



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:25 PM UTC

PDB ID : 8PA2 / pdb_00008pa2
Title : Crystal structure of alcohol dehydrogenase/ketoreductase variant from
Thermus thermophilus apo form
Authors : Rozeboom, H.J.; Janssen, D.B.
Deposited on : 2023-06-07
Resolution : 2.10 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

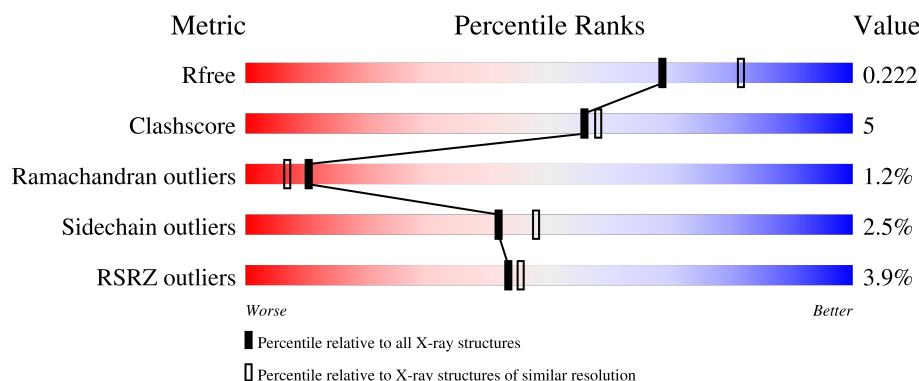
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	264	4% 84% 9% 6%
1	B	264	2% 81% 11% 6%
1	C	264	6% 88% 5% 6%
1	D	264	2% 84% 9% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7995 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Oxidoreductase, short-chain dehydrogenase/reductase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1856	1175	334	342	5			
1	B	249	Total	C	N	O	S	0	0	0
			1856	1175	334	342	5			
1	C	248	Total	C	N	O	S	0	0	0
			1848	1170	333	341	4			
1	D	249	Total	C	N	O	S	0	0	0
			1856	1175	334	342	5			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q5SLC4
A	-6	GLY	-	expression tag	UNP Q5SLC4
A	-5	HIS	-	expression tag	UNP Q5SLC4
A	-4	HIS	-	expression tag	UNP Q5SLC4
A	-3	HIS	-	expression tag	UNP Q5SLC4
A	-2	HIS	-	expression tag	UNP Q5SLC4
A	-1	HIS	-	expression tag	UNP Q5SLC4
A	0	HIS	-	expression tag	UNP Q5SLC4
A	126	PRO	VAL	engineered mutation	UNP Q5SLC4
A	128	PRO	GLY	engineered mutation	UNP Q5SLC4
A	137	TYR	VAL	engineered mutation	UNP Q5SLC4
A	138	LEU	GLN	engineered mutation	UNP Q5SLC4
A	181	PHE	ALA	engineered mutation	UNP Q5SLC4
A	187	LEU	VAL	engineered mutation	UNP Q5SLC4
A	190	LEU	ALA	engineered mutation	UNP Q5SLC4
A	204	MET	TRP	engineered mutation	UNP Q5SLC4
A	245	LEU	MET	engineered mutation	UNP Q5SLC4
B	-7	MET	-	initiating methionine	UNP Q5SLC4
B	-6	GLY	-	expression tag	UNP Q5SLC4
B	-5	HIS	-	expression tag	UNP Q5SLC4
B	-4	HIS	-	expression tag	UNP Q5SLC4

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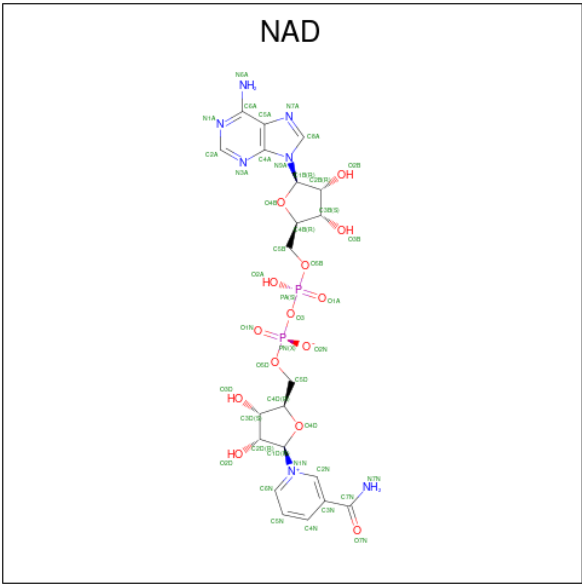
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q5SLC4
B	-2	HIS	-	expression tag	UNP Q5SLC4
B	-1	HIS	-	expression tag	UNP Q5SLC4
B	0	HIS	-	expression tag	UNP Q5SLC4
B	126	PRO	VAL	engineered mutation	UNP Q5SLC4
B	128	PRO	GLY	engineered mutation	UNP Q5SLC4
B	137	TYR	VAL	engineered mutation	UNP Q5SLC4
B	138	LEU	GLN	engineered mutation	UNP Q5SLC4
B	181	PHE	ALA	engineered mutation	UNP Q5SLC4
B	187	LEU	VAL	engineered mutation	UNP Q5SLC4
B	190	LEU	ALA	engineered mutation	UNP Q5SLC4
B	204	MET	TRP	engineered mutation	UNP Q5SLC4
B	245	LEU	MET	engineered mutation	UNP Q5SLC4
C	-7	MET	-	initiating methionine	UNP Q5SLC4
C	-6	GLY	-	expression tag	UNP Q5SLC4
C	-5	HIS	-	expression tag	UNP Q5SLC4
C	-4	HIS	-	expression tag	UNP Q5SLC4
C	-3	HIS	-	expression tag	UNP Q5SLC4
C	-2	HIS	-	expression tag	UNP Q5SLC4
C	-1	HIS	-	expression tag	UNP Q5SLC4
C	0	HIS	-	expression tag	UNP Q5SLC4
C	126	PRO	VAL	engineered mutation	UNP Q5SLC4
C	128	PRO	GLY	engineered mutation	UNP Q5SLC4
C	137	TYR	VAL	engineered mutation	UNP Q5SLC4
C	138	LEU	GLN	engineered mutation	UNP Q5SLC4
C	181	PHE	ALA	engineered mutation	UNP Q5SLC4
C	187	LEU	VAL	engineered mutation	UNP Q5SLC4
C	190	LEU	ALA	engineered mutation	UNP Q5SLC4
C	204	MET	TRP	engineered mutation	UNP Q5SLC4
C	245	LEU	MET	engineered mutation	UNP Q5SLC4
D	-7	MET	-	initiating methionine	UNP Q5SLC4
D	-6	GLY	-	expression tag	UNP Q5SLC4
D	-5	HIS	-	expression tag	UNP Q5SLC4
D	-4	HIS	-	expression tag	UNP Q5SLC4
D	-3	HIS	-	expression tag	UNP Q5SLC4
D	-2	HIS	-	expression tag	UNP Q5SLC4
D	-1	HIS	-	expression tag	UNP Q5SLC4
D	0	HIS	-	expression tag	UNP Q5SLC4
D	126	PRO	VAL	engineered mutation	UNP Q5SLC4
D	128	PRO	GLY	engineered mutation	UNP Q5SLC4
D	137	TYR	VAL	engineered mutation	UNP Q5SLC4
D	138	LEU	GLN	engineered mutation	UNP Q5SLC4

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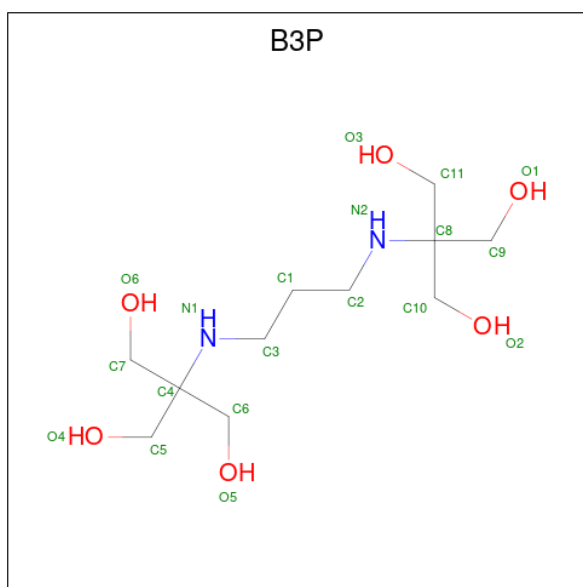
Chain	Residue	Modelled	Actual	Comment	Reference
D	181	PHE	ALA	engineered mutation	UNP Q5SLC4
D	187	LEU	VAL	engineered mutation	UNP Q5SLC4
D	190	LEU	ALA	engineered mutation	UNP Q5SLC4
D	204	MET	TRP	engineered mutation	UNP Q5SLC4
D	245	LEU	MET	engineered mutation	UNP Q5SLC4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (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		

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	O	
			19	11	2	6	
							0
							0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O		
			6	3	3		
						0	0
4	C	1	Total	C	O		
			6	3	3		
						0	0
4	D	1	Total	C	O		
			6	3	3		
						0	0

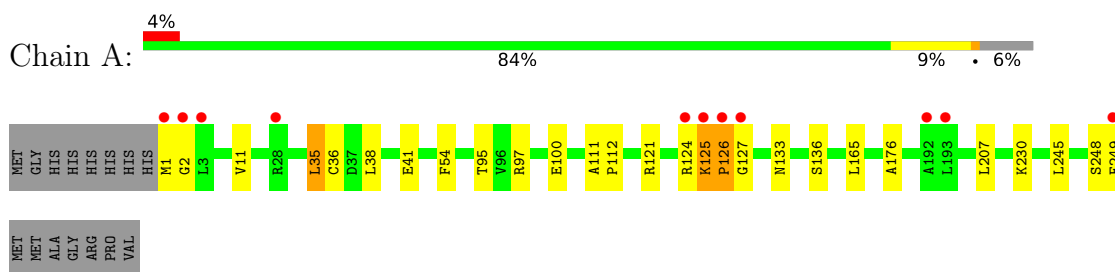
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total 84	O 84	0	0
5	B	96	Total 96	O 96	0	0
5	C	85	Total 85	O 85	0	0
5	D	101	Total 101	O 101	0	0

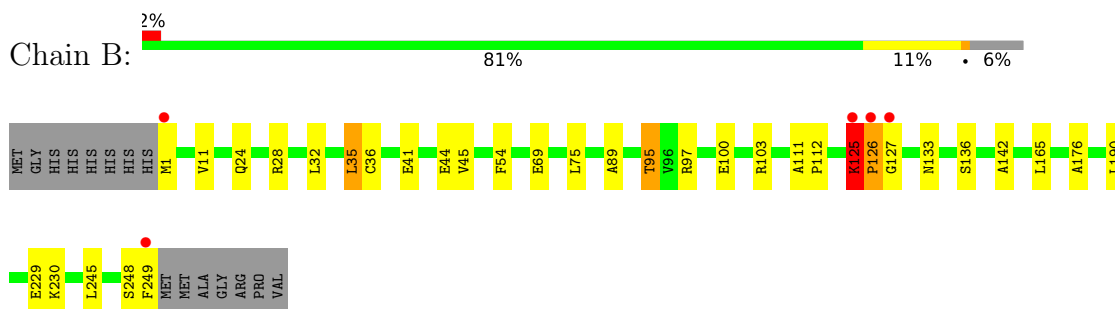
3 Residue-property plots [i](#)

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.

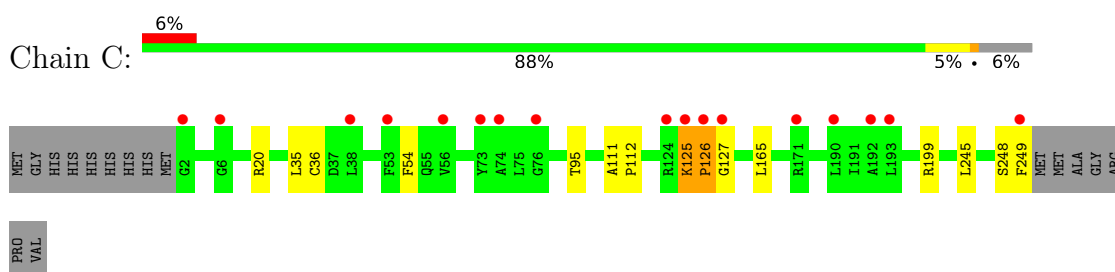
- Molecule 1: Oxidoreductase, short-chain dehydrogenase/reductase family



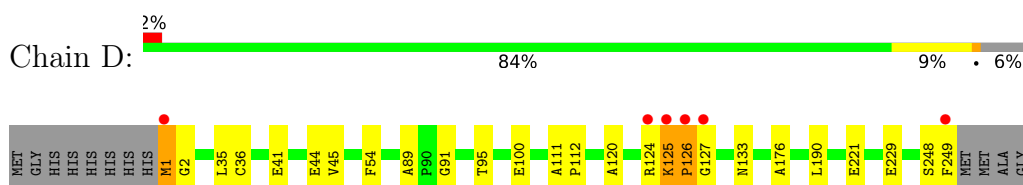
- Molecule 1: Oxidoreductase, short-chain dehydrogenase/reductase family



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.98Å 92.94Å 79.60Å 90.00° 107.87° 90.00°	Depositor
Resolution (Å)	46.50 – 2.10 46.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (46.50-2.10) 96.8 (46.50-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.215 0.187 , 0.222	Depositor DCC
R_{free} test set	2752 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.7	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	0.95	EDS
Total number of atoms	7995	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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: B3P, GOL, 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	0/1884	1.35	0/2554
1	B	1.05	0/1884	1.36	0/2554
1	C	1.00	0/1876	1.35	1/2544 (0.0%)
1	D	1.03	1/1884 (0.1%)	1.35	1/2554 (0.0%)
All	All	1.02	1/7528 (0.0%)	1.35	2/10206 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLY	C-O	5.73	1.28	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	THR	CA-CB-OG1	7.57	120.96	109.60
1	C	199	ARG	CB-CG-CD	5.35	123.60	111.30

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	1856	0	1906	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1856	0	1906	23	0
1	C	1848	0	1894	10	0
1	D	1856	0	1906	21	0
2	A	44	0	26	2	0
2	B	44	0	26	3	0
2	C	44	0	26	1	0
2	D	44	0	26	3	0
3	A	19	0	26	1	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	84	0	0	1	0
5	B	96	0	0	7	0
5	C	85	0	0	2	0
5	D	101	0	0	5	0
All	All	7995	0	7766	73	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 5.

All (73) 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:125:LYS:HB2	1:B:126:PRO:HD3	1.34	1.07
1:A:165:LEU:HD11	1:C:248:SER:HB2	1.67	0.77
1:B:229:GLU:OE2	5:B:401:HOH:O	2.06	0.74
1:B:125:LYS:HB2	1:B:126:PRO:CD	2.16	0.74
1:D:89:ALA:CB	1:D:100:GLU:HG3	2.17	0.74
1:D:229:GLU:OE2	5:D:401:HOH:O	2.06	0.73
2:C:302:NAD:H52A	5:C:437:HOH:O	1.88	0.73
1:D:89:ALA:HB1	1:D:100:GLU:CG	2.19	0.72
1:B:69:GLU:OE2	5:B:402:HOH:O	2.07	0.72
1:A:248:SER:HB2	1:C:165:LEU:HD11	1.73	0.70
1:D:125:LYS:HB2	1:D:126:PRO:HD3	1.73	0.70
1:C:125:LYS:HB2	1:C:126:PRO:HD3	1.73	0.69
2:A:301:NAD:H52A	5:A:444:HOH:O	1.93	0.67
1:C:125:LYS:CB	1:C:126:PRO:HD3	2.26	0.66
1:B:89:ALA:CB	1:B:100:GLU:HG3	2.26	0.65
1:D:125:LYS:CB	1:D:126:PRO:HD3	2.26	0.65
1:B:95:THR:HG22	5:B:447:HOH:O	1.97	0.64
1:D:89:ALA:HB1	1:D:100:GLU:HG3	1.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB1	1:B:100:GLU:HG3	1.82	0.61
2:D:302:NAD:C5B	5:D:443:HOH:O	2.49	0.60
1:B:95:THR:CG2	5:B:447:HOH:O	2.50	0.60
2:B:301:NAD:H52A	5:B:451:HOH:O	2.02	0.60
1:A:111:ALA:HB3	1:A:112:PRO:HD3	1.85	0.59
1:C:111:ALA:HB3	1:C:112:PRO:HD3	1.86	0.58
1:B:111:ALA:HB3	1:B:112:PRO:HD3	1.85	0.58
1:D:111:ALA:HB3	1:D:112:PRO:HD3	1.86	0.58
1:B:248:SER:OG	1:B:249:PHE:N	2.37	0.56
2:B:301:NAD:C5B	5:B:451:HOH:O	2.53	0.56
1:A:248:SER:OG	1:A:249:PHE:N	2.38	0.56
1:C:245:LEU:C	1:C:245:LEU:HD23	2.31	0.55
1:B:245:LEU:C	1:B:245:LEU:HD23	2.32	0.55
1:B:136:SER:HB2	2:B:301:NAD:H6N	1.88	0.55
2:D:302:NAD:H51A	5:D:443:HOH:O	2.04	0.55
1:D:1:MET:HE2	1:D:2:GLY:N	2.22	0.54
1:D:248:SER:OG	1:D:249:PHE:N	2.38	0.54
1:C:20:ARG:NH1	5:C:401:HOH:O	2.38	0.53
1:D:89:ALA:CB	1:D:100:GLU:CG	2.84	0.52
1:B:32:LEU:HD12	1:B:32:LEU:N	2.25	0.51
1:D:126:PRO:HD2	5:D:433:HOH:O	2.11	0.50
1:B:190:LEU:C	1:B:190:LEU:HD23	2.37	0.50
2:D:302:NAD:H52A	5:D:443:HOH:O	2.09	0.50
1:D:190:LEU:C	1:D:190:LEU:HD23	2.37	0.50
1:B:103:ARG:NH1	5:B:404:HOH:O	2.47	0.48
1:B:89:ALA:HB2	1:B:100:GLU:HG3	1.96	0.47
1:D:120:ALA:O	1:D:124:ARG:HD3	2.16	0.46
1:C:36:CYS:HA	1:C:54:PHE:O	2.16	0.46
1:A:125:LYS:CB	1:A:126:PRO:CD	2.94	0.45
1:D:1:MET:HE2	1:D:2:GLY:H	1.81	0.45
1:D:36:CYS:HA	1:D:54:PHE:O	2.16	0.45
1:A:1:MET:SD	1:A:2:GLY:N	2.90	0.45
1:D:125:LYS:CB	1:D:126:PRO:CD	2.94	0.45
1:A:36:CYS:HA	1:A:54:PHE:O	2.17	0.45
1:B:44:GLU:HG2	1:B:45:VAL:N	2.31	0.45
1:D:125:LYS:HB2	1:D:126:PRO:CD	2.46	0.45
1:A:125:LYS:HB2	1:A:126:PRO:CD	2.47	0.44
1:B:36:CYS:HA	1:B:54:PHE:O	2.17	0.44
1:D:44:GLU:HG2	1:D:45:VAL:N	2.32	0.44
1:D:89:ALA:HB2	1:D:100:GLU:HG3	1.97	0.44
1:A:133:ASN:O	1:A:176:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH2	1:A:100:GLU:HG3	2.34	0.43
1:B:24:GLN:O	1:B:28:ARG:HG3	2.19	0.43
1:A:136:SER:HB2	2:A:301:NAD:H6N	2.02	0.42
1:B:133:ASN:O	1:B:176:ALA:HA	2.20	0.42
1:B:230:LYS:HD2	1:D:221:GLU:OE1	2.20	0.42
1:C:125:LYS:CB	1:C:126:PRO:CD	2.96	0.41
1:C:248:SER:OG	1:C:249:PHE:N	2.53	0.41
1:A:207:LEU:O	1:A:245:LEU:HD12	2.21	0.41
1:D:133:ASN:O	1:D:176:ALA:HA	2.21	0.41
1:A:11:VAL:O	1:A:35:LEU:HA	2.20	0.41
1:A:121:ARG:O	1:A:124:ARG:NH1	2.54	0.41
1:B:11:VAL:O	1:B:35:LEU:HA	2.20	0.41
3:A:302:B3P:HN1	3:A:302:B3P:H92	1.85	0.40
1:A:248:SER:HB2	1:B:142:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/264 (94%)	238 (96%)	6 (2%)	3 (1%)	10	7
1	B	247/264 (94%)	238 (96%)	6 (2%)	3 (1%)	10	7
1	C	246/264 (93%)	237 (96%)	6 (2%)	3 (1%)	10	7
1	D	247/264 (94%)	239 (97%)	5 (2%)	3 (1%)	10	7
All	All	987/1056 (94%)	952 (96%)	23 (2%)	12 (1%)	10	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLY

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Mol	Chain	Res	Type
1	B	127	GLY
1	C	127	GLY
1	D	127	GLY
1	A	125	LYS
1	C	125	LYS
1	D	125	LYS
1	B	125	LYS
1	B	126	PRO
1	D	126	PRO
1	A	126	PRO
1	C	126	PRO

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	183/195 (94%)	178 (97%)	5 (3%)	39	45
1	B	183/195 (94%)	175 (96%)	8 (4%)	25	26
1	C	182/195 (93%)	180 (99%)	2 (1%)	65	74
1	D	183/195 (94%)	180 (98%)	3 (2%)	55	64
All	All	731/780 (94%)	713 (98%)	18 (2%)	42	48

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

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	LEU
1	A	41	GLU
1	A	95	THR
1	A	230	LYS
1	B	1	MET
1	B	35	LEU
1	B	41	GLU
1	B	75	LEU
1	B	95	THR

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Mol	Chain	Res	Type
1	B	97	ARG
1	B	125	LYS
1	B	165	LEU
1	C	35	LEU
1	C	95	THR
1	D	1	MET
1	D	35	LEU
1	D	41	GLU

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

Mol	Chain	Res	Type
1	A	150	ASN
1	B	24	GLN
1	D	150	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	B	301	-	46,48,48	0.91	1 (2%)	64,73,73	0.98	3 (4%)
2	NAD	C	302	-	46,48,48	0.91	1 (2%)	64,73,73	1.06	7 (10%)
4	GOL	C	301	-	5,5,5	0.21	0	5,5,5	0.47	0
2	NAD	A	301	-	46,48,48	1.14	4 (8%)	64,73,73	0.94	2 (3%)
2	NAD	D	302	-	46,48,48	0.99	1 (2%)	64,73,73	0.96	4 (6%)
3	B3P	A	302	-	18,18,18	0.31	0	23,23,23	0.92	0
4	GOL	D	301	-	5,5,5	0.08	0	5,5,5	0.27	0
4	GOL	B	302	-	5,5,5	0.08	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	301	-	-	8/30/62/62	0/5/5/5
2	NAD	C	302	-	-	8/30/62/62	0/5/5/5
4	GOL	C	301	-	-	3/4/4/4	-
2	NAD	A	301	-	-	6/30/62/62	0/5/5/5
2	NAD	D	302	-	-	10/30/62/62	0/5/5/5
3	B3P	A	302	-	-	9/28/28/28	-
4	GOL	D	301	-	-	2/4/4/4	-
4	GOL	B	302	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	NAD	C2N-N1N	5.69	1.41	1.35
2	A	301	NAD	C2N-N1N	5.68	1.41	1.35
2	B	301	NAD	C2N-N1N	5.11	1.40	1.35
2	C	302	NAD	C2N-N1N	4.21	1.39	1.35
2	A	301	NAD	O4D-C1D	2.83	1.44	1.40
2	A	301	NAD	PA-O3	2.21	1.61	1.59
2	A	301	NAD	PN-O3	2.12	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	NAD	O4B-C1B-N9A	3.50	114.82	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C6N-N1N-C2N	-3.04	119.29	121.88
2	B	301	NAD	C4B-O4B-C1B	-3.02	102.80	109.47
2	C	302	NAD	C6N-N1N-C2N	-3.02	119.31	121.88
2	B	301	NAD	O4B-C1B-N9A	2.95	113.76	108.09
2	D	302	NAD	C4B-O4B-C1B	-2.84	103.21	109.47
2	C	302	NAD	O4B-C1B-N9A	2.64	113.16	108.09
2	B	301	NAD	C6N-N1N-C2N	-2.52	119.73	121.88
2	A	301	NAD	O4B-C1B-N9A	2.50	112.89	108.09
2	D	302	NAD	C6N-N1N-C2N	-2.39	119.84	121.88
2	C	302	NAD	O3-PA-O1A	-2.39	103.52	110.70
2	D	302	NAD	O4B-C1B-C2B	-2.28	101.74	106.62
2	C	302	NAD	O2A-PA-O1A	2.20	122.68	112.44
2	C	302	NAD	C4B-O4B-C1B	-2.14	104.75	109.47
2	C	302	NAD	O3B-C3B-C4B	-2.11	105.02	111.08
2	C	302	NAD	O2N-PN-O1N	2.08	122.14	112.44

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	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	302	NAD	C5B-O5B-PA-O1A
2	C	302	NAD	C5D-O5D-PN-O3
2	C	302	NAD	C5D-O5D-PN-O2N
2	C	302	NAD	O4D-C1D-N1N-C2N
2	D	302	NAD	C5B-O5B-PA-O1A
2	D	302	NAD	C5B-O5B-PA-O3
2	D	302	NAD	C5D-O5D-PN-O3
2	D	302	NAD	C5D-O5D-PN-O1N
2	D	302	NAD	C5D-O5D-PN-O2N
3	A	302	B3P	N1-C4-C7-O6
3	A	302	B3P	C5-C4-C7-O6
3	A	302	B3P	C6-C4-C7-O6
3	A	302	B3P	O3-C11-C8-N2
3	A	302	B3P	O3-C11-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	302	B3P	O3-C11-C8-C10
3	A	302	B3P	C2-C1-C3-N1
4	D	301	GOL	O1-C1-C2-C3
3	A	302	B3P	N1-C4-C5-O4
4	C	301	GOL	O1-C1-C2-O2
2	D	302	NAD	PN-O3-PA-O5B
4	C	301	GOL	O2-C2-C3-O3
4	C	301	GOL	C1-C2-C3-O3
3	A	302	B3P	C7-C4-C5-O4
2	B	301	NAD	C5B-O5B-PA-O3
2	D	302	NAD	C5B-O5B-PA-O2A
2	A	301	NAD	C4B-C5B-O5B-PA
4	D	301	GOL	O1-C1-C2-O2
2	B	301	NAD	C4B-C5B-O5B-PA
2	C	302	NAD	C4B-C5B-O5B-PA
2	D	302	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	C	302	NAD	O4D-C1D-N1N-C6N
2	D	302	NAD	O4D-C1D-N1N-C6N
2	C	302	NAD	PA-O3-PN-O1N
2	B	301	NAD	PN-O3-PA-O5B
4	B	302	GOL	O2-C2-C3-O3
2	C	302	NAD	PA-O3-PN-O2N
2	D	302	NAD	PA-O3-PN-O2N

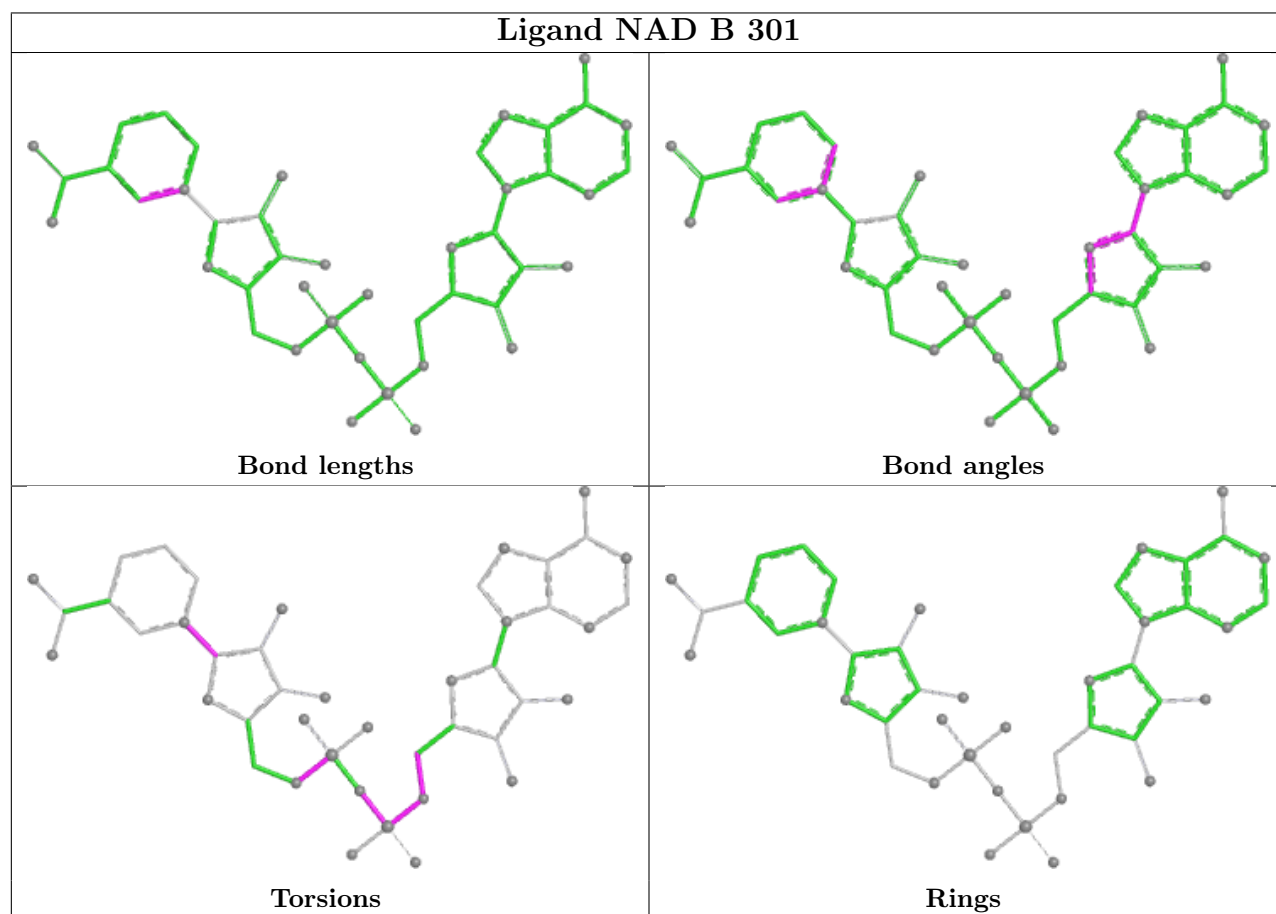
There are no ring outliers.

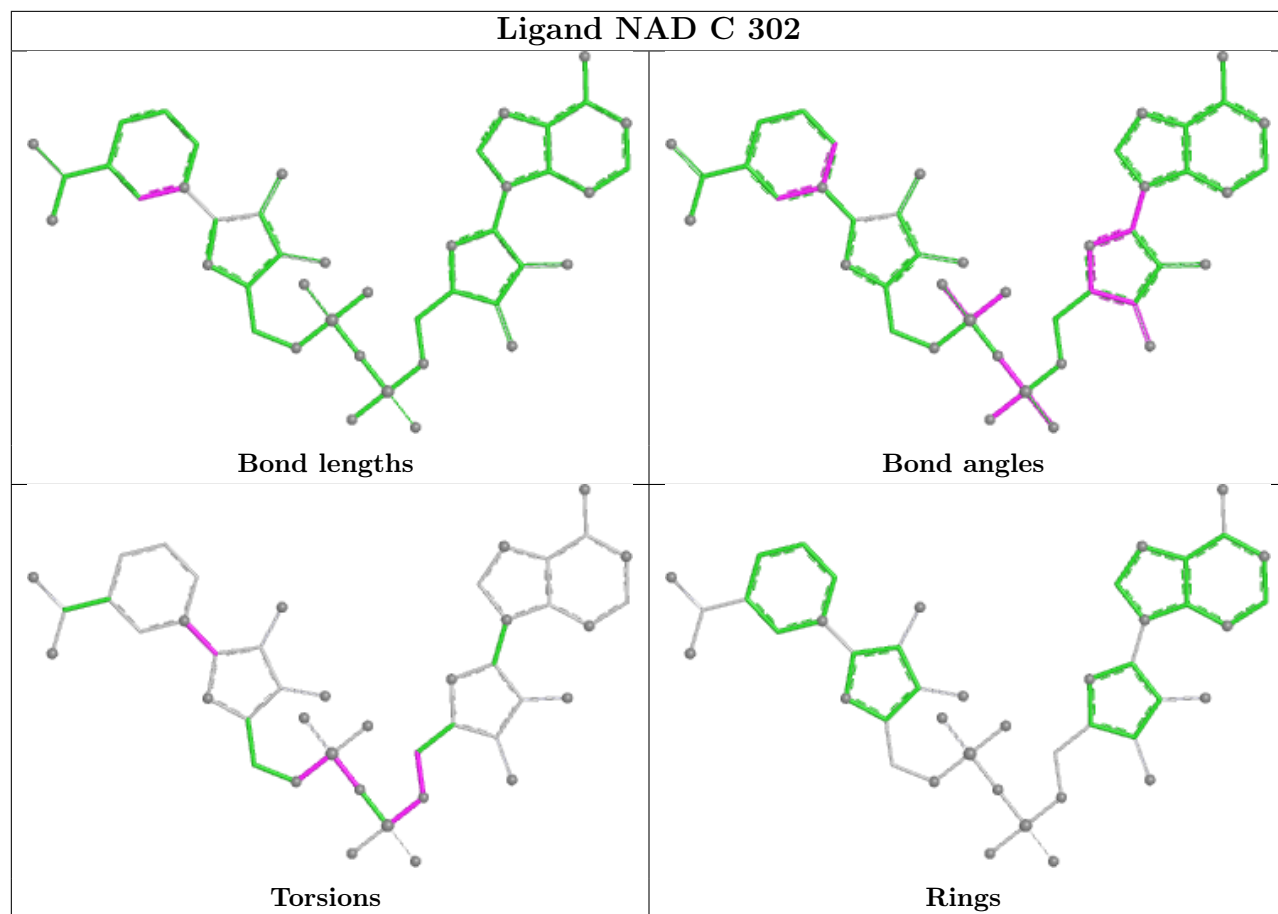
5 monomers are involved in 10 short contacts:

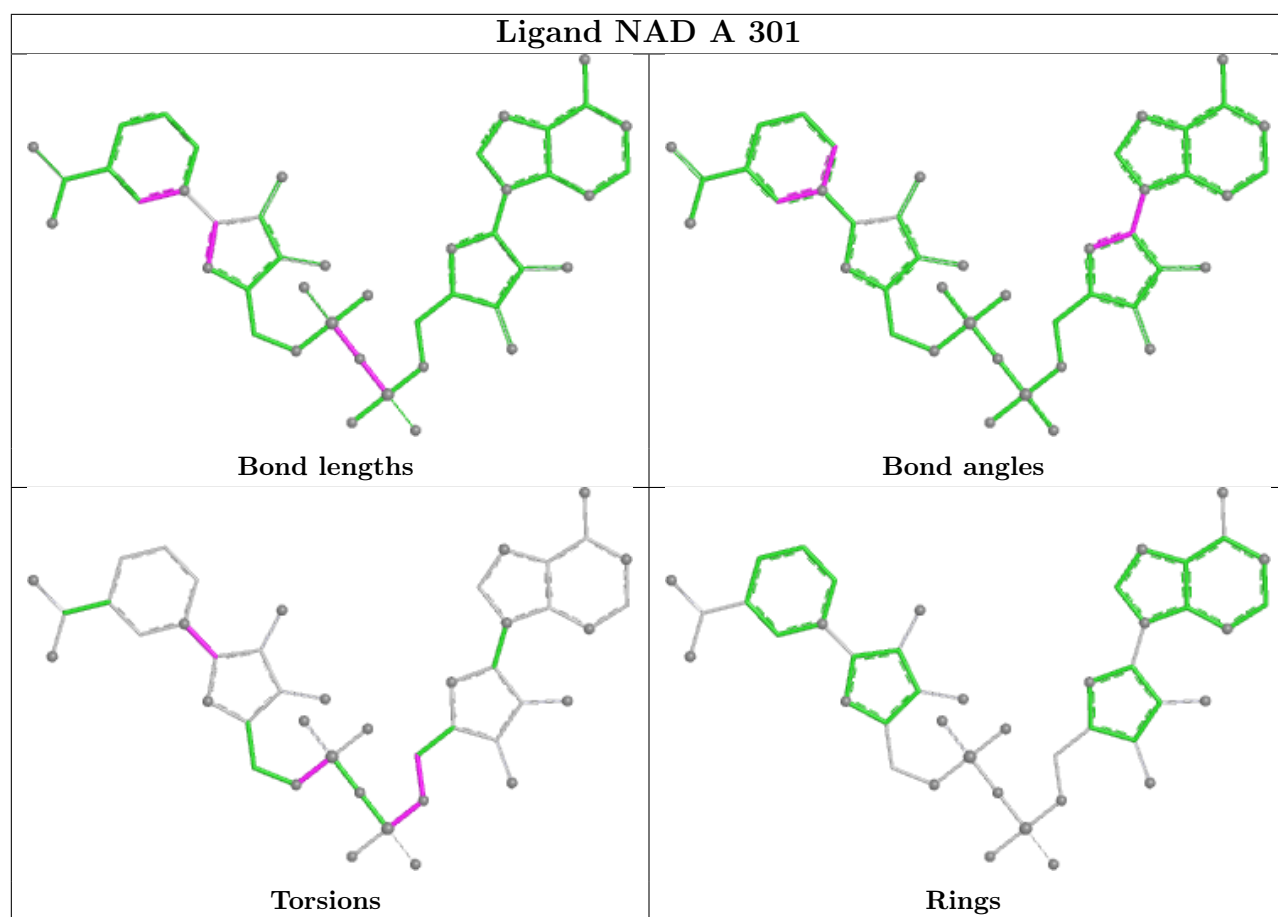
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAD	3	0
2	C	302	NAD	1	0
2	A	301	NAD	2	0
2	D	302	NAD	3	0
3	A	302	B3P	1	0

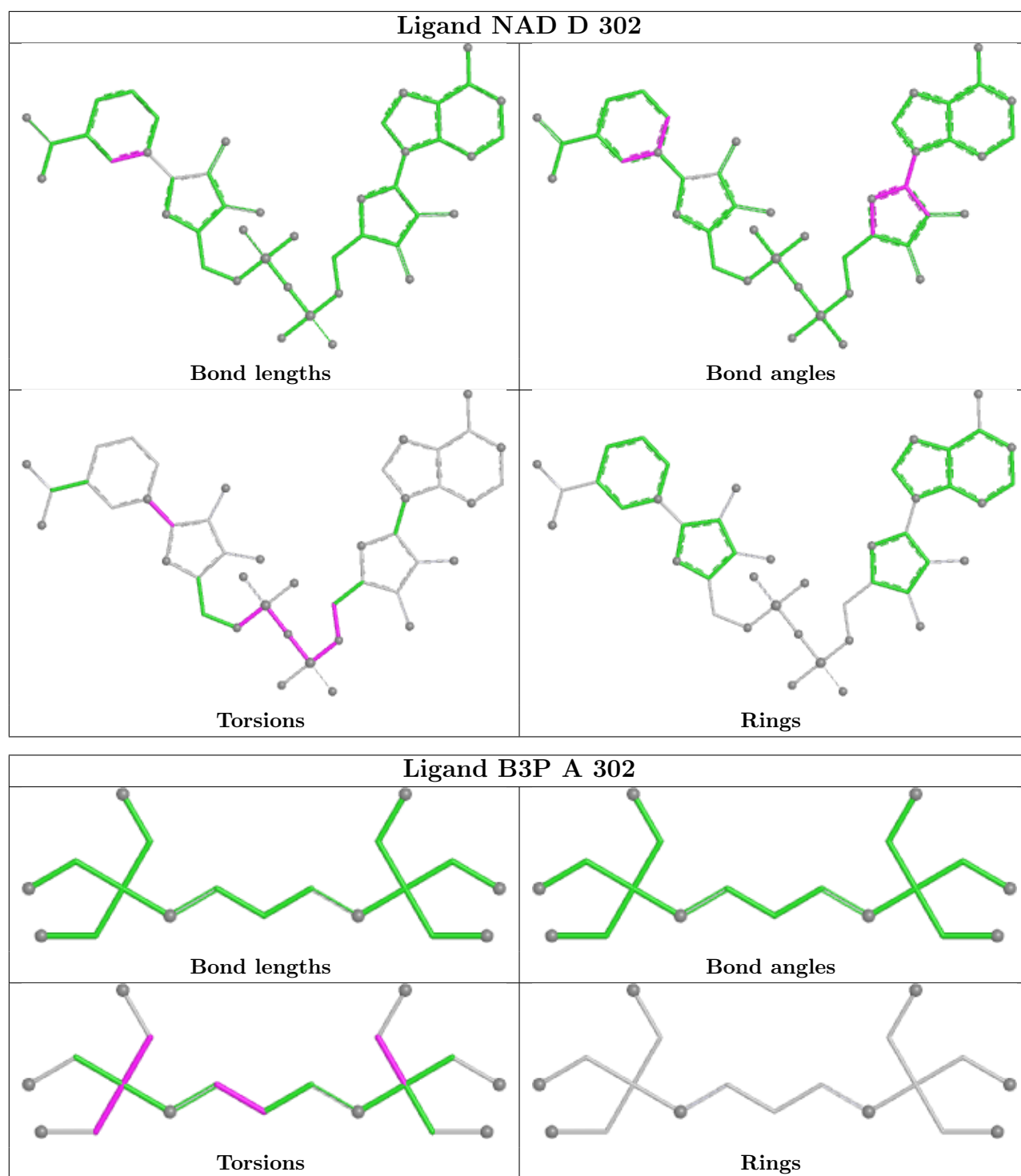
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

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	249/264 (94%)	0.32	11 (4%) 39 41	20, 32, 54, 99	0
1	B	249/264 (94%)	0.21	5 (2%) 65 67	18, 29, 49, 71	0
1	C	248/264 (93%)	0.49	17 (6%) 23 24	21, 33, 57, 112	0
1	D	249/264 (94%)	0.16	6 (2%) 59 62	18, 29, 51, 79	0
All	All	995/1056 (94%)	0.30	39 (3%) 43 45	18, 31, 53, 112	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	5.3
1	C	126	PRO	5.2
1	A	193	LEU	4.2
1	C	127	GLY	4.0
1	C	124	ARG	3.8
1	D	1	MET	3.8
1	A	126	PRO	3.8
1	B	1	MET	3.8
1	D	249	PHE	3.6
1	C	249	PHE	3.4
1	D	127	GLY	3.3
1	A	249	PHE	3.0
1	B	249	PHE	3.0
1	A	124	ARG	2.9
1	A	1	MET	2.9
1	A	2	GLY	2.9
1	C	76	GLY	2.9
1	C	73	TYR	2.9
1	B	126	PRO	2.8
1	C	53	PHE	2.8
1	C	125	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	74	ALA	2.6
1	C	171	ARG	2.6
1	A	125	LYS	2.6
1	C	193	LEU	2.5
1	D	125	LYS	2.4
1	C	190	LEU	2.4
1	A	28	ARG	2.3
1	A	3	LEU	2.3
1	A	127	GLY	2.3
1	C	56	VAL	2.3
1	D	124	ARG	2.3
1	C	192	ALA	2.2
1	D	126	PRO	2.1
1	C	2	GLY	2.1
1	C	6	GLY	2.1
1	A	192	ALA	2.1
1	C	38	LEU	2.0
1	B	125	LYS	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	B3P	A	302	19/19	0.74	0.19	53,63,77,77	0
4	GOL	C	301	6/6	0.82	0.14	39,50,52,60	0
4	GOL	B	302	6/6	0.84	0.14	39,42,46,46	0
4	GOL	D	301	6/6	0.87	0.12	42,47,50,59	0
2	NAD	C	302	44/44	0.94	0.08	27,35,39,43	0

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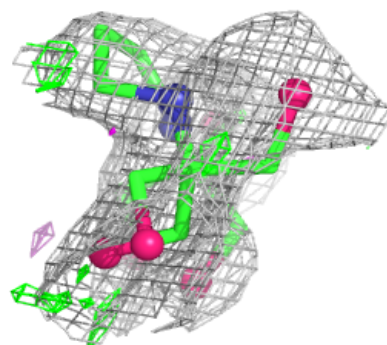
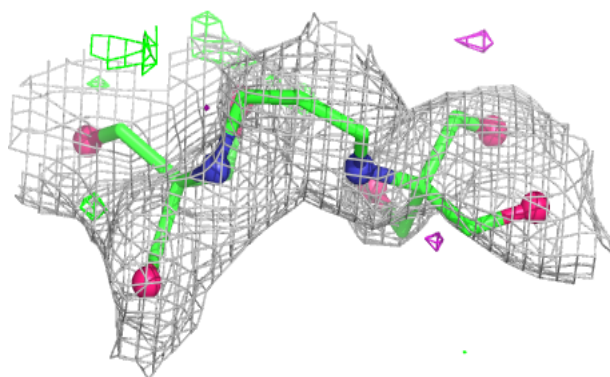
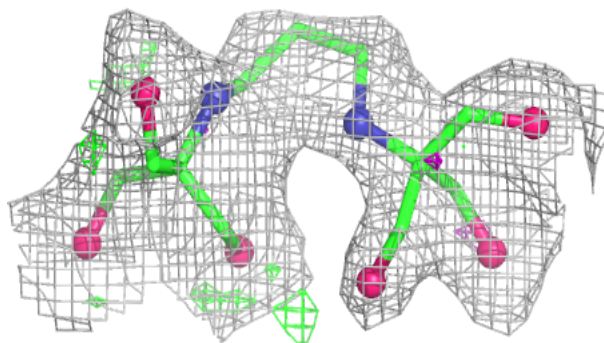
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	302	44/44	0.94	0.07	24,32,37,40	0
2	NAD	A	301	44/44	0.94	0.08	24,30,37,39	0
2	NAD	B	301	44/44	0.95	0.07	23,30,37,39	0

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.

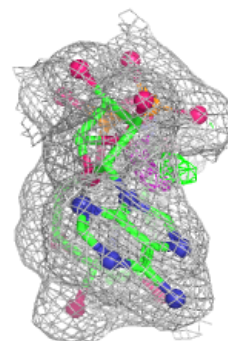
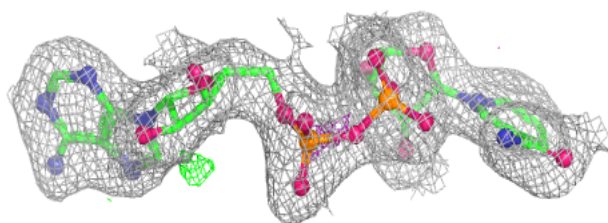
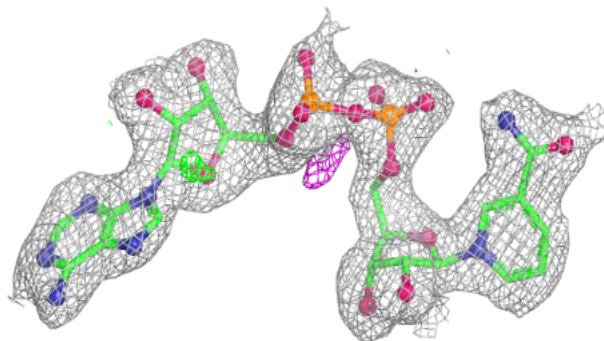
Electron density around B3P A 302:

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

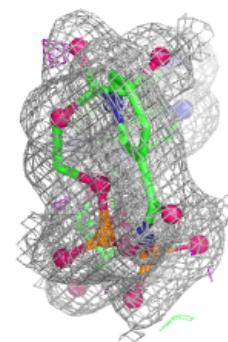
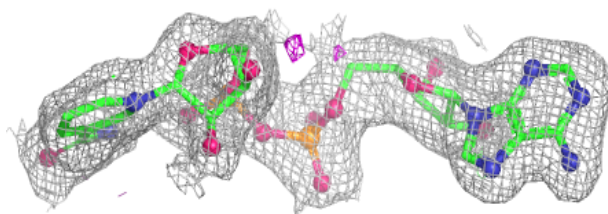
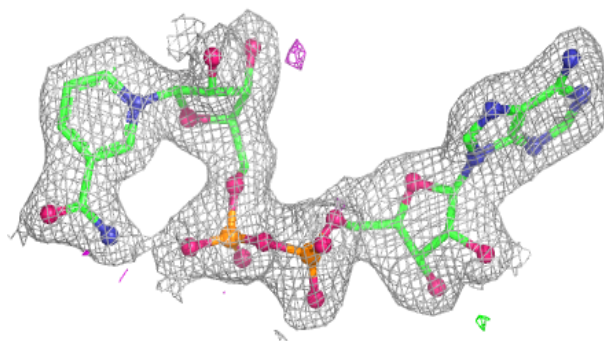


Electron density around NAD C 302:

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

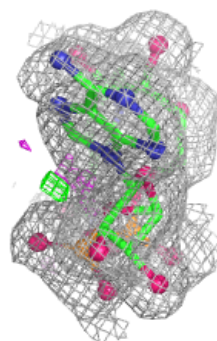
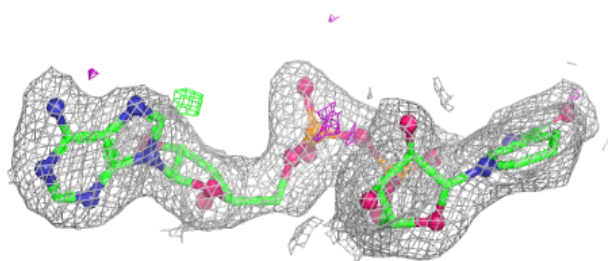
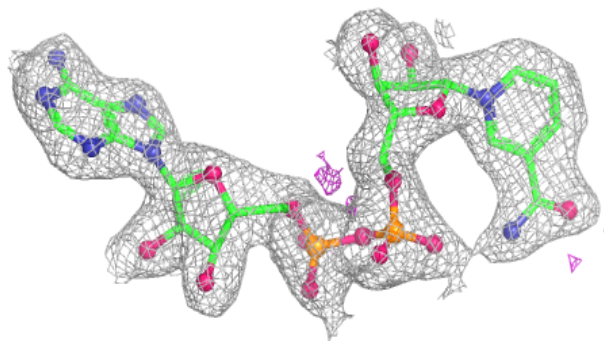
**Electron density around NAD D 302:**

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

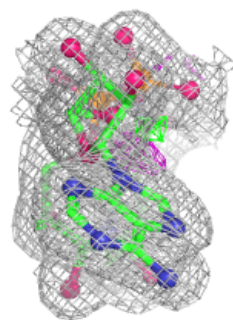
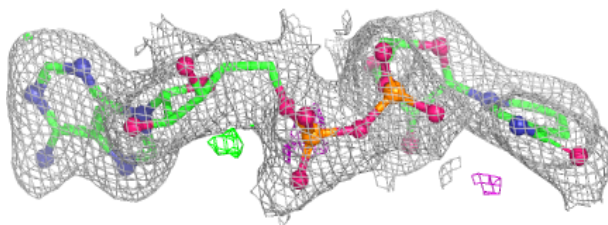
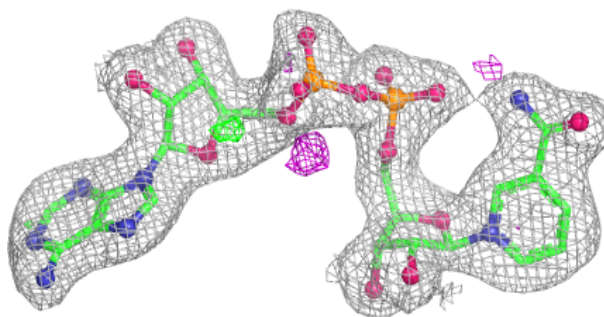


Electron density around NAD A 301:

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

**Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.