



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2022 – 10:12 AM JST

PDB ID : 7X1L  
Title : Malate dehydrogenase from *Geobacillus stearothermophilus* (gs-MDH) delta E311 mutant complexed with Nicotinamide Adenine Dinucleotide (NAD<sup>+</sup>)  
Authors : Shimozawa, Y.; Himiyama, T.; Nakamura, T.; Nishiya, Y.  
Deposited on : 2022-02-24  
Resolution : 2.28 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](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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

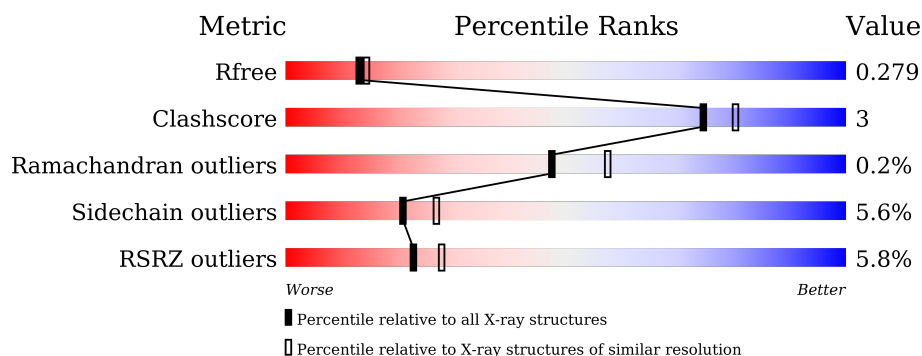
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	A	331	<div> <div>2%</div> <div>82% 11% 7%</div> </div>
1	B	331	<div> <div>3%</div> <div>82% 10% 8%</div> </div>
1	C	331	<div> <div>5%</div> <div>84% 8% 7%</div> </div>
1	D	331	<div> <div>6%</div> <div>81% 11% 7%</div> </div>
1	E	331	<div> <div>8%</div> <div>81% 10% 9%</div> </div>
1	F	331	<div> <div>7%</div> <div>77% 13% 9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2322	1480	384	449	9			
1	B	306	Total	C	N	O	S	0	0	0
			2314	1475	383	448	8			
1	E	300	Total	C	N	O	S	0	0	0
			2272	1450	373	441	8			
1	F	300	Total	C	N	O	S	0	0	0
			2268	1447	372	441	8			
1	C	307	Total	C	N	O	S	0	0	0
			2322	1480	384	449	9			
1	D	307	Total	C	N	O	S	0	0	0
			2322	1480	384	449	9			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A143T1U9
A	-19	GLY	-	expression tag	UNP A0A143T1U9
A	-18	SER	-	expression tag	UNP A0A143T1U9
A	-17	SER	-	expression tag	UNP A0A143T1U9
A	-16	HIS	-	expression tag	UNP A0A143T1U9
A	-15	HIS	-	expression tag	UNP A0A143T1U9
A	-14	HIS	-	expression tag	UNP A0A143T1U9
A	-13	HIS	-	expression tag	UNP A0A143T1U9
A	-12	HIS	-	expression tag	UNP A0A143T1U9
A	-11	HIS	-	expression tag	UNP A0A143T1U9
A	-10	SER	-	expression tag	UNP A0A143T1U9
A	-9	SER	-	expression tag	UNP A0A143T1U9
A	-8	GLY	-	expression tag	UNP A0A143T1U9
A	-7	LEU	-	expression tag	UNP A0A143T1U9
A	-6	VAL	-	expression tag	UNP A0A143T1U9
A	-5	PRO	-	expression tag	UNP A0A143T1U9
A	-4	ARG	-	expression tag	UNP A0A143T1U9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A143T1U9
A	-2	SER	-	expression tag	UNP A0A143T1U9
A	-1	HIS	-	expression tag	UNP A0A143T1U9
B	-20	MET	-	initiating methionine	UNP A0A143T1U9
B	-19	GLY	-	expression tag	UNP A0A143T1U9
B	-18	SER	-	expression tag	UNP A0A143T1U9
B	-17	SER	-	expression tag	UNP A0A143T1U9
B	-16	HIS	-	expression tag	UNP A0A143T1U9
B	-15	HIS	-	expression tag	UNP A0A143T1U9
B	-14	HIS	-	expression tag	UNP A0A143T1U9
B	-13	HIS	-	expression tag	UNP A0A143T1U9
B	-12	HIS	-	expression tag	UNP A0A143T1U9
B	-11	HIS	-	expression tag	UNP A0A143T1U9
B	-10	SER	-	expression tag	UNP A0A143T1U9
B	-9	SER	-	expression tag	UNP A0A143T1U9
B	-8	GLY	-	expression tag	UNP A0A143T1U9
B	-7	LEU	-	expression tag	UNP A0A143T1U9
B	-6	VAL	-	expression tag	UNP A0A143T1U9
B	-5	PRO	-	expression tag	UNP A0A143T1U9
B	-4	ARG	-	expression tag	UNP A0A143T1U9
B	-3	GLY	-	expression tag	UNP A0A143T1U9
B	-2	SER	-	expression tag	UNP A0A143T1U9
B	-1	HIS	-	expression tag	UNP A0A143T1U9
E	-20	MET	-	initiating methionine	UNP A0A143T1U9
E	-19	GLY	-	expression tag	UNP A0A143T1U9
E	-18	SER	-	expression tag	UNP A0A143T1U9
E	-17	SER	-	expression tag	UNP A0A143T1U9
E	-16	HIS	-	expression tag	UNP A0A143T1U9
E	-15	HIS	-	expression tag	UNP A0A143T1U9
E	-14	HIS	-	expression tag	UNP A0A143T1U9
E	-13	HIS	-	expression tag	UNP A0A143T1U9
E	-12	HIS	-	expression tag	UNP A0A143T1U9
E	-11	HIS	-	expression tag	UNP A0A143T1U9
E	-10	SER	-	expression tag	UNP A0A143T1U9
E	-9	SER	-	expression tag	UNP A0A143T1U9
E	-8	GLY	-	expression tag	UNP A0A143T1U9
E	-7	LEU	-	expression tag	UNP A0A143T1U9
E	-6	VAL	-	expression tag	UNP A0A143T1U9
E	-5	PRO	-	expression tag	UNP A0A143T1U9
E	-4	ARG	-	expression tag	UNP A0A143T1U9
E	-3	GLY	-	expression tag	UNP A0A143T1U9
E	-2	SER	-	expression tag	UNP A0A143T1U9

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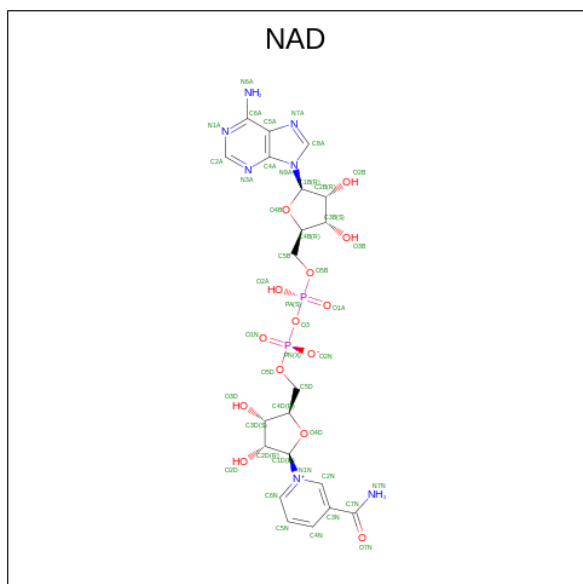
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	HIS	-	expression tag	UNP A0A143T1U9
F	-20	MET	-	initiating methionine	UNP A0A143T1U9
F	-19	GLY	-	expression tag	UNP A0A143T1U9
F	-18	SER	-	expression tag	UNP A0A143T1U9
F	-17	SER	-	expression tag	UNP A0A143T1U9
F	-16	HIS	-	expression tag	UNP A0A143T1U9
F	-15	HIS	-	expression tag	UNP A0A143T1U9
F	-14	HIS	-	expression tag	UNP A0A143T1U9
F	-13	HIS	-	expression tag	UNP A0A143T1U9
F	-12	HIS	-	expression tag	UNP A0A143T1U9
F	-11	HIS	-	expression tag	UNP A0A143T1U9
F	-10	SER	-	expression tag	UNP A0A143T1U9
F	-9	SER	-	expression tag	UNP A0A143T1U9
F	-8	GLY	-	expression tag	UNP A0A143T1U9
F	-7	LEU	-	expression tag	UNP A0A143T1U9
F	-6	VAL	-	expression tag	UNP A0A143T1U9
F	-5	PRO	-	expression tag	UNP A0A143T1U9
F	-4	ARG	-	expression tag	UNP A0A143T1U9
F	-3	GLY	-	expression tag	UNP A0A143T1U9
F	-2	SER	-	expression tag	UNP A0A143T1U9
F	-1	HIS	-	expression tag	UNP A0A143T1U9
C	-20	MET	-	initiating methionine	UNP A0A143T1U9
C	-19	GLY	-	expression tag	UNP A0A143T1U9
C	-18	SER	-	expression tag	UNP A0A143T1U9
C	-17	SER	-	expression tag	UNP A0A143T1U9
C	-16	HIS	-	expression tag	UNP A0A143T1U9
C	-15	HIS	-	expression tag	UNP A0A143T1U9
C	-14	HIS	-	expression tag	UNP A0A143T1U9
C	-13	HIS	-	expression tag	UNP A0A143T1U9
C	-12	HIS	-	expression tag	UNP A0A143T1U9
C	-11	HIS	-	expression tag	UNP A0A143T1U9
C	-10	SER	-	expression tag	UNP A0A143T1U9
C	-9	SER	-	expression tag	UNP A0A143T1U9
C	-8	GLY	-	expression tag	UNP A0A143T1U9
C	-7	LEU	-	expression tag	UNP A0A143T1U9
C	-6	VAL	-	expression tag	UNP A0A143T1U9
C	-5	PRO	-	expression tag	UNP A0A143T1U9
C	-4	ARG	-	expression tag	UNP A0A143T1U9
C	-3	GLY	-	expression tag	UNP A0A143T1U9
C	-2	SER	-	expression tag	UNP A0A143T1U9
C	-1	HIS	-	expression tag	UNP A0A143T1U9
D	-20	MET	-	initiating methionine	UNP A0A143T1U9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	GLY	-	expression tag	UNP A0A143T1U9
D	-18	SER	-	expression tag	UNP A0A143T1U9
D	-17	SER	-	expression tag	UNP A0A143T1U9
D	-16	HIS	-	expression tag	UNP A0A143T1U9
D	-15	HIS	-	expression tag	UNP A0A143T1U9
D	-14	HIS	-	expression tag	UNP A0A143T1U9
D	-13	HIS	-	expression tag	UNP A0A143T1U9
D	-12	HIS	-	expression tag	UNP A0A143T1U9
D	-11	HIS	-	expression tag	UNP A0A143T1U9
D	-10	SER	-	expression tag	UNP A0A143T1U9
D	-9	SER	-	expression tag	UNP A0A143T1U9
D	-8	GLY	-	expression tag	UNP A0A143T1U9
D	-7	LEU	-	expression tag	UNP A0A143T1U9
D	-6	VAL	-	expression tag	UNP A0A143T1U9
D	-5	PRO	-	expression tag	UNP A0A143T1U9
D	-4	ARG	-	expression tag	UNP A0A143T1U9
D	-3	GLY	-	expression tag	UNP A0A143T1U9
D	-2	SER	-	expression tag	UNP A0A143T1U9
D	-1	HIS	-	expression tag	UNP A0A143T1U9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

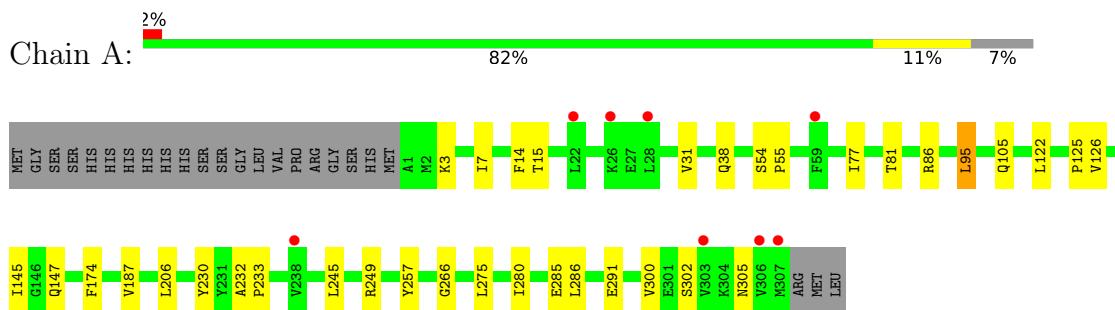
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	45	Total	O	0	0
			45	45		
3	E	11	Total	O	0	0
			11	11		
3	F	7	Total	O	0	0
			7	7		
3	C	34	Total	O	0	0
			34	34		
3	D	27	Total	O	0	0
			27	27		

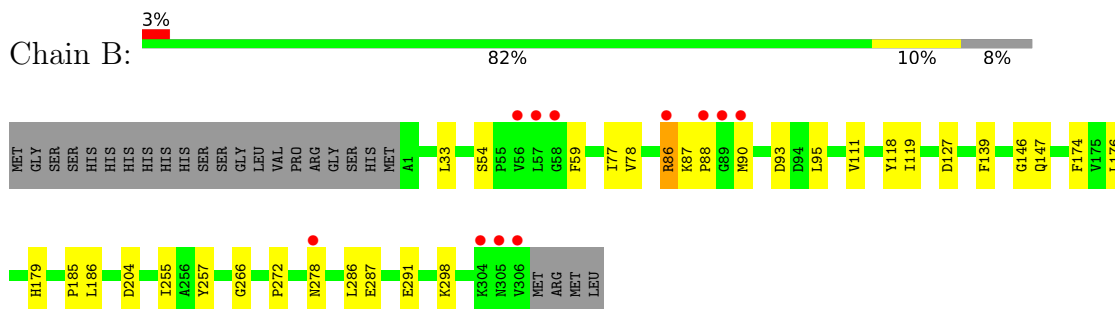
### 3 Residue-property plots [i](#)

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.

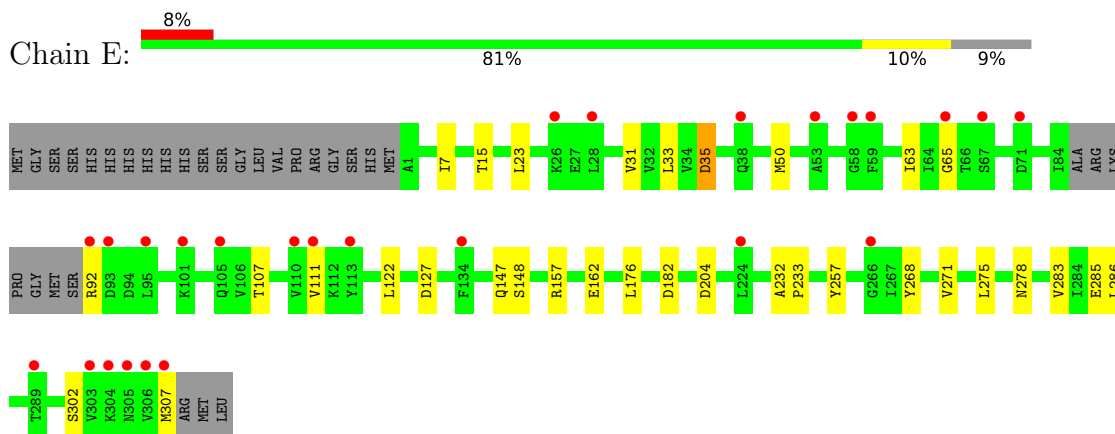
- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.85Å 82.72Å 136.70Å 90.00° 98.59° 90.00°	Depositor
Resolution (Å)	48.63 – 2.28 48.63 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.63-2.28) 99.8 (48.63-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.233 , 0.280 0.236 , 0.279	Depositor DCC
$R_{free}$ test set	6081 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.70	0/2355	0.85	0/3188
1	B	0.72	0/2347	0.81	0/3178
1	C	0.74	0/2355	0.85	0/3188
1	D	0.74	0/2355	0.82	0/3188
1	E	0.71	0/2303	0.83	0/3118
1	F	0.71	0/2299	0.82	0/3112
All	All	0.72	0/14014	0.83	0/18972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2322	0	2396	20	0
1	B	2314	0	2387	12	0
1	C	2322	0	2396	11	0
1	D	2322	0	2396	14	0
1	E	2272	0	2340	16	0
1	F	2268	0	2335	18	0
2	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	1	0
2	F	44	0	26	3	0
3	A	57	0	0	1	0
3	B	45	0	0	0	0
3	C	34	0	0	1	0
3	D	27	0	0	0	0
3	E	11	0	0	3	0
3	F	7	0	0	0	0
All	All	14265	0	14406	90	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 3.

All (90) 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:E:157:ARG:CZ	3:E:501:HOH:O	2.25	0.83
1:E:15:THR:HG21	1:E:122:LEU:CD2	2.10	0.81
1:F:122:LEU:HD22	2:F:400:NAD:H71N	1.50	0.76
1:C:15:THR:HG21	1:C:122:LEU:CD2	2.17	0.75
1:D:15:THR:HG21	1:D:122:LEU:CD2	2.23	0.68
1:E:15:THR:HG21	1:E:122:LEU:HD22	1.77	0.66
1:D:15:THR:HG21	1:D:122:LEU:HD22	1.79	0.65
1:E:35:ASP:OD1	2:E:400:NAD:H1B	1.97	0.62
1:E:157:ARG:NH1	3:E:501:HOH:O	2.30	0.61
1:B:146:GLY:HA3	1:B:255:ILE:HB	1.84	0.60
1:E:182:ASP:OD1	1:E:302:SER:OG	2.11	0.60
1:A:15:THR:HG21	1:A:122:LEU:CD2	2.32	0.59
1:A:15:THR:HG21	1:A:122:LEU:HD22	1.85	0.59
1:A:105:GLN:OE1	2:A:400:NAD:N6A	2.36	0.58
1:C:72:THR:OG1	3:C:501:HOH:O	2.16	0.58
1:B:179:HIS:NE2	2:B:400:NAD:N7N	2.51	0.58
1:B:176:LEU:CD2	1:B:272:PRO:HD3	2.34	0.58
1:E:15:THR:HG21	1:E:122:LEU:HD21	1.88	0.56
1:A:95:LEU:HD13	1:A:125:PRO:HD3	1.88	0.55
1:A:81:THR:O	2:A:400:NAD:H51N	2.06	0.55
1:A:145:ILE:HG12	1:A:280:ILE:CD1	2.38	0.53
1:B:87:LYS:HB3	1:B:88:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:THR:HB	1:F:136:GLU:HG2	1.90	0.53
1:C:153:THR:O	1:C:157:ARG:HG3	2.08	0.53
1:A:187:VAL:HG11	1:A:206:LEU:HD21	1.91	0.52
1:C:15:THR:HG21	1:C:122:LEU:HD21	1.90	0.52
1:A:54:SER:OG	1:A:55:PRO:HD3	2.10	0.52
1:F:183:MET:O	1:F:214:ARG:NH1	2.42	0.51
1:F:23:LEU:HD23	1:F:28:LEU:HD12	1.92	0.50
1:D:50:MET:O	1:D:53:ALA:HB3	2.11	0.50
1:E:157:ARG:NE	3:E:501:HOH:O	2.41	0.50
1:E:271:VAL:HG21	1:E:283:VAL:HG13	1.92	0.50
1:F:15:THR:HG21	1:F:122:LEU:CD1	2.43	0.49
1:C:54:SER:OG	1:C:55:PRO:HD3	2.13	0.49
1:A:14:PHE:HB3	1:A:230:TYR:CG	2.47	0.49
1:F:300:VAL:O	1:F:303:VAL:HG12	2.12	0.49
1:A:232:ALA:HB3	1:A:233:PRO:HD3	1.93	0.49
1:E:7:ILE:HG21	1:E:23:LEU:HD13	1.95	0.47
1:F:15:THR:HG21	1:F:122:LEU:HD12	1.96	0.47
1:A:126:VAL:HG12	3:A:530:HOH:O	2.15	0.46
1:A:187:VAL:CG1	1:A:206:LEU:HD21	2.46	0.46
1:D:54:SER:OG	1:D:55:PRO:HD3	2.16	0.46
1:F:69:TYR:CD1	1:F:109:GLU:HB2	2.50	0.46
1:A:257:TYR:CZ	1:A:266:GLY:HA2	2.51	0.46
1:A:77:ILE:HG13	1:A:245:LEU:HD21	1.96	0.45
1:F:230:TYR:C	1:F:233:PRO:HD2	2.37	0.45
1:B:174:PHE:CE1	1:B:286:LEU:HD11	2.51	0.45
1:C:15:THR:HG21	1:C:122:LEU:HD22	1.97	0.45
1:A:174:PHE:CZ	1:A:286:LEU:HD11	2.52	0.45
1:B:185:PRO:O	1:B:186:LEU:HD12	2.18	0.44
1:C:77:ILE:HG13	1:C:245:LEU:HD21	2.00	0.44
1:E:232:ALA:N	1:E:233:PRO:CD	2.81	0.43
1:B:78:VAL:O	1:B:119:ILE:HA	2.18	0.43
1:D:103:MET:HA	1:D:103:MET:CE	2.49	0.43
1:D:272:PRO:HB2	1:D:284:ILE:HB	2.00	0.43
1:A:257:TYR:OH	1:A:266:GLY:HA2	2.18	0.43
1:D:11:GLY:O	1:D:16:GLY:HA3	2.18	0.43
1:B:111:VAL:HG12	1:B:139:PHE:CZ	2.54	0.43
1:F:111:VAL:HG11	1:F:137:SER:HA	2.00	0.43
1:E:33:LEU:O	1:E:65:GLY:HA2	2.19	0.43
1:D:103:MET:HA	1:D:103:MET:HE2	2.00	0.43
1:B:174:PHE:CZ	1:B:286:LEU:HD11	2.55	0.42
1:F:48:LEU:O	1:F:52:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLU:OE2	1:D:56:VAL:HG13	2.19	0.42
1:F:186:LEU:HD12	1:F:186:LEU:N	2.35	0.42
1:B:54:SER:HB2	1:B:59:PHE:O	2.19	0.42
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.94	0.42
1:C:41:ASN:HB2	1:C:42:PRO:HD3	2.02	0.42
1:D:291:GLU:H	1:D:291:GLU:CD	2.22	0.42
1:E:257:TYR:HB2	1:E:268:TYR:CZ	2.55	0.42
1:F:122:LEU:HD22	2:F:400:NAD:N7N	2.25	0.42
1:A:174:PHE:HZ	1:A:286:LEU:HD11	1.84	0.41
1:F:72:THR:O	1:F:114:SER:OG	2.38	0.41
1:F:122:LEU:O	2:F:400:NAD:H2N	2.21	0.41
1:C:174:PHE:CZ	1:C:286:LEU:HD11	2.55	0.41
1:D:232:ALA:HB3	1:D:233:PRO:HD3	2.01	0.41
1:E:50:MET:HB3	1:E:63:ILE:HD13	2.03	0.41
1:C:296:LEU:O	1:C:300:VAL:HG23	2.21	0.41
1:D:54:SER:HB3	1:D:59:PHE:CE1	2.55	0.41
1:D:269:LEU:HD21	1:D:296:LEU:HD11	2.03	0.41
1:B:257:TYR:CZ	1:B:266:GLY:HA2	2.56	0.40
1:E:107:THR:O	1:E:111:VAL:HG13	2.22	0.40
1:F:192:ALA:HB3	1:F:200:LEU:CD1	2.51	0.40
1:F:206:LEU:O	1:F:210:VAL:HG23	2.21	0.40
1:D:14:PHE:HB3	1:D:230:TYR:CG	2.57	0.40
1:A:7:ILE:O	1:A:31:VAL:HA	2.21	0.40
1:A:300:VAL:C	1:A:302:SER:H	2.25	0.40
1:B:77:ILE:HA	1:B:118:TYR:O	2.21	0.40
1:E:7:ILE:O	1:E:31:VAL:HA	2.21	0.40
1:F:258:LEU:HD11	1:F:269:LEU:HB3	2.04	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	A	305/331 (92%)	298 (98%)	7 (2%)	0	100	100
1	B	304/331 (92%)	296 (97%)	7 (2%)	1 (0%)	41	49
1	C	305/331 (92%)	290 (95%)	14 (5%)	1 (0%)	41	49
1	D	305/331 (92%)	294 (96%)	10 (3%)	1 (0%)	41	49
1	E	296/331 (89%)	290 (98%)	5 (2%)	1 (0%)	41	49
1	F	296/331 (89%)	282 (95%)	14 (5%)	0	100	100
All	All	1811/1986 (91%)	1750 (97%)	57 (3%)	4 (0%)	47	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	ARG
1	E	148	SER
1	C	139	PHE
1	D	148	SER

### 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	A	250/271 (92%)	241 (96%)	9 (4%)	35	47
1	B	249/271 (92%)	237 (95%)	12 (5%)	25	34
1	C	250/271 (92%)	238 (95%)	12 (5%)	25	34
1	D	250/271 (92%)	232 (93%)	18 (7%)	14	17
1	E	245/271 (90%)	233 (95%)	12 (5%)	25	33
1	F	244/271 (90%)	224 (92%)	20 (8%)	11	13
All	All	1488/1626 (92%)	1405 (94%)	83 (6%)	21	27

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	86	ARG
1	A	95	LEU
1	A	147	GLN
1	A	249	ARG
1	A	285	GLU
1	A	291	GLU
1	A	305	ASN
1	B	33	LEU
1	B	86	ARG
1	B	90	MET
1	B	93	ASP
1	B	95	LEU
1	B	127	ASP
1	B	147	GLN
1	B	204	ASP
1	B	278	ASN
1	B	287	GLU
1	B	291	GLU
1	B	298	LYS
1	E	35	ASP
1	E	92	ARG
1	E	127	ASP
1	E	147	GLN
1	E	162	GLU
1	E	176	LEU
1	E	204	ASP
1	E	275	LEU
1	E	278	ASN
1	E	285	GLU
1	E	286	LEU
1	E	307	MET
1	F	3	LYS
1	F	38	GLN
1	F	62	ASN
1	F	92	ARG
1	F	100	GLN
1	F	122	LEU
1	F	127	ASP
1	F	131	TYR
1	F	141	LYS
1	F	145	ILE

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Mol	Chain	Res	Type
1	F	147	GLN
1	F	162	GLU
1	F	172	THR
1	F	176	LEU
1	F	182	ASP
1	F	187	VAL
1	F	265	GLU
1	F	286	LEU
1	F	291	GLU
1	F	303	VAL
1	C	77	ILE
1	C	87	LYS
1	C	92	ARG
1	C	95	LEU
1	C	97	THR
1	C	105	GLN
1	C	127	ASP
1	C	135	LYS
1	C	141	LYS
1	C	187	VAL
1	C	285	GLU
1	C	287	GLU
1	D	3	LYS
1	D	38	GLN
1	D	84	ILE
1	D	87	LYS
1	D	92	ARG
1	D	108	LYS
1	D	126	VAL
1	D	135	LYS
1	D	141	LYS
1	D	172	THR
1	D	175	VAL
1	D	204	ASP
1	D	226	ASN
1	D	228	SER
1	D	286	LEU
1	D	291	GLU
1	D	298	LYS
1	D	306	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	E	226	ASN
1	D	38	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	NAD	B	400	-	42,48,48	0.92	2 (4%)	50,73,73	1.03	5 (10%)
2	NAD	F	400	-	42,48,48	0.75	1 (2%)	50,73,73	0.90	4 (8%)
2	NAD	A	400	-	42,48,48	0.93	2 (4%)	50,73,73	0.99	4 (8%)
2	NAD	C	400	-	42,48,48	0.74	1 (2%)	50,73,73	0.98	2 (4%)
2	NAD	E	400	-	42,48,48	0.71	1 (2%)	50,73,73	0.96	4 (8%)
2	NAD	D	400	-	42,48,48	0.90	1 (2%)	50,73,73	0.91	3 (6%)

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	NAD	B	400	-	-	2/26/62/62	0/5/5/5
2	NAD	F	400	-	-	6/26/62/62	0/5/5/5
2	NAD	A	400	-	-	7/26/62/62	0/5/5/5
2	NAD	C	400	-	-	2/26/62/62	0/5/5/5
2	NAD	E	400	-	-	2/26/62/62	0/5/5/5
2	NAD	D	400	-	-	2/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NAD	C2N-N1N	4.39	1.40	1.35
2	D	400	NAD	C2N-N1N	4.21	1.40	1.35
2	B	400	NAD	C2N-N1N	3.84	1.39	1.35
2	E	400	NAD	C2N-N1N	3.00	1.38	1.35
2	F	400	NAD	C2N-N1N	2.99	1.38	1.35
2	C	400	NAD	C2N-N1N	2.66	1.38	1.35
2	B	400	NAD	C8A-N7A	-2.22	1.30	1.34
2	A	400	NAD	O4D-C1D	2.05	1.43	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAD	C6N-N1N-C2N	-4.32	118.04	121.97
2	D	400	NAD	C6N-N1N-C2N	-3.80	118.51	121.97
2	B	400	NAD	C6N-N1N-C2N	-3.47	118.81	121.97
2	F	400	NAD	C6N-N1N-C2N	-3.40	118.87	121.97
2	E	400	NAD	C6N-N1N-C2N	-3.24	119.02	121.97
2	C	400	NAD	O4D-C1D-C2D	-3.11	102.38	106.93
2	E	400	NAD	C5A-C6A-N6A	2.85	124.69	120.35
2	A	400	NAD	O4B-C1B-C2B	-2.85	102.76	106.93
2	B	400	NAD	O4B-C1B-C2B	-2.84	102.77	106.93
2	C	400	NAD	C6N-N1N-C2N	-2.76	119.46	121.97
2	E	400	NAD	O4D-C1D-C2D	-2.62	103.10	106.93
2	A	400	NAD	C3D-C2D-C1D	2.58	104.86	100.98
2	D	400	NAD	O4B-C1B-C2B	-2.29	103.58	106.93
2	E	400	NAD	O4B-C1B-C2B	-2.15	103.78	106.93
2	D	400	NAD	C5A-C6A-N6A	2.15	123.61	120.35
2	F	400	NAD	O4B-C1B-C2B	-2.12	103.83	106.93
2	B	400	NAD	C5A-C6A-N6A	2.10	123.54	120.35
2	B	400	NAD	O4D-C1D-C2D	-2.08	103.88	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	NAD	C5A-C6A-N6A	2.08	123.52	120.35
2	F	400	NAD	O4D-C1D-C2D	-2.05	103.93	106.93
2	A	400	NAD	C5A-C6A-N6A	2.03	123.44	120.35
2	B	400	NAD	C3N-C7N-N7N	-2.01	115.33	117.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	NAD	O4D-C1D-N1N-C6N
2	E	400	NAD	O4D-C1D-N1N-C6N
2	F	400	NAD	O4D-C1D-N1N-C2N
2	F	400	NAD	O4D-C1D-N1N-C6N
2	F	400	NAD	C2D-C1D-N1N-C2N
2	F	400	NAD	C2D-C1D-N1N-C6N
2	C	400	NAD	O4D-C1D-N1N-C6N
2	D	400	NAD	O4D-C1D-N1N-C6N
2	A	400	NAD	C2N-C3N-C7N-O7N
2	A	400	NAD	C4N-C3N-C7N-O7N
2	A	400	NAD	C4N-C3N-C7N-N7N
2	A	400	NAD	C2N-C3N-C7N-N7N
2	F	400	NAD	O4B-C4B-C5B-O5B
2	A	400	NAD	O4B-C4B-C5B-O5B
2	E	400	NAD	O4B-C4B-C5B-O5B
2	A	400	NAD	PA-O3-PN-O1N
2	A	400	NAD	PA-O3-PN-O2N
2	B	400	NAD	O4B-C4B-C5B-O5B
2	C	400	NAD	O4B-C4B-C5B-O5B
2	D	400	NAD	O4B-C4B-C5B-O5B
2	F	400	NAD	C4N-C3N-C7N-O7N

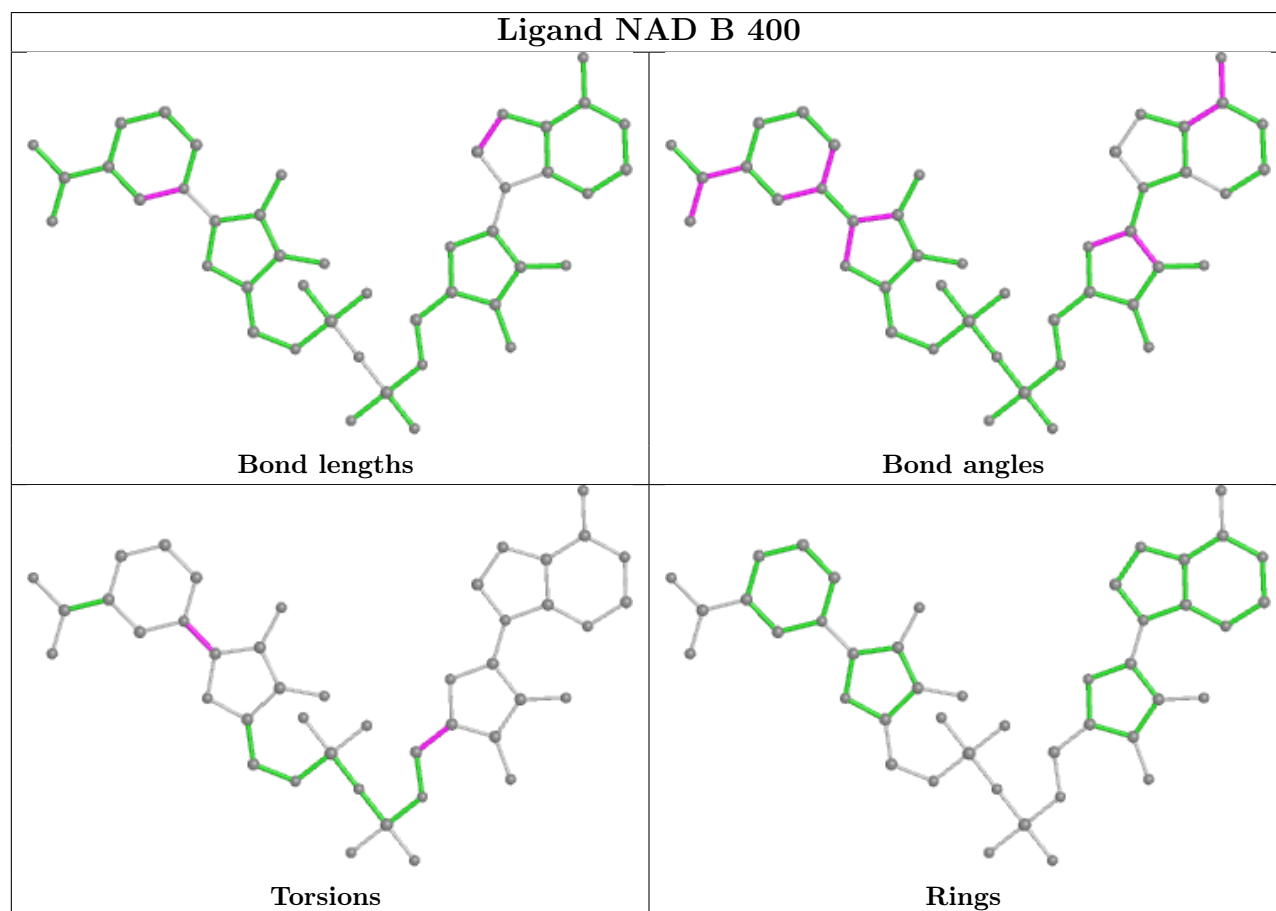
There are no ring outliers.

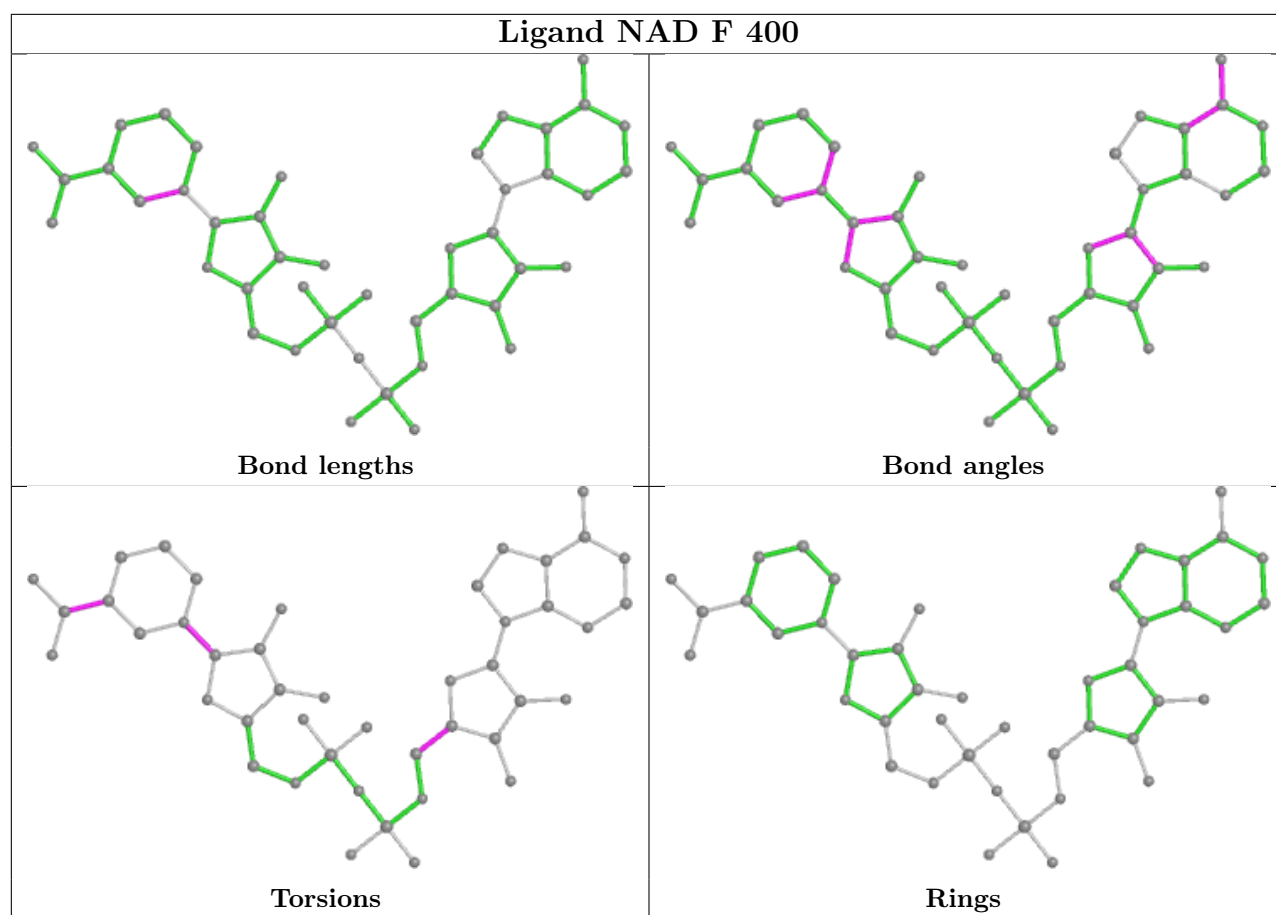
4 monomers are involved in 7 short contacts:

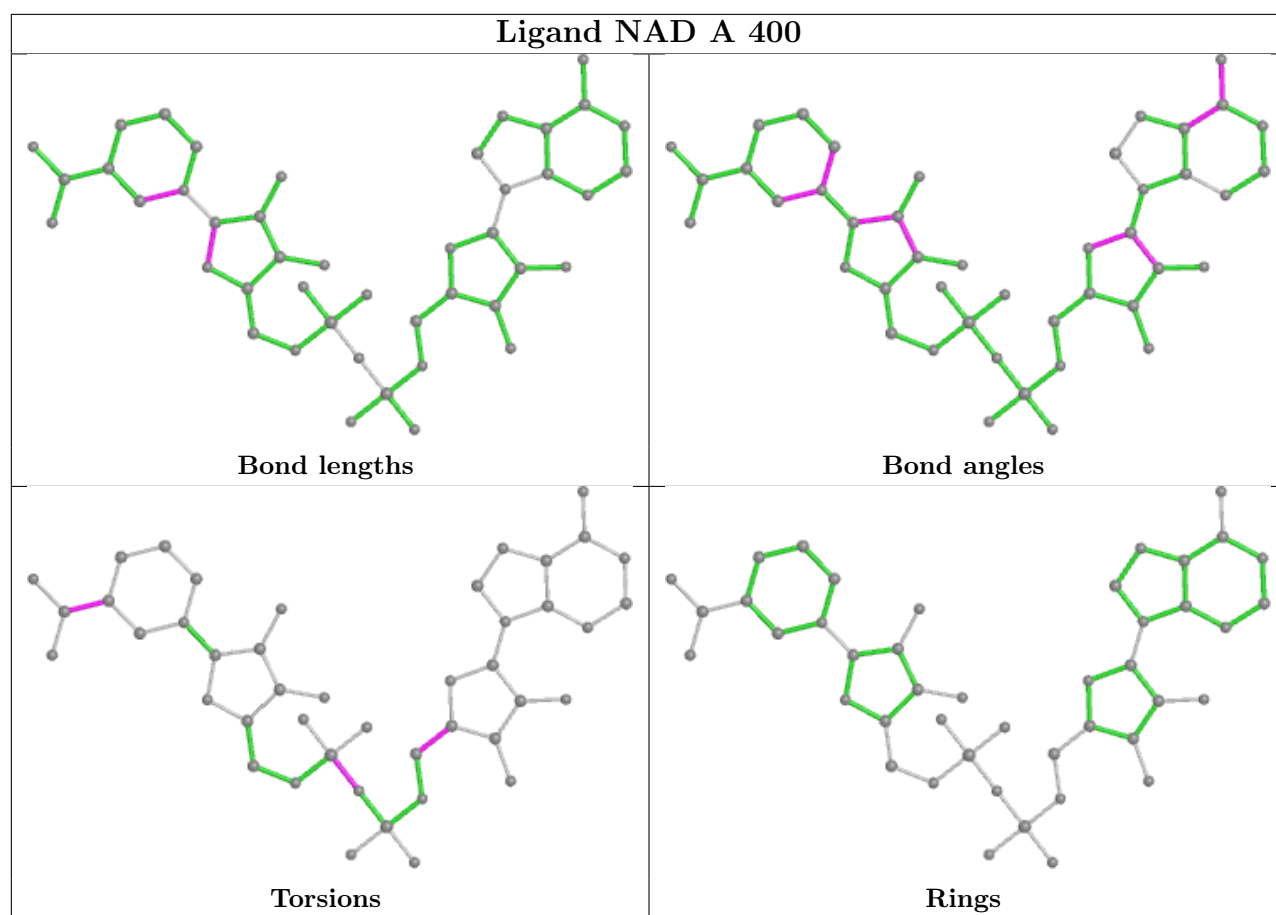
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	NAD	1	0
2	F	400	NAD	3	0
2	A	400	NAD	2	0
2	E	400	NAD	1	0

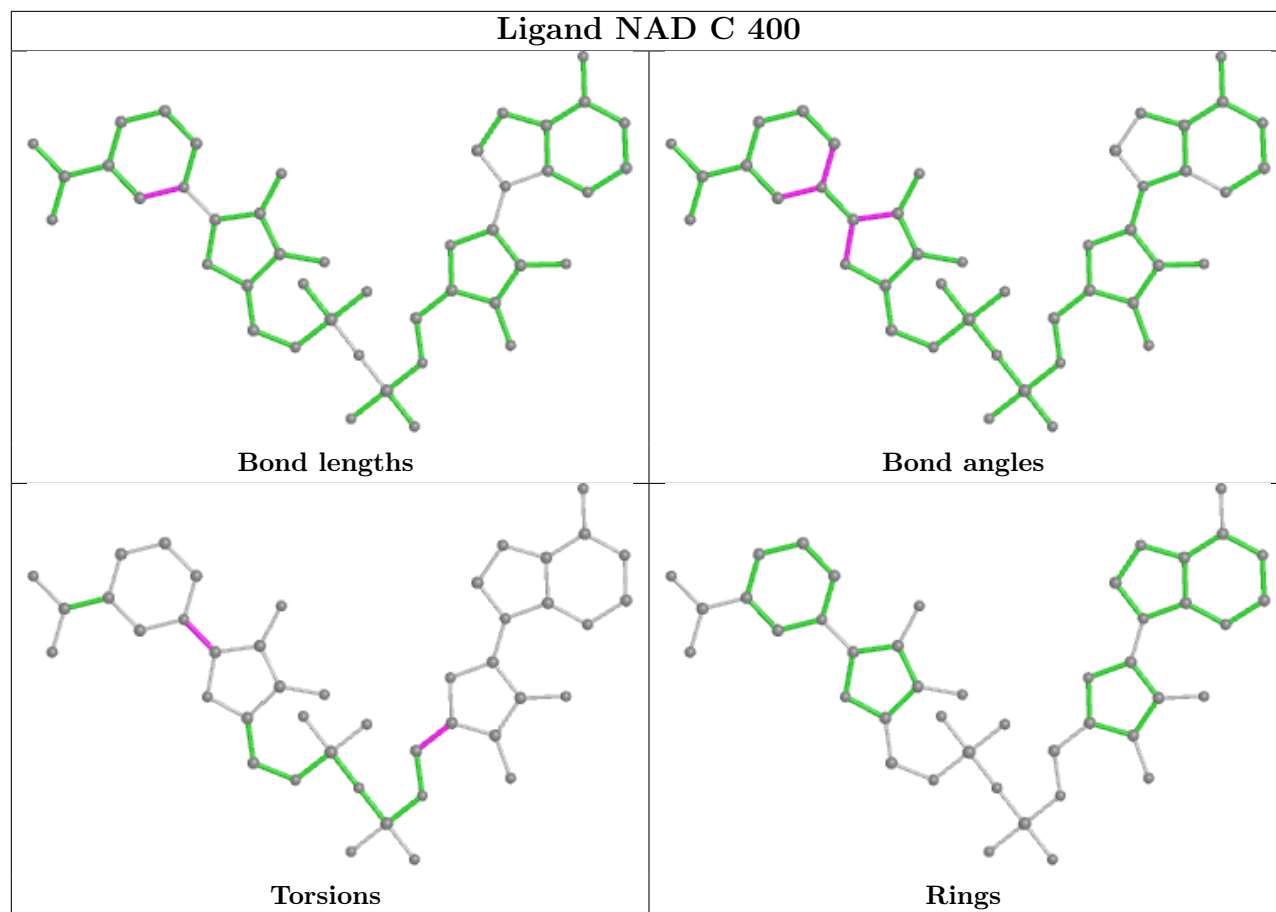
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

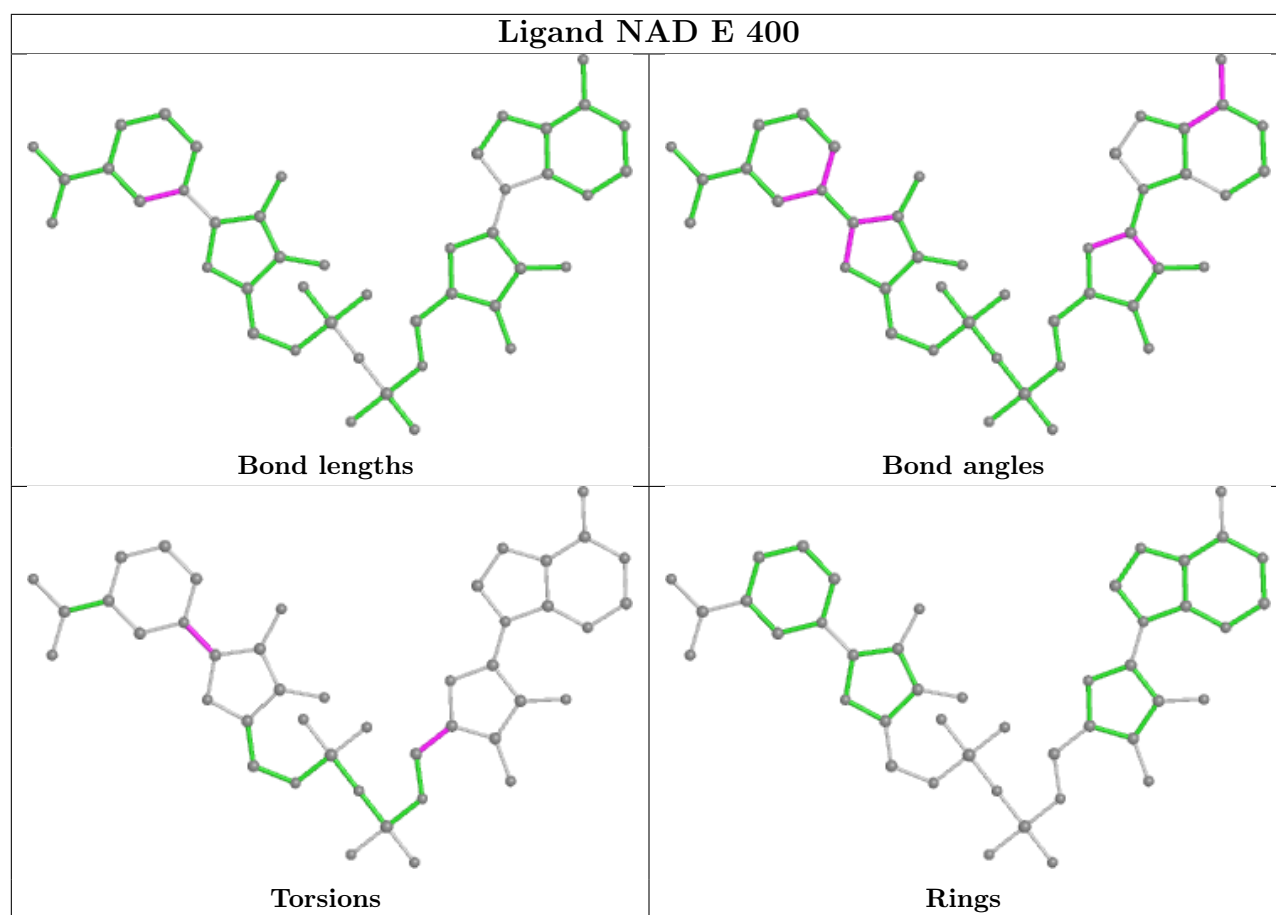


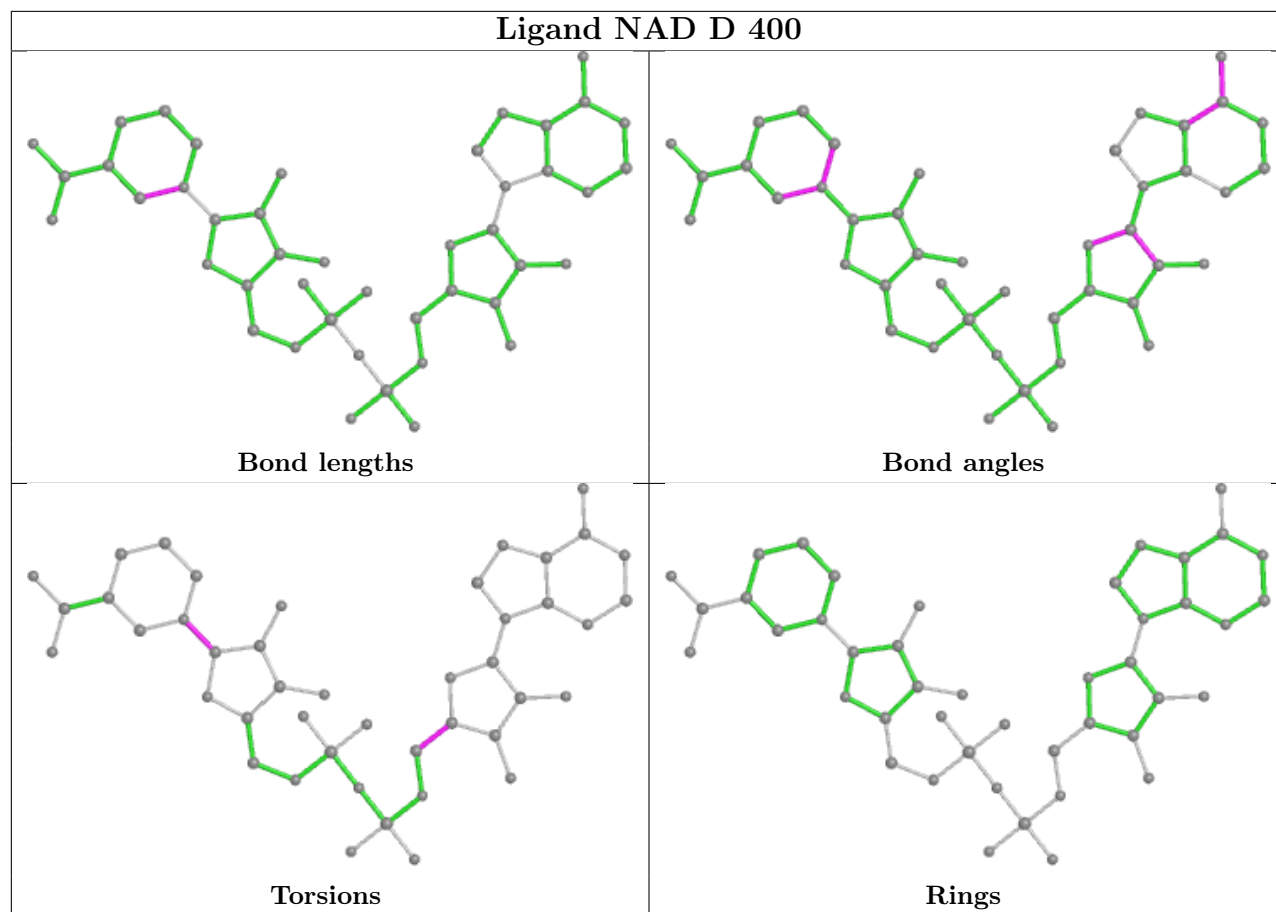












## 5.7 Other polymers [i](#)

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, 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	A	307/331 (92%)	0.20	8 (2%) 56 62	39, 56, 84, 118	0
1	B	306/331 (92%)	0.15	11 (3%) 42 48	41, 58, 89, 139	0
1	C	307/331 (92%)	0.48	16 (5%) 27 32	46, 63, 93, 146	0
1	D	307/331 (92%)	0.50	21 (6%) 17 21	45, 67, 96, 142	0
1	E	300/331 (90%)	0.62	26 (8%) 10 13	52, 70, 112, 151	0
1	F	300/331 (90%)	0.71	24 (8%) 12 15	55, 75, 114, 152	0
All	All	1827/1986 (91%)	0.44	106 (5%) 23 28	39, 65, 101, 152	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	ALA	4.8
1	C	86	ARG	4.6
1	E	303	VAL	4.3
1	F	94	ASP	4.2
1	D	297	ALA	4.1
1	F	113	TYR	4.1
1	E	105	GLN	4.0
1	C	88	PRO	4.0
1	A	307	MET	3.9
1	E	266	GLY	3.7
1	D	57	LEU	3.6
1	D	293	LYS	3.6
1	E	111	VAL	3.5
1	C	306	VAL	3.5
1	F	303	VAL	3.2
1	B	304	LYS	3.2
1	E	305	ASN	3.2
1	E	304	LYS	3.2
1	B	57	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	88	PRO	3.1
1	F	111	VAL	3.1
1	C	91	SER	3.1
1	C	57	LEU	3.1
1	A	303	VAL	3.0
1	F	95	LEU	3.0
1	D	301	GLU	3.0
1	E	224	LEU	2.9
1	F	267	ILE	2.9
1	F	85	ALA	2.9
1	B	89	GLY	2.8
1	E	113	TYR	2.8
1	D	69	TYR	2.8
1	F	112	LYS	2.8
1	E	307	MET	2.7
1	F	226	ASN	2.7
1	E	101	LYS	2.7
1	F	70	ALA	2.7
1	F	262	TYR	2.7
1	A	306	VAL	2.7
1	E	93	ASP	2.6
1	E	289	THR	2.6
1	E	306	VAL	2.6
1	D	288	LEU	2.6
1	F	84	ILE	2.6
1	D	156	PHE	2.6
1	D	196	PRO	2.6
1	F	108	LYS	2.6
1	B	56	VAL	2.6
1	B	306	VAL	2.6
1	E	59	PHE	2.6
1	C	138	GLY	2.6
1	F	98	THR	2.5
1	F	90	MET	2.5
1	D	307	MET	2.5
1	E	65	GLY	2.5
1	D	58	GLY	2.5
1	D	59	PHE	2.5
1	B	58	GLY	2.5
1	E	95	LEU	2.5
1	F	57	LEU	2.5
1	E	134	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	305	ASN	2.5
1	E	110	VAL	2.5
1	E	71	ASP	2.5
1	D	262	TYR	2.5
1	D	305	ASN	2.4
1	E	67	SER	2.4
1	E	92	ARG	2.4
1	D	56	VAL	2.4
1	C	26	LYS	2.4
1	D	298	LYS	2.3
1	B	86	ARG	2.3
1	D	303	VAL	2.3
1	B	278	ASN	2.3
1	A	238	VAL	2.3
1	C	89	GLY	2.3
1	F	34	VAL	2.3
1	A	22	LEU	2.2
1	F	225	GLY	2.2
1	E	38	GLN	2.2
1	D	265	GLU	2.2
1	E	28	LEU	2.2
1	C	278	ASN	2.2
1	D	257	TYR	2.2
1	E	58	GLY	2.2
1	F	109	GLU	2.2
1	C	226	ASN	2.2
1	E	26	LYS	2.1
1	F	140	PRO	2.1
1	F	115	PRO	2.1
1	F	139	PHE	2.1
1	C	87	LYS	2.1
1	D	238	VAL	2.1
1	C	134	PHE	2.1
1	F	25	GLN	2.1
1	A	26	LYS	2.1
1	A	59	PHE	2.1
1	A	28	LEU	2.0
1	D	304	LYS	2.0
1	C	204	ASP	2.0
1	D	267	ILE	2.0
1	C	205	ARG	2.0
1	F	257	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	257	TYR	2.0
1	B	90	MET	2.0
1	E	53	ALA	2.0

## 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](#)

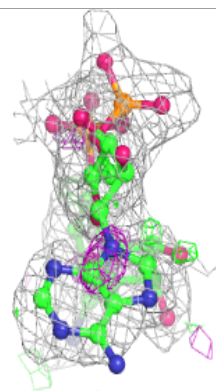
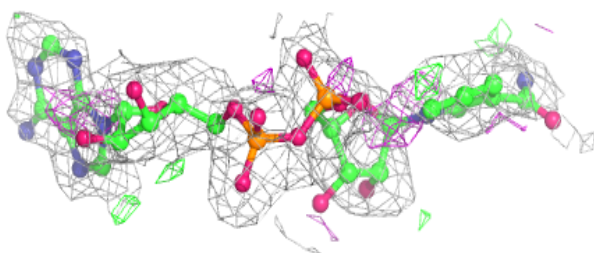
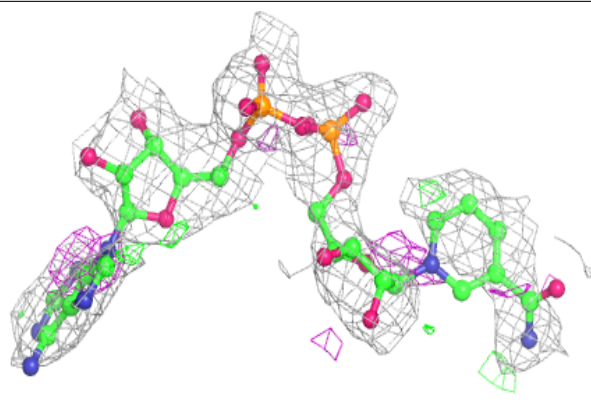
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	A	400	44/44	0.71	0.29	68,93,107,110	0
2	NAD	E	400	44/44	0.89	0.14	62,80,97,99	0
2	NAD	F	400	44/44	0.89	0.16	66,88,101,104	0
2	NAD	D	400	44/44	0.90	0.16	61,79,86,92	0
2	NAD	C	400	44/44	0.92	0.19	54,74,83,87	0
2	NAD	B	400	44/44	0.95	0.14	45,59,70,73	0

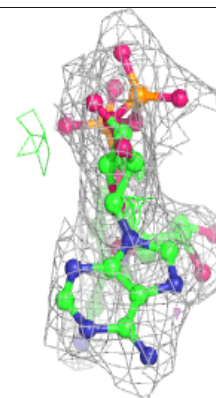
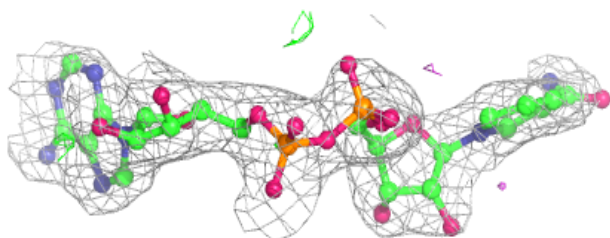
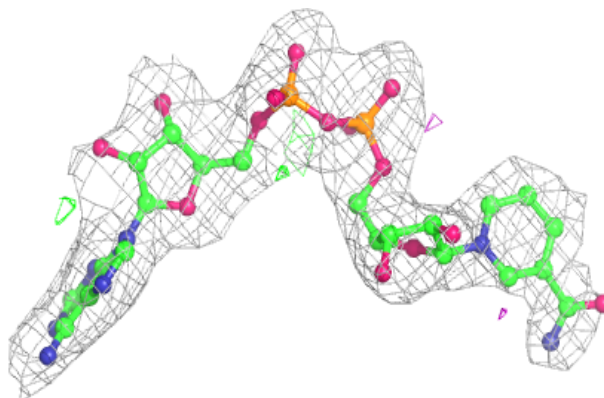
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD A 400:**

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

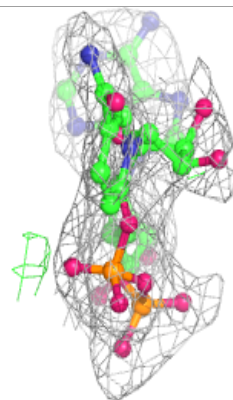
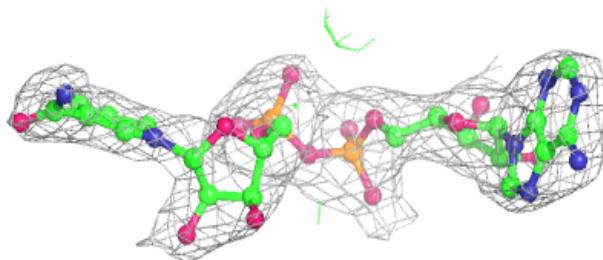
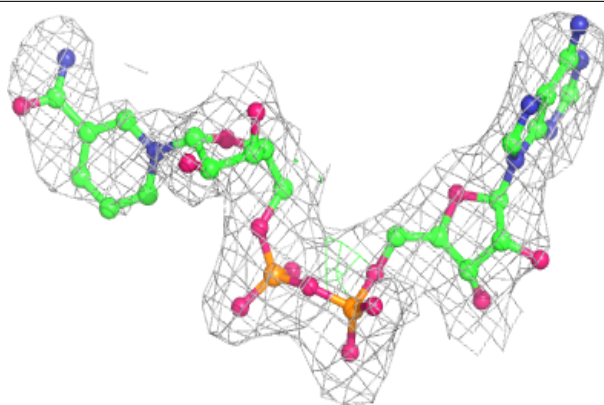
**Electron density around NAD E 400:**

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

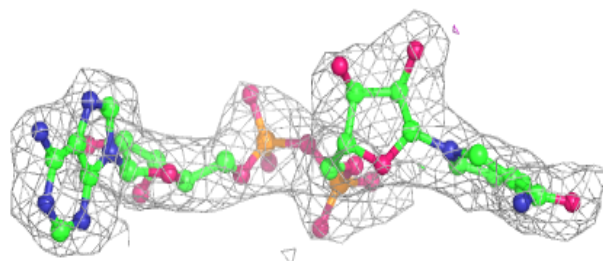
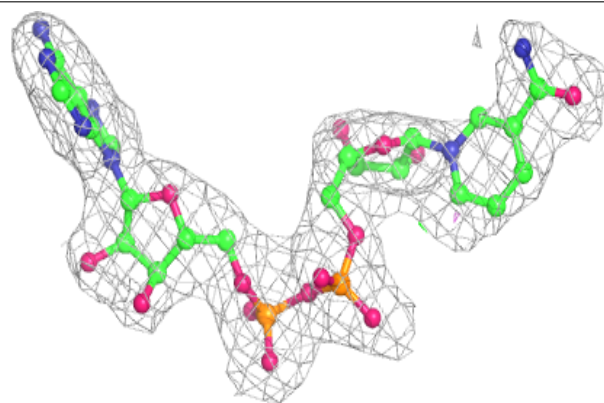


**Electron density around NAD F 400:**

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

**Electron density around NAD D 400:**

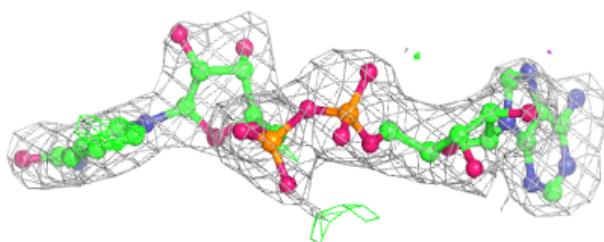
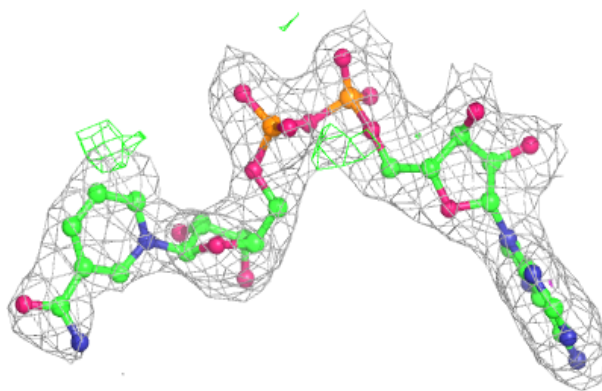
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



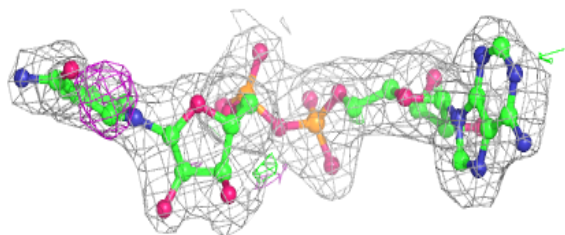
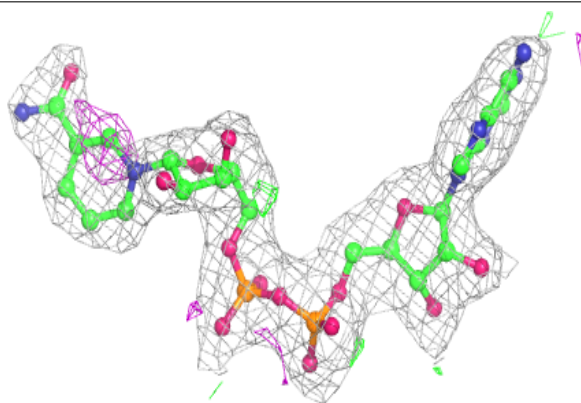


**Electron density around NAD C 400:**

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

**Electron density around NAD B 400:**

$2mF_o-DF_c$  (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.