



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 AM UTC

PDB ID : 2ZTU / pdb_00002ztu
Title : T190A mutant of D-3-hydroxybutyrate dehydrogenase complexed with NAD+
Authors : Nakashima, K.; Nakajima, Y.; Ito, K.; Yoshimoto, T.
Deposited on : 2008-10-09
Resolution : 2.00 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

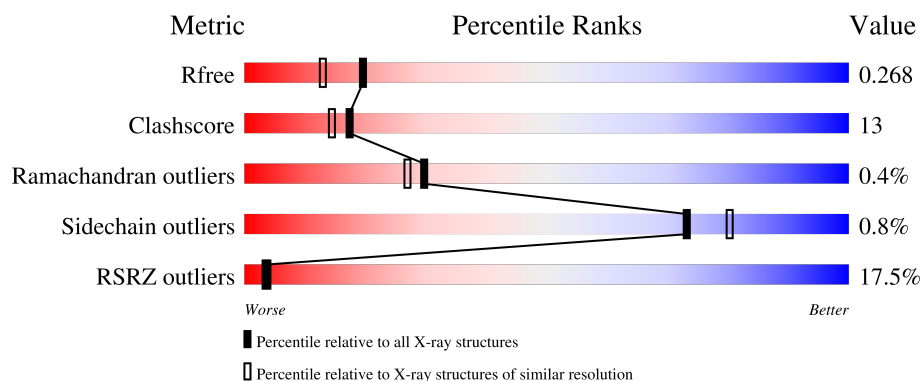
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	260	8% 74% 15% • 10%
1	B	260	43% 45% 33% • 20%
1	C	260	3% 78% 15% 7%
1	D	260	8% 77% 16% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7368 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 D(-)-3-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1688	1064	301	319	4			
1	B	207	Total	C	N	O	S	0	0	0
			1472	928	257	284	3			
1	C	242	Total	C	N	O	S	0	0	0
			1723	1085	308	326	4			
1	D	241	Total	C	N	O	S	0	0	0
			1718	1082	307	325	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ALA	THR	engineered mutation	UNP Q5KST5
B	190	ALA	THR	engineered mutation	UNP Q5KST5
C	190	ALA	THR	engineered mutation	UNP Q5KST5
D	190	ALA	THR	engineered mutation	UNP Q5KST5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



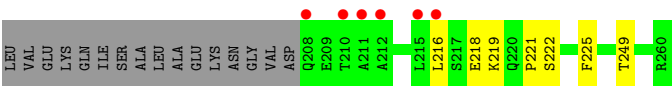
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

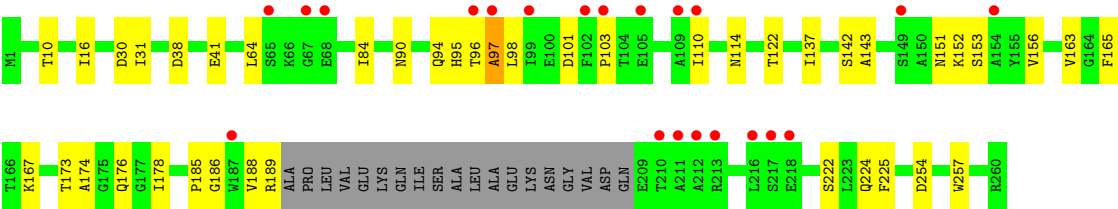
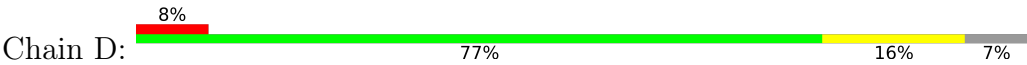
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	82	Total	O	0	0
			82	82		
4	C	223	Total	O	0	0
			223	223		
4	D	186	Total	O	0	0
			186	186		



● Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 106.61Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.00) 98.4 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.268	Depositor DCC
R_{free} test set	4324 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.36	0/1712	0.87	5/2321 (0.2%)
1	B	0.32	0/1493	0.89	4/2030 (0.2%)
1	C	0.42	0/1747	0.91	3/2370 (0.1%)
1	D	0.38	0/1742	0.88	5/2363 (0.2%)
All	All	0.37	0/6694	0.89	17/9084 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ALA	N-CA-C	-7.41	103.34	112.38
1	D	143	ALA	N-CA-C	-6.98	103.69	111.71
1	A	143	ALA	N-CA-C	-6.67	104.03	111.71
1	C	186	GLY	N-CA-C	-6.54	101.40	112.77
1	D	186	GLY	N-CA-C	-6.53	103.14	112.55
1	B	143	ALA	N-CA-C	-6.04	105.18	112.54
1	B	186	GLY	N-CA-C	-5.93	104.01	112.55
1	A	186	GLY	N-CA-C	-5.79	104.21	112.55
1	A	216	LEU	N-CA-C	-5.76	105.58	113.30
1	B	145	GLY	N-CA-C	-5.58	105.91	115.61
1	B	230	GLN	N-CA-C	-5.55	105.13	111.07
1	D	153	SER	N-CA-C	5.42	116.87	111.07
1	D	31	ILE	N-CA-C	5.18	116.83	108.85
1	D	30	ASP	N-CA-C	-5.12	103.28	110.50
1	C	31	ILE	N-CA-C	5.04	117.07	108.86
1	A	30	ASP	N-CA-C	-5.03	103.04	110.48
1	A	64	LEU	N-CA-C	5.02	119.17	113.19

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	1688	0	1718	31	0
1	B	1472	0	1469	83	0
1	C	1723	0	1738	31	0
1	D	1718	0	1736	28	0
2	A	44	0	26	4	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	142	0	0	2	0
4	B	82	0	0	6	0
4	C	223	0	0	3	0
4	D	186	0	0	4	0
All	All	7368	0	6739	169	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 13.

All (169) 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:187:TRP:HE1	1:B:219:LYS:HB2	1.26	0.98
1:B:187:TRP:H	1:B:220:GLN:NE2	1.68	0.91
1:B:62:ALA:HB1	1:B:69:ALA:HB1	1.52	0.91
1:B:16:ILE:HD11	1:B:188:VAL:HG11	1.56	0.87
1:B:89:ASN:HD22	1:B:139:ASN:ND2	1.75	0.84
1:B:187:TRP:H	1:B:220:GLN:HE22	1.21	0.84
1:C:129:MET:HE1	1:C:137:ILE:HD11	1.62	0.79
1:B:187:TRP:N	1:B:220:GLN:HE22	1.79	0.79
1:B:227:THR:OG1	1:B:230:GLN:HG3	1.88	0.73
1:B:25:ALA:HA	4:B:1430:HOH:O	1.91	0.70
1:A:94:GLN:HE21	1:A:95:HIS:H	1.39	0.70
1:B:81:MET:HA	1:B:81:MET:HE2	1.76	0.67
1:B:95:HIS:HB3	1:B:110:ILE:HD11	1.75	0.67
1:B:9:VAL:HG12	1:B:12:SER:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:HD22	1:A:151:ASN:N	1.94	0.66
1:B:128:HIS:O	1:B:132:GLN:HG3	1.96	0.65
1:C:126:LEU:HA	1:C:129:MET:HE3	1.79	0.64
1:B:216:LEU:HD11	1:B:225:PHE:CE1	2.33	0.63
1:A:227:THR:OG1	1:A:230:GLN:HG3	1.98	0.63
1:B:110:ILE:O	1:B:114:ASN:HB2	1.99	0.63
1:B:58:LEU:HD12	1:B:81:MET:HG2	1.82	0.62
1:C:94:GLN:HG3	1:C:95:HIS:N	2.13	0.62
1:B:71:ARG:NH1	1:B:120:HIS:ND1	2.44	0.62
1:C:76:ASN:HB2	4:C:1615:HOH:O	1.99	0.62
1:C:38:ASP:OD2	1:C:41:GLU:HG3	1.99	0.61
1:B:232:GLY:O	1:B:236:VAL:HG23	2.01	0.61
1:B:16:ILE:H	1:B:16:ILE:HD12	1.65	0.61
1:C:125:ALA:CB	1:C:129:MET:HE2	2.30	0.61
1:C:125:ALA:HB1	1:C:129:MET:HE2	1.82	0.60
1:C:126:LEU:HD23	1:C:129:MET:HE3	1.84	0.60
1:B:77:ALA:O	1:B:81:MET:HB2	2.01	0.60
1:A:249:THR:HG21	1:B:252:SER:HB2	1.84	0.59
1:B:216:LEU:HD12	1:B:216:LEU:H	1.67	0.59
1:C:125:ALA:C	1:C:129:MET:HE2	2.29	0.58
1:B:60:ASP:CG	1:B:73:LEU:HD13	2.30	0.57
1:D:189:ARG:HB3	4:D:1338:HOH:O	2.03	0.57
1:B:98:LEU:HD23	1:B:151:ASN:OD1	2.04	0.57
1:D:38:ASP:OD2	1:D:41:GLU:HG3	2.05	0.57
1:A:128:HIS:O	1:A:132:GLN:HG3	2.05	0.57
1:B:126:LEU:HD13	4:D:1559:HOH:O	2.04	0.57
1:D:10:THR:HB	1:D:64:LEU:CD1	2.35	0.57
1:D:163:VAL:HG12	1:D:167:LYS:HE3	1.86	0.56
1:B:78:VAL:HG23	1:B:83:ARG:HA	1.87	0.56
1:D:10:THR:HB	1:D:64:LEU:HD11	1.86	0.56
1:B:83:ARG:HB2	1:B:132:GLN:NE2	2.20	0.55
1:C:189:ARG:HB2	1:C:225:PHE:CG	2.42	0.55
1:B:216:LEU:HD12	1:B:216:LEU:N	2.20	0.55
1:C:216:LEU:HD21	1:C:225:PHE:CE2	2.42	0.55
1:B:89:ASN:HD22	1:B:139:ASN:HD21	1.53	0.54
1:C:222:SER:HA	1:D:174:ALA:HB1	1.89	0.54
1:B:187:TRP:HD1	1:B:220:GLN:NE2	2.04	0.54
1:C:30:ASP:HB3	1:C:81:MET:CE	2.37	0.54
1:B:73:LEU:O	1:B:73:LEU:HD12	2.07	0.54
1:D:167:LYS:HE2	4:D:1435:HOH:O	2.07	0.54
1:B:9:VAL:CG1	1:B:12:SER:HB3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LYS:HE2	4:C:1569:HOH:O	2.08	0.53
1:B:18:LEU:HB3	4:B:1519:HOH:O	2.08	0.53
1:C:30:ASP:HB3	1:C:81:MET:HE3	1.89	0.53
1:D:110:ILE:O	1:D:114:ASN:HB2	2.08	0.53
1:B:241:ASP:HB2	4:B:1498:HOH:O	2.09	0.53
1:B:16:ILE:HD12	1:B:16:ILE:N	2.24	0.53
1:B:105:GLU:N	1:B:105:GLU:OE1	2.42	0.52
1:B:105:GLU:H	1:B:105:GLU:CD	2.18	0.52
1:D:84:ILE:HG23	1:D:84:ILE:O	2.08	0.52
1:A:84:ILE:HG23	1:A:84:ILE:O	2.10	0.52
1:C:129:MET:CE	1:C:137:ILE:HD11	2.36	0.52
1:D:96:THR:O	1:D:97:ALA:HB2	2.10	0.52
1:A:159:LYS:HG2	4:A:1311:HOH:O	2.10	0.51
1:B:60:ASP:CB	1:B:73:LEU:HD13	2.40	0.51
1:D:122:THR:HG23	1:D:137:ILE:HD13	1.94	0.50
1:C:105:GLU:H	1:C:105:GLU:CD	2.19	0.50
1:D:189:ARG:HB2	1:D:225:PHE:CG	2.47	0.50
1:B:78:VAL:HG11	1:B:128:HIS:CE1	2.47	0.50
1:A:249:THR:HG22	1:A:250:THR:H	1.76	0.50
1:B:16:ILE:H	1:B:16:ILE:CD1	2.25	0.50
1:B:183:ILE:O	1:B:185:PRO:HD3	2.11	0.50
1:B:222:SER:O	1:B:224:GLN:HG3	2.11	0.50
1:D:98:LEU:HD23	1:D:151:ASN:OD1	2.11	0.49
1:B:34:ASN:ND2	1:B:64:LEU:HD11	2.27	0.49
1:B:126:LEU:N	1:B:127:PRO:HD2	2.27	0.49
1:A:187:TRP:HE1	1:A:219:LYS:HB2	1.77	0.49
1:D:176:GLN:NE2	4:D:1416:HOH:O	2.43	0.49
1:D:142:SER:HB2	2:D:300:NAD:H6N	1.95	0.49
1:D:189:ARG:HB2	1:D:225:PHE:CD2	2.47	0.49
1:B:240:SER:HB3	4:B:1392:HOH:O	2.12	0.48
1:B:10:THR:HB	1:B:64:LEU:HD11	1.95	0.48
1:B:187:TRP:HB2	1:B:216:LEU:HD23	1.93	0.48
1:D:222:SER:O	1:D:224:GLN:HG3	2.13	0.48
1:B:220:GLN:HG2	1:B:254:ASP:O	2.13	0.48
1:C:163:VAL:HG12	1:C:167:LYS:HE3	1.96	0.48
1:A:122:THR:O	1:A:126:LEU:HG	2.13	0.48
1:A:187:TRP:HB2	1:A:216:LEU:HD11	1.94	0.48
1:D:254:ASP:HB2	1:D:257:TRP:HB3	1.94	0.48
1:C:10:THR:HB	1:C:64:LEU:HD11	1.95	0.48
1:B:68:GLU:H	1:B:68:GLU:CD	2.22	0.47
1:D:94:GLN:HG3	1:D:95:HIS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:HA	1:B:17:GLY:HA3	1.97	0.47
1:B:96:THR:O	1:B:97:ALA:HB2	2.15	0.47
1:B:252:SER:HB3	1:B:254:ASP:OD2	2.14	0.47
1:C:189:ARG:HB3	4:C:1367:HOH:O	2.15	0.47
1:A:142:SER:HB2	2:A:300:NAD:H6N	1.96	0.47
1:B:31:ILE:HG22	1:B:32:VAL:N	2.28	0.46
1:C:84:ILE:O	1:C:84:ILE:HG23	2.15	0.46
1:B:75:ASP:O	1:B:78:VAL:HG12	2.15	0.46
1:B:135:GLY:O	1:B:178:ILE:HA	2.15	0.46
1:B:64:LEU:CD2	1:B:70:VAL:HG22	2.45	0.46
1:B:25:ALA:C	1:B:27:GLN:H	2.24	0.46
1:B:119:PHE:HA	1:B:165:PHE:CZ	2.51	0.45
1:B:16:ILE:CD1	1:B:188:VAL:HG11	2.39	0.45
1:C:219:LYS:O	1:C:221:PRO:HD3	2.16	0.45
1:D:101:ASP:O	1:D:103:PRO:HD3	2.15	0.45
1:A:16:ILE:HB	2:A:300:NAD:H51N	1.98	0.45
1:A:221:PRO:O	1:A:223:LEU:HG	2.16	0.45
1:A:94:GLN:HG3	1:A:95:HIS:N	2.32	0.45
1:A:152:LYS:O	1:A:156:VAL:HG23	2.17	0.45
1:B:158:ALA:O	1:B:162:VAL:HG23	2.16	0.45
1:C:142:SER:HA	1:C:185:PRO:HD2	1.99	0.45
1:B:155:TYR:CZ	1:B:159:LYS:HE3	2.52	0.44
1:A:151:ASN:N	1:A:151:ASN:ND2	2.63	0.44
1:B:31:ILE:CG2	1:B:32:VAL:N	2.80	0.44
1:B:237:PHE:HA	1:B:240:SER:OG	2.17	0.44
1:D:94:GLN:HE21	1:D:95:HIS:H	1.66	0.44
1:A:182:ALA:O	1:A:250:THR:HA	2.18	0.44
1:C:185:PRO:O	2:C:300:NAD:H5N	2.17	0.44
1:D:152:LYS:O	1:D:156:VAL:HG23	2.18	0.44
1:B:122:THR:HG23	1:B:137:ILE:HD13	2.00	0.43
1:D:10:THR:O	1:D:90:ASN:HB3	2.18	0.43
1:A:185:PRO:O	2:A:300:NAD:H5N	2.18	0.43
1:C:218:GLU:HG2	1:C:219:LYS:HG2	2.00	0.43
1:B:125:ALA:O	1:B:129:MET:HG3	2.18	0.43
1:B:22:THR:O	1:B:25:ALA:HB3	2.19	0.43
1:D:185:PRO:O	2:D:300:NAD:H5N	2.19	0.43
1:A:158:ALA:O	1:A:162:VAL:HG23	2.19	0.43
1:B:63:ASP:O	1:B:69:ALA:HB3	2.18	0.43
1:B:99:ILE:HD13	1:D:165:PHE:CZ	2.53	0.43
1:A:187:TRP:CB	1:A:216:LEU:HD11	2.49	0.43
1:A:188:VAL:HG22	1:A:226:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TRP:N	1:B:220:GLN:NE2	2.43	0.43
1:B:257:TRP:CD1	1:B:257:TRP:C	2.97	0.43
1:B:64:LEU:HA	1:B:70:VAL:CG2	2.49	0.43
1:C:181:ASN:OD1	1:C:249:THR:HG22	2.19	0.43
1:B:61:GLY:O	1:B:62:ALA:C	2.61	0.42
1:D:257:TRP:C	1:D:257:TRP:CD1	2.97	0.42
1:A:30:ASP:HB3	1:A:81:MET:CE	2.50	0.42
1:B:31:ILE:HG13	4:B:1430:HOH:O	2.18	0.42
1:A:220:GLN:NE2	1:A:224:GLN:O	2.53	0.42
1:B:101:ASP:O	1:B:103:PRO:HD3	2.20	0.42
1:B:89:ASN:ND2	1:B:139:ASN:ND2	2.56	0.42
1:B:115:LEU:HB2	1:B:158:ALA:HB1	2.02	0.42
1:B:179:THR:HB	1:B:247:THR:HB	2.02	0.42
1:B:176:GLN:O	1:B:178:ILE:HD12	2.20	0.41
1:A:36:PHE:H	2:A:300:NAD:HO2A	1.66	0.41
1:B:32:VAL:CG2	1:B:81:MET:HG3	2.50	0.41
1:D:173:THR:HB	1:D:178:ILE:HB	2.01	0.41
1:C:119:PHE:HA	1:C:165:PHE:CZ	2.55	0.41
1:B:84:ILE:O	1:B:84:ILE:HG23	2.20	0.41
1:A:11:GLY:H	1:A:34:ASN:HD22	1.68	0.41
1:C:10:THR:HB	1:C:64:LEU:CD1	2.51	0.41
1:A:94:GLN:HE22	1:A:155:TYR:HB2	1.85	0.41
1:A:64:LEU:HD22	1:A:70:VAL:HG22	2.03	0.41
1:A:110:ILE:O	1:A:114:ASN:HB2	2.21	0.41
1:A:148:ALA:HB1	1:C:168:VAL:HG22	2.02	0.41
1:C:90:ASN:HD22	1:C:140:ILE:HG13	1.85	0.41
1:A:159:LYS:HE2	4:A:1311:HOH:O	2.21	0.41
1:B:59:TYR:HB3	4:B:1531:HOH:O	2.20	0.40
1:D:16:ILE:HD11	1:D:188:VAL:HG21	2.02	0.40
1:B:10:THR:HB	1:B:64:LEU:CD1	2.51	0.40
1:B:254:ASP:HB2	1:B:257:TRP:CB	2.51	0.40
1:C:96:THR:O	1:C:97:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
1	B	201/260 (77%)	183 (91%)	15 (8%)	3 (2%)	8	4
1	C	238/260 (92%)	230 (97%)	8 (3%)	0	100	100
1	D	237/260 (91%)	226 (95%)	10 (4%)	1 (0%)	30	27
All	All	907/1040 (87%)	863 (95%)	40 (4%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ALA
1	B	97	ALA
1	D	97	ALA
1	B	26	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	166/186 (89%)	164 (99%)	2 (1%)	63	70
1	B	145/186 (78%)	142 (98%)	3 (2%)	47	52
1	C	166/186 (89%)	166 (100%)	0	100	100
1	D	166/186 (89%)	166 (100%)	0	100	100
All	All	643/744 (86%)	638 (99%)	5 (1%)	73	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	249	THR

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Mol	Chain	Res	Type
1	B	105	GLU
1	B	111	LEU
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	94	GLN
1	A	132	GLN
1	A	139	ASN
1	A	151	ASN
1	A	176	GLN
1	A	245	GLN
1	B	76	ASN
1	B	94	GLN
1	B	128	HIS
1	B	139	ASN
1	B	220	GLN
1	B	224	GLN
1	C	90	ASN
1	C	139	ASN
1	C	160	HIS
1	C	176	GLN
1	D	80	GLN
1	D	89	ASN
1	D	132	GLN
1	D	139	ASN
1	D	176	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	D	300	-	46,48,48	2.92	14 (30%)	64,73,73	1.87	9 (14%)
2	NAD	C	300	-	46,48,48	2.88	14 (30%)	64,73,73	1.87	9 (14%)
2	NAD	A	300	-	46,48,48	2.92	14 (30%)	64,73,73	1.90	10 (15%)

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	D	300	-	-	6/30/62/62	0/5/5/5
2	NAD	C	300	-	-	7/30/62/62	0/5/5/5
2	NAD	A	300	-	-	6/30/62/62	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NAD	C2N-N1N	9.72	1.45	1.35
2	D	300	NAD	C2N-N1N	9.70	1.45	1.35
2	C	300	NAD	C2N-N1N	9.69	1.45	1.35
2	D	300	NAD	C4N-C3N	9.65	1.54	1.39
2	A	300	NAD	C4N-C3N	9.57	1.53	1.39
2	C	300	NAD	C4N-C3N	9.45	1.53	1.39
2	A	300	NAD	C5N-C4N	7.83	1.52	1.38
2	C	300	NAD	C5N-C4N	7.83	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	NAD	C5N-C4N	7.73	1.52	1.38
2	D	300	NAD	PN-O3	5.50	1.65	1.59
2	A	300	NAD	PN-O3	5.15	1.65	1.59
2	C	300	NAD	PN-O3	4.96	1.64	1.59
2	A	300	NAD	C2A-N3A	3.78	1.40	1.33
2	A	300	NAD	C6N-N1N	3.65	1.43	1.35
2	D	300	NAD	C2A-N3A	3.62	1.40	1.33
2	D	300	NAD	C6N-N1N	3.60	1.43	1.35
2	C	300	NAD	C2A-N3A	3.55	1.40	1.33
2	A	300	NAD	C4A-N3A	3.54	1.41	1.34
2	C	300	NAD	C6N-N1N	3.51	1.43	1.35
2	D	300	NAD	C4A-N3A	3.43	1.40	1.34
2	C	300	NAD	O4D-C1D	3.37	1.45	1.40
2	C	300	NAD	C4A-N3A	3.34	1.40	1.34
2	D	300	NAD	O4D-C1D	3.08	1.44	1.40
2	A	300	NAD	O4D-C1D	2.95	1.44	1.40
2	C	300	NAD	C2N-C3N	-2.82	1.34	1.39
2	D	300	NAD	C2N-C3N	-2.78	1.34	1.39
2	A	300	NAD	C2N-C3N	-2.62	1.34	1.39
2	A	300	NAD	C5A-N7A	-2.59	1.34	1.39
2	D	300	NAD	C5A-C6A	2.55	1.48	1.41
2	C	300	NAD	C5A-C6A	2.49	1.47	1.41
2	A	300	NAD	C5A-C6A	2.43	1.47	1.41
2	C	300	NAD	C5A-N7A	-2.39	1.34	1.39
2	D	300	NAD	C5A-N7A	-2.37	1.34	1.39
2	A	300	NAD	C3D-C4D	2.25	1.58	1.53
2	D	300	NAD	C3D-C4D	2.23	1.58	1.53
2	D	300	NAD	O4D-C4D	2.13	1.49	1.45
2	A	300	NAD	O4D-C4D	2.11	1.49	1.45
2	C	300	NAD	C6N-C5N	2.11	1.43	1.38
2	C	300	NAD	O4D-C4D	2.10	1.49	1.45
2	A	300	NAD	C6N-C5N	2.07	1.42	1.38
2	C	300	NAD	C3D-C4D	2.06	1.58	1.53
2	D	300	NAD	C6N-C5N	2.05	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	C5N-C4N-C3N	-10.09	110.45	120.36
2	D	300	NAD	C5N-C4N-C3N	-9.80	110.73	120.36
2	C	300	NAD	C5N-C4N-C3N	-9.77	110.76	120.36
2	A	300	NAD	N3A-C2A-N1A	-4.29	122.09	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	NAD	C2A-N1A-C6A	4.27	125.74	118.73
2	D	300	NAD	N3A-C2A-N1A	-4.26	122.13	128.58
2	A	300	NAD	C2A-N1A-C6A	4.21	125.65	118.73
2	C	300	NAD	C2A-N1A-C6A	4.20	125.64	118.73
2	C	300	NAD	N3A-C2A-N1A	-4.17	122.28	128.58
2	A	300	NAD	C6N-N1N-C2N	-3.58	118.83	121.88
2	C	300	NAD	C6N-N1N-C2N	-3.38	119.00	121.88
2	D	300	NAD	C6N-N1N-C2N	-3.33	119.05	121.88
2	D	300	NAD	C4A-N9A-C8A	-2.79	102.81	105.74
2	D	300	NAD	C1B-N9A-C8A	2.76	133.21	127.09
2	A	300	NAD	C1B-N9A-C8A	2.73	133.15	127.09
2	C	300	NAD	C1B-N9A-C8A	2.67	133.03	127.09
2	A	300	NAD	C4A-N9A-C8A	-2.64	102.97	105.74
2	C	300	NAD	C4A-N9A-C8A	-2.64	102.97	105.74
2	C	300	NAD	C5A-N7A-C8A	2.45	107.29	103.45
2	A	300	NAD	C5A-N7A-C8A	2.39	107.21	103.45
2	D	300	NAD	C5A-N7A-C8A	2.30	107.07	103.45
2	D	300	NAD	C2N-C3N-C4N	2.16	120.77	118.26
2	C	300	NAD	C2N-C3N-C4N	2.15	120.76	118.26
2	C	300	NAD	O2B-C2B-C3B	2.08	118.49	111.82
2	A	300	NAD	O2B-C2B-C3B	2.05	118.40	111.82
2	A	300	NAD	C2N-C3N-C4N	2.04	120.63	118.26
2	D	300	NAD	C5A-C4A-N3A	-2.03	123.92	126.72
2	A	300	NAD	C5A-C4A-N3A	-2.00	123.96	126.72

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	PN-O3-PA-O5B
2	A	300	NAD	C5D-O5D-PN-O3
2	A	300	NAD	O4D-C1D-N1N-C6N
2	A	300	NAD	C2D-C1D-N1N-C6N
2	C	300	NAD	C5D-O5D-PN-O3
2	C	300	NAD	C5D-O5D-PN-O2N
2	C	300	NAD	O4D-C1D-N1N-C6N
2	D	300	NAD	C5D-O5D-PN-O3
2	D	300	NAD	C5D-O5D-PN-O1N
2	D	300	NAD	C5D-O5D-PN-O2N
2	A	300	NAD	C5D-O5D-PN-O1N
2	C	300	NAD	C5D-O5D-PN-O1N
2	D	300	NAD	PA-O3-PN-O2N

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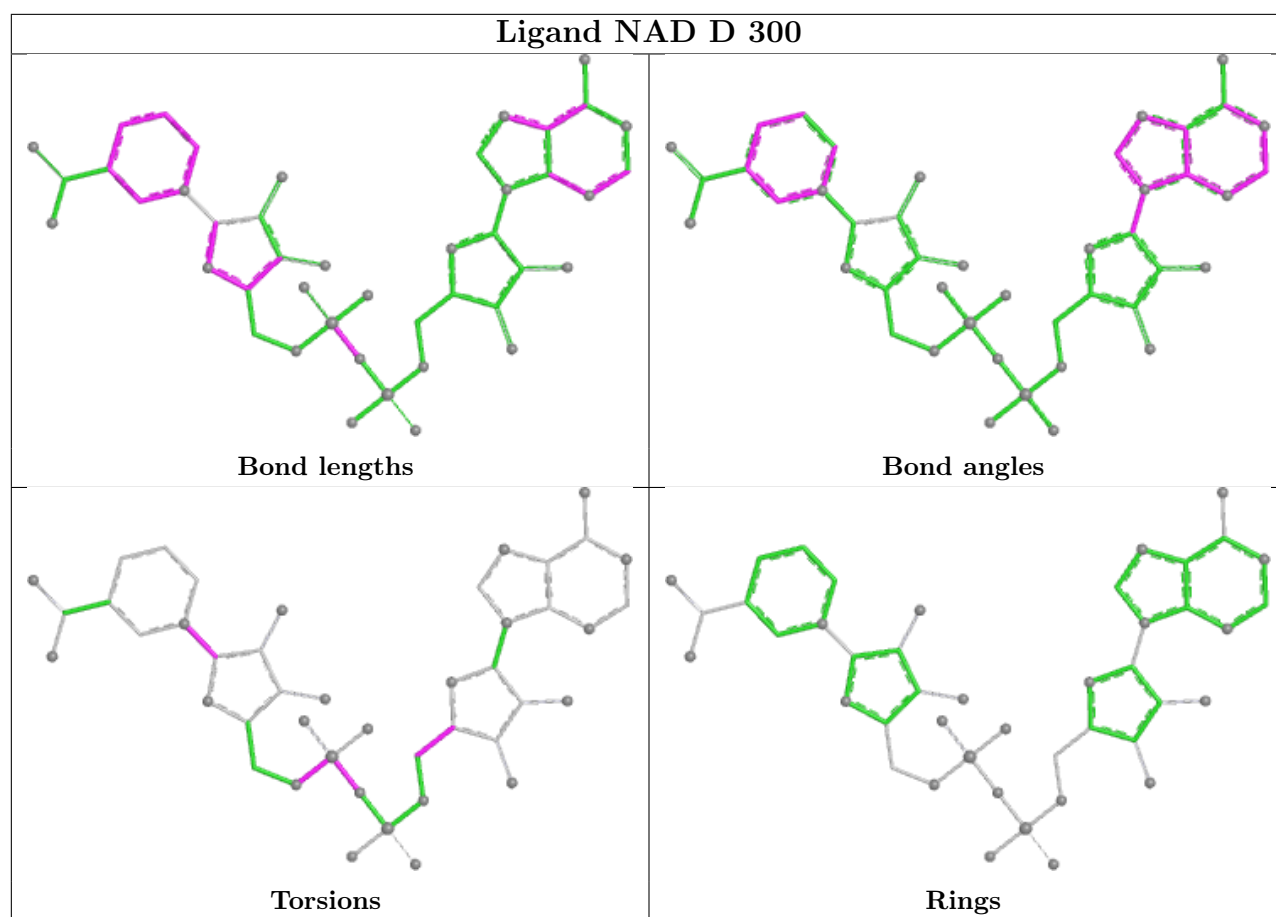
Mol	Chain	Res	Type	Atoms
2	C	300	NAD	C2D-C1D-N1N-C6N
2	D	300	NAD	O4D-C1D-N1N-C6N
2	C	300	NAD	PA-O3-PN-O1N
2	D	300	NAD	O4B-C4B-C5B-O5B
2	C	300	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	O4B-C4B-C5B-O5B

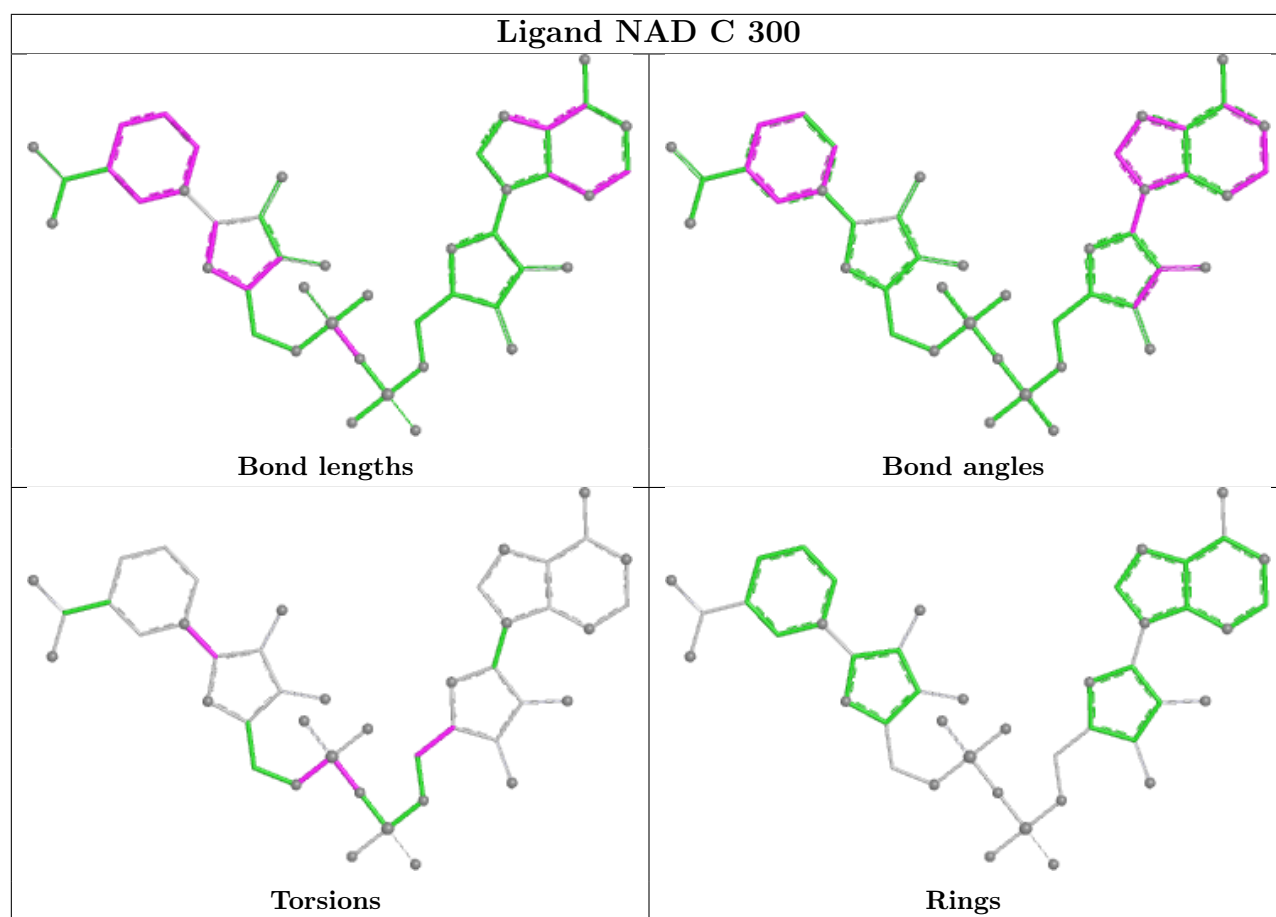
There are no ring outliers.

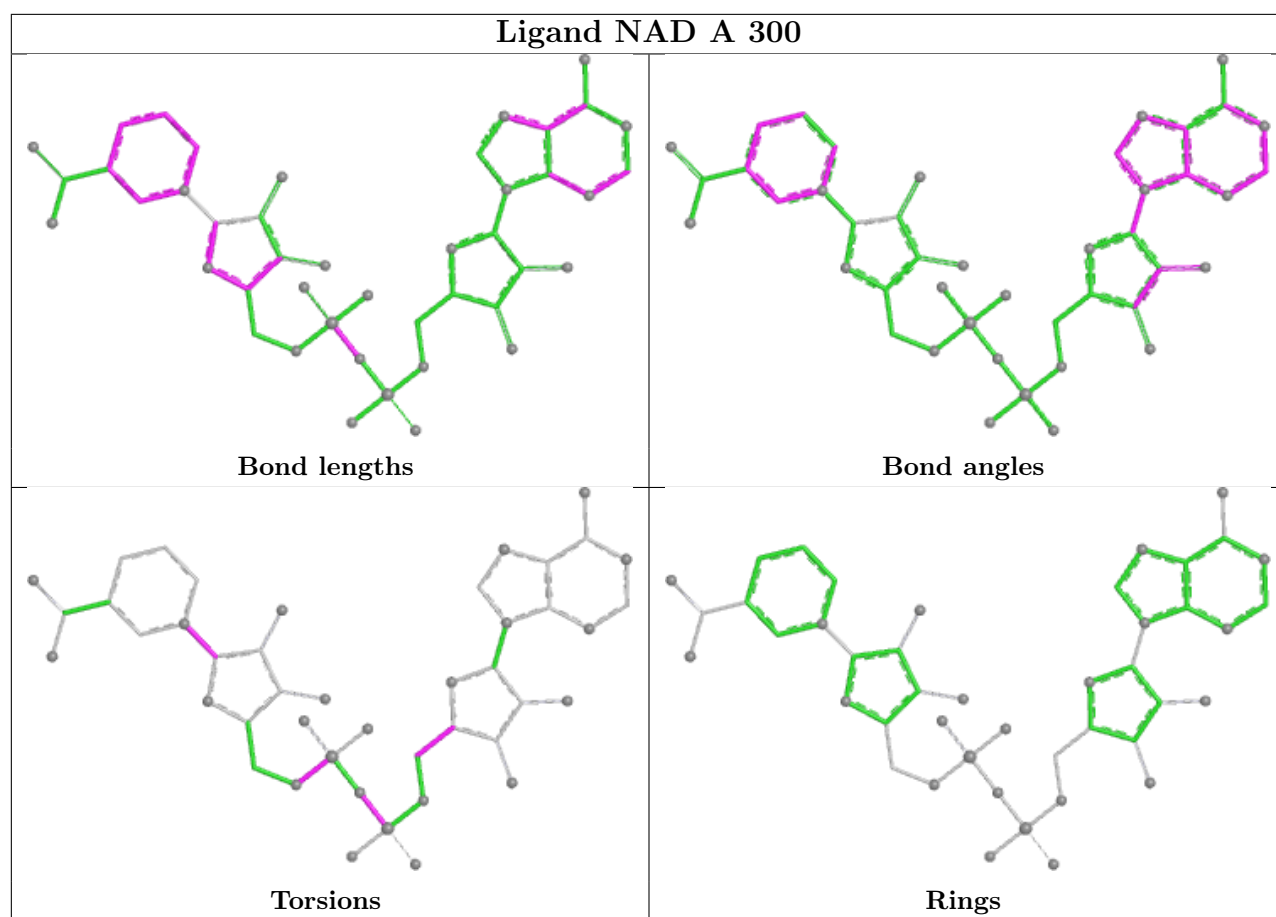
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	NAD	2	0
2	C	300	NAD	1	0
2	A	300	NAD	4	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	235/260 (90%)	0.73	20 (8%) 16 15	12, 30, 50, 61	1 (0%)
1	B	207/260 (79%)	2.27	112 (54%) 0 0	29, 48, 64, 67	0
1	C	242/260 (93%)	-0.06	9 (3%) 45 44	11, 20, 39, 56	1 (0%)
1	D	241/260 (92%)	0.46	21 (8%) 16 15	16, 27, 49, 55	0
All	All	925/1040 (88%)	0.80	162 (17%) 4 3	11, 30, 57, 67	2 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	TRP	5.6
1	B	58	LEU	5.4
1	B	62	ALA	5.3
1	B	187	TRP	5.2
1	B	216	LEU	5.1
1	A	215	LEU	4.9
1	B	26	ALA	4.8
1	B	31	ILE	4.7
1	B	69	ALA	4.5
1	B	18	LEU	4.4
1	B	74	VAL	4.4
1	B	84	ILE	4.4
1	B	36	PHE	4.4
1	B	91	ALA	4.4
1	B	13	THR	4.3
1	B	70	VAL	4.2
1	B	87	LEU	4.2
1	B	81	MET	4.2
1	B	32	VAL	4.1
1	B	59	TYR	4.1
1	B	8	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	217	SER	4.0
1	B	97	ALA	4.0
1	B	21	ALA	3.9
1	B	86	ILE	3.9
1	A	187	TRP	3.8
1	C	210	THR	3.8
1	D	102	PHE	3.8
1	B	9	VAL	3.7
1	B	78	VAL	3.7
1	B	128	HIS	3.7
1	D	212	ALA	3.7
1	B	73	LEU	3.6
1	B	105	GLU	3.6
1	B	88	VAL	3.6
1	B	124	ALA	3.6
1	B	214	GLU	3.6
1	B	93	ILE	3.5
1	C	212	ALA	3.5
1	B	65	SER	3.5
1	B	225	PHE	3.4
1	B	64	LEU	3.4
1	B	133	GLY	3.4
1	A	216	LEU	3.4
1	D	65	SER	3.4
1	B	25	ALA	3.4
1	A	225	PHE	3.4
1	B	229	GLU	3.3
1	B	34	ASN	3.3
1	B	226	VAL	3.3
1	A	44	LYS	3.3
1	B	10	THR	3.2
1	B	180	ALA	3.2
1	B	33	LEU	3.2
1	C	211	ALA	3.2
1	B	63	ASP	3.2
1	B	29	ALA	3.1
1	A	220	GLN	3.1
1	B	188	VAL	3.1
1	B	243	ALA	3.1
1	B	113	LEU	3.1
1	C	208	GLN	3.1
1	D	211	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.0
1	B	20	ILE	3.0
1	B	80	GLN	3.0
1	A	242	ALA	2.9
1	B	125	ALA	2.9
1	A	177	GLY	2.9
1	B	85	ASP	2.9
1	B	23	ALA	2.9
1	D	149	SER	2.9
1	B	215	LEU	2.8
1	D	210	THR	2.8
1	A	237	PHE	2.8
1	D	154	ALA	2.8
1	B	140	ILE	2.8
1	B	19	GLY	2.8
1	D	97	ALA	2.8
1	B	126	LEU	2.8
1	D	216	LEU	2.8
1	B	67	GLY	2.8
1	B	257	TRP	2.8
1	B	102	PHE	2.7
1	B	22	THR	2.7
1	A	222	SER	2.7
1	B	92	GLY	2.7
1	B	134	PHE	2.7
1	D	103	PRO	2.7
1	B	79	ARG	2.7
1	B	24	LEU	2.7
1	B	231	LEU	2.7
1	B	68	GLU	2.7
1	B	76	ASN	2.7
1	B	123	ALA	2.6
1	B	172	GLU	2.6
1	B	221	PRO	2.6
1	B	16	ILE	2.6
1	D	187	TRP	2.6
1	D	99	ILE	2.6
1	B	109	ALA	2.6
1	A	224	GLN	2.6
1	B	77	ALA	2.6
1	B	227	THR	2.6
1	B	11	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	95	HIS	2.5
1	B	90	ASN	2.5
1	B	14	SER	2.5
1	B	217	SER	2.5
1	B	220	GLN	2.5
1	A	221	PRO	2.4
1	B	228	PRO	2.4
1	D	109	ALA	2.4
1	A	131	LYS	2.4
1	B	120	HIS	2.4
1	D	213	ARG	2.4
1	B	155	TYR	2.4
1	B	104	THR	2.4
1	A	189	ARG	2.4
1	B	241	ASP	2.4
1	B	240	SER	2.4
1	B	170	ALA	2.4
1	B	98	LEU	2.4
1	B	17	GLY	2.4
1	B	131	LYS	2.4
1	B	239	ALA	2.3
1	A	132	GLN	2.3
1	A	241	ASP	2.3
1	B	30	ASP	2.3
1	C	189	ARG	2.3
1	B	110	ILE	2.3
1	B	96	THR	2.3
1	A	52	GLN	2.3
1	B	75	ASP	2.3
1	B	175	GLY	2.3
1	B	177	GLY	2.3
1	B	82	GLY	2.3
1	B	186	GLY	2.3
1	D	105	GLU	2.2
1	B	132	GLN	2.2
1	C	52	GLN	2.2
1	D	96	THR	2.2
1	D	68	GLU	2.2
1	B	127	PRO	2.2
1	B	129	MET	2.2
1	A	175	GLY	2.2
1	B	117	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.2
1	B	89	ASN	2.2
1	B	61	GLY	2.2
1	B	66	LYS	2.2
1	C	215	LEU	2.1
1	D	110	ILE	2.1
1	B	15	GLY	2.1
1	B	233	GLY	2.1
1	D	67	GLY	2.1
1	B	244	ALA	2.1
1	D	218	GLU	2.1
1	B	151	ASN	2.1
1	B	182	ALA	2.0
1	B	94	GLN	2.0
1	C	216	LEU	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.

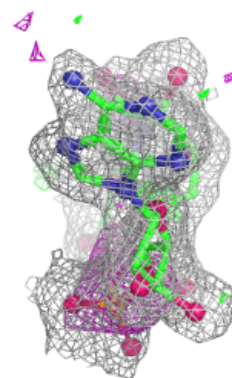
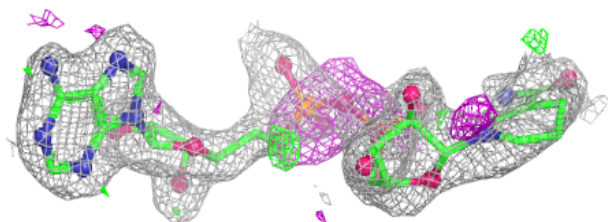
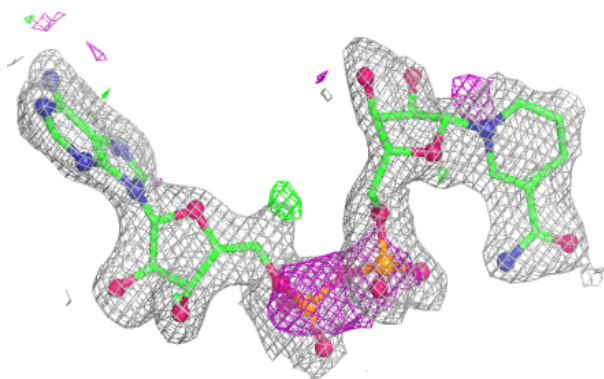
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	401	1/1	0.67	0.34	66,66,66,66	0
2	NAD	D	300	44/44	0.74	0.16	44,60,62,63	0
2	NAD	C	300	44/44	0.84	0.13	31,48,53,54	0
2	NAD	A	300	44/44	0.85	0.13	26,48,54,54	0
3	MG	A	406	1/1	0.90	0.10	39,39,39,39	0

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.

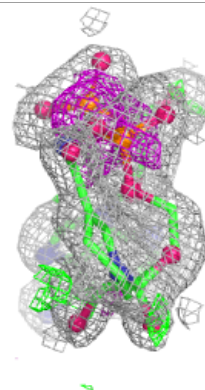
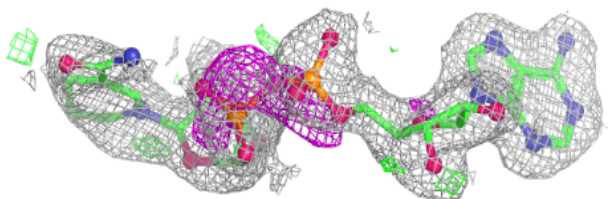
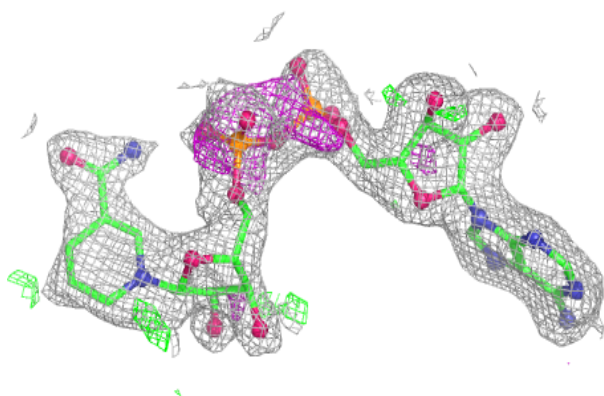
Electron density around NAD D 300:

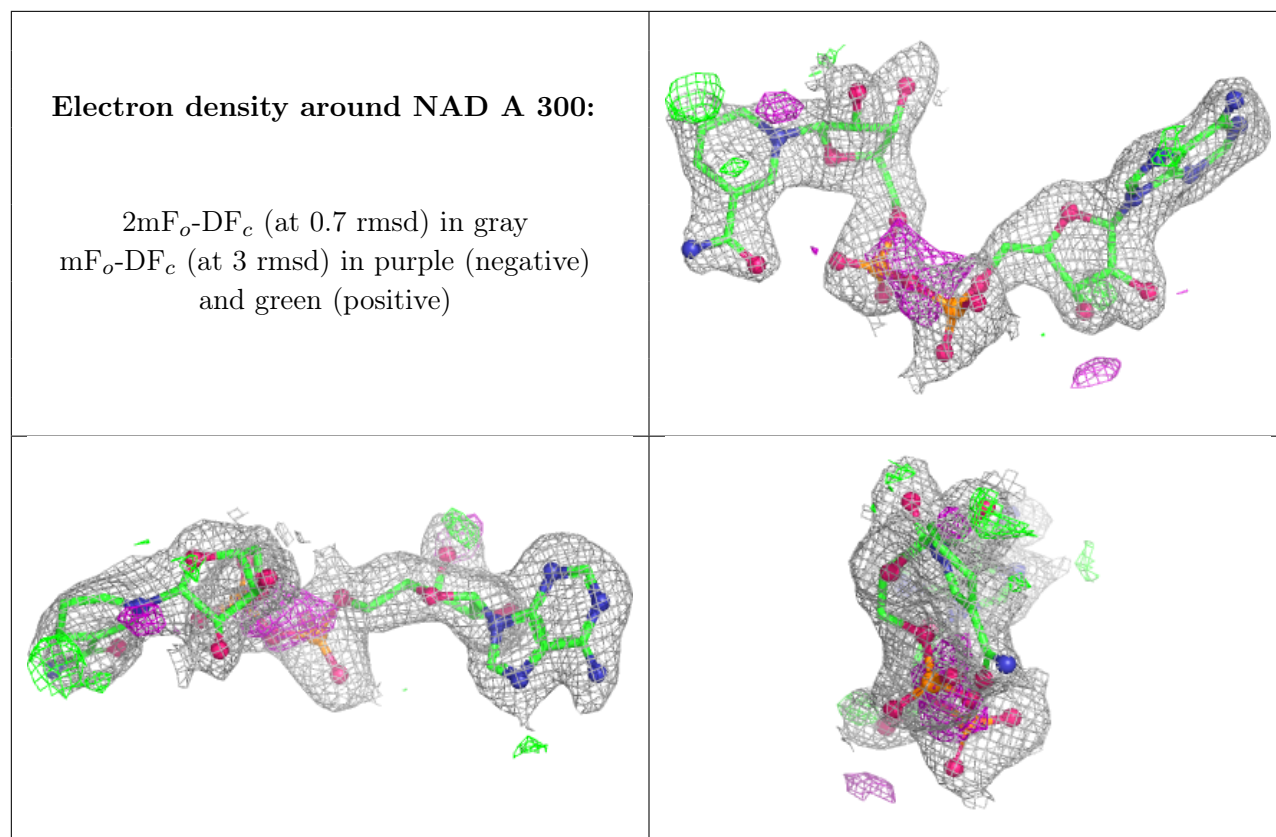
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.