



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 11:14 am BST

PDB ID : 6C8Q  
Title : Crystal structure of NAD synthetase (NadE) from *Enterococcus faecalis* in complex with NAD<sup>+</sup>  
Authors : Stogios, P.J.; Skarina, T.; McChesney, C.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2018-01-25  
Resolution : 2.58 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.

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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	:	2.11
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)	:	2.11

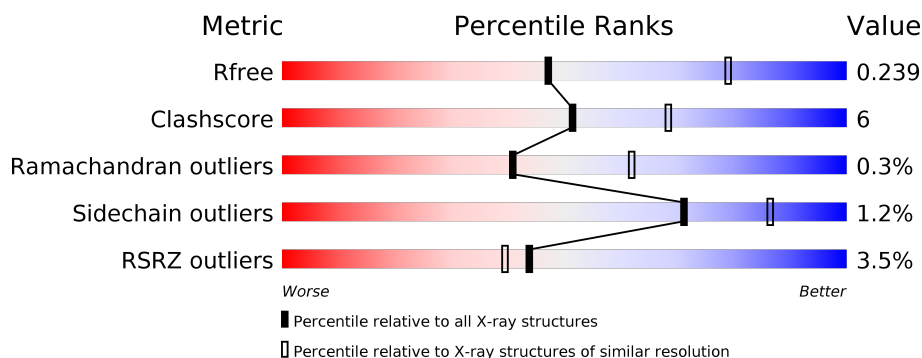
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 88%, yellow 88%, yellow 99%, grey 99%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>0%</span> <span>88%</span> <span>9%</span> <span>•</span> </div> </div>
1	B	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 91%, yellow 91%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>91%</span> <span>6%</span> <span>•</span> </div> </div>
1	C	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 86%, yellow 86%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>86%</span> <span>9%</span> <span>• •</span> </div> </div>
1	D	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 83%, yellow 83%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>83%</span> <span>13%</span> <span>•</span> </div> </div>
1	E	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 83%, yellow 83%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>83%</span> <span>13%</span> <span>•</span> </div> </div>
1	F	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 68%, yellow 68%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>8%</span> <span>68%</span> <span>27%</span> <span>• •</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	275	 3% 84% 12% •
1	H	275	 3% 86% 11% •

## 2 Entry composition

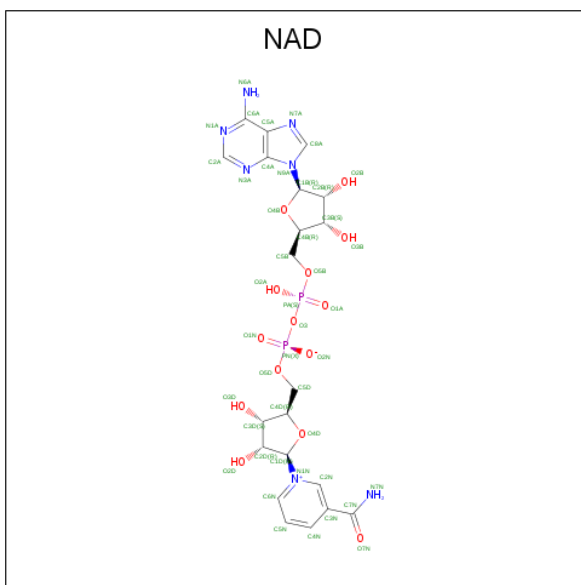
There are 3 unique types of molecules in this entry. The entry contains 17889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NH(3)-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2099	1336	351	406	6			
1	B	266	Total	C	N	O	S	0	1	0
			2082	1328	349	398	7			
1	C	265	Total	C	N	O	S	0	2	0
			2075	1322	348	398	7			
1	D	264	Total	C	N	O	S	0	1	0
			2063	1313	346	398	6			
1	E	263	Total	C	N	O	S	0	1	0
			2055	1307	344	397	7			
1	F	264	Total	C	N	O	S	0	2	0
			2072	1321	348	396	7			
1	G	265	Total	C	N	O	S	0	1	0
			2074	1323	348	397	6			
1	H	267	Total	C	N	O	S	0	2	0
			2094	1337	350	401	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 35	C 15	N 5	O 13	P 2	0	0
2	E	1	Total 36	C 15	N 6	O 13	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	G	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	H	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	174	Total O 174 174	0	0
3	B	131	Total O 136 136	0	5
3	C	125	Total O 128 128	0	3
3	D	80	Total O 81 81	0	1

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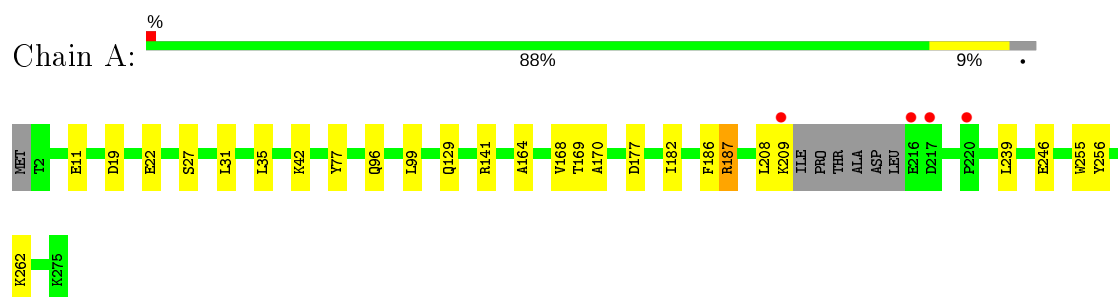
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	128	Total 130	O 130	0	2
3	F	42	Total 43	O 43	0	1
3	G	120	Total 121	O 121	0	1
3	H	127	Total 127	O 127	0	0

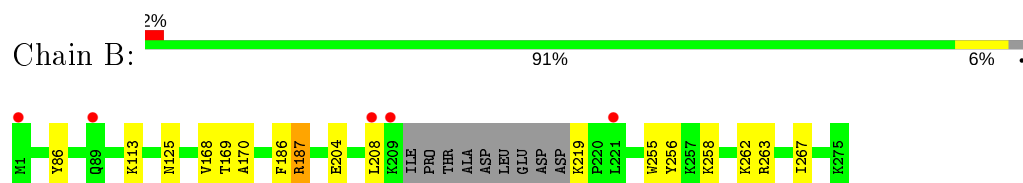
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

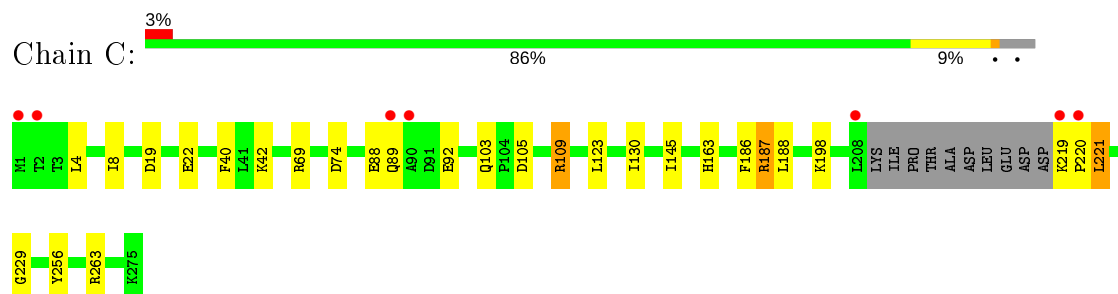
- Molecule 1: NH(3)-dependent NAD(+) synthetase



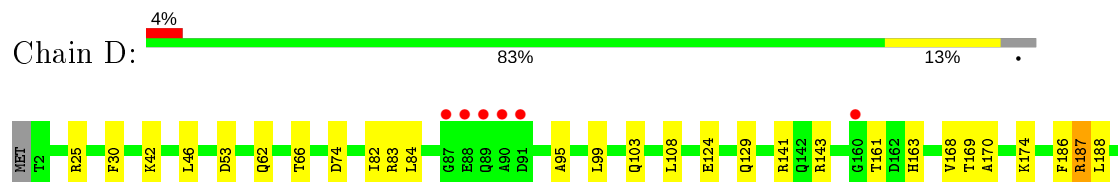
- Molecule 1: NH(3)-dependent NAD(+) synthetase

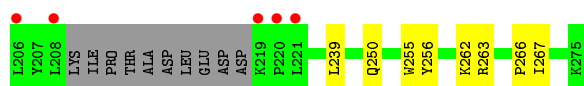


- Molecule 1: NH(3)-dependent NAD(+) synthetase

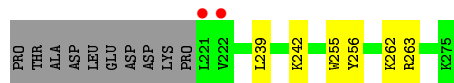
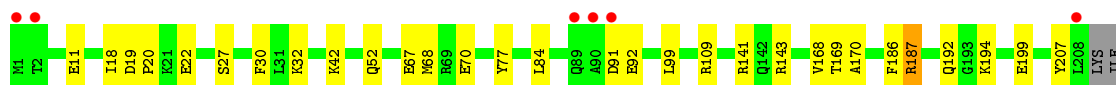
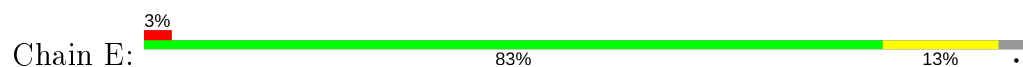


- Molecule 1: NH(3)-dependent NAD(+) synthetase

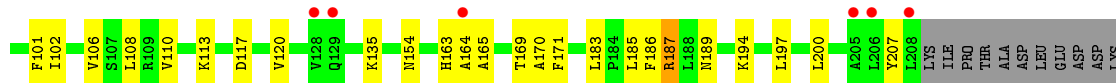
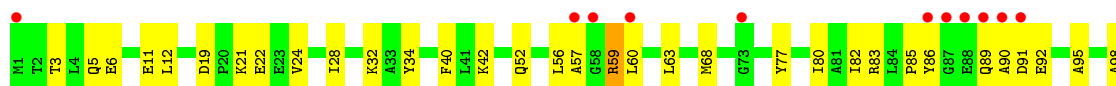




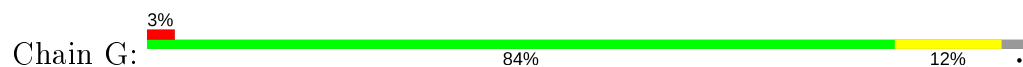
- Molecule 1: NH(3)-dependent NAD(+) synthetase



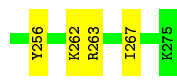
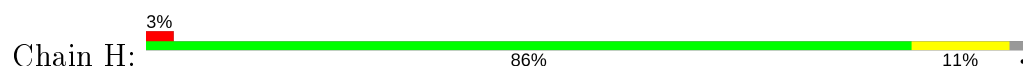
- Molecule 1: NH(3)-dependent NAD(+) synthetase



- Molecule 1: NH(3)-dependent NAD(+) synthetase



- Molecule 1: NH(3)-dependent NAD(+) synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.44Å 85.17Å 175.81Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	24.78 – 2.58 24.78 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.78-2.58) 89.9 (24.78-2.58)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.26 (at 2.57Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.188 , 0.239 0.187 , 0.239	Depositor DCC
$R_{free}$ test set	2020 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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	0.24	0/2139	0.41	0/2887
1	B	0.25	0/2122	0.40	0/2863
1	C	0.24	0/2117	0.40	0/2858
1	D	0.24	0/2102	0.42	0/2838
1	E	0.25	0/2093	0.41	0/2825
1	F	0.27	0/2115	0.47	0/2854
1	G	0.29	0/2114	0.42	0/2853
1	H	0.25	0/2138	0.40	0/2887
All	All	0.25	0/16940	0.42	0/22865

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	2099	0	2094	17	0
1	B	2082	0	2092	13	0
1	C	2075	0	2087	18	0
1	D	2063	0	2064	24	0
1	E	2055	0	2056	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2072	0	2080	62	0
1	G	2074	0	2080	22	0
1	H	2094	0	2102	18	0
2	A	44	0	24	3	0
2	B	44	0	24	2	0
2	C	44	0	24	1	0
2	D	35	0	17	2	0
2	E	36	0	18	2	0
2	F	44	0	24	1	0
2	G	44	0	24	3	0
2	H	44	0	24	2	0
3	A	174	0	0	1	0
3	B	136	0	0	2	0
3	C	128	0	0	1	0
3	D	81	0	0	1	0
3	E	130	0	0	1	0
3	F	43	0	0	0	0
3	G	121	0	0	1	0
3	H	127	0	0	0	0
All	All	17889	0	16834	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (188) 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)
2:B:301:NAD:C1D	2:B:301:NAD:O4D	1.63	1.23
2:B:301:NAD:O4B	2:B:301:NAD:C1B	1.63	1.23
2:G:301:NAD:O4B	2:G:301:NAD:C1B	1.64	1.22
2:F:301:NAD:O4B	2:F:301:NAD:C1B	1.63	1.21
2:E:301:NAD:O4B	2:E:301:NAD:C1B	1.63	1.18
2:A:301:NAD:C1B	2:A:301:NAD:O4B	1.63	1.16
2:C:301:NAD:C1B	2:C:301:NAD:O4B	1.63	1.14
2:D:301:NAD:C1B	2:D:301:NAD:O4B	1.63	1.13
2:H:301:NAD:C1B	2:H:301:NAD:O4B	1.64	1.13
1:F:83[B]:ARG:HH12	1:F:92:GLU:HG3	1.10	1.07
1:F:83[B]:ARG:NH1	1:F:92:GLU:HG3	1.74	1.03
1:F:82:ILE:HD11	1:F:110:VAL:HG23	1.49	0.92
1:F:89:GLN:O	1:F:90:ALA:HB3	1.75	0.87
1:F:40[B]:PHE:HA	1:G:250:GLN:HE22	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40[A]:PHE:HA	1:G:250:GLN:HE22	1.44	0.82
1:F:92:GLU:O	1:F:92:GLU:HG2	1.85	0.76
1:F:194:LYS:HD3	1:F:207:TYR:HB2	1.71	0.73
1:F:83[B]:ARG:HG3	1:F:85:PRO:HD3	1.72	0.71
1:B:256:TYR:HA	1:B:263:ARG:HH22	1.55	0.70
1:F:83[B]:ARG:HH12	1:F:92:GLU:CG	1.99	0.68
1:E:92:GLU:OE2	1:E:109:ARG:NH1	2.27	0.68
1:E:32:LYS:HA	1:E:68:MET:HE1	1.76	0.67
1:F:59:ARG:NH1	1:F:63:LEU:HD21	2.10	0.67
1:E:19:ASP:HB3	1:E:22:GLU:HG2	1.75	0.66
1:F:5:GLN:HB2	1:F:238:TYR:CZ	2.32	0.64
1:B:168:VAL:O	1:B:263:ARG:NH2	2.32	0.62
1:B:170:ALA:HB1	1:B:262:LYS:HD2	1.82	0.62
1:H:170:ALA:HB1	1:H:262:LYS:HD2	1.81	0.62
1:G:172:PHE:HB2	1:G:177:ASP:HB3	1.83	0.60
1:G:83:ARG:NH2	1:G:109:ARG:HD2	2.17	0.60
1:D:267:ILE:HD13	1:F:34:TYR:CE1	2.37	0.60
1:H:42:LYS:NZ	1:H:74:ASP:OD2	2.29	0.59
1:F:89:GLN:O	1:F:90:ALA:CB	2.44	0.59
1:F:59:ARG:O	1:F:63:LEU:HG	2.03	0.58
1:F:170:ALA:HB1	1:F:262:LYS:HD2	1.86	0.58
1:D:168:VAL:HG11	1:D:239:LEU:HD21	1.86	0.58
1:D:169:THR:HA	1:D:255:TRP:HB3	1.86	0.57
1:F:154:ASN:HA	1:G:246:GLU:HB2	1.86	0.57
1:G:256:TYR:HA	1:G:263:ARG:HH22	1.69	0.57
1:E:52:GLN:NE2	3:E:403:HOH:O	2.37	0.57
1:F:59:ARG:HG3	1:F:101:PHE:CE2	2.39	0.57
1:F:120:VAL:HG21	1:F:135:LYS:HE3	1.86	0.57
1:F:238:TYR:CD2	1:F:252:ILE:HD11	2.40	0.57
1:C:69:ARG:NH2	1:C:105:ASP:OD2	2.37	0.57
1:B:256:TYR:HA	1:B:263:ARG:NH2	2.19	0.56
1:C:19:ASP:HB3	1:C:22:GLU:HB3	1.86	0.56
1:E:256:TYR:HA	1:E:263:ARG:HH22	1.69	0.56
1:F:5:GLN:NE2	1:F:238:TYR:O	2.38	0.56
1:H:3:THR:HG22	1:H:6:GLU:HG2	1.88	0.56
1:A:141:ARG:NH2	2:A:301:NAD:O1A	2.38	0.55
1:A:170:ALA:HB1	1:A:262:LYS:HD2	1.87	0.55
2:A:301:NAD:H71N	1:C:229:GLY:HA2	1.71	0.55
1:H:55:THR:HG21	1:H:206:LEU:HD23	1.88	0.55
1:C:256:TYR:HA	1:C:263:ARG:HH22	1.71	0.55
1:F:256:TYR:HA	1:F:263:ARG:HH22	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:ALA:HB1	1:G:262:LYS:HD2	1.88	0.55
1:F:221:LEU:HD23	1:F:221:LEU:H	1.72	0.55
1:A:208:LEU:HD23	1:A:209:LYS:H	1.71	0.55
1:F:32:LYS:HG2	1:F:68:MET:HG3	1.89	0.54
1:A:19:ASP:HB3	1:A:22:GLU:HB3	1.89	0.54
1:D:42:LYS:NZ	1:D:74:ASP:OD2	2.35	0.53
1:F:83[B]:ARG:CZ	1:F:92:GLU:HG3	2.36	0.53
1:F:163:HIS:CE1	1:F:165:ALA:HB3	2.43	0.53
1:D:62:GLN:NE2	1:D:103:GLN:O	2.41	0.53
1:D:256:TYR:HA	1:D:263:ARG:HH22	1.74	0.52
1:F:56:LEU:HD13	1:F:197:LEU:HG	1.90	0.52
1:F:231:THR:HG23	1:F:234:ALA:H	1.74	0.52
1:F:82:ILE:CD1	1:F:108:LEU:HB2	2.39	0.52
1:B:169:THR:HA	1:B:255:TRP:HB3	1.91	0.52
1:G:52:GLN:OE1	1:G:194:LYS:NZ	2.37	0.52
1:A:96:GLN:HA	1:A:99:LEU:HB2	1.90	0.52
1:E:168:VAL:HG11	1:E:239:LEU:HD21	1.90	0.52
1:H:256:TYR:HA	1:H:263:ARG:HH22	1.75	0.52
1:F:95:ALA:O	1:F:98:ALA:N	2.41	0.51
1:A:182:ILE:HG13	1:B:267:ILE:HB	1.93	0.51
1:E:141:ARG:NH2	2:E:301:NAD:O1A	2.43	0.51
1:H:210:ILE:HG23	1:H:211:PRO:HD3	1.92	0.51
1:E:20:PRO:HB2	1:E:199[A]:GLU:HG3	1.92	0.51
1:H:192:GLN:O	1:H:196:LEU:HD12	2.11	0.51
1:F:225:GLU:HA	1:F:228:LEU:HB2	1.93	0.50
1:B:86:TYR:CZ	1:B:113:LYS:HG3	2.47	0.50
1:A:11:GLU:OE1	1:A:256:TYR:OH	2.28	0.50
1:A:31:LEU:O	1:A:35:LEU:HD22	2.11	0.50
1:G:163:HIS:CE1	1:G:165:ALA:HB3	2.47	0.50
1:C:4:LEU:O	1:C:8:ILE:HG12	2.12	0.49
1:G:84:LEU:HD13	1:G:143:ARG:HB3	1.93	0.49
1:E:11:GLU:OE1	1:E:256:TYR:OH	2.25	0.49
1:G:171:PHE:CE2	2:G:301:NAD:H2N	2.48	0.49
1:A:129:GLN:NE2	3:A:408:HOH:O	2.46	0.49
1:A:164:ALA:O	1:A:168:VAL:HG23	2.13	0.49
1:E:169:THR:HA	1:E:255:TRP:HB3	1.95	0.48
1:F:11:GLU:OE1	1:F:256:TYR:OH	2.27	0.48
1:A:168:VAL:HG21	1:A:239:LEU:HD21	1.94	0.48
1:C:42:LYS:NZ	1:C:74:ASP:OD2	2.41	0.48
1:C:123:LEU:HD23	1:G:110:VAL:HG11	1.93	0.48
1:D:267:ILE:HD13	1:F:34:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:VAL:HG22	1:H:80:ILE:HB	1.95	0.48
1:D:141:ARG:NH2	2:D:301:NAD:O1A	2.47	0.47
1:F:82:ILE:HD12	1:F:108:LEU:HB2	1.96	0.47
1:D:62:GLN:O	1:D:66:THR:HG23	2.14	0.47
1:F:254:ASN:O	1:F:258:LYS:HG3	2.15	0.47
1:E:84:LEU:HD13	1:E:143:ARG:HB3	1.96	0.47
1:F:86:TYR:CZ	1:F:113:LYS:HD2	2.50	0.47
1:D:174:LYS:NZ	3:D:407:HOH:O	2.45	0.47
1:F:57:ALA:HB2	1:F:185:LEU:HD21	1.96	0.47
1:E:170:ALA:HB1	1:E:262:LYS:HD2	1.96	0.47
1:D:30:PHE:HZ	1:F:267:ILE:HG22	1.78	0.47
1:D:30:PHE:HB2	1:F:269:ILE:HD13	1.97	0.47
1:C:109:ARG:NH1	3:C:402:HOH:O	2.31	0.46
1:F:19:ASP:HB3	1:F:22:GLU:HB3	1.97	0.46
1:G:119:MET:HE1	1:G:123:LEU:HD11	1.97	0.46
1:C:186:PHE:O	1:C:187:ARG:HB3	2.16	0.46
1:A:169:THR:HA	1:A:255:TRP:HB3	1.96	0.46
1:C:123:LEU:HD13	1:C:130:ILE:HD11	1.96	0.46
1:D:124:GLU:HG2	1:D:129:GLN:HA	1.98	0.46
1:H:137:ASN:OD1	2:H:301:NAD:H6N	2.16	0.46
1:F:56:LEU:O	1:F:60:LEU:HD12	2.16	0.45
1:H:20:PRO:O	1:H:24:VAL:HG23	2.16	0.45
1:F:248:ASP:O	1:F:252:ILE:HG23	2.16	0.45
1:D:53:ASP:HB3	1:D:161:THR:HB	1.98	0.45
1:F:24:VAL:O	1:F:28:ILE:HG12	2.16	0.45
1:H:84:LEU:HD13	1:H:143:ARG:HB3	1.98	0.45
1:B:204:GLU:HB3	1:B:208:LEU:HD13	1.98	0.45
1:B:256:TYR:O	1:B:263:ARG:NH1	2.41	0.45
1:B:258:LYS:NZ	3:B:404:HOH:O	2.36	0.45
1:D:170:ALA:HB1	1:D:262:LYS:HD2	1.99	0.45
1:E:91:ASP:N	1:E:91:ASP:OD1	2.50	0.44
1:H:205:ALA:O	1:H:209:LYS:HD2	2.17	0.44
1:F:59:ARG:HE	1:F:102:ILE:HA	1.82	0.44
1:B:219:LYS:N	3:B:407:HOH:O	2.50	0.44
1:F:164:ALA:HB3	1:F:189:ASN:HA	1.99	0.44
1:F:3:THR:HG23	1:F:6:GLU:H	1.81	0.44
1:C:123:LEU:HD21	1:G:146:THR:HG23	1.99	0.44
1:C:40:PHE:HA	1:D:250:GLN:OE1	2.18	0.44
1:C:221[B]:LEU:H	1:C:221[B]:LEU:HG	1.67	0.43
1:E:67:GLU:O	1:E:70:GLU:HG2	2.18	0.43
1:F:169:THR:HG23	1:F:171:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:OD1	1:A:177:ASP:N	2.51	0.43
1:G:141:ARG:NH2	2:G:301:NAD:O1A	2.51	0.43
1:H:207:TYR:CD2	1:H:208:LEU:HG	2.52	0.43
1:F:186:PHE:O	1:F:187:ARG:HB3	2.18	0.43
1:A:42:LYS:O	1:A:77:TYR:HA	2.19	0.43
1:A:208:LEU:HD23	1:A:209:LYS:N	2.33	0.43
1:F:24:VAL:HG11	1:F:200:LEU:HD21	2.00	0.43
1:G:83:ARG:HH21	1:G:109:ARG:HD2	1.81	0.43
1:E:194:LYS:HG2	1:E:207:TYR:HB2	2.00	0.43
1:A:246:GLU:HB2	1:G:154:ASN:HA	2.01	0.43
1:D:84:LEU:HD22	1:D:143:ARG:HA	2.00	0.43
1:G:244:VAL:HG23	1:G:249:GLN:HB2	2.01	0.43
1:C:88:GLU:HB3	1:C:89:GLN:H	1.70	0.42
1:E:186:PHE:O	1:E:187:ARG:HB3	2.19	0.42
1:E:99:LEU:HD12	1:E:99:LEU:HA	1.90	0.42
1:D:186:PHE:O	1:D:187:ARG:HB3	2.19	0.42
1:C:198:LYS:HB3	1:C:198:LYS:HE2	1.76	0.42
1:F:42:LYS:O	1:F:77:TYR:HA	2.19	0.42
1:A:186:PHE:O	1:A:187:ARG:HB3	2.19	0.42
1:D:82:ILE:HG23	1:D:108:LEU:HB2	2.01	0.42
1:D:83:ARG:HD2	1:D:99:LEU:HD11	2.02	0.42
1:D:83:ARG:HE	1:D:95:ALA:HB1	1.84	0.42
1:H:186:PHE:O	1:H:187:ARG:HB3	2.19	0.42
1:C:145:ILE:HG22	1:G:119:MET:HE2	2.02	0.42
1:C:219:LYS:N	1:C:220:PRO:HD2	2.35	0.42
1:E:18:ILE:HG12	1:E:192:GLN:HG2	2.01	0.42
1:E:256:TYR:HA	1:E:263:ARG:NH2	2.33	0.42
1:G:191:ARG:NH2	1:G:236:ASP:HB2	2.34	0.42
1:F:189:ASN:HB2	1:F:236:ASP:OD1	2.20	0.42
1:F:40[A]:PHE:HA	1:G:250:GLN:NE2	2.24	0.42
1:B:204:GLU:HB3	1:B:208:LEU:HD22	2.01	0.41
1:E:42:LYS:O	1:E:77:TYR:HA	2.20	0.41
1:F:52:GLN:NE2	1:F:194:LYS:HG2	2.35	0.41
1:F:82:ILE:HD13	1:F:108:LEU:HB2	2.02	0.41
1:H:48:ILE:HG21	1:H:99:LEU:HD13	2.02	0.41
1:F:253:GLU:O	1:F:257:LYS:HG2	2.21	0.41
1:F:80:ILE:HA	1:F:106:VAL:HG13	2.03	0.41
1:F:83[B]:ARG:HH22	1:F:92:GLU:HB2	1.86	0.41
1:C:163:HIS:HB2	1:C:188:LEU:O	2.21	0.41
1:F:12:LEU:HD21	1:F:164:ALA:HA	2.02	0.41
1:F:59:ARG:HH11	1:F:63:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:PHE:O	1:B:187:ARG:HB3	2.20	0.41
1:H:208:LEU:C	1:H:211:PRO:HD2	2.41	0.41
1:E:30:PHE:HZ	1:H:267:ILE:HG22	1.84	0.41
1:H:99:LEU:HA	1:H:99:LEU:HD12	1.87	0.41
1:F:238:TYR:CG	1:F:252:ILE:HD11	2.55	0.41
1:D:163:HIS:HB2	1:D:188:LEU:O	2.21	0.40
1:D:266:PRO:HB2	1:F:183:LEU:HD11	2.02	0.40
1:F:117:ASP:HA	1:F:120:VAL:HG12	2.03	0.40
1:D:256:TYR:HA	1:D:263:ARG:NH2	2.34	0.40
1:G:166:GLU:OE1	3:G:401:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/275 (96%)	263 (99%)	1 (0%)	1 (0%)	34	55
1	B	263/275 (96%)	257 (98%)	5 (2%)	1 (0%)	34	55
1	C	263/275 (96%)	255 (97%)	7 (3%)	1 (0%)	34	55
1	D	261/275 (95%)	252 (97%)	8 (3%)	1 (0%)	34	55
1	E	260/275 (94%)	255 (98%)	4 (2%)	1 (0%)	34	55
1	F	262/275 (95%)	251 (96%)	10 (4%)	1 (0%)	34	55
1	G	262/275 (95%)	255 (97%)	7 (3%)	0	100	100
1	H	265/275 (96%)	256 (97%)	8 (3%)	1 (0%)	34	55
All	All	2101/2200 (96%)	2044 (97%)	50 (2%)	7 (0%)	41	62

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	C	187	ARG
1	H	187	ARG
1	A	187	ARG
1	B	187	ARG
1	D	187	ARG
1	E	187	ARG
1	F	187	ARG

### 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	219/224 (98%)	218 (100%)	1 (0%)	88	96
1	B	217/224 (97%)	216 (100%)	1 (0%)	88	96
1	C	217/224 (97%)	212 (98%)	5 (2%)	50	73
1	D	215/224 (96%)	213 (99%)	2 (1%)	78	90
1	E	214/224 (96%)	212 (99%)	2 (1%)	78	90
1	F	216/224 (96%)	212 (98%)	4 (2%)	57	77
1	G	216/224 (96%)	211 (98%)	5 (2%)	50	73
1	H	219/224 (98%)	218 (100%)	1 (0%)	88	96
All	All	1733/1792 (97%)	1712 (99%)	21 (1%)	71	86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	B	125	ASN
1	C	92	GLU
1	C	103	GLN
1	C	109	ARG
1	C	221[A]	LEU
1	C	221[B]	LEU
1	D	25	ARG
1	D	46	LEU

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Mol	Chain	Res	Type
1	E	27	SER
1	E	242	LYS
1	F	21	LYS
1	F	59	ARG
1	F	91	ASP
1	F	221	LEU
1	G	88	GLU
1	G	89	GLN
1	G	91	ASP
1	G	92	GLU
1	G	107	SER
1	H	107	SER

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

Mol	Chain	Res	Type
1	E	142	GLN
1	G	250	GLN
1	H	142	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	F	301	-	42,48,48	5.52	16 (38%)	50,73,73	1.78	7 (14%)
2	NAD	D	301	-	33,38,48	5.38	13 (39%)	37,58,73	1.99	6 (16%)
2	NAD	H	301	-	42,48,48	5.51	16 (38%)	50,73,73	1.70	7 (14%)
2	NAD	B	301	-	42,48,48	5.52	16 (38%)	50,73,73	1.71	7 (14%)
2	NAD	C	301	-	42,48,48	5.51	16 (38%)	50,73,73	1.71	7 (14%)
2	NAD	A	301	-	42,48,48	5.51	16 (38%)	50,73,73	1.73	6 (12%)
2	NAD	G	301	-	42,48,48	5.51	16 (38%)	50,73,73	1.74	7 (14%)
2	NAD	E	301	-	33,39,48	5.05	13 (39%)	38,60,73	1.92	5 (13%)

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	F	301	-	-	4/26/62/62	0/5/5/5
2	NAD	D	301	-	-	8/18/51/62	0/4/4/5
2	NAD	H	301	-	-	4/26/62/62	0/5/5/5
2	NAD	B	301	-	-	7/26/62/62	0/5/5/5
2	NAD	C	301	-	-	3/26/62/62	0/5/5/5
2	NAD	A	301	-	-	5/26/62/62	0/5/5/5
2	NAD	G	301	-	-	8/26/62/62	0/5/5/5
2	NAD	E	301	-	-	4/18/54/62	0/4/4/5

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAD	C2B-C1B	-16.50	1.28	1.53
2	A	301	NAD	C2B-C1B	-16.46	1.28	1.53
2	D	301	NAD	C2B-C1B	-16.44	1.28	1.53
2	F	301	NAD	C2B-C1B	-16.43	1.28	1.53
2	B	301	NAD	C2B-C1B	-16.41	1.28	1.53
2	H	301	NAD	C2B-C1B	-16.40	1.28	1.53
2	H	301	NAD	O4B-C1B	16.40	1.64	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAD	O4B-C1B	16.39	1.64	1.41
2	C	301	NAD	C2B-C1B	-16.39	1.28	1.53
2	B	301	NAD	O4B-C1B	16.38	1.63	1.41
2	C	301	NAD	O4B-C1B	16.34	1.63	1.41
2	D	301	NAD	O4B-C1B	16.33	1.63	1.41
2	A	301	NAD	O4B-C1B	16.33	1.63	1.41
2	F	301	NAD	O4B-C1B	16.29	1.63	1.41
2	G	301	NAD	C2B-C1B	-16.29	1.29	1.53
2	E	301	NAD	O4B-C1B	16.26	1.63	1.41
2	B	301	NAD	O4D-C1D	16.06	1.63	1.41
2	C	301	NAD	O4D-C1D	16.00	1.63	1.41
2	A	301	NAD	O4D-C1D	15.74	1.63	1.41
2	F	301	NAD	O4D-C1D	15.70	1.63	1.41
2	H	301	NAD	O4D-C1D	15.70	1.63	1.41
2	G	301	NAD	O4D-C1D	15.69	1.63	1.41
2	G	301	NAD	C2D-C1D	-14.76	1.31	1.53
2	A	301	NAD	C2D-C1D	-14.67	1.31	1.53
2	H	301	NAD	C2D-C1D	-14.59	1.31	1.53
2	F	301	NAD	C2D-C1D	-14.59	1.31	1.53
2	C	301	NAD	C2D-C1D	-14.37	1.31	1.53
2	B	301	NAD	C2D-C1D	-14.21	1.32	1.53
2	D	301	NAD	C1D-C2D	-11.82	1.32	1.51
2	E	301	NAD	O4D-C1D	9.36	1.63	1.42
2	F	301	NAD	C7N-N7N	9.10	1.50	1.33
2	B	301	NAD	C7N-N7N	9.07	1.50	1.33
2	G	301	NAD	C7N-N7N	9.06	1.50	1.33
2	C	301	NAD	C7N-N7N	9.05	1.50	1.33
2	H	301	NAD	C7N-N7N	9.03	1.50	1.33
2	A	301	NAD	C7N-N7N	8.99	1.50	1.33
2	D	301	NAD	O4D-C1D	8.81	1.63	1.43
2	D	301	NAD	O4D-C4D	-7.48	1.32	1.44
2	E	301	NAD	O4B-C4B	-7.08	1.29	1.45
2	G	301	NAD	O4B-C4B	-6.92	1.29	1.45
2	B	301	NAD	O4B-C4B	-6.92	1.29	1.45
2	F	301	NAD	O4B-C4B	-6.92	1.29	1.45
2	E	301	NAD	C2D-C1D	-6.92	1.31	1.53
2	D	301	NAD	O4B-C4B	-6.89	1.29	1.45
2	C	301	NAD	O4B-C4B	-6.88	1.29	1.45
2	A	301	NAD	O4B-C4B	-6.87	1.29	1.45
2	H	301	NAD	O4B-C4B	-6.85	1.29	1.45
2	C	301	NAD	O4D-C4D	-5.62	1.32	1.45
2	B	301	NAD	O4D-C4D	-5.61	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	O4D-C4D	-5.56	1.32	1.45
2	H	301	NAD	O4D-C4D	-5.55	1.32	1.45
2	A	301	NAD	O4D-C4D	-5.54	1.32	1.45
2	G	301	NAD	O4D-C4D	-5.52	1.32	1.45
2	E	301	NAD	O4D-C4D	-5.45	1.32	1.45
2	G	301	NAD	O2B-C2B	4.50	1.53	1.43
2	F	301	NAD	O2B-C2B	4.43	1.53	1.43
2	A	301	NAD	O2B-C2B	4.43	1.53	1.43
2	C	301	NAD	O2B-C2B	4.42	1.53	1.43
2	B	301	NAD	O2B-C2B	4.42	1.53	1.43
2	D	301	NAD	O2B-C2B	4.41	1.53	1.43
2	E	301	NAD	O2B-C2B	4.41	1.53	1.43
2	H	301	NAD	O2B-C2B	4.40	1.53	1.43
2	C	301	NAD	O3D-C3D	-3.64	1.34	1.43
2	B	301	NAD	O3D-C3D	-3.62	1.34	1.43
2	D	301	NAD	O2D-C2D	3.61	1.51	1.43
2	F	301	NAD	O3D-C3D	-3.58	1.34	1.43
2	H	301	NAD	O3D-C3D	-3.57	1.34	1.43
2	A	301	NAD	O3D-C3D	-3.56	1.34	1.43
2	E	301	NAD	O3D-C3D	-3.52	1.34	1.43
2	D	301	NAD	O3D-C3D	-3.51	1.34	1.43
2	G	301	NAD	O3D-C3D	-3.51	1.34	1.43
2	F	301	NAD	O2D-C2D	3.45	1.51	1.43
2	B	301	NAD	O2D-C2D	3.44	1.51	1.43
2	H	301	NAD	O2D-C2D	3.42	1.51	1.43
2	G	301	NAD	O2D-C2D	3.42	1.51	1.43
2	F	301	NAD	C2N-N1N	3.41	1.39	1.35
2	H	301	NAD	C6A-N6A	3.40	1.46	1.34
2	C	301	NAD	O2D-C2D	3.39	1.51	1.43
2	G	301	NAD	C6A-N6A	3.39	1.46	1.34
2	E	301	NAD	C6A-N6A	3.38	1.46	1.34
2	C	301	NAD	C6A-N6A	3.38	1.46	1.34
2	B	301	NAD	C6A-N6A	3.38	1.46	1.34
2	F	301	NAD	C6A-N6A	3.37	1.46	1.34
2	A	301	NAD	C6A-N6A	3.36	1.46	1.34
2	D	301	NAD	C6A-N6A	3.36	1.46	1.34
2	H	301	NAD	C2N-N1N	3.34	1.39	1.35
2	B	301	NAD	C2N-N1N	3.34	1.39	1.35
2	C	301	NAD	C2N-N1N	3.20	1.38	1.35
2	A	301	NAD	O2D-C2D	3.19	1.50	1.43
2	E	301	NAD	O2D-C2D	3.15	1.50	1.43
2	A	301	NAD	C2N-N1N	3.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAD	C2N-N1N	3.08	1.38	1.35
2	H	301	NAD	O3B-C3B	-2.99	1.35	1.43
2	C	301	NAD	O3B-C3B	-2.97	1.36	1.43
2	B	301	NAD	O3B-C3B	-2.96	1.36	1.43
2	F	301	NAD	O3B-C3B	-2.95	1.36	1.43
2	D	301	NAD	O3B-C3B	-2.95	1.36	1.43
2	E	301	NAD	O3B-C3B	-2.94	1.36	1.43
2	A	301	NAD	O3B-C3B	-2.92	1.36	1.43
2	G	301	NAD	O3B-C3B	-2.92	1.36	1.43
2	A	301	NAD	O7N-C7N	-2.81	1.18	1.24
2	B	301	NAD	O7N-C7N	-2.79	1.18	1.24
2	G	301	NAD	O7N-C7N	-2.79	1.18	1.24
2	C	301	NAD	O7N-C7N	-2.78	1.18	1.24
2	H	301	NAD	O7N-C7N	-2.77	1.18	1.24
2	F	301	NAD	O7N-C7N	-2.76	1.18	1.24
2	E	301	NAD	C5A-C4A	-2.45	1.34	1.40
2	F	301	NAD	C5A-C4A	-2.43	1.34	1.40
2	D	301	NAD	C5A-C4A	-2.40	1.34	1.40
2	B	301	NAD	C5A-C4A	-2.40	1.34	1.40
2	A	301	NAD	C5A-C4A	-2.40	1.34	1.40
2	H	301	NAD	C5A-C4A	-2.39	1.34	1.40
2	G	301	NAD	C5A-C4A	-2.37	1.34	1.40
2	C	301	NAD	C5A-C4A	-2.33	1.34	1.40
2	B	301	NAD	C2A-N3A	2.25	1.35	1.32
2	C	301	NAD	C2A-N3A	2.25	1.35	1.32
2	D	301	NAD	C2A-N3A	2.20	1.35	1.32
2	G	301	NAD	C2A-N3A	2.19	1.35	1.32
2	F	301	NAD	C2A-N3A	2.15	1.35	1.32
2	H	301	NAD	C2A-N3A	2.15	1.35	1.32
2	A	301	NAD	C2A-N3A	2.15	1.35	1.32
2	E	301	NAD	C2A-N3A	2.14	1.35	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAD	C5A-C6A-N6A	6.95	130.92	120.35
2	A	301	NAD	C5A-C6A-N6A	6.92	130.87	120.35
2	F	301	NAD	C5A-C6A-N6A	6.88	130.80	120.35
2	B	301	NAD	C5A-C6A-N6A	6.86	130.77	120.35
2	E	301	NAD	C5A-C6A-N6A	6.85	130.76	120.35
2	D	301	NAD	C5A-C6A-N6A	6.85	130.76	120.35
2	H	301	NAD	C5A-C6A-N6A	6.84	130.75	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAD	C5A-C6A-N6A	6.75	130.62	120.35
2	E	301	NAD	N3A-C2A-N1A	-5.83	119.57	128.68
2	A	301	NAD	N3A-C2A-N1A	-5.81	119.60	128.68
2	F	301	NAD	N3A-C2A-N1A	-5.79	119.62	128.68
2	C	301	NAD	N3A-C2A-N1A	-5.72	119.74	128.68
2	D	301	NAD	N3A-C2A-N1A	-5.71	119.76	128.68
2	H	301	NAD	N3A-C2A-N1A	-5.69	119.79	128.68
2	G	301	NAD	N3A-C2A-N1A	-5.66	119.83	128.68
2	B	301	NAD	N3A-C2A-N1A	-5.59	119.94	128.68
2	G	301	NAD	N6A-C6A-N1A	-4.57	109.09	118.57
2	B	301	NAD	N6A-C6A-N1A	-4.50	109.23	118.57
2	A	301	NAD	N6A-C6A-N1A	-4.49	109.25	118.57
2	F	301	NAD	N6A-C6A-N1A	-4.43	109.38	118.57
2	D	301	NAD	N6A-C6A-N1A	-4.43	109.39	118.57
2	E	301	NAD	N6A-C6A-N1A	-4.42	109.40	118.57
2	H	301	NAD	N6A-C6A-N1A	-4.41	109.42	118.57
2	C	301	NAD	N6A-C6A-N1A	-4.33	109.58	118.57
2	E	301	NAD	C3B-C2B-C1B	3.78	106.67	100.98
2	F	301	NAD	C3B-C2B-C1B	3.64	106.46	100.98
2	D	301	NAD	C3B-C2B-C1B	3.49	106.24	100.98
2	C	301	NAD	C3B-C2B-C1B	3.29	105.94	100.98
2	G	301	NAD	C3B-C2B-C1B	3.07	105.59	100.98
2	D	301	NAD	C1D-C2D-C3D	3.05	106.28	101.63
2	A	301	NAD	C3B-C2B-C1B	3.03	105.53	100.98
2	D	301	NAD	PN-O3-PA	-3.00	122.55	132.83
2	B	301	NAD	C3B-C2B-C1B	2.98	105.47	100.98
2	H	301	NAD	C3B-C2B-C1B	2.73	105.08	100.98
2	G	301	NAD	PN-O3-PA	-2.72	123.51	132.83
2	C	301	NAD	PN-O3-PA	-2.61	123.86	132.83
2	B	301	NAD	PN-O3-PA	-2.53	124.15	132.83
2	F	301	NAD	O4D-C1D-C2D	-2.43	103.37	106.93
2	E	301	NAD	PN-O3-PA	-2.41	124.54	132.83
2	C	301	NAD	C6N-N1N-C2N	-2.37	119.81	121.97
2	H	301	NAD	C6N-N1N-C2N	-2.35	119.84	121.97
2	A	301	NAD	PN-O3-PA	-2.32	124.88	132.83
2	B	301	NAD	C6N-N1N-C2N	-2.30	119.87	121.97
2	H	301	NAD	PN-O3-PA	-2.28	125.00	132.83
2	F	301	NAD	PN-O3-PA	-2.25	125.12	132.83
2	H	301	NAD	O4D-C1D-C2D	-2.24	103.65	106.93
2	F	301	NAD	C6N-N1N-C2N	-2.24	119.94	121.97
2	G	301	NAD	O4D-C1D-C2D	-2.09	103.87	106.93
2	G	301	NAD	C3N-C7N-N7N	2.07	120.23	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C3D-C2D-C1D	2.06	104.08	100.98
2	B	301	NAD	C3N-C7N-N7N	2.06	120.22	117.75
2	C	301	NAD	C3N-C7N-N7N	2.06	120.22	117.75

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	O4D-C4D-C5D-O5D
2	D	301	NAD	C3D-C4D-C5D-O5D
2	B	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	PN-O3-PA-O5B
2	G	301	NAD	C2N-C3N-C7N-O7N
2	G	301	NAD	C2N-C3N-C7N-N7N
2	E	301	NAD	O4D-C4D-C5D-O5D
2	E	301	NAD	C3D-C4D-C5D-O5D
2	G	301	NAD	C4N-C3N-C7N-O7N
2	G	301	NAD	C4N-C3N-C7N-N7N
2	G	301	NAD	O4D-C4D-C5D-O5D
2	A	301	NAD	O4D-C4D-C5D-O5D
2	A	301	NAD	C3D-C4D-C5D-O5D
2	D	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	C4B-C5B-O5B-PA
2	H	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	PN-O3-PA-O1A
2	D	301	NAD	PN-O3-PA-O1A
2	B	301	NAD	C4B-C5B-O5B-PA
2	C	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	C4B-C5B-O5B-PA

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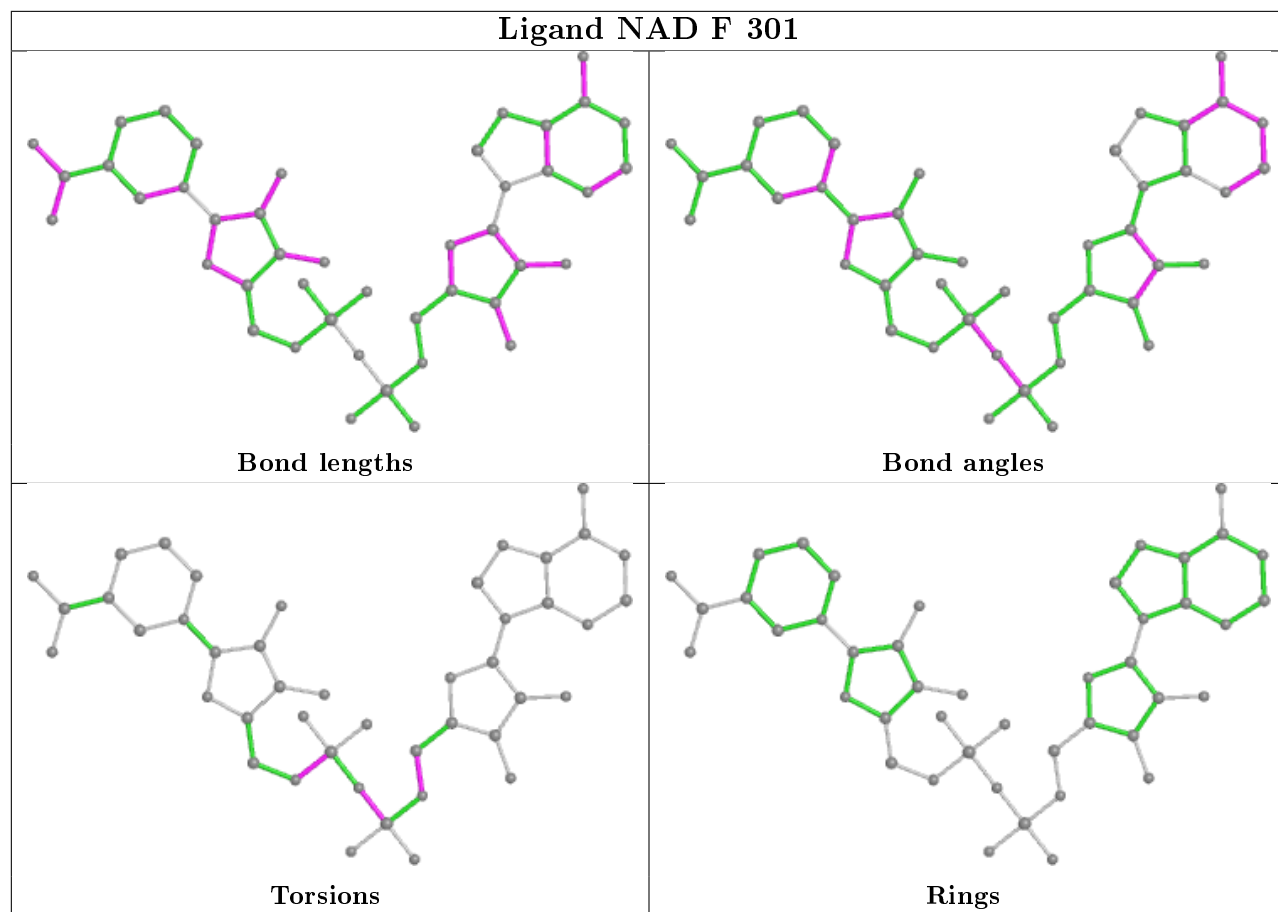
Mol	Chain	Res	Type	Atoms
2	G	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C3D-C4D-C5D-O5D
2	D	301	NAD	O4B-C4B-C5B-O5B
2	B	301	NAD	O4D-C4D-C5D-O5D
2	H	301	NAD	PA-O3-PN-O1N
2	G	301	NAD	PA-O3-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5D-O5D-PN-O1N

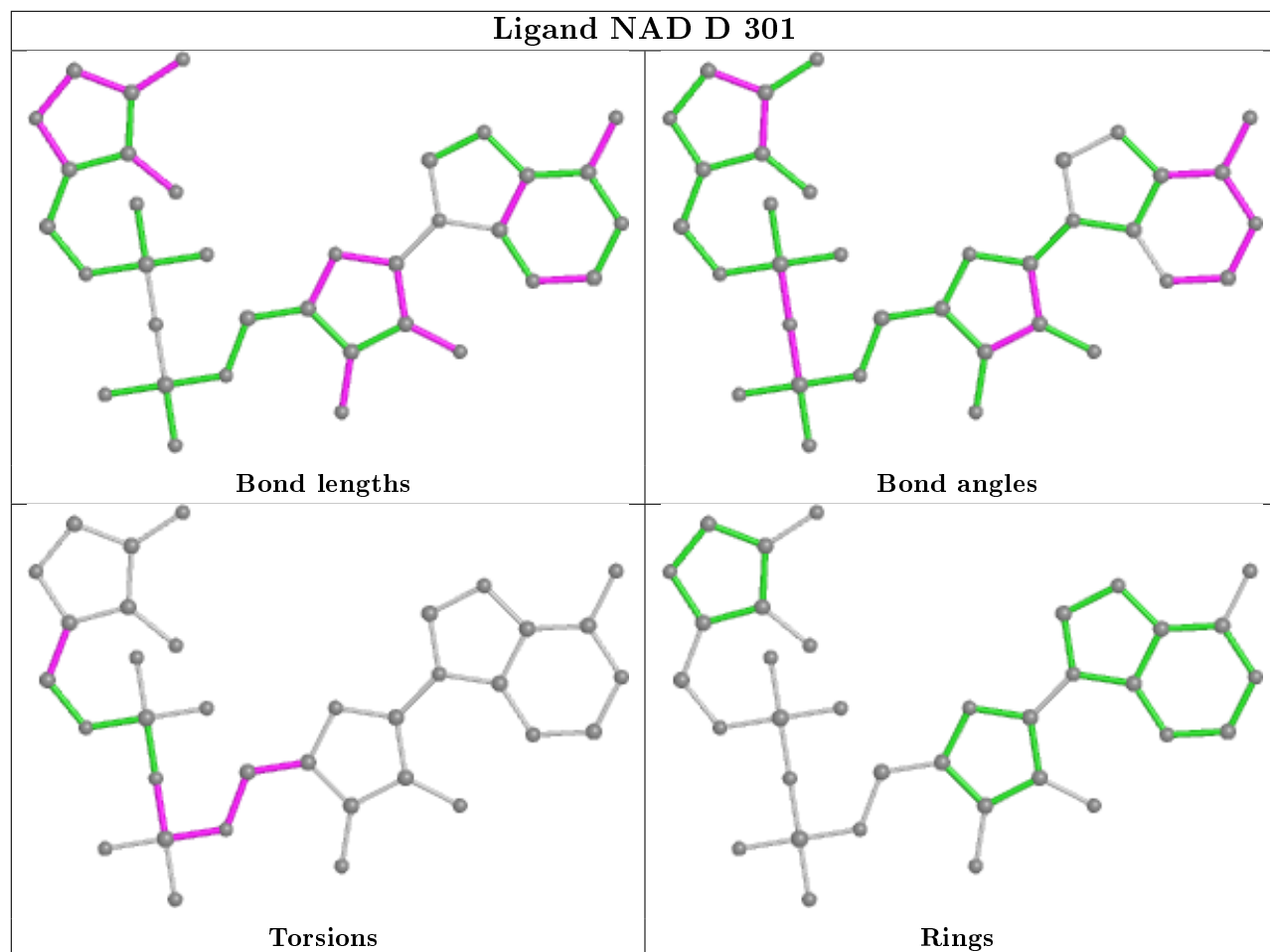
There are no ring outliers.

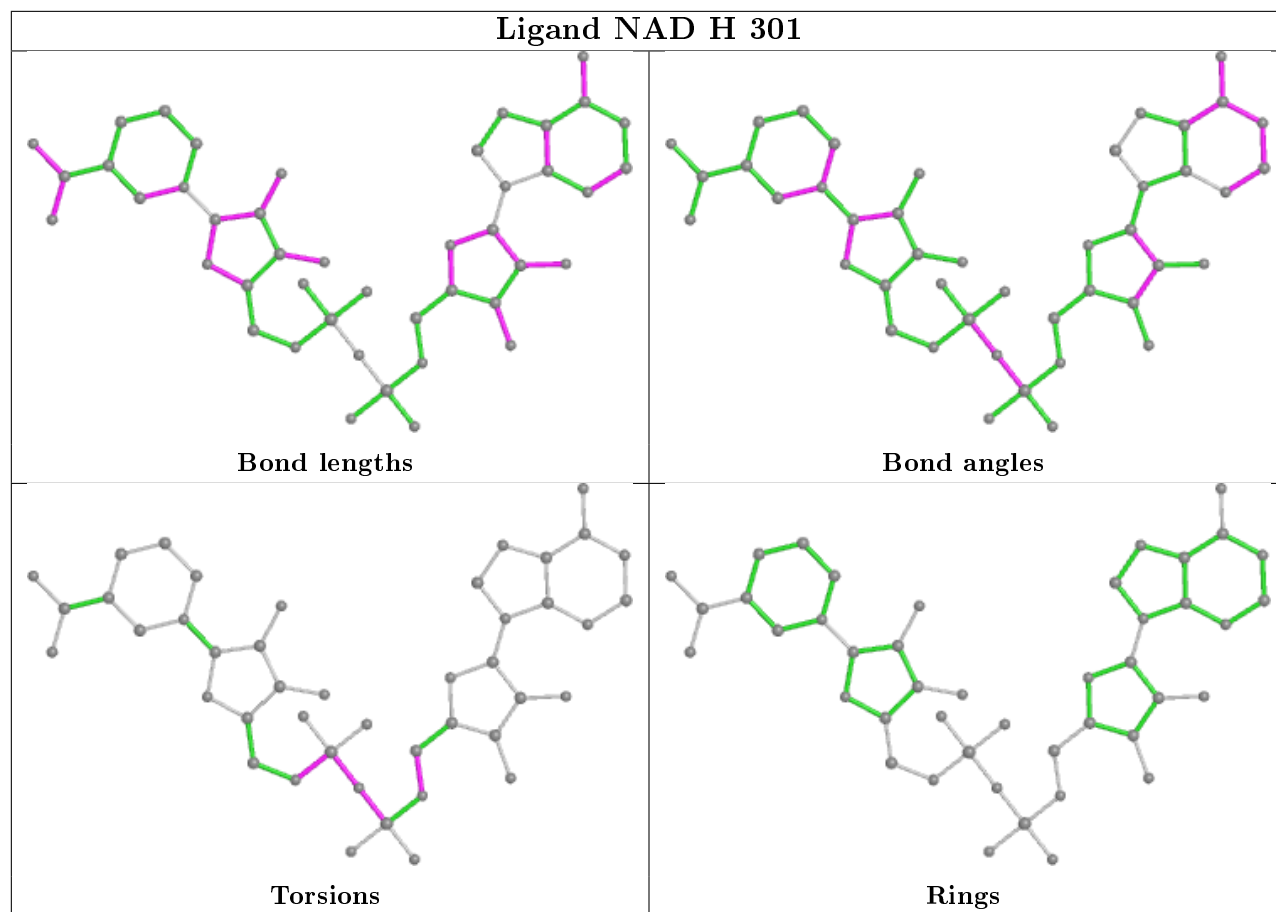
8 monomers are involved in 16 short contacts:

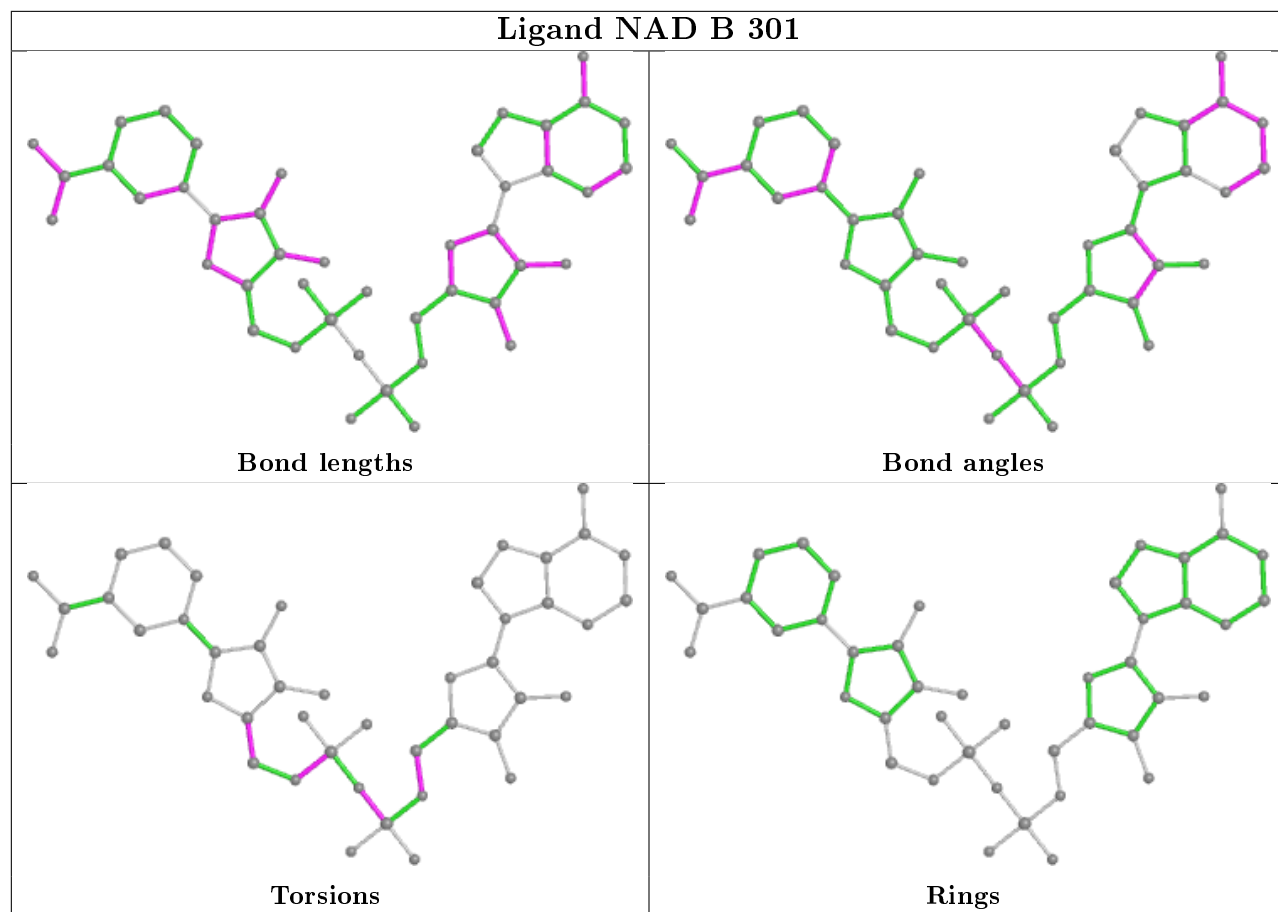
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	NAD	1	0
2	D	301	NAD	2	0
2	H	301	NAD	2	0
2	B	301	NAD	2	0
2	C	301	NAD	1	0
2	A	301	NAD	3	0
2	G	301	NAD	3	0
2	E	301	NAD	2	0

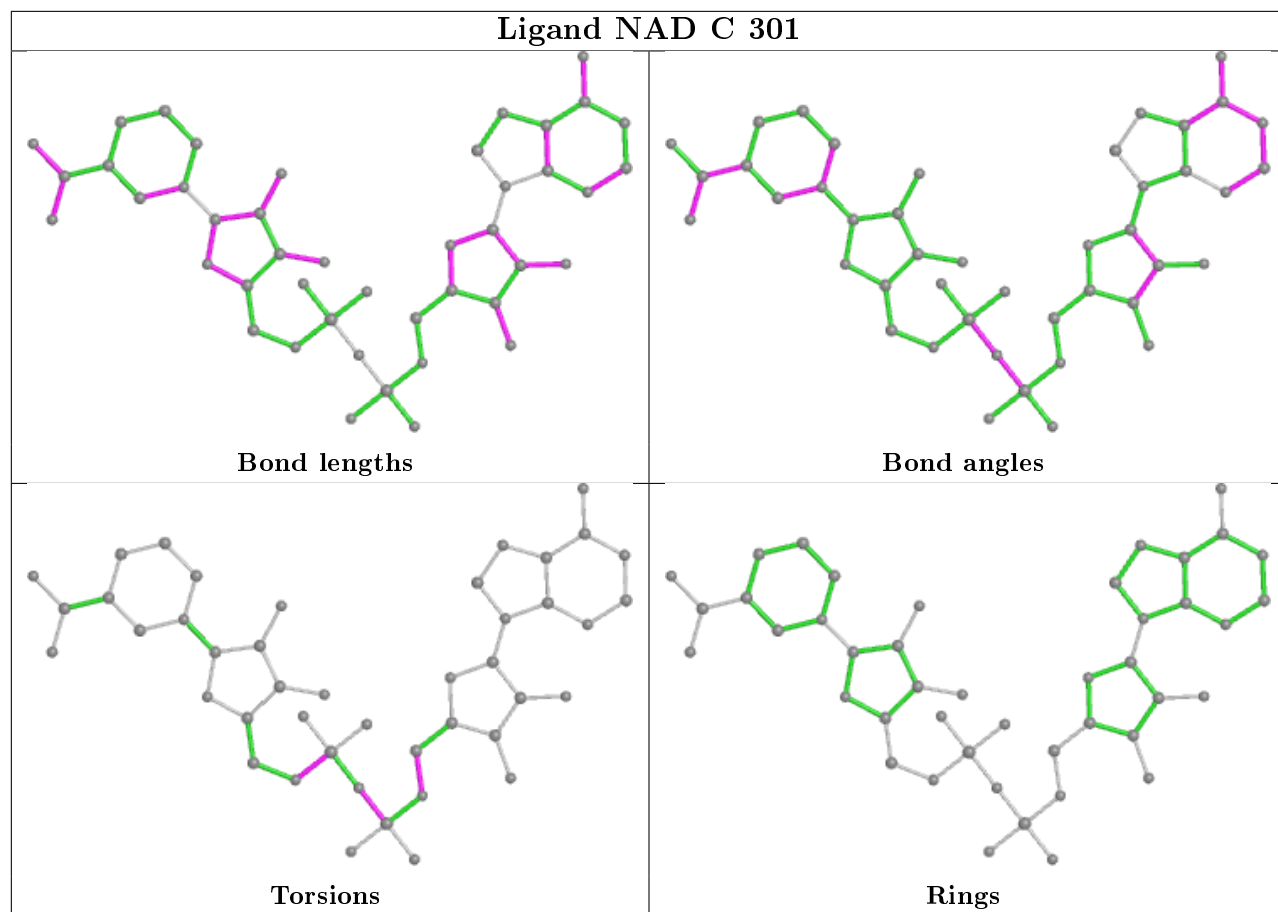
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

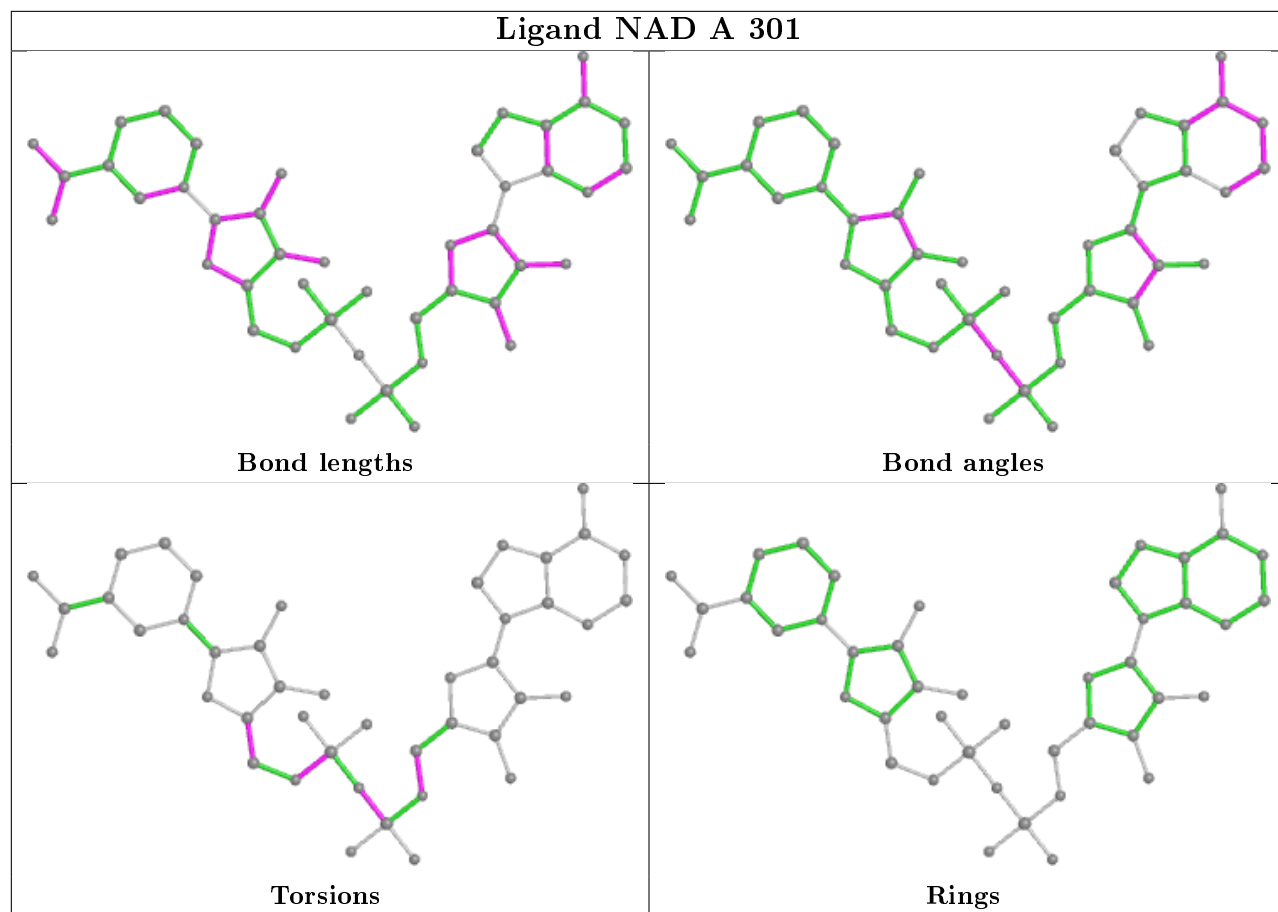


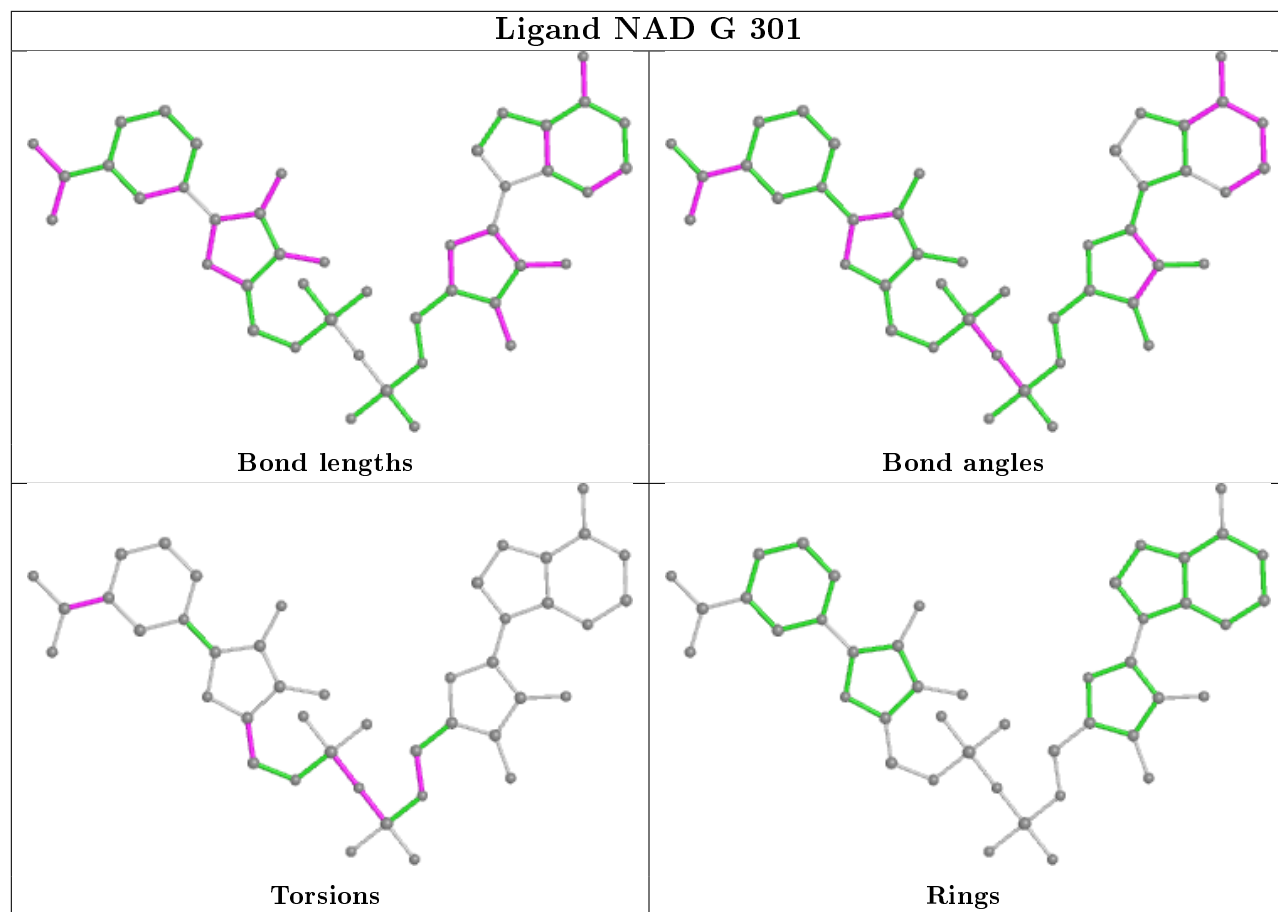




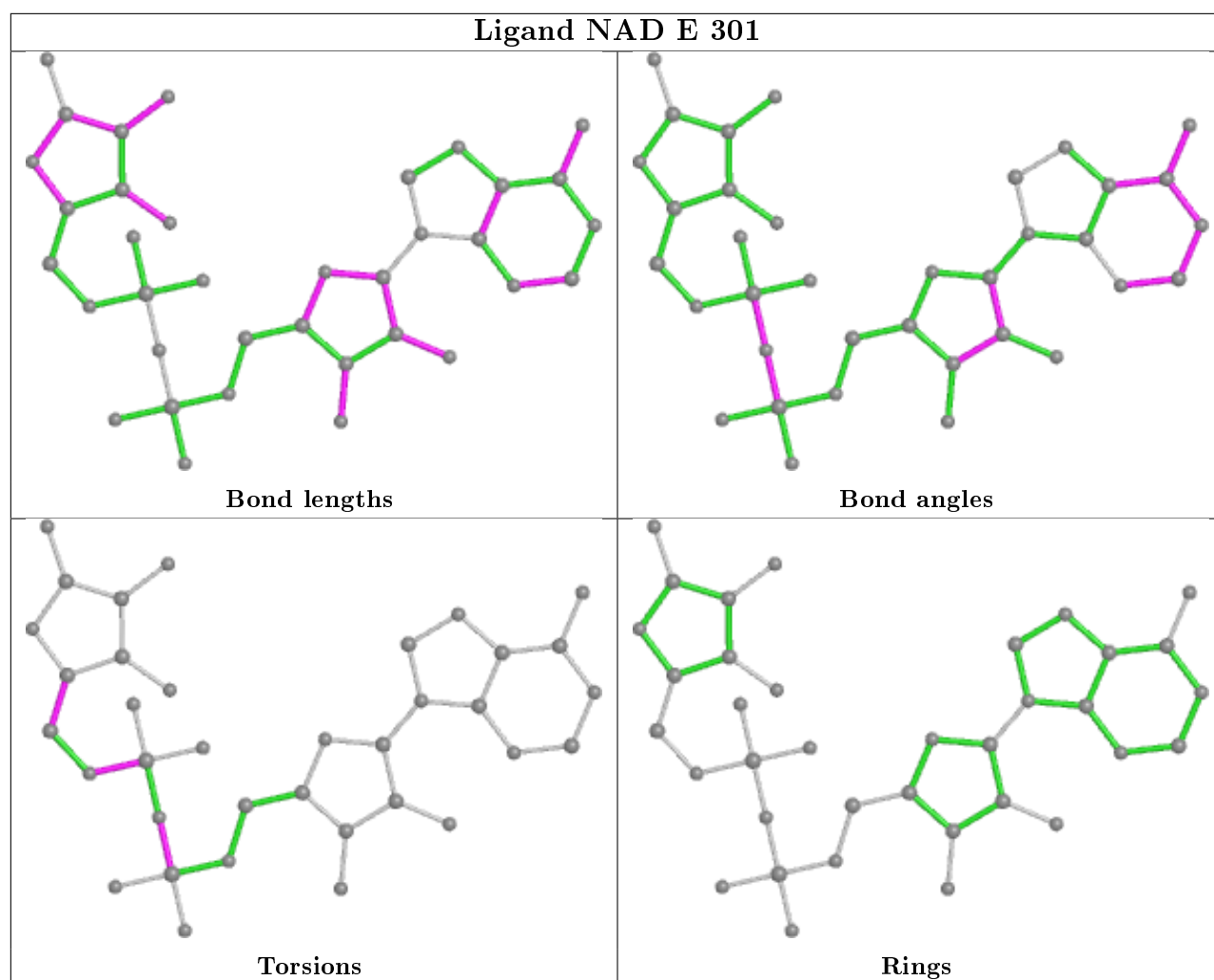












## 5.7 Other polymers [i](#)

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	268/275 (97%)	-0.45	4 (1%) 73 71	30, 43, 68, 166	0
1	B	266/275 (96%)	-0.34	5 (1%) 66 64	31, 47, 86, 133	0
1	C	265/275 (96%)	-0.33	7 (2%) 56 52	37, 51, 85, 166	0
1	D	264/275 (96%)	0.17	11 (4%) 36 32	46, 74, 116, 186	0
1	E	263/275 (95%)	-0.17	8 (3%) 50 46	34, 54, 88, 162	0
1	F	264/275 (96%)	0.53	22 (8%) 11 9	51, 92, 139, 212	0
1	G	265/275 (96%)	-0.15	9 (3%) 45 41	36, 54, 93, 157	0
1	H	267/275 (97%)	-0.15	8 (2%) 50 46	37, 56, 84, 188	0
All	All	2122/2200 (96%)	-0.11	74 (3%) 44 39	30, 56, 112, 212	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	ILE	7.7
1	E	208	LEU	7.0
1	H	211	PRO	6.8
1	E	221	LEU	6.3
1	E	222	VAL	6.2
1	F	222	VAL	6.1
1	F	129	GLN	6.0
1	F	220	PRO	5.9
1	C	90	ALA	5.7
1	H	209	LYS	5.6
1	C	1	MET	5.3
1	F	208	LEU	5.1
1	H	2	THR	4.8
1	E	89	GLN	4.7
1	F	89	GLN	4.7
1	D	89	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	208	LEU	4.3
1	D	220	PRO	4.3
1	F	91	ASP	4.2
1	D	88	GLU	4.1
1	F	1	MET	4.0
1	C	89	GLN	4.0
1	D	219	LYS	3.9
1	C	208	LEU	3.8
1	E	1	MET	3.8
1	F	90	ALA	3.7
1	G	221	LEU	3.7
1	G	220	PRO	3.7
1	F	223	ALA	3.7
1	H	220	PRO	3.6
1	F	206	LEU	3.6
1	F	221	LEU	3.6
1	D	221	LEU	3.5
1	B	89	GLN	3.4
1	D	90	ALA	3.4
1	B	209	LYS	3.4
1	A	217	ASP	3.4
1	F	57	ALA	3.3
1	F	60	LEU	3.3
1	G	207	TYR	3.3
1	A	216	GLU	3.2
1	B	208	LEU	3.1
1	A	220	PRO	3.1
1	D	208	LEU	2.9
1	F	73	GLY	2.9
1	G	88	GLU	2.9
1	C	220	PRO	2.8
1	H	40[A]	PHE	2.8
1	F	164	ALA	2.8
1	B	1	MET	2.8
1	E	91	ASP	2.8
1	D	87	GLY	2.7
1	F	86	TYR	2.7
1	F	87	GLY	2.7
1	G	2	THR	2.6
1	F	205	ALA	2.6
1	G	91	ASP	2.6
1	D	91	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	2	THR	2.6
1	B	221	LEU	2.5
1	H	219	LYS	2.5
1	C	219	LYS	2.5
1	G	219	LYS	2.4
1	G	209	LYS	2.4
1	F	58	GLY	2.4
1	F	128	VAL	2.3
1	F	229	GLY	2.3
1	D	206	LEU	2.3
1	H	221	LEU	2.2
1	D	160	GLY	2.2
1	F	88	GLU	2.2
1	E	90	ALA	2.0
1	A	209	LYS	2.0
1	C	2	THR	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 carbohydrates 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.

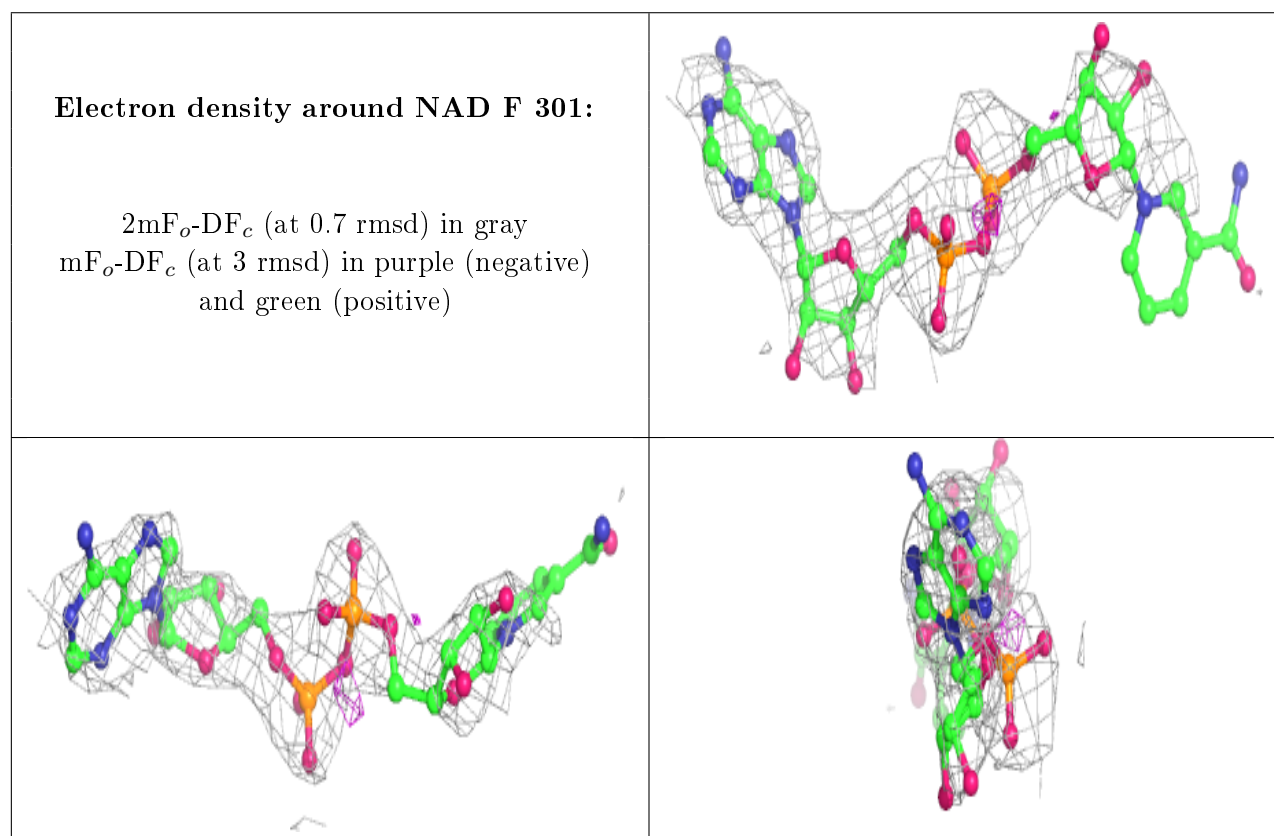
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	F	301	44/44	0.82	0.29	99,108,136,137	0
2	NAD	E	301	36/44	0.91	0.16	76,89,95,100	0
2	NAD	G	301	44/44	0.94	0.16	56,68,103,107	0
2	NAD	C	301	44/44	0.95	0.13	44,53,77,78	0
2	NAD	D	301	35/44	0.95	0.13	59,67,81,84	0
2	NAD	H	301	44/44	0.95	0.16	41,54,105,112	0
2	NAD	B	301	44/44	0.96	0.14	45,52,89,91	0

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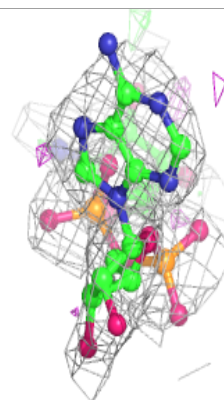
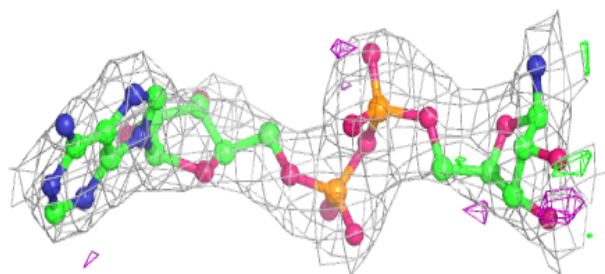
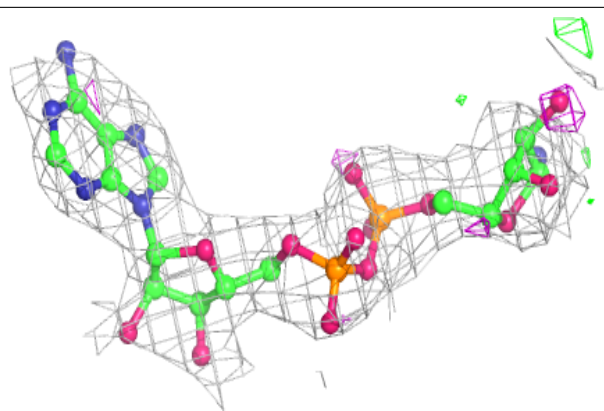
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	A	301	44/44	0.96	0.13	31,44,79,82	0

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.

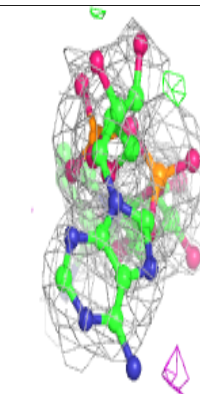
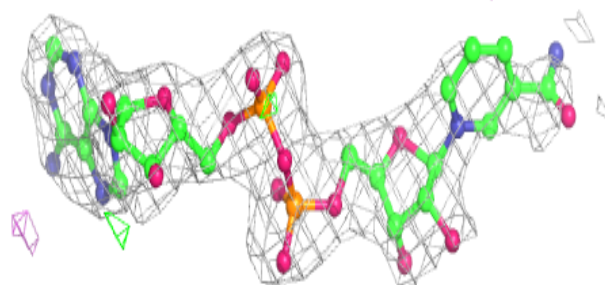
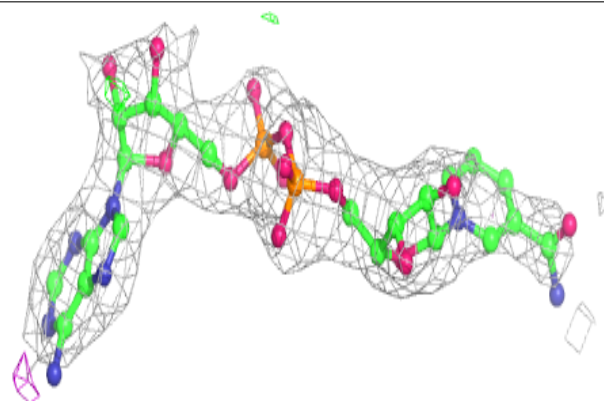


**Electron density around NAD E 301:**

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

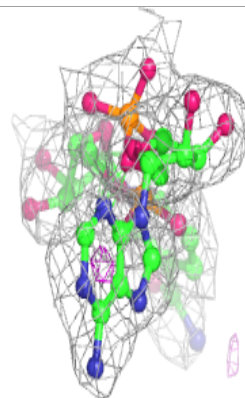
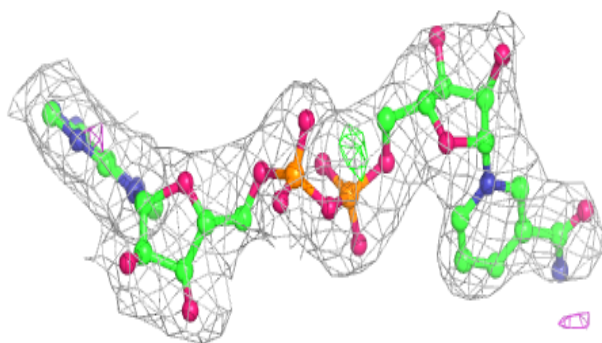
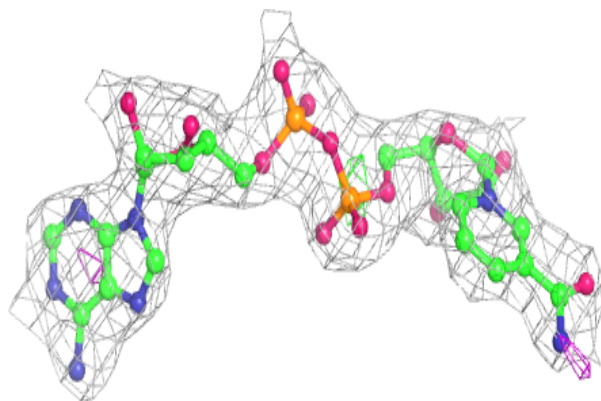
**Electron density around NAD G 301:**

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

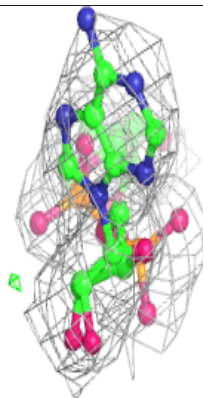
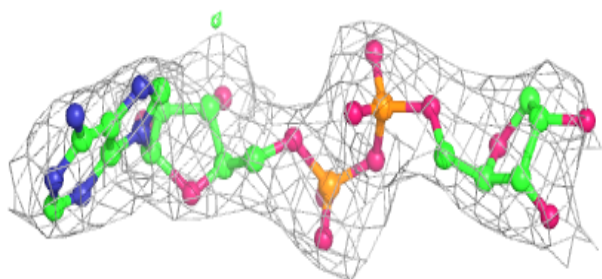
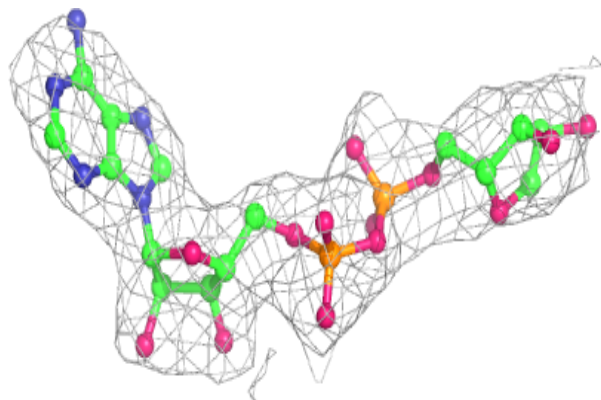


**Electron density around NAD C 301:**

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

**Electron density around NAD D 301:**

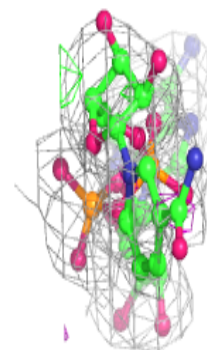
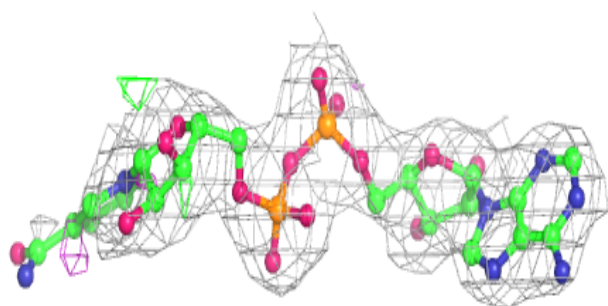
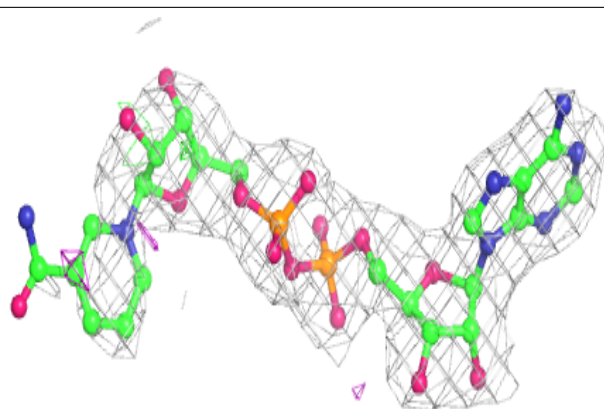
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



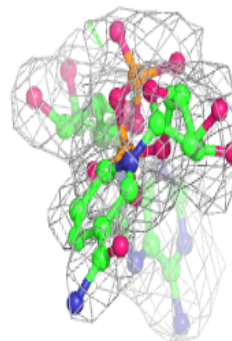
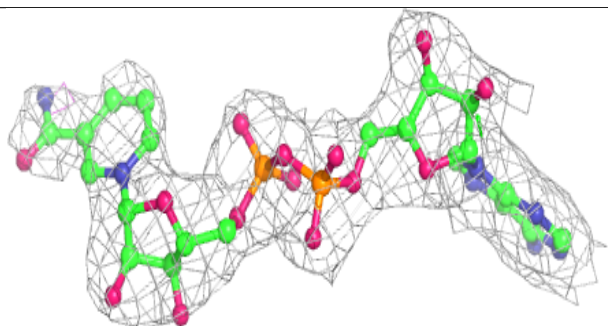
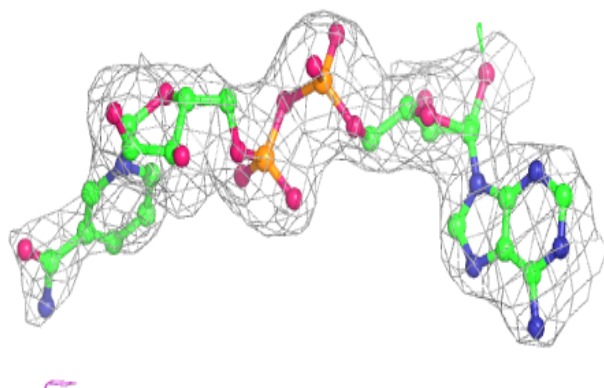


**Electron density around NAD H 301:**

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

**Electron density around NAD B 301:**

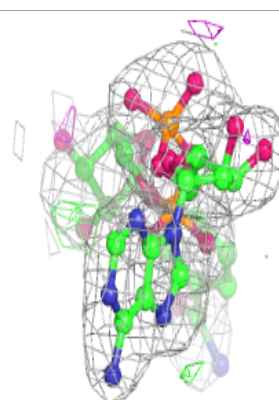
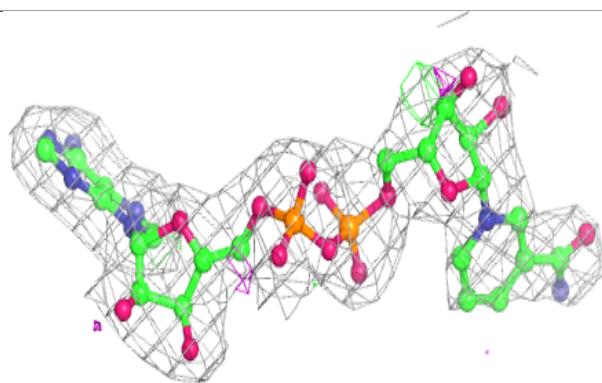
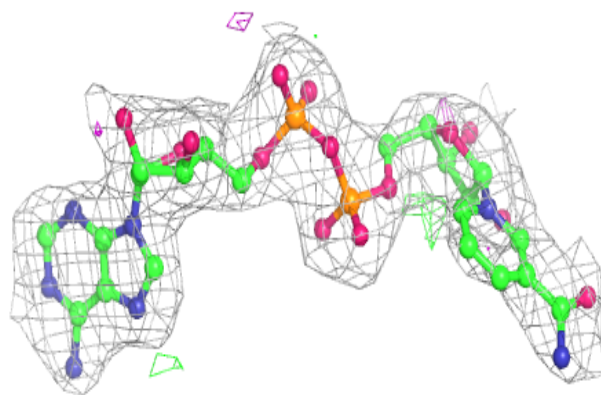
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NAD A 301:**

$2mF_o - DF_c$  (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.