WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 10:22 AM EDT

PDB ID	:	1VM6
Title	:	Crystal structure of Dihydrodipicolinate reductase (TM1520) from Thermotoga maritima at 2.27 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2004-09-03
Resolution	:	2.27 Å(reported)

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

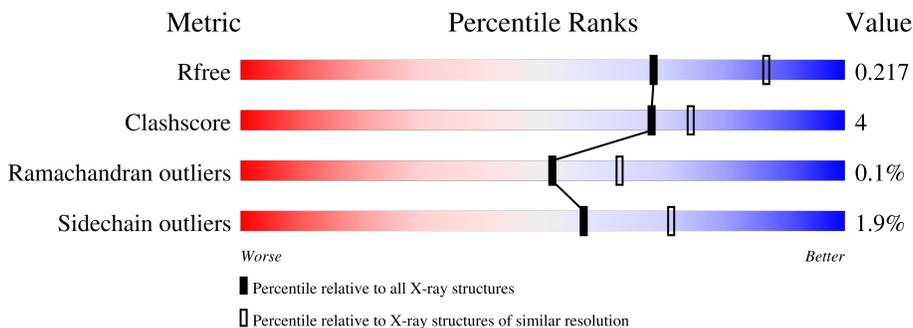|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	Percentile Ranks	Value
Rfree		0.217
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	228	86% 8% 6%
1	B	228	86% 10% •
1	C	228	85% 10% 6%
1	D	228	83% 11% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	218	-	-	X	-
2	ACT	B	218	-	-	X	-
2	ACT	B	221	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7538 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 Dihydrodipicolinate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1667	1073	280	309	5			
1	B	218	Total	C	N	O	S	0	0	0
			1705	1096	292	312	5			
1	C	215	Total	C	N	O	S	0	0	0
			1663	1070	279	309	5			
1	D	217	Total	C	N	O	S	0	1	0
			1699	1092	289	313	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X1K8
A	-10	GLY	-	expression tag	UNP Q9X1K8
A	-9	SER	-	expression tag	UNP Q9X1K8
A	-8	ASP	-	expression tag	UNP Q9X1K8
A	-7	LYS	-	expression tag	UNP Q9X1K8
A	-6	ILE	-	expression tag	UNP Q9X1K8
A	-5	HIS	-	expression tag	UNP Q9X1K8
A	-4	HIS	-	expression tag	UNP Q9X1K8
A	-3	HIS	-	expression tag	UNP Q9X1K8
A	-2	HIS	-	expression tag	UNP Q9X1K8
A	-1	HIS	-	expression tag	UNP Q9X1K8
A	0	HIS	-	expression tag	UNP Q9X1K8
B	-11	MET	-	expression tag	UNP Q9X1K8
B	-10	GLY	-	expression tag	UNP Q9X1K8
B	-9	SER	-	expression tag	UNP Q9X1K8
B	-8	ASP	-	expression tag	UNP Q9X1K8
B	-7	LYS	-	expression tag	UNP Q9X1K8
B	-6	ILE	-	expression tag	UNP Q9X1K8
B	-5	HIS	-	expression tag	UNP Q9X1K8
B	-4	HIS	-	expression tag	UNP Q9X1K8
B	-3	HIS	-	expression tag	UNP Q9X1K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9X1K8
B	-1	HIS	-	expression tag	UNP Q9X1K8
B	0	HIS	-	expression tag	UNP Q9X1K8
C	-11	MET	-	expression tag	UNP Q9X1K8
C	-10	GLY	-	expression tag	UNP Q9X1K8
C	-9	SER	-	expression tag	UNP Q9X1K8
C	-8	ASP	-	expression tag	UNP Q9X1K8
C	-7	LYS	-	expression tag	UNP Q9X1K8
C	-6	ILE	-	expression tag	UNP Q9X1K8
C	-5	HIS	-	expression tag	UNP Q9X1K8
C	-4	HIS	-	expression tag	UNP Q9X1K8
C	-3	HIS	-	expression tag	UNP Q9X1K8
C	-2	HIS	-	expression tag	UNP Q9X1K8
C	-1	HIS	-	expression tag	UNP Q9X1K8
C	0	HIS	-	expression tag	UNP Q9X1K8
D	-11	MET	-	expression tag	UNP Q9X1K8
D	-10	GLY	-	expression tag	UNP Q9X1K8
D	-9	SER	-	expression tag	UNP Q9X1K8
D	-8	ASP	-	expression tag	UNP Q9X1K8
D	-7	LYS	-	expression tag	UNP Q9X1K8
D	-6	ILE	-	expression tag	UNP Q9X1K8
D	-5	HIS	-	expression tag	UNP Q9X1K8
D	-4	HIS	-	expression tag	UNP Q9X1K8
D	-3	HIS	-	expression tag	UNP Q9X1K8
D	-2	HIS	-	expression tag	UNP Q9X1K8
D	-1	HIS	-	expression tag	UNP Q9X1K8
D	0	HIS	-	expression tag	UNP Q9X1K8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

O
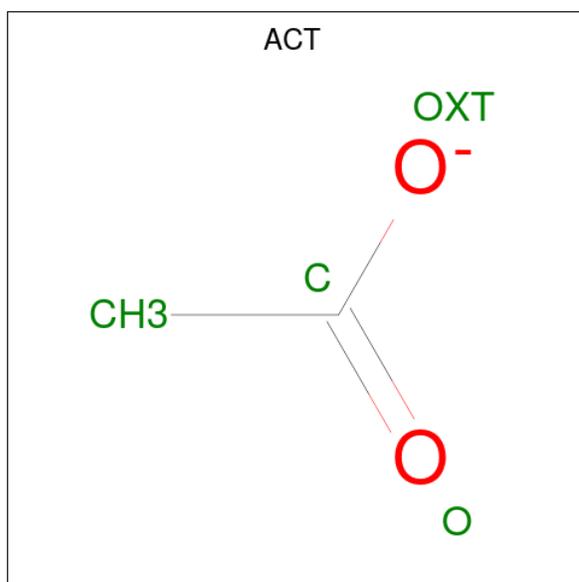
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

NAD

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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 13	C 8	O 5	0	0
4	B	1	Total 13	C 8	O 5	0	0
4	B	1	Total 8	C 5	O 3	0	0
4	C	1	Total 13	C 8	O 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
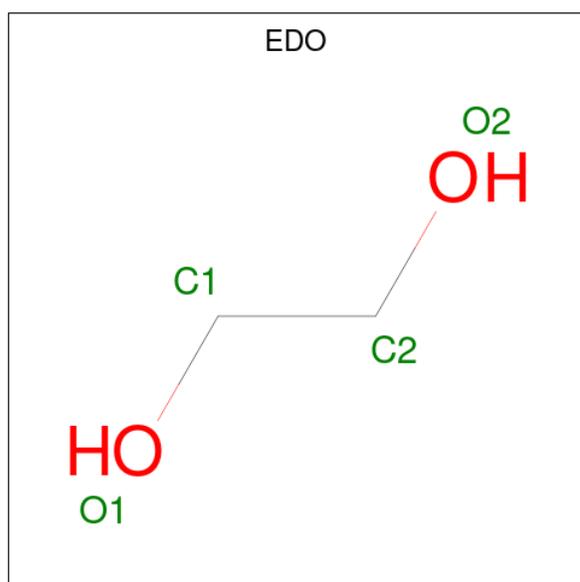
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	93	Total 93	O 93	0	0
6	B	190	Total 190	O 190	0	0
6	C	106	Total 106	O 106	0	0
6	D	140	Total 140	O 140	0	0

3 Residue-property plots ⓘ

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: Dihydrodipicolinate reductase

Chain A:

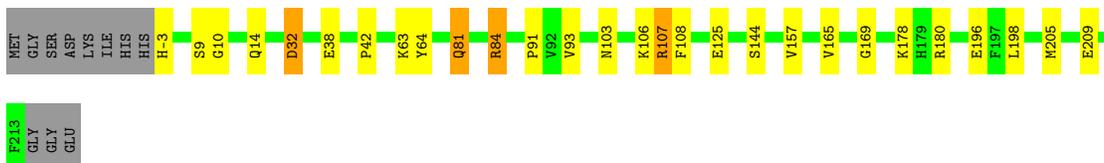- Molecule 1: Dihydrodipicolinate reductase

Chain B:

- Molecule 1: Dihydrodipicolinate reductase

Chain C:

- Molecule 1: Dihydrodipicolinate reductase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.08Å 109.22Å 112.60Å 90.00° 119.23° 90.00°	Depositor
Resolution (Å)	29.03 – 2.27 29.03 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.03-2.27) 95.5 (29.03-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.213 0.176 , 0.217	Depositor DCC
R_{free} test set	3151 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7538	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAD, ACT, PG4

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	0.59	0/1699	0.73	2/2294 (0.1%)
1	B	0.74	1/1741 (0.1%)	0.80	2/2351 (0.1%)
1	C	0.62	0/1694	0.75	2/2286 (0.1%)
1	D	0.65	0/1738	0.78	2/2347 (0.1%)
All	All	0.65	1/6872 (0.0%)	0.77	8/9278 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	GLU	CG-CD	5.16	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	D	180	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	202	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	C	180	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	202	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	180	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	180	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	180	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1667	0	1701	11	0
1	B	1705	0	1733	17	0
1	C	1663	0	1704	14	0
1	D	1699	0	1726	17	0
2	A	8	0	6	2	0
2	B	24	0	18	4	0
2	C	8	0	6	0	0
2	D	8	0	6	0	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	1	0
3	D	44	0	26	0	0
4	B	34	0	45	1	0
4	C	13	0	18	0	0
5	C	4	0	6	0	0
6	A	93	0	0	0	0
6	B	190	0	0	3	0
6	C	106	0	0	0	0
6	D	140	0	0	1	0
All	All	7538	0	7073	54	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 4.

All (54) 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:B:93:VAL:HG23	1:B:198:LEU:HD21	1.61	0.83
1:D:196:GLU:OE2	6:D:411:HOH:O	2.13	0.66
1:A:93:VAL:HG23	1:A:198:LEU:HD21	1.75	0.66
1:C:91:PRO:HB2	1:C:198:LEU:HD22	1.78	0.65
1:B:210:GLU:OE1	6:B:491:HOH:O	2.14	0.64
1:A:91:PRO:HB2	1:A:198:LEU:HD22	1.80	0.64
1:C:93:VAL:HG23	1:C:198:LEU:HD21	1.83	0.61
1:B:193:LYS:NZ	2:B:221:ACT:H1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:SER:OG	1:D:32:ASP:OD1	2.16	0.57
1:B:91:PRO:HB2	1:B:198:LEU:HD22	1.85	0.57
1:C:23:LYS:HG3	1:C:192:LEU:HD21	1.87	0.56
2:A:217:ACT:H1	2:A:218:ACT:H2	1.87	0.55
1:D:106:LYS:HE2	1:D:209:GLU:OE2	2.06	0.55
1:B:193:LYS:HZ3	2:B:221:ACT:H1	1.71	0.55
1:D:103:ASN:O	1:D:107:ARG:HD3	2.08	0.54
1:D:-3:HIS:HA	1:D:196:GLU:OE1	2.09	0.53
1:B:169:GLY:HA3	1:D:157:VAL:HG13	1.89	0.53
1:B:106:LYS:HG2	1:B:145:ALA:HB2	1.92	0.51
1:C:16:ILE:HD13	1:C:46:ILE:HG21	1.93	0.50
2:B:218:ACT:H2	2:B:222:ACT:H3	1.93	0.50
1:C:16:ILE:HD13	1:C:46:ILE:CG2	2.41	0.49
1:A:73:THR:HG21	2:A:218:ACT:H3	1.93	0.49
1:B:106:LYS:HD2	6:B:376:HOH:O	2.13	0.48
1:A:71:GLY:O	3:A:300:NAD:H2N	2.13	0.48
1:B:80:LEU:HD21	4:B:302:PG4:H52	1.96	0.48
1:C:183:SER:O	1:C:186:VAL:HG12	2.13	0.47
1:A:165:VAL:HG22	1:A:178:LYS:HG3	1.97	0.47
1:D:165:VAL:HG22	1:D:178:LYS:HG3	1.96	0.46
1:A:107:ARG:CZ	1:A:209:GLU:OE2	2.64	0.46
1:D:38:GLU:OE2	1:D:63:LYS:NZ	2.40	0.46
1:A:23:LYS:HG3	1:A:192:LEU:HD21	1.99	0.45
1:A:157:VAL:CG1	1:C:169:GLY:HA3	2.46	0.45
1:A:108:PHE:HB3	1:D:108:PHE:CE2	2.52	0.45
1:B:132:LYS:NZ	6:B:361:HOH:O	2.49	0.44
1:B:73:THR:HA	1:B:96:TYR:CE1	2.53	0.44
1:D:91:PRO:HB2	1:D:198:LEU:HD22	1.98	0.44
1:D:42:PRO:HD2	1:D:64:TYR:CG	2.53	0.44
1:B:121:VAL:HA	1:B:167:VAL:O	2.18	0.43
1:D:10:GLY:O	1:D:14:GLN:HG3	2.18	0.43
1:B:178:LYS:HZ2	1:C:178:LYS:HE2	1.84	0.43
1:B:165:VAL:HG22	1:B:178:LYS:HG2	2.01	0.42
1:B:169:GLY:HA3	1:D:157:VAL:CG1	2.49	0.42
1:C:121:VAL:HA	1:C:167:VAL:O	2.19	0.42
1:B:127:HIS:CD2	2:B:218:ACT:H3	2.55	0.42
1:D:93:VAL:HG23	1:D:198:LEU:HD21	2.02	0.42
1:A:121:VAL:O	1:A:150:VAL:HG13	2.20	0.41
1:A:157:VAL:HG13	1:C:169:GLY:HA3	2.02	0.41
1:C:104:VAL:HG22	1:C:212:ILE:HG21	2.02	0.41
1:D:84:ARG:HH12	1:D:205:MET:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:PRO:HD2	1:C:64:TYR:CG	2.56	0.41
1:B:157:VAL:HG13	1:D:169:GLY:HA3	2.02	0.41
1:C:104:VAL:CG2	1:C:212:ILE:HG21	2.52	0.40
1:C:71:GLY:O	3:C:300:NAD:H2N	2.22	0.40
1:D:81:GLN:OE1	1:D:81:GLN:HA	2.21	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	213/228 (93%)	208 (98%)	4 (2%)	1 (0%)	29	34
1	B	216/228 (95%)	214 (99%)	2 (1%)	0	100	100
1	C	213/228 (93%)	208 (98%)	5 (2%)	0	100	100
1	D	216/228 (95%)	212 (98%)	4 (2%)	0	100	100
All	All	858/912 (94%)	842 (98%)	15 (2%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	PHE

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	182/194 (94%)	180 (99%)	2 (1%)	73	84
1	B	187/194 (96%)	184 (98%)	3 (2%)	62	76
1	C	182/194 (94%)	179 (98%)	3 (2%)	62	76
1	D	187/194 (96%)	181 (97%)	6 (3%)	39	52
All	All	738/776 (95%)	724 (98%)	14 (2%)	57	71

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

Mol	Chain	Res	Type
1	A	41	SER
1	A	125	GLU
1	B	-4	HIS
1	B	56	LYS
1	B	125	GLU
1	C	50	SER
1	C	141	LEU
1	C	144	SER
1	D	32	ASP
1	D	81	GLN
1	D	84	ARG
1	D	107	ARG
1	D	125	GLU
1	D	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	#$|Z| > 2$
3	NAD	A	300	-	42,48,48	1.57	3 (7%)	50,73,73	1.32	4 (8%)
2	ACT	B	217	-	3,3,3	0.96	0	3,3,3	1.01	0
5	EDO	C	301	-	3,3,3	0.60	0	2,2,2	0.20	0
2	ACT	B	220	-	3,3,3	1.01	0	3,3,3	1.46	1 (33%)
3	NAD	B	300	-	42,48,48	1.63	3 (7%)	50,73,73	1.26	5 (10%)
4	PG4	B	301	-	12,12,12	0.61	0	11,11,11	0.28	0
2	ACT	C	217	-	3,3,3	0.77	0	3,3,3	1.38	0
4	PG4	B	302	-	12,12,12	0.48	0	11,11,11	0.53	0
2	ACT	A	218	-	3,3,3	0.60	0	3,3,3	1.15	0
2	ACT	D	218	-	3,3,3	0.84	0	3,3,3	0.55	0
3	NAD	C	300	-	42,48,48	1.79	4 (9%)	50,73,73	1.19	3 (6%)
2	ACT	B	221	-	3,3,3	0.43	0	3,3,3	1.99	1 (33%)
4	PG4	B	303	-	7,7,12	0.51	0	6,6,11	0.45	0
2	ACT	B	219	-	3,3,3	0.68	0	3,3,3	1.32	0
2	ACT	A	217	-	3,3,3	0.81	0	3,3,3	1.47	0
2	ACT	D	217	-	3,3,3	0.85	0	3,3,3	0.92	0
2	ACT	B	222	-	3,3,3	0.67	0	3,3,3	1.07	0
2	ACT	C	218	-	3,3,3	0.84	0	3,3,3	1.29	0
2	ACT	B	218	-	3,3,3	0.88	0	3,3,3	1.08	0
3	NAD	D	300	-	42,48,48	1.70	3 (7%)	50,73,73	1.40	5 (10%)
4	PG4	C	302	-	12,12,12	0.67	0	11,11,11	0.46	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
4	PG4	B	302	-	-	5/10/10/10	-
3	NAD	B	300	-	-	4/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	300	-	-	5/26/62/62	0/5/5/5
4	PG4	B	301	-	-	4/10/10/10	-
4	PG4	B	303	-	-	3/5/5/10	-
3	NAD	D	300	-	-	5/26/62/62	0/5/5/5
3	NAD	A	300	-	-	6/26/62/62	0/5/5/5
5	EDO	C	301	-	-	1/1/1/1	-
4	PG4	C	302	-	-	5/10/10/10	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	300	NAD	O7N-C7N	8.74	1.40	1.24
3	D	300	NAD	O7N-C7N	8.64	1.40	1.24
3	B	300	NAD	O7N-C7N	7.65	1.38	1.24
3	A	300	NAD	O7N-C7N	7.18	1.37	1.24
3	C	300	NAD	C2A-N3A	4.34	1.39	1.32
3	B	300	NAD	C2A-N3A	4.25	1.39	1.32
3	A	300	NAD	C2A-N3A	4.21	1.38	1.32
3	D	300	NAD	C2A-N3A	4.12	1.38	1.32
3	B	300	NAD	C2A-N1A	3.34	1.40	1.33
3	C	300	NAD	C2A-N1A	2.94	1.39	1.33
3	A	300	NAD	C2A-N1A	2.75	1.39	1.33
3	D	300	NAD	C2A-N1A	2.26	1.38	1.33
3	C	300	NAD	C2N-N1N	2.16	1.37	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	NAD	N3A-C2A-N1A	-5.85	119.54	128.68
3	D	300	NAD	N3A-C2A-N1A	-5.76	119.68	128.68
3	C	300	NAD	N3A-C2A-N1A	-4.98	120.89	128.68
3	B	300	NAD	N3A-C2A-N1A	-4.80	121.17	128.68
3	A	300	NAD	C3N-C7N-N7N	3.35	121.77	117.75
3	D	300	NAD	C2N-C3N-C4N	2.74	121.36	118.26
2	B	221	ACT	OXT-C-CH3	2.71	126.38	115.18
3	D	300	NAD	C5N-C4N-C3N	-2.70	117.15	120.34
3	B	300	NAD	O4B-C1B-C2B	-2.45	103.34	106.93
3	B	300	NAD	C3N-C7N-N7N	2.37	120.59	117.75
3	C	300	NAD	C1B-N9A-C4A	-2.12	122.92	126.64
3	B	300	NAD	C2N-C3N-C4N	2.11	120.65	118.26
3	D	300	NAD	C6N-N1N-C2N	-2.11	120.06	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	300	NAD	C6N-N1N-C2N	-2.08	120.08	121.97
3	A	300	NAD	O7N-C7N-C3N	-2.07	117.16	119.63
2	B	220	ACT	OXT-C-O	-2.05	114.49	122.05
3	B	300	NAD	C3N-C2N-N1N	-2.03	118.44	120.43
3	A	300	NAD	O2N-PN-O1N	2.03	122.26	112.24
3	D	300	NAD	C1B-N9A-C4A	-2.01	123.10	126.64

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	NAD	O4D-C1D-N1N-C2N
3	A	300	NAD	O4D-C1D-N1N-C6N
3	A	300	NAD	C2D-C1D-N1N-C2N
3	B	300	NAD	O4D-C1D-N1N-C2N
3	B	300	NAD	O4D-C1D-N1N-C6N
3	B	300	NAD	C2D-C1D-N1N-C2N
3	C	300	NAD	O4D-C1D-N1N-C2N
3	C	300	NAD	O4D-C1D-N1N-C6N
3	C	300	NAD	C2D-C1D-N1N-C2N
3	C	300	NAD	C2D-C1D-N1N-C6N
3	D	300	NAD	O4D-C1D-N1N-C2N
3	D	300	NAD	O4D-C1D-N1N-C6N
3	D	300	NAD	C2D-C1D-N1N-C2N
4	C	302	PG4	O2-C3-C4-O3
4	C	302	PG4	O3-C5-C6-O4
4	B	302	PG4	O3-C5-C6-O4
4	B	301	PG4	O4-C7-C8-O5
4	B	301	PG4	O1-C1-C2-O2
4	B	303	PG4	O4-C7-C8-O5
4	B	302	PG4	C1-C2-O2-C3
4	C	302	PG4	C6-C5-O3-C4
4	C	302	PG4	C8-C7-O4-C6
4	B	301	PG4	C1-C2-O2-C3
4	C	302	PG4	O4-C7-C8-O5
5	C	301	EDO	O1-C1-C2-O2
4	B	302	PG4	C6-C5-O3-C4
3	A	300	NAD	PN-O3-PA-O1A
4	B	301	PG4	C4-C3-O2-C2
3	A	300	NAD	O4B-C4B-C5B-O5B
3	B	300	NAD	O4B-C4B-C5B-O5B
4	B	303	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
4	B	303	PG4	O3-C5-C6-O4
3	A	300	NAD	C2D-C1D-N1N-C6N
3	D	300	NAD	C2D-C1D-N1N-C6N
3	C	300	NAD	O4B-C4B-C5B-O5B
3	D	300	NAD	O4B-C4B-C5B-O5B
4	B	302	PG4	O2-C3-C4-O3
4	B	302	PG4	C3-C4-O3-C5

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	NAD	1	0
4	B	302	PG4	1	0
2	A	218	ACT	2	0
3	C	300	NAD	1	0
2	B	221	ACT	2	0
2	A	217	ACT	1	0
2	B	222	ACT	1	0
2	B	218	ACT	2	0

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

Ligand NAD A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 300

Bond lengths

Bond angles

Torsions

Rings
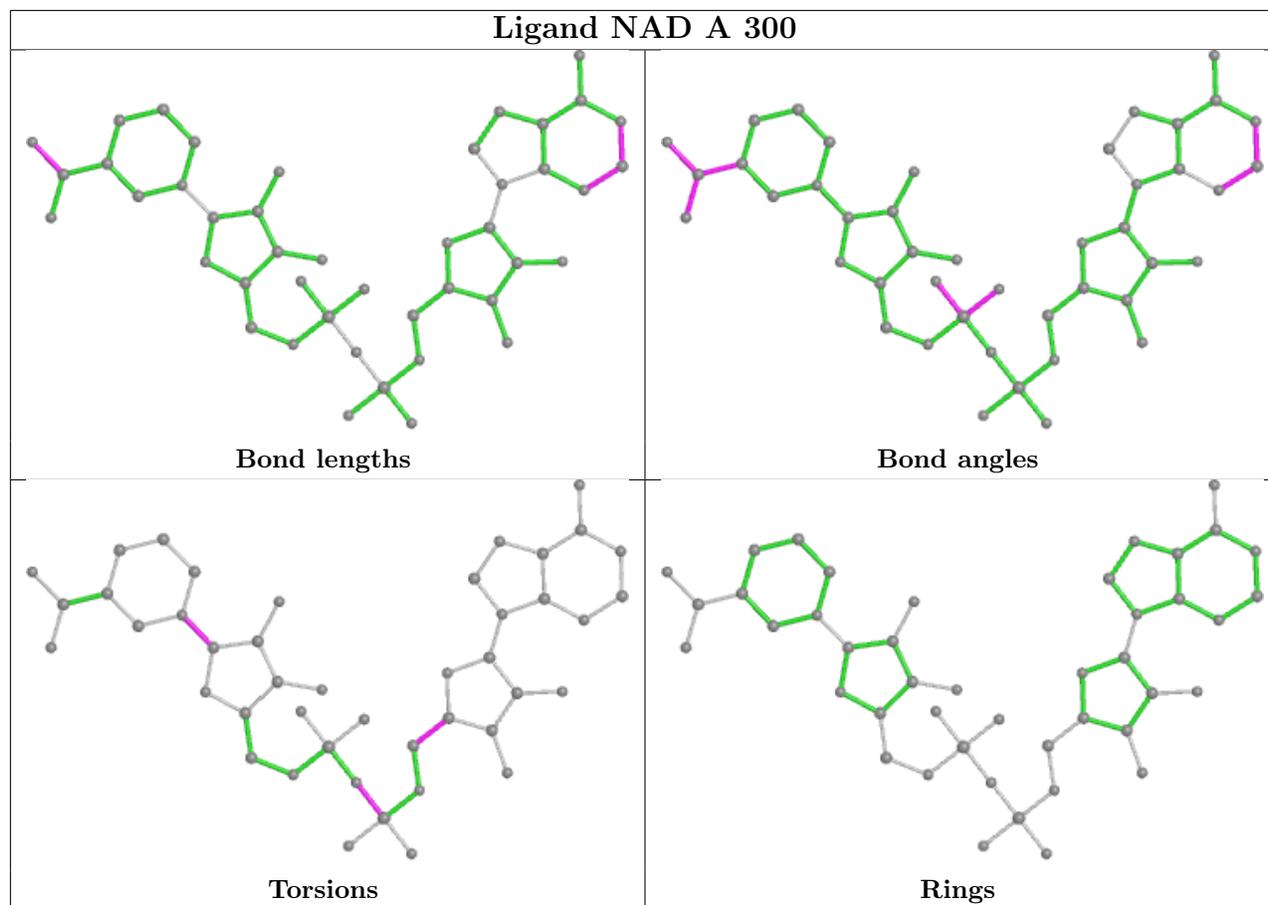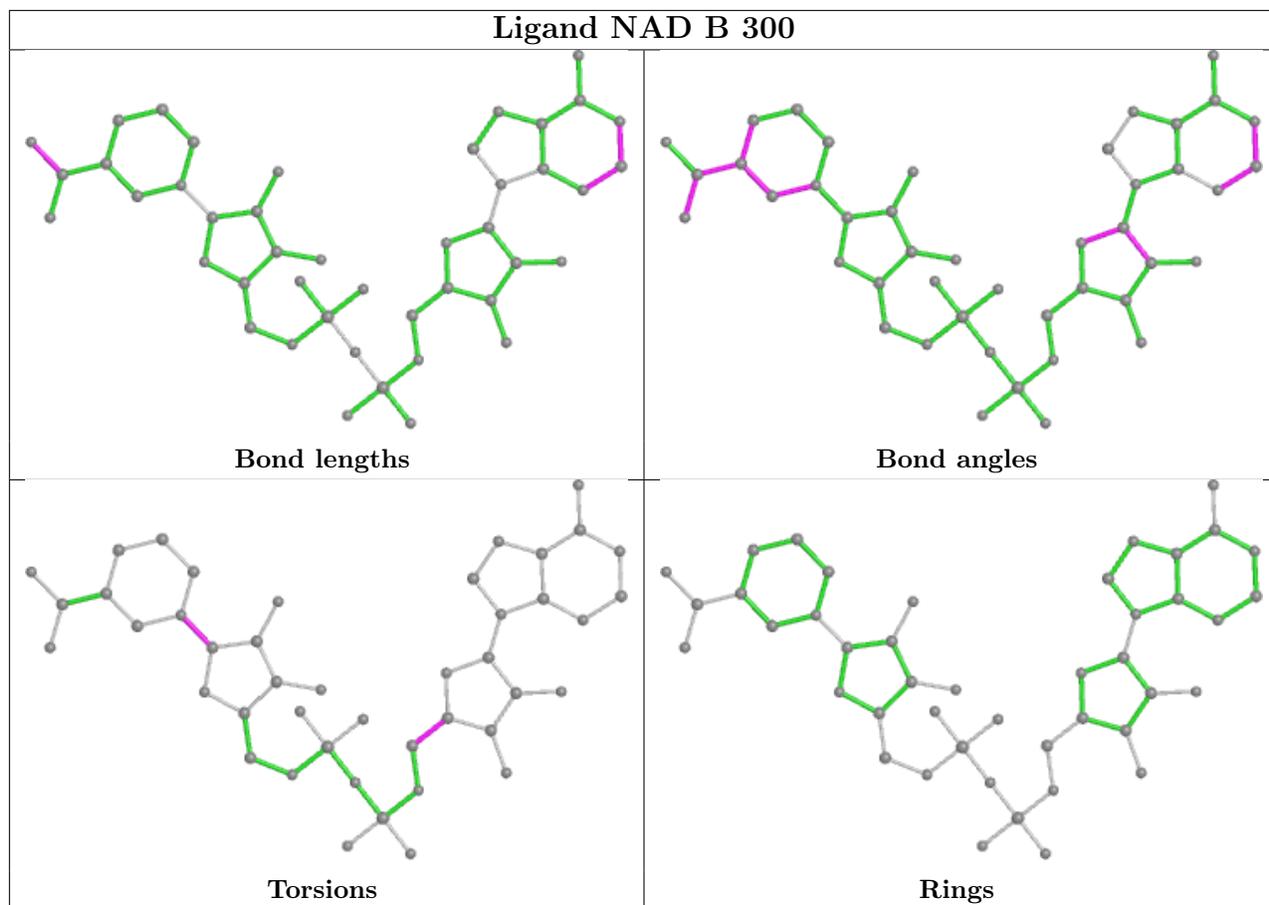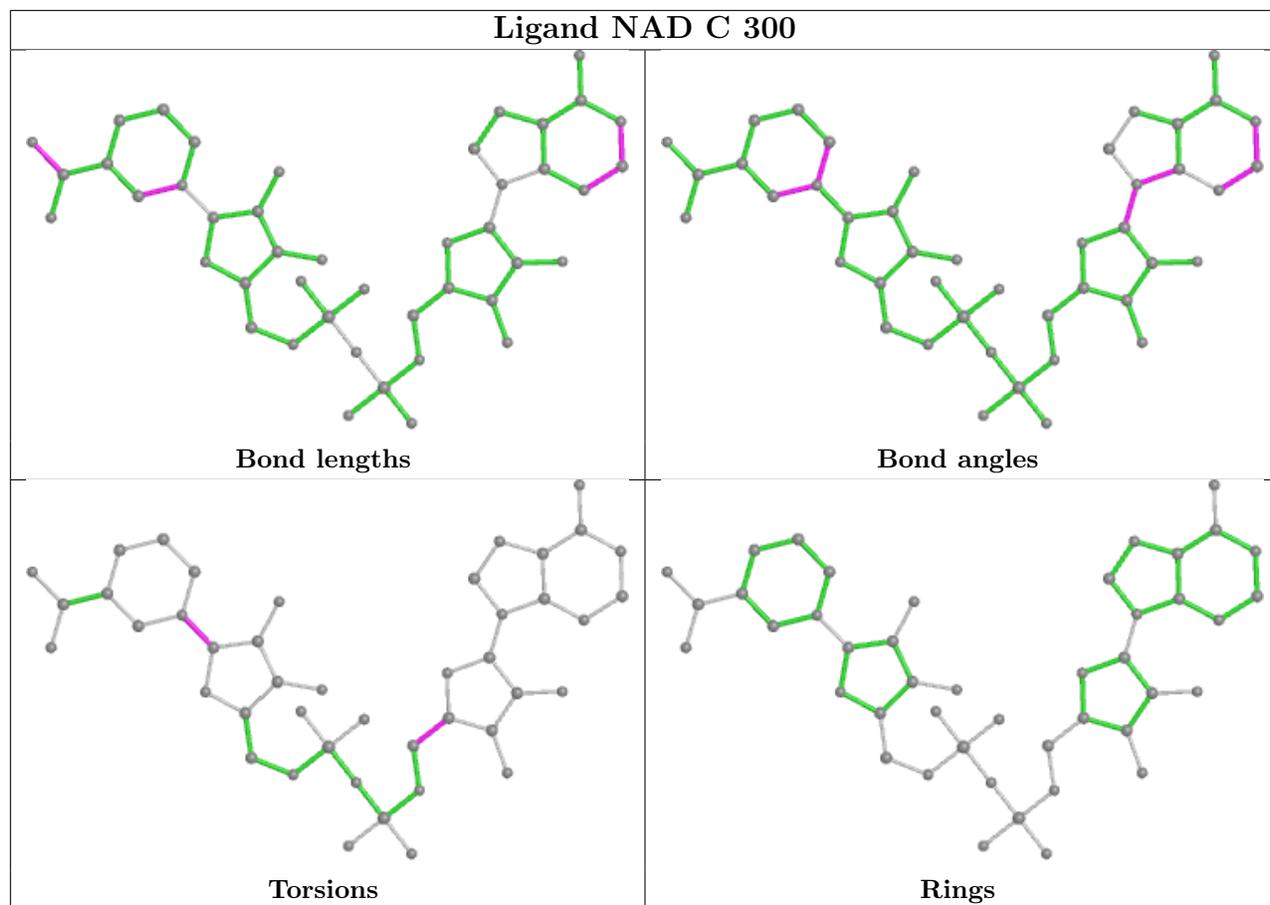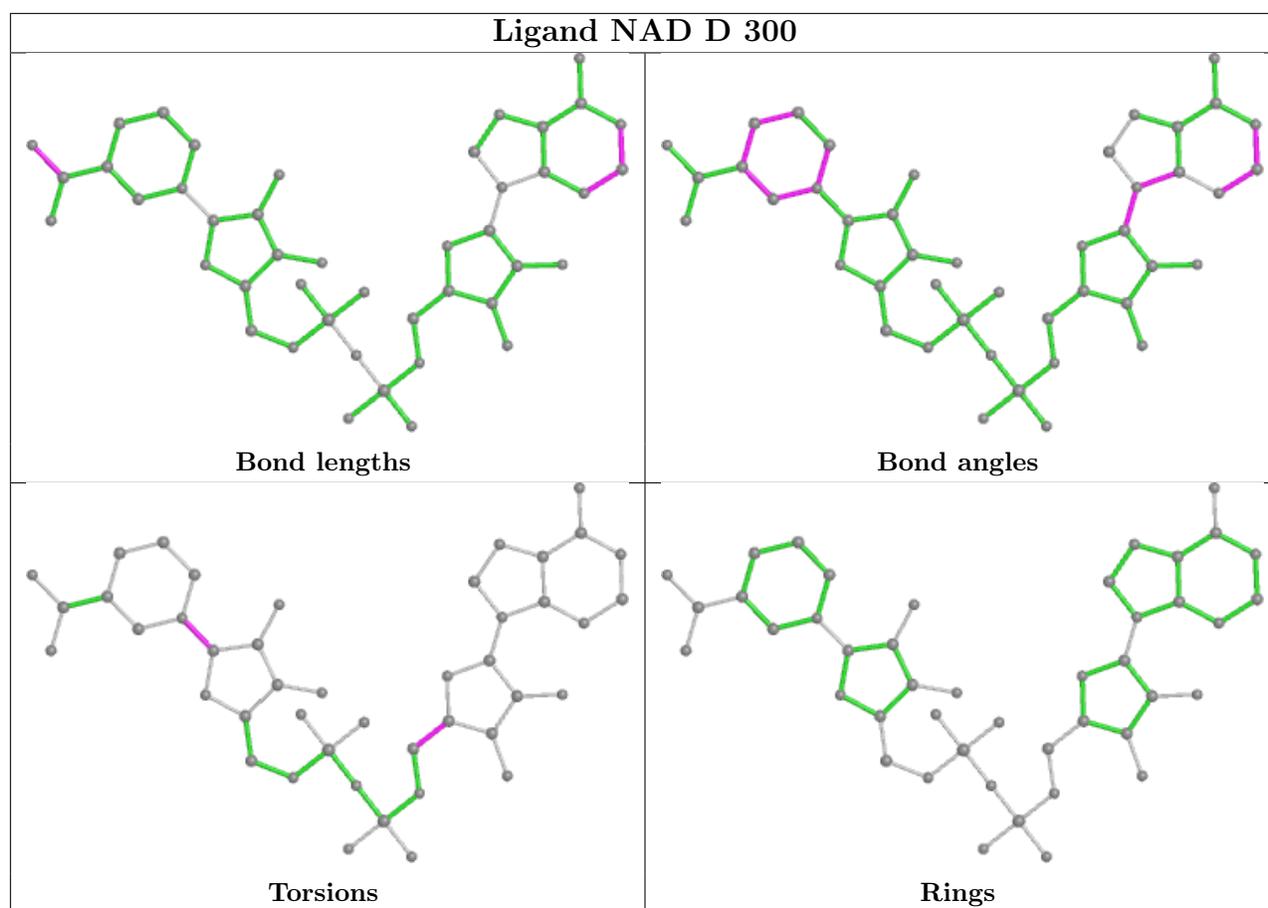
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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.
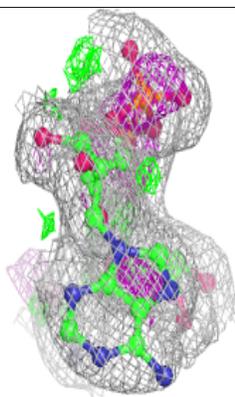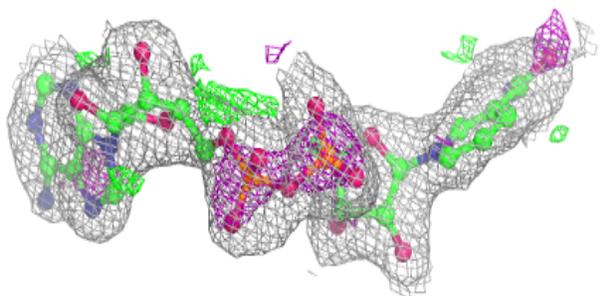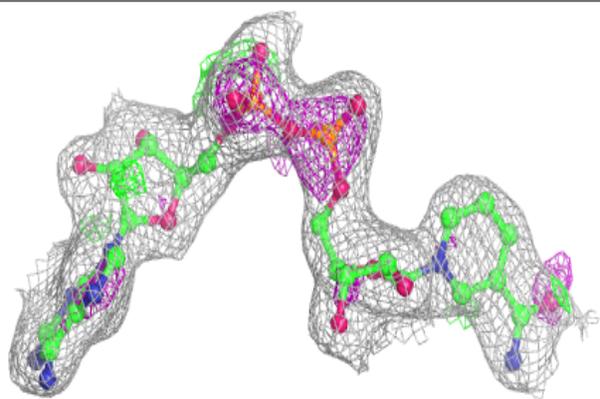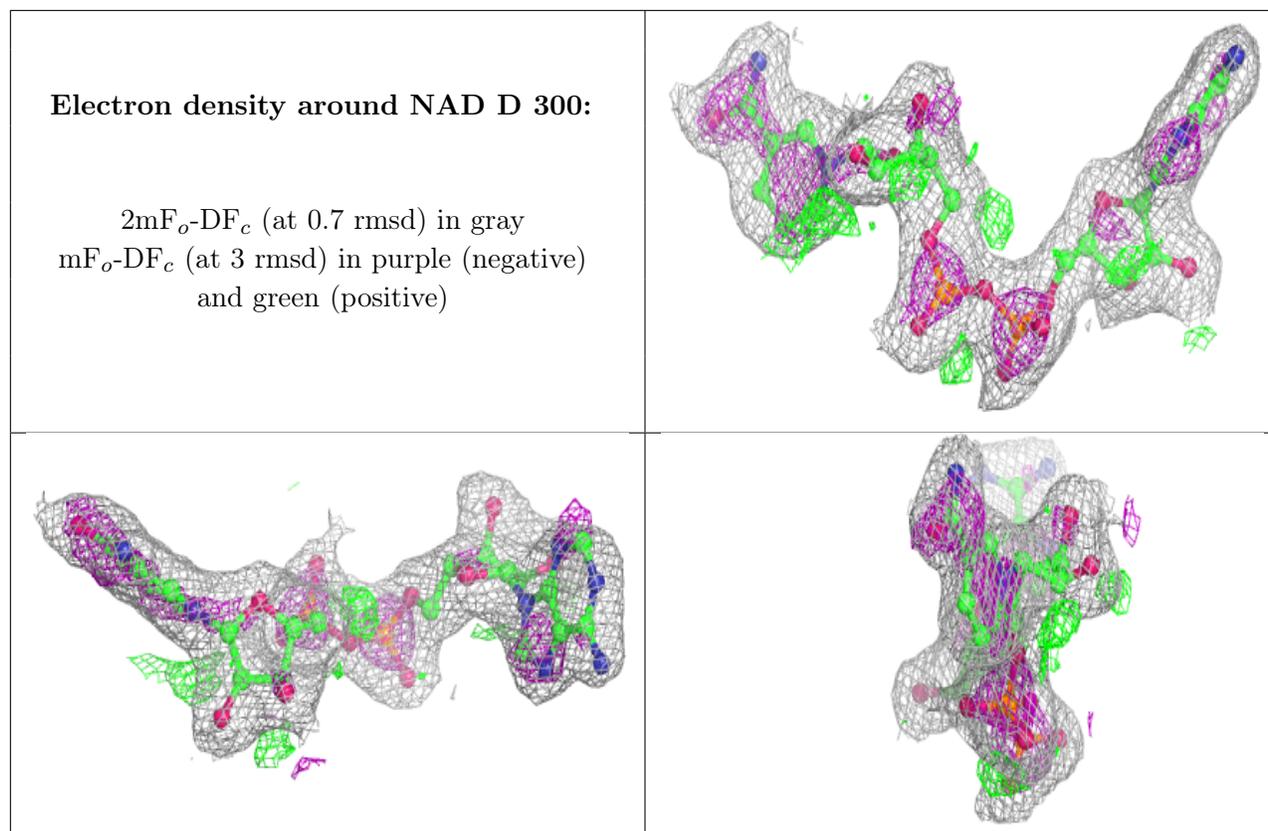

Electron density around NAD A 300:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
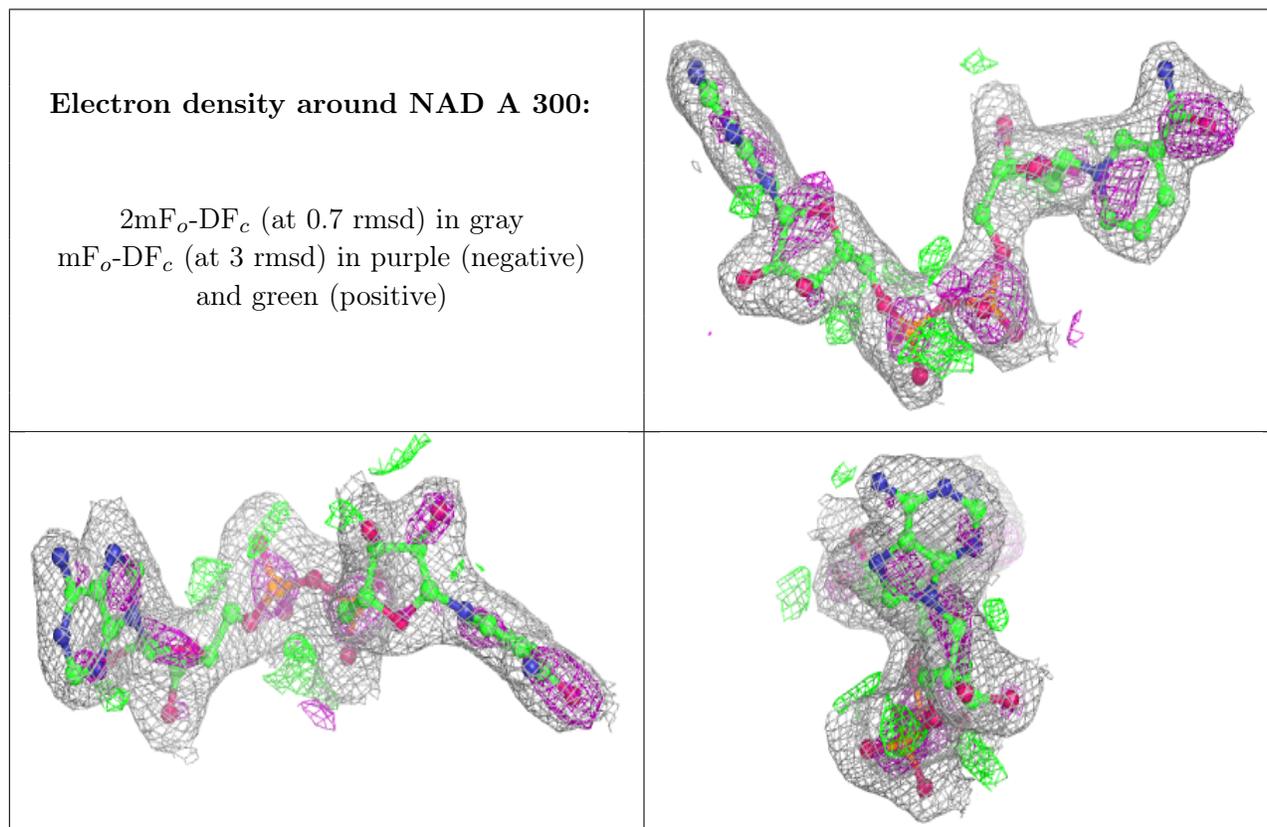
Electron density around NAD B 300:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
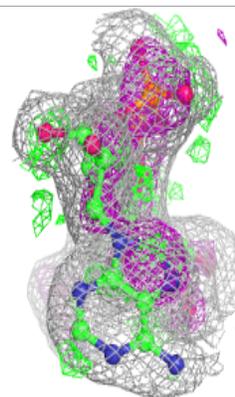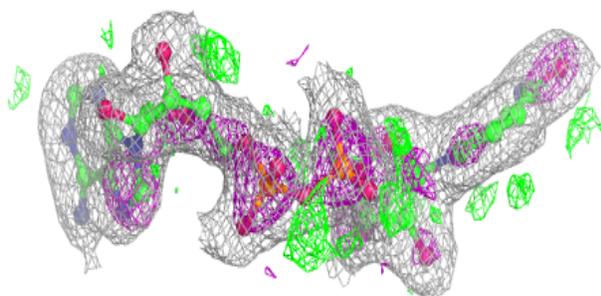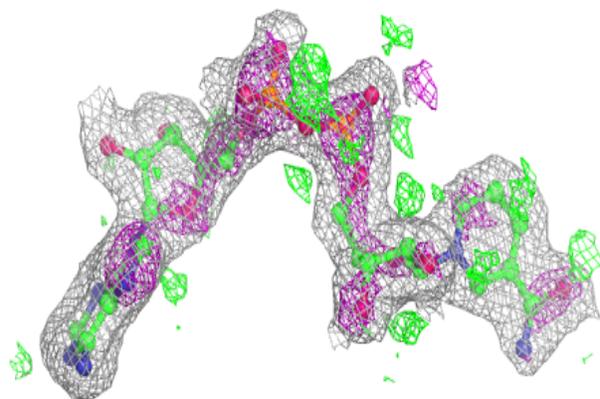
Electron density around NAD C 300:

$2mF_o$-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 300:

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

6.5 Other polymers ⓘ

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