



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 AM UTC

PDB ID : 4MIN / pdb_00004min
Title : Crystal Structure of myo-inositol dehydrogenase from Lactobacillus casei with bound cofactor NAD
Authors : Bertwistle, D.; Sanders, D.A.R.; Palmer, D.R.J.
Deposited on : 2013-09-01
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

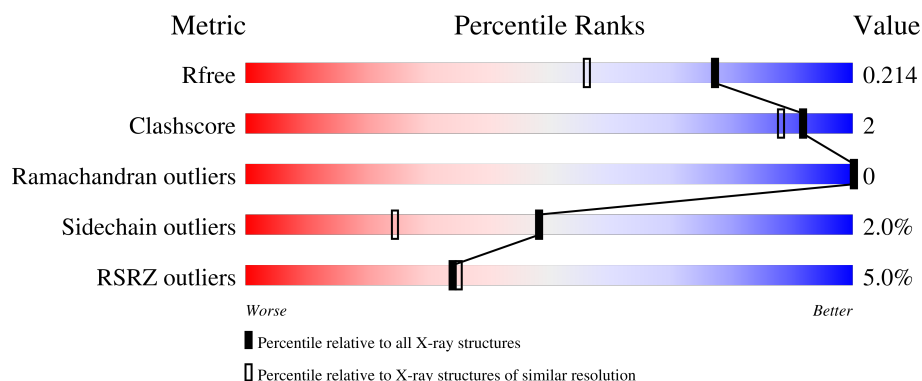
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	351	11% 85% 12% .
1	B	351	3% 85% 10% ..
1	C	351	3% 86% 10% ..
1	D	351	2% 83% 14% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11838 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 Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	2	0
			2632	1663	447	516	6			
1	B	339	Total	C	N	O	S	0	2	0
			2633	1664	448	515	6			
1	C	339	Total	C	N	O	S	0	3	0
			2633	1664	447	516	6			
1	D	339	Total	C	N	O	S	0	5	0
			2652	1676	454	516	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP B3W8L3
A	-10	ARG	-	expression tag	UNP B3W8L3
A	-9	GLY	-	expression tag	UNP B3W8L3
A	-8	SER	-	expression tag	UNP B3W8L3
A	-7	HIS	-	expression tag	UNP B3W8L3
A	-6	HIS	-	expression tag	UNP B3W8L3
A	-5	HIS	-	expression tag	UNP B3W8L3
A	-4	HIS	-	expression tag	UNP B3W8L3
A	-3	HIS	-	expression tag	UNP B3W8L3
A	-2	HIS	-	expression tag	UNP B3W8L3
A	-1	GLY	-	expression tag	UNP B3W8L3
A	0	SER	-	expression tag	UNP B3W8L3
A	292	GLU	GLN	conflict	UNP B3W8L3
B	-11	MET	-	expression tag	UNP B3W8L3
B	-10	ARG	-	expression tag	UNP B3W8L3
B	-9	GLY	-	expression tag	UNP B3W8L3
B	-8	SER	-	expression tag	UNP B3W8L3
B	-7	HIS	-	expression tag	UNP B3W8L3
B	-6	HIS	-	expression tag	UNP B3W8L3
B	-5	HIS	-	expression tag	UNP B3W8L3
B	-4	HIS	-	expression tag	UNP B3W8L3

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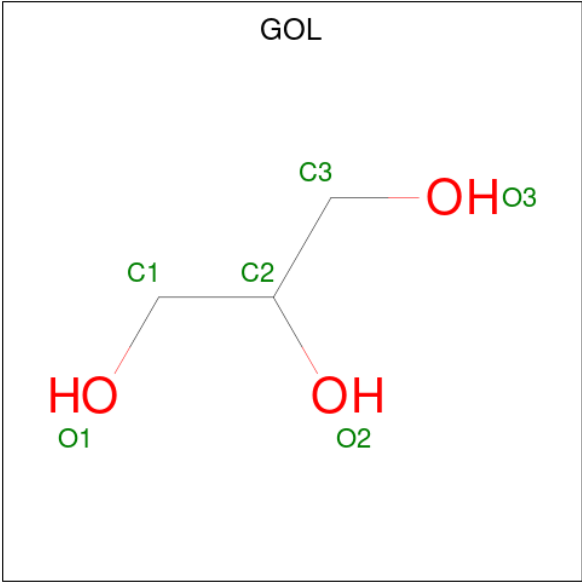
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP B3W8L3
B	-2	HIS	-	expression tag	UNP B3W8L3
B	-1	GLY	-	expression tag	UNP B3W8L3
B	0	SER	-	expression tag	UNP B3W8L3
B	292	GLU	GLN	conflict	UNP B3W8L3
C	-11	MET	-	expression tag	UNP B3W8L3
C	-10	ARG	-	expression tag	UNP B3W8L3
C	-9	GLY	-	expression tag	UNP B3W8L3
C	-8	SER	-	expression tag	UNP B3W8L3
C	-7	HIS	-	expression tag	UNP B3W8L3
C	-6	HIS	-	expression tag	UNP B3W8L3
C	-5	HIS	-	expression tag	UNP B3W8L3
C	-4	HIS	-	expression tag	UNP B3W8L3
C	-3	HIS	-	expression tag	UNP B3W8L3
C	-2	HIS	-	expression tag	UNP B3W8L3
C	-1	GLY	-	expression tag	UNP B3W8L3
C	0	SER	-	expression tag	UNP B3W8L3
C	292	GLU	GLN	conflict	UNP B3W8L3
D	-11	MET	-	expression tag	UNP B3W8L3
D	-10	ARG	-	expression tag	UNP B3W8L3
D	-9	GLY	-	expression tag	UNP B3W8L3
D	-8	SER	-	expression tag	UNP B3W8L3
D	-7	HIS	-	expression tag	UNP B3W8L3
D	-6	HIS	-	expression tag	UNP B3W8L3
D	-5	HIS	-	expression tag	UNP B3W8L3
D	-4	HIS	-	expression tag	UNP B3W8L3
D	-3	HIS	-	expression tag	UNP B3W8L3
D	-2	HIS	-	expression tag	UNP B3W8L3
D	-1	GLY	-	expression tag	UNP B3W8L3
D	0	SER	-	expression tag	UNP B3W8L3
D	292	GLU	GLN	conflict	UNP B3W8L3

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



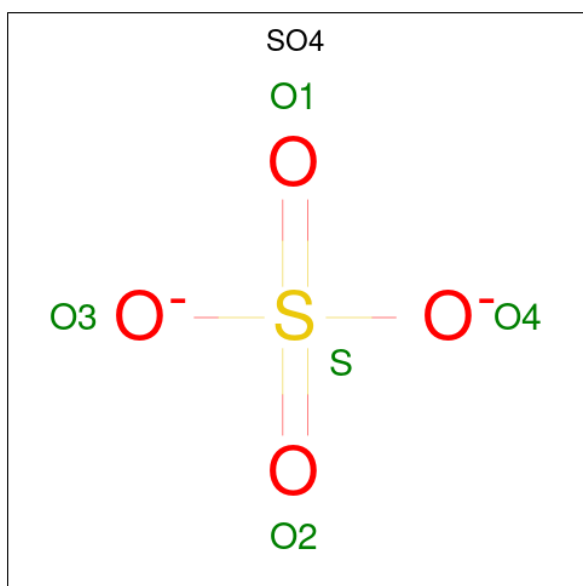
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

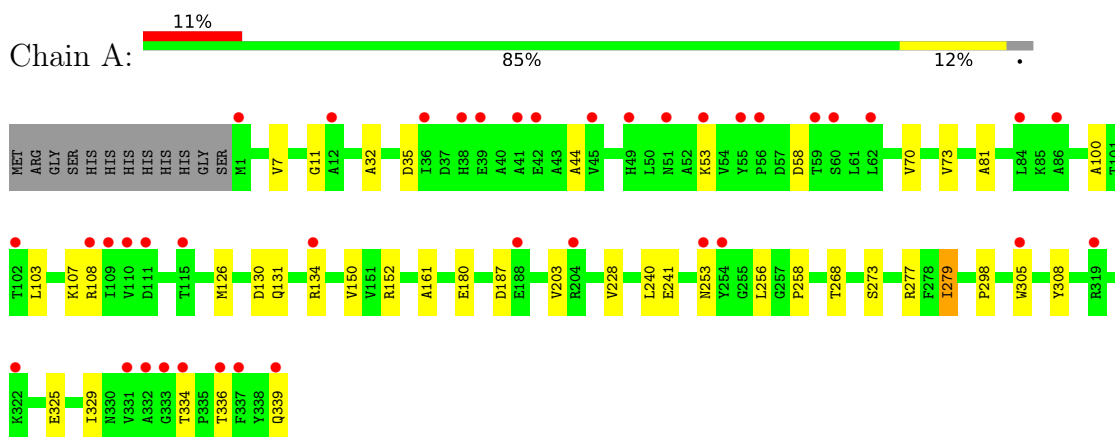
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total 212	O 212	0	0
5	B	271	Total 271	O 271	0	0
5	C	271	Total 271	O 271	0	0
5	D	298	Total 298	O 298	0	0

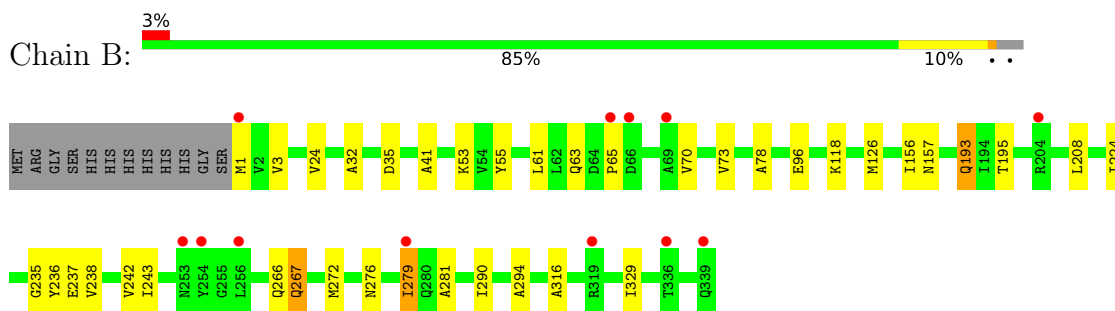
3 Residue-property plots [i](#)

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.

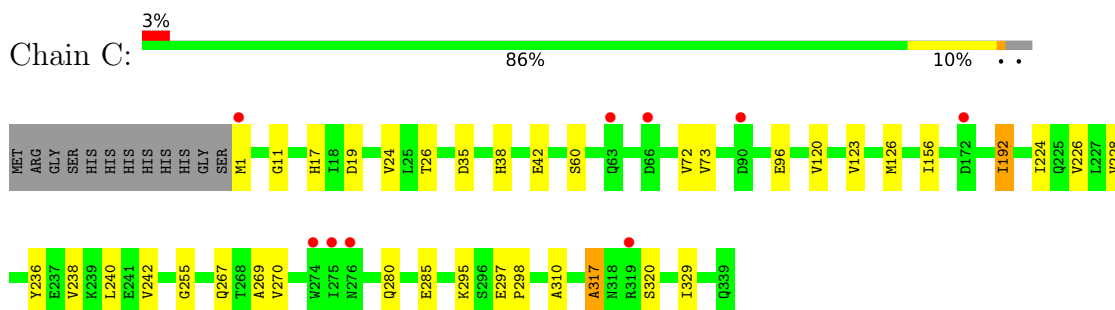
- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase



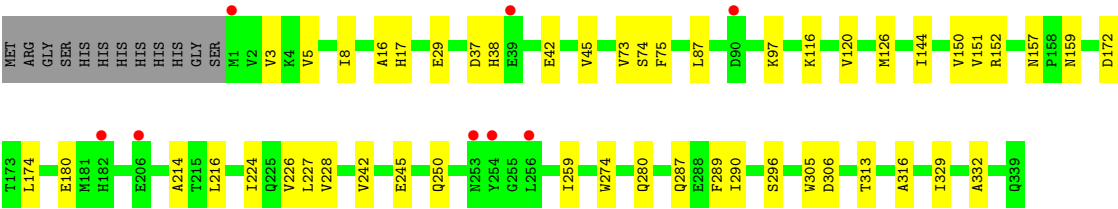
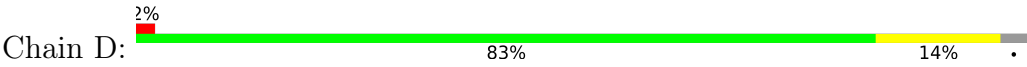
- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase



- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase



- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.56Å 110.51Å 127.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 – 1.60 45.76 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.76-1.60) 100.0 (45.76-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.184 , 0.214 0.184 , 0.214	Depositor DCC
R_{free} test set	9934 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11838	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: NAD, SO4, GOL

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	1.79	24/2685 (0.9%)	0.95	0/3656
1	B	1.79	21/2686 (0.8%)	0.93	3/3657 (0.1%)
1	C	1.77	26/2689 (1.0%)	0.89	2/3661 (0.1%)
1	D	1.81	40/2715 (1.5%)	0.88	0/3696
All	All	1.79	111/10775 (1.0%)	0.91	5/14670 (0.0%)

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	PRO	C-O	-7.99	1.18	1.25
1	D	224	ILE	C-O	-6.63	1.17	1.24
1	A	161	ALA	CA-CB	-6.58	1.42	1.53
1	D	332	ALA	CA-CB	-6.51	1.42	1.53
1	D	151	VAL	C-O	-6.47	1.17	1.24
1	A	298	PRO	C-O	-6.44	1.19	1.25
1	D	5	VAL	C-O	-6.44	1.16	1.24
1	D	226	VAL	C-O	-6.39	1.17	1.24
1	B	156	ILE	C-O	-6.36	1.17	1.24
1	C	238	VAL	C-O	-6.22	1.17	1.24
1	A	32	ALA	CA-CB	-6.19	1.43	1.53
1	A	241	GLU	C-O	-6.13	1.17	1.23
1	D	29	GLU	C-O	-5.99	1.17	1.23
1	A	228	VAL	C-O	-5.96	1.17	1.24
1	A	180	GLU	C-O	-5.89	1.17	1.24
1	C	329	ILE	C-O	-5.89	1.18	1.24
1	B	61	LEU	C-O	-5.85	1.17	1.24
1	D	306	ASP	C-O	-5.85	1.17	1.24
1	A	150	VAL	C-O	-5.83	1.18	1.24
1	D	289	PHE	C-O	-5.82	1.17	1.24
1	B	238	VAL	C-O	-5.82	1.17	1.24
1	D	214	ALA	C-O	-5.80	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	VAL	C-O	-5.79	1.18	1.24
1	C	120	VAL	C-O	-5.78	1.17	1.24
1	C	19	ASP	C-O	-5.77	1.17	1.24
1	C	123	VAL	C-O	-5.73	1.17	1.24
1	A	44	ALA	CA-CB	-5.72	1.44	1.53
1	A	325	GLU	C-O	-5.67	1.17	1.23
1	B	316	ALA	C-O	-5.64	1.17	1.24
1	A	130	ASP	C-O	-5.63	1.17	1.23
1	D	228	VAL	C-O	-5.60	1.18	1.24
1	D	329	ILE	C-O	-5.58	1.18	1.24
1	B	237	GLU	C-O	-5.57	1.17	1.23
1	D	16	ALA	C-O	-5.55	1.17	1.24
1	D	316	ALA	C-O	-5.54	1.17	1.24
1	C	310	ALA	C-O	-5.53	1.17	1.24
1	D	227	LEU	C-O	-5.53	1.17	1.24
1	B	70	VAL	CA-CB	-5.52	1.47	1.54
1	C	224	ILE	C-O	-5.52	1.18	1.24
1	C	255	GLY	C-O	-5.52	1.19	1.23
1	D	180	GLU	C-O	-5.50	1.17	1.24
1	D	214	ALA	CA-CB	-5.49	1.45	1.53
1	D	305	TRP	C-O	-5.49	1.17	1.24
1	A	203	VAL	C-O	-5.46	1.18	1.24
1	C	317	ALA	C-O	-5.45	1.17	1.24
1	C	72	VAL	C-O	-5.44	1.18	1.24
1	D	150	VAL	C-O	-5.44	1.18	1.24
1	B	32	ALA	CA-CB	-5.43	1.44	1.53
1	C	320	SER	C-O	-5.43	1.17	1.24
1	A	11	GLY	C-O	-5.43	1.18	1.24
1	D	242	VAL	C-O	-5.43	1.18	1.24
1	B	3	VAL	C-O	-5.42	1.18	1.24
1	D	8	ILE	C-O	-5.41	1.18	1.24
1	A	70	VAL	C-O	-5.40	1.18	1.24
1	C	269	ALA	CA-CB	-5.39	1.44	1.53
1	C	156	ILE	C-O	-5.39	1.18	1.24
1	C	192	ILE	C-O	-5.39	1.18	1.23
1	D	245	GLU	C-O	-5.38	1.17	1.24
1	D	17	HIS	C-O	-5.38	1.17	1.24
1	C	226	VAL	C-O	-5.34	1.18	1.24
1	A	273	SER	C-O	-5.34	1.18	1.24
1	D	157	ASN	C-O	-5.33	1.17	1.24
1	C	228	VAL	C-O	-5.32	1.18	1.24
1	B	78	ALA	CA-CB	-5.30	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	ILE	C-O	-5.29	1.18	1.24
1	D	120	VAL	C-O	-5.27	1.17	1.24
1	A	277	ARG	C-O	-5.26	1.18	1.24
1	B	208	LEU	C-O	-5.25	1.17	1.24
1	A	258	PRO	C-O	-5.25	1.17	1.23
1	D	216	LEU	C-O	-5.25	1.17	1.24
1	D	250	GLN	C-O	-5.25	1.17	1.23
1	A	268	THR	C-O	-5.23	1.17	1.23
1	D	37	ASP	C-O	-5.22	1.17	1.23
1	A	329	ILE	C-O	-5.22	1.18	1.24
1	C	240	LEU	C-O	-5.21	1.17	1.23
1	B	41	ALA	CA-CB	-5.21	1.45	1.53
1	D	152	ARG	C-O	-5.21	1.17	1.24
1	C	11	GLY	C-O	-5.20	1.18	1.24
1	D	259	ILE	C-O	-5.17	1.18	1.24
1	D	313	THR	C-O	-5.17	1.18	1.24
1	A	187	ASP	C-O	-5.16	1.17	1.23
1	C	236	TYR	C-O	-5.16	1.17	1.24
1	A	100	ALA	CA-CB	-5.15	1.44	1.53
1	A	240	LEU	C-O	-5.15	1.18	1.23
1	B	193[A]	GLN	C-O	-5.14	1.18	1.23
1	B	193[B]	GLN	C-O	-5.14	1.18	1.23
1	D	45	VAL	C-O	-5.14	1.18	1.24
1	B	243	ILE	C-O	-5.13	1.18	1.24
1	A	7	VAL	C-O	-5.13	1.18	1.24
1	C	17	HIS	C-O	-5.13	1.18	1.24
1	D	144	ILE	CG1-CD1	-5.13	1.31	1.51
1	B	329	ILE	C-O	-5.12	1.18	1.24
1	A	152	ARG	C-O	-5.11	1.17	1.24
1	C	270	VAL	C-O	-5.11	1.18	1.24
1	D	159[A]	ASN	C-O	-5.09	1.17	1.23
1	D	159[B]	ASN	C-O	-5.09	1.17	1.23
1	D	75	PHE	C-O	-5.09	1.17	1.23
1	B	235	GLY	C-O	-5.06	1.16	1.24
1	B	236	TYR	C-O	-5.06	1.17	1.24
1	D	280	GLN	C-O	-5.06	1.18	1.24
1	B	157	ASN	C-O	-5.05	1.18	1.24
1	C	60[A]	SER	C-O	-5.05	1.18	1.24
1	C	60[B]	SER	C-O	-5.05	1.18	1.24
1	C	280	GLN	C-O	-5.05	1.18	1.24
1	A	81	ALA	CA-CB	-5.05	1.45	1.53
1	D	287	GLN	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	VAL	C-O	-5.02	1.18	1.24
1	B	281	ALA	C-O	-5.01	1.18	1.24
1	B	242	VAL	C-O	-5.01	1.18	1.24
1	D	290	ILE	C-O	-5.01	1.18	1.24
1	D	174	LEU	C-O	-5.00	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ILE	CB-CA-C	-8.14	101.46	111.88
1	B	24	VAL	CB-CA-C	-6.32	105.43	111.05
1	C	24	VAL	CB-CA-C	-5.58	106.09	111.05
1	B	267	GLN	N-CA-C	5.18	116.94	109.07
1	C	267	GLN	N-CA-C	5.04	116.73	109.07

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	2632	0	2624	8	0
1	B	2633	0	2628	15	0
1	C	2633	0	2630	7	0
1	D	2652	0	2652	4	0
2	A	44	0	24	1	0
2	B	44	0	24	2	0
2	C	44	0	25	2	0
2	D	44	0	24	1	0
3	A	12	0	16	2	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	15	0	0	0	0
4	C	10	0	0	1	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	212	0	0	1	0
5	B	271	0	0	0	0
5	C	271	0	0	0	0
5	D	298	0	0	0	0
All	All	11838	0	10671	34	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 2.

All (34) 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:193[B]:GLN:HE22	1:B:195:THR:HG23	1.27	0.99
1:C:26:THR:OG1	4:C:404:SO4:O2	1.98	0.80
1:B:193[B]:GLN:HE22	1:B:195:THR:CG2	1.99	0.76
1:B:193[B]:GLN:NE2	1:B:195:THR:HG23	2.01	0.76
1:D:38[B]:HIS:HD2	1:D:42:GLU:OE2	1.71	0.73
1:C:38:HIS:HD2	1:C:42:GLU:OE1	1.85	0.60
1:B:1:MET:HE3	1:B:294:ALA:HB1	1.83	0.59
1:A:131:GLN:HG2	1:A:134:ARG:NH2	2.20	0.57
1:C:295:LYS:HE3	1:C:297:GLU:CD	2.29	0.57
3:A:402:GOL:H32	1:B:266:GLN:HG2	1.87	0.56
1:B:53:LYS:HE3	1:B:55:TYR:CE1	2.42	0.55
1:A:35:ASP:OD2	2:A:401:NAD:O3B	2.26	0.54
1:B:53:LYS:HE3	1:B:55:TYR:CZ	2.46	0.50
1:C:192:ILE:HD13	1:C:317:ALA:HB2	1.94	0.50
1:A:305:TRP:CD1	1:A:334:THR:HG23	2.48	0.49
1:C:35:ASP:OD2	2:C:401:NAD:O3B	2.28	0.49
1:B:276:ASN:O	1:B:279:ILE:HG12	2.14	0.46
1:B:96:GLU:HB3	2:B:401:NAD:H1D	1.97	0.46
1:A:131:GLN:HG2	1:A:134:ARG:HH22	1.82	0.44
1:C:38:HIS:CD2	1:C:42:GLU:OE1	2.69	0.43
1:B:1:MET:O	1:B:1:MET:HG2	2.18	0.43
1:B:63:GLN:O	1:B:65:PRO:HD3	2.19	0.43
1:D:274:TRP:CD1	1:D:274:TRP:H	2.37	0.42
1:C:96:GLU:HB3	2:C:401:NAD:H1D	2.02	0.42
3:A:402:GOL:H2	1:B:267:GLN:HA	2.02	0.42
1:D:74:SER:O	2:D:401:NAD:H4D	2.19	0.42
1:A:107:LYS:HD3	1:A:308:TYR:CZ	2.54	0.42
1:B:35:ASP:OD2	2:B:401:NAD:O3B	2.38	0.42
1:B:272:MET:HE3	1:B:272:MET:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:O	1:D:116:LYS:HE3	2.20	0.41
1:B:290:ILE:HD13	1:B:290:ILE:HA	1.87	0.41
1:A:279:ILE:HG12	5:A:541:HOH:O	2.22	0.40
1:A:58:ASP:OD1	1:A:58:ASP:N	2.51	0.40
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.82	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	339/351 (97%)	331 (98%)	8 (2%)	0	100	100
1	B	339/351 (97%)	330 (97%)	9 (3%)	0	100	100
1	C	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
1	D	342/351 (97%)	332 (97%)	10 (3%)	0	100	100
All	All	1360/1404 (97%)	1325 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	284/292 (97%)	274 (96%)	10 (4%)	32	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	284/292 (97%)	281 (99%)	3 (1%)	65	46
1	C	285/292 (98%)	281 (99%)	4 (1%)	59	38
1	D	287/292 (98%)	282 (98%)	5 (2%)	53	30
All	All	1140/1168 (98%)	1118 (98%)	22 (2%)	48	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	73	VAL
1	A	103	LEU
1	A	108	ARG
1	A	126	MET
1	A	253	ASN
1	A	256	LEU
1	A	279	ILE
1	A	336	THR
1	A	339	GLN
1	B	73	VAL
1	B	118	LYS
1	B	126	MET
1	C	1	MET
1	C	73	VAL
1	C	126	MET
1	C	285	GLU
1	D	73	VAL
1	D	97	LYS
1	D	126	MET
1	D	172	ASP
1	D	296	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	233	GLN
1	A	266	GLN
1	A	318	ASN
1	B	131	GLN
1	B	318	ASN

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Mol	Chain	Res	Type
1	B	339	GLN
1	C	38	HIS
1	C	131	GLN
1	C	159	ASN
1	C	233	GLN
1	C	276	ASN
1	C	339	GLN
1	D	49	HIS
1	D	266	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](#)

15 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	GOL	C	402	-	5,5,5	0.71	0	5,5,5	0.40	0
3	GOL	B	402	-	5,5,5	0.96	0	5,5,5	0.44	0
3	GOL	A	402	-	5,5,5	0.66	0	5,5,5	1.10	0
4	SO4	A	406	-	4,4,4	0.67	0	6,6,6	0.44	0
4	SO4	A	404	-	4,4,4	0.76	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	403	-	4,4,4	0.62	0	6,6,6	0.37	0
2	NAD	B	401	-	46,48,48	2.66	20 (43%)	64,73,73	3.78	32 (50%)
4	SO4	D	403	-	4,4,4	0.65	0	6,6,6	0.41	0
4	SO4	A	405	-	4,4,4	0.60	0	6,6,6	0.21	0
4	SO4	C	404	-	4,4,4	0.40	0	6,6,6	0.62	0
2	NAD	A	401	-	46,48,48	2.50	19 (41%)	64,73,73	3.71	31 (48%)
3	GOL	A	403	-	5,5,5	0.73	0	5,5,5	0.75	0
3	GOL	D	402	-	5,5,5	0.74	0	5,5,5	0.42	0
2	NAD	C	401	-	46,48,48	2.43	19 (41%)	64,73,73	3.67	28 (43%)
2	NAD	D	401	-	46,48,48	2.73	21 (45%)	64,73,73	3.69	28 (43%)

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	GOL	C	402	-	-	2/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	A	402	-	-	4/4/4/4	-
2	NAD	B	401	-	-	7/30/62/62	0/5/5/5
2	NAD	A	401	-	-	7/30/62/62	0/5/5/5
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	D	402	-	-	0/4/4/4	-
2	NAD	C	401	-	-	11/30/62/62	0/5/5/5
2	NAD	D	401	-	-	10/30/62/62	0/5/5/5

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAD	PN-O3	-8.69	1.50	1.59
2	D	401	NAD	PN-O3	-8.23	1.50	1.59
2	B	401	NAD	C3N-C7N	-7.79	1.39	1.50
2	D	401	NAD	C3N-C7N	-7.65	1.39	1.50
2	C	401	NAD	C3N-C7N	-7.18	1.39	1.50
2	C	401	NAD	PN-O3	-6.86	1.52	1.59
2	A	401	NAD	PA-O3	-6.01	1.53	1.59
2	A	401	NAD	O3B-C3B	-5.80	1.28	1.43
2	A	401	NAD	C3N-C7N	-5.15	1.42	1.50
2	A	401	NAD	C5A-N7A	-4.94	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAD	PA-O3	-4.90	1.54	1.59
2	A	401	NAD	C8A-N9A	-4.74	1.29	1.37
2	A	401	NAD	C5A-C4A	-4.60	1.30	1.39
2	C	401	NAD	C5A-N7A	-4.52	1.30	1.39
2	B	401	NAD	C8A-N9A	-4.26	1.30	1.37
2	A	401	NAD	C2N-N1N	4.18	1.39	1.35
2	D	401	NAD	C5A-N7A	-4.17	1.31	1.39
2	D	401	NAD	O3B-C3B	-4.08	1.32	1.43
2	C	401	NAD	O3D-C3D	-3.99	1.33	1.43
2	D	401	NAD	C8A-N9A	-3.91	1.30	1.37
2	B	401	NAD	C5A-C4A	-3.67	1.32	1.39
2	B	401	NAD	C5A-N7A	-3.67	1.32	1.39
2	D	401	NAD	O3D-C3D	-3.66	1.33	1.43
2	C	401	NAD	PN-O2N	-3.52	1.39	1.55
2	D	401	NAD	C5A-C4A	-3.51	1.32	1.39
2	D	401	NAD	C2B-C3B	-3.39	1.44	1.53
2	C	401	NAD	C4A-N9A	-3.37	1.30	1.37
2	B	401	NAD	O3D-C3D	-3.31	1.34	1.43
2	A	401	NAD	C4A-N9A	-3.31	1.30	1.37
2	D	401	NAD	C4A-N9A	-3.28	1.30	1.37
2	B	401	NAD	O3B-C3B	-3.26	1.34	1.43
2	B	401	NAD	C4A-N9A	-3.18	1.31	1.37
2	B	401	NAD	PA-O2A	-3.05	1.41	1.55
2	A	401	NAD	PA-O2A	-3.03	1.41	1.55
2	C	401	NAD	PA-O1A	-3.03	1.40	1.50
2	A	401	NAD	PN-O2N	-3.00	1.41	1.55
2	B	401	NAD	PA-O1A	-2.98	1.40	1.50
2	C	401	NAD	C5A-C4A	-2.95	1.33	1.39
2	C	401	NAD	C8A-N9A	-2.93	1.32	1.37
2	D	401	NAD	PN-O2N	-2.89	1.41	1.55
2	A	401	NAD	O2D-C2D	-2.89	1.35	1.43
2	B	401	NAD	O4B-C4B	2.83	1.51	1.45
2	D	401	NAD	PA-O2A	-2.79	1.42	1.55
2	C	401	NAD	O4D-C1D	-2.77	1.37	1.40
2	C	401	NAD	C2N-N1N	2.76	1.38	1.35
2	C	401	NAD	PN-O1N	-2.74	1.41	1.50
2	B	401	NAD	PN-O2N	-2.69	1.42	1.55
2	B	401	NAD	PN-O1N	-2.69	1.41	1.50
2	C	401	NAD	PA-O2A	-2.68	1.42	1.55
2	A	401	NAD	PN-O5D	-2.67	1.48	1.59
2	C	401	NAD	PA-O5B	-2.66	1.49	1.59
2	D	401	NAD	O4D-C1D	-2.64	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C5A-C6A	-2.62	1.33	1.41
2	D	401	NAD	PN-O1N	-2.61	1.41	1.50
2	B	401	NAD	O4D-C1D	-2.58	1.37	1.40
2	D	401	NAD	C4A-N3A	-2.48	1.29	1.34
2	B	401	NAD	C5A-C6A	-2.46	1.34	1.41
2	B	401	NAD	PA-O5B	-2.45	1.49	1.59
2	A	401	NAD	O3D-C3D	-2.45	1.36	1.43
2	D	401	NAD	C5A-C6A	-2.39	1.34	1.41
2	C	401	NAD	C5A-C6A	-2.38	1.34	1.41
2	C	401	NAD	O3B-C3B	-2.34	1.37	1.43
2	B	401	NAD	PA-O3	-2.31	1.57	1.59
2	D	401	NAD	O4B-C4B	2.23	1.50	1.45
2	A	401	NAD	PA-O1A	-2.23	1.43	1.50
2	B	401	NAD	C2A-N1A	2.23	1.37	1.33
2	A	401	NAD	C6A-N6A	-2.20	1.28	1.34
2	B	401	NAD	C2D-C3D	-2.20	1.47	1.53
2	C	401	NAD	C4A-N3A	-2.19	1.30	1.34
2	A	401	NAD	O4D-C1D	-2.18	1.38	1.40
2	B	401	NAD	C1B-N9A	2.16	1.52	1.46
2	D	401	NAD	PA-O5B	-2.14	1.51	1.59
2	D	401	NAD	C6A-N1A	-2.13	1.29	1.35
2	D	401	NAD	PA-O1A	-2.12	1.43	1.50
2	A	401	NAD	PN-O1N	-2.10	1.43	1.50
2	A	401	NAD	C2A-N3A	2.08	1.37	1.33
2	C	401	NAD	C3B-C4B	-2.06	1.47	1.53
2	C	401	NAD	C7N-N7N	-2.03	1.29	1.33
2	D	401	NAD	C1B-N9A	2.01	1.51	1.46

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	O4B-C1B-C2B	-15.13	74.24	106.62
2	B	401	NAD	O4B-C1B-C2B	-13.81	77.07	106.62
2	C	401	NAD	O4B-C1B-C2B	-12.79	79.23	106.62
2	D	401	NAD	O4B-C1B-C2B	-12.75	79.32	106.62
2	A	401	NAD	O4B-C4B-C5B	-9.98	77.36	109.33
2	A	401	NAD	O4D-C4D-C5D	-9.83	77.86	109.33
2	C	401	NAD	O4D-C4D-C3D	-9.49	86.32	105.15
2	B	401	NAD	O4D-C4D-C5D	-9.31	79.53	109.33
2	C	401	NAD	O4D-C4D-C5D	-9.18	79.92	109.33
2	D	401	NAD	O4D-C4D-C3D	-9.07	87.16	105.15
2	D	401	NAD	O4D-C4D-C5D	-8.94	80.69	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	O4D-C4D-C3D	-8.87	87.55	105.15
2	B	401	NAD	O4B-C4B-C5B	-8.74	81.32	109.33
2	D	401	NAD	O4B-C4B-C5B	-8.29	82.77	109.33
2	C	401	NAD	O4B-C4B-C5B	-8.21	83.05	109.33
2	C	401	NAD	O4B-C4B-C3B	-8.20	88.87	105.15
2	A	401	NAD	O4D-C4D-C3D	-8.20	88.88	105.15
2	D	401	NAD	O4B-C4B-C3B	-7.79	89.68	105.15
2	B	401	NAD	O4B-C4B-C3B	-7.59	90.09	105.15
2	A	401	NAD	O4B-C4B-C3B	-7.17	90.92	105.15
2	D	401	NAD	C4D-O4D-C1D	7.11	116.44	109.92
2	B	401	NAD	N3A-C2A-N1A	-6.63	118.54	128.58
2	C	401	NAD	C4D-O4D-C1D	6.59	115.96	109.92
2	D	401	NAD	C6N-N1N-C2N	-6.56	116.30	121.88
2	C	401	NAD	C5B-C4B-C3B	6.35	138.08	115.21
2	D	401	NAD	C5B-C4B-C3B	6.33	138.01	115.21
2	A	401	NAD	N3A-C2A-N1A	-6.08	119.38	128.58
2	B	401	NAD	C6N-N1N-C2N	-6.06	116.72	121.88
2	B	401	NAD	C5B-C4B-C3B	5.71	135.77	115.21
2	A	401	NAD	C6N-N1N-C2N	-5.58	117.13	121.88
2	B	401	NAD	C4D-O4D-C1D	5.37	114.85	109.92
2	B	401	NAD	O3B-C3B-C2B	5.35	128.96	111.82
2	C	401	NAD	C3B-C2B-C1B	-5.34	91.35	101.46
2	A	401	NAD	C5A-C4A-N3A	-5.32	119.39	126.72
2	D	401	NAD	C3B-C2B-C1B	-5.11	91.79	101.46
2	C	401	NAD	O3B-C3B-C2B	4.99	127.82	111.82
2	C	401	NAD	C6N-N1N-C2N	-4.95	117.67	121.88
2	D	401	NAD	C5A-C4A-N3A	-4.95	119.90	126.72
2	A	401	NAD	C5B-C4B-C3B	4.94	133.00	115.21
2	B	401	NAD	C5A-C4A-N3A	-4.94	119.91	126.72
2	D	401	NAD	N3A-C2A-N1A	-4.85	121.25	128.58
2	C	401	NAD	C5A-C4A-N3A	-4.82	120.08	126.72
2	B	401	NAD	C5D-C4D-C3D	4.81	132.52	115.21
2	D	401	NAD	C5D-C4D-C3D	4.80	132.48	115.21
2	A	401	NAD	C5D-C4D-C3D	4.77	132.39	115.21
2	C	401	NAD	N3A-C2A-N1A	-4.68	121.50	128.58
2	B	401	NAD	C5A-C4A-N9A	4.54	110.76	105.81
2	C	401	NAD	C5A-C4A-N9A	4.48	110.70	105.81
2	D	401	NAD	O3B-C3B-C2B	4.45	126.09	111.82
2	B	401	NAD	C3B-C2B-C1B	-4.39	93.16	101.46
2	D	401	NAD	C5A-C4A-N9A	4.35	110.55	105.81
2	A	401	NAD	C5A-C4A-N9A	4.22	110.41	105.81
2	B	401	NAD	C4A-C5A-N7A	-4.08	105.92	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	C5D-C4D-C3D	4.02	129.68	115.21
2	B	401	NAD	C2N-N1N-C1D	3.93	127.82	119.13
2	D	401	NAD	O5B-C5B-C4B	-3.64	96.59	108.99
2	C	401	NAD	C2N-N1N-C1D	3.61	127.10	119.13
2	A	401	NAD	C2N-N1N-C1D	3.60	127.07	119.13
2	A	401	NAD	C2A-N3A-C4A	3.58	120.58	111.83
2	B	401	NAD	O5B-C5B-C4B	-3.58	96.81	108.99
2	B	401	NAD	C2A-N3A-C4A	3.50	120.37	111.83
2	D	401	NAD	O2D-C2D-C3D	-3.44	100.79	111.82
2	D	401	NAD	C2N-N1N-C1D	3.39	126.62	119.13
2	C	401	NAD	C4A-C5A-N7A	-3.38	106.72	110.58
2	C	401	NAD	O3D-C3D-C2D	3.37	122.60	111.82
2	C	401	NAD	C2A-N3A-C4A	3.20	119.64	111.83
2	A	401	NAD	PA-O5B-C5B	3.19	139.62	121.35
2	A	401	NAD	C4A-C5A-N7A	-3.19	106.94	110.58
2	D	401	NAD	O2B-C2B-C3B	-3.09	101.91	111.82
2	C	401	NAD	O2B-C2B-C3B	-3.08	101.94	111.82
2	A	401	NAD	O3D-C3D-C2D	3.06	121.62	111.82
2	D	401	NAD	C2A-N3A-C4A	3.03	119.22	111.83
2	A	401	NAD	C3B-C2B-C1B	-2.99	95.81	101.46
2	C	401	NAD	O5B-C5B-C4B	-2.98	98.84	108.99
2	A	401	NAD	C2D-C3D-C4D	-2.95	96.91	102.61
2	A	401	NAD	C2B-C3B-C4B	-2.90	97.00	102.61
2	A	401	NAD	O2D-C2D-C3D	-2.89	102.55	111.82
2	D	401	NAD	O3D-C3D-C2D	2.84	120.93	111.82
2	D	401	NAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	401	NAD	O2D-C2D-C3D	-2.71	103.13	111.82
2	B	401	NAD	C5N-C4N-C3N	-2.69	117.72	120.36
2	A	401	NAD	C4D-O4D-C1D	2.68	112.38	109.92
2	B	401	NAD	C2N-C3N-C4N	2.68	121.38	118.26
2	D	401	NAD	PA-O5B-C5B	2.62	136.37	121.35
2	B	401	NAD	O2B-C2B-C3B	-2.53	103.72	111.82
2	C	401	NAD	C3N-C7N-N7N	-2.53	114.62	117.74
2	D	401	NAD	C2D-C3D-C4D	-2.49	97.80	102.61
2	B	401	NAD	C6A-C5A-C4A	2.48	120.57	117.18
2	D	401	NAD	O5D-C5D-C4D	2.48	117.45	108.99
2	A	401	NAD	O3B-C3B-C2B	2.47	119.73	111.82
2	B	401	NAD	C5A-N7A-C8A	2.43	107.27	103.45
2	C	401	NAD	O4B-C1B-N9A	2.36	112.62	108.09
2	B	401	NAD	N9A-C8A-N7A	-2.34	110.62	113.94
2	B	401	NAD	O5D-C5D-C4D	2.33	116.94	108.99
2	C	401	NAD	C6N-N1N-C1D	-2.33	115.16	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	O2D-C2D-C3D	-2.32	104.39	111.82
2	A	401	NAD	C3N-C7N-N7N	-2.28	114.93	117.74
2	B	401	NAD	O3D-C3D-C2D	2.28	119.11	111.82
2	C	401	NAD	C5A-N7A-C8A	2.26	107.00	103.45
2	D	401	NAD	C3N-C7N-N7N	-2.25	114.96	117.74
2	D	401	NAD	C5N-C6N-N1N	2.21	123.40	120.38
2	D	401	NAD	C6A-C5A-C4A	2.18	120.16	117.18
2	B	401	NAD	C6N-N1N-C1D	-2.18	115.46	119.73
2	A	401	NAD	C5A-N7A-C8A	2.17	106.86	103.45
2	C	401	NAD	PA-O5B-C5B	2.15	133.64	121.35
2	B	401	NAD	C2D-C3D-C4D	-2.14	98.47	102.61
2	A	401	NAD	O2B-C2B-C1B	-2.11	102.83	110.10
2	C	401	NAD	C6A-C5A-C4A	2.11	120.06	117.18
2	B	401	NAD	PA-O5B-C5B	2.09	133.35	121.35
2	B	401	NAD	C5N-C6N-N1N	2.07	123.20	120.38
2	D	401	NAD	O4B-C1B-N9A	2.06	112.05	108.09
2	A	401	NAD	C6A-C5A-C4A	2.06	120.00	117.18
2	A	401	NAD	C6N-N1N-C1D	-2.06	115.69	119.73
2	A	401	NAD	O5B-PA-O1A	2.05	117.06	108.94
2	C	401	NAD	C2D-C3D-C4D	-2.04	98.66	102.61
2	A	401	NAD	C5N-C6N-N1N	2.04	123.16	120.38
2	B	401	NAD	C3N-C7N-N7N	-2.02	115.24	117.74
2	A	401	NAD	N9A-C8A-N7A	-2.01	111.09	113.94
2	A	401	NAD	O5B-C5B-C4B	-2.00	102.17	108.99

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	C5D-O5D-PN-O2N
3	A	402	GOL	O1-C1-C2-C3
3	A	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
2	A	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	C3D-C4D-C5D-O5D
2	C	401	NAD	C3D-C4D-C5D-O5D
3	C	402	GOL	O1-C1-C2-C3
3	A	402	GOL	O1-C1-C2-O2
2	D	401	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C2B-C1B-N9A-C8A
2	B	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C2B-C1B-N9A-C4A
3	C	402	GOL	O1-C1-C2-O2
2	C	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	PA-O3-PN-O1N
2	A	401	NAD	PA-O3-PN-O2N
2	C	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O2N
2	D	401	NAD	C2B-C1B-N9A-C8A
2	B	401	NAD	C2B-C1B-N9A-C4A
2	C	401	NAD	C2B-C1B-N9A-C4A
2	C	401	NAD	C2B-C1B-N9A-C8A
2	D	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	PA-O3-PN-O1N
2	C	401	NAD	PA-O3-PN-O2N

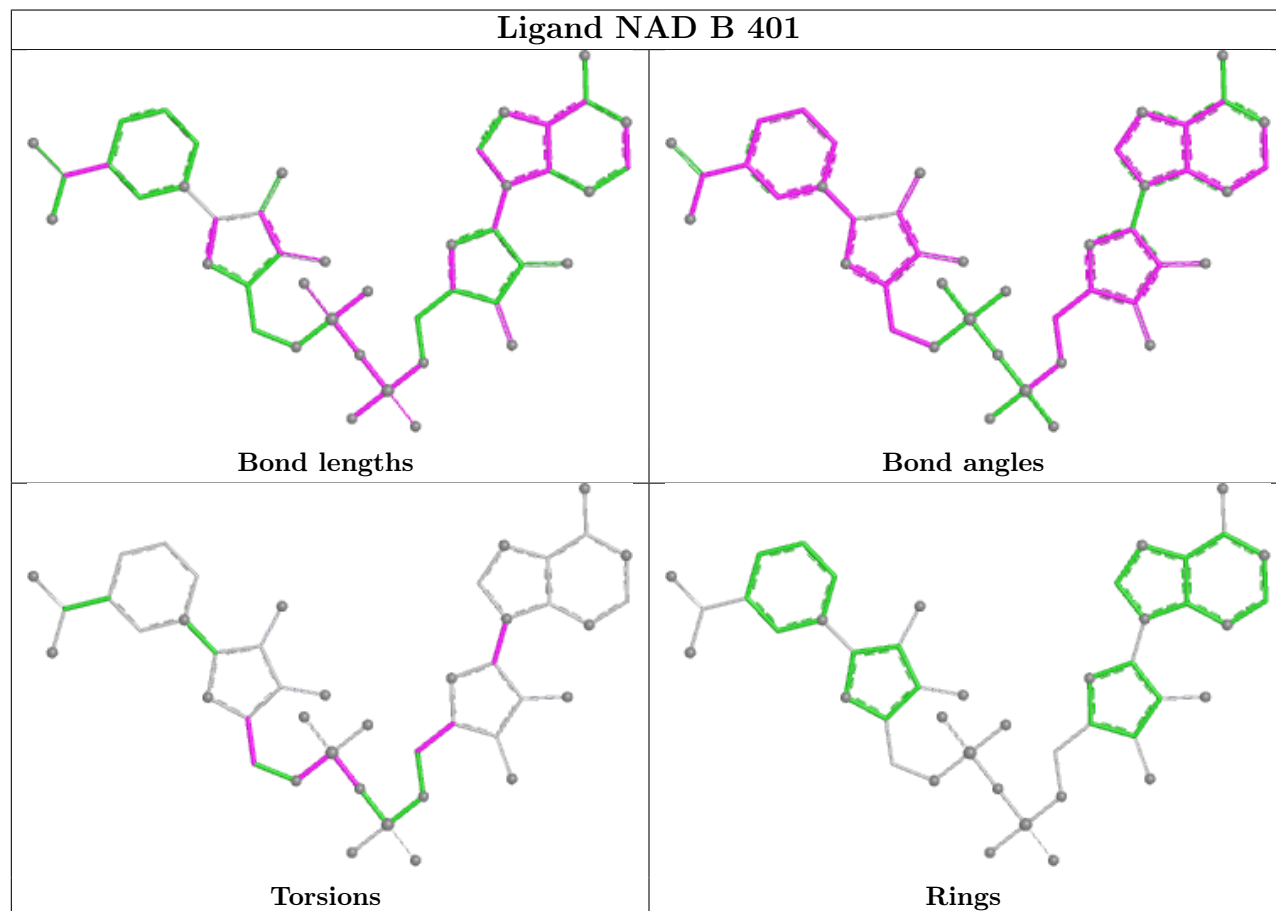
There are no ring outliers.

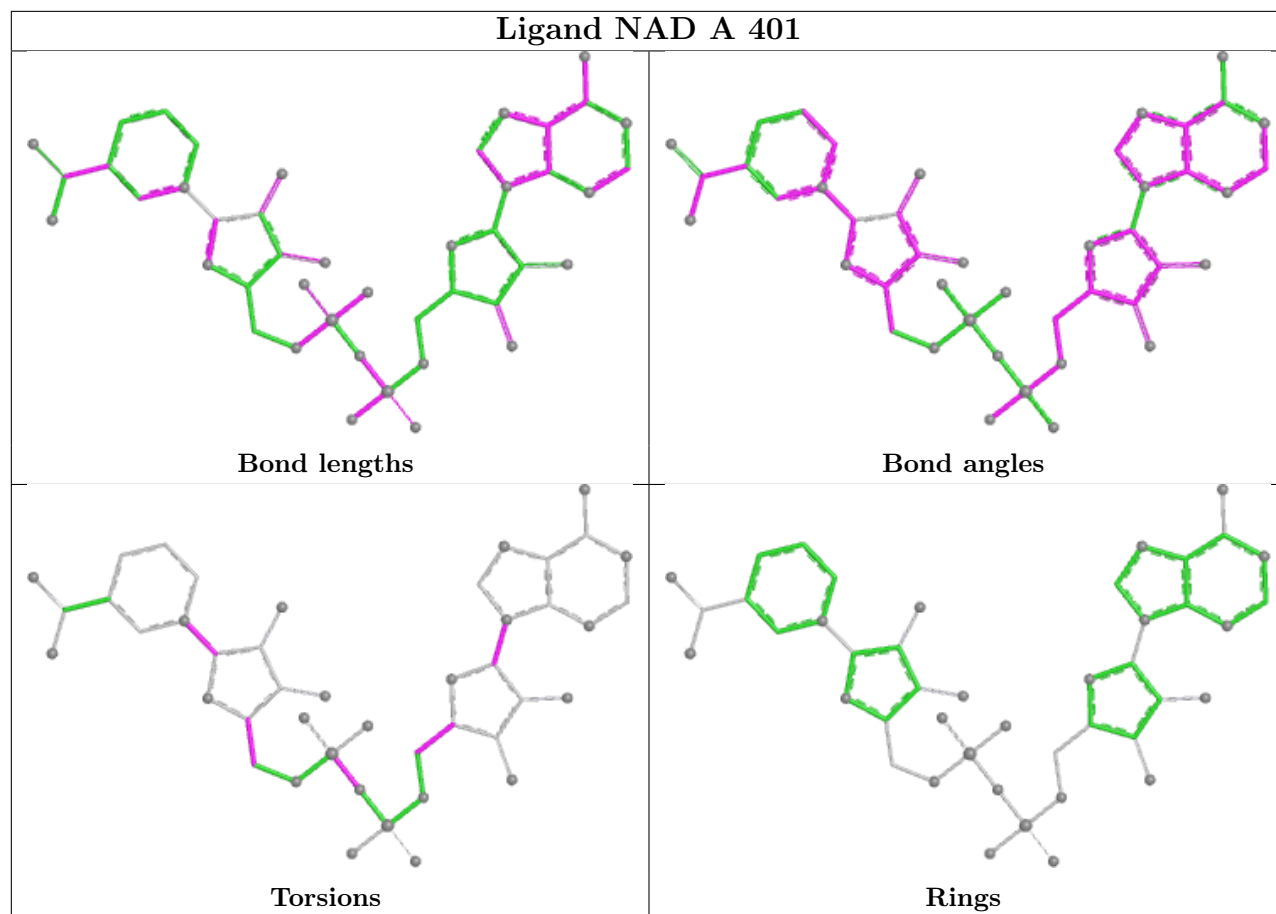
6 monomers are involved in 9 short contacts:

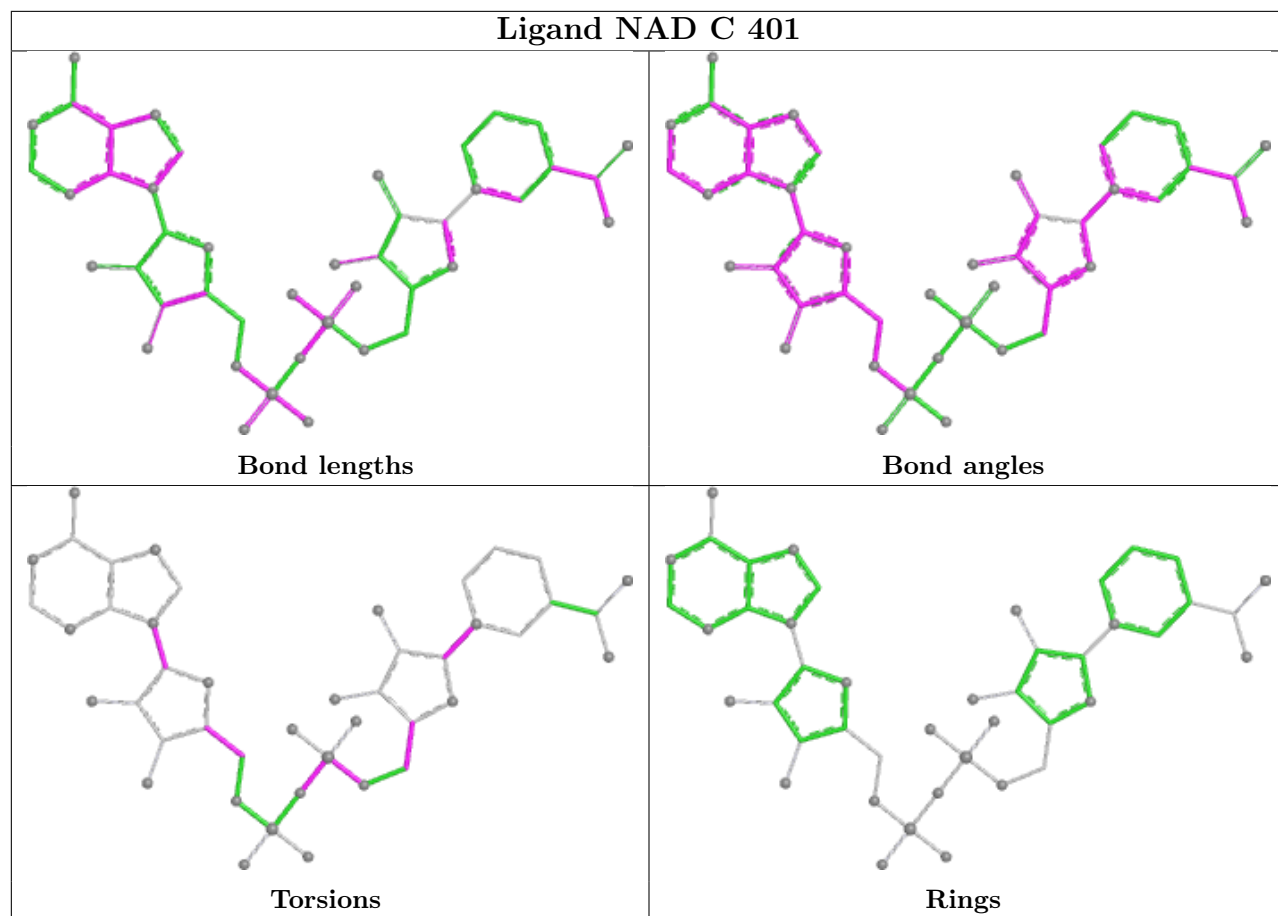
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	2	0
2	B	401	NAD	2	0
4	C	404	SO4	1	0
2	A	401	NAD	1	0
2	C	401	NAD	2	0
2	D	401	NAD	1	0

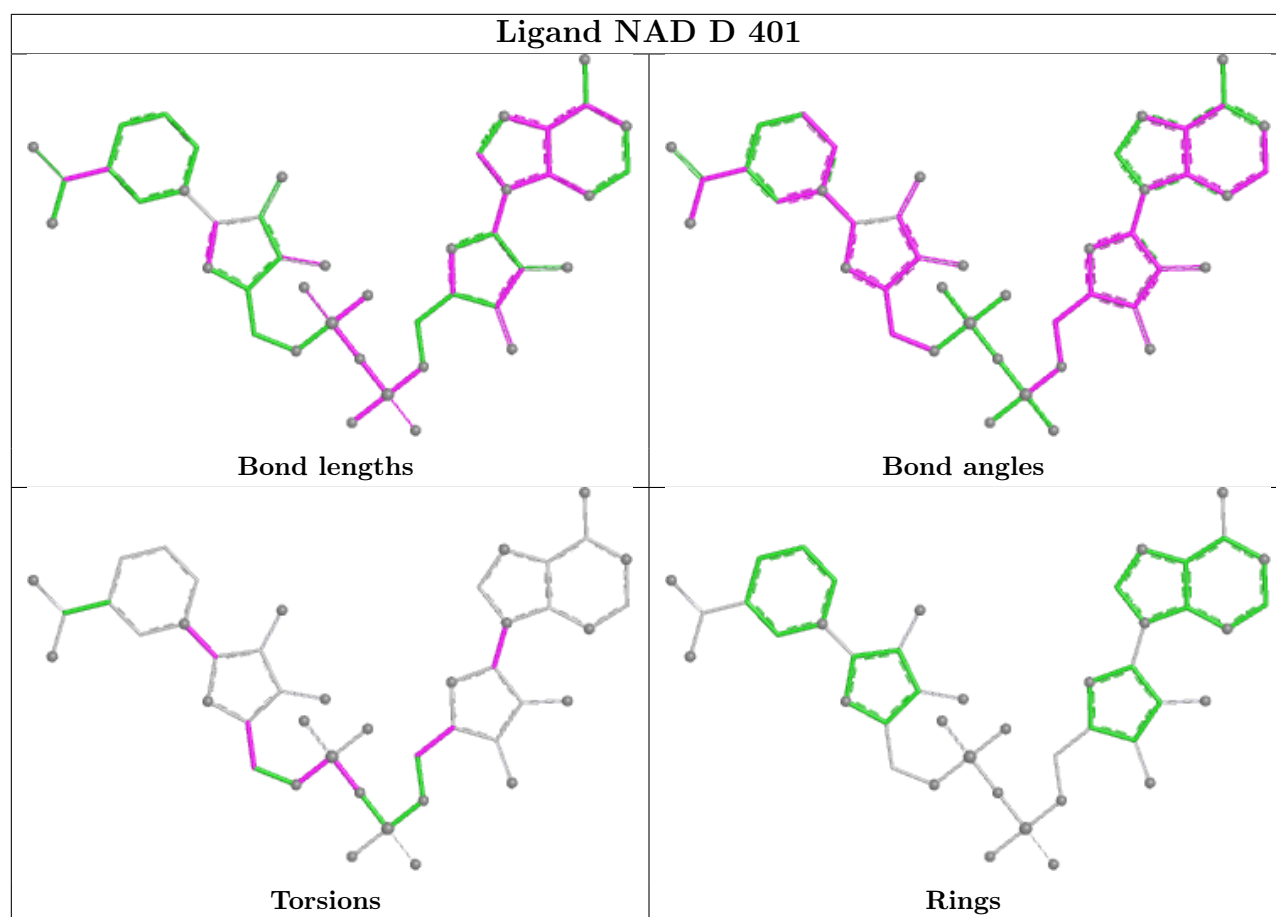
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	339/351 (96%)	0.54	39 (11%) 9 9	14, 23, 37, 54	29 (8%)
1	B	339/351 (96%)	0.22	12 (3%) 47 49	12, 22, 34, 41	20 (5%)
1	C	339/351 (96%)	0.09	9 (2%) 56 59	9, 20, 31, 39	23 (6%)
1	D	339/351 (96%)	-0.07	8 (2%) 59 63	10, 18, 28, 39	24 (7%)
All	All	1356/1404 (96%)	0.19	68 (5%) 34 35	9, 21, 34, 54	96 (7%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	GLY	4.9
1	B	1	MET	4.7
1	C	275	ILE	3.7
1	A	332	ALA	3.5
1	A	331	VAL	3.5
1	D	253	ASN	3.5
1	D	254	TYR	3.5
1	A	253	ASN	3.5
1	D	256	LEU	3.4
1	A	39	GLU	3.4
1	C	1	MET	3.3
1	C	90	ASP	3.3
1	C	274	TRP	3.3
1	A	1	MET	3.1
1	C	276	ASN	3.1
1	A	336	THR	3.1
1	A	51	ASN	2.9
1	D	90	ASP	2.8
1	A	55	TYR	2.8
1	A	109	ILE	2.8
1	B	253	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	38	HIS	2.8
1	A	110	VAL	2.8
1	A	84	LEU	2.7
1	A	337	PHE	2.7
1	B	319	ARG	2.6
1	A	108	ARG	2.6
1	A	134	ARG	2.6
1	A	334	THR	2.5
1	A	56	PRO	2.5
1	C	172	ASP	2.5
1	B	204	ARG	2.5
1	B	66	ASP	2.5
1	A	53	LYS	2.5
1	A	204	ARG	2.4
1	A	115	THR	2.4
1	D	1	MET	2.4
1	C	63	GLN	2.4
1	B	279	ILE	2.4
1	A	188	GLU	2.4
1	A	59	THR	2.4
1	A	36	ILE	2.4
1	D	39	GLU	2.3
1	B	65	PRO	2.3
1	D	182	HIS	2.3
1	A	254	TYR	2.3
1	A	319	ARG	2.3
1	A	86	ALA	2.3
1	A	62	LEU	2.3
1	D	206	GLU	2.3
1	A	322	LYS	2.3
1	C	319	ARG	2.2
1	A	60	SER	2.2
1	C	66	ASP	2.2
1	A	42	GLU	2.2
1	B	256	LEU	2.2
1	A	102	THR	2.2
1	A	41	ALA	2.1
1	A	49	HIS	2.1
1	B	336	THR	2.1
1	B	254	TYR	2.1
1	A	12	ALA	2.1
1	A	111	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	305	TRP	2.1
1	B	69	ALA	2.1
1	B	339	GLN	2.0
1	A	45	VAL	2.0
1	A	339	GLN	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.

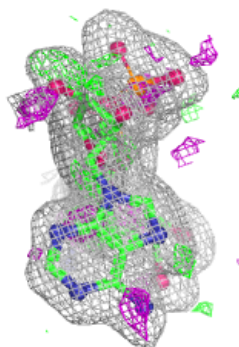
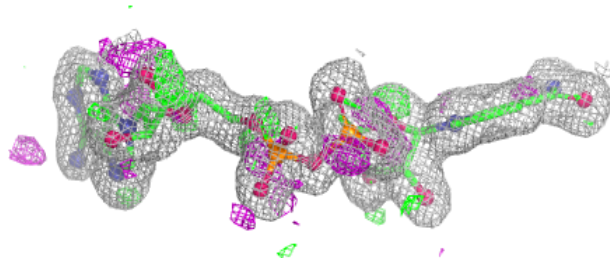
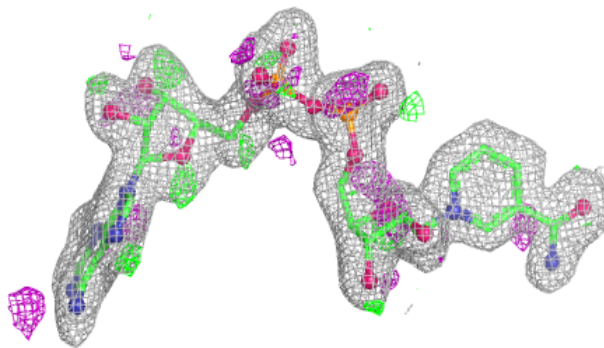
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	404	5/5	0.79	0.18	32,34,37,40	5
3	GOL	A	403	6/6	0.85	0.17	20,21,22,22	6
3	GOL	A	402	6/6	0.86	0.11	31,33,36,37	0
3	GOL	C	402	6/6	0.88	0.11	24,29,29,33	0
3	GOL	B	402	6/6	0.89	0.11	27,28,34,37	0
2	NAD	A	401	44/44	0.90	0.11	23,28,32,36	0
4	SO4	A	405	5/5	0.93	0.12	24,29,34,36	5
2	NAD	B	401	44/44	0.93	0.10	17,21,25,31	0
4	SO4	D	403	5/5	0.93	0.13	26,28,32,33	5
2	NAD	C	401	44/44	0.94	0.09	15,19,23,25	0
3	GOL	D	402	6/6	0.94	0.08	27,30,32,36	0
4	SO4	A	404	5/5	0.94	0.14	23,24,28,28	5
2	NAD	D	401	44/44	0.95	0.08	14,17,20,27	0
4	SO4	C	403	5/5	0.96	0.10	22,23,28,28	5
4	SO4	A	406	5/5	0.97	0.12	19,20,23,25	5

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

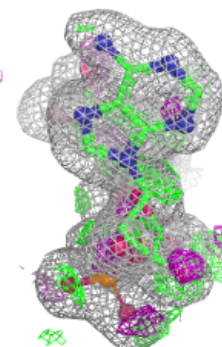
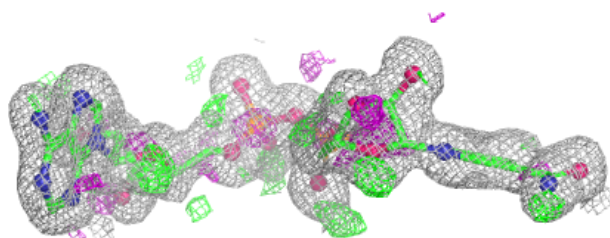
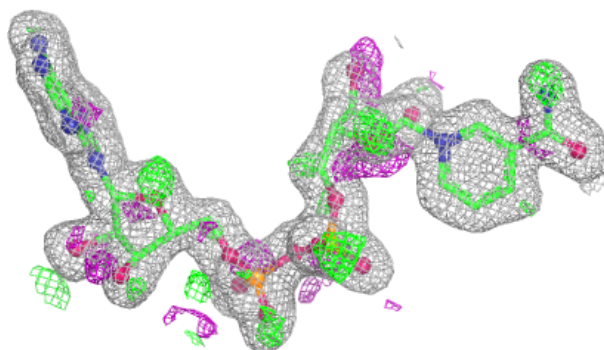
Electron density around NAD A 401:

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



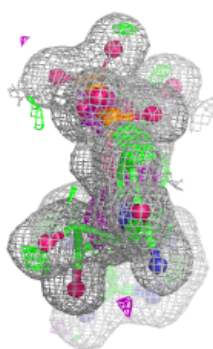
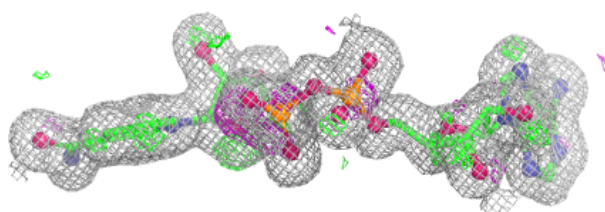
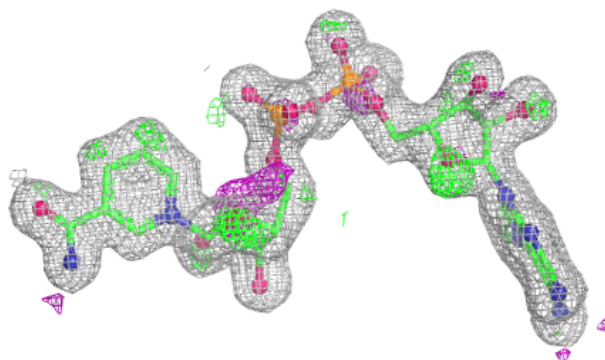
Electron density around NAD B 401:

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

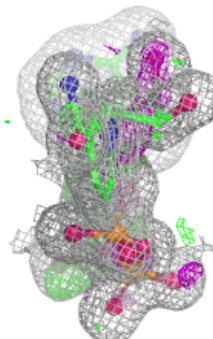
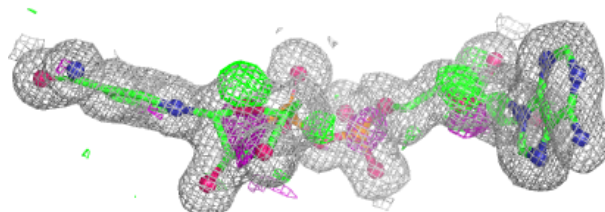
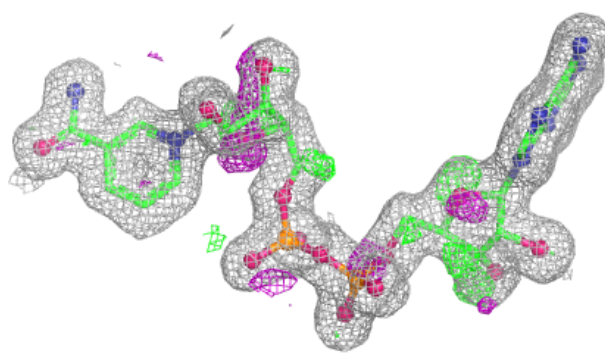


Electron density around NAD C 401:

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

**Electron density around NAD D 401:**

$2mF_o-DF_c$ (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.