



# Full wwPDB X-ray Structure Validation Report

Aug 27, 2023 – 01:19 PM EDT

PDB ID : 3IJR  
Title : 2.05 Angstrom resolution crystal structure of a short chain dehydrogenase from Bacillus anthracis str. 'Ames Ancestor' in complex with NAD+  
Authors : Halavaty, A.S.; Minasov, G.; Skarina, T.; Onopriyenko, O.; Gordon, E.; Kwon, K.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2009-08-04  
Resolution : 2.05 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

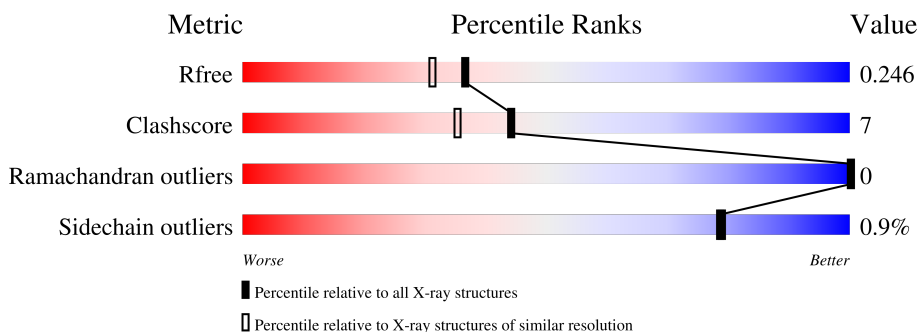
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	291	89% 8% .
1	B	291	87% 9% ..
1	C	291	88% 8% .
1	D	291	89% 8% .
1	E	291	79% 16% .
1	F	291	84% 16%
1	G	291	82% 14% .

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Mol	Chain	Length	Quality of chain
1	H	291	 88% 11%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19037 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 Oxidoreductase, short chain dehydrogenase/reductase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	281	2211	1392	374	439	2	4	0	7	0
1	B	283	2195	1386	371	432	2	4	0	3	0
1	C	281	2201	1390	371	434	2	4	0	6	0
1	D	281	2197	1385	371	435	2	4	0	6	0
1	E	280	2157	1361	364	426	2	4	0	2	0
1	F	290	2263	1425	383	448	2	5	0	5	0
1	G	281	2190	1381	370	433	2	4	0	5	0
1	H	289	2257	1423	383	444	2	5	0	5	0

There are 24 discrepancies between the modelled and reference sequences:

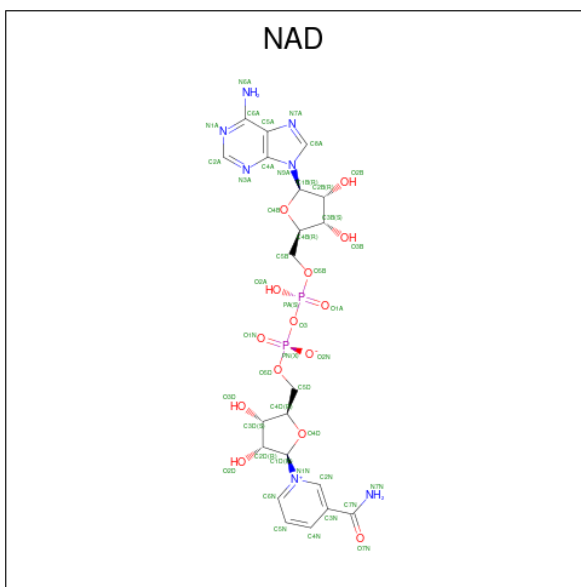
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81UV8
A	-1	ASN	-	expression tag	UNP Q81UV8
A	0	ALA	-	expression tag	UNP Q81UV8
B	-2	SER	-	expression tag	UNP Q81UV8
B	-1	ASN	-	expression tag	UNP Q81UV8
B	0	ALA	-	expression tag	UNP Q81UV8
C	-2	SER	-	expression tag	UNP Q81UV8
C	-1	ASN	-	expression tag	UNP Q81UV8
C	0	ALA	-	expression tag	UNP Q81UV8
D	-2	SER	-	expression tag	UNP Q81UV8
D	-1	ASN	-	expression tag	UNP Q81UV8
D	0	ALA	-	expression tag	UNP Q81UV8
E	-2	SER	-	expression tag	UNP Q81UV8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q81UV8
E	0	ALA	-	expression tag	UNP Q81UV8
F	-2	SER	-	expression tag	UNP Q81UV8
F	-1	ASN	-	expression tag	UNP Q81UV8
F	0	ALA	-	expression tag	UNP Q81UV8
G	-2	SER	-	expression tag	UNP Q81UV8
G	-1	ASN	-	expression tag	UNP Q81UV8
G	0	ALA	-	expression tag	UNP Q81UV8
H	-2	SER	-	expression tag	UNP Q81UV8
H	-1	ASN	-	expression tag	UNP Q81UV8
H	0	ALA	-	expression tag	UNP Q81UV8

- 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		
			Total	C	N	O			P	
2	A	1	Total	44	21	7	14	2	0	0
2	B	1	Total	44	21	7	14	2	0	0
2	C	1	Total	44	21	7	14	2	0	0
2	D	1	Total	44	21	7	14	2	0	0
2	E	1	Total	44	21	7	14	2	0	0

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0



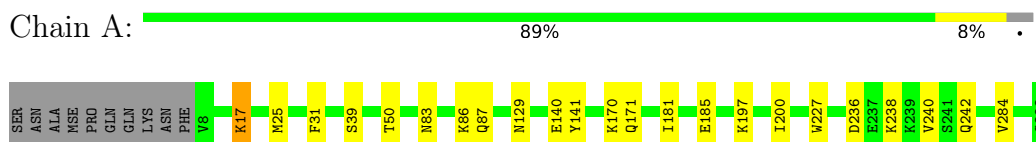
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total 172	O 172	0	5
5	B	127	Total 127	O 127	0	0
5	C	149	Total 151	O 151	0	3
5	D	132	Total 132	O 132	0	1
5	E	68	Total 68	O 68	0	0
5	F	79	Total 79	O 79	0	1
5	G	105	Total 105	O 105	0	0
5	H	102	Total 102	O 102	0	1

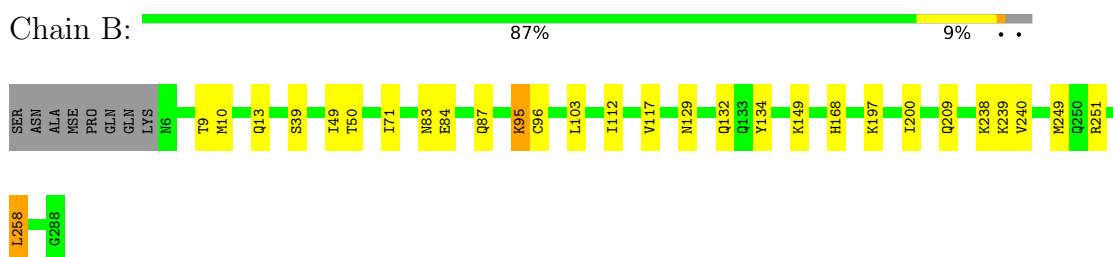
### 3 Residue-property plots [i](#)

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. 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. 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.

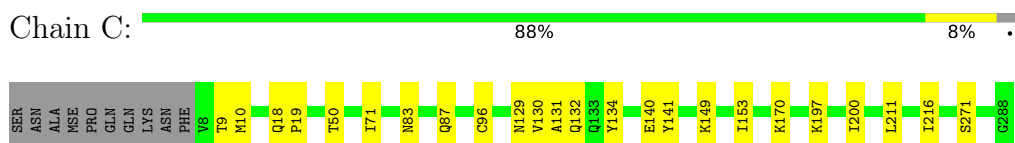
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



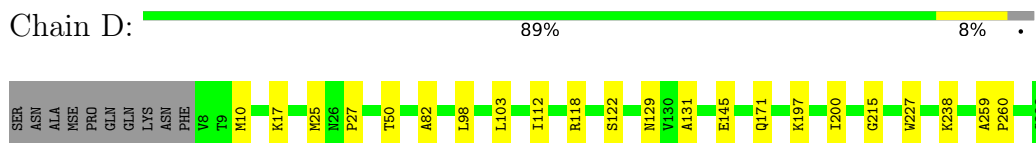
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



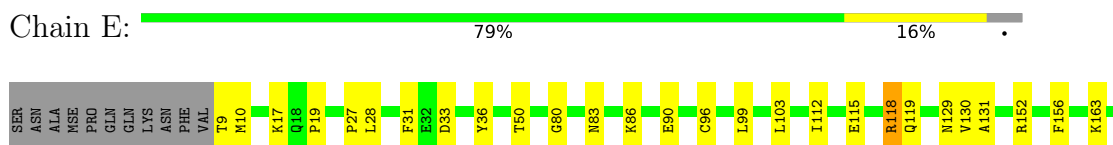
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

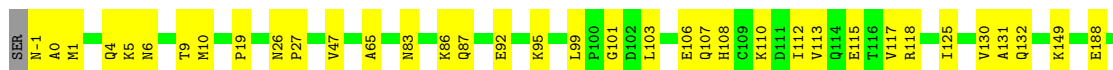
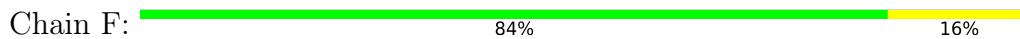


- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

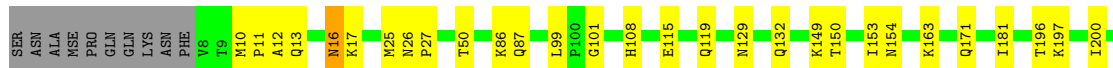
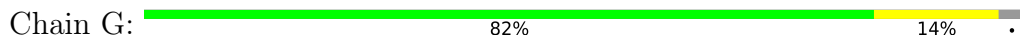




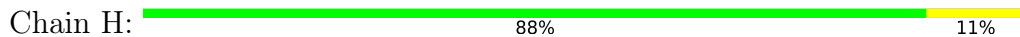
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.75Å 123.20Å 169.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 30.01 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.05) 99.6 (30.01-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.157 , 0.193 0.221 , 0.246	Depositor DCC
$R_{free}$ test set	7373 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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: MG, SO4, 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	0.57	0/2248	0.66	0/3042
1	B	0.55	0/2233	0.66	1/3022 (0.0%)
1	C	0.56	0/2238	0.65	0/3027
1	D	0.53	0/2234	0.65	0/3022
1	E	0.44	0/2194	0.61	0/2969
1	F	0.47	0/2301	0.63	0/3112
1	G	0.48	0/2227	0.63	0/3013
1	H	0.48	0/2295	0.62	0/3103
All	All	0.51	0/17970	0.64	1/24310 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	CA-CB-CG	-5.10	103.58	115.30

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	2211	0	2178	18	0
1	B	2195	0	2169	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2201	0	2183	24	0
1	D	2197	0	2173	20	0
1	E	2157	0	2135	56	0
1	F	2263	0	2231	45	0
1	G	2190	0	2168	30	1
1	H	2257	0	2234	29	0
2	A	44	0	25	1	0
2	B	44	0	25	1	0
2	C	44	0	25	6	0
2	D	44	0	25	1	0
2	E	44	0	25	5	0
2	F	44	0	26	4	0
2	G	44	0	26	0	0
2	H	44	0	25	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	20	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	1	0
4	H	5	0	0	0	0
5	A	172	0	0	5	0
5	B	127	0	0	3	0
5	C	151	0	0	0	0
5	D	132	0	0	2	0
5	E	68	0	0	14	0
5	F	79	0	0	6	0
5	G	105	0	0	1	0
5	H	102	0	0	1	0
All	All	19037	0	17673	237	1

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 7.

All (237) 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:D:10:MSE:HE2	1:D:227:TRP:CE2	1.89	1.06
1:G:10:MSE:HE2	1:G:227:TRP:CZ2	1.95	1.00
1:A:185[B]:GLU:OE2	1:A:284:VAL:HG11	1.60	1.00
1:G:10:MSE:HE1	1:G:27:PRO:HD2	1.41	0.99
1:H:3:GLN:NE2	1:H:6:ASN:HD22	1.64	0.96
1:A:181:ILE:HD11	1:A:185[B]:GLU:OE2	1.69	0.93
1:D:10:MSE:CE	1:D:227:TRP:CE2	2.53	0.90
1:D:10:MSE:HE2	1:D:227:TRP:CD2	2.06	0.90
1:A:83[B]:ASN:HB3	5:A:720[B]:HOH:O	1.77	0.84
1:E:10:MSE:HE2	1:E:227:TRP:CE2	2.12	0.84
1:G:16:ASN:C	1:G:16:ASN:HD22	1.82	0.81
1:E:99:LEU:HD11	5:E:695:HOH:O	1.79	0.81
1:H:87[B]:GLN:HE21	1:H:87[B]:GLN:HA	1.44	0.80
1:H:3:GLN:HE22	1:H:6:ASN:HD22	1.28	0.80
1:A:171:GLN:HG3	5:A:388:HOH:O	1.84	0.78
1:G:132:GLN:HE22	1:G:149:LYS:HE2	1.48	0.78
1:H:3:GLN:HE22	1:H:6:ASN:ND2	1.81	0.78
1:G:10:MSE:HE2	1:G:227:TRP:CE2	2.19	0.77
1:A:83[B]:ASN:O	1:A:87[B]:GLN:HG2	1.86	0.76
1:E:118:ARG:HG3	1:E:118:ARG:HH11	1.51	0.76
1:F:1:MSE:CE	5:F:649:HOH:O	2.34	0.75
1:F:10:MSE:HE2	1:F:10:MSE:HA	1.69	0.74
1:C:10:MSE:HE2	1:C:10:MSE:HA	1.71	0.73
1:A:185[B]:GLU:OE2	1:A:284:VAL:CG1	2.37	0.73
1:C:130[B]:VAL:HG11	1:C:153:ILE:HD11	1.70	0.73
1:E:130:VAL:HG23	2:E:301:NAD:C1B	2.19	0.72
1:H:3:GLN:NE2	1:H:6:ASN:ND2	2.33	0.72
1:F:9:THR:O	1:F:10:MSE:HE3	1.89	0.72
1:E:96:CYS:CB	5:E:694:HOH:O	2.39	0.71
2:A:301:NAD:N7N	5:A:816:HOH:O	2.21	0.70
1:F:1:MSE:HE3	5:F:649:HOH:O	1.92	0.69
1:F:65:ALA:O	1:F:92[B]:GLU:HG2	1.93	0.69
1:E:28:LEU:HD22	5:E:707:HOH:O	1.92	0.69
1:B:9:THR:O	1:B:10:MSE:HE3	1.93	0.68
1:C:132:GLN:HE22	1:C:149:LYS:HE2	1.56	0.68
1:B:10:MSE:HA	1:B:10:MSE:HE2	1.76	0.68
1:E:99:LEU:CD2	1:E:115:GLU:HG2	2.23	0.68
1:C:130[A]:VAL:HG23	2:C:301:NAD:N9A	2.11	0.66
1:G:171:GLN:NE2	5:G:627:HOH:O	2.27	0.65
1:C:130[A]:VAL:HG23	2:C:301:NAD:C1B	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:GLN:NE2	1:F:5:LYS:O	2.30	0.65
1:C:9:THR:O	1:C:10:MSE:HE3	1.97	0.65
1:E:10:MSE:HE3	1:E:27:PRO:HD2	1.77	0.65
1:C:9:THR:O	1:C:10:MSE:CE	2.45	0.64
1:F:4:GLN:NE2	1:F:6:ASN:OD1	2.30	0.64
1:B:83:ASN:O	1:B:87[A]:GLN:HG2	1.99	0.63
1:G:10:MSE:CE	1:G:27:PRO:HD2	2.25	0.62
1:E:90:GLU:HG3	5:E:694:HOH:O	1.99	0.62
1:F:95:LYS:NZ	5:F:566:HOH:O	2.28	0.62
1:E:118:ARG:HH11	1:E:118:ARG:CG	2.11	0.61
1:F:1:MSE:HE2	5:F:649:HOH:O	1.99	0.61
1:F:103:LEU:HD21	1:F:112:ILE:HD13	1.82	0.61
1:F:99:LEU:CD2	1:F:115:GLU:HG2	2.30	0.61
1:E:10:MSE:HE2	1:E:227:TRP:CD2	2.35	0.61
1:E:10:MSE:CE	1:E:27:PRO:HD2	2.31	0.60
1:G:10:MSE:HE3	1:G:11:PRO:HD2	1.82	0.60
1:B:84:GLU:O	1:B:87[B]:GLN:HG2	2.02	0.59
1:D:10:MSE:CE	1:D:27:PRO:HD2	2.33	0.59
1:E:9:THR:HG21	5:E:862:HOH:O	2.01	0.59
1:E:228:THR:HB	1:E:229:PRO:HD2	1.82	0.59
1:H:83:ASN:O	1:H:87[B]:GLN:HG2	2.02	0.59
1:C:197:LYS:HD3	1:C:200:ILE:HD12	1.84	0.59
1:G:10:MSE:HE2	1:G:227:TRP:CH2	2.36	0.59
1:D:10:MSE:CE	1:D:227:TRP:CZ2	2.86	0.58
1:F:132:GLN:HE22	1:F:149:LYS:HE2	1.67	0.58
1:E:99:LEU:HD21	1:E:115:GLU:CG	2.34	0.58
1:B:49:ILE:HG23	1:B:49:ILE:O	2.04	0.57
1:F:115:GLU:OE1	1:F:118:ARG:NH1	2.38	0.57
1:F:99:LEU:HD22	1:F:115:GLU:HG2	1.87	0.57
1:G:10:MSE:CE	1:G:227:TRP:CZ2	2.80	0.56
1:E:31:PHE:HB3	5:E:445:HOH:O	2.06	0.56
1:E:10:MSE:HE2	1:E:227:TRP:CZ2	2.40	0.56
1:H:87[B]:GLN:HE21	1:H:87[B]:GLN:CA	2.15	0.56
1:A:181:ILE:CD1	1:A:185[B]:GLU:OE2	2.51	0.55
1:G:16:ASN:C	1:G:16:ASN:ND2	2.56	0.55
1:C:140[A]:GLU:HG2	1:C:141:TYR:CD1	2.42	0.54
1:E:248:PRO:HG2	1:E:283:GLY:O	2.07	0.54
1:F:131:ALA:HB3	2:F:301:NAD:H3D	1.90	0.54
1:B:197:LYS:HD3	1:B:200:ILE:HD12	1.90	0.54
1:G:25:MSE:HE2	1:G:227:TRP:CE2	2.42	0.54
1:D:197:LYS:HD3	1:D:200:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:-1:ASN:HA	1:F:188:GLU:OE2	2.08	0.54
1:G:50:THR:O	1:G:129:ASN:HB3	2.08	0.54
1:E:197:LYS:HD3	1:E:200:ILE:HD12	1.90	0.53
1:E:96:CYS:HB3	5:E:694:HOH:O	2.04	0.53
1:G:13:GLN:NE2	1:G:26:ASN:O	2.41	0.53
1:C:271:SER:HA	4:C:328:SO4:O4	2.09	0.53
1:H:118:ARG:NE	5:H:782:HOH:O	2.39	0.53
1:A:31:PHE:HB3	5:A:309:HOH:O	2.09	0.53
1:D:145[A]:GLU:OE1	1:D:145[A]:GLU:N	2.40	0.53
5:D:625:HOH:O	1:H:8:VAL:HG21	2.08	0.53
1:H:87[B]:GLN:HA	1:H:87[B]:GLN:NE2	2.20	0.53
1:E:249:MSE:HE3	1:F:274:THR:HG22	1.91	0.53
1:F:92[B]:GLU:HG3	1:F:92[B]:GLU:O	2.09	0.53
1:E:86:LYS:HG2	5:E:694:HOH:O	2.09	0.52
1:H:101:GLY:HA3	1:H:108:HIS:CE1	2.46	0.51
1:B:129:ASN:ND2	2:B:301:NAD:H4D	2.25	0.51
1:G:101:GLY:HA3	1:G:108:HIS:CE1	2.45	0.51
1:B:117:VAL:HG21	1:B:168:HIS:CE1	2.45	0.51
1:E:80:GLY:HA2	5:E:331:HOH:O	2.11	0.51
1:G:153:ILE:HG23	1:G:154:ASN:OD1	2.10	0.51
1:H:170:LYS:N	1:H:173:ASP:OD2	2.34	0.51
1:B:132:GLN:NE2	1:B:134:TYR:OH	2.43	0.51
1:F:92[B]:GLU:O	1:F:92[B]:GLU:CG	2.59	0.51
1:D:10:MSE:HE3	1:D:27:PRO:HD2	1.92	0.50
1:C:130[B]:VAL:HG11	1:C:153:ILE:CD1	2.41	0.50
1:E:278:ILE:HD12	1:F:278:ILE:HD12	1.93	0.50
1:F:107:GLN:HB2	5:F:379:HOH:O	2.10	0.50
1:E:96:CYS:SG	5:E:694:HOH:O	2.59	0.50
1:F:101:GLY:HA3	1:F:108:HIS:CE1	2.46	0.50
1:F:4:GLN:OE1	1:F:6:ASN:OD1	2.30	0.50
1:H:99:LEU:CD2	1:H:115:GLU:HG2	2.42	0.49
1:D:131:ALA:HB3	2:D:301:NAD:H3D	1.95	0.49
1:E:187:ASN:ND2	1:E:190:LEU:HD12	2.27	0.49
1:A:17:LYS:HD2	1:A:17:LYS:C	2.33	0.49
1:B:84:GLU:OE1	5:B:724:HOH:O	2.20	0.49
1:F:130:VAL:HG12	2:F:301:NAD:H1B	1.95	0.49
1:D:25:MSE:HE2	1:D:227:TRP:CE2	2.48	0.49
1:E:99:LEU:HD21	1:E:115:GLU:HG3	1.95	0.49
1:F:10:MSE:HA	1:F:10:MSE:CE	2.41	0.48
1:C:9:THR:O	1:C:10:MSE:HE2	2.13	0.48
1:E:236:ASP:O	1:E:240:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LEU:CD2	1:G:115:GLU:HG2	2.44	0.48
1:G:150:THR:HG22	1:G:196:THR:HG21	1.95	0.48
1:B:71:ILE:O	1:B:96:CYS:HA	2.14	0.48
1:C:130[B]:VAL:HG22	2:C:301:NAD:H1B	1.95	0.48
1:C:132:GLN:NE2	1:C:134:TYR:OH	2.46	0.48
1:E:9:THR:HB	1:E:241:SER:O	2.14	0.48
1:C:50:THR:O	1:C:129:ASN:HB3	2.14	0.48
1:F:197:LYS:HD3	1:F:200:ILE:HD12	1.96	0.48
1:D:10:MSE:HE2	1:D:227:TRP:CZ2	2.45	0.48
1:H:7:PHE:HB2	1:H:10:MSE:HE1	1.94	0.48
1:B:103:LEU:HD21	1:B:112:ILE:HD13	1.96	0.47
1:A:238:LYS:NZ	1:A:242:GLN:HE22	2.12	0.47
1:C:130[A]:VAL:CG2	2:C:301:NAD:C4A	2.92	0.47
1:E:33:ASP:HB3	1:E:36:TYR:HB2	1.97	0.47
1:E:86:LYS:NZ	1:E:86:LYS:HB3	2.29	0.47
1:A:39:SER:HB3	1:B:39:SER:HB3	1.96	0.47
1:B:117:VAL:HG21	1:B:168:HIS:ND1	2.30	0.47
1:H:49:ILE:HG23	1:H:49:ILE:O	2.14	0.47
1:E:118:ARG:CG	1:E:118:ARG:NH1	2.76	0.47
1:B:249:MSE:HE1	1:B:251:ARG:HH21	1.80	0.47
1:E:185[B]:GLU:O	1:H:209[B]:GLN:NE2	2.48	0.47
1:G:278:ILE:HD12	1:H:278:ILE:HD12	1.95	0.47
1:E:259:ALA:HB3	1:E:260:PRO:HD3	1.96	0.46
1:F:125:ILE:HD13	1:F:266:ALA:HB1	1.97	0.46
1:B:209[B]:GLN:NE2	5:B:686:HOH:O	2.48	0.46
1:C:129:ASN:ND2	2:C:301:NAD:H4D	2.30	0.46
1:E:99:LEU:HD21	1:E:115:GLU:HG2	1.93	0.46
1:D:259:ALA:HB3	1:D:260:PRO:HD3	1.97	0.46
1:H:236:ASP:O	1:H:240:VAL:HG23	2.15	0.46
1:H:226:ILE:CD1	1:H:258:LEU:HD11	2.46	0.46
1:D:10:MSE:HE3	1:D:227:TRP:CZ2	2.51	0.46
1:D:171[A]:GLN:HG3	1:D:215:GLY:HA3	1.97	0.46
1:E:246:ASN:OD1	1:E:246:ASN:N	2.39	0.46
1:G:10:MSE:CE	1:G:227:TRP:CE2	2.94	0.46
1:H:129:ASN:ND2	2:H:301:NAD:H4D	2.31	0.45
1:C:83:ASN:O	1:C:87:GLN:HG2	2.15	0.45
1:G:197:LYS:HD3	1:G:200:ILE:HD12	1.98	0.45
1:F:4:GLN:CD	1:F:6:ASN:OD1	2.55	0.45
1:B:132:GLN:NE2	1:B:149:LYS:HE2	2.31	0.45
1:G:12:ALA:HB1	1:G:237:GLU:HB2	1.99	0.45
1:E:99:LEU:CD2	1:E:115:GLU:CG	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:PRO:HG3	2:F:301:NAD:C8A	2.47	0.45
1:G:181:ILE:HD11	1:G:284:VAL:HG11	1.98	0.45
1:A:197:LYS:HD3	1:A:200:ILE:HD12	1.98	0.45
1:A:236:ASP:O	1:A:240:VAL:HG23	2.16	0.45
1:D:103:LEU:HD21	1:D:112:ILE:HD13	1.99	0.45
1:G:163[A]:LYS:NZ	4:G:329:SO4:O4	2.44	0.45
1:G:248:PRO:HG2	1:G:283:GLY:O	2.17	0.45
1:H:231:ILE:HG12	1:H:243:PHE:CZ	2.52	0.45
1:E:99:LEU:HD22	1:E:115:GLU:HG2	1.96	0.45
1:E:103:LEU:HD21	1:E:112:ILE:HD13	1.99	0.45
1:E:249:MSE:HE3	1:F:274:THR:CG2	2.47	0.45
1:A:83[A]:ASN:O	1:A:86:LYS:HB3	2.16	0.44
1:B:132:GLN:HE22	1:B:149:LYS:HE2	1.82	0.44
1:E:130:VAL:HG23	2:E:301:NAD:O4B	2.17	0.44
1:F:83[B]:ASN:O	1:F:87:GLN:HG2	2.17	0.44
1:E:131:ALA:HB3	2:E:301:NAD:H3D	1.99	0.44
1:F:86:LYS:NZ	5:F:618:HOH:O	2.51	0.44
1:F:65:ALA:C	1:F:92[B]:GLU:HG2	2.37	0.44
1:D:50:THR:O	1:D:129:ASN:HB3	2.18	0.44
1:E:214:LYS:HE2	5:E:436:HOH:O	2.18	0.44
1:E:226:ILE:HD12	1:E:258:LEU:HD21	1.99	0.44
1:F:101:GLY:HA3	1:F:108:HIS:NE2	2.33	0.44
1:G:25:MSE:CE	1:G:227:TRP:CE2	3.00	0.44
1:B:13:GLN:HG2	1:B:240:VAL:HG11	1.99	0.43
1:E:86:LYS:CG	5:E:694:HOH:O	2.66	0.43
1:E:17:LYS:HE3	1:E:19:PRO:O	2.18	0.43
1:C:18:GLN:HA	1:C:19:PRO:C	2.38	0.43
1:D:10:MSE:HE1	1:D:27:PRO:HD2	1.99	0.43
1:E:83:ASN:HB3	5:E:331:HOH:O	2.18	0.43
1:H:25:MSE:CE	1:H:227:TRP:CE2	3.00	0.43
1:B:95:LYS:NZ	5:B:843:HOH:O	2.33	0.43
1:A:140:GLU:HG2	1:A:141:TYR:CD1	2.54	0.43
1:B:95:LYS:HG3	1:B:96:CYS:N	2.34	0.42
1:A:50:THR:O	1:A:129:ASN:HB3	2.19	0.42
1:F:106:GLU:HG2	1:F:110:LYS:HE3	2.01	0.42
1:E:130:VAL:HG23	2:E:301:NAD:N9A	2.33	0.42
1:F:26:ASN:HA	1:F:27:PRO:HA	1.90	0.42
1:G:17:LYS:HB2	1:G:17:LYS:HE3	1.81	0.42
1:C:130[A]:VAL:HG21	1:C:153:ILE:HD11	2.00	0.42
1:F:9:THR:O	1:F:10:MSE:CE	2.64	0.42
1:G:259:ALA:HB3	1:G:260:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:GLN:NE2	1:F:149:LYS:HE2	2.34	0.42
1:D:10:MSE:CE	1:D:227:TRP:NE1	2.82	0.42
1:E:9:THR:CG2	5:E:862:HOH:O	2.64	0.42
1:H:259:ALA:HB3	1:H:260:PRO:HD3	2.02	0.42
1:F:83[A]:ASN:O	1:F:86:LYS:HB3	2.20	0.41
1:H:7:PHE:CB	1:H:10:MSE:HE1	2.50	0.41
1:H:74:ALA:HA	1:H:99:LEU:O	2.20	0.41
1:C:130[A]:VAL:HG23	2:C:301:NAD:C4A	2.50	0.41
1:H:212:VAL:HG13	1:H:213:GLN:N	2.35	0.41
1:F:47:VAL:HG22	1:F:125:ILE:HB	2.02	0.41
1:F:231:ILE:HB	1:F:232:PRO:CD	2.50	0.41
1:E:130:VAL:HG23	2:E:301:NAD:H1B	1.98	0.41
1:E:50:THR:O	1:E:129:ASN:HB3	2.21	0.41
1:A:25:MSE:HE2	1:A:227:TRP:CE2	2.55	0.41
1:C:130[B]:VAL:CG1	1:C:131:ALA:N	2.83	0.41
1:F:0:ALA:HB2	1:G:209:GLN:OE1	2.21	0.41
1:E:152:ARG:HA	1:E:156:PHE:CD2	2.56	0.41
1:E:248:PRO:HG2	1:E:283:GLY:C	2.41	0.41
1:H:25:MSE:HE2	1:H:227:TRP:CE2	2.55	0.41
1:B:50:THR:O	1:B:129:ASN:HB3	2.21	0.41
1:C:71:ILE:O	1:C:96:CYS:HA	2.21	0.41
1:A:86:LYS:NZ	5:A:313:HOH:O	2.54	0.40
1:D:82:ALA:HB1	1:D:98:LEU:HD22	2.04	0.40
1:E:115:GLU:OE2	1:E:119:GLN:NE2	2.54	0.40
1:F:236[B]:ASP:O	1:F:240:VAL:HG23	2.21	0.40
1:C:211:LEU:HB3	1:C:216:ILE:HB	2.03	0.40
1:D:122[B]:SER:OG	5:D:590:HOH:O	2.21	0.40
1:F:113:VAL:O	1:F:117:VAL:HG23	2.22	0.40
1:E:115:GLU:CD	1:E:118:ARG:HH12	2.25	0.40
1:E:163:LYS:HG3	1:H:140:GLU:HA	2.03	0.40
1:G:236:ASP:O	1:G:240:VAL:HG23	2.22	0.40
1:H:91:LYS:HB2	1:H:91:LYS:HE3	1.93	0.40
1:F:103:LEU:HD12	2:F:301:NAD:C2A	2.52	0.40

All (1) 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)
1:G:86:LYS:NZ	1:G:119:GLN:O[2_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	A	286/291 (98%)	275 (96%)	11 (4%)	0	100	100
1	B	284/291 (98%)	272 (96%)	12 (4%)	0	100	100
1	C	285/291 (98%)	274 (96%)	11 (4%)	0	100	100
1	D	285/291 (98%)	275 (96%)	10 (4%)	0	100	100
1	E	280/291 (96%)	269 (96%)	11 (4%)	0	100	100
1	F	293/291 (101%)	280 (96%)	13 (4%)	0	100	100
1	G	284/291 (98%)	275 (97%)	9 (3%)	0	100	100
1	H	292/291 (100%)	284 (97%)	8 (3%)	0	100	100
All	All	2289/2328 (98%)	2204 (96%)	85 (4%)	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	A	242/239 (101%)	240 (99%)	2 (1%)	81	82
1	B	240/239 (100%)	236 (98%)	4 (2%)	60	57
1	C	241/239 (101%)	240 (100%)	1 (0%)	91	91
1	D	241/239 (101%)	238 (99%)	3 (1%)	71	70
1	E	236/239 (99%)	234 (99%)	2 (1%)	81	82
1	F	248/239 (104%)	247 (100%)	1 (0%)	91	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	240/239 (100%)	237 (99%)	3 (1%)	69	67
1	H	247/239 (103%)	245 (99%)	2 (1%)	81	82
All	All	1935/1912 (101%)	1917 (99%)	18 (1%)	78	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	170	LYS
1	B	95	LYS
1	B	238	LYS
1	B	239	LYS
1	B	258	LEU
1	C	170	LYS
1	D	17	LYS
1	D	118	ARG
1	D	238	LYS
1	E	118	ARG
1	E	239	LYS
1	F	258	LEU
1	G	16	ASN
1	G	87	GLN
1	G	239	LYS
1	H	17	LYS
1	H	231	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	B	129	ASN
1	B	132	GLN
1	C	129	ASN
1	C	132	GLN
1	C	171	GLN
1	D	30	GLN
1	E	250	GLN
1	F	4	GLN
1	F	87	GLN
1	F	132	GLN

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Mol	Chain	Res	Type
1	G	16	ASN
1	G	132	GLN
1	G	250	GLN
1	H	3	GLN
1	H	30	GLN
1	H	213	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](#)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

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	A	301	3	42,48,48	1.71	2 (4%)	50,73,73	1.24	4 (8%)
2	NAD	F	301	3	42,48,48	1.76	4 (9%)	50,73,73	1.36	5 (10%)
2	NAD	C	301	3	42,48,48	1.71	3 (7%)	50,73,73	1.40	5 (10%)
4	SO4	G	330	-	4,4,4	0.13	0	6,6,6	0.27	0
4	SO4	A	323	-	4,4,4	0.14	0	6,6,6	0.22	0
4	SO4	D	324	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	F	322	-	4,4,4	0.13	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	H	301	3	42,48,48	1.79	3 (7%)	50,73,73	1.16	2 (4%)
4	SO4	C	320	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	E	319	-	4,4,4	0.11	0	6,6,6	0.13	0
4	SO4	F	326	-	4,4,4	0.16	0	6,6,6	0.10	0
2	NAD	G	301	3	42,48,48	1.71	3 (7%)	50,73,73	1.23	4 (8%)
4	SO4	G	329	-	4,4,4	0.13	0	6,6,6	0.06	0
2	NAD	B	301	3	42,48,48	1.75	3 (7%)	50,73,73	1.24	5 (10%)
2	NAD	D	301	3	42,48,48	1.70	3 (7%)	50,73,73	1.42	7 (14%)
4	SO4	H	325	-	4,4,4	0.09	0	6,6,6	0.11	0
4	SO4	B	318	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	C	321	-	4,4,4	0.19	0	6,6,6	0.27	0
4	SO4	A	317	-	4,4,4	0.20	0	6,6,6	0.56	0
4	SO4	C	328	-	4,4,4	0.16	0	6,6,6	0.28	0
2	NAD	E	301	3	42,48,48	1.76	3 (7%)	50,73,73	1.26	4 (8%)
4	SO4	C	327	-	4,4,4	0.12	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	H	301	3	-	7/26/62/62	0/5/5/5
2	NAD	A	301	3	-	6/26/62/62	0/5/5/5
2	NAD	F	301	3	-	6/26/62/62	0/5/5/5
2	NAD	C	301	3	-	6/26/62/62	0/5/5/5
2	NAD	B	301	3	-	7/26/62/62	0/5/5/5
2	NAD	D	301	3	-	5/26/62/62	0/5/5/5
2	NAD	E	301	3	-	9/26/62/62	0/5/5/5
2	NAD	G	301	3	-	5/26/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	O7N-C7N	9.31	1.42	1.24
2	H	301	NAD	O7N-C7N	9.31	1.42	1.24
2	E	301	NAD	O7N-C7N	9.18	1.41	1.24
2	A	301	NAD	O7N-C7N	9.17	1.41	1.24
2	G	301	NAD	O7N-C7N	9.04	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	O7N-C7N	9.00	1.41	1.24
2	C	301	NAD	O7N-C7N	8.89	1.41	1.24
2	D	301	NAD	O7N-C7N	8.71	1.40	1.24
2	B	301	NAD	C2A-N3A	4.12	1.38	1.32
2	C	301	NAD	C2A-N3A	3.99	1.38	1.32
2	D	301	NAD	C2A-N3A	3.97	1.38	1.32
2	E	301	NAD	C2A-N3A	3.93	1.38	1.32
2	H	301	NAD	C2A-N3A	3.74	1.38	1.32
2	F	301	NAD	C2A-N3A	3.63	1.37	1.32
2	G	301	NAD	C2A-N3A	3.51	1.37	1.32
2	A	301	NAD	C2A-N3A	3.51	1.37	1.32
2	H	301	NAD	C2A-N1A	2.71	1.39	1.33
2	D	301	NAD	C2A-N1A	2.58	1.38	1.33
2	B	301	NAD	C2A-N1A	2.45	1.38	1.33
2	F	301	NAD	C2A-N1A	2.33	1.38	1.33
2	E	301	NAD	C2A-N1A	2.32	1.38	1.33
2	G	301	NAD	C2A-N1A	2.24	1.38	1.33
2	C	301	NAD	C2A-N1A	2.17	1.37	1.33
2	F	301	NAD	C2N-N1N	2.13	1.37	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	N3A-C2A-N1A	-5.96	119.36	128.68
2	C	301	NAD	N3A-C2A-N1A	-5.91	119.44	128.68
2	D	301	NAD	N3A-C2A-N1A	-5.71	119.75	128.68
2	E	301	NAD	N3A-C2A-N1A	-5.65	119.84	128.68
2	A	301	NAD	N3A-C2A-N1A	-5.51	120.06	128.68
2	H	301	NAD	N3A-C2A-N1A	-5.49	120.09	128.68
2	G	301	NAD	N3A-C2A-N1A	-5.47	120.12	128.68
2	B	301	NAD	N3A-C2A-N1A	-5.25	120.47	128.68
2	B	301	NAD	C3N-C7N-N7N	3.23	121.63	117.75
2	D	301	NAD	O4D-C1D-C2D	-3.19	102.26	106.93
2	C	301	NAD	C3N-C7N-N7N	2.98	121.33	117.75
2	G	301	NAD	C3B-C2B-C1B	2.89	105.33	100.98
2	F	301	NAD	C3B-C2B-C1B	2.76	105.13	100.98
2	D	301	NAD	C3N-C7N-N7N	2.72	121.01	117.75
2	E	301	NAD	C3N-C7N-N7N	2.67	120.95	117.75
2	C	301	NAD	O4D-C1D-C2D	-2.59	103.14	106.93
2	E	301	NAD	C3B-C2B-C1B	2.58	104.87	100.98
2	C	301	NAD	O7N-C7N-N7N	-2.57	118.93	122.58
2	F	301	NAD	O7N-C7N-N7N	-2.57	118.93	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	O7N-C7N-N7N	-2.53	118.98	122.58
2	D	301	NAD	C3B-C2B-C1B	2.48	104.71	100.98
2	G	301	NAD	PN-O3-PA	-2.46	124.38	132.83
2	F	301	NAD	PN-O3-PA	-2.46	124.38	132.83
2	B	301	NAD	C3B-C2B-C1B	2.44	104.65	100.98
2	B	301	NAD	O7N-C7N-N7N	-2.43	119.12	122.58
2	A	301	NAD	C3B-C2B-C1B	2.37	104.55	100.98
2	H	301	NAD	C3B-C2B-C1B	2.36	104.53	100.98
2	C	301	NAD	PN-O3-PA	-2.20	125.29	132.83
2	A	301	NAD	PN-O3-PA	-2.15	125.44	132.83
2	D	301	NAD	PN-O3-PA	-2.15	125.46	132.83
2	E	301	NAD	O4D-C1D-C2D	-2.12	103.82	106.93
2	D	301	NAD	C2N-C3N-C4N	2.12	120.66	118.26
2	B	301	NAD	O4D-C1D-C2D	-2.11	103.85	106.93
2	D	301	NAD	O2N-PN-O1N	2.10	122.60	112.24
2	F	301	NAD	O7N-C7N-C3N	2.02	122.05	119.63
2	G	301	NAD	C4A-C5A-N7A	-2.01	107.31	109.40

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5B-O5B-PA-O1A
2	E	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O2N
2	G	301	NAD	PN-O3-PA-O5B
2	G	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	H	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	C3B-C4B-C5B-O5B
2	B	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5B-O5B-PA-O2A
2	G	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5B-O5B-PA-O3
2	F	301	NAD	C5D-O5D-PN-O3
2	F	301	NAD	O4B-C4B-C5B-O5B
2	H	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	C5B-O5B-PA-O2A
2	C	301	NAD	C5D-O5D-PN-O2N
2	D	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	C5B-O5B-PA-O2A
2	G	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	C4B-C5B-O5B-PA

There are no ring outliers.

9 monomers are involved in 21 short contacts:

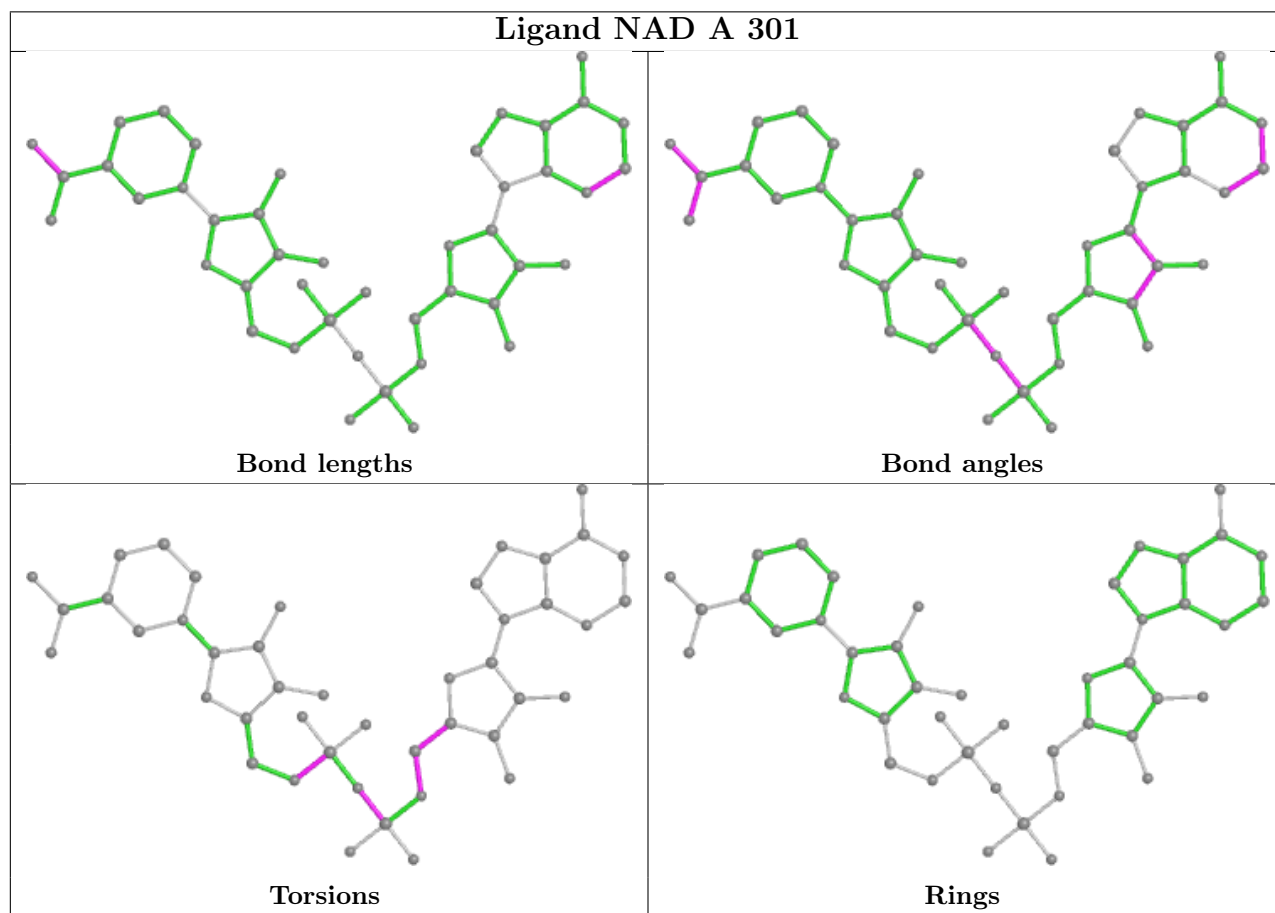
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
2	F	301	NAD	4	0
2	C	301	NAD	6	0
2	H	301	NAD	1	0
4	G	329	SO4	1	0
2	B	301	NAD	1	0

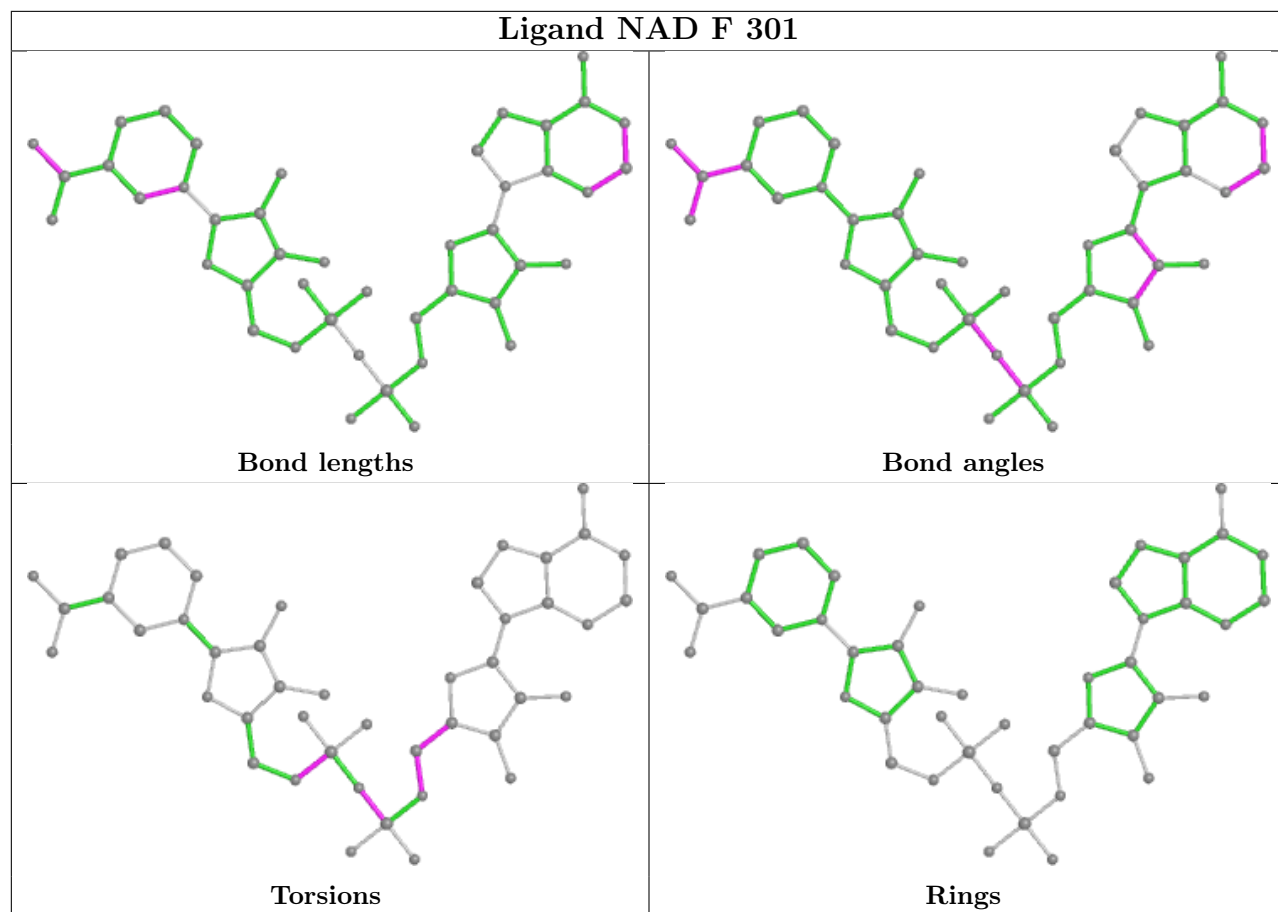
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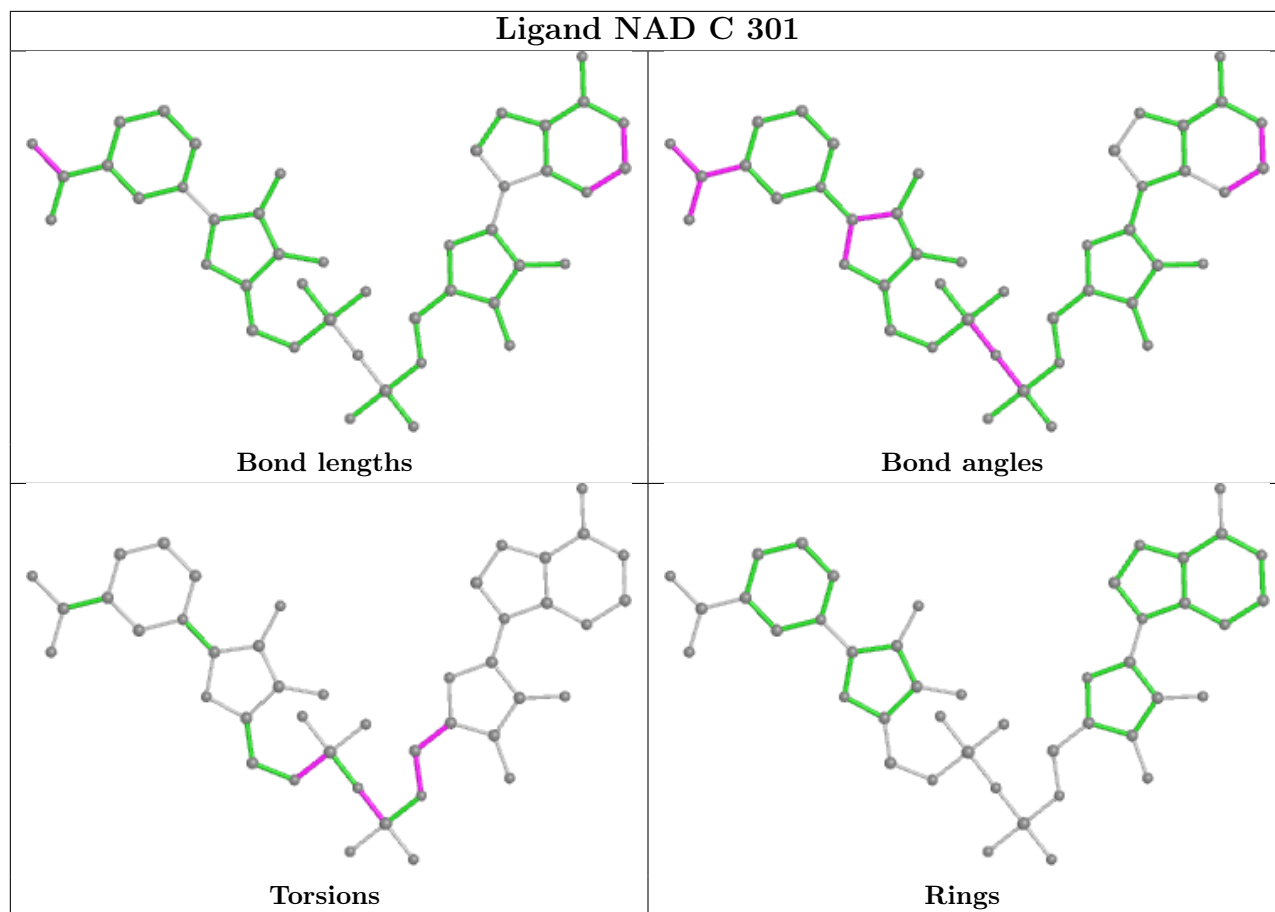
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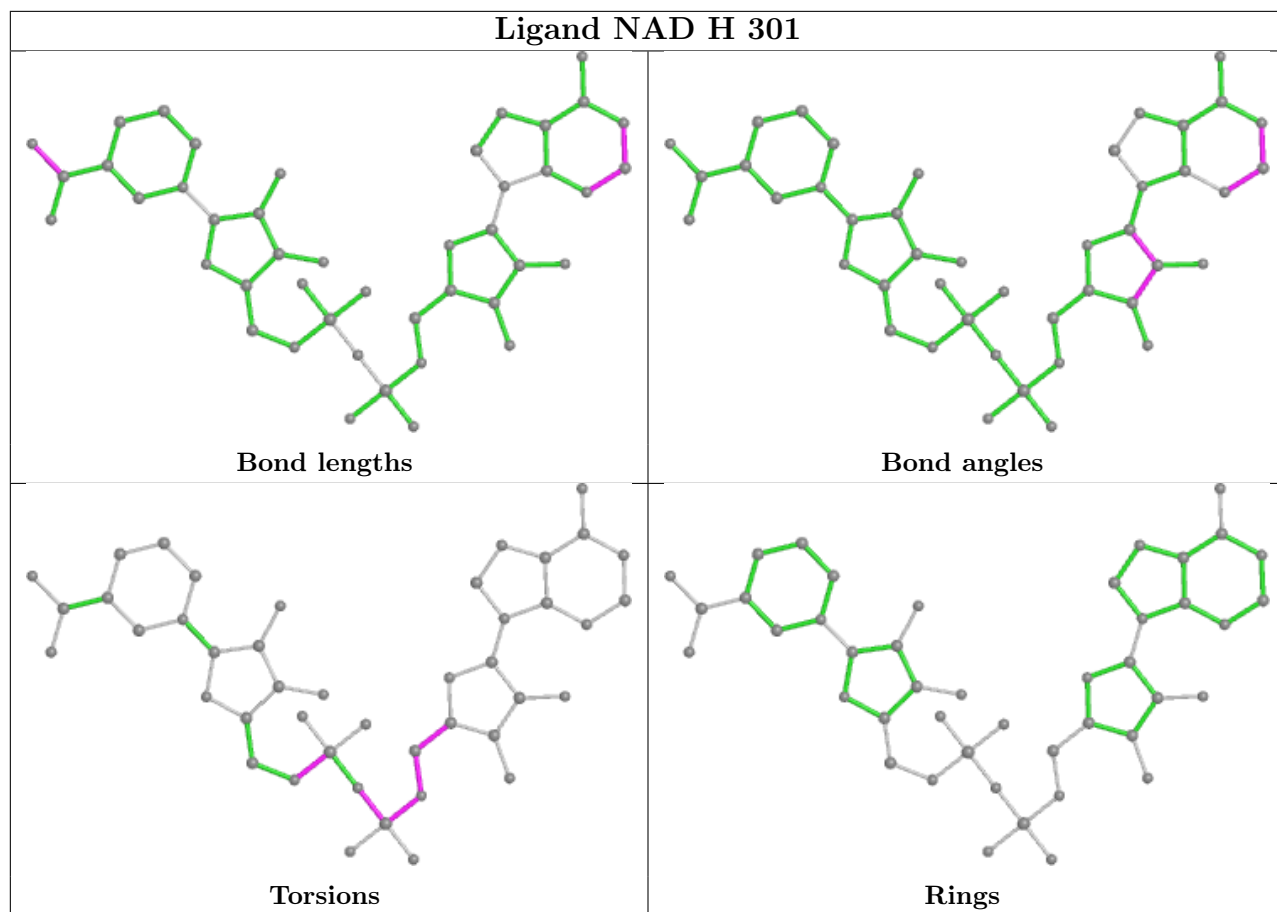
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	NAD	1	0
4	C	328	SO4	1	0
2	E	301	NAD	5	0

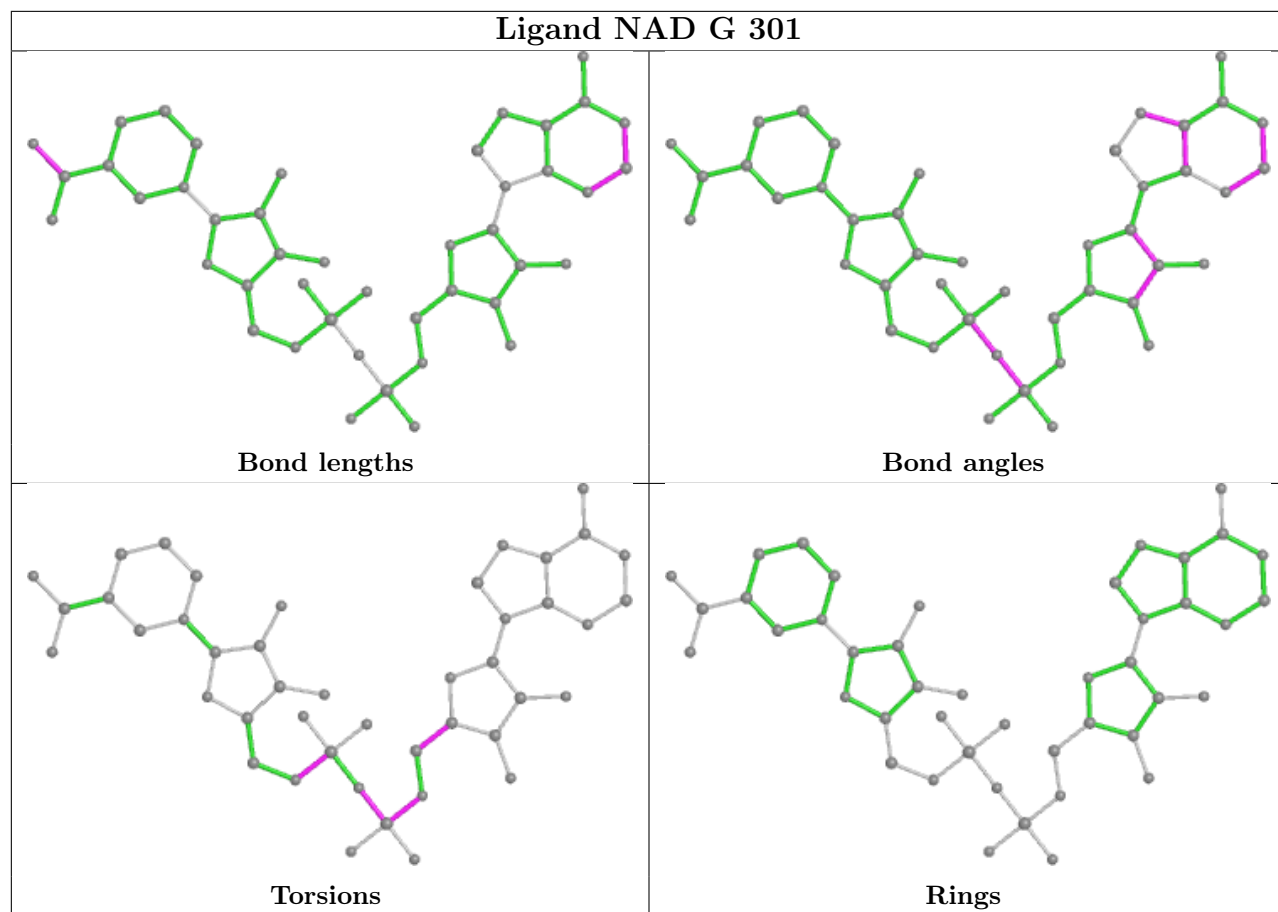
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



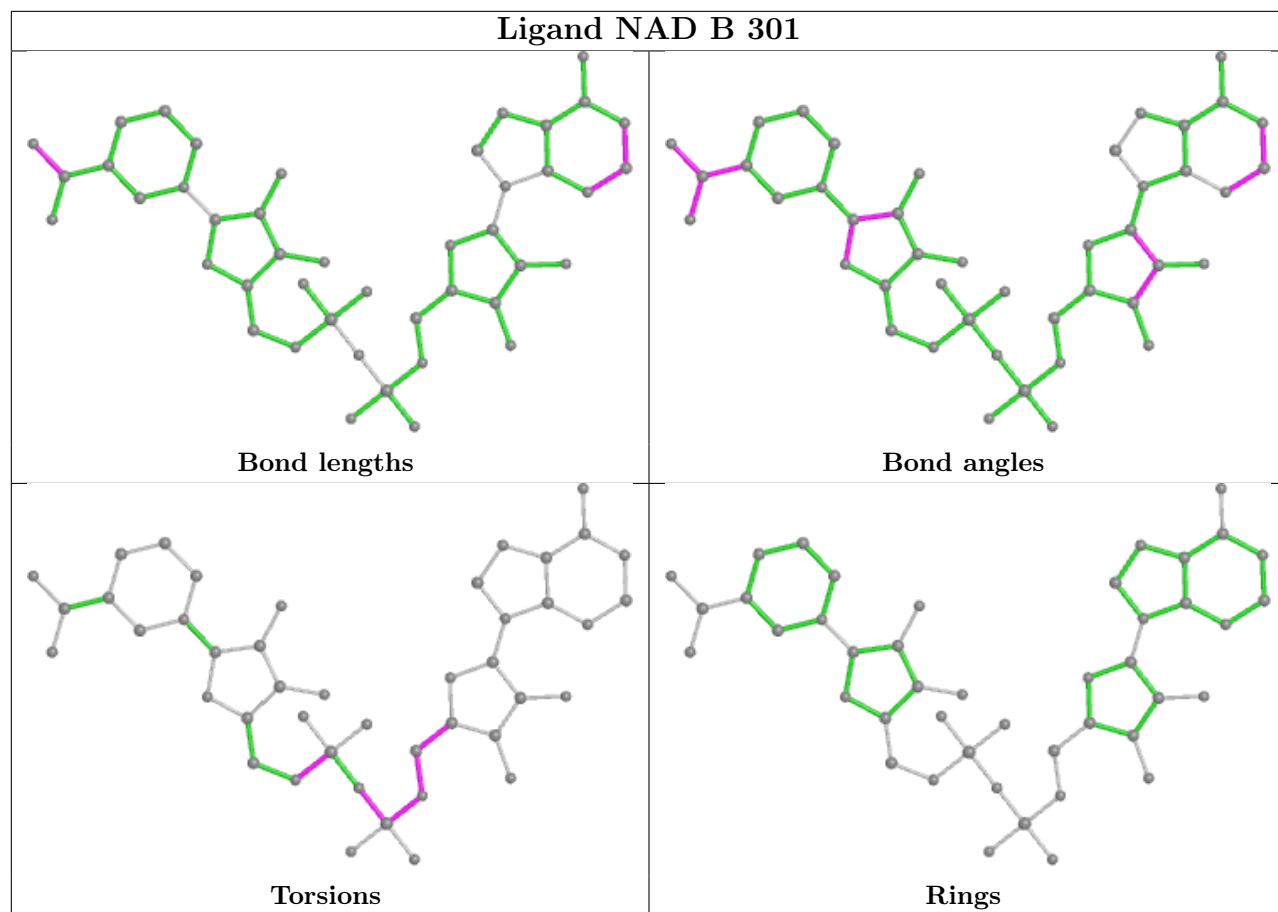


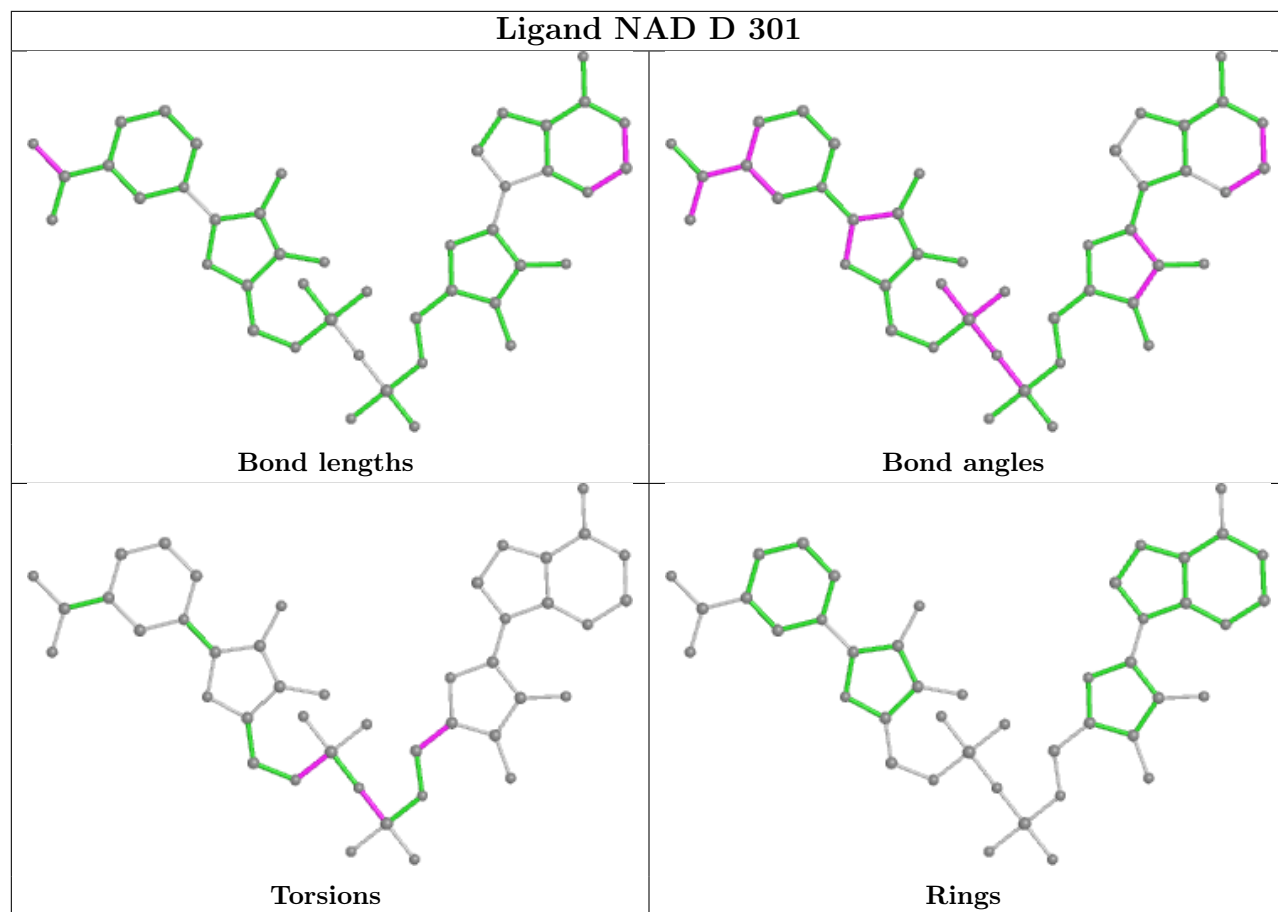


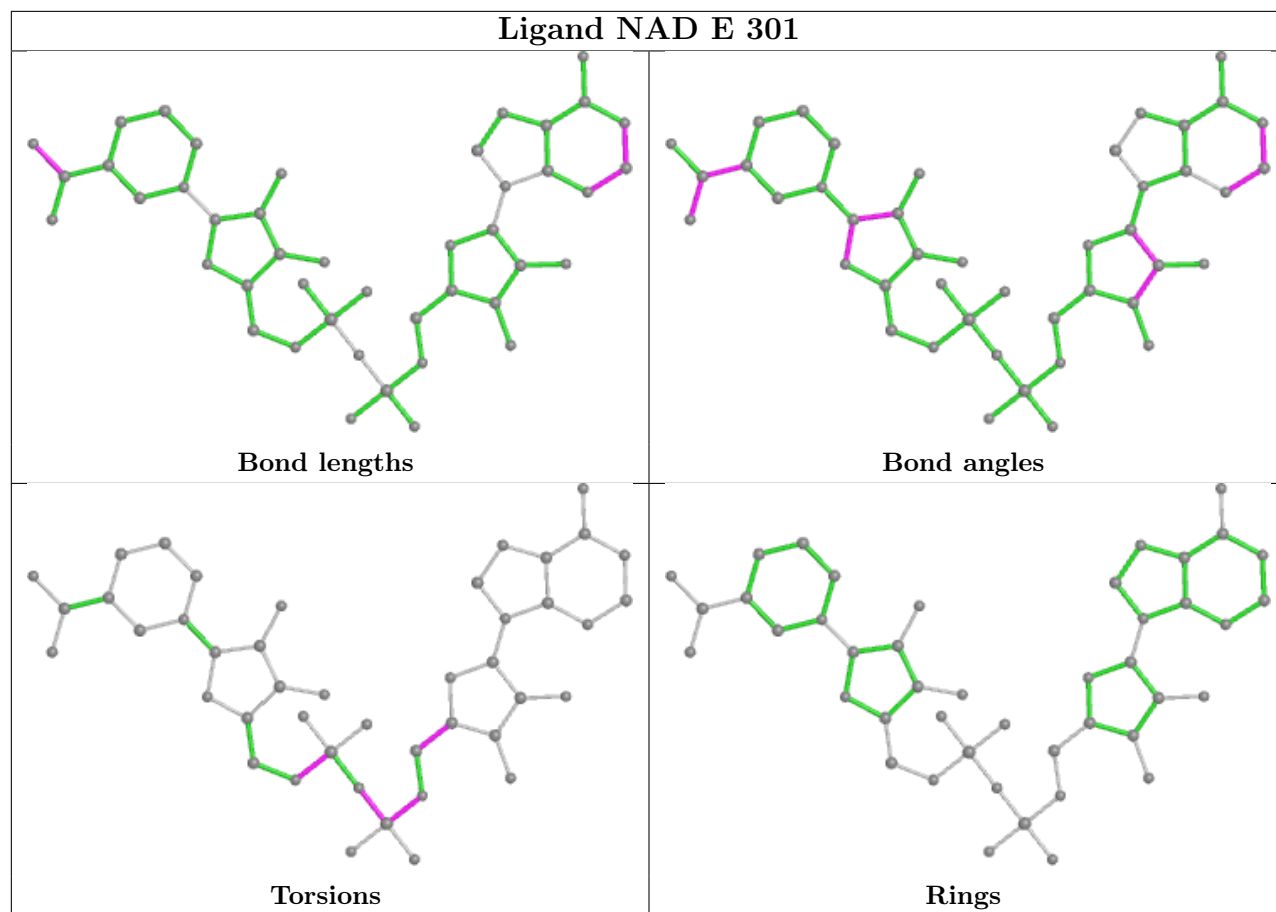












## 5.7 Other polymers [i](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

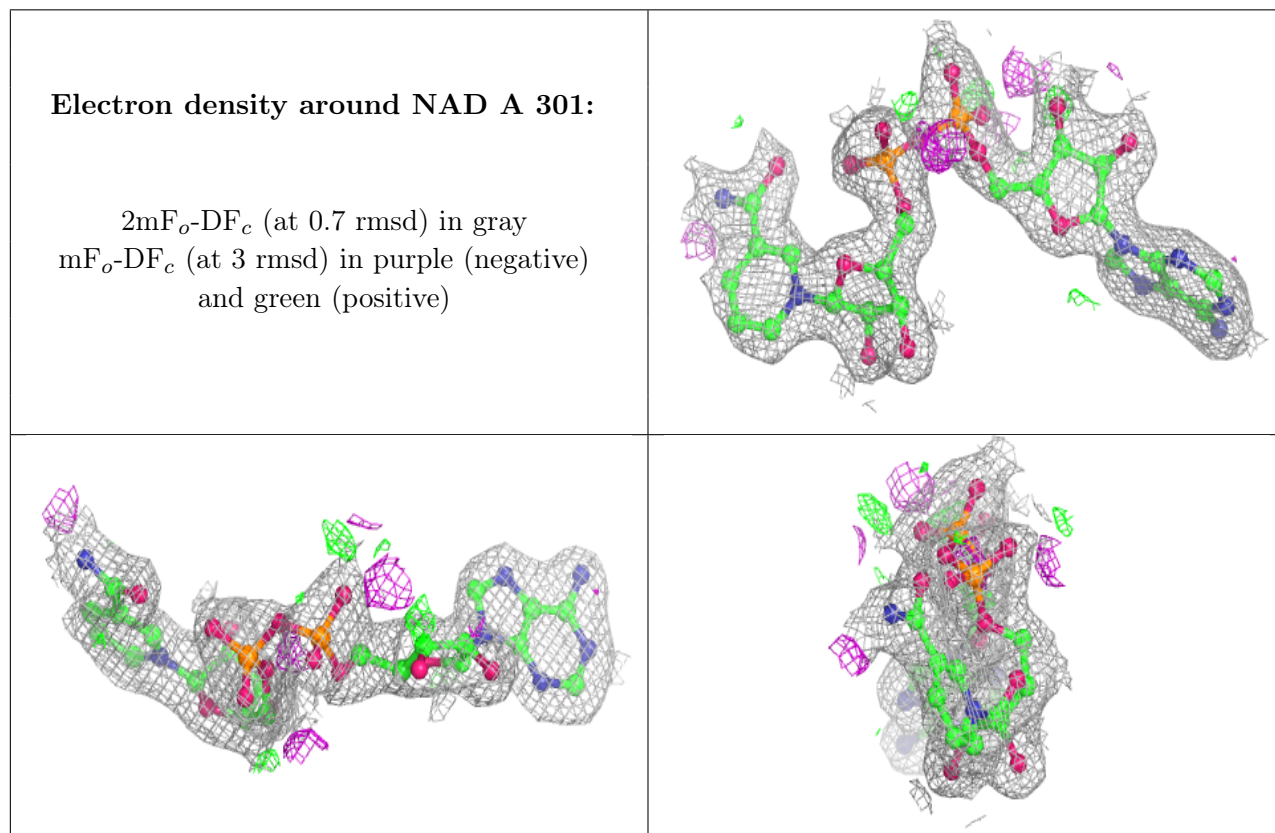
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

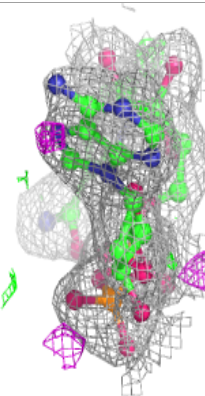
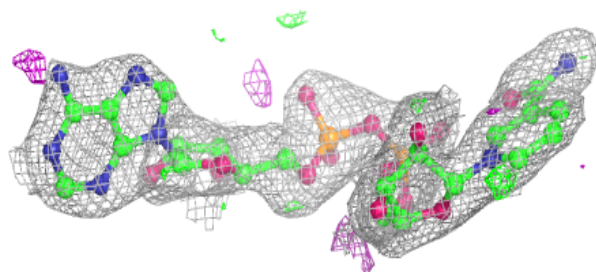
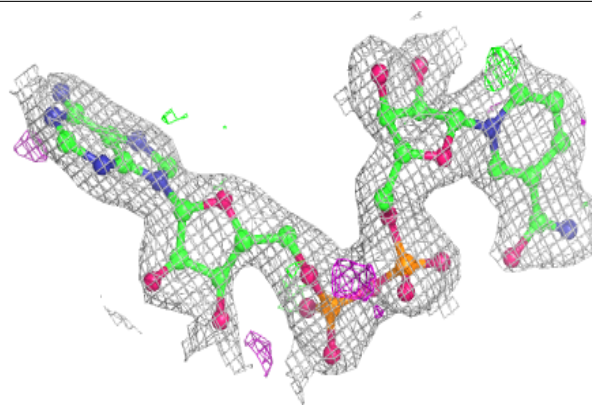
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

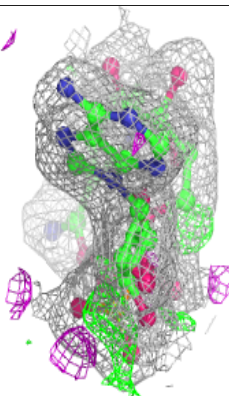
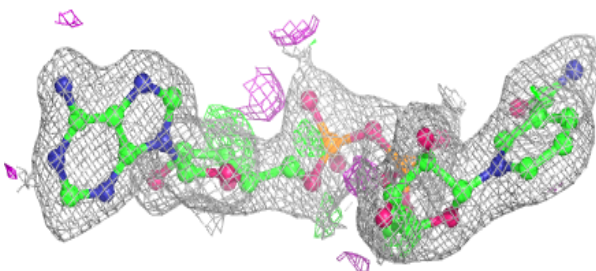
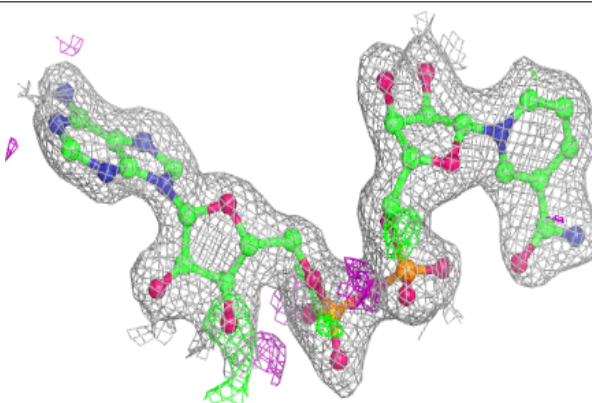


**Electron density around NAD B 301:**

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

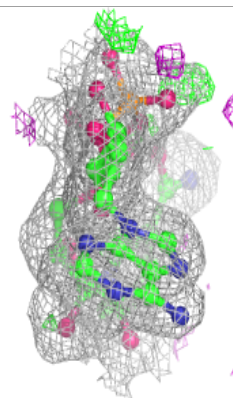
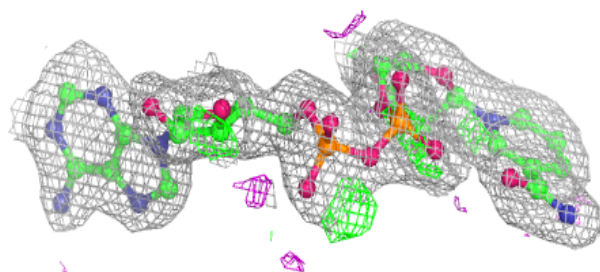
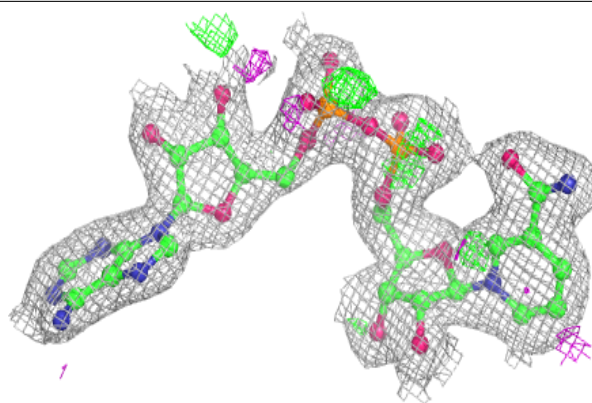
**Electron density around NAD C 301:**

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

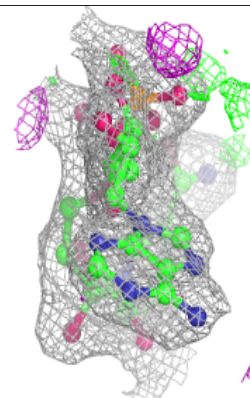
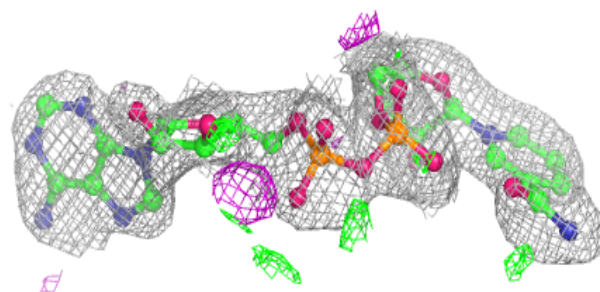
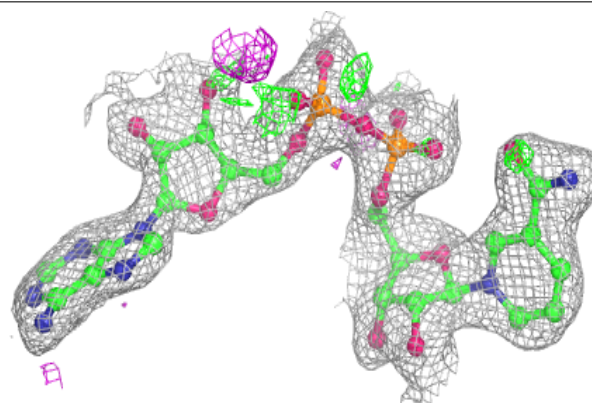


**Electron density around NAD D 301:**

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

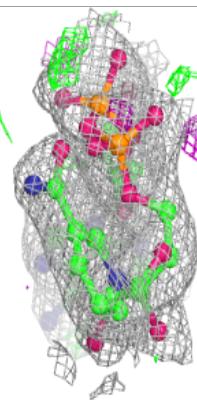
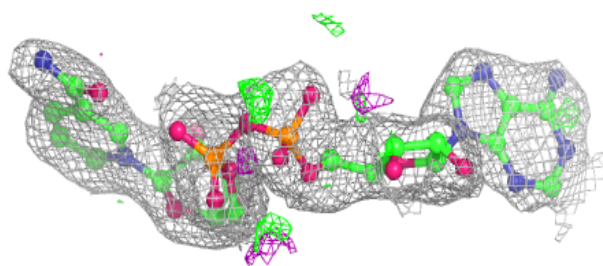
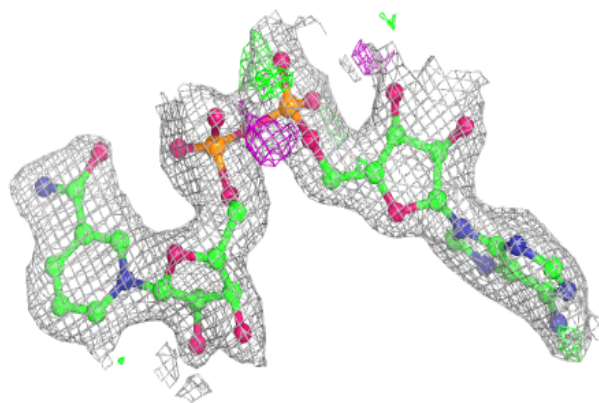
**Electron density around NAD E 301:**

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

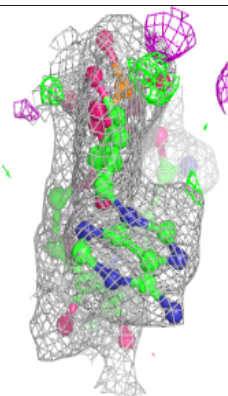
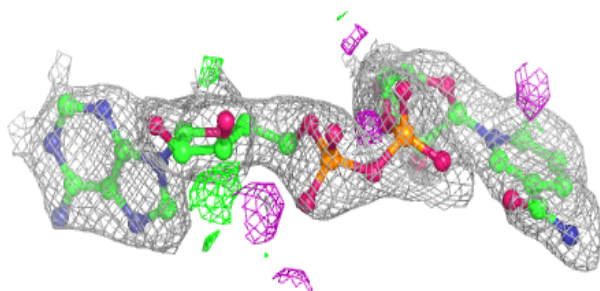
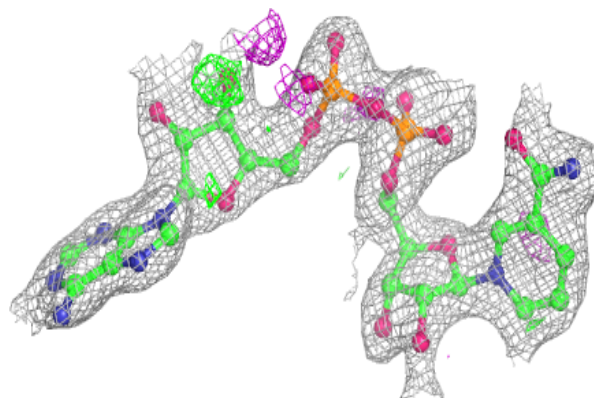


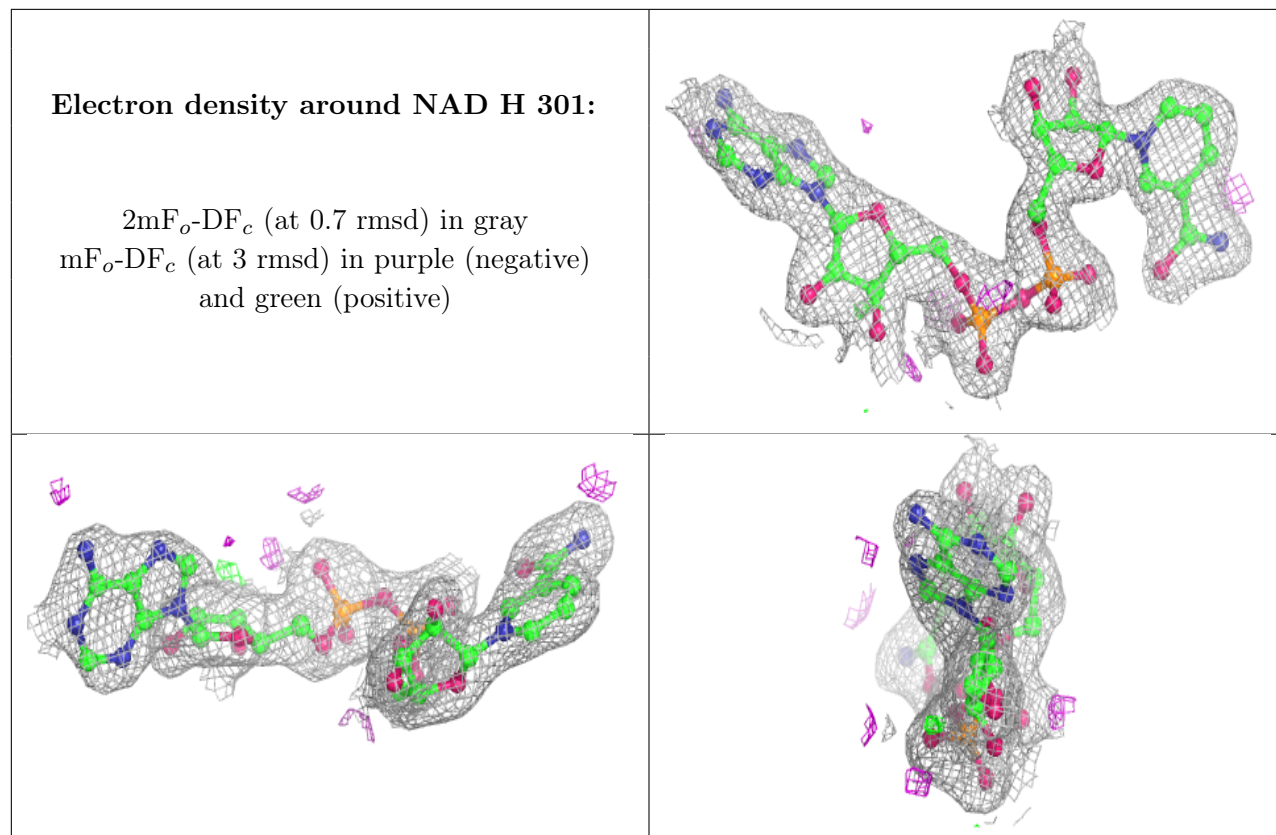
**Electron density around NAD F 301:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.