



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:09 AM UTC

PDB ID : 2OXI / pdb_00002oxi
Title : REFINED CRYSTAL STRUCTURE OF CU-SUBSTITUTED ALCOHOL
DEHYDROGENASE AT 2.1 ANGSTROMS RESOLUTION
Authors : Al-Karadaghi, S.; Cedergren-Zeppezauer, E.S.
Deposited on : 1993-11-08
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

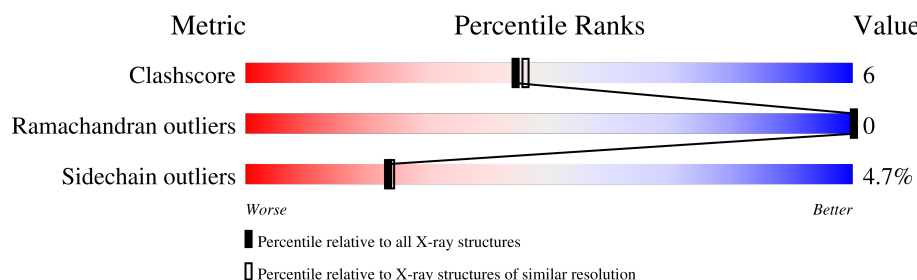
1 Overall quality at a glance

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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	378	-	-	X	-
5	DMS	B	378	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6125 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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	89	3	0
			2791	1772	472	521	26			
1	B	374	Total	C	N	O	S	64	2	0
			2789	1771	472	521	25			

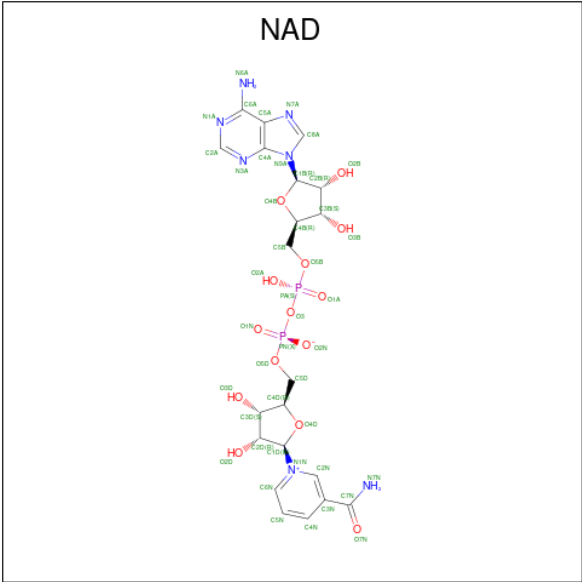
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

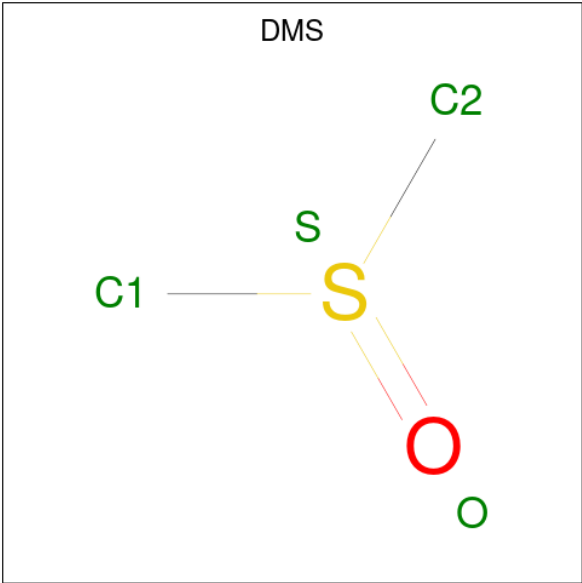
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total 222	O 222	0	0
6	B	223	Total 223	O 223	0	0

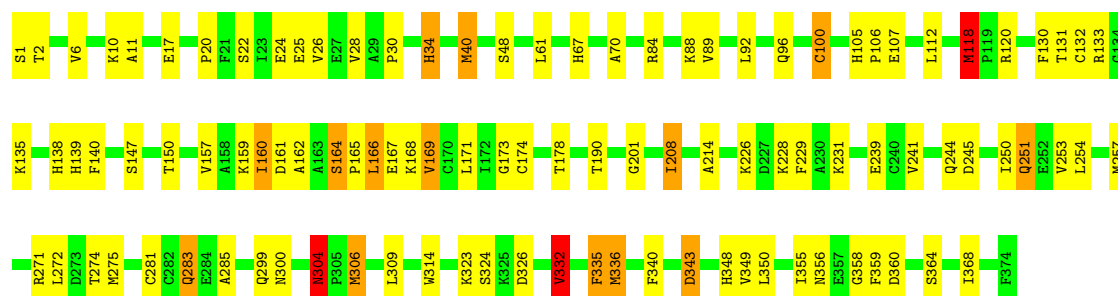
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

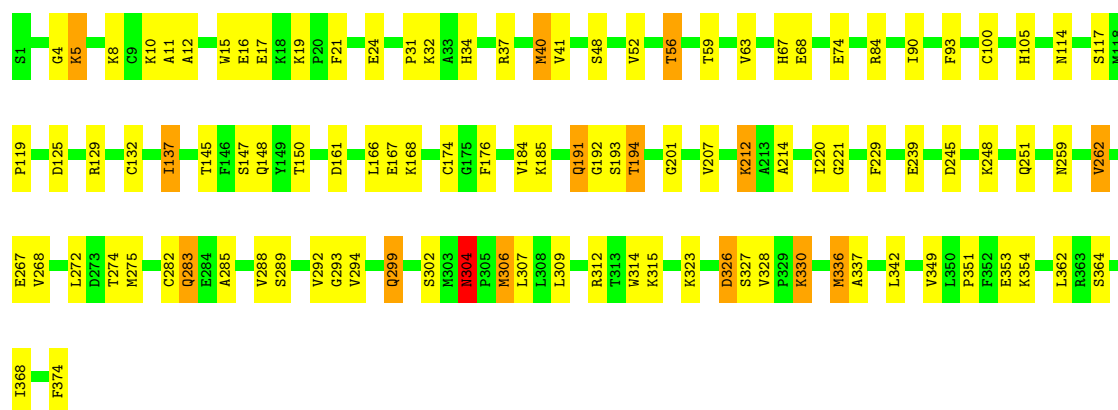
• Molecule 1: ALCOHOL DEHYDROGENASE

Chain A: 



• Molecule 1: ALCOHOL DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.40Å 180.60Å 50.80Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6125	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.27	15/2855 (0.5%)	1.91	71/3858 (1.8%)
1	B	1.33	19/2849 (0.7%)	1.94	76/3850 (2.0%)
All	All	1.30	34/5704 (0.6%)	1.93	147/7708 (1.9%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	THR	C-O	-8.64	1.13	1.23
1	A	161	ASP	N-CA	8.04	1.56	1.46
1	B	184	VAL	CA-CB	7.86	1.64	1.54
1	A	162	ALA	CA-C	-7.66	1.42	1.52
1	B	161	ASP	C-O	-6.72	1.15	1.23
1	A	348	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	34	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	67	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	160	ILE	CA-C	6.44	1.60	1.52
1	A	67	HIS	CD2-NE2	-6.40	1.30	1.37
1	B	105	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	157	VAL	CA-CB	6.19	1.63	1.54
1	A	105	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	221	GLY	CA-C	-5.93	1.48	1.52
1	A	162	ALA	C-N	-5.79	1.25	1.33
1	B	192	GLY	C-N	-5.63	1.25	1.33
1	B	145	THR	CA-CB	5.63	1.62	1.53
1	B	119	PRO	CA-CB	-5.55	1.46	1.53
1	A	138	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	56	THR	CA-CB	5.52	1.62	1.53
1	B	328	VAL	CA-CB	5.52	1.57	1.54
1	A	34	HIS	CD2-NE2	-5.43	1.31	1.37
1	B	90	ILE	CA-CB	5.43	1.59	1.54
1	B	63	VAL	CA-CB	5.38	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	GLU	CA-CB	-5.31	1.45	1.53
1	A	139	HIS	CG-ND1	-5.30	1.32	1.38
1	B	34	HIS	CG-ND1	-5.26	1.32	1.38
1	B	137	ILE	C-O	-5.25	1.17	1.24
1	A	162	ALA	N-CA	-5.25	1.39	1.46
1	B	294	VAL	CA-CB	5.22	1.59	1.53
1	A	355	ILE	CA-CB	5.21	1.60	1.54
1	B	194	THR	N-CA	5.17	1.52	1.46
1	A	67	HIS	CG-ND1	-5.15	1.32	1.38
1	B	293	GLY	CA-C	5.14	1.56	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	MET	CG-SD-CE	-13.65	70.87	100.90
1	B	304	ASN	OD1-CG-ND2	-12.02	110.58	122.60
1	B	74	GLU	N-CA-C	-10.99	99.38	113.12
1	A	283	GLN	OE1-CD-NE2	-9.92	112.68	122.60
1	B	299	GLN	OE1-CD-NE2	-9.56	113.04	122.60
1	A	1	SER	CA-C-O	-9.27	105.03	120.80
1	A	332	VAL	N-CA-C	-8.74	102.31	110.53
1	A	300	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	A	245	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	300	ASN	CB-CG-ND2	8.38	128.97	116.40
1	B	342	LEU	N-CA-C	-8.21	103.72	114.31
1	A	105	HIS	CB-CG-CD2	-8.11	120.66	131.20
1	B	328	VAL	CA-C-N	8.07	127.37	118.97
1	B	328	VAL	C-N-CA	8.07	127.37	118.97
1	A	251	GLN	OE1-CD-NE2	-7.95	114.65	122.60
1	A	360	ASP	CA-CB-CG	7.93	120.53	112.60
1	A	2	THR	N-CA-C	7.91	123.03	113.23
1	B	304	ASN	CB-CG-ND2	7.83	128.15	116.40
1	A	304	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	B	292	VAL	N-CA-C	-7.75	105.61	112.12
1	A	34	HIS	CB-CG-CD2	-7.72	121.16	131.20
1	B	40	MET	CG-SD-CE	-7.59	84.19	100.90
1	A	229	PHE	N-CA-C	7.54	119.50	111.28
1	A	1	SER	CA-CB-OG	-7.51	96.07	111.10
1	B	167	GLU	CA-CB-CG	7.50	129.10	114.10
1	B	330	LYS	N-CA-CB	-7.35	99.31	110.12
1	A	304	ASN	CB-CG-ND2	7.35	127.43	116.40
1	A	118	MET	CA-CB-CG	7.30	128.69	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	CYS	CA-C-N	7.17	131.58	120.82
1	B	100	CYS	C-N-CA	7.17	131.58	120.82
1	B	117	SER	CB-CA-C	-7.03	99.85	110.88
1	B	328	VAL	N-CA-CB	-7.02	104.97	110.45
1	B	5	LYS	CB-CG-CD	-7.00	95.20	111.30
1	B	193	SER	N-CA-CB	-6.99	99.83	110.45
1	A	100	CYS	CA-C-N	6.99	129.95	120.38
1	A	100	CYS	C-N-CA	6.99	129.95	120.38
1	A	168	LYS	N-CA-C	-6.92	102.20	111.96
1	A	306	MET	CG-SD-CE	6.91	116.10	100.90
1	B	93	PHE	CA-CB-CG	6.85	120.65	113.80
1	B	148	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	130	PHE	CA-CB-CG	6.68	120.48	113.80
1	B	328	VAL	CA-C-O	-6.67	114.22	118.69
1	B	15	TRP	CG-CD1-NE1	-6.56	101.67	110.20
1	A	138	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	A	326	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	67	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	212	LYS	N-CA-C	-6.38	104.41	111.36
1	B	368	ILE	N-CA-C	-6.37	96.09	109.34
1	A	105	HIS	CB-CG-ND1	6.35	132.22	122.70
1	B	4	GLY	N-CA-C	-6.35	106.91	115.36
1	A	356	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	368	ILE	N-CA-C	-6.33	96.17	109.34
1	A	120	ARG	N-CA-C	-6.27	105.79	113.50
1	A	364	SER	O-C-N	-6.26	114.22	122.42
1	B	105	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	B	168	LYS	CB-CG-CD	-6.25	96.92	111.30
1	B	299	GLN	CG-CD-NE2	6.20	125.69	116.40
1	A	166	LEU	N-CA-C	6.18	120.38	112.34
1	A	20	PRO	N-CA-C	-6.18	102.14	111.41
1	A	343	ASP	N-CA-C	6.14	122.05	113.57
1	A	201	GLY	O-C-N	-6.14	116.89	122.96
1	B	166	LEU	CA-C-O	-6.13	112.92	119.97
1	B	364	SER	N-CA-C	-6.12	105.57	113.16
1	B	59	THR	O-C-N	-6.09	117.59	121.85
1	A	228	LYS	N-CA-C	-6.02	105.89	113.18
1	B	191	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	105	HIS	CA-C-N	5.99	125.61	119.56
1	A	105	HIS	C-N-CA	5.99	125.61	119.56
1	A	169	VAL	N-CA-C	5.99	120.79	113.00
1	B	174	CYS	CA-C-N	5.96	126.56	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	CYS	C-N-CA	5.96	126.56	119.94
1	A	6	VAL	O-C-N	-5.95	116.60	122.67
1	B	34	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	B	201	GLY	O-C-N	-5.93	117.08	122.96
1	B	67	HIS	O-C-N	-5.93	115.74	121.85
1	B	125	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	275	MET	N-CA-C	-5.89	104.94	111.36
1	A	171	LEU	N-CA-C	5.86	119.96	112.34
1	A	244	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	362	LEU	N-CA-C	-5.81	105.02	111.36
1	A	133	ARG	CA-CB-CG	-5.79	102.51	114.10
1	B	41	VAL	N-CA-CB	-5.79	102.15	111.82
1	B	304	ASN	CA-C-O	-5.78	115.05	119.32
1	A	107	GLU	CA-C-O	-5.76	112.80	118.97
1	B	283	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	B	262	VAL	O-C-N	-5.74	115.39	122.57
1	B	90	ILE	CA-C-O	-5.74	115.04	119.98
1	B	245	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	327	SER	N-CA-C	5.66	118.65	111.69
1	A	332	VAL	N-CA-CB	-5.63	103.36	110.57
1	B	15	TRP	CB-CG-CD1	-5.61	118.49	126.90
1	B	220	ILE	O-C-N	-5.58	116.59	122.95
1	A	167	GLU	CB-CG-CD	5.56	122.06	112.60
1	B	15	TRP	CD1-CG-CD2	5.56	115.20	106.30
1	A	30	PRO	CB-CA-C	5.53	117.67	110.92
1	A	96	GLN	CG-CD-NE2	-5.52	108.12	116.40
1	B	214	ALA	N-CA-C	-5.50	106.52	113.18
1	A	214	ALA	N-CA-C	-5.48	106.55	113.18
1	B	374	PHE	CA-CB-CG	-5.48	108.32	113.80
1	B	274	THR	N-CA-C	-5.44	106.14	112.89
1	B	337	ALA	CA-C-N	5.44	130.07	122.08
1	B	337	ALA	C-N-CA	5.44	130.07	122.08
1	A	348	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	B	114	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	251	GLN	CA-CB-CG	5.38	124.85	114.10
1	B	185	LYS	N-CA-CB	-5.36	102.63	110.40
1	A	226	LYS	CA-CB-CG	5.35	124.81	114.10
1	A	358	GLY	O-C-N	-5.34	117.06	122.19
1	A	20	PRO	O-C-N	5.33	129.50	123.00
1	A	164	SER	CB-CA-C	-5.33	101.26	109.62
1	B	52	VAL	CG1-CB-CG2	-5.31	99.11	110.80
1	A	25	GLU	CA-CB-CG	-5.31	103.48	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	140	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	8	LYS	O-C-N	-5.27	117.31	123.27
1	A	323	LYS	N-CA-C	-5.26	102.12	109.96
1	B	229	PHE	N-CA-C	5.26	117.01	111.28
1	A	135	LYS	CA-C-N	5.25	125.01	119.76
1	A	135	LYS	C-N-CA	5.25	125.01	119.76
1	B	176	PHE	CA-C-O	-5.25	115.50	120.90
1	A	173	GLY	N-CA-C	-5.24	108.16	114.66
1	A	178	THR	CA-C-O	-5.21	115.35	120.82
1	A	335	PHE	N-CA-C	-5.21	105.61	111.28
1	A	314	TRP	O-C-N	-5.19	117.12	123.30
1	B	323	LYS	N-CA-C	-5.19	101.96	109.59
1	A	17	GLU	CA-CB-CG	5.18	124.47	114.10
1	A	208	ILE	O-C-N	-5.18	116.85	121.87
1	A	348	HIS	CB-CG-ND1	5.17	130.45	122.70
1	A	106	PRO	N-CA-C	5.15	120.30	113.86
1	B	67	HIS	CB-CG-ND1	5.15	130.42	122.70
1	B	56	THR	N-CA-CB	-5.14	102.31	110.28
1	B	207	VAL	O-C-N	-5.14	116.88	121.87
1	A	340	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	15	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	A	168	LYS	O-C-N	-5.12	116.14	122.19
1	A	359	PHE	CA-CB-CG	-5.12	108.68	113.80
1	B	349	VAL	O-C-N	-5.12	117.86	123.18
1	B	314	TRP	CG-CD1-NE1	-5.11	103.56	110.20
1	B	17	GLU	CB-CG-CD	-5.10	103.93	112.60
1	A	324	SER	N-CA-C	5.09	116.51	111.07
1	B	326	ASP	N-CA-C	5.07	116.89	111.36
1	B	351	PRO	CB-CA-C	5.05	117.60	110.98
1	B	15	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	28	VAL	CA-CB-CG1	-5.02	101.86	110.40
1	A	133	ARG	N-CA-C	5.02	118.36	111.54
1	B	330	LYS	O-C-N	-5.02	116.80	122.12
1	B	137	ILE	O-C-N	-5.00	117.78	122.98

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	2791	0	2851	37	0
1	B	2789	0	2850	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	0	0
5	A	4	0	6	6	0
5	B	4	0	6	5	0
6	A	222	0	0	2	0
6	B	223	0	0	0	0
All	All	6125	0	5765	66	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 6.

All (66) 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:48:SER:CB	5:B:378:DMS:H13	1.74	1.18
1:B:48:SER:OG	5:B:378:DMS:H13	1.44	1.17
1:A:48:SER:HB3	5:A:378:DMS:H13	1.43	0.98
1:B:48:SER:OG	5:B:378:DMS:C1	2.13	0.94
1:B:48:SER:HB3	5:B:378:DMS:H13	1.58	0.85
1:A:48:SER:CB	5:A:378:DMS:H13	2.08	0.83
1:A:251:GLN:HA	1:A:281[B]:CYS:SG	2.27	0.75
1:B:40:MET:HE1	1:B:150:THR:HG22	1.72	0.70
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.64	0.63
1:B:336:MET:HA	1:B:336:MET:HE2	1.82	0.62
1:A:160:ILE:HB	1:A:332:VAL:HG11	1.82	0.60
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.86	0.58
1:A:40:MET:CE	1:A:150:THR:HG22	2.35	0.57
1:A:283:GLN:NE2	1:A:285:ALA:H	2.05	0.54
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASN:HD22	1:B:306:MET:H	1.56	0.54
1:A:48:SER:CB	5:A:378:DMS:C1	2.84	0.53
1:B:282[B]:CYS:SG	1:B:288:VAL:O	2.66	0.53
1:A:254:LEU:HD12	1:A:281[B]:CYS:SG	2.49	0.52
1:B:31:PRO:HD3	1:B:37:ARG:HB2	1.91	0.52
1:B:272:LEU:HD11	1:B:299:GLN:HE21	1.74	0.52
1:B:283:GLN:HE22	1:B:285:ALA:HB3	1.75	0.52
1:A:34:HIS:HE1	6:A:542:HOH:O	1.93	0.52
1:A:336:MET:HA	1:A:336:MET:HE2	1.90	0.52
1:A:166:LEU:HA	1:A:169:VAL:HG22	1.92	0.50
1:B:283:GLN:NE2	1:B:285:ALA:H	2.09	0.50
1:A:165:PRO:HD3	1:A:336:MET:HE1	1.92	0.50
1:B:132:CYS:HB3	1:B:137:ILE:HD11	1.94	0.50
1:A:304:ASN:ND2	1:A:306:MET:H	2.10	0.49
1:B:194:THR:HG22	1:B:262:VAL:HG12	1.96	0.48
1:A:253:VAL:O	1:A:257:MET:HG3	2.12	0.48
1:B:304:ASN:ND2	1:B:306:MET:H	2.12	0.48
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.96	0.47
1:A:241:VAL:HG21	1:A:250:ILE:HD11	1.97	0.46
1:B:326:ASP:O	1:B:330:LYS:HE2	2.16	0.46
1:B:48:SER:OG	5:B:378:DMS:H12	2.11	0.45
1:A:48:SER:OG	5:A:378:DMS:C1	2.64	0.45
1:A:174:CYS:SG	4:A:377:NAD:H5N	2.57	0.45
1:A:92:LEU:HA	6:A:443:HOH:O	2.16	0.45
1:A:304:ASN:HD22	1:A:306:MET:H	1.65	0.45
1:A:165:PRO:HG2	1:A:335:PHE:HE2	1.82	0.45
1:B:16:GLU:HG3	1:B:19:LYS:HG2	1.98	0.44
1:A:283:GLN:HE22	1:A:285:ALA:H	1.64	0.44
1:B:267:GLU:HG3	1:B:275:MET:HA	2.00	0.44
1:B:16:GLU:HG3	1:B:19:LYS:CG	2.48	0.43
1:A:70:ALA:HB1	1:A:166:LEU:HD22	2.00	0.42
1:B:32:LYS:HD2	1:B:129:ARG:NH2	2.33	0.42
1:A:118:MET:HE2	1:A:118:MET:HB2	1.98	0.42
1:A:48:SER:HB3	5:A:378:DMS:C1	2.31	0.42
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.20	0.42
1:B:272:LEU:HD11	1:B:299:GLN:HB3	2.02	0.42
1:A:272:LEU:HD11	1:A:299:GLN:HB3	2.00	0.42
1:A:88:LYS:HE2	1:A:166:LEU:HG	2.02	0.42
1:B:12:ALA:HB1	1:B:21:PHE:HB3	2.01	0.41
1:A:40:MET:HE3	1:A:150:THR:HG22	2.02	0.41
1:A:11:ALA:HA	1:A:147:SER:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:OG	5:A:378:DMS:H12	2.19	0.41
1:A:208:ILE:HD13	1:A:208:ILE:HG21	1.92	0.41
1:A:349:VAL:O	1:A:350:LEU:HD23	2.21	0.41
1:B:10:LYS:HA	1:B:24:GLU:O	2.21	0.41
1:B:40:MET:HE1	1:B:150:THR:CG2	2.47	0.41
1:B:282[B]:CYS:SG	1:B:288:VAL:C	3.04	0.40
1:B:307:LEU:O	1:B:312:ARG:HD2	2.22	0.40
1:B:11:ALA:HA	1:B:147:SER:HA	2.02	0.40
1:B:282[B]:CYS:SG	1:B:289:SER:HB2	2.61	0.40
1:A:10:LYS:HA	1:A:24:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	375/374 (100%)	359 (96%)	16 (4%)	0	100	100
1	B	374/374 (100%)	358 (96%)	16 (4%)	0	100	100
All	All	749/748 (100%)	717 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	311/308 (101%)	297 (96%)	14 (4%)	24	25
1	B	310/308 (101%)	295 (95%)	15 (5%)	23	23
All	All	621/616 (101%)	592 (95%)	29 (5%)	23	24

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	40	MET
1	A	61	LEU
1	A	84	ARG
1	A	118	MET
1	A	131	THR
1	A	164	SER
1	A	231	LYS
1	A	239	GLU
1	A	304	ASN
1	A	309	LEU
1	A	332	VAL
1	A	336	MET
1	A	343	ASP
1	B	5	LYS
1	B	56	THR
1	B	84	ARG
1	B	191	GLN
1	B	212	LYS
1	B	239	GLU
1	B	248	LYS
1	B	268	VAL
1	B	302	SER
1	B	304	ASN
1	B	309	LEU
1	B	315	LYS
1	B	336	MET
1	B	353	GLU
1	B	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	304	ASN
1	B	124	GLN
1	B	283	GLN
1	B	299	GLN
1	B	304	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMS	B	378	-	3,3,3	0.52	0	3,3,3	2.57	2 (66%)
5	DMS	A	378	-	3,3,3	0.10	0	3,3,3	1.19	0
4	NAD	B	377	-	46,48,48	1.14	5 (10%)	64,73,73	2.04	13 (20%)
4	NAD	A	377	-	46,48,48	1.21	5 (10%)	64,73,73	1.93	14 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	B	377	-	-	10/30/62/62	0/5/5/5
4	NAD	A	377	-	-	4/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	377	NAD	C2N-N1N	3.77	1.39	1.35
4	A	377	NAD	O4D-C1D	3.36	1.45	1.40
4	B	377	NAD	O4D-C1D	3.13	1.45	1.40
4	B	377	NAD	C2N-N1N	2.83	1.38	1.35
4	A	377	NAD	C5A-N7A	-2.80	1.34	1.39
4	A	377	NAD	PA-O3	2.50	1.62	1.59
4	B	377	NAD	C5A-N7A	-2.39	1.34	1.39
4	B	377	NAD	C6N-N1N	2.28	1.40	1.35
4	A	377	NAD	PN-O3	2.08	1.61	1.59
4	B	377	NAD	C4A-N9A	-2.07	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	377	NAD	C5A-C4A-N3A	-7.34	116.61	126.72
4	B	377	NAD	N3A-C4A-N9A	6.61	138.41	127.17
4	A	377	NAD	C5A-C4A-N3A	-6.20	118.18	126.72
4	A	377	NAD	N3A-C4A-N9A	6.14	137.61	127.17
4	A	377	NAD	C6A-C5A-N7A	-4.93	122.58	132.09
4	B	377	NAD	C6A-C5A-C4A	4.85	123.80	117.18
4	A	377	NAD	C6A-C5A-C4A	4.66	123.55	117.18
4	B	377	NAD	C6A-C5A-N7A	-4.17	124.04	132.09
4	B	377	NAD	N3A-C2A-N1A	-3.59	123.15	128.58
4	B	377	NAD	O7N-C7N-C3N	-3.43	115.41	119.60
4	B	377	NAD	C2A-N3A-C4A	3.39	120.11	111.83
5	B	378	DMS	O-S-C2	3.35	123.25	106.49
4	B	377	NAD	C4D-O4D-C1D	-3.34	106.87	109.92
4	A	377	NAD	N3A-C2A-N1A	-3.31	123.57	128.58
4	B	377	NAD	O4B-C4B-C5B	-3.28	98.82	109.33
4	B	377	NAD	C2N-C3N-C4N	2.84	121.57	118.26
4	A	377	NAD	C2N-C3N-C4N	2.75	121.45	118.26
4	A	377	NAD	C2A-N3A-C4A	2.70	118.43	111.83
4	A	377	NAD	N6A-C6A-N1A	2.60	124.17	118.38
5	B	378	DMS	C2-S-C1	-2.59	85.14	98.42
4	A	377	NAD	O4B-C1B-N9A	2.54	112.97	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	377	NAD	C6N-N1N-C2N	-2.52	119.74	121.88
4	A	377	NAD	O5B-C5B-C4B	-2.49	100.52	108.99
4	A	377	NAD	O3D-C3D-C4D	-2.44	104.08	111.08
4	B	377	NAD	C4A-N9A-C8A	2.41	108.27	105.74
4	A	377	NAD	C4A-C5A-N7A	2.40	113.33	110.58
4	B	377	NAD	O4D-C4D-C5D	-2.28	102.03	109.33
4	B	377	NAD	N6A-C6A-N1A	2.10	123.06	118.38
4	A	377	NAD	O2A-PA-O1A	2.07	122.09	112.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	377	NAD	O4D-C1D-N1N-C2N
4	A	377	NAD	O4D-C1D-N1N-C6N
4	A	377	NAD	C2D-C1D-N1N-C2N
4	A	377	NAD	C2D-C1D-N1N-C6N
4	B	377	NAD	C5B-O5B-PA-O2A
4	B	377	NAD	O4D-C1D-N1N-C2N
4	B	377	NAD	O4D-C1D-N1N-C6N
4	B	377	NAD	C2D-C1D-N1N-C2N
4	B	377	NAD	C3B-C4B-C5B-O5B
4	B	377	NAD	C5B-O5B-PA-O1A
4	B	377	NAD	C5B-O5B-PA-O3
4	B	377	NAD	C2D-C1D-N1N-C6N
4	B	377	NAD	C2B-C1B-N9A-C8A
4	B	377	NAD	O4B-C4B-C5B-O5B

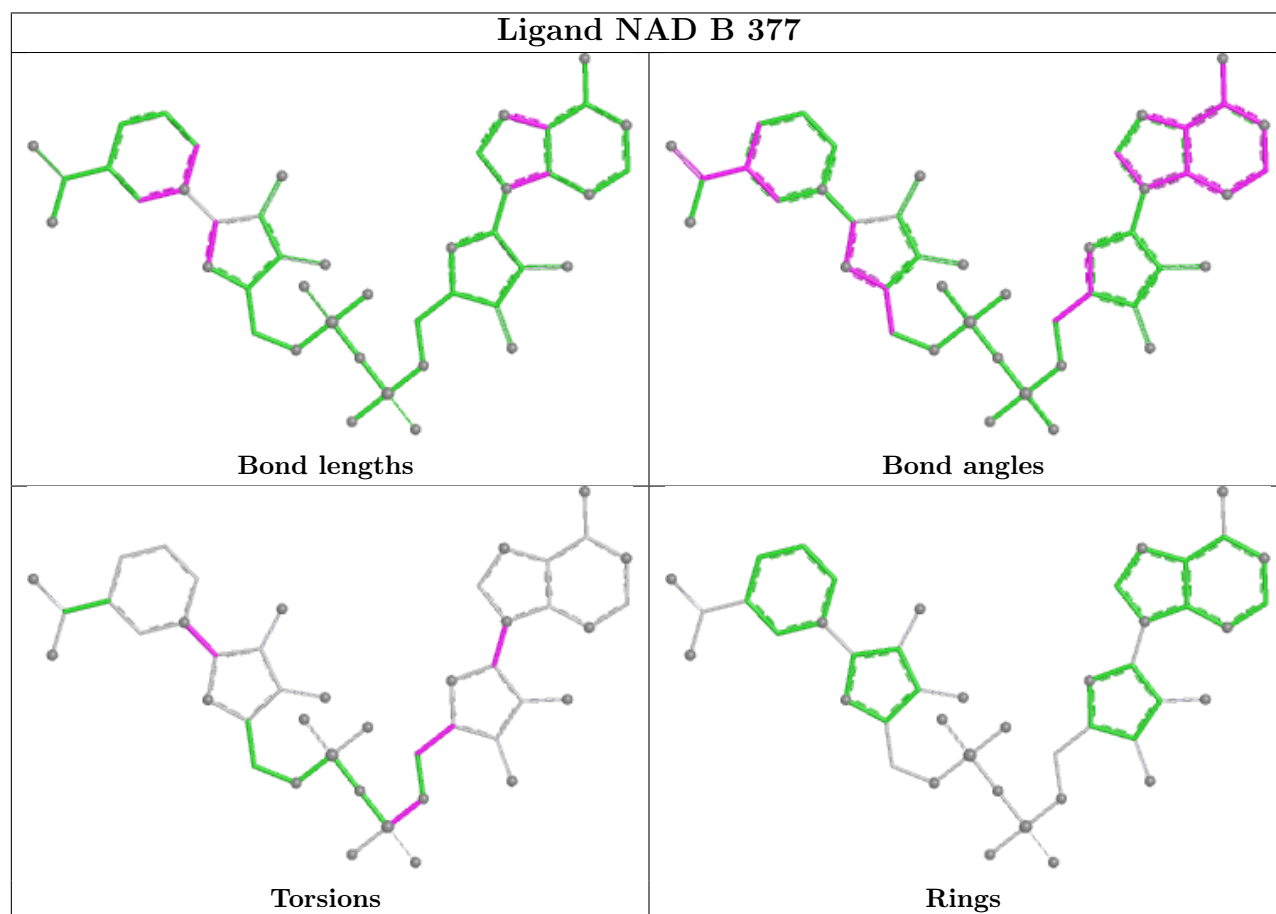
There are no ring outliers.

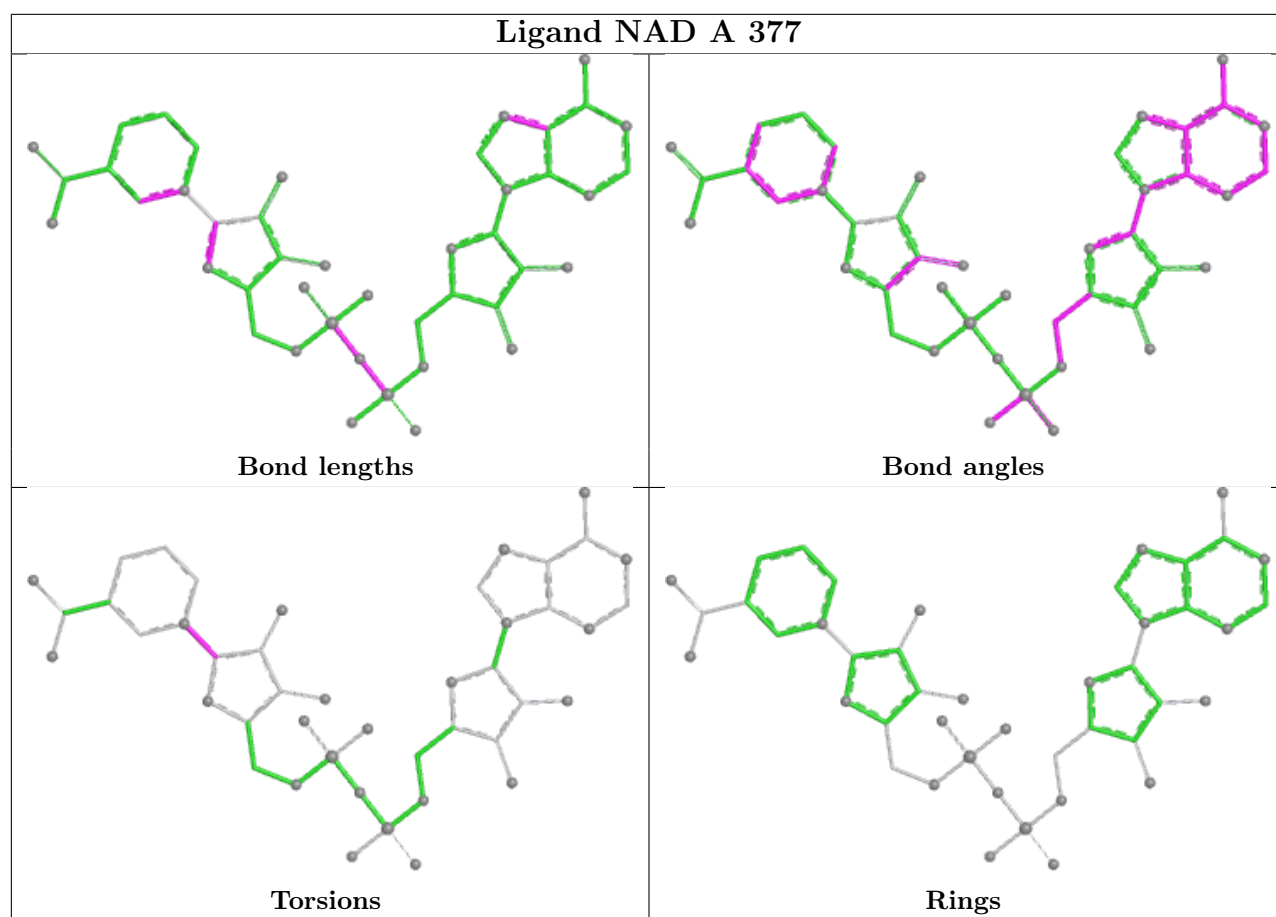
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	378	DMS	5	0
5	A	378	DMS	6	0
4	A	377	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.