



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2020 – 05:26 PM GMT

PDB ID : 6T8Z  
Title : NAD<sup>+</sup>-dependent fungal formate dehydrogenase from *Chaetomium thermophilum*: A ternary complex with the oxidised form of the cofactor NAD<sup>+</sup> and the substrate formate both at a primary and secondary sites.  
Authors : Isupov, M.N.; Yelmazer, B.; De Rose, S.A.; Littlechild, J.A.  
Deposited on : 2019-10-25  
Resolution : 1.21 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6  
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) : 2.14.6

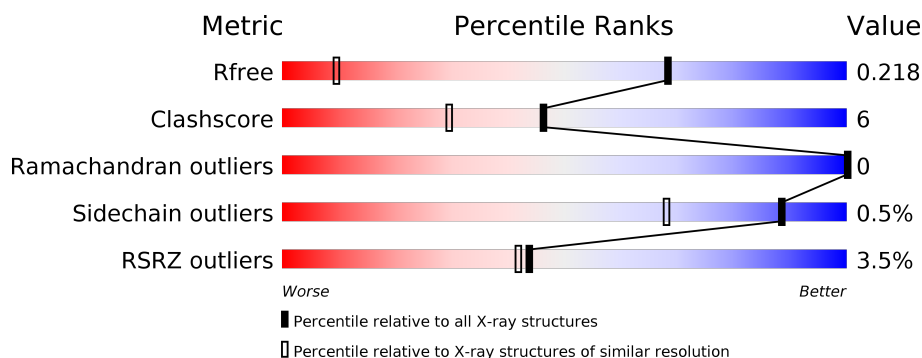
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.21 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	1232 (1.24-1.20)
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	410	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	BBB	410	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>9%</div> </div> </div>
1	CCC	410	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	DDD	410	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	AAA	504	-	-	X	-
3	FMT	BBB	1003	-	-	X	-
3	FMT	CCC	404	-	-	X	-
3	FMT	DDD	404	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27590 atoms, of which 12962 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	373	Total	C	H	N	O	S	119	30	0
			6279	1957	3183	554	574	11			
1	BBB	375	Total	C	H	N	O	S	120	28	0
			6254	1956	3164	547	577	10			
1	CCC	373	Total	C	H	N	O	S	119	36	0
			6352	1980	3231	555	576	10			
1	DDD	374	Total	C	H	N	O	S	122	28	0
			6239	1946	3160	550	573	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-33	MET	-	initiating methionine	UNP G0SGU4
AAA	-32	ALA	-	expression tag	UNP G0SGU4
AAA	-31	HIS	-	expression tag	UNP G0SGU4
AAA	-30	HIS	-	expression tag	UNP G0SGU4
AAA	-29	HIS	-	expression tag	UNP G0SGU4
AAA	-28	HIS	-	expression tag	UNP G0SGU4
AAA	-27	HIS	-	expression tag	UNP G0SGU4
AAA	-26	HIS	-	expression tag	UNP G0SGU4
AAA	-25	VAL	-	expression tag	UNP G0SGU4
AAA	-24	GLY	-	expression tag	UNP G0SGU4
AAA	-23	THR	-	expression tag	UNP G0SGU4
AAA	-22	GLY	-	expression tag	UNP G0SGU4
AAA	-21	SER	-	expression tag	UNP G0SGU4
AAA	-20	ASN	-	expression tag	UNP G0SGU4
AAA	-19	ASP	-	expression tag	UNP G0SGU4
AAA	-18	ASP	-	expression tag	UNP G0SGU4
AAA	-17	ASP	-	expression tag	UNP G0SGU4
AAA	-16	ASP	-	expression tag	UNP G0SGU4
AAA	-15	LYS	-	expression tag	UNP G0SGU4
AAA	-14	SER	-	expression tag	UNP G0SGU4
AAA	-13	PRO	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-12	ASP	-	expression tag	UNP G0SGU4
AAA	-11	PRO	-	expression tag	UNP G0SGU4
AAA	-10	ASN	-	expression tag	UNP G0SGU4
AAA	-9	TRP	-	expression tag	UNP G0SGU4
AAA	-8	GLU	-	expression tag	UNP G0SGU4
AAA	-7	LEU	-	expression tag	UNP G0SGU4
AAA	-6	VAL	-	expression tag	UNP G0SGU4
AAA	-5	TYR	-	expression tag	UNP G0SGU4
AAA	-4	THR	-	expression tag	UNP G0SGU4
AAA	-3	ALA	-	expression tag	UNP G0SGU4
AAA	-2	ARG	-	expression tag	UNP G0SGU4
AAA	-1	LEU	-	expression tag	UNP G0SGU4
AAA	0	GLN	-	expression tag	UNP G0SGU4
AAA	371	HIS	-	expression tag	UNP G0SGU4
AAA	372	HIS	-	expression tag	UNP G0SGU4
AAA	373	HIS	-	expression tag	UNP G0SGU4
AAA	374	HIS	-	expression tag	UNP G0SGU4
AAA	375	HIS	-	expression tag	UNP G0SGU4
AAA	376	HIS	-	expression tag	UNP G0SGU4
BBB	-33	MET	-	initiating methionine	UNP G0SGU4
BBB	-32	ALA	-	expression tag	UNP G0SGU4
BBB	-31	HIS	-	expression tag	UNP G0SGU4
BBB	-30	HIS	-	expression tag	UNP G0SGU4
BBB	-29	HIS	-	expression tag	UNP G0SGU4
BBB	-28	HIS	-	expression tag	UNP G0SGU4
BBB	-27	HIS	-	expression tag	UNP G0SGU4
BBB	-26	HIS	-	expression tag	UNP G0SGU4
BBB	-25	VAL	-	expression tag	UNP G0SGU4
BBB	-24	GLY	-	expression tag	UNP G0SGU4
BBB	-23	THR	-	expression tag	UNP G0SGU4
BBB	-22	GLY	-	expression tag	UNP G0SGU4
BBB	-21	SER	-	expression tag	UNP G0SGU4
BBB	-20	ASN	-	expression tag	UNP G0SGU4
BBB	-19	ASP	-	expression tag	UNP G0SGU4
BBB	-18	ASP	-	expression tag	UNP G0SGU4
BBB	-17	ASP	-	expression tag	UNP G0SGU4
BBB	-16	ASP	-	expression tag	UNP G0SGU4
BBB	-15	LYS	-	expression tag	UNP G0SGU4
BBB	-14	SER	-	expression tag	UNP G0SGU4
BBB	-13	PRO	-	expression tag	UNP G0SGU4
BBB	-12	ASP	-	expression tag	UNP G0SGU4
BBB	-11	PRO	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-10	ASN	-	expression tag	UNP G0SGU4
BBB	-9	TRP	-	expression tag	UNP G0SGU4
BBB	-8	GLU	-	expression tag	UNP G0SGU4
BBB	-7	LEU	-	expression tag	UNP G0SGU4
BBB	-6	VAL	-	expression tag	UNP G0SGU4
BBB	-5	TYR	-	expression tag	UNP G0SGU4
BBB	-4	THR	-	expression tag	UNP G0SGU4
BBB	-3	ALA	-	expression tag	UNP G0SGU4
BBB	-2	ARG	-	expression tag	UNP G0SGU4
BBB	-1	LEU	-	expression tag	UNP G0SGU4
BBB	0	GLN	-	expression tag	UNP G0SGU4
BBB	371	HIS	-	expression tag	UNP G0SGU4
BBB	372	HIS	-	expression tag	UNP G0SGU4
BBB	373	HIS	-	expression tag	UNP G0SGU4
BBB	374	HIS	-	expression tag	UNP G0SGU4
BBB	375	HIS	-	expression tag	UNP G0SGU4
BBB	376	HIS	-	expression tag	UNP G0SGU4
CCC	-33	MET	-	initiating methionine	UNP G0SGU4
CCC	-32	ALA	-	expression tag	UNP G0SGU4
CCC	-31	HIS	-	expression tag	UNP G0SGU4
CCC	-30	HIS	-	expression tag	UNP G0SGU4
CCC	-29	HIS	-	expression tag	UNP G0SGU4
CCC	-28	HIS	-	expression tag	UNP G0SGU4
CCC	-27	HIS	-	expression tag	UNP G0SGU4
CCC	-26	HIS	-	expression tag	UNP G0SGU4
CCC	-25	VAL	-	expression tag	UNP G0SGU4
CCC	-24	GLY	-	expression tag	UNP G0SGU4
CCC	-23	THR	-	expression tag	UNP G0SGU4
CCC	-22	GLY	-	expression tag	UNP G0SGU4
CCC	-21	SER	-	expression tag	UNP G0SGU4
CCC	-20	ASN	-	expression tag	UNP G0SGU4
CCC	-19	ASP	-	expression tag	UNP G0SGU4
CCC	-18	ASP	-	expression tag	UNP G0SGU4
CCC	-17	ASP	-	expression tag	UNP G0SGU4
CCC	-16	ASP	-	expression tag	UNP G0SGU4
CCC	-15	LYS	-	expression tag	UNP G0SGU4
CCC	-14	SER	-	expression tag	UNP G0SGU4
CCC	-13	PRO	-	expression tag	UNP G0SGU4
CCC	-12	ASP	-	expression tag	UNP G0SGU4
CCC	-11	PRO	-	expression tag	UNP G0SGU4
CCC	-10	ASN	-	expression tag	UNP G0SGU4
CCC	-9	TRP	-	expression tag	UNP G0SGU4

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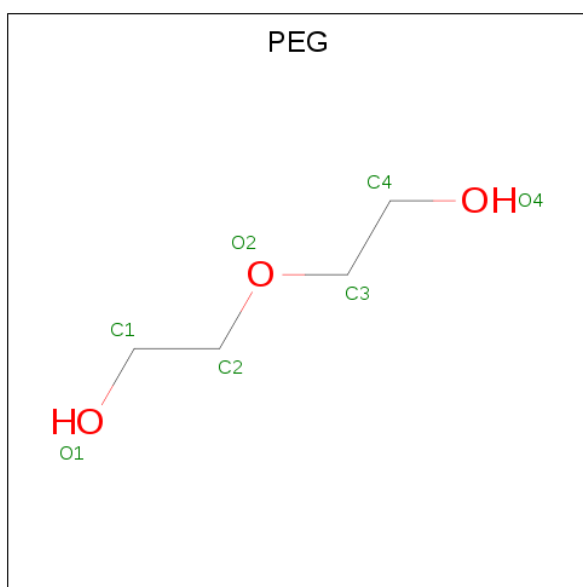
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-8	GLU	-	expression tag	UNP G0SGU4
CCC	-7	LEU	-	expression tag	UNP G0SGU4
CCC	-6	VAL	-	expression tag	UNP G0SGU4
CCC	-5	TYR	-	expression tag	UNP G0SGU4
CCC	-4	THR	-	expression tag	UNP G0SGU4
CCC	-3	ALA	-	expression tag	UNP G0SGU4
CCC	-2	ARG	-	expression tag	UNP G0SGU4
CCC	-1	LEU	-	expression tag	UNP G0SGU4
CCC	0	GLN	-	expression tag	UNP G0SGU4
CCC	371	HIS	-	expression tag	UNP G0SGU4
CCC	372	HIS	-	expression tag	UNP G0SGU4
CCC	373	HIS	-	expression tag	UNP G0SGU4
CCC	374	HIS	-	expression tag	UNP G0SGU4
CCC	375	HIS	-	expression tag	UNP G0SGU4
CCC	376	HIS	-	expression tag	UNP G0SGU4
DDD	-33	MET	-	initiating methionine	UNP G0SGU4
DDD	-32	ALA	-	expression tag	UNP G0SGU4
DDD	-31	HIS	-	expression tag	UNP G0SGU4
DDD	-30	HIS	-	expression tag	UNP G0SGU4
DDD	-29	HIS	-	expression tag	UNP G0SGU4
DDD	-28	HIS	-	expression tag	UNP G0SGU4
DDD	-27	HIS	-	expression tag	UNP G0SGU4
DDD	-26	HIS	-	expression tag	UNP G0SGU4
DDD	-25	VAL	-	expression tag	UNP G0SGU4
DDD	-24	GLY	-	expression tag	UNP G0SGU4
DDD	-23	THR	-	expression tag	UNP G0SGU4
DDD	-22	GLY	-	expression tag	UNP G0SGU4
DDD	-21	SER	-	expression tag	UNP G0SGU4
DDD	-20	ASN	-	expression tag	UNP G0SGU4
DDD	-19	ASP	-	expression tag	UNP G0SGU4
DDD	-18	ASP	-	expression tag	UNP G0SGU4
DDD	-17	ASP	-	expression tag	UNP G0SGU4
DDD	-16	ASP	-	expression tag	UNP G0SGU4
DDD	-15	LYS	-	expression tag	UNP G0SGU4
DDD	-14	SER	-	expression tag	UNP G0SGU4
DDD	-13	PRO	-	expression tag	UNP G0SGU4
DDD	-12	ASP	-	expression tag	UNP G0SGU4
DDD	-11	PRO	-	expression tag	UNP G0SGU4
DDD	-10	ASN	-	expression tag	UNP G0SGU4
DDD	-9	TRP	-	expression tag	UNP G0SGU4
DDD	-8	GLU	-	expression tag	UNP G0SGU4
DDD	-7	LEU	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-6	VAL	-	expression tag	UNP G0SGU4
DDD	-5	TYR	-	expression tag	UNP G0SGU4
DDD	-4	THR	-	expression tag	UNP G0SGU4
DDD	-3	ALA	-	expression tag	UNP G0SGU4
DDD	-2	ARG	-	expression tag	UNP G0SGU4
DDD	-1	LEU	-	expression tag	UNP G0SGU4
DDD	0	GLN	-	expression tag	UNP G0SGU4
DDD	371	HIS	-	expression tag	UNP G0SGU4
DDD	372	HIS	-	expression tag	UNP G0SGU4
DDD	373	HIS	-	expression tag	UNP G0SGU4
DDD	374	HIS	-	expression tag	UNP G0SGU4
DDD	375	HIS	-	expression tag	UNP G0SGU4
DDD	376	HIS	-	expression tag	UNP G0SGU4

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		

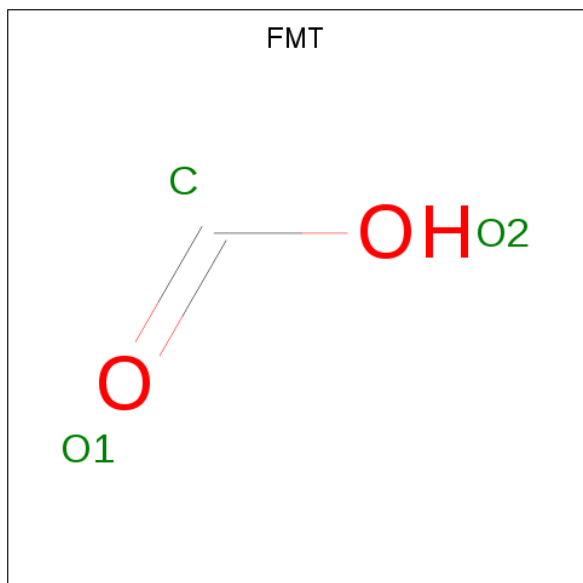
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	DDD	1	Total	C	H	O	1	0
			17	4	10	3		
2	DDD	1	Total	C	H	O	1	0
			17	4	10	3		

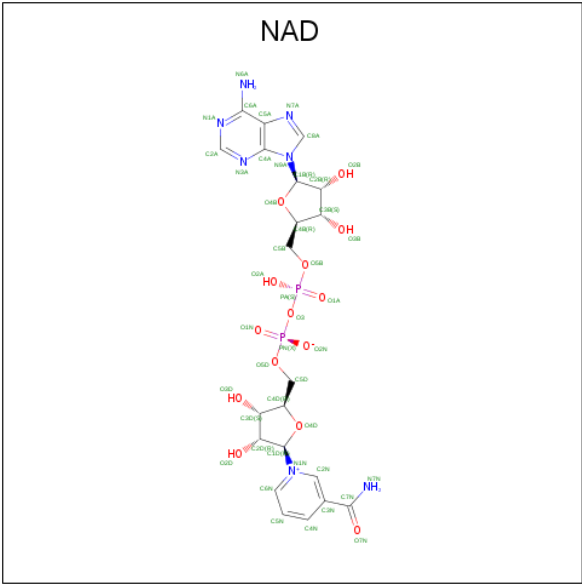
- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	0	0
			4	1	1	2		
3	AAA	1	Total	C	H	O	0	0
			4	1	1	2		
3	BBB	1	Total	C	H	O	0	0
			4	1	1	2		
3	BBB	1	Total	C	H	O	0	0
			4	1	1	2		
3	CCC	1	Total	C	H	O	0	0
			4	1	1	2		
3	CCC	1	Total	C	H	O	0	0
			4	1	1	2		
3	DDD	1	Total	C	H	O	0	0
			4	1	1	2		
3	DDD	1	Total	C	H	O	0	0
			4	1	1	2		

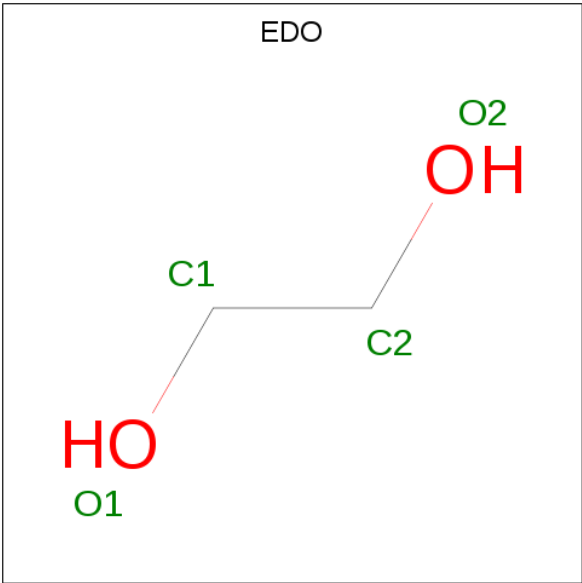
- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	P	8	0
			70	21	26	7	14	2		
4	BBB	1	Total	C	H	N	O	P	8	0
			70	21	26	7	14	2		
4	CCC	1	Total	C	H	N	O	P	8	0
			70	21	26	7	14	2		
4	DDD	1	Total	C	H	N	O	P	8	0
			70	21	26	7	14	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0
5	CCC	1	Total C H O 10 2 6 2	1	0

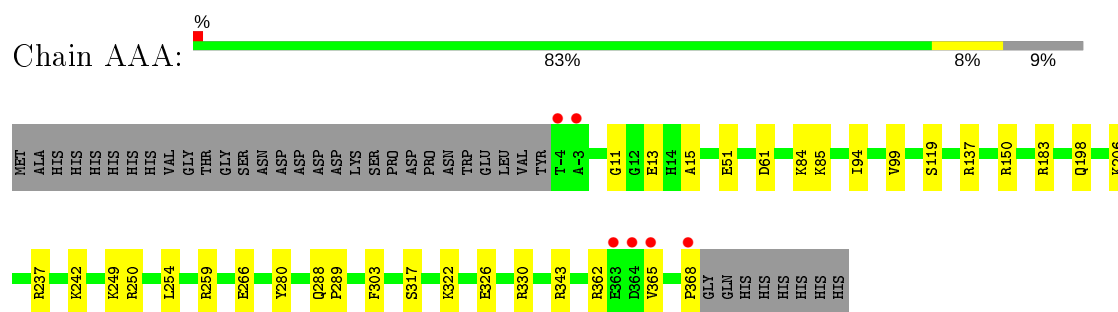
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	522	Total O 522 522	0	0
6	BBB	468	Total O 468 468	0	0
6	CCC	449	Total O 449 449	0	0
6	DDD	526	Total O 526 526	0	0

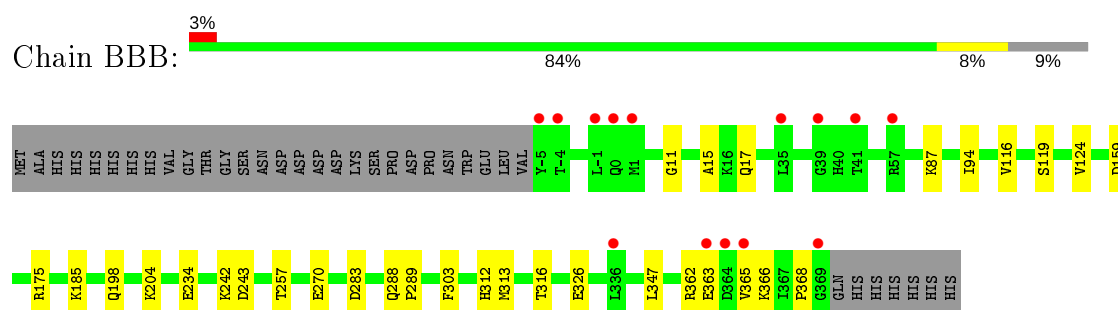
### 3 Residue-property plots [i](#)

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.

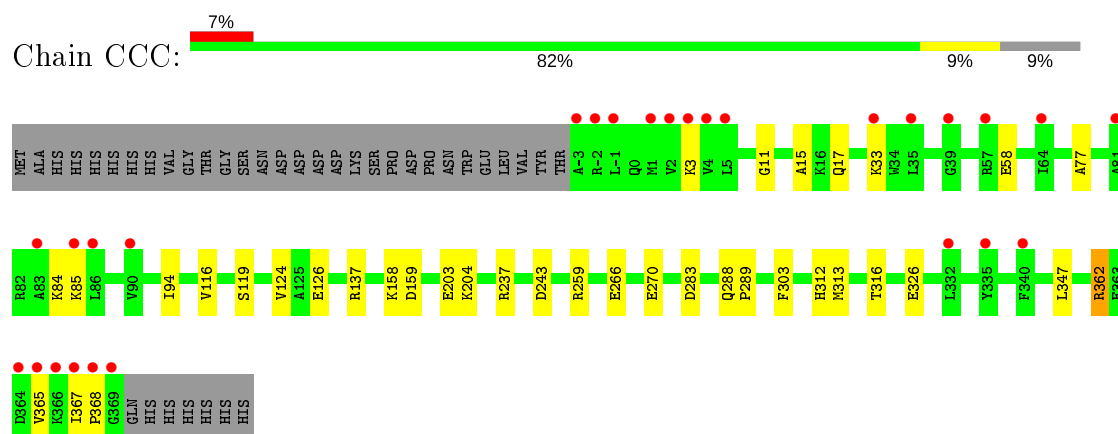
- Molecule 1: Formate dehydrogenase



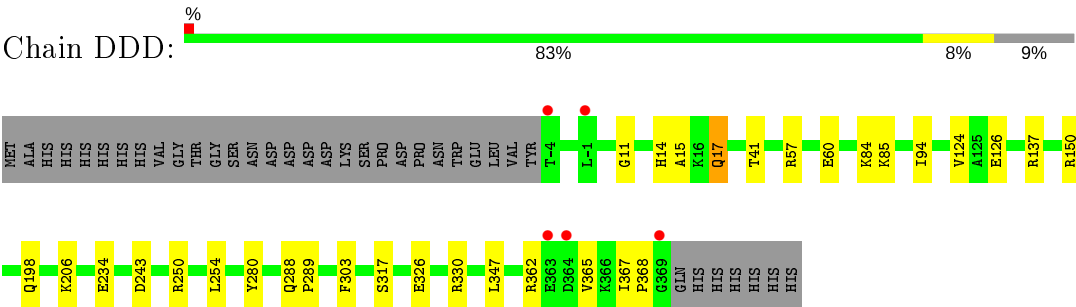
- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.40 Å   94.52 Å   94.33 Å 85.69°   89.93°   81.94°	Depositor
Resolution (Å)	47.03 – 1.21 47.03 – 1.21	Depositor EDS
% Data completeness (in resolution range)	89.1 (47.03-1.21) 89.1 (47.03-1.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 1.21 Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.188   ,   0.211 0.197   ,   0.218	Depositor DCC
$R_{free}$ test set	23228 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	27590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: FMT, PEG, EDO, 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	AAA	0.75	2/3227 (0.1%)	0.86	3/4347 (0.1%)
1	BBB	0.72	0/3222	0.86	1/4344 (0.0%)
1	CCC	0.72	1/3276 (0.0%)	0.86	1/4410 (0.0%)
1	DDD	0.76	1/3210 (0.0%)	0.85	2/4327 (0.0%)
All	All	0.74	4/12935 (0.0%)	0.86	7/17428 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1
1	CCC	0	2
1	DDD	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	317	SER	CA-CB	-5.97	1.44	1.52
1	CCC	126	GLU	CD-OE2	-5.29	1.19	1.25
1	AAA	317	SER	CA-CB	-5.17	1.45	1.52
1	AAA	266	GLU	CD-OE1	5.16	1.31	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	259	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	BBB	175	ARG	NE-CZ-NH2	-5.79	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	259	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	AAA	183	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	DDD	126	GLU	OE1-CD-OE2	5.43	129.81	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	ARG	Sidechain
1	CCC	137	ARG	Sidechain
1	CCC	362	ARG	Peptide
1	DDD	137	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3096	3183	3197	33	0
1	BBB	3090	3164	3180	37	0
1	CCC	3121	3231	3255	42	0
1	DDD	3079	3160	3176	42	0
2	AAA	14	20	20	0	0
2	BBB	7	10	10	0	0
2	CCC	14	20	20	0	0
2	DDD	14	20	20	0	0
3	AAA	6	2	2	3	0
3	BBB	6	2	2	3	0
3	CCC	6	2	2	3	0
3	DDD	6	2	2	3	0
4	AAA	44	26	26	2	0
4	BBB	44	26	26	3	0
4	CCC	44	26	26	2	0
4	DDD	44	26	26	2	0
5	AAA	20	30	30	6	0
5	BBB	4	6	6	1	0
5	CCC	4	6	6	0	0
6	AAA	522	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	468	0	0	20	0
6	CCC	449	0	0	15	0
6	DDD	526	0	0	18	0
All	All	14628	12962	13032	161	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 161 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:DDD:303[A]:PHE:HE2	6:DDD:871:HOH:O	1.12	1.31
1:BBB:204[B]:LYS:HE2	6:BBB:1291:HOH:O	1.21	1.29
1:DDD:326[B]:GLU:OE1	6:DDD:511:HOH:O	1.58	1.20
1:DDD:243[B]:ASP:OD2	6:DDD:512:HOH:O	1.62	1.17
1:BBB:303[B]:PHE:CE2	6:BBB:1350:HOH:O	2.02	1.12

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	401/410 (98%)	391 (98%)	10 (2%)	0	100	100
1	BBB	401/410 (98%)	391 (98%)	10 (2%)	0	100	100
1	CCC	407/410 (99%)	396 (97%)	11 (3%)	0	100	100
1	DDD	400/410 (98%)	389 (97%)	11 (3%)	0	100	100
All	All	1609/1640 (98%)	1567 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	336/340 (99%)	334 (99%)	2 (1%)	86	64
1	BBB	335/340 (98%)	331 (99%)	4 (1%)	71	37
1	CCC	341/340 (100%)	339 (99%)	2 (1%)	86	64
1	DDD	334/340 (98%)	332 (99%)	2 (1%)	86	64
All	All	1346/1360 (99%)	1336 (99%)	10 (1%)	88	60

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	363	GLU
1	BBB	366	LYS
1	CCC	17[B]	GLN
1	BBB	17[B]	GLN
1	CCC	17[A]	GLN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	AAA	506	-	3,3,3	0.23	0	2,2,2	0.47	0
3	FMT	DDD	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PEG	AAA	501	-	6,6,6	0.11	0	5,5,5	0.16	0
5	EDO	BBB	1005	-	3,3,3	0.13	0	2,2,2	0.41	0
4	NAD	DDD	405	-	42,48,48	0.88	2 (4%)	50,73,73	1.03	2 (4%)
3	FMT	CCC	404	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	AAA	505	-	42,48,48	0.96	3 (7%)	50,73,73	0.97	2 (4%)
3	FMT	CCC	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PEG	DDD	401	-	6,6,6	0.29	0	5,5,5	0.22	0
5	EDO	AAA	509	-	3,3,3	0.44	0	2,2,2	0.96	0
2	PEG	BBB	1001	-	6,6,6	0.21	0	5,5,5	0.21	0
5	EDO	AAA	508	-	3,3,3	0.18	0	2,2,2	1.01	0
2	PEG	DDD	402	-	6,6,6	0.18	0	5,5,5	0.11	0
5	EDO	CCC	406	-	3,3,3	0.13	0	2,2,2	0.40	0
5	EDO	AAA	507	-	3,3,3	0.07	0	2,2,2	0.44	0
2	PEG	CCC	402	-	6,6,6	0.19	0	5,5,5	0.15	0
2	PEG	AAA	502	-	6,6,6	0.20	0	5,5,5	0.13	0
3	FMT	BBB	1002	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	DDD	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	BBB	1004	-	42,48,48	0.93	1 (2%)	50,73,73	1.06	4 (8%)
4	NAD	CCC	405	-	42,48,48	0.77	1 (2%)	50,73,73	0.90	1 (2%)
3	FMT	AAA	504	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	BBB	1003	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	AAA	510	-	3,3,3	0.10	0	2,2,2	0.36	0
3	FMT	AAA	503	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PEG	CCC	401	-	6,6,6	0.23	0	5,5,5	0.28	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
5	EDO	AAA	506	-	-	0/1/1/1	-
5	EDO	AAA	509	-	-	1/1/1/1	-
2	PEG	BBB	1001	-	-	0/4/4/4	-
2	PEG	AAA	501	-	-	1/4/4/4	-
5	EDO	AAA	508	-	-	1/1/1/1	-
5	EDO	BBB	1005	-	-	1/1/1/1	-
4	NAD	AAA	505	-	-	2/26/62/62	0/5/5/5
2	PEG	DDD	402	-	-	0/4/4/4	-
2	PEG	DDD	401	-	-	1/4/4/4	-
5	EDO	CCC	406	-	-	0/1/1/1	-
4	NAD	DDD	405	-	-	2/26/62/62	0/5/5/5
5	EDO	AAA	510	-	-	0/1/1/1	-
5	EDO	AAA	507	-	-	1/1/1/1	-
2	PEG	CCC	402	-	-	1/4/4/4	-
2	PEG	AAA	502	-	-	0/4/4/4	-
4	NAD	BBB	1004	-	-	2/26/62/62	0/5/5/5
4	NAD	CCC	405	-	-	2/26/62/62	0/5/5/5
2	PEG	CCC	401	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	1004	NAD	C2N-N1N	3.62	1.39	1.35
4	AAA	505	NAD	C4N-C3N	2.63	1.43	1.39
4	DDD	405	NAD	C8A-N7A	-2.41	1.30	1.34
4	AAA	505	NAD	C8A-N7A	-2.36	1.30	1.34
4	AAA	505	NAD	C2N-N1N	2.35	1.37	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	1004	NAD	C6N-N1N-C2N	-3.33	118.94	121.97
4	DDD	405	NAD	O4B-C1B-C2B	-3.23	102.20	106.93
4	CCC	405	NAD	C5A-C6A-N6A	3.07	125.02	120.35
4	AAA	505	NAD	C6N-N1N-C2N	-2.85	119.38	121.97
4	AAA	505	NAD	O4B-C1B-C2B	-2.75	102.90	106.93

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

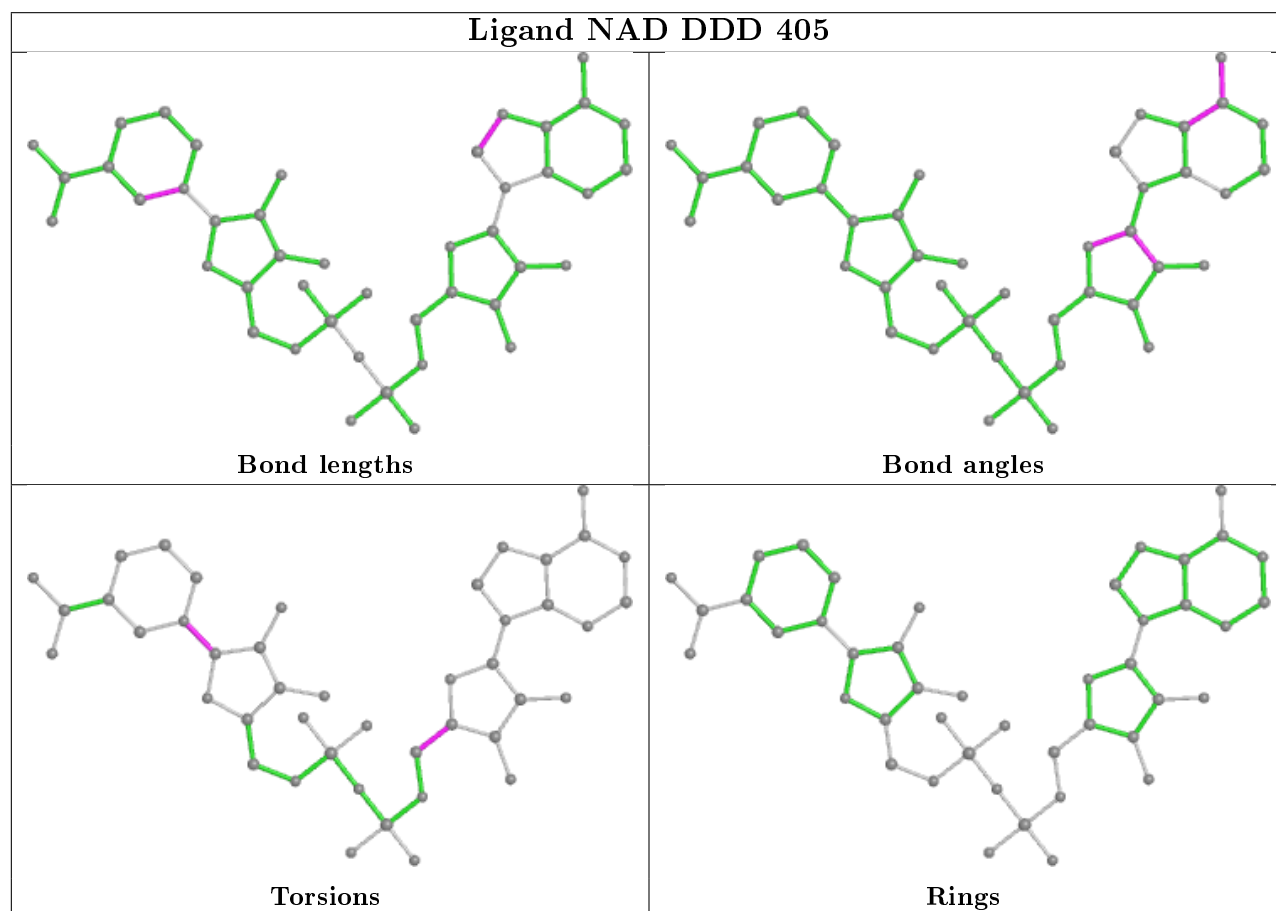
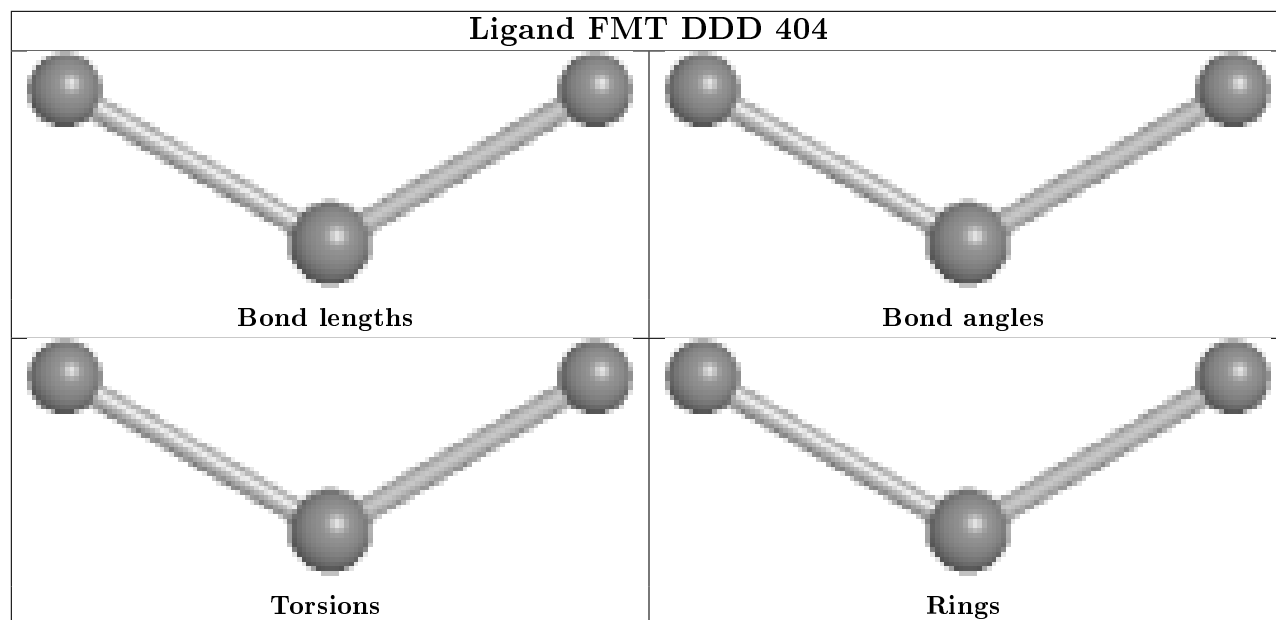
Mol	Chain	Res	Type	Atoms
4	AAA	505	NAD	O4D-C1D-N1N-C6N
4	DDD	405	NAD	O4D-C1D-N1N-C6N
4	BBB	1004	NAD	O4D-C1D-N1N-C6N
4	CCC	405	NAD	O4D-C1D-N1N-C6N
5	BBB	1005	EDO	O1-C1-C2-O2

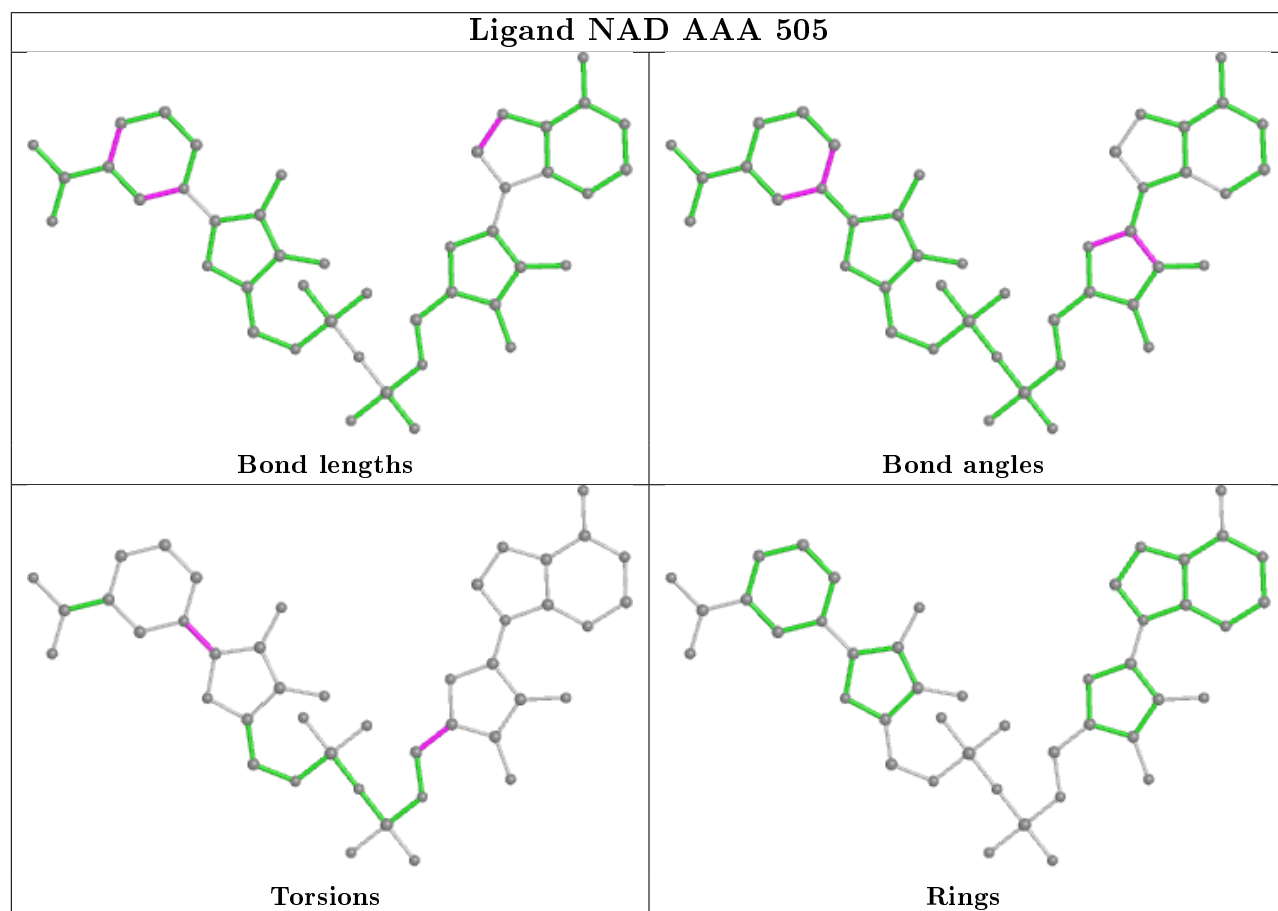
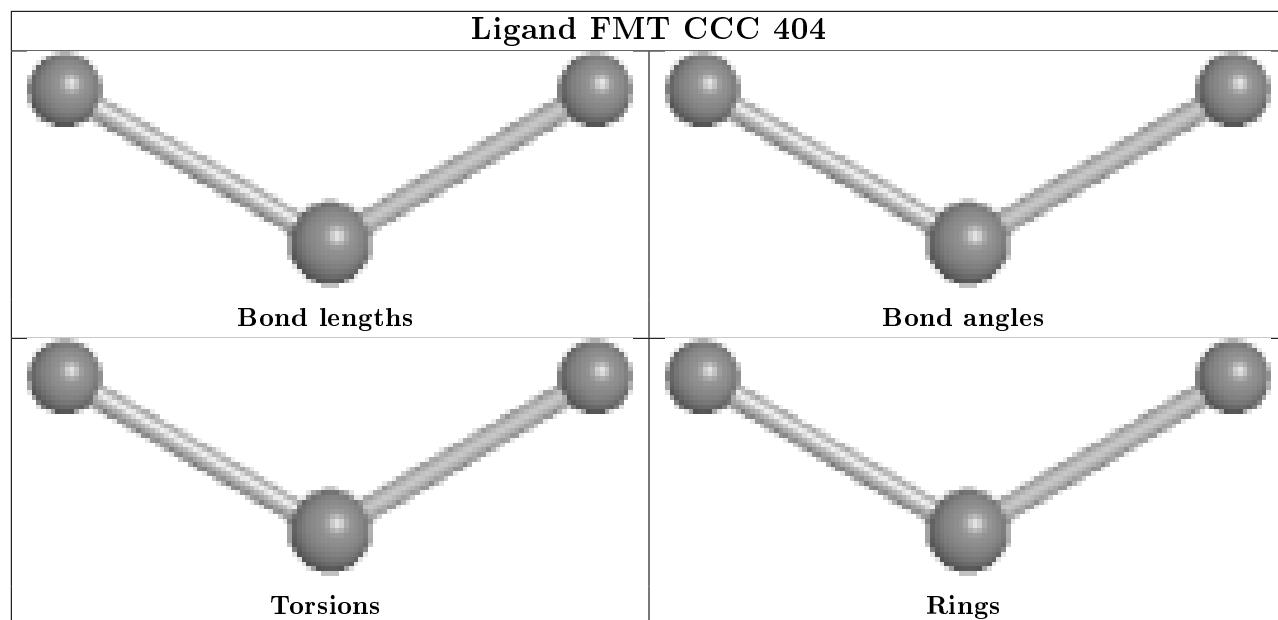
There are no ring outliers.

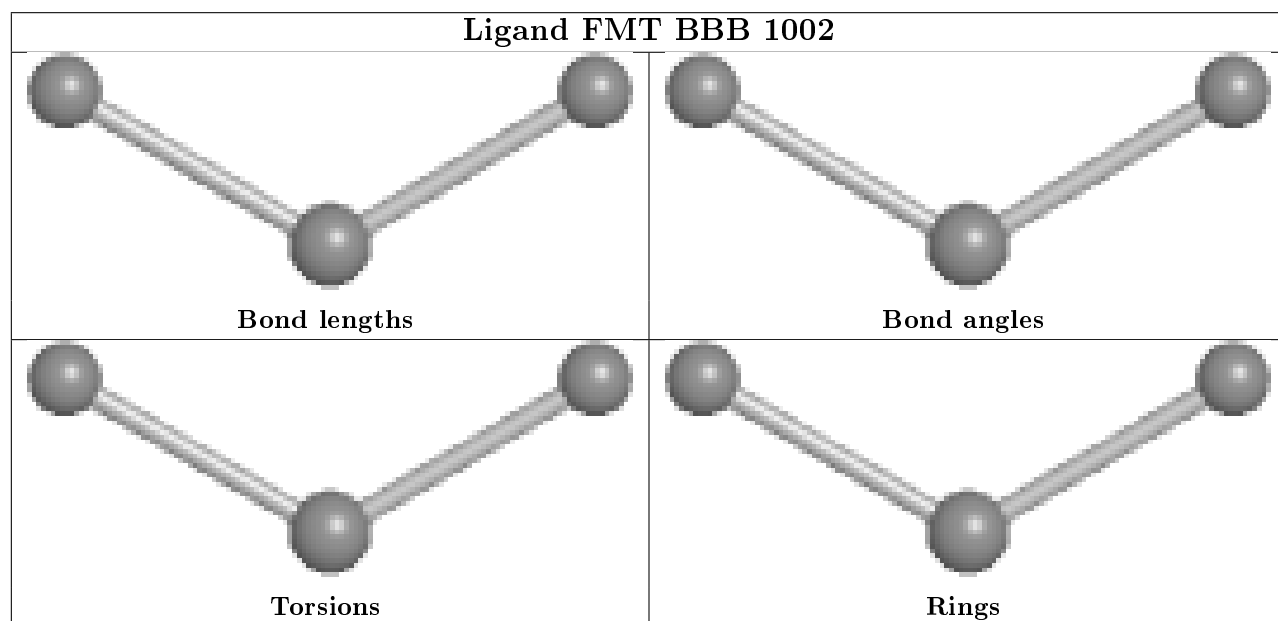
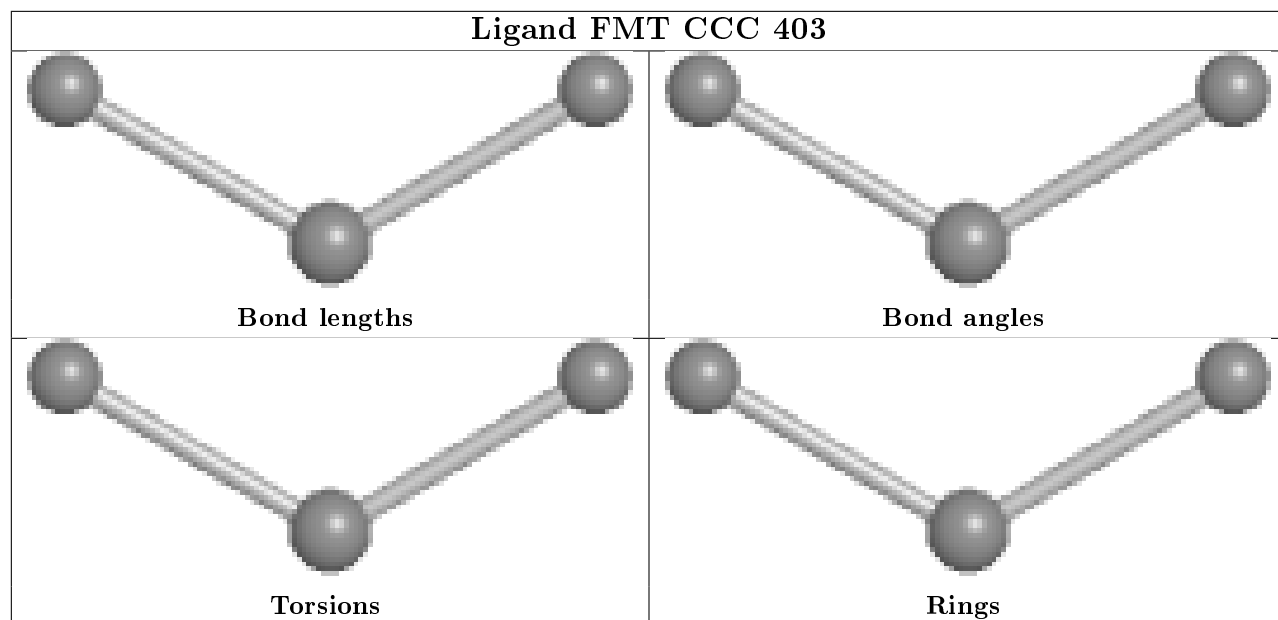
12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	506	EDO	1	0
3	DDD	404	FMT	3	0
5	BBB	1005	EDO	1	0
4	DDD	405	NAD	2	0
3	CCC	404	FMT	3	0
4	AAA	505	NAD	2	0
5	AAA	509	EDO	3	0
5	AAA	508	EDO	2	0
4	BBB	1004	NAD	3	0
4	CCC	405	NAD	2	0
3	AAA	504	FMT	3	0
3	BBB	1003	FMT	3	0

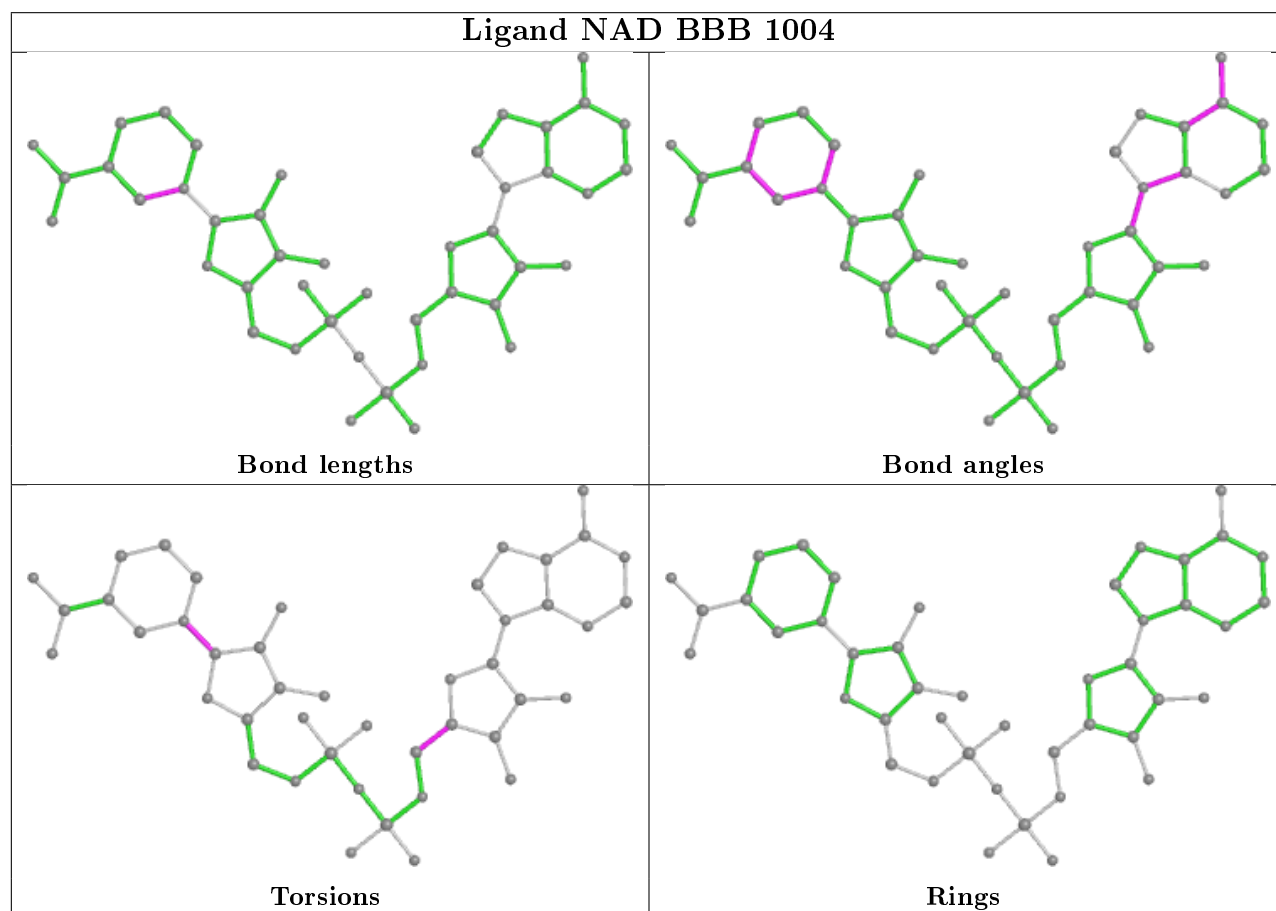
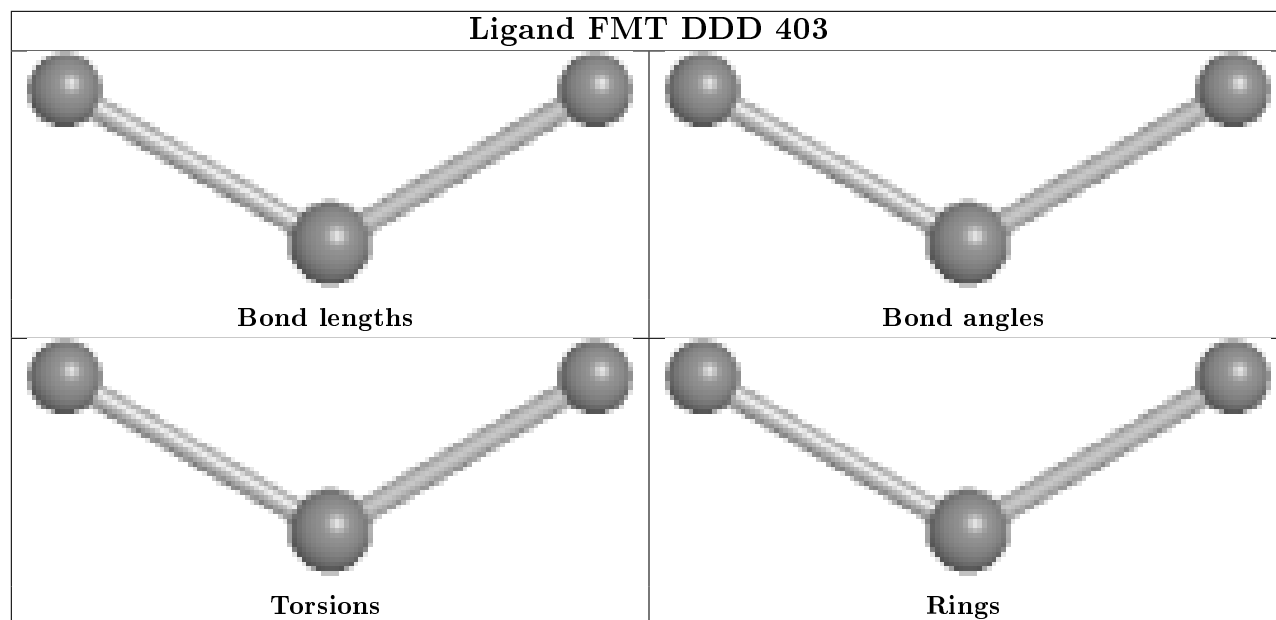
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

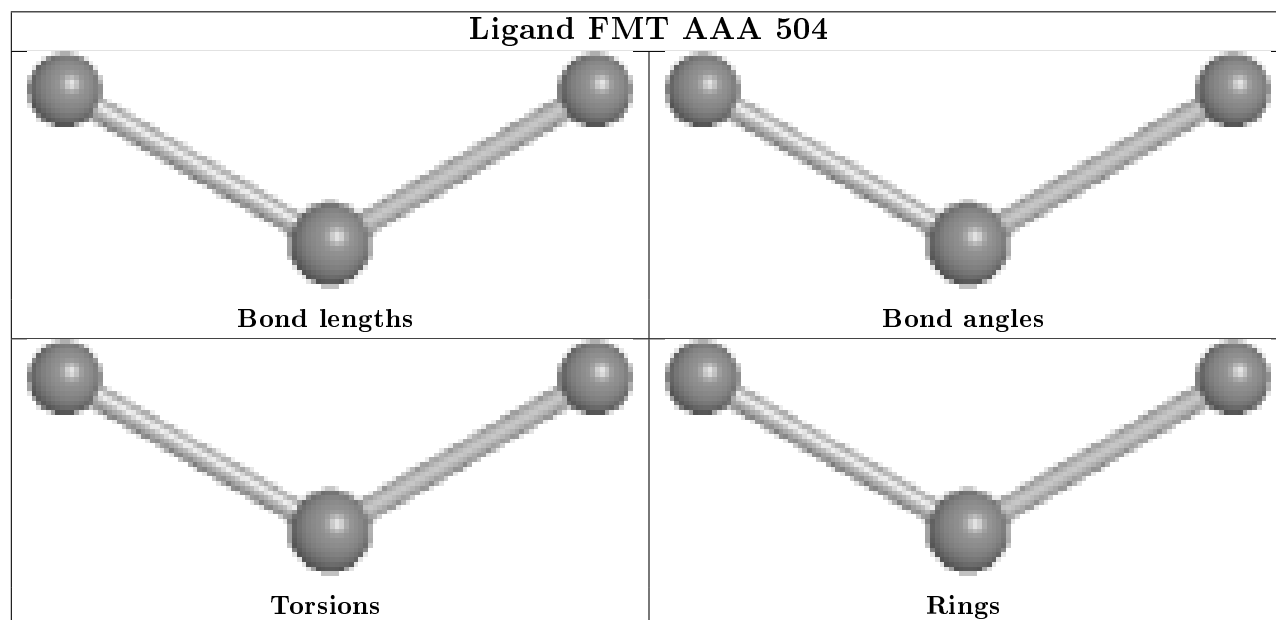
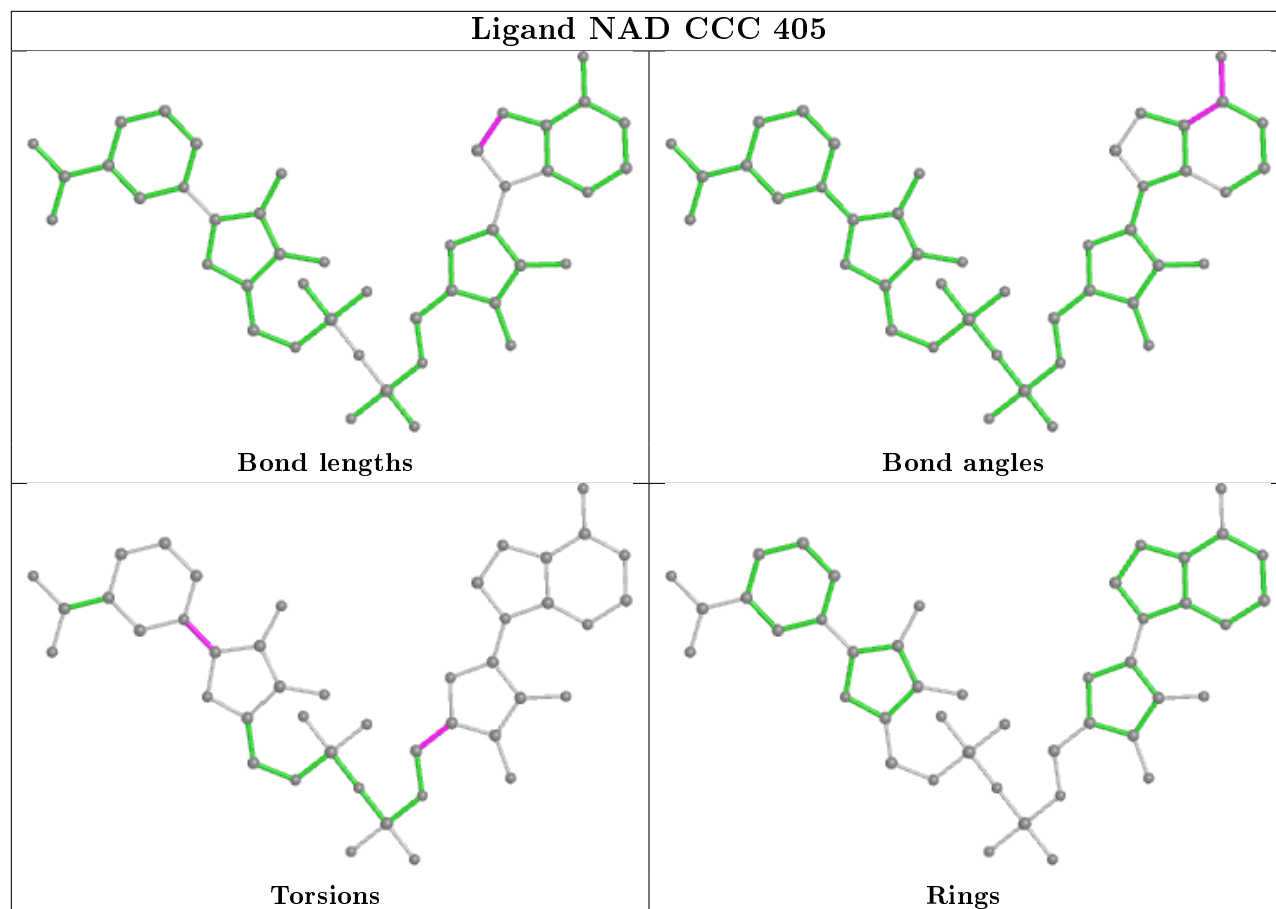


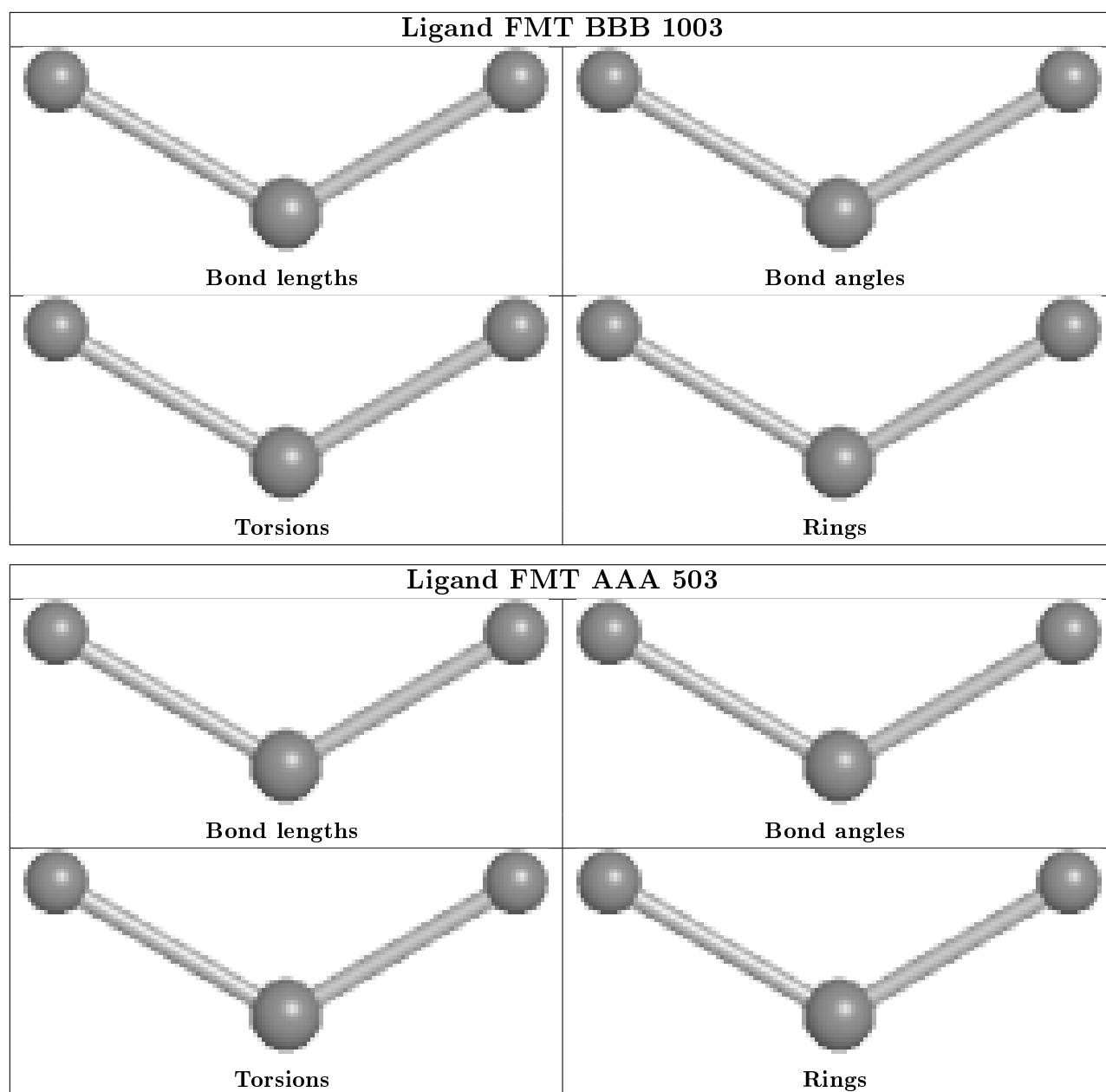












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	373/410 (90%)	-0.17	6 (1%) 72 69	9, 15, 30, 83	0
1	BBB	375/410 (91%)	0.01	14 (3%) 41 40	9, 16, 36, 99	0
1	CCC	373/410 (90%)	0.35	27 (7%) 15 13	8, 17, 41, 98	1 (0%)
1	DDD	374/410 (91%)	-0.06	5 (1%) 77 75	8, 16, 34, 82	0
All	All	1495/1640 (91%)	0.03	52 (3%) 44 42	8, 16, 36, 99	1 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	369	GLY	6.3
1	CCC	-1	LEU	5.9
1	CCC	365	VAL	5.5
1	CCC	364	ASP	4.9
1	BBB	369	GLY	4.9

### 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](#)

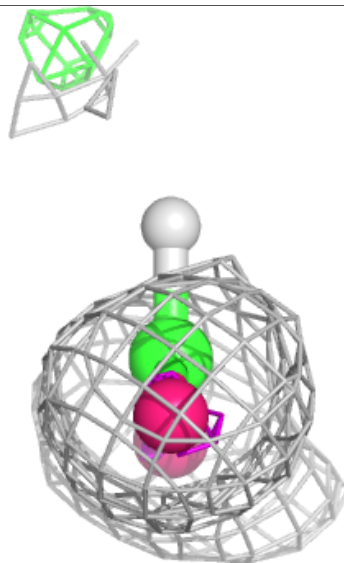
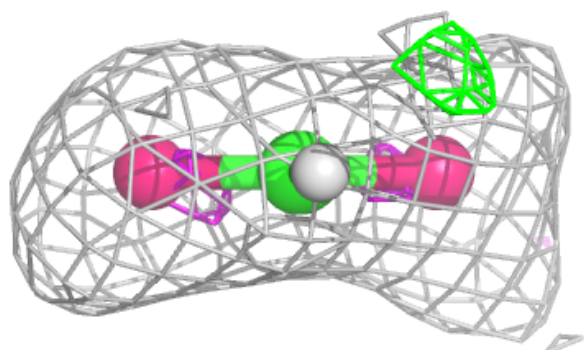
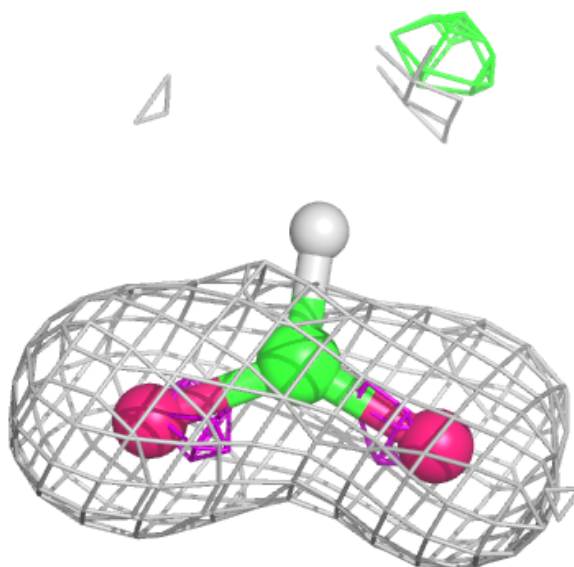
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	CCC	406	4/4	0.83	0.13	24,28,35,35	10
5	EDO	AAA	509	4/4	0.85	0.16	23,23,36,36	1
2	PEG	CCC	402	7/7	0.87	0.09	39,41,58,58	1
5	EDO	AAA	508	4/4	0.87	0.19	22,33,38,38	1
5	EDO	AAA	510	4/4	0.87	0.07	30,33,39,39	1
5	EDO	BBB	1005	4/4	0.89	0.07	36,37,41,41	1
5	EDO	AAA	507	4/4	0.90	0.10	39,39,44,44	1
3	FMT	BBB	1002	3/3	0.90	0.11	21,26,26,30	0
5	EDO	AAA	506	4/4	0.92	0.09	27,32,35,35	1
3	FMT	CCC	404	3/3	0.92	0.09	18,23,32,32	0
2	PEG	DDD	402	7/7	0.92	0.10	27,37,53,53	1
3	FMT	CCC	403	3/3	0.92	0.07	21,25,25,33	0
3	FMT	DDD	403	3/3	0.93	0.08	21,25,25,27	0
3	FMT	AAA	503	3/3	0.94	0.11	19,21,21,33	0
2	PEG	AAA	502	7/7	0.94	0.07	26,30,40,40	1
2	PEG	DDD	401	7/7	0.94	0.10	20,23,59,59	1
3	FMT	DDD	404	3/3	0.95	0.09	18,20,27,27	0
3	FMT	BBB	1003	3/3	0.95	0.07	18,20,31,31	0
2	PEG	BBB	1001	7/7	0.95	0.11	18,20,66,66	1
2	PEG	CCC	401	7/7	0.95	0.10	17,23,54,54	1
2	PEG	AAA	501	7/7	0.96	0.07	18,21,50,50	1
3	FMT	AAA	504	3/3	0.97	0.07	14,18,21,21	0
4	NAD	DDD	405	44/44	0.98	0.07	8,12,14,15	8
4	NAD	BBB	1004	44/44	0.98	0.06	10,12,14,14	8
4	NAD	CCC	405	44/44	0.98	0.06	10,13,16,17	8
4	NAD	AAA	505	44/44	0.98	0.07	9,11,14,15	8

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.

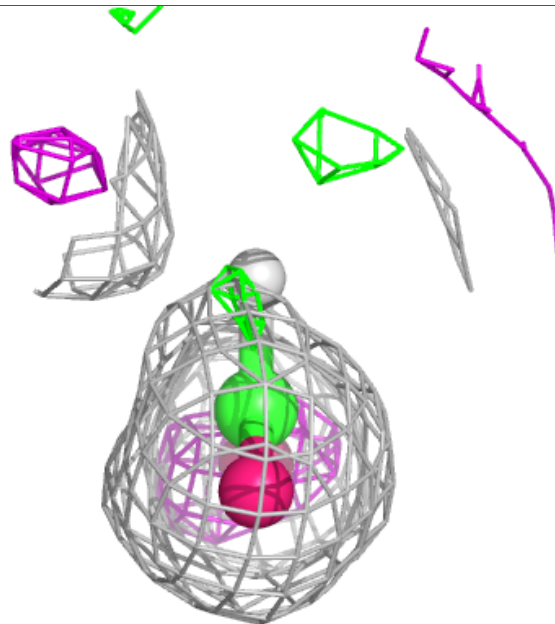
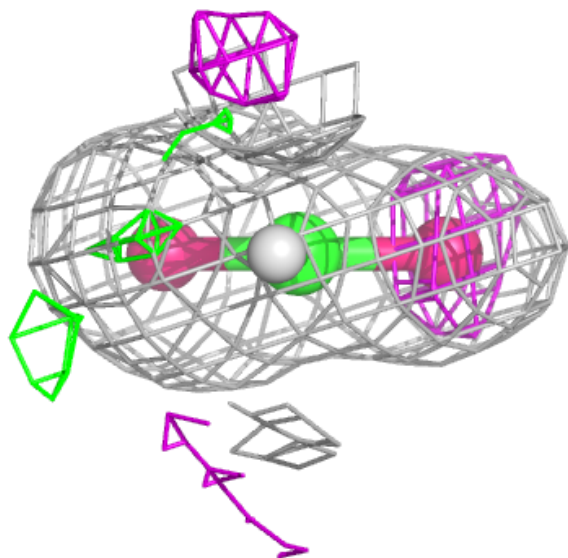
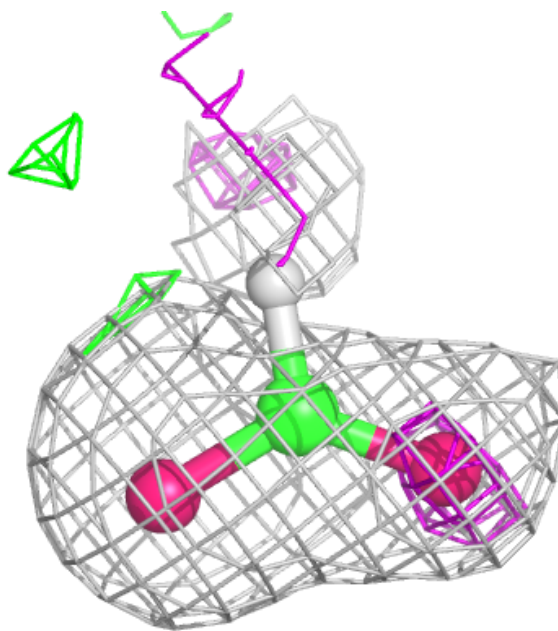
**Electron density around FMT BBB 1002:**

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



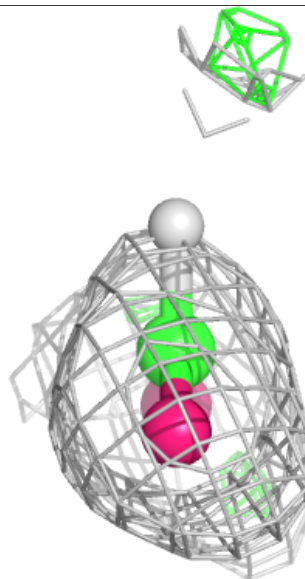
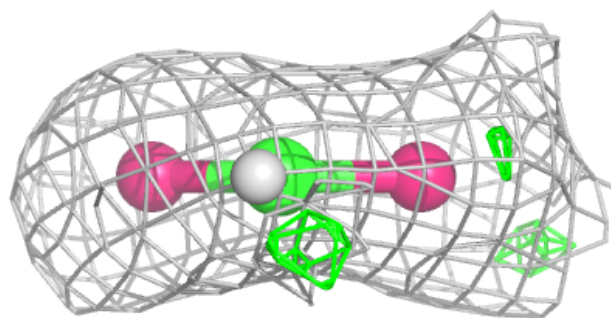
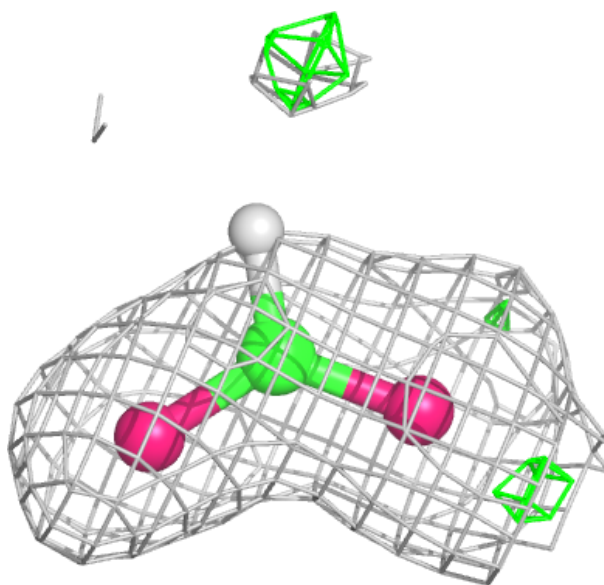
**Electron density around FMT CCC 404:**

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



**Electron density around FMT CCC 403:**

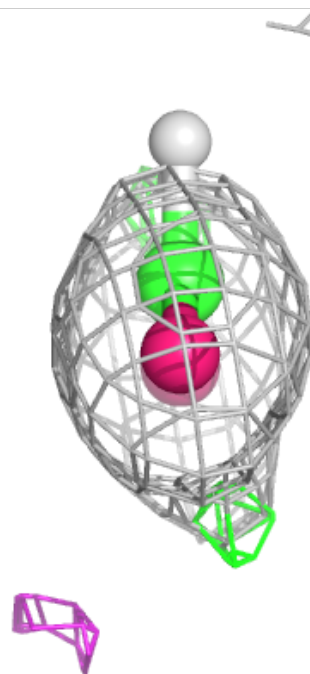
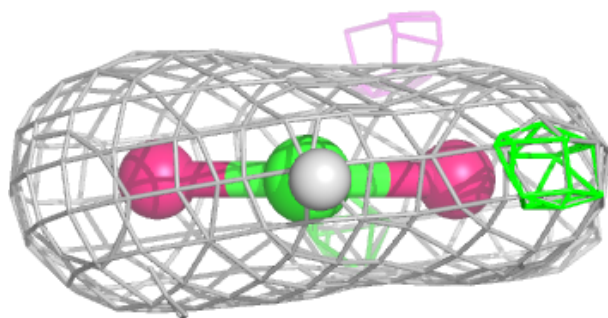
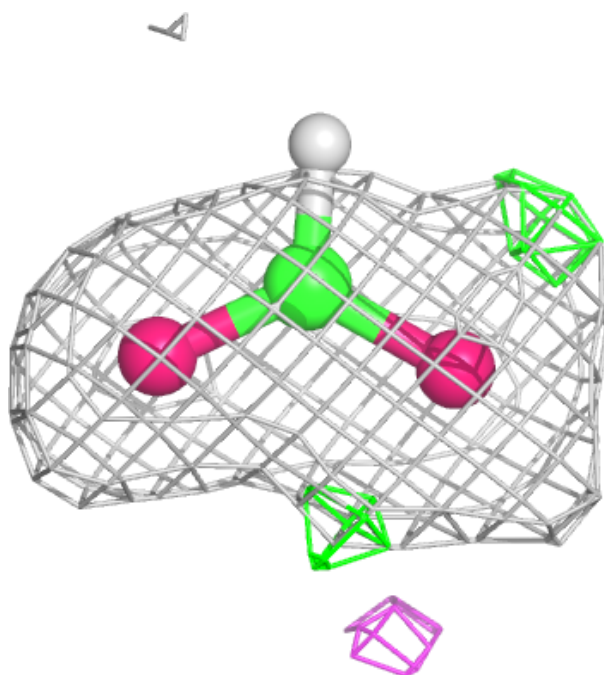
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





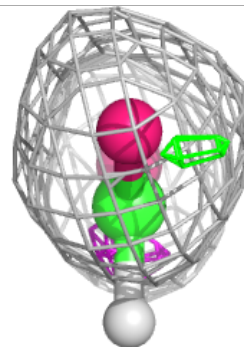
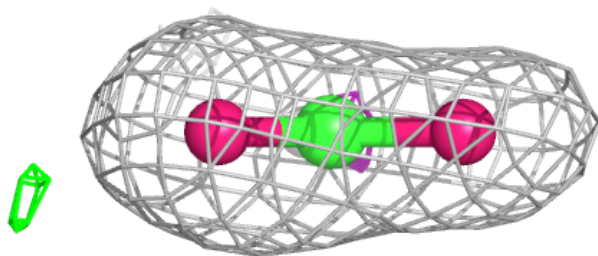
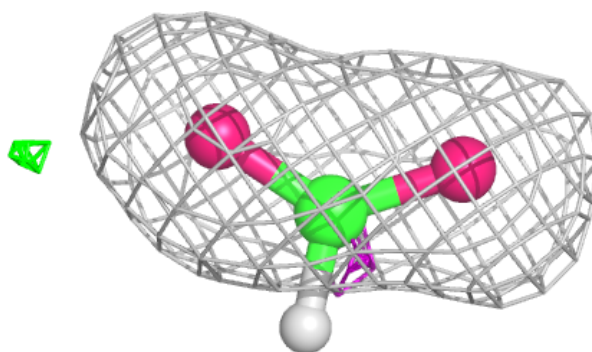
**Electron density around FMT DDD 403:**

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



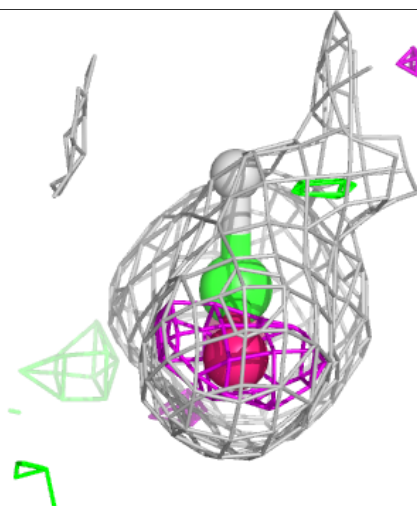
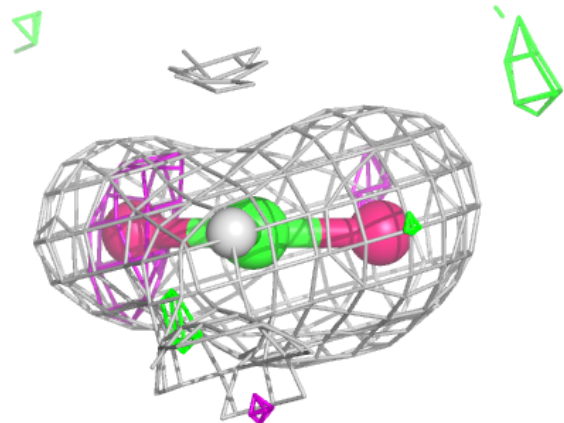
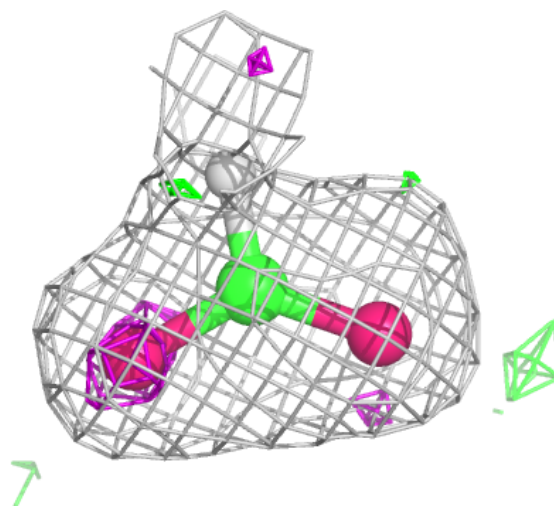
**Electron density around FMT AAA 503:**

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



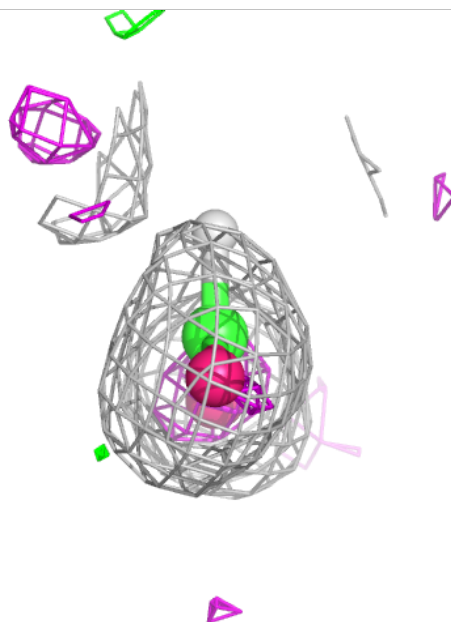
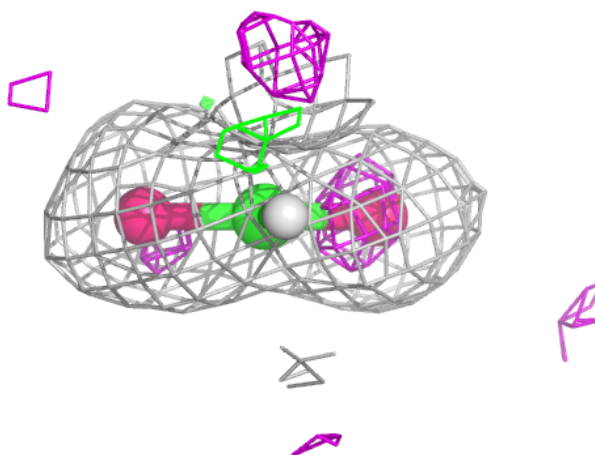
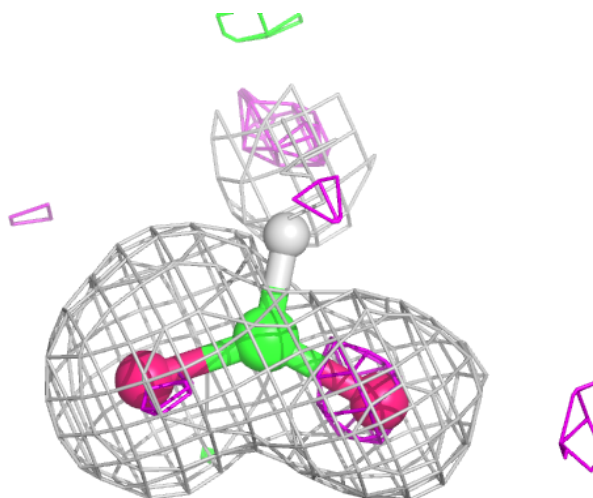
**Electron density around FMT DDD 404:**

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



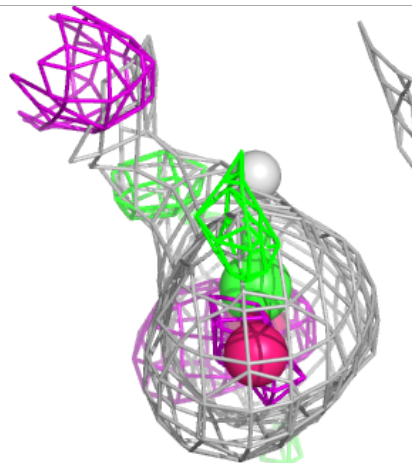
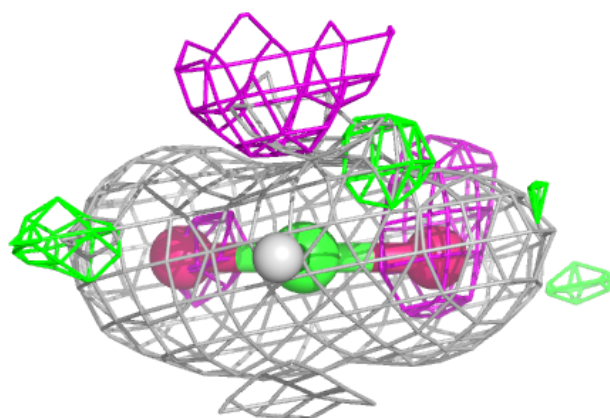
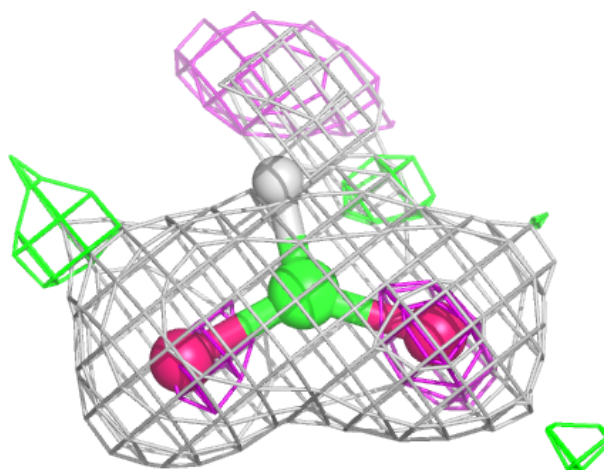
**Electron density around FMT BBB 1003:**

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



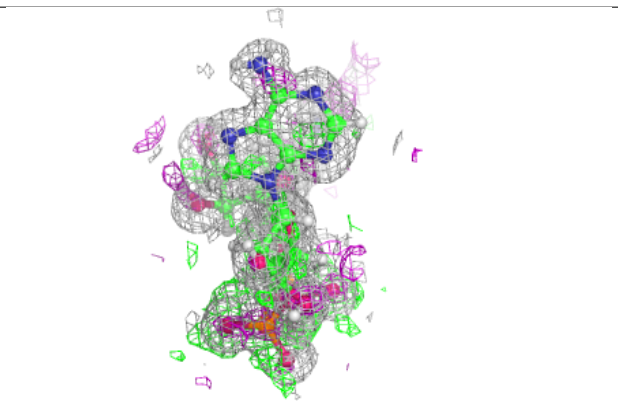
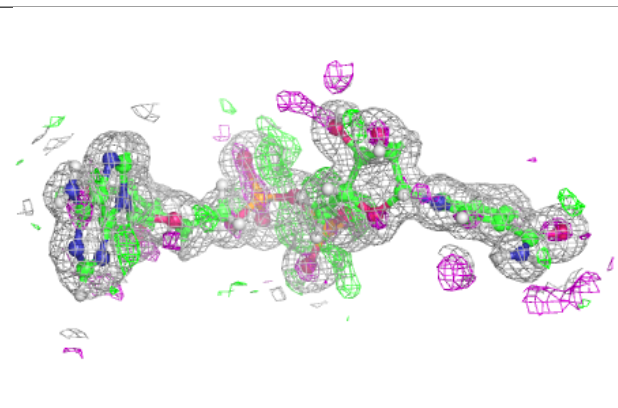
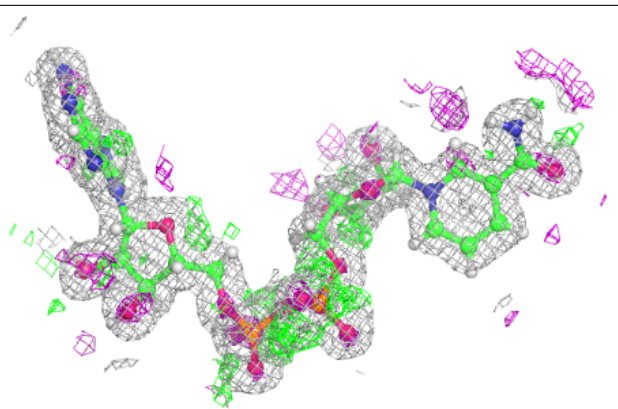
**Electron density around FMT AAA 504:**

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

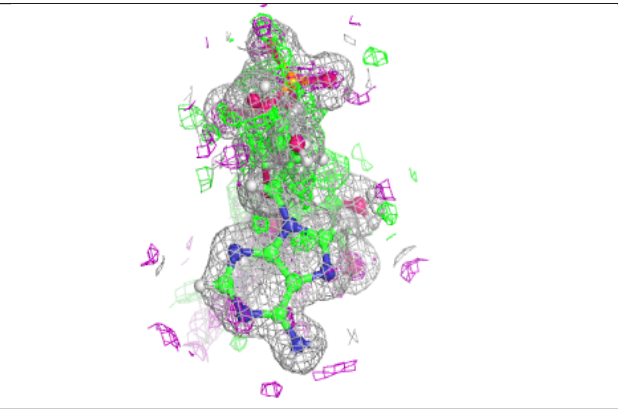
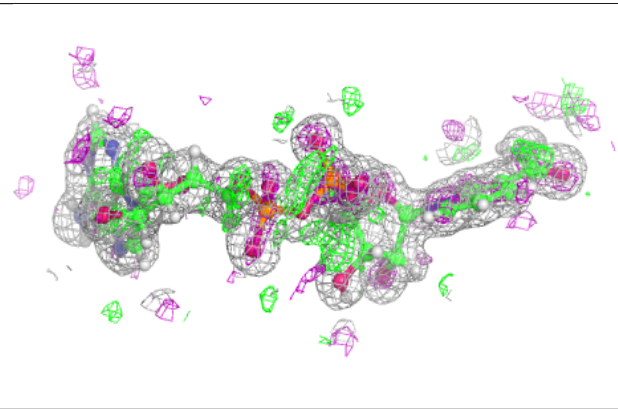
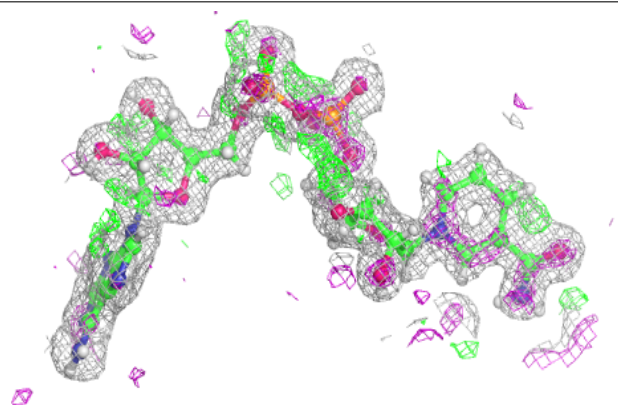


**Electron density around NAD DDD 405:**

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

**Electron density around NAD BBB 1004:**

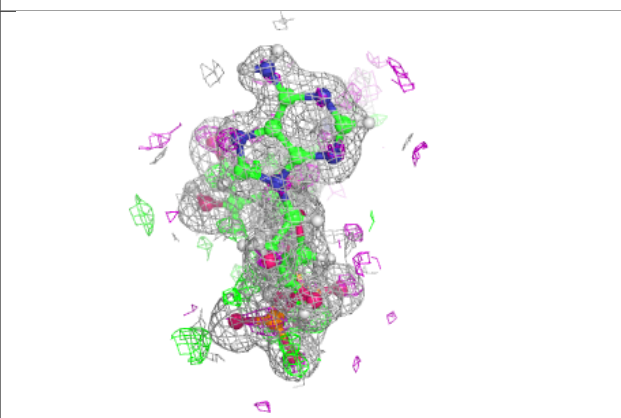
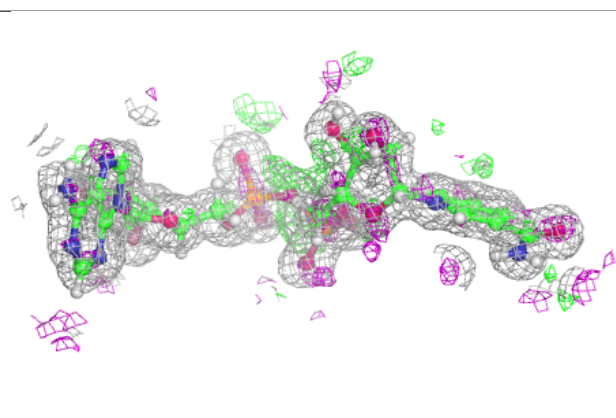
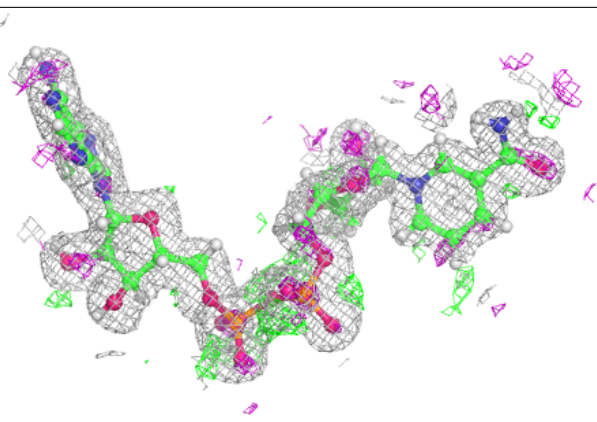
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



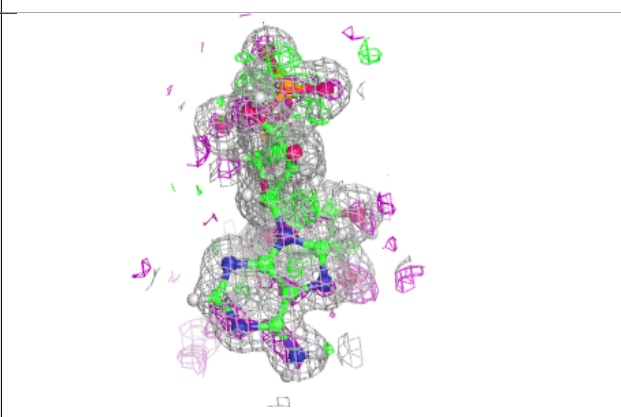
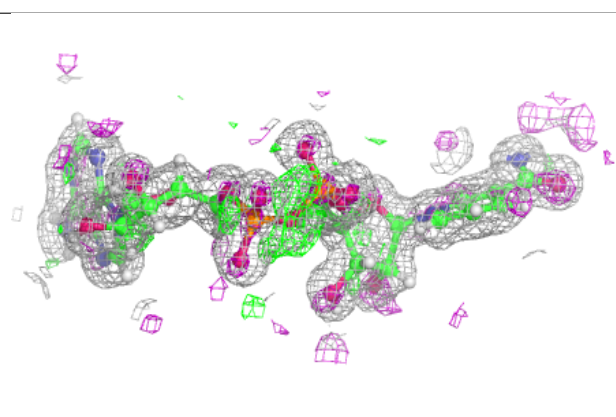
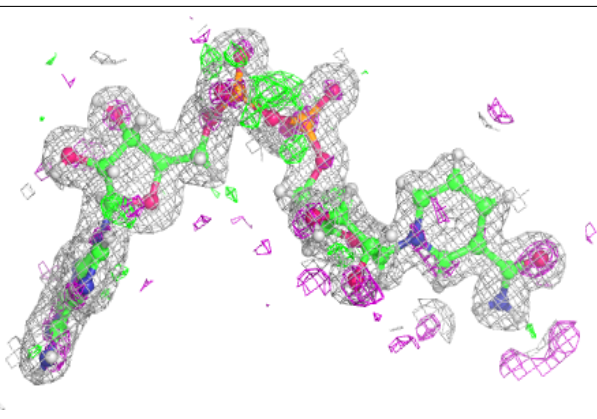


**Electron density around NAD CCC 405:**

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

**Electron density around NAD AAA 505:**

$2mF_o-DF_c$  (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.