



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:44 AM UTC

PDB ID : 6T8Z / pdb_00006t8z
Title : NAD⁺-dependent fungal formate dehydrogenase from *Chaetomium thermophilum*: A ternary complex with the oxidised form of the cofactor NAD⁺ 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 Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

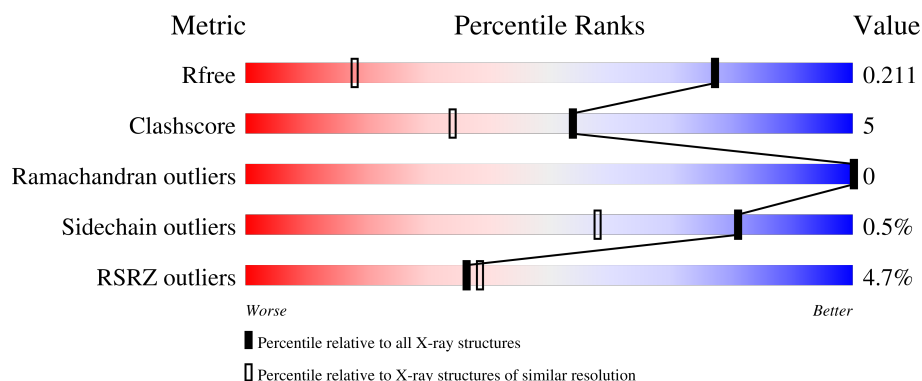
1 Overall quality at a glance

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}	180053	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0% 83% 8% 9%
1	BBB	410	3% 84% 7% 9%
1	CCC	410	10% 83% 8% 9%
1	DDD	410	3% 84% 7% 9%

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	FMT	AAA	504	-	-	X	-
3	FMT	BBB	1003	-	-	X	-
3	FMT	CCC	404	-	-	X	-
3	FMT	DDD	404	-	-	X	-
5	EDO	AAA	509	-	-	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

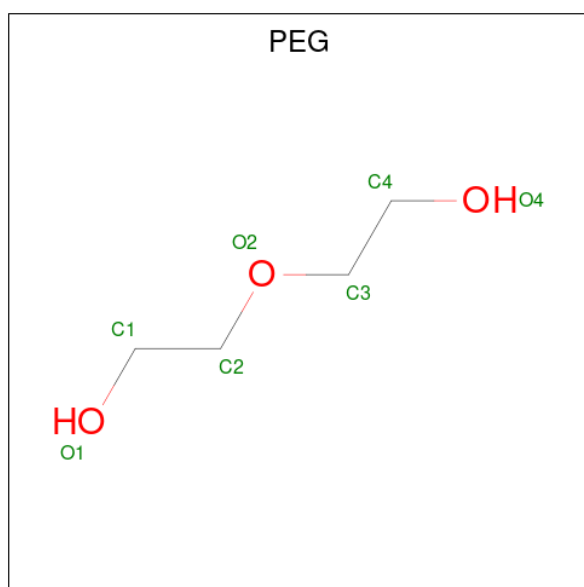
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-8	GLU	-	expression tag	UNP G0SGU4
CCC	-7	LEU	-	expression tag	UNP G0SGU4
CCC	-6	VAL	-	expression tag	UNP G0SGU4
CCC	-5	TYR	-	expression tag	UNP G0SGU4
CCC	-4	THR	-	expression tag	UNP G0SGU4
CCC	-3	ALA	-	expression tag	UNP G0SGU4
CCC	-2	ARG	-	expression 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

Continued on next page...

Continued from previous page...

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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



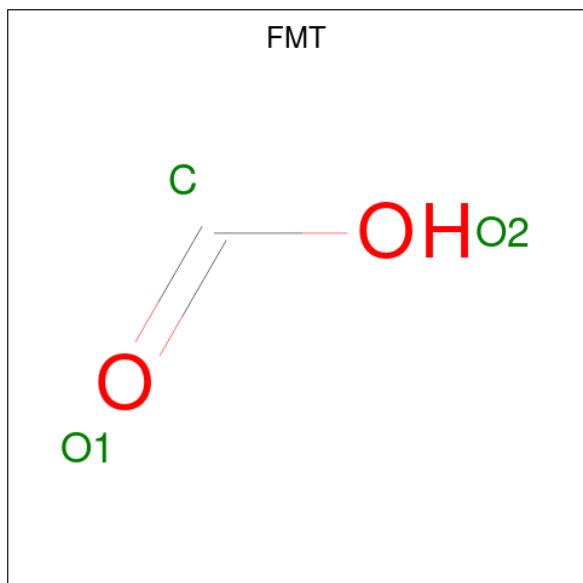
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		

Continued on next page...

Continued from previous page...

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		

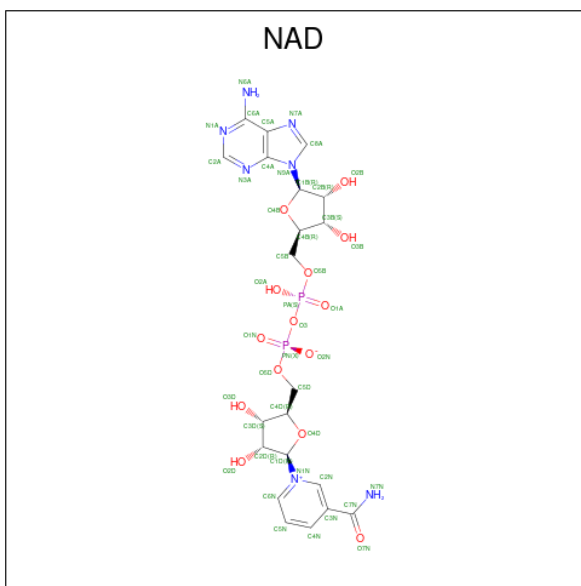
- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



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		

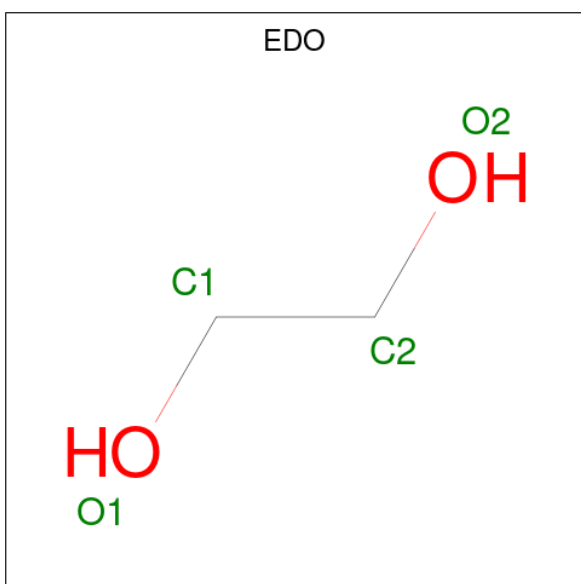
- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

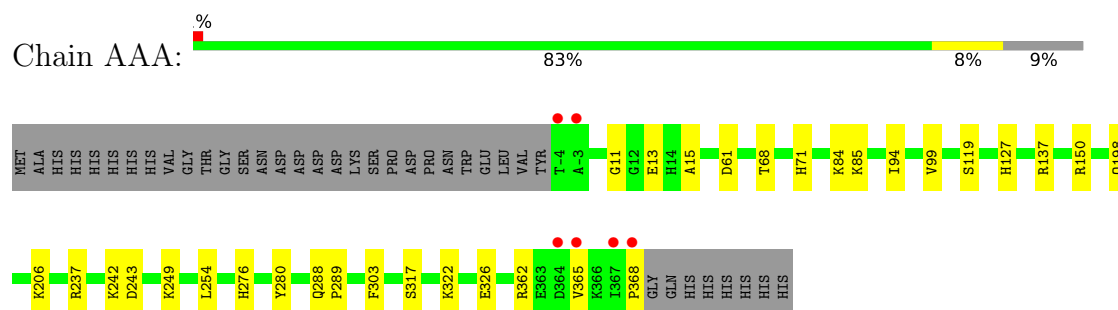
- Molecule 6 is water.

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

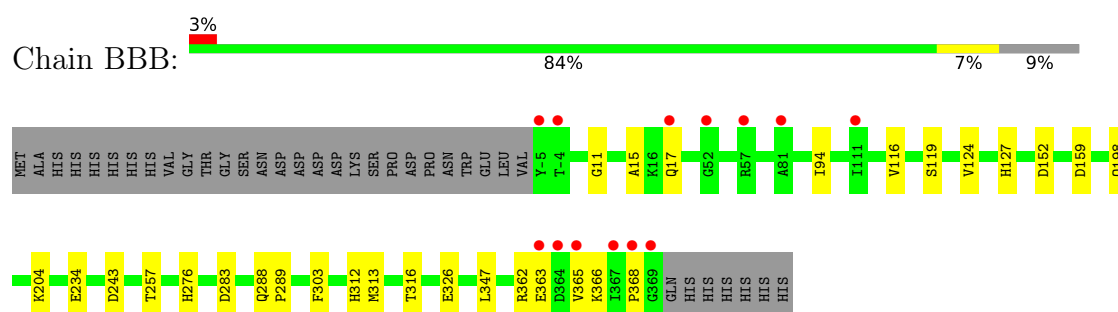
3 Residue-property plots [i](#)

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.

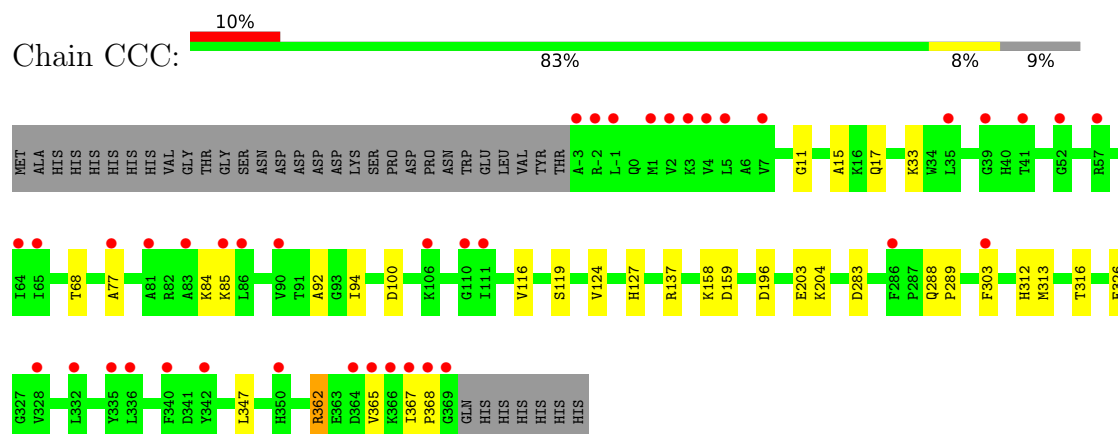
- Molecule 1: Formate dehydrogenase



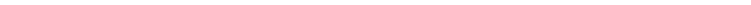
- Molecule 1: Formate dehydrogenase

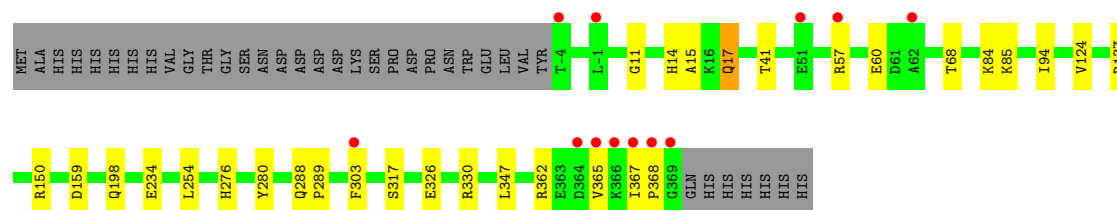


- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase

Chain DDD:  3% 84% 7% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.40Å 94.52Å 94.33Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.21Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.188 , 0.211 0.188 , 0.211	Depositor DCC
R_{free} test set	23228 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, FMT, EDO, PEG

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	1.03	3/3227 (0.1%)	1.14	2/4347 (0.0%)
1	BBB	0.99	2/3222 (0.1%)	1.14	1/4344 (0.0%)
1	CCC	1.01	2/3276 (0.1%)	1.16	3/4410 (0.1%)
1	DDD	1.05	1/3210 (0.0%)	1.15	2/4327 (0.0%)
All	All	1.02	8/12935 (0.1%)	1.15	8/17428 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	127	HIS	CE1-NE2	6.52	1.39	1.32
1	AAA	127	HIS	CE1-NE2	6.44	1.39	1.32
1	DDD	317	SER	CA-CB	-5.87	1.44	1.53
1	BBB	127	HIS	CE1-NE2	5.67	1.38	1.32
1	AAA	71	HIS	CE1-NE2	5.20	1.37	1.32
1	AAA	317	SER	CA-CB	-5.11	1.45	1.53
1	BBB	152	ASP	C-O	5.04	1.28	1.23
1	CCC	100	ASP	C-O	5.01	1.30	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	68	THR	CB-CA-C	6.05	118.20	110.16
1	DDD	68	THR	CB-CA-C	5.78	117.87	109.20
1	DDD	276	HIS	CA-CB-CG	-5.70	108.10	113.80
1	AAA	68	THR	CB-CA-C	5.64	117.66	110.16
1	BBB	276	HIS	CA-CB-CG	-5.28	108.52	113.80
1	CCC	92	ALA	O-C-N	5.24	129.64	122.41
1	AAA	276	HIS	CA-CB-CG	-5.02	108.78	113.80
1	CCC	196	ASP	CA-CB-CG	5.00	117.60	112.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3096	3183	3197	29	0
1	BBB	3090	3164	3180	23	0
1	CCC	3121	3231	3255	35	0
1	DDD	3079	3160	3176	31	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	20	30	30	8	0
5	BBB	4	6	6	1	0
5	CCC	4	6	6	0	0
6	AAA	522	0	0	15	0
6	BBB	468	0	0	6	0
6	CCC	449	0	0	9	0
6	DDD	526	0	0	7	0
All	All	14628	12962	13032	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (125) 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:BBB:159[A]:ASP:OD1	1:BBB:303[A]:PHE:CE2	2.15	0.99
1:CCC:159[B]:ASP:OD1	1:CCC:303[B]:PHE:CE2	2.18	0.96
1:AAA:249:LYS:NZ	5:AAA:509:EDO:H22	1.82	0.94
1:DDD:159[B]:ASP:OD2	1:DDD:303[B]:PHE:CD2	2.27	0.88
5:AAA:509:EDO:H11	6:AAA:837:HOH:O	1.77	0.84
1:CCC:159[B]:ASP:OD1	1:CCC:303[B]:PHE:HE2	1.56	0.84
1:DDD:159[B]:ASP:OD1	1:DDD:303[B]:PHE:CE2	2.32	0.83
1:DDD:159[B]:ASP:OD2	1:DDD:303[B]:PHE:HD2	1.62	0.81
1:BBB:159[A]:ASP:OD1	1:BBB:303[A]:PHE:HE2	1.56	0.81
1:AAA:99:VAL:O	5:AAA:508:EDO:H11	1.81	0.81
1:CCC:159[B]:ASP:OD2	1:CCC:303[B]:PHE:CD2	2.36	0.79
1:CCC:159[B]:ASP:CG	1:CCC:303[B]:PHE:CD2	2.62	0.77
1:CCC:203[B]:GLU:CD	6:CCC:519:HOH:O	2.27	0.77
1:DDD:159[B]:ASP:CG	1:DDD:303[B]:PHE:HD2	1.93	0.76
1:DDD:159[B]:ASP:CG	1:DDD:303[B]:PHE:CD2	2.63	0.76
1:BBB:159[A]:ASP:CG	1:BBB:303[A]:PHE:CD2	2.65	0.75
1:CCC:159[B]:ASP:CG	1:CCC:303[B]:PHE:HD2	1.95	0.73
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CD2	2.56	0.73
1:CCC:159[B]:ASP:OD2	1:CCC:303[B]:PHE:HD2	1.73	0.72
1:DDD:159[B]:ASP:OD1	1:DDD:303[B]:PHE:HE2	1.71	0.71
1:BBB:159[A]:ASP:OD1	1:BBB:303[A]:PHE:CD2	2.43	0.70
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CG	2.59	0.70
1:CCC:77:ALA:O	6:CCC:513:HOH:O	2.09	0.69
1:BBB:159[A]:ASP:CG	1:BBB:303[A]:PHE:HD2	2.01	0.68
1:DDD:330[B]:ARG:HD3	6:DDD:810:HOH:O	1.92	0.68
1:CCC:159[B]:ASP:OD1	1:CCC:303[B]:PHE:CD2	2.47	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:57[B]:ARG:HB3	1:DDD:57[B]:ARG:NH1	2.09	0.67
1:AAA:249:LYS:HZ2	5:AAA:509:EDO:H22	1.59	0.66
5:BBB:1005:EDO:H11	6:BBB:1456:HOH:O	1.94	0.66
1:BBB:94:ILE:O	3:BBB:1003:FMT:H	1.95	0.66
1:CCC:94:ILE:O	3:CCC:404:FMT:H	1.95	0.66
1:DDD:60:GLU:O	1:DDD:84[B]:LYS:HD2	1.95	0.66
1:CCC:326[B]:GLU:OE1	6:CCC:514:HOH:O	2.15	0.64
1:BBB:243[B]:ASP:OD2	6:BBB:1112:HOH:O	2.15	0.63
1:DDD:288:GLN:HA	1:DDD:289:PRO:C	2.23	0.63
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CD1	2.66	0.63
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CE2	2.67	0.62
1:DDD:94:ILE:O	3:DDD:404:FMT:H	2.00	0.62
1:AAA:242[B]:LYS:HG2	6:AAA:706:HOH:O	2.01	0.61
1:CCC:288:GLN:HA	1:CCC:289:PRO:C	2.25	0.61
1:AAA:249:LYS:HZ1	5:AAA:509:EDO:H22	1.64	0.61
1:BBB:159[A]:ASP:OD2	1:BBB:303[A]:PHE:CD2	2.53	0.61
1:AAA:150[B]:ARG:NH1	6:AAA:620:HOH:O	2.31	0.60
1:DDD:159[B]:ASP:OD1	1:DDD:303[B]:PHE:CD2	2.55	0.60
1:AAA:288:GLN:HA	1:AAA:289:PRO:C	2.25	0.60
1:BBB:288:GLN:HA	1:BBB:289:PRO:C	2.26	0.59
1:AAA:237[B]:ARG:NH1	6:AAA:623:HOH:O	2.35	0.58
3:AAA:504:FMT:C	4:AAA:505:NAD:C4N	2.81	0.58
1:DDD:60:GLU:O	1:DDD:84[B]:LYS:CD	2.52	0.57
1:DDD:57[B]:ARG:HB3	1:DDD:57[B]:ARG:HH11	1.69	0.57
1:CCC:33[A]:LYS:HD3	6:CCC:593:HOH:O	2.04	0.56
1:DDD:84[B]:LYS:HD3	1:DDD:85:LYS:HG2	1.86	0.56
1:CCC:203[B]:GLU:HG3	6:CCC:519:HOH:O	2.06	0.56
1:AAA:206[B]:LYS:HG3	6:AAA:699:HOH:O	2.07	0.55
1:AAA:99:VAL:O	5:AAA:508:EDO:C1	2.54	0.55
1:DDD:14:HIS:HA	1:DDD:17[B]:GLN:HG2	1.90	0.54
1:CCC:347:LEU:HD12	1:CCC:368:PRO:HG2	1.90	0.54
1:CCC:303[A]:PHE:HD2	6:CCC:789:HOH:O	1.90	0.54
1:AAA:94:ILE:O	3:AAA:504:FMT:H	2.09	0.52
1:BBB:198:GLN:NE2	6:BBB:1119:HOH:O	2.42	0.52
1:AAA:237[B]:ARG:NH2	6:AAA:619:HOH:O	2.30	0.52
1:CCC:203[B]:GLU:CG	6:CCC:519:HOH:O	2.58	0.52
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CE1	2.78	0.52
1:DDD:326[A]:GLU:HG3	6:DDD:635:HOH:O	2.09	0.51
3:DDD:404:FMT:C	4:DDD:405:NAD:C4N	2.89	0.51
1:AAA:198:GLN:NE2	6:AAA:628:HOH:O	2.42	0.51
1:AAA:61:ASP:HB2	1:AAA:85[A]:LYS:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:158[B]:LYS:NZ	1:CCC:303[B]:PHE:CZ	2.79	0.50
1:BBB:326[A]:GLU:HG3	6:BBB:1286:HOH:O	2.12	0.50
1:BBB:347:LEU:HD12	1:BBB:368:PRO:HG2	1.93	0.50
1:DDD:362:ARG:HB2	1:DDD:365:VAL:HG23	1.94	0.50
1:CCC:94:ILE:O	3:CCC:404:FMT:C	2.59	0.49
1:BBB:234[B]:GLU:HG2	6:BBB:1282:HOH:O	2.14	0.47
1:CCC:362:ARG:HB2	1:CCC:365:VAL:HG23	1.96	0.47
1:AAA:326[A]:GLU:HG3	6:AAA:814:HOH:O	2.13	0.47
1:BBB:362:ARG:HB2	1:BBB:365:VAL:CG1	2.44	0.47
1:DDD:347:LEU:HD12	1:DDD:368:PRO:HG2	1.95	0.47
1:AAA:303[B]:PHE:HD2	6:AAA:849:HOH:O	1.94	0.47
3:CCC:404:FMT:C	4:CCC:405:NAD:C4N	2.93	0.47
1:DDD:198:GLN:NE2	6:DDD:528:HOH:O	2.47	0.47
1:AAA:237[B]:ARG:NH1	6:AAA:619:HOH:O	2.29	0.47
1:AAA:84:LYS:HE3	1:AAA:84:LYS:HA	1.97	0.47
1:CCC:124:VAL:HG21	4:CCC:405:NAD:C4N	2.45	0.46
1:BBB:94:ILE:O	3:BBB:1003:FMT:C	2.63	0.46
1:BBB:124:VAL:HG21	4:BBB:1004:NAD:C4N	2.45	0.46
1:AAA:119:SER:N	5:AAA:506:EDO:H11	2.31	0.46
1:BBB:362:ARG:HB2	1:BBB:365:VAL:HG13	1.98	0.46
1:CCC:11:GLY:HA3	1:CCC:15:ALA:HB2	1.98	0.46
3:BBB:1003:FMT:C	4:BBB:1004:NAD:C4N	2.94	0.45
1:BBB:283:ASP:O	1:BBB:312:HIS:HA	2.17	0.45
1:CCC:85[A]:LYS:HD2	6:CCC:837:HOH:O	2.16	0.45
1:AAA:362:ARG:HB2	1:AAA:365:VAL:HG23	1.99	0.45
3:AAA:504:FMT:H	4:AAA:505:NAD:C4N	2.46	0.45
1:CCC:365:VAL:HG12	1:CCC:367:ILE:CD1	2.47	0.45
1:DDD:365:VAL:HG12	1:DDD:367:ILE:CD1	2.47	0.44
1:AAA:85[A]:LYS:HB3	1:AAA:85[A]:LYS:HE2	1.61	0.44
1:CCC:365:VAL:CG1	1:CCC:367:ILE:CD1	2.95	0.44
1:DDD:365:VAL:CG1	1:DDD:367:ILE:CD1	2.96	0.43
1:AAA:303[B]:PHE:CD2	6:AAA:849:HOH:O	2.57	0.43
1:DDD:94:ILE:O	3:DDD:404:FMT:C	2.65	0.43
1:BBB:11:GLY:HA3	1:BBB:15:ALA:HB2	2.00	0.43
1:BBB:204[B]:LYS:HD2	6:BBB:1425:HOH:O	2.18	0.43
1:CCC:313:MET:HA	1:CCC:316:THR:HG22	2.00	0.43
1:CCC:84[B]:LYS:HG3	1:CCC:85[B]:LYS:HE2	2.00	0.43
1:DDD:11:GLY:HA3	1:DDD:15:ALA:HB2	2.00	0.43
1:AAA:11:GLY:HA3	1:AAA:15:ALA:HB2	2.01	0.42
1:AAA:243[A]:ASP:CG	6:AAA:666:HOH:O	2.61	0.42
1:AAA:303[B]:PHE:CE2	6:AAA:849:HOH:O	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:204[A]:LYS:HD2	6:CCC:821:HOH:O	2.18	0.42
1:CCC:283:ASP:O	1:CCC:312:HIS:HA	2.19	0.42
1:AAA:368:PRO:HD2	6:AAA:650:HOH:O	2.18	0.42
1:CCC:116:VAL:HG12	1:CCC:119:SER:HB3	2.01	0.42
1:DDD:234:GLU:HG3	6:DDD:857:HOH:O	2.19	0.42
1:DDD:17[A]:GLN:HG3	6:DDD:525:HOH:O	2.20	0.42
1:DDD:254:LEU:O	1:DDD:280:TYR:HA	2.20	0.42
1:DDD:41[A]:THR:HG23	6:DDD:522:HOH:O	2.19	0.42
1:DDD:124:VAL:HG21	4:DDD:405:NAD:C4N	2.50	0.41
1:BBB:116:VAL:HG12	1:BBB:119:SER:HB3	2.03	0.41
1:AAA:249:LYS:HZ2	5:AAA:509:EDO:C2	2.29	0.41
1:AAA:322[B]:LYS:HD2	6:AAA:835:HOH:O	2.20	0.41
1:BBB:313:MET:HA	1:BBB:316:THR:HG22	2.03	0.41
1:DDD:150[B]:ARG:NH1	6:DDD:537:HOH:O	2.52	0.41
1:BBB:257:THR:O	4:BBB:1004:NAD:H2N	2.20	0.40
1:AAA:254:LEU:O	1:AAA:280:TYR:HA	2.21	0.40
1:DDD:84[A]:LYS:HE3	1:DDD:84[A]:LYS:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	78	52
1	BBB	335/340 (98%)	331 (99%)	4 (1%)	63	28
1	CCC	341/340 (100%)	339 (99%)	2 (1%)	78	52
1	DDD	334/340 (98%)	332 (99%)	2 (1%)	78	52
All	All	1346/1360 (99%)	1336 (99%)	10 (1%)	81	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13[A]	GLU
1	AAA	13[B]	GLU
1	BBB	17[A]	GLN
1	BBB	17[B]	GLN
1	BBB	363	GLU
1	BBB	366	LYS
1	CCC	17[A]	GLN
1	CCC	17[B]	GLN
1	DDD	17[A]	GLN
1	DDD	17[B]	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	PEG	AAA	501	-	6,6,6	0.11	0	5,5,5	0.16	0
4	NAD	BBB	1004	-	46,48,48	1.08	3 (6%)	64,73,73	1.07	4 (6%)
2	PEG	BBB	1001	-	6,6,6	0.21	0	5,5,5	0.20	0
5	EDO	AAA	508	-	3,3,3	0.17	0	2,2,2	0.90	0
3	FMT	DDD	404	-	2,2,2	0.84	0	1,1,1	0.38	0
3	FMT	BBB	1003	-	2,2,2	1.34	0	1,1,1	0.53	0
5	EDO	AAA	506	-	3,3,3	0.23	0	2,2,2	0.38	0
5	EDO	BBB	1005	-	3,3,3	0.13	0	2,2,2	0.33	0
2	PEG	AAA	502	-	6,6,6	0.20	0	5,5,5	0.13	0
3	FMT	DDD	403	-	2,2,2	0.62	0	1,1,1	0.08	0
3	FMT	AAA	504	-	2,2,2	0.99	0	1,1,1	0.70	0
5	EDO	AAA	510	-	3,3,3	0.10	0	2,2,2	0.29	0
3	FMT	AAA	503	-	2,2,2	0.38	0	1,1,1	0.21	0
2	PEG	CCC	401	-	6,6,6	0.22	0	5,5,5	0.28	0
5	EDO	CCC	406	-	3,3,3	0.13	0	2,2,2	0.32	0
4	NAD	DDD	405	-	46,48,48	0.82	2 (4%)	64,73,73	1.05	4 (6%)
3	FMT	BBB	1002	-	2,2,2	0.78	0	1,1,1	0.13	0
3	FMT	CCC	404	-	2,2,2	0.64	0	1,1,1	0.14	0
3	FMT	CCC	403	-	2,2,2	0.86	0	1,1,1	0.03	0
2	PEG	DDD	402	-	6,6,6	0.18	0	5,5,5	0.11	0
4	NAD	CCC	405	-	46,48,48	1.29	2 (4%)	64,73,73	0.93	2 (3%)
4	NAD	AAA	505	-	46,48,48	0.86	2 (4%)	64,73,73	0.92	2 (3%)
5	EDO	AAA	507	-	3,3,3	0.07	0	2,2,2	0.35	0
5	EDO	AAA	509	-	3,3,3	0.44	0	2,2,2	0.85	0
2	PEG	DDD	401	-	6,6,6	0.29	0	5,5,5	0.23	0
2	PEG	CCC	402	-	6,6,6	0.19	0	5,5,5	0.14	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	CCC	406	-	-	0/1/1/1	-
2	PEG	AAA	501	-	-	1/4/4/4	-
4	NAD	AAA	505	-	-	2/30/62/62	0/5/5/5
2	PEG	BBB	1001	-	-	0/4/4/4	-
4	NAD	BBB	1004	-	-	3/30/62/62	0/5/5/5
4	NAD	DDD	405	-	-	3/30/62/62	0/5/5/5
5	EDO	AAA	507	-	-	1/1/1/1	-
5	EDO	AAA	510	-	-	0/1/1/1	-
5	EDO	AAA	508	-	-	1/1/1/1	-
5	EDO	AAA	509	-	-	1/1/1/1	-
2	PEG	DDD	401	-	-	1/4/4/4	-
5	EDO	AAA	506	-	-	0/1/1/1	-
5	EDO	BBB	1005	-	-	1/1/1/1	-
2	PEG	CCC	402	-	-	1/4/4/4	-
2	PEG	AAA	502	-	-	0/4/4/4	-
2	PEG	DDD	402	-	-	0/4/4/4	-
4	NAD	CCC	405	-	-	2/30/62/62	0/5/5/5
2	PEG	CCC	401	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CCC	405	NAD	PN-O3	6.90	1.66	1.59
4	BBB	1004	NAD	C2N-N1N	3.99	1.39	1.35
4	BBB	1004	NAD	PN-O3	3.80	1.63	1.59
4	CCC	405	NAD	PA-O3	-3.69	1.55	1.59
4	AAA	505	NAD	C4N-C3N	2.90	1.43	1.39
4	AAA	505	NAD	C2N-N1N	2.58	1.37	1.35
4	DDD	405	NAD	C2N-N1N	2.49	1.37	1.35
4	DDD	405	NAD	PN-O3	2.41	1.62	1.59
4	BBB	1004	NAD	PA-O3	-2.13	1.57	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DDD	405	NAD	O2A-PA-O3	3.80	117.54	107.27
4	BBB	1004	NAD	C6N-N1N-C2N	-3.45	118.94	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	1004	NAD	O2A-PA-O3	3.23	116.01	107.27
4	AAA	505	NAD	C6N-N1N-C2N	-2.94	119.38	121.88
4	CCC	405	NAD	O2A-PA-O3	2.63	114.39	107.27
4	CCC	405	NAD	C4D-O4D-C1D	2.28	112.02	109.92
4	BBB	1004	NAD	C1B-N9A-C8A	2.28	132.16	127.09
4	DDD	405	NAD	C6A-C5A-C4A	-2.07	114.35	117.18
4	AAA	505	NAD	O2A-PA-O3	2.07	112.87	107.27
4	DDD	405	NAD	O4B-C1B-C2B	-2.06	102.20	106.62
4	DDD	405	NAD	C5A-C4A-N3A	2.06	129.55	126.72
4	BBB	1004	NAD	C2N-C3N-C4N	2.04	120.63	118.26

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	505	NAD	O4D-C1D-N1N-C6N
4	BBB	1004	NAD	O4D-C1D-N1N-C6N
4	CCC	405	NAD	O4D-C1D-N1N-C6N
4	DDD	405	NAD	O4D-C1D-N1N-C6N
5	AAA	509	EDO	O1-C1-C2-O2
5	BBB	1005	EDO	O1-C1-C2-O2
5	AAA	508	EDO	O1-C1-C2-O2
2	DDD	401	PEG	O2-C3-C4-O4
2	CCC	401	PEG	C1-C2-O2-C3
2	AAA	501	PEG	C1-C2-O2-C3
2	CCC	402	PEG	C1-C2-O2-C3
2	CCC	401	PEG	O1-C1-C2-O2
4	AAA	505	NAD	O4D-C1D-N1N-C2N
4	BBB	1004	NAD	O4D-C1D-N1N-C2N
4	CCC	405	NAD	O4D-C1D-N1N-C2N
4	DDD	405	NAD	O4D-C1D-N1N-C2N
5	AAA	507	EDO	O1-C1-C2-O2
4	DDD	405	NAD	C2B-C1B-N9A-C8A
4	BBB	1004	NAD	C2B-C1B-N9A-C8A

There are no ring outliers.

12 monomers are involved in 25 short contacts:

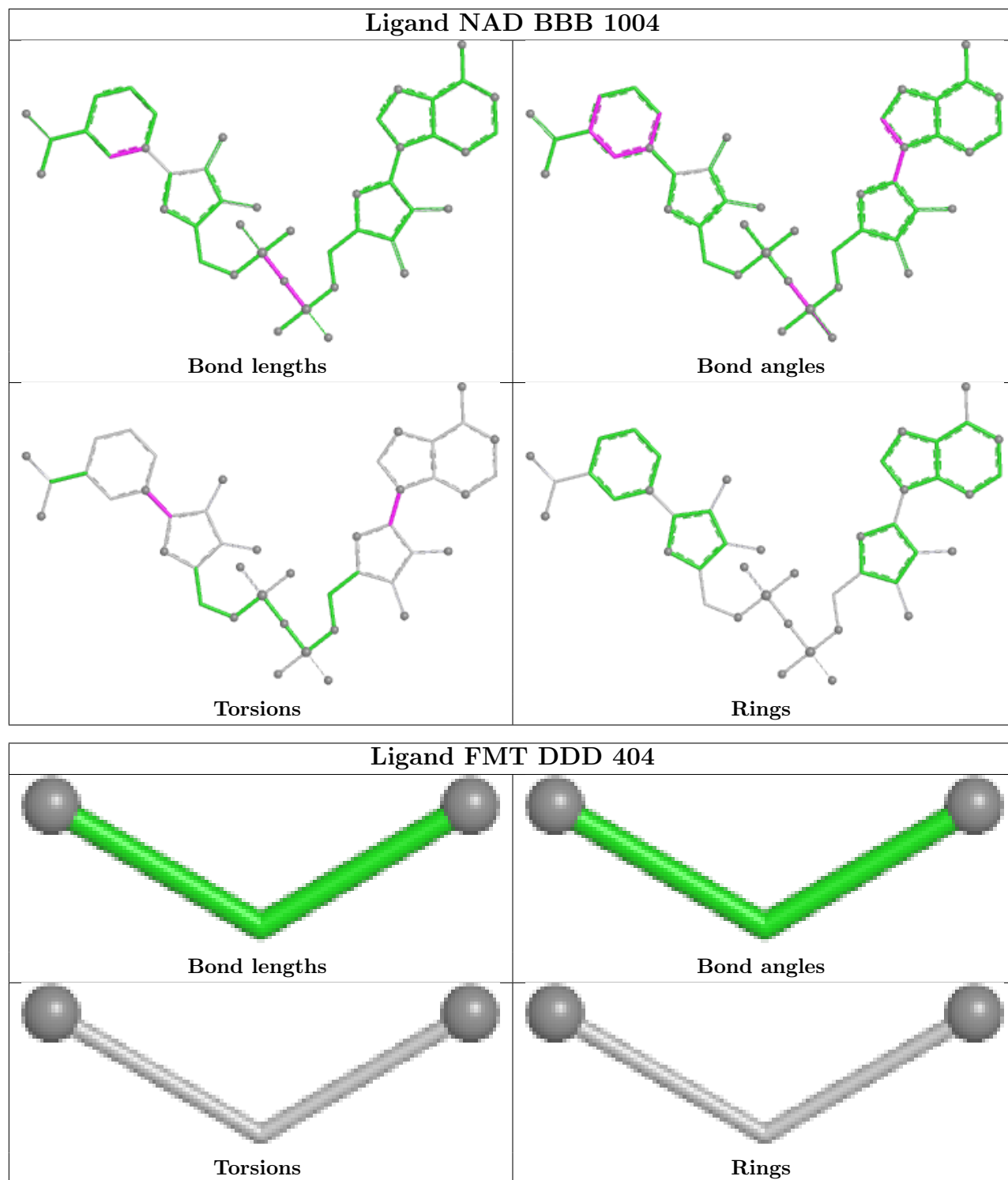
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	1004	NAD	3	0
5	AAA	508	EDO	2	0

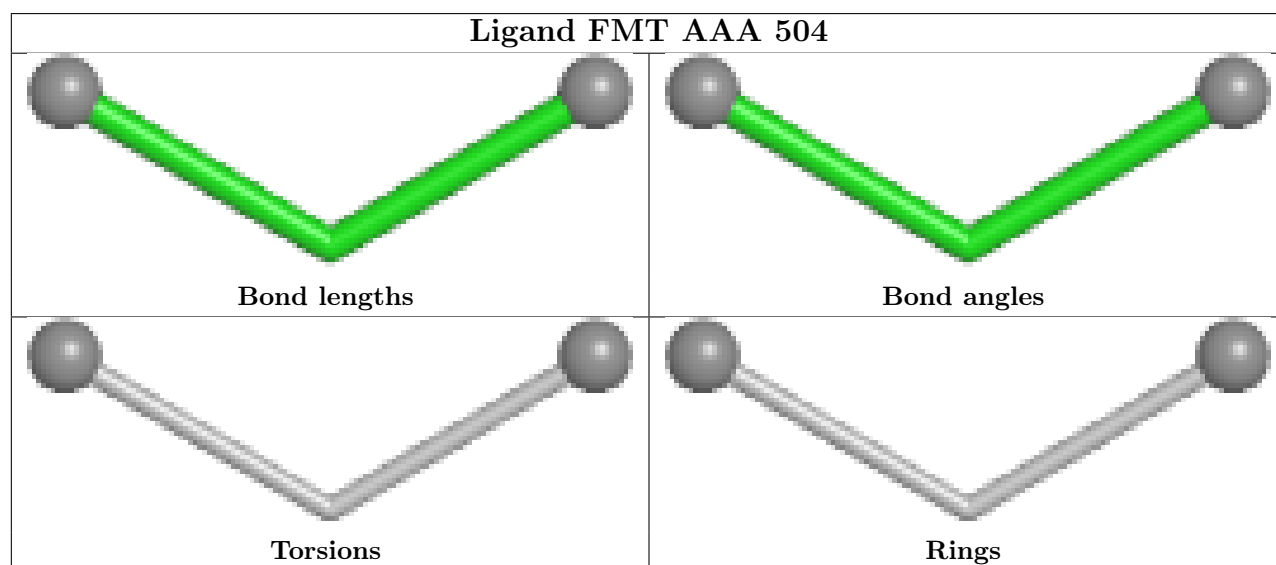
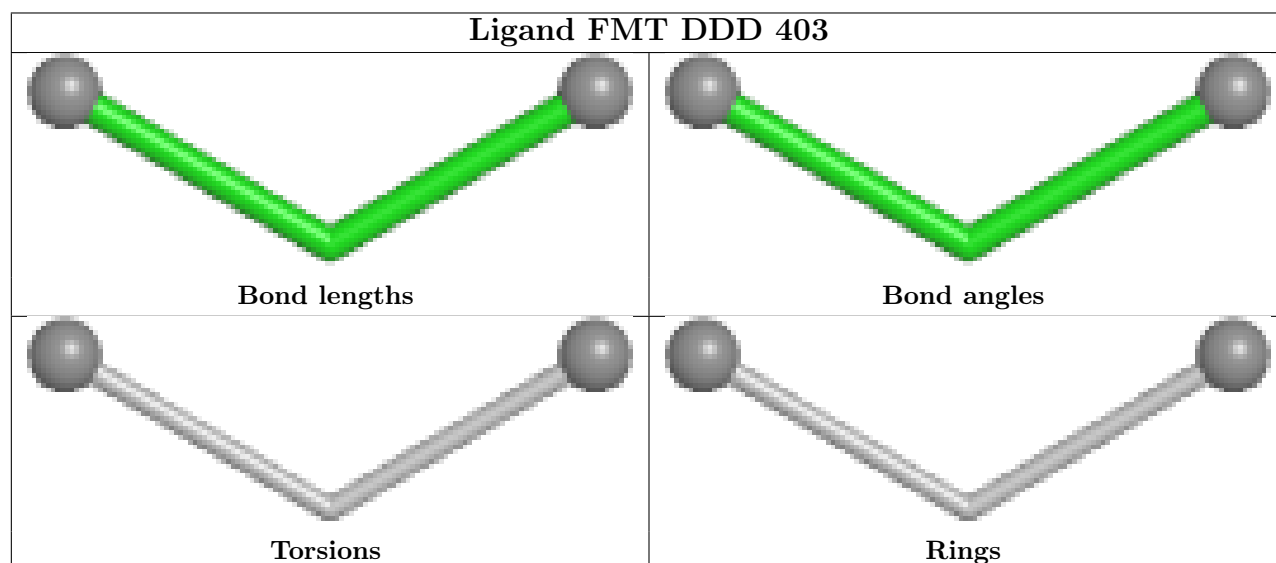
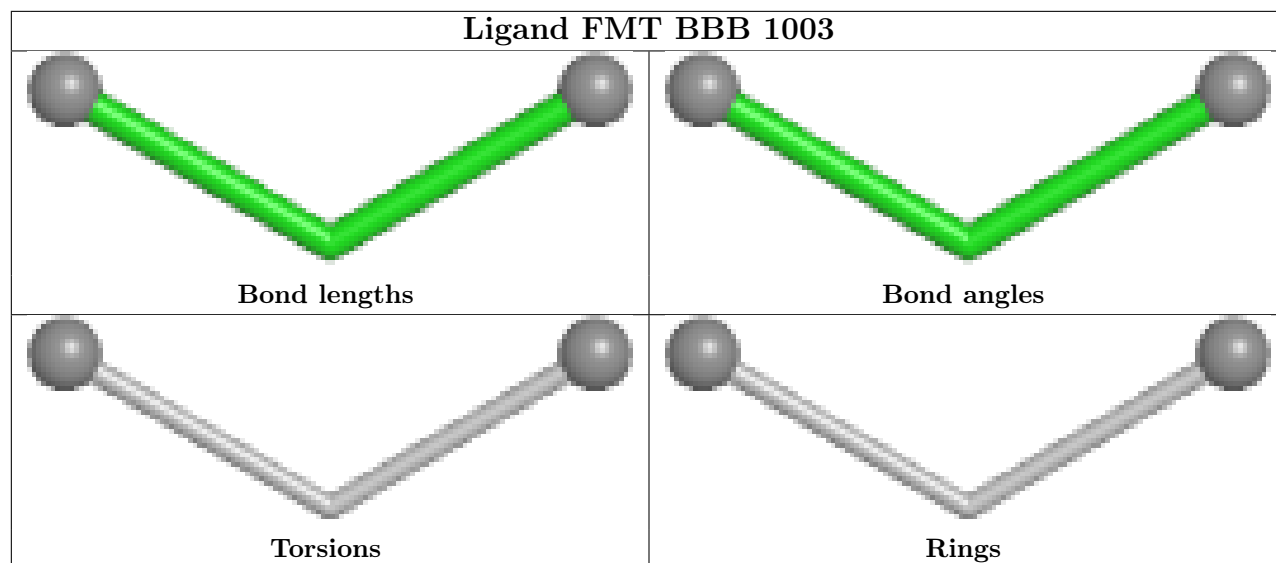
Continued on next page...

Continued from previous page...

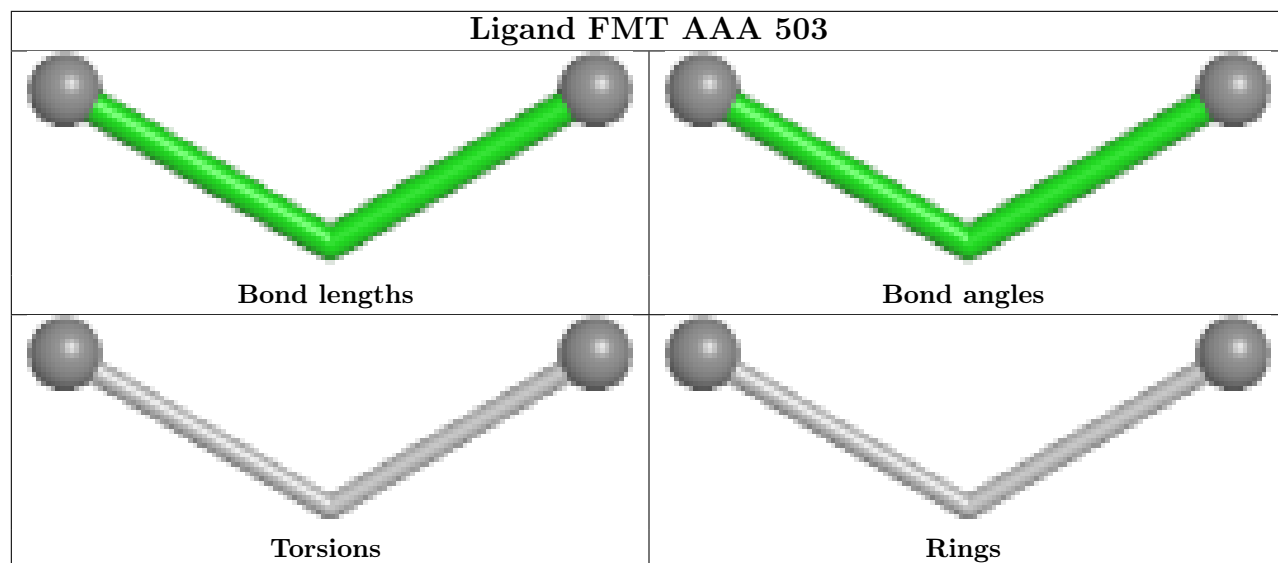
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	404	FMT	3	0
3	BBB	1003	FMT	3	0
5	AAA	506	EDO	1	0
5	BBB	1005	EDO	1	0
3	AAA	504	FMT	3	0
4	DDD	405	NAD	2	0
3	CCC	404	FMT	3	0
4	CCC	405	NAD	2	0
4	AAA	505	NAD	2	0
5	AAA	509	EDO	5	0

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.

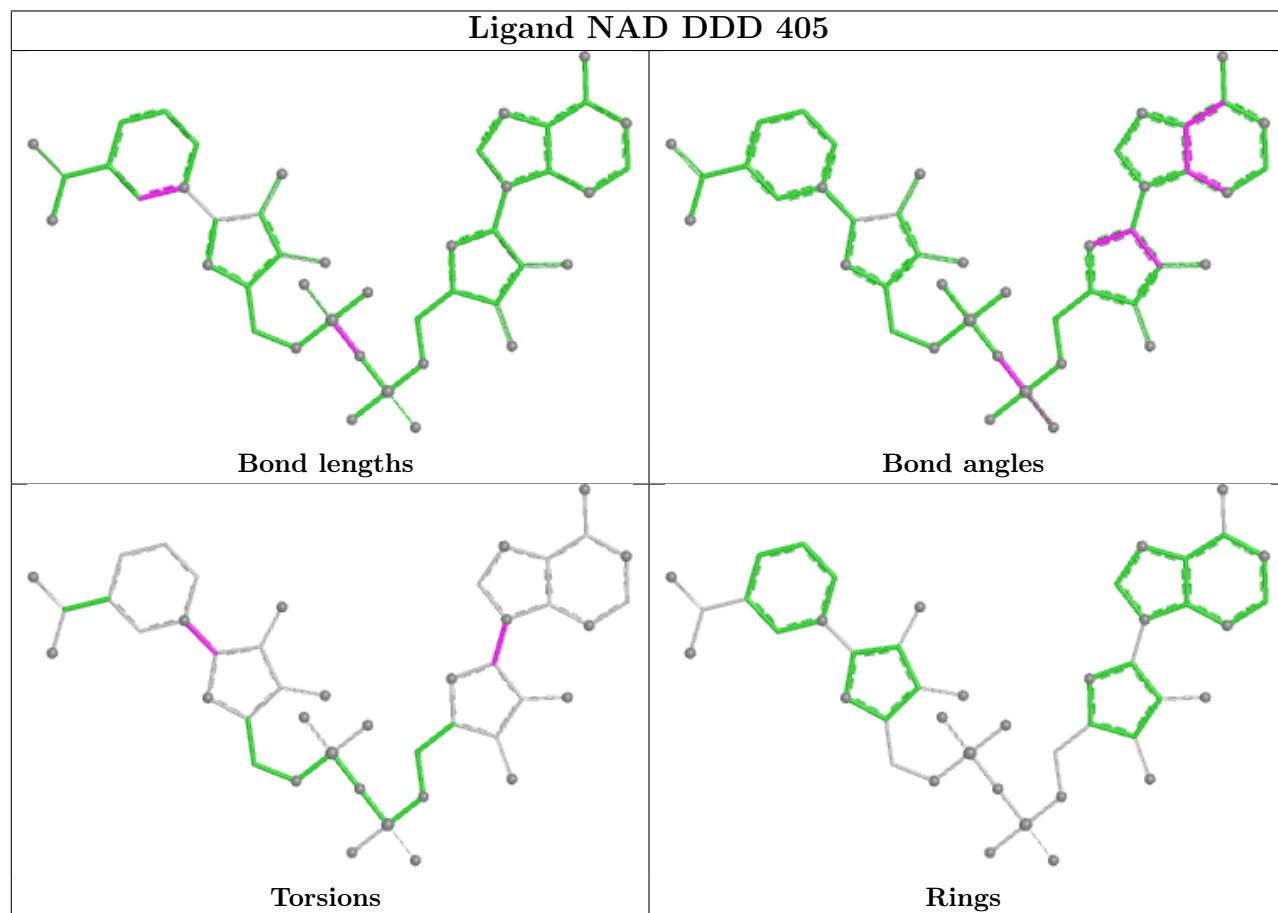


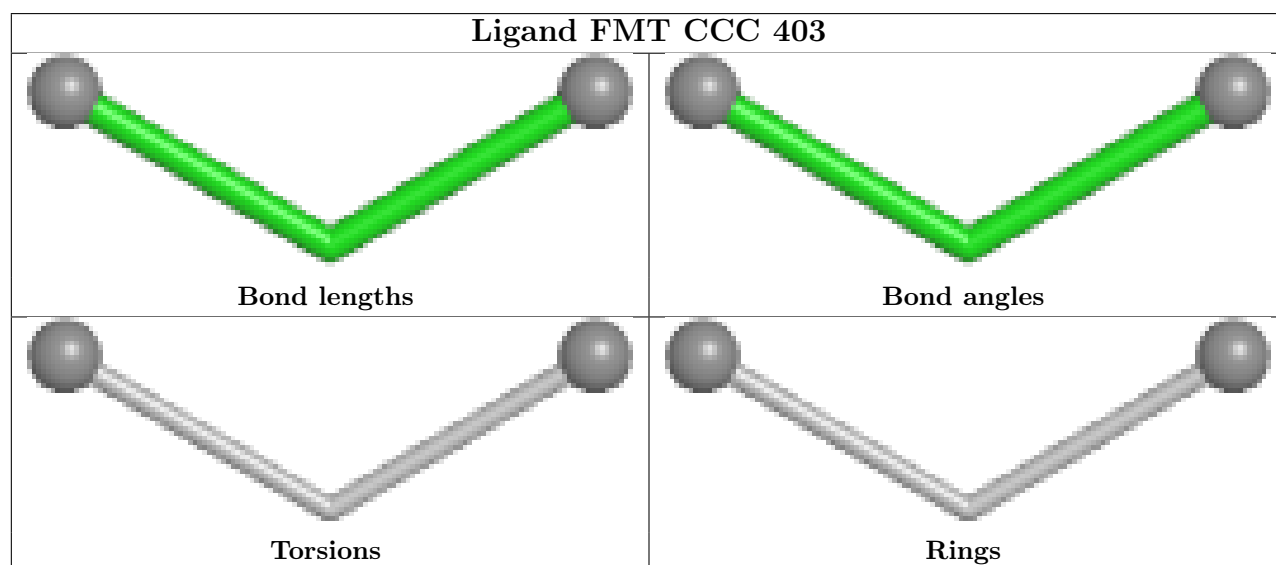
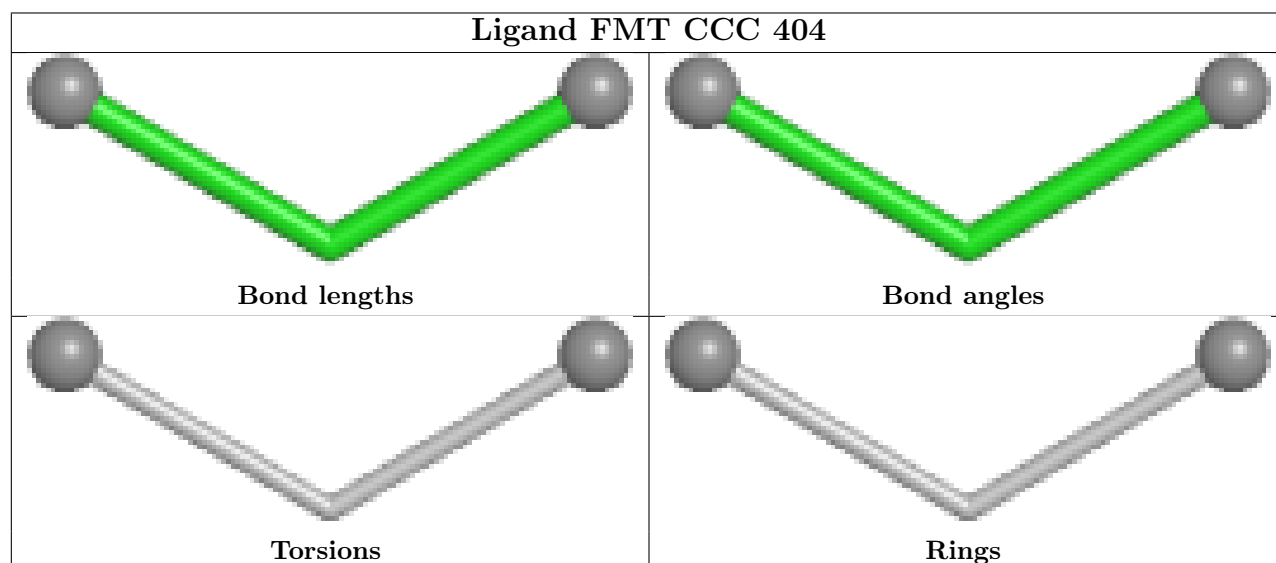
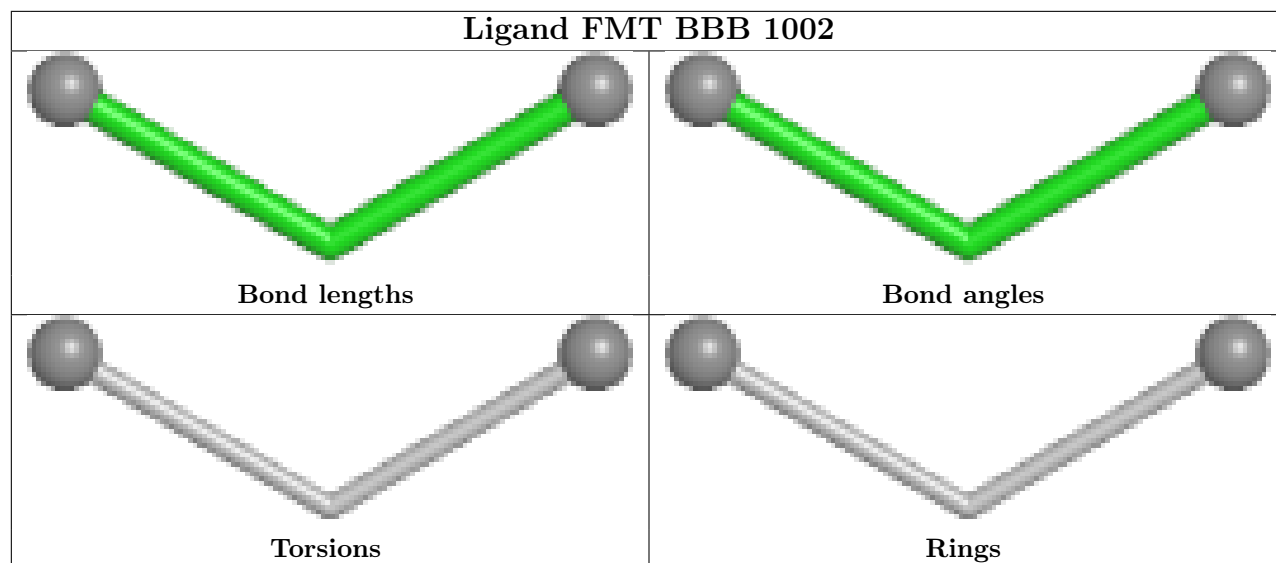


Ligand FMT AAA 503

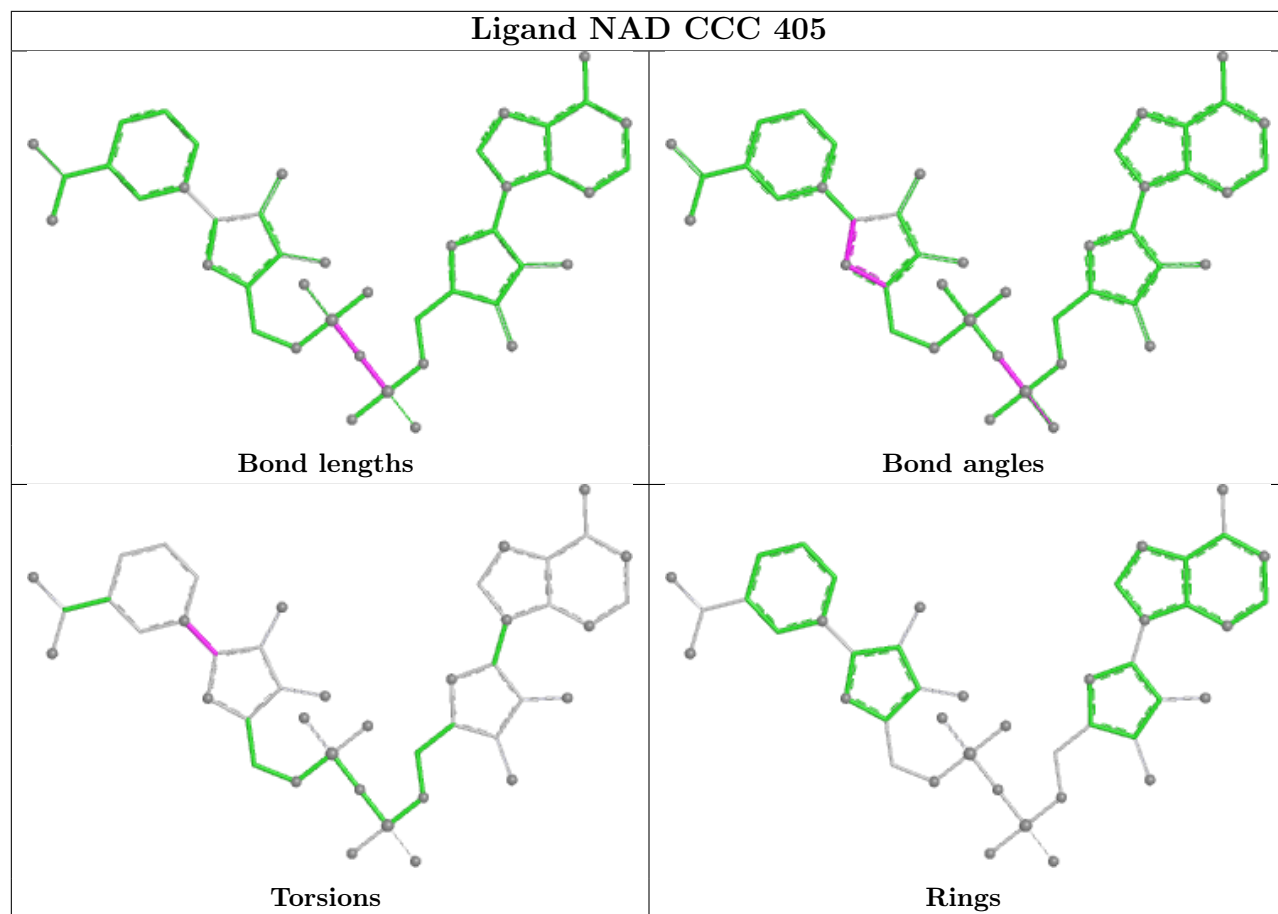


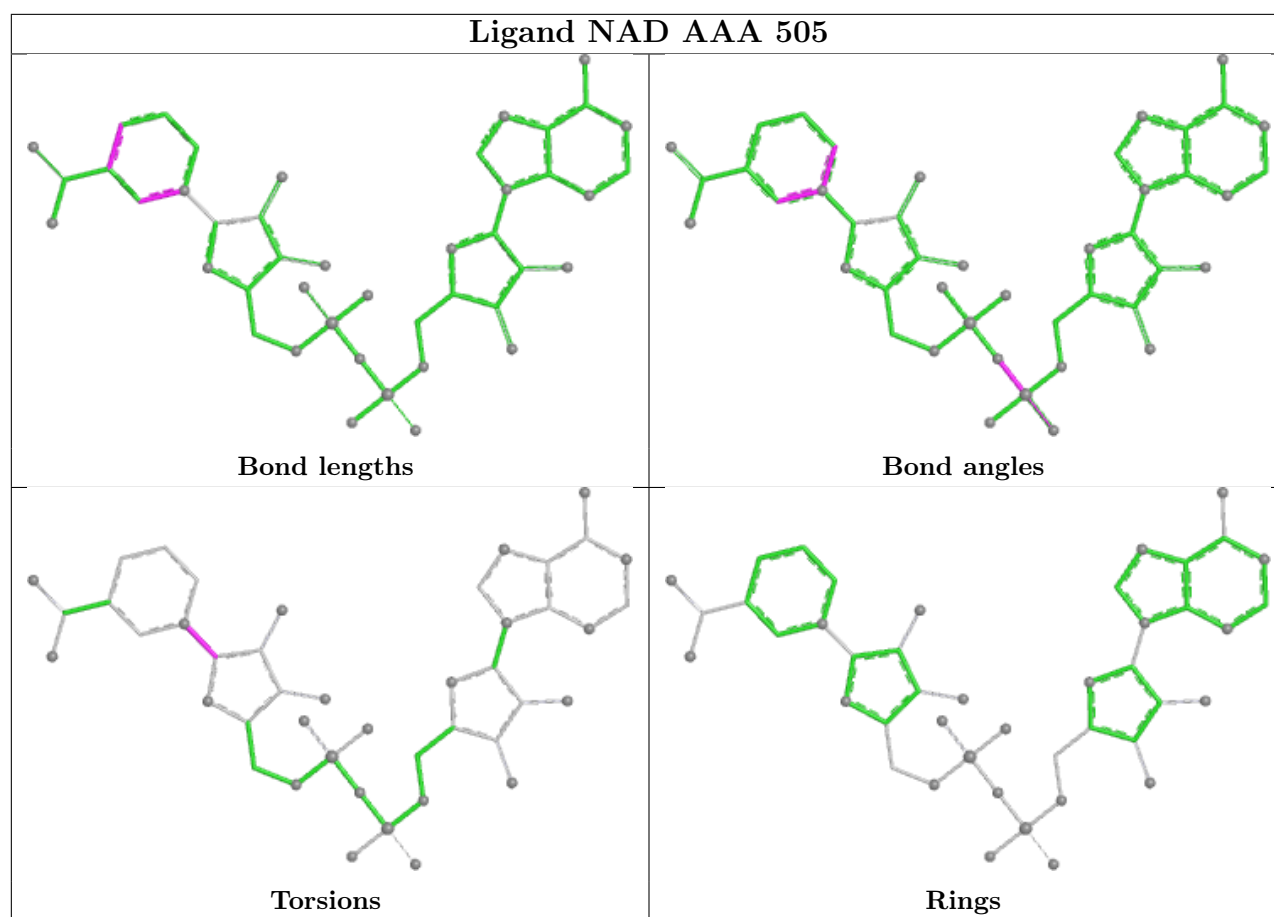
Ligand NAD DDD 405





Ligand NAD CCC 405





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	373/410 (90%)	0.08	6 (1%) 70 71	7, 14, 28, 84	30 (8%)
1	BBB	375/410 (91%)	0.22	13 (3%) 47 48	8, 15, 35, 95	28 (7%)
1	CCC	373/410 (90%)	0.58	40 (10%) 11 12	7, 16, 38, 100	36 (9%)
1	DDD	374/410 (91%)	0.23	12 (3%) 50 51	8, 15, 33, 84	28 (7%)
All	All	1495/1640 (91%)	0.28	71 (4%) 36 38	7, 15, 35, 100	122 (8%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	368	PRO	5.6
1	CCC	369	GLY	5.3
1	CCC	365	VAL	5.2
1	CCC	368	PRO	4.6
1	DDD	367	ILE	4.5
1	CCC	364	ASP	4.5
1	BBB	369	GLY	4.0
1	AAA	367	ILE	4.0
1	CCC	367	ILE	4.0
1	BBB	364	ASP	3.8
1	BBB	367	ILE	3.8
1	CCC	-3	ALA	3.8
1	CCC	303[A]	PHE	3.8
1	DDD	369	GLY	3.7
1	BBB	368	PRO	3.7
1	CCC	85[A]	LYS	3.7
1	CCC	86	LEU	3.7
1	CCC	5	LEU	3.6
1	DDD	-4	THR	3.5
1	CCC	3[A]	LYS	3.5
1	CCC	81	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	365	VAL	3.4
1	BBB	365	VAL	3.4
1	CCC	83	ALA	3.4
1	CCC	-1	LEU	3.3
1	CCC	1	MET	3.3
1	BBB	52[A]	GLY	3.3
1	DDD	303[A]	PHE	3.2
1	CCC	4	VAL	3.2
1	DDD	368	PRO	3.2
1	BBB	-4	THR	3.1
1	DDD	365	VAL	3.1
1	DDD	366	LYS	3.0
1	CCC	2	VAL	2.9
1	CCC	340	PHE	2.8
1	CCC	110	GLY	2.7
1	CCC	-2	ARG	2.7
1	BBB	111	ILE	2.7
1	BBB	-5	TYR	2.7
1	DDD	51[A]	GLU	2.7
1	CCC	336	LEU	2.7
1	BBB	363	GLU	2.6
1	AAA	-4	THR	2.6
1	CCC	52[A]	GLY	2.5
1	BBB	57[A]	ARG	2.5
1	AAA	-3	ALA	2.5
1	CCC	335	TYR	2.4
1	CCC	65	ILE	2.4
1	DDD	62	ALA	2.4
1	CCC	366	LYS	2.3
1	CCC	64	ILE	2.3
1	CCC	111	ILE	2.3
1	CCC	35	LEU	2.3
1	CCC	90	VAL	2.3
1	CCC	286	PHE	2.3
1	CCC	106[A]	LYS	2.3
1	CCC	39	GLY	2.3
1	BBB	81	ALA	2.2
1	CCC	332	LEU	2.2
1	DDD	-1	LEU	2.2
1	CCC	41[A]	THR	2.2
1	DDD	57[A]	ARG	2.2
1	CCC	328	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	364	ASP	2.1
1	BBB	17[A]	GLN	2.1
1	CCC	57[A]	ARG	2.1
1	CCC	77	ALA	2.1
1	CCC	7	VAL	2.1
1	CCC	342	TYR	2.0
1	CCC	350	HIS	2.0
1	DDD	364	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	CCC	402	7/7	0.84	0.16	39,41,58,58	1
5	EDO	CCC	406	4/4	0.85	0.15	24,28,35,35	10
5	EDO	AAA	507	4/4	0.86	0.15	39,39,44,44	1
5	EDO	AAA	510	4/4	0.87	0.12	30,33,39,39	1
5	EDO	AAA	508	4/4	0.87	0.12	22,33,38,38	1
5	EDO	AAA	509	4/4	0.88	0.11	23,23,36,36	1
5	EDO	BBB	1005	4/4	0.90	0.11	36,37,41,41	1
3	FMT	CCC	403	3/3	0.90	0.10	21,25,25,33	0
3	FMT	CCC	404	3/3	0.92	0.11	18,23,32,32	0
5	EDO	AAA	506	4/4	0.92	0.10	27,32,35,35	1
3	FMT	BBB	1002	3/3	0.92	0.09	21,26,26,30	0
2	PEG	BBB	1001	7/7	0.92	0.11	18,20,66,66	1
3	FMT	DDD	404	3/3	0.93	0.11	18,20,27,27	0
2	PEG	DDD	402	7/7	0.93	0.09	27,37,53,53	1
2	PEG	DDD	401	7/7	0.94	0.10	20,23,59,59	1

Continued on next page...

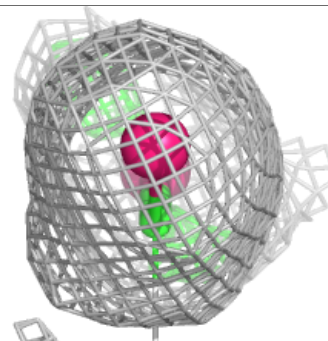
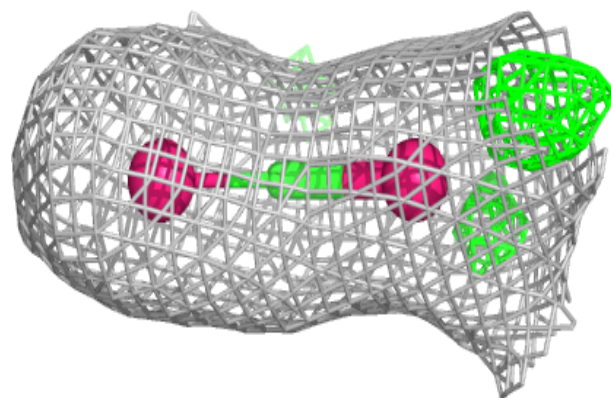
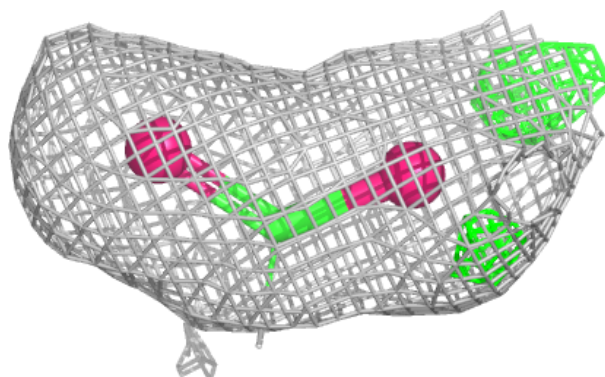
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	CCC	401	7/7	0.94	0.11	17,23,54,54	1
3	FMT	AAA	503	3/3	0.94	0.10	19,21,21,33	0
3	FMT	DDD	403	3/3	0.94	0.10	21,25,25,27	0
3	FMT	BBB	1003	3/3	0.95	0.11	18,20,31,31	0
2	PEG	AAA	502	7/7	0.95	0.08	26,30,40,40	1
3	FMT	AAA	504	3/3	0.96	0.07	14,18,21,21	0
2	PEG	AAA	501	7/7	0.96	0.09	18,21,50,50	1
4	NAD	BBB	1004	44/44	0.98	0.05	10,12,14,14	8
4	NAD	CCC	405	44/44	0.98	0.05	10,13,16,17	8
4	NAD	AAA	505	44/44	0.98	0.05	9,11,14,15	8
4	NAD	DDD	405	44/44	0.99	0.05	8,12,14,15	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.

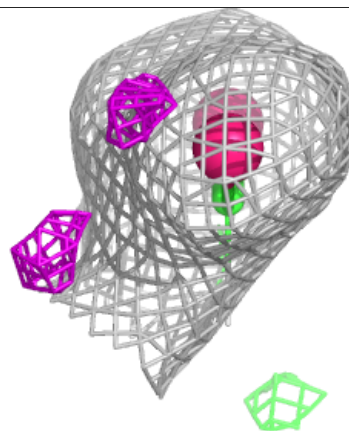
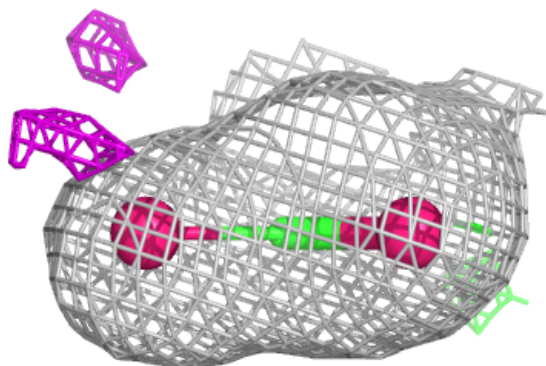
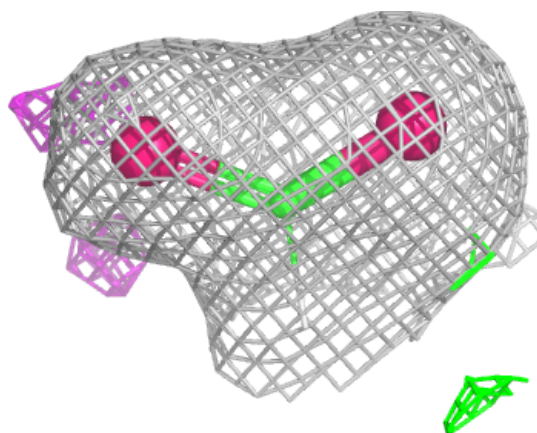
Electron density around FMT CCC 403:

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



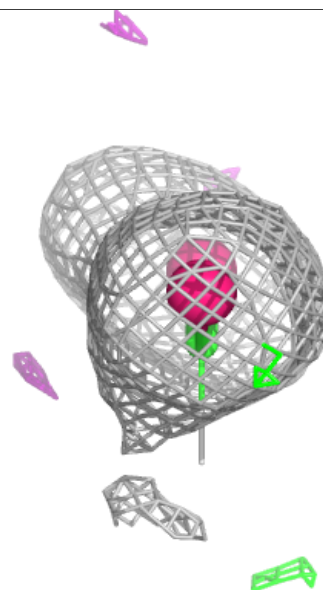
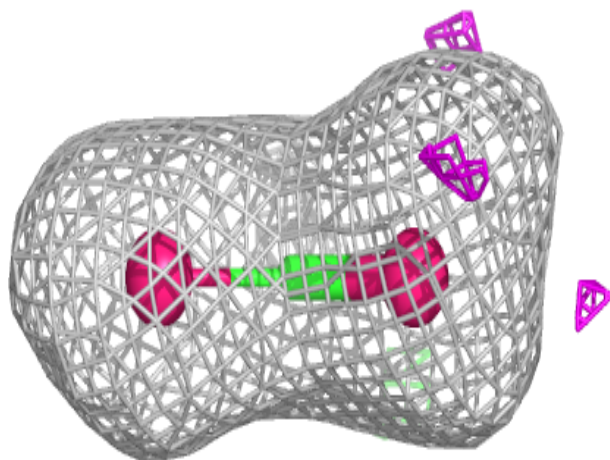
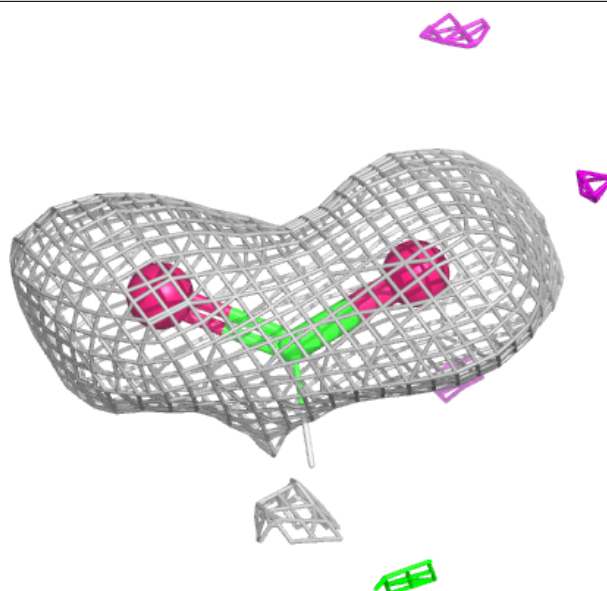
Electron density around FMT CCC 404:

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



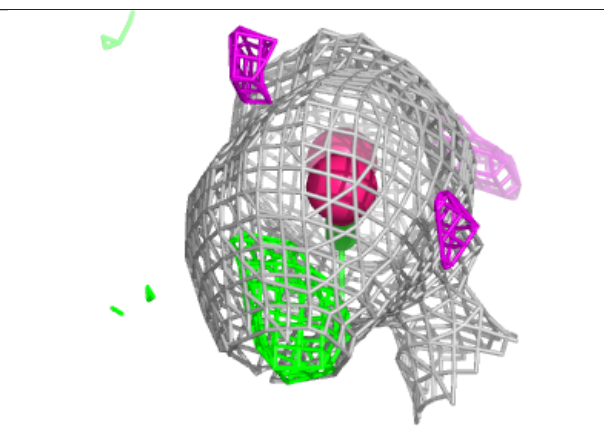
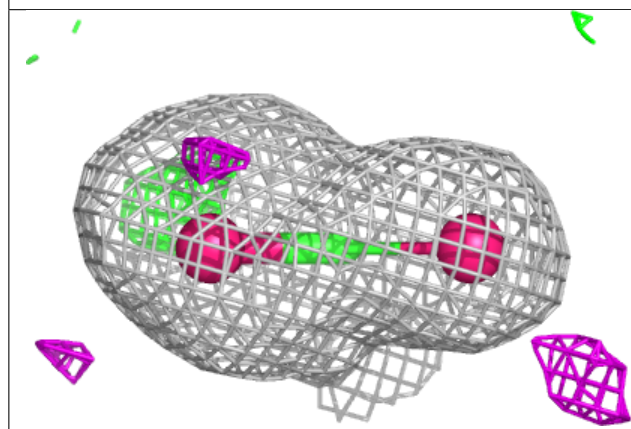
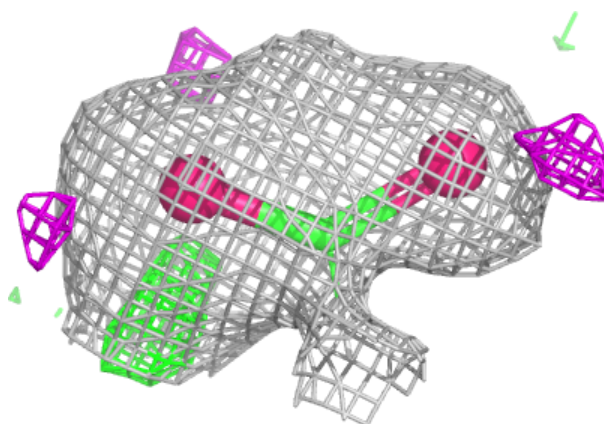
Electron density around FMT BBB 1002:

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

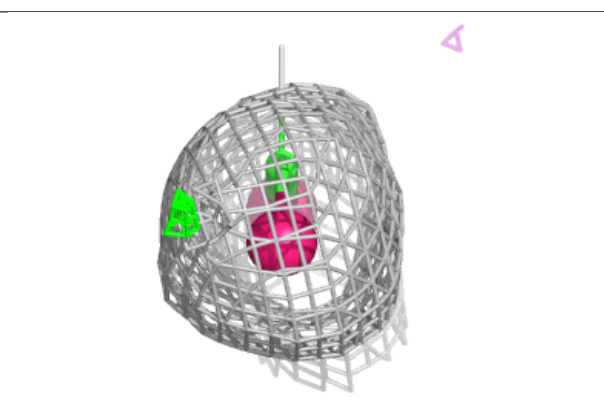
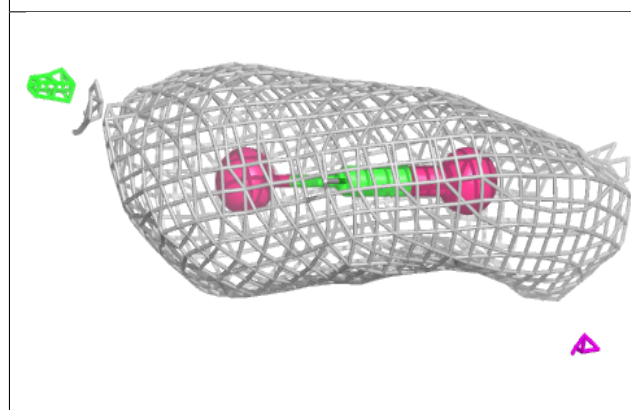
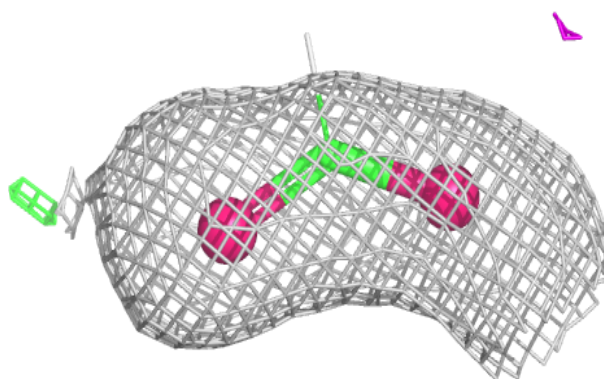


Electron density around FMT DDD 404:

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

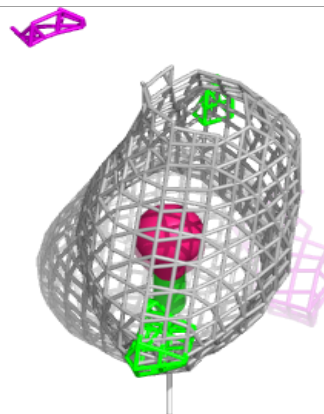
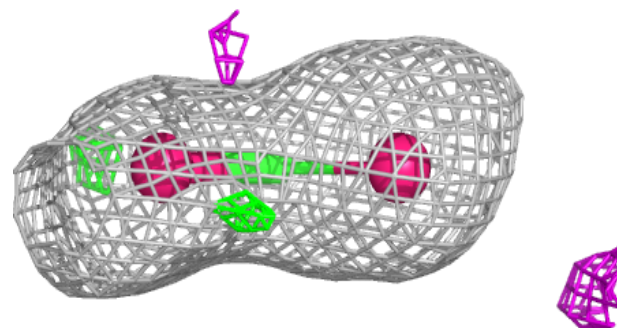
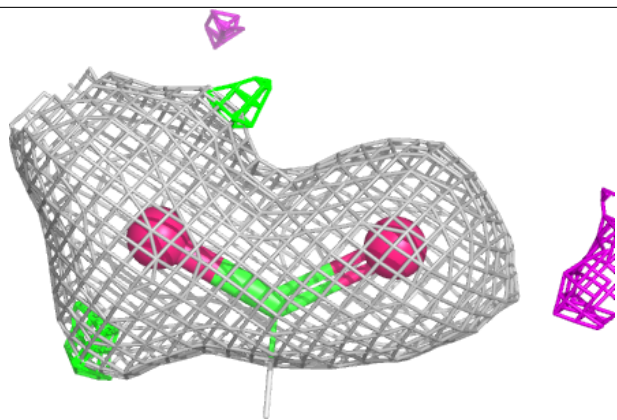
**Electron density around FMT AAA 503:**

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

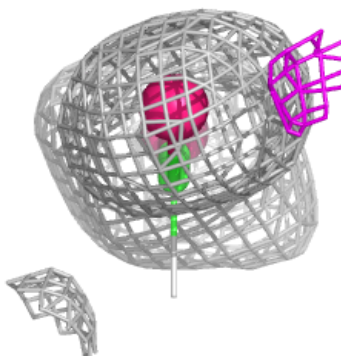
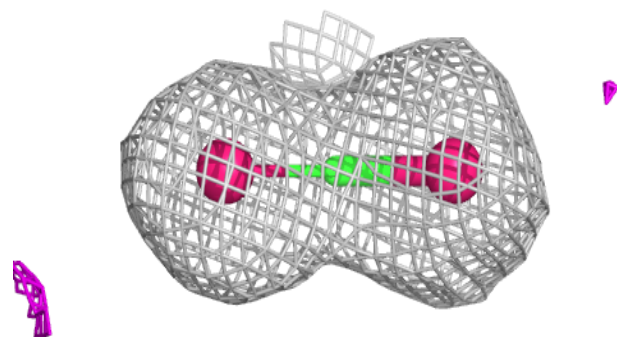
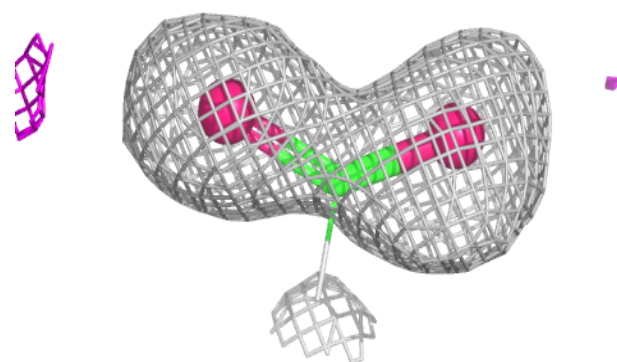


Electron density around FMT DDD 403:

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

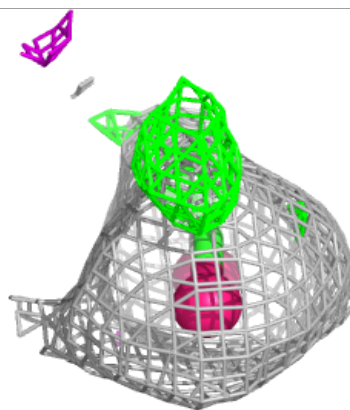
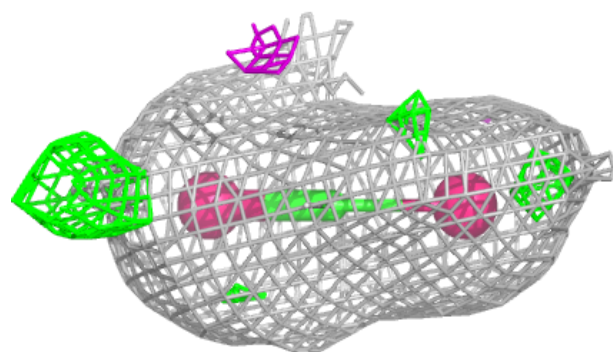
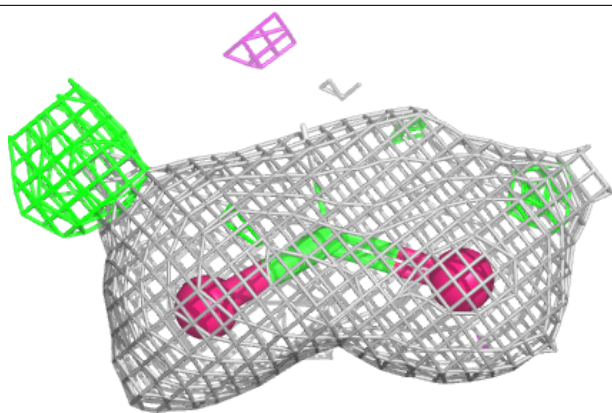
**Electron density around FMT BBB 1003:**

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

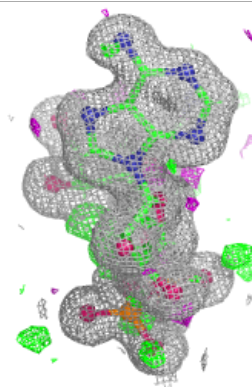
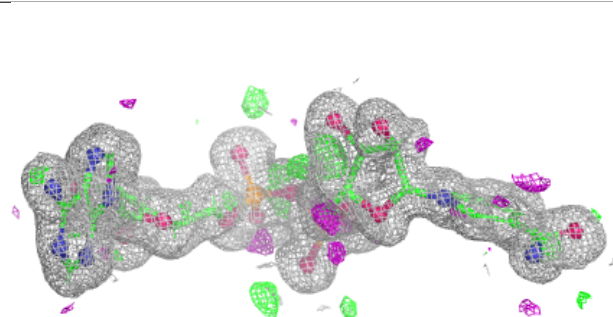
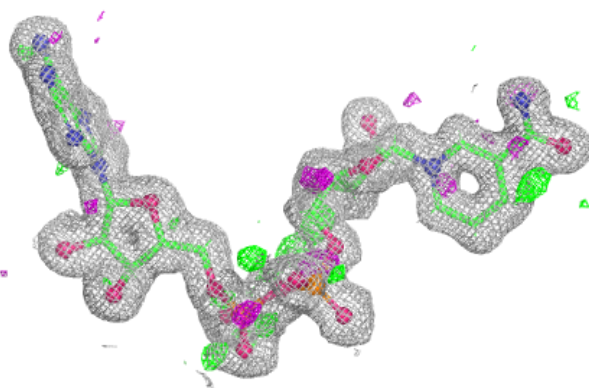


Electron density around FMT AAA 504:

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

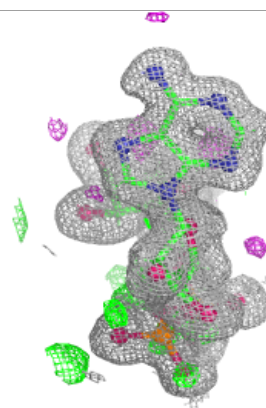
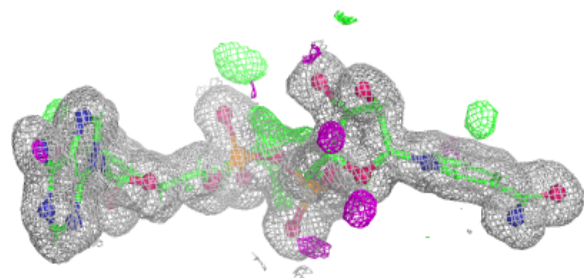
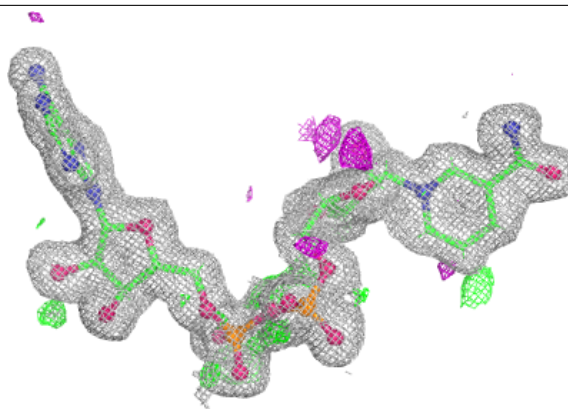
**Electron density around NAD BBB 1004:**

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

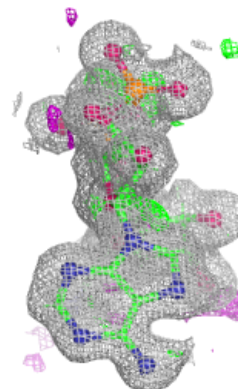
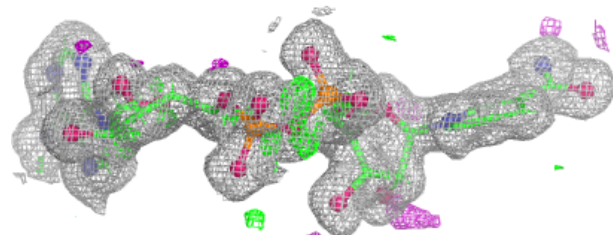
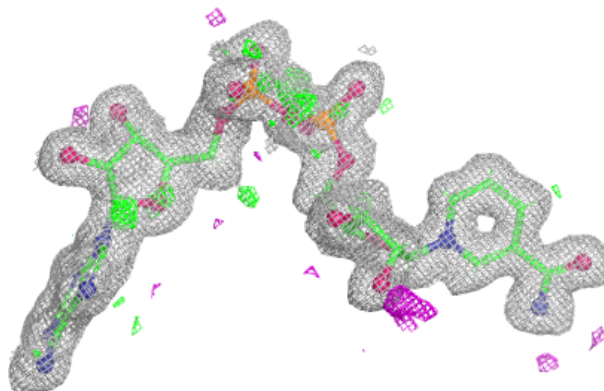


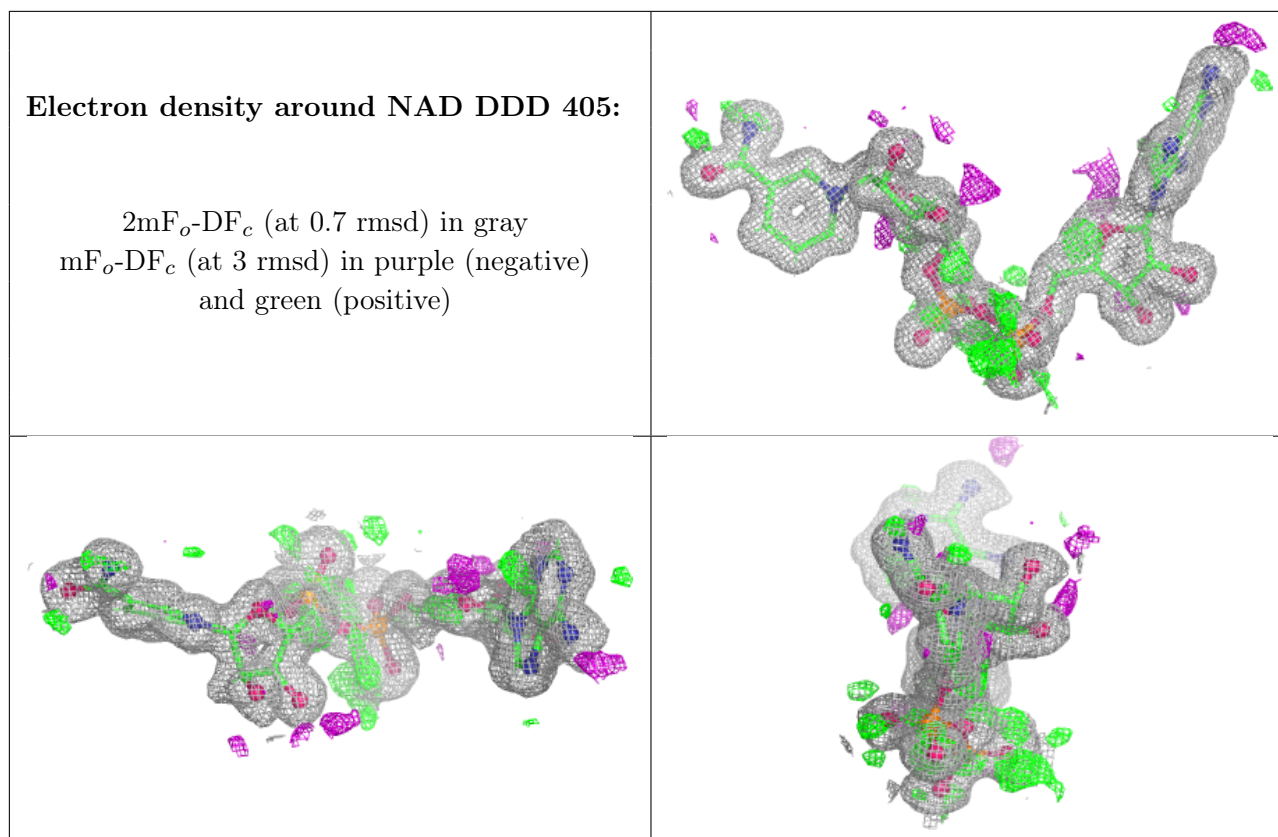
Electron density around NAD CCC 405:

$2mF_o-DF_c$ (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.