



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 02:09 PM EDT

PDB ID : 6T94  
Title : NAD<sup>+</sup>-dependent fungal formate dehydrogenase from *Chaetomium thermophilum*: A complex of N120C mutant protein with the reduced form of the cofactor NADH.  
Authors : Isupov, M.N.; Yelmazer, B.; De Rose, S.A.; Littlechild, J.A.  
Deposited on : 2019-10-25  
Resolution : 1.15 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

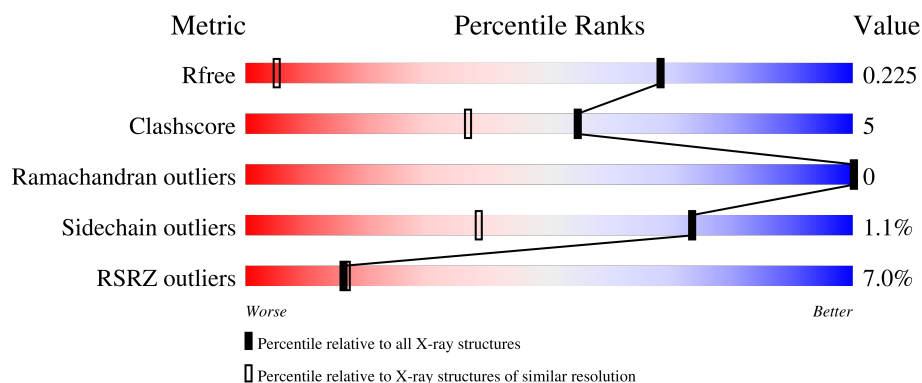
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 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	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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  $\geq 3$ , 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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <span style="flex-grow: 1; border-bottom: 1px solid black; position: relative;"> <span style="position: absolute; right: 0; top: -5px;">82%</span> <span style="position: absolute; left: 0; bottom: -5px;">7%</span> <span style="position: absolute; right: 0; bottom: -5px;">10%</span> </span> </div> </div>
1	BBB	410	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>10%</span> <span style="flex-grow: 1; border-bottom: 1px solid black; position: relative;"> <span style="position: absolute; right: 0; top: -5px;">83%</span> <span style="position: absolute; left: 0; bottom: -5px;">8%</span> <span style="position: absolute; right: 0; bottom: -5px;">9%</span> </span> </div> </div>
1	CCC	410	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>13%</span> <span style="flex-grow: 1; border-bottom: 1px solid black; position: relative;"> <span style="position: absolute; right: 0; top: -5px;">82%</span> <span style="position: absolute; left: 0; bottom: -5px;">8%</span> <span style="position: absolute; right: 0; bottom: -5px;">10%</span> </span> </div> </div>
1	DDD	410	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <span style="flex-grow: 1; border-bottom: 1px solid black; position: relative;"> <span style="position: absolute; right: 0; top: -5px;">82%</span> <span style="position: absolute; left: 0; bottom: -5px;">7%</span> <span style="position: absolute; right: 0; bottom: -5px;">10%</span> </span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27255 atoms, of which 12811 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	367	Total	C	H	N	O	S	119	33	0
			6210	1935	3148	547	566	14			
1	BBB	374	Total	C	H	N	O	S	119	34	0
			6312	1973	3195	549	582	13			
1	CCC	371	Total	C	H	N	O	S	115	31	0
			6259	1951	3177	550	569	12			
1	DDD	367	Total	C	H	N	O	S	120	28	0
			6104	1906	3085	536	563	14			

There are 164 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	120	CYS	ASN	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-11	PRO	-	expression tag	UNP G0SGU4
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	120	CYS	ASN	engineered mutation	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

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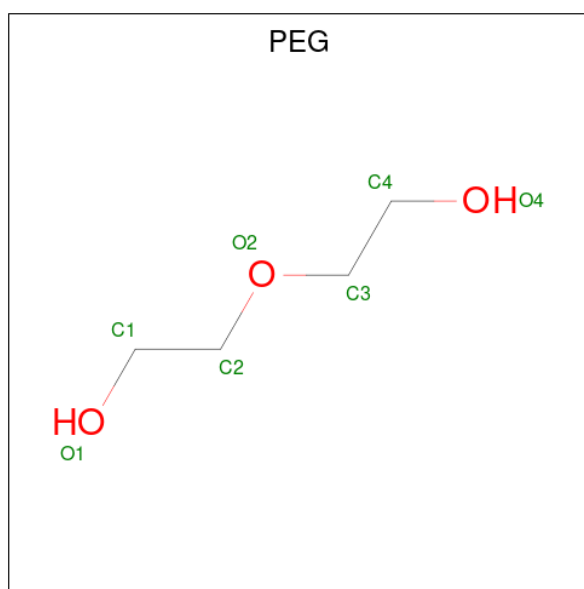
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-10	ASN	-	expression tag	UNP G0SGU4
CCC	-9	TRP	-	expression tag	UNP G0SGU4
CCC	-8	GLU	-	expression tag	UNP G0SGU4
CCC	-7	LEU	-	expression tag	UNP G0SGU4
CCC	-6	VAL	-	expression tag	UNP G0SGU4
CCC	-5	TYR	-	expression tag	UNP G0SGU4
CCC	-4	THR	-	expression 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	120	CYS	ASN	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-9	TRP	-	expression tag	UNP G0SGU4
DDD	-8	GLU	-	expression tag	UNP G0SGU4
DDD	-7	LEU	-	expression tag	UNP G0SGU4
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	120	CYS	ASN	engineered mutation	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>).



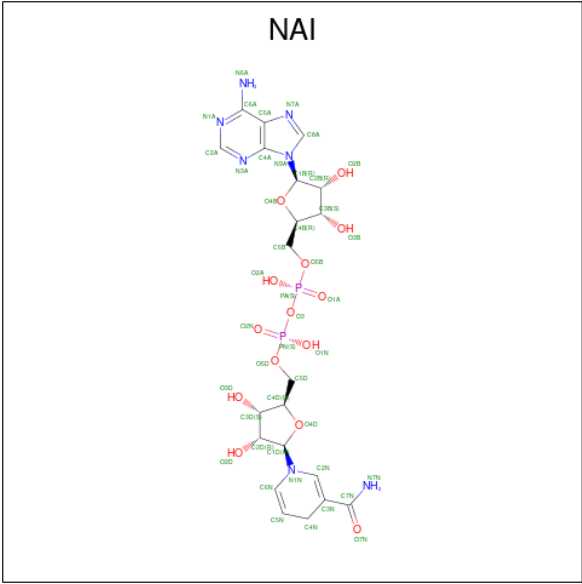
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		

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

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	AAA	1	71	21	27	7	14	4	0
			Total	C	H	N	O		
3	BBB	1	71	21	27	7	14	4	0
			Total	C	H	N	O		
3	CCC	1	71	21	27	7	14	4	0
			Total	C	H	N	O		
3	DDD	1	71	21	27	7	14	4	0
			Total	C	H	N	O		

- Molecule 4 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
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
4	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
4	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
4	DDD	1	Total	C	H	O	1	0
			10	2	6	2		

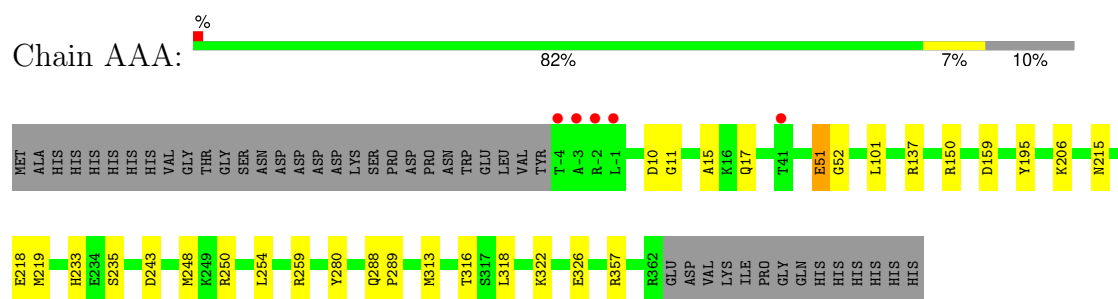
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	515	Total	O	0	0
			515	515		
5	BBB	454	Total	O	0	0
			454	454		
5	CCC	448	Total	O	0	0
			448	448		
5	DDD	504	Total	O	0	0
			504	504		

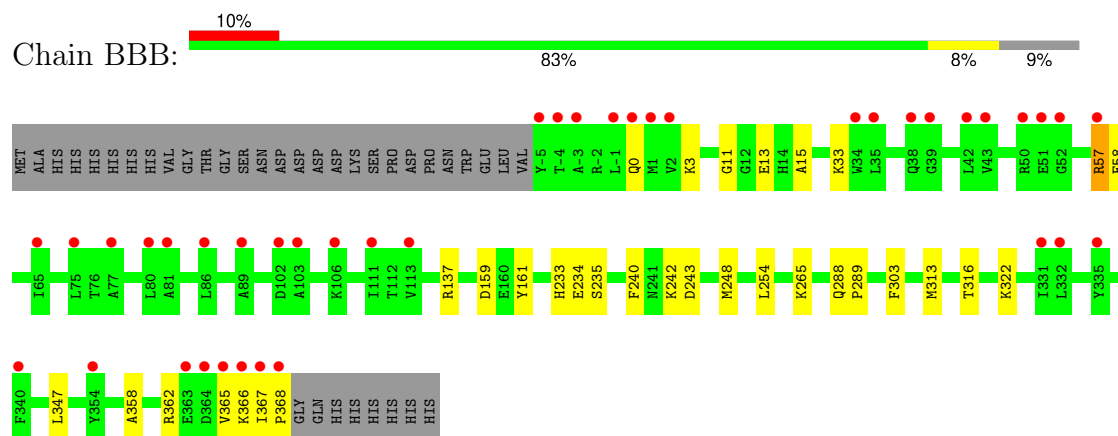
### 3 Residue-property plots [i](#)

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.

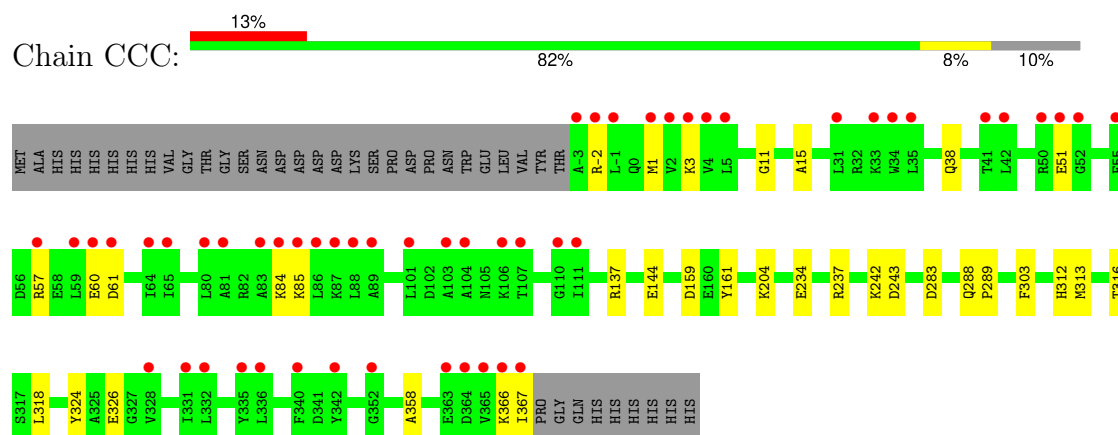
#### • Molecule 1: Formate dehydrogenase



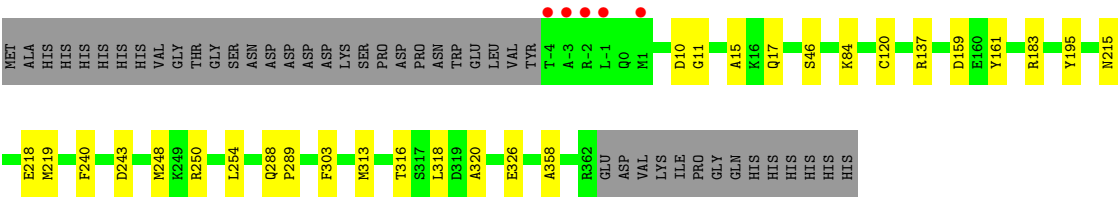
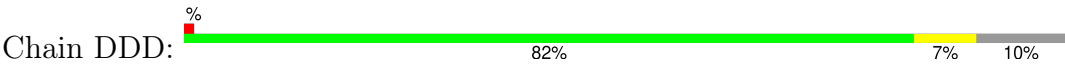
#### • Molecule 1: Formate dehydrogenase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	50.73Å 94.75Å 94.60Å 85.96° 89.97° 81.58°	Depositor
Resolution (Å)	68.90 – 1.15 68.91 – 1.15	Depositor EDS
% Data completeness (in resolution range)	86.8 (68.90-1.15) 86.8 (68.91-1.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.15Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.196 , 0.218 0.205 , 0.225	Depositor DCC
$R_{free}$ test set	26885 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	27255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.47% 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

### 5.1 Standard geometry

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

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	0/3198	0.89	3/4306 (0.1%)
1	BBB	0.74	0/3261	0.88	0/4395
1	CCC	0.78	1/3218 (0.0%)	0.92	1/4333 (0.0%)
1	DDD	0.81	0/3146	0.95	2/4241 (0.0%)
All	All	0.77	1/12823 (0.0%)	0.91	6/17275 (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	BBB	0	1
1	CCC	0	1
1	DDD	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	144	GLU	CD-OE2	-5.12	1.20	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	250	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	DDD	183	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	DDD	250	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	AAA	280	TYR	CB-CG-CD2	5.84	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	324	TYR	CB-CG-CD1	5.61	124.37	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	ARG	Sidechain
1	BBB	137	ARG	Sidechain
1	CCC	137	ARG	Sidechain
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	3062	3148	3163	33	0
1	BBB	3117	3195	3214	26	0
1	CCC	3082	3177	3194	41	0
1	DDD	3019	3085	3099	32	0
2	AAA	14	20	20	1	0
2	CCC	7	10	10	0	0
2	DDD	14	20	20	0	0
3	AAA	44	27	27	1	0
3	BBB	44	27	27	2	0
3	CCC	44	27	27	2	0
3	DDD	44	27	27	1	0
4	AAA	16	24	24	5	0
4	BBB	4	6	6	0	0
4	CCC	4	6	6	1	0
4	DDD	8	12	12	0	0
5	AAA	515	0	0	18	2
5	BBB	454	0	0	7	2
5	CCC	448	0	0	14	0
5	DDD	504	0	0	10	0
All	All	14444	12811	12876	133	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 133 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:150[A]:ARG:NH1	5:AAA:607:HOH:O	1.65	1.28
1:DDD:243[A]:ASP:OD1	5:DDD:502:HOH:O	1.73	1.07
1:BBB:13[B]:GLU:OE2	5:BBB:1006:HOH:O	1.74	1.05
1:CCC:3[A]:LYS:NZ	1:CCC:85[A]:LYS:HZ1	1.53	1.05
1:AAA:195:TYR:HB2	1:AAA:219[B]:MET:HE2	1.44	0.98

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:647:HOH:O	5:BBB:1387:HOH:O[1_455]	2.19	0.01
5:AAA:894:HOH:O	5:BBB:1074:HOH:O[1_455]	2.19	0.01

## 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	398/410 (97%)	388 (98%)	10 (2%)	0	100	100
1	BBB	406/410 (99%)	394 (97%)	12 (3%)	0	100	100
1	CCC	400/410 (98%)	389 (97%)	11 (3%)	0	100	100
1	DDD	393/410 (96%)	382 (97%)	11 (3%)	0	100	100
All	All	1597/1640 (97%)	1553 (97%)	44 (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	333/340 (98%)	329 (99%)	4 (1%)	71	35
1	BBB	341/340 (100%)	334 (98%)	7 (2%)	53	13
1	CCC	335/340 (98%)	328 (98%)	7 (2%)	53	13
1	DDD	328/340 (96%)	326 (99%)	2 (1%)	86	59
All	All	1337/1360 (98%)	1317 (98%)	20 (2%)	73	27

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	234[A]	GLU
1	CCC	367	ILE
1	DDD	159[B]	ASP
1	DDD	159[A]	ASP
1	BBB	57[B]	ARG

Sometimes 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

17 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	DDD	401	-	6,6,6	0.36	0	5,5,5	0.18	0
2	PEG	CCC	401	-	6,6,6	0.25	0	5,5,5	0.13	0
4	EDO	AAA	506	-	3,3,3	0.34	0	2,2,2	0.40	0
4	EDO	AAA	504	-	3,3,3	0.13	0	2,2,2	0.45	0
3	NAI	AAA	503	-	43,48,48	1.16	4 (9%)	50,73,73	1.55	10 (20%)
2	PEG	DDD	402	-	6,6,6	0.15	0	5,5,5	0.12	0
4	EDO	AAA	507	-	3,3,3	0.21	0	2,2,2	0.52	0
4	EDO	AAA	505	-	3,3,3	0.14	0	2,2,2	0.39	0
4	EDO	DDD	404	-	3,3,3	0.12	0	2,2,2	0.29	0
4	EDO	BBB	902	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PEG	AAA	502	-	6,6,6	0.22	0	5,5,5	0.11	0
4	EDO	CCC	403	-	3,3,3	0.14	0	2,2,2	0.72	0
2	PEG	AAA	501	-	6,6,6	0.21	0	5,5,5	0.13	0
3	NAI	BBB	901	-	43,48,48	1.14	3 (6%)	50,73,73	1.62	6 (12%)
4	EDO	DDD	405	-	3,3,3	0.44	0	2,2,2	0.57	0
3	NAI	CCC	402	-	43,48,48	1.36	4 (9%)	50,73,73	1.69	9 (18%)
3	NAI	DDD	403	-	43,48,48	1.71	5 (11%)	50,73,73	1.73	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	DDD	401	-	-	4/4/4/4	-
2	PEG	CCC	401	-	-	1/4/4/4	-
4	EDO	AAA	506	-	-	1/1/1/1	-
4	EDO	AAA	504	-	-	1/1/1/1	-
3	NAI	AAA	503	-	-	1/25/72/72	0/5/5/5
2	PEG	DDD	402	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	507	-	-	0/1/1/1	-
4	EDO	AAA	505	-	-	1/1/1/1	-
4	EDO	DDD	404	-	-	1/1/1/1	-
4	EDO	BBB	902	-	-	1/1/1/1	-
2	PEG	AAA	502	-	-	3/4/4/4	-
4	EDO	CCC	403	-	-	1/1/1/1	-
2	PEG	AAA	501	-	-	1/4/4/4	-
3	NAI	BBB	901	-	-	2/25/72/72	0/5/5/5
4	EDO	DDD	405	-	-	0/1/1/1	-
3	NAI	CCC	402	-	-	1/25/72/72	0/5/5/5
3	NAI	DDD	403	-	-	1/25/72/72	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	403	NAI	PN-O3	7.26	1.67	1.59
3	DDD	403	NAI	C2A-N1A	4.08	1.41	1.33
3	CCC	402	NAI	PN-O3	3.84	1.63	1.59
3	CCC	402	NAI	C4N-C5N	-3.48	1.40	1.49
3	DDD	403	NAI	O4B-C1B	3.24	1.45	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	403	NAI	N3A-C2A-N1A	-6.52	119.82	128.67
3	BBB	901	NAI	N3A-C2A-N1A	-6.02	120.50	128.67
3	AAA	503	NAI	N3A-C2A-N1A	-5.58	121.10	128.67
3	BBB	901	NAI	C4A-C5A-N7A	-5.30	103.74	109.34
3	DDD	403	NAI	C1B-N9A-C4A	-4.77	118.27	126.64

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	401	PEG	C1-C2-O2-C3
2	CCC	401	PEG	O1-C1-C2-O2
2	DDD	401	PEG	O1-C1-C2-O2
2	DDD	402	PEG	O2-C3-C4-O4
4	AAA	505	EDO	O1-C1-C2-O2

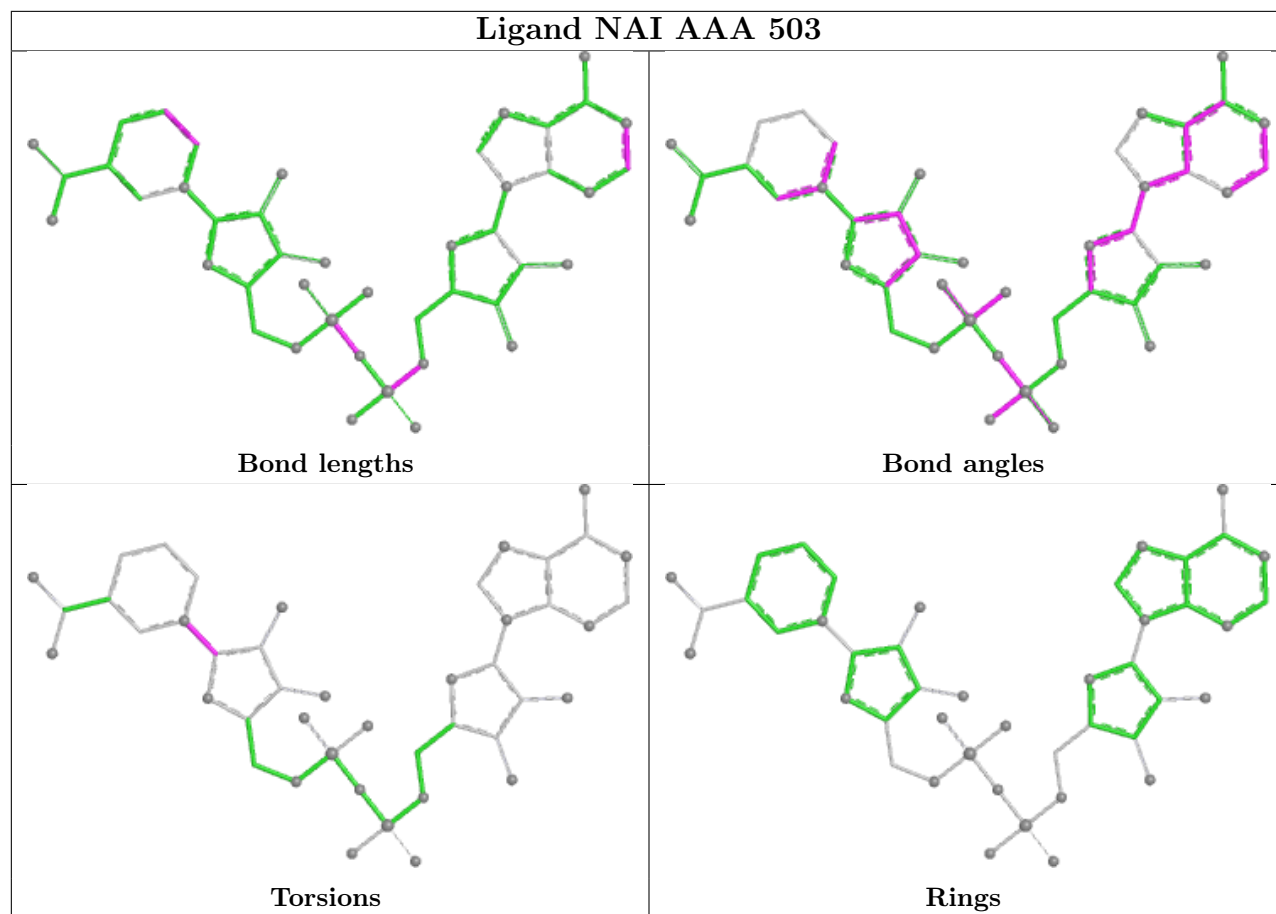
There are no ring outliers.

9 monomers are involved in 12 short contacts:

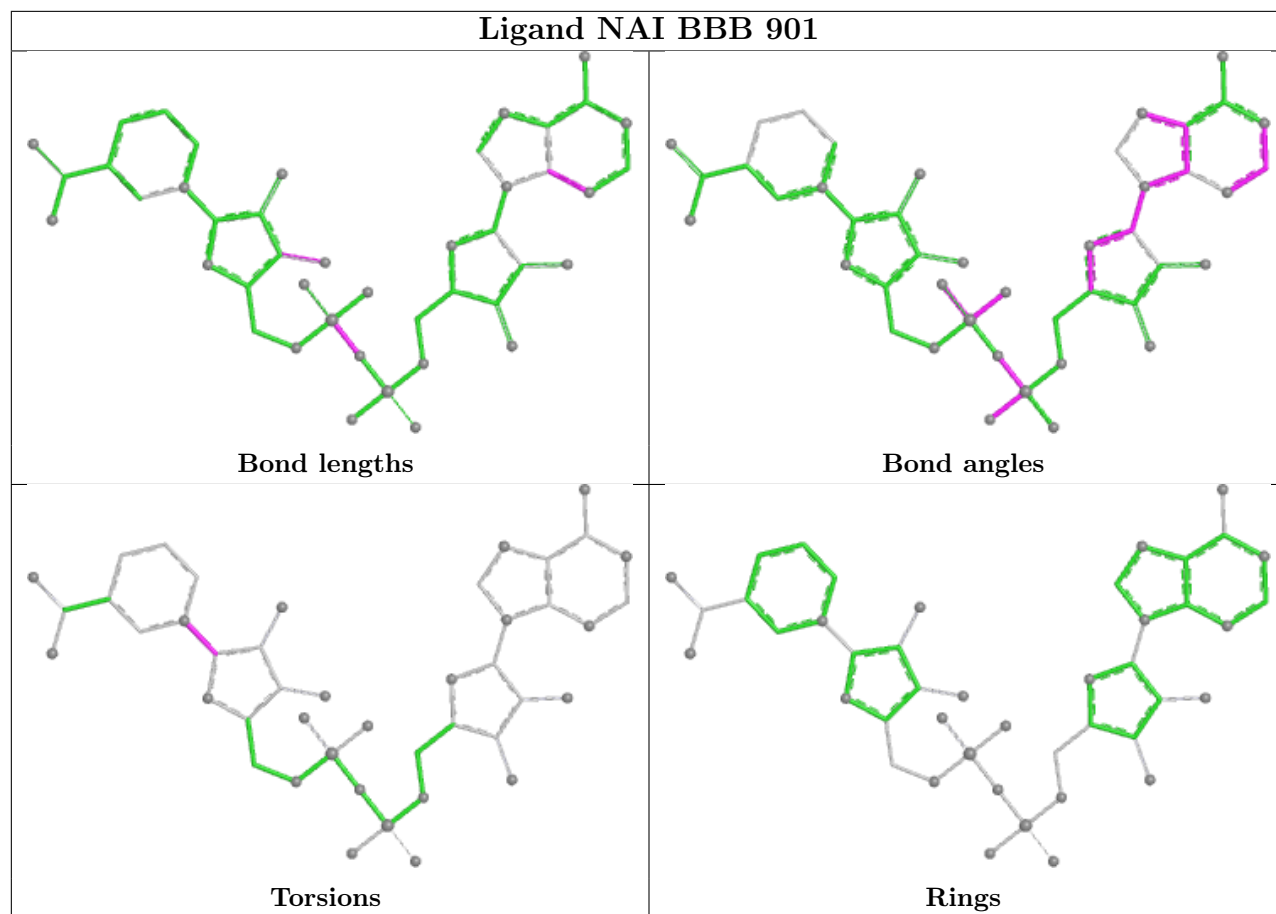
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	504	EDO	1	0
3	AAA	503	NAI	1	0
4	AAA	507	EDO	3	0
4	AAA	505	EDO	1	0
2	AAA	502	PEG	1	0
4	CCC	403	EDO	1	0
3	BBB	901	NAI	2	0
3	CCC	402	NAI	2	0
3	DDD	403	NAI	1	0

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

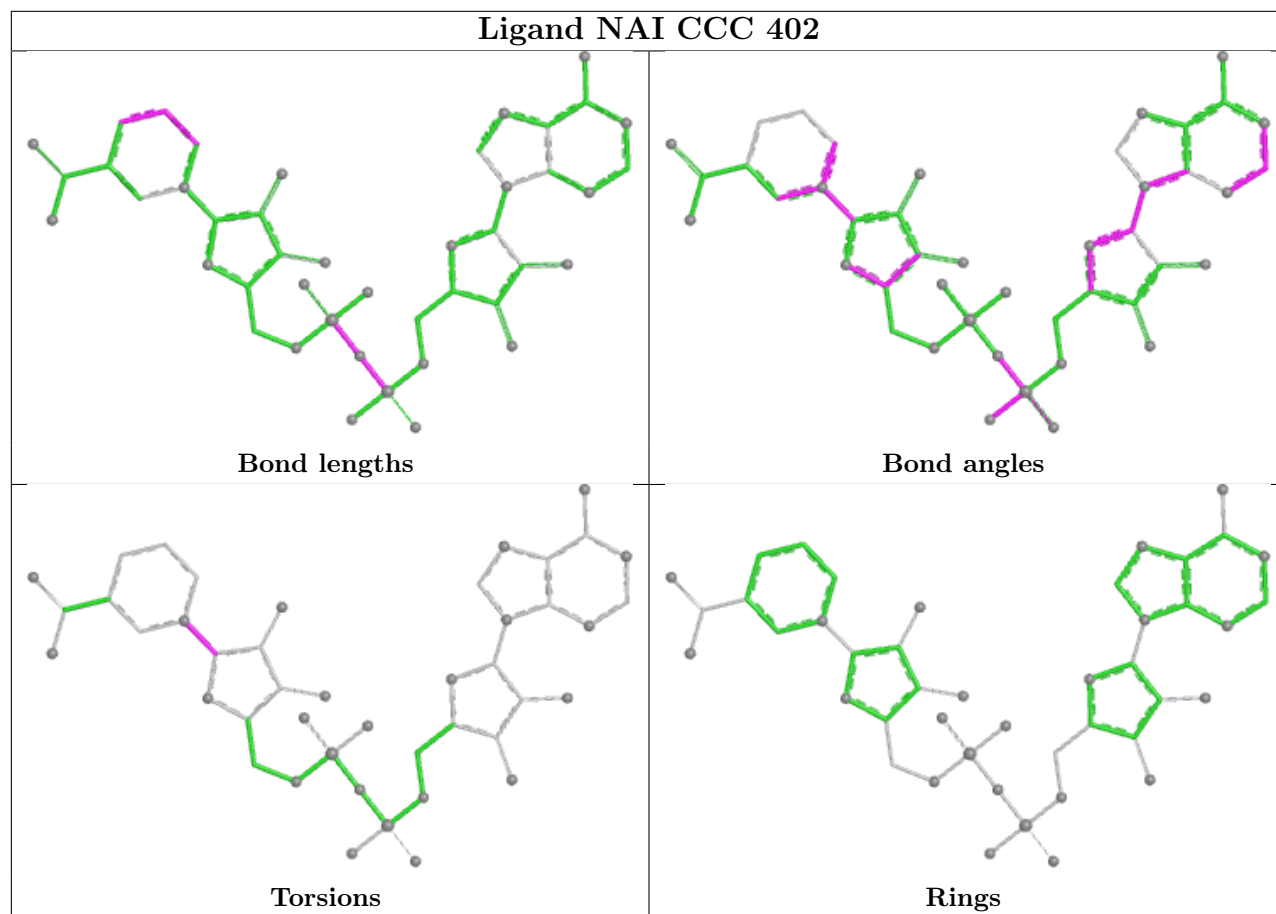
## Ligand NAI AAA 503

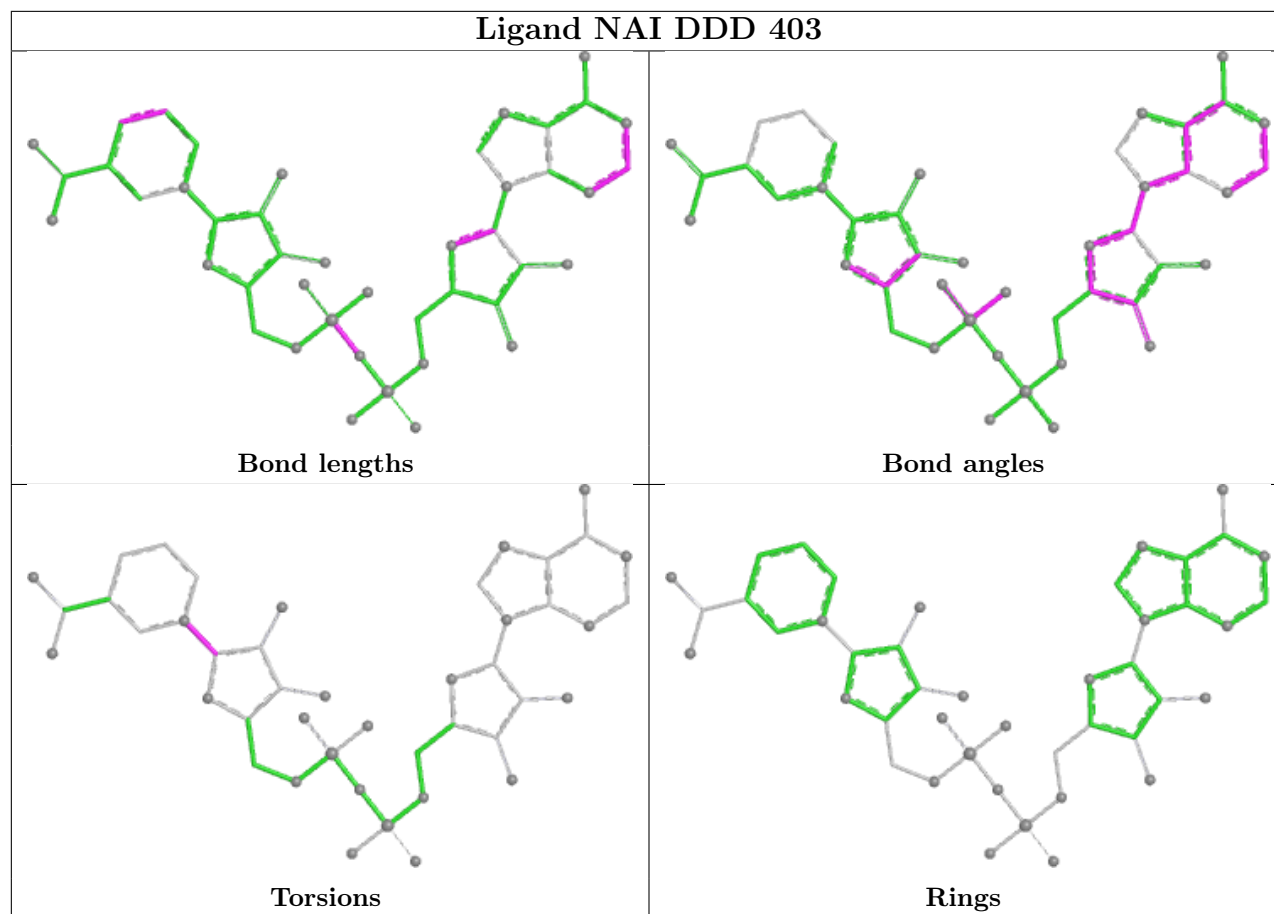


## Ligand NAI BBB 901



## Ligand NAI CCC 402





## 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	367/410 (89%)	-0.02	5 (1%) 75 73	10, 17, 33, 89	0
1	BBB	374/410 (91%)	0.45	40 (10%) 6 7	10, 20, 45, 109	0
1	CCC	371/410 (90%)	0.60	53 (14%) 2 4	9, 19, 45, 128	0
1	DDD	367/410 (89%)	0.08	5 (1%) 75 73	9, 16, 36, 77	0
All	All	1479/1640 (90%)	0.28	103 (6%) 16 17	9, 18, 41, 128	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	365	VAL	11.2
1	CCC	364	ASP	8.9
1	BBB	365	VAL	8.1
1	AAA	-4	THR	7.8
1	CCC	-1	LEU	7.5

### 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.

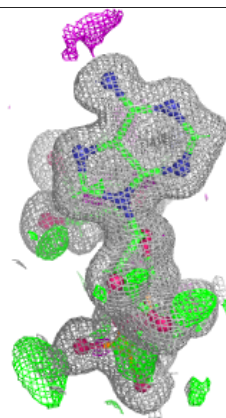
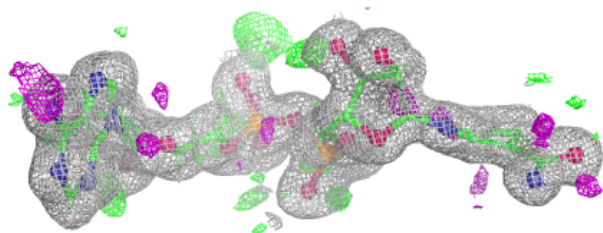
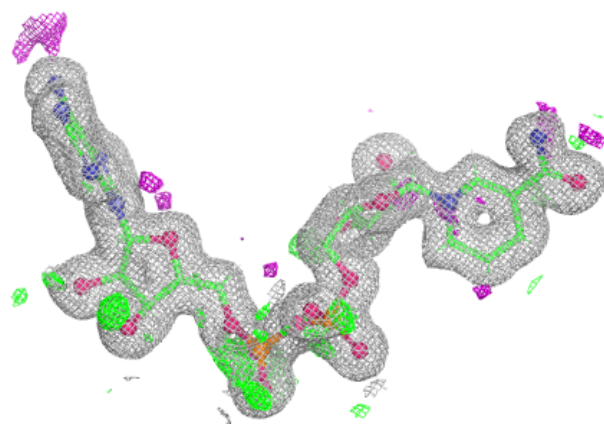


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	DDD	404	4/4	0.69	0.21	49,53,66,66	1
4	EDO	AAA	505	4/4	0.70	0.19	49,51,60,60	1
4	EDO	AAA	507	4/4	0.82	0.18	31,39,52,52	1
2	PEG	AAA	502	7/7	0.86	0.14	33,40,70,70	1
4	EDO	AAA	506	4/4	0.86	0.12	38,39,41,41	1
2	PEG	CCC	401	7/7	0.87	0.10	27,31,48,48	1
4	EDO	DDD	405	4/4	0.87	0.11	30,32,37,37	1
4	EDO	CCC	403	4/4	0.88	0.15	25,37,55,55	1
2	PEG	AAA	501	7/7	0.93	0.11	25,27,80,80	1
2	PEG	DDD	401	7/7	0.93	0.09	20,24,47,47	1
2	PEG	DDD	402	7/7	0.93	0.16	40,59,84,84	1
4	EDO	BBB	902	4/4	0.94	0.06	25,26,37,37	1
4	EDO	AAA	504	4/4	0.96	0.18	24,33,57,57	1
3	NAI	CCC	402	44/44	0.97	0.06	12,15,18,19	4
3	NAI	DDD	403	44/44	0.98	0.07	10,12,14,17	4
3	NAI	AAA	503	44/44	0.99	0.06	10,13,15,16	4
3	NAI	BBB	901	44/44	0.99	0.05	13,16,20,20	4

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.

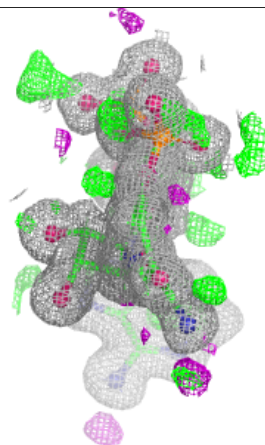
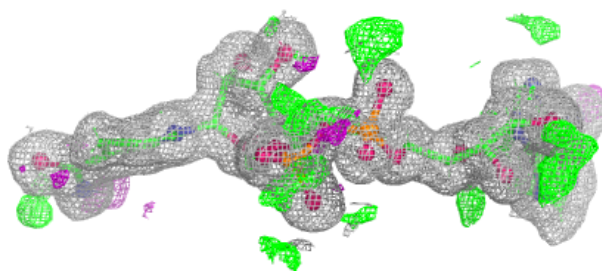
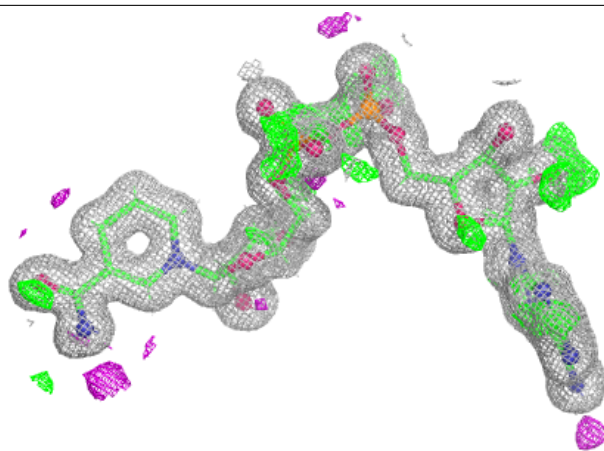
**Electron density around NAI CCC 402:**

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

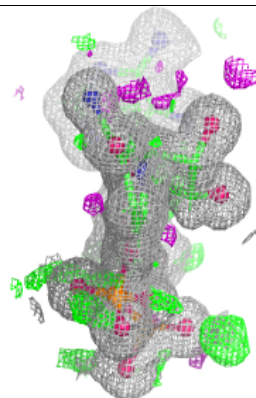
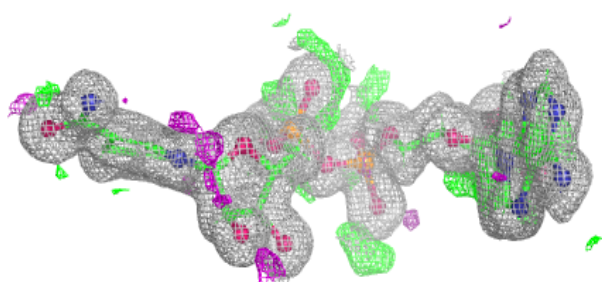
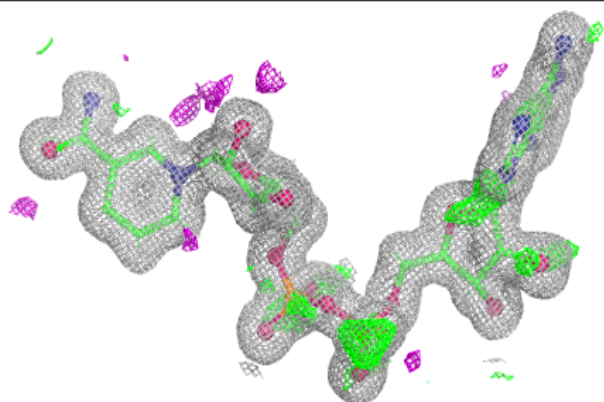


**Electron density around NAI DDD 403:**

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

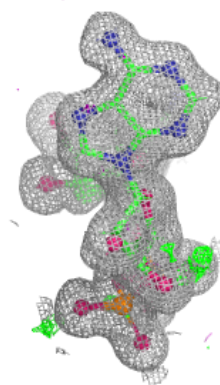
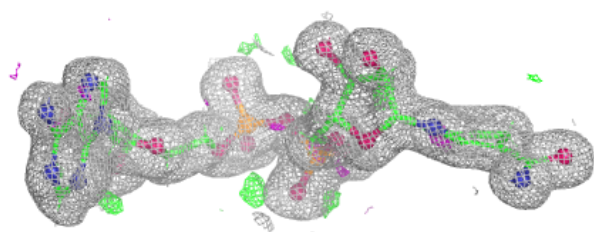
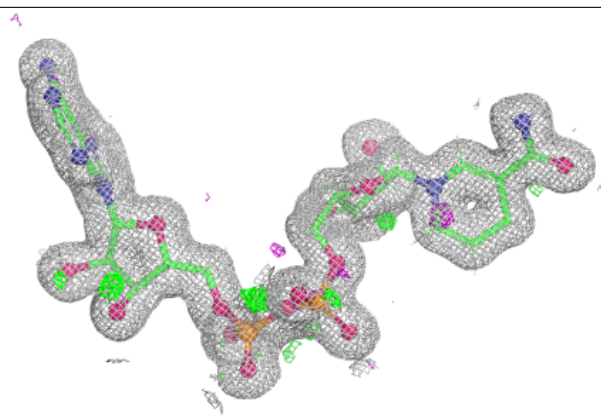
**Electron density around NAI AAA 503:**

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



**Electron density around NAI BBB 901:**

$2mF_o-DF_c$  (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.