wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 04:23 pm BST

PDB ID	:	8AJU
Title	:	Crystal structure of the Q65A mutant of S-adenosyl-L-homocysteine hydrolase from Pseudomonas aeruginosa cocrystallized with adenosine in the presence of K+ cations
Authors	:	Drozdzal, P.; Wozniak, K.; Malecki, P.; Gawel, M.; Komorowska, M.; Brzezinski, K.
Deposited on	:	2022-07-28
Resolution	:	1.65 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 (1)) were used in the production of this report:

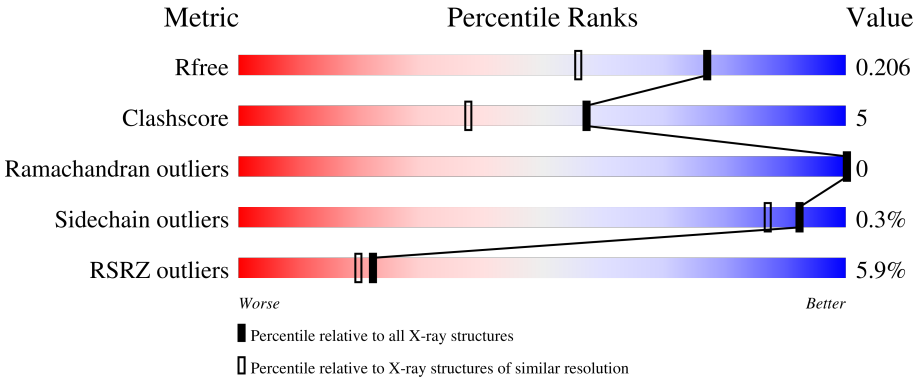
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	AAA	472	3% 89% 8%
1	CCC	472	8% 89% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

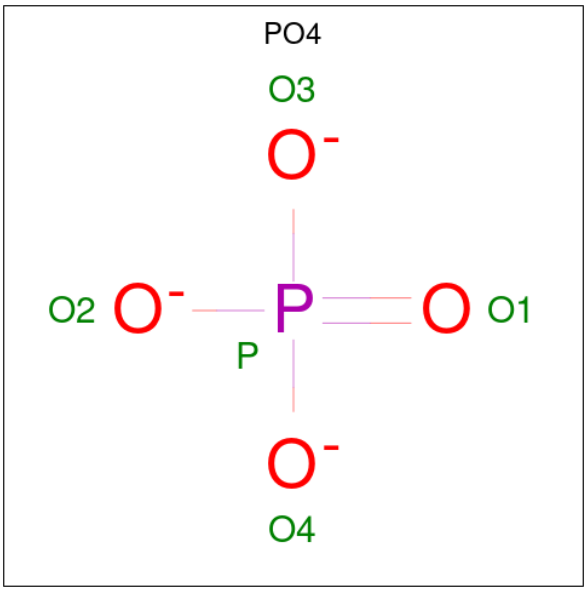
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	460	Total	C	N	O	S	43	19	0
			3676	2317	638	697	24			
1	CCC	460	Total	C	N	O	S	58	17	0
			3650	2303	629	693	25			

There are 8 discrepancies between the modelled and reference sequences:

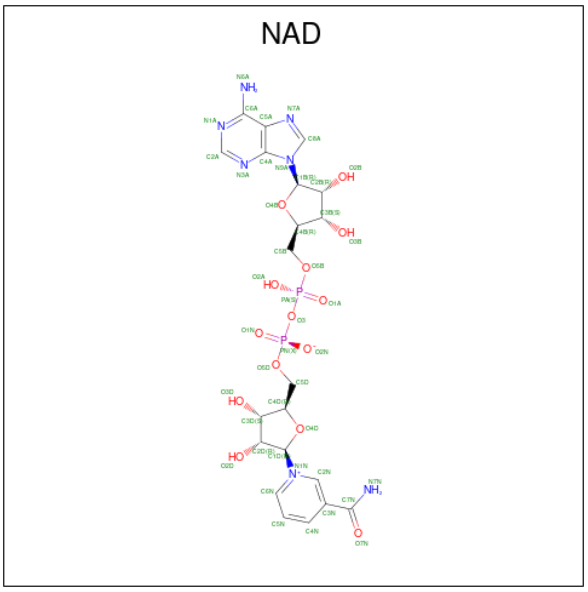
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	SER	-	expression tag	UNP Q9I685
AAA	-1	ASN	-	expression tag	UNP Q9I685
AAA	0	ALA	-	expression tag	UNP Q9I685
AAA	65	ALA	GLN	engineered mutation	UNP Q9I685
CCC	-2	SER	-	expression tag	UNP Q9I685
CCC	-1	ASN	-	expression tag	UNP Q9I685
CCC	0	ALA	-	expression tag	UNP Q9I685
CCC	65	ALA	GLN	engineered mutation	UNP Q9I685

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O P 5 4 1	0	0
2	CCC	1	Total O P 5 4 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O P 44 21 7 14 2	0	0

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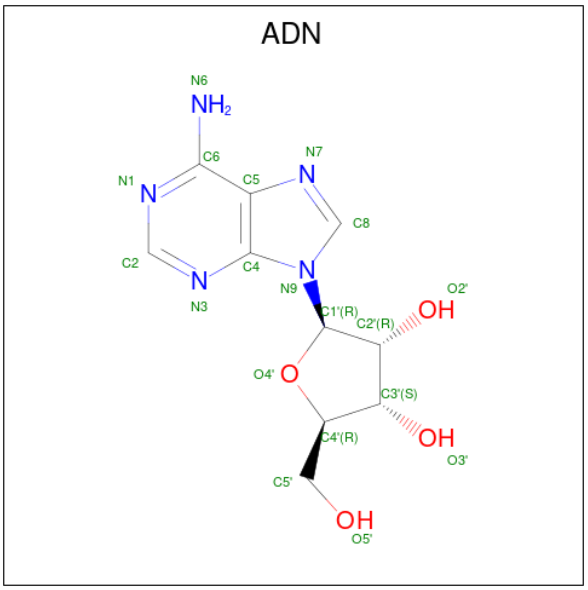
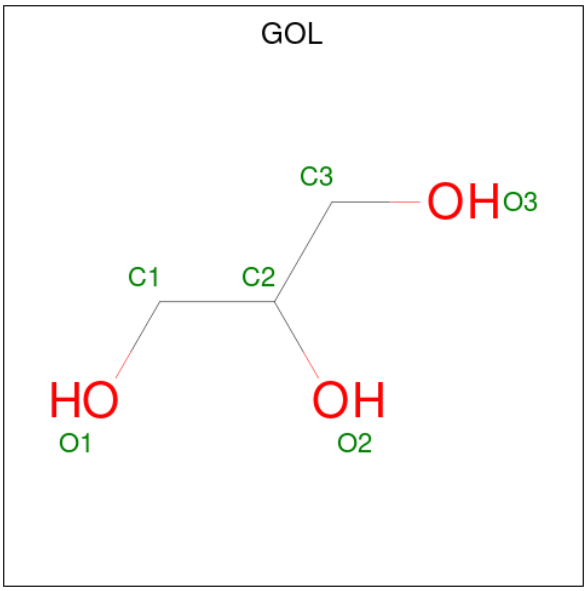
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	CCC	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	0	0
			19	10	5	4		
4	CCC	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

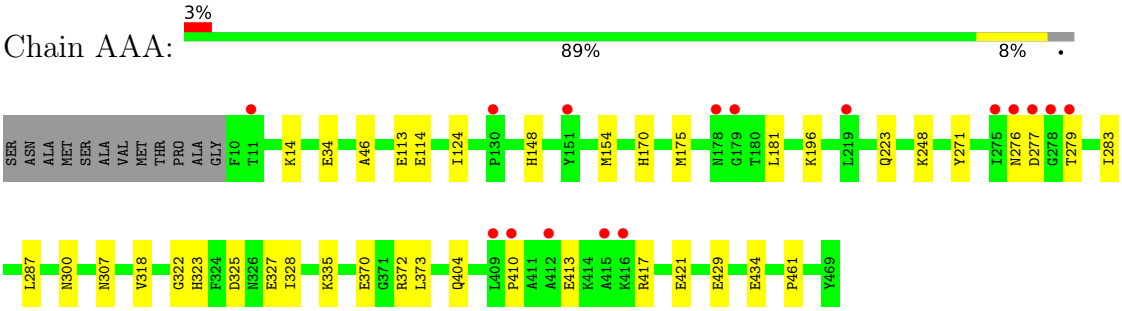
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	579	Total O 579 579	0	0
6	CCC	540	Total O 540 540	0	0

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.

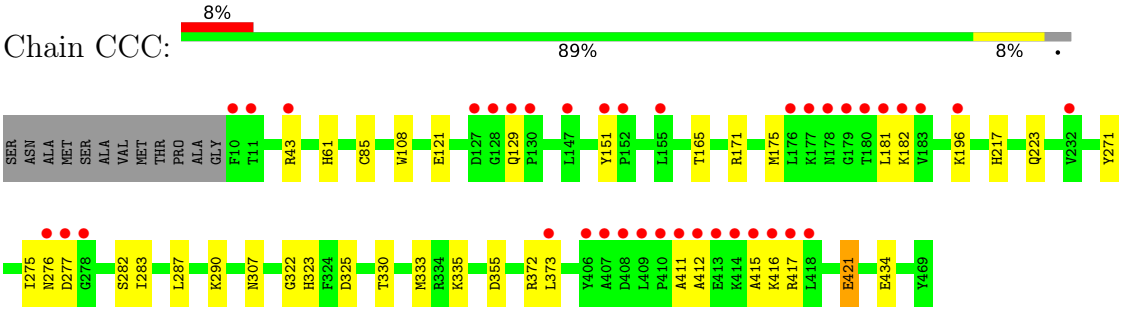
• Molecule 1: Adenosylhomocysteinase

Chain AAA:



• Molecule 1: Adenosylhomocysteinase

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.13Å 85.92Å 125.57Å 90.00° 131.18° 90.00°	Depositor
Resolution (Å)	41.68 – 1.65 41.68 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.68-1.65) 99.1 (41.68-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.198 0.177 , 0.206	Depositor DCC
R_{free} test set	2101 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.7	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	0.97	EDS
Total number of atoms	8587	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.07% 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: PO4, ADN, NAD, GOL

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	AAA	0.85	7/3760 (0.2%)	0.85	1/5080 (0.0%)
1	CCC	0.96	9/3750 (0.2%)	0.85	1/5066 (0.0%)
All	All	0.91	16/7510 (0.2%)	0.85	2/10146 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CCC	0	1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	421	GLU	CD-OE1	-15.62	1.08	1.25
1	CCC	421	GLU	CD-OE2	11.00	1.37	1.25
1	CCC	417	ARG	CD-NE	9.93	1.63	1.46
1	CCC	412	ALA	CA-CB	-8.58	1.34	1.52
1	CCC	434	GLU	CD-OE2	7.43	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	411	ALA	N-CA-CB	6.44	119.12	110.10
1	AAA	170	HIS	CG-ND1-CE1	5.05	115.26	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	421	GLU	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3676	0	3685	31	0
1	CCC	3650	0	3670	36	0
2	AAA	5	0	0	0	0
2	CCC	5	0	0	0	0
3	AAA	44	0	26	1	0
3	CCC	44	0	26	2	0
4	AAA	19	0	13	1	0
4	CCC	19	0	13	1	0
5	CCC	6	0	8	3	0
6	AAA	579	0	0	12	0
6	CCC	540	0	0	13	0
All	All	8587	0	7441	72	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 5.

The worst 5 of 72 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:AAA:335:LYS:HD2	6:AAA:1173:HOH:O	1.44	1.18
1:AAA:277[B]:ASP:OD1	1:AAA:279:THR:OG1	1.70	1.09
1:AAA:14:LYS:NZ	6:AAA:705:HOH:O	1.92	1.01
1:CCC:325[A]:ASP:O	6:CCC:904:HOH:O	1.77	1.00
1:AAA:372[B]:ARG:CZ	6:AAA:706:HOH:O	2.09	1.00

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	AAA	476/472 (101%)	466 (98%)	10 (2%)	0	100	100
1	CCC	475/472 (101%)	463 (98%)	12 (2%)	0	100	100
All	All	951/944 (101%)	929 (98%)	22 (2%)	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	AAA	393/384 (102%)	393 (100%)	0	100	100
1	CCC	392/384 (102%)	390 (100%)	2 (0%)	88	80
All	All	785/768 (102%)	783 (100%)	2 (0%)	92	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	165	THR
1	CCC	217	HIS

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	CCC	804	-	5,5,5	0.06	0	5,5,5	0.30	0
4	ADN	AAA	603	-	18,21,21	0.54	0	18,31,31	1.06	2 (11%)
3	NAD	CCC	802	-	42,48,48	0.91	2 (4%)	50,73,73	0.99	2 (4%)
2	PO4	AAA	601	-	4,4,4	1.69	1 (25%)	6,6,6	0.69	0
2	PO4	CCC	803	-	4,4,4	0.57	0	6,6,6	0.32	0
4	ADN	CCC	801	-	18,21,21	0.61	0	18,31,31	1.12	1 (5%)
3	NAD	AAA	602	-	42,48,48	0.81	3 (7%)	50,73,73	0.98	4 (8%)

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
5	GOL	CCC	804	-	-	0/4/4/4	-
4	ADN	AAA	603	-	-	0/2/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	CCC	802	-	-	5/26/62/62	0/5/5/5
4	ADN	CCC	801	-	-	0/2/22/22	0/3/3/3
3	NAD	AAA	602	-	-	5/26/62/62	0/5/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	802	NAD	C2N-N1N	3.24	1.38	1.35
2	AAA	601	PO4	P-O1	3.04	1.58	1.50
3	CCC	802	NAD	O4D-C1D	2.28	1.44	1.41
3	AAA	602	NAD	C8A-N7A	-2.20	1.30	1.34
3	AAA	602	NAD	C2N-N1N	2.18	1.37	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	802	NAD	C6N-N1N-C2N	-3.55	118.74	121.97
4	CCC	801	ADN	C5-C6-N6	3.06	125.00	120.35
4	AAA	603	ADN	C5-C6-N6	2.83	124.65	120.35
3	AAA	602	NAD	C5A-C6A-N6A	2.70	124.46	120.35
3	AAA	602	NAD	C6N-N1N-C2N	-2.69	119.53	121.97

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	602	NAD	O4D-C1D-N1N-C2N
3	AAA	602	NAD	O4D-C1D-N1N-C6N
3	AAA	602	NAD	C2D-C1D-N1N-C2N
3	AAA	602	NAD	C2D-C1D-N1N-C6N
3	CCC	802	NAD	O4D-C1D-N1N-C2N

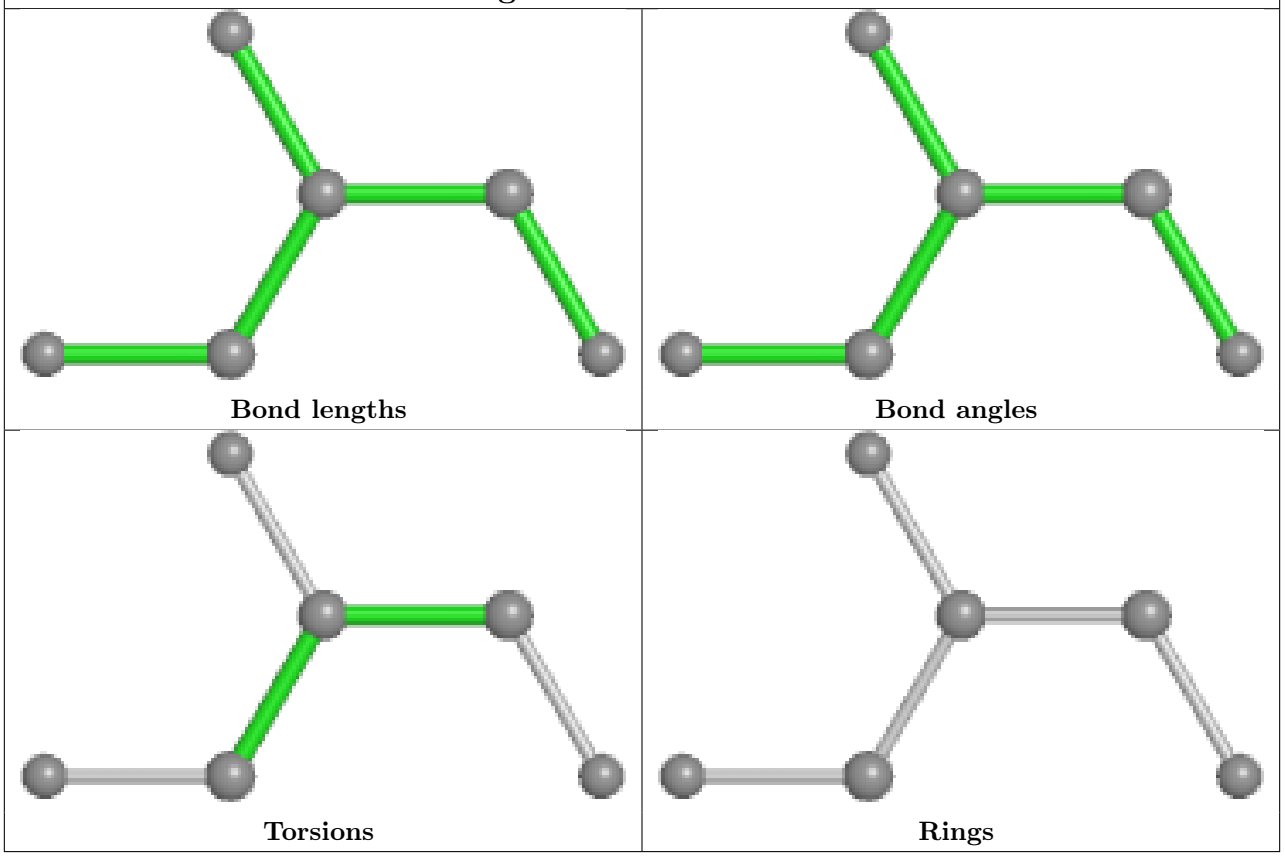
There are no ring outliers.

5 monomers are involved in 6 short contacts:

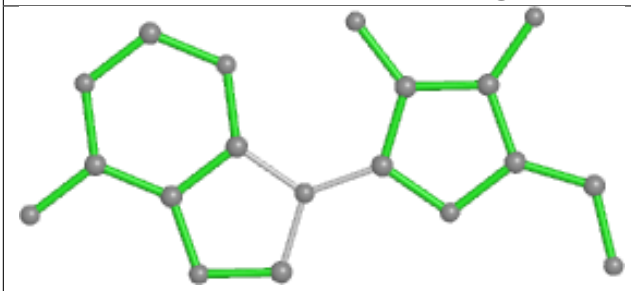
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	CCC	804	GOL	3	0
4	AAA	603	ADN	1	0
3	CCC	802	NAD	2	0
4	CCC	801	ADN	1	0
3	AAA	602	NAD	1	0

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.

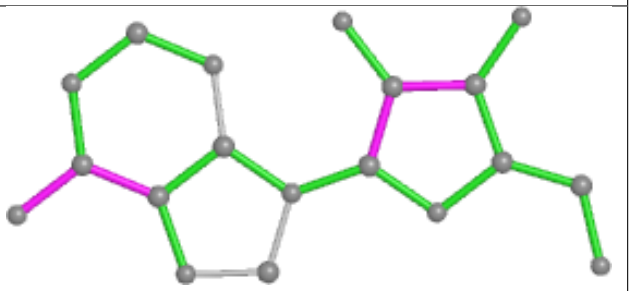
Ligand GOL CCC 804



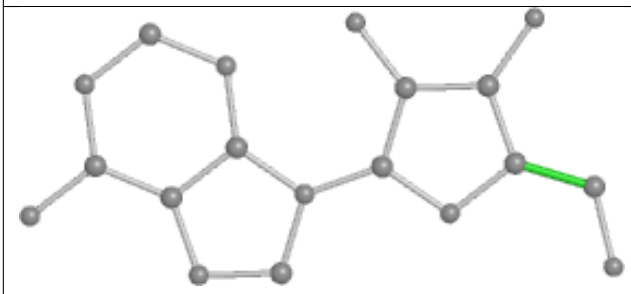
Ligand ADN AAA 603



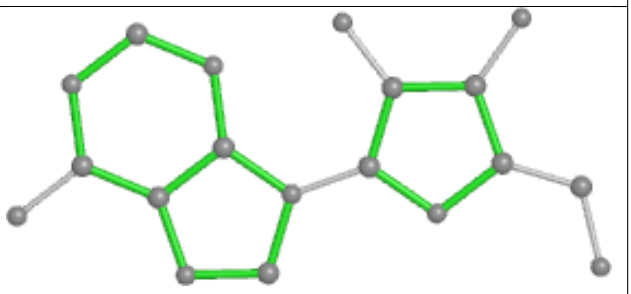
Bond lengths



Bond angles

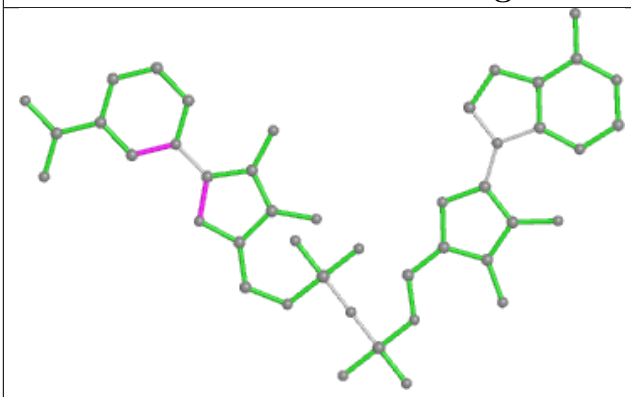


Torsions

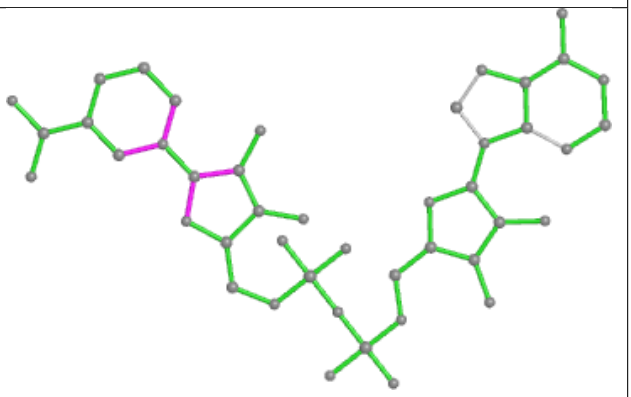


Rings

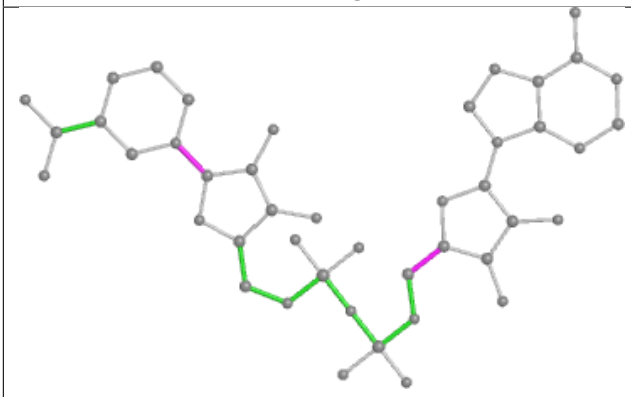
Ligand NAD CCC 802



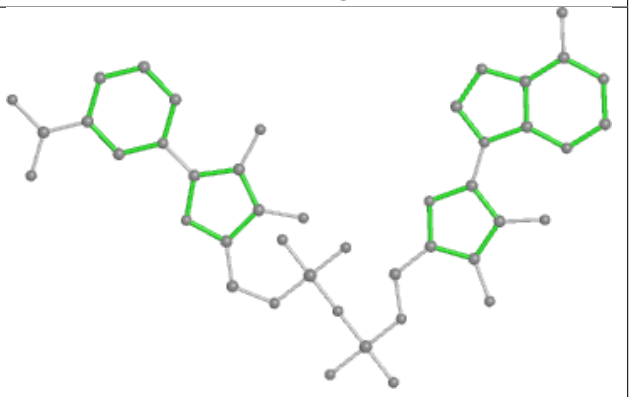
Bond lengths



Bond angles

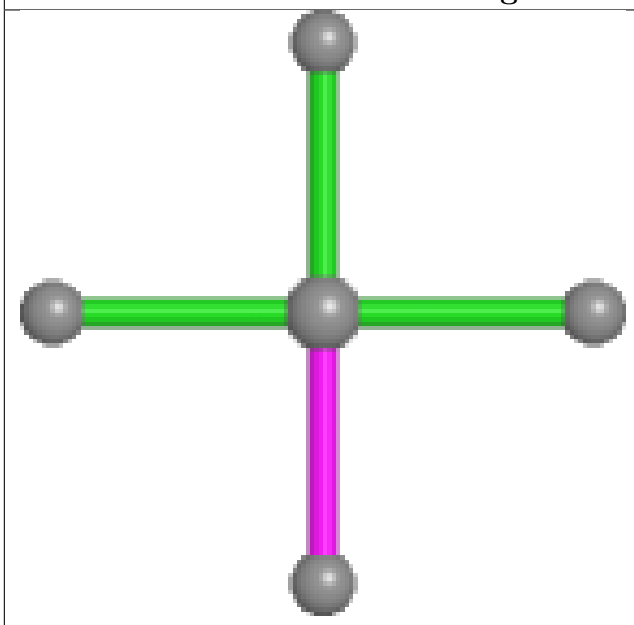


Torsions

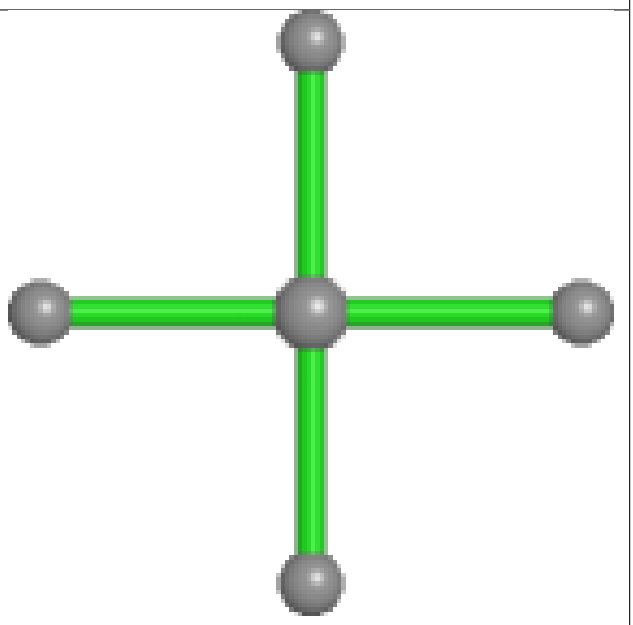


Rings

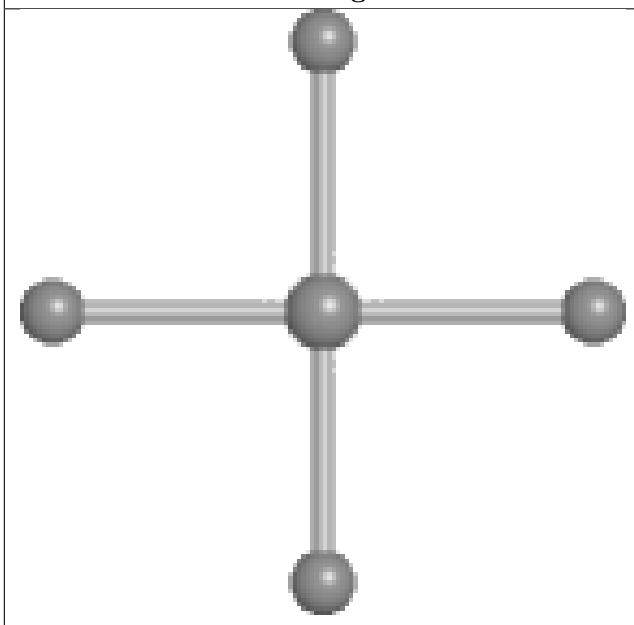
Ligand PO4 AAA 601



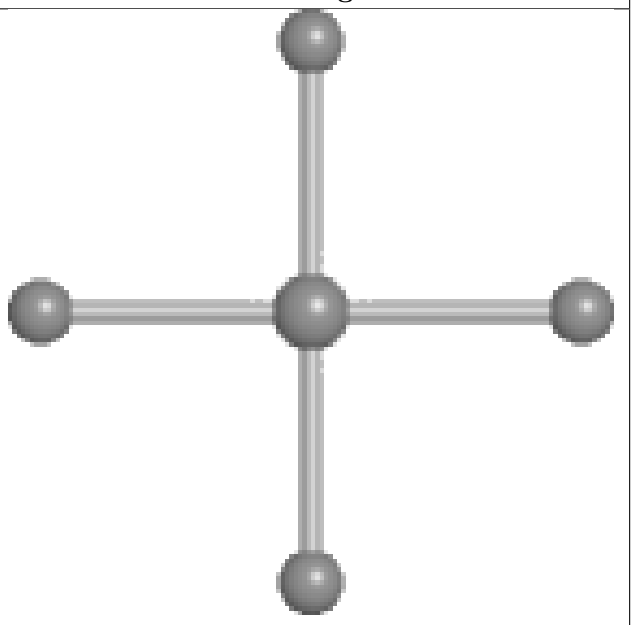
Bond lengths



Bond angles

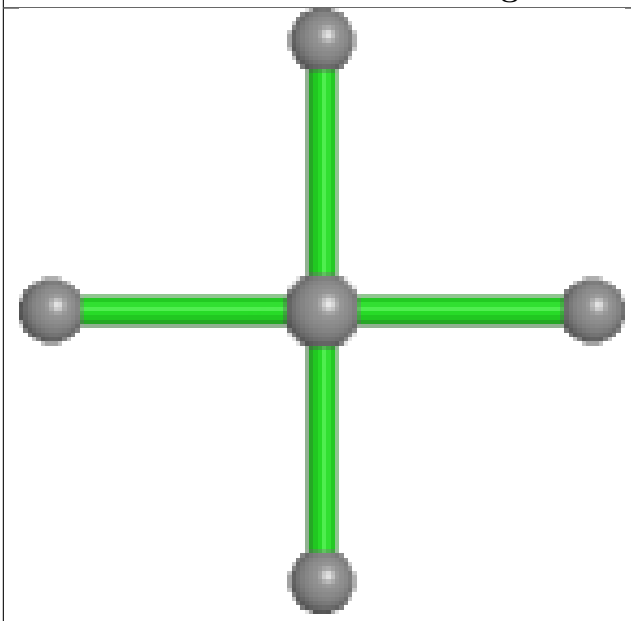


Torsions

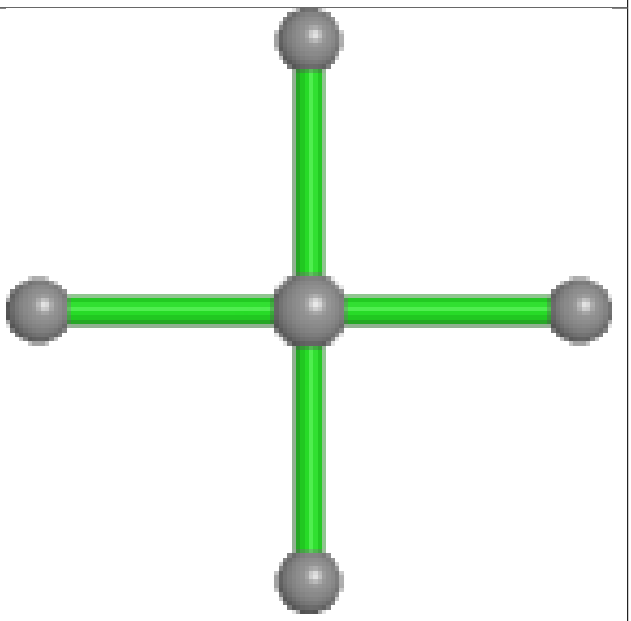


Rings

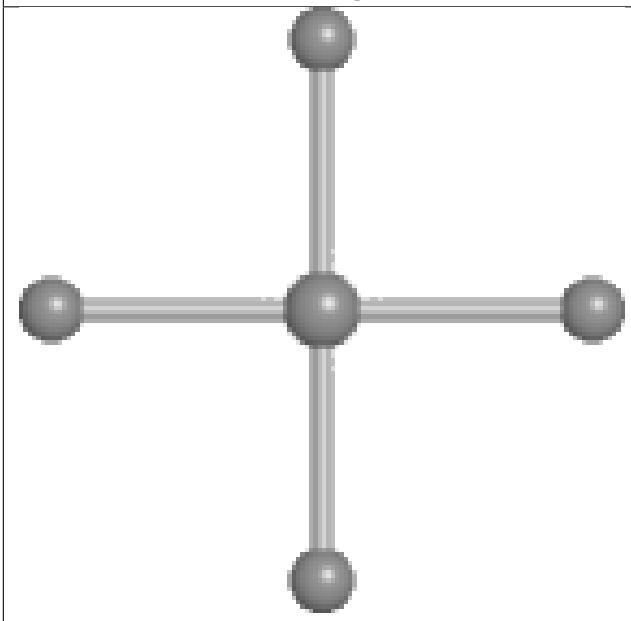
Ligand PO4 CCC 803



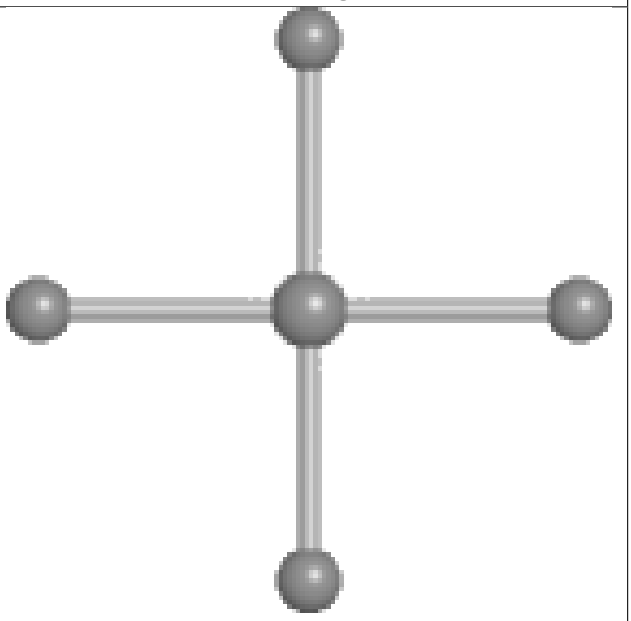
Bond lengths



Bond angles

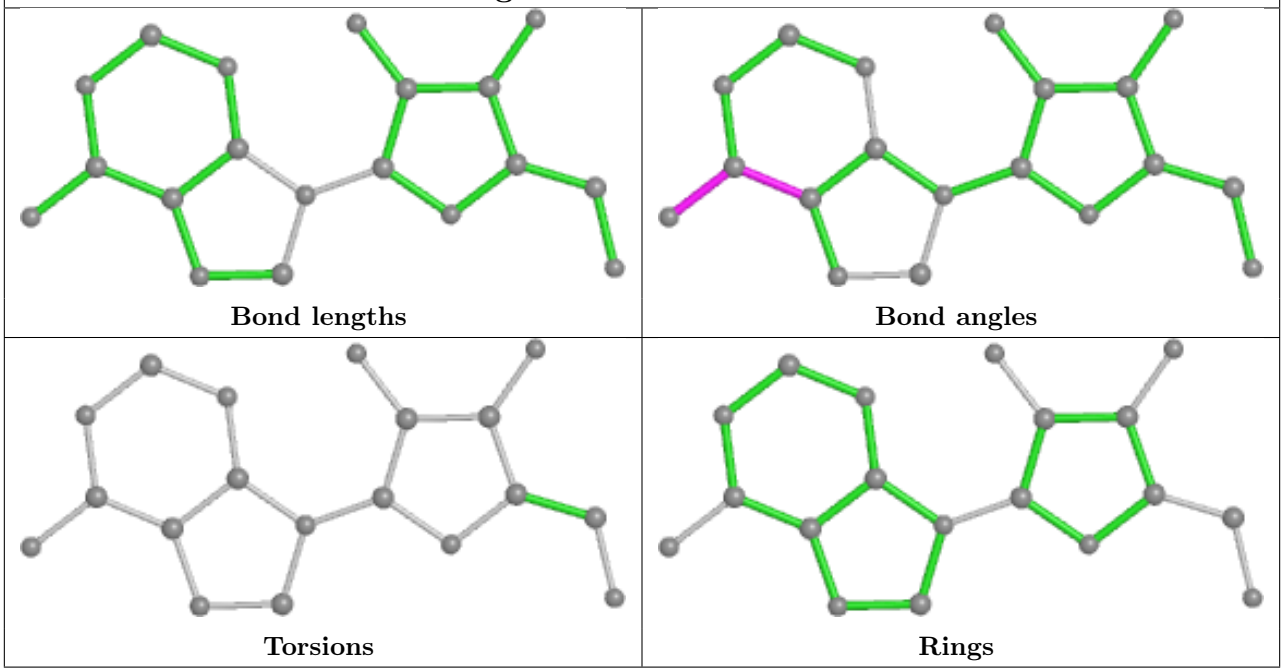


Torsions

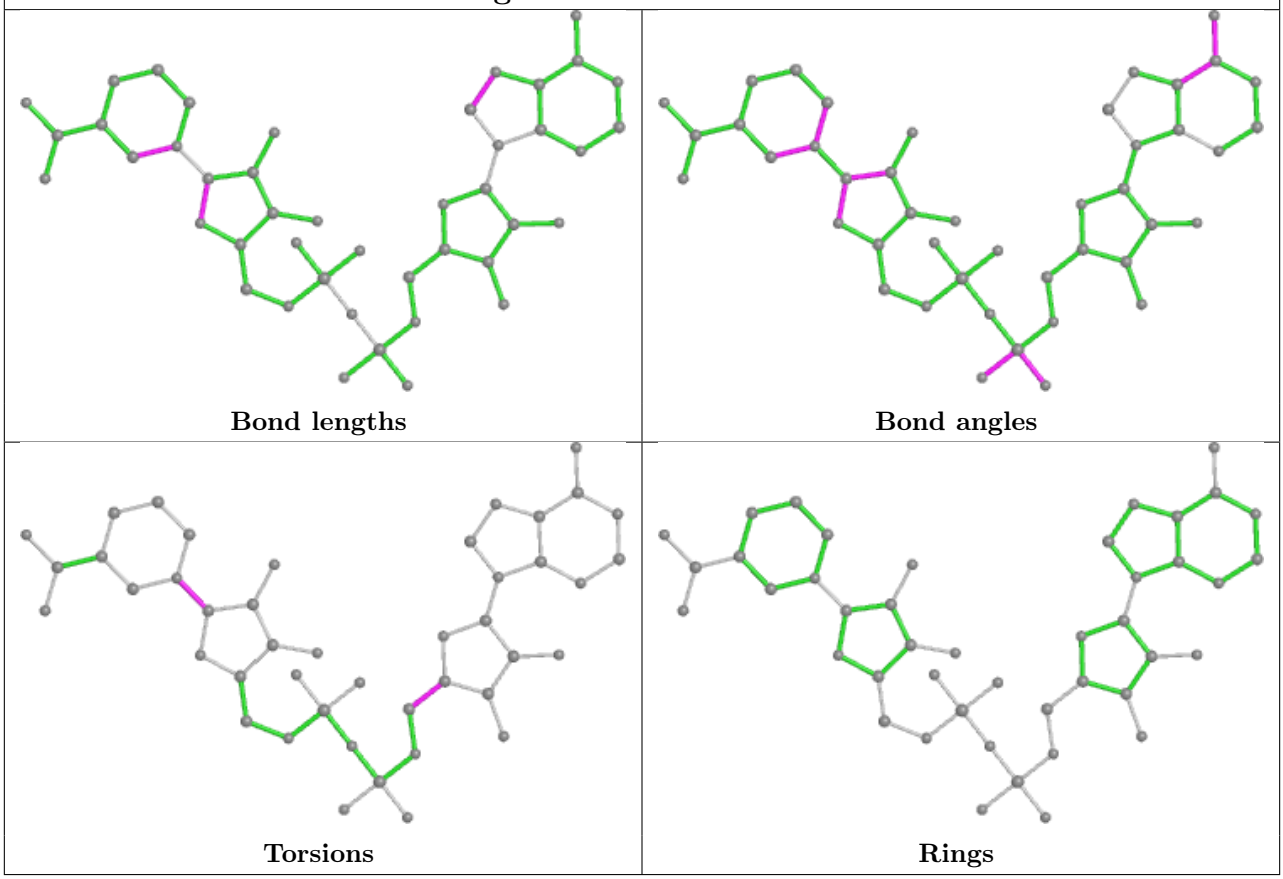


Rings

Ligand ADN CCC 801



Ligand NAD AAA 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	460/472 (97%)	0.26	16 (3%) 44 42	22, 30, 46, 55	28 (6%)
1	CCC	460/472 (97%)	0.53	38 (8%) 11 9	22, 31, 55, 80	31 (6%)
All	All	920/944 (97%)	0.39	54 (5%) 22 20	22, 30, 49, 80	59 (6%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	409	LEU	7.4
1	CCC	412	ALA	6.4
1	CCC	415	ALA	6.2
1	CCC	410	PRO	5.6
1	AAA	415	ALA	5.2

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

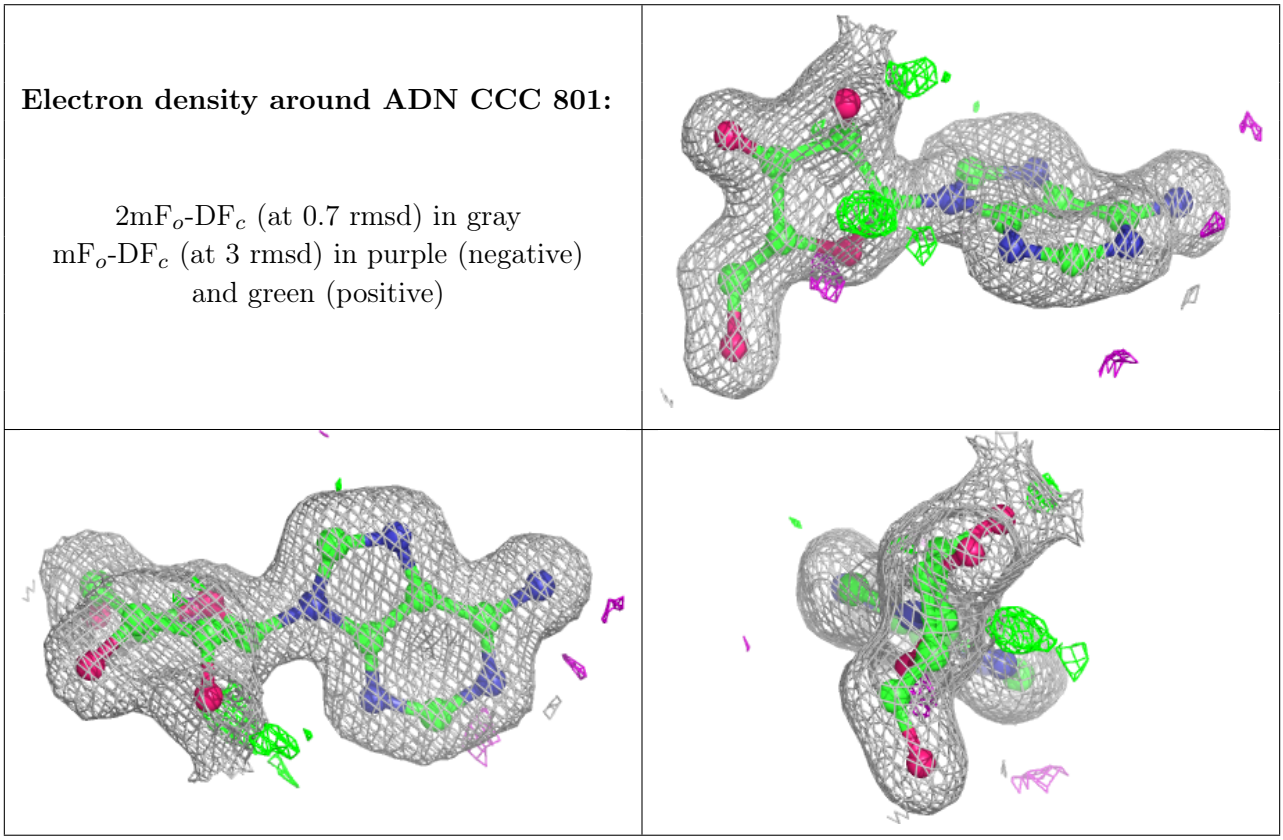
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ADN	CCC	801	19/19	0.91	0.11	25,29,39,41	0
5	GOL	CCC	804	6/6	0.91	0.15	53,57,59,59	0
4	ADN	AAA	603	19/19	0.93	0.11	23,28,34,36	0
3	NAD	CCC	802	44/44	0.95	0.09	23,27,28,31	0
3	NAD	AAA	602	44/44	0.95	0.09	23,27,30,31	0
2	PO4	AAA	601	5/5	0.97	0.07	29,30,31,32	0
2	PO4	CCC	803	5/5	0.98	0.06	30,31,33,33	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.

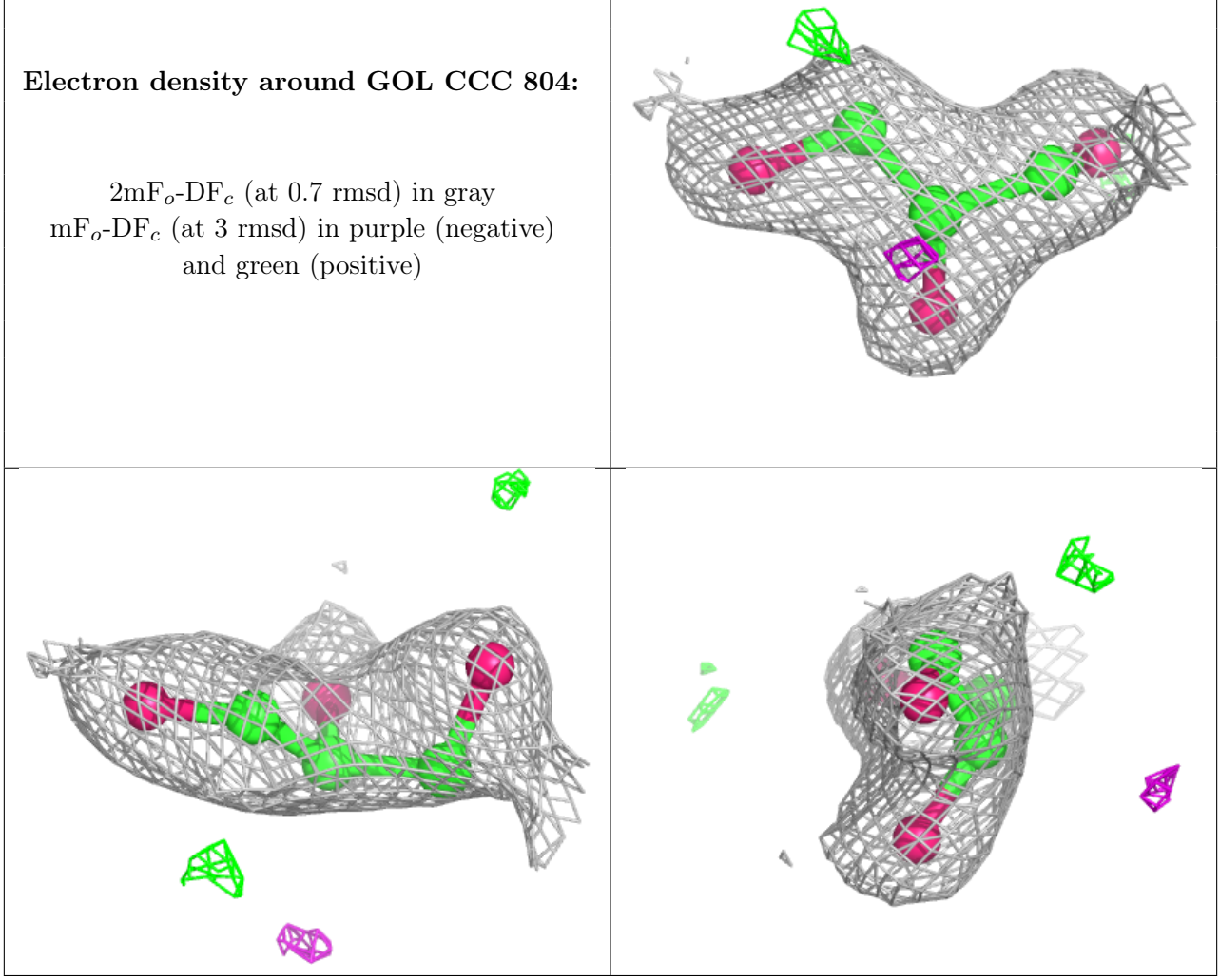
Electron density around ADN CCC 801:

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



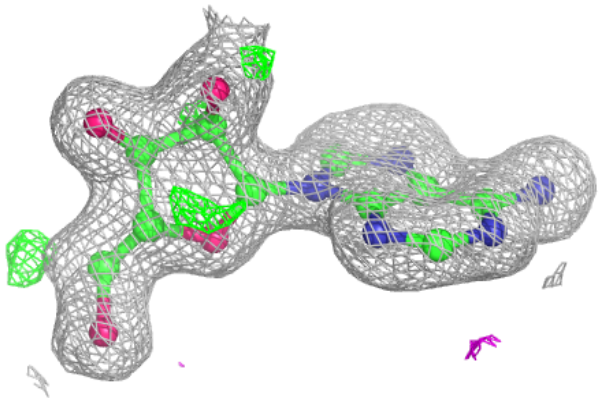
Electron density around GOL CCC 804:

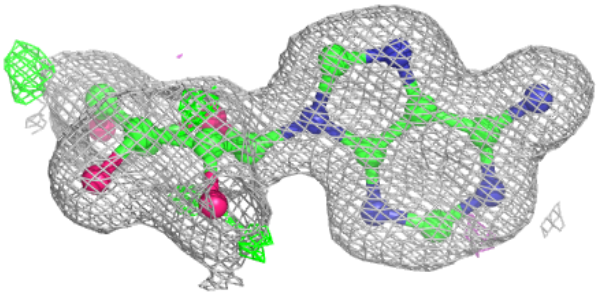
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

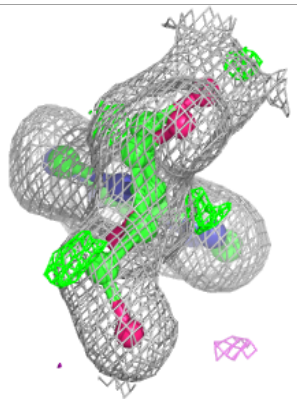


Electron density around ADN AAA 603:

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

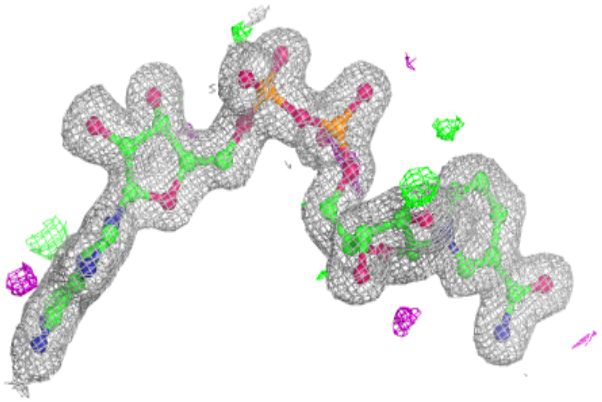


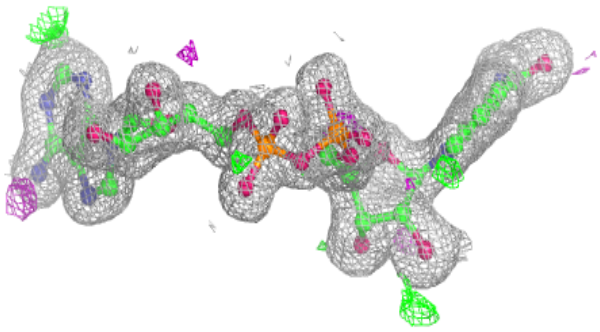


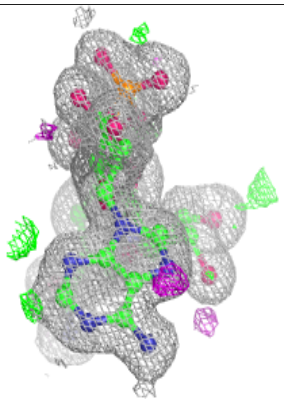


Electron density around NAD CCC 802:

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

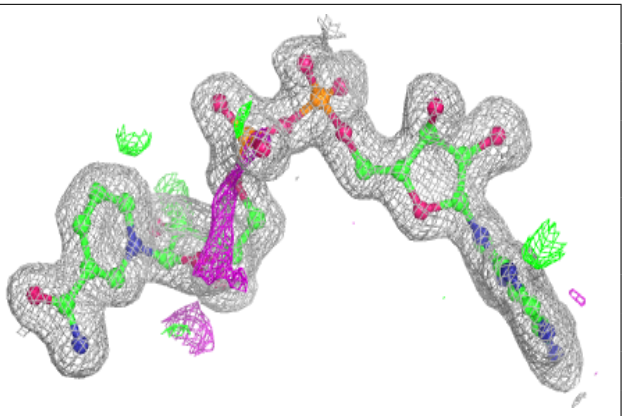


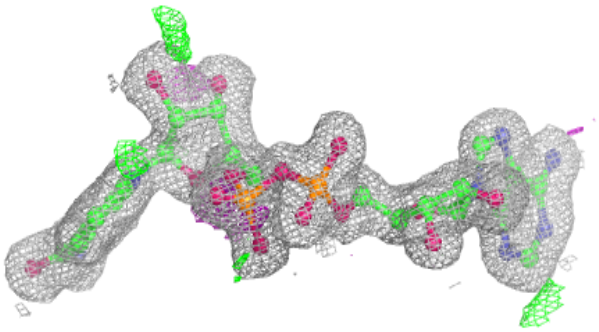


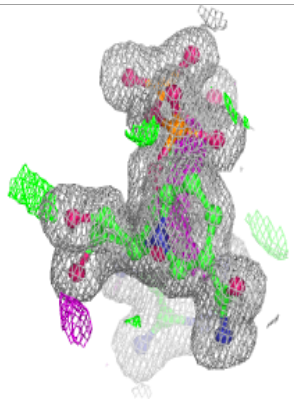


Electron density around NAD AAA 602:

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

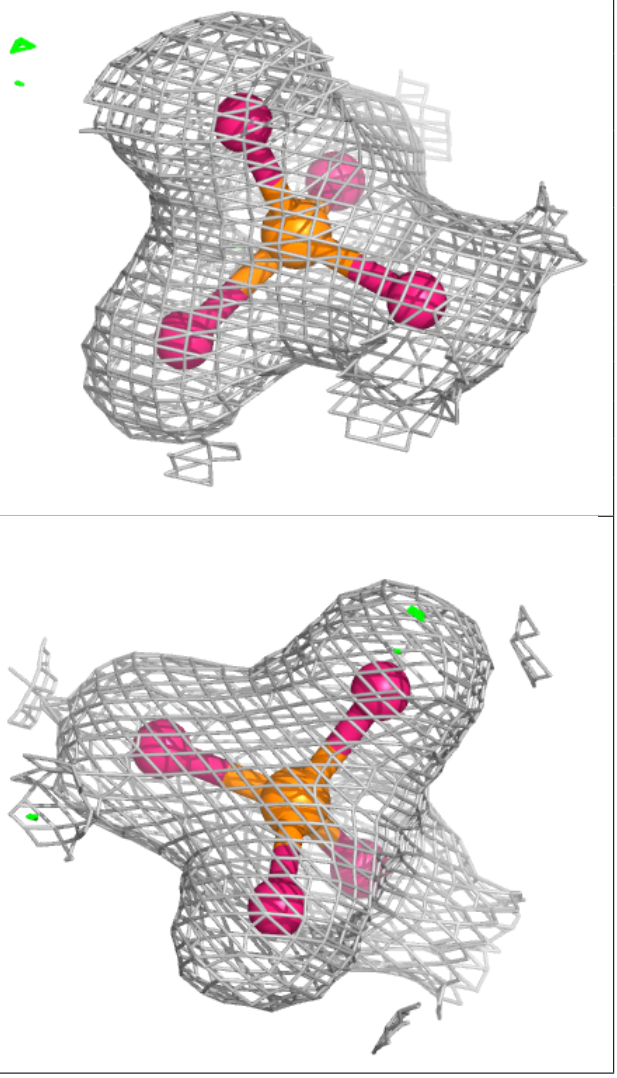






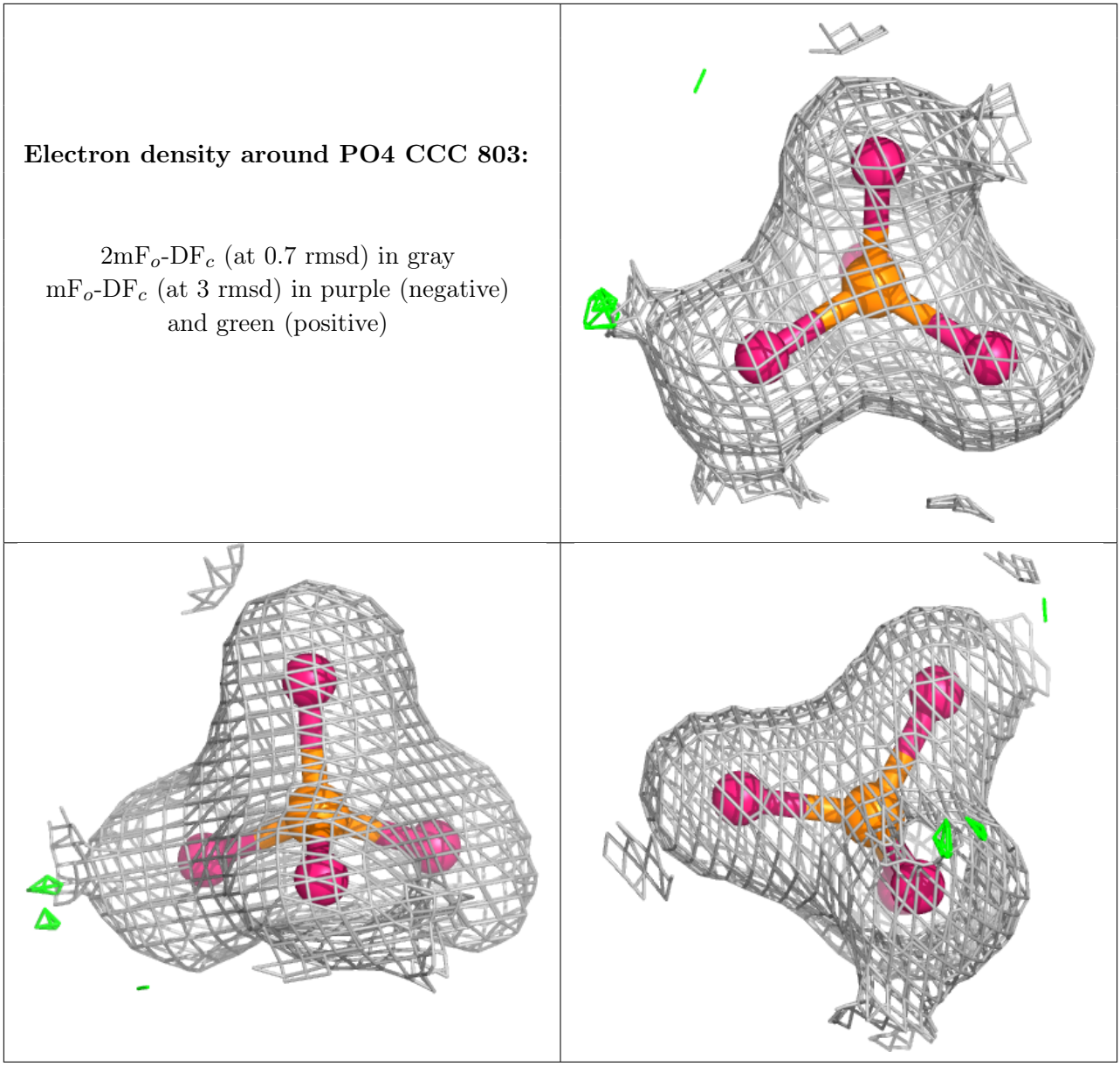
Electron density around PO4 AAA 601:

$2mF_o$-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 CCC 803:

$2mF_o$-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.