wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 02:17 AM EDT

PDB ID	:	4JAY
Title	:	Crystal structure of P. aeruginosa MurB in complex with NADP+
Authors	:	Chen, M.W.; Lohkamp, B.; Schnell, R.; Lescar, J.; Schneider, G.
Deposited on	:	2013-02-19
Resolution	:	2.23 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:

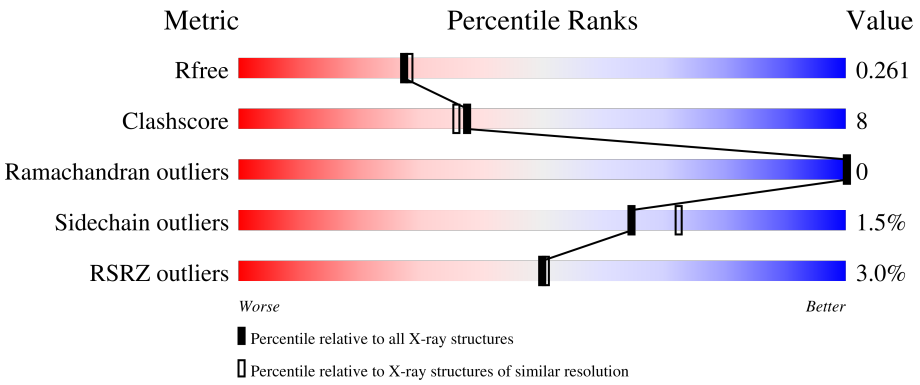
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	340	2% 84% 15% •
1	B	340	4% 85% 14% •
1	C	340	3% 85% 14% •
1	D	340	3% 85% 14% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11404 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 UDP-N-acetylenolpyruvoylglucosamine reductase.

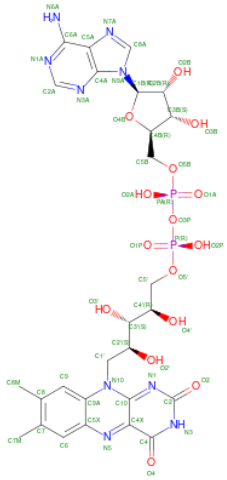
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2645	1657	498	485	5	0	0	0
1	B	338	2645	1657	498	485	5	0	0	0
1	C	338	2645	1657	498	485	5	0	0	0
1	D	338	2645	1657	498	485	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9HZM7
B	0	SER	-	expression tag	UNP Q9HZM7
C	0	SER	-	expression tag	UNP Q9HZM7
D	0	SER	-	expression tag	UNP Q9HZM7

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

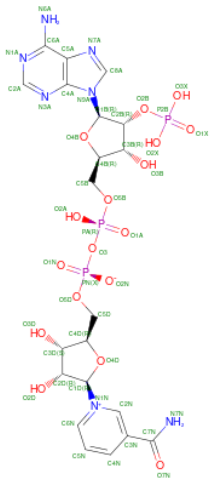
FAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0

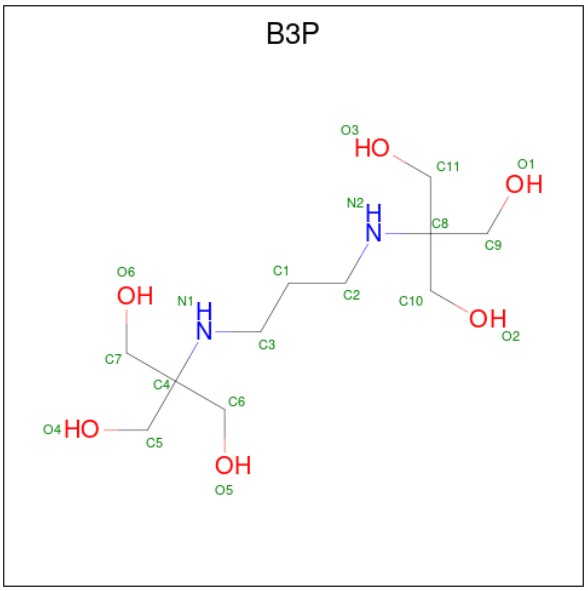
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0
3	C	1	48	21	7	17	3	0	0
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	19	11	2	6	0	0
4	B	1	19	11	2	6	0	0
4	C	1	19	11	2	6	0	0
4	D	1	19	11	2	6	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	A	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

- Molecule 6 is water.

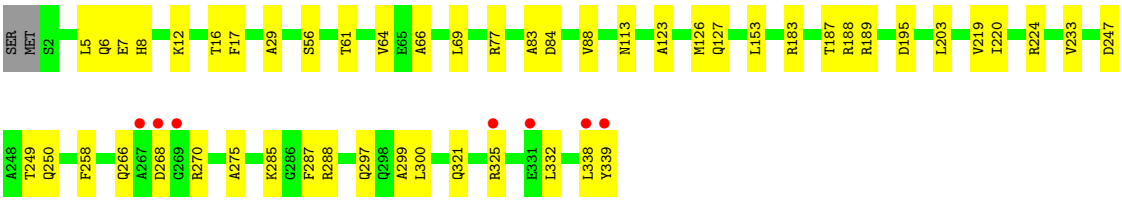
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	84	Total O 84 84	0	0
6	C	76	Total O 76 76	0	0
6	D	82	Total O 82 82	0	0

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.

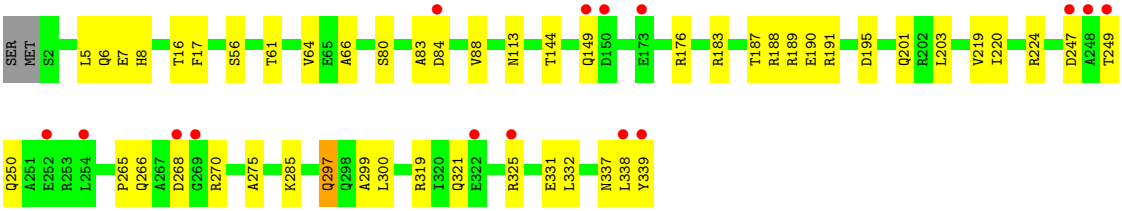
• Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

Chain A:



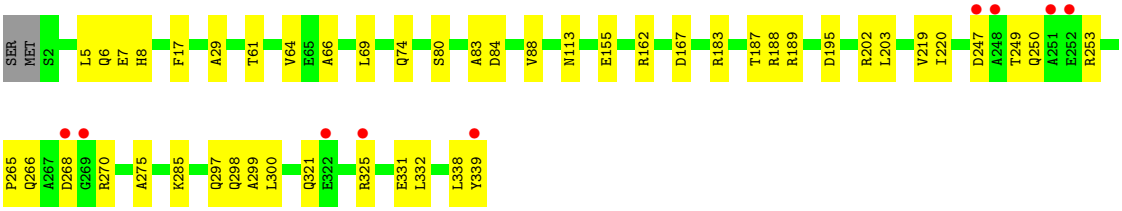
• Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

Chain B:



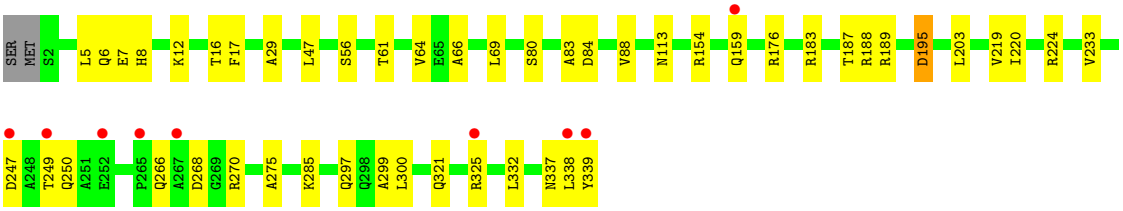
• Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

Chain C:



• Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

Chain D:


SER
MET
S2
L5
Q6
E7
H8
K12
T16
F17
A29
L47
S56
T61
V64
E65
A66
L69
S80
A83
D84
V88
N113
R154
Q159
R176
R183
T187
R188
R189
D195
L203
V219
I220
R224
V233
D247
A248
T249
Q250
A251
E252
P265
Q266
A267
D268
G269
R270
A275
K285
Q297
Q298
A299
L300
Q321
R325
L332
N337
L338
Y339

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.70Å 154.35Å 64.47Å 90.00° 102.26° 90.00°	Depositor
Resolution (Å)	54.33 – 2.23 54.27 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.1 (54.33-2.23) 98.1 (54.27-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.258 0.227 , 0.261	Depositor DCC
R_{free} test set	3529 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11404	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 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, B3P, NAP, FAD

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	0.71	0/2692	0.82	1/3643 (0.0%)
1	B	0.70	0/2692	0.82	1/3643 (0.0%)
1	C	0.70	0/2692	0.83	2/3643 (0.1%)
1	D	0.72	0/2692	0.83	1/3643 (0.0%)
All	All	0.71	0/10768	0.83	5/14572 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	224	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	224	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	162	ARG	CG-CD-NE	5.53	123.42	111.80
1	A	224	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	167	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2657	43	0
1	B	2645	0	2657	45	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2645	0	2657	38	0
1	D	2645	0	2657	45	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	19	0	26	0	0
4	B	19	0	26	1	0
4	C	19	0	26	0	0
4	D	19	0	26	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	98	0	0	9	1
6	B	84	0	0	13	0
6	C	76	0	0	6	0
6	D	82	0	0	10	0
All	All	11404	0	10956	170	5

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 8.

The worst 5 of 170 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:B:321:GLN:HB3	1:B:325:ARG:NH1	1.64	1.12
1:A:321:GLN:HB3	1:A:325:ARG:NH1	1.63	1.12
1:D:321:GLN:HB3	1:D:325:ARG:NH1	1.64	1.10
1:C:321:GLN:HB3	1:C:325:ARG:NH1	1.67	1.08
1:D:159:GLN:HB2	6:D:519:HOH:O	1.61	1.01

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:NH2	1:B:176:ARG:NH2[2_556]	1.71	0.49
1:B:149:GLN:OE1	1:B:176:ARG:NH1[2_556]	1.75	0.45
6:A:1179:HOH:O	6:A:1179:HOH:O[2_656]	1.89	0.31
1:B:176:ARG:CZ	1:B:176:ARG:NH1[2_556]	2.00	0.20
1:B:149:GLN:CD	1:B:176:ARG:NH1[2_556]	2.07	0.13

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	336/340 (99%)	330 (98%)	6 (2%)	0	100	100
1	B	336/340 (99%)	329 (98%)	7 (2%)	0	100	100
1	C	336/340 (99%)	328 (98%)	8 (2%)	0	100	100
1	D	336/340 (99%)	330 (98%)	6 (2%)	0	100	100
All	All	1344/1360 (99%)	1317 (98%)	27 (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	A	270/272 (99%)	267 (99%)	3 (1%)	73	80
1	B	270/272 (99%)	266 (98%)	4 (2%)	65	72
1	C	270/272 (99%)	265 (98%)	5 (2%)	57	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	270/272 (99%)	266 (98%)	4 (2%)	65	72
All	All	1080/1088 (99%)	1064 (98%)	16 (2%)	65	72

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	195	ASP
1	D	80	SER
1	C	74	GLN
1	D	17	PHE
1	C	17	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	GLN
1	C	298	GLN
1	D	298	GLN
1	D	74	GLN
1	D	101	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 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	FAD	D	402	-	53,58,58	1.52	9 (16%)	68,89,89	1.63	14 (20%)
3	NAP	A	1002	5	45,52,52	0.98	2 (4%)	56,80,80	1.58	12 (21%)
4	B3P	B	404	-	18,18,18	1.05	2 (11%)	21,23,23	1.43	3 (14%)
4	B3P	C	404	-	18,18,18	0.98	1 (5%)	21,23,23	1.44	2 (9%)
2	FAD	A	1001	-	53,58,58	1.62	8 (15%)	68,89,89	1.50	12 (17%)
2	FAD	C	402	-	53,58,58	1.38	9 (16%)	68,89,89	1.73	14 (20%)
3	NAP	C	403	5	45,52,52	0.92	1 (2%)	56,80,80	1.56	11 (19%)
3	NAP	B	403	5	45,52,52	1.02	4 (8%)	56,80,80	1.67	13 (23%)
3	NAP	D	403	5	45,52,52	0.98	3 (6%)	56,80,80	1.45	11 (19%)
4	B3P	A	1003	-	18,18,18	0.66	0	21,23,23	1.59	3 (14%)
2	FAD	B	402	-	53,58,58	1.53	9 (16%)	68,89,89	1.30	9 (13%)
4	B3P	D	404	-	18,18,18	0.88	1 (5%)	21,23,23	1.34	4 (19%)

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	FAD	D	402	-	-	2/30/50/50	0/6/6/6
3	NAP	A	1002	5	-	2/31/67/67	0/5/5/5
4	B3P	B	404	-	-	10/28/28/28	-
4	B3P	C	404	-	-	15/28/28/28	-
2	FAD	A	1001	-	-	7/30/50/50	0/6/6/6
2	FAD	C	402	-	-	3/30/50/50	0/6/6/6
3	NAP	C	403	5	-	2/31/67/67	0/5/5/5
3	NAP	B	403	5	-	2/31/67/67	0/5/5/5
3	NAP	D	403	5	-	4/31/67/67	0/5/5/5
4	B3P	A	1003	-	-	12/28/28/28	-
2	FAD	B	402	-	-	3/30/50/50	0/6/6/6
4	B3P	D	404	-	-	10/28/28/28	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	O4B-C1B	4.75	1.47	1.41
2	B	402	FAD	C9A-C5X	4.37	1.48	1.41
2	C	402	FAD	C9A-C5X	4.03	1.47	1.41
2	D	402	FAD	C9A-C5X	3.97	1.47	1.41
2	A	1001	FAD	O4-C4	3.84	1.30	1.23

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	402	FAD	N3A-C2A-N1A	-4.87	121.06	128.68
3	A	1002	NAP	N3A-C2A-N1A	-4.76	121.24	128.68
4	A	1003	B3P	C3-N1-C4	4.57	122.56	116.08
4	B	404	B3P	C3-N1-C4	4.46	122.41	116.08
2	C	402	FAD	C2A-N1A-C6A	4.31	126.12	118.75

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	C5B-O5B-PA-O1A
2	A	1001	FAD	N10-C1'-C2'-O2'
2	A	1001	FAD	N10-C1'-C2'-C3'
2	B	402	FAD	N10-C1'-C2'-O2'
2	B	402	FAD	N10-C1'-C2'-C3'

There are no ring outliers.

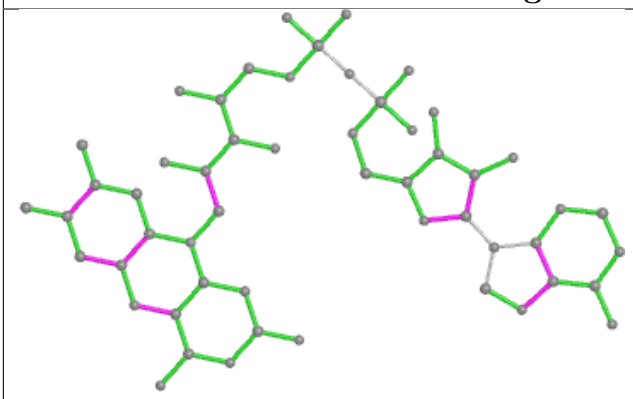
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	B3P	1	0
2	A	1001	FAD	2	0
3	B	403	NAP	1	0
4	D	404	B3P	1	0

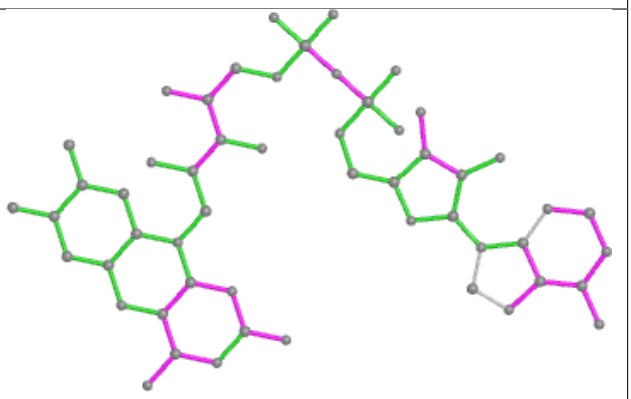
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

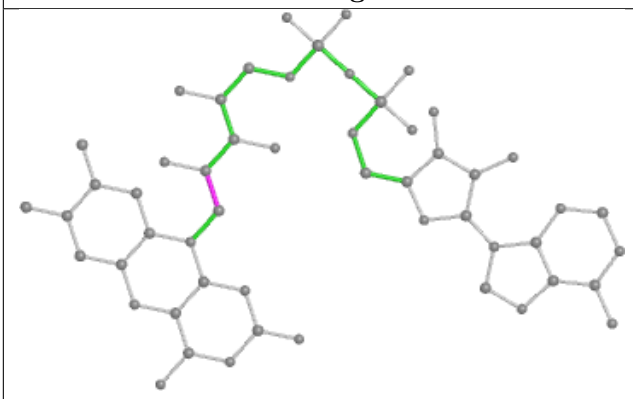
Ligand FAD D 402



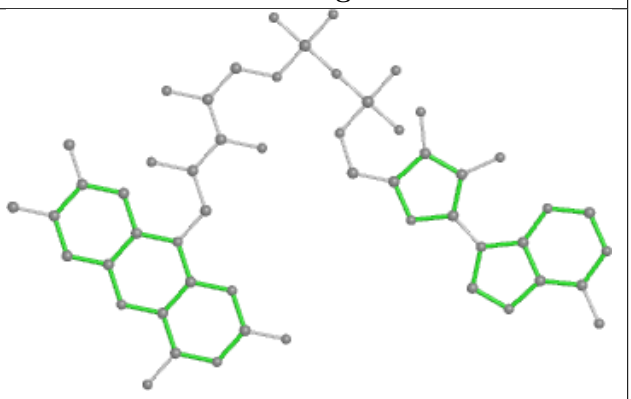
Bond lengths



Bond angles

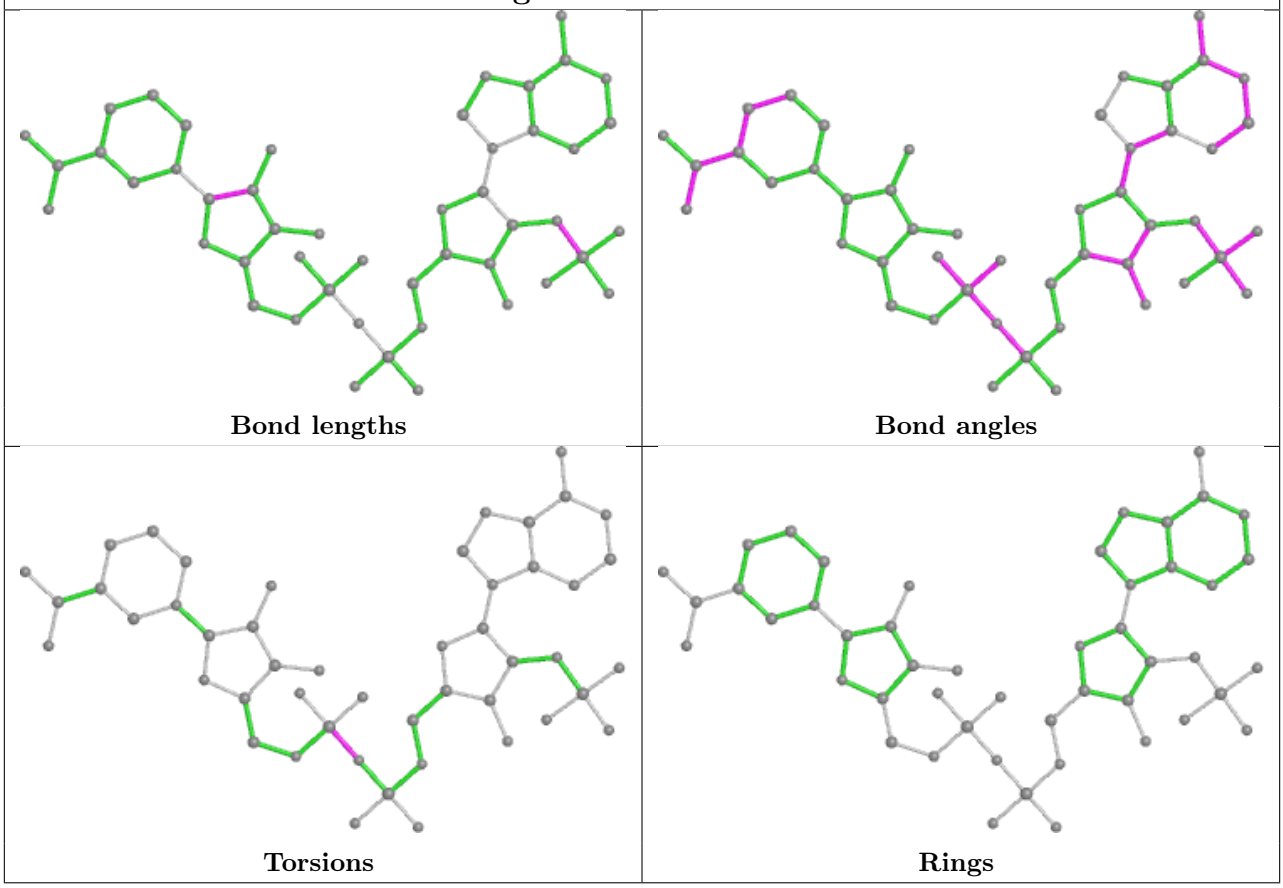


Torsions

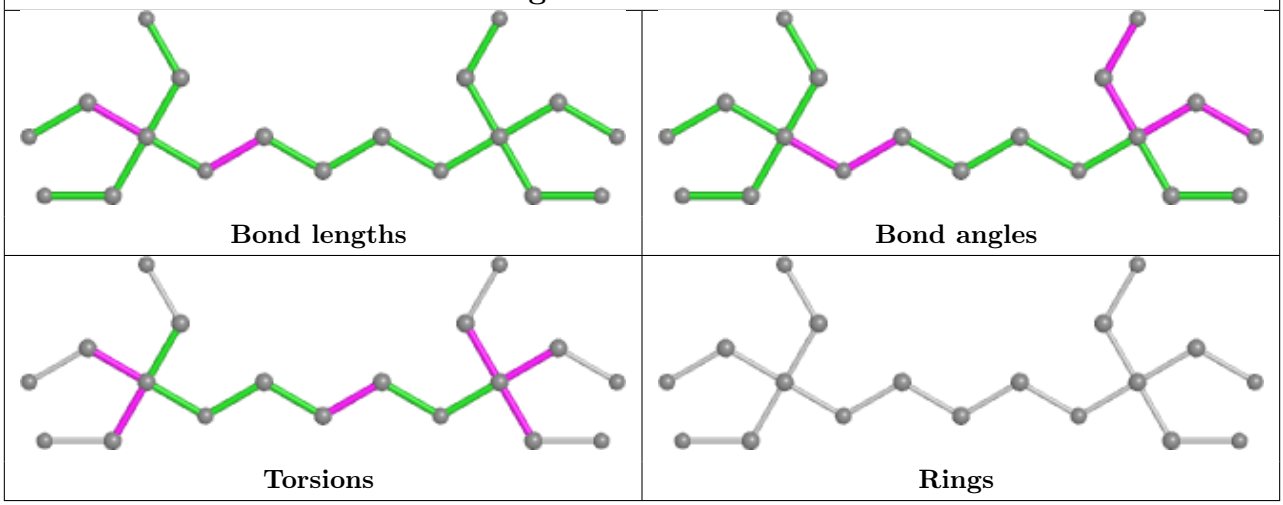


Rings

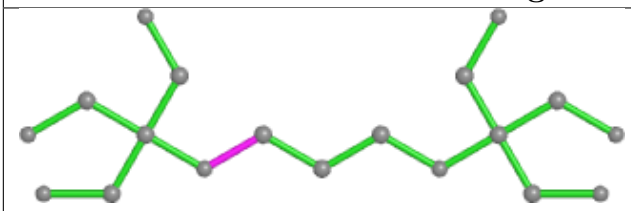
Ligand NAP A 1002



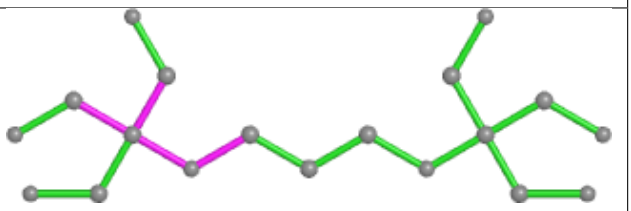
Ligand B3P B 404



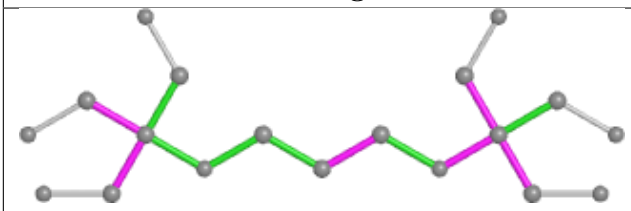
Ligand B3P C 404



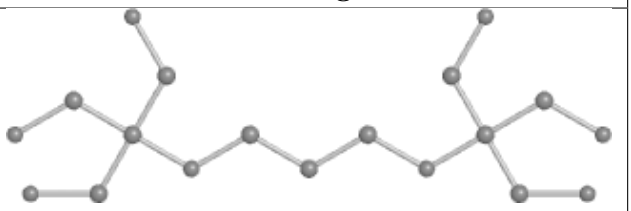
Bond lengths



Bond angles

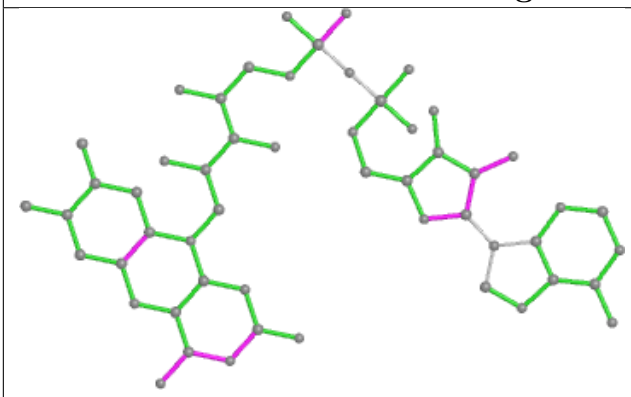


Torsions

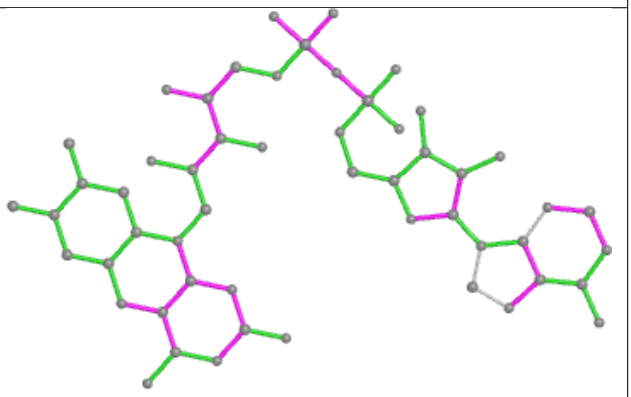


Rings

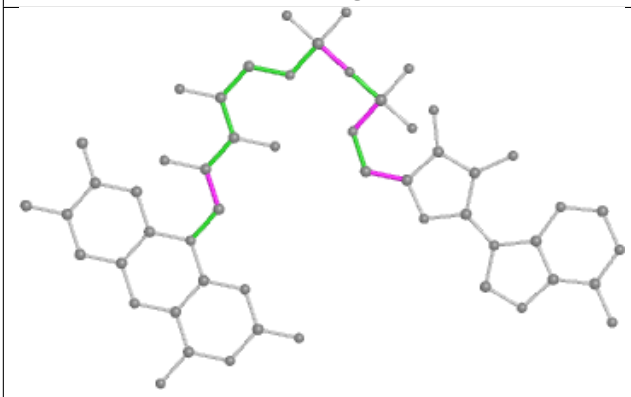
Ligand FAD A 1001



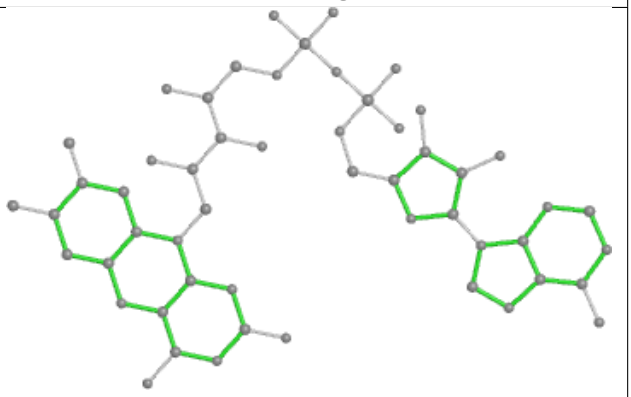
Bond lengths



Bond angles

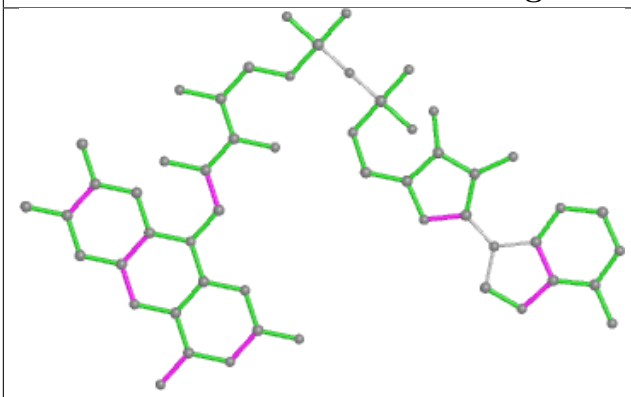


Torsions

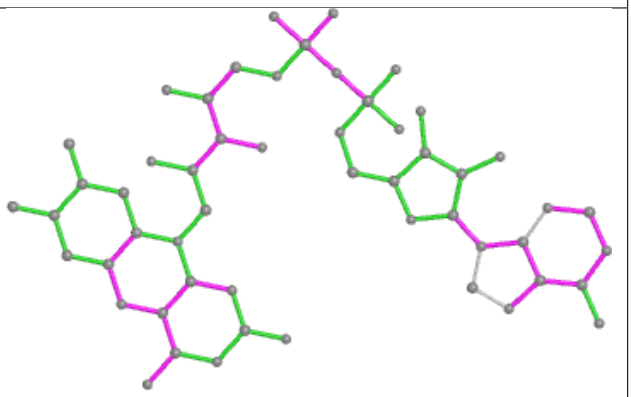


Rings

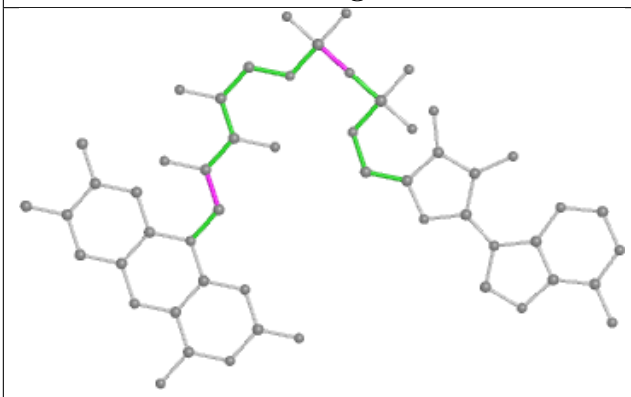
Ligand FAD C 402



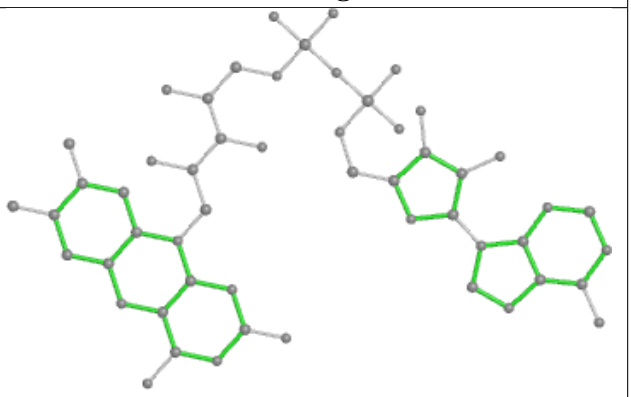
Bond lengths



Bond angles

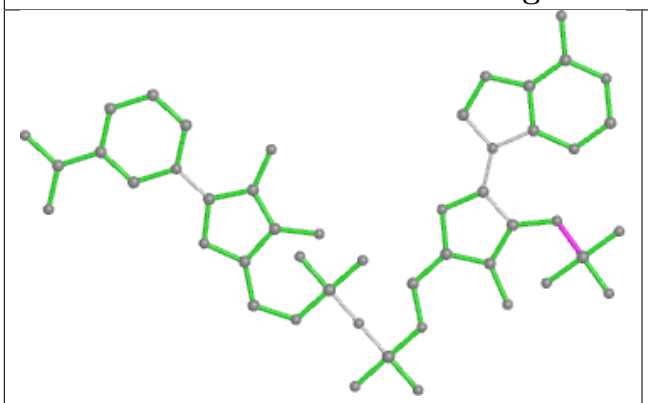


Torsions



Rings

Ligand NAP C 403



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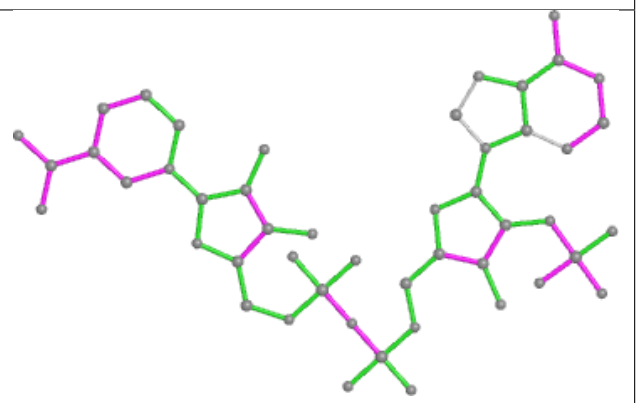
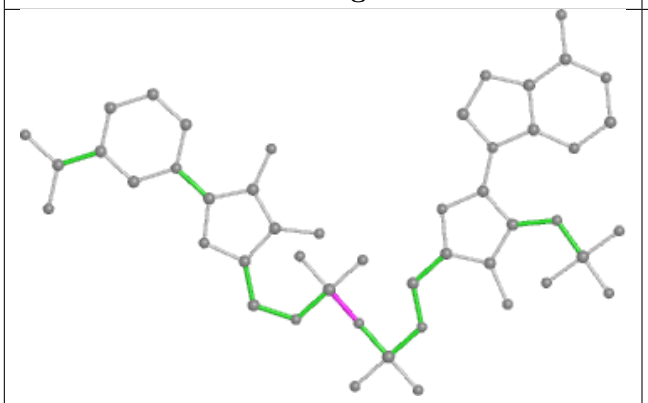
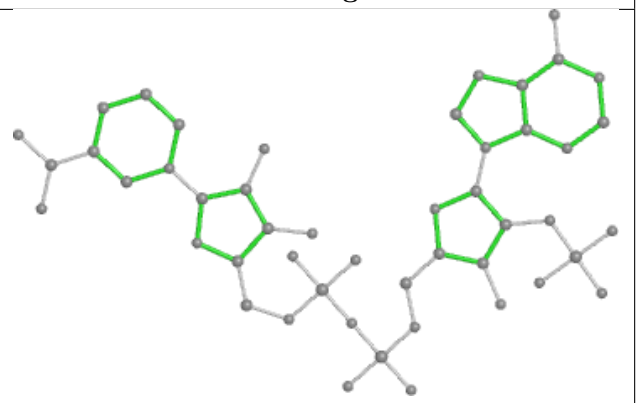


Bond angles

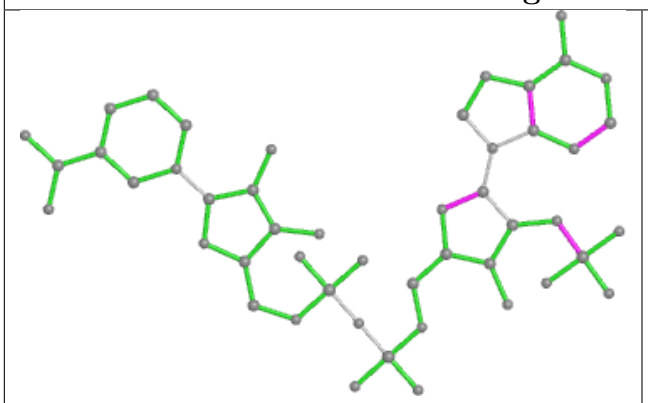


Torsions

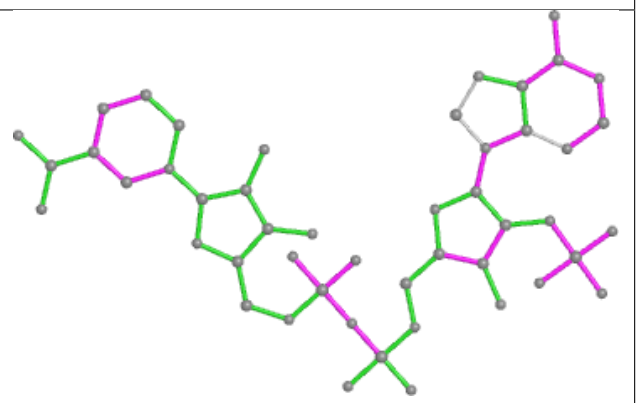


Rings

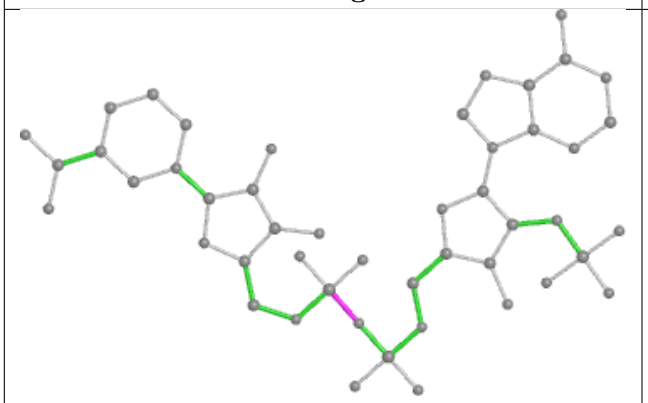
Ligand NAP B 403



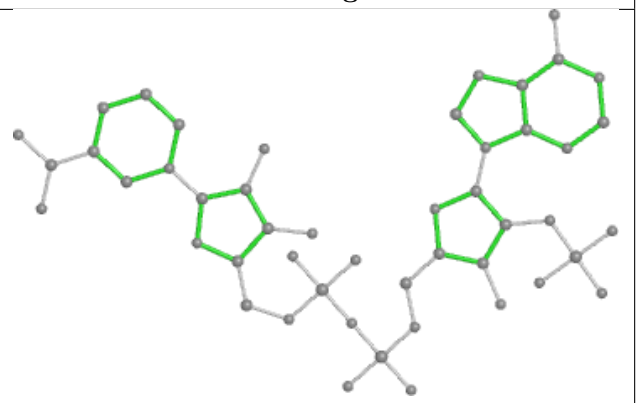
Bond lengths



Bond angles

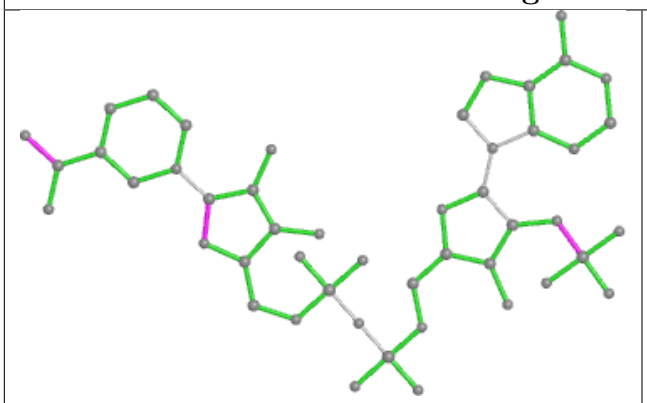


Torsions

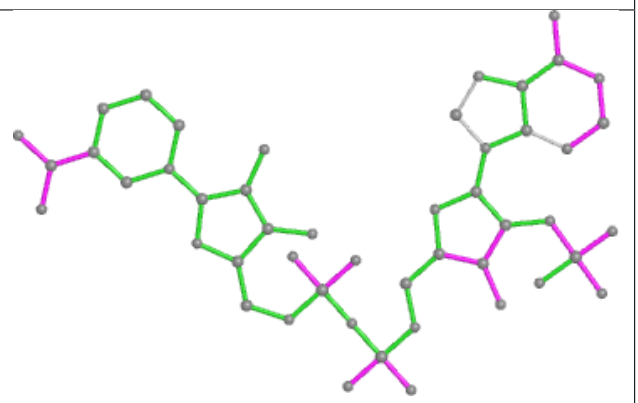


Rings

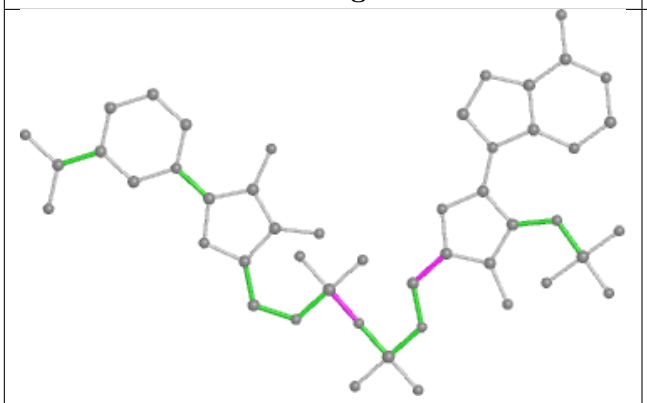
Ligand NAP D 403



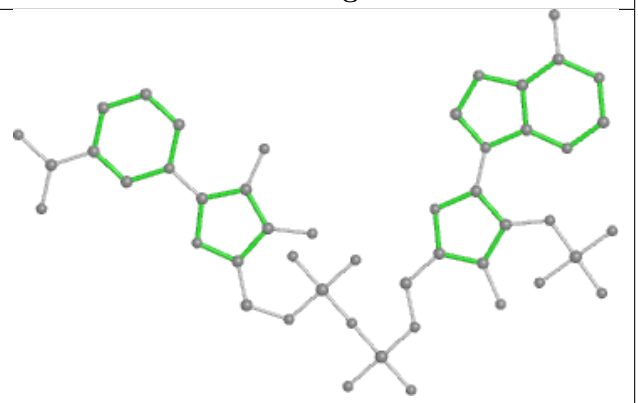
Bond lengths



Bond angles

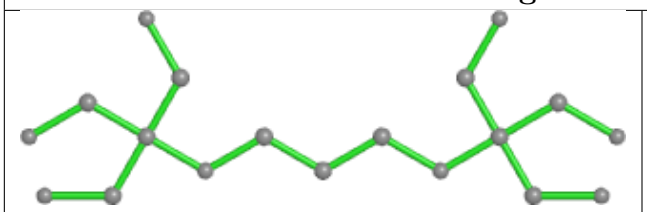


Torsions

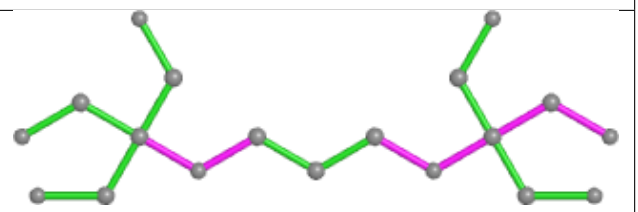


Rings

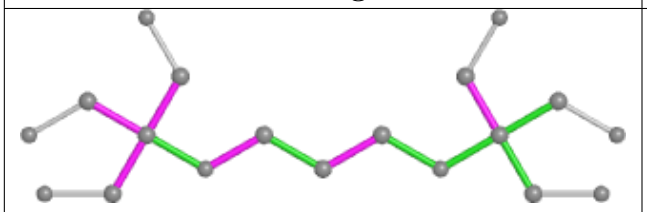
Ligand B3P A 1003



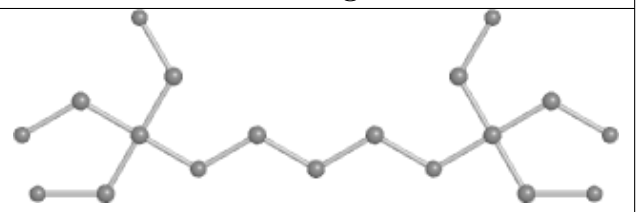
Bond lengths



Bond angles

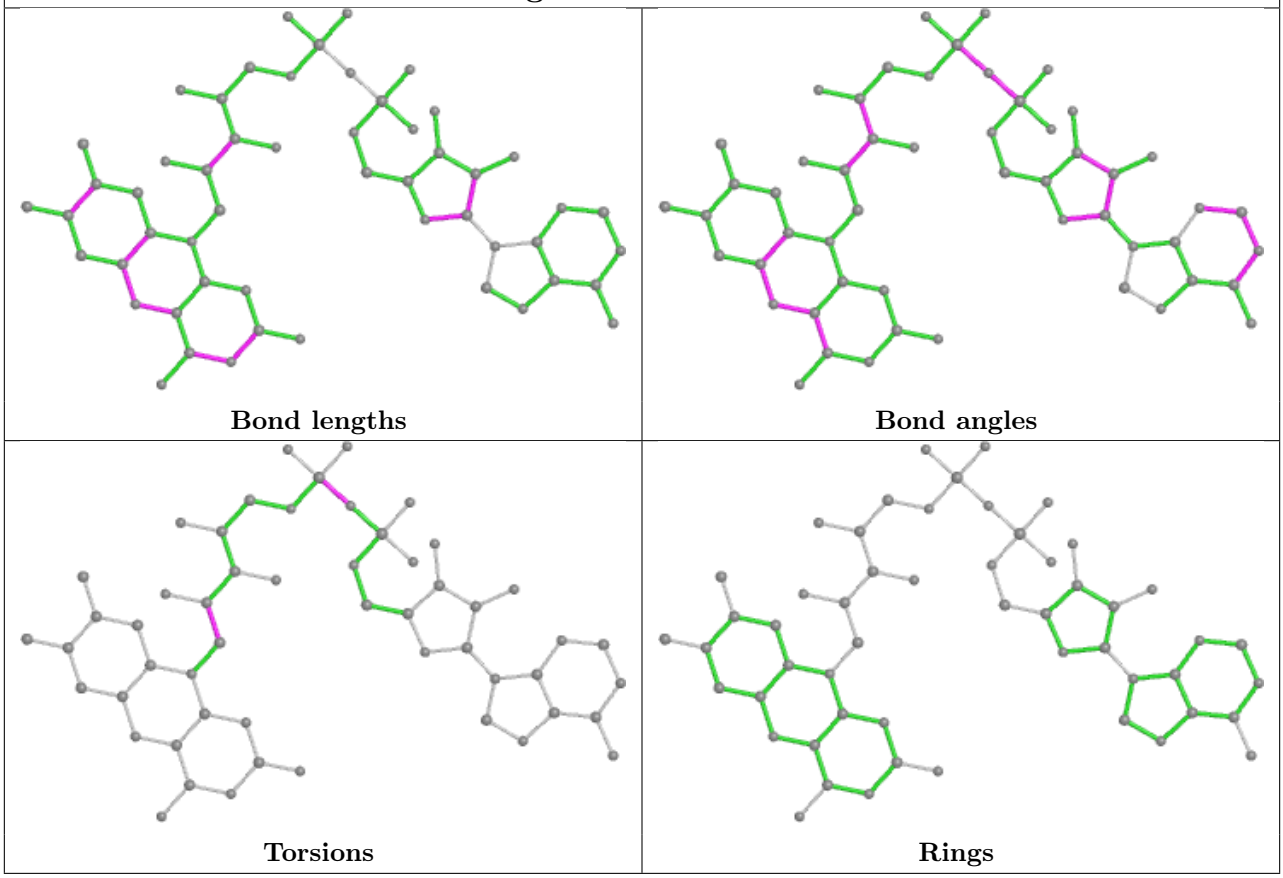


Torsions

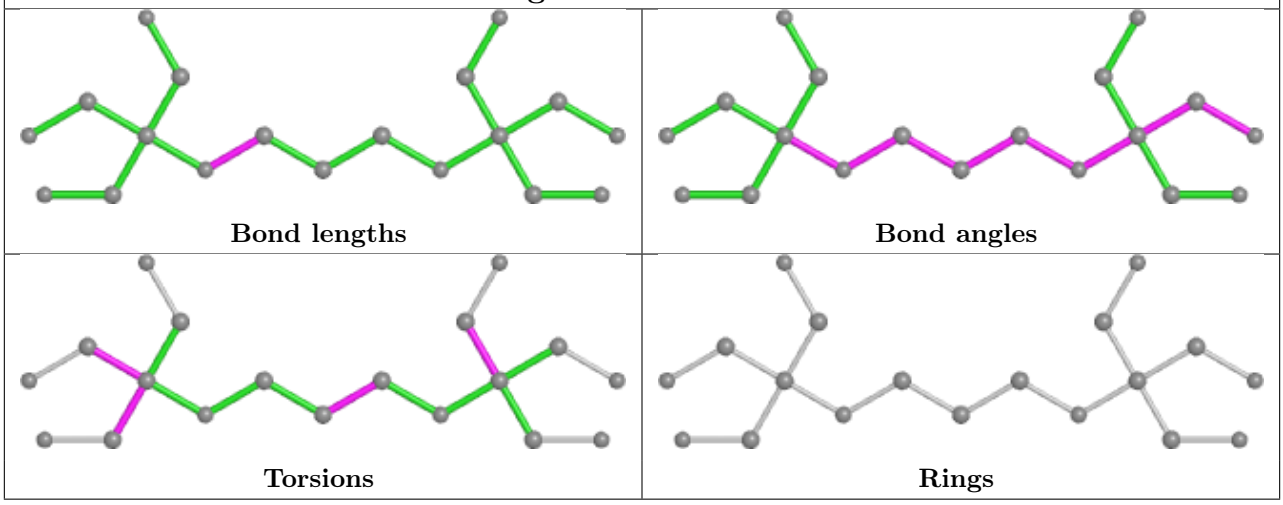


Rings

Ligand FAD B 402



Ligand B3P D 404



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	338/340 (99%)	0.08	7 (2%)	63	65	13, 28, 53, 71	0
1	B	338/340 (99%)	0.25	15 (4%)	34	34	16, 31, 61, 87	0
1	C	338/340 (99%)	0.16	9 (2%)	54	55	14, 31, 65, 97	0
1	D	338/340 (99%)	0.11	9 (2%)	54	55	14, 29, 57, 84	0
All	All	1352/1360 (99%)	0.15	40 (2%)	50	50	13, 30, 58, 97	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	ALA	5.4
1	C	339	TYR	5.1
1	B	149	GLN	4.4
1	B	247	ASP	4.2
1	B	248	ALA	3.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

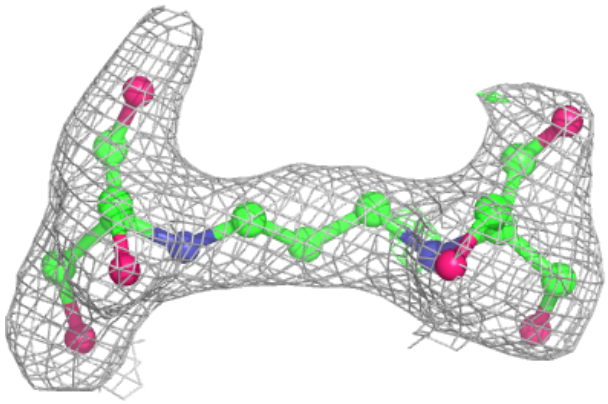
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

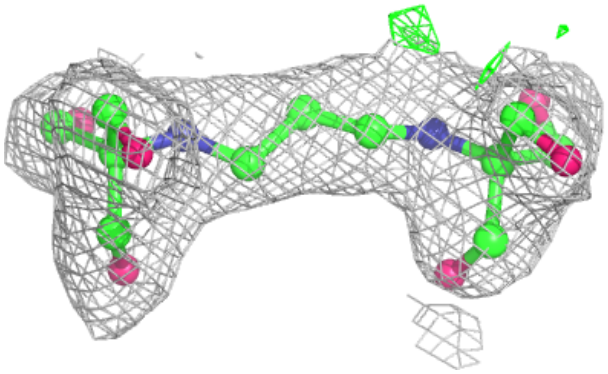
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	B3P	B	404	19/19	0.93	0.14	25,31,48,50	0
4	B3P	C	404	19/19	0.93	0.14	27,34,43,49	0
4	B3P	D	404	19/19	0.93	0.13	23,33,43,49	0
4	B3P	A	1003	19/19	0.94	0.13	23,24,40,47	0
3	NAP	B	403	48/48	0.95	0.12	14,25,34,37	0
3	NAP	C	403	48/48	0.96	0.12	17,26,37,45	0
3	NAP	D	403	48/48	0.96	0.13	15,24,31,35	0
3	NAP	A	1002	48/48	0.96	0.11	13,23,29,31	0
2	FAD	C	402	53/53	0.97	0.12	12,16,20,21	0
2	FAD	A	1001	53/53	0.97	0.12	9,11,15,16	0
2	FAD	B	402	53/53	0.97	0.11	12,15,16,18	0
2	FAD	D	402	53/53	0.98	0.11	11,14,16,18	0
5	K	C	401	1/1	0.98	0.08	19,19,19,19	0
5	K	B	401	1/1	0.99	0.05	16,16,16,16	0
5	K	A	1004	1/1	0.99	0.08	20,20,20,20	0
5	K	D	401	1/1	0.99	0.09	19,19,19,19	0

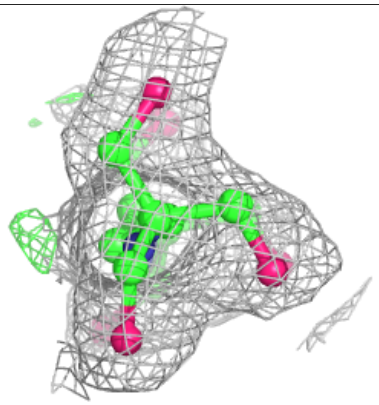
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P B 404:

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

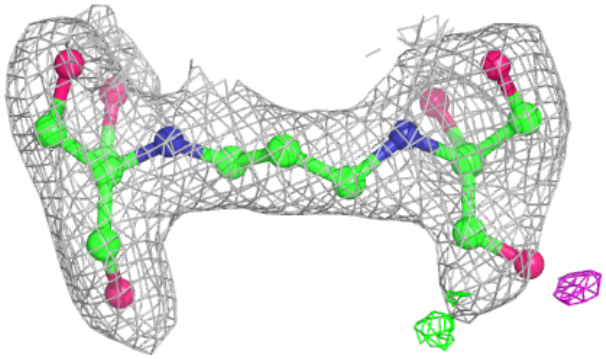


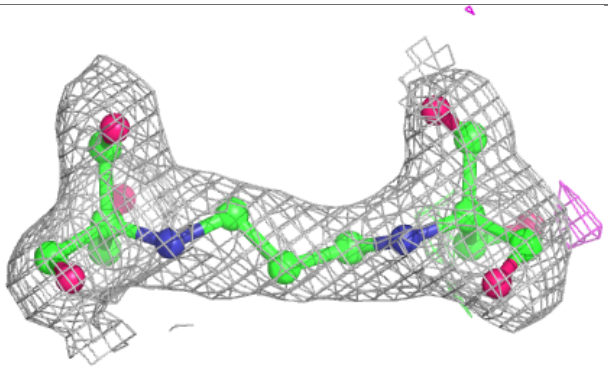


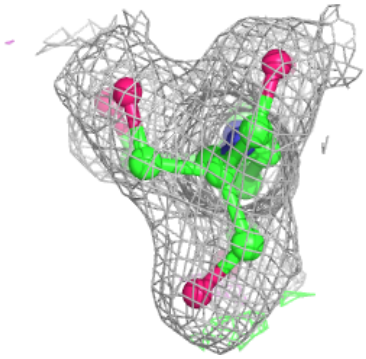


Electron density around B3P C 404:

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

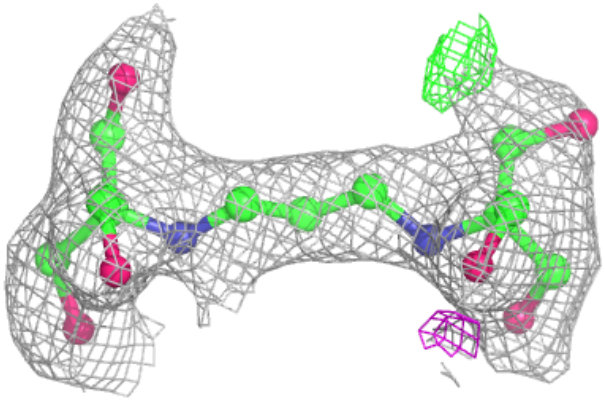


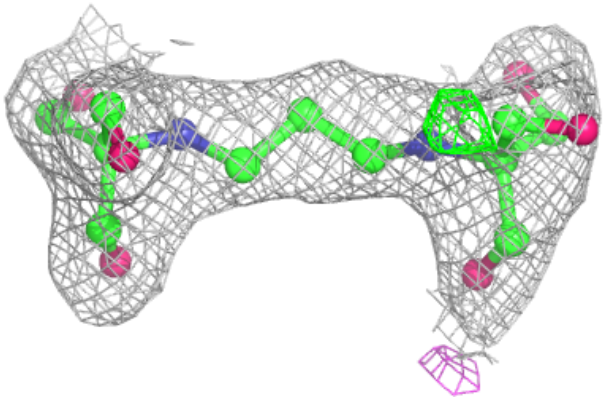




Electron density around B3P D 404:

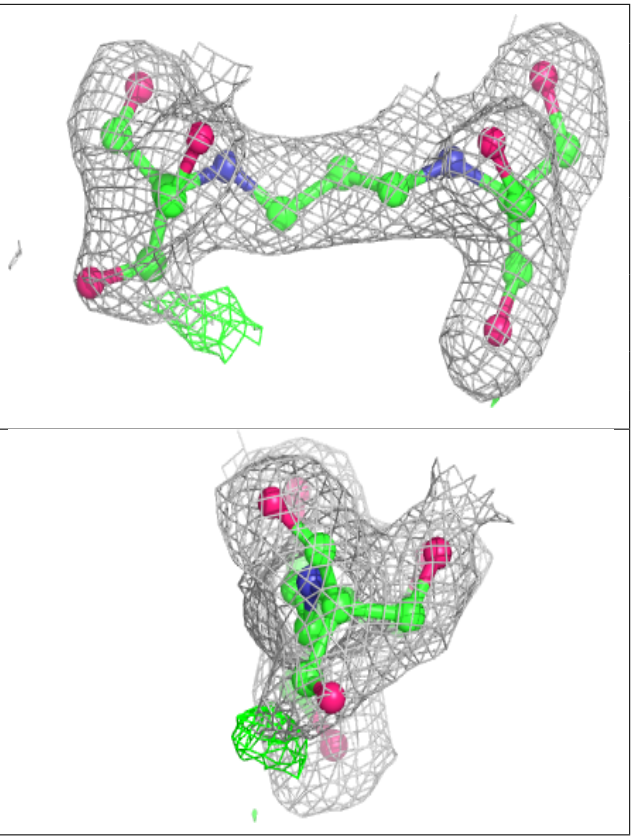
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





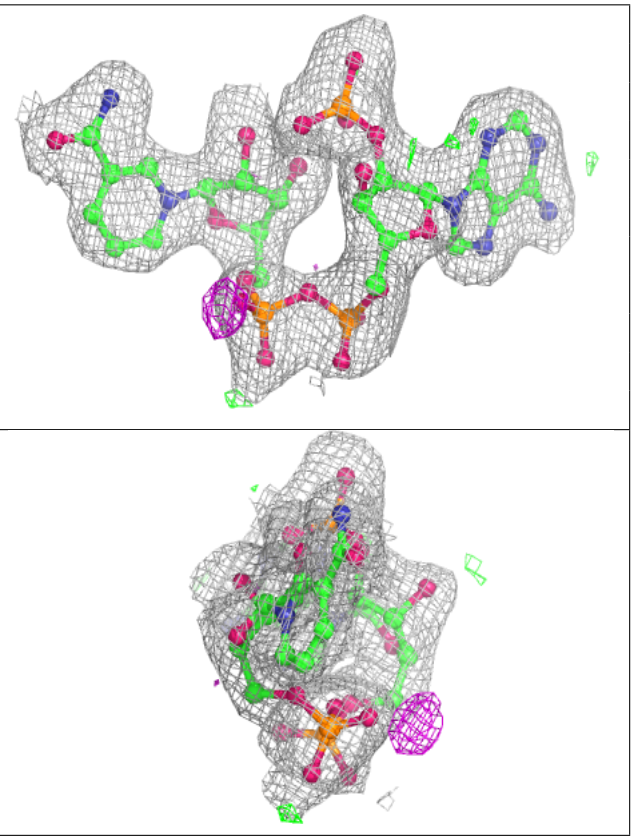
Electron density around B3P A 1003:

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



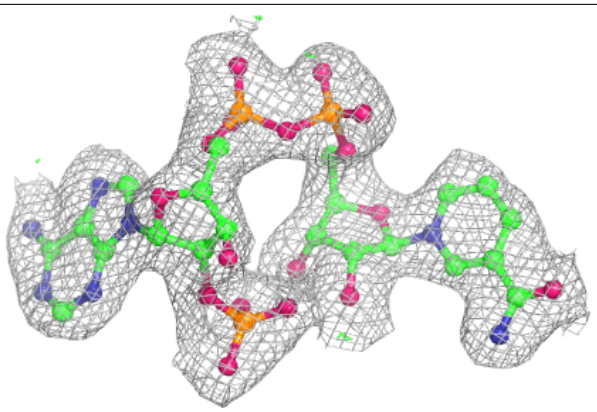
Electron density around NAP B 403:

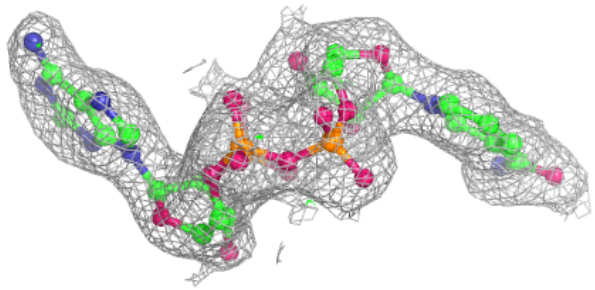
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

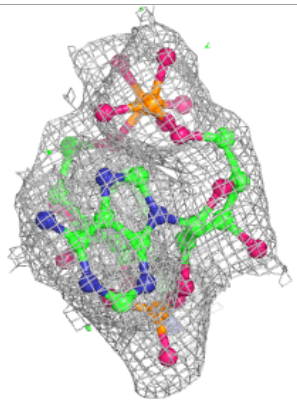


Electron density around NAP C 403:

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

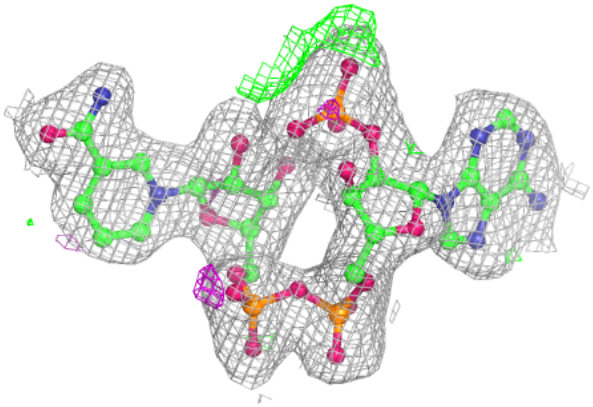


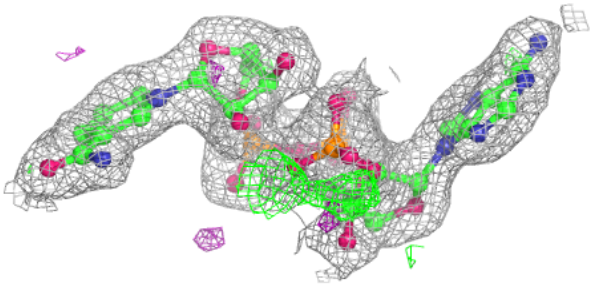


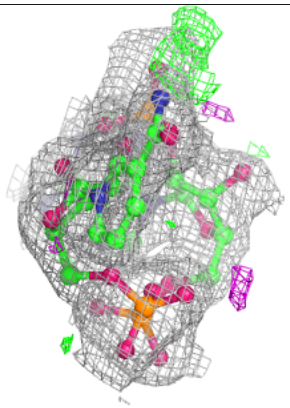


Electron density around NAP D 403:

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

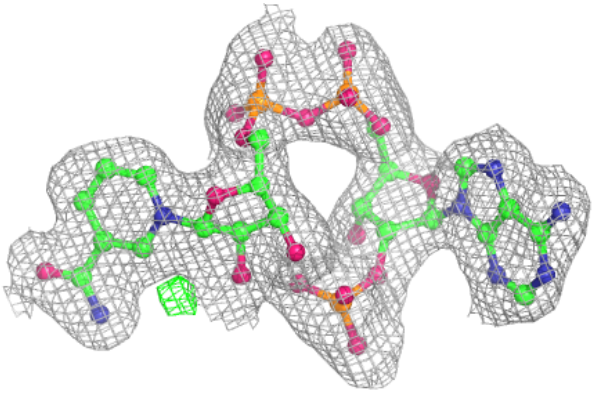


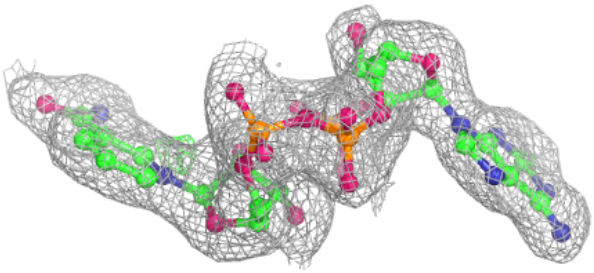


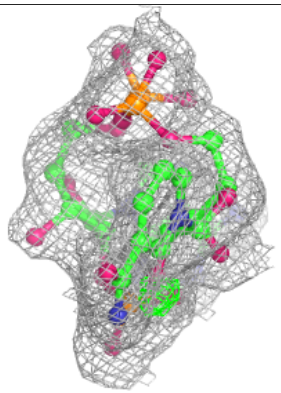


Electron density around NAP A 1002:

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

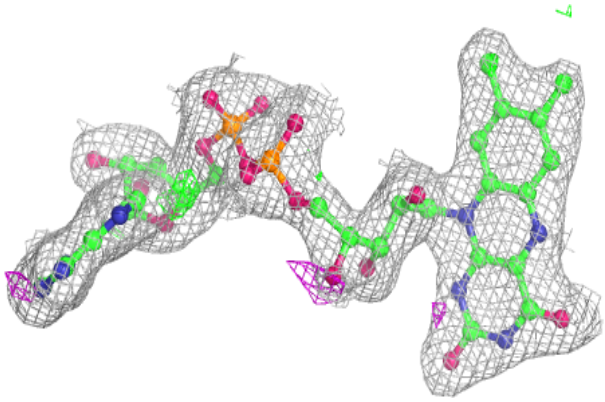


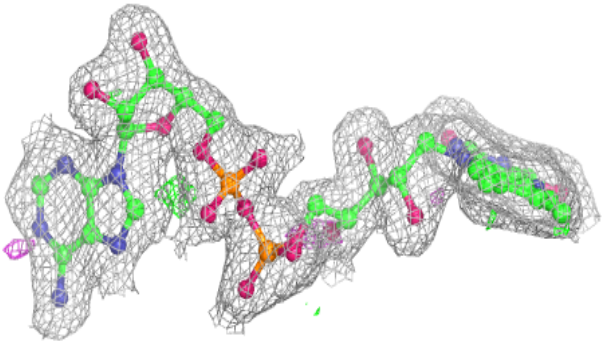


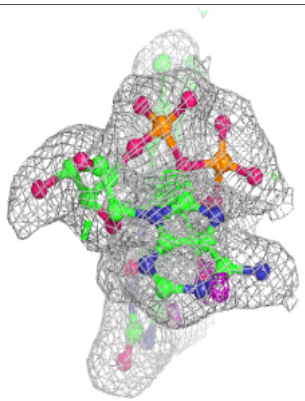


Electron density around FAD C 402:

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

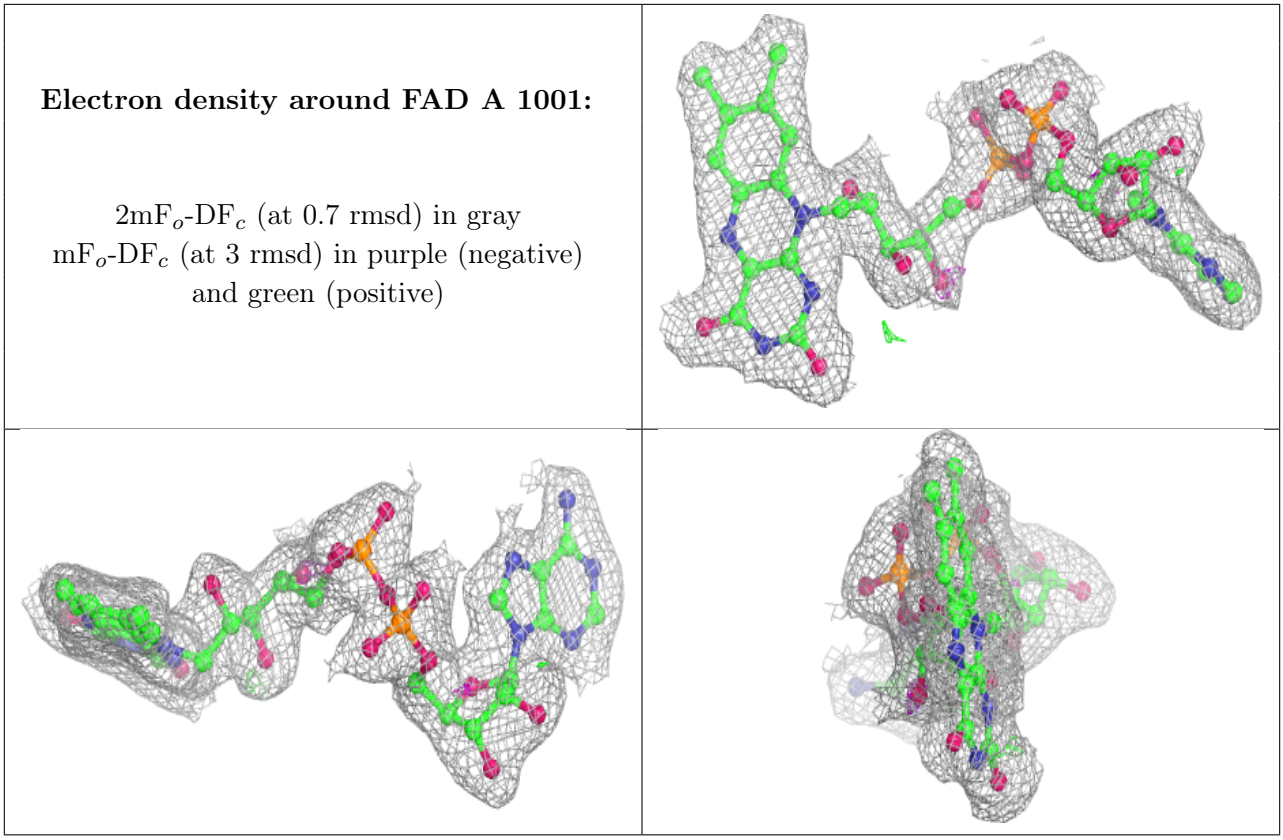






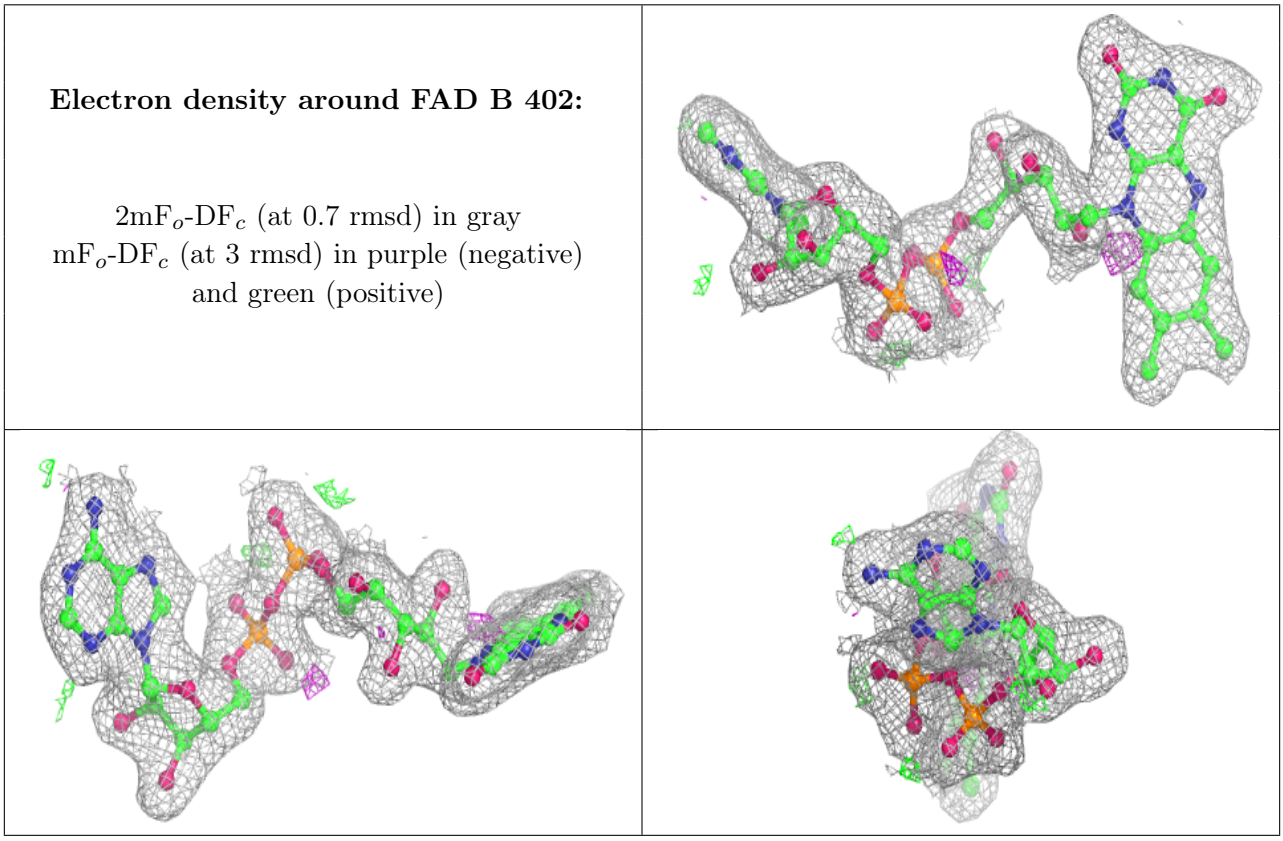
Electron density around FAD A 1001:

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



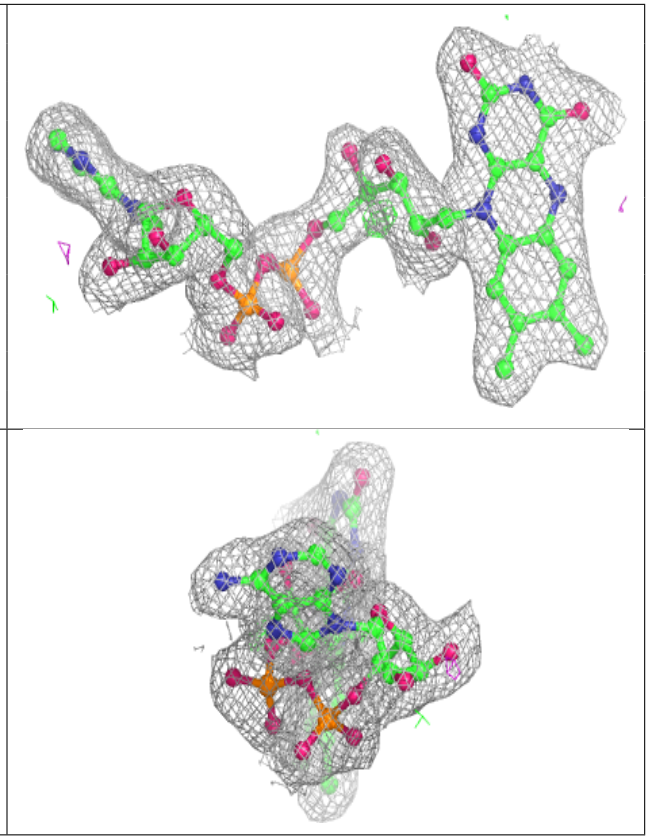
Electron density around FAD B 402:

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



Electron density around FAD D 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.