



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:27 AM UTC

PDB ID : 8QC8 / pdb_00008qc8
Title : Crystal structure of NAD-dependent glycoside hydrolase from *Flavobacterium* sp. (strain K172) in complex with co-factor NAD⁺
Authors : Pickles, I.B.; Sharma, M.; Davies, G.J.
Deposited on : 2023-08-25
Resolution : 2.35 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

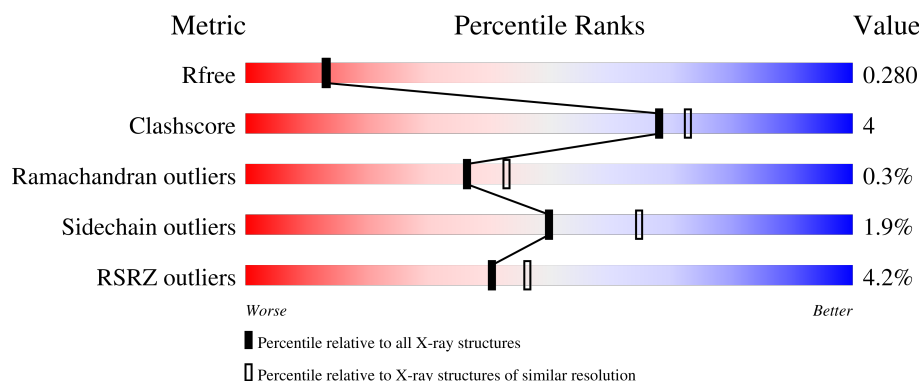
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	393	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11279 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 Gfo/Idh/MocA family oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	367	Total	C	N	O	S	0	0	0
			2785	1766	476	530	13			
1	C	364	Total	C	N	O	S	0	0	0
			2758	1748	473	525	12			
1	D	339	Total	C	N	O	S	0	0	0
			2513	1585	440	476	12			
1	A	364	Total	C	N	O	S	0	0	0
			2767	1752	472	530	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	initiating methionine	UNP A0A7D7VZ79
B	-11	GLY	-	expression tag	UNP A0A7D7VZ79
B	-10	SER	-	expression tag	UNP A0A7D7VZ79
B	-9	SER	-	expression tag	UNP A0A7D7VZ79
B	-8	HIS	-	expression tag	UNP A0A7D7VZ79
B	-7	HIS	-	expression tag	UNP A0A7D7VZ79
B	-6	HIS	-	expression tag	UNP A0A7D7VZ79
B	-5	HIS	-	expression tag	UNP A0A7D7VZ79
B	-4	HIS	-	expression tag	UNP A0A7D7VZ79
B	-3	HIS	-	expression tag	UNP A0A7D7VZ79
B	-2	SER	-	expression tag	UNP A0A7D7VZ79
B	-1	SER	-	expression tag	UNP A0A7D7VZ79
B	0	GLY	-	expression tag	UNP A0A7D7VZ79
C	-12	MET	-	initiating methionine	UNP A0A7D7VZ79
C	-11	GLY	-	expression tag	UNP A0A7D7VZ79
C	-10	SER	-	expression tag	UNP A0A7D7VZ79
C	-9	SER	-	expression tag	UNP A0A7D7VZ79
C	-8	HIS	-	expression tag	UNP A0A7D7VZ79
C	-7	HIS	-	expression tag	UNP A0A7D7VZ79
C	-6	HIS	-	expression tag	UNP A0A7D7VZ79
C	-5	HIS	-	expression tag	UNP A0A7D7VZ79

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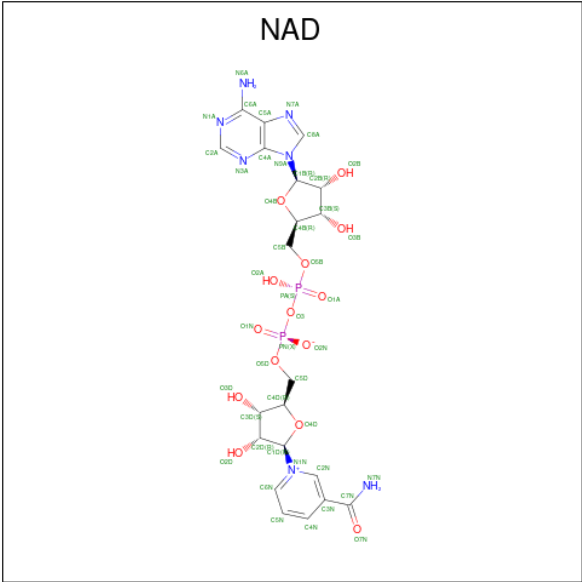
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP A0A7D7VZ79
C	-3	HIS	-	expression tag	UNP A0A7D7VZ79
C	-2	SER	-	expression tag	UNP A0A7D7VZ79
C	-1	SER	-	expression tag	UNP A0A7D7VZ79
C	0	GLY	-	expression tag	UNP A0A7D7VZ79
D	-12	MET	-	initiating methionine	UNP A0A7D7VZ79
D	-11	GLY	-	expression tag	UNP A0A7D7VZ79
D	-10	SER	-	expression tag	UNP A0A7D7VZ79
D	-9	SER	-	expression tag	UNP A0A7D7VZ79
D	-8	HIS	-	expression tag	UNP A0A7D7VZ79
D	-7	HIS	-	expression tag	UNP A0A7D7VZ79
D	-6	HIS	-	expression tag	UNP A0A7D7VZ79
D	-5	HIS	-	expression tag	UNP A0A7D7VZ79
D	-4	HIS	-	expression tag	UNP A0A7D7VZ79
D	-3	HIS	-	expression tag	UNP A0A7D7VZ79
D	-2	SER	-	expression tag	UNP A0A7D7VZ79
D	-1	SER	-	expression tag	UNP A0A7D7VZ79
D	0	GLY	-	expression tag	UNP A0A7D7VZ79
A	-12	MET	-	initiating methionine	UNP A0A7D7VZ79
A	-11	GLY	-	expression tag	UNP A0A7D7VZ79
A	-10	SER	-	expression tag	UNP A0A7D7VZ79
A	-9	SER	-	expression tag	UNP A0A7D7VZ79
A	-8	HIS	-	expression tag	UNP A0A7D7VZ79
A	-7	HIS	-	expression tag	UNP A0A7D7VZ79
A	-6	HIS	-	expression tag	UNP A0A7D7VZ79
A	-5	HIS	-	expression tag	UNP A0A7D7VZ79
A	-4	HIS	-	expression tag	UNP A0A7D7VZ79
A	-3	HIS	-	expression tag	UNP A0A7D7VZ79
A	-2	SER	-	expression tag	UNP A0A7D7VZ79
A	-1	SER	-	expression tag	UNP A0A7D7VZ79
A	0	GLY	-	expression tag	UNP A0A7D7VZ79

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

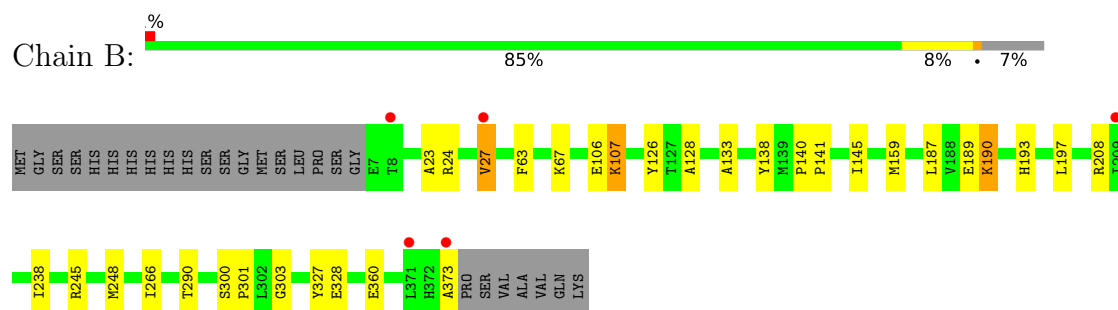
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	78	Total	O	0	0
			78	78		
4	C	71	Total	O	0	0
			71	71		
4	D	38	Total	O	0	0
			38	38		
4	A	63	Total	O	0	0
			63	63		

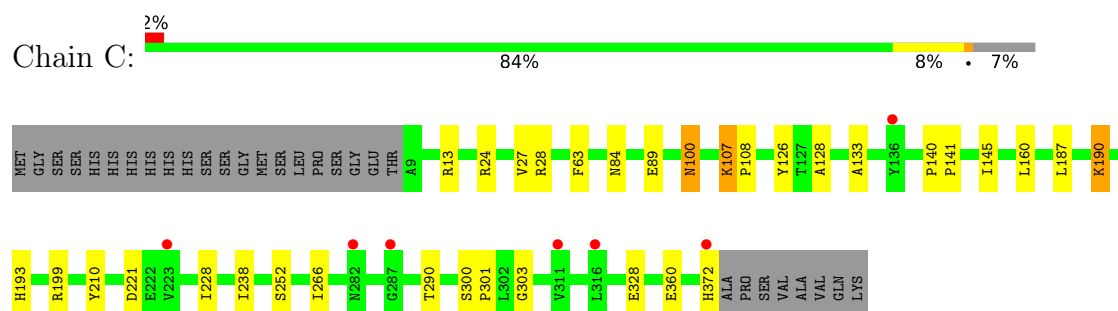
3 Residue-property plots [i](#)

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.

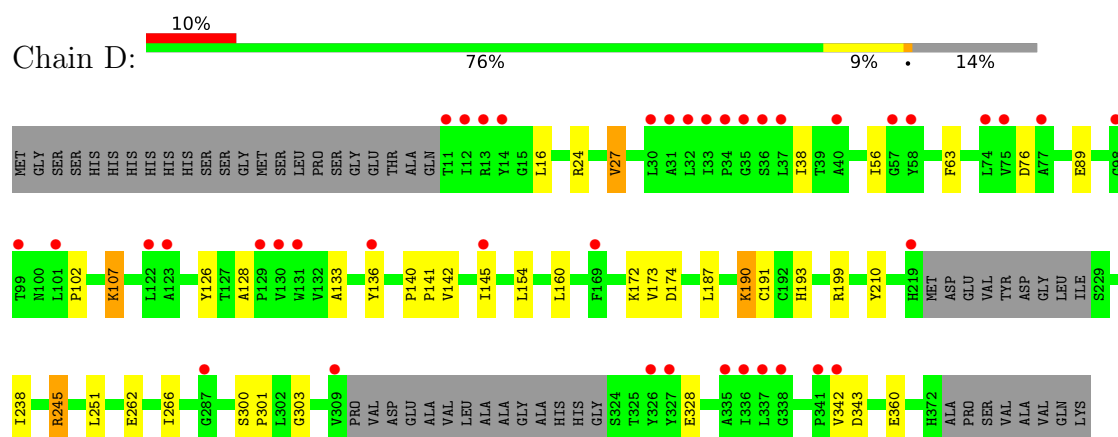
- Molecule 1: Gfo/Idh/MocA family oxidoreductase



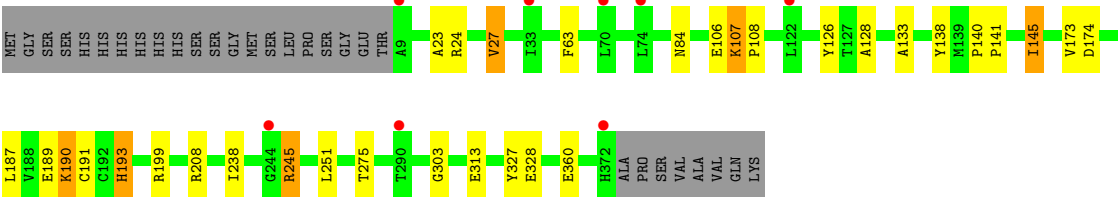
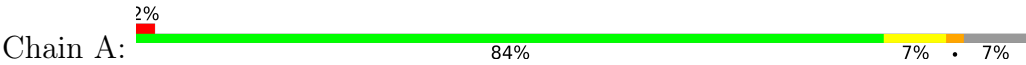
- Molecule 1: Gfo/Idh/MocA family oxidoreductase



- Molecule 1: Gfo/Idh/MocA family oxidoreductase



- Molecule 1: Gfo/Idh/MocA family oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.78Å 161.49Å 175.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.45 – 2.35 59.45 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (59.45-2.35) 99.6 (59.45-2.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.229 , 0.278 0.232 , 0.280	Depositor DCC
R_{free} test set	4904 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	1.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11279	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1227e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PO4

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	0/2828	0.97	2/3851 (0.1%)
1	B	0.59	0/2846	0.95	1/3874 (0.0%)
1	C	0.57	0/2818	0.97	4/3837 (0.1%)
1	D	0.56	0/2566	0.97	2/3494 (0.1%)
All	All	0.58	0/11058	0.97	9/15056 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	4
1	D	0	3
All	All	0	11

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	HIS	CB-CA-C	-6.70	99.66	110.79
1	D	193	HIS	CA-CB-CG	6.21	120.01	113.80
1	C	372	HIS	CA-C-O	-6.16	110.32	120.80
1	D	343	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	193	HIS	CA-CB-CG	5.47	119.28	113.80
1	C	100	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	193	HIS	CB-CA-C	-5.43	101.44	110.68
1	B	189	GLU	CB-CG-CD	5.22	121.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLU	CB-CG-CD	5.10	121.27	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	245	ARG	Sidechain
1	B	24	ARG	Sidechain
1	C	13	ARG	Sidechain
1	C	199	ARG	Sidechain
1	C	24	ARG	Sidechain
1	C	28	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	24	ARG	Sidechain
1	D	245	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2767	0	2675	20	0
1	B	2785	0	2708	24	0
1	C	2758	0	2683	17	0
1	D	2513	0	2381	24	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	1	0
4	A	63	0	0	1	0
4	B	78	0	0	1	0
4	C	71	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	38	0	0	1	0
All	All	11279	0	10551	78	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 (78) 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:A:107:LYS:HE2	1:A:107:LYS:C	2.18	0.69
1:C:107:LYS:HE2	1:C:107:LYS:C	2.18	0.68
1:B:145:ILE:HG23	1:B:266:ILE:HD11	1.78	0.65
1:C:145:ILE:HG23	1:C:266:ILE:HD11	1.80	0.64
1:D:145:ILE:HG23	1:D:266:ILE:HD11	1.83	0.60
1:D:238:ILE:HD11	1:A:238:ILE:HG13	1.86	0.58
1:B:238:ILE:HG13	1:C:238:ILE:HD11	1.85	0.57
1:D:136:TYR:OH	1:D:262:GLU:HG2	2.04	0.57
1:A:145:ILE:HD13	1:A:275:THR:HG22	1.87	0.56
1:B:107:LYS:O	1:B:107:LYS:HE2	2.06	0.56
1:B:107:LYS:HE2	1:B:107:LYS:C	2.31	0.56
1:D:107:LYS:O	1:D:107:LYS:HE2	2.07	0.55
1:D:107:LYS:HE2	1:D:107:LYS:C	2.32	0.54
1:B:238:ILE:HD11	1:C:238:ILE:HG13	1.90	0.53
1:A:245:ARG:HH11	1:A:245:ARG:HG3	1.74	0.53
1:D:238:ILE:HG13	1:A:238:ILE:HD11	1.91	0.52
1:A:190:LYS:HA	1:A:190:LYS:HE2	1.93	0.51
1:B:140:PRO:HB2	1:B:141:PRO:HD3	1.93	0.50
1:B:208:ARG:NH1	1:C:210:TYR:OH	2.41	0.50
1:C:140:PRO:HB2	1:C:141:PRO:HD3	1.94	0.49
1:B:190:LYS:HA	1:B:190:LYS:HE2	1.94	0.49
1:A:140:PRO:HB2	1:A:141:PRO:HD3	1.94	0.48
1:D:140:PRO:HB2	1:D:141:PRO:HD3	1.96	0.48
1:C:126:TYR:CE2	1:C:128:ALA:HB3	2.49	0.47
1:D:38:ILE:HD12	1:D:56:ILE:HG23	1.97	0.47
1:D:187:LEU:HB2	1:D:360:GLU:HG2	1.96	0.47
1:A:145:ILE:HD13	1:A:275:THR:CG2	2.44	0.47
1:B:187:LEU:HB2	1:B:360:GLU:HG2	1.96	0.47
1:C:221:ASP:HA	1:C:228:ILE:HD11	1.97	0.46
1:D:210:TYR:OH	1:A:208:ARG:NH1	2.46	0.46
1:C:190:LYS:HE2	1:C:190:LYS:HA	1.97	0.46
1:B:126:TYR:CE2	1:B:128:ALA:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LYS:HA	1:D:190:LYS:HE2	1.98	0.45
1:A:193:HIS:CD2	4:A:530:HOH:O	2.70	0.45
1:D:126:TYR:CE2	1:D:128:ALA:HB3	2.51	0.45
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.80	0.45
1:D:136:TYR:CE1	1:D:142:VAL:HG21	2.52	0.45
1:B:138:TYR:HB3	1:B:327:TYR:HB2	1.99	0.44
1:C:133:ALA:HA	1:C:328:GLU:OE2	2.17	0.44
1:D:191:CYS:SG	1:D:251:LEU:HD22	2.58	0.44
1:B:300:SER:HA	1:B:301:PRO:HA	1.88	0.44
1:C:160:LEU:HD13	1:C:266:ILE:HG12	2.00	0.44
1:B:248:MET:HE3	1:B:248:MET:HB3	1.94	0.44
1:B:373:ALA:C	4:B:502:HOH:O	2.61	0.43
1:B:107:LYS:C	1:B:107:LYS:CE	2.91	0.43
1:D:173:VAL:O	1:D:174:ASP:HB2	2.17	0.43
1:C:300:SER:HA	1:C:301:PRO:HA	1.90	0.43
1:A:126:TYR:CE2	1:A:128:ALA:HB3	2.54	0.43
1:D:107:LYS:C	1:D:107:LYS:CE	2.91	0.43
1:A:106:GLU:HA	1:A:133:ALA:HB3	2.01	0.43
1:D:342:VAL:N	4:D:501:HOH:O	2.27	0.43
1:A:138:TYR:HB3	1:A:327:TYR:HB2	2.01	0.43
1:B:145:ILE:HG23	1:B:266:ILE:CD1	2.46	0.43
1:C:187:LEU:HB2	1:C:360:GLU:HG2	2.00	0.43
1:D:172:LYS:HB3	3:D:402:NAD:O1A	2.19	0.43
1:D:133:ALA:HA	1:D:328:GLU:OE2	2.19	0.42
1:B:106:GLU:HA	1:B:133:ALA:HB3	2.01	0.42
1:B:159:MET:SD	1:C:252:SER:HB2	2.59	0.42
1:C:100:ASN:HB2	4:C:537:HOH:O	2.20	0.42
1:D:76:ASP:O	1:D:102:PRO:HD2	2.20	0.42
1:A:63:PHE:CD1	1:A:63:PHE:N	2.88	0.41
1:A:187:LEU:HB2	1:A:360:GLU:HG2	2.01	0.41
1:A:191:CYS:SG	1:A:251:LEU:HD22	2.60	0.41
1:D:16:LEU:HD11	1:D:27:VAL:HG12	2.02	0.41
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.91	0.41
1:D:160:LEU:HD13	1:D:266:ILE:HG12	2.02	0.41
1:A:133:ALA:HA	1:A:328:GLU:OE2	2.20	0.41
1:A:84:ASN:CG	1:A:108:PRO:HD2	2.46	0.41
1:B:107:LYS:HD2	1:B:193:HIS:CE1	2.55	0.41
1:A:23:ALA:O	1:A:27:VAL:HG13	2.21	0.41
1:A:173:VAL:O	1:A:174:ASP:HB2	2.19	0.41
1:C:63:PHE:CD1	1:C:63:PHE:N	2.88	0.41
1:D:63:PHE:CD1	1:D:63:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:PHE:CD1	1:B:63:PHE:N	2.88	0.41
1:B:23:ALA:O	1:B:27:VAL:HG13	2.21	0.40
1:C:84:ASN:CG	1:C:108:PRO:HD2	2.46	0.40
1:B:133:ALA:HA	1:B:328:GLU:OE2	2.21	0.40
1:D:300:SER:HA	1:D:301:PRO:HA	1.89	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	362/393 (92%)	355 (98%)	6 (2%)	1 (0%)	36	43
1	B	365/393 (93%)	356 (98%)	8 (2%)	1 (0%)	36	43
1	C	362/393 (92%)	351 (97%)	10 (3%)	1 (0%)	36	43
1	D	333/393 (85%)	322 (97%)	10 (3%)	1 (0%)	36	43
All	All	1422/1572 (90%)	1384 (97%)	34 (2%)	4 (0%)	36	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	GLY
1	C	303	GLY
1	D	303	GLY
1	A	303	GLY

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	286/320 (89%)	281 (98%)	5 (2%)	53	68
1	B	287/320 (90%)	282 (98%)	5 (2%)	53	68
1	C	285/320 (89%)	280 (98%)	5 (2%)	51	66
1	D	250/320 (78%)	244 (98%)	6 (2%)	43	57
All	All	1108/1280 (87%)	1087 (98%)	21 (2%)	50	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	67	LYS
1	B	107	LYS
1	B	190	LYS
1	B	290	THR
1	C	27	VAL
1	C	89	GLU
1	C	107	LYS
1	C	190	LYS
1	C	290	THR
1	D	27	VAL
1	D	89	GLU
1	D	107	LYS
1	D	154	LEU
1	D	190	LYS
1	D	245	ARG
1	A	27	VAL
1	A	107	LYS
1	A	145	ILE
1	A	190	LYS
1	A	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	ASN
1	B	261	GLN
1	C	29	ASN
1	C	171	HIS

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Mol	Chain	Res	Type
1	C	261	GLN
1	D	29	ASN
1	D	100	ASN
1	D	171	HIS
1	D	261	GLN
1	A	100	ASN
1	A	158	HIS
1	A	261	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	D	402	-	46,48,48	0.73	1 (2%)	64,73,73	0.91	3 (4%)
3	NAD	A	402	-	46,48,48	0.89	2 (4%)	64,73,73	0.68	1 (1%)
2	PO4	C	401	-	4,4,4	1.36	1 (25%)	6,6,6	0.71	0
2	PO4	C	402	-	4,4,4	0.77	0	6,6,6	0.52	0
2	PO4	A	401	-	4,4,4	1.80	1 (25%)	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	401	-	4,4,4	1.20	1 (25%)	6,6,6	0.62	0
3	NAD	B	402	-	46,48,48	0.85	4 (8%)	64,73,73	0.79	1 (1%)
2	PO4	B	401	-	4,4,4	1.79	1 (25%)	6,6,6	0.76	0
3	NAD	C	404	-	46,48,48	0.69	1 (2%)	64,73,73	0.82	1 (1%)
2	PO4	C	403	-	4,4,4	1.56	1 (25%)	6,6,6	0.37	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
3	NAD	D	402	-	-	11/30/62/62	0/5/5/5
3	NAD	B	402	-	-	7/30/62/62	0/5/5/5
3	NAD	A	402	-	-	9/30/62/62	0/5/5/5
3	NAD	C	404	-	-	4/30/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAD	PA-O3	3.99	1.63	1.59
2	A	401	PO4	P-O1	3.42	1.58	1.50
2	B	401	PO4	P-O1	3.41	1.58	1.50
2	C	403	PO4	P-O1	2.94	1.57	1.50
3	D	402	NAD	C2N-N1N	2.86	1.38	1.35
3	B	402	NAD	PA-O3	2.69	1.62	1.59
3	A	402	NAD	C2N-N1N	2.68	1.37	1.35
3	C	404	NAD	C2N-N1N	2.58	1.37	1.35
3	B	402	NAD	O4D-C1D	2.30	1.43	1.40
3	B	402	NAD	C2N-N1N	2.26	1.37	1.35
3	B	402	NAD	PN-O3	2.16	1.61	1.59
2	C	401	PO4	P-O3	2.12	1.60	1.54
2	D	401	PO4	P-O1	2.11	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NAD	C6N-N1N-C2N	-2.42	119.82	121.88
3	B	402	NAD	C6N-N1N-C2N	-2.37	119.86	121.88
3	C	404	NAD	O2N-PN-O3	2.34	113.59	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	NAD	O2B-C2B-C3B	2.09	118.52	111.82
3	A	402	NAD	O3-PA-O1A	-2.08	104.43	110.70
3	D	402	NAD	O3-PN-O1N	-2.07	104.49	110.70

There are no chirality outliers.

All (31) torsion outliers are listed below:

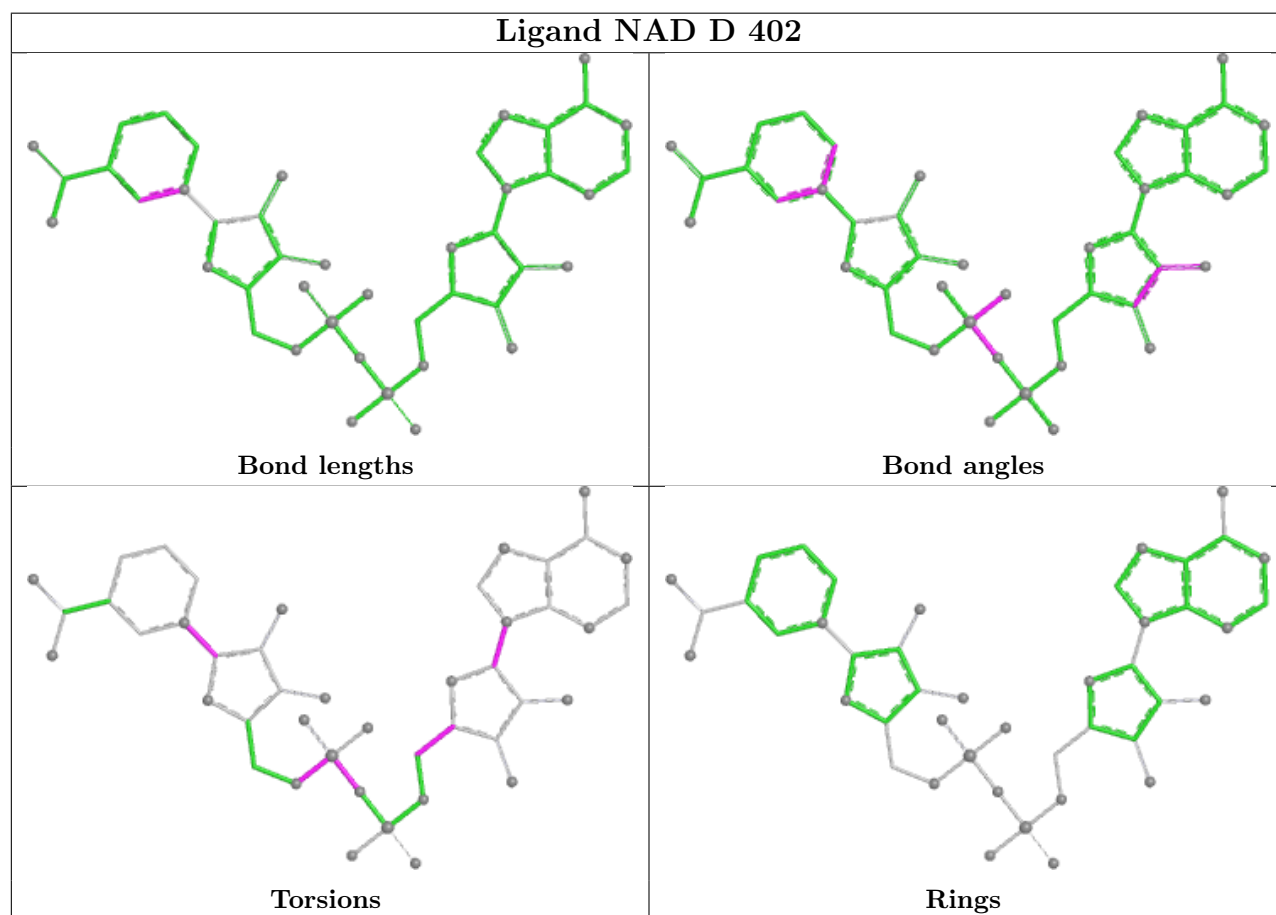
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	D	402	NAD	C5D-O5D-PN-O3
3	D	402	NAD	C5D-O5D-PN-O2N
3	D	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	D	402	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	C2B-C1B-N9A-C8A
3	C	404	NAD	C2B-C1B-N9A-C8A
3	D	402	NAD	C3B-C4B-C5B-O5B
3	D	402	NAD	C2B-C1B-N9A-C8A
3	A	402	NAD	C2B-C1B-N9A-C8A
3	D	402	NAD	C5D-O5D-PN-O1N
3	D	402	NAD	PA-O3-PN-O2N
3	B	402	NAD	C2B-C1B-N9A-C4A
3	C	404	NAD	C2B-C1B-N9A-C4A
3	D	402	NAD	C2B-C1B-N9A-C4A
3	B	402	NAD	C2D-C1D-N1N-C2N
3	C	404	NAD	O4D-C1D-N1N-C2N
3	D	402	NAD	O4D-C1D-N1N-C2N
3	D	402	NAD	O4B-C1B-N9A-C8A
3	A	402	NAD	O4B-C1B-N9A-C8A
3	B	402	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	O4B-C1B-N9A-C8A
3	C	404	NAD	O4B-C1B-N9A-C8A
3	A	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	PA-O3-PN-O1N
3	A	402	NAD	PA-O3-PN-O2N
3	A	402	NAD	C2B-C1B-N9A-C4A

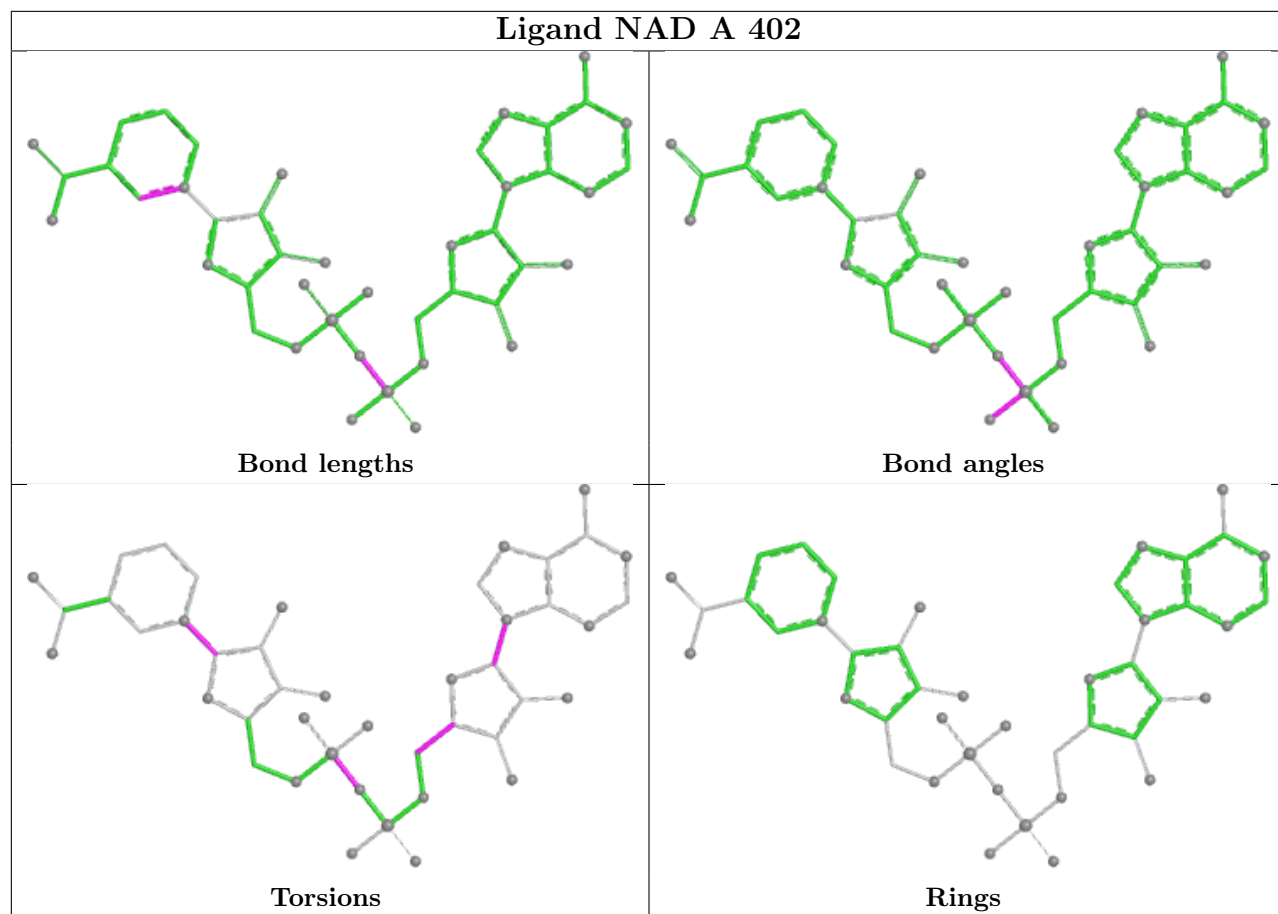
There are no ring outliers.

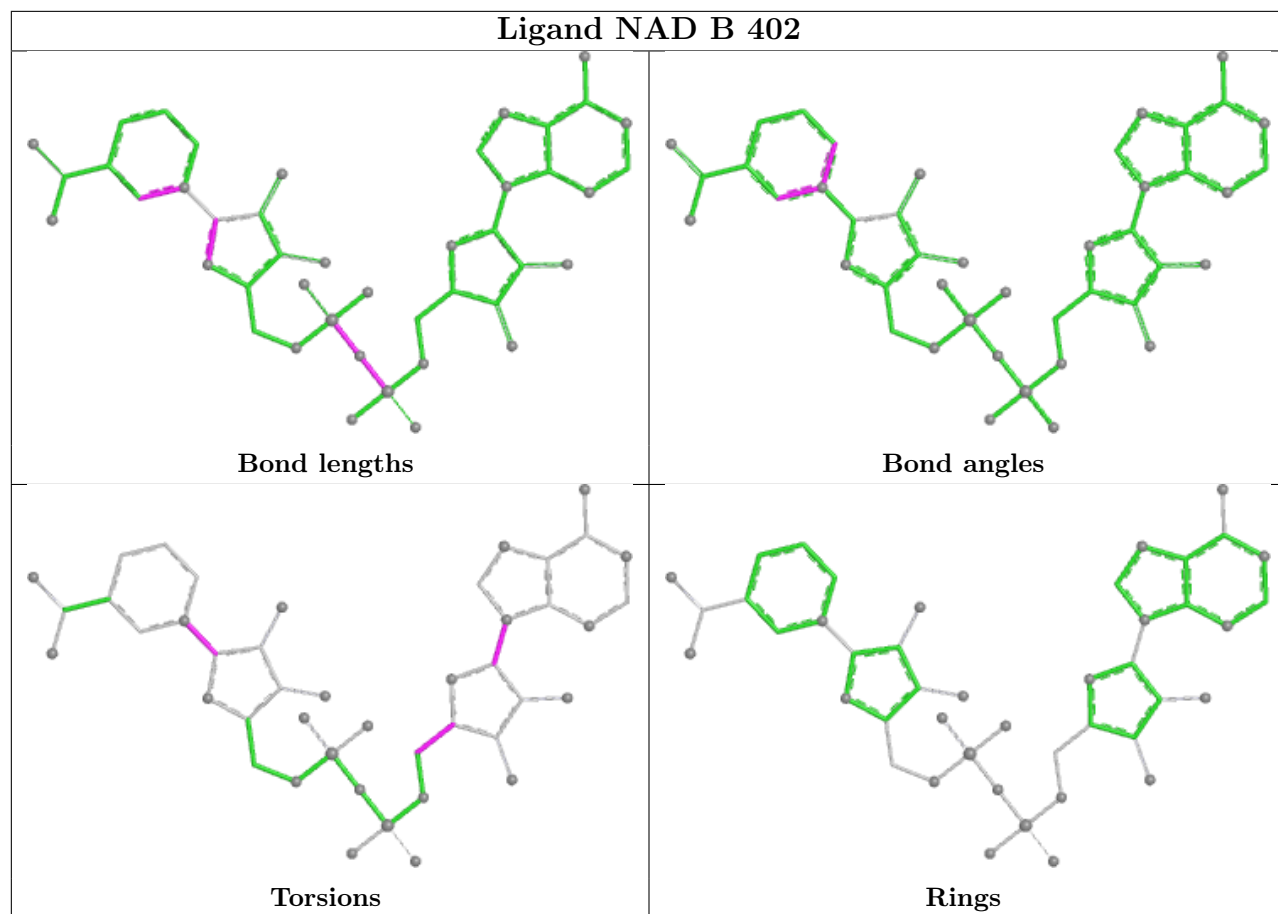
1 monomer is involved in 1 short contact:

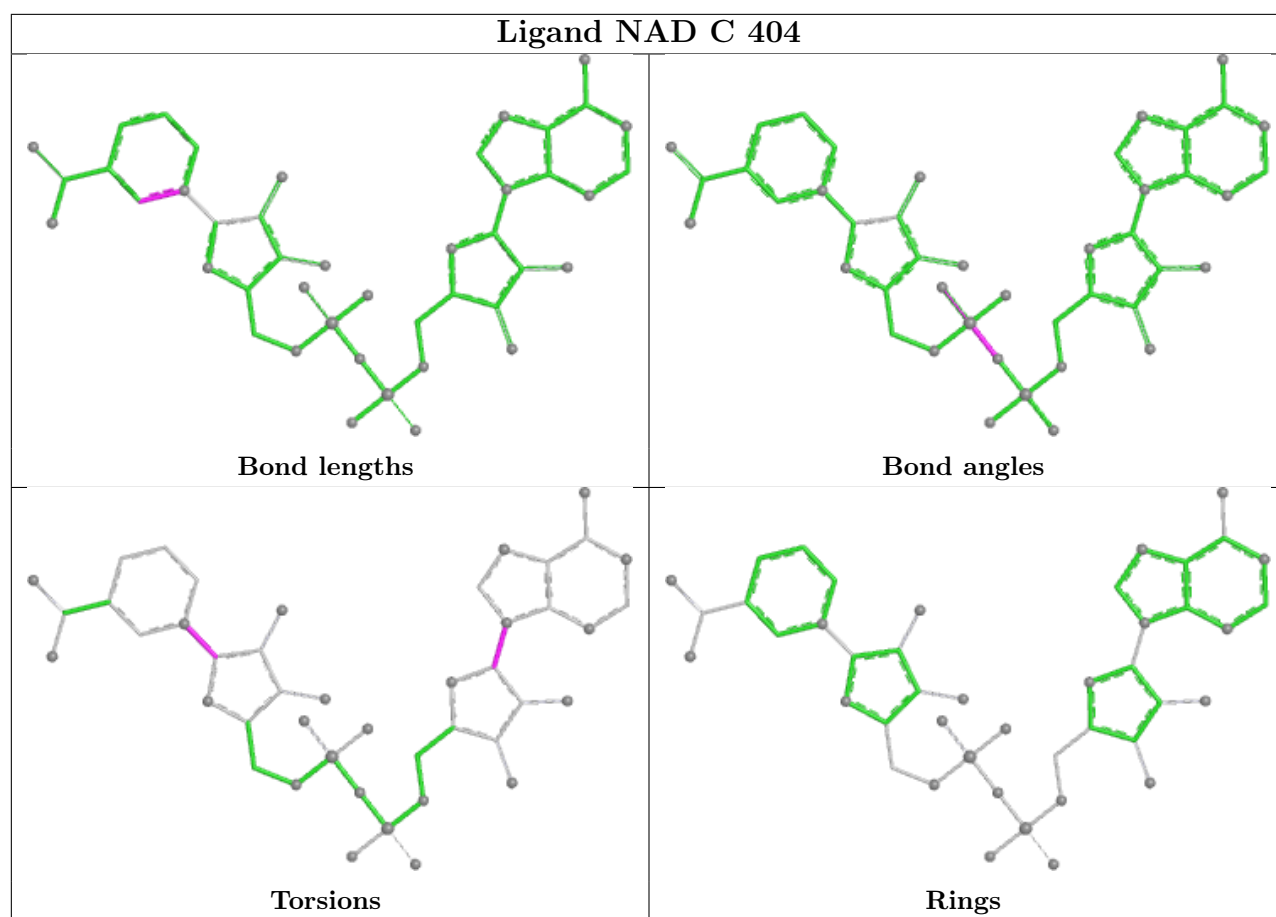
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	NAD	1	0

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 [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	364/393 (92%)	0.39	8 (2%) 62 67	31, 53, 81, 105	0
1	B	367/393 (93%)	0.34	5 (1%) 73 78	31, 52, 81, 106	0
1	C	364/393 (92%)	0.30	7 (1%) 66 71	34, 51, 83, 118	0
1	D	339/393 (86%)	0.90	40 (11%) 9 10	36, 65, 104, 129	0
All	All	1434/1572 (91%)	0.47	60 (4%) 40 46	31, 54, 90, 129	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	4.8
1	D	336	ILE	4.1
1	D	32	LEU	4.0
1	D	57	GLY	4.0
1	D	77	ALA	3.5
1	D	37	LEU	3.5
1	D	74	LEU	3.5
1	B	373	ALA	3.4
1	D	14	TYR	3.3
1	A	372	HIS	3.3
1	D	33	ILE	3.3
1	A	74	LEU	3.3
1	D	12	ILE	3.2
1	D	129	PRO	3.1
1	D	130	VAL	3.1
1	D	36	SER	3.0
1	D	341	PRO	3.0
1	D	337	LEU	2.9
1	B	209	ILE	2.9
1	D	327	TYR	2.9
1	A	9	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	2.7
1	C	287	GLY	2.7
1	D	136	TYR	2.7
1	B	8	THR	2.6
1	D	335	ALA	2.6
1	D	11	THR	2.6
1	D	35	GLY	2.6
1	D	101	LEU	2.6
1	D	58	TYR	2.6
1	D	326	TYR	2.6
1	D	145	ILE	2.6
1	D	131	TRP	2.5
1	C	372	HIS	2.5
1	A	244	GLY	2.5
1	C	311	VAL	2.4
1	D	75	VAL	2.4
1	D	342	VAL	2.4
1	D	30	LEU	2.4
1	D	13	ARG	2.4
1	D	40	ALA	2.4
1	D	34	PRO	2.3
1	D	219	HIS	2.3
1	C	136	TYR	2.3
1	D	98	GLY	2.3
1	C	223	VAL	2.3
1	D	309	VAL	2.3
1	D	287	GLY	2.2
1	B	371	LEU	2.2
1	B	27	VAL	2.2
1	A	122	LEU	2.1
1	D	169	PHE	2.1
1	D	122	LEU	2.1
1	C	282	ASN	2.1
1	A	33	ILE	2.1
1	D	338	GLY	2.0
1	D	99	THR	2.0
1	A	290	THR	2.0
1	D	123	ALA	2.0
1	C	316	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](#)

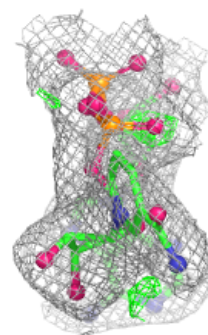
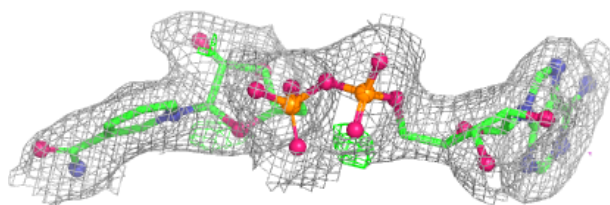
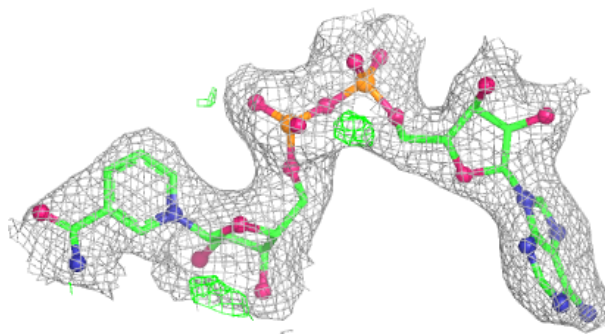
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	PO4	C	403	5/5	0.49	0.13	72,80,92,109	0
2	PO4	D	401	5/5	0.72	0.11	57,64,84,95	0
2	PO4	C	402	5/5	0.75	0.10	79,79,101,110	0
2	PO4	B	401	5/5	0.76	0.13	57,61,93,94	0
2	PO4	C	401	5/5	0.80	0.19	51,61,78,96	0
2	PO4	A	401	5/5	0.84	0.13	46,56,78,82	0
3	NAD	D	402	44/44	0.95	0.07	34,50,59,77	0
3	NAD	C	404	44/44	0.96	0.06	31,39,44,48	0
3	NAD	B	402	44/44	0.97	0.06	25,34,39,45	0
3	NAD	A	402	44/44	0.97	0.06	28,37,45,47	0

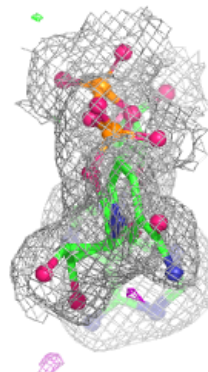
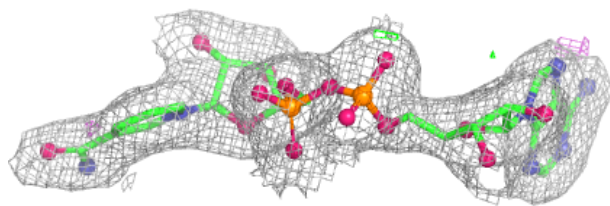
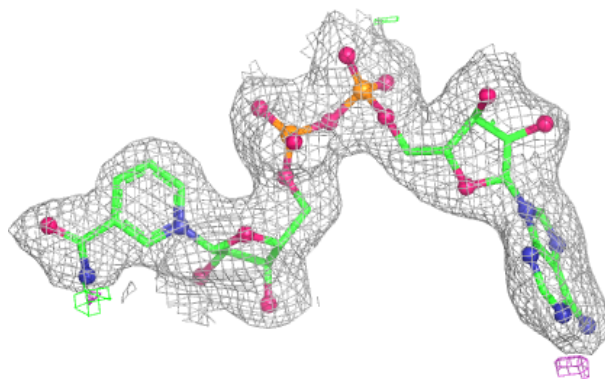
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 402:

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

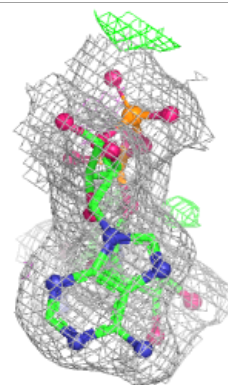
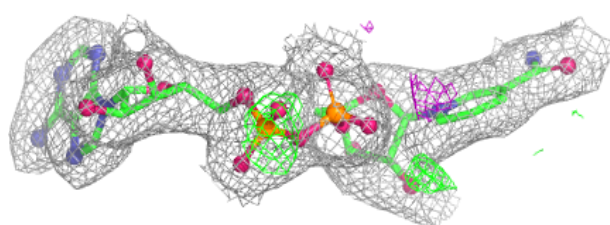
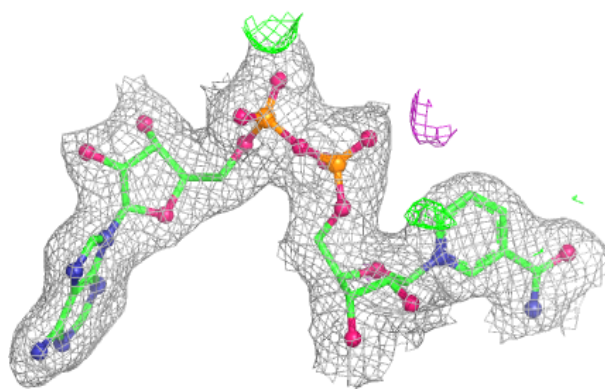
**Electron density around NAD C 404:**

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

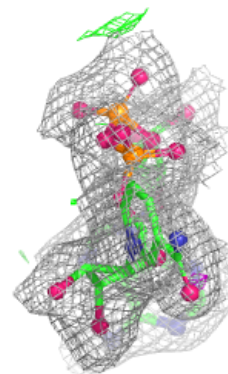
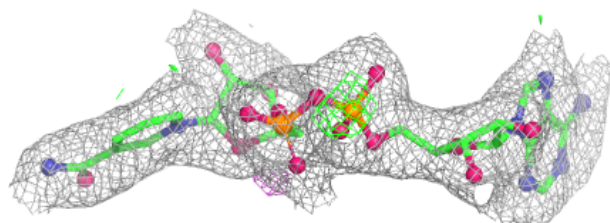
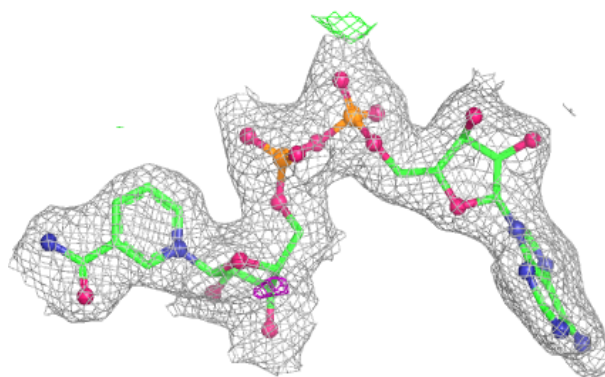


Electron density around NAD B 402:

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

**Electron density around NAD A 402:**

$2mF_o-DF_c$ (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.