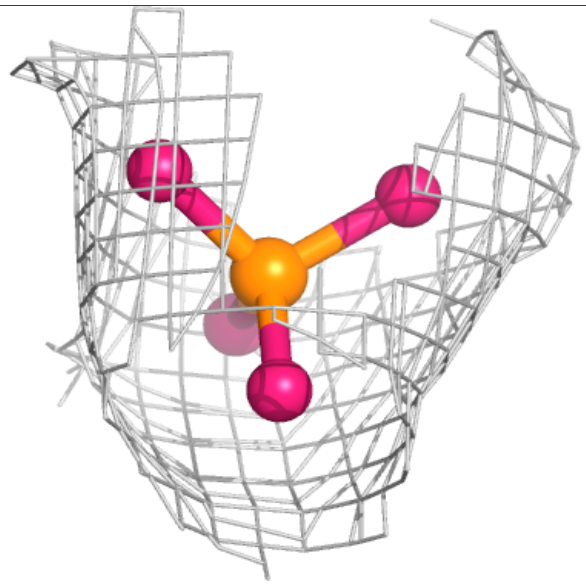
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PO4 C 702:

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

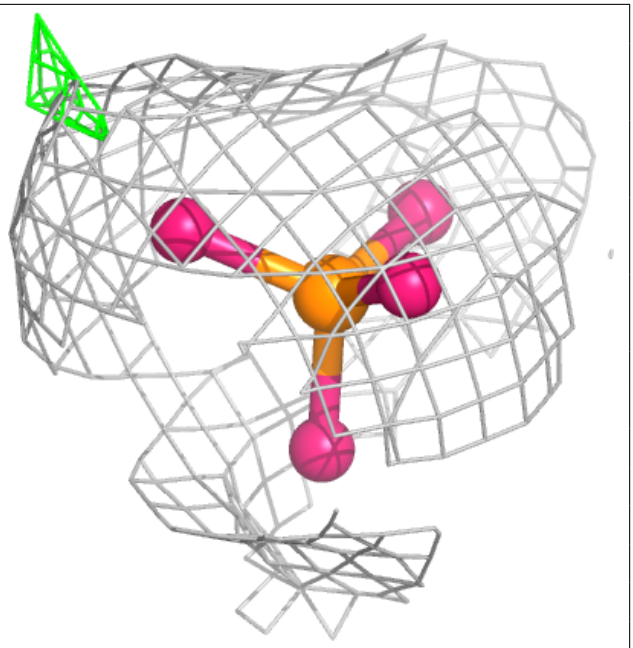


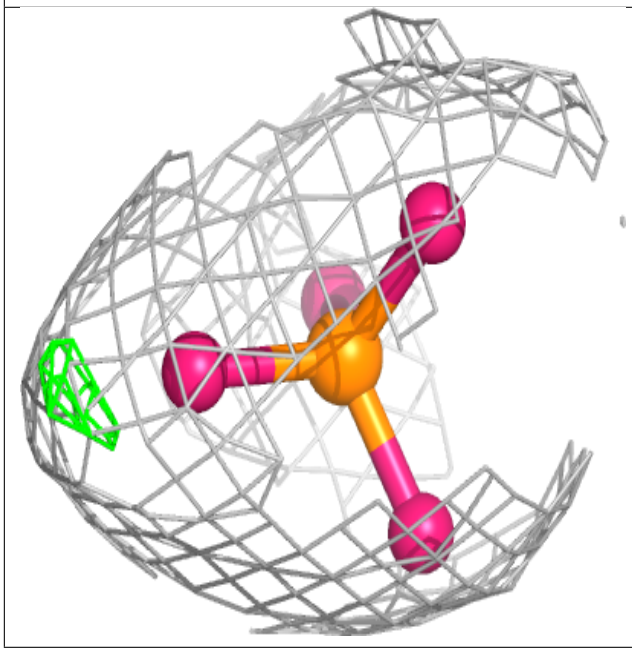


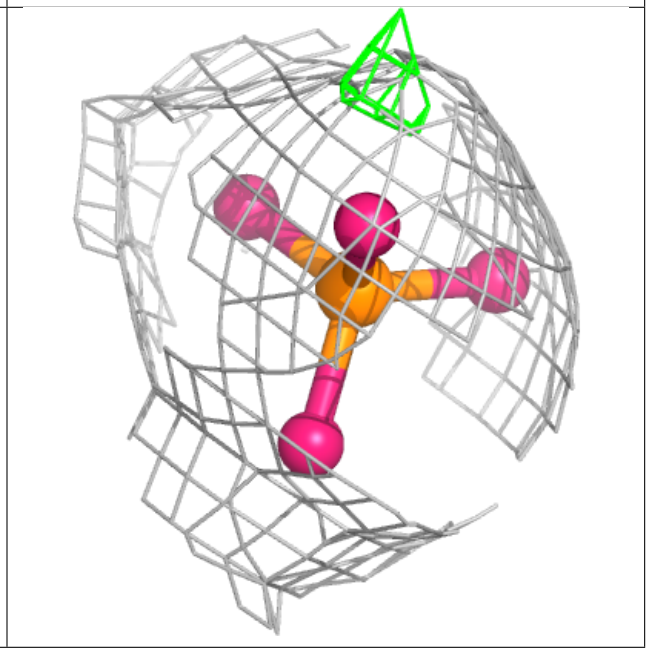


Electron density around PO4 B 702:

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

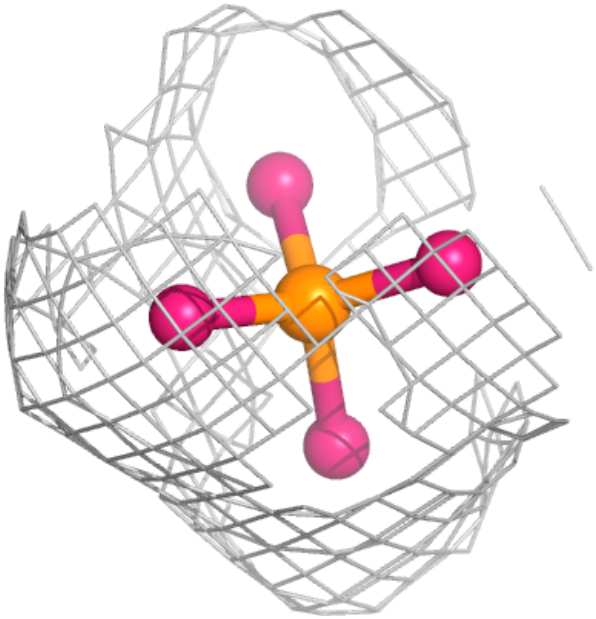


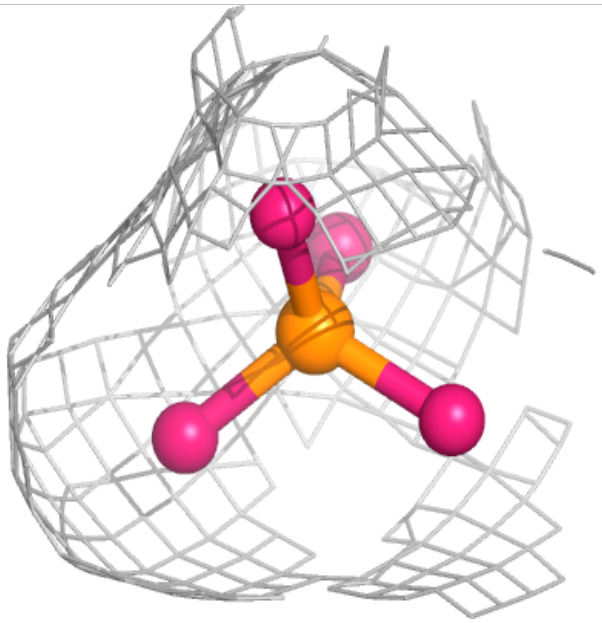


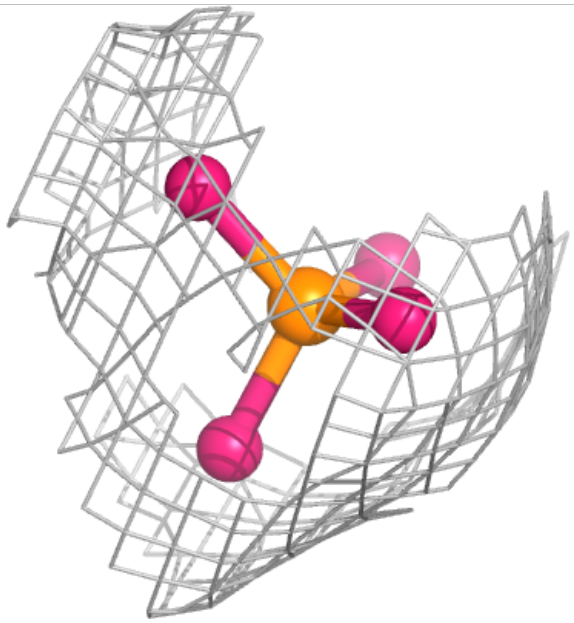


Electron density around PO4 D 701:

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

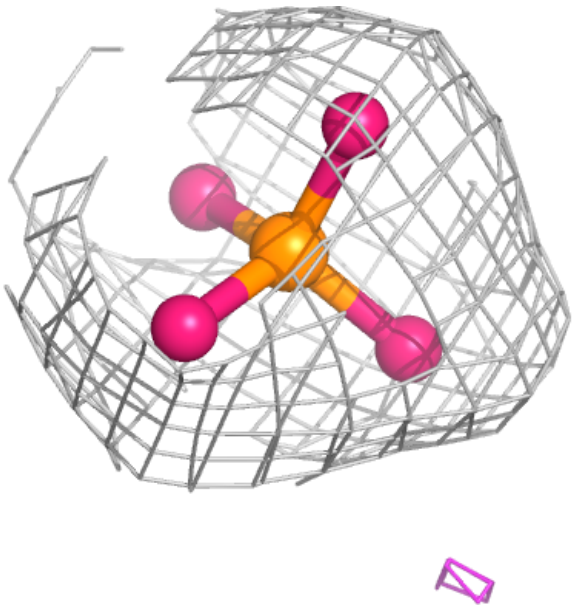


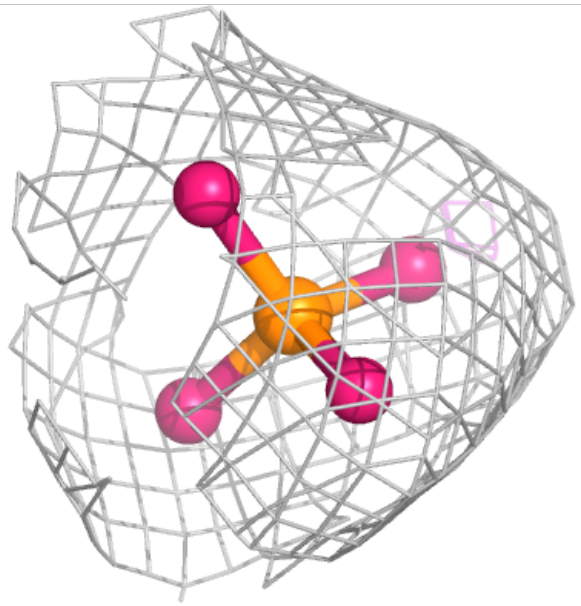


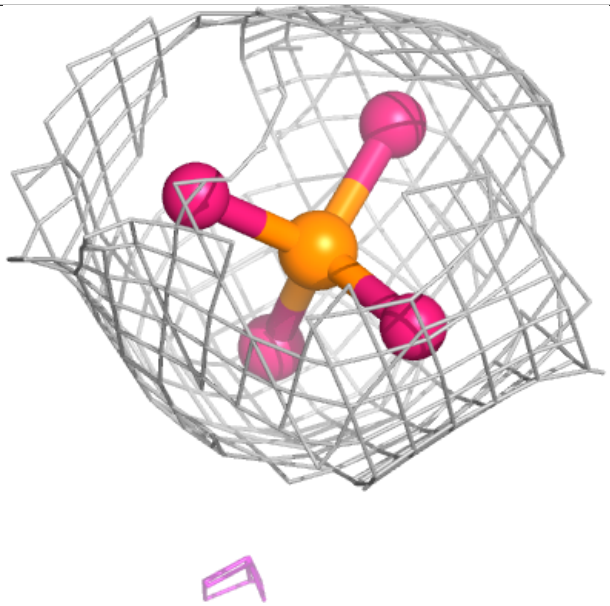


Electron density around PO4 A 702:

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

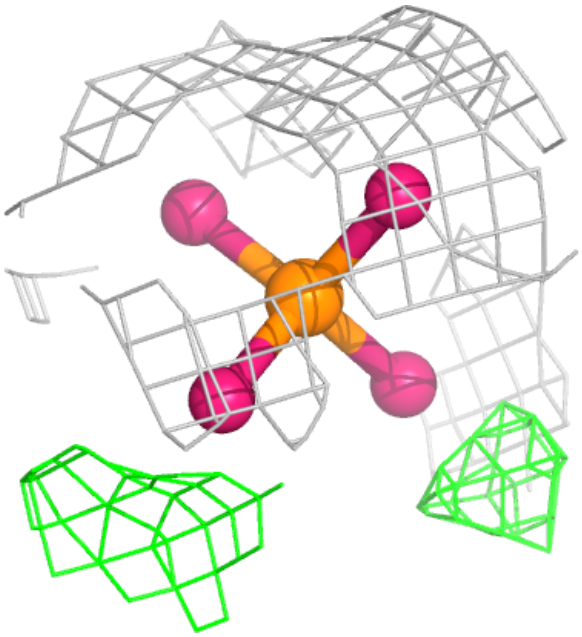


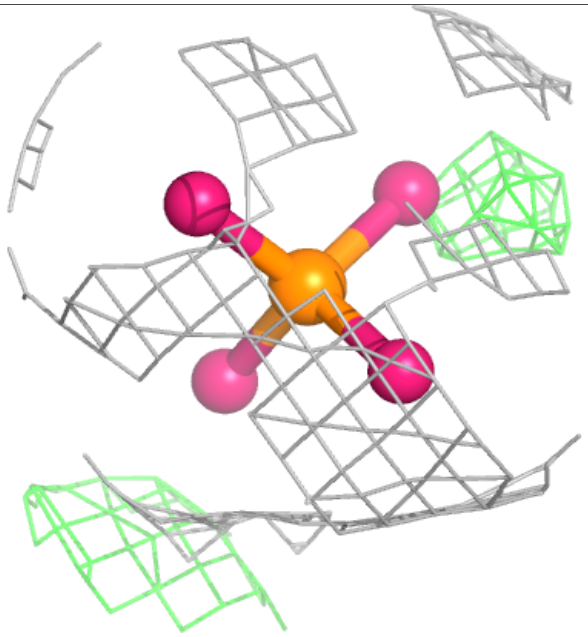


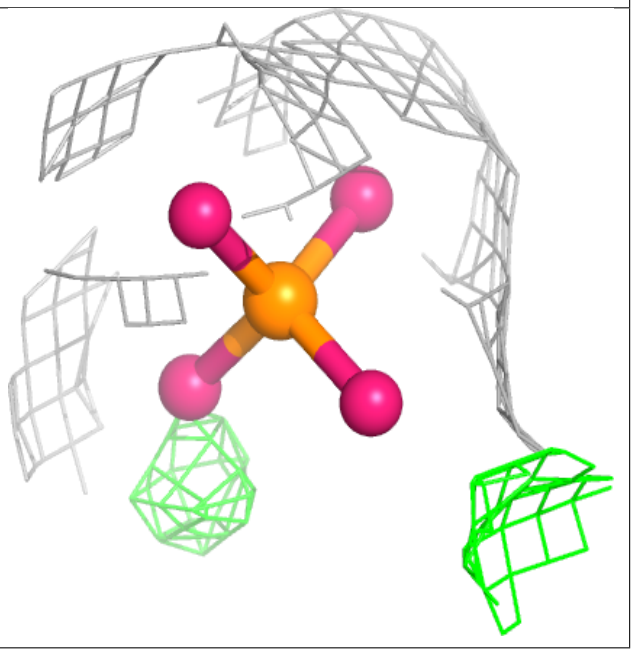


Electron density around PO4 F 702:

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

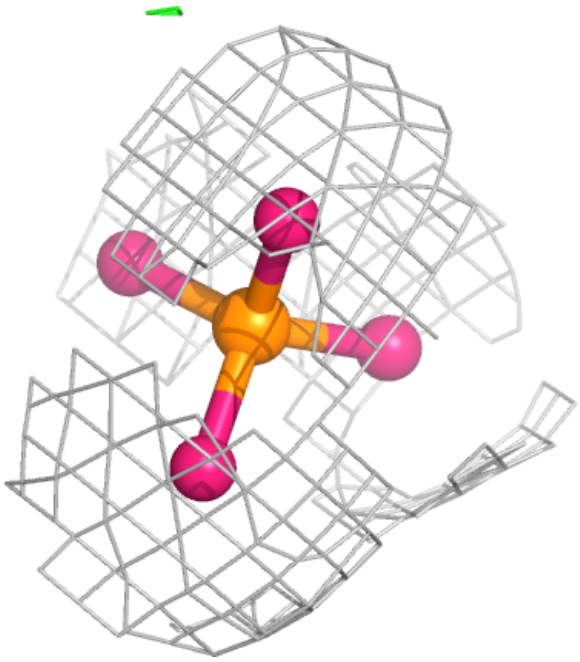


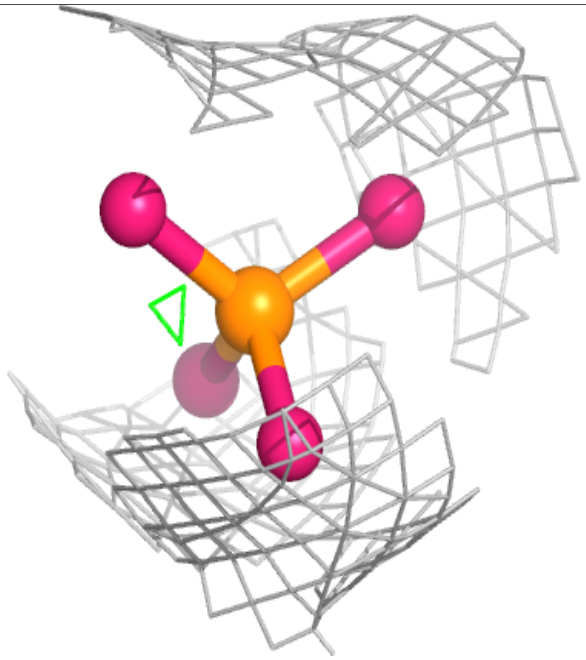


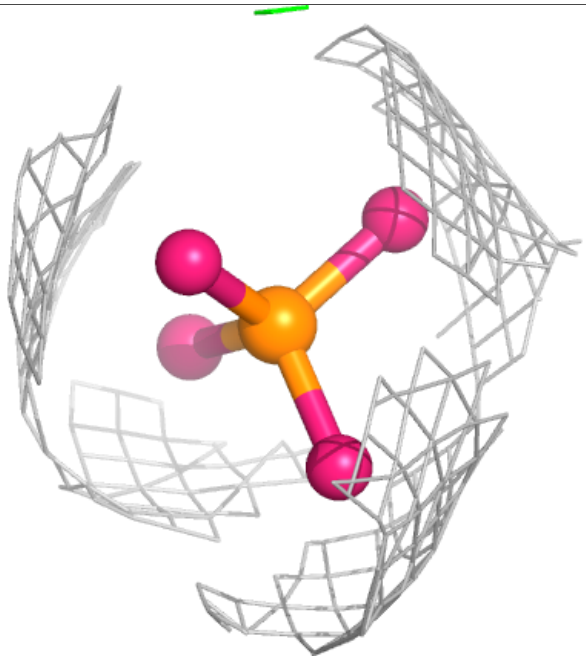


Electron density around PO4 E 702:

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

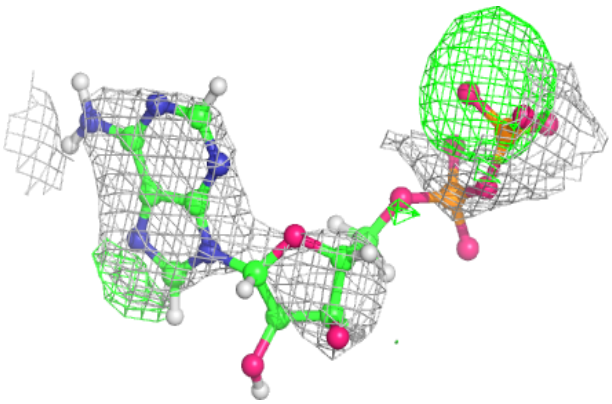


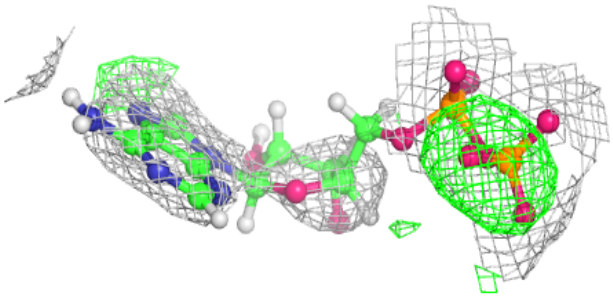


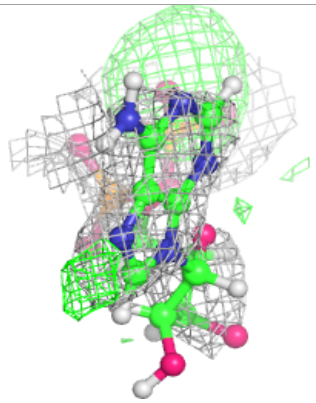


Electron density around ADP A 701:

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

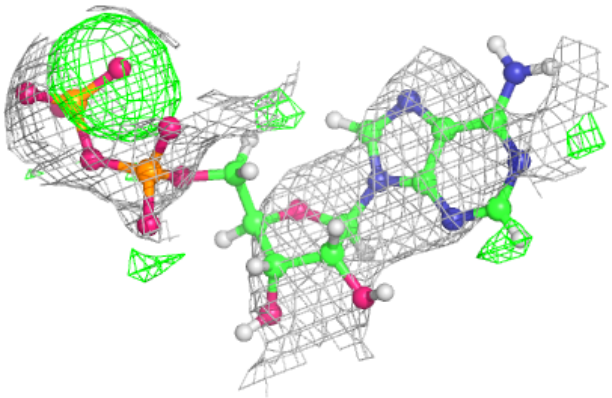


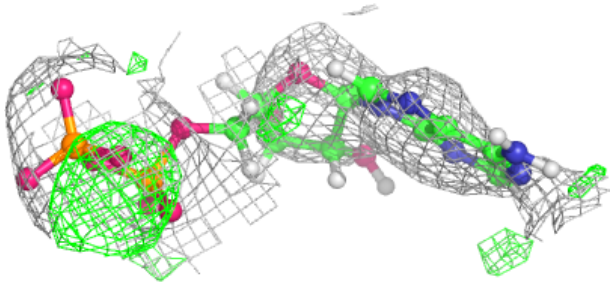


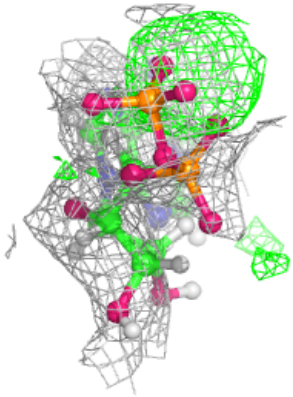


Electron density around ADP C 701:

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

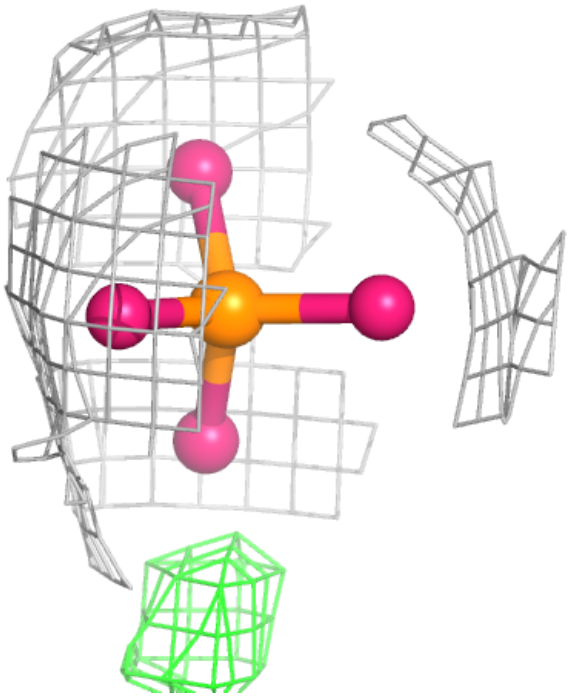


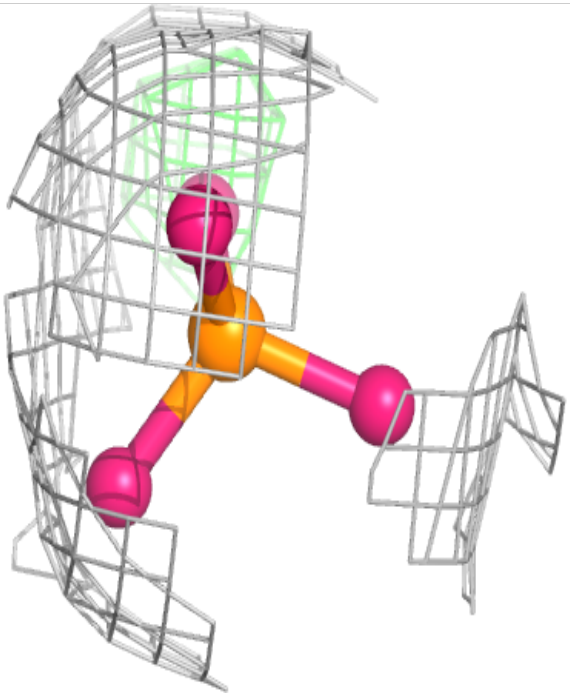




Electron density around PO4 D 702:

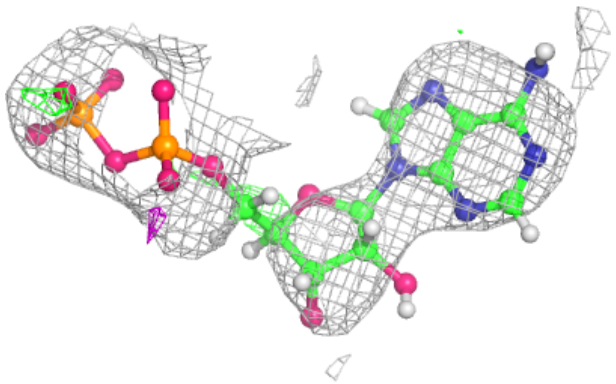
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

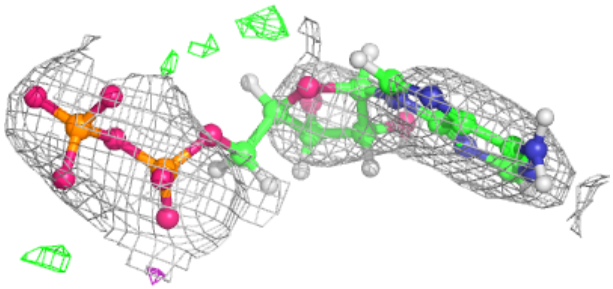


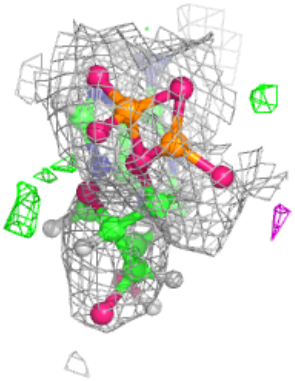


Electron density around ADP B 701:

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

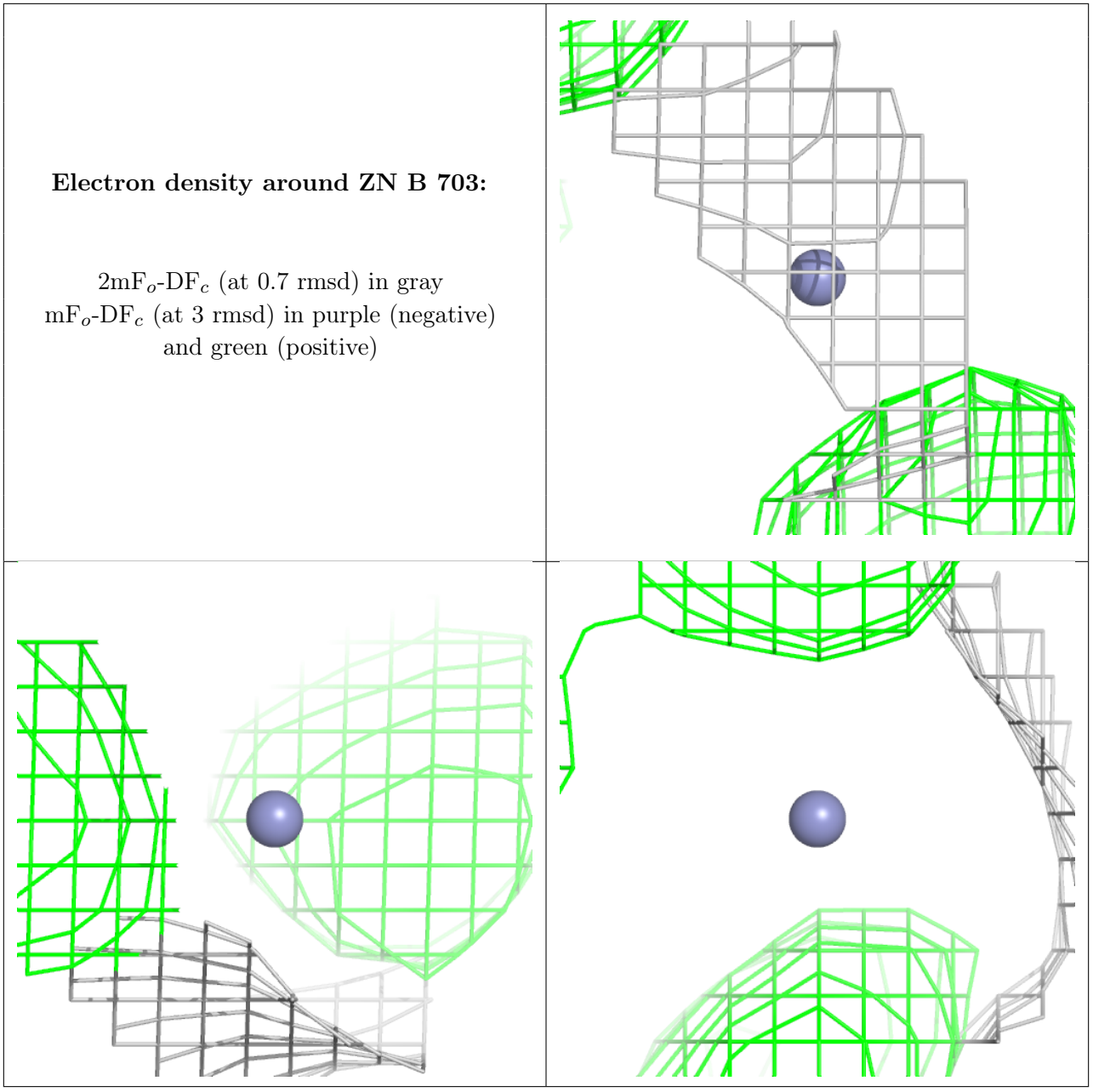






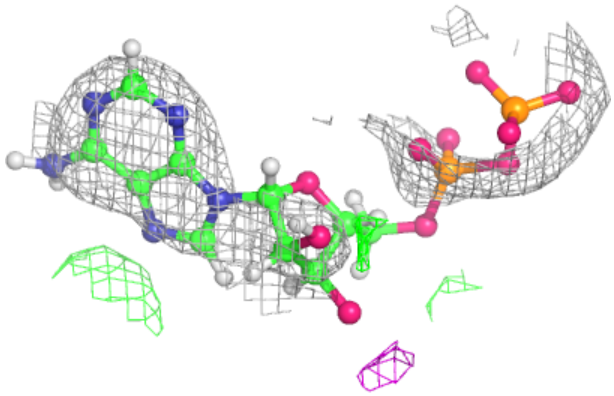
Electron density around ZN B 703:

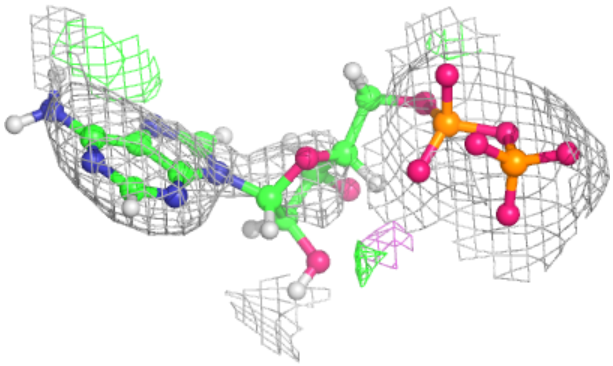
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

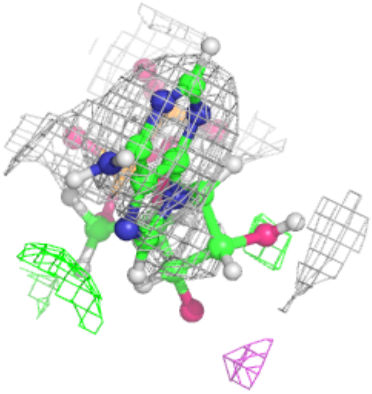


Electron density around ADP E 701:

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

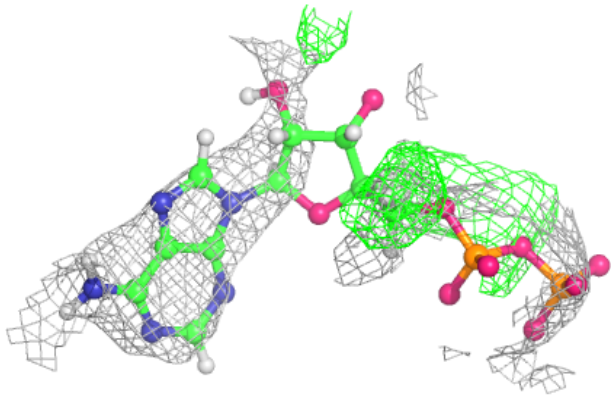


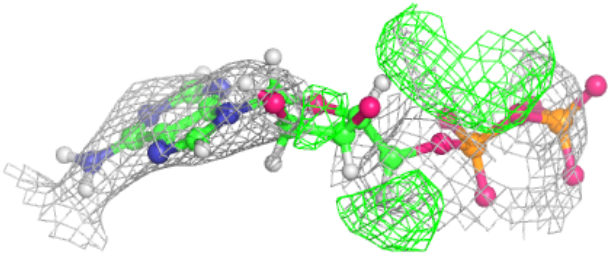


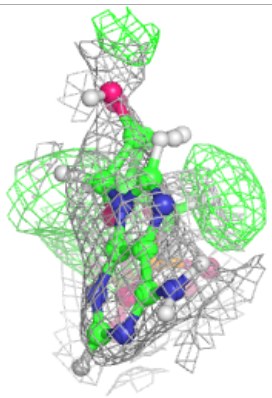


Electron density around ADP F 701:

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

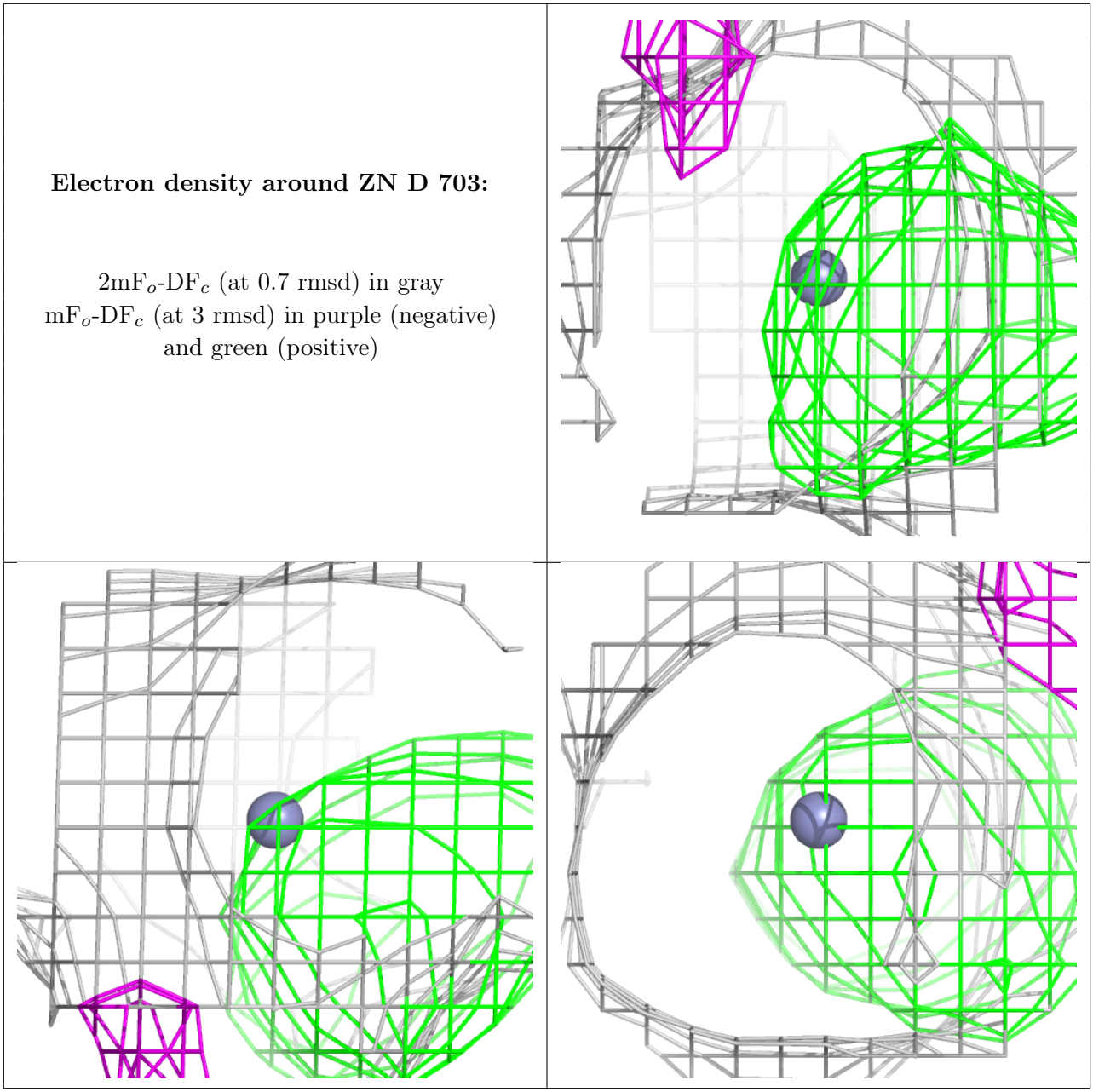






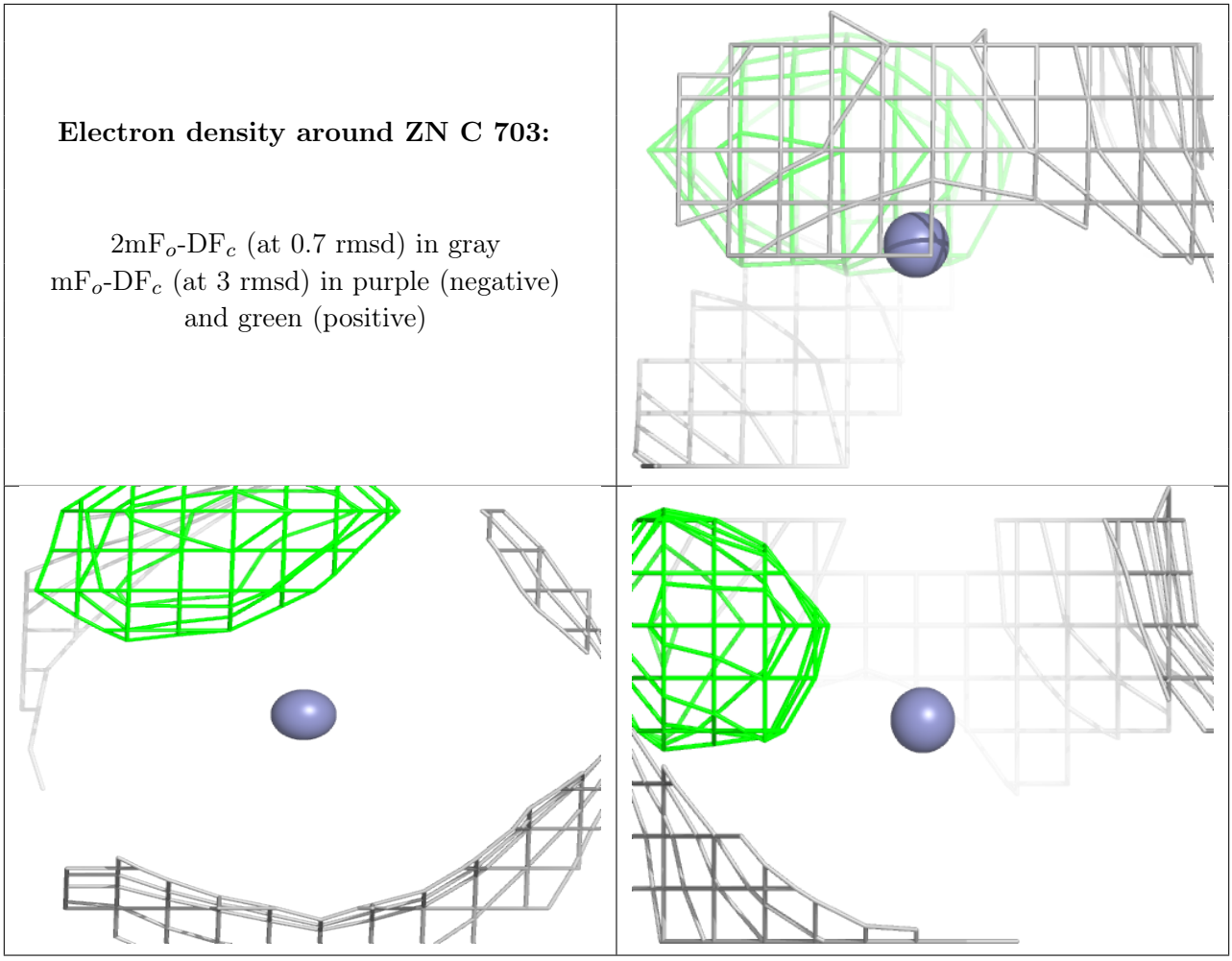
Electron density around ZN D 703:

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



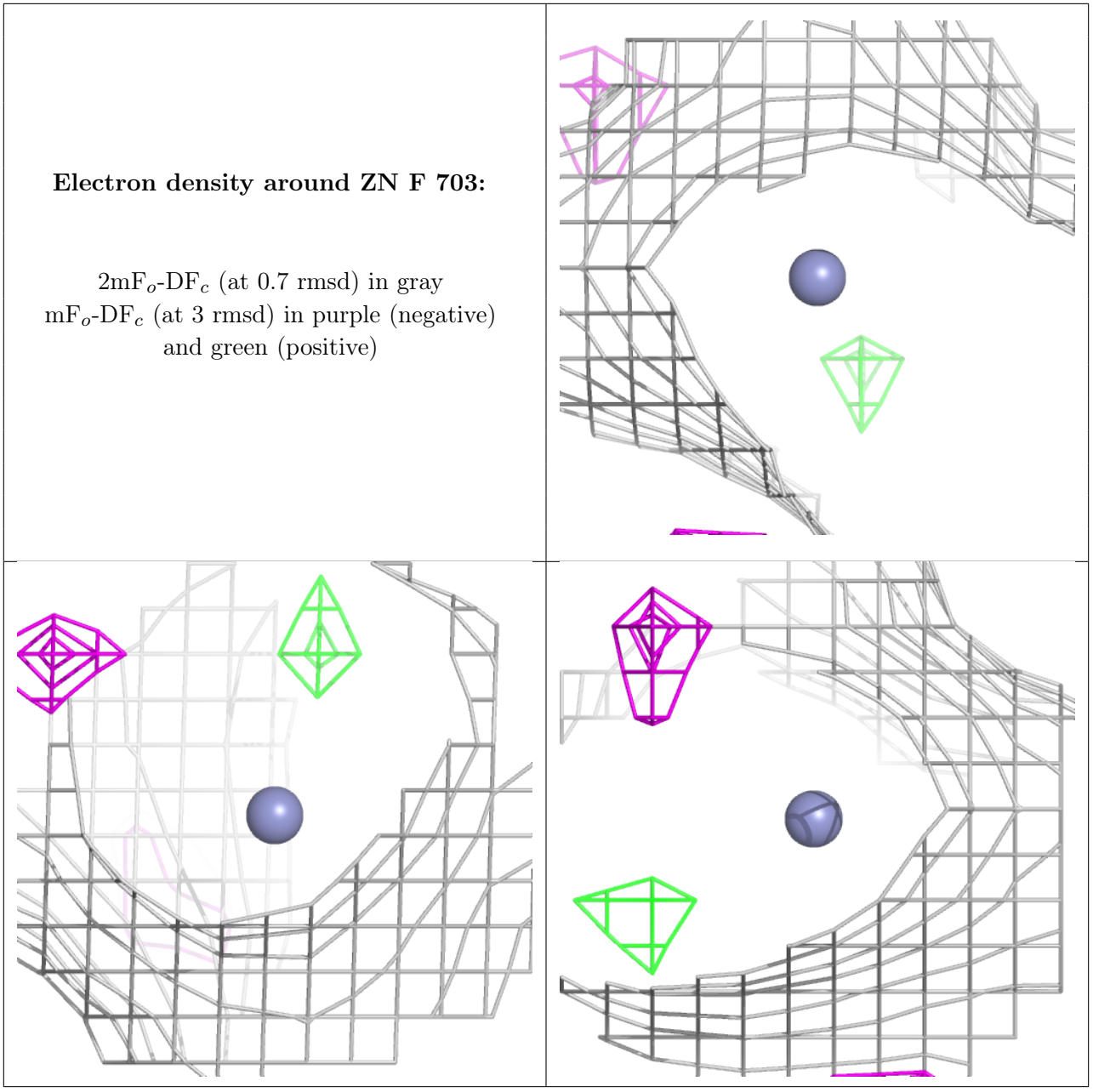
Electron density around ZN C 703:

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



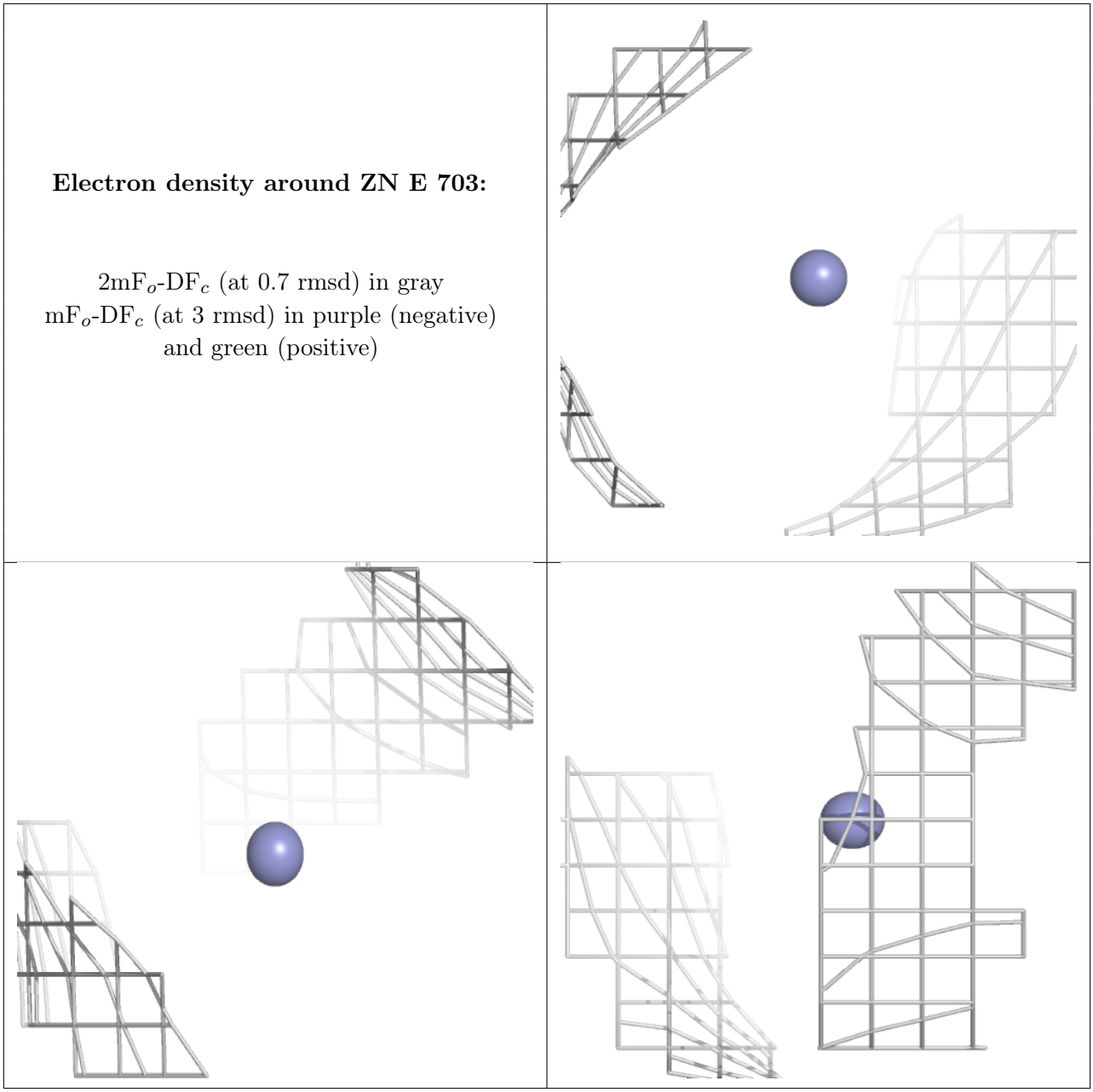
Electron density around ZN F 703:

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



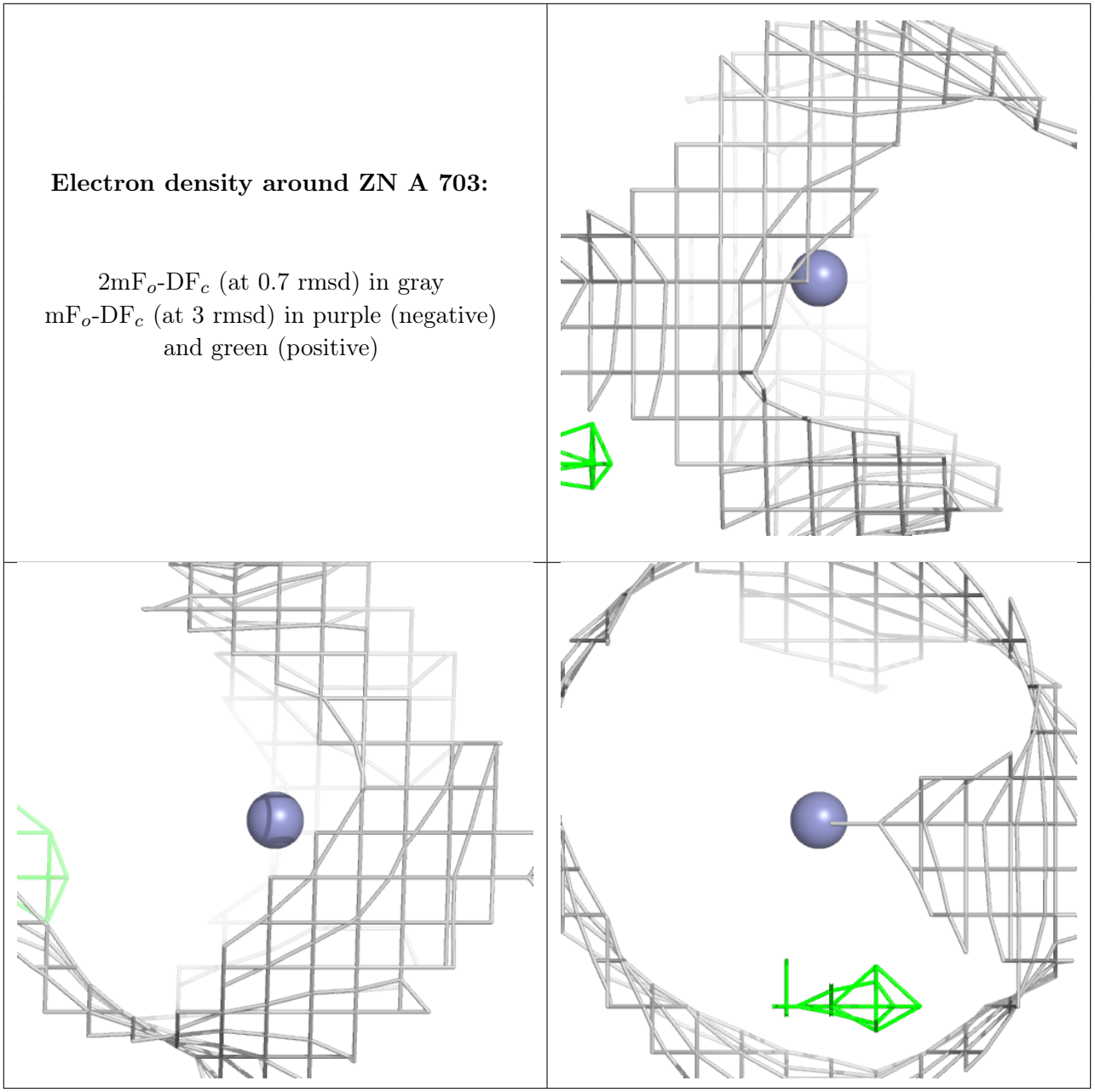
Electron density around ZN E 703:

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



Electron density around ZN A 703:

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



6.5 Other polymers (i)

There are no such residues in this entry.