wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 09:38 AM BST

PDB ID	:	1UP7
Title	:	Structure of the 6-phospho-beta glucosidase from Thermotoga maritima at 2.4 Angstrom resolution in the tetragonal form with NAD and glucose-6-phosphate
Authors	:	Varrot, A.; Yip, V.L.; Withers, S.G.; Davies, G.J.
Deposited on	:	2003-09-29
Resolution	:	2.40 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 following versions of software and data (see references (1)) were used in the production of this report:

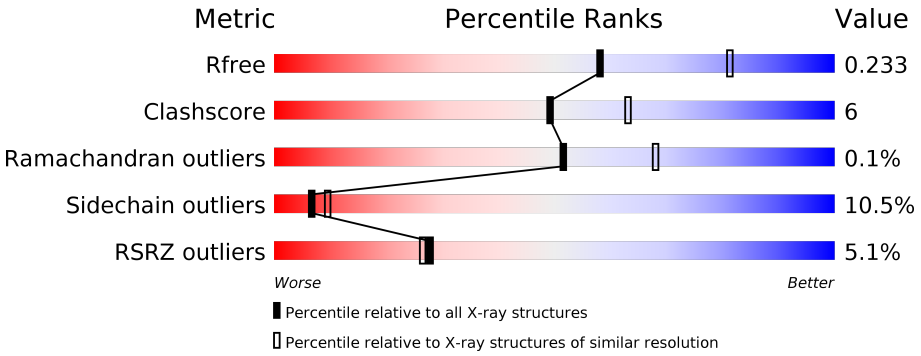
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	417	4% 77% 18%
1	B	417	5% 78% 16%
1	C	417	2% 76% 19%
1	D	417	4% 75% 20%
1	E	417	8% 76% 18%
1	F	417	6% 77% 19%

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Mol	Chain	Length	Quality of chain
1	G	417	4% 78% 18%
1	H	417	6% 73% 22%

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	G6P	A	1417	X	-	-	-
3	G6P	B	1417	X	-	-	-
3	G6P	C	1417	X	-	-	-
3	G6P	D	1417	X	-	-	-
3	G6P	E	1417	X	-	-	-
3	G6P	F	1417	X	-	-	-
3	G6P	G	1417	X	-	-	-
3	G6P	H	1417	X	-	-	-

2 Entry composition (i)

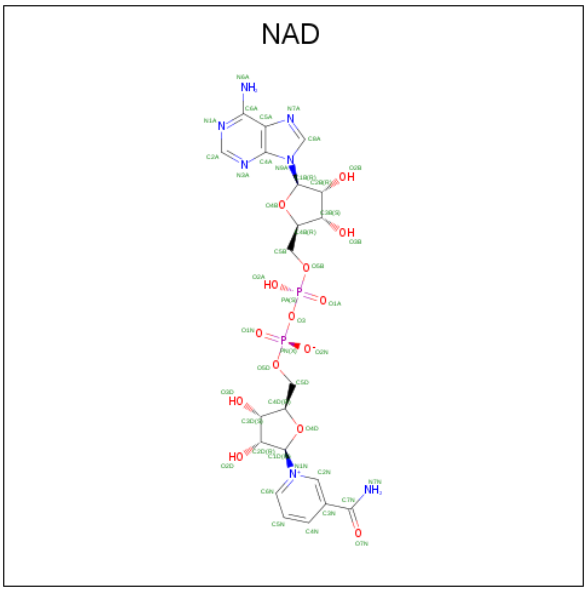
There are 5 unique types of molecules in this entry. The entry contains 27816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-PHOSPHO-BETA-GLUCOSIDASE.

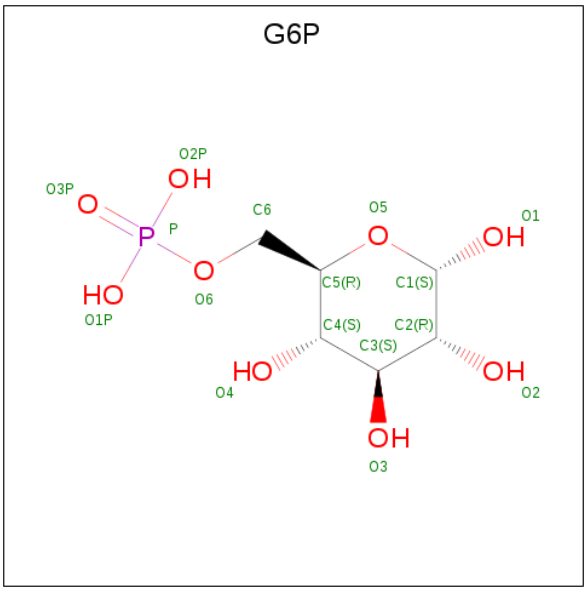
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	10	0	0
			3362	2166	563	624	9			
1	B	409	Total	C	N	O	S	74	0	0
			3318	2139	553	617	9			
1	C	409	Total	C	N	O	S	26	1	0
			3325	2144	553	618	10			
1	D	409	Total	C	N	O	S	51	0	0
			3317	2137	552	619	9			
1	E	406	Total	C	N	O	S	154	0	0
			3294	2124	548	613	9			
1	F	411	Total	C	N	O	S	116	0	0
			3333	2148	555	621	9			
1	G	409	Total	C	N	O	S	77	0	0
			3318	2139	553	617	9			
1	H	407	Total	C	N	O	S	86	0	0
			3300	2127	549	615	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



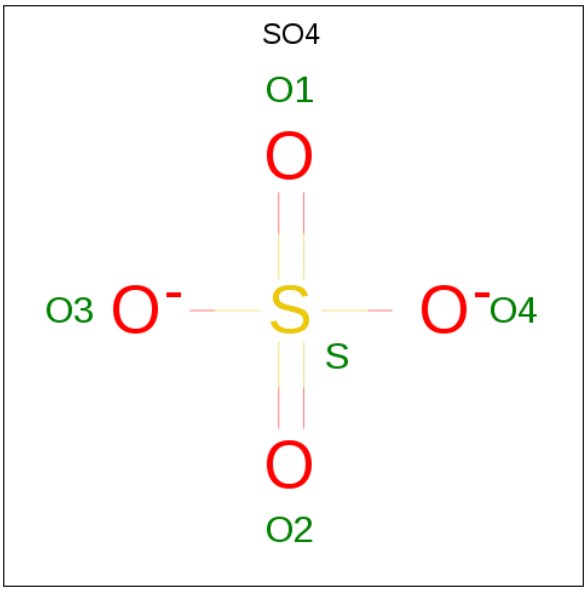
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 16 6 9 1	0	0
3	B	1	Total C O P 16 6 9 1	0	0
3	C	1	Total C O P 16 6 9 1	0	0
3	D	1	Total C O P 16 6 9 1	0	0
3	E	1	Total C O P 16 6 9 1	0	0
3	F	1	Total C O P 16 6 9 1	0	0
3	G	1	Total C O P 16 6 9 1	0	0
3	H	1	Total C O P 16 6 9 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

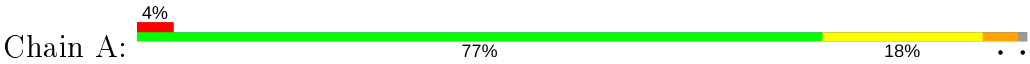
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	149	Total O 149 149	0	0
5	B	103	Total O 103 103	0	0
5	C	108	Total O 108 108	0	0
5	D	91	Total O 91 91	0	0
5	E	78	Total O 78 78	0	0
5	F	83	Total O 83 83	0	0
5	G	81	Total O 81 81	0	0
5	H	66	Total O 66 66	0	0

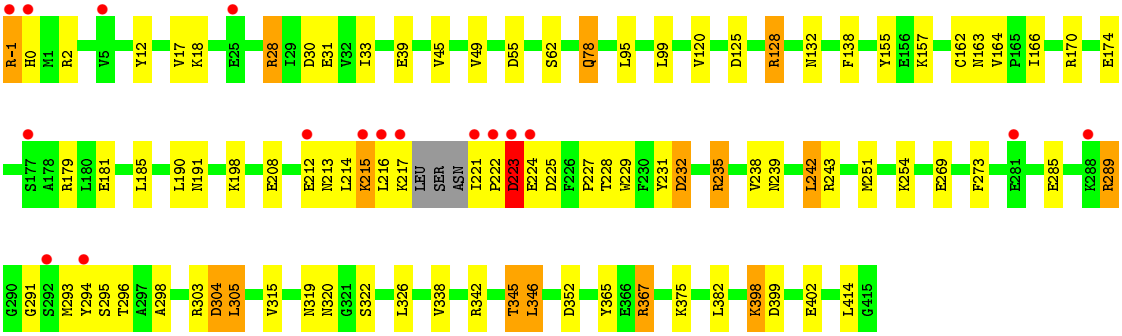
3 Residue-property plots (i)

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: 6-PHOSPHO-BETA-GLUCOSIDASE

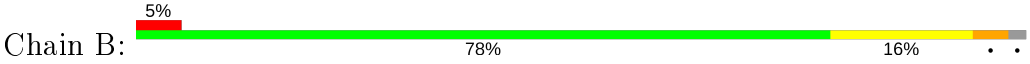
Chain A:

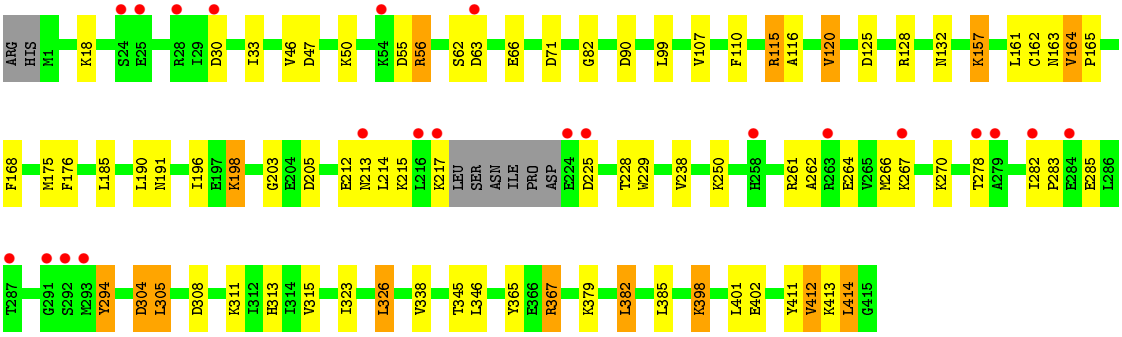




- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

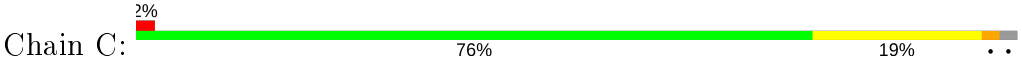
Chain B:

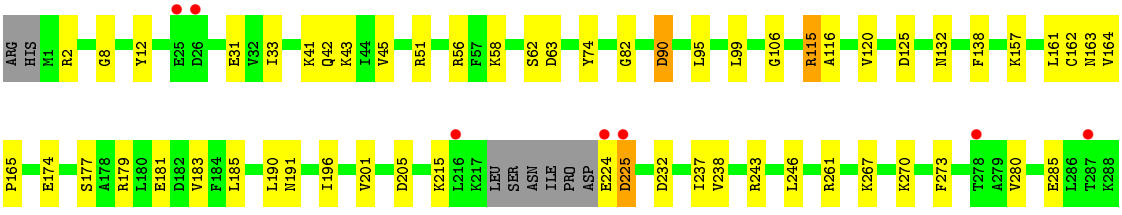


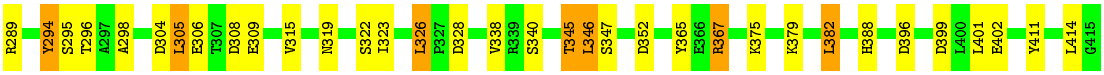


- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain C:

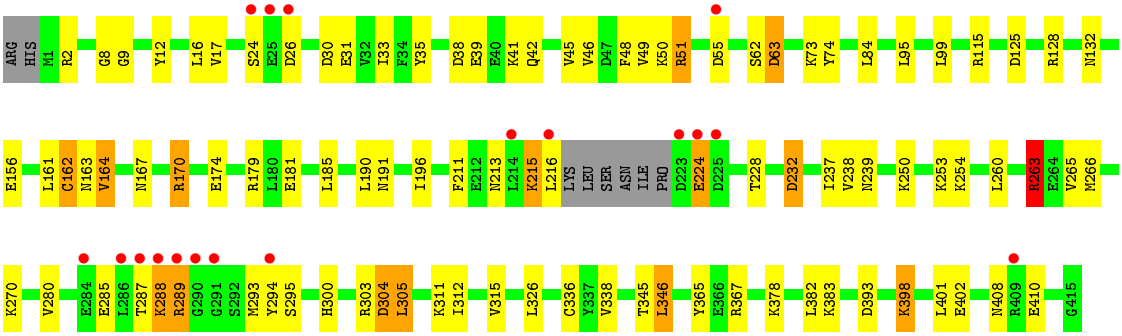






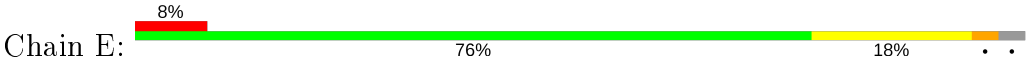
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

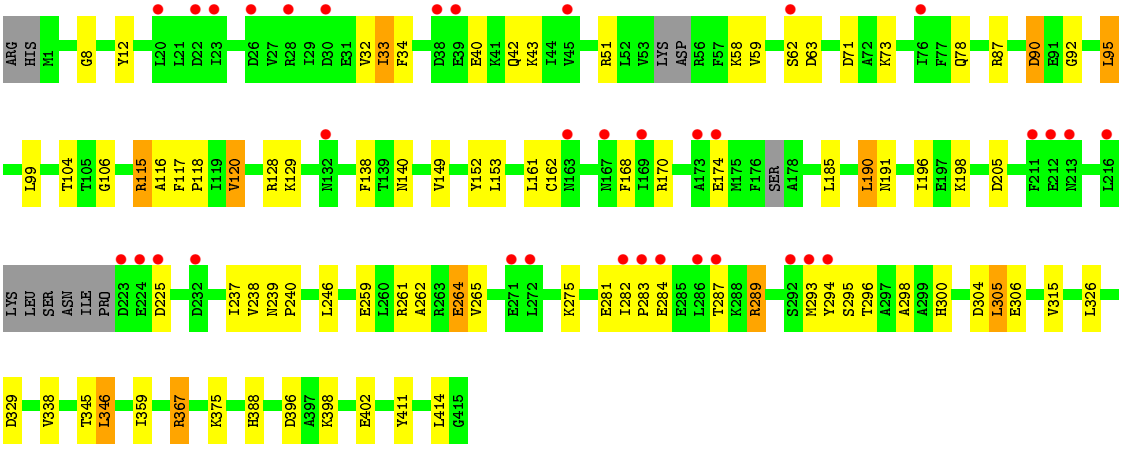
Chain D:



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

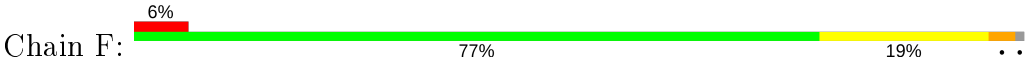
Chain E:

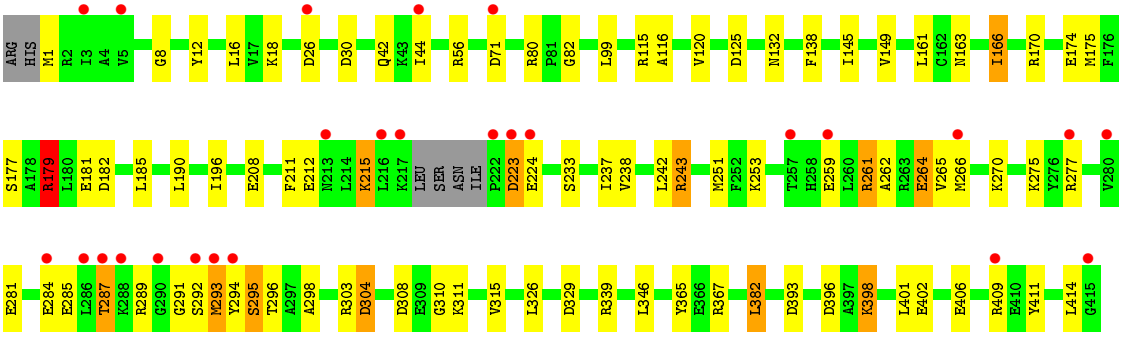




• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

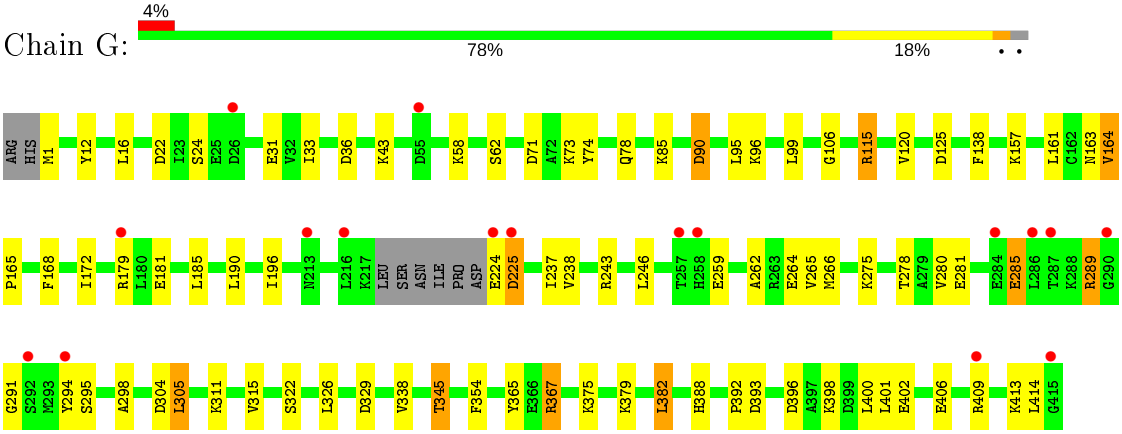
Chain F:





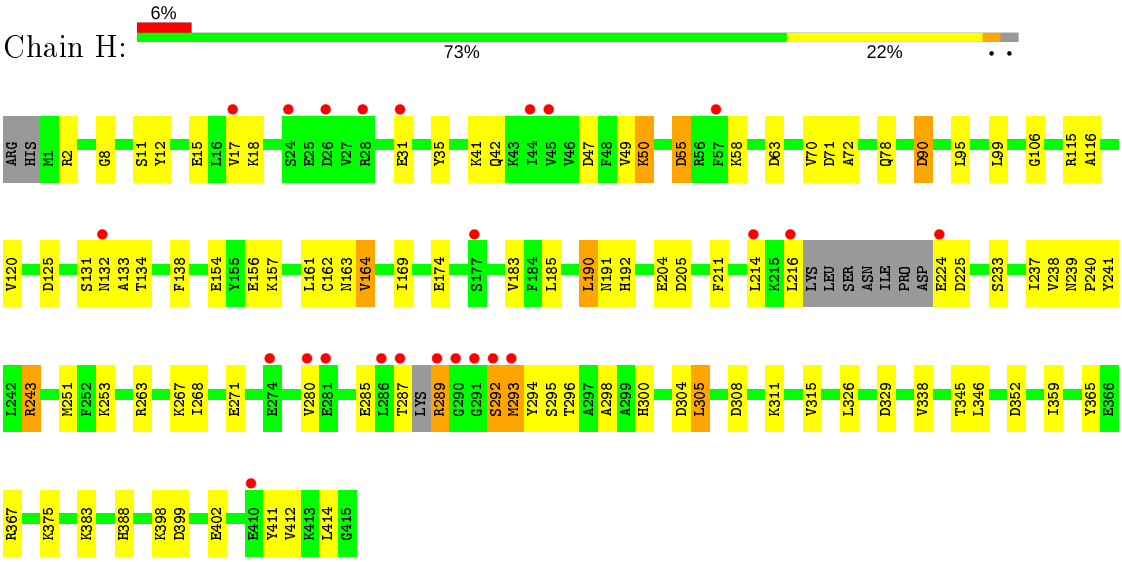
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain G:



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.13Å 178.13Å 278.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.96-2.40) 98.3 (19.96-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.240 0.196 , 0.233	Depositor DCC
R_{free} test set	16459 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27816	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.65% 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: G6P, SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.74	0/3429	0.88	10/4620 (0.2%)
1	B	0.65	0/3383	0.86	12/4557 (0.3%)
1	C	0.68	0/3391	0.90	15/4567 (0.3%)
1	D	0.74	1/3382 (0.0%)	0.87	11/4557 (0.2%)
1	E	0.68	4/3357 (0.1%)	0.85	12/4521 (0.3%)
1	F	0.53	0/3399	0.79	11/4579 (0.2%)
1	G	0.60	0/3383	0.83	13/4557 (0.3%)
1	H	0.57	1/3364 (0.0%)	0.78	12/4532 (0.3%)
All	All	0.65	6/27088 (0.0%)	0.85	96/36490 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	ARG	CZ-NH1	23.24	1.63	1.33
1	D	51	ARG	NE-CZ	8.03	1.43	1.33
1	E	51	ARG	NE-CZ	7.98	1.43	1.33
1	E	59	VAL	CB-CG2	6.38	1.66	1.52
1	H	50	LYS	CB-CG	5.79	1.68	1.52

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	51	ARG	NE-CZ-NH2	-21.85	109.37	120.30
1	C	115	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	E	51	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	C	225	ASP	CB-CG-OD2	8.93	126.34	118.30
1	G	115	ARG	NE-CZ-NH2	-8.58	116.01	120.30

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	3362	0	3397	53	0
1	B	3318	0	3355	38	0
1	C	3325	0	3363	40	0
1	D	3317	0	3346	51	0
1	E	3294	0	3322	43	0
1	F	3333	0	3367	35	0
1	G	3318	0	3355	29	0
1	H	3300	0	3328	48	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	1	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	2	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	2	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	149	0	0	2	0
5	B	103	0	0	1	0
5	C	108	0	0	0	0
5	D	91	0	0	1	0
5	E	78	0	0	0	0
5	F	83	0	0	1	0
5	G	81	0	0	1	0
5	H	66	0	0	0	0
All	All	27816	0	27129	313	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 6.

The worst 5 of 313 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:A:235:ARG:HH11	1:A:235:ARG:HG2	0.97	1.07
1:H:162:CYS:HB2	1:H:191:ASN:ND2	1.80	0.96
1:A:235:ARG:NH1	1:A:235:ARG:HG2	1.76	0.92
1:E:162:CYS:HB2	1:E:191:ASN:HD21	1.34	0.91
1:B:398:LYS:O	1:B:402:GLU:HG3	1.72	0.87

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	410/417 (98%)	402 (98%)	6 (2%)	2 (0%)	29 41
1	B	405/417 (97%)	400 (99%)	5 (1%)	0	100 100
1	C	406/417 (97%)	399 (98%)	7 (2%)	0	100 100
1	D	405/417 (97%)	397 (98%)	6 (2%)	2 (0%)	29 41
1	E	398/417 (95%)	392 (98%)	6 (2%)	0	100 100
1	F	407/417 (98%)	399 (98%)	8 (2%)	0	100 100
1	G	405/417 (97%)	397 (98%)	8 (2%)	0	100 100
1	H	401/417 (96%)	391 (98%)	10 (2%)	0	100 100
All	All	3237/3336 (97%)	3177 (98%)	56 (2%)	4 (0%)	51 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO
1	A	223	ASP

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Mol	Chain	Res	Type
1	D	288	LYS
1	D	285	GLU

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	366/369 (99%)	330 (90%)	36 (10%)	8 11
1	B	361/369 (98%)	327 (91%)	34 (9%)	8 13
1	C	362/369 (98%)	329 (91%)	33 (9%)	9 14
1	D	361/369 (98%)	318 (88%)	43 (12%)	5 6
1	E	358/369 (97%)	327 (91%)	31 (9%)	10 15
1	F	363/369 (98%)	318 (88%)	45 (12%)	4 5
1	G	361/369 (98%)	325 (90%)	36 (10%)	7 11
1	H	359/369 (97%)	314 (88%)	45 (12%)	4 5
All	All	2891/2952 (98%)	2588 (90%)	303 (10%)	7 9

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	326	LEU
1	E	326	LEU
1	H	263	ARG
1	D	367	ARG
1	E	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	300	HIS
1	E	42	GLN
1	H	300	HIS

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Mol	Chain	Res	Type
1	D	320	ASN
1	E	191	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
3	G6P	H	1417	-	16,16,16	0.46	0	24,24,24	0.99	1 (4%)
2	NAD	B	1416	-	42,48,48	1.85	3 (7%)	50,73,73	1.25	5 (10%)
2	NAD	A	1416	-	42,48,48	1.85	5 (11%)	50,73,73	1.40	7 (14%)
2	NAD	D	1416	-	42,48,48	1.81	3 (7%)	50,73,73	1.24	4 (8%)
2	NAD	C	1416	-	42,48,48	1.80	3 (7%)	50,73,73	1.26	4 (8%)
2	NAD	F	1416	-	42,48,48	1.75	3 (7%)	50,73,73	1.30	4 (8%)
2	NAD	E	1416	-	42,48,48	1.77	3 (7%)	50,73,73	1.37	4 (8%)
2	NAD	H	1416	-	42,48,48	1.69	3 (7%)	50,73,73	1.25	4 (8%)
2	NAD	G	1416	-	42,48,48	1.80	3 (7%)	50,73,73	1.34	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	G6P	A	1417	-	16,16,16	0.71	0	24,24,24	1.20	2 (8%)
3	G6P	C	1417	-	16,16,16	0.70	0	24,24,24	1.12	1 (4%)
3	G6P	G	1417	-	16,16,16	0.64	0	24,24,24	1.02	2 (8%)
3	G6P	D	1417	-	16,16,16	0.44	0	24,24,24	0.92	0
4	SO4	C	1418	-	4,4,4	0.61	0	6,6,6	0.38	0
3	G6P	F	1417	-	16,16,16	0.51	0	24,24,24	1.00	2 (8%)
4	SO4	A	1418	-	4,4,4	0.37	0	6,6,6	0.54	0
3	G6P	E	1417	-	16,16,16	0.56	0	24,24,24	0.83	0
3	G6P	B	1417	-	16,16,16	0.46	0	24,24,24	0.70	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
3	G6P	H	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
2	NAD	B	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	A	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	D	1416	-	-	11/26/62/62	0/5/5/5
2	NAD	C	1416	-	-	10/26/62/62	0/5/5/5
2	NAD	F	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	E	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	H	1416	-	-	7/26/62/62	0/5/5/5
2	NAD	G	1416	-	-	9/26/62/62	0/5/5/5
3	G6P	A	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	G	1417	-	1/1/6/6	5/6/26/26	0/1/1/1
3	G6P	D	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	F	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	C	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	E	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	B	1417	-	1/1/6/6	2/6/26/26	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1416	NAD	O7N-C7N	9.70	1.42	1.24
2	G	1416	NAD	O7N-C7N	9.49	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1416	NAD	O7N-C7N	9.49	1.42	1.24
2	A	1416	NAD	O7N-C7N	9.30	1.42	1.24
2	C	1416	NAD	O7N-C7N	9.17	1.41	1.24

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1416	NAD	N3A-C2A-N1A	-6.15	119.07	128.68
2	F	1416	NAD	N3A-C2A-N1A	-5.95	119.37	128.68
2	G	1416	NAD	N3A-C2A-N1A	-5.91	119.44	128.68
2	H	1416	NAD	N3A-C2A-N1A	-5.77	119.66	128.68
2	E	1416	NAD	N3A-C2A-N1A	-5.72	119.74	128.68

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1417	G6P	C1
3	A	1417	G6P	C1
3	G	1417	G6P	C1
3	D	1417	G6P	C1
3	F	1417	G6P	C1

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1417	G6P	C4-C5-C6-O6
3	H	1417	G6P	O5-C5-C6-O6
2	D	1416	NAD	C5B-O5B-PA-O1A
2	D	1416	NAD	C5B-O5B-PA-O2A
2	D	1416	NAD	PN-O3-PA-O5B

There are no ring outliers.

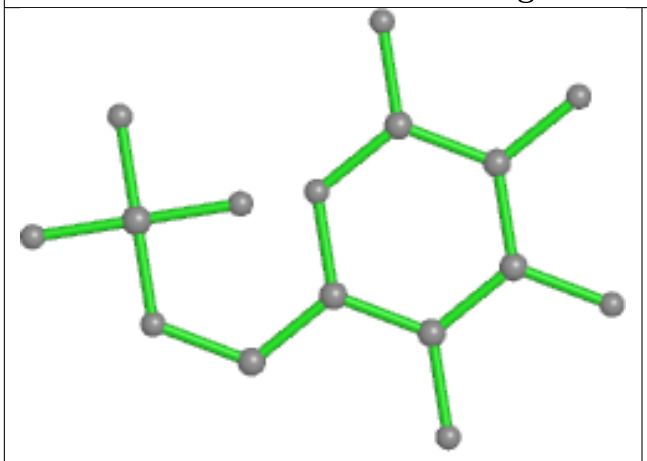
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1417	G6P	2	0
2	F	1416	NAD	2	0
2	E	1416	NAD	1	0
3	D	1417	G6P	2	0

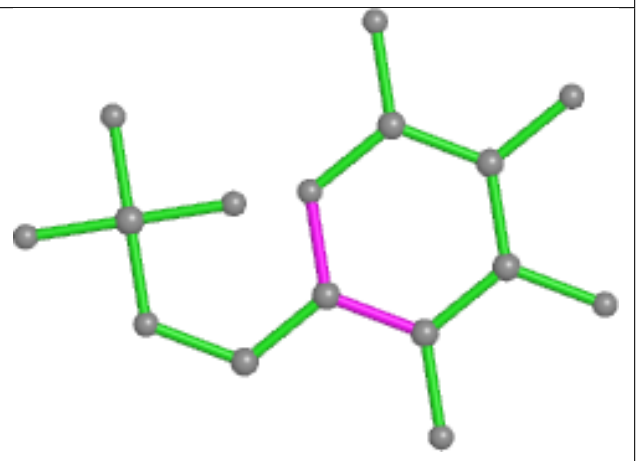
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

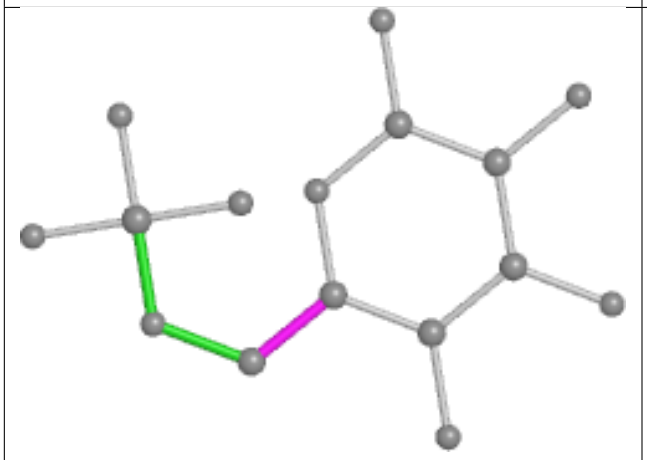
Ligand G6P H 1417



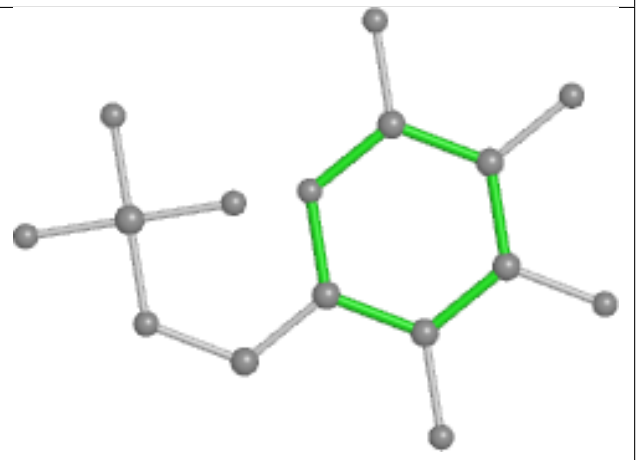
Bond lengths



Bond angles

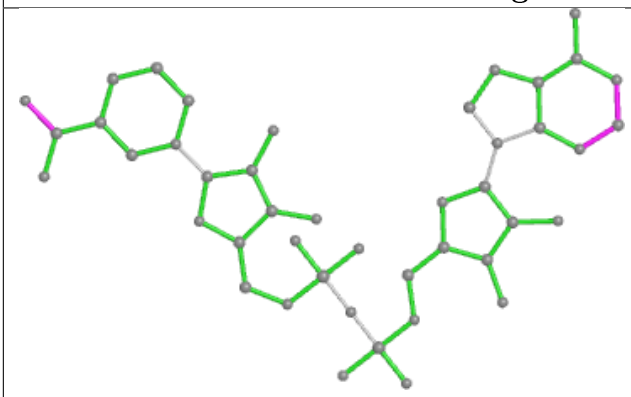


Torsions

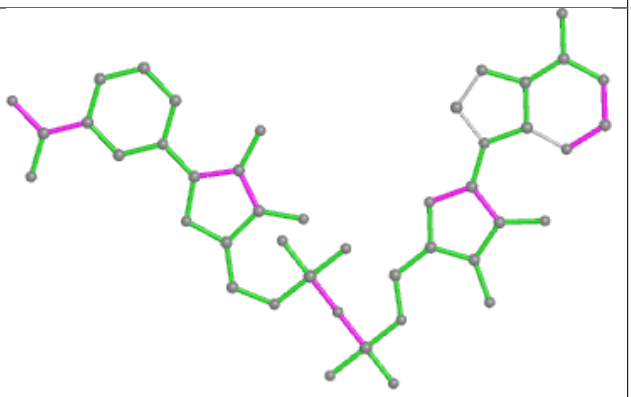


Rings

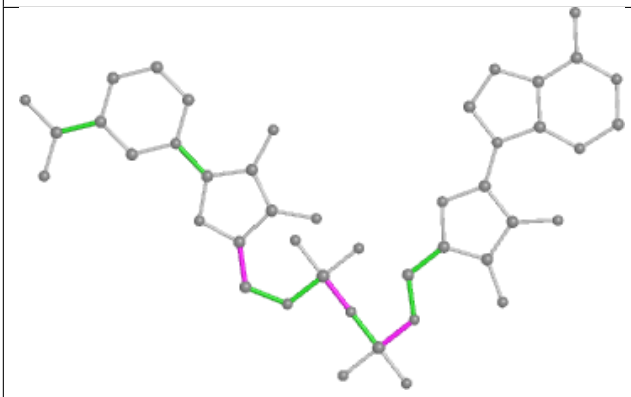
Ligand NAD B 1416



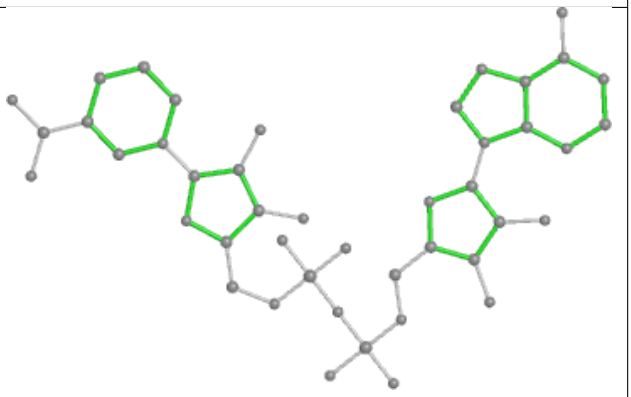
Bond lengths



Bond angles

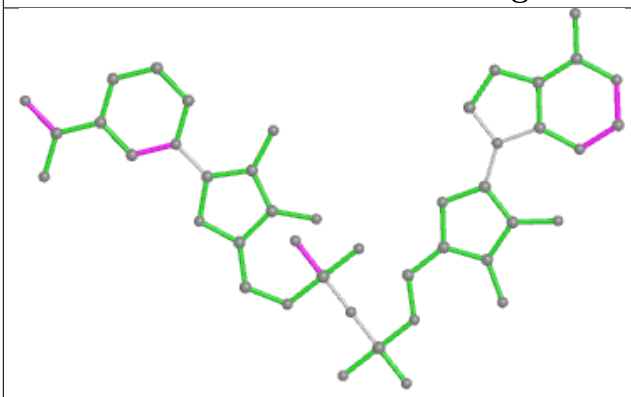


Torsions

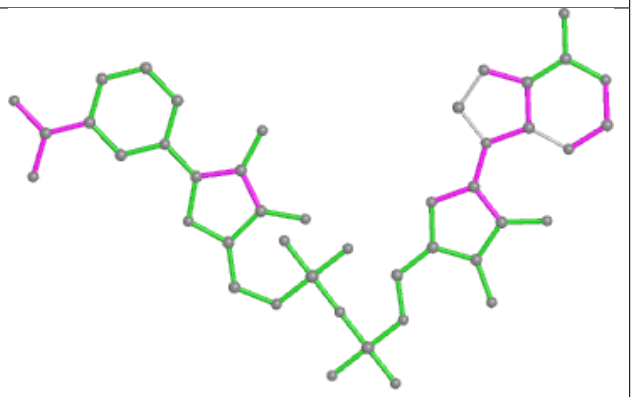


Rings

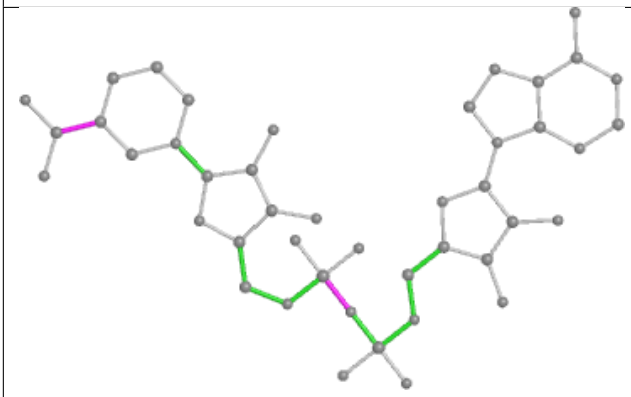
Ligand NAD A 1416



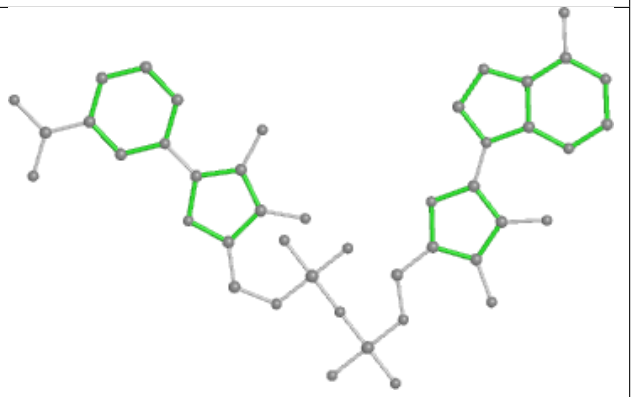
Bond lengths



Bond angles

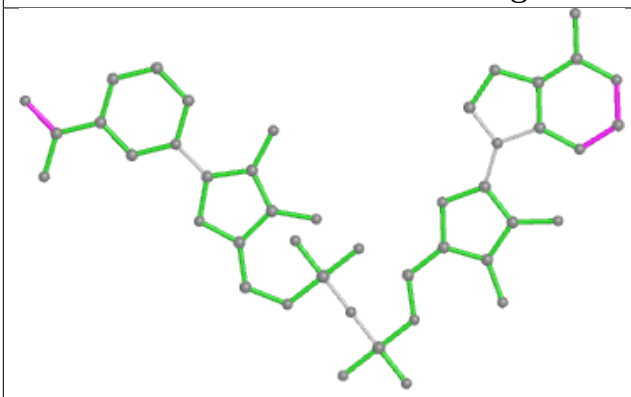


Torsions

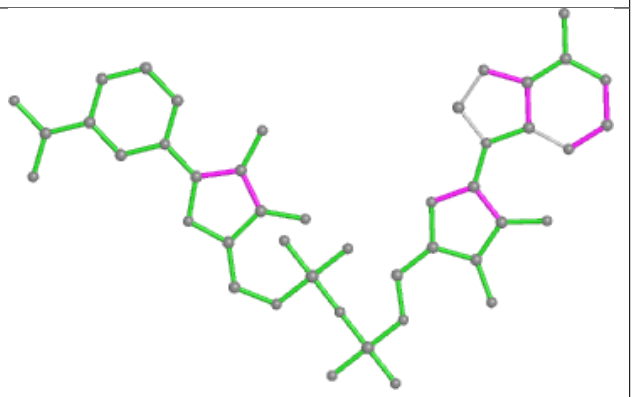


Rings

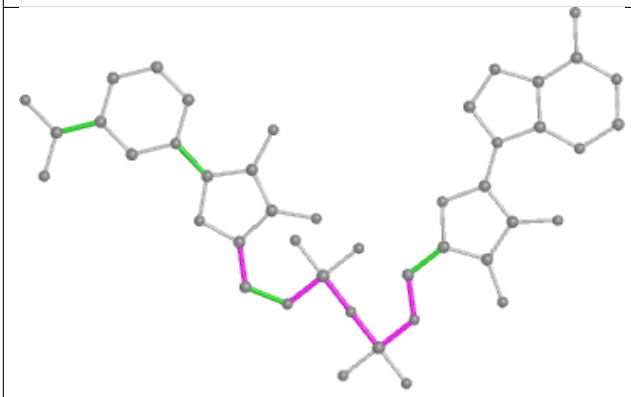
Ligand NAD D 1416



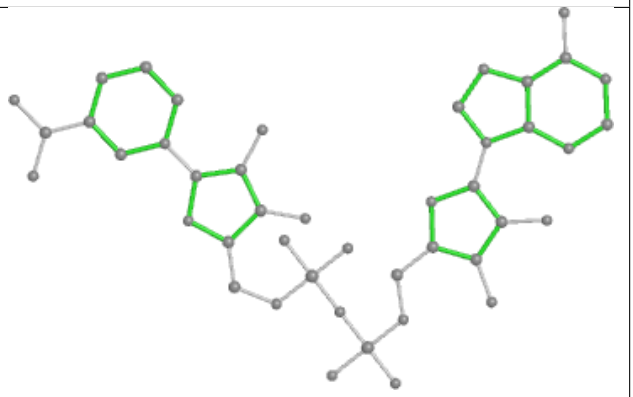
Bond lengths



Bond angles

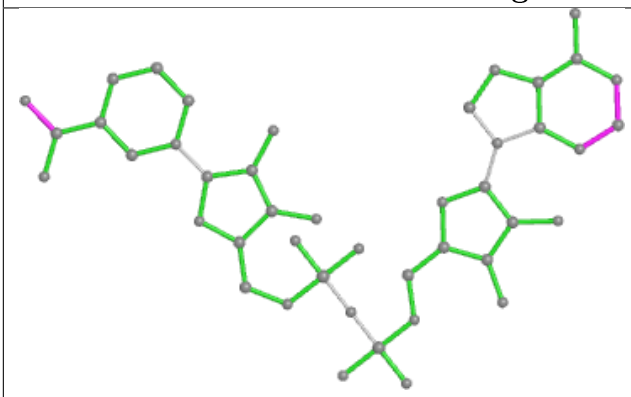


Torsions

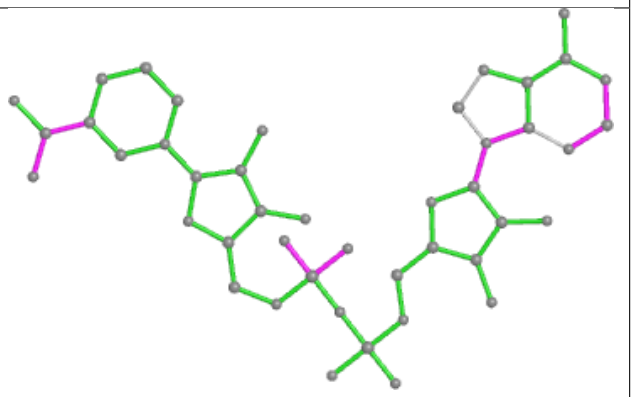


Rings

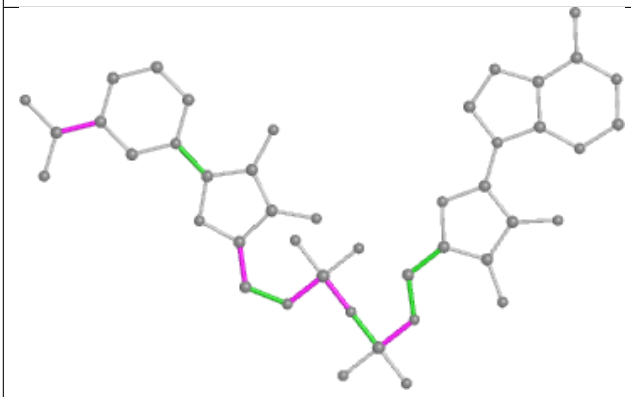
Ligand NAD C 1416



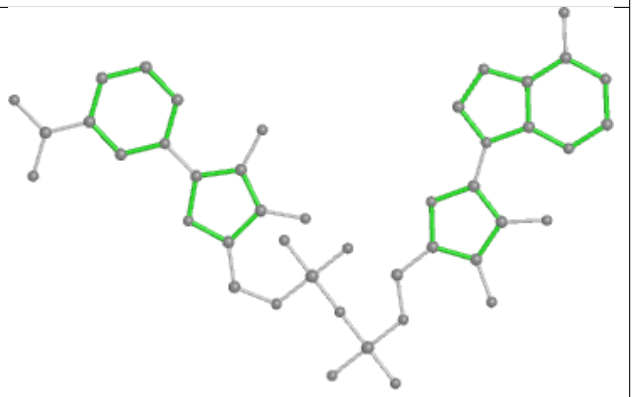
Bond lengths



Bond angles

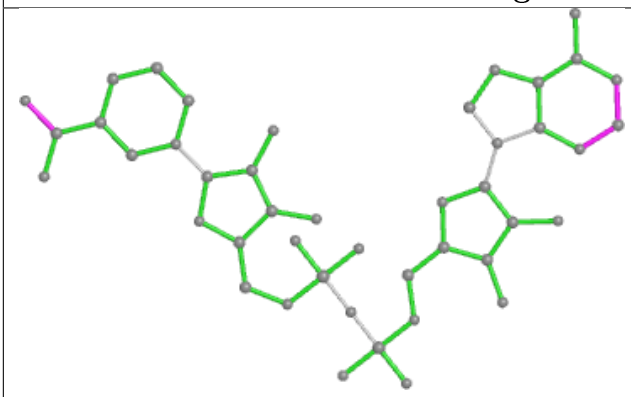


Torsions

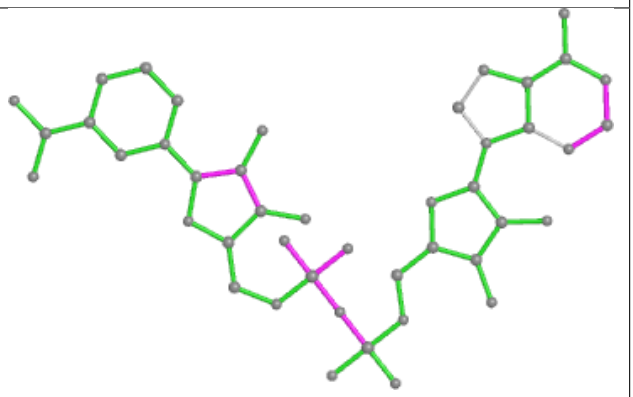


Rings

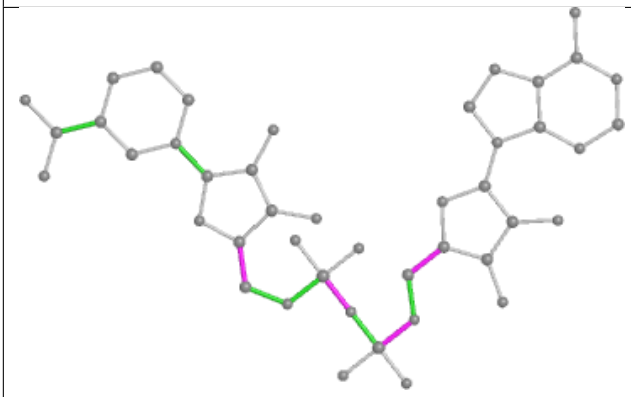
Ligand NAD F 1416



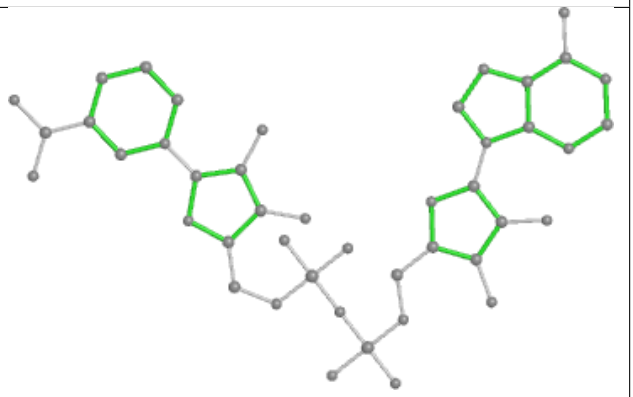
Bond lengths



Bond angles

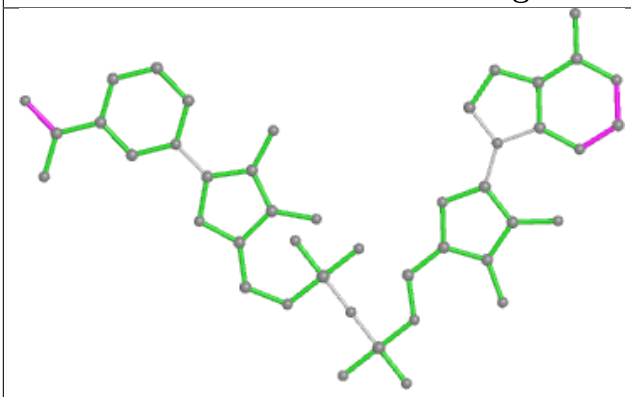


Torsions

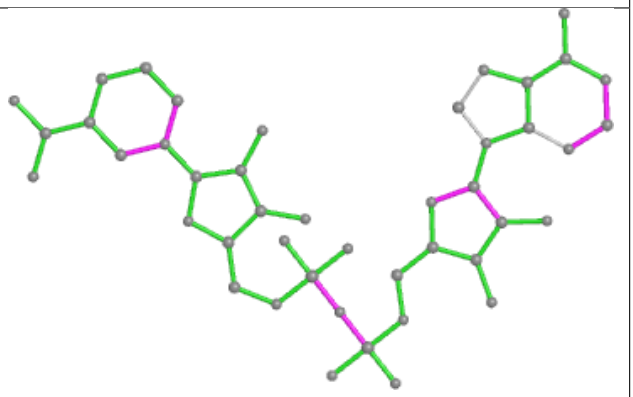


Rings

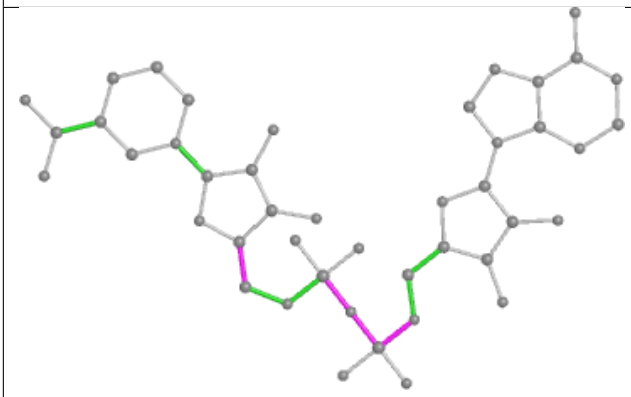
Ligand NAD E 1416



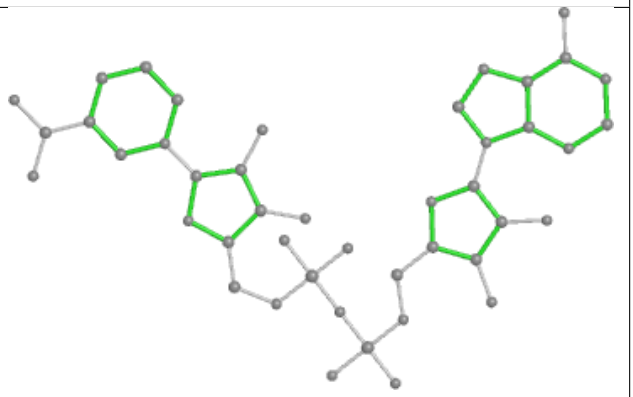
Bond lengths



Bond angles

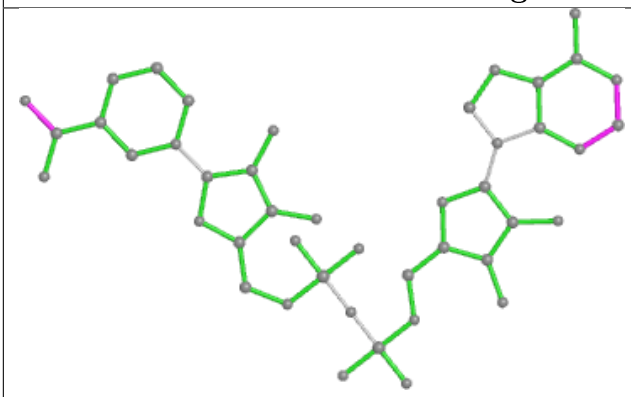


Torsions

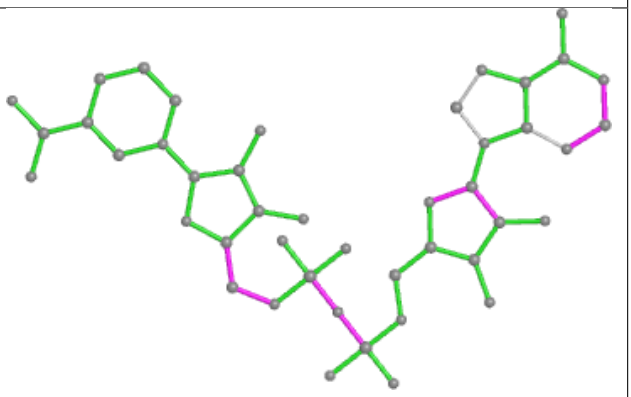


Rings

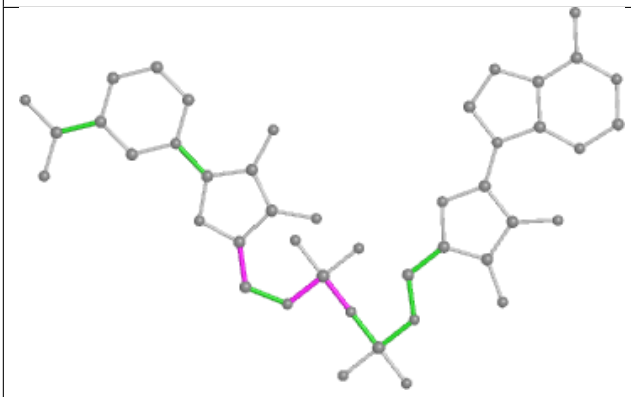
Ligand NAD H 1416



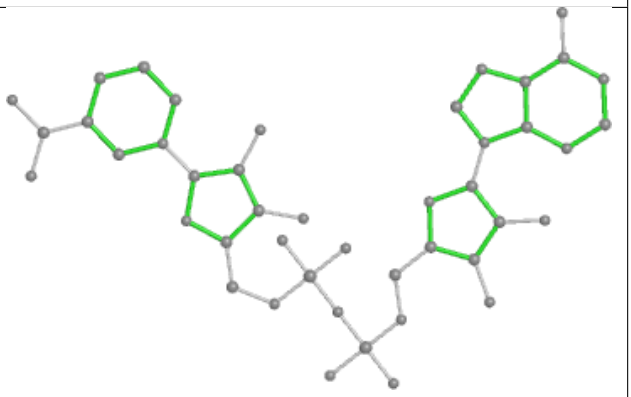
Bond lengths



Bond angles

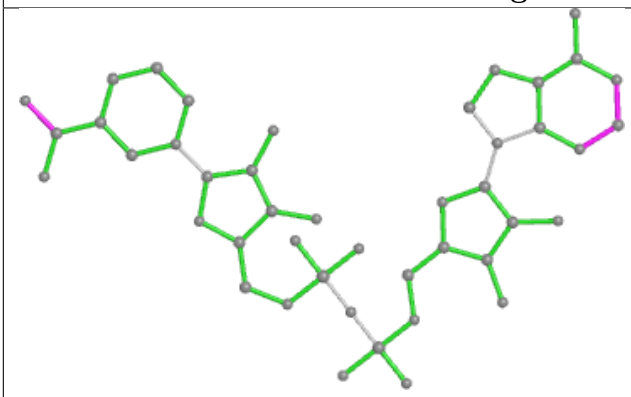


Torsions

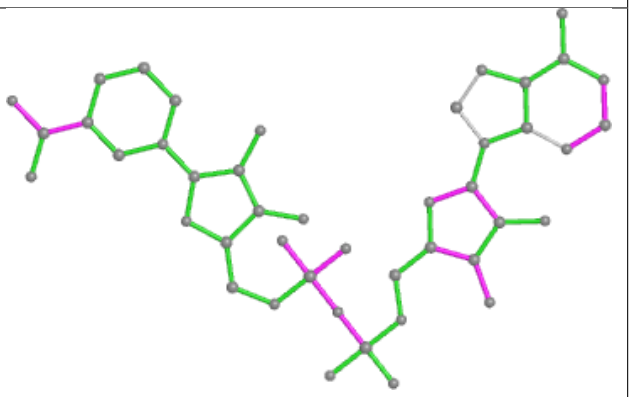


Rings

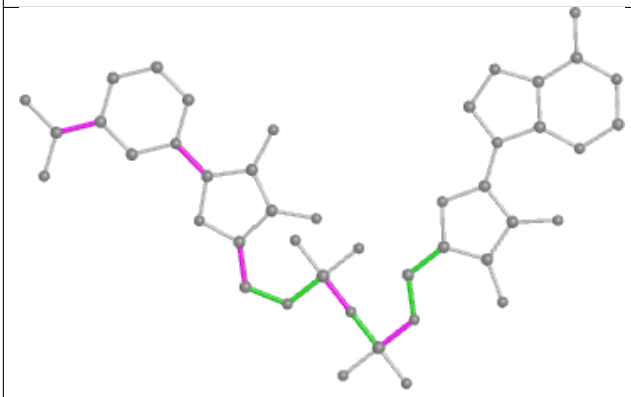
Ligand NAD G 1416



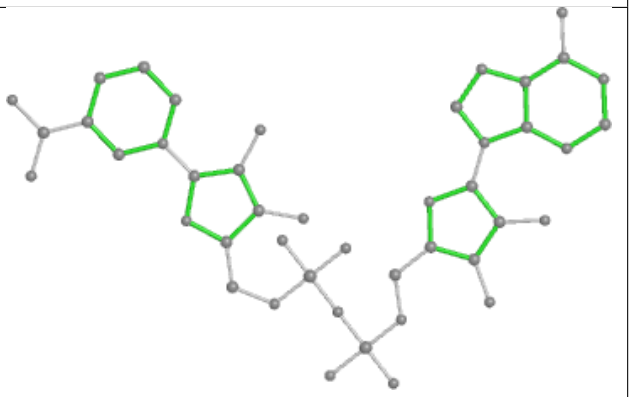
Bond lengths



Bond angles

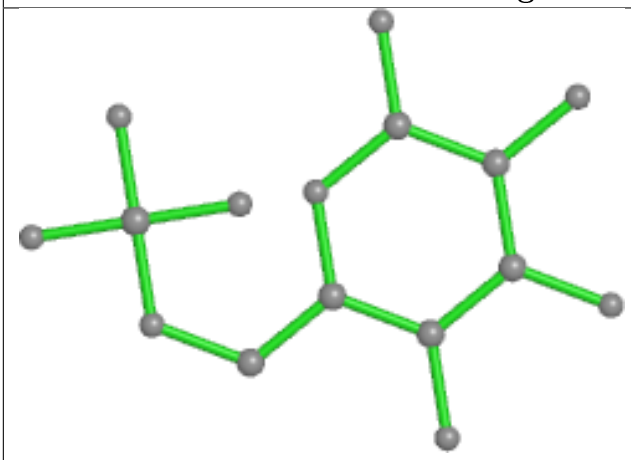


Torsions

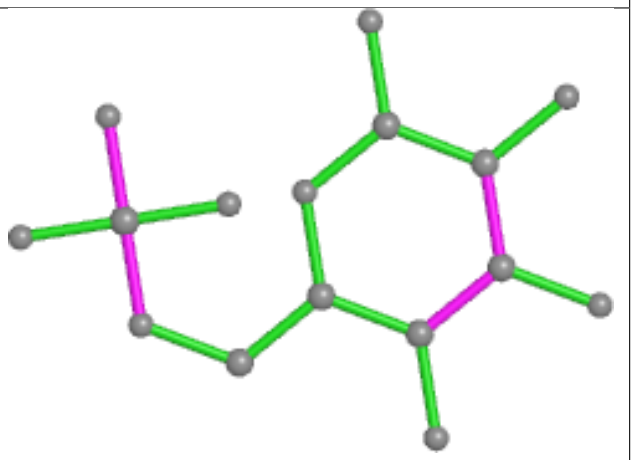


Rings

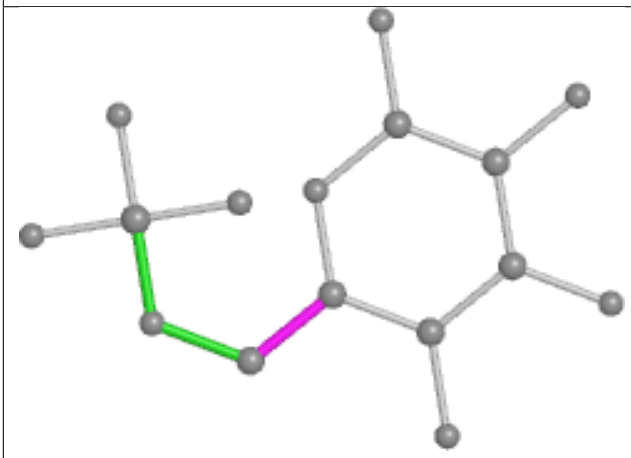
Ligand G6P A 1417



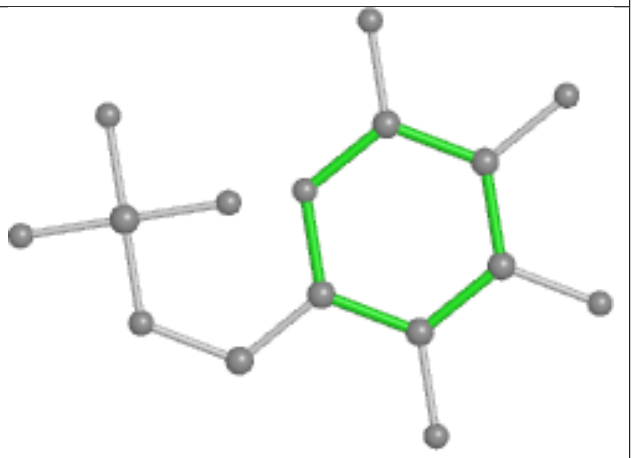
Bond lengths



Bond angles

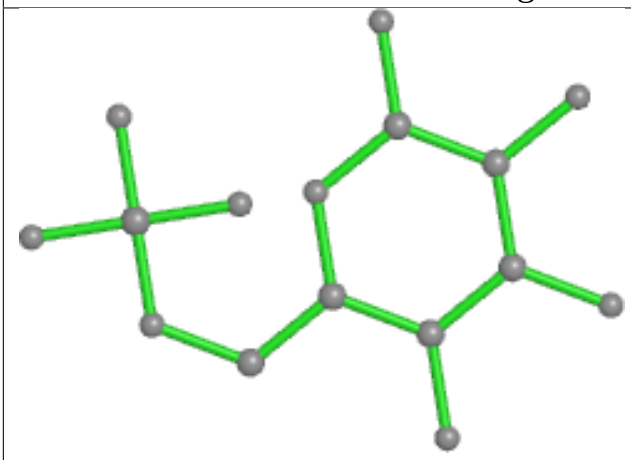


Torsions

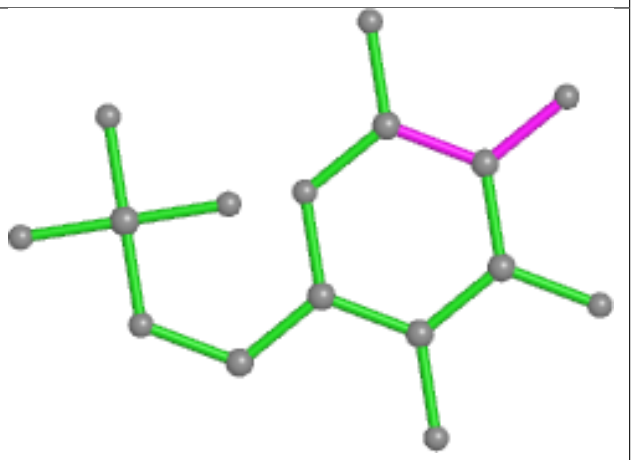


Rings

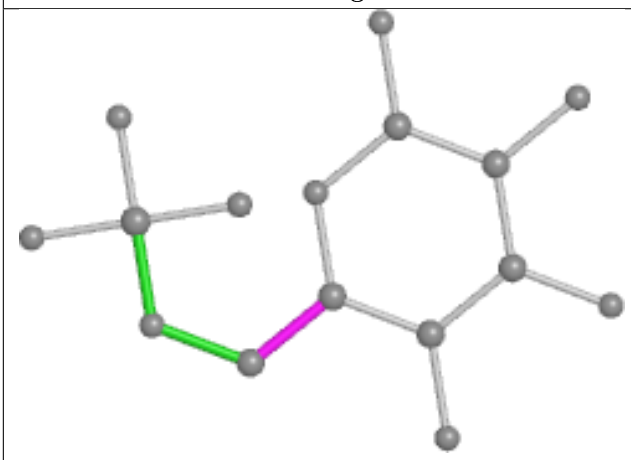
Ligand G6P C 1417



Bond lengths



Bond angles



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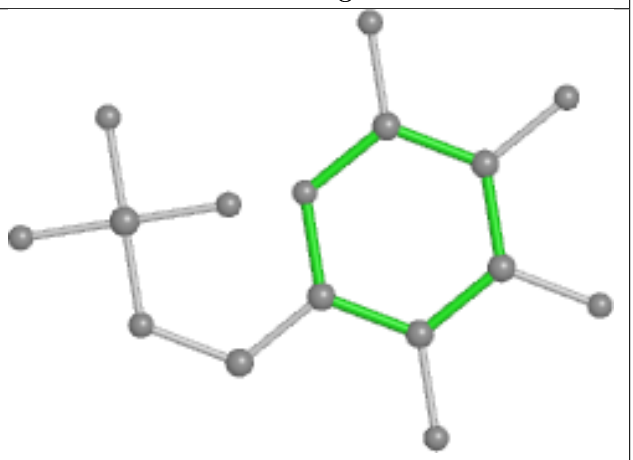
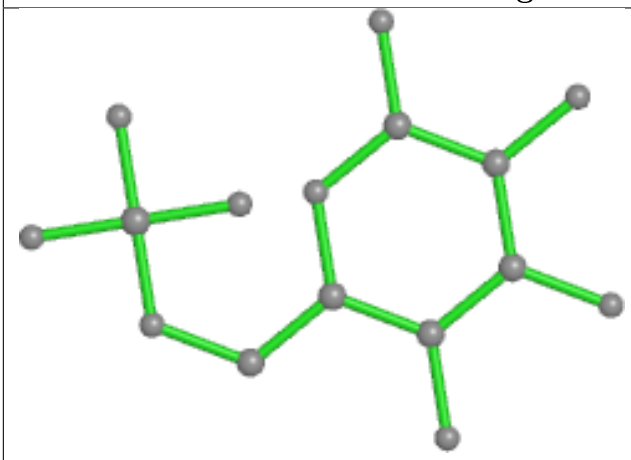
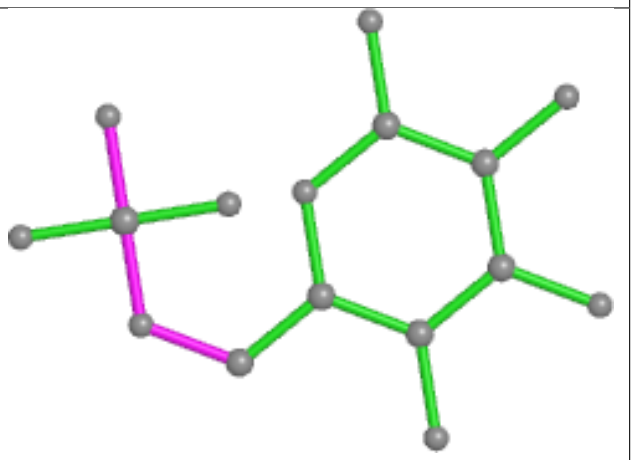


Rings

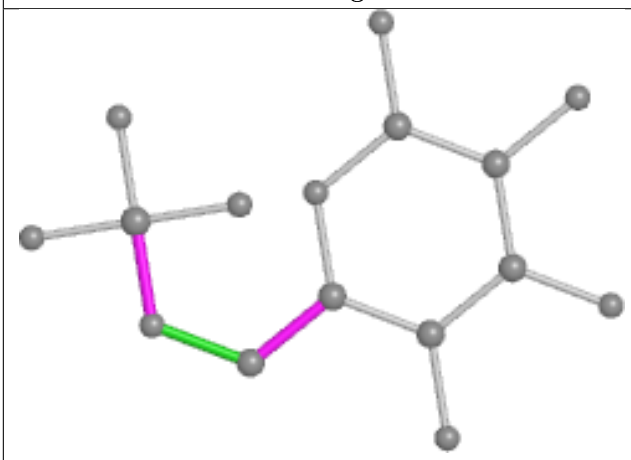
Ligand G6P G 1417



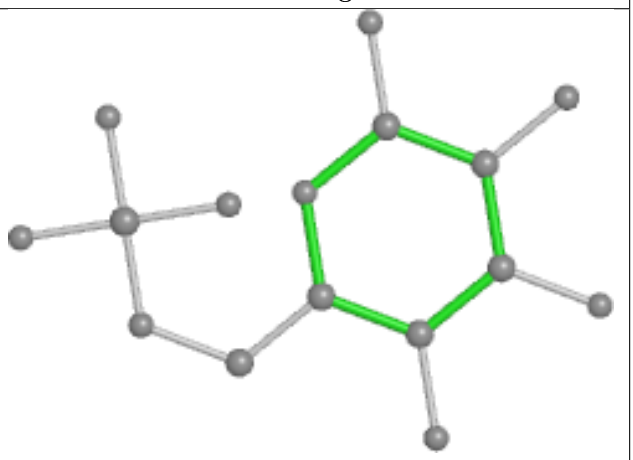
Bond lengths



Bond angles

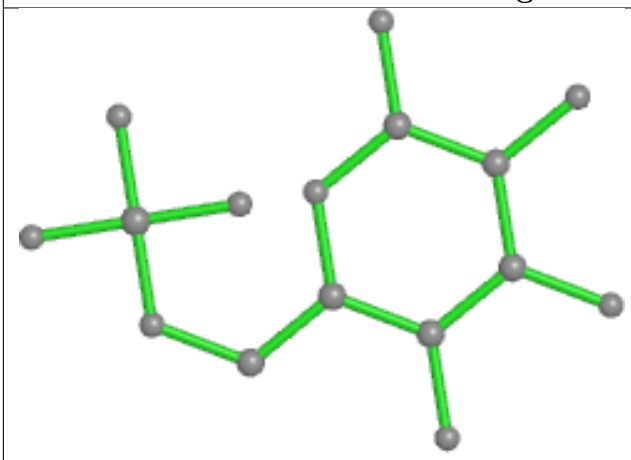


Torsions

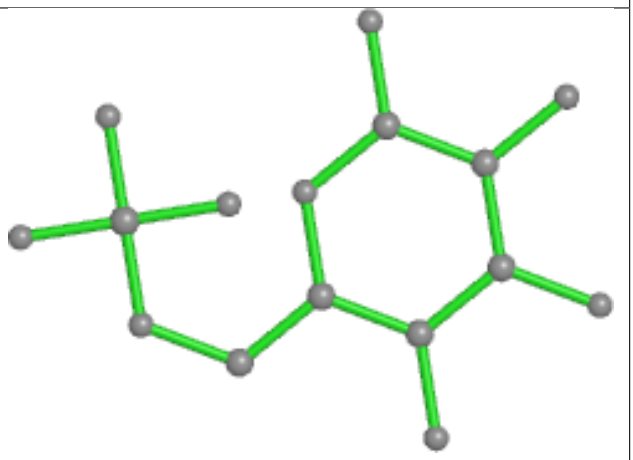


Rings

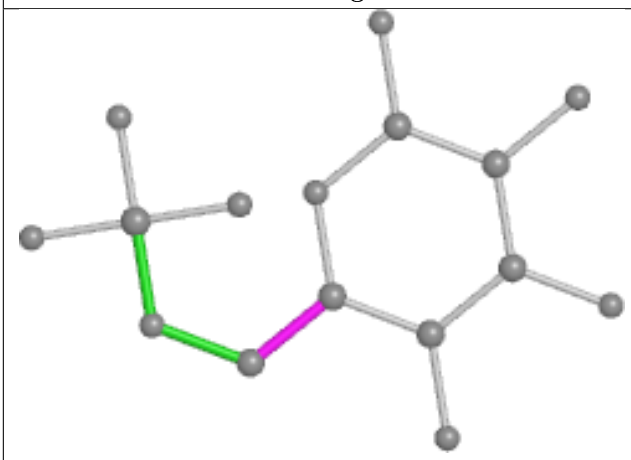
Ligand G6P D 1417



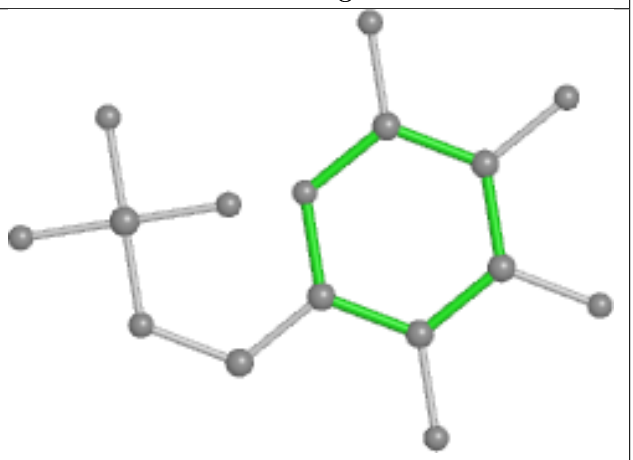
Bond lengths



Bond angles

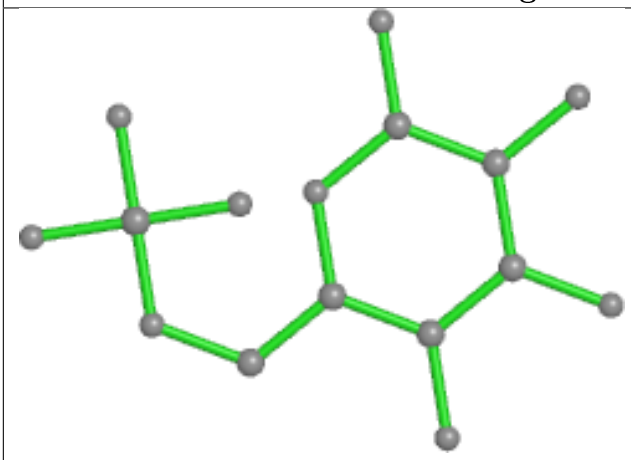


Torsions

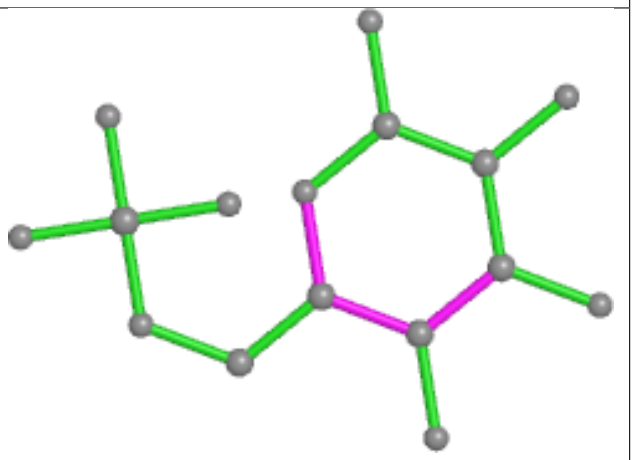


Rings

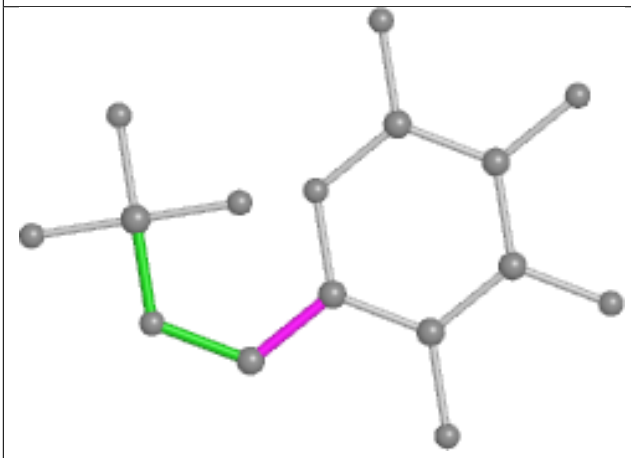
Ligand G6P F 1417



Bond lengths



Bond angles



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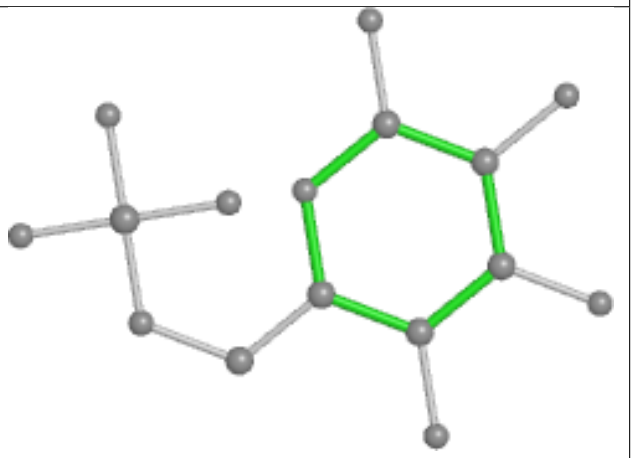
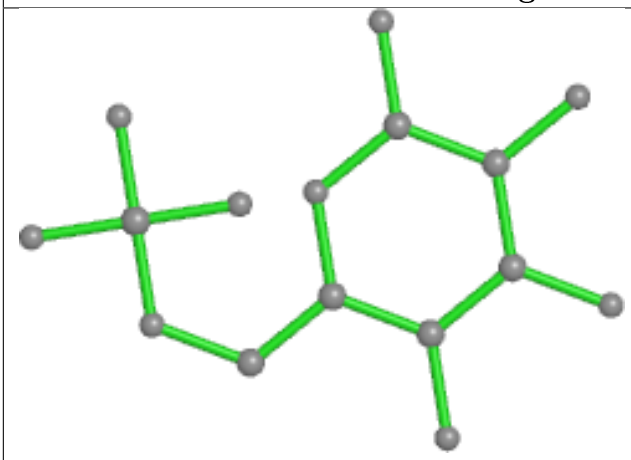
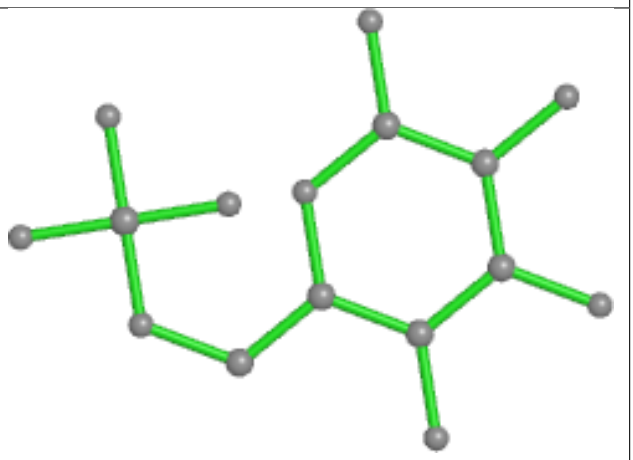


Rings

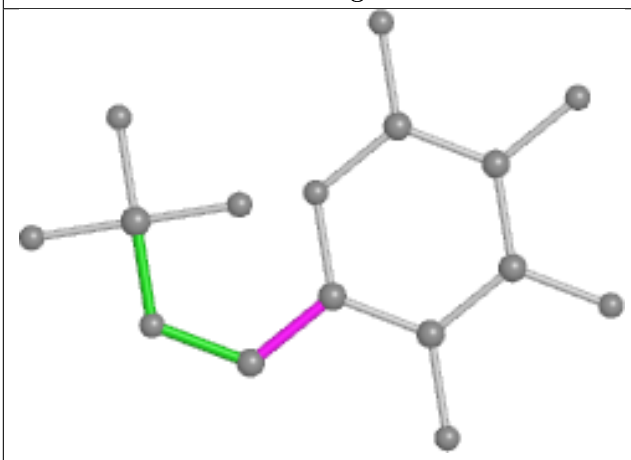
Ligand G6P E 1417



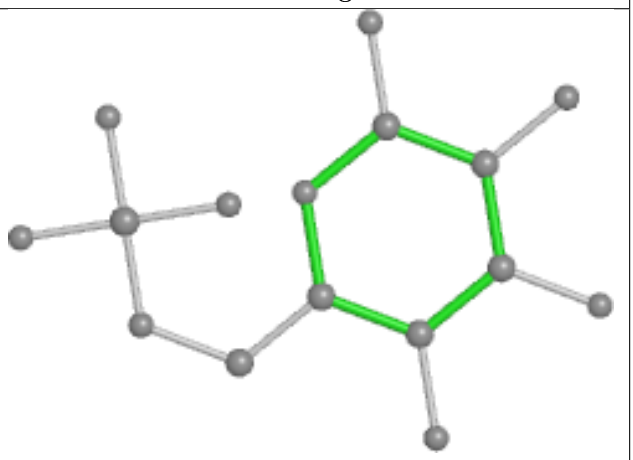
Bond lengths



Bond angles

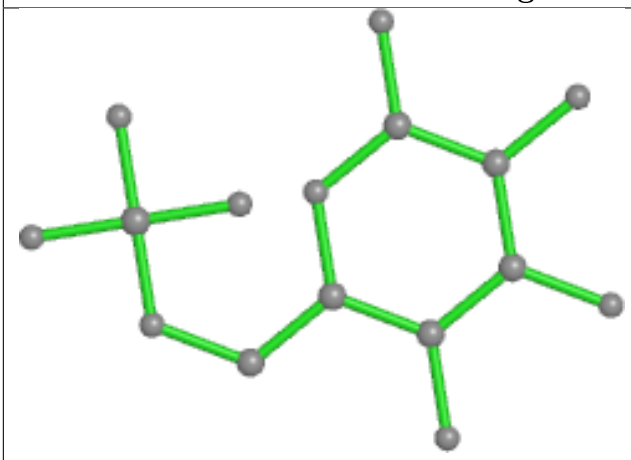


Torsions

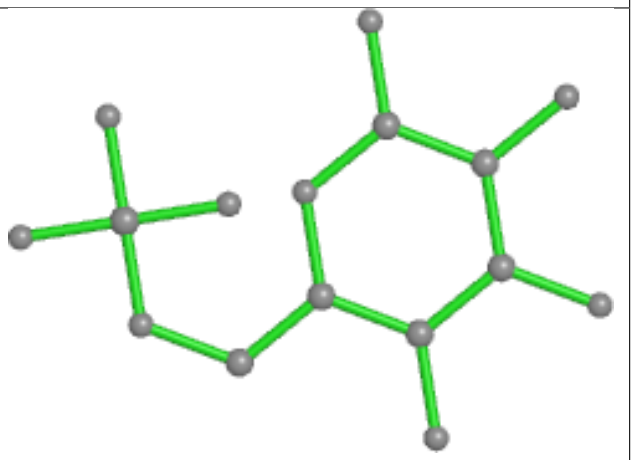


Rings

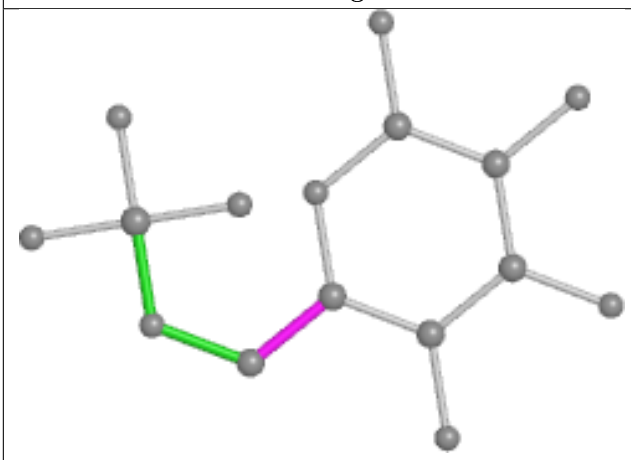
Ligand G6P B 1417



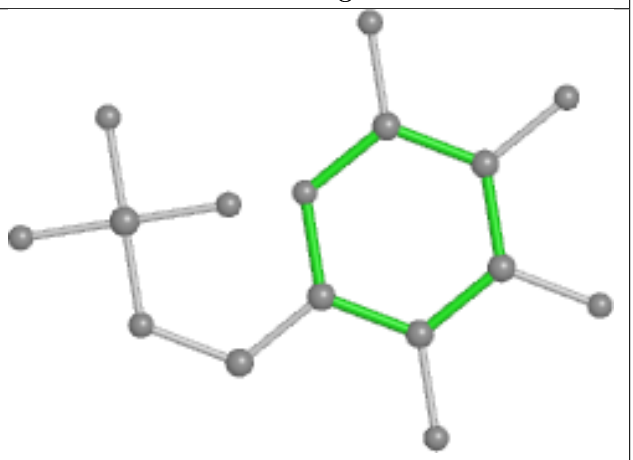
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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	A	414/417 (99%)	-0.13	17 (4%)	37	36	13, 19, 26, 58	3 (0%)
1	B	409/417 (98%)	0.02	22 (5%)	25	24	12, 19, 25, 31	22 (5%)
1	C	409/417 (98%)	-0.20	7 (1%)	70	68	13, 19, 25, 31	13 (3%)
1	D	409/417 (98%)	-0.13	18 (4%)	34	33	13, 19, 27, 39	18 (4%)
1	E	406/417 (97%)	0.27	35 (8%)	10	9	13, 19, 24, 30	41 (10%)
1	F	411/417 (98%)	0.13	26 (6%)	20	18	13, 19, 25, 36	31 (7%)
1	G	409/417 (98%)	-0.12	17 (4%)	36	35	13, 19, 25, 30	22 (5%)
1	H	407/417 (97%)	0.02	24 (5%)	22	21	13, 19, 26, 36	25 (6%)
All	All	3274/3336 (98%)	-0.02	166 (5%)	28	26	12, 19, 25, 58	175 (5%)

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	6.9
1	F	216	LEU	5.8
1	A	222	PRO	5.8
1	D	223	ASP	5.7
1	F	222	PRO	5.3

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)

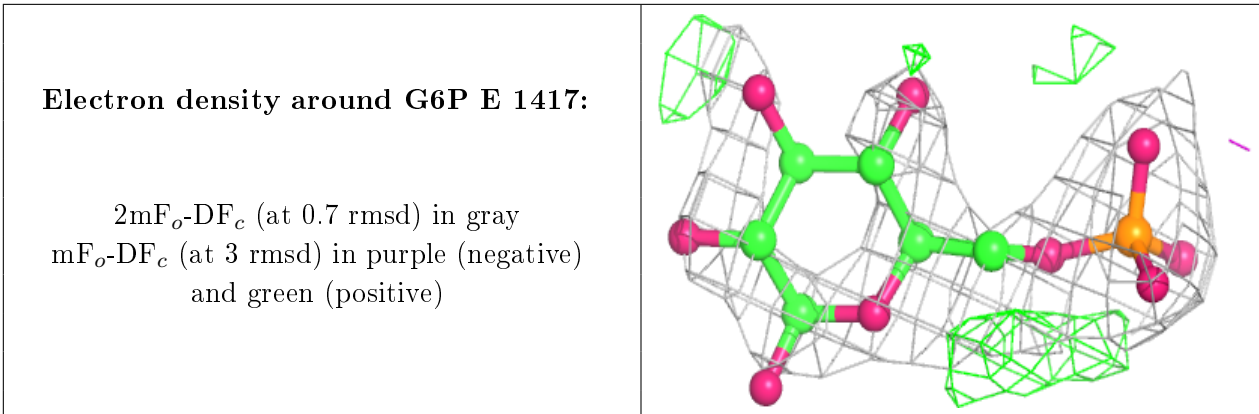
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	SO4	A	1418	5/5	0.81	0.25	57,59,61,62	0
3	G6P	E	1417	16/16	0.82	0.31	36,39,40,40	16
3	G6P	F	1417	16/16	0.83	0.31	47,52,54,55	16
4	SO4	C	1418	5/5	0.83	0.21	53,54,61,63	0
3	G6P	D	1417	16/16	0.85	0.27	43,47,48,49	16
3	G6P	H	1417	16/16	0.85	0.28	43,48,49,51	16
2	NAD	E	1416	44/44	0.87	0.30	31,33,39,41	44
3	G6P	G	1417	16/16	0.87	0.28	62,70,71,71	0
3	G6P	A	1417	16/16	0.90	0.24	46,58,60,60	0
2	NAD	F	1416	44/44	0.90	0.38	21,35,41,45	44
3	G6P	B	1417	16/16	0.91	0.32	37,42,45,45	16
2	NAD	H	1416	44/44	0.93	0.44	24,28,35,39	44
3	G6P	C	1417	16/16	0.93	0.30	58,69,71,71	0
2	NAD	B	1416	44/44	0.95	0.12	34,52,64,69	0
2	NAD	D	1416	44/44	0.96	0.11	31,44,54,55	0
2	NAD	G	1416	44/44	0.97	0.10	30,48,59,62	0
2	NAD	A	1416	44/44	0.98	0.09	21,35,49,52	0
2	NAD	C	1416	44/44	0.98	0.09	24,41,53,59	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.

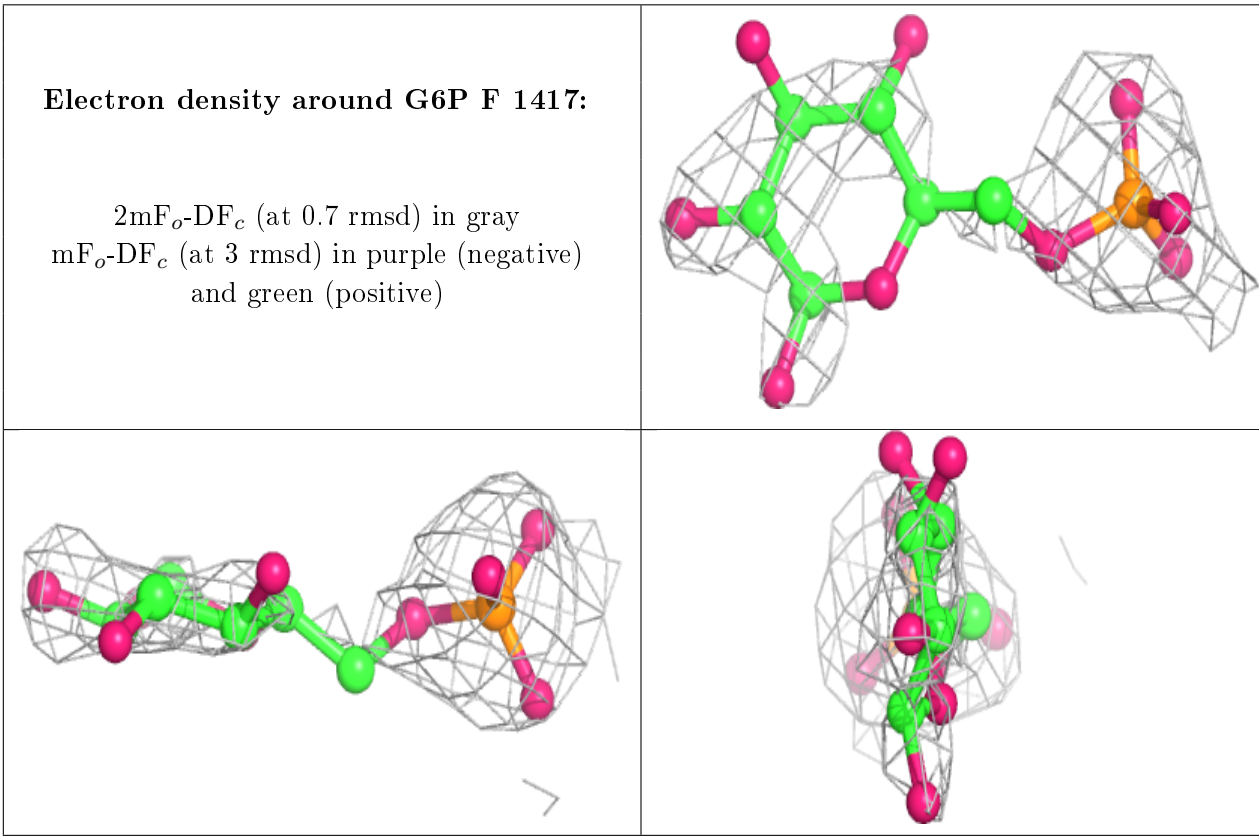
Electron density around G6P E 1417:

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



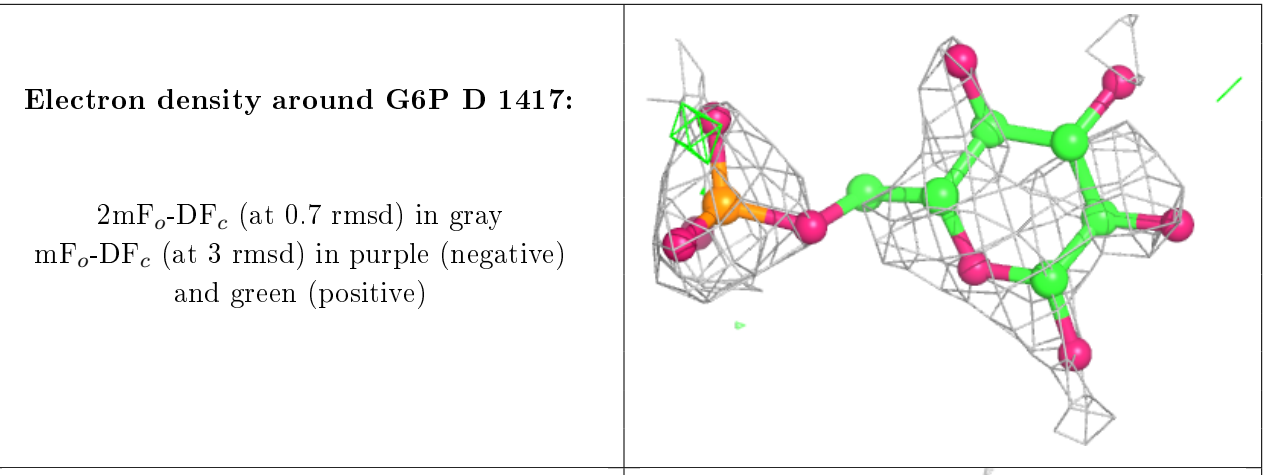
Electron density around G6P F 1417:

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



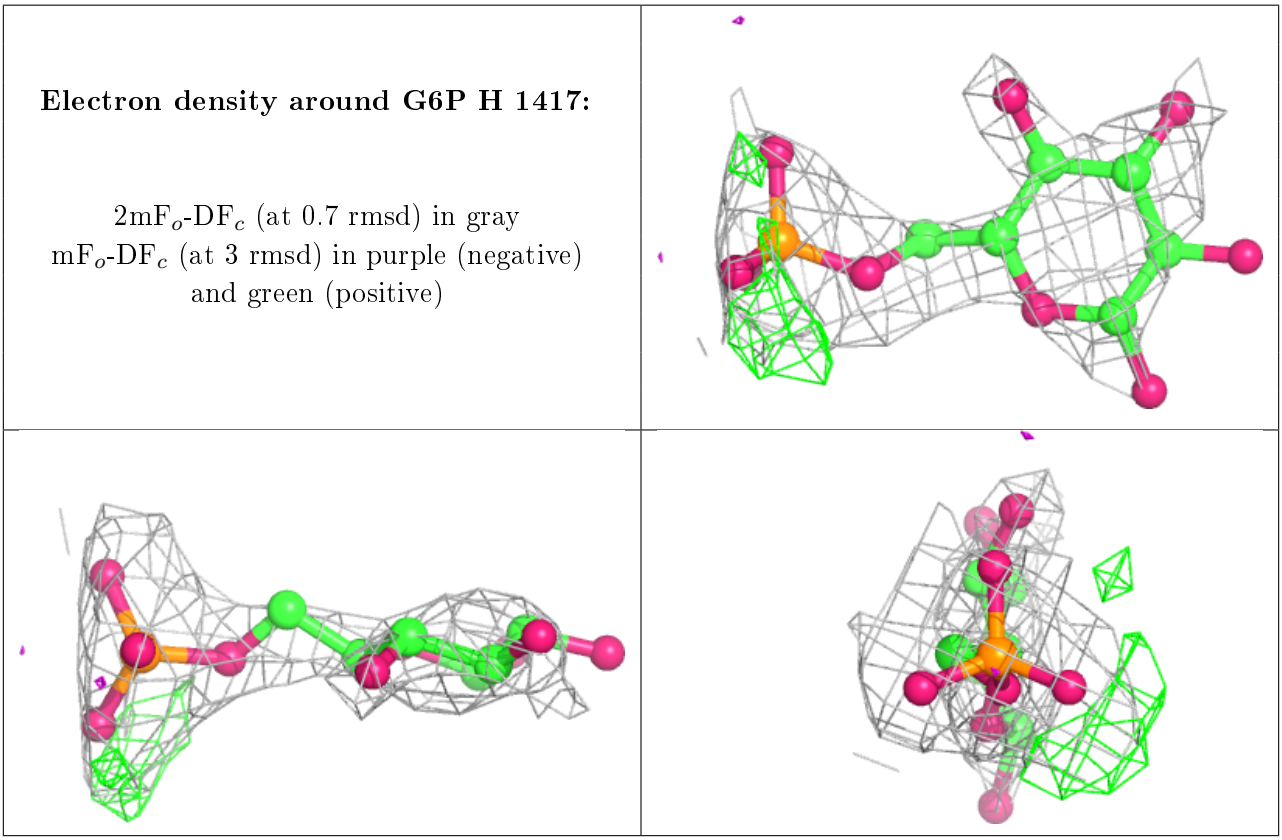
Electron density around G6P D 1417:

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



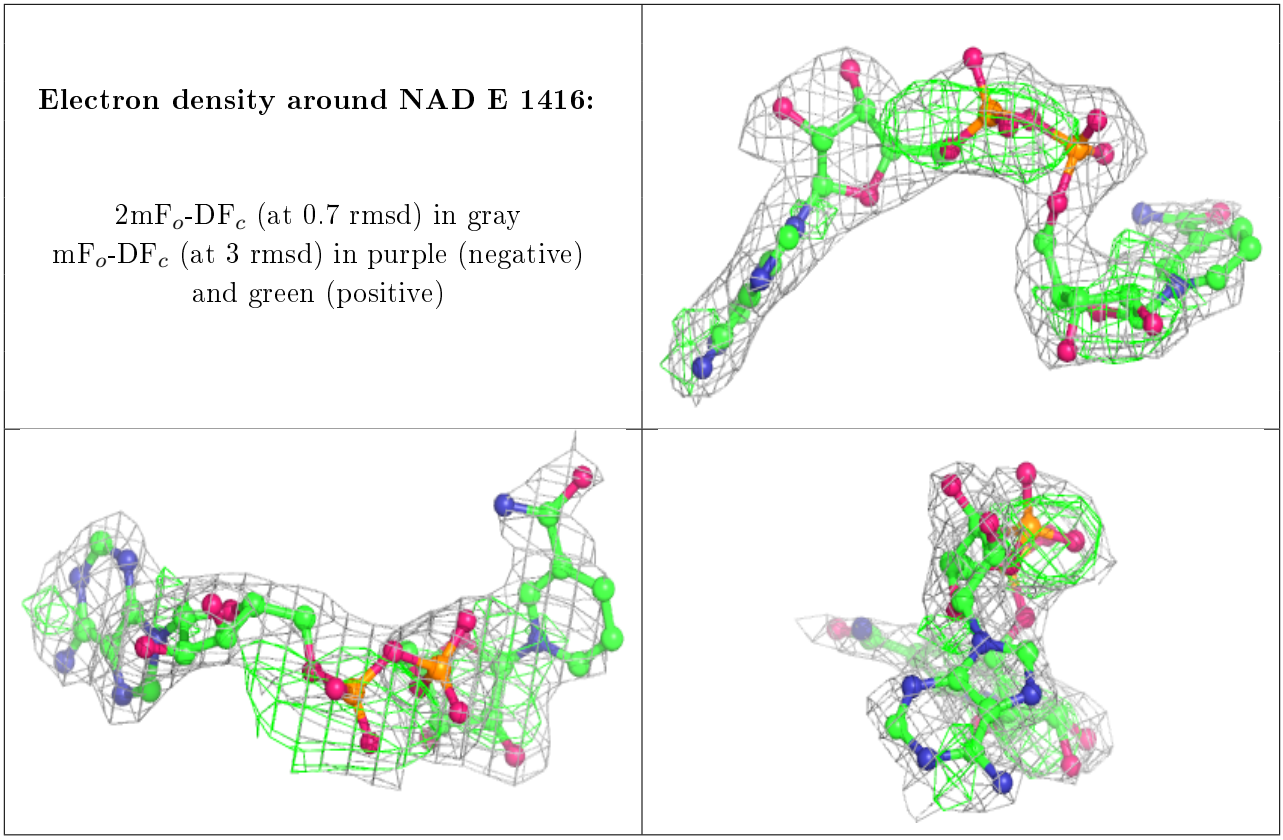
Electron density around G6P H 1417:

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



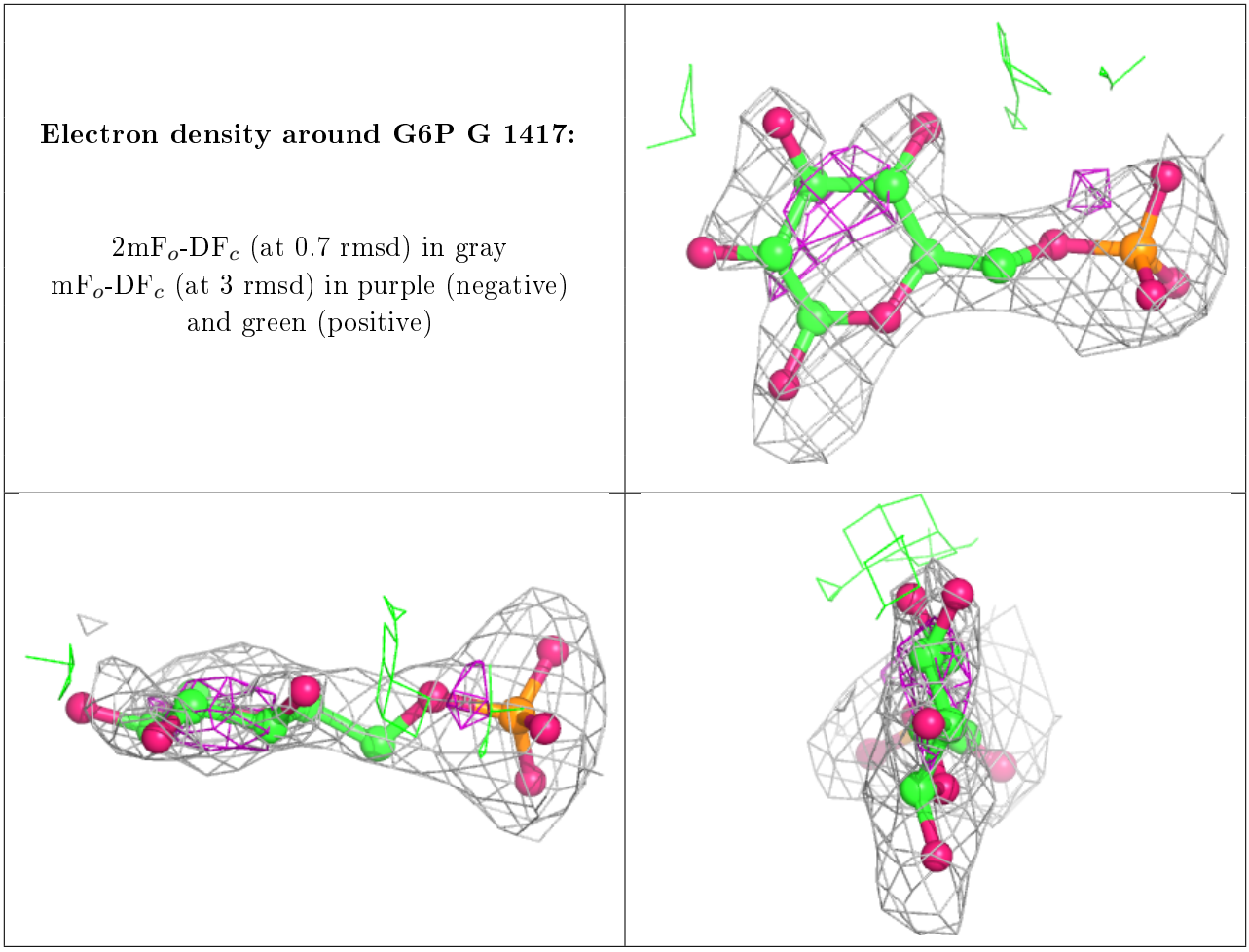
Electron density around NAD E 1416:

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



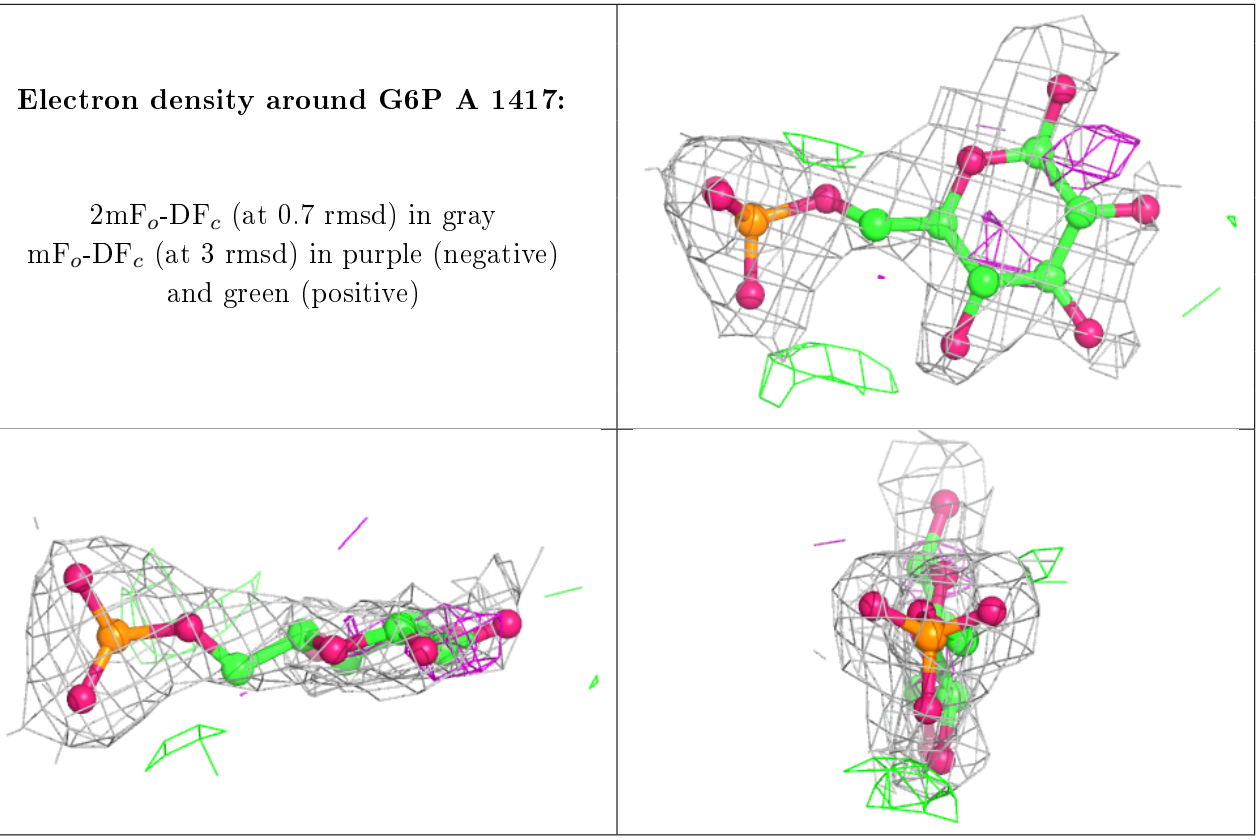
Electron density around G6P G 1417:

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



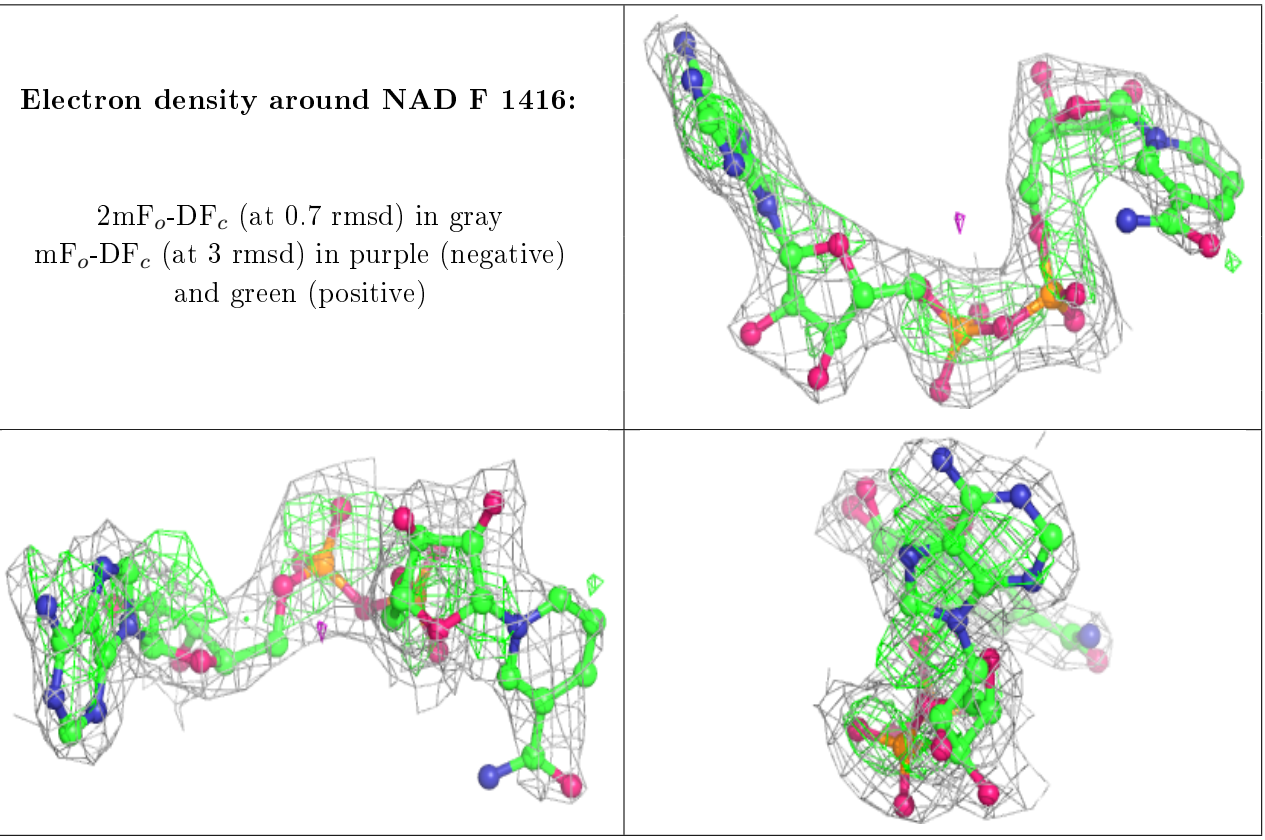
Electron density around G6P A 1417:

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



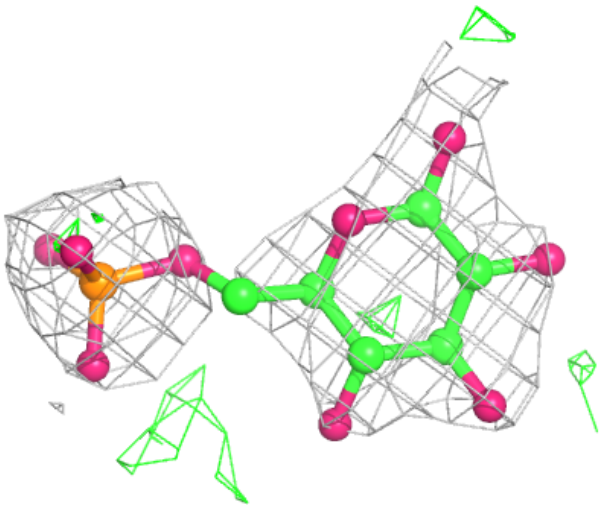
Electron density around NAD F 1416:

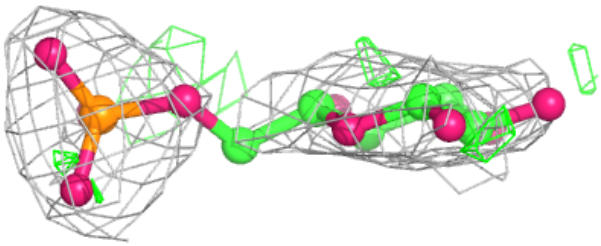
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

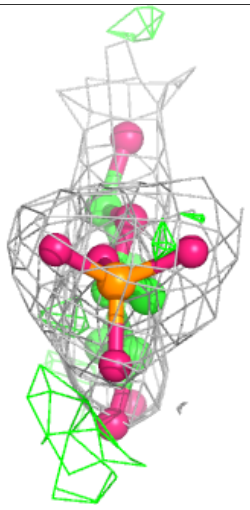


Electron density around G6P B 1417:

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

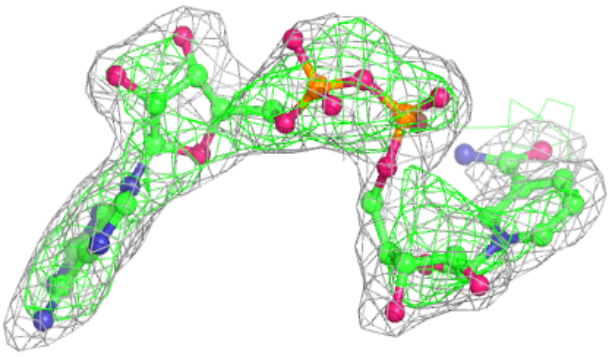


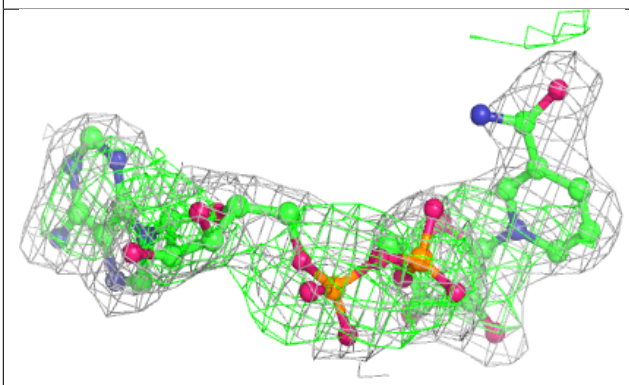


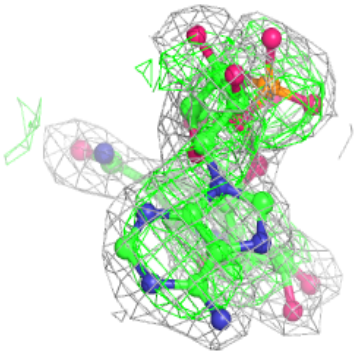


Electron density around NAD H 1416:

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

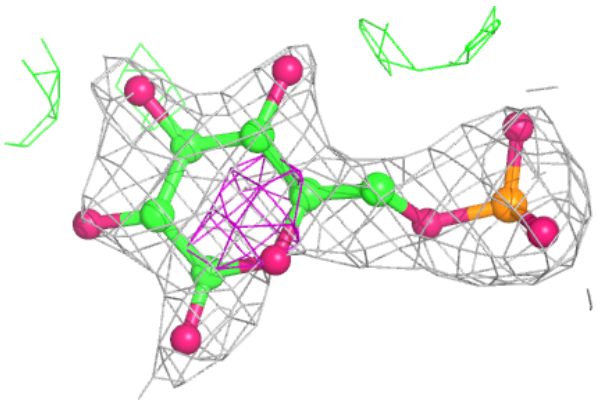


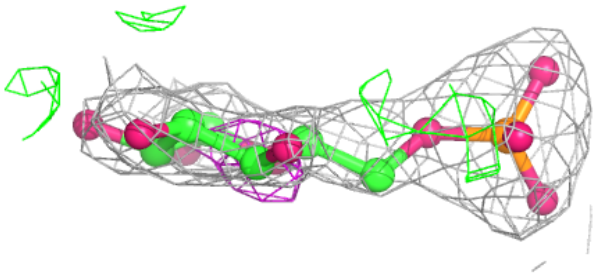


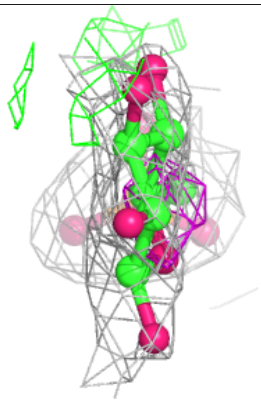


Electron density around G6P C 1417:

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

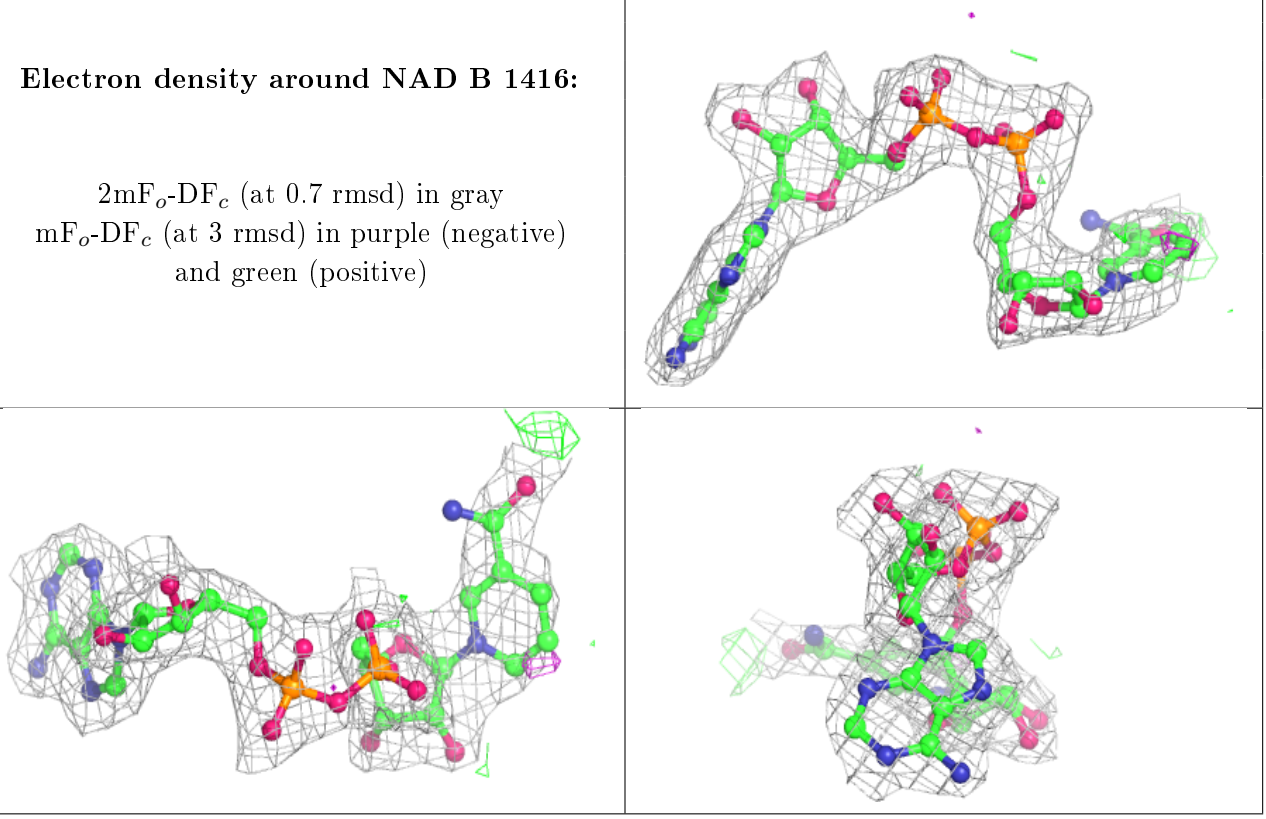






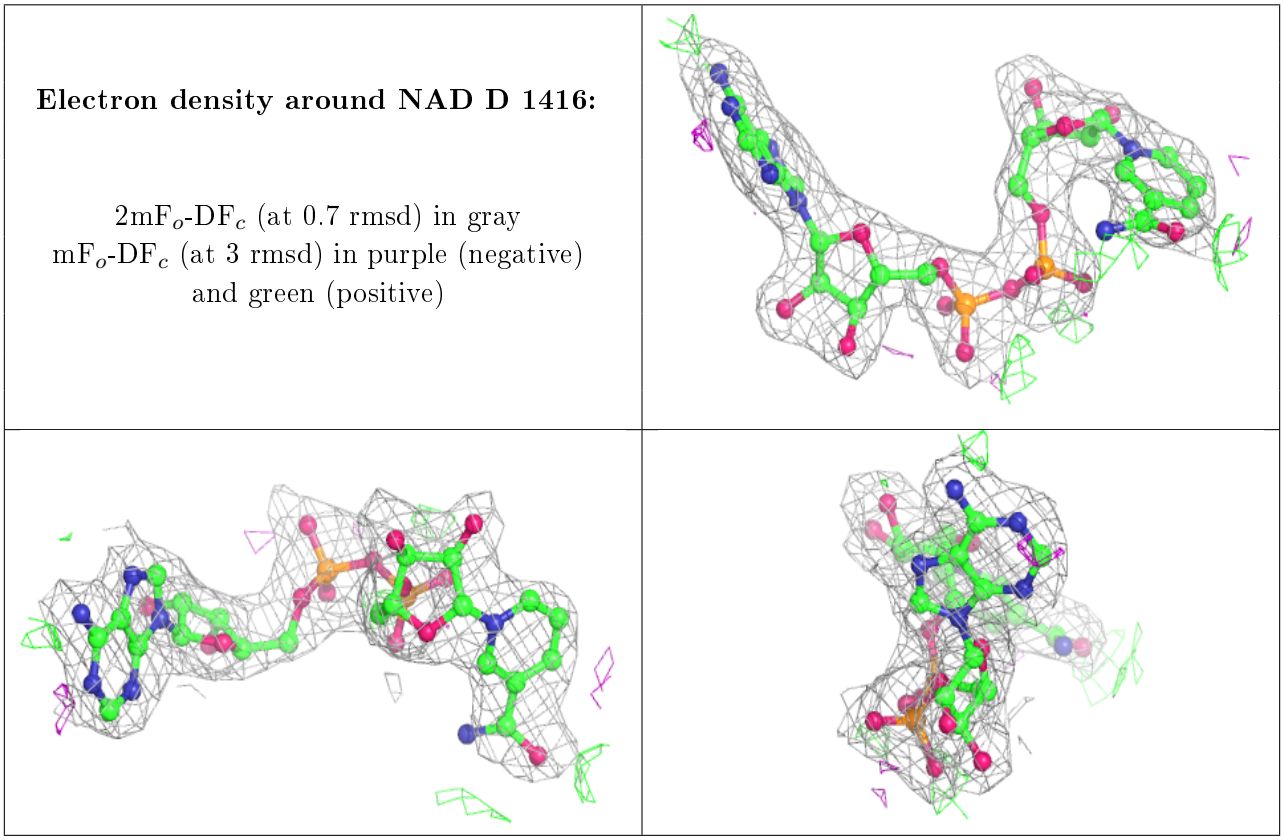
Electron density around NAD B 1416:

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



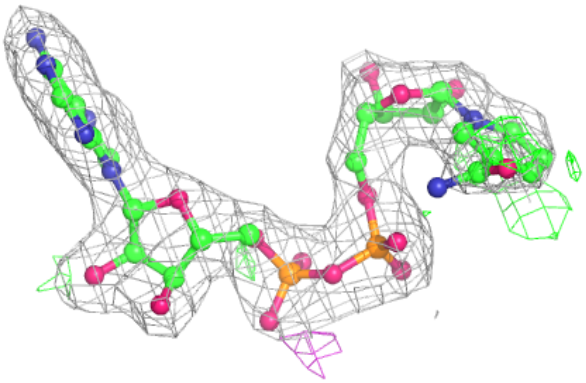
Electron density around NAD D 1416:

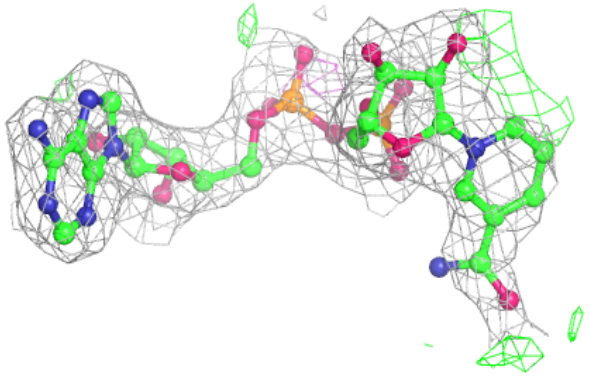
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

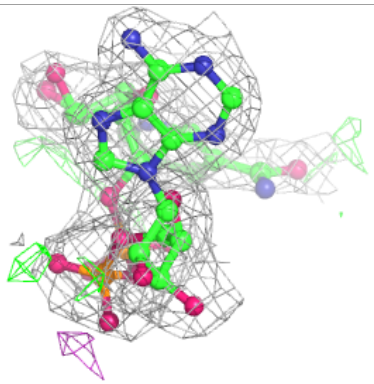


Electron density around NAD G 1416:

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

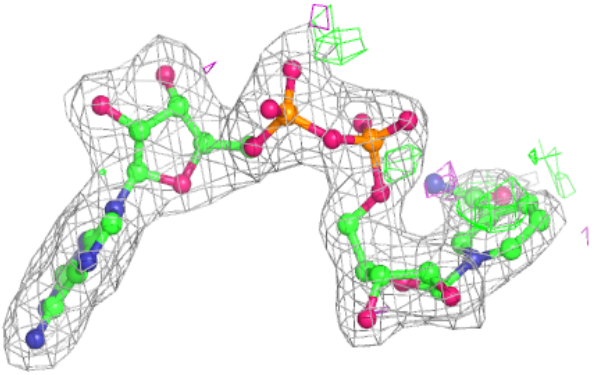


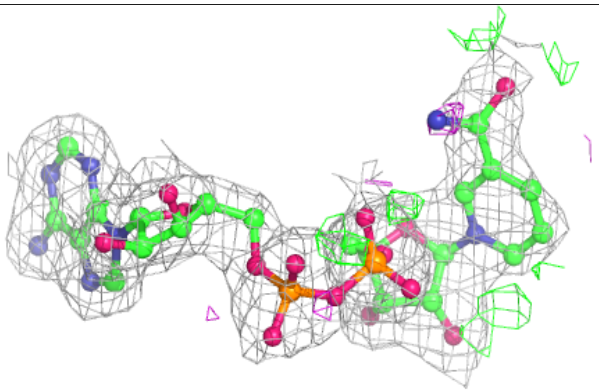


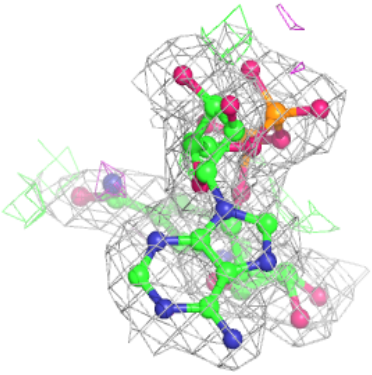


Electron density around NAD A 1416:

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

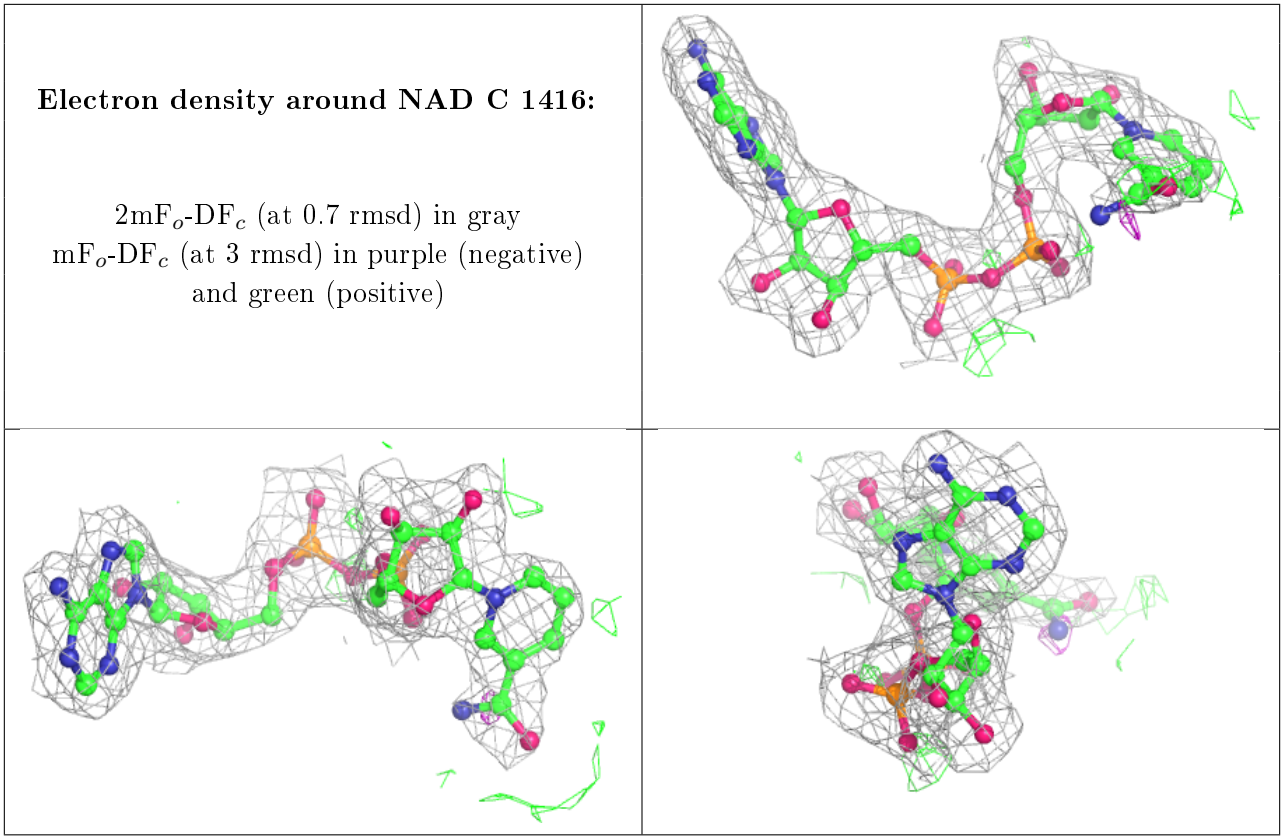






Electron density around NAD C 1416:

$2mF_o$-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.