



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:30 PM UTC

PDB ID : 6OW4 / pdb_00006ow4
Title : Structure of the NADH-bound form of 20beta-Hydroxysteroid Dehydrogenase from Bifidobacterium adolescentis strain L2-32
Authors : Mythen, S.M.; Pollet, R.M.; Koropatkin, N.M.; Ridlon, J.M.
Deposited on : 2019-05-09
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

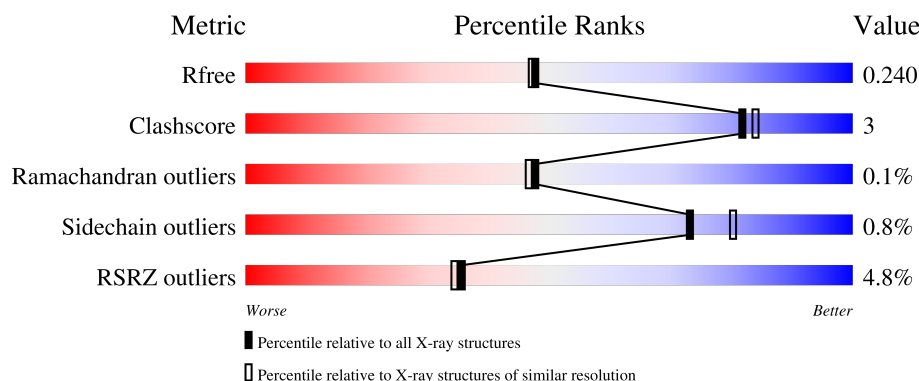
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	294	0% 87% 7% 5%
1	B	294	3% 87% 6% 7%
1	C	294	3% 89% 5% 6%
1	D	294	3% 86% 7% 7%
1	E	294	5% 89% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	294	11% 88% 8%
1	G	294	5% 86% 7% 6%
1	H	294	5% 93%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17642 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2108	1317	366	415	10			
1	B	274	Total	C	N	O	S	0	0	0
			2063	1289	359	405	10			
1	C	277	Total	C	N	O	S	0	0	0
			2091	1304	365	412	10			
1	D	274	Total	C	N	O	S	0	0	0
			2063	1289	359	405	10			
1	E	280	Total	C	N	O	S	0	0	0
			2120	1326	367	417	10			
1	F	284	Total	C	N	O	S	0	1	0
			2159	1349	377	423	10			
1	G	277	Total	C	N	O	S	0	0	0
			2093	1308	363	413	9			
1	H	283	Total	C	N	O	S	0	0	0
			2142	1338	372	422	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	SER	conflict	UNP A7A7R9
B	181	ALA	SER	conflict	UNP A7A7R9
C	181	ALA	SER	conflict	UNP A7A7R9
D	181	ALA	SER	conflict	UNP A7A7R9
E	181	ALA	SER	conflict	UNP A7A7R9
F	181	ALA	SER	conflict	UNP A7A7R9
G	181	ALA	SER	conflict	UNP A7A7R9
H	181	ALA	SER	conflict	UNP A7A7R9

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



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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	56	Total	O	0	0
			56	56		
3	C	54	Total	O	0	0
			54	54		
3	D	61	Total	O	0	0
			61	61		

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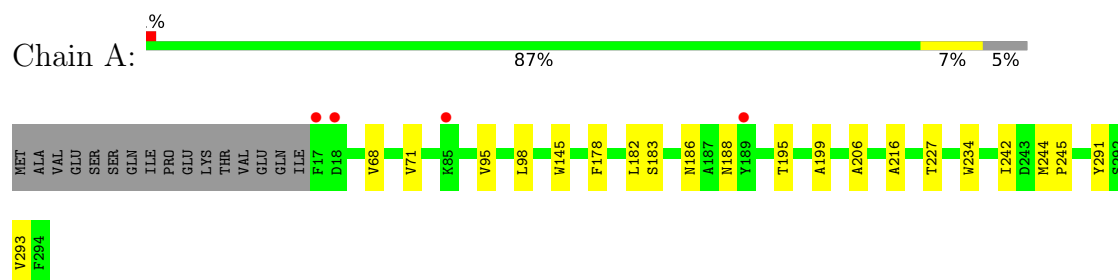
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	55	Total 55	O 55	0	0
3	F	48	Total 48	O 48	0	0
3	G	48	Total 48	O 48	0	0
3	H	48	Total 48	O 48	0	0

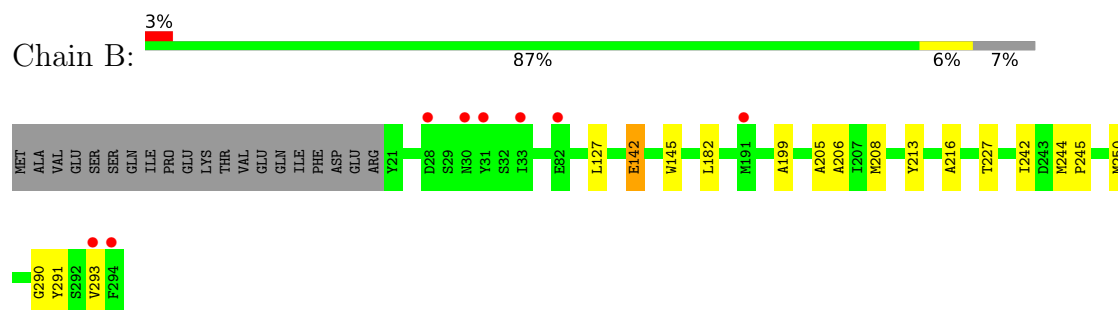
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

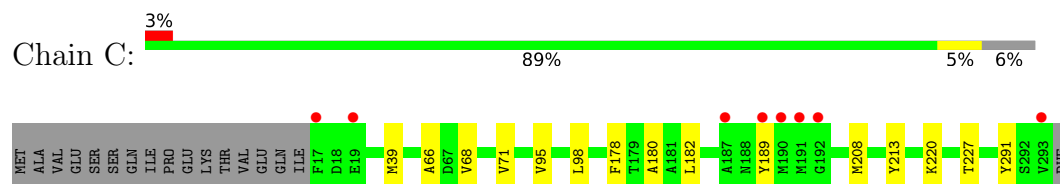
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



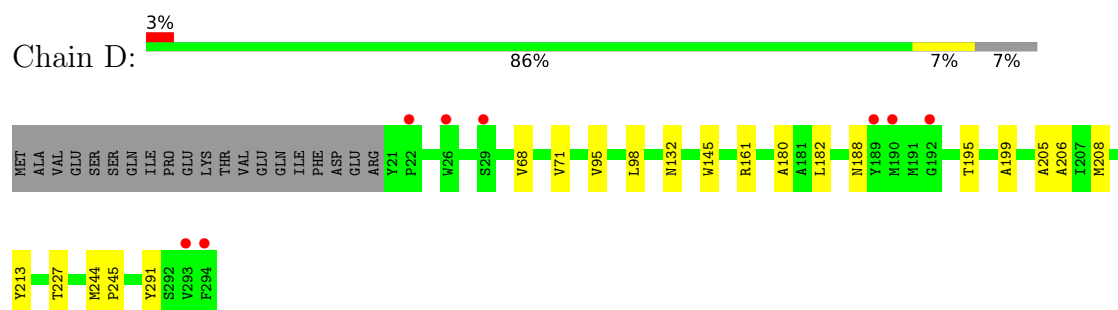
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



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

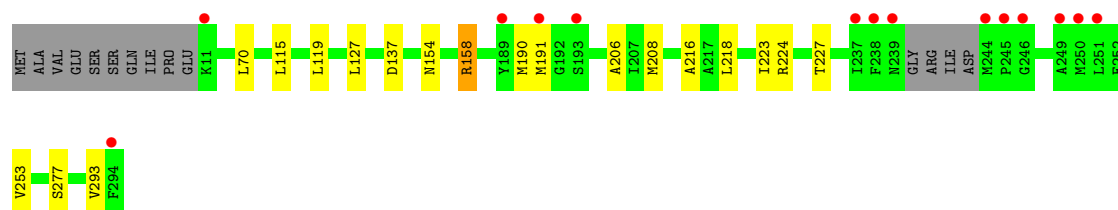


- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



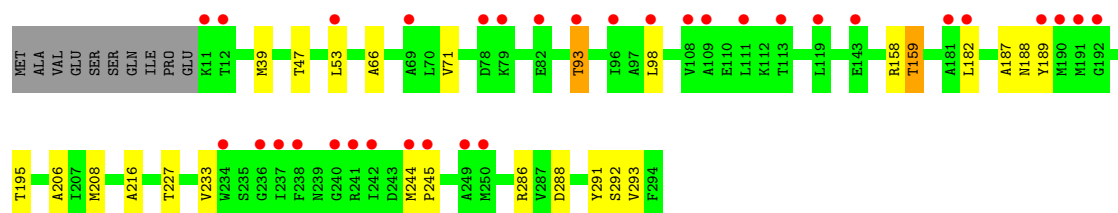
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain E: 



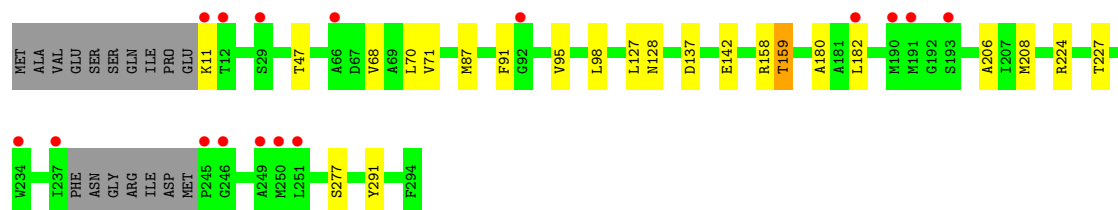
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain F: 

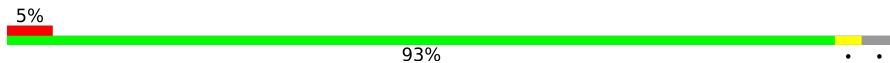


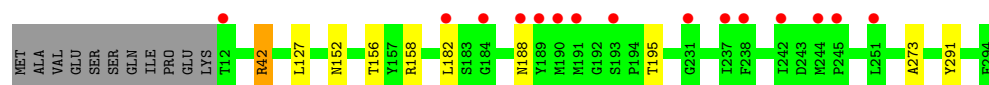
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain G: 



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

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.08Å 134.71Å 96.40Å 90.00° 100.15° 90.00°	Depositor
Resolution (Å)	103.71 – 1.99 103.71 – 1.99	Depositor EDS
% Data completeness (in resolution range)	52.0 (103.71-1.99) 52.0 (103.71-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.238 (Not available) , 0.240	Depositor DCC
R_{free} test set	3672 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17642	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6129e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.99	0/2151	1.47	0/2918
1	B	1.06	2/2102 (0.1%)	1.49	0/2853
1	C	1.00	0/2130	1.47	0/2890
1	D	1.00	0/2102	1.47	0/2853
1	E	1.00	0/2159	1.48	1/2928 (0.0%)
1	F	1.00	0/2202	1.50	0/2986
1	G	1.00	0/2131	1.48	0/2890
1	H	1.00	0/2182	1.47	0/2961
All	All	1.01	2/17159 (0.0%)	1.48	1/23279 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	GLU	CD-OE1	-11.68	1.03	1.25
1	B	142	GLU	CD-OE2	11.57	1.47	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	158	ARG	CG-CD-NE	-6.00	98.80	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	142	GLU	Sidechain

5.2 Too-close contacts

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	2108	0	2040	14	0
1	B	2063	0	2002	11	0
1	C	2091	0	2025	9	0
1	D	2063	0	2002	13	0
1	E	2120	0	2056	13	0
1	F	2159	0	2101	17	0
1	G	2093	0	2033	15	0
1	H	2142	0	2075	5	0
2	A	44	0	25	0	0
2	B	44	0	25	0	0
2	C	44	0	25	0	0
2	D	44	0	25	0	0
2	E	44	0	25	0	0
2	F	44	0	25	0	0
2	G	44	0	25	0	0
2	H	44	0	25	0	0
3	A	81	0	0	0	0
3	B	56	0	0	0	0
3	C	54	0	0	0	0
3	D	61	0	0	0	0
3	E	55	0	0	0	0
3	F	48	0	0	1	0
3	G	48	0	0	1	0
3	H	48	0	0	1	0
All	All	17642	0	16534	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (85) 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:F:47:THR:HG21	1:F:159:THR:HG21	1.70	0.72
1:G:47:THR:HG21	1:G:159:THR:HG21	1.72	0.71
1:H:42:ARG:NH2	1:H:273:ALA:O	2.24	0.71
1:A:216:ALA:HB2	1:E:293:VAL:HG11	1.78	0.66
1:B:290:GLY:O	1:B:293:VAL:HG22	1.98	0.63
1:B:216:ALA:HB2	1:F:293:VAL:HG11	1.81	0.62
1:A:182:LEU:HD21	1:A:291:TYR:CD1	2.36	0.61
1:E:224:ARG:NH2	1:E:277:SER:OG	2.34	0.61
1:A:182:LEU:HD21	1:A:291:TYR:CG	2.36	0.60
1:A:293:VAL:HG11	1:E:216:ALA:HB2	1.84	0.59
1:B:242:ILE:HD13	1:B:250:MET:HE1	1.88	0.56
1:B:206:ALA:HB2	1:E:206:ALA:HB2	1.89	0.55
1:G:208:MET:HA	1:G:227:THR:HG21	1.88	0.55
1:E:208:MET:HA	1:E:227:THR:HG21	1.89	0.55
1:B:182:LEU:HD11	1:B:291:TYR:CE1	2.43	0.53
1:F:182:LEU:HD13	1:F:291:TYR:CD1	2.44	0.52
1:E:154:ASN:HB3	1:E:158:ARG:NH2	2.24	0.52
1:F:182:LEU:HD11	1:F:288:ASP:CB	2.40	0.52
1:D:206:ALA:HB2	1:G:206:ALA:HB2	1.92	0.52
1:D:161:ARG:NH2	1:G:142:GLU:OE2	2.43	0.52
1:F:53:LEU:HD21	1:F:233:VAL:HG11	1.92	0.52
1:E:293:VAL:HG12	1:F:187:ALA:HB3	1.92	0.51
1:B:208:MET:HA	1:B:227:THR:HG21	1.93	0.51
1:H:182:LEU:HD23	1:H:291:TYR:CD1	2.47	0.50
1:D:208:MET:HA	1:D:227:THR:HG21	1.94	0.49
1:F:66:ALA:O	1:F:93:THR:HG21	2.12	0.49
1:F:208:MET:HA	1:F:227:THR:HG21	1.94	0.49
1:A:244:MET:HB3	1:A:245:PRO:HD3	1.94	0.49
1:G:224:ARG:NH2	1:G:277:SER:OG	2.46	0.48
1:D:182:LEU:HD11	1:D:291:TYR:CE1	2.49	0.48
1:A:206:ALA:HB2	1:F:206:ALA:HB2	1.96	0.47
1:F:188:ASN:HB2	1:F:195:THR:OG1	2.14	0.47
1:G:182:LEU:HD21	1:G:291:TYR:CD1	2.49	0.47
1:D:145:TRP:CE3	1:D:199:ALA:HB2	2.49	0.47
1:E:115:LEU:O	1:E:119:LEU:HB2	2.15	0.47
1:G:158:ARG:NH1	3:G:401:HOH:O	2.39	0.47
1:C:208:MET:HA	1:C:227:THR:HG21	1.96	0.47
1:G:68:VAL:O	1:G:95:VAL:HA	2.14	0.47
1:E:154:ASN:HB3	1:E:158:ARG:HH22	1.80	0.47
1:D:71:VAL:HA	1:D:98:LEU:O	2.15	0.47
1:B:145:TRP:CE3	1:B:199:ALA:HB2	2.50	0.46
1:F:286:ARG:HH11	1:F:292:SER:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HA	1:A:98:LEU:O	2.16	0.45
1:A:178:PHE:HB2	1:A:227:THR:HG22	1.99	0.45
1:G:70:LEU:HD11	1:G:87:MET:CE	2.47	0.45
1:H:158:ARG:NH2	3:H:402:HOH:O	2.42	0.45
1:A:291:TYR:CD1	1:A:291:TYR:C	2.94	0.45
1:D:68:VAL:O	1:D:95:VAL:HA	2.17	0.45
1:B:293:VAL:HG21	1:F:216:ALA:HB2	1.99	0.44
1:G:291:TYR:CD1	1:G:291:TYR:C	2.95	0.44
1:B:213:TYR:OH	1:E:137:ASP:HA	2.18	0.44
1:F:71:VAL:HA	1:F:98:LEU:O	2.17	0.44
1:D:188:ASN:HB2	1:D:195:THR:OG1	2.18	0.44
1:G:47:THR:O	1:G:128:ASN:HB3	2.17	0.43
1:G:47:THR:CG2	1:G:159:THR:HG21	2.45	0.43
1:D:291:TYR:C	1:D:291:TYR:CD1	2.96	0.43
1:C:178:PHE:HB2	1:C:227:THR:HG22	2.00	0.43
1:F:39:MET:HB3	1:F:66:ALA:HB2	2.01	0.43
1:B:244:MET:N	1:B:245:PRO:HD2	2.34	0.43
1:D:182:LEU:C	1:D:182:LEU:HD13	2.44	0.42
1:F:158:ARG:NH2	3:F:404:HOH:O	2.52	0.42
1:F:244:MET:N	1:F:245:PRO:HD2	2.34	0.42
1:G:71:VAL:HA	1:G:98:LEU:O	2.20	0.42
1:B:205:ALA:HA	1:B:208:MET:HE3	2.01	0.42
1:C:68:VAL:O	1:C:95:VAL:HA	2.19	0.42
1:C:182:LEU:HD21	1:C:291:TYR:CD1	2.55	0.42
1:D:244:MET:HB3	1:D:245:PRO:HD3	2.01	0.42
1:A:188:ASN:HB2	1:A:195:THR:OG1	2.19	0.42
1:C:182:LEU:HD11	1:C:291:TYR:CD1	2.55	0.42
1:C:213:TYR:CD2	1:C:213:TYR:C	2.98	0.42
1:A:183:SER:HA	1:A:186:ASN:O	2.20	0.42
1:H:188:ASN:HB2	1:H:195:THR:OG1	2.20	0.41
1:A:145:TRP:CE3	1:A:199:ALA:HB2	2.54	0.41
1:A:234:TRP:HZ3	1:A:242:ILE:HD11	1.86	0.41
1:A:68:VAL:O	1:A:95:VAL:HA	2.20	0.41
1:C:71:VAL:HA	1:C:98:LEU:O	2.20	0.41
1:D:205:ALA:HA	1:D:208:MET:HE3	2.03	0.41
1:C:39:MET:HB3	1:C:66:ALA:HB2	2.02	0.41
1:E:253:VAL:HG12	1:F:189:TYR:CE1	2.55	0.41
1:H:152:ASN:O	1:H:156:THR:OG1	2.33	0.41
1:D:213:TYR:OH	1:G:137:ASP:HA	2.21	0.41
1:E:190:MET:C	1:E:191:MET:HG2	2.45	0.41
1:G:182:LEU:HD21	1:G:291:TYR:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HD21	1:C:291:TYR:CE1	2.56	0.40
1:E:218:LEU:HB3	1:E:223:ILE:HB	2.03	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	277/294 (94%)	262 (95%)	15 (5%)	0	100	100
1	B	272/294 (92%)	256 (94%)	16 (6%)	0	100	100
1	C	275/294 (94%)	259 (94%)	15 (6%)	1 (0%)	30	27
1	D	272/294 (92%)	259 (95%)	12 (4%)	1 (0%)	30	27
1	E	276/294 (94%)	262 (95%)	14 (5%)	0	100	100
1	F	283/294 (96%)	266 (94%)	17 (6%)	0	100	100
1	G	273/294 (93%)	259 (95%)	13 (5%)	1 (0%)	30	27
1	H	281/294 (96%)	263 (94%)	18 (6%)	0	100	100
All	All	2209/2352 (94%)	2086 (94%)	120 (5%)	3 (0%)	48	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	180	ALA
1	D	180	ALA
1	G	180	ALA

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	219/233 (94%)	219 (100%)	0	100	100
1	B	214/233 (92%)	213 (100%)	1 (0%)	81	87
1	C	217/233 (93%)	215 (99%)	2 (1%)	70	78
1	D	214/233 (92%)	213 (100%)	1 (0%)	81	87
1	E	221/233 (95%)	219 (99%)	2 (1%)	70	78
1	F	225/233 (97%)	223 (99%)	2 (1%)	70	78
1	G	218/233 (94%)	214 (98%)	4 (2%)	51	58
1	H	223/233 (96%)	221 (99%)	2 (1%)	70	78
All	All	1751/1864 (94%)	1737 (99%)	14 (1%)	73	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	LEU
1	C	189	TYR
1	C	220	LYS
1	D	132	ASN
1	E	70	LEU
1	E	127	LEU
1	F	93	THR
1	F	159	THR
1	G	11	LYS
1	G	91	PHE
1	G	127	LEU
1	G	159	THR
1	H	42	ARG
1	H	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	186	ASN
1	B	132	ASN
1	B	186	ASN
1	G	56	ASN
1	G	132	ASN

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 oligosaccharides 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	E	301	-	46,48,48	3.95	19 (41%)	64,73,73	2.12	18 (28%)
2	NAD	H	301	-	46,48,48	3.91	18 (39%)	64,73,73	2.11	19 (29%)
2	NAD	A	301	-	46,48,48	3.92	17 (36%)	64,73,73	2.19	20 (31%)
2	NAD	G	301	-	46,48,48	3.96	18 (39%)	64,73,73	2.13	19 (29%)
2	NAD	D	301	-	46,48,48	3.89	18 (39%)	64,73,73	2.09	19 (29%)
2	NAD	F	301	-	46,48,48	3.95	18 (39%)	64,73,73	2.16	19 (29%)
2	NAD	C	301	-	46,48,48	3.96	19 (41%)	64,73,73	2.20	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	301	-	46,48,48	3.94	18 (39%)	64,73,73	2.18	19 (29%)

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	E	301	-	-	8/30/62/62	0/5/5/5
2	NAD	H	301	-	-	9/30/62/62	0/5/5/5
2	NAD	A	301	-	-	8/30/62/62	0/5/5/5
2	NAD	G	301	-	-	8/30/62/62	0/5/5/5
2	NAD	D	301	-	-	9/30/62/62	0/5/5/5
2	NAD	F	301	-	-	10/30/62/62	0/5/5/5
2	NAD	C	301	-	-	3/30/62/62	0/5/5/5
2	NAD	B	301	-	-	9/30/62/62	0/5/5/5

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	O4D-C1D	16.61	1.62	1.40
2	G	301	NAD	O4D-C1D	16.60	1.62	1.40
2	E	301	NAD	O4D-C1D	16.55	1.62	1.40
2	F	301	NAD	O4D-C1D	16.45	1.62	1.40
2	D	301	NAD	O4D-C1D	16.36	1.62	1.40
2	B	301	NAD	O4D-C1D	16.35	1.62	1.40
2	H	301	NAD	O4D-C1D	16.35	1.62	1.40
2	C	301	NAD	O4D-C1D	16.32	1.62	1.40
2	G	301	NAD	C3B-C4B	-10.23	1.27	1.53
2	E	301	NAD	C3B-C4B	-10.23	1.27	1.53
2	H	301	NAD	C3B-C4B	-10.19	1.27	1.53
2	F	301	NAD	C3B-C4B	-10.18	1.27	1.53
2	D	301	NAD	C3B-C4B	-10.11	1.27	1.53
2	C	301	NAD	C3B-C4B	-10.07	1.27	1.53
2	B	301	NAD	C3B-C4B	-10.02	1.27	1.53
2	A	301	NAD	C3B-C4B	-10.02	1.27	1.53
2	F	301	NAD	C2B-C1B	-8.19	1.27	1.53
2	D	301	NAD	C2B-C1B	-8.13	1.27	1.53
2	H	301	NAD	C2B-C1B	-8.11	1.28	1.53
2	G	301	NAD	C2B-C1B	-8.11	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAD	C2B-C1B	-8.09	1.28	1.53
2	E	301	NAD	C2B-C1B	-8.07	1.28	1.53
2	B	301	NAD	C2B-C1B	-8.07	1.28	1.53
2	A	301	NAD	C2B-C1B	-8.01	1.28	1.53
2	E	301	NAD	O4D-C4D	-6.35	1.30	1.45
2	F	301	NAD	O4D-C4D	-6.33	1.30	1.45
2	H	301	NAD	O4D-C4D	-6.29	1.31	1.45
2	C	301	NAD	O4D-C4D	-6.17	1.31	1.45
2	D	301	NAD	O4D-C4D	-6.17	1.31	1.45
2	G	301	NAD	O4D-C4D	-6.07	1.31	1.45
2	A	301	NAD	O4D-C4D	-6.05	1.31	1.45
2	B	301	NAD	O4D-C4D	-6.04	1.31	1.45
2	C	301	NAD	O4B-C4B	5.83	1.58	1.45
2	A	301	NAD	O4B-C4B	5.67	1.57	1.45
2	B	301	NAD	O4B-C4B	5.51	1.57	1.45
2	D	301	NAD	O4B-C4B	5.46	1.57	1.45
2	B	301	NAD	C7N-N7N	5.45	1.43	1.33
2	C	301	NAD	C7N-N7N	5.42	1.42	1.33
2	G	301	NAD	C7N-N7N	5.40	1.42	1.33
2	E	301	NAD	O4B-C4B	5.40	1.57	1.45
2	F	301	NAD	O4B-C4B	5.39	1.57	1.45
2	E	301	NAD	PA-O3	5.38	1.65	1.59
2	G	301	NAD	O4B-C4B	5.38	1.57	1.45
2	E	301	NAD	C7N-N7N	5.33	1.42	1.33
2	H	301	NAD	O4B-C4B	5.33	1.56	1.45
2	G	301	NAD	PA-O3	5.32	1.65	1.59
2	F	301	NAD	C7N-N7N	5.26	1.42	1.33
2	A	301	NAD	C7N-N7N	5.24	1.42	1.33
2	G	301	NAD	O4B-C1B	5.18	1.54	1.42
2	F	301	NAD	PA-O3	5.18	1.65	1.59
2	B	301	NAD	O4B-C1B	5.16	1.53	1.42
2	H	301	NAD	PA-O3	5.14	1.65	1.59
2	C	301	NAD	O4B-C1B	5.14	1.53	1.42
2	D	301	NAD	O4B-C1B	5.13	1.53	1.42
2	A	301	NAD	O4B-C1B	5.13	1.53	1.42
2	F	301	NAD	O4B-C1B	5.08	1.53	1.42
2	C	301	NAD	PA-O3	5.07	1.65	1.59
2	C	301	NAD	C2B-C3B	5.06	1.67	1.53
2	H	301	NAD	C2B-C3B	5.04	1.67	1.53
2	H	301	NAD	O4B-C1B	5.00	1.53	1.42
2	H	301	NAD	C7N-N7N	4.99	1.42	1.33
2	A	301	NAD	C2B-C3B	4.96	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	C2B-C3B	4.96	1.66	1.53
2	E	301	NAD	C2B-C3B	4.95	1.66	1.53
2	D	301	NAD	PA-O3	4.95	1.64	1.59
2	F	301	NAD	C2B-C3B	4.94	1.66	1.53
2	E	301	NAD	O4B-C1B	4.91	1.53	1.42
2	B	301	NAD	PA-O3	4.91	1.64	1.59
2	D	301	NAD	C7N-N7N	4.90	1.42	1.33
2	D	301	NAD	C2B-C3B	4.85	1.66	1.53
2	G	301	NAD	C2B-C3B	4.83	1.66	1.53
2	A	301	NAD	PA-O3	4.40	1.64	1.59
2	B	301	NAD	C2N-N1N	4.35	1.39	1.35
2	C	301	NAD	C2N-N1N	4.11	1.39	1.35
2	A	301	NAD	C2N-N1N	3.96	1.39	1.35
2	F	301	NAD	C2N-N1N	3.95	1.39	1.35
2	D	301	NAD	C2N-N1N	3.83	1.39	1.35
2	H	301	NAD	C2N-N1N	3.82	1.39	1.35
2	G	301	NAD	C2N-N1N	3.72	1.39	1.35
2	E	301	NAD	C2N-N1N	3.60	1.38	1.35
2	B	301	NAD	C6A-N6A	3.54	1.43	1.34
2	C	301	NAD	C6A-N6A	3.53	1.43	1.34
2	A	301	NAD	C6A-N6A	3.50	1.43	1.34
2	G	301	NAD	C6A-N6A	3.50	1.43	1.34
2	E	301	NAD	C6A-N6A	3.48	1.43	1.34
2	D	301	NAD	C6A-N6A	3.48	1.43	1.34
2	F	301	NAD	C6A-N6A	3.47	1.43	1.34
2	B	301	NAD	C3N-C7N	3.46	1.55	1.50
2	H	301	NAD	C6A-N6A	3.46	1.43	1.34
2	C	301	NAD	C3N-C7N	3.25	1.55	1.50
2	G	301	NAD	C3N-C7N	3.25	1.55	1.50
2	C	301	NAD	C2A-N3A	3.20	1.39	1.33
2	B	301	NAD	C2A-N3A	3.14	1.39	1.33
2	G	301	NAD	C2A-N3A	3.13	1.39	1.33
2	F	301	NAD	C3N-C7N	3.12	1.55	1.50
2	F	301	NAD	C2A-N3A	3.10	1.39	1.33
2	A	301	NAD	C3N-C7N	3.05	1.55	1.50
2	D	301	NAD	C2A-N3A	2.98	1.39	1.33
2	H	301	NAD	C2A-N3A	2.96	1.39	1.33
2	E	301	NAD	C2A-N3A	2.93	1.39	1.33
2	H	301	NAD	C3N-C7N	2.92	1.54	1.50
2	E	301	NAD	C3N-C7N	2.86	1.54	1.50
2	A	301	NAD	C2A-N3A	2.84	1.39	1.33
2	F	301	NAD	O2D-C2D	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	O2D-C2D	2.54	1.49	1.43
2	H	301	NAD	O2D-C2D	2.53	1.49	1.43
2	A	301	NAD	O2D-C2D	2.53	1.49	1.43
2	E	301	NAD	O2D-C2D	2.49	1.49	1.43
2	D	301	NAD	C3N-C7N	2.47	1.54	1.50
2	C	301	NAD	PN-O3	2.39	1.62	1.59
2	D	301	NAD	O2D-C2D	2.39	1.48	1.43
2	G	301	NAD	O2D-C2D	2.39	1.48	1.43
2	G	301	NAD	PN-O3	2.37	1.62	1.59
2	C	301	NAD	O2D-C2D	2.36	1.48	1.43
2	G	301	NAD	C8A-N7A	2.34	1.36	1.31
2	F	301	NAD	C8A-N7A	2.33	1.36	1.31
2	C	301	NAD	C5A-N7A	-2.31	1.34	1.39
2	D	301	NAD	O3D-C3D	-2.29	1.37	1.43
2	E	301	NAD	PN-O3	2.27	1.62	1.59
2	C	301	NAD	C2A-N1A	2.27	1.38	1.33
2	H	301	NAD	C8A-N7A	2.26	1.36	1.31
2	E	301	NAD	C8A-N7A	2.26	1.36	1.31
2	E	301	NAD	C2A-N1A	2.25	1.37	1.33
2	D	301	NAD	C2A-N1A	2.24	1.37	1.33
2	F	301	NAD	O3D-C3D	-2.23	1.37	1.43
2	C	301	NAD	O3D-C3D	-2.23	1.37	1.43
2	F	301	NAD	C2A-N1A	2.22	1.37	1.33
2	H	301	NAD	O3D-C3D	-2.21	1.37	1.43
2	B	301	NAD	C8A-N7A	2.21	1.35	1.31
2	B	301	NAD	C2A-N1A	2.20	1.37	1.33
2	D	301	NAD	C5A-N7A	-2.20	1.35	1.39
2	D	301	NAD	C8A-N7A	2.19	1.35	1.31
2	G	301	NAD	C2A-N1A	2.18	1.37	1.33
2	B	301	NAD	O3D-C3D	-2.17	1.37	1.43
2	A	301	NAD	O3D-C3D	-2.17	1.37	1.43
2	A	301	NAD	C8A-N7A	2.16	1.35	1.31
2	C	301	NAD	C8A-N7A	2.15	1.35	1.31
2	G	301	NAD	O3D-C3D	-2.12	1.37	1.43
2	H	301	NAD	C5A-N7A	-2.09	1.35	1.39
2	A	301	NAD	C2A-N1A	2.08	1.37	1.33
2	H	301	NAD	C2A-N1A	2.08	1.37	1.33
2	F	301	NAD	C5A-N7A	-2.07	1.35	1.39
2	E	301	NAD	O3D-C3D	-2.07	1.37	1.43
2	B	301	NAD	C5A-N7A	-2.06	1.35	1.39
2	E	301	NAD	C5A-N7A	-2.01	1.35	1.39

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	N6A-C6A-N1A	-6.29	104.38	118.38
2	G	301	NAD	N6A-C6A-N1A	-6.23	104.51	118.38
2	A	301	NAD	N6A-C6A-N1A	-6.14	104.71	118.38
2	B	301	NAD	N6A-C6A-N1A	-6.10	104.78	118.38
2	E	301	NAD	N6A-C6A-N1A	-6.01	104.98	118.38
2	H	301	NAD	N6A-C6A-N1A	-5.98	105.06	118.38
2	C	301	NAD	N6A-C6A-N1A	-5.92	105.18	118.38
2	E	301	NAD	N3A-C2A-N1A	-5.79	119.82	128.58
2	G	301	NAD	N3A-C2A-N1A	-5.77	119.85	128.58
2	D	301	NAD	N6A-C6A-N1A	-5.73	105.62	118.38
2	F	301	NAD	N3A-C2A-N1A	-5.73	119.92	128.58
2	H	301	NAD	N3A-C2A-N1A	-5.72	119.92	128.58
2	A	301	NAD	N3A-C2A-N1A	-5.71	119.93	128.58
2	C	301	NAD	N3A-C2A-N1A	-5.71	119.94	128.58
2	B	301	NAD	N3A-C2A-N1A	-5.67	120.00	128.58
2	D	301	NAD	N3A-C2A-N1A	-5.62	120.07	128.58
2	E	301	NAD	C4A-N9A-C1B	-5.49	113.80	126.63
2	F	301	NAD	C4A-N9A-C1B	-5.32	114.18	126.63
2	C	301	NAD	C5A-C4A-N3A	-5.24	119.50	126.72
2	G	301	NAD	C4A-N9A-C1B	-5.20	114.46	126.63
2	H	301	NAD	C4A-N9A-C1B	-5.19	114.50	126.63
2	D	301	NAD	C4A-N9A-C1B	-5.14	114.60	126.63
2	B	301	NAD	C5A-C6A-N6A	5.06	135.82	123.29
2	H	301	NAD	C5A-C4A-N3A	-5.06	119.75	126.72
2	F	301	NAD	C5A-C6A-N6A	5.03	135.75	123.29
2	A	301	NAD	C5A-C6A-N6A	5.01	135.70	123.29
2	G	301	NAD	C5A-C6A-N6A	5.01	135.69	123.29
2	B	301	NAD	C4A-N9A-C1B	-5.01	114.92	126.63
2	F	301	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	C	301	NAD	C4A-N9A-C1B	-4.95	115.05	126.63
2	A	301	NAD	C5A-C4A-N3A	-4.95	119.90	126.72
2	B	301	NAD	C5A-C4A-N3A	-4.91	119.96	126.72
2	A	301	NAD	C4A-N9A-C1B	-4.89	115.20	126.63
2	D	301	NAD	C5A-C6A-N6A	4.85	135.29	123.29
2	E	301	NAD	C1B-N9A-C8A	4.84	137.84	127.09
2	E	301	NAD	C5A-C6A-N6A	4.84	135.27	123.29
2	G	301	NAD	C5A-C4A-N3A	-4.80	120.10	126.72
2	C	301	NAD	C5A-C6A-N6A	4.80	135.18	123.29
2	H	301	NAD	C5A-C6A-N6A	4.73	134.99	123.29
2	F	301	NAD	C1B-N9A-C8A	4.72	137.56	127.09
2	E	301	NAD	C5A-C4A-N3A	-4.68	120.27	126.72
2	G	301	NAD	C1B-N9A-C8A	4.64	137.39	127.09
2	C	301	NAD	C1B-N9A-C8A	4.60	137.31	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	NAD	C1B-N9A-C8A	4.58	137.26	127.09
2	D	301	NAD	C5A-C4A-N3A	-4.54	120.47	126.72
2	D	301	NAD	C1B-N9A-C8A	4.49	137.06	127.09
2	B	301	NAD	C1B-N9A-C8A	4.44	136.95	127.09
2	A	301	NAD	C1B-N9A-C8A	4.40	136.87	127.09
2	F	301	NAD	N9A-C8A-N7A	-4.11	108.11	113.94
2	E	301	NAD	N9A-C8A-N7A	-4.05	108.19	113.94
2	H	301	NAD	N9A-C8A-N7A	-4.02	108.23	113.94
2	D	301	NAD	N9A-C8A-N7A	-3.92	108.38	113.94
2	B	301	NAD	N9A-C8A-N7A	-3.84	108.49	113.94
2	C	301	NAD	C4B-O4B-C1B	-3.82	101.04	109.47
2	G	301	NAD	N9A-C8A-N7A	-3.80	108.54	113.94
2	C	301	NAD	N3A-C4A-N9A	3.64	133.36	127.17
2	C	301	NAD	N9A-C8A-N7A	-3.64	108.78	113.94
2	H	301	NAD	N3A-C4A-N9A	3.58	133.26	127.17
2	A	301	NAD	N9A-C8A-N7A	-3.57	108.87	113.94
2	A	301	NAD	C3N-C7N-N7N	3.56	122.13	117.74
2	B	301	NAD	C3N-C7N-N7N	3.52	122.08	117.74
2	A	301	NAD	N3A-C4A-N9A	3.49	133.10	127.17
2	F	301	NAD	N3A-C4A-N9A	3.42	132.99	127.17
2	B	301	NAD	N3A-C4A-N9A	3.41	132.97	127.17
2	H	301	NAD	C2A-N3A-C4A	3.36	120.04	111.83
2	E	301	NAD	N3A-C4A-N9A	3.35	132.86	127.17
2	G	301	NAD	N3A-C4A-N9A	3.34	132.85	127.17
2	C	301	NAD	C2A-N3A-C4A	3.31	119.93	111.83
2	F	301	NAD	C2A-N3A-C4A	3.29	119.87	111.83
2	D	301	NAD	C4D-O4D-C1D	-3.26	106.94	109.92
2	A	301	NAD	C2A-N3A-C4A	3.26	119.78	111.83
2	G	301	NAD	C2A-N3A-C4A	3.24	119.74	111.83
2	D	301	NAD	N3A-C4A-N9A	3.23	132.66	127.17
2	B	301	NAD	C2A-N3A-C4A	3.20	119.65	111.83
2	E	301	NAD	C2A-N3A-C4A	3.19	119.62	111.83
2	C	301	NAD	C4D-O4D-C1D	-3.18	107.01	109.92
2	G	301	NAD	C3N-C7N-N7N	3.08	121.53	117.74
2	C	301	NAD	O4B-C1B-N9A	3.08	114.00	108.09
2	D	301	NAD	C2A-N3A-C4A	2.95	119.03	111.83
2	B	301	NAD	C3B-C2B-C1B	2.94	107.03	101.46
2	A	301	NAD	C6N-N1N-C2N	-2.94	119.37	121.88
2	B	301	NAD	O7N-C7N-N7N	-2.94	118.36	122.62
2	F	301	NAD	C6N-N1N-C2N	-2.92	119.40	121.88
2	A	301	NAD	O7N-C7N-N7N	-2.84	118.52	122.62
2	C	301	NAD	C3N-C7N-N7N	2.83	121.22	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	C5A-N7A-C8A	2.82	107.88	103.45
2	H	301	NAD	C6N-N1N-C2N	-2.78	119.51	121.88
2	B	301	NAD	C4D-O4D-C1D	-2.77	107.39	109.92
2	A	301	NAD	C3B-C2B-C1B	2.76	106.69	101.46
2	F	301	NAD	C3N-C7N-N7N	2.76	121.14	117.74
2	E	301	NAD	C4B-O4B-C1B	-2.74	103.41	109.47
2	D	301	NAD	C4B-O4B-C1B	-2.74	103.42	109.47
2	A	301	NAD	C4B-O4B-C1B	-2.73	103.45	109.47
2	B	301	NAD	C5A-N7A-C8A	2.72	107.73	103.45
2	A	301	NAD	C4D-O4D-C1D	-2.72	107.43	109.92
2	H	301	NAD	C5A-N7A-C8A	2.70	107.69	103.45
2	E	301	NAD	C6N-N1N-C2N	-2.67	119.61	121.88
2	E	301	NAD	C5A-N7A-C8A	2.64	107.60	103.45
2	C	301	NAD	C5A-N7A-C8A	2.63	107.58	103.45
2	G	301	NAD	C6N-N1N-C2N	-2.63	119.64	121.88
2	B	301	NAD	C4B-O4B-C1B	-2.61	103.70	109.47
2	G	301	NAD	O7N-C7N-N7N	-2.59	118.87	122.62
2	H	301	NAD	O7N-C7N-N7N	-2.56	118.92	122.62
2	C	301	NAD	C6N-N1N-C2N	-2.55	119.70	121.88
2	D	301	NAD	C3B-C2B-C1B	2.54	106.28	101.46
2	C	301	NAD	C6A-C5A-C4A	2.54	120.65	117.18
2	A	301	NAD	O2N-PN-O3	2.54	114.15	107.27
2	B	301	NAD	C6N-N1N-C2N	-2.54	119.72	121.88
2	G	301	NAD	C5A-N7A-C8A	2.54	107.44	103.45
2	D	301	NAD	C5A-N7A-C8A	2.53	107.43	103.45
2	C	301	NAD	O7N-C7N-N7N	-2.53	118.96	122.62
2	H	301	NAD	C4B-O4B-C1B	-2.49	103.98	109.47
2	G	301	NAD	C4B-O4B-C1B	-2.48	103.99	109.47
2	E	301	NAD	C4A-N9A-C8A	2.48	108.34	105.74
2	C	301	NAD	O4B-C1B-C2B	-2.47	101.33	106.62
2	G	301	NAD	C3B-C2B-C1B	2.47	106.13	101.46
2	A	301	NAD	C5A-N7A-C8A	2.46	107.32	103.45
2	D	301	NAD	C6A-C5A-C4A	2.46	120.53	117.18
2	D	301	NAD	C4A-N9A-C8A	2.46	108.32	105.74
2	F	301	NAD	C4B-O4B-C1B	-2.43	104.11	109.47
2	H	301	NAD	C3B-C2B-C1B	2.42	106.04	101.46
2	D	301	NAD	C6N-N1N-C2N	-2.40	119.83	121.88
2	F	301	NAD	C3B-C2B-C1B	2.40	106.01	101.46
2	H	301	NAD	C3N-C7N-N7N	2.40	120.69	117.74
2	F	301	NAD	C4A-N9A-C8A	2.40	108.25	105.74
2	H	301	NAD	C4A-N9A-C8A	2.39	108.24	105.74
2	F	301	NAD	O7N-C7N-N7N	-2.37	119.19	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAD	C6A-C5A-C4A	2.37	120.41	117.18
2	B	301	NAD	C2B-C3B-C4B	2.36	107.18	102.61
2	E	301	NAD	C3B-C2B-C1B	2.36	105.92	101.46
2	D	301	NAD	C2B-C3B-C4B	2.36	107.16	102.61
2	G	301	NAD	C2B-C3B-C4B	2.32	107.09	102.61
2	H	301	NAD	C2B-C3B-C4B	2.31	107.07	102.61
2	G	301	NAD	C4A-N9A-C8A	2.30	108.15	105.74
2	D	301	NAD	O7N-C7N-N7N	-2.27	119.33	122.62
2	E	301	NAD	C2B-C3B-C4B	2.27	107.00	102.61
2	B	301	NAD	C4A-N9A-C8A	2.26	108.11	105.74
2	E	301	NAD	C4D-O4D-C1D	-2.25	107.86	109.92
2	E	301	NAD	C3N-C7N-N7N	2.22	120.47	117.74
2	G	301	NAD	C4D-O4D-C1D	-2.20	107.91	109.92
2	H	301	NAD	C6A-C5A-C4A	2.20	120.18	117.18
2	D	301	NAD	C3N-C7N-N7N	2.19	120.44	117.74
2	H	301	NAD	C4D-O4D-C1D	-2.18	107.93	109.92
2	A	301	NAD	C6A-C5A-C4A	2.17	120.15	117.18
2	F	301	NAD	C6A-C5A-C4A	2.17	120.14	117.18
2	F	301	NAD	C2B-C3B-C4B	2.13	106.72	102.61
2	A	301	NAD	C4A-N9A-C8A	2.07	107.91	105.74
2	C	301	NAD	C3B-C2B-C1B	2.06	105.36	101.46
2	A	301	NAD	C2B-C3B-C4B	2.04	106.56	102.61
2	F	301	NAD	C4D-O4D-C1D	-2.04	108.05	109.92
2	G	301	NAD	C6A-C5A-C4A	2.04	119.97	117.18
2	E	301	NAD	C6A-C5A-C4A	2.01	119.93	117.18

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	C5B-O5B-PA-O1A
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5B-O5B-PA-O2A
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	E	301	NAD	C5B-O5B-PA-O2A
2	E	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5B-O5B-PA-O1A
2	F	301	NAD	C5B-O5B-PA-O2A
2	F	301	NAD	C5B-O5B-PA-O3
2	F	301	NAD	C5D-O5D-PN-O3
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	O4D-C4D-C5D-O5D
2	H	301	NAD	C5B-O5B-PA-O1A
2	H	301	NAD	C5B-O5B-PA-O2A
2	H	301	NAD	C5B-O5B-PA-O3
2	H	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O2N
2	G	301	NAD	C3D-C4D-C5D-O5D
2	A	301	NAD	PA-O3-PN-O1N
2	D	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5B-O5B-PA-O2A
2	A	301	NAD	C5B-O5B-PA-O3
2	A	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	C5B-O5B-PA-O3
2	C	301	NAD	C5D-O5D-PN-O2N
2	D	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	C5B-O5B-PA-O1A
2	E	301	NAD	C5B-O5B-PA-O3
2	E	301	NAD	C5D-O5D-PN-O2N
2	G	301	NAD	C5B-O5B-PA-O1A
2	G	301	NAD	C5B-O5B-PA-O2A
2	G	301	NAD	C5B-O5B-PA-O3
2	F	301	NAD	PN-O3-PA-O1A
2	G	301	NAD	PA-O3-PN-O1N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	D	301	NAD	O4D-C1D-N1N-C6N
2	E	301	NAD	O4D-C1D-N1N-C6N

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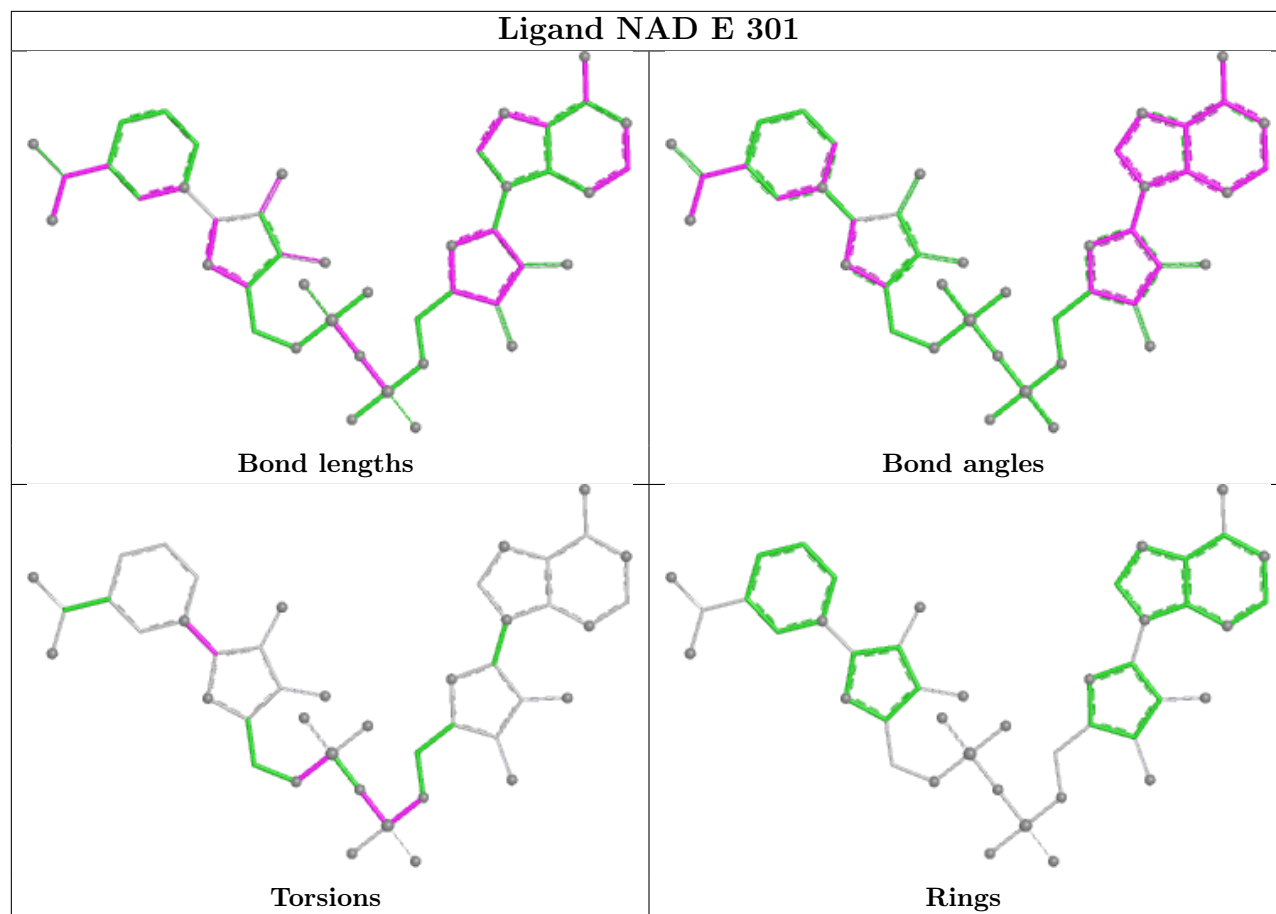
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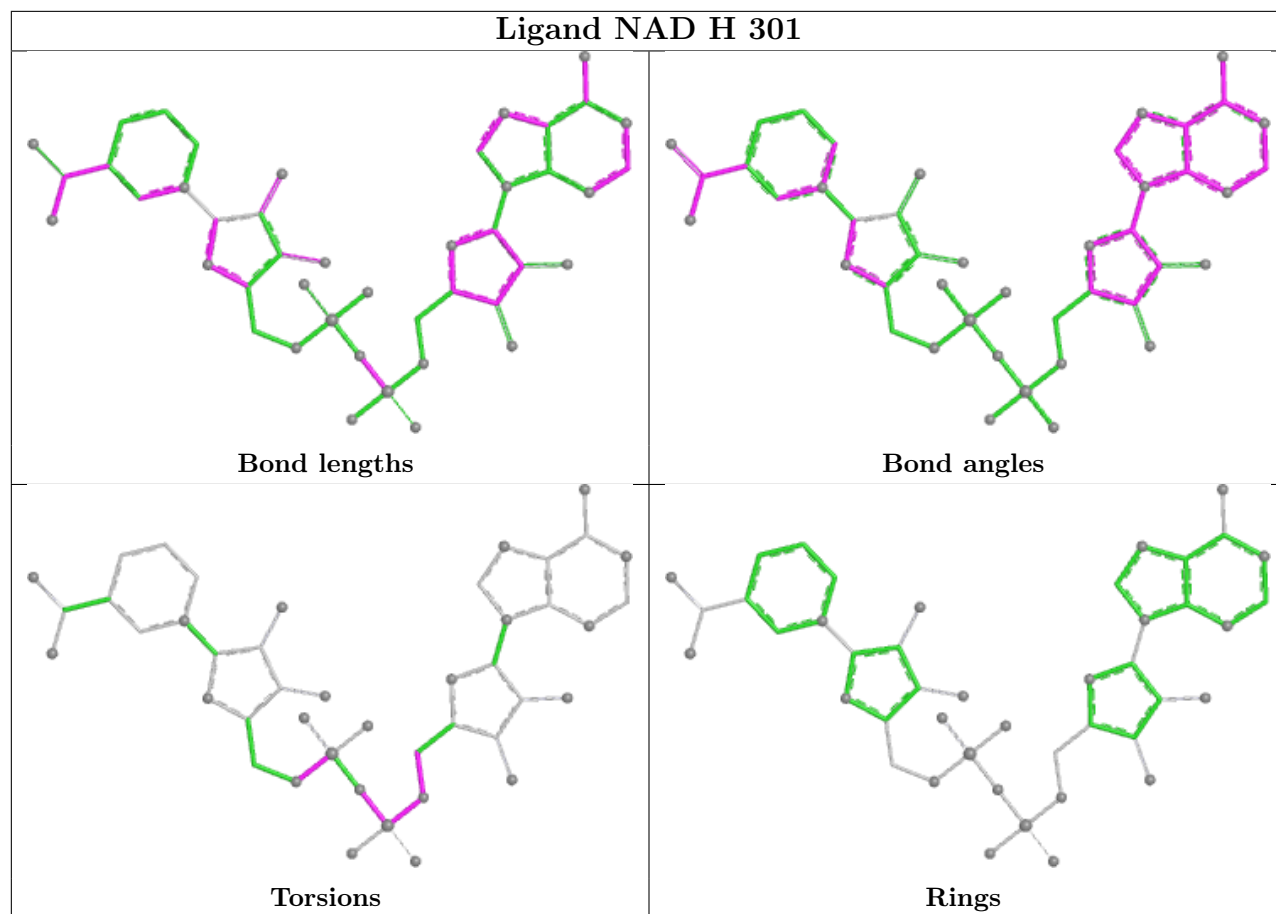
Mol	Chain	Res	Type	Atoms
2	B	301	NAD	PN-O3-PA-O1A
2	B	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	O4B-C4B-C5B-O5B
2	G	301	NAD	PA-O3-PN-O2N
2	F	301	NAD	C4B-C5B-O5B-PA
2	D	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	PA-O3-PN-O2N
2	H	301	NAD	PN-O3-PA-O2A
2	B	301	NAD	O4B-C4B-C5B-O5B

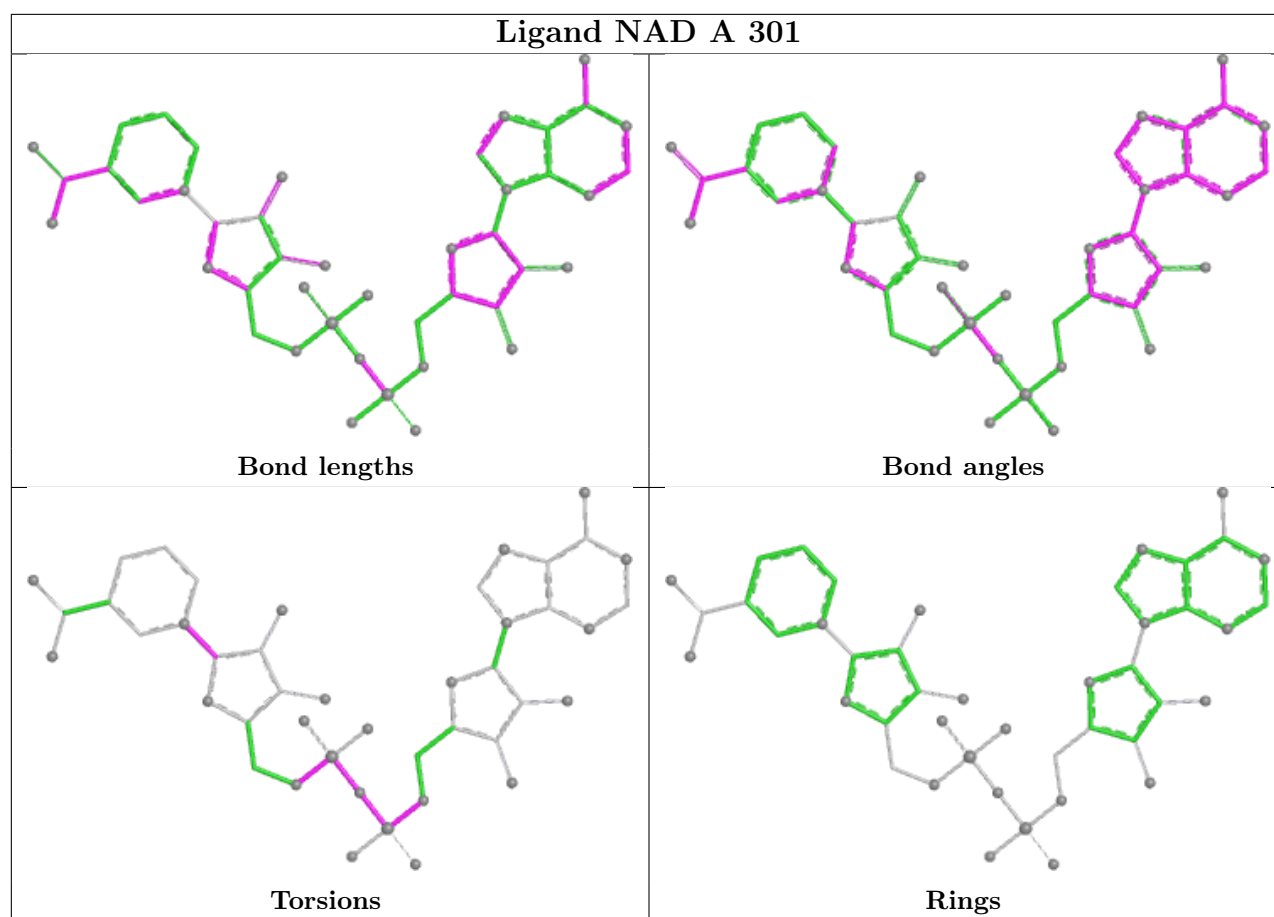
There are no ring outliers.

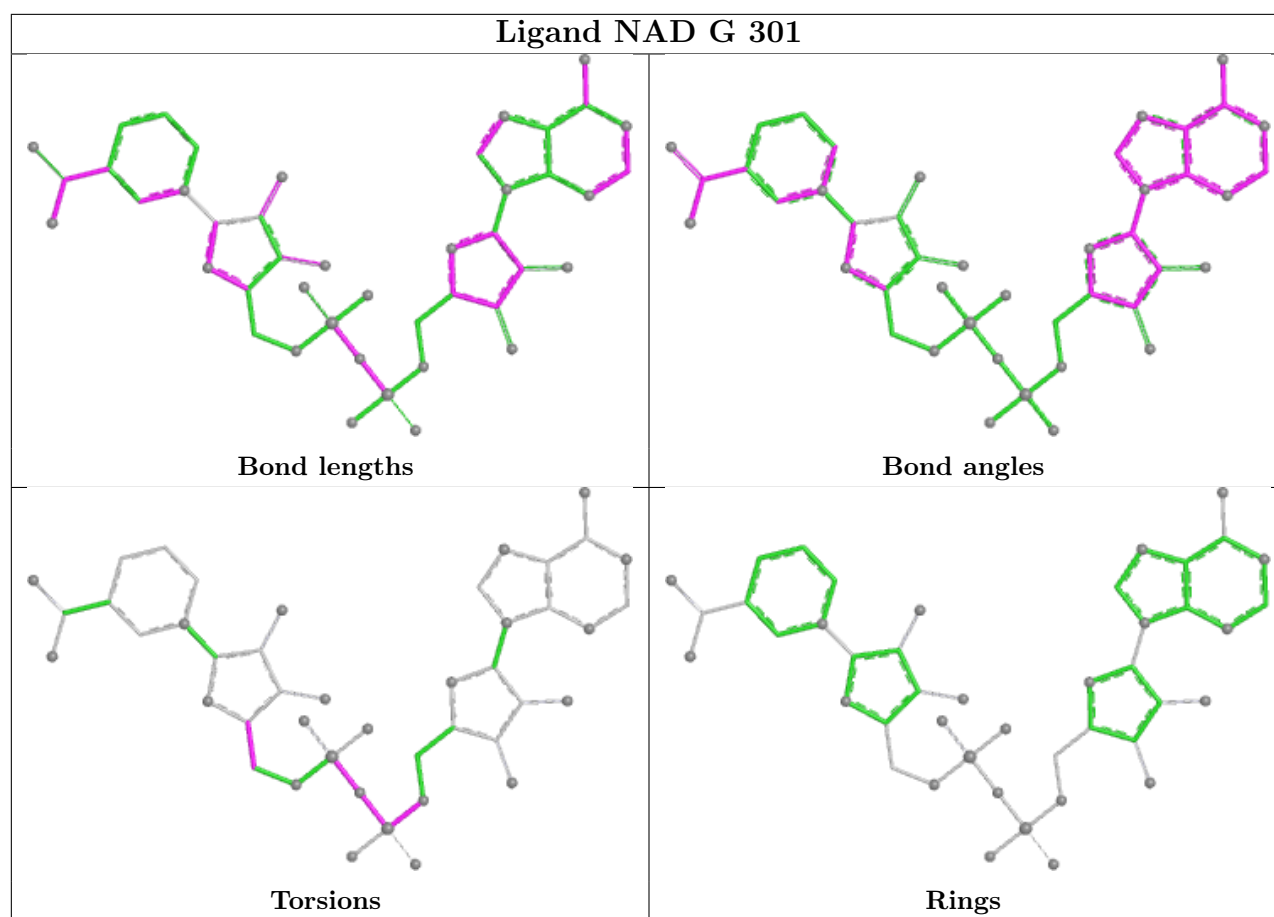
No monomer is involved in short contacts.

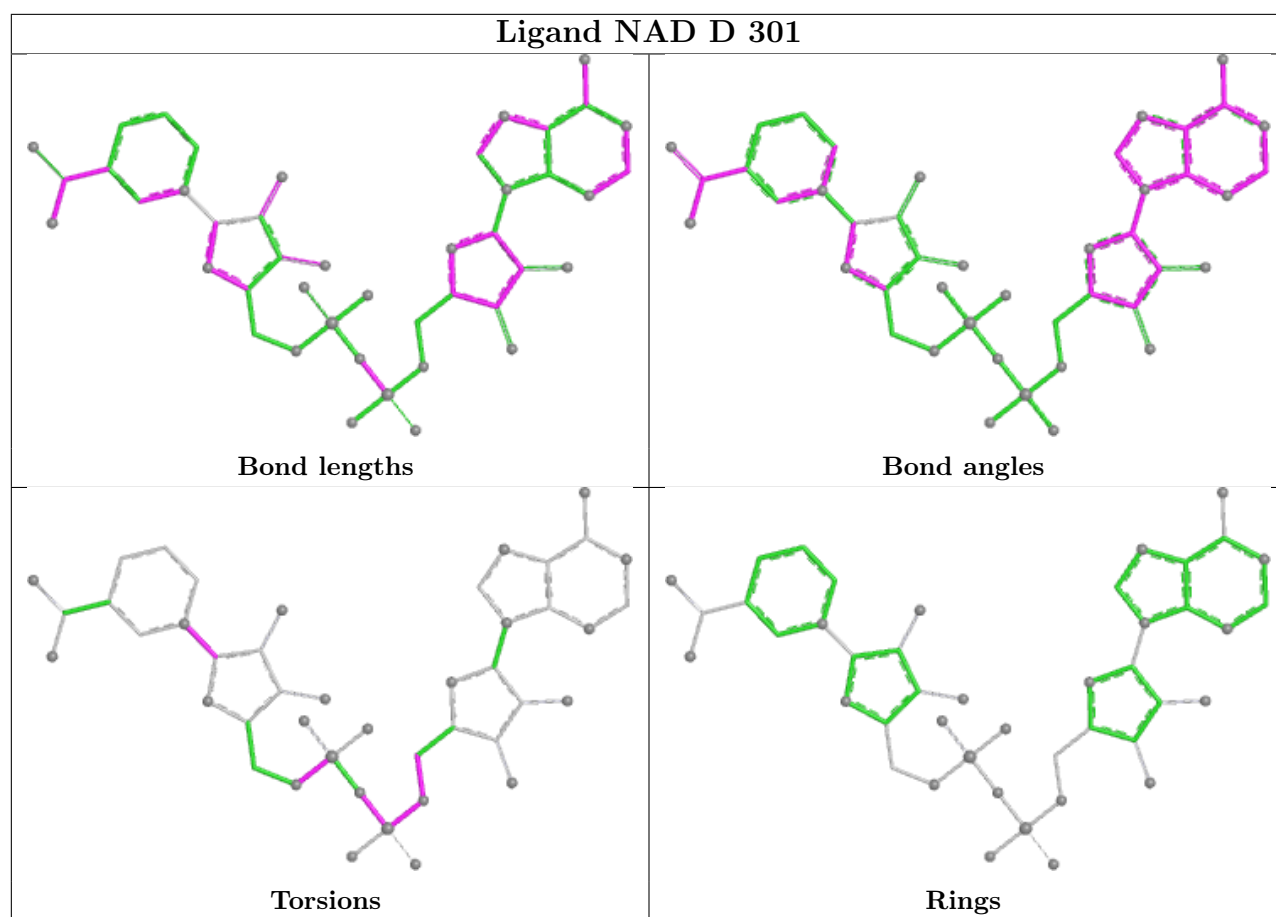
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

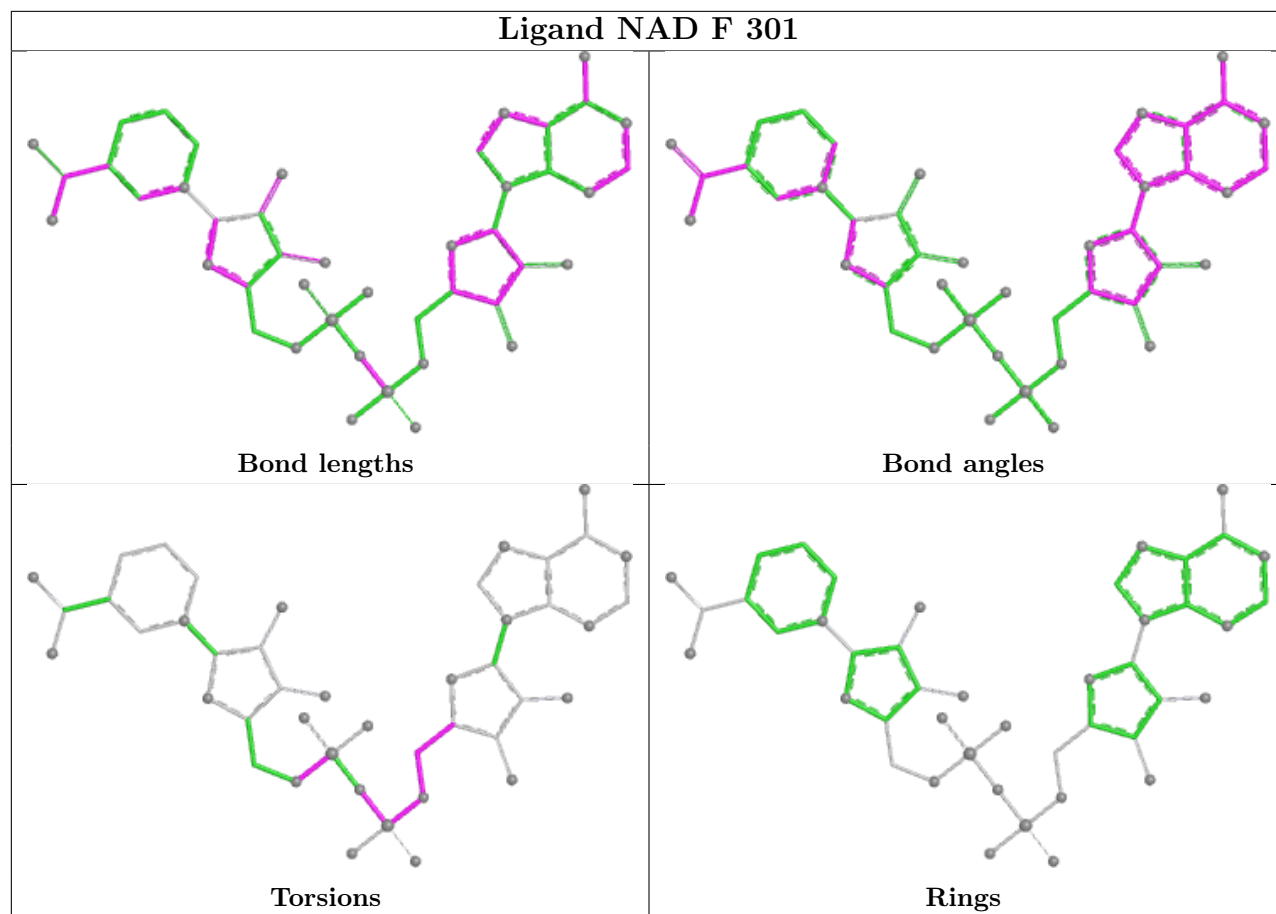


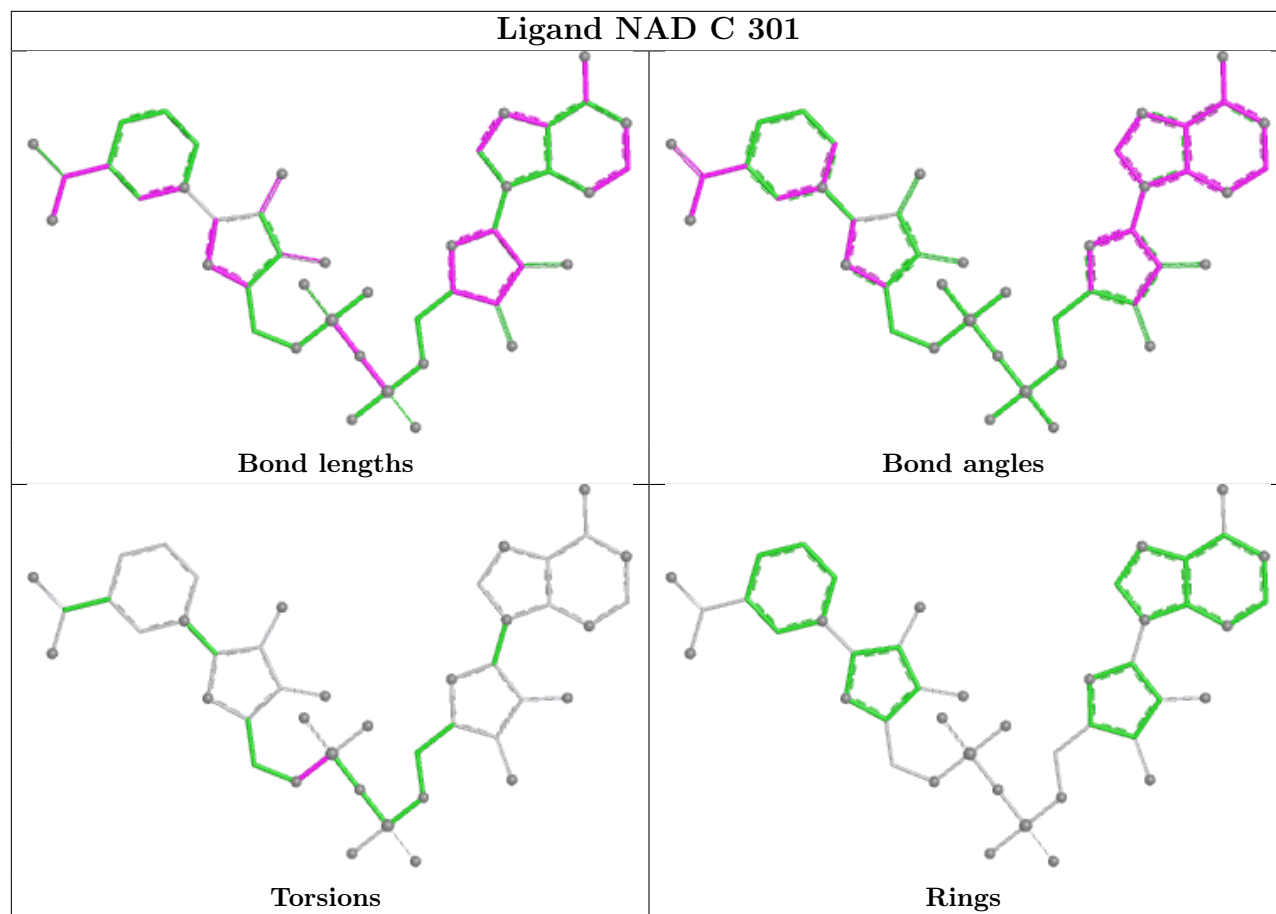


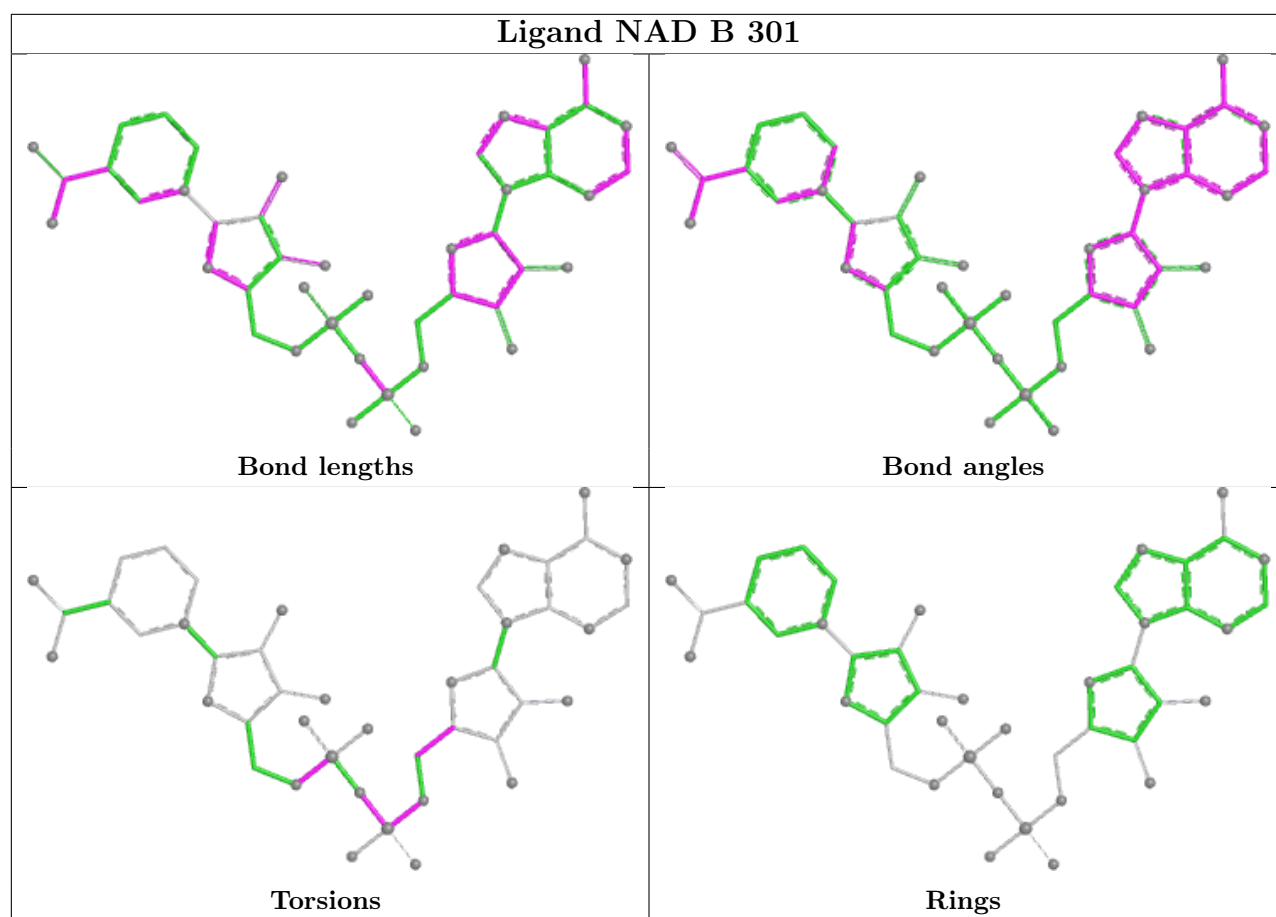












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	278/294 (94%)	0.06	4 (1%) 73 73	12, 20, 36, 71	1 (0%)
1	B	274/294 (93%)	0.28	8 (2%) 53 52	14, 24, 44, 62	0
1	C	277/294 (94%)	0.16	8 (2%) 53 52	14, 23, 36, 61	0
1	D	274/294 (93%)	0.08	8 (2%) 53 52	12, 20, 38, 49	0
1	E	280/294 (95%)	0.26	14 (5%) 34 33	12, 23, 48, 83	0
1	F	284/294 (96%)	0.79	33 (11%) 9 8	18, 34, 65, 80	1 (0%)
1	G	277/294 (94%)	0.42	16 (5%) 29 27	13, 28, 47, 73	0
1	H	283/294 (96%)	0.28	15 (5%) 32 31	14, 24, 48, 68	0
All	All	2227/2352 (94%)	0.29	106 (4%) 35 34	12, 24, 49, 83	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	238	PHE	7.4
1	F	237	ILE	6.9
1	G	245	PRO	6.6
1	F	182	LEU	4.8
1	E	237	ILE	4.7
1	E	245	PRO	4.6
1	E	244	MET	4.5
1	F	189	TYR	4.3
1	E	191	MET	4.0
1	H	189	TYR	3.9
1	H	182	LEU	3.9
1	E	246	GLY	3.9
1	G	246	GLY	3.7
1	F	12	THR	3.7
1	C	190	MET	3.7
1	A	17	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	193	SER	3.6
1	C	17	PHE	3.6
1	F	242	ILE	3.5
1	C	191	MET	3.5
1	E	238	PHE	3.4
1	F	93	THR	3.4
1	F	191	MET	3.4
1	A	18	ASP	3.4
1	B	294	PHE	3.4
1	F	11	LYS	3.3
1	H	238	PHE	3.3
1	F	245	PRO	3.2
1	B	191	MET	3.1
1	C	187	ALA	3.1
1	G	234	TRP	3.1
1	C	192	GLY	3.1
1	F	190	MET	3.0
1	F	234	TRP	3.0
1	G	11	LYS	2.9
1	F	244	MET	2.9
1	G	250	MET	2.8
1	F	240	GLY	2.8
1	E	11	LYS	2.8
1	G	191	MET	2.8
1	G	249	ALA	2.8
1	B	30	ASN	2.7
1	B	28	ASP	2.7
1	G	92	GLY	2.7
1	F	113	THR	2.6
1	C	19	GLU	2.6
1	F	119	LEU	2.6
1	C	293	VAL	2.6
1	E	294	PHE	2.6
1	B	82	GLU	2.5
1	D	190	MET	2.5
1	E	251	LEU	2.5
1	F	53	LEU	2.5
1	H	244	MET	2.5
1	H	245	PRO	2.5
1	D	192	GLY	2.5
1	G	182	LEU	2.5
1	B	33	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	231	GLY	2.4
1	D	294	PHE	2.4
1	F	249	ALA	2.4
1	G	66	ALA	2.4
1	H	191	MET	2.4
1	F	98	LEU	2.4
1	B	31	TYR	2.4
1	H	12	THR	2.4
1	F	82	GLU	2.4
1	E	193	SER	2.4
1	D	189	TYR	2.3
1	E	250	MET	2.3
1	F	109	ALA	2.3
1	G	190	MET	2.3
1	H	237	ILE	2.3
1	F	143	GLU	2.3
1	D	26	TRP	2.2
1	F	192	GLY	2.2
1	D	29	SER	2.2
1	F	96	ILE	2.2
1	E	189	TYR	2.2
1	F	250	MET	2.2
1	G	12	THR	2.2
1	F	111	LEU	2.2
1	F	181	ALA	2.2
1	E	239	ASN	2.2
1	A	85	LYS	2.2
1	H	190	MET	2.1
1	G	237	ILE	2.1
1	F	69	ALA	2.1
1	F	78	ASP	2.1
1	G	29	SER	2.1
1	F	241	ARG	2.1
1	H	188	ASN	2.1
1	A	189	TYR	2.1
1	C	189	TYR	2.1
1	F	108	VAL	2.1
1	G	251	LEU	2.1
1	H	251	LEU	2.1
1	F	79	LYS	2.0
1	E	249	ALA	2.0
1	G	193	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	242	ILE	2.0
1	F	236	GLY	2.0
1	H	184	GLY	2.0
1	D	22	PRO	2.0
1	B	293	VAL	2.0
1	D	293	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

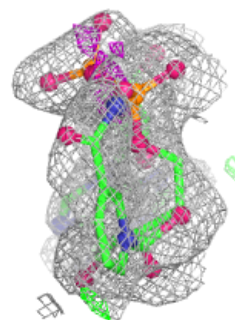
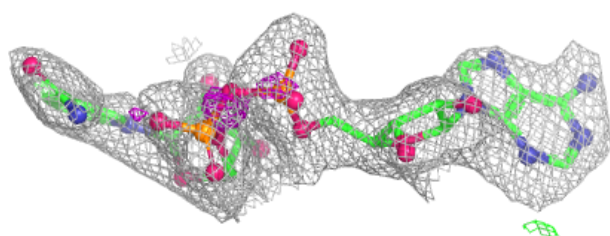
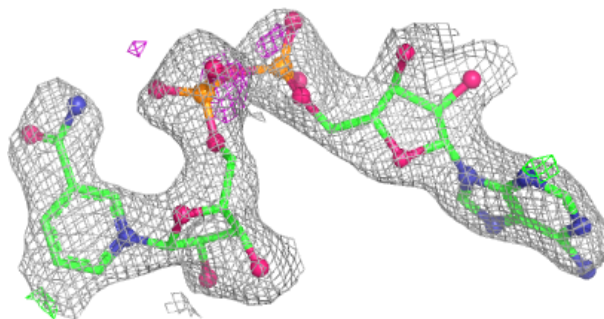
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	F	301	44/44	0.88	0.10	34,42,44,46	0
2	NAD	G	301	44/44	0.89	0.10	27,33,38,43	0
2	NAD	E	301	44/44	0.91	0.08	22,26,29,31	0
2	NAD	H	301	44/44	0.92	0.09	25,28,30,31	0
2	NAD	B	301	44/44	0.94	0.07	17,21,23,24	0
2	NAD	A	301	44/44	0.95	0.07	15,18,19,20	0
2	NAD	C	301	44/44	0.95	0.07	15,19,21,22	0
2	NAD	D	301	44/44	0.96	0.06	15,18,19,19	0

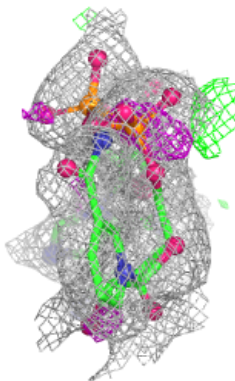
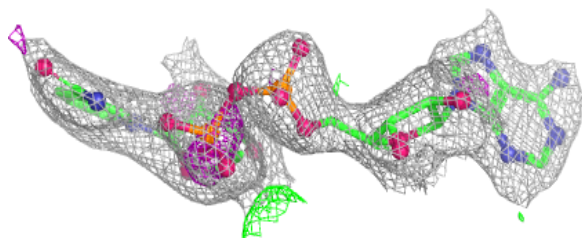
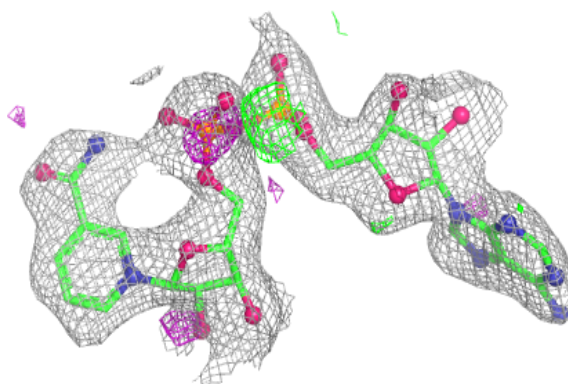
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

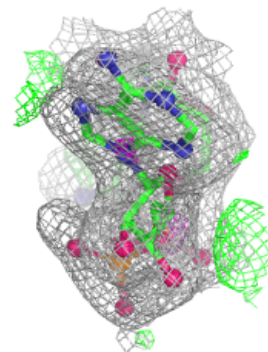
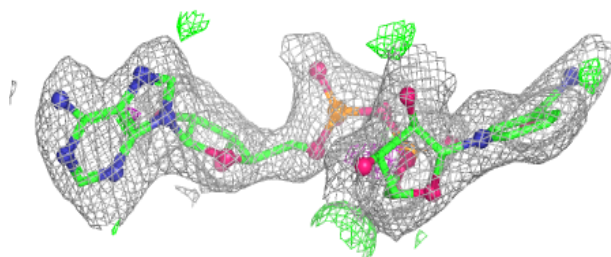
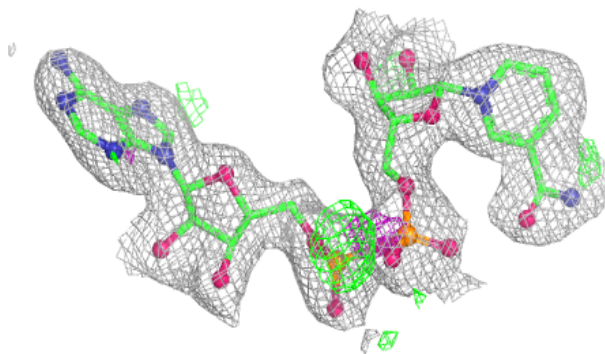
**Electron density around NAD G 301:**

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

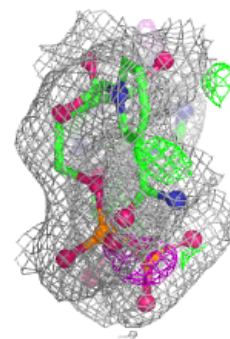
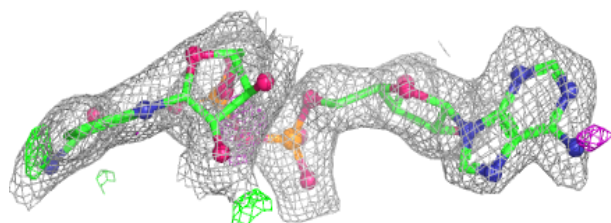
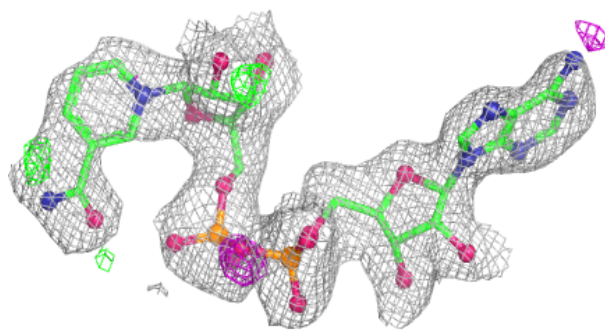


Electron density around NAD E 301:

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

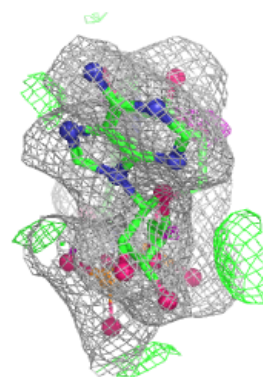
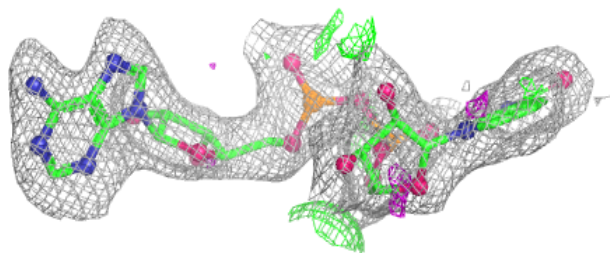
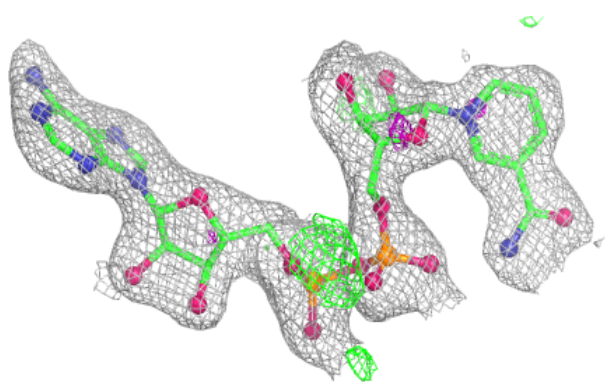
**Electron density around NAD H 301:**

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

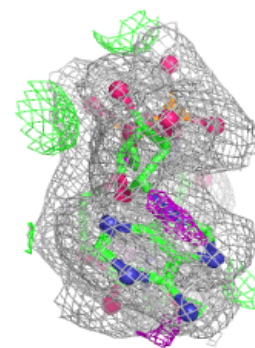
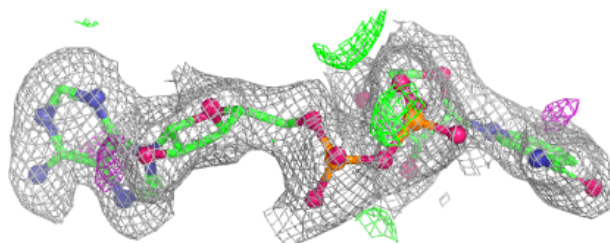
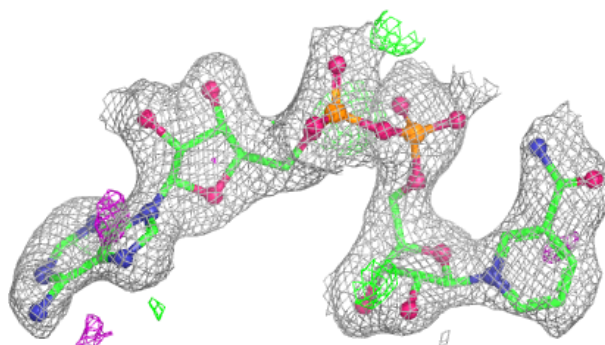


Electron density around NAD B 301:

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

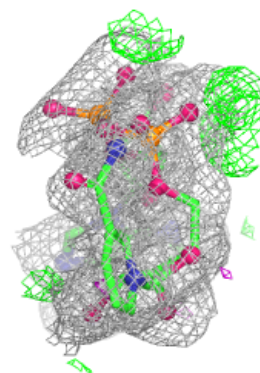
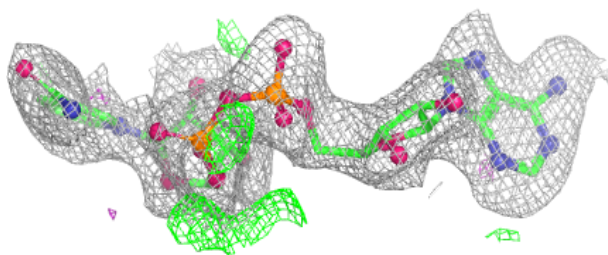
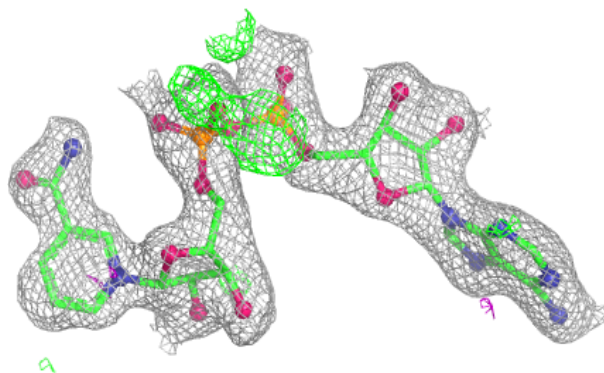
**Electron density around NAD A 301:**

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

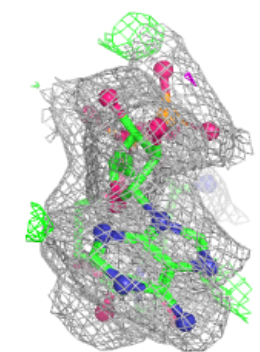
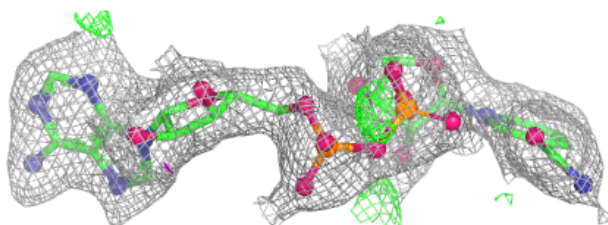
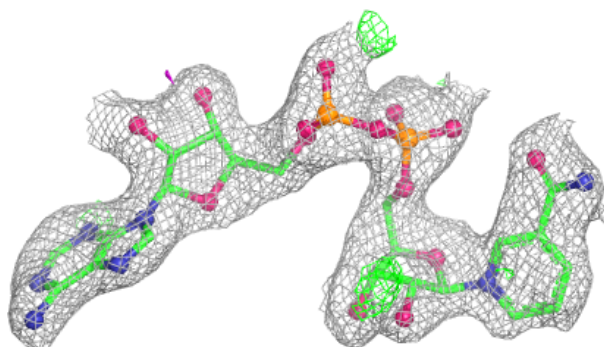


Electron density around NAD C 301:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.